



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:01 AM UTC

PDB ID : 7COU / pdb_00007cou
Title : Structure of cyanobacterial photosystem II in the dark S1 state
Authors : Li, H.; Shen, J.-R.; Suga, M.
Deposited on : 2020-08-05
Resolution : 2.25 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

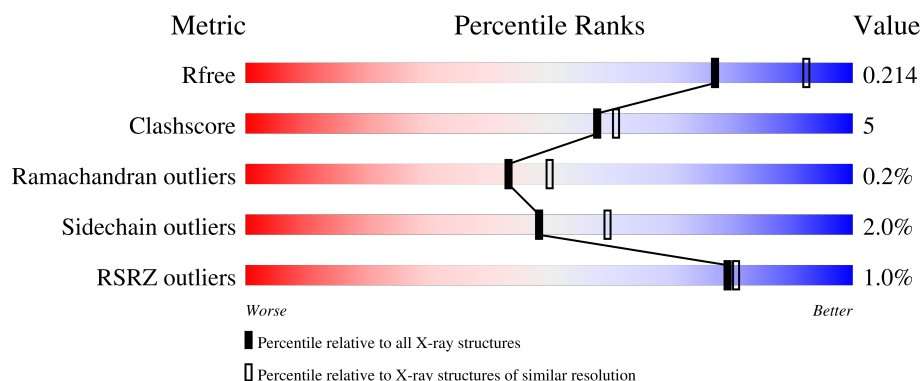
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.



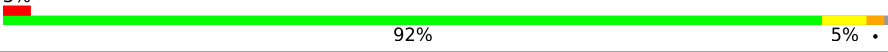
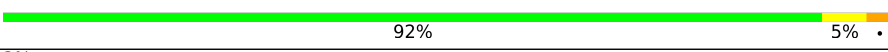
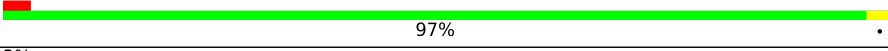
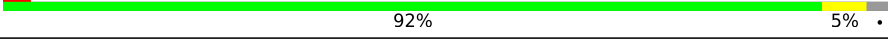
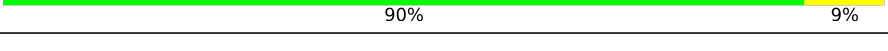
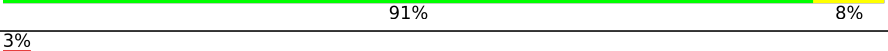
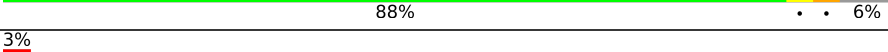
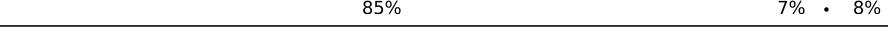
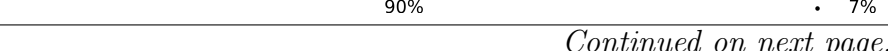
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	505	
2	b	505	
3	C	455	

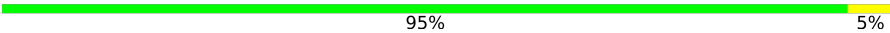
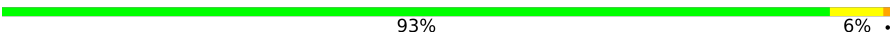
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Mol	Chain	Length	Quality of chain
3	c	455	 91% 8%
4	D	342	 92% 8%
4	d	342	 89% 10% .
5	E	84	 69% 27% .
5	e	84	 85% 7% . 6%
6	F	44	 64% 14% 23%
6	f	44	 64% 7% 30%
7	H	65	 92% 5% . .
7	h	65	 89% 8% . .
8	I	38	 92% 5% .
8	i	38	 97% .
9	J	39	 82% 8% 8% .
9	j	39	 85% 15%
10	K	37	 86% 14%
10	k	37	 84% 16%
11	L	37	 89% 8% .
11	l	37	 92% 5% .
12	M	36	 78% 14% 8%
12	m	36	 75% 17% . 6%
13	O	244	 90% 9%
13	o	244	 91% 8%
14	T	32	 88% . . 6%
14	t	32	 88% 6% 6%
15	U	104	 85% 7% . 8%
15	u	104	 90% . 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	503	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	403	X	-	-	-
23	CLA	D	404	X	-	-	-
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	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	c	515	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 53138 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	2	0
			2634	1725	433	461	15			
1	a	334	Total	C	N	O	S	0	3	0
			2642	1731	434	462	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
a	279	PRO	ARG	conflict	UNP P51765

- 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	10	0
			4050	2650	677	710	13			
2	b	504	Total	C	N	O	S	0	4	0
			3998	2622	665	698	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3513	2295	588	617	13			
3	c	455	Total	C	N	O	S	0	2	0
			3534	2311	591	619	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O		0	1	0
			668	435	108	125				
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
			517	345	85	85	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 reaction center protein K.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054
k	33	LEU	PHE	conflict	UNP P19054
k	39	TRP	VAL	conflict	UNP P19054

- 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
			304	203	48	53			
11	l	36	Total	C	N	O	0	1	0
			304	203	48	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			268	179	39	49	1			
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	8	LEU	PHE	conflict	UNP P12312

- 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	3	0
			1886	1177	318	386	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	o	243	Total	C	N	O	S	0	2	0
			1879	1173	317	384	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	S	0	0	0
			765	486	128	151				
15	u	97	Total	C	N	O	S	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	S	0	0	0
			281	188	45	48				
17	x	38	Total	C	N	O	S	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		
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).



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

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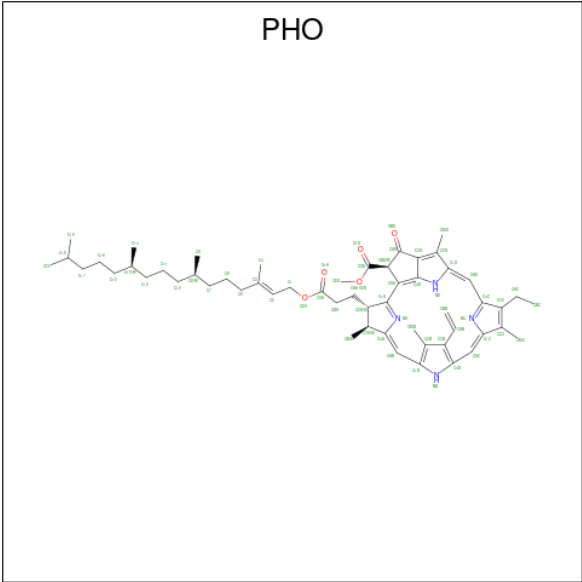
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23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55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

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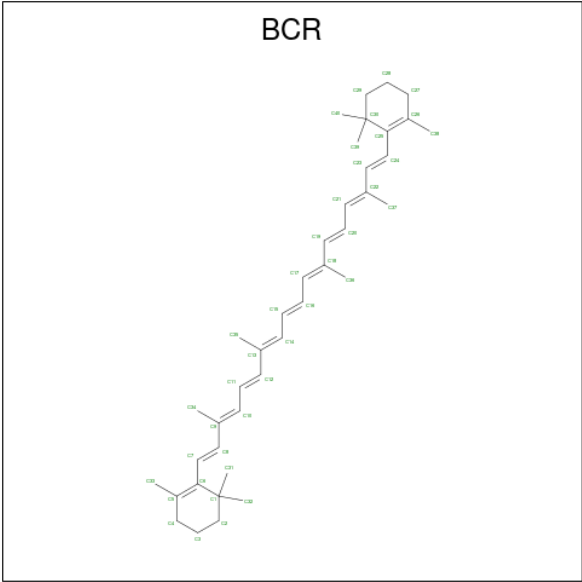
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



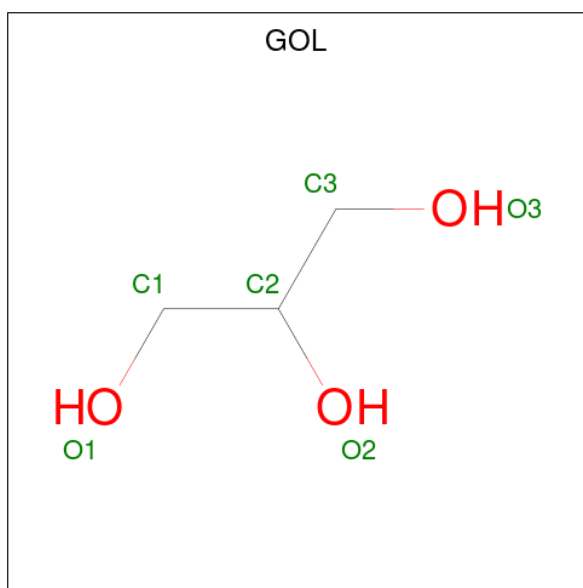
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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
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

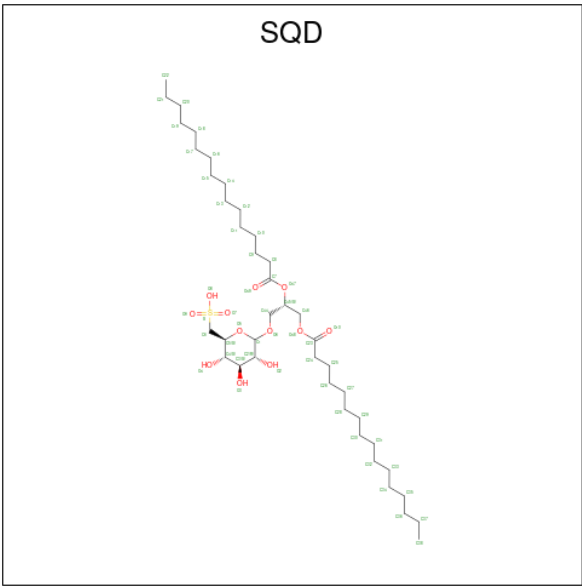
- Molecule 26 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	O	0	0
			6	3	3		
26	B	1	Total	C	O	0	0
			6	3	3		
26	B	1	Total	C	O	0	0
			6	3	3		
26	B	1	Total	C	O	0	0
			6	3	3		
26	C	1	Total	C	O	0	0
			6	3	3		
26	O	1	Total	C	O	0	0
			6	3	3		
26	a	1	Total	C	O	0	0
			6	3	3		
26	b	1	Total	C	O	0	0
			6	3	3		
26	b	1	Total	C	O	0	0
			6	3	3		
26	c	1	Total	C	O	0	0
			6	3	3		
26	o	1	Total	C	O	0	0
			6	3	3		
26	v	1	Total	C	O	0	0
			6	3	3		

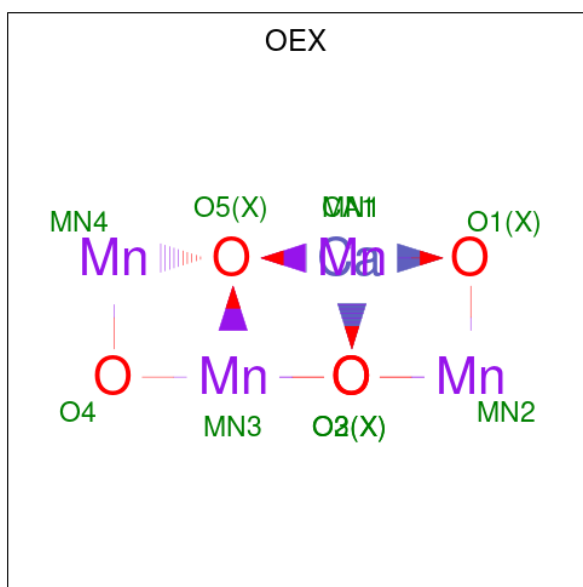
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



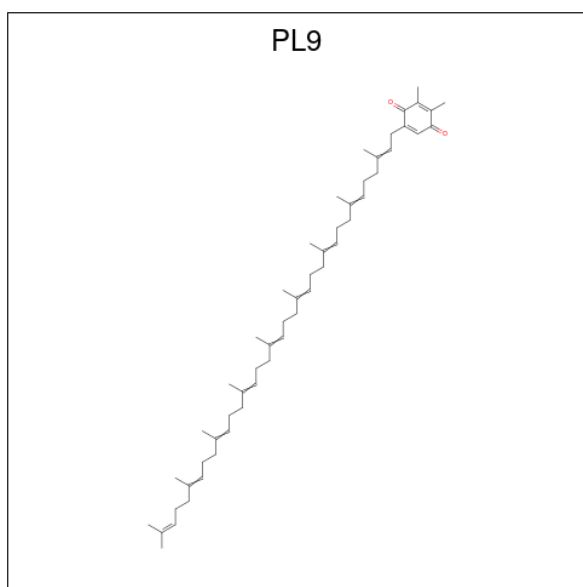
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	C	1	Total	C	O	S	0	0
			54	41	12	1		
27	D	1	Total	C	O	S	0	0
			43	30	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn₄O₅).



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: C₅₃H₈₀O₂).



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

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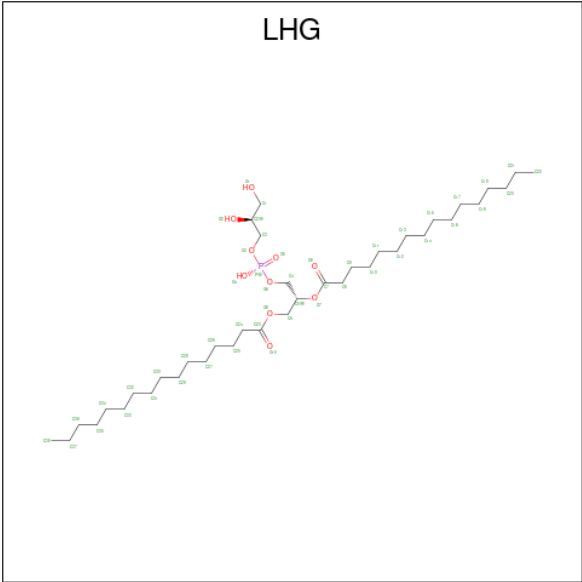
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	D	1	Total	C	O	0	0
			55	53	2		
29	a	1	Total	C	O	0	0
			55	53	2		
29	d	1	Total	C	O	0	0
			55	53	2		

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

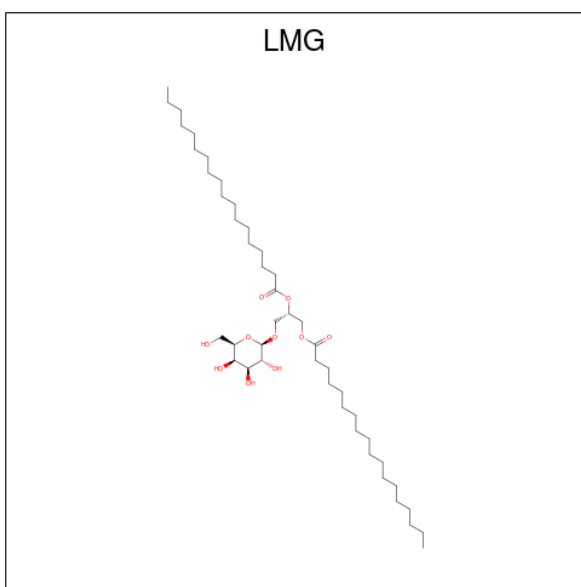
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	C	1	Total	C	O	0	0
			34	29	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	M	1	Total	C		0	0
			10	10			
30	X	1	Total	C	O	0	0
			18	16	2		
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	3	Total	C	O	0	0
			71	63	8		
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			

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



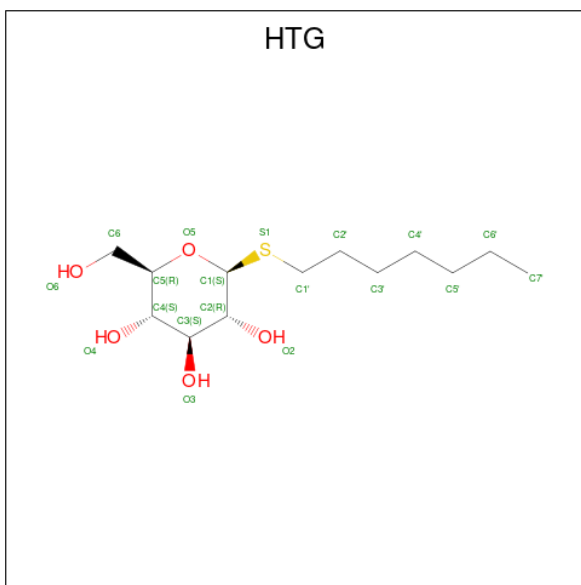
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			42	31	10	1		
31	b	1	Total	C	O	P	0	0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

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



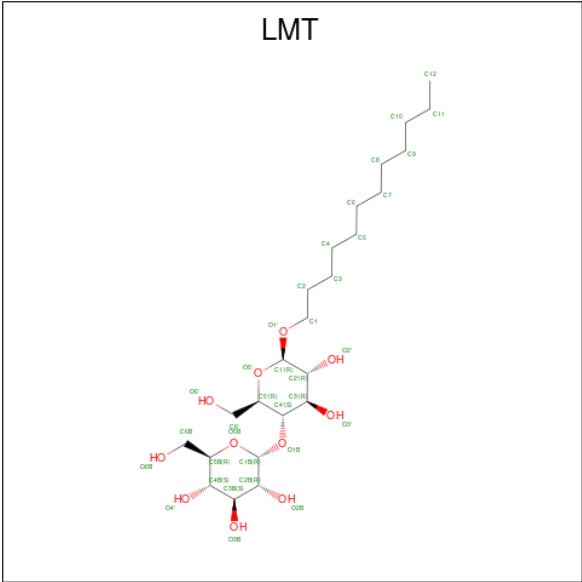
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	D	1	Total	C	O	0	0
			51	41	10		
32	Z	1	Total	C	O	0	0
			37	27	10		
32	c	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total	C	O	0	0
			51	41	10		
32	d	1	Total	C	O	0	0
			51	41	10		
32	m	1	Total	C	O	0	0
			51	41	10		
32	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 33 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



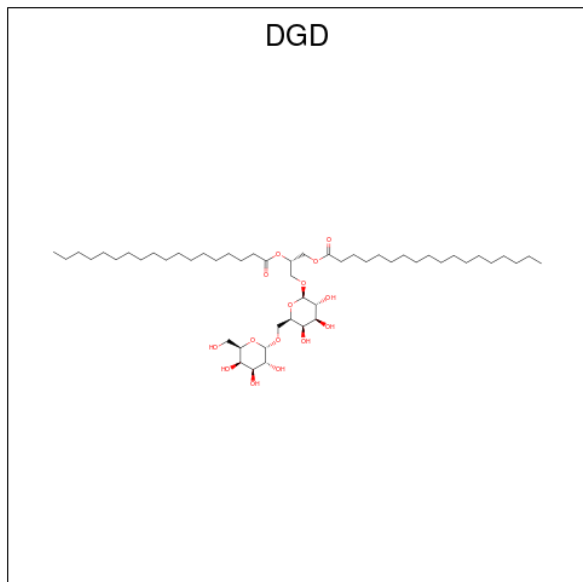
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	C	1	Total 19	C 13	O 5	S 1	0	0
33	D	1	Total 16	C 10	O 5	S 1	0	0
33	V	1	Total 11	C 6	O 5		0	0
33	b	1	Total 19	C 13	O 5	S 1	0	0
33	b	1	Total 19	C 13	O 5	S 1	0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

- Molecule 34 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

- 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).

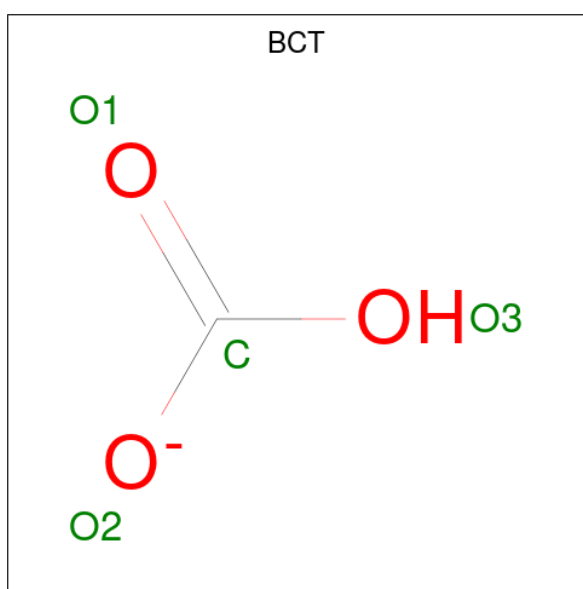
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	C	1	Total	Ca	0	0
			1	1		
36	F	1	Total	Ca	0	0
			1	1		

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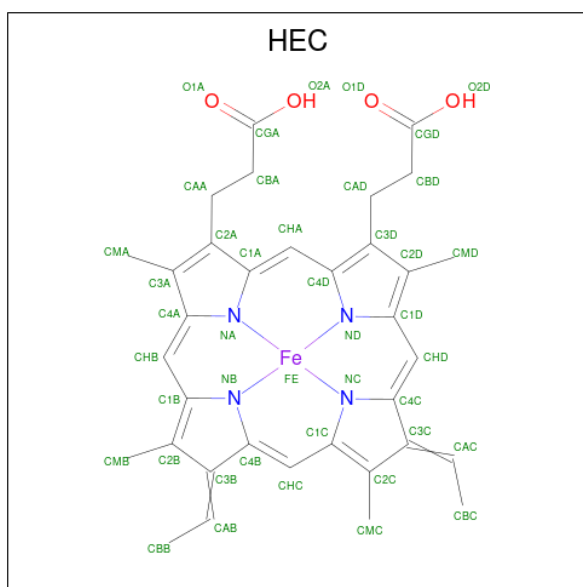
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total	Ca	0	0
			1	1		
36	a	1	Total	Ca	0	0
			1	1		
36	c	2	Total	Ca	0	0
			2	2		
36	o	1	Total	Ca	0	0
			1	1		

- Molecule 37 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	D	1	Total	C	O	0	0
			4	1	3		
37	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 38 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
38	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
38	V	1	Total	C	Fe	N	O	
			43	34	1	4	4	
38	e	1	Total	C	Fe	N	O	
			43	34	1	4	4	
38	v	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	143	Total	O		
			143	143	0	0
40	B	223	Total	O		
			223	223	0	0
40	C	203	Total	O		
			203	203	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	D	136	Total O 136 136	0	0
40	E	27	Total O 27 27	0	0
40	F	9	Total O 9 9	0	0
40	H	26	Total O 26 26	0	0
40	I	5	Total O 5 5	0	0
40	J	5	Total O 5 5	0	0
40	K	7	Total O 7 7	0	0
40	L	6	Total O 6 6	0	0
40	M	17	Total O 17 17	0	0
40	O	125	Total O 125 125	0	0
40	T	16	Total O 16 16	0	0
40	U	56	Total O 56 56	0	0
40	V	102	Total O 102 102	0	0
40	X	9	Total O 9 9	0	0
40	Y	1	Total O 1 1	0	0
40	R	1	Total O 1 1	0	0
40	a	143	Total O 143 143	0	0
40	b	234	Total O 234 234	0	0
40	c	174	Total O 174 174	0	0
40	d	125	Total O 125 125	0	0
40	e	16	Total O 16 16	0	0

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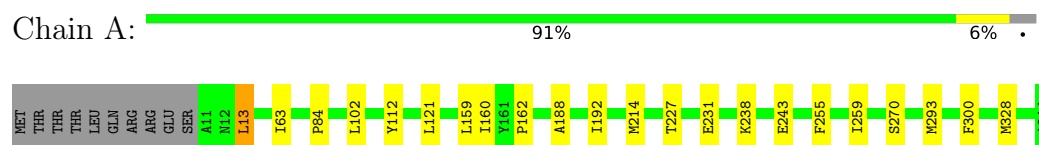
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	f	4	Total 4	O 4	0	0
40	h	23	Total 23	O 23	0	0
40	i	2	Total 2	O 2	0	0
40	j	3	Total 3	O 3	0	0
40	k	5	Total 5	O 5	0	0
40	l	7	Total 7	O 7	0	0
40	m	11	Total 11	O 11	0	0
40	o	99	Total 99	O 99	0	0
40	t	11	Total 11	O 11	0	0
40	u	71	Total 71	O 71	0	0
40	v	60	Total 60	O 60	0	0
40	x	9	Total 9	O 9	0	0
40	y	4	Total 4	O 4	0	0

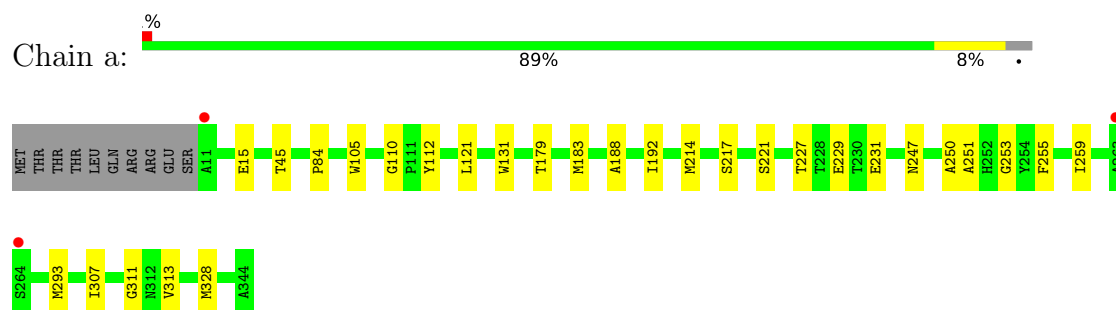
3 Residue-property plots

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

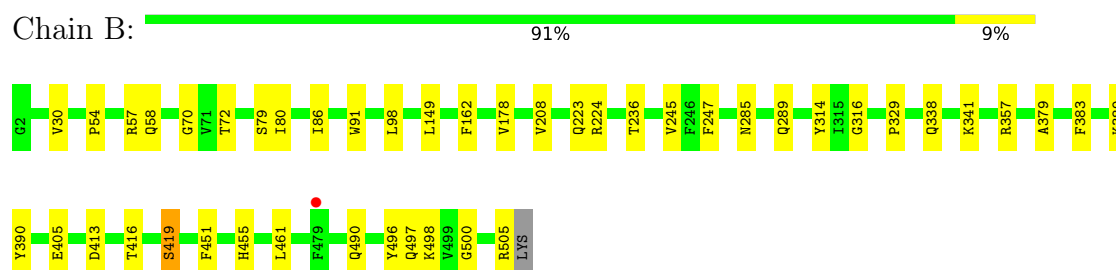
• Molecule 1: Photosystem II protein D1



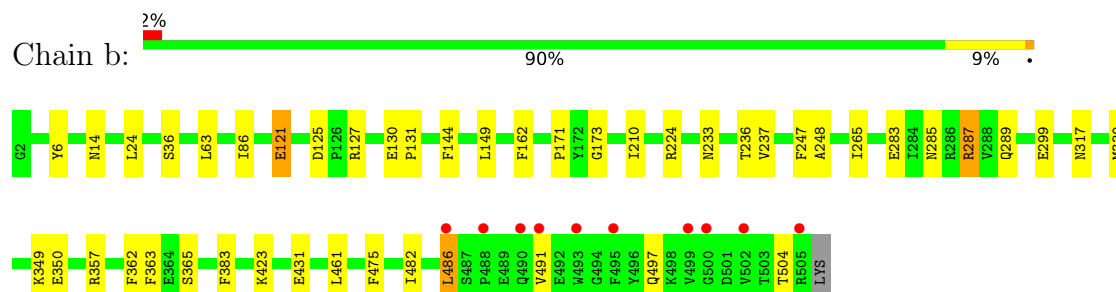
• Molecule 1: Photosystem II protein D1



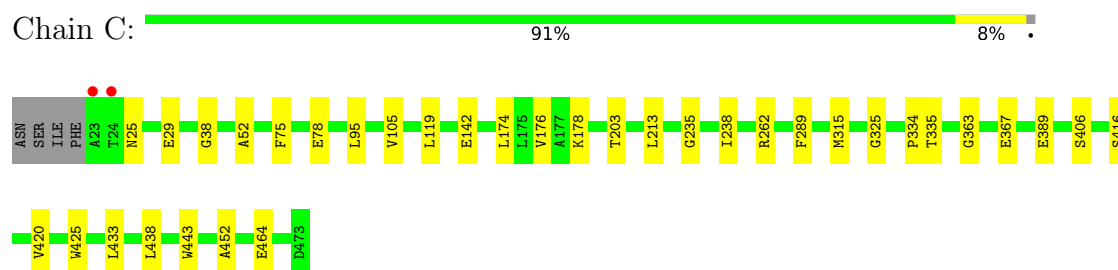
• Molecule 2: Photosystem II CP47 reaction center protein



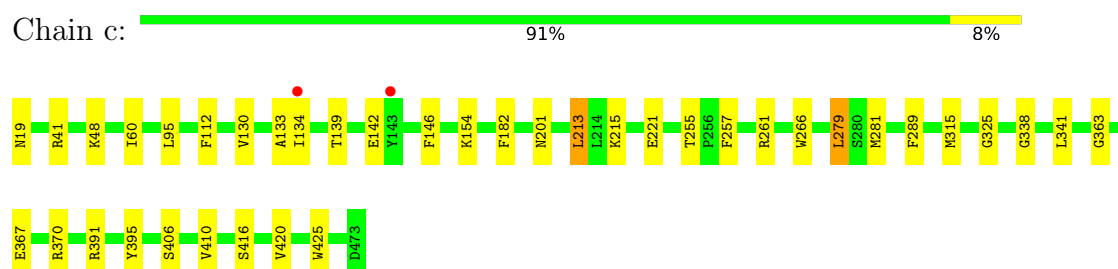
• Molecule 2: Photosystem II CP47 reaction center protein



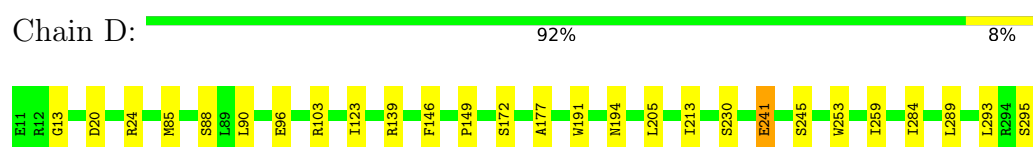
- Molecule 3: Photosystem II CP43 reaction center protein



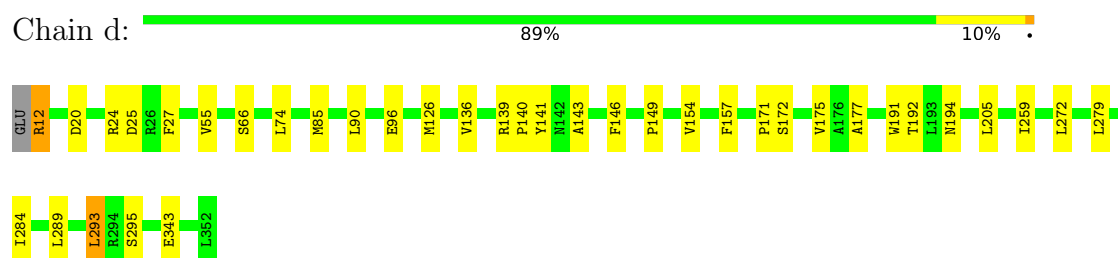
- Molecule 3: Photosystem II CP43 reaction center protein



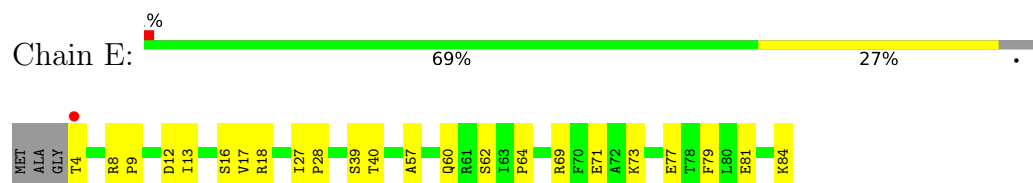
- Molecule 4: Photosystem II D2 protein



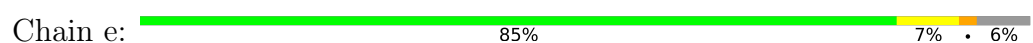
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha

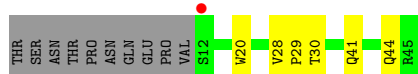


- Molecule 5: Cytochrome b559 subunit alpha

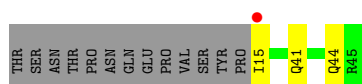




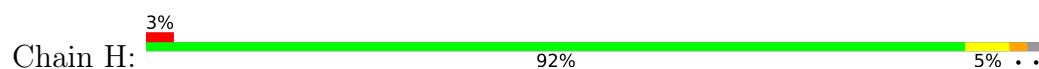
- Molecule 6: Cytochrome b559 subunit beta



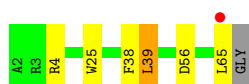
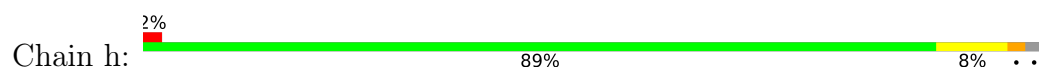
- Molecule 6: Cytochrome b559 subunit beta



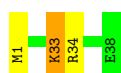
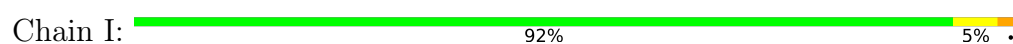
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



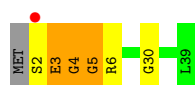
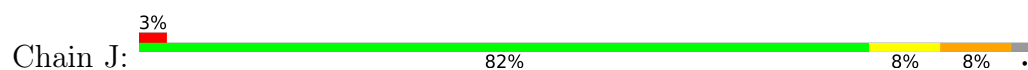
- Molecule 8: Photosystem II reaction center protein I



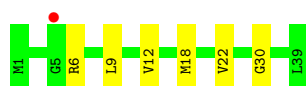
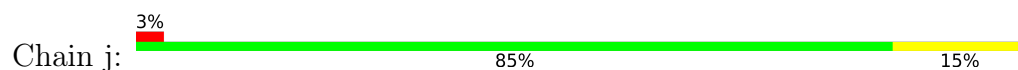
- Molecule 8: Photosystem II reaction center protein I



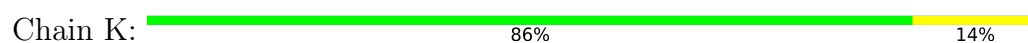
- Molecule 9: Photosystem II reaction center protein J



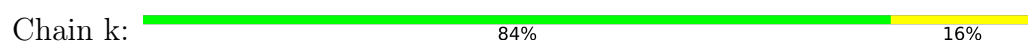
- Molecule 9: Photosystem II reaction center protein J



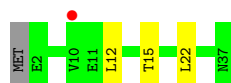
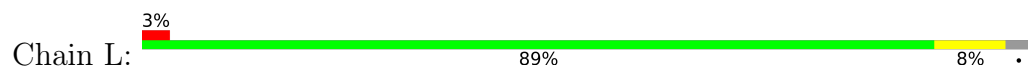
- Molecule 10: Photosystem II reaction center protein K



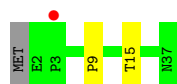
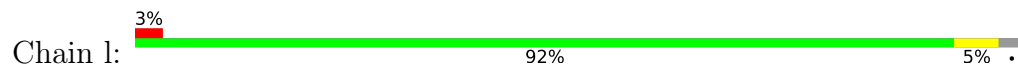
- Molecule 10: Photosystem II reaction center protein K



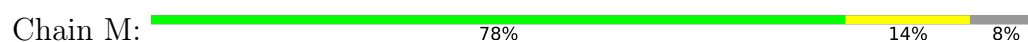
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 17% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  90% 9%



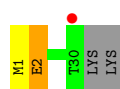
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  91% 8%



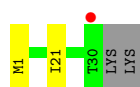
- Molecule 14: Photosystem II reaction center protein T

Chain T:  3% 88% 6% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 88% 6% 6%



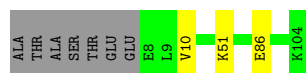
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  85% 7% 8%

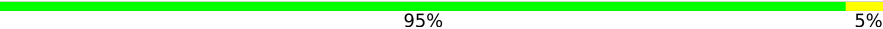


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  90% 7%



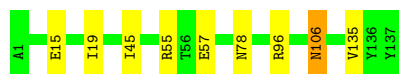
- Molecule 16: Cytochrome c-550

Chain V:  95% 5%



- Molecule 16: Cytochrome c-550

Chain v:  93% 6% .



- Molecule 17: Photosystem II reaction center protein X

Chain X:  88% 8% 5%



- Molecule 17: Photosystem II reaction center protein X

Chain x:  82% 12% 5%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  7% 73% 23% .



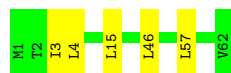
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  77% 20% .

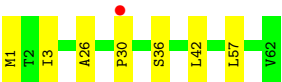
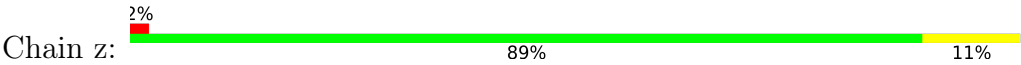


- Molecule 19: Photosystem II reaction center protein Z

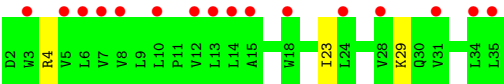
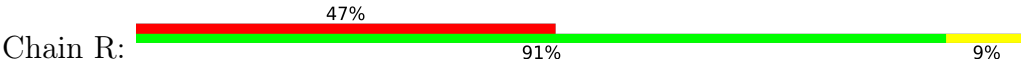
Chain Z:  92% 8%



- Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	126.15Å 232.70Å 288.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.97 – 2.25 39.97 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.0 (39.97-2.25) 85.6 (39.97-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.169 , 0.211 0.171 , 0.214	Depositor DCC
R_{free} test set	20023 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	53138	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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: SQD, MG, GOL, HTG, CA, FE2, HEC, BCT, PL9, DGD, LMT, CL, PHO, OEX, LMG, BCR, LHG, FME, CLA, UNL

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	0.37	0/2719	0.55	0/3708
1	a	0.34	0/2727	0.50	0/3719
2	B	0.34	0/4190	0.49	0/5708
2	b	0.31	0/4138	0.49	0/5640
3	C	0.29	0/3626	0.46	0/4936
3	c	0.27	0/3648	0.43	0/4966
4	D	0.36	0/2821	0.52	0/3844
4	d	0.33	0/2812	0.49	0/3832
5	E	0.26	0/687	0.45	0/936
5	e	0.24	0/667	0.40	0/908
6	F	0.25	0/284	0.39	0/387
6	f	0.22	0/257	0.43	0/349
7	H	0.27	0/530	0.50	0/723
7	h	0.25	0/519	0.48	0/708
8	I	0.24	0/311	0.36	0/419
8	i	0.26	0/311	0.41	0/419
9	J	0.23	0/278	0.37	0/376
9	j	0.23	0/283	0.39	0/383
10	K	0.25	0/303	0.46	0/416
10	k	0.24	0/303	0.44	0/416
11	L	0.40	0/311	0.47	0/423
11	l	0.33	0/311	0.50	0/423
12	M	0.35	0/261	0.51	0/357
12	m	0.35	0/262	0.50	0/357
13	O	0.30	0/1917	0.48	0/2599
13	o	0.28	0/1910	0.46	0/2589
14	T	0.36	0/257	0.42	0/349
14	t	0.35	0/257	0.41	0/349
15	U	0.33	0/776	0.53	0/1052
15	u	0.29	0/785	0.52	0/1064
16	V	0.29	0/1085	0.46	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.26	0/1085	0.41	0/1473
17	X	0.22	0/284	0.36	0/384
17	x	0.18	0/284	0.31	0/384
18	Y	0.20	0/216	0.37	0/289
18	y	0.18	0/216	0.38	0/289
19	Z	0.18	0/490	0.33	0/669
19	z	0.18	0/490	0.33	0/669
20	R	0.19	0/279	0.33	0/383
All	All	0.31	0/42890	0.47	0/58368

There are no bond length outliers.

There are no bond angle outliers.

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	2531	14	0
1	a	2642	0	2541	23	0
2	B	4050	0	3894	31	0
2	b	3998	0	3852	36	0
3	C	3513	0	3424	23	0
3	c	3534	0	3446	26	0
4	D	2726	0	2627	23	0
4	d	2717	0	2621	25	0
5	E	668	0	652	16	0
5	e	648	0	634	7	0
6	F	275	0	282	5	0
6	f	250	0	261	3	0
7	H	517	0	542	4	0
7	h	506	0	529	5	0
8	I	314	0	328	2	0
8	i	314	0	328	0	0
9	J	272	0	279	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	4	0
10	K	293	0	305	1	0
10	k	293	0	305	3	0
11	L	304	0	314	2	0
11	l	304	0	314	2	0
12	M	268	0	285	4	0
12	m	269	0	288	5	0
13	O	1886	0	1856	14	0
13	o	1879	0	1850	11	0
14	T	258	0	261	1	0
14	t	258	0	261	1	0
15	U	765	0	767	4	0
15	u	774	0	773	1	0
16	V	1064	0	1073	4	0
16	v	1064	0	1073	6	0
17	X	281	0	312	2	0
17	x	281	0	312	4	0
18	Y	215	0	246	4	0
18	y	215	0	246	3	0
19	Z	479	0	516	2	0
19	z	479	0	516	2	0
20	R	273	0	305	2	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	10	0
23	B	1040	0	1152	32	0
23	C	845	0	936	30	0
23	D	130	0	144	2	0
23	a	260	0	288	9	0
23	b	1040	0	1152	32	0
23	c	845	0	936	30	0
23	d	130	0	144	1	0
24	A	128	0	148	3	0
24	a	128	0	148	5	0
25	A	40	0	56	2	0
25	B	120	0	168	7	0
25	C	80	0	112	1	0
25	D	40	0	56	0	0
25	H	40	0	56	3	0
25	K	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	40	0	56	4	0
25	Y	40	0	56	1	0
25	a	40	0	56	2	0
25	b	120	0	168	9	0
25	c	80	0	112	5	0
25	d	40	0	56	1	0
25	h	40	0	56	3	0
25	k	40	0	56	1	0
25	t	40	0	56	5	0
25	y	40	0	56	2	0
26	A	6	0	8	0	0
26	B	18	0	24	0	0
26	C	6	0	8	0	0
26	O	6	0	8	0	0
26	a	6	0	8	0	0
26	b	12	0	16	1	0
26	c	6	0	8	1	0
26	o	6	0	8	0	0
26	v	6	0	8	1	0
27	A	54	0	78	1	0
27	B	54	0	78	0	0
27	C	54	0	77	3	0
27	D	43	0	53	0	0
27	a	108	0	155	2	0
27	b	54	0	78	1	0
27	f	43	0	53	2	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	55	0	80	5	0
29	D	55	0	80	2	0
29	a	55	0	80	6	0
29	d	55	0	80	1	0
30	A	28	0	0	0	0
30	B	33	0	0	1	0
30	C	34	0	0	0	0
30	D	57	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
30	a	30	0	0	0	0
30	b	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	c	32	0	0	0	0
30	d	71	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
31	A	49	0	74	2	0
31	D	98	0	148	6	0
31	E	42	0	57	2	0
31	L	49	0	74	2	0
31	a	42	0	57	5	0
31	b	49	0	74	0	0
31	d	147	0	222	10	0
32	B	51	0	72	3	0
32	C	153	0	216	4	0
32	D	51	0	72	1	0
32	Z	37	0	44	0	0
32	c	153	0	216	5	0
32	d	51	0	71	2	0
32	m	51	0	72	2	0
32	z	39	0	48	2	0
33	B	57	0	78	4	0
33	C	19	0	26	0	0
33	D	16	0	17	1	0
33	V	11	0	10	0	0
33	b	57	0	78	3	0
33	c	19	0	26	1	0
33	h	16	0	17	1	0
34	B	60	0	81	0	0
34	C	35	0	46	2	0
34	D	35	0	46	2	0
34	E	35	0	46	1	0
34	M	70	0	92	3	0
34	a	70	0	92	3	0
34	b	50	0	70	1	0
34	e	35	0	46	0	0
34	m	35	0	46	0	0
34	t	26	0	35	0	0
35	C	186	0	246	9	0
35	H	62	0	82	1	0
35	c	186	0	246	3	0
35	h	62	0	82	0	0
36	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	F	1	0	0	0	0
36	O	1	0	0	0	0
36	a	1	0	0	0	0
36	c	2	0	0	0	0
36	o	1	0	0	0	0
37	D	4	0	0	0	0
37	d	4	0	0	0	0
38	E	43	0	32	1	0
38	V	43	0	30	1	0
38	e	43	0	32	2	0
38	v	43	0	30	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	A	143	0	0	0	0
40	B	223	0	0	1	0
40	C	203	0	0	1	0
40	D	136	0	0	3	0
40	E	27	0	0	0	0
40	F	9	0	0	1	0
40	H	26	0	0	1	0
40	I	5	0	0	0	0
40	J	5	0	0	0	0
40	K	7	0	0	0	0
40	L	6	0	0	0	0
40	M	17	0	0	0	0
40	O	125	0	0	1	0
40	R	1	0	0	0	0
40	T	16	0	0	0	0
40	U	56	0	0	0	0
40	V	102	0	0	0	0
40	X	9	0	0	0	0
40	Y	1	0	0	0	0
40	a	143	0	0	0	0
40	b	234	0	0	1	0
40	c	174	0	0	3	0
40	d	125	0	0	0	0
40	e	16	0	0	0	0
40	f	4	0	0	1	0
40	h	23	0	0	0	0
40	i	2	0	0	0	0
40	j	3	0	0	0	0
40	k	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	l	7	0	0	0	0
40	m	11	0	0	0	0
40	o	99	0	0	0	0
40	t	11	0	0	0	0
40	u	71	0	0	0	0
40	v	60	0	0	1	0
40	x	9	0	0	0	0
40	y	4	0	0	0	0
All	All	53138	0	51938	468	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 5.

All (468) 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:c:515:CLA:HBB1	25:c:516:BCR:H24C	1.57	0.86
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.58	0.83
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.61	0.82
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.62	0.82
4:d:192:THR:HG23	23:d:402:CLA:HBC2	1.62	0.81
1:A:214:MET:HG2	29:A:413:PL9:H102	1.64	0.79
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.65	0.78
23:c:505:CLA:HBB1	23:c:514:CLA:H41	1.65	0.77
23:c:506:CLA:H201	31:d:408:LHG:H352	1.68	0.75
23:b:604:CLA:H42	23:b:605:CLA:H2	1.70	0.73
23:C:512:CLA:H52	31:D:408:LHG:H371	1.70	0.73
23:B:601:CLA:H12	23:B:601:CLA:H71	1.71	0.72
6:F:44:GLN:NE2	40:F:201:HOH:O	2.23	0.71
23:C:505:CLA:HBB1	23:C:505:CLA:HHC	1.73	0.71
23:b:606:CLA:H72	25:b:619:BCR:H311	1.72	0.70
2:b:121:GLU:HG2	7:h:4:ARG:HG2	1.74	0.69
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.74	0.68
3:C:325:GLY:O	15:U:51:LYS:NZ	2.26	0.68
23:c:507:CLA:CMD	23:c:509:CLA:HAB	2.25	0.66
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.78	0.65
2:b:171:PRO:HD3	7:h:65:LEU:HD13	1.78	0.65
23:b:606:CLA:H72	25:b:619:BCR:HC7	1.79	0.65
27:A:411:SQD:H301	23:b:606:CLA:H202	1.78	0.64
16:v:106:ASN:OD1	16:v:106:ASN:N	2.30	0.63
32:c:501:LMG:H242	23:c:507:CLA:HBB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:482:ILE:HD12	2:b:486:LEU:HD12	1.79	0.63
5:E:40:THR:HB	20:R:4:ARG:HD2	1.80	0.63
23:B:615:CLA:H2	23:B:616:CLA:HBB2	1.81	0.62
1:a:45:THR:HG23	23:a:405:CLA:H201	1.81	0.62
25:t:102:BCR:HC8	25:t:102:BCR:H311	1.81	0.62
32:B:621:LMG:O10	12:M:4:ASN:ND2	2.32	0.62
27:a:410:SQD:H271	31:d:408:LHG:H141	1.80	0.62
3:C:174:LEU:HB3	23:C:504:CLA:H152	1.82	0.62
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.83	0.61
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.81	0.61
3:c:261:ARG:NH2	40:c:603:HOH:O	2.34	0.60
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.36	0.60
33:B:622:HTG:H1	34:a:413:LMT:H12	1.83	0.60
32:C:521:LMG:H181	18:Y:25:ILE:HG12	1.83	0.60
23:b:601:CLA:H72	23:b:601:CLA:H2	1.83	0.60
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.02	0.60
2:B:498:LYS:HD2	4:D:20:ASP:HA	1.84	0.59
2:b:461:LEU:HD21	4:d:284:ILE:HD11	1.85	0.59
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.85	0.59
23:b:615:CLA:HHC	23:b:615:CLA:HBB1	1.85	0.59
23:B:604:CLA:H42	23:B:605:CLA:H2	1.84	0.58
3:c:279:LEU:HD22	23:c:511:CLA:HED2	1.85	0.58
1:a:227:THR:HB	1:a:231:GLU:HG3	1.85	0.58
2:b:357:ARG:NH1	26:b:628:GOL:O3	2.32	0.58
32:z:101:LMG:H302	32:z:101:LMG:H141	1.84	0.58
34:D:402:LMT:H21	33:b:622:HTG:H3	1.85	0.58
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.39	0.58
32:C:502:LMG:H391	35:C:518:DGD:HB51	1.86	0.58
32:D:413:LMG:H412	6:F:30:THR:HG21	1.84	0.57
2:B:341:LYS:HA	2:B:405[A]:GLU:HG2	1.85	0.57
13:O:27:ARG:NH1	13:O:202:ALA:O	2.38	0.57
3:C:262:ARG:NH2	34:C:526:LMT:O2'	2.35	0.57
23:C:510:CLA:H203	35:C:519:DGD:HA92	1.87	0.57
4:D:24:ARG:NH2	40:D:503:HOH:O	2.34	0.57
15:U:86:GLU:H	15:U:86:GLU:CD	2.11	0.57
24:a:407:PHO:HAB	4:d:205:LEU:HD13	1.85	0.57
1:a:214:MET:HG2	29:a:415:PL9:H103	1.85	0.57
25:B:618:BCR:H363	25:t:102:BCR:H19C	1.86	0.57
3:c:325:GLY:O	15:u:51:LYS:NZ	2.29	0.57
31:d:407:LHG:HC62	11:l:15:THR:HG23	1.87	0.56
4:D:123:ILE:HD11	35:H:102:DGD:HAH2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:503:CLA:C4D	23:c:505:CLA:H2	2.35	0.56
31:d:408:LHG:H342	31:d:408:LHG:H151	1.87	0.56
25:y:101:BCR:H321	25:y:101:BCR:HC8	1.88	0.55
2:b:24:LEU:HD21	23:b:616:CLA:HAB	1.88	0.55
23:B:602:CLA:HHC	23:B:602:CLA:HBB1	1.89	0.55
25:T:101:BCR:H311	25:T:101:BCR:HC8	1.88	0.55
27:a:410:SQD:H141	31:d:408:LHG:H152	1.87	0.55
5:e:68:ASP:O	5:e:72:ALA:HB2	2.07	0.55
13:o:39:ARG:HG3	13:o:246:ALA:HB2	1.89	0.55
23:B:612:CLA:HBB1	23:B:612:CLA:HMB1	1.89	0.55
23:b:616:CLA:H91	25:b:619:BCR:H14C	1.90	0.54
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.43	0.54
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.36	0.54
32:C:502:LMG:H161	35:C:518:DGD:HA82	1.89	0.54
11:L:22:LEU:HD23	31:L:101:LHG:H172	1.90	0.54
23:c:503:CLA:C3D	23:c:505:CLA:H2	2.37	0.54
3:c:182:PHE:HA	33:c:523:HTG:H61	1.90	0.53
2:B:285:ASN:O	2:B:289:GLN:HG2	2.08	0.53
13:O:68:THR:HG22	13:O:110[A]:MET:HG2	1.91	0.53
4:d:24:ARG:HD3	17:x:37:VAL:HG22	1.89	0.53
23:a:408:CLA:H192	23:c:507:CLA:H142	1.91	0.53
16:v:45:ILE:HD13	26:v:201:GOL:H11	1.91	0.53
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.44	0.53
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.91	0.52
1:a:105:TRP:CE2	1:a:110:GLY:HA3	2.45	0.52
23:A:408:CLA:H171	23:C:508:CLA:H121	1.92	0.52
2:b:497:GLN:HB2	2:b:504:THR:HB	1.91	0.52
3:c:146:PHE:HZ	23:c:514:CLA:HBB2	1.74	0.52
3:C:452:ALA:O	8:I:34:ARG:NH2	2.43	0.52
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	1.92	0.52
13:O:58:ASN:ND2	40:O:402:HOH:O	2.27	0.52
4:D:85:MET:CE	4:D:96:GLU:HG2	2.40	0.52
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.91	0.52
25:T:101:BCR:H351	27:b:620:SQD:H223	1.91	0.51
23:a:405:CLA:HHC	23:a:405:CLA:HBB1	1.93	0.51
4:d:20:ASP:HB3	17:x:37:VAL:HG21	1.90	0.51
2:B:490:GLN:HE21	2:B:500:GLY:HA2	1.75	0.51
1:a:183:MET:HA	23:a:404:CLA:HMD1	1.93	0.51
25:t:102:BCR:H382	25:t:102:BCR:H23C	1.92	0.51
23:C:503:CLA:H193	23:C:509:CLA:H13	1.93	0.51
13:O:33:ASP:OD2	13:O:35:SER:OG	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:285:ASN:O	2:b:289:GLN:HG2	2.10	0.51
23:A:405:CLA:HHC	23:A:405:CLA:HBB1	1.93	0.51
23:B:615:CLA:H71	23:B:616:CLA:H172	1.92	0.51
16:V:12:LEU:HD23	16:V:17:LYS:HG2	1.93	0.51
1:a:121[A]:LEU:HG	32:c:501:LMG:H171	1.93	0.51
1:a:307[B]:ILE:HG22	1:a:313:VAL:HA	1.92	0.51
1:A:300:PHE:HZ	35:C:520:DGD:HB61	1.74	0.51
24:A:407:PHO:HAB	4:D:205:LEU:HD13	1.91	0.51
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.93	0.51
3:C:406:SER:HA	3:C:420:VAL:HG23	1.92	0.51
13:O:42:ARG:O	13:O:241:ALA:HA	2.11	0.51
2:B:247:PHE:CE1	23:B:602:CLA:H102	2.46	0.51
19:Z:4:LEU:HD22	19:Z:57:LEU:HD11	1.94	0.51
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.94	0.50
4:D:139:ARG:NH2	40:D:508:HOH:O	2.44	0.50
3:c:215:LYS:HD3	3:c:221:GLU:O	2.11	0.50
23:c:507:CLA:HMD3	23:c:509:CLA:HAB	1.92	0.50
3:C:178:LYS:HB2	23:C:504:CLA:H172	1.93	0.50
5:E:73:LYS:NZ	5:E:77:GLU:OE2	2.35	0.50
5:E:60:GLN:HG2	5:E:62[B]:SER:H	1.75	0.50
13:o:37:THR:HB	13:o:246:ALA:HB3	1.93	0.50
1:a:15:GLU:HB2	34:a:418:LMT:H6'2	1.94	0.50
10:k:20:PRO:HB3	18:y:21:GLN:HG3	1.94	0.50
29:D:406:PL9:H311	31:L:101:LHG:H201	1.94	0.49
23:c:510:CLA:HBC3	23:c:512:CLA:H71	1.94	0.49
4:d:157:PHE:CE2	4:d:171:PRO:HG2	2.47	0.49
23:c:511:CLA:HBB1	23:c:511:CLA:HMB1	1.94	0.49
13:o:83:GLY:HA2	13:o:98:GLU:HG3	1.93	0.49
2:B:413:ASP:OD2	2:B:416:THR:OG1	2.22	0.49
35:c:519:DGD:HAT1	35:c:520:DGD:HBE2	1.95	0.49
13:o:58:ASN:C	13:o:60:ARG:H	2.21	0.49
2:b:491:VAL:HG13	4:d:136:VAL:HG13	1.94	0.49
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.47	0.49
25:H:101:BCR:H331	25:H:101:BCR:C8	2.43	0.49
5:e:14:ILE:HD12	9:j:12:VAL:HG11	1.94	0.49
1:A:121[A]:LEU:HG	32:C:502:LMG:H182	1.95	0.48
23:c:513:CLA:HBB1	23:c:513:CLA:HMB3	1.93	0.48
2:B:341:LYS:NZ	33:B:623:HTG:O2	2.29	0.48
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.48	0.48
1:A:84:PRO:HA	1:A:112:TYR:CG	2.48	0.48
23:C:510:CLA:HBC3	23:C:512:CLA:H71	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:221[A]:SER:HB2	4:d:139:ARG:O	2.14	0.48
5:E:8:ARG:NH1	5:E:13:ILE:HG12	2.29	0.48
31:A:416:LHG:H142	23:B:607:CLA:H201	1.95	0.48
9:j:6:ARG:HH21	9:j:6:ARG:HA	1.78	0.48
23:C:508:CLA:HMC2	23:C:509:CLA:H102	1.95	0.48
13:O:181:GLU:H	13:O:181:GLU:HG2	1.45	0.48
3:c:213:LEU:HD23	23:c:508:CLA:H202	1.96	0.48
23:B:609:CLA:HHC	23:B:609:CLA:HBB1	1.95	0.48
15:U:70:ARG:HH21	15:U:74:ILE:HD11	1.79	0.48
10:K:20:PRO:HB3	18:Y:21:GLN:HG3	1.96	0.47
10:k:21:LEU:HD13	18:y:24:MET:HE2	1.96	0.47
2:B:149:LEU:HD13	23:B:604:CLA:H171	1.96	0.47
23:C:503:CLA:HBB1	23:C:503:CLA:HHC	1.94	0.47
31:D:407:LHG:HC62	11:L:15:THR:HG23	1.96	0.47
5:E:60:GLN:HG2	5:E:62[A]:SER:H	1.78	0.47
29:a:415:PL9:H272	29:a:415:PL9:H251	1.45	0.47
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.49	0.47
23:B:604:CLA:HBB1	23:B:604:CLA:HMB1	1.96	0.47
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.96	0.47
1:a:84:PRO:HA	1:a:112:TYR:CG	2.49	0.47
2:b:237:VAL:HG22	23:b:610:CLA:HBC2	1.96	0.47
23:C:507:CLA:HAA1	23:C:507:CLA:HBD	1.97	0.47
23:b:605:CLA:HAA1	23:b:605:CLA:HBD	1.96	0.47
4:d:194:ASN:HA	4:d:295:SER:OG	2.15	0.47
1:A:270:SER:HB2	27:C:501:SQD:O49	2.15	0.47
23:A:406:CLA:HED1	35:C:520:DGD:HAE2	1.96	0.47
23:B:613:CLA:H162	23:B:613:CLA:H121	1.62	0.47
3:C:464:GLU:OE2	4:D:245:SER:OG	2.31	0.47
5:e:26:THR:HB	38:e:102:HEC:HAB	1.95	0.47
23:A:408:CLA:H41	23:A:408:CLA:H61	1.57	0.47
23:b:606:CLA:H122	23:b:606:CLA:H162	1.73	0.47
13:o:142:PHE:HB2	13:o:199:LEU:HB2	1.97	0.47
16:V:126:LEU:HB3	16:V:129:LYS:HB2	1.96	0.47
23:c:514:CLA:H121	23:c:515:CLA:H142	1.97	0.47
2:b:248:ALA:HB2	23:b:603:CLA:H52	1.97	0.47
23:c:515:CLA:HBB1	25:c:516:BCR:H371	1.96	0.47
19:z:1:MET:HE3	19:z:57:LEU:HD22	1.96	0.47
2:B:98:LEU:HD13	33:B:622:HTG:H7'1	1.97	0.47
23:c:510:CLA:H122	23:c:510:CLA:H162	1.44	0.47
5:e:18:ARG:HH11	38:e:102:HEC:HBA2	1.80	0.46
4:d:126:MET:HE3	4:d:143:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:c:520:DGD:HAH1	32:d:412:LMG:H201	1.96	0.46
25:a:409:BCR:H24C	25:a:409:BCR:H371	1.62	0.46
2:b:247:PHE:HB2	23:b:608:CLA:HBC1	1.98	0.46
23:c:513:CLA:H191	32:z:101:LMG:H242	1.97	0.46
4:D:146:PHE:O	4:D:149:PRO:HD2	2.15	0.46
23:a:405:CLA:HBA1	23:a:405:CLA:C4A	2.45	0.46
23:b:605:CLA:H62	23:b:605:CLA:H41	1.78	0.46
1:A:102:LEU:HD12	33:b:625:HTG:H61	1.98	0.46
25:B:617:BCR:H11C	25:B:617:BCR:H341	1.82	0.46
13:O:69:LYS:HE2	13:O:69:LYS:HB2	1.69	0.46
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.97	0.46
3:C:363:GLY:O	3:C:367:GLU:HG2	2.17	0.46
3:c:370:ARG:NH1	40:c:609:HOH:O	2.49	0.46
31:a:419:LHG:HC32	5:e:10:PHE:H	1.80	0.45
31:a:419:LHG:O5	5:e:10:PHE:HB2	2.16	0.45
19:z:26:ALA:HB1	19:z:36:SER:HB3	1.97	0.45
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.98	0.45
31:A:416:LHG:H361	23:B:613:CLA:H51	1.98	0.45
23:b:614:CLA:H162	23:b:614:CLA:H122	1.64	0.45
40:B:873:HOH:O	13:O:179:GLU:HG3	2.15	0.45
9:J:3:GLU:O	9:J:5:GLY:N	2.49	0.45
23:b:608:CLA:H142	7:h:39:LEU:HD11	1.97	0.45
1:a:253:GLY:HA3	2:b:491:VAL:HG12	1.98	0.45
3:c:363:GLY:O	3:c:367:GLU:HG2	2.17	0.45
4:d:141:TYR:OH	31:d:406:LHG:O4	2.34	0.45
29:A:413:PL9:HC2	29:A:413:PL9:H103	1.98	0.45
3:C:38:GLY:HA3	23:C:513:CLA:HMD2	1.98	0.45
25:K:101:BCR:H24C	25:K:101:BCR:H371	1.64	0.45
23:C:506:CLA:H41	23:C:506:CLA:H62	1.72	0.45
4:D:194:ASN:HA	4:D:295:SER:OG	2.16	0.45
5:E:18:ARG:H	9:J:2:SER:N	2.14	0.45
29:a:415:PL9:H503	17:x:24:THR:OG1	2.17	0.45
31:d:406:LHG:H212	12:m:18:PRO:HG3	1.99	0.45
1:A:159:LEU:C	1:A:162:PRO:HD2	2.41	0.45
23:B:614:CLA:H202	32:B:621:LMG:H412	1.98	0.45
27:C:501:SQD:H171	31:D:408:LHG:H181	1.99	0.45
23:C:503:CLA:C3D	23:C:505:CLA:H2	2.47	0.45
34:M:101:LMT:H6D	11:l:9:PRO:HA	1.99	0.45
2:b:224:ARG:HH21	34:b:621:LMT:H12	1.81	0.45
23:A:406:CLA:H193	31:E:101:LHG:H172	1.99	0.45
25:B:617:BCR:H24C	25:B:617:BCR:H371	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.16	0.45
24:a:417:PHO:HBC3	4:d:279:LEU:HD22	1.98	0.45
2:b:431:GLU:HG2	40:b:883:HOH:O	2.16	0.45
2:B:72:THR:HG22	2:B:80:ILE:HD11	1.99	0.45
18:Y:20:ALA:O	18:Y:24:MET:HG2	2.17	0.45
2:B:338:GLN:O	13:o:58:ASN:ND2	2.49	0.44
23:A:408:CLA:H193	23:C:508:CLA:H91	1.99	0.44
3:C:443:TRP:CZ2	23:C:510:CLA:HMD1	2.52	0.44
1:a:214:MET:HE2	1:a:255:PHE:HE1	1.81	0.44
25:B:619:BCR:H331	25:B:619:BCR:C8	2.47	0.44
3:c:130:VAL:O	3:c:134:ILE:HG12	2.17	0.44
6:f:44:GLN:HG3	40:f:204:HOH:O	2.18	0.44
2:B:149:LEU:HD12	2:B:149:LEU:HA	1.77	0.44
23:B:615:CLA:H152	23:B:615:CLA:H112	1.64	0.44
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.83	0.44
3:c:48:LYS:HG2	3:c:133:ALA:O	2.16	0.44
3:C:203:THR:O	3:C:235:GLY:HA3	2.17	0.44
8:I:33:LYS:HB3	8:I:34:ARG:H	1.55	0.44
2:B:419:SER:HB3	33:B:623:HTG:H4'2	1.99	0.44
5:E:17:VAL:HG23	9:J:6:ARG:HD3	2.00	0.44
12:m:12:ALA:O	12:m:16:LEU:HB2	2.18	0.44
23:B:604:CLA:H91	23:B:604:CLA:H111	1.80	0.44
23:B:605:CLA:HAA1	23:B:605:CLA:HBD	2.00	0.44
23:C:504:CLA:H192	23:C:504:CLA:H162	1.73	0.44
25:T:101:BCR:H19C	25:b:618:BCR:H363	2.00	0.44
2:b:24:LEU:HD21	23:b:616:CLA:CAB	2.47	0.44
25:A:409:BCR:H24C	25:A:409:BCR:H371	1.71	0.44
3:C:334:PRO:HA	13:O:153:THR:OG1	2.18	0.44
23:C:508:CLA:H152	23:C:508:CLA:H18	1.82	0.44
23:a:406:CLA:H143	23:a:406:CLA:H161	1.86	0.44
2:b:36:SER:OG	25:b:618:BCR:H362	2.18	0.44
2:b:283:GLU:OE2	2:b:287:ARG:NH1	2.46	0.44
2:B:86:ILE:H	2:B:86:ILE:HG13	1.70	0.44
2:B:223:GLN:HG2	7:H:21:VAL:HG21	1.99	0.44
23:C:503:CLA:C4D	23:C:505:CLA:H2	2.48	0.44
31:a:419:LHG:HC91	4:d:27:PHE:HZ	1.83	0.44
3:c:425:TRP:CD1	23:c:506:CLA:HMA2	2.53	0.44
31:d:407:LHG:H321	14:t:21:ILE:HD11	2.00	0.44
31:d:408:LHG:H342	31:d:408:LHG:H372	1.88	0.44
25:y:101:BCR:H15C	25:y:101:BCR:H351	1.84	0.44
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C:519:DGD:HBF2	35:C:519:DGD:HBE2	1.63	0.43
5:E:16:SER:HB3	9:J:4:GLY:HA2	2.00	0.43
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.00	0.43
25:H:101:BCR:H331	25:H:101:BCR:HC8	2.00	0.43
23:a:408:CLA:H102	23:a:408:CLA:H62	1.30	0.43
23:c:505:CLA:H101	23:c:505:CLA:H62	1.69	0.43
23:c:509:CLA:H203	23:c:509:CLA:H161	1.62	0.43
2:B:497:GLN:HE22	17:X:38:GLN:HB2	1.82	0.43
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.47	0.43
23:b:608:CLA:H162	23:b:608:CLA:H192	1.75	0.43
3:c:410:VAL:HG13	26:c:502:GOL:H32	1.99	0.43
23:c:511:CLA:H142	23:c:511:CLA:H112	1.84	0.43
18:Y:23:THR:HB	18:Y:24:MET:HE2	2.00	0.43
2:B:58:GLN:C	2:B:329:PRO:HB3	2.43	0.43
2:B:496:TYR:CE1	2:B:505:ARG:HB2	2.53	0.43
3:C:438:LEU:HD11	23:C:507:CLA:HBB1	2.00	0.43
23:b:605:CLA:H192	23:b:609:CLA:HBB2	2.00	0.43
25:b:619:BCR:H11C	25:b:619:BCR:H341	1.80	0.43
25:h:102:BCR:H331	25:h:102:BCR:C8	2.48	0.43
2:B:451:PHE:CE1	2:B:455:HIS:CE1	3.07	0.43
27:C:501:SQD:H271	31:D:408:LHG:H152	1.98	0.43
23:b:613:CLA:H121	32:m:101:LMG:H242	1.99	0.43
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.00	0.43
12:M:33:GLN:HG3	34:M:101:LMT:O4'	2.18	0.43
32:c:501:LMG:H411	32:c:501:LMG:H232	2.00	0.43
4:d:55:VAL:O	4:d:66:SER:HB3	2.19	0.43
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.53	0.43
5:E:77:GLU:O	5:E:81:GLU:HG2	2.19	0.43
24:a:407:PHO:ND	24:a:407:PHO:NC	2.67	0.43
25:a:409:BCR:H11C	25:a:409:BCR:H341	1.83	0.43
32:c:521:LMG:H362	10:k:30:VAL:HG21	2.00	0.43
6:f:15:ILE:HG23	27:f:101:SQD:H92	2.01	0.43
25:B:618:BCR:H381	25:t:102:BCR:H341	2.01	0.43
25:b:618:BCR:H24C	25:b:618:BCR:H371	1.81	0.43
3:c:41:ARG:NH1	23:c:513:CLA:HMD1	2.33	0.43
23:A:404:CLA:CBD	23:A:405:CLA:HAC2	2.49	0.43
2:B:162:PHE:O	23:B:606:CLA:HHD	2.19	0.43
4:D:24:ARG:HD3	17:X:37:VAL:HG22	2.00	0.43
2:b:144:PHE:CE1	2:b:210:ILE:HG23	2.54	0.43
23:C:509:CLA:H92	23:C:509:CLA:H61	1.70	0.43
34:M:101:LMT:H6'1	12:m:32:GLN:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:217:SER:HA	4:d:272:LEU:HD12	1.99	0.43
3:c:281:MET:HE3	3:c:281:MET:HB2	1.81	0.43
25:A:409:BCR:H11C	25:A:409:BCR:H341	1.91	0.42
1:a:131:TRP:CH2	23:c:507:CLA:HAA2	2.54	0.42
23:a:405:CLA:H52	29:d:405:PL9:H151	2.01	0.42
3:c:60:ILE:HG22	23:c:505:CLA:HHD	2.01	0.42
9:j:18:MET:O	9:j:22:VAL:HG23	2.19	0.42
1:A:63:ILE:HB	3:C:335:THR:HG21	2.01	0.42
23:B:615:CLA:H2	23:B:616:CLA:CBB	2.49	0.42
3:C:52:ALA:HB2	23:C:513:CLA:HMA2	2.01	0.42
1:a:247:ASN:HB3	2:b:482:ILE:HD11	2.01	0.42
23:b:603:CLA:HAB	23:b:605:CLA:H152	2.01	0.42
23:b:613:CLA:H72	23:b:613:CLA:H111	1.80	0.42
3:c:95:LEU:HD21	23:c:503:CLA:OBD	2.18	0.42
24:A:415:PHO:NC	24:A:415:PHO:ND	2.66	0.42
23:B:603:CLA:CGA	23:B:603:CLA:H3A	2.49	0.42
3:c:338:GLY:HA3	3:c:341:LEU:O	2.20	0.42
32:c:501:LMG:H382	35:c:518:DGD:HB51	2.00	0.42
2:B:70:GLY:HA2	2:B:178:VAL:HG21	2.00	0.42
25:T:101:BCR:HC7	25:T:101:BCR:H331	1.59	0.42
2:b:149:LEU:HD23	23:b:603:CLA:HBC1	2.00	0.42
13:o:42:ARG:O	13:o:241:ALA:HA	2.19	0.42
1:A:13:LEU:HD13	1:A:13:LEU:HA	1.80	0.42
2:b:130[B]:GLU:HG3	2:b:131:PRO:HD2	2.01	0.42
23:c:515:CLA:H62	23:c:515:CLA:H41	1.90	0.42
4:d:85:MET:HE2	4:d:90:LEU:HD21	2.00	0.42
23:C:508:CLA:H3A	23:C:508:CLA:HBA1	1.74	0.42
2:b:86:ILE:H	2:b:86:ILE:HG13	1.74	0.42
23:b:606:CLA:H192	23:b:606:CLA:H161	1.85	0.42
3:c:19:ASN:ND2	40:c:612:HOH:O	2.52	0.42
7:h:38:PHE:HB2	25:h:102:BCR:C10	2.49	0.42
4:D:13:GLY:HA3	33:D:411:HTG:H62	2.02	0.42
5:E:9:PRO:HA	31:E:101:LHG:HC31	2.01	0.42
34:a:418:LMT:H102	34:a:418:LMT:H71	1.95	0.42
4:d:343:GLU:HG2	16:v:135:VAL:HG11	2.02	0.42
25:t:102:BCR:HC7	25:t:102:BCR:H331	1.63	0.42
29:A:413:PL9:H301	29:A:413:PL9:H322	1.83	0.42
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.02	0.42
3:c:112:PHE:HE2	25:c:516:BCR:HC31	1.85	0.42
25:c:516:BCR:H15C	25:c:516:BCR:H351	1.84	0.42
23:A:408:CLA:H192	23:A:408:CLA:H161	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:H:101:BCR:H24C	25:H:101:BCR:H371	1.72	0.42
23:b:613:CLA:H112	23:b:613:CLA:H151	1.79	0.42
25:b:619:BCR:H15C	25:b:619:BCR:H351	1.90	0.42
25:d:404:BCR:H15C	25:d:404:BCR:H351	1.84	0.42
13:o:200:ASN:O	13:o:213:GLY:HA3	2.20	0.42
3:C:389:GLU:OE2	40:C:601:HOH:O	2.22	0.42
3:c:213:LEU:HD21	25:c:517:BCR:C19	2.49	0.42
3:C:433:LEU:HD22	23:C:504:CLA:HMC3	2.01	0.41
23:C:514:CLA:H101	23:C:515:CLA:H141	2.02	0.41
35:C:520:DGD:HB91	35:C:520:DGD:HB62	1.78	0.41
31:D:408:LHG:H281	31:D:408:LHG:H251	1.81	0.41
13:O:147:ASN:OD1	13:O:194:LYS:HE3	2.19	0.41
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.97	0.41
12:m:4:ASN:ND2	32:m:101:LMG:O10	2.52	0.41
12:m:16:LEU:HD12	12:m:16:LEU:HA	1.83	0.41
23:B:602:CLA:H203	23:B:602:CLA:H162	1.76	0.41
23:B:607:CLA:H122	32:B:621:LMG:H241	2.02	0.41
34:D:402:LMT:H62	33:b:622:HTG:H4'1	2.02	0.41
5:E:57:ALA:HB1	5:E:84:LYS:NZ	2.35	0.41
13:O:193:THR:HG21	13:O:220:LEU:HD12	2.01	0.41
20:R:29:LYS:HE2	20:R:29:LYS:HB3	1.74	0.41
1:a:179:THR:O	1:a:183:MET:HG3	2.20	0.41
24:a:417:PHO:ND	24:a:417:PHO:NC	2.69	0.41
2:b:233:ASN:O	2:b:236:THR:HG22	2.20	0.41
23:b:604:CLA:H172	23:b:604:CLA:H13	1.62	0.41
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.02	0.41
25:B:618:BCR:C8	25:B:618:BCR:H331	2.48	0.41
4:D:241:GLU:H	4:D:241:GLU:CD	2.29	0.41
5:E:64:PRO:HB2	5:E:79:PHE:CD1	2.56	0.41
19:Z:15:LEU:HD22	19:Z:46:LEU:HD23	2.02	0.41
1:a:251:ALA:HB3	29:a:415:PL9:H532	2.02	0.41
23:b:616:CLA:H92	23:b:616:CLA:H62	1.87	0.41
3:c:154:LYS:HE3	3:c:266:TRP:CD2	2.55	0.41
4:d:74:LEU:HD22	4:d:175:VAL:HG11	2.03	0.41
13:o:234:LYS:HB2	13:o:234:LYS:HE2	1.88	0.41
16:v:57:GLU:H	16:v:57:GLU:CD	2.26	0.41
29:A:413:PL9:H171	29:A:413:PL9:H151	1.80	0.41
2:B:91:TRP:HE1	30:B:626:UNL:C10	2.33	0.41
23:B:613:CLA:H143	23:B:613:CLA:H111	1.79	0.41
3:C:433:LEU:HD13	23:C:504:CLA:CHC	2.51	0.41
29:D:406:PL9:H401	29:D:406:PL9:H422	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:E:103:HEC:C2A	6:F:20:TRP:HE1	2.33	0.41
2:b:6:TYR:OH	31:d:406:LHG:HC2	2.20	0.41
23:b:615:CLA:H8	23:b:615:CLA:H122	1.87	0.41
1:A:160:ILE:HD11	35:C:518:DGD:HBT2	2.02	0.41
1:A:227:THR:HB	1:A:231:GLU:HG3	2.03	0.41
2:b:349:LYS:HG3	2:b:350:GLU:OE1	2.21	0.41
2:b:497:GLN:HE22	17:x:38:GLN:H	1.68	0.41
3:c:391:ARG:HD2	3:c:395:TYR:CZ	2.56	0.41
23:c:514:CLA:HBA2	23:c:514:CLA:H3A	1.84	0.41
2:B:461:LEU:HD21	4:D:284:ILE:HD11	2.03	0.41
4:D:146:PHE:C	4:D:149:PRO:HD2	2.45	0.41
23:c:507:CLA:HAA1	23:c:507:CLA:HBD	2.02	0.41
13:O:24:ASP:HA	13:O:203:LYS:HE2	2.02	0.41
2:B:30:VAL:HG12	23:B:605:CLA:HHD	2.03	0.41
23:a:405:CLA:H161	23:a:405:CLA:H141	1.88	0.41
24:a:417:PHO:HBC2	24:a:417:PHO:HHD	2.02	0.41
31:a:419:LHG:H241	31:a:419:LHG:HC61	1.91	0.41
2:b:162:PHE:O	23:b:606:CLA:HHD	2.20	0.41
23:b:609:CLA:NC	25:h:102:BCR:H332	2.36	0.41
4:d:293:LEU:HD12	4:d:293:LEU:HA	1.96	0.41
23:A:404:CLA:H143	24:A:407:PHO:H61	2.02	0.41
2:B:357[B]:ARG:NH2	4:D:337:GLU:O	2.50	0.41
23:B:610:CLA:H92	23:B:610:CLA:H61	1.90	0.41
35:C:518:DGD:HA81	35:C:518:DGD:HAE1	1.89	0.41
4:D:230:SER:HB2	40:D:579:HOH:O	2.20	0.41
31:D:408:LHG:H361	31:D:408:LHG:H142	2.03	0.41
12:M:25:LEU:HD23	12:M:25:LEU:HA	1.91	0.41
1:a:121[B]:LEU:HD23	1:a:121[B]:LEU:HA	1.94	0.41
29:a:415:PL9:H453	27:f:101:SQD:H262	2.02	0.41
3:c:257:PHE:O	3:c:261:ARG:HG3	2.20	0.41
3:c:406:SER:HA	3:c:420:VAL:HG23	2.01	0.41
5:e:12:ASP:OD1	5:e:12:ASP:N	2.53	0.41
18:y:22:LEU:HA	18:y:25:ILE:HG22	2.02	0.41
23:B:616:CLA:H62	23:B:616:CLA:H41	1.46	0.41
3:C:119:LEU:HA	3:C:119:LEU:HD12	1.85	0.41
2:b:475:PHE:CD2	4:d:140:PRO:HG3	2.56	0.41
23:A:404:CLA:HMB3	23:A:404:CLA:HBB1	2.04	0.40
23:B:614:CLA:H92	23:B:614:CLA:H61	1.83	0.40
23:D:403:CLA:HBC3	23:D:403:CLA:CHD	2.51	0.40
16:V:93:PRO:HG3	16:V:101:PHE:CD1	2.55	0.40
29:a:415:PL9:H272	31:a:419:LHG:H223	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:k:101:BCR:H15C	25:k:101:BCR:H351	1.87	0.40
25:B:618:BCR:H24C	25:B:618:BCR:H371	1.87	0.40
3:C:176:VAL:HG21	3:C:238:ILE:HG13	2.03	0.40
23:C:505:CLA:HBB1	23:C:505:CLA:CHC	2.47	0.40
34:C:526:LMT:H3'	34:C:526:LMT:H1B	1.92	0.40
16:V:41:HIS:CD2	38:V:201:HEC:NB	2.89	0.40
2:b:125:ASP:OD1	2:b:127:ARG:NH1	2.53	0.40
25:b:617:BCR:H24C	25:b:617:BCR:H371	1.72	0.40
4:d:12:ARG:HB2	4:d:12:ARG:NH2	2.36	0.40
4:d:146:PHE:C	4:d:149:PRO:HD2	2.46	0.40
7:h:25:TRP:CD2	33:h:101:HTG:H1'1	2.56	0.40
13:o:210:GLU:OE2	13:o:240:TYR:OH	2.35	0.40
23:B:614:CLA:HAA1	23:B:614:CLA:HBD	2.03	0.40
25:C:517:BCR:H24C	25:C:517:BCR:H371	1.87	0.40
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.57	0.40
23:D:403:CLA:HAA2	23:D:403:CLA:HBD	2.04	0.40
7:H:12[B]:ARG:HD2	40:H:219:HOH:O	2.21	0.40
13:O:234:LYS:HB2	13:O:234:LYS:HE2	1.82	0.40
1:a:307[A]:ILE:CG2	1:a:311:GLY:HA2	2.51	0.40
2:b:363:PHE:HB3	2:b:365:SER:O	2.21	0.40
23:B:606:CLA:H161	23:B:606:CLA:H122	1.56	0.40
5:E:39:SER:O	34:E:102:LMT:O4'	2.40	0.40
2:b:317:ASN:HA	2:b:330:MET:HE1	2.02	0.40
3:c:139:THR:OG1	3:c:142:GLU:OE2	2.36	0.40
32:d:412:LMG:H221	32:d:412:LMG:H191	1.92	0.40
29:A:413:PL9:H101	29:A:413:PL9:C13	2.51	0.40
23:B:610:CLA:H122	23:B:615:CLA:HAA1	2.03	0.40
3:C:95:LEU:HD21	23:C:503:CLA:OBD	2.21	0.40
3:C:425:TRP:CD1	23:C:506:CLA:HMA2	2.56	0.40
23:C:508:CLA:H93	23:C:508:CLA:H61	1.89	0.40
15:U:73:GLN:O	15:U:77:GLU:HG3	2.21	0.40
23:b:606:CLA:H141	23:b:616:CLA:H121	2.03	0.40
16:v:55:ARG:HD2	40:v:318:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/344 (97%)	330 (99%)	3 (1%)	1 (0%)	36	40
1	a	335/344 (97%)	328 (98%)	6 (2%)	1 (0%)	36	40
2	B	512/505 (101%)	505 (99%)	7 (1%)	0	100	100
2	b	506/505 (100%)	497 (98%)	9 (2%)	0	100	100
3	C	453/455 (100%)	443 (98%)	8 (2%)	2 (0%)	30	31
3	c	455/455 (100%)	444 (98%)	10 (2%)	1 (0%)	43	50
4	D	340/342 (99%)	329 (97%)	11 (3%)	0	100	100
4	d	339/342 (99%)	331 (98%)	8 (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%)	61 (97%)	2 (3%)	0	100	100
7	h	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
8	I	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	33 (92%)	0	3 (8%)	0	0
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	244/244 (100%)	237 (97%)	6 (2%)	1 (0%)	30	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	243/244 (100%)	236 (97%)	7 (3%)	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%)	92 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	3
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5246/5384 (97%)	5129 (98%)	107 (2%)	10 (0%)	43	50

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416	SER
9	J	4	GLY
9	J	5	GLY
13	O	61	GLN
9	J	3	GLU
1	a	259	ILE
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	271/279 (97%)	268 (99%)	3 (1%)	65	75
1	a	272/279 (98%)	271 (100%)	1 (0%)	84	89
2	B	412/403 (102%)	406 (98%)	6 (2%)	57	68
2	b	406/403 (101%)	399 (98%)	7 (2%)	53	65
3	C	356/356 (100%)	349 (98%)	7 (2%)	48	59
3	c	358/356 (101%)	352 (98%)	6 (2%)	53	65
4	D	277/277 (100%)	274 (99%)	3 (1%)	65	75
4	d	276/277 (100%)	271 (98%)	5 (2%)	51	63
5	E	73/73 (100%)	70 (96%)	3 (4%)	27	33
5	e	70/73 (96%)	67 (96%)	3 (4%)	26	31
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	20
7	h	54/54 (100%)	52 (96%)	2 (4%)	30	37
8	I	34/34 (100%)	33 (97%)	1 (3%)	37	47
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	36
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	2
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	5
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	47
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%)	28 (93%)	2 (7%)	15	14
13	O	209/207 (101%)	206 (99%)	3 (1%)	59	70
13	o	208/207 (100%)	203 (98%)	5 (2%)	43	54
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	36
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	83/89 (93%)	80 (96%)	3 (4%)	31	39
15	u	84/89 (94%)	82 (98%)	2 (2%)	43	54
16	V	117/117 (100%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	v	117/117 (100%)	114 (97%)	3 (3%)	40	50
17	X	31/33 (94%)	30 (97%)	1 (3%)	34	43
17	x	31/33 (94%)	29 (94%)	2 (6%)	15	14
18	Y	22/23 (96%)	20 (91%)	2 (9%)	9	7
18	y	22/23 (96%)	20 (91%)	2 (9%)	9	7
19	Z	52/52 (100%)	51 (98%)	1 (2%)	50	61
19	z	52/52 (100%)	50 (96%)	2 (4%)	29	36
20	R	29/29 (100%)	28 (97%)	1 (3%)	32	40
All	All	4352/4403 (99%)	4263 (98%)	89 (2%)	48	59

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

Mol	Chain	Res	Type
1	A	13	LEU
1	A	238	LYS
1	A	243	GLU
2	B	79	SER
2	B	208	VAL
2	B	236	THR
2	B	245	VAL
2	B	389	LYS
2	B	419	SER
3	C	25	ASN
3	C	29	GLU
3	C	78	GLU
3	C	142	GLU
3	C	213	LEU
3	C	289	PHE
3	C	315	MET
4	D	241	GLU
4	D	259	ILE
4	D	293	LEU
5	E	4	THR
5	E	12	ASP
5	E	71	GLU
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	39	LEU
8	I	33	LYS

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Mol	Chain	Res	Type
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
10	K	27	VAL
11	L	12	LEU
13	O	60	ARG
13	O	118	LEU
13	O	181	GLU
14	T	2	GLU
15	U	10	VAL
15	U	56	GLU
15	U	86	GLU
17	X	2	THR
18	Y	19	ILE
18	Y	30	ILE
19	Z	3	ILE
20	R	23	ILE
1	a	229	GLU
2	b	14	ASN
2	b	63	LEU
2	b	121	GLU
2	b	287	ARG
2	b	299	GLU
2	b	362	PHE
2	b	486	LEU
3	c	201	ASN
3	c	213	LEU
3	c	255	THR
3	c	279	LEU
3	c	289	PHE
3	c	315	MET
4	d	12	ARG
4	d	25	ASP
4	d	154	VAL
4	d	259	ILE
4	d	293	LEU
5	e	12	ASP
5	e	14	ILE
5	e	71	GLU
7	h	39	LEU
7	h	56	ASP
9	j	9	LEU

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Mol	Chain	Res	Type
10	k	10	LYS
10	k	17	ILE
10	k	19	ASP
12	m	5	GLN
12	m	16	LEU
13	o	25	THR
13	o	37	THR
13	o	69	LYS
13	o	80	GLN
13	o	118	LEU
15	u	10	VAL
15	u	86	GLU
16	v	15	GLU
16	v	19	ILE
16	v	106	ASN
17	x	15	LEU
17	x	21	LEU
18	y	18	VAL
18	y	45	ASN
19	z	3	ILE
19	z	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	296	ASN
2	B	331	ASN
2	B	490	GLN
3	C	201	ASN
3	C	322	GLN
4	D	98	GLN
4	D	186	GLN
13	O	231	HIS
15	U	78	ASN
15	U	81	HIS
1	a	165	GLN
2	b	179	GLN
2	b	331	ASN
3	c	19	ASN
3	c	373	ASN
13	o	80	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.70	0	8,9,11	1.04	1 (12%)
12	FME	m	1	12	8,9,10	0.59	0	8,9,11	1.50	2 (25%)
14	FME	t	1	14	8,9,10	0.67	0	8,9,11	1.66	2 (25%)
14	FME	T	1	14	8,9,10	0.73	0	8,9,11	1.36	2 (25%)
8	FME	i	1	8	8,9,10	0.60	0	8,9,11	0.97	1 (12%)
12	FME	M	1	12	8,9,10	0.64	0	8,9,11	1.58	3 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-

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	CA-N-CN	-3.25	117.82	122.82
12	M	1	FME	CA-N-CN	-3.08	118.08	122.82
14	t	1	FME	O-C-CA	-2.65	117.96	124.77
14	T	1	FME	O-C-CA	-2.52	118.29	124.77
14	T	1	FME	CA-N-CN	-2.36	119.19	122.82
12	m	1	FME	C-CA-N	2.36	114.04	109.50
12	m	1	FME	O-C-CA	-2.28	118.90	124.77
12	M	1	FME	O1-CN-N	-2.09	119.93	125.32
8	I	1	FME	O-C-CA	-2.07	119.44	124.77
8	i	1	FME	O-C-CA	-2.07	119.44	124.77
12	M	1	FME	O-C-CA	-2.00	119.61	124.77

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
12	M	1	FME	O-C-CA-CB
12	m	1	FME	O1-CN-N-CA
12	m	1	FME	CB-CA-N-CN
14	t	1	FME	O-C-CA-CB
14	t	1	FME	O1-CN-N-CA
12	M	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 216 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 183 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	$\# Z > 2$
33	HTG	B	623	-	19,19,19	0.75	1 (5%)	23,24,24	1.67	4 (17%)
23	CLA	b	605	-	69,73,73	1.98	20 (28%)	82,113,113	2.82	27 (32%)
24	PHO	A	407	-	58,69,69	2.65	14 (24%)	55,99,99	2.90	17 (30%)
23	CLA	a	405	40	69,73,73	2.07	18 (26%)	82,113,113	2.74	32 (39%)
33	HTG	h	101	-	16,16,19	1.05	1 (6%)	20,21,24	2.01	5 (25%)
23	CLA	b	616	-	69,73,73	1.97	19 (27%)	82,113,113	2.78	34 (41%)
25	BCR	B	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.35	9 (16%)
32	LMG	C	502	-	51,51,55	0.93	2 (3%)	59,59,63	1.03	3 (5%)
23	CLA	c	505	-	69,73,73	2.04	19 (27%)	82,113,113	2.66	29 (35%)
34	LMT	M	103	-	36,36,36	0.46	0	47,47,47	1.04	2 (4%)
23	CLA	A	405	40	69,73,73	2.01	19 (27%)	82,113,113	2.73	33 (40%)
25	BCR	b	619	-	41,41,41	1.18	2 (4%)	56,56,56	1.51	12 (21%)
23	CLA	B	611	-	69,73,73	2.00	19 (27%)	82,113,113	2.81	34 (41%)
23	CLA	c	508	-	69,73,73	2.02	20 (28%)	82,113,113	2.65	31 (37%)
27	SQD	D	412	-	41,43,54	1.10	2 (4%)	51,54,65	1.76	10 (19%)
23	CLA	C	506	40	69,73,73	1.98	21 (30%)	82,113,113	2.65	32 (39%)
35	DGD	h	103	-	63,63,67	0.91	3 (4%)	77,77,81	1.01	3 (3%)
23	CLA	c	509	40	69,73,73	2.06	18 (26%)	82,113,113	2.75	30 (36%)
24	PHO	a	417	-	58,69,69	2.80	13 (22%)	55,99,99	3.08	14 (25%)
31	LHG	d	408	-	48,48,48	0.90	2 (4%)	51,54,54	1.08	3 (5%)
23	CLA	B	612	-	69,73,73	1.92	18 (26%)	82,113,113	2.81	31 (37%)
25	BCR	A	409	-	41,41,41	1.05	1 (2%)	56,56,56	1.47	10 (17%)
34	LMT	m	103	-	36,36,36	0.46	0	47,47,47	1.00	3 (6%)
31	LHG	E	101	-	41,41,48	1.05	2 (4%)	44,47,54	1.04	2 (4%)
32	LMG	c	522	-	51,51,55	0.96	2 (3%)	59,59,63	1.11	5 (8%)
33	HTG	C	523	-	19,19,19	0.85	1 (5%)	23,24,24	1.24	1 (4%)
25	BCR	C	516	-	41,41,41	1.01	1 (2%)	56,56,56	1.62	9 (16%)
32	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.16	3 (5%)
23	CLA	C	508	-	69,73,73	2.06	20 (28%)	82,113,113	2.66	33 (40%)
23	CLA	B	613	-	69,73,73	1.94	18 (26%)	82,113,113	2.66	29 (35%)
23	CLA	B	603	-	69,73,73	2.00	19 (27%)	82,113,113	2.78	30 (36%)
23	CLA	d	402	-	69,73,73	1.95	19 (27%)	82,113,113	2.63	33 (40%)
23	CLA	c	513	3	69,73,73	2.00	19 (27%)	82,113,113	2.72	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	OEX	a	414	1,3,40	0,15,15	-	-	-		
34	LMT	E	102	-	36,36,36	0.52	1 (2%)	47,47,47	0.86	1 (2%)
23	CLA	C	515	-	69,73,73	2.02	20 (28%)	82,113,113	2.69	31 (37%)
27	SQD	a	410	-	52,54,54	0.92	2 (3%)	62,65,65	1.63	11 (17%)
23	CLA	B	605	-	69,73,73	2.03	19 (27%)	82,113,113	2.68	30 (36%)
23	CLA	A	408	-	69,73,73	2.04	20 (28%)	82,113,113	2.65	33 (40%)
23	CLA	C	505	-	69,73,73	2.02	19 (27%)	82,113,113	2.72	28 (34%)
23	CLA	c	510	-	69,73,73	2.08	20 (28%)	82,113,113	2.72	30 (36%)
34	LMT	C	526	-	36,36,36	0.50	1 (2%)	47,47,47	1.06	3 (6%)
26	GOL	o	302	-	5,5,5	0.86	0	5,5,5	1.12	1 (20%)
23	CLA	c	514	-	69,73,73	2.03	19 (27%)	82,113,113	2.71	33 (40%)
23	CLA	b	609	-	69,73,73	2.00	21 (30%)	82,113,113	2.59	32 (39%)
23	CLA	C	503	-	69,73,73	1.97	20 (28%)	82,113,113	2.78	31 (37%)
23	CLA	b	602	-	69,73,73	2.05	20 (28%)	82,113,113	2.75	33 (40%)
25	BCR	b	617	-	41,41,41	1.12	1 (2%)	56,56,56	1.53	8 (14%)
27	SQD	b	620	-	52,54,54	0.98	2 (3%)	62,65,65	1.53	9 (14%)
26	GOL	a	411	-	5,5,5	0.91	0	5,5,5	1.12	1 (20%)
26	GOL	c	502	-	5,5,5	1.12	0	5,5,5	0.96	0
25	BCR	B	618	-	41,41,41	0.95	1 (2%)	56,56,56	1.41	6 (10%)
34	LMT	B	628	-	36,36,36	0.42	0	47,47,47	1.10	3 (6%)
26	GOL	B	629	-	5,5,5	1.06	0	5,5,5	0.94	0
33	HTG	b	622	-	19,19,19	1.03	1 (5%)	23,24,24	1.37	3 (13%)
33	HTG	V	202	-	11,11,19	0.21	0	15,15,24	1.22	2 (13%)
23	CLA	A	406	40	69,73,73	2.03	20 (28%)	82,113,113	2.66	29 (35%)
31	LHG	d	407	-	48,48,48	0.89	2 (4%)	51,54,54	1.02	4 (7%)
23	CLA	B	601	40	69,73,73	2.07	21 (30%)	82,113,113	2.69	30 (36%)
34	LMT	b	621	-	25,25,36	0.52	0	30,30,47	0.58	0
33	HTG	B	625	-	19,19,19	0.95	2 (10%)	23,24,24	1.04	1 (4%)
23	CLA	B	606	-	69,73,73	1.99	20 (28%)	82,113,113	2.73	31 (37%)
23	CLA	a	408	-	69,73,73	1.98	20 (28%)	82,113,113	2.69	31 (37%)
29	PL9	a	415	-	55,55,55	0.66	2 (3%)	68,69,69	2.00	21 (30%)
23	CLA	d	403	-	69,73,73	2.08	21 (30%)	82,113,113	2.74	32 (39%)
35	DGD	c	519	-	63,63,67	0.85	2 (3%)	77,77,81	1.01	4 (5%)
32	LMG	d	412	39	51,51,55	0.93	2 (3%)	59,59,63	0.87	2 (3%)
26	GOL	b	628	-	5,5,5	1.00	0	5,5,5	1.15	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	HEC	v	202	16	46,50,50	1.88	6 (13%)	58,82,82	1.94	6 (10%)
25	BCR	a	409	-	41,41,41	1.09	1 (2%)	56,56,56	1.48	10 (17%)
29	PL9	D	406	-	55,55,55	0.69	2 (3%)	68,69,69	1.66	17 (25%)
35	DGD	C	519	-	63,63,67	0.90	3 (4%)	77,77,81	1.10	4 (5%)
35	DGD	c	520	-	63,63,67	0.89	3 (4%)	77,77,81	1.03	6 (7%)
23	CLA	c	506	40	69,73,73	2.03	20 (28%)	82,113,113	2.73	32 (39%)
26	GOL	b	624	-	5,5,5	1.00	0	5,5,5	1.14	0
23	CLA	b	607	40	69,73,73	2.02	18 (26%)	82,113,113	2.67	31 (37%)
26	GOL	B	624	-	5,5,5	0.91	0	5,5,5	1.10	0
24	PHO	A	415	-	58,69,69	2.71	14 (24%)	55,99,99	2.83	18 (32%)
25	BCR	C	517	-	41,41,41	1.02	1 (2%)	56,56,56	1.57	10 (17%)
25	BCR	h	102	-	41,41,41	1.08	1 (2%)	56,56,56	1.31	7 (12%)
23	CLA	B	610	40	69,73,73	2.03	20 (28%)	82,113,113	2.70	31 (37%)
23	CLA	B	602	-	69,73,73	2.05	20 (28%)	82,113,113	2.74	32 (39%)
27	SQD	C	501	-	52,54,54	0.88	2 (3%)	62,65,65	1.88	11 (17%)
29	PL9	A	413	-	55,55,55	0.68	2 (3%)	68,69,69	1.87	21 (30%)
32	LMG	c	521	-	51,51,55	0.92	2 (3%)	59,59,63	1.02	3 (5%)
23	CLA	C	510	-	69,73,73	2.01	20 (28%)	82,113,113	2.70	30 (36%)
23	CLA	D	403	-	69,73,73	1.97	19 (27%)	82,113,113	2.79	31 (37%)
25	BCR	T	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.59	12 (21%)
23	CLA	c	507	-	69,73,73	2.01	19 (27%)	82,113,113	2.61	30 (36%)
32	LMG	Z	101	-	37,37,55	1.02	3 (8%)	45,45,63	1.54	6 (13%)
23	CLA	A	404	-	69,73,73	2.01	19 (27%)	82,113,113	2.70	33 (40%)
26	GOL	A	410	-	5,5,5	1.17	0	5,5,5	0.88	0
23	CLA	b	601	40	69,73,73	2.10	20 (28%)	82,113,113	2.67	29 (35%)
32	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.11	4 (8%)
34	LMT	D	402	-	36,36,36	0.53	1 (2%)	47,47,47	0.86	1 (2%)
32	LMG	C	522	-	51,51,55	1.01	3 (5%)	59,59,63	1.32	5 (8%)
23	CLA	B	616	-	69,73,73	1.95	20 (28%)	82,113,113	2.67	31 (37%)
31	LHG	D	408	-	48,48,48	0.90	2 (4%)	51,54,54	0.97	3 (5%)
34	LMT	e	101	-	36,36,36	0.53	1 (2%)	47,47,47	1.04	2 (4%)
35	DGD	C	520	-	63,63,67	0.84	2 (3%)	77,77,81	1.04	5 (6%)
23	CLA	D	404	-	69,73,73	2.04	18 (26%)	82,113,113	2.67	30 (36%)
34	LMT	a	418	-	36,36,36	0.45	0	47,47,47	0.94	1 (2%)
25	BCR	Y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.85	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	GOL	C	524	-	5,5,5	1.13	0	5,5,5	1.01	0
23	CLA	C	509	40	69,73,73	1.99	19 (27%)	82,113,113	2.63	28 (34%)
32	LMG	C	521	-	51,51,55	0.99	2 (3%)	59,59,63	1.04	3 (5%)
35	DGD	H	102	-	63,63,67	0.83	3 (4%)	77,77,81	1.05	7 (9%)
25	BCR	D	405	-	41,41,41	1.07	1 (2%)	56,56,56	1.66	13 (23%)
35	DGD	c	518	-	63,63,67	0.90	2 (3%)	77,77,81	1.05	6 (7%)
23	CLA	B	604	-	69,73,73	2.00	21 (30%)	82,113,113	2.61	31 (37%)
23	CLA	c	504	-	69,73,73	2.00	19 (27%)	82,113,113	2.61	29 (35%)
31	LHG	b	629	-	48,48,48	0.90	2 (4%)	51,54,54	1.05	3 (5%)
23	CLA	C	513	3	69,73,73	2.03	22 (31%)	82,113,113	2.65	30 (36%)
32	LMG	D	413	39	51,51,55	0.84	3 (5%)	59,59,63	0.96	3 (5%)
35	DGD	C	518	-	63,63,67	0.88	2 (3%)	77,77,81	1.00	3 (3%)
28	OEX	A	412	1,3,40	0,15,15	-	-	-	-	-
24	PHO	a	407	-	58,69,69	2.65	14 (24%)	55,99,99	2.97	16 (29%)
23	CLA	C	504	-	69,73,73	1.98	20 (28%)	82,113,113	2.62	30 (36%)
25	BCR	c	517	-	41,41,41	1.08	1 (2%)	56,56,56	1.44	13 (23%)
33	HTG	c	523	-	19,19,19	0.88	1 (5%)	23,24,24	1.30	1 (4%)
38	HEC	e	102	5,6	46,50,50	1.75	11 (23%)	58,82,82	1.69	13 (22%)
25	BCR	H	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.36	7 (12%)
23	CLA	B	615	-	69,73,73	1.93	17 (24%)	82,113,113	2.71	31 (37%)
23	CLA	b	606	-	69,73,73	1.94	21 (30%)	82,113,113	2.83	32 (39%)
25	BCR	c	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.44	8 (14%)
23	CLA	a	404	-	69,73,73	1.97	20 (28%)	82,113,113	2.73	32 (39%)
31	LHG	a	419	-	41,41,48	1.05	2 (4%)	44,47,54	0.98	2 (4%)
26	GOL	O	302	-	5,5,5	0.90	0	5,5,5	1.08	0
23	CLA	c	515	-	69,73,73	2.04	20 (28%)	82,113,113	2.67	32 (39%)
26	GOL	B	627	-	5,5,5	1.05	0	5,5,5	1.23	0
37	BCT	d	401	21	3,3,3	0.50	0	2,3,3	1.70	1 (50%)
33	HTG	B	622	-	19,19,19	0.93	1 (5%)	23,24,24	1.53	4 (17%)
34	LMT	t	101	-	26,26,36	0.56	1 (3%)	31,31,47	1.16	4 (12%)
23	CLA	B	614	-	69,73,73	1.96	19 (27%)	82,113,113	2.88	31 (37%)
23	CLA	c	503	-	69,73,73	2.01	19 (27%)	82,113,113	2.67	30 (36%)
34	LMT	b	627	-	25,25,36	0.46	0	30,30,47	0.90	1 (3%)
31	LHG	L	101	-	48,48,48	0.92	3 (6%)	51,54,54	1.12	4 (7%)
27	SQD	f	101	-	41,43,54	1.10	2 (4%)	51,54,65	1.27	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	HTG	D	411	-	16,16,19	0.98	2 (12%)	20,21,24	1.15	1 (5%)
33	HTG	b	623	-	19,19,19	0.91	1 (5%)	23,24,24	1.41	2 (8%)
23	CLA	b	613	-	69,73,73	1.99	18 (26%)	82,113,113	2.69	31 (37%)
31	LHG	d	406	-	48,48,48	0.89	2 (4%)	51,54,54	1.14	5 (9%)
33	HTG	b	625	-	19,19,19	0.91	2 (10%)	23,24,24	1.23	3 (13%)
29	PL9	d	405	-	55,55,55	0.65	1 (1%)	68,69,69	1.61	13 (19%)
34	LMT	a	413	-	36,36,36	0.60	1 (2%)	47,47,47	1.16	4 (8%)
26	GOL	v	201	-	5,5,5	1.21	0	5,5,5	0.89	0
23	CLA	B	608	-	69,73,73	1.97	20 (28%)	82,113,113	2.68	32 (39%)
23	CLA	B	607	40	69,73,73	2.01	19 (27%)	82,113,113	2.64	32 (39%)
23	CLA	b	608	-	69,73,73	2.03	20 (28%)	82,113,113	2.67	32 (39%)
25	BCR	b	618	-	41,41,41	1.04	1 (2%)	56,56,56	1.30	8 (14%)
25	BCR	B	619	-	41,41,41	1.04	1 (2%)	56,56,56	1.31	8 (14%)
23	CLA	c	512	-	69,73,73	1.96	20 (28%)	82,113,113	2.61	31 (37%)
23	CLA	C	507	-	69,73,73	1.97	20 (28%)	82,113,113	2.62	29 (35%)
25	BCR	K	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.42	9 (16%)
38	HEC	V	201	16	46,50,50	1.92	7 (15%)	58,82,82	1.76	8 (13%)
23	CLA	b	615	-	69,73,73	1.98	18 (26%)	82,113,113	2.65	32 (39%)
25	BCR	d	404	-	41,41,41	1.15	1 (2%)	56,56,56	1.75	11 (19%)
32	LMG	c	501	-	51,51,55	0.93	2 (3%)	59,59,63	1.09	3 (5%)
23	CLA	C	512	-	69,73,73	2.03	20 (28%)	82,113,113	2.69	31 (37%)
27	SQD	a	412	-	52,54,54	0.98	2 (3%)	62,65,65	1.25	5 (8%)
23	CLA	b	603	-	69,73,73	2.03	20 (28%)	82,113,113	2.78	31 (37%)
37	BCT	D	401	21	3,3,3	0.44	0	2,3,3	1.20	0
31	LHG	A	416	-	48,48,48	0.89	2 (4%)	51,54,54	1.14	6 (11%)
25	BCR	y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.63	10 (17%)
25	BCR	k	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.46	11 (19%)
31	LHG	D	407	-	48,48,48	0.89	3 (6%)	51,54,54	1.01	3 (5%)
23	CLA	b	610	40	69,73,73	2.02	20 (28%)	82,113,113	2.74	32 (39%)
23	CLA	b	612	-	69,73,73	1.98	19 (27%)	82,113,113	2.75	29 (35%)
23	CLA	b	604	-	69,73,73	2.00	19 (27%)	82,113,113	2.62	31 (37%)
23	CLA	a	406	40	69,73,73	1.92	18 (26%)	82,113,113	2.71	31 (37%)
23	CLA	C	514	-	69,73,73	2.02	20 (28%)	82,113,113	2.65	31 (37%)
23	CLA	c	511	-	69,73,73	2.07	20 (28%)	82,113,113	2.67	30 (36%)
34	LMT	M	101	-	36,36,36	0.45	0	47,47,47	0.99	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMG	m	101	-	51,51,55	0.90	2 (3%)	59,59,63	1.12	5 (8%)
25	BCR	t	102	-	41,41,41	1.07	1 (2%)	56,56,56	1.44	9 (16%)
34	LMT	B	630	-	25,25,36	0.44	0	30,30,47	1.02	2 (6%)
23	CLA	b	614	-	69,73,73	1.97	20 (28%)	82,113,113	2.76	32 (39%)
27	SQD	B	620	-	52,54,54	0.98	2 (3%)	62,65,65	1.42	8 (12%)
38	HEC	E	103	5,6	46,50,50	1.75	10 (21%)	58,82,82	1.73	15 (25%)
23	CLA	B	609	-	69,73,73	1.97	18 (26%)	82,113,113	2.73	30 (36%)
23	CLA	b	611	-	69,73,73	1.95	20 (28%)	82,113,113	2.71	30 (36%)
23	CLA	C	511	-	69,73,73	2.08	19 (27%)	82,113,113	2.65	31 (37%)
27	SQD	A	411	-	52,54,54	0.99	2 (3%)	62,65,65	1.23	7 (11%)

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
33	HTG	B	623	-	-	4/10/30/30	0/1/1/1
23	CLA	b	605	-	1/1/15/20	6/39/115/115	-
24	PHO	A	407	-	-	0/37/103/103	0/5/6/6
23	CLA	a	405	40	1/1/15/20	9/39/115/115	-
33	HTG	h	101	-	-	1/7/27/30	0/1/1/1
23	CLA	b	616	-	1/1/15/20	6/39/115/115	-
25	BCR	B	617	-	-	0/29/63/63	0/2/2/2
32	LMG	C	502	-	-	25/46/66/70	0/1/1/1
23	CLA	c	505	-	1/1/15/20	1/39/115/115	-
34	LMT	M	103	-	-	9/21/61/61	0/2/2/2
23	CLA	A	405	40	1/1/15/20	3/39/115/115	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	B	611	-	1/1/15/20	3/39/115/115	-
23	CLA	c	508	-	1/1/15/20	11/39/115/115	-
27	SQD	D	412	-	-	15/38/58/69	0/1/1/1
23	CLA	C	506	40	1/1/15/20	7/39/115/115	-
35	DGD	h	103	-	-	14/51/91/95	0/2/2/2
23	CLA	c	509	40	1/1/15/20	7/39/115/115	-
24	PHO	a	417	-	-	2/37/103/103	0/5/6/6
31	LHG	d	408	-	-	10/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	612	-	1/1/15/20	2/39/115/115	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
34	LMT	m	103	-	-	7/21/61/61	0/2/2/2
31	LHG	E	101	-	-	14/46/46/53	-
32	LMG	c	522	-	-	9/46/66/70	0/1/1/1
33	HTG	C	523	-	-	1/10/30/30	0/1/1/1
25	BCR	C	516	-	-	2/29/63/63	0/2/2/2
32	LMG	B	621	-	-	11/46/66/70	0/1/1/1
23	CLA	C	508	-	1/1/15/20	10/39/115/115	-
23	CLA	B	613	-	1/1/15/20	8/39/115/115	-
23	CLA	B	603	-	1/1/15/20	6/39/115/115	-
23	CLA	c	513	3	1/1/15/20	8/39/115/115	-
23	CLA	d	402	-	1/1/15/20	3/39/115/115	-
34	LMT	E	102	-	-	7/21/61/61	0/2/2/2
23	CLA	C	515	-	-	14/39/115/115	-
27	SQD	a	410	-	-	14/49/69/69	0/1/1/1
23	CLA	B	605	-	1/1/15/20	3/39/115/115	-
23	CLA	A	408	-	1/1/15/20	9/39/115/115	-
23	CLA	C	505	-	1/1/15/20	4/39/115/115	-
23	CLA	c	510	-	1/1/15/20	8/39/115/115	-
34	LMT	C	526	-	-	8/21/61/61	0/2/2/2
26	GOL	o	302	-	-	2/4/4/4	-
23	CLA	c	514	-	1/1/15/20	14/39/115/115	-
23	CLA	b	609	-	1/1/15/20	7/39/115/115	-
23	CLA	C	503	-	1/1/15/20	4/39/115/115	-
23	CLA	b	602	-	1/1/15/20	5/39/115/115	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
27	SQD	b	620	-	-	26/49/69/69	0/1/1/1
26	GOL	a	411	-	-	4/4/4/4	-
26	GOL	c	502	-	-	0/4/4/4	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
34	LMT	B	628	-	-	9/21/61/61	0/2/2/2
26	GOL	B	629	-	-	0/4/4/4	-
33	HTG	b	622	-	-	2/10/30/30	0/1/1/1
33	HTG	V	202	-	-	1/2/19/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	406	40	-	6/39/115/115	-
31	LHG	d	407	-	-	19/53/53/53	-
23	CLA	B	601	40	1/1/15/20	9/39/115/115	-
34	LMT	b	621	-	-	7/17/37/61	0/1/1/2
33	HTG	B	625	-	-	3/10/30/30	0/1/1/1
23	CLA	B	606	-	1/1/15/20	9/39/115/115	-
23	CLA	a	408	-	1/1/15/20	16/39/115/115	-
29	PL9	a	415	-	-	13/53/73/73	0/1/1/1
23	CLA	d	403	-	1/1/15/20	7/39/115/115	-
35	DGD	c	519	-	-	17/51/91/95	0/2/2/2
32	LMG	d	412	39	-	8/46/66/70	0/1/1/1
26	GOL	b	628	-	-	0/4/4/4	-
38	HEC	v	202	16	-	6/14/54/54	-
25	BCR	a	409	-	-	1/29/63/63	0/2/2/2
29	PL9	D	406	-	-	8/53/73/73	0/1/1/1
35	DGD	C	519	-	-	16/51/91/95	0/2/2/2
35	DGD	c	520	-	-	10/51/91/95	0/2/2/2
23	CLA	c	506	40	1/1/15/20	5/39/115/115	-
26	GOL	b	624	-	-	3/4/4/4	-
23	CLA	b	607	40	1/1/15/20	0/39/115/115	-
26	GOL	B	624	-	-	2/4/4/4	-
24	PHO	A	415	-	-	2/37/103/103	0/5/6/6
25	BCR	C	517	-	-	0/29/63/63	0/2/2/2
25	BCR	h	102	-	-	0/29/63/63	0/2/2/2
23	CLA	B	610	40	1/1/15/20	5/39/115/115	-
23	CLA	B	602	-	1/1/15/20	5/39/115/115	-
27	SQD	C	501	-	-	12/49/69/69	0/1/1/1
29	PL9	A	413	-	-	15/53/73/73	0/1/1/1
32	LMG	c	521	-	-	6/46/66/70	0/1/1/1
23	CLA	C	510	-	1/1/15/20	3/39/115/115	-
23	CLA	D	403	-	1/1/15/20	6/39/115/115	-
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
23	CLA	c	507	-	1/1/15/20	4/39/115/115	-
32	LMG	Z	101	-	-	9/31/51/70	0/1/1/1
23	CLA	A	404	-	1/1/15/20	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	GOL	A	410	-	-	2/4/4/4	-
23	CLA	b	601	40	1/1/15/20	16/39/115/115	-
32	LMG	z	101	-	-	8/34/54/70	0/1/1/1
34	LMT	D	402	-	-	8/21/61/61	0/2/2/2
32	LMG	C	522	-	-	12/46/66/70	0/1/1/1
23	CLA	B	616	-	1/1/15/20	10/39/115/115	-
31	LHG	D	408	-	-	13/53/53/53	-
34	LMT	e	101	-	-	8/21/61/61	0/2/2/2
35	DGD	C	520	-	-	10/51/91/95	0/2/2/2
23	CLA	D	404	-	1/1/15/20	9/39/115/115	-
34	LMT	a	418	-	-	4/21/61/61	0/2/2/2
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
26	GOL	C	524	-	-	0/4/4/4	-
23	CLA	C	509	40	1/1/15/20	7/39/115/115	-
32	LMG	C	521	-	-	10/46/66/70	0/1/1/1
35	DGD	H	102	-	-	13/51/91/95	0/2/2/2
25	BCR	D	405	-	-	6/29/63/63	0/2/2/2
35	DGD	c	518	-	-	19/51/91/95	0/2/2/2
23	CLA	B	604	-	1/1/15/20	9/39/115/115	-
23	CLA	c	504	-	1/1/15/20	7/39/115/115	-
31	LHG	b	629	-	-	14/53/53/53	-
23	CLA	C	513	3	1/1/15/20	2/39/115/115	-
32	LMG	D	413	39	-	8/46/66/70	0/1/1/1
35	DGD	C	518	-	-	15/51/91/95	0/2/2/2
24	PHO	a	407	-	-	3/37/103/103	0/5/6/6
23	CLA	C	504	-	-	9/39/115/115	-
25	BCR	c	517	-	-	0/29/63/63	0/2/2/2
33	HTG	c	523	-	-	3/10/30/30	0/1/1/1
38	HEC	e	102	5,6	-	7/14/54/54	-
25	BCR	H	101	-	-	1/29/63/63	0/2/2/2
23	CLA	B	615	-	1/1/15/20	9/39/115/115	-
23	CLA	b	606	-	1/1/15/20	11/39/115/115	-
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
23	CLA	a	404	-	1/1/15/20	6/39/115/115	-
31	LHG	a	419	-	-	18/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	GOL	O	302	-	-	4/4/4/4	-
23	CLA	c	515	-	1/1/15/20	9/39/115/115	-
26	GOL	B	627	-	-	0/4/4/4	-
33	HTG	B	622	-	-	4/10/30/30	0/1/1/1
34	LMT	t	101	-	-	6/17/38/61	0/1/1/2
23	CLA	B	614	-	1/1/15/20	12/39/115/115	-
23	CLA	c	503	-	1/1/15/20	4/39/115/115	-
34	LMT	b	627	-	-	9/17/37/61	0/1/1/2
31	LHG	L	101	-	-	13/53/53/53	-
27	SQD	f	101	-	-	19/38/58/69	0/1/1/1
33	HTG	D	411	-	-	2/7/27/30	0/1/1/1
33	HTG	b	623	-	-	2/10/30/30	0/1/1/1
23	CLA	b	613	-	1/1/15/20	5/39/115/115	-
31	LHG	d	406	-	-	14/53/53/53	-
33	HTG	b	625	-	-	4/10/30/30	0/1/1/1
29	PL9	d	405	-	-	6/53/73/73	0/1/1/1
34	LMT	a	413	-	-	7/21/61/61	0/2/2/2
26	GOL	v	201	-	-	2/4/4/4	-
23	CLA	B	608	-	-	1/39/115/115	-
23	CLA	B	607	40	1/1/15/20	3/39/115/115	-
23	CLA	b	608	-	-	2/39/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	c	512	-	1/1/15/20	6/39/115/115	-
23	CLA	C	507	-	1/1/15/20	8/39/115/115	-
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
38	HEC	V	201	16	-	6/14/54/54	-
23	CLA	b	615	-	1/1/15/20	8/39/115/115	-
25	BCR	d	404	-	-	4/29/63/63	0/2/2/2
32	LMG	c	501	-	-	18/46/66/70	0/1/1/1
23	CLA	C	512	-	1/1/15/20	10/39/115/115	-
27	SQD	a	412	-	-	17/49/69/69	0/1/1/1
23	CLA	b	603	-	1/1/15/20	3/39/115/115	-
31	LHG	A	416	-	-	16/53/53/53	-
25	BCR	y	101	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	k	101	-	-	2/29/63/63	0/2/2/2
31	LHG	D	407	-	-	11/53/53/53	-
23	CLA	b	610	40	1/1/15/20	8/39/115/115	-
23	CLA	b	612	-	1/1/15/20	4/39/115/115	-
23	CLA	b	604	-	1/1/15/20	10/39/115/115	-
23	CLA	a	406	40	-	8/39/115/115	-
23	CLA	C	514	-	1/1/15/20	11/39/115/115	-
23	CLA	c	511	-	1/1/15/20	15/39/115/115	-
34	LMT	M	101	-	-	6/21/61/61	0/2/2/2
32	LMG	m	101	-	-	11/46/66/70	0/1/1/1
25	BCR	t	102	-	-	4/29/63/63	0/2/2/2
34	LMT	B	630	-	-	5/17/37/61	0/1/1/2
23	CLA	b	614	-	1/1/15/20	10/39/115/115	-
27	SQD	B	620	-	-	17/49/69/69	0/1/1/1
38	HEC	E	103	5,6	-	8/14/54/54	-
23	CLA	B	609	-	1/1/15/20	4/39/115/115	-
23	CLA	b	611	-	1/1/15/20	4/39/115/115	-
23	CLA	C	511	-	1/1/15/20	5/39/115/115	-
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1

