



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 05:33 AM UTC

PDB ID : 5WS5 / pdb_00005ws5
Title : Native XFEL structure of photosystem II (preflash dark dataset)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2016-12-05
Resolution : 2.35 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

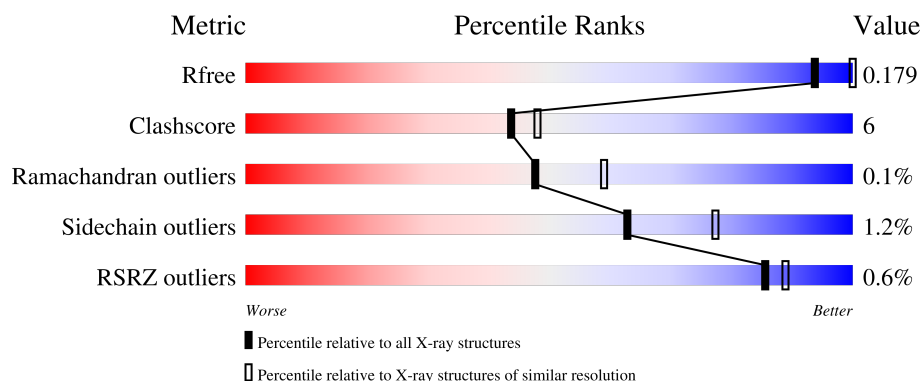
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.



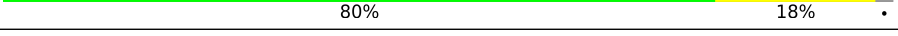
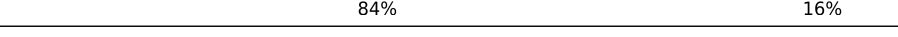
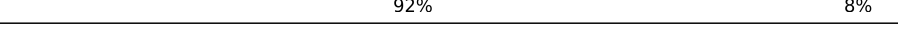
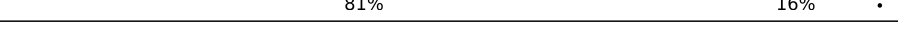
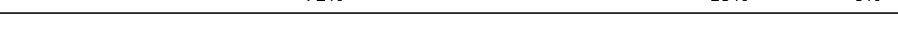
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	344	 87% 10% .
1	a	344	 84% 13% .
2	B	505	 89% 10% .
2	b	505	 92% 8%
3	C	455	 91% 7% .

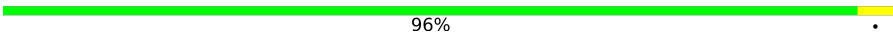
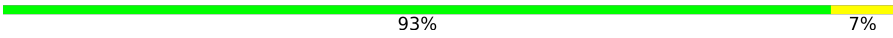
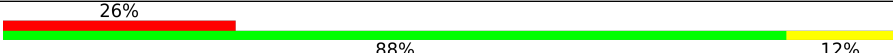
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Mol	Chain	Length	Quality of chain
3	c	455	 89% 10% .
4	D	342	 89% 11%
4	d	342	 90% 9%
5	E	84	 80% 17% .
5	e	84	 80% 14% 6%
6	F	44	 57% 20% 23%
6	f	44	 59% 11% 30%
7	H	65	 85% 14% .
7	h	65	 80% 18% .
8	I	38	 82% 18%
8	i	38	 84% 16%
9	J	39	 85% 13% .
9	j	39	 92% 8%
10	K	37	 81% 16% .
10	k	37	 84% 14% .
11	L	37	 89% 8% .
11	l	37	 89% 8% .
12	M	36	 83% 8% 8%
12	m	36	 72% 19% 6%
13	O	244	 86% 13%
13	o	244	 91% 9%
14	T	32	 88% . . 6%
14	t	32	 72% 16% 6% 6%
15	U	104	 84% 9% 8%
15	u	104	 88% 6% 7%

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Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	X	40	
17	x	40	
18	Y	30	
18	y	30	
19	Z	62	
19	z	62	
20	R	34	

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	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	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	D	406	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	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	c	514	X	-	-	-
23	CLA	d	402	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	403	X	-	-	-
27	GOL	B	625	-	-	X	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 52545 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	4	0
			2636	1730	431	460	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 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	4	0
			3536	2316	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	64	Total	C	N	O	S	0	0	0
			506	339	81	84	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 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 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	4	0
			1883	1178	315	385	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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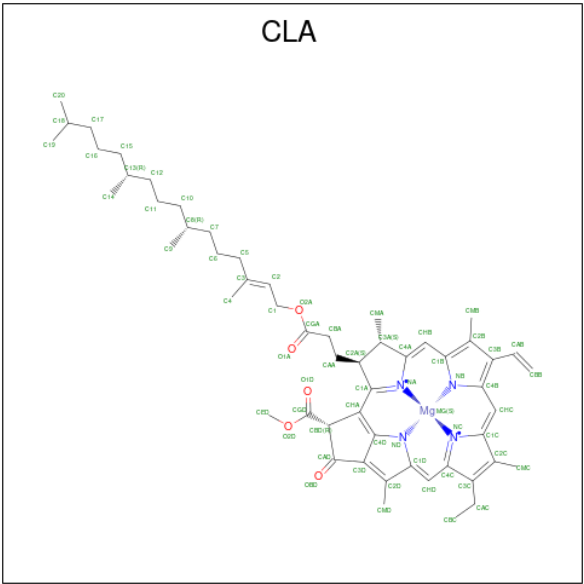
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

- 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

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

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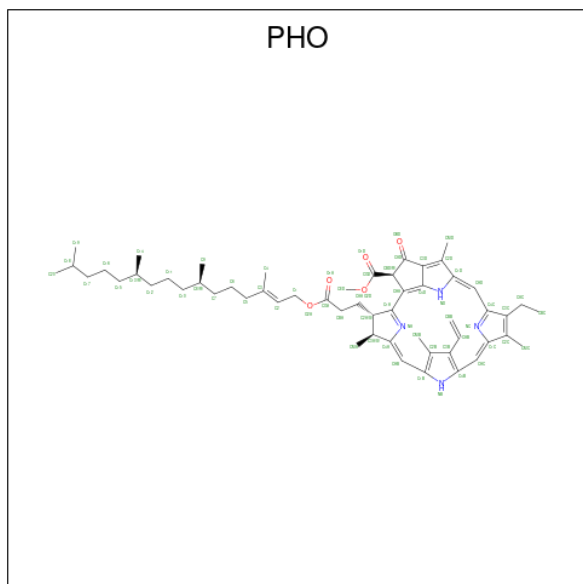
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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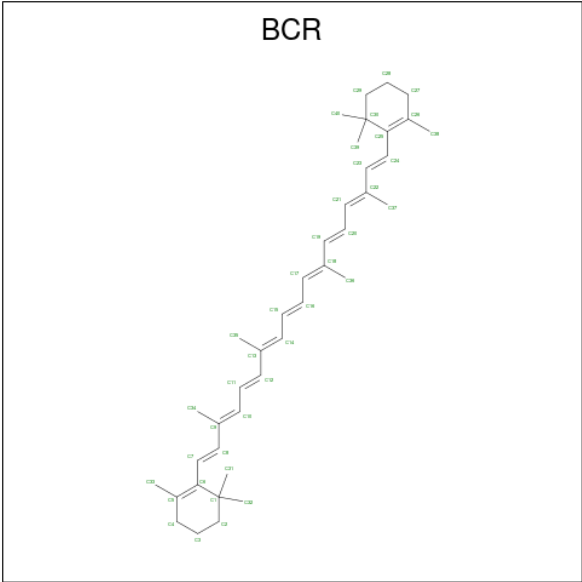
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- 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	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		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



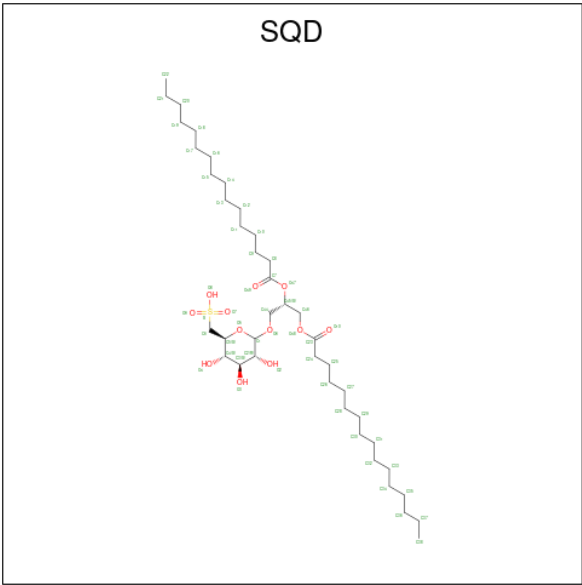
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total 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).



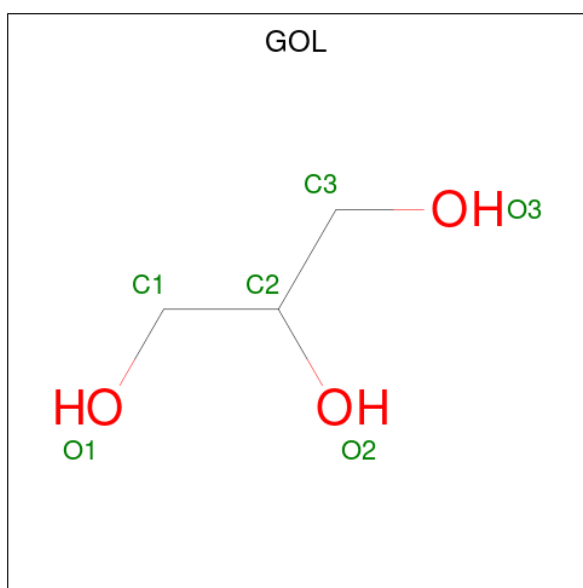
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	F	1	Total	C	O	S	0	0
			43	30	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	b	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

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



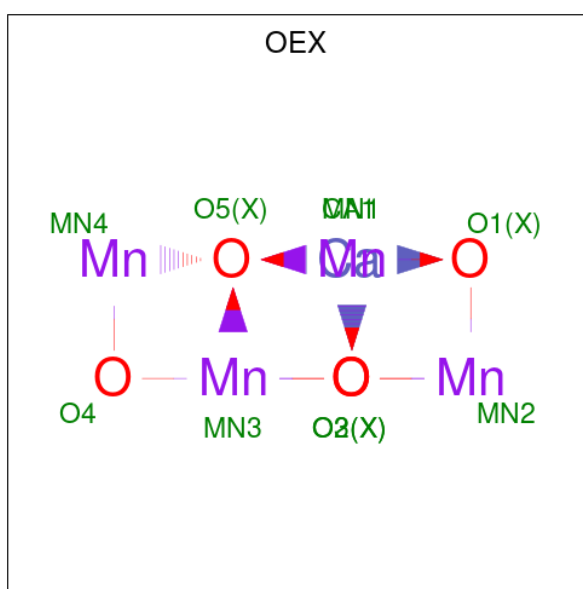
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	V	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		

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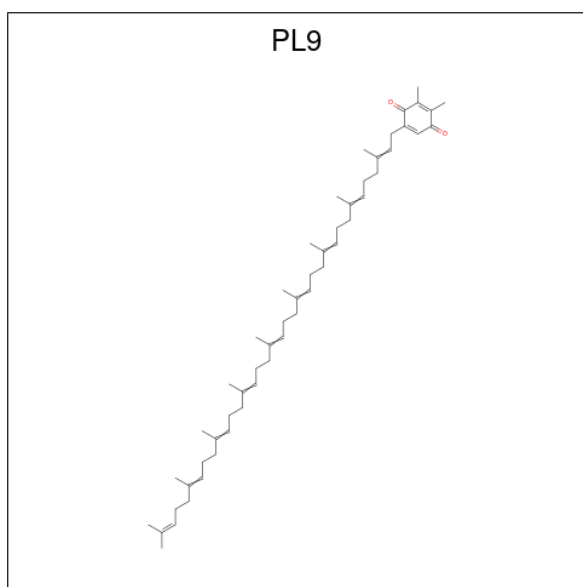
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	c	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	0
			6	3	3		

- 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:).

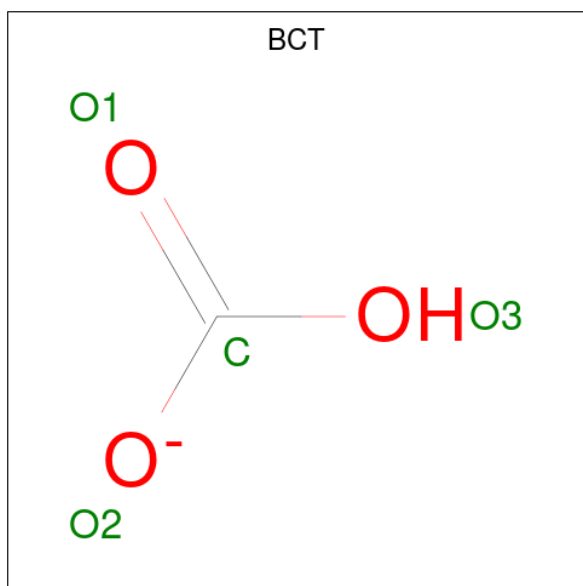
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	0
			34	29	5		
30	M	1	Total	C		0	0
			10	10			
30	X	1	Total	C	O	0	0
		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

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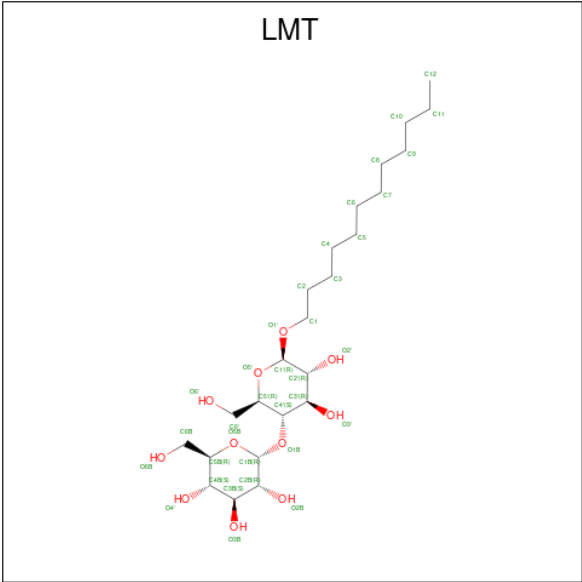
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	1	Total	C	O	0	0
			33	28	5		
30	c	1	Total	C	O	0	0
			32	27	5		
30	d	2	Total	C	O	0	0
			53	47	6		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
			10	10			
30	x	1	Total	C	O	0	0
			18	16	2		

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



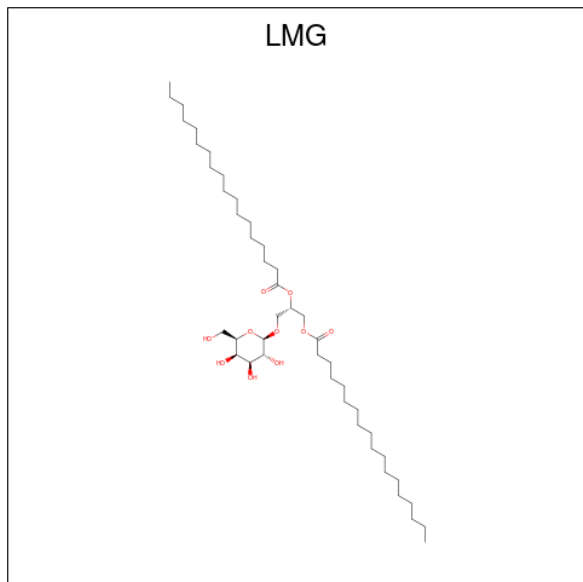
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			4	1	3		
31	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



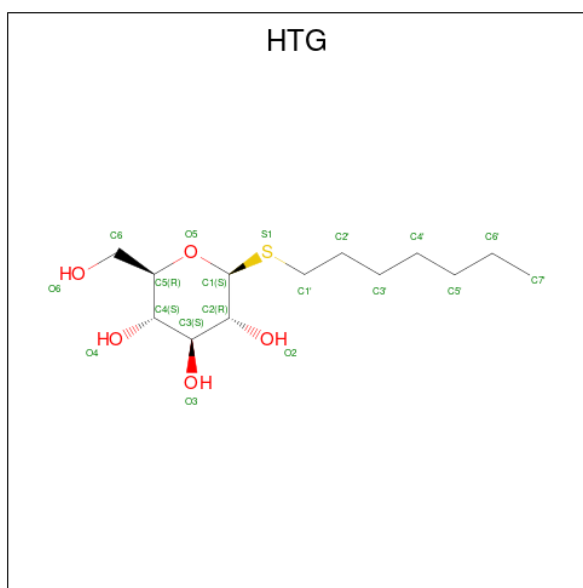
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			35	24	11		
32	D	1	Total	C	O	0	0
			35	24	11		
32	E	1	Total	C	O	0	0
			35	24	11		
32	I	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			25	19	6		
32	b	1	Total	C	O	0	0
			25	19	6		
32	e	1	Total	C	O	0	0
			35	24	11		
32	m	1	Total	C	O	0	0
			35	24	11		
32	t	1	Total	C	O	0	0
			25	19	6		
32	t	1	Total	C	O	0	0
			26	19	7		

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



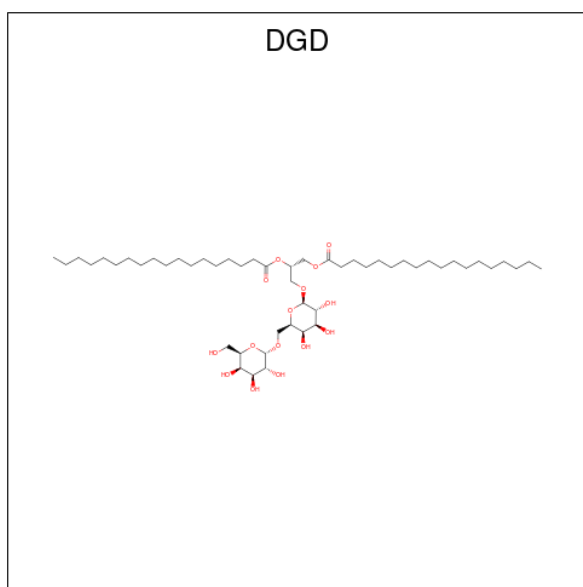
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	D	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	d	1	Total	C	O	0	0
			51	41	10		
33	m	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: $C_{13}H_{26}O_5S$).



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	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	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		

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 36 is CALCIUM ION (CCD ID: CA) (formula: Ca).

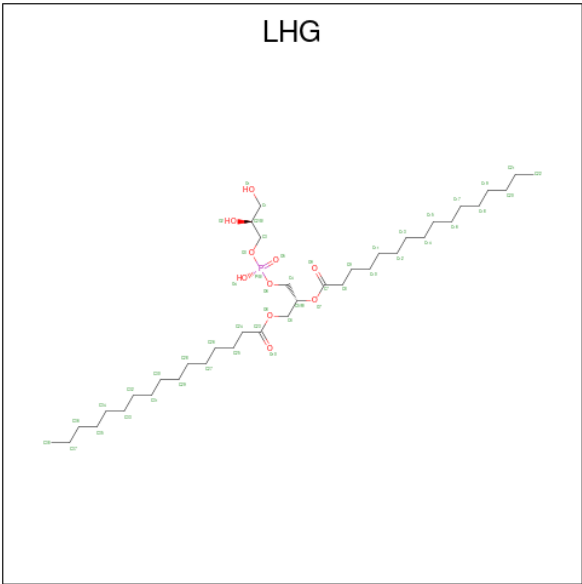
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	C	1	Total	Ca	0	0
			1	1		
36	F	1	Total	Ca	0	0
			1	1		
36	O	1	Total	Ca	0	0
			1	1		
36	c	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	f	1	Total	Ca	0	0
			1	1		
36	o	1	Total	Ca	0	0
			1	1		

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



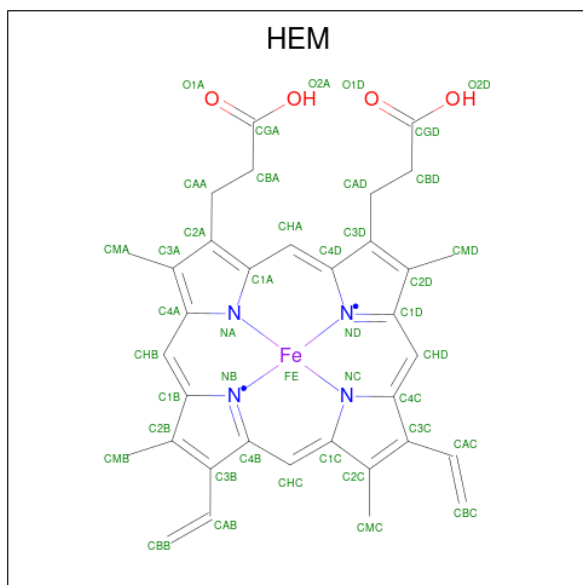
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	E	1	Total	C	O	P	0	0
			42	31	10	1		
37	L	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	1	1	Total	C	O	P	0	0
			49	38	10	1		

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

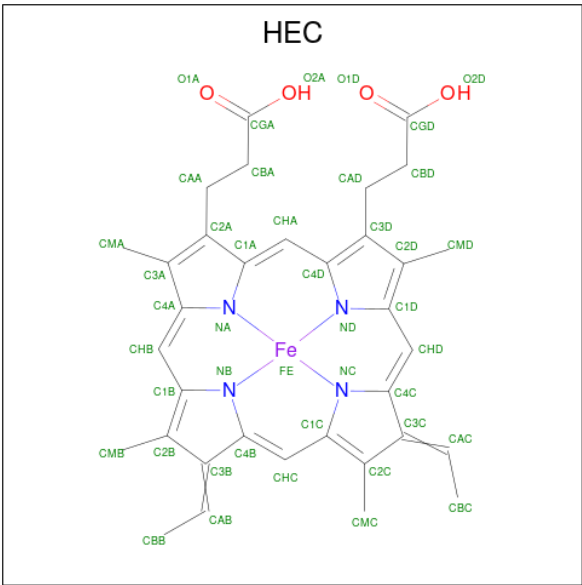


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
38	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	130	Total	O	0	0
			130	130		
41	B	167	Total	O	0	0
			167	167		
41	C	144	Total	O	0	0
			144	144		
41	D	122	Total	O	0	0
			122	122		
41	E	15	Total	O	0	0
			15	15		
41	F	4	Total	O	0	0
			4	4		
41	H	19	Total	O	0	0
			19	19		
41	I	6	Total	O	0	0
			6	6		
41	J	5	Total	O	0	0
			5	5		
41	K	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	L	3	Total 3	O 3	0	0
41	M	7	Total 7	O 7	0	0
41	O	71	Total 71	O 71	0	0
41	T	9	Total 9	O 9	0	0
41	U	32	Total 32	O 32	0	0
41	V	67	Total 67	O 67	0	0
41	X	1	Total 1	O 1	0	0
41	Y	1	Total 1	O 1	0	0
41	a	133	Total 133	O 133	0	0
41	b	193	Total 193	O 193	0	0
41	c	142	Total 142	O 142	0	0
41	d	114	Total 114	O 114	0	0
41	e	8	Total 8	O 8	0	0
41	f	4	Total 4	O 4	0	0
41	h	16	Total 16	O 16	0	0
41	i	3	Total 3	O 3	0	0
41	j	2	Total 2	O 2	0	0
41	k	3	Total 3	O 3	0	0
41	l	4	Total 4	O 4	0	0
41	m	15	Total 15	O 15	0	0
41	o	77	Total 77	O 77	0	0

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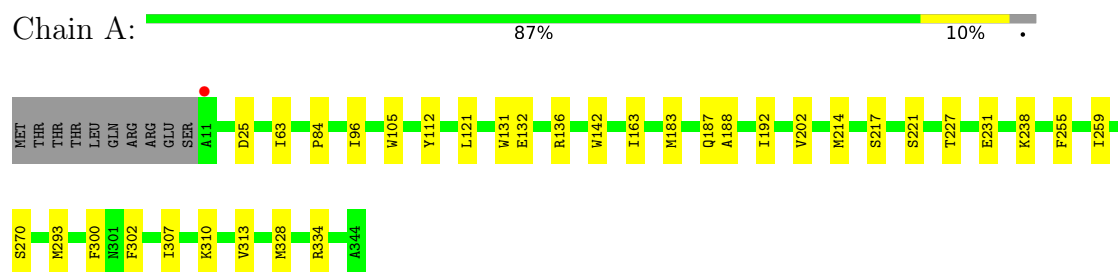
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	t	6	Total 6	O 6	0	0
41	u	47	Total 47	O 47	0	0
41	v	47	Total 47	O 47	0	0
41	x	2	Total 2	O 2	0	0
41	y	1	Total 1	O 1	0	0

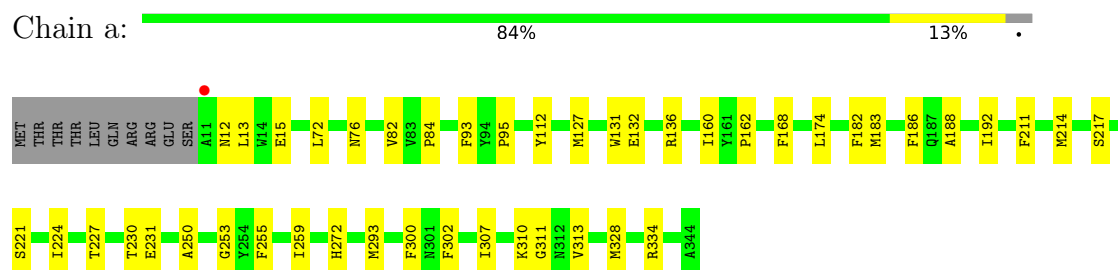
3 Residue-property plots

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

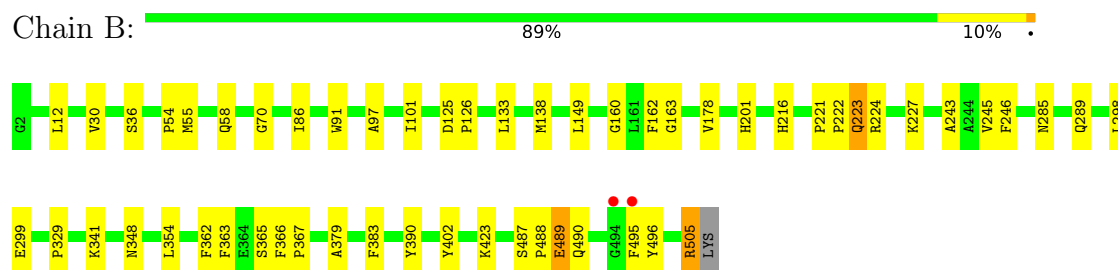
- Molecule 1: Photosystem II D1 protein



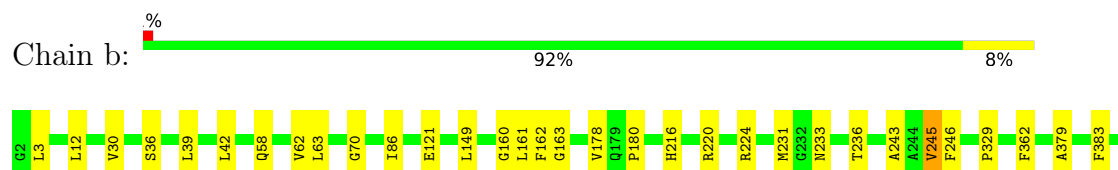
- Molecule 1: Photosystem II D1 protein

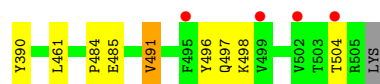


- Molecule 2: Photosystem II CP47 reaction center protein



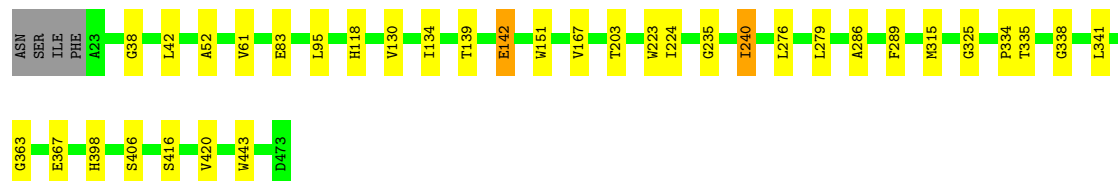
- Molecule 2: Photosystem II CP47 reaction center protein





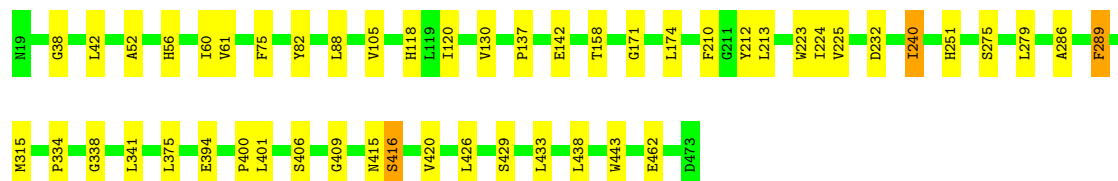
• Molecule 3: Photosystem II CP43 protein

Chain C: 91% 7% .



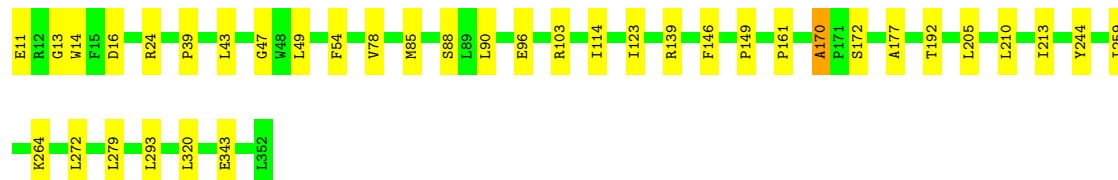
• Molecule 3: Photosystem II CP43 protein

Chain c: 89% 10% .



• Molecule 4: Photosystem II D2 protein

Chain D: 89% 11% .



• Molecule 4: Photosystem II D2 protein

Chain d: 90% 9% .



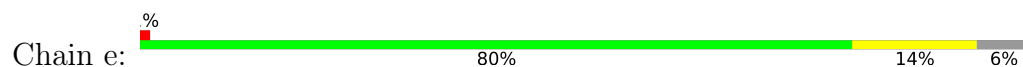
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 80% 17% .





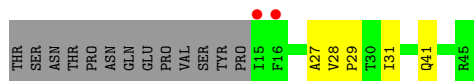
- Molecule 5: Cytochrome b559 subunit alpha



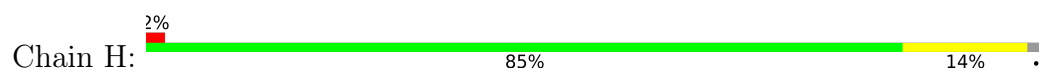
- Molecule 6: Cytochrome b559 subunit beta



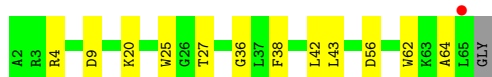
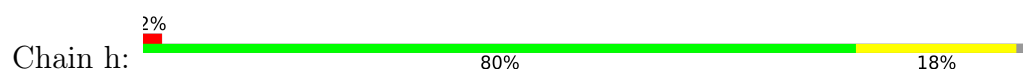
- Molecule 6: Cytochrome b559 subunit beta



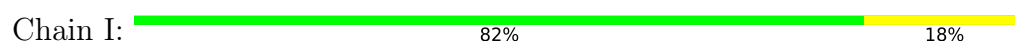
- Molecule 7: Photosystem II reaction center protein H



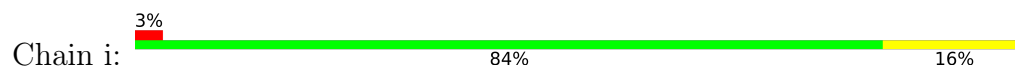
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



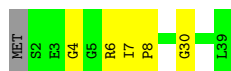
- Molecule 8: Photosystem II reaction center protein I





- Molecule 9: Photosystem II reaction center protein J

Chain J: 85% 13% .



- Molecule 9: Photosystem II reaction center protein J

Chain j: 92% 8%



- Molecule 10: Photosystem II protein K

Chain K: 81% 16% .



- Molecule 10: Photosystem II protein K

Chain k: 84% 14% .



- Molecule 11: Photosystem II reaction center protein L

Chain L: 89% 8% .



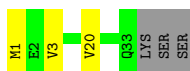
- Molecule 11: Photosystem II reaction center protein L

Chain l: 89% 8% .



- Molecule 12: Photosystem II protein M

Chain M: 83% 8% 8%



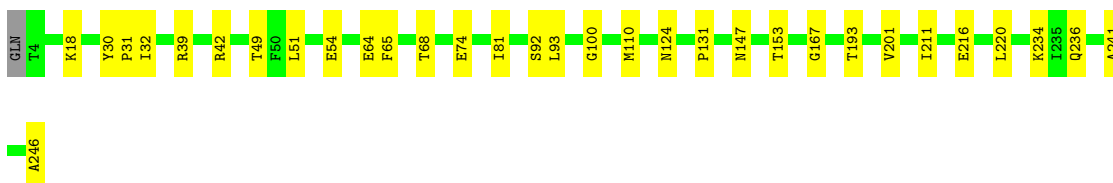
- Molecule 12: Photosystem II protein M

Chain m: 72% 19% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 86% 13%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 91% 9%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 3% 88% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 3% 72% 16% 6% 6%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 84% 9% 8%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  88% 6% 7%



- Molecule 16: Cytochrome c-550

Chain V:  96% .



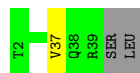
- Molecule 16: Cytochrome c-550

Chain v:  93% 7%



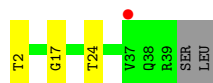
- Molecule 17: Photosystem II reaction center protein X

Chain X:  92% . 5%



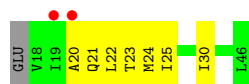
- Molecule 17: Photosystem II reaction center protein X

Chain x:  2% 88% 8% 5%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  7% 73% 23% .

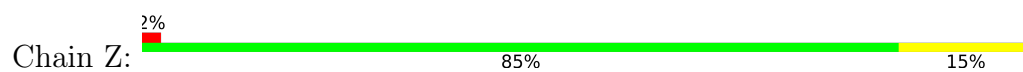


- Molecule 18: Photosystem II reaction center protein Ycf12

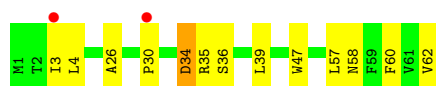
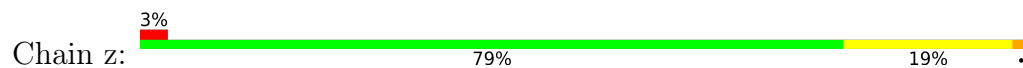
Chain y:  73% 23% .



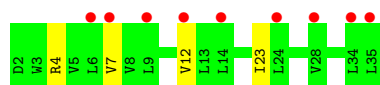
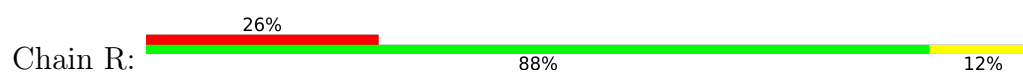
- Molecule 19: Photosystem II reaction center protein Z



- 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	124.70Å 229.89Å 285.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 20.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.35) 99.8 (20.00-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.133 , 0.171 0.144 , 0.179	Depositor DCC
R_{free} test set	17049 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 89.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52545	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.60	0/2728	0.85	1/3719 (0.0%)
1	a	0.57	0/2733	0.85	0/3727
2	B	0.56	0/4171	0.80	0/5683
2	b	0.55	0/4138	0.80	2/5640 (0.0%)
3	C	0.54	0/3626	0.81	0/4936
3	c	0.51	0/3662	0.81	0/4985
4	D	0.60	0/2827	0.81	2/3852 (0.1%)
4	d	0.56	0/2818	0.81	2/3840 (0.1%)
5	E	0.51	0/687	0.83	0/936
5	e	0.49	0/667	0.81	0/908
6	F	0.59	0/284	0.79	0/387
6	f	0.54	0/257	0.82	0/349
7	H	0.49	0/530	0.80	0/723
7	h	0.45	0/519	0.77	0/708
8	I	0.49	0/311	0.76	0/419
8	i	0.48	0/311	0.77	0/419
9	J	0.46	0/278	0.82	0/376
9	j	0.44	0/283	0.77	0/383
10	K	0.47	0/303	0.79	0/416
10	k	0.49	0/303	0.83	0/416
11	L	0.58	0/311	0.68	0/423
11	l	0.57	0/311	0.71	0/423
12	M	0.62	0/261	1.00	0/357
12	m	0.57	0/262	0.95	0/357
13	O	0.54	0/1926	0.81	0/2611
13	o	0.53	0/1910	0.82	2/2589 (0.1%)
14	T	0.63	0/257	0.79	0/349
14	t	0.56	0/257	0.77	0/349
15	U	0.53	0/776	0.78	0/1052
15	u	0.53	0/785	0.76	0/1064
16	V	0.52	0/1085	0.79	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.48	0/1085	0.78	0/1473
17	X	0.47	0/284	0.79	0/384
17	x	0.45	0/284	0.77	0/384
18	Y	0.44	0/216	0.81	0/289
18	y	0.44	0/216	0.91	0/289
19	Z	0.41	0/490	0.84	0/669
19	z	0.41	0/490	0.84	0/669
20	R	0.44	0/279	0.74	0/383
All	All	0.54	0/42921	0.81	9/58409 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	55	GLU	CA-C-N	6.24	126.19	119.76
13	o	55	GLU	C-N-CA	6.24	126.19	119.76
4	d	170	ALA	CA-C-N	-6.21	113.55	119.76
4	d	170	ALA	C-N-CA	-6.21	113.55	119.76
2	b	163	GLY	CA-C-N	5.79	125.48	119.64
2	b	163	GLY	C-N-CA	5.79	125.48	119.64
4	D	170	ALA	CA-C-N	-5.39	114.37	119.76
4	D	170	ALA	C-N-CA	-5.39	114.37	119.76
1	A	142	TRP	N-CA-C	5.07	119.16	112.92

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	23	0
1	a	2636	0	2549	33	0
2	B	4007	0	3879	45	0
2	b	3986	0	3855	37	0
3	C	3501	0	3428	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3536	0	3463	37	0
4	D	2729	0	2632	29	0
4	d	2720	0	2626	23	0
5	E	665	0	653	15	0
5	e	648	0	634	9	0
6	F	275	0	282	7	0
6	f	250	0	261	5	0
7	H	514	0	542	7	0
7	h	506	0	529	14	0
8	I	314	0	328	5	0
8	i	314	0	328	2	0
9	J	272	0	279	4	0
9	j	277	0	284	2	0
10	K	293	0	305	6	0
10	k	293	0	305	3	0
11	L	301	0	315	2	0
11	l	301	0	315	3	0
12	M	265	0	286	2	0
12	m	269	0	288	10	0
13	O	1883	0	1865	20	0
13	o	1873	0	1852	13	0
14	T	258	0	261	2	0
14	t	258	0	261	6	0
15	U	765	0	767	5	0
15	u	774	0	773	4	0
16	V	1064	0	1073	3	0
16	v	1064	0	1073	6	0
17	X	281	0	312	1	0
17	x	281	0	312	3	0
18	Y	215	0	246	5	0
18	y	215	0	246	3	0
19	Z	479	0	516	4	0
19	z	479	0	516	8	0
20	R	273	0	305	4	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	260	0	288	14	0
23	B	1040	0	1152	40	0
23	C	845	0	936	43	0
23	D	130	0	144	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	a	260	0	288	11	0
23	b	1040	0	1152	41	0
23	c	845	0	936	51	0
23	d	130	0	144	6	0
24	A	128	0	148	5	0
24	a	128	0	148	6	0
25	A	40	0	56	1	0
25	B	120	0	168	8	0
25	C	80	0	112	6	0
25	D	40	0	56	4	0
25	H	40	0	56	3	0
25	K	40	0	56	2	0
25	T	40	0	56	8	0
25	Y	40	0	56	3	0
25	a	40	0	56	2	0
25	b	120	0	168	11	0
25	c	80	0	112	10	0
25	d	40	0	56	1	0
25	h	40	0	56	4	0
25	k	40	0	56	2	0
25	t	40	0	56	6	0
25	y	40	0	56	2	0
26	A	108	0	156	6	0
26	B	54	0	78	3	0
26	F	43	0	53	2	0
26	a	108	0	156	3	0
26	b	54	0	78	4	0
26	f	43	0	53	2	0
27	A	6	0	8	0	0
27	B	12	0	16	4	0
27	C	6	0	8	0	0
27	V	6	0	8	0	0
27	a	12	0	16	2	0
27	b	6	0	8	0	0
27	c	6	0	8	0	0
27	v	6	0	8	0	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	55	0	80	4	0
29	D	55	0	80	0	0
29	a	55	0	80	7	0
29	d	55	0	80	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	A	28	0	0	0	0
30	B	33	0	0	1	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	33	0	0	0	0
30	c	32	0	0	1	0
30	d	53	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	4	0	0	0	0
31	a	4	0	0	0	0
32	A	35	0	46	2	0
32	D	35	0	46	2	0
32	E	35	0	46	1	0
32	I	35	0	46	1	0
32	M	70	0	92	5	0
32	a	70	0	92	4	0
32	b	50	0	70	2	0
32	e	35	0	46	0	0
32	m	35	0	46	2	0
32	t	51	0	70	1	0
33	B	51	0	72	0	0
33	C	153	0	216	7	0
33	D	51	0	72	2	0
33	Z	37	0	44	2	0
33	a	51	0	72	1	0
33	c	102	0	144	3	0
33	d	51	0	71	1	0
33	m	51	0	72	0	0
33	z	39	0	48	1	0
34	B	57	0	78	4	0
34	C	19	0	26	0	0
34	D	16	0	17	2	0
34	V	11	0	10	0	0
34	b	57	0	78	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	c	19	0	26	0	0
34	d	16	0	17	2	0
35	C	186	0	246	8	0
35	H	62	0	82	2	0
35	c	186	0	246	7	0
35	h	62	0	82	0	0
36	C	1	0	0	0	0
36	F	1	0	0	0	0
36	O	1	0	0	0	0
36	c	2	0	0	0	0
36	f	1	0	0	0	0
36	o	1	0	0	0	0
37	D	147	0	222	4	0
37	E	42	0	57	3	0
37	L	49	0	74	1	0
37	d	147	0	222	12	0
37	e	42	0	57	2	0
37	l	49	0	74	0	0
38	E	43	0	30	4	0
38	e	43	0	30	5	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	130	0	0	1	0
41	B	167	0	0	1	0
41	C	144	0	0	2	0
41	D	122	0	0	2	0
41	E	15	0	0	0	0
41	F	4	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	3	0	0	0	0
41	M	7	0	0	0	0
41	O	71	0	0	0	0
41	T	9	0	0	0	0
41	U	32	0	0	0	0
41	V	67	0	0	0	0
41	X	1	0	0	0	0
41	Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	a	133	0	0	0	0
41	b	193	0	0	0	0
41	c	142	0	0	2	0
41	d	114	0	0	2	0
41	e	8	0	0	0	0
41	f	4	0	0	0	0
41	h	16	0	0	0	0
41	i	3	0	0	0	0
41	j	2	0	0	0	0
41	k	3	0	0	0	0
41	l	4	0	0	0	0
41	m	15	0	0	1	0
41	o	77	0	0	0	0
41	t	6	0	0	0	0
41	u	47	0	0	0	0
41	v	47	0	0	2	0
41	x	2	0	0	0	0
41	y	1	0	0	0	0
All	All	52545	0	51977	630	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 (630) 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	1.43	0.99
23:C:514:CLA:HBB1	25:C:515:BCR:H24C	1.48	0.93
23:B:604:CLA:H42	23:B:605:CLA:H2	1.50	0.91
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.51	0.90
25:b:619:BCR:H331	25:b:619:BCR:HC8	1.58	0.85
4:d:192:THR:HG23	23:d:402:CLA:HBC2	1.61	0.82
25:H:101:BCR:HC8	25:H:101:BCR:H331	1.64	0.80
1:a:253:GLY:HA3	2:b:491:VAL:HG12	1.66	0.77
2:b:121:GLU:HG2	7:h:4:ARG:HG2	1.65	0.77
23:c:514:CLA:HBB1	25:c:515:BCR:H24C	1.68	0.74
23:B:601:CLA:H12	23:B:601:CLA:H71	1.70	0.73
3:c:279:LEU:HD22	23:c:510:CLA:HED2	1.69	0.73
26:a:411:SQD:H141	37:d:408:LHG:H152	1.69	0.73
23:c:506:CLA:CMD	23:c:508:CLA:HAB	2.18	0.73
23:C:506:CLA:CMD	23:C:508:CLA:HAB	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:409:GLY:O	41:c:601:HOH:O	2.06	0.73
23:A:406:CLA:H152	29:A:414:PL9:H252	1.70	0.72
8:I:37:LEU:O	41:I:201:HOH:O	2.07	0.71
10:K:15:TYR:OH	19:Z:58:ASN:ND2	2.22	0.71
23:a:409:CLA:H152	23:c:507:CLA:H142	1.72	0.71
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.74	0.70
32:E:102:LMT:H3O2	32:E:102:LMT:H2O1	1.39	0.70
13:O:124:ASN:HD22	13:O:147:ASN:HD22	1.40	0.70
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.73	0.70
33:D:415:LMG:H412	6:F:30:THR:HG21	1.74	0.69
23:c:504:CLA:HBB1	23:c:513:CLA:H41	1.73	0.69
1:A:25:ASP:OD1	41:A:501:HOH:O	2.10	0.69
13:o:124:ASN:HD22	13:o:147:ASN:HD22	1.38	0.69
29:A:414:PL9:H253	23:D:405:CLA:H141	1.73	0.69
23:c:510:CLA:H192	23:c:513:CLA:HHD	1.74	0.68
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.76	0.67
2:B:54:PRO:HB3	27:B:625:GOL:H11	1.75	0.67
23:c:512:CLA:H191	33:z:101:LMG:H242	1.77	0.67
25:t:103:BCR:H311	25:t:103:BCR:HC8	1.75	0.67
3:C:286:ALA:HB2	23:C:503:CLA:HMD1	1.77	0.67
23:C:506:CLA:HMD3	23:C:508:CLA:HAB	1.76	0.66
4:D:11:GLU:OE2	41:D:501:HOH:O	2.12	0.66
33:Z:101:LMG:HO4	33:Z:101:LMG:HO5	1.43	0.66
24:A:353:PHO:H3A	23:D:405:CLA:H142	1.77	0.66
2:b:224:ARG:HH11	32:b:621:LMT:H12	1.61	0.66
5:e:9:PRO:HA	37:e:101:LHG:HC31	1.78	0.65
23:B:606:CLA:H192	23:B:616:CLA:H101	1.76	0.65
25:d:404:BCR:H383	33:d:412:LMG:H171	1.80	0.64
26:a:411:SQD:H271	37:d:408:LHG:H141	1.79	0.64
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.79	0.64
23:B:602:CLA:HHC	23:B:602:CLA:HBB1	1.78	0.63
29:a:416:PL9:H28	37:e:101:LHG:H222	1.80	0.63
1:A:121[B]:LEU:HD11	23:C:506:CLA:H122	1.78	0.63
4:D:14:TRP:CD1	34:D:414:HTG:H61	2.32	0.63
29:a:416:PL9:H512	26:f:102:SQD:H292	1.78	0.63
23:c:505:CLA:H42	35:c:518:DGD:HB42	1.81	0.63
3:c:438:LEU:HD11	23:c:506:CLA:HBB1	1.81	0.63
37:D:411:LHG:H132	37:D:411:LHG:H372	1.79	0.62
1:a:72:LEU:HD11	32:a:414:LMT:H52	1.79	0.62
34:B:622:HTG:H1	32:a:414:LMT:H21	1.80	0.62
13:O:68:THR:HG22	13:O:110[B]:MET:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:606:CLA:HHC	23:b:606:CLA:HBB1	1.81	0.62
35:C:517:DGD:O1A	41:C:601:HOH:O	2.16	0.62
3:C:406:SER:HA	3:C:420:VAL:HG23	1.82	0.61
23:C:509:CLA:HBC3	23:C:511:CLA:H71	1.82	0.61
2:b:497:GLN:HB2	2:b:504:THR:HB	1.83	0.61
13:o:58:ASN:HD21	13:o:61:GLN:HB2	1.64	0.61
23:a:406:CLA:HHC	23:a:406:CLA:HBB1	1.82	0.61
23:B:603:CLA:H191	7:H:39:LEU:HD12	1.84	0.60
5:e:67:THR:H	5:e:75:GLN:HE22	1.50	0.60
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	1.82	0.60
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.83	0.60
25:y:101:BCR:H321	25:y:101:BCR:HC8	1.84	0.59
25:T:101:BCR:H311	25:T:101:BCR:HC8	1.84	0.59
18:Y:23:THR:HB	18:Y:24:MET:HE2	1.84	0.59
1:a:227:THR:HB	1:a:231:GLU:HG3	1.84	0.59
23:c:509:CLA:HBC3	23:c:511:CLA:H71	1.84	0.59
1:a:211:PHE:CD2	29:a:416:PL9:H101	2.38	0.59
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.84	0.58
33:c:520:LMG:H172	33:c:520:LMG:H312	1.84	0.58
3:C:279:LEU:HD22	23:C:510:CLA:HED2	1.84	0.58
23:A:405:CLA:HHC	23:A:405:CLA:HBB1	1.85	0.58
34:B:622:HTG:H61	32:a:414:LMT:H6E	1.84	0.58
1:A:227:THR:HB	1:A:231:GLU:HG3	1.85	0.58
1:A:270:SER:HB2	26:A:410:SQD:O49	2.04	0.58
37:d:407:LHG:H322	14:t:21:ILE:HD11	1.84	0.57
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.86	0.57
23:c:509:CLA:HBC2	37:d:408:LHG:H362	1.85	0.57
23:c:514:CLA:HBB1	25:c:515:BCR:H371	1.86	0.57
7:h:56:ASP:OD1	17:x:2:THR:OG1	2.22	0.57
1:a:15:GLU:HB2	32:a:420:LMT:H6'2	1.86	0.57
23:A:408:CLA:H193	23:C:507:CLA:H101	1.86	0.57
23:b:602:CLA:H101	23:b:609:CLA:H193	1.87	0.57
32:M:101:LMT:H102	23:b:614:CLA:H92	1.87	0.57
8:i:35:LYS:O	8:i:37:LEU:N	2.38	0.57
23:c:502:CLA:C4D	23:c:504:CLA:H2	2.35	0.57
38:e:87:HEM:HAC	6:f:27:ALA:HB1	1.87	0.57
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.87	0.57
32:A:359:LMT:H71	2:b:39:LEU:HD13	1.87	0.56
25:B:618:BCR:H363	25:t:103:BCR:H19C	1.87	0.56
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.86	0.56
2:b:216:HIS:HE1	23:b:609:CLA:C1A	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:406:SER:HA	3:c:420:VAL:HG23	1.88	0.56
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.88	0.55
4:D:123:ILE:HD11	35:H:102:DGD:HAH2	1.87	0.55
32:M:101:LMT:H6D	11:l:9:PRO:HA	1.87	0.55
23:b:615:CLA:HHC	23:b:615:CLA:HBB1	1.89	0.55
3:C:325:GLY:O	15:U:51:LYS:NZ	2.37	0.55
5:E:40:THR:HB	20:R:4:ARG:HG2	1.88	0.55
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.87	0.55
26:A:410:SQD:H251	37:D:411:LHG:H131	1.89	0.55
5:e:26:THR:HB	38:e:87:HEM:HAB	1.89	0.55
23:C:507:CLA:H62	32:I:101:LMT:H91	1.89	0.55
37:d:406:LHG:H212	12:m:18:PRO:HG3	1.87	0.55
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.19	0.55
3:c:286:ALA:HB2	23:c:503:CLA:HMD1	1.87	0.55
23:C:514:CLA:HBB1	25:C:515:BCR:H371	1.89	0.54
25:b:619:BCR:H331	25:b:619:BCR:C8	2.32	0.54
23:C:504:CLA:HBB1	23:C:513:CLA:H41	1.90	0.54
13:o:124:ASN:ND2	13:o:147:ASN:HD22	2.05	0.54
13:O:39:ARG:HB2	13:O:246:ALA:HB2	1.88	0.54
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.42	0.54
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.42	0.54
10:K:20:PRO:HB3	18:Y:21:GLN:HG3	1.90	0.54
23:B:614:CLA:H43	26:B:620:SQD:H111	1.89	0.54
2:b:12:LEU:HB2	23:b:612:CLA:HMC2	1.90	0.54
23:c:506:CLA:HMD3	23:c:508:CLA:HAB	1.90	0.54
1:a:183:MET:HA	23:a:405:CLA:HMD1	1.90	0.54
23:C:514:CLA:H171	25:C:515:BCR:H373	1.90	0.54
23:B:616:CLA:HHC	23:B:616:CLA:HBB1	1.89	0.53
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.44	0.53
24:a:353:PHO:H61	23:d:402:CLA:H111	1.89	0.53
19:z:35:ARG:HH21	19:z:39:LEU:HD11	1.73	0.53
1:A:84:PRO:HA	1:A:112:TYR:CG	2.43	0.53
4:d:141:TYR:OH	37:d:406:LHG:O4	2.16	0.53
13:O:42:ARG:O	13:O:241:ALA:HA	2.09	0.53
12:m:5:GLN:H	12:m:5:GLN:NE2	2.07	0.53
6:F:15:ILE:HD13	20:R:23:ILE:HD11	1.91	0.53
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.90	0.53
23:c:505:CLA:H151	23:c:509:CLA:H143	1.89	0.53
2:B:299:GLU:HG2	2:B:402:TYR:HD1	1.74	0.53
37:E:101:LHG:O2	6:F:19:ARG:NH1	2.42	0.53
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:620:SQD:H462	26:b:620:SQD:H1	1.91	0.52
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.09	0.52
24:a:408:PHO:HAB	4:d:205:LEU:HD13	1.90	0.52
3:c:52:ALA:HB2	23:c:512:CLA:HMA2	1.91	0.52
33:c:521:LMG:H232	33:c:521:LMG:H391	1.92	0.52
2:B:285:ASN:O	2:B:289:GLN:HG2	2.10	0.52
13:O:92:SER:HB3	13:O:131:PRO:HA	1.91	0.52
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.45	0.52
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.45	0.52
23:b:607:CLA:HBC3	25:b:618:BCR:HC8	1.90	0.52
1:a:84:PRO:HA	1:a:112:TYR:CG	2.45	0.52
1:A:183:MET:HA	23:A:404:CLA:HMD1	1.92	0.51
5:E:30:LEU:HD23	20:R:12:VAL:HG22	1.90	0.51
13:O:124:ASN:ND2	13:O:147:ASN:HD22	2.06	0.51
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.92	0.51
24:A:407:PHO:HAB	4:D:205:LEU:HD13	1.92	0.51
4:D:192:THR:HG23	23:D:405:CLA:HBC2	1.92	0.51
25:T:101:BCR:H351	26:b:620:SQD:H211	1.92	0.51
23:B:602:CLA:H101	23:B:609:CLA:H193	1.92	0.51
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.93	0.51
23:C:502:CLA:C4D	23:C:504:CLA:H2	2.41	0.51
26:a:411:SQD:H301	23:c:509:CLA:H71	1.93	0.51
37:d:407:LHG:HC62	11:l:15:THR:HG23	1.92	0.51
23:a:405:CLA:H201	37:d:407:LHG:H161	1.92	0.51
25:B:619:BCR:H331	25:B:619:BCR:C8	2.40	0.51
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.46	0.51
4:D:24:ARG:NH2	26:F:101:SQD:O4	2.44	0.51
10:K:25:LEU:HD22	25:Y:101:BCR:H332	1.93	0.51
5:E:60:GLN:HG2	5:E:62[B]:SER:H	1.77	0.50
25:H:101:BCR:H331	25:H:101:BCR:C8	2.36	0.50
16:v:12:LEU:HD12	16:v:69:ILE:HB	1.92	0.50
13:O:124:ASN:HD22	13:O:147:ASN:ND2	2.06	0.50
23:c:513:CLA:O2D	23:c:514:CLA:HBB2	2.11	0.50
2:B:149:LEU:HD13	23:B:604:CLA:H171	1.93	0.50
29:A:414:PL9:H503	26:F:101:SQD:H341	1.92	0.50
26:B:620:SQD:H381	32:m:103:LMT:H121	1.92	0.50
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.92	0.50
33:C:501:LMG:H142	23:C:506:CLA:H203	1.94	0.50
1:a:214:MET:HG2	29:a:416:PL9:H103	1.94	0.50
12:m:5:GLN:HB3	41:m:213:HOH:O	2.12	0.50
23:D:406:CLA:HBB1	23:D:406:CLA:HHC	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:13:GLY:HA3	34:D:414:HTG:H62	1.93	0.49
19:z:34:ASP:OD1	19:z:34:ASP:N	2.44	0.49
25:B:619:BCR:H331	25:B:619:BCR:HC8	1.94	0.49
23:C:502:CLA:C3D	23:C:504:CLA:H2	2.42	0.49
32:M:103:LMT:O3'	32:M:103:LMT:O2B	2.26	0.49
2:b:491:VAL:HG13	4:d:136:VAL:HG13	1.93	0.49
25:T:101:BCR:H19C	25:b:618:BCR:H363	1.95	0.49
5:E:60:GLN:HG2	5:E:62[A]:SER:H	1.77	0.49
1:A:163:ILE:HD11	35:C:517:DGD:HA22	1.93	0.49
2:B:299:GLU:HG3	41:B:824:HOH:O	2.10	0.49
35:c:519:DGD:HBH2	37:d:408:LHG:H211	1.95	0.49
19:z:57:LEU:HA	19:z:60:PHE:HD1	1.78	0.49
23:c:506:CLA:HAA1	23:c:506:CLA:HBD	1.94	0.49
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.93	0.49
2:b:233:ASN:O	2:b:236:THR:HG22	2.13	0.49
2:B:490:GLN:HG3	2:B:496:TYR:HE2	1.77	0.49
3:C:334:PRO:HA	13:O:153:THR:OG1	2.13	0.49
33:C:501:LMG:H121	23:C:506:CLA:H201	1.95	0.48
30:c:525:UNL:O6	41:c:602:HOH:O	2.20	0.48
19:z:26:ALA:HB1	19:z:36:SER:HB3	1.94	0.48
2:B:58:GLN:C	2:B:329:PRO:HB3	2.38	0.48
23:B:602:CLA:H203	23:B:602:CLA:H162	1.56	0.48
1:a:221[A]:SER:HB2	4:d:139:ARG:O	2.13	0.48
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.47	0.48
3:c:137:PRO:HG3	23:c:514:CLA:HED3	1.95	0.48
16:V:126:LEU:HB3	16:V:129:LYS:HB2	1.93	0.48
2:b:162:PHE:O	23:b:606:CLA:HHD	2.13	0.48
10:k:15:TYR:OH	19:z:58:ASN:ND2	2.43	0.48
13:O:193:THR:HG21	13:O:220:LEU:HD12	1.94	0.48
23:b:606:CLA:H162	23:b:606:CLA:H122	1.49	0.48
3:c:212:TYR:OH	3:c:232:ASP:OD2	2.27	0.48
2:B:54:PRO:HB2	27:B:625:GOL:H31	1.96	0.48
34:B:622:HTG:O5	27:a:412:GOL:H11	2.13	0.48
25:B:618:BCR:H381	25:t:103:BCR:H341	1.96	0.48
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.95	0.48
13:O:49[A]:THR:OG1	13:O:236:GLN:HB2	2.14	0.48
2:B:363:PHE:HB3	2:B:365:SER:O	2.14	0.48
3:C:95:LEU:HD21	23:C:502:CLA:OBD	2.14	0.48
32:D:404:LMT:H5'	30:D:413:UNL:O9	2.14	0.48
23:a:406:CLA:HBA1	23:a:406:CLA:C4A	2.43	0.48
3:c:60:ILE:HG22	23:c:504:CLA:HHD	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:40:ILE:HD12	13:o:95:PHE:CD1	2.48	0.48
26:A:410:SQD:H122	26:A:410:SQD:H152	1.67	0.47
3:C:95:LEU:HD13	23:C:503:CLA:H142	1.95	0.47
35:C:518:DGD:HAE2	35:C:518:DGD:HA81	1.69	0.47
13:o:42:ARG:O	13:o:241:ALA:HA	2.14	0.47
18:Y:22:LEU:HA	18:Y:25:ILE:HG22	1.96	0.47
2:b:245:VAL:HG22	23:b:612:CLA:H202	1.96	0.47
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.80	0.47
10:k:16:ALA:O	10:k:19:ASP:HB2	2.14	0.47
23:A:404:CLA:CBD	23:A:405:CLA:HAC2	2.45	0.47
23:B:615:CLA:HHC	23:B:615:CLA:HBB1	1.97	0.47
23:c:503:CLA:H61	23:c:513:CLA:H42	1.96	0.47
32:A:359:LMT:H21	34:b:622:HTG:H1	1.96	0.47
3:C:38:GLY:HA3	23:C:512:CLA:HMD2	1.97	0.47
3:c:82:TYR:OH	3:c:394:GLU:OE2	2.26	0.47
4:d:85:MET:HE2	4:d:90:LEU:HD21	1.95	0.47
13:o:216:GLU:CD	13:o:234:LYS:HD2	2.40	0.47
2:B:36[A]:SER:OG	25:B:618:BCR:H362	2.14	0.47
2:B:55:MET:HE3	27:B:625:GOL:H32	1.97	0.47
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.50	0.47
2:B:489:GLU:HB3	2:B:495:PHE:CD1	2.50	0.47
23:a:405:CLA:CBD	23:a:406:CLA:HAC2	2.45	0.47
2:b:62:VAL:HB	23:b:605:CLA:HED3	1.97	0.47
3:c:120:ILE:HG23	19:z:47:TRP:CH2	2.50	0.47
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.96	0.47
2:B:54:PRO:CB	27:B:625:GOL:H11	2.45	0.47
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.97	0.47
23:b:613:CLA:H112	23:b:613:CLA:H151	1.60	0.47
2:B:12:LEU:HB2	23:B:612:CLA:HMC2	1.97	0.47
2:B:223:GLN:HG2	7:H:21:VAL:HG21	1.97	0.47
25:B:618:BCR:H382	25:t:103:BCR:H11C	1.96	0.47
5:E:27:ILE:HD11	38:E:103:HEM:HBC2	1.96	0.47
1:a:272:HIS:CD2	4:d:218:VAL:HG21	2.50	0.47
24:a:353:PHO:HBC3	4:d:279:LEU:HD22	1.97	0.47
23:b:616:CLA:H92	23:b:616:CLA:H62	1.70	0.47
4:D:54:PHE:O	5:E:49:THR:OG1	2.27	0.47
13:O:18:LYS:NZ	13:O:74[A]:GLU:OE2	2.48	0.47
7:H:43:LEU:HA	7:H:43:LEU:HD12	1.77	0.46
32:M:103:LMT:H11	12:m:6:LEU:HD11	1.97	0.46
2:b:58:GLN:C	2:b:329:PRO:HB3	2.41	0.46
13:o:43:LEU:HB3	13:o:81:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:SER:HA	4:D:272:LEU:HD12	1.96	0.46
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.14	0.46
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.71	0.46
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.49	0.46
10:K:17:ILE:H	10:K:17:ILE:HD13	1.81	0.46
1:a:334:ARG:HD3	4:d:320:LEU:HD13	1.96	0.46
14:T:2:GLU:H	14:T:2:GLU:CD	2.22	0.46
1:a:217:SER:O	1:a:221[A]:SER:HB3	2.16	0.46
19:Z:33:TRP:HZ2	33:Z:101:LMG:HC61	1.80	0.46
13:o:124:ASN:HD22	13:o:147:ASN:ND2	2.10	0.46
23:b:614:CLA:H62	23:b:614:CLA:H41	1.51	0.46
24:A:353:PHO:HBC2	24:A:353:PHO:HHD	1.98	0.46
24:a:353:PHO:HBC2	24:a:353:PHO:HHD	1.98	0.46
2:b:498:LYS:NZ	4:d:20:ASP:OD1	2.42	0.46
26:b:620:SQD:H62	11:l:7:ARG:NH1	2.30	0.46
4:D:16:ASP:OD2	32:D:404:LMT:H6E	2.15	0.46
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.98	0.46
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.50	0.46
23:B:614:CLA:HAA1	23:B:614:CLA:HBD	1.97	0.46
2:b:36:SER:OG	25:b:618:BCR:H362	2.16	0.46
7:h:38:PHE:HB2	25:h:101:BCR:C10	2.45	0.46
16:v:64:PRO:HD2	16:v:66:ARG:NH2	2.31	0.46
3:C:276:LEU:HD23	23:C:510:CLA:HED1	1.97	0.46
23:C:509:CLA:H142	23:C:509:CLA:H111	1.76	0.46
2:b:224:ARG:NH1	4:d:16:ASP:OD2	2.44	0.46
2:b:231:MET:HE2	23:b:610:CLA:HMC1	1.97	0.46
1:A:310:LYS:HD2	16:V:1:ALA:HB1	1.98	0.45
2:B:160:GLY:HA2	2:B:163:GLY:O	2.16	0.45
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.99	0.45
3:C:83:GLU:OE2	3:C:398:HIS:NE2	2.47	0.45
1:A:132:GLU:O	1:A:136:ARG:HG2	2.17	0.45
3:C:42:LEU:HD21	23:C:512:CLA:H2A	1.98	0.45
11:L:26:VAL:HG11	37:L:101:LHG:H201	1.99	0.45
33:C:501:LMG:H211	35:C:517:DGD:HA82	1.97	0.45
23:C:507:CLA:HMC2	23:C:508:CLA:H102	1.99	0.45
25:D:407:BCR:H381	33:D:415:LMG:H231	1.99	0.45
13:O:81:ILE:HA	13:O:100:GLY:HA3	1.99	0.45
23:b:613:CLA:HBB1	23:b:613:CLA:HMB1	1.97	0.45
3:c:171:GLY:O	3:c:174:LEU:HB2	2.16	0.45
4:d:61:HIS:O	41:d:501:HOH:O	2.20	0.45
1:A:121[B]:LEU:HD21	23:C:506:CLA:H172	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.51	0.45
5:E:12:ASP:OD2	9:J:4:GLY:HA3	2.16	0.45
3:c:429:SER:HA	35:c:518:DGD:HBW1	1.98	0.45
13:o:51:LEU:HB3	13:o:65:PHE:HB3	1.98	0.45
26:A:412:SQD:H301	23:b:606:CLA:H202	1.98	0.45
23:B:613:CLA:H121	23:B:613:CLA:H162	1.70	0.45
13:O:51:LEU:HB3	13:O:65:PHE:HB3	1.99	0.45
13:O:216:GLU:CD	13:O:234:LYS:HD2	2.42	0.45
35:c:518:DGD:HA61	35:c:518:DGD:HAN2	1.99	0.45
8:i:2:GLU:O	8:i:6:ILE:HG12	2.16	0.45
23:B:604:CLA:HBB1	23:B:604:CLA:HMB1	1.99	0.45
2:b:30:VAL:HG12	23:b:605:CLA:HHD	1.97	0.45
23:c:509:CLA:H93	37:d:408:LHG:H162	1.99	0.45
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.99	0.45
29:A:414:PL9:H151	29:A:414:PL9:H171	1.54	0.45
25:H:101:BCR:H24C	25:H:101:BCR:H371	1.73	0.45
23:c:514:CLA:H202	33:c:521:LMG:H402	1.98	0.45
25:c:515:BCR:H341	25:c:515:BCR:H11C	1.72	0.45
1:A:63:ILE:HB	3:C:335:THR:HG21	1.99	0.45
33:C:501:LMG:H161	33:C:501:LMG:H191	1.84	0.45
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.47	0.45
1:A:131:TRP:CH2	23:C:506:CLA:HAA2	2.52	0.45
1:a:131:TRP:CH2	23:c:506:CLA:HAA2	2.52	0.45
1:a:230:THR:O	2:b:3:LEU:HD23	2.17	0.45
23:a:405:CLA:H202	23:a:405:CLA:H162	1.82	0.45
23:c:509:CLA:H203	35:c:518:DGD:HA92	1.98	0.45
4:d:210:LEU:HA	4:d:213:ILE:HG22	1.99	0.45
10:k:20:PRO:HB3	18:y:21:GLN:HG3	1.98	0.45
35:C:518:DGD:HAN1	35:C:518:DGD:HAW1	1.73	0.44
13:O:32:ILE:HG13	13:O:93:LEU:HD11	1.98	0.44
1:a:307[A]:ILE:CG2	1:a:311:GLY:HA2	2.48	0.44
1:a:310:LYS:HD2	16:v:1:ALA:HB1	1.98	0.44
25:a:410:BCR:H11C	25:a:410:BCR:H341	1.85	0.44
3:c:61:VAL:HG12	3:c:118:HIS:O	2.17	0.44
23:c:513:CLA:H91	23:c:513:CLA:H112	1.75	0.44
23:A:406:CLA:HED1	35:C:519:DGD:HAE2	1.99	0.44
3:C:223:TRP:CG	3:C:224:ILE:H	2.35	0.44
5:E:9:PRO:HA	37:E:101:LHG:HC31	1.99	0.44
1:a:224:ILE:HG23	2:b:484:PRO:HA	1.99	0.44
3:C:443:TRP:CZ2	23:C:509:CLA:HMD1	2.52	0.44
38:E:103:HEM:HAC	6:F:27:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:506:CLA:H192	23:c:506:CLA:H162	1.80	0.44
13:o:83:GLY:HA2	13:o:98:GLU:HG3	2.00	0.44
16:v:47:LYS:NZ	41:v:303:HOH:O	2.50	0.44
23:A:408:CLA:H151	23:C:507:CLA:H13	1.98	0.44
24:A:353:PHO:NC	24:A:353:PHO:ND	2.64	0.44
10:K:24:VAL:HG13	18:Y:25:ILE:HD13	1.98	0.44
25:T:101:BCR:H24C	25:T:101:BCR:H371	1.83	0.44
29:a:416:PL9:H503	17:x:24:THR:OG1	2.17	0.44
3:c:443:TRP:CZ2	23:c:509:CLA:HMD1	2.52	0.44
23:c:511:CLA:H122	23:c:511:CLA:H161	1.80	0.44
16:v:2:GLU:HB2	41:v:336:HOH:O	2.17	0.44
1:A:221[A]:SER:HB2	4:D:139:ARG:O	2.16	0.44
4:D:78:VAL:HG11	4:D:114:ILE:HD12	2.00	0.44
29:a:416:PL9:H151	29:a:416:PL9:H171	1.54	0.44
23:C:511:CLA:H112	23:C:511:CLA:H152	1.55	0.44
35:C:517:DGD:HG11	41:C:601:HOH:O	2.18	0.44
4:D:244:TYR:OH	4:D:264:LYS:HE2	2.16	0.44
8:I:17:LEU:HD22	8:I:21:PHE:HE2	1.82	0.44
25:T:101:BCR:H331	25:T:101:BCR:HC7	1.62	0.44
26:A:410:SQD:H112	26:A:410:SQD:H81	1.67	0.44
2:B:489:GLU:HB3	2:B:495:PHE:CG	2.52	0.44
23:C:504:CLA:HBB1	23:C:504:CLA:HHC	2.00	0.44
2:b:161:LEU:HD12	2:b:161:LEU:HA	1.86	0.44
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.51	0.44
23:c:511:CLA:H2	23:c:511:CLA:HED2	2.00	0.44
35:c:517:DGD:HAN1	35:c:517:DGD:HAW2	1.74	0.44
23:B:613:CLA:H161	23:B:613:CLA:H192	1.77	0.44
25:Y:101:BCR:H15C	25:Y:101:BCR:H351	1.90	0.44
3:c:415:ASN:O	3:c:416[B]:SER:HB2	2.18	0.44
23:c:511:CLA:H111	23:c:511:CLA:H142	1.66	0.44
4:d:14:TRP:CD1	34:d:411:HTG:H61	2.52	0.44
2:b:496:TYR:HB2	41:d:608:HOH:O	2.18	0.44
26:B:620:SQD:H383	26:B:620:SQD:H351	1.81	0.43
3:C:151:TRP:CZ3	23:C:510:CLA:H202	2.52	0.43
23:C:506:CLA:H93	23:C:506:CLA:H111	1.75	0.43
25:C:516:BCR:H15C	25:C:516:BCR:H351	1.86	0.43
37:D:411:LHG:H382	37:D:411:LHG:H112	1.99	0.43
6:F:21:VAL:O	6:F:25:THR:HG23	2.17	0.43
1:a:300:PHE:HB3	1:a:302:PHE:CE1	2.53	0.43
23:b:601:CLA:H72	23:b:601:CLA:H2	1.99	0.43
23:c:506:CLA:HMD2	23:c:508:CLA:HAB	1.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:d:403:CLA:H2	17:x:17:GLY:HA3	2.00	0.43
18:y:22:LEU:HA	18:y:25:ILE:HG22	1.99	0.43
23:C:511:CLA:H2	23:C:511:CLA:HED2	1.99	0.43
1:a:132:GLU:O	1:a:136:ARG:HG2	2.18	0.43
3:c:223:TRP:CG	3:c:224:ILE:H	2.36	0.43
37:d:408:LHG:H302	37:d:408:LHG:H332	1.69	0.43
7:h:38:PHE:HB2	25:h:101:BCR:H10C	2.00	0.43
35:H:102:DGD:HB91	35:H:102:DGD:HBW2	1.93	0.43
32:M:103:LMT:H2O1	32:M:103:LMT:H3O2	1.63	0.43
3:c:275:SER:HB3	23:c:510:CLA:HED3	2.00	0.43
23:c:509:CLA:H162	23:c:509:CLA:H122	1.77	0.43
4:d:148:ALA:HB3	4:d:149:PRO:HD3	2.00	0.43
38:e:87:HEM:CAC	6:f:27:ALA:HB1	2.48	0.43
9:j:6:ARG:HA	9:j:6:ARG:NH2	2.33	0.43
25:k:101:BCR:H371	25:k:101:BCR:H24C	1.62	0.43
2:b:461:LEU:HD21	4:d:284:ILE:HD11	1.99	0.43
23:c:513:CLA:H92	23:c:513:CLA:H62	1.84	0.43
15:u:17:LEU:HD23	15:u:17:LEU:HA	1.85	0.43
23:C:506:CLA:HAA1	23:C:506:CLA:HBD	2.01	0.43
15:U:64:ILE:HA	15:U:65:PRO:HD3	1.87	0.43
23:a:406:CLA:H203	23:a:406:CLA:H162	1.81	0.43
2:b:220:ARG:HG3	7:h:20:LYS:HG2	2.00	0.43
3:c:213[B]:LEU:HD11	25:c:516:BCR:H373	2.01	0.43
6:f:28:VAL:HB	6:f:29:PRO:HD3	2.00	0.43
2:B:201:HIS:HB2	23:B:602:CLA:CHB	2.48	0.43
2:B:223:GLN:OE1	2:B:227:LYS:HD2	2.18	0.43
23:C:511:CLA:H192	23:C:511:CLA:HBC3	2.00	0.43
23:a:407:CLA:C4A	23:a:407:CLA:HBA1	2.48	0.43
25:c:516:BCR:H15C	25:c:516:BCR:H351	1.87	0.43
12:m:28:GLN:O	12:m:32:GLN:HG3	2.18	0.43
3:C:52:ALA:HB2	23:C:512:CLA:HMA2	2.01	0.43
10:K:15:TYR:CE1	19:Z:5:PHE:HZ	2.37	0.43
2:b:42:LEU:HD23	2:b:42:LEU:HA	1.83	0.43
23:b:615:CLA:H92	23:b:615:CLA:H61	1.85	0.43
23:c:506:CLA:HBC2	25:c:516:BCR:H341	2.01	0.43
2:B:489:GLU:HG2	2:B:495:PHE:CE2	2.54	0.43
1:a:160:ILE:HD11	35:c:517:DGD:HBT1	2.01	0.43
2:b:149:LEU:HG	23:b:606:CLA:HBB2	2.01	0.43
23:b:607:CLA:H91	23:b:607:CLA:H112	1.79	0.43
3:c:38:GLY:HA3	23:c:512:CLA:HMD2	2.01	0.43
3:c:42:LEU:HD21	23:c:512:CLA:H2A	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:146:PHE:O	4:d:149:PRO:HD2	2.18	0.43
7:h:4:ARG:HH11	7:h:9:ASP:CG	2.27	0.43
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.89	0.43
2:B:162:PHE:O	23:B:606:CLA:HHD	2.19	0.43
23:B:605:CLA:HMC3	23:B:615:CLA:H43	1.99	0.43
5:E:27:ILE:CD1	38:E:103:HEM:HBC2	2.48	0.43
2:b:86:ILE:H	2:b:86:ILE:HG13	1.65	0.43
23:c:510:CLA:CMB	23:c:512:CLA:HBB1	2.49	0.43
25:c:516:BCR:H341	25:c:516:BCR:H11C	1.93	0.43
34:d:411:HTG:H1	7:h:25:TRP:CD1	2.54	0.43
25:t:103:BCR:HC7	25:t:103:BCR:H331	1.62	0.43
23:C:514:CLA:H161	33:C:521:LMG:H421	1.99	0.43
5:E:45:ASP:OD2	20:R:4:ARG:NH2	2.52	0.43
15:U:48:LEU:HA	15:U:48:LEU:HD23	1.80	0.43
23:b:602:CLA:H203	23:b:602:CLA:H161	1.76	0.43
14:t:20:ALA:O	14:t:24:ARG:HB3	2.18	0.43
23:A:408:CLA:HMC2	25:A:409:BCR:H12C	2.01	0.42
25:B:618:BCR:H24C	25:B:618:BCR:H371	1.74	0.42
3:C:203:THR:O	3:C:235:GLY:HA3	2.19	0.42
4:d:126:MET:HE3	4:d:143:ALA:O	2.19	0.42
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.54	0.42
12:m:5:GLN:HA	14:t:1:FME:HE1	2.01	0.42
12:m:6:LEU:HD23	12:m:6:LEU:HA	1.87	0.42
2:B:423:LYS:HA	2:B:423:LYS:HD3	1.81	0.42
23:B:605:CLA:H192	23:B:609:CLA:HBB2	2.01	0.42
7:H:62:TRP:C	7:H:64:ALA:H	2.27	0.42
25:K:102:BCR:H24C	25:K:102:BCR:H371	1.64	0.42
23:a:406:CLA:H52	29:d:405:PL9:H151	2.01	0.42
3:c:130:VAL:HG22	23:c:512:CLA:H91	2.01	0.42
2:B:133:LEU:HB3	2:B:138:MET:SD	2.59	0.42
2:B:505:ARG:HD3	2:B:505:ARG:C	2.44	0.42
25:B:618:BCR:H15C	25:B:618:BCR:H351	1.86	0.42
25:C:515:BCR:H24C	25:C:515:BCR:H371	1.76	0.42
4:D:146:PHE:O	4:D:149:PRO:HD2	2.19	0.42
37:E:101:LHG:H261	37:E:101:LHG:H291	1.65	0.42
19:Z:26:ALA:HB1	19:Z:36:SER:HB3	2.01	0.42
23:b:605:CLA:HAA1	23:b:605:CLA:HBD	2.00	0.42
19:z:35:ARG:NH2	19:z:39:LEU:HD11	2.34	0.42
23:A:404:CLA:H192	23:A:404:CLA:H161	1.75	0.42
8:I:33:LYS:HB3	8:I:34:ARG:H	1.62	0.42
23:b:604:CLA:H172	23:b:604:CLA:H13	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:614:CLA:H122	23:b:614:CLA:H162	1.70	0.42
23:d:403:CLA:H142	7:h:36:GLY:HA3	2.00	0.42
7:h:62:TRP:C	7:h:64:ALA:H	2.28	0.42
14:t:15:ALA:HA	25:t:103:BCR:H12C	2.01	0.42
1:A:202:VAL:HG11	23:A:406:CLA:C3D	2.49	0.42
23:B:603:CLA:HAB	23:B:605:CLA:H171	2.02	0.42
23:B:614:CLA:H61	32:m:103:LMT:H82	2.02	0.42
12:M:20:VAL:HG22	12:m:20:VAL:HG11	2.01	0.42
13:O:32:ILE:HG21	13:O:93:LEU:HD21	2.01	0.42
25:T:101:BCR:H11C	25:T:101:BCR:H341	1.81	0.42
1:a:307[B]:ILE:HG22	1:a:313:VAL:HA	2.02	0.42
3:c:338:GLY:HA3	3:c:341:LEU:O	2.19	0.42
25:h:101:BCR:H331	25:h:101:BCR:C8	2.49	0.42
18:y:38:LEU:O	18:y:42:ARG:HG2	2.18	0.42
2:B:86:ILE:H	2:B:86:ILE:HG13	1.74	0.42
4:D:24:ARG:HD3	17:X:37:VAL:HG22	2.02	0.42
25:K:102:BCR:H15C	25:K:102:BCR:H351	1.89	0.42
1:a:127:MET:HE3	23:c:506:CLA:HMB2	2.00	0.42
24:a:353:PHO:H72	24:a:353:PHO:H112	1.80	0.42
23:b:612:CLA:H171	23:b:613:CLA:HBB2	2.00	0.42
3:c:334:PRO:HA	13:o:153:THR:OG1	2.20	0.42
1:A:187:GLN:HB2	23:A:404:CLA:HAC2	2.02	0.42
23:A:408:CLA:H112	23:A:408:CLA:H142	1.67	0.42
2:B:223:GLN:HE21	2:B:223:GLN:HB3	1.62	0.42
13:O:201:VAL:HG22	13:O:211:ILE:HD12	2.01	0.42
3:c:400:PRO:C	3:c:401:LEU:HD12	2.44	0.42
23:d:403:CLA:H142	23:d:403:CLA:H112	1.91	0.42
13:o:40:ILE:HG12	13:o:243:ILE:HD13	2.02	0.42
2:B:97:ALA:O	2:B:101:ILE:HG12	2.20	0.42
23:B:603:CLA:H2	23:B:605:CLA:H91	2.01	0.42
4:D:49:LEU:HD13	25:D:407:BCR:C15	2.49	0.42
23:b:606:CLA:H161	23:b:606:CLA:H192	1.80	0.42
23:c:502:CLA:C3D	23:c:504:CLA:H2	2.50	0.42
15:u:45:LEU:HD23	15:u:45:LEU:HA	1.82	0.42
1:A:307:ILE:HD13	1:A:313:VAL:HA	2.02	0.42
23:B:612:CLA:HBB1	23:B:612:CLA:HMB1	2.01	0.42
13:O:30:TYR:HA	13:O:31:PRO:HD3	1.84	0.42
25:T:101:BCR:H11C	25:b:618:BCR:H382	2.02	0.42
18:Y:20:ALA:O	18:Y:24:MET:HG2	2.20	0.42
1:a:162:PRO:HB3	1:a:168:PHE:HA	2.02	0.42
23:b:603:CLA:H193	7:h:42:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:608:CLA:H192	23:b:608:CLA:H162	1.89	0.42
26:b:620:SQD:H212	26:b:620:SQD:H181	1.90	0.42
23:c:507:CLA:H162	23:c:507:CLA:H122	1.66	0.42
23:d:403:CLA:H41	23:d:403:CLA:H61	1.64	0.42
24:A:353:PHO:HBC3	4:D:279:LEU:HD22	2.02	0.42
2:B:30:VAL:HG12	23:B:605:CLA:HHD	2.02	0.42
23:B:609:CLA:HHC	23:B:609:CLA:HBB1	2.02	0.42
23:B:615:CLA:H152	23:B:615:CLA:H112	1.50	0.42
4:D:47:GLY:HA2	25:D:407:BCR:C33	2.50	0.42
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.02	0.41
23:B:613:CLA:H51	37:D:409:LHG:H361	2.02	0.41
9:J:6:ARG:HG3	41:J:201:HOH:O	2.20	0.41
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.02	0.41
33:a:419:LMG:H241	33:a:419:LMG:H211	1.74	0.41
25:b:617:BCR:H24C	25:b:617:BCR:H371	1.83	0.41
1:A:300:PHE:HB3	1:A:302:PHE:CE1	2.55	0.41
2:B:201:HIS:HB2	23:B:602:CLA:C1B	2.50	0.41
25:D:407:BCR:H15C	25:D:407:BCR:H351	1.87	0.41
25:a:410:BCR:H24C	25:a:410:BCR:H371	1.84	0.41
23:b:607:CLA:HBD	23:b:607:CLA:HAA1	2.02	0.41
25:b:619:BCR:HC7	25:b:619:BCR:H311	1.78	0.41
23:c:505:CLA:H62	23:c:505:CLA:H41	1.90	0.41
25:y:101:BCR:H15C	25:y:101:BCR:H351	1.85	0.41
2:B:91:TRP:HE1	30:B:627:UNL:C10	2.33	0.41
2:B:348:ASN:HB3	2:B:354:LEU:HD11	2.02	0.41
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.02	0.41
5:e:14:ILE:O	5:e:20:TRP:NE1	2.50	0.41
15:u:42:TYR:HA	15:u:43:PRO:HA	1.80	0.41
2:B:487:SER:HA	2:B:488:PRO:HD3	1.92	0.41
23:C:508:CLA:H61	23:C:508:CLA:H92	1.80	0.41
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.01	0.41
13:O:54:GLU:HG2	13:O:64:GLU:O	2.21	0.41
2:b:224:ARG:NH1	32:b:621:LMT:H1'	2.36	0.41
3:c:120:ILE:HG23	19:z:47:TRP:HH2	1.84	0.41
5:e:66:VAL:HA	5:e:75:GLN:NE2	2.35	0.41
5:e:68:ASP:O	5:e:72:ALA:HB2	2.21	0.41
4:D:343:GLU:HG2	16:V:135:VAL:HG11	2.03	0.41
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.55	0.41
23:b:605:CLA:H62	23:b:605:CLA:H41	1.70	0.41
25:c:516:BCR:H24C	25:c:516:BCR:H371	1.84	0.41
23:B:610:CLA:H61	23:B:610:CLA:H92	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:515:BCR:H15C	25:C:515:BCR:H351	1.83	0.41
4:D:210:LEU:HA	4:D:213:ILE:HG22	2.03	0.41
25:T:101:BCR:H341	25:b:618:BCR:H381	2.01	0.41
3:c:56:HIS:HB2	23:c:510:CLA:HMB1	2.03	0.41
37:d:408:LHG:H122	37:d:408:LHG:C38	2.50	0.41
5:e:18:ARG:HH11	38:e:87:HEM:HBA2	1.85	0.41
7:h:43:LEU:HA	7:h:43:LEU:HD12	1.79	0.41
14:t:8:PHE:HA	32:t:101:LMT:H123	2.03	0.41
16:v:126:LEU:HB3	16:v:129:LYS:HB2	2.02	0.41
2:B:221:PRO:HA	2:B:222:PRO:HD3	1.99	0.41
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.85	0.41
4:D:293:LEU:HD12	4:D:293:LEU:HA	1.95	0.41
8:I:17:LEU:HD23	8:I:17:LEU:HA	1.90	0.41
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.55	0.41
26:A:412:SQD:H262	26:A:412:SQD:H291	1.78	0.41
2:B:341:LYS:NZ	34:B:623:HTG:O2	2.40	0.41
23:B:606:CLA:H151	23:B:616:CLA:H122	2.02	0.41
3:C:130:VAL:O	3:C:134:ILE:HG12	2.20	0.41
3:C:363:GLY:O	3:C:367:GLU:HG2	2.21	0.41
1:a:93:PHE:CD1	1:a:95:PRO:HD3	2.55	0.41
1:a:182:PHE:O	1:a:186:PHE:HB2	2.21	0.41
23:c:508:CLA:O1D	23:c:510:CLA:H102	2.21	0.41
1:A:334:ARG:HD3	4:D:320:LEU:HD13	2.03	0.41
23:A:405:CLA:H152	23:A:405:CLA:H111	1.90	0.41
2:B:224:ARG:HD2	41:D:501:HOH:O	2.20	0.41
23:B:603:CLA:CGA	23:B:603:CLA:H3A	2.50	0.41
23:B:603:CLA:H61	23:B:603:CLA:H102	1.84	0.41
3:C:167:VAL:HG13	23:C:513:CLA:H71	2.03	0.41
5:E:25:ILE:O	5:E:28:PRO:HD2	2.21	0.41
23:b:609:CLA:HMD1	7:h:27:THR:HB	2.03	0.41
23:b:613:CLA:H141	23:b:613:CLA:H162	1.57	0.41
23:b:614:CLA:H112	23:b:614:CLA:H72	1.82	0.41
25:b:617:BCR:H15C	25:b:617:BCR:H351	1.98	0.41
3:c:210:PHE:HD2	3:c:213[B]:LEU:HD12	1.86	0.41
3:c:433:LEU:HD13	23:c:503:CLA:CHC	2.51	0.41
23:c:511:CLA:HBA1	23:c:511:CLA:H3A	1.80	0.41
12:m:5:GLN:H	12:m:5:GLN:HE21	1.68	0.41
23:A:404:CLA:CAD	23:A:405:CLA:HAC2	2.51	0.41
5:E:23:HIS:CD2	38:E:103:HEM:NC	2.89	0.41
7:H:37:LEU:HA	7:H:37:LEU:HD23	1.84	0.41
1:a:72:LEU:HA	1:a:72:LEU:HD23	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:82:VAL:HB	1:a:174:LEU:HB2	2.02	0.41
1:a:211:PHE:HD2	29:a:416:PL9:H101	1.86	0.41
23:b:603:CLA:H3A	23:b:603:CLA:CGA	2.50	0.41
23:b:615:CLA:HMA1	23:b:616:CLA:CBB	2.51	0.41
3:C:61:VAL:HG12	3:C:118:HIS:O	2.21	0.40
23:C:505:CLA:H41	23:C:505:CLA:H62	1.66	0.40
11:L:20:GLY:O	11:L:24[A]:ILE:HG12	2.21	0.40
1:a:76:ASN:HD22	27:a:418:GOL:H32	1.86	0.40
24:a:408:PHO:ND	24:a:408:PHO:NC	2.70	0.40
3:c:225:VAL:HG13	3:c:289:PHE:HA	2.03	0.40
38:e:87:HEM:HMC2	6:f:31:ILE:HG13	2.03	0.40
26:f:102:SQD:H261	26:f:102:SQD:H291	1.69	0.40
23:B:605:CLA:HBD	23:B:605:CLA:HAA1	2.03	0.40
3:C:139:THR:OG1	3:C:142:GLU:OE2	2.32	0.40
3:C:338:GLY:HA3	3:C:341:LEU:O	2.21	0.40
33:C:501:LMG:H391	35:C:517:DGD:HB51	2.04	0.40
23:C:509:CLA:H122	23:C:509:CLA:H162	1.86	0.40
8:I:18:LEU:HD23	8:I:18:LEU:HA	1.88	0.40
23:c:508:CLA:HAA2	23:c:508:CLA:HBD	2.02	0.40
25:c:515:BCR:H24C	25:c:515:BCR:H371	1.77	0.40
25:c:515:BCR:H15C	25:c:515:BCR:H351	1.81	0.40
5:e:68:ASP:OD1	5:e:71:GLU:N	2.53	0.40
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.90	0.40
4:D:39:PRO:O	4:D:43:LEU:HG	2.21	0.40
9:J:7:ILE:HA	9:J:8:PRO:HD3	1.95	0.40
23:a:405:CLA:HBD	23:a:406:CLA:HAC2	2.02	0.40
23:b:609:CLA:NC	25:h:101:BCR:H332	2.37	0.40
23:b:614:CLA:H203	23:b:614:CLA:H161	1.98	0.40
23:b:614:CLA:HAA1	23:b:614:CLA:HBD	2.03	0.40
25:b:618:BCR:H351	25:b:618:BCR:H15C	1.85	0.40
23:B:604:CLA:HBA2	23:B:612:CLA:H152	2.02	0.40
23:B:614:CLA:H62	23:B:614:CLA:H41	1.58	0.40
33:C:501:LMG:H232	23:C:506:CLA:C9	2.50	0.40
23:C:506:CLA:H3A	23:C:506:CLA:HBA2	1.88	0.40
23:C:506:CLA:H112	23:C:506:CLA:H72	1.93	0.40
2:b:498:LYS:HB3	2:b:504:THR:HG21	2.02	0.40
3:c:88:LEU:HD23	3:c:88:LEU:HA	1.83	0.40
3:c:158:THR:O	3:c:251:HIS:HB3	2.21	0.40
3:c:375:LEU:HA	3:c:375:LEU:HD23	1.87	0.40
3:c:426:LEU:HD23	3:c:426:LEU:HA	1.97	0.40
25:k:101:BCR:H15C	25:k:101:BCR:H351	1.91	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%)	331 (99%)	3 (1%)	1 (0%)	36	43
1	a	336/344 (98%)	331 (98%)	4 (1%)	1 (0%)	36	43
2	B	510/505 (101%)	505 (99%)	5 (1%)	0	100	100
2	b	506/505 (100%)	500 (99%)	6 (1%)	0	100	100
3	C	453/455 (100%)	443 (98%)	8 (2%)	2 (0%)	30	34
3	c	457/455 (100%)	446 (98%)	9 (2%)	2 (0%)	30	34
4	D	341/342 (100%)	333 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	333 (98%)	7 (2%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
7	h	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	4	2
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	245/244 (100%)	238 (97%)	7 (3%)	0	100	100
13	o	243/244 (100%)	237 (98%)	6 (2%)	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%)	130 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	Y	27/30 (90%)	27 (100%)	0	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	59 (98%)	0	1 (2%)	7	6
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	6
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5251/5384 (98%)	5147 (98%)	95 (2%)	9 (0%)	48	52

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
1	a	259	ILE
3	c	416[A]	SER
3	c	416[B]	SER
19	Z	30	PRO
19	z	30	PRO
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	86
1	a	273/279 (98%)	271 (99%)	2 (1%)	76	86
2	B	410/403 (102%)	405 (99%)	5 (1%)	63	77
2	b	406/403 (101%)	401 (99%)	5 (1%)	63	77
3	C	356/356 (100%)	352 (99%)	4 (1%)	65	79
3	c	360/356 (101%)	354 (98%)	6 (2%)	53	68
4	D	278/277 (100%)	277 (100%)	1 (0%)	84	91
4	d	277/277 (100%)	276 (100%)	1 (0%)	84	91
5	E	73/73 (100%)	73 (100%)	0	100	100
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	55/54 (102%)	52 (94%)	3 (6%)	19	24
7	h	54/54 (100%)	54 (100%)	0	100	100
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	34 (100%)	0	100	100
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	39
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	7
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	7
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%)	30 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	33	44
13	O	210/207 (101%)	210 (100%)	0	100	100
13	o	208/207 (100%)	206 (99%)	2 (1%)	68	81
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	39
14	t	26/28 (93%)	25 (96%)	1 (4%)	29	39
15	U	83/89 (93%)	82 (99%)	1 (1%)	63	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	117/117 (100%)	116 (99%)	1 (1%)	70	82
16	v	117/117 (100%)	116 (99%)	1 (1%)	70	82
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	32
18	y	22/23 (96%)	20 (91%)	2 (9%)	9	9
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18	22
19	z	52/52 (100%)	48 (92%)	4 (8%)	12	13
20	R	29/29 (100%)	28 (97%)	1 (3%)	32	43
All	All	4357/4403 (99%)	4302 (99%)	55 (1%)	63	76

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238[A]	LYS
1	A	238[B]	LYS
2	B	223	GLN
2	B	245	VAL
2	B	362	PHE
2	B	489	GLU
2	B	505	ARG
3	C	142	GLU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
4	D	259	ILE
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	65	LEU
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
14	T	2	GLU
15	U	70	ARG
16	V	15	GLU
18	Y	30	ILE
19	Z	3	ILE

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Mol	Chain	Res	Type
19	Z	4	LEU
19	Z	62	VAL
20	R	7	VAL
1	a	12	ASN
1	a	13	LEU
2	b	63	LEU
2	b	245	VAL
2	b	362	PHE
2	b	485	GLU
2	b	491	VAL
3	c	142	GLU
3	c	240	ILE
3	c	289	PHE
3	c	315	MET
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	259	ILE
9	j	2	SER
10	k	10	LYS
10	k	17	ILE
10	k	19	ASP
12	m	5	GLN
13	o	25	THR
13	o	118	LEU
14	t	2	GLU
16	v	15	GLU
18	y	30	ILE
18	y	45	ASN
19	z	3	ILE
19	z	4	LEU
19	z	34	ASP
19	z	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	165	GLN
2	B	53	ASN
2	B	331	ASN
3	C	28	GLN
3	C	201	ASN

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Mol	Chain	Res	Type
4	D	83	ASN
4	D	186	GLN
6	F	44	GLN
12	M	28	GLN
13	O	124	ASN
13	O	130	GLN
19	Z	58	ASN
1	a	165	GLN
2	b	53	ASN
2	b	331	ASN
2	b	374	ASN
3	c	44	ASN
3	c	201	ASN
4	d	83	ASN
5	e	75	GLN
12	m	5	GLN
13	o	124	ASN
13	o	130	GLN
15	u	78	ASN
19	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.62	0	8,9,11	1.10	1 (12%)
12	FME	M	1	12	8,9,10	0.62	0	8,9,11	1.40	2 (25%)
14	FME	T	1	14	8,9,10	0.60	0	8,9,11	1.88	3 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	i	1	8	8,9,10	0.61	0	8,9,11	1.31	1 (12%)
14	FME	t	1	14	8,9,10	0.65	0	8,9,11	1.56	2 (25%)
12	FME	m	1	12	8,9,10	0.60	0	8,9,11	1.42	2 (25%)

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

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

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	CB-CA-N	-3.57	104.02	110.52
14	t	1	FME	O-C-CA	-2.71	117.79	124.77
14	t	1	FME	CA-N-CN	-2.55	118.89	122.82
12	m	1	FME	CA-N-CN	-2.50	118.98	122.82
12	M	1	FME	O-C-CA	-2.37	118.67	124.77
8	i	1	FME	O-C-CA	-2.33	118.79	124.77
12	m	1	FME	O1-CN-N	-2.24	119.53	125.32
8	I	1	FME	O-C-CA	-2.22	119.07	124.77
14	T	1	FME	CG-CB-CA	2.19	119.57	112.87
12	M	1	FME	CA-N-CN	-2.14	119.53	122.82
14	T	1	FME	O-C-CA	-2.10	119.36	124.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	O1-CN-N-CA
12	M	1	FME	O1-CN-N-CA
12	m	1	FME	O1-CN-N-CA

Continued on next page...

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Mol	Chain	Res	Type	Atoms
8	i	1	FME	O1-CN-N-CA
14	t	1	FME	CB-CA-N-CN

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, 15 are monoatomic and 18 are unknown - leaving 181 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	D	406	4	69,73,73	2.01	18 (26%)	82,113,113	2.71	32 (39%)
25	BCR	B	617	-	41,41,41	1.03	1 (2%)	56,56,56	1.58	10 (17%)
33	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.20	6 (10%)
33	LMG	d	412	39	51,51,55	0.89	2 (3%)	59,59,63	1.06	3 (5%)
25	BCR	Y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.76	14 (25%)
35	DGD	c	518	-	63,63,67	0.90	3 (4%)	77,77,81	0.98	4 (5%)
24	PHO	A	353	-	58,69,69	2.70	13 (22%)	55,99,99	3.19	18 (32%)
25	BCR	b	619	-	41,41,41	1.05	1 (2%)	56,56,56	1.55	13 (23%)
23	CLA	c	507	3	69,73,73	2.00	18 (26%)	82,113,113	2.59	31 (37%)
32	LMT	a	414	-	36,36,36	0.56	1 (2%)	47,47,47	1.11	4 (8%)
23	CLA	A	408	1	69,73,73	2.00	20 (28%)	82,113,113	2.82	33 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	m	103	-	36,36,36	0.47	0	47,47,47	0.93	1 (2%)
27	GOL	V	201	-	5,5,5	0.43	0	5,5,5	0.51	0
25	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.54	11 (19%)
33	LMG	C	521	-	51,51,55	1.00	3 (5%)	59,59,63	1.26	4 (6%)
25	BCR	y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.79	13 (23%)
24	PHO	a	408	-	58,69,69	2.72	12 (20%)	55,99,99	3.10	17 (30%)
31	BCT	A	348	21	3,3,3	0.53	0	2,3,3	1.11	0
26	SQD	b	620	-	52,54,54	0.98	2 (3%)	62,65,65	1.54	9 (14%)
23	CLA	B	603	2	69,73,73	1.92	20 (28%)	82,113,113	2.80	34 (41%)
27	GOL	a	412	-	5,5,5	0.34	0	5,5,5	0.50	0
34	HTG	B	622	-	19,19,19	0.95	1 (5%)	23,24,24	1.48	5 (21%)
29	PL9	a	416	-	55,55,55	0.65	2 (3%)	68,69,69	2.01	23 (33%)
32	LMT	A	359	-	36,36,36	0.59	1 (2%)	47,47,47	0.89	1 (2%)
26	SQD	B	620	-	52,54,54	0.97	3 (5%)	62,65,65	1.43	8 (12%)
23	CLA	C	509	3	69,73,73	2.00	21 (30%)	82,113,113	2.62	30 (36%)
23	CLA	b	609	2	69,73,73	1.98	20 (28%)	82,113,113	2.72	31 (37%)
33	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.17	4 (6%)
26	SQD	a	411	-	52,54,54	0.88	2 (3%)	62,65,65	1.68	13 (20%)
23	CLA	c	510	3	69,73,73	2.05	20 (28%)	82,113,113	2.76	33 (40%)
23	CLA	B	606	2	69,73,73	1.90	19 (27%)	82,113,113	2.84	32 (39%)
32	LMT	e	102	-	36,36,36	0.52	1 (2%)	47,47,47	0.93	2 (4%)
34	HTG	C	522	-	19,19,19	0.86	1 (5%)	23,24,24	1.27	2 (8%)
29	PL9	A	414	-	55,55,55	0.65	2 (3%)	68,69,69	2.01	24 (35%)
23	CLA	b	603	2	69,73,73	1.98	20 (28%)	82,113,113	2.76	34 (41%)
23	CLA	c	513	3	69,73,73	1.99	19 (27%)	82,113,113	2.76	33 (40%)
23	CLA	C	508	41	69,73,73	1.99	18 (26%)	82,113,113	2.65	29 (35%)
35	DGD	c	519	-	63,63,67	0.86	3 (4%)	77,77,81	1.05	6 (7%)
23	CLA	C	507	3	69,73,73	1.99	20 (28%)	82,113,113	2.65	34 (41%)
34	HTG	b	625	-	19,19,19	0.86	2 (10%)	23,24,24	1.31	3 (13%)
35	DGD	c	517	-	63,63,67	0.83	2 (3%)	77,77,81	1.14	8 (10%)
29	PL9	D	408	-	55,55,55	0.67	1 (1%)	68,69,69	1.76	19 (27%)
32	LMT	I	101	-	36,36,36	0.51	1 (2%)	47,47,47	1.12	3 (6%)
33	LMG	a	419	-	51,51,55	0.92	2 (3%)	59,59,63	1.13	6 (10%)
23	CLA	b	612	2	69,73,73	1.96	20 (28%)	82,113,113	2.67	29 (35%)
23	CLA	C	503	3	69,73,73	1.99	20 (28%)	82,113,113	2.66	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	512	3	69,73,73	1.99	20 (28%)	82,113,113	2.58	31 (37%)
23	CLA	b	606	2	69,73,73	1.96	19 (27%)	82,113,113	2.75	33 (40%)
23	CLA	C	510	3	69,73,73	2.02	21 (30%)	82,113,113	2.67	32 (39%)
25	BCR	c	515	-	41,41,41	1.06	1 (2%)	56,56,56	1.83	16 (28%)
25	BCR	C	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.59	9 (16%)
23	CLA	B	616	2	69,73,73	1.99	19 (27%)	82,113,113	2.67	28 (34%)
23	CLA	C	513	3	69,73,73	2.01	20 (28%)	82,113,113	2.67	31 (37%)
23	CLA	a	406	41	69,73,73	2.01	18 (26%)	82,113,113	2.77	30 (36%)
23	CLA	B	609	2	69,73,73	1.99	17 (24%)	82,113,113	2.67	27 (32%)
27	GOL	c	501	-	5,5,5	0.32	0	5,5,5	0.45	0
34	HTG	b	623	-	19,19,19	0.97	1 (5%)	23,24,24	1.55	1 (4%)
38	HEM	E	103	5,6	50,50,50	1.51	7 (14%)	67,82,82	1.74	15 (22%)
23	CLA	c	506	3	69,73,73	1.97	19 (27%)	82,113,113	2.58	30 (36%)
23	CLA	C	506	3	69,73,73	1.97	19 (27%)	82,113,113	2.68	33 (40%)
25	BCR	d	404	-	41,41,41	1.10	1 (2%)	56,56,56	1.89	16 (28%)
23	CLA	C	502	3	69,73,73	1.93	20 (28%)	82,113,113	2.76	31 (37%)
27	GOL	A	411	-	5,5,5	0.40	0	5,5,5	0.25	0
23	CLA	B	604	2	69,73,73	1.94	19 (27%)	82,113,113	2.67	33 (40%)
25	BCR	b	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.54	6 (10%)
23	CLA	A	405	41	69,73,73	2.02	18 (26%)	82,113,113	2.76	33 (40%)
23	CLA	c	502	3	69,73,73	2.02	20 (28%)	82,113,113	2.68	32 (39%)
34	HTG	d	411	-	16,16,19	1.06	2 (12%)	20,21,24	1.49	2 (10%)
23	CLA	D	405	4	69,73,73	1.85	19 (27%)	82,113,113	2.71	32 (39%)
35	DGD	C	519	-	63,63,67	0.83	3 (4%)	77,77,81	1.05	6 (7%)
23	CLA	a	409	1	69,73,73	1.96	19 (27%)	82,113,113	2.65	34 (41%)
23	CLA	a	405	1	69,73,73	2.00	20 (28%)	82,113,113	2.64	36 (43%)
32	LMT	M	103	-	36,36,36	0.46	0	47,47,47	0.93	2 (4%)
23	CLA	c	503	3	69,73,73	1.92	20 (28%)	82,113,113	2.66	30 (36%)
33	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.13	5 (8%)
26	SQD	A	412	-	52,54,54	0.95	2 (3%)	62,65,65	1.18	9 (14%)
31	BCT	a	404	21	3,3,3	0.51	0	2,3,3	1.13	0
35	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.02	5 (6%)
23	CLA	c	514	3	69,73,73	2.05	21 (30%)	82,113,113	2.69	32 (39%)
33	LMG	D	415	39	51,51,55	0.88	3 (5%)	59,59,63	0.89	3 (5%)
25	BCR	T	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.70	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	604	2	69,73,73	1.92	18 (26%)	82,113,113	2.72	31 (37%)
23	CLA	A	406	41	69,73,73	1.96	19 (27%)	82,113,113	2.70	32 (39%)
23	CLA	b	611	2	69,73,73	1.93	18 (26%)	82,113,113	2.81	30 (36%)
25	BCR	a	410	-	41,41,41	1.00	1 (2%)	56,56,56	1.62	13 (23%)
32	LMT	D	404	-	36,36,36	0.43	0	47,47,47	1.10	4 (8%)
33	LMG	z	101	-	39,39,55	1.07	2 (5%)	47,47,63	1.10	4 (8%)
32	LMT	a	420	-	36,36,36	0.49	1 (2%)	47,47,47	0.93	1 (2%)
33	LMG	Z	101	-	37,37,55	1.02	3 (8%)	45,45,63	1.48	7 (15%)
23	CLA	B	611	2	69,73,73	1.99	19 (27%)	82,113,113	2.68	31 (37%)
29	PL9	d	405	-	55,55,55	0.67	1 (1%)	68,69,69	1.79	19 (27%)
35	DGD	h	102	-	63,63,67	0.85	2 (3%)	77,77,81	0.98	4 (5%)
25	BCR	B	618	-	41,41,41	0.93	1 (2%)	56,56,56	1.63	15 (26%)
23	CLA	b	610	41	69,73,73	1.98	20 (28%)	82,113,113	2.76	32 (39%)
23	CLA	b	615	2	69,73,73	1.97	18 (26%)	82,113,113	2.67	30 (36%)
27	GOL	B	625	-	5,5,5	0.62	0	5,5,5	0.79	0
37	LHG	D	410	-	48,48,48	0.87	3 (6%)	51,54,54	1.00	3 (5%)
23	CLA	C	511	3	69,73,73	2.01	20 (28%)	82,113,113	2.79	32 (39%)
27	GOL	b	624	-	5,5,5	0.30	0	5,5,5	0.57	0
37	LHG	D	411	-	48,48,48	0.90	2 (4%)	51,54,54	1.02	3 (5%)
34	HTG	V	203	-	11,11,19	0.24	0	15,15,24	1.06	1 (6%)
23	CLA	b	605	2	69,73,73	1.94	19 (27%)	82,113,113	2.88	30 (36%)
23	CLA	c	504	3	69,73,73	2.01	19 (27%)	82,113,113	2.69	29 (35%)
23	CLA	C	504	3	69,73,73	1.97	20 (28%)	82,113,113	2.70	32 (39%)
32	LMT	b	621	-	25,25,36	0.48	0	30,30,47	0.72	0
26	SQD	A	410	-	52,54,54	0.87	2 (3%)	62,65,65	1.91	12 (19%)
37	LHG	L	101	-	48,48,48	0.94	3 (6%)	51,54,54	1.09	2 (3%)
32	LMT	E	102	-	36,36,36	0.51	1 (2%)	47,47,47	0.89	0
37	LHG	D	409	-	48,48,48	0.91	3 (6%)	51,54,54	1.18	6 (11%)
25	BCR	D	407	-	41,41,41	1.06	1 (2%)	56,56,56	1.95	15 (26%)
23	CLA	C	505	41	69,73,73	1.98	20 (28%)	82,113,113	2.70	31 (37%)
37	LHG	l	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.12	5 (9%)
23	CLA	B	608	2	69,73,73	1.94	21 (30%)	82,113,113	2.65	31 (37%)
37	LHG	e	101	-	41,41,48	1.04	2 (4%)	44,47,54	0.95	2 (4%)
34	HTG	b	622	-	19,19,19	0.97	1 (5%)	23,24,24	1.67	4 (17%)
23	CLA	b	614	2	69,73,73	1.91	20 (28%)	82,113,113	2.76	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PHO	A	407	-	58,69,69	2.59	14 (24%)	55,99,99	3.06	19 (34%)
23	CLA	c	505	41	69,73,73	1.97	20 (28%)	82,113,113	2.78	34 (41%)
23	CLA	d	403	4	69,73,73	2.02	20 (28%)	82,113,113	2.78	36 (43%)
32	LMT	t	101	-	25,25,36	0.53	1 (4%)	30,30,47	1.04	1 (3%)
23	CLA	a	407	41	69,73,73	1.96	19 (27%)	82,113,113	2.74	32 (39%)
23	CLA	b	607	41	69,73,73	1.92	18 (26%)	82,113,113	2.71	31 (37%)
34	HTG	D	414	-	16,16,19	0.95	2 (12%)	20,21,24	1.39	1 (5%)
37	LHG	d	406	-	48,48,48	0.89	3 (6%)	51,54,54	1.11	4 (7%)
37	LHG	d	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.08	3 (5%)
28	OEX	a	415	41,1,3	0,15,15	-	-	-	-	-
24	PHO	a	353	-	58,69,69	2.75	13 (22%)	55,99,99	3.07	17 (30%)
32	LMT	b	627	-	25,25,36	0.53	1 (4%)	30,30,47	0.76	0
33	LMG	c	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.06	4 (6%)
38	HEM	e	87	5,6	50,50,50	1.54	8 (16%)	67,82,82	1.63	13 (19%)
23	CLA	B	610	41	69,73,73	2.00	21 (30%)	82,113,113	2.67	33 (40%)
26	SQD	F	101	-	41,43,54	1.11	3 (7%)	51,54,65	1.75	11 (21%)
32	LMT	t	102	-	26,26,36	0.57	1 (3%)	31,31,47	0.97	2 (6%)
25	BCR	t	103	-	41,41,41	1.00	1 (2%)	56,56,56	1.77	15 (26%)
25	BCR	H	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.52	12 (21%)
33	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.32	6 (10%)
37	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.17	5 (11%)
25	BCR	A	409	-	41,41,41	1.04	1 (2%)	56,56,56	1.61	14 (25%)
35	DGD	H	102	-	63,63,67	0.83	3 (4%)	77,77,81	1.00	4 (5%)
23	CLA	d	402	4	69,73,73	1.93	19 (27%)	82,113,113	2.65	32 (39%)
40	HEC	v	202	16	46,50,50	1.78	9 (19%)	58,82,82	1.73	13 (22%)
23	CLA	b	608	2	69,73,73	2.02	20 (28%)	82,113,113	2.70	35 (42%)
26	SQD	a	413	-	52,54,54	1.00	2 (3%)	62,65,65	1.18	7 (11%)
27	GOL	B	624	-	5,5,5	0.37	0	5,5,5	0.59	0
23	CLA	B	601	41	69,73,73	2.06	21 (30%)	82,113,113	2.72	31 (37%)
23	CLA	B	612	2	69,73,73	1.89	19 (27%)	82,113,113	2.74	34 (41%)
23	CLA	b	613	2	69,73,73	1.98	19 (27%)	82,113,113	2.68	30 (36%)
25	BCR	K	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.64	12 (21%)
23	CLA	B	605	2	69,73,73	1.97	19 (27%)	82,113,113	2.83	32 (39%)
28	OEX	A	413	41,1,3	0,15,15	-	-	-	-	-
23	CLA	B	607	41	69,73,73	1.97	19 (27%)	82,113,113	2.76	33 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GOL	a	418	-	5,5,5	0.38	0	5,5,5	0.71	0
25	BCR	c	516	-	41,41,41	1.05	2 (4%)	56,56,56	1.63	12 (21%)
25	BCR	C	516	-	41,41,41	1.08	1 (2%)	56,56,56	1.65	14 (25%)
32	LMT	M	101	-	36,36,36	0.48	0	47,47,47	1.07	3 (6%)
23	CLA	b	601	41	69,73,73	2.08	22 (31%)	82,113,113	2.63	28 (34%)
27	GOL	v	201	-	5,5,5	0.42	0	5,5,5	0.38	0
34	HTG	B	623	-	19,19,19	0.84	1 (5%)	23,24,24	1.34	3 (13%)
40	HEC	V	202	16	46,50,50	1.71	8 (17%)	58,82,82	1.70	13 (22%)
34	HTG	B	626	-	19,19,19	0.92	2 (10%)	23,24,24	1.43	4 (17%)
25	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.59	13 (23%)
25	BCR	b	618	-	41,41,41	1.02	1 (2%)	56,56,56	1.46	11 (19%)
23	CLA	c	511	3	69,73,73	1.98	20 (28%)	82,113,113	2.72	34 (41%)
23	CLA	C	514	3	69,73,73	2.03	20 (28%)	82,113,113	2.71	32 (39%)
23	CLA	c	509	3	69,73,73	2.00	19 (27%)	82,113,113	2.72	30 (36%)
37	LHG	d	407	-	48,48,48	0.88	3 (6%)	51,54,54	1.02	3 (5%)
23	CLA	c	508	41	69,73,73	1.97	18 (26%)	82,113,113	2.71	30 (36%)
33	LMG	c	521	-	51,51,55	0.96	2 (3%)	59,59,63	1.17	5 (8%)
23	CLA	B	614	2	69,73,73	1.94	19 (27%)	82,113,113	2.98	32 (39%)
34	HTG	c	522	-	19,19,19	0.90	1 (5%)	23,24,24	1.39	1 (4%)
35	DGD	C	517	-	63,63,67	0.83	2 (3%)	77,77,81	1.23	8 (10%)
23	CLA	A	404	1	69,73,73	1.97	19 (27%)	82,113,113	2.77	32 (39%)
23	CLA	b	602	2	69,73,73	2.01	19 (27%)	82,113,113	2.79	35 (42%)
23	CLA	b	616	2	69,73,73	1.99	18 (26%)	82,113,113	2.71	33 (40%)
26	SQD	f	102	-	41,43,54	1.10	2 (4%)	51,54,65	1.44	9 (17%)
27	GOL	C	523	-	5,5,5	0.48	0	5,5,5	0.14	0
23	CLA	B	615	2	69,73,73	1.94	18 (26%)	82,113,113	2.68	33 (40%)
23	CLA	c	512	3	69,73,73	1.98	18 (26%)	82,113,113	2.72	29 (35%)
23	CLA	B	613	2	69,73,73	1.99	19 (27%)	82,113,113	2.69	31 (37%)
25	BCR	h	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.37	7 (12%)
23	CLA	B	602	2	69,73,73	2.05	19 (27%)	82,113,113	2.77	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	D	406	4	1/1/15/20	7/39/115/115	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
33	LMG	m	101	-	-	14/46/66/70	0/1/1/1
33	LMG	d	412	39	-	7/46/66/70	0/1/1/1
25	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
35	DGD	c	518	-	-	11/51/91/95	0/2/2/2
24	PHO	A	353	-	-	1/37/103/103	0/5/6/6
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	c	507	3	1/1/15/20	11/39/115/115	-
32	LMT	a	414	-	-	7/21/61/61	0/2/2/2
23	CLA	A	408	1	1/1/15/20	13/39/115/115	-
32	LMT	m	103	-	-	6/21/61/61	0/2/2/2
27	GOL	V	201	-	-	2/4/4/4	-
25	BCR	B	619	-	-	2/29/63/63	0/2/2/2
33	LMG	C	521	-	-	9/46/66/70	0/1/1/1
25	BCR	y	101	-	-	5/29/63/63	0/2/2/2
24	PHO	a	408	-	-	5/37/103/103	0/5/6/6
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
23	CLA	B	603	2	1/1/15/20	4/39/115/115	-
27	GOL	a	412	-	-	4/4/4/4	-
34	HTG	B	622	-	-	5/10/30/30	0/1/1/1
29	PL9	a	416	-	-	16/53/73/73	0/1/1/1
32	LMT	A	359	-	-	3/21/61/61	0/2/2/2
26	SQD	B	620	-	-	18/49/69/69	0/1/1/1
23	CLA	C	509	3	1/1/15/20	2/39/115/115	-
23	CLA	b	609	2	1/1/15/20	8/39/115/115	-
33	LMG	B	621	-	-	15/46/66/70	0/1/1/1
26	SQD	a	411	-	-	10/49/69/69	0/1/1/1
23	CLA	c	510	3	1/1/15/20	13/39/115/115	-
23	CLA	B	606	2	1/1/15/20	8/39/115/115	-
32	LMT	e	102	-	-	7/21/61/61	0/2/2/2
34	HTG	C	522	-	-	1/10/30/30	0/1/1/1
29	PL9	A	414	-	-	16/53/73/73	0/1/1/1
23	CLA	b	603	2	1/1/15/20	5/39/115/115	-
23	CLA	c	513	3	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	508	41	1/1/15/20	8/39/115/115	-
35	DGD	c	519	-	-	7/51/91/95	0/2/2/2
23	CLA	C	507	3	1/1/15/20	11/39/115/115	-
34	HTG	b	625	-	-	4/10/30/30	0/1/1/1
35	DGD	c	517	-	-	21/51/91/95	0/2/2/2
29	PL9	D	408	-	-	7/53/73/73	0/1/1/1
32	LMT	I	101	-	-	9/21/61/61	0/2/2/2
33	LMG	a	419	-	-	12/46/66/70	0/1/1/1
23	CLA	b	612	2	1/1/15/20	2/39/115/115	-
23	CLA	C	503	3	1/1/15/20	8/39/115/115	-
23	CLA	C	512	3	1/1/15/20	4/39/115/115	-
23	CLA	b	606	2	1/1/15/20	5/39/115/115	-
23	CLA	C	510	3	1/1/15/20	4/39/115/115	-
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
23	CLA	B	616	2	1/1/15/20	7/39/115/115	-
23	CLA	C	513	3	1/1/15/20	10/39/115/115	-
23	CLA	a	406	41	-	3/39/115/115	-
23	CLA	B	609	2	1/1/15/20	3/39/115/115	-
27	GOL	c	501	-	-	0/4/4/4	-
34	HTG	b	623	-	-	4/10/30/30	0/1/1/1
38	HEM	E	103	5,6	-	8/14/54/54	-
23	CLA	c	506	3	1/1/15/20	3/39/115/115	-
23	CLA	C	506	3	1/1/15/20	7/39/115/115	-
25	BCR	d	404	-	-	6/29/63/63	0/2/2/2
23	CLA	C	502	3	1/1/15/20	4/39/115/115	-
27	GOL	A	411	-	-	2/4/4/4	-
23	CLA	B	604	2	1/1/15/20	7/39/115/115	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	A	405	41	1/1/15/20	2/39/115/115	-
23	CLA	c	502	3	1/1/15/20	3/39/115/115	-
34	HTG	d	411	-	-	0/7/27/30	0/1/1/1
23	CLA	D	405	4	1/1/15/20	5/39/115/115	-
35	DGD	C	519	-	-	14/51/91/95	0/2/2/2
23	CLA	a	409	1	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	405	1	1/1/15/20	2/39/115/115	-
32	LMT	M	103	-	-	10/21/61/61	0/2/2/2
23	CLA	c	503	3	1/1/15/20	7/39/115/115	-
33	LMG	C	520	-	-	12/46/66/70	0/1/1/1
26	SQD	A	412	-	-	11/49/69/69	0/1/1/1
35	DGD	C	518	-	-	16/51/91/95	0/2/2/2
23	CLA	c	514	3	1/1/15/20	8/39/115/115	-
33	LMG	D	415	39	-	10/46/66/70	0/1/1/1
25	BCR	T	101	-	-	3/29/63/63	0/2/2/2
23	CLA	b	604	2	1/1/15/20	5/39/115/115	-
23	CLA	b	611	2	1/1/15/20	4/39/115/115	-
23	CLA	A	406	41	-	6/39/115/115	-
25	BCR	a	410	-	-	0/29/63/63	0/2/2/2
32	LMT	D	404	-	-	7/21/61/61	0/2/2/2
33	LMG	z	101	-	-	8/34/54/70	0/1/1/1
32	LMT	a	420	-	-	5/21/61/61	0/2/2/2
33	LMG	Z	101	-	-	11/31/51/70	0/1/1/1
23	CLA	B	611	2	1/1/15/20	2/39/115/115	-
29	PL9	d	405	-	-	7/53/73/73	0/1/1/1
35	DGD	h	102	-	-	10/51/91/95	0/2/2/2
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	b	610	41	1/1/15/20	9/39/115/115	-
23	CLA	b	615	2	1/1/15/20	5/39/115/115	-
27	GOL	B	625	-	-	3/4/4/4	-
37	LHG	D	410	-	-	15/53/53/53	-
23	CLA	C	511	3	1/1/15/20	12/39/115/115	-
27	GOL	b	624	-	-	0/4/4/4	-
37	LHG	D	411	-	-	14/53/53/53	-
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
23	CLA	b	605	2	1/1/15/20	4/39/115/115	-
23	CLA	c	504	3	1/1/15/20	1/39/115/115	-
23	CLA	C	504	3	1/1/15/20	3/39/115/115	-
32	LMT	b	621	-	-	7/17/37/61	0/1/1/2
26	SQD	A	410	-	-	15/49/69/69	0/1/1/1
37	LHG	L	101	-	-	18/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMT	E	102	-	-	8/21/61/61	0/2/2/2
37	LHG	D	409	-	-	10/53/53/53	-
25	BCR	D	407	-	-	6/29/63/63	0/2/2/2
23	CLA	C	505	41	1/1/15/20	6/39/115/115	-
37	LHG	l	101	-	-	18/53/53/53	-
23	CLA	B	608	2	-	3/39/115/115	-
37	LHG	e	101	-	-	11/46/46/53	-
34	HTG	b	622	-	-	4/10/30/30	0/1/1/1
23	CLA	b	614	2	1/1/15/20	11/39/115/115	-
24	PHO	A	407	-	-	2/37/103/103	0/5/6/6
23	CLA	c	505	41	1/1/15/20	4/39/115/115	-
23	CLA	d	403	4	1/1/15/20	7/39/115/115	-
32	LMT	t	101	-	-	6/17/37/61	0/1/1/2
23	CLA	b	607	41	1/1/15/20	4/39/115/115	-
23	CLA	a	407	41	-	6/39/115/115	-
34	HTG	D	414	-	-	0/7/27/30	0/1/1/1
37	LHG	d	406	-	-	5/53/53/53	-
37	LHG	d	408	-	-	13/53/53/53	-
24	PHO	a	353	-	-	2/37/103/103	0/5/6/6
32	LMT	b	627	-	-	8/17/37/61	0/1/1/2
33	LMG	c	520	-	-	15/46/66/70	0/1/1/1
38	HEM	e	87	5,6	-	9/14/54/54	-
23	CLA	B	610	41	1/1/15/20	4/39/115/115	-
26	SQD	F	101	-	-	14/38/58/69	0/1/1/1
32	LMT	t	102	-	-	5/17/38/61	0/1/1/2
25	BCR	t	103	-	-	5/29/63/63	0/2/2/2
25	BCR	H	101	-	-	5/29/63/63	0/2/2/2
33	LMG	C	501	-	-	13/46/66/70	0/1/1/1
37	LHG	E	101	-	-	18/46/46/53	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
35	DGD	H	102	-	-	14/51/91/95	0/2/2/2
23	CLA	d	402	4	1/1/15/20	4/39/115/115	-
40	HEC	v	202	16	-	6/14/54/54	-
23	CLA	b	608	2	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	a	413	-	-	16/49/69/69	0/1/1/1
27	GOL	B	624	-	-	4/4/4/4	-
23	CLA	B	601	41	1/1/15/20	12/39/115/115	-
23	CLA	B	612	2	1/1/15/20	3/39/115/115	-
23	CLA	b	613	2	1/1/15/20	7/39/115/115	-
25	BCR	K	102	-	-	1/29/63/63	0/2/2/2
23	CLA	B	605	2	1/1/15/20	6/39/115/115	-
23	CLA	B	607	41	1/1/15/20	3/39/115/115	-
27	GOL	a	418	-	-	2/4/4/4	-
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
32	LMT	M	101	-	-	4/21/61/61	0/2/2/2
23	CLA	b	601	41	1/1/15/20	18/39/115/115	-
27	GOL	v	201	-	-	2/4/4/4	-
34	HTG	B	623	-	-	4/10/30/30	0/1/1/1
40	HEC	V	202	16	-	6/14/54/54	-
34	HTG	B	626	-	-	2/10/30/30	0/1/1/1
25	BCR	k	101	-	-	2/29/63/63	0/2/2/2
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	c	511	3	1/1/15/20	9/39/115/115	-
23	CLA	C	514	3	1/1/15/20	7/39/115/115	-
23	CLA	c	509	3	1/1/15/20	1/39/115/115	-
37	LHG	d	407	-	-	15/53/53/53	-
23	CLA	c	508	41	1/1/15/20	8/39/115/115	-
33	LMG	c	521	-	-	7/46/66/70	0/1/1/1
23	CLA	B	614	2	1/1/15/20	10/39/115/115	-
34	HTG	c	522	-	-	4/10/30/30	0/1/1/1
35	DGD	C	517	-	-	14/51/91/95	0/2/2/2
23	CLA	A	404	1	1/1/15/20	3/39/115/115	-
23	CLA	b	602	2	1/1/15/20	3/39/115/115	-
23	CLA	b	616	2	1/1/15/20	10/39/115/115	-
26	SQD	f	102	-	-	13/38/58/69	0/1/1/1
27	GOL	C	523	-	-	2/4/4/4	-
23	CLA	B	615	2	1/1/15/20	8/39/115/115	-
23	CLA	c	512	3	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	613	2	1/1/15/20	6/39/115/115	-
25	BCR	h	101	-	-	0/29/63/63	0/2/2/2
23	CLA	B	602	2	1/1/15/20	6/39/115/115	-