All (1587) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	417	PHO	C1B-C2B	9.19	1.49	1.39
24	A	407	PHO	C1D-C2D	9.02	1.49	1.39
24	a	417	PHO	C1D-C2D	8.87	1.49	1.39
24	a	407	PHO	C1B-C2B	8.80	1.49	1.39
24	A	415	PHO	C1D-C2D	8.39	1.48	1.39
24	A	415	PHO	C1B-C2B	8.37	1.48	1.39
24	A	407	PHO	C1B-C2B	8.29	1.48	1.39
24	a	407	PHO	C1D-C2D	8.27	1.48	1.39
24	a	417	PHO	C3B-C4B	8.00	1.49	1.41
24	A	415	PHO	C4D-CHA	7.58	1.50	1.39
38	V	201	HEC	CAC-C3C	7.01	1.57	1.35
24	A	415	PHO	C3B-C2B	6.92	1.49	1.40
24	a	417	PHO	C4D-CHA	6.86	1.49	1.39
24	A	407	PHO	C4D-CHA	6.81	1.49	1.39
38	v	202	HEC	CAC-C3C	6.60	1.56	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407	PHO	C4D-CHA	6.58	1.49	1.39
24	A	415	PHO	C3B-C4B	6.56	1.48	1.41
38	V	201	HEC	CAB-C3B	6.46	1.56	1.35
24	a	407	PHO	C3B-C2B	6.27	1.48	1.40
24	a	417	PHO	C3B-C2B	6.24	1.48	1.40
24	a	407	PHO	C3B-C4B	6.13	1.47	1.41
38	v	202	HEC	CAB-C3B	6.08	1.54	1.35
24	A	407	PHO	C3B-C2B	6.06	1.48	1.40
24	A	407	PHO	C3B-C4B	6.00	1.47	1.41
24	a	407	PHO	C3D-C2D	5.87	1.49	1.39
24	A	415	PHO	C3D-C2D	5.77	1.49	1.39
24	a	417	PHO	C3D-C2D	5.76	1.49	1.39
23	C	510	CLA	C3C-C2C	5.72	1.49	1.36
23	B	610	CLA	C3C-C2C	5.71	1.49	1.36
23	a	408	CLA	C3C-C2C	5.61	1.48	1.36
23	a	405	CLA	C3C-C2C	5.61	1.48	1.36
38	v	202	HEC	C3D-C2D	5.58	1.53	1.38
23	b	601	CLA	C3C-C2C	5.58	1.48	1.36
23	c	510	CLA	C3C-C2C	5.56	1.48	1.36
23	C	509	CLA	C3C-C2C	5.53	1.48	1.36
23	a	404	CLA	C3C-C2C	5.49	1.48	1.36
23	d	403	CLA	C1D-ND	5.48	1.45	1.37
23	B	601	CLA	C3C-C2C	5.44	1.48	1.36
23	C	514	CLA	C3C-C2C	5.44	1.48	1.36
24	A	407	PHO	OBD-CAD	5.44	1.29	1.22
23	B	614	CLA	C3C-C2C	5.41	1.48	1.36
23	A	406	CLA	C3C-C2C	5.39	1.48	1.36
23	d	403	CLA	C3C-C2C	5.39	1.48	1.36
25	d	404	BCR	C23-C22	-5.38	1.34	1.46
23	c	504	CLA	C3C-C2C	5.37	1.48	1.36
23	b	606	CLA	C3C-C2C	5.35	1.48	1.36
23	C	505	CLA	C3C-C2C	5.34	1.48	1.36
23	C	513	CLA	O2D-CGD	5.34	1.46	1.33
23	a	405	CLA	C1D-ND	5.33	1.44	1.37
23	b	615	CLA	C3C-C2C	5.32	1.48	1.36
23	C	503	CLA	C3C-C2C	5.32	1.48	1.36
23	b	605	CLA	C3C-C2C	5.31	1.48	1.36
23	c	504	CLA	O2D-CGD	5.30	1.46	1.33
23	c	513	CLA	C3C-C2C	5.28	1.48	1.36
23	D	403	CLA	C3C-C2C	5.27	1.48	1.36
23	B	602	CLA	CHC-C1C	5.27	1.49	1.38
38	V	201	HEC	C3D-C2D	5.25	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	C3C-C2C	5.24	1.48	1.36
23	b	601	CLA	C1D-ND	5.22	1.44	1.37
23	c	507	CLA	C3C-C2C	5.21	1.48	1.36
23	b	603	CLA	C3C-C2C	5.20	1.48	1.36
23	C	515	CLA	C1D-ND	5.20	1.44	1.37
23	D	404	CLA	C1D-ND	5.20	1.44	1.37
23	c	506	CLA	C1D-ND	5.20	1.44	1.37
23	c	505	CLA	C3C-C2C	5.18	1.47	1.36
23	B	602	CLA	C3C-C2C	5.17	1.47	1.36
23	c	514	CLA	C3C-C2C	5.17	1.47	1.36
23	b	613	CLA	C3C-C2C	5.17	1.47	1.36
23	B	611	CLA	O2D-CGD	5.16	1.45	1.33
23	A	404	CLA	C3C-C2C	5.16	1.47	1.36
23	A	405	CLA	C3C-C2C	5.15	1.47	1.36
23	b	614	CLA	O2D-CGD	5.14	1.45	1.33
23	A	408	CLA	C3C-C2C	5.14	1.47	1.36
23	b	602	CLA	O2D-CGD	5.14	1.45	1.33
23	c	510	CLA	O2D-CGD	5.14	1.45	1.33
23	c	509	CLA	C1D-ND	5.14	1.44	1.37
23	D	404	CLA	C3C-C2C	5.12	1.47	1.36
23	B	611	CLA	C3C-C2C	5.12	1.47	1.36
23	b	613	CLA	O2D-CGD	5.12	1.45	1.33
23	c	514	CLA	CHC-C1C	5.12	1.48	1.38
23	b	609	CLA	C3C-C2C	5.12	1.47	1.36
23	B	603	CLA	C3C-C2C	5.11	1.47	1.36
25	b	619	BCR	C23-C22	-5.11	1.35	1.46
23	c	515	CLA	O2D-CGD	5.11	1.45	1.33
23	C	515	CLA	C3C-C2C	5.11	1.47	1.36
23	c	508	CLA	C3C-C2C	5.11	1.47	1.36
23	B	608	CLA	C3C-C2C	5.09	1.47	1.36
23	c	511	CLA	C1D-ND	5.09	1.44	1.37
23	d	402	CLA	C3C-C2C	5.09	1.47	1.36
23	B	604	CLA	C3C-C2C	5.08	1.47	1.36
23	b	607	CLA	C3C-C2C	5.08	1.47	1.36
23	B	601	CLA	O2D-CGD	5.08	1.45	1.33
23	A	406	CLA	O2D-CGD	5.07	1.45	1.33
24	a	417	PHO	OBD-CAD	5.06	1.28	1.22
23	c	511	CLA	O2D-CGD	5.06	1.45	1.33
23	C	511	CLA	C3C-C2C	5.06	1.47	1.36
23	b	602	CLA	C3C-C2C	5.06	1.47	1.36
23	c	509	CLA	C3C-C2C	5.05	1.47	1.36
25	t	102	BCR	C23-C22	-5.05	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	C1D-ND	5.05	1.44	1.37
23	B	605	CLA	C3C-C2C	5.05	1.47	1.36
24	a	417	PHO	O2D-CGD	5.05	1.45	1.33
23	B	611	CLA	C1D-ND	5.05	1.44	1.37
23	b	603	CLA	O2D-CGD	5.04	1.45	1.33
23	c	509	CLA	CHC-C1C	5.04	1.48	1.38
23	C	504	CLA	CHC-C1C	5.04	1.48	1.38
23	B	605	CLA	CHC-C1C	5.03	1.48	1.38
23	A	404	CLA	C1D-ND	5.03	1.44	1.37
23	A	408	CLA	O2D-CGD	5.03	1.45	1.33
23	b	614	CLA	C3C-C2C	5.02	1.47	1.36
23	c	515	CLA	C3C-C2C	5.02	1.47	1.36
23	c	508	CLA	O2D-CGD	5.01	1.45	1.33
23	b	612	CLA	C3C-C2C	5.01	1.47	1.36
23	c	515	CLA	CHC-C1C	5.01	1.48	1.38
23	c	509	CLA	O2D-CGD	5.01	1.45	1.33
23	c	503	CLA	C3C-C2C	5.00	1.47	1.36
23	C	507	CLA	C3C-C2C	5.00	1.47	1.36
23	c	512	CLA	C3C-C2C	5.00	1.47	1.36
23	c	506	CLA	O2D-CGD	5.00	1.45	1.33
23	C	504	CLA	O2D-CGD	4.99	1.45	1.33
23	b	609	CLA	CHC-C1C	4.99	1.48	1.38
23	d	403	CLA	CHC-C1C	4.99	1.48	1.38
23	b	609	CLA	O2D-CGD	4.99	1.45	1.33
23	C	511	CLA	C1D-ND	4.99	1.44	1.37
24	A	407	PHO	C3D-C2D	4.98	1.48	1.39
23	b	610	CLA	O2D-CGD	4.98	1.45	1.33
23	c	514	CLA	O2D-CGD	4.97	1.45	1.33
24	a	407	PHO	OBD-CAD	4.97	1.28	1.22
23	b	604	CLA	O2D-CGD	4.97	1.45	1.33
23	b	608	CLA	O2D-CGD	4.96	1.45	1.33
25	k	101	BCR	C23-C22	-4.96	1.35	1.46
23	c	510	CLA	C1D-ND	4.96	1.44	1.37
25	c	517	BCR	C23-C22	-4.96	1.35	1.46
23	C	512	CLA	C3C-C2C	4.95	1.47	1.36
23	C	508	CLA	O2D-CGD	4.95	1.45	1.33
23	D	404	CLA	O2D-CGD	4.94	1.45	1.33
23	b	616	CLA	O2D-CGD	4.94	1.45	1.33
25	H	101	BCR	C23-C22	-4.94	1.35	1.46
23	b	601	CLA	O2D-CGD	4.94	1.45	1.33
23	B	616	CLA	C3C-C2C	4.94	1.47	1.36
23	B	606	CLA	C3C-C2C	4.93	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	O2D-CGD	4.92	1.45	1.33
23	C	504	CLA	C3C-C2C	4.92	1.47	1.36
23	C	508	CLA	CHD-C1D	4.92	1.48	1.38
23	b	608	CLA	C3C-C2C	4.92	1.47	1.36
23	B	607	CLA	C3C-C2C	4.91	1.47	1.36
23	b	616	CLA	C3C-C2C	4.91	1.47	1.36
23	a	405	CLA	CHC-C1C	4.91	1.48	1.38
23	c	506	CLA	C3C-C2C	4.91	1.47	1.36
23	c	511	CLA	C3C-C2C	4.90	1.47	1.36
23	b	611	CLA	C3C-C2C	4.90	1.47	1.36
23	A	408	CLA	CHC-C1C	4.90	1.48	1.38
25	K	101	BCR	C23-C22	-4.90	1.35	1.46
23	b	604	CLA	C1D-ND	4.89	1.44	1.37
23	B	615	CLA	O2D-CGD	4.89	1.45	1.33
23	c	513	CLA	C1D-ND	4.88	1.44	1.37
23	C	512	CLA	O2D-CGD	4.87	1.45	1.33
25	C	516	BCR	C23-C22	-4.87	1.35	1.46
23	C	512	CLA	C1D-ND	4.87	1.44	1.37
23	a	405	CLA	O2D-CGD	4.87	1.45	1.33
23	B	615	CLA	C3C-C2C	4.86	1.47	1.36
23	c	515	CLA	C1D-ND	4.85	1.44	1.37
23	B	603	CLA	O2D-CGD	4.85	1.45	1.33
23	a	404	CLA	C1D-ND	4.85	1.44	1.37
23	b	613	CLA	C1D-ND	4.85	1.44	1.37
23	c	508	CLA	C1D-ND	4.84	1.44	1.37
23	a	406	CLA	CHC-C1C	4.84	1.48	1.38
25	c	516	BCR	C23-C22	-4.84	1.35	1.46
25	a	409	BCR	C23-C22	-4.84	1.35	1.46
23	c	503	CLA	C1D-ND	4.82	1.44	1.37
23	C	505	CLA	C1D-ND	4.81	1.44	1.37
23	a	408	CLA	CHC-C1C	4.81	1.48	1.38
23	C	506	CLA	C3C-C2C	4.81	1.47	1.36
23	C	506	CLA	O2D-CGD	4.81	1.45	1.33
23	c	507	CLA	CHC-C1C	4.81	1.48	1.38
23	b	614	CLA	CHC-C1C	4.81	1.48	1.38
23	C	507	CLA	CHC-C1C	4.81	1.48	1.38
25	b	617	BCR	C23-C22	-4.81	1.35	1.46
23	b	605	CLA	C1D-ND	4.81	1.44	1.37
23	B	604	CLA	O2D-CGD	4.80	1.45	1.33
24	A	415	PHO	O2D-CGD	4.80	1.45	1.33
23	C	508	CLA	C3C-C2C	4.80	1.47	1.36
23	A	406	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	616	CLA	O2D-CGD	4.79	1.45	1.33
25	D	405	BCR	C23-C22	-4.79	1.35	1.46
23	B	601	CLA	CHC-C1C	4.78	1.48	1.38
23	C	508	CLA	C1D-ND	4.78	1.44	1.37
23	b	601	CLA	CHC-C1C	4.77	1.48	1.38
24	a	407	PHO	O2D-CGD	4.76	1.44	1.33
23	B	605	CLA	O2D-CGD	4.76	1.44	1.33
23	A	405	CLA	CHC-C1C	4.76	1.48	1.38
23	C	506	CLA	CHC-C1C	4.76	1.48	1.38
23	c	513	CLA	O2D-CGD	4.76	1.44	1.33
25	y	101	BCR	C23-C22	-4.75	1.35	1.46
23	c	503	CLA	O2D-CGD	4.75	1.44	1.33
23	C	505	CLA	O2D-CGD	4.75	1.44	1.33
23	C	512	CLA	CHC-C1C	4.74	1.48	1.38
23	D	404	CLA	CHC-C1C	4.74	1.48	1.38
23	b	608	CLA	CHC-C1C	4.74	1.48	1.38
23	B	602	CLA	C1D-ND	4.74	1.44	1.37
23	a	406	CLA	C3C-C2C	4.73	1.47	1.36
23	b	601	CLA	O2A-CGA	4.73	1.47	1.33
23	b	615	CLA	C1D-ND	4.73	1.44	1.37
23	c	505	CLA	C1D-ND	4.72	1.44	1.37
23	b	615	CLA	O2D-CGD	4.72	1.44	1.33
23	c	507	CLA	O2D-CGD	4.72	1.44	1.33
25	b	618	BCR	C23-C22	-4.72	1.35	1.46
23	C	514	CLA	CHC-C1C	4.71	1.47	1.38
23	b	605	CLA	O2D-CGD	4.71	1.44	1.33
23	c	510	CLA	CHC-C1C	4.71	1.47	1.38
23	c	503	CLA	CHC-C1C	4.71	1.47	1.38
23	B	604	CLA	CHC-C1C	4.71	1.47	1.38
23	B	612	CLA	CHC-C1C	4.71	1.47	1.38
23	B	613	CLA	O2D-CGD	4.70	1.44	1.33
23	C	515	CLA	O2D-CGD	4.70	1.44	1.33
23	c	504	CLA	CHC-C1C	4.69	1.47	1.38
23	c	504	CLA	C1D-ND	4.69	1.44	1.37
23	C	507	CLA	O2D-CGD	4.68	1.44	1.33
23	c	513	CLA	CHC-C1C	4.68	1.47	1.38
23	A	404	CLA	CHC-C1C	4.67	1.47	1.38
23	A	405	CLA	O2D-CGD	4.67	1.44	1.33
23	B	609	CLA	C3C-C2C	4.66	1.46	1.36
23	B	606	CLA	O2D-CGD	4.66	1.44	1.33
24	A	415	PHO	OBD-CAD	4.66	1.28	1.22
23	b	606	CLA	C1D-ND	4.65	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	CHC-C1C	4.65	1.47	1.38
23	C	514	CLA	O2D-CGD	4.65	1.44	1.33
23	b	603	CLA	C1D-ND	4.64	1.44	1.37
23	B	612	CLA	O2D-CGD	4.64	1.44	1.33
23	B	601	CLA	O2A-CGA	4.63	1.46	1.33
24	A	407	PHO	O2D-CGD	4.63	1.44	1.33
23	A	408	CLA	C1D-ND	4.63	1.43	1.37
23	B	603	CLA	CHC-C1C	4.62	1.47	1.38
23	b	602	CLA	CHC-C1C	4.62	1.47	1.38
23	C	510	CLA	CHC-C1C	4.62	1.47	1.38
23	C	513	CLA	C3C-C2C	4.61	1.46	1.36
23	b	603	CLA	CHC-C1C	4.61	1.47	1.38
23	c	512	CLA	C1D-ND	4.61	1.43	1.37
23	b	611	CLA	CHC-C1C	4.60	1.47	1.38
23	b	611	CLA	O2D-CGD	4.60	1.44	1.33
23	b	610	CLA	CHC-C1C	4.60	1.47	1.38
23	C	514	CLA	C1D-ND	4.60	1.43	1.37
23	B	615	CLA	CHC-C1C	4.60	1.47	1.38
23	c	508	CLA	CHC-C1C	4.60	1.47	1.38
23	C	513	CLA	CHC-C1C	4.59	1.47	1.38
23	B	601	CLA	C1D-ND	4.59	1.43	1.37
23	C	511	CLA	O2D-CGD	4.59	1.44	1.33
23	b	601	CLA	CHD-C1D	4.59	1.47	1.38
23	c	505	CLA	O2D-CGD	4.59	1.44	1.33
23	B	612	CLA	C3C-C2C	4.58	1.46	1.36
25	C	517	BCR	C23-C22	-4.58	1.36	1.46
23	B	613	CLA	CHC-C1C	4.58	1.47	1.38
25	h	102	BCR	C23-C22	-4.58	1.36	1.46
23	C	509	CLA	CHC-C1C	4.57	1.47	1.38
23	b	604	CLA	C3C-C2C	4.57	1.46	1.36
23	a	404	CLA	O2D-CGD	4.57	1.44	1.33
23	b	602	CLA	C1D-ND	4.56	1.43	1.37
25	B	619	BCR	C23-C22	-4.56	1.36	1.46
23	B	614	CLA	C1D-ND	4.56	1.43	1.37
23	c	505	CLA	CHC-C1C	4.56	1.47	1.38
23	C	505	CLA	CHC-C1C	4.55	1.47	1.38
23	B	602	CLA	CHD-C1D	4.55	1.47	1.38
23	B	610	CLA	CHC-C1C	4.55	1.47	1.38
23	C	510	CLA	O2D-CGD	4.54	1.44	1.33
23	b	613	CLA	CHC-C1C	4.54	1.47	1.38
23	B	615	CLA	C1D-ND	4.54	1.43	1.37
23	C	510	CLA	C1D-ND	4.54	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	CHC-C1C	4.53	1.47	1.38
27	A	411	SQD	O48-C23	4.53	1.46	1.33
23	b	606	CLA	CHC-C1C	4.53	1.47	1.38
23	C	509	CLA	O2D-CGD	4.53	1.44	1.33
23	C	511	CLA	CHD-C1D	4.53	1.47	1.38
23	c	511	CLA	CHC-C1C	4.53	1.47	1.38
25	A	409	BCR	C23-C22	-4.52	1.36	1.46
23	A	404	CLA	O2D-CGD	4.51	1.44	1.33
23	B	615	CLA	C3D-C2D	4.51	1.51	1.39
23	B	608	CLA	C1D-ND	4.50	1.43	1.37
23	B	609	CLA	CHC-C1C	4.48	1.47	1.38
23	A	406	CLA	CHD-C1D	4.48	1.47	1.38
23	b	611	CLA	O2A-CGA	4.47	1.46	1.33
25	B	617	BCR	C23-C22	-4.47	1.36	1.46
23	D	403	CLA	O2D-CGD	4.47	1.44	1.33
23	B	614	CLA	O2D-CGD	4.47	1.44	1.33
23	C	503	CLA	CHC-C1C	4.47	1.47	1.38
23	B	607	CLA	O2D-CGD	4.47	1.44	1.33
23	c	506	CLA	CHC-C1C	4.46	1.47	1.38
23	a	408	CLA	O2D-CGD	4.46	1.44	1.33
23	B	602	CLA	O2D-CGD	4.46	1.44	1.33
23	C	503	CLA	C1D-ND	4.46	1.43	1.37
23	C	503	CLA	O2D-CGD	4.45	1.44	1.33
23	B	608	CLA	CHC-C1C	4.45	1.47	1.38
23	b	602	CLA	CHD-C1D	4.44	1.47	1.38
23	c	514	CLA	C1D-ND	4.44	1.43	1.37
23	B	605	CLA	CHC-C4B	4.44	1.49	1.39
23	B	612	CLA	CHB-C1B	4.44	1.49	1.39
23	b	607	CLA	CHD-C1D	4.44	1.47	1.38
23	c	513	CLA	CHB-C1B	4.44	1.49	1.39
23	a	404	CLA	CHC-C1C	4.44	1.47	1.38
31	E	101	LHG	O8-C23	4.43	1.46	1.33
23	B	609	CLA	O2A-CGA	4.43	1.46	1.33
23	d	402	CLA	O2D-CGD	4.43	1.44	1.33
31	a	419	LHG	O7-C7	4.42	1.46	1.34
23	a	405	CLA	O2A-CGA	4.42	1.46	1.33
23	C	508	CLA	CHC-C1C	4.42	1.47	1.38
23	D	403	CLA	CHC-C1C	4.42	1.47	1.38
23	d	403	CLA	O2D-CGD	4.42	1.44	1.33
23	c	505	CLA	CHD-C1D	4.41	1.47	1.38
32	C	522	LMG	O7-C10	4.41	1.46	1.34
23	c	510	CLA	CHD-C1D	4.41	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	521	LMG	O8-C28	4.40	1.46	1.33
23	d	402	CLA	O2A-CGA	4.40	1.46	1.33
23	b	605	CLA	CHC-C1C	4.40	1.47	1.38
38	e	102	HEC	CBC-CAC	-4.40	1.33	1.49
23	c	507	CLA	CHD-C1D	4.40	1.47	1.38
32	z	101	LMG	O8-C28	4.38	1.46	1.33
23	C	514	CLA	CHD-C1D	4.38	1.47	1.38
23	a	406	CLA	O2D-CGD	4.38	1.44	1.33
23	B	607	CLA	C1D-ND	4.37	1.43	1.37
23	b	607	CLA	CHC-C1C	4.37	1.47	1.38
23	C	513	CLA	C1D-ND	4.37	1.43	1.37
25	Y	101	BCR	C23-C22	-4.37	1.36	1.46
32	C	522	LMG	O8-C28	4.37	1.46	1.33
23	d	403	CLA	C3D-C2D	4.37	1.50	1.39
23	B	601	CLA	CHD-C1D	4.36	1.46	1.38
23	B	606	CLA	CHD-C1D	4.36	1.46	1.38
23	C	515	CLA	CHC-C1C	4.36	1.47	1.38
31	a	419	LHG	O8-C23	4.36	1.46	1.33
23	c	513	CLA	O2A-CGA	4.36	1.46	1.33
23	b	604	CLA	CHC-C1C	4.35	1.47	1.38
27	a	412	SQD	O47-C7	4.35	1.46	1.34
38	E	103	HEC	CBC-CAC	-4.35	1.33	1.49
35	c	520	DGD	O1G-C1A	4.35	1.46	1.33
23	A	406	CLA	C1B-NB	-4.35	1.32	1.37
27	D	412	SQD	O47-C7	4.35	1.46	1.34
23	c	510	CLA	O2A-CGA	4.35	1.46	1.33
32	c	522	LMG	O7-C10	4.35	1.46	1.34
23	B	606	CLA	CHC-C1C	4.35	1.47	1.38
25	T	101	BCR	C23-C22	-4.35	1.36	1.46
23	D	403	CLA	O2A-CGA	4.34	1.46	1.33
23	b	608	CLA	C1D-ND	4.34	1.43	1.37
27	f	101	SQD	O47-C7	4.34	1.46	1.34
38	e	102	HEC	CBB-CAB	-4.34	1.33	1.49
23	B	616	CLA	CHC-C1C	4.34	1.47	1.38
23	b	608	CLA	CHD-C1D	4.34	1.46	1.38
23	B	605	CLA	C1D-ND	4.33	1.43	1.37
32	c	522	LMG	O8-C28	4.33	1.46	1.33
23	c	512	CLA	CHC-C1C	4.33	1.47	1.38
32	C	521	LMG	O7-C10	4.33	1.46	1.34
27	B	620	SQD	O48-C23	4.33	1.46	1.33
23	B	604	CLA	C1D-ND	4.33	1.43	1.37
23	c	514	CLA	O2A-CGA	4.33	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	O2D-CGD	4.32	1.43	1.33
23	C	515	CLA	CHD-C1D	4.32	1.46	1.38
23	B	602	CLA	CHC-C4B	4.32	1.49	1.39
23	a	405	CLA	C3D-C2D	4.32	1.50	1.39
23	b	612	CLA	C1D-ND	4.32	1.43	1.37
27	a	412	SQD	O48-C23	4.32	1.45	1.33
23	C	511	CLA	CHC-C1C	4.32	1.47	1.38
23	C	509	CLA	C1D-ND	4.32	1.43	1.37
23	b	614	CLA	C1D-ND	4.32	1.43	1.37
32	Z	101	LMG	O7-C10	4.32	1.46	1.34
27	b	620	SQD	O47-C7	4.31	1.46	1.34
32	d	412	LMG	O8-C28	4.31	1.45	1.33
23	B	610	CLA	C1D-ND	4.31	1.43	1.37
27	B	620	SQD	O47-C7	4.31	1.46	1.34
23	B	609	CLA	C1D-ND	4.30	1.43	1.37
23	b	602	CLA	O2A-CGA	4.30	1.45	1.33
23	A	405	CLA	C1D-ND	4.30	1.43	1.37
23	c	515	CLA	CHD-C1D	4.29	1.46	1.38
23	c	512	CLA	O2D-CGD	4.29	1.43	1.33
27	b	620	SQD	O48-C23	4.29	1.45	1.33
23	c	503	CLA	CHB-C1B	4.29	1.49	1.39
23	b	612	CLA	O2D-CGD	4.28	1.43	1.33
23	d	403	CLA	CHD-C4C	4.28	1.49	1.39
23	B	611	CLA	CHC-C1C	4.28	1.47	1.38
23	C	508	CLA	CHD-C4C	4.28	1.48	1.39
23	D	404	CLA	CHD-C1D	4.28	1.46	1.38
23	B	614	CLA	CHC-C1C	4.27	1.47	1.38
23	b	609	CLA	CHD-C1D	4.27	1.46	1.38
38	E	103	HEC	CBB-CAB	-4.27	1.33	1.49
23	c	509	CLA	CHD-C4C	4.27	1.48	1.39
23	A	408	CLA	CHD-C1D	4.26	1.46	1.38
23	d	403	CLA	O2A-CGA	4.26	1.45	1.33
23	d	402	CLA	CHC-C1C	4.26	1.47	1.38
23	C	511	CLA	CHD-C4C	4.26	1.48	1.39
23	b	601	CLA	CHD-C4C	4.25	1.48	1.39
23	B	605	CLA	CHD-C1D	4.25	1.46	1.38
32	C	502	LMG	O8-C28	4.25	1.45	1.33
23	D	404	CLA	CHB-C1B	4.24	1.48	1.39
23	b	616	CLA	CHC-C1C	4.24	1.47	1.38
23	D	403	CLA	CHD-C4C	4.24	1.48	1.39
32	B	621	LMG	O8-C28	4.24	1.45	1.33
23	B	613	CLA	C3C-C2C	4.24	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	C1D-ND	4.23	1.43	1.37
23	b	602	CLA	CHD-C4C	4.23	1.48	1.39
23	B	614	CLA	C4B-NB	-4.23	1.32	1.37
23	C	515	CLA	O2A-CGA	4.22	1.45	1.33
23	C	509	CLA	O2A-CGA	4.22	1.45	1.33
38	E	103	HEC	CAB-C3B	4.22	1.48	1.35
23	B	610	CLA	CHD-C1D	4.22	1.46	1.38
27	f	101	SQD	O48-C23	4.22	1.45	1.33
23	c	509	CLA	CHC-C4B	4.22	1.48	1.39
23	c	515	CLA	O2A-CGA	4.22	1.45	1.33
23	a	408	CLA	O2A-CGA	4.21	1.45	1.33
23	C	513	CLA	O2A-CGA	4.21	1.45	1.33
23	D	403	CLA	CHB-C1B	4.21	1.48	1.39
23	c	509	CLA	CHD-C1D	4.20	1.46	1.38
23	d	403	CLA	CHD-C1D	4.20	1.46	1.38
32	m	101	LMG	O8-C28	4.20	1.45	1.33
23	A	405	CLA	CHD-C1D	4.20	1.46	1.38
23	c	514	CLA	CHD-C1D	4.20	1.46	1.38
23	c	512	CLA	CHB-C1B	4.20	1.48	1.39
23	c	508	CLA	CHD-C1D	4.20	1.46	1.38
23	C	508	CLA	O2A-CGA	4.19	1.45	1.33
32	c	501	LMG	O8-C28	4.19	1.45	1.33
23	b	610	CLA	OBD-CAD	4.19	1.29	1.22
23	b	610	CLA	C1D-ND	4.19	1.43	1.37
23	c	511	CLA	CHD-C1D	4.19	1.46	1.38
23	B	608	CLA	O2D-CGD	4.19	1.43	1.33
23	b	608	CLA	CHD-C4C	4.18	1.48	1.39
23	B	609	CLA	CHD-C1D	4.18	1.46	1.38
23	b	611	CLA	C1D-ND	4.18	1.43	1.37
23	c	509	CLA	O2A-CGA	4.17	1.45	1.33
23	A	408	CLA	CHD-C4C	4.17	1.48	1.39
35	h	103	DGD	O1G-C1A	4.17	1.45	1.33
32	c	521	LMG	O7-C10	4.17	1.46	1.34
35	c	518	DGD	O1G-C1A	4.17	1.45	1.33
23	C	510	CLA	O2A-CGA	4.16	1.45	1.33
23	D	403	CLA	CHD-C1D	4.16	1.46	1.38
23	b	614	CLA	O2A-CGA	4.16	1.45	1.33
32	c	521	LMG	O8-C28	4.15	1.45	1.33
23	C	507	CLA	CHD-C1D	4.15	1.46	1.38
23	c	512	CLA	CHD-C1D	4.15	1.46	1.38
23	b	608	CLA	O2A-CGA	4.15	1.45	1.33
23	C	509	CLA	CHD-C1D	4.15	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	515	CLA	CHD-C4C	4.14	1.48	1.39
23	b	612	CLA	C1B-NB	-4.14	1.32	1.37
23	B	610	CLA	O2D-CGD	4.14	1.43	1.33
23	B	602	CLA	CHD-C4C	4.14	1.48	1.39
23	C	503	CLA	O2A-CGA	4.14	1.45	1.33
23	a	404	CLA	OBD-CAD	4.13	1.29	1.22
31	E	101	LHG	O7-C7	4.13	1.46	1.34
23	a	406	CLA	O2A-CGA	4.13	1.45	1.33
27	D	412	SQD	O48-C23	4.13	1.45	1.33
23	B	606	CLA	O2A-CGA	4.13	1.45	1.33
23	A	408	CLA	O2A-CGA	4.12	1.45	1.33
23	b	612	CLA	CHB-C1B	4.12	1.48	1.39
32	z	101	LMG	O7-C10	4.12	1.45	1.34
27	a	410	SQD	O48-C23	4.12	1.45	1.33
23	B	610	CLA	OBD-CAD	4.11	1.29	1.22
23	C	514	CLA	O2A-CGA	4.11	1.45	1.33
31	L	101	LHG	O8-C23	4.11	1.45	1.33
23	B	616	CLA	C1D-ND	4.11	1.43	1.37
27	A	411	SQD	O47-C7	4.11	1.45	1.34
31	d	408	LHG	O7-C7	4.11	1.45	1.34
23	B	607	CLA	CHB-C1B	4.11	1.48	1.39
23	c	511	CLA	O2A-CGA	4.10	1.45	1.33
23	c	504	CLA	CHD-C1D	4.10	1.46	1.38
23	c	506	CLA	CHD-C1D	4.10	1.46	1.38
31	b	629	LHG	O7-C7	4.10	1.45	1.34
27	a	410	SQD	O47-C7	4.10	1.45	1.34
23	C	511	CLA	OBD-CAD	4.09	1.29	1.22
35	C	518	DGD	O1G-C1A	4.09	1.45	1.33
23	C	511	CLA	C3D-C2D	4.09	1.50	1.39
23	c	514	CLA	CHC-C4B	4.09	1.48	1.39
35	C	518	DGD	O2G-C1B	4.09	1.45	1.34
35	C	520	DGD	O1G-C1A	4.09	1.45	1.33
23	b	603	CLA	CHD-C1D	4.09	1.46	1.38
23	b	613	CLA	C3D-C2D	4.08	1.50	1.39
23	C	503	CLA	CHD-C1D	4.08	1.46	1.38
23	b	603	CLA	OBD-CAD	4.08	1.29	1.22
23	b	611	CLA	CHB-C1B	4.08	1.48	1.39
23	b	612	CLA	CHC-C1C	4.08	1.46	1.38
24	A	407	PHO	O2A-CGA	4.08	1.45	1.33
23	C	506	CLA	C1D-ND	4.08	1.43	1.37
23	C	507	CLA	CHD-C4C	4.08	1.48	1.39
23	c	503	CLA	O2A-CGA	4.08	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	C3D-C2D	4.08	1.50	1.39
23	C	506	CLA	O2A-CGA	4.07	1.45	1.33
23	C	504	CLA	C3D-C2D	4.07	1.50	1.39
23	B	612	CLA	O2A-CGA	4.07	1.45	1.33
23	B	604	CLA	CHD-C4C	4.07	1.48	1.39
23	b	602	CLA	C3D-C2D	4.06	1.50	1.39
23	B	605	CLA	O2A-CGA	4.06	1.45	1.33
23	B	616	CLA	O2A-CGA	4.05	1.45	1.33
23	b	616	CLA	C1D-ND	4.05	1.43	1.37
23	B	603	CLA	O2A-CGA	4.05	1.45	1.33
23	C	512	CLA	C3D-C2D	4.05	1.50	1.39
23	c	511	CLA	C3D-C2D	4.05	1.50	1.39
23	b	604	CLA	C3D-C2D	4.05	1.50	1.39
23	B	607	CLA	CHD-C1D	4.05	1.46	1.38
23	c	508	CLA	O2A-CGA	4.05	1.45	1.33
23	b	612	CLA	O2A-CGA	4.05	1.45	1.33
35	C	519	DGD	O2G-C1B	4.04	1.45	1.34
23	b	610	CLA	CHD-C1D	4.04	1.46	1.38
23	c	503	CLA	CHD-C4C	4.03	1.48	1.39
23	C	511	CLA	O2A-CGA	4.03	1.45	1.33
23	c	511	CLA	CHD-C4C	4.03	1.48	1.39
23	c	507	CLA	CHC-C4B	4.03	1.48	1.39
23	a	404	CLA	CHD-C4C	4.03	1.48	1.39
23	b	607	CLA	C3D-C2D	4.03	1.50	1.39
35	C	519	DGD	O1G-C1A	4.02	1.45	1.33
23	B	615	CLA	O2A-CGA	4.02	1.45	1.33
23	C	505	CLA	O2A-CGA	4.02	1.45	1.33
23	C	515	CLA	C3D-C2D	4.02	1.50	1.39
23	c	510	CLA	C3D-C2D	4.02	1.50	1.39
23	c	507	CLA	CHD-C4C	4.02	1.48	1.39
23	B	614	CLA	CHB-C1B	4.02	1.48	1.39
27	C	501	SQD	O48-C23	4.02	1.45	1.33
23	B	608	CLA	O2A-CGA	4.02	1.45	1.33
23	c	506	CLA	C3D-C2D	4.02	1.50	1.39
23	c	508	CLA	CHD-C4C	4.02	1.48	1.39
23	C	506	CLA	C3D-C2D	4.01	1.49	1.39
23	a	405	CLA	CHD-C1D	4.01	1.46	1.38
32	c	501	LMG	O7-C10	4.01	1.45	1.34
23	B	615	CLA	OBD-CAD	4.01	1.29	1.22
35	c	519	DGD	O1G-C1A	4.01	1.45	1.33
23	B	601	CLA	CHC-C4B	4.01	1.48	1.39
23	C	504	CLA	CHD-C1D	4.00	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	CHD-C1D	4.00	1.46	1.38
23	C	507	CLA	C1D-ND	4.00	1.43	1.37
32	C	502	LMG	O7-C10	4.00	1.45	1.34
35	c	518	DGD	O2G-C1B	4.00	1.45	1.34
23	C	504	CLA	C1D-ND	4.00	1.43	1.37
35	h	103	DGD	O2G-C1B	4.00	1.45	1.34
23	C	512	CLA	CHC-C4B	4.00	1.48	1.39
23	B	613	CLA	O2A-CGA	4.00	1.45	1.33
23	c	506	CLA	CHD-C4C	4.00	1.48	1.39
23	c	507	CLA	C1D-ND	4.00	1.43	1.37
23	B	605	CLA	C3D-C2D	4.00	1.49	1.39
38	e	102	HEC	CAB-C3B	3.99	1.48	1.35
23	B	611	CLA	CHD-C1D	3.99	1.46	1.38
23	B	603	CLA	C3D-C2D	3.99	1.49	1.39
23	c	504	CLA	O2A-CGA	3.99	1.45	1.33
23	B	607	CLA	CHD-C4C	3.99	1.48	1.39
23	b	614	CLA	CHB-C1B	3.98	1.48	1.39
23	b	605	CLA	CHD-C1D	3.98	1.46	1.38
23	A	405	CLA	O2A-CGA	3.98	1.44	1.33
23	B	603	CLA	C1D-ND	3.98	1.43	1.37
23	a	408	CLA	C1D-ND	3.98	1.43	1.37
23	C	505	CLA	C3D-C2D	3.97	1.49	1.39
23	b	607	CLA	C1B-NB	-3.97	1.32	1.37
23	B	610	CLA	CHC-C4B	3.97	1.48	1.39
23	b	615	CLA	O2A-CGA	3.97	1.44	1.33
32	m	101	LMG	O7-C10	3.97	1.45	1.34
23	C	505	CLA	CHD-C4C	3.97	1.48	1.39
23	c	510	CLA	CHD-C4C	3.97	1.48	1.39
23	B	613	CLA	C3D-C2D	3.96	1.49	1.39
23	a	404	CLA	CHD-C1D	3.96	1.46	1.38
23	C	510	CLA	CHB-C1B	3.96	1.48	1.39
23	B	608	CLA	CHD-C1D	3.96	1.46	1.38
23	B	604	CLA	CHD-C1D	3.96	1.46	1.38
23	c	512	CLA	CHD-C4C	3.96	1.48	1.39
23	C	510	CLA	C3D-C2D	3.96	1.49	1.39
23	c	504	CLA	C3D-C2D	3.96	1.49	1.39
23	b	609	CLA	O2A-CGA	3.96	1.44	1.33
23	B	601	CLA	CHD-C4C	3.96	1.48	1.39
23	B	610	CLA	CHD-C4C	3.96	1.48	1.39
23	C	513	CLA	CHD-C1D	3.95	1.46	1.38
23	c	508	CLA	C3D-C2D	3.95	1.49	1.39
23	b	604	CLA	CHD-C1D	3.95	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	CHD-C1D	3.95	1.46	1.38
32	d	412	LMG	O7-C10	3.95	1.45	1.34
23	c	515	CLA	C3D-C2D	3.95	1.49	1.39
23	b	607	CLA	CHB-C1B	3.94	1.48	1.39
23	C	506	CLA	CHB-C1B	3.94	1.48	1.39
23	C	512	CLA	CHD-C1D	3.94	1.46	1.38
23	b	609	CLA	C1D-ND	3.93	1.43	1.37
23	B	610	CLA	C3D-C2D	3.93	1.49	1.39
23	C	515	CLA	CHD-C4C	3.93	1.48	1.39
23	c	509	CLA	OBD-CAD	3.93	1.29	1.22
23	B	604	CLA	O2A-CGA	3.93	1.44	1.33
35	C	520	DGD	O2G-C1B	3.93	1.45	1.34
23	b	616	CLA	CHD-C1D	3.93	1.46	1.38
23	c	511	CLA	CHB-C1B	3.93	1.48	1.39
23	B	605	CLA	OBD-CAD	3.93	1.29	1.22
23	b	612	CLA	CHD-C1D	3.93	1.46	1.38
23	C	513	CLA	CHD-C4C	3.92	1.48	1.39
23	A	408	CLA	CHC-C4B	3.92	1.48	1.39
23	C	503	CLA	CHC-C4B	3.92	1.48	1.39
23	c	509	CLA	C3D-C2D	3.92	1.49	1.39
23	c	505	CLA	CHD-C4C	3.92	1.48	1.39
23	c	506	CLA	CHB-C1B	3.92	1.48	1.39
23	b	606	CLA	O2D-CGD	3.92	1.42	1.33
23	C	513	CLA	C3D-C2D	3.91	1.49	1.39
23	B	616	CLA	CHB-C1B	3.91	1.48	1.39
23	A	406	CLA	CHC-C4B	3.91	1.48	1.39
23	c	510	CLA	OBD-CAD	3.91	1.29	1.22
23	c	507	CLA	O2A-CGA	3.91	1.44	1.33
23	b	610	CLA	CHC-C4B	3.90	1.48	1.39
23	A	406	CLA	CHD-C4C	3.90	1.48	1.39
23	B	614	CLA	O2A-CGA	3.90	1.44	1.33
23	B	607	CLA	OBD-CAD	3.90	1.29	1.22
23	C	512	CLA	CHB-C1B	3.89	1.48	1.39
23	b	604	CLA	CHC-C4B	3.89	1.48	1.39
23	a	406	CLA	C3D-C2D	3.89	1.49	1.39
23	C	512	CLA	CHD-C4C	3.89	1.48	1.39
23	B	609	CLA	C3D-C2D	3.89	1.49	1.39
23	b	616	CLA	O2A-CGA	3.89	1.44	1.33
23	B	601	CLA	C3D-C2D	3.89	1.49	1.39
23	c	504	CLA	CHB-C1B	3.89	1.48	1.39
23	C	515	CLA	CHB-C1B	3.88	1.48	1.39
23	b	605	CLA	CHD-C4C	3.88	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	CHB-C1B	3.88	1.48	1.39
23	c	507	CLA	CHB-C1B	3.88	1.48	1.39
23	c	505	CLA	O2A-CGA	3.88	1.44	1.33
23	b	603	CLA	O2A-CGA	3.88	1.44	1.33
23	b	609	CLA	C3D-C2D	3.87	1.49	1.39
31	D	408	LHG	O7-C7	3.87	1.45	1.34
23	a	408	CLA	CHC-C4B	3.87	1.48	1.39
23	b	611	CLA	CHD-C4C	3.87	1.48	1.39
23	b	604	CLA	CHD-C4C	3.87	1.48	1.39
23	A	405	CLA	C3D-C2D	3.87	1.49	1.39
23	C	507	CLA	CHB-C1B	3.87	1.48	1.39
23	B	611	CLA	CHB-C1B	3.87	1.48	1.39
38	E	103	HEC	CAC-C3C	3.86	1.47	1.35
31	d	406	LHG	O8-C23	3.86	1.44	1.33
23	c	505	CLA	CHB-C1B	3.86	1.48	1.39
23	B	613	CLA	CHB-C1B	3.86	1.48	1.39
23	b	603	CLA	CHB-C1B	3.86	1.48	1.39
23	c	505	CLA	CHC-C4B	3.85	1.48	1.39
23	B	609	CLA	CHD-C4C	3.85	1.48	1.39
23	B	608	CLA	CHD-C4C	3.85	1.48	1.39
23	B	612	CLA	CHC-C4B	3.85	1.48	1.39
23	b	604	CLA	O2A-CGA	3.84	1.44	1.33
23	B	613	CLA	C1D-ND	3.84	1.42	1.37
23	A	405	CLA	CHB-C1B	3.84	1.48	1.39
23	C	508	CLA	C3D-C2D	3.84	1.49	1.39
23	A	405	CLA	CHC-C4B	3.84	1.48	1.39
23	b	606	CLA	OBD-CAD	3.84	1.29	1.22
23	B	607	CLA	O2A-CGA	3.84	1.44	1.33
23	A	408	CLA	C3D-C2D	3.84	1.49	1.39
23	B	613	CLA	CHD-C1D	3.84	1.45	1.38
23	C	505	CLA	CHC-C4B	3.84	1.48	1.39
23	B	606	CLA	C3D-C2D	3.83	1.49	1.39
38	e	102	HEC	CAC-C3C	3.83	1.47	1.35
31	d	408	LHG	O8-C23	3.83	1.44	1.33
23	C	512	CLA	O2A-CGA	3.83	1.44	1.33
23	A	404	CLA	CHB-C1B	3.83	1.48	1.39
23	b	605	CLA	CHC-C4B	3.83	1.48	1.39
23	B	602	CLA	O2A-CGA	3.83	1.44	1.33
23	A	406	CLA	C3D-C2D	3.83	1.49	1.39
23	C	514	CLA	C3D-C2D	3.83	1.49	1.39
23	c	510	CLA	CHB-C1B	3.83	1.48	1.39
23	A	404	CLA	C3D-C2D	3.82	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	CHB-C1B	3.82	1.48	1.39
35	H	102	DGD	O1G-C1A	3.82	1.44	1.33
23	B	602	CLA	C3D-C2D	3.82	1.49	1.39
24	a	407	PHO	O2A-CGA	3.82	1.44	1.33
23	b	615	CLA	CHD-C4C	3.82	1.47	1.39
23	C	507	CLA	CHC-C4B	3.82	1.48	1.39
31	D	407	LHG	O7-C7	3.81	1.45	1.34
23	c	503	CLA	CHD-C1D	3.81	1.45	1.38
31	d	407	LHG	O8-C23	3.81	1.44	1.33
23	c	514	CLA	C3D-C2D	3.80	1.49	1.39
23	b	616	CLA	CHD-C4C	3.80	1.47	1.39
23	b	601	CLA	OBD-CAD	3.80	1.29	1.22
23	b	610	CLA	C3D-C2D	3.80	1.49	1.39
23	b	613	CLA	O2A-CGA	3.80	1.44	1.33
23	c	513	CLA	CHD-C1D	3.80	1.45	1.38
23	B	615	CLA	CHB-C1B	3.80	1.47	1.39
23	C	504	CLA	O2A-CGA	3.80	1.44	1.33
23	C	510	CLA	CHD-C1D	3.80	1.45	1.38
23	b	616	CLA	OBD-CAD	3.80	1.29	1.22
32	B	621	LMG	O7-C10	3.79	1.45	1.34
35	c	519	DGD	O2G-C1B	3.79	1.45	1.34
35	c	520	DGD	O2G-C1B	3.79	1.45	1.34
23	d	403	CLA	CHC-C4B	3.79	1.47	1.39
23	d	402	CLA	OBD-CAD	3.79	1.29	1.22
23	b	605	CLA	OBD-CAD	3.79	1.29	1.22
23	B	614	CLA	CHC-C4B	3.79	1.47	1.39
23	c	504	CLA	CHD-C4C	3.79	1.47	1.39
23	d	402	CLA	CHD-C1D	3.78	1.45	1.38
25	B	618	BCR	C23-C22	-3.78	1.37	1.46
24	a	417	PHO	O2A-CGA	3.78	1.44	1.33
23	C	514	CLA	CHD-C4C	3.78	1.47	1.39
23	a	405	CLA	CHD-C4C	3.78	1.47	1.39
23	C	511	CLA	CHB-C1B	3.78	1.47	1.39
23	b	615	CLA	C3D-C2D	3.78	1.49	1.39
23	b	606	CLA	CHD-C4C	3.78	1.47	1.39
23	A	406	CLA	O2A-CGA	3.78	1.44	1.33
23	a	408	CLA	CHD-C1D	3.78	1.45	1.38
23	a	405	CLA	CHB-C1B	3.78	1.47	1.39
23	a	406	CLA	C1D-ND	3.77	1.42	1.37
23	C	504	CLA	OBD-CAD	3.77	1.29	1.22
23	a	404	CLA	C3D-C2D	3.77	1.49	1.39
23	b	609	CLA	CHD-C4C	3.77	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	101	LHG	O7-C7	3.77	1.44	1.34
23	b	606	CLA	CHD-C1D	3.77	1.45	1.38
23	B	609	CLA	CHC-C4B	3.77	1.47	1.39
23	B	609	CLA	CHB-C1B	3.77	1.47	1.39
23	c	503	CLA	C3D-C2D	3.77	1.49	1.39
23	C	504	CLA	CHB-C1B	3.76	1.47	1.39
23	D	404	CLA	O2A-CGA	3.76	1.44	1.33
23	c	507	CLA	C3D-C2D	3.76	1.49	1.39
23	c	508	CLA	CHB-C1B	3.76	1.47	1.39
23	b	603	CLA	CHD-C4C	3.76	1.47	1.39
23	a	408	CLA	CHB-C1B	3.76	1.47	1.39
23	b	616	CLA	CHB-C1B	3.76	1.47	1.39
23	B	611	CLA	C3D-C2D	3.76	1.49	1.39
23	d	402	CLA	CHB-C1B	3.75	1.47	1.39
23	B	603	CLA	CHB-C1B	3.75	1.47	1.39
23	b	602	CLA	CHC-C4B	3.75	1.47	1.39
23	b	610	CLA	CHD-C4C	3.75	1.47	1.39
23	C	509	CLA	CHD-C4C	3.75	1.47	1.39
23	c	514	CLA	CHD-C4C	3.74	1.47	1.39
23	c	508	CLA	OBD-CAD	3.74	1.28	1.22
23	c	512	CLA	C3D-C2D	3.74	1.49	1.39
23	D	404	CLA	CHD-C4C	3.73	1.47	1.39
23	c	513	CLA	C3D-C2D	3.73	1.49	1.39
23	c	503	CLA	CHC-C4B	3.73	1.47	1.39
23	B	610	CLA	CHB-C1B	3.73	1.47	1.39
23	c	513	CLA	CHD-C4C	3.73	1.47	1.39
23	B	608	CLA	C3D-C2D	3.73	1.49	1.39
23	b	614	CLA	C3D-C2D	3.73	1.49	1.39
31	b	629	LHG	O8-C23	3.73	1.44	1.33
23	a	406	CLA	CHD-C1D	3.73	1.45	1.38
23	C	505	CLA	CHB-C1B	3.72	1.47	1.39
23	B	611	CLA	OBD-CAD	3.72	1.28	1.22
23	C	506	CLA	CHD-C1D	3.72	1.45	1.38
23	b	604	CLA	CHB-C1B	3.72	1.47	1.39
31	A	416	LHG	O8-C23	3.72	1.44	1.33
23	C	509	CLA	C3D-C2D	3.72	1.49	1.39
23	c	508	CLA	CHC-C4B	3.72	1.47	1.39
23	C	503	CLA	CHD-C4C	3.72	1.47	1.39
23	a	404	CLA	CHB-C1B	3.71	1.47	1.39
23	b	616	CLA	CHC-C4B	3.71	1.47	1.39
31	A	416	LHG	O7-C7	3.71	1.44	1.34
23	d	402	CLA	C3D-C2D	3.70	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	514	CLA	CHC-C4B	3.70	1.47	1.39
23	b	608	CLA	CHB-C1B	3.70	1.47	1.39
23	b	616	CLA	C3D-C2D	3.70	1.49	1.39
23	C	511	CLA	C4B-NB	-3.70	1.33	1.37
23	a	406	CLA	OBD-CAD	3.69	1.28	1.22
23	C	504	CLA	CHC-C4B	3.69	1.47	1.39
31	d	407	LHG	O7-C7	3.69	1.44	1.34
23	b	613	CLA	CHB-C1B	3.69	1.47	1.39
24	A	415	PHO	O2A-CGA	3.69	1.44	1.33
23	b	607	CLA	CHD-C4C	3.69	1.47	1.39
23	D	404	CLA	C3D-C2D	3.69	1.49	1.39
23	B	604	CLA	C3D-C2D	3.69	1.49	1.39
23	b	613	CLA	CHD-C4C	3.68	1.47	1.39
23	D	404	CLA	CHC-C4B	3.68	1.47	1.39
23	b	603	CLA	C3D-C2D	3.68	1.49	1.39
23	b	612	CLA	C3D-C2D	3.68	1.49	1.39
23	B	603	CLA	CHD-C4C	3.68	1.47	1.39
23	b	605	CLA	C1B-NB	-3.67	1.33	1.37
23	c	512	CLA	CHC-C4B	3.67	1.47	1.39
23	b	608	CLA	C3D-C2D	3.67	1.49	1.39
23	C	511	CLA	CHC-C4B	3.67	1.47	1.39
23	b	603	CLA	CHC-C4B	3.67	1.47	1.39
23	b	614	CLA	CHC-C4B	3.67	1.47	1.39
23	B	616	CLA	CHD-C1D	3.66	1.45	1.38
23	B	616	CLA	C3D-C2D	3.66	1.49	1.39
23	C	506	CLA	CHC-C4B	3.66	1.47	1.39
23	b	611	CLA	CHD-C1D	3.66	1.45	1.38
23	b	606	CLA	CHC-C4B	3.66	1.47	1.39
23	A	405	CLA	CHD-C4C	3.66	1.47	1.39
23	b	601	CLA	CHC-C4B	3.66	1.47	1.39
23	b	607	CLA	O2A-CGA	3.66	1.44	1.33
23	B	606	CLA	CHD-C4C	3.65	1.47	1.39
23	d	402	CLA	CHD-C4C	3.65	1.47	1.39
23	B	604	CLA	CHB-C1B	3.65	1.47	1.39
23	c	515	CLA	CHB-C1B	3.65	1.47	1.39
23	C	514	CLA	OBD-CAD	3.65	1.28	1.22
23	B	611	CLA	O2A-CGA	3.65	1.44	1.33
23	C	505	CLA	OBD-CAD	3.65	1.28	1.22
23	a	406	CLA	CHD-C4C	3.65	1.47	1.39
23	c	513	CLA	CHC-C4B	3.65	1.47	1.39
27	C	501	SQD	O47-C7	3.65	1.44	1.34
23	b	615	CLA	CHC-C4B	3.64	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	CHB-C1B	3.64	1.47	1.39
23	C	509	CLA	CHC-C4B	3.64	1.47	1.39
23	a	405	CLA	CHC-C4B	3.64	1.47	1.39
23	c	506	CLA	O2A-CGA	3.64	1.44	1.33
23	b	609	CLA	CHC-C4B	3.64	1.47	1.39
23	c	514	CLA	CHB-C1B	3.64	1.47	1.39
23	C	509	CLA	CHB-C1B	3.64	1.47	1.39
23	B	604	CLA	CHC-C4B	3.64	1.47	1.39
23	b	605	CLA	CHB-C1B	3.64	1.47	1.39
23	A	406	CLA	OBD-CAD	3.64	1.28	1.22
23	a	408	CLA	C3D-C2D	3.64	1.48	1.39
23	C	507	CLA	C3D-C2D	3.63	1.48	1.39
31	d	406	LHG	O7-C7	3.63	1.44	1.34
23	b	613	CLA	CHD-C1D	3.63	1.45	1.38
23	B	607	CLA	CHC-C4B	3.63	1.47	1.39
31	D	408	LHG	O8-C23	3.63	1.43	1.33
23	d	402	CLA	C1D-ND	3.63	1.42	1.37
23	a	406	CLA	CHB-C1B	3.63	1.47	1.39
23	b	601	CLA	CHB-C1B	3.62	1.47	1.39
23	B	616	CLA	OBD-CAD	3.62	1.28	1.22
23	c	505	CLA	C3D-C2D	3.62	1.48	1.39
23	C	508	CLA	CHB-C1B	3.62	1.47	1.39
23	b	610	CLA	CHB-C1B	3.62	1.47	1.39
23	b	606	CLA	O2A-CGA	3.61	1.43	1.33
23	B	601	CLA	OBD-CAD	3.61	1.28	1.22
23	b	605	CLA	O2A-CGA	3.61	1.43	1.33
23	b	614	CLA	CHD-C4C	3.61	1.47	1.39
31	D	407	LHG	O8-C23	3.60	1.43	1.33
23	d	403	CLA	CHB-C1B	3.60	1.47	1.39
23	D	403	CLA	C4B-NB	-3.60	1.33	1.37
23	C	508	CLA	OBD-CAD	3.60	1.28	1.22
23	C	503	CLA	CHB-C1B	3.60	1.47	1.39
23	b	615	CLA	OBD-CAD	3.60	1.28	1.22
23	C	506	CLA	CHD-C4C	3.60	1.47	1.39
23	A	404	CLA	CHD-C1D	3.59	1.45	1.38
23	c	514	CLA	OBD-CAD	3.59	1.28	1.22
23	b	605	CLA	C3D-C2D	3.59	1.48	1.39
23	D	403	CLA	C1D-ND	3.59	1.42	1.37
23	B	603	CLA	C1B-NB	-3.59	1.33	1.37
23	B	611	CLA	CHD-C4C	3.59	1.47	1.39
23	C	503	CLA	OBD-CAD	3.58	1.28	1.22
23	b	611	CLA	CHC-C4B	3.58	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	OBD-CAD	3.58	1.28	1.22
23	B	607	CLA	C3D-C2D	3.58	1.48	1.39
23	B	612	CLA	C3D-C2D	3.58	1.48	1.39
23	A	405	CLA	C1B-NB	-3.58	1.33	1.37
23	C	515	CLA	CHC-C4B	3.58	1.47	1.39
32	D	413	LMG	O8-C28	3.58	1.43	1.33
23	C	514	CLA	CHB-C1B	3.58	1.47	1.39
23	b	615	CLA	CHB-C1B	3.58	1.47	1.39
23	C	507	CLA	O2A-CGA	3.57	1.43	1.33
23	D	404	CLA	OBD-CAD	3.56	1.28	1.22
23	a	408	CLA	C1B-NB	-3.56	1.33	1.37
23	b	602	CLA	OBD-CAD	3.55	1.28	1.22
23	B	604	CLA	OBD-CAD	3.55	1.28	1.22
23	C	505	CLA	CHD-C1D	3.55	1.45	1.38
23	c	511	CLA	OBD-CAD	3.54	1.28	1.22
23	c	506	CLA	CHC-C4B	3.54	1.47	1.39
23	B	614	CLA	CHD-C4C	3.54	1.47	1.39
23	b	612	CLA	CHC-C4B	3.54	1.47	1.39
23	B	603	CLA	CHC-C4B	3.54	1.47	1.39
23	B	606	CLA	CHB-C1B	3.54	1.47	1.39
23	B	614	CLA	C3D-C2D	3.53	1.48	1.39
23	c	515	CLA	CHC-C4B	3.53	1.47	1.39
23	B	608	CLA	OBD-CAD	3.53	1.28	1.22
23	A	408	CLA	OBD-CAD	3.53	1.28	1.22
23	C	503	CLA	C3D-C2D	3.52	1.48	1.39
23	b	604	CLA	C1B-NB	-3.52	1.33	1.37
23	C	504	CLA	CHD-C4C	3.52	1.47	1.39
23	d	402	CLA	CHC-C4B	3.51	1.47	1.39
23	B	610	CLA	C1B-NB	-3.51	1.33	1.37
33	b	622	HTG	C1'-S1	-3.51	1.76	1.81
23	c	511	CLA	C1B-NB	-3.50	1.33	1.37
23	B	603	CLA	OBD-CAD	3.50	1.28	1.22
23	C	510	CLA	CHC-C4B	3.50	1.47	1.39
23	b	608	CLA	OBD-CAD	3.50	1.28	1.22
23	c	506	CLA	OBD-CAD	3.50	1.28	1.22
23	B	603	CLA	CHD-C1D	3.50	1.45	1.38
23	A	404	CLA	O2A-CGA	3.50	1.43	1.33
23	c	504	CLA	CHC-C4B	3.50	1.47	1.39
23	b	608	CLA	CHC-C4B	3.49	1.47	1.39
23	B	613	CLA	C1B-NB	-3.49	1.33	1.37
23	B	616	CLA	CHD-C4C	3.49	1.47	1.39
23	B	610	CLA	O2A-CGA	3.49	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	CHD-C4C	3.49	1.47	1.39
23	b	610	CLA	C1B-NB	-3.48	1.33	1.37
23	A	404	CLA	CHD-C4C	3.48	1.47	1.39
23	C	511	CLA	C1B-NB	-3.48	1.33	1.37
23	b	604	CLA	OBD-CAD	3.48	1.28	1.22
23	B	605	CLA	CHD-C4C	3.47	1.47	1.39
23	B	615	CLA	CHC-C4B	3.47	1.47	1.39
23	a	408	CLA	CHD-C4C	3.46	1.47	1.39
23	A	404	CLA	C1B-NB	-3.46	1.33	1.37
23	d	403	CLA	OBD-CAD	3.46	1.28	1.22
23	B	613	CLA	CHC-C4B	3.45	1.47	1.39
23	B	611	CLA	C1B-NB	-3.44	1.33	1.37
23	B	616	CLA	CHC-C4B	3.44	1.47	1.39
23	b	612	CLA	OBD-CAD	3.44	1.28	1.22
23	C	515	CLA	OBD-CAD	3.43	1.28	1.22
23	B	613	CLA	OBD-CAD	3.43	1.28	1.22
23	D	403	CLA	C3D-C2D	3.43	1.48	1.39
23	B	612	CLA	C1C-C2C	3.43	1.51	1.44
23	B	604	CLA	C1B-NB	-3.43	1.33	1.37
23	b	611	CLA	C3D-C2D	3.43	1.48	1.39
23	a	405	CLA	OBD-CAD	3.42	1.28	1.22
23	B	608	CLA	CHC-C4B	3.42	1.47	1.39
23	A	404	CLA	CHC-C4B	3.42	1.47	1.39
23	C	512	CLA	OBD-CAD	3.42	1.28	1.22
23	C	513	CLA	C4B-NB	-3.42	1.33	1.37
23	C	513	CLA	CHC-C4B	3.42	1.47	1.39
23	b	607	CLA	OBD-CAD	3.41	1.28	1.22
23	C	513	CLA	OBD-CAD	3.41	1.28	1.22
23	B	607	CLA	C1B-NB	-3.41	1.33	1.37
23	b	602	CLA	CHB-C1B	3.41	1.47	1.39
23	b	607	CLA	C1B-C2B	3.40	1.51	1.43
23	B	602	CLA	CHB-C1B	3.39	1.47	1.39
23	B	612	CLA	C1B-NB	-3.39	1.33	1.37
23	b	610	CLA	O2A-CGA	3.39	1.43	1.33
23	b	606	CLA	C3D-C2D	3.38	1.48	1.39
23	D	404	CLA	C1B-NB	-3.38	1.33	1.37
23	A	404	CLA	C4B-NB	-3.38	1.33	1.37
23	B	613	CLA	CHD-C4C	3.37	1.46	1.39
23	c	509	CLA	CHB-C1B	3.37	1.47	1.39
23	b	607	CLA	CHC-C4B	3.36	1.47	1.39
32	D	413	LMG	O7-C10	3.36	1.43	1.34
23	c	505	CLA	C4C-C3C	3.36	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	C1B-NB	-3.36	1.33	1.37
23	c	513	CLA	OBD-CAD	3.35	1.28	1.22
23	B	615	CLA	CHD-C4C	3.35	1.46	1.39
23	B	611	CLA	CHC-C4B	3.35	1.46	1.39
23	c	504	CLA	OBD-CAD	3.35	1.28	1.22
23	A	408	CLA	CHB-C1B	3.35	1.46	1.39
23	c	512	CLA	O2A-CGA	3.33	1.43	1.33
23	b	606	CLA	C1B-NB	-3.33	1.33	1.37
23	b	613	CLA	OBD-CAD	3.32	1.28	1.22
23	c	513	CLA	C1B-C2B	3.32	1.50	1.43
23	C	510	CLA	OBD-CAD	3.32	1.28	1.22
23	b	608	CLA	C4B-NB	-3.32	1.33	1.37
33	h	101	HTG	C1'-S1	-3.32	1.76	1.81
23	B	615	CLA	CHD-C1D	3.31	1.44	1.38
23	C	514	CLA	C1B-NB	-3.31	1.33	1.37
23	B	601	CLA	C1B-NB	-3.31	1.33	1.37
23	c	508	CLA	C1B-NB	-3.30	1.33	1.37
23	B	612	CLA	C1D-ND	3.30	1.42	1.37
23	B	614	CLA	OBD-CAD	3.30	1.28	1.22
23	C	509	CLA	OBD-CAD	3.29	1.28	1.22
23	c	511	CLA	CHC-C4B	3.29	1.46	1.39
23	C	507	CLA	C1B-NB	-3.29	1.33	1.37
23	A	408	CLA	C1B-NB	-3.29	1.33	1.37
23	C	508	CLA	CHC-C4B	3.29	1.46	1.39
23	A	405	CLA	OBD-CAD	3.28	1.28	1.22
23	c	507	CLA	OBD-CAD	3.27	1.28	1.22
23	B	612	CLA	CHD-C1D	3.27	1.44	1.38
35	H	102	DGD	O2G-C1B	3.27	1.43	1.34
23	B	606	CLA	C1B-NB	-3.27	1.33	1.37
23	C	507	CLA	OBD-CAD	3.27	1.28	1.22
23	c	510	CLA	CHC-C4B	3.26	1.46	1.39
23	a	406	CLA	C1B-NB	-3.26	1.33	1.37
23	b	614	CLA	OBD-CAD	3.26	1.28	1.22
23	B	601	CLA	CHB-C1B	3.26	1.46	1.39
23	a	405	CLA	C1B-C2B	3.25	1.50	1.43
23	B	612	CLA	OBD-CAD	3.25	1.28	1.22
23	b	612	CLA	CHD-C4C	3.24	1.46	1.39
23	a	404	CLA	CHC-C4B	3.24	1.46	1.39
23	B	611	CLA	C1B-C2B	3.24	1.50	1.43
33	b	623	HTG	C1'-S1	-3.22	1.76	1.81
23	b	603	CLA	C1B-C2B	3.22	1.50	1.43
23	C	512	CLA	C1B-NB	-3.21	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	CHC-C4B	3.21	1.46	1.39
23	B	615	CLA	C1B-C2B	3.20	1.50	1.43
23	c	511	CLA	C4C-C3C	3.20	1.50	1.45
23	C	512	CLA	C4B-NB	-3.20	1.33	1.37
23	B	606	CLA	CHC-C4B	3.20	1.46	1.39
23	A	404	CLA	OBD-CAD	3.20	1.28	1.22
38	e	102	HEC	C1D-ND	-3.19	1.33	1.39
23	c	515	CLA	OBD-CAD	3.19	1.28	1.22
23	b	616	CLA	C1B-NB	-3.19	1.33	1.37
23	a	404	CLA	O2A-CGA	3.18	1.42	1.33
23	A	406	CLA	C1D-ND	3.18	1.42	1.37
33	B	622	HTG	C1'-S1	-3.18	1.76	1.81
23	a	406	CLA	CHC-C4B	3.18	1.46	1.39
23	c	505	CLA	OBD-CAD	3.17	1.27	1.22
23	C	507	CLA	C1B-C2B	3.17	1.50	1.43
23	b	613	CLA	C1B-C2B	3.17	1.50	1.43
23	b	612	CLA	C1B-C2B	3.17	1.50	1.43
23	B	607	CLA	C1B-C2B	3.17	1.50	1.43
23	a	408	CLA	OBD-CAD	3.16	1.27	1.22
23	C	506	CLA	OBD-CAD	3.16	1.27	1.22
23	C	509	CLA	C4B-NB	-3.16	1.33	1.37
23	c	503	CLA	C4B-NB	-3.16	1.33	1.37
23	B	614	CLA	C1B-C2B	3.16	1.50	1.43
23	B	602	CLA	C1C-C2C	3.15	1.50	1.44
23	b	613	CLA	C4B-NB	-3.15	1.33	1.37
23	B	609	CLA	C1B-NB	-3.15	1.33	1.37
23	d	402	CLA	C1B-NB	-3.15	1.33	1.37
23	C	504	CLA	C1B-C2B	3.12	1.50	1.43
23	b	612	CLA	C4B-NB	-3.12	1.33	1.37
23	b	609	CLA	C1B-NB	-3.12	1.33	1.37
23	D	403	CLA	CHC-C4B	3.12	1.46	1.39
23	B	616	CLA	C1B-C2B	3.11	1.50	1.43
23	c	510	CLA	C1B-C2B	3.11	1.50	1.43
23	b	610	CLA	C4B-NB	-3.11	1.33	1.37
23	C	508	CLA	C1B-NB	-3.11	1.33	1.37
23	b	609	CLA	OBD-CAD	3.10	1.27	1.22
23	b	606	CLA	CHB-C1B	3.10	1.46	1.39
23	B	602	CLA	OBD-CAD	3.09	1.27	1.22
23	C	510	CLA	C4B-NB	-3.08	1.33	1.37
23	C	508	CLA	C4B-NB	-3.08	1.33	1.37
23	C	515	CLA	C1B-C2B	3.08	1.50	1.43
23	B	604	CLA	C4D-CHA	3.08	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	C1B-C2B	3.06	1.50	1.43
23	b	611	CLA	C1B-C2B	3.06	1.50	1.43
23	c	506	CLA	C4B-NB	-3.06	1.33	1.37
23	B	609	CLA	OBD-CAD	3.05	1.27	1.22
23	c	505	CLA	C1B-C2B	3.04	1.50	1.43
23	A	405	CLA	C4D-CHA	3.04	1.48	1.38
23	B	603	CLA	C1B-C2B	3.04	1.50	1.43
23	D	403	CLA	OBD-CAD	3.03	1.27	1.22
23	B	605	CLA	CHB-C1B	3.03	1.46	1.39
23	C	506	CLA	C1B-NB	-3.03	1.33	1.37
23	C	508	CLA	C4C-C3C	3.02	1.50	1.45
23	B	612	CLA	CHD-C4C	3.01	1.46	1.39
23	d	403	CLA	C1B-NB	-3.01	1.33	1.37
23	b	611	CLA	OBD-CAD	3.01	1.27	1.22
23	c	511	CLA	C4B-NB	-3.00	1.33	1.37
23	A	406	CLA	CHB-C1B	3.00	1.46	1.39
23	D	403	CLA	C1B-NB	-3.00	1.33	1.37
23	c	503	CLA	C1B-NB	-2.99	1.33	1.37
23	c	503	CLA	OBD-CAD	2.99	1.27	1.22
23	b	601	CLA	C1B-NB	-2.99	1.33	1.37
23	b	615	CLA	C1B-NB	-2.99	1.33	1.37
23	a	408	CLA	C1B-C2B	2.98	1.50	1.43
23	b	604	CLA	C4D-CHA	2.98	1.48	1.38
23	A	404	CLA	C1B-C2B	2.98	1.50	1.43
23	B	616	CLA	C4B-NB	-2.98	1.33	1.37
23	c	511	CLA	C1B-C2B	2.98	1.50	1.43
23	c	512	CLA	C1B-C2B	2.97	1.50	1.43
23	b	604	CLA	C1B-C2B	2.97	1.50	1.43
23	B	604	CLA	C1B-C2B	2.97	1.50	1.43
23	B	602	CLA	C1B-NB	-2.97	1.34	1.37
23	C	506	CLA	C4B-NB	-2.97	1.34	1.37
33	D	411	HTG	C1'-S1	-2.97	1.77	1.81
23	C	513	CLA	C4D-CHA	2.97	1.48	1.38
23	B	607	CLA	C4D-CHA	2.96	1.48	1.38
23	B	606	CLA	OBD-CAD	2.96	1.27	1.22
23	c	512	CLA	C4D-CHA	2.96	1.48	1.38
23	c	505	CLA	C1C-C2C	2.95	1.50	1.44
23	c	510	CLA	C4B-NB	-2.95	1.34	1.37
33	b	625	HTG	C1'-S1	-2.95	1.77	1.81
23	B	608	CLA	C4B-NB	-2.94	1.34	1.37
23	b	610	CLA	C1B-C2B	2.94	1.50	1.43
23	b	601	CLA	C1B-C2B	2.93	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	C1B-NB	-2.93	1.34	1.37
23	C	513	CLA	C1B-C2B	2.93	1.50	1.43
23	C	509	CLA	C4D-CHA	2.93	1.48	1.38
23	b	614	CLA	C1B-C2B	2.93	1.50	1.43
23	a	408	CLA	C1C-C2C	2.92	1.50	1.44
33	c	523	HTG	C1'-S1	-2.92	1.77	1.81
33	B	625	HTG	C1'-S1	-2.92	1.77	1.81
23	b	615	CLA	C1B-C2B	2.92	1.50	1.43
23	C	506	CLA	C4D-CHA	2.92	1.48	1.38
23	d	402	CLA	C1B-C2B	2.91	1.50	1.43
23	c	509	CLA	C1B-NB	-2.91	1.34	1.37
38	E	103	HEC	C1D-ND	-2.90	1.34	1.39
23	d	402	CLA	C4B-NB	-2.90	1.34	1.37
23	B	616	CLA	C1B-NB	-2.90	1.34	1.37
23	b	609	CLA	C4B-NB	-2.90	1.34	1.37
23	B	608	CLA	C4D-CHA	2.89	1.48	1.38
23	D	404	CLA	C1B-C2B	2.89	1.49	1.43
23	c	509	CLA	C1C-C2C	2.89	1.50	1.44
23	B	606	CLA	C4D-CHA	2.89	1.48	1.38
23	B	612	CLA	C4B-NB	-2.89	1.34	1.37
23	C	515	CLA	C1B-NB	-2.88	1.34	1.37
23	b	616	CLA	C1B-C2B	2.88	1.49	1.43
23	B	606	CLA	C4B-NB	-2.88	1.34	1.37
23	c	507	CLA	C4C-C3C	2.88	1.49	1.45
23	b	616	CLA	C4D-CHA	2.87	1.48	1.38
23	b	602	CLA	C4B-NB	-2.87	1.34	1.37
23	B	607	CLA	C4C-C3C	2.86	1.49	1.45
33	C	523	HTG	C1'-S1	-2.86	1.77	1.81
23	c	509	CLA	C4D-CHA	2.86	1.48	1.38
23	C	507	CLA	C4C-C3C	2.86	1.49	1.45
23	b	615	CLA	C4C-C3C	2.86	1.49	1.45
23	C	511	CLA	C1B-C2B	2.86	1.49	1.43
23	D	403	CLA	C1B-C2B	2.86	1.49	1.43
23	a	404	CLA	C1B-C2B	2.86	1.49	1.43
23	b	615	CLA	C4D-CHA	2.86	1.48	1.38
29	A	413	PL9	C6-C5	2.86	1.49	1.35
23	B	614	CLA	C4D-CHA	2.86	1.48	1.38
23	c	514	CLA	C1B-NB	-2.85	1.34	1.37
23	b	602	CLA	C1B-NB	-2.85	1.34	1.37
24	A	415	PHO	CHA-CBD	-2.85	1.48	1.51
23	C	505	CLA	C1B-NB	-2.84	1.34	1.37
23	C	510	CLA	C1B-NB	-2.84	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	e	102	HEC	C4D-ND	-2.84	1.34	1.39
23	c	510	CLA	C1B-NB	-2.84	1.34	1.37
23	C	515	CLA	C4B-NB	-2.83	1.34	1.37
23	B	606	CLA	C1B-C2B	2.83	1.49	1.43
23	b	606	CLA	C4B-NB	-2.83	1.34	1.37
23	b	608	CLA	C4D-CHA	2.83	1.48	1.38
23	C	505	CLA	C4B-NB	-2.83	1.34	1.37
23	C	514	CLA	C4D-CHA	2.83	1.48	1.38
23	b	608	CLA	C1B-NB	-2.83	1.34	1.37
23	B	603	CLA	C1C-C2C	2.82	1.50	1.44
23	C	506	CLA	C1C-C2C	2.82	1.50	1.44
23	C	504	CLA	C4B-NB	-2.82	1.34	1.37
23	B	608	CLA	C1B-NB	-2.82	1.34	1.37
23	a	405	CLA	C1B-NB	-2.82	1.34	1.37
23	c	505	CLA	C1B-NB	-2.82	1.34	1.37
23	C	503	CLA	C1B-C2B	2.81	1.49	1.43
23	C	512	CLA	C1C-C2C	2.81	1.50	1.44
23	B	613	CLA	C4C-C3C	2.81	1.49	1.45
23	b	609	CLA	C4D-CHA	2.81	1.48	1.38
23	c	511	CLA	C4D-CHA	2.81	1.48	1.38
23	b	605	CLA	C1B-C2B	2.81	1.49	1.43
23	D	403	CLA	C4D-CHA	2.80	1.48	1.38
23	C	508	CLA	C4D-CHA	2.80	1.48	1.38
38	E	103	HEC	C4D-ND	-2.80	1.34	1.39
23	c	505	CLA	C4D-CHA	2.79	1.48	1.38
23	B	602	CLA	C3B-C4B	2.79	1.50	1.42
23	B	612	CLA	C1B-C2B	2.79	1.49	1.43
29	a	415	PL9	C6-C5	2.79	1.48	1.35
23	c	506	CLA	C4C-C3C	2.78	1.49	1.45
23	d	402	CLA	C4D-CHA	2.77	1.47	1.38
23	c	504	CLA	C4B-NB	-2.77	1.34	1.37
23	C	503	CLA	C4D-CHA	2.77	1.47	1.38
23	C	503	CLA	C1C-C2C	2.77	1.50	1.44
23	c	513	CLA	C4D-CHA	2.76	1.47	1.38
23	B	611	CLA	C1C-C2C	2.76	1.50	1.44
23	c	515	CLA	C4B-NB	-2.76	1.34	1.37
23	B	613	CLA	C1B-C2B	2.76	1.49	1.43
23	C	511	CLA	C4C-C3C	2.75	1.49	1.45
23	B	613	CLA	C1C-C2C	2.75	1.50	1.44
23	C	511	CLA	C4D-CHA	2.75	1.47	1.38
23	b	616	CLA	C4B-NB	-2.75	1.34	1.37
23	B	609	CLA	C1B-C2B	2.75	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	C4B-NB	-2.75	1.34	1.37
23	C	512	CLA	C4D-CHA	2.74	1.47	1.38
23	a	406	CLA	C4B-NB	-2.74	1.34	1.37
23	B	610	CLA	C4D-CHA	2.74	1.47	1.38
23	C	503	CLA	C3B-C4B	2.74	1.50	1.42
23	c	506	CLA	C4D-CHA	2.74	1.47	1.38
23	C	510	CLA	C4D-CHA	2.73	1.47	1.38
23	c	514	CLA	C4D-CHA	2.73	1.47	1.38
23	c	507	CLA	C4D-CHA	2.73	1.47	1.38
23	c	515	CLA	C1C-C2C	2.73	1.50	1.44
23	A	405	CLA	C4B-NB	-2.73	1.34	1.37
23	A	408	CLA	C4D-CHA	2.73	1.47	1.38
23	C	507	CLA	C4D-CHA	2.73	1.47	1.38
23	b	608	CLA	C3D-C4D	-2.72	1.38	1.44
23	b	603	CLA	C4B-NB	-2.72	1.34	1.37
23	a	404	CLA	C1B-NB	-2.71	1.34	1.37
23	c	507	CLA	C1B-C2B	2.71	1.49	1.43
23	C	513	CLA	C4C-C3C	2.71	1.49	1.45
23	C	514	CLA	C1B-C2B	2.71	1.49	1.43
23	c	506	CLA	C1B-NB	-2.70	1.34	1.37
23	C	505	CLA	C1B-C2B	2.70	1.49	1.43
23	D	404	CLA	C1C-C2C	2.70	1.50	1.44
23	b	602	CLA	C4D-CHA	2.70	1.47	1.38
23	C	508	CLA	C1B-C2B	2.69	1.49	1.43
23	a	404	CLA	C4B-NB	-2.69	1.34	1.37
23	b	607	CLA	C4D-CHA	2.69	1.47	1.38
23	c	506	CLA	C1B-C2B	2.69	1.49	1.43
23	b	607	CLA	C4B-NB	-2.69	1.34	1.37
23	b	610	CLA	C1C-C2C	2.69	1.50	1.44
23	b	603	CLA	C1C-C2C	2.68	1.50	1.44
23	B	611	CLA	C4D-CHA	2.68	1.47	1.38
23	b	608	CLA	C1B-C2B	2.68	1.49	1.43
23	B	614	CLA	C4C-C3C	2.68	1.49	1.45
23	c	507	CLA	C1C-C2C	2.67	1.49	1.44
23	B	603	CLA	C4D-CHA	2.67	1.47	1.38
23	b	603	CLA	C4D-CHA	2.67	1.47	1.38
23	c	513	CLA	C1B-NB	-2.67	1.34	1.37
23	A	404	CLA	C4C-C3C	2.67	1.49	1.45
23	c	515	CLA	C1B-C2B	2.67	1.49	1.43
23	b	616	CLA	C3D-C4D	-2.67	1.38	1.44
23	C	507	CLA	C1C-C2C	2.67	1.49	1.44
23	c	515	CLA	C1B-NB	-2.67	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	C4C-C3C	2.67	1.49	1.45
23	B	605	CLA	C4B-NB	-2.66	1.34	1.37
23	B	615	CLA	C4D-CHA	2.66	1.47	1.38
23	C	509	CLA	C1B-C2B	2.66	1.49	1.43
23	b	610	CLA	C4D-CHA	2.66	1.47	1.38
23	B	609	CLA	C4D-CHA	2.66	1.47	1.38
23	b	614	CLA	C4D-CHA	2.66	1.47	1.38
23	B	610	CLA	C4B-NB	-2.66	1.34	1.37
23	b	611	CLA	C1B-NB	-2.66	1.34	1.37
23	b	614	CLA	C1B-NB	-2.66	1.34	1.37
23	c	509	CLA	C4B-NB	-2.66	1.34	1.37
23	c	503	CLA	C4D-CHA	2.66	1.47	1.38
23	B	605	CLA	C1B-C2B	2.65	1.49	1.43
23	B	603	CLA	C4B-NB	-2.65	1.34	1.37
23	C	511	CLA	C1C-C2C	2.64	1.49	1.44
23	c	514	CLA	C1C-C2C	2.64	1.49	1.44
23	C	515	CLA	C4D-CHA	2.64	1.47	1.38
23	a	405	CLA	C1C-C2C	2.64	1.49	1.44
23	c	515	CLA	C4D-CHA	2.64	1.47	1.38
23	B	616	CLA	C4D-CHA	2.64	1.47	1.38
23	C	503	CLA	C1B-NB	-2.64	1.34	1.37
23	b	602	CLA	C1B-C2B	2.64	1.49	1.43
23	b	606	CLA	C4D-CHA	2.64	1.47	1.38
23	d	402	CLA	C4C-C3C	2.64	1.49	1.45
23	a	405	CLA	C4D-CHA	2.63	1.47	1.38
23	b	608	CLA	C4C-C3C	2.63	1.49	1.45
23	A	404	CLA	C1C-C2C	2.63	1.49	1.44
23	C	515	CLA	C1C-C2C	2.63	1.49	1.44
23	B	614	CLA	CHD-C1D	2.63	1.43	1.38
23	A	405	CLA	C1B-C2B	2.63	1.49	1.43
23	C	509	CLA	C1B-NB	-2.62	1.34	1.37
32	Z	101	LMG	O8-C28	2.62	1.46	1.33
23	C	513	CLA	C1C-C2C	2.62	1.49	1.44
23	A	406	CLA	C4D-CHA	2.62	1.47	1.38
23	B	613	CLA	C4D-CHA	2.61	1.47	1.38
23	c	506	CLA	C3B-C2B	2.61	1.50	1.41
23	B	602	CLA	C4D-CHA	2.61	1.47	1.38
23	c	512	CLA	C1B-NB	-2.61	1.34	1.37
38	E	103	HEC	C1B-NB	-2.60	1.34	1.39
23	c	508	CLA	C1B-C2B	2.60	1.49	1.43
23	b	601	CLA	C4B-NB	-2.60	1.34	1.37
23	A	406	CLA	C3B-C4B	2.60	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	C1B-C2B	2.60	1.49	1.43
23	A	406	CLA	C4B-NB	-2.60	1.34	1.37
23	c	503	CLA	C1B-C2B	2.60	1.49	1.43
23	D	404	CLA	C4D-CHA	2.60	1.47	1.38
23	B	601	CLA	C1B-C2B	2.60	1.49	1.43
23	d	403	CLA	C4B-NB	-2.59	1.34	1.37
23	C	512	CLA	C1B-C2B	2.59	1.49	1.43
23	a	408	CLA	C4D-CHA	2.59	1.47	1.38
23	b	603	CLA	C4C-C3C	2.59	1.49	1.45
23	b	601	CLA	C4D-CHA	2.59	1.47	1.38
23	c	510	CLA	C4D-CHA	2.59	1.47	1.38
23	B	602	CLA	C3D-C4D	-2.59	1.38	1.44
23	C	510	CLA	C1B-C2B	2.59	1.49	1.43
23	b	601	CLA	C3B-C4B	2.59	1.50	1.42
23	c	507	CLA	C3B-C4B	2.59	1.50	1.42
23	B	605	CLA	C4D-CHA	2.58	1.47	1.38
23	b	612	CLA	C3B-C2B	2.58	1.49	1.41
23	A	405	CLA	C3B-C4B	2.58	1.50	1.42
23	b	613	CLA	C4D-CHA	2.58	1.47	1.38
23	B	605	CLA	C1C-C2C	2.58	1.49	1.44
23	c	503	CLA	C3D-C4D	-2.58	1.38	1.44
23	B	608	CLA	C1B-C2B	2.58	1.49	1.43
23	a	406	CLA	C4D-CHA	2.58	1.47	1.38
23	A	406	CLA	C1B-C2B	2.57	1.49	1.43
23	B	607	CLA	C4B-NB	-2.57	1.34	1.37
23	A	404	CLA	C4D-CHA	2.57	1.47	1.38
23	B	602	CLA	C4C-C3C	2.57	1.49	1.45
23	C	514	CLA	C4B-NB	-2.57	1.34	1.37
23	C	505	CLA	C3B-C4B	2.57	1.50	1.42
38	e	102	HEC	C1B-NB	-2.57	1.34	1.39
23	B	601	CLA	C4D-CHA	2.56	1.47	1.38
29	d	405	PL9	C6-C5	2.56	1.47	1.35
23	C	504	CLA	C4D-CHA	2.56	1.47	1.38
23	C	504	CLA	C3B-C4B	2.56	1.50	1.42
23	a	406	CLA	C1B-C2B	2.56	1.49	1.43
23	B	605	CLA	C3B-C4B	2.55	1.50	1.42
23	A	408	CLA	C1B-C2B	2.55	1.49	1.43
23	d	403	CLA	C4D-CHA	2.55	1.47	1.38
23	B	608	CLA	C3D-C4D	-2.55	1.38	1.44
23	a	408	CLA	C4B-NB	-2.55	1.34	1.37
23	A	405	CLA	C1C-C2C	2.55	1.49	1.44
34	a	413	LMT	O1'-C1'	2.55	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	415	PHO	C1B-NB	-2.55	1.34	1.38
38	E	103	HEC	C4B-NB	-2.55	1.34	1.39
23	C	505	CLA	C4D-CHA	2.54	1.47	1.38
23	c	505	CLA	C4B-NB	-2.54	1.34	1.37
23	B	601	CLA	C3B-C4B	2.54	1.50	1.42
23	c	507	CLA	C3D-C4D	-2.54	1.38	1.44
23	d	402	CLA	C3D-C4D	-2.54	1.38	1.44
23	C	504	CLA	C1C-C2C	2.54	1.49	1.44
23	c	508	CLA	C4D-CHA	2.53	1.47	1.38
23	a	405	CLA	C3B-C4B	2.53	1.50	1.42
23	c	515	CLA	C3B-C4B	2.53	1.50	1.42
23	C	510	CLA	C3B-C2B	2.53	1.49	1.41
23	b	612	CLA	C4D-CHA	2.53	1.47	1.38
23	b	613	CLA	C4C-C3C	2.53	1.49	1.45
24	A	407	PHO	CBD-CGD	-2.53	1.49	1.52
23	a	404	CLA	C4D-CHA	2.53	1.47	1.38
23	c	514	CLA	C4C-C3C	2.53	1.49	1.45
33	B	625	HTG	C1-S1	-2.53	1.76	1.80
23	C	512	CLA	C4C-C3C	2.53	1.49	1.45
23	B	610	CLA	C4C-C3C	2.52	1.49	1.45
23	B	601	CLA	C4B-NB	-2.51	1.34	1.37
23	b	602	CLA	C1C-C2C	2.51	1.49	1.44
23	B	612	CLA	C4D-CHA	2.51	1.47	1.38
23	B	615	CLA	C1B-NB	-2.51	1.34	1.37
23	b	606	CLA	C1C-C2C	2.51	1.49	1.44
23	a	406	CLA	C1C-C2C	2.51	1.49	1.44
23	c	504	CLA	C3B-C4B	2.51	1.50	1.42
23	b	611	CLA	C4D-CHA	2.51	1.47	1.38
23	c	514	CLA	C4B-NB	-2.50	1.34	1.37
35	h	103	DGD	O5D-C1E	2.50	1.44	1.40
23	c	515	CLA	C3D-C4D	-2.50	1.38	1.44
23	c	512	CLA	C3D-C4D	-2.50	1.38	1.44
23	C	514	CLA	C3D-C4D	-2.49	1.38	1.44
23	D	404	CLA	C3B-C4B	2.49	1.50	1.42
23	c	504	CLA	C4D-CHA	2.49	1.46	1.38
38	v	202	HEC	CMC-C2C	2.49	1.55	1.50
23	c	514	CLA	C1B-C2B	2.49	1.49	1.43
23	C	509	CLA	C3D-C4D	-2.48	1.38	1.44
23	b	609	CLA	C1C-C2C	2.48	1.49	1.44
23	b	608	CLA	C3B-C4B	2.48	1.50	1.42
23	c	510	CLA	C3B-C2B	2.48	1.49	1.41
23	B	604	CLA	C1C-C2C	2.48	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	e	102	HEC	C4B-NB	-2.48	1.34	1.39
23	C	513	CLA	C3B-C4B	2.48	1.49	1.42
23	B	606	CLA	C3D-C4D	-2.48	1.38	1.44
23	C	509	CLA	C4C-C3C	2.48	1.49	1.45
23	A	404	CLA	C3B-C2B	2.47	1.49	1.41
23	C	513	CLA	C1B-NB	-2.47	1.34	1.37
23	d	403	CLA	C3B-C4B	2.47	1.49	1.42
23	A	408	CLA	C4B-NB	-2.47	1.34	1.37
23	b	607	CLA	C1C-C2C	2.47	1.49	1.44
23	d	403	CLA	C1B-C2B	2.47	1.48	1.43
23	c	505	CLA	C3D-C4D	-2.46	1.38	1.44
23	A	408	CLA	C4C-C3C	2.46	1.49	1.45
23	b	605	CLA	C4D-CHA	2.46	1.46	1.38
23	c	512	CLA	C1C-C2C	2.46	1.49	1.44
23	b	603	CLA	C1B-NB	-2.46	1.34	1.37
23	C	510	CLA	C3D-C4D	-2.46	1.38	1.44
23	B	609	CLA	C3D-C4D	-2.46	1.38	1.44
23	B	609	CLA	C1C-C2C	2.46	1.49	1.44
23	A	408	CLA	C1C-C2C	2.46	1.49	1.44
23	B	612	CLA	C3B-C2B	2.45	1.49	1.41
23	b	612	CLA	C4C-C3C	2.45	1.49	1.45
38	V	201	HEC	CMC-C2C	2.45	1.55	1.50
33	B	623	HTG	C1'-S1	-2.44	1.78	1.81
23	d	402	CLA	C1C-C2C	2.44	1.49	1.44
23	D	403	CLA	C3D-C4D	-2.44	1.38	1.44
23	c	506	CLA	C1D-C2D	2.44	1.50	1.45
23	b	603	CLA	C3D-C4D	-2.44	1.38	1.44
23	b	610	CLA	C3D-C4D	-2.43	1.38	1.44
23	b	602	CLA	C3D-C4D	-2.43	1.38	1.44
23	d	403	CLA	C1C-C2C	2.43	1.49	1.44
23	c	514	CLA	C3B-C4B	2.43	1.49	1.42
23	b	609	CLA	C3B-C4B	2.43	1.49	1.42
23	c	507	CLA	C4B-NB	-2.43	1.34	1.37
23	c	503	CLA	C1C-C2C	2.43	1.49	1.44
23	b	605	CLA	C3B-C4B	2.42	1.49	1.42
23	b	613	CLA	C3B-C2B	2.42	1.49	1.41
23	c	509	CLA	C1B-C2B	2.41	1.48	1.43
23	b	611	CLA	C3B-C2B	2.41	1.49	1.41
23	b	606	CLA	C3B-C4B	2.41	1.49	1.42
23	B	601	CLA	C4C-C3C	2.41	1.49	1.45
38	E	103	HEC	C1A-C2A	-2.41	1.41	1.45
23	b	615	CLA	C3B-C4B	2.41	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	C3D-C4D	-2.41	1.38	1.44
24	A	415	PHO	C4B-NB	-2.41	1.34	1.38
23	C	508	CLA	C1D-C2D	2.41	1.50	1.45
23	b	611	CLA	C3D-C4D	-2.40	1.38	1.44
23	b	613	CLA	C1C-C2C	2.40	1.49	1.44
23	a	406	CLA	C3B-C4B	2.40	1.49	1.42
23	c	515	CLA	C4C-C3C	2.40	1.49	1.45
23	c	511	CLA	C1C-C2C	2.40	1.49	1.44
23	B	601	CLA	C1C-C2C	2.40	1.49	1.44
23	b	604	CLA	C1C-C2C	2.40	1.49	1.44
23	A	405	CLA	C4C-C3C	2.39	1.49	1.45
23	d	402	CLA	C3B-C2B	2.39	1.49	1.41
23	b	612	CLA	C1C-C2C	2.39	1.49	1.44
23	c	513	CLA	C3B-C2B	2.39	1.49	1.41
23	B	613	CLA	C4B-NB	-2.39	1.34	1.37
23	C	514	CLA	C3B-C2B	2.38	1.49	1.41
23	c	506	CLA	C1C-C2C	2.38	1.49	1.44
23	b	603	CLA	C3B-C2B	2.38	1.49	1.41
23	b	614	CLA	C3B-C4B	2.38	1.49	1.42
23	C	505	CLA	C1C-C2C	2.38	1.49	1.44
23	a	406	CLA	C3D-C4D	-2.37	1.38	1.44
23	B	611	CLA	C4B-NB	-2.37	1.34	1.37
23	C	505	CLA	C4C-C3C	2.37	1.49	1.45
23	b	605	CLA	C4B-NB	-2.37	1.34	1.37
23	B	614	CLA	C3B-C4B	2.36	1.49	1.42
23	A	408	CLA	C3D-C4D	-2.36	1.38	1.44
23	C	507	CLA	C3D-C4D	-2.36	1.38	1.44
23	c	505	CLA	C3B-C4B	2.36	1.49	1.42
24	a	417	PHO	C1B-NB	-2.36	1.34	1.38
23	C	514	CLA	C1C-C2C	2.36	1.49	1.44
23	c	507	CLA	C1B-NB	-2.35	1.34	1.37
35	H	102	DGD	O5D-C1E	2.35	1.44	1.40
29	D	406	PL9	C6-C5	2.35	1.46	1.35
23	C	504	CLA	C3D-C4D	-2.35	1.38	1.44
23	b	609	CLA	C3B-C2B	2.35	1.49	1.41
23	C	509	CLA	C1C-C2C	2.35	1.49	1.44
23	B	608	CLA	C3B-C2B	2.35	1.49	1.41
23	B	602	CLA	C4B-NB	-2.35	1.34	1.37
24	A	407	PHO	C3D-C4D	-2.35	1.38	1.41
29	A	413	PL9	C2-C3	2.34	1.40	1.34
23	B	615	CLA	C3B-C4B	2.34	1.49	1.42
23	b	602	CLA	C3B-C4B	2.34	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	403	CLA	C3D-C4D	-2.34	1.38	1.44
23	B	610	CLA	C1B-C2B	2.34	1.48	1.43
23	b	616	CLA	C3B-C2B	2.34	1.49	1.41
23	b	616	CLA	C1C-C2C	2.34	1.49	1.44
23	b	614	CLA	C4B-NB	-2.34	1.34	1.37
23	A	406	CLA	C4C-C3C	2.33	1.49	1.45
23	B	604	CLA	C4C-C3C	2.33	1.49	1.45
38	V	201	HEC	CMA-C3A	2.33	1.55	1.50
32	Z	101	LMG	O1-C1	2.33	1.44	1.40
24	a	417	PHO	C3A-C2A	-2.33	1.52	1.54
23	c	508	CLA	C3D-C4D	-2.33	1.38	1.44
23	B	609	CLA	C3B-C4B	2.33	1.49	1.42
23	B	614	CLA	C3D-C4D	-2.33	1.38	1.44
23	c	511	CLA	C3B-C2B	2.33	1.49	1.41
23	B	609	CLA	C4C-C3C	2.33	1.49	1.45
23	B	612	CLA	C4C-C3C	2.33	1.49	1.45
23	B	616	CLA	C3B-C2B	2.33	1.49	1.41
23	B	613	CLA	C3B-C2B	2.32	1.49	1.41
23	B	603	CLA	C3B-C4B	2.32	1.49	1.42
23	C	512	CLA	C3D-C4D	-2.32	1.39	1.44
23	c	509	CLA	C3B-C4B	2.32	1.49	1.42
23	c	512	CLA	C4C-C3C	2.32	1.49	1.45
23	C	513	CLA	C3B-C2B	2.31	1.49	1.41
33	b	625	HTG	C1-S1	-2.31	1.76	1.80
23	b	614	CLA	C3B-C2B	2.31	1.49	1.41
23	c	504	CLA	C1C-C2C	2.31	1.49	1.44
23	B	604	CLA	C3B-C4B	2.31	1.49	1.42
23	C	503	CLA	C3D-C4D	-2.31	1.39	1.44
23	B	603	CLA	C3B-C2B	2.31	1.48	1.41
23	B	608	CLA	C4C-C3C	2.30	1.48	1.45
23	c	503	CLA	C4C-C3C	2.30	1.48	1.45
23	D	404	CLA	C4B-NB	-2.30	1.34	1.37
23	B	610	CLA	C3B-C2B	2.30	1.48	1.41
23	c	510	CLA	C4C-C3C	2.30	1.48	1.45
23	b	610	CLA	C4C-C3C	2.30	1.48	1.45
25	b	619	BCR	C30-C25	-2.29	1.50	1.53
23	B	616	CLA	C1C-C2C	2.29	1.49	1.44
23	B	606	CLA	C3B-C2B	2.29	1.48	1.41
34	t	101	LMT	O1'-C1'	2.29	1.44	1.40
23	B	603	CLA	C4C-C3C	2.29	1.48	1.45
23	c	513	CLA	C4C-C3C	2.29	1.48	1.45
23	C	511	CLA	C3B-C2B	2.28	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	C3B-C2B	2.28	1.48	1.41
23	B	608	CLA	C3B-C4B	2.28	1.49	1.42
23	c	503	CLA	C3B-C4B	2.28	1.49	1.42
23	c	504	CLA	C3B-C2B	2.28	1.48	1.41
23	C	504	CLA	C1B-NB	-2.28	1.34	1.37
23	b	611	CLA	C1C-C2C	2.27	1.49	1.44
23	C	508	CLA	C3D-C4D	-2.26	1.39	1.44
23	b	607	CLA	C4C-C3C	2.26	1.48	1.45
24	a	417	PHO	C4B-NB	-2.26	1.34	1.38
23	B	607	CLA	C1C-C2C	2.26	1.49	1.44
23	b	602	CLA	C3B-C2B	2.25	1.48	1.41
23	C	508	CLA	C1C-C2C	2.25	1.49	1.44
23	B	605	CLA	C4C-C3C	2.25	1.48	1.45
23	B	604	CLA	C3B-C2B	2.25	1.48	1.41
24	a	407	PHO	C1B-NB	-2.25	1.34	1.38
23	b	612	CLA	C3D-C4D	-2.24	1.39	1.44
23	b	605	CLA	C3D-C4D	-2.24	1.39	1.44
23	b	606	CLA	C3D-C4D	-2.24	1.39	1.44
23	c	512	CLA	C3B-C2B	2.24	1.48	1.41
23	c	513	CLA	C1C-C2C	2.24	1.49	1.44
23	b	614	CLA	C4C-C3C	2.23	1.48	1.45
23	B	615	CLA	C1C-C2C	2.23	1.49	1.44
23	b	611	CLA	C3B-C4B	2.23	1.49	1.42
23	C	503	CLA	C4B-NB	-2.23	1.34	1.37
23	b	611	CLA	C4B-NB	-2.23	1.34	1.37
23	b	611	CLA	C4C-C3C	2.23	1.48	1.45
23	b	604	CLA	C4B-NB	-2.23	1.34	1.37
23	b	604	CLA	C3B-C2B	2.23	1.48	1.41
23	c	512	CLA	C4B-NB	-2.23	1.34	1.37
23	b	616	CLA	C3B-C4B	2.23	1.49	1.42
23	B	605	CLA	C3D-C4D	-2.22	1.39	1.44
24	a	407	PHO	CBD-CGD	-2.22	1.49	1.52
23	B	611	CLA	C3B-C4B	2.22	1.49	1.42
23	C	506	CLA	C3B-C4B	2.22	1.49	1.42
23	B	610	CLA	C3B-C4B	2.22	1.49	1.42
23	C	512	CLA	C3B-C4B	2.21	1.49	1.42
23	c	514	CLA	C3D-C4D	-2.21	1.39	1.44
23	C	510	CLA	C4C-C3C	2.21	1.48	1.45
23	b	609	CLA	C4C-C3C	2.21	1.48	1.45
23	D	403	CLA	C3B-C2B	2.21	1.48	1.41
23	c	508	CLA	C3B-C2B	2.21	1.48	1.41
23	c	512	CLA	C3B-C4B	2.20	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	D	402	LMT	O1'-C1'	2.20	1.43	1.40
23	B	616	CLA	C3D-C4D	-2.20	1.39	1.44
24	a	407	PHO	C3A-C2A	-2.20	1.52	1.54
23	b	607	CLA	C1A-CHA	2.20	1.52	1.43
23	b	608	CLA	C1C-C2C	2.20	1.49	1.44
31	L	101	LHG	O7-C5	-2.20	1.41	1.46
23	C	514	CLA	C4C-C3C	2.19	1.48	1.45
23	b	614	CLA	C1C-C2C	2.19	1.49	1.44
23	b	601	CLA	C3B-C2B	2.19	1.48	1.41
23	A	405	CLA	C3D-C4D	-2.19	1.39	1.44
23	B	614	CLA	C1C-C2C	2.19	1.49	1.44
23	C	503	CLA	C4C-C3C	2.19	1.48	1.45
23	B	604	CLA	C3D-C4D	-2.19	1.39	1.44
23	b	606	CLA	C3B-C2B	2.19	1.48	1.41
23	C	513	CLA	C3D-C4D	-2.19	1.39	1.44
23	a	404	CLA	C3B-C2B	2.19	1.48	1.41
23	b	609	CLA	C3D-C4D	-2.18	1.39	1.44
23	B	616	CLA	C3B-C4B	2.18	1.49	1.42
23	B	601	CLA	C3D-C4D	-2.18	1.39	1.44
23	B	616	CLA	C1C-NC	-2.18	1.34	1.37
23	b	601	CLA	C3D-C4D	-2.18	1.39	1.44
23	b	609	CLA	C1B-C2B	2.18	1.48	1.43
23	C	515	CLA	C4C-C3C	2.18	1.48	1.45
23	B	601	CLA	C3B-C2B	2.17	1.48	1.41
23	B	611	CLA	C3B-C2B	2.17	1.48	1.41
23	C	510	CLA	C1C-C2C	2.17	1.48	1.44
23	b	603	CLA	C3B-C4B	2.16	1.49	1.42
34	E	102	LMT	O1'-C1'	2.16	1.43	1.40
29	D	406	PL9	C2-C3	2.16	1.40	1.34
23	D	403	CLA	C1C-C2C	2.16	1.48	1.44
32	C	522	LMG	O1-C1	2.16	1.43	1.40
23	b	608	CLA	C3B-C2B	2.16	1.48	1.41
23	A	408	CLA	C3B-C4B	2.16	1.49	1.42
23	c	511	CLA	C3B-C4B	2.16	1.49	1.42
24	a	407	PHO	C4B-NB	-2.16	1.34	1.38
23	C	515	CLA	C3D-C4D	-2.15	1.39	1.44
34	C	526	LMT	O1'-C1'	2.15	1.43	1.40
23	B	606	CLA	C3B-C4B	2.15	1.49	1.42
23	d	403	CLA	C1D-C2D	2.15	1.49	1.45
23	b	610	CLA	C3B-C4B	2.15	1.49	1.42
23	B	614	CLA	C1B-NB	-2.15	1.35	1.37
23	B	610	CLA	C1C-C2C	2.15	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	E	103	HEC	C3C-C4C	-2.15	1.42	1.46
23	c	510	CLA	C3D-C4D	-2.15	1.39	1.44
38	v	202	HEC	C3B-C2B	-2.15	1.33	1.41
23	C	506	CLA	C3B-C2B	2.14	1.48	1.41
23	a	408	CLA	C3D-C4D	-2.14	1.39	1.44
23	C	506	CLA	C3D-C4D	-2.14	1.39	1.44
23	d	403	CLA	C4C-C3C	2.14	1.48	1.45
29	a	415	PL9	C2-C3	2.14	1.40	1.34
23	C	515	CLA	C3B-C2B	2.13	1.48	1.41
23	a	408	CLA	C3B-C4B	2.13	1.48	1.42
24	A	415	PHO	C3D-C4D	-2.13	1.38	1.41
23	A	406	CLA	C1C-NC	-2.13	1.34	1.37
23	a	405	CLA	C4B-NB	-2.13	1.35	1.37
23	A	408	CLA	C3B-C2B	2.13	1.48	1.41
23	b	614	CLA	C3D-C4D	-2.13	1.39	1.44
23	a	404	CLA	C1C-C2C	2.13	1.48	1.44
23	C	503	CLA	C3B-C2B	2.12	1.48	1.41
23	A	404	CLA	C1D-C2D	2.12	1.49	1.45
23	c	508	CLA	C3B-C4B	2.12	1.48	1.42
23	b	609	CLA	C1D-C2D	2.12	1.49	1.45
23	B	602	CLA	C1B-C2B	2.12	1.48	1.43
23	B	607	CLA	C3B-C4B	2.11	1.48	1.42
23	B	611	CLA	C3D-C4D	-2.11	1.39	1.44
23	c	511	CLA	C3D-C4D	-2.11	1.39	1.44
23	b	615	CLA	C4B-NB	-2.11	1.35	1.37
34	e	101	LMT	O1'-C1'	2.11	1.43	1.40
23	B	601	CLA	C1D-C2D	2.11	1.49	1.45
23	b	606	CLA	C1B-C2B	2.11	1.48	1.43
24	A	415	PHO	C3A-C2A	-2.11	1.52	1.54
23	C	504	CLA	C4C-C3C	2.10	1.48	1.45
23	a	404	CLA	C3D-C4D	-2.10	1.39	1.44
38	e	102	HEC	C3C-C4C	-2.10	1.42	1.46
23	C	508	CLA	C3B-C4B	2.10	1.48	1.42
23	c	508	CLA	C1C-C2C	2.10	1.48	1.44
24	A	407	PHO	C1D-ND	-2.10	1.34	1.38
23	C	511	CLA	C3D-C4D	-2.10	1.39	1.44
23	b	604	CLA	C3B-C4B	2.10	1.48	1.42
23	b	605	CLA	C1D-C2D	2.09	1.49	1.45
32	D	413	LMG	O7-C8	-2.09	1.41	1.46
33	D	411	HTG	C1-S1	-2.09	1.77	1.80
23	c	504	CLA	C1B-NB	-2.09	1.35	1.37
23	b	605	CLA	C1C-C2C	2.09	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	v	202	HEC	CMD-C2D	2.09	1.55	1.50
38	V	201	HEC	CMD-C2D	2.09	1.55	1.50
23	c	504	CLA	C3D-C4D	-2.09	1.39	1.44
23	C	513	CLA	C1C-NC	-2.09	1.34	1.37
23	D	403	CLA	C4C-C3C	2.08	1.48	1.45
23	C	512	CLA	C3B-C2B	2.08	1.48	1.41
23	C	513	CLA	C1A-CHA	2.08	1.51	1.43
23	b	604	CLA	C4C-C3C	2.08	1.48	1.45
24	A	407	PHO	C4B-NB	-2.08	1.34	1.38
23	c	515	CLA	C3B-C2B	2.08	1.48	1.41
23	b	601	CLA	C1C-C2C	2.08	1.48	1.44
23	C	507	CLA	C4B-NB	-2.08	1.35	1.37
23	b	615	CLA	C3D-C4D	-2.08	1.39	1.44
23	A	406	CLA	C3D-C4D	-2.07	1.39	1.44
23	C	514	CLA	C3B-C4B	2.07	1.48	1.42
23	c	510	CLA	C1C-C2C	2.06	1.48	1.44
23	B	606	CLA	C1C-C2C	2.06	1.48	1.44
23	c	510	CLA	C3B-C4B	2.06	1.48	1.42
23	A	406	CLA	C1C-C2C	2.06	1.48	1.44
23	C	507	CLA	C3B-C4B	2.06	1.48	1.42
35	c	520	DGD	O2G-C2G	-2.06	1.41	1.46
23	b	610	CLA	C3B-C2B	2.06	1.48	1.41
23	c	508	CLA	C4C-C3C	2.06	1.48	1.45
23	B	607	CLA	C3D-C4D	-2.06	1.39	1.44
23	c	506	CLA	C3D-C4D	-2.06	1.39	1.44
38	e	102	HEC	C4A-C3A	-2.05	1.41	1.45
23	D	404	CLA	C3D-C4D	-2.05	1.39	1.44
23	C	506	CLA	C4C-C3C	2.05	1.48	1.45
23	a	408	CLA	C3B-C2B	2.05	1.48	1.41
23	C	506	CLA	C1A-CHA	2.04	1.51	1.43
23	b	605	CLA	C4C-C3C	2.04	1.48	1.45
23	C	505	CLA	MG-NA	2.04	2.11	2.06
31	D	407	LHG	O7-C5	-2.04	1.41	1.46
23	B	606	CLA	MG-NA	2.04	2.11	2.06
23	B	604	CLA	C4B-NB	-2.03	1.35	1.37
23	a	404	CLA	C4C-C3C	2.03	1.48	1.45
23	B	615	CLA	C3D-C4D	-2.03	1.39	1.44
23	a	404	CLA	C3B-C4B	2.03	1.48	1.42
38	e	102	HEC	C1D-C2D	2.03	1.47	1.43
24	A	407	PHO	C1B-NB	-2.03	1.35	1.38
38	V	201	HEC	C3B-C2B	-2.03	1.34	1.41
35	C	519	DGD	O5D-C1E	2.03	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	417	PHO	CHA-CBD	-2.02	1.49	1.51
23	C	515	CLA	C3B-C4B	2.02	1.48	1.42
23	B	602	CLA	CHB-C4A	-2.02	1.32	1.37
23	C	510	CLA	C3B-C4B	2.02	1.48	1.42
23	a	408	CLA	C4C-C3C	2.02	1.48	1.45
23	C	504	CLA	C3B-C2B	2.02	1.48	1.41
23	a	405	CLA	C3D-C4D	-2.01	1.39	1.44
23	b	606	CLA	C1D-C2D	2.01	1.49	1.45
23	c	509	CLA	C1D-C2D	2.01	1.49	1.45
23	B	604	CLA	MG-NA	2.01	2.11	2.06
23	b	606	CLA	C4C-C3C	2.01	1.48	1.45
23	d	403	CLA	C3B-C2B	2.01	1.47	1.41
23	c	513	CLA	C3B-C4B	2.01	1.48	1.42
23	c	513	CLA	C4B-NB	-2.01	1.35	1.37
23	B	608	CLA	C1C-C2C	2.01	1.48	1.44
24	a	407	PHO	C1D-ND	-2.00	1.35	1.38
23	C	507	CLA	C3B-C2B	2.00	1.47	1.41
23	b	601	CLA	C1D-C2D	2.00	1.49	1.45

All (2810) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	407	PHO	C2D-C1D-ND	11.72	117.90	109.43
24	a	417	PHO	C2D-C1D-ND	11.38	117.66	109.43
24	A	415	PHO	C2D-C1D-ND	10.59	117.08	109.43
24	A	407	PHO	C2D-C1D-ND	10.53	117.04	109.43
23	c	513	CLA	C1D-ND-C4D	-10.46	98.97	106.31
23	b	605	CLA	C1D-ND-C4D	-10.44	98.99	106.31
23	B	614	CLA	C1D-ND-C4D	-10.39	99.02	106.31
23	B	612	CLA	C1D-ND-C4D	-10.22	99.14	106.31
23	C	505	CLA	C1D-ND-C4D	-10.21	99.15	106.31
23	a	406	CLA	C1D-ND-C4D	-10.16	99.18	106.31
38	v	202	HEC	CBB-CAB-C3B	-10.05	107.35	127.43
23	c	504	CLA	C1D-ND-C4D	-9.96	99.32	106.31
23	C	503	CLA	C1D-ND-C4D	-9.95	99.33	106.31
23	D	403	CLA	C1D-ND-C4D	-9.93	99.35	106.31
23	B	611	CLA	C1D-ND-C4D	-9.86	99.40	106.31
23	B	601	CLA	C1D-ND-C4D	-9.76	99.47	106.31
23	b	603	CLA	C1D-ND-C4D	-9.66	99.53	106.31
23	A	405	CLA	C1D-ND-C4D	-9.66	99.53	106.31
23	b	614	CLA	C1D-ND-C4D	-9.63	99.56	106.31
23	b	606	CLA	C1D-ND-C4D	-9.62	99.56	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	C1D-ND-C4D	-9.61	99.57	106.31
23	B	607	CLA	C1D-ND-C4D	-9.56	99.61	106.31
23	B	603	CLA	C1D-ND-C4D	-9.56	99.61	106.31
23	d	403	CLA	C1D-ND-C4D	-9.56	99.61	106.31
23	c	503	CLA	C1D-ND-C4D	-9.55	99.61	106.31
23	a	408	CLA	C1D-ND-C4D	-9.54	99.62	106.31
23	b	615	CLA	C1D-ND-C4D	-9.50	99.65	106.31
23	C	515	CLA	C1D-ND-C4D	-9.47	99.67	106.31
24	a	407	PHO	O2D-CGD-CBD	9.45	121.33	110.95
23	D	404	CLA	C1D-ND-C4D	-9.41	99.71	106.31
23	B	605	CLA	C1D-ND-C4D	-9.41	99.71	106.31
24	a	417	PHO	O2D-CGD-CBD	9.40	121.27	110.95
23	b	611	CLA	C1D-ND-C4D	-9.40	99.72	106.31
23	B	609	CLA	C1D-ND-C4D	-9.40	99.72	106.31
23	B	608	CLA	C1D-ND-C4D	-9.33	99.77	106.31
23	A	406	CLA	C1D-ND-C4D	-9.31	99.78	106.31
23	A	404	CLA	C1D-ND-C4D	-9.30	99.78	106.31
23	b	601	CLA	C1D-ND-C4D	-9.26	99.81	106.31
23	c	505	CLA	C1D-ND-C4D	-9.26	99.82	106.31
23	c	508	CLA	C1D-ND-C4D	-9.24	99.83	106.31
23	B	615	CLA	C1D-ND-C4D	-9.23	99.84	106.31
23	B	616	CLA	C1D-ND-C4D	-9.22	99.85	106.31
23	c	515	CLA	C1D-ND-C4D	-9.20	99.86	106.31
23	a	405	CLA	C1D-ND-C4D	-9.16	99.88	106.31
23	C	513	CLA	C1D-ND-C4D	-9.15	99.89	106.31
23	c	509	CLA	C1D-ND-C4D	-9.10	99.92	106.31
23	C	506	CLA	C1D-ND-C4D	-9.10	99.93	106.31
23	C	507	CLA	C1D-ND-C4D	-9.07	99.95	106.31
23	C	504	CLA	C1D-ND-C4D	-9.02	99.99	106.31
23	C	510	CLA	C1D-ND-C4D	-9.01	99.99	106.31
23	a	404	CLA	C1D-ND-C4D	-9.01	99.99	106.31
23	c	514	CLA	C1D-ND-C4D	-8.99	100.00	106.31
23	b	610	CLA	C1D-ND-C4D	-8.96	100.02	106.31
23	B	613	CLA	C1D-ND-C4D	-8.91	100.06	106.31
23	b	607	CLA	C1D-ND-C4D	-8.90	100.07	106.31
23	b	609	CLA	C1D-ND-C4D	-8.90	100.07	106.31
23	C	511	CLA	C1D-ND-C4D	-8.88	100.08	106.31
23	C	512	CLA	C1D-ND-C4D	-8.81	100.13	106.31
23	c	510	CLA	C1D-ND-C4D	-8.80	100.14	106.31
23	c	507	CLA	C1D-ND-C4D	-8.75	100.17	106.31
23	c	511	CLA	C1D-ND-C4D	-8.75	100.17	106.31
23	C	509	CLA	C1D-ND-C4D	-8.74	100.18	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	CLA	C1D-ND-C4D	-8.72	100.19	106.31
23	b	608	CLA	C1D-ND-C4D	-8.70	100.21	106.31
23	b	616	CLA	C1D-ND-C4D	-8.67	100.23	106.31
23	b	613	CLA	C1D-ND-C4D	-8.66	100.24	106.31
23	b	602	CLA	C1D-ND-C4D	-8.64	100.25	106.31
23	c	512	CLA	C1D-ND-C4D	-8.60	100.28	106.31
23	C	508	CLA	C1D-ND-C4D	-8.58	100.29	106.31
23	B	610	CLA	C1D-ND-C4D	-8.44	100.39	106.31
24	A	415	PHO	O2D-CGD-CBD	8.44	120.22	110.95
23	d	402	CLA	C1D-ND-C4D	-8.42	100.41	106.31
23	C	514	CLA	C1D-ND-C4D	-8.27	100.51	106.31
23	B	606	CLA	C1D-ND-C4D	-8.23	100.54	106.31
23	b	604	CLA	C1D-ND-C4D	-8.18	100.57	106.31
23	b	612	CLA	C1D-ND-C4D	-8.13	100.61	106.31
23	B	602	CLA	C1D-ND-C4D	-8.12	100.61	106.31
23	B	602	CLA	C4A-NA-C1A	-8.04	103.01	106.68
24	A	407	PHO	C3B-C4B-NB	8.00	112.68	107.46
23	B	604	CLA	C1D-ND-C4D	-7.98	100.71	106.31
23	B	614	CLA	C2D-C1D-ND	7.75	117.80	110.13
23	B	612	CLA	C2D-C1D-ND	7.56	117.61	110.13
38	V	201	HEC	CBB-CAB-C3B	-7.50	112.45	127.43
23	b	602	CLA	C4A-NA-C1A	-7.39	103.31	106.68
24	A	415	PHO	C3B-C4B-NB	7.32	112.24	107.46
23	B	609	CLA	C4A-NA-C1A	-7.28	103.36	106.68
24	a	417	PHO	C3B-C4B-NB	7.25	112.19	107.46
23	B	615	CLA	CHD-C4C-C3C	-7.24	114.22	124.77
23	D	403	CLA	C4A-NA-C1A	-7.18	103.40	106.68
23	b	611	CLA	CMD-C2D-C1D	7.17	137.35	124.73
23	B	606	CLA	CMD-C2D-C1D	7.16	137.34	124.73
24	a	407	PHO	C3B-C4B-NB	7.15	112.13	107.46
23	b	606	CLA	C4A-NA-C1A	-7.09	103.44	106.68
23	C	508	CLA	CMD-C2D-C1D	7.06	137.16	124.73
23	b	606	CLA	CMD-C2D-C1D	6.99	137.04	124.73
23	C	505	CLA	C2D-C1D-ND	6.99	117.04	110.13
23	B	611	CLA	CHD-C4C-C3C	-6.96	114.63	124.77
23	a	406	CLA	C2D-C1D-ND	6.96	117.01	110.13
27	C	501	SQD	O6-C1-C2	6.94	118.82	108.27
23	b	605	CLA	CMD-C2D-C1D	6.91	136.89	124.73
24	A	407	PHO	O2D-CGD-CBD	6.90	118.53	110.95
23	c	513	CLA	C2D-C1D-ND	6.89	116.95	110.13
23	B	615	CLA	C2D-C1D-ND	6.87	116.92	110.13
23	B	610	CLA	CMD-C2D-C1D	6.86	136.80	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	O2D-CGD-CBD	6.83	123.17	111.23
23	b	605	CLA	CHD-C4C-C3C	-6.81	114.84	124.77
23	A	405	CLA	C2D-C1D-ND	6.81	116.86	110.13
23	c	509	CLA	CMD-C2D-C1D	6.81	136.71	124.73
23	c	506	CLA	CMD-C2D-C1D	6.76	136.64	124.73
23	B	603	CLA	C2D-C1D-ND	6.75	116.81	110.13
24	A	407	PHO	C2B-C1B-NB	6.71	114.28	109.43
23	c	503	CLA	CMD-C2D-C1D	6.69	136.52	124.73
23	B	612	CLA	O2D-CGD-CBD	6.69	122.93	111.23
23	B	612	CLA	CHD-C4C-C3C	-6.69	115.02	124.77
23	b	608	CLA	CMD-C2D-C1D	6.68	136.50	124.73
23	a	408	CLA	CHD-C4C-C3C	-6.68	115.03	124.77
23	a	405	CLA	CHD-C4C-C3C	-6.68	115.03	124.77
23	C	509	CLA	CMD-C2D-C1D	6.68	136.49	124.73
23	B	604	CLA	O2D-CGD-CBD	6.67	122.90	111.23
23	B	611	CLA	C2D-C1D-ND	6.63	116.69	110.13
23	B	613	CLA	C2D-C1D-ND	6.63	116.69	110.13
23	b	614	CLA	C2D-C1D-ND	6.61	116.67	110.13
23	b	607	CLA	C2D-C1D-ND	6.58	116.64	110.13
24	a	417	PHO	C2B-C1B-NB	6.58	114.19	109.43
23	b	616	CLA	C4A-NA-C1A	-6.58	103.68	106.68
23	B	614	CLA	CMD-C2D-C1D	6.56	136.27	124.73
23	b	601	CLA	CMD-C2D-C1D	6.55	136.26	124.73
23	B	611	CLA	CMD-C2D-C1D	6.55	136.26	124.73
23	C	507	CLA	O2D-CGD-CBD	6.54	122.67	111.23
23	a	406	CLA	CHD-C4C-C3C	-6.54	115.24	124.77
23	C	506	CLA	C2D-C1D-ND	6.51	116.57	110.13
23	B	608	CLA	CMD-C2D-C1D	6.50	136.18	124.73
23	c	509	CLA	O2D-CGD-CBD	6.49	122.57	111.23
23	B	616	CLA	C2D-C1D-ND	6.49	116.55	110.13
23	C	503	CLA	CMD-C2D-C1D	6.48	136.14	124.73
23	b	613	CLA	C2D-C1D-ND	6.48	116.54	110.13
23	b	616	CLA	CHD-C4C-C3C	-6.46	115.35	124.77
23	a	405	CLA	C2D-C1D-ND	6.46	116.52	110.13
23	a	408	CLA	C2D-C1D-ND	6.46	116.52	110.13
23	B	606	CLA	C4A-NA-C1A	-6.46	103.73	106.68
23	C	515	CLA	CHD-C4C-C3C	-6.46	115.35	124.77
23	B	614	CLA	CHD-C4C-C3C	-6.46	115.36	124.77
23	c	504	CLA	C2D-C1D-ND	6.45	116.51	110.13
23	b	604	CLA	O2D-CGD-CBD	6.44	122.49	111.23
23	B	602	CLA	CMD-C2D-C1D	6.44	136.06	124.73
23	c	515	CLA	CMD-C2D-C1D	6.43	136.06	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	C2D-C1D-ND	6.43	116.49	110.13
23	b	615	CLA	C2D-C1D-ND	6.43	116.49	110.13
23	B	603	CLA	CHD-C4C-C3C	-6.42	115.41	124.77
23	b	610	CLA	O2D-CGD-CBD	6.40	122.42	111.23
38	v	202	HEC	CBC-CAC-C3C	-6.40	114.64	127.43
23	a	404	CLA	CMD-C2D-C1D	6.40	136.00	124.73
23	B	616	CLA	CHD-C4C-C3C	-6.40	115.45	124.77
23	c	504	CLA	CHD-C4C-C3C	-6.40	115.45	124.77
23	b	610	CLA	CHD-C4C-C3C	-6.39	115.46	124.77
23	C	510	CLA	CHD-C4C-C3C	-6.37	115.48	124.77
23	B	605	CLA	CHD-C4C-C3C	-6.36	115.49	124.77
23	C	505	CLA	CHD-C4C-C3C	-6.36	115.51	124.77
23	c	513	CLA	CHD-C4C-C3C	-6.35	115.51	124.77
23	B	601	CLA	O2D-CGD-CBD	6.35	122.32	111.23
23	C	514	CLA	CHD-C4C-C3C	-6.34	115.53	124.77
23	C	503	CLA	CHD-C4C-C3C	-6.33	115.54	124.77
23	B	609	CLA	CMD-C2D-C1D	6.33	135.88	124.73
23	b	608	CLA	C4A-NA-C1A	-6.33	103.79	106.68
23	B	610	CLA	O2D-CGD-CBD	6.33	122.29	111.23
23	d	403	CLA	CMD-C2D-C1D	6.32	135.85	124.73
23	B	607	CLA	C2D-C1D-ND	6.31	116.38	110.13
23	C	505	CLA	C4A-NA-C1A	-6.31	103.80	106.68
23	b	616	CLA	CMD-C2D-C1D	6.31	135.84	124.73
23	C	510	CLA	C2D-C1D-ND	6.30	116.37	110.13
23	b	605	CLA	C2D-C1D-ND	6.30	116.37	110.13
23	C	505	CLA	CMD-C2D-C1D	6.30	135.83	124.73
23	C	512	CLA	CMD-C2D-C1D	6.30	135.82	124.73
23	c	505	CLA	CMD-C2D-C1D	6.30	135.82	124.73
23	b	611	CLA	C2D-C1D-ND	6.29	116.35	110.13
23	D	403	CLA	C2D-C1D-ND	6.29	116.35	110.13
23	c	514	CLA	O2D-CGD-CBD	6.29	122.23	111.23
23	B	603	CLA	C4A-NA-C1A	-6.28	103.81	106.68
23	B	606	CLA	O2D-CGD-CBD	6.27	122.19	111.23
23	c	503	CLA	C2D-C1D-ND	6.25	116.31	110.13
23	C	513	CLA	CMD-C2D-C1D	6.24	135.72	124.73
23	C	504	CLA	C2D-C1D-ND	6.24	116.30	110.13
23	b	603	CLA	CMD-C2D-C1D	6.22	135.69	124.73
23	b	614	CLA	CMD-C2D-C1D	6.21	135.66	124.73
23	D	404	CLA	CMD-C2D-C1D	6.20	135.65	124.73
23	b	602	CLA	O2D-CGD-CBD	6.20	122.06	111.23
23	B	601	CLA	CMD-C2D-C1D	6.20	135.64	124.73
23	c	510	CLA	C2D-C1D-ND	6.19	116.25	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	O2D-CGD-CBD	6.18	122.03	111.23
23	D	404	CLA	CHD-C4C-C3C	-6.17	115.77	124.77
23	B	614	CLA	C3D-C2D-C1D	-6.16	97.42	105.83
23	c	509	CLA	CHD-C4C-C3C	-6.16	115.79	124.77
23	b	612	CLA	CHD-C4C-C3C	-6.16	115.79	124.77
23	C	503	CLA	O2D-CGD-CBD	6.16	121.99	111.23
23	c	512	CLA	CMD-C2D-C1D	6.15	135.56	124.73
23	b	605	CLA	C4A-NA-C1A	-6.15	103.87	106.68
23	C	509	CLA	C2D-C1D-ND	6.15	116.21	110.13
23	b	606	CLA	O2D-CGD-CBD	6.15	121.97	111.23
23	c	509	CLA	C2D-C1D-ND	6.14	116.20	110.13
23	c	507	CLA	O2D-CGD-CBD	6.13	121.95	111.23
23	C	509	CLA	O2D-CGD-CBD	6.11	121.90	111.23
23	b	612	CLA	CMD-C2D-C1D	6.08	135.43	124.73
23	C	514	CLA	CMD-C2D-C1D	6.07	135.41	124.73
23	C	504	CLA	CHD-C4C-C3C	-6.06	115.94	124.77
27	C	501	SQD	C1-O5-C5	-6.06	101.88	113.72
23	D	403	CLA	CMD-C2D-C1D	6.06	135.40	124.73
23	B	608	CLA	C2D-C1D-ND	6.06	116.12	110.13
23	B	604	CLA	CHD-C4C-C3C	-6.05	115.96	124.77
23	C	513	CLA	C2D-C1D-ND	6.04	116.11	110.13
23	A	404	CLA	CMD-C2D-C1D	6.04	135.37	124.73
23	c	505	CLA	C4A-NA-C1A	-6.03	103.93	106.68
24	a	407	PHO	C2B-C1B-NB	6.03	113.79	109.43
23	B	609	CLA	C2D-C1D-ND	6.03	116.09	110.13
23	C	515	CLA	C2D-C1D-ND	6.03	116.09	110.13
23	b	606	CLA	CHD-C4C-C3C	-6.02	115.99	124.77
23	b	614	CLA	CHD-C4C-C3C	-6.02	116.00	124.77
23	c	508	CLA	CMD-C2D-C1D	6.02	135.32	124.73
24	a	417	PHO	C1-C2-C3	-6.02	116.34	126.20
23	c	510	CLA	O2D-CGD-CBD	6.01	121.73	111.23
23	C	514	CLA	O2D-CGD-CBD	5.99	121.70	111.23
23	b	611	CLA	CHD-C4C-C3C	-5.99	116.04	124.77
23	b	615	CLA	CMD-C2D-C1D	5.98	135.26	124.73
23	d	403	CLA	C2D-C1D-ND	5.98	116.04	110.13
23	b	601	CLA	CHD-C4C-C3C	-5.98	116.06	124.77
23	c	515	CLA	C2D-C1D-ND	5.97	116.04	110.13
23	B	616	CLA	O2D-CGD-CBD	5.97	121.67	111.23
23	c	508	CLA	CHD-C4C-C3C	-5.96	116.08	124.77
23	c	510	CLA	CHD-C4C-C3C	-5.96	116.08	124.77
23	b	616	CLA	C2D-C1D-ND	5.96	116.02	110.13
23	A	408	CLA	CMD-C2D-C1D	5.96	135.22	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	CHD-C4C-C3C	-5.96	116.09	124.77
23	c	512	CLA	CHD-C4C-C3C	-5.95	116.10	124.77
23	C	509	CLA	CHD-C4C-C3C	-5.95	116.10	124.77
23	b	613	CLA	CMD-C2D-C1D	5.94	135.19	124.73
23	b	612	CLA	O2D-CGD-CBD	5.94	121.61	111.23
23	b	609	CLA	C2D-C1D-ND	5.94	116.00	110.13
23	b	603	CLA	CHD-C4C-C3C	-5.94	116.12	124.77
23	c	506	CLA	C2D-C1D-ND	5.93	115.99	110.13
23	c	508	CLA	C2D-C1D-ND	5.93	115.99	110.13
23	c	514	CLA	C2D-C1D-ND	5.92	115.99	110.13
23	b	604	CLA	C2D-C1D-ND	5.92	115.98	110.13
23	B	603	CLA	O2D-CGD-CBD	5.92	121.58	111.23
23	D	404	CLA	C2D-C1D-ND	5.92	115.98	110.13
23	B	605	CLA	C2D-C1D-ND	5.91	115.98	110.13
23	b	603	CLA	C2D-C1D-ND	5.90	115.97	110.13
23	B	609	CLA	CHD-C4C-C3C	-5.90	116.17	124.77
23	b	609	CLA	CHD-C4C-C3C	-5.89	116.19	124.77
23	A	406	CLA	C2D-C1D-ND	5.88	115.94	110.13
23	b	606	CLA	C2D-C1D-ND	5.88	115.94	110.13
23	B	602	CLA	CHD-C4C-C3C	-5.86	116.23	124.77
23	b	602	CLA	CMD-C2D-C1D	5.86	135.05	124.73
23	b	603	CLA	O2D-CGD-CBD	5.86	121.47	111.23
23	c	513	CLA	CMD-C2D-C1D	5.86	135.04	124.73
23	c	514	CLA	CHD-C4C-C3C	-5.85	116.24	124.77
23	C	515	CLA	CMD-C2D-C1D	5.85	135.03	124.73
23	b	609	CLA	CMD-C2D-C1D	5.85	135.03	124.73
23	C	512	CLA	CHD-C4C-C3C	-5.84	116.25	124.77
24	A	415	PHO	C2B-C1B-NB	5.84	113.65	109.43
23	B	608	CLA	CHD-C4C-C3C	-5.84	116.26	124.77
23	B	614	CLA	O2D-CGD-CBD	5.84	121.43	111.23
23	A	408	CLA	C2D-C1D-ND	5.83	115.90	110.13
23	b	610	CLA	C2D-C1D-ND	5.82	115.89	110.13
23	A	406	CLA	C4A-NA-C1A	-5.81	104.03	106.68
23	b	613	CLA	CHD-C4C-C3C	-5.79	116.33	124.77
23	B	610	CLA	C2D-C1D-ND	5.79	115.86	110.13
23	C	507	CLA	CMD-C2D-C1D	5.79	134.92	124.73
24	A	407	PHO	C4D-ND-C1D	-5.78	101.95	108.87
23	c	507	CLA	C4A-NA-C1A	-5.78	104.04	106.68
23	A	406	CLA	CHD-C4C-C3C	-5.78	116.35	124.77
23	b	601	CLA	O2D-CGD-CBD	5.77	121.32	111.23
23	c	507	CLA	CHD-C4C-C3C	-5.77	116.36	124.77
23	B	601	CLA	C2D-C1D-ND	5.77	115.84	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	C2D-C1D-ND	5.77	115.84	110.13
23	b	612	CLA	C2C-C1C-NC	5.75	116.02	109.98
23	c	505	CLA	C2D-C1D-ND	5.75	115.81	110.13
23	d	402	CLA	C2C-C1C-NC	5.74	116.02	109.98
23	b	604	CLA	CHD-C4C-C3C	-5.74	116.40	124.77
24	a	417	PHO	C4D-ND-C1D	-5.74	101.99	108.87
23	C	507	CLA	CHD-C4C-C3C	-5.74	116.41	124.77
23	c	506	CLA	O2D-CGD-CBD	5.73	121.25	111.23
23	B	615	CLA	CMD-C2D-C1D	5.72	134.80	124.73
23	B	606	CLA	CHD-C4C-C3C	-5.71	116.44	124.77
23	A	405	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
23	c	503	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
23	c	515	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
23	B	613	CLA	CHD-C4C-C3C	-5.70	116.46	124.77
23	C	510	CLA	O2D-CGD-CBD	5.70	121.19	111.23
23	c	511	CLA	CMD-C2D-C1D	5.69	134.75	124.73
23	b	612	CLA	C2D-C1D-ND	5.68	115.75	110.13
23	B	601	CLA	CHD-C4C-C3C	-5.68	116.49	124.77
23	C	513	CLA	CHD-C4C-C3C	-5.68	116.50	124.77
27	D	412	SQD	O6-C1-C2	5.67	116.89	108.27
25	Y	101	BCR	C33-C5-C6	-5.67	118.29	124.48
23	d	403	CLA	CHD-C4C-C3C	-5.67	116.51	124.77
23	c	510	CLA	C2C-C1C-NC	5.66	115.93	109.98
23	a	404	CLA	CHD-C4C-C3C	-5.66	116.52	124.77
23	C	511	CLA	CMD-C2D-C1D	5.65	134.68	124.73
23	C	504	CLA	CMD-C2D-C1D	5.64	134.66	124.73
24	a	407	PHO	C4D-ND-C1D	-5.63	102.12	108.87
23	b	601	CLA	C2D-C1D-ND	5.63	115.69	110.13
23	c	511	CLA	C2D-C1D-ND	5.62	115.69	110.13
23	B	605	CLA	C4A-NA-C1A	-5.62	104.12	106.68
23	c	507	CLA	CMD-C2D-C1D	5.61	134.61	124.73
23	b	607	CLA	CMD-C2D-C1D	5.61	134.60	124.73
23	A	405	CLA	CMD-C2D-C1D	5.61	134.60	124.73
23	C	508	CLA	C4A-NA-C1A	-5.60	104.12	106.68
23	b	607	CLA	CHD-C4C-C3C	-5.60	116.61	124.77
23	B	604	CLA	C2D-C1D-ND	5.60	115.67	110.13
23	A	408	CLA	C4A-NA-C1A	-5.58	104.13	106.68
23	C	512	CLA	C2D-C1D-ND	5.58	115.65	110.13
23	c	509	CLA	C4A-NA-C1A	-5.58	104.13	106.68
23	C	511	CLA	C2C-C1C-NC	5.58	115.84	109.98
23	A	408	CLA	CHD-C4C-C3C	-5.57	116.66	124.77
23	a	405	CLA	CMD-C2D-C1D	5.56	134.53	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	CMD-C2D-C1D	5.56	134.53	124.73
23	b	612	CLA	C4A-NA-C1A	-5.56	104.14	106.68
23	c	514	CLA	C4A-NA-C1A	-5.55	104.15	106.68
23	B	607	CLA	CMD-C2D-C1D	5.54	134.49	124.73
23	B	614	CLA	C2C-C1C-NC	5.54	115.80	109.98
27	b	620	SQD	O6-C1-C2	5.53	116.68	108.27
23	A	406	CLA	CMD-C2D-C1D	5.51	134.43	124.73
23	C	511	CLA	C2D-C1D-ND	5.51	115.58	110.13
23	c	514	CLA	CMD-C2D-C1D	5.50	134.42	124.73
23	A	405	CLA	C3D-C2D-C1D	-5.49	98.33	105.83
23	C	510	CLA	CMD-C2D-C1D	5.49	134.40	124.73
23	b	613	CLA	C2C-C1C-NC	5.49	115.75	109.98
23	d	402	CLA	CHD-C4C-C3C	-5.49	116.77	124.77
23	b	604	CLA	C2C-C1C-NC	5.48	115.74	109.98
23	C	512	CLA	O2D-CGD-CBD	5.48	120.81	111.23
23	A	404	CLA	C2D-C1D-ND	5.48	115.55	110.13
23	B	613	CLA	C2C-C1C-NC	5.47	115.73	109.98
23	d	403	CLA	C4A-NA-C1A	-5.47	104.19	106.68
23	d	402	CLA	C2D-C1D-ND	5.46	115.53	110.13
23	c	509	CLA	C3B-C2B-C1B	-5.46	100.73	107.17
23	a	408	CLA	C4A-NA-C1A	-5.46	104.19	106.68
23	C	511	CLA	CHD-C4C-C3C	-5.46	116.82	124.77
23	b	610	CLA	CMD-C2D-C1D	5.45	134.33	124.73
23	B	616	CLA	C4A-NA-C1A	-5.44	104.20	106.68
23	b	606	CLA	C2B-C1B-NB	5.44	115.96	110.33
23	D	403	CLA	C2C-C1C-NC	5.43	115.68	109.98
24	A	407	PHO	C3D-C4D-ND	5.42	114.66	107.71
23	b	615	CLA	CHD-C4C-C3C	-5.42	116.87	124.77
23	c	505	CLA	CHD-C4C-C3C	-5.40	116.90	124.77
23	B	613	CLA	CMD-C2D-C1D	5.39	134.22	124.73
23	B	613	CLA	C1-C2-C3	-5.38	117.38	126.20
23	c	506	CLA	CHD-C4C-C3C	-5.38	116.93	124.77
23	C	514	CLA	C2D-C1D-ND	5.37	115.44	110.13
23	B	616	CLA	CMD-C2D-C1D	5.37	134.18	124.73
23	a	405	CLA	O2D-CGD-CBD	5.36	120.60	111.23
23	C	506	CLA	C2C-C1C-NC	5.34	115.59	109.98
23	b	615	CLA	C2C-C1C-NC	5.34	115.59	109.98
23	b	611	CLA	C4A-NA-C1A	-5.33	104.25	106.68
23	b	604	CLA	CMD-C2D-C1D	5.32	134.09	124.73
23	C	507	CLA	C2D-C1D-ND	5.31	115.38	110.13
23	b	610	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
23	b	609	CLA	C4A-NA-C1A	-5.31	104.26	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	403	CLA	O2D-CGD-CBD	5.30	120.50	111.23
23	C	514	CLA	C4A-NA-C1A	-5.30	104.26	106.68
23	b	615	CLA	C4A-NA-C1A	-5.30	104.26	106.68
23	a	404	CLA	C2C-C1C-NC	5.29	115.54	109.98
23	a	404	CLA	C2D-C1D-ND	5.29	115.36	110.13
23	B	607	CLA	C2C-C1C-NC	5.29	115.54	109.98
23	c	514	CLA	C2B-C1B-NB	5.29	115.81	110.33
23	d	403	CLA	C2B-C1B-NB	5.28	115.80	110.33
27	a	410	SQD	O6-C1-C2	5.27	116.28	108.27
23	c	512	CLA	C2D-C1D-ND	5.26	115.34	110.13
33	b	623	HTG	C1'-S1-C1	5.26	111.81	100.45
23	c	512	CLA	C2C-C1C-NC	5.26	115.51	109.98
23	B	612	CLA	C3C-C4C-NC	5.26	117.17	110.43
23	C	510	CLA	C2C-C1C-NC	5.25	115.50	109.98
23	B	610	CLA	C4A-NA-C1A	-5.25	104.28	106.68
23	B	602	CLA	C2B-C1B-NB	5.25	115.77	110.33
23	c	514	CLA	C3B-C2B-C1B	-5.25	100.98	107.17
23	B	614	CLA	C3B-C2B-C1B	-5.25	100.98	107.17
23	b	602	CLA	CHD-C4C-C3C	-5.25	117.12	124.77
25	D	405	BCR	C7-C8-C9	-5.24	118.48	126.23
23	C	508	CLA	C2C-C1C-NC	5.24	115.49	109.98
23	B	605	CLA	C2B-C1B-NB	5.24	115.76	110.33
23	b	601	CLA	C4A-NA-C1A	-5.24	104.29	106.68
25	y	101	BCR	C33-C5-C6	-5.24	118.77	124.48
23	C	511	CLA	C3B-C2B-C1B	-5.23	101.00	107.17
23	A	405	CLA	C2C-C1C-NC	5.23	115.47	109.98
24	a	417	PHO	C3D-C4D-ND	5.23	114.41	107.71
23	B	606	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
23	B	611	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
23	c	505	CLA	C2C-C1C-NC	5.21	115.46	109.98
23	b	613	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
25	d	404	BCR	C7-C8-C9	-5.21	118.53	126.23
27	b	620	SQD	O47-C7-C8	5.21	122.75	111.48
23	b	611	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
23	c	510	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
23	C	506	CLA	O2D-CGD-CBD	5.20	120.33	111.23
23	B	606	CLA	C2C-C1C-NC	5.20	115.45	109.98
23	B	605	CLA	C3B-C2B-C1B	-5.20	101.04	107.17
23	c	510	CLA	CMD-C2D-C1D	5.19	133.86	124.73
23	b	613	CLA	C3B-C2B-C1B	-5.19	101.06	107.17
23	A	404	CLA	CHD-C4C-C3C	-5.19	117.21	124.77
23	D	403	CLA	CHD-C4C-C3C	-5.18	117.22	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	C4A-NA-C1A	-5.18	104.32	106.68
23	A	404	CLA	C3B-C2B-C1B	-5.17	101.07	107.17
23	b	602	CLA	C2D-C1D-ND	5.15	115.23	110.13
23	B	610	CLA	CHD-C4C-C3C	-5.15	117.27	124.77
23	C	504	CLA	C4A-NA-C1A	-5.14	104.33	106.68
23	C	507	CLA	C4A-NA-C1A	-5.14	104.33	106.68
23	c	503	CLA	O2D-CGD-CBD	5.14	120.21	111.23
27	C	501	SQD	C1-C2-C3	-5.13	99.21	110.01
23	B	604	CLA	CMD-C2D-C1D	5.13	133.76	124.73
23	C	505	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
23	C	506	CLA	CMD-C2D-C1D	5.12	133.75	124.73
23	c	511	CLA	C2C-C1C-NC	5.12	115.36	109.98
23	C	513	CLA	O2D-CGD-CBD	5.12	120.18	111.23
23	c	509	CLA	C2B-C1B-NB	5.12	115.64	110.33
23	c	508	CLA	C2C-C1C-NC	5.12	115.36	109.98
23	B	603	CLA	CMD-C2D-C1D	5.12	133.74	124.73
23	a	405	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
23	B	612	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
23	b	616	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
23	c	507	CLA	C2D-C1D-ND	5.10	115.17	110.13
23	a	406	CLA	CMD-C2D-C1D	5.10	133.71	124.73
23	a	405	CLA	C2C-C1C-NC	5.09	115.33	109.98
23	a	406	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
23	c	508	CLA	C4A-NA-C1A	-5.09	104.36	106.68
23	c	503	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
23	c	510	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
23	C	512	CLA	C2C-C1C-NC	5.08	115.31	109.98
23	c	504	CLA	O2D-CGD-CBD	5.08	120.10	111.23
23	A	406	CLA	C3D-C4D-ND	5.07	118.23	109.99
23	b	608	CLA	C2D-C1D-ND	5.06	115.14	110.13
33	B	623	HTG	C1'-S1-C1	5.06	111.37	100.45
23	b	607	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
23	B	613	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	B	607	CLA	CHD-C4C-C3C	-5.05	117.41	124.77
23	b	603	CLA	C2C-C1C-NC	5.05	115.28	109.98
23	c	511	CLA	O2D-CGD-CBD	5.04	120.04	111.23
23	c	507	CLA	C2C-C1C-NC	5.04	115.28	109.98
33	c	523	HTG	C1'-S1-C1	5.03	111.32	100.45
23	B	609	CLA	CMB-C2B-C1B	5.03	133.08	125.42
23	c	506	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
23	C	509	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
23	b	614	CLA	C3D-C2D-C1D	-5.03	98.97	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	415	PHO	C4D-ND-C1D	-5.03	102.85	108.87
23	b	615	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
23	a	408	CLA	CMD-C2D-C1D	5.02	133.57	124.73
23	B	602	CLA	O2D-CGD-CBD	5.02	120.01	111.23
24	a	407	PHO	C3D-C4D-ND	5.02	114.14	107.71
23	b	608	CLA	CHD-C4C-C3C	-5.02	117.46	124.77
23	c	511	CLA	CHD-C4C-C3C	-5.02	117.46	124.77
23	B	604	CLA	C4A-NA-C1A	-5.02	104.39	106.68
23	b	608	CLA	O2D-CGD-CBD	5.00	119.97	111.23
23	A	404	CLA	C2C-C1C-NC	4.99	115.23	109.98
23	C	509	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
23	B	602	CLA	C2D-C1D-ND	4.98	115.06	110.13
27	f	101	SQD	O47-C7-C8	4.98	122.26	111.48
23	C	506	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
23	B	604	CLA	C2C-C1C-NC	4.98	115.21	109.98
23	C	504	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
23	d	403	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
23	D	403	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
23	B	603	CLA	C2C-C1C-NC	4.96	115.20	109.98
23	b	605	CLA	O2D-CGD-CBD	4.96	119.91	111.23
23	B	605	CLA	CMD-C2D-C1D	4.96	133.46	124.73
23	B	605	CLA	O2D-CGD-CBD	4.96	119.90	111.23
23	b	607	CLA	C2C-C1C-NC	4.96	115.19	109.98
23	B	602	CLA	C3B-C2B-C1B	-4.96	101.33	107.17
23	B	615	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
23	c	509	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
23	b	602	CLA	C3B-C2B-C1B	-4.95	101.34	107.17
29	a	415	PL9	C7-C3-C4	4.95	120.98	116.91
23	C	511	CLA	O2D-CGD-CBD	4.94	119.86	111.23
23	b	603	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
23	b	605	CLA	C3D-C4D-ND	4.93	118.01	109.99
23	c	506	CLA	C2C-C1C-NC	4.93	115.16	109.98
23	C	510	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
33	C	523	HTG	C1'-S1-C1	4.93	111.09	100.45
23	B	612	CLA	CMD-C2D-C1D	4.93	133.41	124.73
23	C	515	CLA	O2D-CGD-CBD	4.93	119.84	111.23
23	b	610	CLA	C2C-C1C-NC	4.93	115.16	109.98
23	c	513	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
23	C	507	CLA	C2C-C1C-NC	4.93	115.16	109.98
23	C	513	CLA	C3B-C2B-C1B	-4.92	101.36	107.17
23	B	616	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
23	C	512	CLA	C4A-NA-C1A	-4.92	104.44	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	403	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
23	B	616	CLA	C3D-C2D-C1D	-4.91	99.12	105.83
23	A	404	CLA	C4A-NA-C1A	-4.91	104.44	106.68
23	C	515	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
23	c	515	CLA	C2B-C1B-NB	4.91	115.42	110.33
27	D	412	SQD	O47-C7-C8	4.91	122.10	111.48
23	B	601	CLA	C4A-NA-C1A	-4.91	104.44	106.68
23	B	615	CLA	C2C-C1C-NC	4.90	115.13	109.98
23	B	610	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
23	B	601	CLA	C3D-C4D-ND	4.90	117.95	109.99
23	B	605	CLA	C3D-C4D-ND	4.90	117.95	109.99
23	D	404	CLA	O2D-CGD-CBD	4.90	119.80	111.23
23	c	511	CLA	CAC-C3C-C4C	4.90	131.16	124.79
23	C	515	CLA	C2C-C1C-NC	4.90	115.13	109.98
23	C	512	CLA	C1-C2-C3	-4.90	118.18	126.20
23	c	513	CLA	O2D-CGD-CBD	4.89	119.78	111.23
23	c	505	CLA	O2D-CGD-CBD	4.89	119.78	111.23
23	c	504	CLA	CMD-C2D-C1D	4.89	133.34	124.73
23	b	601	CLA	C2B-C1B-NB	4.89	115.39	110.33
23	a	408	CLA	O2D-CGD-CBD	4.88	119.77	111.23
23	B	609	CLA	C2C-C1C-NC	4.88	115.11	109.98
23	b	614	CLA	C3B-C2B-C1B	-4.88	101.41	107.17
25	b	617	BCR	C7-C8-C9	-4.88	119.01	126.23
23	A	406	CLA	O2D-CGD-CBD	4.88	119.77	111.23
23	b	606	CLA	C3B-C2B-C1B	-4.88	101.41	107.17
23	b	608	CLA	C2B-C1B-NB	4.88	115.39	110.33
23	b	605	CLA	C3D-C2D-C1D	-4.88	99.18	105.83
23	C	503	CLA	C3D-C2D-C1D	-4.88	99.18	105.83
23	C	513	CLA	C2B-C1B-NB	4.88	115.38	110.33
23	c	511	CLA	C4A-NA-C1A	-4.87	104.45	106.68
23	B	603	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
23	B	608	CLA	C2C-C1C-NC	4.87	115.10	109.98
23	c	515	CLA	C4A-NA-C1A	-4.87	104.46	106.68
23	C	508	CLA	C2D-C1D-ND	4.87	114.94	110.13
23	b	614	CLA	C2B-C1B-NB	4.86	115.37	110.33
23	A	408	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	C	510	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
23	C	503	CLA	C2C-C1C-NC	4.85	115.07	109.98
23	b	616	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
23	A	408	CLA	C3B-C2B-C1B	-4.85	101.46	107.17
23	C	514	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
23	C	513	CLA	C2C-C1C-NC	4.84	115.06	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	C2B-C1B-NB	4.83	115.34	110.33
23	C	505	CLA	C2C-C1C-NC	4.83	115.06	109.98
23	A	404	CLA	CAA-C2A-C3A	-4.83	99.95	113.00
23	b	616	CLA	C2B-C1B-NB	4.83	115.33	110.33
23	b	608	CLA	C3B-C2B-C1B	-4.82	101.48	107.17
23	c	511	CLA	C1-C2-C3	-4.82	118.30	126.20
23	c	510	CLA	C2B-C1B-NB	4.82	115.33	110.33
23	d	402	CLA	C4A-NA-C1A	-4.82	104.48	106.68
23	A	405	CLA	O2D-CGD-CBD	4.82	119.65	111.23
23	B	601	CLA	C2B-C1B-NB	4.82	115.32	110.33
23	A	408	CLA	C2B-C1B-NB	4.81	115.32	110.33
23	b	611	CLA	C2C-C1C-NC	4.81	115.03	109.98
23	c	515	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
23	A	408	CLA	C2C-C1C-NC	4.80	115.02	109.98
23	c	507	CLA	C3B-C2B-C1B	-4.80	101.52	107.17
23	B	608	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	B	608	CLA	C4A-NA-C1A	-4.79	104.49	106.68
23	b	614	CLA	C2C-C1C-NC	4.79	115.01	109.98
23	b	610	CLA	C2B-C1B-NB	4.78	115.28	110.33
23	B	611	CLA	O2D-CGD-CBD	4.78	119.58	111.23
23	c	506	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
23	c	512	CLA	O2D-CGD-CBD	4.77	119.57	111.23
23	B	607	CLA	O2D-CGD-CBD	4.77	119.57	111.23
23	b	602	CLA	C2C-C1C-NC	4.77	114.99	109.98
23	b	612	CLA	C3B-C4B-NB	4.76	114.78	110.53
23	a	404	CLA	C2B-C1B-NB	4.76	115.26	110.33
23	C	509	CLA	C2C-C1C-NC	4.76	114.98	109.98
23	c	507	CLA	C2B-C1B-NB	4.75	115.25	110.33
29	a	415	PL9	C15-C14-C16	4.74	123.46	115.23
27	B	620	SQD	O6-C1-C2	4.74	115.48	108.27
23	B	611	CLA	C2C-C1C-NC	4.74	114.96	109.98
23	B	609	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	d	402	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
23	a	408	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	D	403	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	c	511	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
23	c	504	CLA	C3D-C4D-ND	4.74	117.69	109.99
23	C	504	CLA	O2D-CGD-CBD	4.74	119.51	111.23
23	b	609	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
29	a	415	PL9	C37-C38-C39	-4.73	116.80	127.62
23	C	509	CLA	C4A-NA-C1A	-4.73	104.52	106.68
23	a	406	CLA	C4A-NA-C1A	-4.73	104.52	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	CLA	C3D-C4D-ND	4.73	117.67	109.99
23	D	404	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
23	c	508	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
23	D	403	CLA	C3D-C4D-ND	4.73	117.67	109.99
23	c	515	CLA	C3B-C2B-C1B	-4.72	101.60	107.17
23	a	406	CLA	C3D-C4D-ND	4.72	117.67	109.99
23	d	403	CLA	C3D-C4D-ND	4.72	117.67	109.99
23	B	608	CLA	O2D-CGD-CBD	4.72	119.49	111.23
23	c	504	CLA	C2C-C1C-NC	4.72	114.94	109.98
23	C	504	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
23	b	603	CLA	C4A-NA-C1A	-4.72	104.53	106.68
23	b	609	CLA	O2D-CGD-CBD	4.72	119.48	111.23
23	C	514	CLA	C2B-C1B-NB	4.71	115.21	110.33
23	a	404	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
23	C	508	CLA	O2D-CGD-CBD	4.71	119.46	111.23
23	A	405	CLA	C1C-C2C-C3C	-4.70	102.03	106.98
23	C	513	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	C	512	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
23	b	601	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
23	B	603	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
23	d	403	CLA	CHD-C1D-ND	-4.70	118.19	124.80
23	B	616	CLA	C2C-C1C-NC	4.69	114.91	109.98
23	b	607	CLA	C4A-NA-C1A	-4.69	104.54	106.68
23	C	505	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
23	c	504	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	b	608	CLA	C2C-C1C-NC	4.69	114.91	109.98
23	B	607	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
23	a	404	CLA	C4A-NA-C1A	-4.69	104.54	106.68
23	c	513	CLA	C2C-C1C-NC	4.68	114.90	109.98
25	Y	101	BCR	C16-C17-C18	-4.67	120.73	127.28
24	A	415	PHO	C1-C2-C3	-4.66	118.56	126.20
23	B	612	CLA	O2D-CGD-O1D	-4.66	114.78	123.85
23	b	606	CLA	O2D-CGD-O1D	-4.66	114.78	123.85
33	h	101	HTG	O5-C5-C4	4.65	118.09	109.70
25	C	516	BCR	C7-C8-C9	-4.65	119.35	126.23
23	b	604	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
23	B	616	CLA	C3C-C4C-NC	4.65	116.38	110.43
23	C	508	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
23	a	404	CLA	C1D-CHD-C4C	-4.64	116.15	126.02
23	c	503	CLA	C2C-C1C-NC	4.64	114.86	109.98
23	b	612	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	C	504	CLA	CMB-C2B-C1B	4.64	132.48	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
23	b	601	CLA	C3D-C4D-ND	4.64	117.53	109.99
23	C	510	CLA	C2B-C1B-NB	4.64	115.13	110.33
23	D	403	CLA	CHD-C1D-ND	-4.63	118.28	124.80
23	a	404	CLA	C3B-C4B-NB	4.63	114.67	110.53
23	B	615	CLA	C3C-C4C-NC	4.63	116.37	110.43
23	c	509	CLA	CHD-C1D-ND	-4.63	118.28	124.80
23	c	506	CLA	C3D-C4D-ND	4.63	117.51	109.99
23	b	603	CLA	C1D-CHD-C4C	-4.62	116.19	126.02
23	A	406	CLA	C2B-C1B-NB	4.62	115.12	110.33
23	C	515	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
23	c	505	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
23	A	408	CLA	C1-C2-C3	-4.61	118.64	126.20
23	c	513	CLA	C3D-C4D-ND	4.61	117.48	109.99
23	C	511	CLA	C4A-NA-C1A	-4.61	104.58	106.68
23	c	511	CLA	C2B-C1B-NB	4.60	115.10	110.33
23	c	506	CLA	CHD-C1D-ND	-4.60	118.33	124.80
23	b	606	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
23	D	404	CLA	C4A-NA-C1A	-4.60	104.58	106.68
23	C	505	CLA	C2B-C1B-NB	4.60	115.09	110.33
32	Z	101	LMG	O7-C10-C11	4.60	121.43	111.48
23	B	614	CLA	CHD-C1D-ND	-4.60	118.33	124.80
23	B	603	CLA	C3C-C4C-NC	4.59	116.31	110.43
23	A	406	CLA	C2C-C1C-NC	4.59	114.80	109.98
23	a	405	CLA	C1C-C2C-C3C	-4.58	102.16	106.98
23	B	615	CLA	C4A-NA-C1A	-4.57	104.59	106.68
23	b	602	CLA	C3D-C4D-ND	4.57	117.42	109.99
23	b	612	CLA	C3B-C2B-C1B	-4.57	101.79	107.17
23	b	612	CLA	C3C-C4C-NC	4.57	116.28	110.43
23	C	508	CLA	C3D-C4D-ND	4.56	117.40	109.99
25	C	517	BCR	C7-C8-C9	-4.56	119.49	126.23
23	C	514	CLA	C2C-C1C-NC	4.56	114.77	109.98
23	C	508	CLA	CHD-C4C-C3C	-4.56	118.13	124.77
23	b	611	CLA	O2D-CGD-CBD	4.56	119.19	111.23
23	C	511	CLA	C2B-C1B-NB	4.55	115.05	110.33
23	c	512	CLA	C4A-NA-C1A	-4.55	104.60	106.68
23	b	605	CLA	C3B-C2B-C1B	-4.55	101.81	107.17
23	b	612	CLA	C1-C2-C3	-4.55	118.75	126.20
23	C	508	CLA	CHD-C1D-ND	-4.55	118.40	124.80
23	b	605	CLA	C2B-C1B-NB	4.55	115.04	110.33
23	c	514	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
23	B	610	CLA	C2C-C1C-NC	4.54	114.75	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	C3B-C2B-C1B	-4.54	101.82	107.17
23	a	408	CLA	C3C-C4C-NC	4.54	116.24	110.43
23	b	613	CLA	C2B-C1B-NB	4.54	115.03	110.33
23	D	403	CLA	C1C-C2C-C3C	-4.54	102.21	106.98
23	b	601	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	C	503	CLA	C2B-C1B-NB	4.53	115.02	110.33
23	b	607	CLA	O2D-CGD-CBD	4.53	119.14	111.23
23	C	512	CLA	C2B-C1B-NB	4.52	115.02	110.33
23	C	507	CLA	C3D-C4D-ND	4.52	117.34	109.99
23	b	605	CLA	CHD-C1D-ND	-4.52	118.44	124.80
23	B	614	CLA	C1C-C2C-C3C	-4.52	102.22	106.98
25	b	619	BCR	C38-C26-C25	-4.52	119.55	124.48
23	C	508	CLA	C2B-C1B-NB	4.52	115.01	110.33
23	B	605	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
23	b	611	CLA	C3B-C2B-C1B	-4.51	101.85	107.17
23	b	603	CLA	C3D-C4D-ND	4.51	117.31	109.99
23	c	515	CLA	C2C-C1C-NC	4.51	114.72	109.98
23	b	609	CLA	C3B-C2B-C1B	-4.50	101.86	107.17
23	C	514	CLA	C3D-C2D-C1D	-4.50	99.68	105.83
23	B	610	CLA	CAC-C3C-C4C	4.50	130.65	124.79
23	C	507	CLA	C3B-C2B-C1B	-4.50	101.86	107.17
23	B	608	CLA	C2B-C1B-NB	4.50	114.99	110.33
27	B	620	SQD	O47-C7-C8	4.50	121.22	111.48
33	h	101	HTG	C1'-S1-C1	4.50	110.17	100.45
23	c	507	CLA	C3D-C4D-ND	4.49	117.29	109.99
23	B	606	CLA	CHD-C1D-ND	-4.49	118.48	124.80
23	b	603	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
23	B	609	CLA	C3D-C4D-ND	4.49	117.28	109.99
23	B	612	CLA	C3B-C2B-C1B	-4.49	101.88	107.17
23	c	505	CLA	CAC-C3C-C4C	4.49	130.63	124.79
23	C	506	CLA	C3B-C2B-C1B	-4.48	101.88	107.17
23	d	402	CLA	C1C-C2C-C3C	-4.48	102.26	106.98
33	D	411	HTG	C1'-S1-C1	4.48	110.12	100.45
23	a	404	CLA	C3D-C4D-ND	4.48	117.27	109.99
23	c	511	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	b	610	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	C	512	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	c	503	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
23	a	405	CLA	C4A-NA-C1A	-4.47	104.64	106.68
23	B	613	CLA	C3C-C4C-NC	4.47	116.16	110.43
23	a	405	CLA	C1D-CHD-C4C	-4.47	116.52	126.02
33	h	101	HTG	C1-O5-C5	4.47	120.58	112.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	CLA	C2B-C1B-NB	4.47	114.96	110.33
23	b	606	CLA	CHD-C1D-ND	-4.47	118.52	124.80
23	c	514	CLA	C2C-C1C-NC	4.47	114.67	109.98
23	B	604	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
23	C	510	CLA	C3C-C4C-NC	4.45	116.14	110.43
23	C	506	CLA	C1C-C2C-C3C	-4.45	102.30	106.98
23	b	607	CLA	C3B-C4B-NB	4.45	114.51	110.53
23	C	515	CLA	C3D-C4D-ND	4.45	117.22	109.99
23	a	408	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
23	c	506	CLA	C2B-C1B-NB	4.45	114.94	110.33
23	c	504	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
24	A	415	PHO	C3D-C4D-ND	4.45	113.41	107.71
38	E	103	HEC	CHC-C4B-NB	4.44	129.29	124.45
23	c	508	CLA	C3D-C4D-ND	4.44	117.21	109.99
23	B	605	CLA	C3C-C4C-NC	4.44	116.12	110.43
38	V	201	HEC	CBC-CAC-C3C	-4.44	118.55	127.43
23	B	602	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	b	611	CLA	CHD-C1D-ND	-4.44	118.56	124.80
23	b	601	CLA	C2C-C1C-NC	4.43	114.64	109.98
23	a	404	CLA	C1C-C2C-C3C	-4.43	102.32	106.98
23	B	609	CLA	C3C-C4C-NC	4.43	116.10	110.43
25	t	102	BCR	C33-C5-C6	-4.43	119.65	124.48
23	c	503	CLA	CHD-C1D-ND	-4.43	118.57	124.80
23	C	515	CLA	C2B-C1B-NB	4.42	114.91	110.33
23	b	614	CLA	C3D-C4D-ND	4.42	117.17	109.99
23	b	616	CLA	C1D-CHD-C4C	-4.42	116.62	126.02
23	b	615	CLA	C2B-C1B-NB	4.42	114.91	110.33
23	a	404	CLA	CAA-C2A-C3A	-4.42	101.07	113.00
23	c	505	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
23	C	505	CLA	C3D-C4D-ND	4.41	117.15	109.99
23	C	504	CLA	C2C-C1C-NC	4.41	114.61	109.98
23	B	609	CLA	C2B-C1B-NB	4.41	114.90	110.33
23	B	604	CLA	C1D-CHD-C4C	-4.40	116.66	126.02
23	B	603	CLA	C2B-C1B-NB	4.40	114.89	110.33
23	B	610	CLA	C3B-C2B-C1B	-4.40	101.98	107.17
23	b	613	CLA	C3C-C4C-NC	4.40	116.06	110.43
23	B	614	CLA	C2B-C1B-NB	4.40	114.89	110.33
23	C	511	CLA	C3D-C4D-ND	4.40	117.13	109.99
23	B	601	CLA	C2C-C1C-NC	4.40	114.60	109.98
38	e	102	HEC	CHC-C4B-NB	4.40	129.24	124.45
23	a	406	CLA	O2D-CGD-CBD	4.39	118.91	111.23
23	c	510	CLA	C3B-C4B-NB	4.39	114.45	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	C3D-C4D-ND	4.39	117.12	109.99
23	B	607	CLA	C3D-C4D-ND	4.39	117.12	109.99
23	c	515	CLA	CHD-C1D-ND	-4.39	118.63	124.80
23	C	506	CLA	C3C-C4C-NC	4.39	116.05	110.43
23	B	609	CLA	O2D-CGD-CBD	4.39	118.90	111.23
23	a	406	CLA	C3B-C2B-C1B	-4.38	102.00	107.17
23	A	405	CLA	C3D-C4D-ND	4.38	117.11	109.99
23	B	606	CLA	C3B-C2B-C1B	-4.38	102.00	107.17
23	b	610	CLA	C4A-NA-C1A	-4.38	104.68	106.68
23	c	505	CLA	C3C-C4C-NC	4.38	116.04	110.43
29	d	405	PL9	C42-C43-C44	-4.38	117.61	127.62
23	B	604	CLA	C3B-C2B-C1B	-4.38	102.01	107.17
23	C	505	CLA	CHD-C1D-ND	-4.37	118.65	124.80
23	D	404	CLA	C2C-C1C-NC	4.37	114.57	109.98
23	B	616	CLA	C2B-C1B-NB	4.37	114.86	110.33
23	C	503	CLA	C3D-C4D-ND	4.37	117.08	109.99
23	B	603	CLA	C3D-C4D-ND	4.37	117.08	109.99
23	B	602	CLA	CMC-C2C-C1C	4.36	131.85	125.03
23	C	504	CLA	C3D-C4D-ND	4.36	117.08	109.99
23	C	512	CLA	C1C-C2C-C3C	-4.36	102.39	106.98
23	c	510	CLA	C1C-C2C-C3C	-4.36	102.39	106.98
23	C	513	CLA	C3B-C4B-NB	4.36	114.42	110.53
23	c	507	CLA	C3C-C4C-NC	4.36	116.01	110.43
23	a	406	CLA	C2B-C1B-NB	4.35	114.84	110.33
23	B	612	CLA	C2C-C1C-NC	4.35	114.55	109.98
32	C	522	LMG	O6-C5-C4	4.35	117.53	109.70
23	B	613	CLA	O2D-CGD-CBD	4.35	118.83	111.23
23	c	503	CLA	C3D-C4D-ND	4.34	117.04	109.99
23	B	611	CLA	C3B-C2B-C1B	-4.34	102.05	107.17
23	C	510	CLA	C4A-NA-C1A	-4.34	104.70	106.68
27	a	410	SQD	O47-C7-C8	4.34	120.86	111.48
23	b	616	CLA	C2C-C1C-NC	4.34	114.54	109.98
23	a	408	CLA	C3D-C4D-ND	4.34	117.03	109.99
23	c	503	CLA	C2B-C1B-NB	4.33	114.82	110.33
23	a	406	CLA	C2C-C1C-NC	4.33	114.53	109.98
23	C	512	CLA	C3D-C4D-ND	4.33	117.02	109.99
23	c	511	CLA	C3B-C4B-NB	4.32	114.39	110.53
23	C	513	CLA	C3D-C4D-ND	4.32	117.02	109.99
23	A	405	CLA	C2B-C1B-NB	4.32	114.81	110.33
23	C	511	CLA	C1-C2-C3	-4.32	119.11	126.20
23	C	504	CLA	C2B-C1B-NB	4.32	114.81	110.33
23	b	605	CLA	C2C-C1C-NC	4.32	114.52	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	CLA	CHD-C1D-ND	-4.32	118.73	124.80
23	b	609	CLA	CHD-C1D-ND	-4.31	118.73	124.80
23	B	601	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
32	c	501	LMG	O7-C10-C11	4.31	120.81	111.48
23	b	610	CLA	C3D-C4D-ND	4.31	116.99	109.99
25	C	516	BCR	C33-C5-C6	-4.31	119.78	124.48
23	b	609	CLA	C2B-C1B-NB	4.31	114.79	110.33
23	B	613	CLA	C3B-C4B-NB	4.30	114.37	110.53
23	c	505	CLA	C3D-C4D-ND	4.30	116.98	109.99
23	D	403	CLA	C1-C2-C3	-4.29	119.16	126.20
23	b	606	CLA	C3D-C4D-ND	4.29	116.96	109.99
23	b	608	CLA	C3D-C4D-ND	4.29	116.96	109.99
23	C	504	CLA	C3C-C4C-NC	4.29	115.93	110.43
23	b	604	CLA	C1C-C2C-C3C	-4.29	102.47	106.98
23	B	601	CLA	CHD-C1D-ND	-4.29	118.77	124.80
24	a	417	PHO	C4-C3-C5	4.29	122.67	115.23
23	A	406	CLA	CHD-C1D-ND	-4.28	118.78	124.80
23	b	611	CLA	C2B-C1B-NB	4.28	114.77	110.33
23	A	404	CLA	C3B-C4B-NB	4.28	114.35	110.53
23	b	615	CLA	C3B-C2B-C1B	-4.28	102.12	107.17
23	B	610	CLA	C2B-C1B-NB	4.28	114.76	110.33
23	b	601	CLA	CHD-C1D-ND	-4.28	118.78	124.80
23	c	514	CLA	C3D-C4D-ND	4.27	116.93	109.99
23	c	508	CLA	C3B-C2B-C1B	-4.27	102.14	107.17
23	c	515	CLA	C3D-C4D-ND	4.27	116.92	109.99
23	c	515	CLA	O2D-CGD-CBD	4.27	118.69	111.23
23	B	611	CLA	C3D-C4D-ND	4.26	116.92	109.99
23	D	404	CLA	C3D-C4D-ND	4.26	116.91	109.99
23	b	615	CLA	C3D-C4D-ND	4.26	116.91	109.99
23	C	503	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
23	B	608	CLA	CHD-C1D-ND	-4.26	118.81	124.80
23	C	514	CLA	C1D-CHD-C4C	-4.25	116.98	126.02
23	b	613	CLA	C1-C2-C3	-4.25	119.23	126.20
23	B	615	CLA	C1D-CHD-C4C	-4.25	116.98	126.02
23	B	606	CLA	C2B-C1B-NB	4.25	114.73	110.33
23	a	406	CLA	CHD-C1D-ND	-4.25	118.83	124.80
23	b	611	CLA	C3D-C4D-ND	4.24	116.89	109.99
23	a	408	CLA	C2C-C1C-NC	4.24	114.44	109.98
23	A	404	CLA	O2D-CGD-CBD	4.24	118.65	111.23
23	b	613	CLA	C3B-C4B-NB	4.24	114.32	110.53
23	B	613	CLA	C3B-C2B-C1B	-4.24	102.17	107.17
23	B	607	CLA	C4A-NA-C1A	-4.24	104.75	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	C1D-CHD-C4C	-4.23	117.02	126.02
23	d	402	CLA	C3D-C4D-ND	4.23	116.86	109.99
23	b	607	CLA	C3B-C2B-C1B	-4.23	102.19	107.17
23	b	609	CLA	C2C-C1C-NC	4.23	114.42	109.98
23	c	503	CLA	O2D-CGD-O1D	-4.23	115.62	123.85
23	a	405	CLA	C3B-C2B-C1B	-4.22	102.19	107.17
23	c	513	CLA	C3B-C2B-C1B	-4.22	102.19	107.17
23	a	404	CLA	O2D-CGD-CBD	4.22	118.61	111.23
23	c	512	CLA	C1C-C2C-C3C	-4.22	102.54	106.98
23	C	510	CLA	C1D-CHD-C4C	-4.22	117.05	126.02
23	B	604	CLA	C2B-C1B-NB	4.22	114.70	110.33
23	b	603	CLA	C2B-C1B-NB	4.22	114.70	110.33
23	D	404	CLA	C2B-C1B-NB	4.22	114.70	110.33
23	d	403	CLA	C2C-C1C-NC	4.21	114.41	109.98
23	A	404	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
23	c	511	CLA	C3D-C4D-ND	4.21	116.83	109.99
23	B	611	CLA	C3B-C4B-NB	4.21	114.29	110.53
23	C	515	CLA	C3C-C4C-NC	4.21	115.82	110.43
23	A	406	CLA	C3D-C2D-C1D	-4.21	100.09	105.83
23	c	508	CLA	C1C-C2C-C3C	-4.21	102.56	106.98
23	b	608	CLA	CHD-C1D-ND	-4.20	118.89	124.80
23	B	604	CLA	C3C-C4C-NC	4.20	115.81	110.43
23	B	611	CLA	C2B-C1B-NB	4.20	114.68	110.33
23	C	511	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
23	b	614	CLA	CHD-C1D-ND	-4.20	118.89	124.80
23	B	612	CLA	C3D-C4D-ND	4.20	116.81	109.99
23	a	405	CLA	C3D-C4D-ND	4.20	116.81	109.99
23	c	512	CLA	C3D-C4D-ND	4.19	116.80	109.99
23	D	403	CLA	C2B-C1B-NB	4.19	114.67	110.33
23	a	405	CLA	C2B-C1B-NB	4.19	114.67	110.33
23	C	506	CLA	C3D-C4D-ND	4.19	116.79	109.99
23	B	608	CLA	C3D-C4D-ND	4.19	116.79	109.99
23	A	405	CLA	CHD-C1D-ND	-4.18	118.91	124.80
23	b	604	CLA	C3B-C4B-NB	4.18	114.27	110.53
23	B	607	CLA	C1C-C2C-C3C	-4.18	102.58	106.98
23	B	606	CLA	C3B-C4B-NB	4.18	114.26	110.53
23	B	609	CLA	CHD-C1D-ND	-4.18	118.92	124.80
23	B	610	CLA	C3D-C4D-ND	4.18	116.78	109.99
23	D	404	CLA	CAC-C3C-C4C	4.18	130.22	124.79
23	c	505	CLA	C1D-CHD-C4C	-4.18	117.14	126.02
23	b	610	CLA	C3C-C4C-NC	4.17	115.78	110.43
23	c	509	CLA	C2C-C1C-NC	4.17	114.36	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	CHD-C1D-ND	-4.17	118.93	124.80
23	b	602	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
23	B	609	CLA	C3B-C2B-C1B	-4.17	102.25	107.17
23	A	408	CLA	O2D-CGD-CBD	4.17	118.52	111.23
23	B	611	CLA	C1D-CHD-C4C	-4.17	117.16	126.02
23	B	612	CLA	CMC-C2C-C1C	4.17	131.54	125.03
23	c	504	CLA	C1C-C2C-C3C	-4.17	102.60	106.98
23	c	508	CLA	C2B-C1B-NB	4.16	114.64	110.33
23	b	606	CLA	C2C-C1C-NC	4.16	114.36	109.98
32	C	522	LMG	O7-C10-C11	4.16	120.48	111.48
23	B	613	CLA	C1C-C2C-C3C	-4.16	102.61	106.98
23	c	512	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
23	d	402	CLA	C3D-C2D-C1D	-4.15	100.16	105.83
23	c	510	CLA	C1-C2-C3	-4.15	119.39	126.20
23	C	508	CLA	C3D-C2D-C1D	-4.15	100.16	105.83
32	B	621	LMG	O7-C10-C11	4.15	120.47	111.48
23	c	512	CLA	C3B-C2B-C1B	-4.15	102.28	107.17
23	C	513	CLA	CHD-C1D-ND	-4.15	118.96	124.80
23	d	402	CLA	C2B-C1B-NB	4.15	114.63	110.33
23	B	607	CLA	C3B-C2B-C1B	-4.15	102.28	107.17
23	c	510	CLA	C3D-C4D-ND	4.15	116.73	109.99
23	B	611	CLA	C3C-C4C-NC	4.15	115.74	110.43
23	b	608	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
23	A	408	CLA	C3D-C4D-ND	4.15	116.73	109.99
23	b	604	CLA	C3C-C4C-NC	4.15	115.74	110.43
27	a	412	SQD	O47-C7-C8	4.14	120.44	111.48
23	c	509	CLA	CMC-C2C-C1C	4.14	131.51	125.03
29	a	415	PL9	C27-C28-C29	-4.14	118.14	127.62
23	B	615	CLA	C3D-C4D-ND	4.14	116.72	109.99
23	B	602	CLA	C3D-C4D-ND	4.14	116.71	109.99
23	C	505	CLA	C1D-CHD-C4C	-4.14	117.23	126.02
23	c	510	CLA	C1D-CHD-C4C	-4.14	117.23	126.02
23	B	613	CLA	CAC-C3C-C4C	4.13	130.17	124.79
23	b	610	CLA	C1D-CHD-C4C	-4.13	117.23	126.02
23	c	508	CLA	CHD-C1D-ND	-4.13	118.99	124.80
23	a	408	CLA	C2B-C1B-NB	4.13	114.61	110.33
23	c	505	CLA	C2B-C1B-NB	4.13	114.61	110.33
23	B	610	CLA	CHD-C1D-ND	-4.13	118.99	124.80
23	c	513	CLA	C3B-C4B-NB	4.13	114.22	110.53
23	A	406	CLA	C3B-C2B-C1B	-4.12	102.31	107.17
23	C	508	CLA	CAC-C3C-C4C	4.12	130.15	124.79
23	c	508	CLA	O2D-CGD-CBD	4.12	118.43	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	515	CLA	C1D-CHD-C4C	-4.12	117.27	126.02
23	C	510	CLA	C3D-C4D-ND	4.12	116.68	109.99
29	A	413	PL9	C15-C14-C16	4.11	122.36	115.23
23	C	510	CLA	C3B-C4B-NB	4.11	114.20	110.53
23	d	402	CLA	C3B-C4B-NB	4.10	114.19	110.53
25	b	617	BCR	C33-C5-C6	-4.10	120.01	124.48
23	b	612	CLA	C2B-C1B-NB	4.10	114.58	110.33
23	b	607	CLA	O2D-CGD-O1D	-4.10	115.86	123.85
23	B	615	CLA	CMB-C2B-C1B	4.09	131.64	125.42
34	M	103	LMT	O5'-C5'-C4'	4.08	118.16	109.72
23	B	613	CLA	C3D-C4D-ND	4.08	116.62	109.99
23	c	512	CLA	C1D-CHD-C4C	-4.08	117.36	126.02
23	D	404	CLA	C3C-C4C-NC	4.08	115.65	110.43
23	C	508	CLA	C1C-C2C-C3C	-4.07	102.69	106.98
23	B	613	CLA	C2B-C1B-NB	4.07	114.55	110.33
23	B	614	CLA	C3D-C4D-ND	4.07	116.61	109.99
23	C	503	CLA	C1C-C2C-C3C	-4.07	102.70	106.98
23	B	607	CLA	CHD-C1D-ND	-4.06	119.08	124.80
23	b	612	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
23	b	603	CLA	C3C-C4C-NC	4.06	115.63	110.43
23	B	603	CLA	CHD-C1D-ND	-4.06	119.09	124.80
23	B	602	CLA	CAC-C3C-C4C	4.06	130.07	124.79
34	C	526	LMT	C1'-O5'-C5'	4.06	121.64	113.72
23	C	503	CLA	CHD-C1D-ND	-4.06	119.09	124.80
23	c	509	CLA	C3D-C4D-ND	4.05	116.58	109.99
23	b	607	CLA	C3D-C4D-ND	4.05	116.58	109.99
23	b	613	CLA	C1C-C2C-C3C	-4.05	102.72	106.98
23	C	506	CLA	C2B-C1B-NB	4.05	114.52	110.33
23	c	504	CLA	C2B-C1B-NB	4.05	114.52	110.33
23	a	404	CLA	CHD-C1D-ND	-4.04	119.11	124.80
23	b	605	CLA	C1D-CHD-C4C	-4.04	117.42	126.02
23	B	616	CLA	C3D-C4D-ND	4.04	116.56	109.99
23	c	509	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
23	C	514	CLA	C3C-C4C-NC	4.04	115.61	110.43
29	a	415	PL9	C7-C3-C2	-4.04	118.63	123.39
38	e	102	HEC	CHD-C4C-NC	4.04	128.85	124.45
23	C	507	CLA	C2B-C1B-NB	4.04	114.51	110.33
23	a	408	CLA	C1D-CHD-C4C	-4.03	117.45	126.02
23	A	405	CLA	CBC-CAC-C3C	-4.03	101.49	112.42
23	a	406	CLA	C3C-C4C-NC	4.03	115.59	110.43
23	b	607	CLA	CAA-C2A-C3A	-4.03	102.11	113.00
23	B	606	CLA	C1D-CHD-C4C	-4.02	117.47	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
23	B	611	CLA	C4A-NA-C1A	-4.02	104.84	106.68
23	C	509	CLA	CHD-C1D-ND	-4.02	119.14	124.80
23	D	404	CLA	C1D-CHD-C4C	-4.02	117.48	126.02
23	B	605	CLA	C2C-C1C-NC	4.02	114.20	109.98
23	D	403	CLA	O2D-CGD-CBD	4.01	118.25	111.23
35	C	519	DGD	O2G-C1B-C2B	4.01	120.16	111.48
23	B	611	CLA	CMC-C2C-C1C	4.01	131.31	125.03
29	A	413	PL9	C7-C3-C4	4.01	120.22	116.91
23	b	601	CLA	C1D-CHD-C4C	-4.01	117.50	126.02
23	C	514	CLA	C3D-C4D-ND	4.00	116.50	109.99
23	D	404	CLA	C3B-C2B-C1B	-4.00	102.45	107.17
23	b	610	CLA	CMB-C2B-C1B	4.00	131.51	125.42
35	C	520	DGD	O2G-C1B-C2B	4.00	120.13	111.48
32	C	521	LMG	O7-C10-C11	4.00	120.13	111.48
23	B	602	CLA	CHD-C1D-ND	-4.00	119.18	124.80
38	V	201	HEC	C4D-ND-C1D	4.00	112.33	105.82
23	B	615	CLA	CED-O2D-CGD	4.00	124.98	115.92
23	C	507	CLA	CMB-C2B-C1B	3.99	131.50	125.42
33	B	622	HTG	O5-C1-C2	3.99	115.82	110.32
23	B	602	CLA	CAA-C2A-C3A	-3.99	102.23	113.00
23	B	612	CLA	C1-C2-C3	-3.98	119.67	126.20
23	c	504	CLA	CHD-C1D-ND	-3.98	119.20	124.80
23	A	408	CLA	CHD-C1D-ND	-3.98	119.20	124.80
23	b	614	CLA	C4A-NA-C1A	-3.98	104.86	106.68
23	C	511	CLA	C1C-C2C-C3C	-3.98	102.80	106.98
31	E	101	LHG	O7-C7-C8	3.98	120.08	111.48
23	D	403	CLA	C3B-C4B-NB	3.98	114.08	110.53
23	B	606	CLA	C1C-C2C-C3C	-3.98	102.80	106.98
23	B	602	CLA	C2C-C1C-NC	3.97	114.16	109.98
25	T	101	BCR	C15-C16-C17	-3.97	115.39	123.52
23	B	615	CLA	O2D-CGD-CBD	3.97	118.17	111.23
23	b	603	CLA	CAA-C2A-C3A	-3.97	102.27	113.00
23	C	504	CLA	CHD-C1D-ND	-3.97	119.22	124.80
23	c	503	CLA	C1C-C2C-C3C	-3.96	102.81	106.98
23	b	611	CLA	C3C-C4C-NC	3.96	115.51	110.43
23	B	614	CLA	C3C-C4C-NC	3.96	115.50	110.43
23	b	607	CLA	CHD-C1D-ND	-3.96	119.23	124.80
23	c	512	CLA	C2B-C1B-NB	3.96	114.43	110.33
23	b	609	CLA	C3C-C4C-NC	3.96	115.50	110.43
23	b	607	CLA	C1C-C2C-C3C	-3.96	102.82	106.98
23	b	604	CLA	C3B-C2B-C1B	-3.96	102.51	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	O2D-CGD-O1D	-3.95	116.15	123.85
23	c	512	CLA	C3B-C4B-NB	3.95	114.06	110.53
23	c	508	CLA	C1D-CHD-C4C	-3.95	117.63	126.02
23	b	611	CLA	C3B-C4B-NB	3.95	114.05	110.53
23	B	607	CLA	CMB-C2B-C1B	3.95	131.43	125.42
23	C	509	CLA	C1D-CHD-C4C	-3.94	117.64	126.02
23	C	509	CLA	C3C-C4C-NC	3.94	115.48	110.43
23	b	616	CLA	C3C-C4C-NC	3.94	115.48	110.43
23	b	616	CLA	C3D-C4D-ND	3.94	116.39	109.99
23	b	606	CLA	C1D-CHD-C4C	-3.94	117.65	126.02
23	c	514	CLA	C1D-CHD-C4C	-3.93	117.66	126.02
23	b	612	CLA	C1D-CHD-C4C	-3.93	117.66	126.02
23	C	506	CLA	C3B-C4B-NB	3.93	114.04	110.53
23	C	515	CLA	C3B-C4B-NB	3.93	114.04	110.53
23	b	612	CLA	O2D-CGD-O1D	-3.93	116.20	123.85
23	c	506	CLA	C3B-C4B-NB	3.93	114.03	110.53
27	a	410	SQD	C1-C2-C3	-3.93	101.75	110.01
23	a	405	CLA	CMB-C2B-C1B	3.93	131.40	125.42
23	C	503	CLA	C3C-C4C-NC	3.92	115.45	110.43
23	B	612	CLA	CAC-C3C-C4C	3.92	129.89	124.79
23	C	507	CLA	C3C-C4C-NC	3.92	115.45	110.43
23	A	405	CLA	C3B-C2B-C1B	-3.92	102.55	107.17
23	c	513	CLA	C3C-C4C-NC	3.92	115.45	110.43
32	c	522	LMG	O7-C10-C11	3.91	119.95	111.48
23	c	506	CLA	C4A-NA-C1A	-3.91	104.89	106.68
23	B	611	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
23	b	615	CLA	CHD-C1D-ND	-3.91	119.30	124.80
23	C	511	CLA	C3B-C4B-NB	3.91	114.02	110.53
33	b	622	HTG	C1-O5-C5	3.90	119.56	112.56
23	b	610	CLA	O2A-CGA-CBA	3.90	123.73	111.83
23	b	607	CLA	C3C-C4C-NC	3.90	115.43	110.43
23	D	404	CLA	CMB-C2B-C1B	3.90	131.36	125.42
23	b	602	CLA	CHD-C1D-ND	-3.90	119.31	124.80
23	C	510	CLA	O2D-CGD-O1D	-3.90	116.26	123.85
23	C	506	CLA	CHD-C1D-ND	-3.90	119.32	124.80
23	c	505	CLA	CMB-C2B-C1B	3.90	131.35	125.42
31	d	408	LHG	O7-C7-C8	3.89	119.91	111.48
23	C	508	CLA	C3B-C4B-NB	3.89	114.01	110.53
25	y	101	BCR	C15-C14-C13	-3.89	121.82	127.28
23	c	513	CLA	C1-C2-C3	-3.89	119.82	126.20
23	d	402	CLA	O2D-CGD-CBD	3.89	118.03	111.23
23	B	613	CLA	CMC-C2C-C1C	3.89	131.11	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Z	101	LMG	C1-C2-C3	3.88	118.18	110.01
23	b	604	CLA	C2B-C1B-NB	3.88	114.35	110.33
23	b	602	CLA	CAA-C2A-C3A	-3.88	102.51	113.00
23	c	503	CLA	C4A-NA-C1A	-3.88	104.91	106.68
23	b	613	CLA	C3D-C4D-ND	3.88	116.29	109.99
23	C	513	CLA	CAC-C3C-C4C	3.88	129.84	124.79
23	b	608	CLA	C1-C2-C3	-3.88	119.84	126.20
23	B	614	CLA	C3B-C4B-NB	3.88	113.99	110.53
23	b	602	CLA	C1-C2-C3	-3.87	119.86	126.20
24	A	407	PHO	CBC-CAC-C3C	-3.87	107.33	112.87
23	C	511	CLA	C3C-C4C-NC	3.87	115.39	110.43
23	B	610	CLA	O2D-CGD-O1D	-3.87	116.32	123.85
23	B	607	CLA	C3B-C4B-NB	3.86	113.98	110.53
23	A	406	CLA	CMB-C2B-C1B	3.86	131.30	125.42
23	b	606	CLA	C3C-C4C-NC	3.86	115.37	110.43
23	c	515	CLA	C3C-C4C-NC	3.85	115.37	110.43
32	C	502	LMG	O7-C10-C11	3.85	119.82	111.48
23	c	515	CLA	C1D-CHD-C4C	-3.85	117.83	126.02
23	b	606	CLA	C4-C3-C5	3.85	121.91	115.23
25	B	618	BCR	C29-C30-C25	3.85	116.03	110.44
23	B	611	CLA	CHD-C1D-ND	-3.85	119.38	124.80
23	c	506	CLA	CAC-C3C-C4C	3.85	129.80	124.79
23	B	602	CLA	C3C-C4C-NC	3.85	115.36	110.43
23	d	402	CLA	C3C-C4C-NC	3.85	115.36	110.43
23	A	404	CLA	C1C-C2C-C3C	-3.84	102.94	106.98
23	b	615	CLA	C1D-CHD-C4C	-3.84	117.85	126.02
23	b	608	CLA	C1C-C2C-C3C	-3.84	102.94	106.98
23	b	614	CLA	C1C-C2C-C3C	-3.84	102.94	106.98
25	D	405	BCR	C38-C26-C25	-3.84	120.30	124.48
23	b	615	CLA	CMB-C2B-C1B	3.84	131.26	125.42
24	A	407	PHO	CMA-C3A-C4A	-3.84	106.34	114.61
23	A	408	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
23	b	607	CLA	C2B-C1B-NB	3.83	114.30	110.33
23	B	616	CLA	C3B-C4B-NB	3.83	113.95	110.53
23	c	511	CLA	C1D-CHD-C4C	-3.83	117.89	126.02
23	C	509	CLA	C2B-C1B-NB	3.82	114.29	110.33
27	C	501	SQD	O47-C7-C8	3.82	119.75	111.48
23	b	612	CLA	C4B-C3B-C2B	-3.82	102.56	107.30
23	B	604	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
27	D	412	SQD	C44-O6-C1	-3.81	105.62	113.80
23	b	615	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
23	b	610	CLA	CAA-C2A-C3A	-3.81	102.69	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	C3C-C4C-NC	3.81	115.31	110.43
23	B	613	CLA	CHD-C1D-ND	-3.81	119.44	124.80
25	Y	101	BCR	C15-C14-C13	-3.81	121.94	127.28
23	B	603	CLA	C1C-C2C-C3C	-3.80	102.98	106.98
27	a	412	SQD	O48-C23-C24	3.80	123.42	111.83
23	B	606	CLA	C3C-C4C-NC	3.80	115.30	110.43
23	C	512	CLA	CHD-C1D-ND	-3.80	119.46	124.80
23	c	510	CLA	O2D-CGD-O1D	-3.80	116.46	123.85
23	C	507	CLA	C3D-C2D-C1D	-3.80	100.65	105.83
23	b	604	CLA	C3D-C4D-ND	3.80	116.16	109.99
38	E	103	HEC	CBC-CAC-C3C	-3.79	119.85	127.43
23	c	510	CLA	C3C-C4C-NC	3.79	115.28	110.43
23	a	405	CLA	C3C-C4C-NC	3.79	115.28	110.43
23	C	504	CLA	C1-C2-C3	-3.78	120.00	126.20
23	C	506	CLA	O2D-CGD-O1D	-3.78	116.49	123.85
23	C	509	CLA	C3D-C4D-ND	3.78	116.14	109.99
23	b	605	CLA	C4-C3-C5	3.78	121.78	115.23
23	B	605	CLA	C1D-CHD-C4C	-3.78	117.99	126.02
23	C	503	CLA	O2D-CGD-O1D	-3.77	116.50	123.85
25	d	404	BCR	C33-C5-C6	-3.77	120.37	124.48
25	h	102	BCR	C7-C8-C9	-3.77	120.66	126.23
23	b	613	CLA	O2A-CGA-CBA	3.77	123.32	111.83
23	b	613	CLA	O2A-CGA-O1A	-3.76	114.21	123.63
23	b	608	CLA	C3B-C4B-NB	3.76	113.89	110.53
23	b	610	CLA	C1C-C2C-C3C	-3.76	103.02	106.98
23	b	605	CLA	C3C-C4C-NC	3.76	115.25	110.43
23	c	514	CLA	C3C-C4C-NC	3.76	115.25	110.43
23	b	603	CLA	C3B-C4B-NB	3.76	113.89	110.53
23	c	514	CLA	C1-C2-C3	-3.76	120.04	126.20
23	C	513	CLA	C3C-C4C-NC	3.76	115.24	110.43
23	C	507	CLA	CHD-C1D-ND	-3.76	119.52	124.80
23	c	507	CLA	C3D-C2D-C1D	-3.75	100.71	105.83
23	d	402	CLA	C1-C2-C3	-3.75	120.06	126.20
29	A	413	PL9	C27-C28-C29	-3.75	119.05	127.62
23	A	404	CLA	O2A-CGA-CBA	3.75	123.25	111.83
23	B	607	CLA	C2B-C1B-NB	3.75	114.21	110.33
23	d	402	CLA	C1D-CHD-C4C	-3.74	118.07	126.02
23	C	515	CLA	CHD-C1D-ND	-3.74	119.54	124.80
23	B	608	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
23	c	508	CLA	C3B-C4B-NB	3.74	113.87	110.53
23	B	601	CLA	C1D-CHD-C4C	-3.73	118.09	126.02
23	b	611	CLA	C1C-C2C-C3C	-3.73	103.06	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	C3B-C4B-NB	3.73	113.86	110.53
23	B	615	CLA	CHD-C1D-ND	-3.73	119.55	124.80
25	C	517	BCR	C33-C5-C6	-3.73	120.42	124.48
23	c	504	CLA	C3C-C4C-NC	3.73	115.20	110.43
23	c	506	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
27	a	410	SQD	C1-O5-C5	-3.73	106.44	113.72
23	b	614	CLA	C3C-C4C-NC	3.73	115.20	110.43
23	B	605	CLA	CHD-C1D-ND	-3.73	119.56	124.80
23	B	615	CLA	CMC-C2C-C1C	3.73	130.86	125.03
23	b	603	CLA	C1C-C2C-C3C	-3.72	103.06	106.98
23	d	403	CLA	C1C-C2C-C3C	-3.72	103.06	106.98
23	C	503	CLA	C1-C2-C3	-3.72	120.11	126.20
23	B	615	CLA	C1C-C2C-C3C	-3.72	103.07	106.98
35	c	519	DGD	O2G-C1B-C2B	3.72	119.52	111.48
23	C	512	CLA	C1D-CHD-C4C	-3.71	118.13	126.02
23	B	605	CLA	CMB-C2B-C1B	3.71	131.07	125.42
23	C	507	CLA	O2D-CGD-O1D	-3.71	116.63	123.85
23	C	513	CLA	C1D-CHD-C4C	-3.71	118.14	126.02
27	D	412	SQD	C1-C2-C3	-3.70	102.22	110.01
23	B	611	CLA	C1-C2-C3	-3.70	120.13	126.20
38	E	103	HEC	CAD-CBD-CGD	3.70	123.48	113.67
23	C	510	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
23	A	408	CLA	C1D-CHD-C4C	-3.70	118.16	126.02
23	B	604	CLA	C3D-C4D-ND	3.70	116.00	109.99
23	b	614	CLA	C1D-CHD-C4C	-3.70	118.16	126.02
23	B	612	CLA	C4C-C3C-C2C	-3.69	101.51	106.89
23	B	615	CLA	C3B-C2B-C1B	-3.69	102.82	107.17
23	a	405	CLA	C3B-C4B-NB	3.69	113.82	110.53
23	C	515	CLA	C4A-NA-C1A	-3.69	105.00	106.68
23	d	403	CLA	O2D-CGD-O1D	-3.69	116.67	123.85
23	D	404	CLA	CHD-C1D-ND	-3.69	119.61	124.80
23	B	604	CLA	O2D-CGD-O1D	-3.68	116.69	123.85
23	A	406	CLA	CAA-C2A-C3A	-3.68	103.06	113.00
23	B	610	CLA	C3C-C4C-NC	3.68	115.14	110.43
23	b	601	CLA	C3B-C4B-NB	3.68	113.81	110.53
23	B	606	CLA	O2D-CGD-O1D	-3.68	116.69	123.85
23	B	608	CLA	C3C-C4C-NC	3.68	115.14	110.43
23	C	505	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
32	C	522	LMG	C3-C4-C5	3.67	116.89	110.23
23	b	610	CLA	C1-C2-C3	-3.67	120.18	126.20
23	A	405	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
23	C	511	CLA	CHD-C1D-ND	-3.67	119.64	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	411	SQD	O47-C7-C8	3.67	119.42	111.48
32	c	521	LMG	O7-C10-C11	3.67	119.41	111.48
25	d	404	BCR	C15-C14-C13	-3.67	122.14	127.28
23	C	514	CLA	C3B-C4B-NB	3.66	113.80	110.53
23	c	512	CLA	C3C-C4C-NC	3.66	115.12	110.43
23	B	607	CLA	CAA-C2A-C3A	-3.66	103.11	113.00
33	V	202	HTG	C1-O5-C5	3.66	117.09	112.19
23	b	605	CLA	CHD-C4C-NC	3.66	129.90	124.23
32	z	101	LMG	O7-C10-C11	3.66	119.39	111.48
23	b	604	CLA	C1D-CHD-C4C	-3.65	118.25	126.02
23	D	404	CLA	CMC-C2C-C1C	3.65	130.74	125.03
23	c	510	CLA	C4A-NA-C1A	-3.65	105.01	106.68
23	B	602	CLA	C1D-CHD-C4C	-3.65	118.25	126.02
29	D	406	PL9	C42-C43-C44	-3.65	119.26	127.62
23	a	406	CLA	C1D-CHD-C4C	-3.65	118.26	126.02
23	A	406	CLA	C3C-C4C-NC	3.65	115.11	110.43
23	b	602	CLA	C1D-CHD-C4C	-3.65	118.26	126.02
23	B	612	CLA	CHD-C1D-ND	-3.65	119.67	124.80
23	C	507	CLA	C1D-CHD-C4C	-3.64	118.28	126.02
25	k	101	BCR	C29-C30-C25	3.64	115.73	110.44
24	a	407	PHO	C1-C2-C3	-3.64	120.23	126.20
23	b	613	CLA	CHD-C1D-ND	-3.64	119.68	124.80
23	b	608	CLA	O2D-CGD-O1D	-3.64	116.77	123.85
35	c	518	DGD	O2G-C1B-C2B	3.64	119.35	111.48
23	a	406	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
27	a	410	SQD	C44-O6-C1	-3.63	106.01	113.80
23	B	604	CLA	C1-C2-C3	-3.63	120.25	126.20
23	c	513	CLA	C2B-C1B-NB	3.63	114.09	110.33
23	B	614	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
23	B	612	CLA	C2B-C1B-NB	3.63	114.09	110.33
23	B	605	CLA	C4C-C3C-C2C	-3.63	101.61	106.89
23	C	511	CLA	C1D-CHD-C4C	-3.63	118.31	126.02
23	a	405	CLA	O2D-CGD-O1D	-3.62	116.79	123.85
23	C	512	CLA	C3C-C4C-NC	3.62	115.07	110.43
23	B	606	CLA	C3D-C4D-ND	3.62	115.88	109.99
23	d	402	CLA	CHD-C1D-ND	-3.62	119.70	124.80
23	C	507	CLA	C1C-C2C-C3C	-3.62	103.17	106.98
23	C	509	CLA	O2D-CGD-O1D	-3.62	116.80	123.85
23	b	604	CLA	C4B-C3B-C2B	-3.62	102.80	107.30
23	A	408	CLA	CAA-C2A-C3A	-3.62	103.23	113.00
23	c	507	CLA	CHD-C1D-ND	-3.61	119.72	124.80
38	e	102	HEC	CBC-CAC-C3C	-3.61	120.21	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
23	b	607	CLA	C1D-CHD-C4C	-3.61	118.34	126.02
23	c	504	CLA	C1D-CHD-C4C	-3.61	118.34	126.02
23	b	605	CLA	CMB-C2B-C1B	3.61	130.91	125.42
38	E	103	HEC	CHD-C4C-NC	3.61	128.38	124.45
23	B	616	CLA	C1D-CHD-C4C	-3.61	118.35	126.02
23	b	614	CLA	C3B-C4B-NB	3.61	113.75	110.53
23	B	610	CLA	O2A-CGA-CBA	3.61	122.83	111.83
23	b	612	CLA	C3D-C4D-ND	3.61	115.85	109.99
23	C	510	CLA	C4C-C3C-C2C	-3.60	101.65	106.89
23	C	511	CLA	CAC-C3C-C4C	3.60	129.48	124.79
25	d	404	BCR	C38-C26-C25	-3.60	120.56	124.48
23	c	514	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
25	a	409	BCR	C24-C23-C22	-3.60	120.91	126.23
23	a	408	CLA	O2D-CGD-O1D	-3.60	116.84	123.85
23	b	605	CLA	O2D-CGD-O1D	-3.60	116.85	123.85
23	c	505	CLA	CHD-C1D-ND	-3.60	119.74	124.80
23	B	603	CLA	C1D-CHD-C4C	-3.59	118.38	126.02
23	c	515	CLA	C1C-C2C-C3C	-3.59	103.20	106.98
23	b	609	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
23	B	608	CLA	C1D-CHD-C4C	-3.59	118.40	126.02
23	A	406	CLA	C1C-C2C-C3C	-3.59	103.21	106.98
23	b	602	CLA	CAC-C3C-C4C	3.58	129.45	124.79
38	E	103	HEC	CHA-C1A-NA	3.58	128.35	124.45
23	b	602	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
23	B	616	CLA	C4C-C3C-C2C	-3.57	101.69	106.89
23	b	603	CLA	O2A-CGA-O1A	-3.57	114.69	123.63
23	b	607	CLA	CBC-CAC-C3C	-3.57	102.74	112.42
23	B	603	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
23	a	405	CLA	CHD-C1D-ND	-3.57	119.78	124.80
23	b	616	CLA	CHD-C1D-ND	-3.57	119.78	124.80
23	a	406	CLA	CMC-C2C-C1C	3.56	130.60	125.03
25	K	101	BCR	C7-C8-C9	-3.56	120.97	126.23
23	b	615	CLA	C3C-C4C-NC	3.56	114.99	110.43
23	b	614	CLA	C1-C2-C3	-3.56	120.37	126.20
23	c	505	CLA	C4C-C3C-C2C	-3.56	101.71	106.89
31	d	406	LHG	O7-C7-C8	3.56	119.17	111.48
25	c	516	BCR	C11-C10-C9	-3.55	122.29	127.28
23	B	602	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
23	b	604	CLA	C4A-NA-C1A	-3.55	105.06	106.68
23	b	603	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
23	C	509	CLA	C1C-C2C-C3C	-3.55	103.25	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	C1D-CHD-C4C	-3.55	118.48	126.02
23	B	610	CLA	CAA-C2A-C3A	-3.55	103.41	113.00
23	b	613	CLA	C4A-NA-C1A	-3.55	105.06	106.68
23	b	604	CLA	C1-C2-C3	-3.55	120.39	126.20
23	B	616	CLA	CHD-C1D-ND	-3.55	119.81	124.80
23	B	614	CLA	C1D-CHD-C4C	-3.54	118.49	126.02
23	A	408	CLA	C3C-C4C-NC	3.54	114.97	110.43
23	b	603	CLA	CMB-C2B-C1B	3.54	130.81	125.42
23	c	503	CLA	C3C-C4C-NC	3.54	114.96	110.43
23	c	509	CLA	C3C-C4C-NC	3.53	114.96	110.43
23	C	515	CLA	CMB-C2B-C1B	3.53	130.80	125.42
23	c	511	CLA	CHD-C1D-ND	-3.53	119.83	124.80
23	B	605	CLA	O2A-CGA-O1A	-3.53	114.79	123.63
32	m	101	LMG	O7-C10-C11	3.53	119.12	111.48
23	d	402	CLA	CAA-C2A-C3A	-3.53	103.47	113.00
23	B	612	CLA	C1D-CHD-C4C	-3.53	118.53	126.02
27	C	501	SQD	C44-O6-C1	-3.52	106.24	113.80
23	c	511	CLA	C3C-C4C-NC	3.52	114.94	110.43
23	B	608	CLA	C3B-C4B-NB	3.52	113.68	110.53
23	a	408	CLA	C3B-C4B-NB	3.52	113.67	110.53
31	a	419	LHG	O7-C7-C8	3.52	119.10	111.48
23	C	515	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
29	D	406	PL9	C53-C6-C1	3.52	122.48	115.28
25	c	517	BCR	C7-C8-C9	-3.52	121.03	126.23
31	D	408	LHG	O7-C7-C8	3.52	119.09	111.48
23	C	506	CLA	C1D-CHD-C4C	-3.52	118.55	126.02
23	a	405	CLA	CHD-C4C-NC	3.52	129.68	124.23
23	A	404	CLA	C1D-CHD-C4C	-3.51	118.55	126.02
23	B	605	CLA	CAC-C3C-C4C	3.51	129.36	124.79
23	C	512	CLA	C3B-C4B-NB	3.51	113.67	110.53
23	B	601	CLA	C1C-C2C-C3C	-3.51	103.29	106.98
23	B	605	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
24	A	407	PHO	C1A-C2A-C3A	-3.51	99.50	102.84
23	A	405	CLA	C3C-C4C-NC	3.51	114.92	110.43
23	A	405	CLA	C3B-C4B-NB	3.51	113.66	110.53
23	c	507	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
23	B	613	CLA	C4A-NA-C1A	-3.50	105.08	106.68
23	b	612	CLA	O2A-CGA-CBA	3.50	122.51	111.83
23	c	513	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
23	c	509	CLA	C1D-CHD-C4C	-3.50	118.58	126.02
23	b	613	CLA	O2D-CGD-CBD	3.50	117.34	111.23
23	C	512	CLA	CMC-C2C-C1C	3.50	130.50	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
31	A	416	LHG	O8-C23-O10	-3.49	114.89	123.63
23	b	603	CLA	CHD-C1D-ND	-3.49	119.89	124.80
23	a	408	CLA	C4C-C3C-C2C	-3.49	101.82	106.89
29	A	413	PL9	C37-C38-C39	-3.49	119.65	127.62
23	B	601	CLA	C3C-C4C-NC	3.48	114.89	110.43
27	C	501	SQD	O9-S-C6	3.48	111.96	106.76
25	b	617	BCR	C29-C30-C25	3.48	115.50	110.44
23	B	607	CLA	C3C-C4C-NC	3.48	114.89	110.43
23	B	611	CLA	CHD-C4C-NC	3.48	129.62	124.23
27	B	620	SQD	C3-C4-C5	3.48	116.54	110.23
23	b	614	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
23	b	609	CLA	C1-C2-C3	-3.48	120.50	126.20
23	c	511	CLA	C1C-C2C-C3C	-3.48	103.33	106.98
23	b	616	CLA	C1-C2-C3	-3.47	120.51	126.20
23	b	608	CLA	C1D-CHD-C4C	-3.47	118.64	126.02
23	B	613	CLA	C4B-C3B-C2B	-3.47	102.99	107.30
23	B	615	CLA	C2B-C1B-NB	3.46	113.92	110.33
23	C	504	CLA	C1C-C2C-C3C	-3.46	103.34	106.98
23	A	405	CLA	CMB-C2B-C1B	3.46	130.69	125.42
38	e	102	HEC	CAD-CBD-CGD	3.46	122.85	113.67
25	K	101	BCR	C24-C23-C22	-3.46	121.11	126.23
23	b	615	CLA	C3B-C4B-NB	3.46	113.62	110.53
23	c	508	CLA	C3C-C4C-NC	3.46	114.86	110.43
25	c	517	BCR	C33-C5-C6	-3.46	120.71	124.48
23	c	507	CLA	CMB-C2B-C1B	3.45	130.68	125.42
23	B	603	CLA	C3B-C4B-NB	3.45	113.61	110.53
23	A	405	CLA	C4B-C3B-C2B	-3.45	103.01	107.30
23	c	509	CLA	CMB-C2B-C1B	3.45	130.67	125.42
23	C	505	CLA	O2D-CGD-CBD	3.45	117.25	111.23
34	a	413	LMT	O5'-C5'-C4'	3.44	116.84	109.72
23	B	606	CLA	C4B-C3B-C2B	-3.44	103.03	107.30
23	C	510	CLA	CHD-C1D-ND	-3.43	119.97	124.80
23	c	512	CLA	C4-C3-C5	3.43	121.19	115.23
23	A	404	CLA	C3C-C4C-NC	3.43	114.83	110.43
23	B	604	CLA	O2A-CGA-O1A	-3.43	115.05	123.63
23	c	515	CLA	C3B-C4B-NB	3.43	113.59	110.53
23	B	607	CLA	O2D-CGD-O1D	-3.42	117.18	123.85
23	c	507	CLA	O2D-CGD-O1D	-3.42	117.18	123.85
23	B	612	CLA	C3B-C4B-NB	3.42	113.59	110.53
23	b	615	CLA	CAC-C3C-C4C	3.42	129.24	124.79
23	D	403	CLA	C3C-C4C-NC	3.42	114.81	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	CLA	C1C-C2C-C3C	-3.42	103.38	106.98
24	A	415	PHO	O2D-CGD-O1D	-3.42	117.19	123.85
23	b	616	CLA	C3B-C4B-NB	3.42	113.58	110.53
25	C	516	BCR	C15-C14-C13	-3.41	122.49	127.28
23	c	504	CLA	C4A-NA-C1A	-3.41	105.12	106.68
25	d	404	BCR	C28-C27-C26	-3.41	107.97	114.06
23	C	514	CLA	CHD-C1D-ND	-3.41	120.01	124.80
25	B	618	BCR	C15-C14-C13	-3.40	122.50	127.28
23	C	508	CLA	C1-C2-C3	-3.40	120.62	126.20
23	A	404	CLA	C2A-C1A-CHA	-3.40	117.96	123.87
23	B	614	CLA	CHC-C1C-C2C	-3.40	117.28	126.95
23	B	609	CLA	C1C-C2C-C3C	-3.40	103.40	106.98
23	c	515	CLA	CAC-C3C-C4C	3.40	129.22	124.79
23	C	505	CLA	C1-C2-C3	-3.40	120.62	126.20
23	C	513	CLA	C1C-C2C-C3C	-3.40	103.40	106.98
23	b	606	CLA	C1C-C2C-C3C	-3.40	103.40	106.98
23	C	506	CLA	C1-C2-C3	-3.39	120.64	126.20
23	D	404	CLA	C1C-C2C-C3C	-3.39	103.42	106.98
23	c	506	CLA	C3C-C4C-NC	3.38	114.77	110.43
23	c	512	CLA	CHD-C1D-ND	-3.38	120.04	124.80
23	c	505	CLA	C3B-C4B-NB	3.38	113.55	110.53
23	c	514	CLA	CHD-C1D-ND	-3.38	120.04	124.80
23	b	603	CLA	O2A-CGA-CBA	3.38	122.15	111.83
23	c	515	CLA	C1-C2-C3	-3.38	120.66	126.20
25	a	409	BCR	C38-C26-C25	-3.38	120.80	124.48
23	d	403	CLA	C1D-CHD-C4C	-3.38	118.84	126.02
23	C	508	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
23	b	602	CLA	C3C-C4C-NC	3.38	114.76	110.43
23	C	504	CLA	C1D-CHD-C4C	-3.38	118.84	126.02
23	b	615	CLA	CHC-C1C-C2C	-3.38	117.35	126.95
23	b	607	CLA	C4B-C3B-C2B	-3.38	103.10	107.30
23	B	612	CLA	C4A-NA-C1A	-3.38	105.14	106.68
29	A	413	PL9	C25-C24-C26	3.37	121.09	115.23
23	B	603	CLA	C4C-C3C-C2C	-3.37	101.98	106.89
23	C	508	CLA	C1D-CHD-C4C	-3.37	118.85	126.02
31	L	101	LHG	O7-C7-C8	3.37	118.78	111.48
23	c	506	CLA	C1D-CHD-C4C	-3.37	118.85	126.02
23	A	406	CLA	C1D-CHD-C4C	-3.37	118.86	126.02
23	c	510	CLA	CHD-C1D-ND	-3.37	120.06	124.80
23	b	601	CLA	C3C-C4C-NC	3.37	114.75	110.43
25	b	619	BCR	C24-C23-C22	-3.37	121.25	126.23
23	c	503	CLA	C3B-C4B-NB	3.37	113.54	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	CMC-C2C-C1C	3.37	130.30	125.03
23	c	511	CLA	C4B-C3B-C2B	-3.37	103.12	107.30
23	D	404	CLA	C3B-C4B-NB	3.37	113.53	110.53
23	B	611	CLA	C4B-C3B-C2B	-3.36	103.12	107.30
24	A	415	PHO	C1A-C2A-C3A	-3.36	99.64	102.84
23	c	513	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
23	b	613	CLA	CAC-C3C-C4C	3.36	129.16	124.79
25	B	617	BCR	C7-C8-C9	-3.36	121.27	126.23
23	A	404	CLA	O2A-CGA-O1A	-3.36	115.23	123.63
23	B	616	CLA	C1C-C2C-C3C	-3.36	103.45	106.98
23	a	408	CLA	C1C-C2C-C3C	-3.36	103.45	106.98
23	C	507	CLA	C3B-C4B-NB	3.36	113.53	110.53
23	c	503	CLA	C1D-CHD-C4C	-3.35	118.89	126.02
23	b	615	CLA	O2D-CGD-CBD	3.35	117.09	111.23
23	C	506	CLA	CMC-C2C-C1C	3.35	130.27	125.03
23	b	610	CLA	O2D-CGD-O1D	-3.35	117.32	123.85
23	c	507	CLA	C4C-C3C-C2C	-3.35	102.01	106.89
23	c	512	CLA	CBC-CAC-C3C	-3.35	103.34	112.42
23	C	505	CLA	CMB-C2B-C1B	3.35	130.51	125.42
23	C	515	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
23	C	514	CLA	C1C-C2C-C3C	-3.34	103.46	106.98
23	c	507	CLA	C1D-CHD-C4C	-3.34	118.92	126.02
23	B	615	CLA	CHD-C4C-NC	3.34	129.41	124.23
27	A	411	SQD	C3-C4-C5	3.34	116.29	110.23
31	d	406	LHG	O8-C23-O10	-3.34	115.27	123.63
29	A	413	PL9	C10-C9-C11	3.34	121.02	115.23
23	A	405	CLA	CAA-C2A-C3A	-3.33	103.99	113.00
23	a	408	CLA	CHD-C1D-ND	-3.33	120.11	124.80
27	a	410	SQD	O9-S-C6	3.33	111.73	106.76
35	c	520	DGD	O2G-C1B-C2B	3.33	118.68	111.48
23	b	612	CLA	CAC-C3C-C4C	3.33	129.12	124.79
23	c	512	CLA	CMC-C2C-C1C	3.33	130.23	125.03
23	c	513	CLA	C4A-NA-C1A	-3.32	105.16	106.68
23	b	609	CLA	C4C-C3C-C2C	-3.32	102.06	106.89
23	B	606	CLA	CHC-C1C-C2C	-3.32	117.51	126.95
23	b	604	CLA	CMC-C2C-C1C	3.32	130.22	125.03
25	D	405	BCR	C24-C23-C22	-3.32	121.33	126.23
23	b	604	CLA	CAC-C3C-C4C	3.32	129.11	124.79
23	c	508	CLA	C4B-C3B-C2B	-3.32	103.18	107.30
27	C	501	SQD	O48-C23-C24	3.31	121.94	111.83
23	a	404	CLA	C1-C2-C3	-3.31	120.78	126.20
25	a	409	BCR	C11-C10-C9	-3.31	122.64	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	C4A-NA-C1A	-3.31	105.17	106.68
23	B	609	CLA	C1D-CHD-C4C	-3.31	118.99	126.02
23	B	610	CLA	C1C-C2C-C3C	-3.31	103.50	106.98
23	c	511	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
23	b	608	CLA	CAC-C3C-C4C	3.30	129.09	124.79
23	B	614	CLA	CMC-C2C-C1C	3.30	130.19	125.03
23	c	504	CLA	CHD-C4C-NC	3.30	129.34	124.23
25	H	101	BCR	C38-C26-C25	-3.29	120.90	124.48
23	A	405	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
38	v	202	HEC	C4D-ND-C1D	3.28	111.18	105.82
34	e	101	LMT	C4B-C3B-C2B	3.28	116.59	110.83
23	b	601	CLA	C4-C3-C5	3.28	120.93	115.23
25	H	101	BCR	C16-C17-C18	-3.28	122.67	127.28
25	h	102	BCR	C38-C26-C25	-3.28	120.90	124.48
23	b	612	CLA	C4C-C3C-C2C	-3.28	102.12	106.89
23	C	514	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
23	a	405	CLA	CAA-C2A-C3A	-3.28	104.14	113.00
23	a	404	CLA	CHC-C1C-C2C	-3.28	117.64	126.95
29	D	406	PL9	C42-C41-C39	-3.28	102.33	113.19
38	e	102	HEC	CBD-CAD-C3D	-3.27	103.48	112.53
23	b	611	CLA	C1D-CHD-C4C	-3.27	119.06	126.02
23	A	406	CLA	C4B-C3B-C2B	-3.27	103.24	107.30
23	c	514	CLA	CMB-C2B-C1B	3.27	130.40	125.42
23	C	514	CLA	C1-C2-C3	-3.27	120.85	126.20
23	B	610	CLA	C4C-C3C-C2C	-3.26	102.14	106.89
23	C	509	CLA	C4C-C3C-C2C	-3.26	102.14	106.89
23	A	406	CLA	C4C-C3C-C2C	-3.26	102.14	106.89
23	b	605	CLA	C4C-C3C-C2C	-3.26	102.14	106.89
23	b	616	CLA	C1C-C2C-C3C	-3.26	103.55	106.98
23	a	404	CLA	C3C-C4C-NC	3.26	114.61	110.43
23	B	601	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
23	b	612	CLA	CHD-C1D-ND	-3.26	120.22	124.80
32	C	522	LMG	O8-C28-C29	3.26	121.77	111.83
23	b	609	CLA	C1C-C2C-C3C	-3.26	103.56	106.98
25	K	101	BCR	C38-C26-C25	-3.25	120.93	124.48
23	C	503	CLA	C3B-C4B-NB	3.25	113.44	110.53
25	H	101	BCR	C7-C8-C9	-3.25	121.42	126.23
23	C	514	CLA	C4C-C3C-C2C	-3.25	102.16	106.89
23	b	614	CLA	CHC-C1C-C2C	-3.25	117.72	126.95
23	C	508	CLA	CBC-CAC-C3C	-3.25	103.62	112.42
23	B	609	CLA	C4C-C3C-C2C	-3.25	102.17	106.89
29	d	405	PL9	C40-C39-C41	3.25	120.86	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	CMC-C2C-C1C	3.25	130.11	125.03
23	b	602	CLA	C3B-C4B-NB	3.25	113.43	110.53
23	A	404	CLA	CAC-C3C-C4C	3.24	129.01	124.79
23	B	604	CLA	C3B-C4B-NB	3.24	113.42	110.53
23	C	515	CLA	C4C-C3C-C2C	-3.24	102.17	106.89
29	a	415	PL9	C37-C36-C34	-3.24	102.44	113.19
32	B	621	LMG	O8-C28-C29	3.24	121.72	111.83
23	d	402	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
25	k	101	BCR	C15-C14-C13	-3.24	122.73	127.28
23	c	509	CLA	CHD-C4C-NC	3.24	129.25	124.23
31	A	416	LHG	O7-C7-C8	3.24	118.49	111.48
23	B	607	CLA	C1D-CHD-C4C	-3.24	119.14	126.02
23	C	515	CLA	C1-C2-C3	-3.23	120.90	126.20
24	a	417	PHO	O2D-CGD-O1D	-3.23	117.55	123.85
25	T	101	BCR	C33-C5-C6	-3.23	120.95	124.48
23	d	403	CLA	CAA-C2A-C3A	-3.23	104.26	113.00
23	B	601	CLA	O2A-CGA-CBA	3.23	121.69	111.83
25	b	618	BCR	C15-C14-C13	-3.23	122.75	127.28
23	B	607	CLA	CBC-CAC-C3C	-3.23	103.67	112.42
23	C	513	CLA	C4-C3-C5	3.23	120.83	115.23
23	c	512	CLA	C4B-C3B-C2B	-3.23	103.29	107.30
23	B	603	CLA	CMC-C2C-C1C	3.23	130.07	125.03
29	a	415	PL9	C42-C43-C44	-3.22	120.24	127.62
23	b	613	CLA	C4C-C3C-C2C	-3.22	102.20	106.89
23	a	406	CLA	CAA-C2A-C3A	-3.22	104.29	113.00
25	y	101	BCR	C38-C26-C25	-3.22	120.97	124.48
23	a	408	CLA	CAA-C2A-C3A	-3.22	104.29	113.00
23	b	611	CLA	O2A-CGA-CBA	3.22	121.66	111.83
23	B	607	CLA	C4-C3-C5	3.22	120.82	115.23
29	A	413	PL9	C7-C8-C9	-3.22	121.29	126.83
24	a	417	PHO	CMB-C2B-C3B	3.22	131.11	124.68
23	b	610	CLA	C4C-C3C-C2C	-3.22	102.21	106.89
23	C	508	CLA	CHC-C1C-C2C	-3.22	117.81	126.95
23	A	405	CLA	C4A-NA-C1A	-3.22	105.21	106.68
23	C	512	CLA	CBC-CAC-C3C	-3.21	103.71	112.42
23	c	506	CLA	C1-O2A-CGA	3.21	124.43	116.65
27	A	411	SQD	O48-C23-C24	3.21	121.62	111.83
27	a	410	SQD	O8-S-C6	3.20	112.16	105.97
23	B	602	CLA	C1C-C2C-C3C	-3.20	103.61	106.98
23	b	601	CLA	CHD-C4C-NC	3.20	129.20	124.23
23	A	406	CLA	O2A-CGA-O1A	-3.20	115.62	123.63
23	b	613	CLA	C1D-CHD-C4C	-3.20	119.22	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	CHD-C1D-ND	-3.20	120.30	124.80
25	K	101	BCR	C33-C5-C6	-3.20	121.00	124.48
29	d	405	PL9	C10-C9-C11	3.20	120.78	115.23
23	b	610	CLA	CHD-C1D-ND	-3.19	120.31	124.80
23	C	505	CLA	CHD-C4C-NC	3.19	129.18	124.23
25	b	618	BCR	C29-C30-C25	3.19	115.08	110.44
27	b	620	SQD	C1-C2-C3	-3.19	103.30	110.01
23	b	609	CLA	C1D-CHD-C4C	-3.19	119.24	126.02
23	B	615	CLA	C4B-C3B-C2B	-3.19	103.34	107.30
38	E	103	HEC	CBD-CAD-C3D	-3.19	103.72	112.53
23	b	616	CLA	CHD-C4C-NC	3.19	129.18	124.23
23	c	504	CLA	CMC-C2C-C1C	3.18	130.01	125.03
23	C	511	CLA	CMC-C2C-C1C	3.18	130.01	125.03
23	B	601	CLA	C3B-C4B-NB	3.18	113.37	110.53
23	c	513	CLA	C4B-C3B-C2B	-3.18	103.35	107.30
23	b	605	CLA	C2A-C1A-CHA	-3.18	118.35	123.87
23	a	406	CLA	CHD-C4C-NC	3.18	129.16	124.23
23	d	403	CLA	C3C-C4C-NC	3.18	114.50	110.43
23	d	402	CLA	O2A-CGA-CBA	3.18	121.52	111.83
29	a	415	PL9	C25-C24-C26	3.17	120.74	115.23
23	b	612	CLA	O2A-CGA-O1A	-3.17	115.69	123.63
31	b	629	LHG	O7-C7-C8	3.17	118.34	111.48
23	C	504	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
23	C	510	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
23	c	513	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
23	b	606	CLA	C3B-C4B-NB	3.17	113.36	110.53
23	C	513	CLA	C4B-C3B-C2B	-3.17	103.37	107.30
23	a	404	CLA	C4B-C3B-C2B	-3.17	103.37	107.30
24	A	415	PHO	C4-C3-C5	3.16	120.72	115.23
23	c	508	CLA	CAA-C2A-C3A	-3.16	104.46	113.00
38	V	201	HEC	CBD-CAD-C3D	-3.16	103.80	112.53
23	D	403	CLA	C1D-CHD-C4C	-3.16	119.30	126.02
35	C	519	DGD	O1G-C1A-C2A	3.16	121.46	111.83
29	d	405	PL9	C53-C6-C1	3.16	121.74	115.28
23	b	616	CLA	C4C-C3C-C2C	-3.15	102.30	106.89
23	B	614	CLA	CHD-C4C-NC	3.15	129.12	124.23
23	c	514	CLA	CMC-C2C-C1C	3.15	129.96	125.03
25	Y	101	BCR	C37-C22-C23	3.15	122.90	118.09
23	c	508	CLA	CBC-CAC-C3C	-3.15	103.89	112.42
32	C	521	LMG	O8-C28-C29	3.14	121.42	111.83
23	D	404	CLA	CAA-C2A-C3A	-3.14	104.50	113.00
29	a	415	PL9	C20-C19-C21	3.14	120.68	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	O2A-CGA-CBA	3.14	121.41	111.83
35	C	518	DGD	O2G-C1B-C2B	3.14	118.27	111.48
32	m	101	LMG	O8-C28-C29	3.14	121.40	111.83
23	C	512	CLA	C4-C3-C5	3.13	120.67	115.23
23	B	612	CLA	C1C-C2C-C3C	-3.13	103.69	106.98
23	d	403	CLA	CMC-C2C-C1C	3.13	129.93	125.03
23	B	607	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
29	A	413	PL9	C20-C19-C21	3.13	120.66	115.23
23	B	614	CLA	O2A-CGA-CBA	3.13	121.38	111.83
23	C	506	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
23	C	509	CLA	CMB-C2B-C1B	3.13	130.18	125.42
38	e	102	HEC	CBB-CAB-C3B	-3.13	121.18	127.43
23	c	515	CLA	CMC-C2C-C1C	3.13	129.92	125.03
23	b	612	CLA	CMC-C2C-C1C	3.12	129.92	125.03
29	D	406	PL9	C45-C44-C46	3.12	120.65	115.23
23	D	403	CLA	CBC-CAC-C3C	-3.12	103.95	112.42
23	c	503	CLA	O2A-CGA-O1A	-3.12	115.82	123.63
23	D	404	CLA	C4B-C3B-C2B	-3.12	103.42	107.30
31	d	406	LHG	O8-C23-C24	3.12	121.35	111.83
29	a	415	PL9	C22-C23-C24	-3.12	120.48	127.62
23	c	508	CLA	CHD-C4C-NC	3.12	129.06	124.23
25	a	409	BCR	C33-C5-C6	-3.12	121.08	124.48
23	b	611	CLA	C4B-C3B-C2B	-3.12	103.43	107.30
23	c	514	CLA	C4-C3-C5	3.11	120.63	115.23
23	c	514	CLA	CAC-C3C-C4C	3.11	128.84	124.79
25	b	619	BCR	C7-C8-C9	-3.11	121.64	126.23
23	C	513	CLA	C4C-C3C-C2C	-3.11	102.37	106.89
34	C	526	LMT	O1B-C4'-C3'	3.11	115.13	107.23
29	D	406	PL9	C10-C9-C11	3.11	120.62	115.23
23	c	510	CLA	CHC-C1C-C2C	-3.11	118.12	126.95
23	a	408	CLA	O2A-CGA-CBA	3.11	121.31	111.83
23	b	605	CLA	C1C-C2C-C3C	-3.10	103.72	106.98
23	c	504	CLA	CMB-C2B-C1B	3.10	130.14	125.42
38	v	202	HEC	CBD-CAD-C3D	-3.10	103.95	112.53
25	c	516	BCR	C15-C14-C13	-3.10	122.93	127.28
23	b	610	CLA	O2A-CGA-O1A	-3.10	115.87	123.63
23	d	403	CLA	CMB-C2B-C1B	3.10	130.14	125.42
24	a	407	PHO	O2A-CGA-CBA	3.10	121.28	111.83
23	d	403	CLA	O2A-CGA-CBA	3.10	121.28	111.83
23	b	604	CLA	O2A-CGA-O1A	-3.10	115.88	123.63
29	A	413	PL9	C7-C3-C2	-3.10	119.74	123.39
23	b	613	CLA	C4-C3-C5	3.10	120.60	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	CHD-C4C-NC	3.10	129.03	124.23
23	d	402	CLA	C4-C3-C5	3.10	120.60	115.23
23	a	404	CLA	C4-C3-C5	3.09	120.59	115.23
23	C	503	CLA	C4B-C3B-C2B	-3.09	103.46	107.30
23	b	603	CLA	C4C-C3C-C2C	-3.09	102.40	106.89
23	b	604	CLA	CHC-C1C-C2C	-3.08	118.18	126.95
23	B	611	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
23	C	503	CLA	CHD-C4C-NC	3.08	129.01	124.23
24	A	407	PHO	C1-C2-C3	-3.08	121.15	126.20
23	B	601	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
23	C	504	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
23	B	614	CLA	O2A-CGA-O1A	-3.08	115.92	123.63
35	H	102	DGD	O1G-C1A-C2A	3.08	121.22	111.83
23	B	611	CLA	CAC-C3C-C4C	3.08	128.79	124.79
23	b	601	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
23	B	604	CLA	C4-C3-C5	3.08	120.57	115.23
23	b	610	CLA	C3B-C4B-NB	3.07	113.27	110.53
23	c	505	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
23	B	603	CLA	C4B-C3B-C2B	-3.07	103.48	107.30
25	b	619	BCR	C11-C10-C9	-3.07	122.97	127.28
23	c	510	CLA	O2A-CGA-CBA	3.07	121.20	111.83
23	d	403	CLA	C3B-C4B-NB	3.07	113.27	110.53
32	Z	101	LMG	O6-C1-C2	3.07	116.68	110.37
23	A	408	CLA	C3B-C4B-NB	3.07	113.27	110.53
23	D	403	CLA	O2A-CGA-CBA	3.07	121.19	111.83
23	d	403	CLA	CHD-C4C-NC	3.07	128.99	124.23
23	c	511	CLA	C4C-C3C-C2C	-3.07	102.43	106.89
23	B	604	CLA	C4C-C3C-C2C	-3.07	102.43	106.89
23	a	406	CLA	C1-C2-C3	-3.07	121.17	126.20
23	A	404	CLA	C4B-C3B-C2B	-3.07	103.49	107.30
23	D	403	CLA	CAA-C2A-C3A	-3.07	104.71	113.00
23	C	507	CLA	CAC-C3C-C4C	3.07	128.78	124.79
23	C	505	CLA	C4C-C3C-C2C	-3.07	102.43	106.89
23	c	505	CLA	C1C-C2C-C3C	-3.06	103.76	106.98
27	B	620	SQD	O48-C23-C24	3.06	121.17	111.83
23	B	601	CLA	C4C-C3C-C2C	-3.06	102.43	106.89
23	B	604	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
23	b	601	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
23	b	616	CLA	O2A-CGA-CBA	3.06	121.16	111.83
23	c	508	CLA	C1-C2-C3	-3.06	121.19	126.20
23	a	405	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
25	d	404	BCR	C40-C30-C25	-3.06	105.45	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	406	PL9	C22-C23-C24	-3.06	120.63	127.62
23	A	408	CLA	CMB-C2B-C1B	3.06	130.07	125.42
23	d	402	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
23	B	607	CLA	CHC-C1C-C2C	-3.05	118.27	126.95
23	B	612	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
23	c	505	CLA	CMC-C2C-C1C	3.05	129.80	125.03
23	B	610	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
23	a	404	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
23	b	613	CLA	CHC-C1C-C2C	-3.05	118.29	126.95
23	C	511	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
23	B	608	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
31	b	629	LHG	O8-C23-C24	3.05	121.12	111.83
23	B	605	CLA	C4-C3-C5	3.05	120.52	115.23
23	B	610	CLA	C1D-CHD-C4C	-3.05	119.55	126.02
23	b	612	CLA	C4-C3-C5	3.05	120.51	115.23
23	b	607	CLA	CHC-C1C-C2C	-3.05	118.29	126.95
25	B	617	BCR	C11-C10-C9	-3.04	123.01	127.28
23	D	404	CLA	C4C-C3C-C2C	-3.04	102.46	106.89
23	B	612	CLA	O2A-CGA-CBA	3.04	121.11	111.83
23	b	601	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
23	b	608	CLA	C4B-C3B-C2B	-3.04	103.53	107.30
23	A	406	CLA	C1-C2-C3	-3.04	121.22	126.20
23	B	615	CLA	C4-C3-C5	3.03	120.50	115.23
23	b	606	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
23	c	509	CLA	O2A-CGA-CBA	3.03	121.08	111.83
23	B	611	CLA	CBC-CAC-C3C	-3.03	104.20	112.42
23	a	408	CLA	C4-C3-C5	3.03	120.49	115.23
23	b	616	CLA	OBD-CAD-C3D	-3.03	121.34	128.42
27	D	412	SQD	O8-S-C6	3.03	111.82	105.97
29	D	406	PL9	C37-C38-C39	-3.03	120.70	127.62
23	C	510	CLA	CHC-C1C-C2C	-3.03	118.35	126.95
23	B	609	CLA	CAC-C3C-C4C	3.03	128.73	124.79
25	A	409	BCR	C24-C23-C22	-3.02	121.76	126.23
32	c	521	LMG	O8-C28-C29	3.02	121.06	111.83
35	h	103	DGD	O2G-C1B-C2B	3.02	118.02	111.48
23	c	507	CLA	CAC-C3C-C4C	3.02	128.72	124.79
25	T	101	BCR	C11-C10-C9	-3.02	123.05	127.28
34	e	101	LMT	C1B-C2B-C3B	3.02	116.35	110.01
33	B	622	HTG	C1-C2-C3	3.02	116.44	110.55
23	B	615	CLA	C4C-C3C-C2C	-3.01	102.50	106.89
23	b	608	CLA	C3C-C4C-NC	3.01	114.29	110.43
24	a	407	PHO	O1D-CGD-CBD	-3.01	120.16	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	C1-C2-C3	-3.01	121.27	126.20
23	a	408	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
23	C	513	CLA	CHC-C1C-C2C	-3.01	118.40	126.95
23	c	515	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
23	b	604	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
23	b	603	CLA	C4-C3-C5	3.01	120.45	115.23
29	d	405	PL9	C51-C49-C50	3.01	121.51	114.59
23	B	601	CLA	CAC-C3C-C4C	3.01	128.70	124.79
29	A	413	PL9	C22-C23-C24	-3.01	120.74	127.62
23	D	403	CLA	CHC-C1C-C2C	-3.00	118.42	126.95
23	a	406	CLA	C4C-C3C-C2C	-3.00	102.52	106.89
23	C	506	CLA	CBC-CAC-C3C	-3.00	104.29	112.42
23	B	603	CLA	C4-C3-C5	3.00	120.43	115.23
31	D	408	LHG	O8-C23-O10	-3.00	116.13	123.63
23	A	405	CLA	C4-C3-C5	3.00	120.43	115.23
23	b	614	CLA	CBC-CAC-C3C	-3.00	104.29	112.42
23	C	514	CLA	C4B-C3B-C2B	-3.00	103.58	107.30
23	c	514	CLA	CMA-C3A-C4A	-3.00	103.72	111.77
32	c	522	LMG	O8-C28-C29	2.99	120.96	111.83
23	b	611	CLA	CHC-C1C-C2C	-2.99	118.45	126.95
29	A	413	PL9	C17-C18-C19	-2.99	120.78	127.62
23	C	511	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
31	A	416	LHG	O8-C23-C24	2.99	120.94	111.83
23	C	506	CLA	C4A-NA-C1A	-2.99	105.32	106.68
23	C	508	CLA	C4B-C3B-C2B	-2.98	103.59	107.30
35	H	102	DGD	O1G-C1A-O1A	-2.98	116.17	123.63
23	c	504	CLA	C1-C2-C3	-2.98	121.31	126.20
23	C	514	CLA	CHD-C4C-NC	2.98	128.85	124.23
23	B	612	CLA	C4-C3-C5	2.98	120.40	115.23
25	B	617	BCR	C33-C5-C6	-2.98	121.23	124.48
23	c	505	CLA	C4-C3-C5	2.98	120.40	115.23
23	C	506	CLA	CMB-C2B-C1B	2.98	129.95	125.42
23	b	606	CLA	C4B-C3B-C2B	-2.97	103.60	107.30
23	c	513	CLA	CHC-C1C-C2C	-2.97	118.50	126.95
23	C	507	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
25	B	619	BCR	C38-C26-C25	-2.97	121.24	124.48
25	d	404	BCR	C29-C30-C25	2.97	114.75	110.44
24	a	407	PHO	CMA-C3A-C4A	-2.97	108.21	114.61
23	b	601	CLA	CHC-C1C-C2C	-2.97	118.51	126.95
23	B	609	CLA	CHC-C1C-C2C	-2.97	118.51	126.95
23	C	514	CLA	C4-C3-C5	2.97	120.38	115.23
23	d	402	CLA	CHC-C1C-C2C	-2.97	118.52	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	C4B-C3B-C2B	-2.97	103.61	107.30
23	C	515	CLA	CHD-C4C-NC	2.96	128.83	124.23
25	k	101	BCR	C24-C23-C22	-2.96	121.85	126.23
23	B	608	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
23	c	515	CLA	O2A-CGA-CBA	2.96	120.86	111.83
23	B	602	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
23	b	611	CLA	CAC-C3C-C4C	2.96	128.64	124.79
32	Z	101	LMG	C4-C3-C2	2.96	116.02	110.83
23	a	404	CLA	CHD-C4C-NC	2.96	128.82	124.23
23	c	506	CLA	CMC-C2C-C1C	2.96	129.65	125.03
23	c	506	CLA	CHC-C1C-C2C	-2.96	118.55	126.95
23	b	604	CLA	O2A-CGA-CBA	2.96	120.85	111.83
23	b	612	CLA	OBD-CAD-C3D	-2.96	121.51	128.42
23	c	510	CLA	C4B-C3B-C2B	-2.95	103.63	107.30
32	d	412	LMG	O7-C10-C11	2.95	117.87	111.48
29	D	406	PL9	C40-C39-C41	2.95	120.35	115.23
23	B	606	CLA	C4-C3-C5	2.95	120.34	115.23
23	c	510	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
31	d	407	LHG	C6-C5-C4	-2.94	104.92	111.78
31	E	101	LHG	O8-C23-C24	2.94	120.81	111.83
23	b	615	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
23	B	616	CLA	O2A-CGA-CBA	2.94	120.81	111.83
23	B	613	CLA	C4-C3-C5	2.94	120.33	115.23
23	b	611	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
23	A	405	CLA	CHC-C1C-C2C	-2.94	118.59	126.95
23	b	614	CLA	CHD-C4C-NC	2.94	128.79	124.23
23	c	511	CLA	CHC-C1C-C2C	-2.94	118.60	126.95
23	c	512	CLA	CHC-C1C-C2C	-2.94	118.60	126.95
23	B	610	CLA	CHC-C1C-C2C	-2.94	118.60	126.95
23	c	512	CLA	CHD-C4C-NC	2.94	128.78	124.23
32	z	101	LMG	O8-C28-C29	2.93	120.78	111.83
38	e	102	HEC	CHA-C1A-NA	2.93	127.65	124.45
25	D	405	BCR	C10-C11-C12	-2.93	114.71	123.20
23	B	603	CLA	CAA-C2A-C3A	-2.93	105.09	113.00
31	d	407	LHG	O7-C7-C8	2.93	117.81	111.48
23	c	508	CLA	CHC-C1C-C2C	-2.93	118.63	126.95
23	a	406	CLA	O2A-CGA-O1A	-2.93	116.31	123.63
35	c	520	DGD	O1G-C1A-C2A	2.93	120.75	111.83
23	c	505	CLA	C1-C2-C3	-2.92	121.41	126.20
23	c	509	CLA	O1D-CGD-CBD	-2.92	118.75	124.52
25	A	409	BCR	C31-C1-C6	-2.92	105.66	110.24
23	A	406	CLA	C3B-C4B-NB	2.92	113.14	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	D	413	LMG	O8-C28-O10	-2.92	116.32	123.63
23	C	507	CLA	CHC-C1C-C2C	-2.92	118.64	126.95
23	A	408	CLA	C4-C3-C5	2.92	120.30	115.23
23	B	604	CLA	CHC-C1C-C2C	-2.92	118.65	126.95
23	b	610	CLA	CHD-C4C-NC	2.92	128.76	124.23
23	C	514	CLA	O2A-CGA-CBA	2.92	120.72	111.83
23	C	514	CLA	CHC-C1C-C2C	-2.91	118.67	126.95
25	T	101	BCR	C15-C14-C13	2.91	131.37	127.28
25	C	516	BCR	C16-C17-C18	-2.91	123.19	127.28
25	b	619	BCR	C39-C30-C25	-2.91	105.68	110.24
23	b	611	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
24	a	417	PHO	C4A-C3A-C2A	-2.91	100.07	102.84
23	C	508	CLA	CMB-C2B-C1B	2.91	129.85	125.42
23	c	506	CLA	C4B-C3B-C2B	-2.91	103.69	107.30
23	C	512	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
24	a	407	PHO	C1A-C2A-C3A	-2.90	100.08	102.84
23	B	609	CLA	C3B-C4B-NB	2.90	113.12	110.53
29	A	413	PL9	C42-C43-C44	-2.90	120.98	127.62
27	a	412	SQD	O48-C23-O10	-2.90	116.37	123.63
29	d	405	PL9	C37-C38-C39	-2.90	120.98	127.62
23	B	610	CLA	CAA-CBA-CGA	-2.90	104.97	113.21
23	c	503	CLA	CBC-CAC-C3C	-2.90	104.56	112.42
35	C	520	DGD	O1G-C1A-C2A	2.90	120.68	111.83
23	C	515	CLA	CMC-C2C-C1C	2.90	129.56	125.03
23	a	408	CLA	CHD-C4C-NC	2.90	128.72	124.23
23	b	612	CLA	CHC-C1C-C2C	-2.89	118.73	126.95
23	c	512	CLA	O2A-CGA-O1A	-2.89	116.39	123.63
23	B	613	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
23	C	511	CLA	O2A-CGA-O1A	-2.89	116.40	123.63
23	b	613	CLA	CMB-C2B-C1B	2.89	129.82	125.42
23	C	512	CLA	O2A-CGA-CBA	2.89	120.64	111.83
23	b	616	CLA	CBC-CAC-C3C	-2.89	104.60	112.42
25	A	409	BCR	C15-C14-C13	-2.89	123.23	127.28
23	c	503	CLA	O2A-CGA-CBA	2.88	120.63	111.83
23	b	615	CLA	C4C-C3C-C2C	-2.88	102.69	106.89
23	B	609	CLA	O2A-CGA-CBA	2.88	120.63	111.83
23	C	510	CLA	C4-C3-C5	2.88	120.23	115.23
25	t	102	BCR	C2-C1-C6	2.88	114.62	110.44
23	B	601	CLA	C2A-C1A-CHA	-2.88	118.87	123.87
34	a	413	LMT	C1B-O5B-C5B	2.88	119.35	113.72
23	b	611	CLA	CMC-C2C-C1C	2.88	129.53	125.03
23	a	406	CLA	CMB-C2B-C1B	2.88	129.80	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	403	CLA	O2A-CGA-O1A	-2.88	116.43	123.63
23	b	607	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
23	B	602	CLA	CMB-C2B-C1B	2.88	129.80	125.42
23	A	404	CLA	CMC-C2C-C1C	2.88	129.53	125.03
23	C	503	CLA	CMB-C2B-C1B	2.87	129.80	125.42
23	a	405	CLA	CMA-C3A-C2A	-2.87	102.87	113.98
23	B	616	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
27	f	101	SQD	O48-C23-C24	2.87	120.59	111.83
23	d	403	CLA	CAC-C3C-C4C	2.87	128.53	124.79
27	a	412	SQD	O7-S-C6	2.87	111.04	106.76
23	c	506	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
31	D	407	LHG	O8-C23-O10	-2.87	116.45	123.63
23	b	610	CLA	CAA-CBA-CGA	-2.87	105.06	113.21
23	C	511	CLA	O2A-CGA-CBA	2.87	120.58	111.83
25	K	101	BCR	C10-C11-C12	-2.87	114.89	123.20
23	C	512	CLA	CHD-C4C-NC	2.87	128.68	124.23
23	B	606	CLA	C4C-C3C-C2C	-2.87	102.72	106.89
23	c	503	CLA	C4B-C3B-C2B	-2.86	103.74	107.30
23	c	513	CLA	C4-C3-C5	2.86	120.20	115.23
25	D	405	BCR	C37-C22-C23	2.86	122.46	118.09
23	a	404	CLA	O2A-CGA-CBA	2.86	120.56	111.83
23	b	613	CLA	C4B-C3B-C2B	-2.86	103.75	107.30
23	b	602	CLA	CMC-C2C-C1C	2.86	129.50	125.03
23	a	408	CLA	CMA-C3A-C2A	-2.86	102.94	113.98
25	B	618	BCR	C37-C22-C23	2.86	122.45	118.09
23	C	505	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
31	D	408	LHG	O8-C23-C24	2.85	120.54	111.83
23	c	515	CLA	C4B-C3B-C2B	-2.85	103.75	107.30
32	D	413	LMG	O8-C28-C29	2.85	120.53	111.83
23	c	503	CLA	CMC-C2C-C1C	2.85	129.49	125.03
23	A	404	CLA	C4C-C3C-C2C	-2.85	102.75	106.89
23	B	615	CLA	CHC-C1C-C2C	-2.85	118.85	126.95
23	C	503	CLA	CBC-CAC-C3C	-2.85	104.70	112.42
23	C	511	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
23	B	616	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
23	C	512	CLA	CAC-C3C-C4C	2.85	128.49	124.79
23	c	511	CLA	C1-O2A-CGA	2.84	123.54	116.65
23	b	605	CLA	CED-O2D-CGD	2.84	122.37	115.92
29	A	413	PL9	C32-C33-C34	-2.84	121.11	127.62
23	b	606	CLA	O2A-CGA-O1A	-2.84	116.52	123.63
23	b	606	CLA	CHD-C4C-NC	2.84	128.64	124.23
23	c	510	CLA	CHD-C4C-NC	2.84	128.64	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	CMC-C2C-C1C	2.84	129.47	125.03
23	a	404	CLA	O2A-CGA-O1A	-2.84	116.52	123.63
23	D	403	CLA	C2A-C1A-CHA	-2.84	118.94	123.87
23	b	605	CLA	O2A-CGA-O1A	-2.84	116.53	123.63
23	b	609	CLA	C4B-C3B-C2B	-2.84	103.77	107.30
23	A	405	CLA	CHD-C4C-NC	2.84	128.63	124.23
23	b	607	CLA	C1-O2A-CGA	2.84	123.52	116.65
23	b	602	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
23	c	509	CLA	CBC-CAC-C3C	-2.83	104.74	112.42
23	C	505	CLA	C3B-C4B-NB	2.83	113.06	110.53
23	B	610	CLA	CMB-C2B-C1B	2.83	129.73	125.42
23	b	603	CLA	CHC-C1C-C2C	-2.83	118.90	126.95
23	D	404	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
23	a	408	CLA	O2A-CGA-O1A	-2.83	116.56	123.63
23	c	503	CLA	C4C-C3C-C2C	-2.83	102.78	106.89
23	B	601	CLA	CHD-C4C-NC	2.83	128.61	124.23
23	b	603	CLA	C2A-C1A-CHA	-2.83	118.96	123.87
23	b	608	CLA	CBC-CAC-C3C	-2.83	104.76	112.42
23	B	611	CLA	C4C-C3C-C2C	-2.83	102.78	106.89
23	b	608	CLA	CHC-C1C-C2C	-2.83	118.92	126.95
23	a	405	CLA	CHC-C1C-C2C	-2.82	118.92	126.95
24	a	417	PHO	CBA-CAA-C2A	-2.82	105.46	113.78
29	A	413	PL9	C53-C6-C1	2.82	121.06	115.28
23	C	508	CLA	C3C-C4C-NC	2.82	114.05	110.43
23	a	406	CLA	C3B-C4B-NB	2.82	113.05	110.53
23	C	511	CLA	CHC-C1C-C2C	-2.82	118.93	126.95
23	b	614	CLA	C4C-C3C-C2C	-2.82	102.79	106.89
31	d	408	LHG	O8-C23-C24	2.82	120.43	111.83
23	C	508	CLA	CMC-C2C-C1C	2.82	129.44	125.03
23	B	608	CLA	CHD-C4C-NC	2.82	128.60	124.23
25	k	101	BCR	C3-C4-C5	-2.82	109.03	114.06
29	D	406	PL9	C51-C49-C50	2.82	121.07	114.59
23	A	408	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
23	B	610	CLA	C3B-C4B-NB	2.81	113.04	110.53
23	b	614	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
23	c	503	CLA	CHC-C1C-C2C	-2.81	118.96	126.95
23	a	408	CLA	CMB-C2B-C1B	2.81	129.70	125.42
23	A	406	CLA	CHC-C1C-C2C	-2.81	118.96	126.95
23	D	403	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
23	B	605	CLA	C2A-C1A-CHA	-2.81	118.99	123.87
23	B	608	CLA	CHC-C1C-C2C	-2.81	118.96	126.95
23	c	503	CLA	CHD-C4C-NC	2.81	128.59	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	C1-C2-C3	-2.81	121.60	126.20
23	c	507	CLA	O2A-CGA-CBA	2.81	120.39	111.83
23	b	616	CLA	O2A-CGA-O1A	-2.81	116.61	123.63
23	D	404	CLA	O2A-CGA-CBA	2.80	120.38	111.83
23	D	404	CLA	CHD-C4C-NC	2.80	128.57	124.23
23	b	614	CLA	C4-C3-C5	2.80	120.09	115.23
23	C	509	CLA	CHC-C1C-C2C	-2.80	118.99	126.95
34	b	627	LMT	C1'-O5'-C5'	2.80	119.19	113.72
23	c	514	CLA	C4C-C3C-C2C	-2.80	102.82	106.89
23	B	613	CLA	C1D-CHD-C4C	-2.80	120.07	126.02
33	b	625	HTG	C1'-S1-C1	2.80	106.49	100.45
23	a	406	CLA	C4B-C3B-C2B	-2.80	103.83	107.30
23	b	605	CLA	CHC-C1C-C2C	-2.79	119.00	126.95
23	c	514	CLA	O2A-CGA-CBA	2.79	120.36	111.83
23	b	606	CLA	CHC-C1C-C2C	-2.79	119.01	126.95
23	B	603	CLA	CMB-C2B-C1B	2.79	129.67	125.42
23	C	505	CLA	C4-C3-C5	2.79	120.07	115.23
23	B	605	CLA	CMC-C2C-C1C	2.79	129.39	125.03
23	c	503	CLA	CAC-C3C-C4C	2.79	128.42	124.79
25	c	516	BCR	C38-C26-C25	-2.78	121.45	124.48
23	c	508	CLA	CMC-C2C-C1C	2.78	129.38	125.03
27	C	501	SQD	O48-C23-O10	-2.78	116.68	123.63
33	B	623	HTG	C1-O5-C5	2.78	117.54	112.56
38	V	201	HEC	C2A-C1A-NA	-2.78	107.64	110.32
23	A	406	CLA	CHD-C4C-NC	2.77	128.53	124.23
23	c	515	CLA	CAA-C2A-C3A	-2.77	105.50	113.00
23	a	406	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
23	b	601	CLA	CMB-C2B-C1B	2.77	129.64	125.42
23	c	505	CLA	C4B-C3B-C2B	-2.77	103.85	107.30
23	d	403	CLA	C1-C2-C3	-2.77	121.66	126.20
23	b	611	CLA	O2A-CGA-O1A	-2.77	116.70	123.63
23	C	508	CLA	C2A-C1A-CHA	-2.77	119.06	123.87
23	B	611	CLA	CMB-C2B-C1B	2.77	129.64	125.42
23	C	503	CLA	C4-C3-C5	2.77	120.03	115.23
23	a	408	CLA	C2A-C1A-CHA	-2.77	119.06	123.87
23	B	602	CLA	CHB-C1B-C2B	-2.77	119.39	127.43
25	t	102	BCR	C1-C6-C7	2.77	123.15	115.65
23	c	504	CLA	C3B-C4B-NB	2.76	113.00	110.53
23	A	408	CLA	CHC-C1C-C2C	-2.76	119.10	126.95
35	C	519	DGD	O1G-C1A-O1A	-2.76	116.72	123.63
35	h	103	DGD	O1G-C1A-C2A	2.76	120.25	111.83
23	c	514	CLA	CHD-C4C-NC	2.76	128.51	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	h	101	HTG	C3-C4-C5	2.76	115.23	110.23
23	B	605	CLA	O2A-CGA-CBA	2.76	120.25	111.83
23	C	503	CLA	C4C-C3C-C2C	-2.76	102.88	106.89
23	C	507	CLA	CMC-C2C-C1C	2.75	129.34	125.03
23	B	611	CLA	CED-O2D-CGD	2.75	122.16	115.92
31	d	407	LHG	O8-C23-O10	-2.75	116.74	123.63
23	C	509	CLA	O2A-CGA-CBA	2.75	120.23	111.83
23	B	601	CLA	CHC-C1C-C2C	-2.75	119.12	126.95
23	c	506	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
24	a	407	PHO	O2D-CGD-O1D	-2.75	118.50	123.85
23	b	601	CLA	O2A-CGA-CBA	2.74	120.20	111.83
23	c	508	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
23	B	604	CLA	O2A-CGA-CBA	2.74	120.20	111.83
23	c	513	CLA	O2A-CGA-CBA	2.74	120.19	111.83
23	B	614	CLA	CAC-C3C-C4C	2.74	128.36	124.79
23	B	616	CLA	CHC-C1C-C2C	-2.74	119.16	126.95
23	c	507	CLA	CHC-C1C-C2C	-2.74	119.16	126.95
25	t	102	BCR	C21-C20-C19	-2.74	115.27	123.20
25	b	617	BCR	C16-C17-C18	-2.74	123.44	127.28
23	c	514	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
23	b	616	CLA	C4B-C3B-C2B	-2.74	103.90	107.30
33	b	625	HTG	O5-C5-C4	2.74	114.63	109.70
23	B	613	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
23	B	606	CLA	CAC-C3C-C4C	2.73	128.34	124.79
27	b	620	SQD	O48-C23-C24	2.73	120.16	111.83
23	C	513	CLA	C1-C2-C3	-2.73	121.72	126.20
23	B	614	CLA	C4C-C3C-C2C	-2.73	102.92	106.89
32	D	413	LMG	O7-C10-C11	2.73	117.39	111.48
23	C	513	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
23	C	515	CLA	C4B-C3B-C2B	-2.73	103.91	107.30
23	B	615	CLA	CAC-C3C-C4C	2.73	128.34	124.79
23	B	604	CLA	CHD-C1D-ND	-2.73	120.96	124.80
25	C	516	BCR	C37-C22-C23	2.73	122.25	118.09
23	C	512	CLA	CHC-C1C-C2C	-2.73	119.20	126.95
25	C	517	BCR	C38-C26-C25	-2.72	121.51	124.48
23	B	610	CLA	CMC-C2C-C1C	2.72	129.29	125.03
23	b	602	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
23	B	603	CLA	O2A-CGA-CBA	2.72	120.14	111.83
23	b	605	CLA	C3B-C4B-NB	2.72	112.96	110.53
25	K	101	BCR	C15-C14-C13	-2.72	123.46	127.28
29	a	415	PL9	C10-C9-C11	2.72	119.95	115.23
33	B	625	HTG	C1'-S1-C1	2.72	106.32	100.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	415	PL9	C32-C33-C34	-2.71	121.41	127.62
23	A	406	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
27	A	411	SQD	O5-C5-C4	2.71	114.59	109.70
25	A	409	BCR	C38-C26-C25	-2.71	121.53	124.48
33	b	622	HTG	C1'-S1-C1	2.71	106.30	100.45
23	b	603	CLA	CAC-C3C-C4C	2.71	128.31	124.79
23	b	611	CLA	CHD-C4C-NC	2.71	128.43	124.23
23	b	611	CLA	CBC-CAC-C3C	-2.71	105.08	112.42
23	b	603	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
25	Y	101	BCR	C34-C9-C8	2.71	122.22	118.09
23	b	602	CLA	CHC-C1C-C2C	-2.71	119.25	126.95
32	Z	101	LMG	C9-C8-C7	-2.71	105.47	111.78
29	D	406	PL9	C25-C24-C26	2.71	119.93	115.23
23	b	615	CLA	C1-C2-C3	-2.71	121.76	126.20
23	B	609	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
23	c	507	CLA	CMC-C2C-C1C	2.70	129.26	125.03
23	C	507	CLA	C4B-C3B-C2B	-2.70	103.94	107.30
23	c	510	CLA	CAA-C2A-C3A	-2.70	105.69	113.00
23	B	602	CLA	O2A-CGA-CBA	2.70	120.08	111.83
32	c	522	LMG	O6-C5-C4	2.70	114.57	109.70
23	C	504	CLA	C3B-C4B-NB	2.70	112.94	110.53
31	D	407	LHG	O7-C7-C8	2.70	117.33	111.48
31	L	101	LHG	O8-C23-C24	2.70	120.07	111.83
23	c	506	CLA	C4-C3-C5	2.70	119.92	115.23
23	c	504	CLA	C4B-C3B-C2B	-2.70	103.94	107.30
23	c	508	CLA	O2A-CGA-O1A	-2.70	116.88	123.63
23	c	504	CLA	C4C-C3C-C2C	-2.70	102.96	106.89
23	b	616	CLA	CHC-C1C-C2C	-2.70	119.28	126.95
29	d	405	PL9	C27-C28-C29	-2.70	121.45	127.62
23	C	509	CLA	CHD-C4C-NC	2.70	128.41	124.23
23	A	406	CLA	O2A-CGA-CBA	2.70	120.06	111.83
23	C	506	CLA	C4C-C3C-C2C	-2.70	102.97	106.89
23	C	506	CLA	C1-O2A-CGA	2.70	123.18	116.65
23	b	602	CLA	C2A-C1A-CHA	-2.69	119.19	123.87
23	C	504	CLA	O2A-CGA-CBA	2.69	120.05	111.83
23	b	614	CLA	O2A-CGA-CBA	2.69	120.05	111.83
23	B	602	CLA	CHD-C4C-NC	2.69	128.41	124.23
25	y	101	BCR	C10-C11-C12	-2.69	115.40	123.20
23	c	515	CLA	CMB-C2B-C1B	2.69	129.52	125.42
23	B	608	CLA	CMA-C3A-C4A	-2.69	104.54	111.77
23	B	608	CLA	O2A-CGA-CBA	2.69	120.04	111.83
23	B	616	CLA	CAC-C3C-C4C	2.69	128.29	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	C4B-C3B-C2B	-2.69	103.96	107.30
23	C	515	CLA	CHC-C1C-C2C	-2.69	119.31	126.95
25	d	404	BCR	C21-C20-C19	-2.69	115.42	123.20
23	c	509	CLA	C4-C3-C5	2.69	119.89	115.23
25	y	101	BCR	C24-C23-C22	-2.69	122.26	126.23
23	a	405	CLA	C1-O2A-CGA	2.68	123.15	116.65
23	C	508	CLA	O2A-CGA-CBA	2.68	120.02	111.83
23	c	512	CLA	CAC-C3C-C4C	2.68	128.28	124.79
25	C	516	BCR	C11-C10-C9	-2.68	123.52	127.28
23	B	610	CLA	CMA-C3A-C4A	-2.68	104.56	111.77
23	B	602	CLA	O2A-CGA-O1A	-2.68	116.92	123.63
23	b	611	CLA	C1-C2-C3	-2.68	121.80	126.20
27	a	410	SQD	O48-C23-C24	2.68	120.01	111.83
23	A	404	CLA	CHC-C1C-C2C	-2.68	119.33	126.95
23	b	606	CLA	C1-O2A-CGA	2.68	123.14	116.65
23	b	609	CLA	CBC-CAC-C3C	-2.68	105.15	112.42
23	C	515	CLA	CAC-C3C-C4C	2.68	128.28	124.79
29	a	415	PL9	C45-C44-C46	2.68	119.88	115.23
25	C	517	BCR	C36-C18-C19	2.68	122.18	118.09
34	B	628	LMT	C1-O1'-C1'	-2.68	109.11	113.68
23	B	605	CLA	CHD-C4C-NC	2.68	128.38	124.23
33	b	625	HTG	C1-O5-C5	2.68	117.36	112.56
23	C	510	CLA	CHD-C4C-NC	2.68	128.38	124.23
23	d	402	CLA	C4C-C3C-C2C	-2.68	103.00	106.89
23	a	406	CLA	O2A-CGA-CBA	2.68	119.99	111.83
23	b	605	CLA	C4B-C3B-C2B	-2.67	103.98	107.30
23	c	509	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
25	B	619	BCR	C29-C30-C25	2.67	114.32	110.44
29	A	413	PL9	C30-C29-C31	2.67	119.87	115.23
23	c	512	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
29	a	415	PL9	C17-C18-C19	-2.67	121.51	127.62
23	B	606	CLA	CBC-CAC-C3C	-2.67	105.18	112.42
23	B	603	CLA	O2A-CGA-O1A	-2.67	116.95	123.63
23	c	514	CLA	O1D-CGD-CBD	-2.67	119.25	124.52
23	B	601	CLA	CMB-C2B-C1B	2.67	129.49	125.42
23	B	607	CLA	O2A-CGA-O1A	-2.67	116.95	123.63
23	b	602	CLA	C11-C12-C13	-2.67	107.09	115.97
23	A	408	CLA	CHD-C4C-NC	2.67	128.37	124.23
23	c	515	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
23	B	605	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
23	c	508	CLA	O2A-CGA-CBA	2.67	119.97	111.83
23	a	405	CLA	C4C-C3C-C2C	-2.67	103.01	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	CAC-C3C-C4C	2.67	128.26	124.79
25	B	619	BCR	C24-C23-C22	-2.67	122.29	126.23
23	c	509	CLA	O2A-CGA-O1A	-2.67	116.96	123.63
23	d	403	CLA	CHC-C1C-C2C	-2.67	119.37	126.95
23	A	404	CLA	CAA-C2A-C1A	-2.67	103.24	111.97
25	c	516	BCR	C16-C17-C18	-2.67	123.54	127.28
23	b	616	CLA	CMC-C2C-C1C	2.66	129.20	125.03
23	b	608	CLA	C4C-C3C-C2C	-2.66	103.01	106.89
23	b	607	CLA	C4-C3-C5	2.66	119.85	115.23
25	H	101	BCR	C24-C23-C22	-2.66	122.30	126.23
23	A	408	CLA	C4B-C3B-C2B	-2.66	103.99	107.30
23	b	608	CLA	C2A-C1A-CHA	-2.66	119.25	123.87
23	a	405	CLA	C2A-C1A-CHA	-2.66	119.25	123.87
23	C	504	CLA	C4-C3-C5	2.66	119.84	115.23
23	d	403	CLA	C4B-C3B-C2B	-2.66	104.00	107.30
23	b	615	CLA	O2A-CGA-CBA	2.66	119.94	111.83
24	A	407	PHO	CBA-CAA-C2A	-2.66	105.95	113.78
23	C	513	CLA	CMC-C2C-C1C	2.66	129.18	125.03
23	B	614	CLA	CMB-C2B-C1B	2.65	129.46	125.42
23	c	514	CLA	CHC-C1C-C2C	-2.65	119.40	126.95
25	H	101	BCR	C11-C10-C9	-2.65	123.56	127.28
27	a	412	SQD	C3-C4-C5	2.65	115.04	110.23
23	b	613	CLA	CMC-C2C-C1C	2.65	129.18	125.03
23	A	408	CLA	CBC-CAC-C3C	-2.65	105.23	112.42
31	d	406	LHG	C5-O7-C7	-2.65	111.45	117.80
23	B	614	CLA	C2A-C1A-CHA	-2.65	119.27	123.87
23	B	613	CLA	O2A-CGA-CBA	2.65	119.91	111.83
33	B	622	HTG	C1-O5-C5	2.65	117.31	112.56
31	a	419	LHG	O8-C23-C24	2.65	119.91	111.83
23	B	611	CLA	CHC-C1C-C2C	-2.65	119.43	126.95
31	b	629	LHG	O8-C23-O10	-2.64	117.01	123.63
27	b	620	SQD	C3-C4-C5	2.64	115.02	110.23
23	a	404	CLA	CHB-C4A-NA	2.64	128.21	124.40
24	A	407	PHO	C4-C3-C5	2.64	119.81	115.23
23	A	404	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
23	C	505	CLA	C4B-C3B-C2B	-2.64	104.02	107.30
23	C	508	CLA	CAA-C2A-C3A	-2.64	105.87	113.00
25	A	409	BCR	C33-C5-C6	-2.64	121.61	124.48
29	a	415	PL9	C53-C6-C1	2.64	120.68	115.28
23	b	603	CLA	CMA-C3A-C2A	-2.64	103.78	113.98
23	c	504	CLA	CHC-C1C-C2C	-2.64	119.45	126.95
29	D	406	PL9	C2-C1-C6	2.63	122.13	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	C4C-C3C-C2C	-2.63	103.06	106.89
29	d	405	PL9	C25-C24-C26	2.63	119.80	115.23
23	C	508	CLA	CGD-CBD-CAD	-2.63	102.33	110.85
31	d	408	LHG	O8-C23-O10	-2.63	117.05	123.63
23	C	506	CLA	CHC-C1C-C2C	-2.63	119.47	126.95
25	T	101	BCR	C21-C20-C19	-2.63	115.58	123.20
23	c	504	CLA	CBC-CAC-C3C	-2.63	105.29	112.42
23	c	505	CLA	O2A-CGA-O1A	-2.63	117.05	123.63
23	c	507	CLA	C3B-C4B-NB	2.63	112.88	110.53
23	c	506	CLA	CHD-C4C-NC	2.63	128.31	124.23
35	c	520	DGD	O3G-C3G-C2G	-2.63	104.43	110.82
38	e	102	HEC	CHA-C4D-ND	2.62	128.62	123.86
23	c	506	CLA	C2A-C1A-CHA	-2.62	119.31	123.87
23	b	609	CLA	CHD-C4C-NC	2.62	128.30	124.23
23	B	614	CLA	C4-C3-C5	2.62	119.78	115.23
23	b	615	CLA	C7-C6-C5	-2.62	106.28	113.26
23	C	504	CLA	CHC-C1C-C2C	-2.62	119.51	126.95
23	b	607	CLA	CMB-C2B-C1B	2.62	129.40	125.42
23	B	610	CLA	C1-C2-C3	-2.61	121.92	126.20
25	t	102	BCR	C37-C22-C23	2.61	122.08	118.09
23	B	611	CLA	O2A-CGA-O1A	-2.61	117.09	123.63
27	D	412	SQD	O48-C23-C24	2.61	119.80	111.83
23	c	503	CLA	C1-C2-C3	-2.61	121.92	126.20
23	C	515	CLA	C2A-C1A-CHA	-2.61	119.34	123.87
23	B	603	CLA	CHD-C4C-NC	2.61	128.28	124.23
23	b	610	CLA	CHC-C1C-C2C	-2.61	119.53	126.95
23	B	611	CLA	C2A-C1A-CHA	-2.61	119.34	123.87
24	a	407	PHO	CBA-CAA-C2A	-2.61	106.10	113.78
23	D	404	CLA	CHC-C1C-C2C	-2.61	119.54	126.95
25	B	618	BCR	C37-C22-C21	-2.60	118.60	122.82
23	b	604	CLA	C4C-C3C-C2C	-2.60	103.10	106.89
23	B	610	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
29	D	406	PL9	C30-C29-C31	2.60	119.74	115.23
23	b	604	CLA	C11-C12-C13	-2.60	107.32	115.97
23	b	610	CLA	C4-C3-C5	2.60	119.74	115.23
23	A	408	CLA	O2A-CGA-CBA	2.60	119.76	111.83
25	t	102	BCR	C7-C6-C5	-2.60	115.57	121.56
23	c	514	CLA	CBA-CAA-C2A	-2.60	106.06	113.79
23	C	513	CLA	CHD-C4C-NC	2.60	128.26	124.23
23	d	403	CLA	C4C-C3C-C2C	-2.60	103.11	106.89
23	B	606	CLA	CHD-C4C-NC	2.60	128.26	124.23
25	B	619	BCR	C7-C8-C9	-2.60	122.39	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	C2A-C1A-CHA	-2.60	119.36	123.87
23	c	509	CLA	C1-C2-C3	-2.59	121.95	126.20
31	D	407	LHG	O8-C23-C24	2.59	119.74	111.83
23	a	404	CLA	CAA-CBA-CGA	-2.59	105.84	113.21
23	b	608	CLA	CHD-C4C-NC	2.59	128.25	124.23
23	b	608	CLA	O2A-CGA-CBA	2.59	119.74	111.83
23	d	403	CLA	C2A-C1A-CHA	-2.59	119.37	123.87
23	b	603	CLA	CHD-C4C-NC	2.59	128.25	124.23
25	C	517	BCR	C15-C16-C17	-2.59	118.22	123.52
23	c	503	CLA	C2A-C1A-CHA	-2.59	119.38	123.87
33	B	623	HTG	C1-C2-C3	2.59	115.61	110.55
23	C	509	CLA	C3B-C4B-NB	2.58	112.83	110.53
23	C	515	CLA	C1-O2A-CGA	2.58	122.90	116.65
23	C	503	CLA	CHC-C1C-C2C	-2.58	119.62	126.95
23	B	604	CLA	CHD-C4C-NC	2.58	128.22	124.23
23	b	609	CLA	CHC-C1C-C2C	-2.57	119.64	126.95
23	c	503	CLA	CMB-C2B-C1B	2.57	129.34	125.42
25	C	517	BCR	C29-C30-C25	2.57	114.17	110.44
25	k	101	BCR	C34-C9-C8	2.57	122.01	118.09
23	b	613	CLA	CED-O2D-CGD	2.57	121.74	115.92
23	b	609	CLA	CAC-C3C-C4C	2.56	128.12	124.79
23	a	405	CLA	O2A-CGA-CBA	2.56	119.65	111.83
25	b	617	BCR	C24-C23-C22	-2.56	122.44	126.23
23	A	408	CLA	CAC-C3C-C4C	2.56	128.12	124.79
23	b	610	CLA	CBC-CAC-C3C	-2.56	105.48	112.42
25	B	619	BCR	C21-C20-C19	-2.56	115.79	123.20
23	B	603	CLA	CHC-C1C-C2C	-2.56	119.68	126.95
23	c	508	CLA	C4-C3-C5	2.55	119.66	115.23
24	A	407	PHO	O2A-CGA-CBA	2.55	119.62	111.83
23	c	513	CLA	CMB-C2B-C1B	2.55	129.30	125.42
23	b	604	CLA	O1D-CGD-CBD	-2.55	119.49	124.52
23	a	405	CLA	CBC-CAC-C3C	-2.55	105.50	112.42
35	c	520	DGD	C2G-O2G-C1B	-2.55	111.69	117.80
23	C	507	CLA	C1-C2-C3	-2.55	122.02	126.20
23	A	408	CLA	CMC-C2C-C1C	2.55	129.02	125.03
23	C	512	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
25	d	404	BCR	C10-C11-C12	-2.55	115.82	123.20
27	a	410	SQD	C45-O47-C7	-2.55	111.70	117.80
23	C	511	CLA	CMB-C2B-C1B	2.55	129.29	125.42
23	a	404	CLA	C2A-C1A-CHA	-2.54	119.45	123.87
25	b	619	BCR	C21-C20-C19	-2.54	115.83	123.20
23	c	515	CLA	CHD-C4C-NC	2.54	128.17	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	CHD-C4C-NC	2.54	128.17	124.23
23	b	606	CLA	CAA-C2A-C3A	-2.54	106.14	113.00
25	Y	101	BCR	C28-C27-C26	-2.54	109.53	114.06
23	C	515	CLA	C4-C3-C5	2.54	119.63	115.23
24	A	415	PHO	CMB-C2B-C3B	2.54	129.75	124.68
23	c	508	CLA	C4C-C3C-C2C	-2.54	103.20	106.89
23	C	515	CLA	O2A-CGA-CBA	2.54	119.57	111.83
23	c	512	CLA	O2A-CGA-CBA	2.54	119.57	111.83
23	A	406	CLA	CMA-C3A-C2A	-2.54	104.18	113.98
38	V	201	HEC	C3D-C4D-ND	-2.54	107.34	110.15
23	D	403	CLA	CMC-C2C-C1C	2.53	128.99	125.03
23	C	504	CLA	CAC-C3C-C4C	2.53	128.09	124.79
25	c	517	BCR	C38-C26-C25	-2.53	121.72	124.48
29	A	413	PL9	C40-C39-C41	2.53	119.62	115.23
23	B	608	CLA	CBC-CAC-C3C	-2.53	105.57	112.42
25	A	409	BCR	C16-C17-C18	-2.53	123.74	127.28
25	C	516	BCR	C20-C21-C22	-2.52	123.74	127.28
23	C	504	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
23	b	615	CLA	CHD-C4C-NC	2.52	128.14	124.23
25	T	101	BCR	C1-C6-C7	2.52	122.49	115.65
23	C	504	CLA	CHD-C4C-NC	2.52	128.14	124.23
23	C	507	CLA	CHD-C4C-NC	2.52	128.14	124.23
25	T	101	BCR	C29-C30-C25	2.52	114.10	110.44
23	B	609	CLA	C4-C3-C5	2.52	119.60	115.23
23	c	513	CLA	C2A-C1A-CHA	-2.52	119.50	123.87
23	c	505	CLA	CHC-C1C-C2C	-2.52	119.80	126.95
29	d	405	PL9	C20-C19-C21	2.52	119.60	115.23
25	D	405	BCR	C21-C20-C19	-2.52	115.91	123.20
23	B	613	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
27	A	411	SQD	O48-C23-O10	-2.51	117.34	123.63
31	d	407	LHG	O8-C23-C24	2.51	119.49	111.83
27	D	412	SQD	C1-O5-C5	-2.51	108.82	113.72
25	C	517	BCR	C37-C22-C23	2.51	121.92	118.09
25	Y	101	BCR	C36-C18-C19	2.51	121.92	118.09
23	b	615	CLA	CBC-CAC-C3C	-2.51	105.62	112.42
23	b	616	CLA	CAC-C3C-C4C	2.51	128.05	124.79
23	c	504	CLA	C2A-C1A-CHA	-2.51	119.52	123.87
33	B	622	HTG	O2-C2-C3	-2.51	104.47	110.38
23	b	602	CLA	CHD-C4C-NC	2.51	128.12	124.23
23	B	603	CLA	C2A-C1A-CHA	-2.51	119.52	123.87
23	c	510	CLA	CMB-C2B-C1B	2.50	129.23	125.42
25	h	102	BCR	C16-C17-C18	-2.50	123.77	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	k	101	BCR	C11-C10-C9	-2.50	123.77	127.28
35	H	102	DGD	O2G-C1B-C2B	2.50	116.90	111.48
25	B	618	BCR	C28-C27-C26	-2.50	109.59	114.06
23	D	403	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
23	b	608	CLA	C4-C3-C5	2.50	119.56	115.23
25	b	619	BCR	C8-C9-C10	2.50	122.94	119.01
23	B	616	CLA	CMB-C2B-C1B	2.50	129.22	125.42
23	C	509	CLA	O2A-CGA-O1A	-2.50	117.39	123.63
25	D	405	BCR	C29-C30-C25	2.49	114.06	110.44
25	D	405	BCR	C40-C30-C25	-2.49	106.33	110.24
25	t	102	BCR	C7-C8-C9	-2.49	122.55	126.23
23	c	512	CLA	C4C-C3C-C2C	-2.49	103.26	106.89
23	c	506	CLA	CMB-C2B-C1B	2.49	129.22	125.42
23	A	405	CLA	CMA-C3A-C4A	-2.49	105.07	111.77
23	b	609	CLA	O2A-CGA-CBA	2.49	119.43	111.83
23	b	602	CLA	C4-C3-C5	2.49	119.55	115.23
23	c	505	CLA	C2A-C1A-CHA	-2.49	119.54	123.87
23	c	512	CLA	C11-C10-C8	-2.49	107.69	115.97
23	a	406	CLA	CHC-C1C-C2C	-2.49	119.87	126.95
23	c	510	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
23	B	611	CLA	OBD-CAD-C3D	-2.49	122.60	128.42
29	a	415	PL9	C7-C8-C9	-2.48	122.55	126.83
25	y	101	BCR	C16-C17-C18	-2.48	123.80	127.28
25	D	405	BCR	C33-C5-C6	-2.48	121.78	124.48
25	k	101	BCR	C36-C18-C19	2.48	121.88	118.09
23	b	602	CLA	CMA-C3A-C2A	-2.48	104.39	113.98
23	b	615	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
25	C	517	BCR	C3-C4-C5	-2.48	109.63	114.06
33	B	623	HTG	O5-C1-C2	2.48	113.73	110.32
25	b	618	BCR	C3-C4-C5	-2.48	109.64	114.06
23	c	510	CLA	C6-C7-C8	-2.48	107.73	115.97
24	a	417	PHO	C4-C3-C2	-2.48	117.26	123.63
23	a	404	CLA	CMA-C3A-C2A	-2.48	104.40	113.98
23	B	608	CLA	CAC-C3C-C4C	2.48	128.01	124.79
35	c	519	DGD	O1G-C1A-C2A	2.48	119.38	111.83
23	b	614	CLA	C2A-C1A-CHA	-2.47	119.57	123.87
23	a	404	CLA	C4C-C3C-C2C	-2.47	103.29	106.89
23	C	505	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
33	h	101	HTG	C1-C2-C3	-2.47	105.71	110.55
23	B	614	CLA	CAA-C2A-C3A	-2.47	106.31	113.00
25	B	617	BCR	C16-C17-C18	-2.47	123.81	127.28
23	D	403	CLA	C4C-C3C-C2C	-2.47	103.29	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	514	CLA	CHB-C4A-NA	2.47	127.97	124.40
25	T	101	BCR	C16-C17-C18	-2.47	123.81	127.28
23	b	601	CLA	C2A-C1A-CHA	-2.47	119.58	123.87
23	B	608	CLA	CMC-C2C-C1C	2.47	128.89	125.03
34	M	101	LMT	O1'-C1'-C2'	2.47	112.02	108.27
23	c	513	CLA	CAC-C3C-C4C	2.47	128.00	124.79
23	c	511	CLA	CAA-C2A-C3A	-2.47	106.34	113.00
23	b	606	CLA	C1-C2-C3	-2.46	122.16	126.20
23	c	506	CLA	CAA-C2A-C3A	-2.46	106.35	113.00
34	M	103	LMT	C1'-O5'-C5'	2.46	118.52	113.72
24	A	407	PHO	CMB-C2B-C3B	2.46	129.59	124.68
24	A	415	PHO	OBD-CAD-C3D	-2.46	124.06	127.89
23	b	611	CLA	C2A-C1A-CHA	-2.46	119.60	123.87
23	b	614	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
29	d	405	PL9	C35-C34-C36	2.45	119.48	115.23
25	C	516	BCR	C23-C24-C25	-2.45	120.45	127.00
27	A	411	SQD	O7-S-C6	2.45	110.41	106.76
35	C	518	DGD	O1G-C1A-O1A	-2.45	117.50	123.63
25	Y	101	BCR	C38-C26-C25	-2.45	121.82	124.48
23	A	405	CLA	C2A-C1A-CHA	-2.44	119.62	123.87
29	D	406	PL9	C27-C28-C29	-2.44	122.03	127.62
23	B	609	CLA	C1-O2A-CGA	2.44	122.56	116.65
25	B	619	BCR	C10-C11-C12	-2.44	116.13	123.20
23	b	609	CLA	CMC-C2C-C1C	2.44	128.84	125.03
23	c	510	CLA	C4-C3-C5	2.44	119.46	115.23
23	b	607	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
31	d	406	LHG	O7-C7-O9	-2.44	118.01	123.70
25	y	101	BCR	C21-C20-C19	-2.44	116.14	123.20
23	B	616	CLA	CMC-C2C-C1C	2.43	128.84	125.03
23	c	509	CLA	C4C-C3C-C2C	-2.43	103.35	106.89
23	C	513	CLA	CMB-C2B-C1B	2.43	129.12	125.42
23	B	614	CLA	C4B-C3B-C2B	-2.43	104.28	107.30
23	A	405	CLA	C4C-C3C-C2C	-2.43	103.35	106.89
23	b	608	CLA	C11-C10-C8	-2.43	107.88	115.97
23	c	515	CLA	C2A-C1A-CHA	-2.43	119.65	123.87
23	b	606	CLA	CHB-C1B-C2B	-2.43	120.38	127.43
25	b	617	BCR	C40-C30-C25	-2.43	106.44	110.24
23	b	602	CLA	CMB-C2B-C1B	2.43	129.11	125.42
32	C	521	LMG	O8-C28-O10	-2.42	117.56	123.63
23	b	603	CLA	CMC-C2C-C1C	2.42	128.82	125.03
38	V	201	HEC	CAD-CBD-CGD	-2.42	107.24	113.67
23	c	509	CLA	CAC-C3C-C4C	2.42	127.94	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	C2A-C1A-CHA	-2.42	119.66	123.87
23	a	405	CLA	CAA-CBA-CGA	2.42	120.08	113.21
23	C	503	CLA	OBD-CAD-C3D	-2.42	122.76	128.42
38	E	103	HEC	O2D-CGD-CBD	2.42	121.64	114.00
23	b	603	CLA	CBC-CAC-C3C	-2.42	105.87	112.42
23	c	507	CLA	CBC-CAC-C3C	-2.42	105.87	112.42
38	E	103	HEC	CBB-CAB-C3B	-2.42	122.61	127.43
23	d	403	CLA	CMA-C3A-C2A	-2.42	104.64	113.98
23	c	504	CLA	O2A-CGA-CBA	2.42	119.20	111.83
25	c	516	BCR	C33-C5-C6	-2.41	121.85	124.48
25	h	102	BCR	C36-C18-C17	-2.41	118.91	122.82
23	A	405	CLA	OBD-CAD-C3D	-2.41	122.78	128.42
23	C	510	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
25	k	101	BCR	C2-C1-C6	2.41	113.94	110.44
23	D	403	CLA	CHD-C4C-NC	2.41	127.97	124.23
23	B	608	CLA	CHB-C4A-NA	2.41	127.88	124.40
38	E	103	HEC	C2A-C1A-NA	-2.41	108.00	110.32
23	b	607	CLA	CHD-C4C-NC	2.41	127.96	124.23
23	C	512	CLA	C4C-C3C-C2C	-2.41	103.39	106.89
23	B	615	CLA	C2A-C1A-CHA	-2.40	119.70	123.87
23	B	605	CLA	CHC-C1C-C2C	-2.40	120.12	126.95
23	b	606	CLA	C2A-C1A-CHA	-2.40	119.70	123.87
25	b	619	BCR	C15-C14-C13	-2.40	123.91	127.28
23	D	404	CLA	C4-C3-C5	2.40	119.39	115.23
31	L	101	LHG	O4-P-O5	2.40	123.61	112.44
25	T	101	BCR	C12-C13-C14	-2.40	115.24	119.01
23	B	609	CLA	C2A-C1A-CHA	-2.40	119.71	123.87
23	C	509	CLA	CBC-CAC-C3C	-2.40	105.93	112.42
23	c	508	CLA	CGD-CBD-CAD	-2.40	103.09	110.85
38	v	202	HEC	C2A-C1A-NA	-2.40	108.01	110.32
34	t	101	LMT	O1'-C1'-C2'	2.39	111.91	108.27
23	B	612	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
23	C	510	CLA	CHB-C4A-NA	2.39	127.85	124.40
23	A	404	CLA	CHD-C4C-NC	2.39	127.94	124.23
38	e	102	HEC	C4C-NC-C1C	2.39	109.72	105.82
27	f	101	SQD	O47-C7-O49	-2.39	118.11	123.70
23	b	616	CLA	C4-C3-C5	2.39	119.38	115.23
23	B	611	CLA	C4-C3-C5	2.39	119.38	115.23
23	b	607	CLA	CMC-C2C-C1C	2.39	128.77	125.03
23	B	608	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
25	y	101	BCR	C1-C6-C7	2.39	122.13	115.65
24	a	407	PHO	O2A-CGA-O1A	-2.39	117.66	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
23	C	508	CLA	C4C-C3C-C2C	-2.38	103.42	106.89
25	a	409	BCR	C7-C8-C9	-2.38	122.71	126.23
25	T	101	BCR	C3-C4-C5	-2.38	109.80	114.06
23	b	612	CLA	CHD-C4C-NC	2.38	127.93	124.23
35	c	518	DGD	C2G-O2G-C1B	-2.38	112.09	117.80
23	c	515	CLA	CED-O2D-CGD	2.38	121.31	115.92
23	c	506	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
29	A	413	PL9	C45-C44-C46	2.38	119.35	115.23
23	b	608	CLA	O2A-CGA-O1A	-2.38	117.69	123.63
25	C	517	BCR	C21-C20-C19	-2.38	116.32	123.20
25	C	517	BCR	C11-C10-C9	-2.38	123.95	127.28
27	D	412	SQD	O47-C7-O49	-2.37	118.15	123.70
23	c	512	CLA	CMB-C2B-C1B	2.37	129.03	125.42
23	b	610	CLA	C4B-C3B-C2B	-2.37	104.35	107.30
23	C	504	CLA	CMC-C2C-C1C	2.37	128.74	125.03
23	A	405	CLA	CAA-CBA-CGA	2.37	119.94	113.21
25	b	619	BCR	C29-C30-C25	2.37	113.88	110.44
25	H	101	BCR	C10-C11-C12	-2.37	116.33	123.20
23	c	514	CLA	C3B-C4B-NB	2.37	112.64	110.53
23	b	609	CLA	C4-C3-C5	2.37	119.34	115.23
23	C	506	CLA	OBD-CAD-C3D	-2.36	122.89	128.42
23	C	503	CLA	CAC-C3C-C4C	2.36	127.86	124.79
23	B	606	CLA	OBD-CAD-C3D	-2.36	122.89	128.42
23	B	602	CLA	C1-C2-C3	-2.36	122.33	126.20
23	B	615	CLA	C1-C2-C3	-2.36	122.33	126.20
38	E	103	HEC	O2A-CGA-CBA	2.36	121.47	114.00
23	C	507	CLA	C4-C3-C5	2.36	119.33	115.23
27	b	620	SQD	O7-S-C6	2.36	110.28	106.76
27	f	101	SQD	C46-C45-C44	-2.36	106.28	111.78
23	c	513	CLA	CBC-CAC-C3C	-2.36	106.02	112.42
25	Y	101	BCR	C10-C11-C12	-2.36	116.36	123.20
23	B	616	CLA	C1-O2A-CGA	2.36	122.36	116.65
23	C	506	CLA	CAA-C2A-C3A	-2.36	106.62	113.00
25	c	517	BCR	C15-C16-C17	-2.36	118.69	123.52
32	c	522	LMG	O8-C28-O10	-2.36	117.73	123.63
23	B	607	CLA	CAC-C3C-C4C	2.36	127.86	124.79
23	C	513	CLA	C1-O2A-CGA	2.36	122.35	116.65
23	a	404	CLA	CAA-C2A-C1A	-2.36	104.26	111.97
23	B	612	CLA	C2A-C1A-CHA	-2.36	119.78	123.87
23	C	504	CLA	C2A-C1A-CHA	-2.35	119.78	123.87
27	b	620	SQD	O8-S-C6	2.35	110.51	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	CMC-C2C-C1C	2.35	128.71	125.03
23	b	607	CLA	CAA-CBA-CGA	2.35	119.87	113.21
23	a	408	CLA	CHC-C1C-C2C	-2.35	120.28	126.95
25	b	618	BCR	C11-C10-C9	-2.35	123.99	127.28
23	a	408	CLA	OBD-CAD-C3D	-2.35	122.93	128.42
23	B	601	CLA	CAA-C2A-C3A	-2.35	106.66	113.00
23	B	616	CLA	C2A-C1A-CHA	-2.35	119.80	123.87
23	B	615	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
23	C	506	CLA	C2A-C1A-CHA	-2.34	119.80	123.87
23	B	609	CLA	CMC-C2C-C1C	2.34	128.69	125.03
25	T	101	BCR	C7-C6-C5	-2.34	116.16	121.56
24	a	417	PHO	O1D-CGD-CBD	-2.34	121.17	124.72
23	C	506	CLA	CHD-C4C-NC	2.34	127.86	124.23
23	C	512	CLA	CMB-C2B-C1B	2.34	128.98	125.42
23	b	604	CLA	CHD-C4C-NC	2.34	127.86	124.23
23	C	512	CLA	C4-C3-C2	-2.34	117.62	123.63
25	c	516	BCR	C20-C21-C22	-2.34	124.00	127.28
23	d	403	CLA	C4-C3-C5	2.34	119.29	115.23
23	B	603	CLA	CAC-C3C-C4C	2.34	127.83	124.79
25	h	102	BCR	C10-C11-C12	-2.34	116.42	123.20
23	A	408	CLA	CMA-C3A-C2A	-2.34	104.94	113.98
25	c	517	BCR	C21-C20-C19	-2.34	116.43	123.20
23	c	509	CLA	CHC-C1C-C2C	-2.34	120.31	126.95
25	b	617	BCR	C39-C30-C25	-2.34	106.58	110.24
34	B	628	LMT	O1B-C4'-C3'	2.33	113.17	107.23
23	d	402	CLA	C2A-C1A-CHA	-2.33	119.82	123.87
23	a	408	CLA	CMC-C2C-C1C	2.33	128.68	125.03
23	B	615	CLA	C11-C10-C8	-2.33	108.21	115.97
23	b	605	CLA	C1-C2-C3	-2.33	122.37	126.20
23	B	607	CLA	C2A-C1A-CHA	-2.33	119.82	123.87
23	b	601	CLA	C1-O2A-CGA	2.33	122.30	116.65
23	b	614	CLA	CMB-C2B-C1B	2.33	128.97	125.42
34	a	418	LMT	C1B-O1B-C4'	-2.33	112.46	117.98
32	m	101	LMG	O8-C28-O10	-2.33	117.80	123.63
23	B	608	CLA	C2A-C1A-CHA	-2.33	119.83	123.87
23	d	402	CLA	CHD-C4C-NC	2.33	127.84	124.23
35	H	102	DGD	C3G-O3G-C1D	-2.33	108.81	113.80
23	c	506	CLA	CBC-CAC-C3C	-2.33	106.11	112.42
25	h	102	BCR	C34-C9-C8	2.33	121.64	118.09
23	c	505	CLA	O2A-CGA-CBA	2.32	118.92	111.83
23	c	511	CLA	CMB-C2B-C1B	2.32	128.95	125.42
34	t	101	LMT	O5'-C5'-C4'	2.32	114.52	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	C4-C3-C5	2.32	119.25	115.23
23	A	406	CLA	CAC-C3C-C4C	2.32	127.81	124.79
23	b	602	CLA	O2A-CGA-CBA	2.32	118.90	111.83
23	C	508	CLA	CHD-C4C-NC	2.32	127.83	124.23
23	B	607	CLA	O2A-CGA-CBA	2.32	118.90	111.83
23	C	505	CLA	O2A-CGA-CBA	2.31	118.89	111.83
23	c	513	CLA	CMC-C2C-C1C	2.31	128.65	125.03
38	e	102	HEC	O2D-CGD-CBD	2.31	121.30	114.00
23	B	605	CLA	C3B-C4B-NB	2.31	112.59	110.53
25	H	101	BCR	C29-C30-C25	2.31	113.79	110.44
29	D	406	PL9	O2-C1-C6	-2.31	116.81	120.48
25	a	409	BCR	C3-C4-C5	-2.31	109.94	114.06
35	c	519	DGD	O6E-C5E-C6E	2.31	112.16	106.44
23	C	504	CLA	CBC-CAC-C3C	-2.31	106.16	112.42
35	c	518	DGD	O1G-C1A-O1A	-2.31	117.86	123.63
23	C	513	CLA	O2A-CGA-CBA	2.31	118.86	111.83
23	c	507	CLA	C4B-C3B-C2B	-2.30	104.44	107.30
23	c	507	CLA	O2A-CGA-O1A	-2.30	117.86	123.63
23	b	606	CLA	CAC-C3C-C4C	2.30	127.78	124.79
35	c	518	DGD	O3G-C3G-C2G	-2.30	105.22	110.82
23	b	606	CLA	CBC-CAC-C3C	-2.30	106.18	112.42
38	E	103	HEC	CBA-CAA-C2A	-2.30	106.17	112.53
23	B	602	CLA	CHC-C1C-C2C	-2.30	120.41	126.95
27	f	101	SQD	O5-C1-C2	2.30	115.10	110.37
24	A	415	PHO	C4A-C3A-C2A	-2.30	100.65	102.84
23	B	612	CLA	CHD-C4C-NC	2.30	127.80	124.23
23	C	511	CLA	CHD-C4C-NC	2.30	127.80	124.23
27	a	410	SQD	O47-C7-O49	-2.30	118.33	123.70
23	a	405	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
23	c	515	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
23	B	614	CLA	OBD-CAD-C3D	-2.29	123.06	128.42
38	e	102	HEC	CHB-C1B-NB	2.29	128.02	123.86
31	A	416	LHG	C5-O7-C7	-2.29	112.32	117.80
25	b	619	BCR	C34-C9-C10	-2.29	119.11	122.82
23	B	604	CLA	CMC-C2C-C1C	2.29	128.61	125.03
25	y	101	BCR	C37-C22-C23	2.29	121.58	118.09
23	C	514	CLA	OBD-CAD-C3D	-2.29	123.07	128.42
23	d	402	CLA	C4-C3-C2	-2.29	117.75	123.63
25	t	102	BCR	C20-C21-C22	-2.29	124.07	127.28
25	Y	101	BCR	C29-C30-C25	2.28	113.76	110.44
25	c	517	BCR	C32-C1-C6	-2.28	106.66	110.24
35	C	518	DGD	O1G-C1A-C2A	2.28	118.80	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	514	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
25	A	409	BCR	C36-C18-C19	2.28	121.57	118.09
23	B	614	CLA	C1-C2-C3	-2.28	122.46	126.20
23	B	616	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
23	b	609	CLA	C3B-C4B-NB	2.28	112.56	110.53
23	C	507	CLA	O2A-CGA-O1A	-2.28	117.94	123.63
23	b	607	CLA	CMA-C3A-C2A	-2.27	105.19	113.98
23	C	510	CLA	CAC-C3C-C4C	2.27	127.75	124.79
23	c	513	CLA	C1-O2A-CGA	2.27	122.16	116.65
23	A	404	CLA	CHB-C4A-NA	2.27	127.68	124.40
23	C	506	CLA	CAC-C3C-C4C	2.27	127.75	124.79
34	B	630	LMT	C1'-O5'-C5'	2.27	118.16	113.72
23	A	408	CLA	C2A-C1A-CHA	-2.27	119.93	123.87
23	b	606	CLA	CMC-C2C-C1C	2.27	128.58	125.03
25	Y	101	BCR	C21-C20-C19	-2.27	116.63	123.20
23	c	508	CLA	CAC-C3C-C4C	2.27	127.74	124.79
25	K	101	BCR	C29-C30-C25	2.27	113.73	110.44
32	C	502	LMG	O8-C28-C29	2.27	118.74	111.83
25	B	619	BCR	C37-C22-C21	-2.27	119.15	122.82
24	a	407	PHO	CBC-CAC-C3C	-2.27	109.63	112.87
25	B	617	BCR	C29-C30-C25	2.26	113.73	110.44
23	C	512	CLA	C2A-C1A-CHA	-2.26	119.94	123.87
23	A	405	CLA	CMA-C3A-C2A	-2.26	105.23	113.98
23	c	504	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
35	h	103	DGD	O4D-C4D-C3D	-2.26	105.04	110.38
23	b	611	CLA	OBD-CAD-C3D	-2.26	123.13	128.42
25	h	102	BCR	C24-C23-C22	-2.26	122.89	126.23
25	Y	101	BCR	C1-C6-C7	2.26	121.78	115.65
25	b	619	BCR	C16-C17-C18	-2.26	124.11	127.28
23	c	515	CLA	CBC-CAC-C3C	-2.26	106.30	112.42
23	C	506	CLA	C4-C3-C5	2.25	119.14	115.23
29	a	415	PL9	C35-C34-C36	2.25	119.14	115.23
23	b	616	CLA	CMB-C2B-C1B	2.25	128.85	125.42
23	B	607	CLA	C1-O2A-CGA	2.25	122.10	116.65
23	B	609	CLA	CHD-C4C-NC	2.25	127.72	124.23
35	c	518	DGD	O6D-C1D-O3G	-2.25	104.73	110.04
32	Z	101	LMG	C1-O6-C5	2.25	118.11	113.72
23	B	603	CLA	CMA-C3A-C2A	-2.25	105.28	113.98
23	c	509	CLA	CHB-C1B-C2B	-2.25	120.90	127.43
23	b	615	CLA	C11-C12-C13	-2.25	108.49	115.97
23	C	514	CLA	CBC-CAC-C3C	-2.25	106.33	112.42
23	d	402	CLA	CBC-CAC-C3C	-2.25	106.33	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	C1-O2A-CGA	2.24	122.08	116.65
27	B	620	SQD	O48-C23-O10	-2.24	118.02	123.63
32	m	101	LMG	C9-C8-C7	-2.24	106.56	111.78
23	B	608	CLA	C11-C12-C13	-2.24	108.52	115.97
23	B	607	CLA	CHD-C4C-NC	2.24	127.70	124.23
23	A	404	CLA	CMA-C3A-C2A	-2.24	105.34	113.98
23	c	506	CLA	O2A-CGA-CBA	2.24	118.65	111.83
23	d	402	CLA	O2A-CGA-O1A	-2.24	118.04	123.63
32	B	621	LMG	O8-C28-O10	-2.24	118.04	123.63
23	C	514	CLA	CHB-C4A-NA	2.23	127.62	124.40
34	m	103	LMT	O6'-C6'-C5'	-2.23	103.73	111.33
23	B	611	CLA	O2A-CGA-CBA	2.23	118.64	111.83
25	a	409	BCR	C10-C11-C12	-2.23	116.73	123.20
27	f	101	SQD	O8-S-C6	2.23	110.28	105.97
29	D	406	PL9	C32-C33-C34	-2.23	122.52	127.62
25	K	101	BCR	C36-C18-C19	2.23	121.49	118.09
23	c	515	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
25	B	619	BCR	C37-C22-C23	2.23	121.49	118.09
25	Y	101	BCR	C35-C13-C12	2.23	121.49	118.09
25	T	101	BCR	C2-C1-C6	2.22	113.67	110.44
23	b	612	CLA	C2A-C1A-CHA	-2.22	120.01	123.87
34	M	101	LMT	O1B-C1B-C2B	2.22	113.56	108.09
32	c	521	LMG	O8-C28-O10	-2.22	118.06	123.63
23	B	613	CLA	CBC-CAC-C3C	-2.22	106.39	112.42
23	D	404	CLA	C1-O2A-CGA	2.22	122.03	116.65
25	C	516	BCR	C38-C26-C25	-2.22	122.06	124.48
23	a	406	CLA	CAC-C3C-C4C	2.22	127.68	124.79
23	C	505	CLA	CMC-C2C-C1C	2.22	128.50	125.03
23	C	509	CLA	C4B-C3B-C2B	-2.22	104.54	107.30
23	b	613	CLA	CHB-C4A-NA	2.22	127.61	124.40
23	B	604	CLA	C6-C7-C8	-2.22	108.58	115.97
29	A	413	PL9	C35-C34-C36	2.22	119.08	115.23
25	b	618	BCR	C15-C16-C17	-2.22	118.97	123.52
23	A	405	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
32	z	101	LMG	C8-O7-C10	-2.22	112.49	117.80
23	c	503	CLA	OBD-CAD-C3D	-2.22	123.23	128.42
23	b	601	CLA	CAA-C2A-C3A	-2.22	107.01	113.00
23	C	506	CLA	O2A-CGA-CBA	2.21	118.58	111.83
23	D	403	CLA	C4-C3-C5	2.21	119.07	115.23
31	A	416	LHG	O7-C7-O9	-2.21	118.54	123.70
23	c	507	CLA	C2A-C1A-CHA	-2.21	120.03	123.87
23	C	510	CLA	C1-C2-C3	-2.21	122.58	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	501	SQD	O9-S-O7	-2.21	106.64	113.82
23	A	408	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
24	A	407	PHO	CMC-C2C-C1C	2.20	128.70	124.73
29	D	406	PL9	C25-C24-C23	-2.20	117.97	123.63
23	B	601	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
23	B	605	CLA	C1-C2-C3	-2.20	122.59	126.20
23	a	406	CLA	CBC-CAC-C3C	-2.20	106.46	112.42
23	B	602	CLA	C2A-C1A-CHA	-2.20	120.05	123.87
32	c	501	LMG	C30-C29-C28	-2.20	105.64	113.69
29	d	405	PL9	C22-C23-C24	-2.20	122.59	127.62
23	C	511	CLA	C2A-C1A-CHA	-2.20	120.05	123.87
23	a	408	CLA	CBC-CAC-C3C	-2.20	106.46	112.42
23	C	504	CLA	C4B-C3B-C2B	-2.20	104.57	107.30
38	E	103	HEC	CMD-C2D-C1D	2.20	128.76	125.42
23	A	405	CLA	CHB-C4A-NA	2.20	127.57	124.40
25	c	517	BCR	C24-C23-C22	-2.20	122.99	126.23
34	B	628	LMT	O1B-C4'-C5'	-2.20	103.72	109.48
25	b	618	BCR	C37-C22-C21	-2.19	119.26	122.82
23	B	615	CLA	CBC-CAC-C3C	-2.19	106.47	112.42
35	C	520	DGD	O1G-C1A-O1A	-2.19	118.14	123.63
32	d	412	LMG	O8-C28-C29	2.19	118.52	111.83
35	C	520	DGD	O6E-C1E-O5D	-2.19	104.86	110.04
23	b	611	CLA	CMB-C2B-C1B	2.19	128.76	125.42
23	c	507	CLA	CHD-C4C-NC	2.19	127.63	124.23
23	B	605	CLA	CAA-C2A-C3A	-2.19	107.08	113.00
23	D	404	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
23	a	406	CLA	C2A-C1A-CHA	-2.19	120.07	123.87
25	D	405	BCR	C3-C4-C5	-2.19	110.16	114.06
23	C	508	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
23	C	509	CLA	C1-C2-C3	-2.19	122.61	126.20
29	a	415	PL9	C30-C29-C31	2.18	119.02	115.23
25	B	617	BCR	C34-C9-C10	-2.18	119.28	122.82
23	b	601	CLA	CBC-CAC-C3C	-2.18	106.50	112.42
23	B	608	CLA	CAA-C2A-C3A	-2.18	107.10	113.00
27	D	412	SQD	O5-C1-C2	-2.18	105.89	110.37
24	A	415	PHO	C6-C5-C3	-2.18	108.16	113.47
27	f	101	SQD	O7-S-C6	2.18	110.01	106.76
29	d	405	PL9	C36-C34-C33	-2.18	116.27	121.17
23	B	606	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
23	C	503	CLA	CAA-C2A-C3A	-2.18	107.11	113.00
23	B	602	CLA	C11-C12-C13	-2.18	108.73	115.97
23	B	604	CLA	CHA-C1A-NA	-2.18	121.46	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	CHD-C4C-NC	2.18	127.61	124.23
25	Y	101	BCR	C11-C10-C9	-2.18	124.23	127.28
23	B	613	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
25	c	516	BCR	C28-C27-C26	-2.17	110.19	114.06
23	c	506	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
23	c	511	CLA	CHD-C4C-NC	2.17	127.60	124.23
23	C	515	CLA	CBC-CAC-C3C	-2.17	106.54	112.42
23	B	605	CLA	C4B-C3B-C2B	-2.17	104.60	107.30
23	b	609	CLA	CAA-C2A-C3A	-2.17	107.14	113.00
35	c	518	DGD	O1G-C1A-C2A	2.17	118.45	111.83
23	B	601	CLA	C4-C3-C5	2.17	118.99	115.23
37	d	401	BCT	O2-C-O1	2.17	125.22	119.68
23	B	610	CLA	CHD-C4C-NC	2.17	127.59	124.23
23	b	613	CLA	CMA-C3A-C4A	-2.17	105.95	111.77
23	b	610	CLA	O1D-CGD-CBD	-2.17	120.25	124.52
38	E	103	HEC	CHB-C1B-NB	2.17	127.79	123.86
27	B	620	SQD	O5-C5-C4	2.17	113.60	109.70
23	A	408	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
23	B	606	CLA	O2A-CGA-CBA	2.16	118.43	111.83
23	a	405	CLA	CAC-C3C-C2C	2.16	131.53	127.56
23	B	612	CLA	OBD-CAD-C3D	-2.16	123.37	128.42
29	a	415	PL9	C47-C48-C49	-2.16	120.44	127.64
25	c	516	BCR	C8-C7-C6	-2.16	121.23	127.00
23	c	512	CLA	C2A-C1A-CHA	-2.16	120.12	123.87
32	c	501	LMG	O6-C5-C4	2.16	113.59	109.70
23	A	404	CLA	CMB-C2B-C3B	2.16	131.62	126.55
23	C	503	CLA	C2A-C1A-CHA	-2.16	120.13	123.87
25	D	405	BCR	C28-C27-C26	-2.15	110.22	114.06
34	B	630	LMT	O5'-C1'-C2'	2.15	114.79	110.37
24	A	407	PHO	O1D-CGD-CBD	-2.15	121.46	124.72
24	A	415	PHO	O2A-CGA-O1A	-2.15	118.24	123.63
23	C	507	CLA	O2A-CGA-CBA	2.15	118.40	111.83
24	A	407	PHO	OBD-CAD-C3D	-2.15	124.54	127.89
32	C	522	LMG	O8-C28-O10	-2.15	118.25	123.63
34	C	526	LMT	O5'-C5'-C4'	2.15	114.16	109.72
23	b	614	CLA	CAC-C3C-C4C	2.15	127.58	124.79
23	B	606	CLA	CHA-C1A-NA	-2.15	121.53	126.39
23	c	508	CLA	C2A-C1A-CHA	-2.15	120.14	123.87
23	D	403	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
23	C	509	CLA	OBD-CAD-C3D	-2.14	123.41	128.42
26	b	628	GOL	C3-C2-C1	-2.14	103.94	111.80
23	B	611	CLA	CHB-C4A-NA	2.14	127.49	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C11-C12-C13	-2.14	108.85	115.97
23	b	608	CLA	C11-C12-C13	-2.14	108.85	115.97
23	b	614	CLA	CMC-C2C-C1C	2.14	128.38	125.03
23	b	606	CLA	O2A-CGA-CBA	2.14	118.36	111.83
23	C	503	CLA	O2A-CGA-CBA	2.14	118.35	111.83
23	C	511	CLA	C16-C15-C13	-2.13	108.87	115.97
25	b	617	BCR	C21-C20-C19	-2.13	117.02	123.20
34	t	101	LMT	C2'-C3'-C4'	2.13	114.52	109.68
23	b	615	CLA	CMC-C2C-C1C	2.13	128.36	125.03
29	D	406	PL9	C12-C13-C14	-2.13	122.75	127.62
23	B	607	CLA	CMA-C3A-C2A	-2.13	105.75	113.98
23	a	405	CLA	CMC-C2C-C1C	2.13	128.36	125.03
25	Y	101	BCR	C15-C16-C17	-2.13	119.16	123.52
25	A	409	BCR	C28-C27-C26	-2.13	110.26	114.06
23	d	403	CLA	CBC-CAC-C3C	-2.13	106.65	112.42
23	C	508	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
24	A	415	PHO	C4D-CHA-CBD	2.13	109.47	108.45
23	B	602	CLA	CED-O2D-CGD	2.13	120.74	115.92
25	k	101	BCR	C7-C8-C9	-2.13	123.09	126.23
23	B	607	CLA	CMC-C2C-C1C	2.12	128.35	125.03
23	D	403	CLA	CMA-C3A-C2A	-2.12	105.77	113.98
25	b	618	BCR	C38-C26-C25	-2.12	122.17	124.48
31	A	416	LHG	O4-P-O5	2.12	122.32	112.44
23	A	408	CLA	CHB-C4A-NA	2.12	127.46	124.40
29	a	415	PL9	C51-C49-C50	2.12	119.47	114.59
25	c	517	BCR	C37-C22-C23	2.12	121.33	118.09
23	B	612	CLA	CHB-C4A-NA	2.12	127.46	124.40
23	b	604	CLA	CHA-C1A-NA	-2.12	121.59	126.39
23	C	510	CLA	OBD-CAD-C3D	-2.12	123.46	128.42
23	b	609	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
25	c	517	BCR	C36-C18-C19	2.12	121.32	118.09
23	B	604	CLA	CAC-C3C-C4C	2.12	127.54	124.79
33	b	623	HTG	C1-O5-C5	2.12	116.36	112.56
23	b	604	CLA	C6-C7-C8	-2.12	108.94	115.97
23	d	402	CLA	C6-C5-C3	2.11	118.62	113.47
23	C	510	CLA	C1-O2A-CGA	2.11	121.77	116.65
25	k	101	BCR	C10-C11-C12	-2.11	117.08	123.20
23	a	404	CLA	CMA-C3A-C4A	-2.11	106.10	111.77
23	B	611	CLA	C1-O2A-CGA	2.11	121.76	116.65
38	E	103	HEC	C4C-NC-C1C	2.11	109.26	105.82
23	B	604	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
24	A	415	PHO	O2A-CGA-CBA	2.11	118.26	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	520	DGD	O2G-C1B-O1B	-2.11	118.78	123.70
23	C	505	CLA	C2A-C1A-CHA	-2.11	120.21	123.87
23	b	609	CLA	C2A-C1A-CHA	-2.11	120.21	123.87
23	b	610	CLA	CHB-C4A-NA	2.11	127.44	124.40
25	k	101	BCR	C16-C17-C18	-2.10	124.33	127.28
34	m	103	LMT	O5B-C5B-C6B	2.10	111.65	106.44
38	E	103	HEC	C4B-NB-C1B	2.10	109.25	105.82
23	C	505	CLA	CBC-CAC-C3C	-2.10	106.72	112.42
25	b	618	BCR	C8-C7-C6	-2.10	121.39	127.00
23	b	602	CLA	CAA-CBA-CGA	-2.10	107.24	113.21
27	a	410	SQD	O48-C23-O10	-2.10	118.37	123.63
25	d	404	BCR	C24-C23-C22	-2.10	123.13	126.23
27	f	101	SQD	O48-C23-O10	-2.10	118.38	123.63
23	b	614	CLA	CAA-C2A-C3A	-2.10	107.33	113.00
23	C	515	CLA	CAA-C2A-C3A	-2.10	107.33	113.00
23	b	616	CLA	C2A-C1A-CHA	-2.10	120.23	123.87
29	A	413	PL9	C16-C14-C13	-2.10	116.46	121.17
34	m	103	LMT	C1'-C2'-C3'	2.10	114.42	110.01
25	c	517	BCR	C2-C1-C6	2.09	113.48	110.44
23	a	406	CLA	C4-C3-C5	2.09	118.86	115.23
23	b	609	CLA	CHB-C1B-C2B	-2.09	121.35	127.43
23	c	505	CLA	OBD-CAD-C3D	-2.09	123.53	128.42
23	c	504	CLA	C4-C3-C5	2.09	118.86	115.23
25	A	409	BCR	C15-C16-C17	-2.09	119.25	123.52
23	B	609	CLA	CHA-C1A-NA	-2.09	121.66	126.39
23	B	616	CLA	CBC-CAC-C3C	-2.09	106.76	112.42
23	c	514	CLA	CHA-C1A-NA	-2.09	121.67	126.39
23	C	514	CLA	C2A-C1A-CHA	-2.09	120.25	123.87
23	b	609	CLA	C7-C6-C5	-2.09	107.70	113.26
23	c	507	CLA	C4-C3-C5	2.09	118.85	115.23
23	b	615	CLA	C1-O2A-CGA	2.09	121.70	116.65
23	C	510	CLA	O2A-CGA-CBA	2.08	118.19	111.83
23	c	514	CLA	C4B-C3B-C2B	-2.08	104.71	107.30
23	B	613	CLA	CHB-C4A-NA	2.08	127.40	124.40
23	A	404	CLA	C7-C6-C5	-2.08	107.72	113.26
25	B	617	BCR	C21-C20-C19	-2.08	117.17	123.20
23	B	615	CLA	C1-O2A-CGA	2.08	121.69	116.65
34	D	402	LMT	O5'-C5'-C4'	2.08	114.02	109.72
23	b	615	CLA	CHA-C1A-NA	-2.08	121.69	126.39
25	D	405	BCR	C37-C22-C21	-2.08	119.45	122.82
35	H	102	DGD	O6E-C5E-C6E	2.08	111.59	106.44
23	C	514	CLA	CAC-C3C-C4C	2.08	127.49	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	OBD-CAD-C3D	-2.08	123.56	128.42
38	e	102	HEC	CHD-C1D-ND	2.07	127.62	123.86
34	M	101	LMT	C1B-C2B-C3B	2.07	114.37	110.01
23	C	507	CLA	C2A-C1A-CHA	-2.07	120.27	123.87
23	c	511	CLA	C2A-C1A-CHA	-2.07	120.27	123.87
38	v	202	HEC	CBA-CAA-C2A	-2.07	106.81	112.53
23	B	616	CLA	C4-C3-C5	2.07	118.82	115.23
25	Y	101	BCR	C36-C18-C17	-2.07	119.46	122.82
23	B	612	CLA	C11-C12-C13	-2.07	109.09	115.97
27	C	501	SQD	O47-C7-O49	-2.07	118.88	123.70
25	B	617	BCR	C24-C23-C22	-2.07	123.18	126.23
23	c	514	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
23	c	504	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
25	y	101	BCR	C29-C28-C27	-2.06	106.74	111.28
23	C	513	CLA	C11-C10-C8	-2.06	109.11	115.97
23	B	610	CLA	CMA-C3A-C2A	-2.06	106.02	113.98
25	a	409	BCR	C15-C16-C17	-2.06	119.31	123.52
29	A	413	PL9	C51-C49-C50	2.06	119.33	114.59
25	t	102	BCR	C3-C4-C5	-2.06	110.38	114.06
23	B	609	CLA	C1-C2-C3	-2.06	122.82	126.20
23	A	404	CLA	CAA-CBA-CGA	-2.06	107.36	113.21
25	A	409	BCR	C34-C9-C8	2.06	121.23	118.09
34	E	102	LMT	O5'-C5'-C4'	2.06	113.98	109.72
23	C	511	CLA	CED-O2D-CGD	2.06	120.58	115.92
23	c	509	CLA	CHA-C1A-NA	-2.05	121.74	126.39
23	B	614	CLA	C4A-NA-C1A	-2.05	105.74	106.68
25	a	409	BCR	C34-C9-C8	2.05	121.22	118.09
25	B	618	BCR	C33-C5-C6	-2.05	122.24	124.48
23	d	402	CLA	CHB-C4A-NA	2.05	127.36	124.40
23	B	602	CLA	CAA-CBA-CGA	-2.05	107.38	113.21
23	C	513	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
32	c	522	LMG	C9-C8-C7	-2.05	107.01	111.78
38	e	102	HEC	C2A-C1A-NA	-2.05	108.35	110.32
25	K	101	BCR	C3-C4-C5	-2.05	110.41	114.06
23	b	613	CLA	CHB-C1B-NB	-2.05	120.98	124.05
23	b	614	CLA	CED-O2D-CGD	2.05	120.56	115.92
25	d	404	BCR	C23-C24-C25	-2.04	121.54	127.00
23	b	604	CLA	C11-C10-C8	-2.04	109.17	115.97
23	B	602	CLA	C11-C10-C8	-2.04	109.17	115.97
25	c	517	BCR	C20-C21-C22	-2.04	124.41	127.28
35	C	519	DGD	O2G-C1B-O1B	-2.04	118.93	123.70
24	a	407	PHO	CMC-C2C-C1C	2.04	128.41	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	405	PL9	C47-C48-C49	-2.04	120.83	127.64
32	C	502	LMG	O7-C10-O9	-2.04	118.93	123.70
35	H	102	DGD	O2G-C1B-O1B	-2.04	118.93	123.70
23	C	509	CLA	C4-C3-C5	2.04	118.77	115.23
34	t	101	LMT	O2'-C2'-C3'	-2.04	105.57	110.38
23	A	405	CLA	O2A-CGA-CBA	2.04	118.06	111.83
25	b	619	BCR	C2-C1-C6	2.04	113.40	110.44
23	b	601	CLA	CHB-C4A-NA	2.04	127.34	124.40
33	b	622	HTG	O2-C2-C1	2.04	113.92	110.30
27	B	620	SQD	C1-C2-C3	-2.04	105.72	110.01
27	D	412	SQD	O48-C23-O10	-2.04	118.53	123.63
25	a	409	BCR	C8-C7-C6	-2.04	121.56	127.00
29	A	413	PL9	C47-C48-C49	-2.04	120.85	127.64
35	c	519	DGD	C2G-O2G-C1B	-2.04	112.92	117.80
29	a	415	PL9	C47-C46-C44	-2.04	106.44	113.19
23	B	616	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
35	c	520	DGD	O6E-C5E-C4E	2.03	113.36	109.70
25	c	517	BCR	C15-C14-C13	-2.03	124.42	127.28
23	b	616	CLA	CHA-C1A-NA	-2.03	121.79	126.39
23	B	612	CLA	CAA-C2A-C3A	-2.03	107.50	113.00
38	V	201	HEC	CMD-C2D-C1D	2.03	128.51	125.42
23	d	402	CLA	CMA-C3A-C4A	-2.03	106.31	111.77
23	B	606	CLA	CMC-C2C-C1C	2.03	128.21	125.03
23	B	613	CLA	CHD-C4C-NC	2.03	127.38	124.23
23	c	511	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
23	C	514	CLA	CBA-CAA-C2A	-2.03	107.76	113.79
23	d	402	CLA	CMC-C2C-C1C	2.03	128.20	125.03
32	m	101	LMG	O1-C7-C8	-2.03	105.89	110.82
23	b	616	CLA	CMA-C3A-C4A	-2.03	106.33	111.77
27	b	620	SQD	O47-C7-O49	-2.03	118.97	123.70
23	B	601	CLA	CHB-C4A-NA	2.03	127.32	124.40
23	b	608	CLA	CHB-C1B-C2B	-2.02	121.55	127.43
27	b	620	SQD	C44-O6-C1	-2.02	109.46	113.80
23	c	510	CLA	C2A-C1A-CHA	-2.02	120.36	123.87
26	o	302	GOL	C3-C2-C1	-2.02	104.39	111.80
25	c	517	BCR	C29-C30-C25	2.02	113.37	110.44
27	B	620	SQD	O7-S-C6	2.02	109.77	106.76
26	a	411	GOL	C3-C2-C1	-2.02	104.39	111.80
23	D	403	CLA	C11-C12-C13	-2.02	109.26	115.97
23	c	510	CLA	CHB-C4A-NA	2.02	127.31	124.40
32	z	101	LMG	C9-C8-C7	-2.02	107.08	111.78
23	B	606	CLA	CHB-C1B-C2B	-2.02	121.57	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L	101	LHG	O8-C23-O10	-2.02	118.58	123.63
35	c	520	DGD	O2G-C1B-O1B	-2.02	118.99	123.70
25	D	405	BCR	C30-C25-C24	2.01	121.11	115.65
27	A	411	SQD	O8-S-C6	2.01	109.86	105.97
33	V	202	HTG	C6-C5-C4	-2.01	108.08	113.02
24	A	415	PHO	C7-C6-C5	-2.01	107.91	113.26
23	c	515	CLA	C4-C3-C5	2.01	118.72	115.23
23	c	512	CLA	C11-C12-C13	-2.01	109.29	115.97
23	B	604	CLA	C11-C12-C13	-2.01	109.30	115.97
23	c	513	CLA	C11-C10-C8	-2.01	109.30	115.97
23	b	615	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
34	a	413	LMT	C1'-O5'-C5'	2.00	117.63	113.72
35	H	102	DGD	C2G-O2G-C1B	-2.00	113.00	117.80
34	a	413	LMT	O1B-C1B-C2B	2.00	113.02	108.09
27	C	501	SQD	C45-O47-C7	-2.00	113.00	117.80
23	D	404	CLA	CMA-C3A-C2A	-2.00	106.24	113.98
23	b	616	CLA	CMA-C3A-C2A	-2.00	106.24	113.98
25	B	617	BCR	C15-C14-C13	-2.00	124.47	127.28