All (1581) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	353	PHO	C1D-C2D	9.50	1.49	1.39
24	a	408	PHO	C1B-C2B	9.41	1.49	1.39
24	A	353	PHO	C1D-C2D	8.75	1.49	1.39
24	A	407	PHO	C1D-C2D	8.59	1.48	1.39
24	a	408	PHO	C1D-C2D	8.58	1.48	1.39
24	a	353	PHO	C1B-C2B	8.40	1.48	1.39
24	A	353	PHO	C1B-C2B	7.87	1.48	1.39
24	a	408	PHO	C3B-C4B	7.76	1.49	1.41
24	A	407	PHO	C1B-C2B	7.64	1.47	1.39
24	A	353	PHO	C3B-C4B	7.30	1.48	1.41
24	a	353	PHO	C3B-C4B	7.30	1.48	1.41
24	a	408	PHO	C4D-CHA	6.92	1.49	1.39
24	A	407	PHO	C4D-CHA	6.84	1.49	1.39
24	A	353	PHO	C3B-C2B	6.68	1.49	1.40
24	A	353	PHO	C4D-CHA	6.43	1.49	1.39
24	a	408	PHO	C3B-C2B	6.32	1.48	1.40
24	A	407	PHO	C3B-C4B	6.09	1.47	1.41
24	A	407	PHO	C3B-C2B	6.09	1.48	1.40
24	a	353	PHO	C4D-CHA	6.04	1.48	1.39
24	a	353	PHO	C3B-C2B	5.91	1.48	1.40
24	a	353	PHO	C3D-C2D	5.73	1.49	1.39
24	a	408	PHO	C3D-C2D	5.57	1.49	1.39
23	c	513	CLA	C3C-C2C	5.54	1.48	1.36
23	C	509	CLA	C3C-C2C	5.53	1.48	1.36
23	c	509	CLA	C3C-C2C	5.51	1.48	1.36
24	A	353	PHO	C3D-C2D	5.47	1.49	1.39
23	b	605	CLA	C3C-C2C	5.45	1.48	1.36
23	C	513	CLA	C3C-C2C	5.44	1.48	1.36
23	b	610	CLA	C3C-C2C	5.43	1.48	1.36
23	B	601	CLA	C3C-C2C	5.40	1.48	1.36
23	B	602	CLA	CHC-C1C	5.40	1.49	1.38
23	C	511	CLA	C3C-C2C	5.36	1.48	1.36
23	B	602	CLA	C3C-C2C	5.36	1.48	1.36
23	C	508	CLA	C3C-C2C	5.35	1.48	1.36
23	a	406	CLA	C3C-C2C	5.34	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	514	CLA	C3C-C2C	5.32	1.48	1.36
24	A	353	PHO	OBD-CAD	5.32	1.29	1.22
38	e	87	HEM	FE-NB	5.31	2.11	1.94
24	A	407	PHO	C3D-C2D	5.31	1.48	1.39
23	b	601	CLA	C3C-C2C	5.30	1.48	1.36
23	b	613	CLA	C3C-C2C	5.28	1.48	1.36
23	b	602	CLA	CHC-C1C	5.26	1.49	1.38
23	b	615	CLA	C3C-C2C	5.26	1.48	1.36
23	B	611	CLA	C3C-C2C	5.26	1.48	1.36
25	b	617	BCR	C23-C22	-5.26	1.34	1.46
25	B	619	BCR	C23-C22	-5.26	1.34	1.46
23	C	510	CLA	C3C-C2C	5.25	1.48	1.36
23	b	616	CLA	CHC-C1C	5.25	1.49	1.38
23	B	614	CLA	C3C-C2C	5.24	1.48	1.36
23	b	613	CLA	O2D-CGD	5.24	1.46	1.33
23	b	608	CLA	C3C-C2C	5.24	1.48	1.36
23	d	403	CLA	CHC-C1C	5.23	1.49	1.38
23	b	606	CLA	C3C-C2C	5.23	1.48	1.36
23	B	610	CLA	C3C-C2C	5.22	1.48	1.36
23	c	502	CLA	C3C-C2C	5.22	1.48	1.36
23	b	612	CLA	C3C-C2C	5.22	1.48	1.36
23	B	607	CLA	C3C-C2C	5.21	1.48	1.36
24	a	353	PHO	OBD-CAD	5.20	1.29	1.22
25	k	101	BCR	C23-C22	-5.20	1.34	1.46
23	c	510	CLA	C3C-C2C	5.20	1.48	1.36
23	A	408	CLA	C3C-C2C	5.20	1.48	1.36
23	c	507	CLA	C3C-C2C	5.19	1.48	1.36
23	B	604	CLA	C3C-C2C	5.18	1.48	1.36
25	C	516	BCR	C23-C22	-5.16	1.34	1.46
23	D	406	CLA	C3C-C2C	5.16	1.47	1.36
23	b	602	CLA	C3C-C2C	5.16	1.47	1.36
23	B	613	CLA	O2D-CGD	5.15	1.45	1.33
23	b	604	CLA	C3C-C2C	5.15	1.47	1.36
25	C	515	BCR	C23-C22	-5.15	1.34	1.46
23	C	514	CLA	C3C-C2C	5.15	1.47	1.36
23	B	608	CLA	C3C-C2C	5.15	1.47	1.36
23	b	603	CLA	C3C-C2C	5.15	1.47	1.36
23	A	404	CLA	C3C-C2C	5.13	1.47	1.36
25	d	404	BCR	C23-C22	-5.12	1.35	1.46
23	C	512	CLA	O2D-CGD	5.11	1.45	1.33
23	C	505	CLA	C3C-C2C	5.11	1.47	1.36
23	d	403	CLA	C3C-C2C	5.11	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	C1D-ND	5.11	1.44	1.37
23	A	405	CLA	C3C-C2C	5.10	1.47	1.36
25	c	515	BCR	C23-C22	-5.09	1.35	1.46
23	B	616	CLA	C3C-C2C	5.09	1.47	1.36
23	a	407	CLA	C3C-C2C	5.09	1.47	1.36
23	A	406	CLA	C3C-C2C	5.08	1.47	1.36
23	c	510	CLA	O2D-CGD	5.08	1.45	1.33
23	B	605	CLA	C3C-C2C	5.08	1.47	1.36
23	b	607	CLA	C3C-C2C	5.07	1.47	1.36
23	C	511	CLA	CHC-C1C	5.07	1.48	1.38
23	C	507	CLA	C3C-C2C	5.06	1.47	1.36
23	C	502	CLA	C3C-C2C	5.06	1.47	1.36
23	C	508	CLA	CHC-C1C	5.06	1.48	1.38
23	B	609	CLA	C3C-C2C	5.06	1.47	1.36
23	c	512	CLA	C3C-C2C	5.06	1.47	1.36
23	b	616	CLA	C3C-C2C	5.05	1.47	1.36
23	C	506	CLA	C3C-C2C	5.05	1.47	1.36
23	C	504	CLA	C3C-C2C	5.05	1.47	1.36
23	B	609	CLA	O2D-CGD	5.05	1.45	1.33
23	C	514	CLA	CHC-C1C	5.04	1.48	1.38
38	E	103	HEM	FE-NB	5.03	2.10	1.94
23	d	402	CLA	C3C-C2C	5.03	1.47	1.36
23	B	605	CLA	C1D-ND	5.03	1.44	1.37
23	a	409	CLA	C3C-C2C	5.03	1.47	1.36
23	c	506	CLA	O2D-CGD	5.01	1.45	1.33
23	a	406	CLA	O2D-CGD	5.00	1.45	1.33
23	c	504	CLA	C3C-C2C	5.00	1.47	1.36
23	C	513	CLA	CHC-C1C	4.99	1.48	1.38
23	c	509	CLA	O2D-CGD	4.99	1.45	1.33
23	c	509	CLA	CHC-C1C	4.98	1.48	1.38
23	b	616	CLA	O2D-CGD	4.98	1.45	1.33
23	b	614	CLA	C3C-C2C	4.98	1.47	1.36
23	c	506	CLA	C3C-C2C	4.98	1.47	1.36
25	K	102	BCR	C23-C22	-4.98	1.35	1.46
23	D	406	CLA	O2D-CGD	4.97	1.45	1.33
23	c	513	CLA	CHC-C1C	4.97	1.48	1.38
25	c	516	BCR	C23-C22	-4.95	1.35	1.46
23	B	611	CLA	C1D-ND	4.95	1.44	1.37
23	b	608	CLA	O2D-CGD	4.94	1.45	1.33
25	A	409	BCR	C23-C22	-4.94	1.35	1.46
23	c	507	CLA	O2D-CGD	4.94	1.45	1.33
23	a	406	CLA	C1D-ND	4.94	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	C3C-C2C	4.94	1.47	1.36
23	c	512	CLA	C1D-ND	4.94	1.44	1.37
23	a	405	CLA	O2D-CGD	4.93	1.45	1.33
23	a	405	CLA	C3C-C2C	4.93	1.47	1.36
23	c	514	CLA	C1D-ND	4.93	1.44	1.37
23	D	406	CLA	CHC-C1C	4.93	1.48	1.38
25	y	101	BCR	C23-C22	-4.92	1.35	1.46
23	b	601	CLA	O2D-CGD	4.91	1.45	1.33
23	b	603	CLA	O2D-CGD	4.91	1.45	1.33
23	A	405	CLA	CHC-C1C	4.90	1.48	1.38
24	a	353	PHO	O2D-CGD	4.90	1.45	1.33
25	b	619	BCR	C23-C22	-4.90	1.35	1.46
23	c	503	CLA	C3C-C2C	4.90	1.47	1.36
23	B	610	CLA	CHC-C1C	4.90	1.48	1.38
23	B	616	CLA	CHC-C1C	4.90	1.48	1.38
23	C	503	CLA	C3C-C2C	4.89	1.47	1.36
23	B	606	CLA	C3C-C2C	4.89	1.47	1.36
23	c	505	CLA	C3C-C2C	4.88	1.47	1.36
23	c	505	CLA	O2D-CGD	4.88	1.45	1.33
23	C	507	CLA	O2D-CGD	4.87	1.45	1.33
23	B	601	CLA	O2D-CGD	4.87	1.45	1.33
23	B	601	CLA	CHC-C1C	4.87	1.48	1.38
23	A	405	CLA	O2D-CGD	4.87	1.45	1.33
25	T	101	BCR	C23-C22	-4.87	1.35	1.46
23	A	408	CLA	CHC-C1C	4.86	1.48	1.38
23	b	609	CLA	O2D-CGD	4.86	1.45	1.33
23	a	407	CLA	C1D-ND	4.86	1.44	1.37
24	A	353	PHO	O2D-CGD	4.86	1.45	1.33
23	c	504	CLA	CHD-C1D	4.85	1.47	1.38
23	c	511	CLA	C3C-C2C	4.85	1.47	1.36
23	B	603	CLA	C3C-C2C	4.85	1.47	1.36
23	B	612	CLA	C3C-C2C	4.84	1.47	1.36
23	C	505	CLA	O2D-CGD	4.83	1.45	1.33
23	D	405	CLA	C3C-C2C	4.82	1.47	1.36
25	D	407	BCR	C23-C22	-4.82	1.35	1.46
25	B	617	BCR	C23-C22	-4.82	1.35	1.46
25	t	103	BCR	C23-C22	-4.82	1.35	1.46
23	c	510	CLA	CHC-C1C	4.82	1.48	1.38
25	b	618	BCR	C23-C22	-4.81	1.35	1.46
23	c	508	CLA	O2D-CGD	4.81	1.45	1.33
23	c	511	CLA	C1D-ND	4.81	1.44	1.37
23	c	514	CLA	CHC-C1C	4.80	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	O2D-CGD	4.80	1.45	1.33
23	B	605	CLA	CHC-C1C	4.80	1.48	1.38
23	b	606	CLA	CHC-C1C	4.79	1.48	1.38
23	b	609	CLA	C3C-C2C	4.79	1.47	1.36
24	A	407	PHO	O2D-CGD	4.79	1.45	1.33
23	c	511	CLA	O2D-CGD	4.78	1.45	1.33
23	b	614	CLA	O2D-CGD	4.78	1.45	1.33
23	b	605	CLA	O2D-CGD	4.78	1.45	1.33
23	c	502	CLA	CHC-C1C	4.78	1.48	1.38
23	B	609	CLA	CHC-C1C	4.78	1.48	1.38
23	d	402	CLA	O2D-CGD	4.77	1.45	1.33
23	b	610	CLA	CHC-C1C	4.77	1.48	1.38
23	C	506	CLA	CHC-C1C	4.76	1.48	1.38
23	B	614	CLA	O2D-CGD	4.76	1.44	1.33
23	B	601	CLA	O2A-CGA	4.76	1.47	1.33
23	C	514	CLA	O2D-CGD	4.75	1.44	1.33
23	a	409	CLA	CHC-C1C	4.74	1.48	1.38
23	B	602	CLA	C1D-ND	4.74	1.44	1.37
23	B	602	CLA	O2D-CGD	4.74	1.44	1.33
23	c	510	CLA	C1D-ND	4.74	1.44	1.37
23	A	405	CLA	C1D-ND	4.74	1.44	1.37
23	C	503	CLA	O2D-CGD	4.73	1.44	1.33
23	c	508	CLA	C3C-C2C	4.73	1.47	1.36
23	c	506	CLA	CHC-C1C	4.73	1.48	1.38
23	C	502	CLA	CHC-C1C	4.72	1.47	1.38
25	H	101	BCR	C23-C22	-4.72	1.35	1.46
23	A	406	CLA	O2D-CGD	4.72	1.44	1.33
23	a	406	CLA	CHC-C1C	4.71	1.47	1.38
23	B	615	CLA	O2D-CGD	4.71	1.44	1.33
23	B	613	CLA	C3C-C2C	4.69	1.46	1.36
23	c	514	CLA	O2D-CGD	4.69	1.44	1.33
23	b	615	CLA	CHC-C1C	4.69	1.47	1.38
23	B	614	CLA	CHC-C1C	4.69	1.47	1.38
26	F	101	SQD	O47-C7	4.69	1.47	1.34
23	B	605	CLA	O2D-CGD	4.69	1.44	1.33
23	C	512	CLA	CHC-C1C	4.69	1.47	1.38
23	C	514	CLA	C1D-ND	4.68	1.44	1.37
23	B	611	CLA	O2D-CGD	4.68	1.44	1.33
23	A	408	CLA	O2D-CGD	4.68	1.44	1.33
23	b	607	CLA	O2D-CGD	4.68	1.44	1.33
25	a	410	BCR	C23-C22	-4.67	1.35	1.46
23	C	506	CLA	O2D-CGD	4.67	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	C1D-ND	4.67	1.44	1.37
23	B	616	CLA	O2D-CGD	4.66	1.44	1.33
23	d	402	CLA	CHC-C1C	4.66	1.47	1.38
23	C	511	CLA	O2D-CGD	4.66	1.44	1.33
23	C	503	CLA	CHC-C1C	4.66	1.47	1.38
23	B	601	CLA	C1D-ND	4.66	1.44	1.37
23	B	615	CLA	C3C-C2C	4.66	1.46	1.36
23	B	604	CLA	O2D-CGD	4.65	1.44	1.33
25	h	101	BCR	C23-C22	-4.65	1.36	1.46
23	C	504	CLA	CHC-C1C	4.64	1.47	1.38
23	b	612	CLA	O2D-CGD	4.63	1.44	1.33
23	c	513	CLA	O2D-CGD	4.63	1.44	1.33
23	B	612	CLA	O2D-CGD	4.62	1.44	1.33
23	b	609	CLA	C1D-ND	4.62	1.43	1.37
23	c	504	CLA	CHC-C1C	4.62	1.47	1.38
23	C	505	CLA	CHD-C1D	4.61	1.47	1.38
23	b	601	CLA	CHD-C1D	4.61	1.47	1.38
23	b	611	CLA	CHC-C1C	4.60	1.47	1.38
23	C	510	CLA	C1D-ND	4.60	1.43	1.37
23	C	509	CLA	O2D-CGD	4.59	1.44	1.33
23	b	601	CLA	O2A-CGA	4.59	1.46	1.33
23	B	615	CLA	CHC-C1C	4.59	1.47	1.38
23	b	608	CLA	CHC-C1C	4.59	1.47	1.38
23	c	511	CLA	CHC-C1C	4.58	1.47	1.38
23	C	509	CLA	C1D-ND	4.58	1.43	1.37
23	b	609	CLA	CHC-C1C	4.58	1.47	1.38
23	b	611	CLA	O2D-CGD	4.57	1.44	1.33
23	b	604	CLA	O2D-CGD	4.57	1.44	1.33
23	B	610	CLA	O2D-CGD	4.57	1.44	1.33
25	Y	101	BCR	C23-C22	-4.56	1.36	1.46
23	C	513	CLA	C1D-ND	4.56	1.43	1.37
23	b	615	CLA	O2D-CGD	4.55	1.44	1.33
23	a	407	CLA	CHC-C1C	4.55	1.47	1.38
23	A	406	CLA	CHC-C1C	4.55	1.47	1.38
23	C	505	CLA	CHC-C1C	4.55	1.47	1.38
23	b	605	CLA	C1D-ND	4.54	1.43	1.37
23	C	507	CLA	C1D-ND	4.54	1.43	1.37
23	D	406	CLA	C1D-ND	4.54	1.43	1.37
23	a	407	CLA	O2D-CGD	4.54	1.44	1.33
23	c	503	CLA	C1D-ND	4.54	1.43	1.37
23	C	510	CLA	O2D-CGD	4.54	1.44	1.33
23	a	406	CLA	O2A-CGA	4.53	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404	CLA	CHC-C1C	4.53	1.47	1.38
23	c	502	CLA	CHD-C1D	4.53	1.47	1.38
33	C	521	LMG	O7-C10	4.53	1.47	1.34
23	B	615	CLA	C1D-ND	4.52	1.43	1.37
23	c	502	CLA	C1D-ND	4.51	1.43	1.37
23	b	615	CLA	C1D-ND	4.50	1.43	1.37
23	c	503	CLA	O2D-CGD	4.50	1.44	1.33
23	c	502	CLA	O2D-CGD	4.50	1.44	1.33
23	c	514	CLA	CHD-C1D	4.50	1.47	1.38
23	c	503	CLA	CHC-C1C	4.50	1.47	1.38
23	B	603	CLA	CHC-C1C	4.50	1.47	1.38
23	C	503	CLA	C1D-ND	4.49	1.43	1.37
23	c	509	CLA	C1D-ND	4.49	1.43	1.37
23	B	603	CLA	O2D-CGD	4.49	1.44	1.33
23	d	403	CLA	C1D-ND	4.49	1.43	1.37
23	b	611	CLA	C1D-ND	4.48	1.43	1.37
23	c	512	CLA	CHC-C1C	4.48	1.47	1.38
23	C	511	CLA	C1D-ND	4.48	1.43	1.37
23	c	512	CLA	O2D-CGD	4.48	1.44	1.33
23	c	508	CLA	CHC-C1C	4.48	1.47	1.38
26	a	413	SQD	O48-C23	4.48	1.46	1.33
23	a	405	CLA	CHD-C1D	4.47	1.47	1.38
23	b	616	CLA	C1D-ND	4.47	1.43	1.37
24	A	407	PHO	OBD-CAD	4.47	1.28	1.22
23	C	504	CLA	C1D-ND	4.46	1.43	1.37
23	C	504	CLA	O2D-CGD	4.46	1.44	1.33
23	b	603	CLA	CHC-C1C	4.45	1.47	1.38
23	c	504	CLA	C1D-ND	4.45	1.43	1.37
23	C	510	CLA	CHD-C1D	4.45	1.47	1.38
23	B	602	CLA	CHD-C1D	4.44	1.47	1.38
23	A	404	CLA	O2D-CGD	4.44	1.44	1.33
23	C	509	CLA	CHC-C1C	4.43	1.47	1.38
23	A	404	CLA	C1D-ND	4.43	1.43	1.37
23	b	601	CLA	CHC-C1C	4.43	1.47	1.38
23	A	408	CLA	C1D-ND	4.42	1.43	1.37
23	D	405	CLA	O2D-CGD	4.42	1.44	1.33
37	E	101	LHG	O8-C23	4.42	1.46	1.33
23	b	607	CLA	CHC-C1C	4.41	1.47	1.38
23	c	507	CLA	C1D-ND	4.41	1.43	1.37
23	C	507	CLA	CHD-C1D	4.41	1.47	1.38
23	c	504	CLA	O2D-CGD	4.41	1.44	1.33
23	B	616	CLA	C1D-ND	4.41	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	O2A-CGA	4.41	1.46	1.33
23	B	604	CLA	CHC-C1C	4.40	1.47	1.38
23	C	513	CLA	O2D-CGD	4.40	1.44	1.33
23	C	508	CLA	O2D-CGD	4.40	1.44	1.33
23	C	514	CLA	CHD-C1D	4.40	1.47	1.38
23	a	409	CLA	O2D-CGD	4.40	1.44	1.33
23	b	613	CLA	CHC-C1C	4.39	1.47	1.38
26	f	102	SQD	O47-C7	4.39	1.46	1.34
23	a	405	CLA	C1D-ND	4.39	1.43	1.37
23	B	607	CLA	CHC-C1C	4.37	1.47	1.38
23	c	507	CLA	CHC-C1C	4.37	1.47	1.38
23	b	614	CLA	CHC-C1C	4.37	1.47	1.38
23	C	512	CLA	C3C-C2C	4.36	1.46	1.36
23	c	508	CLA	C1D-ND	4.36	1.43	1.37
33	C	521	LMG	O8-C28	4.35	1.46	1.33
26	A	412	SQD	O48-C23	4.35	1.46	1.33
37	e	101	LHG	O8-C23	4.35	1.46	1.33
33	Z	101	LMG	O7-C10	4.35	1.46	1.34
24	a	408	PHO	O2D-CGD	4.34	1.43	1.33
40	V	202	HEC	CAC-C3C	4.34	1.49	1.35
23	b	609	CLA	CHD-C1D	4.34	1.46	1.38
33	z	101	LMG	O8-C28	4.34	1.46	1.33
23	C	507	CLA	CHC-C1C	4.33	1.47	1.38
33	c	520	LMG	O8-C28	4.32	1.45	1.33
33	B	621	LMG	O8-C28	4.32	1.45	1.33
40	v	202	HEC	CBC-CAC	-4.31	1.33	1.49
23	b	602	CLA	C1D-ND	4.31	1.43	1.37
33	c	521	LMG	O8-C28	4.31	1.45	1.33
23	C	513	CLA	O2A-CGA	4.30	1.45	1.33
23	B	607	CLA	O2D-CGD	4.30	1.43	1.33
37	l	101	LHG	O8-C23	4.30	1.45	1.33
35	c	518	DGD	O1G-C1A	4.30	1.45	1.33
23	b	612	CLA	CHC-C1C	4.29	1.47	1.38
23	B	608	CLA	O2D-CGD	4.29	1.43	1.33
33	C	520	LMG	O8-C28	4.29	1.45	1.33
23	C	506	CLA	C1D-ND	4.29	1.43	1.37
23	B	611	CLA	CHC-C1C	4.29	1.47	1.38
26	b	620	SQD	O47-C7	4.29	1.46	1.34
23	b	608	CLA	C1D-ND	4.29	1.43	1.37
23	C	512	CLA	O2A-CGA	4.28	1.45	1.33
23	d	403	CLA	CHD-C1D	4.28	1.46	1.38
23	c	513	CLA	O2A-CGA	4.28	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	O2A-CGA	4.28	1.45	1.33
23	B	609	CLA	C1D-ND	4.28	1.43	1.37
23	c	505	CLA	CHC-C1C	4.27	1.47	1.38
23	c	507	CLA	CHD-C1D	4.26	1.46	1.38
33	c	521	LMG	O7-C10	4.26	1.46	1.34
23	C	510	CLA	CHC-C1C	4.26	1.47	1.38
23	D	405	CLA	CHC-C1C	4.26	1.47	1.38
23	B	610	CLA	C1D-ND	4.25	1.43	1.37
23	b	604	CLA	C1D-ND	4.25	1.43	1.37
26	B	620	SQD	O47-C7	4.25	1.46	1.34
37	e	101	LHG	O7-C7	4.25	1.46	1.34
23	C	502	CLA	CHD-C1D	4.24	1.46	1.38
23	b	606	CLA	O2D-CGD	4.23	1.43	1.33
40	v	202	HEC	CAC-C3C	4.23	1.48	1.35
23	C	513	CLA	CHD-C1D	4.23	1.46	1.38
26	f	102	SQD	O48-C23	4.23	1.45	1.33
23	B	606	CLA	CHC-C1C	4.23	1.47	1.38
23	B	604	CLA	C1D-ND	4.23	1.43	1.37
23	b	601	CLA	CHD-C4C	4.23	1.48	1.39
23	B	606	CLA	O2D-CGD	4.23	1.43	1.33
23	C	502	CLA	O2D-CGD	4.22	1.43	1.33
23	c	508	CLA	CHD-C4C	4.22	1.48	1.39
23	B	613	CLA	CHC-C1C	4.22	1.46	1.38
23	B	612	CLA	CHC-C1C	4.22	1.46	1.38
33	C	501	LMG	O8-C28	4.22	1.45	1.33
23	B	609	CLA	O2A-CGA	4.22	1.45	1.33
23	C	506	CLA	CHD-C1D	4.21	1.46	1.38
23	b	610	CLA	CHD-C1D	4.20	1.46	1.38
23	c	507	CLA	C3D-C2D	4.20	1.50	1.39
23	a	409	CLA	O2A-CGA	4.20	1.45	1.33
23	b	602	CLA	CHD-C1D	4.20	1.46	1.38
23	B	612	CLA	C1B-NB	-4.20	1.32	1.37
23	C	514	CLA	O2A-CGA	4.20	1.45	1.33
23	B	615	CLA	C3D-C2D	4.19	1.50	1.39
23	B	606	CLA	O2A-CGA	4.19	1.45	1.33
26	B	620	SQD	O48-C23	4.19	1.45	1.33
23	c	508	CLA	O2A-CGA	4.19	1.45	1.33
23	c	514	CLA	O2A-CGA	4.19	1.45	1.33
23	b	608	CLA	O2A-CGA	4.18	1.45	1.33
23	b	606	CLA	CHD-C1D	4.18	1.46	1.38
23	C	503	CLA	CHD-C1D	4.17	1.46	1.38
23	C	507	CLA	O2A-CGA	4.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	CHD-C1D	4.17	1.46	1.38
23	A	405	CLA	CHC-C4B	4.17	1.48	1.39
23	C	512	CLA	CHD-C1D	4.17	1.46	1.38
23	A	408	CLA	O2A-CGA	4.17	1.45	1.33
23	B	601	CLA	CHD-C1D	4.17	1.46	1.38
23	c	513	CLA	CHD-C1D	4.17	1.46	1.38
40	V	202	HEC	CBC-CAC	-4.17	1.34	1.49
40	V	202	HEC	CBB-CAB	-4.16	1.34	1.49
26	a	413	SQD	O47-C7	4.16	1.46	1.34
23	B	609	CLA	CHD-C1D	4.16	1.46	1.38
26	b	620	SQD	O48-C23	4.16	1.45	1.33
23	b	601	CLA	C3D-C2D	4.16	1.50	1.39
23	A	405	CLA	C3D-C2D	4.16	1.50	1.39
33	C	520	LMG	O7-C10	4.16	1.46	1.34
23	d	403	CLA	O2A-CGA	4.16	1.45	1.33
23	B	603	CLA	C1D-ND	4.16	1.43	1.37
24	A	407	PHO	O2A-CGA	4.15	1.45	1.33
24	a	408	PHO	OBD-CAD	4.15	1.27	1.22
23	a	407	CLA	C3D-C2D	4.15	1.50	1.39
40	v	202	HEC	CAB-C3B	4.15	1.48	1.35
23	C	508	CLA	C1D-ND	4.15	1.43	1.37
38	E	103	HEM	FE-NC	4.15	2.08	1.95
23	c	512	CLA	O2A-CGA	4.15	1.45	1.33
23	b	606	CLA	C1D-ND	4.15	1.43	1.37
23	a	406	CLA	C3D-C2D	4.14	1.50	1.39
37	L	101	LHG	O8-C23	4.14	1.45	1.33
23	C	508	CLA	O2A-CGA	4.14	1.45	1.33
23	b	610	CLA	CHC-C4B	4.14	1.48	1.39
40	v	202	HEC	CBB-CAB	-4.14	1.34	1.49
23	B	613	CLA	O2A-CGA	4.14	1.45	1.33
40	V	202	HEC	CAB-C3B	4.14	1.48	1.35
23	a	405	CLA	CHC-C1C	4.13	1.46	1.38
23	c	514	CLA	CHD-C4C	4.13	1.48	1.39
37	d	408	LHG	O8-C23	4.13	1.45	1.33
33	m	101	LMG	O8-C28	4.13	1.45	1.33
23	C	502	CLA	O2A-CGA	4.13	1.45	1.33
23	c	510	CLA	O2A-CGA	4.13	1.45	1.33
35	c	519	DGD	O1G-C1A	4.13	1.45	1.33
23	c	502	CLA	CHD-C4C	4.12	1.48	1.39
23	C	513	CLA	C3D-C2D	4.12	1.50	1.39
23	c	509	CLA	O2A-CGA	4.12	1.45	1.33
26	A	410	SQD	O48-C23	4.12	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	406	CLA	CHD-C1D	4.12	1.46	1.38
23	c	510	CLA	CHD-C1D	4.12	1.46	1.38
33	C	501	LMG	O7-C10	4.11	1.45	1.34
23	C	504	CLA	CHD-C1D	4.11	1.46	1.38
23	b	610	CLA	O2D-CGD	4.11	1.43	1.33
37	d	408	LHG	O7-C7	4.10	1.45	1.34
23	C	509	CLA	C3D-C2D	4.10	1.50	1.39
23	b	608	CLA	CHD-C1D	4.09	1.46	1.38
23	C	508	CLA	CHC-C4B	4.09	1.48	1.39
23	d	403	CLA	O2D-CGD	4.09	1.43	1.33
23	b	602	CLA	CHC-C4B	4.09	1.48	1.39
25	B	618	BCR	C23-C22	-4.09	1.37	1.46
23	B	608	CLA	C1D-ND	4.09	1.43	1.37
26	A	412	SQD	O47-C7	4.09	1.45	1.34
23	C	508	CLA	CHD-C1D	4.09	1.46	1.38
23	C	514	CLA	CHD-C4C	4.09	1.48	1.39
23	c	511	CLA	CHD-C1D	4.08	1.46	1.38
23	C	503	CLA	O2A-CGA	4.08	1.45	1.33
23	b	616	CLA	CHD-C1D	4.08	1.46	1.38
23	b	612	CLA	O2A-CGA	4.08	1.45	1.33
23	C	512	CLA	C3D-C2D	4.08	1.50	1.39
33	a	419	LMG	O8-C28	4.07	1.45	1.33
23	c	511	CLA	CHB-C1B	4.07	1.48	1.39
35	h	102	DGD	O1G-C1A	4.07	1.45	1.33
23	b	616	CLA	O2A-CGA	4.07	1.45	1.33
23	D	406	CLA	CHC-C4B	4.06	1.48	1.39
26	a	411	SQD	O48-C23	4.06	1.45	1.33
23	b	613	CLA	C1D-ND	4.06	1.43	1.37
23	c	504	CLA	O2A-CGA	4.06	1.45	1.33
23	b	610	CLA	C1D-ND	4.06	1.43	1.37
23	B	614	CLA	C1D-ND	4.06	1.43	1.37
37	E	101	LHG	O7-C7	4.06	1.45	1.34
23	d	403	CLA	CHC-C4B	4.05	1.48	1.39
24	a	353	PHO	O2A-CGA	4.05	1.45	1.33
23	c	512	CLA	CHB-C1B	4.05	1.48	1.39
23	b	613	CLA	C3D-C2D	4.05	1.50	1.39
35	C	518	DGD	O1G-C1A	4.05	1.45	1.33
23	b	605	CLA	CHC-C1C	4.05	1.46	1.38
23	c	509	CLA	C3D-C2D	4.05	1.50	1.39
23	B	608	CLA	CHD-C1D	4.04	1.46	1.38
23	B	611	CLA	CHD-C1D	4.04	1.46	1.38
23	b	602	CLA	O2A-CGA	4.03	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C3D-C2D	4.03	1.50	1.39
23	C	509	CLA	CHD-C1D	4.03	1.46	1.38
23	c	506	CLA	CHC-C4B	4.02	1.48	1.39
23	b	615	CLA	CHD-C1D	4.02	1.46	1.38
23	d	402	CLA	CHC-C4B	4.02	1.48	1.39
23	B	604	CLA	CHD-C1D	4.01	1.46	1.38
23	b	604	CLA	CHC-C1C	4.01	1.46	1.38
23	B	615	CLA	CHD-C1D	4.01	1.46	1.38
23	b	613	CLA	O2A-CGA	4.01	1.45	1.33
23	D	405	CLA	O2A-CGA	4.01	1.45	1.33
23	d	403	CLA	CHD-C4C	4.01	1.48	1.39
23	C	512	CLA	C1D-ND	4.01	1.43	1.37
23	b	615	CLA	C3D-C2D	4.00	1.49	1.39
23	c	502	CLA	O2A-CGA	4.00	1.45	1.33
23	c	512	CLA	C3D-C2D	4.00	1.49	1.39
23	d	402	CLA	O2A-CGA	4.00	1.45	1.33
23	c	511	CLA	CHD-C4C	4.00	1.48	1.39
23	C	511	CLA	CHD-C4C	4.00	1.48	1.39
33	a	419	LMG	O7-C10	4.00	1.45	1.34
26	F	101	SQD	O48-C23	4.00	1.45	1.33
23	c	506	CLA	CHD-C1D	3.99	1.46	1.38
23	b	607	CLA	C1B-NB	-3.99	1.32	1.37
23	C	510	CLA	CHD-C4C	3.99	1.48	1.39
23	B	602	CLA	CHC-C4B	3.99	1.48	1.39
38	e	87	HEM	FE-NC	3.99	2.08	1.95
23	B	610	CLA	C3D-C2D	3.98	1.49	1.39
23	B	605	CLA	CHB-C1B	3.98	1.48	1.39
23	B	616	CLA	CHD-C1D	3.98	1.46	1.38
23	b	606	CLA	O2A-CGA	3.98	1.44	1.33
33	c	520	LMG	O7-C10	3.98	1.45	1.34
33	z	101	LMG	O7-C10	3.98	1.45	1.34
23	B	601	CLA	CHC-C4B	3.97	1.48	1.39
23	b	612	CLA	C1D-ND	3.97	1.43	1.37
23	c	508	CLA	OBD-CAD	3.97	1.29	1.22
23	B	607	CLA	OBD-CAD	3.97	1.29	1.22
23	c	504	CLA	CHD-C4C	3.97	1.48	1.39
23	c	508	CLA	C3D-C2D	3.97	1.49	1.39
23	C	511	CLA	O2A-CGA	3.96	1.44	1.33
23	C	505	CLA	C1D-ND	3.96	1.43	1.37
23	c	507	CLA	CHD-C4C	3.96	1.48	1.39
23	A	406	CLA	C3D-C2D	3.96	1.49	1.39
23	c	507	CLA	O2A-CGA	3.95	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	O2A-CGA	3.95	1.44	1.33
23	B	612	CLA	CHB-C1B	3.95	1.48	1.39
23	B	611	CLA	C3D-C2D	3.95	1.49	1.39
23	b	611	CLA	C3D-C2D	3.95	1.49	1.39
23	c	513	CLA	C1D-ND	3.94	1.43	1.37
23	B	607	CLA	O2A-CGA	3.94	1.44	1.33
35	c	517	DGD	O1G-C1A	3.94	1.44	1.33
23	B	605	CLA	CHC-C4B	3.94	1.48	1.39
23	d	403	CLA	C3D-C2D	3.94	1.49	1.39
23	B	609	CLA	C3D-C2D	3.94	1.49	1.39
33	d	412	LMG	O8-C28	3.94	1.44	1.33
23	a	409	CLA	C1B-NB	-3.94	1.32	1.37
23	B	615	CLA	OBD-CAD	3.94	1.29	1.22
23	C	514	CLA	C3D-C2D	3.94	1.49	1.39
23	a	409	CLA	C3D-C2D	3.93	1.49	1.39
23	C	510	CLA	O2A-CGA	3.93	1.44	1.33
37	D	411	LHG	O7-C7	3.93	1.45	1.34
23	B	613	CLA	C3D-C2D	3.93	1.49	1.39
23	b	602	CLA	CHD-C4C	3.93	1.48	1.39
23	A	406	CLA	CHD-C1D	3.93	1.46	1.38
23	b	616	CLA	CHC-C4B	3.93	1.48	1.39
23	B	606	CLA	C1D-ND	3.93	1.43	1.37
23	b	611	CLA	O2A-CGA	3.92	1.44	1.33
23	b	604	CLA	O2A-CGA	3.92	1.44	1.33
23	b	614	CLA	O2A-CGA	3.92	1.44	1.33
23	B	608	CLA	C3D-C2D	3.92	1.49	1.39
23	B	613	CLA	C1B-NB	-3.92	1.32	1.37
23	A	408	CLA	CHD-C4C	3.92	1.48	1.39
23	C	510	CLA	OBD-CAD	3.91	1.29	1.22
23	c	509	CLA	CHC-C4B	3.91	1.48	1.39
23	B	613	CLA	C1D-ND	3.91	1.43	1.37
23	A	405	CLA	O2A-CGA	3.91	1.44	1.33
23	a	405	CLA	CHD-C4C	3.91	1.48	1.39
23	b	611	CLA	CHB-C1B	3.91	1.48	1.39
23	B	610	CLA	OBD-CAD	3.91	1.29	1.22
23	C	509	CLA	O2A-CGA	3.91	1.44	1.33
23	b	613	CLA	CHD-C1D	3.91	1.46	1.38
23	a	407	CLA	O2A-CGA	3.90	1.44	1.33
33	d	412	LMG	O7-C10	3.90	1.45	1.34
23	C	513	CLA	CHD-C4C	3.90	1.48	1.39
23	B	604	CLA	CHB-C1B	3.90	1.48	1.39
23	C	509	CLA	CHB-C1B	3.90	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	519	DGD	O1G-C1A	3.90	1.44	1.33
23	B	605	CLA	C3D-C2D	3.89	1.49	1.39
23	C	506	CLA	O2A-CGA	3.89	1.44	1.33
23	c	512	CLA	CHD-C1D	3.89	1.46	1.38
23	C	510	CLA	C3D-C2D	3.89	1.49	1.39
23	c	510	CLA	CHD-C4C	3.89	1.48	1.39
23	B	614	CLA	CHC-C4B	3.89	1.48	1.39
23	C	503	CLA	C3D-C2D	3.89	1.49	1.39
23	C	506	CLA	CHB-C1B	3.89	1.48	1.39
23	C	511	CLA	CHD-C1D	3.89	1.46	1.38
23	B	603	CLA	C3D-C2D	3.89	1.49	1.39
23	b	608	CLA	OBD-CAD	3.89	1.29	1.22
23	a	407	CLA	CHD-C4C	3.88	1.48	1.39
35	C	517	DGD	O2G-C1B	3.88	1.45	1.34
23	c	510	CLA	C3D-C2D	3.88	1.49	1.39
23	a	409	CLA	C1D-ND	3.88	1.43	1.37
23	b	608	CLA	CHD-C4C	3.88	1.48	1.39
23	C	513	CLA	CHC-C4B	3.87	1.48	1.39
23	B	616	CLA	CHD-C4C	3.87	1.48	1.39
23	A	405	CLA	CHB-C1B	3.87	1.48	1.39
23	B	613	CLA	CHD-C1D	3.87	1.46	1.38
23	B	610	CLA	CHC-C4B	3.87	1.48	1.39
23	B	601	CLA	C3D-C2D	3.87	1.49	1.39
23	b	606	CLA	CHD-C4C	3.87	1.48	1.39
23	B	602	CLA	O2A-CGA	3.86	1.44	1.33
23	A	404	CLA	CHD-C1D	3.86	1.45	1.38
23	b	612	CLA	CHD-C1D	3.86	1.45	1.38
23	c	502	CLA	CHB-C1B	3.86	1.48	1.39
23	C	502	CLA	CHC-C4B	3.86	1.48	1.39
23	C	507	CLA	CHD-C4C	3.86	1.48	1.39
23	c	505	CLA	C3D-C2D	3.86	1.49	1.39
23	B	607	CLA	CHD-C1D	3.86	1.45	1.38
23	A	404	CLA	CHC-C4B	3.86	1.48	1.39
35	H	102	DGD	O1G-C1A	3.86	1.44	1.33
23	B	602	CLA	CHD-C4C	3.86	1.48	1.39
23	C	507	CLA	C3D-C2D	3.85	1.49	1.39
23	B	610	CLA	CHD-C1D	3.85	1.45	1.38
23	c	506	CLA	C1D-ND	3.85	1.42	1.37
23	B	611	CLA	CHD-C4C	3.85	1.48	1.39
23	b	614	CLA	C1D-ND	3.85	1.42	1.37
23	D	406	CLA	CHB-C1B	3.85	1.48	1.39
23	c	506	CLA	CHB-C1B	3.84	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404	CLA	C3D-C2D	3.84	1.49	1.39
23	b	602	CLA	C3D-C2D	3.84	1.49	1.39
23	C	505	CLA	CHD-C4C	3.84	1.47	1.39
26	a	411	SQD	O47-C7	3.83	1.45	1.34
23	C	503	CLA	CHD-C4C	3.83	1.47	1.39
23	c	502	CLA	C3D-C2D	3.83	1.49	1.39
23	C	504	CLA	CHD-C4C	3.83	1.47	1.39
23	A	406	CLA	O2A-CGA	3.83	1.44	1.33
23	c	503	CLA	CHD-C1D	3.83	1.45	1.38
23	B	610	CLA	CHB-C1B	3.82	1.48	1.39
23	A	404	CLA	CHD-C4C	3.82	1.47	1.39
23	c	514	CLA	C3D-C2D	3.82	1.49	1.39
23	C	502	CLA	C1D-ND	3.82	1.42	1.37
23	c	512	CLA	CHD-C4C	3.82	1.47	1.39
23	c	502	CLA	CHC-C4B	3.82	1.48	1.39
23	c	506	CLA	O2A-CGA	3.82	1.44	1.33
23	D	406	CLA	C3D-C2D	3.82	1.49	1.39
23	a	405	CLA	C3D-C2D	3.82	1.49	1.39
23	B	604	CLA	O2A-CGA	3.82	1.44	1.33
23	B	612	CLA	C3D-C2D	3.82	1.49	1.39
23	A	408	CLA	C3D-C2D	3.82	1.49	1.39
23	b	611	CLA	CHC-C4B	3.82	1.48	1.39
23	c	513	CLA	OBD-CAD	3.81	1.29	1.22
23	A	404	CLA	C1B-NB	-3.81	1.32	1.37
23	c	510	CLA	CHB-C1B	3.81	1.48	1.39
35	c	518	DGD	O2G-C1B	3.80	1.45	1.34
23	C	508	CLA	CHD-C4C	3.80	1.47	1.39
23	b	616	CLA	CHD-C4C	3.79	1.47	1.39
23	A	406	CLA	CHD-C4C	3.79	1.47	1.39
23	a	406	CLA	CHD-C1D	3.79	1.45	1.38
23	C	502	CLA	CHD-C4C	3.79	1.47	1.39
23	D	406	CLA	OBD-CAD	3.79	1.29	1.22
23	D	405	CLA	CHD-C1D	3.79	1.45	1.38
23	B	608	CLA	CHC-C1C	3.79	1.46	1.38
23	b	609	CLA	CHD-C4C	3.79	1.47	1.39
23	C	504	CLA	O2A-CGA	3.79	1.44	1.33
33	D	415	LMG	O8-C28	3.79	1.44	1.33
23	b	603	CLA	CHD-C1D	3.78	1.45	1.38
37	d	406	LHG	O8-C23	3.78	1.44	1.33
23	B	616	CLA	C3D-C2D	3.78	1.49	1.39
23	a	407	CLA	CHD-C1D	3.78	1.45	1.38
35	C	518	DGD	O2G-C1B	3.78	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	C1D-ND	3.77	1.42	1.37
23	c	506	CLA	CHD-C4C	3.77	1.47	1.39
23	b	609	CLA	CHB-C1B	3.77	1.47	1.39
37	D	409	LHG	O8-C23	3.77	1.44	1.33
23	B	610	CLA	CHD-C4C	3.77	1.47	1.39
33	B	621	LMG	O7-C10	3.77	1.44	1.34
35	h	102	DGD	O2G-C1B	3.77	1.44	1.34
23	A	405	CLA	CHD-C1D	3.76	1.45	1.38
23	b	609	CLA	C3D-C2D	3.76	1.49	1.39
23	b	609	CLA	O2A-CGA	3.76	1.44	1.33
23	a	405	CLA	CHB-C1B	3.76	1.47	1.39
35	C	517	DGD	O1G-C1A	3.76	1.44	1.33
23	C	505	CLA	C3D-C2D	3.76	1.49	1.39
23	B	609	CLA	CHC-C4B	3.76	1.47	1.39
23	b	611	CLA	CHD-C4C	3.76	1.47	1.39
23	B	603	CLA	CHD-C1D	3.76	1.45	1.38
23	C	505	CLA	O2A-CGA	3.75	1.44	1.33
23	b	610	CLA	CHD-C4C	3.75	1.47	1.39
23	b	615	CLA	CHD-C4C	3.75	1.47	1.39
23	b	616	CLA	C3D-C2D	3.75	1.49	1.39
23	A	405	CLA	OBD-CAD	3.75	1.28	1.22
23	a	409	CLA	CHD-C1D	3.75	1.45	1.38
23	C	508	CLA	C3D-C2D	3.74	1.49	1.39
23	B	609	CLA	C1B-NB	-3.74	1.32	1.37
23	B	608	CLA	CHB-C1B	3.74	1.47	1.39
23	B	607	CLA	CHD-C4C	3.74	1.47	1.39
23	C	512	CLA	CHB-C1B	3.74	1.47	1.39
37	L	101	LHG	O7-C7	3.74	1.44	1.34
23	B	605	CLA	CHD-C1D	3.73	1.45	1.38
23	A	406	CLA	C1D-ND	3.73	1.42	1.37
23	c	503	CLA	C3D-C2D	3.73	1.49	1.39
23	B	613	CLA	CHD-C4C	3.73	1.47	1.39
23	C	506	CLA	CHD-C4C	3.73	1.47	1.39
23	c	503	CLA	CHB-C1B	3.72	1.47	1.39
23	c	505	CLA	CHD-C1D	3.72	1.45	1.38
23	c	513	CLA	CHC-C4B	3.71	1.47	1.39
23	B	608	CLA	O2A-CGA	3.71	1.44	1.33
23	C	514	CLA	CHB-C1B	3.71	1.47	1.39
23	c	513	CLA	C3D-C2D	3.71	1.49	1.39
23	b	615	CLA	C1B-NB	-3.71	1.33	1.37
23	c	505	CLA	CHB-C1B	3.71	1.47	1.39
23	b	613	CLA	CHB-C1B	3.70	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	OBD-CAD	3.70	1.28	1.22
23	C	511	CLA	C3D-C2D	3.70	1.49	1.39
23	C	510	CLA	CHB-C1B	3.70	1.47	1.39
23	B	607	CLA	C1D-ND	3.69	1.42	1.37
23	b	608	CLA	C3D-C2D	3.69	1.49	1.39
23	C	512	CLA	CHD-C4C	3.69	1.47	1.39
23	b	613	CLA	CHC-C4B	3.69	1.47	1.39
23	B	609	CLA	CHB-C1B	3.69	1.47	1.39
23	B	601	CLA	CHD-C4C	3.69	1.47	1.39
23	a	406	CLA	CHD-C4C	3.69	1.47	1.39
37	D	411	LHG	O8-C23	3.68	1.44	1.33
23	A	408	CLA	CHC-C4B	3.68	1.47	1.39
23	B	607	CLA	C1B-NB	-3.68	1.33	1.37
23	C	511	CLA	CHC-C4B	3.68	1.47	1.39
35	c	517	DGD	O2G-C1B	3.68	1.44	1.34
23	b	605	CLA	CHD-C4C	3.68	1.47	1.39
23	d	403	CLA	OBD-CAD	3.67	1.28	1.22
35	c	519	DGD	O2G-C1B	3.67	1.44	1.34
23	c	513	CLA	CHD-C4C	3.67	1.47	1.39
23	b	603	CLA	CHB-C1B	3.67	1.47	1.39
23	b	612	CLA	C3D-C2D	3.66	1.49	1.39
23	c	505	CLA	OBD-CAD	3.66	1.28	1.22
23	C	503	CLA	OBD-CAD	3.66	1.28	1.22
23	b	609	CLA	OBD-CAD	3.66	1.28	1.22
23	C	504	CLA	C3D-C2D	3.66	1.49	1.39
23	c	511	CLA	C3D-C2D	3.66	1.49	1.39
23	b	614	CLA	CHD-C1D	3.66	1.45	1.38
23	c	504	CLA	C3D-C2D	3.66	1.49	1.39
23	b	604	CLA	CHD-C1D	3.66	1.45	1.38
23	a	406	CLA	CHC-C4B	3.66	1.47	1.39
23	c	507	CLA	OBD-CAD	3.66	1.28	1.22
23	b	601	CLA	CHB-C1B	3.66	1.47	1.39
23	b	607	CLA	CHD-C1D	3.65	1.45	1.38
23	A	408	CLA	CHD-C1D	3.65	1.45	1.38
23	b	614	CLA	C3D-C2D	3.65	1.48	1.39
23	B	603	CLA	O2A-CGA	3.65	1.44	1.33
23	c	504	CLA	CHC-C4B	3.65	1.47	1.39
23	C	505	CLA	CHB-C1B	3.65	1.47	1.39
23	c	507	CLA	C1B-NB	-3.65	1.33	1.37
23	b	603	CLA	O2A-CGA	3.64	1.44	1.33
23	d	402	CLA	C1B-NB	-3.64	1.33	1.37
23	b	605	CLA	C3D-C2D	3.64	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	CHB-C1B	3.64	1.47	1.39
26	A	410	SQD	O47-C7	3.64	1.44	1.34
23	b	606	CLA	C1B-NB	-3.64	1.33	1.37
23	a	409	CLA	CHD-C4C	3.64	1.47	1.39
23	C	503	CLA	CHC-C4B	3.63	1.47	1.39
33	m	101	LMG	O7-C10	3.63	1.44	1.34
23	C	502	CLA	CHB-C1B	3.63	1.47	1.39
23	b	611	CLA	CHD-C1D	3.63	1.45	1.38
23	b	604	CLA	C3D-C2D	3.63	1.48	1.39
23	b	607	CLA	C3D-C2D	3.63	1.48	1.39
23	B	606	CLA	C3D-C2D	3.62	1.48	1.39
23	B	607	CLA	CHB-C1B	3.62	1.47	1.39
23	b	601	CLA	OBD-CAD	3.62	1.28	1.22
23	b	606	CLA	C3D-C2D	3.62	1.48	1.39
23	C	514	CLA	CHC-C4B	3.62	1.47	1.39
23	C	506	CLA	C1B-NB	-3.62	1.33	1.37
23	B	608	CLA	CHD-C4C	3.62	1.47	1.39
23	b	605	CLA	CHB-C1B	3.62	1.47	1.39
23	B	613	CLA	CHB-C1B	3.62	1.47	1.39
23	b	602	CLA	OBD-CAD	3.62	1.28	1.22
23	b	605	CLA	OBD-CAD	3.62	1.28	1.22
23	C	511	CLA	CHB-C1B	3.62	1.47	1.39
23	B	614	CLA	C4B-NB	-3.61	1.33	1.37
23	b	603	CLA	C3D-C2D	3.61	1.48	1.39
23	C	512	CLA	OBD-CAD	3.61	1.28	1.22
23	b	612	CLA	CHD-C4C	3.61	1.47	1.39
23	c	504	CLA	CHB-C1B	3.61	1.47	1.39
23	c	503	CLA	CHD-C4C	3.61	1.47	1.39
23	c	503	CLA	O2A-CGA	3.60	1.43	1.33
23	d	402	CLA	C3D-C2D	3.60	1.48	1.39
23	C	509	CLA	OBD-CAD	3.60	1.28	1.22
37	d	407	LHG	O7-C7	3.60	1.44	1.34
23	b	607	CLA	CHB-C1B	3.60	1.47	1.39
23	C	510	CLA	C4B-NB	-3.60	1.33	1.37
23	C	502	CLA	C3D-C2D	3.60	1.48	1.39
23	b	608	CLA	CHB-C1B	3.60	1.47	1.39
23	c	511	CLA	OBD-CAD	3.60	1.28	1.22
23	B	611	CLA	O2A-CGA	3.60	1.43	1.33
23	c	510	CLA	CHC-C4B	3.60	1.47	1.39
23	B	614	CLA	O2A-CGA	3.60	1.43	1.33
23	B	605	CLA	CHD-C4C	3.59	1.47	1.39
23	b	614	CLA	CHB-C1B	3.59	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	CHC-C4B	3.59	1.47	1.39
33	D	415	LMG	O7-C10	3.59	1.44	1.34
23	D	406	CLA	CHD-C4C	3.58	1.47	1.39
23	b	605	CLA	CHD-C1D	3.58	1.45	1.38
23	b	613	CLA	CHD-C4C	3.58	1.47	1.39
23	b	610	CLA	OBD-CAD	3.58	1.28	1.22
23	a	407	CLA	OBD-CAD	3.58	1.28	1.22
23	C	505	CLA	CHC-C4B	3.58	1.47	1.39
23	B	611	CLA	CHB-C1B	3.58	1.47	1.39
23	c	506	CLA	C3D-C2D	3.57	1.48	1.39
34	B	622	HTG	C1'-S1	-3.57	1.76	1.81
23	b	606	CLA	CHC-C4B	3.56	1.47	1.39
23	B	603	CLA	CHC-C4B	3.56	1.47	1.39
23	B	613	CLA	C4B-NB	-3.56	1.33	1.37
23	D	405	CLA	CHD-C4C	3.56	1.47	1.39
23	B	610	CLA	O2A-CGA	3.56	1.43	1.33
23	A	408	CLA	CHB-C1B	3.56	1.47	1.39
35	H	102	DGD	O2G-C1B	3.56	1.44	1.34
23	B	601	CLA	OBD-CAD	3.55	1.28	1.22
23	B	616	CLA	OBD-CAD	3.55	1.28	1.22
23	B	612	CLA	CHD-C1D	3.55	1.45	1.38
23	b	605	CLA	C1B-NB	-3.54	1.33	1.37
23	b	613	CLA	C4B-NB	-3.54	1.33	1.37
23	C	504	CLA	CHC-C4B	3.54	1.47	1.39
23	c	514	CLA	CHC-C4B	3.54	1.47	1.39
23	B	614	CLA	C3D-C2D	3.54	1.48	1.39
23	b	614	CLA	CHD-C4C	3.54	1.47	1.39
23	B	611	CLA	OBD-CAD	3.53	1.28	1.22
23	B	608	CLA	C1B-NB	-3.53	1.33	1.37
23	b	607	CLA	O2A-CGA	3.53	1.43	1.33
23	c	508	CLA	CHC-C4B	3.53	1.47	1.39
37	D	409	LHG	O7-C7	3.53	1.44	1.34
23	B	613	CLA	OBD-CAD	3.53	1.28	1.22
37	d	407	LHG	O8-C23	3.52	1.43	1.33
23	B	614	CLA	CHB-C1B	3.52	1.47	1.39
23	c	507	CLA	CHB-C1B	3.52	1.47	1.39
23	c	509	CLA	CHB-C1B	3.52	1.47	1.39
23	B	605	CLA	O2A-CGA	3.52	1.43	1.33
23	B	606	CLA	CHB-C1B	3.52	1.47	1.39
23	D	406	CLA	C1B-NB	-3.52	1.33	1.37
23	B	611	CLA	C1B-NB	-3.52	1.33	1.37
23	b	605	CLA	O2A-CGA	3.52	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	604	CLA	CHB-C1B	3.52	1.47	1.39
23	b	610	CLA	CHB-C1B	3.51	1.47	1.39
23	c	509	CLA	CHD-C4C	3.51	1.47	1.39
23	b	612	CLA	C4B-NB	-3.51	1.33	1.37
23	B	603	CLA	CHD-C4C	3.51	1.47	1.39
23	B	609	CLA	OBD-CAD	3.51	1.28	1.22
23	A	408	CLA	C4B-NB	-3.51	1.33	1.37
23	b	607	CLA	C1D-ND	3.51	1.42	1.37
23	B	616	CLA	CHC-C4B	3.51	1.47	1.39
23	b	604	CLA	CHD-C4C	3.50	1.47	1.39
23	c	514	CLA	CHB-C1B	3.50	1.47	1.39
23	a	406	CLA	CHB-C1B	3.50	1.47	1.39
23	d	402	CLA	CHB-C1B	3.50	1.47	1.39
23	D	406	CLA	O2A-CGA	3.50	1.43	1.33
23	c	511	CLA	O2A-CGA	3.50	1.43	1.33
35	C	519	DGD	O2G-C1B	3.50	1.44	1.34
23	D	405	CLA	C3D-C2D	3.50	1.48	1.39
23	C	513	CLA	OBD-CAD	3.50	1.28	1.22
23	B	612	CLA	C1D-ND	3.50	1.42	1.37
23	c	505	CLA	O2A-CGA	3.49	1.43	1.33
23	C	507	CLA	CHC-C4B	3.49	1.47	1.39
23	c	510	CLA	OBD-CAD	3.49	1.28	1.22
23	b	615	CLA	CHC-C4B	3.49	1.47	1.39
23	B	614	CLA	CHD-C4C	3.49	1.47	1.39
23	c	505	CLA	CHD-C4C	3.49	1.47	1.39
23	c	511	CLA	CHC-C4B	3.49	1.47	1.39
23	B	604	CLA	C1B-NB	-3.49	1.33	1.37
23	C	507	CLA	CHB-C1B	3.49	1.47	1.39
23	B	607	CLA	C3D-C2D	3.49	1.48	1.39
23	b	608	CLA	CHC-C4B	3.48	1.47	1.39
23	A	405	CLA	C1B-NB	-3.48	1.33	1.37
37	l	101	LHG	O7-C7	3.48	1.44	1.34
23	B	609	CLA	CHD-C4C	3.48	1.47	1.39
23	B	606	CLA	C4B-NB	-3.47	1.33	1.37
23	B	611	CLA	C4B-NB	-3.47	1.33	1.37
23	d	402	CLA	CHD-C1D	3.47	1.45	1.38
23	A	404	CLA	OBD-CAD	3.47	1.28	1.22
23	C	507	CLA	C1B-NB	-3.46	1.33	1.37
23	d	402	CLA	OBD-CAD	3.46	1.28	1.22
23	B	606	CLA	CHD-C1D	3.46	1.45	1.38
34	b	622	HTG	C1'-S1	-3.46	1.76	1.81
34	d	411	HTG	C1'-S1	-3.45	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406	CLA	OBD-CAD	3.45	1.28	1.22
23	a	409	CLA	CHC-C4B	3.45	1.47	1.39
23	C	503	CLA	CHB-C1B	3.45	1.47	1.39
23	c	507	CLA	CHC-C4B	3.44	1.47	1.39
23	C	509	CLA	CHD-C4C	3.44	1.47	1.39
23	C	504	CLA	OBD-CAD	3.44	1.28	1.22
23	c	509	CLA	OBD-CAD	3.44	1.28	1.22
37	D	410	LHG	O7-C7	3.43	1.44	1.34
23	B	612	CLA	CHC-C4B	3.43	1.47	1.39
23	B	602	CLA	OBD-CAD	3.43	1.28	1.22
23	b	610	CLA	O2A-CGA	3.43	1.43	1.33
37	d	406	LHG	O7-C7	3.43	1.44	1.34
23	b	610	CLA	C1B-NB	-3.43	1.33	1.37
23	a	405	CLA	OBD-CAD	3.43	1.28	1.22
23	b	610	CLA	C3D-C2D	3.42	1.48	1.39
23	A	406	CLA	CHB-C1B	3.42	1.47	1.39
23	a	409	CLA	CHB-C1B	3.42	1.47	1.39
23	B	604	CLA	CHC-C4B	3.42	1.47	1.39
23	b	607	CLA	CHD-C4C	3.42	1.47	1.39
23	C	511	CLA	C1B-NB	-3.41	1.33	1.37
23	b	612	CLA	CHC-C4B	3.41	1.47	1.39
23	C	504	CLA	CHB-C1B	3.41	1.47	1.39
23	A	408	CLA	OBD-CAD	3.41	1.28	1.22
23	C	514	CLA	OBD-CAD	3.41	1.28	1.22
23	A	406	CLA	CHC-C4B	3.41	1.47	1.39
34	b	623	HTG	C1'-S1	-3.41	1.76	1.81
23	a	405	CLA	O2A-CGA	3.41	1.43	1.33
23	a	405	CLA	C1B-NB	-3.41	1.33	1.37
23	b	604	CLA	CHC-C4B	3.40	1.47	1.39
23	b	612	CLA	C1B-NB	-3.40	1.33	1.37
23	B	606	CLA	CHD-C4C	3.40	1.46	1.39
23	C	506	CLA	CHC-C4B	3.40	1.47	1.39
23	B	603	CLA	C1B-NB	-3.40	1.33	1.37
23	d	403	CLA	CHB-C1B	3.40	1.47	1.39
24	A	353	PHO	O2A-CGA	3.40	1.43	1.33
23	C	511	CLA	OBD-CAD	3.39	1.28	1.22
23	c	505	CLA	CHC-C4B	3.39	1.47	1.39
23	a	406	CLA	OBD-CAD	3.39	1.28	1.22
23	b	605	CLA	CHC-C4B	3.39	1.47	1.39
23	B	604	CLA	CHD-C4C	3.39	1.46	1.39
23	c	512	CLA	CHC-C4B	3.39	1.47	1.39
23	b	615	CLA	OBD-CAD	3.39	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	CHC-C4B	3.38	1.47	1.39
23	b	613	CLA	C1B-NB	-3.38	1.33	1.37
23	c	505	CLA	C4B-NB	-3.38	1.33	1.37
23	c	504	CLA	OBD-CAD	3.38	1.28	1.22
23	c	509	CLA	CHD-C1D	3.37	1.45	1.38
23	b	612	CLA	CHB-C1B	3.37	1.47	1.39
37	D	410	LHG	O8-C23	3.36	1.43	1.33
23	c	503	CLA	CHC-C4B	3.36	1.47	1.39
23	B	607	CLA	CHC-C4B	3.36	1.46	1.39
23	B	608	CLA	C4B-NB	-3.36	1.33	1.37
23	b	603	CLA	CHD-C4C	3.36	1.46	1.39
23	B	615	CLA	CHB-C1B	3.35	1.46	1.39
38	e	87	HEM	C1B-NB	-3.35	1.34	1.40
23	b	609	CLA	CHC-C4B	3.35	1.46	1.39
23	c	503	CLA	OBD-CAD	3.35	1.28	1.22
23	b	601	CLA	CHC-C4B	3.35	1.46	1.39
23	B	615	CLA	CHD-C4C	3.35	1.46	1.39
23	c	510	CLA	C1B-NB	-3.35	1.33	1.37
23	B	612	CLA	O2A-CGA	3.34	1.43	1.33
23	b	614	CLA	CHC-C4B	3.34	1.46	1.39
23	B	602	CLA	C1B-NB	-3.34	1.33	1.37
23	a	406	CLA	C1B-NB	-3.33	1.33	1.37
23	b	608	CLA	C4B-NB	-3.33	1.33	1.37
23	c	512	CLA	OBD-CAD	3.33	1.28	1.22
23	B	601	CLA	C1B-NB	-3.33	1.33	1.37
23	B	601	CLA	CHB-C1B	3.33	1.46	1.39
23	B	606	CLA	CHC-C4B	3.32	1.46	1.39
23	C	502	CLA	OBD-CAD	3.32	1.28	1.22
23	B	604	CLA	C3D-C2D	3.32	1.48	1.39
23	C	513	CLA	CHB-C1B	3.32	1.46	1.39
23	A	405	CLA	CHD-C4C	3.32	1.46	1.39
23	c	510	CLA	C4B-NB	-3.32	1.33	1.37
23	b	603	CLA	C4B-NB	-3.31	1.33	1.37
23	D	405	CLA	C1D-ND	3.31	1.42	1.37
23	a	407	CLA	CHB-C1B	3.30	1.46	1.39
23	b	616	CLA	CHB-C1B	3.30	1.46	1.39
23	a	407	CLA	C1B-NB	-3.29	1.33	1.37
23	b	602	CLA	CHB-C1B	3.29	1.46	1.39
23	C	506	CLA	C3D-C2D	3.29	1.48	1.39
23	B	603	CLA	CHB-C1B	3.29	1.46	1.39
23	C	508	CLA	OBD-CAD	3.29	1.28	1.22
23	c	502	CLA	OBD-CAD	3.29	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	514	CLA	OBD-CAD	3.29	1.28	1.22
23	b	616	CLA	C1B-NB	-3.28	1.33	1.37
23	C	508	CLA	CHB-C1B	3.28	1.46	1.39
23	B	614	CLA	CHD-C1D	3.28	1.44	1.38
23	C	510	CLA	CHC-C4B	3.28	1.46	1.39
23	b	604	CLA	OBD-CAD	3.27	1.28	1.22
23	a	405	CLA	C4B-NB	-3.25	1.33	1.37
23	b	608	CLA	C1B-NB	-3.25	1.33	1.37
23	c	513	CLA	C1B-NB	-3.25	1.33	1.37
23	B	615	CLA	CHC-C4B	3.25	1.46	1.39
23	b	606	CLA	OBD-CAD	3.25	1.28	1.22
23	d	402	CLA	C1D-ND	3.24	1.42	1.37
23	C	508	CLA	C1B-NB	-3.24	1.33	1.37
23	D	405	CLA	CHB-C1B	3.23	1.46	1.39
38	e	87	HEM	C4D-ND	-3.23	1.34	1.40
23	c	513	CLA	CHB-C1B	3.23	1.46	1.39
23	A	404	CLA	CHB-C1B	3.22	1.46	1.39
24	a	408	PHO	O2A-CGA	3.22	1.42	1.33
23	b	601	CLA	C1B-NB	-3.22	1.33	1.37
23	c	506	CLA	OBD-CAD	3.21	1.28	1.22
23	c	508	CLA	CHB-C1B	3.21	1.46	1.39
23	A	408	CLA	C1B-NB	-3.21	1.33	1.37
23	A	404	CLA	O2A-CGA	3.20	1.42	1.33
23	C	513	CLA	C1B-NB	-3.20	1.33	1.37
23	B	602	CLA	CHB-C1B	3.18	1.46	1.39
40	v	202	HEC	C1B-NB	-3.18	1.33	1.39
23	b	604	CLA	C1B-NB	-3.18	1.33	1.37
23	b	615	CLA	CHB-C1B	3.18	1.46	1.39
23	B	607	CLA	C4B-NB	-3.17	1.33	1.37
23	C	512	CLA	CHC-C4B	3.17	1.46	1.39
23	b	607	CLA	C1B-C2B	3.17	1.50	1.43
23	C	509	CLA	CHC-C4B	3.16	1.46	1.39
23	B	606	CLA	C1B-NB	-3.16	1.33	1.37
23	D	405	CLA	C1B-NB	-3.16	1.33	1.37
23	B	611	CLA	CHC-C4B	3.16	1.46	1.39
23	C	505	CLA	OBD-CAD	3.16	1.27	1.22
23	A	406	CLA	C1B-NB	-3.15	1.33	1.37
23	B	616	CLA	C1B-NB	-3.14	1.33	1.37
23	c	506	CLA	C4B-NB	-3.14	1.33	1.37
23	c	514	CLA	C1B-NB	-3.14	1.33	1.37
23	C	512	CLA	C4B-NB	-3.14	1.33	1.37
23	b	603	CLA	C1B-NB	-3.14	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	CHB-C1B	3.13	1.46	1.39
23	C	503	CLA	C4B-NB	-3.13	1.33	1.37
23	b	616	CLA	OBD-CAD	3.13	1.27	1.22
23	c	503	CLA	C1B-NB	-3.13	1.33	1.37
23	d	402	CLA	CHD-C4C	3.12	1.46	1.39
23	B	614	CLA	C1B-NB	-3.12	1.33	1.37
23	b	601	CLA	C4B-NB	-3.12	1.33	1.37
23	b	612	CLA	OBD-CAD	3.11	1.27	1.22
23	A	406	CLA	C4B-NB	-3.11	1.33	1.37
23	a	405	CLA	CHC-C4B	3.11	1.46	1.39
23	C	511	CLA	C4B-NB	-3.10	1.33	1.37
23	B	610	CLA	C4B-NB	-3.10	1.33	1.37
23	C	505	CLA	C1B-NB	-3.10	1.33	1.37
23	c	502	CLA	C4B-NB	-3.08	1.33	1.37
23	b	614	CLA	C1B-NB	-3.07	1.33	1.37
23	b	604	CLA	C1B-C2B	3.07	1.50	1.43
23	b	611	CLA	OBD-CAD	3.07	1.27	1.22
23	b	607	CLA	OBD-CAD	3.07	1.27	1.22
34	c	522	HTG	C1'-S1	-3.07	1.77	1.81
40	v	202	HEC	C4D-ND	-3.07	1.33	1.39
23	c	512	CLA	C1B-NB	-3.06	1.33	1.37
23	C	504	CLA	C1B-NB	-3.06	1.33	1.37
23	B	612	CLA	OBD-CAD	3.05	1.27	1.22
23	D	405	CLA	CHC-C4B	3.05	1.46	1.39
23	B	612	CLA	CHD-C4C	3.05	1.46	1.39
23	c	508	CLA	C1B-NB	-3.04	1.33	1.37
23	C	507	CLA	OBD-CAD	3.04	1.27	1.22
23	B	601	CLA	C4B-NB	-3.03	1.33	1.37
23	C	506	CLA	C1B-C2B	3.03	1.50	1.43
23	C	503	CLA	C1B-NB	-3.03	1.33	1.37
23	c	511	CLA	C1B-NB	-3.02	1.33	1.37
23	d	402	CLA	C4B-NB	-3.02	1.33	1.37
23	c	509	CLA	C4B-NB	-3.01	1.33	1.37
40	v	202	HEC	C1D-ND	-3.01	1.33	1.39
23	B	606	CLA	OBD-CAD	3.01	1.27	1.22
23	B	608	CLA	OBD-CAD	3.01	1.27	1.22
23	c	505	CLA	C1B-NB	-3.00	1.33	1.37
23	C	506	CLA	OBD-CAD	2.99	1.27	1.22
23	b	607	CLA	CHC-C4B	2.99	1.46	1.39
23	B	612	CLA	C4B-NB	-2.98	1.33	1.37
23	b	609	CLA	C1B-NB	-2.98	1.33	1.37
24	A	353	PHO	CHA-CBD	-2.98	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	C4B-NB	-2.97	1.34	1.37
23	C	505	CLA	C4B-NB	-2.96	1.34	1.37
24	a	353	PHO	C3A-C2A	-2.96	1.52	1.54
23	b	614	CLA	OBD-CAD	2.95	1.27	1.22
23	c	504	CLA	C1B-NB	-2.94	1.34	1.37
23	b	605	CLA	C4B-NB	-2.94	1.34	1.37
34	B	626	HTG	C1'-S1	-2.94	1.77	1.81
23	c	514	CLA	C4B-NB	-2.94	1.34	1.37
23	a	409	CLA	C1B-C2B	2.94	1.50	1.43
23	b	614	CLA	C1B-C2B	2.94	1.50	1.43
23	B	602	CLA	C1C-C2C	2.94	1.50	1.44
40	V	202	HEC	C1B-NB	-2.93	1.34	1.39
38	E	103	HEM	C4D-ND	-2.93	1.35	1.40
23	b	610	CLA	C4B-NB	-2.93	1.34	1.37
23	B	604	CLA	C1B-C2B	2.93	1.50	1.43
38	E	103	HEM	C1B-NB	-2.92	1.35	1.40
29	a	416	PL9	C6-C5	2.92	1.49	1.35
34	B	623	HTG	C1'-S1	-2.92	1.77	1.81
23	c	512	CLA	C4B-NB	-2.91	1.34	1.37
23	C	504	CLA	C4B-NB	-2.91	1.34	1.37
23	B	614	CLA	OBD-CAD	2.91	1.27	1.22
23	A	404	CLA	C4B-NB	-2.90	1.34	1.37
23	B	603	CLA	OBD-CAD	2.90	1.27	1.22
23	b	603	CLA	C1C-C2C	2.90	1.50	1.44
23	B	616	CLA	C1B-C2B	2.90	1.49	1.43
23	C	507	CLA	C4B-NB	-2.89	1.34	1.37
23	c	508	CLA	C4B-NB	-2.89	1.34	1.37
23	c	509	CLA	C1B-NB	-2.89	1.34	1.37
23	B	607	CLA	C4D-CHA	2.89	1.48	1.38
29	A	414	PL9	C6-C5	2.89	1.49	1.35
23	b	601	CLA	C1B-C2B	2.88	1.49	1.43
34	b	625	HTG	C1'-S1	-2.88	1.77	1.81
34	D	414	HTG	C1'-S1	-2.88	1.77	1.81
23	C	509	CLA	C1B-C2B	2.87	1.49	1.43
24	A	407	PHO	C4B-NB	-2.87	1.33	1.38
23	d	403	CLA	C3B-C4B	2.87	1.51	1.42
23	c	504	CLA	C4C-C3C	2.87	1.49	1.45
23	b	611	CLA	C1B-NB	-2.86	1.34	1.37
23	c	504	CLA	C4B-NB	-2.86	1.34	1.37
23	a	409	CLA	OBD-CAD	2.85	1.27	1.22
34	C	522	HTG	C1'-S1	-2.85	1.77	1.81
23	d	403	CLA	C4B-NB	-2.84	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	353	PHO	C1B-NB	-2.84	1.33	1.38
24	A	353	PHO	C3A-C2A	-2.84	1.52	1.54
23	b	604	CLA	C4B-NB	-2.84	1.34	1.37
38	E	103	HEM	C1C-C2C	-2.84	1.39	1.45
23	C	514	CLA	C4B-NB	-2.84	1.34	1.37
23	c	502	CLA	C1B-NB	-2.84	1.34	1.37
23	B	605	CLA	OBD-CAD	2.84	1.27	1.22
23	a	407	CLA	C4B-NB	-2.84	1.34	1.37
23	C	510	CLA	C1B-C2B	2.83	1.49	1.43
23	B	608	CLA	CHC-C4B	2.83	1.45	1.39
23	B	606	CLA	C1B-C2B	2.83	1.49	1.43
23	C	502	CLA	C1B-NB	-2.82	1.34	1.37
23	b	614	CLA	C4B-NB	-2.82	1.34	1.37
23	B	615	CLA	C1B-C2B	2.82	1.49	1.43
23	B	604	CLA	C4D-CHA	2.82	1.48	1.38
23	C	506	CLA	C3D-C4D	-2.82	1.37	1.44
23	c	512	CLA	C1B-C2B	2.81	1.49	1.43
23	c	511	CLA	C4B-NB	-2.81	1.34	1.37
23	c	508	CLA	C4D-CHA	2.81	1.48	1.38
23	B	610	CLA	C1B-NB	-2.80	1.34	1.37
23	C	512	CLA	C1B-C2B	2.80	1.49	1.43
23	b	607	CLA	C4B-NB	-2.80	1.34	1.37
23	b	606	CLA	C3B-C4B	2.80	1.50	1.42
40	V	202	HEC	C4D-ND	-2.79	1.34	1.39
23	c	506	CLA	C1B-NB	-2.79	1.34	1.37
23	C	507	CLA	C4D-CHA	2.79	1.48	1.38
24	a	408	PHO	C4B-NB	-2.79	1.33	1.38
23	C	514	CLA	C1B-NB	-2.79	1.34	1.37
23	b	613	CLA	C4D-CHA	2.79	1.48	1.38
23	B	603	CLA	C4B-NB	-2.79	1.34	1.37
23	D	406	CLA	C1C-C2C	2.79	1.50	1.44
23	c	512	CLA	C4D-CHA	2.79	1.47	1.38
23	a	407	CLA	CHC-C4B	2.78	1.45	1.39
23	C	508	CLA	C4D-CHA	2.78	1.47	1.38
23	c	505	CLA	C1B-C2B	2.78	1.49	1.43
23	B	615	CLA	C1B-NB	-2.78	1.34	1.37
23	D	405	CLA	OBD-CAD	2.78	1.27	1.22
24	a	353	PHO	C4B-NB	-2.78	1.33	1.38
23	c	503	CLA	C1B-C2B	2.78	1.49	1.43
23	c	510	CLA	C1B-C2B	2.78	1.49	1.43
23	c	510	CLA	C4D-CHA	2.77	1.47	1.38
23	C	506	CLA	C4B-NB	-2.77	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C4D-CHA	2.77	1.47	1.38
23	b	615	CLA	C1B-C2B	2.77	1.49	1.43
23	c	503	CLA	C4B-NB	-2.77	1.34	1.37
23	c	507	CLA	C4B-NB	-2.77	1.34	1.37
38	e	87	HEM	C1C-C2C	-2.76	1.39	1.45
23	a	405	CLA	C1B-C2B	2.76	1.49	1.43
23	b	613	CLA	OBD-CAD	2.76	1.27	1.22
23	C	508	CLA	C1C-C2C	2.75	1.50	1.44
23	C	510	CLA	C1B-NB	-2.75	1.34	1.37
23	C	504	CLA	C4D-CHA	2.75	1.47	1.38
23	C	505	CLA	C3D-C4D	-2.74	1.38	1.44
23	C	505	CLA	C1B-C2B	2.74	1.49	1.43
23	C	511	CLA	C3D-C4D	-2.74	1.38	1.44
23	C	512	CLA	C1C-C2C	2.74	1.50	1.44
23	B	605	CLA	C1B-C2B	2.74	1.49	1.43
23	A	405	CLA	C1C-C2C	2.74	1.50	1.44
23	b	610	CLA	C3D-C4D	-2.74	1.38	1.44
23	C	510	CLA	C4D-CHA	2.73	1.47	1.38
23	C	509	CLA	C1B-NB	-2.73	1.34	1.37
23	C	504	CLA	C4C-C3C	2.73	1.49	1.45
23	B	605	CLA	C1B-NB	-2.73	1.34	1.37
23	B	604	CLA	OBD-CAD	2.73	1.27	1.22
23	d	402	CLA	C3D-C4D	-2.73	1.38	1.44
23	a	409	CLA	C4B-NB	-2.73	1.34	1.37
23	c	505	CLA	C1C-C2C	2.72	1.50	1.44
23	A	405	CLA	C4D-CHA	2.72	1.47	1.38
23	B	604	CLA	C4B-NB	-2.72	1.34	1.37
23	c	504	CLA	C4D-CHA	2.72	1.47	1.38
23	B	604	CLA	C3D-C4D	-2.72	1.38	1.44
23	b	604	CLA	C4D-CHA	2.71	1.47	1.38
23	c	507	CLA	C4D-CHA	2.71	1.47	1.38
23	b	606	CLA	C1B-C2B	2.71	1.49	1.43
23	C	511	CLA	C4D-CHA	2.70	1.47	1.38
23	B	601	CLA	C1B-C2B	2.70	1.49	1.43
23	b	608	CLA	C4D-CHA	2.70	1.47	1.38
23	B	608	CLA	C1B-C2B	2.70	1.49	1.43
23	C	503	CLA	C1B-C2B	2.70	1.49	1.43
23	b	616	CLA	C4D-CHA	2.70	1.47	1.38
23	c	513	CLA	C4D-CHA	2.70	1.47	1.38
40	v	202	HEC	C4B-NB	-2.70	1.34	1.39
23	b	602	CLA	C3B-C4B	2.70	1.50	1.42
23	B	613	CLA	C4C-C3C	2.70	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C1B-NB	-2.69	1.34	1.37
23	b	602	CLA	C1B-NB	-2.69	1.34	1.37
23	b	610	CLA	C4D-CHA	2.69	1.47	1.38
23	b	603	CLA	C1B-C2B	2.69	1.49	1.43
24	A	353	PHO	C4B-NB	-2.69	1.33	1.38
23	c	511	CLA	C1B-C2B	2.68	1.49	1.43
23	b	601	CLA	C4D-CHA	2.68	1.47	1.38
23	b	611	CLA	C1B-C2B	2.68	1.49	1.43
23	c	502	CLA	C4D-CHA	2.68	1.47	1.38
23	B	616	CLA	C4D-CHA	2.68	1.47	1.38
23	C	511	CLA	C1B-C2B	2.68	1.49	1.43
23	b	607	CLA	C4D-CHA	2.68	1.47	1.38
23	b	609	CLA	C4D-CHA	2.67	1.47	1.38
23	B	613	CLA	C4D-CHA	2.66	1.47	1.38
23	D	406	CLA	C1B-C2B	2.66	1.49	1.43
23	C	502	CLA	C4D-CHA	2.66	1.47	1.38
23	B	608	CLA	C4D-CHA	2.66	1.47	1.38
23	C	514	CLA	C1C-C2C	2.65	1.49	1.44
23	A	406	CLA	C3D-C4D	-2.65	1.38	1.44
23	b	602	CLA	C1C-C2C	2.65	1.49	1.44
23	c	506	CLA	C4D-CHA	2.65	1.47	1.38
23	B	601	CLA	C4D-CHA	2.65	1.47	1.38
23	a	409	CLA	C4D-CHA	2.65	1.47	1.38
23	b	612	CLA	C4D-CHA	2.65	1.47	1.38
23	D	405	CLA	C4B-NB	-2.65	1.34	1.37
23	a	405	CLA	C3D-C4D	-2.64	1.38	1.44
23	C	513	CLA	C4D-CHA	2.64	1.47	1.38
23	D	405	CLA	C4D-CHA	2.64	1.47	1.38
23	b	615	CLA	C4D-CHA	2.63	1.47	1.38
23	B	606	CLA	C4D-CHA	2.63	1.47	1.38
23	c	506	CLA	C1C-C2C	2.63	1.49	1.44
23	b	616	CLA	C3D-C4D	-2.63	1.38	1.44
33	Z	101	LMG	O8-C28	2.63	1.46	1.33
23	a	407	CLA	C4D-CHA	2.63	1.47	1.38
23	A	406	CLA	C1B-C2B	2.62	1.49	1.43
23	B	603	CLA	C1B-C2B	2.62	1.49	1.43
23	c	509	CLA	C4D-CHA	2.62	1.47	1.38
23	B	612	CLA	C3B-C2B	2.62	1.50	1.41
23	b	613	CLA	C1B-C2B	2.61	1.49	1.43
29	D	408	PL9	C6-C5	2.61	1.48	1.35
23	b	608	CLA	C3D-C4D	-2.61	1.38	1.44
23	C	502	CLA	C1C-C2C	2.61	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	V	202	HEC	C1D-ND	-2.61	1.34	1.39
23	C	506	CLA	C1C-C2C	2.60	1.49	1.44
32	A	359	LMT	O1'-C1'	2.60	1.44	1.40
23	b	603	CLA	C4C-C3C	2.60	1.49	1.45
23	C	505	CLA	C4D-CHA	2.60	1.47	1.38
29	d	405	PL9	C6-C5	2.60	1.48	1.35
23	a	406	CLA	C4D-CHA	2.60	1.47	1.38
23	D	405	CLA	C1C-C2C	2.60	1.49	1.44
23	c	514	CLA	C1C-C2C	2.60	1.49	1.44
23	C	507	CLA	C4C-C3C	2.60	1.49	1.45
23	D	405	CLA	C3D-C4D	-2.60	1.38	1.44
23	B	612	CLA	C4D-CHA	2.60	1.47	1.38
23	c	511	CLA	C4D-CHA	2.60	1.47	1.38
23	B	611	CLA	C1B-C2B	2.59	1.49	1.43
23	c	513	CLA	C4B-NB	-2.59	1.34	1.37
23	c	509	CLA	C1C-C2C	2.59	1.49	1.44
23	c	502	CLA	C4C-C3C	2.59	1.49	1.45
23	c	508	CLA	C1B-C2B	2.59	1.49	1.43
23	B	614	CLA	C4D-CHA	2.59	1.47	1.38
23	c	504	CLA	C1B-C2B	2.59	1.49	1.43
23	B	601	CLA	C3B-C4B	2.58	1.50	1.42
23	C	505	CLA	C4C-C3C	2.58	1.49	1.45
23	a	406	CLA	C4B-NB	-2.58	1.34	1.37
23	B	610	CLA	C4D-CHA	2.58	1.47	1.38
23	A	405	CLA	C4B-NB	-2.57	1.34	1.37
23	d	402	CLA	C4D-CHA	2.57	1.47	1.38
23	d	403	CLA	C1B-NB	-2.57	1.34	1.37
23	A	408	CLA	C4D-CHA	2.56	1.47	1.38
23	a	405	CLA	C4D-CHA	2.56	1.47	1.38
23	B	605	CLA	C4D-CHA	2.56	1.47	1.38
23	c	505	CLA	C4C-C3C	2.56	1.49	1.45
23	c	506	CLA	C1B-C2B	2.56	1.49	1.43
23	A	404	CLA	C4C-C3C	2.56	1.49	1.45
23	C	502	CLA	C1B-C2B	2.56	1.49	1.43
23	A	404	CLA	C1B-C2B	2.55	1.49	1.43
23	B	602	CLA	C3B-C4B	2.55	1.50	1.42
23	B	616	CLA	C3D-C4D	-2.55	1.38	1.44
23	b	607	CLA	C4C-C3C	2.55	1.49	1.45
23	B	614	CLA	C1C-C2C	2.55	1.49	1.44
23	b	605	CLA	C1B-C2B	2.55	1.49	1.43
23	B	603	CLA	C4D-CHA	2.55	1.47	1.38
38	E	103	HEM	C3C-C4C	-2.54	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	C4D-CHA	2.54	1.47	1.38
23	A	404	CLA	C4D-CHA	2.54	1.47	1.38
23	A	405	CLA	C1B-C2B	2.54	1.49	1.43
23	B	607	CLA	C4C-C3C	2.54	1.49	1.45
23	b	611	CLA	C4D-CHA	2.54	1.47	1.38
23	b	612	CLA	C1B-C2B	2.54	1.49	1.43
23	B	607	CLA	C1C-C2C	2.54	1.49	1.44
23	C	502	CLA	C3D-C4D	-2.54	1.38	1.44
23	D	405	CLA	C3B-C2B	2.54	1.49	1.41
23	C	510	CLA	C4C-C3C	2.54	1.49	1.45
23	a	406	CLA	C1B-C2B	2.53	1.49	1.43
23	C	513	CLA	C1C-C2C	2.53	1.49	1.44
23	D	406	CLA	C3B-C4B	2.53	1.50	1.42
23	b	602	CLA	C4D-CHA	2.53	1.47	1.38
35	c	519	DGD	O2G-C2G	-2.53	1.40	1.46
23	A	406	CLA	C4C-C3C	2.53	1.49	1.45
23	B	614	CLA	C3D-C4D	-2.53	1.38	1.44
23	b	609	CLA	C1B-C2B	2.53	1.49	1.43
23	B	602	CLA	C4D-CHA	2.53	1.47	1.38
23	B	605	CLA	C4B-NB	-2.53	1.34	1.37
23	b	616	CLA	C3B-C4B	2.52	1.50	1.42
23	c	514	CLA	C1B-C2B	2.51	1.49	1.43
23	B	607	CLA	C3D-C4D	-2.51	1.38	1.44
23	B	613	CLA	C1C-C2C	2.51	1.49	1.44
23	d	403	CLA	C1B-C2B	2.51	1.49	1.43
23	C	507	CLA	C3D-C4D	-2.51	1.38	1.44
23	b	603	CLA	C3D-C4D	-2.51	1.38	1.44
23	c	502	CLA	C3D-C4D	-2.51	1.38	1.44
23	C	503	CLA	C4D-CHA	2.50	1.47	1.38
23	b	603	CLA	C4D-CHA	2.50	1.47	1.38
23	c	506	CLA	C3D-C4D	-2.50	1.38	1.44
23	C	509	CLA	C4D-CHA	2.50	1.47	1.38
23	B	603	CLA	C1C-C2C	2.50	1.49	1.44
23	B	615	CLA	C1C-C2C	2.50	1.49	1.44
23	C	514	CLA	C1B-C2B	2.50	1.49	1.43
34	B	626	HTG	C1-S1	-2.49	1.76	1.80
23	c	502	CLA	C1B-C2B	2.49	1.49	1.43
23	C	509	CLA	C4C-C3C	2.49	1.49	1.45
23	C	503	CLA	C3D-C4D	-2.49	1.38	1.44
23	b	606	CLA	C3D-C4D	-2.49	1.38	1.44
23	b	606	CLA	C4D-CHA	2.49	1.46	1.38
23	C	512	CLA	C4C-C3C	2.49	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C3B-C2B	2.49	1.49	1.41
23	c	505	CLA	C4D-CHA	2.48	1.46	1.38
23	C	514	CLA	C4D-CHA	2.48	1.46	1.38
23	D	406	CLA	C4B-NB	-2.48	1.34	1.37
23	B	609	CLA	C4D-CHA	2.48	1.46	1.38
23	B	615	CLA	C4B-NB	-2.48	1.34	1.37
23	B	605	CLA	C1C-C2C	2.48	1.49	1.44
23	c	510	CLA	C1C-C2C	2.48	1.49	1.44
23	B	605	CLA	C3B-C4B	2.48	1.49	1.42
23	C	508	CLA	C1B-C2B	2.48	1.48	1.43
23	B	612	CLA	C1B-C2B	2.48	1.48	1.43
23	B	612	CLA	C1C-C2C	2.47	1.49	1.44
23	b	607	CLA	C1C-C2C	2.47	1.49	1.44
23	a	405	CLA	C4C-C3C	2.47	1.49	1.45
23	b	615	CLA	C4C-C3C	2.47	1.49	1.45
23	B	610	CLA	C3D-C4D	-2.47	1.38	1.44
23	C	506	CLA	C4D-CHA	2.46	1.46	1.38
23	c	504	CLA	C1C-C2C	2.46	1.49	1.44
23	b	609	CLA	C4B-NB	-2.46	1.34	1.37
23	B	608	CLA	C3D-C4D	-2.46	1.38	1.44
23	b	614	CLA	C4D-CHA	2.46	1.46	1.38
23	C	504	CLA	C1B-C2B	2.46	1.48	1.43
23	c	513	CLA	C1B-C2B	2.46	1.48	1.43
23	c	514	CLA	C3B-C4B	2.45	1.49	1.42
23	C	509	CLA	C3D-C4D	-2.45	1.38	1.44
35	C	519	DGD	O2G-C2G	-2.45	1.40	1.46
23	B	603	CLA	C3B-C2B	2.45	1.49	1.41
23	B	616	CLA	C1C-NC	-2.45	1.34	1.37
23	c	513	CLA	C1C-C2C	2.45	1.49	1.44
23	d	402	CLA	C1C-C2C	2.45	1.49	1.44
23	c	514	CLA	C4D-CHA	2.45	1.46	1.38
23	B	611	CLA	C4D-CHA	2.44	1.46	1.38
23	b	612	CLA	C3B-C2B	2.44	1.49	1.41
23	b	615	CLA	C4B-NB	-2.44	1.34	1.37
24	A	407	PHO	CHA-CBD	-2.44	1.48	1.51
23	B	607	CLA	C1B-C2B	2.44	1.48	1.43
23	b	603	CLA	C3B-C2B	2.44	1.49	1.41
23	C	513	CLA	C1B-C2B	2.44	1.48	1.43
23	c	514	CLA	C3D-C4D	-2.44	1.38	1.44
23	C	502	CLA	C3B-C4B	2.44	1.49	1.42
23	A	405	CLA	C3B-C4B	2.44	1.49	1.42
23	a	407	CLA	C3D-C4D	-2.43	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C3B-C4B	2.43	1.49	1.42
23	c	507	CLA	C1B-C2B	2.43	1.48	1.43
23	b	613	CLA	C3B-C2B	2.43	1.49	1.41
40	V	202	HEC	C4B-NB	-2.43	1.35	1.39
23	B	614	CLA	C1B-C2B	2.43	1.48	1.43
23	B	609	CLA	C3B-C4B	2.43	1.49	1.42
23	c	509	CLA	C3B-C2B	2.42	1.49	1.41
23	B	608	CLA	C1C-NC	-2.42	1.34	1.37
23	C	504	CLA	C3B-C4B	2.42	1.49	1.42
23	b	610	CLA	C1B-C2B	2.42	1.48	1.43
23	C	514	CLA	C3B-C4B	2.42	1.49	1.42
23	b	605	CLA	C4D-CHA	2.42	1.46	1.38
23	a	409	CLA	C1C-C2C	2.42	1.49	1.44
23	c	510	CLA	C3B-C4B	2.42	1.49	1.42
23	b	606	CLA	C1C-C2C	2.41	1.49	1.44
23	A	405	CLA	C3D-C4D	-2.41	1.38	1.44
23	c	511	CLA	C1C-C2C	2.41	1.49	1.44
23	b	609	CLA	C4C-C3C	2.41	1.49	1.45
23	d	402	CLA	C1B-C2B	2.41	1.48	1.43
23	c	503	CLA	C1C-C2C	2.41	1.49	1.44
23	C	508	CLA	C3D-C4D	-2.41	1.38	1.44
23	B	606	CLA	C3D-C4D	-2.41	1.38	1.44
23	C	505	CLA	C1C-C2C	2.41	1.49	1.44
23	b	609	CLA	C1C-C2C	2.41	1.49	1.44
23	C	513	CLA	C4B-NB	-2.41	1.34	1.37
23	b	606	CLA	C4B-NB	-2.41	1.34	1.37
23	c	509	CLA	C1B-C2B	2.40	1.48	1.43
23	c	511	CLA	C3D-C4D	-2.40	1.38	1.44
23	d	403	CLA	C4D-CHA	2.40	1.46	1.38
23	B	605	CLA	C3D-C4D	-2.40	1.38	1.44
38	e	87	HEM	C1D-ND	-2.40	1.34	1.38
23	D	405	CLA	C1B-C2B	2.40	1.48	1.43
23	D	406	CLA	C4D-CHA	2.39	1.46	1.38
23	c	508	CLA	C1C-C2C	2.39	1.49	1.44
23	b	602	CLA	C1B-C2B	2.39	1.48	1.43
23	a	407	CLA	C1B-C2B	2.39	1.48	1.43
23	B	615	CLA	C3B-C4B	2.39	1.49	1.42
37	D	410	LHG	O7-C5	-2.39	1.41	1.46
23	B	610	CLA	C1B-C2B	2.39	1.48	1.43
23	B	602	CLA	C3D-C4D	-2.39	1.38	1.44
23	B	604	CLA	C1C-C2C	2.39	1.49	1.44
23	B	613	CLA	C3B-C2B	2.39	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	C1C-C2C	2.39	1.49	1.44
23	C	502	CLA	C4B-NB	-2.39	1.34	1.37
23	c	505	CLA	C3B-C2B	2.38	1.49	1.41
23	b	616	CLA	C1C-C2C	2.38	1.49	1.44
23	c	504	CLA	C3B-C4B	2.38	1.49	1.42
23	B	616	CLA	C1C-C2C	2.38	1.49	1.44
23	A	406	CLA	C3B-C4B	2.38	1.49	1.42
23	b	614	CLA	C4C-C3C	2.38	1.49	1.45
23	C	504	CLA	C1C-C2C	2.37	1.49	1.44
23	B	609	CLA	C1C-C2C	2.37	1.49	1.44
23	c	513	CLA	C3B-C4B	2.37	1.49	1.42
23	C	513	CLA	C3B-C4B	2.37	1.49	1.42
23	c	510	CLA	C3D-C4D	-2.37	1.38	1.44
23	C	508	CLA	C4B-NB	-2.36	1.34	1.37
23	C	510	CLA	C1C-C2C	2.36	1.49	1.44
32	a	414	LMT	O1'-C1'	2.36	1.44	1.40
23	c	502	CLA	C3B-C4B	2.36	1.49	1.42
23	a	407	CLA	C3B-C4B	2.36	1.49	1.42
23	B	601	CLA	C1C-C2C	2.35	1.49	1.44
23	B	610	CLA	C3B-C4B	2.35	1.49	1.42
23	a	409	CLA	C3B-C4B	2.35	1.49	1.42
23	b	601	CLA	C3B-C4B	2.35	1.49	1.42
23	d	403	CLA	C3D-C4D	-2.35	1.38	1.44
23	B	610	CLA	C4C-C3C	2.35	1.49	1.45
23	C	510	CLA	C3B-C2B	2.35	1.49	1.41
23	C	503	CLA	C3B-C4B	2.34	1.49	1.42
23	A	408	CLA	C1B-C2B	2.34	1.48	1.43
23	B	602	CLA	C4C-C3C	2.34	1.49	1.45
25	B	619	BCR	C30-C25	-2.34	1.50	1.53
37	d	407	LHG	O7-C5	-2.34	1.41	1.46
23	c	507	CLA	C3D-C4D	-2.34	1.38	1.44
23	A	406	CLA	C1C-C2C	2.34	1.49	1.44
23	B	609	CLA	C1B-C2B	2.34	1.48	1.43
23	c	503	CLA	C3D-C4D	-2.34	1.38	1.44
23	b	611	CLA	C3B-C2B	2.33	1.49	1.41
23	a	406	CLA	C3B-C4B	2.33	1.49	1.42
23	b	609	CLA	C3D-C4D	-2.33	1.38	1.44
23	b	610	CLA	C1C-C2C	2.33	1.49	1.44
23	B	615	CLA	C4D-CHA	2.33	1.46	1.38
23	a	405	CLA	C3B-C2B	2.33	1.49	1.41
23	c	509	CLA	C3B-C4B	2.32	1.49	1.42
37	L	101	LHG	O7-C5	-2.32	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	C3D-C4D	-2.32	1.39	1.44
23	B	615	CLA	C3D-C4D	-2.32	1.39	1.44
23	C	509	CLA	C1C-C2C	2.32	1.49	1.44
23	D	405	CLA	C4C-C3C	2.32	1.49	1.45
23	A	408	CLA	C1C-NC	-2.32	1.34	1.37
23	A	406	CLA	C4D-CHA	2.32	1.46	1.38
23	B	611	CLA	C3D-C4D	-2.32	1.39	1.44
23	C	504	CLA	C3D-C4D	-2.32	1.39	1.44
23	b	612	CLA	C3D-C4D	-2.32	1.39	1.44
23	C	502	CLA	C4C-C3C	2.32	1.49	1.45
24	a	408	PHO	C1D-ND	-2.31	1.34	1.38
23	b	602	CLA	C4C-C3C	2.31	1.49	1.45
23	C	509	CLA	C3B-C2B	2.31	1.49	1.41
23	C	512	CLA	C3D-C4D	-2.31	1.39	1.44
23	C	508	CLA	C3B-C4B	2.31	1.49	1.42
23	A	404	CLA	C3B-C2B	2.31	1.49	1.41
23	b	602	CLA	C3D-C4D	-2.31	1.39	1.44
23	c	514	CLA	C4C-C3C	2.31	1.49	1.45
37	D	409	LHG	O7-C5	-2.31	1.41	1.46
23	c	503	CLA	C3B-C2B	2.31	1.48	1.41
23	a	409	CLA	C3D-C4D	-2.30	1.39	1.44
23	B	609	CLA	C3D-C4D	-2.30	1.39	1.44
23	b	616	CLA	C4B-NB	-2.30	1.34	1.37
23	b	610	CLA	C3B-C2B	2.30	1.48	1.41
23	c	504	CLA	C3D-C4D	-2.29	1.39	1.44
23	A	404	CLA	C3D-C4D	-2.29	1.39	1.44
23	c	506	CLA	C3B-C4B	2.29	1.49	1.42
23	B	601	CLA	C3D-C4D	-2.29	1.39	1.44
23	b	613	CLA	C1C-C2C	2.28	1.49	1.44
23	c	512	CLA	C1C-C2C	2.28	1.49	1.44
23	c	509	CLA	C3D-C4D	-2.28	1.39	1.44
23	b	604	CLA	C3B-C2B	2.28	1.48	1.41
23	b	611	CLA	C4B-NB	-2.28	1.34	1.37
23	B	611	CLA	C1C-C2C	2.28	1.49	1.44
23	d	403	CLA	C1C-C2C	2.27	1.49	1.44
23	b	608	CLA	C4C-C3C	2.27	1.48	1.45
23	B	606	CLA	C3B-C4B	2.27	1.49	1.42
23	b	612	CLA	C3B-C4B	2.27	1.49	1.42
23	b	616	CLA	C1B-C2B	2.27	1.48	1.43
23	c	507	CLA	C4C-C3C	2.27	1.48	1.45
23	b	608	CLA	C3B-C2B	2.26	1.48	1.41
23	b	602	CLA	C4B-NB	-2.26	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	C1C-NC	-2.26	1.34	1.37
23	B	603	CLA	C3D-C4D	-2.26	1.39	1.44
23	c	510	CLA	C3B-C2B	2.26	1.48	1.41
23	b	612	CLA	C1C-C2C	2.25	1.49	1.44
23	C	505	CLA	C3B-C2B	2.25	1.48	1.41
23	B	603	CLA	C3B-C4B	2.25	1.49	1.42
23	b	615	CLA	C3B-C4B	2.25	1.49	1.42
23	c	502	CLA	C1C-C2C	2.25	1.49	1.44
23	b	614	CLA	C3B-C2B	2.25	1.48	1.41
23	B	608	CLA	C3B-C2B	2.25	1.48	1.41
23	d	402	CLA	C4C-C3C	2.25	1.48	1.45
23	A	408	CLA	C1C-C2C	2.24	1.49	1.44
24	A	353	PHO	C1D-ND	-2.24	1.34	1.38
23	b	608	CLA	C1B-C2B	2.24	1.48	1.43
23	c	513	CLA	C3D-C4D	-2.24	1.39	1.44
23	a	407	CLA	C4C-C3C	2.24	1.48	1.45
23	b	609	CLA	C3B-C4B	2.23	1.49	1.42
23	b	604	CLA	C1C-C2C	2.23	1.49	1.44
32	t	102	LMT	O1'-C1'	2.22	1.43	1.40
23	B	602	CLA	C4B-NB	-2.22	1.34	1.37
23	C	511	CLA	C1C-C2C	2.22	1.49	1.44
23	B	612	CLA	C4C-C3C	2.21	1.48	1.45
23	b	601	CLA	C3D-C4D	-2.21	1.39	1.44
23	C	509	CLA	C1C-NC	-2.21	1.34	1.37
23	D	406	CLA	C3D-C4D	-2.21	1.39	1.44
24	A	407	PHO	C1B-NB	-2.20	1.34	1.38
23	B	606	CLA	C1C-C2C	2.20	1.49	1.44
23	C	514	CLA	C3D-C4D	-2.20	1.39	1.44
23	b	612	CLA	C4C-C3C	2.20	1.48	1.45
23	c	502	CLA	C3B-C2B	2.20	1.48	1.41
23	c	505	CLA	C3D-C4D	-2.19	1.39	1.44
23	A	404	CLA	C1C-C2C	2.19	1.49	1.44
23	b	608	CLA	C3B-C4B	2.19	1.49	1.42
23	B	608	CLA	C1C-C2C	2.19	1.49	1.44
23	C	510	CLA	C3D-C4D	-2.19	1.39	1.44
23	b	610	CLA	C3B-C4B	2.18	1.49	1.42
23	B	614	CLA	C3B-C2B	2.18	1.48	1.41
23	b	601	CLA	C1D-C2D	2.18	1.49	1.45
23	B	611	CLA	C3B-C2B	2.18	1.48	1.41
23	c	511	CLA	C3B-C2B	2.18	1.48	1.41
23	B	610	CLA	C1C-C2C	2.18	1.48	1.44
23	b	601	CLA	C4C-C3C	2.18	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	C3B-C2B	2.18	1.48	1.41
23	c	506	CLA	C4C-C3C	2.18	1.48	1.45
23	b	607	CLA	C3D-C4D	-2.17	1.39	1.44
23	b	615	CLA	C3D-C4D	-2.17	1.39	1.44
23	c	512	CLA	C3D-C4D	-2.17	1.39	1.44
24	A	407	PHO	C3D-C4D	-2.17	1.38	1.41
23	C	510	CLA	C1C-NC	-2.17	1.34	1.37
23	C	513	CLA	C3D-C4D	-2.17	1.39	1.44
23	A	408	CLA	C3B-C2B	2.17	1.48	1.41
23	b	601	CLA	C3B-C2B	2.16	1.48	1.41
23	b	610	CLA	C4C-C3C	2.16	1.48	1.45
24	a	353	PHO	CHA-CBD	-2.16	1.49	1.51
40	v	202	HEC	C4A-C3A	-2.16	1.41	1.45
32	t	101	LMT	O1'-C1'	2.15	1.43	1.40
23	B	610	CLA	C3B-C2B	2.15	1.48	1.41
23	C	502	CLA	C3B-C2B	2.15	1.48	1.41
23	C	510	CLA	C3B-C4B	2.15	1.49	1.42
23	c	503	CLA	C4C-C3C	2.15	1.48	1.45
29	a	416	PL9	C2-C3	2.15	1.40	1.34
23	B	616	CLA	C3B-C2B	2.15	1.48	1.41
23	b	613	CLA	C3D-C4D	-2.14	1.39	1.44
23	d	403	CLA	C1D-C2D	2.14	1.49	1.45
35	H	102	DGD	O5D-C1E	2.14	1.43	1.40
23	B	614	CLA	C3B-C4B	2.14	1.49	1.42
32	I	101	LMT	O1'-C1'	2.14	1.43	1.40
23	C	511	CLA	C3B-C2B	2.13	1.48	1.41
33	Z	101	LMG	O1-C1	2.13	1.43	1.40
23	C	513	CLA	C3B-C2B	2.13	1.48	1.41
23	B	606	CLA	C3B-C2B	2.12	1.48	1.41
23	B	604	CLA	C3B-C2B	2.12	1.48	1.41
23	b	614	CLA	C1C-C2C	2.12	1.48	1.44
23	C	507	CLA	C3B-C2B	2.12	1.48	1.41
23	B	613	CLA	C1B-C2B	2.12	1.48	1.43
23	C	511	CLA	C3B-C4B	2.12	1.48	1.42
23	B	608	CLA	C4C-C3C	2.12	1.48	1.45
32	e	102	LMT	O1'-C1'	2.12	1.43	1.40
23	b	603	CLA	C3B-C4B	2.11	1.48	1.42
23	C	503	CLA	C4C-C3C	2.11	1.48	1.45
23	B	610	CLA	C1C-NC	-2.11	1.34	1.37
23	A	408	CLA	C3D-C4D	-2.11	1.39	1.44
23	B	602	CLA	C1B-C2B	2.11	1.48	1.43
23	B	601	CLA	C3B-C2B	2.11	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	C3B-C4B	2.10	1.48	1.42
23	b	606	CLA	C3B-C2B	2.10	1.48	1.41
23	c	508	CLA	C3D-C4D	-2.10	1.39	1.44
32	a	420	LMT	O1'-C1'	2.10	1.43	1.40
23	a	409	CLA	C4C-C3C	2.10	1.48	1.45
38	e	87	HEM	C3B-C4B	2.10	1.49	1.44
23	C	513	CLA	C4C-C3C	2.10	1.48	1.45
37	d	406	LHG	O7-C5	-2.09	1.41	1.46
23	a	406	CLA	C3D-C4D	-2.09	1.39	1.44
23	B	601	CLA	C1C-NC	-2.09	1.34	1.37
23	b	605	CLA	C1C-C2C	2.09	1.48	1.44
23	d	403	CLA	C3B-C2B	2.09	1.48	1.41
23	b	614	CLA	C3B-C4B	2.09	1.48	1.42
23	c	507	CLA	C3B-C4B	2.09	1.48	1.42
33	D	415	LMG	O7-C8	-2.09	1.41	1.46
23	a	405	CLA	C1C-C2C	2.09	1.48	1.44
23	B	604	CLA	CBD-CAD	-2.08	1.47	1.56
23	b	605	CLA	C3D-C4D	-2.08	1.39	1.44
23	c	514	CLA	C3B-C2B	2.08	1.48	1.41
23	C	507	CLA	C1B-C2B	2.08	1.48	1.43
23	b	604	CLA	C3D-C4D	-2.08	1.39	1.44
33	C	521	LMG	O1-C1	2.08	1.43	1.40
23	a	406	CLA	C1C-C2C	2.08	1.48	1.44
23	C	506	CLA	C3B-C4B	2.07	1.48	1.42
23	c	508	CLA	C3B-C2B	2.07	1.48	1.41
23	d	402	CLA	C3B-C2B	2.07	1.48	1.41
34	b	625	HTG	C1-S1	-2.07	1.77	1.80
23	C	506	CLA	C3B-C2B	2.07	1.48	1.41
38	E	103	HEM	C4B-NB	-2.07	1.34	1.38
23	A	408	CLA	C3B-C4B	2.07	1.48	1.42
32	b	627	LMT	O1'-C1'	2.07	1.43	1.40
23	b	601	CLA	C1C-NC	-2.07	1.34	1.37
29	A	414	PL9	C2-C3	2.06	1.39	1.34
23	B	608	CLA	C3B-C4B	2.06	1.48	1.42
23	b	601	CLA	C1C-C2C	2.06	1.48	1.44
23	B	607	CLA	C3B-C2B	2.06	1.48	1.41
23	c	513	CLA	C3B-C2B	2.06	1.48	1.41
34	D	414	HTG	C1-S1	-2.06	1.77	1.80
24	A	407	PHO	C1D-ND	-2.06	1.34	1.38
23	C	511	CLA	C4C-C3C	2.06	1.48	1.45
23	b	605	CLA	C1D-C2D	2.06	1.49	1.45
35	c	518	DGD	O3G-C1D	2.05	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	C3B-C2B	2.05	1.48	1.41
23	b	605	CLA	C3B-C2B	2.05	1.48	1.41
23	C	509	CLA	C3B-C4B	2.05	1.48	1.42
23	b	611	CLA	C1C-C2C	2.05	1.48	1.44
32	E	102	LMT	O1'-C1'	2.05	1.43	1.40
23	C	505	CLA	C3B-C4B	2.05	1.48	1.42
23	C	514	CLA	C3B-C2B	2.05	1.48	1.41
23	C	512	CLA	C3B-C4B	2.05	1.48	1.42
23	b	613	CLA	C4C-C3C	2.04	1.48	1.45
23	c	511	CLA	C3B-C4B	2.04	1.48	1.42
26	F	101	SQD	O6-C1	2.04	1.43	1.40
34	d	411	HTG	C1-S1	-2.04	1.77	1.80
23	B	613	CLA	C3D-C4D	-2.04	1.39	1.44
23	c	511	CLA	C4C-C3C	2.04	1.48	1.45
25	c	516	BCR	C1-C6	-2.04	1.51	1.53
23	B	605	CLA	C3B-C2B	2.04	1.48	1.41
23	a	407	CLA	C1C-C2C	2.03	1.48	1.44
23	C	514	CLA	C1D-C2D	2.03	1.49	1.45
23	B	601	CLA	C4C-C3C	2.03	1.48	1.45
23	c	514	CLA	C1D-C2D	2.03	1.49	1.45
23	B	612	CLA	C3D-C4D	-2.03	1.39	1.44
38	e	87	HEM	C4B-NB	-2.03	1.34	1.38
23	C	503	CLA	C1C-C2C	2.02	1.48	1.44
23	a	405	CLA	O2D-CED	-2.02	1.40	1.45
23	b	609	CLA	C3B-C2B	2.02	1.48	1.41
26	B	620	SQD	O6-C1	2.01	1.43	1.40
23	B	611	CLA	C4C-C3C	2.01	1.48	1.45
23	c	503	CLA	C3B-C4B	2.01	1.48	1.42
24	a	408	PHO	C1B-NB	-2.01	1.35	1.38
23	B	603	CLA	C4C-C3C	2.01	1.48	1.45
23	C	507	CLA	C3B-C4B	2.01	1.48	1.42
23	C	503	CLA	C3B-C2B	2.00	1.47	1.41
23	c	510	CLA	C4C-C3C	2.00	1.48	1.45
23	C	507	CLA	C1C-C2C	2.00	1.48	1.44