All (64) 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
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	503	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	403	CLA	ND
23	D	404	CLA	ND
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
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	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	c	515	CLA	ND

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

All (1261) 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	504	CLA	C2B-C3B-CAB-CBB
23	C	504	CLA	C4B-C3B-CAB-CBB
23	C	504	CLA	C14-C13-C15-C16
23	C	507	CLA	C2B-C3B-CAB-CBB
23	C	507	CLA	C4B-C3B-CAB-CBB
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	C2B-C3B-CAB-CBB
23	b	606	CLA	C4B-C3B-CAB-CBB
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	C2B-C3B-CAB-CBB
23	b	616	CLA	C4B-C3B-CAB-CBB
23	c	504	CLA	C2B-C3B-CAB-CBB
23	c	504	CLA	C4B-C3B-CAB-CBB
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
25	D	405	BCR	C21-C22-C23-C24
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	b	619	BCR	C7-C8-C9-C10
25	b	619	BCR	C7-C8-C9-C34
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
26	B	624	GOL	C1-C2-C3-O3
26	O	302	GOL	O1-C1-C2-C3
26	O	302	GOL	C1-C2-C3-O3
26	O	302	GOL	O2-C2-C3-O3
26	a	411	GOL	O1-C1-C2-C3
26	b	624	GOL	C1-C2-C3-O3
26	v	201	GOL	O1-C1-C2-C3
27	A	411	SQD	O6-C44-C45-O47
27	B	620	SQD	O49-C7-O47-C45
27	D	412	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
27	D	412	SQD	C8-C7-O47-C45
27	a	412	SQD	C5-C6-S-O7
27	a	412	SQD	C5-C6-S-O8
27	a	412	SQD	C5-C6-S-O9
27	b	620	SQD	O49-C7-O47-C45
27	b	620	SQD	C8-C7-O47-C45
27	f	101	SQD	O5-C1-O6-C44
27	f	101	SQD	C8-C7-O47-C45
27	f	101	SQD	C5-C6-S-O7
27	f	101	SQD	C5-C6-S-O8
27	f	101	SQD	C5-C6-S-O9
31	D	407	LHG	C3-O3-P-O4
31	D	407	LHG	C3-O3-P-O6
31	E	101	LHG	C3-O3-P-O4
31	E	101	LHG	C3-O3-P-O5
31	E	101	LHG	C3-O3-P-O6
31	E	101	LHG	C4-O6-P-O5
31	E	101	LHG	O10-C23-O8-C6
31	E	101	LHG	C24-C23-O8-C6
31	L	101	LHG	C4-O6-P-O3
31	L	101	LHG	C4-O6-P-O4
31	L	101	LHG	C4-O6-P-O5
31	a	419	LHG	C3-O3-P-O4
31	a	419	LHG	C3-O3-P-O5
31	a	419	LHG	C3-O3-P-O6
31	a	419	LHG	C4-O6-P-O4
31	a	419	LHG	O10-C23-O8-C6
31	a	419	LHG	C24-C23-O8-C6
31	b	629	LHG	C4-O6-P-O3
31	b	629	LHG	C4-O6-P-O5
31	d	406	LHG	C3-O3-P-O4
31	d	406	LHG	C4-O6-P-O5
31	d	407	LHG	O2-C2-C3-O3
31	d	407	LHG	C3-O3-P-O4
31	d	407	LHG	C3-O3-P-O6
31	d	407	LHG	C4-O6-P-O4
32	C	522	LMG	C11-C10-O7-C8
32	Z	101	LMG	O9-C10-O7-C8
32	Z	101	LMG	C11-C10-O7-C8
32	c	501	LMG	C2-C1-O1-C7
32	c	522	LMG	C11-C10-O7-C8
32	z	101	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
32	z	101	LMG	C11-C10-O7-C8
33	b	622	HTG	C2'-C1'-S1-C1
34	B	630	LMT	C2'-C1'-O1'-C1
34	B	630	LMT	O5'-C1'-O1'-C1
34	C	526	LMT	C3'-C4'-O1B-C1B
34	C	526	LMT	C2'-C1'-O1'-C1
34	C	526	LMT	O5'-C1'-O1'-C1
34	E	102	LMT	O5'-C1'-O1'-C1
34	b	621	LMT	O5'-C1'-O1'-C1
34	t	101	LMT	O5'-C1'-O1'-C1
38	E	103	HEC	C2B-C3B-CAB-CBB
38	E	103	HEC	C4B-C3B-CAB-CBB
38	E	103	HEC	C2C-C3C-CAC-CBC
38	E	103	HEC	C4C-C3C-CAC-CBC
38	V	201	HEC	C2B-C3B-CAB-CBB
38	V	201	HEC	C4B-C3B-CAB-CBB
38	V	201	HEC	C2C-C3C-CAC-CBC
38	V	201	HEC	C4C-C3C-CAC-CBC
38	e	102	HEC	C2B-C3B-CAB-CBB
38	e	102	HEC	C4B-C3B-CAB-CBB
38	e	102	HEC	C2C-C3C-CAC-CBC
38	e	102	HEC	C4C-C3C-CAC-CBC
38	v	202	HEC	C2B-C3B-CAB-CBB
38	v	202	HEC	C2C-C3C-CAC-CBC
38	v	202	HEC	C4C-C3C-CAC-CBC
34	B	628	LMT	C4'-C5'-C6'-O6'
27	f	101	SQD	O49-C7-O47-C45
32	C	522	LMG	O9-C10-O7-C8
32	z	101	LMG	O9-C10-O7-C8
23	A	408	CLA	C3-C5-C6-C7
23	B	614	CLA	C3-C5-C6-C7
23	a	408	CLA	C3-C5-C6-C7
23	c	508	CLA	C3-C5-C6-C7
23	C	505	CLA	CBD-CGD-O2D-CED
27	B	620	SQD	C8-C7-O47-C45
23	B	605	CLA	C4-C3-C5-C6
23	B	616	CLA	C4-C3-C5-C6
23	C	506	CLA	C4-C3-C5-C6
23	D	404	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	c	506	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	c	509	CLA	C4-C3-C5-C6
23	c	515	CLA	C4-C3-C5-C6
23	d	403	CLA	C4-C3-C5-C6
29	A	413	PL9	C12-C11-C9-C10
29	A	413	PL9	C15-C14-C16-C17
29	A	413	PL9	C25-C24-C26-C27
23	B	605	CLA	C2-C3-C5-C6
23	C	506	CLA	C2-C3-C5-C6
23	D	404	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	c	509	CLA	C2-C3-C5-C6
23	c	515	CLA	C2-C3-C5-C6
23	d	403	CLA	C2-C3-C5-C6
23	B	616	CLA	C3-C5-C6-C7
27	f	101	SQD	C24-C23-O48-C46
32	c	522	LMG	O9-C10-O7-C8
34	B	628	LMT	C3'-C4'-O1B-C1B
34	e	101	LMT	O5'-C5'-C6'-O6'
34	E	102	LMT	C4'-C5'-C6'-O6'
27	f	101	SQD	O10-C23-O48-C46
34	M	103	LMT	C4'-C5'-C6'-O6'
23	c	514	CLA	C3-C5-C6-C7
32	C	522	LMG	O6-C5-C6-O5
33	b	625	HTG	O5-C5-C6-O6
23	A	408	CLA	C4-C3-C5-C6
23	B	603	CLA	C4-C3-C5-C6
23	C	509	CLA	C4-C3-C5-C6
23	a	408	CLA	C4-C3-C5-C6
29	a	415	PL9	C25-C24-C26-C27
23	A	408	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
29	A	413	PL9	C13-C14-C16-C17
29	a	415	PL9	C23-C24-C26-C27
32	C	502	LMG	O6-C5-C6-O5
32	c	522	LMG	O6-C5-C6-O5
29	A	413	PL9	C14-C16-C17-C18
29	A	413	PL9	C19-C21-C22-C23
29	D	406	PL9	C39-C41-C42-C43
29	a	415	PL9	C19-C21-C22-C23
29	d	405	PL9	C39-C41-C42-C43
23	C	503	CLA	CBD-CGD-O2D-CED
34	B	628	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
27	B	620	SQD	O5-C1-O6-C44
34	D	402	LMT	O5'-C1'-O1'-C1
34	M	103	LMT	O5'-C1'-O1'-C1
34	a	413	LMT	O5'-C1'-O1'-C1
34	a	418	LMT	O5'-C1'-O1'-C1
34	b	627	LMT	O5'-C1'-O1'-C1
34	e	101	LMT	O5'-C1'-O1'-C1
23	c	513	CLA	CBD-CGD-O2D-CED
34	B	628	LMT	O5B-C5B-C6B-O6B
34	C	526	LMT	O5B-C5B-C6B-O6B
23	C	514	CLA	C3-C5-C6-C7
31	d	407	LHG	C1-C2-C3-O3
23	B	601	CLA	CBA-CGA-O2A-C1
23	C	514	CLA	CBA-CGA-O2A-C1
23	c	511	CLA	CBA-CGA-O2A-C1
34	C	526	LMT	C4B-C5B-C6B-O6B
33	D	411	HTG	C4-C5-C6-O6
33	c	523	HTG	C4-C5-C6-O6
23	b	615	CLA	C13-C15-C16-C17
23	b	614	CLA	C4-C3-C5-C6
29	a	415	PL9	C15-C14-C16-C17
23	B	616	CLA	C2-C3-C5-C6
23	C	509	CLA	C2-C3-C5-C6
23	a	408	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
23	c	506	CLA	C2-C3-C5-C6
29	A	413	PL9	C23-C24-C26-C27
29	a	415	PL9	C13-C14-C16-C17
23	d	403	CLA	C3-C5-C6-C7
23	B	610	CLA	C11-C12-C13-C14
23	B	611	CLA	C11-C12-C13-C14
23	C	514	CLA	C6-C7-C8-C9
23	C	515	CLA	C14-C13-C15-C16
23	c	508	CLA	C6-C7-C8-C9
23	c	511	CLA	C11-C10-C8-C9
23	c	514	CLA	C6-C7-C8-C9
32	C	502	LMG	C4-C5-C6-O5
23	C	505	CLA	O1D-CGD-O2D-CED
27	f	101	SQD	C2-C1-O6-C44
34	D	402	LMT	C2'-C1'-O1'-C1
34	E	102	LMT	C2'-C1'-O1'-C1
34	M	103	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
34	a	413	LMT	C2'-C1'-O1'-C1
34	a	418	LMT	C2'-C1'-O1'-C1
34	b	627	LMT	C2'-C1'-O1'-C1
34	e	101	LMT	C2'-C1'-O1'-C1
34	e	101	LMT	C4'-C5'-C6'-O6'
25	D	405	BCR	C37-C22-C23-C24
34	E	102	LMT	O5'-C5'-C6'-O6'
32	Z	101	LMG	C10-C11-C12-C13
23	c	511	CLA	O1A-CGA-O2A-C1
32	c	501	LMG	O6-C5-C6-O5
34	B	628	LMT	C4B-C5B-C6B-O6B
32	B	621	LMG	O9-C10-O7-C8
32	B	621	LMG	C11-C10-O7-C8
27	a	412	SQD	O6-C44-C45-O47
23	A	408	CLA	C5-C6-C7-C8
23	B	615	CLA	C13-C15-C16-C17
23	c	511	CLA	C2-C1-O2A-CGA
23	B	604	CLA	C8-C10-C11-C12
23	B	606	CLA	C10-C11-C12-C13
23	B	614	CLA	C10-C11-C12-C13
23	b	613	CLA	CBD-CGD-O2D-CED
23	a	408	CLA	C6-C7-C8-C10
34	C	526	LMT	O1'-C1-C2-C3
29	a	415	PL9	C24-C26-C27-C28
29	a	415	PL9	C29-C31-C32-C33
23	C	510	CLA	C5-C6-C7-C8
23	b	601	CLA	C10-C11-C12-C13
35	c	518	DGD	C1A-C2A-C3A-C4A
35	c	519	DGD	C1B-C2B-C3B-C4B
23	B	613	CLA	C15-C16-C17-C18
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
23	C	507	CLA	C8-C10-C11-C12
23	C	507	CLA	C15-C16-C17-C18
23	b	616	CLA	C13-C15-C16-C17
23	c	506	CLA	C5-C6-C7-C8
27	D	412	SQD	C23-C24-C25-C26
32	c	501	LMG	C10-C11-C12-C13
23	C	514	CLA	O1A-CGA-O2A-C1
23	C	508	CLA	C3-C5-C6-C7
32	c	501	LMG	O6-C1-O1-C7
34	M	101	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
35	C	519	DGD	O6E-C1E-O5D-C6D
33	D	411	HTG	O5-C5-C6-O6
33	c	523	HTG	O5-C5-C6-O6
34	M	103	LMT	O5'-C5'-C6'-O6'
23	C	512	CLA	C5-C6-C7-C8
23	C	514	CLA	C13-C15-C16-C17
23	a	406	CLA	C10-C11-C12-C13
23	B	601	CLA	O1A-CGA-O2A-C1
34	M	101	LMT	C4B-C5B-C6B-O6B
23	B	614	CLA	C8-C10-C11-C12
23	B	608	CLA	C13-C15-C16-C17
27	A	411	SQD	C7-C8-C9-C10
23	B	615	CLA	C10-C11-C12-C13
23	C	514	CLA	C15-C16-C17-C18
23	a	406	CLA	C8-C10-C11-C12
23	b	605	CLA	C8-C10-C11-C12
23	c	503	CLA	CBD-CGD-O2D-CED
23	C	504	CLA	C13-C15-C16-C17
25	T	101	BCR	C13-C14-C15-C16
31	E	101	LHG	C11-C10-C9-C8
23	A	405	CLA	C15-C16-C17-C18
23	B	603	CLA	C8-C10-C11-C12
23	B	606	CLA	C15-C16-C17-C18
23	B	614	CLA	C5-C6-C7-C8
23	B	615	CLA	C5-C6-C7-C8
23	C	506	CLA	C8-C10-C11-C12
23	C	508	CLA	C10-C11-C12-C13
23	b	606	CLA	C13-C15-C16-C17
23	b	611	CLA	C15-C16-C17-C18
23	c	510	CLA	C10-C11-C12-C13
27	C	501	SQD	C7-C8-C9-C10
23	C	508	CLA	C8-C10-C11-C12
23	C	510	CLA	C10-C11-C12-C13
23	c	508	CLA	C15-C16-C17-C18
23	C	515	CLA	CBD-CGD-O2D-CED
23	B	601	CLA	C5-C6-C7-C8
23	B	602	CLA	C8-C10-C11-C12
23	D	404	CLA	C10-C11-C12-C13
23	a	408	CLA	C5-C6-C7-C8
23	c	514	CLA	C10-C11-C12-C13
34	M	101	LMT	O5B-C5B-C6B-O6B
23	B	603	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	D	412	SQD	C2-C1-O6-C44
32	C	502	LMG	C2-C1-O1-C7
34	M	101	LMT	C2'-C1'-O1'-C1
34	b	621	LMT	C2'-C1'-O1'-C1
35	C	519	DGD	C2E-C1E-O5D-C6D
23	B	602	CLA	C15-C16-C17-C18
35	C	519	DGD	C1A-C2A-C3A-C4A
29	A	413	PL9	C24-C26-C27-C28
33	B	623	HTG	C1'-C2'-C3'-C4'
35	c	518	DGD	C2A-C3A-C4A-C5A
23	b	604	CLA	CBD-CGD-O2D-CED
23	C	508	CLA	C13-C15-C16-C17
25	D	405	BCR	C7-C8-C9-C34
25	k	101	BCR	C7-C8-C9-C34
25	t	102	BCR	C11-C12-C13-C35
27	C	501	SQD	C11-C10-C9-C8
34	B	628	LMT	C5'-C4'-O1B-C1B
23	B	610	CLA	C2A-CAA-CBA-CGA
26	A	410	GOL	C1-C2-C3-O3
26	a	411	GOL	C1-C2-C3-O3
26	o	302	GOL	C1-C2-C3-O3
31	A	416	LHG	O1-C1-C2-C3
31	D	408	LHG	O1-C1-C2-C3
31	d	406	LHG	O1-C1-C2-C3
27	D	412	SQD	C7-C8-C9-C10
23	b	615	CLA	C16-C17-C18-C20
23	c	504	CLA	C16-C17-C18-C19
35	C	519	DGD	CBB-CCB-CDB-CEB
23	B	604	CLA	C3-C5-C6-C7
23	a	405	CLA	C15-C16-C17-C18
32	C	502	LMG	O6-C1-O1-C7
23	B	611	CLA	C8-C10-C11-C12
23	C	504	CLA	C15-C16-C17-C18
23	c	512	CLA	C10-C11-C12-C13
23	B	616	CLA	C2-C1-O2A-CGA
23	b	615	CLA	C16-C17-C18-C19
23	A	408	CLA	C15-C16-C17-C18
27	a	412	SQD	C16-C17-C18-C19
35	c	519	DGD	C9A-CAA-CBA-CCA
27	C	501	SQD	C15-C16-C17-C18
31	D	408	LHG	C29-C30-C31-C32
32	C	502	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
32	D	413	LMG	C19-C20-C21-C22
32	c	521	LMG	C32-C33-C34-C35
32	c	521	LMG	C36-C37-C38-C39
32	d	412	LMG	C21-C22-C23-C24
27	b	620	SQD	C24-C23-O48-C46
31	L	101	LHG	C25-C26-C27-C28
31	a	419	LHG	C13-C14-C15-C16
32	C	502	LMG	C34-C35-C36-C37
35	c	518	DGD	CAB-CBB-CCB-CDB
35	c	519	DGD	C7A-C8A-C9A-CAA
26	B	624	GOL	O2-C2-C3-O3
26	v	201	GOL	O1-C1-C2-O2
31	D	408	LHG	C32-C33-C34-C35
32	m	101	LMG	C32-C33-C34-C35
23	C	503	CLA	O1D-CGD-O2D-CED
23	B	616	CLA	C4B-C3B-CAB-CBB
23	C	506	CLA	C4B-C3B-CAB-CBB
23	b	602	CLA	C4B-C3B-CAB-CBB
23	c	509	CLA	C4B-C3B-CAB-CBB
31	E	101	LHG	C23-C24-C25-C26
31	d	407	LHG	C33-C34-C35-C36
32	C	522	LMG	C36-C37-C38-C39
34	m	103	LMT	O5'-C5'-C6'-O6'
23	a	408	CLA	C16-C17-C18-C19
31	a	419	LHG	C17-C18-C19-C20
35	H	102	DGD	C5B-C6B-C7B-C8B
23	B	613	CLA	C10-C11-C12-C13
27	C	501	SQD	C8-C7-O47-C45
32	C	502	LMG	C11-C10-O7-C8
35	C	518	DGD	C3A-C4A-C5A-C6A
32	z	101	LMG	C4-C5-C6-O5
23	b	606	CLA	C12-C13-C15-C16
27	B	620	SQD	C30-C31-C32-C33
27	D	412	SQD	C30-C31-C32-C33
31	D	407	LHG	C32-C33-C34-C35
31	a	419	LHG	C25-C26-C27-C28
34	b	621	LMT	C5-C6-C7-C8
35	h	103	DGD	CAA-CBA-CCA-CDA
32	d	412	LMG	C28-C29-C30-C31
32	Z	101	LMG	C16-C17-C18-C19
35	C	520	DGD	C6B-C7B-C8B-C9B
27	a	410	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	D	413	LMG	C35-C36-C37-C38
35	H	102	DGD	C9B-CAB-CBB-CCB
23	B	602	CLA	C13-C15-C16-C17
23	c	515	CLA	C10-C11-C12-C13
23	a	408	CLA	C16-C17-C18-C20
23	b	610	CLA	C16-C17-C18-C19
23	c	504	CLA	C16-C17-C18-C20
23	c	511	CLA	C16-C17-C18-C20
27	B	620	SQD	C14-C15-C16-C17
27	D	412	SQD	C24-C23-O48-C46
27	C	501	SQD	O6-C44-C45-C46
31	a	419	LHG	C4-C5-C6-O8
27	a	412	SQD	C25-C26-C27-C28
31	D	408	LHG	C33-C34-C35-C36
31	d	408	LHG	C28-C29-C30-C31
32	C	502	LMG	C37-C38-C39-C40
35	C	518	DGD	C4B-C5B-C6B-C7B
23	b	604	CLA	C13-C15-C16-C17
31	D	408	LHG	C12-C13-C14-C15
31	E	101	LHG	C27-C28-C29-C30
31	a	419	LHG	C18-C19-C20-C21
31	d	408	LHG	C29-C30-C31-C32
32	C	521	LMG	C37-C38-C39-C40
32	D	413	LMG	C12-C13-C14-C15
32	m	101	LMG	C38-C39-C40-C41
27	D	412	SQD	C24-C25-C26-C27
32	B	621	LMG	C32-C33-C34-C35
35	C	518	DGD	C5A-C6A-C7A-C8A
35	h	103	DGD	CAB-CBB-CCB-CDB
35	h	103	DGD	CCB-CDB-CEB-CFB
34	B	630	LMT	C4-C5-C6-C7
34	e	101	LMT	C5-C6-C7-C8
35	C	519	DGD	C8A-C9A-CAA-CBA
35	c	519	DGD	C7B-C8B-C9B-CAB
33	V	202	HTG	O5-C5-C6-O6
31	d	407	LHG	C28-C29-C30-C31
32	C	502	LMG	C12-C13-C14-C15
23	b	602	CLA	C2B-C3B-CAB-CBB
23	c	509	CLA	C2B-C3B-CAB-CBB
31	b	629	LHG	C16-C17-C18-C19
23	C	504	CLA	C3-C5-C6-C7
23	b	604	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	E	101	LHG	C7-C8-C9-C10
27	b	620	SQD	O10-C23-O48-C46
27	C	501	SQD	O49-C7-O47-C45
32	C	502	LMG	O9-C10-O7-C8
23	B	604	CLA	C4-C3-C5-C6
23	b	604	CLA	C8-C10-C11-C12
31	d	406	LHG	C23-C24-C25-C26
23	C	512	CLA	CBA-CGA-O2A-C1
23	d	403	CLA	CBA-CGA-O2A-C1
32	C	521	LMG	C30-C31-C32-C33
32	c	501	LMG	C30-C31-C32-C33
35	c	519	DGD	O6E-C1E-O5D-C6D
23	c	513	CLA	O1D-CGD-O2D-CED
34	t	101	LMT	C2'-C1'-O1'-C1
23	C	507	CLA	C5-C6-C7-C8
27	D	412	SQD	C29-C30-C31-C32
32	C	502	LMG	C18-C19-C20-C21
27	b	620	SQD	C28-C29-C30-C31
31	b	629	LHG	C14-C15-C16-C17
35	h	103	DGD	C9A-CAA-CBA-CCA
35	C	518	DGD	O6D-C5D-C6D-O5D
27	a	410	SQD	C34-C35-C36-C37
34	M	103	LMT	O1'-C1-C2-C3
27	b	620	SQD	C10-C11-C12-C13
34	a	418	LMT	C4-C5-C6-C7
34	a	413	LMT	C1-C2-C3-C4
34	B	630	LMT	O1'-C1-C2-C3
34	D	402	LMT	C3-C4-C5-C6
35	C	519	DGD	C9B-CAB-CBB-CCB
33	B	623	HTG	C2'-C3'-C4'-C5'
27	D	412	SQD	O10-C23-O48-C46
25	d	404	BCR	C7-C8-C9-C34
25	y	101	BCR	C37-C22-C23-C24
23	c	511	CLA	C3-C5-C6-C7
25	y	101	BCR	C21-C22-C23-C24
35	c	519	DGD	CBB-CCB-CDB-CEB
23	c	511	CLA	C16-C17-C18-C19
27	C	501	SQD	C18-C19-C20-C21
24	a	407	PHO	C4-C3-C5-C6
29	a	415	PL9	C30-C29-C31-C32
31	D	407	LHG	C16-C17-C18-C19
23	b	606	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	b	616	CLA	C10-C11-C12-C13
32	C	521	LMG	C21-C22-C23-C24
23	C	512	CLA	O1A-CGA-O2A-C1
23	d	403	CLA	O1A-CGA-O2A-C1
23	B	601	CLA	C3-C5-C6-C7
24	a	417	PHO	C2C-C3C-CAC-CBC
32	d	412	LMG	C10-C11-C12-C13
34	B	630	LMT	C1-C2-C3-C4
27	b	620	SQD	C14-C15-C16-C17
32	C	521	LMG	C17-C18-C19-C20
32	C	502	LMG	C17-C18-C19-C20
33	h	101	HTG	O5-C5-C6-O6
27	C	501	SQD	O6-C44-C45-O47
27	A	411	SQD	C29-C30-C31-C32
32	C	521	LMG	C31-C32-C33-C34
34	D	402	LMT	C5-C6-C7-C8
31	A	416	LHG	C34-C35-C36-C37
31	E	101	LHG	C24-C25-C26-C27
35	C	519	DGD	CAB-CBB-CCB-CDB
31	d	407	LHG	C30-C31-C32-C33
32	C	521	LMG	C29-C30-C31-C32
32	m	101	LMG	C39-C40-C41-C42
23	b	601	CLA	C2-C1-O2A-CGA
23	b	610	CLA	C16-C17-C18-C20
27	D	412	SQD	C34-C35-C36-C37
31	d	407	LHG	C32-C33-C34-C35
32	C	522	LMG	C18-C19-C20-C21
35	C	518	DGD	C5B-C6B-C7B-C8B
24	a	407	PHO	C2-C3-C5-C6
31	A	416	LHG	C26-C27-C28-C29
31	D	407	LHG	C12-C13-C14-C15
31	L	101	LHG	C17-C18-C19-C20
33	b	623	HTG	O5-C5-C6-O6
35	c	519	DGD	C6A-C7A-C8A-C9A
32	m	101	LMG	C14-C15-C16-C17
34	b	627	LMT	C11-C10-C9-C8
32	D	413	LMG	O6-C5-C6-O5
31	d	407	LHG	C34-C35-C36-C37
32	c	522	LMG	C30-C31-C32-C33
23	B	604	CLA	C13-C15-C16-C17
26	a	411	GOL	O1-C1-C2-O2
26	a	411	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
31	d	406	LHG	O1-C1-C2-O2
23	D	404	CLA	C3-C5-C6-C7
34	B	628	LMT	C11-C10-C9-C8
27	a	410	SQD	C30-C31-C32-C33
23	C	503	CLA	C1A-C2A-CAA-CBA
34	t	101	LMT	C2-C3-C4-C5
23	c	511	CLA	C15-C16-C17-C18
31	a	419	LHG	O6-C4-C5-C6
23	A	406	CLA	C12-C13-C15-C16
23	C	504	CLA	C12-C13-C15-C16
23	C	512	CLA	C12-C13-C15-C16
23	C	515	CLA	C12-C13-C15-C16
23	D	403	CLA	C12-C13-C15-C16
23	D	404	CLA	C12-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C10
23	c	507	CLA	C11-C12-C13-C15
35	c	520	DGD	C8B-C9B-CAB-CBB
33	b	625	HTG	S1-C1'-C2'-C3'
23	B	604	CLA	C16-C17-C18-C20
35	c	518	DGD	O6E-C5E-C6E-O5E
23	b	608	CLA	C13-C15-C16-C17
27	a	410	SQD	C7-C8-C9-C10
23	b	601	CLA	C4-C3-C5-C6
23	b	601	CLA	C2-C3-C5-C6
23	c	512	CLA	C2-C3-C5-C6
35	h	103	DGD	CDB-CEB-CFB-CGB
23	b	601	CLA	CBD-CGD-O2D-CED
23	a	404	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C14-C13-C15-C16
23	a	408	CLA	C11-C10-C8-C9
23	b	606	CLA	C6-C7-C8-C9
32	B	621	LMG	C28-C29-C30-C31
23	B	615	CLA	C8-C10-C11-C12
31	b	629	LHG	C27-C28-C29-C30
32	d	412	LMG	O6-C5-C6-O5
32	C	502	LMG	C28-C29-C30-C31
27	B	620	SQD	C44-C45-C46-O48
27	a	410	SQD	O6-C44-C45-C46
27	a	412	SQD	O6-C44-C45-C46
32	Z	101	LMG	C7-C8-C9-O8
35	c	519	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
23	b	610	CLA	C13-C15-C16-C17
31	D	408	LHG	C28-C29-C30-C31
32	C	502	LMG	C11-C12-C13-C14
35	c	518	DGD	CAA-CBA-CCA-CDA
23	a	408	CLA	CBA-CGA-O2A-C1
23	c	513	CLA	CBA-CGA-O2A-C1
23	c	514	CLA	CBA-CGA-O2A-C1
35	C	518	DGD	O6E-C5E-C6E-O5E
34	b	627	LMT	C5-C6-C7-C8
35	h	103	DGD	CCA-CDA-CEA-CFA
34	t	101	LMT	C3-C4-C5-C6
33	B	625	HTG	O5-C5-C6-O6
23	B	609	CLA	C13-C15-C16-C17
27	f	101	SQD	C25-C26-C27-C28
23	c	513	CLA	O1A-CGA-O2A-C1
23	c	512	CLA	C4-C3-C5-C6
29	d	405	PL9	C15-C14-C16-C17
29	A	413	PL9	C12-C11-C9-C8
29	D	406	PL9	C28-C29-C31-C32
29	a	415	PL9	C28-C29-C31-C32
29	d	405	PL9	C13-C14-C16-C17
35	C	520	DGD	O6E-C5E-C6E-O5E
34	b	621	LMT	C3-C4-C5-C6
31	A	416	LHG	C23-C24-C25-C26
27	a	410	SQD	C26-C27-C28-C29
35	c	518	DGD	O6D-C5D-C6D-O5D
23	a	408	CLA	O1A-CGA-O2A-C1
23	b	611	CLA	C8-C10-C11-C12
35	c	518	DGD	C5A-C6A-C7A-C8A
34	M	103	LMT	C2B-C1B-O1B-C4'
32	c	501	LMG	C17-C18-C19-C20
34	m	103	LMT	C7-C8-C9-C10
35	h	103	DGD	C5B-C6B-C7B-C8B
32	C	522	LMG	C17-C18-C19-C20
23	b	601	CLA	CBA-CGA-O2A-C1
32	c	522	LMG	C29-C28-O8-C9
23	c	514	CLA	C15-C16-C17-C18
31	b	629	LHG	C13-C14-C15-C16
23	B	604	CLA	C16-C17-C18-C19
32	c	501	LMG	C16-C17-C18-C19
31	b	629	LHG	O6-C4-C5-O7
27	a	412	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
23	c	507	CLA	C2-C3-C5-C6
27	a	410	SQD	C33-C34-C35-C36
31	E	101	LHG	C10-C11-C12-C13
27	a	410	SQD	O6-C44-C45-O47
27	b	620	SQD	O47-C45-C46-O48
35	C	519	DGD	CDA-CEA-CFA-CGA
34	D	402	LMT	C4-C5-C6-C7
35	C	519	DGD	C2A-C3A-C4A-C5A
35	C	519	DGD	C3A-C4A-C5A-C6A
35	C	520	DGD	C4B-C5B-C6B-C7B
33	B	623	HTG	C4'-C5'-C6'-C7'
31	L	101	LHG	C24-C25-C26-C27
32	c	522	LMG	C29-C30-C31-C32
35	C	519	DGD	C6B-C7B-C8B-C9B
33	b	622	HTG	S1-C1'-C2'-C3'
23	b	601	CLA	C3-C5-C6-C7
32	C	521	LMG	C12-C13-C14-C15
23	C	511	CLA	C13-C15-C16-C17
27	b	620	SQD	C31-C32-C33-C34
34	B	628	LMT	C4-C5-C6-C7
34	b	621	LMT	C3'-C4'-O1B-C1B
23	D	403	CLA	C15-C16-C17-C18
27	A	411	SQD	C17-C18-C19-C20
35	c	518	DGD	C2A-C1A-O1G-C1G
35	c	520	DGD	C2A-C1A-O1G-C1G
31	L	101	LHG	C12-C13-C14-C15
34	b	627	LMT	C4'-C5'-C6'-O6'
27	A	411	SQD	C16-C17-C18-C19
32	C	502	LMG	C35-C36-C37-C38
31	d	406	LHG	C16-C17-C18-C19
32	c	521	LMG	C31-C32-C33-C34
23	b	613	CLA	O1D-CGD-O2D-CED
23	b	615	CLA	C4-C3-C5-C6
23	b	606	CLA	C15-C16-C17-C18
29	a	415	PL9	C2-C3-C7-C8
31	d	406	LHG	C29-C30-C31-C32
26	O	302	GOL	O1-C1-C2-O2
26	b	624	GOL	O2-C2-C3-O3
23	A	406	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	C	512	CLA	C14-C13-C15-C16
23	C	515	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	D	404	CLA	C14-C13-C15-C16
23	a	408	CLA	C6-C7-C8-C9
23	b	614	CLA	C6-C7-C8-C9
23	a	405	CLA	C13-C15-C16-C17
23	c	510	CLA	C8-C10-C11-C12
23	C	509	CLA	C4B-C3B-CAB-CBB
23	c	515	CLA	C4B-C3B-CAB-CBB
23	a	404	CLA	C16-C17-C18-C19
27	a	412	SQD	C19-C20-C21-C22
34	M	101	LMT	C7-C8-C9-C10
33	B	625	HTG	C4'-C5'-C6'-C7'
31	b	629	LHG	O6-C4-C5-C6
27	A	411	SQD	C30-C31-C32-C33
27	b	620	SQD	C13-C14-C15-C16
27	b	620	SQD	C25-C26-C27-C28
23	B	614	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	C	515	CLA	C11-C10-C8-C7
23	a	408	CLA	C11-C10-C8-C7
23	c	506	CLA	C12-C13-C15-C16
23	d	402	CLA	C11-C12-C13-C15
23	D	403	CLA	C10-C11-C12-C13
32	C	502	LMG	C13-C14-C15-C16
23	b	612	CLA	C8-C10-C11-C12
32	Z	101	LMG	O6-C5-C6-O5
31	A	416	LHG	C32-C33-C34-C35
35	C	518	DGD	C4D-C5D-C6D-O5D
23	C	507	CLA	C4-C3-C5-C6
23	C	508	CLA	C3A-C2A-CAA-CBA
32	D	413	LMG	C30-C31-C32-C33
35	h	103	DGD	O2G-C1B-C2B-C3B
29	D	406	PL9	C13-C14-C16-C17
32	c	522	LMG	O6-C1-O1-C7
23	b	601	CLA	O1A-CGA-O2A-C1
35	c	519	DGD	CBA-CCA-CDA-CEA
35	c	520	DGD	CBA-CCA-CDA-CEA
32	c	522	LMG	O10-C28-O8-C9
33	b	625	HTG	C4-C5-C6-O6
23	b	611	CLA	C10-C11-C12-C13
32	c	501	LMG	C29-C30-C31-C32
32	z	101	LMG	C19-C20-C21-C22
27	A	411	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
27	f	101	SQD	O6-C44-C45-C46
29	A	413	PL9	C9-C11-C12-C13
31	E	101	LHG	C4-C5-C6-O8
32	C	522	LMG	C7-C8-C9-O8
34	C	526	LMT	C3-C4-C5-C6
35	C	518	DGD	C6B-C7B-C8B-C9B
23	a	405	CLA	CBD-CGD-O2D-CED
23	b	614	CLA	C16-C17-C18-C19
32	z	101	LMG	O6-C5-C6-O5
23	C	515	CLA	C4-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
29	D	406	PL9	C15-C14-C16-C17
23	b	615	CLA	C2-C3-C5-C6
35	C	519	DGD	C5A-C6A-C7A-C8A
35	H	102	DGD	CCA-CDA-CEA-CFA
23	c	503	CLA	O1D-CGD-O2D-CED
27	a	412	SQD	C18-C19-C20-C21
23	B	614	CLA	C16-C17-C18-C20
31	a	419	LHG	O6-C4-C5-O7
23	c	515	CLA	C2B-C3B-CAB-CBB
25	D	405	BCR	C23-C24-C25-C30
23	C	509	CLA	C5-C6-C7-C8
23	c	511	CLA	C10-C11-C12-C13
34	b	621	LMT	C6-C7-C8-C9
32	d	412	LMG	C38-C39-C40-C41
23	c	513	CLA	C8-C10-C11-C12
31	E	101	LHG	O7-C5-C6-O8
32	C	502	LMG	O1-C7-C8-O7
29	A	413	PL9	C4-C3-C7-C8
29	a	415	PL9	C4-C3-C7-C8
34	M	103	LMT	O5B-C1B-O1B-C4'
23	c	514	CLA	O1A-CGA-O2A-C1
29	D	406	PL9	C30-C29-C31-C32
23	b	615	CLA	C15-C16-C17-C18
27	B	620	SQD	C24-C25-C26-C27
31	D	407	LHG	C11-C12-C13-C14
32	C	521	LMG	C36-C37-C38-C39
23	c	506	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C12-C13-C14
35	C	520	DGD	C2A-C3A-C4A-C5A
27	B	620	SQD	C19-C20-C21-C22
27	a	412	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
27	D	412	SQD	O5-C1-O6-C44
32	B	621	LMG	C34-C35-C36-C37
31	D	408	LHG	C9-C10-C11-C12
35	c	518	DGD	C4D-C5D-C6D-O5D
33	b	625	HTG	C4'-C5'-C6'-C7'
31	A	416	LHG	O1-C1-C2-O2
23	C	507	CLA	C2-C3-C5-C6
23	c	514	CLA	C16-C17-C18-C20
32	m	101	LMG	C11-C10-O7-C8
35	H	102	DGD	C9A-CAA-CBA-CCA
23	A	408	CLA	C13-C15-C16-C17
32	C	521	LMG	C13-C14-C15-C16
32	m	101	LMG	C33-C34-C35-C36
23	a	404	CLA	C16-C17-C18-C20
23	b	613	CLA	C15-C16-C17-C18
32	C	522	LMG	C32-C33-C34-C35
23	a	406	CLA	C11-C12-C13-C15
23	c	511	CLA	C11-C10-C8-C7
31	d	408	LHG	C11-C10-C9-C8
25	D	405	BCR	C7-C8-C9-C10
25	d	404	BCR	C7-C8-C9-C10
25	k	101	BCR	C7-C8-C9-C10
25	t	102	BCR	C11-C12-C13-C14
31	a	419	LHG	C26-C27-C28-C29
35	C	519	DGD	C9A-CAA-CBA-CCA
35	c	519	DGD	C5D-C6D-O5D-C1E
32	C	522	LMG	C33-C34-C35-C36
32	c	501	LMG	C32-C33-C34-C35
23	C	515	CLA	C16-C17-C18-C19
27	a	412	SQD	O10-C23-O48-C46
35	c	520	DGD	O1A-C1A-O1G-C1G
23	B	609	CLA	C2-C3-C5-C6
23	C	511	CLA	C3-C5-C6-C7
27	B	620	SQD	C46-C45-O47-C7
27	b	620	SQD	C46-C45-O47-C7
27	b	620	SQD	C18-C19-C20-C21
23	b	602	CLA	C10-C11-C12-C13
32	m	101	LMG	C29-C30-C31-C32
32	c	522	LMG	C4-C5-C6-O5
32	c	501	LMG	O9-C10-O7-C8
23	C	515	CLA	O1D-CGD-O2D-CED
32	C	502	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	C	501	SQD	C14-C15-C16-C17
23	B	609	CLA	C4-C3-C5-C6
35	c	519	DGD	CDA-CEA-CFA-CGA
35	h	103	DGD	C7B-C8B-C9B-CAB
29	A	413	PL9	C2-C3-C7-C8
23	b	603	CLA	C13-C15-C16-C17
31	d	407	LHG	C13-C14-C15-C16
31	b	629	LHG	C9-C10-C11-C12
34	m	103	LMT	C6-C7-C8-C9
32	Z	101	LMG	O7-C8-C9-O8
32	c	501	LMG	O1-C7-C8-O7
23	C	508	CLA	C11-C10-C8-C9
23	B	603	CLA	C16-C17-C18-C20
23	a	405	CLA	C2C-C3C-CAC-CBC
31	d	407	LHG	C31-C32-C33-C34
35	H	102	DGD	CBB-CCB-CDB-CEB
35	c	518	DGD	O1A-C1A-O1G-C1G
35	H	102	DGD	C7A-C8A-C9A-CAA
23	B	606	CLA	C8-C10-C11-C12
23	C	507	CLA	C10-C11-C12-C13
23	b	601	CLA	C8-C10-C11-C12
33	B	622	HTG	C2'-C3'-C4'-C5'
27	a	410	SQD	C11-C12-C13-C14
32	c	501	LMG	C11-C10-O7-C8
25	H	101	BCR	C9-C10-C11-C12
35	c	519	DGD	C2E-C1E-O5D-C6D
23	c	513	CLA	C16-C17-C18-C19
35	C	519	DGD	C6A-C7A-C8A-C9A
23	b	616	CLA	C4-C3-C5-C6
27	A	411	SQD	O49-C7-O47-C45
23	A	408	CLA	C8-C10-C11-C12
32	D	413	LMG	C38-C39-C40-C41
23	B	615	CLA	C16-C17-C18-C20
35	C	520	DGD	C9A-CAA-CBA-CCA
35	C	518	DGD	C7A-C8A-C9A-CAA
33	B	625	HTG	C2'-C3'-C4'-C5'
27	A	411	SQD	C8-C7-O47-C45
23	B	614	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C20
34	B	628	LMT	C6-C7-C8-C9
23	B	615	CLA	C4B-C3B-CAB-CBB
23	a	406	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	a	406	CLA	C4B-C3B-CAB-CBB
23	b	609	CLA	C4B-C3B-CAB-CBB
23	c	503	CLA	C4B-C3B-CAB-CBB
23	c	508	CLA	C1A-C2A-CAA-CBA
23	c	514	CLA	C4B-C3B-CAB-CBB
31	d	407	LHG	C24-C23-O8-C6
23	b	601	CLA	CAA-CBA-CGA-O2A
35	H	102	DGD	O2G-C1B-C2B-C3B
33	b	623	HTG	C3'-C4'-C5'-C6'
34	b	627	LMT	C7-C8-C9-C10
31	a	419	LHG	C19-C20-C21-C22
31	b	629	LHG	C12-C13-C14-C15
32	z	101	LMG	C10-C11-C12-C13
32	C	502	LMG	C36-C37-C38-C39
23	B	610	CLA	C15-C16-C17-C18
32	c	501	LMG	C4-C5-C6-O5
32	m	101	LMG	O9-C10-O7-C8
23	B	616	CLA	C12-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C10
23	b	610	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	c	508	CLA	C6-C7-C8-C10
23	c	510	CLA	C6-C7-C8-C10
23	c	510	CLA	C11-C12-C13-C15
32	B	621	LMG	C20-C21-C22-C23
23	A	408	CLA	C16-C17-C18-C19
23	C	515	CLA	C16-C17-C18-C20
27	B	620	SQD	C11-C12-C13-C14
35	C	518	DGD	CDB-CEB-CFB-CGB
31	d	408	LHG	C9-C10-C11-C12
35	H	102	DGD	CBA-CCA-CDA-CEA
31	d	408	LHG	C2-C3-O3-P
29	D	406	PL9	C45-C44-C46-C47
38	v	202	HEC	C4B-C3B-CAB-CBB
32	C	522	LMG	C37-C38-C39-C40
29	D	406	PL9	C43-C44-C46-C47
23	B	604	CLA	C2C-C3C-CAC-CBC
23	a	404	CLA	C15-C16-C17-C18
27	a	412	SQD	C31-C32-C33-C34
23	B	606	CLA	C16-C17-C18-C20
23	D	404	CLA	C8-C10-C11-C12
23	B	607	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
34	b	627	LMT	O5'-C5'-C6'-O6'
31	d	408	LHG	O10-C23-O8-C6
27	B	620	SQD	O47-C45-C46-O48
27	f	101	SQD	O6-C44-C45-O47
31	a	419	LHG	O7-C5-C6-O8
32	C	522	LMG	O7-C8-C9-O8
23	b	604	CLA	O1D-CGD-O2D-CED
31	d	407	LHG	C29-C30-C31-C32
31	d	408	LHG	C24-C23-O8-C6
23	b	604	CLA	C16-C17-C18-C20
27	b	620	SQD	C44-C45-C46-O48
32	c	501	LMG	O1-C7-C8-C9
32	C	502	LMG	O8-C28-C29-C30
31	d	407	LHG	O10-C23-O8-C6
23	B	601	CLA	CAD-CBD-CGD-O2D
23	C	504	CLA	CAD-CBD-CGD-O2D
23	C	508	CLA	CAD-CBD-CGD-O2D
23	b	605	CLA	CAD-CBD-CGD-O2D
23	b	609	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O2D
23	c	508	CLA	CAD-CBD-CGD-O2D
31	D	407	LHG	C28-C29-C30-C31
27	b	620	SQD	O5-C1-O6-C44
32	B	621	LMG	C15-C16-C17-C18
35	c	520	DGD	CDB-CEB-CFB-CGB
35	c	520	DGD	C2B-C3B-C4B-C5B
23	C	513	CLA	O1A-CGA-O2A-C1
31	A	416	LHG	O10-C23-O8-C6
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	616	CLA	CHA-CBD-CGD-O1D
23	B	616	CLA	CHA-CBD-CGD-O2D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	C	508	CLA	CAD-CBD-CGD-O1D
23	C	511	CLA	CHA-CBD-CGD-O1D
23	C	511	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
23	c	508	CLA	CAD-CBD-CGD-O1D
23	c	511	CLA	CHA-CBD-CGD-O1D
23	c	511	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	D	407	LHG	C4-O6-P-O3
31	a	419	LHG	C4-O6-P-O3
31	d	406	LHG	C3-O3-P-O5
31	d	406	LHG	C3-O3-P-O6
31	d	406	LHG	C4-O6-P-O3
23	B	615	CLA	C2B-C3B-CAB-CBB
23	B	616	CLA	C2B-C3B-CAB-CBB
23	C	506	CLA	C2B-C3B-CAB-CBB
23	a	406	CLA	C2B-C3B-CAB-CBB
25	d	404	BCR	C23-C24-C25-C30
23	B	604	CLA	C2-C3-C5-C6
29	a	415	PL9	C43-C44-C46-C47
27	b	620	SQD	C15-C16-C17-C18
23	D	403	CLA	C13-C15-C16-C17
25	Y	101	BCR	C37-C22-C23-C24
25	b	619	BCR	C37-C22-C23-C24
31	D	408	LHG	C2-C3-O3-P
32	C	502	LMG	C21-C22-C23-C24
35	C	520	DGD	C8A-C9A-CAA-CBA
23	A	405	CLA	C2C-C3C-CAC-CBC
27	f	101	SQD	C29-C30-C31-C32
31	D	408	LHG	C30-C31-C32-C33
27	a	412	SQD	C34-C35-C36-C37
35	h	103	DGD	CDA-CEA-CFA-CGA
38	e	102	HEC	C2A-CAA-CBA-CGA
31	d	408	LHG	C10-C11-C12-C13
34	a	413	LMT	C6-C7-C8-C9
23	B	605	CLA	C10-C11-C12-C13
23	b	616	CLA	C2-C3-C5-C6
35	C	520	DGD	C5B-C6B-C7B-C8B
27	a	412	SQD	C24-C25-C26-C27
23	A	406	CLA	C16-C17-C18-C19
27	a	410	SQD	C19-C20-C21-C22
23	b	615	CLA	C14-C13-C15-C16
23	d	402	CLA	C11-C12-C13-C14
23	b	614	CLA	C12-C13-C15-C16
23	c	515	CLA	C12-C13-C15-C16
31	A	416	LHG	C1-C2-C3-O3
23	c	513	CLA	C16-C17-C18-C20
23	c	514	CLA	C16-C17-C18-C19
31	A	416	LHG	C24-C23-O8-C6
31	d	408	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
34	a	418	LMT	C6-C7-C8-C9
34	D	402	LMT	C7-C8-C9-C10
23	B	603	CLA	C16-C17-C18-C19
31	b	629	LHG	C10-C11-C12-C13
23	B	601	CLA	CAA-CBA-CGA-O2A
34	m	103	LMT	C4'-C5'-C6'-O6'
31	d	407	LHG	C25-C26-C27-C28
31	L	101	LHG	C23-C24-C25-C26
27	a	410	SQD	C11-C10-C9-C8
27	B	620	SQD	C9-C10-C11-C12
29	d	405	PL9	C45-C44-C46-C47
35	C	520	DGD	C1B-C2B-C3B-C4B
35	c	520	DGD	O6D-C5D-C6D-O5D
35	C	518	DGD	C3B-C4B-C5B-C6B
23	B	615	CLA	C16-C17-C18-C19
33	B	623	HTG	C2'-C1'-S1-C1
25	Y	101	BCR	C21-C22-C23-C24
25	b	619	BCR	C21-C22-C23-C24
35	c	519	DGD	C2G-C3G-O3G-C1D
27	C	501	SQD	C12-C13-C14-C15
32	C	522	LMG	C4-C5-C6-O5
23	c	509	CLA	C5-C6-C7-C8
34	t	101	LMT	C2-C1-O1'-C1'
27	b	620	SQD	C35-C36-C37-C38
23	B	616	CLA	C14-C13-C15-C16
23	a	406	CLA	C11-C12-C13-C14
23	b	610	CLA	C14-C13-C15-C16
23	c	510	CLA	C11-C12-C13-C14
23	A	406	CLA	C4B-C3B-CAB-CBB
23	a	408	CLA	C4B-C3B-CAB-CBB
35	c	519	DGD	C1A-C2A-C3A-C4A
27	B	620	SQD	C11-C10-C9-C8
24	a	407	PHO	C8-C10-C11-C12
23	c	510	CLA	C13-C15-C16-C17
29	D	406	PL9	C35-C34-C36-C37
29	a	415	PL9	C45-C44-C46-C47
34	m	103	LMT	C2'-C1'-O1'-C1
33	B	622	HTG	C3'-C4'-C5'-C6'
34	b	621	LMT	C4-C5-C6-C7
23	B	613	CLA	C12-C13-C15-C16
23	B	615	CLA	C11-C12-C13-C15
23	b	606	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	c	510	CLA	C12-C13-C15-C16
23	c	512	CLA	C12-C13-C15-C16
23	A	404	CLA	C13-C15-C16-C17
23	C	513	CLA	CBA-CGA-O2A-C1
23	A	406	CLA	C16-C17-C18-C20
27	a	412	SQD	C27-C28-C29-C30
32	C	521	LMG	C32-C33-C34-C35
27	D	412	SQD	O47-C45-C46-O48
35	C	518	DGD	CCB-CDB-CEB-CFB
23	a	404	CLA	C2C-C3C-CAC-CBC
33	B	622	HTG	C1'-C2'-C3'-C4'
23	a	405	CLA	C4C-C3C-CAC-CBC
31	D	407	LHG	C10-C11-C12-C13
34	m	103	LMT	O5'-C1'-O1'-C1
31	d	408	LHG	C35-C36-C37-C38
23	b	612	CLA	C10-C11-C12-C13
27	b	620	SQD	C17-C18-C19-C20
27	a	410	SQD	C31-C32-C33-C34
32	m	101	LMG	C30-C31-C32-C33
23	b	613	CLA	C2-C1-O2A-CGA
23	b	601	CLA	O1D-CGD-O2D-CED
31	L	101	LHG	C11-C12-C13-C14
31	d	407	LHG	C26-C27-C28-C29
35	c	518	DGD	CCA-CDA-CEA-CFA
23	B	610	CLA	C13-C15-C16-C17
23	C	510	CLA	C13-C15-C16-C17
23	C	512	CLA	C8-C10-C11-C12
32	C	502	LMG	C32-C33-C34-C35
35	C	518	DGD	C2A-C3A-C4A-C5A
23	B	613	CLA	C11-C12-C13-C14
23	b	606	CLA	C11-C10-C8-C9
23	b	609	CLA	C6-C7-C8-C9
23	c	510	CLA	C6-C7-C8-C9
23	c	515	CLA	C6-C7-C8-C9
35	C	519	DGD	C5B-C6B-C7B-C8B
23	B	603	CLA	C13-C15-C16-C17
27	b	620	SQD	C26-C27-C28-C29
31	d	407	LHG	C9-C10-C11-C12
35	h	103	DGD	C8B-C9B-CAB-CBB
26	A	410	GOL	O2-C2-C3-O3
26	o	302	GOL	O2-C2-C3-O3
34	a	413	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
38	v	202	HEC	CAD-CBD-CGD-O1D
23	B	614	CLA	C2A-CAA-CBA-CGA
23	C	503	CLA	C2A-CAA-CBA-CGA
31	L	101	LHG	C32-C33-C34-C35
34	E	102	LMT	O1'-C1-C2-C3
23	A	406	CLA	C2B-C3B-CAB-CBB
23	B	607	CLA	C2B-C3B-CAB-CBB
23	C	509	CLA	C2B-C3B-CAB-CBB
23	a	408	CLA	C2B-C3B-CAB-CBB
23	b	601	CLA	C2B-C3B-CAB-CBB
23	b	609	CLA	C2B-C3B-CAB-CBB
23	c	503	CLA	C2B-C3B-CAB-CBB
23	c	514	CLA	C2B-C3B-CAB-CBB
25	D	405	BCR	C23-C24-C25-C26
25	b	617	BCR	C1-C6-C7-C8
34	t	101	LMT	C4-C5-C6-C7
35	c	518	DGD	C2B-C3B-C4B-C5B
23	b	606	CLA	C16-C17-C18-C19
23	c	508	CLA	C16-C17-C18-C19
23	C	508	CLA	C4-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
29	A	413	PL9	C45-C44-C46-C47
38	v	202	HEC	CAD-CBD-CGD-O2D
23	B	611	CLA	C11-C12-C13-C15
23	C	514	CLA	C12-C13-C15-C16
23	b	604	CLA	C12-C13-C15-C16
23	c	511	CLA	C6-C7-C8-C10
35	C	520	DGD	CBA-CCA-CDA-CEA
38	E	103	HEC	CAD-CBD-CGD-O1D
27	A	411	SQD	C15-C16-C17-C18
27	a	412	SQD	C30-C31-C32-C33
31	d	406	LHG	C27-C28-C29-C30
32	c	501	LMG	C18-C19-C20-C21
34	e	101	LMT	C4-C5-C6-C7
23	C	515	CLA	C2-C3-C5-C6
29	A	413	PL9	C43-C44-C46-C47
27	D	412	SQD	C33-C34-C35-C36
23	B	614	CLA	C6-C7-C8-C9
23	C	514	CLA	C14-C13-C15-C16
23	a	406	CLA	C14-C13-C15-C16
27	f	101	SQD	C28-C29-C30-C31
23	C	515	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	B	606	CLA	C16-C17-C18-C19
23	B	604	CLA	C4C-C3C-CAC-CBC
32	C	502	LMG	C16-C17-C18-C19
38	E	103	HEC	CAD-CBD-CGD-O2D
23	A	404	CLA	C2A-CAA-CBA-CGA
31	D	407	LHG	C34-C35-C36-C37
31	b	629	LHG	C32-C33-C34-C35
34	e	101	LMT	C2-C1-O1'-C1'
35	c	518	DGD	C5B-C6B-C7B-C8B
23	c	508	CLA	C4-C3-C5-C6
32	B	621	LMG	C37-C38-C39-C40
23	b	604	CLA	C16-C17-C18-C19
23	D	403	CLA	C4B-C3B-CAB-CBB
23	a	405	CLA	C16-C17-C18-C20
33	c	523	HTG	S1-C1'-C2'-C3'
27	a	410	SQD	C27-C28-C29-C30
38	V	201	HEC	CAD-CBD-CGD-O1D
32	c	501	LMG	C19-C20-C21-C22
27	f	101	SQD	O47-C45-C46-O48
35	c	519	DGD	CCB-CDB-CEB-CFB
23	a	405	CLA	O1D-CGD-O2D-CED
35	c	520	DGD	O6E-C5E-C6E-O5E
34	M	101	LMT	C2-C3-C4-C5
31	A	416	LHG	O2-C2-C3-O3
38	V	201	HEC	CAD-CBD-CGD-O2D
23	B	606	CLA	C11-C10-C8-C9
23	d	403	CLA	C14-C13-C15-C16
24	A	415	PHO	C6-C7-C8-C9
35	c	518	DGD	C5D-C6D-O5D-C1E
34	b	627	LMT	C1-C2-C3-C4
23	C	508	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
33	C	523	HTG	C4-C5-C6-O6
23	B	609	CLA	C3A-C2A-CAA-CBA
31	A	416	LHG	C30-C31-C32-C33
29	d	405	PL9	C43-C44-C46-C47
26	b	624	GOL	O1-C1-C2-C3
23	c	504	CLA	C3-C5-C6-C7
35	c	520	DGD	CCB-CDB-CEB-CFB
27	B	620	SQD	C7-C8-C9-C10
23	B	602	CLA	O2A-C1-C2-C3
35	H	102	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
23	b	610	CLA	C15-C16-C17-C18
23	B	612	CLA	C10-C11-C12-C13
23	b	605	CLA	C13-C15-C16-C17
34	E	102	LMT	C6-C7-C8-C9
27	C	501	SQD	C10-C11-C12-C13
32	d	412	LMG	C29-C30-C31-C32
32	d	412	LMG	C12-C13-C14-C15
32	z	101	LMG	C15-C16-C17-C18
31	D	408	LHG	O1-C1-C2-O2
27	b	620	SQD	C12-C13-C14-C15
34	e	101	LMT	C2B-C1B-O1B-C4'
31	L	101	LHG	C29-C30-C31-C32
34	E	102	LMT	C7-C8-C9-C10
34	M	103	LMT	C6-C7-C8-C9
35	h	103	DGD	C6A-C7A-C8A-C9A
35	c	519	DGD	C5B-C6B-C7B-C8B
32	B	621	LMG	C17-C18-C19-C20
35	h	103	DGD	O1B-C1B-C2B-C3B
23	b	601	CLA	C6-C7-C8-C9
23	b	610	CLA	C11-C12-C13-C14
23	B	613	CLA	CAA-CBA-CGA-O2A
23	C	512	CLA	CAA-CBA-CGA-O2A
27	A	411	SQD	C24-C25-C26-C27
23	A	408	CLA	C12-C13-C15-C16
23	B	601	CLA	C6-C7-C8-C10
23	B	606	CLA	C11-C10-C8-C7
23	B	606	CLA	C12-C13-C15-C16
23	b	611	CLA	C6-C7-C8-C10
23	d	403	CLA	C12-C13-C15-C16
23	A	404	CLA	C2B-C3B-CAB-CBB
23	C	515	CLA	C2B-C3B-CAB-CBB
23	D	403	CLA	C2B-C3B-CAB-CBB
25	C	516	BCR	C1-C6-C7-C8
25	a	409	BCR	C1-C6-C7-C8
25	b	617	BCR	C5-C6-C7-C8
25	d	404	BCR	C23-C24-C25-C26
25	t	102	BCR	C1-C6-C7-C8
25	t	102	BCR	C5-C6-C7-C8
25	y	101	BCR	C23-C24-C25-C30
27	f	101	SQD	O48-C23-C24-C25
27	b	620	SQD	C11-C10-C9-C8
31	d	406	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
32	m	101	LMG	C37-C38-C39-C40
23	a	408	CLA	C2-C1-O2A-CGA
23	a	405	CLA	C16-C17-C18-C19
29	d	405	PL9	C34-C36-C37-C38
34	a	413	LMT	C9-C10-C11-C12
35	c	518	DGD	O2G-C1B-C2B-C3B
23	C	505	CLA	C5-C6-C7-C8
32	Z	101	LMG	O7-C10-C11-C12
23	C	512	CLA	C2-C3-C5-C6
23	B	613	CLA	C13-C15-C16-C17
33	B	622	HTG	C2'-C1'-S1-C1
32	c	521	LMG	C10-C11-C12-C13
23	C	514	CLA	CAA-CBA-CGA-O2A
31	b	629	LHG	O7-C7-C8-C9
31	D	407	LHG	C17-C18-C19-C20
32	B	621	LMG	C29-C30-C31-C32
31	d	406	LHG	O8-C23-C24-C25
34	a	413	LMT	C2-C3-C4-C5
31	A	416	LHG	C29-C30-C31-C32
35	h	103	DGD	C6B-C7B-C8B-C9B
23	C	512	CLA	C4-C3-C5-C6
27	f	101	SQD	C33-C34-C35-C36
23	a	408	CLA	C15-C16-C17-C18
27	b	620	SQD	C27-C28-C29-C30
32	c	501	LMG	C37-C38-C39-C40
23	c	505	CLA	C15-C16-C17-C18
27	b	620	SQD	O48-C23-C24-C25
32	D	413	LMG	O7-C10-C11-C12
34	b	627	LMT	C2-C1-O1'-C1'
23	c	508	CLA	C13-C15-C16-C17
27	B	620	SQD	C33-C34-C35-C36
23	b	604	CLA	C14-C13-C15-C16
23	c	511	CLA	C6-C7-C8-C9
23	b	613	CLA	CAA-CBA-CGA-O2A
23	c	514	CLA	CAA-CBA-CGA-O2A
31	A	416	LHG	O8-C23-C24-C25
27	D	412	SQD	C44-C45-C46-O48
24	A	415	PHO	C2C-C3C-CAC-CBC
35	c	519	DGD	C2B-C3B-C4B-C5B
23	b	602	CLA	C13-C15-C16-C17
23	B	607	CLA	C4B-C3B-CAB-CBB
23	C	515	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	a	405	CLA	C1A-C2A-CAA-CBA
34	M	103	LMT	C3-C4-C5-C6
23	b	602	CLA	C8-C10-C11-C12
31	D	408	LHG	O8-C23-C24-C25
31	L	101	LHG	O7-C7-C8-C9
32	C	502	LMG	O7-C10-C11-C12
31	d	407	LHG	C14-C15-C16-C17
35	c	518	DGD	O1G-C1A-C2A-C3A
34	C	526	LMT	C4-C5-C6-C7
31	L	101	LHG	C18-C19-C20-C21
32	B	621	LMG	C14-C15-C16-C17
23	c	508	CLA	C16-C17-C18-C20
32	c	521	LMG	O7-C10-C11-C12
31	A	416	LHG	C11-C10-C9-C8
31	A	416	LHG	C33-C34-C35-C36
34	m	103	LMT	O1'-C1-C2-C3
27	B	620	SQD	C5-C6-S-O7
27	B	620	SQD	C5-C6-S-O9
31	a	419	LHG	C16-C17-C18-C19
23	B	613	CLA	C2-C1-O2A-CGA
23	c	513	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2-C1-O2A-CGA
23	B	610	CLA	C11-C12-C13-C15
23	b	609	CLA	C12-C13-C15-C16
23	c	514	CLA	C6-C7-C8-C10
32	c	501	LMG	C36-C37-C38-C39
38	e	102	HEC	CAD-CBD-CGD-O2D
23	c	512	CLA	CAA-CBA-CGA-O2A
34	D	402	LMT	C1-C2-C3-C4
23	C	505	CLA	C15-C16-C17-C18
38	E	103	HEC	CAA-CBA-CGA-O1A
38	e	102	HEC	CAD-CBD-CGD-O1D
23	b	612	CLA	CAA-CBA-CGA-O2A
27	f	101	SQD	O10-C23-C24-C25
35	C	518	DGD	C2B-C3B-C4B-C5B
23	C	514	CLA	CAA-CBA-CGA-O1A
35	H	102	DGD	O1B-C1B-C2B-C3B
35	c	518	DGD	O1B-C1B-C2B-C3B
32	d	412	LMG	C19-C20-C21-C22
23	B	601	CLA	C6-C7-C8-C9
23	D	404	CLA	C11-C10-C8-C9
23	c	515	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
27	C	501	SQD	C28-C29-C30-C31
34	D	402	LMT	C4'-C5'-C6'-O6'
25	C	516	BCR	C11-C12-C13-C35
31	b	629	LHG	O9-C7-C8-C9
23	b	609	CLA	C2-C3-C5-C6
23	C	512	CLA	CAA-CBA-CGA-O1A
31	d	406	LHG	O10-C23-C24-C25
32	c	521	LMG	O9-C10-C11-C12
31	D	408	LHG	C25-C26-C27-C28
23	A	405	CLA	C4C-C3C-CAC-CBC
23	c	514	CLA	CAA-CBA-CGA-O1A
31	A	416	LHG	O10-C23-C24-C25
23	a	404	CLA	C4C-C3C-CAC-CBC
32	m	101	LMG	C8-C7-O1-C1
35	C	518	DGD	C5D-C6D-O5D-C1E
35	C	519	DGD	C2G-C3G-O3G-C1D
35	H	102	DGD	C2G-C3G-O3G-C1D
35	H	102	DGD	O1G-C1G-C2G-O2G
23	B	613	CLA	CAA-CBA-CGA-O1A
32	Z	101	LMG	O9-C10-C11-C12
35	c	518	DGD	O1A-C1A-C2A-C3A
23	B	602	CLA	C2A-CAA-CBA-CGA
35	H	102	DGD	O1G-C1G-C2G-C3G
27	f	101	SQD	C23-C24-C25-C26
23	c	511	CLA	C8-C10-C11-C12
23	B	612	CLA	CAA-CBA-CGA-O2A
38	E	103	HEC	CAA-CBA-CGA-O2A
31	D	408	LHG	O10-C23-C24-C25
23	C	511	CLA	CAD-CBD-CGD-O2D
23	b	601	CLA	CAD-CBD-CGD-O2D
23	D	404	CLA	C5-C6-C7-C8
32	D	413	LMG	O9-C10-C11-C12
35	c	518	DGD	O6E-C1E-O5D-C6D
23	C	514	CLA	C2-C1-O2A-CGA
23	C	515	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	c	515	CLA	C2-C1-O2A-CGA
23	d	402	CLA	C2-C1-O2A-CGA
29	A	413	PL9	C46-C47-C48-C49
23	b	612	CLA	CAA-CBA-CGA-O1A
27	b	620	SQD	O10-C23-C24-C25
35	C	520	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
35	c	520	DGD	O1G-C1A-C2A-C3A
23	c	512	CLA	CAA-CBA-CGA-O1A
27	b	620	SQD	C19-C20-C21-C22
27	a	410	SQD	C25-C26-C27-C28
24	a	417	PHO	CBD-CGD-O2D-CED
32	C	502	LMG	O9-C10-C11-C12
27	b	620	SQD	C30-C31-C32-C33

There are no ring outliers.

138 monomers are involved in 270 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	B	623	HTG	2	0
23	b	605	CLA	6	0
24	A	407	PHO	2	0
23	a	405	CLA	5	0
33	h	101	HTG	1	0
23	b	616	CLA	5	0
25	B	617	BCR	2	0
32	C	502	LMG	3	0
23	c	505	CLA	5	0
23	A	405	CLA	2	0
25	b	619	BCR	5	0
23	c	508	CLA	1	0
23	C	506	CLA	2	0
23	c	509	CLA	3	0
24	a	417	PHO	3	0
31	d	408	LHG	5	0
23	B	612	CLA	1	0
25	A	409	BCR	2	0
31	E	101	LHG	2	0
32	B	621	LMG	3	0
23	C	508	CLA	6	0
23	B	613	CLA	3	0
23	B	603	CLA	1	0
23	d	402	CLA	1	0
23	c	513	CLA	3	0
34	E	102	LMT	1	0
23	C	515	CLA	1	0
27	a	410	SQD	2	0
23	B	605	CLA	4	0
23	A	408	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	505	CLA	4	0
23	c	510	CLA	2	0
34	C	526	LMT	2	0
23	c	514	CLA	4	0
23	b	609	CLA	2	0
23	C	503	CLA	5	0
25	b	617	BCR	1	0
27	b	620	SQD	1	0
26	c	502	GOL	1	0
25	B	618	BCR	4	0
33	b	622	HTG	2	0
23	A	406	CLA	2	0
31	d	407	LHG	2	0
23	B	601	CLA	1	0
34	b	621	LMT	1	0
23	B	606	CLA	2	0
23	a	408	CLA	2	0
29	a	415	PL9	6	0
35	c	519	DGD	1	0
32	d	412	LMG	2	0
26	b	628	GOL	1	0
25	a	409	BCR	2	0
29	D	406	PL9	2	0
35	C	519	DGD	2	0
35	c	520	DGD	2	0
23	c	506	CLA	2	0
24	A	415	PHO	1	0
25	C	517	BCR	1	0
25	h	102	BCR	3	0
23	B	610	CLA	2	0
23	B	602	CLA	3	0
27	C	501	SQD	3	0
29	A	413	PL9	5	0
32	c	521	LMG	1	0
23	C	510	CLA	3	0
23	D	403	CLA	2	0
25	T	101	BCR	4	0
23	c	507	CLA	6	0
23	A	404	CLA	3	0
23	b	601	CLA	1	0
32	z	101	LMG	2	0
34	D	402	LMT	2	0

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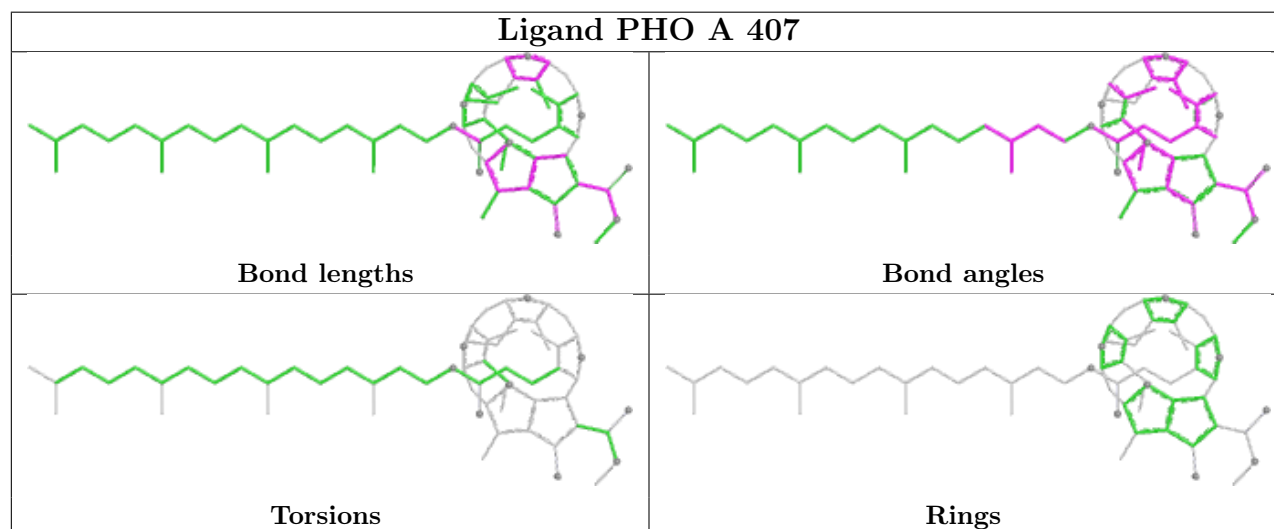
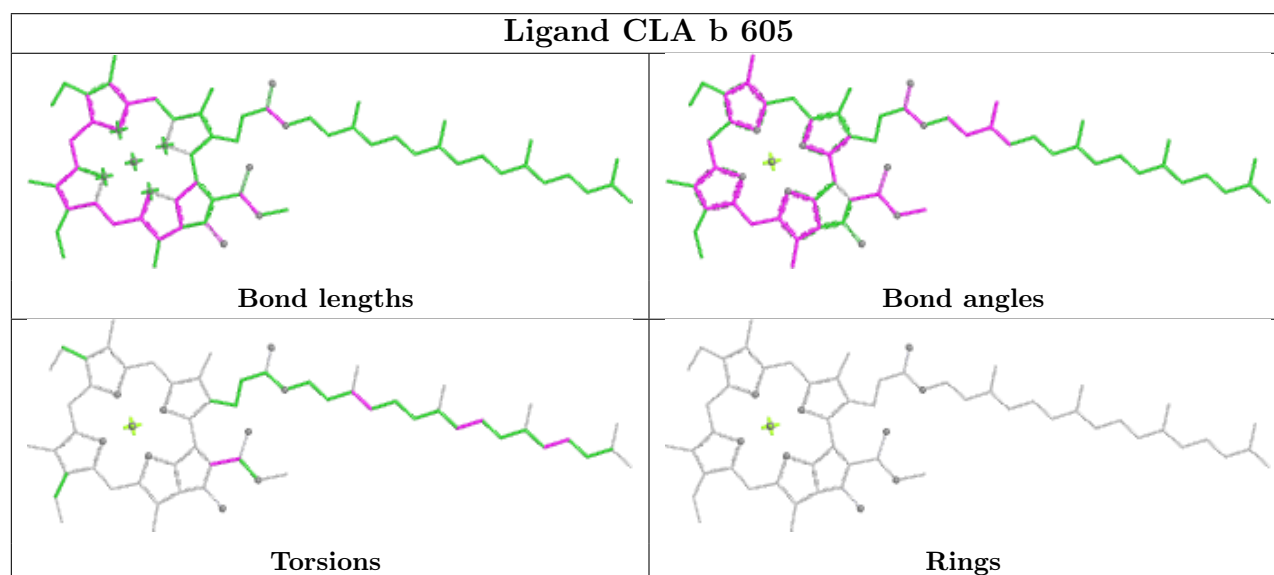
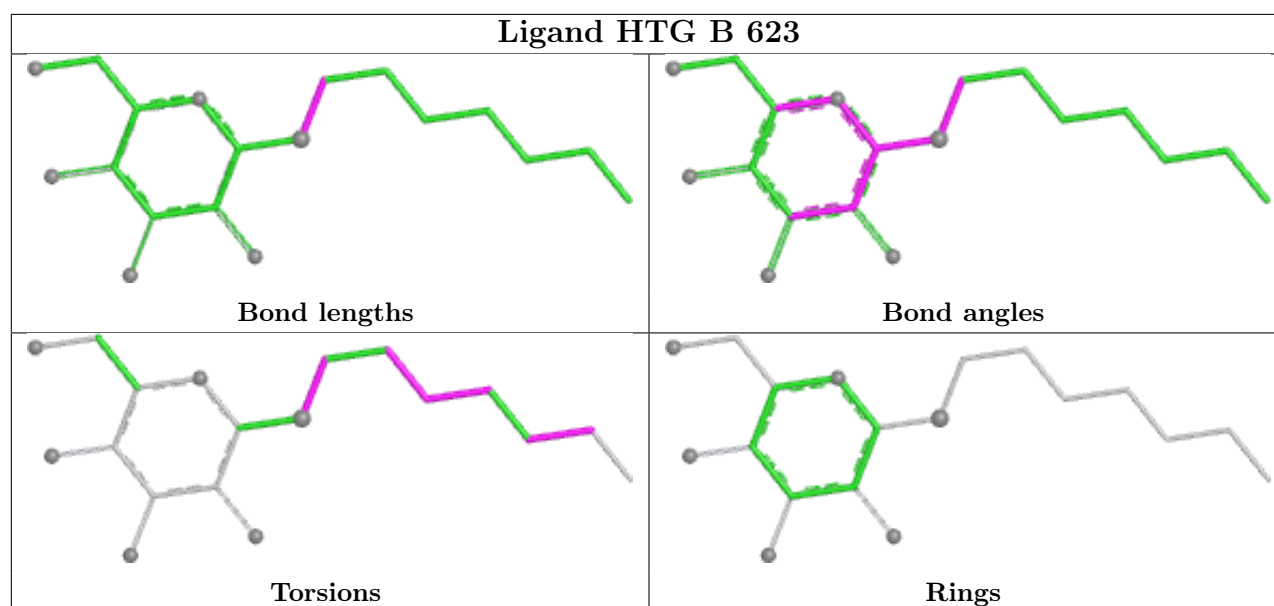
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	616	CLA	5	0
31	D	408	LHG	5	0
35	C	520	DGD	3	0
34	a	418	LMT	2	0
25	Y	101	BCR	1	0
23	C	509	CLA	3	0
32	C	521	LMG	1	0
35	H	102	DGD	1	0
35	c	518	DGD	1	0
23	B	604	CLA	4	0
23	C	513	CLA	2	0
32	D	413	LMG	1	0
35	C	518	DGD	4	0
24	a	407	PHO	2	0
23	C	504	CLA	5	0
25	c	517	BCR	1	0
33	c	523	HTG	1	0
38	e	102	HEC	2	0
25	H	101	BCR	3	0
23	B	615	CLA	5	0
23	b	606	CLA	7	0
25	c	516	BCR	4	0
23	a	404	CLA	1	0
31	a	419	LHG	5	0
23	c	515	CLA	4	0
33	B	622	HTG	2	0
23	B	614	CLA	3	0
23	c	503	CLA	3	0
31	L	101	LHG	2	0
27	f	101	SQD	2	0
33	D	411	HTG	1	0
23	b	613	CLA	3	0
31	d	406	LHG	3	0
33	b	625	HTG	1	0
29	d	405	PL9	1	0
34	a	413	LMT	1	0
26	v	201	GOL	1	0
23	B	607	CLA	2	0
23	b	608	CLA	3	0
25	b	618	BCR	3	0
25	B	619	BCR	1	0
23	c	512	CLA	1	0

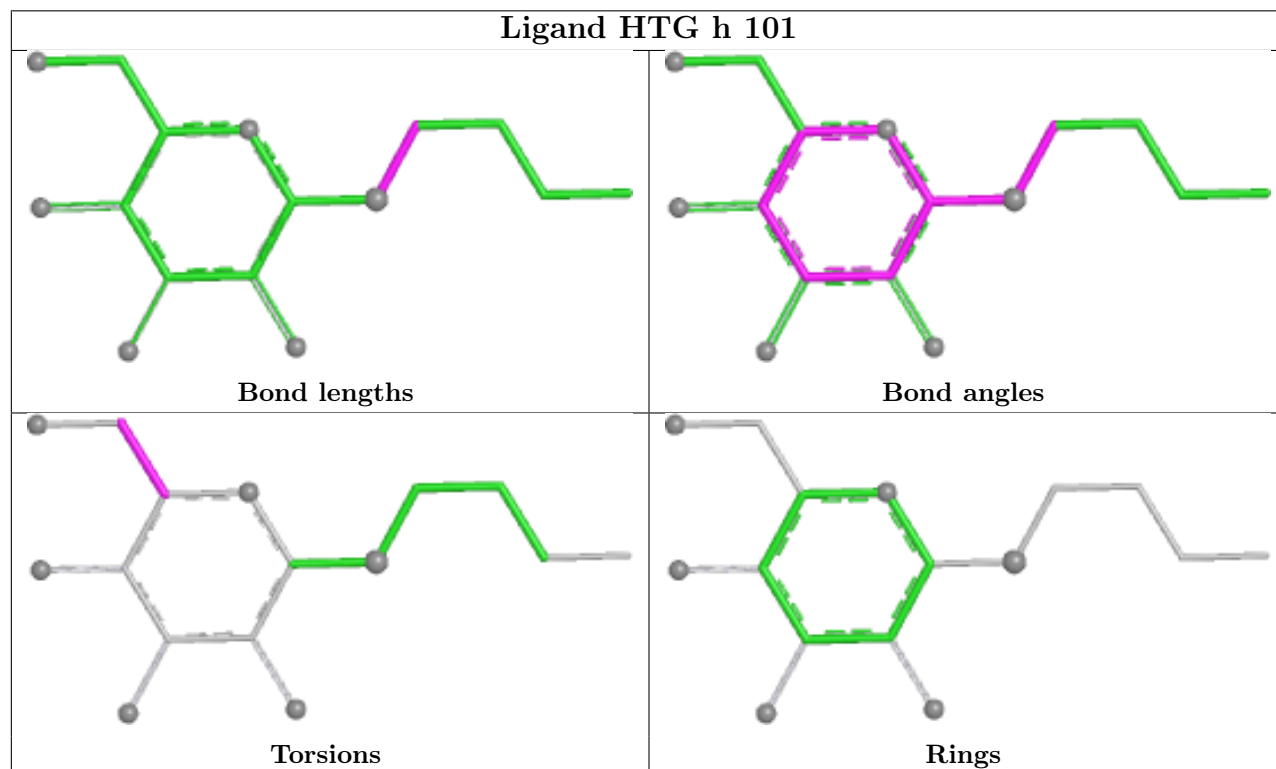
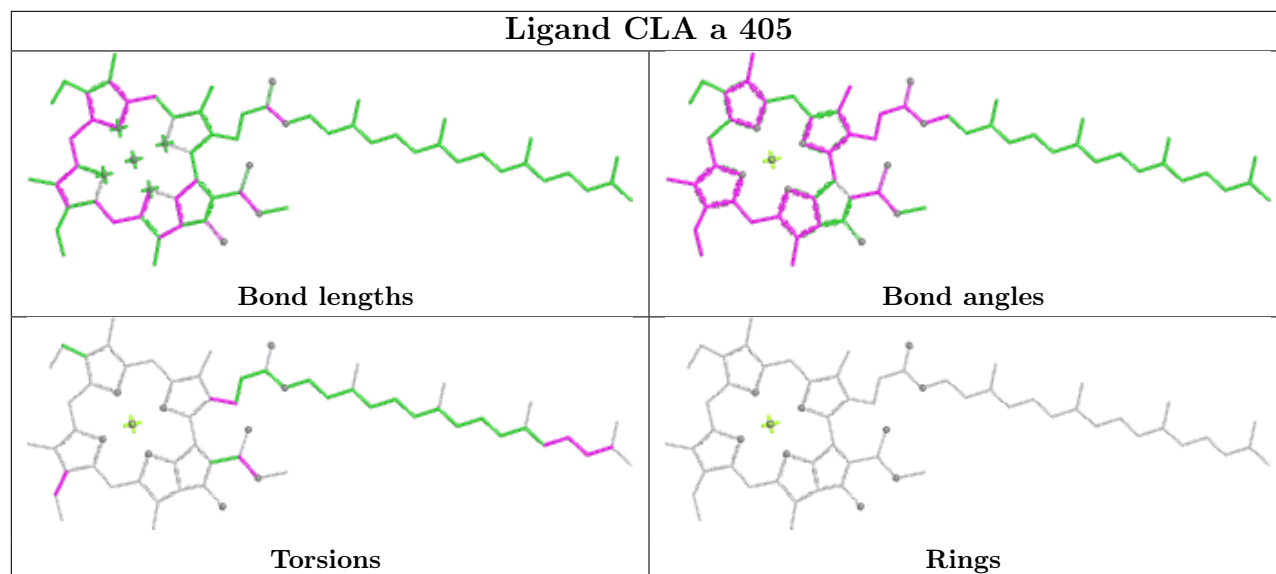
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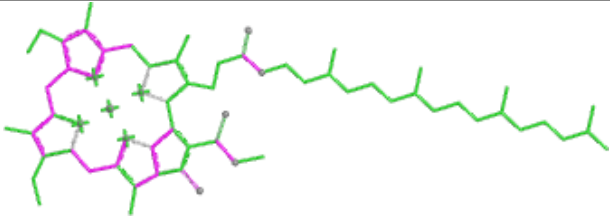
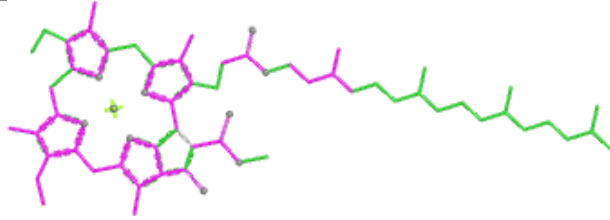
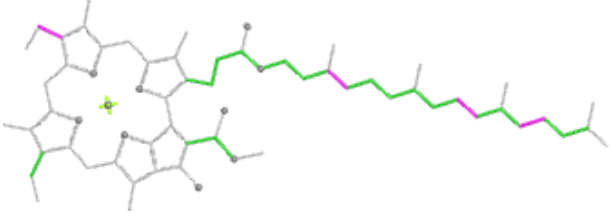
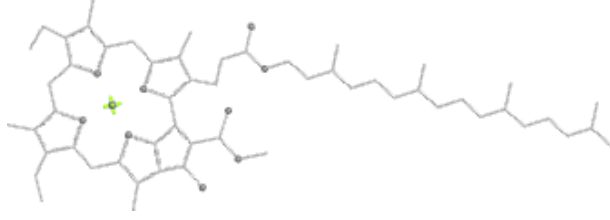
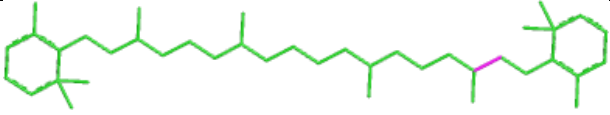
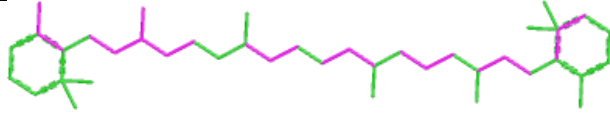
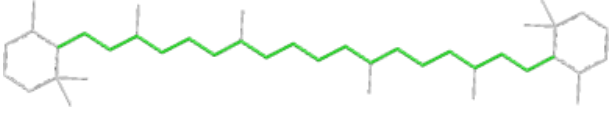
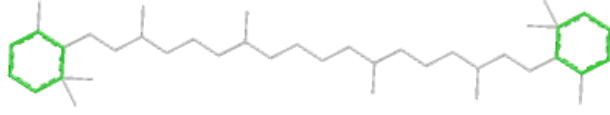
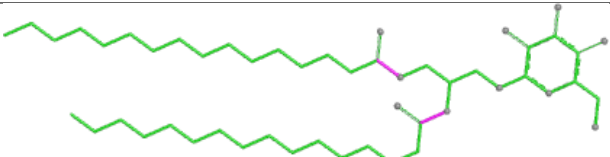
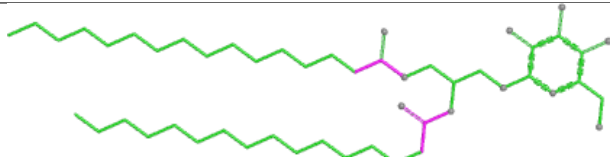
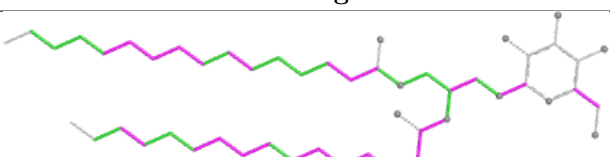
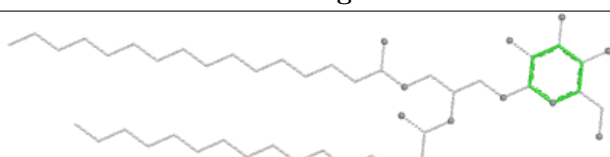
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	507	CLA	2	0
25	K	101	BCR	1	0
38	V	201	HEC	1	0
23	b	615	CLA	2	0
25	d	404	BCR	1	0
32	c	501	LMG	4	0
23	C	512	CLA	2	0
23	b	603	CLA	3	0
31	A	416	LHG	2	0
25	y	101	BCR	2	0
25	k	101	BCR	1	0
31	D	407	LHG	1	0
23	b	610	CLA	1	0
23	b	604	CLA	2	0
23	a	406	CLA	1	0
23	C	514	CLA	1	0
23	c	511	CLA	3	0
34	M	101	LMT	3	0
32	m	101	LMG	2	0
25	t	102	BCR	5	0
23	b	614	CLA	1	0
38	E	103	HEC	1	0
23	B	609	CLA	1	0
27	A	411	SQD	1	0

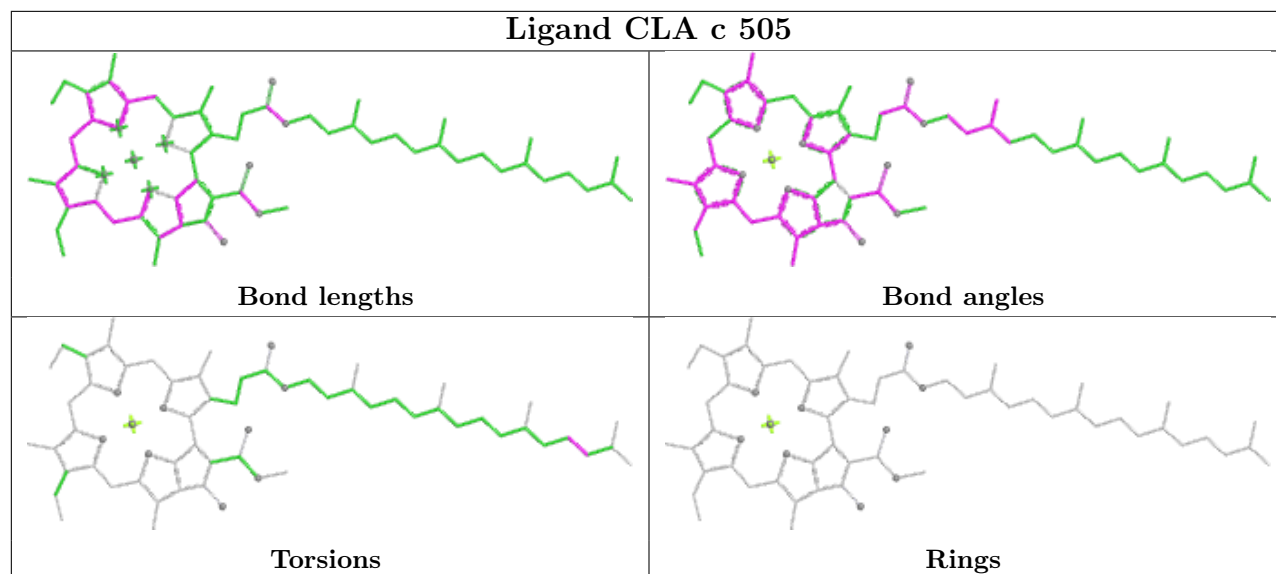
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



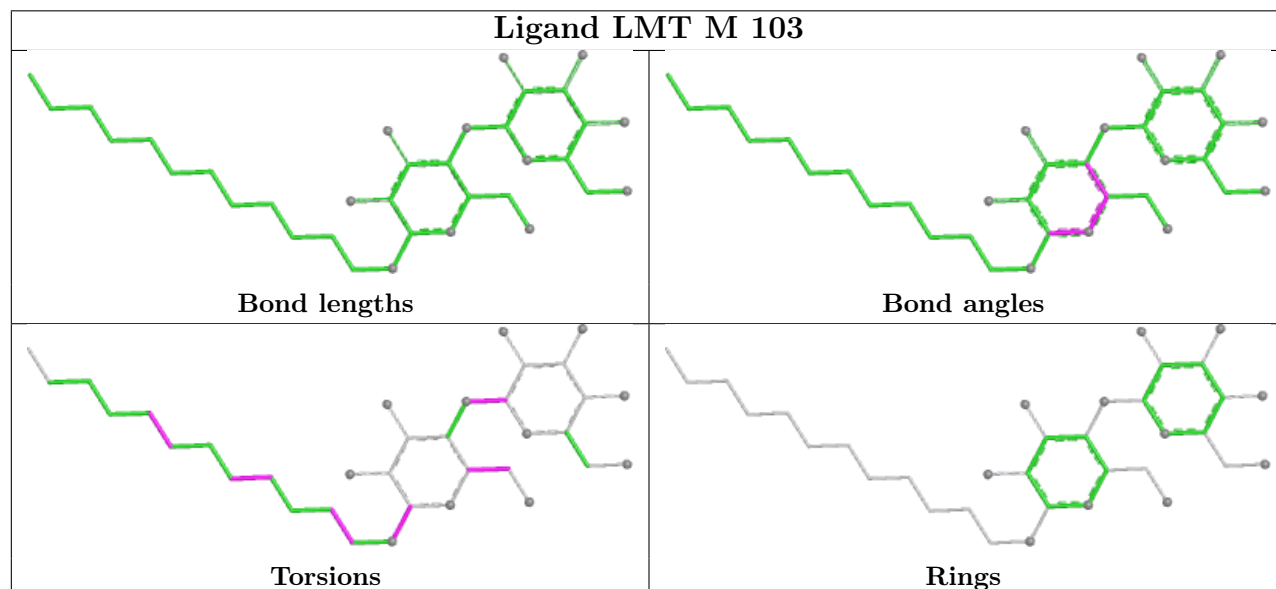


Ligand CLA b 616	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

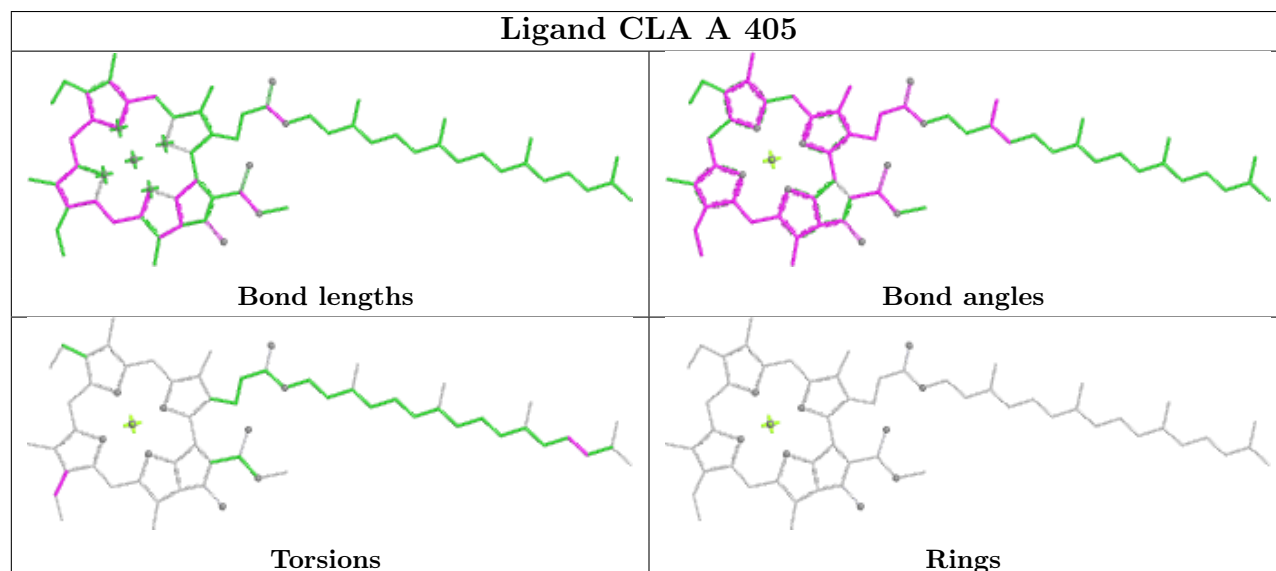
Ligand CLA c 505



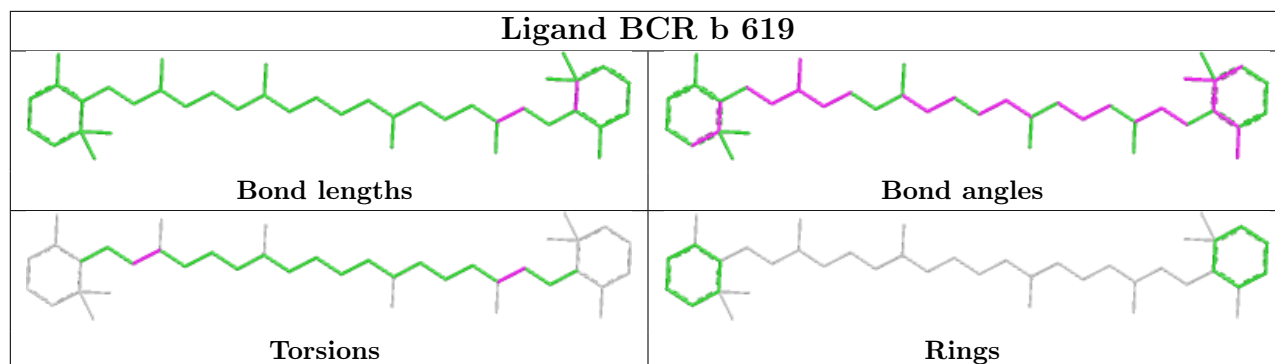
Ligand LMT M 103



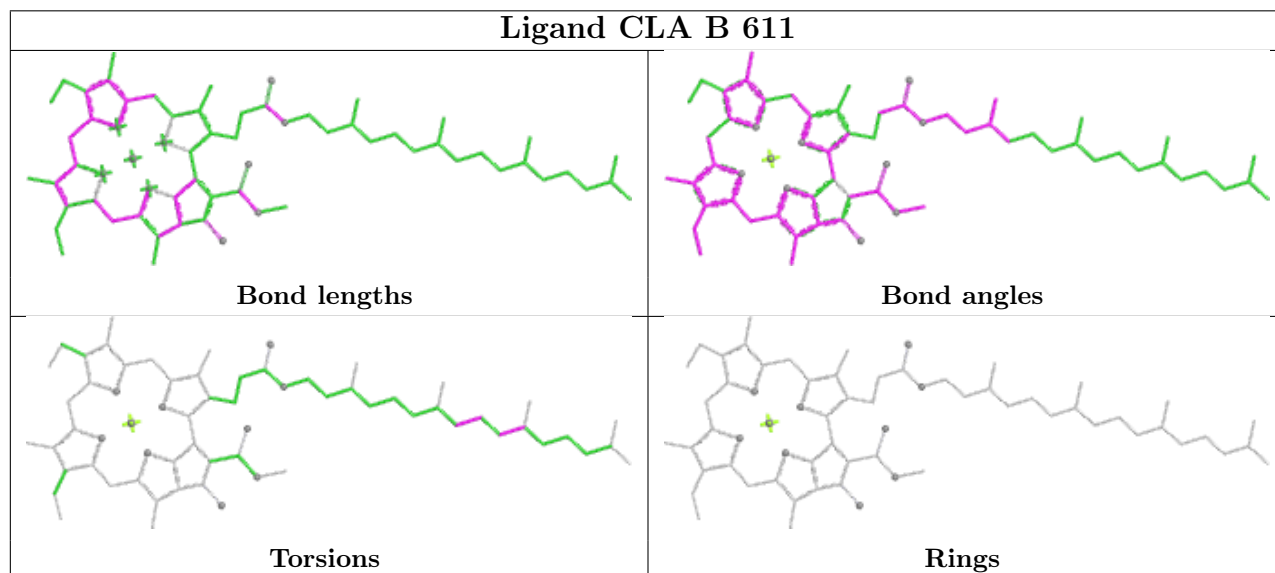
Ligand CLA A 405



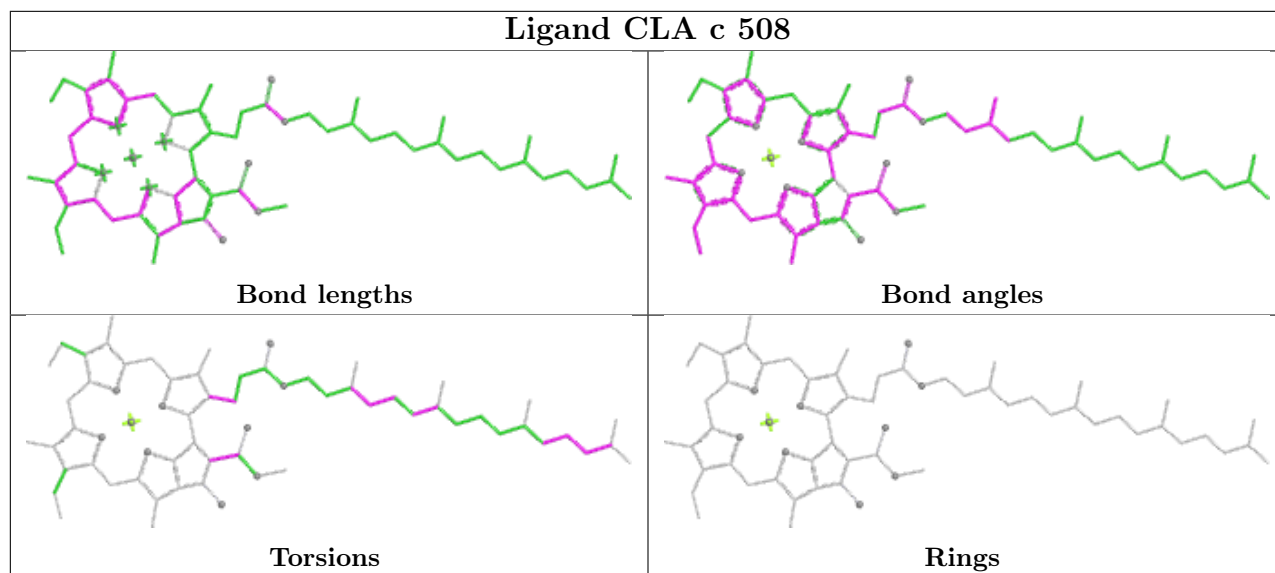
Ligand BCR b 619

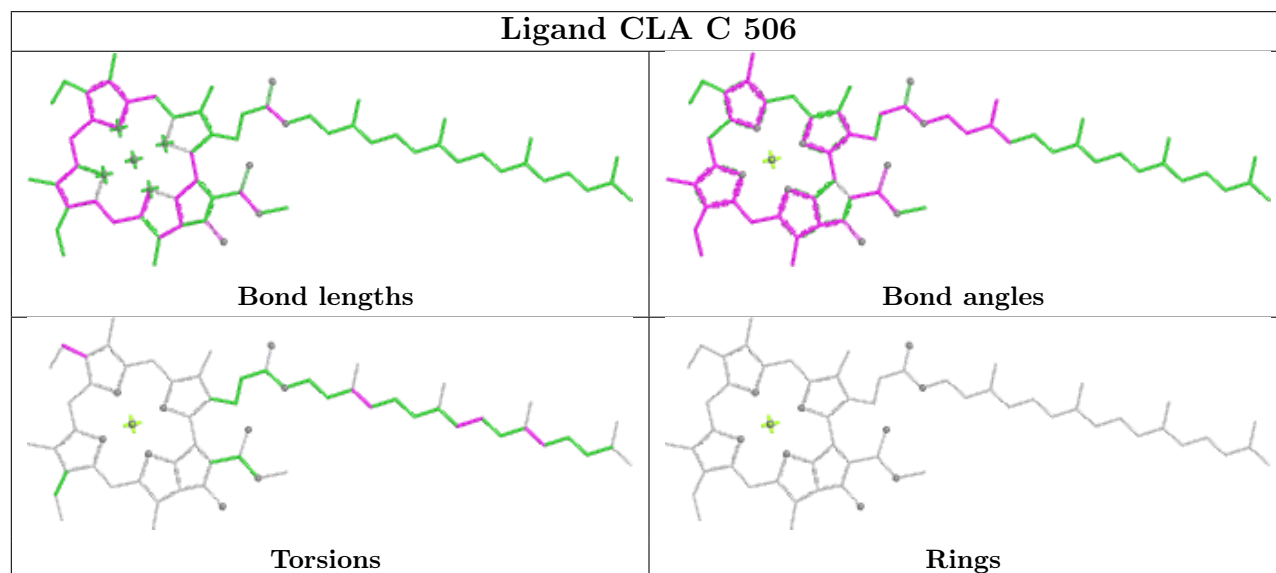
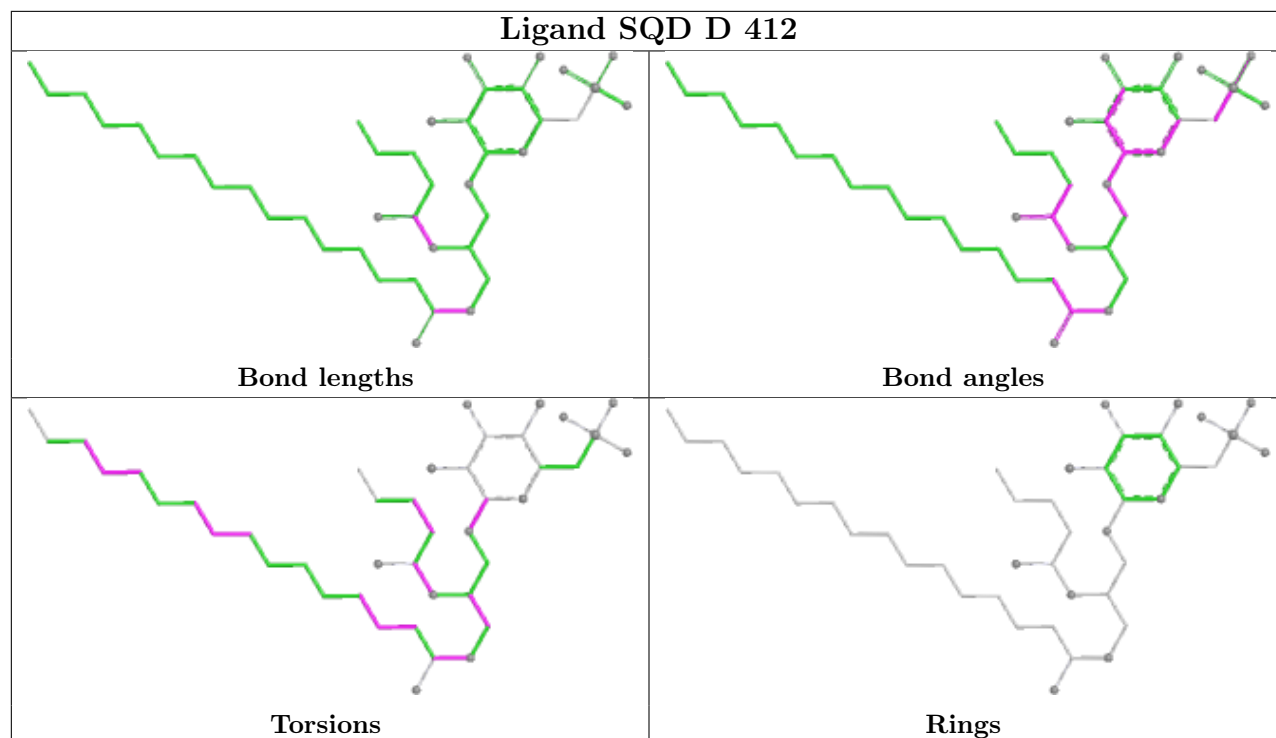


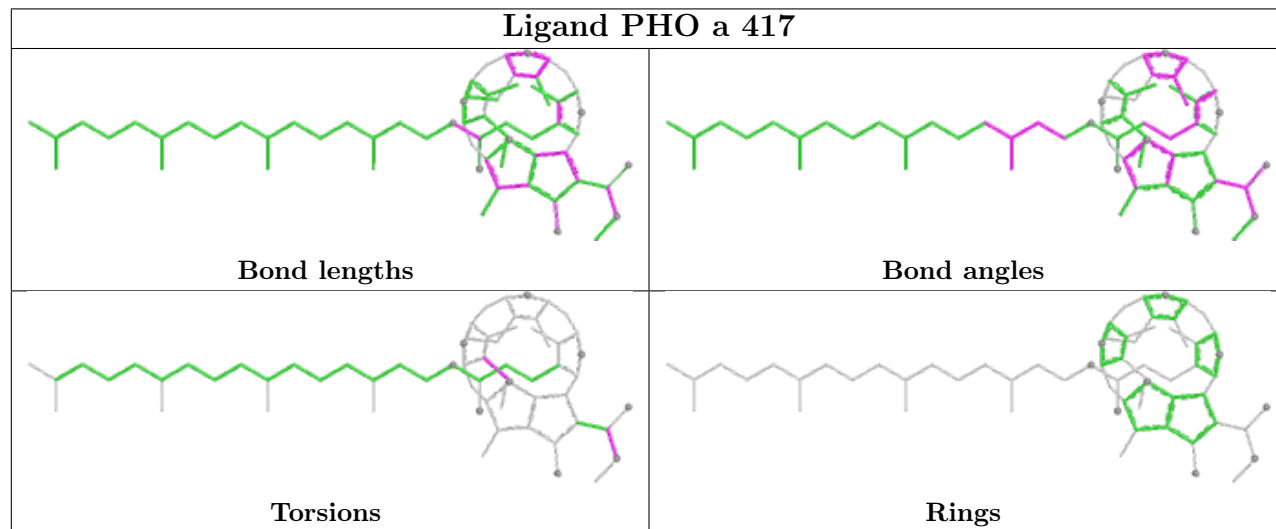
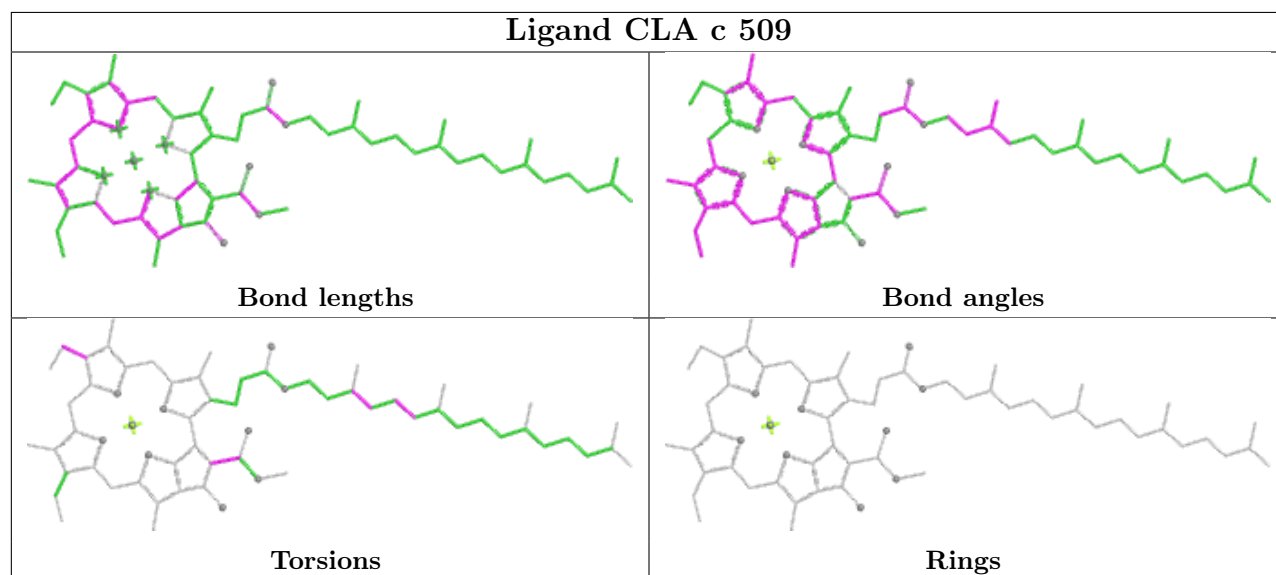
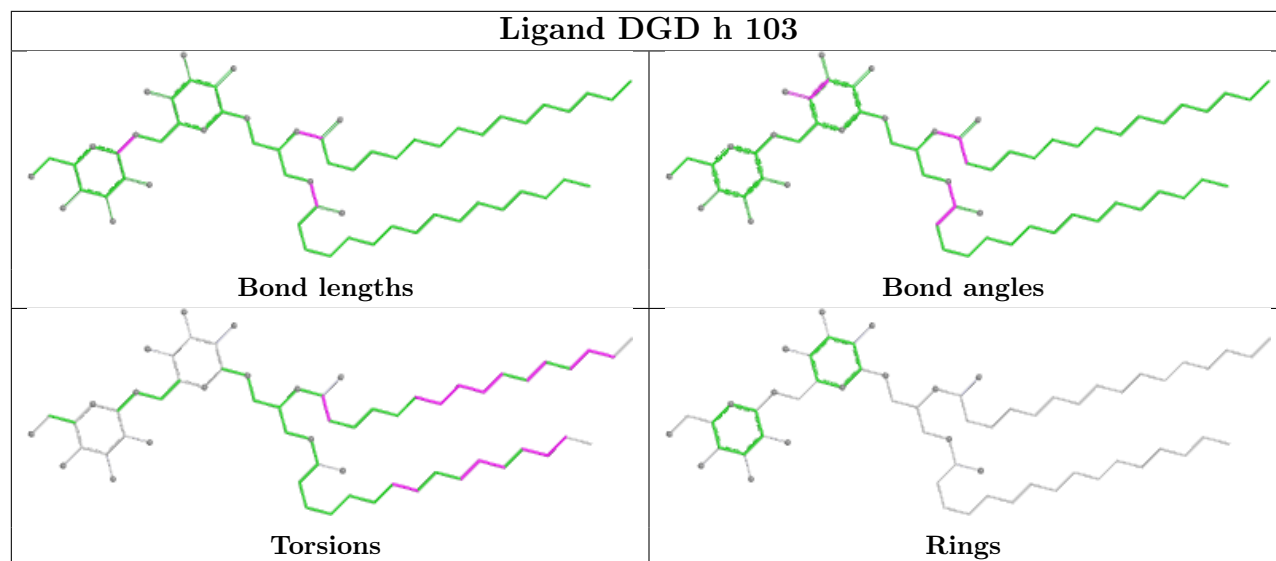
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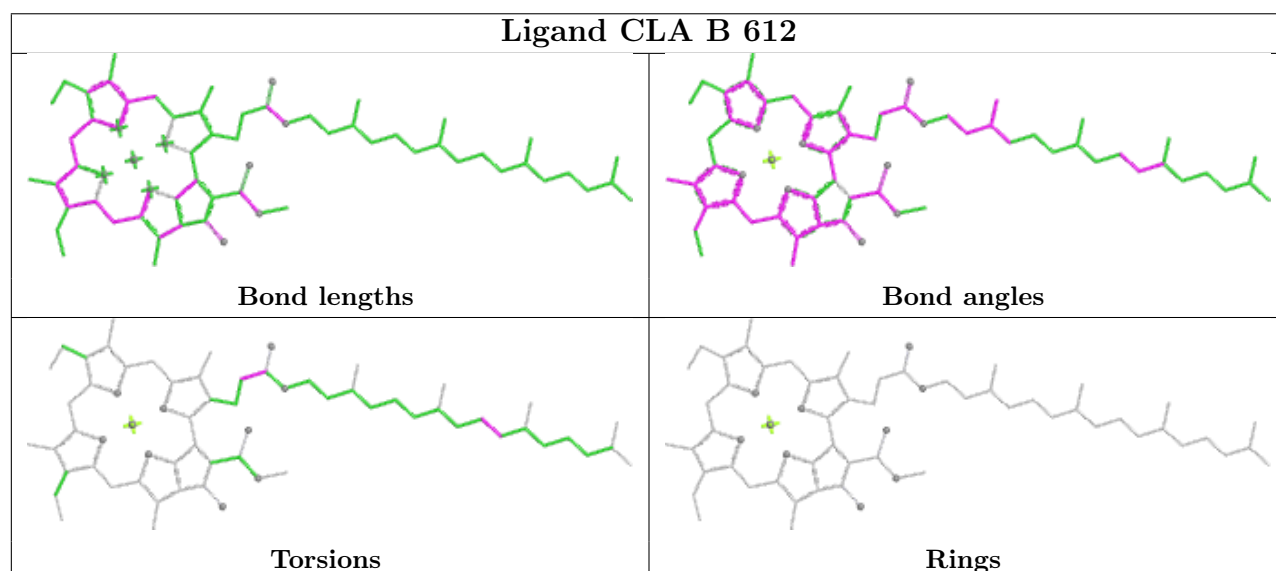
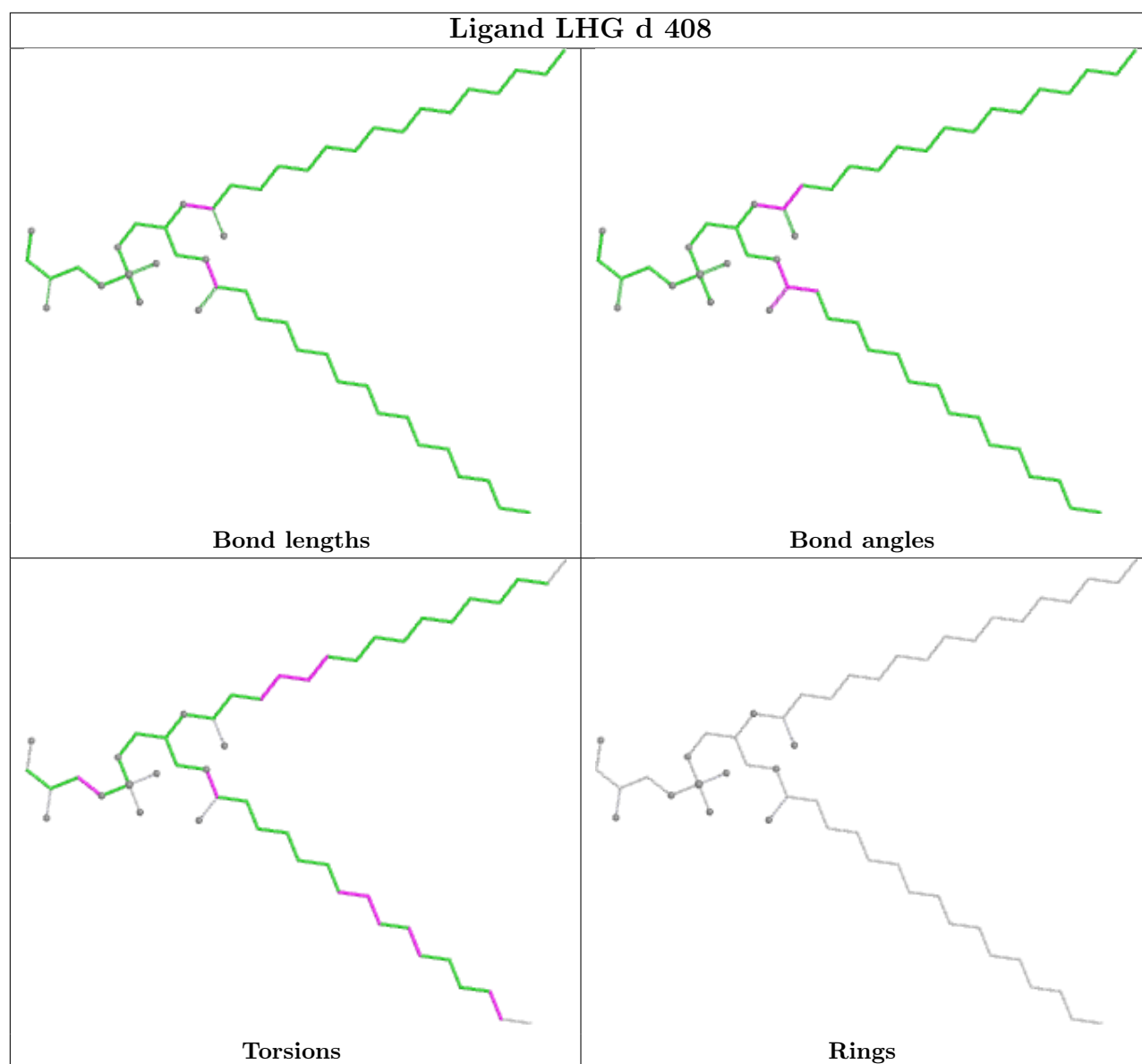


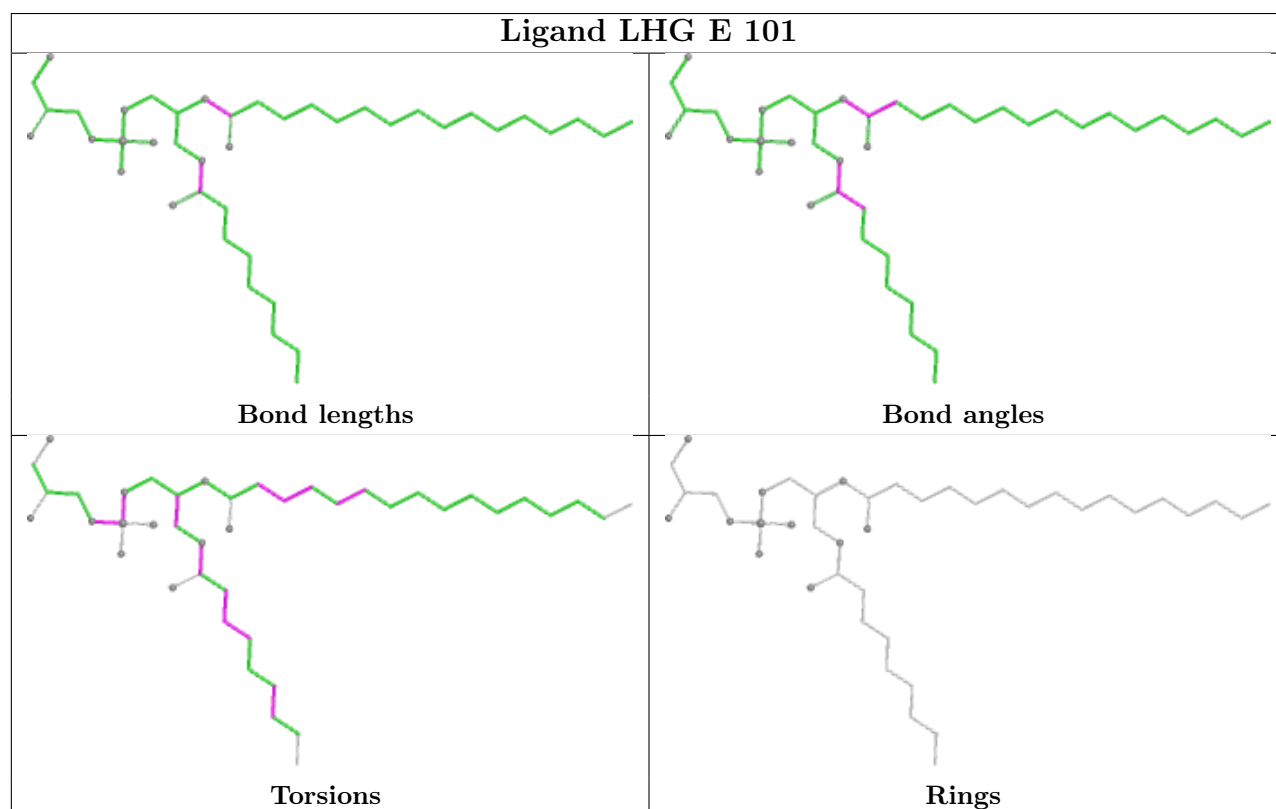
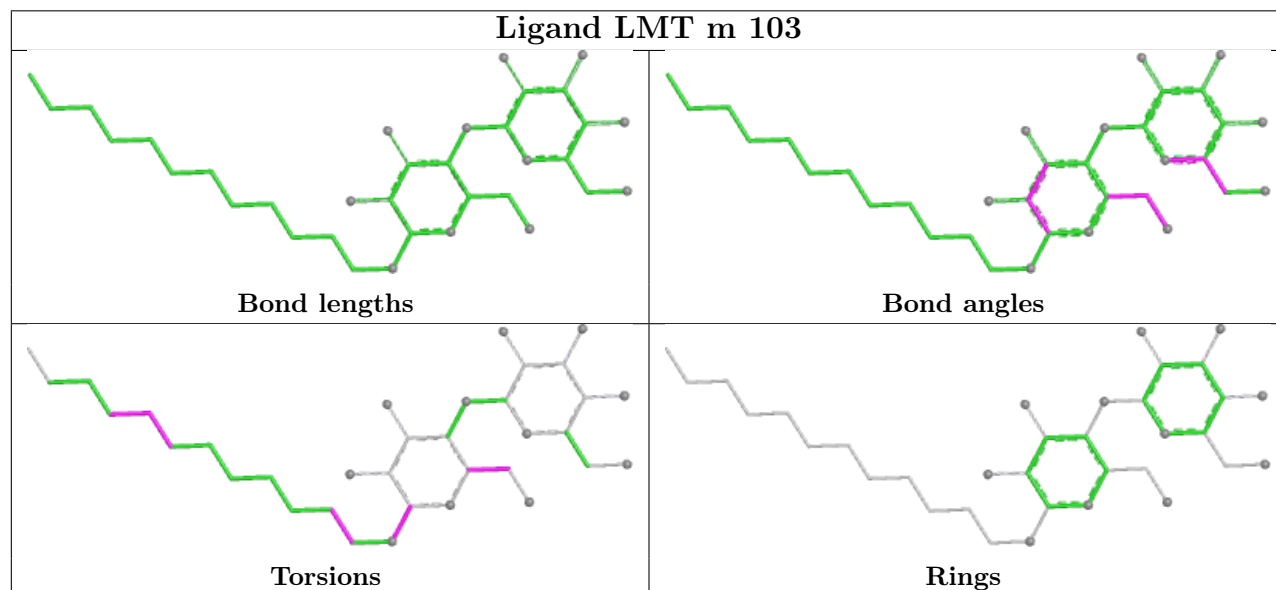
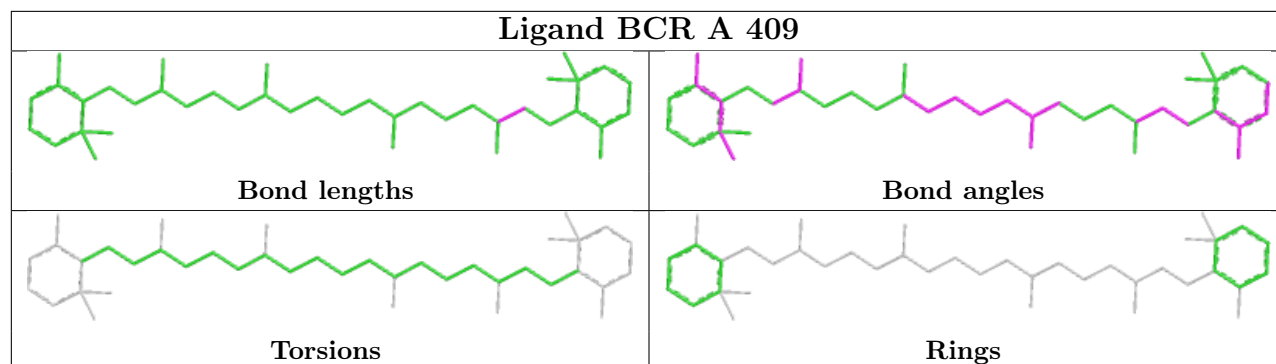
Ligand CLA c 508

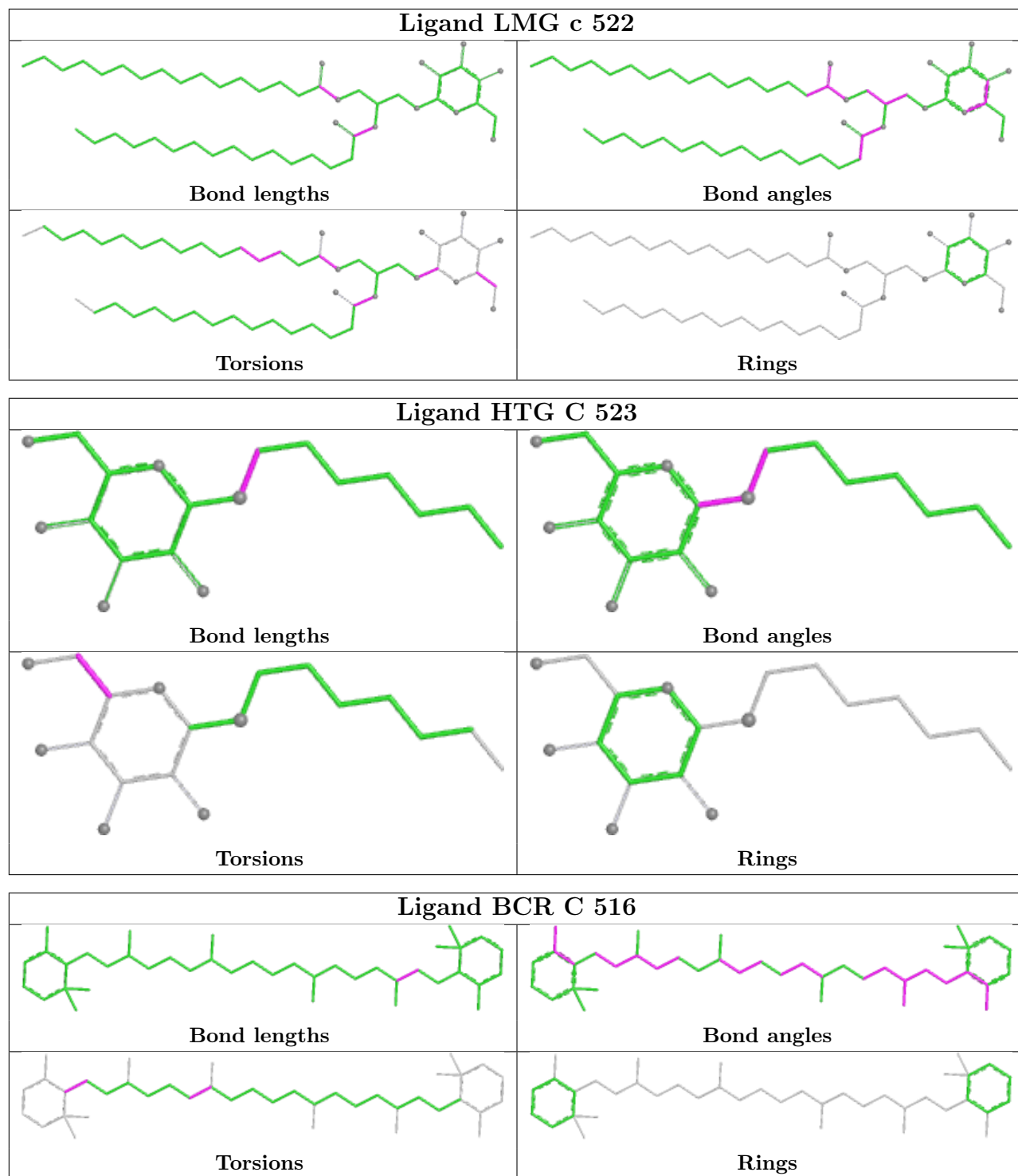


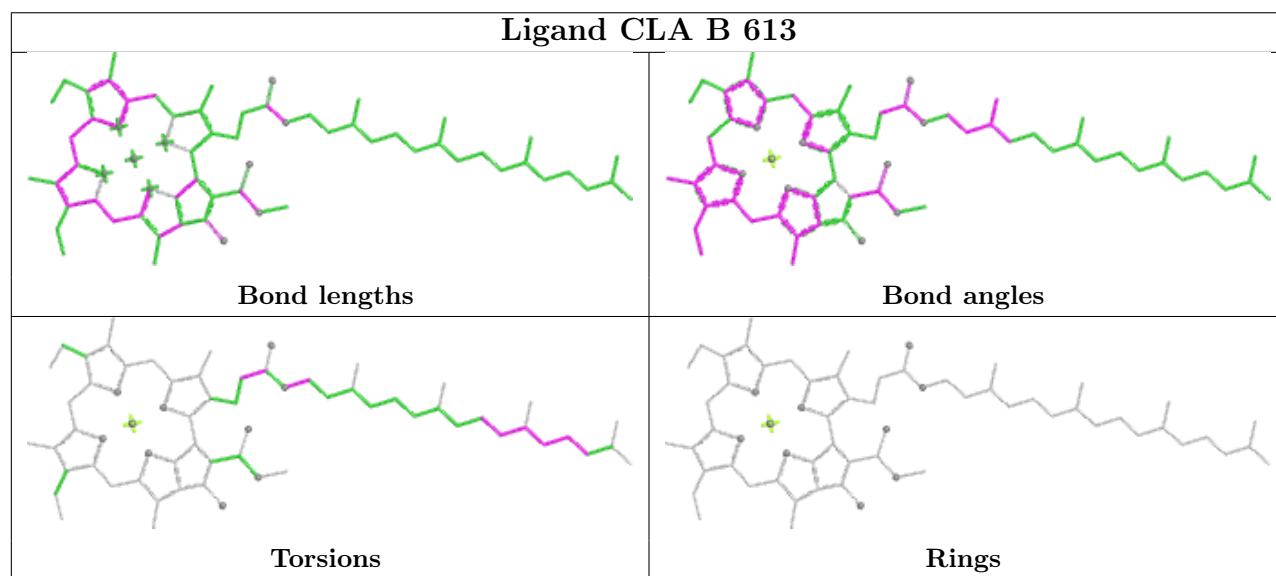
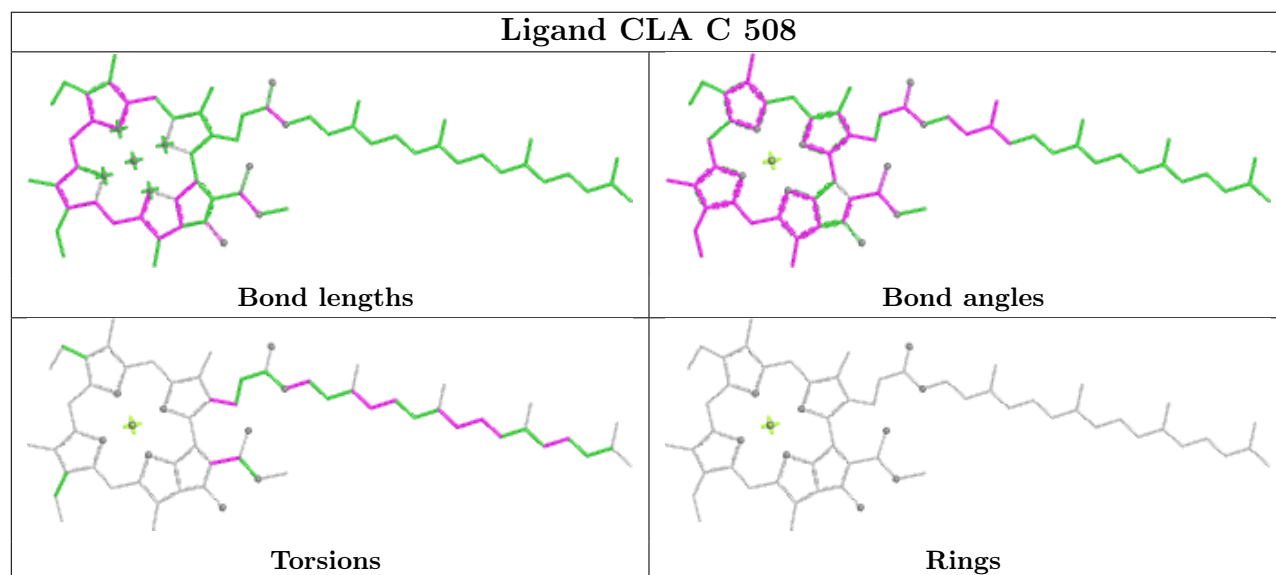
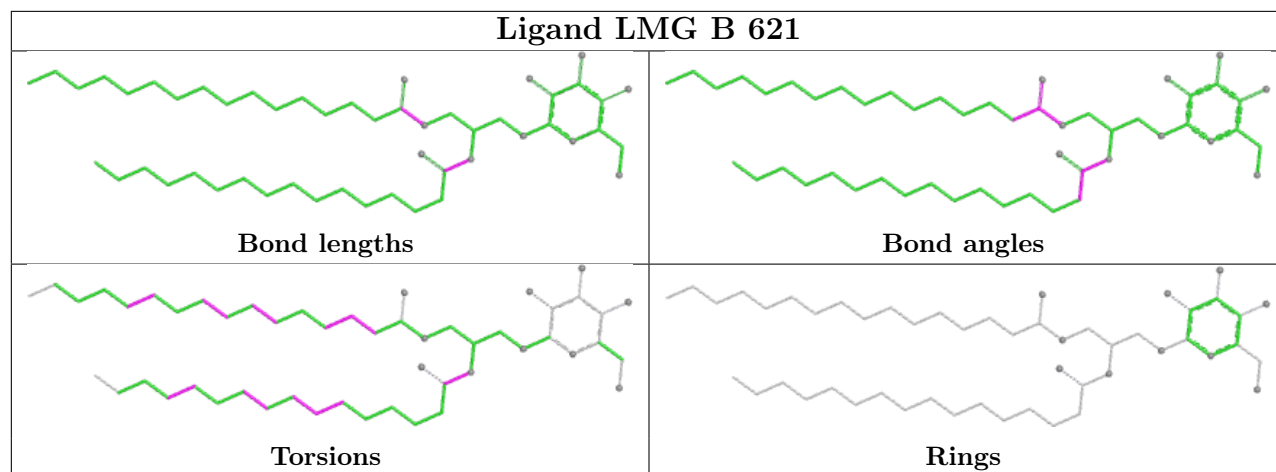




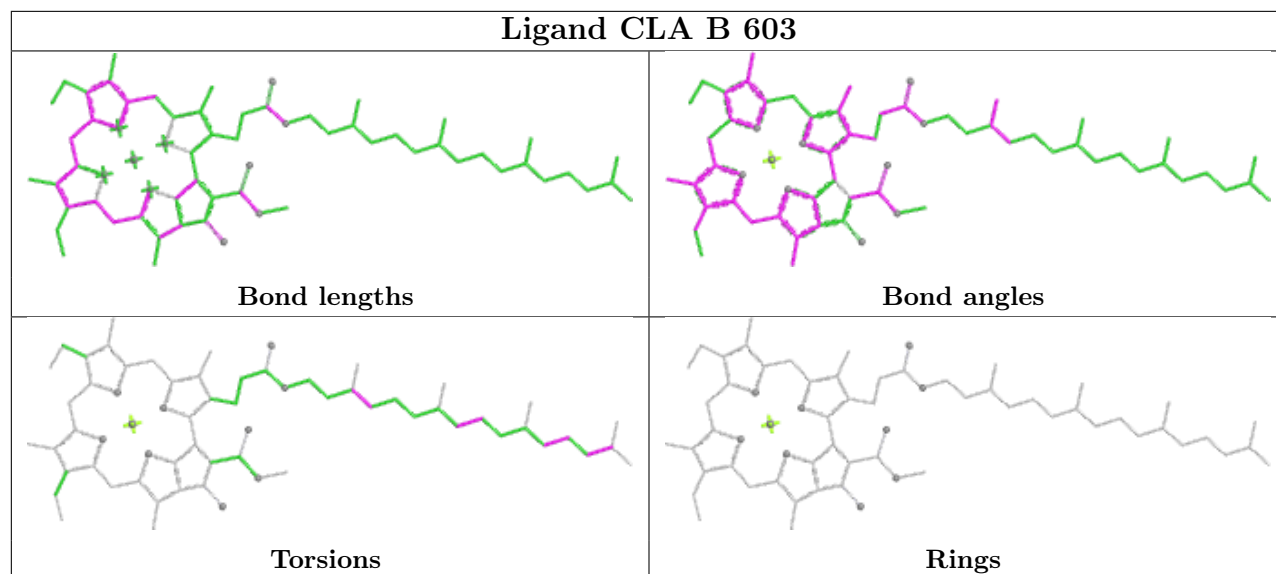




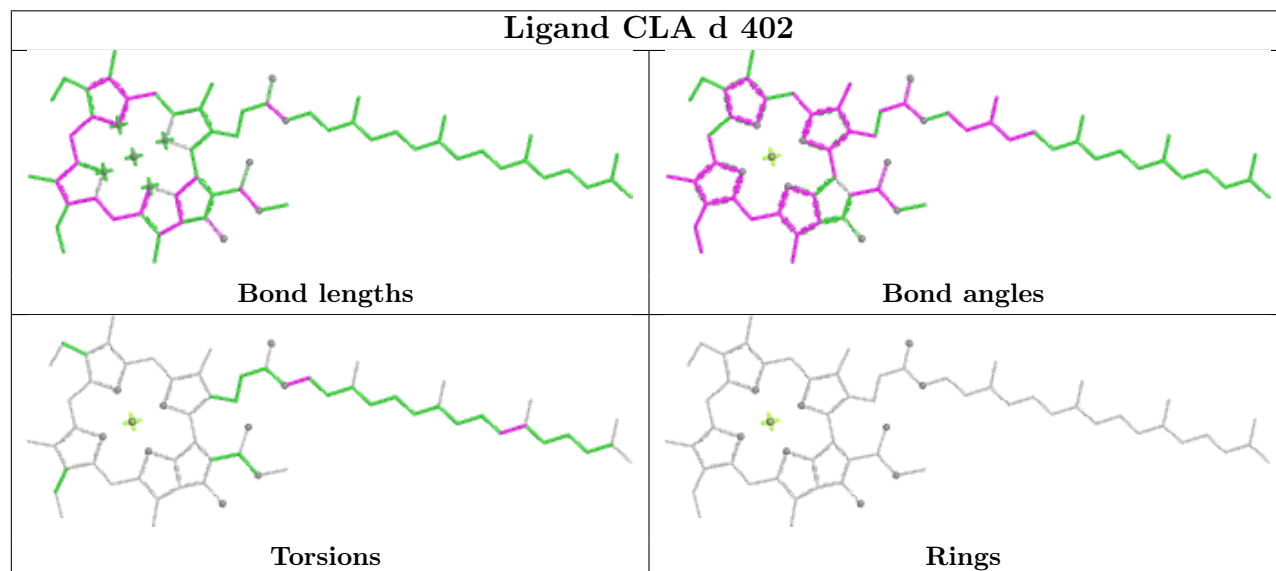




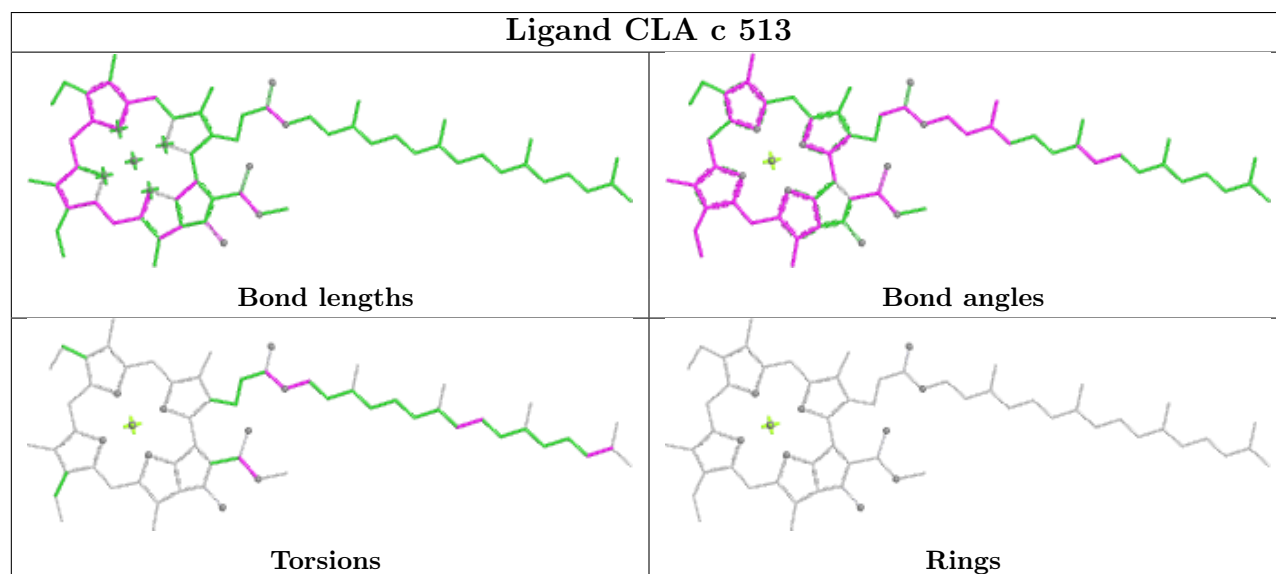
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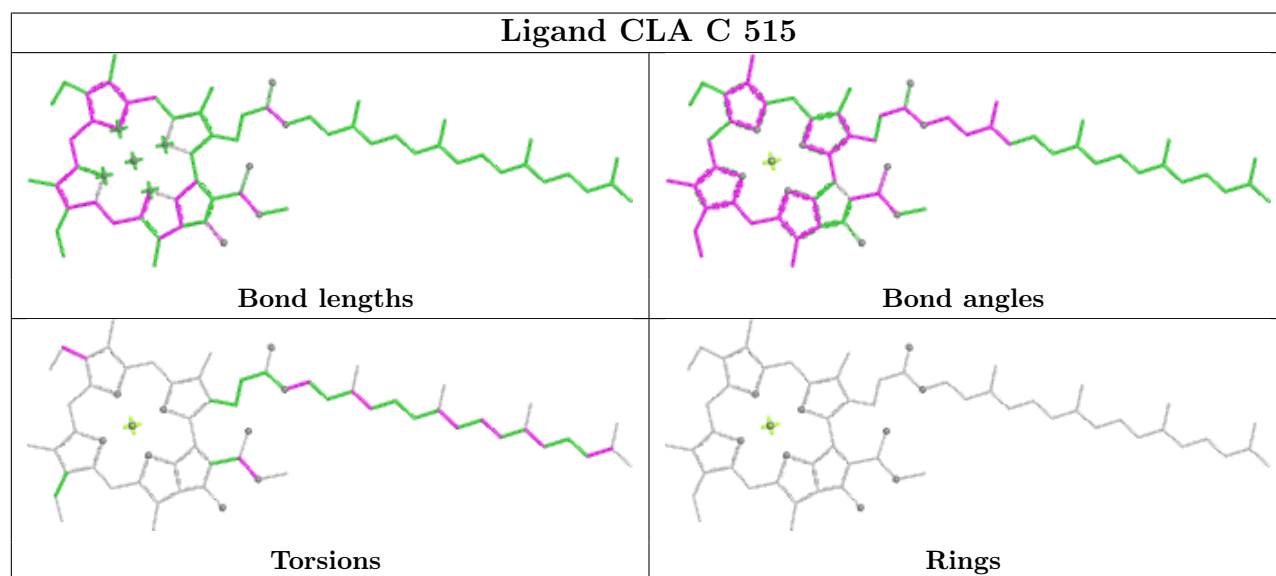
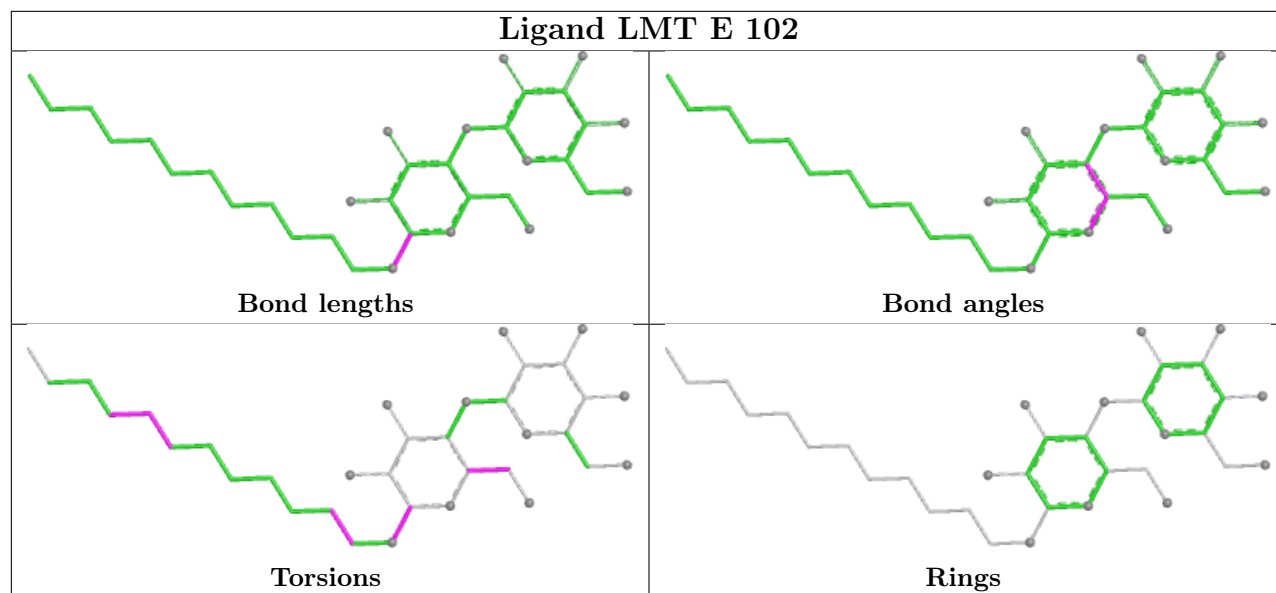


Ligand CLA d 402

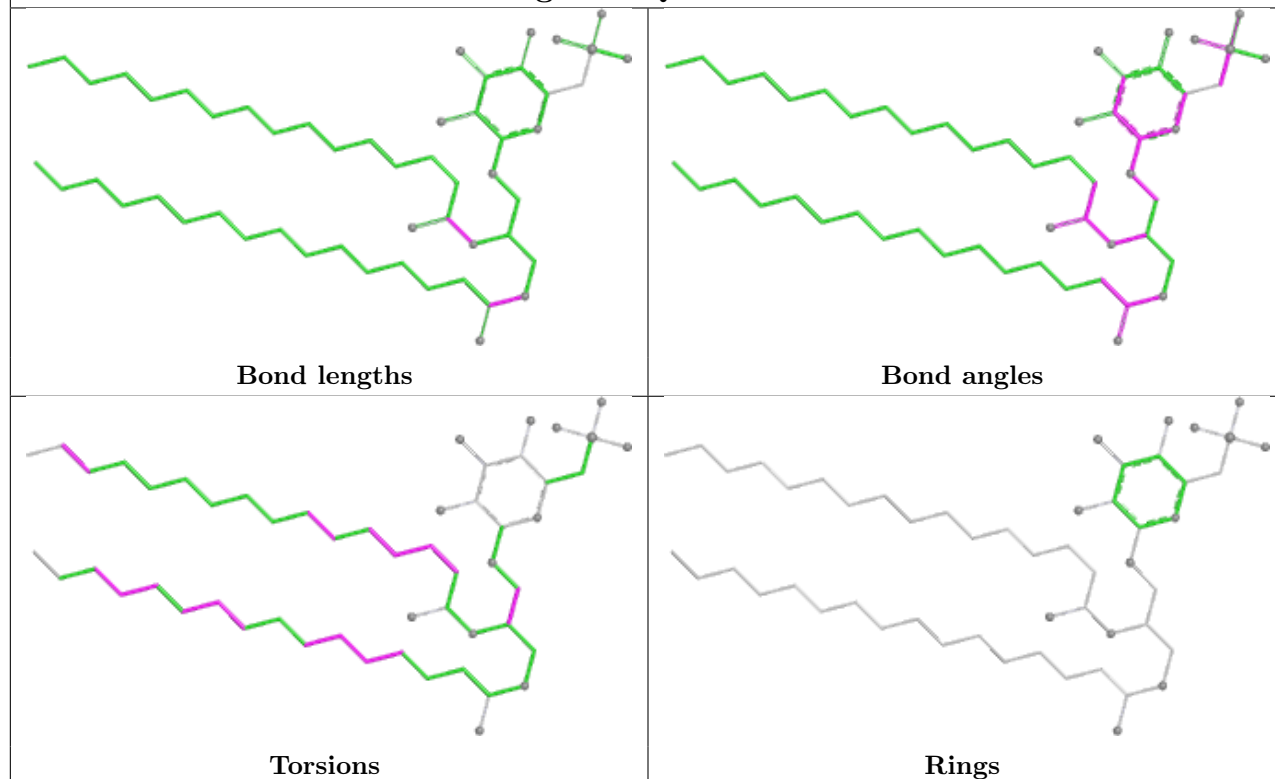


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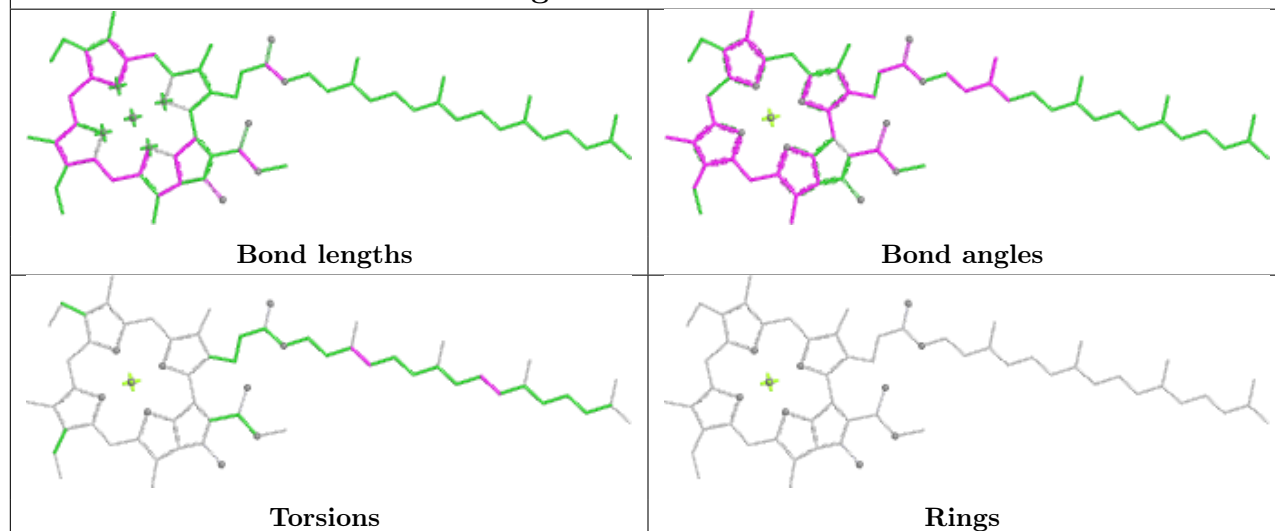




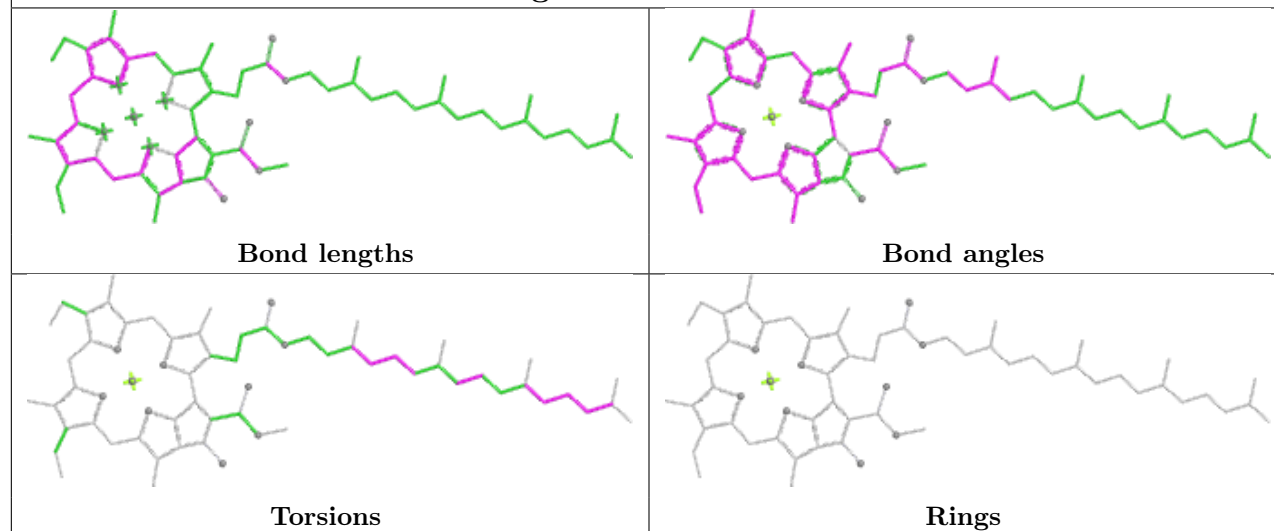
Ligand SQD a 410



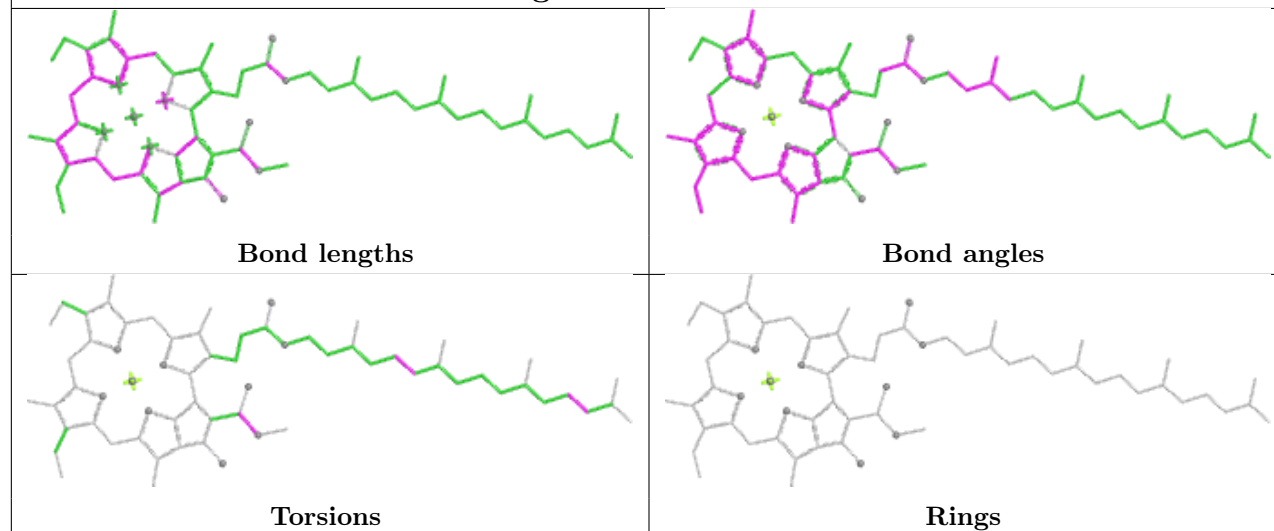
Ligand CLA B 605



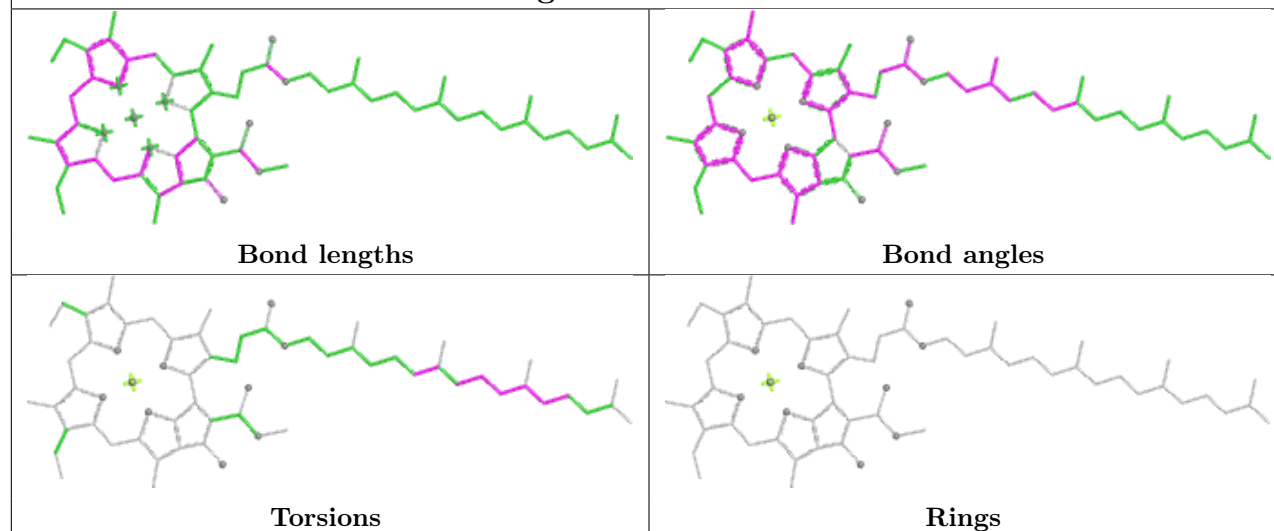
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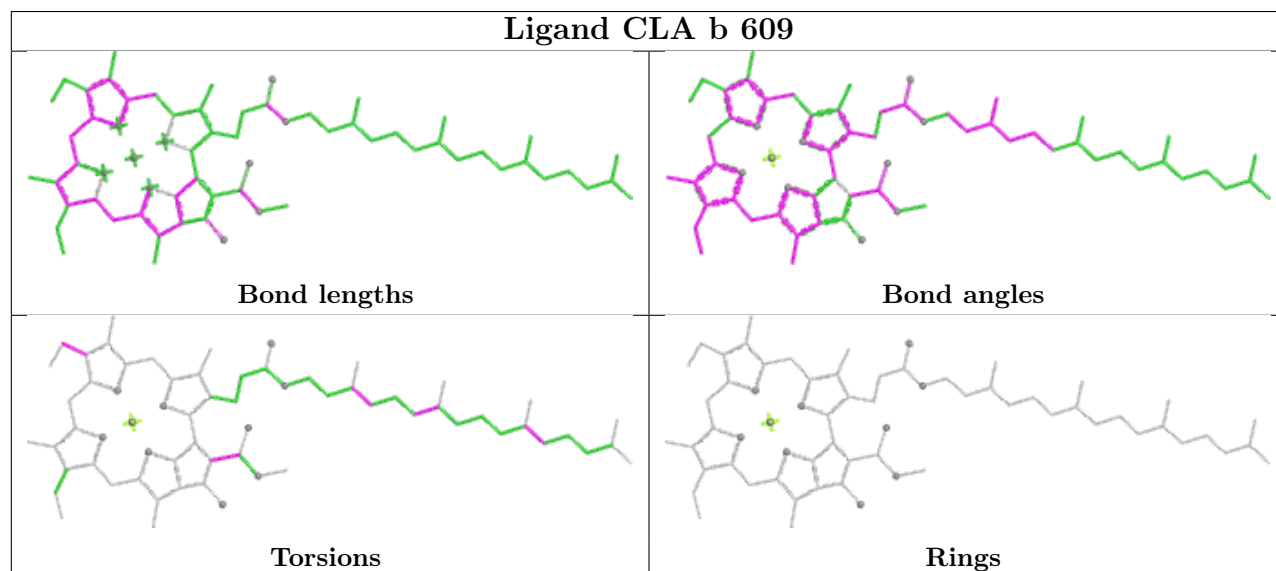
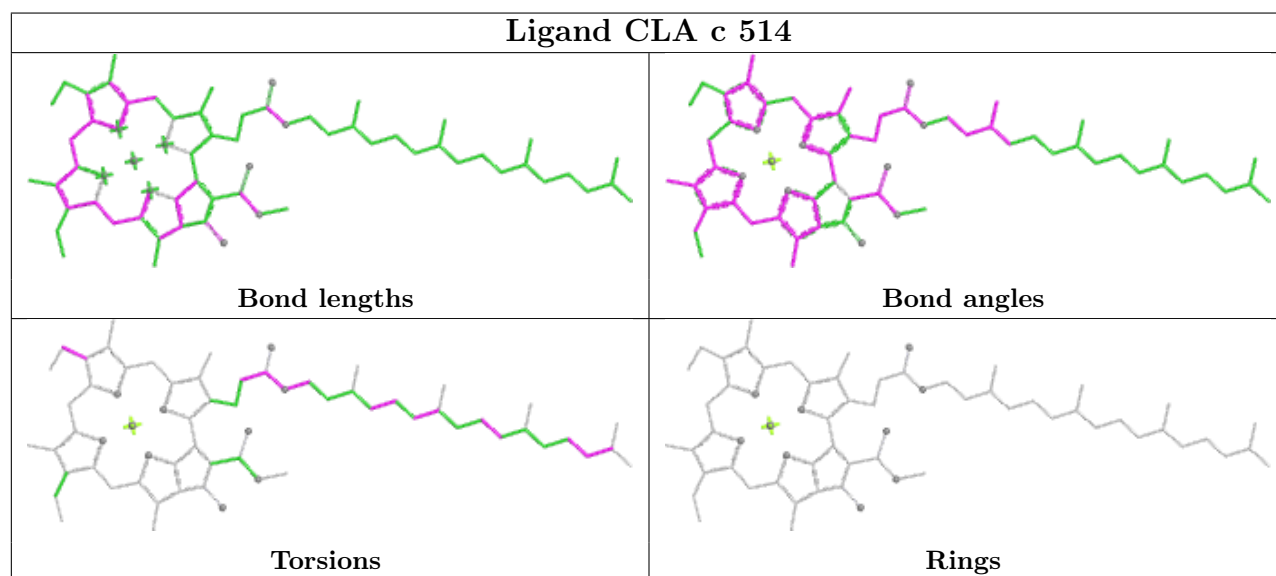
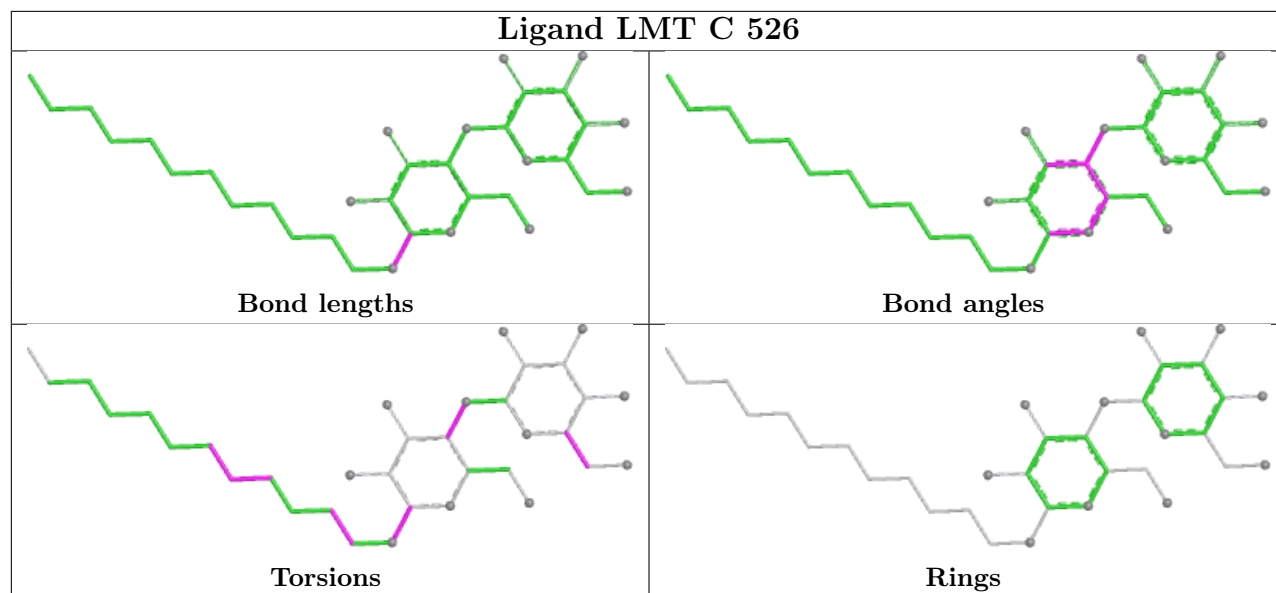


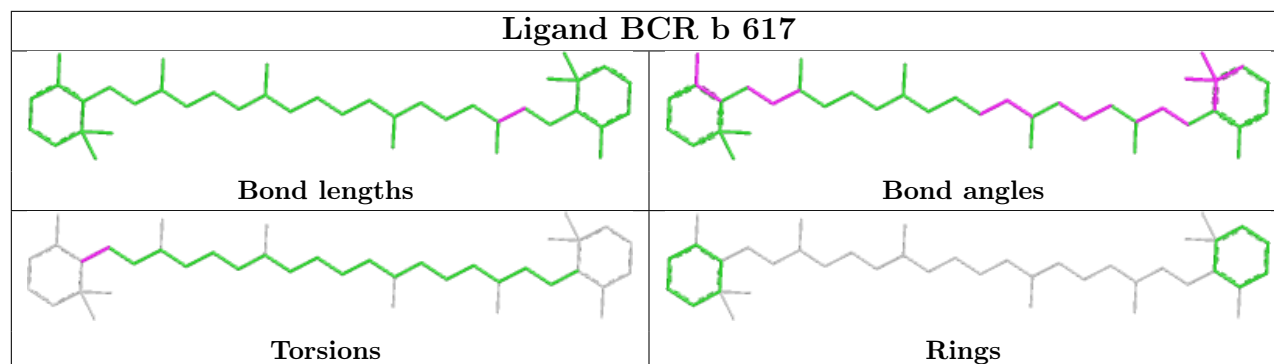
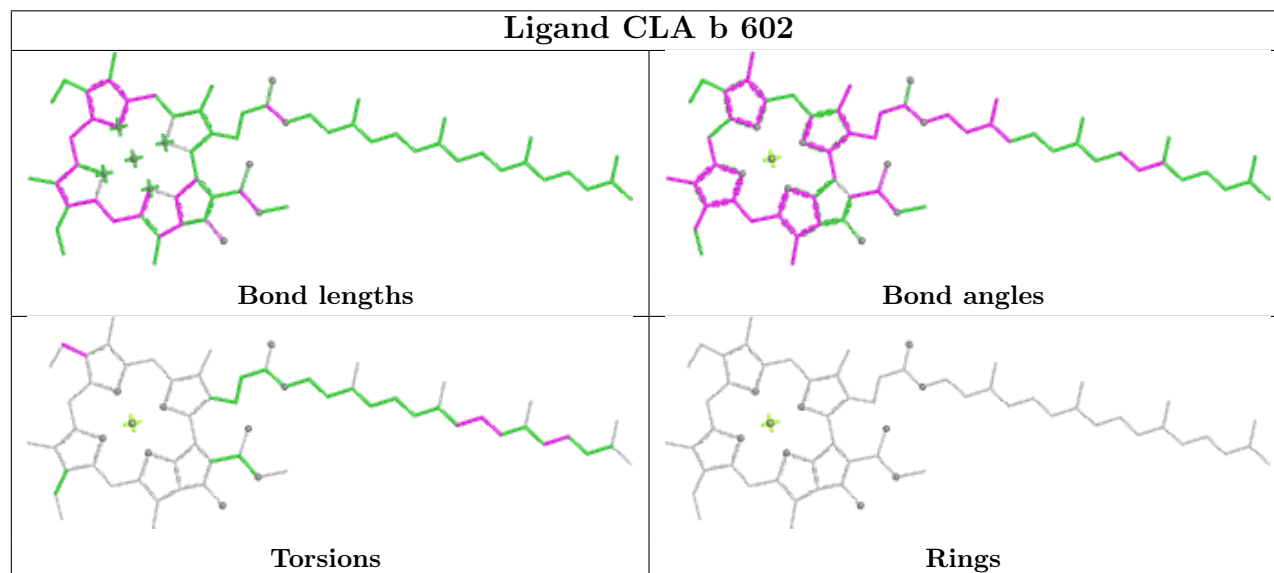
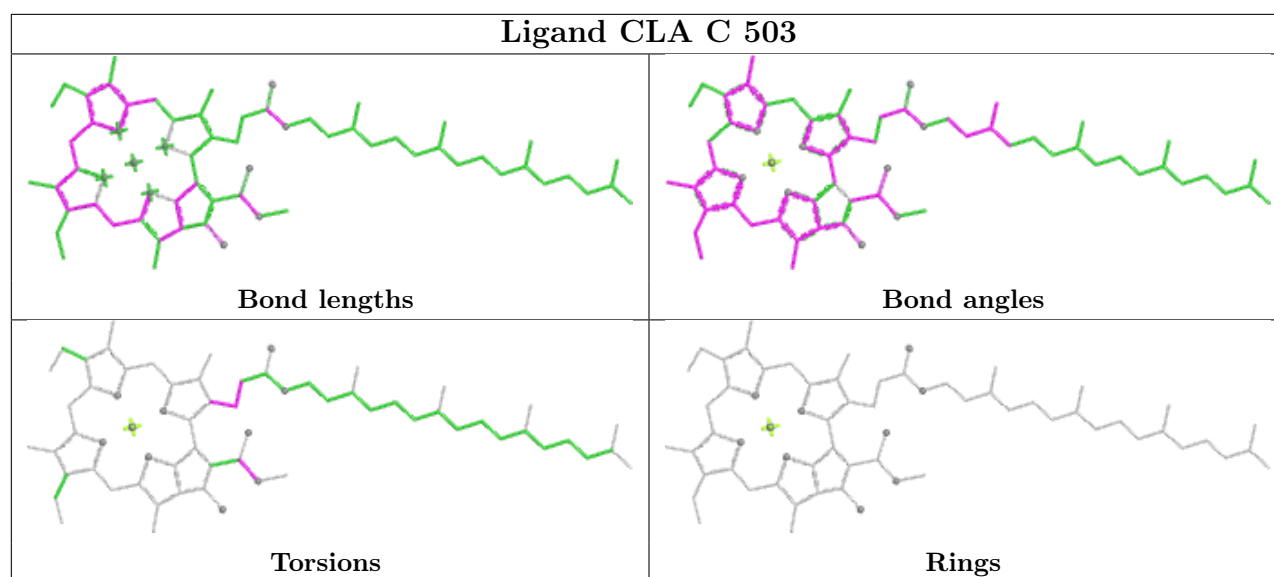
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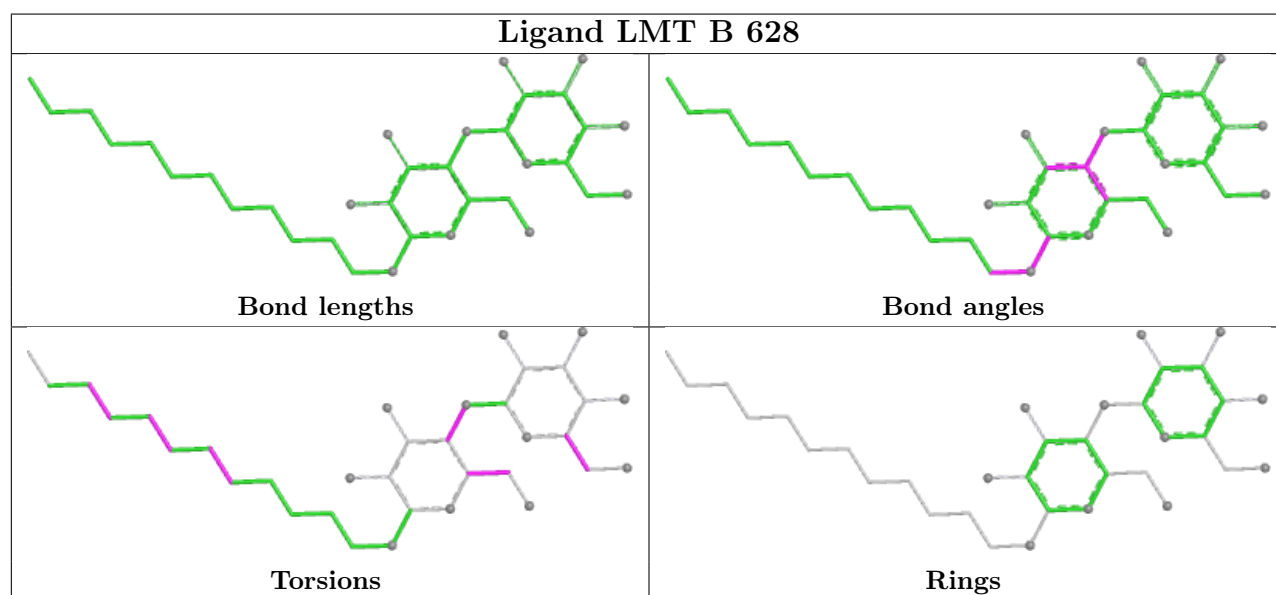
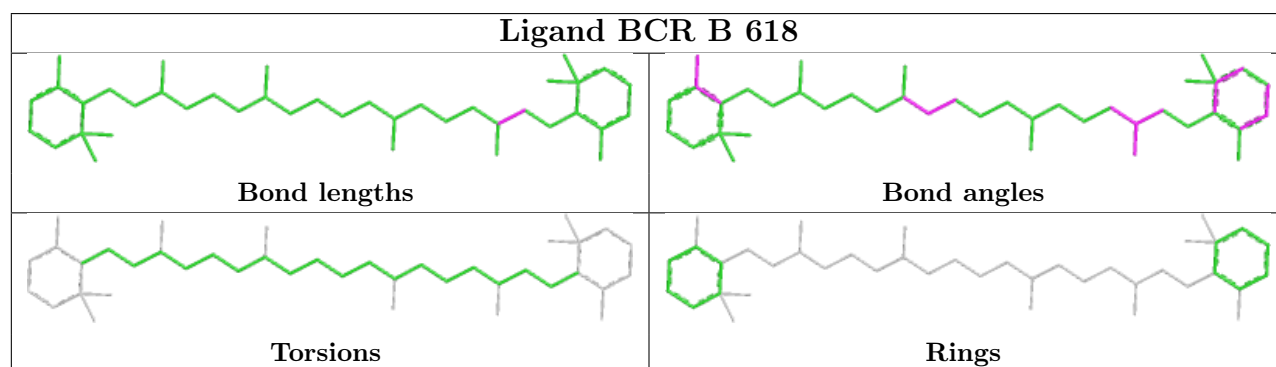
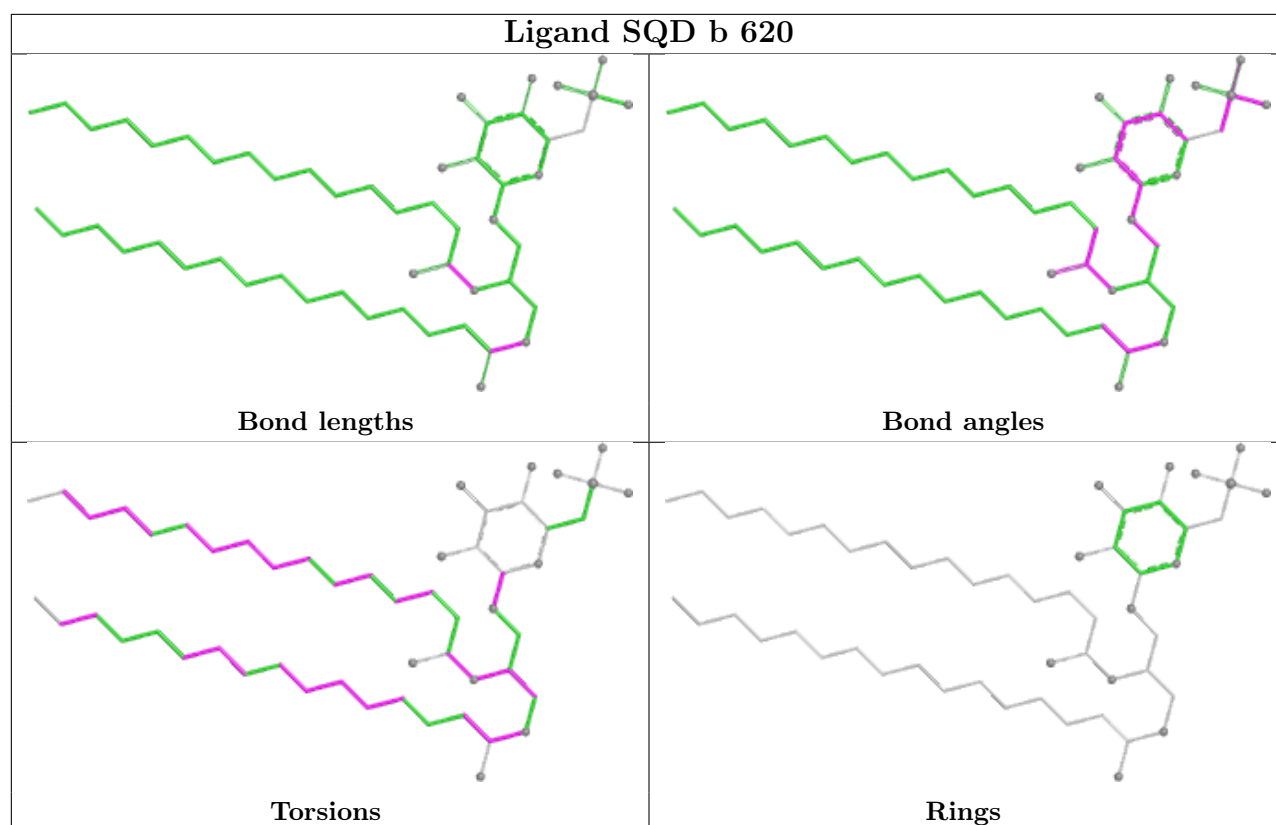