All (2970) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	353	PHO	C2D-C1D-ND	12.09	118.17	109.43
24	A	407	PHO	C2D-C1D-ND	11.39	117.66	109.43
24	a	408	PHO	C2D-C1D-ND	10.78	117.22	109.43
24	a	353	PHO	C2D-C1D-ND	10.55	117.06	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	CLA	C1D-ND-C4D	-10.52	98.93	106.31
23	b	605	CLA	C1D-ND-C4D	-10.50	98.95	106.31
23	B	614	CLA	C1D-ND-C4D	-10.47	98.97	106.31
23	C	502	CLA	C1D-ND-C4D	-10.18	99.17	106.31
24	a	408	PHO	O2D-CGD-CBD	10.07	122.01	110.95
23	C	514	CLA	C1D-ND-C4D	-10.06	99.26	106.31
23	a	406	CLA	C1D-ND-C4D	-9.99	99.30	106.31
23	B	605	CLA	C1D-ND-C4D	-9.86	99.39	106.31
23	a	407	CLA	C1D-ND-C4D	-9.83	99.41	106.31
23	B	607	CLA	C1D-ND-C4D	-9.83	99.41	106.31
23	b	607	CLA	C1D-ND-C4D	-9.81	99.43	106.31
23	B	609	CLA	C1D-ND-C4D	-9.81	99.43	106.31
23	c	505	CLA	C1D-ND-C4D	-9.78	99.45	106.31
23	d	403	CLA	C1D-ND-C4D	-9.74	99.48	106.31
23	c	514	CLA	C1D-ND-C4D	-9.70	99.51	106.31
23	D	406	CLA	C1D-ND-C4D	-9.65	99.54	106.31
23	A	405	CLA	C1D-ND-C4D	-9.65	99.54	106.31
23	b	611	CLA	C1D-ND-C4D	-9.62	99.56	106.31
23	b	609	CLA	C1D-ND-C4D	-9.56	99.60	106.31
24	a	408	PHO	C3B-C4B-NB	9.48	113.64	107.46
23	C	504	CLA	C1D-ND-C4D	-9.48	99.66	106.31
23	b	608	CLA	C1D-ND-C4D	-9.44	99.69	106.31
23	B	601	CLA	C1D-ND-C4D	-9.42	99.70	106.31
23	A	406	CLA	C1D-ND-C4D	-9.40	99.72	106.31
23	b	614	CLA	C1D-ND-C4D	-9.39	99.72	106.31
23	b	615	CLA	C1D-ND-C4D	-9.39	99.73	106.31
23	C	510	CLA	C1D-ND-C4D	-9.37	99.73	106.31
23	B	615	CLA	C1D-ND-C4D	-9.37	99.74	106.31
23	b	606	CLA	C1D-ND-C4D	-9.35	99.75	106.31
23	c	503	CLA	C1D-ND-C4D	-9.35	99.75	106.31
23	A	404	CLA	C1D-ND-C4D	-9.32	99.77	106.31
23	c	509	CLA	C1D-ND-C4D	-9.31	99.78	106.31
23	c	502	CLA	C1D-ND-C4D	-9.29	99.80	106.31
24	A	353	PHO	O2D-CGD-CBD	9.28	121.14	110.95
23	B	612	CLA	C1D-ND-C4D	-9.28	99.80	106.31
23	c	512	CLA	C1D-ND-C4D	-9.28	99.80	106.31
23	b	602	CLA	C1D-ND-C4D	-9.23	99.83	106.31
23	D	405	CLA	C1D-ND-C4D	-9.23	99.84	106.31
23	c	513	CLA	C1D-ND-C4D	-9.17	99.88	106.31
23	B	616	CLA	C1D-ND-C4D	-9.16	99.89	106.31
23	b	610	CLA	C1D-ND-C4D	-9.16	99.89	106.31
23	B	606	CLA	C1D-ND-C4D	-9.15	99.89	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	C1D-ND-C4D	-9.12	99.91	106.31
23	c	510	CLA	C1D-ND-C4D	-9.08	99.94	106.31
23	C	503	CLA	C1D-ND-C4D	-9.07	99.95	106.31
23	c	508	CLA	C1D-ND-C4D	-9.03	99.98	106.31
23	c	504	CLA	C1D-ND-C4D	-9.02	99.98	106.31
23	C	512	CLA	C1D-ND-C4D	-8.99	100.00	106.31
23	C	505	CLA	C1D-ND-C4D	-8.97	100.02	106.31
24	a	353	PHO	O2D-CGD-CBD	8.95	120.78	110.95
23	B	603	CLA	C1D-ND-C4D	-8.94	100.04	106.31
23	b	601	CLA	C1D-ND-C4D	-8.88	100.08	106.31
23	d	402	CLA	C1D-ND-C4D	-8.87	100.09	106.31
23	C	513	CLA	C1D-ND-C4D	-8.84	100.11	106.31
23	C	508	CLA	C1D-ND-C4D	-8.80	100.14	106.31
23	B	613	CLA	C1D-ND-C4D	-8.79	100.14	106.31
23	b	616	CLA	C1D-ND-C4D	-8.79	100.15	106.31
23	c	506	CLA	C1D-ND-C4D	-8.72	100.20	106.31
23	c	511	CLA	C1D-ND-C4D	-8.71	100.20	106.31
23	b	612	CLA	C1D-ND-C4D	-8.71	100.20	106.31
23	b	604	CLA	C1D-ND-C4D	-8.69	100.22	106.31
23	C	511	CLA	C1D-ND-C4D	-8.68	100.22	106.31
23	B	611	CLA	C1D-ND-C4D	-8.68	100.22	106.31
23	B	608	CLA	C1D-ND-C4D	-8.67	100.23	106.31
23	B	602	CLA	C1D-ND-C4D	-8.66	100.23	106.31
23	b	613	CLA	C1D-ND-C4D	-8.64	100.25	106.31
23	c	507	CLA	C1D-ND-C4D	-8.48	100.36	106.31
23	B	602	CLA	C4A-NA-C1A	-8.47	102.81	106.68
23	a	409	CLA	C1D-ND-C4D	-8.47	100.37	106.31
23	C	506	CLA	C1D-ND-C4D	-8.46	100.38	106.31
23	B	610	CLA	C1D-ND-C4D	-8.42	100.41	106.31
24	A	407	PHO	C3B-C4B-NB	8.36	112.91	107.46
23	C	507	CLA	C1D-ND-C4D	-8.32	100.47	106.31
23	C	509	CLA	C1D-ND-C4D	-8.27	100.51	106.31
23	B	604	CLA	C1D-ND-C4D	-8.13	100.61	106.31
24	A	407	PHO	O2D-CGD-CBD	7.86	119.58	110.95
23	a	405	CLA	C1D-ND-C4D	-7.82	100.83	106.31
24	A	353	PHO	C2B-C1B-NB	7.72	115.01	109.43
24	a	353	PHO	C3B-C4B-NB	7.66	112.45	107.46
24	A	353	PHO	C3B-C4B-NB	7.55	112.38	107.46
23	b	602	CLA	C4A-NA-C1A	-7.54	103.24	106.68
23	c	504	CLA	C4A-NA-C1A	-7.50	103.26	106.68
24	a	408	PHO	C2B-C1B-NB	7.39	114.77	109.43
23	C	504	CLA	C4A-NA-C1A	-7.37	103.31	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407	PHO	C2B-C1B-NB	7.26	114.68	109.43
23	B	614	CLA	C2D-C1D-ND	7.15	117.21	110.13
23	B	605	CLA	CHD-C4C-C3C	-7.13	114.38	124.77
23	C	506	CLA	CMD-C2D-C1D	7.11	137.24	124.73
23	B	614	CLA	O2D-CGD-CBD	7.04	123.54	111.23
23	b	607	CLA	C2D-C1D-ND	7.04	117.09	110.13
23	C	511	CLA	CMD-C2D-C1D	7.00	137.06	124.73
23	c	509	CLA	CHD-C4C-C3C	-6.98	114.59	124.77
23	c	508	CLA	O2D-CGD-CBD	6.97	123.41	111.23
23	A	408	CLA	C2D-C1D-ND	6.96	117.02	110.13
23	c	511	CLA	CMD-C2D-C1D	6.93	136.94	124.73
23	B	601	CLA	O2D-CGD-CBD	6.88	123.25	111.23
23	C	508	CLA	CMD-C2D-C1D	6.85	136.80	124.73
23	b	605	CLA	CMD-C2D-C1D	6.85	136.79	124.73
23	b	616	CLA	C4A-NA-C1A	-6.85	103.56	106.68
23	c	509	CLA	C2D-C1D-ND	6.81	116.87	110.13
23	B	612	CLA	CHD-C4C-C3C	-6.79	114.87	124.77
23	B	612	CLA	C2D-C1D-ND	6.74	116.80	110.13
23	b	605	CLA	CHD-C4C-C3C	-6.73	114.95	124.77
23	C	504	CLA	CMD-C2D-C1D	6.72	136.56	124.73
23	A	405	CLA	CHD-C4C-C3C	-6.72	114.98	124.77
23	c	504	CLA	CMD-C2D-C1D	6.72	136.56	124.73
23	b	605	CLA	C2D-C1D-ND	6.72	116.77	110.13
23	c	505	CLA	CMD-C2D-C1D	6.71	136.54	124.73
23	B	615	CLA	CHD-C4C-C3C	-6.70	115.00	124.77
23	b	606	CLA	C4A-NA-C1A	-6.70	103.62	106.68
23	C	507	CLA	CMD-C2D-C1D	6.69	136.50	124.73
23	B	606	CLA	CHD-C4C-C3C	-6.68	115.03	124.77
23	b	611	CLA	C2D-C1D-ND	6.67	116.72	110.13
23	c	514	CLA	CMD-C2D-C1D	6.66	136.46	124.73
23	B	604	CLA	CHD-C4C-C3C	-6.66	115.07	124.77
23	A	405	CLA	C2D-C1D-ND	6.65	116.71	110.13
23	B	614	CLA	CMD-C2D-C1D	6.65	136.44	124.73
23	B	602	CLA	CMD-C2D-C1D	6.65	136.44	124.73
23	B	606	CLA	C4A-NA-C1A	-6.65	103.65	106.68
24	a	353	PHO	C2B-C1B-NB	6.64	114.23	109.43
23	c	508	CLA	CMD-C2D-C1D	6.63	136.41	124.73
23	c	510	CLA	CMD-C2D-C1D	6.61	136.37	124.73
23	d	403	CLA	CMD-C2D-C1D	6.61	136.37	124.73
23	B	616	CLA	O2D-CGD-CBD	6.61	122.78	111.23
23	b	611	CLA	C4A-NA-C1A	-6.60	103.67	106.68
23	a	406	CLA	C2D-C1D-ND	6.60	116.66	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	C2D-C1D-ND	6.60	116.66	110.13
23	b	614	CLA	C2D-C1D-ND	6.57	116.63	110.13
26	A	410	SQD	O6-C1-C2	6.55	118.23	108.27
23	c	505	CLA	C2D-C1D-ND	6.55	116.61	110.13
23	B	605	CLA	C2D-C1D-ND	6.54	116.60	110.13
23	b	613	CLA	C2D-C1D-ND	6.53	116.59	110.13
23	B	607	CLA	C2D-C1D-ND	6.52	116.58	110.13
23	b	611	CLA	CMD-C2D-C1D	6.52	136.21	124.73
23	b	602	CLA	CMD-C2D-C1D	6.50	136.18	124.73
23	B	609	CLA	C2D-C1D-ND	6.50	116.56	110.13
23	B	609	CLA	CHD-C4C-C3C	-6.49	115.31	124.77
23	b	616	CLA	CHD-C4C-C3C	-6.48	115.32	124.77
23	C	508	CLA	CHD-C4C-C3C	-6.48	115.32	124.77
25	D	407	BCR	C7-C8-C9	-6.48	116.65	126.23
23	B	606	CLA	O2D-CGD-CBD	6.47	122.54	111.23
23	D	405	CLA	C2D-C1D-ND	6.47	116.53	110.13
23	b	610	CLA	CMD-C2D-C1D	6.46	136.10	124.73
23	B	616	CLA	CHD-C4C-C3C	-6.45	115.36	124.77
23	c	513	CLA	O2D-CGD-CBD	6.45	122.51	111.23
23	c	512	CLA	CHD-C4C-C3C	-6.44	115.38	124.77
23	c	510	CLA	C1-C2-C3	-6.44	115.64	126.20
23	b	611	CLA	CHD-C4C-C3C	-6.44	115.38	124.77
23	b	601	CLA	CMD-C2D-C1D	6.44	136.07	124.73
23	c	502	CLA	CMD-C2D-C1D	6.43	136.06	124.73
23	B	614	CLA	CHD-C4C-C3C	-6.42	115.41	124.77
23	a	406	CLA	CHD-C4C-C3C	-6.42	115.41	124.77
23	B	603	CLA	CHD-C4C-C3C	-6.41	115.43	124.77
23	B	607	CLA	CMD-C2D-C1D	6.39	135.98	124.73
23	A	408	CLA	CHD-C4C-C3C	-6.39	115.46	124.77
23	C	505	CLA	CMD-C2D-C1D	6.39	135.97	124.73
23	b	613	CLA	CHD-C4C-C3C	-6.37	115.48	124.77
23	B	615	CLA	C2D-C1D-ND	6.37	116.43	110.13
23	a	407	CLA	C2D-C1D-ND	6.36	116.42	110.13
23	D	406	CLA	C2D-C1D-ND	6.36	116.42	110.13
23	b	615	CLA	CMD-C2D-C1D	6.36	135.92	124.73
23	C	506	CLA	CHD-C4C-C3C	-6.35	115.52	124.77
23	c	512	CLA	C2D-C1D-ND	6.33	116.39	110.13
26	F	101	SQD	O6-C1-C2	6.33	117.89	108.27
23	B	603	CLA	O2D-CGD-CBD	6.32	122.28	111.23
23	A	404	CLA	CMD-C2D-C1D	6.32	135.85	124.73
23	D	406	CLA	CHD-C4C-C3C	-6.31	115.57	124.77
23	B	616	CLA	CMD-C2D-C1D	6.31	135.84	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	CMD-C2D-C1D	6.29	135.80	124.73
23	c	513	CLA	CHD-C4C-C3C	-6.28	115.61	124.77
23	B	604	CLA	CMD-C2D-C1D	6.28	135.79	124.73
23	C	513	CLA	CHD-C4C-C3C	-6.27	115.63	124.77
23	B	601	CLA	CHD-C4C-C3C	-6.27	115.63	124.77
23	b	604	CLA	C2D-C1D-ND	6.27	116.33	110.13
23	b	616	CLA	CMD-C2D-C1D	6.25	135.73	124.73
23	B	601	CLA	CMD-C2D-C1D	6.24	135.71	124.73
23	B	611	CLA	CHD-C4C-C3C	-6.23	115.69	124.77
23	c	512	CLA	CMD-C2D-C1D	6.23	135.70	124.73
23	c	503	CLA	CHD-C4C-C3C	-6.22	115.70	124.77
23	c	506	CLA	CHD-C4C-C3C	-6.22	115.70	124.77
23	C	508	CLA	O2D-CGD-CBD	6.22	122.11	111.23
23	B	606	CLA	CMD-C2D-C1D	6.22	135.68	124.73
23	b	604	CLA	CHD-C4C-C3C	-6.21	115.72	124.77
23	b	603	CLA	CHD-C4C-C3C	-6.20	115.73	124.77
23	D	405	CLA	C4A-NA-C1A	-6.19	103.86	106.68
23	c	503	CLA	C2D-C1D-ND	6.17	116.24	110.13
23	b	616	CLA	O2D-CGD-CBD	6.17	122.01	111.23
23	B	613	CLA	C2D-C1D-ND	6.16	116.22	110.13
23	c	513	CLA	C2D-C1D-ND	6.16	116.22	110.13
23	b	604	CLA	CMD-C2D-C1D	6.16	135.57	124.73
23	C	502	CLA	C2D-C1D-ND	6.15	116.21	110.13
23	A	406	CLA	CMD-C2D-C1D	6.15	135.56	124.73
23	b	609	CLA	CMD-C2D-C1D	6.14	135.54	124.73
23	B	613	CLA	C1-C2-C3	-6.14	116.14	126.20
23	B	603	CLA	C4A-NA-C1A	-6.14	103.88	106.68
23	b	606	CLA	CMD-C2D-C1D	6.12	135.51	124.73
23	b	610	CLA	CHD-C4C-C3C	-6.12	115.86	124.77
23	c	505	CLA	CHD-C4C-C3C	-6.11	115.86	124.77
23	B	610	CLA	CMD-C2D-C1D	6.11	135.48	124.73
24	A	353	PHO	C4D-ND-C1D	-6.11	101.56	108.87
23	C	508	CLA	C2D-C1D-ND	6.10	116.17	110.13
23	a	406	CLA	CMD-C2D-C1D	6.10	135.47	124.73
23	C	511	CLA	CHD-C4C-C3C	-6.10	115.88	124.77
23	d	402	CLA	CHD-C4C-C3C	-6.10	115.89	124.77
23	b	614	CLA	CMD-C2D-C1D	6.09	135.45	124.73
23	D	406	CLA	CMD-C2D-C1D	6.09	135.45	124.73
23	a	407	CLA	CMD-C2D-C1D	6.08	135.44	124.73
23	b	606	CLA	CHD-C4C-C3C	-6.08	115.91	124.77
23	C	514	CLA	C2D-C1D-ND	6.08	116.14	110.13
23	C	504	CLA	C2D-C1D-ND	6.06	116.13	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	C2D-C1D-ND	6.06	116.12	110.13
23	B	611	CLA	CMD-C2D-C1D	6.05	135.39	124.73
23	c	506	CLA	O2D-CGD-CBD	6.05	121.81	111.23
23	b	603	CLA	C4A-NA-C1A	-6.04	103.92	106.68
23	A	408	CLA	CMD-C2D-C1D	6.04	135.37	124.73
23	b	607	CLA	CMD-C2D-C1D	6.04	135.37	124.73
23	b	603	CLA	O2D-CGD-CBD	6.04	121.78	111.23
23	c	508	CLA	C2D-C1D-ND	6.03	116.10	110.13
23	C	511	CLA	O2D-CGD-CBD	6.02	121.76	111.23
23	C	513	CLA	O2D-CGD-CBD	6.01	121.73	111.23
23	C	502	CLA	CMD-C2D-C1D	6.00	135.29	124.73
23	b	612	CLA	CHD-C4C-C3C	-5.99	116.04	124.77
23	A	406	CLA	C2D-C1D-ND	5.99	116.06	110.13
23	c	511	CLA	CHD-C4C-C3C	-5.99	116.04	124.77
23	b	610	CLA	O2D-CGD-CBD	5.99	121.70	111.23
23	B	609	CLA	CMD-C2D-C1D	5.99	135.27	124.73
23	C	509	CLA	CHD-C4C-C3C	-5.98	116.05	124.77
23	c	508	CLA	CHD-C4C-C3C	-5.97	116.06	124.77
23	b	608	CLA	C2D-C1D-ND	5.96	116.03	110.13
23	B	610	CLA	CHD-C4C-C3C	-5.96	116.08	124.77
23	B	616	CLA	C2D-C1D-ND	5.95	116.02	110.13
23	B	605	CLA	CMD-C2D-C1D	5.95	135.20	124.73
23	B	601	CLA	C2D-C1D-ND	5.94	116.00	110.13
23	b	609	CLA	C2D-C1D-ND	5.94	116.00	110.13
23	C	514	CLA	CHD-C4C-C3C	-5.93	116.12	124.77
23	B	608	CLA	CHD-C4C-C3C	-5.93	116.12	124.77
23	b	609	CLA	C4A-NA-C1A	-5.93	103.97	106.68
24	a	353	PHO	C3D-C4D-ND	5.92	115.30	107.71
23	b	606	CLA	C2D-C1D-ND	5.92	115.99	110.13
23	b	601	CLA	O2D-CGD-CBD	5.92	121.58	111.23
23	C	513	CLA	C2D-C1D-ND	5.92	115.98	110.13
23	C	514	CLA	CMD-C2D-C1D	5.91	135.14	124.73
23	C	506	CLA	C4A-NA-C1A	-5.91	103.98	106.68
23	C	502	CLA	O2D-CGD-CBD	5.91	121.55	111.23
23	b	602	CLA	CHD-C4C-C3C	-5.89	116.18	124.77
23	C	503	CLA	CMD-C2D-C1D	5.89	135.09	124.73
23	B	604	CLA	O2D-CGD-CBD	5.89	121.52	111.23
23	C	503	CLA	C2D-C1D-ND	5.88	115.95	110.13
23	B	612	CLA	O2D-CGD-CBD	5.88	121.51	111.23
24	a	353	PHO	C4D-ND-C1D	-5.87	101.83	108.87
23	C	503	CLA	CHD-C4C-C3C	-5.87	116.22	124.77
23	a	409	CLA	C2D-C1D-ND	5.87	115.93	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C4A-NA-C1A	-5.86	104.00	106.68
34	b	623	HTG	C1'-S1-C1	5.86	113.10	100.45
23	B	605	CLA	O2D-CGD-CBD	5.85	121.46	111.23
23	b	604	CLA	O2D-CGD-CBD	5.85	121.46	111.23
23	C	512	CLA	CHD-C4C-C3C	-5.85	116.24	124.77
23	c	510	CLA	C2D-C1D-ND	5.85	115.92	110.13
23	C	510	CLA	CMD-C2D-C1D	5.85	135.03	124.73
23	d	403	CLA	C4A-NA-C1A	-5.84	104.02	106.68
23	C	512	CLA	C2D-C1D-ND	5.84	115.90	110.13
24	A	407	PHO	C4D-ND-C1D	-5.83	101.88	108.87
23	d	403	CLA	C2D-C1D-ND	5.83	115.89	110.13
23	A	404	CLA	C2D-C1D-ND	5.83	115.89	110.13
23	c	510	CLA	CHD-C4C-C3C	-5.82	116.28	124.77
23	c	502	CLA	O2D-CGD-CBD	5.82	121.41	111.23
23	B	602	CLA	CHD-C4C-C3C	-5.81	116.31	124.77
23	c	513	CLA	C4A-NA-C1A	-5.80	104.03	106.68
23	a	409	CLA	CHD-C4C-C3C	-5.79	116.32	124.77
24	a	353	PHO	C1-C2-C3	-5.79	116.70	126.20
23	C	502	CLA	CHD-C4C-C3C	-5.79	116.34	124.77
23	B	611	CLA	C2D-C1D-ND	5.78	115.85	110.13
23	b	614	CLA	O2D-CGD-CBD	5.78	121.33	111.23
26	b	620	SQD	O6-C1-C2	5.78	117.05	108.27
23	B	603	CLA	C2D-C1D-ND	5.78	115.84	110.13
23	B	609	CLA	C4A-NA-C1A	-5.78	104.04	106.68
23	C	505	CLA	C2D-C1D-ND	5.78	115.84	110.13
23	c	502	CLA	C4A-NA-C1A	-5.77	104.05	106.68
23	B	610	CLA	O2D-CGD-CBD	5.77	121.32	111.23
23	b	606	CLA	O2D-CGD-CBD	5.77	121.32	111.23
23	c	509	CLA	O2D-CGD-CBD	5.76	121.31	111.23
23	b	608	CLA	CHD-C4C-C3C	-5.76	116.37	124.77
23	a	405	CLA	C2C-C1C-NC	5.76	116.03	109.98
23	b	609	CLA	CHD-C4C-C3C	-5.76	116.38	124.77
23	d	402	CLA	C2D-C1D-ND	5.75	115.81	110.13
23	a	405	CLA	CMD-C2D-C1D	5.75	134.85	124.73
23	b	616	CLA	C2D-C1D-ND	5.74	115.81	110.13
23	C	513	CLA	C4A-NA-C1A	-5.74	104.06	106.68
23	d	403	CLA	C2B-C1B-NB	5.73	116.27	110.33
23	a	407	CLA	CHD-C4C-C3C	-5.73	116.42	124.77
23	C	510	CLA	C2D-C1D-ND	5.73	115.79	110.13
23	C	505	CLA	O2D-CGD-CBD	5.72	121.22	111.23
23	A	405	CLA	CMD-C2D-C1D	5.71	134.78	124.73
23	c	502	CLA	C2D-C1D-ND	5.71	115.78	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	C2D-C1D-ND	5.71	115.78	110.13
23	B	610	CLA	C2D-C1D-ND	5.71	115.77	110.13
23	b	601	CLA	CHD-C4C-C3C	-5.70	116.46	124.77
23	b	611	CLA	O2D-CGD-CBD	5.69	121.17	111.23
23	b	602	CLA	C2D-C1D-ND	5.69	115.75	110.13
23	d	403	CLA	CHD-C4C-C3C	-5.68	116.49	124.77
23	c	514	CLA	C2D-C1D-ND	5.68	115.75	110.13
23	b	607	CLA	CHD-C4C-C3C	-5.67	116.50	124.77
23	B	607	CLA	CHD-C4C-C3C	-5.67	116.50	124.77
23	c	504	CLA	C2D-C1D-ND	5.67	115.73	110.13
23	c	503	CLA	CMD-C2D-C1D	5.66	134.70	124.73
23	B	608	CLA	C2D-C1D-ND	5.66	115.73	110.13
23	A	404	CLA	CHD-C4C-C3C	-5.65	116.53	124.77
23	b	612	CLA	C4A-NA-C1A	-5.65	104.10	106.68
23	b	604	CLA	C2C-C1C-NC	5.64	115.90	109.98
23	B	602	CLA	O2D-CGD-CBD	5.63	121.08	111.23
23	b	613	CLA	C4A-NA-C1A	-5.63	104.11	106.68
23	b	603	CLA	C2D-C1D-ND	5.63	115.69	110.13
23	B	615	CLA	CMD-C2D-C1D	5.62	134.62	124.73
23	c	514	CLA	C4A-NA-C1A	-5.61	104.12	106.68
23	D	405	CLA	CHD-C4C-C3C	-5.60	116.61	124.77
23	C	504	CLA	CHD-C4C-C3C	-5.59	116.62	124.77
23	C	506	CLA	O2D-CGD-CBD	5.59	120.99	111.23
23	b	614	CLA	CHD-C4C-C3C	-5.57	116.65	124.77
23	B	608	CLA	CMD-C2D-C1D	5.57	134.54	124.73
23	D	405	CLA	CMD-C2D-C1D	5.57	134.53	124.73
23	c	503	CLA	O2D-CGD-CBD	5.54	120.91	111.23
23	C	509	CLA	O2D-CGD-CBD	5.53	120.91	111.23
23	b	610	CLA	C2D-C1D-ND	5.53	115.60	110.13
23	c	514	CLA	CHD-C4C-C3C	-5.53	116.71	124.77
23	D	406	CLA	C4A-NA-C1A	-5.52	104.16	106.68
23	B	616	CLA	C4A-NA-C1A	-5.51	104.16	106.68
23	d	402	CLA	CMD-C2D-C1D	5.51	134.44	124.73
23	b	615	CLA	CHD-C4C-C3C	-5.50	116.76	124.77
23	B	604	CLA	C2D-C1D-ND	5.50	115.56	110.13
23	c	507	CLA	CHD-C4C-C3C	-5.49	116.76	124.77
23	c	513	CLA	CMD-C2D-C1D	5.49	134.40	124.73
26	F	101	SQD	O47-C7-C8	5.49	123.35	111.48
23	c	511	CLA	C2D-C1D-ND	5.48	115.55	110.13
34	D	414	HTG	C1'-S1-C1	5.48	112.29	100.45
23	A	406	CLA	CHD-C4C-C3C	-5.48	116.78	124.77
23	B	613	CLA	CMD-C2D-C1D	5.47	134.36	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	403	CLA	C3B-C2B-C1B	-5.47	100.72	107.17
23	B	614	CLA	C3D-C2D-C1D	-5.47	98.37	105.83
23	c	507	CLA	CMD-C2D-C1D	5.45	134.33	124.73
23	C	503	CLA	C4A-NA-C1A	-5.45	104.19	106.68
23	D	405	CLA	C2C-C1C-NC	5.45	115.71	109.98
23	b	615	CLA	C4A-NA-C1A	-5.45	104.19	106.68
23	b	612	CLA	O2D-CGD-CBD	5.44	120.75	111.23
23	c	513	CLA	C2B-C1B-NB	5.44	115.97	110.33
23	b	605	CLA	O2D-CGD-CBD	5.43	120.73	111.23
23	C	511	CLA	C2D-C1D-ND	5.43	115.50	110.13
23	c	512	CLA	O2D-CGD-CBD	5.43	120.72	111.23
23	b	607	CLA	C3D-C2D-C1D	-5.43	98.42	105.83
23	c	506	CLA	CMD-C2D-C1D	5.42	134.27	124.73
23	C	509	CLA	C2D-C1D-ND	5.42	115.49	110.13
23	c	507	CLA	C2C-C1C-NC	5.42	115.67	109.98
23	D	406	CLA	O2D-CGD-CBD	5.41	120.68	111.23
23	b	605	CLA	C4A-NA-C1A	-5.41	104.21	106.68
23	C	510	CLA	CHD-C4C-C3C	-5.40	116.89	124.77
23	C	511	CLA	C3B-C2B-C1B	-5.40	100.80	107.17
23	B	602	CLA	C2D-C1D-ND	5.40	115.47	110.13
23	a	407	CLA	C4A-NA-C1A	-5.39	104.22	106.68
23	b	602	CLA	O2D-CGD-CBD	5.39	120.66	111.23
23	b	606	CLA	C2B-C1B-NB	5.38	115.91	110.33
23	B	607	CLA	C2C-C1C-NC	5.38	115.63	109.98
23	b	610	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
23	b	612	CLA	C2D-C1D-ND	5.37	115.44	110.13
23	C	507	CLA	C2D-C1D-ND	5.36	115.43	110.13
23	C	507	CLA	C4A-NA-C1A	-5.36	104.23	106.68
23	C	509	CLA	C2C-C1C-NC	5.36	115.61	109.98
23	c	506	CLA	C2D-C1D-ND	5.34	115.41	110.13
23	d	403	CLA	O2D-CGD-CBD	5.34	120.56	111.23
26	A	410	SQD	C1-O5-C5	-5.33	103.30	113.72
23	b	601	CLA	C2D-C1D-ND	5.33	115.40	110.13
23	C	507	CLA	C2C-C1C-NC	5.33	115.58	109.98
23	a	406	CLA	C4A-NA-C1A	-5.33	104.25	106.68
24	A	353	PHO	C3D-C4D-ND	5.30	114.50	107.71
23	C	507	CLA	CHD-C4C-C3C	-5.29	117.06	124.77
23	B	613	CLA	C2C-C1C-NC	5.29	115.54	109.98
23	B	615	CLA	C4A-NA-C1A	-5.28	104.27	106.68
23	B	604	CLA	C1-C2-C3	-5.28	117.55	126.20
23	C	509	CLA	CMD-C2D-C1D	5.27	134.00	124.73
24	a	408	PHO	C4D-ND-C1D	-5.26	102.56	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	d	411	HTG	C1'-S1-C1	5.26	111.82	100.45
23	B	614	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
23	C	503	CLA	O2D-CGD-CBD	5.26	120.42	111.23
23	b	613	CLA	C2C-C1C-NC	5.26	115.50	109.98
23	C	511	CLA	C2B-C1B-NB	5.26	115.78	110.33
23	c	502	CLA	CHD-C4C-C3C	-5.25	117.12	124.77
23	c	509	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
23	c	513	CLA	C3B-C2B-C1B	-5.24	100.99	107.17
23	c	509	CLA	C4A-NA-C1A	-5.24	104.29	106.68
23	a	409	CLA	O2D-CGD-CBD	5.23	120.37	111.23
23	b	612	CLA	C2C-C1C-NC	5.23	115.47	109.98
23	b	609	CLA	O2D-CGD-CBD	5.22	120.35	111.23
25	y	101	BCR	C33-C5-C6	-5.22	118.79	124.48
34	c	522	HTG	C1'-S1-C1	5.21	111.70	100.45
23	c	506	CLA	C4A-NA-C1A	-5.21	104.30	106.68
23	C	511	CLA	C1-C2-C3	-5.21	117.67	126.20
23	A	405	CLA	C3D-C2D-C1D	-5.21	98.73	105.83
24	A	407	PHO	C3D-C4D-ND	5.19	114.36	107.71
23	C	505	CLA	C2C-C1C-NC	5.19	115.44	109.98
23	B	608	CLA	C2C-C1C-NC	5.19	115.44	109.98
23	B	603	CLA	CMD-C2D-C1D	5.18	133.86	124.73
26	A	410	SQD	O47-C7-C8	5.18	122.68	111.48
23	B	613	CLA	CHD-C4C-C3C	-5.17	117.23	124.77
23	A	408	CLA	C4A-NA-C1A	-5.17	104.32	106.68
23	b	612	CLA	CMD-C2D-C1D	5.17	133.83	124.73
23	B	605	CLA	C3D-C2D-C1D	-5.16	98.78	105.83
23	b	610	CLA	C4A-NA-C1A	-5.15	104.33	106.68
25	Y	101	BCR	C33-C5-C6	-5.15	118.87	124.48
23	b	603	CLA	CMD-C2D-C1D	5.15	133.79	124.73
23	b	607	CLA	C2C-C1C-NC	5.14	115.39	109.98
23	C	505	CLA	C4A-NA-C1A	-5.14	104.33	106.68
26	f	102	SQD	O47-C7-C8	5.14	122.60	111.48
23	c	505	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
23	C	513	CLA	C2B-C1B-NB	5.13	115.64	110.33
23	C	514	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
23	c	510	CLA	O2D-CGD-CBD	5.12	120.18	111.23
23	c	505	CLA	C2C-C1C-NC	5.12	115.36	109.98
23	b	613	CLA	CMD-C2D-C1D	5.12	133.74	124.73
23	B	611	CLA	C4A-NA-C1A	-5.11	104.35	106.68
23	A	404	CLA	C2C-C1C-NC	5.11	115.35	109.98
23	A	408	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
23	b	614	CLA	C3D-C2D-C1D	-5.11	98.86	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	CMD-C2D-C1D	5.11	133.73	124.73
29	A	414	PL9	C7-C8-C9	-5.11	118.03	126.83
23	a	409	CLA	CMD-C2D-C1D	5.10	133.72	124.73
23	B	611	CLA	O2D-CGD-CBD	5.10	120.15	111.23
23	B	606	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
23	a	407	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
26	a	411	SQD	O47-C7-C8	5.09	122.50	111.48
23	b	613	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
24	A	353	PHO	C1-C2-C3	-5.09	117.86	126.20
26	a	411	SQD	O6-C1-C2	5.08	116.00	108.27
23	b	605	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
23	A	404	CLA	C4A-NA-C1A	-5.07	104.36	106.68
23	c	504	CLA	C2C-C1C-NC	5.07	115.31	109.98
23	b	603	CLA	C2C-C1C-NC	5.07	115.31	109.98
23	c	505	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
23	c	508	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
23	B	606	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
23	A	408	CLA	C3B-C2B-C1B	-5.07	101.20	107.17
23	b	616	CLA	C2B-C1B-NB	5.06	115.58	110.33
23	C	510	CLA	C2C-C1C-NC	5.05	115.29	109.98
25	b	617	BCR	C7-C8-C9	-5.05	118.77	126.23
23	B	614	CLA	C1-C2-C3	-5.04	117.94	126.20
40	V	202	HEC	CHC-C4B-NB	5.04	129.94	124.45
23	c	511	CLA	C1-C2-C3	-5.03	117.95	126.20
23	c	510	CLA	C4A-NA-C1A	-5.03	104.38	106.68
23	B	601	CLA	C2B-C1B-NB	5.03	115.54	110.33
23	B	607	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
25	d	404	BCR	C38-C26-C25	-5.03	119.00	124.48
23	b	611	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
23	C	502	CLA	C4A-NA-C1A	-5.02	104.39	106.68
23	C	510	CLA	C3B-C2B-C1B	-5.02	101.26	107.17
23	b	614	CLA	C3B-C2B-C1B	-5.01	101.26	107.17
23	C	507	CLA	O2D-CGD-CBD	5.01	119.99	111.23
23	B	610	CLA	C4A-NA-C1A	-5.01	104.39	106.68
23	B	611	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
23	C	512	CLA	C3B-C2B-C1B	-5.00	101.28	107.17
23	B	613	CLA	C4A-NA-C1A	-5.00	104.40	106.68
23	C	505	CLA	CHD-C4C-C3C	-5.00	117.49	124.77
23	c	509	CLA	C3B-C2B-C1B	-4.99	101.28	107.17
23	B	609	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
23	b	604	CLA	C1C-C2C-C3C	-4.99	101.73	106.98
23	C	514	CLA	C4A-NA-C1A	-4.99	104.40	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	406	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
23	C	513	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
23	b	615	CLA	C2C-C1C-NC	4.99	115.22	109.98
23	b	602	CLA	C2B-C1B-NB	4.99	115.50	110.33
23	B	612	CLA	C3C-C4C-NC	4.99	116.82	110.43
23	a	405	CLA	C3B-C4B-NB	4.98	114.98	110.53
23	C	514	CLA	C2B-C1B-NB	4.98	115.49	110.33
23	c	504	CLA	CHD-C4C-C3C	-4.98	117.51	124.77
23	c	514	CLA	C2B-C1B-NB	4.97	115.48	110.33
26	B	620	SQD	O6-C1-C2	4.97	115.82	108.27
25	C	515	BCR	C7-C8-C9	-4.97	118.88	126.23
23	d	402	CLA	C2C-C1C-NC	4.97	115.20	109.98
23	b	605	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
23	D	405	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
23	C	508	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
23	b	611	CLA	C1-C2-C3	-4.96	118.07	126.20
23	C	513	CLA	CMD-C2D-C1D	4.95	133.45	124.73
23	B	613	CLA	C3B-C2B-C1B	-4.95	101.33	107.17
23	B	614	CLA	C4A-NA-C1A	-4.95	104.42	106.68
26	b	620	SQD	O47-C7-C8	4.95	122.19	111.48
24	a	408	PHO	C3D-C4D-ND	4.95	114.05	107.71
23	B	601	CLA	C3B-C2B-C1B	-4.94	101.34	107.17
23	C	514	CLA	C3D-C4D-ND	4.94	118.02	109.99
23	C	502	CLA	C3D-C4D-ND	4.94	118.02	109.99
23	d	403	CLA	C3D-C4D-ND	4.94	118.01	109.99
23	B	612	CLA	C2C-C1C-NC	4.94	115.17	109.98
23	B	607	CLA	C1C-C2C-C3C	-4.93	101.79	106.98
23	B	606	CLA	C2C-C1C-NC	4.93	115.16	109.98
23	b	601	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
23	b	613	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
29	D	408	PL9	C42-C43-C44	-4.91	116.37	127.62
23	b	604	CLA	C3D-C2D-C1D	-4.91	99.12	105.83
23	C	512	CLA	C2C-C1C-NC	4.91	115.14	109.98
23	C	503	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
23	B	602	CLA	C2B-C1B-NB	4.90	115.41	110.33
40	v	202	HEC	CHC-C4B-NB	4.90	129.79	124.45
38	E	103	HEM	CHC-C4B-NB	4.90	129.69	124.42
23	b	610	CLA	C2B-C1B-NB	4.89	115.39	110.33
23	b	608	CLA	C4A-NA-C1A	-4.89	104.45	106.68
23	b	614	CLA	C1-C2-C3	-4.89	118.19	126.20
23	b	608	CLA	C2B-C1B-NB	4.88	115.39	110.33
23	c	512	CLA	C3D-C2D-C1D	-4.88	99.17	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	C3B-C2B-C1B	-4.88	101.42	107.17
23	b	601	CLA	C4A-NA-C1A	-4.88	104.45	106.68
23	B	614	CLA	C2B-C1B-NB	4.88	115.38	110.33
23	b	614	CLA	C2C-C1C-NC	4.88	115.10	109.98
23	B	611	CLA	C2C-C1C-NC	4.87	115.10	109.98
23	b	610	CLA	C1-C2-C3	-4.87	118.21	126.20
23	A	404	CLA	CAA-C2A-C3A	-4.87	99.84	113.00
23	B	608	CLA	O2D-CGD-CBD	4.87	119.74	111.23
23	D	406	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
23	d	402	CLA	C1-C2-C3	-4.86	118.23	126.20
23	c	503	CLA	C2C-C1C-NC	4.86	115.08	109.98
23	b	615	CLA	C2B-C1B-NB	4.86	115.36	110.33
25	d	404	BCR	C7-C8-C9	-4.86	119.05	126.23
23	b	605	CLA	C3D-C4D-ND	4.86	117.88	109.99
23	b	606	CLA	C3B-C2B-C1B	-4.86	101.45	107.17
23	B	611	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
23	b	605	CLA	CHD-C1D-ND	-4.85	117.97	124.80
23	A	406	CLA	C4A-NA-C1A	-4.85	104.47	106.68
23	c	514	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
23	C	510	CLA	O2D-CGD-CBD	4.84	119.70	111.23
23	b	612	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
23	C	504	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
33	C	501	LMG	O7-C10-C11	4.83	121.93	111.48
23	B	614	CLA	O2D-CGD-O1D	-4.83	114.45	123.85
23	b	608	CLA	O2D-CGD-CBD	4.82	119.66	111.23
23	A	404	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
23	C	506	CLA	C2D-C1D-ND	4.82	114.90	110.13
23	d	403	CLA	CHD-C1D-ND	-4.82	118.02	124.80
23	B	607	CLA	C4A-NA-C1A	-4.82	104.48	106.68
23	c	506	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
23	c	504	CLA	O2D-CGD-CBD	4.82	119.65	111.23
23	A	406	CLA	C3D-C4D-ND	4.82	117.82	109.99
23	a	409	CLA	C4A-NA-C1A	-4.82	104.48	106.68
23	A	408	CLA	C3D-C4D-ND	4.81	117.81	109.99
25	c	515	BCR	C11-C10-C9	-4.81	120.53	127.28
23	c	503	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
23	c	505	CLA	O2D-CGD-CBD	4.81	119.64	111.23
23	B	603	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
23	c	514	CLA	C3D-C4D-ND	4.81	117.80	109.99
23	c	510	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
23	B	604	CLA	C2C-C1C-NC	4.81	115.03	109.98
23	B	616	CLA	C3D-C2D-C1D	-4.81	99.27	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
25	b	617	BCR	C33-C5-C6	-4.80	119.25	124.48
23	C	504	CLA	C2B-C1B-NB	4.80	115.30	110.33
23	b	616	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	c	511	CLA	C4A-NA-C1A	-4.79	104.49	106.68
23	c	502	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
23	B	615	CLA	CMB-C2B-C1B	4.78	132.70	125.42
23	c	511	CLA	O2D-CGD-CBD	4.78	119.58	111.23
23	B	611	CLA	C2B-C1B-NB	4.77	115.28	110.33
23	B	607	CLA	O2D-CGD-CBD	4.77	119.57	111.23
23	C	512	CLA	CMD-C2D-C1D	4.77	133.12	124.73
23	C	508	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
23	C	505	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
23	a	409	CLA	C2B-C1B-NB	4.76	115.27	110.33
23	c	508	CLA	C2C-C1C-NC	4.76	114.98	109.98
23	C	507	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
23	B	615	CLA	C3D-C2D-C1D	-4.75	99.34	105.83
23	a	405	CLA	C1C-C2C-C3C	-4.75	101.98	106.98
23	c	504	CLA	C2B-C1B-NB	4.75	115.25	110.33
23	b	603	CLA	C3B-C2B-C1B	-4.75	101.57	107.17
23	b	612	CLA	C2B-C1B-NB	4.75	115.25	110.33
23	A	408	CLA	C2B-C1B-NB	4.74	115.25	110.33
23	a	409	CLA	C2C-C1C-NC	4.74	114.96	109.98
23	a	407	CLA	C3D-C4D-ND	4.74	117.69	109.99
23	C	505	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
23	B	610	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
25	c	516	BCR	C7-C8-C9	-4.74	119.22	126.23
23	a	405	CLA	CHD-C4C-C3C	-4.74	117.87	124.77
23	c	512	CLA	C2C-C1C-NC	4.73	114.95	109.98
40	v	202	HEC	CBB-CAB-C3B	-4.73	117.99	127.43
23	C	504	CLA	C2C-C1C-NC	4.72	114.94	109.98
23	b	608	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
23	b	614	CLA	C4A-NA-C1A	-4.72	104.53	106.68
23	b	604	CLA	C4A-NA-C1A	-4.71	104.53	106.68
23	b	608	CLA	C3B-C2B-C1B	-4.71	101.61	107.17
23	C	504	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
23	A	404	CLA	C2B-C1B-NB	4.71	115.21	110.33
23	A	406	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
23	B	604	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
23	c	508	CLA	CHD-C1D-ND	-4.70	118.18	124.80
23	B	613	CLA	C2B-C1B-NB	4.70	115.20	110.33
23	A	406	CLA	C2B-C1B-NB	4.70	115.20	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
23	b	609	CLA	C2C-C1C-NC	4.70	114.92	109.98
23	a	405	CLA	C4A-NA-C1A	-4.70	104.54	106.68
23	B	609	CLA	C3D-C4D-ND	4.70	117.62	109.99
23	a	405	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
23	c	508	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	c	509	CLA	C2B-C1B-NB	4.69	115.19	110.33
23	C	508	CLA	C4A-NA-C1A	-4.69	104.54	106.68
23	C	502	CLA	C2C-C1C-NC	4.68	114.90	109.98
23	D	405	CLA	C1C-C2C-C3C	-4.68	102.06	106.98
23	B	612	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
23	c	504	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
23	C	503	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
23	C	506	CLA	C2C-C1C-NC	4.68	114.90	109.98
23	A	405	CLA	O2D-CGD-CBD	4.68	119.40	111.23
23	B	614	CLA	C2C-C1C-NC	4.67	114.89	109.98
23	B	601	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
23	b	606	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
33	C	520	LMG	O7-C10-C11	4.66	121.57	111.48
23	b	601	CLA	C2C-C1C-NC	4.66	114.88	109.98
23	a	406	CLA	C3D-C4D-ND	4.66	117.56	109.99
23	b	601	CLA	C2B-C1B-NB	4.66	115.16	110.33
23	c	510	CLA	C2B-C1B-NB	4.66	115.16	110.33
23	b	602	CLA	C3D-C4D-ND	4.66	117.56	109.99
23	B	604	CLA	C4A-NA-C1A	-4.66	104.55	106.68
23	c	503	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
23	b	603	CLA	C1D-CHD-C4C	-4.65	116.13	126.02
23	B	612	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
23	b	613	CLA	C1-C2-C3	-4.65	118.58	126.20
23	B	613	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	b	615	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	c	506	CLA	C3C-C4C-NC	4.64	116.37	110.43
23	a	407	CLA	C2C-C1C-NC	4.63	114.85	109.98
23	d	402	CLA	C4A-NA-C1A	-4.63	104.56	106.68
37	E	101	LHG	O7-C7-C8	4.63	121.49	111.48
23	C	509	CLA	C1-C2-C3	-4.63	118.61	126.20
23	c	505	CLA	C2B-C1B-NB	4.63	115.12	110.33
23	B	608	CLA	C4A-NA-C1A	-4.63	104.57	106.68
23	b	604	CLA	C3B-C2B-C1B	-4.63	101.72	107.17
23	b	615	CLA	C3B-C2B-C1B	-4.63	101.72	107.17
23	b	607	CLA	O2D-CGD-CBD	4.62	119.31	111.23
25	B	617	BCR	C33-C5-C6	-4.62	119.44	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407	CLA	O2D-CGD-CBD	4.62	119.31	111.23
23	c	511	CLA	C2C-C1C-NC	4.62	114.83	109.98
23	d	402	CLA	C3B-C2B-C1B	-4.62	101.73	107.17
23	a	407	CLA	C2B-C1B-NB	4.62	115.11	110.33
23	b	609	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
23	c	510	CLA	C3D-C2D-C1D	-4.61	99.55	105.83
23	B	606	CLA	C2B-C1B-NB	4.60	115.10	110.33
23	C	503	CLA	C1-C2-C3	-4.60	118.66	126.20
23	C	510	CLA	C3D-C4D-ND	4.60	117.47	109.99
23	c	511	CLA	C3B-C2B-C1B	-4.60	101.75	107.17
23	c	507	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	B	603	CLA	C2C-C1C-NC	4.59	114.81	109.98
23	A	405	CLA	CBC-CAC-C3C	-4.59	99.97	112.42
23	c	502	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
23	C	512	CLA	C3D-C4D-ND	4.59	117.45	109.99
23	C	511	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
23	B	605	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
23	B	610	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
23	b	601	CLA	C3D-C4D-ND	4.59	117.44	109.99
23	B	602	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
23	C	505	CLA	C1-C2-C3	-4.58	118.69	126.20
23	b	605	CLA	C2C-C1C-NC	4.58	114.79	109.98
23	c	502	CLA	C2C-C1C-NC	4.58	114.79	109.98
23	b	611	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
23	A	406	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	b	608	CLA	C2C-C1C-NC	4.58	114.79	109.98
23	B	606	CLA	C3C-C4C-NC	4.58	116.29	110.43
23	B	602	CLA	CAA-C2A-C3A	-4.58	100.64	113.00
23	B	605	CLA	C1D-CHD-C4C	-4.57	116.30	126.02
23	C	502	CLA	C1-C2-C3	-4.57	118.71	126.20
23	c	506	CLA	C2C-C1C-NC	4.57	114.78	109.98
23	b	609	CLA	C3D-C4D-ND	4.56	117.41	109.99
23	b	615	CLA	C3D-C4D-ND	4.56	117.40	109.99
23	C	514	CLA	O2D-CGD-CBD	4.55	119.19	111.23
23	D	405	CLA	C3B-C2B-C1B	-4.55	101.80	107.17
25	t	103	BCR	C33-C5-C6	-4.55	119.52	124.48
23	c	513	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
23	c	514	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
23	B	603	CLA	C2B-C1B-NB	4.55	115.05	110.33
23	B	601	CLA	C3D-C4D-ND	4.55	117.38	109.99
23	B	607	CLA	C3D-C4D-ND	4.54	117.37	109.99
23	b	603	CLA	C3D-C4D-ND	4.54	117.37	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	C3B-C2B-C1B	-4.54	101.81	107.17
33	Z	101	LMG	O7-C10-C11	4.54	121.31	111.48
23	a	409	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
23	a	406	CLA	C2B-C1B-NB	4.54	115.03	110.33
23	c	502	CLA	C3D-C4D-ND	4.54	117.36	109.99
23	D	405	CLA	C1-C2-C3	-4.53	118.77	126.20
23	b	607	CLA	C4A-NA-C1A	-4.53	104.61	106.68
23	C	502	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	A	404	CLA	C3D-C4D-ND	4.53	117.35	109.99
23	B	604	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	A	406	CLA	CHD-C1D-ND	-4.53	118.43	124.80
23	c	509	CLA	C2C-C1C-NC	4.52	114.73	109.98
23	c	502	CLA	C2B-C1B-NB	4.52	115.01	110.33
23	D	406	CLA	C2B-C1B-NB	4.52	115.01	110.33
23	c	511	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
23	B	609	CLA	O2D-CGD-CBD	4.51	119.12	111.23
23	d	403	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
23	C	510	CLA	C2B-C1B-NB	4.51	115.00	110.33
23	A	408	CLA	CHD-C1D-ND	-4.51	118.46	124.80
23	C	514	CLA	C3D-C2D-C1D	-4.50	99.68	105.83
23	c	514	CLA	CHD-C1D-ND	-4.50	118.46	124.80
23	a	409	CLA	C3B-C2B-C1B	-4.50	101.86	107.17
23	B	615	CLA	C2C-C1C-NC	4.50	114.71	109.98
29	d	405	PL9	C42-C43-C44	-4.49	117.34	127.62
23	c	508	CLA	C1C-C2C-C3C	-4.49	102.25	106.98
23	a	406	CLA	C3B-C2B-C1B	-4.49	101.88	107.17
23	B	614	CLA	C3D-C4D-ND	4.49	117.28	109.99
23	B	609	CLA	C2C-C1C-NC	4.49	114.69	109.98
23	C	512	CLA	C2B-C1B-NB	4.48	114.98	110.33
23	b	610	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
23	B	605	CLA	C4A-NA-C1A	-4.48	104.63	106.68
23	C	502	CLA	C2B-C1B-NB	4.48	114.98	110.33
23	d	402	CLA	C3C-C4C-NC	4.48	116.17	110.43
23	a	406	CLA	CHD-C1D-ND	-4.48	118.49	124.80
23	c	505	CLA	C3D-C4D-ND	4.48	117.27	109.99
23	b	607	CLA	CHD-C1D-ND	-4.48	118.50	124.80
23	a	406	CLA	C2C-C1C-NC	4.48	114.69	109.98
23	C	513	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
23	B	607	CLA	C3B-C2B-C1B	-4.47	101.90	107.17
23	c	502	CLA	CHD-C1D-ND	-4.47	118.51	124.80
25	b	619	BCR	C7-C8-C9	-4.47	119.62	126.23
23	B	602	CLA	C3D-C2D-C1D	-4.47	99.73	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	406	CLA	C3D-C4D-ND	4.47	117.25	109.99
23	A	408	CLA	C1-C2-C3	-4.47	118.88	126.20
23	b	607	CLA	C3D-C4D-ND	4.47	117.25	109.99
29	a	416	PL9	C7-C3-C4	4.47	120.59	116.91
23	c	504	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
23	b	614	CLA	C2B-C1B-NB	4.46	114.95	110.33
23	B	608	CLA	C3B-C2B-C1B	-4.46	101.91	107.17
23	a	407	CLA	CHD-C1D-ND	-4.46	118.53	124.80
23	b	608	CLA	C1-C2-C3	-4.46	118.90	126.20
34	b	622	HTG	C1-O5-C5	4.45	120.55	112.56
23	D	406	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
23	C	502	CLA	CHD-C1D-ND	-4.45	118.54	124.80
23	b	606	CLA	C3D-C4D-ND	4.45	117.22	109.99
23	B	615	CLA	C3B-C2B-C1B	-4.45	101.93	107.17
23	C	509	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
23	C	503	CLA	C2B-C1B-NB	4.45	114.94	110.33
23	B	614	CLA	CHD-C1D-ND	-4.44	118.55	124.80
23	A	405	CLA	C3D-C4D-ND	4.44	117.21	109.99
23	b	614	CLA	C3D-C4D-ND	4.44	117.21	109.99
23	C	509	CLA	C3C-C4C-NC	4.44	116.12	110.43
23	C	506	CLA	C3B-C2B-C1B	-4.44	101.94	107.17
23	b	608	CLA	C3D-C4D-ND	4.44	117.20	109.99
23	c	514	CLA	C2C-C1C-NC	4.44	114.64	109.98
23	b	602	CLA	CHD-C1D-ND	-4.43	118.56	124.80
23	B	605	CLA	C3D-C4D-ND	4.43	117.18	109.99
23	A	404	CLA	O2A-CGA-CBA	4.42	125.33	111.83
34	B	623	HTG	C1'-S1-C1	4.42	110.00	100.45
23	c	511	CLA	C2B-C1B-NB	4.42	114.91	110.33
23	b	610	CLA	C3D-C4D-ND	4.42	117.17	109.99
23	C	504	CLA	C3D-C4D-ND	4.42	117.17	109.99
23	B	609	CLA	C3C-C4C-NC	4.42	116.09	110.43
23	a	405	CLA	C3D-C4D-ND	4.42	117.17	109.99
23	D	405	CLA	CHD-C1D-ND	-4.42	118.59	124.80
23	C	511	CLA	C2C-C1C-NC	4.41	114.62	109.98
23	C	503	CLA	C2C-C1C-NC	4.41	114.61	109.98
23	b	611	CLA	C2C-C1C-NC	4.41	114.61	109.98
23	a	405	CLA	C2B-C1B-NB	4.41	114.90	110.33
23	B	602	CLA	C3D-C4D-ND	4.41	117.15	109.99
23	a	407	CLA	C1-C2-C3	-4.41	118.98	126.20
23	C	514	CLA	CHD-C1D-ND	-4.41	118.60	124.80
23	B	610	CLA	C2C-C1C-NC	4.40	114.61	109.98
34	C	522	HTG	C1'-S1-C1	4.40	109.96	100.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
23	B	612	CLA	C1-C2-C3	-4.40	118.99	126.20
23	b	602	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
26	A	410	SQD	C1-C2-C3	-4.40	100.75	110.01
23	d	402	CLA	C3D-C4D-ND	4.40	117.13	109.99
40	V	202	HEC	CBB-CAB-C3B	-4.40	118.65	127.43
23	B	603	CLA	C3D-C4D-ND	4.39	117.13	109.99
23	b	601	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
23	A	404	CLA	CHD-C1D-ND	-4.39	118.62	124.80
23	C	505	CLA	C3D-C4D-ND	4.39	117.12	109.99
23	c	503	CLA	C3D-C4D-ND	4.39	117.12	109.99
23	b	612	CLA	C1-C2-C3	-4.38	119.01	126.20
23	b	603	CLA	C3C-C4C-NC	4.38	116.04	110.43
23	A	406	CLA	C2C-C1C-NC	4.38	114.58	109.98
23	B	615	CLA	C2B-C1B-NB	4.38	114.87	110.33
23	B	616	CLA	C3D-C4D-ND	4.38	117.11	109.99
23	a	406	CLA	C1C-C2C-C3C	-4.38	102.38	106.98
23	B	608	CLA	C3D-C4D-ND	4.38	117.10	109.99
23	a	405	CLA	C2D-C1D-ND	4.37	114.45	110.13
23	c	507	CLA	C4A-NA-C1A	-4.37	104.68	106.68
23	C	503	CLA	C3D-C4D-ND	4.37	117.09	109.99
23	b	611	CLA	C3D-C4D-ND	4.37	117.09	109.99
23	c	504	CLA	C3D-C4D-ND	4.37	117.09	109.99
23	b	609	CLA	C1-C2-C3	-4.37	119.05	126.20
23	B	604	CLA	C1D-CHD-C4C	-4.36	116.74	126.02
23	A	404	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
23	c	506	CLA	C3D-C4D-ND	4.36	117.08	109.99
23	c	514	CLA	O2D-CGD-CBD	4.36	118.84	111.23
23	B	615	CLA	C3D-C4D-ND	4.35	117.06	109.99
23	a	407	CLA	C3B-C2B-C1B	-4.35	102.04	107.17
23	b	606	CLA	CHD-C1D-ND	-4.35	118.68	124.80
23	c	505	CLA	CHD-C1D-ND	-4.35	118.68	124.80
23	C	513	CLA	C3D-C4D-ND	4.34	117.05	109.99
23	B	612	CLA	CMD-C2D-C1D	4.34	132.38	124.73
25	D	407	BCR	C38-C26-C25	-4.34	119.75	124.48
23	B	601	CLA	C4A-NA-C1A	-4.34	104.70	106.68
23	B	603	CLA	C1D-CHD-C4C	-4.34	116.80	126.02
23	B	604	CLA	C3C-C4C-NC	4.34	115.98	110.43
23	D	405	CLA	O2D-CGD-CBD	4.33	118.81	111.23
23	C	512	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
23	A	408	CLA	C2C-C1C-NC	4.33	114.53	109.98
23	c	510	CLA	C2C-C1C-NC	4.33	114.53	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	C2C-C1C-NC	4.33	114.53	109.98
23	c	513	CLA	C2C-C1C-NC	4.33	114.53	109.98
23	C	505	CLA	C2B-C1B-NB	4.32	114.81	110.33
23	C	509	CLA	C3B-C4B-NB	4.32	114.39	110.53
38	E	103	HEM	CAD-CBD-CGD	4.32	125.12	113.67
23	c	508	CLA	C3D-C4D-ND	4.32	117.01	109.99
23	a	405	CLA	CAA-C2A-C3A	-4.31	101.35	113.00
38	e	87	HEM	CHC-C4B-NB	4.31	129.06	124.42
25	B	617	BCR	C7-C8-C9	-4.31	119.86	126.23
23	b	613	CLA	C1C-C2C-C3C	-4.31	102.45	106.98
25	H	101	BCR	C16-C17-C18	-4.30	121.24	127.28
33	C	521	LMG	O7-C10-C11	4.30	120.79	111.48
23	A	406	CLA	O2D-CGD-CBD	4.30	118.75	111.23
23	d	402	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
23	c	513	CLA	C3D-C4D-ND	4.30	116.97	109.99
23	B	605	CLA	C3C-C4C-NC	4.30	115.94	110.43
23	B	605	CLA	CMB-C2B-C1B	4.30	131.96	125.42
23	b	615	CLA	CHD-C1D-ND	-4.29	118.76	124.80
23	C	510	CLA	C1-C2-C3	-4.29	119.16	126.20
23	C	509	CLA	C3D-C4D-ND	4.29	116.96	109.99
23	C	510	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
23	b	605	CLA	C2B-C1B-NB	4.29	114.77	110.33
23	b	607	CLA	C3B-C4B-NB	4.28	114.35	110.53
23	A	405	CLA	CHD-C1D-ND	-4.28	118.78	124.80
23	B	613	CLA	C3D-C4D-ND	4.28	116.94	109.99
23	c	507	CLA	C1C-C2C-C3C	-4.28	102.48	106.98
23	C	507	CLA	CHD-C1D-ND	-4.28	118.78	124.80
23	c	513	CLA	C1-C2-C3	-4.27	119.19	126.20
23	C	505	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
23	B	601	CLA	C2C-C1C-NC	4.27	114.47	109.98
23	B	615	CLA	C3C-C4C-NC	4.27	115.90	110.43
23	b	607	CLA	C3C-C4C-NC	4.27	115.89	110.43
23	C	504	CLA	CHD-C1D-ND	-4.26	118.80	124.80
23	B	606	CLA	C1D-CHD-C4C	-4.26	116.96	126.02
23	c	507	CLA	C3D-C4D-ND	4.26	116.91	109.99
23	b	612	CLA	C3D-C4D-ND	4.26	116.91	109.99
23	A	406	CLA	CMB-C2B-C1B	4.26	131.90	125.42
23	B	616	CLA	C2B-C1B-NB	4.26	114.74	110.33
23	C	505	CLA	CHD-C1D-ND	-4.26	118.81	124.80
23	b	601	CLA	CHD-C1D-ND	-4.26	118.81	124.80
23	B	605	CLA	C2B-C1B-NB	4.25	114.74	110.33
23	C	504	CLA	C1-C2-C3	-4.25	119.23	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C3D-C4D-ND	4.25	116.90	109.99
23	b	612	CLA	C3C-C4C-NC	4.25	115.88	110.43
23	b	616	CLA	C1D-CHD-C4C	-4.25	116.99	126.02
23	B	612	CLA	C3D-C4D-ND	4.25	116.89	109.99
23	B	608	CLA	C2B-C1B-NB	4.25	114.73	110.33
23	b	613	CLA	C2B-C1B-NB	4.25	114.73	110.33
23	B	605	CLA	C2C-C1C-NC	4.25	114.44	109.98
29	a	416	PL9	C32-C33-C34	-4.25	117.90	127.62
23	C	506	CLA	C3C-C4C-NC	4.25	115.87	110.43
23	C	512	CLA	O2D-CGD-CBD	4.24	118.65	111.23
23	B	608	CLA	C3B-C4B-NB	4.24	114.32	110.53
23	C	509	CLA	C3B-C2B-C1B	-4.24	102.17	107.17
25	d	404	BCR	C24-C23-C22	-4.24	119.97	126.23
23	B	613	CLA	CAC-C3C-C4C	4.24	130.30	124.79
23	A	405	CLA	C3B-C2B-C1B	-4.24	102.18	107.17
23	b	608	CLA	CHD-C1D-ND	-4.24	118.84	124.80
23	c	508	CLA	C4A-NA-C1A	-4.23	104.75	106.68
23	c	510	CLA	C3D-C4D-ND	4.23	116.86	109.99
32	I	101	LMT	C1'-O5'-C5'	4.22	121.97	113.72
23	B	607	CLA	CHD-C1D-ND	-4.22	118.86	124.80
26	B	620	SQD	O47-C7-C8	4.22	120.61	111.48
23	B	614	CLA	C1C-C2C-C3C	-4.22	102.55	106.98
23	B	606	CLA	CHD-C1D-ND	-4.21	118.88	124.80
23	b	603	CLA	C2B-C1B-NB	4.21	114.69	110.33
23	D	405	CLA	C3D-C4D-ND	4.21	116.82	109.99
23	b	611	CLA	C2B-C1B-NB	4.21	114.69	110.33
23	c	509	CLA	C3C-C4C-NC	4.20	115.81	110.43
23	c	509	CLA	C3D-C4D-ND	4.20	116.81	109.99
23	B	610	CLA	C3D-C4D-ND	4.19	116.81	109.99
23	B	605	CLA	O2D-CGD-O1D	-4.19	115.68	123.85
23	B	609	CLA	CHD-C1D-ND	-4.19	118.90	124.80
23	B	603	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
24	A	407	PHO	CBC-CAC-C3C	-4.19	106.87	112.87
23	B	611	CLA	C1-C2-C3	-4.19	119.33	126.20
23	b	613	CLA	C3C-C4C-NC	4.19	115.79	110.43
23	b	611	CLA	CHD-C1D-ND	-4.19	118.91	124.80
23	C	510	CLA	C4A-NA-C1A	-4.18	104.77	106.68
23	C	508	CLA	CHD-C1D-ND	-4.18	118.92	124.80
23	C	509	CLA	C4A-NA-C1A	-4.18	104.77	106.68
23	C	503	CLA	CMB-C2B-C1B	4.18	131.78	125.42
23	c	503	CLA	C4A-NA-C1A	-4.18	104.77	106.68
23	B	610	CLA	C2B-C1B-NB	4.18	114.66	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	C1D-CHD-C4C	-4.17	117.16	126.02
23	c	504	CLA	CHD-C1D-ND	-4.17	118.94	124.80
23	B	603	CLA	C3C-C4C-NC	4.17	115.77	110.43
23	A	405	CLA	C2B-C1B-NB	4.16	114.64	110.33
23	b	616	CLA	C3D-C4D-ND	4.16	116.75	109.99
25	C	516	BCR	C7-C8-C9	-4.16	120.09	126.23
23	C	507	CLA	C3D-C4D-ND	4.15	116.74	109.99
23	C	508	CLA	C3C-C4C-NC	4.15	115.74	110.43
23	B	605	CLA	C4-C3-C5	4.15	122.42	115.23
23	d	402	CLA	O2D-CGD-CBD	4.15	118.48	111.23
23	c	512	CLA	C3D-C4D-ND	4.15	116.72	109.99
23	C	508	CLA	C2B-C1B-NB	4.14	114.62	110.33
23	C	506	CLA	C3D-C4D-ND	4.14	116.71	109.99
23	b	603	CLA	C3D-C2D-C1D	-4.14	100.19	105.83
23	C	513	CLA	C2C-C1C-NC	4.13	114.32	109.98
23	b	615	CLA	O2D-CGD-CBD	4.13	118.45	111.23
23	A	405	CLA	C1C-C2C-C3C	-4.13	102.64	106.98
23	c	508	CLA	C2B-C1B-NB	4.13	114.61	110.33
23	a	409	CLA	C3D-C4D-ND	4.12	116.69	109.99
23	B	602	CLA	CHD-C1D-ND	-4.12	119.00	124.80
23	B	604	CLA	C1C-C2C-C3C	-4.12	102.64	106.98
25	Y	101	BCR	C16-C17-C18	-4.12	121.50	127.28
23	c	504	CLA	C1D-CHD-C4C	-4.12	117.27	126.02
23	c	511	CLA	C3D-C4D-ND	4.12	116.68	109.99
23	C	510	CLA	CHD-C1D-ND	-4.11	119.01	124.80
23	d	402	CLA	C2B-C1B-NB	4.11	114.59	110.33
23	C	507	CLA	C1C-C2C-C3C	-4.11	102.66	106.98
23	b	604	CLA	C3C-C4C-NC	4.11	115.69	110.43
23	c	512	CLA	CHD-C1D-ND	-4.11	119.02	124.80
23	a	406	CLA	O2D-CGD-CBD	4.10	118.40	111.23
23	C	508	CLA	C2C-C1C-NC	4.10	114.29	109.98
23	c	511	CLA	CHD-C1D-ND	-4.10	119.03	124.80
23	c	509	CLA	C1C-C2C-C3C	-4.10	102.67	106.98
23	c	505	CLA	C3B-C4B-NB	4.09	114.19	110.53
23	c	502	CLA	O2D-CGD-O1D	-4.09	115.88	123.85
23	C	502	CLA	C1C-C2C-C3C	-4.09	102.67	106.98
23	B	611	CLA	C3D-C4D-ND	4.09	116.64	109.99
23	C	502	CLA	O2D-CGD-O1D	-4.09	115.88	123.85
23	B	616	CLA	C3C-C4C-NC	4.09	115.67	110.43
23	C	507	CLA	C3B-C2B-C1B	-4.09	102.35	107.17
23	c	510	CLA	C1D-CHD-C4C	-4.09	117.33	126.02
23	c	507	CLA	C1-C2-C3	-4.09	119.50	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	C1D-CHD-C4C	-4.09	117.34	126.02
23	c	506	CLA	C1D-CHD-C4C	-4.09	117.34	126.02
23	C	506	CLA	C1D-CHD-C4C	-4.08	117.34	126.02
23	B	616	CLA	C3B-C2B-C1B	-4.08	102.36	107.17
23	c	512	CLA	O2D-CGD-O1D	-4.08	115.90	123.85
23	B	610	CLA	C3C-C4C-NC	4.08	115.66	110.43
23	A	405	CLA	C4A-NA-C1A	-4.08	104.82	106.68
23	C	504	CLA	C1D-CHD-C4C	-4.08	117.35	126.02
23	c	507	CLA	C3B-C4B-NB	4.08	114.17	110.53
23	C	507	CLA	C2B-C1B-NB	4.08	114.55	110.33
23	B	612	CLA	C2B-C1B-NB	4.07	114.55	110.33
23	b	612	CLA	C1D-CHD-C4C	-4.07	117.37	126.02
23	b	611	CLA	C3C-C4C-NC	4.07	115.64	110.43
23	c	512	CLA	C1D-CHD-C4C	-4.06	117.38	126.02
23	c	503	CLA	C2B-C1B-NB	4.06	114.54	110.33
23	c	506	CLA	C2B-C1B-NB	4.06	114.54	110.33
23	C	512	CLA	C3C-C4C-NC	4.06	115.63	110.43
23	B	613	CLA	C3C-C4C-NC	4.05	115.62	110.43
23	B	610	CLA	O2A-CGA-CBA	4.05	124.19	111.83
23	C	512	CLA	C1-C2-C3	-4.05	119.56	126.20
23	B	601	CLA	CHD-C1D-ND	-4.04	119.11	124.80
25	c	515	BCR	C20-C21-C22	-4.04	121.61	127.28
23	a	406	CLA	C1D-CHD-C4C	-4.03	117.45	126.02
23	c	513	CLA	C3C-C4C-NC	4.03	115.59	110.43
23	b	607	CLA	C3B-C2B-C1B	-4.03	102.42	107.17
23	c	505	CLA	C3C-C4C-NC	4.02	115.58	110.43
23	c	512	CLA	C2B-C1B-NB	4.02	114.50	110.33
23	B	604	CLA	C2B-C1B-NB	4.02	114.50	110.33
23	C	511	CLA	C1D-CHD-C4C	-4.02	117.47	126.02
23	C	513	CLA	C3C-C4C-NC	4.02	115.58	110.43
23	c	507	CLA	O2D-CGD-CBD	4.02	118.25	111.23
23	c	504	CLA	CAC-C3C-C4C	4.01	130.00	124.79
23	a	409	CLA	C3B-C4B-NB	4.00	114.10	110.53
23	c	509	CLA	C1D-CHD-C4C	-4.00	117.51	126.02
23	c	507	CLA	C2B-C1B-NB	4.00	114.48	110.33
23	C	510	CLA	C3B-C4B-NB	4.00	114.10	110.53
25	K	102	BCR	C7-C8-C9	-4.00	120.32	126.23
23	C	506	CLA	C3D-C2D-C1D	-4.00	100.38	105.83
23	b	604	CLA	C1-C2-C3	-4.00	119.65	126.20
23	c	505	CLA	C1C-C2C-C3C	-4.00	102.78	106.98
23	B	601	CLA	C1D-CHD-C4C	-3.99	117.53	126.02
23	a	406	CLA	CBC-CAC-C3C	-3.99	101.60	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	515	BCR	C15-C14-C13	-3.99	121.68	127.28
23	D	406	CLA	CHD-C1D-ND	-3.99	119.19	124.80
23	b	612	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
23	B	615	CLA	CHD-C1D-ND	-3.99	119.19	124.80
23	C	511	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
23	B	601	CLA	O2D-CGD-O1D	-3.99	116.09	123.85
23	c	511	CLA	C1D-CHD-C4C	-3.98	117.55	126.02
26	A	410	SQD	C45-O47-C7	-3.98	108.26	117.80
23	C	508	CLA	C3D-C4D-ND	3.98	116.46	109.99
23	b	602	CLA	C2C-C1C-NC	3.98	114.16	109.98
23	B	611	CLA	C3C-C4C-NC	3.98	115.52	110.43
25	H	101	BCR	C11-C10-C9	-3.98	121.70	127.28
25	T	101	BCR	C11-C10-C9	-3.97	121.71	127.28
25	C	515	BCR	C33-C5-C6	-3.97	120.15	124.48
29	a	416	PL9	C7-C3-C2	-3.97	118.71	123.39
23	B	614	CLA	C3C-C4C-NC	3.97	115.52	110.43
25	c	515	BCR	C15-C14-C13	-3.97	121.71	127.28
23	c	512	CLA	C1-C2-C3	-3.96	119.70	126.20
23	B	608	CLA	C1C-C2C-C3C	-3.96	102.81	106.98
23	D	406	CLA	C3C-C4C-NC	3.96	115.50	110.43
23	c	513	CLA	C1D-CHD-C4C	-3.96	117.60	126.02
23	B	613	CLA	C1C-C2C-C3C	-3.96	102.81	106.98
23	D	405	CLA	C3C-C4C-NC	3.96	115.50	110.43
23	a	409	CLA	C3C-C4C-NC	3.96	115.50	110.43
23	B	608	CLA	C1D-CHD-C4C	-3.96	117.61	126.02
23	b	606	CLA	C2C-C1C-NC	3.96	114.14	109.98
23	b	613	CLA	O2D-CGD-CBD	3.96	118.15	111.23
23	C	512	CLA	CAC-C3C-C4C	3.95	129.93	124.79
23	c	503	CLA	C1D-CHD-C4C	-3.95	117.62	126.02
23	A	405	CLA	C2C-C1C-NC	3.95	114.13	109.98
23	c	512	CLA	C4A-NA-C1A	-3.95	104.88	106.68
23	b	615	CLA	C1D-CHD-C4C	-3.95	117.62	126.02
23	B	607	CLA	C2B-C1B-NB	3.95	114.42	110.33
23	B	602	CLA	O2D-CGD-O1D	-3.95	116.17	123.85
24	a	408	PHO	O2D-CGD-O1D	-3.95	116.17	123.85
23	c	510	CLA	CHD-C1D-ND	-3.95	119.25	124.80
23	B	611	CLA	C3B-C4B-NB	3.94	114.05	110.53
23	B	605	CLA	O2A-CGA-O1A	-3.94	113.77	123.63
25	y	101	BCR	C38-C26-C25	-3.94	120.18	124.48
23	C	514	CLA	C2C-C1C-NC	3.94	114.12	109.98
23	b	607	CLA	C1C-C2C-C3C	-3.94	102.84	106.98
25	k	101	BCR	C24-C23-C22	-3.94	120.41	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C1D-CHD-C4C	-3.94	117.65	126.02
23	b	610	CLA	O2A-CGA-CBA	3.94	123.84	111.83
23	b	609	CLA	CHD-C1D-ND	-3.93	119.27	124.80
35	c	517	DGD	O2G-C1B-C2B	3.93	119.99	111.48
23	b	608	CLA	C1C-C2C-C3C	-3.93	102.85	106.98
29	A	414	PL9	C37-C38-C39	-3.93	118.63	127.62
23	B	603	CLA	O2A-CGA-O1A	-3.93	113.81	123.63
26	a	411	SQD	C45-O47-C7	-3.93	108.40	117.80
29	a	416	PL9	C7-C8-C9	-3.93	120.07	126.83
25	D	407	BCR	C15-C14-C13	-3.92	121.78	127.28
23	a	406	CLA	CAA-C2A-C3A	-3.92	102.41	113.00
23	b	606	CLA	C1D-CHD-C4C	-3.92	117.69	126.02
23	d	403	CLA	C1-C2-C3	-3.91	119.78	126.20
23	b	610	CLA	CHD-C1D-ND	-3.91	119.29	124.80
23	b	613	CLA	C3D-C4D-ND	3.91	116.35	109.99
23	B	611	CLA	C1D-CHD-C4C	-3.91	117.70	126.02
34	B	626	HTG	C1'-S1-C1	3.91	108.90	100.45
23	A	404	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
23	C	509	CLA	C1D-CHD-C4C	-3.91	117.72	126.02
23	A	405	CLA	C1D-CHD-C4C	-3.90	117.72	126.02
23	c	503	CLA	C1C-C2C-C3C	-3.90	102.87	106.98
33	C	521	LMG	O6-C5-C4	3.90	116.73	109.70
29	d	405	PL9	C10-C9-C11	3.90	122.00	115.23
23	c	503	CLA	C3C-C4C-NC	3.90	115.42	110.43
23	B	606	CLA	C3D-C4D-ND	3.90	116.32	109.99
23	B	616	CLA	C2C-C1C-NC	3.90	114.08	109.98
23	c	514	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
23	C	504	CLA	C4-C3-C5	3.89	121.98	115.23
25	K	102	BCR	C3-C4-C5	-3.89	107.12	114.06
23	b	605	CLA	C1C-C2C-C3C	-3.89	102.89	106.98
23	b	601	CLA	C1D-CHD-C4C	-3.89	117.76	126.02
23	C	514	CLA	C1-C2-C3	-3.89	119.83	126.20
23	B	612	CLA	C4A-NA-C1A	-3.88	104.91	106.68
35	C	517	DGD	O2G-C1B-C2B	3.88	119.88	111.48
33	B	621	LMG	O7-C10-C11	3.88	119.88	111.48
38	E	103	HEM	CHD-C4C-NC	3.88	128.68	124.45
23	A	406	CLA	C1-C2-C3	-3.88	119.84	126.20
23	C	512	CLA	C3B-C4B-NB	3.88	113.99	110.53
33	c	520	LMG	O7-C10-C11	3.87	119.86	111.48
29	A	414	PL9	C7-C3-C2	-3.87	118.82	123.39
23	b	606	CLA	C3C-C4C-NC	3.87	115.39	110.43
23	C	511	CLA	CHD-C1D-ND	-3.87	119.35	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	CHD-C1D-ND	-3.87	119.36	124.80
23	a	405	CLA	C1D-CHD-C4C	-3.87	117.80	126.02
23	B	603	CLA	O2D-CGD-O1D	-3.87	116.32	123.85
23	C	506	CLA	C2B-C1B-NB	3.86	114.33	110.33
23	B	601	CLA	C3C-C4C-NC	3.86	115.38	110.43
23	c	507	CLA	C1D-CHD-C4C	-3.86	117.81	126.02
23	A	404	CLA	O2A-CGA-O1A	-3.86	113.97	123.63
23	c	511	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
23	a	407	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
23	b	614	CLA	CHD-C1D-ND	-3.86	119.38	124.80
23	b	604	CLA	C3D-C4D-ND	3.86	116.25	109.99
23	b	609	CLA	C1D-CHD-C4C	-3.85	117.84	126.02
23	c	511	CLA	C3B-C4B-NB	3.85	113.97	110.53
23	C	509	CLA	C2B-C1B-NB	3.85	114.32	110.33
23	b	616	CLA	C3C-C4C-NC	3.85	115.36	110.43
23	B	612	CLA	O2D-CGD-O1D	-3.84	116.37	123.85
23	C	503	CLA	C1D-CHD-C4C	-3.84	117.86	126.02
23	a	409	CLA	C1D-CHD-C4C	-3.84	117.86	126.02
23	b	604	CLA	C2B-C1B-NB	3.84	114.31	110.33
23	b	613	CLA	C3B-C4B-NB	3.84	113.96	110.53
23	C	509	CLA	O2D-CGD-O1D	-3.84	116.38	123.85
23	C	510	CLA	C1C-C2C-C3C	-3.84	102.95	106.98
23	B	609	CLA	C2B-C1B-NB	3.83	114.30	110.33
23	A	404	CLA	C3B-C4B-NB	3.83	113.95	110.53
26	a	411	SQD	C1-O5-C5	-3.83	106.23	113.72
23	C	506	CLA	CMB-C2B-C1B	3.83	131.25	125.42
23	A	408	CLA	C1D-CHD-C4C	-3.83	117.88	126.02
23	b	603	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
23	b	605	CLA	CHD-C4C-NC	3.83	130.17	124.23
23	b	612	CLA	C3B-C4B-NB	3.83	113.95	110.53
23	C	512	CLA	C1D-CHD-C4C	-3.83	117.88	126.02
29	a	416	PL9	C22-C23-C24	-3.83	118.86	127.62
23	B	614	CLA	C1D-CHD-C4C	-3.83	117.89	126.02
23	b	605	CLA	C1D-CHD-C4C	-3.82	117.89	126.02
23	c	506	CLA	C3D-C2D-C1D	-3.82	100.61	105.83
23	C	507	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
23	D	406	CLA	C1D-CHD-C4C	-3.82	117.90	126.02
23	a	407	CLA	C1D-CHD-C4C	-3.82	117.90	126.02
23	B	602	CLA	C2C-C1C-NC	3.82	114.00	109.98
23	a	405	CLA	O2D-CGD-CBD	3.82	117.91	111.23
23	a	409	CLA	CAA-C2A-C3A	-3.82	102.68	113.00
23	c	513	CLA	CHD-C1D-ND	-3.81	119.43	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	605	CLA	O2D-CGD-O1D	-3.81	116.42	123.85
23	c	504	CLA	C3C-C4C-NC	3.81	115.31	110.43
23	B	602	CLA	C3C-C4C-NC	3.81	115.31	110.43
23	B	608	CLA	C3C-C4C-NC	3.81	115.31	110.43
23	b	614	CLA	C3C-C4C-NC	3.81	115.31	110.43
23	b	609	CLA	C3B-C2B-C1B	-3.81	102.68	107.17
23	D	406	CLA	C2C-C1C-NC	3.81	113.98	109.98
23	A	405	CLA	CHD-C4C-NC	3.80	130.13	124.23
23	a	409	CLA	C1C-C2C-C3C	-3.80	102.98	106.98
23	a	407	CLA	CAA-C2A-C3A	-3.80	102.74	113.00
33	d	412	LMG	O7-C10-C11	3.79	119.69	111.48
24	a	353	PHO	O2D-CGD-O1D	-3.79	116.47	123.85
23	A	404	CLA	C1D-CHD-C4C	-3.79	117.96	126.02
29	a	416	PL9	C37-C38-C39	-3.79	118.95	127.62
23	b	611	CLA	C1D-CHD-C4C	-3.79	117.97	126.02
23	C	514	CLA	C3C-C4C-NC	3.79	115.28	110.43
23	B	606	CLA	C1C-C2C-C3C	-3.79	103.00	106.98
23	d	403	CLA	O2D-CGD-O1D	-3.79	116.48	123.85
33	C	521	LMG	C3-C4-C5	3.78	117.09	110.23
23	A	408	CLA	C3C-C4C-NC	3.78	115.27	110.43
23	B	616	CLA	CHD-C1D-ND	-3.78	119.48	124.80
34	b	625	HTG	C1'-S1-C1	3.78	108.61	100.45
26	f	102	SQD	C1-O5-C5	3.78	121.10	113.72
23	c	512	CLA	C1C-C2C-C3C	-3.77	103.01	106.98
23	B	610	CLA	CAA-C2A-C3A	-3.77	102.80	113.00
26	B	620	SQD	O7-S-C6	3.77	112.39	106.76
23	c	502	CLA	C1C-C2C-C3C	-3.77	103.02	106.98
23	C	508	CLA	C1D-CHD-C4C	-3.77	118.01	126.02
23	b	609	CLA	C3C-C4C-NC	3.76	115.25	110.43
23	C	504	CLA	O2D-CGD-CBD	3.76	117.81	111.23
23	B	614	CLA	O2A-CGA-O1A	-3.76	114.21	123.63
23	b	609	CLA	O2D-CGD-O1D	-3.76	116.52	123.85
23	b	614	CLA	C1D-CHD-C4C	-3.76	118.03	126.02
23	C	502	CLA	C1D-CHD-C4C	-3.76	118.03	126.02
23	B	608	CLA	CHD-C1D-ND	-3.76	119.52	124.80
23	B	616	CLA	C1D-CHD-C4C	-3.76	118.04	126.02
23	B	613	CLA	O2D-CGD-CBD	3.75	117.79	111.23
23	c	507	CLA	C3B-C2B-C1B	-3.75	102.75	107.17
23	b	612	CLA	C3D-C2D-C1D	-3.75	100.71	105.83
24	A	353	PHO	O2D-CGD-O1D	-3.75	116.55	123.85
29	A	414	PL9	C32-C33-C34	-3.75	119.05	127.62
23	c	512	CLA	C3C-C4C-NC	3.75	115.23	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
23	c	507	CLA	C4B-C3B-C2B	-3.73	102.66	107.30
23	A	404	CLA	C3C-C4C-NC	3.73	115.21	110.43
23	b	604	CLA	C3B-C4B-NB	3.73	113.86	110.53
23	b	608	CLA	C3B-C4B-NB	3.73	113.86	110.53
23	C	503	CLA	CHD-C1D-ND	-3.73	119.55	124.80
25	b	618	BCR	C15-C14-C13	-3.73	122.05	127.28
23	a	405	CLA	C3D-C2D-C1D	-3.73	100.74	105.83
23	b	613	CLA	C1D-CHD-C4C	-3.73	118.09	126.02
23	c	510	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
25	K	102	BCR	C24-C23-C22	-3.73	120.72	126.23
38	E	103	HEM	CBD-CAD-C3D	-3.73	102.23	112.53
23	B	613	CLA	C3B-C4B-NB	3.73	113.86	110.53
23	b	604	CLA	CHD-C1D-ND	-3.72	119.56	124.80
23	C	513	CLA	C1-C2-C3	-3.72	120.10	126.20
23	b	602	CLA	O2D-CGD-O1D	-3.72	116.61	123.85
23	b	616	CLA	CHD-C1D-ND	-3.72	119.57	124.80
23	B	612	CLA	C4C-C3C-C2C	-3.71	101.49	106.89
23	c	502	CLA	C1-C2-C3	-3.71	120.12	126.20
23	B	607	CLA	C1D-CHD-C4C	-3.71	118.14	126.02
23	B	611	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
33	c	521	LMG	O7-C10-C11	3.70	119.50	111.48
23	D	405	CLA	C2B-C1B-NB	3.70	114.17	110.33
23	C	509	CLA	C4C-C3C-C2C	-3.70	101.50	106.89
25	a	410	BCR	C20-C21-C22	-3.70	122.09	127.28
23	B	603	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
23	B	613	CLA	CMC-C2C-C1C	3.70	130.81	125.03
23	B	616	CLA	C4C-C3C-C2C	-3.70	101.51	106.89
23	b	602	CLA	CMB-C2B-C1B	3.69	131.04	125.42
33	a	419	LMG	O7-C10-C11	3.69	119.47	111.48
24	A	407	PHO	C1A-C2A-C3A	-3.68	99.33	102.84
33	C	501	LMG	C7-O1-C1	-3.68	105.90	113.80
23	C	505	CLA	C1D-CHD-C4C	-3.68	118.20	126.02
23	C	503	CLA	C3C-C4C-NC	3.68	115.14	110.43
25	B	618	BCR	C29-C30-C25	3.68	115.78	110.44
23	c	503	CLA	O2D-CGD-O1D	-3.67	116.70	123.85
23	b	610	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
23	b	610	CLA	O2D-CGD-O1D	-3.67	116.71	123.85
23	c	505	CLA	C1D-CHD-C4C	-3.66	118.23	126.02
23	b	610	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
23	c	508	CLA	CMB-C2B-C1B	3.66	130.99	125.42
23	a	406	CLA	CHD-C4C-NC	3.66	129.91	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	C1D-CHD-C4C	-3.66	118.24	126.02
23	C	505	CLA	CAC-C3C-C4C	3.65	129.54	124.79
23	b	614	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
37	d	408	LHG	O7-C7-C8	3.65	119.38	111.48
25	Y	101	BCR	C15-C14-C13	-3.64	122.17	127.28
23	A	408	CLA	O2D-CGD-CBD	3.64	117.60	111.23
23	A	405	CLA	CAA-C2A-C3A	-3.64	103.16	113.00
23	d	402	CLA	C1D-CHD-C4C	-3.64	118.28	126.02
23	B	608	CLA	O2D-CGD-O1D	-3.64	116.76	123.85
25	c	515	BCR	C16-C17-C18	-3.64	122.17	127.28
23	C	504	CLA	C3C-C4C-NC	3.64	115.09	110.43
23	C	502	CLA	C3C-C4C-NC	3.64	115.09	110.43
25	A	409	BCR	C24-C23-C22	-3.64	120.86	126.23
25	B	618	BCR	C15-C14-C13	-3.64	122.18	127.28
37	L	101	LHG	O7-C7-C8	3.64	119.35	111.48
29	A	414	PL9	C10-C9-C11	3.64	121.54	115.23
23	d	402	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
23	C	514	CLA	C1D-CHD-C4C	-3.63	118.30	126.02
23	B	605	CLA	CHD-C1D-ND	-3.63	119.70	124.80
23	c	514	CLA	C3C-C4C-NC	3.62	115.07	110.43
23	B	610	CLA	C4C-C3C-C2C	-3.62	101.62	106.89
23	b	601	CLA	O2D-CGD-O1D	-3.62	116.81	123.85
23	c	510	CLA	C3B-C4B-NB	3.62	113.76	110.53
23	b	609	CLA	C2B-C1B-NB	3.61	114.07	110.33
23	B	611	CLA	CHD-C1D-ND	-3.61	119.72	124.80
23	b	603	CLA	C3B-C4B-NB	3.61	113.75	110.53
23	c	514	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
23	c	503	CLA	CHD-C1D-ND	-3.61	119.72	124.80
23	C	506	CLA	CHD-C1D-ND	-3.60	119.73	124.80
23	B	610	CLA	C1-C2-C3	-3.60	120.30	126.20
23	C	505	CLA	C3B-C4B-NB	3.60	113.74	110.53
23	b	610	CLA	C3C-C4C-NC	3.60	115.04	110.43
23	B	610	CLA	C1D-CHD-C4C	-3.60	118.37	126.02
24	A	353	PHO	C1A-C2A-C3A	-3.60	99.42	102.84
38	e	87	HEM	CHD-C4C-NC	3.60	128.37	124.45
23	B	604	CLA	C3D-C4D-ND	3.60	115.83	109.99
23	C	503	CLA	O2D-CGD-O1D	-3.60	116.85	123.85
23	B	616	CLA	CMB-C2B-C1B	3.59	130.89	125.42
33	m	101	LMG	O7-C10-C11	3.59	119.25	111.48
23	B	609	CLA	C1D-CHD-C4C	-3.59	118.38	126.02
26	a	413	SQD	O47-C7-C8	3.59	119.25	111.48
23	a	405	CLA	O2A-CGA-CBA	3.59	122.78	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	C1-C2-C3	-3.59	120.32	126.20
23	C	508	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
38	e	87	HEM	CHA-C4D-ND	3.59	128.80	124.37
23	b	602	CLA	C3C-C4C-NC	3.59	115.02	110.43
23	B	612	CLA	C3B-C4B-NB	3.58	113.73	110.53
23	B	615	CLA	C1C-C2C-C3C	-3.58	103.21	106.98
23	b	602	CLA	C1D-CHD-C4C	-3.58	118.41	126.02
23	C	513	CLA	CHD-C1D-ND	-3.58	119.76	124.80
23	B	615	CLA	O2D-CGD-CBD	3.58	117.48	111.23
23	d	403	CLA	C2C-C1C-NC	3.58	113.74	109.98
25	k	101	BCR	C29-C30-C25	3.57	115.63	110.44
29	d	405	PL9	C32-C33-C34	-3.57	119.45	127.62
23	b	604	CLA	C1D-CHD-C4C	-3.57	118.43	126.02
23	C	508	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
23	A	406	CLA	C3C-C4C-NC	3.57	115.00	110.43
29	D	408	PL9	C37-C38-C39	-3.57	119.46	127.62
23	C	506	CLA	C1C-C2C-C3C	-3.57	103.23	106.98
40	V	202	HEC	CHA-C1A-NA	3.56	128.33	124.45
35	C	517	DGD	C3G-C2G-C1G	-3.56	103.48	111.78
23	b	607	CLA	C2B-C1B-NB	3.56	114.02	110.33
23	b	609	CLA	CAC-C3C-C4C	3.56	129.42	124.79
29	A	414	PL9	C27-C28-C29	-3.56	119.48	127.62
23	A	408	CLA	C1C-C2C-C3C	-3.56	103.24	106.98
23	b	614	CLA	CAC-C3C-C4C	3.55	129.41	124.79
23	B	615	CLA	CMC-C2C-C1C	3.55	130.58	125.03
23	B	616	CLA	O2D-CGD-O1D	-3.54	116.95	123.85
23	b	608	CLA	C1D-CHD-C4C	-3.54	118.49	126.02
23	c	506	CLA	C1-C2-C3	-3.54	120.39	126.20
23	b	611	CLA	O2D-CGD-O1D	-3.54	116.95	123.85
23	b	603	CLA	CAA-C2A-C3A	-3.54	103.44	113.00
33	C	501	LMG	O1-C1-C2	3.54	113.65	108.27
23	c	513	CLA	C1C-C2C-C3C	-3.54	103.26	106.98
23	A	406	CLA	C1C-C2C-C3C	-3.54	103.26	106.98
23	C	510	CLA	C3C-C4C-NC	3.54	114.96	110.43
23	b	615	CLA	C3B-C4B-NB	3.54	113.69	110.53
23	c	509	CLA	CHD-C1D-ND	-3.54	119.83	124.80
23	b	616	CLA	C4C-C3C-C2C	-3.53	101.75	106.89
23	c	508	CLA	O2D-CGD-O1D	-3.53	116.97	123.85
23	C	508	CLA	CMB-C2B-C1B	3.53	130.79	125.42
35	c	518	DGD	O2G-C1B-C2B	3.53	119.11	111.48
23	b	606	CLA	O2D-CGD-O1D	-3.53	116.99	123.85
23	B	610	CLA	CHD-C1D-ND	-3.52	119.84	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414	PL9	C15-C14-C16	3.52	121.34	115.23
23	C	512	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
23	c	512	CLA	C4-C3-C5	3.52	121.34	115.23
23	c	504	CLA	CMB-C2B-C1B	3.52	130.77	125.42
23	b	601	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
23	C	509	CLA	C1C-C2C-C3C	-3.51	103.28	106.98
23	B	605	CLA	CHD-C4C-NC	3.51	129.68	124.23
23	a	409	CLA	O2D-CGD-O1D	-3.51	117.01	123.85
23	b	603	CLA	O2A-CGA-O1A	-3.51	114.84	123.63
23	c	511	CLA	C3C-C4C-NC	3.51	114.92	110.43
23	C	512	CLA	CHD-C1D-ND	-3.51	119.87	124.80
23	D	405	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
23	C	512	CLA	C4A-NA-C1A	-3.51	105.08	106.68
23	b	607	CLA	C4B-C3B-C2B	-3.51	102.94	107.30
23	c	503	CLA	C1-C2-C3	-3.51	120.45	126.20
23	c	506	CLA	C4C-C3C-C2C	-3.51	101.79	106.89
23	B	602	CLA	C1D-CHD-C4C	-3.50	118.57	126.02
23	B	609	CLA	C4B-C3B-C2B	-3.50	102.95	107.30
23	b	608	CLA	C3C-C4C-NC	3.50	114.91	110.43
23	B	603	CLA	C4-C3-C5	3.50	121.30	115.23
23	a	405	CLA	CHD-C1D-ND	-3.50	119.88	124.80
23	B	608	CLA	C4B-C3B-C2B	-3.50	102.95	107.30
37	l	101	LHG	O8-C23-C24	3.50	122.50	111.83
29	a	416	PL9	C15-C14-C16	3.50	121.30	115.23
23	c	502	CLA	C1D-CHD-C4C	-3.50	118.59	126.02
23	b	603	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
23	b	615	CLA	CMB-C2B-C1B	3.49	130.73	125.42
23	B	613	CLA	CHD-C1D-ND	-3.49	119.90	124.80
23	b	606	CLA	C4-C3-C5	3.48	121.28	115.23
29	A	414	PL9	C17-C18-C19	-3.48	119.65	127.62
23	b	613	CLA	CHD-C1D-ND	-3.48	119.91	124.80
23	d	402	CLA	CHD-C1D-ND	-3.48	119.91	124.80
37	d	406	LHG	O7-C7-C8	3.47	119.00	111.48
23	A	405	CLA	C3C-C4C-NC	3.47	114.88	110.43
23	a	405	CLA	C4B-C3B-C2B	-3.47	102.98	107.30
29	a	416	PL9	C27-C28-C29	-3.47	119.68	127.62
33	z	101	LMG	O7-C10-C11	3.47	118.99	111.48
23	d	402	CLA	CAA-C2A-C3A	-3.47	103.62	113.00
33	Z	101	LMG	C1-C2-C3	3.47	117.31	110.01
23	b	605	CLA	C3C-C4C-NC	3.47	114.87	110.43
23	c	506	CLA	CMB-C2B-C1B	3.46	130.69	125.42
23	b	609	CLA	C1C-C2C-C3C	-3.46	103.34	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	CLA	C3B-C4B-NB	3.46	113.62	110.53
23	b	612	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
23	b	602	CLA	C1C-C2C-C3C	-3.46	103.34	106.98
23	c	509	CLA	CHD-C4C-NC	3.45	129.59	124.23
23	B	608	CLA	C1-C2-C3	-3.45	120.54	126.20
25	t	103	BCR	C7-C8-C9	-3.45	121.13	126.23
37	l	101	LHG	O7-C7-C8	3.45	118.95	111.48
33	c	521	LMG	O6-C5-C4	3.45	115.92	109.70
23	C	506	CLA	C3B-C4B-NB	3.45	113.61	110.53
23	C	503	CLA	C1C-C2C-C3C	-3.45	103.36	106.98
23	B	603	CLA	CBC-CAC-C3C	-3.44	103.08	112.42
23	C	511	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
23	B	616	CLA	C3B-C4B-NB	3.44	113.60	110.53
23	C	512	CLA	CMC-C2C-C1C	3.44	130.41	125.03
23	C	507	CLA	C1-C2-C3	-3.44	120.56	126.20
23	C	505	CLA	C3C-C4C-NC	3.43	114.83	110.43
23	b	602	CLA	CAA-C2A-C3A	-3.43	103.72	113.00
25	A	409	BCR	C33-C5-C6	-3.43	120.74	124.48
23	b	615	CLA	C3C-C4C-NC	3.43	114.82	110.43
23	B	607	CLA	C3C-C4C-NC	3.42	114.82	110.43
23	B	609	CLA	C1C-C2C-C3C	-3.42	103.38	106.98
23	c	504	CLA	C1C-C2C-C3C	-3.42	103.38	106.98
23	C	507	CLA	C3C-C4C-NC	3.42	114.81	110.43
23	A	408	CLA	CAA-C2A-C3A	-3.42	103.76	113.00
25	D	407	BCR	C37-C22-C23	3.41	123.30	118.09
29	a	416	PL9	C42-C43-C44	-3.41	119.81	127.62
23	d	403	CLA	C1D-CHD-C4C	-3.41	118.77	126.02
23	C	511	CLA	C3B-C4B-NB	3.41	113.58	110.53
23	b	610	CLA	O2A-CGA-O1A	-3.41	115.09	123.63
34	V	203	HTG	C1-O5-C5	3.41	116.75	112.19
23	C	504	CLA	C1C-C2C-C3C	-3.41	103.40	106.98
34	B	622	HTG	C1-O5-C5	3.40	118.67	112.56
23	B	603	CLA	O2A-CGA-CBA	3.40	122.21	111.83
23	c	508	CLA	C1D-CHD-C4C	-3.40	118.79	126.02
23	c	505	CLA	C4A-NA-C1A	-3.40	105.13	106.68
23	B	606	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
23	a	405	CLA	CHC-C1C-C2C	-3.40	117.28	126.95
23	B	604	CLA	C3B-C4B-NB	3.40	113.56	110.53
23	C	509	CLA	C4B-C3B-C2B	-3.40	103.08	107.30
25	d	404	BCR	C15-C14-C13	-3.40	122.51	127.28
25	A	409	BCR	C16-C17-C18	-3.40	122.52	127.28
23	c	507	CLA	C3C-C4C-NC	3.39	114.78	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	C3C-C4C-NC	3.39	114.78	110.43
23	C	511	CLA	C4-C3-C5	3.39	121.12	115.23
29	a	416	PL9	C30-C29-C31	3.39	121.11	115.23
24	a	408	PHO	CMA-C3A-C4A	-3.38	107.32	114.61
23	C	511	CLA	C3C-C4C-NC	3.38	114.76	110.43
23	B	612	CLA	C1C-C2C-C3C	-3.38	103.42	106.98
32	M	103	LMT	O5'-C5'-C4'	3.38	116.71	109.72
23	B	614	CLA	C4-C3-C5	3.38	121.09	115.23
23	B	603	CLA	CHD-C1D-ND	-3.38	120.05	124.80
25	C	516	BCR	C33-C5-C6	-3.38	120.80	124.48
23	B	615	CLA	C11-C10-C8	-3.38	104.75	115.97
23	C	507	CLA	C1D-CHD-C4C	-3.37	118.85	126.02
23	c	509	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
23	d	402	CLA	O2A-CGA-CBA	3.37	122.11	111.83
25	C	516	BCR	C16-C17-C18	-3.37	122.55	127.28
23	B	603	CLA	CAA-C2A-C3A	-3.36	103.91	113.00
23	B	605	CLA	C4C-C3C-C2C	-3.36	101.99	106.89
23	B	606	CLA	C3B-C4B-NB	3.36	113.53	110.53
23	b	614	CLA	C3B-C4B-NB	3.36	113.53	110.53
23	b	604	CLA	CMB-C2B-C1B	3.36	130.54	125.42
23	b	601	CLA	C4-C3-C5	3.36	121.06	115.23
23	a	409	CLA	C4B-C3B-C2B	-3.36	103.13	107.30
23	A	406	CLA	CAA-C2A-C3A	-3.36	103.93	113.00
23	b	603	CLA	O2A-CGA-CBA	3.35	122.06	111.83
23	d	403	CLA	C1C-C2C-C3C	-3.35	103.46	106.98
23	c	510	CLA	C3C-C4C-NC	3.35	114.72	110.43
37	D	409	LHG	O8-C23-O10	-3.35	115.25	123.63
24	a	353	PHO	C4-C3-C5	3.35	121.04	115.23
23	B	601	CLA	C1C-C2C-C3C	-3.35	103.46	106.98
23	B	609	CLA	C3B-C2B-C1B	-3.34	103.23	107.17
23	b	606	CLA	C1C-C2C-C3C	-3.34	103.47	106.98
23	c	511	CLA	C4-C3-C5	3.34	121.03	115.23
23	b	614	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
23	c	510	CLA	C1-O2A-CGA	3.34	124.73	116.65
23	C	514	CLA	C1C-C2C-C3C	-3.34	103.47	106.98
25	D	407	BCR	C24-C23-C22	-3.33	121.30	126.23
23	b	601	CLA	C3C-C4C-NC	3.33	114.70	110.43
26	A	412	SQD	O47-C7-C8	3.33	118.69	111.48
25	h	101	BCR	C16-C17-C18	-3.33	122.61	127.28
23	a	409	CLA	CHD-C1D-ND	-3.33	120.12	124.80
23	c	512	CLA	CHD-C4C-NC	3.33	129.39	124.23
25	y	101	BCR	C15-C14-C13	-3.32	122.62	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	101	BCR	C15-C16-C17	-3.32	116.72	123.52
23	B	601	CLA	C4C-C3C-C2C	-3.32	102.06	106.89
23	a	406	CLA	C3C-C4C-NC	3.32	114.68	110.43
34	b	622	HTG	C1'-S1-C1	3.32	107.62	100.45
23	C	513	CLA	C4C-C3C-C2C	-3.32	102.06	106.89
25	D	407	BCR	C33-C5-C6	-3.32	120.86	124.48
23	b	612	CLA	C4B-C3B-C2B	-3.31	103.18	107.30
23	c	502	CLA	C3C-C4C-NC	3.31	114.67	110.43
23	b	611	CLA	C1C-C2C-C3C	-3.31	103.50	106.98
23	c	507	CLA	CHC-C1C-C2C	-3.31	117.54	126.95
23	c	504	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
25	b	618	BCR	C7-C8-C9	-3.31	121.34	126.23
23	c	503	CLA	C3B-C4B-NB	3.31	113.48	110.53
23	b	616	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
23	D	406	CLA	CMC-C2C-C1C	3.31	130.20	125.03
37	d	406	LHG	O8-C23-O10	-3.30	115.36	123.63
23	C	511	CLA	CHD-C4C-NC	3.30	129.35	124.23
26	A	410	SQD	C44-O6-C1	-3.30	106.71	113.80
23	D	406	CLA	CMB-C2B-C1B	3.30	130.45	125.42
23	B	610	CLA	CAC-C3C-C4C	3.30	129.09	124.79
25	B	619	BCR	C38-C26-C25	-3.30	120.88	124.48
29	a	416	PL9	C17-C18-C19	-3.30	120.08	127.62
33	C	520	LMG	O8-C28-C29	3.30	121.89	111.83
23	B	612	CLA	C4B-C3B-C2B	-3.30	103.20	107.30
23	B	609	CLA	CMB-C2B-C1B	3.29	130.43	125.42
23	B	607	CLA	C4-C3-C5	3.29	120.94	115.23
23	C	514	CLA	C2A-C1A-CHA	-3.29	118.16	123.87
23	b	605	CLA	O2A-CGA-O1A	-3.29	115.40	123.63
23	a	407	CLA	C3B-C4B-NB	3.29	113.47	110.53
23	a	407	CLA	C3C-C4C-NC	3.29	114.64	110.43
37	D	411	LHG	O8-C23-O10	-3.28	115.41	123.63
23	B	608	CLA	O2A-CGA-O1A	-3.28	115.42	123.63
23	b	616	CLA	CHD-C4C-NC	3.28	129.32	124.23
23	b	605	CLA	CED-O2D-CGD	3.28	123.35	115.92
23	c	503	CLA	CMB-C2B-C1B	3.28	130.41	125.42
23	b	612	CLA	C4-C3-C5	3.27	120.91	115.23
23	C	507	CLA	CAC-C3C-C4C	3.27	129.05	124.79
23	A	405	CLA	CMC-C2C-C1C	3.27	130.15	125.03
23	b	616	CLA	O2A-CGA-CBA	3.27	121.81	111.83
25	a	410	BCR	C29-C30-C25	3.27	115.18	110.44
23	A	406	CLA	C3B-C4B-NB	3.27	113.44	110.53
23	c	512	CLA	C3B-C4B-NB	3.26	113.44	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	516	BCR	C38-C26-C25	-3.26	120.92	124.48
23	b	616	CLA	CMB-C2B-C1B	3.26	130.39	125.42
23	C	514	CLA	CMB-C2B-C1B	3.26	130.38	125.42
23	a	406	CLA	CMB-C2B-C1B	3.26	130.38	125.42
29	D	408	PL9	C27-C28-C29	-3.26	120.17	127.62
26	A	410	SQD	O7-S-C6	3.26	111.62	106.76
23	B	606	CLA	C4C-C3C-C2C	-3.26	102.15	106.89
25	C	516	BCR	C11-C10-C9	-3.26	122.71	127.28
23	B	609	CLA	C4C-C3C-C2C	-3.26	102.15	106.89
26	B	620	SQD	O48-C23-C24	3.25	121.76	111.83
23	d	402	CLA	C4C-C3C-C2C	-3.25	102.16	106.89
25	t	103	BCR	C3-C4-C5	-3.25	108.26	114.06
25	T	101	BCR	C12-C13-C14	-3.25	113.90	119.01
23	C	507	CLA	C4B-C3B-C2B	-3.25	103.26	107.30
23	A	408	CLA	CHD-C4C-NC	3.25	129.27	124.23
23	b	604	CLA	C11-C12-C13	-3.25	105.18	115.97
37	D	409	LHG	O8-C23-C24	3.24	121.73	111.83
23	C	514	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
38	E	103	HEM	CHD-C1D-ND	3.24	127.91	124.42
23	b	607	CLA	C4C-C3C-C2C	-3.24	102.18	106.89
29	D	408	PL9	C40-C39-C41	3.24	120.85	115.23
25	B	617	BCR	C16-C17-C18	-3.23	122.74	127.28
23	c	507	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
25	t	103	BCR	C11-C10-C9	-3.23	122.75	127.28
23	b	607	CLA	C1D-CHD-C4C	-3.23	119.15	126.02
23	a	409	CLA	C4-C3-C5	3.23	120.83	115.23
23	B	616	CLA	C4B-C3B-C2B	-3.23	103.29	107.30
38	E	103	HEM	C1B-NB-C4B	3.23	109.03	105.21
23	B	613	CLA	O2A-CGA-CBA	3.23	121.67	111.83
23	c	507	CLA	CBC-CAC-C3C	-3.23	103.67	112.42
40	V	202	HEC	CHD-C4C-NC	3.23	127.97	124.45
23	c	509	CLA	C1-C2-C3	-3.22	120.92	126.20
26	a	413	SQD	O48-C23-C24	3.22	121.66	111.83
26	a	411	SQD	O8-S-C6	3.22	112.19	105.97
32	M	101	LMT	O1'-C1'-C2'	3.22	113.16	108.27
25	A	409	BCR	C15-C14-C13	-3.22	122.76	127.28
23	C	510	CLA	O2A-CGA-CBA	3.22	121.65	111.83
25	k	101	BCR	C11-C10-C9	-3.22	122.77	127.28
23	C	507	CLA	CHC-C1C-C2C	-3.22	117.81	126.95
23	b	608	CLA	C4B-C3B-C2B	-3.22	103.30	107.30
23	c	504	CLA	C3B-C4B-NB	3.22	113.40	110.53
29	d	405	PL9	C37-C38-C39	-3.21	120.27	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	C1D-CHD-C4C	-3.21	119.19	126.02
23	b	612	CLA	O2A-CGA-CBA	3.21	121.63	111.83
37	D	409	LHG	O7-C7-C8	3.21	118.43	111.48
23	a	409	CLA	CBC-CAC-C3C	-3.21	103.71	112.42
23	B	614	CLA	CMC-C2C-C1C	3.21	130.05	125.03
25	c	515	BCR	C33-C5-C6	-3.21	120.98	124.48
23	a	405	CLA	C1-C2-C3	-3.21	120.94	126.20
23	B	613	CLA	C1D-CHD-C4C	-3.21	119.20	126.02
23	D	406	CLA	C1C-C2C-C3C	-3.21	103.61	106.98
23	b	615	CLA	CHC-C1C-C2C	-3.21	117.83	126.95
25	a	410	BCR	C11-C10-C9	-3.21	122.78	127.28
23	c	512	CLA	CBC-CAC-C3C	-3.20	103.73	112.42
23	c	513	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
23	b	612	CLA	C4C-C3C-C2C	-3.20	102.23	106.89
23	b	612	CLA	CHD-C1D-ND	-3.20	120.30	124.80
23	b	603	CLA	C4C-C3C-C2C	-3.20	102.23	106.89
38	e	87	HEM	CHD-C1D-ND	3.20	127.87	124.42
23	b	613	CLA	C4-C3-C5	3.20	120.78	115.23
29	d	405	PL9	C40-C39-C41	3.20	120.78	115.23
23	d	403	CLA	C3C-C4C-NC	3.20	114.53	110.43
23	C	506	CLA	C4C-C3C-C2C	-3.20	102.24	106.89
23	B	607	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
23	b	605	CLA	C4-C3-C5	3.20	120.78	115.23
23	B	605	CLA	C1C-C2C-C3C	-3.20	103.62	106.98
23	C	507	CLA	C3B-C4B-NB	3.20	113.38	110.53
26	a	411	SQD	C1-C2-C3	-3.20	103.29	110.01
23	B	610	CLA	O2A-CGA-O1A	-3.19	115.64	123.63
23	D	405	CLA	C3B-C4B-NB	3.19	113.38	110.53
23	B	602	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
25	c	515	BCR	C24-C23-C22	-3.19	121.52	126.23
23	b	604	CLA	O2A-CGA-CBA	3.19	121.56	111.83
25	t	103	BCR	C35-C13-C12	3.18	122.95	118.09
23	b	616	CLA	C2C-C1C-NC	3.18	113.33	109.98
23	b	611	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
23	a	405	CLA	O2A-CGA-O1A	-3.18	115.67	123.63
23	a	409	CLA	O2A-CGA-CBA	3.18	121.53	111.83
23	A	405	CLA	O2A-CGA-O1A	-3.18	115.67	123.63
23	C	510	CLA	CAC-C3C-C4C	3.18	128.93	124.79
23	b	616	CLA	C1-C2-C3	-3.18	120.99	126.20
23	c	508	CLA	C4-C3-C5	3.18	120.74	115.23
23	C	505	CLA	CMC-C2C-C1C	3.17	130.00	125.03
23	c	508	CLA	CMC-C2C-C1C	3.17	130.00	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	C4-C3-C5	3.17	120.73	115.23
23	b	603	CLA	CHD-C1D-ND	-3.17	120.34	124.80
23	A	404	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
23	c	508	CLA	CHD-C4C-NC	3.17	129.15	124.23
23	B	607	CLA	C3B-C4B-NB	3.17	113.36	110.53
37	D	411	LHG	O7-C7-C8	3.17	118.33	111.48
25	c	516	BCR	C21-C20-C19	-3.17	114.03	123.20
29	A	414	PL9	C42-C43-C44	-3.16	120.39	127.62
23	A	408	CLA	C4C-C3C-C2C	-3.16	102.29	106.89
23	b	605	CLA	CMB-C2B-C1B	3.16	130.23	125.42
23	a	405	CLA	C3C-C4C-NC	3.16	114.47	110.43
23	c	511	CLA	CBC-CAC-C3C	-3.15	103.87	112.42
23	c	508	CLA	CBC-CAC-C3C	-3.15	103.87	112.42
23	B	607	CLA	C1-C2-C3	-3.15	121.03	126.20
23	B	611	CLA	C4C-C3C-C2C	-3.15	102.31	106.89
23	A	408	CLA	C3B-C4B-NB	3.15	113.34	110.53
23	c	510	CLA	C4B-C3B-C2B	-3.15	103.39	107.30
23	b	609	CLA	C4B-C3B-C2B	-3.15	103.39	107.30
23	C	511	CLA	O2A-CGA-CBA	3.15	121.43	111.83
23	B	613	CLA	C4B-C3B-C2B	-3.15	103.39	107.30
23	B	615	CLA	CHD-C4C-NC	3.14	129.10	124.23
23	c	513	CLA	C4C-C3C-C2C	-3.14	102.32	106.89
23	b	610	CLA	CHD-C4C-NC	3.14	129.10	124.23
23	b	603	CLA	C2A-C1A-CHA	-3.14	118.42	123.87
23	a	409	CLA	CMA-C3A-C2A	-3.14	101.84	113.98
23	c	505	CLA	CAC-C3C-C4C	3.14	128.87	124.79
23	c	507	CLA	C4-C3-C5	3.14	120.67	115.23
26	A	412	SQD	O48-C23-C24	3.14	121.40	111.83
25	K	102	BCR	C10-C11-C12	-3.13	114.12	123.20
23	d	402	CLA	C4-C3-C5	3.13	120.67	115.23
23	c	506	CLA	C1C-C2C-C3C	-3.13	103.68	106.98
25	D	407	BCR	C10-C11-C12	-3.13	114.13	123.20
23	B	602	CLA	C1C-C2C-C3C	-3.13	103.69	106.98
37	e	101	LHG	O7-C7-C8	3.13	118.25	111.48
29	d	405	PL9	C20-C19-C21	3.13	120.65	115.23
25	D	407	BCR	C16-C17-C18	-3.13	122.89	127.28
23	A	405	CLA	CMA-C3A-C2A	-3.13	101.90	113.98
23	c	513	CLA	C4-C3-C5	3.12	120.65	115.23
23	B	601	CLA	C3B-C4B-NB	3.12	113.32	110.53
23	B	614	CLA	C2A-C1A-CHA	-3.12	118.45	123.87
23	C	508	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
29	A	414	PL9	C35-C34-C36	3.12	120.64	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	410	BCR	C7-C8-C9	-3.12	121.62	126.23
23	b	611	CLA	O2A-CGA-O1A	-3.12	115.83	123.63
23	C	502	CLA	CMB-C2B-C1B	3.12	130.16	125.42
23	B	614	CLA	CHD-C4C-NC	3.12	129.06	124.23
23	C	513	CLA	C1C-C2C-C3C	-3.12	103.70	106.98
25	B	619	BCR	C24-C23-C22	-3.12	121.63	126.23
23	b	607	CLA	CAC-C3C-C4C	3.11	128.84	124.79
23	C	502	CLA	CMC-C2C-C1C	3.11	129.90	125.03
40	v	202	HEC	CHD-C4C-NC	3.11	127.84	124.45
23	b	605	CLA	C2A-C1A-CHA	-3.11	118.47	123.87
23	A	406	CLA	CAC-C3C-C4C	3.11	128.84	124.79
23	D	406	CLA	C4-C3-C5	3.11	120.62	115.23
23	c	505	CLA	C4C-C3C-C2C	-3.11	102.37	106.89
23	b	610	CLA	CAA-C2A-C3A	-3.11	104.61	113.00
23	b	606	CLA	C4C-C3C-C2C	-3.11	102.37	106.89
23	c	514	CLA	C3B-C4B-NB	3.10	113.30	110.53
23	B	608	CLA	C4C-C3C-C2C	-3.10	102.38	106.89
23	B	603	CLA	C3B-C4B-NB	3.10	113.30	110.53
23	c	511	CLA	CHD-C4C-NC	3.10	129.04	124.23
23	b	603	CLA	C4B-C3B-C2B	-3.10	103.45	107.30
23	C	513	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
23	C	507	CLA	CAA-C2A-C3A	-3.10	104.63	113.00
23	b	616	CLA	CAC-C3C-C4C	3.10	128.82	124.79
23	c	502	CLA	CAC-C3C-C4C	3.10	128.82	124.79
23	c	506	CLA	CAC-C3C-C4C	3.09	128.82	124.79
23	c	504	CLA	C4C-C3C-C2C	-3.09	102.39	106.89
23	A	406	CLA	C4C-C3C-C2C	-3.09	102.39	106.89
23	B	607	CLA	CMB-C2B-C1B	3.09	130.13	125.42
38	e	87	HEM	CAD-CBD-CGD	3.09	121.86	113.67
23	B	607	CLA	CBC-CAC-C3C	-3.09	104.05	112.42
23	c	507	CLA	CAA-C2A-C3A	-3.09	104.66	113.00
25	T	101	BCR	C33-C5-C6	-3.09	121.12	124.48
23	B	612	CLA	CHD-C1D-ND	-3.09	120.46	124.80
37	d	406	LHG	O8-C23-C24	3.09	121.24	111.83
23	C	503	CLA	C4C-C3C-C2C	-3.08	102.41	106.89
23	c	506	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
25	t	103	BCR	C21-C20-C19	-3.08	114.28	123.20
23	B	614	CLA	C3B-C4B-NB	3.08	113.28	110.53
23	B	604	CLA	O2A-CGA-O1A	-3.08	115.93	123.63
23	b	609	CLA	C3B-C4B-NB	3.08	113.28	110.53
23	c	510	CLA	CHD-C4C-NC	3.07	129.00	124.23
23	C	514	CLA	C4C-C3C-C2C	-3.07	102.42	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	521	LMG	O8-C28-C29	3.07	121.20	111.83
23	C	506	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
23	C	502	CLA	CBC-CAC-C3C	-3.07	104.09	112.42
23	c	512	CLA	CMB-C2B-C1B	3.07	130.09	125.42
23	c	510	CLA	CAC-C3C-C4C	3.07	128.78	124.79
29	A	414	PL9	C22-C23-C24	-3.07	120.60	127.62
23	B	601	CLA	CHD-C4C-NC	3.07	128.99	124.23
23	D	406	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
23	d	403	CLA	CHD-C4C-NC	3.06	128.98	124.23
25	C	516	BCR	C15-C14-C13	-3.06	122.98	127.28
23	a	407	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
23	b	611	CLA	CHD-C4C-NC	3.06	128.98	124.23
35	C	518	DGD	O1G-C1A-C2A	3.06	121.17	111.83
23	C	509	CLA	CHD-C1D-ND	-3.06	120.50	124.80
23	B	610	CLA	C1C-C2C-C3C	-3.06	103.76	106.98
23	C	511	CLA	CBC-CAC-C3C	-3.06	104.13	112.42
33	Z	101	LMG	O6-C1-C2	3.06	116.65	110.37
23	B	614	CLA	CBC-CAC-C3C	-3.06	104.13	112.42
23	A	404	CLA	CAC-C3C-C4C	3.06	128.77	124.79
26	a	411	SQD	O47-C7-O49	-3.06	116.56	123.70
23	b	614	CLA	CMB-C2B-C1B	3.05	130.07	125.42
23	a	407	CLA	CHC-C1C-C2C	-3.05	118.27	126.95
23	b	602	CLA	C1-C2-C3	-3.05	121.20	126.20
23	B	616	CLA	CHD-C4C-NC	3.05	128.96	124.23
23	C	504	CLA	CAC-C3C-C4C	3.05	128.76	124.79
37	E	101	LHG	O8-C23-C24	3.05	121.13	111.83
35	C	518	DGD	O2G-C1B-C2B	3.05	118.07	111.48
25	h	101	BCR	C38-C26-C25	-3.05	121.16	124.48
23	B	604	CLA	CHD-C1D-ND	-3.05	120.52	124.80
23	B	607	CLA	CAA-C2A-C3A	-3.04	104.77	113.00
23	C	506	CLA	CMC-C2C-C1C	3.04	129.79	125.03
33	B	621	LMG	O8-C28-C29	3.04	121.12	111.83
23	b	611	CLA	C3B-C4B-NB	3.04	113.25	110.53
23	d	403	CLA	CMC-C2C-C1C	3.04	129.79	125.03
23	B	604	CLA	CHD-C4C-NC	3.04	128.95	124.23
23	a	407	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
25	b	619	BCR	C38-C26-C25	-3.04	121.17	124.48
25	y	101	BCR	C16-C17-C18	-3.04	123.02	127.28
23	C	513	CLA	O2A-CGA-CBA	3.04	121.10	111.83
23	C	512	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
23	a	407	CLA	CHD-C4C-NC	3.04	128.94	124.23
23	D	406	CLA	C4C-C3C-C2C	-3.04	102.47	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407	PHO	C1-C2-C3	-3.04	121.22	126.20
25	h	101	BCR	C7-C8-C9	-3.04	121.75	126.23
23	A	405	CLA	CMB-C2B-C1B	3.03	130.04	125.42
23	A	404	CLA	CAA-CBA-CGA	-3.03	104.59	113.21
23	B	615	CLA	C3B-C4B-NB	3.03	113.24	110.53
23	b	609	CLA	CMB-C2B-C1B	3.03	130.04	125.42
23	C	514	CLA	CMC-C2C-C1C	3.03	129.77	125.03
23	C	508	CLA	CHD-C4C-NC	3.03	128.93	124.23
23	c	511	CLA	C4B-C3B-C2B	-3.03	103.54	107.30
23	B	604	CLA	CMB-C2B-C1B	3.03	130.03	125.42
23	b	608	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
37	D	411	LHG	O8-C23-C24	3.02	121.06	111.83
23	B	615	CLA	C4C-C3C-C2C	-3.02	102.49	106.89
23	b	615	CLA	C11-C10-C8	-3.02	105.91	115.97
23	B	610	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
23	C	510	CLA	C4C-C3C-C2C	-3.02	102.49	106.89
23	C	504	CLA	C4C-C3C-C2C	-3.02	102.49	106.89
23	D	406	CLA	CHD-C4C-NC	3.02	128.91	124.23
29	a	416	PL9	C10-C9-C11	3.02	120.47	115.23
25	B	618	BCR	C11-C10-C9	-3.02	123.04	127.28
24	A	353	PHO	C6-C5-C3	-3.02	106.12	113.47
23	B	614	CLA	O2A-CGA-CBA	3.02	121.04	111.83
25	d	404	BCR	C33-C5-C6	-3.02	121.19	124.48
23	B	601	CLA	O2A-CGA-CBA	3.02	121.04	111.83
23	b	614	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
33	m	101	LMG	O8-C28-C29	3.02	121.03	111.83
40	v	202	HEC	CHA-C1A-NA	3.02	127.74	124.45
23	c	514	CLA	CAC-C3C-C4C	3.01	128.71	124.79
25	C	515	BCR	C16-C17-C18	-3.01	123.05	127.28
23	D	406	CLA	CAC-C3C-C4C	3.01	128.71	124.79
25	a	410	BCR	C38-C26-C25	-3.01	121.20	124.48
23	b	609	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
23	b	603	CLA	C7-C6-C5	-3.01	105.24	113.26
29	d	405	PL9	C12-C13-C14	-3.01	120.73	127.62
23	C	509	CLA	CHC-C1C-C2C	-3.01	118.40	126.95
23	A	408	CLA	CMA-C3A-C2A	-3.01	102.36	113.98
29	d	405	PL9	C7-C8-C9	-3.00	121.66	126.83
23	B	603	CLA	C4C-C3C-C2C	-3.00	102.52	106.89
23	A	404	CLA	CMC-C2C-C1C	3.00	129.72	125.03
25	T	101	BCR	C2-C1-C6	3.00	114.80	110.44
23	B	611	CLA	C4B-C3B-C2B	-3.00	103.58	107.30
23	C	506	CLA	C4B-C3B-C2B	-3.00	103.58	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	CHD-C4C-NC	3.00	128.88	124.23
25	K	102	BCR	C15-C14-C13	-3.00	123.08	127.28
23	c	514	CLA	C4C-C3C-C2C	-2.99	102.53	106.89
23	b	601	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
23	C	507	CLA	O2A-CGA-CBA	2.99	120.95	111.83
26	b	620	SQD	C1-O5-C5	-2.99	107.88	113.72
23	c	510	CLA	O2A-CGA-CBA	2.99	120.95	111.83
23	d	402	CLA	O2A-CGA-O1A	-2.99	116.15	123.63
23	a	405	CLA	CAA-C2A-C1A	-2.99	102.18	111.97
23	A	406	CLA	C2A-C1A-CHA	-2.99	118.68	123.87
23	A	406	CLA	O2A-CGA-O1A	-2.99	116.16	123.63
23	b	603	CLA	CMC-C2C-C1C	2.99	129.70	125.03
23	a	409	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
25	B	618	BCR	C28-C27-C26	-2.98	108.74	114.06
23	B	612	CLA	C4-C3-C5	2.98	120.40	115.23
29	D	408	PL9	C10-C9-C11	2.98	120.40	115.23
23	C	510	CLA	CHC-C1C-C2C	-2.98	118.48	126.95
23	b	613	CLA	C4C-C3C-C2C	-2.98	102.56	106.89
26	b	620	SQD	C3-C4-C5	2.98	115.63	110.23
23	C	504	CLA	CHC-C1C-C2C	-2.98	118.48	126.95
23	c	509	CLA	C4C-C3C-C2C	-2.98	102.56	106.89
23	b	601	CLA	CHC-C1C-C2C	-2.98	118.49	126.95
38	E	103	HEM	CHB-C1B-NB	2.97	128.04	124.37
23	b	601	CLA	CHD-C4C-NC	2.97	128.84	124.23
34	B	622	HTG	O5-C1-C2	2.97	114.41	110.32
23	A	404	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
23	b	604	CLA	CHC-C1C-C2C	-2.97	118.51	126.95
24	a	353	PHO	CMB-C2B-C3B	2.97	130.61	124.68
23	a	406	CLA	O2A-CGA-CBA	2.97	120.88	111.83
23	b	610	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
23	c	505	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
25	Y	101	BCR	C28-C27-C26	-2.96	108.78	114.06
23	B	603	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
38	e	87	HEM	CHB-C1B-NB	2.96	128.03	124.37
23	A	408	CLA	O2A-CGA-CBA	2.96	120.86	111.83
23	B	612	CLA	O2A-CGA-O1A	-2.96	116.23	123.63
25	y	101	BCR	C10-C11-C12	-2.96	114.63	123.20
23	A	408	CLA	CMA-C3A-C4A	-2.96	103.83	111.77
23	c	514	CLA	CMC-C2C-C1C	2.96	129.65	125.03
37	D	410	LHG	O8-C23-O10	-2.96	116.24	123.63
23	a	405	CLA	C4-C3-C5	2.95	120.36	115.23
23	b	615	CLA	C4B-C3B-C2B	-2.95	103.63	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	102	BCR	C2-C1-C6	2.95	114.73	110.44
38	e	87	HEM	C1B-NB-C4B	2.95	108.70	105.21
25	b	618	BCR	C38-C26-C25	-2.95	121.26	124.48
23	C	510	CLA	C4B-C3B-C2B	-2.95	103.63	107.30
23	d	403	CLA	CAA-C2A-C3A	-2.95	105.03	113.00
32	I	101	LMT	O1B-C4'-C3'	2.95	114.73	107.23
40	V	202	HEC	CBC-CAC-C3C	-2.95	121.54	127.43
23	b	613	CLA	O2A-CGA-CBA	2.95	120.82	111.83
26	a	411	SQD	O48-C23-C24	2.95	120.82	111.83
25	H	101	BCR	C38-C26-C25	-2.95	121.27	124.48
23	B	603	CLA	CHD-C4C-NC	2.95	128.80	124.23
40	v	202	HEC	CBC-CAC-C3C	-2.94	121.55	127.43
23	B	608	CLA	CHC-C1C-C2C	-2.94	118.58	126.95
23	b	606	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
23	c	506	CLA	CHD-C1D-ND	-2.94	120.66	124.80
23	c	513	CLA	CHD-C4C-NC	2.94	128.79	124.23
23	c	511	CLA	CHC-C1C-C2C	-2.94	118.59	126.95
23	B	607	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
23	b	602	CLA	CHD-C4C-NC	2.94	128.79	124.23
23	C	513	CLA	CHD-C4C-NC	2.94	128.79	124.23
23	B	611	CLA	CHD-C4C-NC	2.94	128.78	124.23
25	T	101	BCR	C35-C13-C12	2.94	122.57	118.09
23	B	606	CLA	O2A-CGA-CBA	2.93	120.78	111.83
23	B	608	CLA	CMA-C3A-C4A	-2.93	103.89	111.77
25	c	516	BCR	C33-C5-C6	-2.93	121.28	124.48
23	b	614	CLA	CHC-C1C-C2C	-2.93	118.61	126.95
23	b	604	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
33	a	419	LMG	O6-C5-C4	2.93	114.98	109.70
23	b	606	CLA	C3B-C4B-NB	2.93	113.14	110.53
23	b	612	CLA	CHC-C1C-C2C	-2.93	118.63	126.95
25	t	103	BCR	C1-C6-C7	2.93	123.58	115.65
23	c	512	CLA	CHC-C1C-C2C	-2.92	118.64	126.95
25	y	101	BCR	C37-C22-C23	2.92	122.55	118.09
23	C	510	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
23	C	502	CLA	C4-C3-C5	2.92	120.30	115.23
25	Y	101	BCR	C10-C11-C12	-2.92	114.74	123.20
23	a	405	CLA	C2A-C1A-CHA	-2.92	118.80	123.87
23	B	608	CLA	O2A-CGA-CBA	2.92	120.73	111.83
23	b	609	CLA	CBC-CAC-C3C	-2.92	104.52	112.42
24	A	353	PHO	C4-C3-C5	2.92	120.29	115.23
23	c	513	CLA	O2A-CGA-CBA	2.91	120.71	111.83
23	C	505	CLA	C4B-C3B-C2B	-2.91	103.68	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	406	CLA	CMA-C3A-C2A	-2.91	102.73	113.98
24	A	407	PHO	CMA-C3A-C4A	-2.91	108.34	114.61
23	D	406	CLA	CAA-C2A-C3A	-2.91	105.14	113.00
29	d	405	PL9	C27-C28-C29	-2.91	120.97	127.62
25	Y	101	BCR	C37-C22-C23	2.91	122.53	118.09
25	b	619	BCR	C2-C1-C6	2.91	114.66	110.44
25	B	618	BCR	C24-C23-C22	-2.91	121.94	126.23
24	a	408	PHO	C1A-C2A-C3A	-2.90	100.08	102.84
23	a	406	CLA	CHC-C1C-C2C	-2.90	118.70	126.95
23	B	613	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
23	b	614	CLA	CMC-C2C-C1C	2.90	129.57	125.03
38	e	87	HEM	C4D-ND-C1D	2.90	108.64	105.21
23	B	604	CLA	O2A-CGA-CBA	2.90	120.68	111.83
23	B	611	CLA	CHC-C1C-C2C	-2.90	118.70	126.95
23	c	514	CLA	C2A-C1A-CHA	-2.90	118.83	123.87
23	c	511	CLA	O2A-CGA-O1A	-2.90	116.38	123.63
23	b	602	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
23	C	507	CLA	CBC-CAC-C3C	-2.89	104.57	112.42
23	b	613	CLA	CHD-C4C-NC	2.89	128.72	124.23
35	c	519	DGD	O1G-C1A-C2A	2.89	120.66	111.83
37	d	408	LHG	O8-C23-C24	2.89	120.66	111.83
23	C	511	CLA	O2A-CGA-O1A	-2.89	116.39	123.63
23	C	512	CLA	C4B-C3B-C2B	-2.89	103.70	107.30
23	C	512	CLA	C4-C3-C5	2.89	120.25	115.23
25	C	515	BCR	C24-C23-C22	-2.89	121.96	126.23
23	C	504	CLA	CMB-C2B-C1B	2.89	129.82	125.42
23	b	605	CLA	C1-C2-C3	-2.89	121.47	126.20
23	c	503	CLA	CMC-C2C-C1C	2.89	129.55	125.03
23	c	505	CLA	CED-O2D-CGD	2.89	122.47	115.92
23	c	503	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
25	B	617	BCR	C31-C1-C6	-2.89	105.72	110.24
23	c	510	CLA	CMC-C2C-C1C	2.89	129.54	125.03
23	B	604	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
35	c	519	DGD	O2G-C1B-C2B	2.89	117.72	111.48
23	b	608	CLA	CHD-C4C-NC	2.89	128.71	124.23
23	b	605	CLA	C4C-C3C-C2C	-2.88	102.69	106.89
23	c	505	CLA	CMC-C2C-C1C	2.88	129.54	125.03
23	B	604	CLA	C4C-C3C-C2C	-2.88	102.69	106.89
23	a	409	CLA	CHC-C1C-C2C	-2.88	118.76	126.95
26	A	410	SQD	O48-C23-C24	2.88	120.62	111.83
23	C	505	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
23	B	615	CLA	CAC-C3C-C4C	2.88	128.54	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F	101	SQD	C44-O6-C1	-2.88	107.63	113.80
23	c	512	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
23	b	608	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
23	b	606	CLA	CHD-C4C-NC	2.88	128.69	124.23
23	c	505	CLA	CHC-C1C-C2C	-2.88	118.78	126.95
23	b	615	CLA	C4C-C3C-C2C	-2.88	102.71	106.89
23	d	403	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
23	b	601	CLA	CMB-C2B-C1B	2.87	129.80	125.42
25	T	101	BCR	C36-C18-C19	2.87	122.48	118.09
23	b	604	CLA	CMC-C2C-C1C	2.87	129.52	125.03
23	C	505	CLA	CHC-C1C-C2C	-2.87	118.78	126.95
23	c	502	CLA	CHC-C1C-C2C	-2.87	118.78	126.95
25	C	516	BCR	C38-C26-C25	-2.87	121.35	124.48
25	B	619	BCR	C2-C1-C6	2.87	114.61	110.44
25	b	618	BCR	C28-C27-C26	-2.87	108.94	114.06
23	A	406	CLA	O2A-CGA-CBA	2.87	120.58	111.83
23	d	403	CLA	CBC-CAC-C3C	-2.87	104.65	112.42
29	D	408	PL9	C7-C8-C9	-2.87	121.89	126.83
23	B	606	CLA	CHD-C4C-NC	2.86	128.67	124.23
23	B	607	CLA	CHC-C1C-C2C	-2.86	118.81	126.95
23	c	502	CLA	C3B-C4B-NB	2.86	113.09	110.53
23	b	614	CLA	O2A-CGA-CBA	2.86	120.57	111.83
25	T	101	BCR	C3-C4-C5	-2.86	108.95	114.06
23	D	405	CLA	C1D-CHD-C4C	-2.86	119.94	126.02
23	A	405	CLA	C4B-C3B-C2B	-2.86	103.74	107.30
35	H	102	DGD	O2G-C1B-C2B	2.86	117.67	111.48
23	b	603	CLA	C4-C3-C5	2.86	120.19	115.23
23	c	514	CLA	CAA-C2A-C3A	-2.86	105.28	113.00
23	c	511	CLA	O2A-CGA-CBA	2.86	120.55	111.83
23	b	607	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
23	b	609	CLA	C4-C3-C5	2.86	120.18	115.23
23	c	504	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
24	a	353	PHO	C4A-C3A-C2A	-2.85	100.12	102.84
23	b	611	CLA	C2A-C1A-CHA	-2.85	118.92	123.87
23	B	602	CLA	CMB-C2B-C1B	2.85	129.76	125.42
23	B	609	CLA	C3B-C4B-NB	2.85	113.08	110.53
23	C	502	CLA	CAC-C3C-C4C	2.85	128.50	124.79
23	b	602	CLA	C2A-C1A-CHA	-2.85	118.92	123.87
25	A	409	BCR	C11-C10-C9	-2.85	123.28	127.28
25	B	619	BCR	C3-C4-C5	-2.85	108.98	114.06
23	b	601	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
23	c	503	CLA	O2A-CGA-CBA	2.85	120.51	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	C3B-C4B-NB	2.85	113.07	110.53
23	B	607	CLA	CHD-C4C-NC	2.84	128.64	124.23
33	z	101	LMG	O8-C28-C29	2.84	120.50	111.83
23	b	613	CLA	C4B-C3B-C2B	-2.84	103.77	107.30
23	D	406	CLA	C4B-C3B-C2B	-2.84	103.77	107.30
23	D	405	CLA	CHC-C1C-C2C	-2.84	118.88	126.95
33	c	520	LMG	O8-C28-C29	2.84	120.49	111.83
29	A	414	PL9	C20-C19-C21	2.84	120.15	115.23
23	a	405	CLA	CAC-C3C-C4C	2.84	128.48	124.79
23	b	609	CLA	CMC-C2C-C1C	2.84	129.47	125.03
26	A	410	SQD	O9-S-C6	2.83	110.99	106.76
23	C	503	CLA	CHD-C4C-NC	2.83	128.63	124.23
23	c	503	CLA	C4B-C3B-C2B	-2.83	103.78	107.30
35	C	517	DGD	O6D-C1D-O3G	-2.83	103.35	110.04
29	a	416	PL9	C35-C34-C36	2.83	120.14	115.23
23	b	608	CLA	CHC-C1C-C2C	-2.83	118.90	126.95
23	C	510	CLA	O2A-CGA-O1A	-2.83	116.54	123.63
23	c	502	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
23	B	601	CLA	C4B-C3B-C2B	-2.83	103.78	107.30
23	D	405	CLA	C4B-C3B-C2B	-2.83	103.79	107.30
23	b	615	CLA	C4-C3-C5	2.83	120.13	115.23
23	b	614	CLA	O2A-CGA-O1A	-2.83	116.56	123.63
23	c	503	CLA	CHC-C1C-C2C	-2.83	118.92	126.95
23	C	506	CLA	CHD-C4C-NC	2.82	128.61	124.23
23	B	601	CLA	C1-C2-C3	-2.82	121.57	126.20
24	A	353	PHO	CMB-C2B-C3B	2.82	130.32	124.68
23	a	407	CLA	O2A-CGA-CBA	2.82	120.44	111.83
25	B	619	BCR	C34-C9-C8	2.82	122.40	118.09
23	B	613	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
23	C	513	CLA	C4-C3-C5	2.82	120.13	115.23
29	a	416	PL9	C25-C24-C26	2.82	120.13	115.23
24	a	353	PHO	C1A-C2A-C3A	-2.82	100.16	102.84
25	k	101	BCR	C10-C11-C12	-2.82	115.03	123.20
23	A	408	CLA	C4-C3-C5	2.82	120.12	115.23
25	K	102	BCR	C20-C21-C22	-2.82	123.33	127.28
23	C	514	CLA	CHD-C4C-NC	2.82	128.60	124.23
23	d	403	CLA	CAC-C3C-C4C	2.82	128.45	124.79
23	c	503	CLA	O2A-CGA-O1A	-2.81	116.59	123.63
23	C	511	CLA	CHC-C1C-C2C	-2.81	118.95	126.95
25	K	102	BCR	C11-C10-C9	-2.81	123.33	127.28
23	c	503	CLA	CBC-CAC-C3C	-2.81	104.80	112.42
23	c	510	CLA	CBC-CAC-C3C	-2.81	104.81	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	CHD-C4C-NC	2.81	128.58	124.23
23	A	405	CLA	C4-C3-C5	2.80	120.09	115.23
23	B	609	CLA	CHD-C4C-NC	2.80	128.58	124.23
40	v	202	HEC	CBA-CAA-C2A	-2.80	104.78	112.53
35	C	519	DGD	O1G-C1A-C2A	2.80	120.38	111.83
23	a	407	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
23	b	602	CLA	C1-O2A-CGA	2.80	123.42	116.65
23	B	610	CLA	CHC-C1C-C2C	-2.80	119.00	126.95
23	B	603	CLA	CMC-C2C-C1C	2.80	129.40	125.03
23	a	406	CLA	C3B-C4B-NB	2.79	113.03	110.53
23	b	605	CLA	CHC-C1C-C2C	-2.79	119.01	126.95
23	C	502	CLA	CHD-C4C-NC	2.79	128.56	124.23
23	d	402	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
23	A	404	CLA	CHC-C1C-C2C	-2.79	119.01	126.95
23	C	514	CLA	CAC-C3C-C4C	2.79	128.42	124.79
23	B	601	CLA	CMB-C2B-C1B	2.79	129.67	125.42
35	c	517	DGD	C2G-O2G-C1B	-2.79	111.11	117.80
23	d	403	CLA	CMB-C2B-C1B	2.79	129.67	125.42
23	B	608	CLA	CHD-C4C-NC	2.79	128.56	124.23
23	b	613	CLA	CHC-C1C-C2C	-2.79	119.02	126.95
23	b	602	CLA	CMC-C2C-C1C	2.79	129.39	125.03
23	c	514	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
23	c	505	CLA	CHD-C4C-NC	2.79	128.55	124.23
23	D	406	CLA	CBC-CAC-C3C	-2.79	104.86	112.42
29	A	414	PL9	C7-C3-C4	2.79	119.20	116.91
40	V	202	HEC	CHA-C4D-ND	2.78	128.91	123.86
23	c	514	CLA	C4-C3-C5	2.78	120.06	115.23
33	m	101	LMG	C8-O7-C10	-2.78	111.14	117.80
23	C	503	CLA	CHC-C1C-C2C	-2.78	119.04	126.95
23	B	606	CLA	CHC-C1C-C2C	-2.78	119.04	126.95
32	a	414	LMT	C1B-O5B-C5B	2.78	119.15	113.72
25	c	515	BCR	C28-C27-C26	-2.78	109.10	114.06
29	D	408	PL9	C25-C24-C26	2.78	120.06	115.23
23	C	506	CLA	C1-C2-C3	-2.78	121.64	126.20
23	A	406	CLA	C4B-C3B-C2B	-2.78	103.84	107.30
23	B	614	CLA	C4C-C3C-C2C	-2.78	102.85	106.89
23	C	507	CLA	C4C-C3C-C2C	-2.78	102.85	106.89
25	t	103	BCR	C37-C22-C23	2.78	122.33	118.09
23	B	612	CLA	O2A-CGA-CBA	2.78	120.30	111.83
23	a	409	CLA	CAC-C3C-C4C	2.78	128.40	124.79
23	B	606	CLA	C4-C3-C5	2.78	120.05	115.23
25	y	101	BCR	C21-C20-C19	-2.77	115.17	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	CMB-C2B-C1B	2.77	129.64	125.42
23	A	408	CLA	O2A-CGA-O1A	-2.77	116.70	123.63
23	B	603	CLA	CHC-C1C-C2C	-2.77	119.08	126.95
23	b	609	CLA	CHC-C1C-C2C	-2.77	119.08	126.95
26	F	101	SQD	C1-O5-C5	-2.77	108.32	113.72
35	h	102	DGD	O2G-C1B-C2B	2.77	117.47	111.48
23	a	409	CLA	O2A-CGA-O1A	-2.76	116.72	123.63
34	b	622	HTG	O5-C5-C4	2.76	114.68	109.70
29	D	408	PL9	C17-C18-C19	-2.76	121.30	127.62
23	c	508	CLA	CHC-C1C-C2C	-2.76	119.10	126.95
23	B	610	CLA	CAA-CBA-CGA	-2.76	105.37	113.21
35	H	102	DGD	O1G-C1A-C2A	2.76	120.25	111.83
23	b	614	CLA	C2A-C1A-CHA	-2.76	119.08	123.87
25	y	101	BCR	C11-C10-C9	-2.76	123.41	127.28
24	A	407	PHO	CMB-C2B-C3B	2.76	130.19	124.68
25	c	516	BCR	C15-C14-C13	-2.76	123.41	127.28
23	c	503	CLA	CAC-C3C-C4C	2.76	128.38	124.79
23	b	602	CLA	CMA-C3A-C4A	-2.76	104.36	111.77
29	A	414	PL9	C30-C29-C31	2.76	120.01	115.23
23	b	615	CLA	CAC-C3C-C4C	2.76	128.38	124.79
23	B	609	CLA	C1-O2A-CGA	2.76	123.32	116.65
23	a	407	CLA	CMB-C2B-C1B	2.75	129.61	125.42
25	D	407	BCR	C30-C25-C24	2.75	123.12	115.65
23	B	604	CLA	C6-C7-C8	-2.75	106.81	115.97
23	C	502	CLA	CHC-C1C-C2C	-2.75	119.12	126.95
23	c	505	CLA	C2A-C1A-CHA	-2.75	119.09	123.87
23	C	507	CLA	C4-C3-C5	2.75	120.00	115.23
23	d	403	CLA	C2A-C1A-CHA	-2.75	119.10	123.87
25	c	515	BCR	C38-C26-C25	-2.75	121.48	124.48
23	C	503	CLA	C4-C3-C5	2.75	120.00	115.23
29	d	405	PL9	C22-C23-C24	-2.75	121.34	127.62
23	b	607	CLA	CMB-C2B-C1B	2.75	129.60	125.42
23	B	613	CLA	C4-C3-C5	2.75	119.99	115.23
23	A	404	CLA	CAA-C2A-C1A	-2.75	102.98	111.97
23	B	603	CLA	C2A-C1A-CHA	-2.74	119.11	123.87
25	t	103	BCR	C7-C6-C5	-2.74	115.23	121.56
23	c	510	CLA	CHC-C1C-C2C	-2.74	119.16	126.95
23	b	615	CLA	CBC-CAC-C3C	-2.74	104.99	112.42
23	c	513	CLA	C3B-C4B-NB	2.74	112.98	110.53
29	a	416	PL9	C40-C39-C41	2.74	119.98	115.23
23	B	606	CLA	CAA-C2A-C3A	-2.74	105.60	113.00
23	b	606	CLA	O2A-CGA-O1A	-2.74	116.78	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	CLA	C2A-C1A-CHA	-2.74	119.12	123.87
33	D	415	LMG	O7-C10-C11	2.74	117.40	111.48
23	C	504	CLA	C3B-C4B-NB	2.74	112.97	110.53
29	D	408	PL9	C2-C1-C6	2.74	122.25	119.00
23	b	611	CLA	C4B-C3B-C2B	-2.73	103.90	107.30
25	T	101	BCR	C21-C20-C19	-2.73	115.28	123.20
23	b	604	CLA	O1D-CGD-CBD	-2.73	119.13	124.52
23	A	408	CLA	C2A-C1A-CHA	-2.73	119.13	123.87
23	b	611	CLA	CHC-C1C-C2C	-2.73	119.19	126.95
23	b	605	CLA	CBC-CAC-C3C	-2.73	105.02	112.42
23	c	507	CLA	CHD-C4C-NC	2.73	128.46	124.23
24	A	353	PHO	O2A-CGA-O1A	-2.73	116.81	123.63
23	A	404	CLA	O2D-CGD-CBD	2.73	116.00	111.23
23	A	405	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
23	B	605	CLA	C2A-C1A-CHA	-2.72	119.14	123.87
23	B	604	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
23	A	404	CLA	C1-C2-C3	-2.72	121.74	126.20
23	c	505	CLA	CMB-C2B-C1B	2.72	129.56	125.42
23	B	604	CLA	CMC-C2C-C1C	2.72	129.29	125.03
23	C	509	CLA	O2A-CGA-O1A	-2.72	116.82	123.63
26	a	413	SQD	O7-S-C6	2.72	110.82	106.76
34	B	626	HTG	C3-C4-C5	2.72	115.16	110.23
23	b	607	CLA	C4-C3-C5	2.72	119.94	115.23
35	C	519	DGD	O3G-C3G-C2G	-2.72	104.21	110.82
25	d	404	BCR	C3-C4-C5	-2.72	109.21	114.06
23	B	605	CLA	O2A-CGA-CBA	2.72	120.12	111.83
23	B	616	CLA	CHC-C1C-C2C	-2.72	119.23	126.95
23	C	508	CLA	C4-C3-C5	2.72	119.94	115.23
25	d	404	BCR	C40-C30-C25	-2.72	105.98	110.24
23	b	607	CLA	C1-C2-C3	-2.71	121.75	126.20
23	c	504	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
23	A	405	CLA	CMA-C3A-C4A	-2.71	104.48	111.77
23	d	402	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
25	c	515	BCR	C21-C20-C19	-2.71	115.34	123.20
23	c	504	CLA	C1-C2-C3	-2.71	121.75	126.20
23	C	512	CLA	CHC-C1C-C2C	-2.71	119.24	126.95
23	D	406	CLA	C2A-C1A-CHA	-2.71	119.16	123.87
33	c	521	LMG	C3-C4-C5	2.71	115.15	110.23
23	c	511	CLA	CMC-C2C-C1C	2.71	129.27	125.03
23	C	510	CLA	CMB-C2B-C1B	2.71	129.54	125.42
33	C	521	LMG	O8-C28-C29	2.71	120.09	111.83
23	b	606	CLA	CMC-C2C-C1C	2.71	129.27	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	CBC-CAC-C3C	-2.71	105.08	112.42
23	B	611	CLA	O2A-CGA-O1A	-2.71	116.86	123.63
23	C	502	CLA	C3B-C4B-NB	2.71	112.95	110.53
23	C	502	CLA	O2A-CGA-CBA	2.71	120.09	111.83
24	A	407	PHO	O1D-CGD-CBD	-2.71	120.62	124.72
29	D	408	PL9	C12-C13-C14	-2.71	121.43	127.62
23	B	602	CLA	C1-C2-C3	-2.71	121.76	126.20
26	f	102	SQD	O5-C1-C2	2.71	115.93	110.37
23	B	609	CLA	O2A-CGA-CBA	2.71	120.08	111.83
23	b	615	CLA	CHD-C4C-NC	2.70	128.42	124.23
23	c	513	CLA	CHC-C1C-C2C	-2.70	119.27	126.95
23	B	613	CLA	CHC-C1C-C2C	-2.70	119.27	126.95
32	a	414	LMT	O5'-C5'-C4'	2.70	115.31	109.72
23	a	406	CLA	C2A-C1A-CHA	-2.70	119.18	123.87
35	c	519	DGD	O3G-C3G-C2G	-2.70	104.25	110.82
23	c	509	CLA	C3B-C4B-NB	2.70	112.94	110.53
23	b	606	CLA	O2A-CGA-CBA	2.70	120.06	111.83
23	C	503	CLA	CBC-CAC-C3C	-2.70	105.11	112.42
25	B	617	BCR	C15-C14-C13	-2.70	123.50	127.28
25	k	101	BCR	C20-C21-C22	-2.70	123.50	127.28
23	D	405	CLA	O2A-CGA-CBA	2.70	120.06	111.83
23	a	405	CLA	CMA-C3A-C2A	-2.70	103.56	113.98
23	c	510	CLA	C4C-C3C-C2C	-2.70	102.97	106.89
23	C	503	CLA	C3B-C4B-NB	2.69	112.94	110.53
23	D	405	CLA	CAA-C2A-C3A	-2.69	105.72	113.00
23	c	514	CLA	O2A-CGA-CBA	2.69	120.05	111.83
23	D	405	CLA	CBC-CAC-C3C	-2.69	105.12	112.42
23	B	606	CLA	C4B-C3B-C2B	-2.69	103.96	107.30
25	b	618	BCR	C11-C10-C9	-2.69	123.51	127.28
23	C	502	CLA	C4B-C3B-C2B	-2.69	103.96	107.30
23	c	509	CLA	C2A-C1A-CHA	-2.69	119.20	123.87
23	B	612	CLA	CHC-C1C-C2C	-2.69	119.31	126.95
23	B	601	CLA	CHC-C1C-C2C	-2.69	119.31	126.95
33	z	101	LMG	C8-O7-C10	-2.68	111.37	117.80
33	d	412	LMG	O8-C28-O10	-2.68	116.91	123.63
23	B	614	CLA	CHC-C1C-C2C	-2.68	119.32	126.95
23	C	504	CLA	O2A-CGA-O1A	-2.68	116.92	123.63
24	A	353	PHO	C4A-C3A-C2A	-2.68	100.29	102.84
23	C	506	CLA	O2A-CGA-O1A	-2.68	116.92	123.63
23	C	505	CLA	CBC-CAC-C3C	-2.68	105.15	112.42
23	b	611	CLA	CMC-C2C-C1C	2.68	129.22	125.03
23	D	406	CLA	C3B-C4B-NB	2.68	112.92	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	CHC-C1C-C2C	-2.68	119.33	126.95
23	b	601	CLA	C2A-C1A-CHA	-2.68	119.22	123.87
26	A	410	SQD	O47-C7-O49	-2.68	117.44	123.70
23	c	502	CLA	CMB-C2B-C1B	2.68	129.50	125.42
23	C	509	CLA	CAC-C3C-C4C	2.68	128.27	124.79
23	c	513	CLA	CMA-C3A-C4A	-2.68	104.58	111.77
23	B	602	CLA	CHD-C4C-NC	2.68	128.38	124.23
23	c	506	CLA	CMC-C2C-C1C	2.68	129.22	125.03
37	e	101	LHG	O8-C23-C24	2.68	119.99	111.83
23	c	502	CLA	C4B-C3B-C2B	-2.67	103.98	107.30
25	b	619	BCR	C15-C14-C13	-2.67	123.53	127.28
23	C	513	CLA	CHC-C1C-C2C	-2.67	119.35	126.95
23	A	406	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
23	B	616	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
23	b	613	CLA	O2A-CGA-O1A	-2.67	116.95	123.63
25	b	618	BCR	C16-C17-C18	-2.67	123.54	127.28
23	b	611	CLA	O2A-CGA-CBA	2.67	119.97	111.83
23	B	604	CLA	CHC-C1C-C2C	-2.67	119.37	126.95
37	l	101	LHG	O8-C23-O10	-2.67	116.96	123.63
23	b	606	CLA	CHC-C1C-C2C	-2.67	119.37	126.95
23	b	609	CLA	CHD-C4C-NC	2.67	128.36	124.23
25	k	101	BCR	C16-C17-C18	-2.66	123.54	127.28
37	d	407	LHG	O7-C7-C8	2.66	117.24	111.48
23	b	609	CLA	O2A-CGA-CBA	2.66	119.96	111.83
23	B	614	CLA	CAC-C3C-C4C	2.66	128.25	124.79
23	b	606	CLA	CMB-C2B-C1B	2.66	129.47	125.42
23	D	405	CLA	C2A-C1A-CHA	-2.66	119.25	123.87
23	C	510	CLA	CBC-CAC-C3C	-2.66	105.21	112.42
23	a	406	CLA	C4B-C3B-C2B	-2.66	104.00	107.30
25	a	410	BCR	C10-C11-C12	-2.66	115.50	123.20
23	b	607	CLA	C2A-C1A-CHA	-2.66	119.25	123.87
23	C	513	CLA	C3B-C4B-NB	2.66	112.90	110.53
37	D	409	LHG	C5-O7-C7	-2.65	111.44	117.80
23	d	402	CLA	CBC-CAC-C3C	-2.65	105.22	112.42
23	b	610	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
37	d	407	LHG	O8-C23-O10	-2.65	117.00	123.63
23	b	610	CLA	C4-C3-C5	2.65	119.83	115.23
23	a	407	CLA	CAC-C3C-C4C	2.65	128.24	124.79
23	A	408	CLA	C4B-C3B-C2B	-2.65	104.01	107.30
23	B	607	CLA	C1-O2A-CGA	2.65	123.06	116.65
23	b	605	CLA	C3B-C4B-NB	2.65	112.89	110.53
23	B	613	CLA	C7-C6-C5	-2.64	106.21	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	409	BCR	C38-C26-C25	-2.64	121.60	124.48
23	b	616	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
23	b	615	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
23	B	615	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
23	c	502	CLA	C4-C3-C5	2.64	119.81	115.23
38	E	103	HEM	CHA-C4D-ND	2.64	127.63	124.37
37	L	101	LHG	O8-C23-C24	2.64	119.89	111.83
29	d	405	PL9	C17-C18-C19	-2.64	121.58	127.62
24	A	407	PHO	C4A-C3A-C2A	-2.64	100.33	102.84
23	D	405	CLA	CMC-C2C-C1C	2.64	129.16	125.03
23	c	506	CLA	C4-C3-C5	2.64	119.81	115.23
23	c	502	CLA	O2A-CGA-O1A	-2.63	117.04	123.63
23	C	508	CLA	CMC-C2C-C1C	2.63	129.15	125.03
23	B	610	CLA	C4B-C3B-C2B	-2.63	104.03	107.30
23	B	616	CLA	O2A-CGA-CBA	2.63	119.85	111.83
23	c	507	CLA	C4C-C3C-C2C	-2.63	103.06	106.89
23	C	511	CLA	C4C-C3C-C2C	-2.63	103.06	106.89
29	D	408	PL9	C51-C49-C50	2.63	120.64	114.59
23	B	612	CLA	CHD-C4C-NC	2.63	128.31	124.23
23	c	509	CLA	C4B-C3B-C2B	-2.63	104.03	107.30
33	Z	101	LMG	C9-C8-C7	-2.63	105.66	111.78
23	B	603	CLA	C5-C3-C2	-2.63	115.27	121.17
25	D	407	BCR	C3-C4-C5	-2.63	109.37	114.06
23	C	509	CLA	C2A-C1A-CHA	-2.63	119.31	123.87
23	c	510	CLA	C4-C3-C5	2.62	119.78	115.23
23	C	506	CLA	O2A-CGA-CBA	2.62	119.84	111.83
23	c	511	CLA	C4C-C3C-C2C	-2.62	103.07	106.89
29	D	408	PL9	C53-C6-C1	2.62	120.65	115.28
23	B	612	CLA	C6-C5-C3	-2.62	107.08	113.47
25	b	617	BCR	C20-C21-C22	-2.62	123.60	127.28
23	b	606	CLA	CAA-C2A-C3A	-2.62	105.92	113.00
23	C	504	CLA	CHD-C4C-NC	2.62	128.29	124.23
25	c	515	BCR	C8-C7-C6	-2.62	120.01	127.00
24	A	407	PHO	C4D-CHA-CBD	2.62	109.71	108.45
23	A	406	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
23	b	614	CLA	C4B-C3B-C2B	-2.61	104.05	107.30
23	b	604	CLA	C4C-C3C-C2C	-2.61	103.09	106.89
23	d	402	CLA	CAC-C3C-C4C	2.61	128.19	124.79
23	a	409	CLA	CMB-C2B-C1B	2.61	129.39	125.42
23	c	505	CLA	C4-C3-C5	2.61	119.75	115.23
23	b	608	CLA	CMA-C3A-C4A	-2.61	104.77	111.77
35	h	102	DGD	O1G-C1A-C2A	2.61	119.78	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	O2A-CGA-CBA	2.60	119.77	111.83
23	d	402	CLA	CMB-C2B-C1B	2.60	129.38	125.42
23	C	504	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
23	c	511	CLA	CAC-C3C-C4C	2.60	128.17	124.79
23	B	610	CLA	CHD-C4C-NC	2.60	128.26	124.23
23	c	508	CLA	O2A-CGA-CBA	2.60	119.75	111.83
40	v	202	HEC	C2A-C1A-NA	-2.60	107.82	110.32
25	d	404	BCR	C21-C20-C19	-2.60	115.68	123.20
23	B	613	CLA	O2A-CGA-O1A	-2.60	117.14	123.63
26	b	620	SQD	O48-C23-C24	2.59	119.74	111.83
25	B	619	BCR	C15-C14-C13	-2.59	123.64	127.28
23	b	603	CLA	CHC-C1C-C2C	-2.59	119.59	126.95
26	b	620	SQD	O8-S-C6	2.59	110.97	105.97
23	C	512	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
23	c	512	CLA	O2A-CGA-CBA	2.59	119.73	111.83
23	b	612	CLA	C2A-C1A-CHA	-2.59	119.38	123.87
23	c	509	CLA	CAA-C2A-C3A	-2.59	106.01	113.00
23	B	612	CLA	CAC-C3C-C4C	2.59	128.16	124.79
25	c	516	BCR	C37-C22-C23	2.59	122.04	118.09
23	C	502	CLA	C4C-C3C-C2C	-2.59	103.13	106.89
23	A	404	CLA	CHD-C4C-NC	2.59	128.24	124.23
25	a	410	BCR	C33-C5-C6	-2.58	121.67	124.48
23	b	602	CLA	CAC-C3C-C4C	2.58	128.15	124.79
25	A	409	BCR	C8-C7-C6	-2.58	120.10	127.00
23	C	502	CLA	C2A-C1A-CHA	-2.58	119.39	123.87
23	B	611	CLA	CMB-C2B-C1B	2.58	129.35	125.42
23	A	405	CLA	C3B-C4B-NB	2.58	112.83	110.53
23	A	408	CLA	CHC-C1C-C2C	-2.58	119.61	126.95
23	b	607	CLA	CAA-C2A-C3A	-2.58	106.02	113.00
25	k	101	BCR	C15-C14-C13	-2.58	123.66	127.28
40	v	202	HEC	C4B-NB-C1B	2.58	110.03	105.82
23	c	512	CLA	C4B-C3B-C2B	-2.58	104.10	107.30
23	A	406	CLA	CMC-C2C-C1C	2.58	129.06	125.03
23	b	603	CLA	CHD-C4C-NC	2.58	128.22	124.23
23	c	504	CLA	O2A-CGA-CBA	2.57	119.69	111.83
40	V	202	HEC	C2A-C1A-NA	-2.57	107.84	110.32
23	c	502	CLA	O2A-CGA-CBA	2.57	119.68	111.83
25	B	618	BCR	C33-C5-C6	-2.57	121.68	124.48
23	c	514	CLA	CHD-C4C-NC	2.57	128.22	124.23
24	a	408	PHO	O2A-CGA-CBA	2.57	119.67	111.83
25	B	619	BCR	C21-C20-C19	-2.57	115.75	123.20
24	a	408	PHO	O2A-CGA-O1A	-2.57	117.20	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	C4B-C3B-C2B	-2.57	104.11	107.30
25	d	404	BCR	C28-C27-C26	-2.57	109.47	114.06
40	V	202	HEC	C4B-NB-C1B	2.57	110.01	105.82
23	a	406	CLA	C1-C2-C3	-2.57	121.99	126.20
23	B	603	CLA	C6-C7-C8	-2.56	107.44	115.97
23	A	406	CLA	CHD-C4C-NC	2.56	128.21	124.23
35	c	518	DGD	O1G-C1A-C2A	2.56	119.65	111.83
23	b	611	CLA	CBC-CAC-C3C	-2.56	105.48	112.42
23	c	502	CLA	CHD-C4C-NC	2.56	128.20	124.23
23	c	509	CLA	O2A-CGA-CBA	2.56	119.63	111.83
23	C	513	CLA	CMB-C2B-C1B	2.56	129.31	125.42
23	A	405	CLA	O2A-CGA-CBA	2.55	119.62	111.83
23	C	512	CLA	O2A-CGA-CBA	2.55	119.62	111.83
23	C	506	CLA	CHC-C1C-C2C	-2.55	119.69	126.95
23	B	611	CLA	CBC-CAC-C3C	-2.55	105.50	112.42
23	B	606	CLA	CMC-C2C-C1C	2.55	129.02	125.03
23	c	502	CLA	CBC-CAC-C3C	-2.55	105.50	112.42
34	C	522	HTG	C1-O5-C5	2.55	117.14	112.56
32	M	103	LMT	C1'-O5'-C5'	2.55	118.70	113.72
29	D	408	PL9	C22-C23-C24	-2.55	121.79	127.62
25	t	103	BCR	C36-C18-C19	2.55	121.98	118.09
25	C	516	BCR	C15-C16-C17	-2.55	118.30	123.52
26	f	102	SQD	O47-C7-O49	-2.55	117.75	123.70
23	B	609	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
24	a	353	PHO	CBA-CAA-C2A	-2.55	106.28	113.78
23	B	603	CLA	C16-C15-C13	-2.54	107.51	115.97
23	c	502	CLA	CMC-C2C-C1C	2.54	129.01	125.03
23	b	602	CLA	CHC-C1C-C2C	-2.54	119.72	126.95
37	d	407	LHG	O8-C23-C24	2.54	119.59	111.83
23	d	402	CLA	CHC-C1C-C2C	-2.54	119.72	126.95
35	C	517	DGD	C2G-O2G-C1B	-2.54	111.71	117.80
32	t	101	LMT	C1'-O5'-C5'	2.54	118.68	113.72
23	a	409	CLA	CHD-C4C-NC	2.54	128.17	124.23
25	B	617	BCR	C29-C30-C25	2.54	114.13	110.44
25	T	101	BCR	C1-C6-C7	2.54	122.54	115.65
23	B	615	CLA	CBC-CAC-C3C	-2.54	105.54	112.42
23	b	606	CLA	C2A-C1A-CHA	-2.54	119.46	123.87
23	C	505	CLA	C4C-C3C-C2C	-2.54	103.20	106.89
23	B	605	CLA	C7-C6-C5	-2.54	106.50	113.26
40	v	202	HEC	CHB-C1B-NB	2.54	128.46	123.86
23	D	405	CLA	C4C-C3C-C2C	-2.53	103.20	106.89
33	d	412	LMG	O8-C28-C29	2.53	119.56	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	102	SQD	O48-C23-C24	2.53	119.55	111.83
26	F	101	SQD	O48-C23-C24	2.53	119.55	111.83
26	b	620	SQD	C44-O6-C1	-2.53	108.38	113.80
23	C	507	CLA	O2A-CGA-O1A	-2.53	117.31	123.63
23	C	511	CLA	C4B-C3B-C2B	-2.53	104.16	107.30
23	B	615	CLA	C4B-C3B-C2B	-2.53	104.16	107.30
23	B	602	CLA	CHB-C1B-C2B	-2.53	120.09	127.43
26	f	102	SQD	O5-C5-C4	2.53	114.25	109.70
23	C	510	CLA	CHD-C4C-NC	2.53	128.15	124.23
23	B	603	CLA	CAC-C3C-C4C	2.53	128.08	124.79
23	C	506	CLA	CAC-C3C-C4C	2.53	128.08	124.79
23	C	507	CLA	C2A-C1A-CHA	-2.53	119.48	123.87
26	F	101	SQD	O7-S-C6	2.52	110.53	106.76
29	d	405	PL9	C51-C49-C50	2.52	120.40	114.59
23	c	507	CLA	CGD-CBD-CAD	-2.52	102.68	110.85
32	I	101	LMT	O5'-C5'-C4'	2.52	114.94	109.72
37	D	410	LHG	O7-C7-C8	2.52	116.94	111.48
23	B	607	CLA	C2A-C1A-CHA	-2.52	119.49	123.87
23	B	605	CLA	C1-C2-C3	-2.52	122.06	126.20
23	b	612	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
29	A	414	PL9	C45-C44-C46	2.52	119.60	115.23
23	A	404	CLA	CED-O2D-CGD	2.52	121.63	115.92
23	c	505	CLA	C1-C2-C3	-2.52	122.07	126.20
25	D	407	BCR	C28-C27-C26	-2.52	109.56	114.06
23	b	607	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
23	B	614	CLA	C4-C3-C2	-2.52	117.16	123.63
33	D	415	LMG	O8-C28-O10	-2.52	117.33	123.63
23	B	614	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
23	c	512	CLA	CMC-C2C-C1C	2.51	128.96	125.03
23	d	402	CLA	CMC-C2C-C1C	2.51	128.96	125.03
23	B	610	CLA	C3B-C4B-NB	2.51	112.78	110.53
23	C	514	CLA	C4-C3-C5	2.51	119.59	115.23
24	a	353	PHO	C7-C6-C5	-2.51	106.56	113.26
23	C	512	CLA	CHD-C4C-NC	2.51	128.13	124.23
23	C	507	CLA	CHD-C4C-NC	2.51	128.13	124.23
23	C	509	CLA	C4-C3-C5	2.51	119.59	115.23
23	C	513	CLA	C4B-C3B-C2B	-2.51	104.18	107.30
26	F	101	SQD	O8-S-C6	2.51	110.82	105.97
25	c	516	BCR	C11-C10-C9	-2.51	123.76	127.28
23	b	616	CLA	OBD-CAD-C3D	-2.51	122.55	128.42
23	c	514	CLA	CHC-C1C-C2C	-2.51	119.83	126.95
23	B	605	CLA	C3B-C4B-NB	2.51	112.77	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	CMB-C2B-C1B	2.50	129.23	125.42
25	k	101	BCR	C36-C18-C19	2.50	121.91	118.09
25	b	619	BCR	C31-C1-C6	-2.50	106.32	110.24
23	c	514	CLA	C1-C2-C3	-2.50	122.10	126.20
23	C	514	CLA	C3B-C4B-NB	2.50	112.76	110.53
23	c	510	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
25	Y	101	BCR	C21-C20-C19	-2.50	115.96	123.20
25	b	619	BCR	C39-C30-C25	-2.50	106.32	110.24
29	A	414	PL9	C25-C24-C26	2.50	119.56	115.23
35	C	517	DGD	O3G-C3G-C2G	-2.50	104.74	110.82
23	d	403	CLA	C4-C3-C5	2.50	119.56	115.23
23	b	615	CLA	C11-C12-C13	-2.50	107.67	115.97
23	B	605	CLA	CMC-C2C-C1C	2.50	128.93	125.03
33	c	521	LMG	O8-C28-O10	-2.50	117.39	123.63
23	C	513	CLA	CMA-C3A-C4A	-2.49	105.07	111.77
23	a	409	CLA	CMC-C2C-C1C	2.49	128.93	125.03
23	b	611	CLA	CAC-C3C-C4C	2.49	128.03	124.79
25	B	618	BCR	C37-C22-C21	-2.49	118.78	122.82
23	C	503	CLA	C2A-C1A-CHA	-2.49	119.54	123.87
23	B	616	CLA	C2A-C1A-CHA	-2.49	119.55	123.87
25	H	101	BCR	C2-C3-C4	-2.49	105.81	111.28
25	d	404	BCR	C37-C22-C23	2.49	121.89	118.09
23	b	612	CLA	CHD-C4C-NC	2.49	128.09	124.23
23	B	616	CLA	CAC-C3C-C4C	2.49	128.03	124.79
23	D	406	CLA	CMA-C3A-C2A	-2.49	104.37	113.98
23	c	508	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
23	b	603	CLA	CAC-C3C-C4C	2.48	128.02	124.79
23	D	405	CLA	C4-C3-C5	2.48	119.54	115.23
23	B	610	CLA	C6-C7-C8	-2.48	107.71	115.97
23	B	605	CLA	C4B-C3B-C2B	-2.48	104.21	107.30
23	b	604	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
25	h	101	BCR	C10-C11-C12	-2.48	116.01	123.20
34	B	626	HTG	O5-C5-C4	2.48	114.17	109.70
24	A	407	PHO	O2A-CGA-CBA	2.48	119.40	111.83
23	B	607	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
23	b	607	CLA	CMC-C2C-C1C	2.48	128.91	125.03
23	b	608	CLA	CBC-CAC-C3C	-2.48	105.70	112.42
23	B	608	CLA	CHB-C4A-NA	2.48	127.98	124.40
37	d	408	LHG	O8-C23-O10	-2.48	117.43	123.63
25	Y	101	BCR	C34-C9-C8	2.48	121.87	118.09
23	B	611	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
38	e	87	HEM	C4C-NC-C1C	2.47	109.86	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	C4-C3-C5	2.47	119.52	115.23
25	Y	101	BCR	C16-C15-C14	-2.47	118.45	123.52
23	b	613	CLA	CED-O2D-CGD	2.47	121.53	115.92
23	a	407	CLA	C4-C3-C5	2.47	119.52	115.23
23	C	503	CLA	O2A-CGA-CBA	2.47	119.37	111.83
35	H	102	DGD	C2G-O2G-C1B	-2.47	111.89	117.80
23	b	616	CLA	CHC-C1C-C2C	-2.47	119.93	126.95
23	B	610	CLA	CMB-C2B-C1B	2.47	129.18	125.42
23	C	505	CLA	C2A-C1A-CHA	-2.47	119.59	123.87
25	b	618	BCR	C8-C7-C6	-2.47	120.41	127.00
24	a	353	PHO	C4D-CHA-CBD	2.47	109.64	108.45
23	c	507	CLA	CMB-C2B-C1B	2.47	129.17	125.42
23	B	609	CLA	CBC-CAC-C3C	-2.47	105.73	112.42
35	c	517	DGD	O1G-C1A-C2A	2.47	119.35	111.83
35	c	517	DGD	O6D-C1D-O3G	-2.47	104.22	110.04
33	Z	101	LMG	C4-C3-C2	2.47	115.16	110.83
23	B	601	CLA	CAC-C3C-C4C	2.46	128.00	124.79
23	c	505	CLA	CBC-CAC-C3C	-2.46	105.74	112.42
23	b	601	CLA	CBC-CAC-C3C	-2.46	105.74	112.42
25	y	101	BCR	C40-C30-C25	-2.46	106.38	110.24
23	A	408	CLA	CMB-C2B-C1B	2.46	129.16	125.42
23	C	505	CLA	C4-C3-C5	2.46	119.50	115.23
23	B	602	CLA	C2A-C1A-CHA	-2.46	119.60	123.87
23	A	405	CLA	C4C-C3C-C2C	-2.46	103.31	106.89
23	c	506	CLA	CHC-C1C-C2C	-2.46	119.97	126.95
40	V	202	HEC	CHB-C1B-NB	2.46	128.31	123.86
23	A	408	CLA	CMC-C2C-C1C	2.46	128.87	125.03
29	a	416	PL9	C20-C19-C21	2.46	119.49	115.23
23	b	614	CLA	CHD-C4C-NC	2.46	128.04	124.23
25	d	404	BCR	C16-C17-C18	-2.46	123.83	127.28
23	b	610	CLA	CMB-C2B-C1B	2.45	129.16	125.42
23	B	615	CLA	O2A-CGA-CBA	2.45	119.32	111.83
25	B	618	BCR	C2-C1-C6	2.45	114.00	110.44
23	C	507	CLA	CMC-C2C-C1C	2.45	128.87	125.03
23	B	602	CLA	CHC-C1C-C2C	-2.45	119.98	126.95
23	a	407	CLA	CBC-CAC-C3C	-2.45	105.78	112.42
23	A	405	CLA	CHC-C1C-C2C	-2.45	119.99	126.95
23	b	603	CLA	CMA-C3A-C2A	-2.45	104.52	113.98
34	b	625	HTG	C1-O5-C5	2.45	116.95	112.56
25	C	516	BCR	C21-C20-C19	-2.45	116.11	123.20
23	c	509	CLA	CHC-C1C-C2C	-2.45	119.99	126.95
23	b	605	CLA	O2A-CGA-CBA	2.44	119.29	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	H	101	BCR	C15-C14-C13	-2.44	123.85	127.28
23	c	511	CLA	CMB-C2B-C1B	2.44	129.14	125.42
23	C	509	CLA	O2A-CGA-CBA	2.44	119.28	111.83
29	A	414	PL9	C40-C39-C41	2.44	119.47	115.23
23	b	608	CLA	O2A-CGA-CBA	2.44	119.28	111.83
33	m	101	LMG	C7-O1-C1	-2.44	108.56	113.80
25	k	101	BCR	C33-C5-C6	-2.44	121.82	124.48
23	B	606	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
26	b	620	SQD	C1-C2-C3	-2.44	104.88	110.01
23	b	606	CLA	CAC-C3C-C4C	2.44	127.96	124.79
23	B	607	CLA	C4C-C3C-C2C	-2.44	103.34	106.89
32	D	404	LMT	O1B-C4'-C5'	-2.44	103.08	109.48
23	c	508	CLA	C3B-C4B-NB	2.44	112.71	110.53
24	a	408	PHO	CMB-C2B-C3B	2.44	129.55	124.68
23	D	405	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
25	T	101	BCR	C7-C6-C5	-2.44	115.94	121.56
25	H	101	BCR	C16-C15-C14	-2.44	118.53	123.52
23	C	514	CLA	O2A-CGA-CBA	2.44	119.26	111.83
23	B	608	CLA	CAC-C3C-C4C	2.44	127.96	124.79
23	C	510	CLA	CMC-C2C-C1C	2.43	128.84	125.03
23	C	503	CLA	C4B-C3B-C2B	-2.43	104.28	107.30
25	b	618	BCR	C24-C23-C22	-2.43	122.64	126.23
26	f	102	SQD	C4-C3-C2	-2.43	106.56	110.83
23	b	603	CLA	CMB-C2B-C1B	2.43	129.12	125.42
23	A	408	CLA	CAC-C3C-C4C	2.43	127.95	124.79
25	C	515	BCR	C10-C11-C12	-2.43	116.16	123.20
23	b	616	CLA	C4-C3-C5	2.43	119.44	115.23
23	b	610	CLA	CAA-CBA-CGA	-2.43	106.31	113.21
23	c	504	CLA	CMC-C2C-C1C	2.43	128.83	125.03
25	B	618	BCR	C37-C22-C23	2.43	121.80	118.09
33	D	415	LMG	O8-C28-C29	2.43	119.23	111.83
23	B	612	CLA	C2A-C1A-CHA	-2.42	119.66	123.87
23	B	602	CLA	O2A-CGA-CBA	2.42	119.22	111.83
29	A	414	PL9	C53-C6-C1	2.42	120.24	115.28
23	a	406	CLA	C4C-C3C-C2C	-2.42	103.37	106.89
29	a	416	PL9	C45-C44-C46	2.42	119.42	115.23
23	d	402	CLA	C2A-C1A-CHA	-2.42	119.67	123.87
23	d	403	CLA	CHC-C1C-C2C	-2.42	120.08	126.95
38	E	103	HEM	C4C-CHD-C1D	-2.42	120.88	126.02
35	C	518	DGD	O1G-C1A-O1A	-2.41	117.59	123.63
26	A	410	SQD	O48-C23-O10	-2.41	117.59	123.63
29	d	405	PL9	C36-C37-C38	-2.41	100.09	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	CLA	CHB-C4A-NA	2.41	127.88	124.40
23	B	602	CLA	C4B-C3B-C2B	-2.41	104.31	107.30
23	b	607	CLA	CBC-CAC-C3C	-2.41	105.89	112.42
23	b	608	CLA	CMC-C2C-C1C	2.41	128.79	125.03
25	H	101	BCR	C24-C23-C22	-2.41	122.68	126.23
35	H	102	DGD	O1G-C1A-O1A	-2.40	117.61	123.63
23	b	615	CLA	O2A-CGA-CBA	2.40	119.16	111.83
23	C	506	CLA	C11-C10-C8	-2.40	107.99	115.97
23	B	602	CLA	CAC-C3C-C4C	2.40	127.91	124.79
23	C	505	CLA	CMB-C2B-C1B	2.40	129.07	125.42
25	Y	101	BCR	C32-C1-C6	-2.40	106.49	110.24
25	a	410	BCR	C8-C7-C6	-2.40	120.60	127.00
23	B	605	CLA	CBC-CAC-C3C	-2.40	105.93	112.42
23	b	610	CLA	C2A-C1A-CHA	-2.39	119.71	123.87
24	a	408	PHO	CBA-CAA-C2A	-2.39	106.73	113.78
23	B	614	CLA	CMA-C3A-C2A	-2.39	104.73	113.98
26	a	413	SQD	C1-O5-C5	2.39	118.39	113.72
23	C	506	CLA	CBC-CAC-C3C	-2.39	105.94	112.42
23	d	402	CLA	CHD-C4C-NC	2.39	127.94	124.23
26	A	410	SQD	O9-S-O7	-2.39	106.05	113.82
26	B	620	SQD	O48-C23-O10	-2.39	117.65	123.63
25	c	516	BCR	C20-C21-C22	-2.39	123.92	127.28
25	b	617	BCR	C29-C30-C25	2.39	113.91	110.44
23	A	408	CLA	CBC-CAC-C3C	-2.39	105.94	112.42
25	A	409	BCR	C31-C1-C6	-2.39	106.50	110.24
25	B	618	BCR	C10-C11-C12	-2.39	116.28	123.20
23	A	406	CLA	CBC-CAC-C3C	-2.39	105.95	112.42
23	c	506	CLA	CHD-C4C-NC	2.39	127.93	124.23
29	a	416	PL9	C47-C48-C49	-2.38	119.69	127.64
26	a	411	SQD	C3-C4-C5	2.38	114.56	110.23
26	a	413	SQD	O5-C5-C4	2.38	114.00	109.70
23	c	504	CLA	O2A-CGA-O1A	-2.38	117.66	123.63
26	a	411	SQD	O4-C4-C3	-2.38	104.76	110.38
25	D	407	BCR	C24-C25-C26	-2.38	116.07	121.56
23	B	611	CLA	C2A-C1A-CHA	-2.38	119.74	123.87
23	c	513	CLA	C4B-C3B-C2B	-2.38	104.34	107.30
33	C	501	LMG	O8-C28-C29	2.38	119.08	111.83
26	B	620	SQD	C3-C4-C5	2.38	114.54	110.23
23	D	405	CLA	CMA-C3A-C4A	-2.38	105.39	111.77
34	b	625	HTG	O5-C5-C4	2.37	113.98	109.70
37	d	406	LHG	O7-C7-O9	-2.37	118.16	123.70
29	A	414	PL9	C2-C3-C4	2.37	121.97	118.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	h	102	DGD	O1G-C1A-O1A	-2.37	117.69	123.63
23	C	503	CLA	CAC-C3C-C4C	2.37	127.88	124.79
23	B	615	CLA	C1-C2-C3	-2.37	122.31	126.20
34	B	623	HTG	C1-C2-C3	2.37	115.18	110.55
23	B	610	CLA	CMA-C3A-C4A	-2.37	105.40	111.77
23	B	601	CLA	C2A-C1A-CHA	-2.37	119.75	123.87
35	c	519	DGD	O6E-C1E-O5D	-2.37	104.45	110.04
23	c	509	CLA	CMC-C2C-C1C	2.37	128.74	125.03
34	B	622	HTG	O2-C2-C3	-2.37	104.80	110.38
23	c	505	CLA	CHB-C4A-NA	2.37	127.81	124.40
32	e	102	LMT	O5'-C5'-C4'	2.36	114.61	109.72
23	b	613	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
34	B	626	HTG	C1-O5-C5	2.36	116.80	112.56
23	c	508	CLA	C1-C2-C3	-2.36	122.33	126.20
25	H	101	BCR	C2-C1-C6	2.36	113.87	110.44
23	c	509	CLA	C4-C3-C5	2.36	119.33	115.23
23	b	609	CLA	C2A-C1A-CHA	-2.36	119.77	123.87
25	K	102	BCR	C36-C18-C19	2.36	121.70	118.09
25	y	101	BCR	C35-C13-C12	2.36	121.69	118.09
23	B	613	CLA	CAA-C2A-C3A	-2.36	106.62	113.00
29	d	405	PL9	C30-C29-C31	2.36	119.32	115.23
40	V	202	HEC	CBA-CAA-C2A	-2.36	106.01	112.53
26	a	411	SQD	O48-C23-O10	-2.36	117.73	123.63
40	v	202	HEC	CHD-C1D-ND	2.36	128.14	123.86
24	a	353	PHO	CMA-C3A-C4A	-2.36	109.53	114.61
26	F	101	SQD	O47-C7-O49	-2.36	118.19	123.70
32	M	101	LMT	O1B-C1B-C2B	2.36	113.89	108.09
25	c	516	BCR	C23-C24-C25	-2.36	120.70	127.00
23	D	406	CLA	CHC-C1C-C2C	-2.36	120.25	126.95
29	d	405	PL9	C15-C14-C16	2.36	119.32	115.23
23	B	605	CLA	CHC-C1C-C2C	-2.36	120.25	126.95
23	b	612	CLA	C11-C10-C8	-2.35	108.14	115.97
23	D	405	CLA	CHD-C4C-NC	2.35	127.88	124.23
23	C	514	CLA	CHC-C1C-C2C	-2.35	120.26	126.95
23	c	513	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
33	B	621	LMG	O1-C1-C2	-2.35	104.70	108.27
23	b	601	CLA	C1-O2A-CGA	2.35	122.34	116.65
23	C	502	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
23	B	612	CLA	C11-C12-C13	-2.35	108.16	115.97
23	B	607	CLA	CMC-C2C-C1C	2.35	128.70	125.03
23	c	513	CLA	CBC-CAC-C3C	-2.35	106.06	112.42
23	B	602	CLA	C11-C12-C13	-2.35	108.17	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	CBA-CAA-C2A	-2.35	106.81	113.79
25	k	101	BCR	C2-C1-C6	2.35	113.85	110.44
33	z	101	LMG	C7-O1-C1	-2.35	108.77	113.80
26	F	101	SQD	C1-C2-C3	-2.34	105.08	110.01
23	C	512	CLA	CBC-CAC-C3C	-2.34	106.06	112.42
23	c	505	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
23	b	605	CLA	C4B-C3B-C2B	-2.34	104.39	107.30
23	B	615	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
25	K	102	BCR	C38-C26-C25	-2.34	121.93	124.48
23	c	509	CLA	CAC-C3C-C2C	2.34	131.86	127.56
29	D	408	PL9	C42-C41-C39	-2.34	105.43	113.19
25	t	103	BCR	C2-C1-C6	2.34	113.84	110.44
23	a	407	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
23	C	508	CLA	O2A-CGA-CBA	2.34	118.97	111.83
40	V	202	HEC	CBD-CAD-C3D	-2.34	106.06	112.53
23	d	403	CLA	C3B-C4B-NB	2.34	112.62	110.53
23	c	510	CLA	CMB-C2B-C1B	2.34	128.98	125.42
23	A	406	CLA	CMA-C3A-C2A	-2.34	104.95	113.98
25	c	516	BCR	C15-C16-C17	-2.33	118.74	123.52
25	K	102	BCR	C33-C5-C6	-2.33	121.94	124.48
23	b	608	CLA	C11-C10-C8	-2.33	108.22	115.97
35	c	518	DGD	O1G-C1A-O1A	-2.33	117.80	123.63
24	A	353	PHO	O2A-CGA-CBA	2.33	118.93	111.83
23	c	507	CLA	CAC-C3C-C4C	2.33	127.82	124.79
35	C	519	DGD	O2G-C1B-C2B	2.33	116.52	111.48
23	C	508	CLA	CHC-C1C-C2C	-2.32	120.34	126.95
23	B	613	CLA	C2A-C1A-CHA	-2.32	119.84	123.87
23	C	511	CLA	C4-C3-C2	-2.32	117.67	123.63
23	b	616	CLA	C3B-C4B-NB	2.32	112.60	110.53
23	C	509	CLA	CHD-C4C-NC	2.32	127.83	124.23
25	Y	101	BCR	C38-C26-C25	-2.32	121.95	124.48
35	c	517	DGD	O3G-C3G-C2G	-2.32	105.18	110.82
26	A	412	SQD	O48-C23-O10	-2.32	117.83	123.63
23	a	405	CLA	C4C-C3C-C2C	-2.32	103.52	106.89
23	C	510	CLA	C4-C3-C5	2.32	119.25	115.23
23	A	404	CLA	CMA-C3A-C2A	-2.32	105.03	113.98
29	d	405	PL9	C42-C41-C39	-2.32	105.51	113.19
35	C	519	DGD	O2G-C1B-O1B	-2.32	118.29	123.70
23	b	613	CLA	CBC-CAC-C3C	-2.32	106.14	112.42
23	C	506	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
23	C	514	CLA	CBC-CAC-C3C	-2.31	106.14	112.42
23	B	604	CLA	C11-C12-C13	-2.31	108.27	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	617	BCR	C37-C22-C23	2.31	121.62	118.09
23	B	615	CLA	C6-C7-C8	-2.31	108.27	115.97
23	A	404	CLA	C4-C3-C5	2.31	119.24	115.23
23	b	604	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
23	c	507	CLA	O2A-CGA-CBA	2.31	118.88	111.83
23	c	514	CLA	CMB-C2B-C1B	2.31	128.94	125.42
34	b	622	HTG	C6-C5-C4	-2.31	107.35	113.02
35	C	519	DGD	O1G-C1A-O1A	-2.31	117.85	123.63
40	v	202	HEC	CBD-CAD-C3D	-2.31	106.15	112.53
23	B	602	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
23	C	505	CLA	C1-O2A-CGA	2.31	122.24	116.65
23	c	512	CLA	C11-C10-C8	-2.31	108.30	115.97
33	C	520	LMG	O6-C5-C6	2.31	112.16	106.44
33	m	101	LMG	O7-C10-O9	-2.31	118.31	123.70
29	A	414	PL9	C51-C49-C50	2.31	119.89	114.59
37	D	410	LHG	O8-C23-C24	2.30	118.86	111.83
23	B	602	CLA	CMA-C3A-C2A	-2.30	105.07	113.98
23	B	606	CLA	C1-C2-C3	-2.30	122.42	126.20
25	t	103	BCR	C12-C13-C14	-2.30	115.39	119.01
23	c	502	CLA	C2A-C1A-CHA	-2.30	119.87	123.87
29	d	405	PL9	C53-C6-C1	2.30	119.99	115.28
23	B	612	CLA	CMC-C2C-C1C	2.30	128.63	125.03
23	a	409	CLA	CMA-C3A-C4A	-2.30	105.60	111.77
32	t	102	LMT	O1'-C1'-C2'	2.30	111.76	108.27
25	k	101	BCR	C7-C8-C9	-2.30	122.84	126.23
23	c	513	CLA	CHB-C4A-NA	2.29	127.71	124.40
32	e	102	LMT	O1B-C1B-C2B	2.29	113.73	108.09
40	V	202	HEC	CMD-C2D-C1D	2.29	128.91	125.42
25	C	515	BCR	C11-C10-C9	-2.29	124.06	127.28
35	c	519	DGD	O5D-C6D-C5D	-2.29	104.26	109.42
23	c	505	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
25	C	516	BCR	C36-C18-C19	2.29	121.59	118.09
25	c	515	BCR	C34-C9-C8	2.29	121.59	118.09
25	b	619	BCR	C3-C4-C5	-2.29	109.97	114.06
26	A	412	SQD	O8-S-C6	2.29	110.39	105.97
33	Z	101	LMG	C3-C4-C5	2.29	114.38	110.23
23	A	405	CLA	CAA-CBA-CGA	2.29	119.70	113.21
23	b	608	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
33	C	501	LMG	C8-O7-C10	-2.28	112.33	117.80
32	a	414	LMT	O5B-C5B-C4B	2.28	113.81	109.70
25	C	516	BCR	C3-C4-C5	-2.28	109.98	114.06
23	C	514	CLA	CAA-C2A-C3A	-2.28	106.83	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	404	BCR	C16-C15-C14	-2.28	118.85	123.52
23	b	609	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
23	b	616	CLA	CMC-C2C-C1C	2.28	128.60	125.03
37	E	101	LHG	O7-C7-O9	-2.28	118.37	123.70
25	k	101	BCR	C21-C20-C19	-2.28	116.60	123.20
23	C	507	CLA	CMB-C2B-C1B	2.28	128.89	125.42
23	b	602	CLA	O2A-CGA-CBA	2.27	118.77	111.83
23	C	511	CLA	CMB-C2B-C1B	2.27	128.88	125.42
26	a	411	SQD	C44-O6-C1	-2.27	108.92	113.80
23	C	510	CLA	C16-C15-C13	-2.27	108.41	115.97
26	F	101	SQD	C3-C4-C5	2.27	114.35	110.23
23	C	509	CLA	C7-C6-C5	-2.27	107.21	113.26
25	y	101	BCR	C15-C16-C17	-2.27	118.87	123.52
23	b	615	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
23	B	601	CLA	C4-C3-C5	2.27	119.17	115.23
25	a	410	BCR	C37-C22-C21	-2.27	119.14	122.82
23	B	606	CLA	C2A-C1A-CHA	-2.27	119.93	123.87
25	T	101	BCR	C29-C28-C27	-2.27	106.29	111.28
25	D	407	BCR	C29-C30-C25	2.27	113.73	110.44
40	v	202	HEC	CHA-C4D-ND	2.27	127.97	123.86
32	D	404	LMT	O5'-C5'-C4'	2.27	114.41	109.72
24	a	408	PHO	C4-C3-C5	2.27	119.16	115.23
23	c	504	CLA	CBC-CAC-C3C	-2.26	106.28	112.42
23	b	601	CLA	CAA-C2A-C3A	-2.26	106.88	113.00
29	a	416	PL9	C51-C49-C50	2.26	119.79	114.59
23	c	506	CLA	C2A-C1A-CHA	-2.26	119.94	123.87
23	C	513	CLA	CHB-C4A-NA	2.26	127.66	124.40
23	b	613	CLA	CMA-C3A-C4A	-2.26	105.70	111.77
32	D	404	LMT	O1B-C4'-C3'	2.26	112.97	107.23
23	b	602	CLA	CHB-C1B-C2B	-2.26	120.87	127.43
25	Y	101	BCR	C40-C30-C25	-2.26	106.70	110.24
25	b	618	BCR	C15-C16-C17	-2.26	118.90	123.52
23	b	602	CLA	C11-C10-C8	-2.26	108.46	115.97
23	b	604	CLA	C11-C10-C8	-2.26	108.46	115.97
29	A	414	PL9	C37-C36-C34	-2.26	105.70	113.19
25	c	515	BCR	C37-C22-C21	-2.26	119.16	122.82
23	B	608	CLA	CMC-C2C-C1C	2.26	128.56	125.03
29	D	408	PL9	C47-C48-C49	-2.26	120.12	127.64
25	B	617	BCR	C21-C20-C19	-2.25	116.67	123.20
23	C	514	CLA	C4B-C3B-C2B	-2.25	104.50	107.30
23	b	603	CLA	C5-C3-C2	-2.25	116.11	121.17
25	c	515	BCR	C16-C15-C14	-2.25	118.92	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	C2A-C1A-CHA	-2.25	119.97	123.87
23	c	510	CLA	CED-O2D-CGD	2.25	121.01	115.92
23	A	405	CLA	C2A-C1A-CHA	-2.25	119.97	123.87
23	B	608	CLA	C2A-C1A-CHA	-2.25	119.97	123.87
23	c	514	CLA	O2D-CGD-O1D	-2.25	119.48	123.85
23	b	608	CLA	C2A-C1A-CHA	-2.25	119.97	123.87
24	A	407	PHO	CBA-CAA-C2A	-2.24	107.17	113.78
23	b	602	CLA	C11-C12-C13	-2.24	108.50	115.97
23	B	611	CLA	OBD-CAD-C3D	-2.24	123.17	128.42
23	b	605	CLA	CAC-C3C-C2C	2.24	131.68	127.56
29	a	416	PL9	C53-C6-C1	2.24	119.87	115.28
25	d	404	BCR	C30-C25-C24	2.24	121.73	115.65
24	A	353	PHO	C4D-CHA-CBD	2.24	109.53	108.45
23	b	608	CLA	OBD-CAD-C3D	-2.24	123.18	128.42
23	D	406	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
23	b	602	CLA	CMA-C3A-C2A	-2.24	105.32	113.98
23	a	407	CLA	C2A-C1A-CHA	-2.24	119.98	123.87
33	m	101	LMG	O8-C28-O10	-2.24	118.03	123.63
23	b	608	CLA	CAC-C3C-C4C	2.24	127.70	124.79
23	b	614	CLA	CBC-CAC-C3C	-2.24	106.36	112.42
25	C	515	BCR	C21-C20-C19	-2.23	116.73	123.20
25	D	407	BCR	C21-C20-C19	-2.23	116.73	123.20
25	H	101	BCR	C31-C1-C6	-2.23	106.74	110.24
23	b	609	CLA	C16-C15-C13	-2.23	108.55	115.97
23	a	407	CLA	CMA-C3A-C2A	-2.23	105.35	113.98
37	l	101	LHG	O7-C7-O9	-2.23	118.49	123.70
23	b	601	CLA	CAC-C3C-C4C	2.23	127.69	124.79
25	b	619	BCR	C29-C30-C25	2.23	113.68	110.44
37	l	101	LHG	O4-P-O5	2.23	122.81	112.44
25	c	515	BCR	C34-C9-C10	-2.23	119.21	122.82
25	H	101	BCR	C7-C6-C5	2.23	126.68	121.56
25	b	619	BCR	C37-C22-C23	2.23	121.49	118.09
33	a	419	LMG	C7-O1-C1	-2.23	109.02	113.80
23	c	513	CLA	C1-O2A-CGA	2.23	122.04	116.65
23	a	406	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
25	A	409	BCR	C40-C30-C25	-2.22	106.75	110.24
23	a	405	CLA	CMA-C3A-C4A	-2.22	105.80	111.77
23	C	505	CLA	CHD-C4C-NC	2.22	127.68	124.23
32	M	101	LMT	C1-O1'-C1'	-2.22	109.88	113.68
24	a	408	PHO	C4A-C3A-C2A	-2.22	100.72	102.84
25	Y	101	BCR	C29-C28-C27	-2.22	106.39	111.28
23	b	607	CLA	CAA-CBA-CGA	2.22	119.52	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	419	LMG	O8-C28-C29	2.22	118.61	111.83
23	B	607	CLA	OBD-CAD-C3D	-2.22	123.22	128.42
23	B	604	CLA	C11-C10-C8	-2.22	108.58	115.97
23	C	511	CLA	CAA-C2A-C3A	-2.22	107.00	113.00
40	v	202	HEC	O2A-CGA-CBA	2.22	121.01	114.00
32	D	404	LMT	C3B-C4B-C5B	2.22	114.25	110.23
23	B	605	CLA	CAC-C3C-C2C	2.22	131.63	127.56
25	B	619	BCR	C2-C3-C4	-2.22	106.40	111.28
25	y	101	BCR	C23-C24-C25	-2.22	121.07	127.00
25	B	618	BCR	C38-C26-C25	-2.22	122.06	124.48
26	b	620	SQD	O47-C7-O49	-2.22	118.52	123.70
29	D	408	PL9	C15-C14-C16	2.22	119.08	115.23
23	d	403	CLA	CMA-C3A-C2A	-2.22	105.42	113.98
25	B	619	BCR	C20-C21-C22	-2.22	124.17	127.28
25	h	101	BCR	C20-C21-C22	-2.21	124.17	127.28
23	a	405	CLA	CHB-C4A-NA	2.21	127.60	124.40
25	b	619	BCR	C24-C23-C22	-2.21	122.96	126.23
29	A	414	PL9	C47-C48-C49	-2.21	120.26	127.64
23	d	403	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
24	A	353	PHO	OBD-CAD-C3D	-2.21	124.44	127.89
23	c	511	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
26	B	620	SQD	O47-C7-O49	-2.21	118.54	123.70
25	b	619	BCR	C7-C6-C5	2.21	126.65	121.56
23	C	507	CLA	OBD-CAD-C3D	-2.21	123.25	128.42
33	c	520	LMG	O8-C28-O10	-2.21	118.11	123.63
23	B	611	CLA	O2A-CGA-CBA	2.21	118.57	111.83
23	A	405	CLA	C1-C2-C3	-2.21	122.58	126.20
23	c	508	CLA	C4C-C3C-C2C	-2.20	103.68	106.89
24	a	408	PHO	C1-C2-C3	-2.20	122.58	126.20
25	a	410	BCR	C15-C16-C17	-2.20	119.01	123.52
25	b	619	BCR	C21-C20-C19	-2.20	116.81	123.20
23	d	403	CLA	O2A-CGA-CBA	2.20	118.55	111.83
23	a	405	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
23	C	510	CLA	C2A-C1A-CHA	-2.20	120.05	123.87
23	a	405	CLA	CHD-C4C-NC	2.20	127.64	124.23
35	c	519	DGD	O6D-C1D-O3G	-2.20	104.84	110.04
26	a	413	SQD	O48-C23-O10	-2.20	118.13	123.63
23	B	603	CLA	CHB-C1B-C2B	-2.20	121.04	127.43
25	A	409	BCR	C20-C21-C22	-2.20	124.19	127.28
23	C	504	CLA	C4-C3-C2	-2.20	117.98	123.63
23	c	503	CLA	C4-C3-C5	2.20	119.04	115.23
35	C	517	DGD	CDB-CCB-CBB	-2.20	103.26	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	C2A-C1A-CHA	-2.20	120.06	123.87
23	b	616	CLA	C1C-C2C-C3C	-2.20	104.67	106.98
23	B	610	CLA	C2A-C1A-CHA	-2.19	120.06	123.87
23	B	604	CLA	O1D-CGD-CBD	-2.19	120.19	124.52
23	b	611	CLA	CMB-C2B-C1B	2.19	128.76	125.42
23	b	611	CLA	C4-C3-C5	2.19	119.03	115.23
23	C	511	CLA	C6-C7-C8	-2.19	108.68	115.97
25	C	515	BCR	C20-C21-C22	-2.19	124.21	127.28
23	C	514	CLA	C11-C10-C8	-2.19	108.69	115.97
23	B	615	CLA	C2A-C1A-CHA	-2.19	120.07	123.87
34	B	623	HTG	O5-C1-C2	2.19	113.33	110.32
23	a	405	CLA	CMC-C2C-C1C	2.19	128.45	125.03
37	D	409	LHG	O7-C7-O9	-2.19	118.59	123.70
23	B	602	CLA	CED-O2D-CGD	2.19	120.88	115.92
38	E	103	HEM	CHA-C1A-NA	2.19	127.83	123.86
23	B	611	CLA	CMC-C2C-C1C	2.19	128.45	125.03
25	H	101	BCR	C29-C30-C25	2.18	113.61	110.44
23	B	611	CLA	C4-C3-C5	2.18	119.02	115.23
23	b	610	CLA	CMA-C3A-C2A	-2.18	105.55	113.98
23	B	601	CLA	C11-C12-C13	-2.18	108.72	115.97
25	T	101	BCR	C7-C8-C9	-2.18	123.01	126.23
23	B	612	CLA	C7-C6-C5	-2.18	107.45	113.26
25	a	410	BCR	C32-C1-C6	-2.18	106.83	110.24
23	B	609	CLA	CMC-C2C-C1C	2.18	128.44	125.03
23	B	606	CLA	O1D-CGD-CBD	-2.18	120.23	124.52
23	b	604	CLA	C6-C7-C8	-2.18	108.73	115.97
25	B	617	BCR	C11-C10-C9	-2.17	124.23	127.28
25	Y	101	BCR	C36-C18-C19	2.17	121.41	118.09
34	B	622	HTG	C1-C2-C3	2.17	114.80	110.55
23	b	610	CLA	C4B-C3B-C2B	-2.17	104.60	107.30
23	c	510	CLA	C2A-C1A-CHA	-2.17	120.10	123.87
23	C	508	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
23	d	403	CLA	C1-O2A-CGA	2.17	121.90	116.65
23	a	405	CLA	C17-C16-C15	-2.17	103.56	113.28
25	t	103	BCR	C29-C28-C27	-2.17	106.51	111.28
23	c	510	CLA	CAA-C2A-C3A	-2.17	107.14	113.00
25	d	404	BCR	C29-C30-C25	2.17	113.59	110.44
23	B	601	CLA	CAA-C2A-C3A	-2.17	107.15	113.00
23	b	607	CLA	CHD-C4C-NC	2.17	127.59	124.23
40	V	202	HEC	C4C-NC-C1C	2.17	109.35	105.82
23	b	616	CLA	C2A-C1A-CHA	-2.16	120.11	123.87
25	A	409	BCR	C36-C18-C19	2.16	121.39	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	406	CLA	O2A-CGA-CBA	2.16	118.43	111.83
23	B	606	CLA	OBD-CAD-C3D	-2.16	123.36	128.42
38	e	87	HEM	C3B-C4B-NB	-2.16	107.91	109.47
32	t	102	LMT	C1'-O5'-C5'	2.16	117.94	113.72
33	c	520	LMG	O7-C10-O9	-2.16	118.65	123.70
23	C	507	CLA	CED-O2D-CGD	2.16	120.82	115.92
23	C	507	CLA	CGD-CBD-CAD	-2.16	103.85	110.85
23	a	406	CLA	CED-O2D-CGD	2.16	120.81	115.92
23	d	403	CLA	CHB-C4A-NA	2.16	127.52	124.40
25	d	404	BCR	C38-C26-C27	2.16	118.20	113.60
25	B	618	BCR	C21-C20-C19	-2.16	116.95	123.20
23	B	616	CLA	O1D-CGD-CBD	-2.16	120.27	124.52
23	d	403	CLA	C4B-C3B-C2B	-2.15	104.62	107.30
23	C	513	CLA	CHB-C1B-C2B	-2.15	121.17	127.43
23	c	505	CLA	O2A-CGA-CBA	2.15	118.40	111.83
23	B	616	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
23	D	405	CLA	CMB-C2B-C1B	2.15	128.70	125.42
25	h	101	BCR	C37-C22-C21	-2.15	119.33	122.82
32	m	103	LMT	C1'-C2'-C3'	2.15	114.54	110.01
23	B	612	CLA	CMB-C2B-C3B	2.15	131.61	126.55
25	k	101	BCR	C34-C9-C8	2.15	121.37	118.09
33	C	520	LMG	O8-C28-O10	-2.15	118.25	123.63
23	c	512	CLA	CAC-C3C-C4C	2.15	127.59	124.79
25	C	516	BCR	C2-C1-C6	2.15	113.56	110.44
37	E	101	LHG	C5-O7-C7	-2.15	112.66	117.80
37	E	101	LHG	O8-C23-O10	-2.15	118.26	123.63
23	c	511	CLA	C2A-C1A-CHA	-2.15	120.14	123.87
23	a	409	CLA	CHB-C4A-NA	2.15	127.50	124.40
25	a	410	BCR	C40-C30-C25	-2.15	106.88	110.24
23	C	504	CLA	CHA-C1A-NA	-2.15	121.53	126.39
23	b	614	CLA	CMA-C3A-C2A	-2.14	105.69	113.98
25	b	619	BCR	C16-C15-C14	-2.14	119.14	123.52
23	b	607	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
23	D	406	CLA	C1-C2-C3	-2.14	122.69	126.20
29	D	408	PL9	C7-C3-C4	2.14	118.67	116.91
23	C	504	CLA	O2A-CGA-CBA	2.14	118.35	111.83
23	C	511	CLA	CMC-C2C-C1C	2.14	128.37	125.03
25	b	618	BCR	C21-C20-C19	-2.14	117.01	123.20
23	C	509	CLA	CHB-C4A-NA	2.14	127.48	124.40
23	b	608	CLA	C4-C3-C5	2.14	118.94	115.23
34	B	622	HTG	C1'-S1-C1	2.14	105.06	100.45
23	c	506	CLA	C4B-C3B-C2B	-2.13	104.65	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	C11-C10-C8	-2.13	108.88	115.97
37	D	409	LHG	O4-P-O5	2.13	122.36	112.44
38	E	103	HEM	O2A-CGA-CBA	2.13	120.73	114.00
35	c	517	DGD	O1G-C1A-O1A	-2.13	118.30	123.63
26	a	413	SQD	C3-C4-C5	2.13	114.10	110.23
25	C	516	BCR	C37-C22-C23	2.13	121.34	118.09
23	b	603	CLA	CBC-CAC-C3C	-2.13	106.65	112.42
23	b	610	CLA	CMC-C2C-C1C	2.13	128.36	125.03
23	b	613	CLA	CMC-C2C-C1C	2.13	128.36	125.03
23	C	511	CLA	C2A-C1A-CHA	-2.13	120.18	123.87
23	c	513	CLA	CHB-C1B-C2B	-2.13	121.25	127.43
23	c	506	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
23	B	601	CLA	CHB-C4A-NA	2.13	127.47	124.40
23	C	512	CLA	C11-C10-C8	-2.13	108.90	115.97
23	b	616	CLA	CBC-CAC-C3C	-2.13	106.66	112.42
23	C	506	CLA	CHA-C1A-NA	-2.12	121.58	126.39
23	D	405	CLA	OBD-CAD-C3D	-2.12	123.45	128.42
23	b	610	CLA	C3B-C4B-NB	2.12	112.42	110.53
38	e	87	HEM	CHA-C1A-NA	2.12	127.71	123.86
25	B	618	BCR	C16-C17-C18	-2.12	124.30	127.28
23	d	403	CLA	CHB-C1B-C2B	-2.12	121.27	127.43
23	b	606	CLA	C6-C7-C8	-2.12	108.92	115.97
38	E	103	HEM	O2D-CGD-CBD	2.12	120.69	114.00
25	h	101	BCR	C34-C9-C8	2.12	121.32	118.09
25	B	618	BCR	C7-C8-C9	-2.12	123.10	126.23
23	B	608	CLA	C4-C3-C5	2.11	118.90	115.23
23	C	512	CLA	CMB-C2B-C1B	2.11	128.64	125.42
23	B	605	CLA	CAA-C2A-C3A	-2.11	107.29	113.00
29	A	414	PL9	C12-C13-C14	-2.11	122.79	127.62
23	C	514	CLA	CMA-C3A-C2A	-2.11	105.82	113.98
23	C	504	CLA	CMC-C2C-C1C	2.11	128.33	125.03
23	B	613	CLA	CHB-C4A-NA	2.11	127.44	124.40
23	C	505	CLA	C6-C7-C8	-2.11	108.96	115.97
26	f	102	SQD	O7-S-C6	2.11	109.90	106.76
25	B	617	BCR	C10-C11-C12	-2.11	117.09	123.20
23	B	607	CLA	O2A-CGA-CBA	2.11	118.26	111.83
23	c	504	CLA	C2A-C1A-CHA	-2.11	120.21	123.87
23	b	606	CLA	CHB-C1B-C2B	-2.11	121.31	127.43
25	D	407	BCR	C29-C28-C27	-2.10	106.65	111.28
26	B	620	SQD	C1-C2-C3	-2.10	105.58	110.01
23	c	505	CLA	OBD-CAD-C3D	-2.10	123.50	128.42
29	d	405	PL9	C25-C24-C26	2.10	118.88	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	t	103	BCR	C33-C5-C4	2.10	118.08	113.60
23	B	610	CLA	CMC-C2C-C1C	2.10	128.32	125.03
25	B	619	BCR	C10-C11-C12	-2.10	117.11	123.20
23	c	506	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
23	B	609	CLA	C2A-C1A-CHA	-2.10	120.22	123.87
33	C	520	LMG	O7-C10-O9	-2.10	118.80	123.70
26	A	412	SQD	C46-C45-C44	-2.10	106.89	111.78
23	c	509	CLA	CMB-C2B-C3B	2.10	131.48	126.55
23	C	503	CLA	CED-O2D-CGD	2.09	120.67	115.92
33	B	621	LMG	C12-C11-C10	-2.09	106.02	113.69
23	d	402	CLA	CED-O2D-CGD	2.09	120.67	115.92
25	A	409	BCR	C21-C20-C19	-2.09	117.13	123.20
23	b	602	CLA	C4-C3-C5	2.09	118.86	115.23
32	a	420	LMT	O1B-C4'-C3'	2.09	112.55	107.23
23	a	406	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
38	E	103	HEM	CBA-CAA-C2A	-2.09	106.75	112.53
25	b	617	BCR	C15-C16-C17	-2.09	119.24	123.52
25	d	404	BCR	C24-C25-C26	-2.09	116.74	121.56
23	B	612	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
23	a	405	CLA	CBC-CAC-C3C	-2.09	106.76	112.42
23	b	615	CLA	CHA-C1A-NA	-2.09	121.67	126.39
35	C	518	DGD	O5D-C1E-C2E	2.09	111.44	108.27
23	c	511	CLA	CHB-C4A-NA	2.09	127.41	124.40
23	b	602	CLA	C4B-C3B-C2B	-2.08	104.71	107.30
23	c	513	CLA	CHA-C1A-NA	-2.08	121.67	126.39
35	C	519	DGD	C3G-C2G-C1G	-2.08	106.93	111.78
25	A	409	BCR	C29-C30-C25	2.08	113.46	110.44
24	A	407	PHO	O2D-CGD-O1D	-2.08	119.80	123.85
23	b	616	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
25	B	618	BCR	C40-C30-C25	-2.08	106.98	110.24
35	h	102	DGD	C3B-C2B-C1B	-2.08	106.08	113.69
23	c	513	CLA	CBA-CAA-C2A	-2.08	107.61	113.79
35	C	518	DGD	C2G-O2G-C1B	-2.08	112.83	117.80
32	a	414	LMT	C1'-O5'-C5'	2.08	117.77	113.72
23	a	409	CLA	C2A-C1A-CHA	-2.08	120.27	123.87
23	C	504	CLA	CHB-C1B-C2B	-2.08	121.40	127.43
38	e	87	HEM	CBD-CAD-C3D	-2.07	106.80	112.53
23	b	608	CLA	C6-C5-C3	-2.07	108.42	113.47
38	e	87	HEM	CHC-C1C-NC	2.07	126.71	124.45
33	a	419	LMG	C3-C4-C5	2.07	113.99	110.23
26	A	412	SQD	C1-C2-C3	-2.07	105.65	110.01
25	c	516	BCR	C24-C23-C22	-2.07	123.17	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	CMA-C3A-C4A	-2.07	106.20	111.77
23	C	512	CLA	C1-O2A-CGA	2.07	121.66	116.65
38	E	103	HEM	C3B-C4B-NB	-2.07	107.98	109.47
23	C	513	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
23	b	606	CLA	CBC-CAC-C3C	-2.07	106.81	112.42
23	C	504	CLA	CBC-CAC-C3C	-2.07	106.82	112.42
25	B	619	BCR	C16-C15-C14	-2.07	119.29	123.52
24	a	408	PHO	OBD-CAD-C3D	-2.06	124.67	127.89
25	c	516	BCR	C3-C4-C5	-2.06	110.38	114.06
23	C	508	CLA	CHB-C1B-C2B	-2.06	121.44	127.43
23	b	606	CLA	C1-O2A-CGA	2.06	121.64	116.65
23	b	604	CLA	C2A-C1A-CHA	-2.06	120.29	123.87
23	c	506	CLA	C3B-C4B-NB	2.06	112.37	110.53
25	t	103	BCR	C19-C18-C17	-2.06	115.77	119.01
35	c	518	DGD	O5D-C1E-C2E	2.06	111.40	108.27
23	A	406	CLA	CHB-C4A-NA	2.06	127.37	124.40
23	c	508	CLA	C4B-C3B-C2B	-2.06	104.74	107.30
23	B	604	CLA	C4-C3-C5	2.06	118.80	115.23
23	b	603	CLA	C11-C10-C8	-2.06	109.13	115.97
23	b	614	CLA	C4-C3-C2	-2.06	118.35	123.63
23	B	612	CLA	CAA-CBA-CGA	-2.06	107.37	113.21
23	B	604	CLA	C6-C5-C3	-2.05	108.46	113.47
38	E	103	HEM	C2A-C1A-NA	-2.05	107.87	110.15
23	B	613	CLA	CMB-C2B-C3B	2.05	131.38	126.55
23	c	507	CLA	CHB-C4A-NA	2.05	127.36	124.40
23	B	607	CLA	CAA-CBA-CGA	2.05	119.04	113.21
23	c	514	CLA	C11-C10-C8	-2.05	109.15	115.97
24	A	353	PHO	CMA-C3A-C4A	-2.05	110.19	114.61
26	F	101	SQD	O48-C23-O10	-2.05	118.50	123.63
25	a	410	BCR	C34-C9-C8	2.05	121.22	118.09
23	C	504	CLA	C2A-C1A-CHA	-2.05	120.31	123.87
23	C	502	CLA	C11-C12-C13	-2.05	109.16	115.97
23	b	612	CLA	OBD-CAD-C3D	-2.05	123.63	128.42
24	a	353	PHO	O2A-CGA-CBA	2.05	118.08	111.83
23	b	612	CLA	CMB-C2B-C3B	2.05	131.36	126.55
23	c	511	CLA	CAA-C2A-C3A	-2.05	107.47	113.00
23	a	409	CLA	C1-C2-C3	-2.05	122.85	126.20
23	c	508	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
25	C	516	BCR	C35-C13-C12	2.04	121.21	118.09
23	C	508	CLA	C16-C15-C13	-2.04	109.17	115.97
23	c	514	CLA	CBC-CAC-C3C	-2.04	106.88	112.42
23	B	614	CLA	CAA-C2A-C3A	-2.04	107.48	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	CHB-C4A-NA	2.04	127.35	124.40
32	A	359	LMT	O5B-C5B-C4B	2.04	113.38	109.70
23	c	511	CLA	CED-O2D-CGD	2.04	120.55	115.92
25	c	515	BCR	C11-C12-C13	-2.04	120.77	126.36
29	a	416	PL9	C47-C46-C44	-2.04	106.43	113.19
25	K	102	BCR	C29-C30-C25	2.04	113.40	110.44
23	c	507	CLA	C2A-C1A-CHA	-2.04	120.33	123.87
29	a	416	PL9	C10-C9-C8	-2.04	118.40	123.63
25	b	618	BCR	C33-C5-C6	-2.04	122.26	124.48
23	c	502	CLA	CHB-C1B-C2B	-2.03	121.52	127.43
23	b	602	CLA	CHB-C4A-NA	2.03	127.33	124.40
23	C	508	CLA	C6-C7-C8	-2.03	109.21	115.97
24	A	407	PHO	OBD-CAD-C3D	-2.03	124.72	127.89
29	D	408	PL9	C36-C37-C38	-2.03	101.96	112.02
29	a	416	PL9	C12-C13-C14	-2.03	122.97	127.62
26	f	102	SQD	O8-S-C6	2.03	109.89	105.97
25	c	515	BCR	C37-C22-C23	2.03	121.19	118.09
23	c	509	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
35	C	517	DGD	O1G-C1A-O1A	-2.03	118.55	123.63
33	Z	101	LMG	C1-O6-C5	2.03	117.68	113.72
23	c	502	CLA	C6-C7-C8	-2.03	109.23	115.97
24	A	407	PHO	C4-C3-C5	2.03	118.74	115.23
23	c	514	CLA	CED-O2D-CGD	2.03	120.51	115.92
26	A	412	SQD	C1-O5-C5	-2.03	109.77	113.72
23	c	511	CLA	C4-C3-C2	-2.02	118.43	123.63
23	B	615	CLA	CED-O2D-CGD	2.02	120.50	115.92
23	C	512	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
23	B	615	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
23	B	615	CLA	CHA-C1A-NA	-2.02	121.82	126.39
23	a	407	CLA	CMC-C2C-C1C	2.02	128.19	125.03
35	C	517	DGD	O1G-C1A-C2A	2.02	117.99	111.83
23	C	505	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
29	A	414	PL9	C47-C46-C44	-2.02	106.49	113.19
23	B	604	CLA	CHA-C1A-NA	-2.02	121.82	126.39
26	A	412	SQD	C44-O6-C1	-2.02	109.47	113.80
34	d	411	HTG	C1-O5-C5	2.02	116.18	112.56
23	B	602	CLA	CMC-C2C-C1C	2.02	128.18	125.03
25	H	101	BCR	C3-C4-C5	-2.01	110.47	114.06
23	B	601	CLA	CMC-C2C-C1C	2.01	128.18	125.03
29	d	405	PL9	C40-C39-C38	-2.01	118.46	123.63
23	C	506	CLA	C2A-C1A-CHA	-2.01	120.37	123.87
23	c	510	CLA	C4-C3-C2	-2.01	118.46	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	CMC-C2C-C1C	2.01	128.18	125.03
23	c	508	CLA	C6-C7-C8	-2.01	109.28	115.97
25	C	516	BCR	C31-C1-C6	-2.01	107.09	110.24
23	C	510	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
35	c	517	DGD	C3G-C2G-C1G	-2.01	107.10	111.78
23	b	610	CLA	CBC-CAC-C3C	-2.01	106.97	112.42
23	b	608	CLA	C6-C7-C8	-2.01	109.28	115.97
33	C	501	LMG	O7-C10-O9	-2.01	119.01	123.70
29	D	408	PL9	O1-C4-C3	-2.01	118.61	120.73
23	B	603	CLA	C7-C6-C5	-2.01	107.91	113.26
35	c	517	DGD	O2G-C1B-O1B	-2.01	119.01	123.70
23	a	405	CLA	CAA-CBA-CGA	-2.01	107.51	113.21
23	B	608	CLA	CBC-CAC-C3C	-2.01	106.98	112.42
23	C	508	CLA	CAC-C3C-C2C	2.00	131.24	127.56
23	d	403	CLA	C6-C7-C8	-2.00	109.30	115.97
26	a	411	SQD	O9-S-C6	2.00	109.75	106.76
23	C	513	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
33	a	419	LMG	C8-O7-C10	-2.00	113.00	117.80
25	A	409	BCR	C11-C12-C13	-2.00	120.87	126.36
25	b	617	BCR	C32-C1-C6	-2.00	107.10	110.24
23	B	602	CLA	C4-C3-C5	2.00	118.70	115.23
26	A	412	SQD	O6-C1-C2	2.00	111.31	108.27
23	B	611	CLA	C11-C12-C13	-2.00	109.31	115.97
23	B	610	CLA	CHB-C4A-NA	2.00	127.29	124.40
25	y	101	BCR	C1-C6-C7	2.00	121.08	115.65
23	b	616	CLA	O1D-CGD-CBD	-2.00	120.57	124.52