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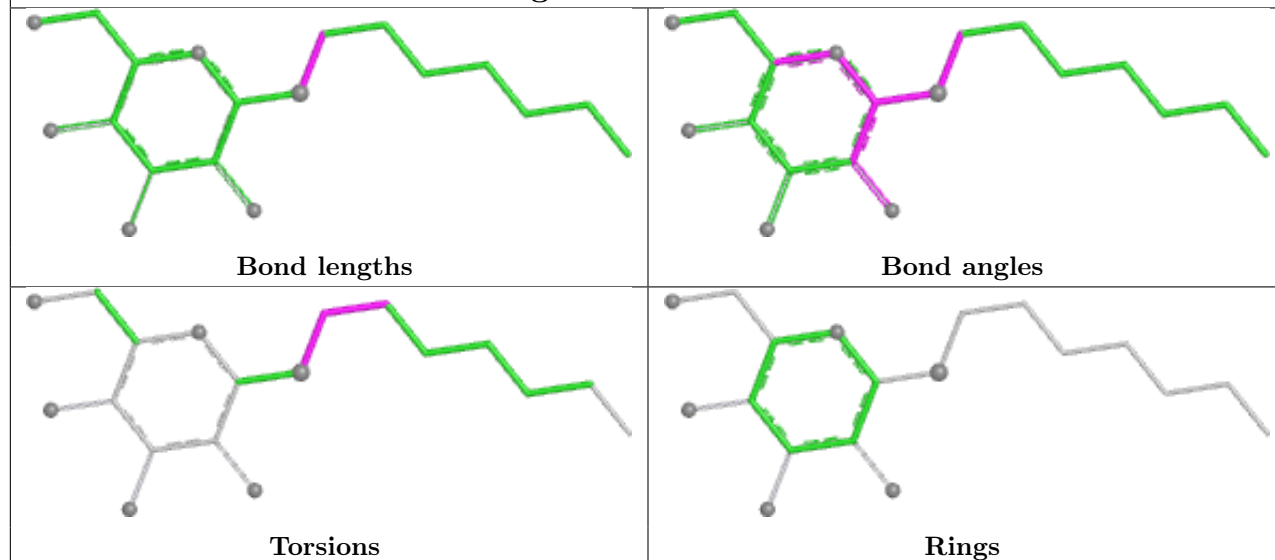




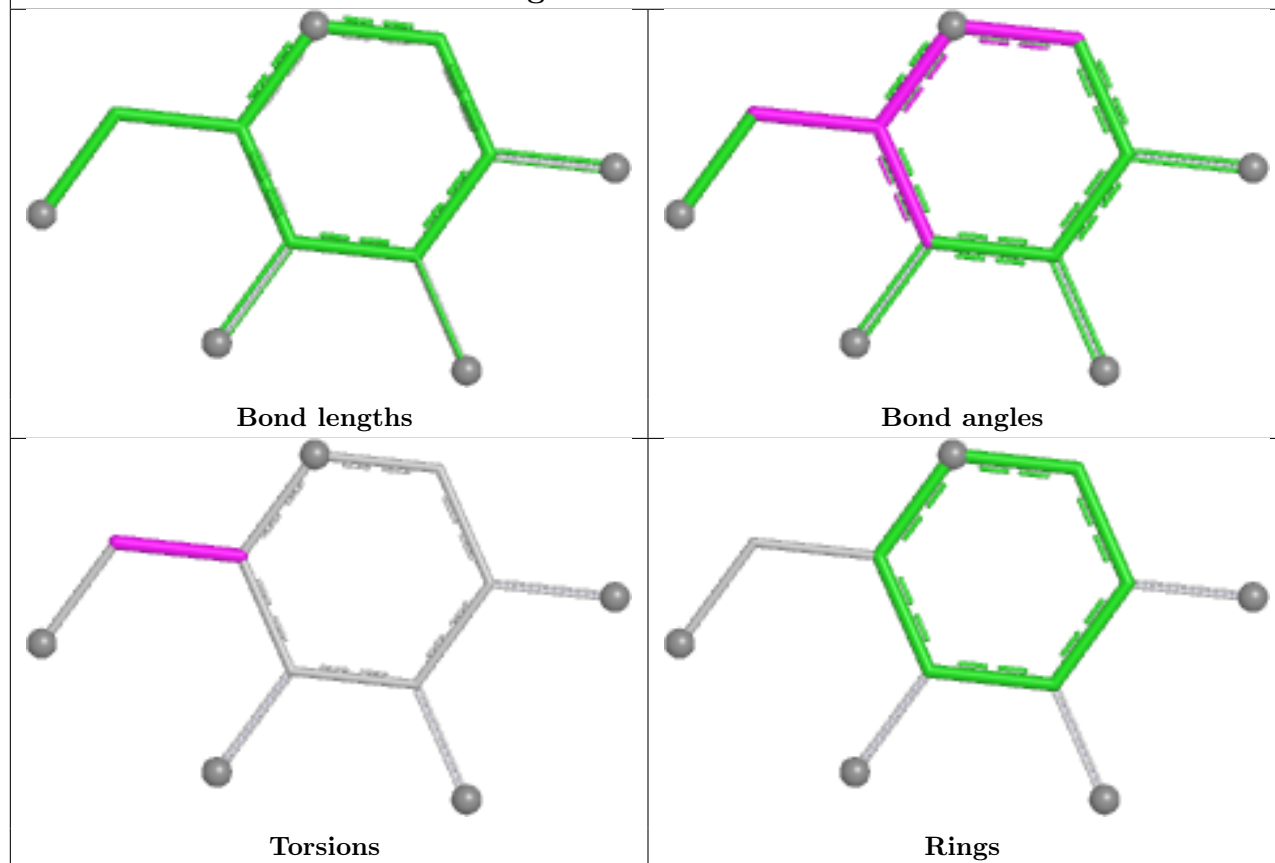


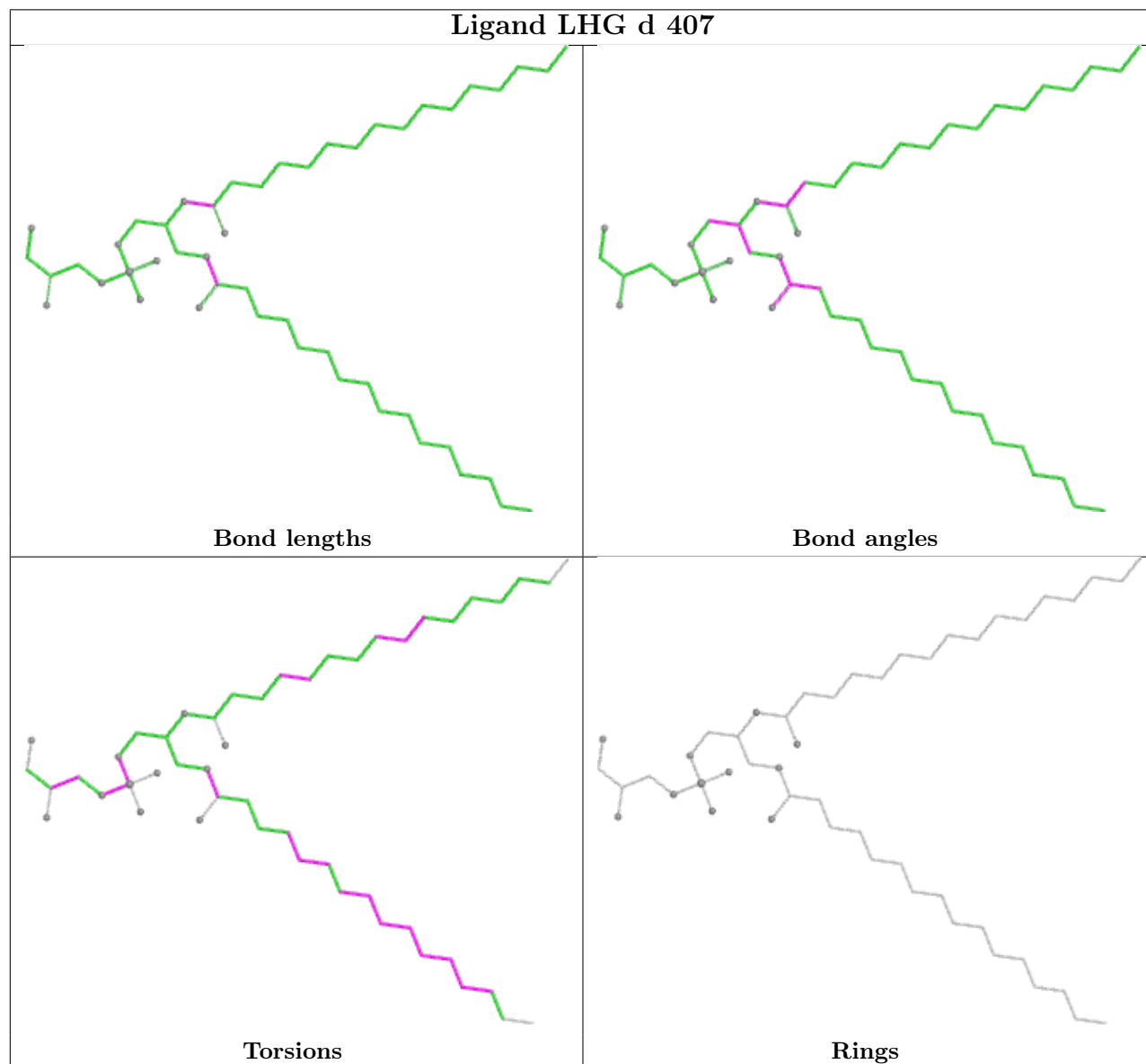
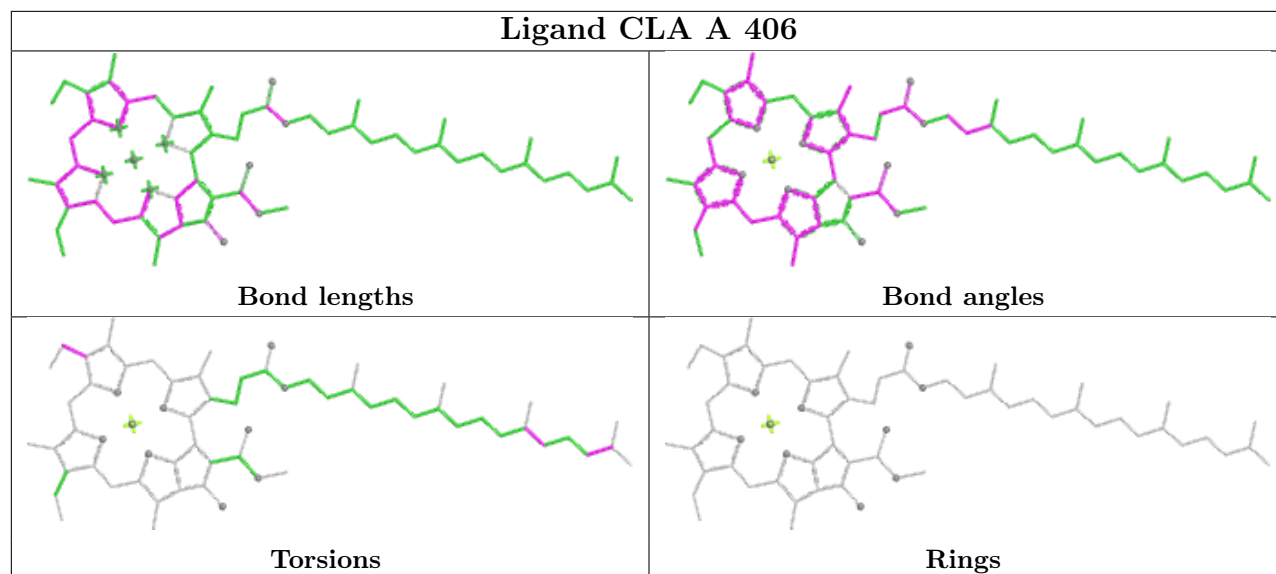


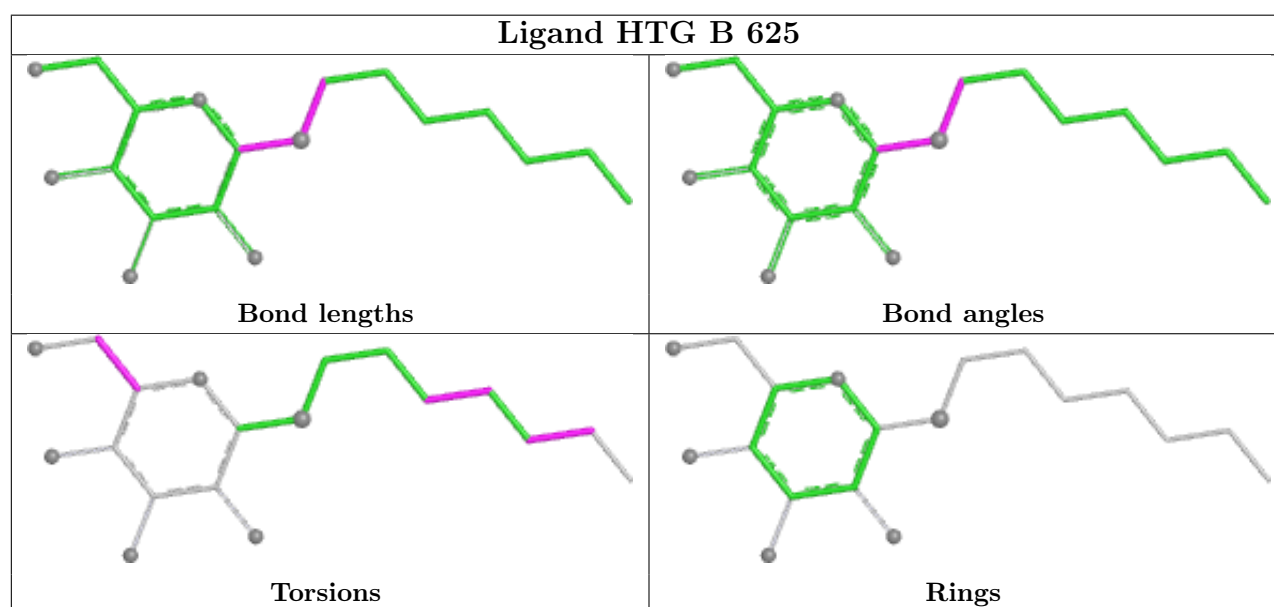
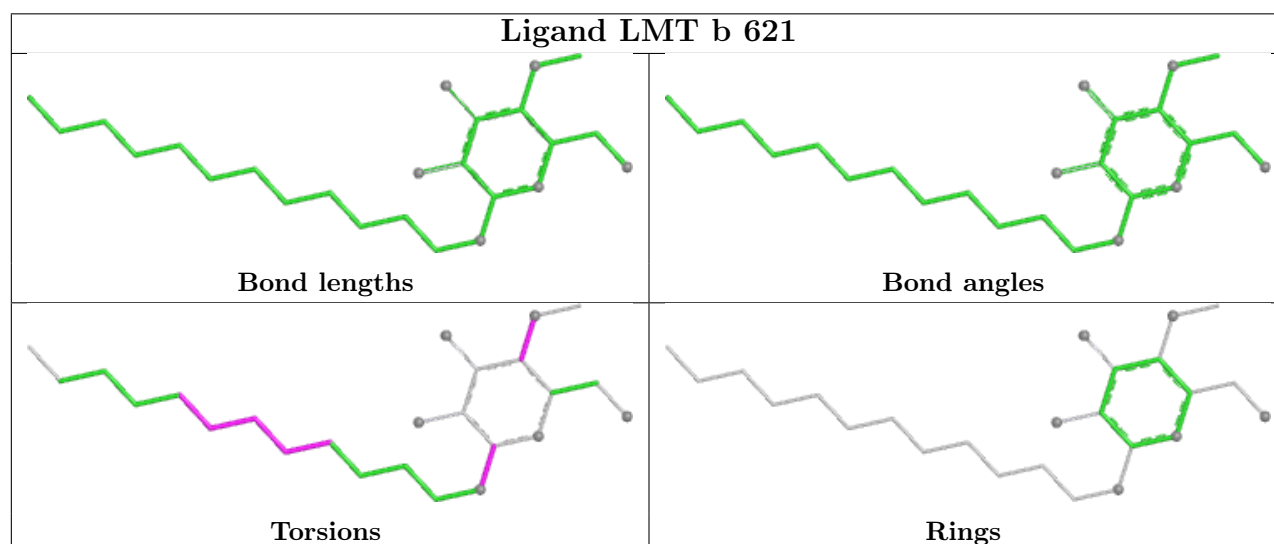
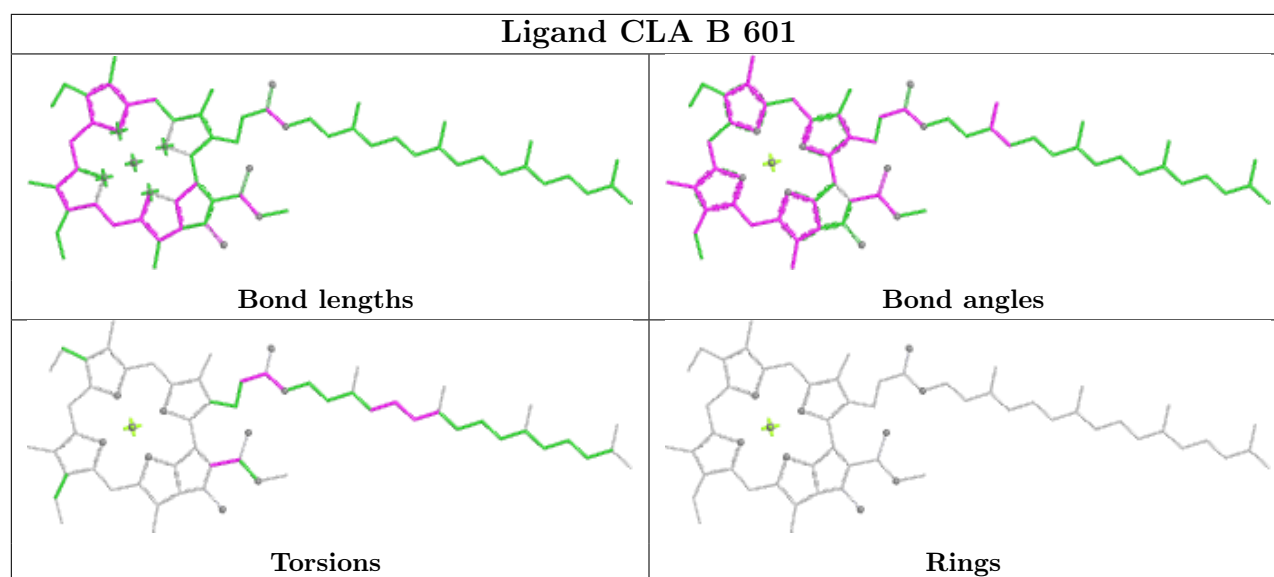
Ligand HTG b 622

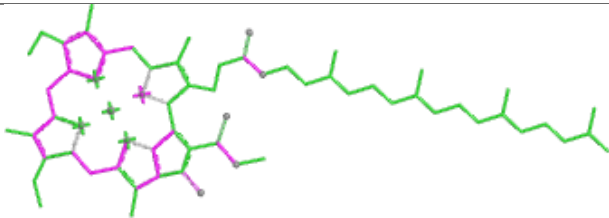
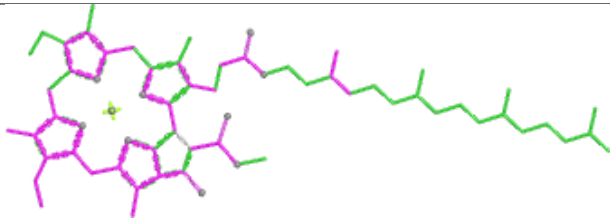
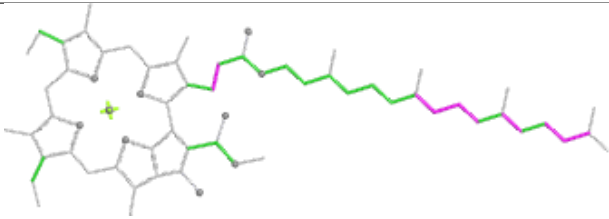
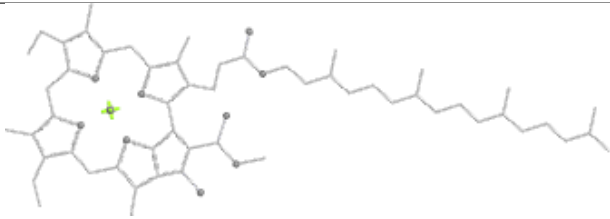


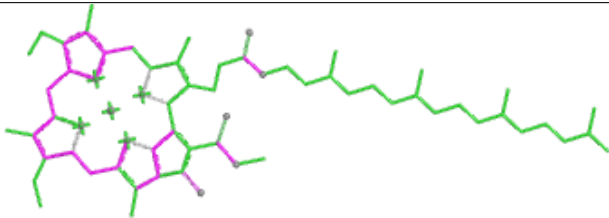
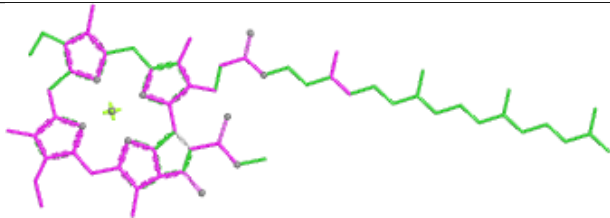
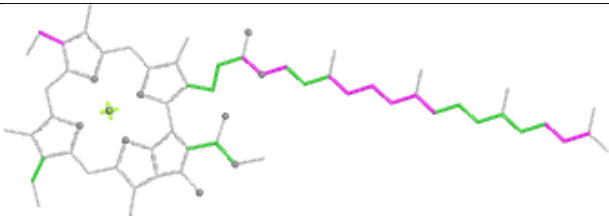
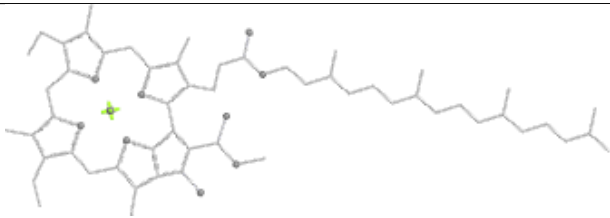
Ligand HTG V 202

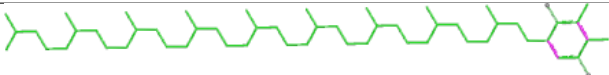
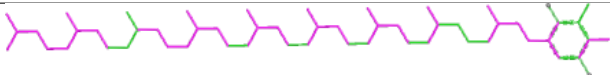
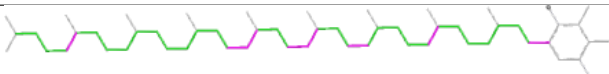


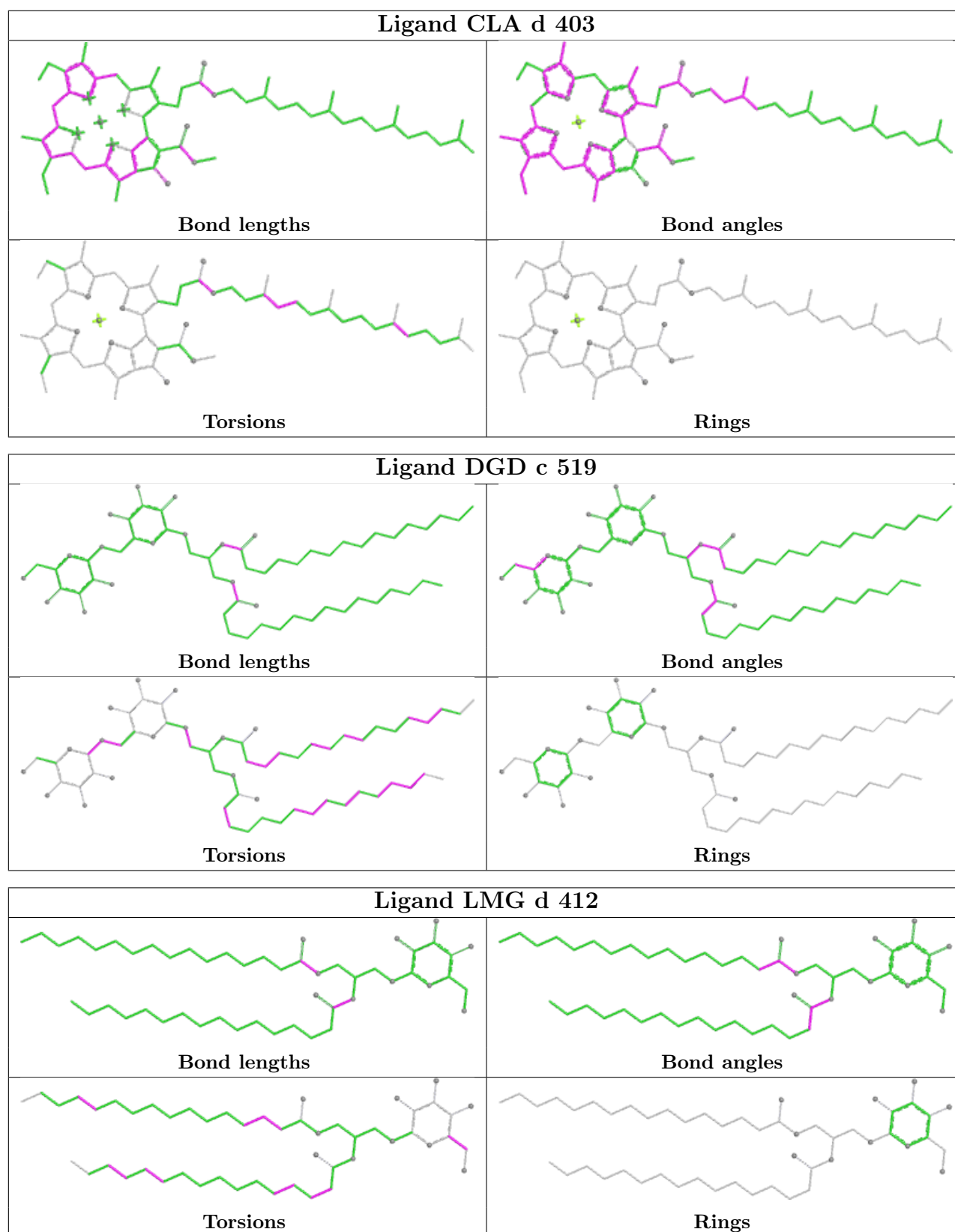




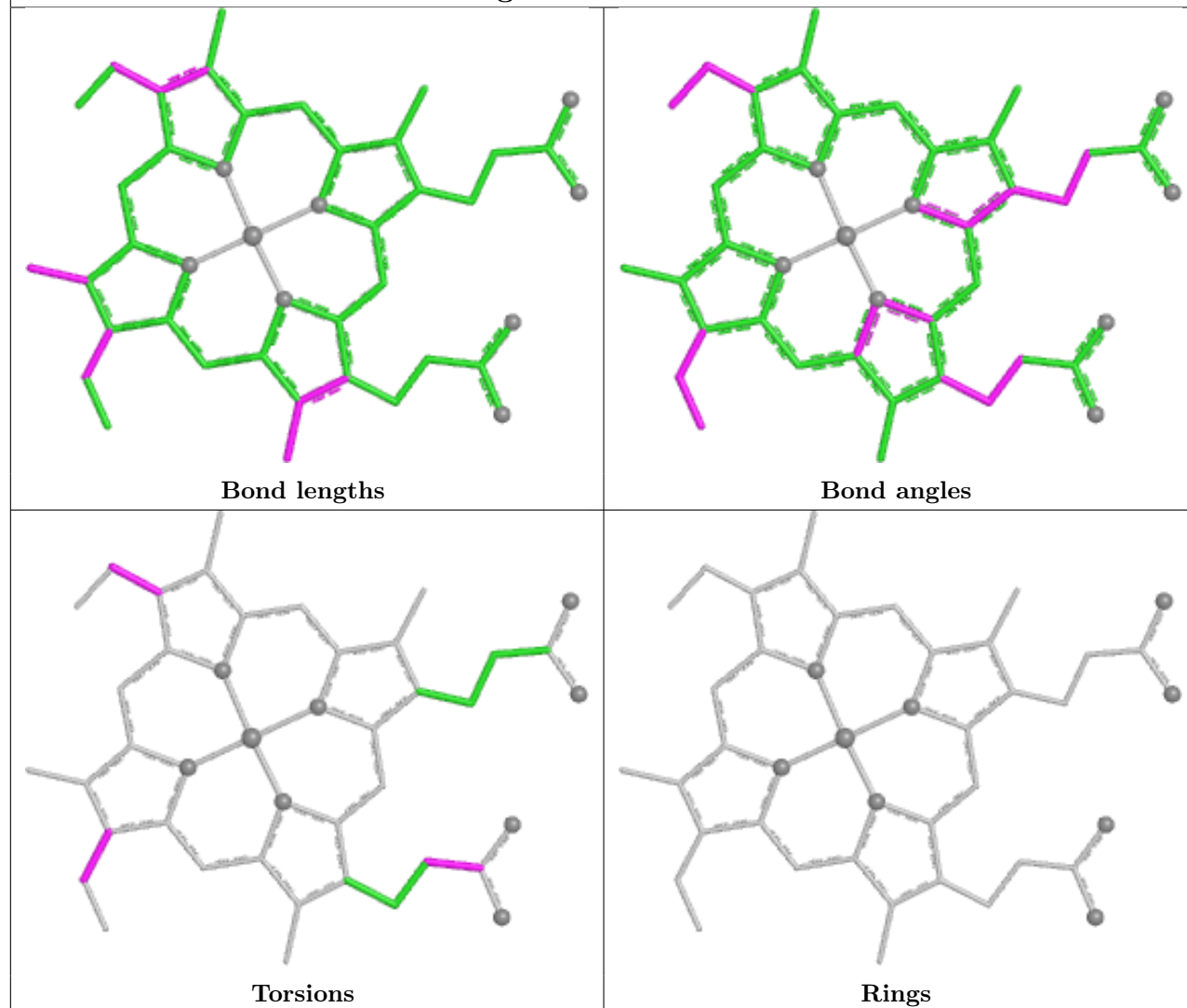
Ligand CLA B 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

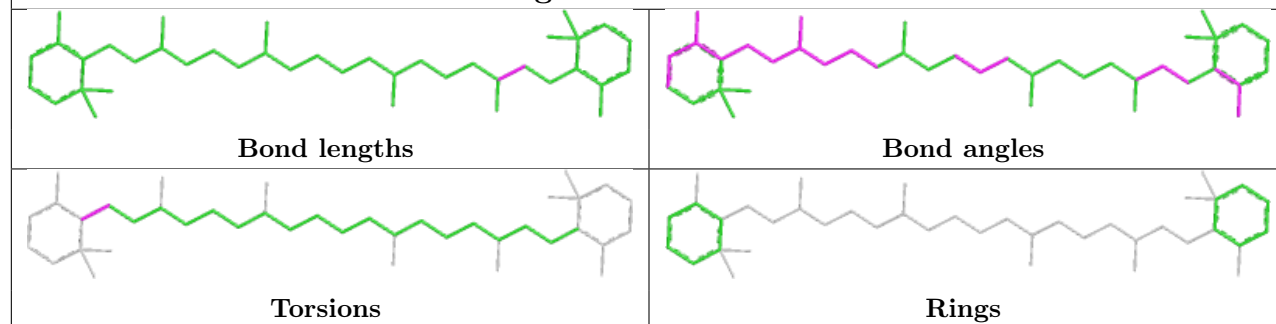
Ligand PL9 a 415	
	
Bond lengths	Bond angles
	
Torsions	Rings

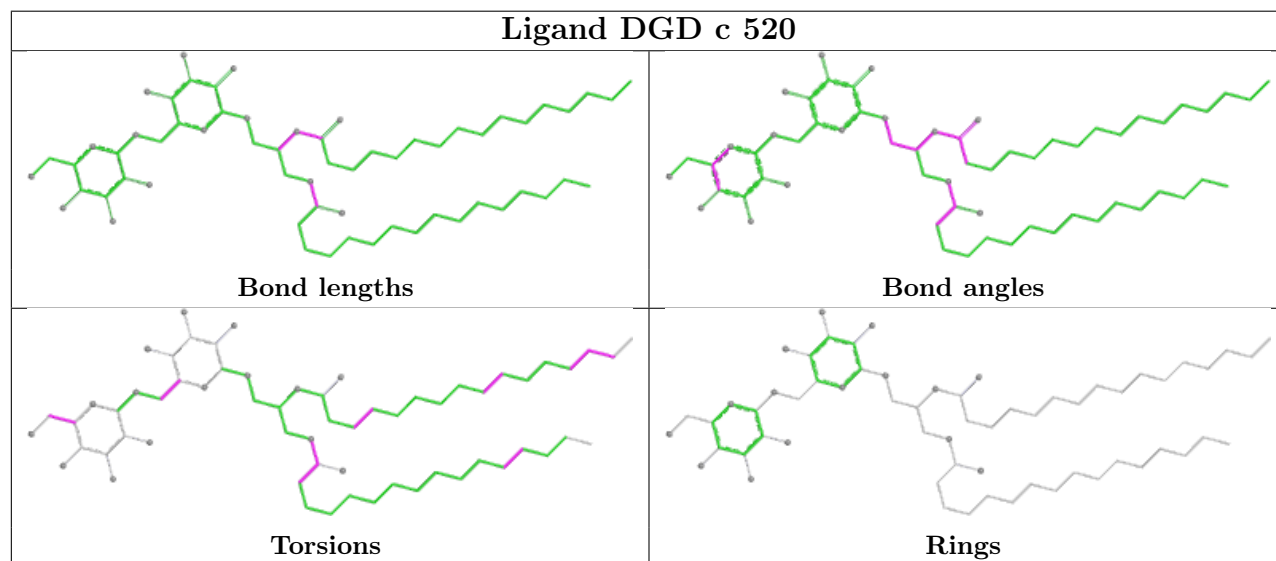
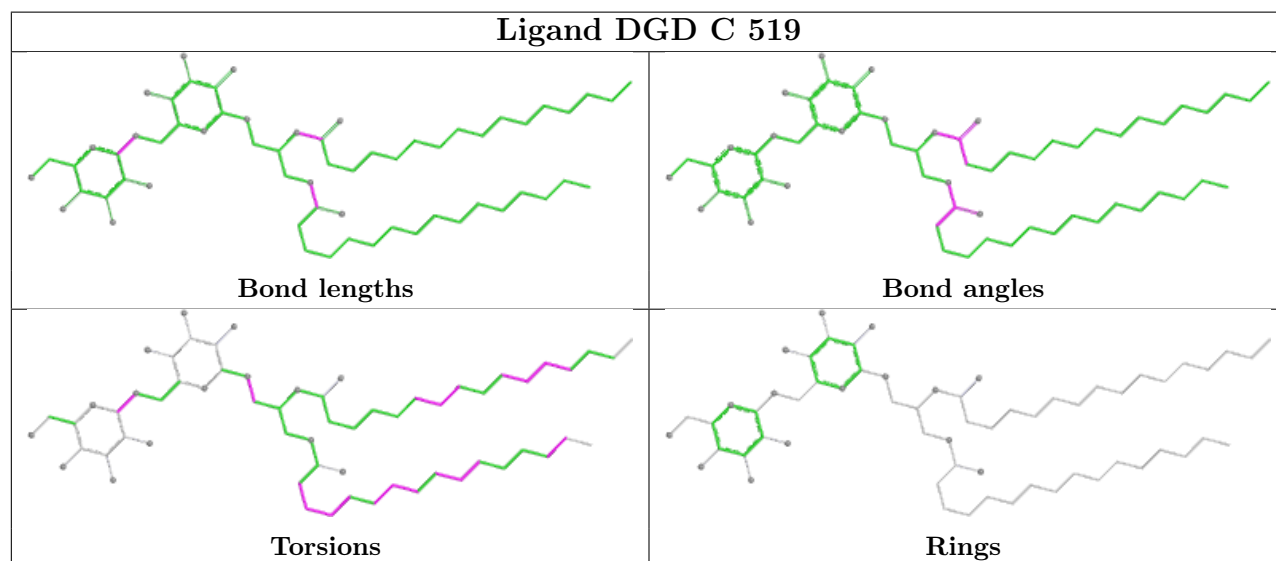
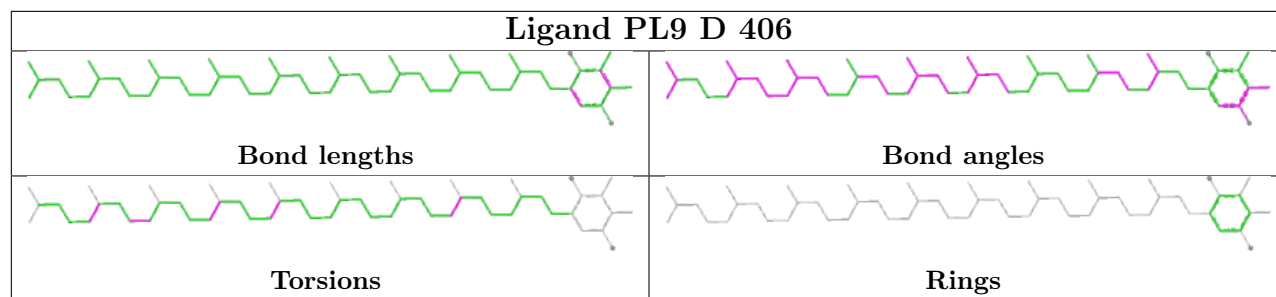


Ligand HEC v 202

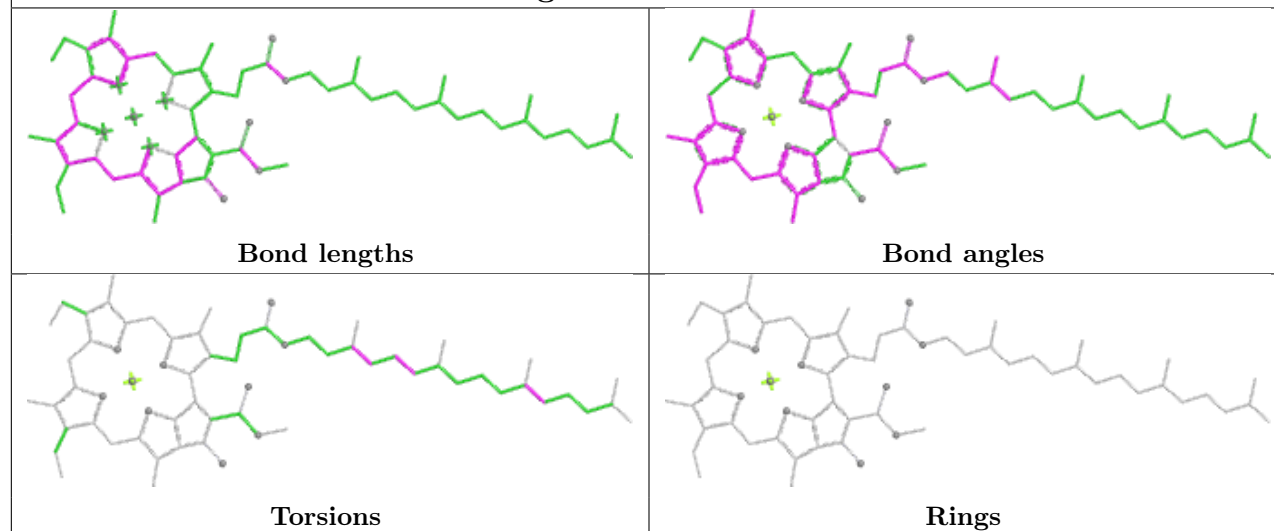


Ligand BCR a 409

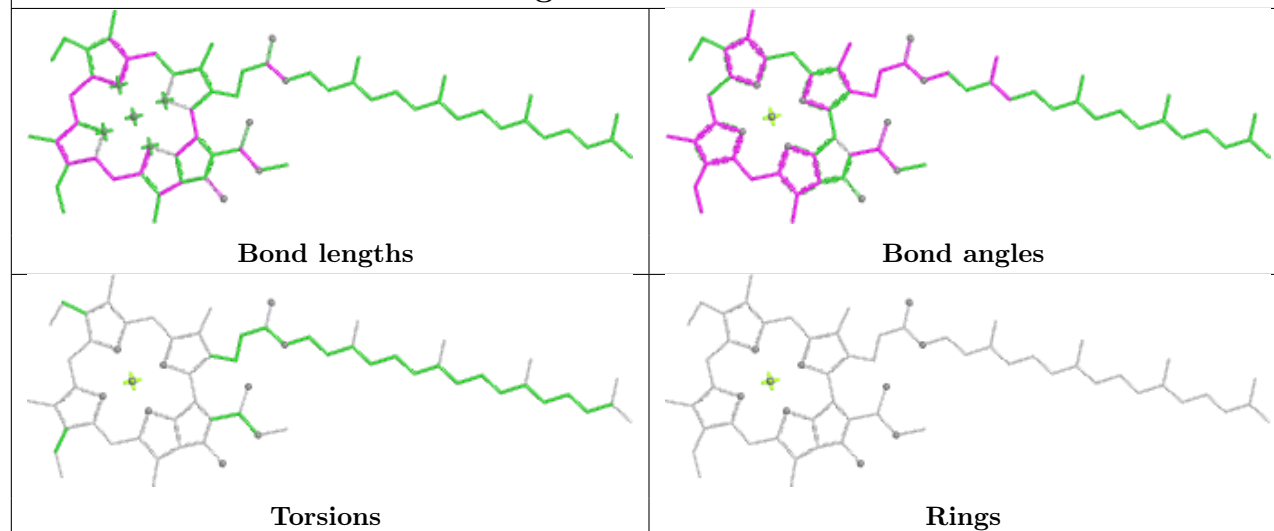




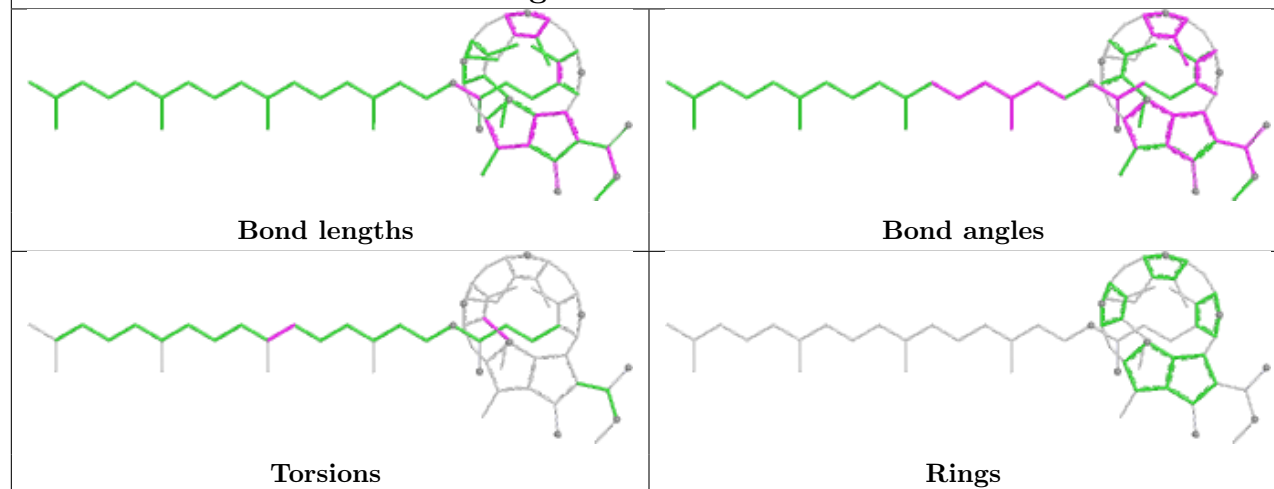
Ligand CLA c 506

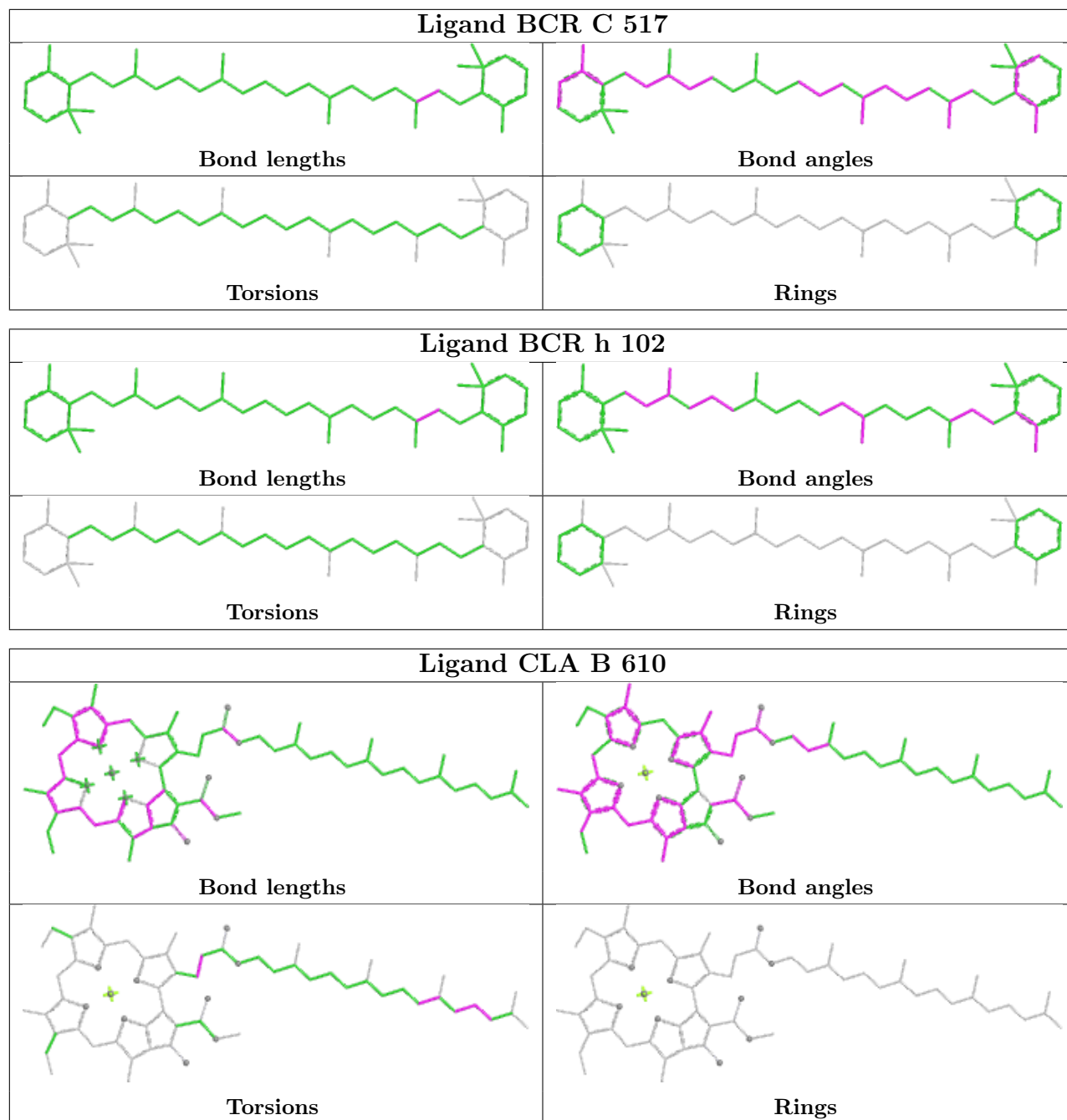


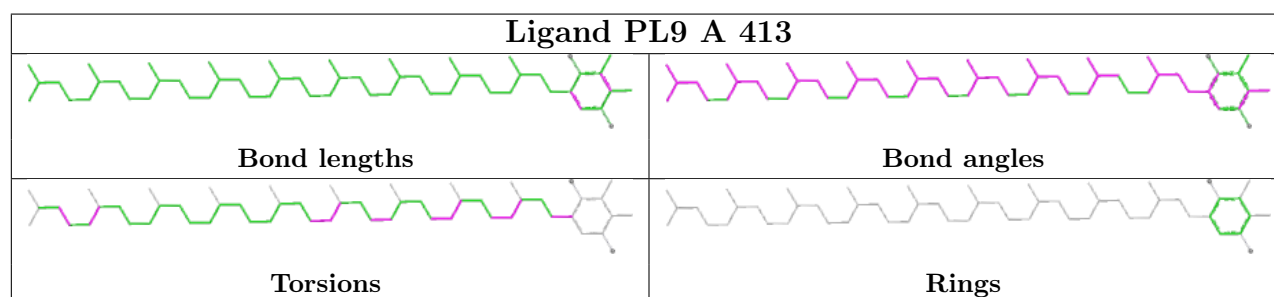
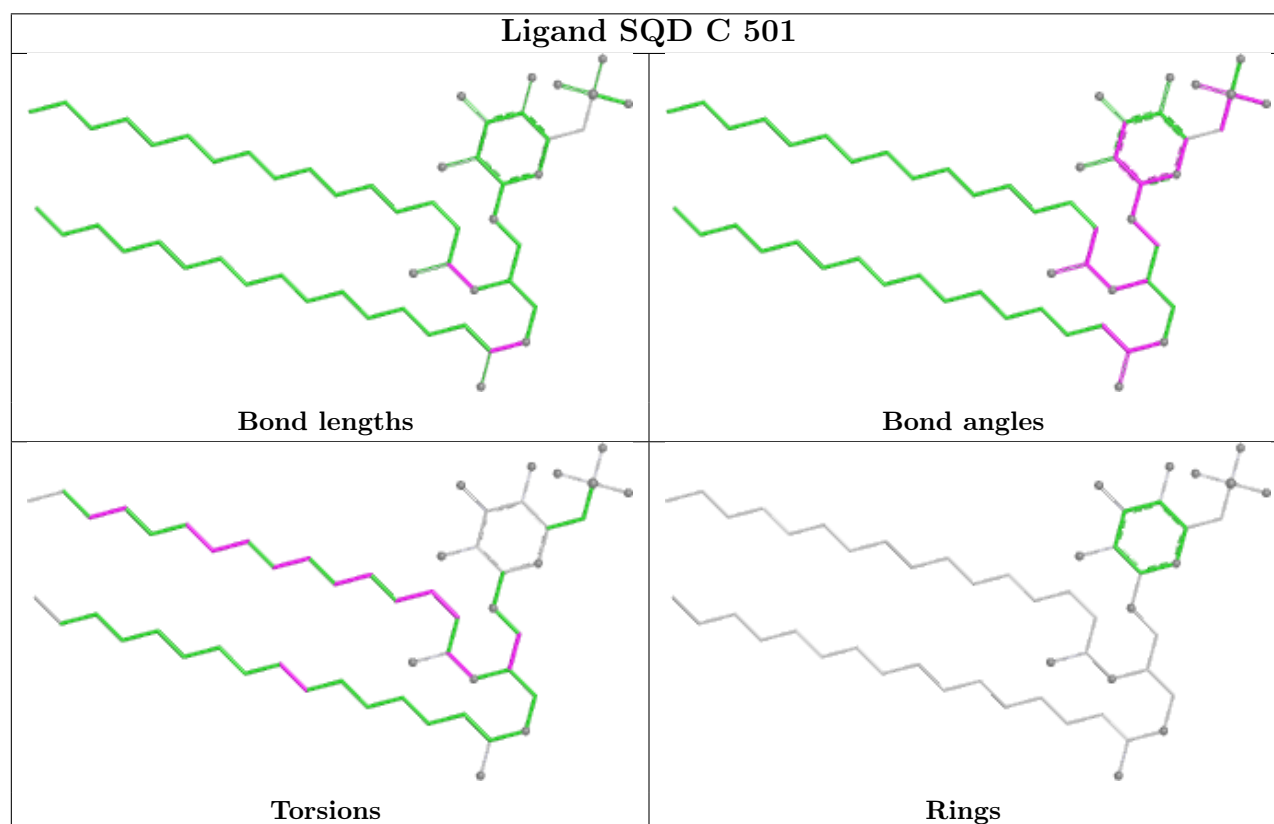
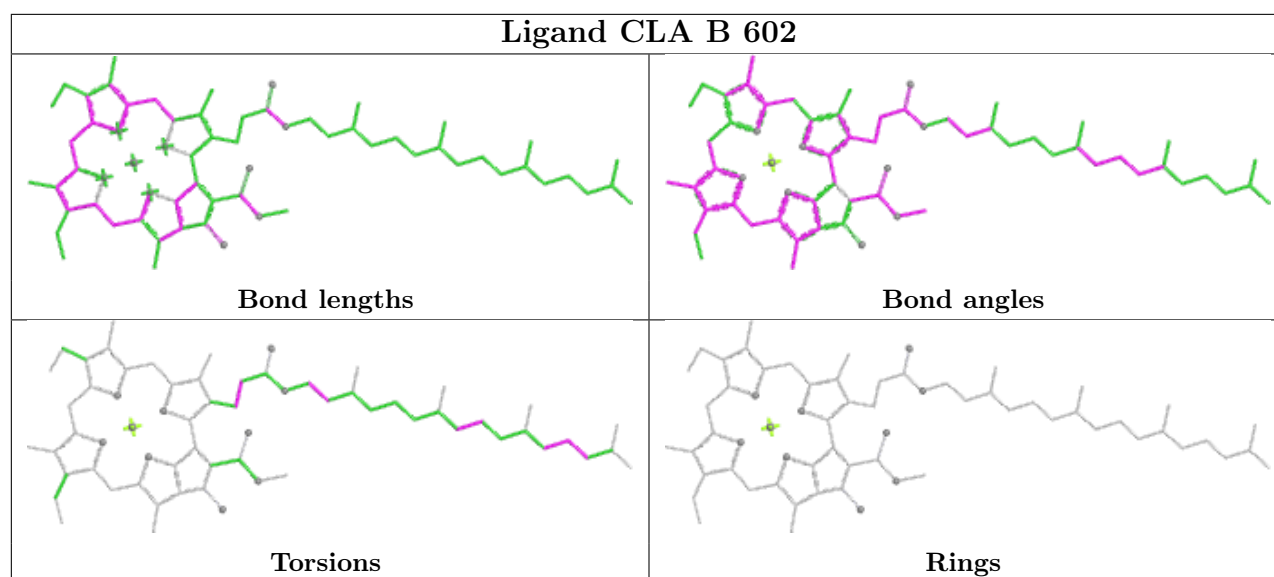
Ligand CLA b 607



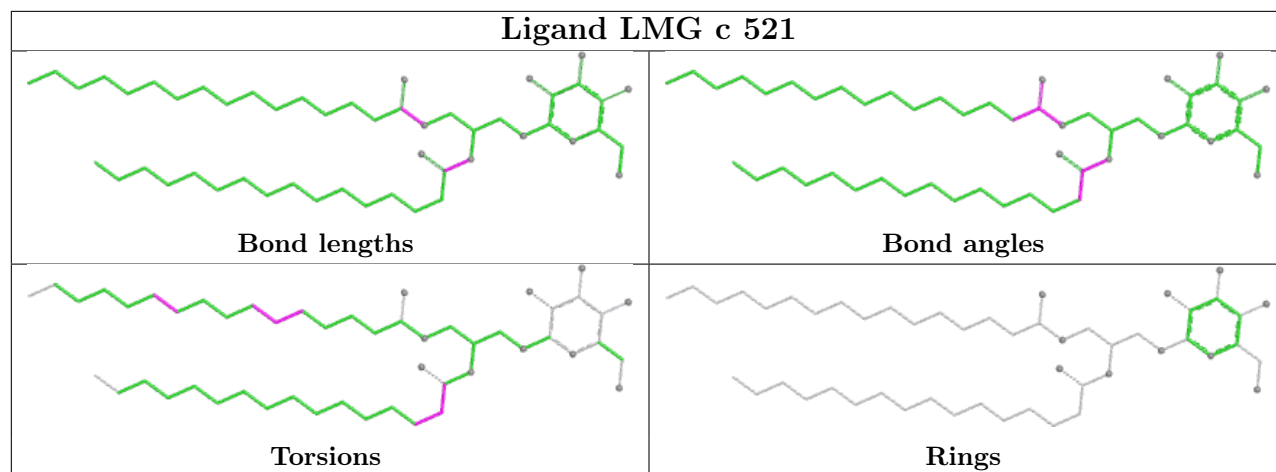
Ligand PHO A 415



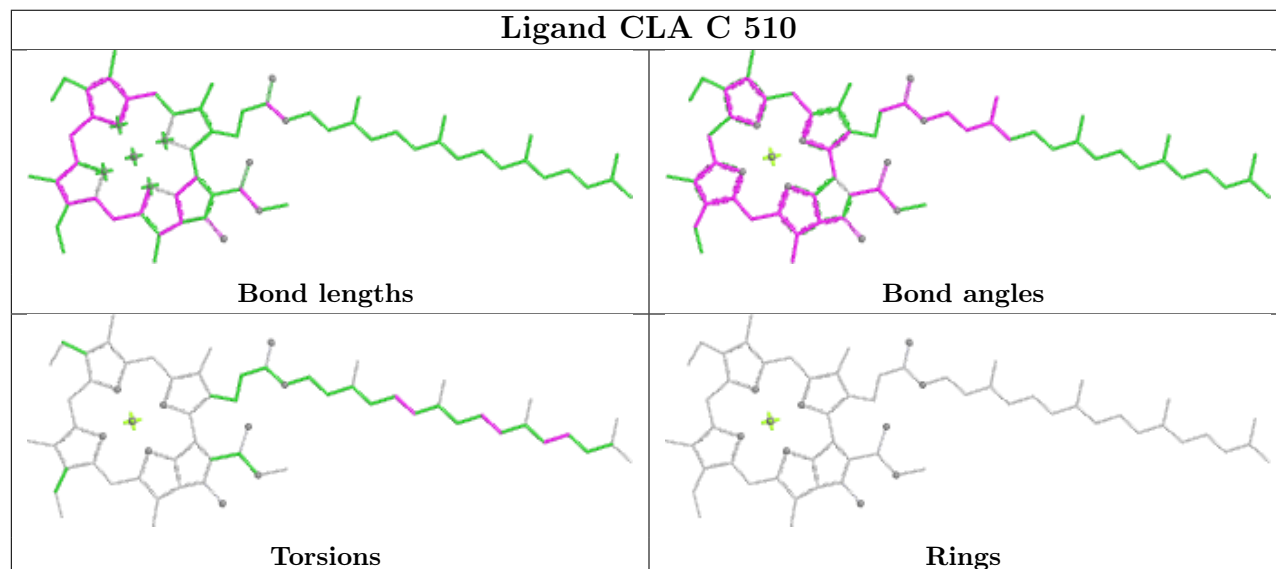




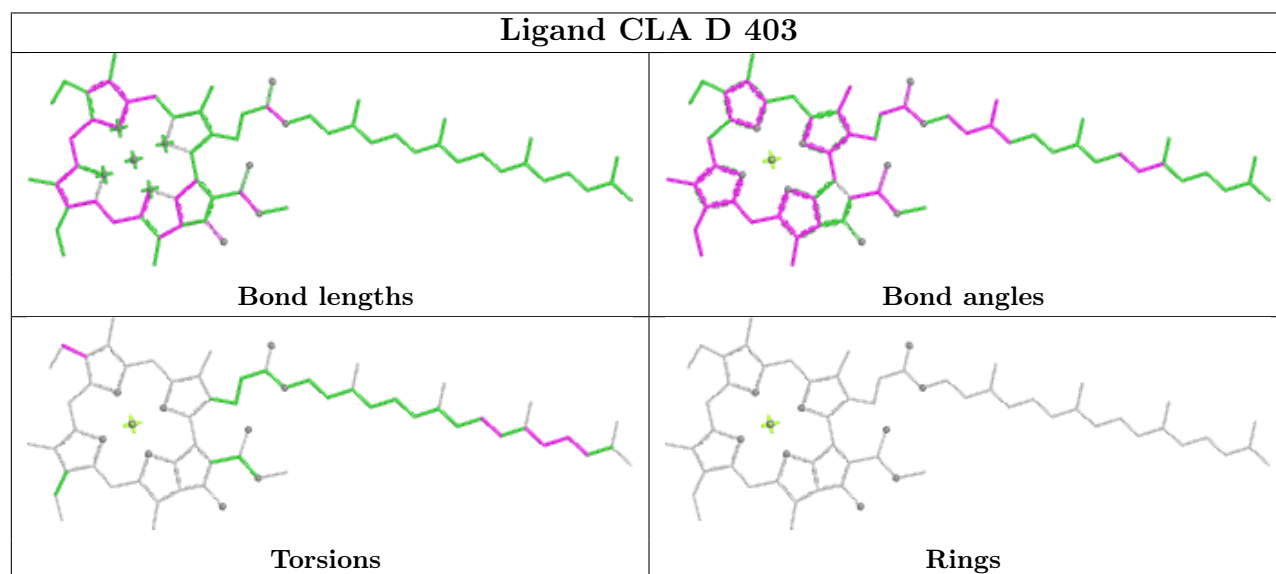
Ligand LMG c 521

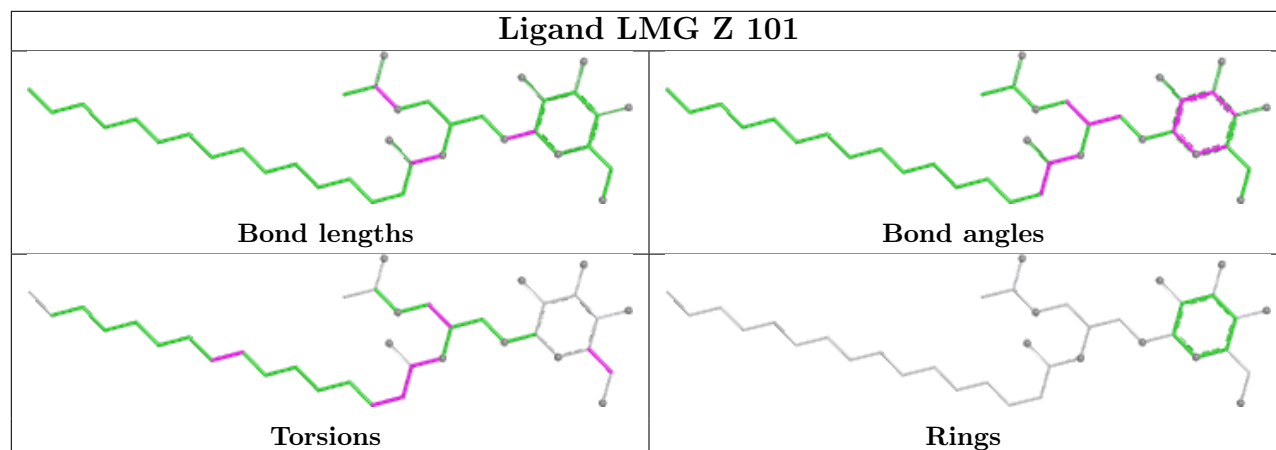
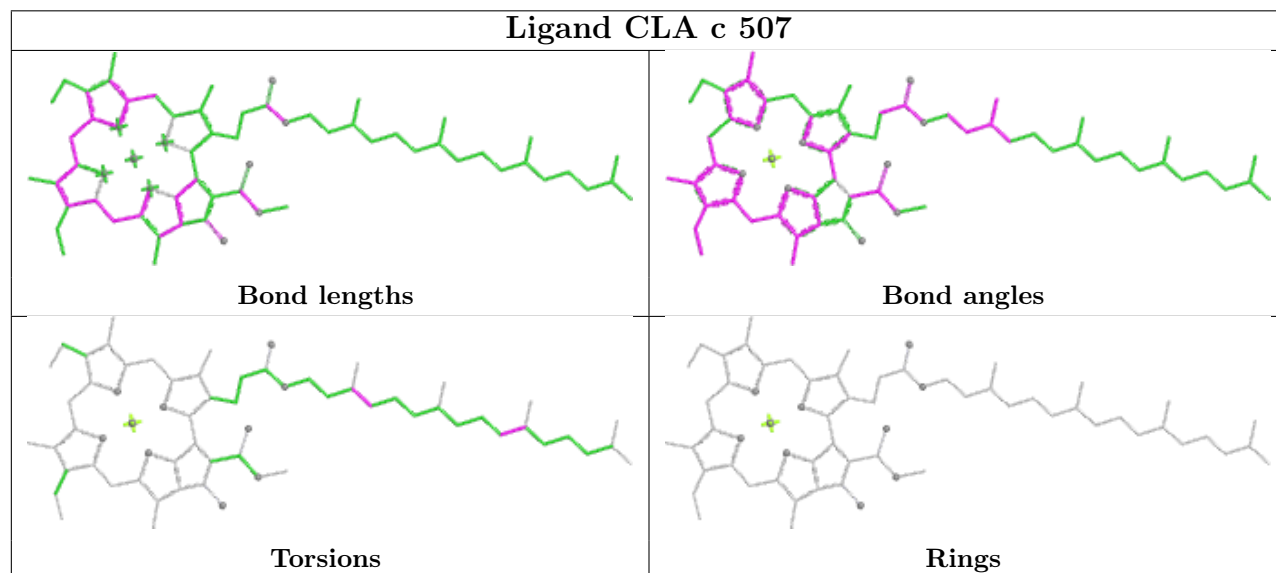
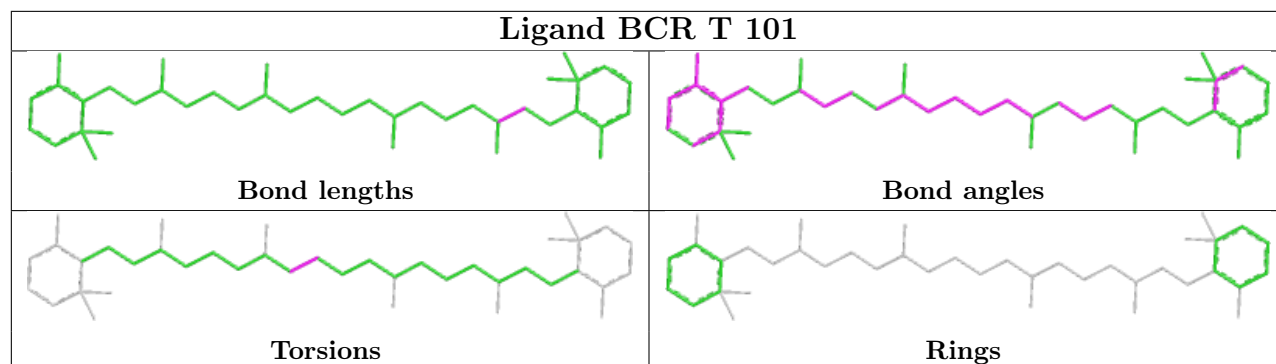


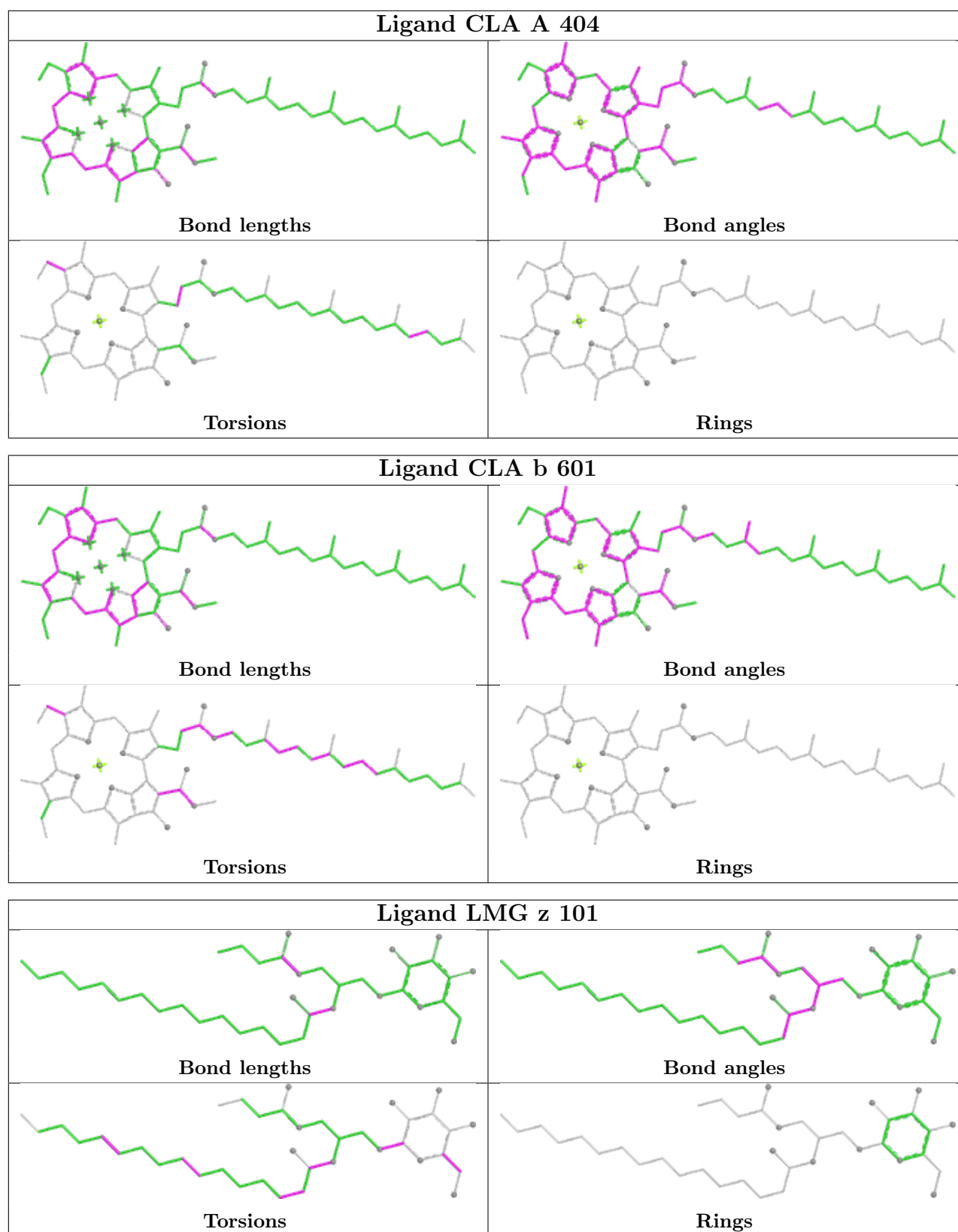
Ligand CLA C 510

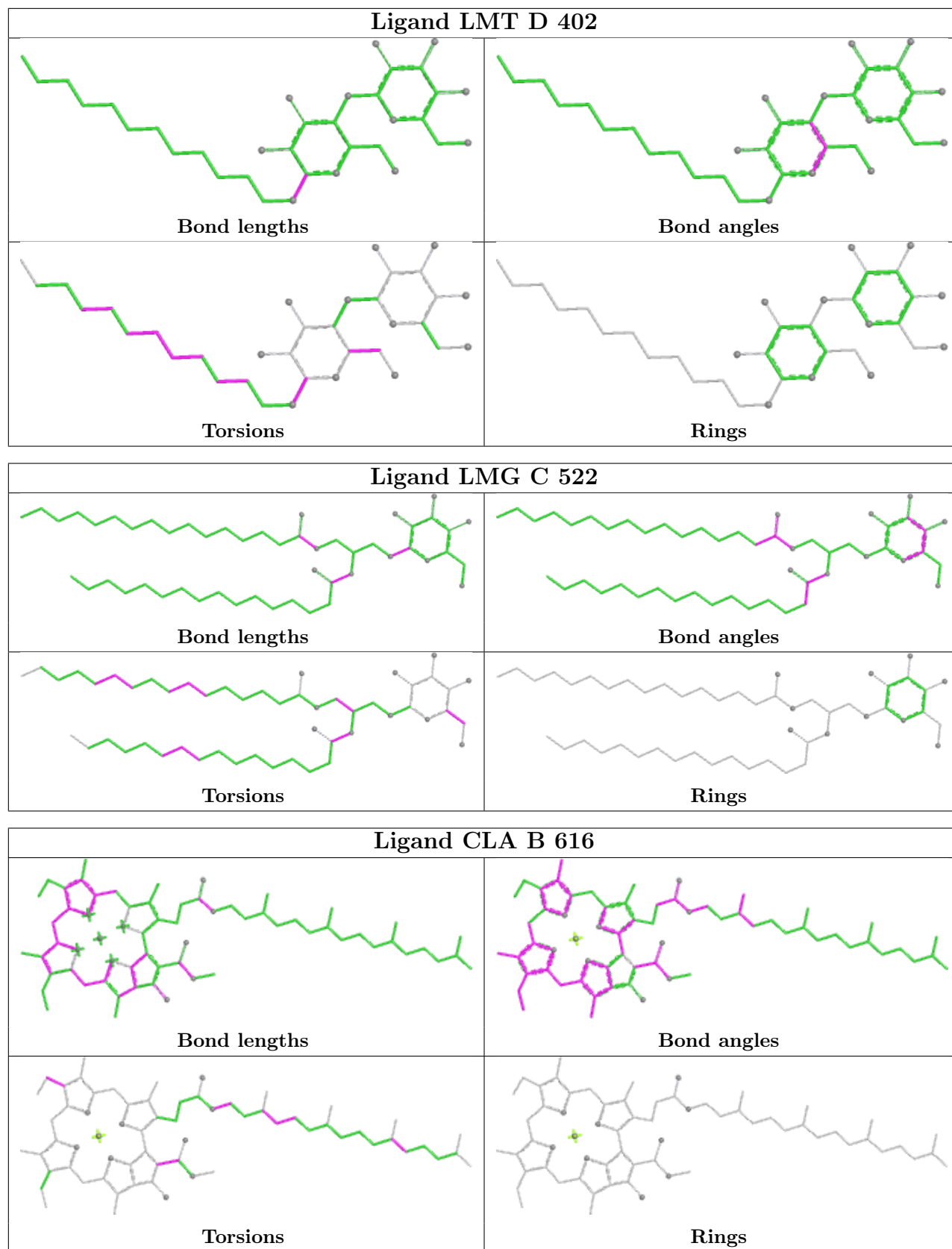


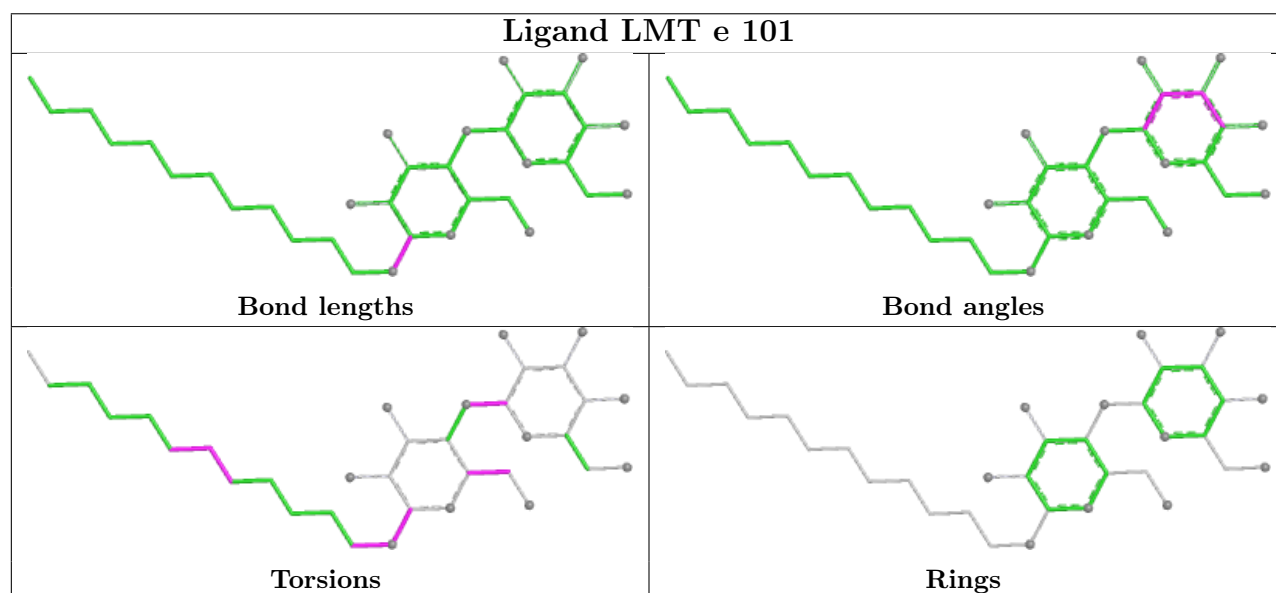
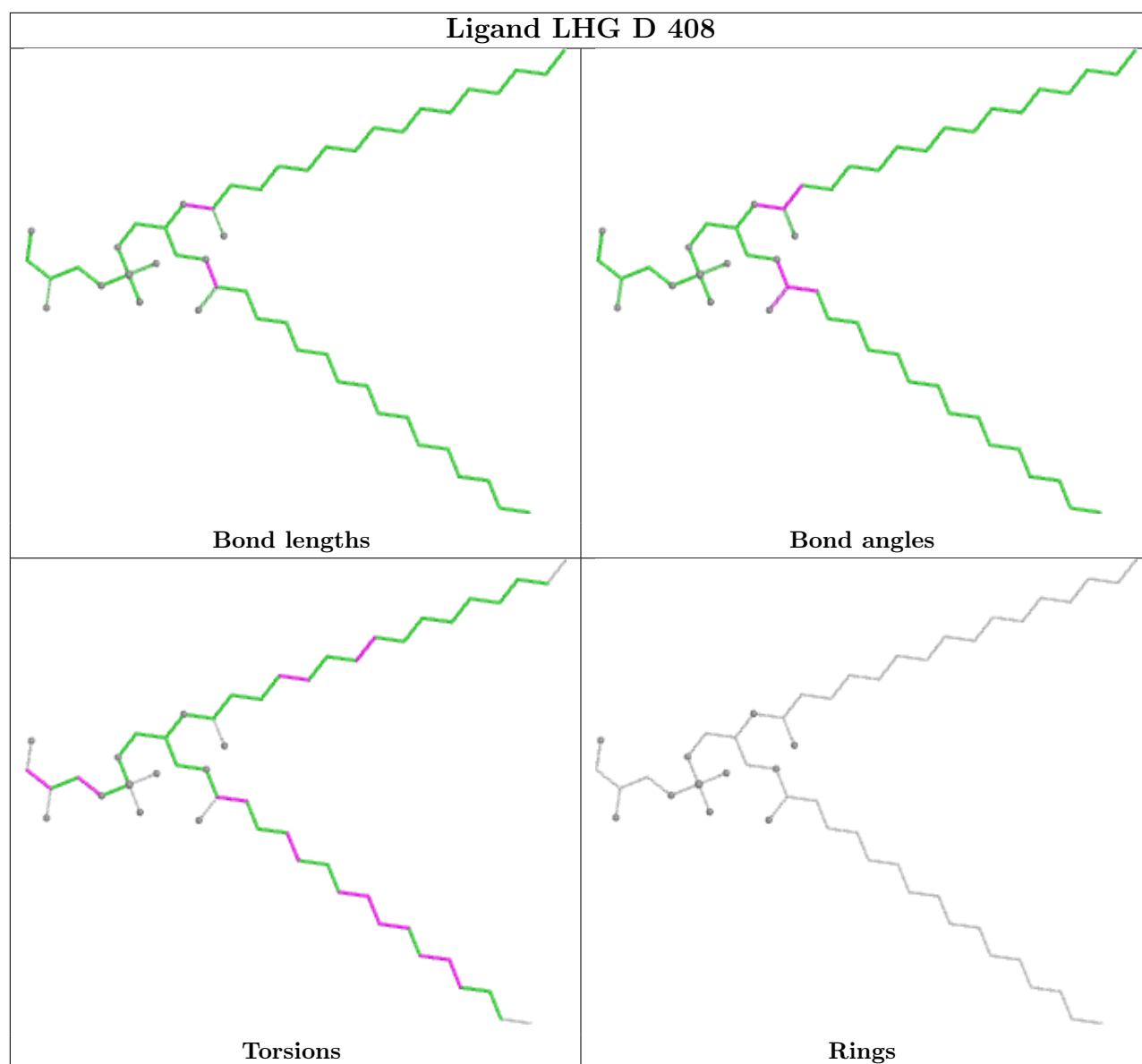
Ligand CLA D 403

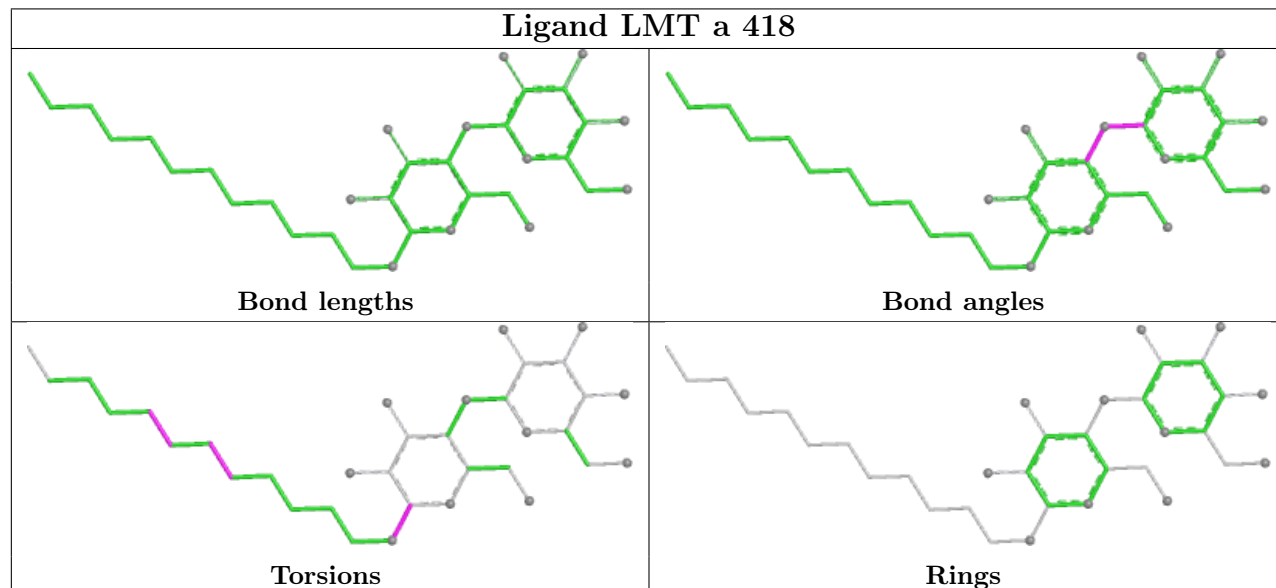
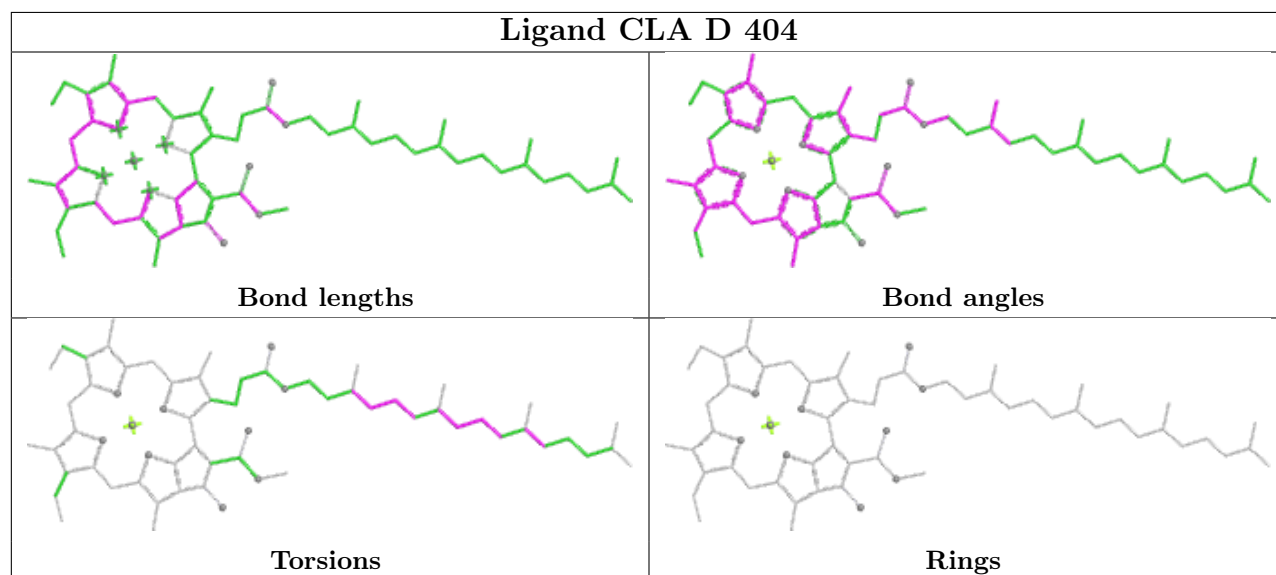
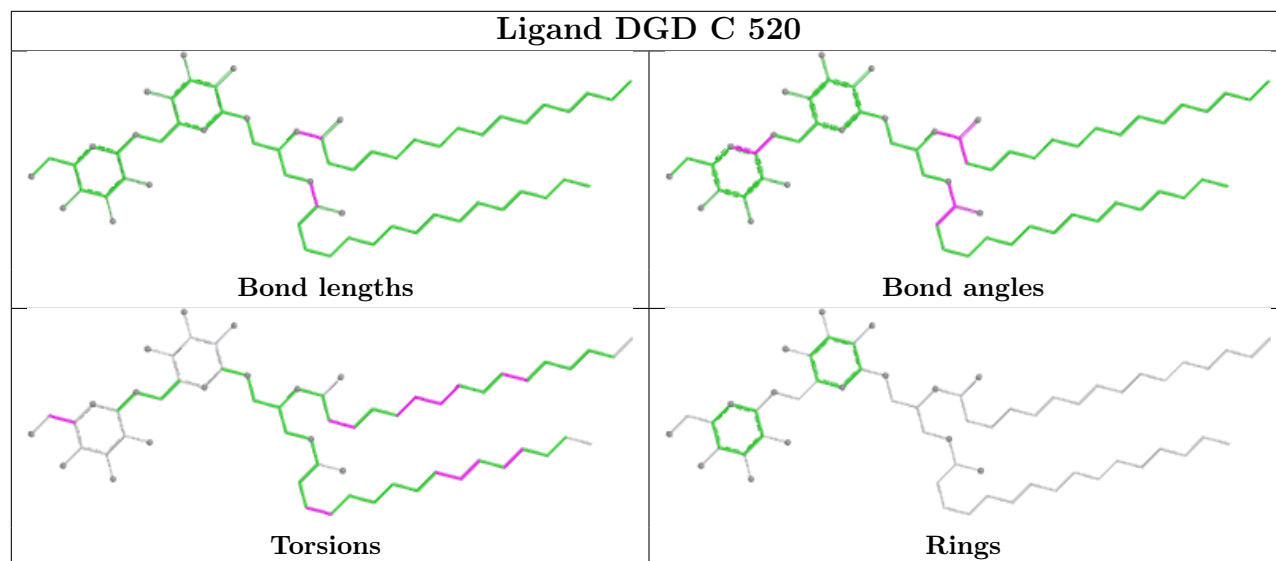


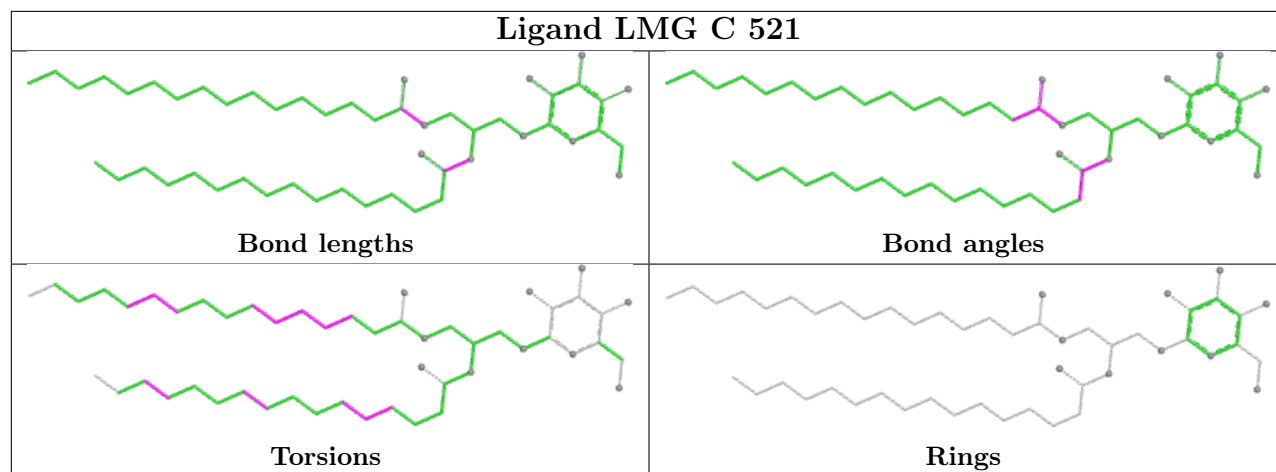
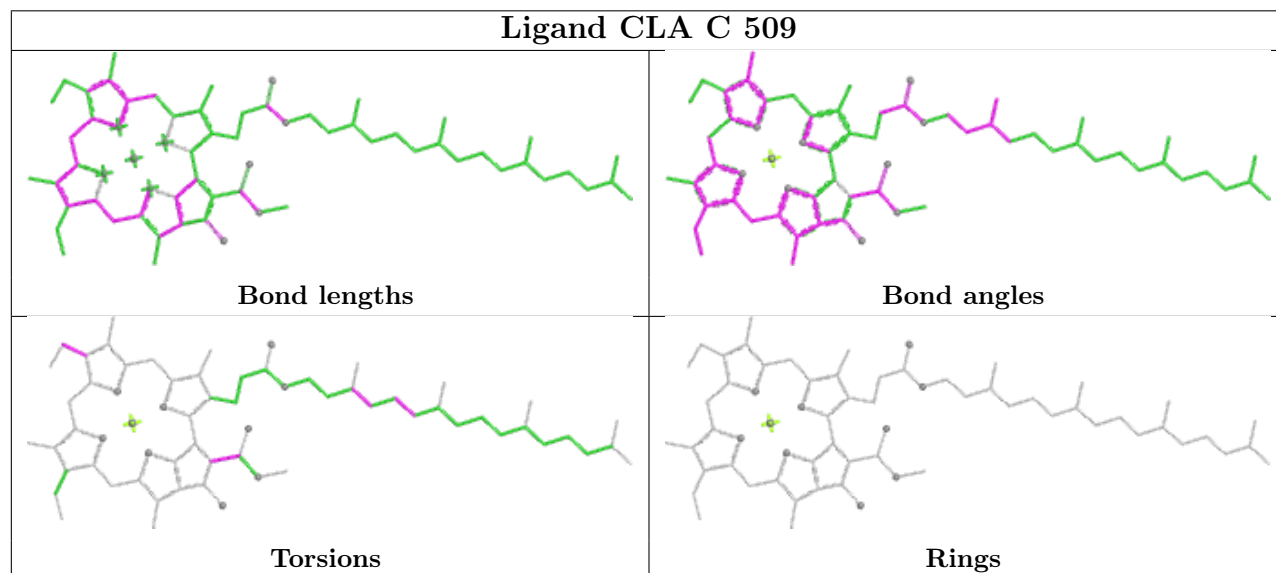
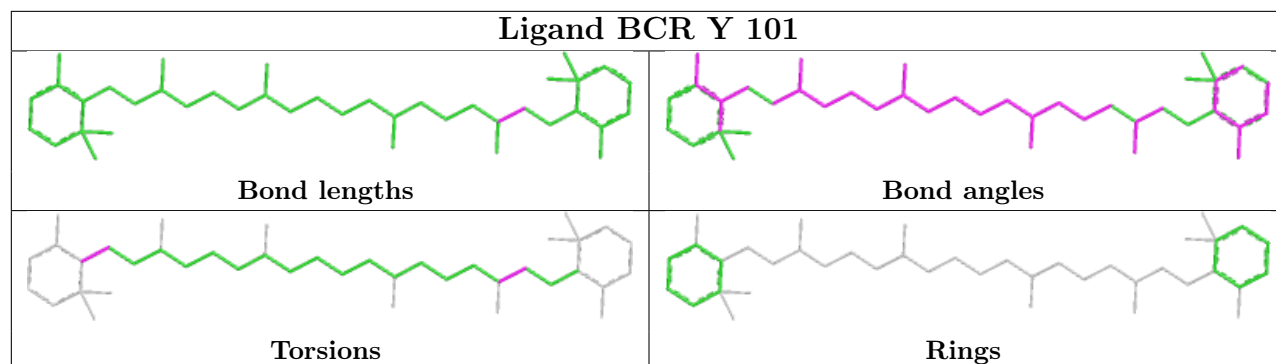


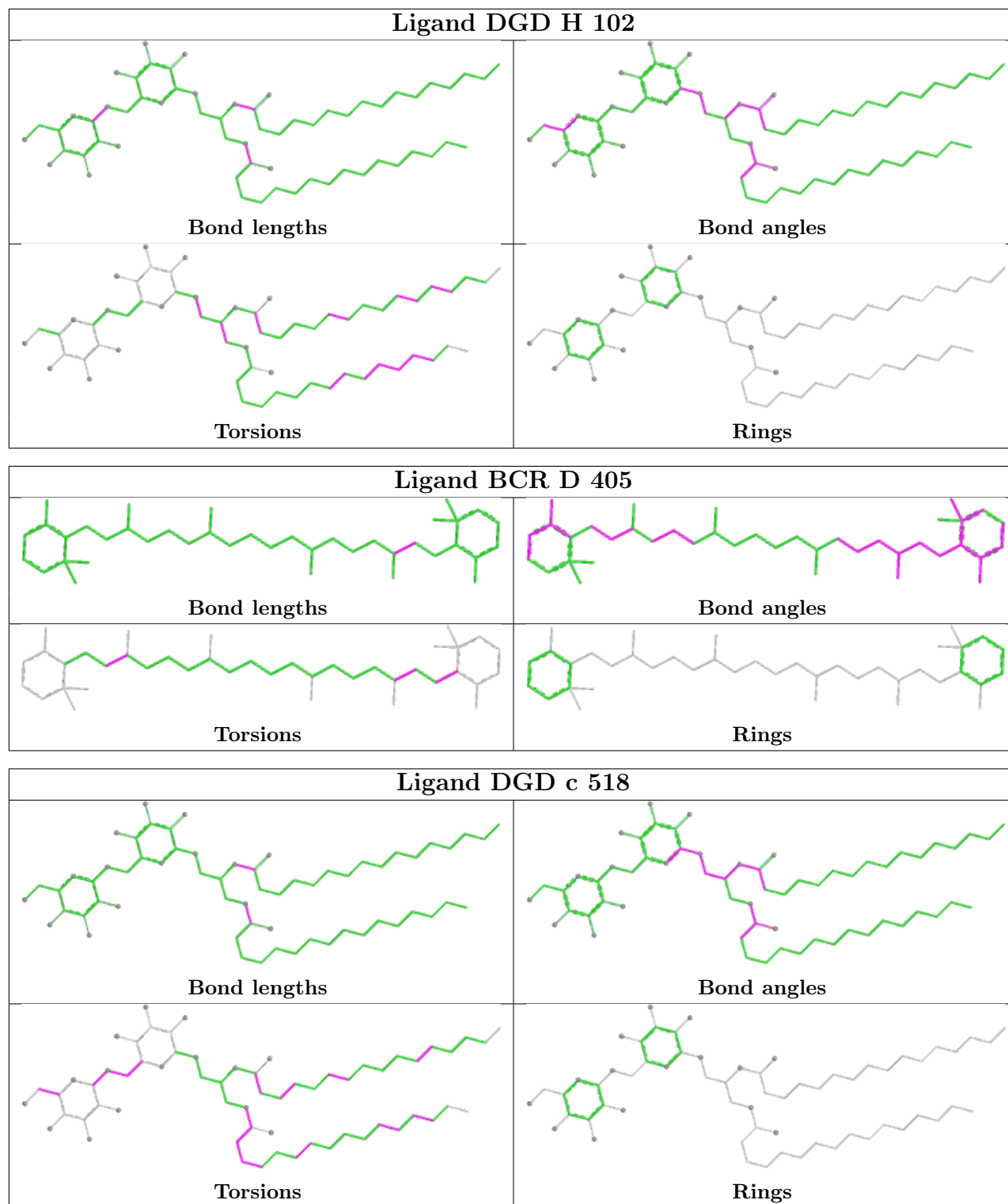


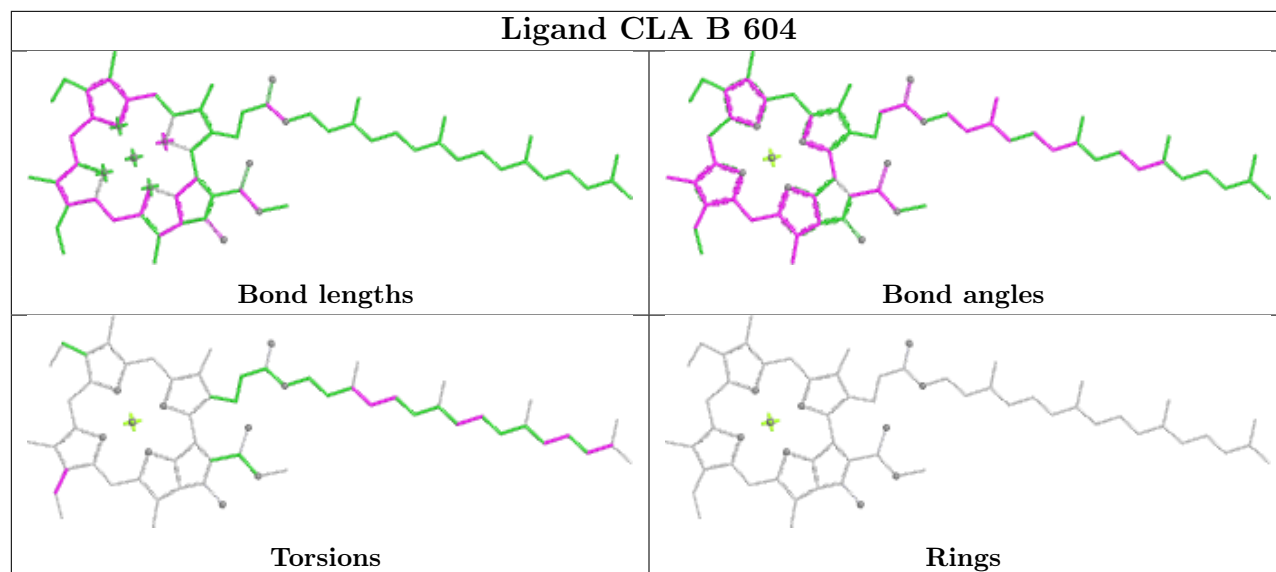
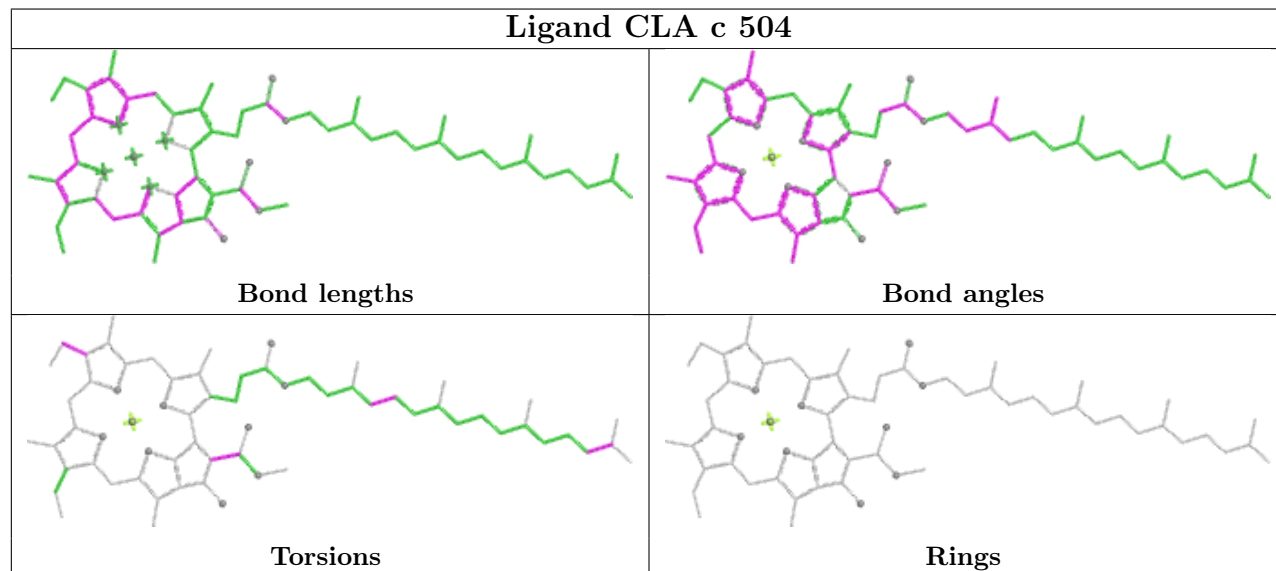


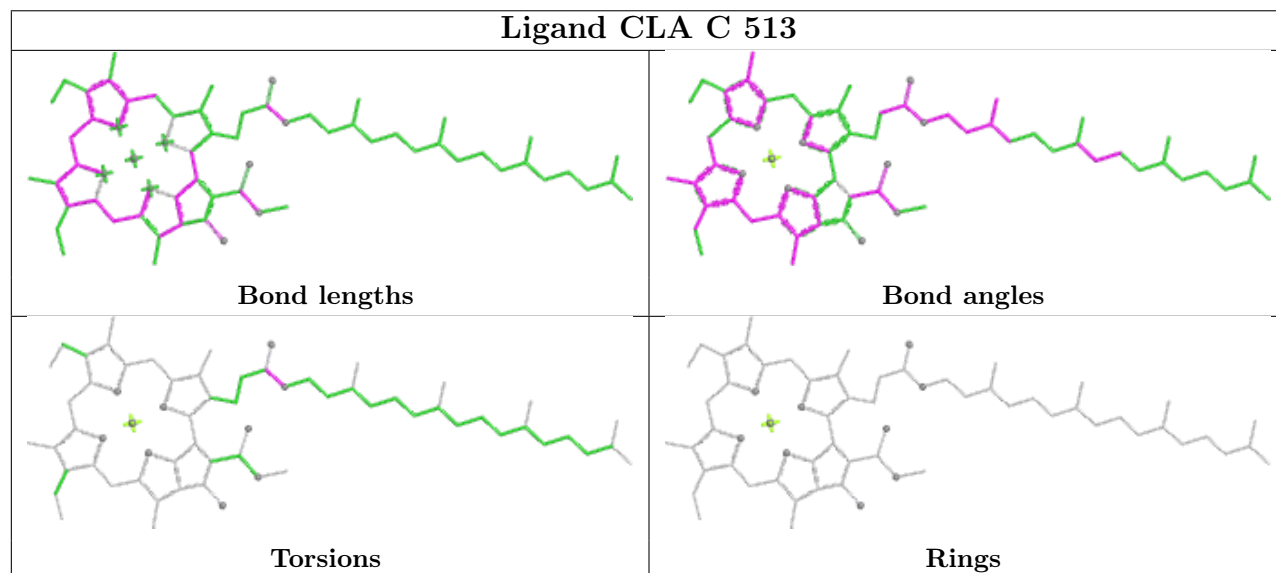
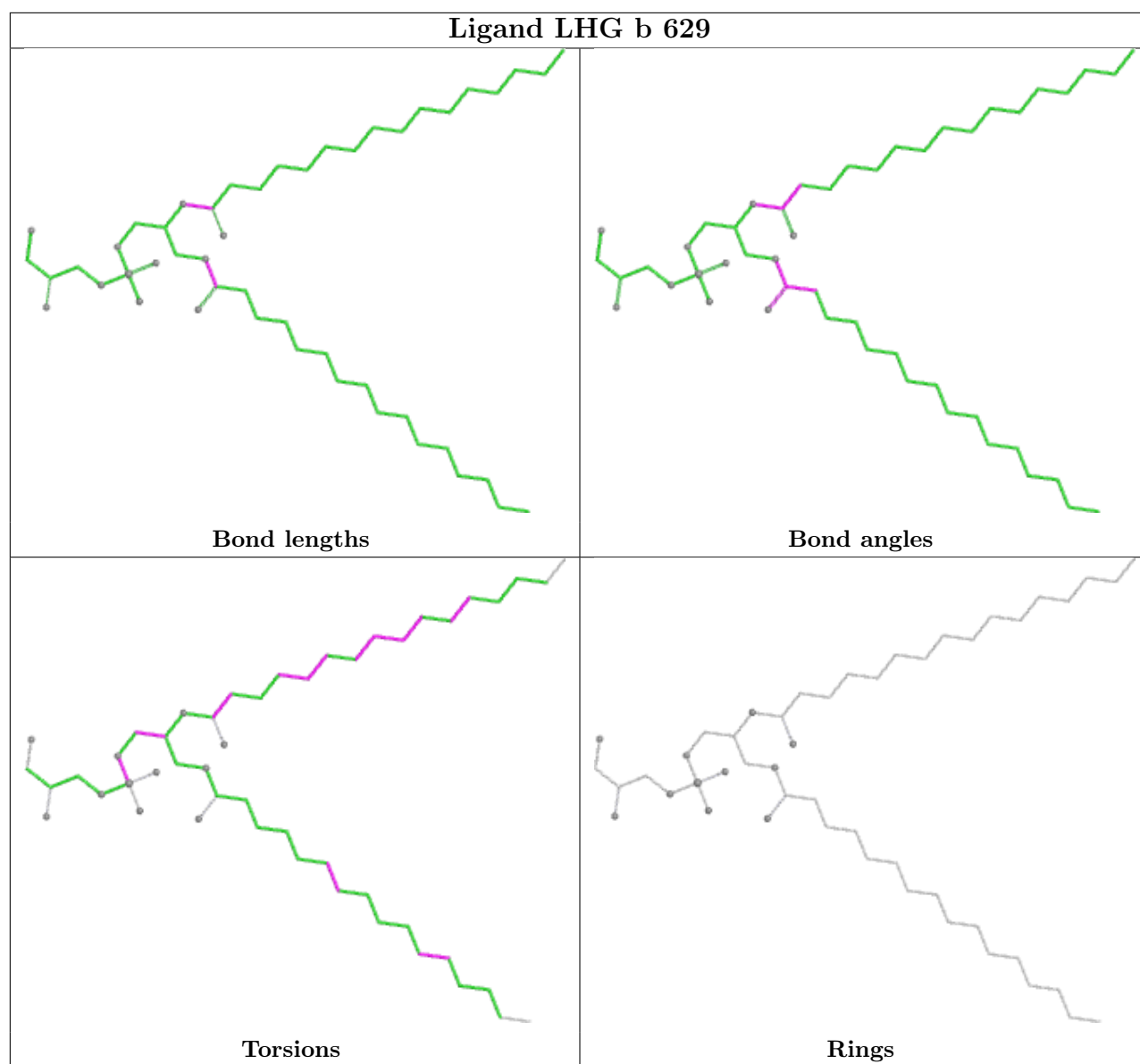


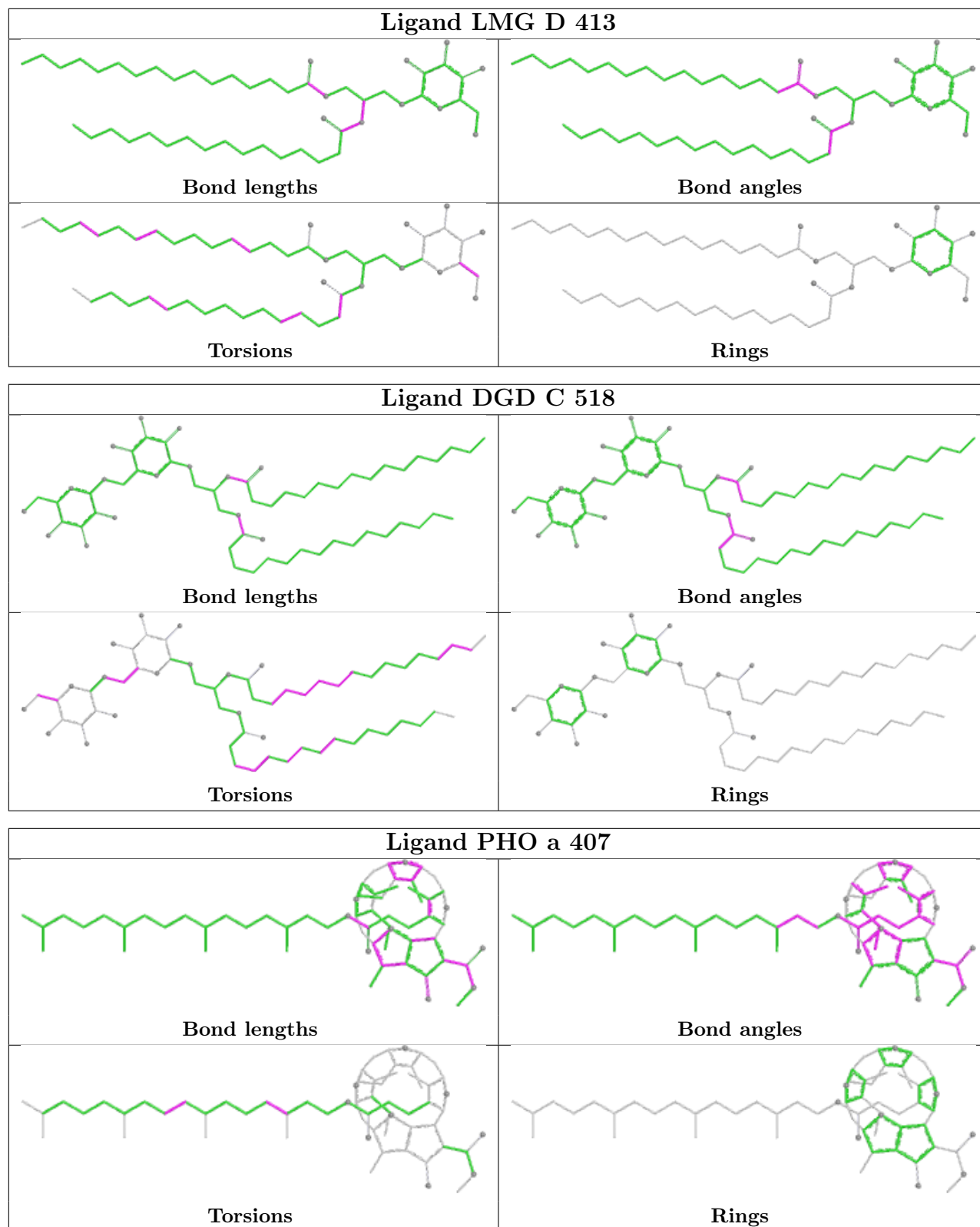


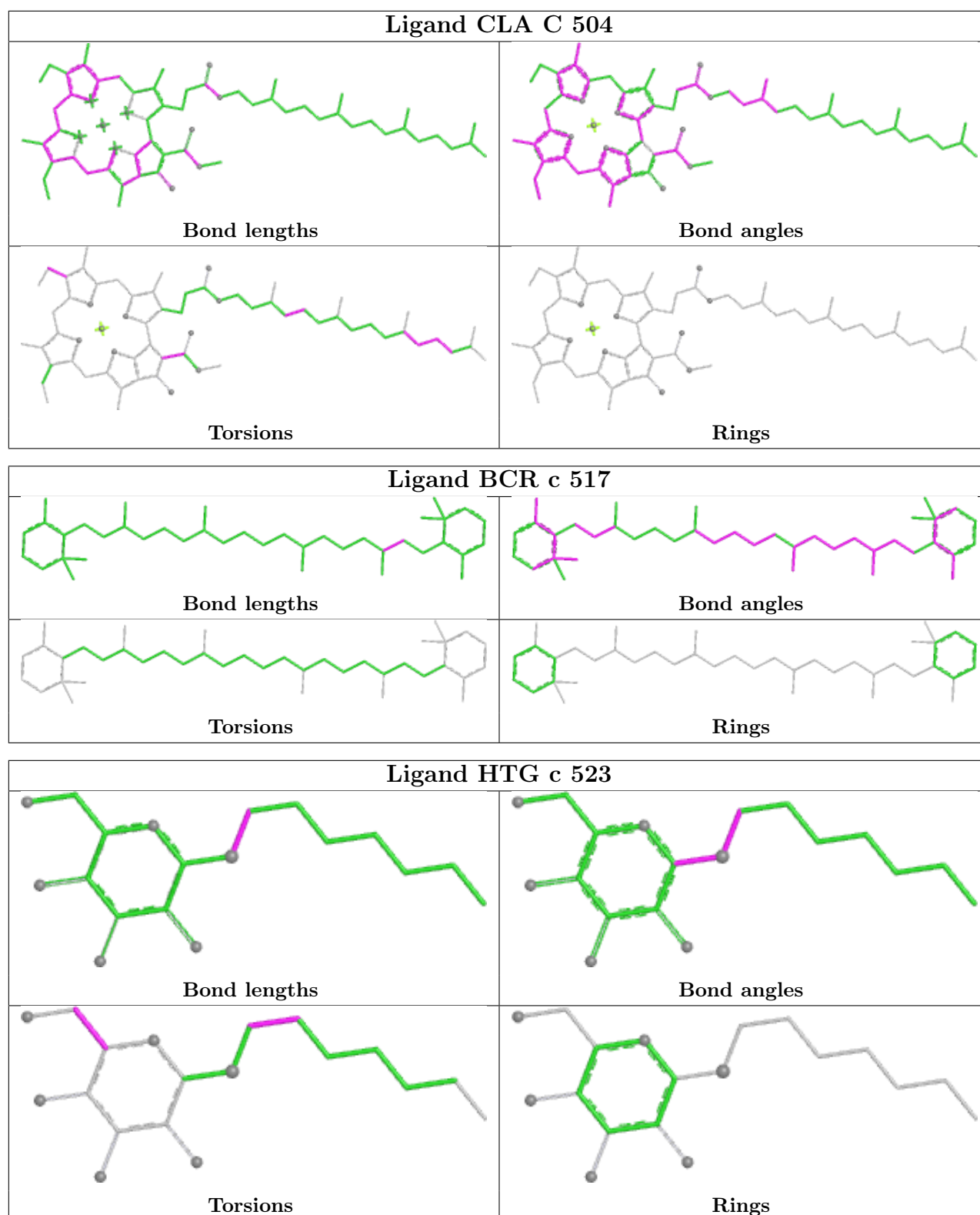




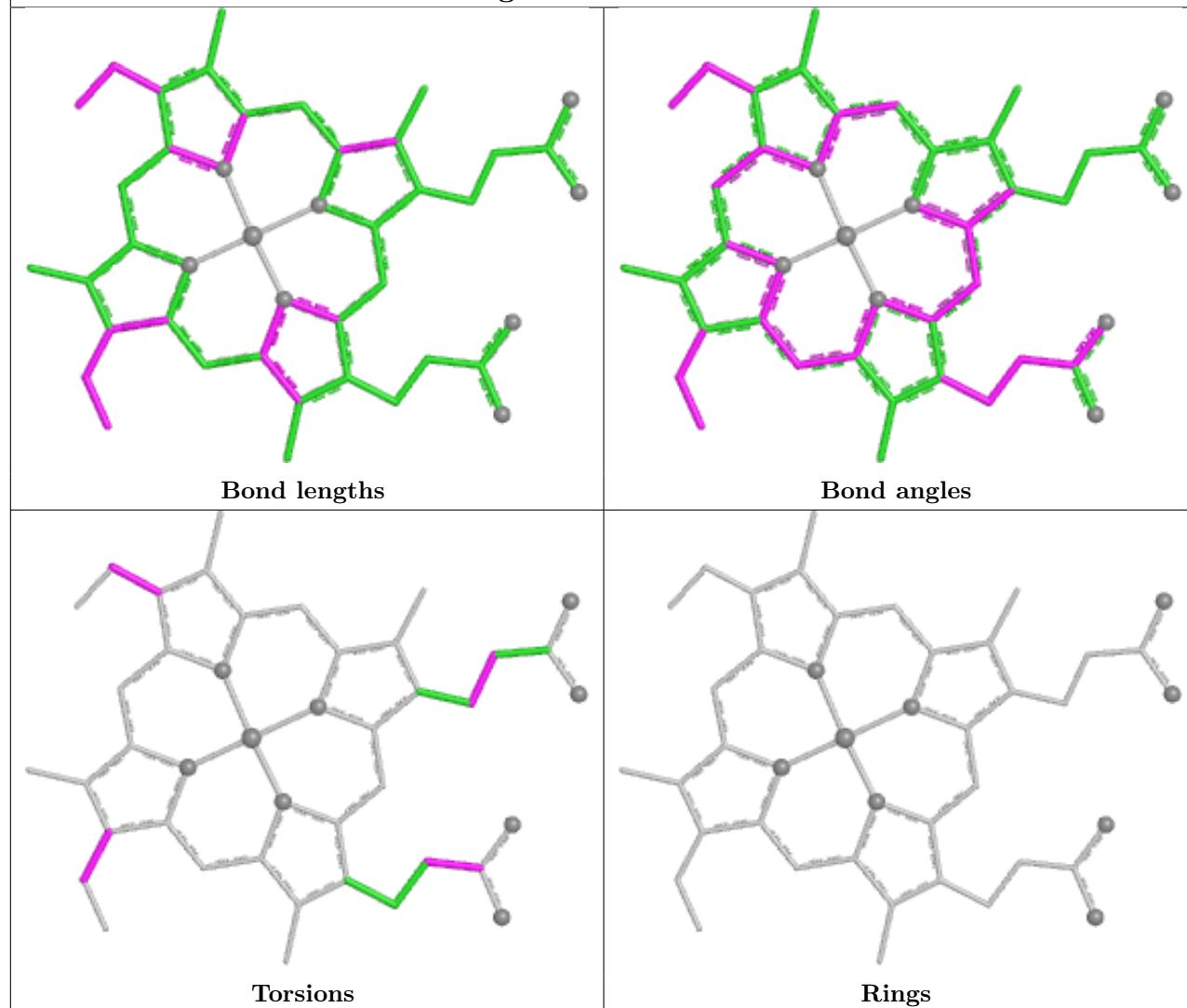
Ligand CLA B 604**Ligand CLA c 504**



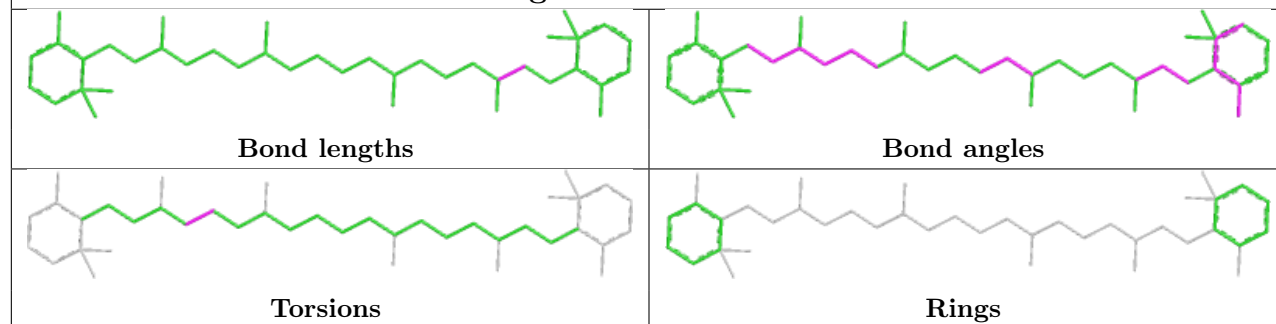


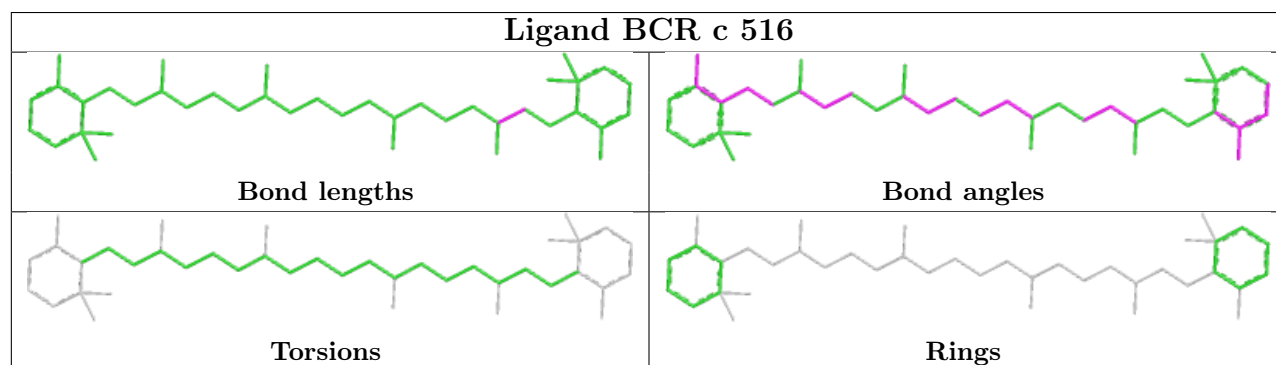
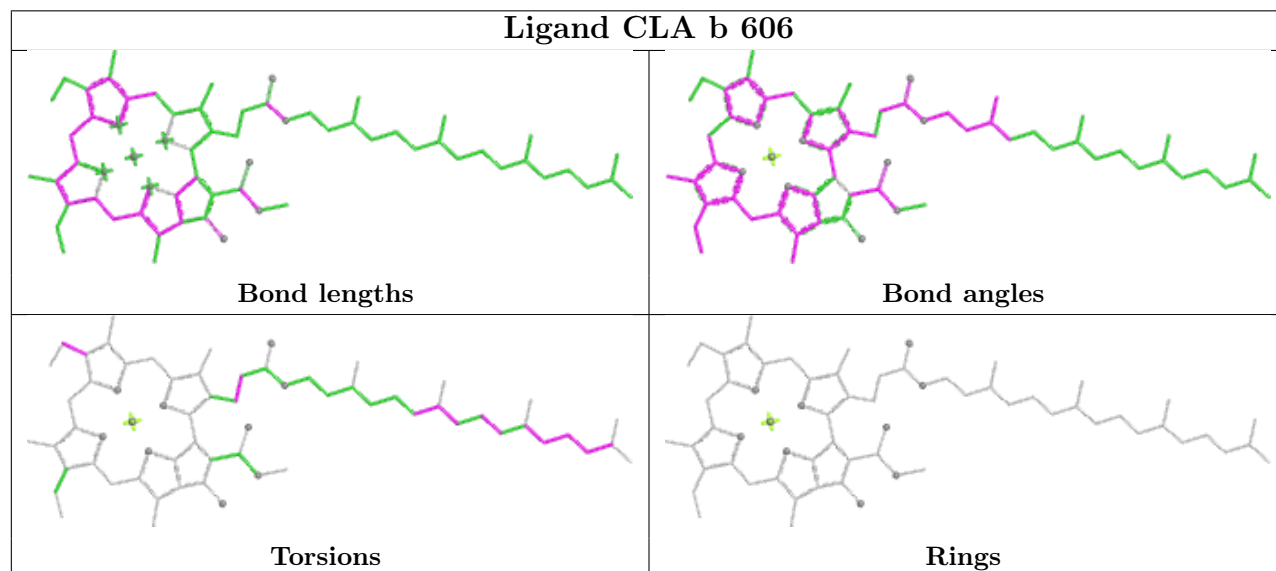
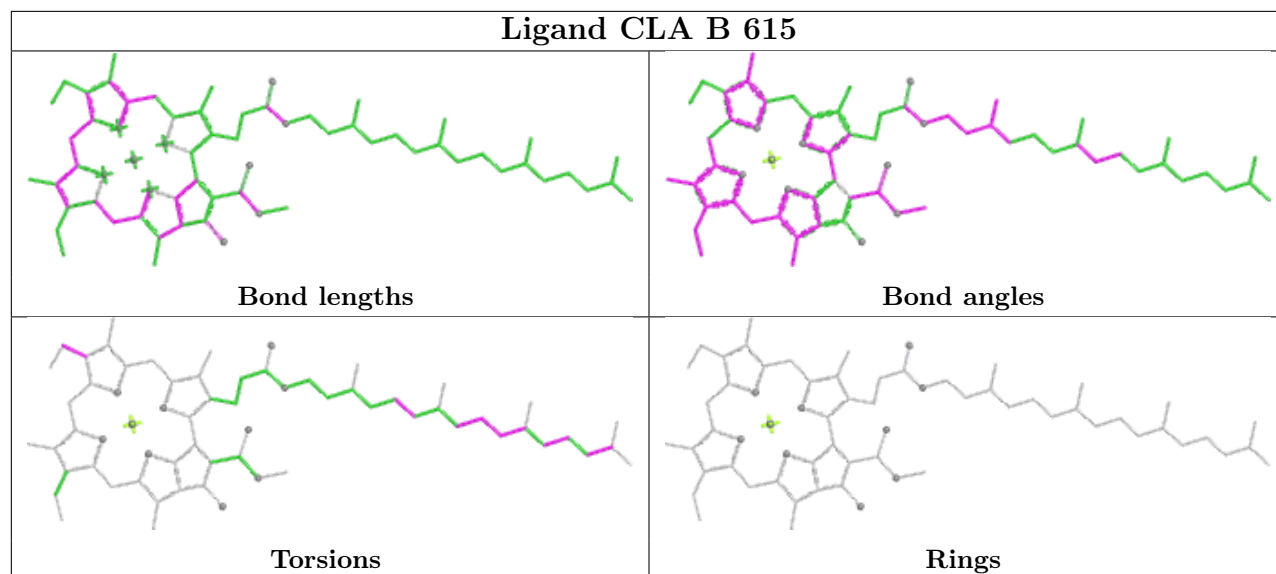


Ligand HEC e 102

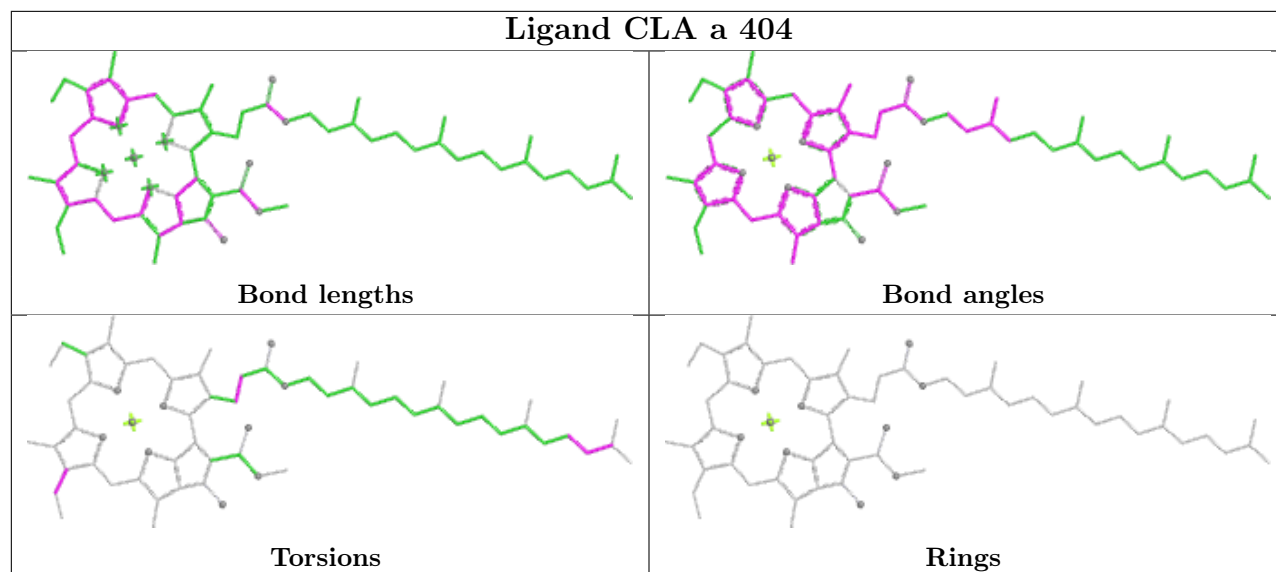


Ligand BCR H 101

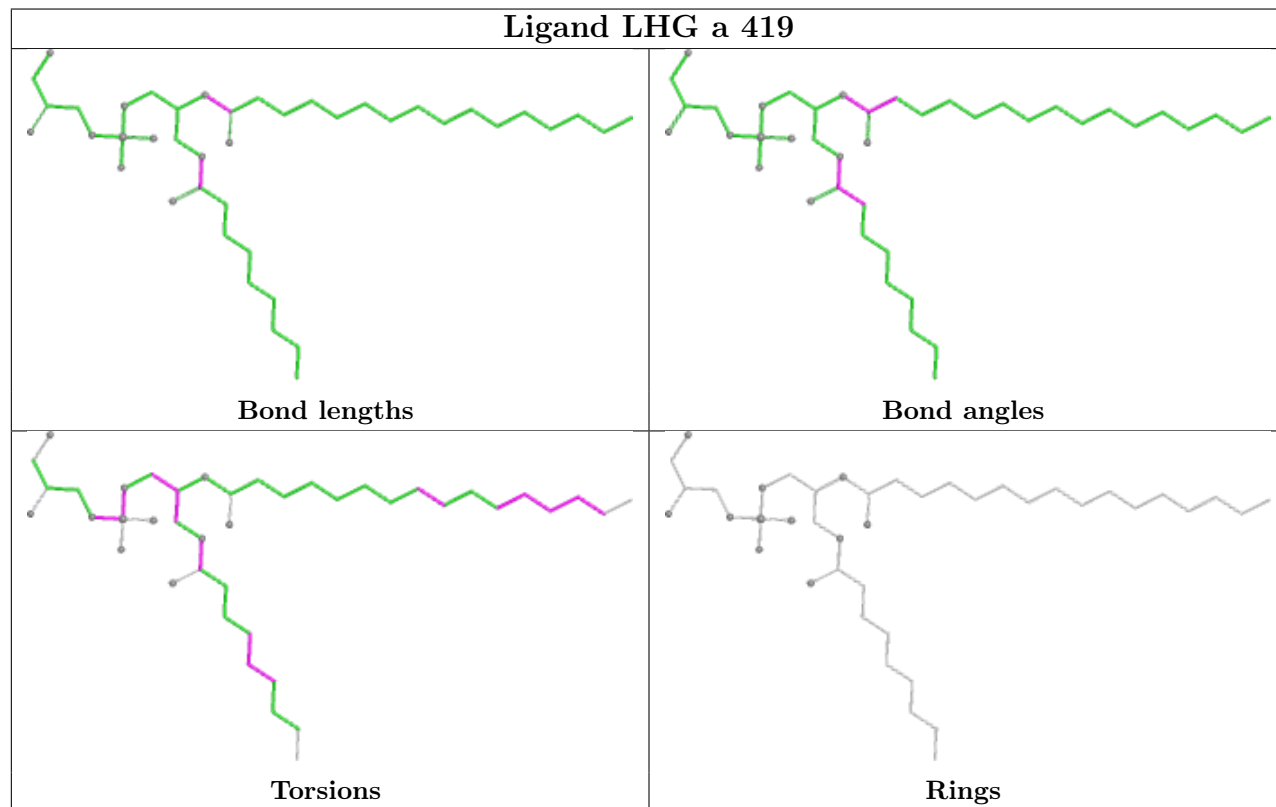




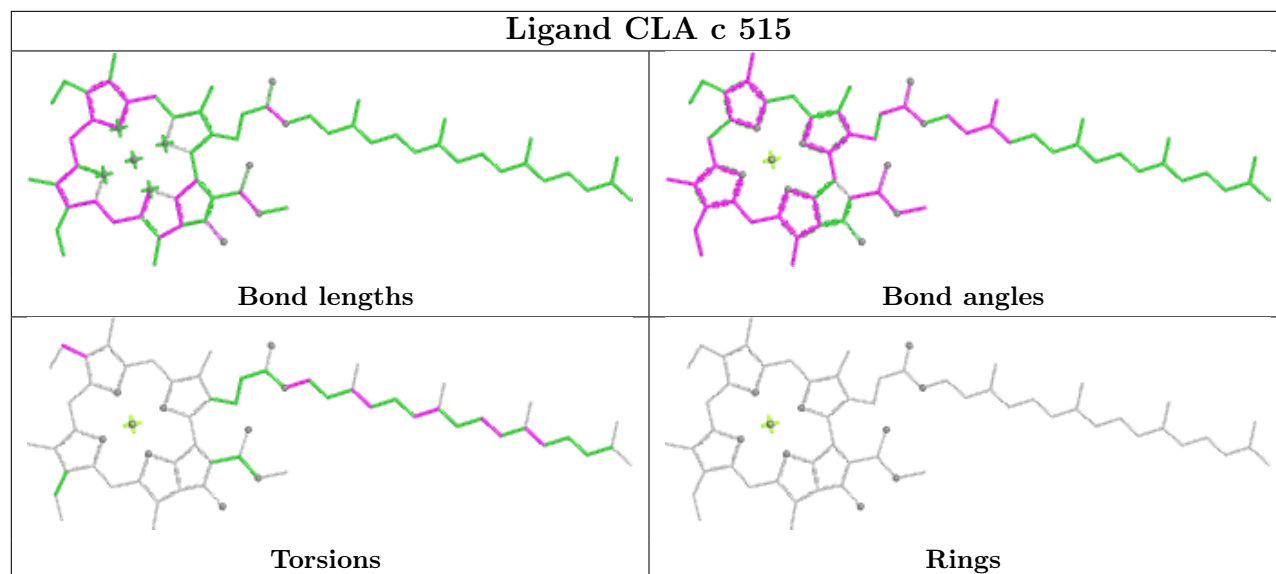
Ligand CLA a 404



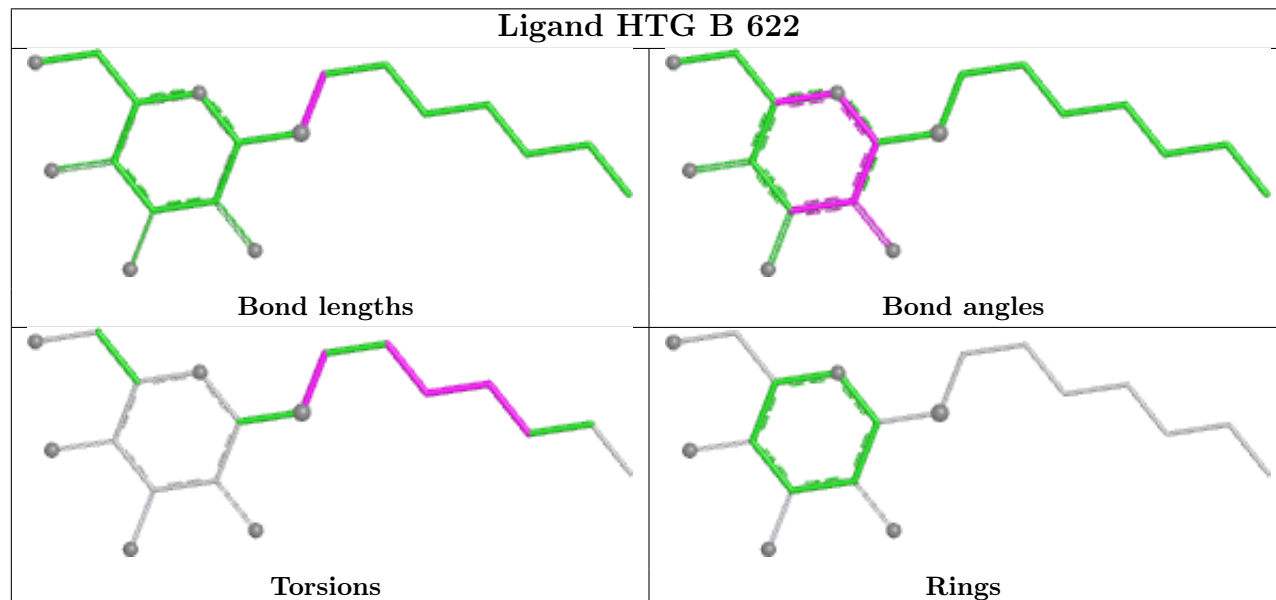
Ligand LHG a 419



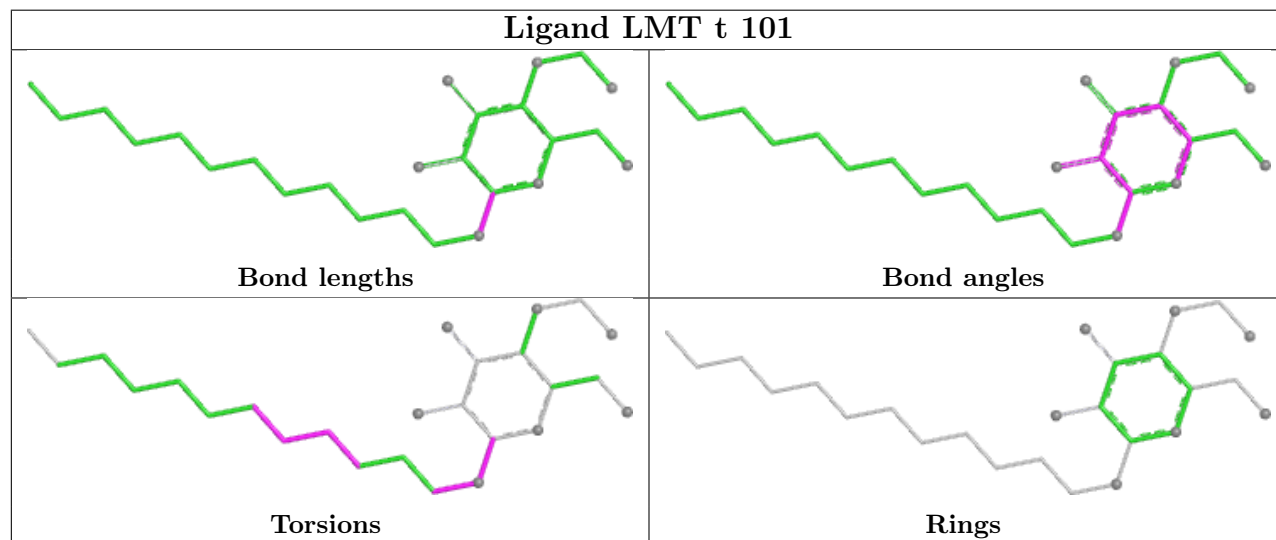
Ligand CLA c 515



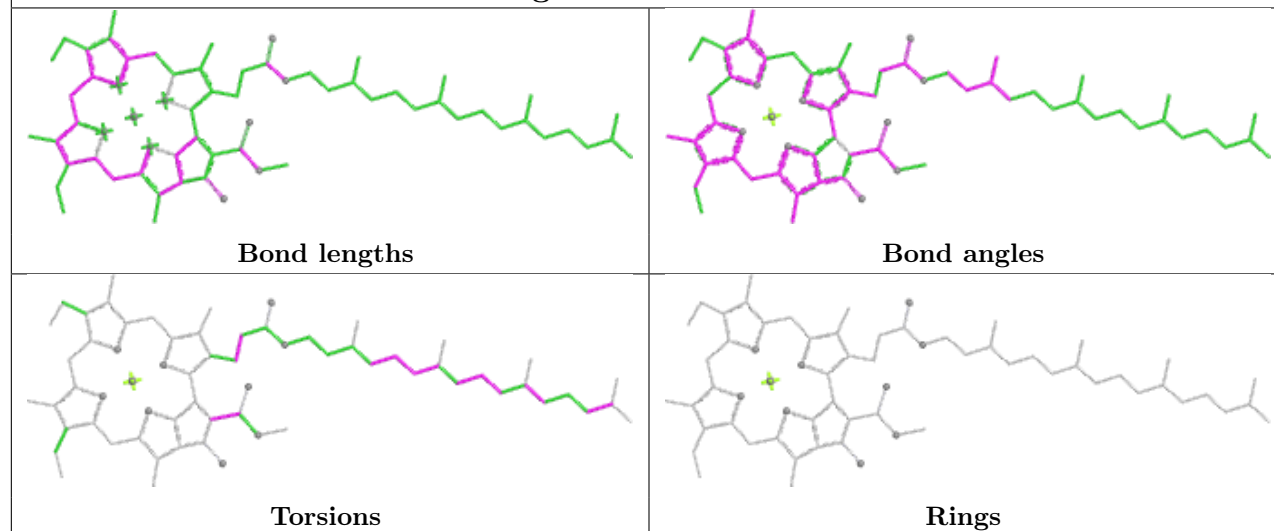
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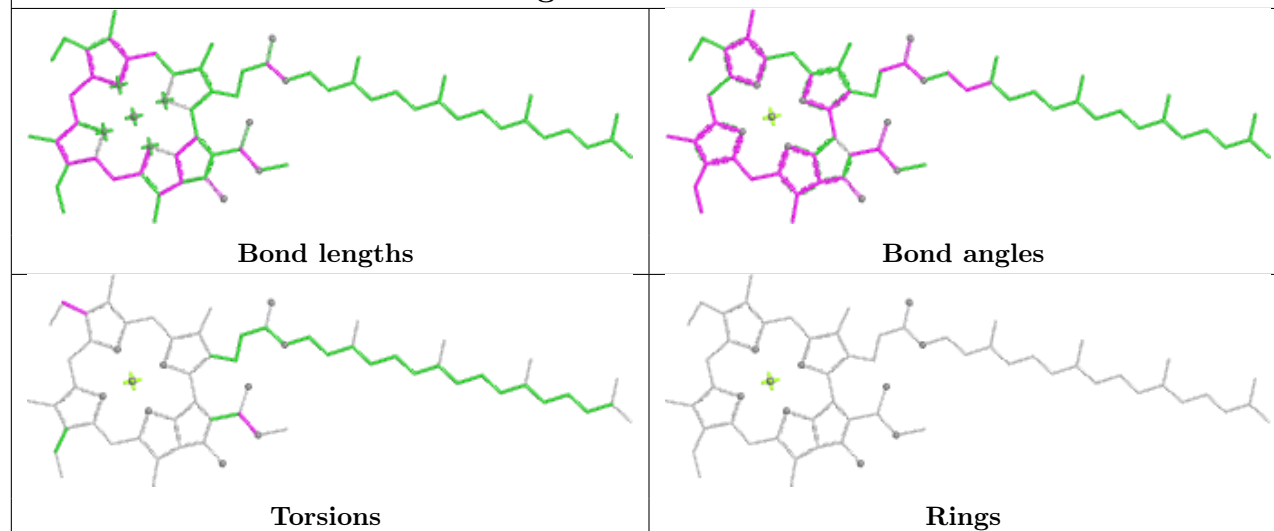
Ligand LMT t 101



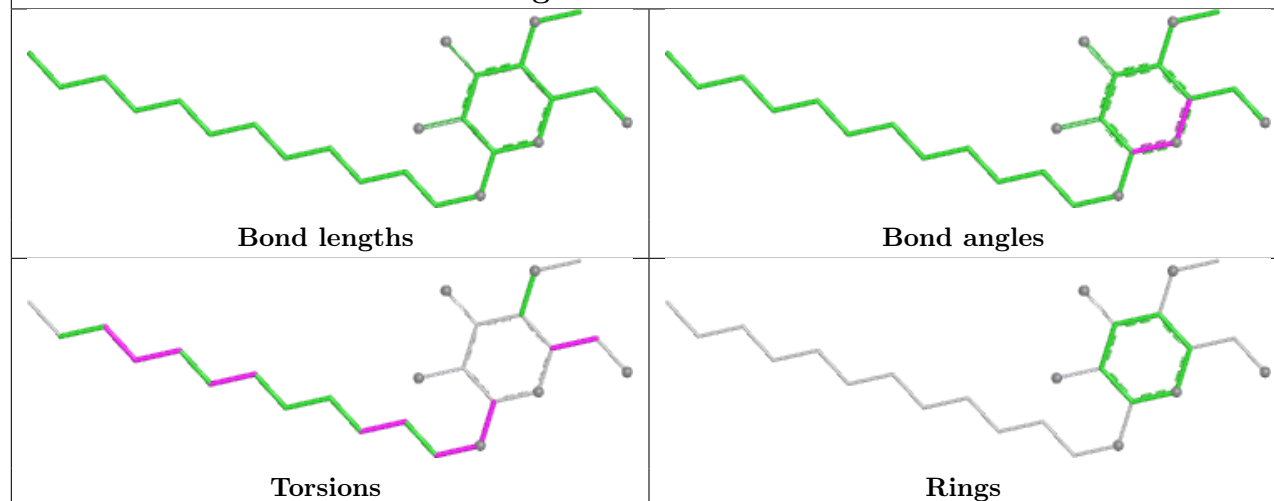
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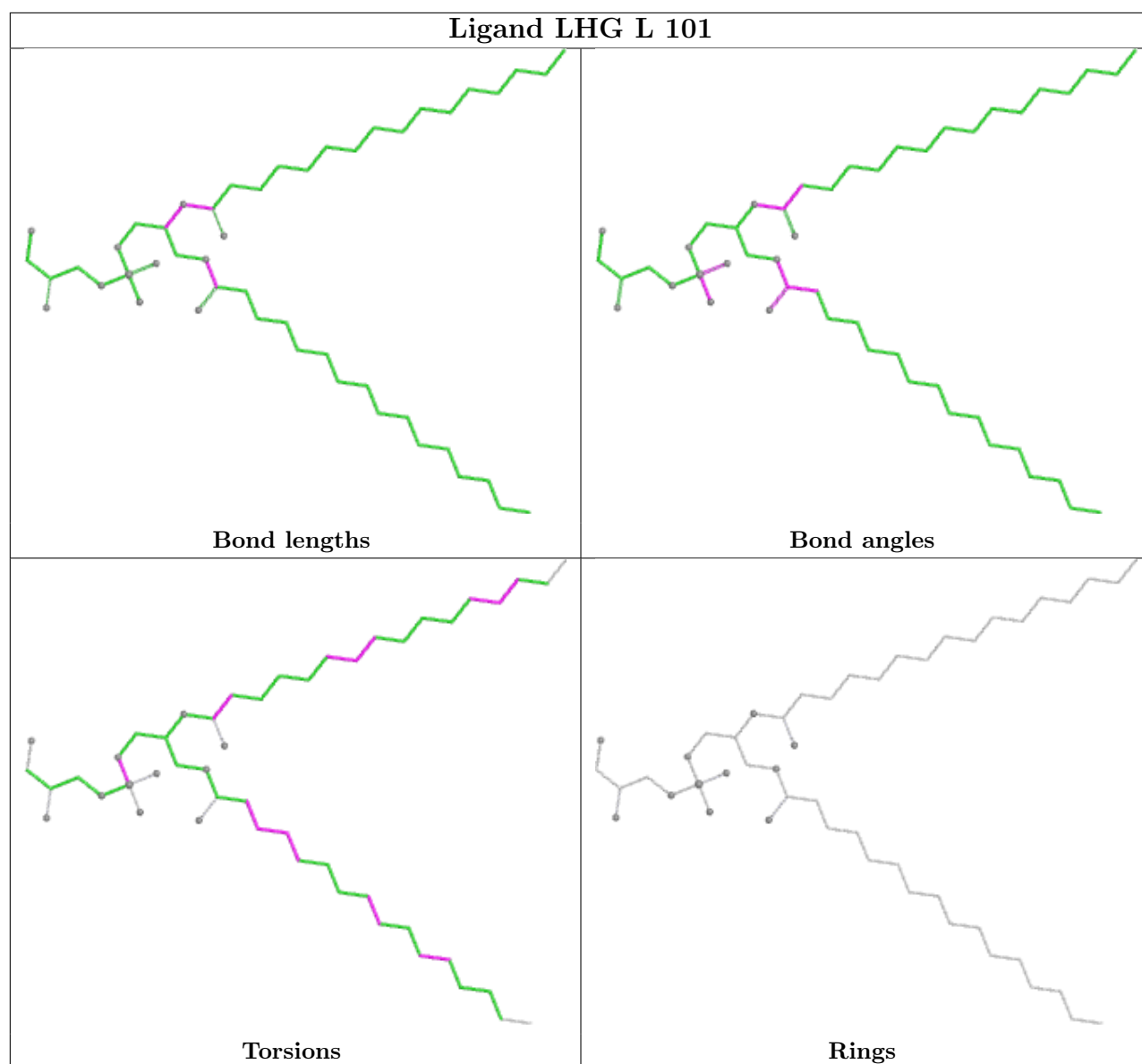


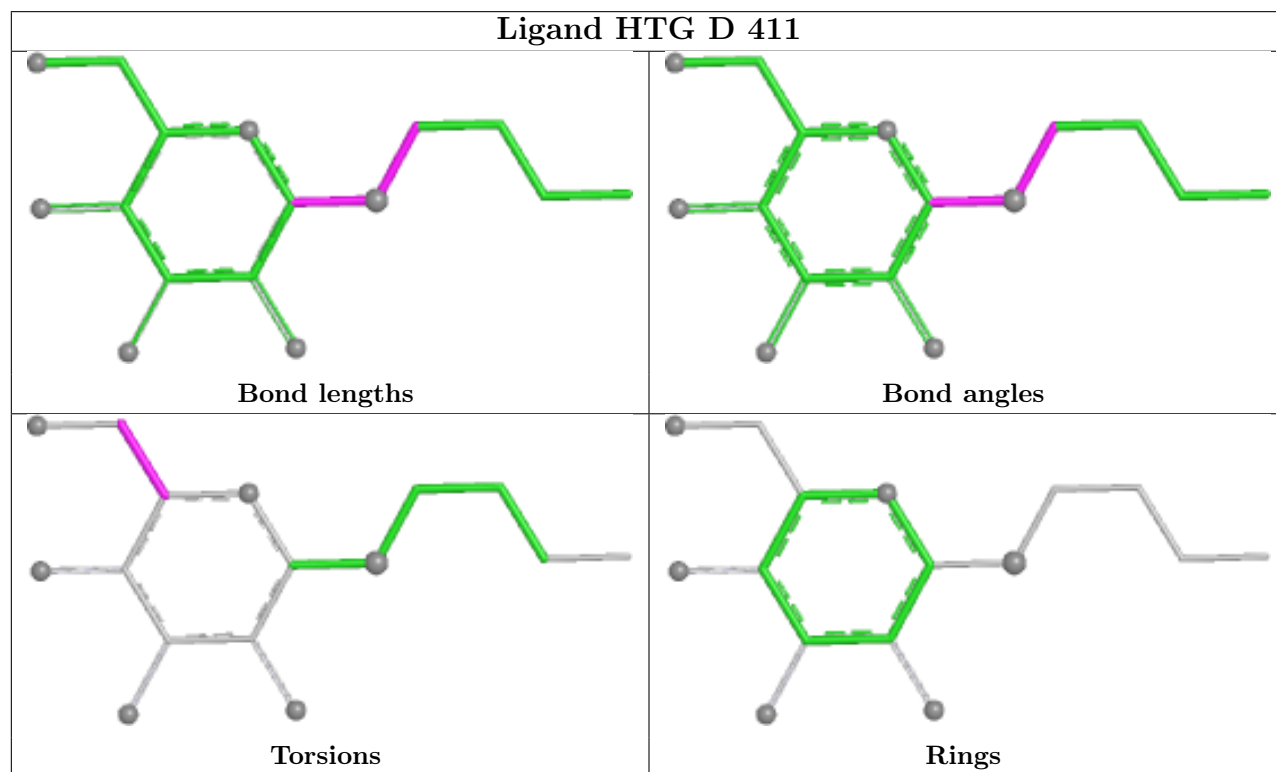
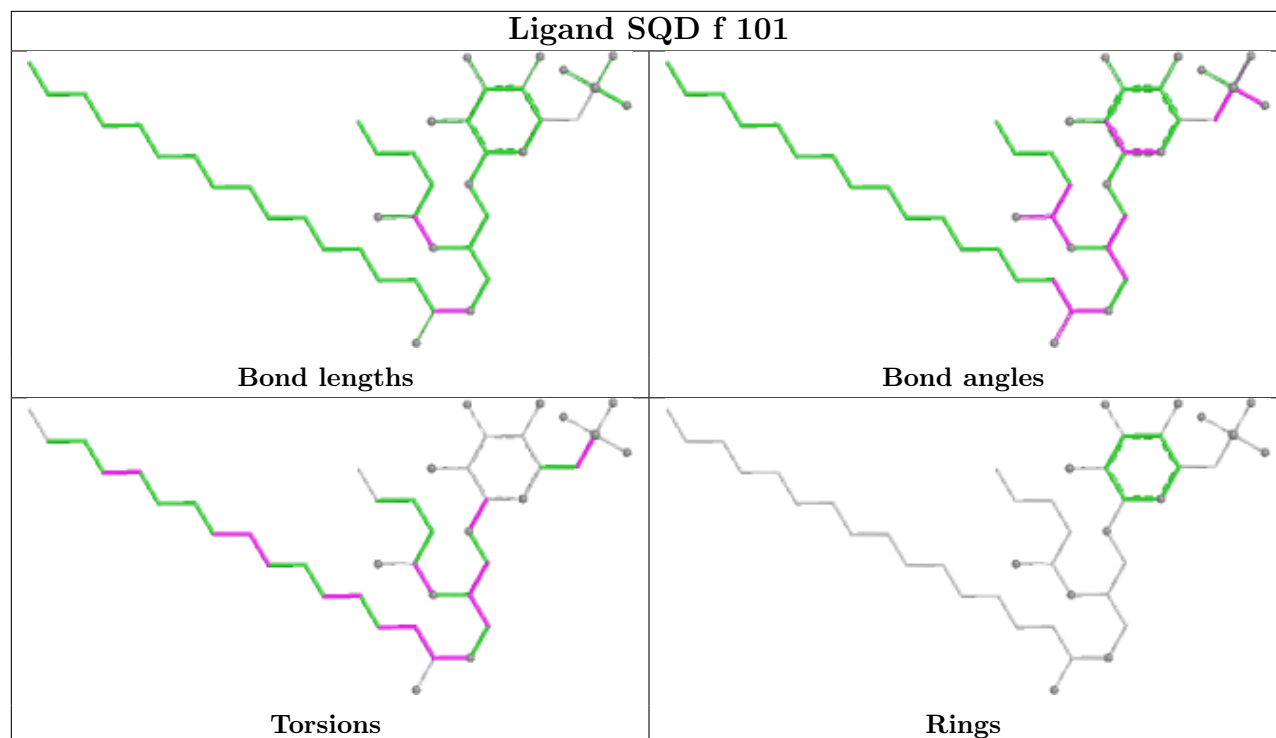
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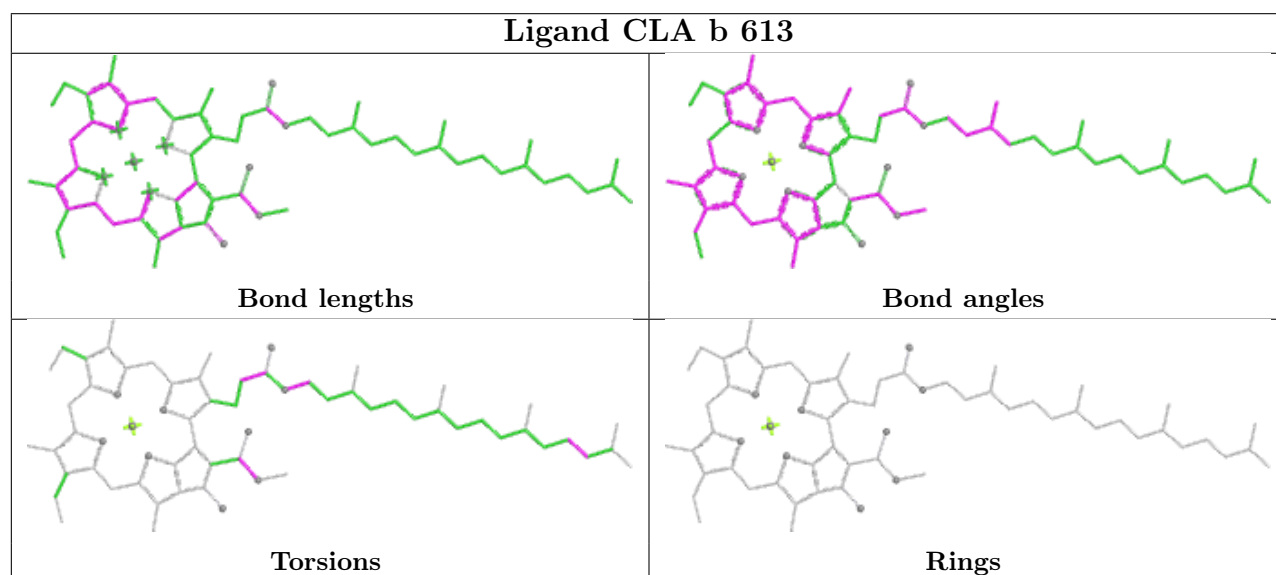
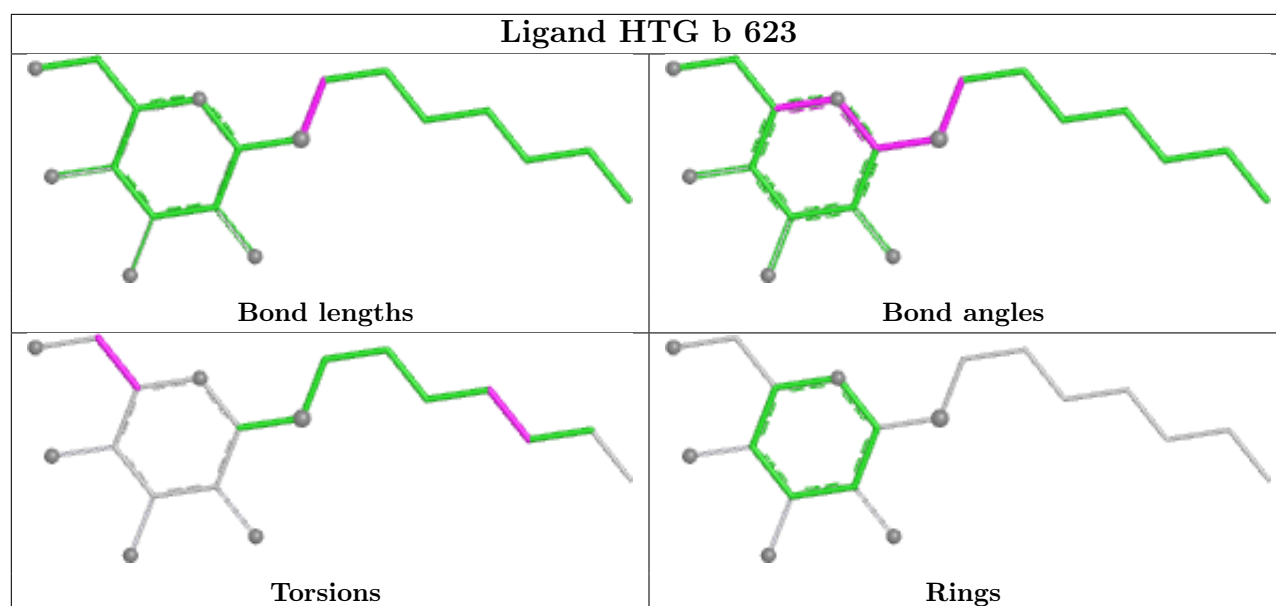


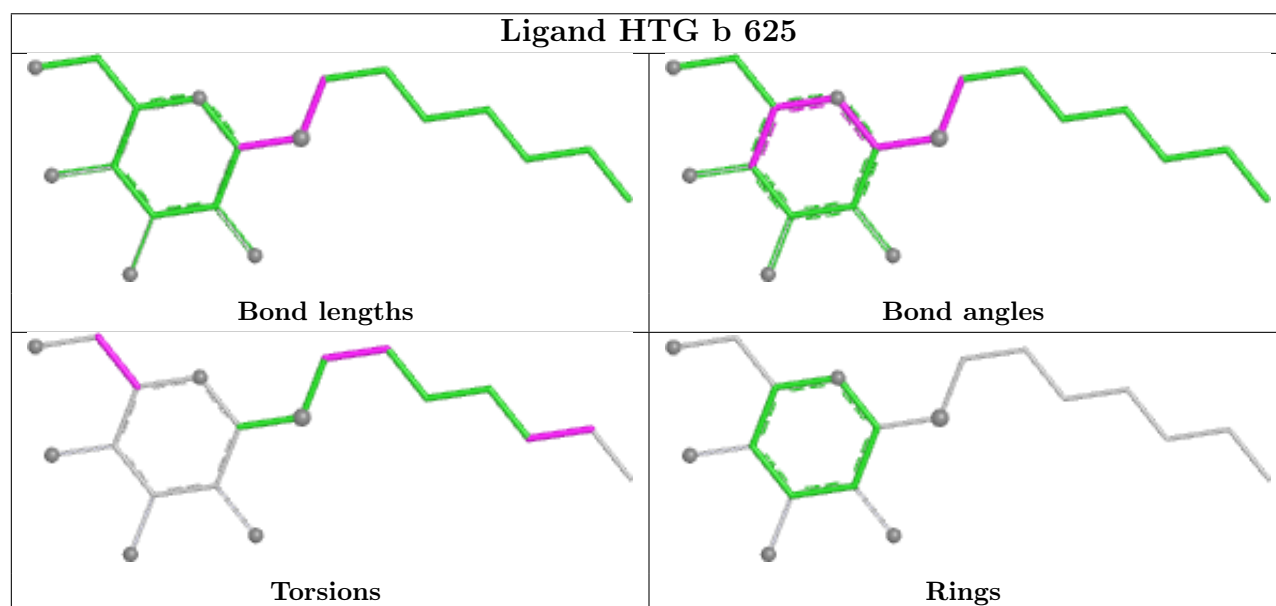
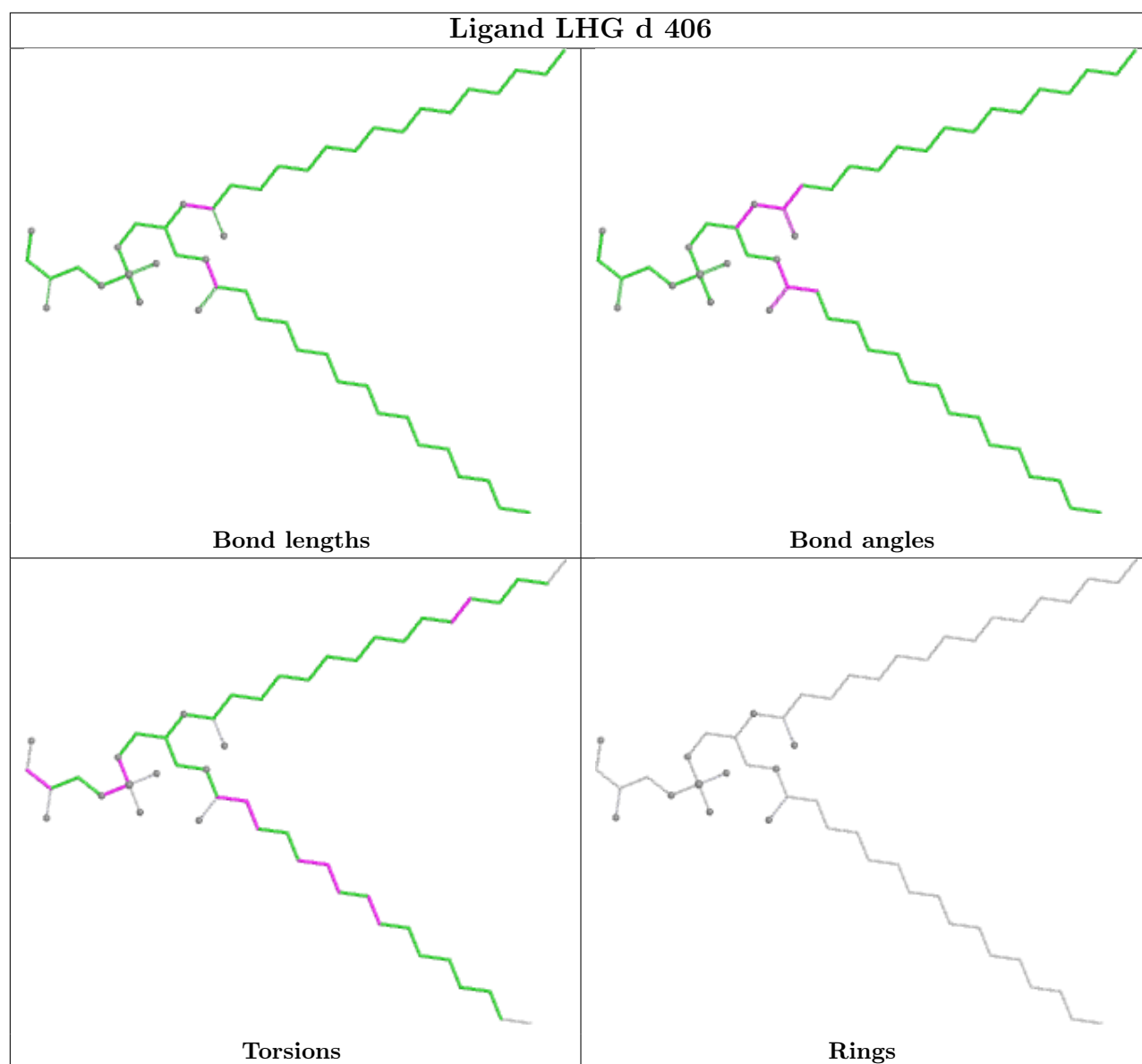
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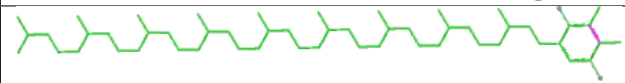
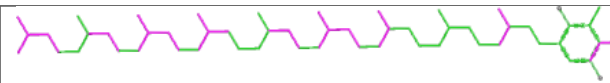
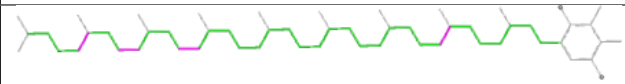
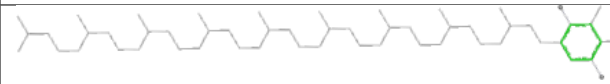


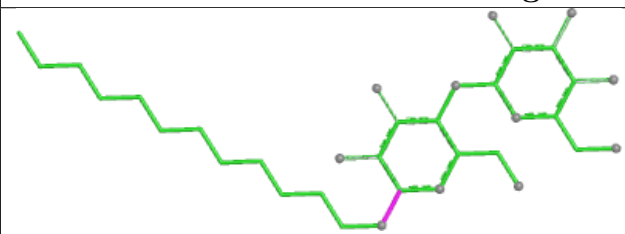
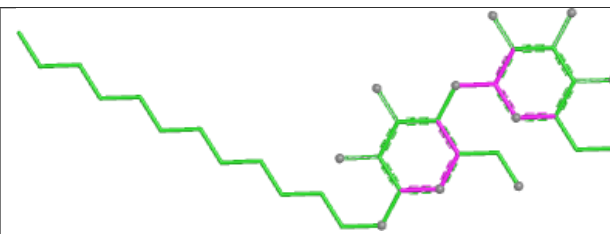
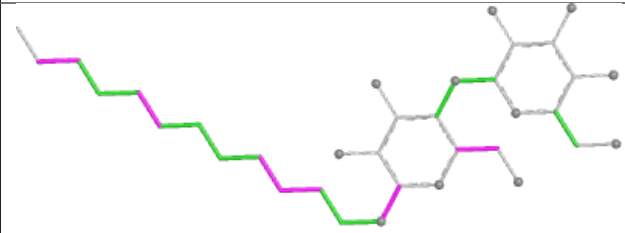
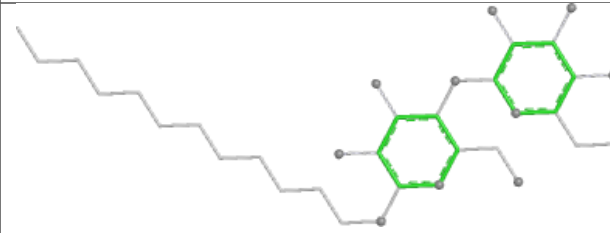


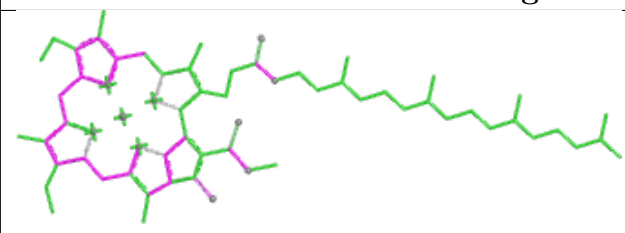
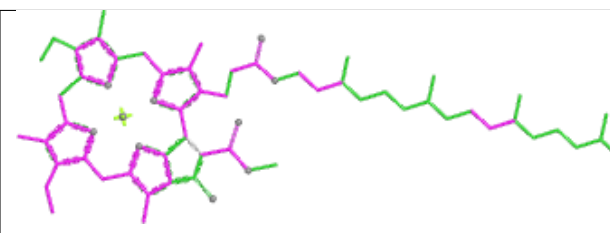
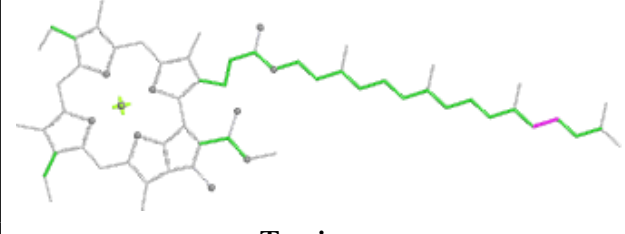
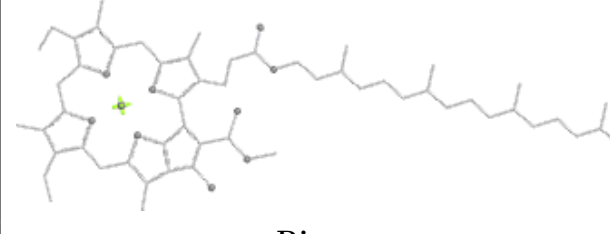


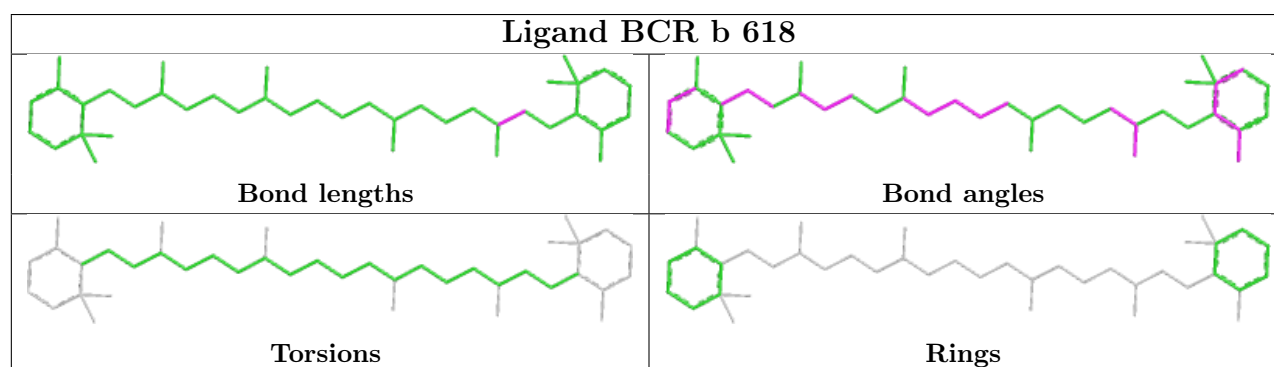
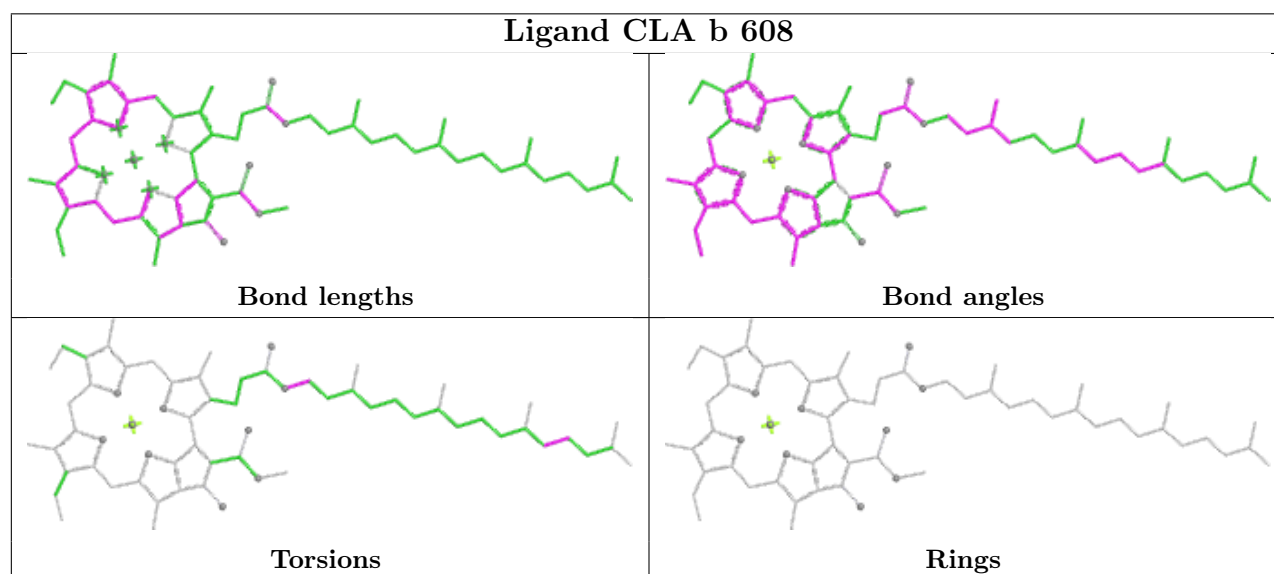
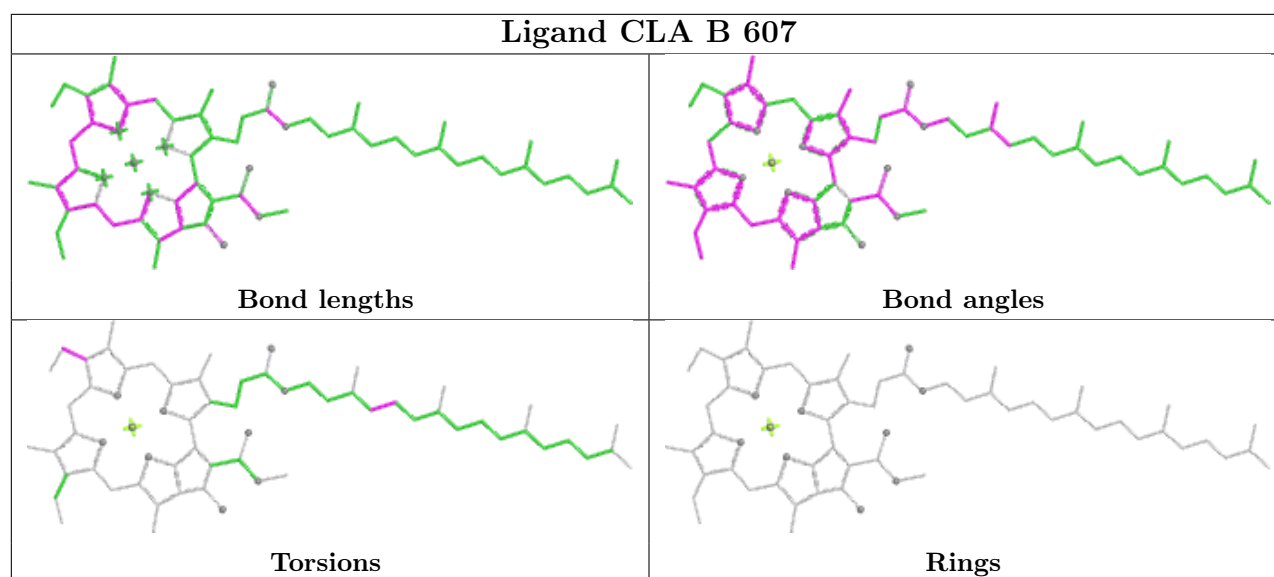


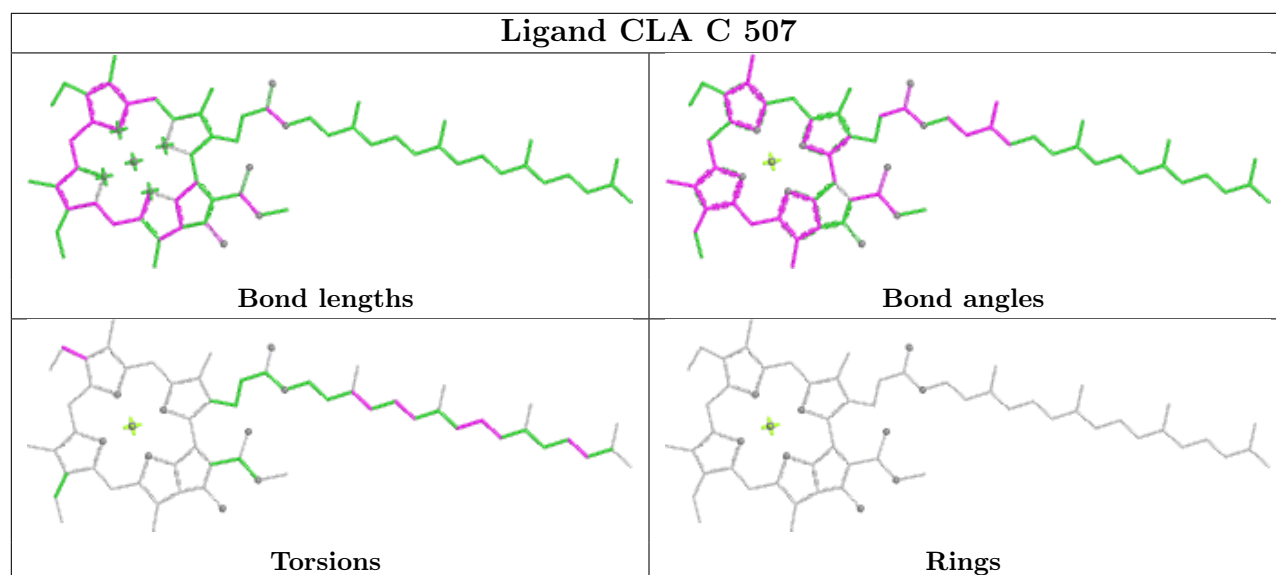
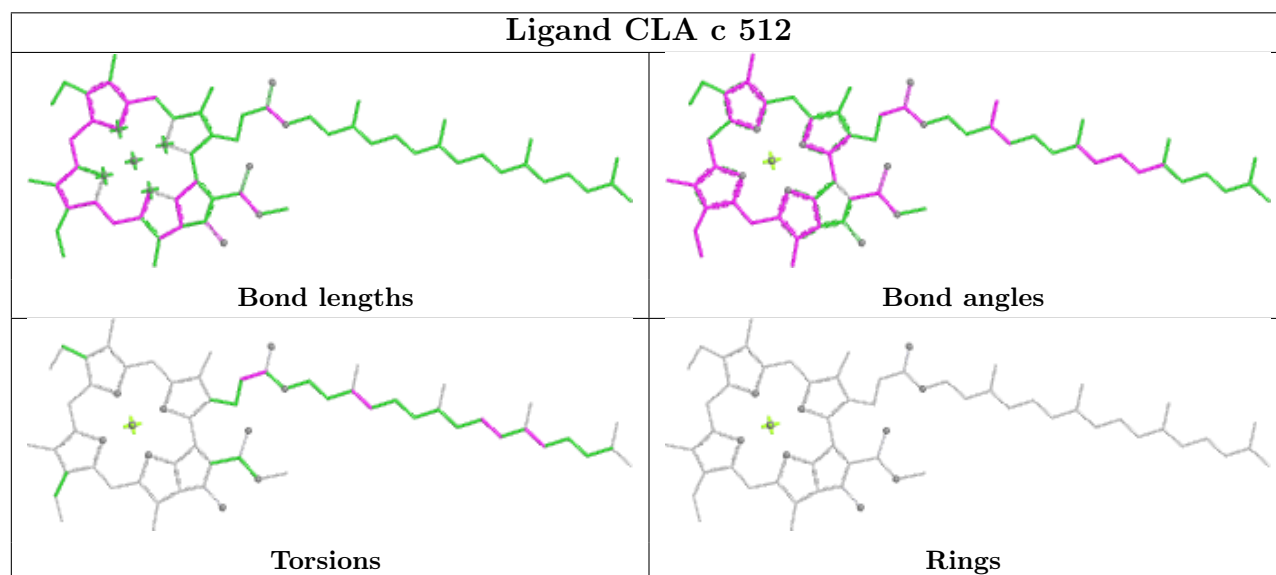
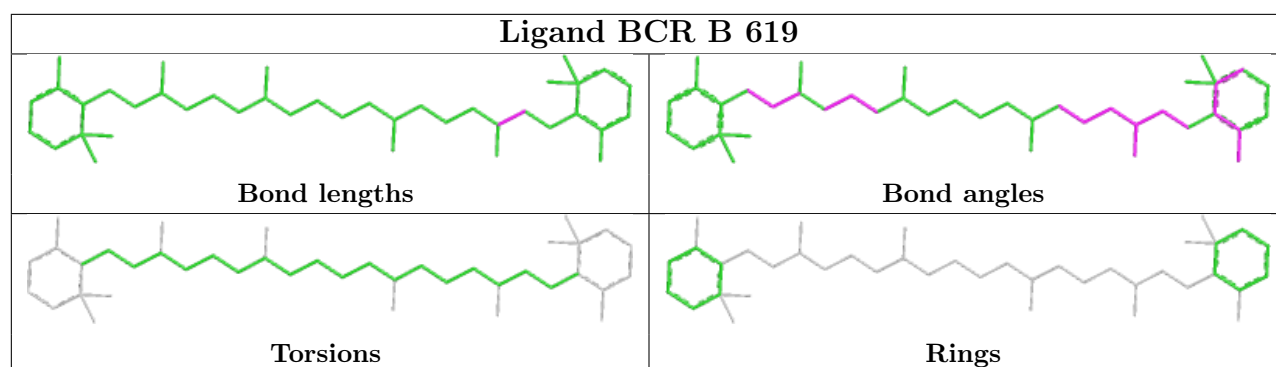


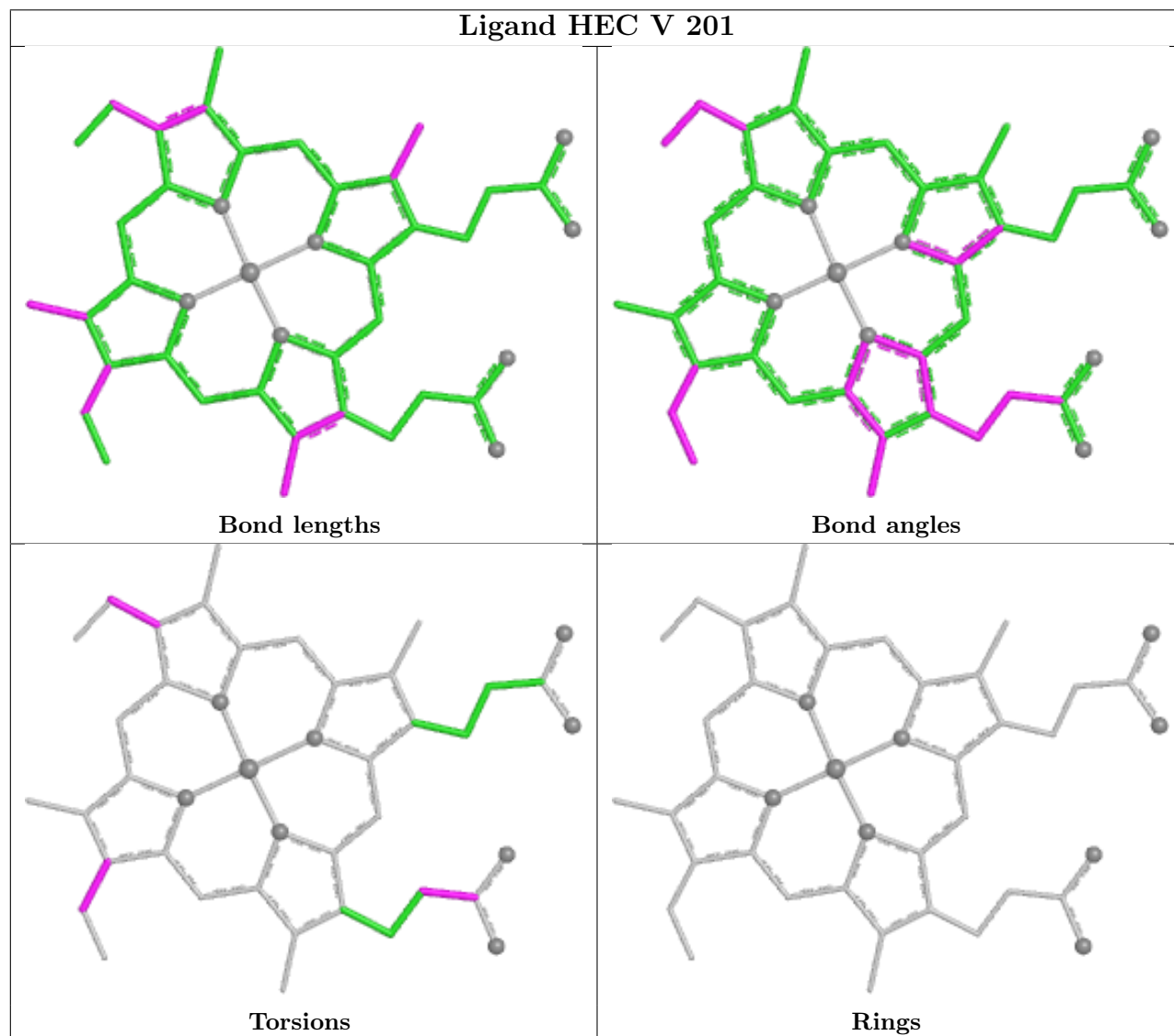
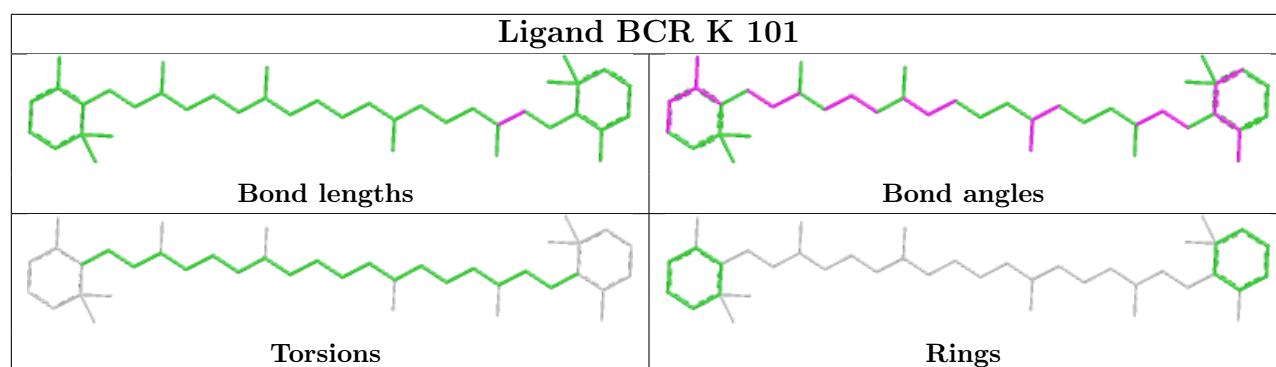
Ligand PL9 d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

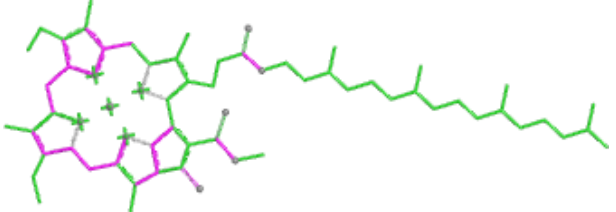
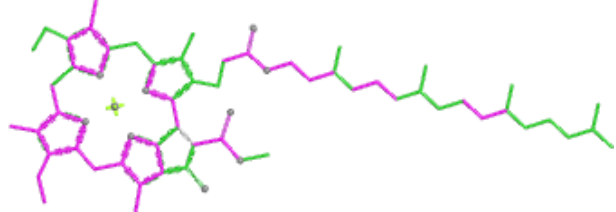
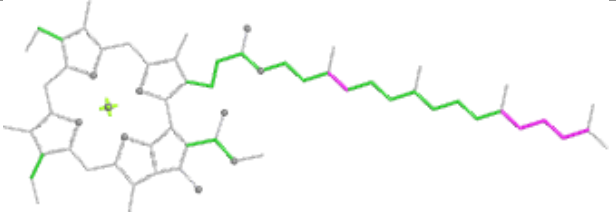
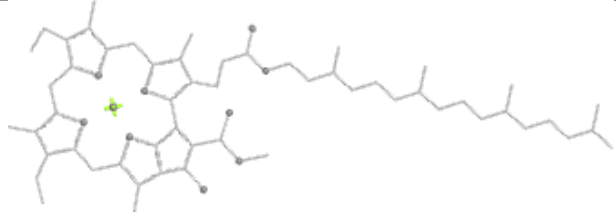
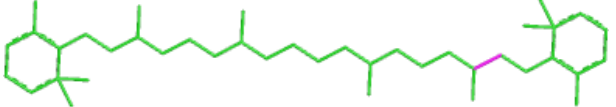
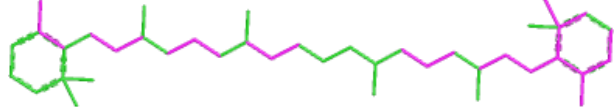
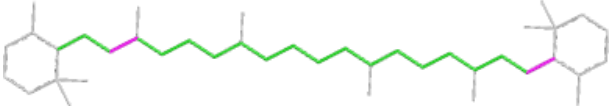
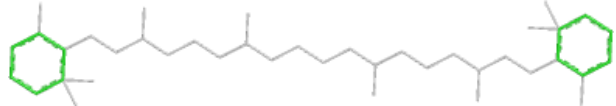
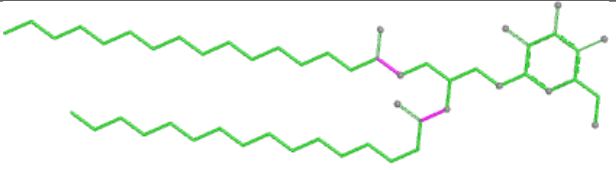
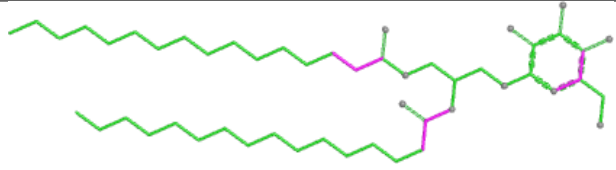
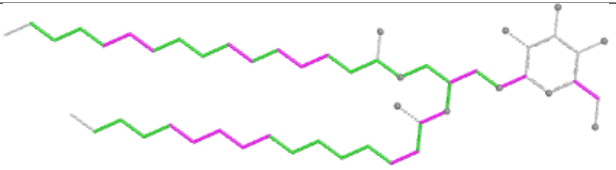
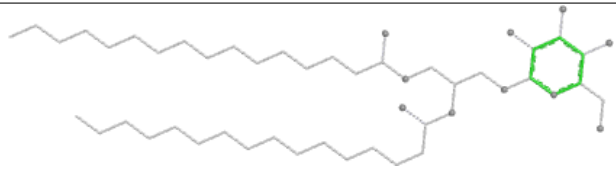
Ligand LMT a 413	
 Bond lengths	 Bond angles
 Torsions	 Rings

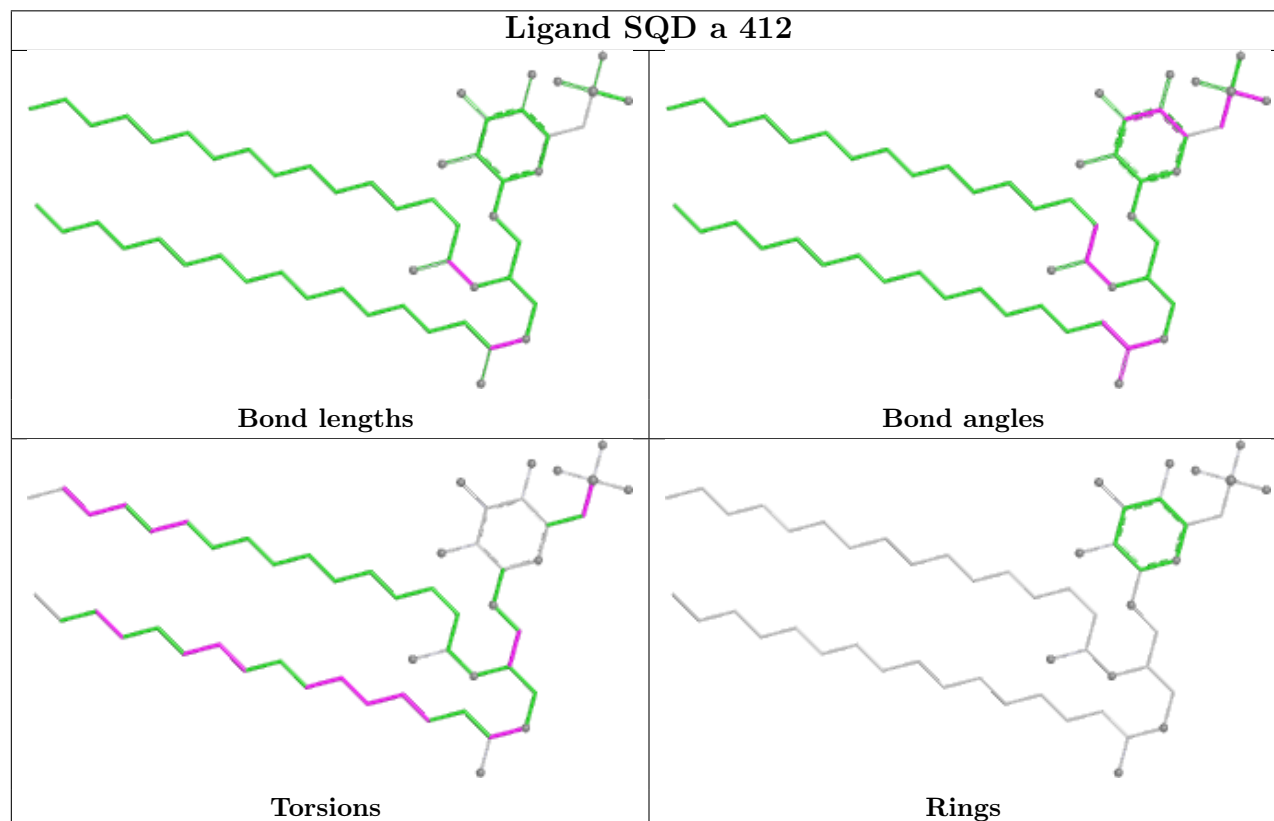
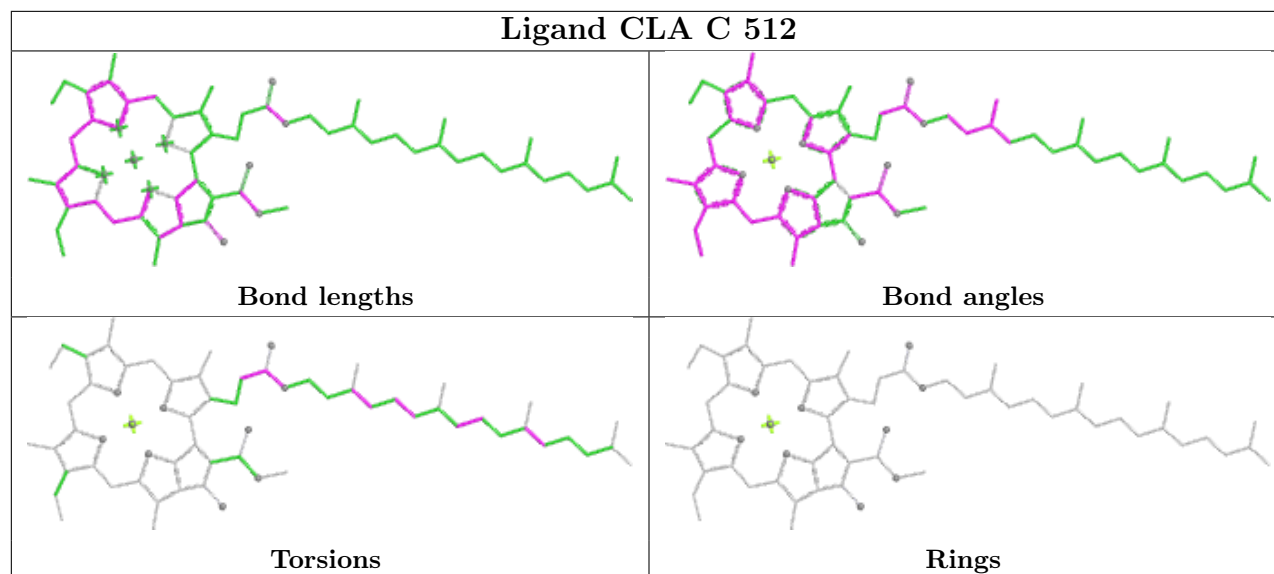
Ligand CLA B 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

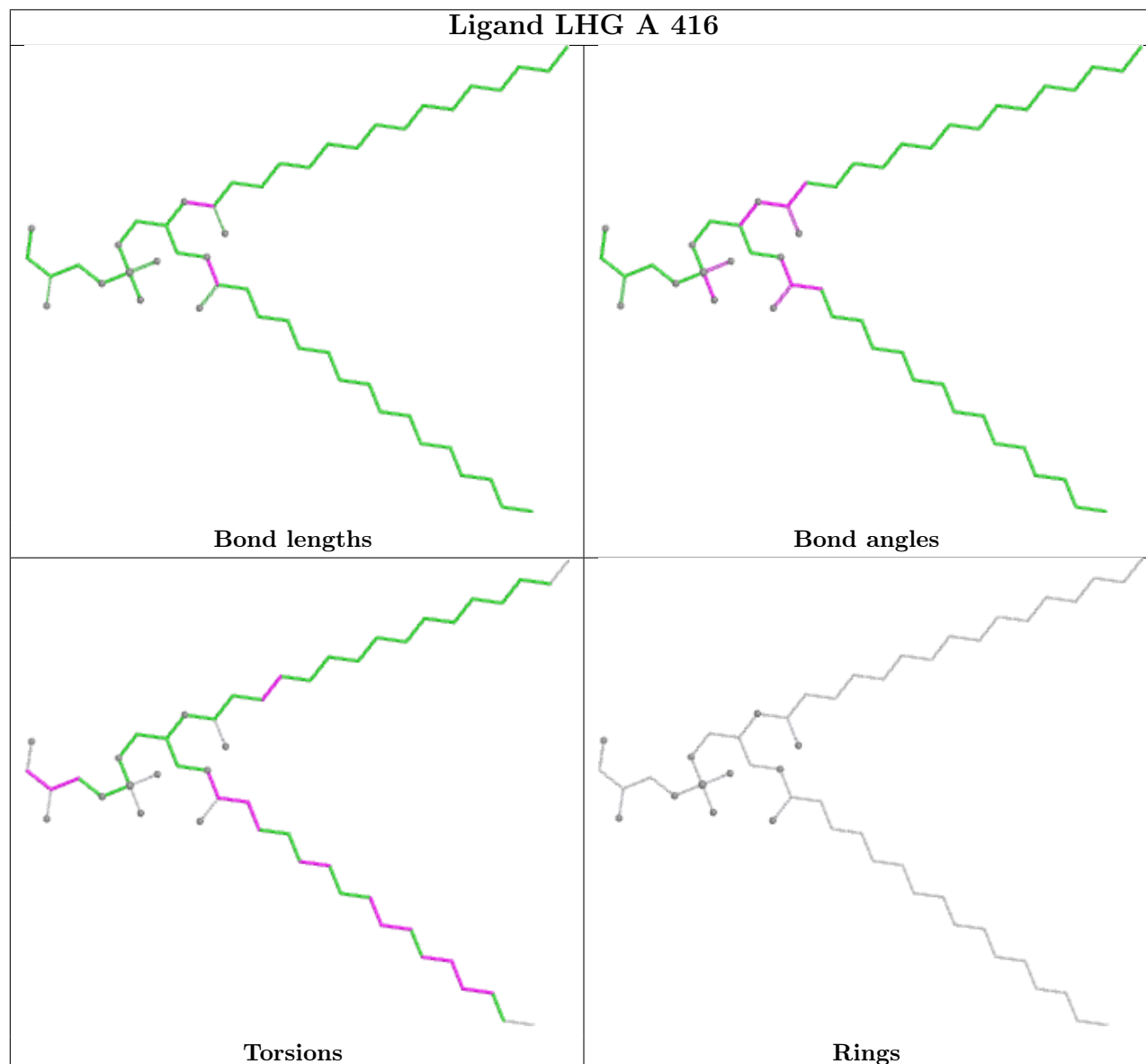
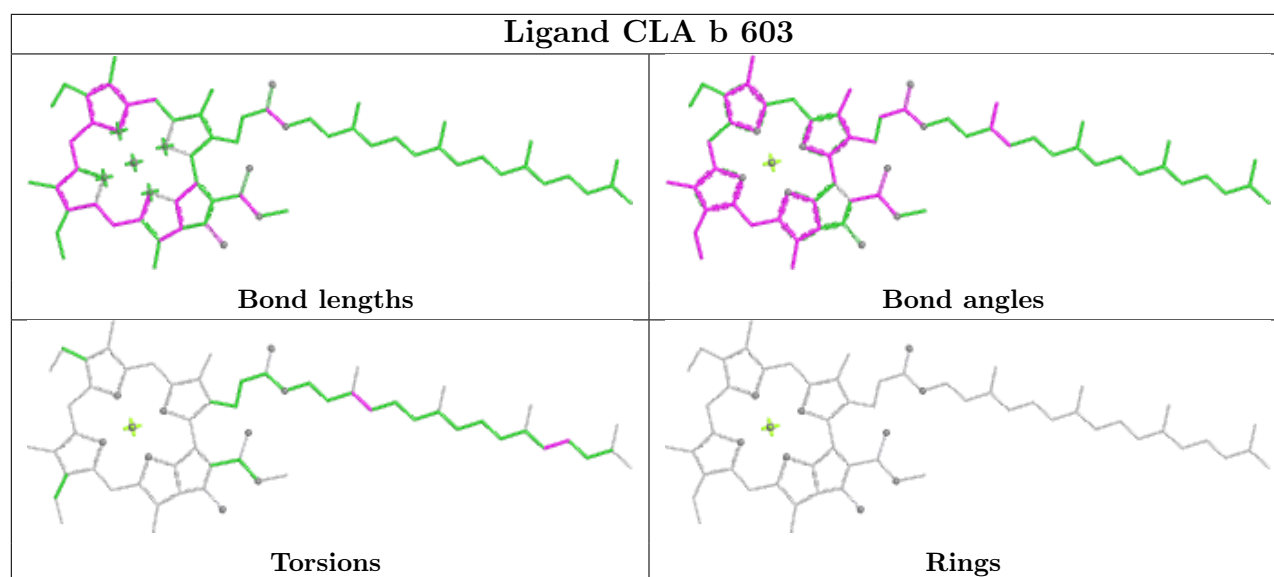


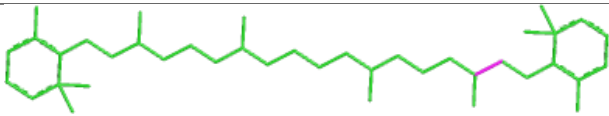
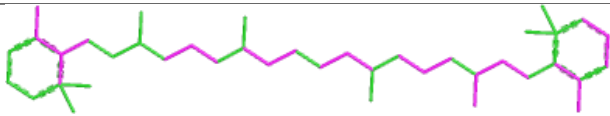
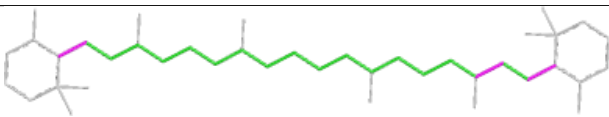
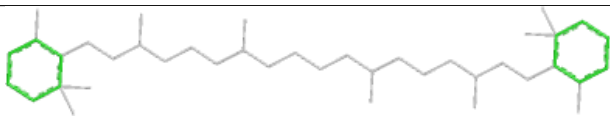


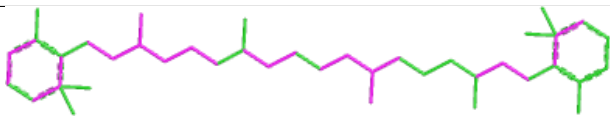
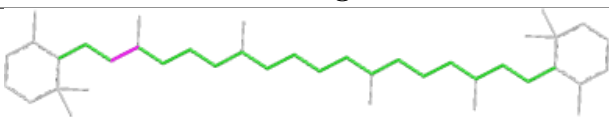
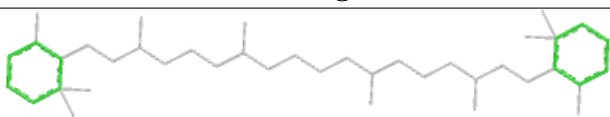


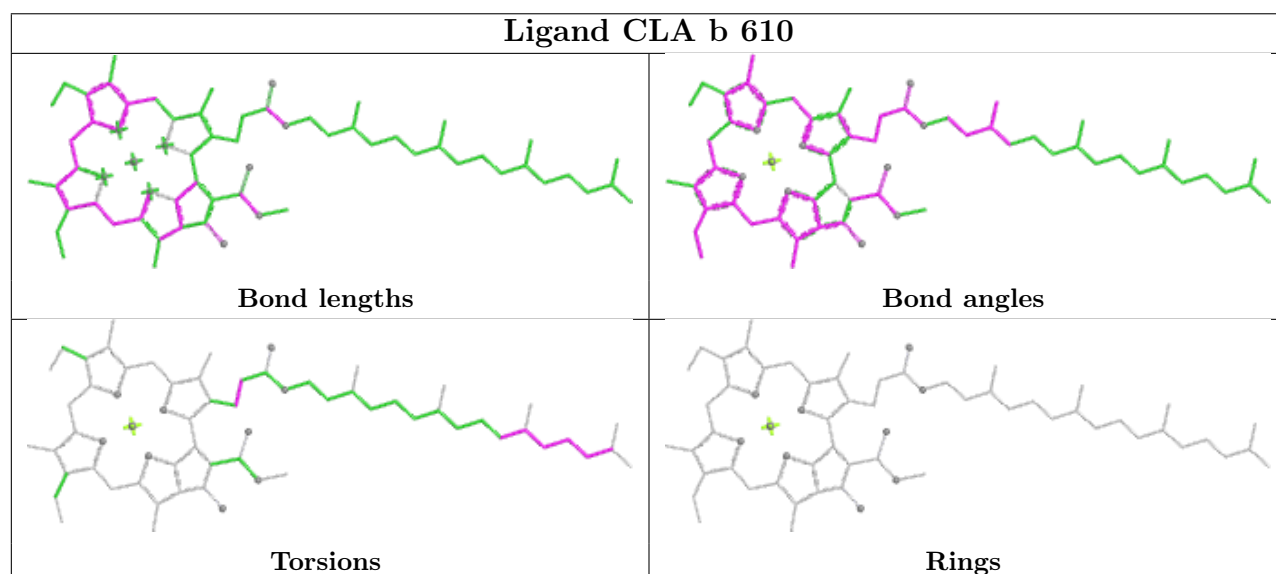
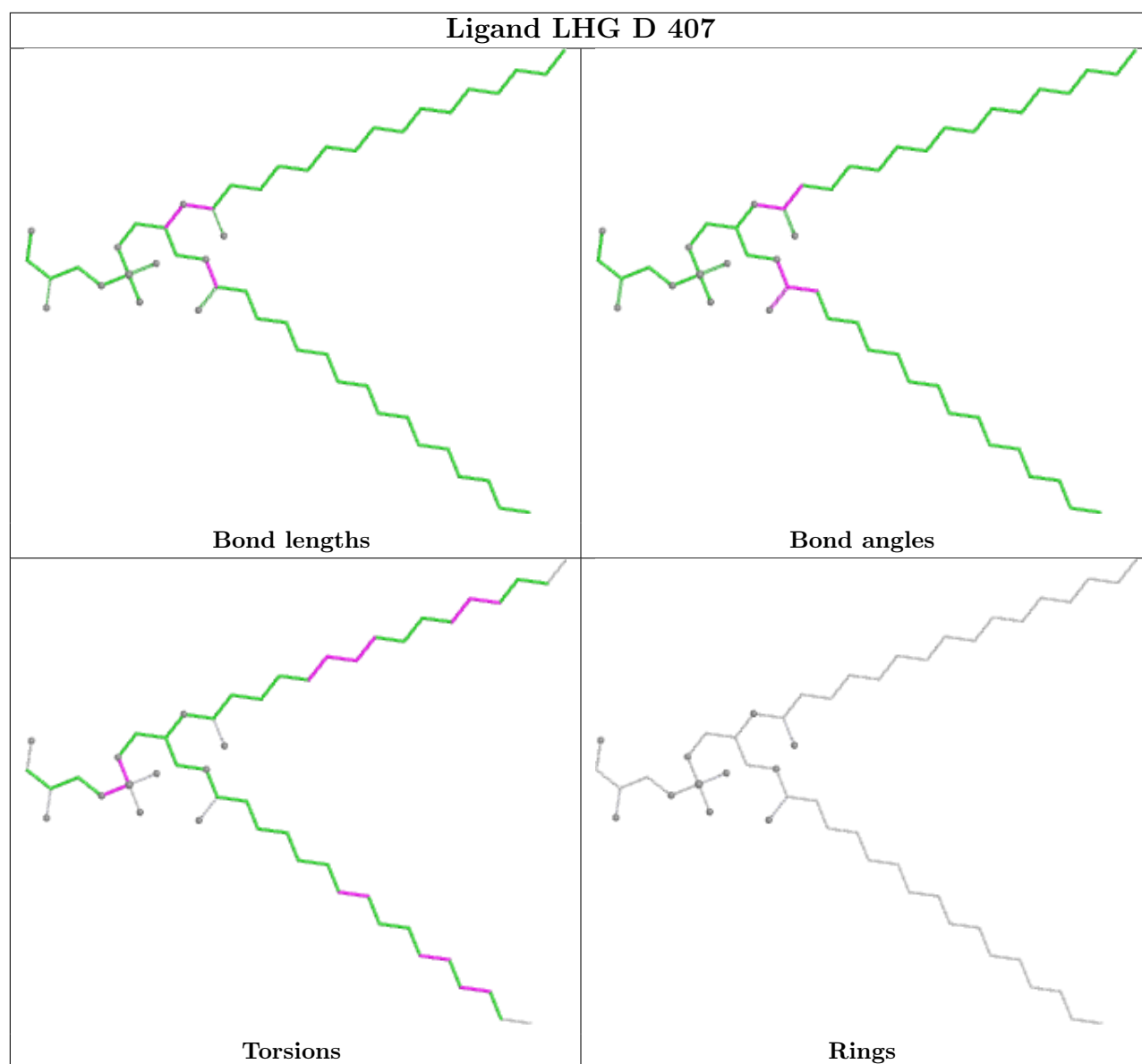
Ligand CLA b 615	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR d 404	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG c 501	
 Bond lengths	 Bond angles
 Torsions	 Rings



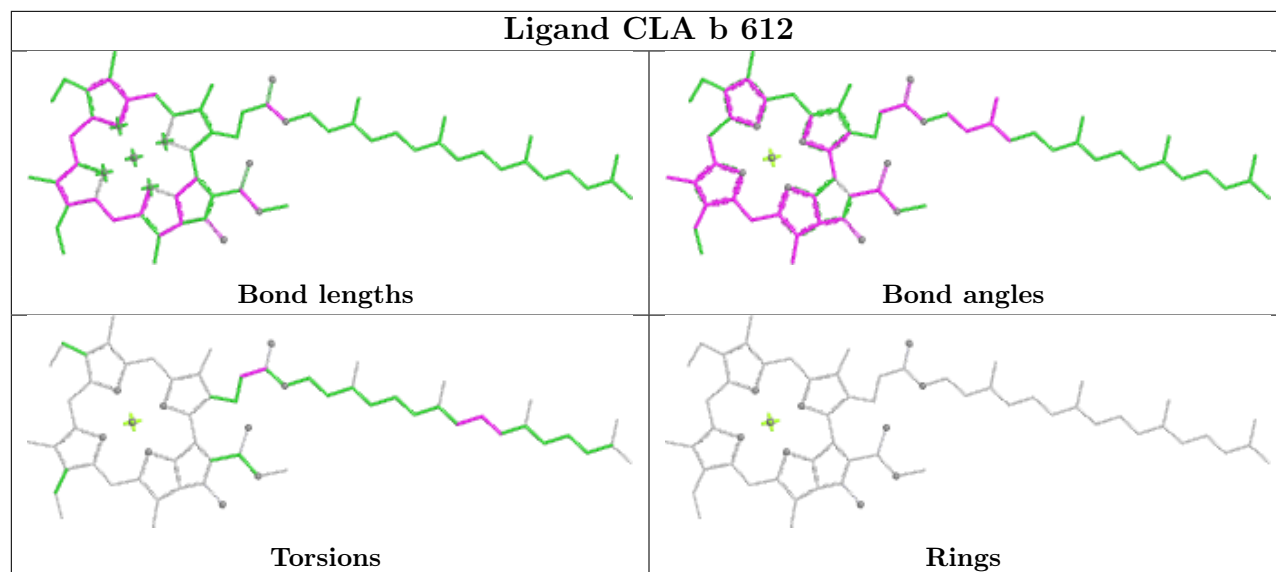


Ligand BCR y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

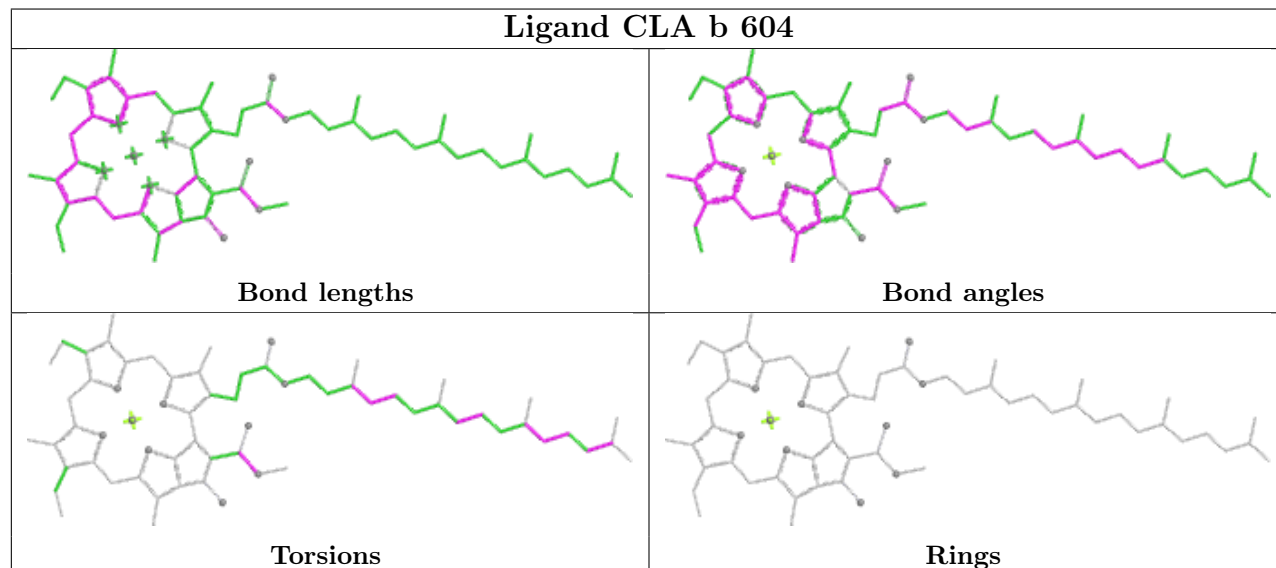
Ligand BCR k 101	
	
Bond lengths	Bond angles
	
Torsions	Rings



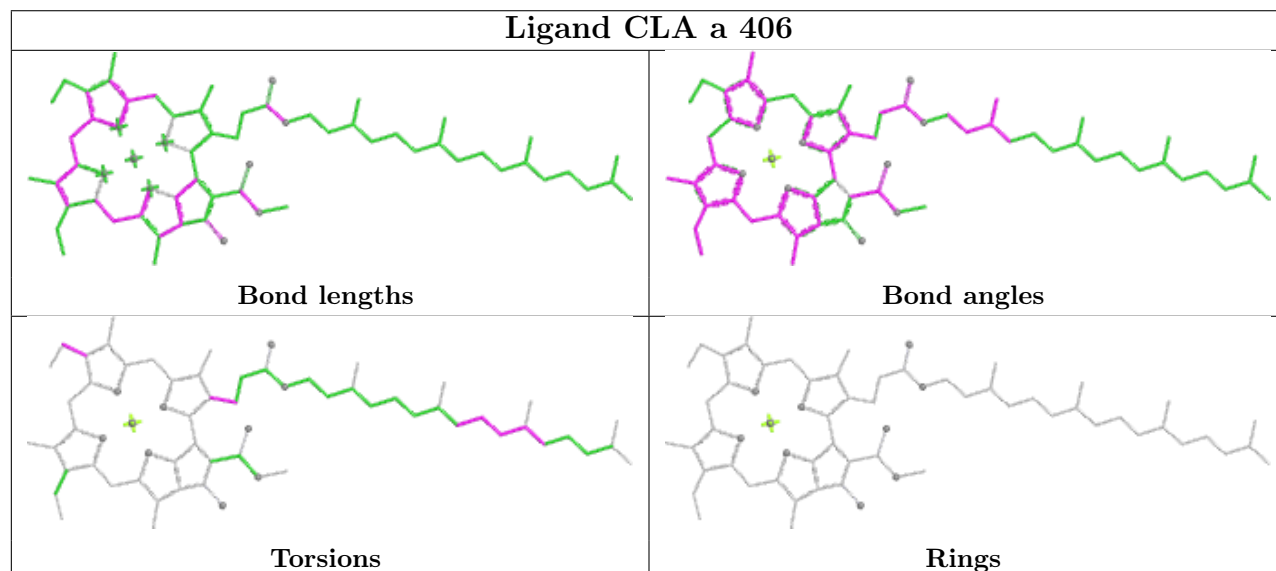
Ligand CLA b 612

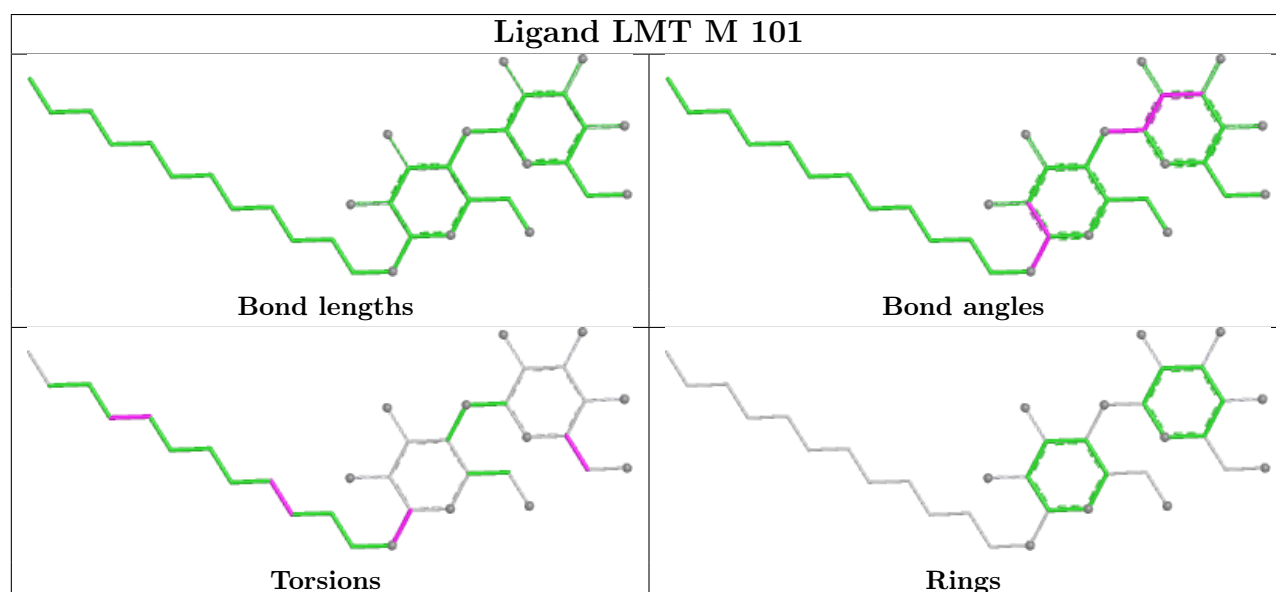
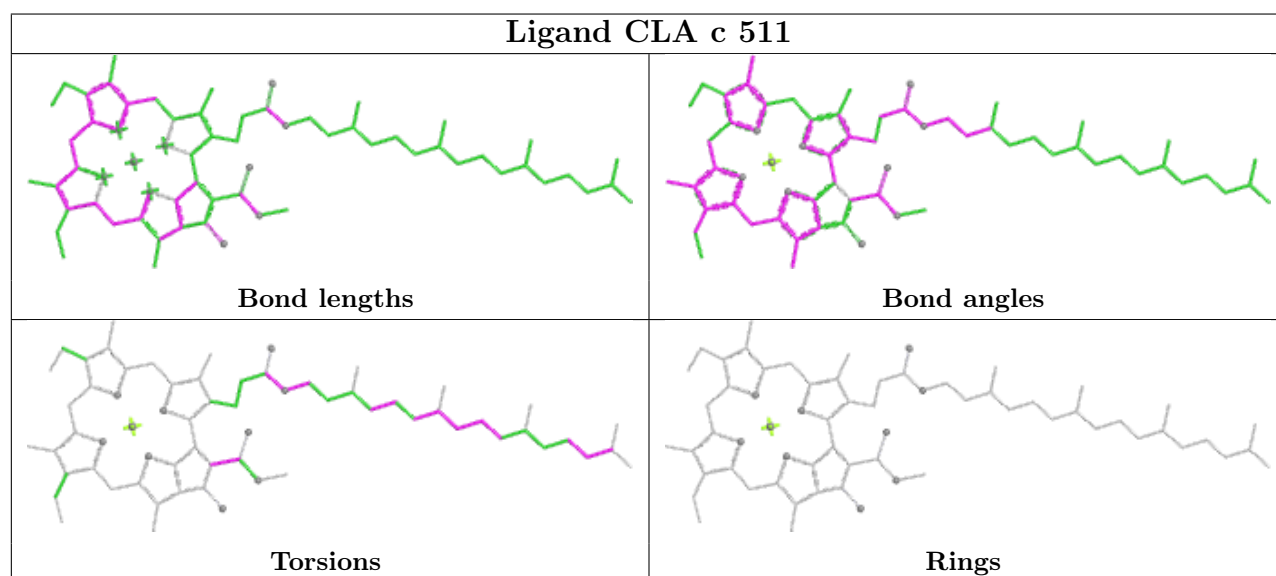
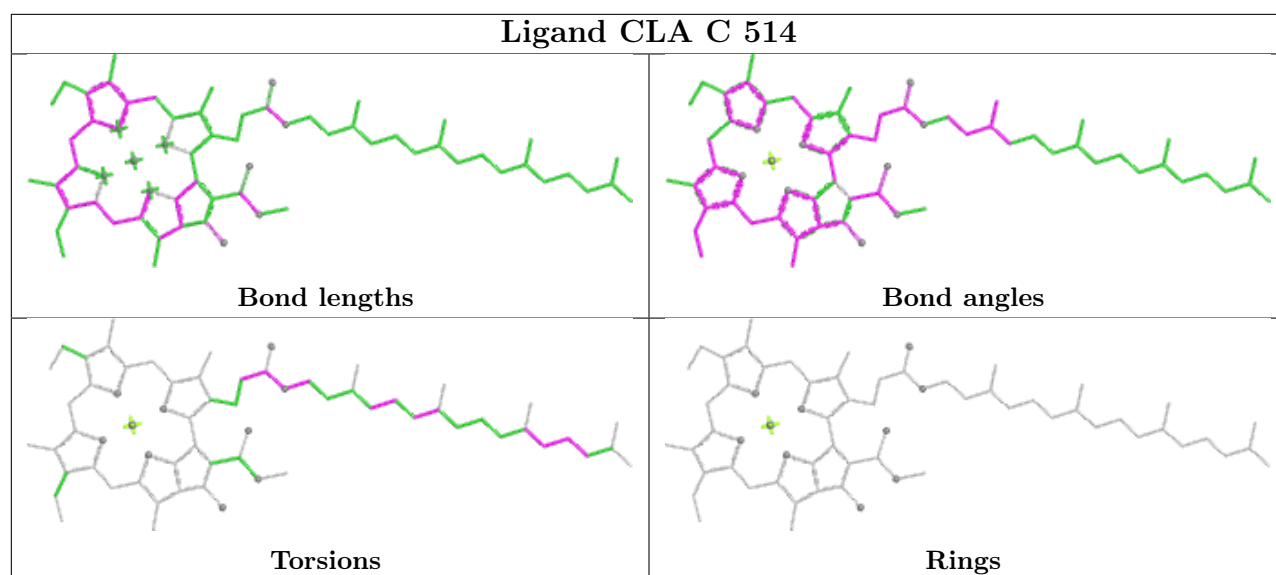


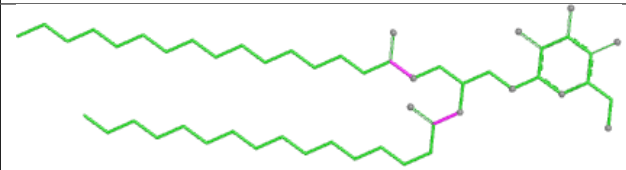
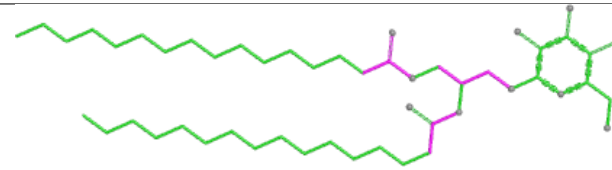
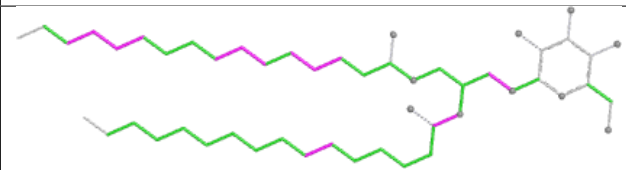
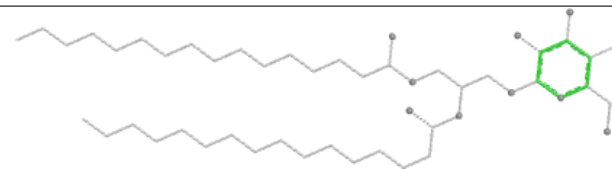
Ligand CLA b 604

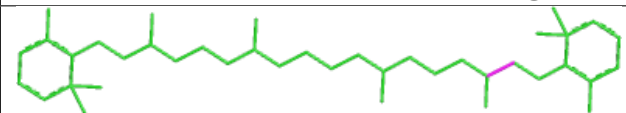
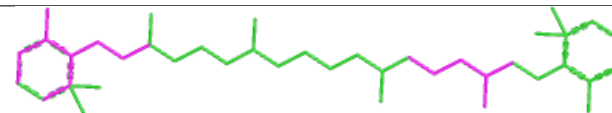
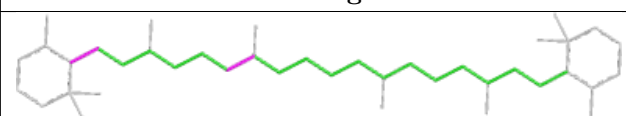
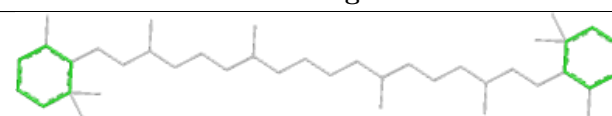


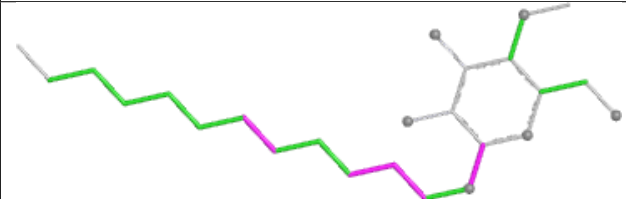
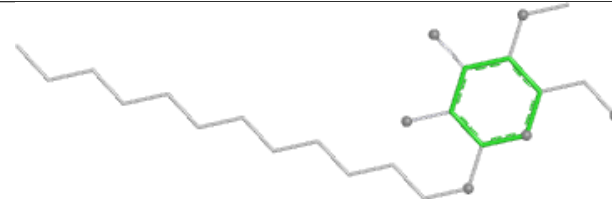
Ligand CLA a 406



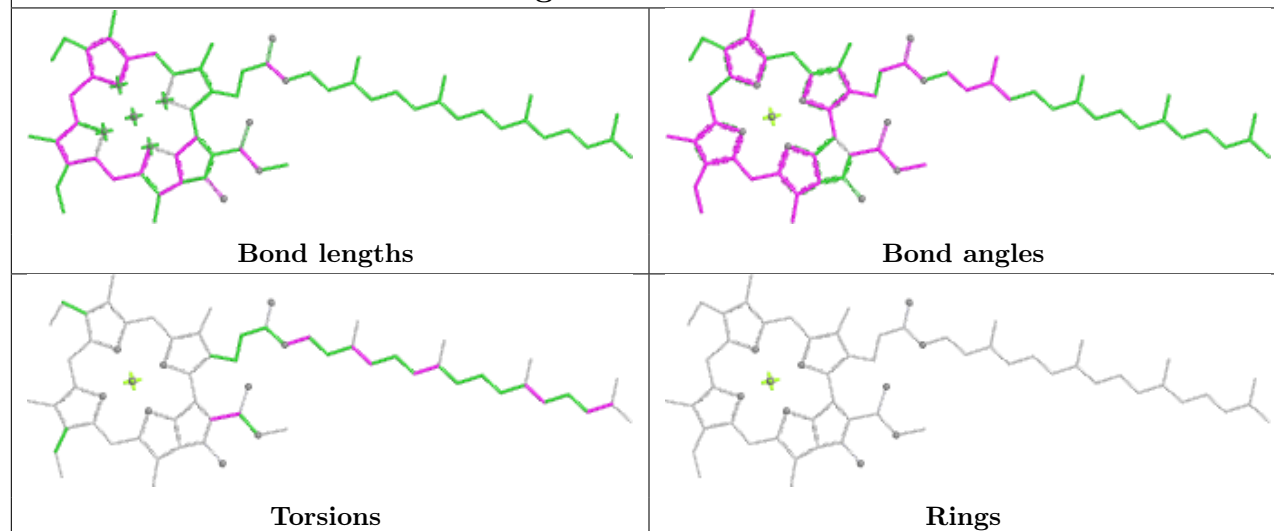


Ligand LMG m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

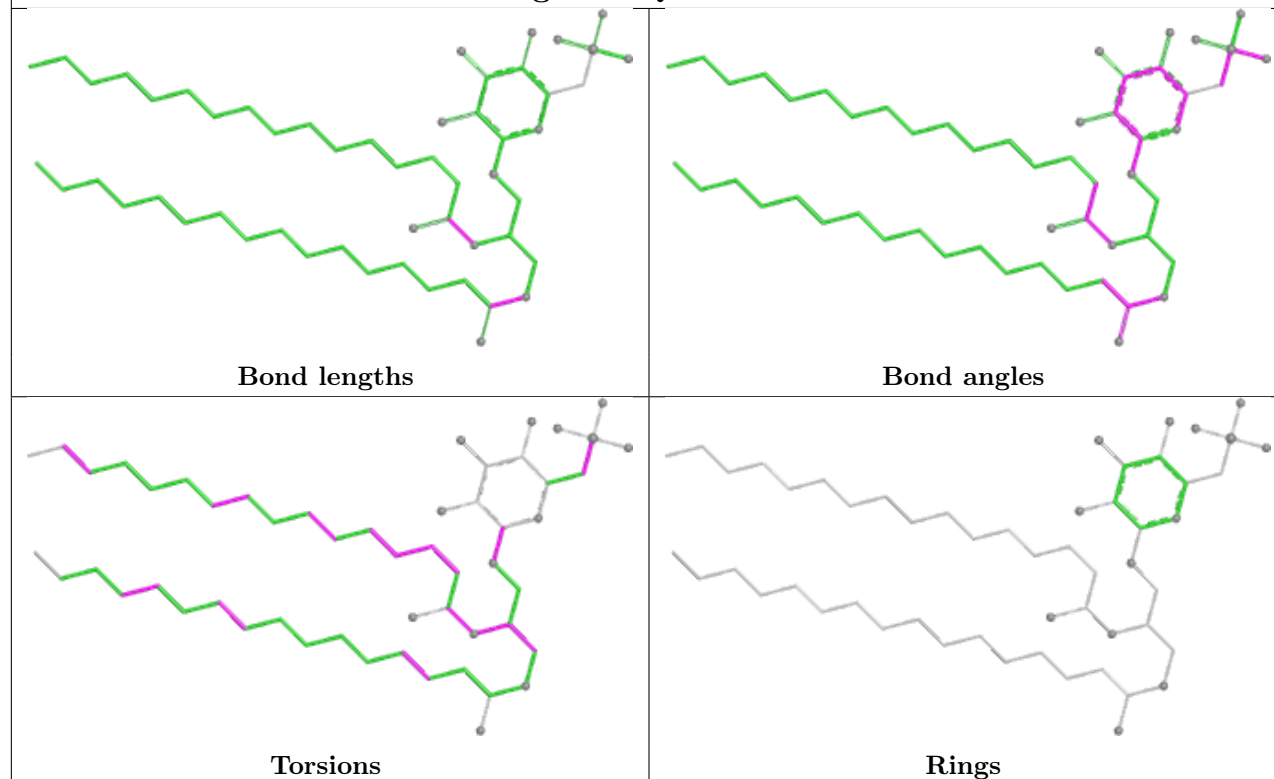
Ligand BCR t 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMT B 630	
	