All (65) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	405	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
23	B	610	CLA	ND

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Mol	Chain	Res	Type	Atom
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	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	C	514	CLA	ND
23	D	405	CLA	ND
23	D	406	CLA	ND
23	a	405	CLA	ND
23	a	409	CLA	ND
23	b	601	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
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	504	CLA	ND
23	c	505	CLA	ND

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Mol	Chain	Res	Type	Atom
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	c	514	CLA	ND
23	d	402	CLA	ND
23	d	403	CLA	ND

All (1203) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	C2B-C3B-CAB-CBB
23	C	503	CLA	C4B-C3B-CAB-CBB
23	C	506	CLA	C2B-C3B-CAB-CBB
23	C	506	CLA	C4B-C3B-CAB-CBB
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	513	CLA	C2B-C3B-CAB-CBB
23	C	513	CLA	C4B-C3B-CAB-CBB
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	C4B-C3B-CAB-CBB
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C2-C1-O2A-CGA
23	c	510	CLA	C11-C10-C8-C9
25	D	407	BCR	C21-C22-C23-C24
25	D	407	BCR	C37-C22-C23-C24
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	b	619	BCR	C5-C6-C7-C8
25	d	404	BCR	C7-C8-C9-C10
25	d	404	BCR	C21-C22-C23-C24
25	d	404	BCR	C37-C22-C23-C24
25	t	103	BCR	C11-C12-C13-C14
25	y	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
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	F	101	SQD	O49-C7-O47-C45
26	F	101	SQD	C8-C7-O47-C45
26	a	413	SQD	O6-C44-C45-O47
26	a	413	SQD	C5-C6-S-O7
26	a	413	SQD	C5-C6-S-O8
26	a	413	SQD	C5-C6-S-O9
26	b	620	SQD	O49-C7-O47-C45
26	b	620	SQD	C8-C7-O47-C45
26	f	102	SQD	O6-C44-C45-O47
26	f	102	SQD	O49-C7-O47-C45
26	f	102	SQD	C8-C7-O47-C45
27	A	411	GOL	O1-C1-C2-C3
27	B	624	GOL	C1-C2-C3-O3
27	B	625	GOL	C1-C2-C3-O3
27	B	625	GOL	O2-C2-C3-O3
27	V	201	GOL	O1-C1-C2-O2
27	V	201	GOL	O1-C1-C2-C3
27	a	412	GOL	C1-C2-C3-O3
27	a	418	GOL	O1-C1-C2-C3
27	v	201	GOL	O1-C1-C2-C3
29	A	414	PL9	C18-C19-C21-C22
29	A	414	PL9	C20-C19-C21-C22
29	a	416	PL9	C28-C29-C31-C32
29	a	416	PL9	C30-C29-C31-C32
32	A	359	LMT	C2'-C1'-O1'-C1
32	A	359	LMT	O5'-C1'-O1'-C1
32	I	101	LMT	O5'-C1'-O1'-C1
32	M	103	LMT	C2'-C1'-O1'-C1
32	M	103	LMT	O5'-C1'-O1'-C1
32	a	414	LMT	O5'-C1'-O1'-C1
32	a	420	LMT	C2'-C1'-O1'-C1
32	a	420	LMT	O5'-C1'-O1'-C1
32	b	621	LMT	O5'-C1'-O1'-C1
32	b	627	LMT	C2'-C1'-O1'-C1
32	b	627	LMT	O5'-C1'-O1'-C1
32	t	101	LMT	C2'-C1'-O1'-C1
32	t	101	LMT	O5'-C1'-O1'-C1
32	t	102	LMT	O5'-C1'-O1'-C1
33	C	501	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
33	C	520	LMG	C11-C10-O7-C8
33	Z	101	LMG	O9-C10-O7-C8
33	Z	101	LMG	C11-C10-O7-C8
33	c	521	LMG	O9-C10-O7-C8
33	c	521	LMG	C11-C10-O7-C8
33	z	101	LMG	O6-C1-O1-C7
33	z	101	LMG	C11-C10-O7-C8
34	B	623	HTG	C2'-C1'-S1-C1
37	D	410	LHG	O2-C2-C3-O3
37	D	410	LHG	C3-O3-P-O4
37	D	410	LHG	C3-O3-P-O6
37	D	410	LHG	C4-O6-P-O3
37	D	410	LHG	C4-O6-P-O4
37	E	101	LHG	C3-O3-P-O4
37	E	101	LHG	C3-O3-P-O5
37	E	101	LHG	C3-O3-P-O6
37	L	101	LHG	C3-O3-P-O4
37	L	101	LHG	C3-O3-P-O6
37	L	101	LHG	C4-O6-P-O3
37	L	101	LHG	C4-O6-P-O4
37	d	407	LHG	O2-C2-C3-O3
37	d	407	LHG	C3-O3-P-O4
37	d	407	LHG	C3-O3-P-O6
37	d	407	LHG	C4-O6-P-O4
37	d	408	LHG	C4-O6-P-O4
37	e	101	LHG	C4-O6-P-O3
37	e	101	LHG	C4-O6-P-O4
37	e	101	LHG	C4-O6-P-O5
37	l	101	LHG	C4-O6-P-O3
37	l	101	LHG	C4-O6-P-O4
37	l	101	LHG	C4-O6-P-O5
38	E	103	HEM	C2C-C3C-CAC-CBC
38	E	103	HEM	C4C-C3C-CAC-CBC
38	e	87	HEM	C2B-C3B-CAB-CBB
38	e	87	HEM	C2C-C3C-CAC-CBC
38	e	87	HEM	C4C-C3C-CAC-CBC
40	V	202	HEC	C2B-C3B-CAB-CBB
40	V	202	HEC	C4B-C3B-CAB-CBB
40	V	202	HEC	C2C-C3C-CAC-CBC
40	V	202	HEC	C4C-C3C-CAC-CBC
40	v	202	HEC	C2B-C3B-CAB-CBB
40	v	202	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
40	v	202	HEC	C2C-C3C-CAC-CBC
40	v	202	HEC	C4C-C3C-CAC-CBC
32	I	101	LMT	C3'-C4'-O1B-C1B
37	E	101	LHG	O10-C23-O8-C6
37	e	101	LHG	O10-C23-O8-C6
37	E	101	LHG	C24-C23-O8-C6
37	e	101	LHG	C24-C23-O8-C6
33	C	520	LMG	O9-C10-O7-C8
33	z	101	LMG	O9-C10-O7-C8
23	B	604	CLA	C3-C5-C6-C7
23	b	616	CLA	C3-C5-C6-C7
23	c	507	CLA	C3-C5-C6-C7
23	C	504	CLA	CBD-CGD-O2D-CED
23	C	514	CLA	CBD-CGD-O2D-CED
26	B	620	SQD	C8-C7-O47-C45
33	C	501	LMG	C11-C10-O7-C8
23	B	603	CLA	C4-C3-C5-C6
23	B	614	CLA	C4-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
23	a	409	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
23	d	403	CLA	C4-C3-C5-C6
29	a	416	PL9	C25-C24-C26-C27
23	B	603	CLA	C2-C3-C5-C6
23	B	614	CLA	C2-C3-C5-C6
23	C	505	CLA	C2-C3-C5-C6
23	a	409	CLA	C2-C3-C5-C6
23	A	408	CLA	C3-C5-C6-C7
23	c	513	CLA	C3-C5-C6-C7
23	d	403	CLA	C3-C5-C6-C7
33	c	521	LMG	O6-C5-C6-O5
32	b	627	LMT	O5'-C5'-C6'-O6'
23	B	616	CLA	C3-C5-C6-C7
23	C	502	CLA	CBD-CGD-O2D-CED
32	E	102	LMT	O5'-C5'-C6'-O6'
32	I	101	LMT	O5B-C5B-C6B-O6B
32	t	101	LMT	O5'-C5'-C6'-O6'
32	D	404	LMT	C3'-C4'-O1B-C1B
32	M	103	LMT	O5'-C5'-C6'-O6'
23	B	605	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	c	508	CLA	C4-C3-C5-C6
29	A	414	PL9	C15-C14-C16-C17
29	a	416	PL9	C15-C14-C16-C17
23	B	605	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	c	508	CLA	C2-C3-C5-C6
23	d	403	CLA	C2-C3-C5-C6
29	A	414	PL9	C13-C14-C16-C17
29	a	416	PL9	C13-C14-C16-C17
29	A	414	PL9	C9-C11-C12-C13
29	A	414	PL9	C14-C16-C17-C18
29	A	414	PL9	C44-C46-C47-C48
29	D	408	PL9	C39-C41-C42-C43
29	a	416	PL9	C14-C16-C17-C18
29	d	405	PL9	C39-C41-C42-C43
33	c	521	LMG	C4-C5-C6-O5
26	B	620	SQD	O5-C1-O6-C44
32	E	102	LMT	O5'-C1'-O1'-C1
32	e	102	LMT	O5'-C1'-O1'-C1
32	D	404	LMT	O5B-C5B-C6B-O6B
33	C	521	LMG	O6-C5-C6-O5
32	D	404	LMT	C4B-C5B-C6B-O6B
23	c	510	CLA	CBA-CGA-O2A-C1
32	b	627	LMT	C4'-C5'-C6'-O6'
32	t	101	LMT	C4'-C5'-C6'-O6'
23	C	508	CLA	C4-C3-C5-C6
23	C	508	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
23	c	505	CLA	C2-C3-C5-C6
29	a	416	PL9	C23-C24-C26-C27
23	B	614	CLA	C3-C5-C6-C7
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	503	CLA	C14-C13-C15-C16
23	C	513	CLA	C6-C7-C8-C9
23	b	616	CLA	C6-C7-C8-C9
23	c	507	CLA	C6-C7-C8-C9
32	E	102	LMT	C4'-C5'-C6'-O6'
32	E	102	LMT	C2'-C1'-O1'-C1
32	a	414	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
32	e	102	LMT	C2'-C1'-O1'-C1
37	E	101	LHG	O2-C2-C3-O3
23	C	514	CLA	O1D-CGD-O2D-CED
25	T	101	BCR	C11-C12-C13-C35
25	b	619	BCR	C7-C8-C9-C34
25	d	404	BCR	C7-C8-C9-C34
25	t	103	BCR	C11-C12-C13-C35
25	b	619	BCR	C7-C8-C9-C10
34	c	522	HTG	C4-C5-C6-O6
23	a	409	CLA	CBA-CGA-O2A-C1
23	b	601	CLA	C2-C1-O2A-CGA
23	c	502	CLA	CBD-CGD-O2D-CED
23	B	601	CLA	C5-C6-C7-C8
23	b	606	CLA	C10-C11-C12-C13
23	b	606	CLA	C13-C15-C16-C17
27	A	411	GOL	O1-C1-C2-O2
27	B	624	GOL	O2-C2-C3-O3
27	a	418	GOL	O1-C1-C2-O2
27	v	201	GOL	O1-C1-C2-O2
26	F	101	SQD	C7-C8-C9-C10
32	D	404	LMT	C5'-C4'-O1B-C1B
35	H	102	DGD	C9B-CAB-CBB-CCB
32	M	103	LMT	O1'-C1-C2-C3
23	c	505	CLA	C4-C3-C5-C6
23	C	504	CLA	O1D-CGD-O2D-CED
32	I	101	LMT	O1'-C1-C2-C3
32	D	404	LMT	O5'-C5'-C6'-O6'
23	B	606	CLA	C13-C15-C16-C17
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
23	B	610	CLA	C13-C15-C16-C17
32	I	101	LMT	C4B-C5B-C6B-O6B
33	z	101	LMG	C4-C5-C6-O5
33	Z	101	LMG	C10-C11-C12-C13
35	C	518	DGD	C1A-C2A-C3A-C4A
23	c	510	CLA	O1A-CGA-O2A-C1
23	C	513	CLA	C3-C5-C6-C7
26	f	102	SQD	C26-C27-C28-C29
23	B	613	CLA	C15-C16-C17-C18
23	B	614	CLA	C8-C10-C11-C12
23	B	614	CLA	C10-C11-C12-C13
23	b	611	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C13-C15-C16-C17
23	c	513	CLA	C10-C11-C12-C13
23	B	608	CLA	C13-C15-C16-C17
23	B	615	CLA	C10-C11-C12-C13
33	B	621	LMG	O6-C5-C6-O5
33	B	621	LMG	C32-C33-C34-C35
33	C	521	LMG	C4-C5-C6-O5
23	B	609	CLA	C13-C15-C16-C17
35	c	518	DGD	C1B-C2B-C3B-C4B
37	L	101	LHG	C23-C24-C25-C26
33	z	101	LMG	O6-C5-C6-O5
23	C	503	CLA	C13-C15-C16-C17
26	A	410	SQD	C8-C7-O47-C45
34	c	522	HTG	S1-C1'-C2'-C3'
35	c	517	DGD	O6D-C5D-C6D-O5D
23	b	608	CLA	C13-C15-C16-C17
26	A	410	SQD	O49-C7-O47-C45
37	D	410	LHG	C1-C2-C3-O3
37	d	407	LHG	C1-C2-C3-O3
23	b	602	CLA	C15-C16-C17-C18
23	c	511	CLA	C10-C11-C12-C13
23	B	616	CLA	C10-C11-C12-C13
23	C	506	CLA	C10-C11-C12-C13
23	A	405	CLA	C15-C16-C17-C18
23	C	507	CLA	C13-C15-C16-C17
32	m	103	LMT	C2'-C1'-O1'-C1
32	t	102	LMT	C2'-C1'-O1'-C1
33	Z	101	LMG	C2-C1-O1-C7
35	C	518	DGD	C2E-C1E-O5D-C6D
23	C	502	CLA	O1D-CGD-O2D-CED
29	a	416	PL9	C9-C11-C12-C13
34	B	622	HTG	C1'-C2'-C3'-C4'
23	C	511	CLA	CBA-CGA-O2A-C1
34	c	522	HTG	O5-C5-C6-O6
23	B	610	CLA	C16-C17-C18-C20
25	B	619	BCR	C7-C8-C9-C34
25	H	101	BCR	C7-C8-C9-C34
25	H	101	BCR	C7-C8-C9-C10
35	C	517	DGD	O6D-C5D-C6D-O5D
23	a	409	CLA	O1A-CGA-O2A-C1
23	b	610	CLA	C2A-CAA-CBA-CGA
27	B	624	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
27	C	523	GOL	O1-C1-C2-C3
27	a	412	GOL	O1-C1-C2-C3
37	D	409	LHG	O1-C1-C2-C3
23	C	511	CLA	C16-C17-C18-C20
23	B	614	CLA	C5-C6-C7-C8
32	m	103	LMT	O5'-C5'-C6'-O6'
23	b	601	CLA	C13-C15-C16-C17
35	c	517	DGD	C4D-C5D-C6D-O5D
32	A	359	LMT	O1'-C1-C2-C3
23	C	510	CLA	C2-C1-O2A-CGA
23	B	610	CLA	C16-C17-C18-C19
32	I	101	LMT	C1-C2-C3-C4
33	B	621	LMG	C36-C37-C38-C39
23	b	606	CLA	C15-C16-C17-C18
26	a	413	SQD	C24-C25-C26-C27
33	C	521	LMG	C35-C36-C37-C38
33	D	415	LMG	C19-C20-C21-C22
34	B	623	HTG	C2'-C3'-C4'-C5'
23	B	601	CLA	CBA-CGA-O2A-C1
26	b	620	SQD	C27-C28-C29-C30
33	B	621	LMG	C17-C18-C19-C20
33	d	412	LMG	C11-C12-C13-C14
35	H	102	DGD	CCA-CDA-CEA-CFA
37	D	411	LHG	C13-C14-C15-C16
37	L	101	LHG	C17-C18-C19-C20
37	L	101	LHG	C25-C26-C27-C28
24	a	353	PHO	C2C-C3C-CAC-CBC
23	C	505	CLA	C4B-C3B-CAB-CBB
23	b	603	CLA	C4B-C3B-CAB-CBB
37	E	101	LHG	C24-C25-C26-C27
23	c	503	CLA	C16-C17-C18-C20
26	A	410	SQD	C9-C10-C11-C12
23	B	606	CLA	C10-C11-C12-C13
23	c	507	CLA	C10-C11-C12-C13
33	B	621	LMG	C11-C10-O7-C8
23	B	613	CLA	C11-C10-C8-C7
23	b	606	CLA	C12-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C10
34	b	622	HTG	S1-C1'-C2'-C3'
33	a	419	LMG	C20-C21-C22-C23
33	m	101	LMG	C38-C39-C40-C41
35	H	102	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
26	a	411	SQD	C30-C31-C32-C33
32	D	404	LMT	C6-C7-C8-C9
35	C	517	DGD	C4D-C5D-C6D-O5D
33	C	520	LMG	C10-C11-C12-C13
23	C	511	CLA	O1A-CGA-O2A-C1
23	C	508	CLA	C5-C6-C7-C8
33	B	621	LMG	O9-C10-O7-C8
26	b	620	SQD	C14-C15-C16-C17
23	d	403	CLA	CBA-CGA-O2A-C1
26	B	620	SQD	C30-C31-C32-C33
33	d	412	LMG	C38-C39-C40-C41
37	D	409	LHG	C32-C33-C34-C35
33	c	520	LMG	C34-C35-C36-C37
26	F	101	SQD	C30-C31-C32-C33
32	t	101	LMT	C3-C4-C5-C6
33	C	521	LMG	C16-C17-C18-C19
35	c	517	DGD	C5A-C6A-C7A-C8A
23	C	508	CLA	C2B-C3B-CAB-CBB
23	C	514	CLA	C2B-C3B-CAB-CBB
23	c	503	CLA	C2B-C3B-CAB-CBB
23	c	508	CLA	C2B-C3B-CAB-CBB
25	D	407	BCR	C23-C24-C25-C26
25	D	407	BCR	C23-C24-C25-C30
25	H	101	BCR	C1-C6-C7-C8
25	H	101	BCR	C5-C6-C7-C8
25	b	617	BCR	C1-C6-C7-C8
25	b	619	BCR	C1-C6-C7-C8
25	d	404	BCR	C23-C24-C25-C26
25	d	404	BCR	C23-C24-C25-C30
26	a	411	SQD	C17-C18-C19-C20
33	Z	101	LMG	C15-C16-C17-C18
23	b	601	CLA	CBA-CGA-O2A-C1
35	h	102	DGD	CAA-CBA-CCA-CDA
37	l	101	LHG	C14-C15-C16-C17
33	z	101	LMG	C10-C11-C12-C13
23	B	601	CLA	O1A-CGA-O2A-C1
23	d	403	CLA	O1A-CGA-O2A-C1
29	a	416	PL9	C4-C3-C7-C8
26	b	620	SQD	C12-C13-C14-C15
33	c	520	LMG	C4-C5-C6-O5
35	c	517	DGD	CAA-CBA-CCA-CDA
35	h	102	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
23	a	409	CLA	C16-C17-C18-C20
26	A	410	SQD	C12-C13-C14-C15
33	C	501	LMG	C18-C19-C20-C21
33	C	520	LMG	C19-C20-C21-C22
33	Z	101	LMG	C19-C20-C21-C22
35	c	517	DGD	C2A-C1A-O1G-C1G
23	b	610	CLA	C11-C12-C13-C14
35	H	102	DGD	CAB-CBB-CCB-CDB
37	d	408	LHG	C27-C28-C29-C30
33	C	521	LMG	C12-C13-C14-C15
32	m	103	LMT	O5'-C1'-O1'-C1
35	C	518	DGD	O6E-C1E-O5D-C6D
26	A	410	SQD	C15-C16-C17-C18
35	c	517	DGD	C2B-C3B-C4B-C5B
34	b	625	HTG	O5-C5-C6-O6
32	I	101	LMT	C2'-C1'-O1'-C1
23	c	513	CLA	C13-C15-C16-C17
26	a	411	SQD	C11-C12-C13-C14
35	c	517	DGD	C9A-CAA-CBA-CCA
35	h	102	DGD	C9A-CAA-CBA-CCA
33	c	520	LMG	C28-C29-C30-C31
33	d	412	LMG	O6-C5-C6-O5
33	C	521	LMG	C15-C16-C17-C18
33	C	521	LMG	C17-C18-C19-C20
33	m	101	LMG	C35-C36-C37-C38
37	e	101	LHG	C26-C27-C28-C29
23	C	510	CLA	C3-C5-C6-C7
33	a	419	LMG	C11-C10-O7-C8
33	m	101	LMG	C11-C10-O7-C8
23	b	613	CLA	C13-C15-C16-C17
26	a	413	SQD	C25-C26-C27-C28
35	H	102	DGD	C7A-C8A-C9A-CAA
37	d	406	LHG	C32-C33-C34-C35
37	L	101	LHG	C12-C13-C14-C15
23	C	503	CLA	C3-C5-C6-C7
23	C	513	CLA	CBA-CGA-O2A-C1
37	L	101	LHG	C13-C14-C15-C16
23	C	507	CLA	C16-C17-C18-C20
23	a	409	CLA	C16-C17-C18-C19
23	c	503	CLA	C16-C17-C18-C19
35	C	517	DGD	C4B-C5B-C6B-C7B
33	C	521	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
32	e	102	LMT	C4-C5-C6-C7
33	C	521	LMG	C33-C34-C35-C36
33	d	412	LMG	C29-C30-C31-C32
32	I	101	LMT	O5'-C5'-C6'-O6'
23	B	601	CLA	C10-C11-C12-C13
33	d	412	LMG	C19-C20-C21-C22
33	m	101	LMG	O9-C10-O7-C8
34	b	623	HTG	O5-C5-C6-O6
23	A	408	CLA	C10-C11-C12-C13
23	B	601	CLA	C15-C16-C17-C18
23	b	614	CLA	C15-C16-C17-C18
38	e	87	HEM	C4B-C3B-CAB-CBB
33	D	415	LMG	C30-C31-C32-C33
23	A	404	CLA	C13-C15-C16-C17
23	b	616	CLA	C5-C6-C7-C8
26	a	411	SQD	C9-C10-C11-C12
35	C	519	DGD	CBA-CCA-CDA-CEA
35	c	518	DGD	C2B-C3B-C4B-C5B
37	E	101	LHG	C11-C10-C9-C8
26	A	410	SQD	O6-C44-C45-O47
33	a	419	LMG	C30-C31-C32-C33
23	b	601	CLA	O1A-CGA-O2A-C1
33	Z	101	LMG	O6-C5-C6-O5
32	e	102	LMT	C2B-C1B-O1B-C4'
32	M	101	LMT	C2-C3-C4-C5
33	m	101	LMG	C39-C40-C41-C42
33	c	520	LMG	C31-C32-C33-C34
23	C	511	CLA	C16-C17-C18-C19
33	D	415	LMG	O6-C5-C6-O5
26	F	101	SQD	C32-C33-C34-C35
37	e	101	LHG	C11-C12-C13-C14
24	A	353	PHO	C2C-C3C-CAC-CBC
37	l	101	LHG	C16-C17-C18-C19
27	a	412	GOL	O2-C2-C3-O3
23	a	406	CLA	C1A-C2A-CAA-CBA
23	C	512	CLA	CBD-CGD-O2D-CED
23	B	615	CLA	C5-C6-C7-C8
23	b	605	CLA	C8-C10-C11-C12
35	C	517	DGD	C5B-C6B-C7B-C8B
35	c	518	DGD	C9A-CAA-CBA-CCA
32	b	621	LMT	C3-C4-C5-C6
33	D	415	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
35	c	517	DGD	O6E-C5E-C6E-O5E
33	m	101	LMG	C14-C15-C16-C17
23	b	601	CLA	C3-C5-C6-C7
23	B	606	CLA	C11-C10-C8-C7
23	B	615	CLA	C11-C12-C13-C15
23	B	616	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	C	511	CLA	C12-C13-C15-C16
23	D	406	CLA	C11-C10-C8-C7
23	a	407	CLA	C11-C12-C13-C15
23	b	614	CLA	C12-C13-C15-C16
23	d	403	CLA	C12-C13-C15-C16
23	C	513	CLA	O1A-CGA-O2A-C1
23	b	613	CLA	C8-C10-C11-C12
23	c	514	CLA	C10-C11-C12-C13
26	F	101	SQD	C23-C24-C25-C26
26	B	620	SQD	C34-C35-C36-C37
37	D	410	LHG	C13-C14-C15-C16
29	A	414	PL9	C12-C11-C9-C10
23	b	609	CLA	C2-C3-C5-C6
29	d	405	PL9	C13-C14-C16-C17
35	C	517	DGD	O6E-C5E-C6E-O5E
23	B	606	CLA	C11-C10-C8-C9
23	B	614	CLA	C14-C13-C15-C16
23	B	616	CLA	C14-C13-C15-C16
23	C	505	CLA	C14-C13-C15-C16
23	D	406	CLA	C11-C10-C8-C9
23	b	614	CLA	C6-C7-C8-C9
33	B	621	LMG	C34-C35-C36-C37
32	E	102	LMT	O1'-C1-C2-C3
33	D	415	LMG	C34-C35-C36-C37
23	c	512	CLA	CBA-CGA-O2A-C1
33	m	101	LMG	C30-C31-C32-C33
33	a	419	LMG	O9-C10-O7-C8
32	b	621	LMT	C2'-C1'-O1'-C1
35	c	517	DGD	C1A-C2A-C3A-C4A
26	A	410	SQD	O6-C44-C45-C46
26	A	412	SQD	O6-C44-C45-C46
26	B	620	SQD	C44-C45-C46-O48
26	b	620	SQD	C44-C45-C46-O48
37	E	101	LHG	C4-C5-C6-O8
26	a	411	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
26	F	101	SQD	C29-C30-C31-C32
23	c	507	CLA	C15-C16-C17-C18
33	C	501	LMG	C36-C37-C38-C39
35	C	519	DGD	CAB-CBB-CCB-CDB
34	B	626	HTG	O5-C5-C6-O6
23	C	507	CLA	C16-C17-C18-C19
32	a	414	LMT	C2-C3-C4-C5
37	L	101	LHG	C24-C25-C26-C27
26	b	620	SQD	C33-C34-C35-C36
35	c	517	DGD	O1A-C1A-O1G-C1G
35	c	518	DGD	C7A-C8A-C9A-CAA
37	d	408	LHG	C33-C34-C35-C36
29	d	405	PL9	C15-C14-C16-C17
29	d	405	PL9	C35-C34-C36-C37
23	c	512	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	C2-C3-C5-C6
29	A	414	PL9	C12-C11-C9-C8
35	c	518	DGD	C7B-C8B-C9B-CAB
23	c	512	CLA	O1A-CGA-O2A-C1
23	B	602	CLA	C15-C16-C17-C18
26	f	102	SQD	C29-C30-C31-C32
26	A	410	SQD	C11-C10-C9-C8
33	C	520	LMG	C36-C37-C38-C39
26	F	101	SQD	C24-C25-C26-C27
26	b	620	SQD	C13-C14-C15-C16
32	b	621	LMT	C4-C5-C6-C7
26	b	620	SQD	C24-C23-O48-C46
35	C	518	DGD	C7B-C8B-C9B-CAB
35	c	519	DGD	C9A-CAA-CBA-CCA
23	b	611	CLA	C8-C10-C11-C12
32	M	101	LMT	O1'-C1-C2-C3
23	B	604	CLA	C13-C15-C16-C17
26	a	413	SQD	C12-C13-C14-C15
32	I	101	LMT	C4-C5-C6-C7
34	B	623	HTG	C1'-C2'-C3'-C4'
26	A	410	SQD	C18-C19-C20-C21
33	c	520	LMG	C33-C34-C35-C36
37	l	101	LHG	C12-C13-C14-C15
23	c	511	CLA	C4-C3-C5-C6
29	A	414	PL9	C25-C24-C26-C27
34	b	625	HTG	C3'-C4'-C5'-C6'
37	d	406	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
26	B	620	SQD	C16-C17-C18-C19
26	a	411	SQD	C34-C35-C36-C37
34	B	626	HTG	C4'-C5'-C6'-C7'
23	B	605	CLA	C13-C15-C16-C17
33	D	415	LMG	C36-C37-C38-C39
33	a	419	LMG	C29-C30-C31-C32
35	C	518	DGD	C8B-C9B-CAB-CBB
37	d	407	LHG	C31-C32-C33-C34
37	E	101	LHG	C14-C15-C16-C17
23	A	408	CLA	CBA-CGA-O2A-C1
37	D	411	LHG	C24-C23-O8-C6
34	b	625	HTG	C4'-C5'-C6'-C7'
23	b	601	CLA	CAA-CBA-CGA-O2A
35	h	102	DGD	O2G-C1B-C2B-C3B
26	B	620	SQD	C11-C12-C13-C14
34	B	622	HTG	C2'-C3'-C4'-C5'
23	b	604	CLA	C13-C15-C16-C17
33	m	101	LMG	C37-C38-C39-C40
33	C	501	LMG	C29-C30-C31-C32
37	D	410	LHG	C28-C29-C30-C31
37	D	411	LHG	C27-C28-C29-C30
26	a	413	SQD	C24-C23-O48-C46
23	A	408	CLA	CBD-CGD-O2D-CED
26	F	101	SQD	C11-C10-C9-C8
35	c	517	DGD	CDB-CEB-CFB-CGB
37	l	101	LHG	C13-C14-C15-C16
32	E	102	LMT	C3-C4-C5-C6
29	A	414	PL9	C45-C44-C46-C47
37	D	409	LHG	C16-C17-C18-C19
26	A	410	SQD	C16-C17-C18-C19
32	E	102	LMT	C2B-C1B-O1B-C4'
26	B	620	SQD	C26-C27-C28-C29
27	B	624	GOL	O1-C1-C2-O2
32	t	102	LMT	C2-C1-O1'-C1'
37	D	409	LHG	O1-C1-C2-O2
23	a	407	CLA	C11-C12-C13-C14
23	d	403	CLA	C14-C13-C15-C16
33	B	621	LMG	C14-C15-C16-C17
35	c	519	DGD	CAA-CBA-CCA-CDA
23	c	508	CLA	C5-C6-C7-C8
23	A	406	CLA	C4B-C3B-CAB-CBB
23	B	606	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	C	508	CLA	C4B-C3B-CAB-CBB
23	C	514	CLA	C4B-C3B-CAB-CBB
23	D	405	CLA	C4B-C3B-CAB-CBB
23	a	409	CLA	C4B-C3B-CAB-CBB
23	c	508	CLA	C4B-C3B-CAB-CBB
23	d	402	CLA	C4B-C3B-CAB-CBB
23	C	509	CLA	C10-C11-C12-C13
38	e	87	HEM	C2A-CAA-CBA-CGA
26	A	412	SQD	C2-C1-O6-C44
35	C	517	DGD	C2E-C1E-O5D-C6D
23	a	406	CLA	C15-C16-C17-C18
37	l	101	LHG	O6-C4-C5-C6
23	B	602	CLA	C11-C12-C13-C15
23	B	605	CLA	C6-C7-C8-C10
23	B	614	CLA	C12-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C7
23	a	409	CLA	C11-C10-C8-C7
37	D	409	LHG	C25-C26-C27-C28
23	B	609	CLA	C3A-C2A-CAA-CBA
23	b	601	CLA	C4-C3-C5-C6
23	b	609	CLA	C3A-C2A-CAA-CBA
29	d	405	PL9	C45-C44-C46-C47
23	c	502	CLA	O1D-CGD-O2D-CED
32	M	101	LMT	C9-C10-C11-C12
26	f	102	SQD	C25-C26-C27-C28
25	y	101	BCR	C37-C22-C23-C24
26	b	620	SQD	C18-C19-C20-C21
33	C	520	LMG	C37-C38-C39-C40
37	E	101	LHG	C25-C26-C27-C28
23	c	511	CLA	CBA-CGA-O2A-C1
26	f	102	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
37	e	101	LHG	C4-C5-C6-O8
23	B	606	CLA	C15-C16-C17-C18
35	c	517	DGD	C7B-C8B-C9B-CAB
35	C	518	DGD	CCB-CDB-CEB-CFB
37	D	410	LHG	C26-C27-C28-C29
32	M	103	LMT	C11-C10-C9-C8
23	b	609	CLA	C4-C3-C5-C6
37	d	406	LHG	C25-C26-C27-C28
37	d	407	LHG	C30-C31-C32-C33
23	b	601	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	A	414	PL9	C43-C44-C46-C47
29	d	405	PL9	C33-C34-C36-C37
32	E	102	LMT	O5B-C1B-O1B-C4'
35	c	518	DGD	CBA-CCA-CDA-CEA
23	B	615	CLA	C16-C17-C18-C20
23	b	616	CLA	C15-C16-C17-C18
32	D	404	LMT	C4'-C5'-C6'-O6'
23	A	406	CLA	C2B-C3B-CAB-CBB
26	a	411	SQD	C10-C11-C12-C13
33	C	501	LMG	C37-C38-C39-C40
33	Z	101	LMG	C17-C18-C19-C20
33	a	419	LMG	O6-C5-C6-O5
37	E	101	LHG	C7-C8-C9-C10
26	b	620	SQD	O47-C45-C46-O48
33	c	520	LMG	C32-C33-C34-C35
29	A	414	PL9	C4-C3-C7-C8
35	c	518	DGD	CAA-CBA-CCA-CDA
23	c	509	CLA	C5-C6-C7-C8
33	B	621	LMG	C28-C29-C30-C31
33	c	521	LMG	C29-C30-C31-C32
29	d	405	PL9	C43-C44-C46-C47
23	B	615	CLA	C16-C17-C18-C19
33	d	412	LMG	C28-C29-C30-C31
23	B	602	CLA	C11-C12-C13-C14
23	C	511	CLA	C14-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C9
23	a	409	CLA	C11-C10-C8-C9
32	a	420	LMT	C6-C7-C8-C9
37	D	411	LHG	C24-C25-C26-C27
26	A	412	SQD	O5-C1-O6-C44
35	c	517	DGD	O6E-C1E-O5D-C6D
23	A	408	CLA	O1A-CGA-O2A-C1
33	a	419	LMG	C35-C36-C37-C38
35	C	518	DGD	CDA-CEA-CFA-CGA
32	b	627	LMT	C1-C2-C3-C4
26	a	413	SQD	C31-C32-C33-C34
26	b	620	SQD	O10-C23-O48-C46
37	L	101	LHG	C14-C15-C16-C17
27	B	625	GOL	O1-C1-C2-O2
27	C	523	GOL	O1-C1-C2-O2
23	c	513	CLA	CBA-CGA-O2A-C1
35	C	519	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
35	c	519	DGD	C2A-C1A-O1G-C1G
23	C	511	CLA	C4-C3-C5-C6
23	C	511	CLA	C2-C3-C5-C6
23	c	506	CLA	C2-C3-C5-C6
35	C	517	DGD	C6A-C7A-C8A-C9A
23	D	406	CLA	C8-C10-C11-C12
33	D	415	LMG	C35-C36-C37-C38
23	C	511	CLA	C8-C10-C11-C12
33	z	101	LMG	C12-C13-C14-C15
34	c	522	HTG	C2'-C3'-C4'-C5'
33	C	520	LMG	C18-C19-C20-C21
23	B	607	CLA	C10-C11-C12-C13
35	C	517	DGD	C3B-C4B-C5B-C6B
23	C	507	CLA	C5-C6-C7-C8
25	t	103	BCR	C7-C8-C9-C34
23	A	406	CLA	C12-C13-C15-C16
23	B	604	CLA	C11-C12-C13-C15
23	C	507	CLA	C11-C12-C13-C15
23	c	510	CLA	C11-C10-C8-C7
32	M	103	LMT	O5B-C5B-C6B-O6B
35	H	102	DGD	C5B-C6B-C7B-C8B
37	D	410	LHG	C17-C18-C19-C20
32	a	414	LMT	C6-C7-C8-C9
23	b	610	CLA	C15-C16-C17-C18
25	B	619	BCR	C7-C8-C9-C10
25	T	101	BCR	C11-C12-C13-C14
25	y	101	BCR	C21-C22-C23-C24
33	C	520	LMG	C16-C17-C18-C19
35	c	517	DGD	C2A-C3A-C4A-C5A
26	a	413	SQD	O10-C23-O48-C46
35	c	518	DGD	C5D-C6D-O5D-C1E
23	B	602	CLA	C13-C15-C16-C17
37	d	408	LHG	C25-C26-C27-C28
23	B	615	CLA	C4-C3-C5-C6
23	c	513	CLA	O1A-CGA-O2A-C1
37	D	411	LHG	O10-C23-O8-C6
38	E	103	HEM	C2B-C3B-CAB-CBB
32	t	102	LMT	O1'-C1-C2-C3
32	M	103	LMT	O5B-C1B-O1B-C4'
26	A	412	SQD	C15-C16-C17-C18
24	a	408	PHO	O2A-C1-C2-C3
26	b	620	SQD	C46-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
35	c	519	DGD	O1A-C1A-O1G-C1G
35	C	518	DGD	CBB-CCB-CDB-CEB
37	E	101	LHG	C10-C11-C12-C13
35	C	517	DGD	C1B-C2B-C3B-C4B
34	b	622	HTG	O5-C5-C6-O6
23	A	408	CLA	O1D-CGD-O2D-CED
23	c	511	CLA	O1A-CGA-O2A-C1
23	b	611	CLA	C13-C15-C16-C17
26	A	412	SQD	C29-C30-C31-C32
33	m	101	LMG	C22-C23-C24-C25
33	B	621	LMG	C18-C19-C20-C21
33	a	419	LMG	C33-C34-C35-C36
35	H	102	DGD	CBA-CCA-CDA-CEA
35	C	517	DGD	O6E-C1E-O5D-C6D
23	C	512	CLA	O1D-CGD-O2D-CED
32	b	627	LMT	C11-C10-C9-C8
26	a	413	SQD	O6-C44-C45-C46
33	c	521	LMG	C7-C8-C9-O8
35	H	102	DGD	O1G-C1G-C2G-C3G
35	h	102	DGD	C4E-C5E-C6E-O5E
23	c	506	CLA	C4-C3-C5-C6
29	D	408	PL9	C45-C44-C46-C47
29	a	416	PL9	C12-C11-C9-C10
35	C	519	DGD	C6B-C7B-C8B-C9B
35	C	519	DGD	O1A-C1A-O1G-C1G
26	B	620	SQD	O47-C45-C46-O48
33	C	501	LMG	O1-C7-C8-O7
35	H	102	DGD	O1G-C1G-C2G-O2G
37	E	101	LHG	O7-C5-C6-O8
37	e	101	LHG	O7-C5-C6-O8
23	B	604	CLA	C11-C12-C13-C14
23	C	507	CLA	C11-C12-C13-C14
23	b	601	CLA	C6-C7-C8-C9
35	h	102	DGD	CBA-CCA-CDA-CEA
37	d	406	LHG	C33-C34-C35-C36
32	e	102	LMT	O5B-C1B-O1B-C4'
35	C	517	DGD	C7A-C8A-C9A-CAA
35	c	517	DGD	C2E-C1E-O5D-C6D
23	b	615	CLA	C10-C11-C12-C13
37	D	411	LHG	C2-C3-O3-P
37	d	408	LHG	C2-C3-O3-P
37	d	407	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
23	b	615	CLA	C5-C6-C7-C8
23	B	615	CLA	C2-C3-C5-C6
26	b	620	SQD	C9-C10-C11-C12
37	l	101	LHG	C27-C28-C29-C30
33	c	520	LMG	C29-C30-C31-C32
23	b	607	CLA	C3-C5-C6-C7
32	M	103	LMT	C2B-C1B-O1B-C4'
23	b	604	CLA	C2C-C3C-CAC-CBC
23	b	601	CLA	C4B-C3B-CAB-CBB
23	c	513	CLA	C4B-C3B-CAB-CBB
23	c	514	CLA	C4B-C3B-CAB-CBB
32	t	101	LMT	C4-C5-C6-C7
33	c	520	LMG	C35-C36-C37-C38
35	C	518	DGD	CCA-CDA-CEA-CFA
23	B	611	CLA	C8-C10-C11-C12
23	B	601	CLA	C11-C10-C8-C7
23	C	507	CLA	C6-C7-C8-C10
23	C	513	CLA	C6-C7-C8-C10
23	b	608	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C10
23	c	507	CLA	C6-C7-C8-C10
23	c	510	CLA	C6-C7-C8-C10
23	d	402	CLA	C11-C12-C13-C15
35	C	519	DGD	O6D-C5D-C6D-O5D
35	h	102	DGD	C6A-C7A-C8A-C9A
37	d	407	LHG	C13-C14-C15-C16
37	e	101	LHG	C24-C25-C26-C27
35	c	517	DGD	C5B-C6B-C7B-C8B
37	D	409	LHG	C24-C25-C26-C27
37	l	101	LHG	O6-C4-C5-O7
37	E	101	LHG	C15-C16-C17-C18
23	B	608	CLA	C3-C5-C6-C7
35	C	517	DGD	CAA-CBA-CCA-CDA
23	A	406	CLA	C14-C13-C15-C16
23	c	510	CLA	C11-C12-C13-C14
23	B	601	CLA	CAA-CBA-CGA-O2A
25	T	101	BCR	C13-C14-C15-C16
23	b	615	CLA	C13-C15-C16-C17
24	a	353	PHO	C8-C10-C11-C12
37	D	411	LHG	C17-C18-C19-C20
37	L	101	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
26	f	102	SQD	O47-C45-C46-O48
23	D	405	CLA	C8-C10-C11-C12
33	C	501	LMG	O1-C7-C8-C9
23	C	509	CLA	C13-C15-C16-C17
37	d	408	LHG	O10-C23-O8-C6
23	B	601	CLA	CAD-CBD-CGD-O2D
23	B	607	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	CAD-CBD-CGD-O2D
23	b	601	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CAD-CBD-CGD-O2D
23	c	507	CLA	CAD-CBD-CGD-O2D
37	d	408	LHG	C9-C10-C11-C12
33	c	520	LMG	C21-C22-C23-C24
23	B	612	CLA	C10-C11-C12-C13
23	B	613	CLA	C13-C15-C16-C17
33	c	520	LMG	C30-C31-C32-C33
34	B	622	HTG	C4'-C5'-C6'-C7'
37	E	101	LHG	C26-C27-C28-C29
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	b	610	CLA	CHA-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
23	c	510	CLA	CHA-CBD-CGD-O1D
23	c	510	CLA	CHA-CBD-CGD-O2D
37	D	410	LHG	C4-O6-P-O5
37	E	101	LHG	C4-O6-P-O5
37	L	101	LHG	C3-O3-P-O5
37	L	101	LHG	C4-O6-P-O5
37	d	407	LHG	C4-O6-P-O3
23	D	406	CLA	C4-C3-C5-C6
23	C	505	CLA	C2B-C3B-CAB-CBB
23	D	405	CLA	C2B-C3B-CAB-CBB
23	b	603	CLA	C2B-C3B-CAB-CBB
23	c	513	CLA	C2B-C3B-CAB-CBB
23	a	409	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
35	h	102	DGD	C9B-CAB-CBB-CCB
35	H	102	DGD	CDA-CEA-CFA-CGA
33	C	501	LMG	O8-C28-C29-C30
32	m	103	LMT	C7-C8-C9-C10
37	D	411	LHG	O1-C1-C2-C3
33	a	419	LMG	C10-C11-C12-C13
37	d	406	LHG	C7-C8-C9-C10
23	b	609	CLA	O1A-CGA-O2A-C1
23	A	405	CLA	C13-C15-C16-C17
26	B	620	SQD	C46-C45-O47-C7
35	C	518	DGD	C9B-CAB-CBB-CCB
35	H	102	DGD	O2G-C1B-C2B-C3B
23	C	506	CLA	C2-C3-C5-C6
29	D	408	PL9	C43-C44-C46-C47
29	a	416	PL9	C12-C11-C9-C8
23	c	507	CLA	C13-C15-C16-C17
23	C	503	CLA	C12-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C10
23	c	514	CLA	C12-C13-C15-C16
23	c	508	CLA	C2A-CAA-CBA-CGA
37	D	411	LHG	C25-C26-C27-C28
23	C	506	CLA	C4-C3-C5-C6
33	B	621	LMG	C33-C34-C35-C36
32	m	103	LMT	C4'-C5'-C6'-O6'
23	D	405	CLA	C16-C17-C18-C20
37	d	408	LHG	C30-C31-C32-C33
23	c	511	CLA	C13-C15-C16-C17
26	A	410	SQD	C14-C15-C16-C17
37	d	408	LHG	C24-C23-O8-C6
23	B	604	CLA	C2C-C3C-CAC-CBC
23	b	610	CLA	C16-C17-C18-C19
26	f	102	SQD	C31-C32-C33-C34
32	b	627	LMT	C4-C5-C6-C7
23	c	512	CLA	O1D-CGD-O2D-CED
32	M	103	LMT	C4'-C5'-C6'-O6'
32	b	621	LMT	C3'-C4'-O1B-C1B
35	C	518	DGD	C2G-C3G-O3G-C1D
35	c	517	DGD	C5D-C6D-O5D-C1E
25	k	101	BCR	C9-C10-C11-C12
29	a	416	PL9	C20-C19-C21-C22
32	M	103	LMT	C4B-C5B-C6B-O6B
37	E	101	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
33	C	520	LMG	O7-C10-C11-C12
35	C	519	DGD	C1B-C2B-C3B-C4B
23	b	608	CLA	C14-C13-C15-C16
23	b	613	CLA	C14-C13-C15-C16
23	b	615	CLA	C14-C13-C15-C16
23	d	402	CLA	C11-C12-C13-C14
26	A	412	SQD	C32-C33-C34-C35
23	b	603	CLA	C13-C15-C16-C17
37	D	409	LHG	C12-C13-C14-C15
33	a	419	LMG	C34-C35-C36-C37
23	b	609	CLA	CBA-CGA-O2A-C1
37	d	407	LHG	C24-C23-O8-C6
33	c	520	LMG	O6-C5-C6-O5
26	a	413	SQD	C27-C28-C29-C30
35	C	518	DGD	CAB-CBB-CCB-CDB
26	A	410	SQD	C13-C14-C15-C16
37	D	411	LHG	C33-C34-C35-C36
37	D	411	LHG	C29-C30-C31-C32
23	C	512	CLA	O1A-CGA-O2A-C1
26	a	413	SQD	C10-C11-C12-C13
38	E	103	HEM	C4B-C3B-CAB-CBB
33	C	520	LMG	C31-C32-C33-C34
23	b	604	CLA	C12-C13-C15-C16
35	c	519	DGD	C7B-C8B-C9B-CAB
35	c	517	DGD	CCB-CDB-CEB-CFB
37	l	101	LHG	C28-C29-C30-C31
35	h	102	DGD	O1B-C1B-C2B-C3B
26	a	413	SQD	C34-C35-C36-C37
23	C	507	CLA	C3A-C2A-CAA-CBA
29	a	416	PL9	C45-C44-C46-C47
23	C	508	CLA	C13-C15-C16-C17
33	m	101	LMG	C13-C14-C15-C16
37	d	408	LHG	C32-C33-C34-C35
34	b	625	HTG	C1'-C2'-C3'-C4'
26	A	412	SQD	C30-C31-C32-C33
37	d	407	LHG	O10-C23-O8-C6
23	A	408	CLA	C5-C6-C7-C8
37	l	101	LHG	C35-C36-C37-C38
37	L	101	LHG	C11-C12-C13-C14
23	B	608	CLA	C2-C1-O2A-CGA
25	k	101	BCR	C19-C20-C21-C22
33	C	501	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
34	b	622	HTG	C2'-C3'-C4'-C5'
23	b	601	CLA	C10-C11-C12-C13
35	C	517	DGD	C3A-C4A-C5A-C6A
29	a	416	PL9	C2-C3-C7-C8
37	D	410	LHG	C9-C10-C11-C12
23	b	601	CLA	CAA-CBA-CGA-O1A
37	d	407	LHG	C9-C10-C11-C12
23	a	407	CLA	C14-C13-C15-C16
23	b	601	CLA	C11-C10-C8-C9
26	A	410	SQD	C32-C33-C34-C35
23	B	601	CLA	C3-C5-C6-C7
33	B	621	LMG	C15-C16-C17-C18
32	m	103	LMT	C11-C10-C9-C8
29	A	414	PL9	C23-C24-C26-C27
29	a	416	PL9	C18-C19-C21-C22
26	F	101	SQD	C2-C1-O6-C44
35	H	102	DGD	CDB-CEB-CFB-CGB
35	C	519	DGD	C7B-C8B-C9B-CAB
23	C	502	CLA	C1A-C2A-CAA-CBA
23	a	407	CLA	C1A-C2A-CAA-CBA
23	b	609	CLA	C1A-C2A-CAA-CBA
23	c	512	CLA	C1A-C2A-CAA-CBA
37	D	411	LHG	C15-C16-C17-C18
40	v	202	HEC	CAD-CBD-CGD-O2D
37	e	101	LHG	C23-C24-C25-C26
23	B	606	CLA	C2B-C3B-CAB-CBB
23	b	601	CLA	C2B-C3B-CAB-CBB
23	c	514	CLA	C2B-C3B-CAB-CBB
25	B	617	BCR	C1-C6-C7-C8
25	b	617	BCR	C5-C6-C7-C8
40	v	202	HEC	CAD-CBD-CGD-O1D
26	B	620	SQD	C31-C32-C33-C34
35	c	519	DGD	C3B-C4B-C5B-C6B
37	D	410	LHG	C33-C34-C35-C36
23	D	405	CLA	C16-C17-C18-C19
32	e	102	LMT	C4'-C5'-C6'-O6'
23	A	408	CLA	C4-C3-C5-C6
35	C	518	DGD	C9A-CAA-CBA-CCA
23	B	616	CLA	C6-C7-C8-C10
23	C	511	CLA	C11-C12-C13-C15
23	b	613	CLA	C11-C12-C13-C15
23	c	514	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	a	408	PHO	C8-C10-C11-C12
26	a	411	SQD	O6-C44-C45-O47
33	c	521	LMG	O7-C8-C9-O8
26	A	412	SQD	C19-C20-C21-C22
34	b	623	HTG	C3'-C4'-C5'-C6'
26	a	413	SQD	C13-C14-C15-C16
25	D	407	BCR	C7-C8-C9-C34
23	B	604	CLA	C4-C3-C5-C6
23	b	616	CLA	C2-C3-C5-C6
29	a	416	PL9	C43-C44-C46-C47
26	F	101	SQD	C27-C28-C29-C30
33	d	412	LMG	C10-C11-C12-C13
33	C	520	LMG	C30-C31-C32-C33
23	a	405	CLA	C2A-CAA-CBA-CGA
23	A	408	CLA	C11-C10-C8-C9
33	D	415	LMG	C37-C38-C39-C40
33	Z	101	LMG	C29-C28-O8-C9
23	b	601	CLA	C8-C10-C11-C12
23	b	616	CLA	C4-C3-C5-C6
29	A	414	PL9	C30-C29-C31-C32
29	D	408	PL9	C35-C34-C36-C37
23	b	605	CLA	C13-C15-C16-C17
38	E	103	HEM	CAD-CBD-CGD-O2D
35	C	519	DGD	O6E-C5E-C6E-O5E
23	b	610	CLA	C16-C17-C18-C20
23	C	512	CLA	CBA-CGA-O2A-C1
38	E	103	HEM	CAD-CBD-CGD-O1D
33	C	520	LMG	C21-C22-C23-C24
26	b	620	SQD	C35-C36-C37-C38
37	D	409	LHG	C26-C27-C28-C29
23	A	404	CLA	C2A-CAA-CBA-CGA
23	C	502	CLA	C2A-CAA-CBA-CGA
35	c	519	DGD	C8A-C9A-CAA-CBA
32	a	414	LMT	C3-C4-C5-C6
38	e	87	HEM	CAA-CBA-CGA-O2A
23	C	506	CLA	C15-C16-C17-C18
37	l	101	LHG	C34-C35-C36-C37
35	H	102	DGD	C7B-C8B-C9B-CAB
23	A	408	CLA	C4B-C3B-CAB-CBB
23	b	607	CLA	C4B-C3B-CAB-CBB
23	c	512	CLA	C4B-C3B-CAB-CBB
23	a	407	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	a	406	CLA	C2C-C3C-CAC-CBC
34	B	623	HTG	C4-C5-C6-O6
33	c	520	LMG	C10-C11-C12-C13
34	b	623	HTG	S1-C1'-C2'-C3'
24	a	408	PHO	CHA-CBD-CGD-O1D
23	b	612	CLA	C13-C15-C16-C17
40	V	202	HEC	CAD-CBD-CGD-O1D
23	b	604	CLA	C4C-C3C-CAC-CBC
35	C	519	DGD	C3B-C4B-C5B-C6B
33	C	501	LMG	C28-C29-C30-C31
33	Z	101	LMG	O6-C1-O1-C7
35	c	518	DGD	O6E-C1E-O5D-C6D
23	A	408	CLA	C11-C10-C8-C7
23	B	603	CLA	C11-C12-C13-C15
26	A	412	SQD	C25-C26-C27-C28
32	b	627	LMT	C5-C6-C7-C8
23	B	603	CLA	C11-C12-C13-C14
23	c	510	CLA	C6-C7-C8-C9
23	c	510	CLA	C14-C13-C15-C16
37	l	101	LHG	C25-C26-C27-C28
35	C	517	DGD	C5D-C6D-O5D-C1E
37	D	409	LHG	C17-C18-C19-C20
33	B	621	LMG	O8-C28-C29-C30
23	A	408	CLA	C2-C1-O2A-CGA
23	C	513	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	c	513	CLA	C2-C1-O2A-CGA
23	A	406	CLA	C3-C5-C6-C7
37	D	411	LHG	C26-C27-C28-C29
23	c	513	CLA	C16-C17-C18-C20
23	c	514	CLA	CBD-CGD-O2D-CED
23	B	604	CLA	C4C-C3C-CAC-CBC
33	a	419	LMG	C31-C32-C33-C34
32	a	414	LMT	O5B-C5B-C6B-O6B
35	c	518	DGD	C2E-C1E-O5D-C6D
40	V	202	HEC	CAD-CBD-CGD-O2D
32	a	414	LMT	C4-C5-C6-C7
34	b	622	HTG	C3'-C4'-C5'-C6'
38	e	87	HEM	CAA-CBA-CGA-O1A
32	M	101	LMT	O5'-C1'-O1'-C1
26	a	413	SQD	C30-C31-C32-C33
26	a	411	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
37	d	407	LHG	C28-C29-C30-C31
26	b	620	SQD	C11-C10-C9-C8
32	a	420	LMT	C4-C5-C6-C7
35	c	517	DGD	CCA-CDA-CEA-CFA
26	A	410	SQD	O47-C7-C8-C9
23	D	406	CLA	C2-C3-C5-C6
23	C	504	CLA	C15-C16-C17-C18
33	B	621	LMG	C35-C36-C37-C38
37	d	407	LHG	C32-C33-C34-C35
32	e	102	LMT	C3-C4-C5-C6
23	C	507	CLA	C6-C7-C8-C9
23	C	513	CLA	C11-C10-C8-C9
23	c	514	CLA	C14-C13-C15-C16
23	C	511	CLA	CAA-CBA-CGA-O2A
33	m	101	LMG	C16-C17-C18-C19
23	B	613	CLA	CAA-CBA-CGA-O2A
29	D	408	PL9	C13-C14-C16-C17
33	m	101	LMG	C21-C22-C23-C24
23	B	616	CLA	C11-C12-C13-C15
23	b	607	CLA	C12-C13-C15-C16
23	b	611	CLA	C12-C13-C15-C16
23	c	507	CLA	C11-C12-C13-C15
23	c	510	CLA	C12-C13-C15-C16
23	c	511	CLA	C6-C7-C8-C10
23	b	614	CLA	C3-C5-C6-C7
23	A	408	CLA	C2B-C3B-CAB-CBB
23	a	409	CLA	C2B-C3B-CAB-CBB
23	b	607	CLA	C2B-C3B-CAB-CBB
23	b	613	CLA	C2B-C3B-CAB-CBB
23	c	512	CLA	C2B-C3B-CAB-CBB
23	d	402	CLA	C2B-C3B-CAB-CBB
25	B	617	BCR	C5-C6-C7-C8
25	t	103	BCR	C1-C6-C7-C8
25	t	103	BCR	C5-C6-C7-C8
25	y	101	BCR	C23-C24-C25-C30
23	B	605	CLA	C8-C10-C11-C12
33	C	501	LMG	C21-C22-C23-C24
37	D	409	LHG	C33-C34-C35-C36
23	B	611	CLA	C16-C17-C18-C20
23	b	613	CLA	CAA-CBA-CGA-O2A
37	l	101	LHG	O7-C7-C8-C9
23	a	405	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
34	C	522	HTG	C4-C5-C6-O6
37	d	408	LHG	C26-C27-C28-C29
24	a	408	PHO	C2-C3-C5-C6
34	B	622	HTG	C2'-C1'-S1-C1
23	B	601	CLA	C2A-CAA-CBA-CGA
23	D	406	CLA	C10-C11-C12-C13
23	b	602	CLA	C10-C11-C12-C13
34	B	622	HTG	S1-C1'-C2'-C3'
33	c	520	LMG	O7-C10-C11-C12
26	A	412	SQD	C26-C27-C28-C29
29	D	408	PL9	C15-C14-C16-C17
26	f	102	SQD	O47-C7-C8-C9
32	t	102	LMT	C5-C6-C7-C8
38	e	87	HEM	CAD-CBD-CGD-O1D
27	a	412	GOL	O1-C1-C2-O2
37	l	101	LHG	C32-C33-C34-C35
35	C	518	DGD	C8A-C9A-CAA-CBA
23	b	614	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C12-C13-C14
23	b	612	CLA	CAA-CBA-CGA-O2A
33	m	101	LMG	O1-C7-C8-C9
23	B	612	CLA	C13-C15-C16-C17
23	a	409	CLA	C8-C10-C11-C12
23	B	609	CLA	C1A-C2A-CAA-CBA
23	a	407	CLA	C4B-C3B-CAB-CBB
23	b	610	CLA	C4B-C3B-CAB-CBB
23	c	506	CLA	C4B-C3B-CAB-CBB
33	B	621	LMG	C4-C5-C6-O5
29	A	414	PL9	C35-C34-C36-C37
26	F	101	SQD	O5-C1-O6-C44
23	c	513	CLA	CAA-CBA-CGA-O2A
33	D	415	LMG	O7-C10-C11-C12
29	D	408	PL9	C36-C37-C38-C39
25	D	407	BCR	C7-C8-C9-C10
33	Z	101	LMG	O7-C10-C11-C12
23	B	610	CLA	C2A-CAA-CBA-CGA
26	F	101	SQD	C31-C32-C33-C34
33	a	419	LMG	C21-C22-C23-C24
23	B	602	CLA	C16-C17-C18-C20
23	c	511	CLA	CAA-CBA-CGA-O2A
26	b	620	SQD	O48-C23-C24-C25
35	c	517	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
38	E	103	HEM	CAA-CBA-CGA-O1A
38	e	87	HEM	CAD-CBD-CGD-O2D
26	B	620	SQD	C5-C6-S-O7
26	B	620	SQD	C5-C6-S-O9
32	b	621	LMT	C11-C10-C9-C8
23	B	613	CLA	C2-C1-O2A-CGA
23	c	507	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2-C1-O2A-CGA
23	A	406	CLA	C11-C10-C8-C7
23	C	506	CLA	C11-C12-C13-C15
23	b	610	CLA	C11-C12-C13-C15
23	b	616	CLA	C11-C12-C13-C15
37	L	101	LHG	C16-C17-C18-C19
24	A	407	PHO	O2A-C1-C2-C3
37	D	410	LHG	C32-C33-C34-C35
35	C	519	DGD	C9B-CAB-CBB-CCB
23	C	513	CLA	C10-C11-C12-C13
23	B	602	CLA	C2A-CAA-CBA-CGA
33	z	101	LMG	O7-C10-C11-C12
26	B	620	SQD	O10-C23-O48-C46
23	A	404	CLA	C15-C16-C17-C18
23	a	409	CLA	C15-C16-C17-C18
38	E	103	HEM	CAA-CBA-CGA-O2A
24	A	407	PHO	C10-C11-C12-C13
23	B	615	CLA	C8-C10-C11-C12
35	C	519	DGD	CAA-CBA-CCA-CDA
26	a	411	SQD	C26-C27-C28-C29
26	f	102	SQD	O49-C7-C8-C9
37	l	101	LHG	O9-C7-C8-C9
23	b	604	CLA	C14-C13-C15-C16
23	b	616	CLA	C11-C12-C13-C14
33	C	501	LMG	C17-C18-C19-C20
33	c	520	LMG	O9-C10-C11-C12
26	B	620	SQD	C11-C10-C9-C8
25	H	101	BCR	C9-C10-C11-C12
24	a	408	PHO	C4-C3-C5-C6
23	C	511	CLA	CAA-CBA-CGA-O1A
33	m	101	LMG	C19-C20-C21-C22
23	B	613	CLA	CAA-CBA-CGA-O1A
23	c	511	CLA	CAA-CBA-CGA-O1A
26	A	410	SQD	O49-C7-C8-C9
26	b	620	SQD	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
37	L	101	LHG	C11-C10-C9-C8
23	c	503	CLA	C3-C5-C6-C7
32	a	420	LMT	O5'-C5'-C6'-O6'
25	K	102	BCR	C7-C8-C9-C10
26	B	620	SQD	C24-C23-O48-C46
23	C	507	CLA	C8-C10-C11-C12
23	b	616	CLA	C10-C11-C12-C13
35	C	518	DGD	C5D-C6D-O5D-C1E
35	h	102	DGD	C2G-C3G-O3G-C1D
33	c	520	LMG	O10-C28-O8-C9
35	C	519	DGD	CDA-CEA-CFA-CGA
23	c	502	CLA	C2A-CAA-CBA-CGA
37	D	410	LHG	C34-C35-C36-C37
23	c	504	CLA	C15-C16-C17-C18
26	F	101	SQD	C28-C29-C30-C31
23	b	613	CLA	CAA-CBA-CGA-O1A
23	c	513	CLA	CAA-CBA-CGA-O1A
35	c	517	DGD	O1B-C1B-C2B-C3B
23	B	612	CLA	C8-C10-C11-C12
23	b	602	CLA	C13-C15-C16-C17
23	c	510	CLA	C13-C15-C16-C17
23	c	513	CLA	C8-C10-C11-C12
35	C	519	DGD	C8B-C9B-CAB-CBB
23	C	507	CLA	CAD-CBD-CGD-O2D
23	D	406	CLA	CAD-CBD-CGD-O2D
23	b	609	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	c	505	CLA	CAD-CBD-CGD-O2D
37	d	408	LHG	C28-C29-C30-C31
33	D	415	LMG	O9-C10-C11-C12
35	c	518	DGD	C5A-C6A-C7A-C8A
32	b	621	LMT	C6-C7-C8-C9
35	C	518	DGD	O2G-C1B-C2B-C3B
37	D	411	LHG	C12-C13-C14-C15
26	B	620	SQD	C12-C13-C14-C15
34	b	623	HTG	C4'-C5'-C6'-C7'
26	f	102	SQD	C28-C29-C30-C31
37	L	101	LHG	O7-C7-C8-C9
37	d	408	LHG	O8-C23-C24-C25
35	H	102	DGD	C2B-C3B-C4B-C5B
23	C	514	CLA	C13-C15-C16-C17
37	l	101	LHG	C17-C18-C19-C20

There are no ring outliers.

146 monomers are involved in 367 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	D	406	CLA	1	0
33	d	412	LMG	1	0
25	Y	101	BCR	3	0
35	c	518	DGD	4	0
24	A	353	PHO	4	0
25	b	619	BCR	3	0
23	c	507	CLA	2	0
32	a	414	LMT	3	0
23	A	408	CLA	4	0
32	m	103	LMT	2	0
25	B	619	BCR	2	0
33	C	521	LMG	1	0
25	y	101	BCR	2	0
24	a	408	PHO	2	0
26	b	620	SQD	4	0
23	B	603	CLA	5	0
27	a	412	GOL	1	0
34	B	622	HTG	3	0
29	a	416	PL9	7	0
32	A	359	LMT	2	0
26	B	620	SQD	3	0
23	C	509	CLA	4	0
23	b	609	CLA	4	0
26	a	411	SQD	3	0
23	c	510	CLA	6	0
23	B	606	CLA	3	0
29	A	414	PL9	4	0
23	b	603	CLA	2	0
23	c	513	CLA	6	0
23	C	508	CLA	4	0
35	c	519	DGD	1	0
23	C	507	CLA	4	0
35	c	517	DGD	2	0
32	I	101	LMT	1	0
33	a	419	LMG	1	0
23	b	612	CLA	3	0
23	C	503	CLA	2	0
23	C	512	CLA	3	0
23	b	606	CLA	6	0
23	C	510	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	515	BCR	5	0
25	C	515	BCR	5	0
23	B	616	CLA	4	0
23	C	513	CLA	2	0
23	a	406	CLA	6	0
23	B	609	CLA	4	0
38	E	103	HEM	4	0
23	c	506	CLA	9	0
23	C	506	CLA	12	0
25	d	404	BCR	1	0
23	C	502	CLA	3	0
23	B	604	CLA	4	0
25	b	617	BCR	2	0
23	A	405	CLA	4	0
23	c	502	CLA	2	0
34	d	411	HTG	2	0
23	D	405	CLA	3	0
35	C	519	DGD	1	0
23	a	409	CLA	1	0
23	a	405	CLA	5	0
32	M	103	LMT	3	0
23	c	503	CLA	3	0
26	A	412	SQD	2	0
35	C	518	DGD	2	0
23	c	514	CLA	5	0
33	D	415	LMG	2	0
25	T	101	BCR	8	0
23	b	604	CLA	2	0
23	A	406	CLA	3	0
25	a	410	BCR	2	0
32	D	404	LMT	2	0
33	z	101	LMG	1	0
32	a	420	LMT	1	0
33	Z	101	LMG	2	0
29	d	405	PL9	1	0
25	B	618	BCR	6	0
23	b	610	CLA	1	0
23	b	615	CLA	3	0
27	B	625	GOL	4	0
23	C	511	CLA	4	0
37	D	411	LHG	3	0
23	b	605	CLA	5	0

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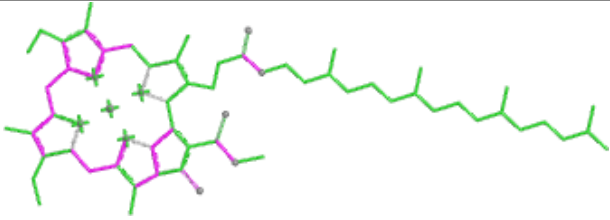
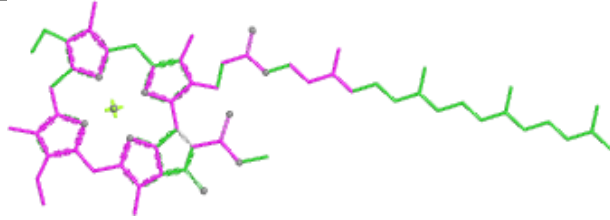
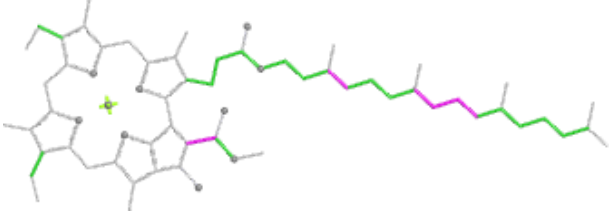
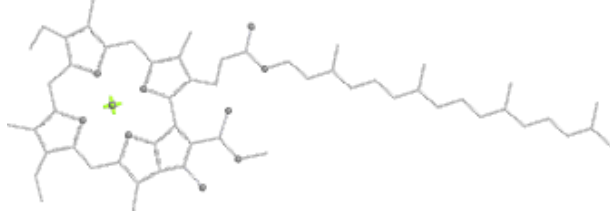
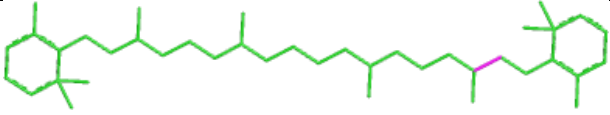
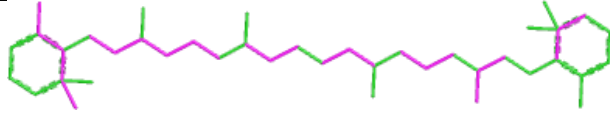
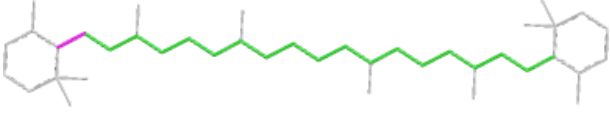
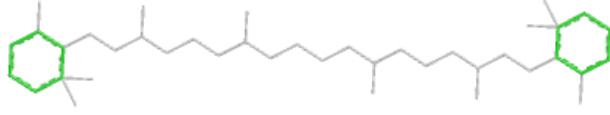
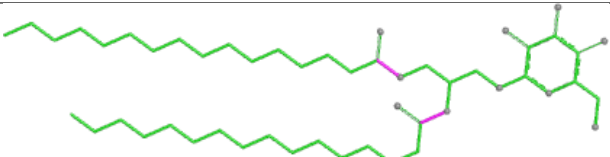
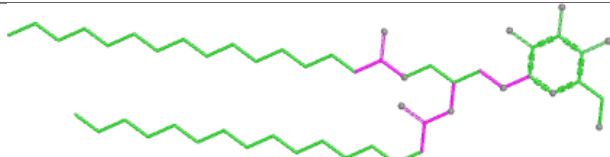
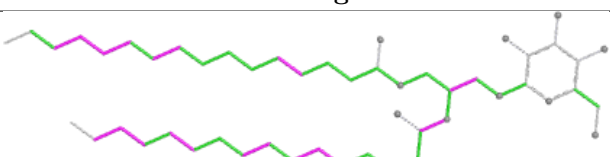
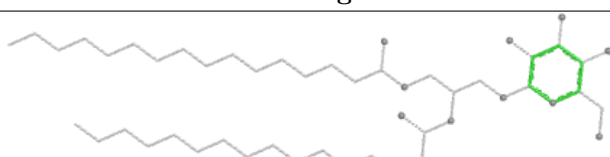
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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23	C	504	CLA	4	0
32	b	621	LMT	2	0
26	A	410	SQD	4	0
37	L	101	LHG	1	0
32	E	102	LMT	1	0
37	D	409	LHG	1	0
25	D	407	BCR	4	0
23	C	505	CLA	1	0
37	e	101	LHG	2	0
34	b	622	HTG	1	0
23	b	614	CLA	6	0
24	A	407	PHO	1	0
23	c	505	CLA	3	0
23	d	403	CLA	4	0
32	t	101	LMT	1	0
23	a	407	CLA	1	0
23	b	607	CLA	3	0
34	D	414	HTG	2	0
37	d	406	LHG	2	0
37	d	408	LHG	7	0
24	a	353	PHO	4	0
33	c	520	LMG	1	0
38	e	87	HEM	5	0
23	B	610	CLA	1	0
26	F	101	SQD	2	0
25	t	103	BCR	6	0
25	H	101	BCR	3	0
33	C	501	LMG	6	0
37	E	101	LHG	3	0
25	A	409	BCR	1	0
35	H	102	DGD	2	0
23	d	402	CLA	2	0
23	b	608	CLA	1	0
23	B	601	CLA	1	0
23	B	612	CLA	3	0
23	b	613	CLA	4	0
25	K	102	BCR	2	0
23	B	605	CLA	8	0
27	a	418	GOL	1	0
25	c	516	BCR	5	0
25	C	516	BCR	1	0

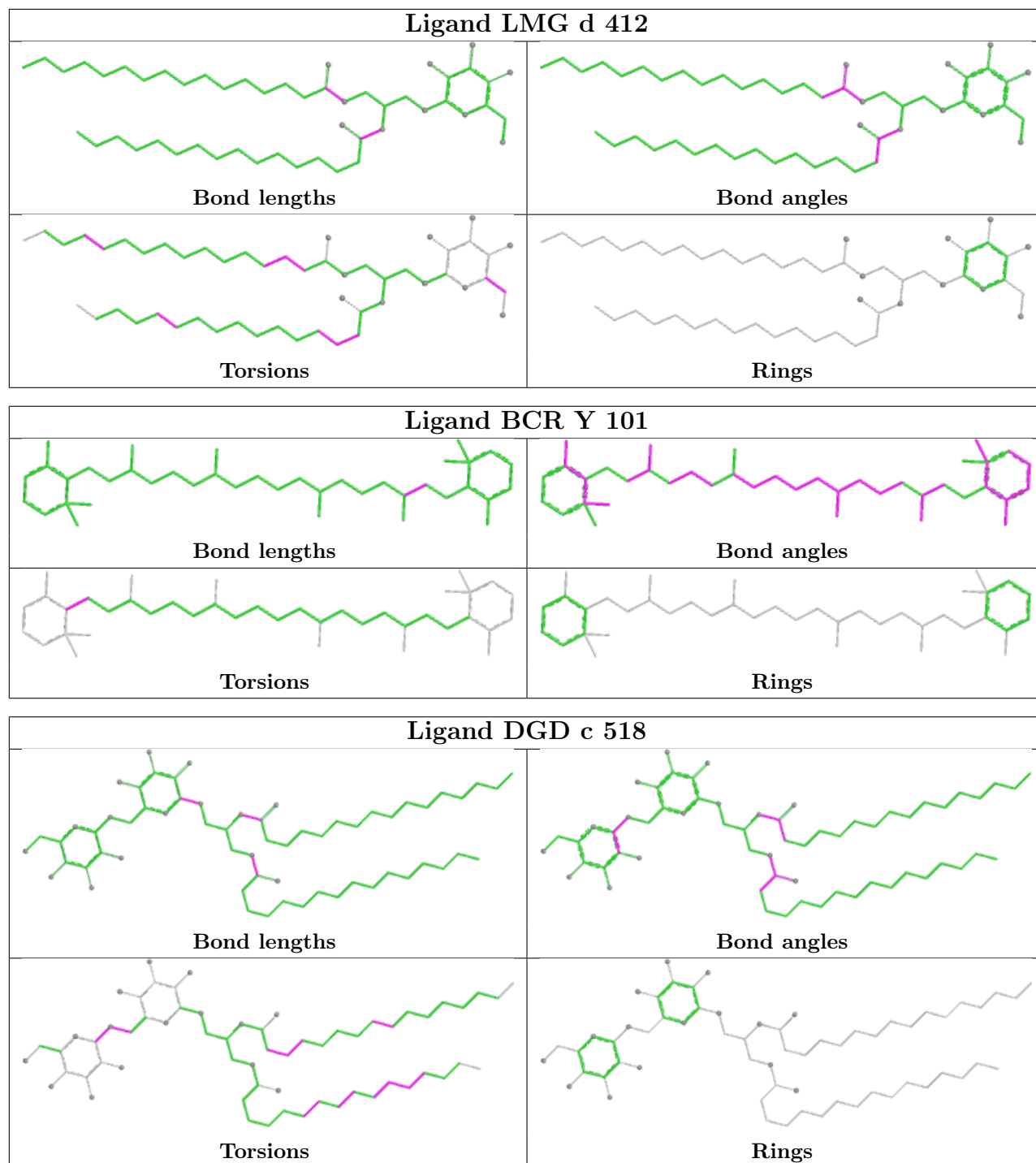
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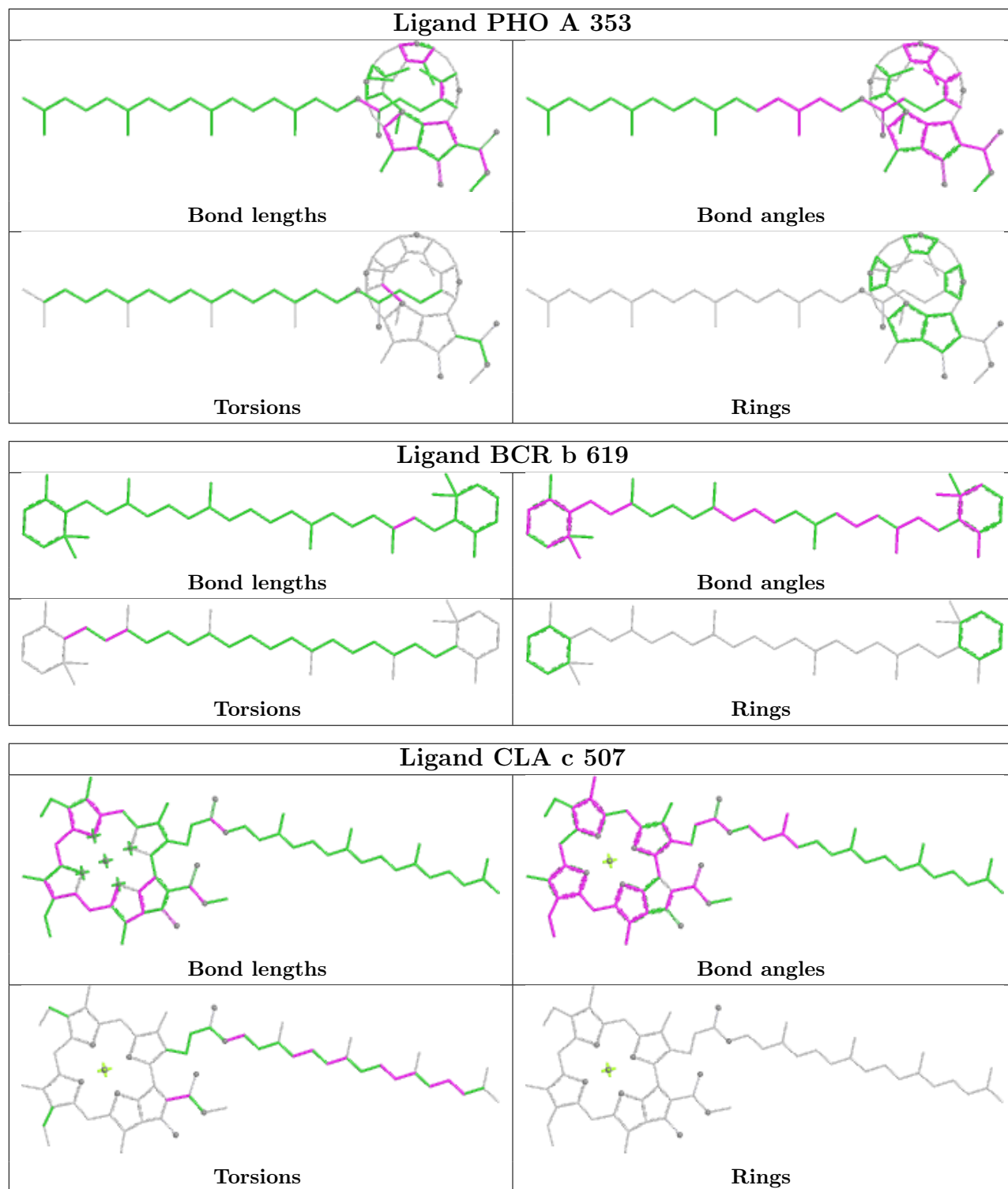
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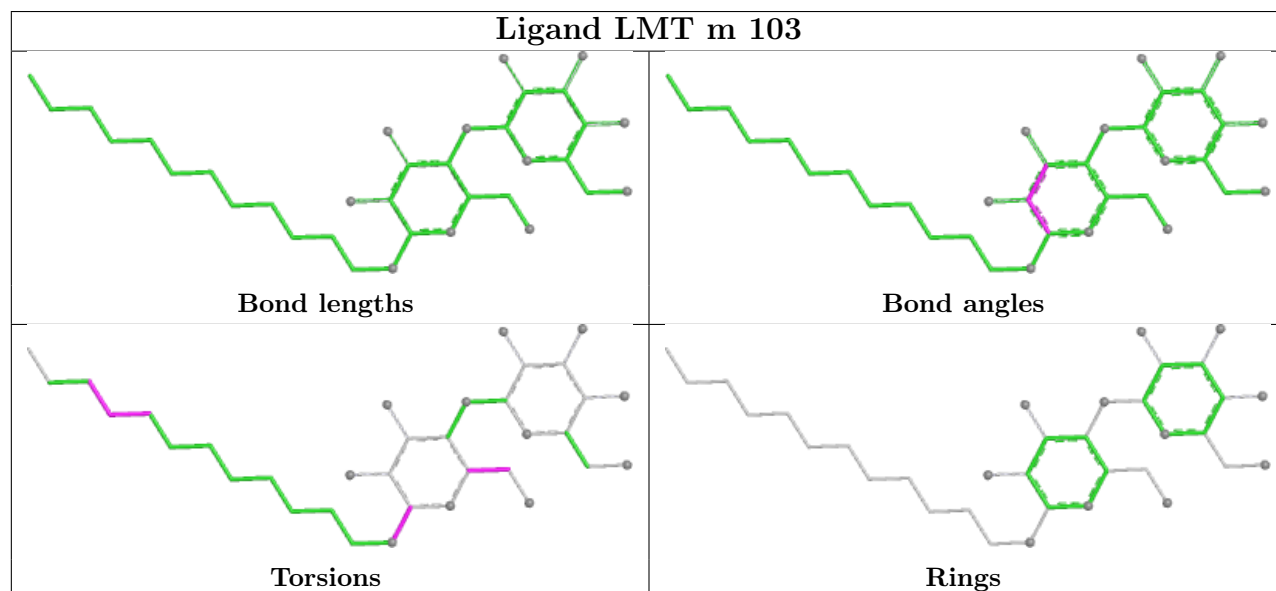
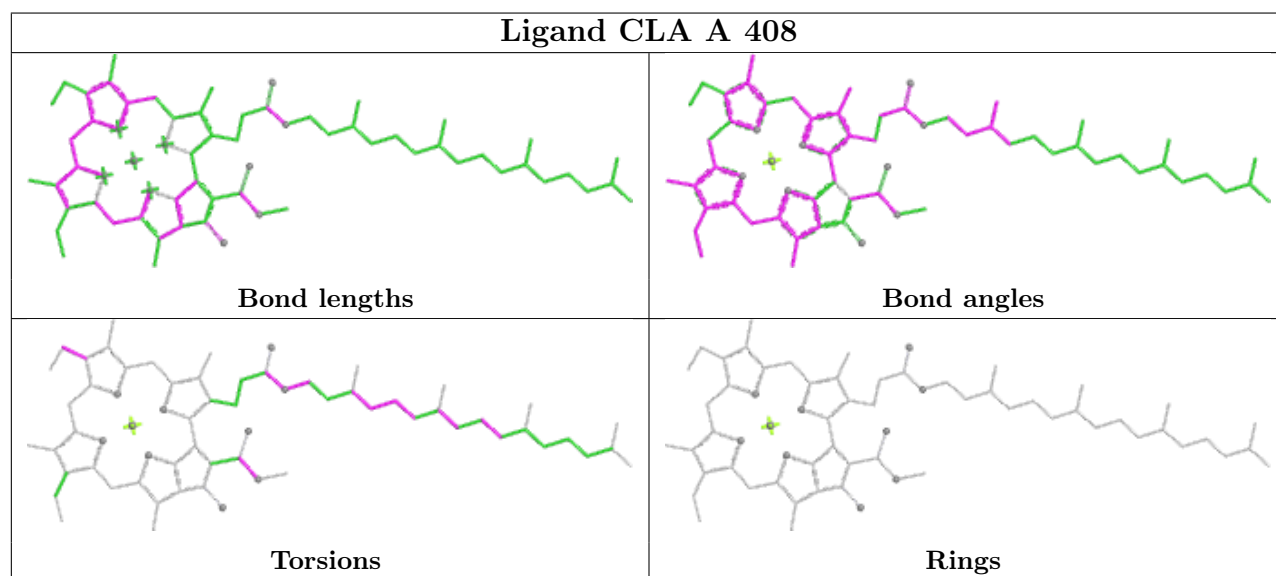
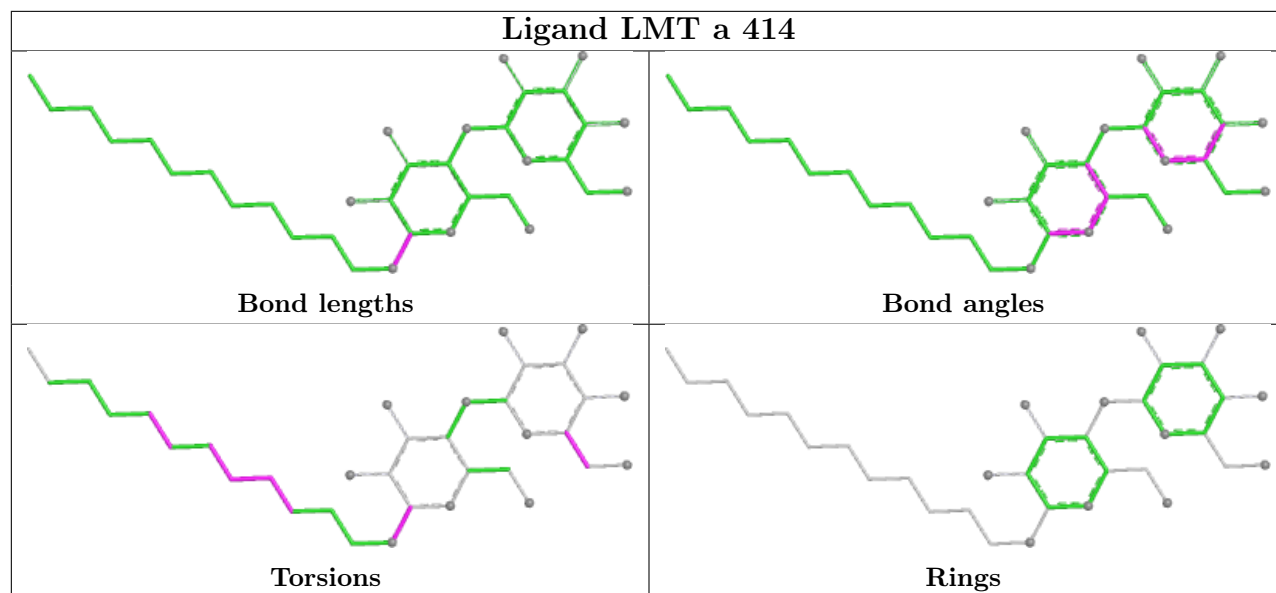
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	M	101	LMT	2	0
23	b	601	CLA	1	0
34	B	623	HTG	1	0
25	k	101	BCR	2	0
25	b	618	BCR	6	0
23	c	511	CLA	5	0
23	C	514	CLA	4	0
23	c	509	CLA	8	0
37	d	407	LHG	3	0
23	c	508	CLA	5	0
33	c	521	LMG	2	0
23	B	614	CLA	4	0
35	C	517	DGD	5	0
23	A	404	CLA	5	0
23	b	602	CLA	2	0
23	b	616	CLA	2	0
26	f	102	SQD	2	0
23	B	615	CLA	3	0
23	c	512	CLA	6	0
23	B	613	CLA	4	0
25	h	101	BCR	4	0
23	B	602	CLA	5	0

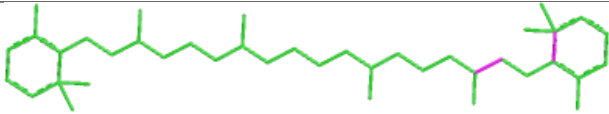
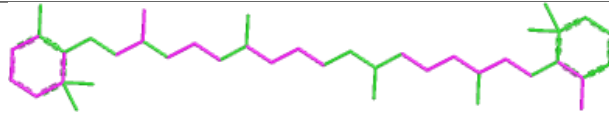
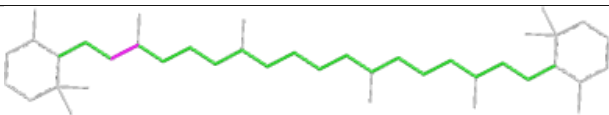
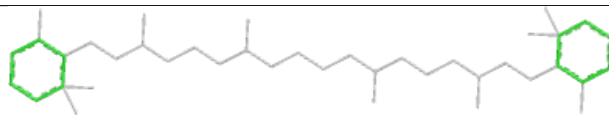
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

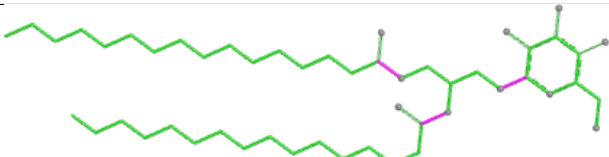
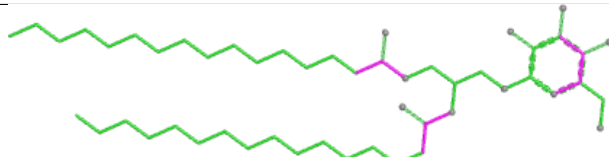
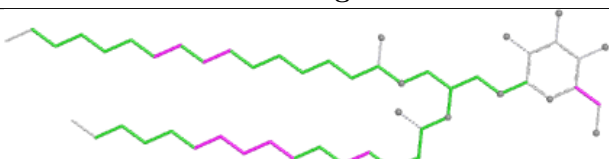
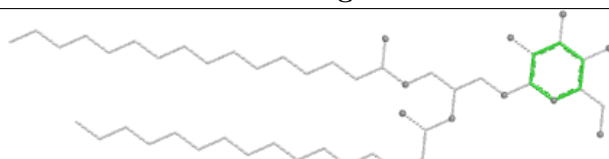
Ligand CLA D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG m 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

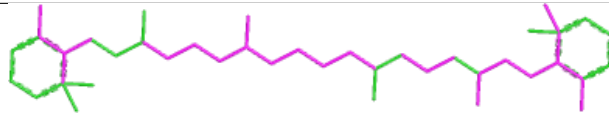
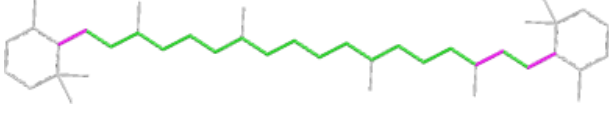
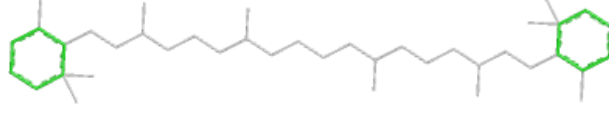


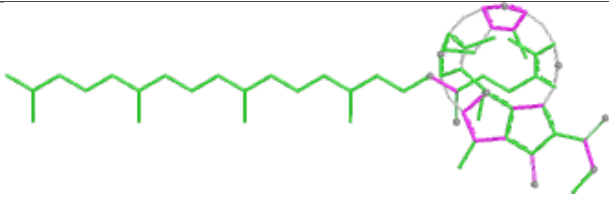
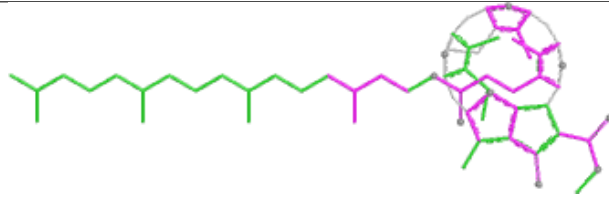
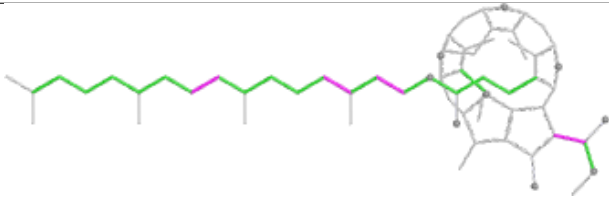
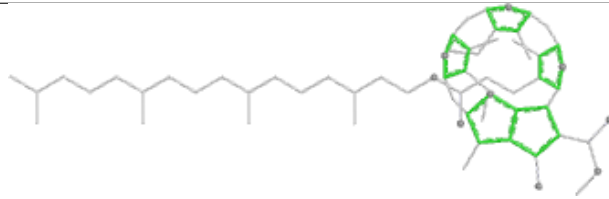


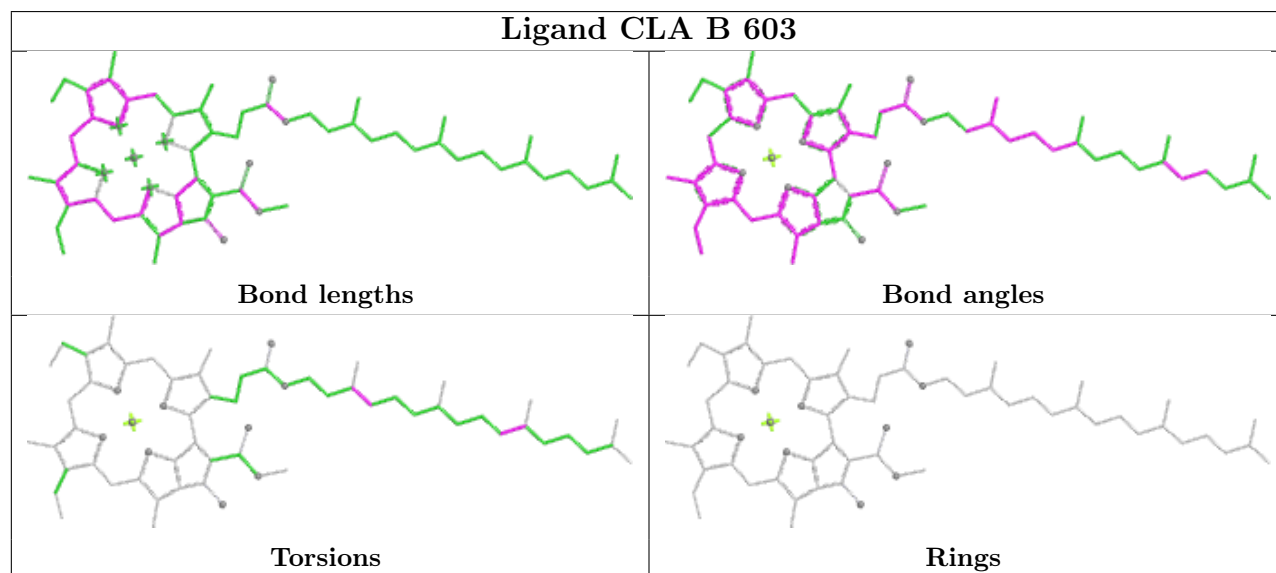
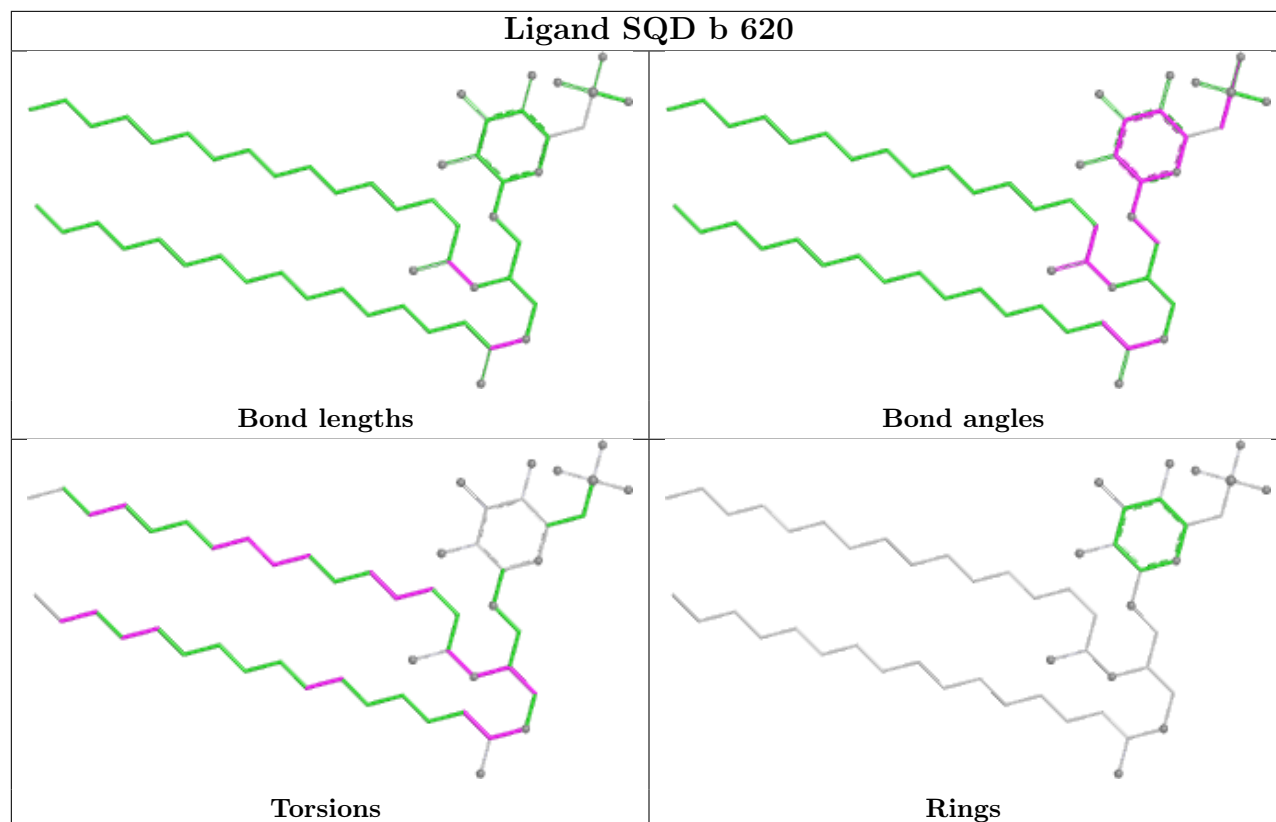


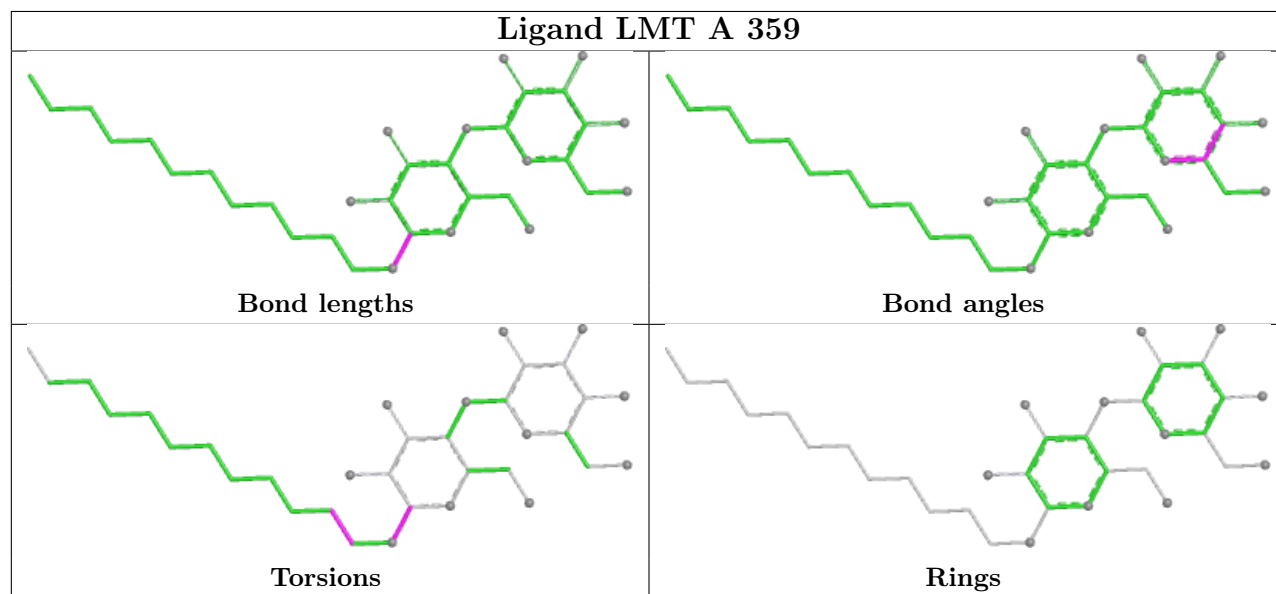
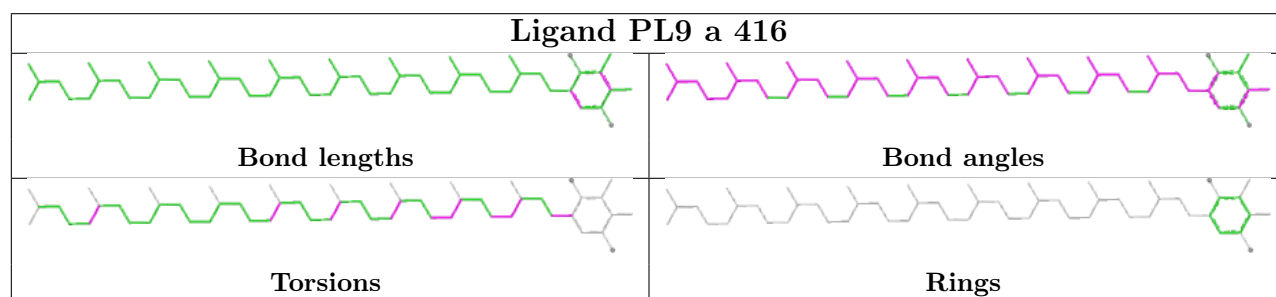
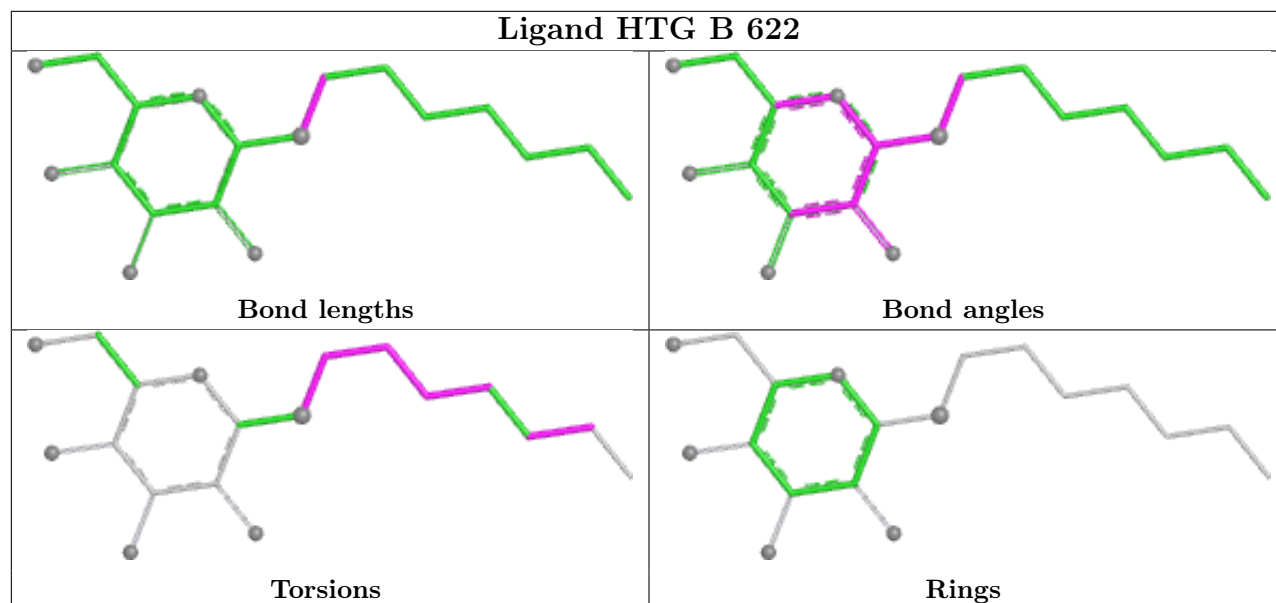
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

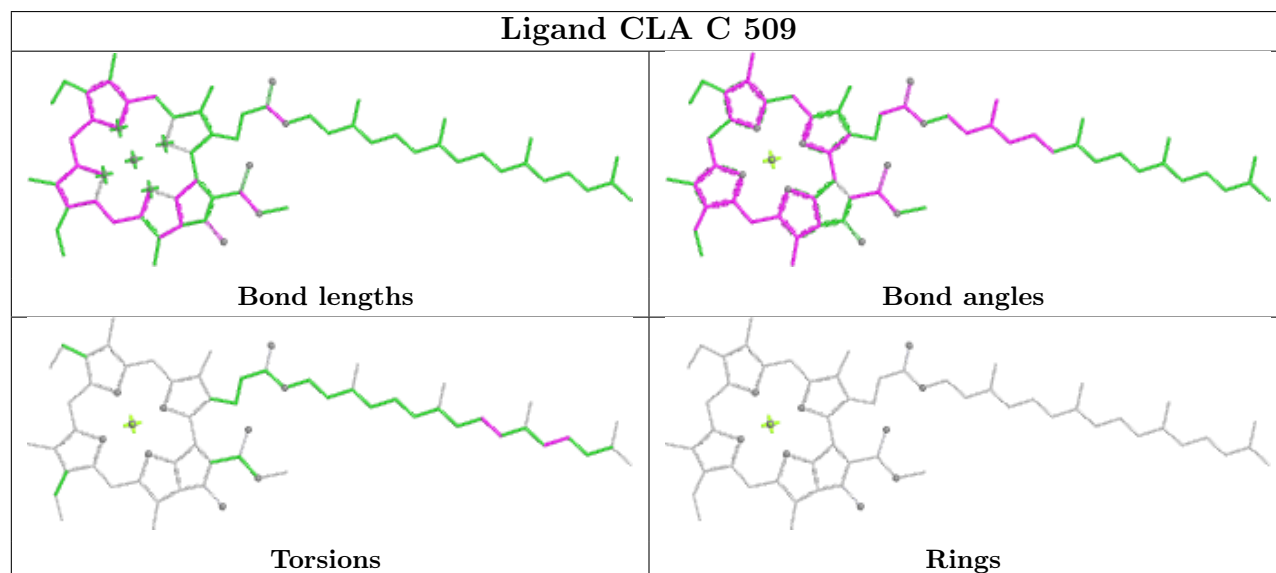
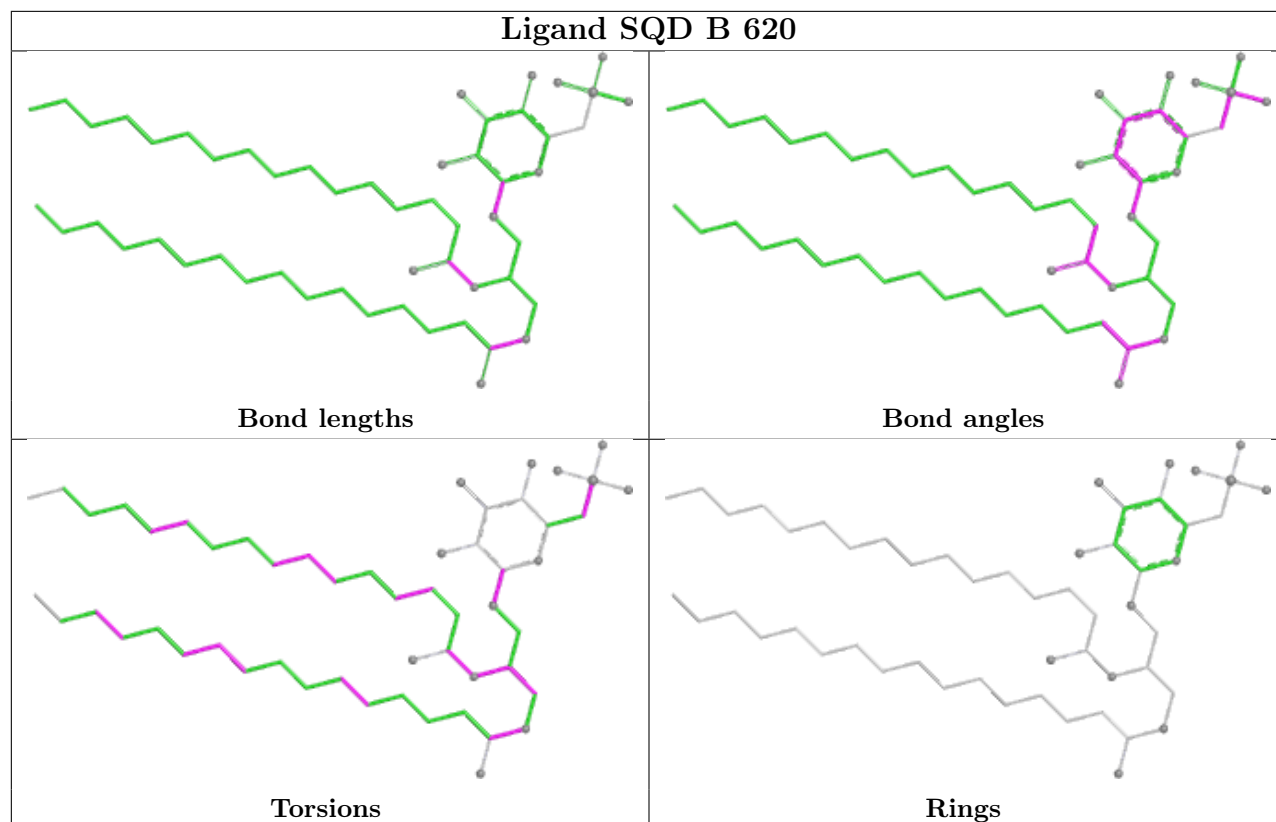
Ligand LMG C 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

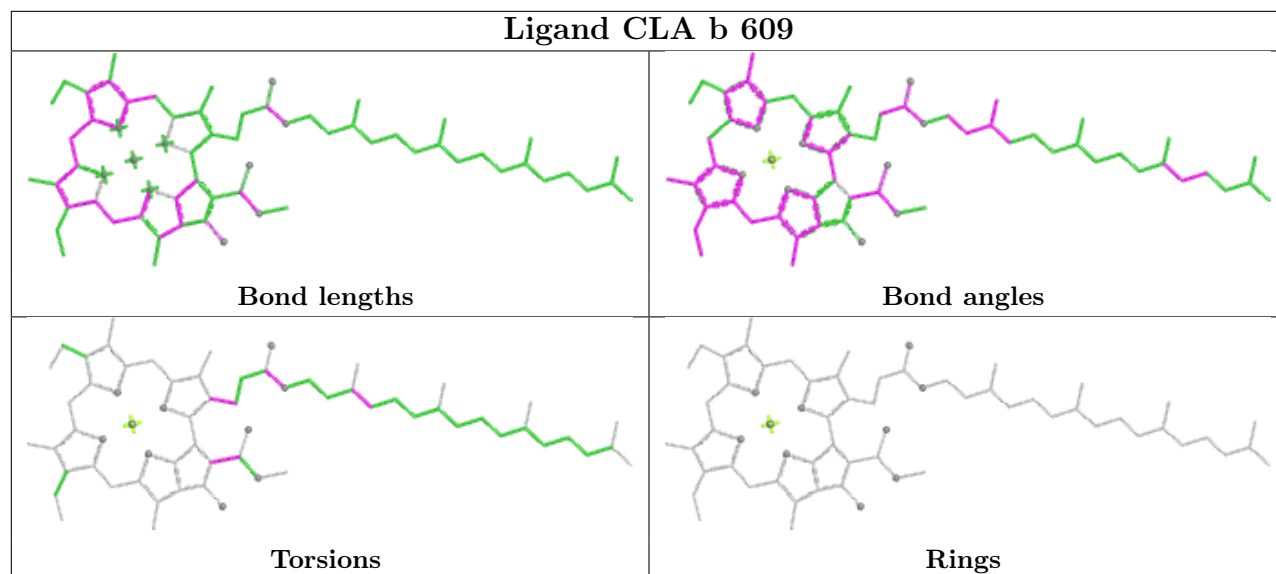
Ligand PHO a 408	
	
Bond lengths	Bond angles
	
Torsions	Rings



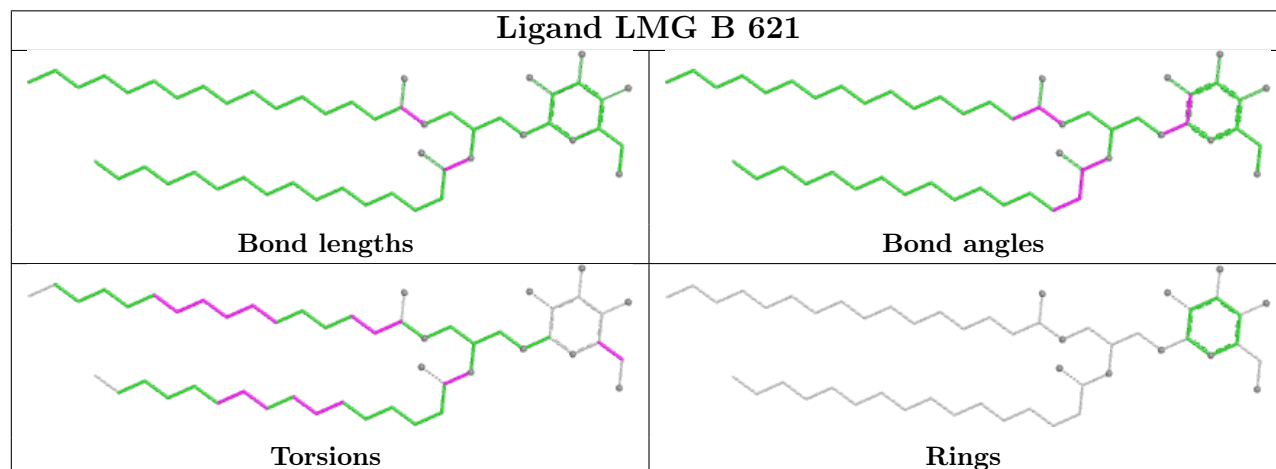


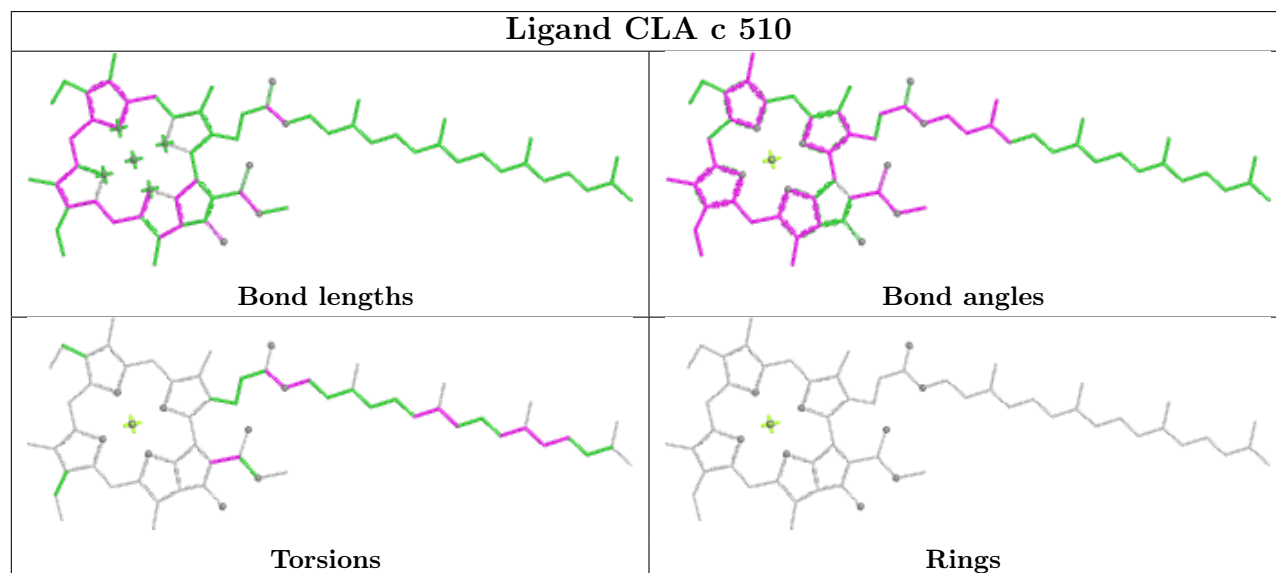
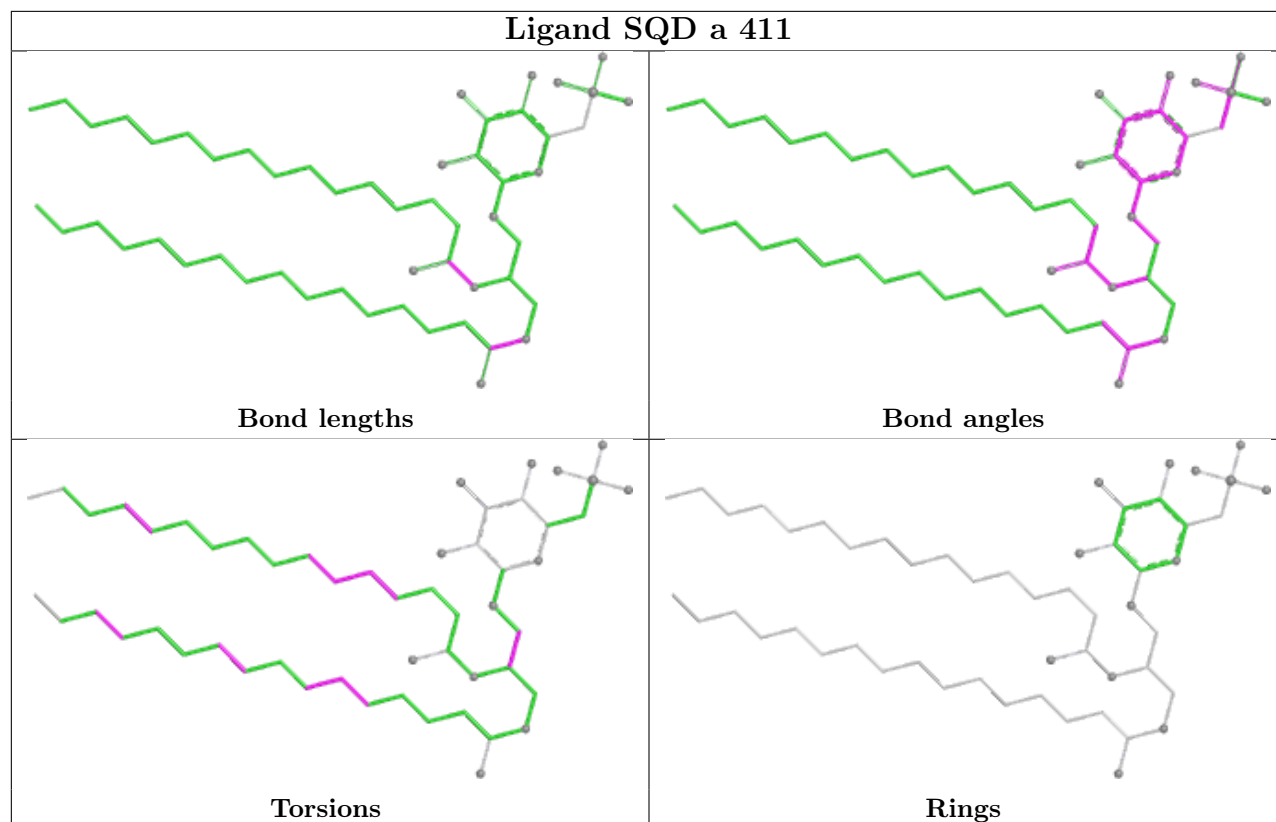


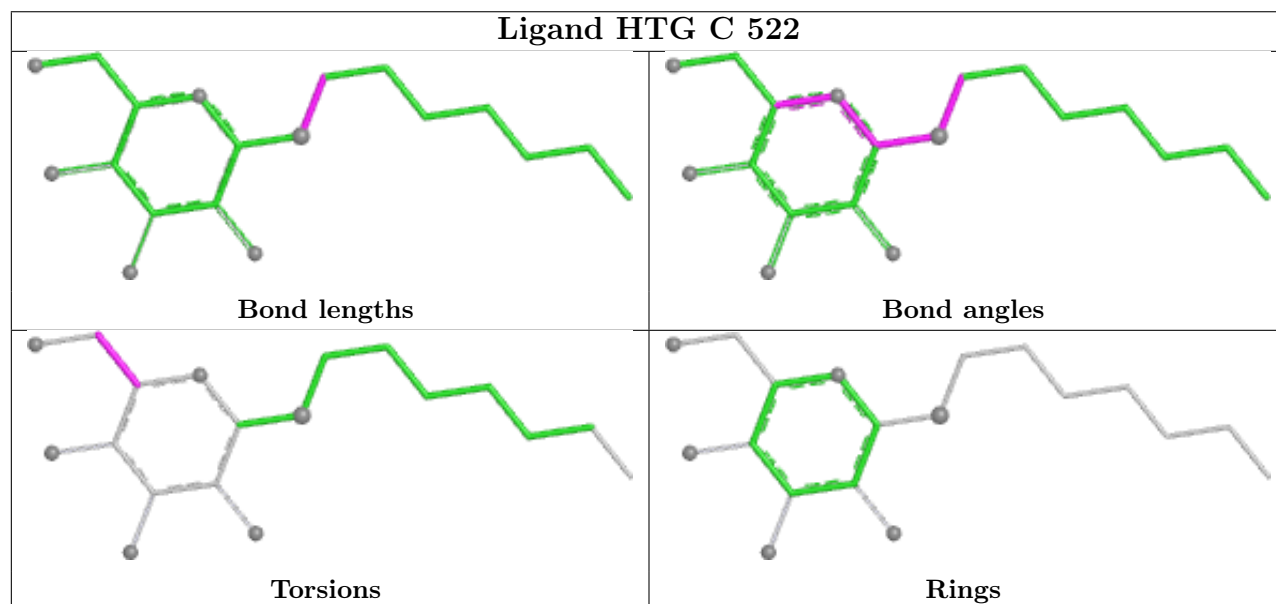
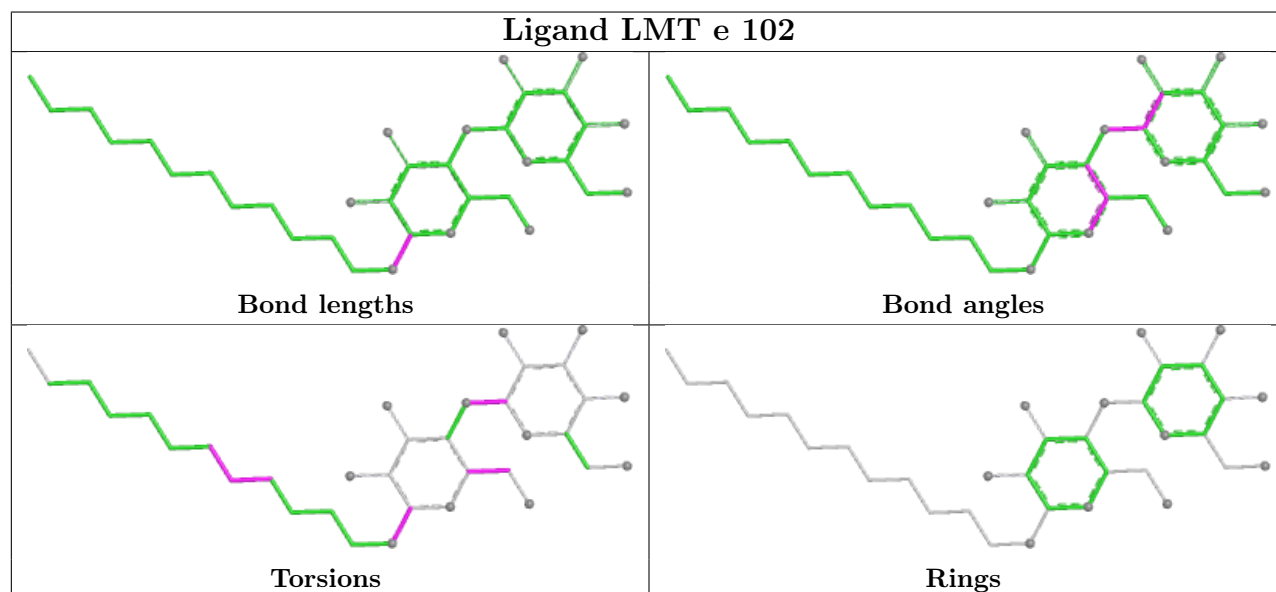
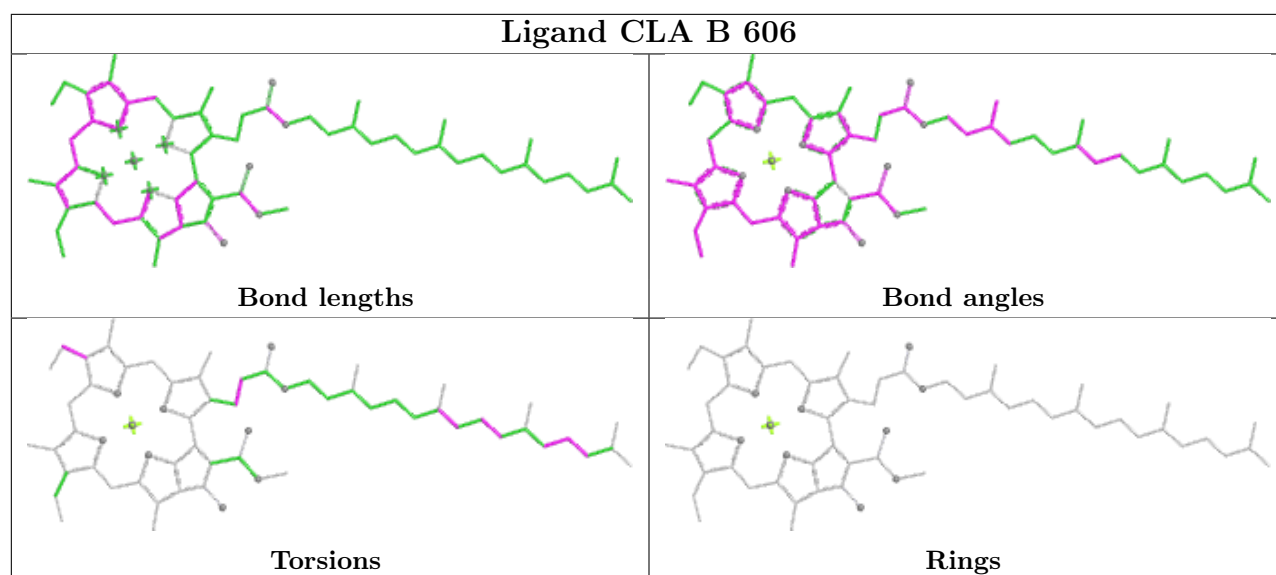
Ligand CLA b 609

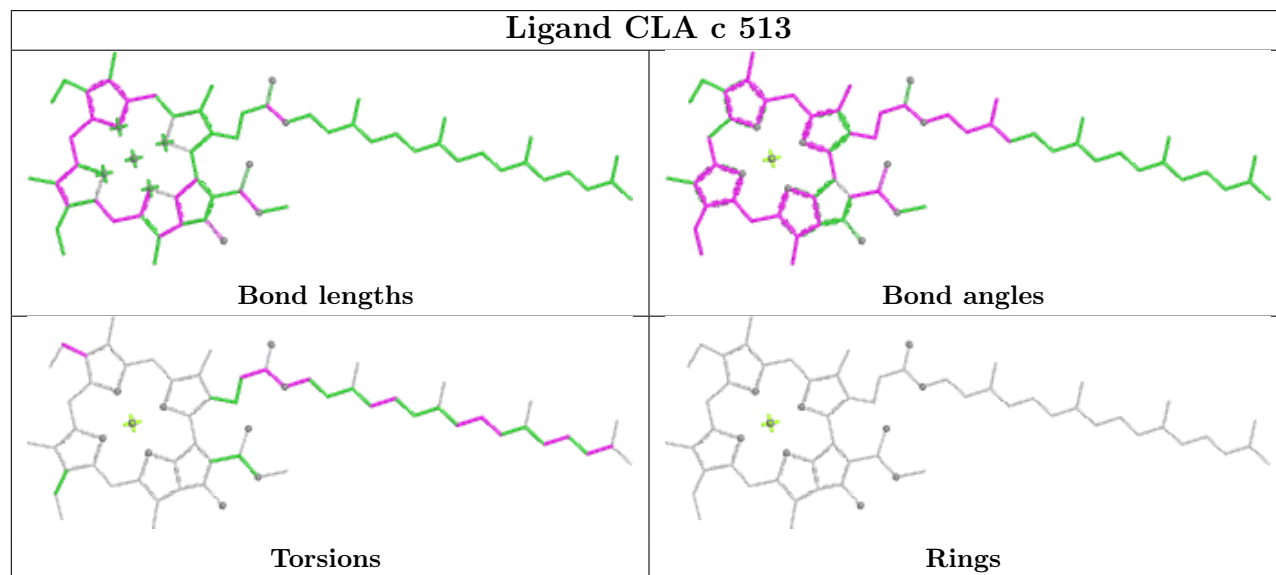
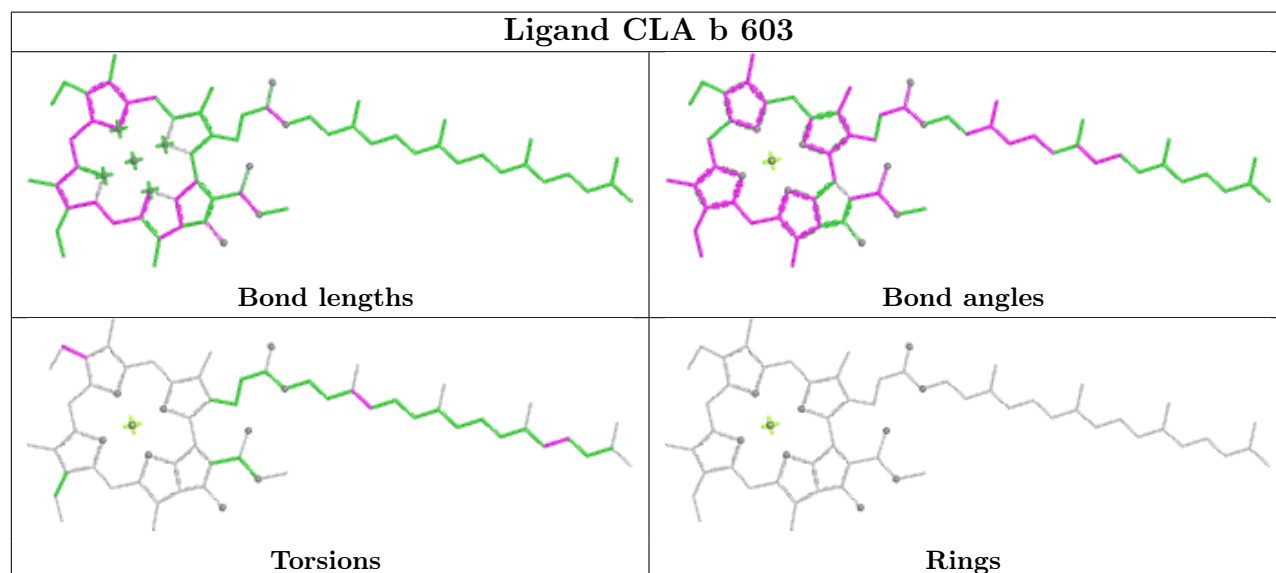
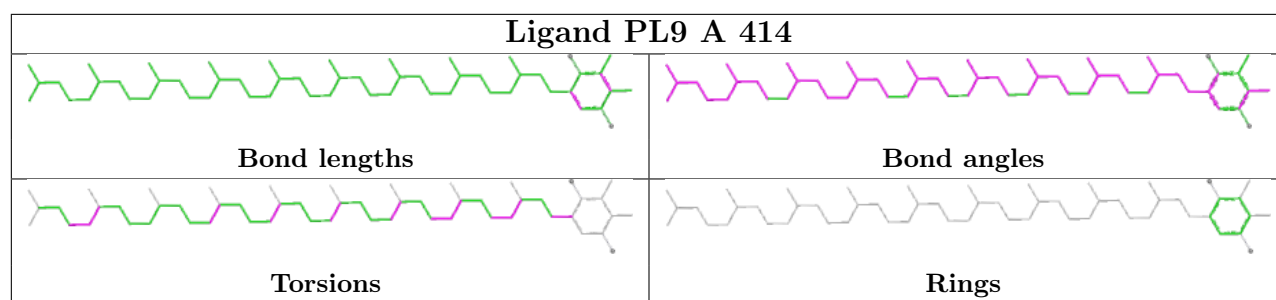


Ligand LMG B 621

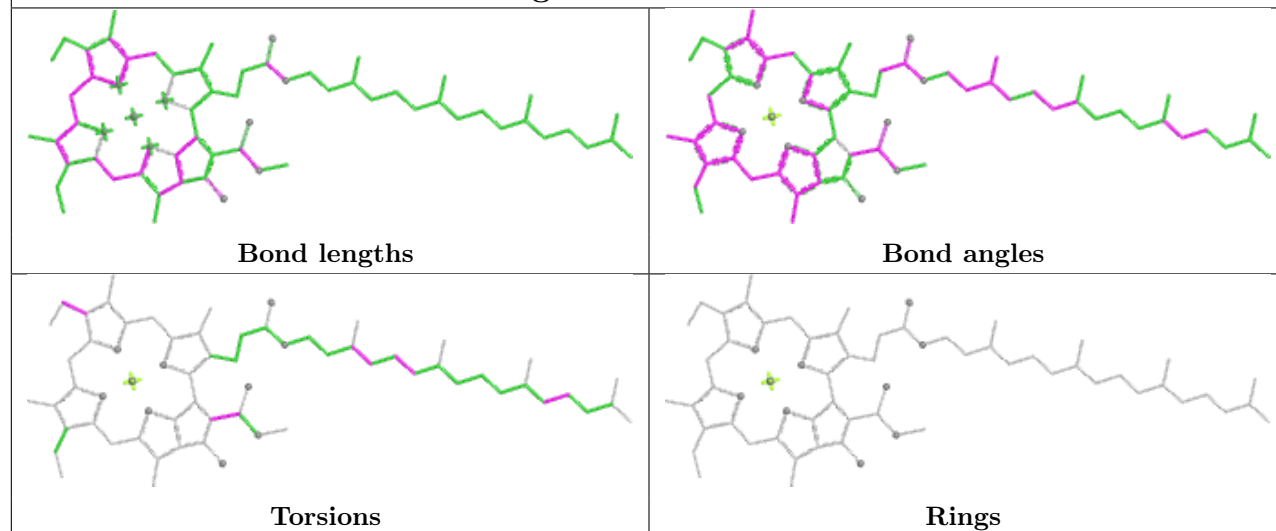




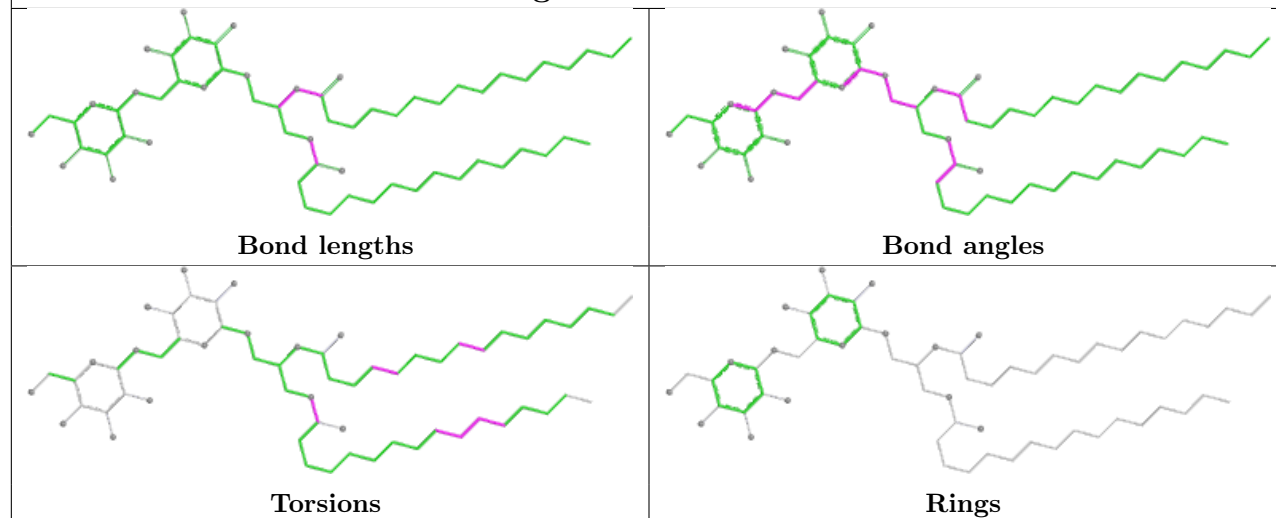




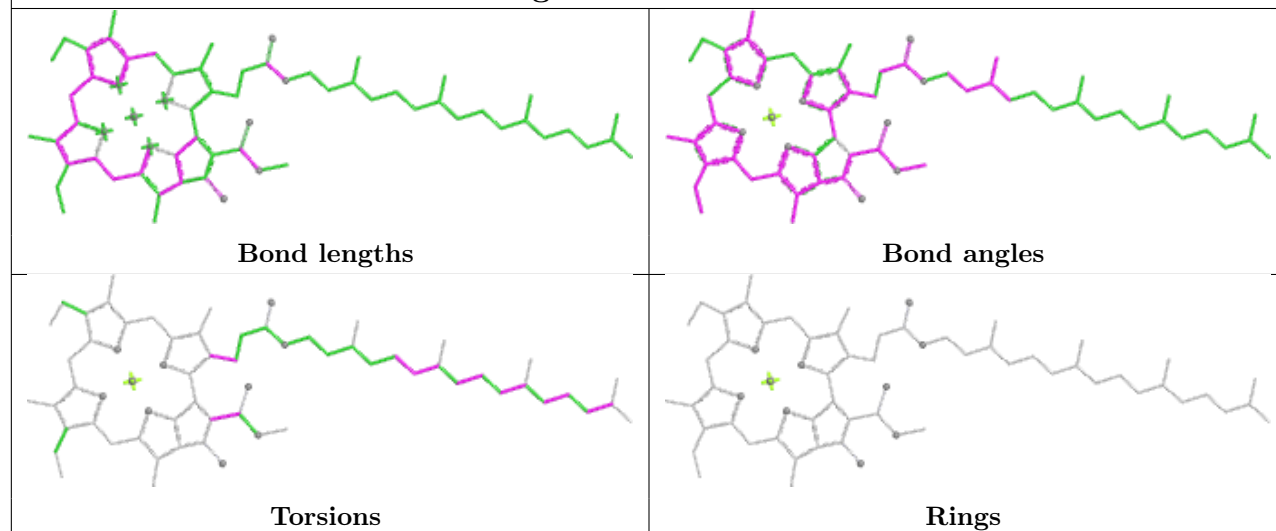
Ligand CLA C 508

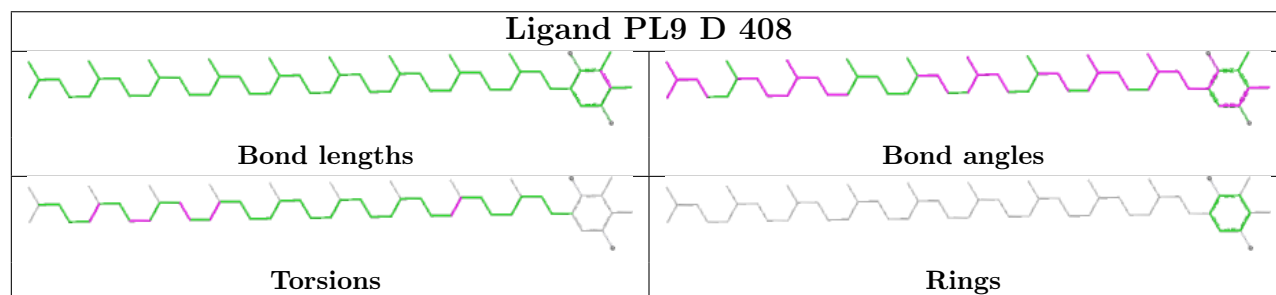
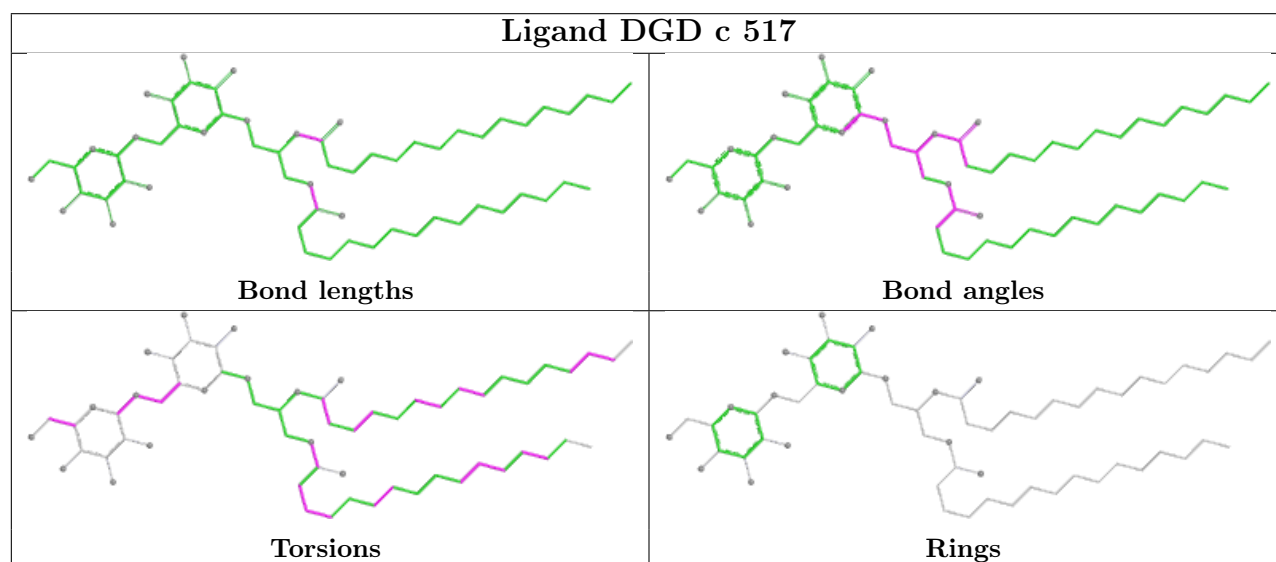
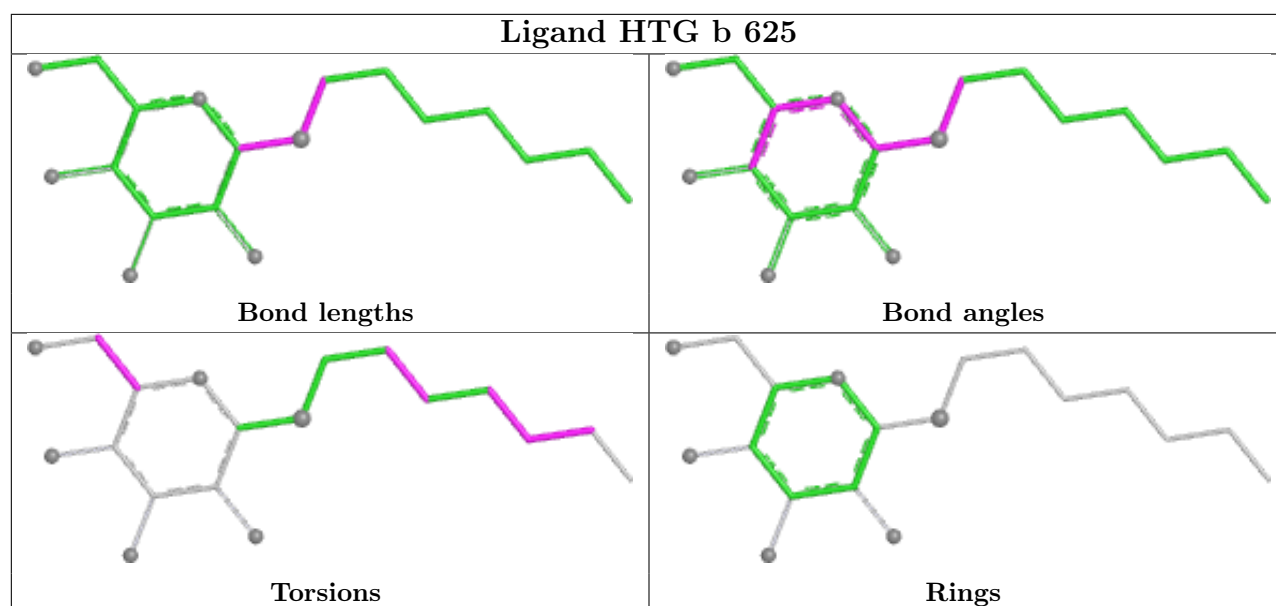


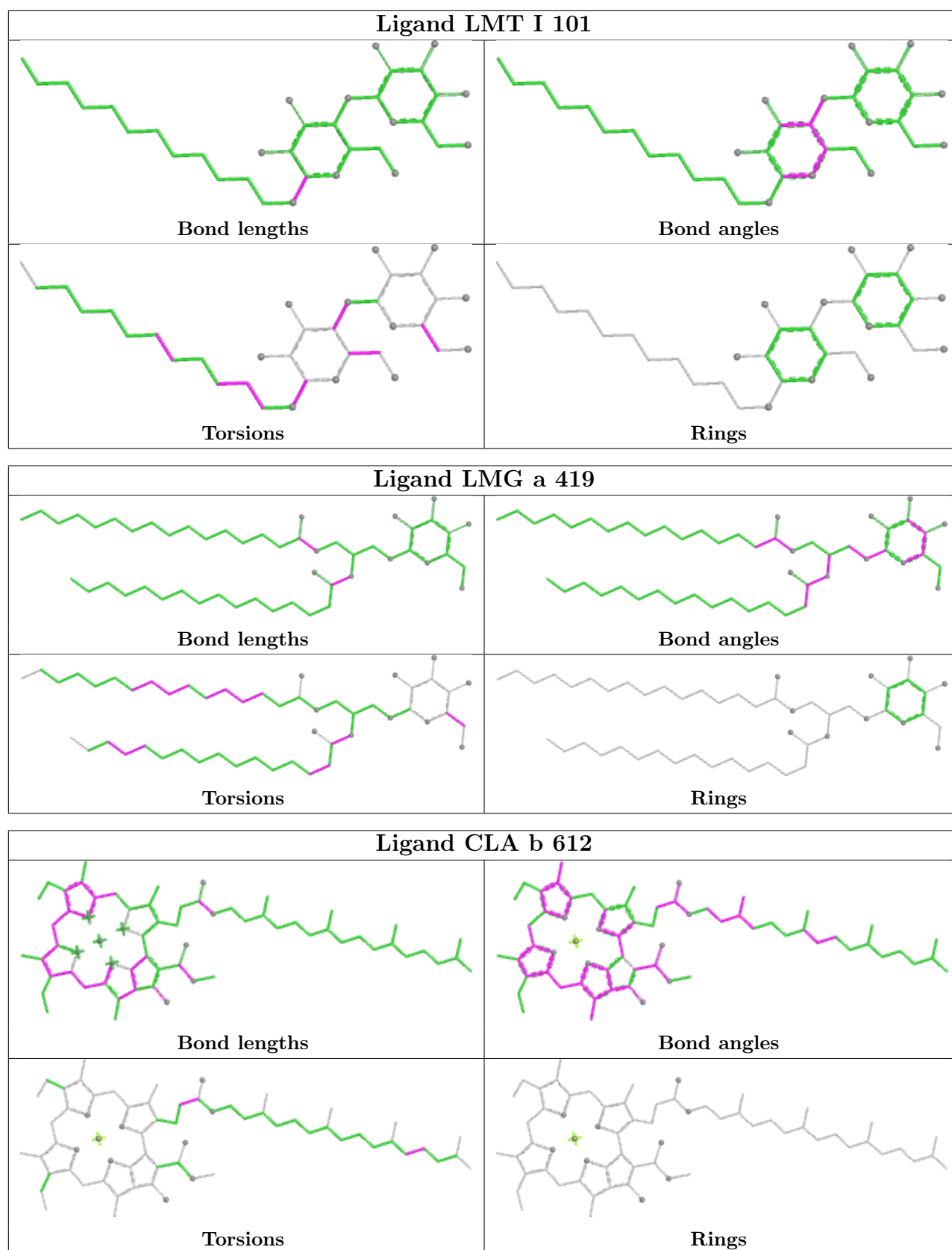
Ligand DGD c 519



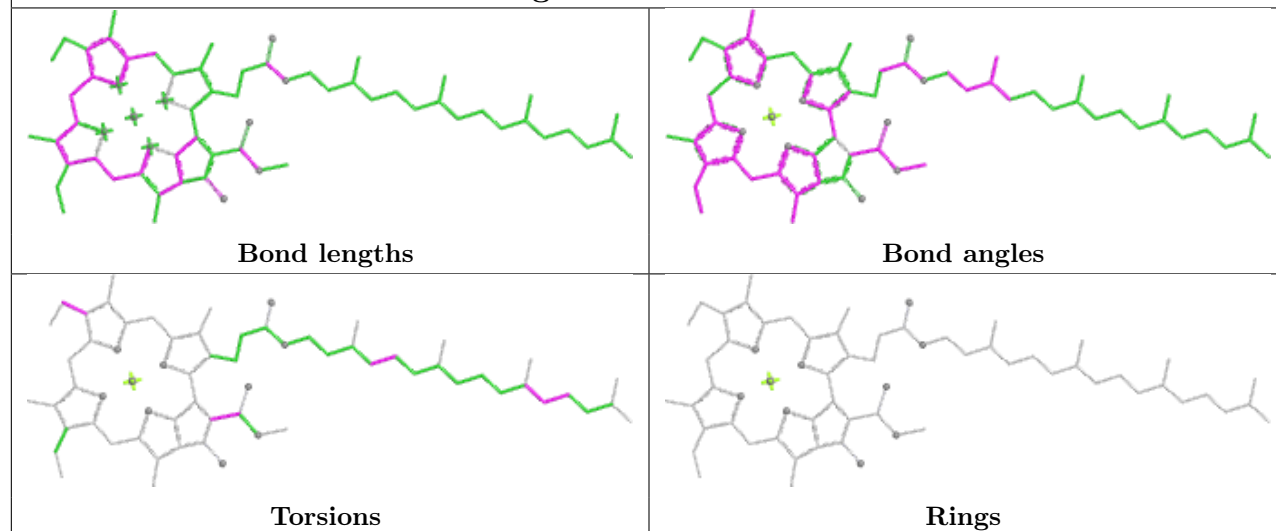
Ligand CLA C 507



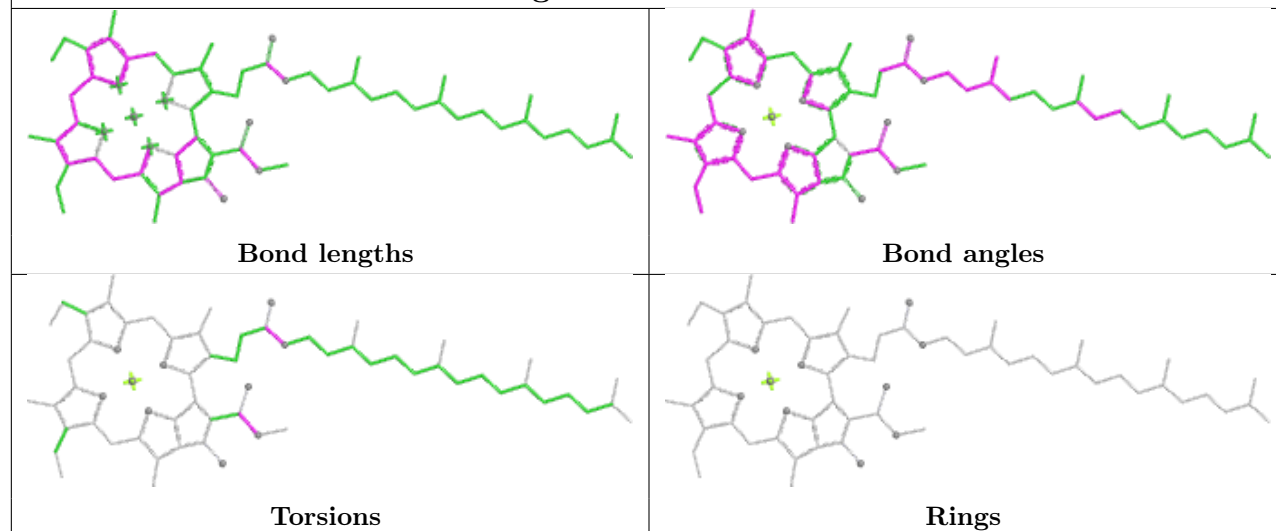




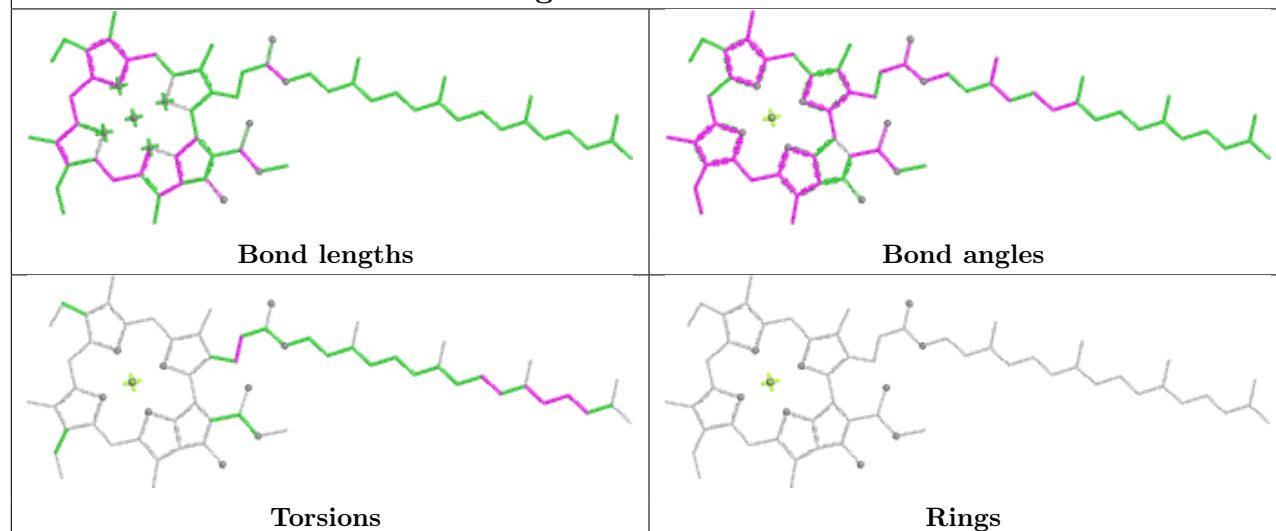
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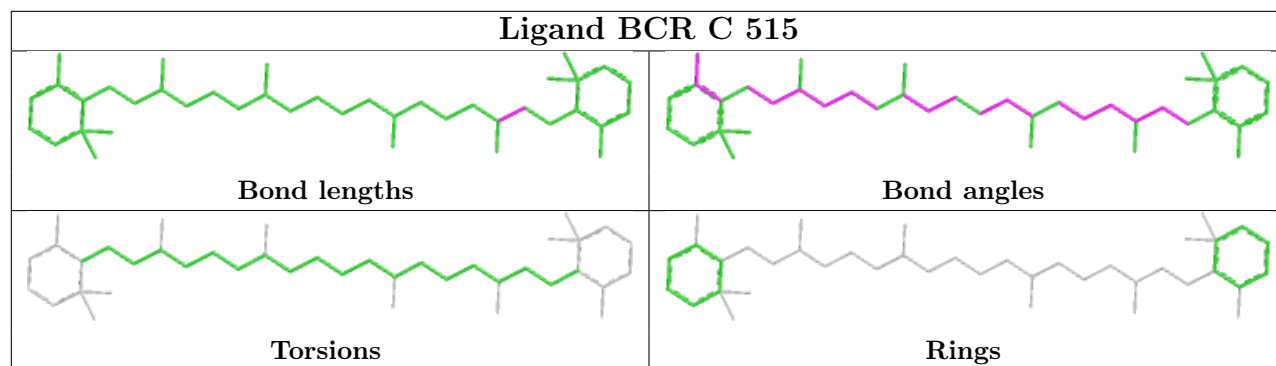
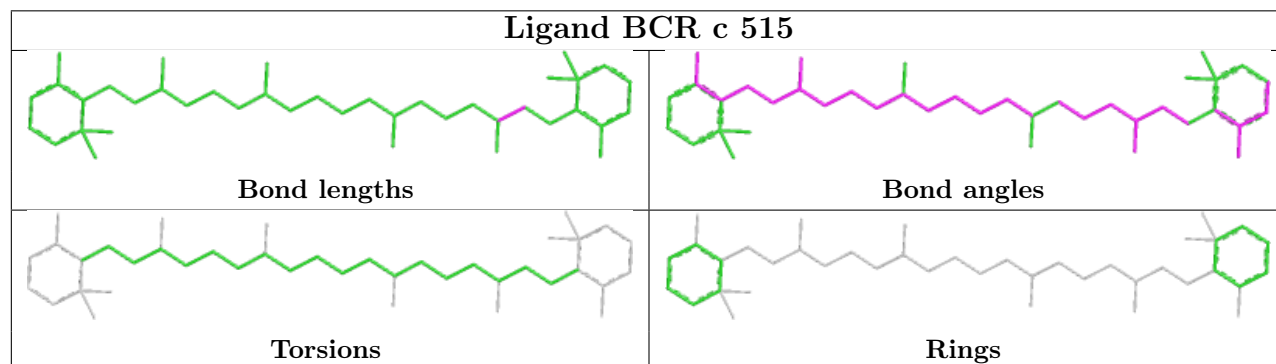
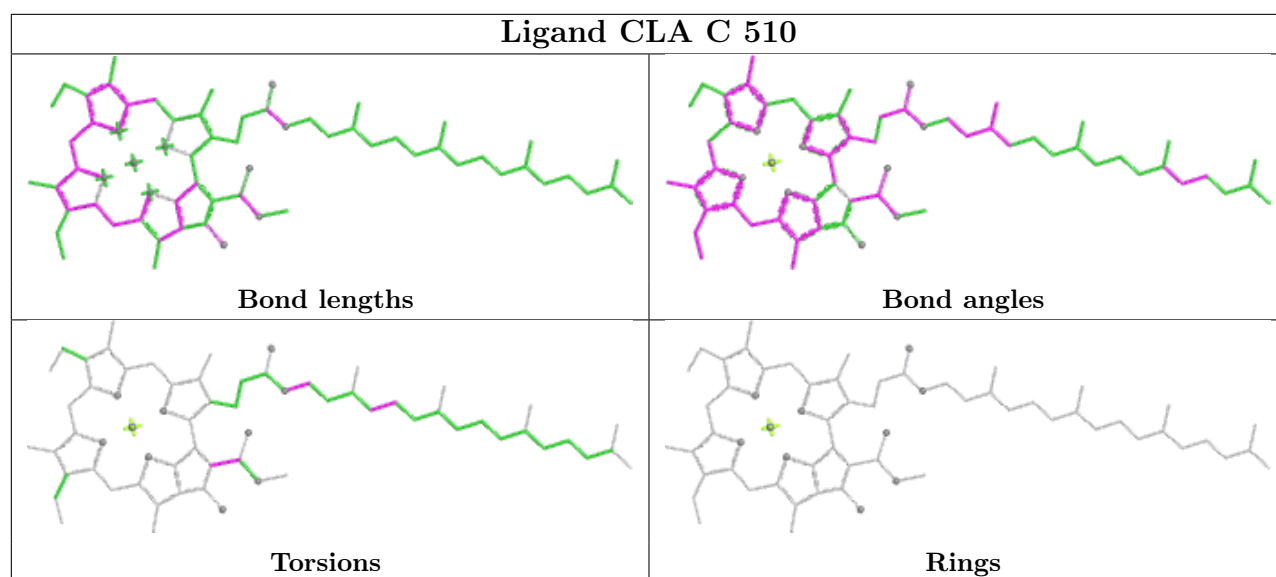


Ligand CLA C 512

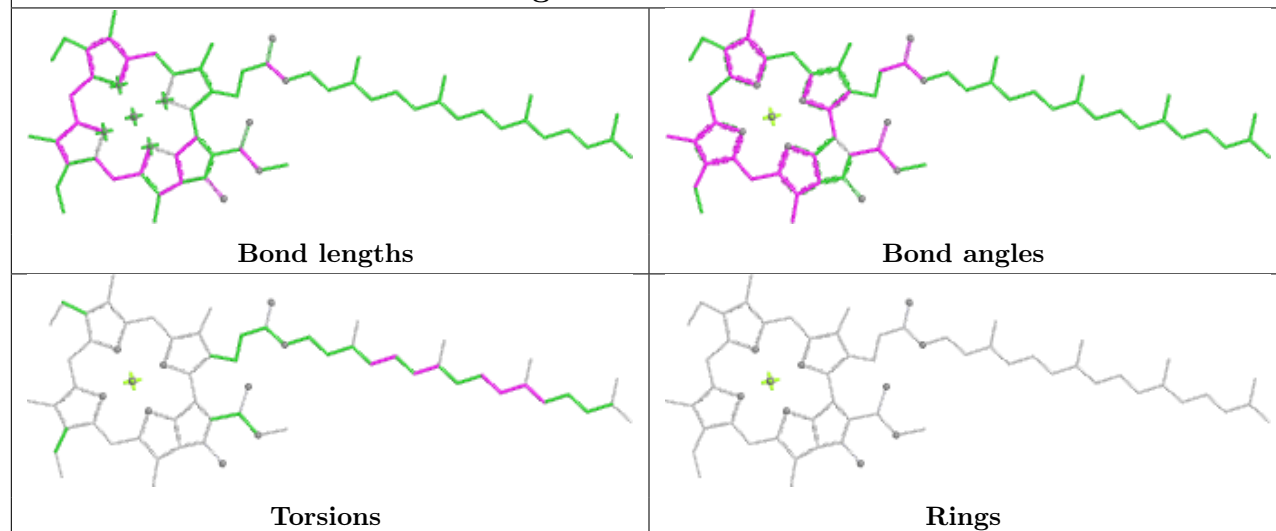


Ligand CLA b 606

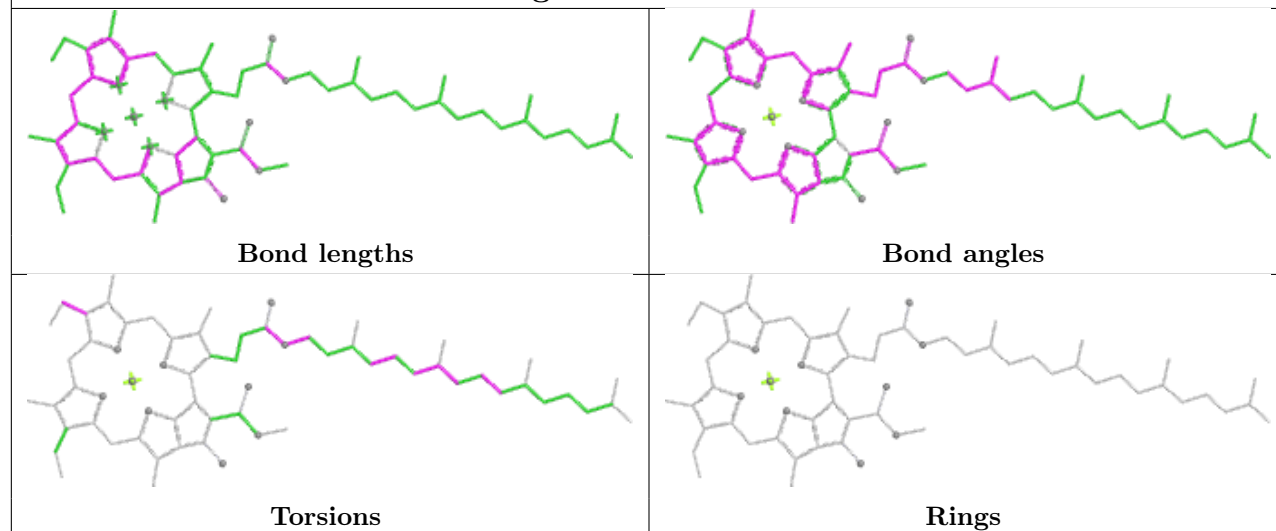




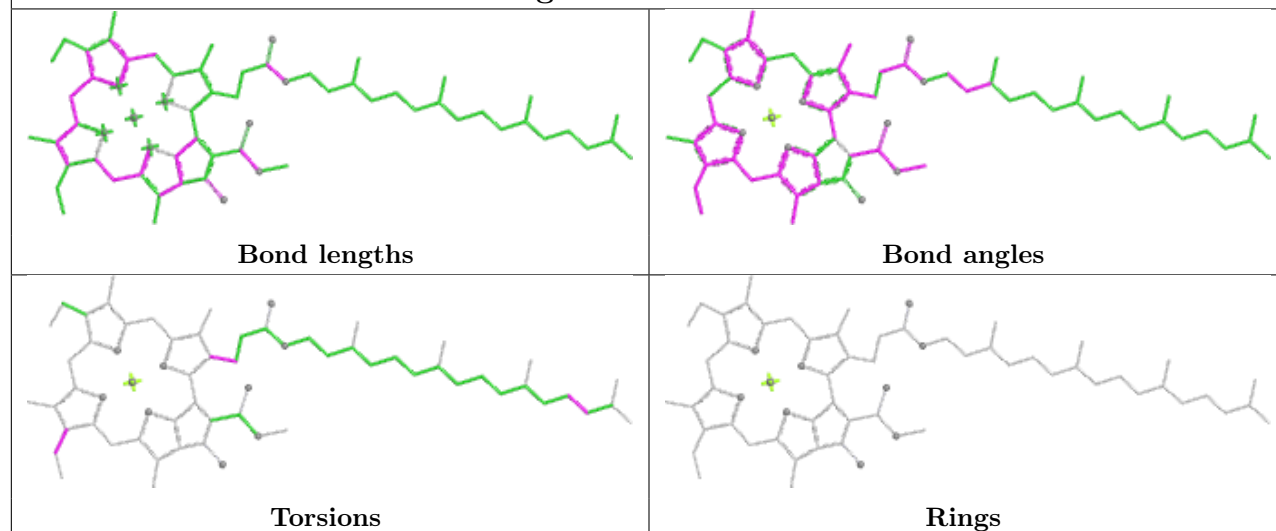
Ligand CLA B 616



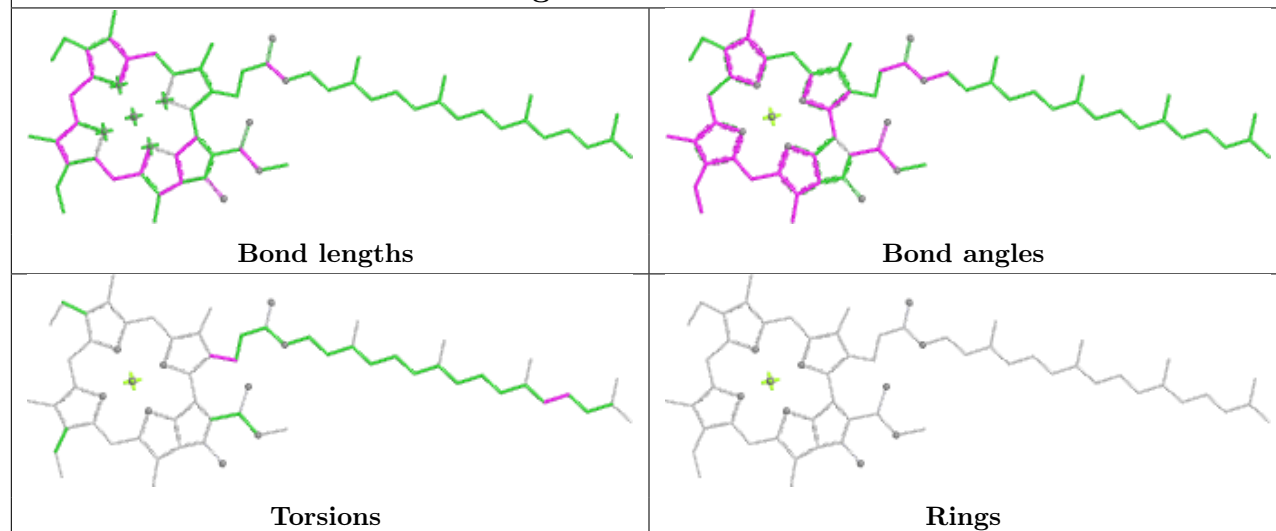
Ligand CLA C 513



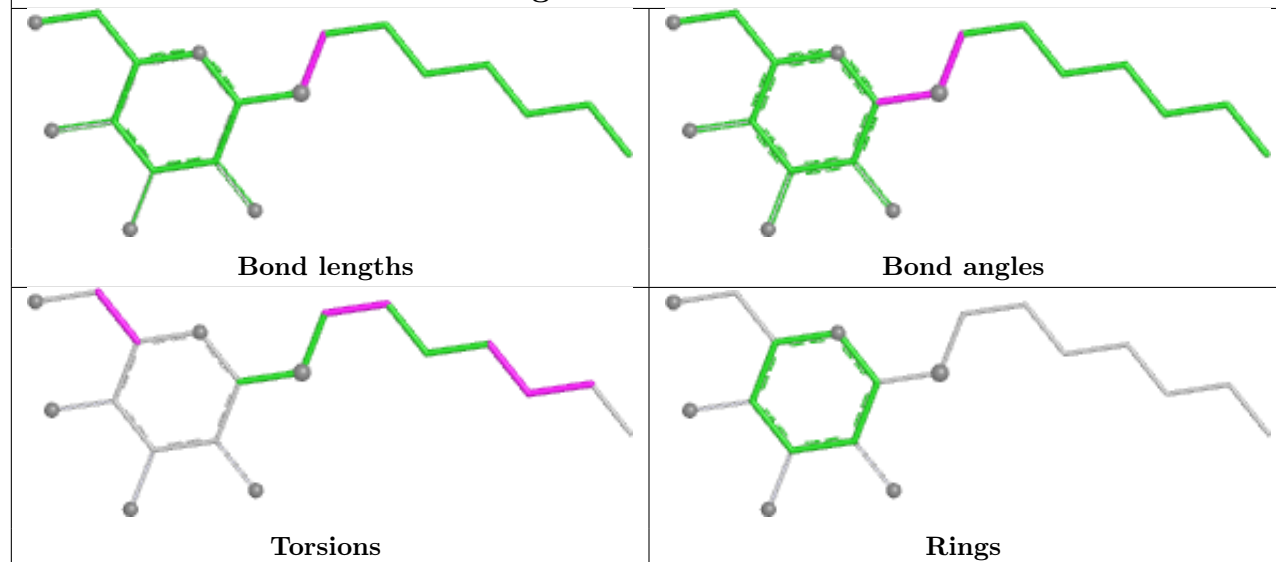
Ligand CLA a 406

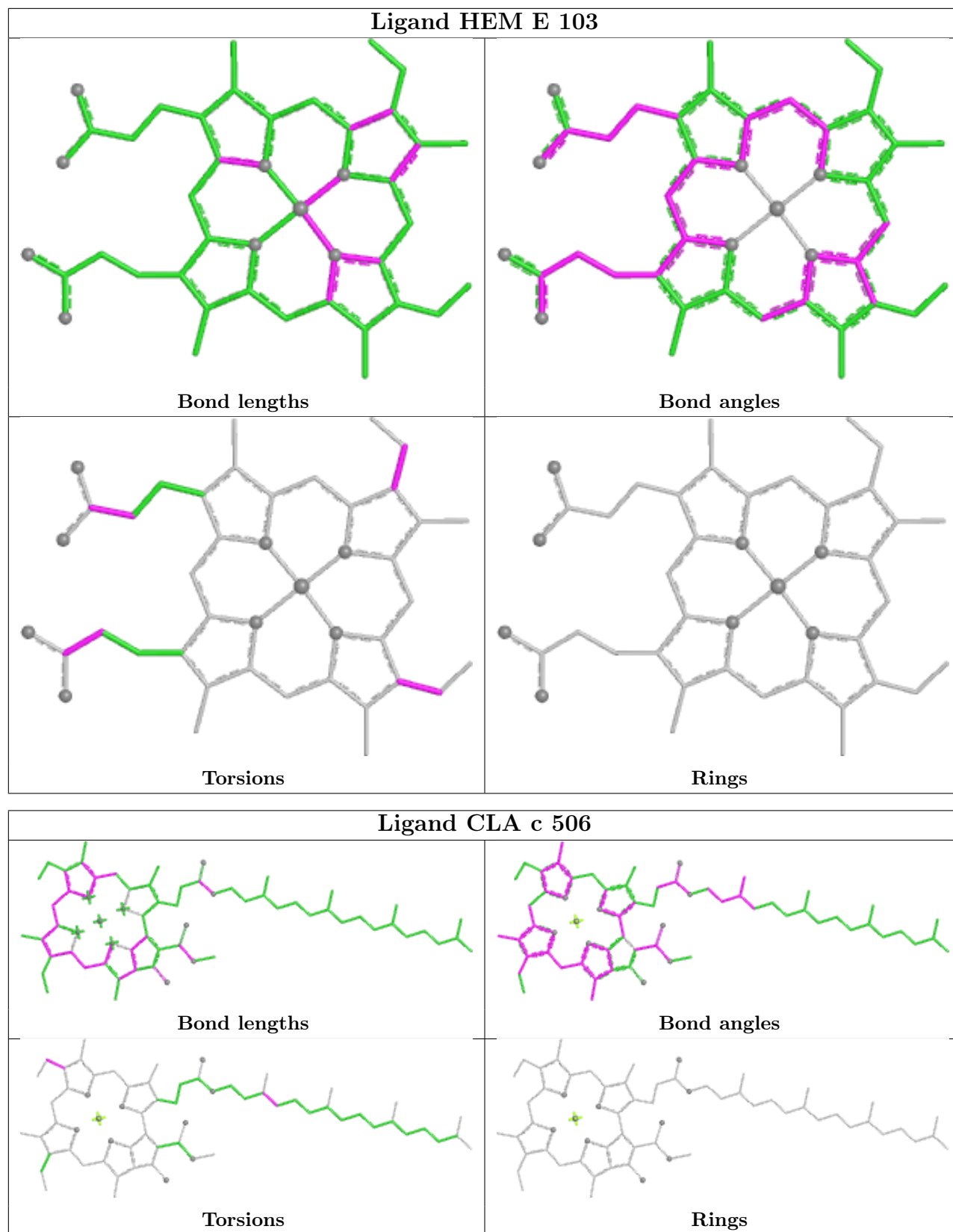


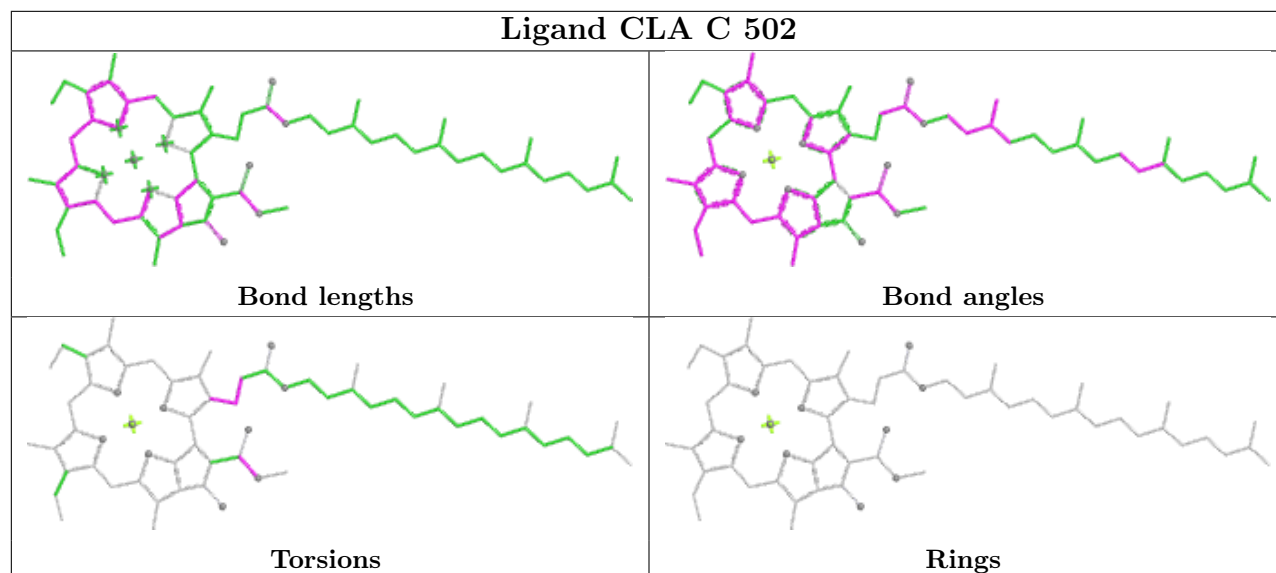
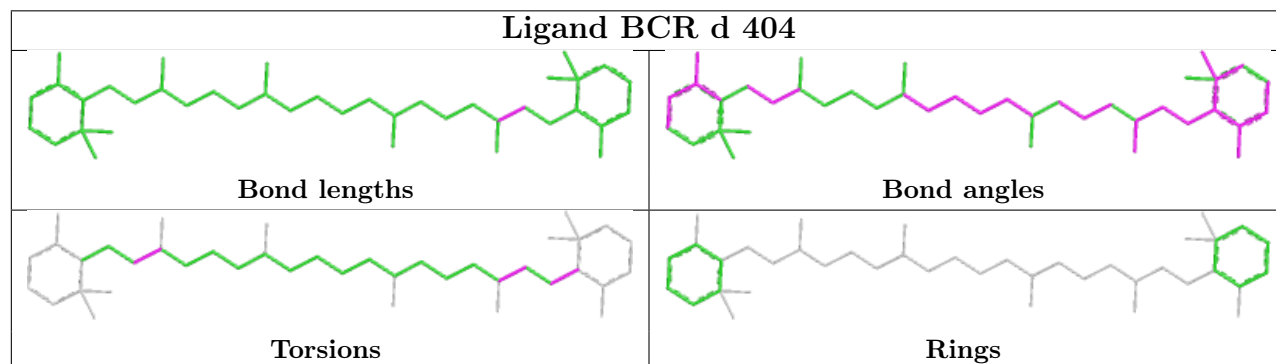
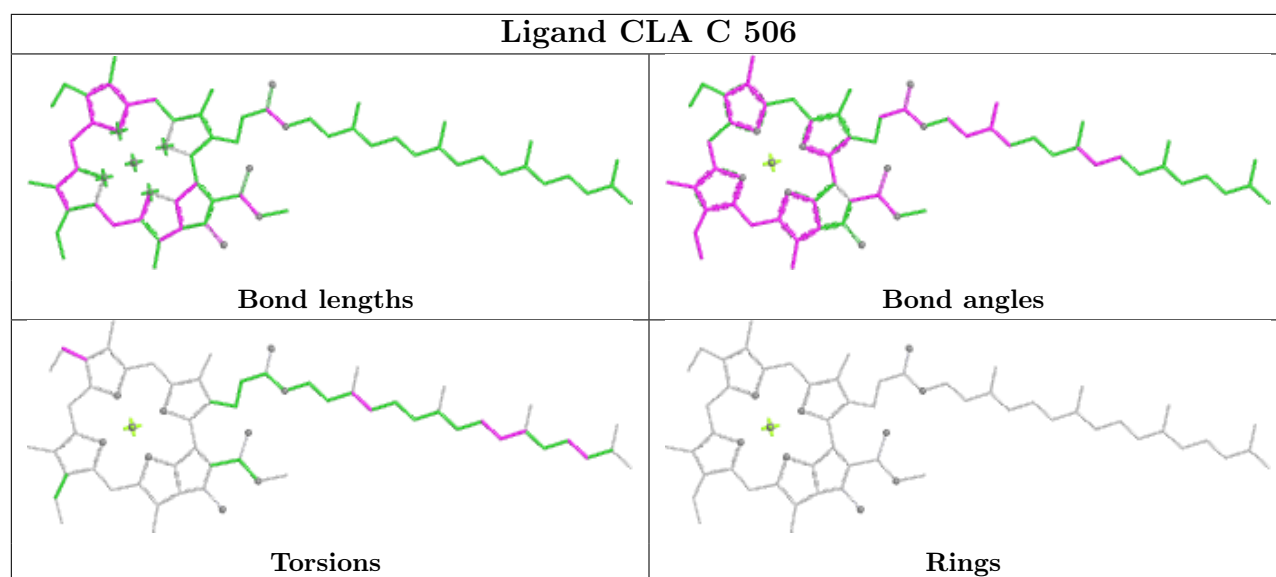
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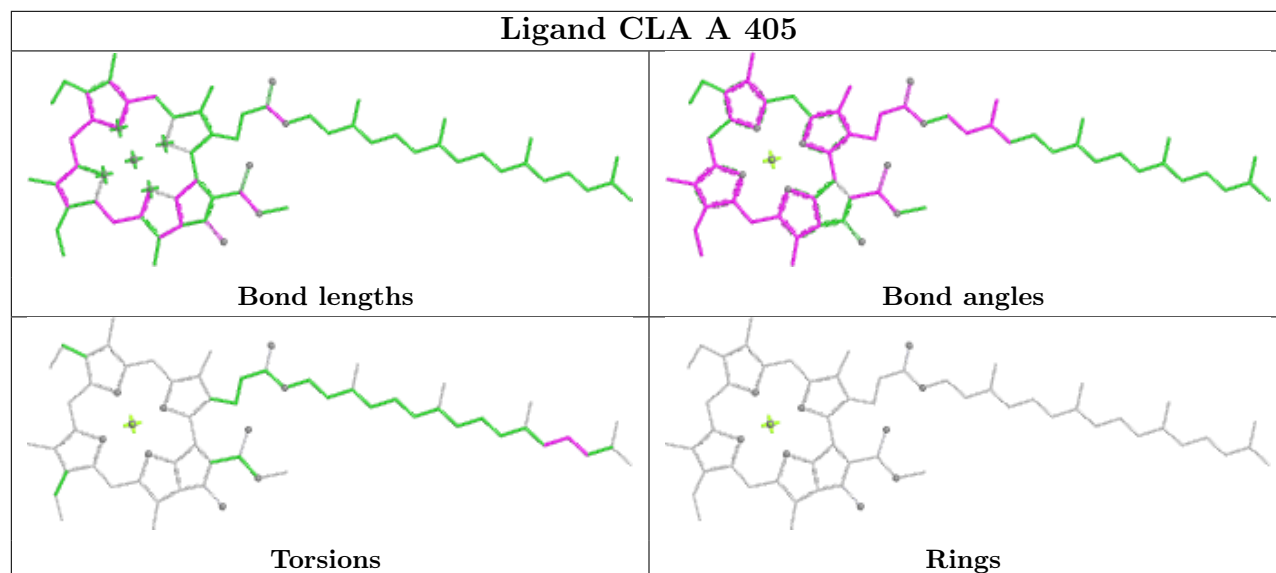
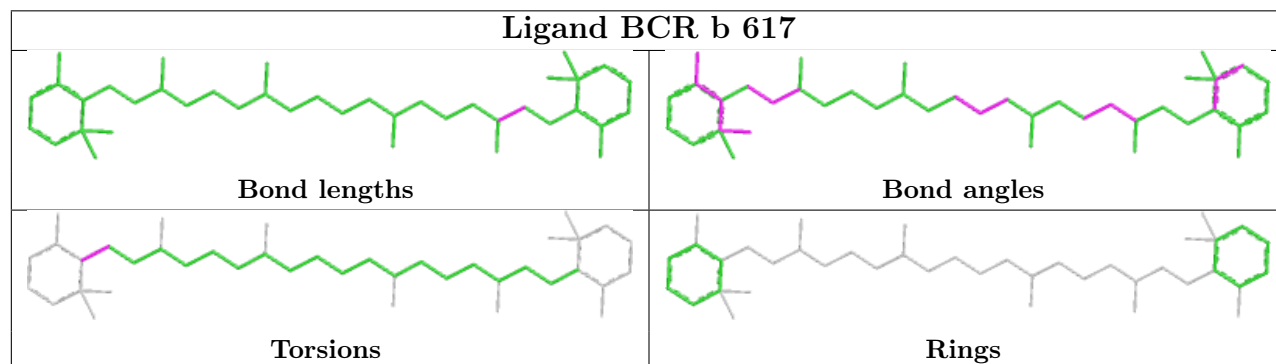
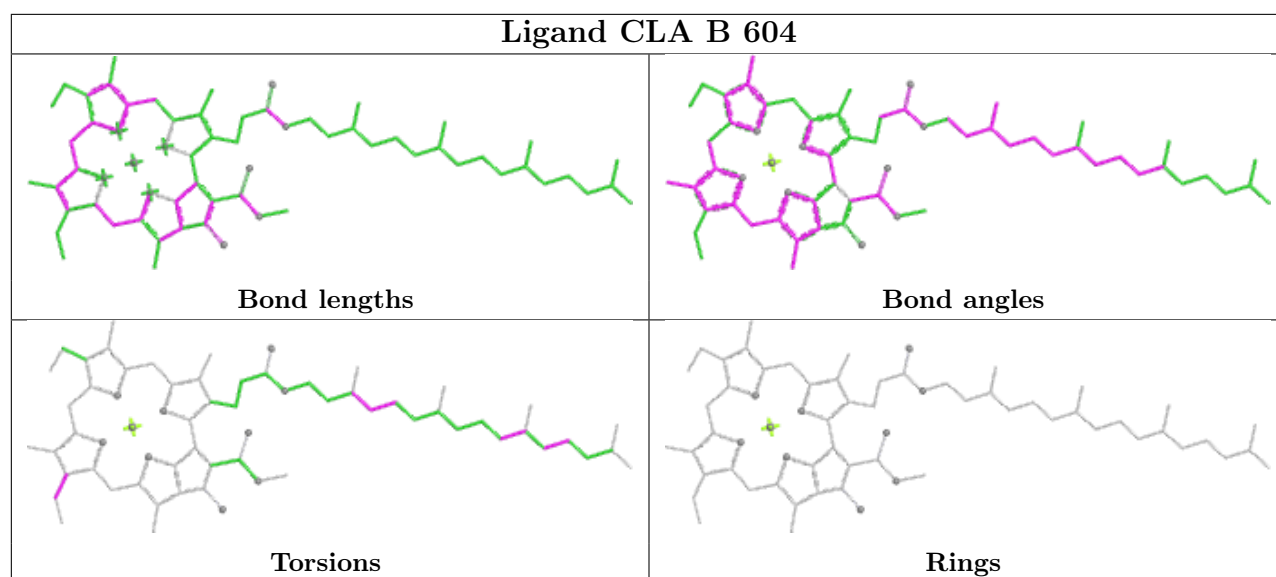


Ligand HTG b 623

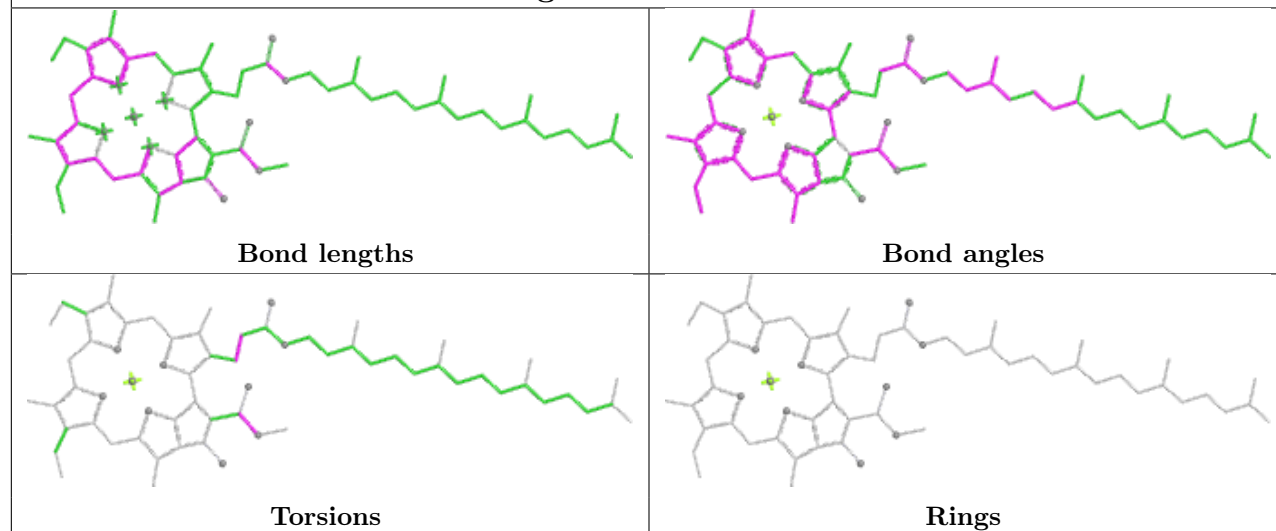




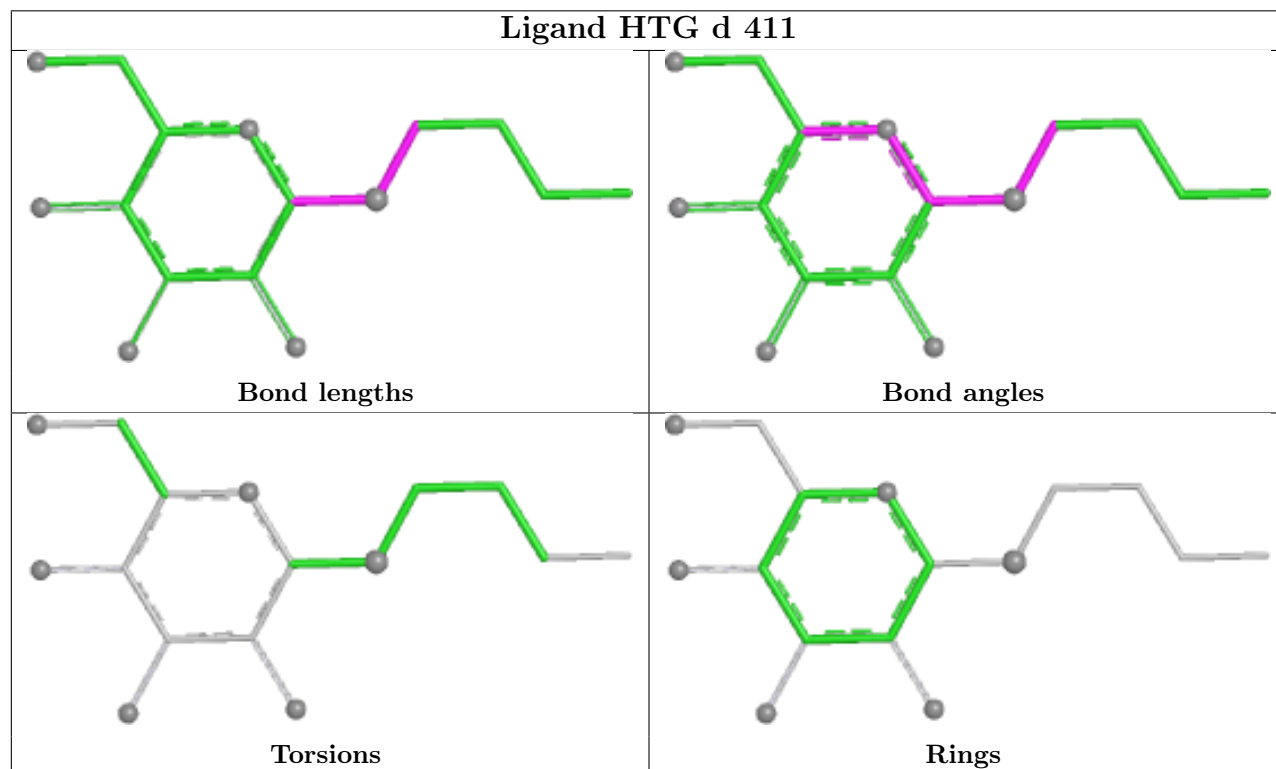




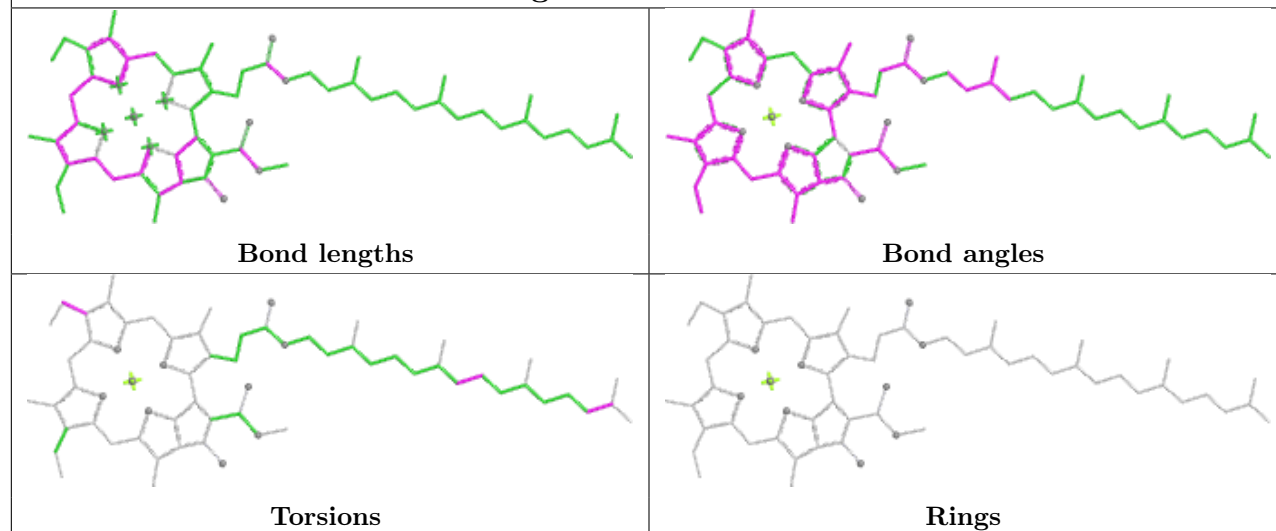
Ligand CLA c 502



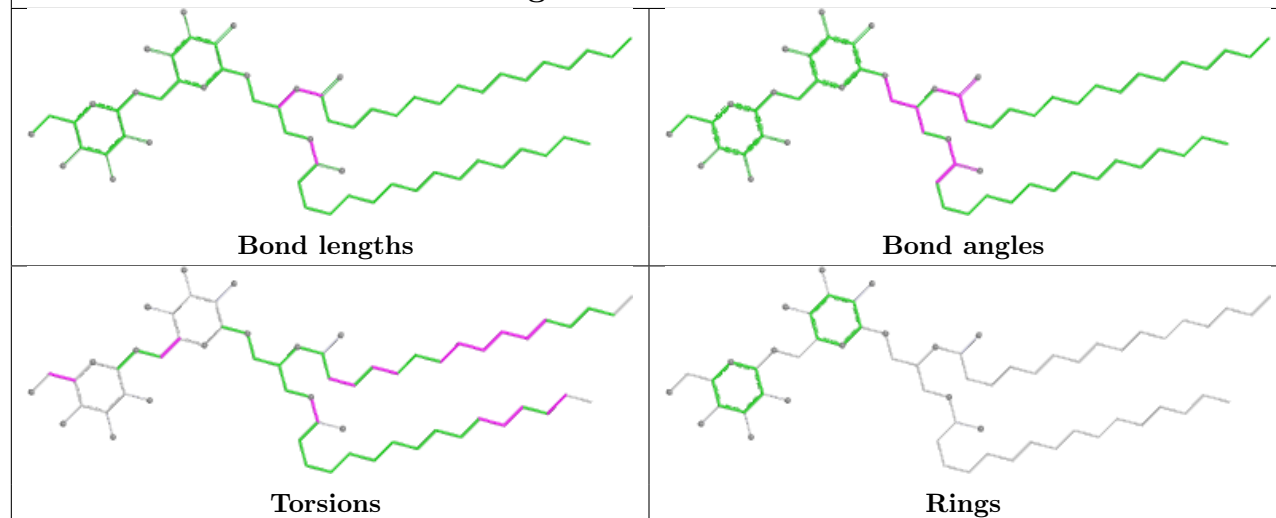
Ligand HTG d 411



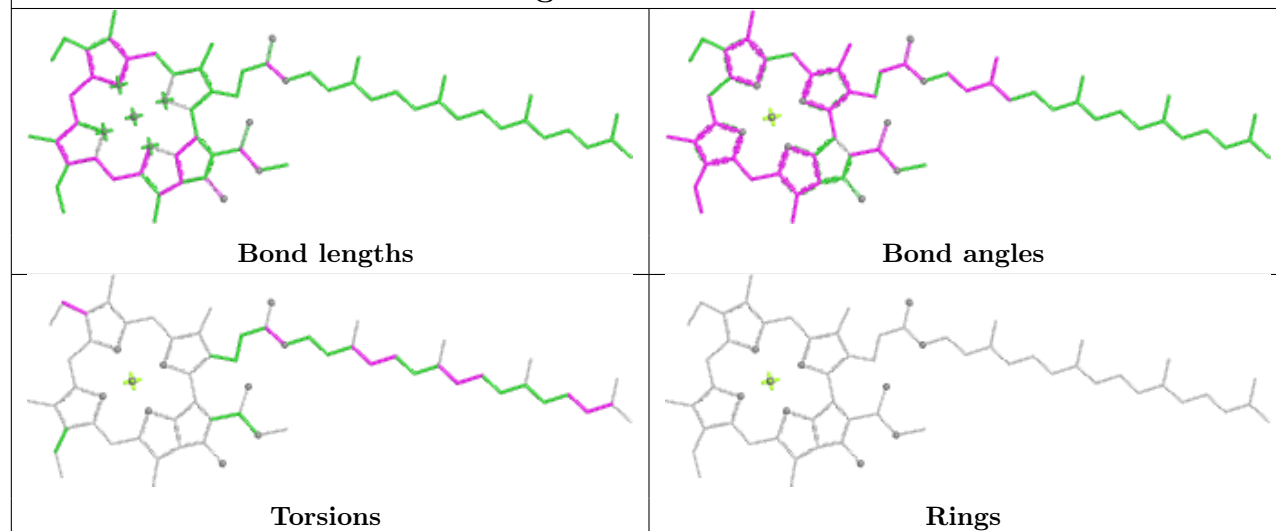
Ligand CLA D 405



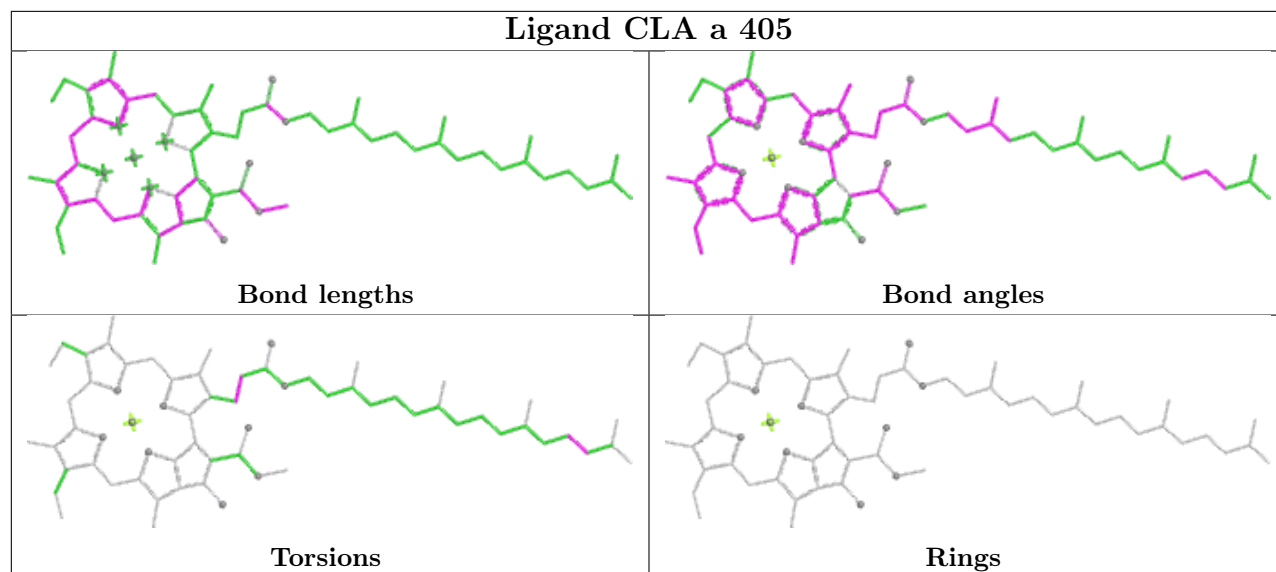
Ligand DGD C 519



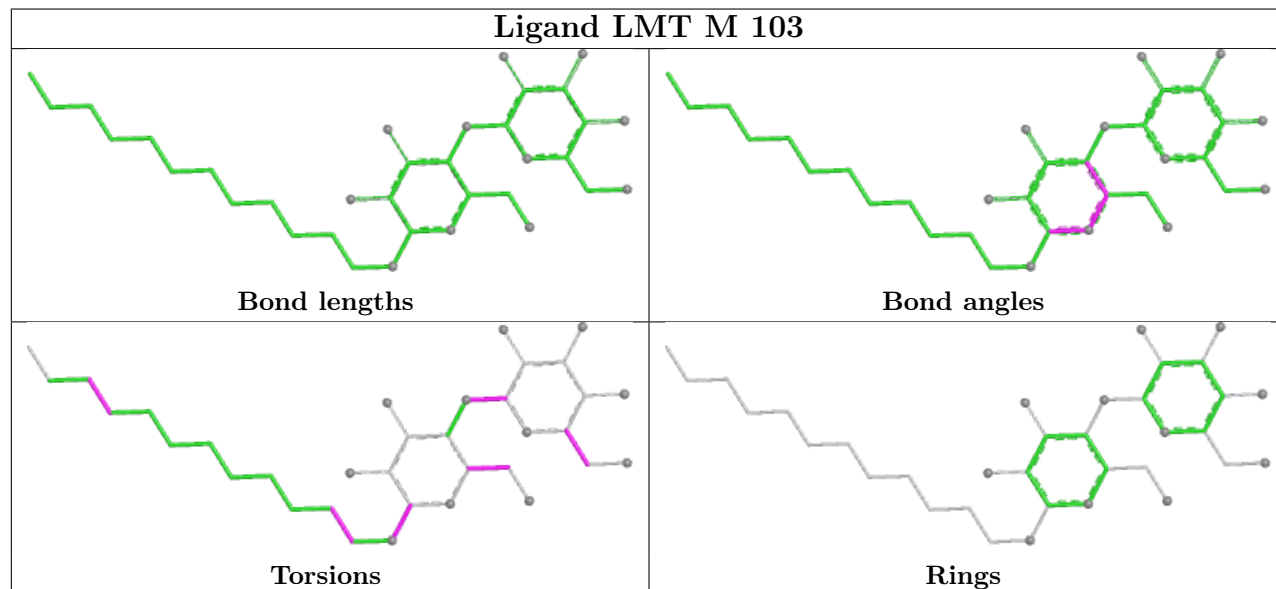
Ligand CLA a 409



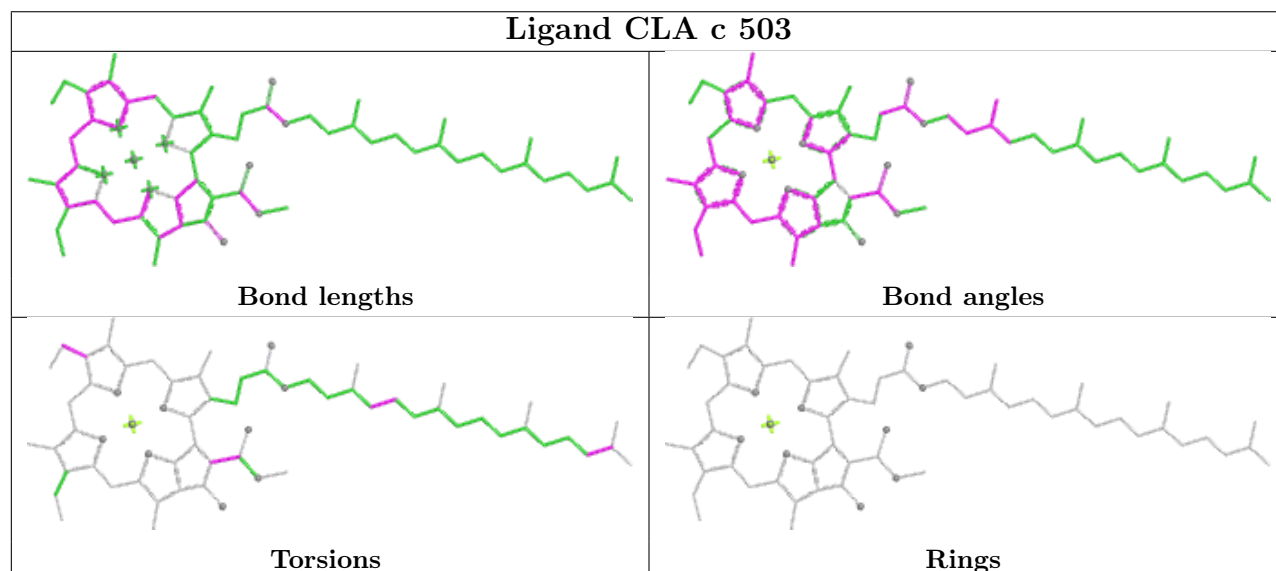
Ligand CLA a 405

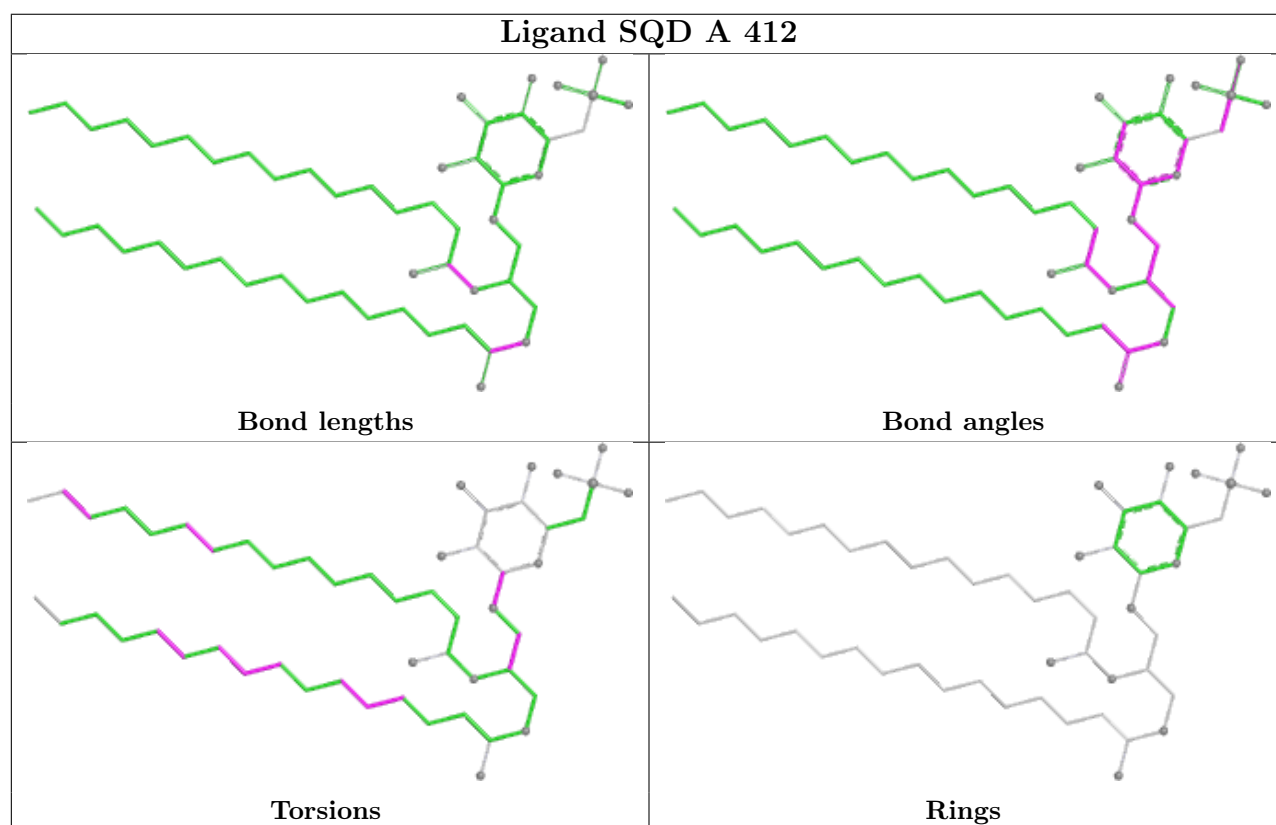
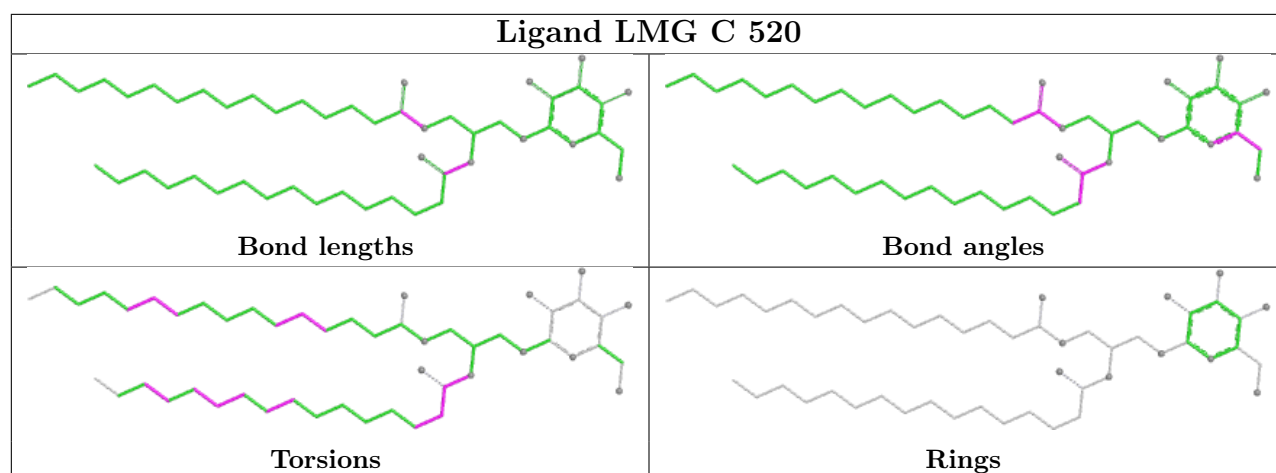


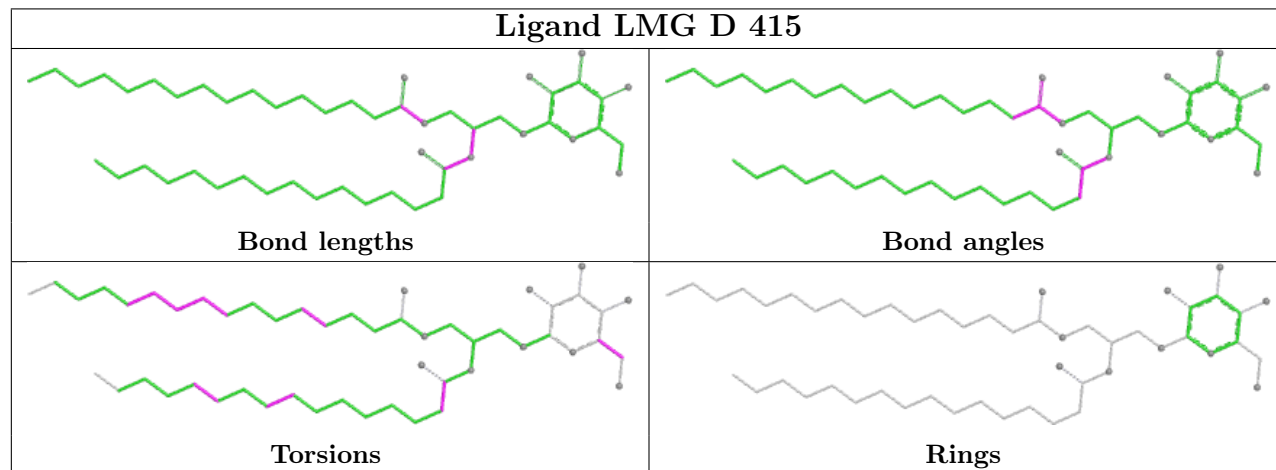
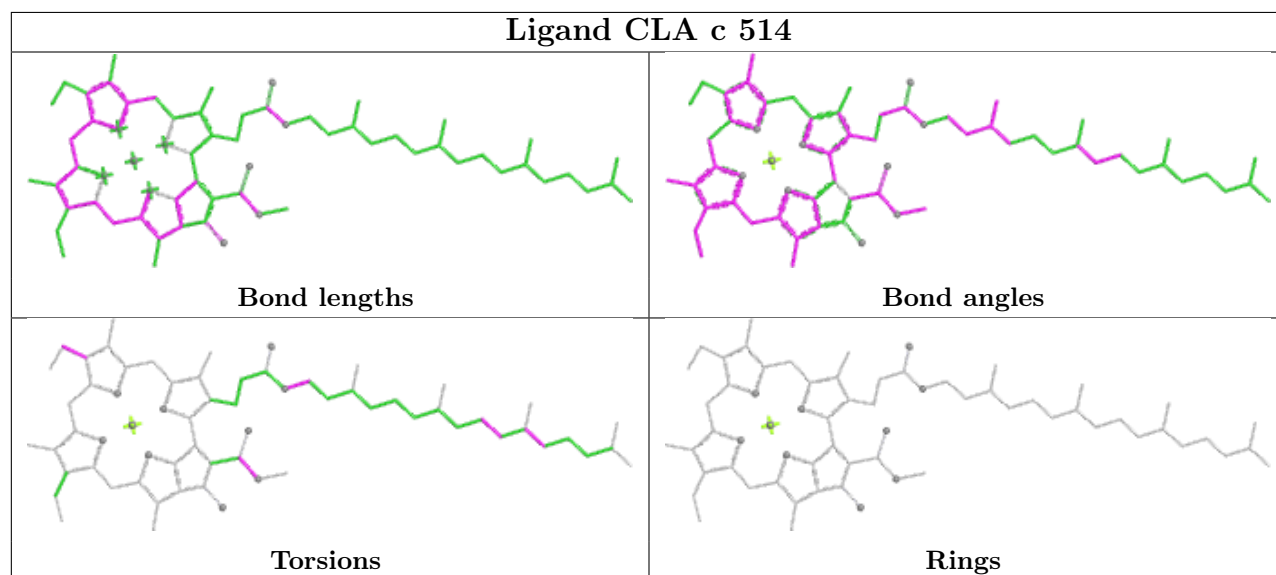
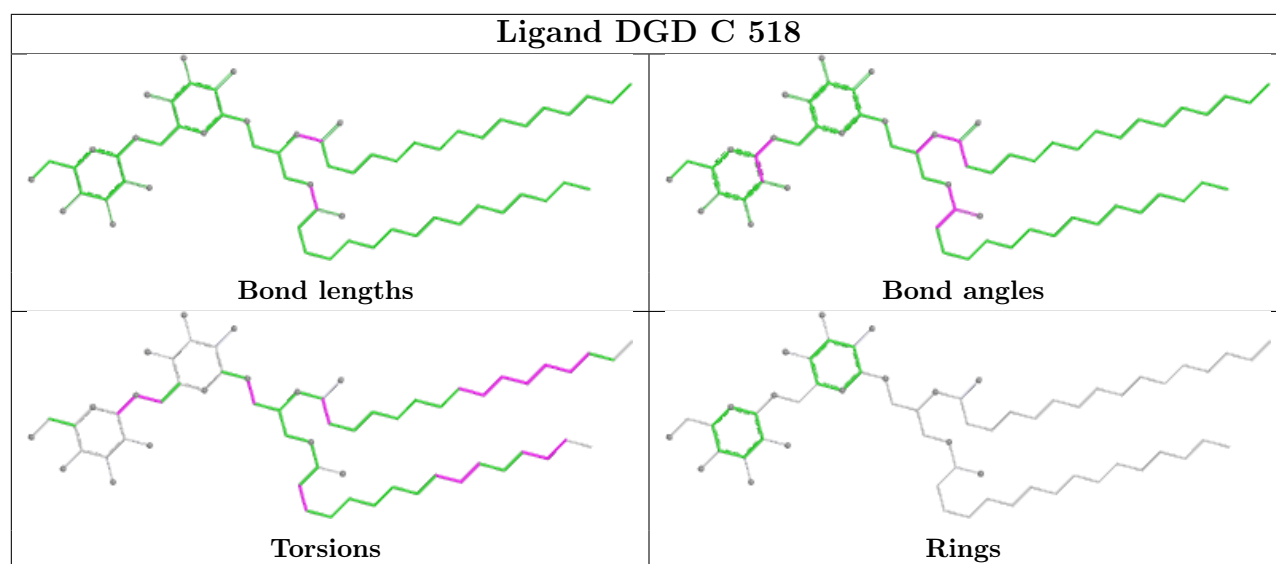
Ligand LMT M 103

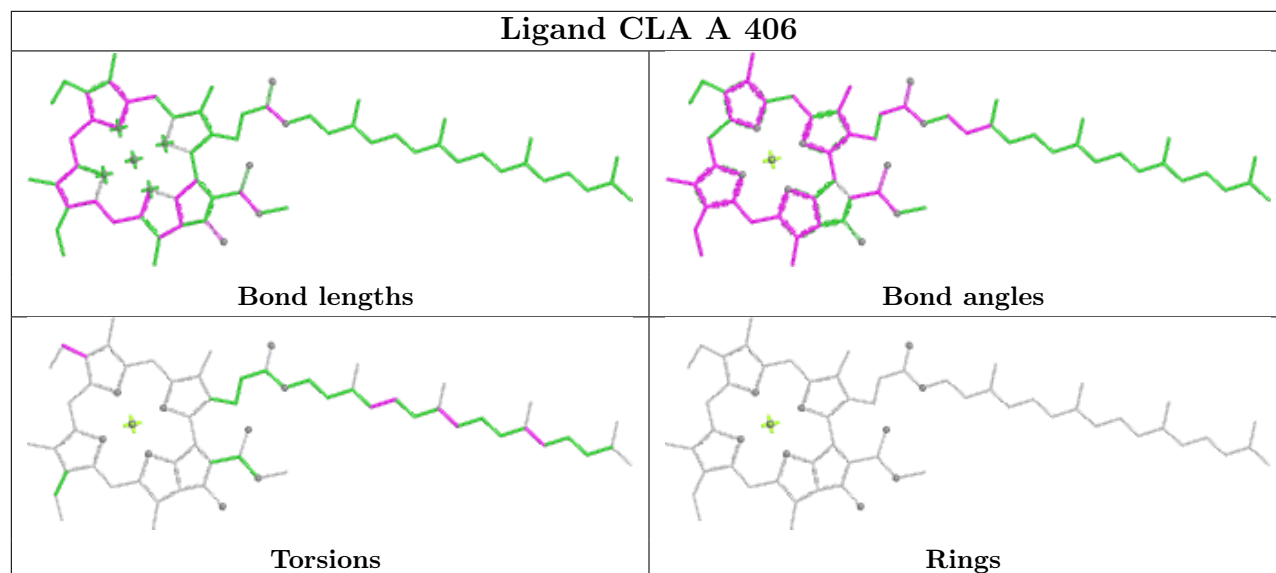
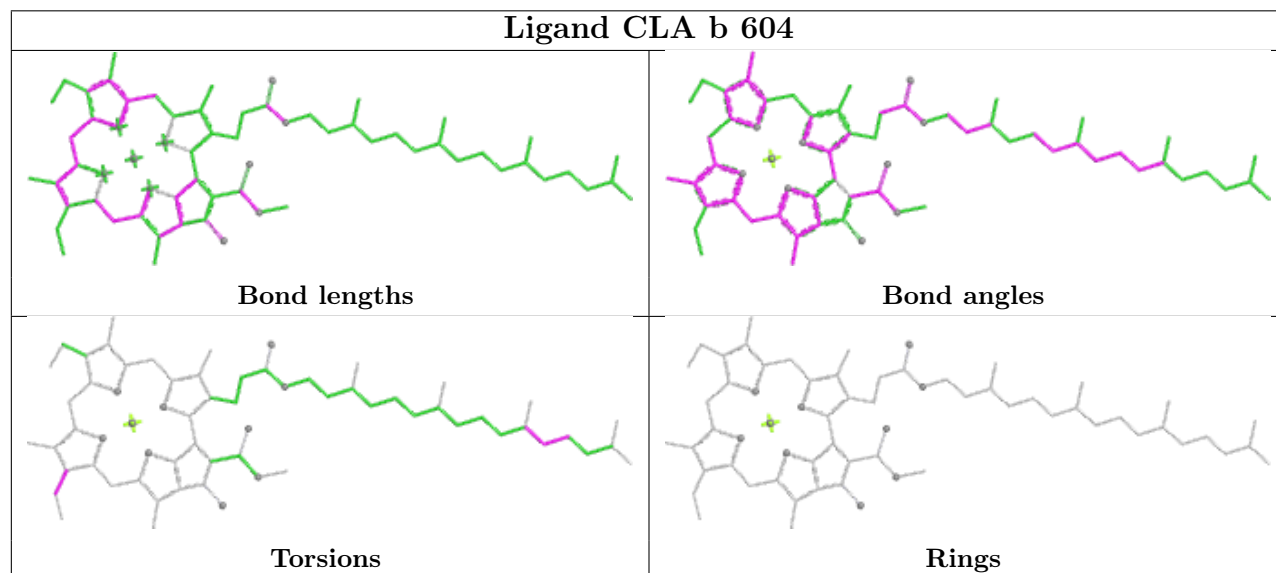
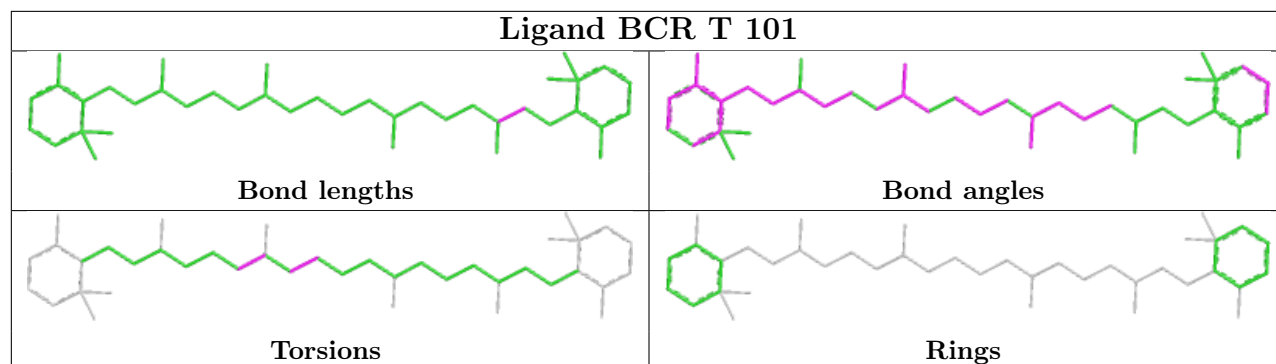


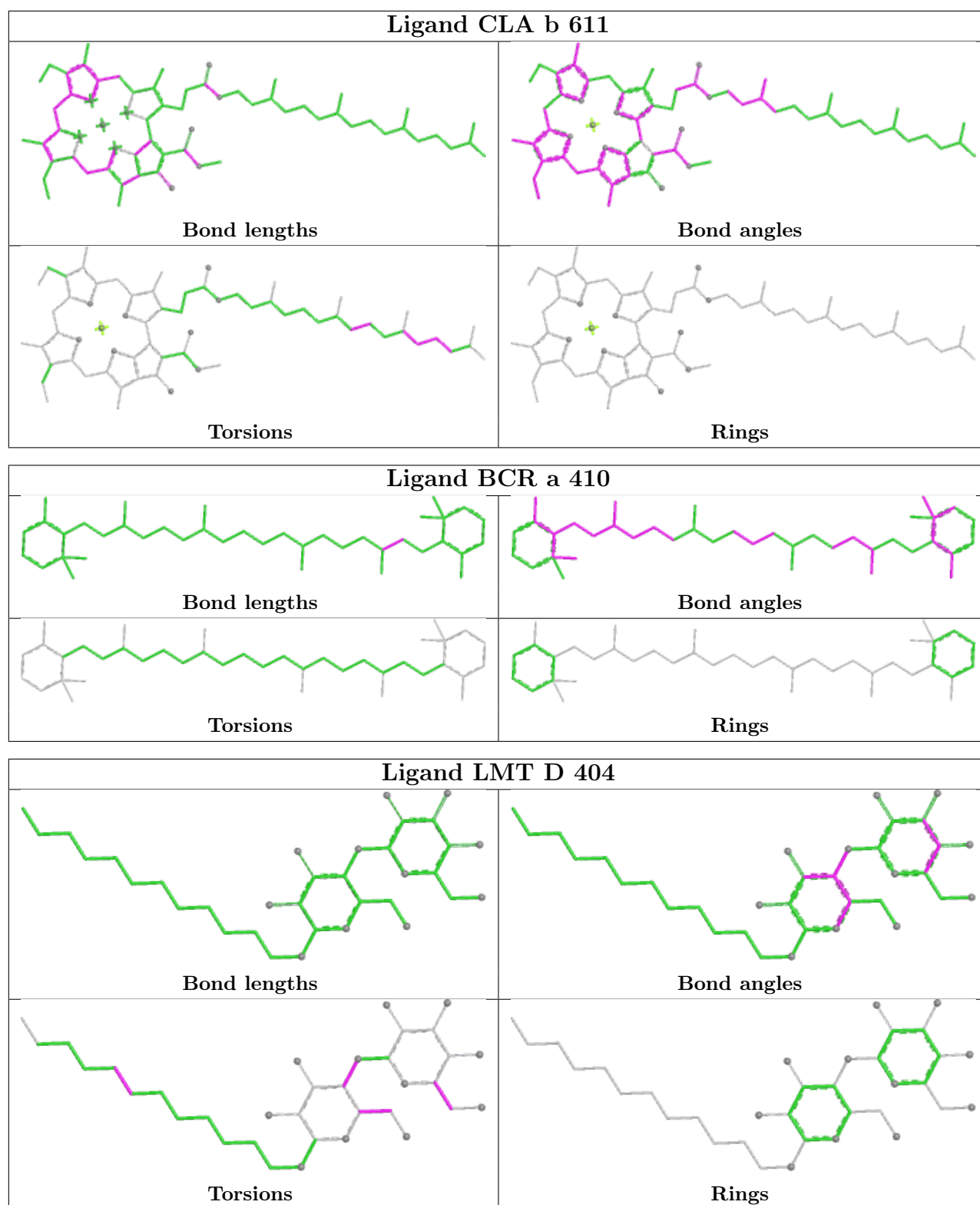
Ligand CLA c 503

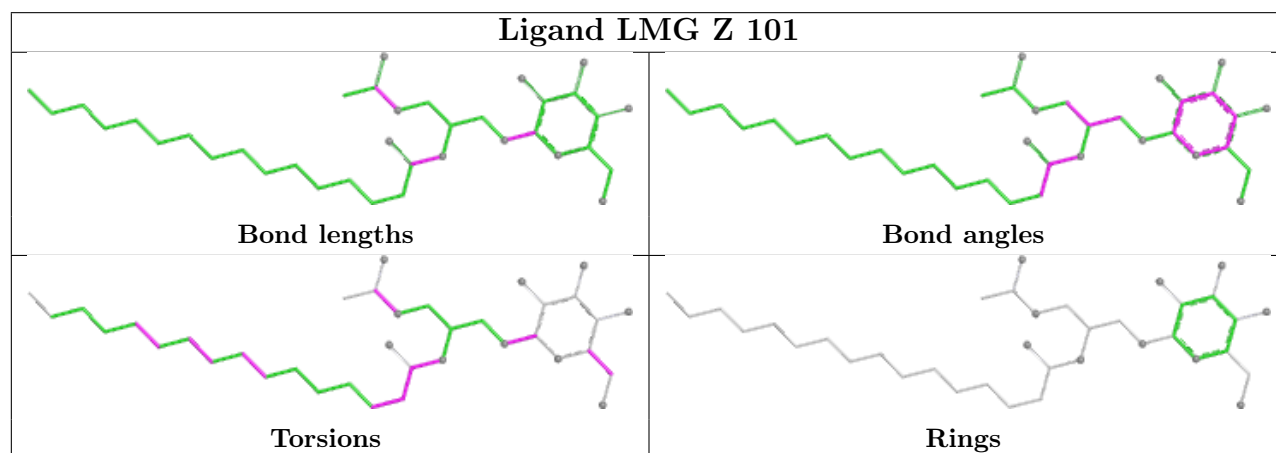
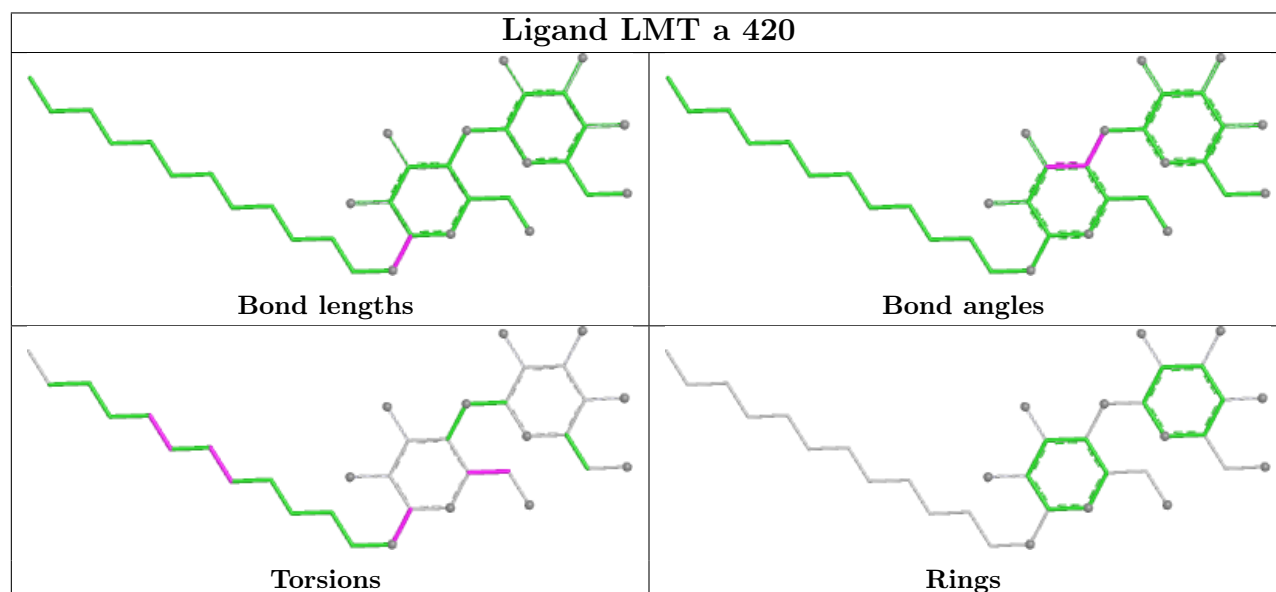
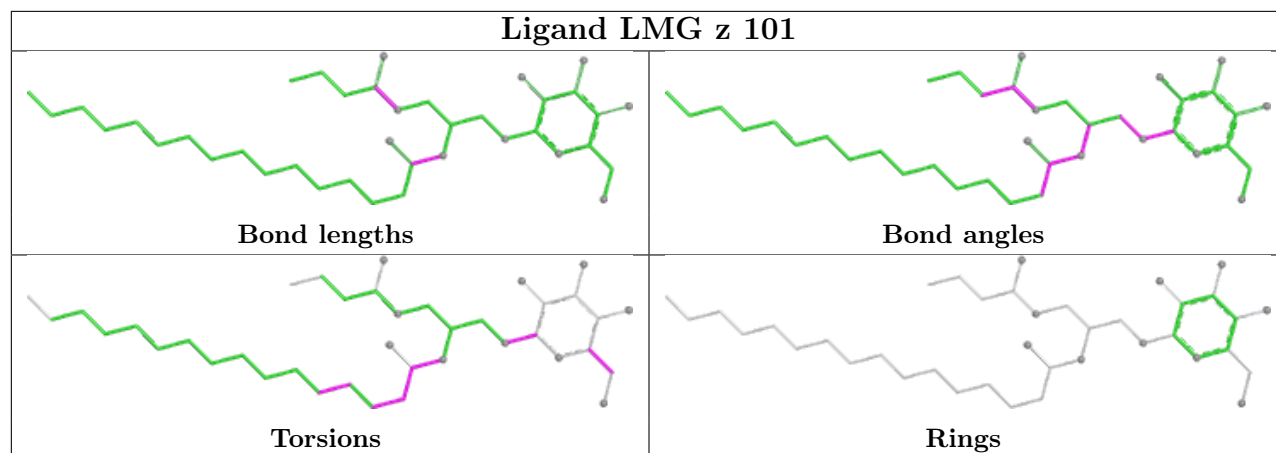


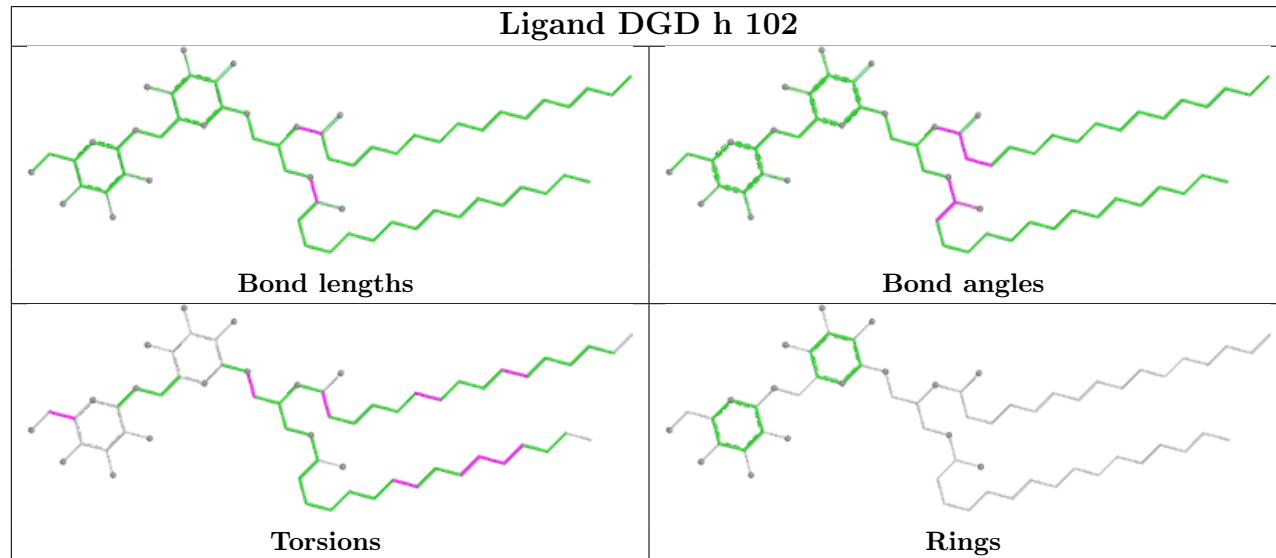
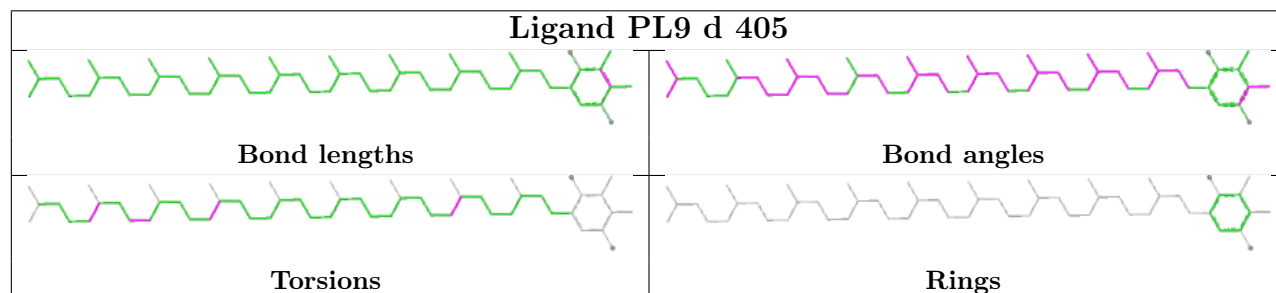
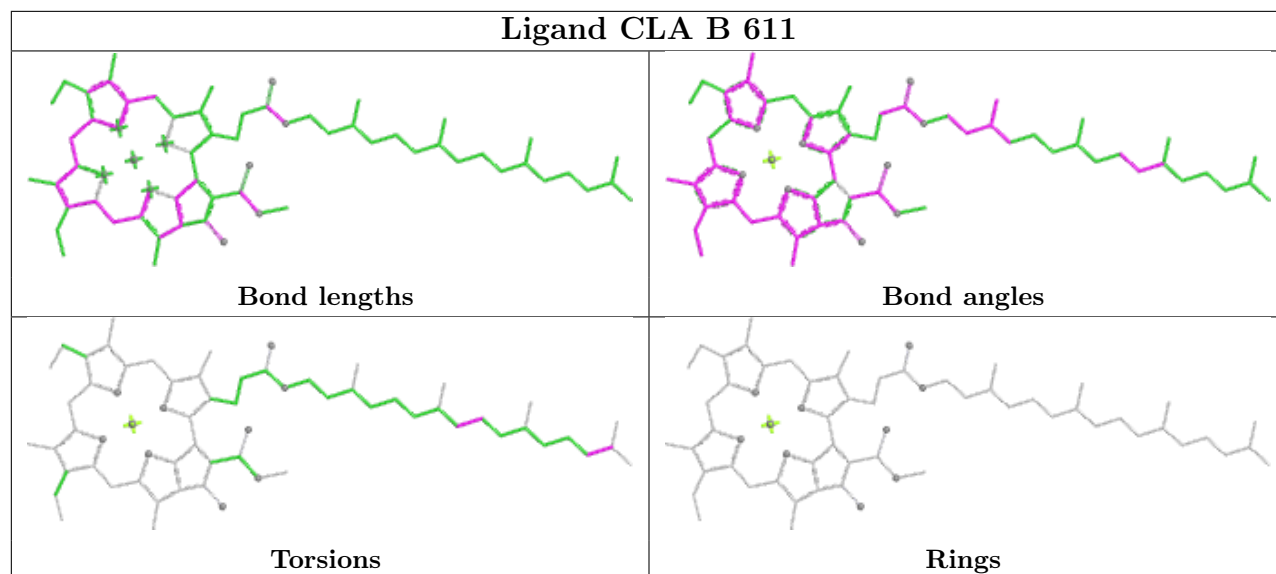


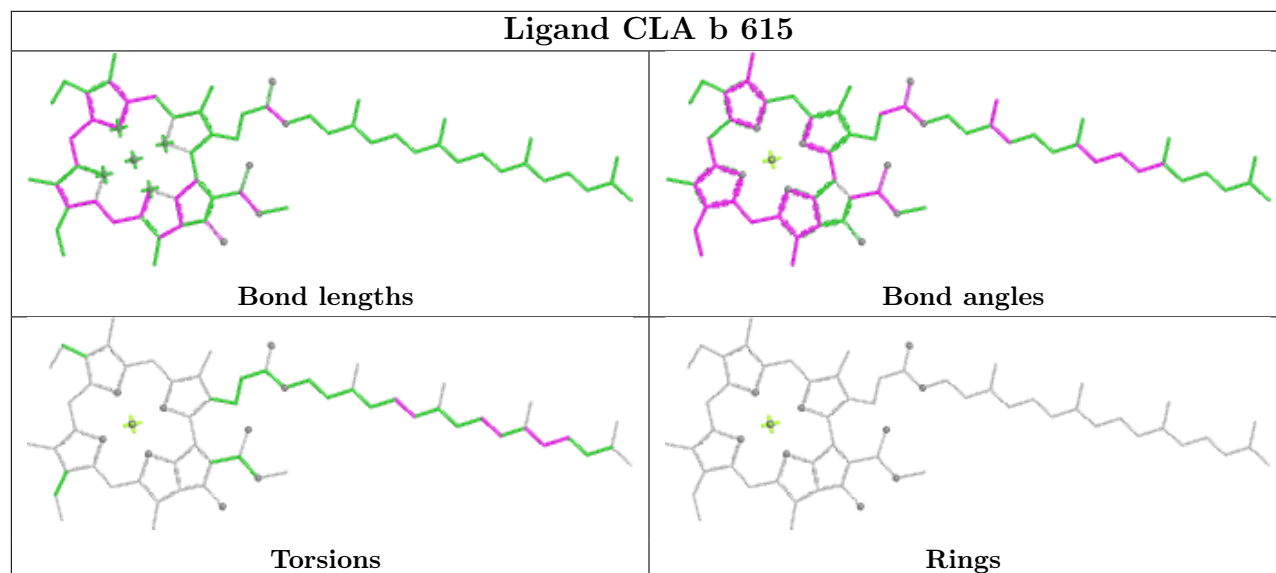
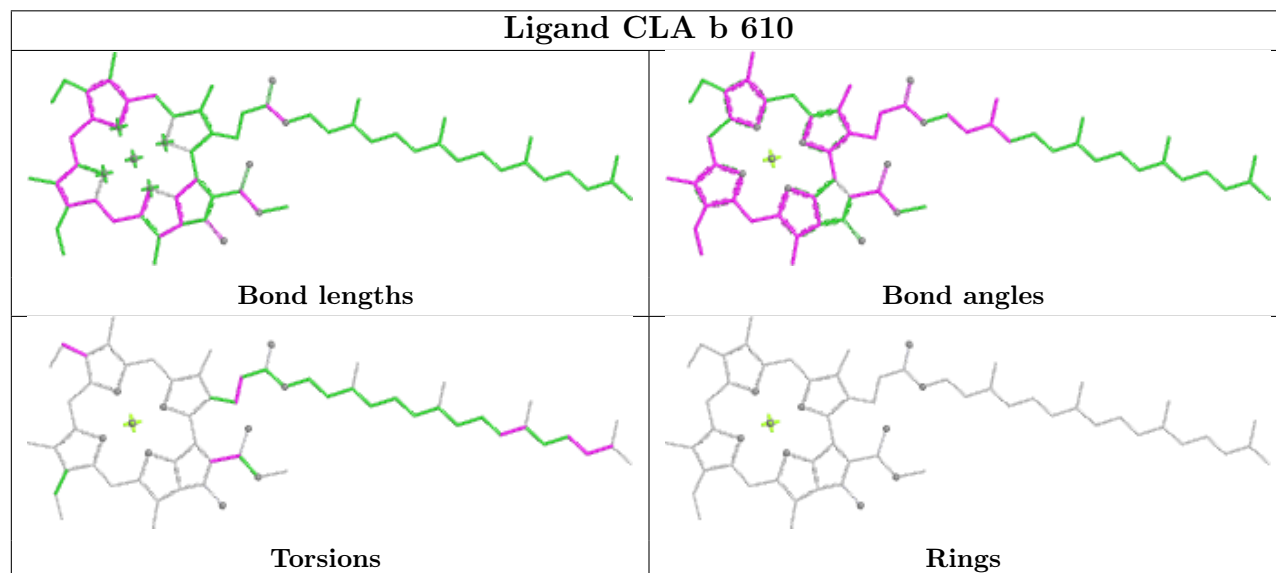
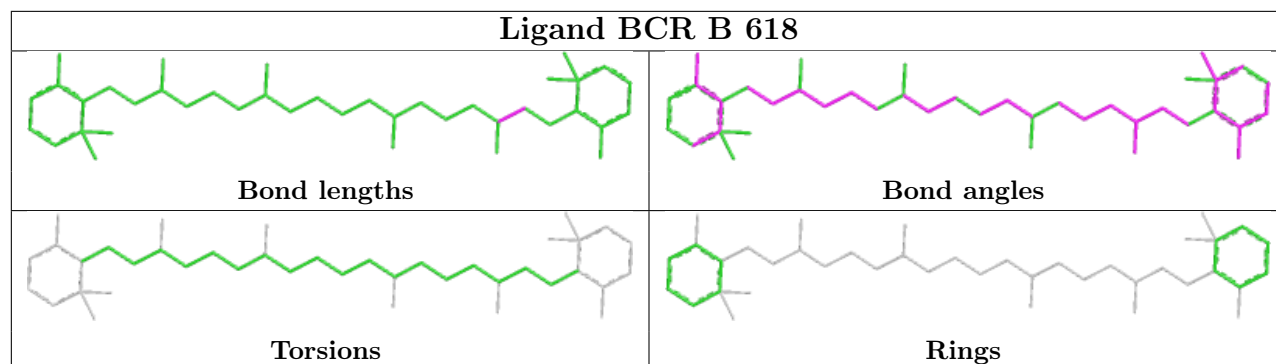


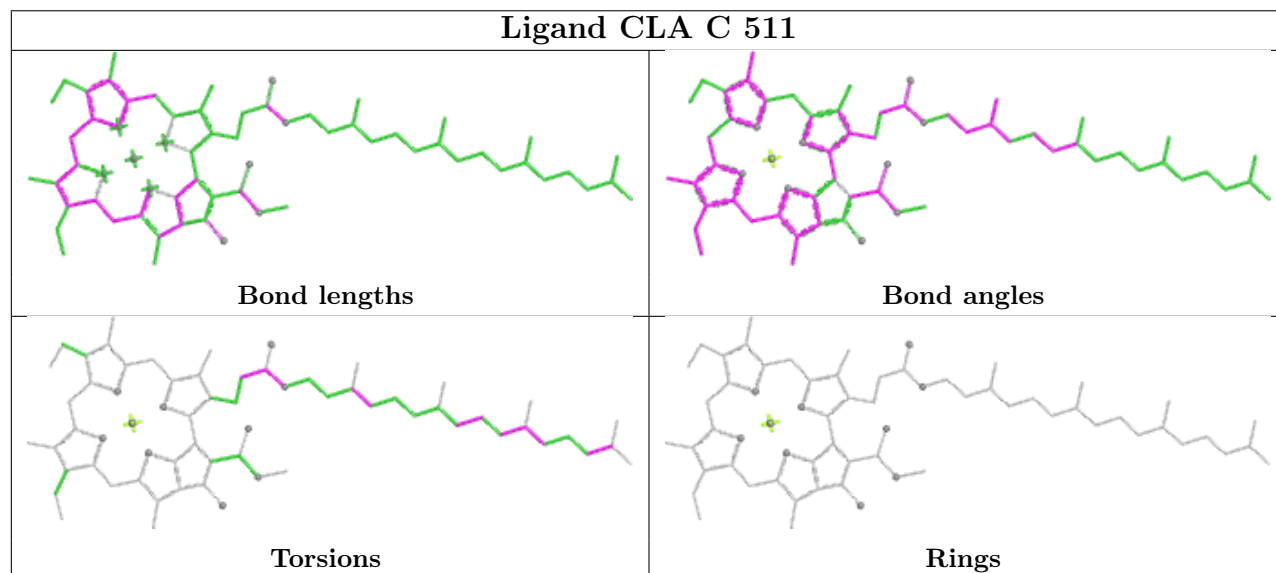
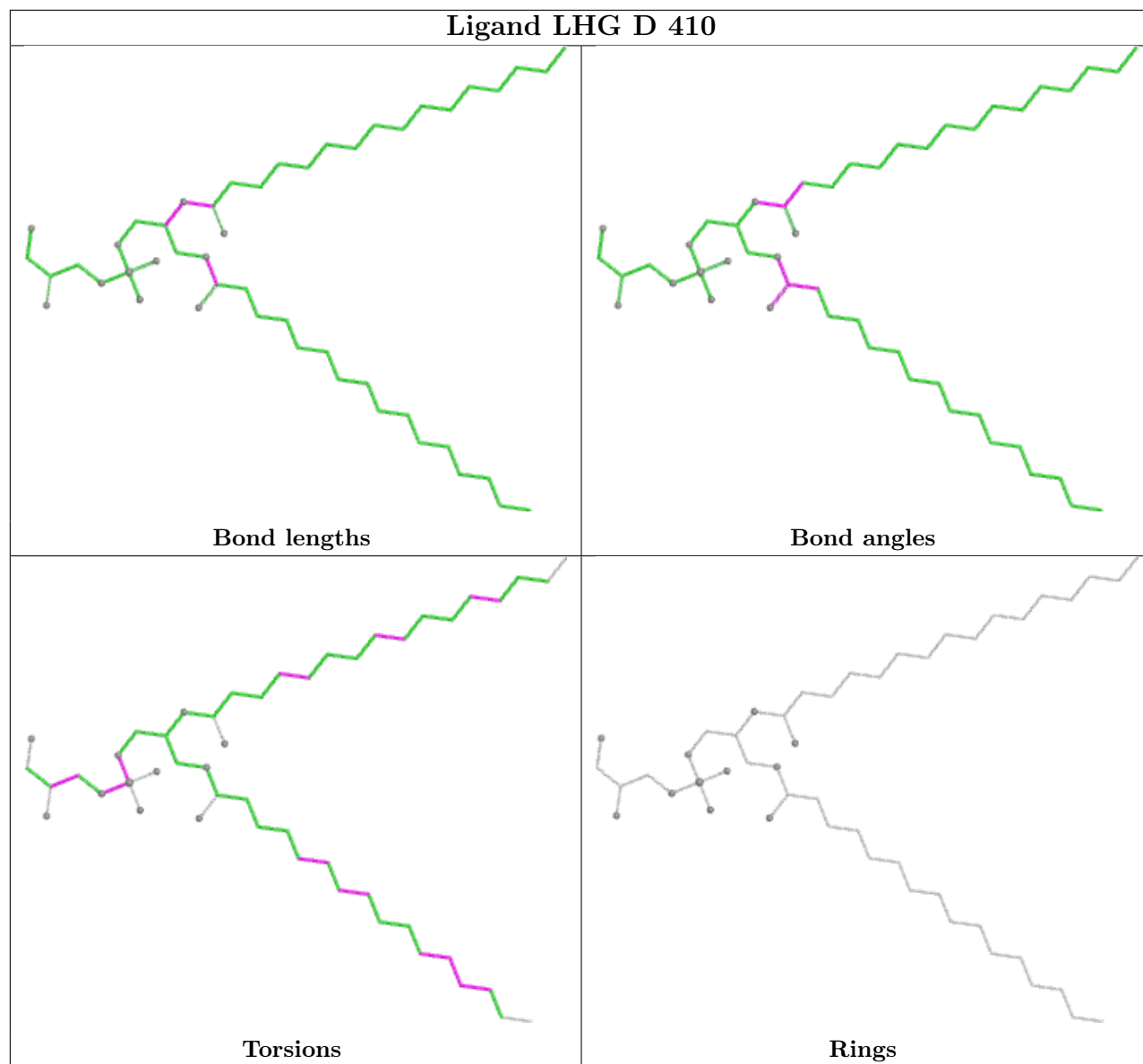


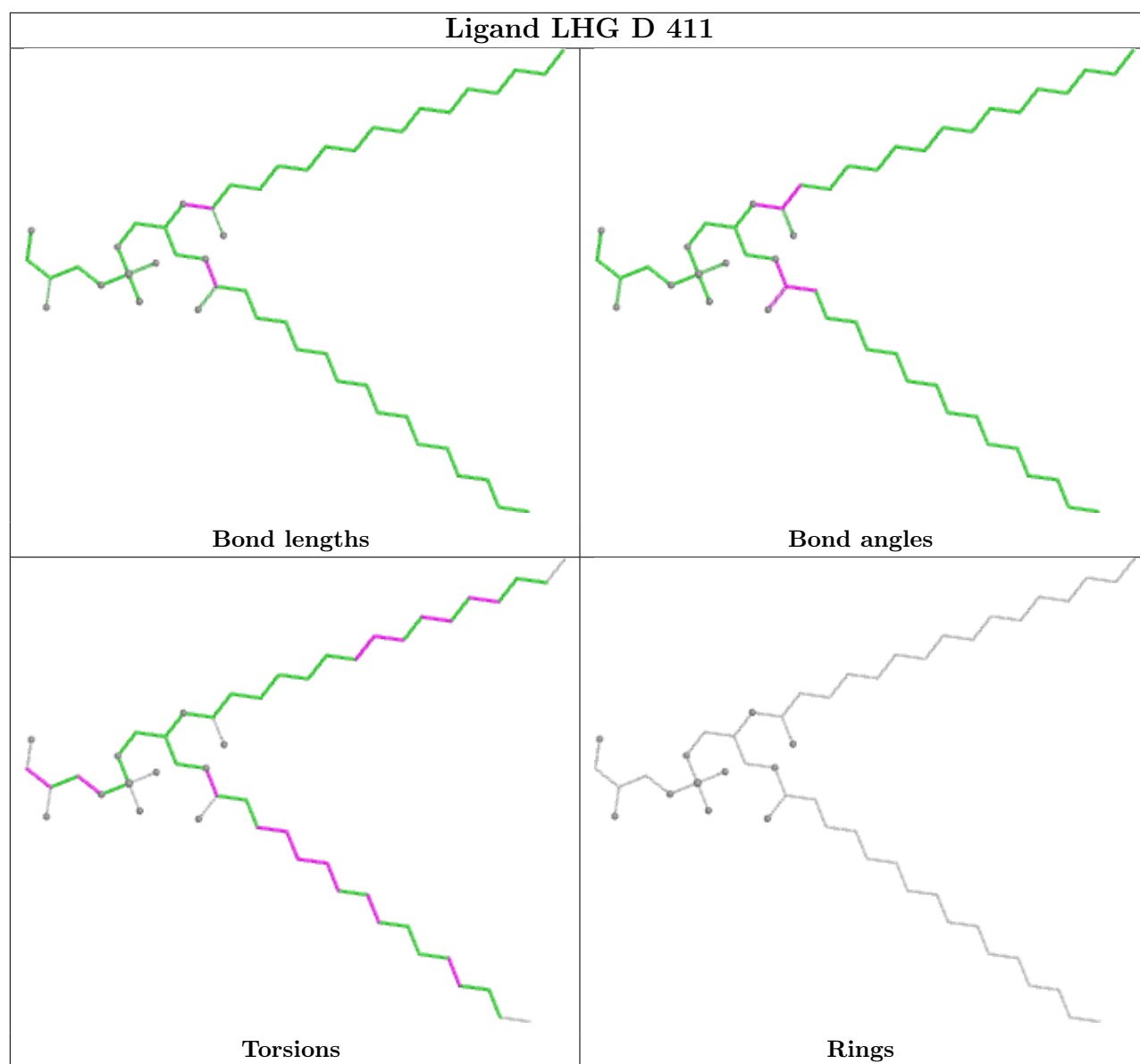


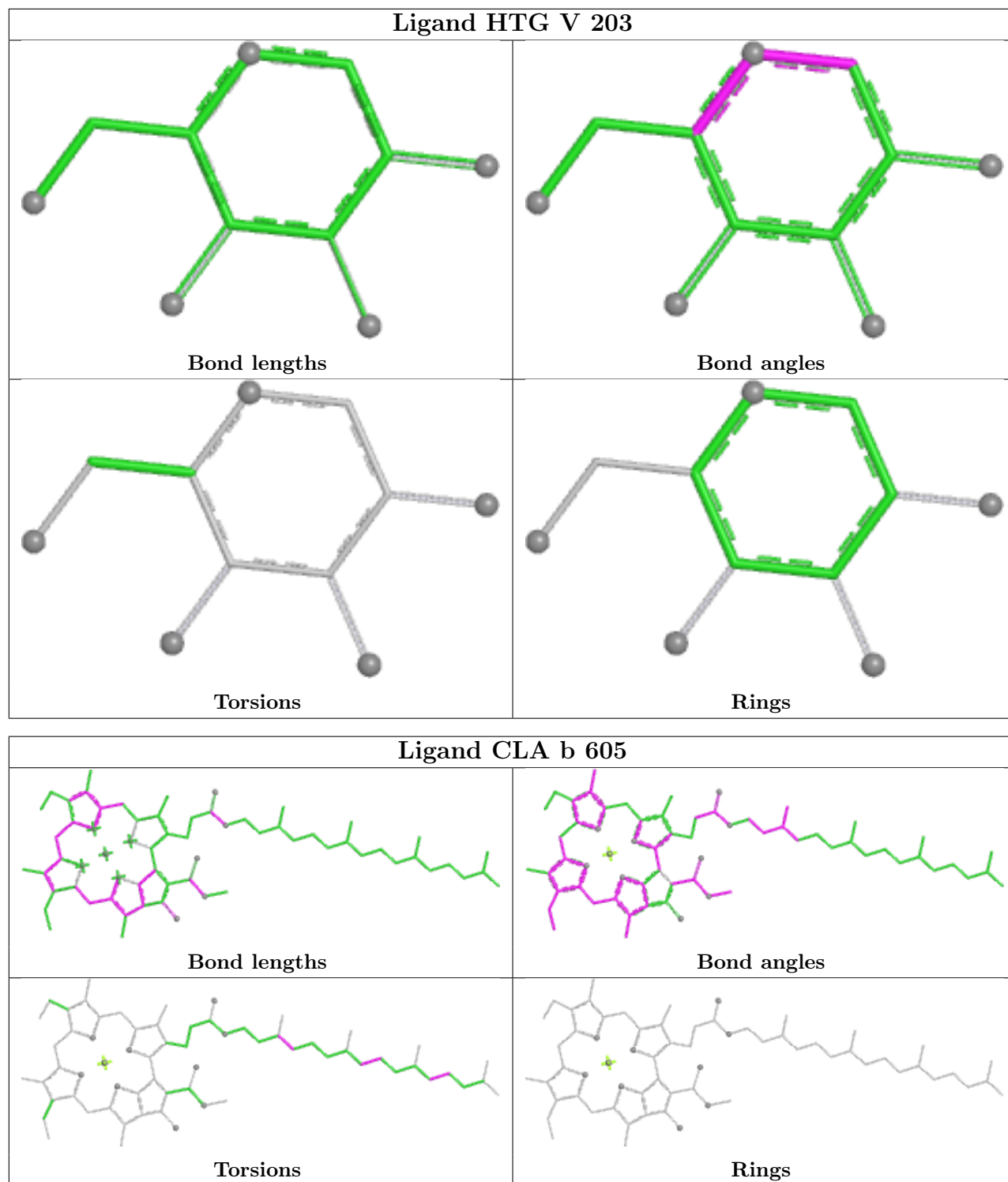


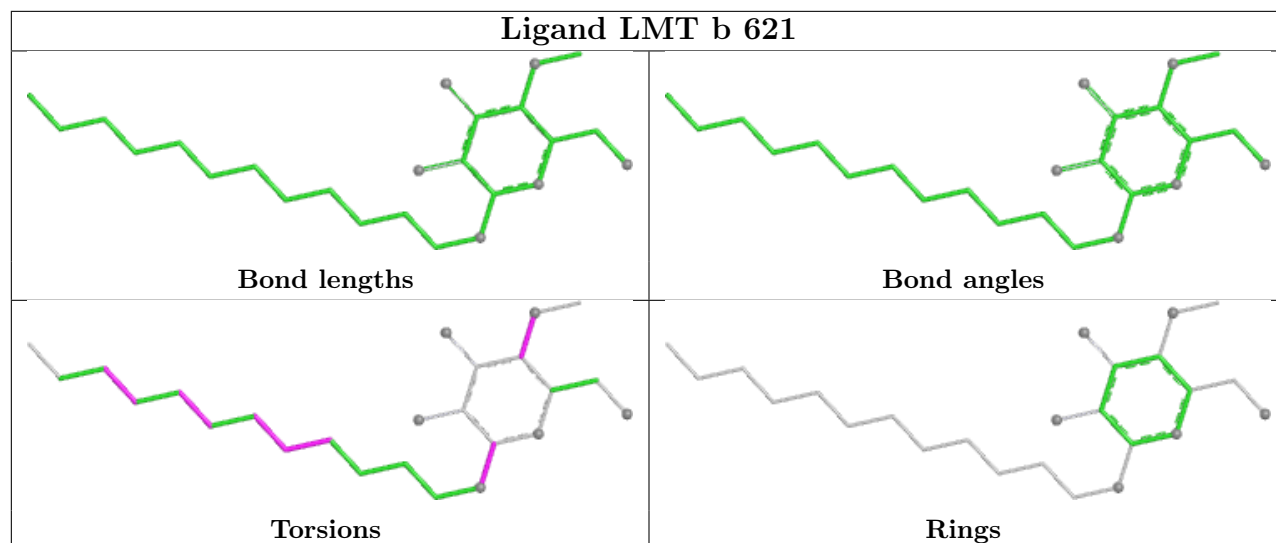
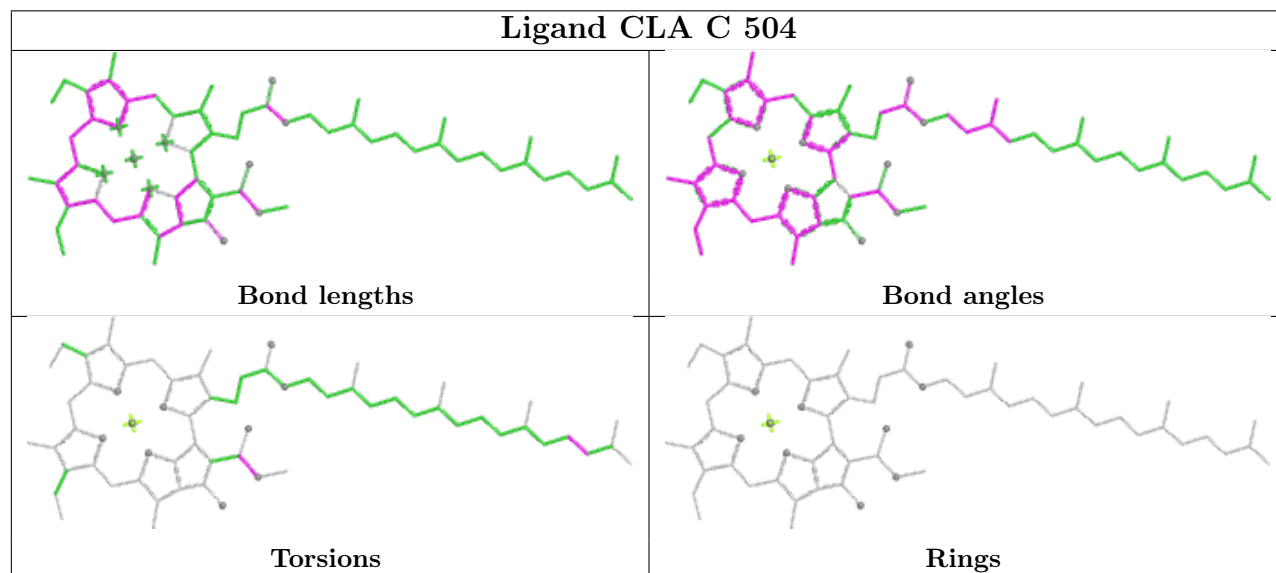
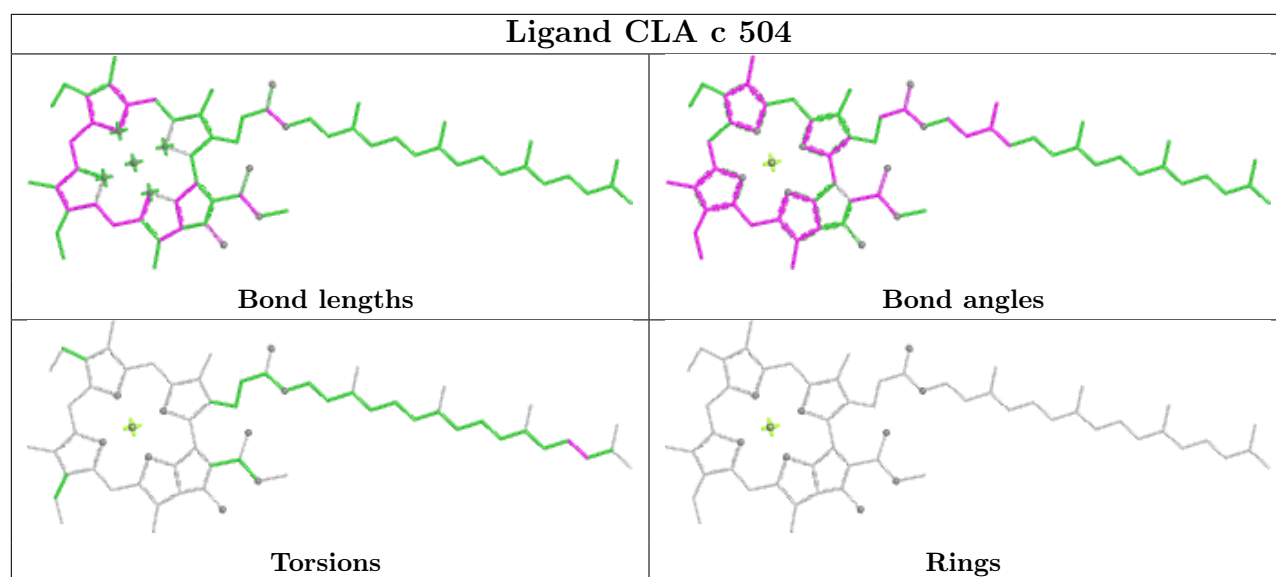


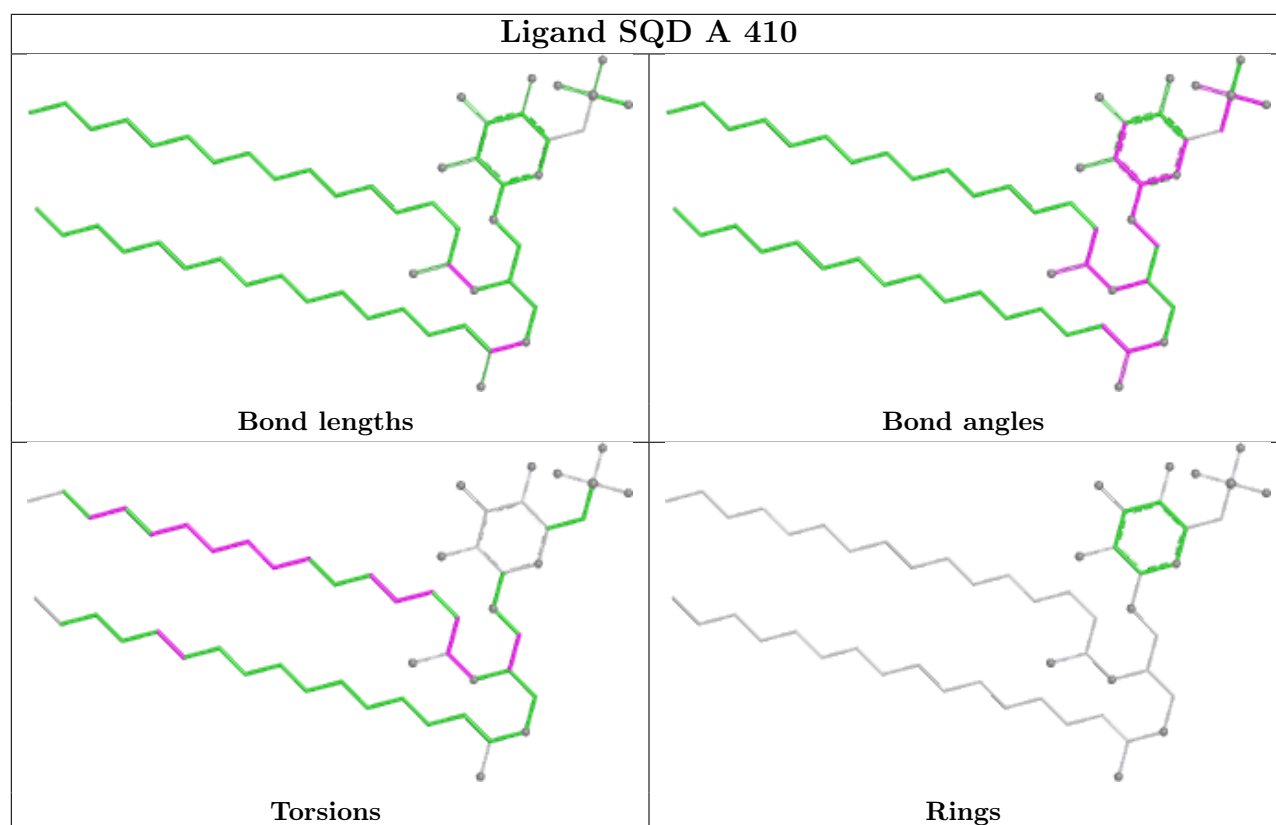


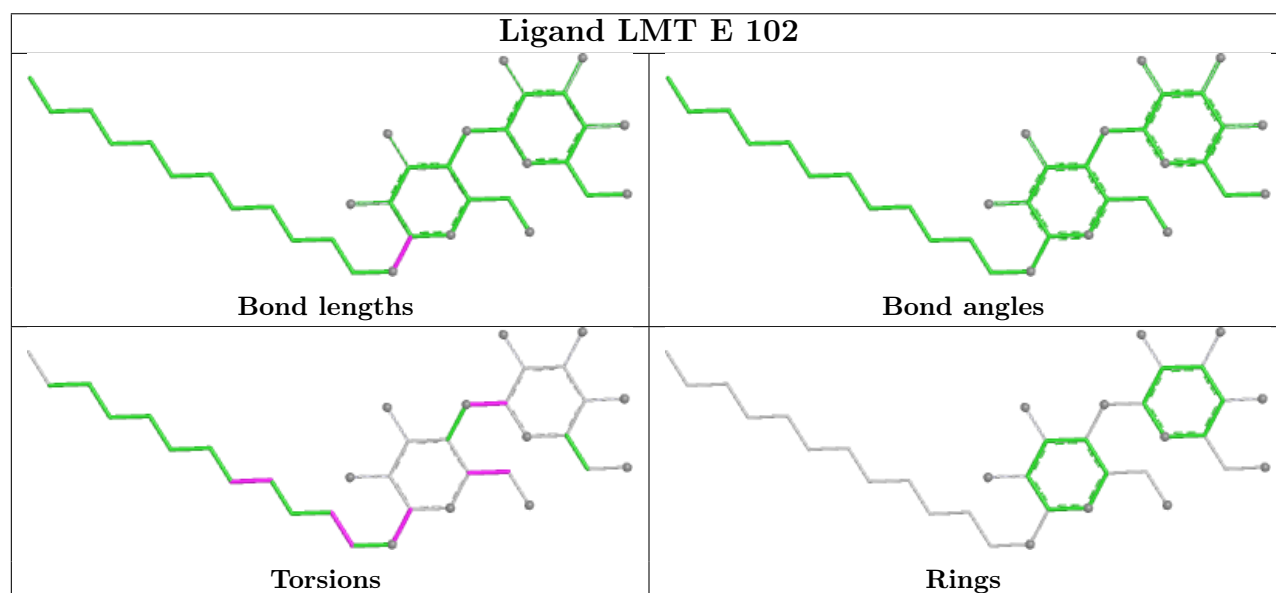
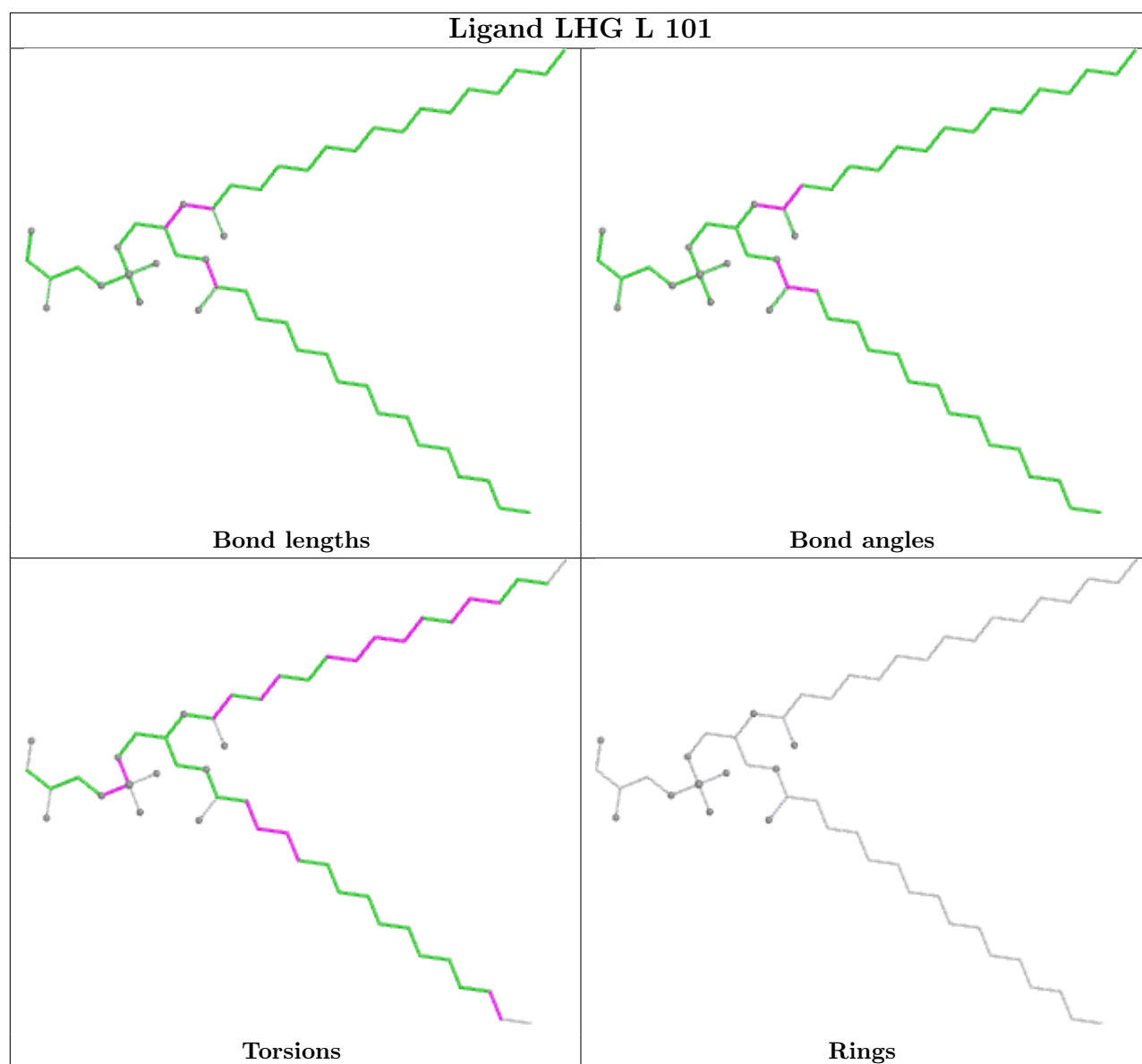


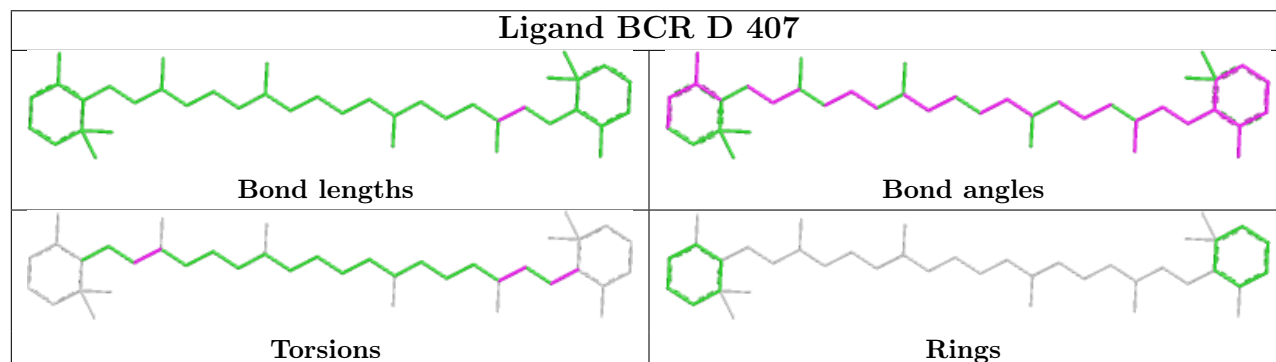
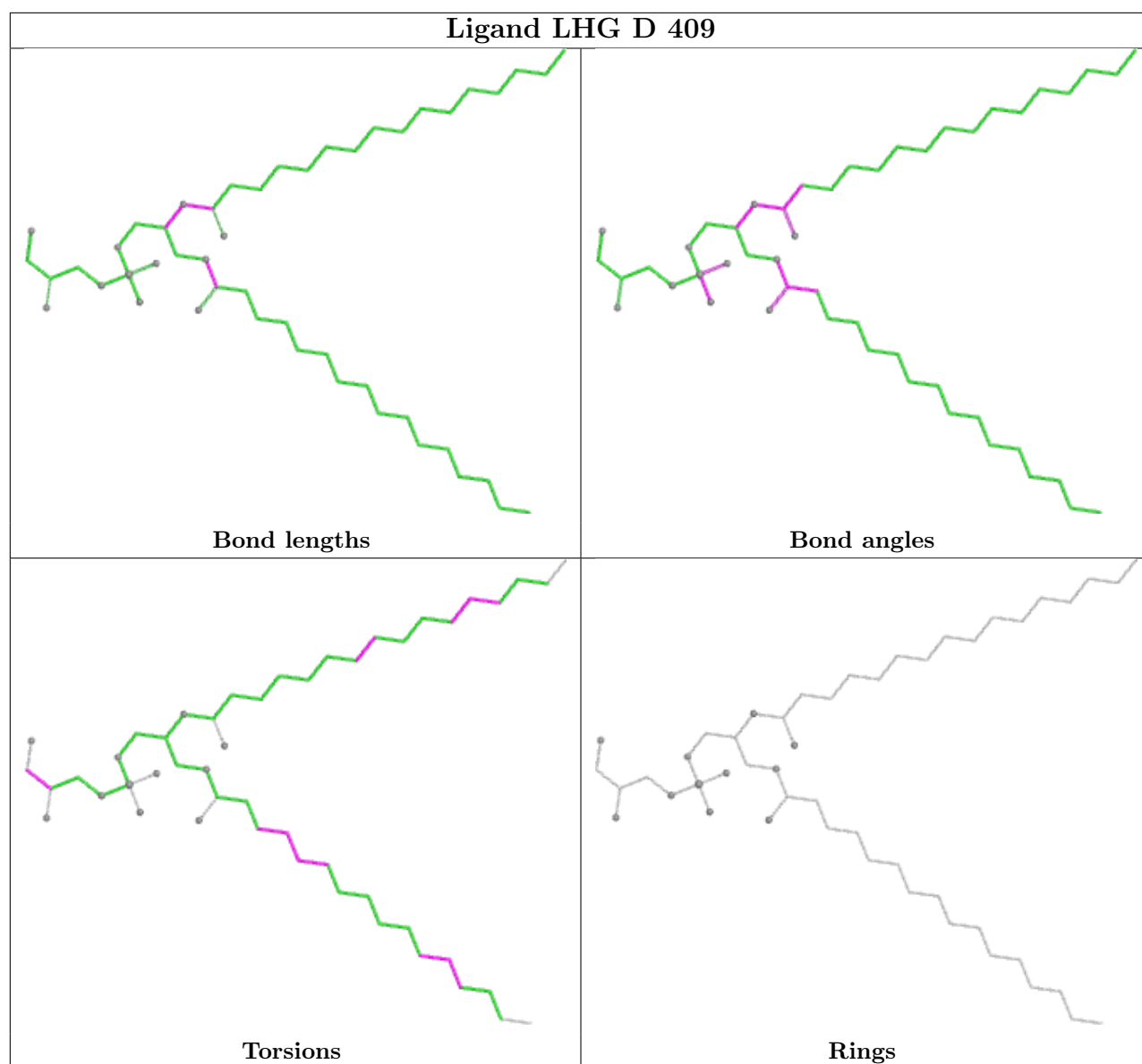


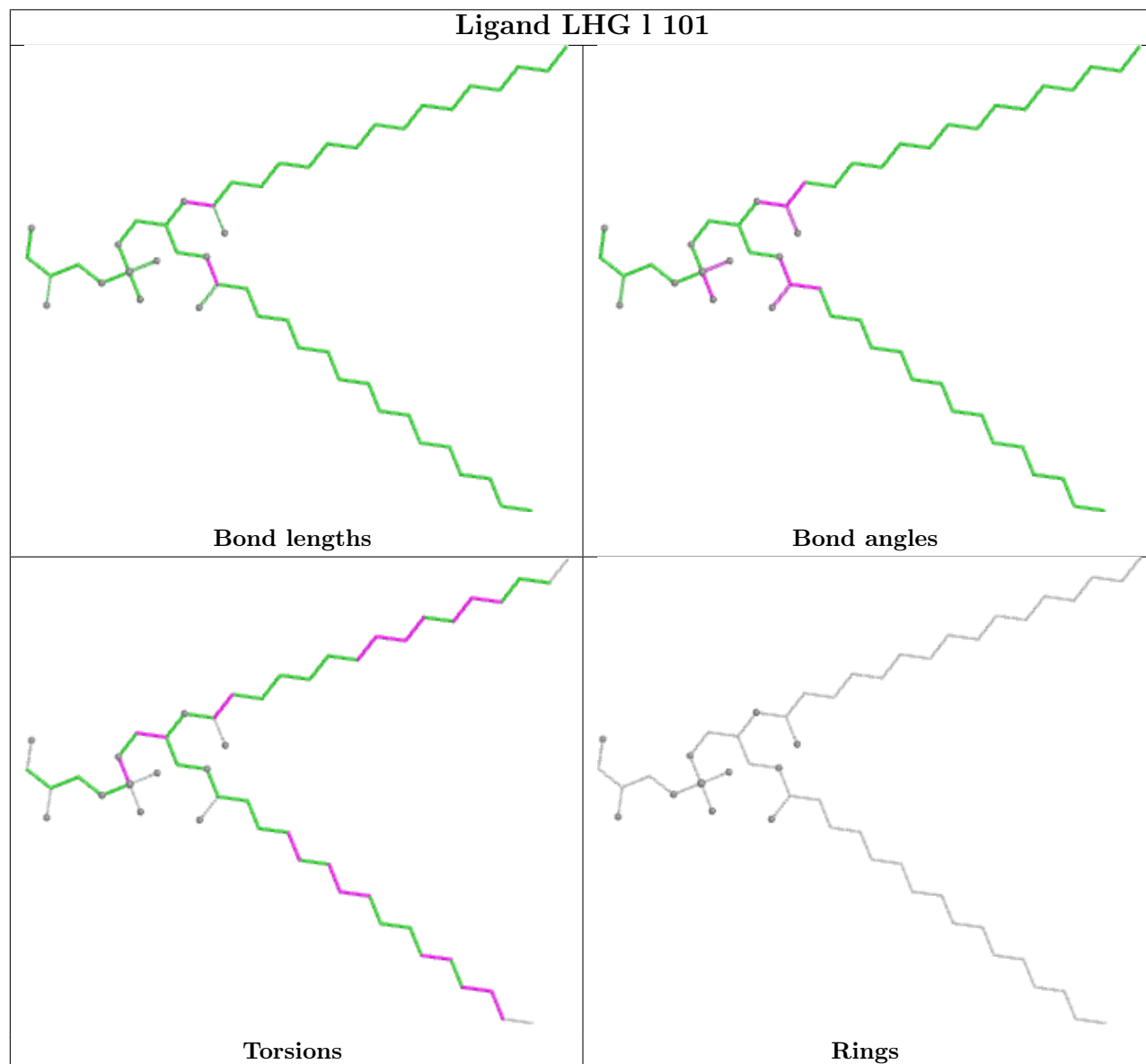
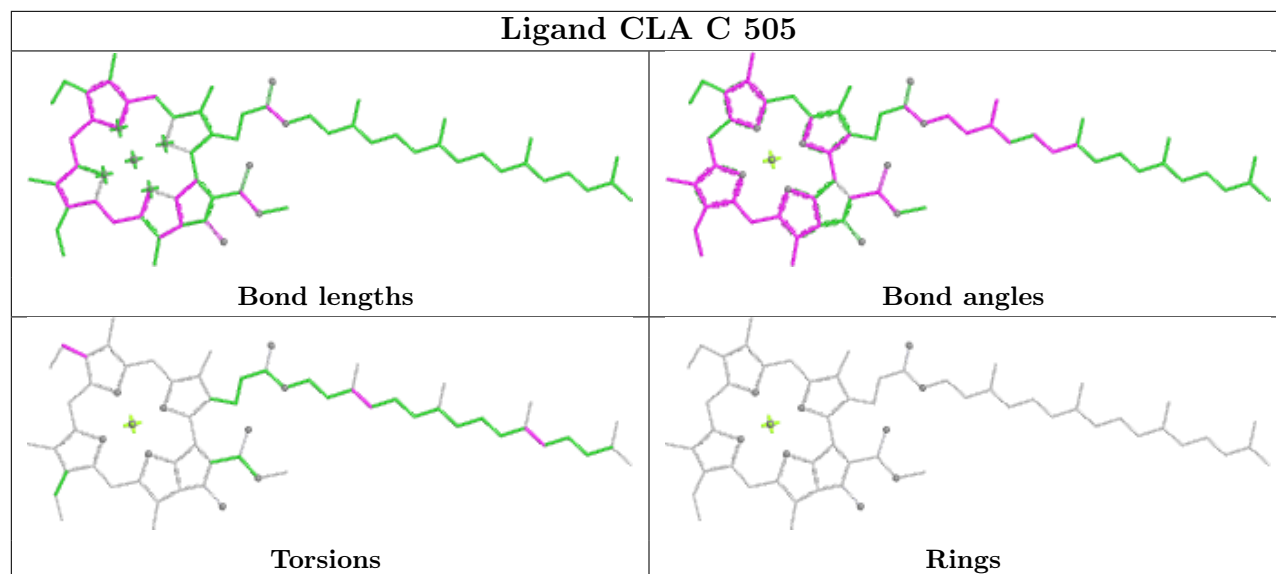


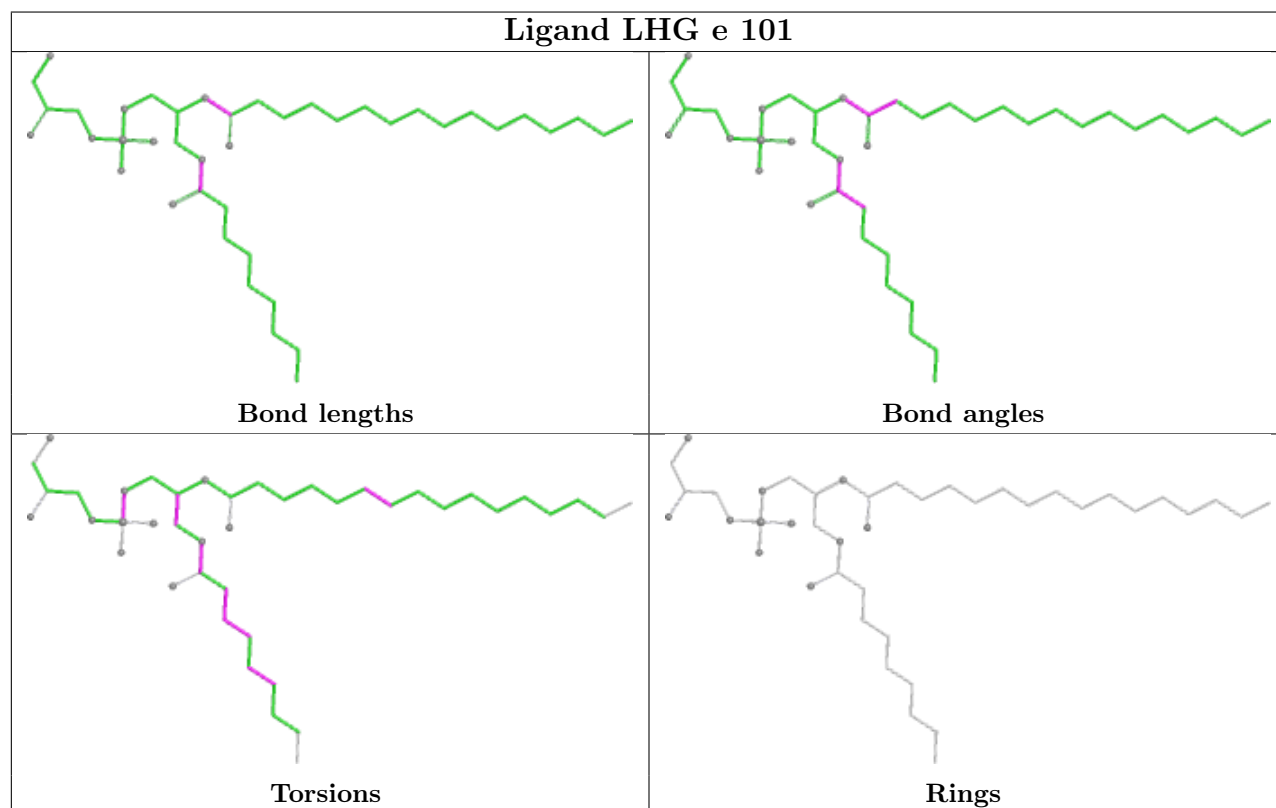
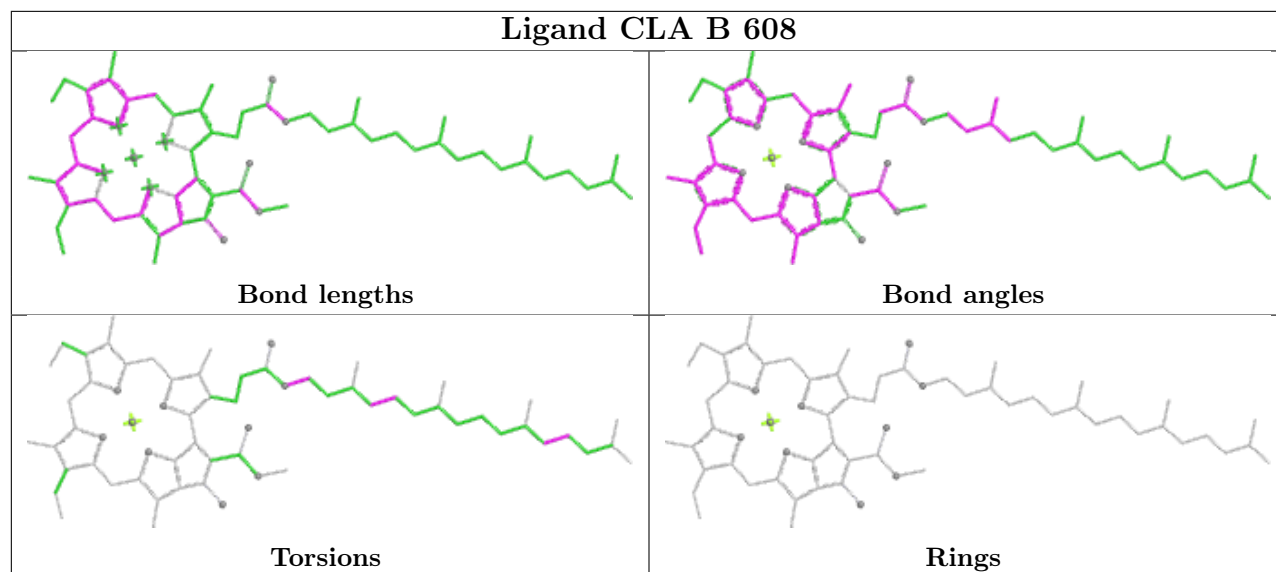


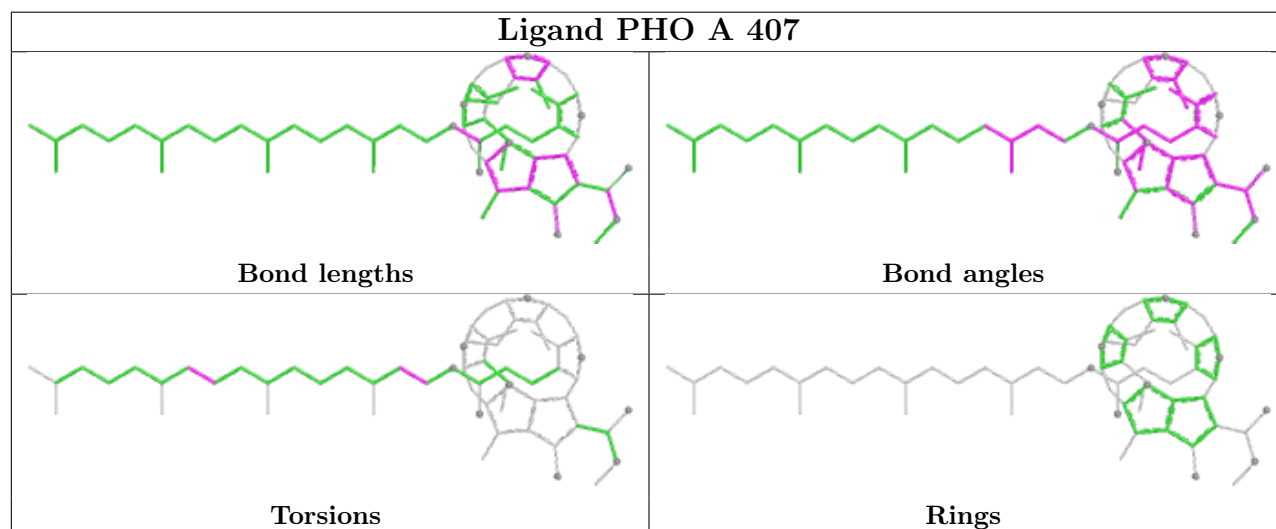
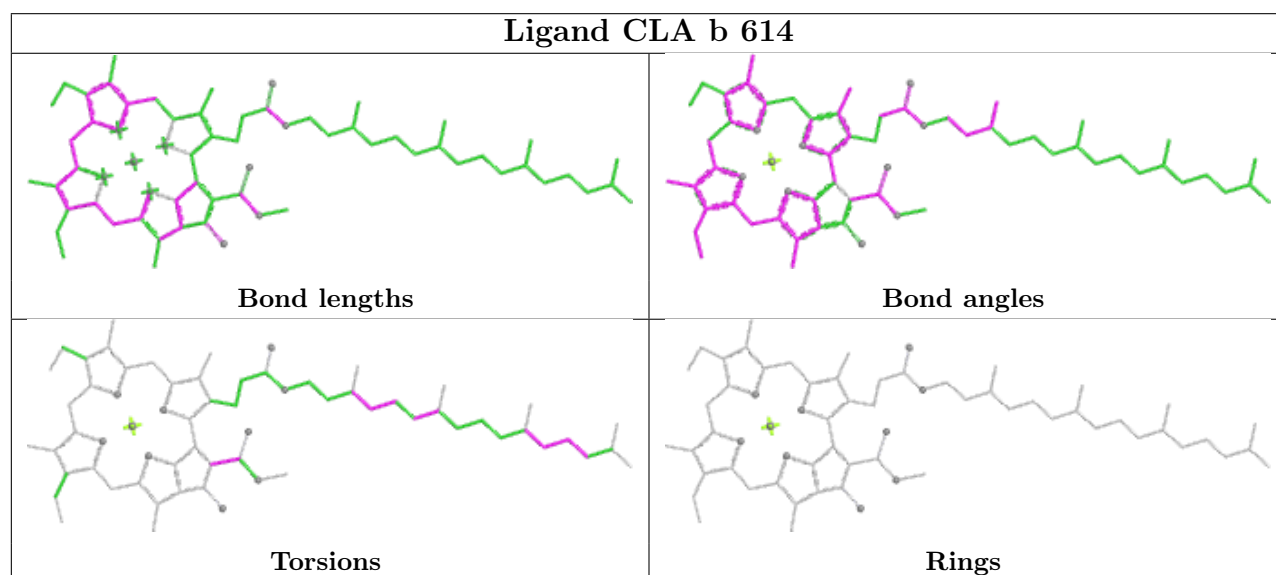
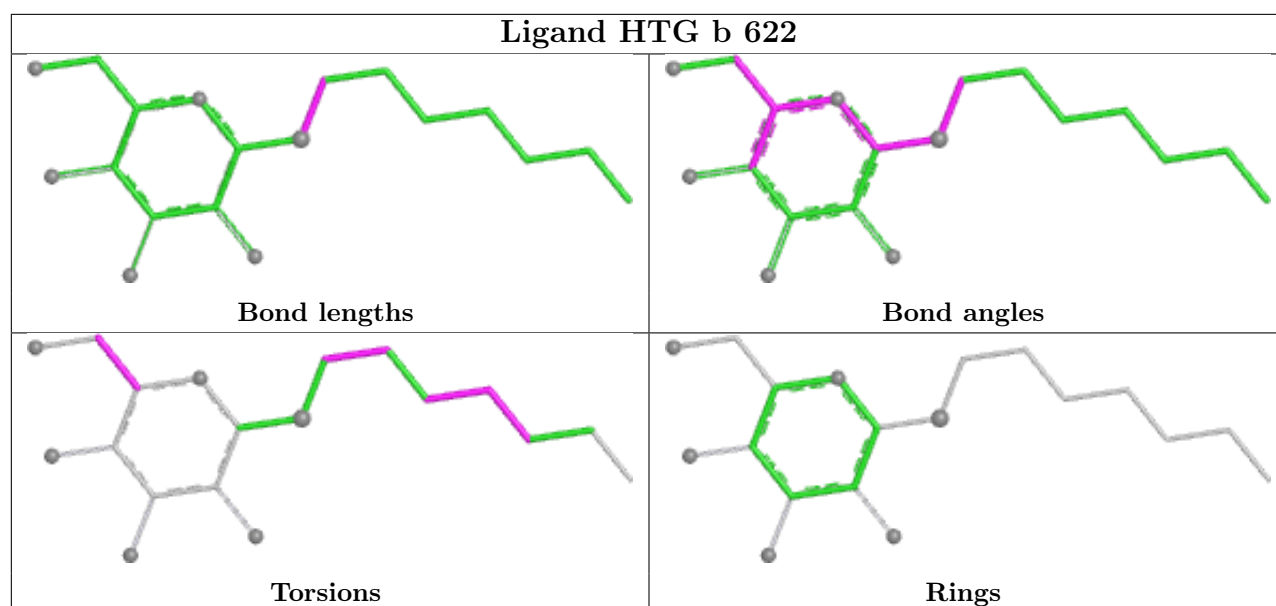




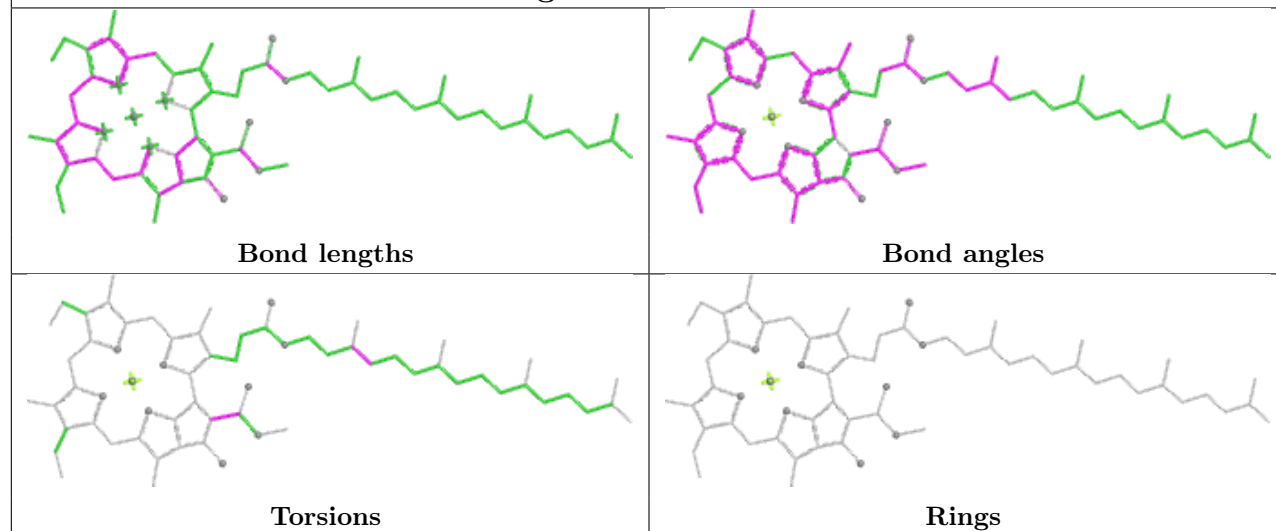




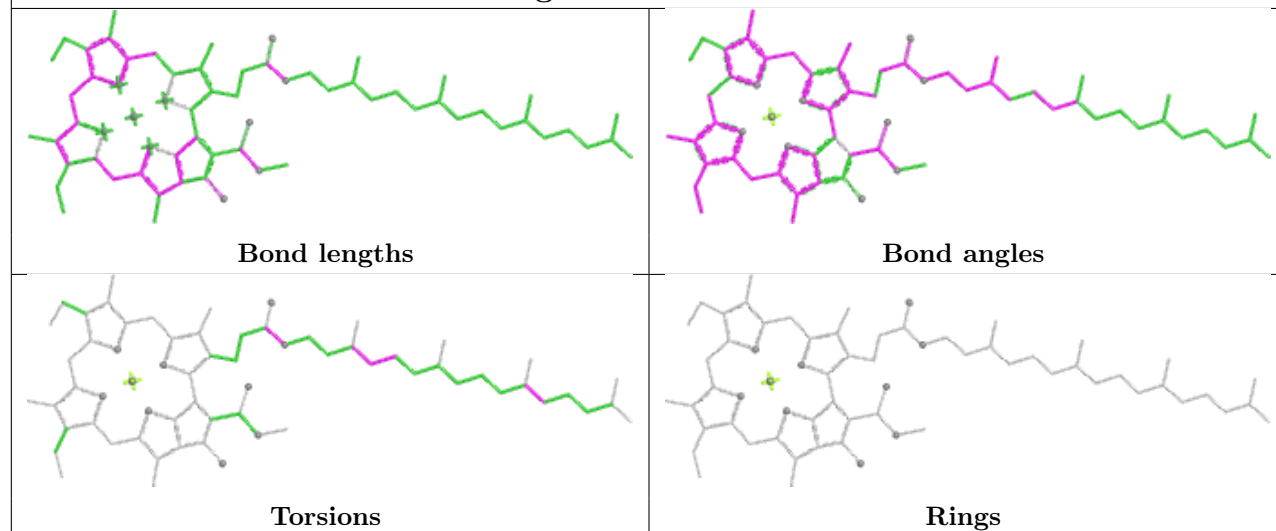




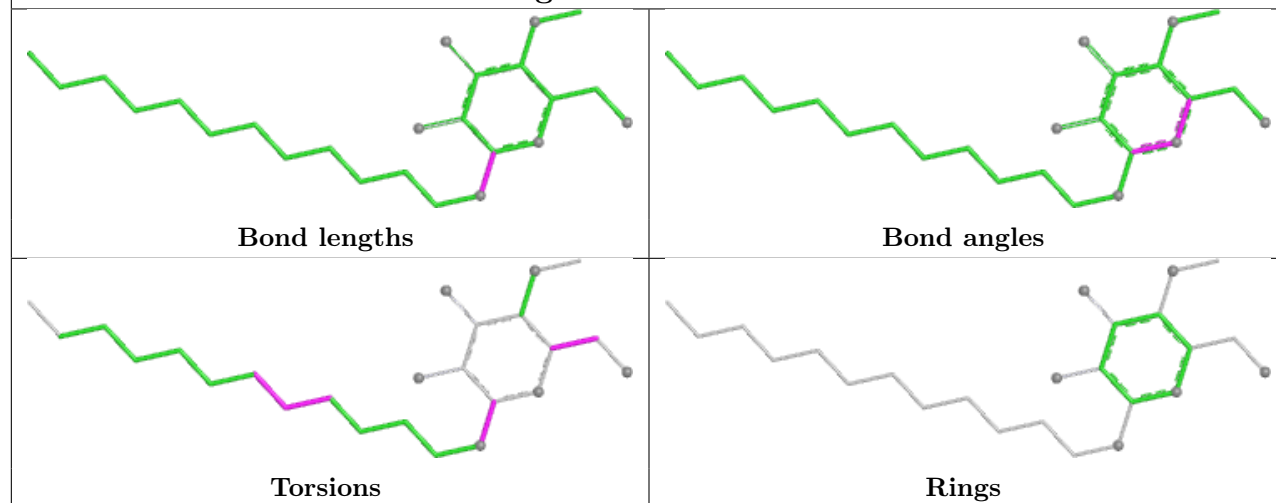
Ligand CLA c 505



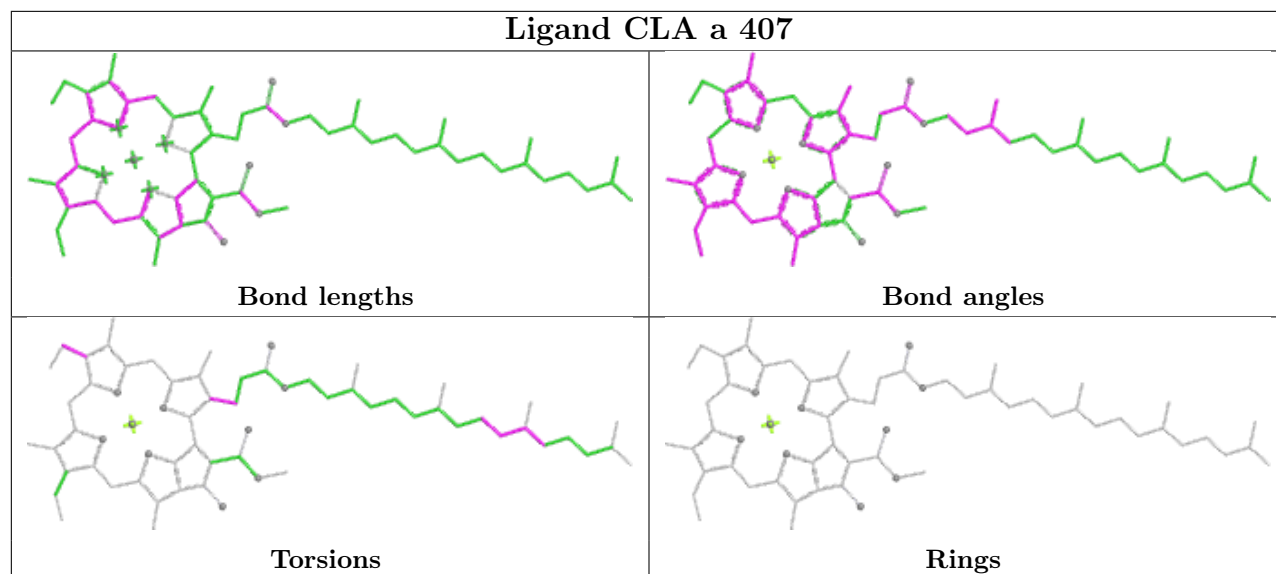
Ligand CLA d 403



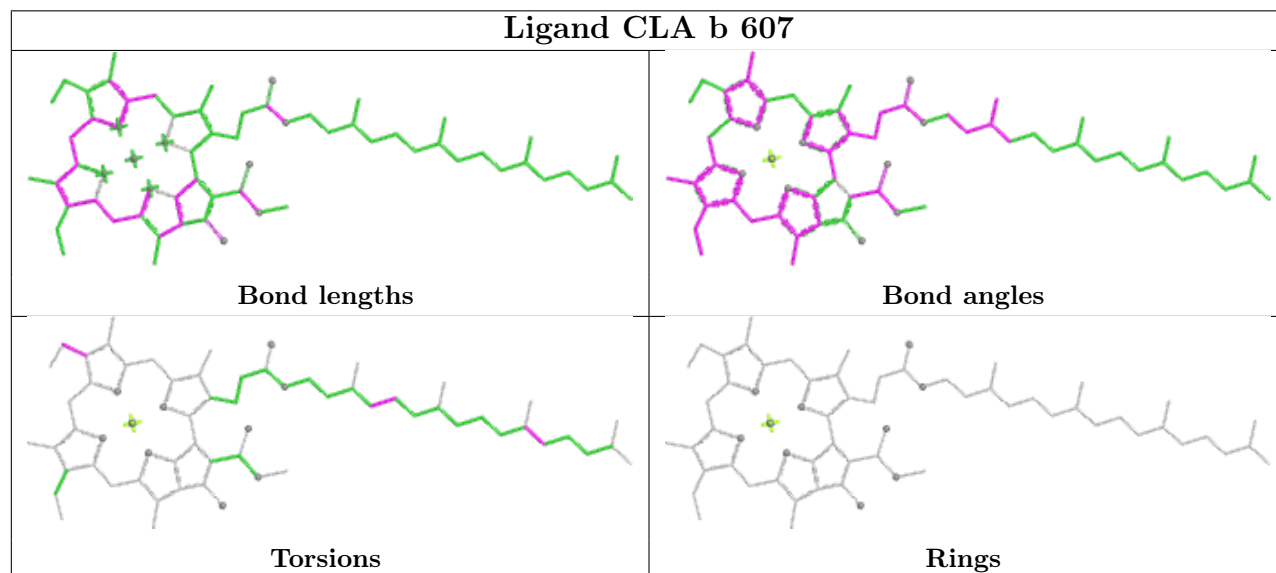
Ligand LMT t 101

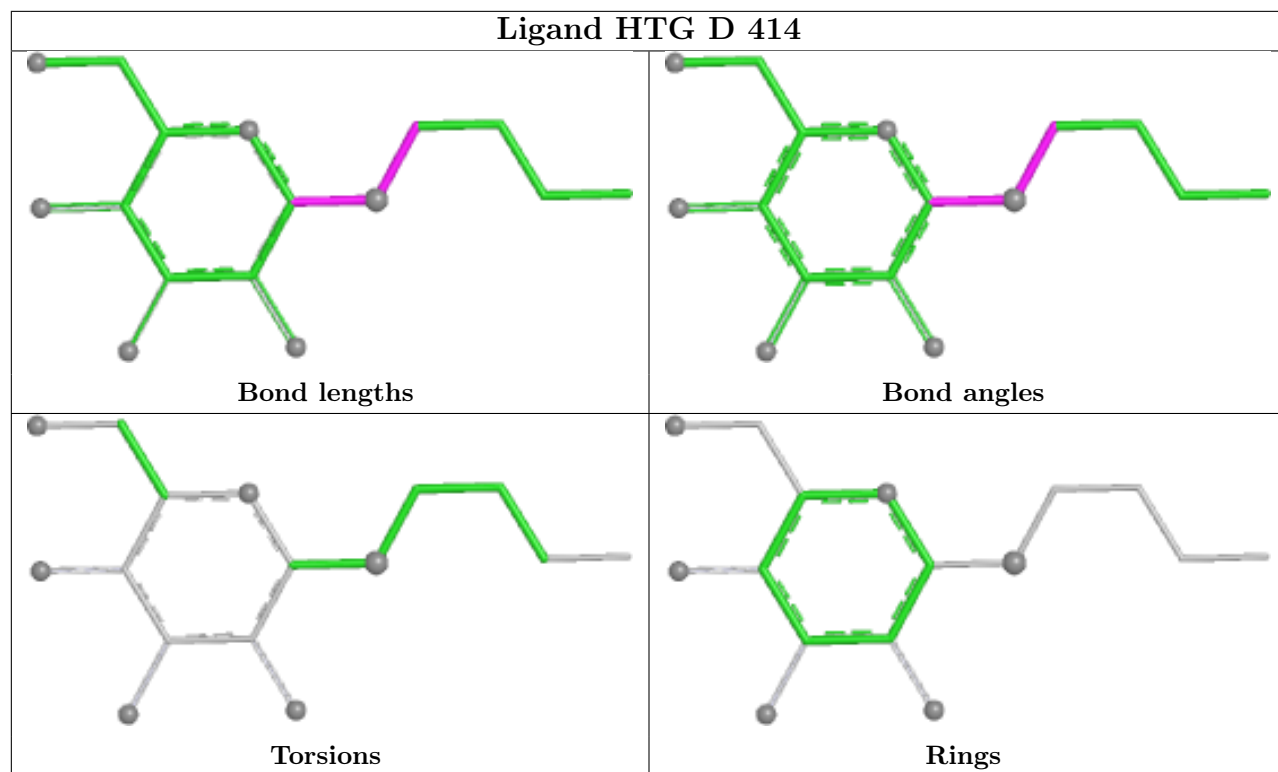


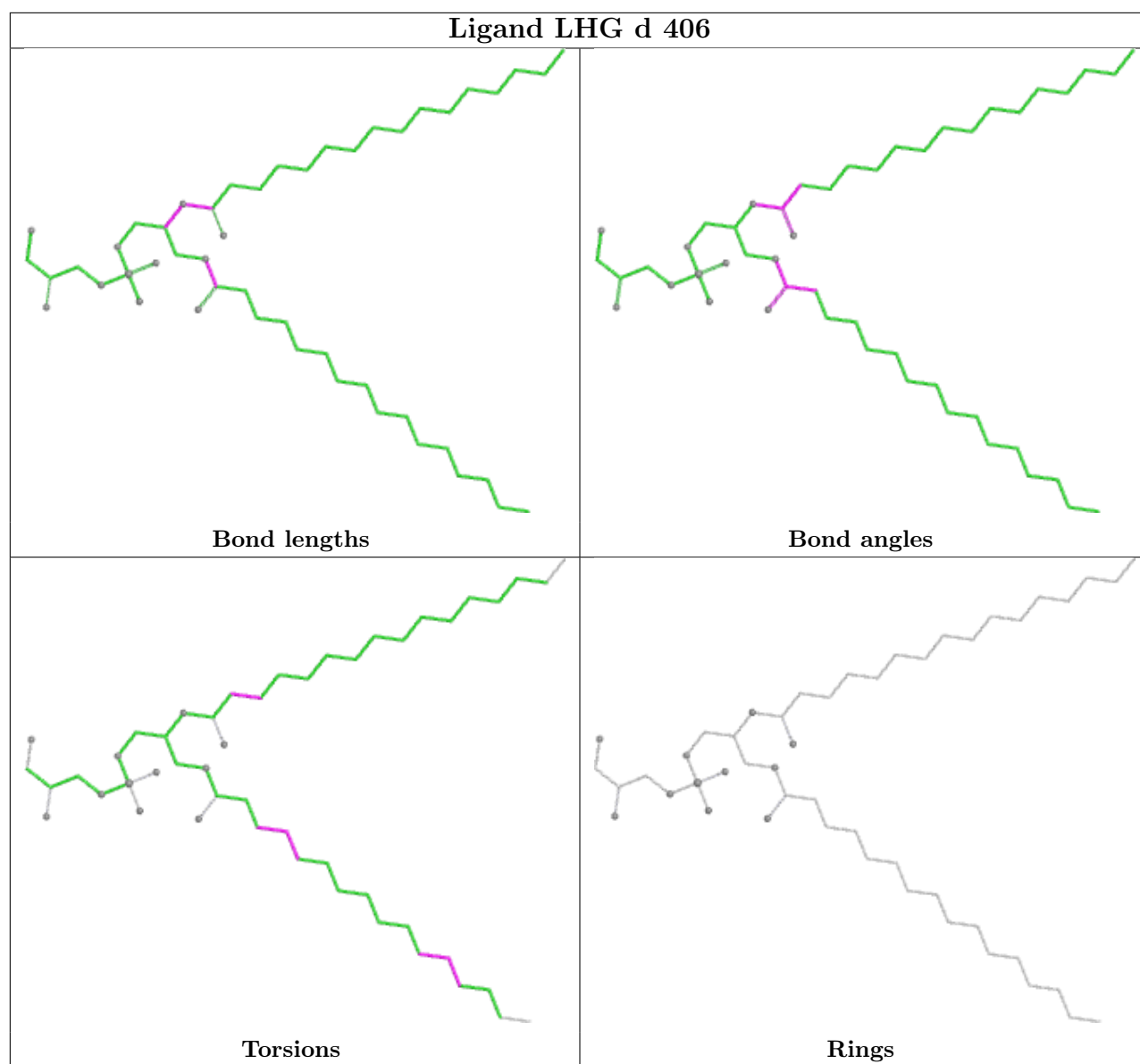
Ligand CLA a 407

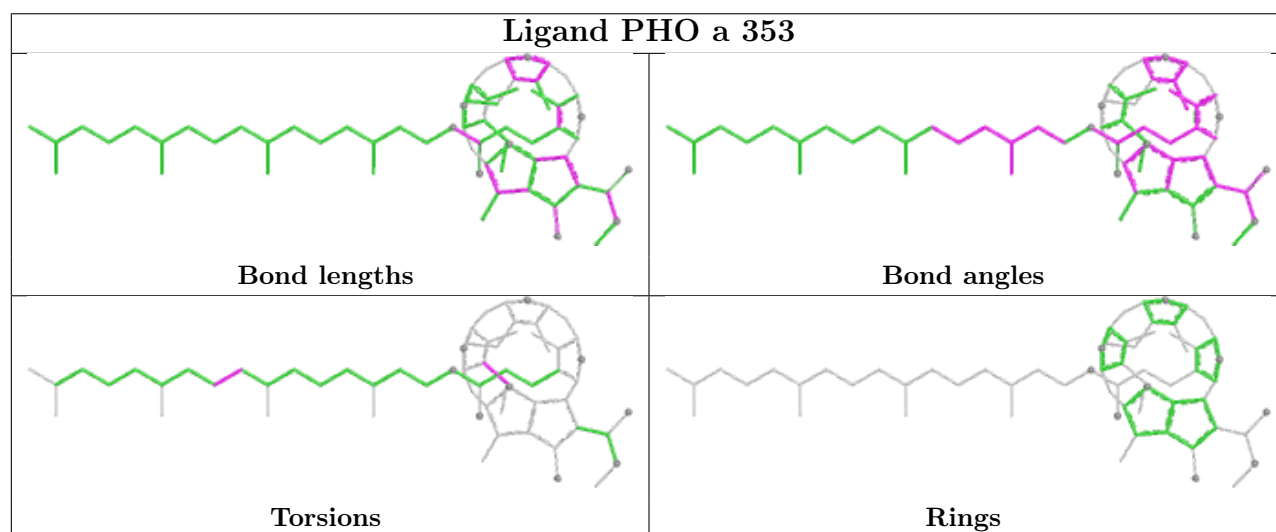
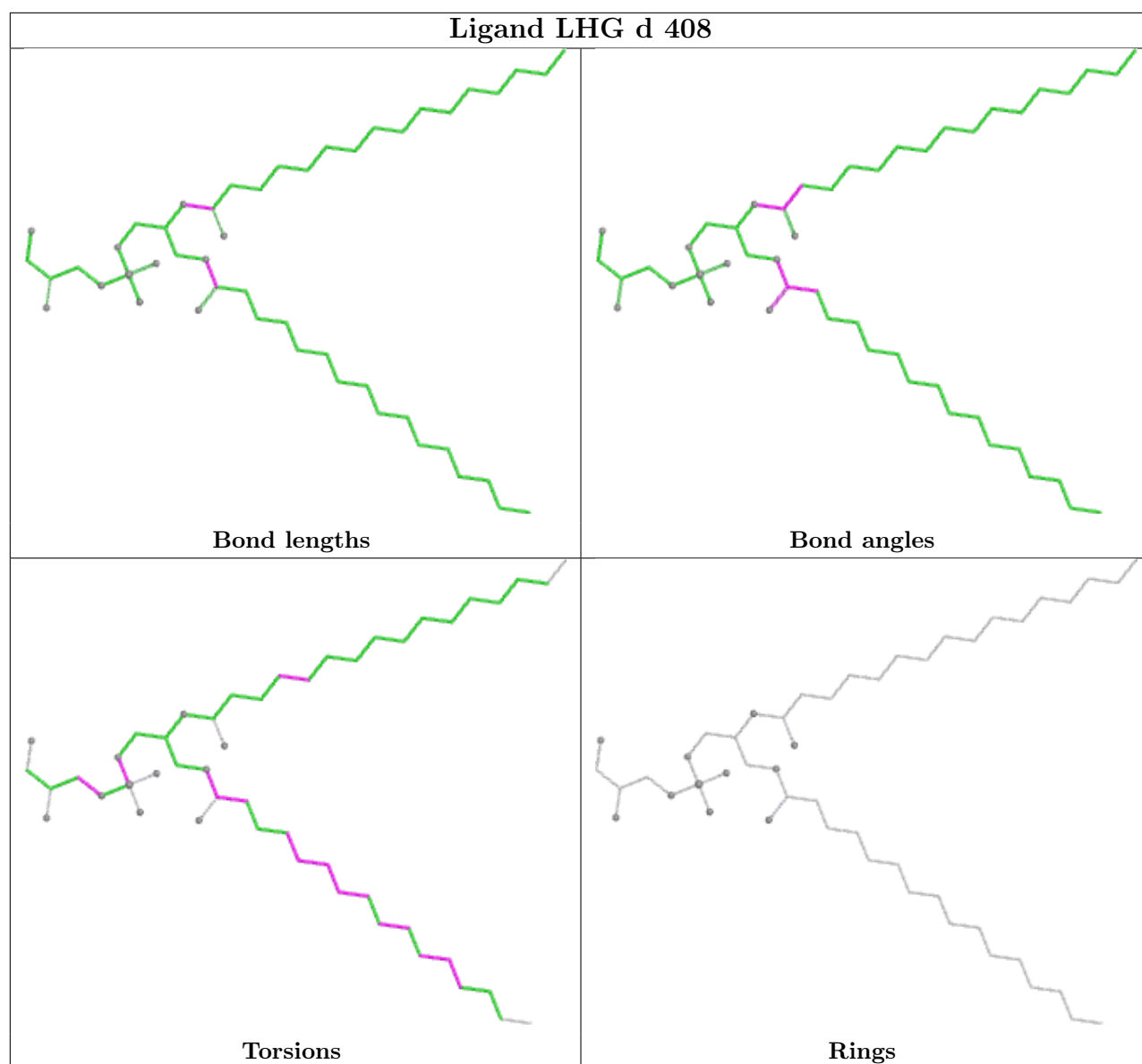


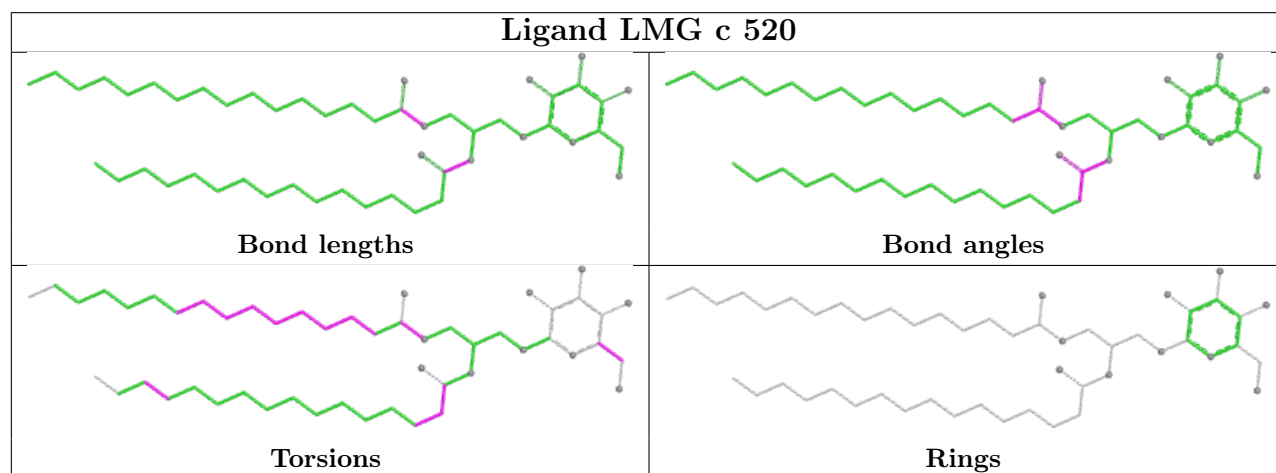
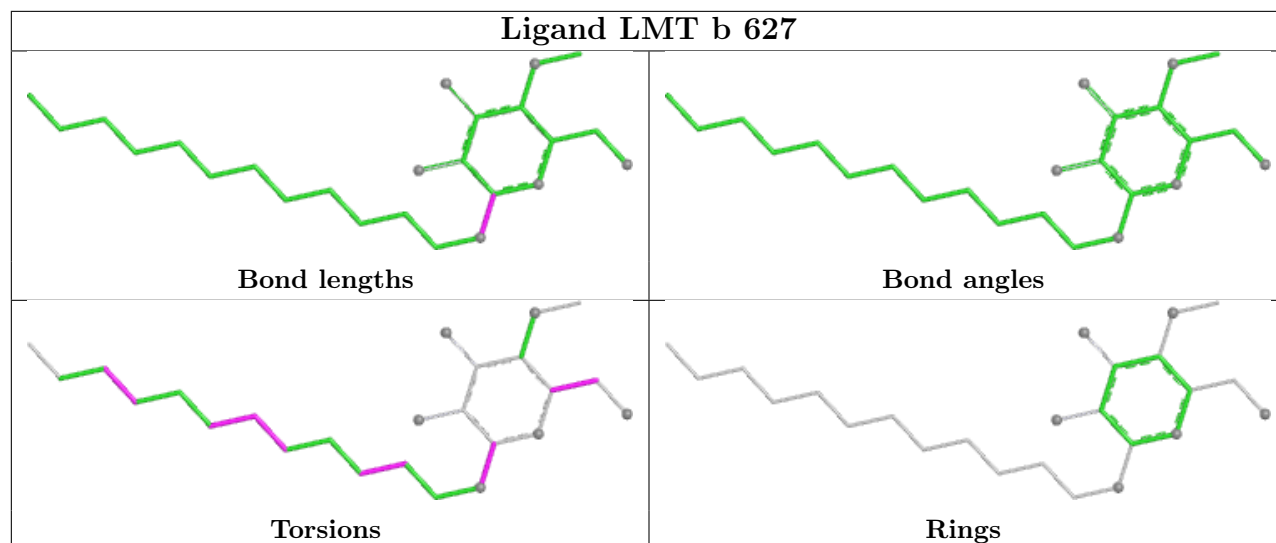
Ligand CLA b 607



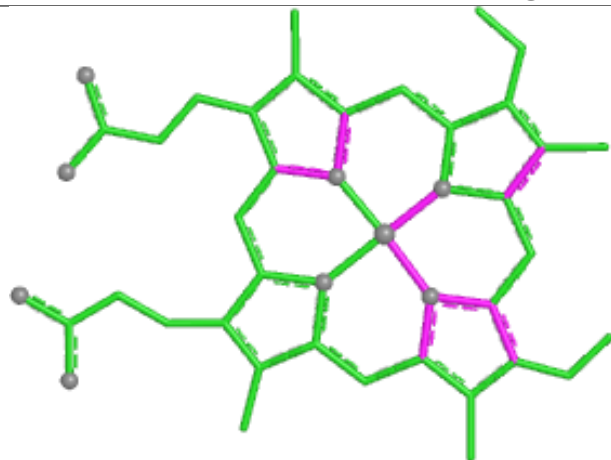




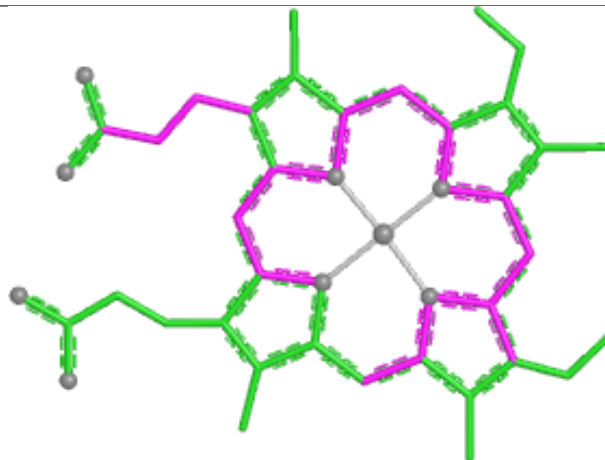




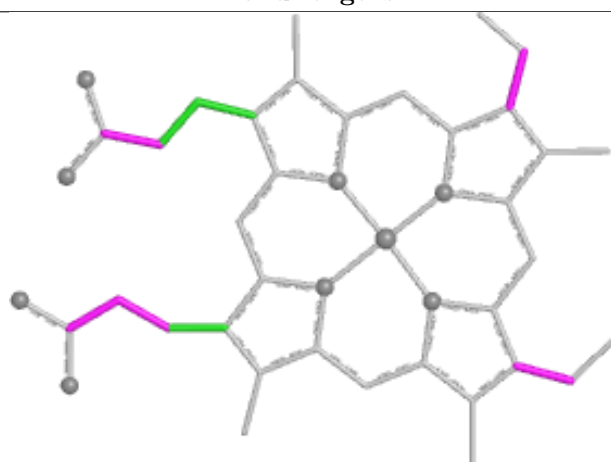
Ligand HEM e 87



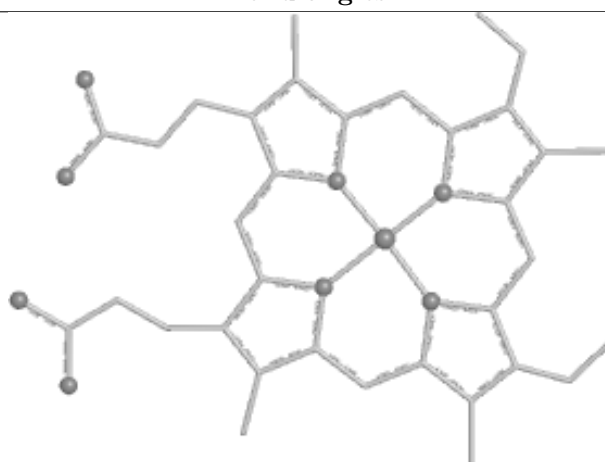
Bond lengths



Bond angles

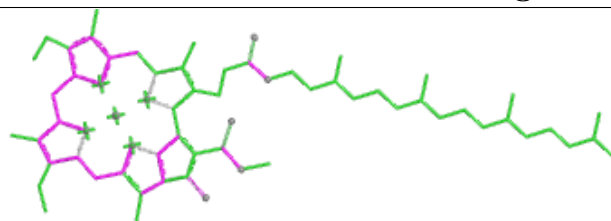


Torsions

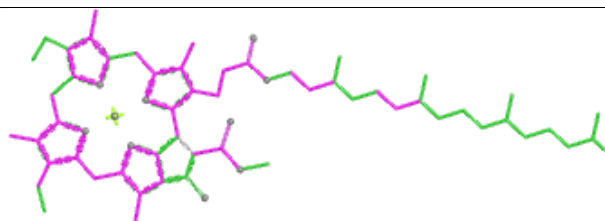


Rings

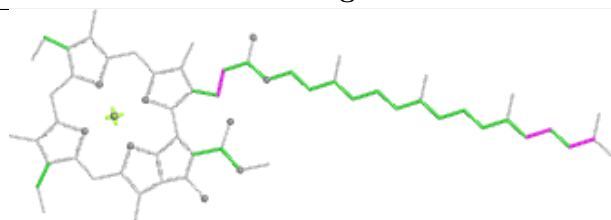
Ligand CLA B 610



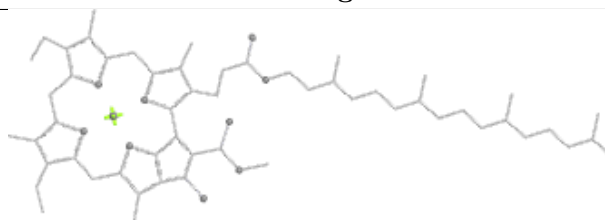
Bond lengths



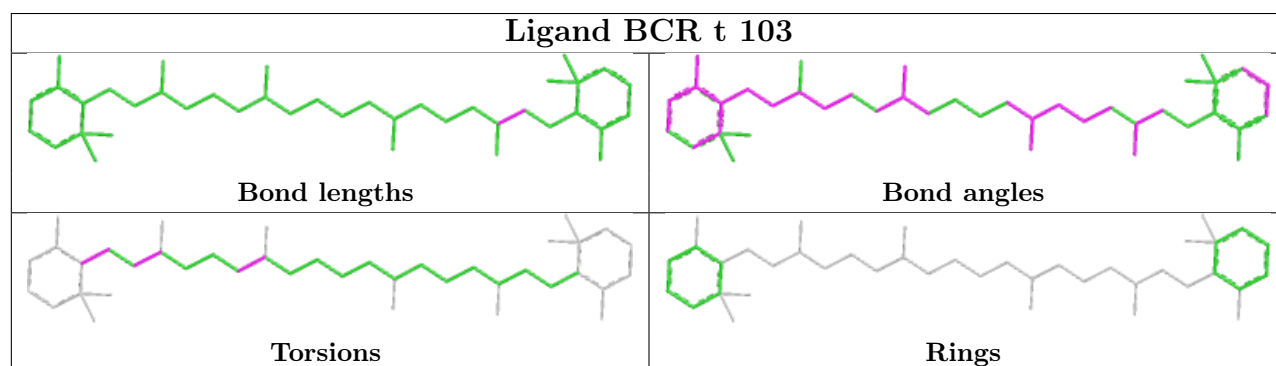
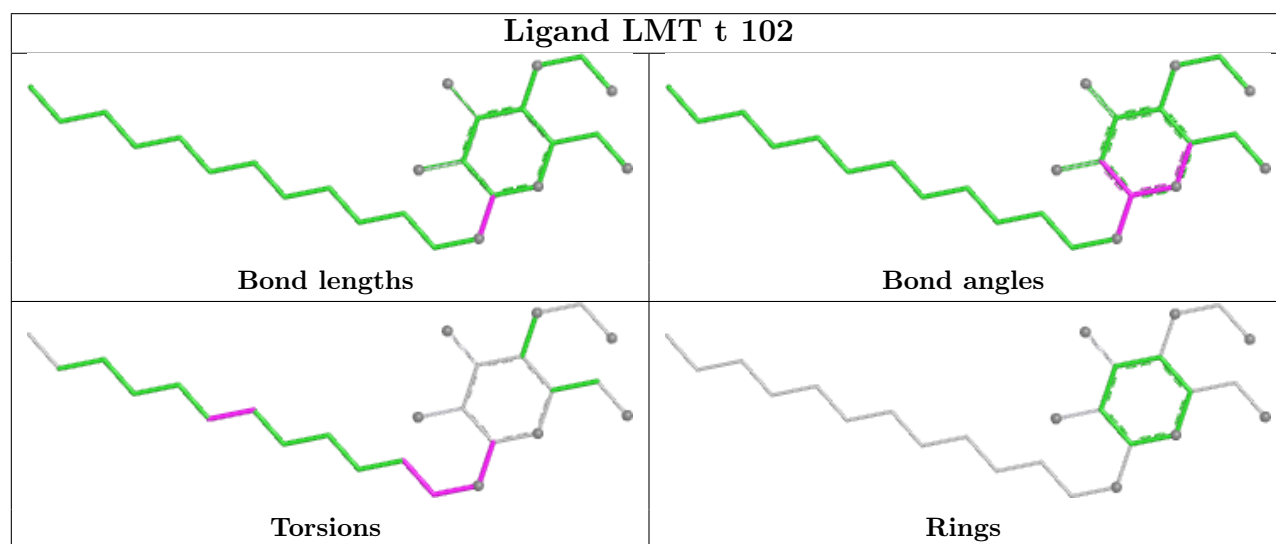
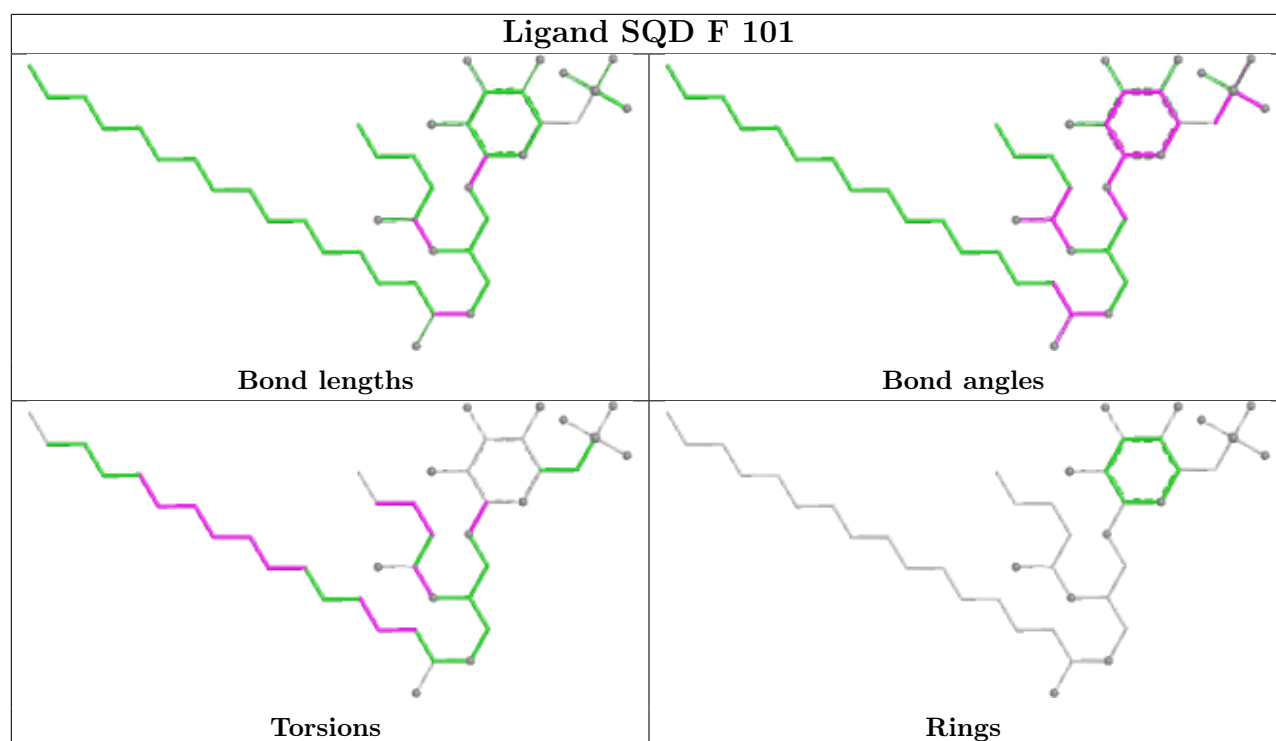
Bond angles

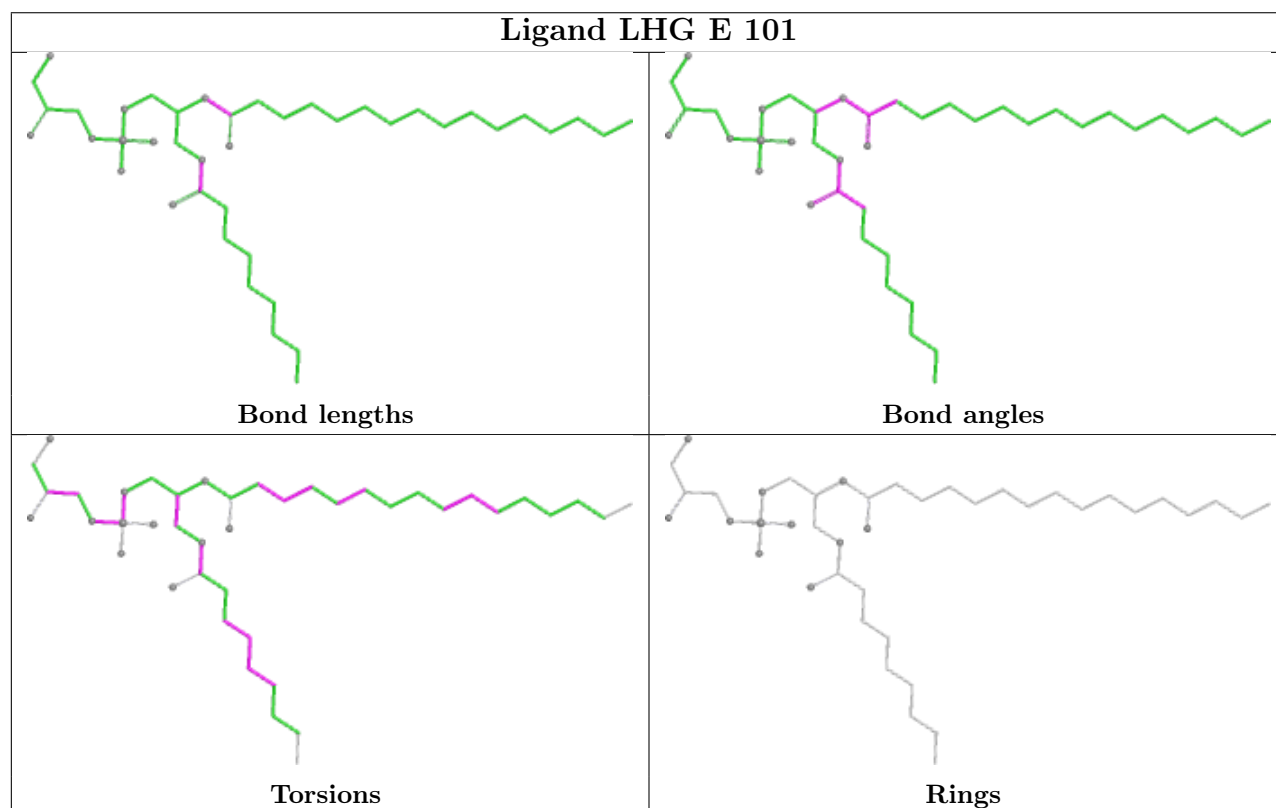
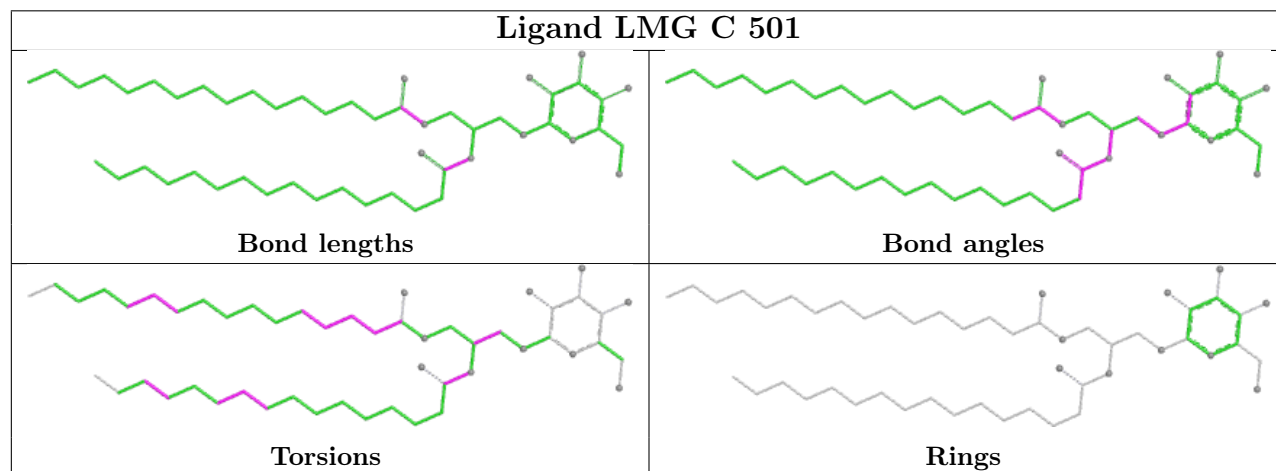
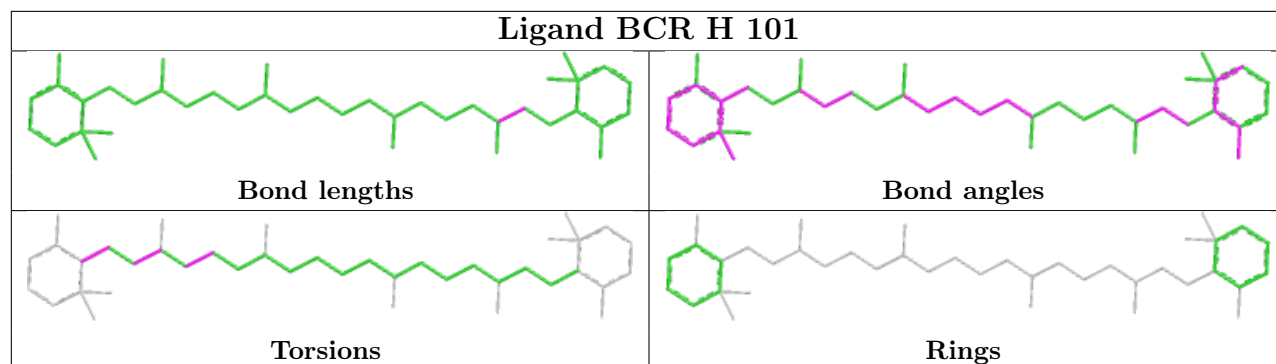


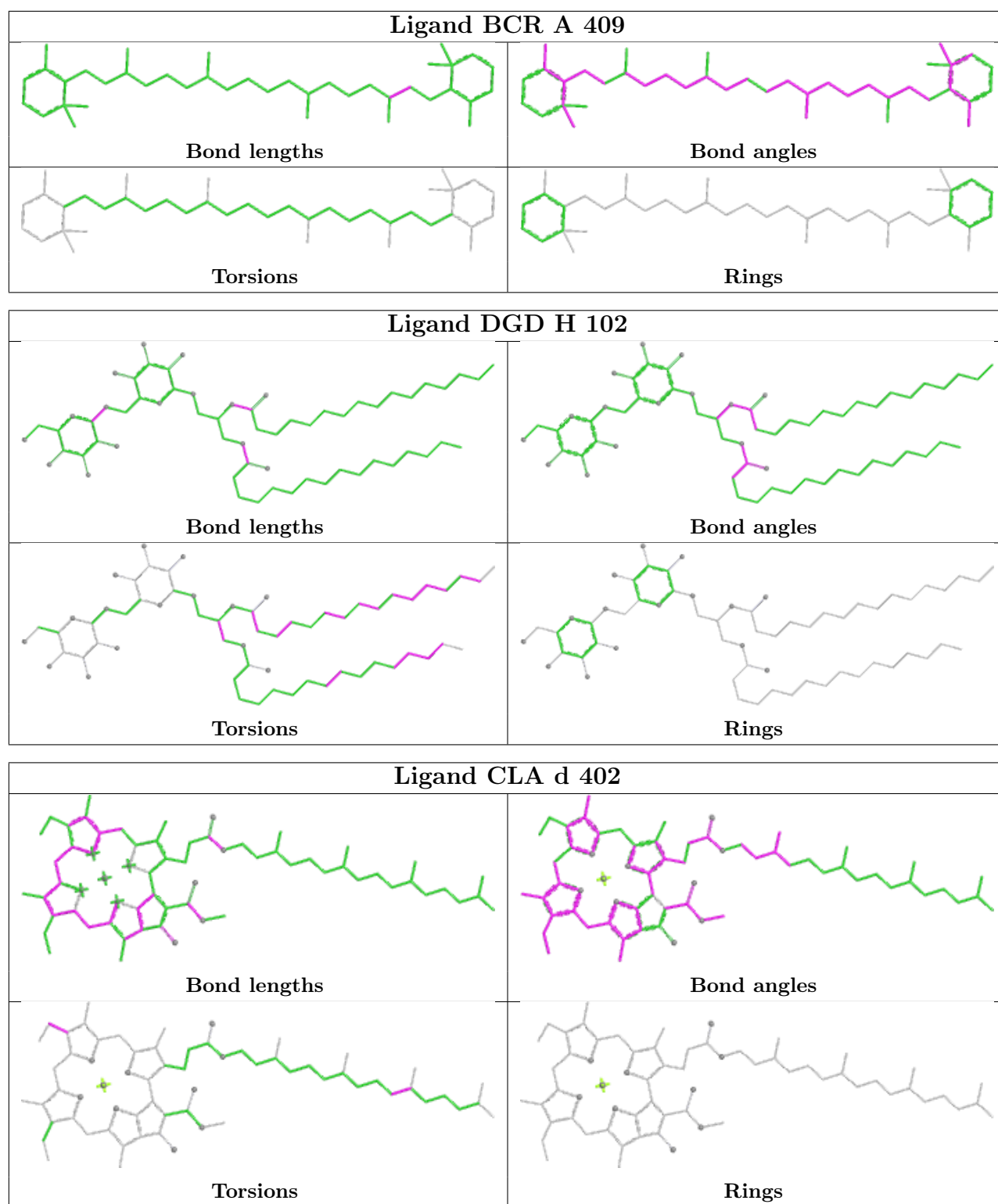
Torsions



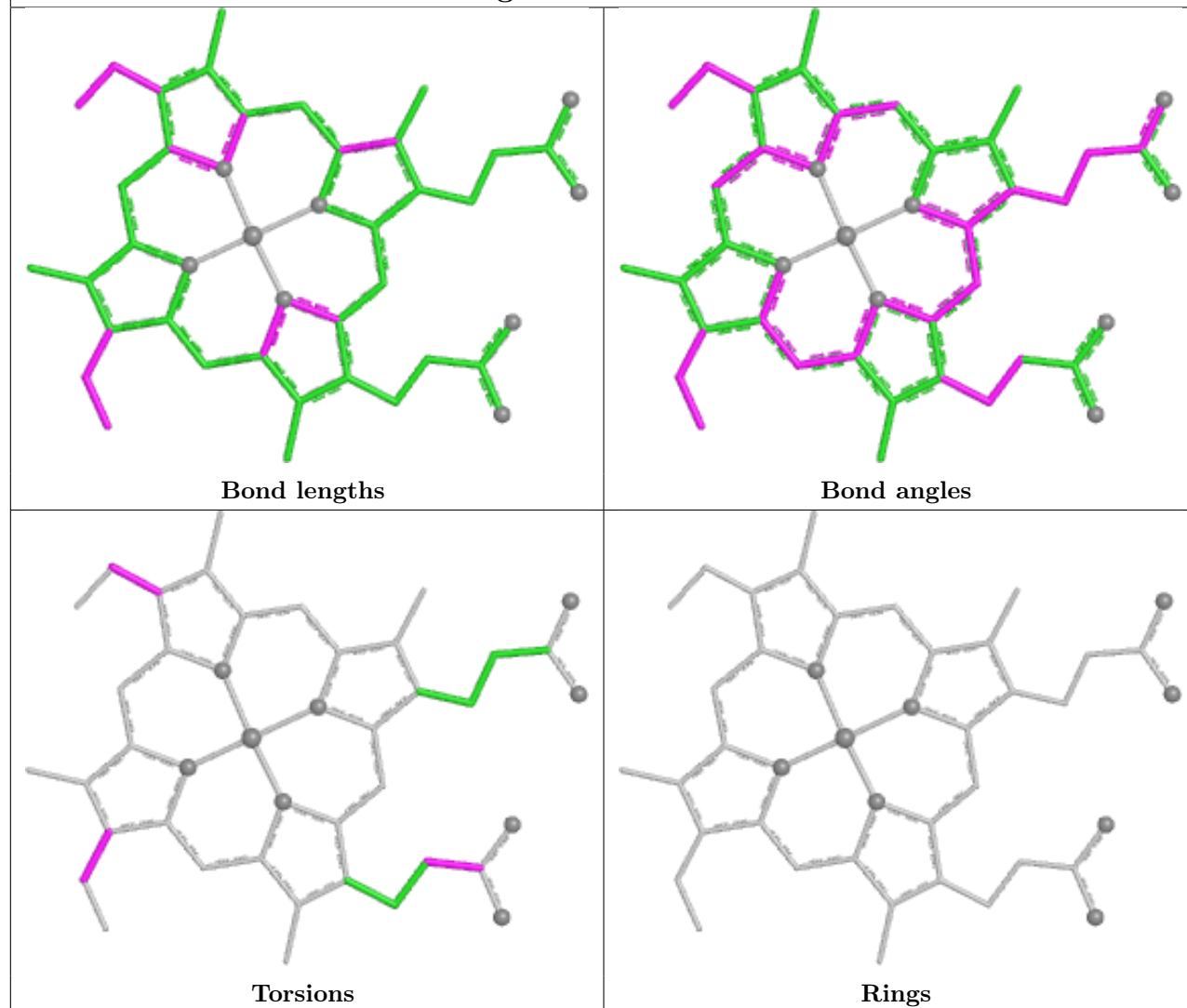
Rings



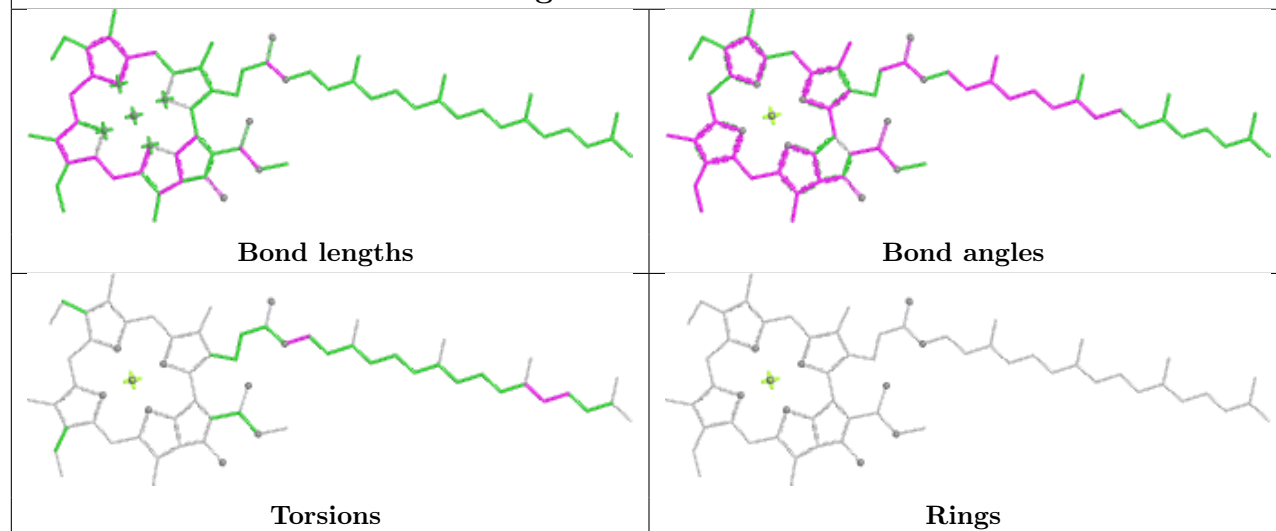




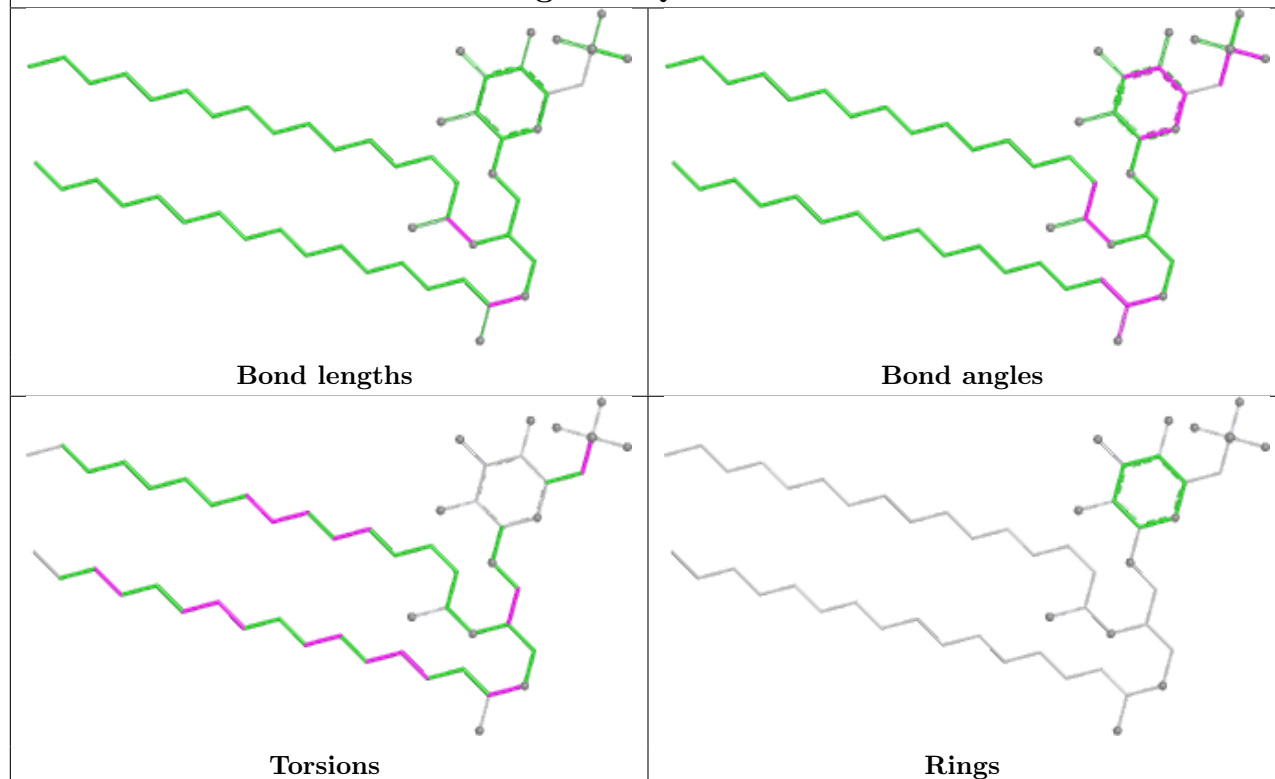
Ligand HEC v 202



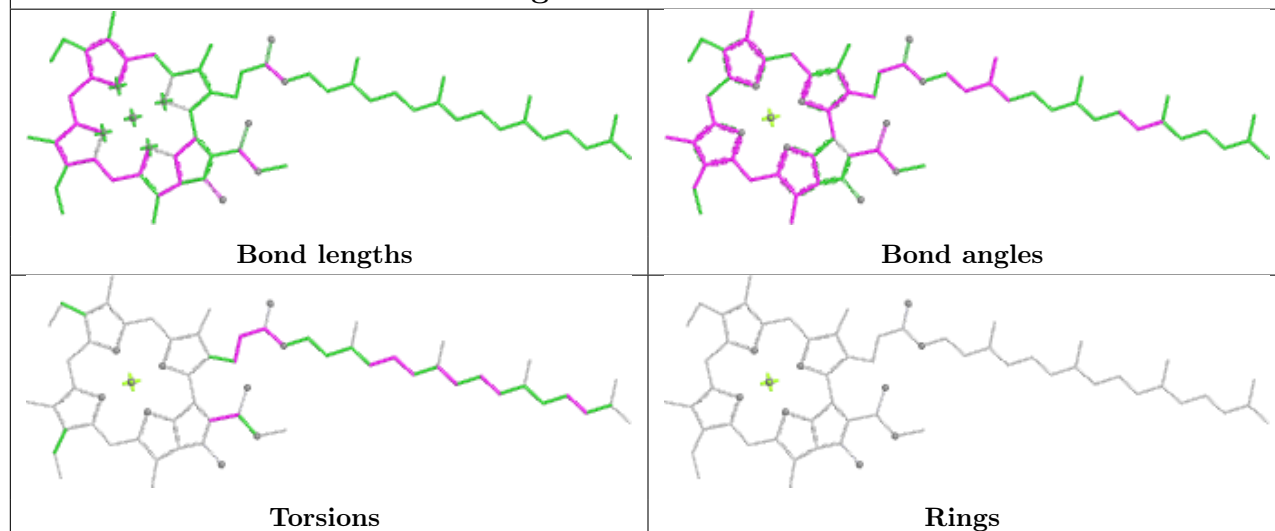
Ligand CLA b 608

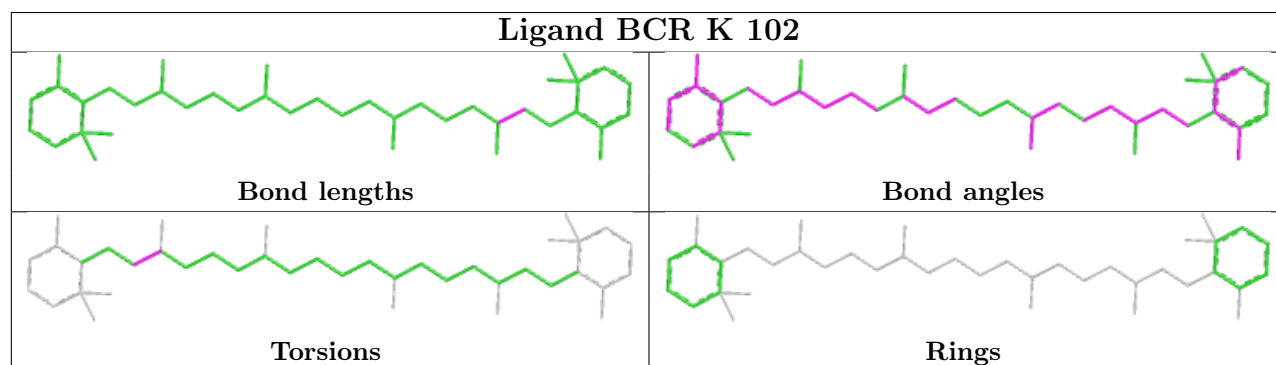
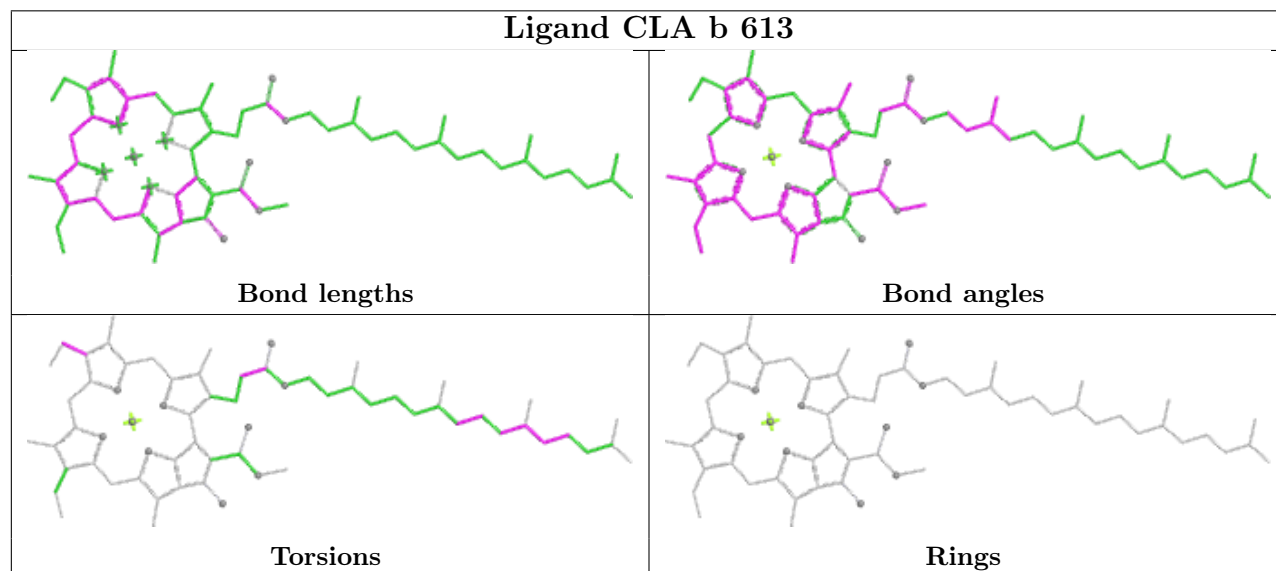
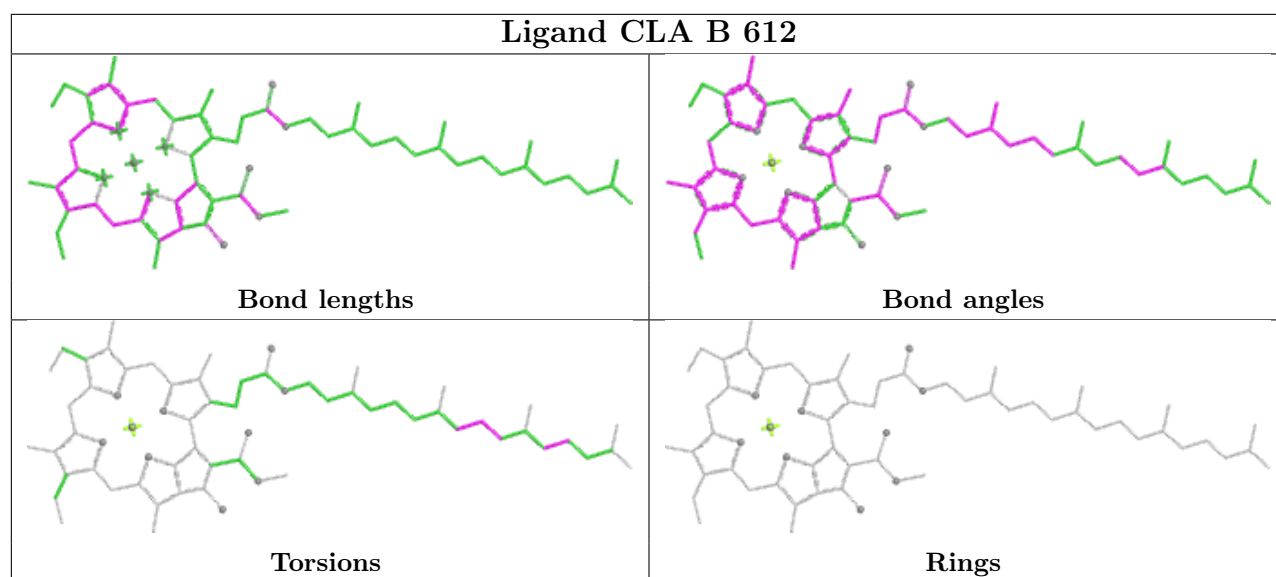


Ligand SQD a 413

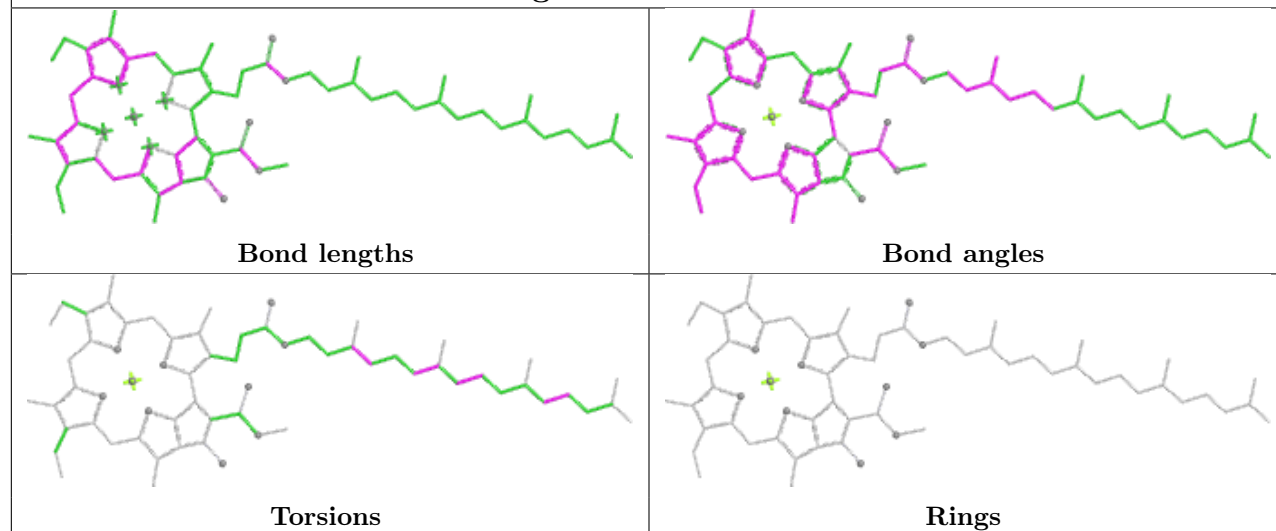


Ligand CLA B 601

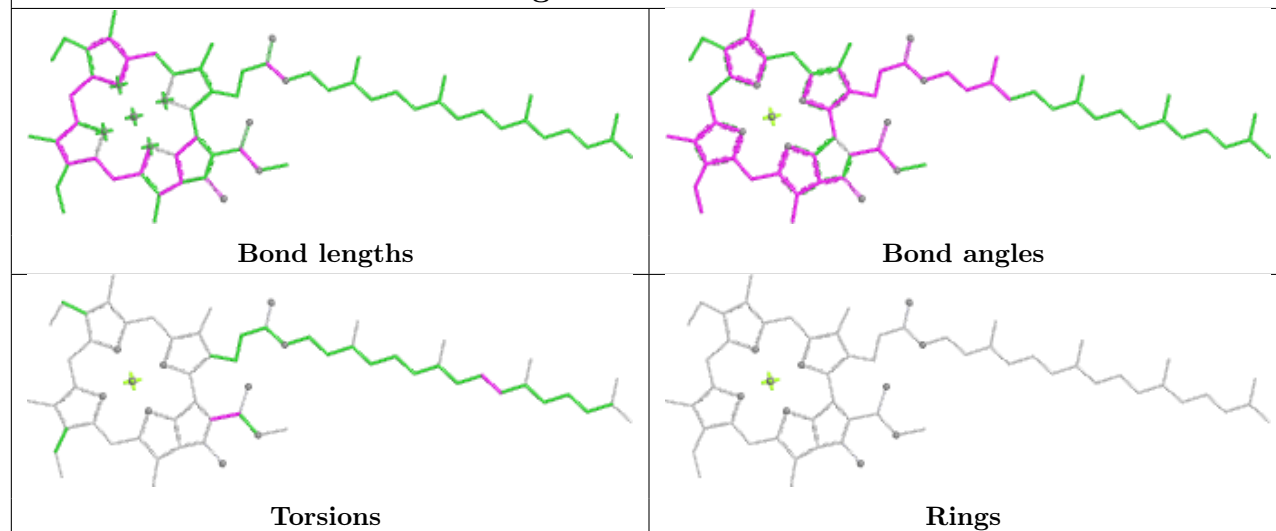




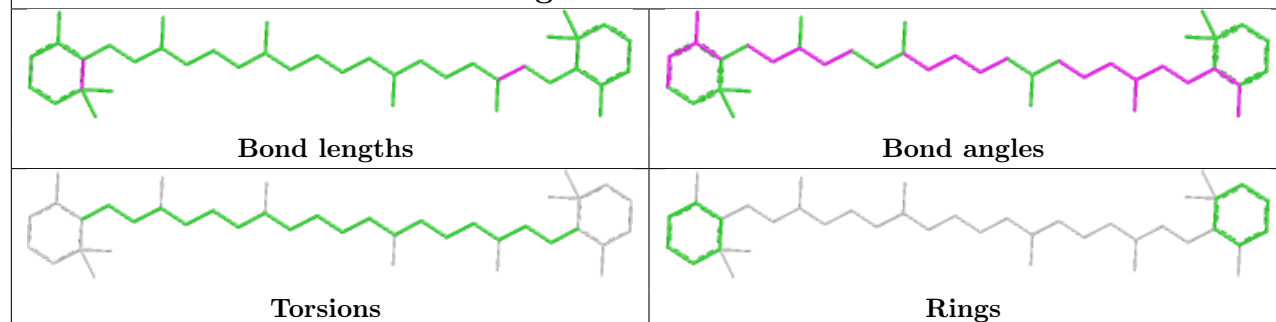
Ligand CLA B 605

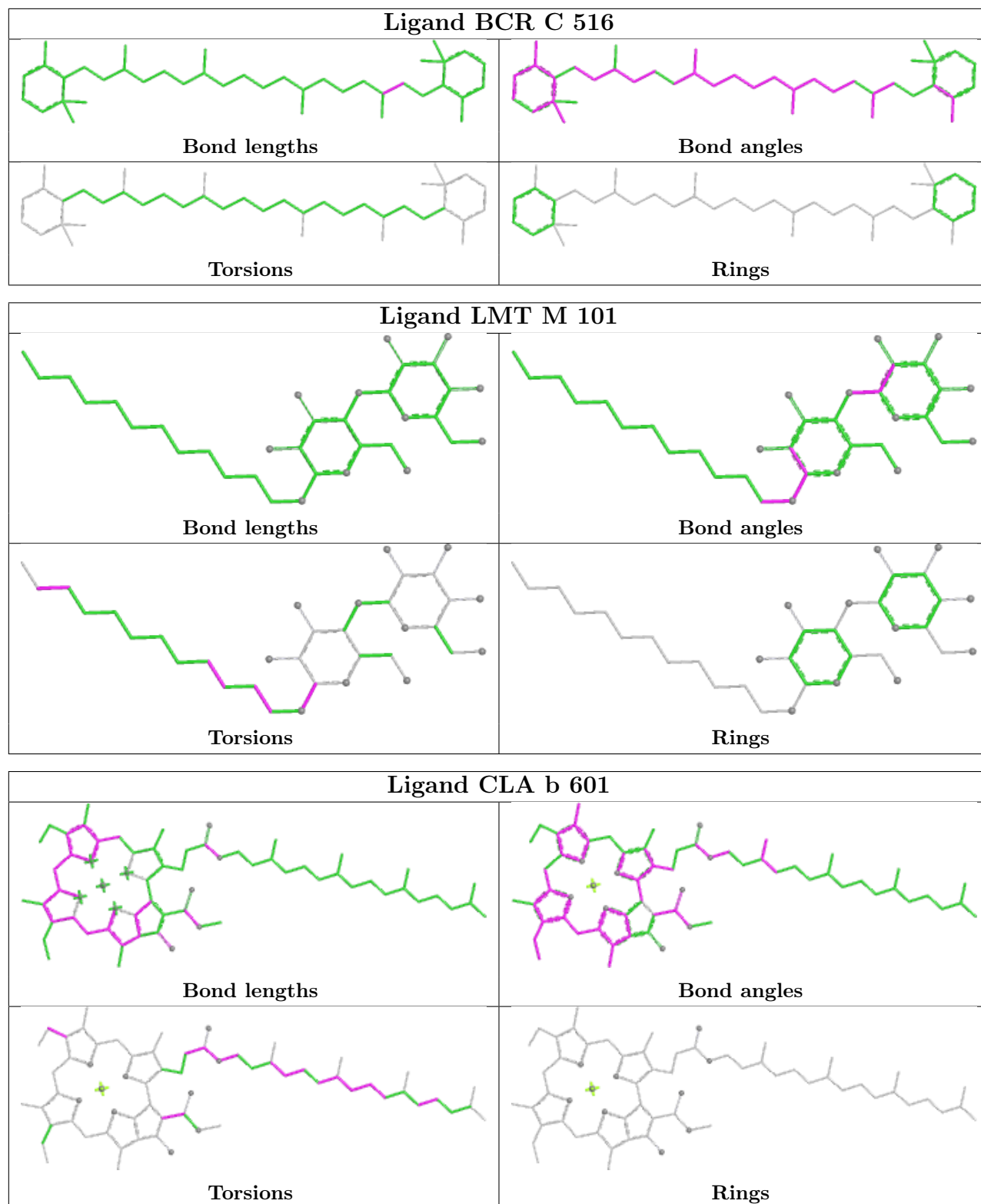


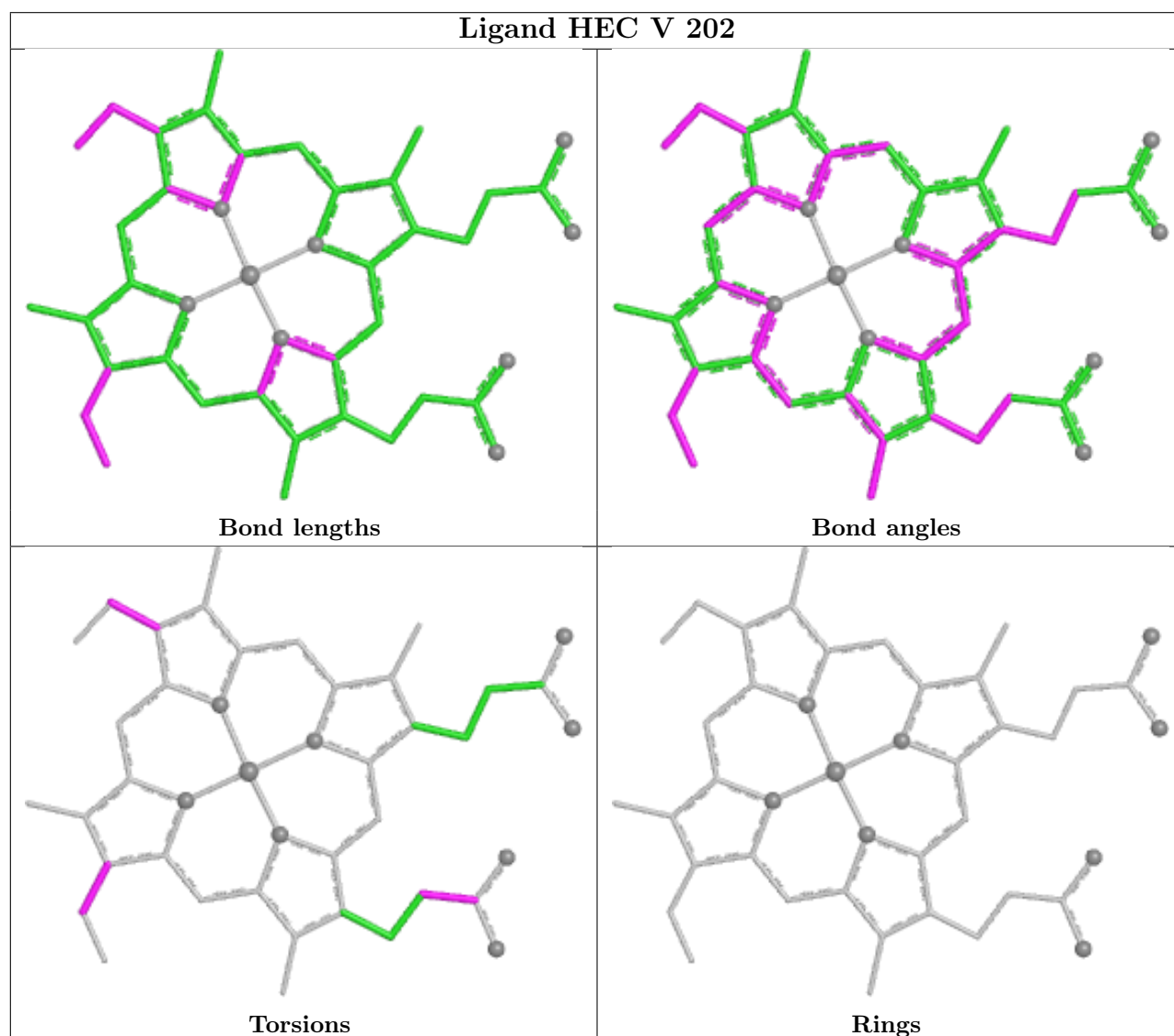
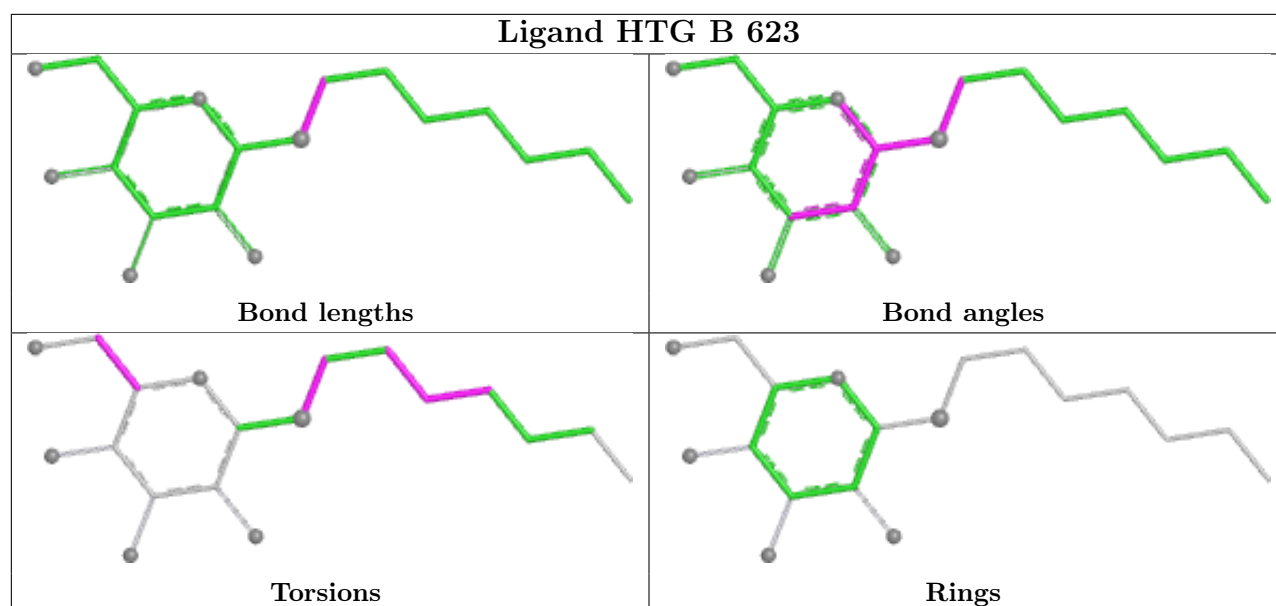
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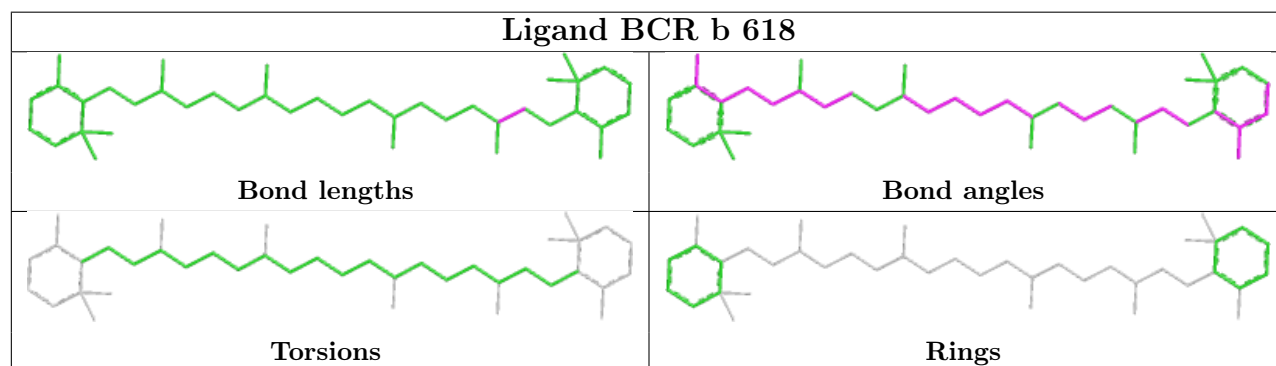
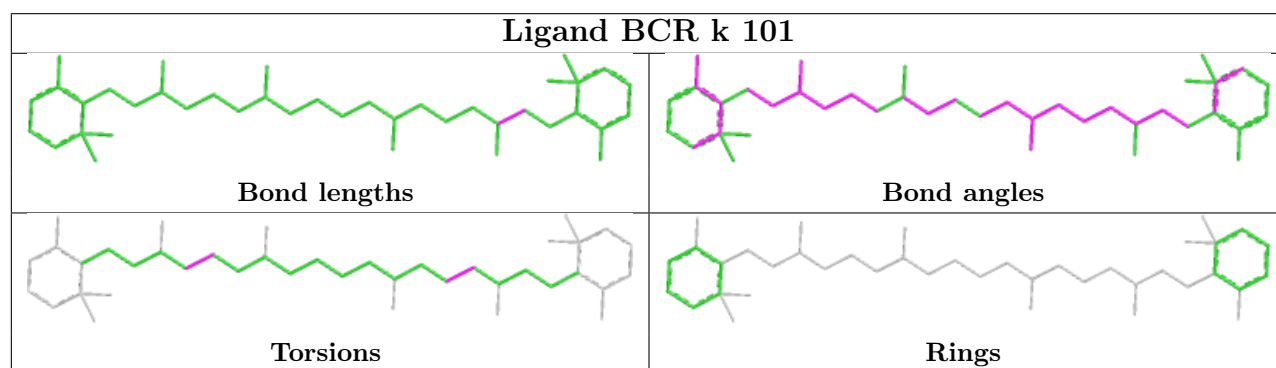
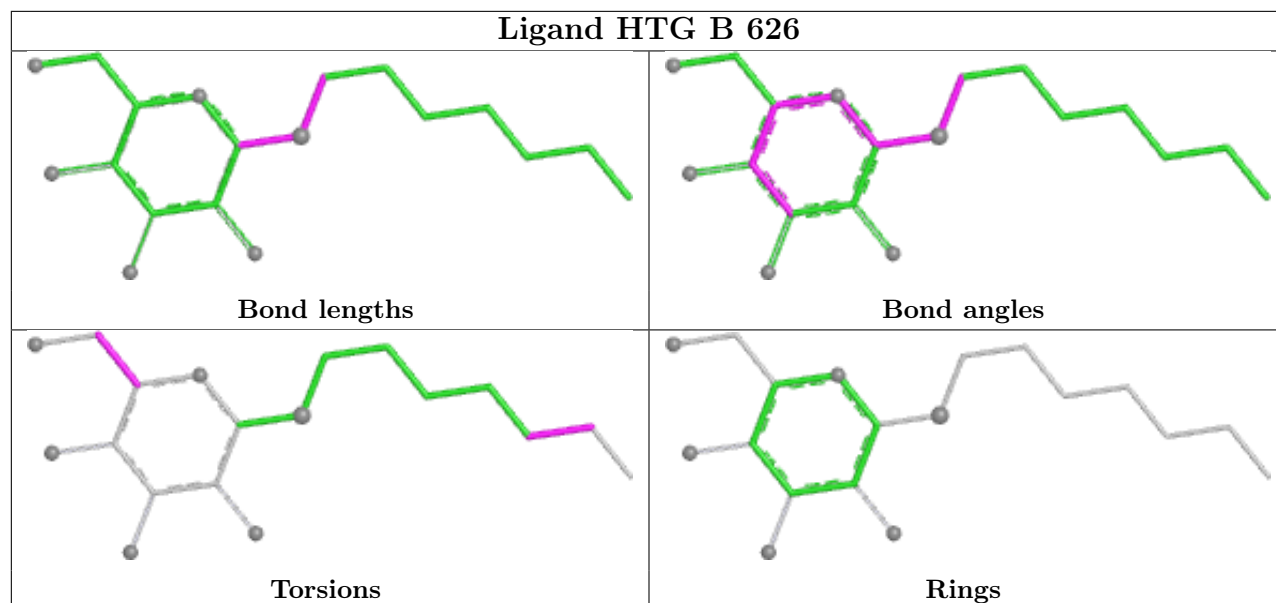


Ligand BCR c 516

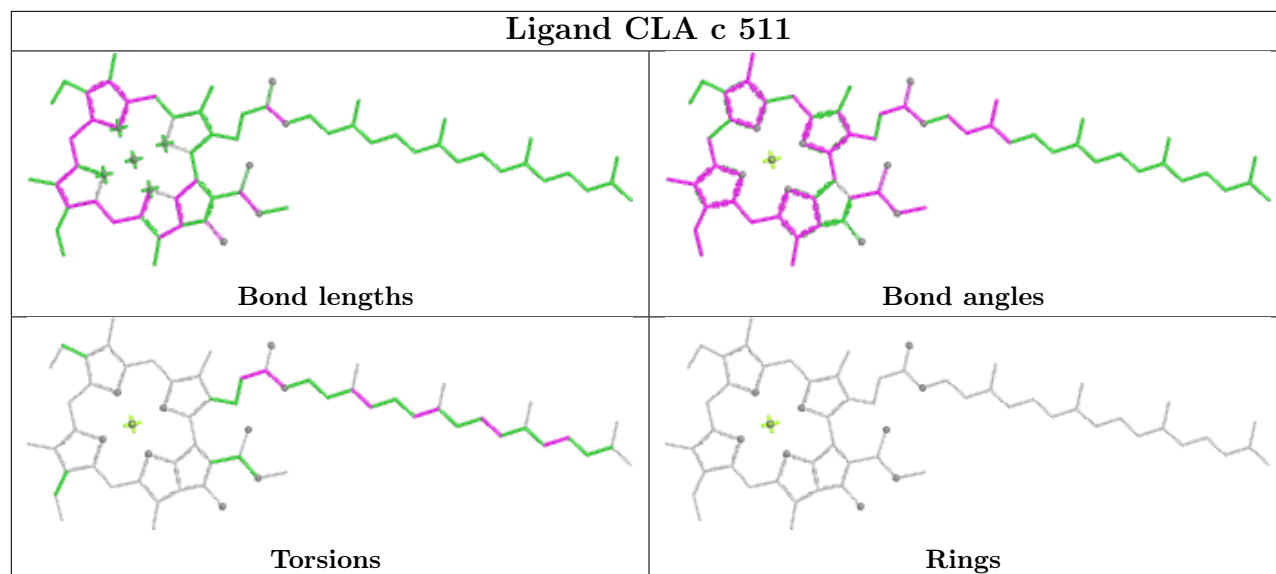




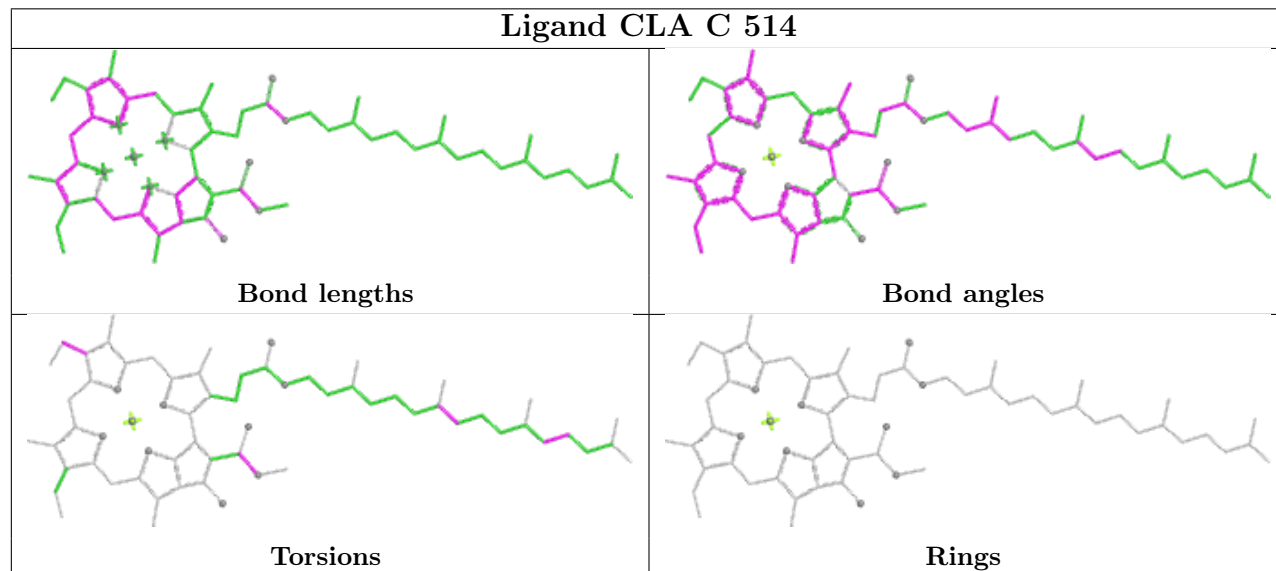




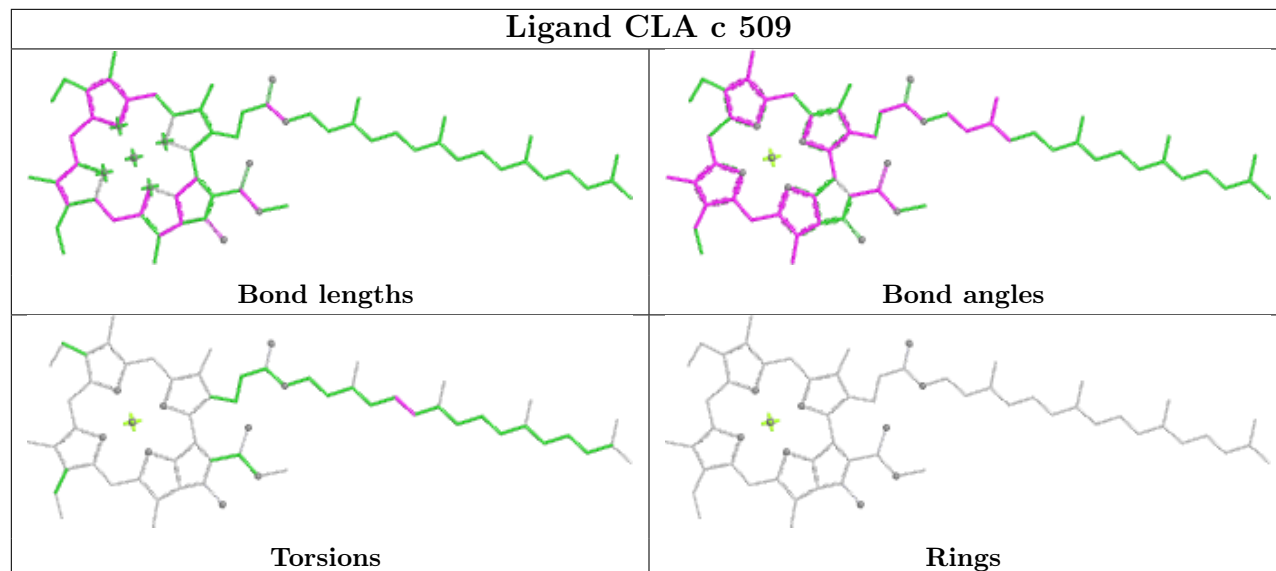
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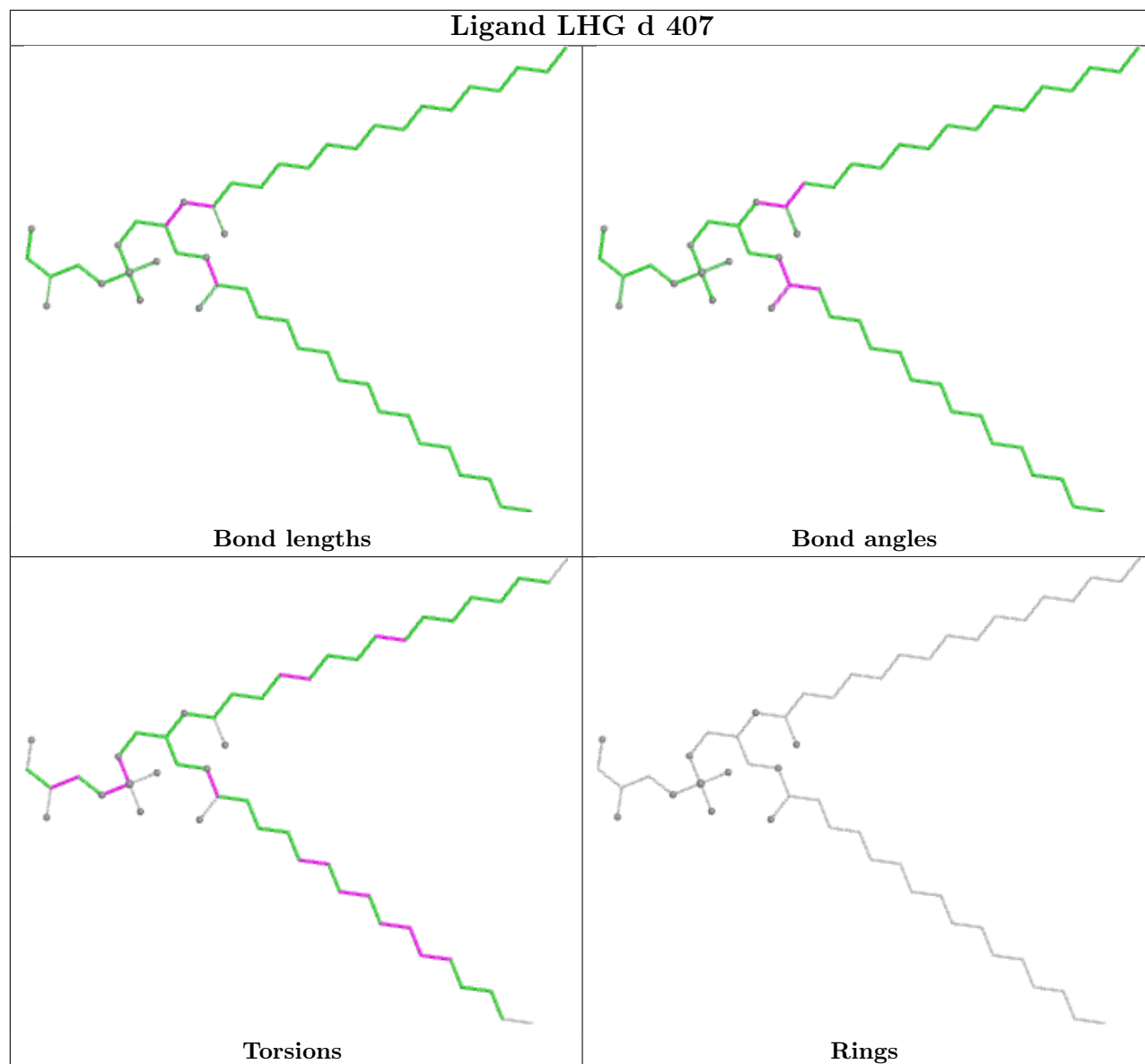
Ligand CLA C 514



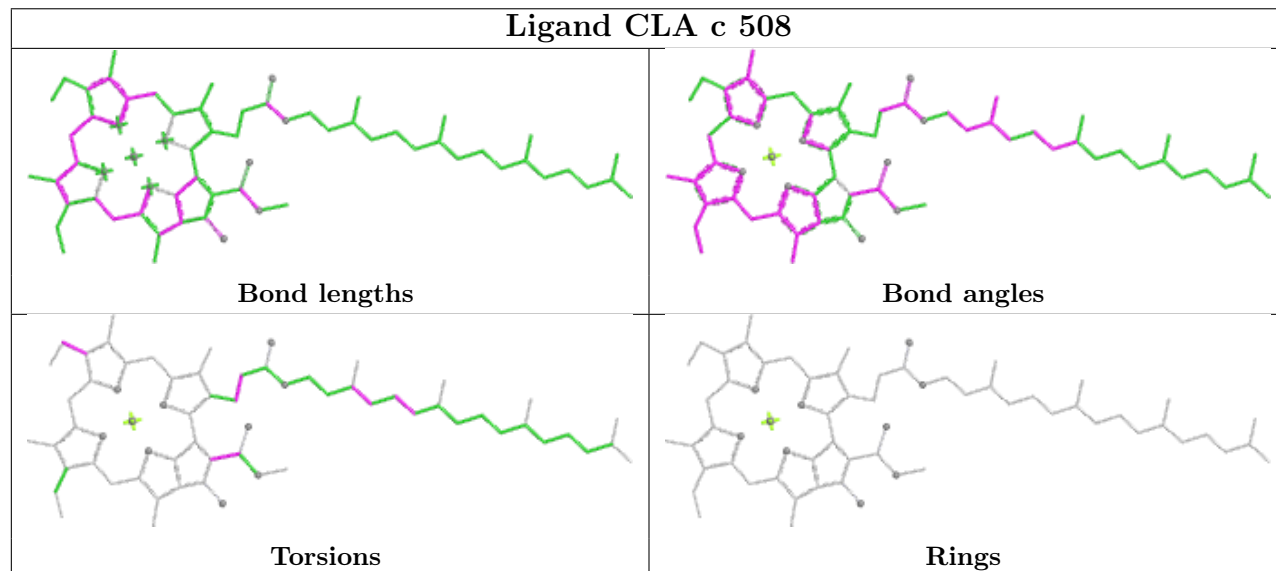
Ligand CLA c 509



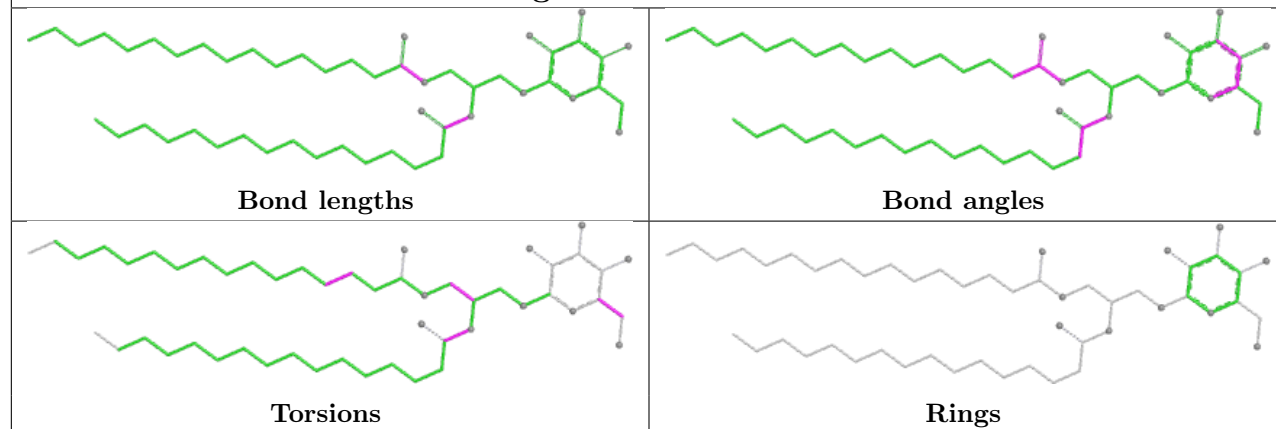
Ligand LHG d 407



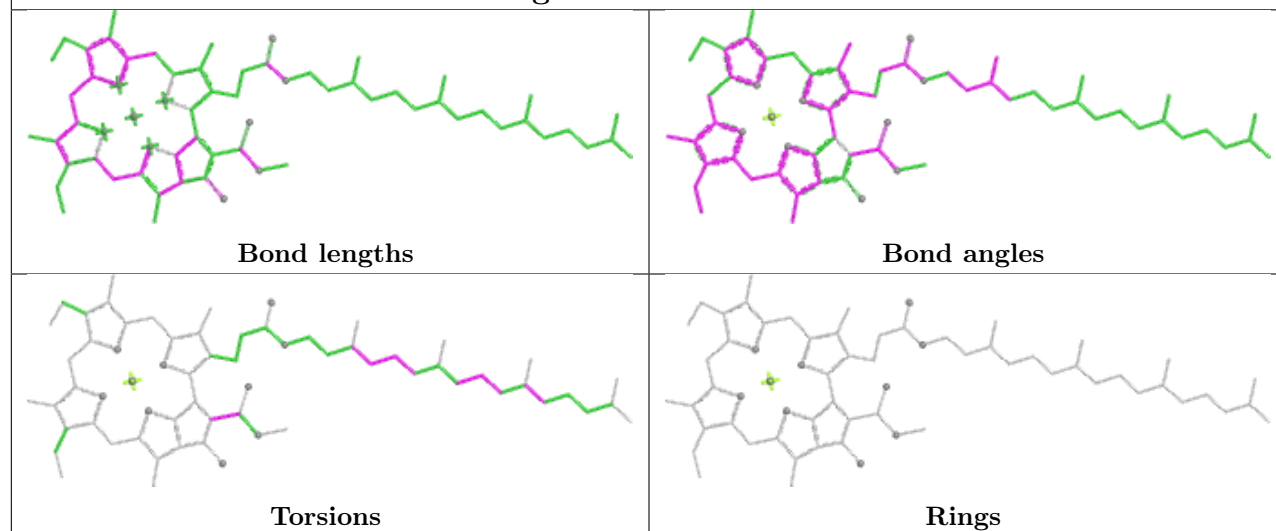
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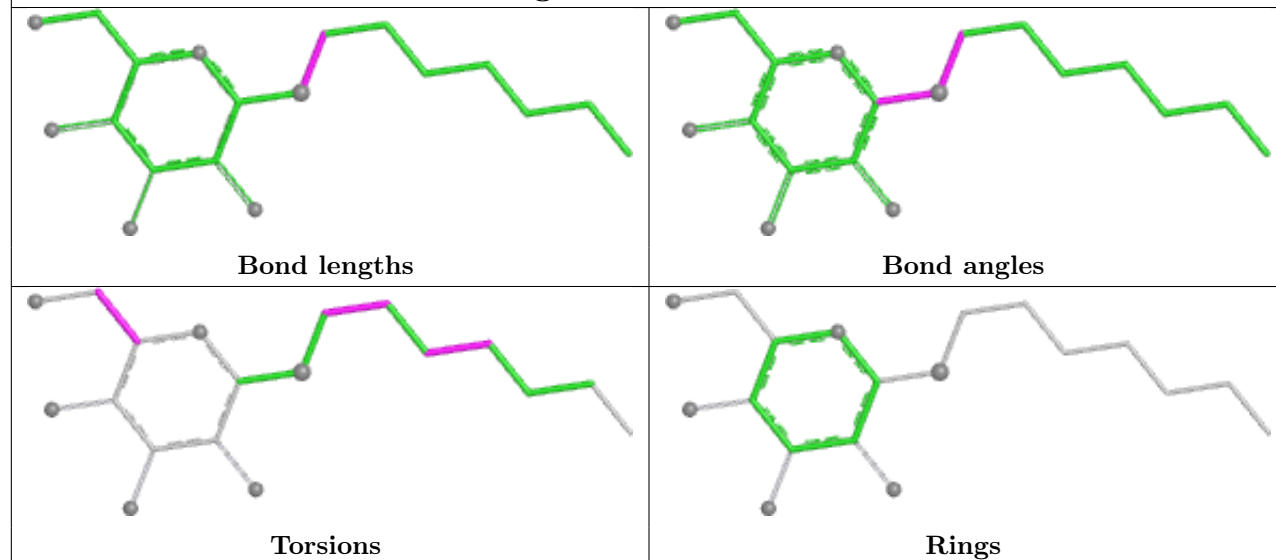
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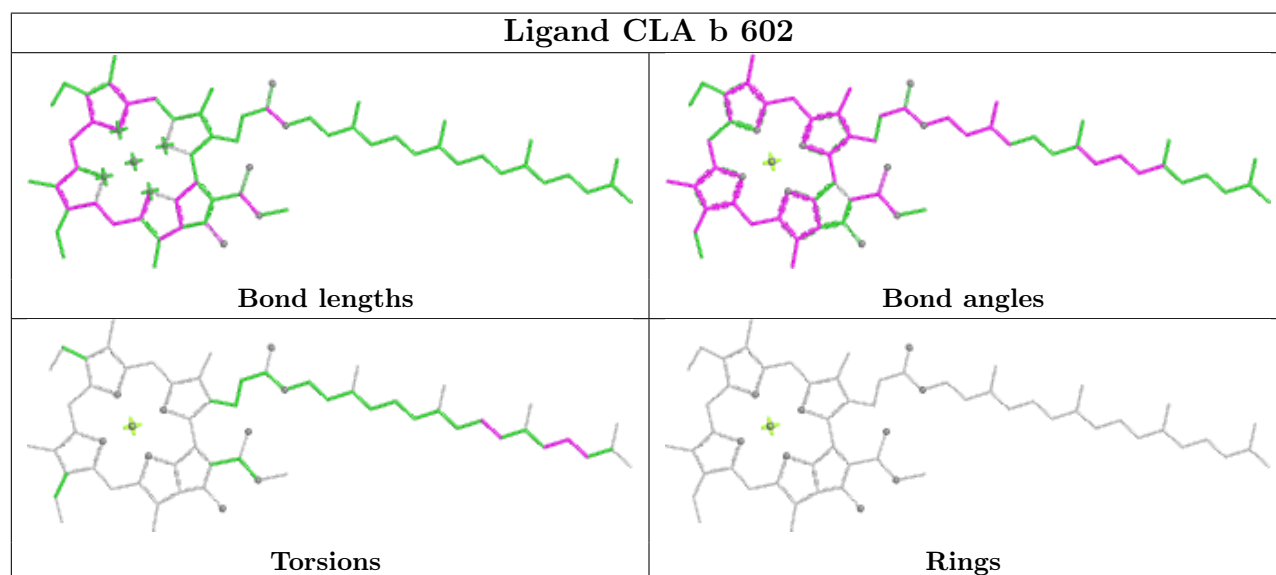
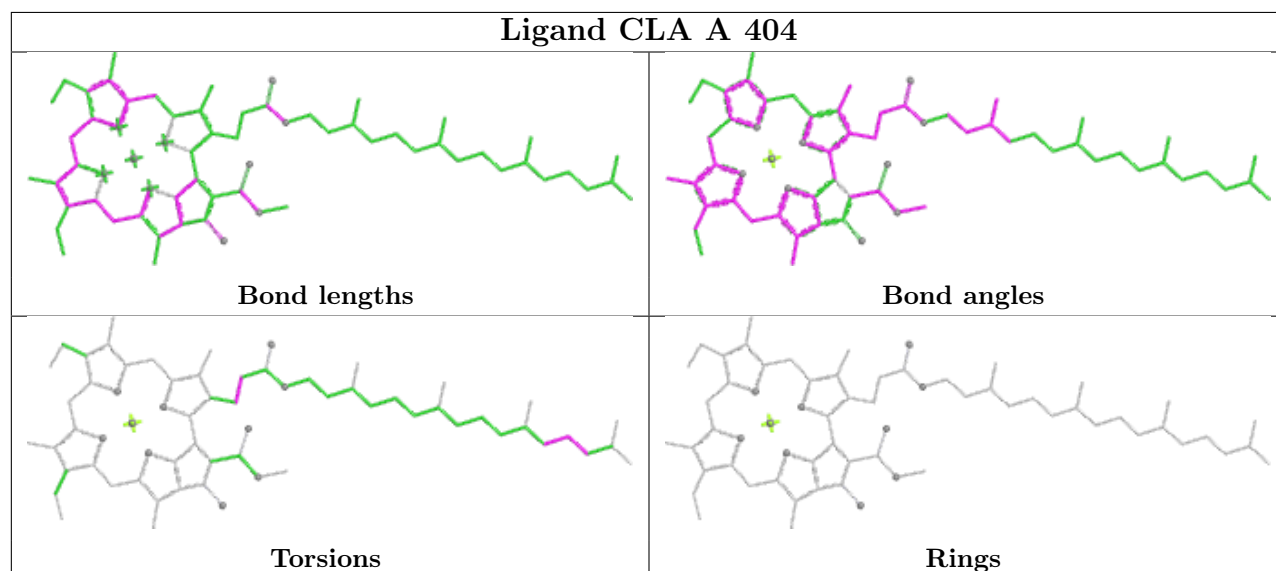
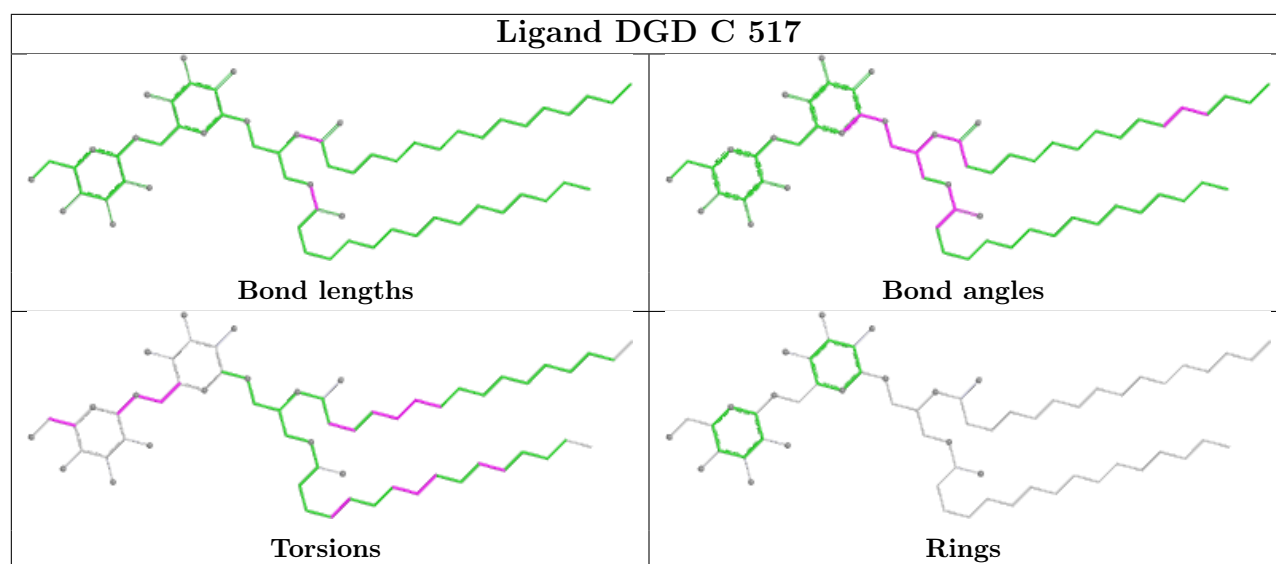


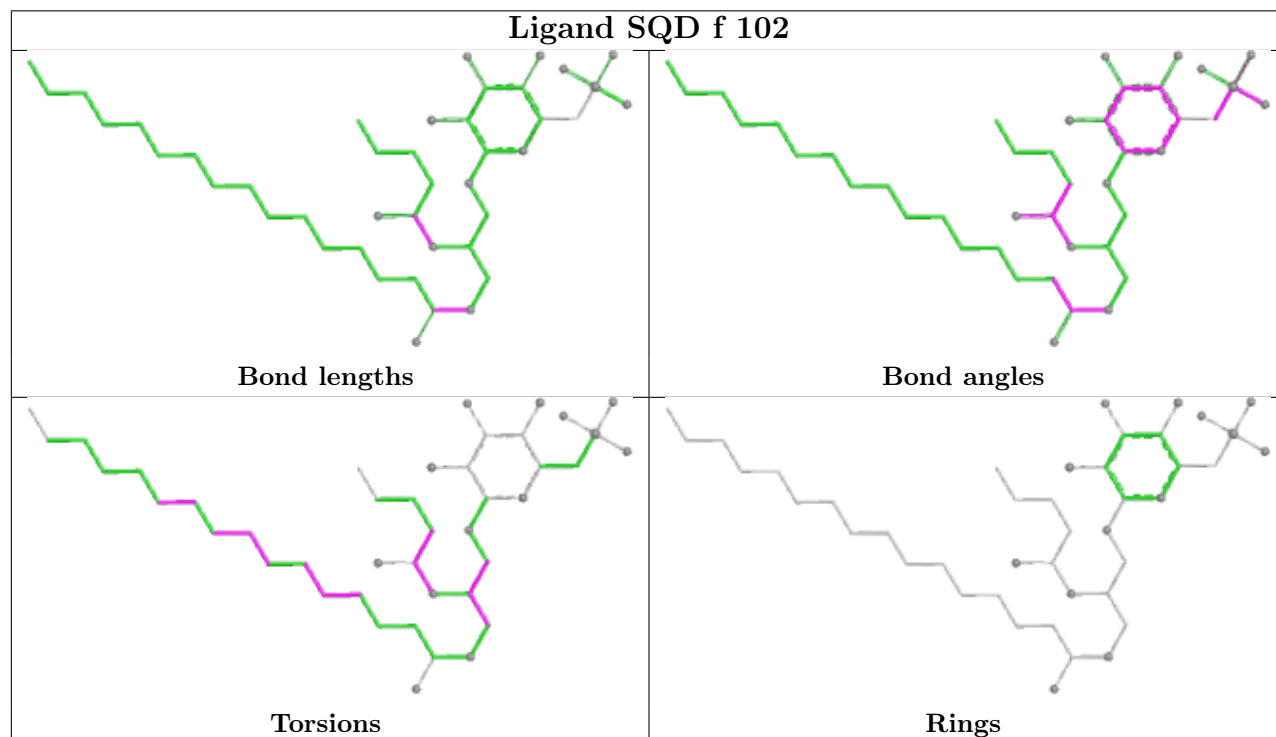
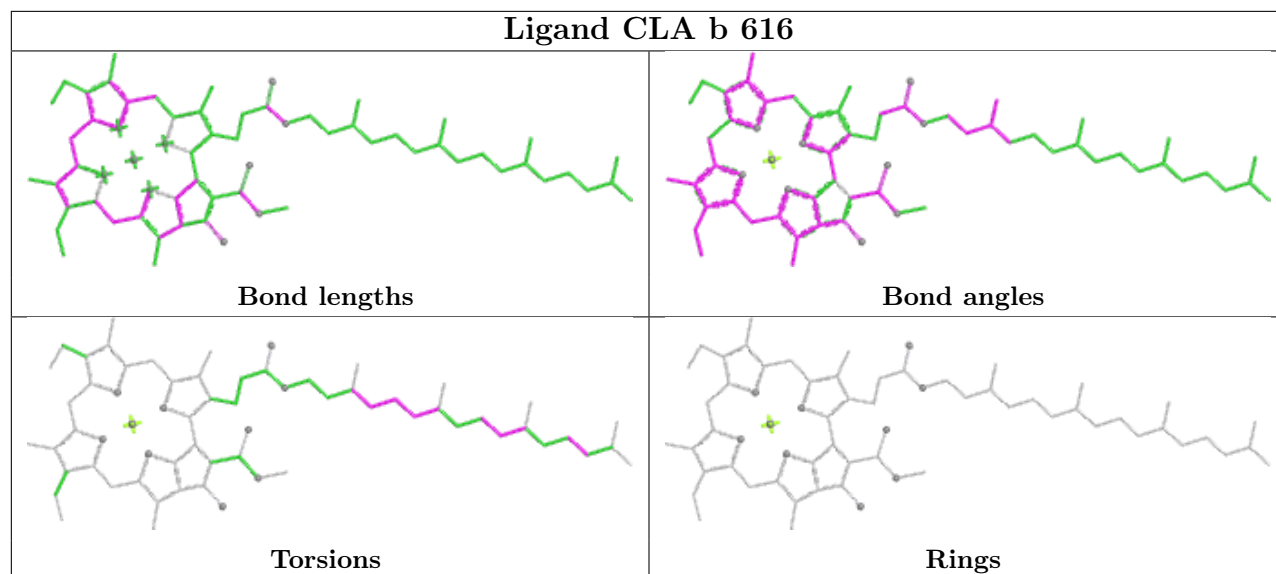
Ligand CLA B 614

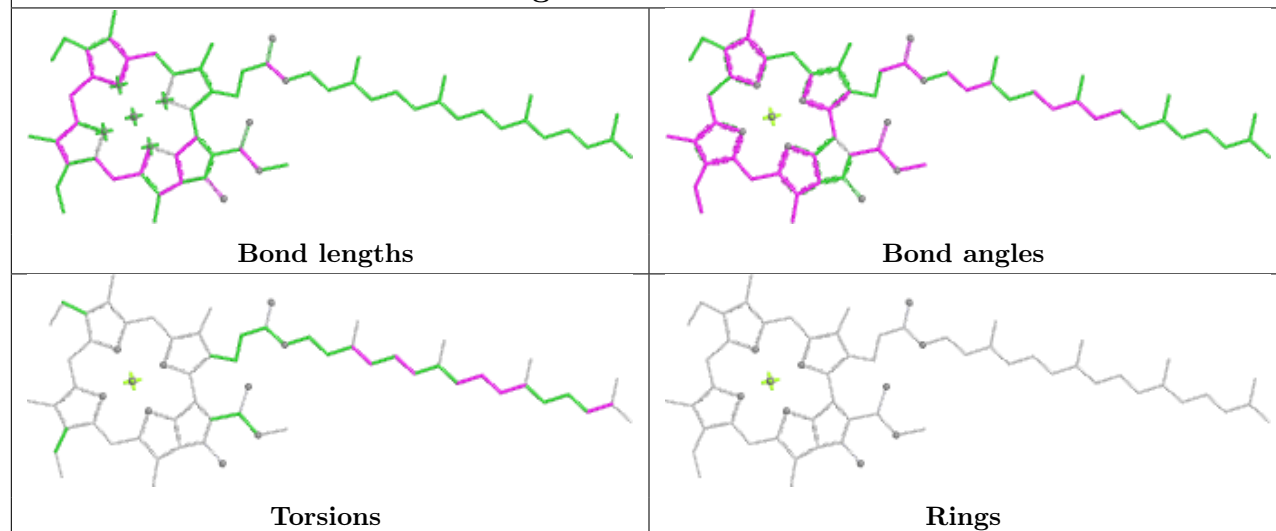
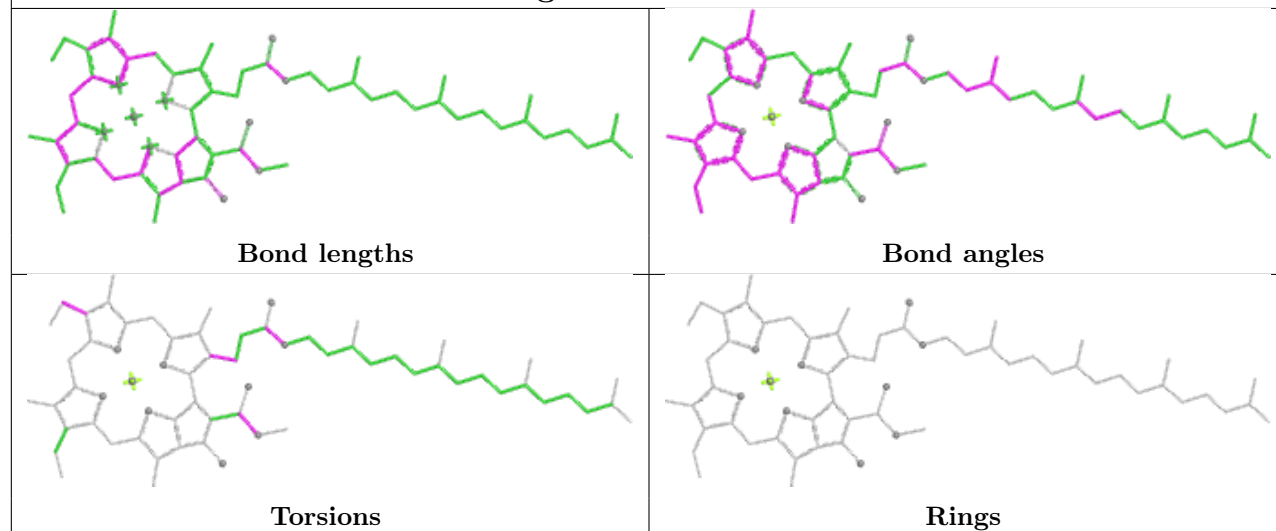
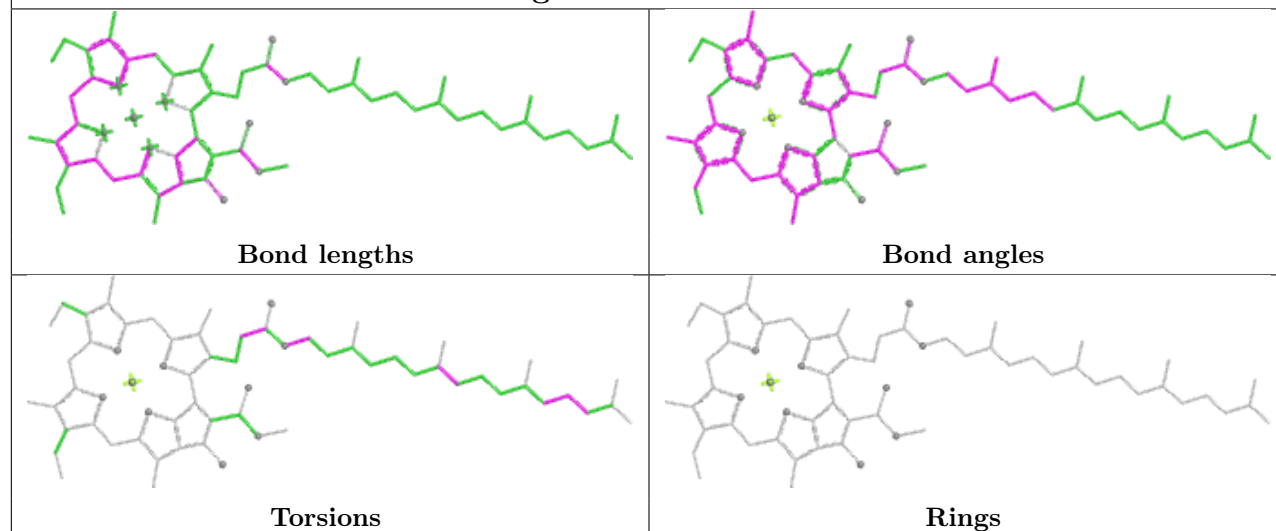


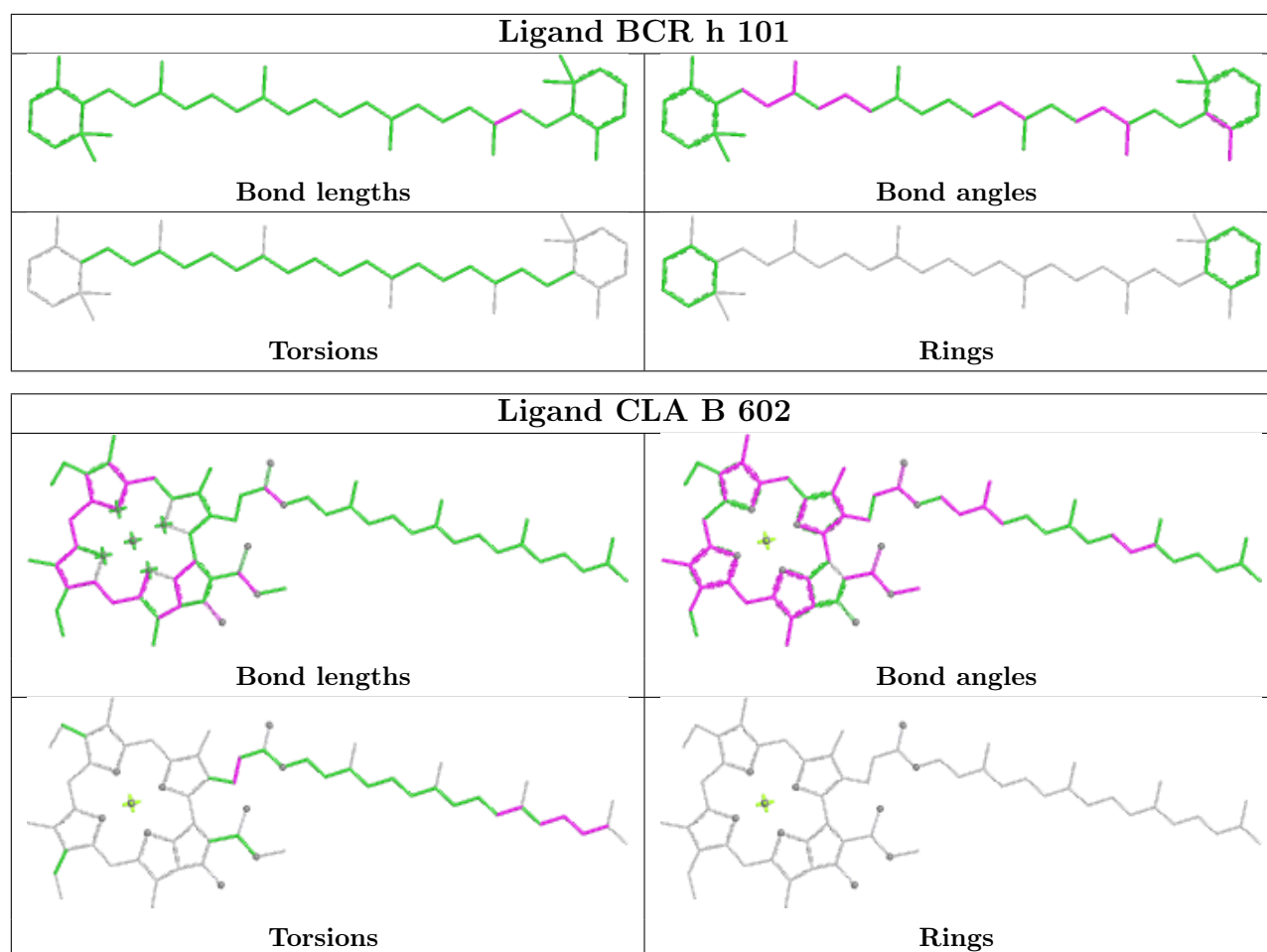
Ligand HTG c 522







Ligand CLA B 615**Ligand CLA c 512****Ligand CLA B 613**



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.61	1 (0%) 90 92	33, 54, 76, 123	3 (0%)
1	a	334/344 (97%)	-0.54	1 (0%) 90 92	34, 58, 88, 134	4 (1%)
2	B	504/505 (99%)	-0.50	2 (0%) 88 91	34, 59, 88, 130	8 (1%)
2	b	504/505 (99%)	-0.42	4 (0%) 82 86	38, 63, 102, 155	4 (0%)
3	C	451/455 (99%)	-0.48	0 100 100	38, 65, 86, 146	4 (0%)
3	c	455/455 (100%)	-0.42	0 100 100	41, 73, 94, 133	4 (0%)
4	D	342/342 (100%)	-0.65	0 100 100	34, 55, 75, 139	1 (0%)
4	d	341/342 (99%)	-0.58	0 100 100	40, 60, 83, 160	1 (0%)
5	E	81/84 (96%)	-0.14	0 100 100	54, 76, 104, 157	1 (1%)
5	e	79/84 (94%)	-0.01	1 (1%) 75 79	68, 85, 123, 148	0
6	F	34/44 (77%)	-0.39	0 100 100	62, 69, 95, 128	0
6	f	31/44 (70%)	-0.16	2 (6%) 25 28	68, 75, 106, 142	0
7	H	64/65 (98%)	-0.33	1 (1%) 70 76	36, 68, 84, 128	1 (1%)
7	h	64/65 (98%)	-0.29	1 (1%) 70 76	61, 75, 93, 140	0
8	I	37/38 (97%)	-0.23	0 100 100	59, 68, 122, 144	0
8	i	37/38 (97%)	-0.18	1 (2%) 56 63	59, 70, 130, 139	0
9	J	38/39 (97%)	-0.18	0 100 100	59, 78, 130, 185	0
9	j	39/39 (100%)	0.07	0 100 100	67, 85, 134, 172	0
10	K	37/37 (100%)	-0.36	0 100 100	68, 75, 93, 103	0
10	k	37/37 (100%)	-0.21	0 100 100	72, 82, 101, 111	0
11	L	36/37 (97%)	-0.50	0 100 100	31, 52, 103, 152	1 (2%)
11	l	36/37 (97%)	-0.53	0 100 100	32, 54, 106, 151	1 (2%)
12	M	32/36 (88%)	-0.45	0 100 100	32, 55, 76, 144	1 (3%)
12	m	33/36 (91%)	-0.45	0 100 100	49, 55, 83, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.38	0 100 100	40, 70, 117, 175	4 (1%)
13	o	243/244 (99%)	-0.31	0 100 100	38, 71, 121, 168	2 (0%)
14	T	29/32 (90%)	-0.59	1 (3%) 48 55	49, 54, 84, 117	0
14	t	29/32 (90%)	-0.58	1 (3%) 48 55	49, 56, 86, 150	0
15	U	96/104 (92%)	-0.48	0 100 100	52, 66, 90, 101	0
15	u	97/104 (93%)	-0.48	0 100 100	58, 68, 86, 131	0
16	V	137/137 (100%)	-0.53	0 100 100	52, 64, 88, 113	0
16	v	137/137 (100%)	-0.39	0 100 100	59, 76, 106, 153	0
17	X	38/40 (95%)	-0.18	0 100 100	65, 79, 102, 123	0
17	x	38/40 (95%)	0.15	1 (2%) 57 63	70, 86, 123, 162	0
18	Y	29/30 (96%)	0.48	2 (6%) 23 26	76, 92, 127, 141	0
18	y	29/30 (96%)	0.27	0 100 100	85, 103, 127, 133	0
19	Z	62/62 (100%)	0.04	1 (1%) 70 76	75, 90, 138, 173	0
19	z	62/62 (100%)	0.41	2 (3%) 50 57	89, 104, 148, 194	0
20	R	34/34 (100%)	1.45	9 (26%) 1 1	103, 130, 154, 159	0
All	All	5283/5384 (98%)	-0.41	31 (0%) 85 89	31, 65, 107, 194	40 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	4.8
7	h	65	LEU	4.3
14	t	30	THR	3.4
20	R	24	LEU	3.1
2	B	494	GLY	3.1
14	T	30	THR	3.0
18	Y	19	ILE	2.9
8	i	37	LEU	2.8
2	b	502	VAL	2.7
20	R	34	LEU	2.6
6	f	16	PHE	2.6
2	b	504	THR	2.5
20	R	6	LEU	2.5
20	R	35	LEU	2.5
1	a	11	ALA	2.4
18	Y	20	ALA	2.4
2	b	495	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
20	R	7	VAL	2.4
20	R	28	VAL	2.4
19	z	3	ILE	2.3
5	e	79	PHE	2.3
2	B	495	PHE	2.3
1	A	11	ALA	2.3
19	z	30	PRO	2.2
6	f	15	ILE	2.2
2	b	499	VAL	2.2
20	R	9	LEU	2.1
19	Z	3	ILE	2.1
17	x	37	VAL	2.1
20	R	14	LEU	2.1
20	R	12	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.96	0.08	49,57,68,72	0
12	FME	m	1	10/11	0.96	0.08	59,67,83,96	0
8	FME	I	1	10/11	0.97	0.07	60,72,75,79	0
14	FME	T	1	10/11	0.97	0.07	53,59,69,70	0
12	FME	M	1	10/11	0.98	0.08	54,65,84,92	0
8	FME	i	1	10/11	0.98	0.05	60,70,79,79	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
34	HTG	c	522	19/19	0.74	0.13	122,143,151,152	0
32	LMT	e	102	35/35	0.75	0.16	132,156,166,171	0
30	UNL	J	101	10/-	0.76	0.19	85,93,100,106	0
32	LMT	A	359	35/35	0.76	0.16	85,123,132,134	0
32	LMT	a	414	35/35	0.77	0.15	77,121,131,134	0
34	HTG	C	522	19/19	0.77	0.13	112,128,136,139	0
32	LMT	a	420	35/35	0.77	0.16	124,142,152,152	0
30	UNL	I	102	40/-	0.78	0.17	83,112,137,141	0
26	SQD	f	102	43/54	0.78	0.15	121,146,161,163	0
30	UNL	a	417	30/-	0.78	0.16	105,118,135,144	0
30	UNL	i	101	40/-	0.78	0.15	91,109,147,151	0
30	UNL	A	415	28/-	0.78	0.17	101,116,129,137	0
30	UNL	K	101	34/-	0.79	0.15	98,118,130,146	0
37	LHG	e	101	42/49	0.79	0.13	108,140,159,166	0
30	UNL	j	101	10/-	0.80	0.15	92,102,116,117	0
32	LMT	E	102	35/35	0.80	0.15	118,142,160,165	0
32	LMT	I	101	35/35	0.80	0.15	112,139,150,154	0
30	UNL	c	525	32/-	0.81	0.15	99,116,133,137	0
30	UNL	m	102	10/-	0.81	0.14	70,81,92,93	0
33	LMG	C	521	51/55	0.81	0.14	91,116,139,141	0
32	LMT	b	621	25/35	0.82	0.14	105,119,144,144	0
34	HTG	D	414	16/19	0.82	0.13	93,117,129,133	0
30	UNL	b	626	33/-	0.83	0.14	88,107,143,146	0
33	LMG	c	521	51/55	0.83	0.12	103,127,143,146	0
34	HTG	d	411	16/19	0.83	0.14	112,133,141,153	0
36	CA	f	103	1/1	0.83	0.14	136,136,136,136	0
32	LMT	M	103	35/35	0.83	0.13	93,135,153,154	0
34	HTG	b	623	19/19	0.84	0.13	103,124,138,158	0
32	LMT	D	404	35/35	0.84	0.13	87,111,134,136	0
34	HTG	B	623	19/19	0.84	0.17	81,103,114,114	0
29	PL9	A	414	55/55	0.84	0.15	90,112,121,124	0
30	UNL	D	413	40/-	0.84	0.13	77,100,127,131	0
33	LMG	Z	101	37/55	0.86	0.14	94,122,137,139	0
27	GOL	v	201	6/6	0.86	0.13	77,89,97,99	0
30	UNL	B	627	33/-	0.86	0.13	76,108,140,145	0
36	CA	F	102	1/1	0.86	0.18	147,147,147,147	0
29	PL9	a	416	55/55	0.86	0.14	104,118,129,130	0
30	UNL	M	102	10/-	0.86	0.10	72,78,87,88	0
33	LMG	z	101	39/55	0.87	0.13	102,127,141,143	0
30	UNL	d	410	36/-	0.87	0.12	84,104,130,135	0
27	GOL	b	624	6/6	0.87	0.12	93,100,106,108	0
26	SQD	a	413	54/54	0.87	0.11	82,98,124,129	0
32	LMT	b	627	25/35	0.87	0.12	68,90,129,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	HTG	B	622	19/19	0.88	0.13	81,91,122,125	0
26	SQD	F	101	43/54	0.88	0.11	91,107,124,129	0
32	LMT	t	101	25/35	0.89	0.12	80,99,127,128	0
32	LMT	t	102	26/35	0.89	0.11	85,105,128,129	0
26	SQD	b	620	54/54	0.89	0.11	78,97,128,130	0
26	SQD	A	412	54/54	0.89	0.10	72,92,109,117	0
26	SQD	B	620	54/54	0.89	0.11	81,100,120,129	0
37	LHG	E	101	42/49	0.89	0.11	95,119,132,134	0
34	HTG	b	622	19/19	0.89	0.12	71,90,118,119	0
27	GOL	a	412	6/6	0.90	0.10	82,88,94,97	0
27	GOL	A	411	6/6	0.90	0.13	79,87,89,100	0
27	GOL	B	625	6/6	0.90	0.15	65,82,86,93	0
34	HTG	V	203	11/19	0.90	0.11	103,119,123,128	0
23	CLA	B	601	65/65	0.91	0.10	69,81,102,119	0
33	LMG	C	501	51/55	0.91	0.11	79,98,110,117	0
33	LMG	C	520	51/55	0.91	0.09	74,94,110,120	0
32	LMT	M	101	35/35	0.91	0.10	69,95,111,113	0
32	LMT	m	103	35/35	0.91	0.11	73,95,108,111	0
33	LMG	c	520	51/55	0.91	0.09	85,101,121,129	0
27	GOL	c	501	6/6	0.91	0.16	73,74,77,78	0
30	UNL	D	412	17/-	0.92	0.09	70,84,100,106	0
33	LMG	a	419	51/55	0.92	0.09	85,100,111,117	0
27	GOL	a	418	6/6	0.92	0.20	65,79,86,90	0
23	CLA	C	514	65/65	0.92	0.09	72,85,107,112	0
23	CLA	b	601	65/65	0.92	0.10	76,88,109,125	0
23	CLA	c	514	65/65	0.92	0.10	83,97,115,122	0
23	CLA	C	507	65/65	0.93	0.09	61,75,112,117	0
23	CLA	c	513	65/65	0.93	0.08	71,87,107,113	0
33	LMG	D	415	51/55	0.93	0.09	62,75,104,108	0
25	BCR	h	101	40/40	0.94	0.08	65,75,84,85	0
23	CLA	b	616	65/65	0.94	0.09	58,67,97,103	0
23	CLA	c	505	65/65	0.94	0.09	63,71,94,111	0
23	CLA	B	616	65/65	0.94	0.11	53,63,108,111	0
33	LMG	B	621	51/55	0.94	0.09	69,78,97,108	0
34	HTG	b	625	19/19	0.94	0.09	79,86,107,111	0
33	LMG	d	412	51/55	0.94	0.09	69,77,107,115	0
33	LMG	m	101	51/55	0.94	0.09	65,77,96,113	0
26	SQD	a	411	54/54	0.94	0.09	79,90,116,119	0
23	CLA	C	513	65/65	0.94	0.08	71,80,101,108	0
25	BCR	D	407	40/40	0.94	0.08	59,68,91,92	0
37	LHG	d	408	49/49	0.94	0.09	64,72,102,105	0
34	HTG	B	626	19/19	0.94	0.08	78,85,96,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	HEM	E	103	43/43	0.94	0.08	65,73,87,116	0
27	GOL	V	201	6/6	0.95	0.11	64,71,83,87	0
23	CLA	A	408	65/65	0.95	0.08	51,59,101,112	0
30	UNL	x	101	18/-	0.95	0.11	82,91,108,111	0
23	CLA	d	403	65/65	0.95	0.08	58,71,98,106	0
25	BCR	C	515	40/40	0.95	0.08	74,79,87,92	0
23	CLA	D	406	65/65	0.95	0.09	55,65,105,108	0
25	BCR	T	101	40/40	0.95	0.06	52,62,69,72	0
25	BCR	d	404	40/40	0.95	0.08	67,78,91,92	0
23	CLA	a	407	65/65	0.95	0.08	52,59,102,109	0
25	BCR	t	103	40/40	0.95	0.07	54,64,79,80	0
25	BCR	y	101	40/40	0.95	0.08	72,79,88,91	0
26	SQD	A	410	54/54	0.95	0.08	70,87,106,114	0
23	CLA	a	409	65/65	0.95	0.09	53,62,108,115	0
23	CLA	C	505	65/65	0.95	0.07	55,63,88,103	0
23	CLA	b	606	65/65	0.95	0.08	55,65,89,102	0
23	CLA	b	614	65/65	0.95	0.07	49,58,92,99	0
23	CLA	B	606	65/65	0.95	0.08	51,59,90,98	0
35	DGD	C	517	62/66	0.95	0.08	55,65,89,93	0
35	DGD	C	518	62/66	0.95	0.08	60,71,105,112	0
35	DGD	c	517	62/66	0.95	0.07	62,69,85,94	0
35	DGD	c	518	62/66	0.95	0.08	64,76,106,114	0
30	UNL	X	101	18/-	0.95	0.09	72,79,98,98	0
36	CA	O	301	1/1	0.95	0.06	121,121,121,121	0
23	CLA	C	509	65/65	0.95	0.08	54,63,97,106	0
37	LHG	D	411	49/49	0.95	0.09	60,67,105,110	0
23	CLA	c	507	65/65	0.95	0.08	71,81,103,112	0
37	LHG	d	406	49/49	0.95	0.08	60,71,88,100	0
23	CLA	c	509	65/65	0.95	0.08	57,69,106,115	0
23	CLA	B	614	65/65	0.95	0.08	48,54,87,95	0
27	GOL	C	523	6/6	0.95	0.10	63,67,73,76	0
23	CLA	A	406	65/65	0.96	0.07	47,54,92,96	0
30	UNL	d	409	17/-	0.96	0.07	78,88,109,111	0
23	CLA	b	607	65/65	0.96	0.07	47,55,76,83	0
25	BCR	A	409	40/40	0.96	0.06	48,55,62,65	0
27	GOL	B	624	6/6	0.96	0.09	85,88,93,95	0
25	BCR	B	618	40/40	0.96	0.06	53,61,74,81	0
25	BCR	B	619	40/40	0.96	0.06	56,64,78,81	0
31	BCT	a	404	4/4	0.96	0.08	59,65,66,76	0
23	CLA	b	609	65/65	0.96	0.07	61,68,82,98	0
23	CLA	C	506	65/65	0.96	0.07	55,63,81,93	0
25	BCR	H	101	40/40	0.96	0.07	58,69,79,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	BCR	K	102	40/40	0.96	0.07	64,72,81,83	0
23	CLA	b	615	65/65	0.96	0.06	56,64,74,80	0
25	BCR	Y	101	40/40	0.96	0.07	67,75,80,82	0
25	BCR	b	618	40/40	0.96	0.06	53,62,71,76	0
29	PL9	D	408	55/55	0.96	0.06	47,55,61,73	0
25	BCR	c	515	40/40	0.96	0.08	86,93,98,101	0
29	PL9	d	405	55/55	0.96	0.07	51,58,66,90	0
35	DGD	C	519	62/66	0.96	0.08	57,66,90,97	0
35	DGD	H	102	62/66	0.96	0.07	59,68,77,78	0
23	CLA	B	602	65/65	0.96	0.07	55,60,76,82	0
23	CLA	c	504	65/65	0.96	0.07	65,72,82,97	0
35	DGD	c	519	62/66	0.96	0.07	64,74,94,102	0
25	BCR	k	101	40/40	0.96	0.07	71,80,90,95	0
23	CLA	B	604	65/65	0.96	0.07	44,53,90,103	0
36	CA	c	523	1/1	0.96	0.11	84,84,84,84	0
23	CLA	c	506	65/65	0.96	0.07	58,69,85,91	0
36	CA	o	301	1/1	0.96	0.05	107,107,107,107	0
37	LHG	D	409	49/49	0.96	0.07	58,69,84,96	0
23	CLA	C	504	65/65	0.96	0.07	58,65,74,84	0
23	CLA	c	508	65/65	0.96	0.08	64,75,83,90	0
23	CLA	b	602	65/65	0.96	0.07	59,66,79,89	0
23	CLA	c	510	65/65	0.96	0.07	61,73,84,92	0
23	CLA	c	512	65/65	0.96	0.08	67,78,91,94	0
37	LHG	l	101	49/49	0.96	0.07	55,65,77,87	0
23	CLA	b	604	65/65	0.96	0.07	49,56,91,101	0
38	HEM	e	87	43/43	0.96	0.09	80,94,117,126	0
23	CLA	B	605	65/65	0.97	0.06	47,54,63,69	0
23	CLA	A	404	65/65	0.97	0.06	43,50,60,70	0
23	CLA	b	608	65/65	0.97	0.05	57,64,79,88	0
23	CLA	B	607	65/65	0.97	0.06	44,52,69,76	0
25	BCR	a	410	40/40	0.97	0.06	51,59,65,67	0
25	BCR	b	617	40/40	0.97	0.06	51,58,65,67	0
23	CLA	b	610	65/65	0.97	0.07	57,64,73,78	0
25	BCR	b	619	40/40	0.97	0.06	56,67,80,82	0
23	CLA	b	611	65/65	0.97	0.06	52,58,68,75	0
25	BCR	c	516	40/40	0.97	0.07	66,74,81,85	0
23	CLA	b	612	65/65	0.97	0.06	53,60,66,77	0
23	CLA	b	613	65/65	0.97	0.06	48,55,84,89	0
23	CLA	B	609	65/65	0.97	0.07	58,64,70,74	0
23	CLA	C	508	65/65	0.97	0.07	59,66,77,79	0
23	CLA	B	610	65/65	0.97	0.07	52,59,69,75	0
23	CLA	c	502	65/65	0.97	0.06	64,72,80,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	c	503	65/65	0.97	0.07	59,69,79,81	0
23	CLA	C	510	65/65	0.97	0.07	57,67,80,86	0
23	CLA	C	511	65/65	0.97	0.07	58,67,77,87	0
23	CLA	C	512	65/65	0.97	0.07	60,73,82,88	0
23	CLA	B	611	65/65	0.97	0.06	46,52,63,68	0
23	CLA	B	612	65/65	0.97	0.06	47,54,61,67	0
23	CLA	D	405	65/65	0.97	0.06	43,50,66,81	0
23	CLA	B	613	65/65	0.97	0.06	47,54,80,87	0
35	DGD	h	102	62/66	0.97	0.07	62,72,79,84	0
23	CLA	c	511	65/65	0.97	0.06	62,71,80,84	0
23	CLA	a	405	65/65	0.97	0.06	48,54,64,81	0
23	CLA	a	406	65/65	0.97	0.05	48,52,63,71	0
23	CLA	B	603	65/65	0.97	0.06	50,58,69,75	0
23	CLA	B	615	65/65	0.97	0.06	48,58,74,77	0
24	PHO	A	353	64/64	0.97	0.06	47,56,61,64	0
37	LHG	D	410	49/49	0.97	0.07	55,61,74,84	0
24	PHO	a	353	64/64	0.97	0.06	53,60,65,67	0
22	CL	a	403	1/1	0.97	0.08	58,58,58,58	0
37	LHG	L	101	49/49	0.97	0.07	55,63,69,84	0
25	BCR	B	617	40/40	0.97	0.05	51,56,63,64	0
37	LHG	d	407	49/49	0.97	0.07	55,62,72,80	0
23	CLA	C	502	65/65	0.97	0.06	56,65,71,76	0
23	CLA	b	603	65/65	0.97	0.06	52,62,78,88	0
23	CLA	C	503	65/65	0.97	0.07	54,62,73,86	0
25	BCR	C	516	40/40	0.97	0.07	59,69,76,80	0
23	CLA	b	605	65/65	0.97	0.06	51,57,70,72	0
23	CLA	A	405	65/65	0.98	0.05	44,51,59,60	0
24	PHO	A	407	64/64	0.98	0.05	46,51,56,59	0
31	BCT	A	348	4/4	0.98	0.05	60,62,64,69	0
23	CLA	B	608	65/65	0.98	0.05	51,59,69,72	0
24	PHO	a	408	64/64	0.98	0.05	49,55,60,66	0
23	CLA	d	402	65/65	0.98	0.06	48,55,66,78	0
39	MG	J	102	1/1	0.98	0.07	64,64,64,64	0
40	HEC	V	202	43/43	0.98	0.06	50,60,63,64	0
40	HEC	v	202	43/43	0.98	0.06	61,70,75,79	0
36	CA	c	524	1/1	0.99	0.03	93,93,93,93	0
22	CL	A	402	1/1	0.99	0.03	51,51,51,51	0
22	CL	A	403	1/1	0.99	0.05	52,52,52,52	0
22	CL	a	402	1/1	0.99	0.02	56,56,56,56	0
28	OEX	A	413	10/10	0.99	0.05	56,57,57,57	0
36	CA	C	524	1/1	0.99	0.09	81,81,81,81	0
28	OEX	a	415	10/10	0.99	0.04	58,62,66,67	0

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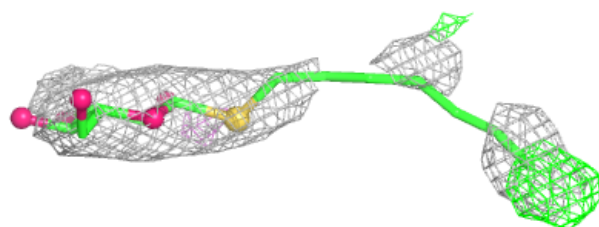
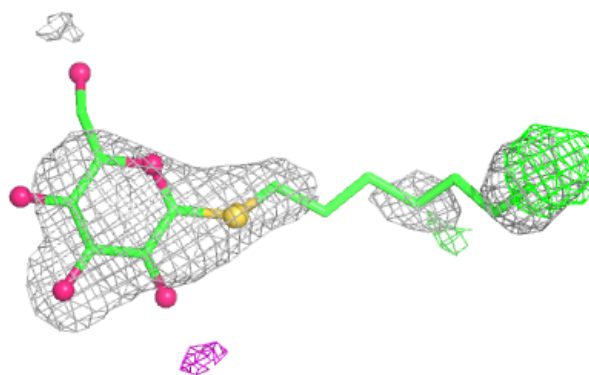
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
39	MG	j	102	1/1	0.99	0.04	70,70,70,70	0
21	FE2	A	401	1/1	0.99	0.03	64,64,64,64	0
21	FE2	a	401	1/1	0.99	0.04	67,67,67,67	0

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.

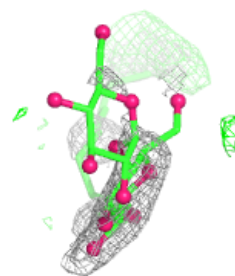
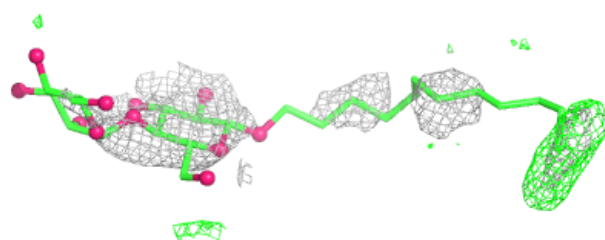
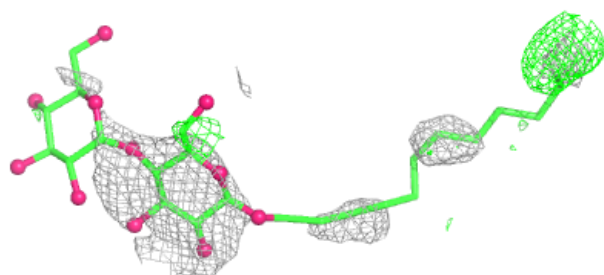
Electron density around HTG c 522:

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

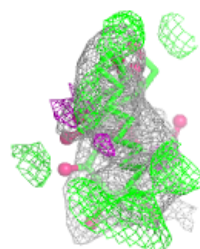
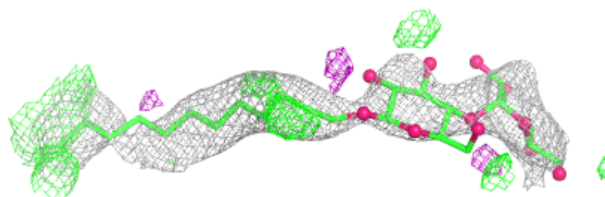
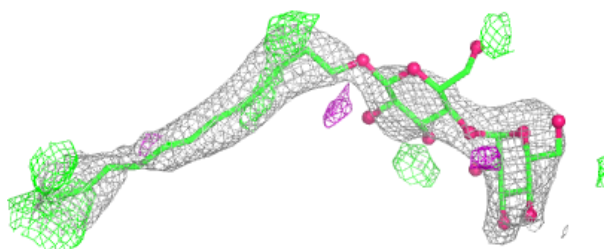


Electron density around LMT e 102:

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

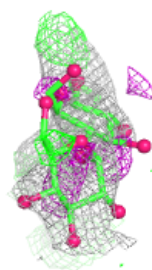
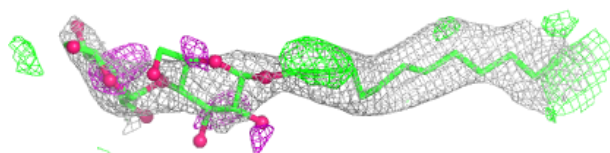
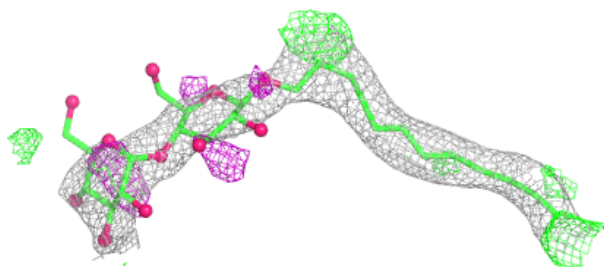
**Electron density around LMT A 359:**

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

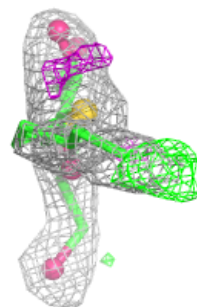
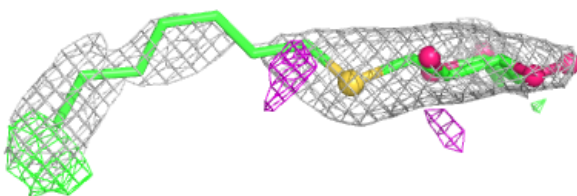
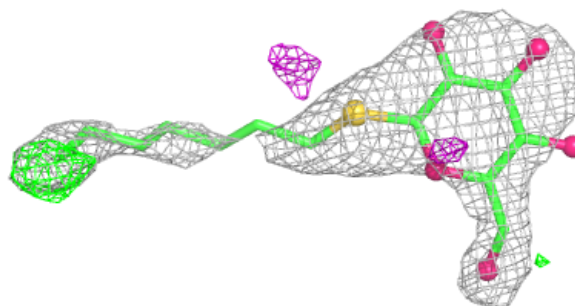


Electron density around LMT a 414:

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

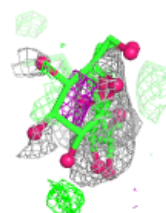
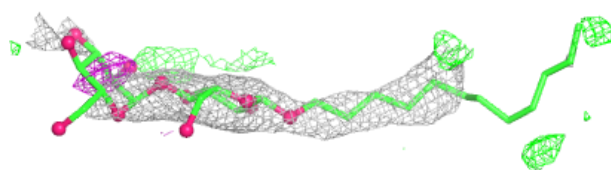
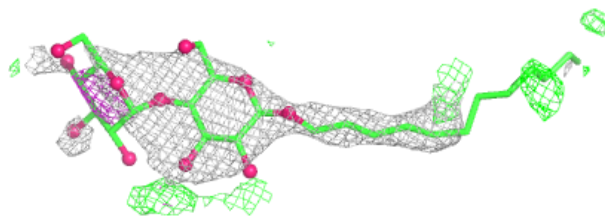
**Electron density around HTG C 522:**

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

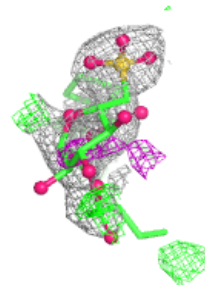
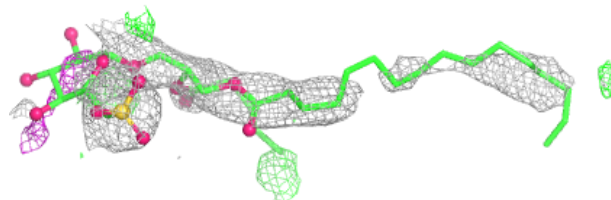
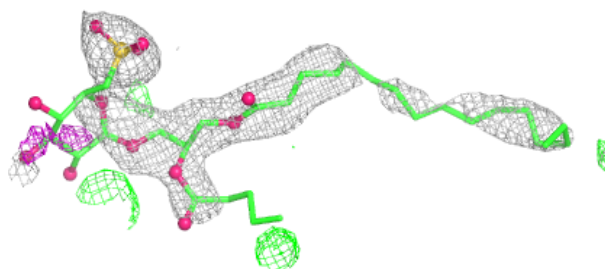


Electron density around LMT a 420:

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

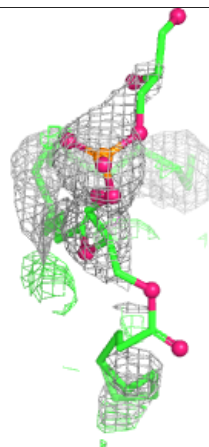
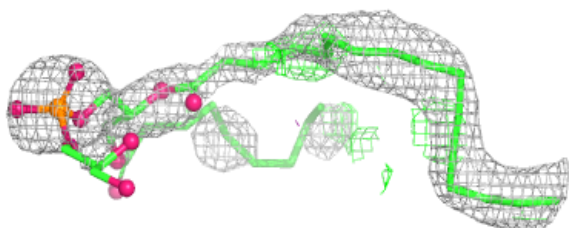
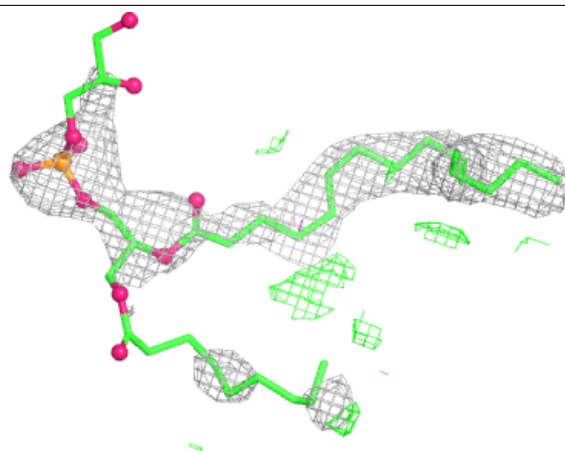
**Electron density around SQD f 102:**

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



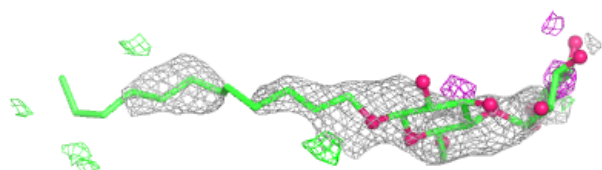
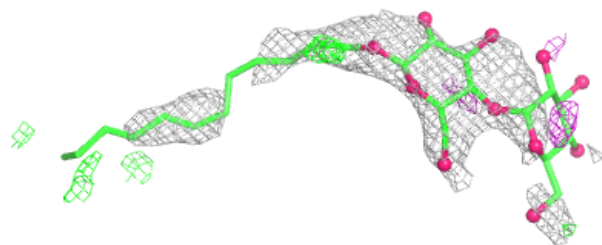
Electron density around LHG e 101:

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

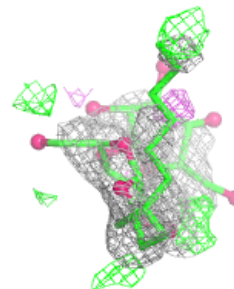
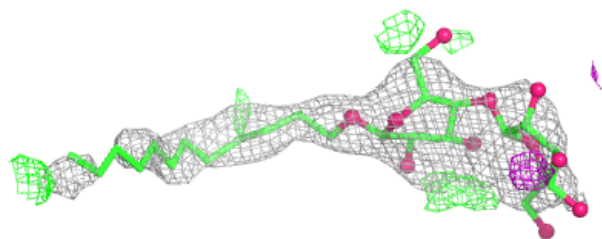
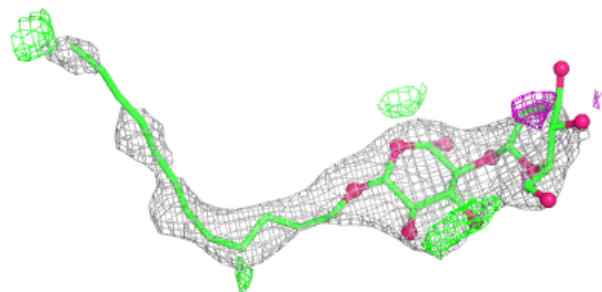


Electron density around LMT E 102:

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

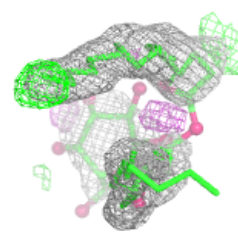
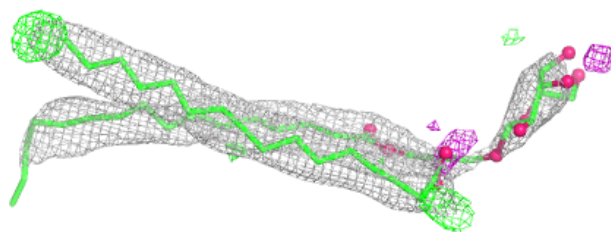
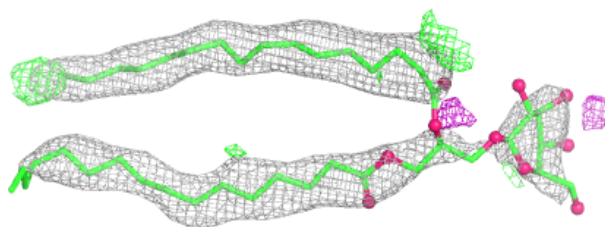
**Electron density around LMT I 101:**

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

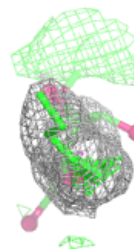
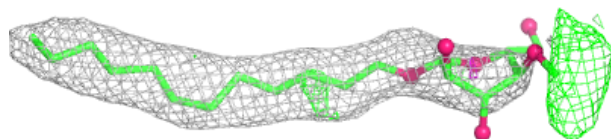
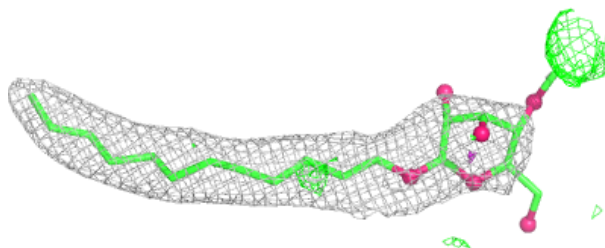


Electron density around LMG C 521:

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

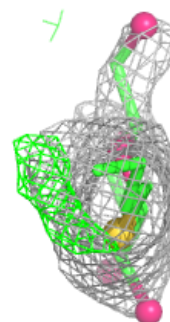
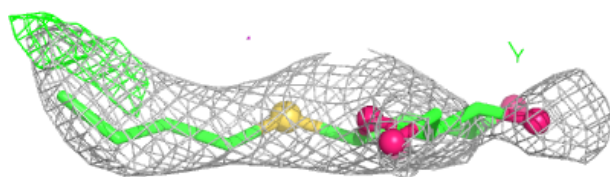
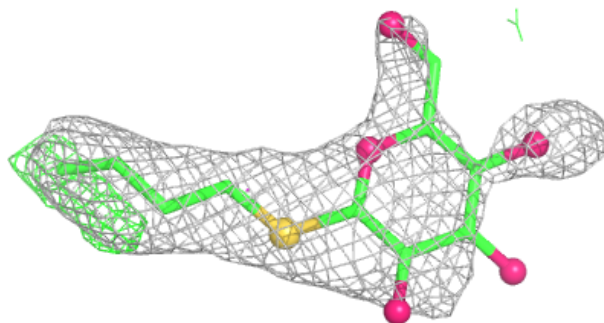
**Electron density around LMT b 621:**

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

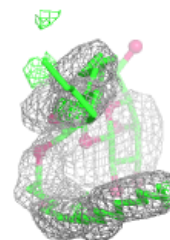
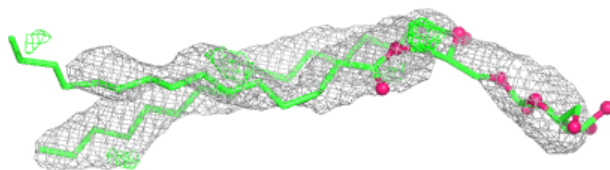
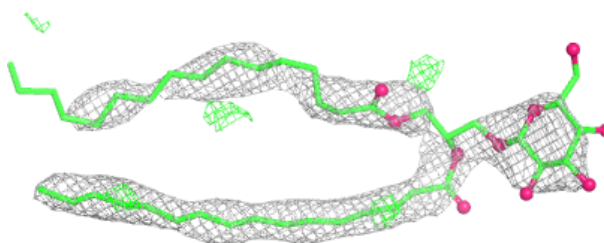


Electron density around HTG D 414:

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

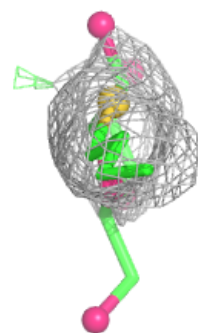
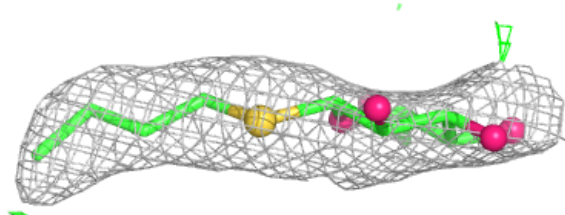
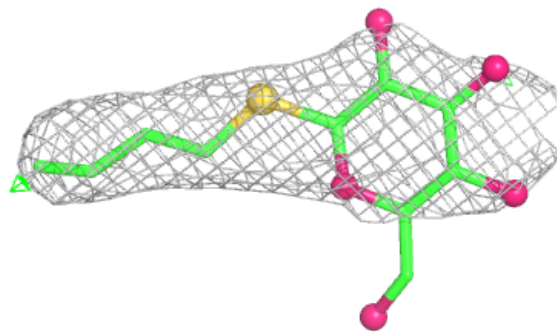
**Electron density around LMG c 521:**

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

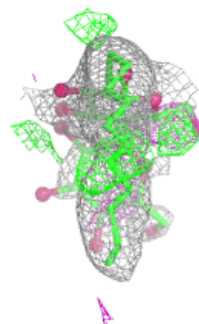
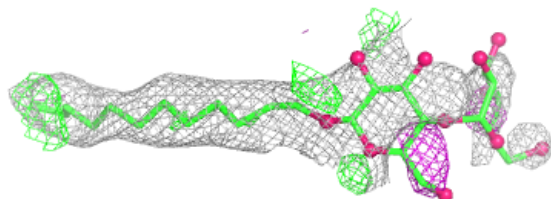
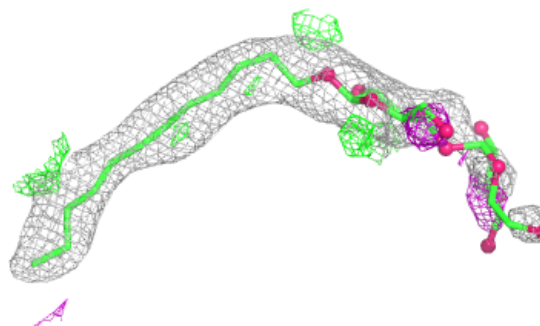


Electron density around HTG d 411:

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

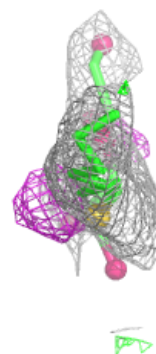
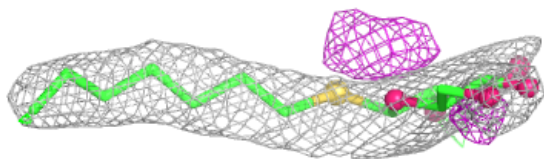
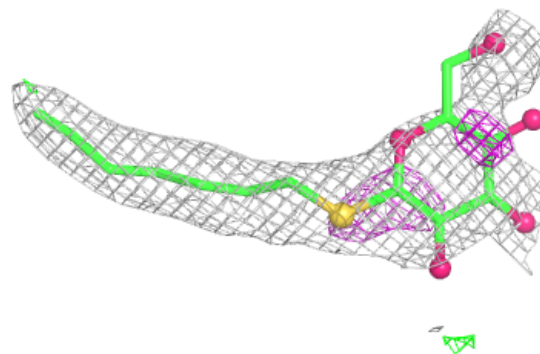
**Electron density around LMT M 103:**

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

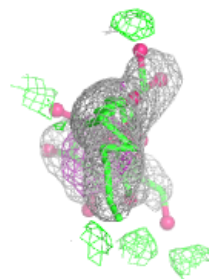
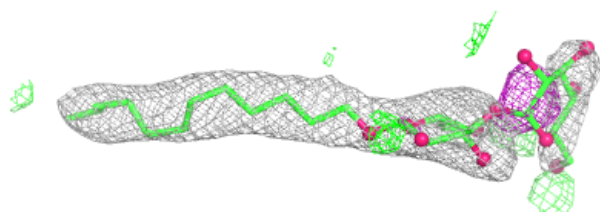
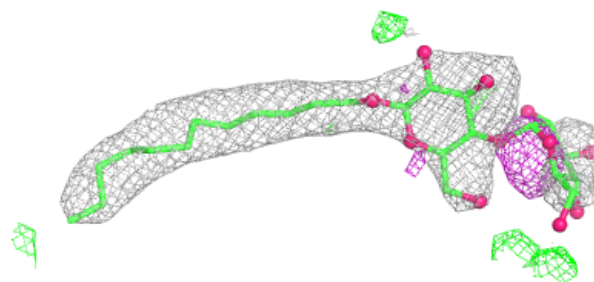


Electron density around HTG b 623:

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

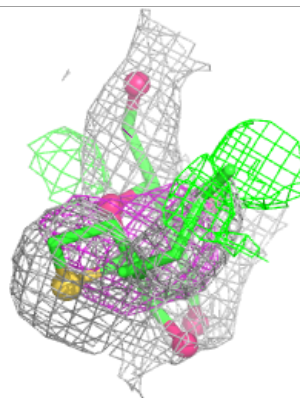
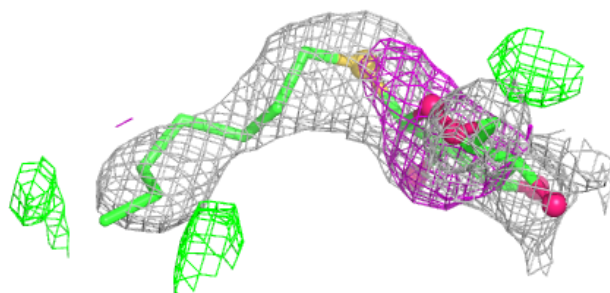
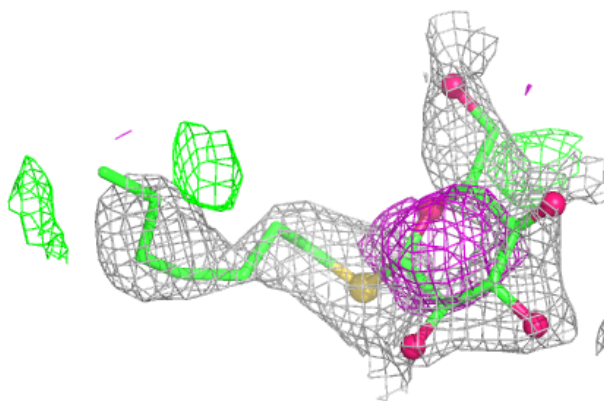
**Electron density around LMT D 404:**

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

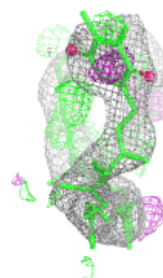
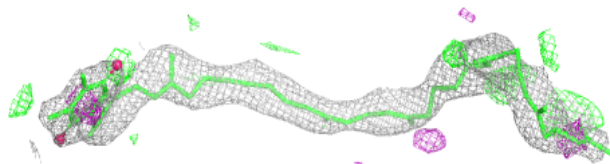
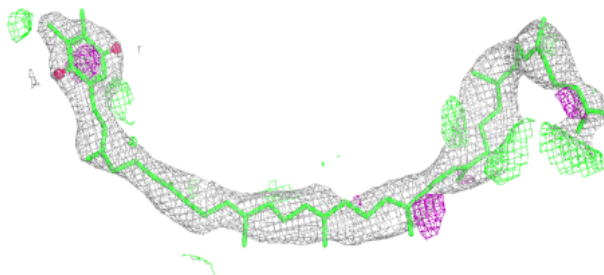


Electron density around HTG B 623:

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

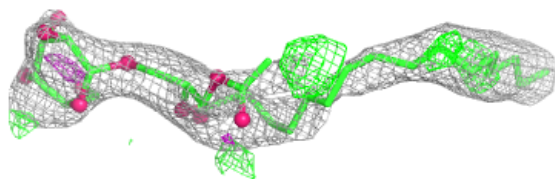
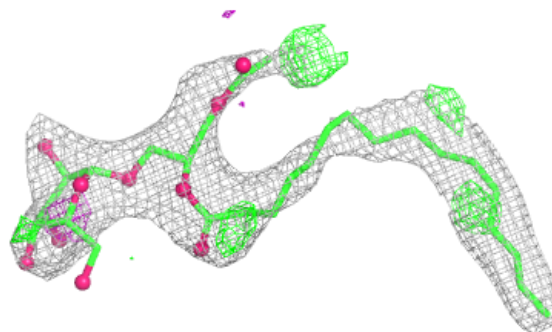
**Electron density around PL9 A 414:**

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

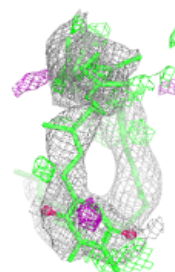
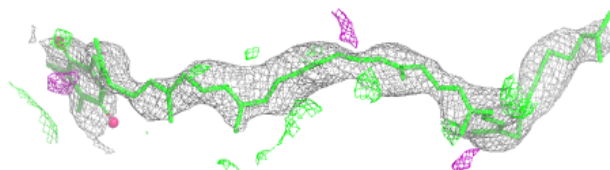
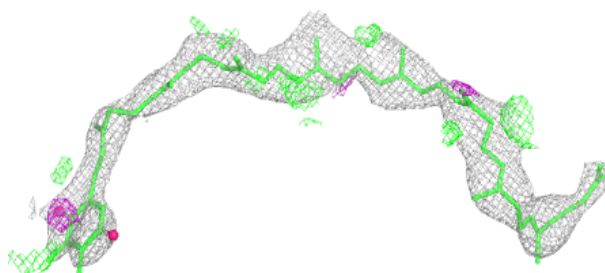


Electron density around LMG Z 101:

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

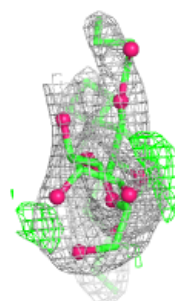
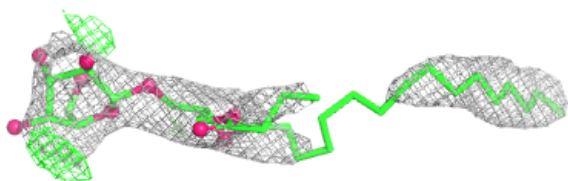
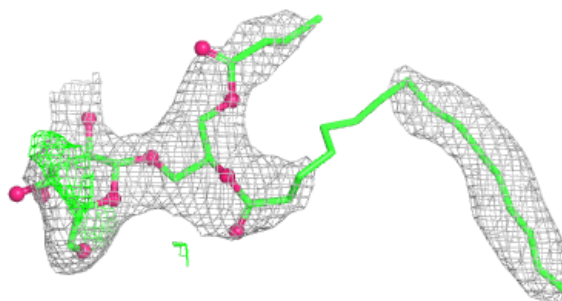
**Electron density around PL9 a 416:**

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

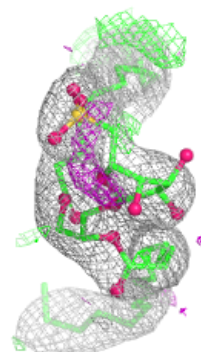
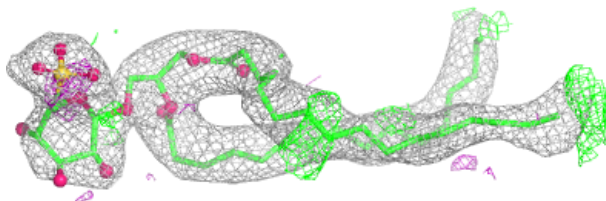
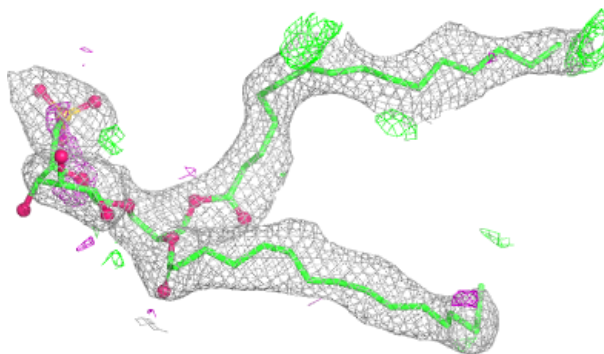


Electron density around LMG z 101:

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

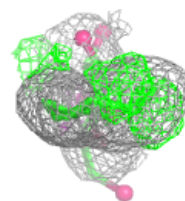
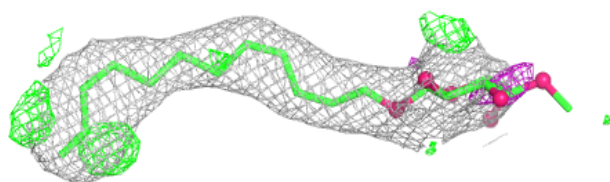
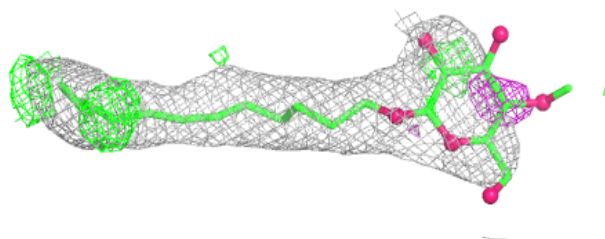
**Electron density around SQD a 413:**

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

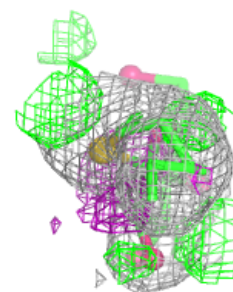
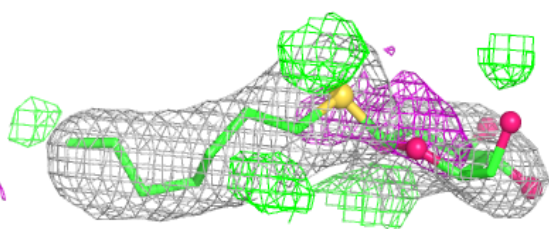
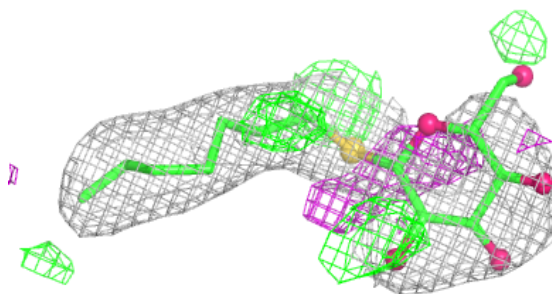


Electron density around LMT b 627:

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

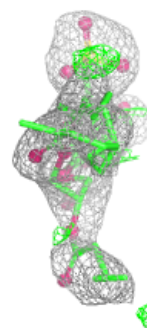
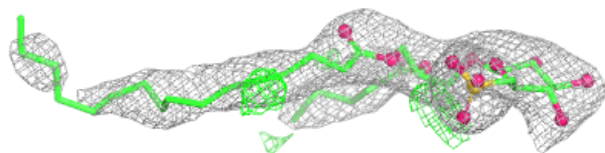
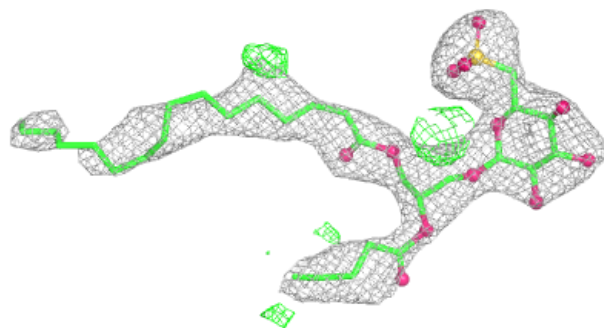
**Electron density around HTG B 622:**

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

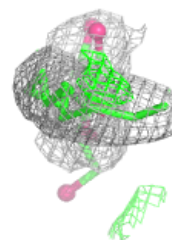
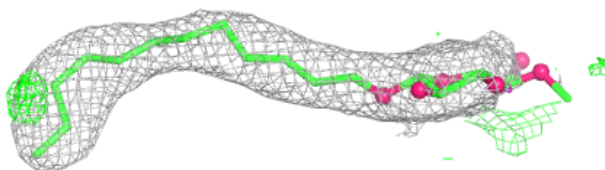
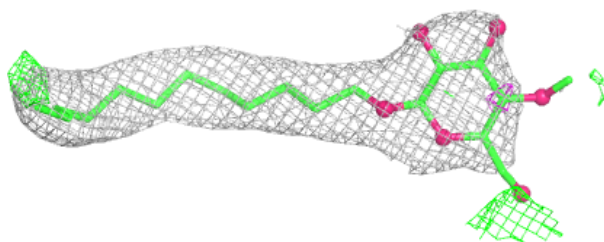


Electron density around SQD F 101:

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

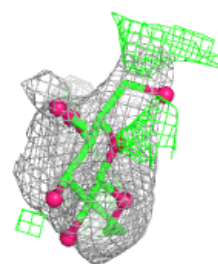
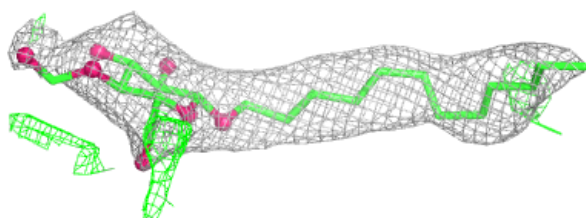
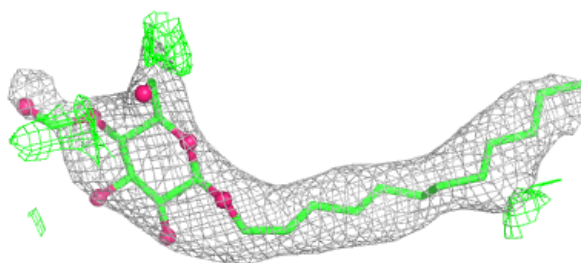
**Electron density around LMT t 101:**

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

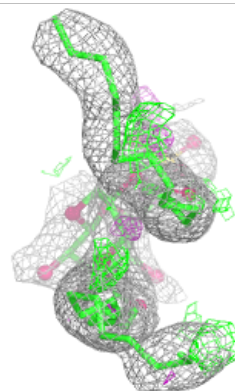
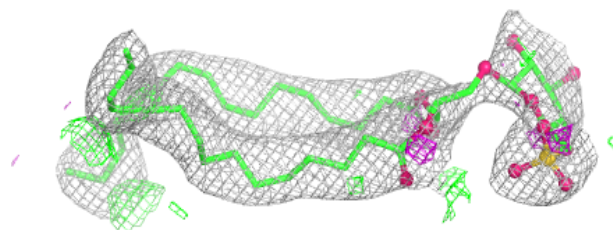
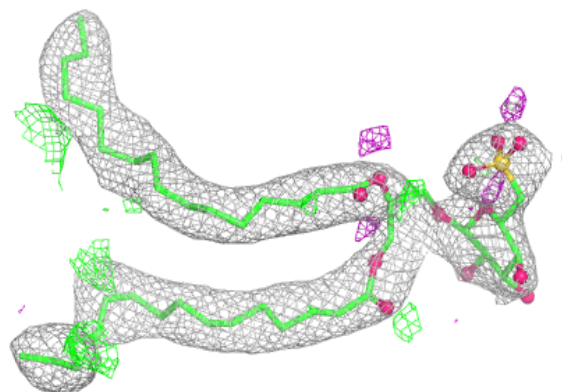


Electron density around LMT t 102:

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

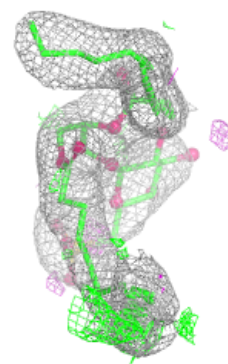
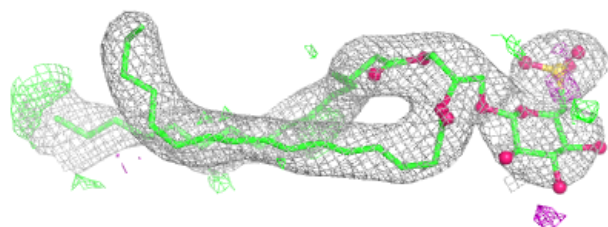
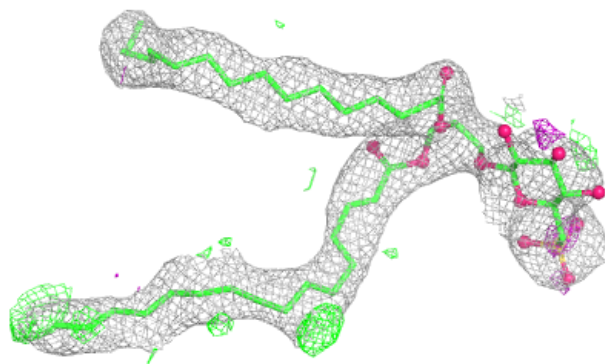
**Electron density around SQD b 620:**

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

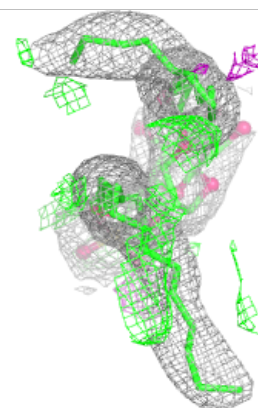
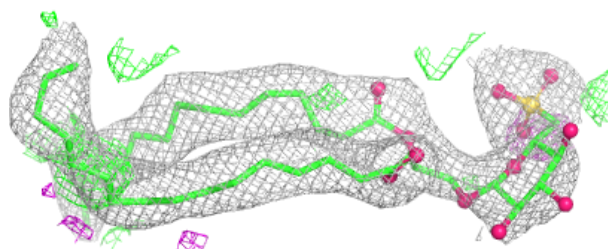
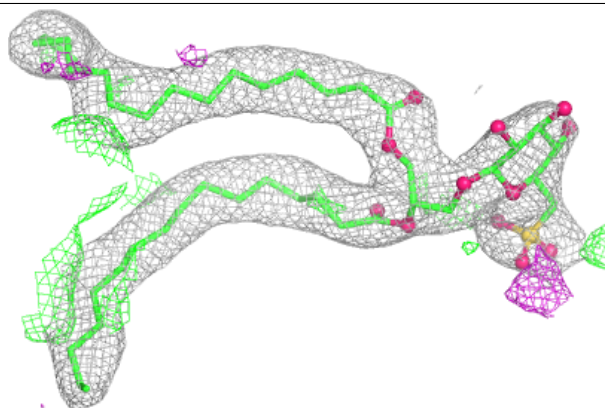


Electron density around SQD A 412:

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

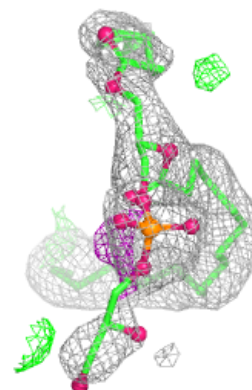
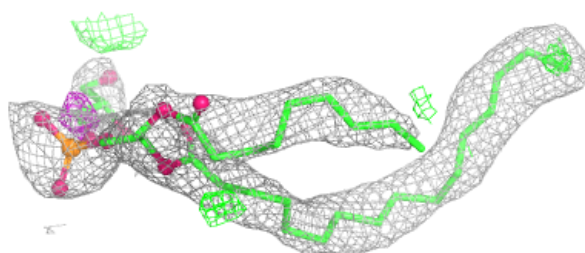
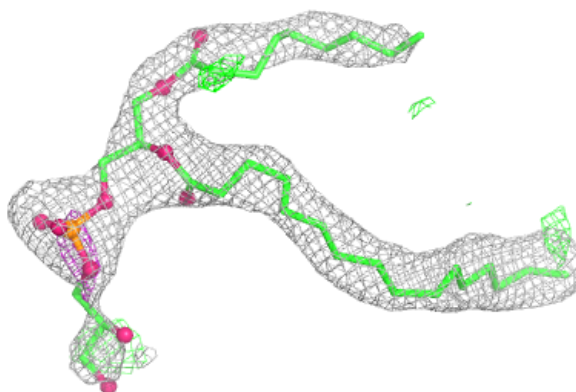
**Electron density around SQD B 620:**

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

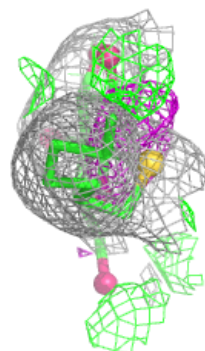
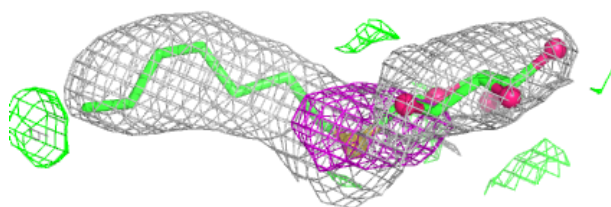
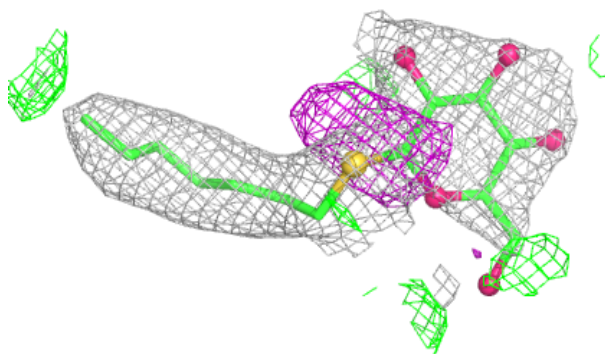


Electron density around LHG E 101:

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

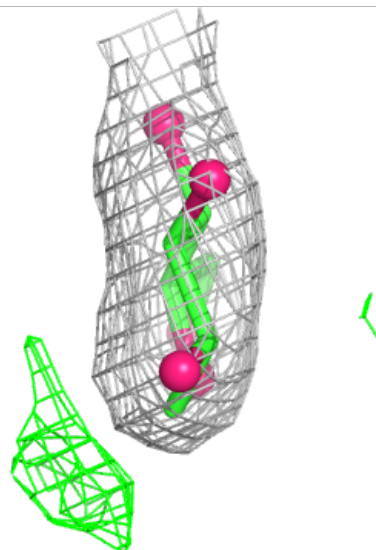
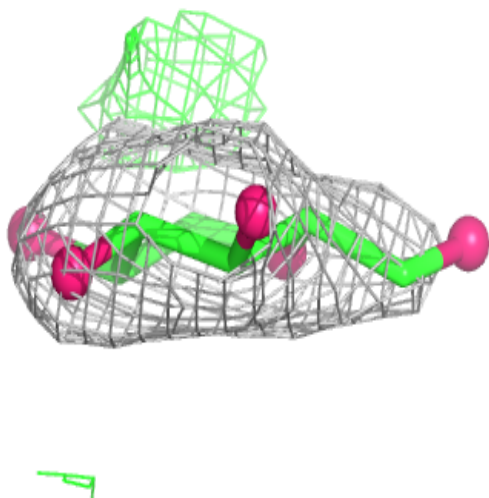
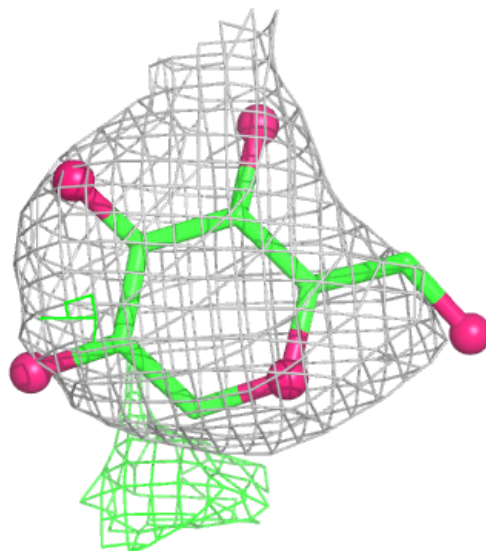
**Electron density around HTG b 622:**

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



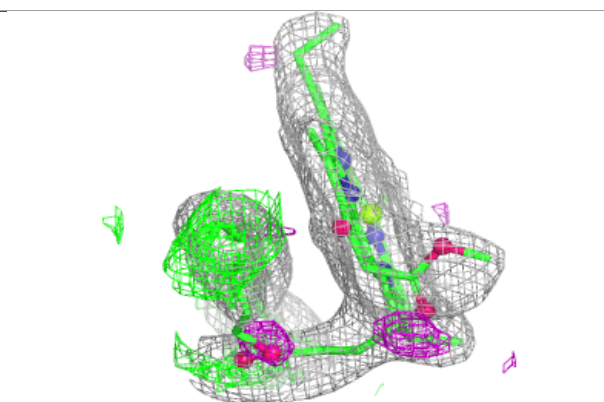
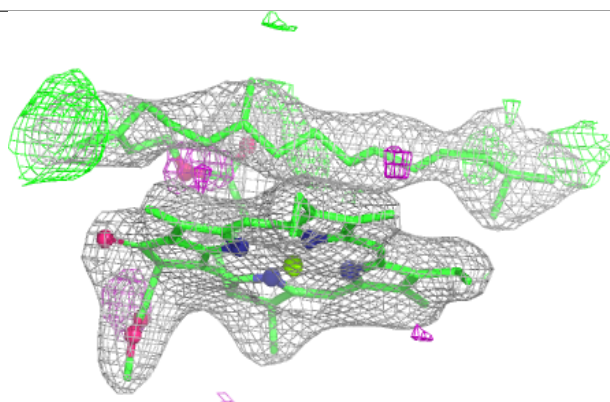
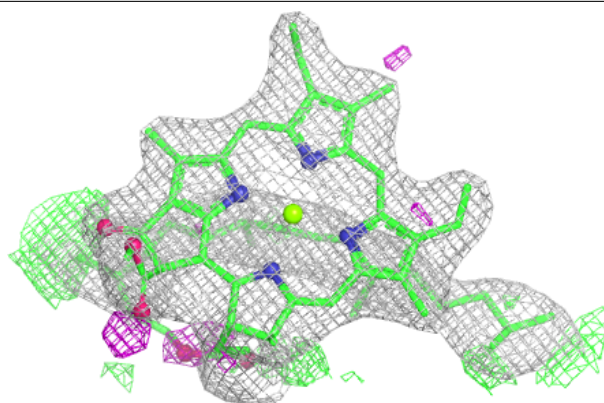
Electron density around HTG V 203:

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

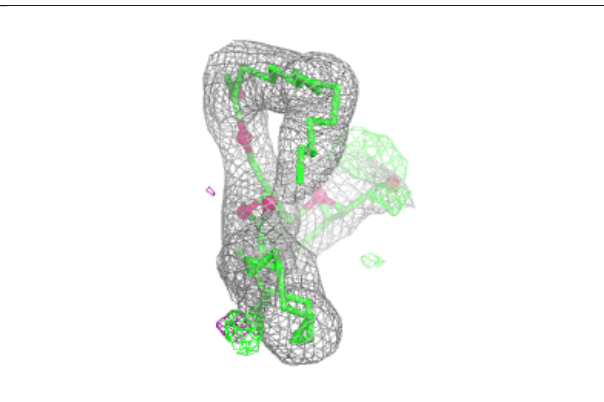
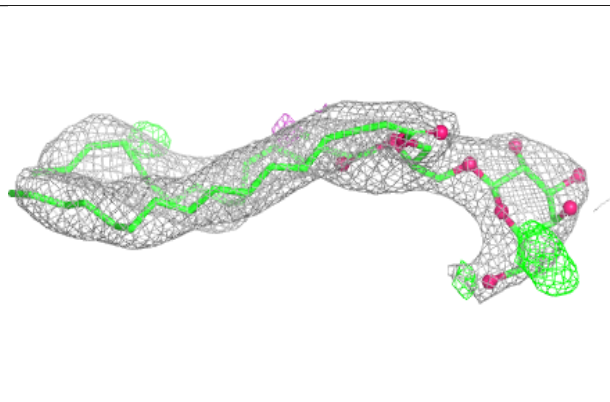
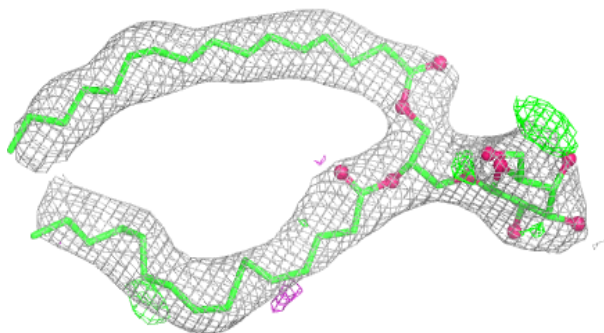


Electron density around CLA B 601:

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

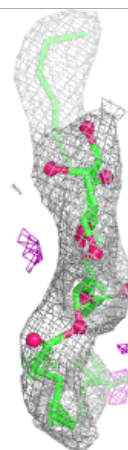
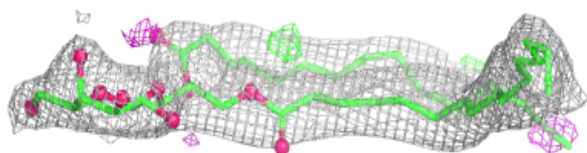
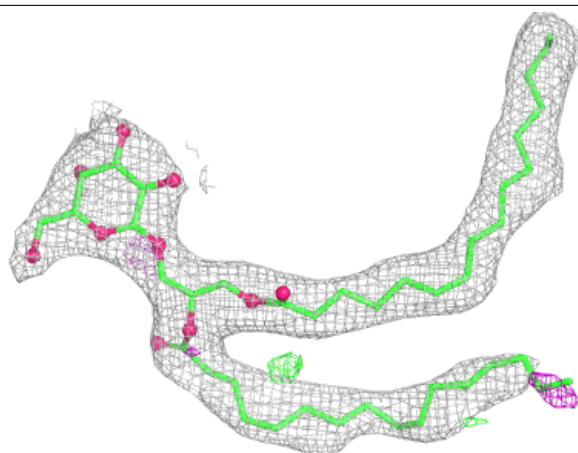
**Electron density around LMG C 501:**

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



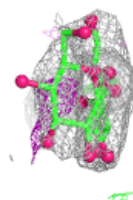
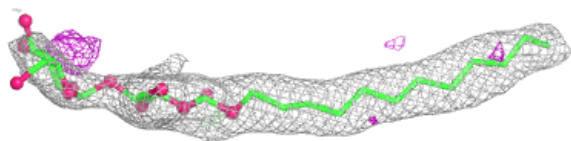
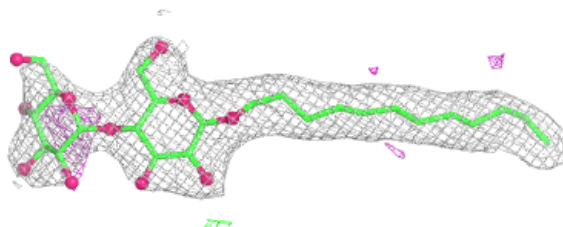
Electron density around LMG C 520:

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

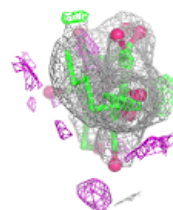
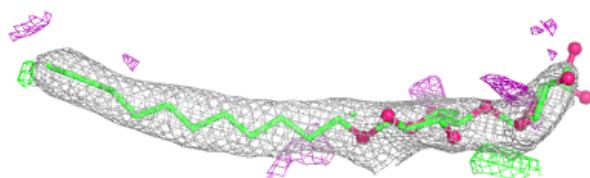
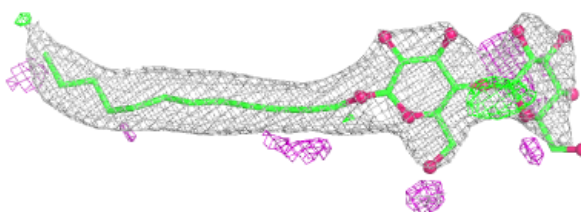


Electron density around LMT M 101:

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

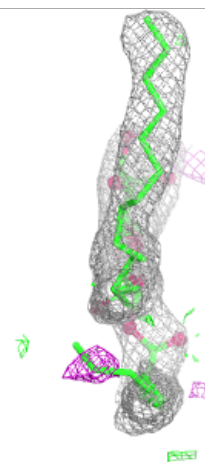
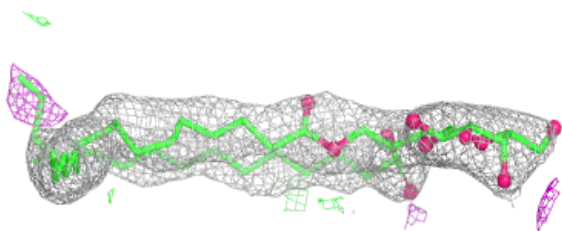
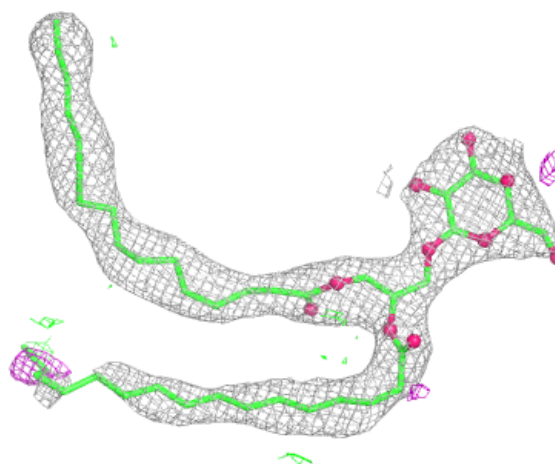
**Electron density around LMT m 103:**

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



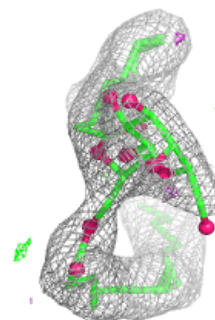
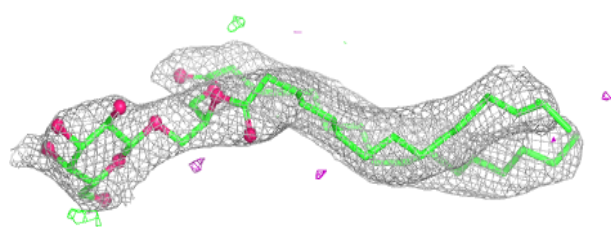
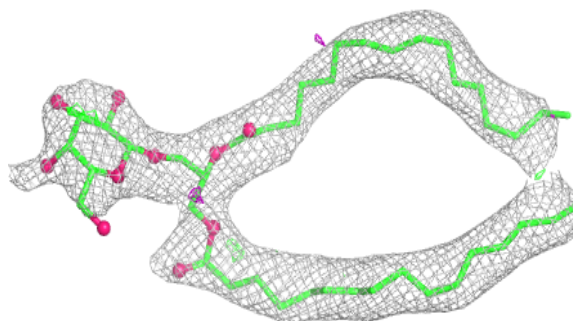
Electron density around LMG c 520:

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

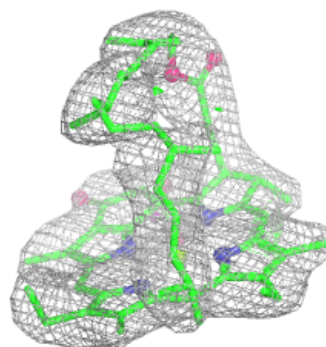
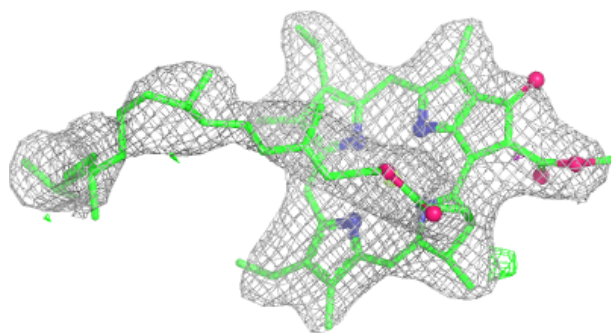
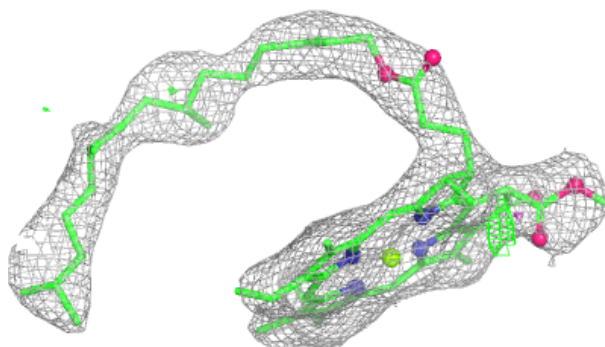


Electron density around LMG a 419:

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

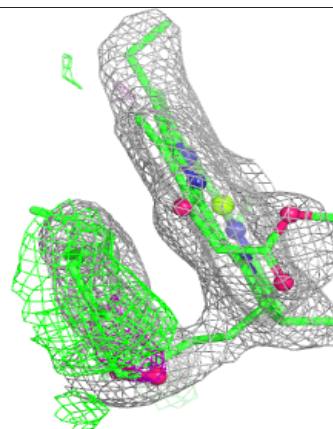
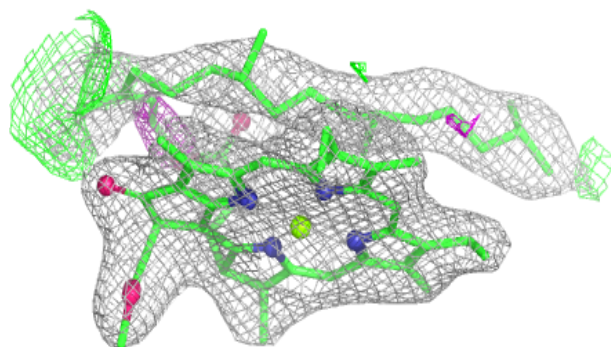
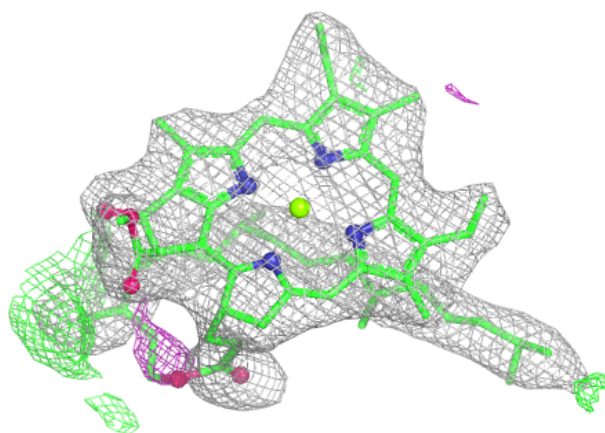
**Electron density around CLA C 514:**

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

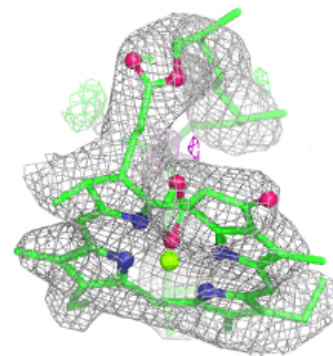
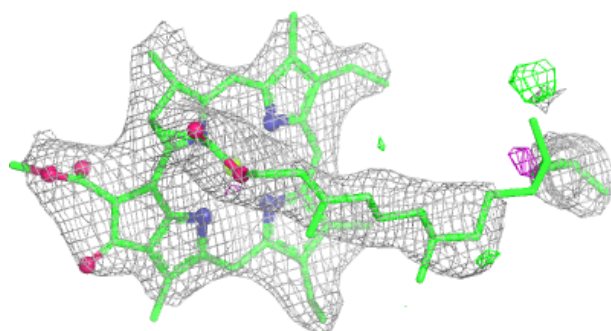
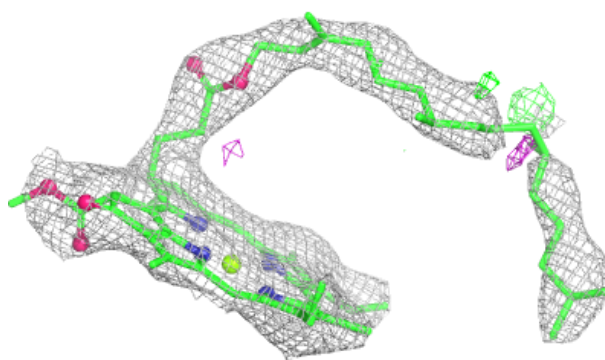


Electron density around CLA b 601:

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

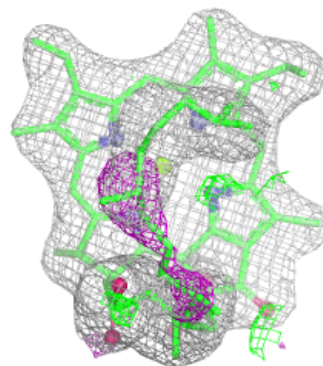
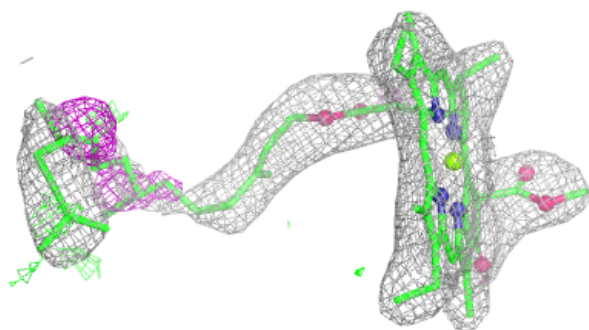
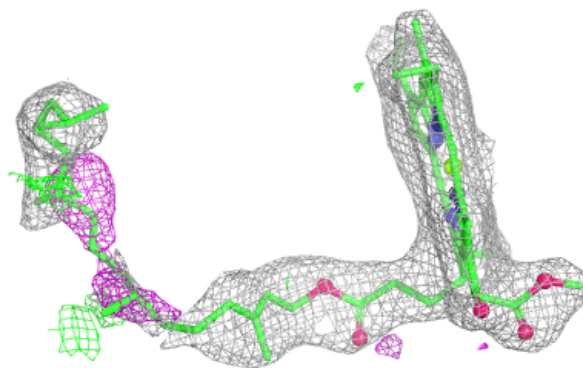
**Electron density around CLA c 514:**

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



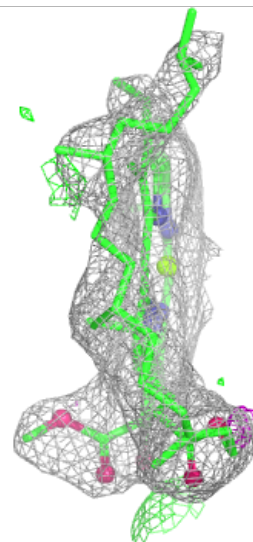
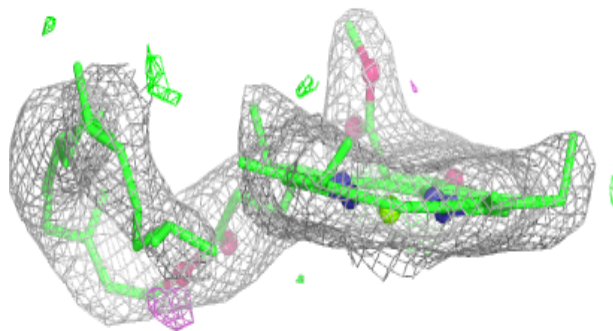
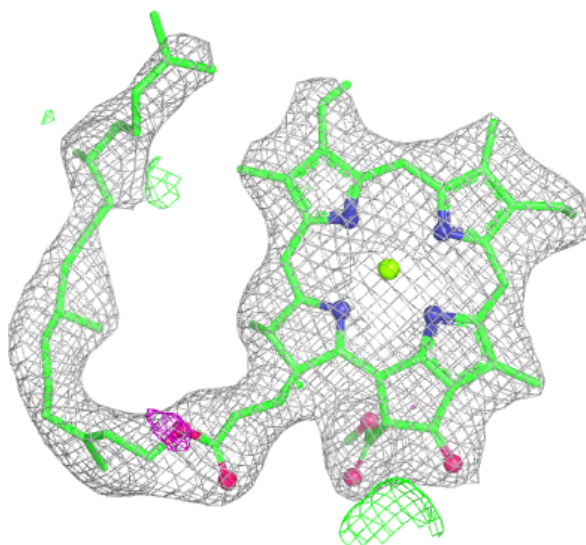
Electron density around CLA C 507:

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



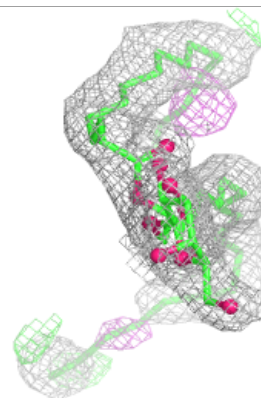
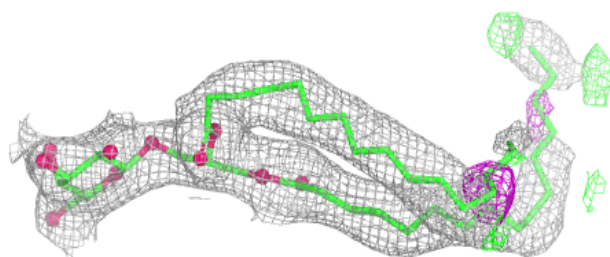
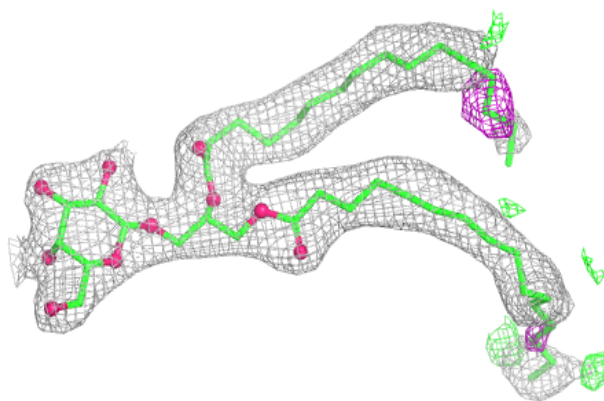
Electron density around CLA c 513:

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

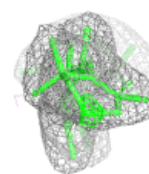
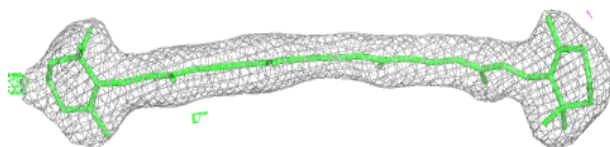
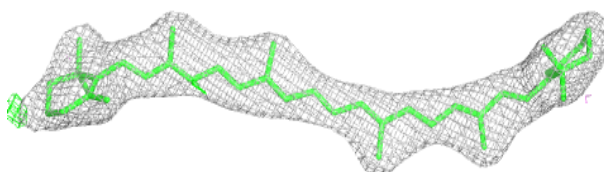


Electron density around LMG D 415:

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

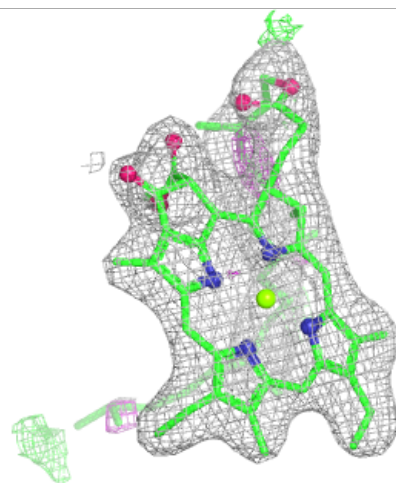
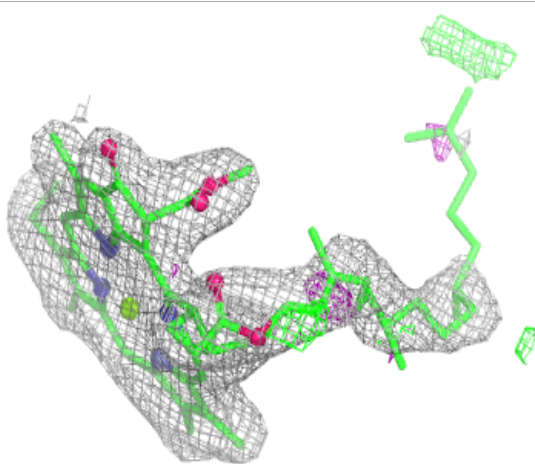
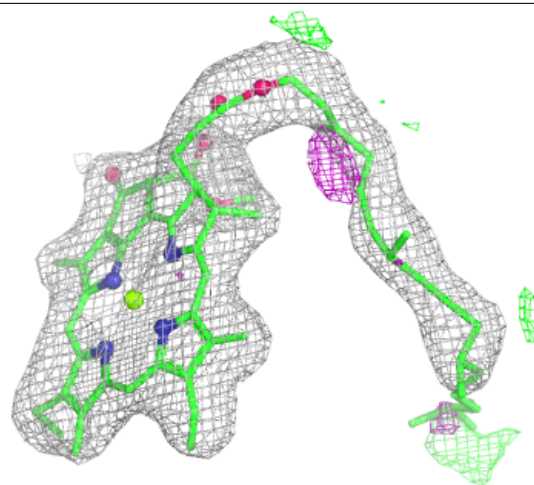
**Electron density around BCR h 101:**

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



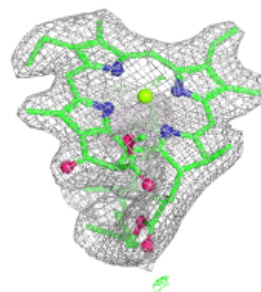
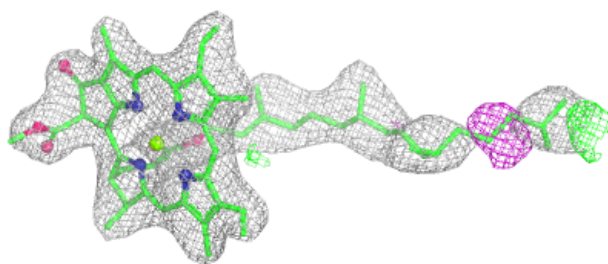
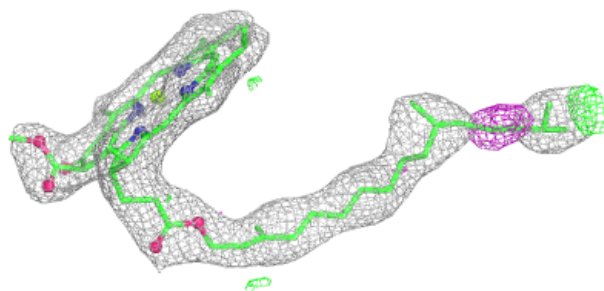
Electron density around CLA b 616:

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



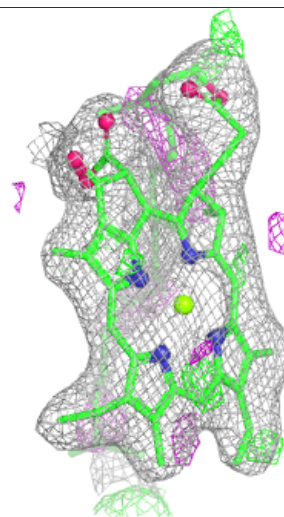
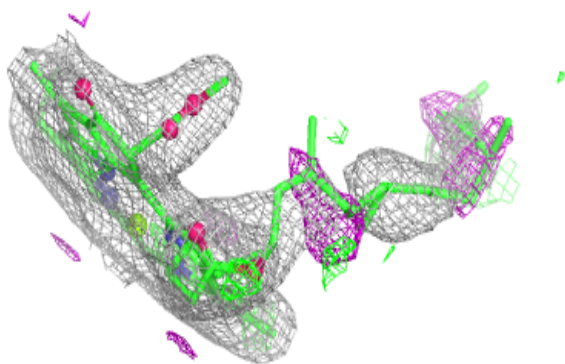
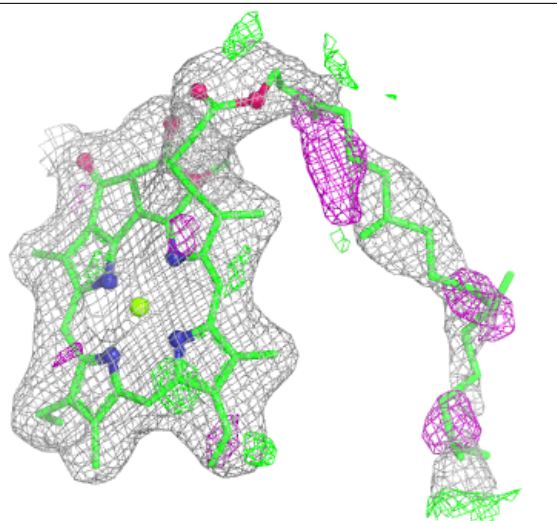
Electron density around CLA c 505:

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



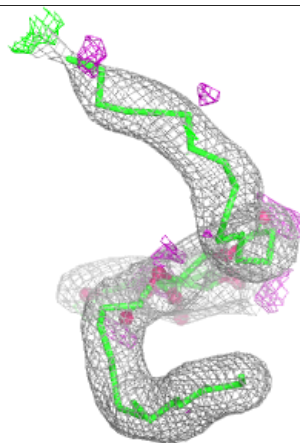
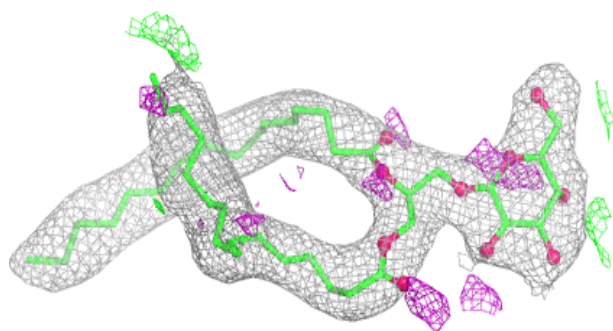
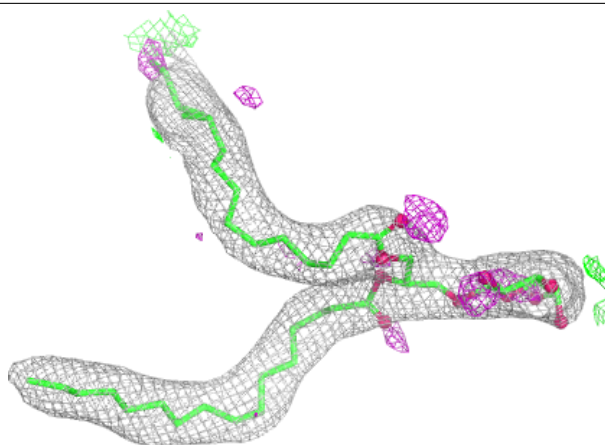
Electron density around CLA B 616:

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

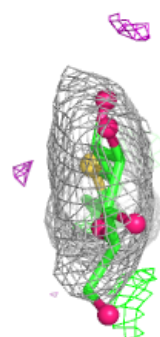
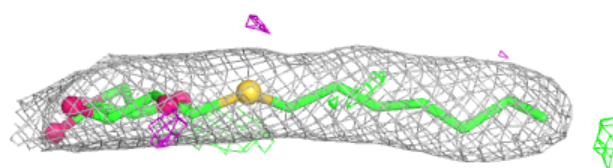
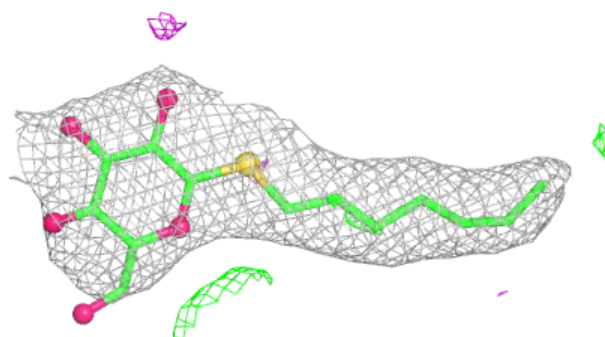


Electron density around LMG B 621:

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

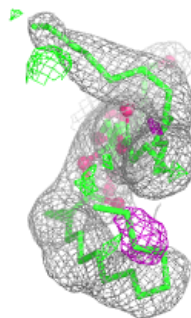
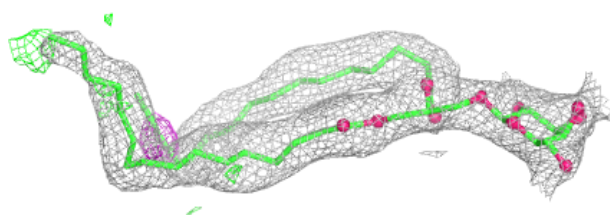
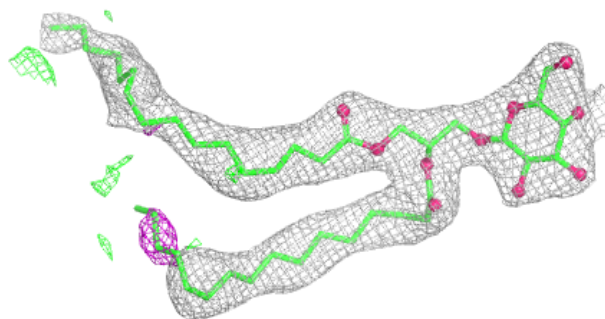
**Electron density around HTG b 625:**

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

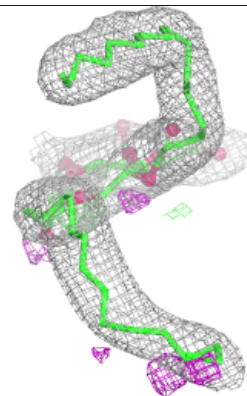
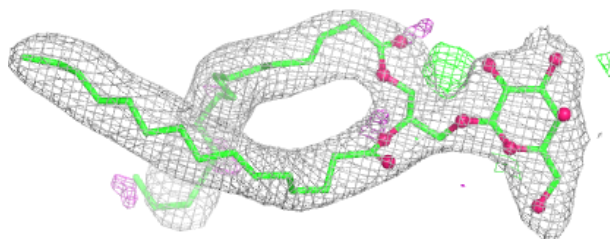
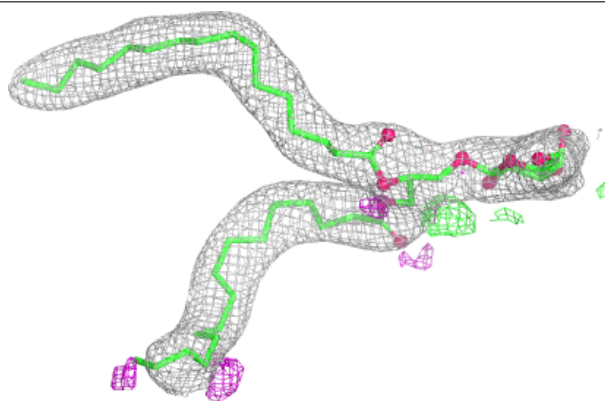


Electron density around LMG d 412:

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

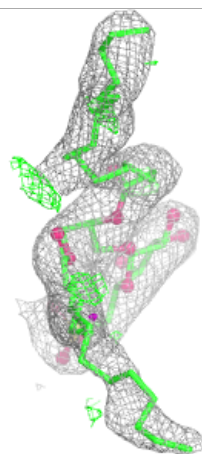
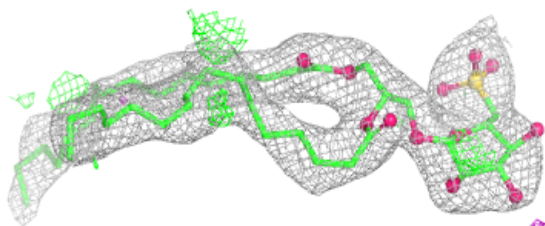
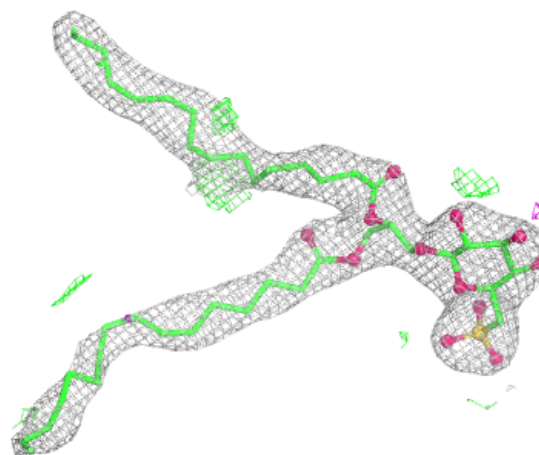
**Electron density around LMG m 101:**

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



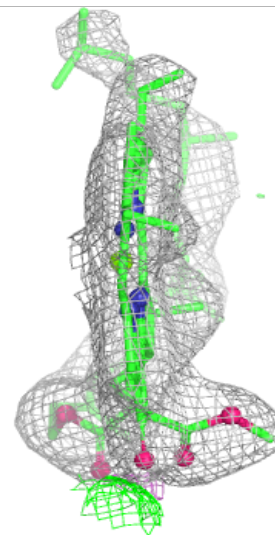
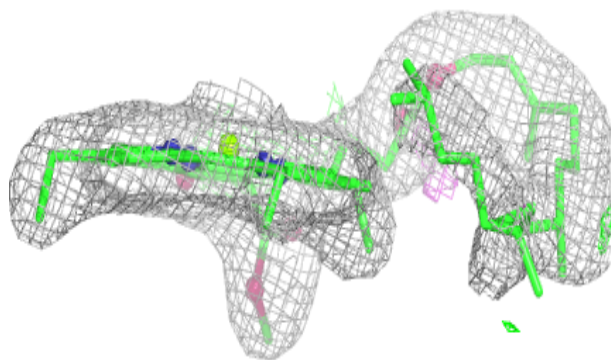
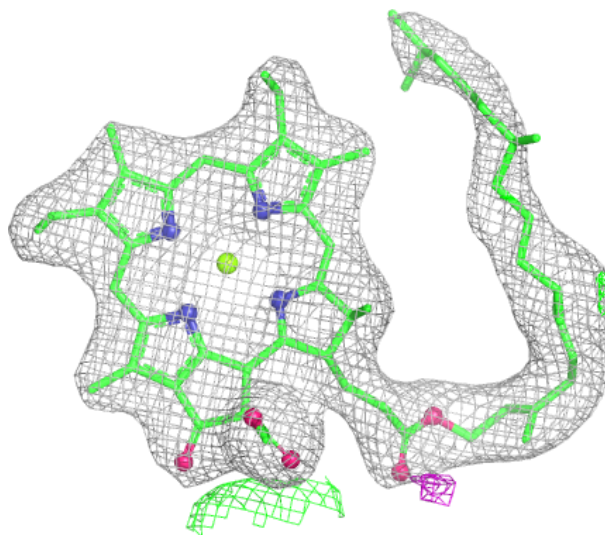
Electron density around SQD a 411:

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



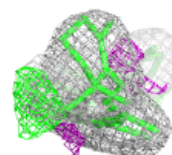
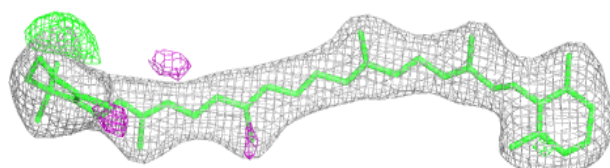
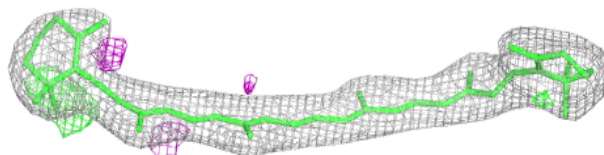
Electron density around CLA C 513:

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

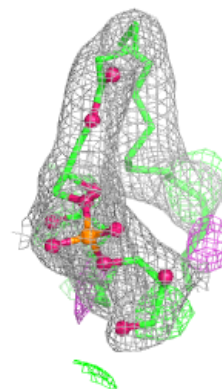
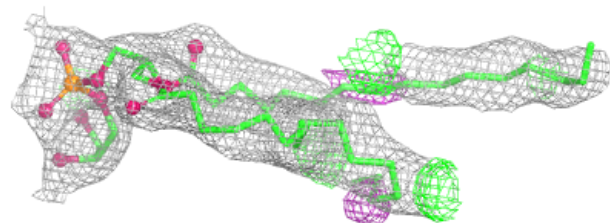
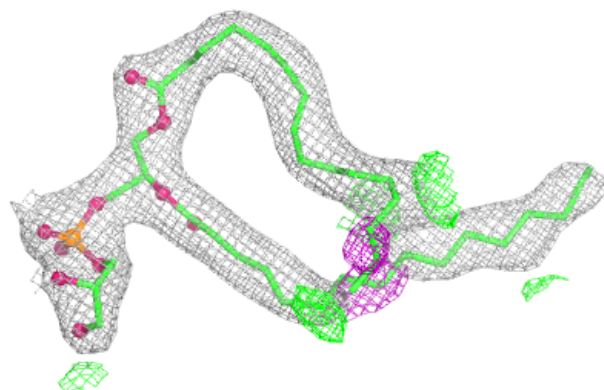


Electron density around BCR D 407:

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

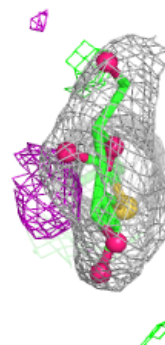
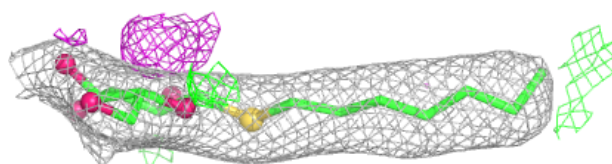
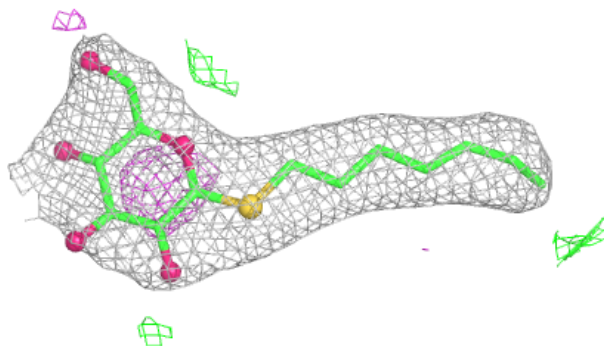
**Electron density around LHG d 408:**

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



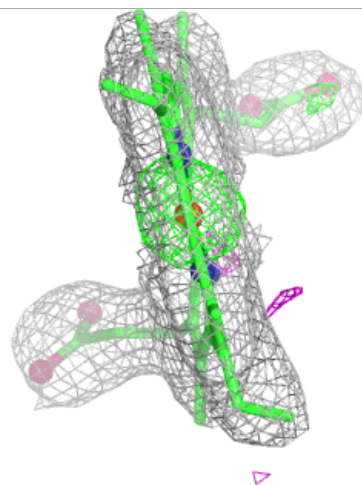
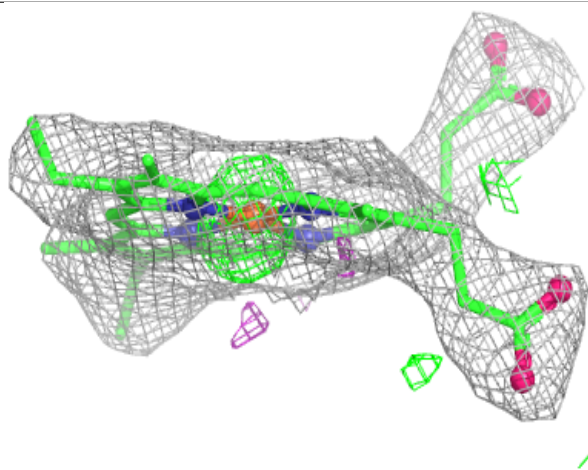
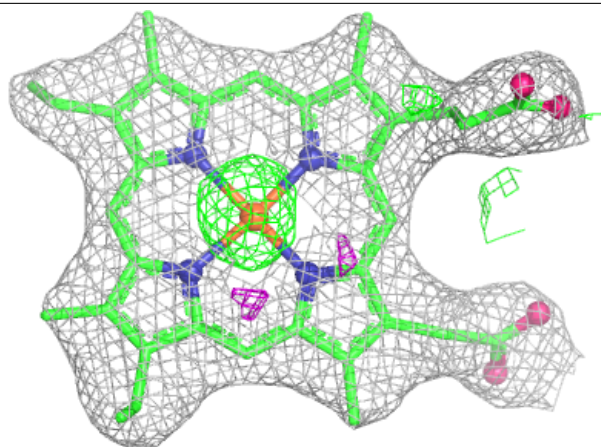
Electron density around HTG B 626:

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



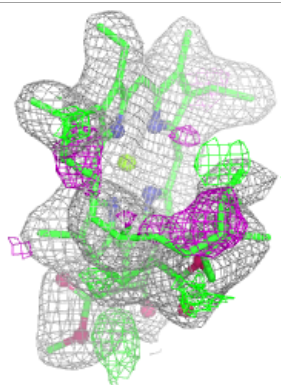
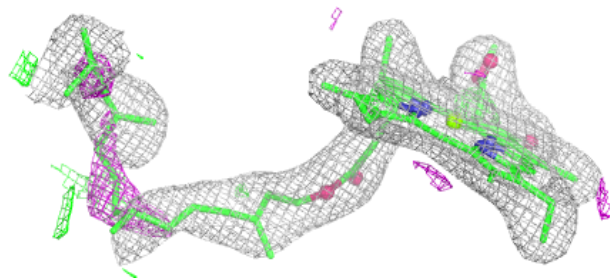
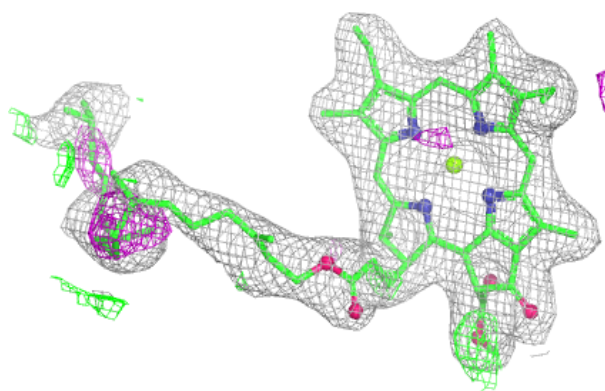
Electron density around HEM E 103:

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

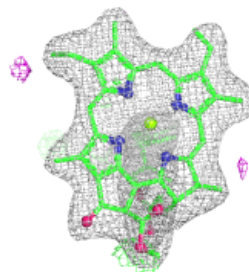
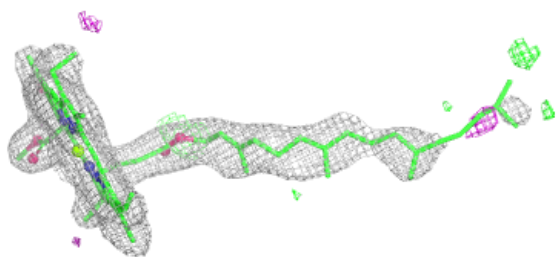
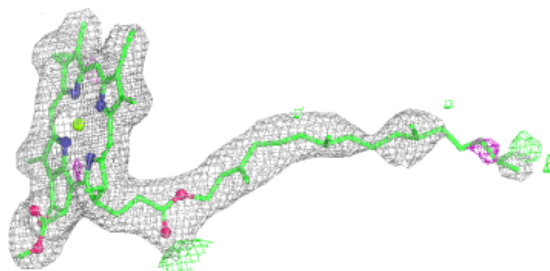


Electron density around CLA A 408:

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

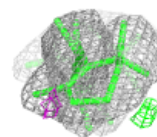
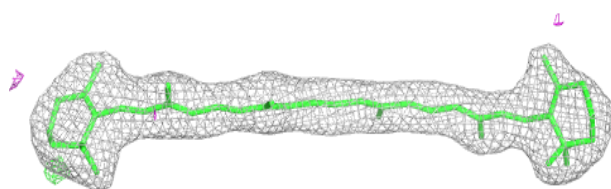
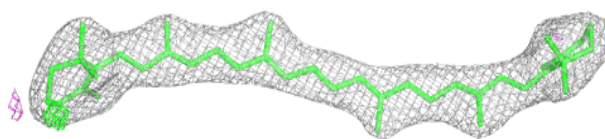
**Electron density around CLA d 403:**

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

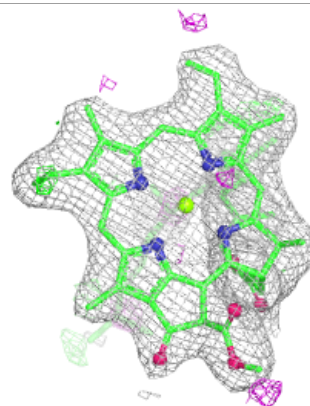
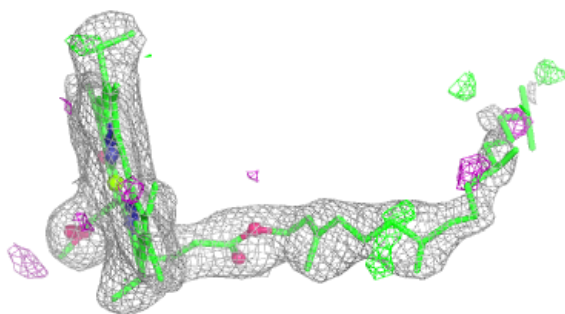
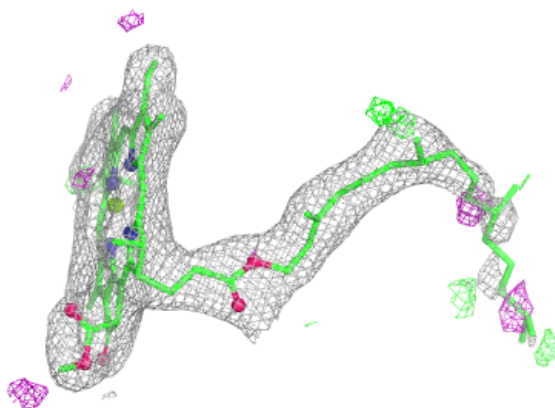


Electron density around BCR C 515:

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

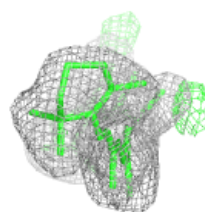
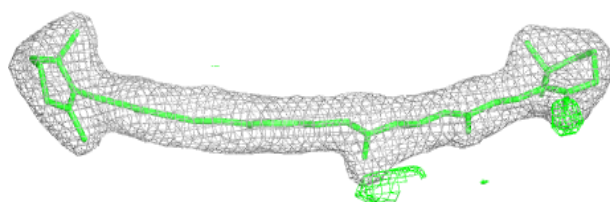
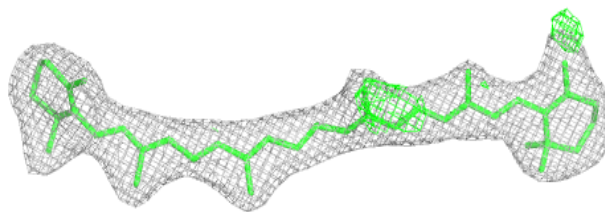
**Electron density around CLA D 406:**

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

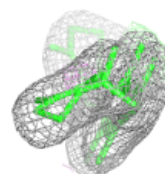
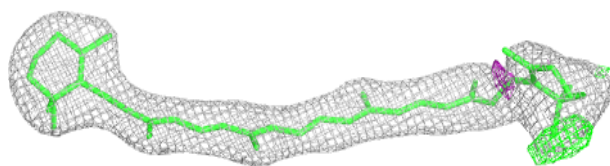
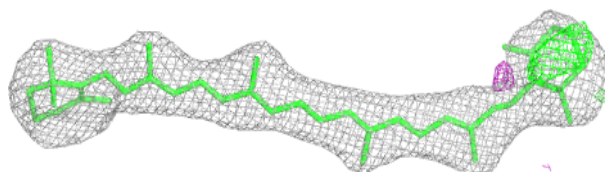


Electron density around BCR T 101:

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

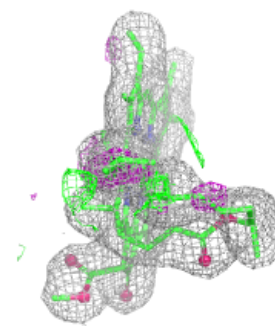
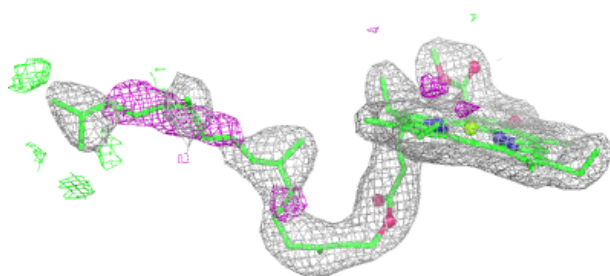
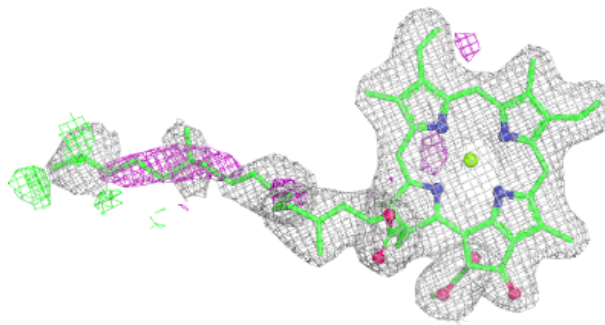
**Electron density around BCR d 404:**

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

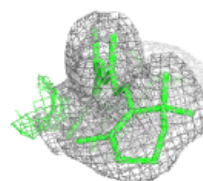
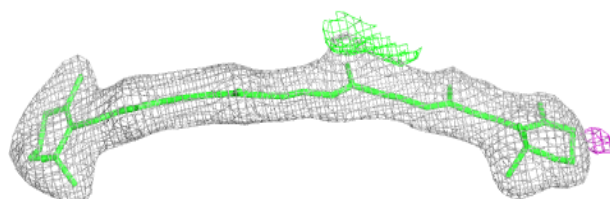
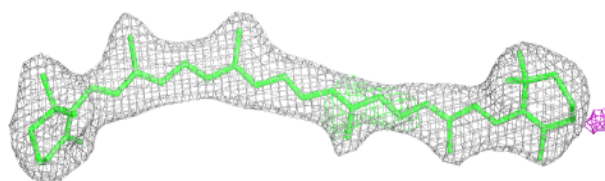


Electron density around CLA a 407:

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

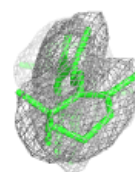
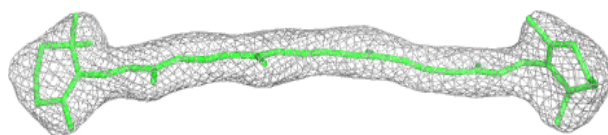
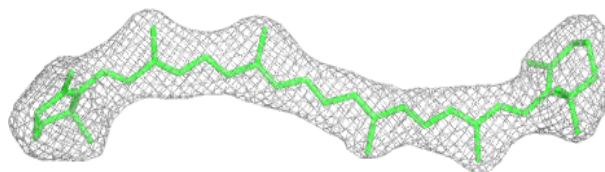
**Electron density around BCR t 103:**

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



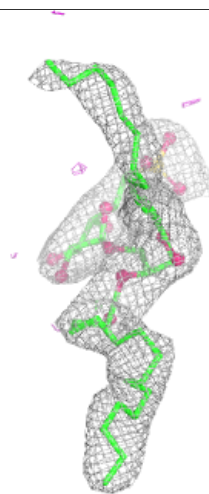
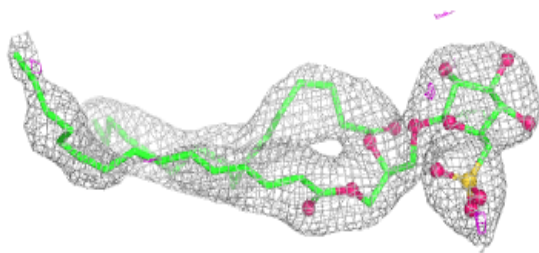
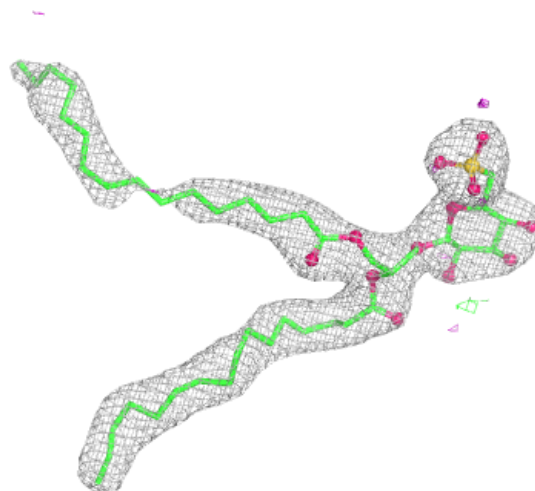
Electron density around BCR y 101:

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



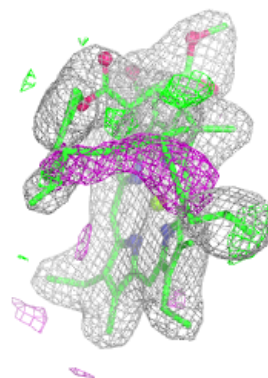
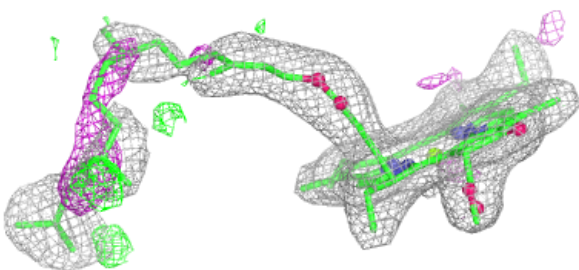
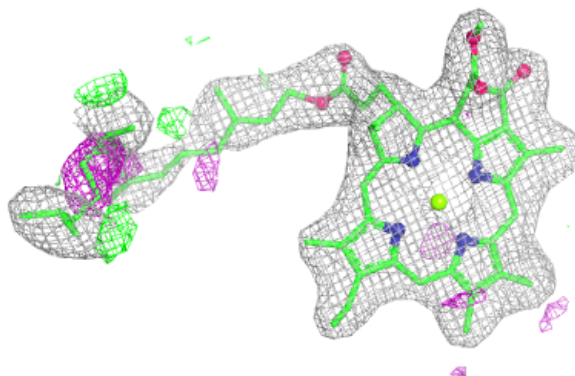
Electron density around SQD A 410:

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

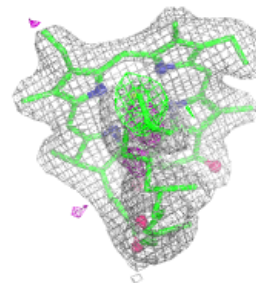
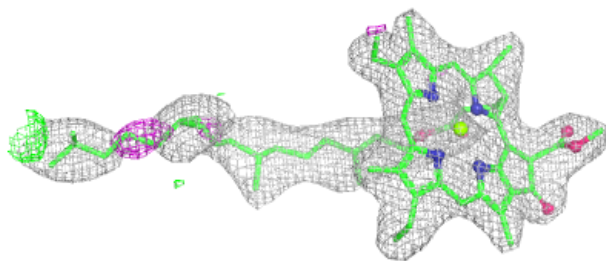
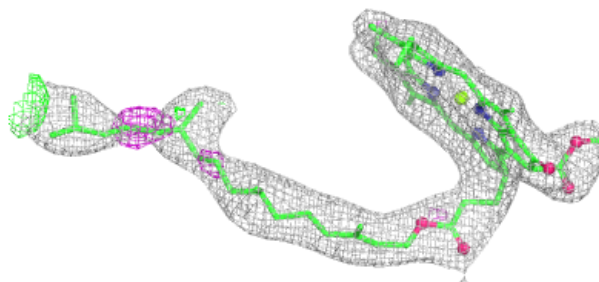


Electron density around CLA a 409:

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

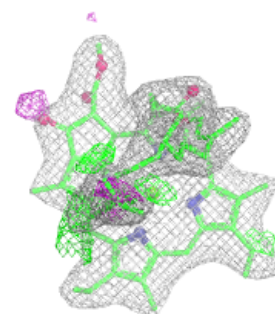
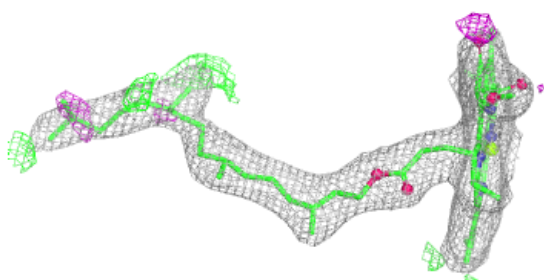
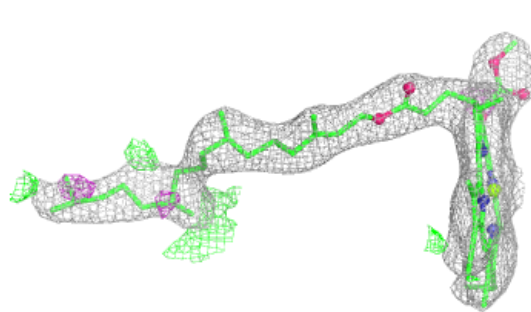
**Electron density around CLA C 505:**

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

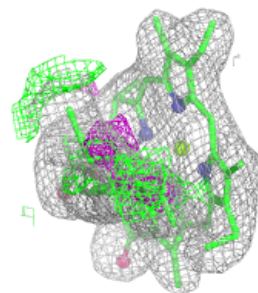
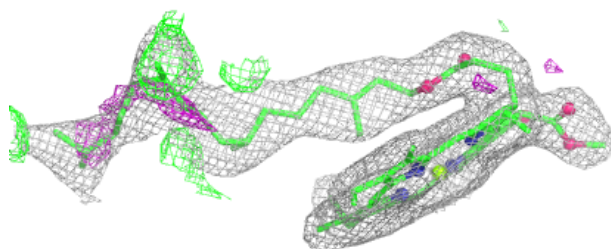
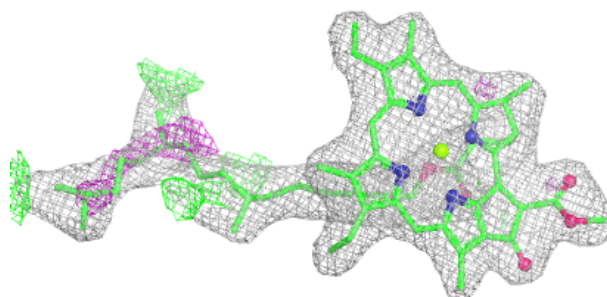


Electron density around CLA b 606:

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

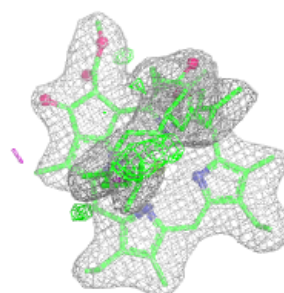
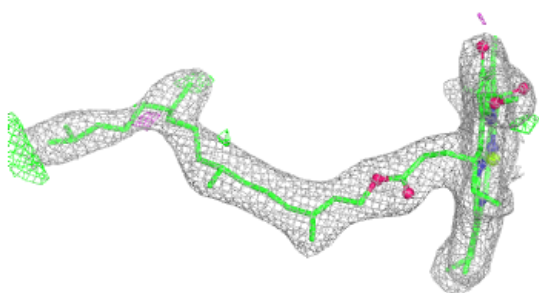
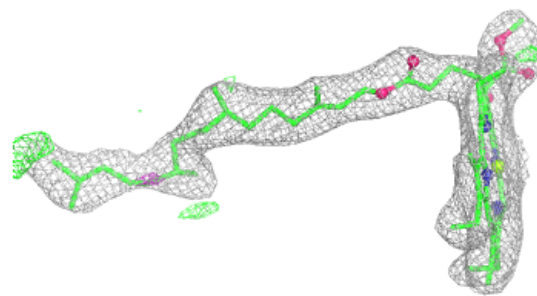
**Electron density around CLA b 614:**

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

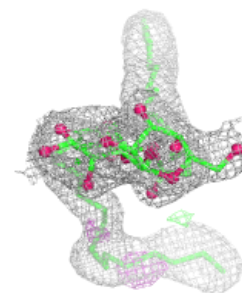
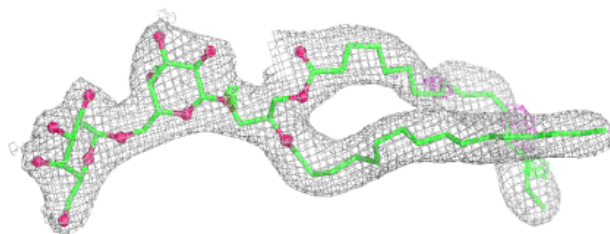
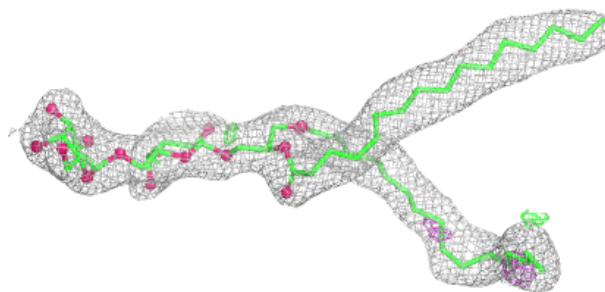


Electron density around CLA B 606:

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

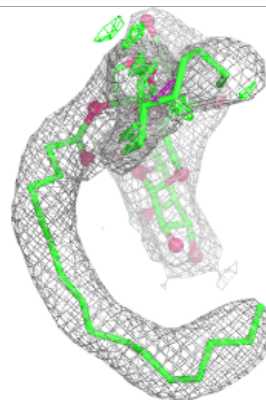
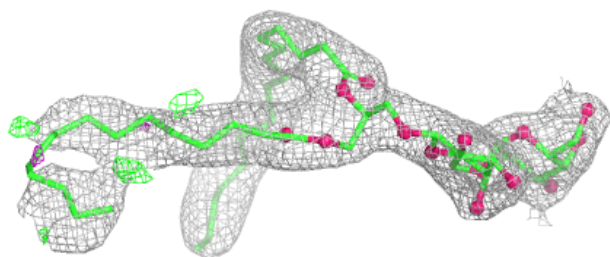
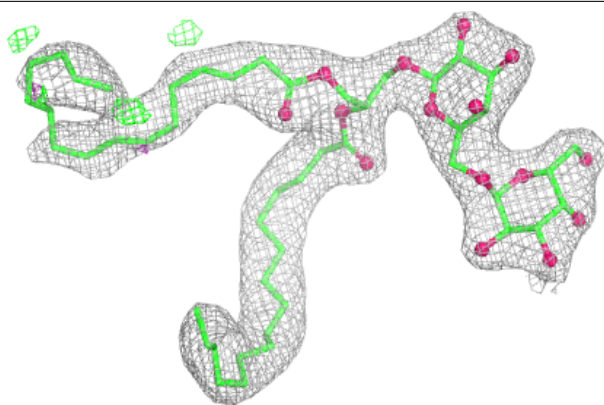
**Electron density around DGD C 517:**

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

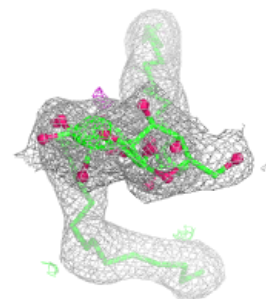
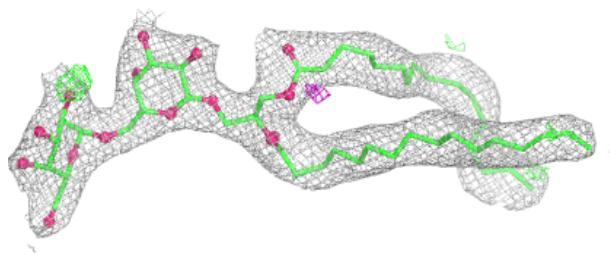
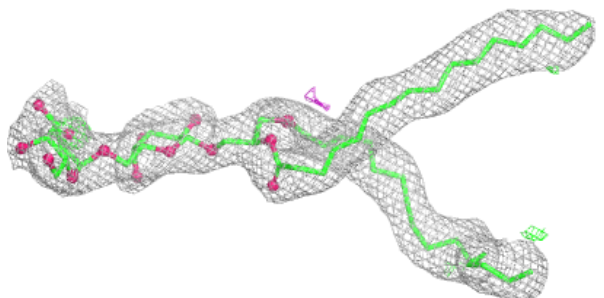


Electron density around DGD C 518:

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

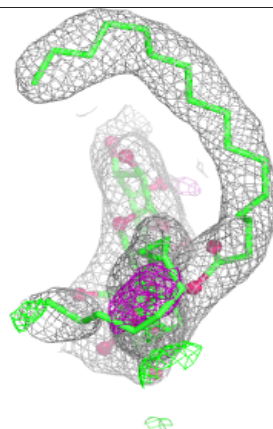
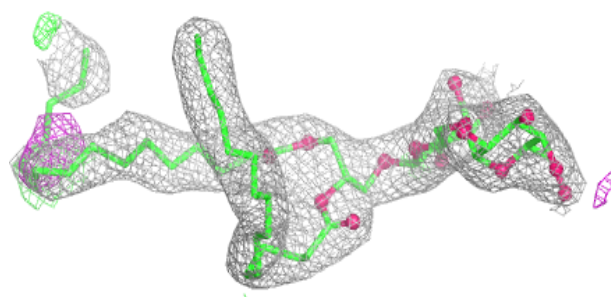
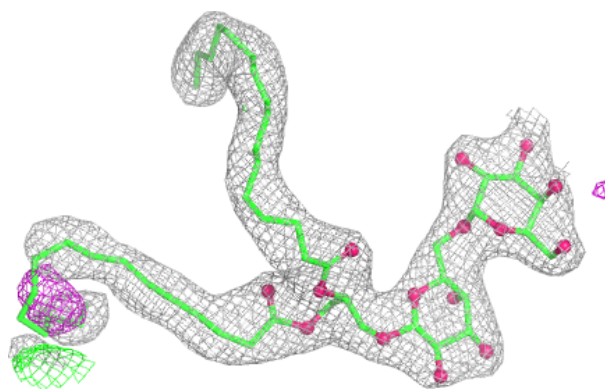
**Electron density around DGD c 517:**

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

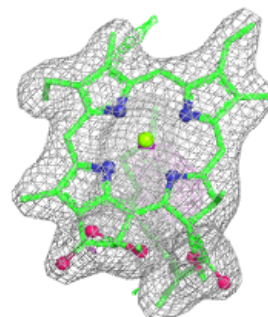
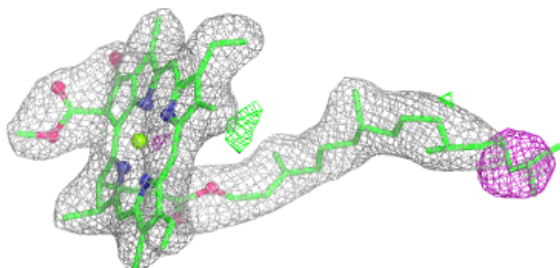
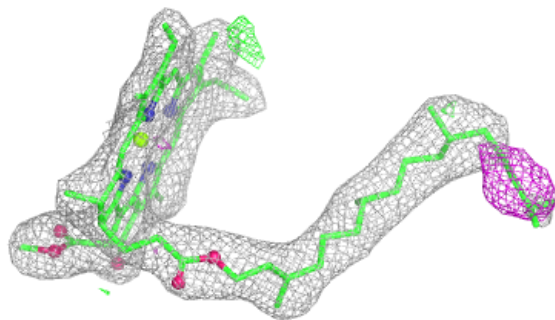


Electron density around DGD c 518:

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

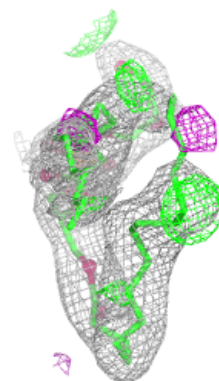
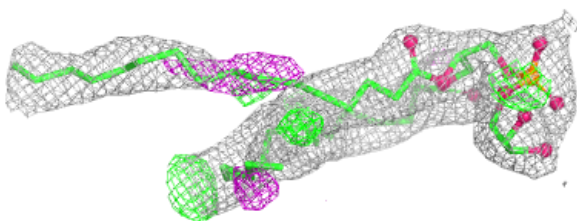
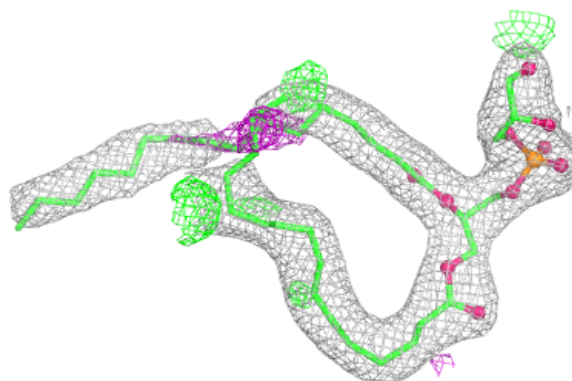
**Electron density around CLA C 509:**

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

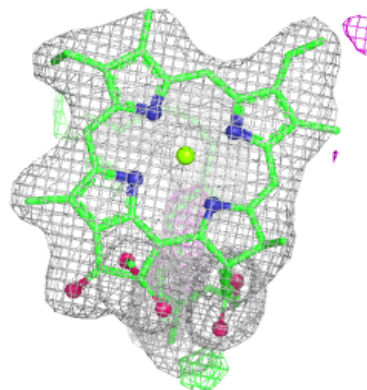
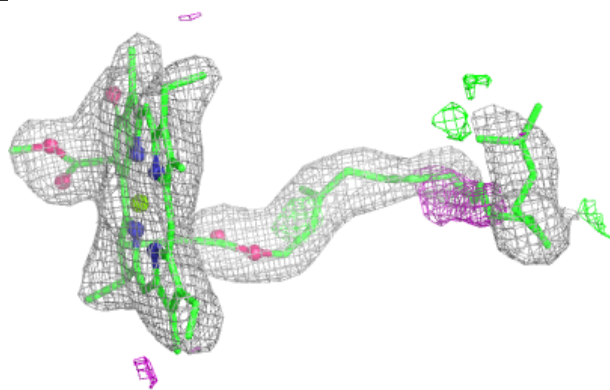
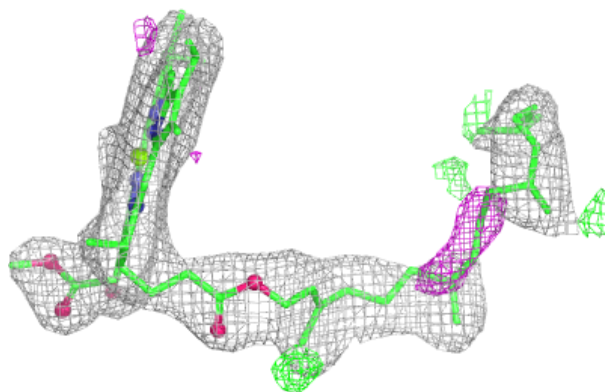


Electron density around LHG D 411:

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

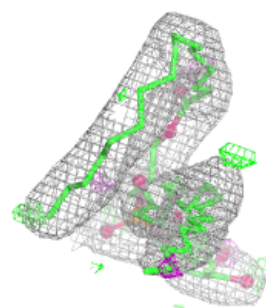
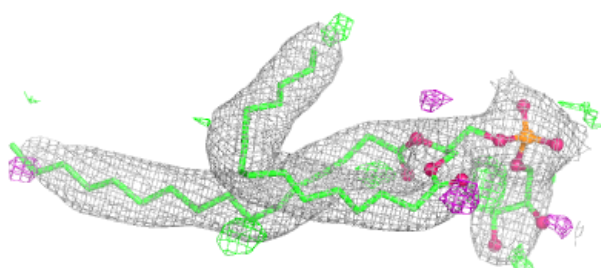
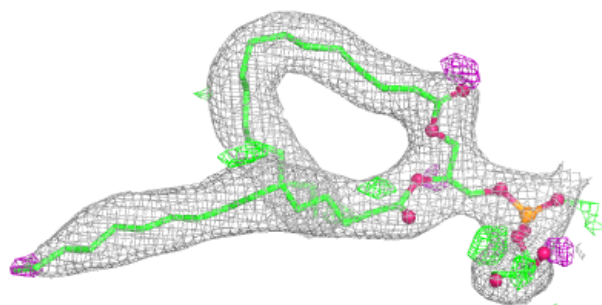
**Electron density around CLA c 507:**

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

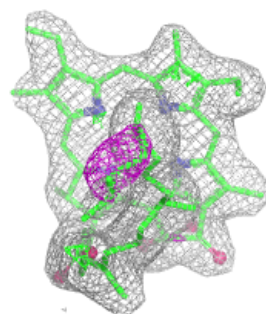
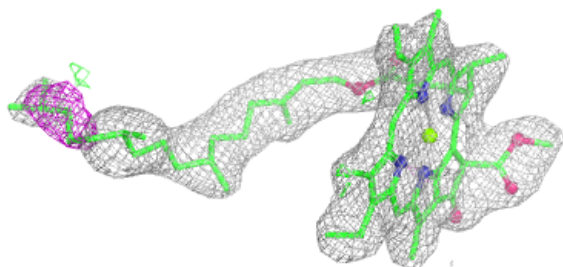
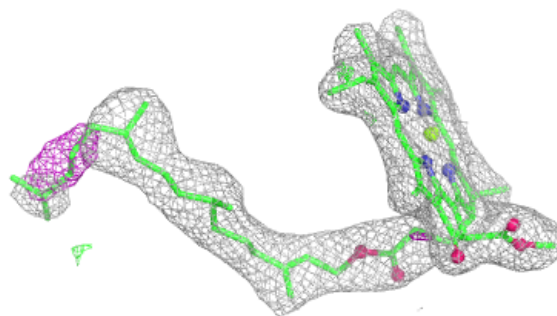


Electron density around LHG d 406:

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

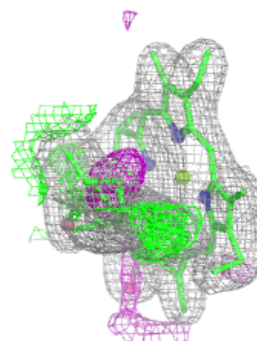
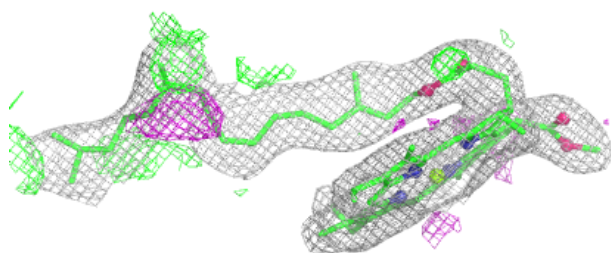
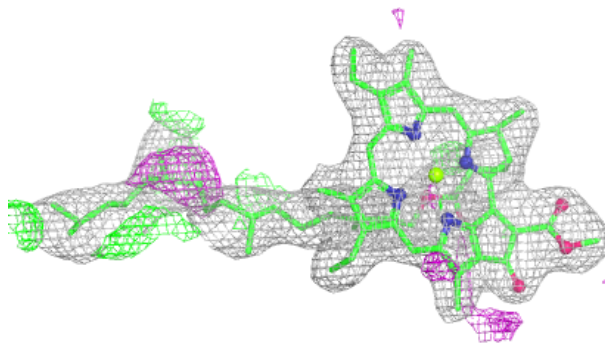
**Electron density around CLA c 509:**

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

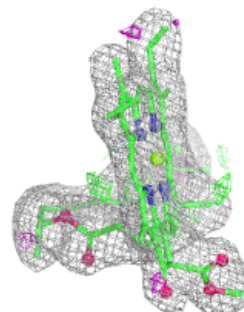
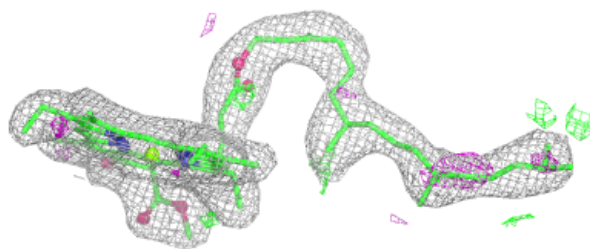
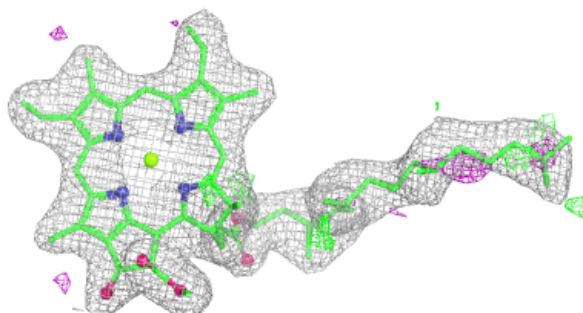


Electron density around CLA B 614:

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

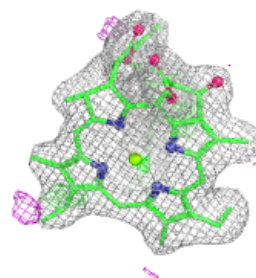
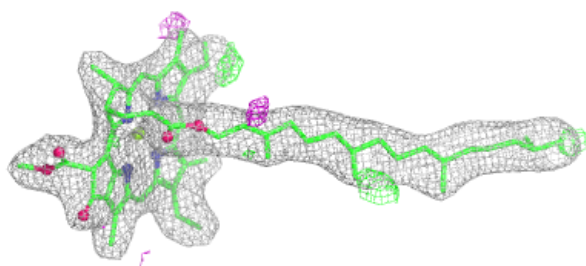
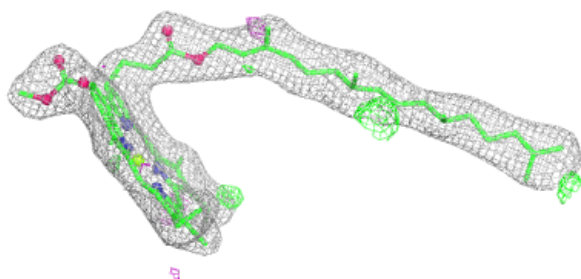
**Electron density around CLA A 406:**

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

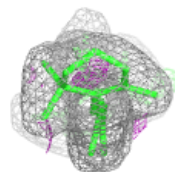
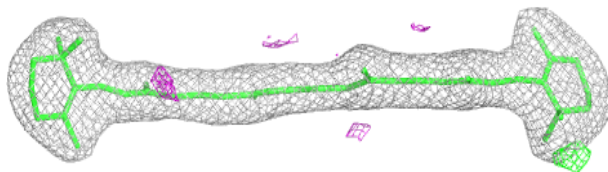
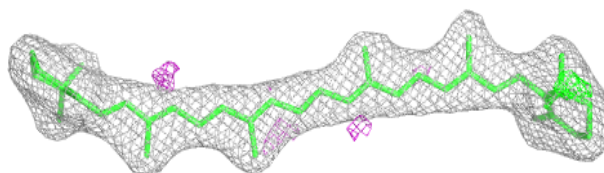


Electron density around CLA b 607:

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

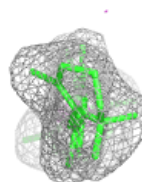
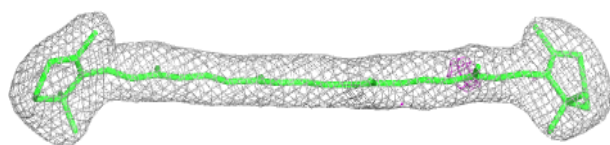
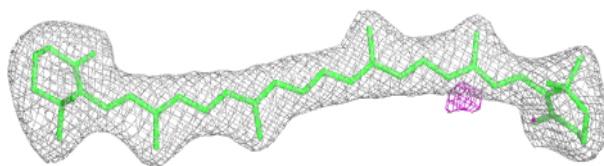
**Electron density around BCR A 409:**

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

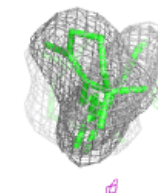
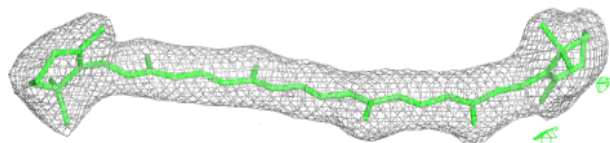
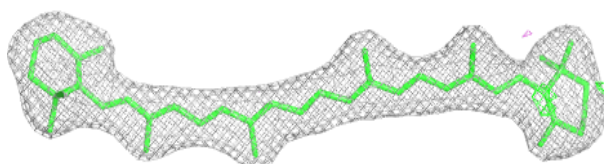


Electron density around BCR B 618:

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

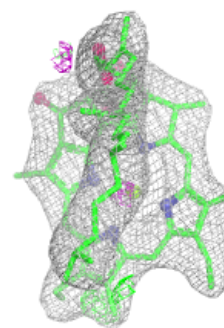
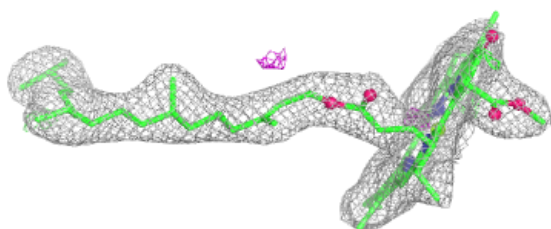
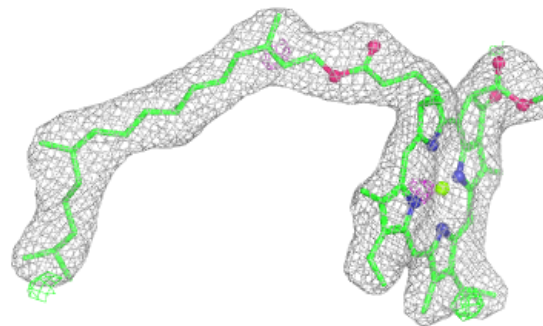
**Electron density around BCR B 619:**

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

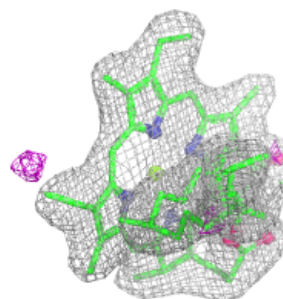
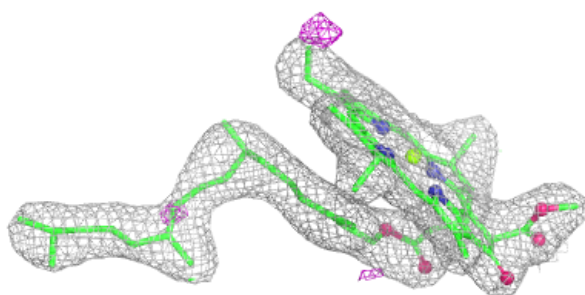
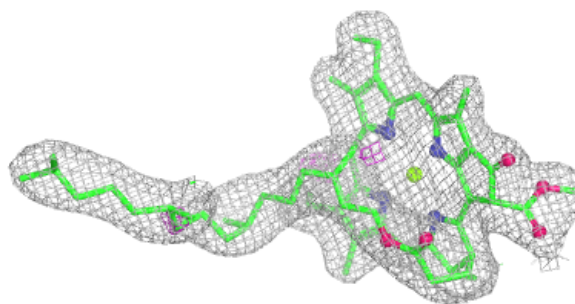


Electron density around CLA b 609:

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

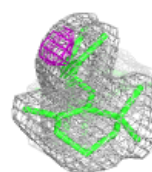
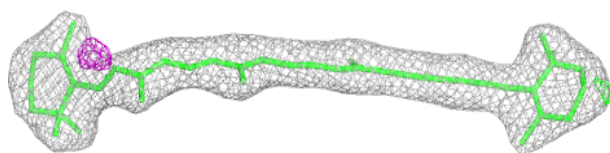
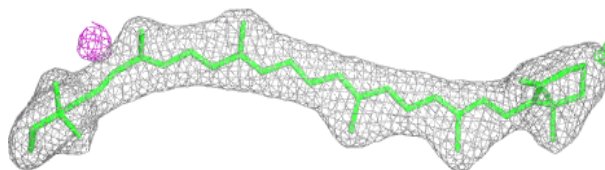
**Electron density around CLA C 506:**

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

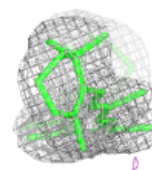
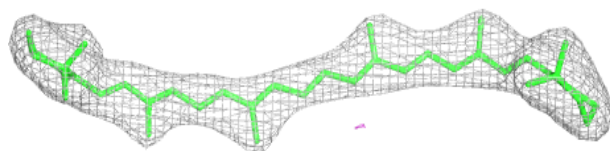
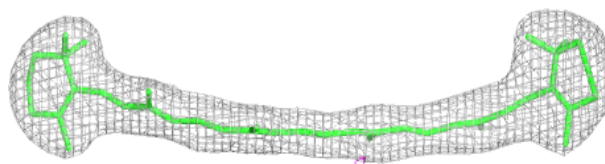


Electron density around BCR H 101:

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

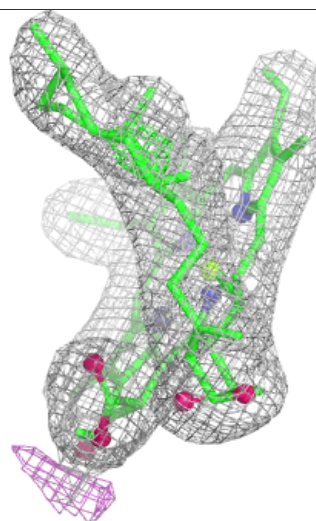
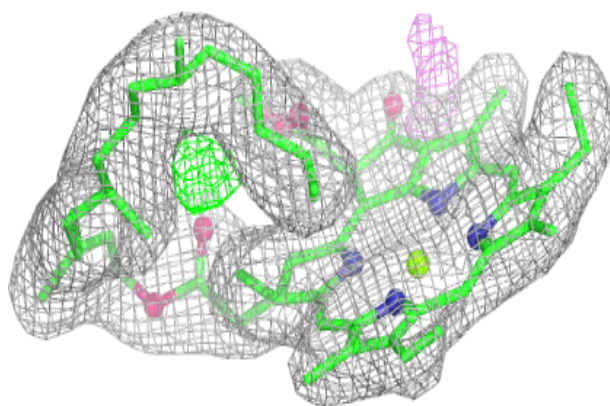
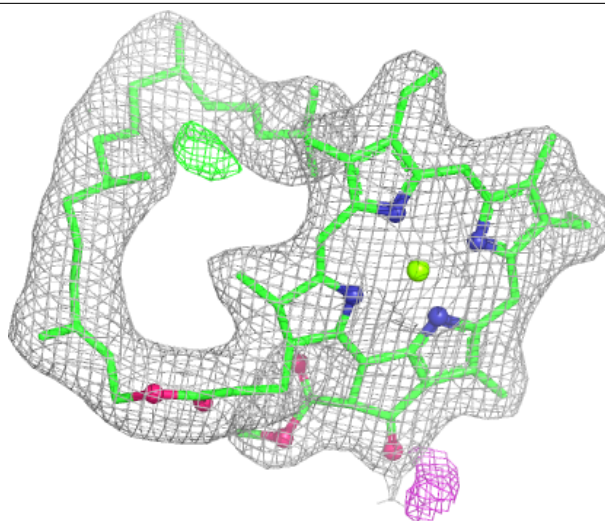
**Electron density around BCR K 102:**

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



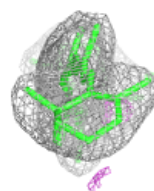
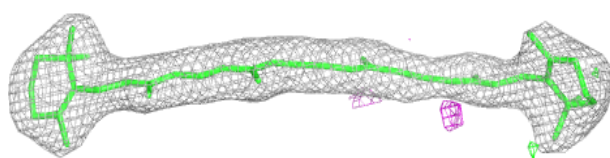
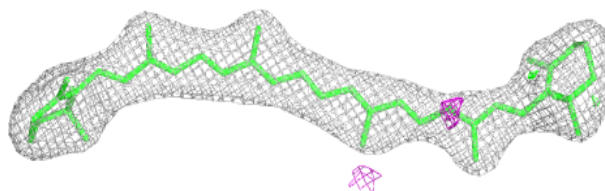
Electron density around CLA b 615:

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

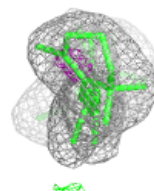
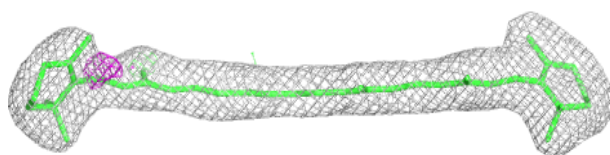
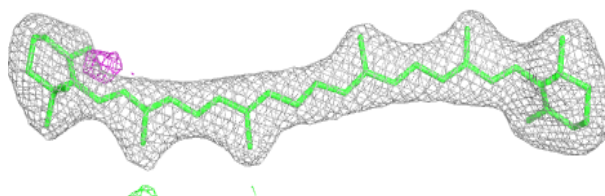


Electron density around BCR Y 101:

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

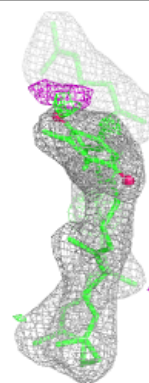
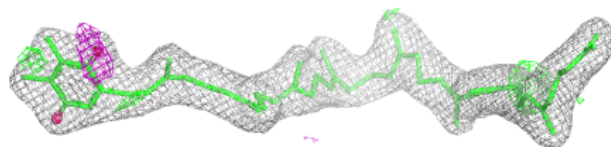
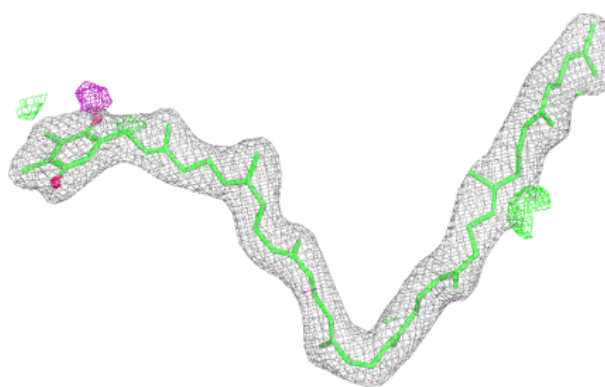
**Electron density around BCR b 618:**

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

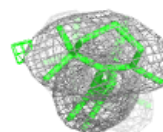
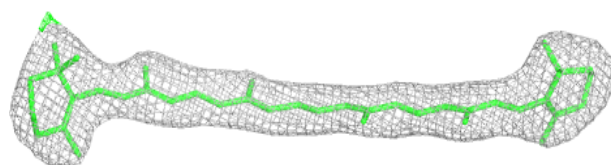


Electron density around PL9 D 408:

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

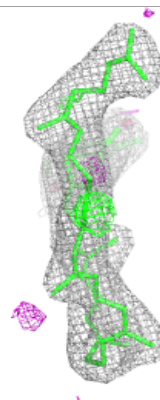
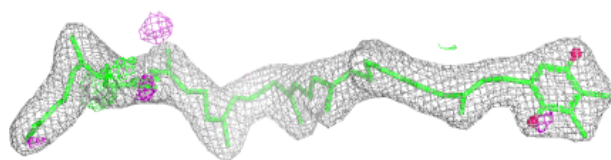
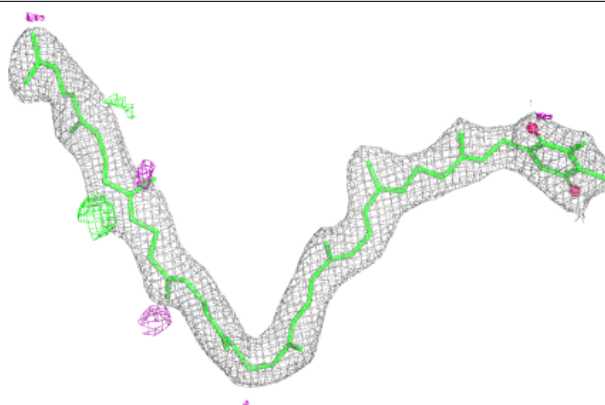
**Electron density around BCR c 515:**

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

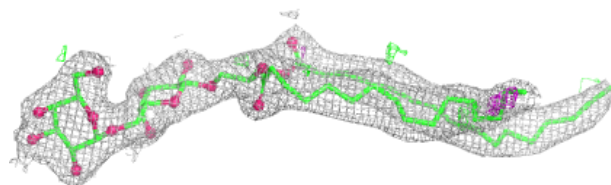
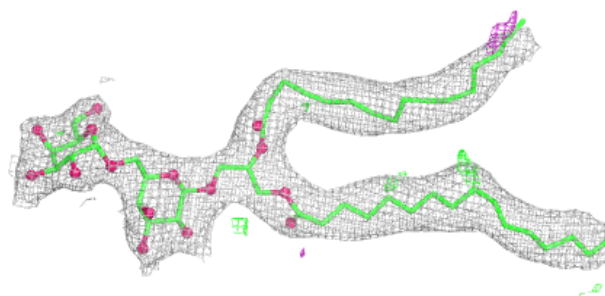


Electron density around PL9 d 405:

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

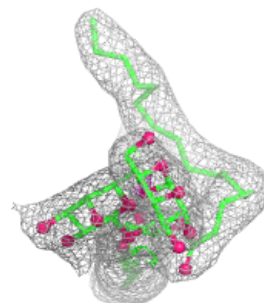
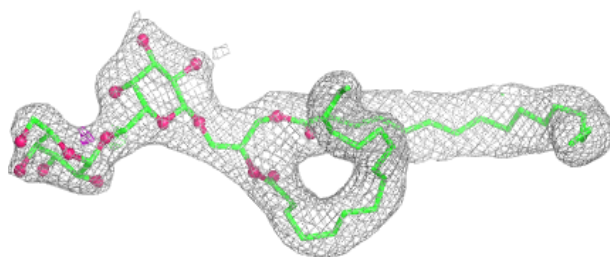
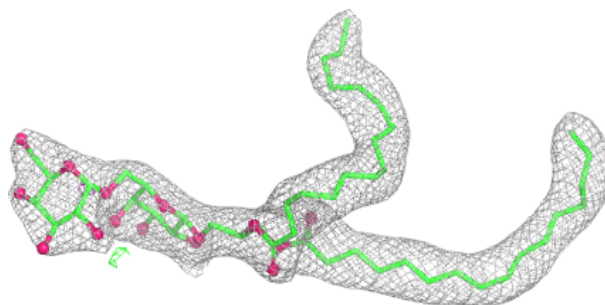
**Electron density around DGD C 519:**

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

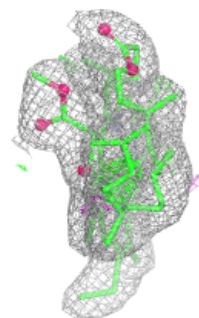
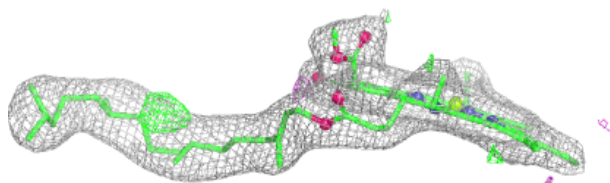
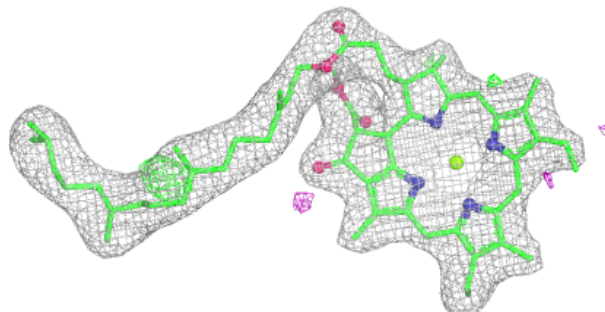


Electron density around DGD H 102:

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

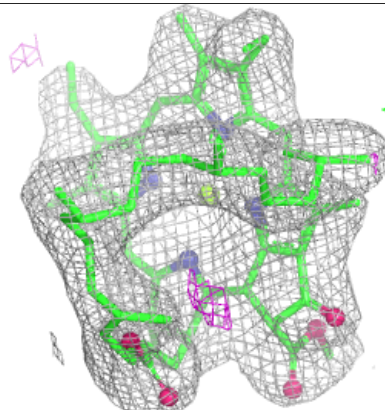
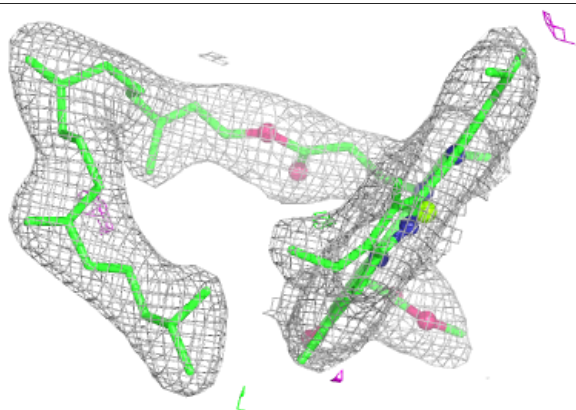
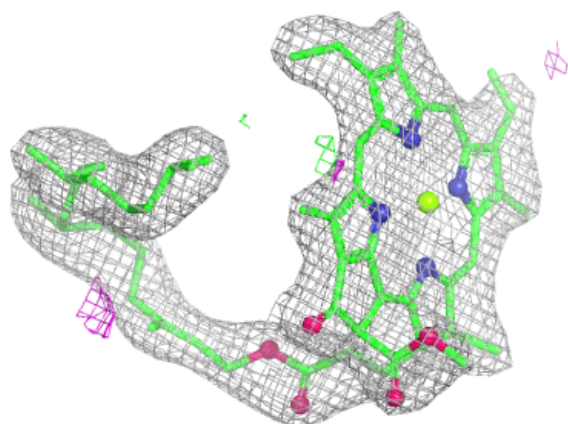
**Electron density around CLA B 602:**

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

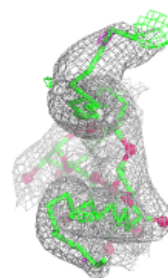
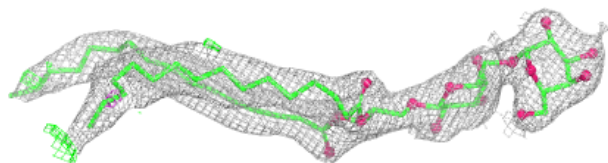
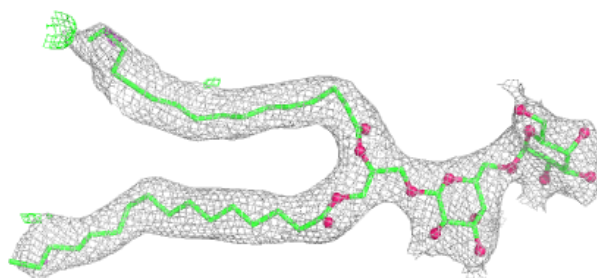


Electron density around CLA c 504:

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

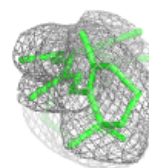
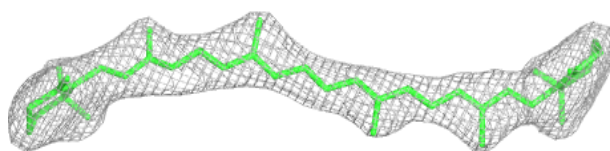
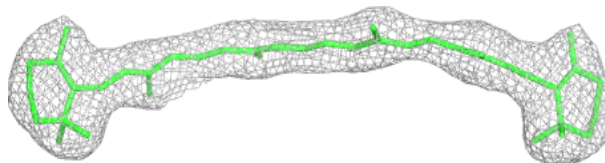
**Electron density around DGD c 519:**

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

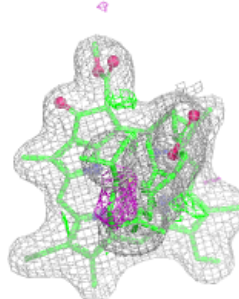
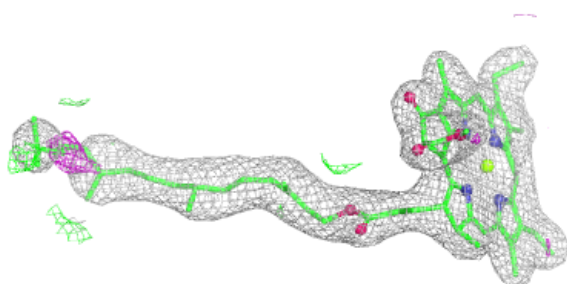
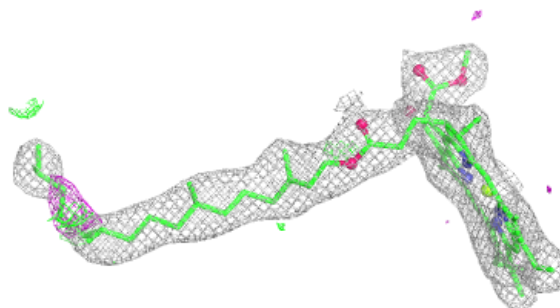


Electron density around BCR k 101:

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

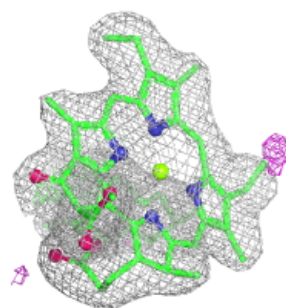
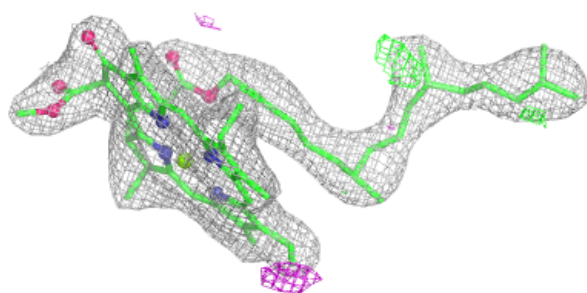
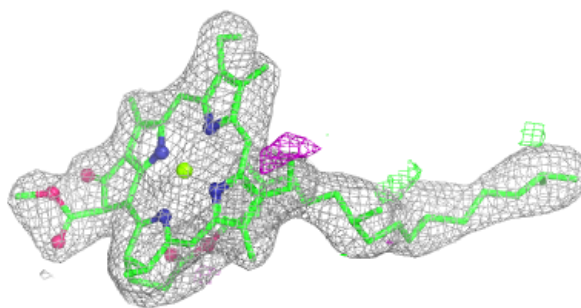
**Electron density around CLA B 604:**

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

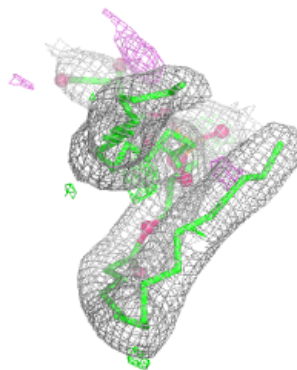
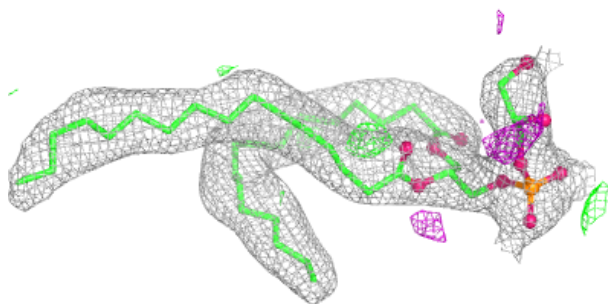
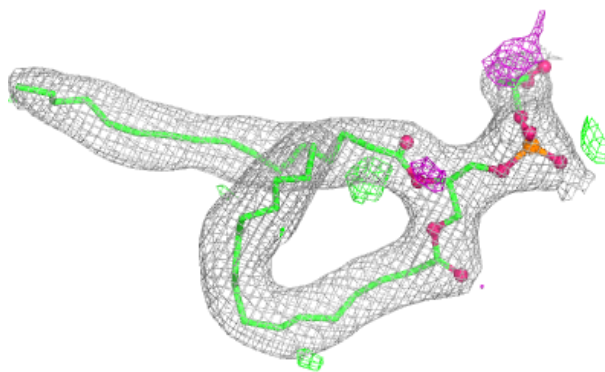


Electron density around CLA c 506:

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

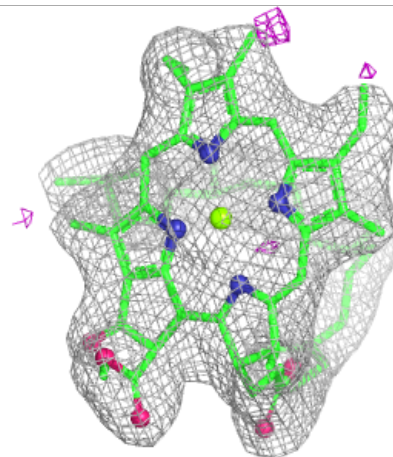
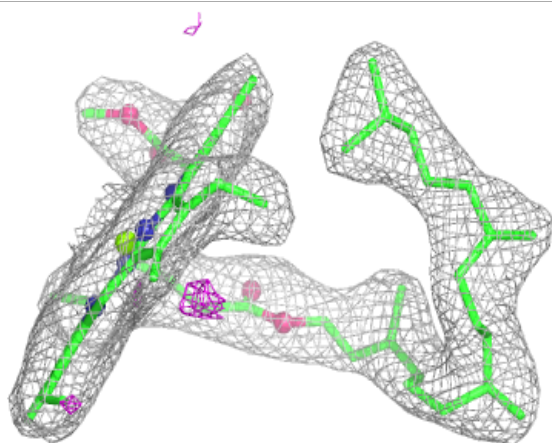
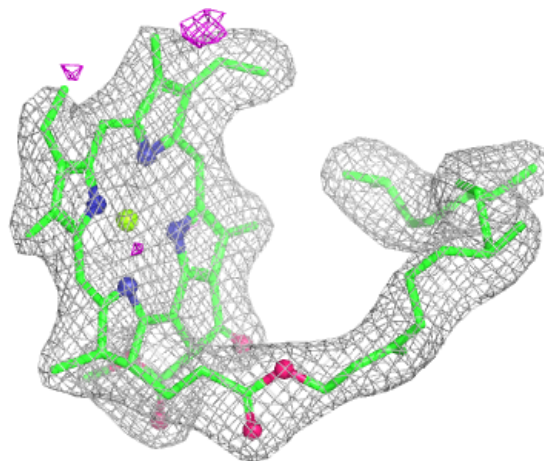
**Electron density around LHG D 409:**

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



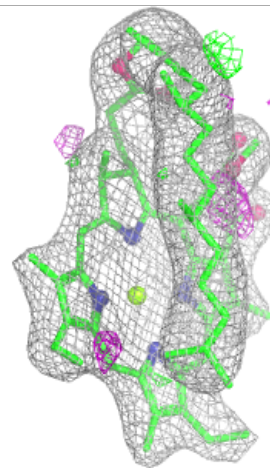
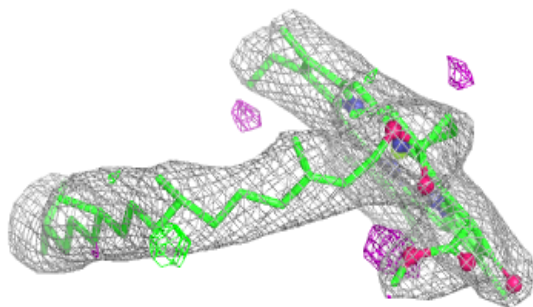
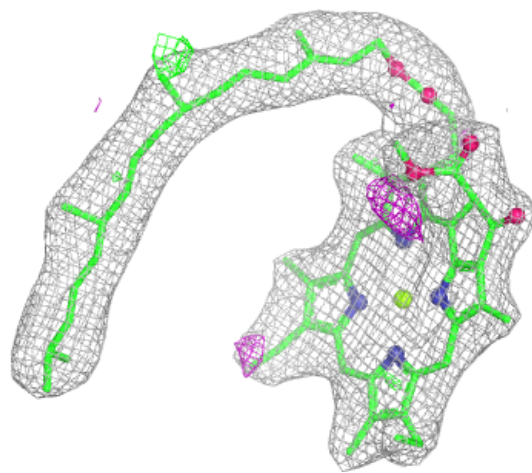
Electron density around CLA C 504:

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



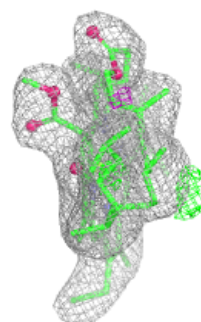
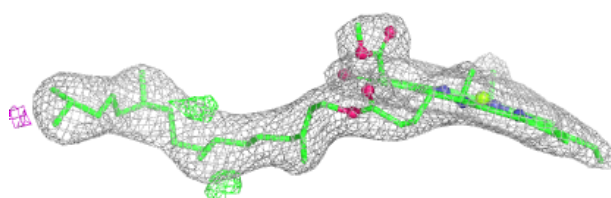
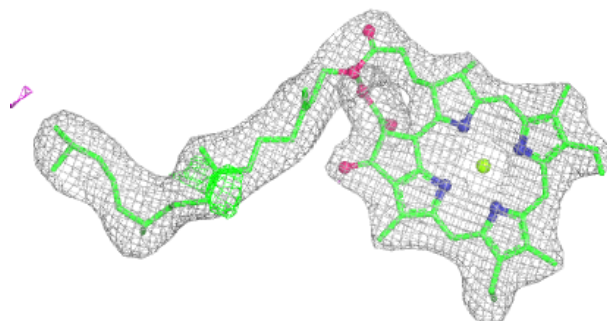
Electron density around CLA c 508:

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



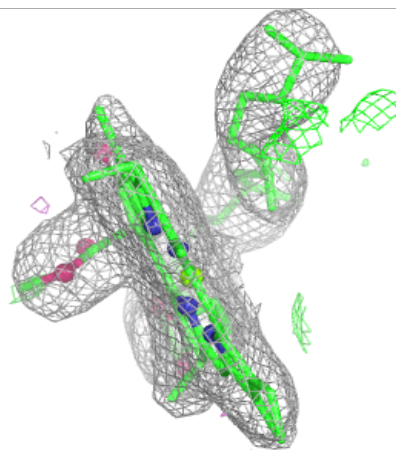
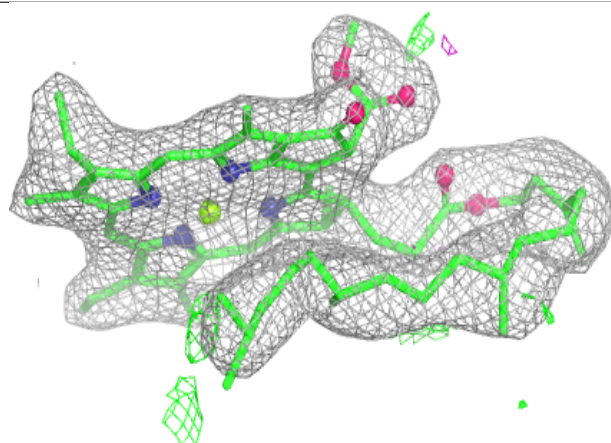
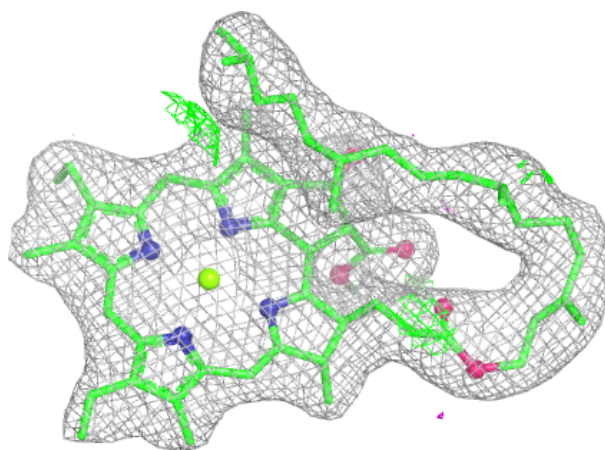
Electron density around CLA b 602:

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



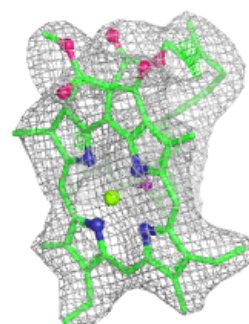
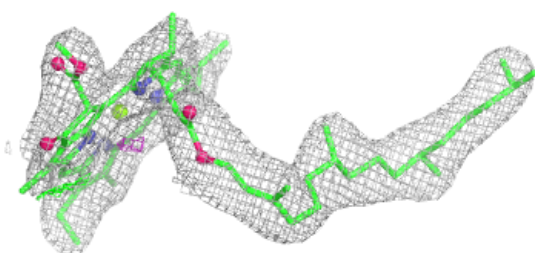
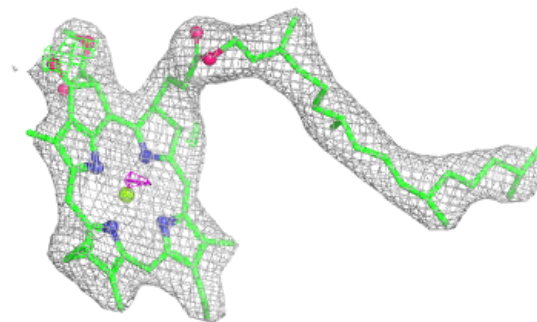
Electron density around CLA c 510:

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



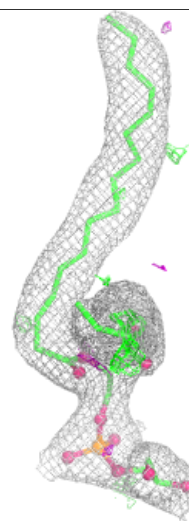
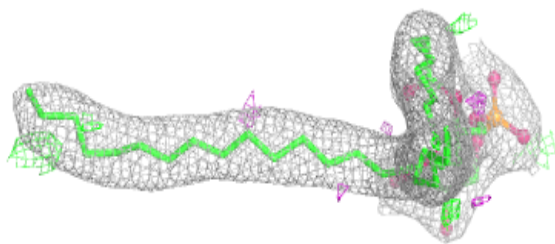
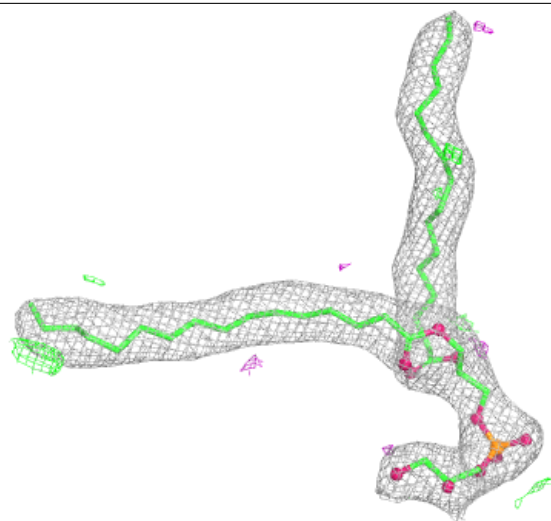
Electron density around CLA c 512:

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



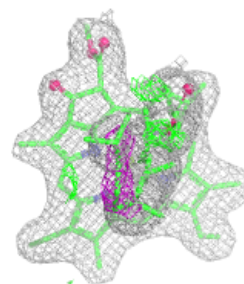
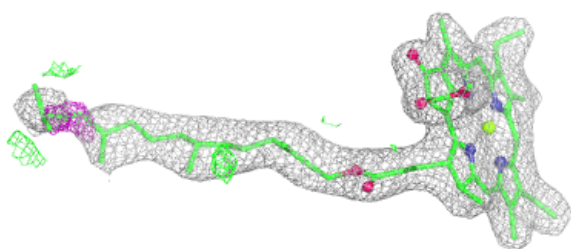
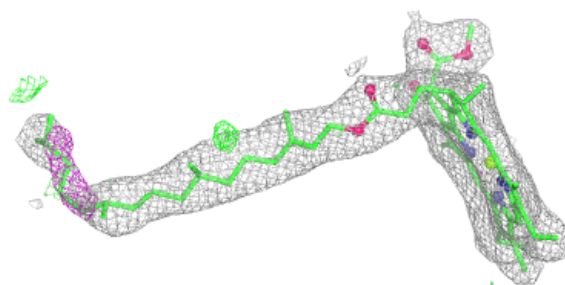
Electron density around LHG 1 101:

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



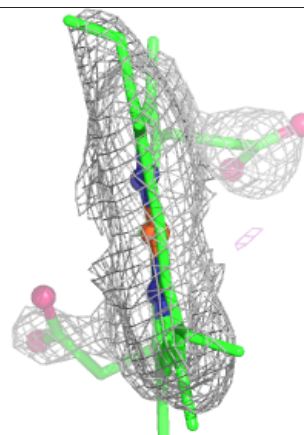
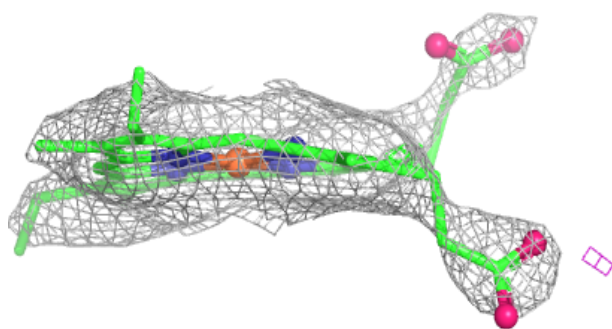
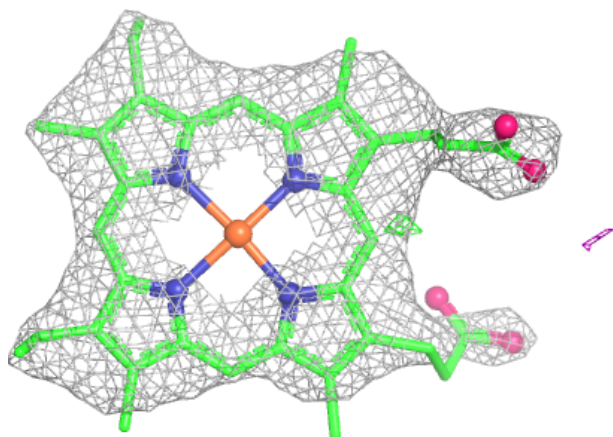
Electron density around CLA b 604:

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



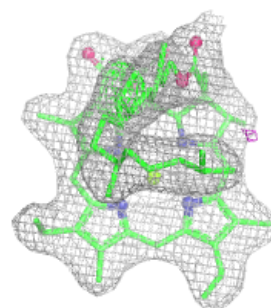
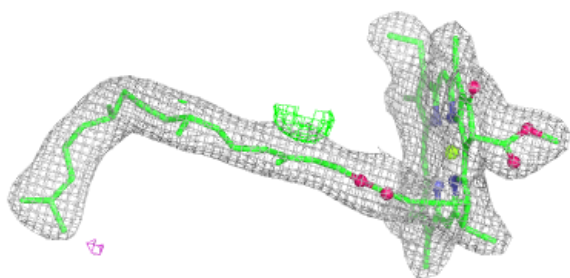
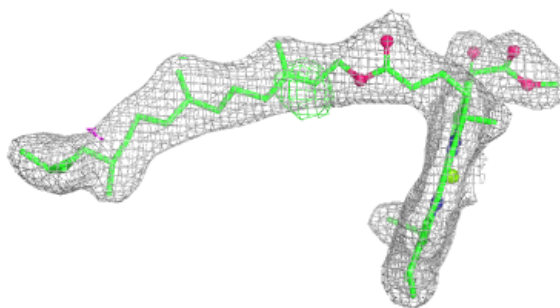
Electron density around HEM e 87:

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

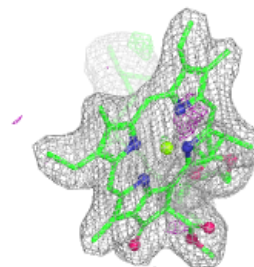
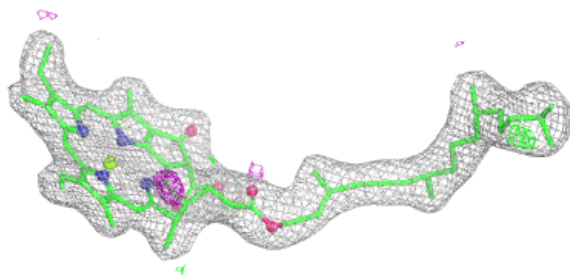
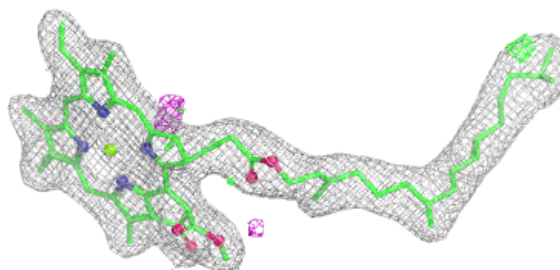


Electron density around CLA B 605:

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

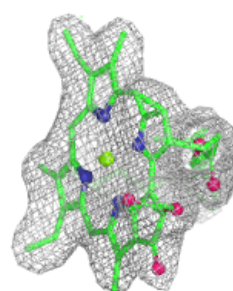
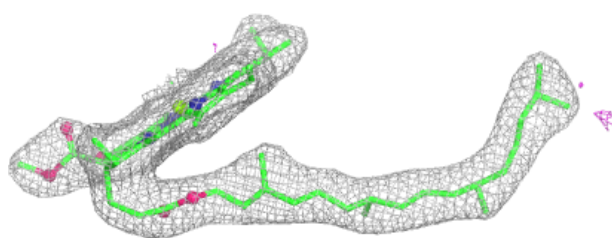
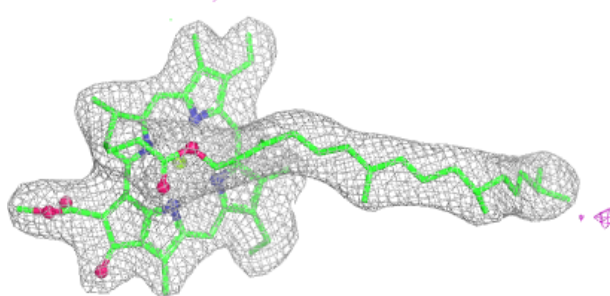
**Electron density around CLA A 404:**

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

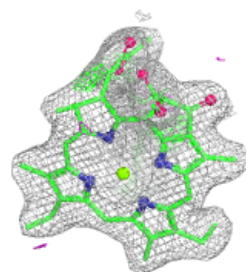
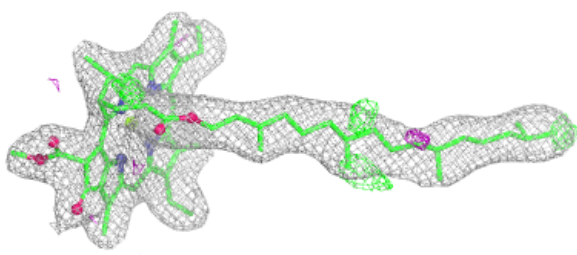
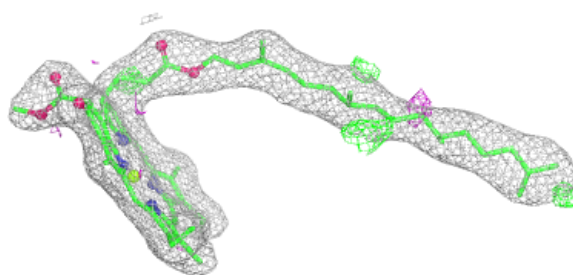


Electron density around CLA b 608:

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

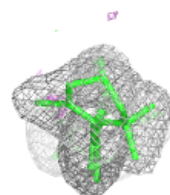
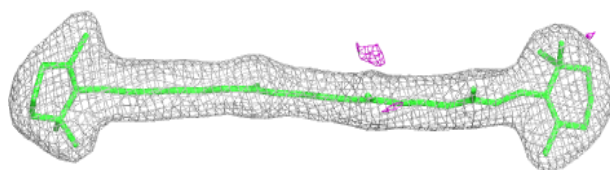
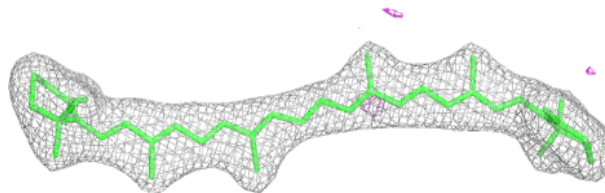
**Electron density around CLA B 607:**

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

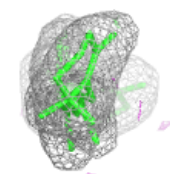
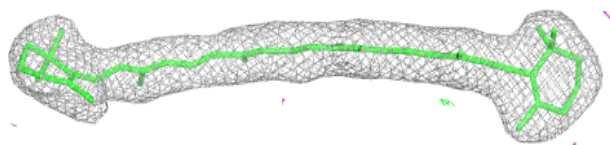
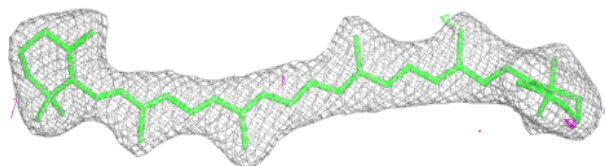


Electron density around BCR a 410:

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

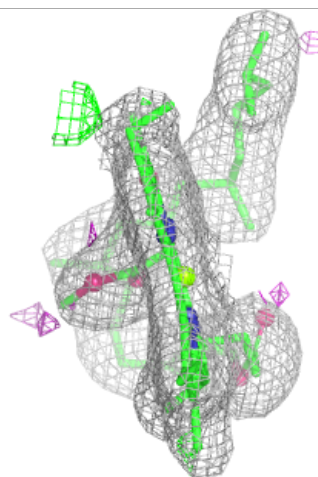
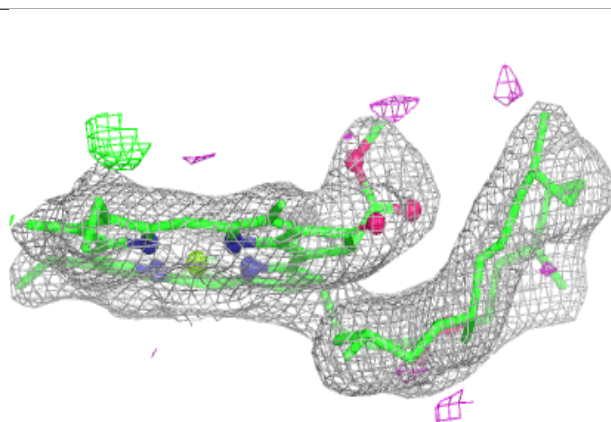
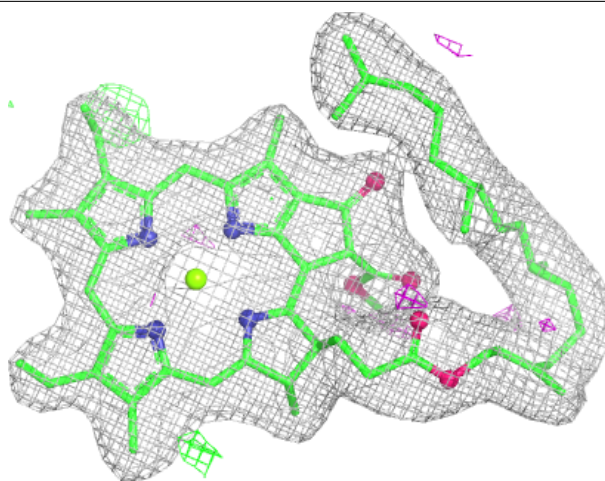
**Electron density around BCR b 617:**

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



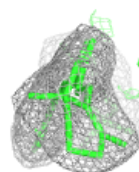
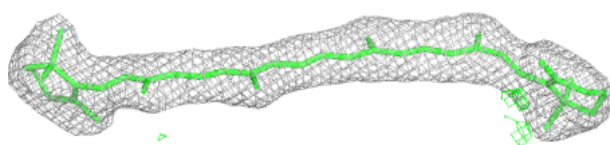
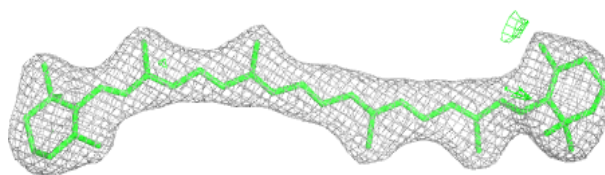
Electron density around CLA b 610:

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



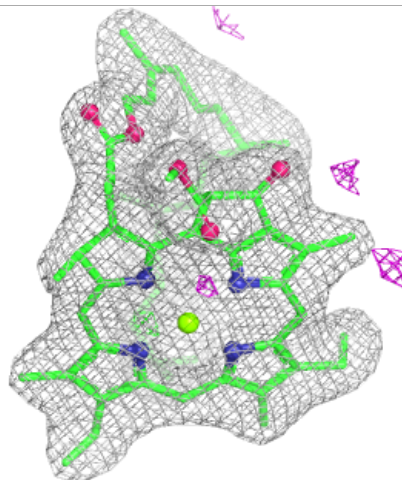
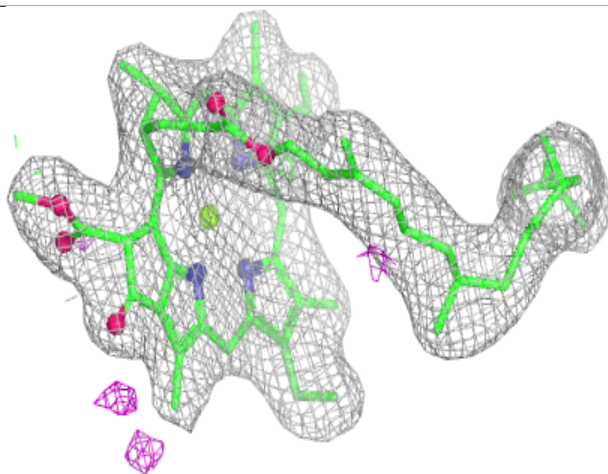
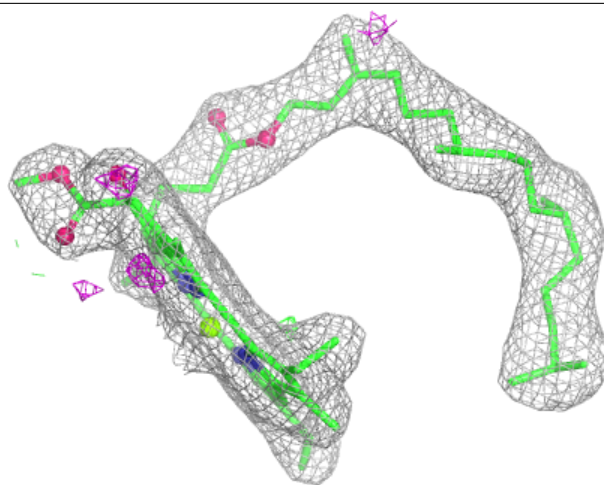
Electron density around BCR b 619:

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



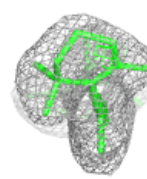
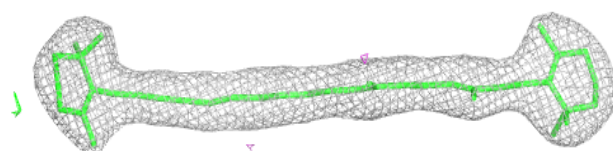
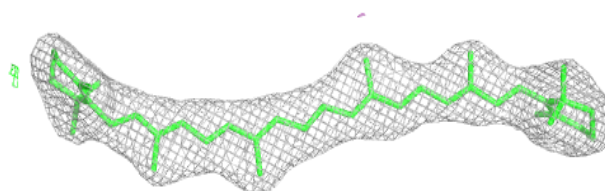
Electron density around CLA b 611:

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

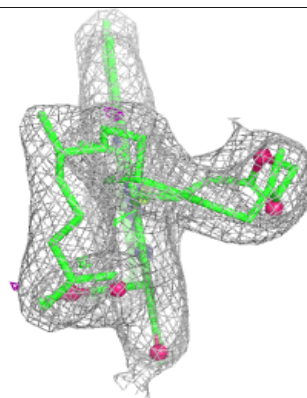
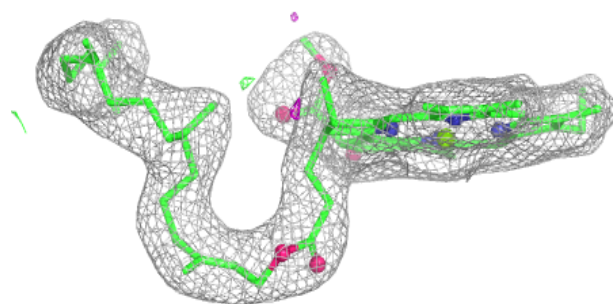
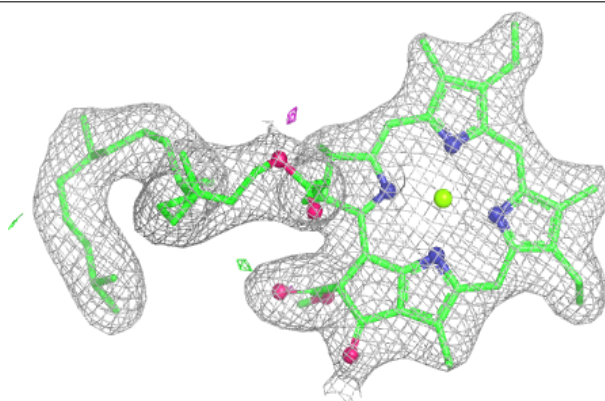


Electron density around BCR c 516:

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

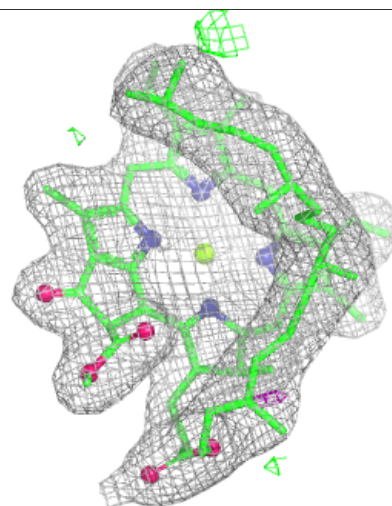
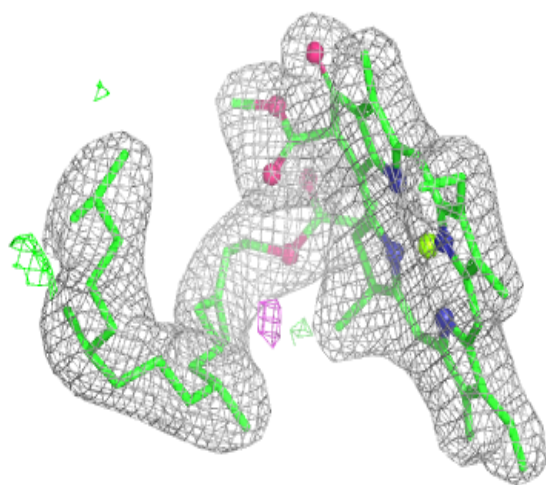
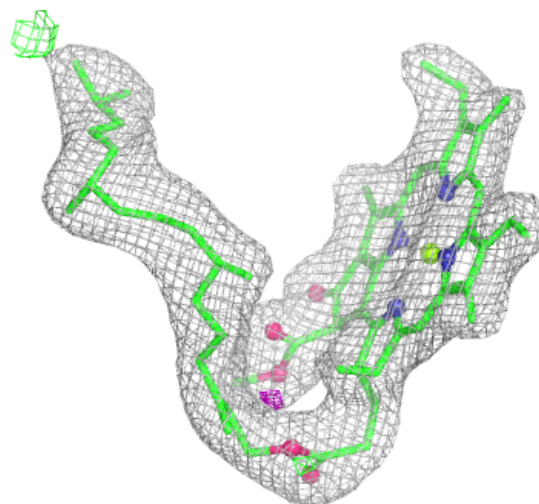
**Electron density around CLA b 612:**

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



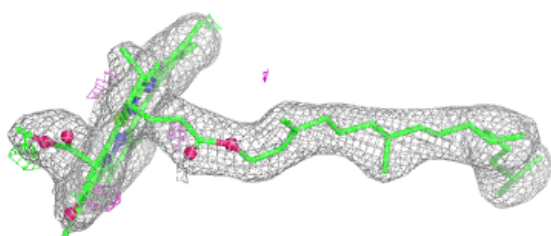
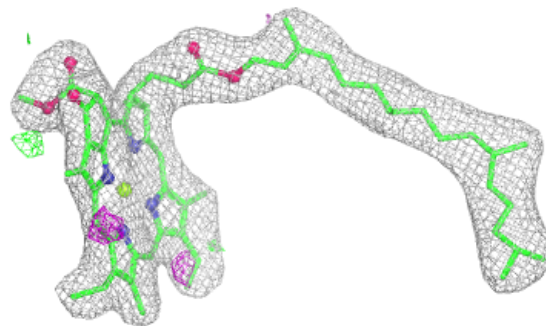
Electron density around CLA b 613:

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



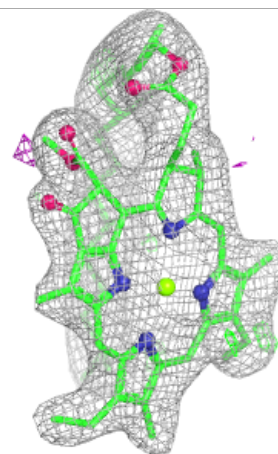
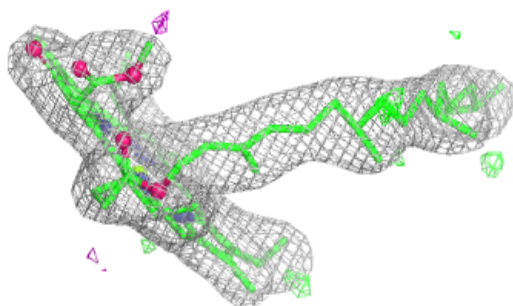
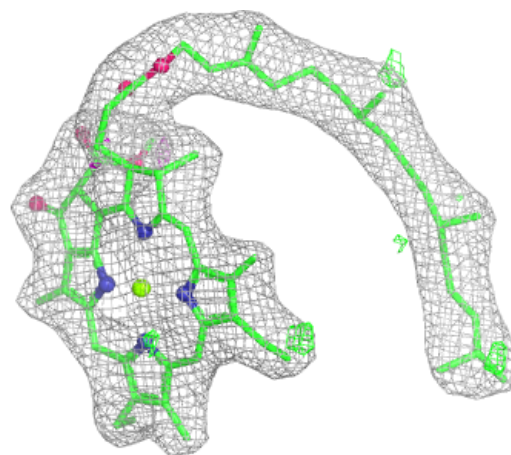
Electron density around CLA B 609:

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



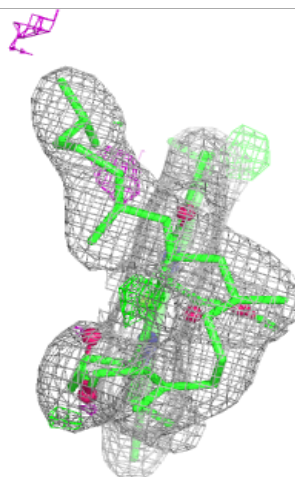
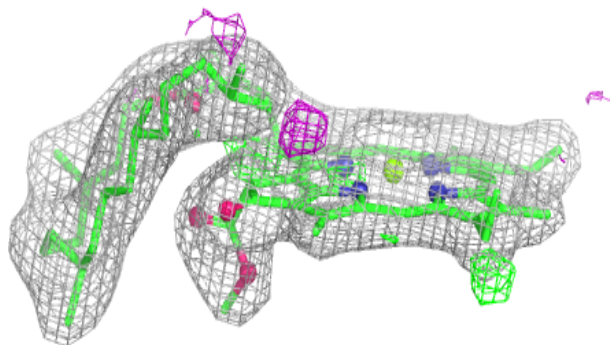
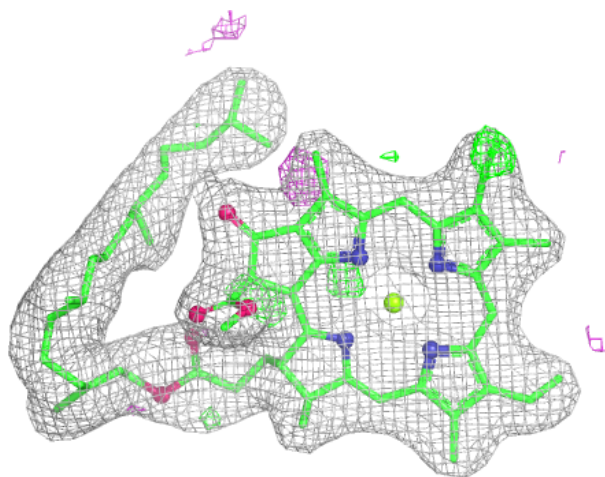
Electron density around CLA C 508:

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



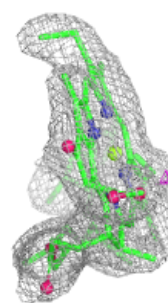
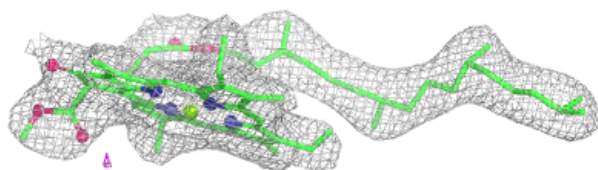
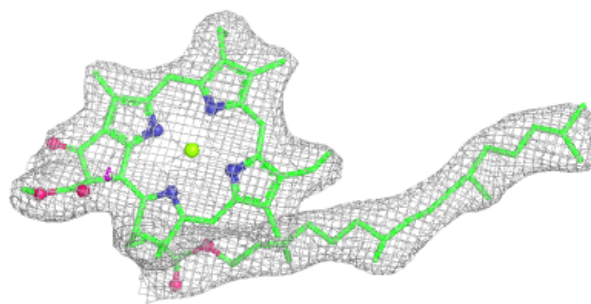
Electron density around CLA B 610:

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

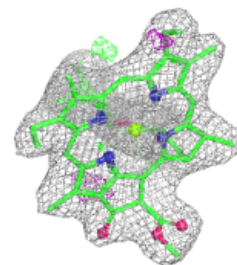
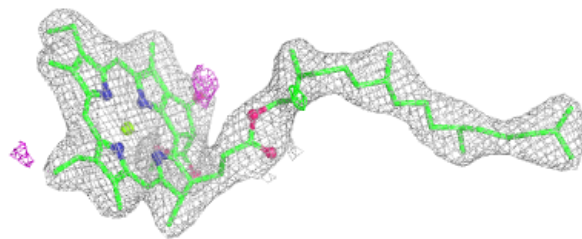
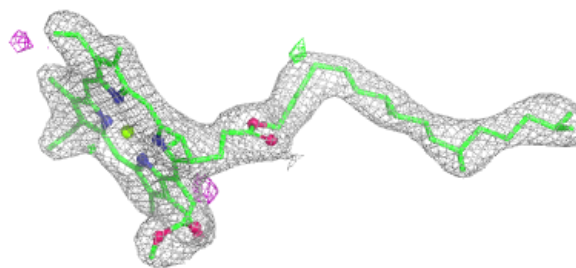


Electron density around CLA c 502:

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

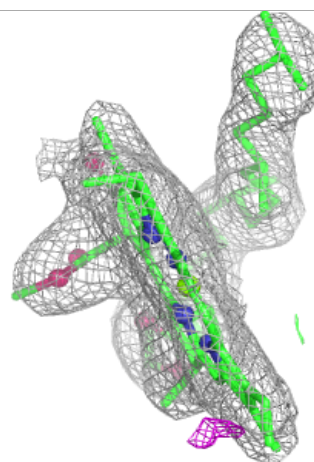
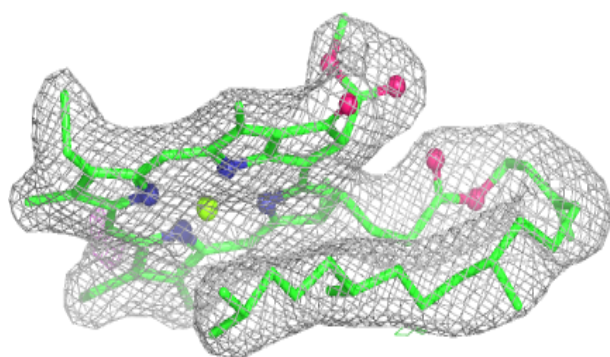
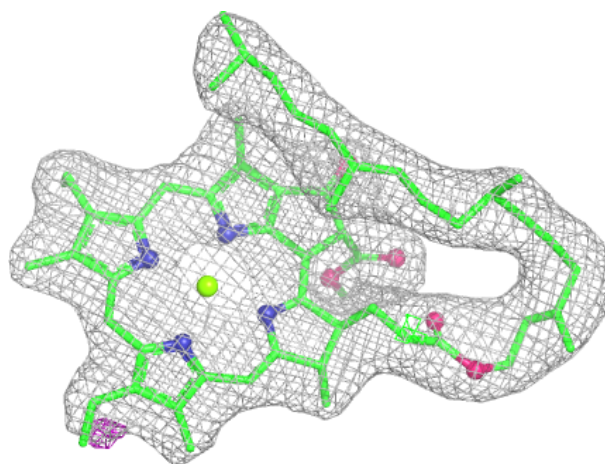
**Electron density around CLA c 503:**

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



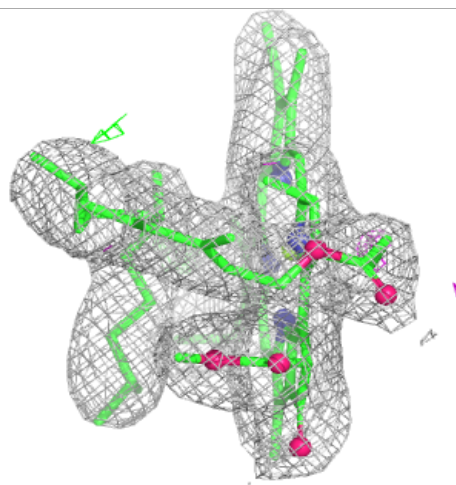
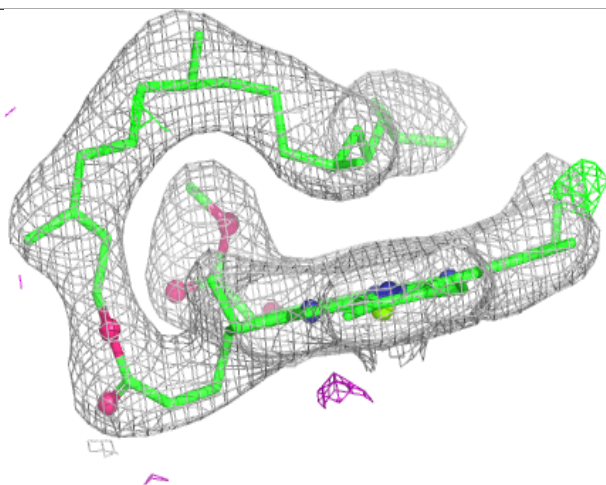
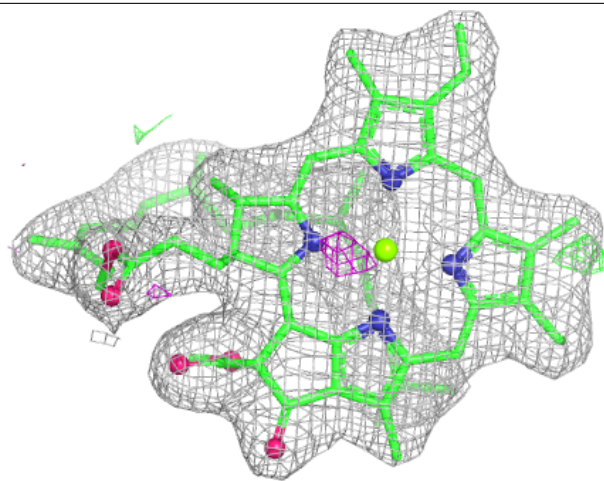
Electron density around CLA C 510:

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



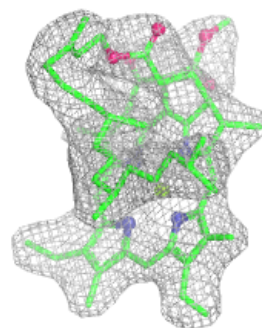
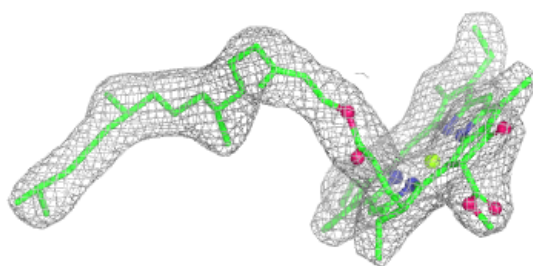
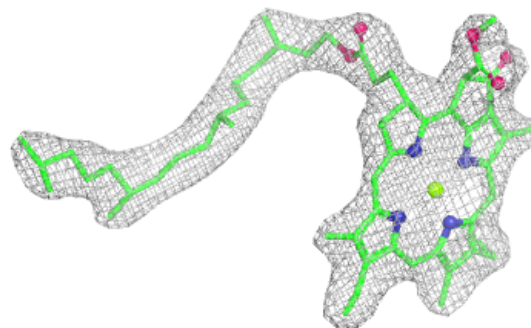
Electron density around CLA C 511:

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



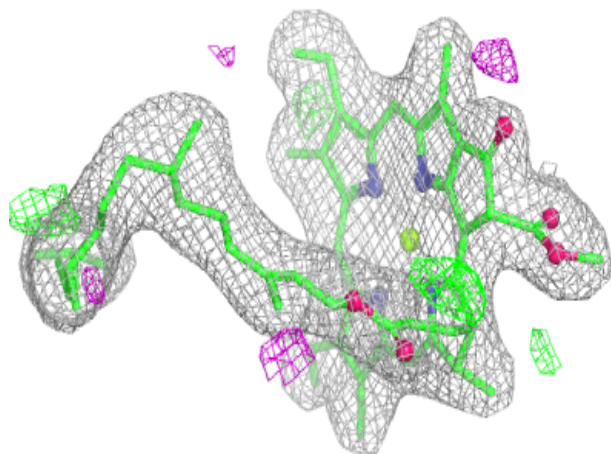
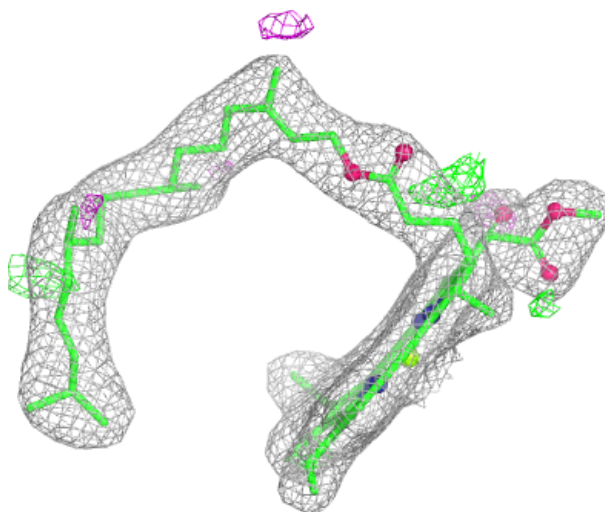
Electron density around CLA C 512:

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



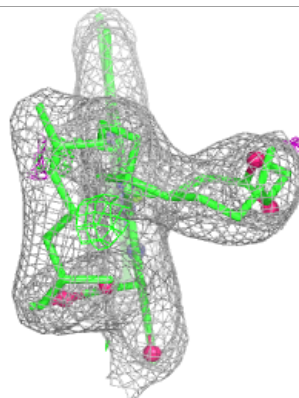
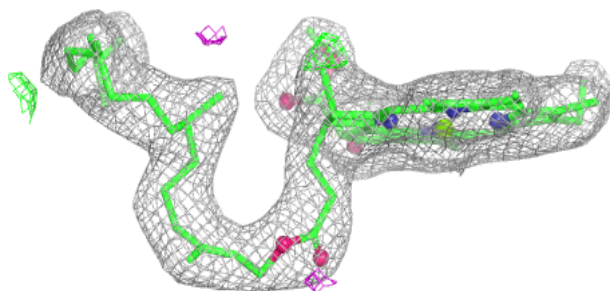
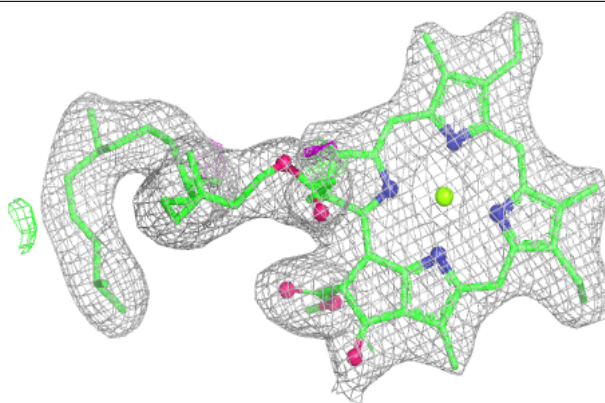
Electron density around CLA B 611:

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

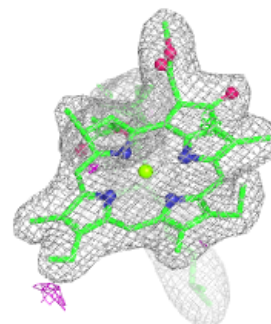
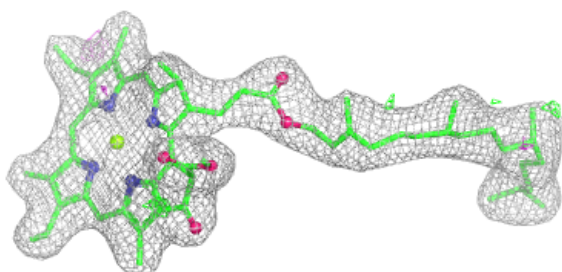
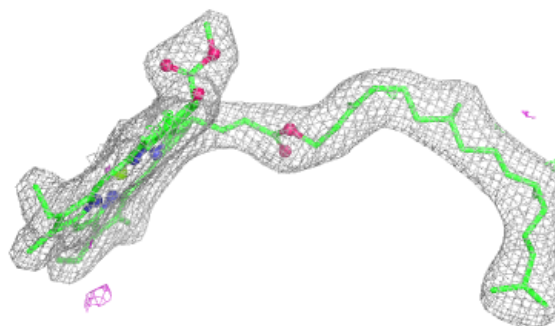


Electron density around CLA B 612:

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

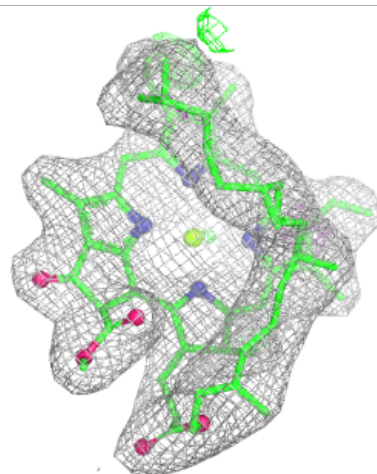
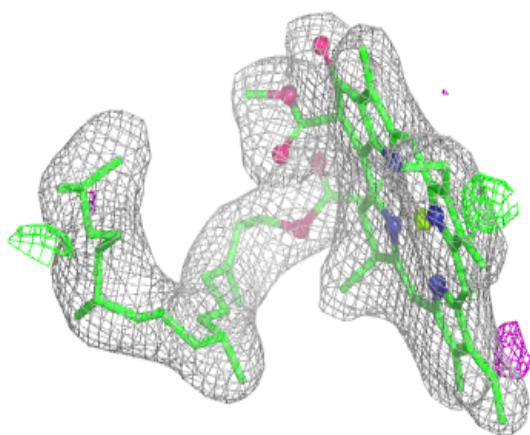
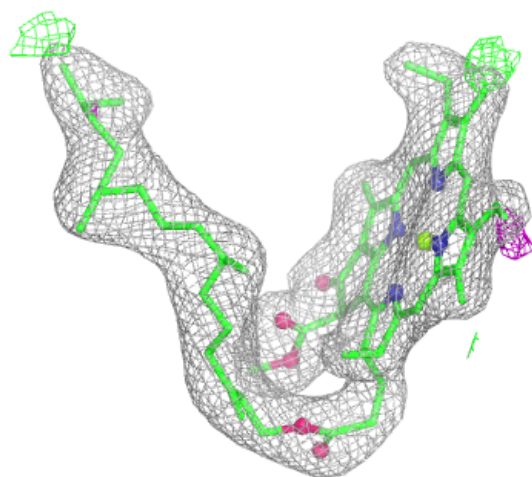
**Electron density around CLA D 405:**

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



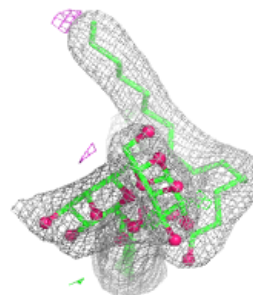
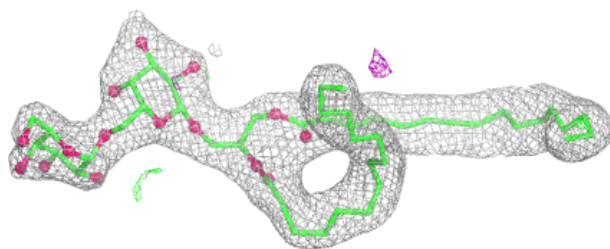
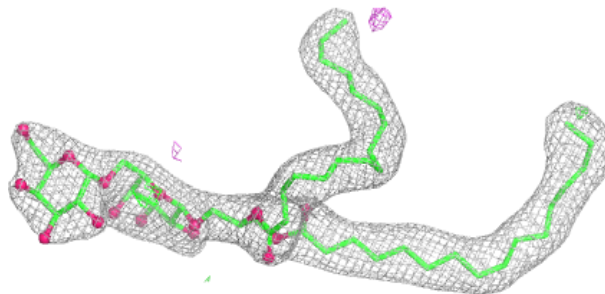
Electron density around CLA B 613:

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



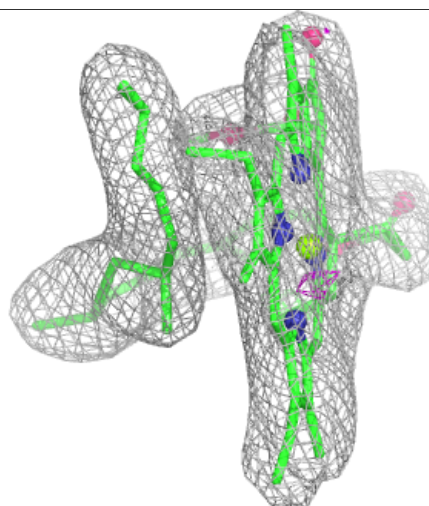
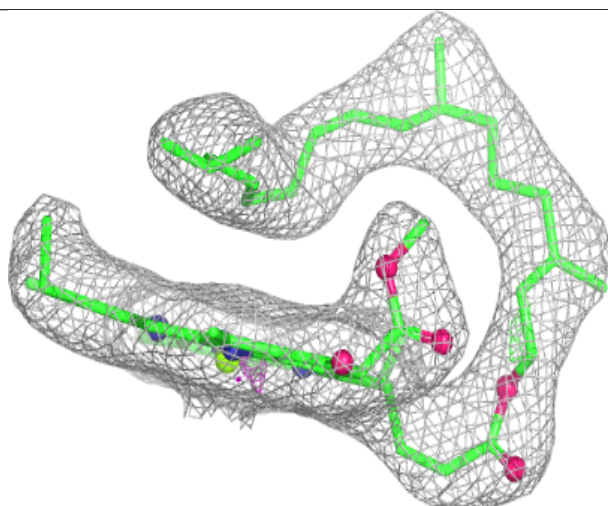
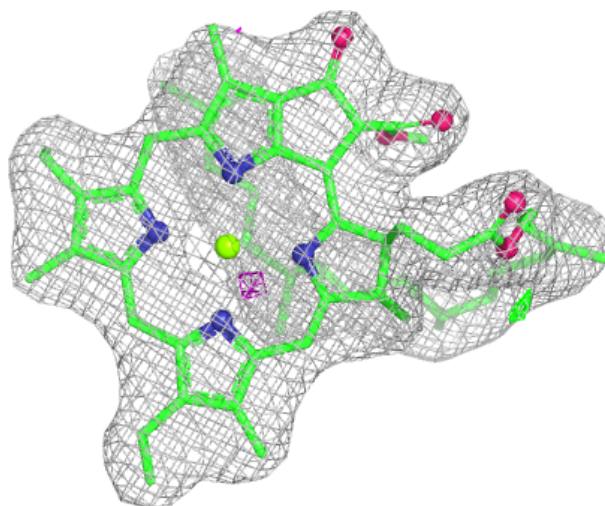
Electron density around DGD h 102:

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



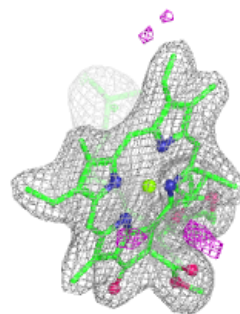
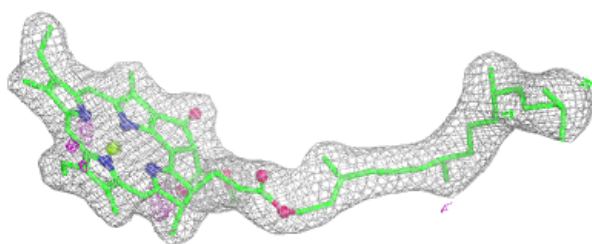
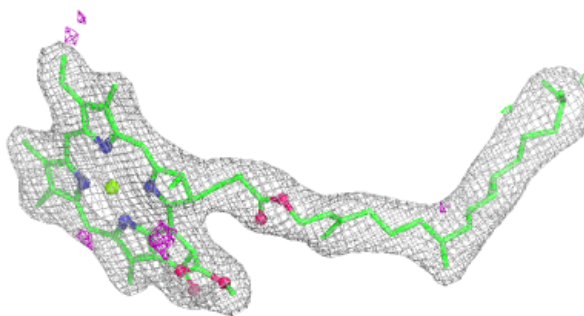
Electron density around CLA c 511:

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

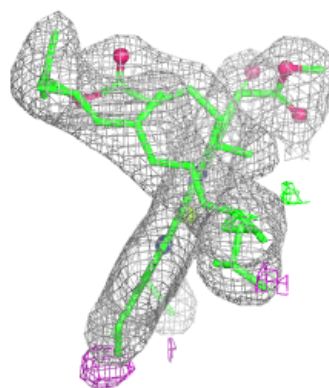
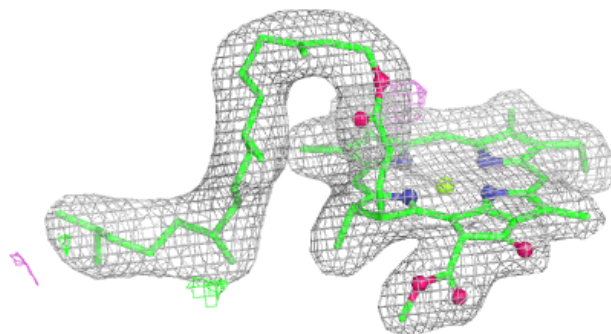
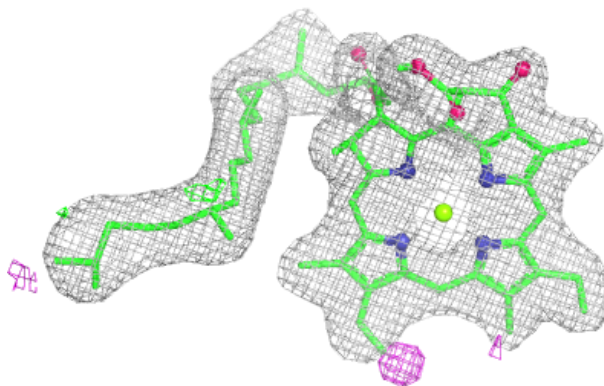


Electron density around CLA a 405:

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

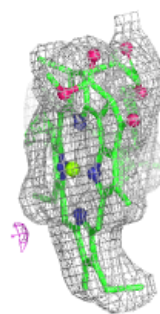
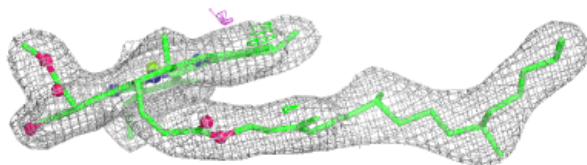
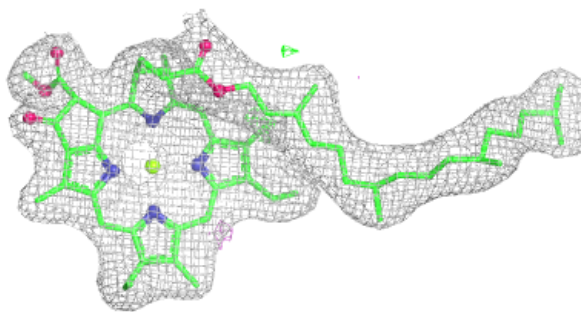
**Electron density around CLA a 406:**

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



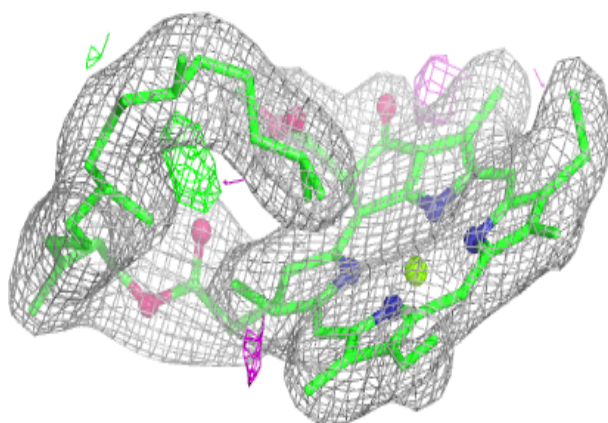
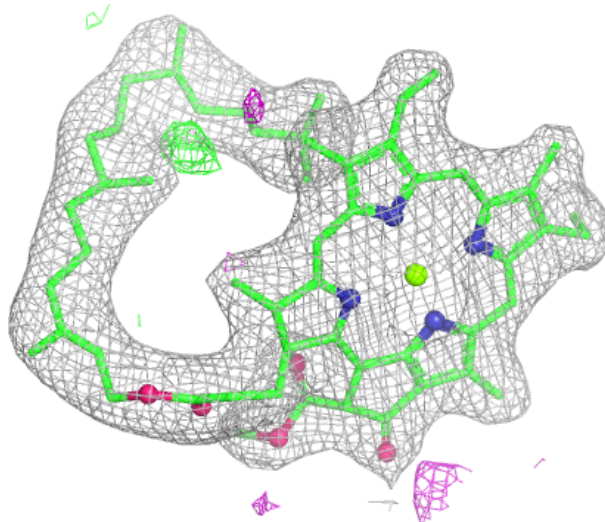
Electron density around CLA B 603:

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



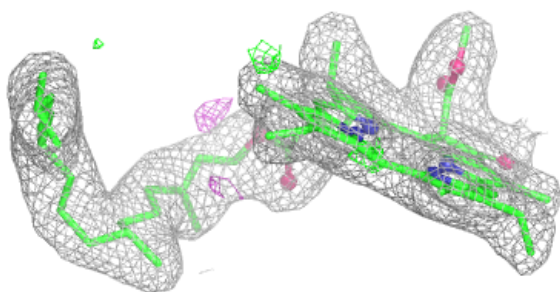
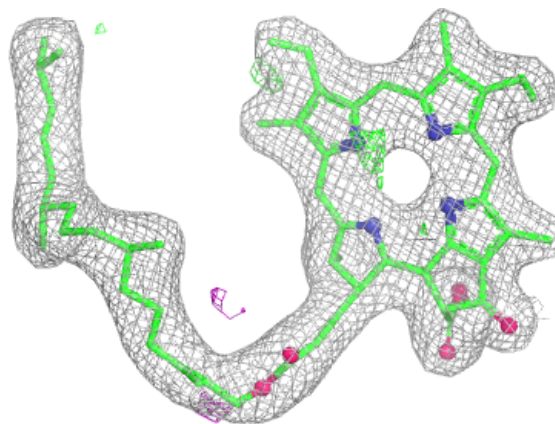
Electron density around CLA B 615:

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



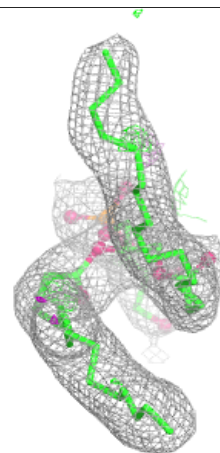
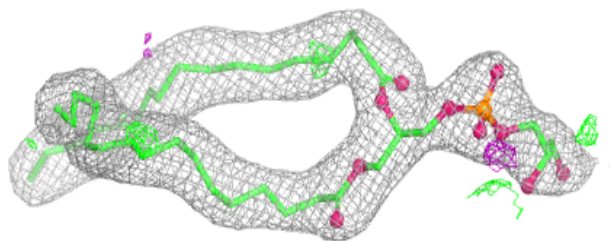
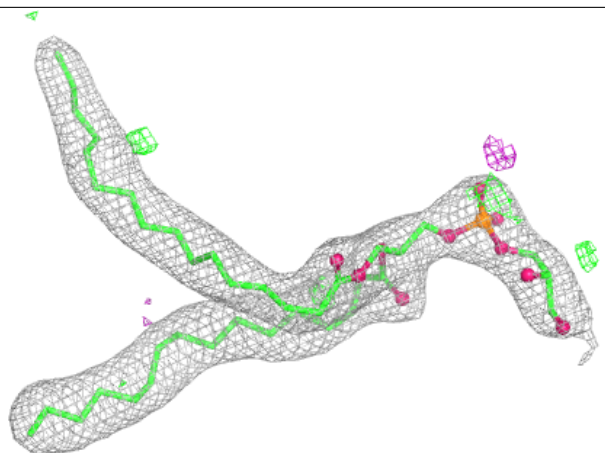
Electron density around PHO A 353:

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



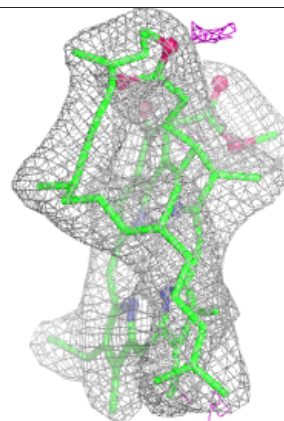
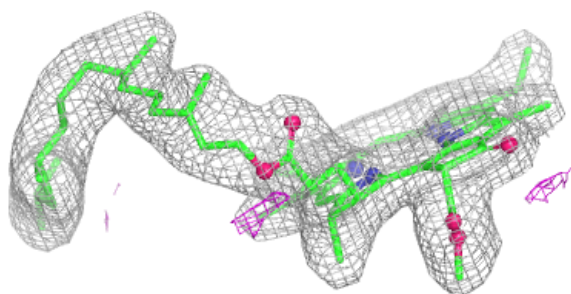
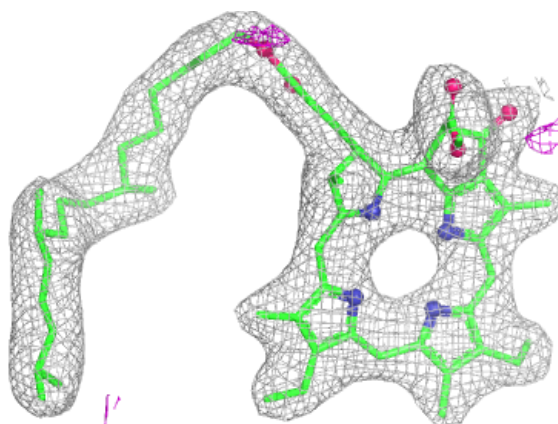
Electron density around LHG D 410:

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



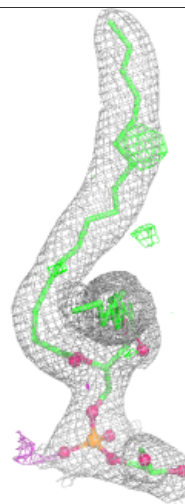
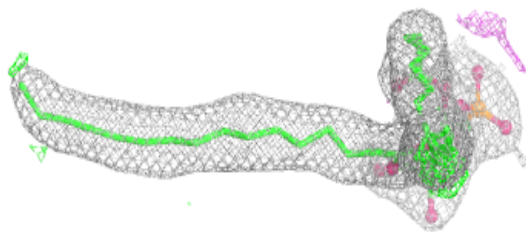
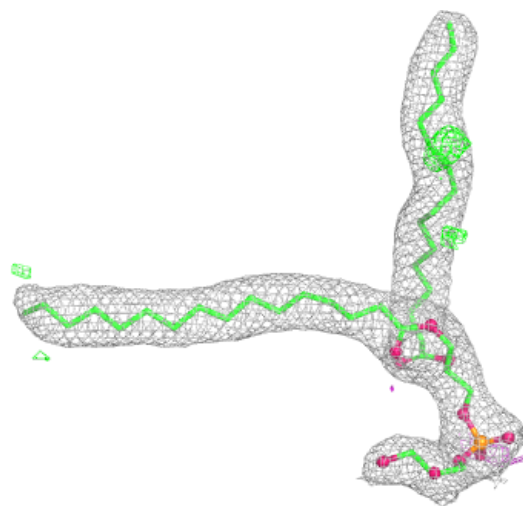
Electron density around PHO a 353:

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



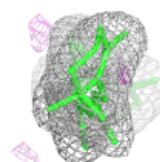
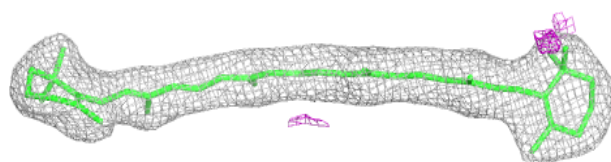
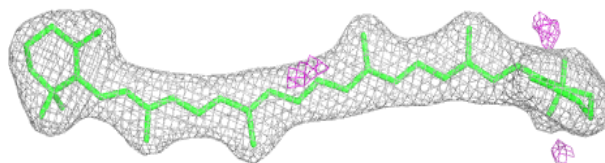
Electron density around LHG L 101:

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



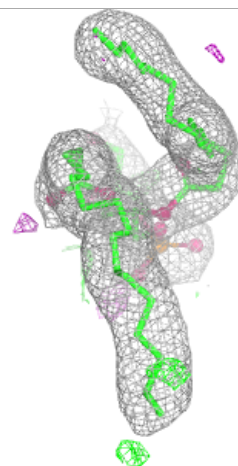
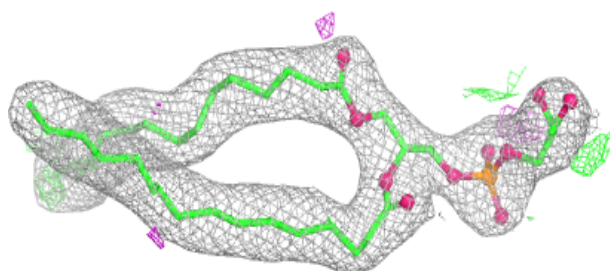
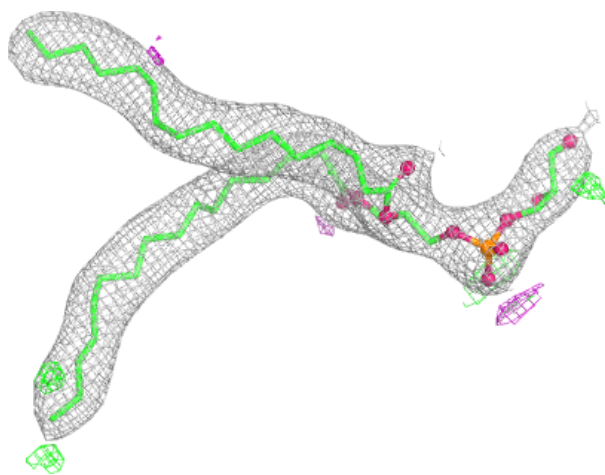
Electron density around BCR B 617:

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



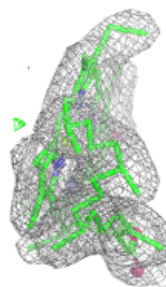
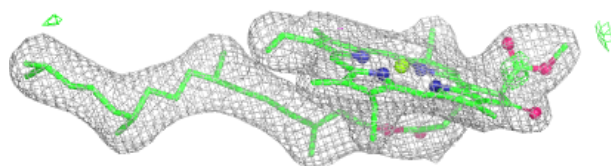
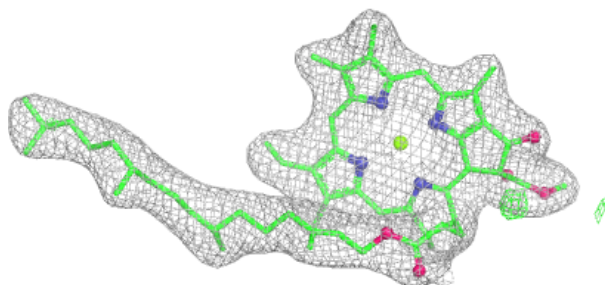
Electron density around LHG d 407:

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

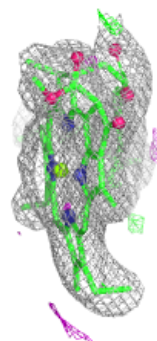
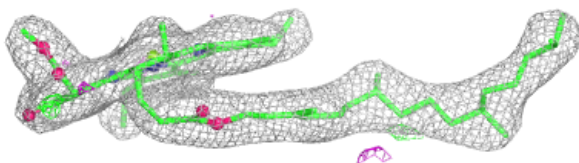
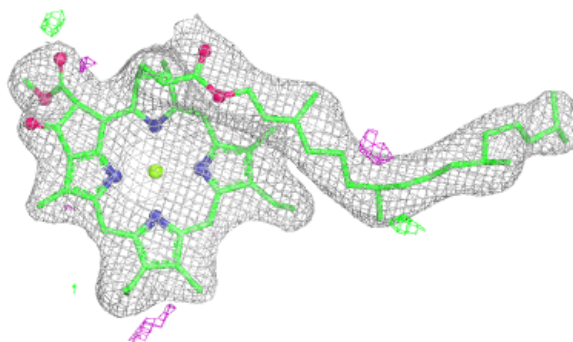


Electron density around CLA C 502:

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

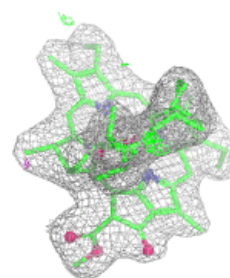
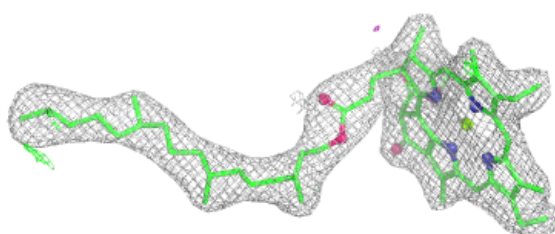
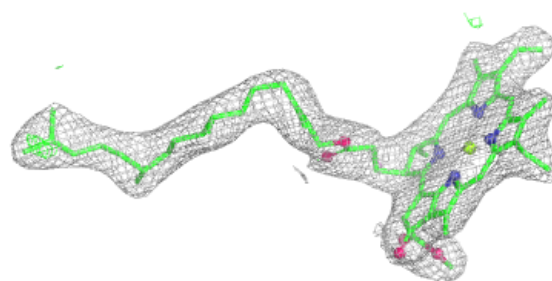
**Electron density around CLA b 603:**

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

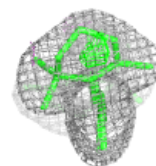
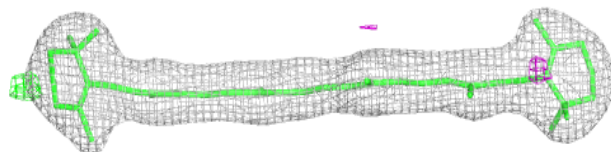
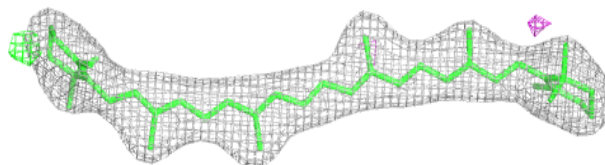


Electron density around CLA C 503:

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

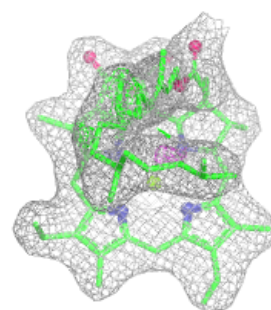
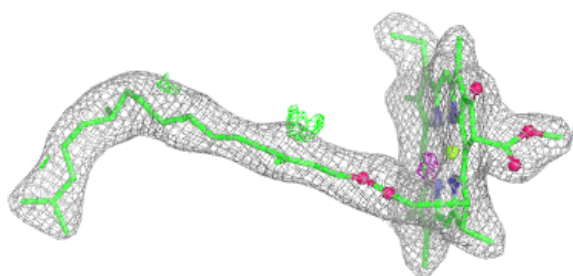
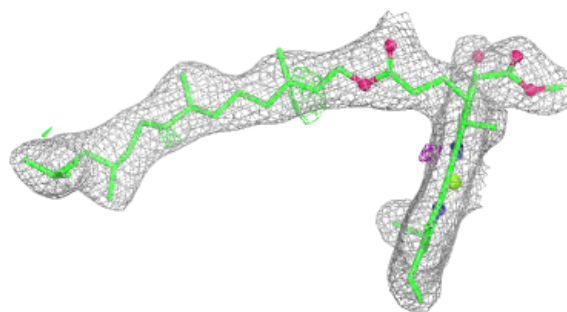
**Electron density around BCR C 516:**

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

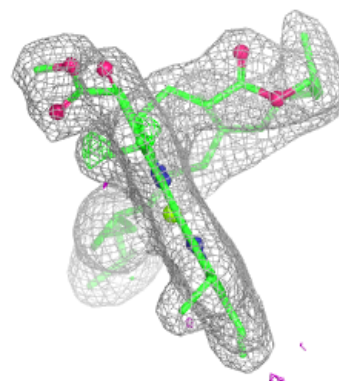
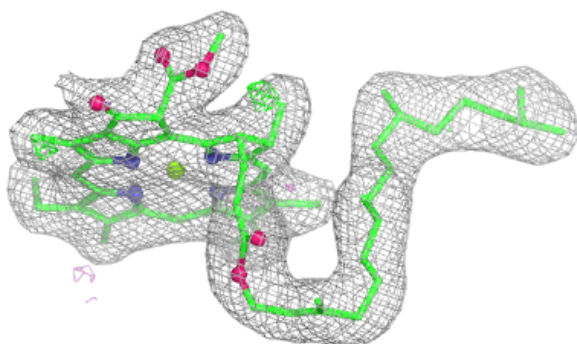
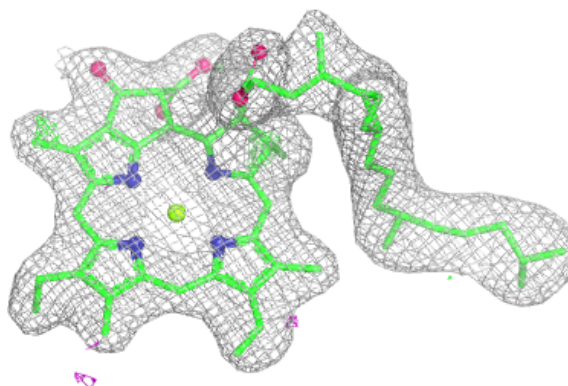


Electron density around CLA b 605:

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

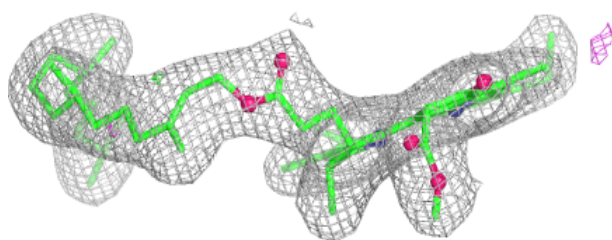
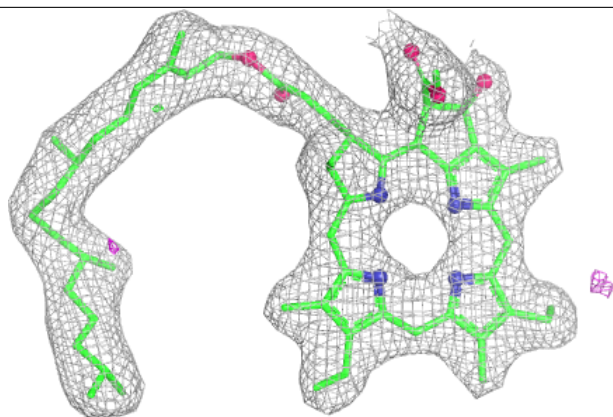
**Electron density around CLA A 405:**

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

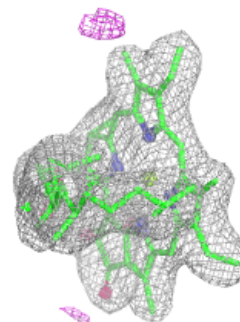
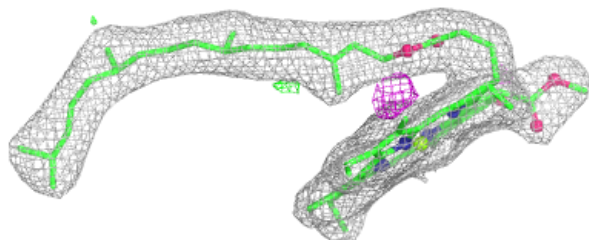
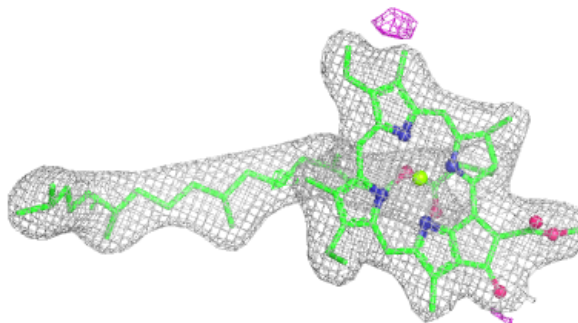


Electron density around PHO A 407:

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

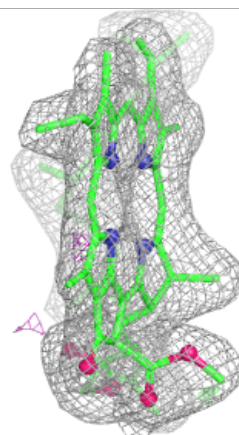
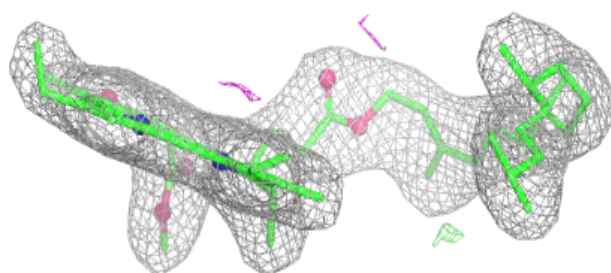
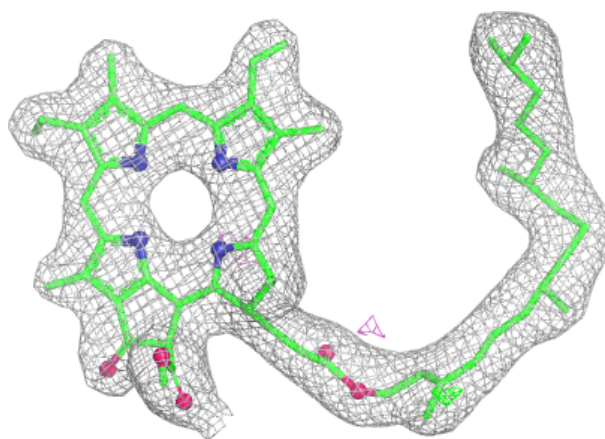
**Electron density around CLA B 608:**

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



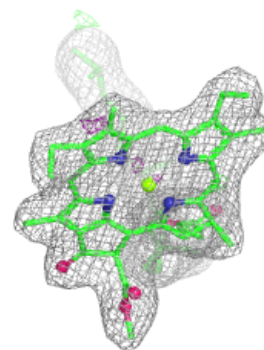
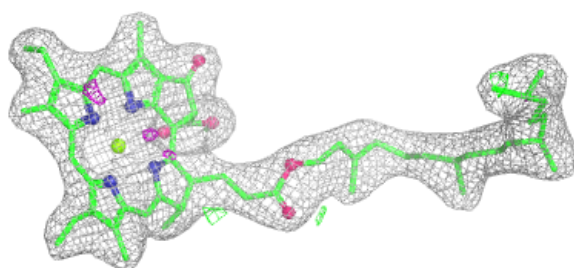
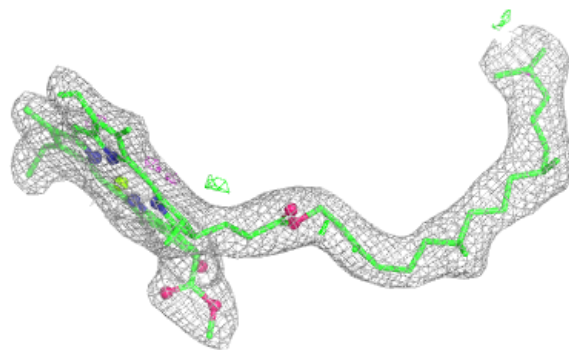
Electron density around PHO a 408:

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



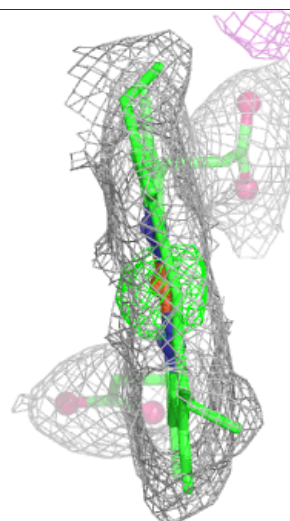
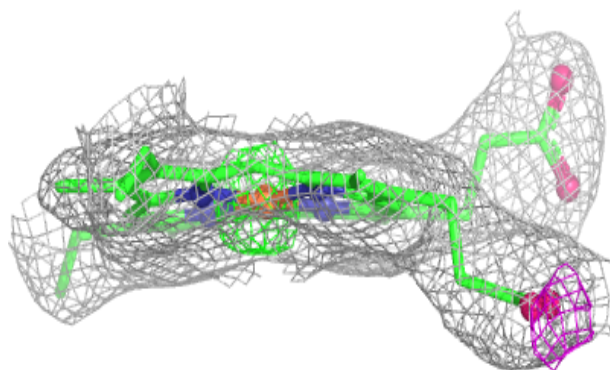
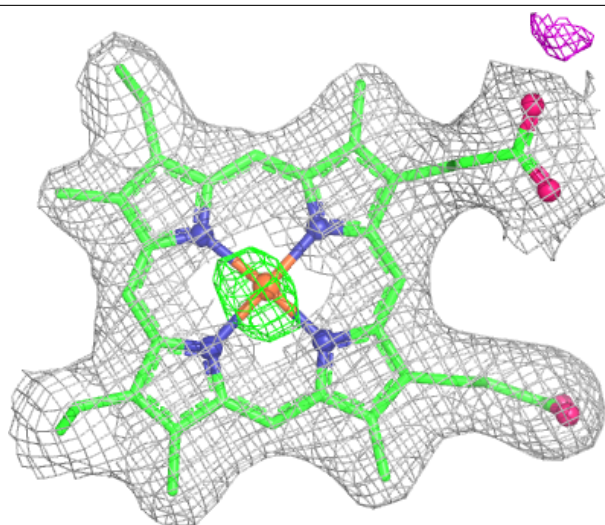
Electron density around CLA d 402:

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



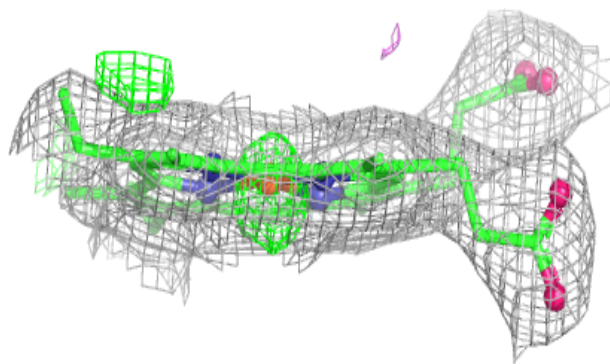
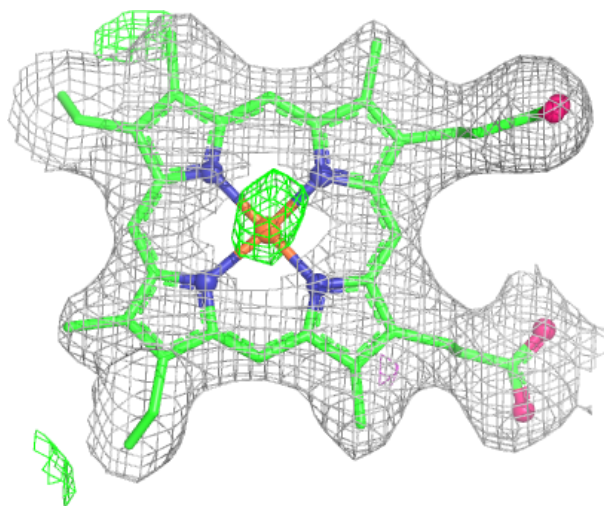
Electron density around HEC V 202:

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



Electron density around HEC v 202:

$2mF_o-DF_c$ (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.