Bond lengths	Bond angles
	
Torsions	Rings

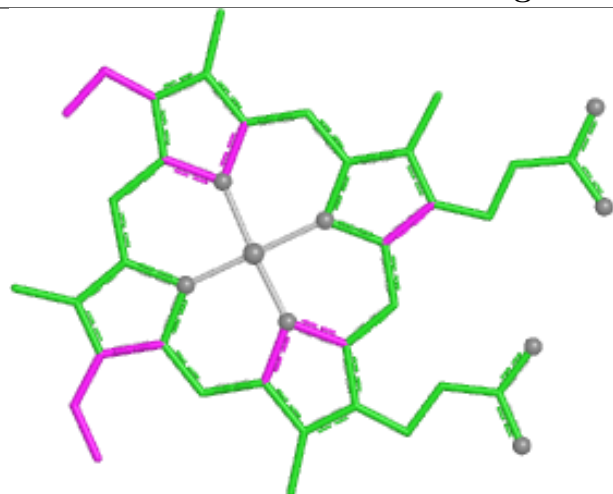
Ligand CLA b 614



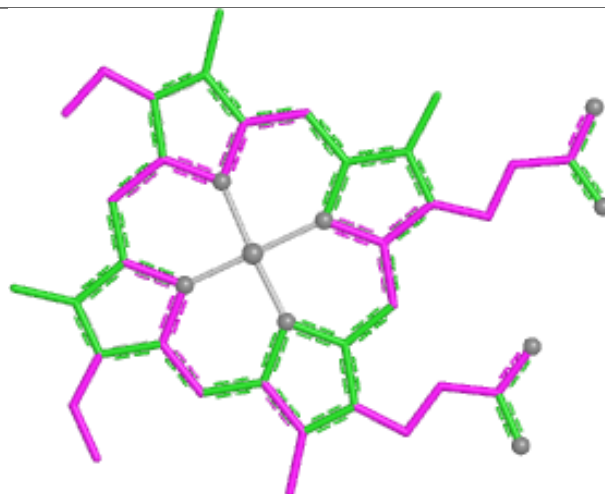
Ligand SQD B 620



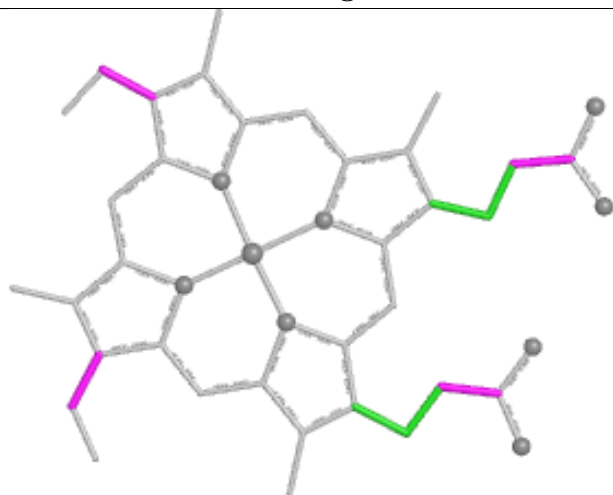
Ligand HEC E 103



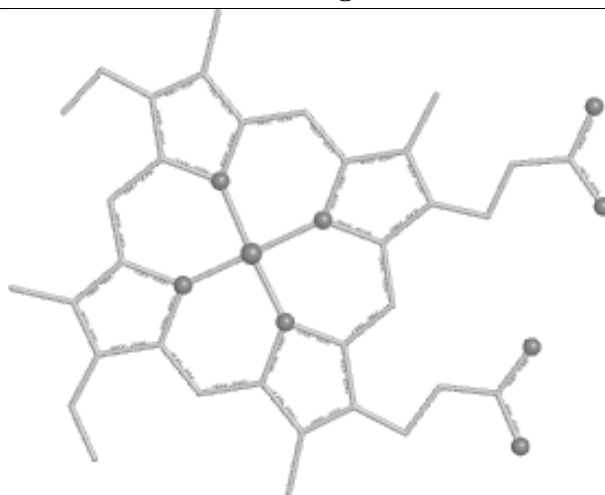
Bond lengths



Bond angles

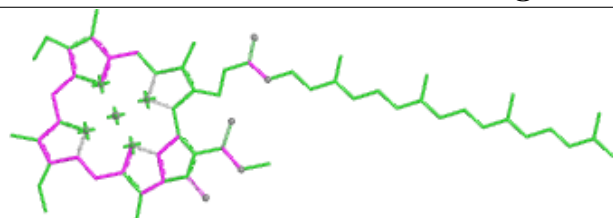


Torsions

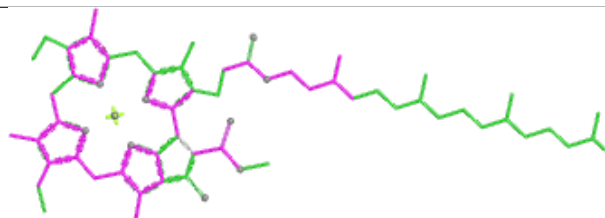


Rings

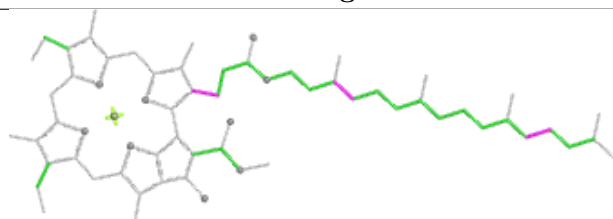
Ligand CLA B 609



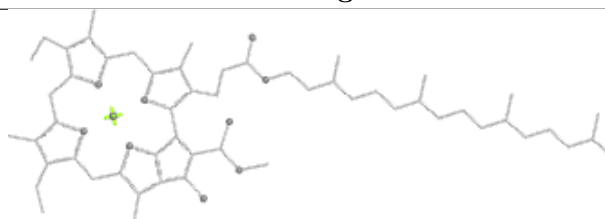
Bond lengths



Bond angles

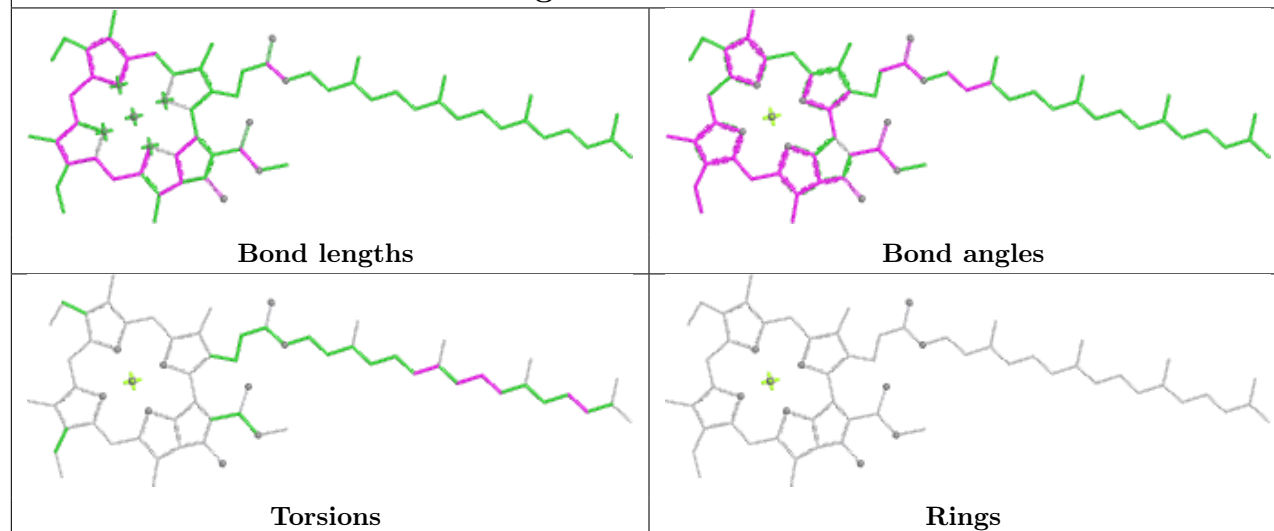


Torsions

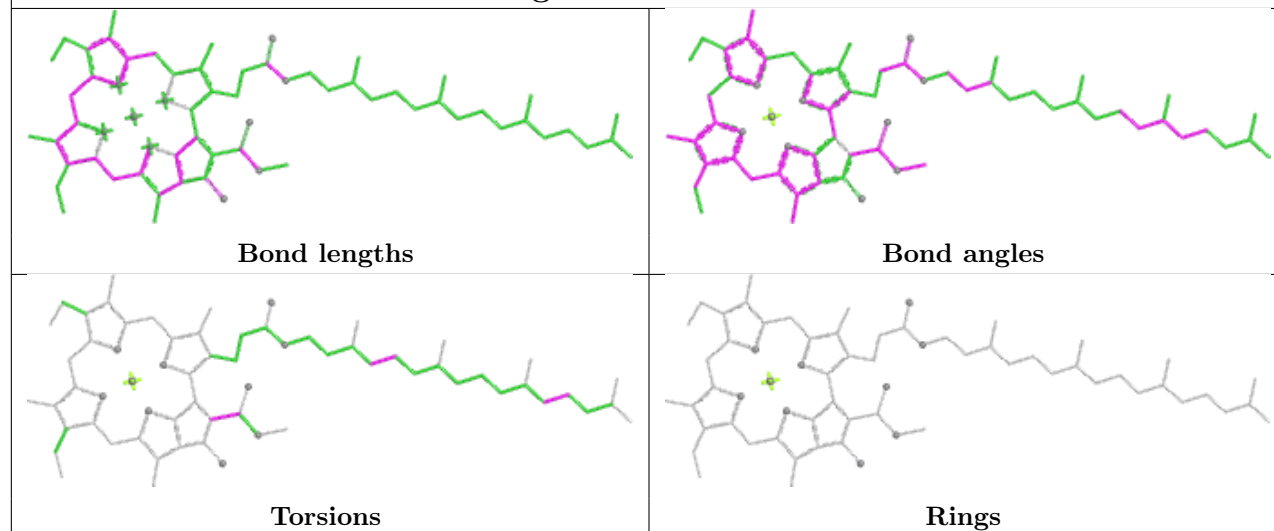


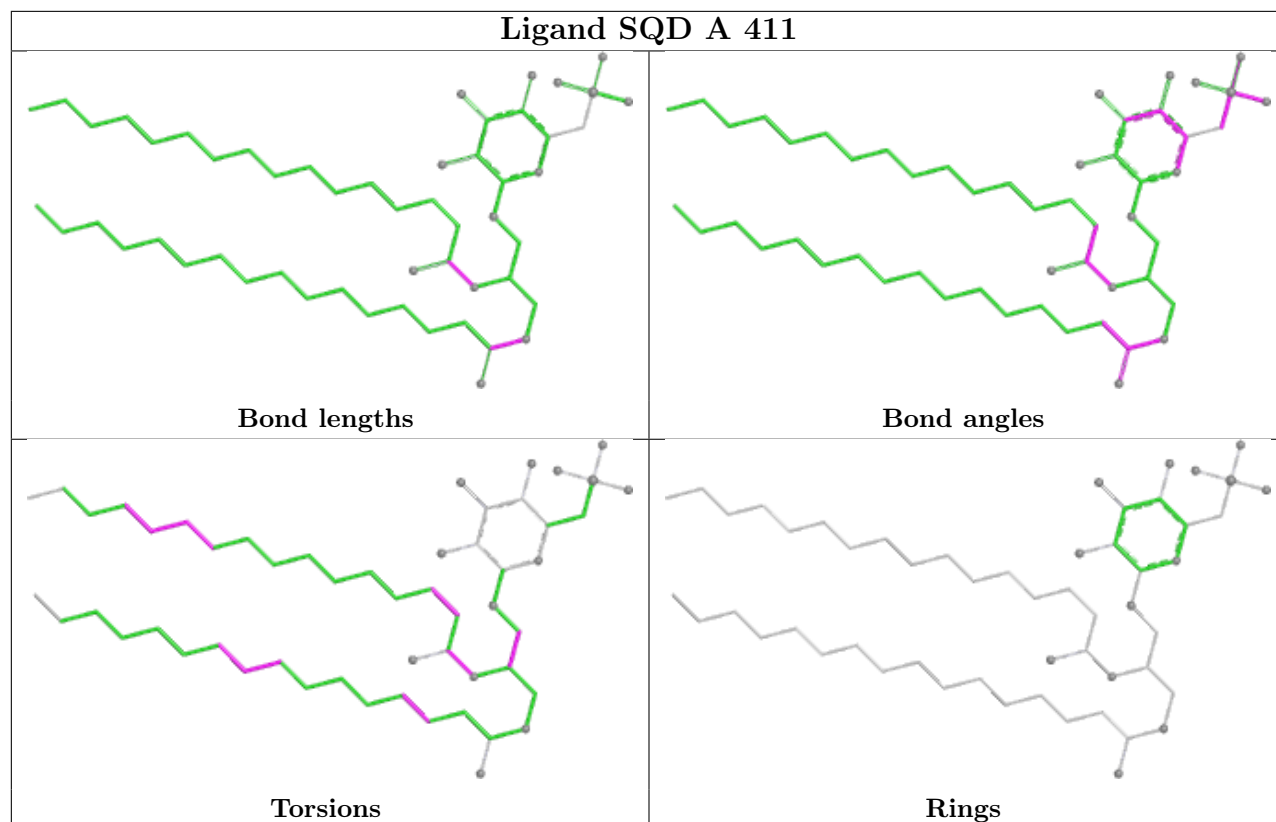
Rings

Ligand CLA b 611



Ligand CLA C 511





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%)	-0.38	0 100 100	22, 41, 67, 126	2 (0%)
1	a	334/344 (97%)	-0.36	3 (0%) 81 82	23, 46, 80, 122	3 (0%)
2	B	504/505 (99%)	-0.31	1 (0%) 91 92	19, 46, 79, 129	10 (1%)
2	b	504/505 (99%)	-0.19	10 (1%) 65 65	22, 50, 92, 164	4 (0%)
3	C	451/455 (99%)	-0.19	2 (0%) 88 89	23, 54, 77, 144	4 (0%)
3	c	455/455 (100%)	-0.18	2 (0%) 88 89	31, 62, 84, 127	2 (0%)
4	D	342/342 (100%)	-0.35	0 100 100	33, 43, 65, 134	0
4	d	341/342 (99%)	-0.39	0 100 100	35, 49, 74, 136	0
5	E	81/84 (96%)	-0.02	1 (1%) 76 77	32, 66, 95, 140	1 (1%)
5	e	79/84 (94%)	-0.02	0 100 100	57, 74, 117, 150	0
6	F	34/44 (77%)	-0.04	1 (2%) 53 54	48, 58, 92, 113	0
6	f	31/44 (70%)	0.04	1 (3%) 50 50	57, 66, 93, 154	0
7	H	64/65 (98%)	0.08	2 (3%) 51 51	29, 58, 77, 105	1 (1%)
7	h	64/65 (98%)	0.08	1 (1%) 70 71	51, 63, 85, 108	0
8	I	37/38 (97%)	0.08	0 100 100	47, 58, 120, 144	0
8	i	37/38 (97%)	-0.11	1 (2%) 56 57	49, 59, 117, 145	0
9	J	38/39 (97%)	-0.01	1 (2%) 57 58	47, 66, 127, 181	0
9	j	39/39 (100%)	0.16	1 (2%) 57 58	55, 74, 135, 179	0
10	K	37/37 (100%)	-0.27	0 100 100	53, 65, 88, 102	0
10	k	37/37 (100%)	-0.16	0 100 100	66, 72, 94, 109	0
11	L	36/37 (97%)	-0.18	1 (2%) 55 55	18, 39, 95, 137	1 (2%)
11	l	36/37 (97%)	-0.19	1 (2%) 55 55	19, 40, 96, 132	1 (2%)
12	M	32/36 (88%)	-0.33	0 100 100	19, 42, 66, 135	1 (3%)
12	m	33/36 (91%)	-0.42	0 100 100	36, 43, 78, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.22	0 100 100	23, 57, 110, 186	3 (1%)
13	o	243/244 (99%)	-0.12	1 (0%) 88 89	24, 59, 124, 166	2 (0%)
14	T	29/32 (90%)	-0.31	1 (3%) 48 48	36, 40, 78, 109	0
14	t	29/32 (90%)	-0.30	1 (3%) 48 48	36, 43, 70, 137	0
15	U	96/104 (92%)	-0.37	0 100 100	41, 53, 85, 90	0
15	u	97/104 (93%)	-0.30	0 100 100	46, 58, 80, 132	0
16	V	137/137 (100%)	-0.39	0 100 100	40, 53, 79, 115	0
16	v	137/137 (100%)	-0.28	0 100 100	47, 68, 96, 138	0
17	X	38/40 (95%)	0.03	0 100 100	56, 68, 93, 110	0
17	x	38/40 (95%)	0.09	0 100 100	60, 74, 114, 163	0
18	Y	29/30 (96%)	0.31	2 (6%) 23 21	66, 82, 139, 159	0
18	y	29/30 (96%)	0.23	0 100 100	77, 89, 119, 120	0
19	Z	62/62 (100%)	0.06	0 100 100	66, 80, 132, 180	0
19	z	62/62 (100%)	0.39	1 (1%) 70 71	77, 94, 135, 178	0
20	R	34/34 (100%)	1.88	16 (47%) 0 0	102, 124, 154, 164	0
All	All	5283/5384 (98%)	-0.21	51 (0%) 79 81	18, 54, 98, 186	35 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	5.3
14	t	30	THR	4.4
7	h	65	LEU	4.1
6	f	15	ILE	3.7
3	C	23	ALA	3.5
20	R	3	TRP	3.4
20	R	24	LEU	3.3
20	R	7	VAL	3.1
20	R	12	VAL	3.1
20	R	10	LEU	3.1
20	R	28	VAL	3.0
20	R	35	LEU	2.9
1	a	11	ALA	2.9
20	R	6	LEU	2.9
14	T	30	THR	2.9
1	a	264	SER	2.8
20	R	34	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
8	i	37	LEU	2.8
2	b	499	VAL	2.8
2	b	486	LEU	2.7
2	b	491	VAL	2.6
9	J	2	SER	2.6
2	b	495	PHE	2.6
2	b	502	VAL	2.6
11	L	10	VAL	2.6
20	R	13	LEU	2.6
20	R	14	LEU	2.6
5	E	4	THR	2.5
20	R	5	VAL	2.5
3	c	134	ILE	2.4
19	z	30	PRO	2.4
20	R	8	VAL	2.4
20	R	18	TRP	2.3
7	H	64	ALA	2.3
18	Y	18	VAL	2.3
11	l	3	PRO	2.2
9	j	5	GLY	2.2
20	R	15	ALA	2.2
18	Y	19	ILE	2.2
20	R	31	VAL	2.2
3	C	24	THR	2.2
2	b	490	GLN	2.1
2	b	500	GLY	2.1
2	b	505	ARG	2.1
1	a	263	ALA	2.1
2	B	479	PHE	2.1
2	b	493	TRP	2.1
13	o	22	LEU	2.1
3	c	143	TYR	2.1
6	F	12	SER	2.0
2	b	488	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	FME	I	1	10/11	0.95	0.08	44,65,72,73	0
14	FME	T	1	10/11	0.96	0.07	40,46,63,64	0
14	FME	t	1	10/11	0.96	0.07	36,43,68,73	0
8	FME	i	1	10/11	0.97	0.06	49,58,67,73	0
12	FME	m	1	10/11	0.97	0.06	41,53,62,76	0
12	FME	M	1	10/11	0.97	0.09	37,50,80,87	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	LMT	E	102	35/35	0.61	0.20	102,145,164,166	0
34	LMT	e	101	35/35	0.64	0.18	122,163,170,171	0
34	LMT	a	413	35/35	0.65	0.21	66,131,140,142	0
34	LMT	C	526	35/35	0.65	0.16	88,140,155,158	0
30	UNL	A	414	28/-	0.67	0.20	83,97,113,115	0
30	UNL	j	101	10/-	0.69	0.27	78,87,93,94	0
33	HTG	b	623	19/19	0.72	0.15	83,144,150,150	0
33	HTG	D	411	16/19	0.72	0.15	91,113,123,129	0
34	LMT	D	402	35/35	0.72	0.21	69,124,137,143	0
30	UNL	J	101	10/-	0.76	0.27	75,79,91,92	0
33	HTG	B	623	19/19	0.78	0.18	61,86,94,95	0
30	UNL	m	102	10/-	0.78	0.21	59,68,91,92	0
31	LHG	a	419	42/49	0.79	0.16	100,147,177,181	0
30	UNL	i	101	40/-	0.79	0.19	69,98,148,152	0
27	SQD	f	101	43/54	0.79	0.16	111,132,160,166	0
30	UNL	a	416	30/-	0.79	0.16	96,111,134,138	0
34	LMT	a	418	35/35	0.79	0.14	118,150,157,158	0
33	HTG	c	523	19/19	0.79	0.14	119,138,143,144	0
30	UNL	C	527	34/-	0.81	0.17	83,110,123,126	0
32	LMG	C	522	51/55	0.81	0.17	69,127,161,165	0
30	UNL	c	526	32/-	0.82	0.17	94,113,130,132	0
30	UNL	I	101	40/-	0.82	0.20	68,107,149,150	0
33	HTG	C	523	19/19	0.82	0.14	106,118,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	GOL	O	302	6/6	0.82	0.10	78,85,86,87	0
26	GOL	B	627	6/6	0.82	0.20	63,92,96,97	0
30	UNL	b	626	33/-	0.82	0.16	63,90,146,148	0
34	LMT	m	103	35/35	0.82	0.14	52,93,109,110	0
30	UNL	M	102	10/-	0.83	0.20	63,73,84,84	0
33	HTG	h	101	16/19	0.83	0.12	103,133,139,143	0
34	LMT	B	628	35/35	0.83	0.13	63,110,126,130	0
34	LMT	M	103	35/35	0.83	0.15	78,152,175,176	0
32	LMG	Z	101	37/55	0.84	0.16	72,123,156,161	0
34	LMT	b	621	25/35	0.84	0.16	89,129,154,154	0
26	GOL	c	502	6/6	0.84	0.18	61,75,77,81	0
33	HTG	V	202	11/19	0.84	0.13	110,119,121,121	0
31	LHG	E	101	42/49	0.85	0.16	72,126,138,141	0
32	LMG	c	522	51/55	0.85	0.15	72,129,152,157	0
33	HTG	b	622	19/19	0.85	0.16	64,71,105,109	0
26	GOL	b	624	6/6	0.85	0.21	86,95,99,105	0
26	GOL	v	201	6/6	0.85	0.20	51,70,78,80	0
34	LMT	M	101	35/35	0.85	0.12	53,98,131,139	0
36	CA	F	101	1/1	0.85	0.12	115,115,115,115	0
27	SQD	A	411	54/54	0.86	0.13	60,82,123,130	0
30	UNL	d	410	36/-	0.86	0.17	70,94,127,130	0
34	LMT	b	627	25/35	0.86	0.15	50,75,135,136	0
30	UNL	B	626	33/-	0.86	0.15	52,108,152,156	0
26	GOL	B	629	6/6	0.86	0.20	103,111,114,116	0
29	PL9	a	415	55/55	0.86	0.23	87,111,124,126	0
32	LMG	z	101	39/55	0.87	0.15	80,128,136,139	0
30	UNL	D	410	40/-	0.87	0.17	56,85,125,129	0
27	SQD	a	412	54/54	0.87	0.12	59,85,125,127	0
26	GOL	A	410	6/6	0.87	0.14	68,68,74,81	0
27	SQD	D	412	43/54	0.87	0.15	74,111,131,138	0
34	LMT	B	630	25/35	0.87	0.14	55,84,135,139	0
23	CLA	b	601	65/65	0.88	0.12	58,80,120,129	0
33	HTG	B	622	19/19	0.88	0.17	61,83,110,111	0
26	GOL	o	302	6/6	0.88	0.16	110,113,118,120	0
27	SQD	b	620	54/54	0.88	0.13	59,88,112,115	0
27	SQD	B	620	54/54	0.88	0.13	54,88,124,129	0
29	PL9	A	413	55/55	0.88	0.20	72,102,112,115	0
32	LMG	C	521	51/55	0.90	0.14	52,87,119,120	0
34	LMT	t	101	26/35	0.90	0.15	77,117,136,140	0
23	CLA	B	601	65/65	0.90	0.11	52,72,115,121	0
26	GOL	a	411	6/6	0.91	0.12	57,68,80,81	0
33	HTG	B	625	19/19	0.91	0.11	65,75,82,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	LMG	C	502	51/55	0.92	0.12	57,84,104,106	0
32	LMG	c	501	51/55	0.92	0.14	60,88,109,117	0
32	LMG	c	521	51/55	0.92	0.14	68,92,125,127	0
23	CLA	c	515	65/65	0.92	0.12	64,83,117,119	0
23	CLA	C	515	65/65	0.92	0.12	59,70,111,114	0
32	LMG	D	413	51/55	0.92	0.12	44,64,111,123	0
30	UNL	D	409	17/-	0.93	0.16	56,77,114,114	0
25	BCR	t	102	40/40	0.93	0.08	37,51,66,70	0
32	LMG	m	101	51/55	0.93	0.11	51,68,96,98	0
26	GOL	b	628	6/6	0.93	0.17	94,100,102,103	0
31	LHG	A	416	49/49	0.93	0.13	41,57,80,87	0
23	CLA	C	506	65/65	0.93	0.11	42,51,85,95	0
25	BCR	B	619	40/40	0.93	0.10	43,53,72,75	0
32	LMG	B	621	51/55	0.93	0.11	49,65,92,114	0
25	BCR	K	101	40/40	0.93	0.10	54,63,69,71	0
26	GOL	C	524	6/6	0.93	0.17	53,56,60,61	0
25	BCR	T	101	40/40	0.93	0.08	37,48,57,61	0
30	UNL	d	409	17/-	0.93	0.13	67,82,97,97	0
33	HTG	b	625	19/19	0.93	0.10	66,72,92,98	0
25	BCR	h	102	40/40	0.93	0.10	50,61,74,75	0
35	DGD	C	519	62/66	0.93	0.12	42,62,116,121	0
30	UNL	d	411	18/-	0.93	0.13	74,78,109,112	0
36	CA	a	420	1/1	0.93	0.10	105,105,105,105	0
27	SQD	C	501	54/54	0.94	0.11	59,79,105,107	0
25	BCR	d	404	40/40	0.94	0.10	52,63,87,92	0
27	SQD	a	410	54/54	0.94	0.12	64,83,117,118	0
23	CLA	b	612	65/65	0.94	0.09	38,46,61,70	0
23	CLA	b	614	65/65	0.94	0.09	35,44,102,105	0
25	BCR	y	101	40/40	0.94	0.09	57,70,83,86	0
23	CLA	b	616	65/65	0.94	0.10	43,55,114,116	0
29	PL9	D	406	55/55	0.94	0.09	32,42,54,60	0
31	LHG	b	629	49/49	0.94	0.11	40,55,71,78	0
26	GOL	B	624	6/6	0.94	0.12	76,87,95,97	0
29	PL9	d	405	55/55	0.94	0.10	35,46,56,61	0
23	CLA	c	509	65/65	0.94	0.10	53,63,73,83	0
23	CLA	c	514	65/65	0.94	0.11	64,77,112,122	0
23	CLA	C	508	65/65	0.94	0.12	51,63,123,130	0
25	BCR	B	618	40/40	0.94	0.08	35,50,63,72	0
23	CLA	B	614	65/65	0.94	0.10	33,43,93,97	0
25	BCR	D	405	40/40	0.94	0.11	45,58,95,103	0
25	BCR	H	101	40/40	0.94	0.09	44,61,71,74	0
23	CLA	a	408	65/65	0.94	0.11	40,48,128,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	UNL	X	101	18/-	0.94	0.12	60,68,98,99	0
23	CLA	B	610	65/65	0.94	0.10	41,48,59,77	0
25	BCR	b	617	40/40	0.94	0.08	35,43,56,58	0
25	BCR	b	618	40/40	0.94	0.08	37,50,67,72	0
25	BCR	c	516	40/40	0.94	0.11	68,83,90,94	0
23	CLA	b	605	65/65	0.95	0.09	35,43,66,75	0
23	CLA	b	606	65/65	0.95	0.09	38,49,110,115	0
25	BCR	c	517	40/40	0.95	0.10	53,65,71,71	0
23	CLA	b	610	65/65	0.95	0.09	43,50,62,73	0
32	LMG	d	412	51/55	0.95	0.11	53,67,111,119	0
23	CLA	C	503	65/65	0.95	0.09	45,53,68,78	0
23	CLA	C	505	65/65	0.95	0.08	47,55,67,72	0
23	CLA	B	606	65/65	0.95	0.09	38,46,101,108	0
23	CLA	c	505	65/65	0.95	0.09	53,63,73,77	0
23	CLA	c	506	65/65	0.95	0.10	49,58,103,110	0
23	CLA	c	507	65/65	0.95	0.09	43,56,83,86	0
23	CLA	c	508	65/65	0.95	0.10	56,69,121,126	0
23	CLA	A	408	65/65	0.95	0.10	38,45,111,119	0
23	CLA	c	510	65/65	0.95	0.09	47,57,127,132	0
23	CLA	C	509	65/65	0.95	0.09	50,57,76,80	0
23	CLA	C	510	65/65	0.95	0.09	43,51,117,130	0
23	CLA	d	403	65/65	0.95	0.09	48,58,115,123	0
24	PHO	A	415	64/64	0.95	0.07	35,43,52,54	0
25	BCR	A	409	40/40	0.95	0.07	33,42,54,58	0
23	CLA	C	513	65/65	0.95	0.09	49,62,77,78	0
23	CLA	C	514	65/65	0.95	0.11	55,65,114,119	0
25	BCR	C	516	40/40	0.95	0.10	59,74,81,83	0
31	LHG	D	407	49/49	0.95	0.09	40,48,64,76	0
31	LHG	D	408	49/49	0.95	0.13	45,57,124,134	0
25	BCR	C	517	40/40	0.95	0.08	49,56,64,73	0
31	LHG	L	101	49/49	0.95	0.10	39,51,65,84	0
23	CLA	B	611	65/65	0.95	0.08	34,39,61,68	0
23	CLA	D	404	65/65	0.95	0.10	44,54,126,133	0
31	LHG	d	406	49/49	0.95	0.11	50,61,76,81	0
31	LHG	d	408	49/49	0.95	0.12	53,65,117,122	0
23	CLA	a	406	65/65	0.95	0.10	39,49,114,118	0
23	CLA	B	603	65/65	0.95	0.09	38,46,62,66	0
35	DGD	C	518	62/66	0.95	0.10	40,54,93,96	0
25	BCR	Y	101	40/40	0.95	0.09	53,64,73,77	0
35	DGD	C	520	62/66	0.95	0.10	40,53,95,108	0
35	DGD	H	102	62/66	0.95	0.10	40,55,67,69	0
35	DGD	c	518	62/66	0.95	0.10	45,58,90,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	DGD	c	519	62/66	0.95	0.09	50,70,107,118	0
35	DGD	c	520	62/66	0.95	0.10	48,60,98,111	0
35	DGD	h	103	62/66	0.95	0.09	50,59,68,71	0
25	BCR	a	409	40/40	0.95	0.07	36,45,56,59	0
23	CLA	B	616	65/65	0.95	0.11	41,52,136,137	0
36	CA	o	301	1/1	0.95	0.05	100,100,100,100	0
37	BCT	d	401	4/4	0.95	0.07	52,54,62,64	0
23	CLA	A	406	65/65	0.96	0.09	34,42,114,117	0
23	CLA	b	611	65/65	0.96	0.08	36,44,70,76	0
23	CLA	B	607	65/65	0.96	0.07	31,40,64,69	0
23	CLA	B	609	65/65	0.96	0.07	43,51,74,81	0
23	CLA	D	403	65/65	0.96	0.07	32,37,53,62	0
23	CLA	c	503	65/65	0.96	0.09	53,61,74,82	0
23	CLA	c	504	65/65	0.96	0.08	48,56,73,83	0
23	CLA	B	602	65/65	0.96	0.08	39,48,72,77	0
23	CLA	a	404	65/65	0.96	0.07	37,41,64,73	0
31	LHG	d	407	49/49	0.96	0.09	41,51,68,78	0
25	BCR	b	619	40/40	0.96	0.08	46,53,74,84	0
23	CLA	a	405	65/65	0.96	0.07	34,40,57,62	0
23	CLA	A	404	65/65	0.96	0.08	33,36,61,75	0
23	CLA	B	613	65/65	0.96	0.08	34,41,89,94	0
23	CLA	B	605	65/65	0.96	0.08	35,41,61,73	0
25	BCR	k	101	40/40	0.96	0.09	58,70,81,81	0
23	CLA	c	511	65/65	0.96	0.09	54,62,86,88	0
23	CLA	c	512	65/65	0.96	0.08	52,59,73,76	0
23	CLA	c	513	65/65	0.96	0.08	55,65,81,85	0
23	CLA	b	602	65/65	0.96	0.08	43,54,70,80	0
23	CLA	b	603	65/65	0.96	0.08	41,50,70,88	0
23	CLA	b	604	65/65	0.96	0.09	34,43,111,119	0
24	PHO	A	407	64/64	0.96	0.07	32,37,47,52	0
23	CLA	C	511	65/65	0.96	0.09	48,56,77,79	0
24	PHO	a	417	64/64	0.96	0.07	39,47,55,60	0
23	CLA	C	512	65/65	0.96	0.08	46,56,78,87	0
25	BCR	B	617	40/40	0.96	0.07	34,45,55,58	0
36	CA	O	301	1/1	0.96	0.06	103,103,103,103	0
23	CLA	b	607	65/65	0.96	0.08	32,40,73,80	0
23	CLA	b	608	65/65	0.96	0.07	45,52,69,76	0
37	BCT	D	401	4/4	0.96	0.08	51,57,61,62	0
23	CLA	b	609	65/65	0.96	0.08	49,57,78,100	0
38	HEC	e	102	43/43	0.96	0.08	64,78,119,130	0
39	MG	J	102	1/1	0.96	0.08	50,50,50,50	0
23	CLA	B	612	65/65	0.97	0.07	35,44,54,59	0

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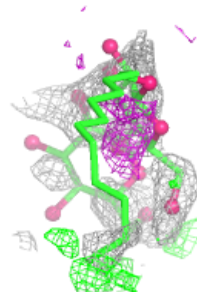
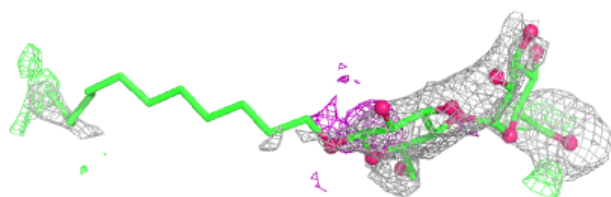
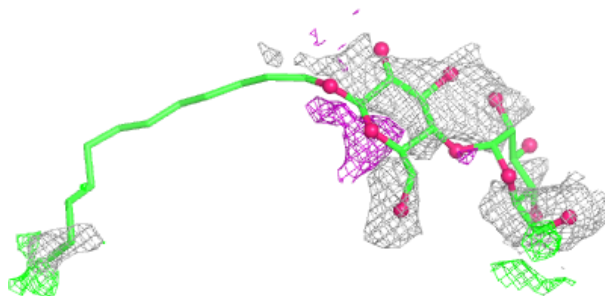
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	CA	C	525	1/1	0.97	0.10	66,66,66,66	0
23	CLA	B	608	65/65	0.97	0.07	39,47,62,65	0
23	CLA	b	613	65/65	0.97	0.07	33,42,84,88	0
23	CLA	C	504	65/65	0.97	0.07	43,50,71,82	0
36	CA	c	524	1/1	0.97	0.07	73,73,73,73	0
23	CLA	b	615	65/65	0.97	0.08	42,50,74,79	0
23	CLA	A	405	65/65	0.97	0.07	31,37,52,56	0
24	PHO	a	407	64/64	0.97	0.06	35,42,47,50	0
38	HEC	E	103	43/43	0.97	0.07	57,65,80,93	0
38	HEC	V	201	43/43	0.97	0.07	43,46,51,54	0
23	CLA	B	615	65/65	0.97	0.07	40,46,77,83	0
38	HEC	v	202	43/43	0.97	0.08	52,58,63,64	0
23	CLA	C	507	65/65	0.97	0.08	43,52,86,93	0
23	CLA	d	402	65/65	0.98	0.06	36,40,68,77	0
22	CL	A	403	1/1	0.98	0.04	40,40,40,40	0
23	CLA	B	604	65/65	0.98	0.08	32,39,110,116	0
39	MG	j	102	1/1	0.98	0.04	60,60,60,60	0
22	CL	a	403	1/1	0.99	0.05	44,44,44,44	0
22	CL	A	402	1/1	0.99	0.04	35,35,35,35	0
36	CA	c	525	1/1	0.99	0.04	80,80,80,80	0
22	CL	a	402	1/1	0.99	0.04	42,42,42,42	0
28	OEX	A	412	10/10	0.99	0.04	35,38,45,46	0
28	OEX	a	414	10/10	0.99	0.03	39,45,49,49	0
21	FE2	A	401	1/1	1.00	0.04	53,53,53,53	0
21	FE2	a	401	1/1	1.00	0.04	57,57,57,57	0

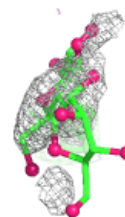
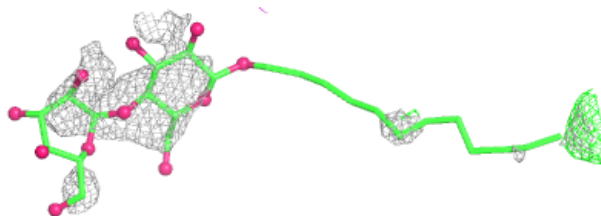
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

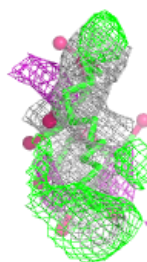
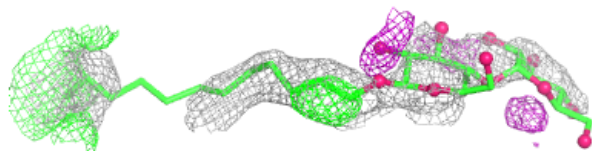
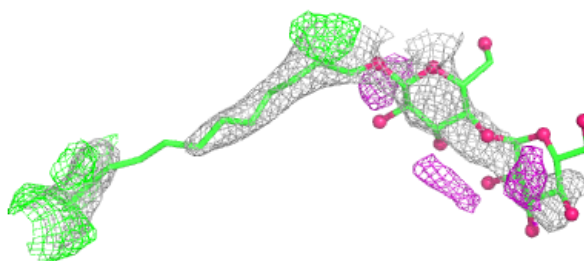
**Electron density around LMT e 101:**

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

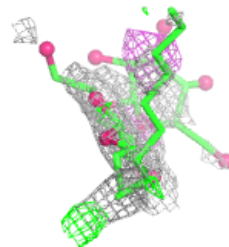
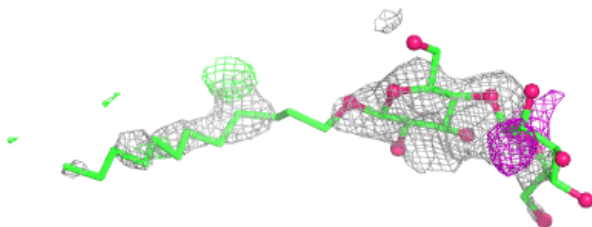
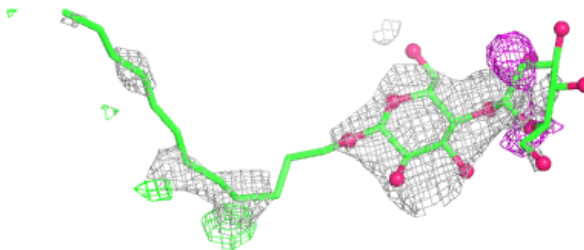


Electron density around LMT a 413:

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

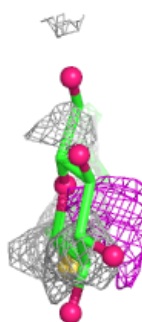
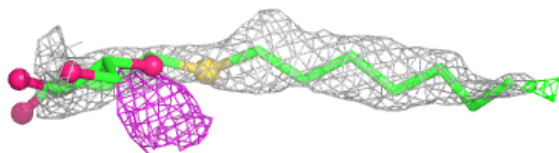
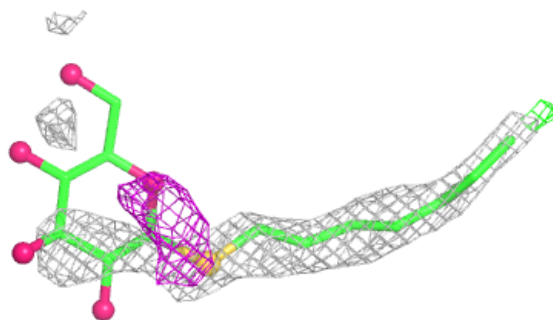
**Electron density around LMT C 526:**

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

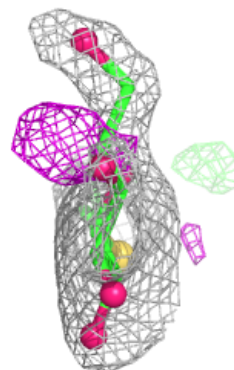
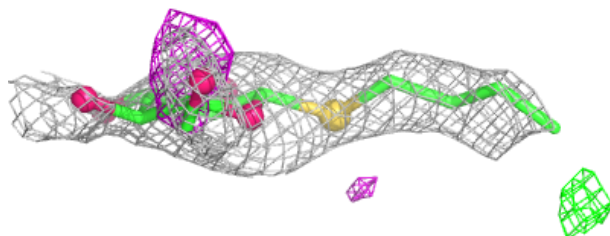
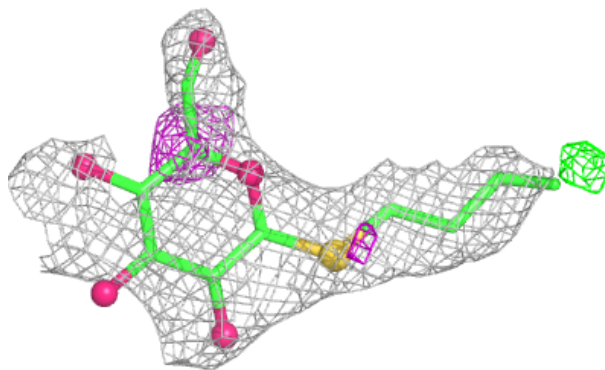


Electron density around HTG b 623:

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

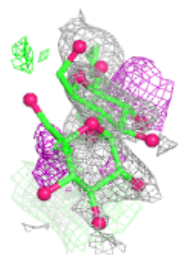
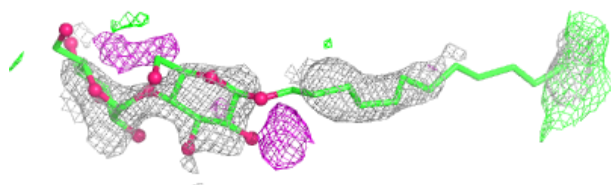
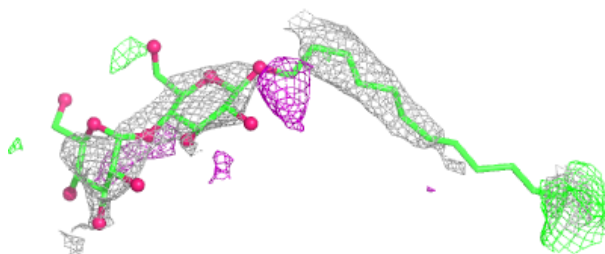
**Electron density around HTG D 411:**

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



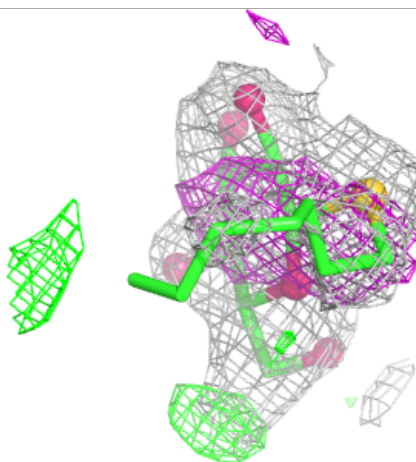
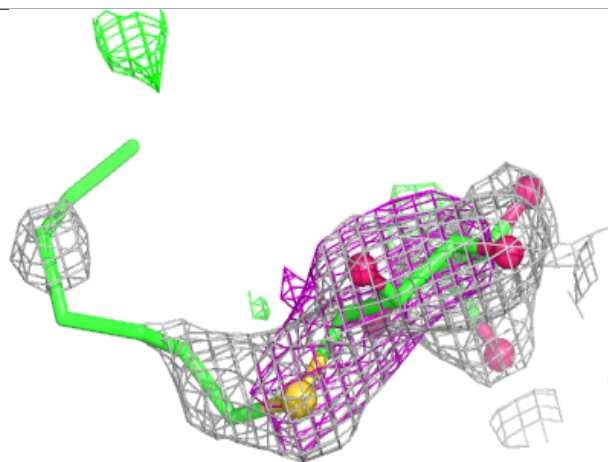
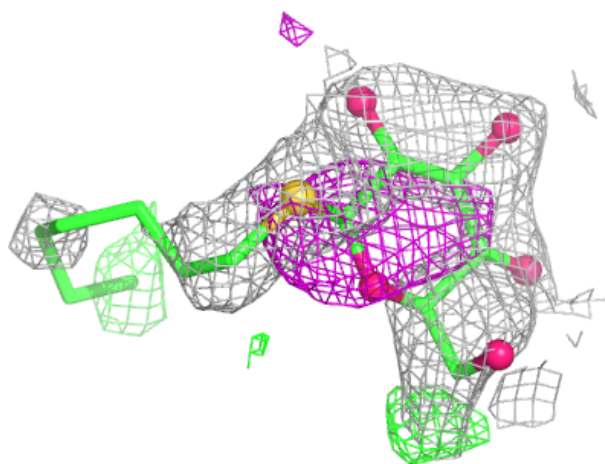
Electron density around LMT D 402:

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



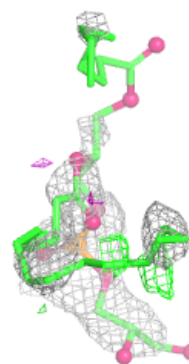
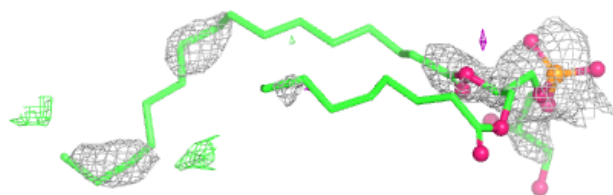
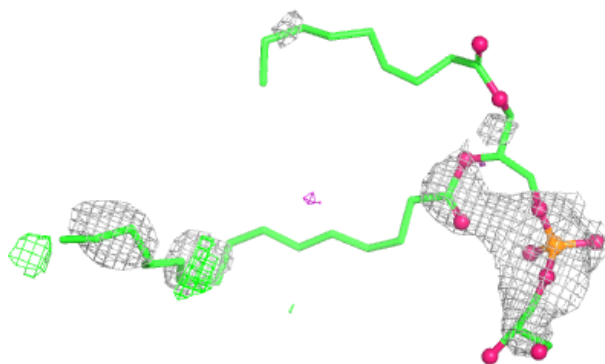
Electron density around HTG B 623:

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

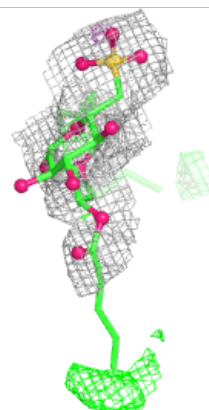
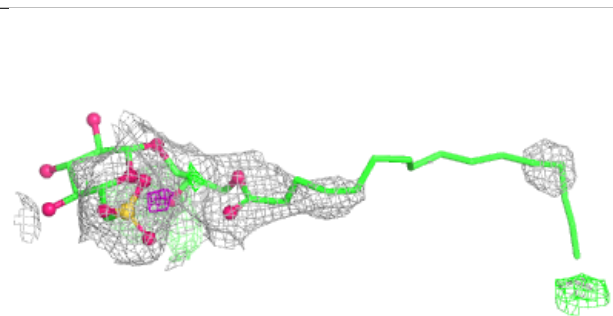
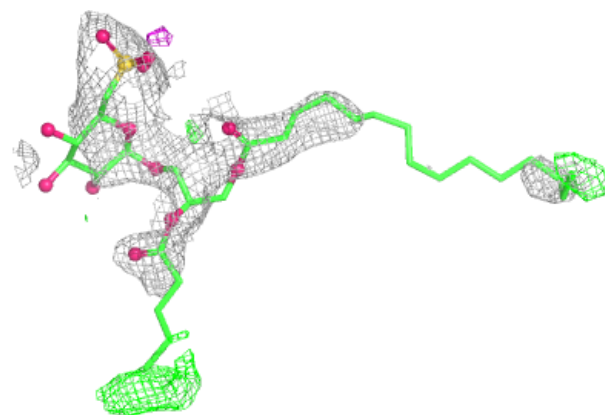


Electron density around LHG a 419:

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

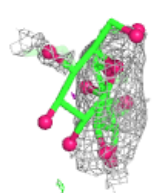
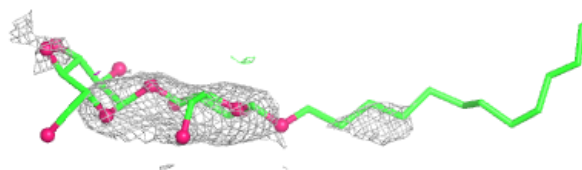
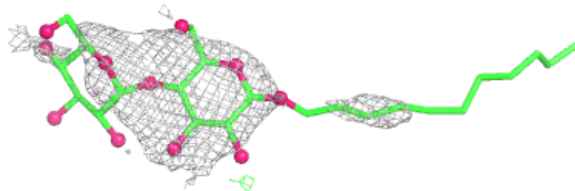
**Electron density around SQD f 101:**

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

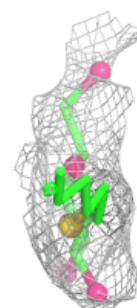
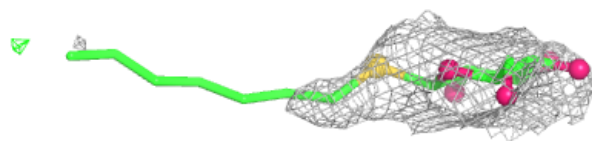
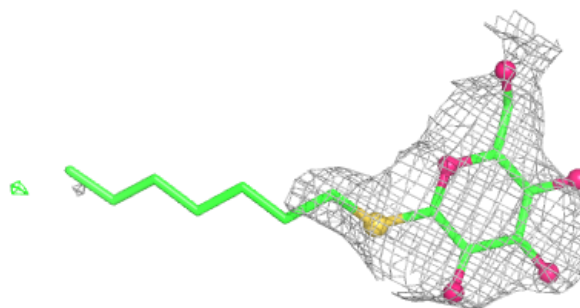


Electron density around LMT a 418:

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

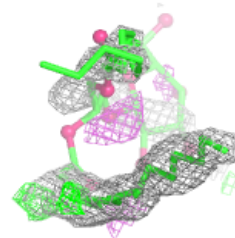
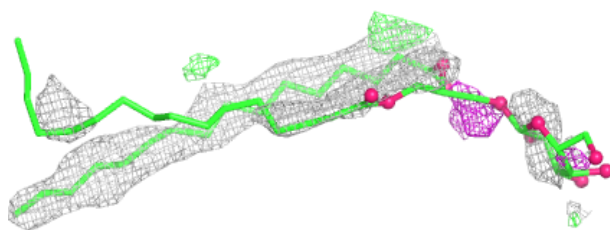
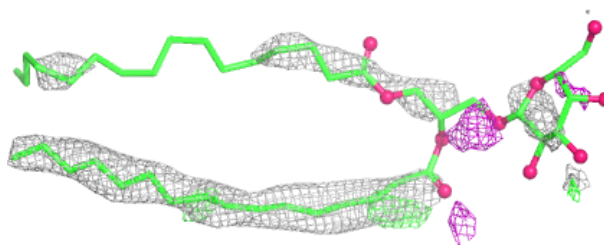
**Electron density around HTG c 523:**

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

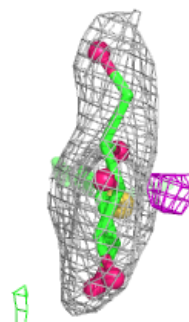
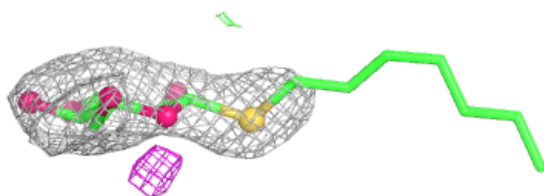
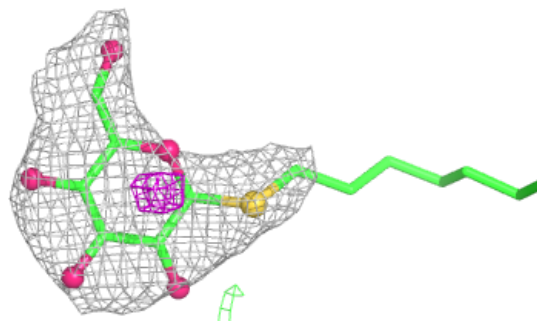


Electron density around LMG C 522:

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

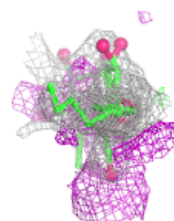
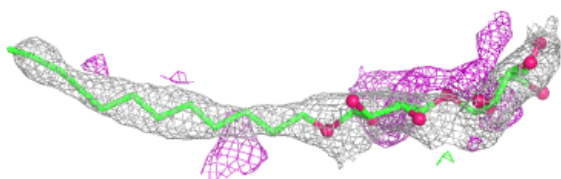
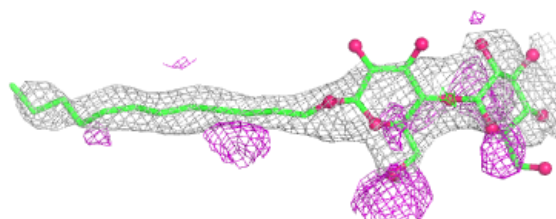
**Electron density around HTG C 523:**

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

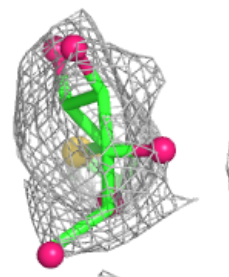
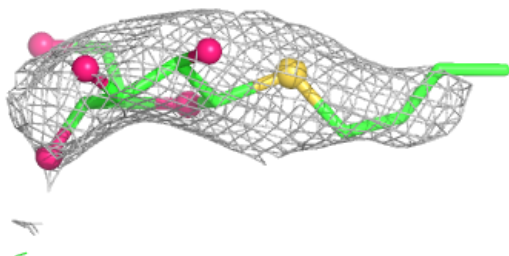
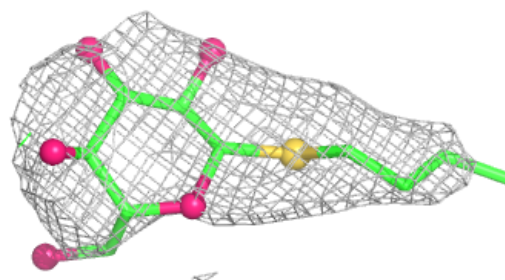


Electron density around LMT m 103:

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

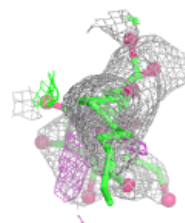
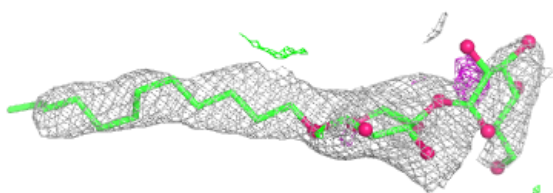
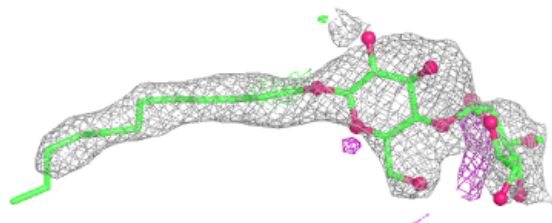
**Electron density around HTG h 101:**

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

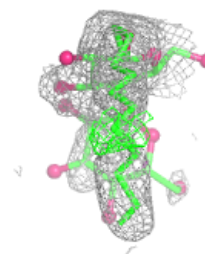
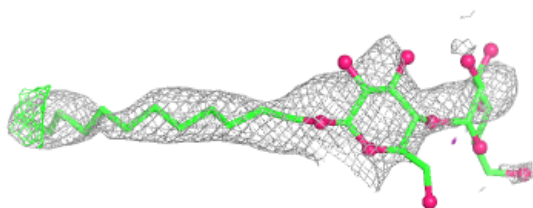
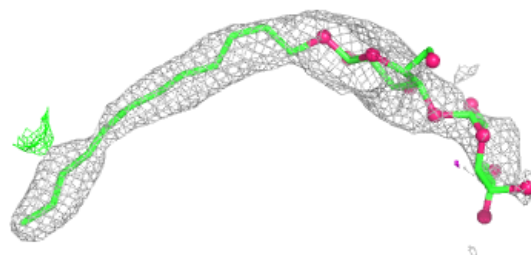


Electron density around LMT B 628:

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

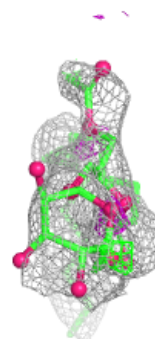
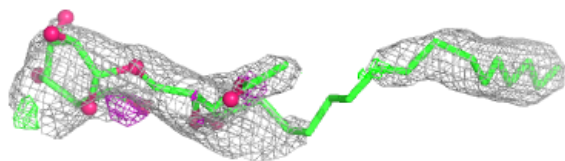
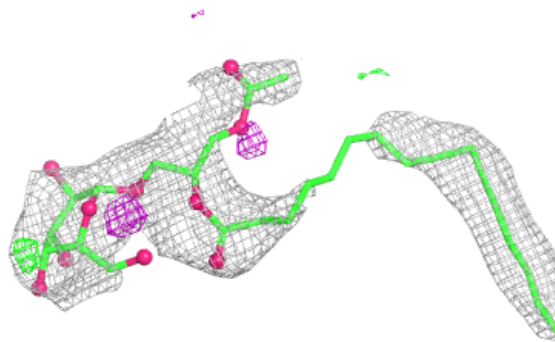
**Electron density around LMT M 103:**

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

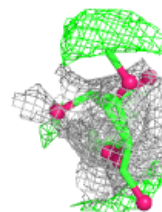
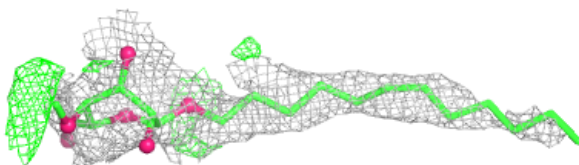
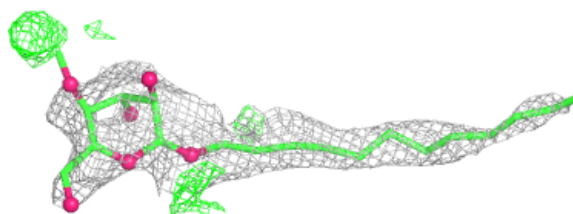


Electron density around LMG Z 101:

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

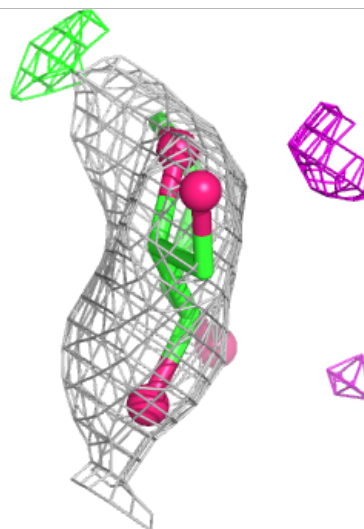
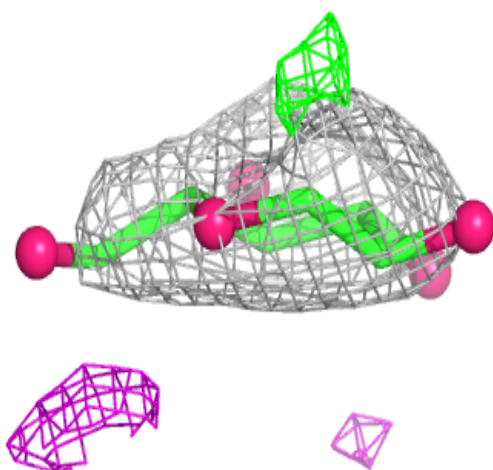
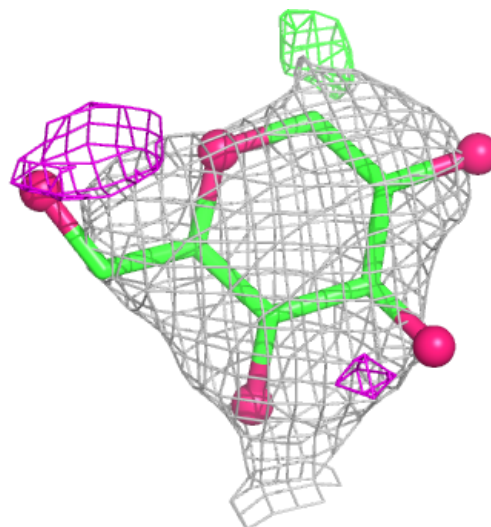
**Electron density around LMT b 621:**

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



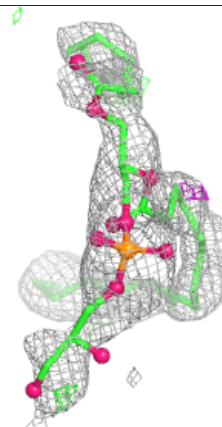
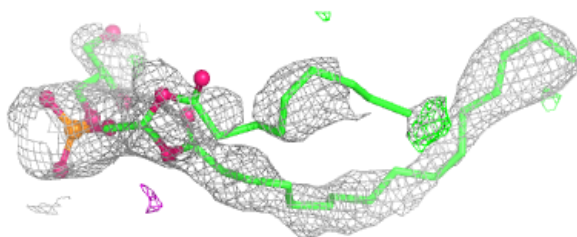
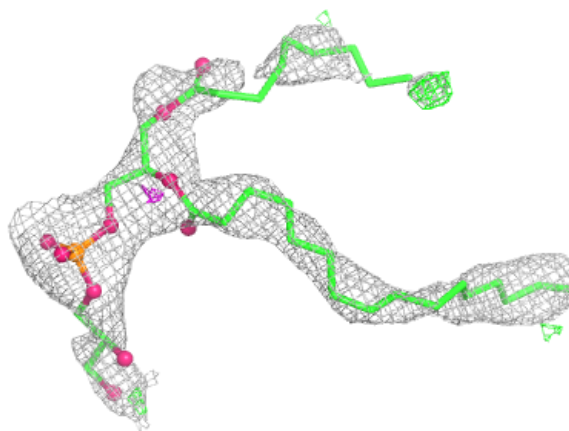
Electron density around HTG V 202:

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

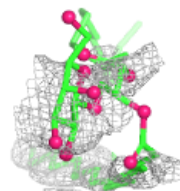
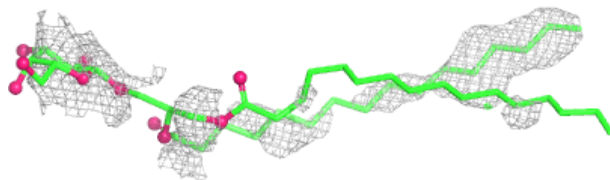
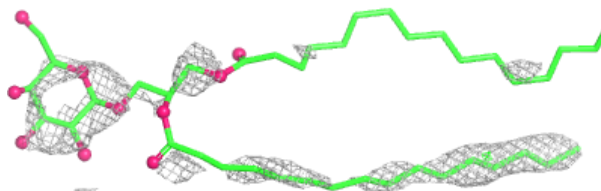


Electron density around LHG E 101:

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

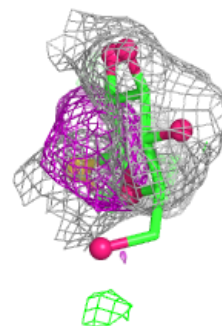
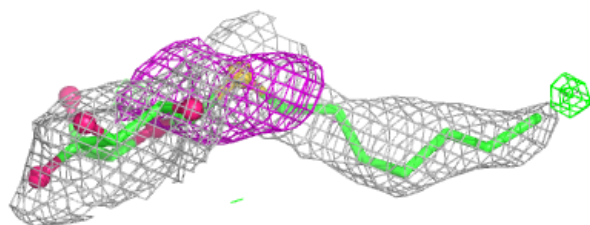
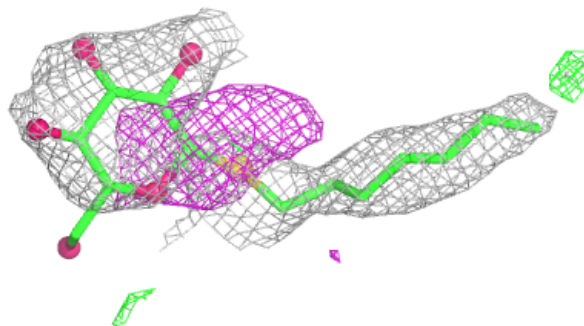
**Electron density around LMG c 522:**

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

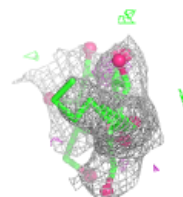
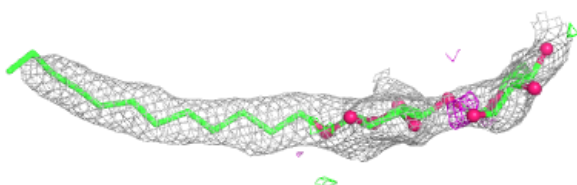
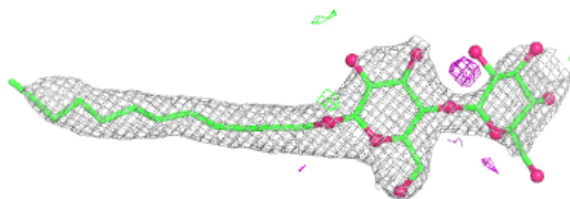


Electron density around HTG b 622:

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

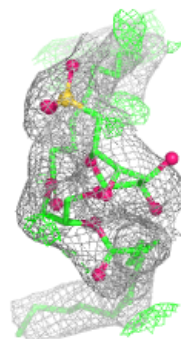
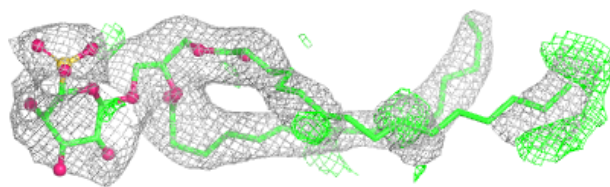
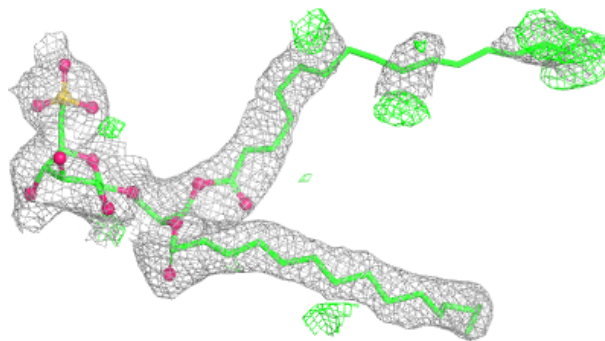
**Electron density around LMT M 101:**

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

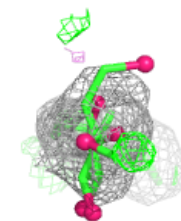
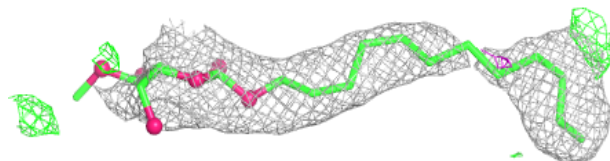
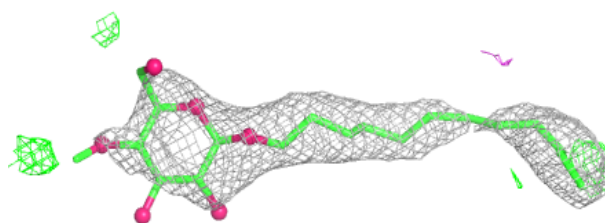


Electron density around SQD A 411:

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

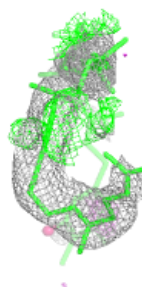
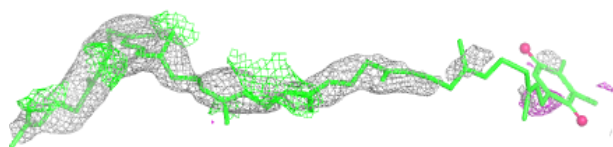
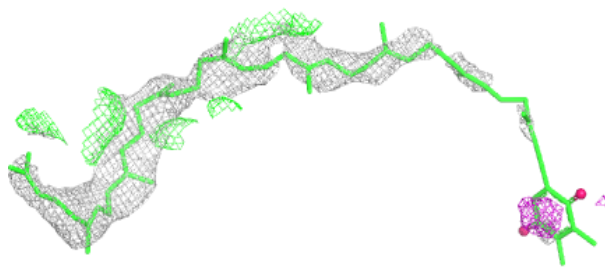
**Electron density around LMT b 627:**

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

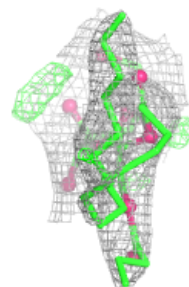
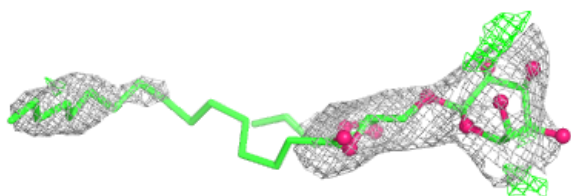
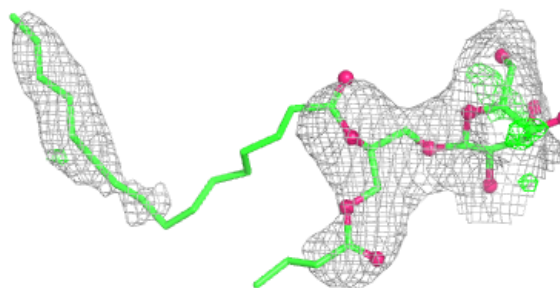


Electron density around PL9 a 415:

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

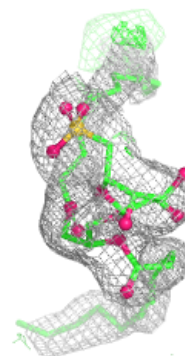
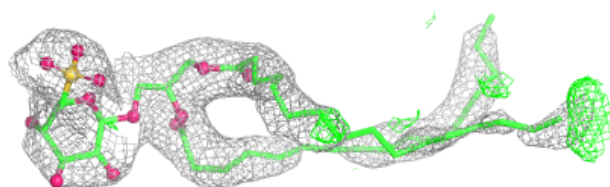
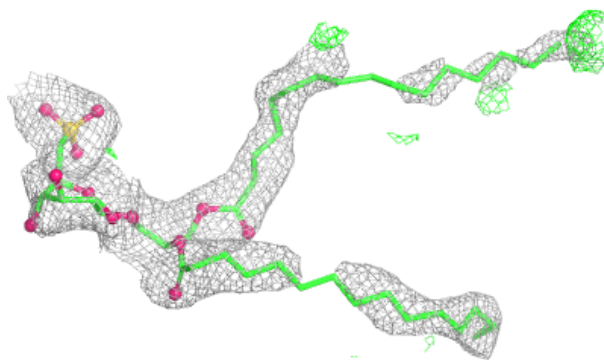
**Electron density around LMG z 101:**

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

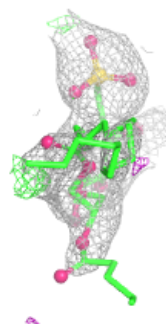
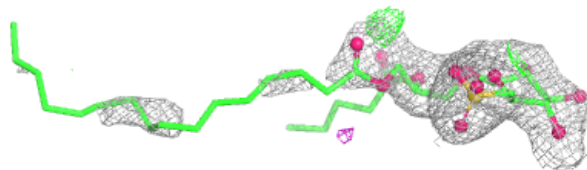
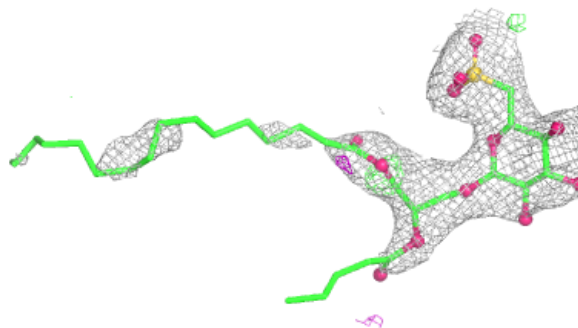


Electron density around SQD a 412:

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

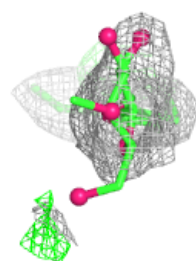
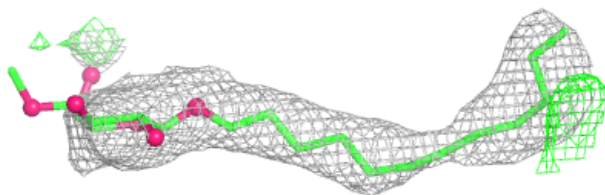
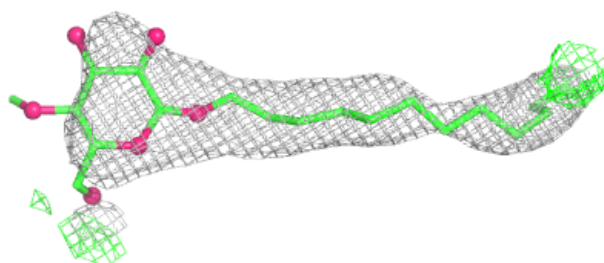
**Electron density around SQD D 412:**

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

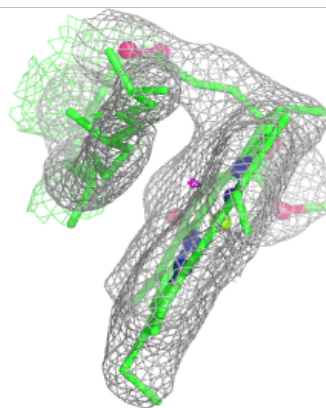
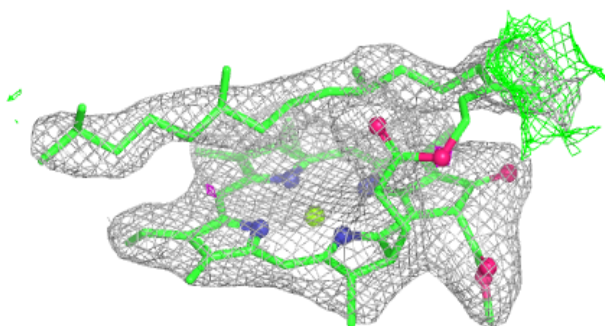
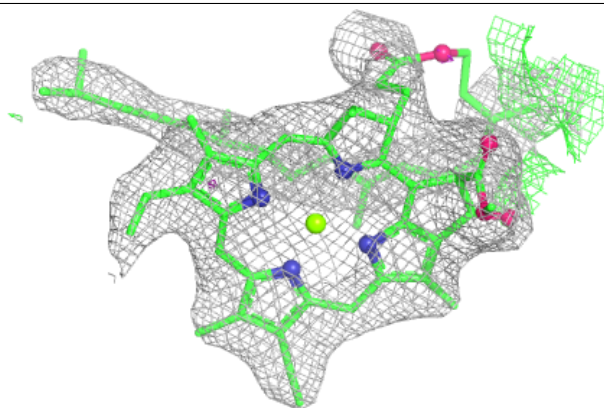


Electron density around LMT B 630:

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

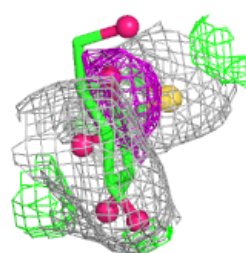
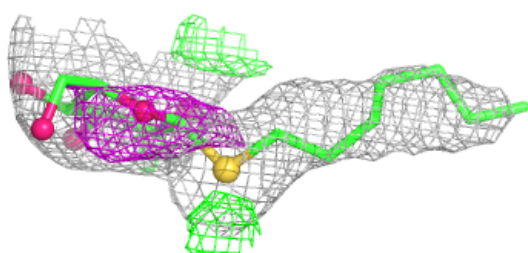
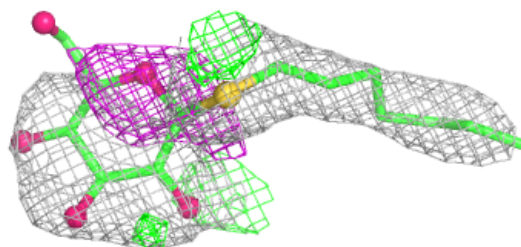
**Electron density around CLA b 601:**

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

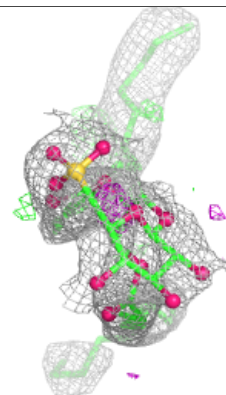
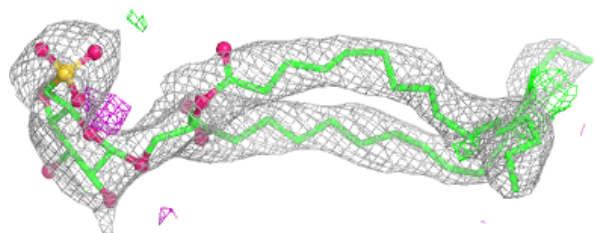
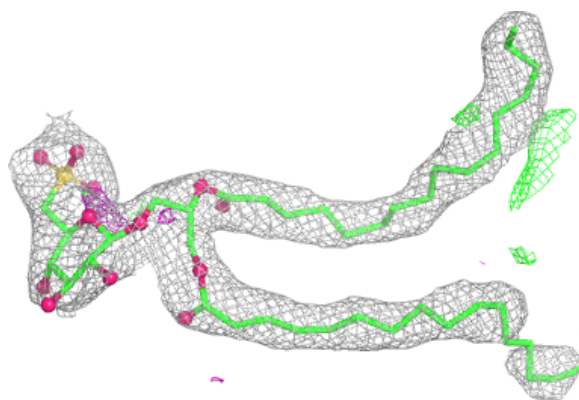


Electron density around HTG B 622:

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

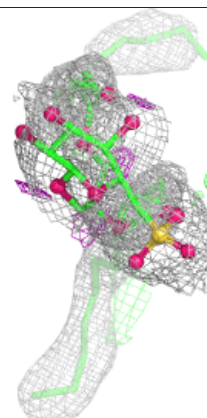
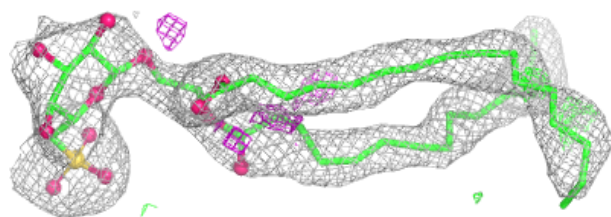
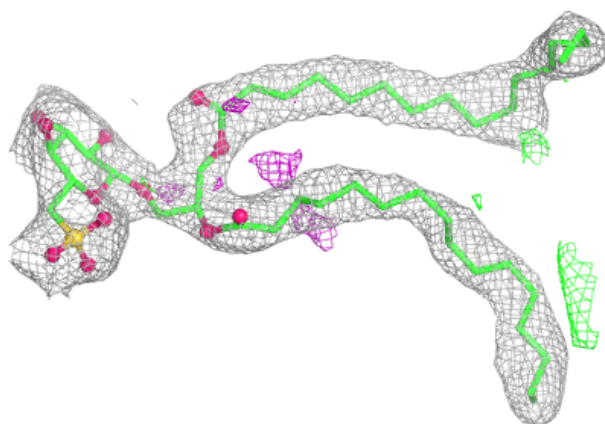
**Electron density around SQD b 620:**

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

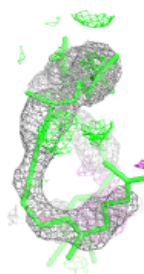
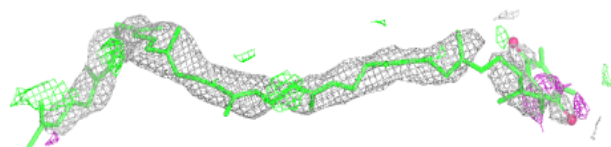
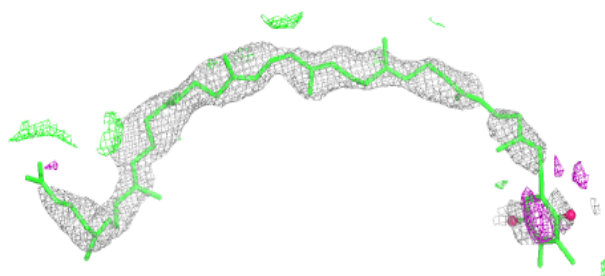


Electron density around SQD B 620:

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

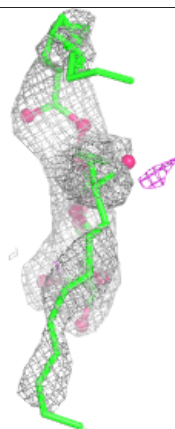
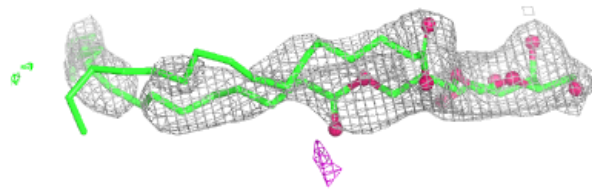
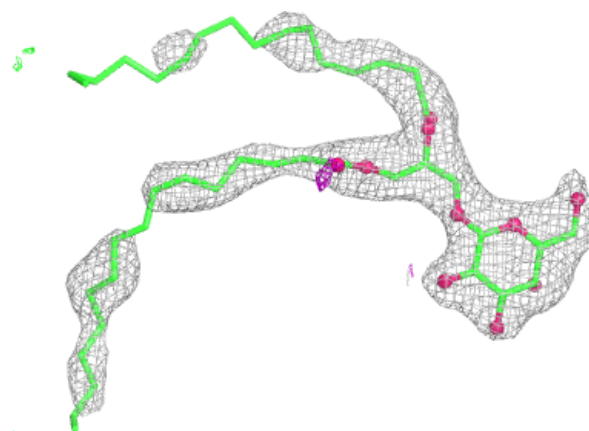
**Electron density around PL9 A 413:**

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

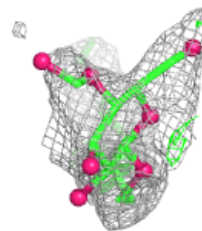
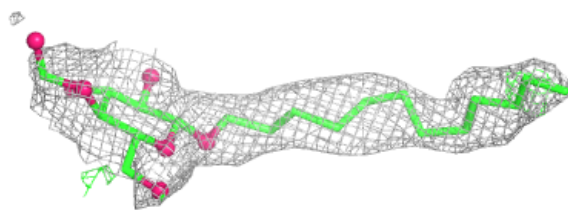
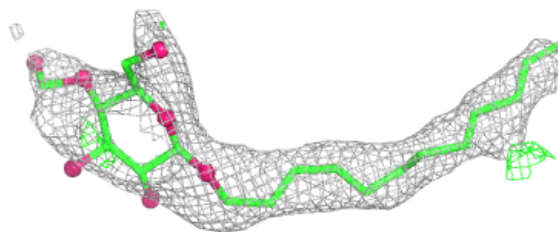


Electron density around LMG C 521:

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

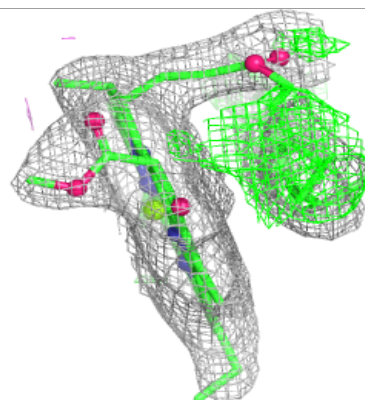
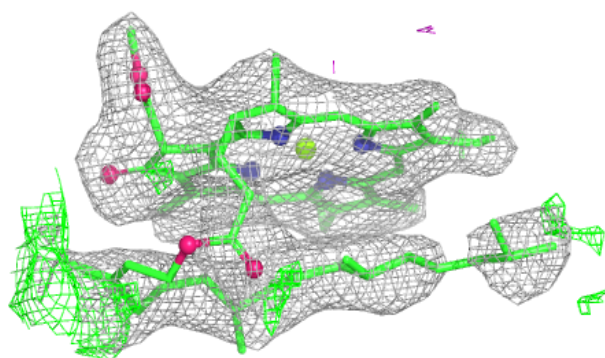
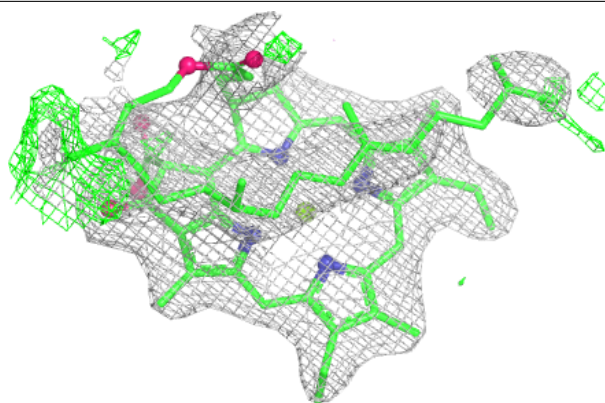
**Electron density around LMT t 101:**

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

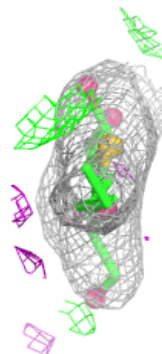
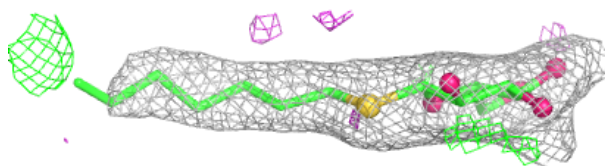
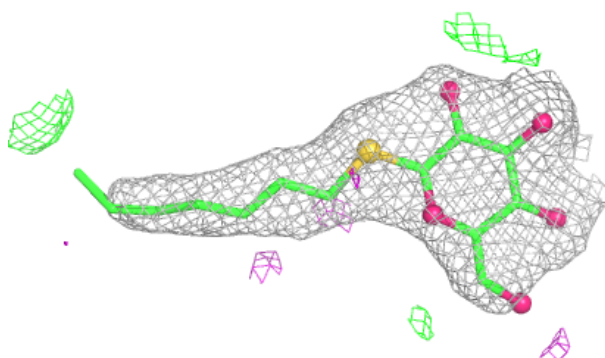


Electron density around CLA B 601:

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

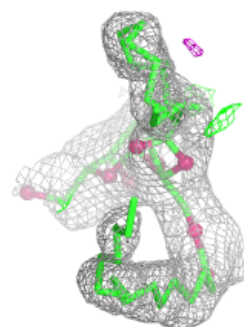
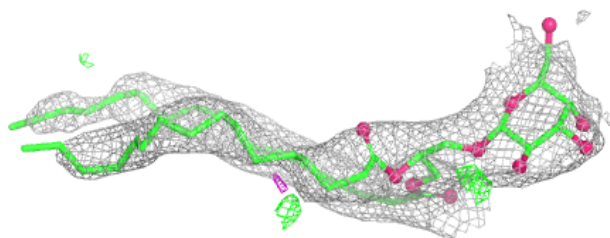
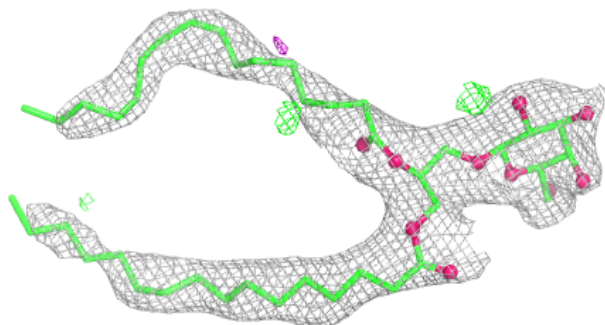
**Electron density around HTG B 625:**

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

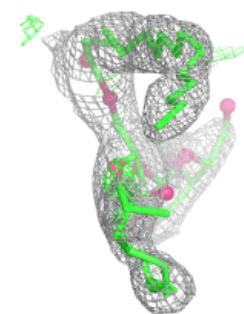
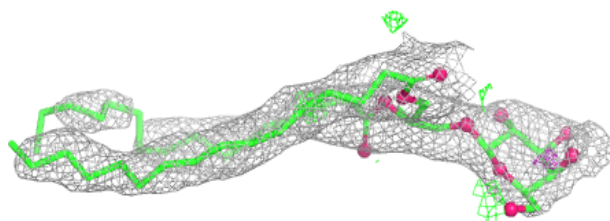
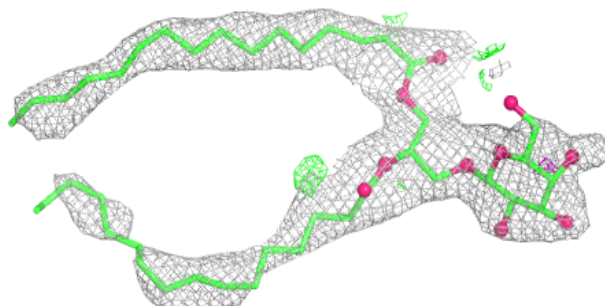


Electron density around LMG C 502:

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

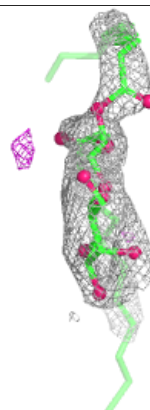
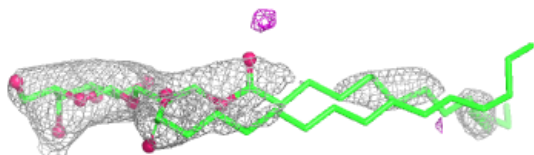
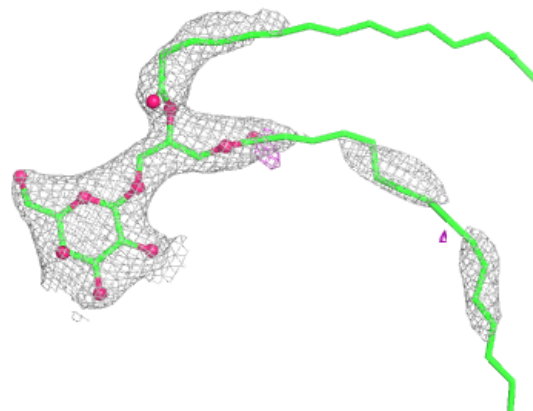
**Electron density around LMG c 501:**

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

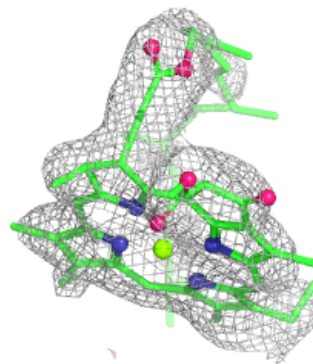
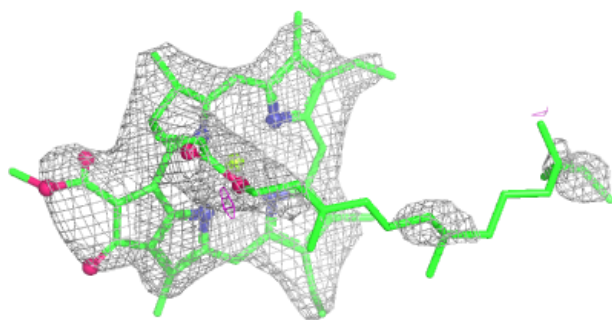
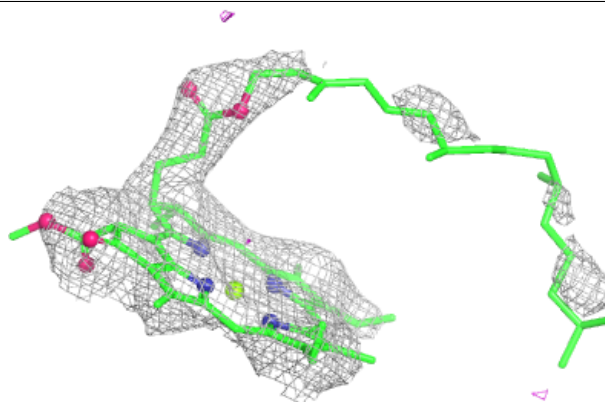


Electron density around LMG c 521:

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

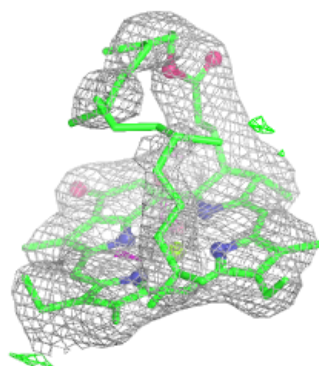
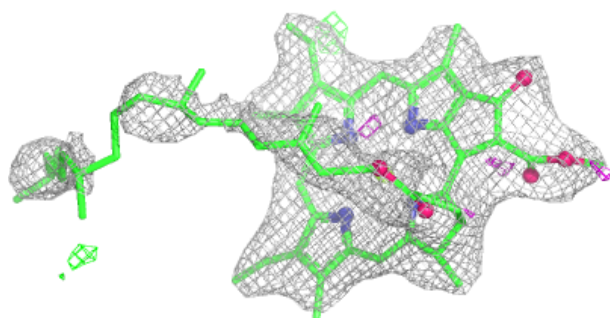
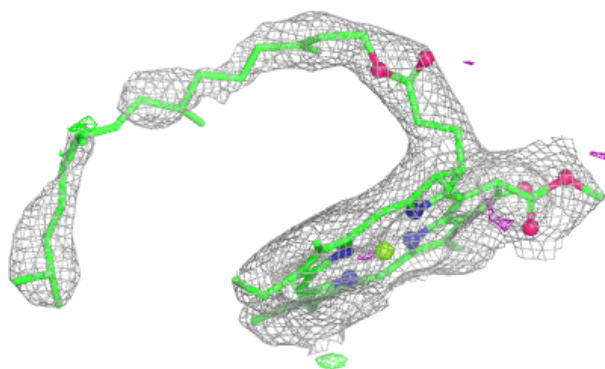
**Electron density around CLA c 515:**

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

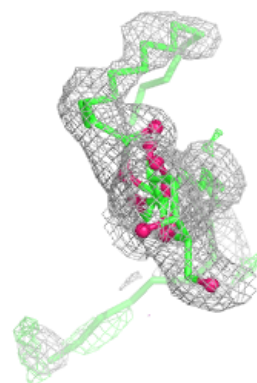
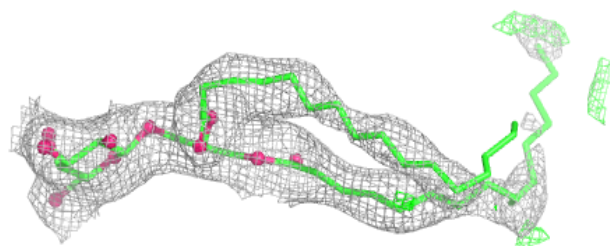
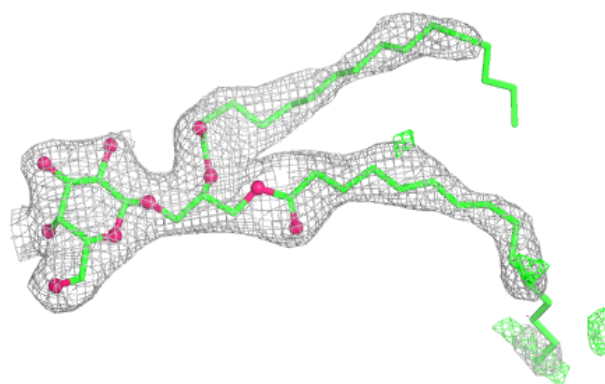


Electron density around CLA C 515:

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

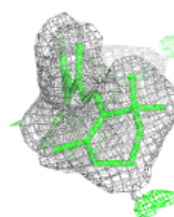
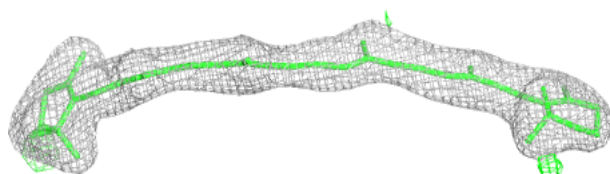
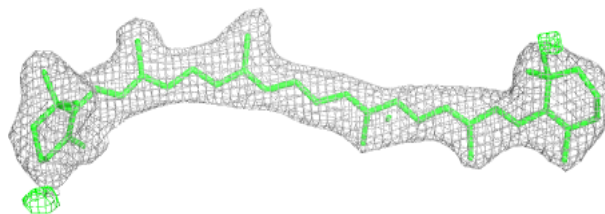
**Electron density around LMG D 413:**

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

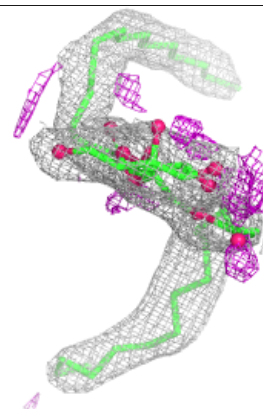
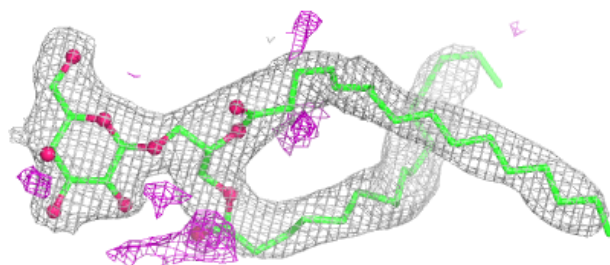
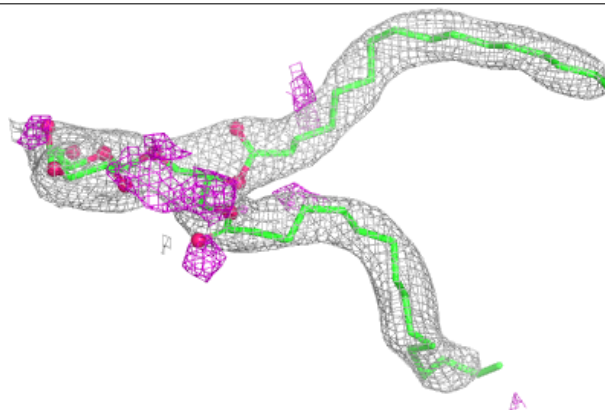


Electron density around BCR t 102:

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

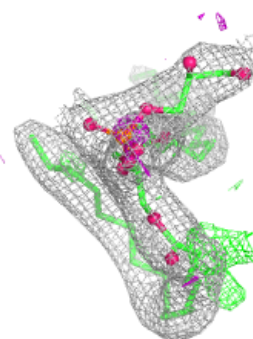
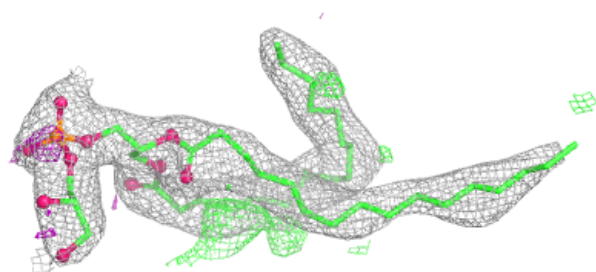
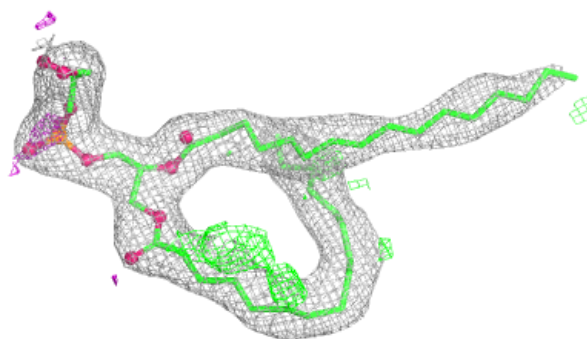
**Electron density around LMG m 101:**

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

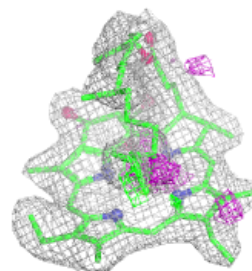
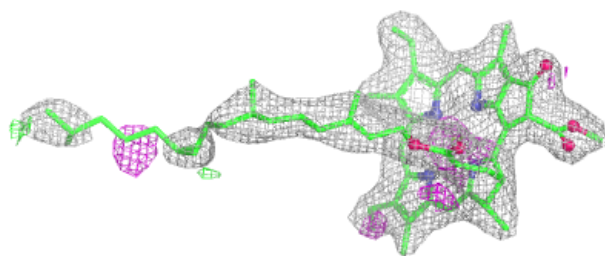
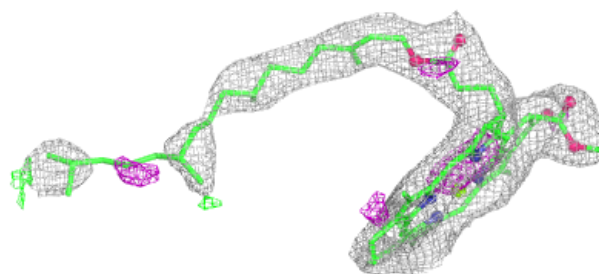


Electron density around LHG A 416:

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

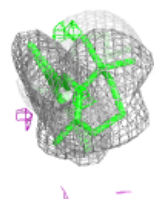
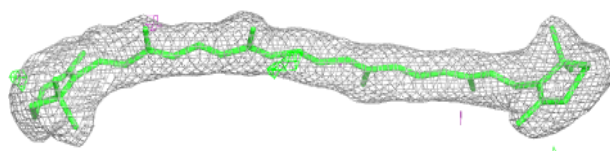
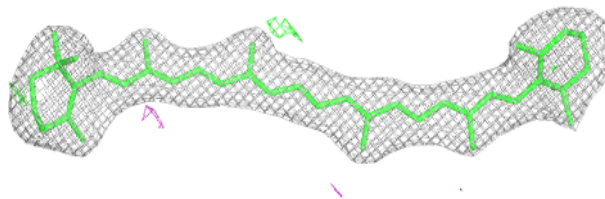
**Electron density around CLA C 506:**

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

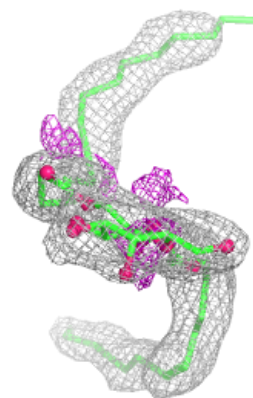
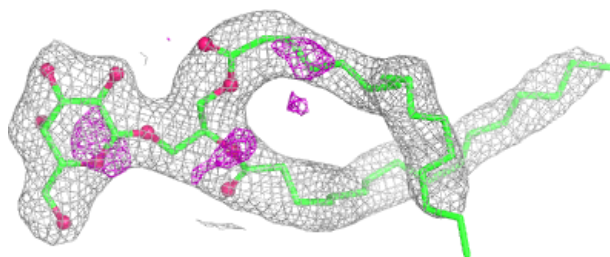
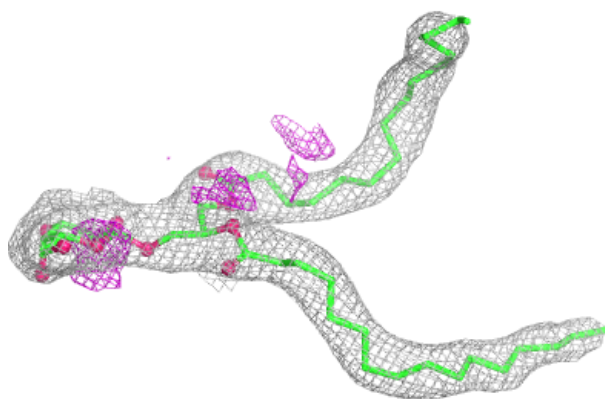


Electron density around BCR B 619:

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

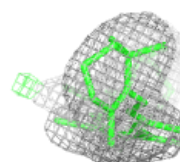
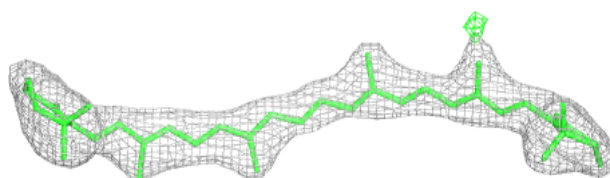
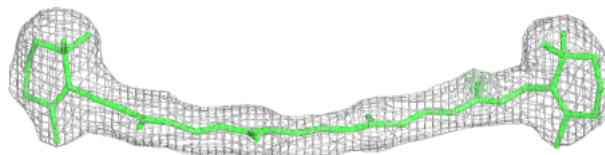
**Electron density around LMG B 621:**

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

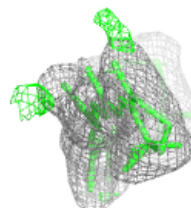
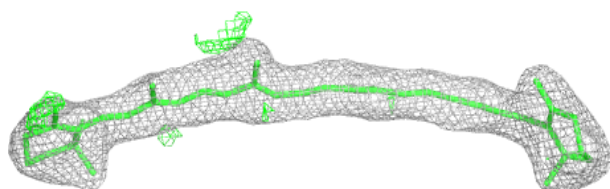
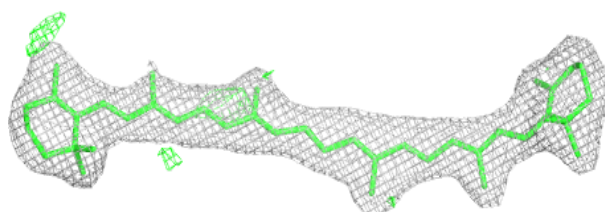


Electron density around BCR K 101:

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

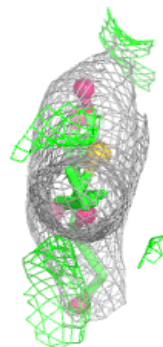
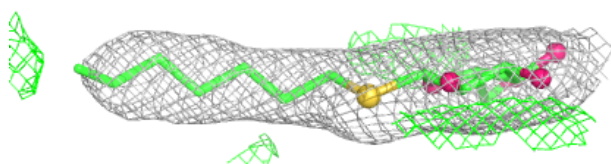
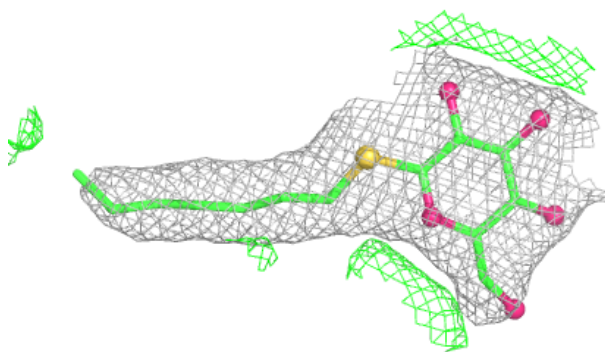
**Electron density around BCR T 101:**

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

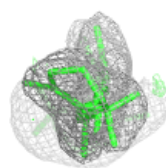
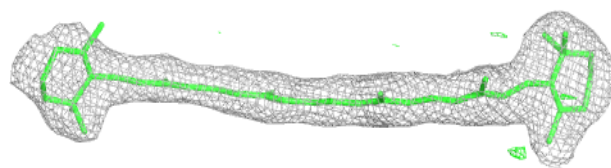


Electron density around HTG b 625:

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

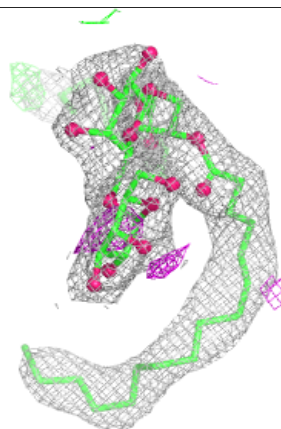
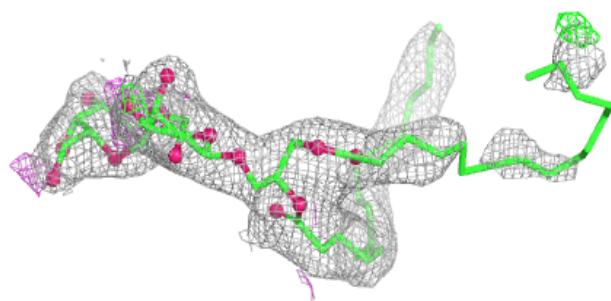
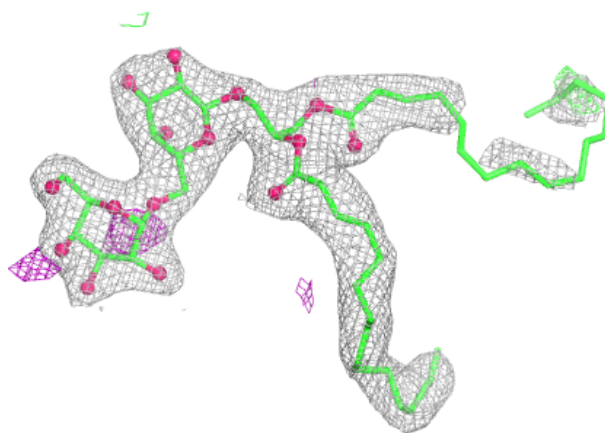
**Electron density around BCR h 102:**

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



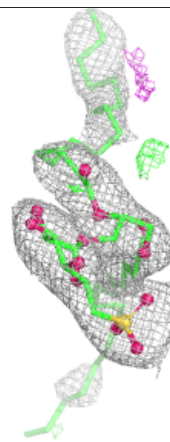
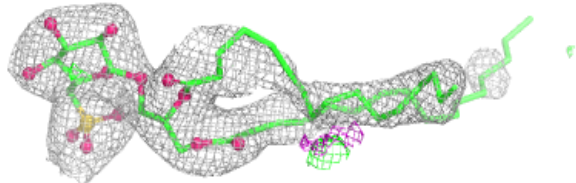
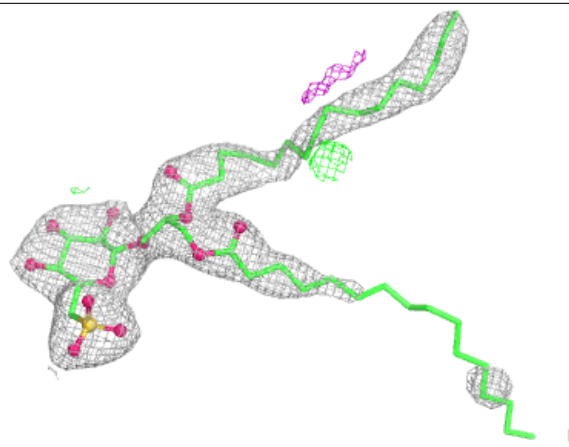
Electron density around DGD C 519:

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

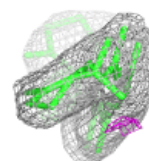
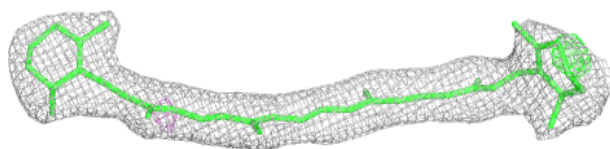
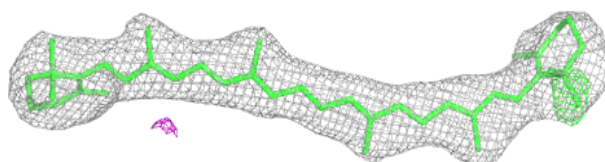


Electron density around SQD C 501:

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

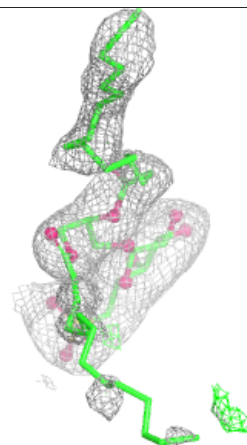
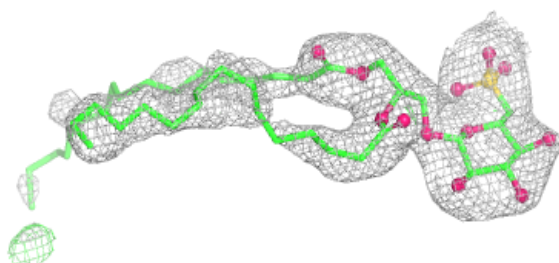
**Electron density around BCR d 404:**

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

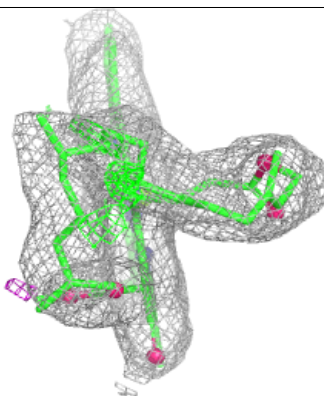
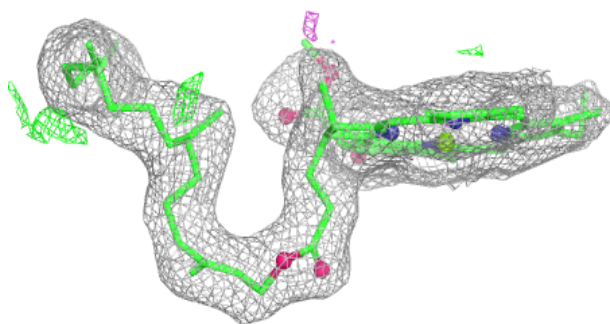
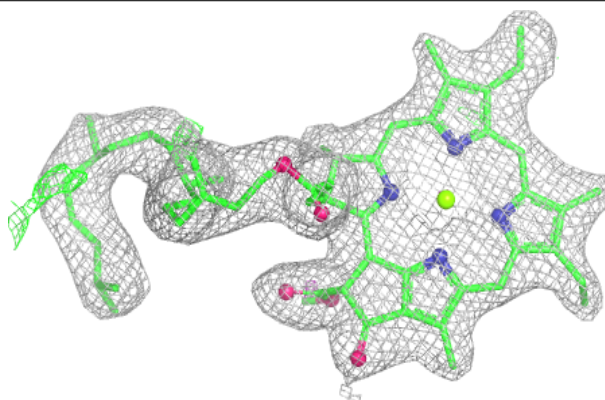


Electron density around SQD a 410:

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

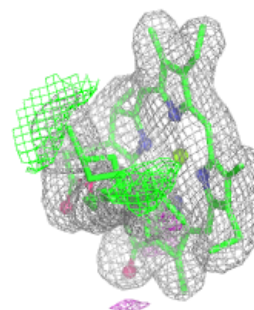
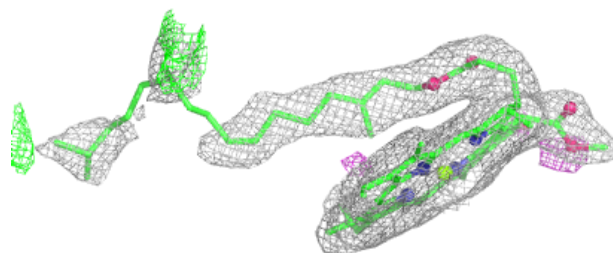
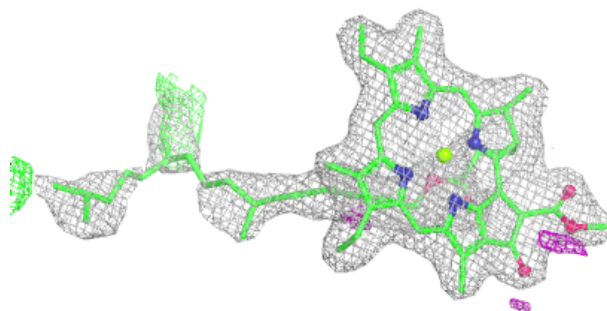
**Electron density around CLA b 612:**

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

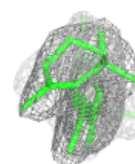
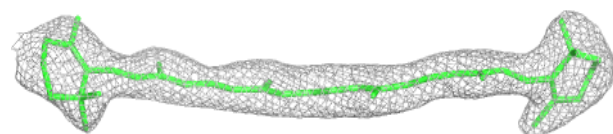
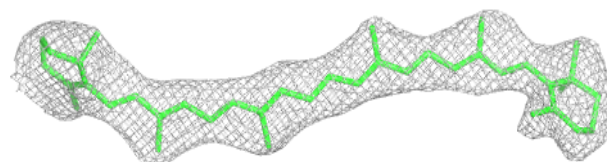


Electron density around CLA b 614:

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

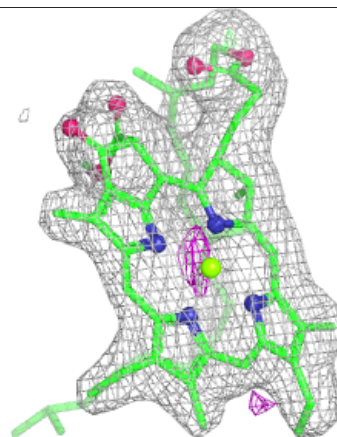
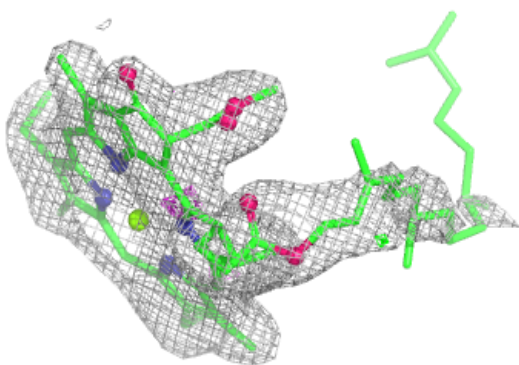
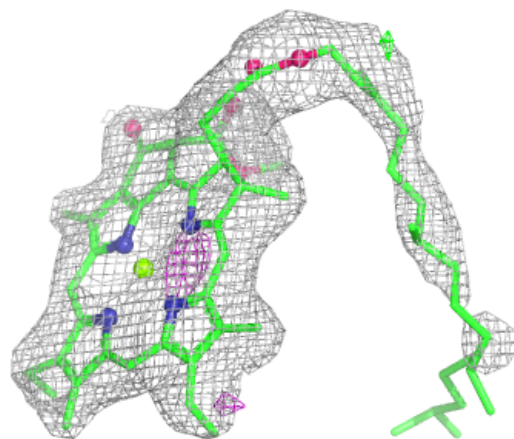
**Electron density around BCR y 101:**

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

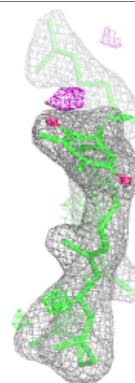
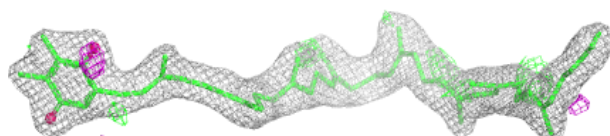
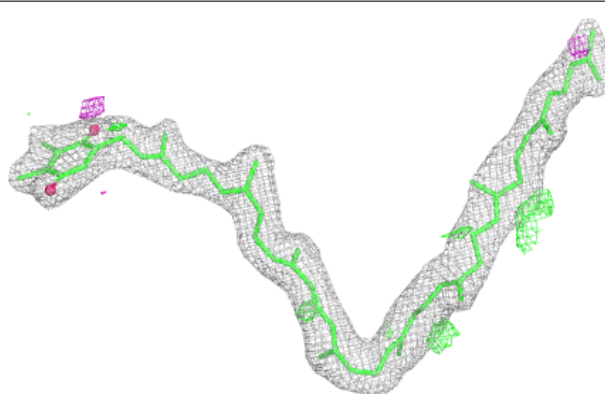


Electron density around CLA b 616:

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

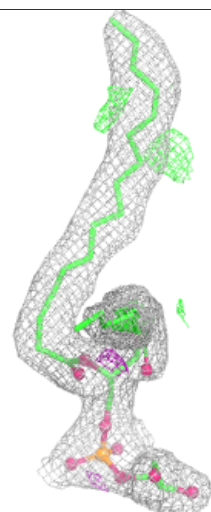
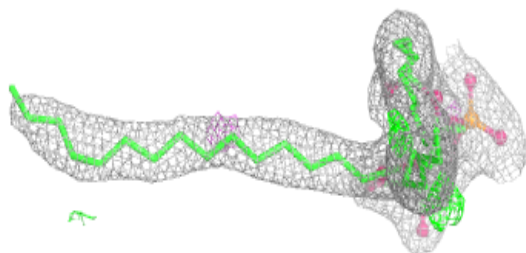
**Electron density around PL9 D 406:**

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



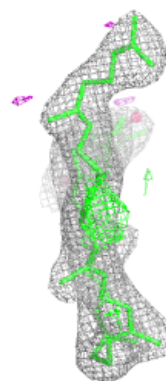
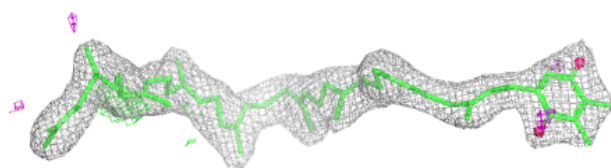
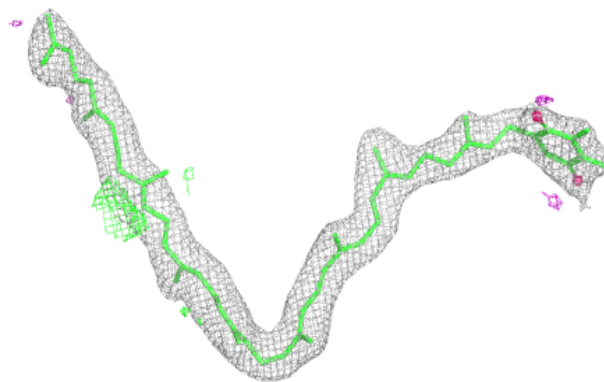
Electron density around LHG b 629:

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



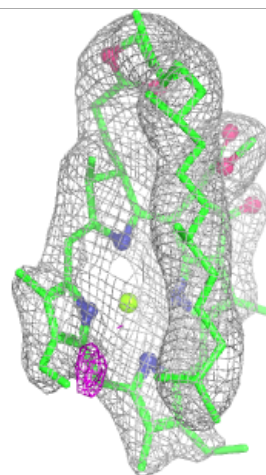
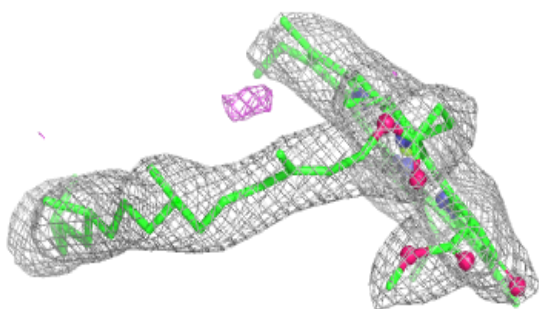
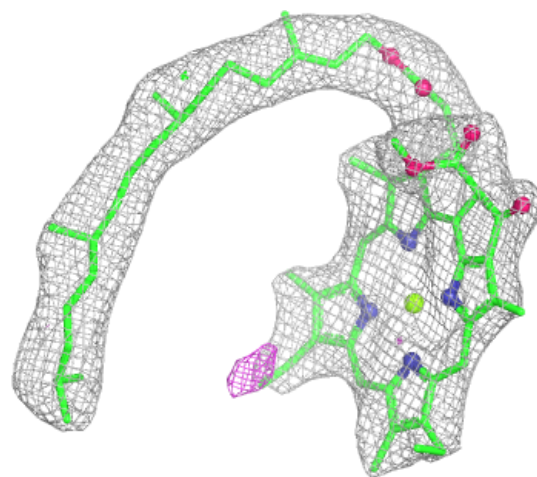
Electron density around PL9 d 405:

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



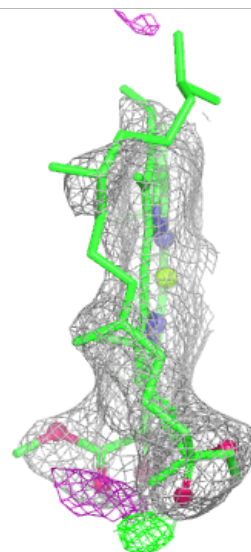
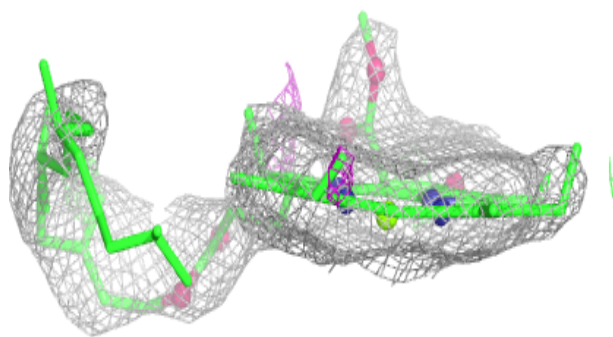
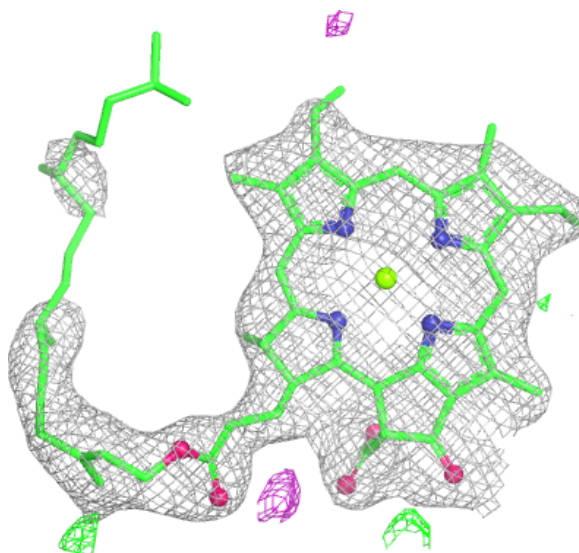
Electron density around CLA c 509:

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



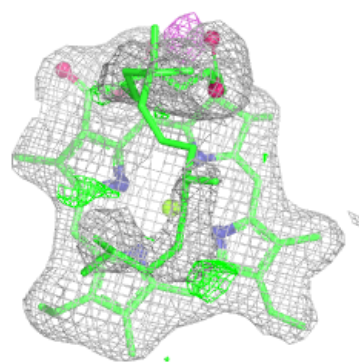
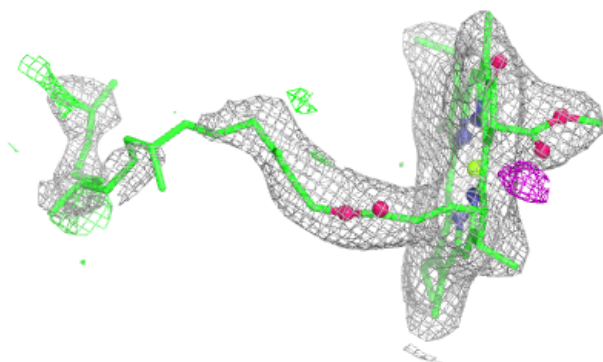
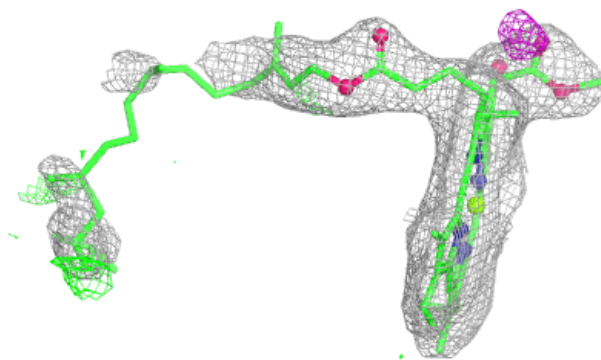
Electron density around CLA c 514:

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

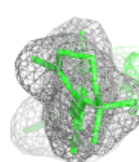
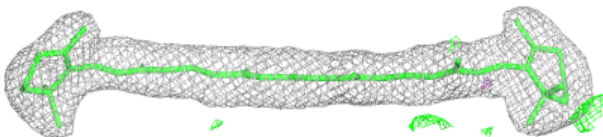
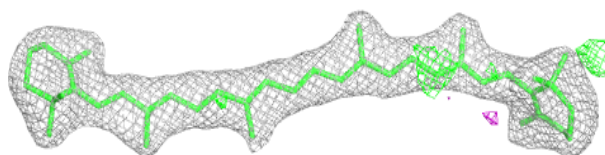


Electron density around CLA C 508:

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

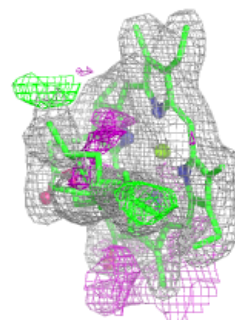
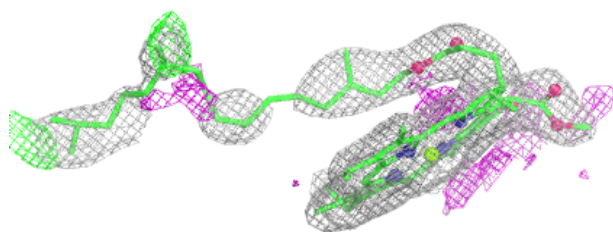
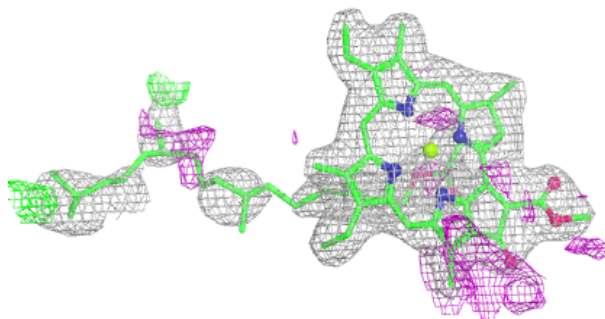
**Electron density around BCR B 618:**

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

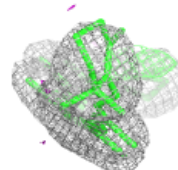
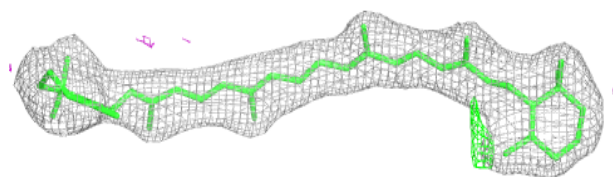
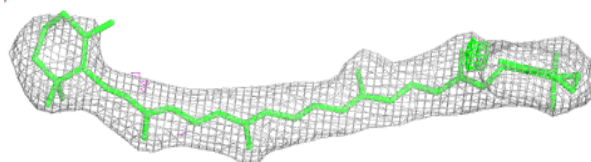


Electron density around CLA B 614:

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

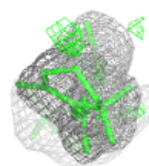
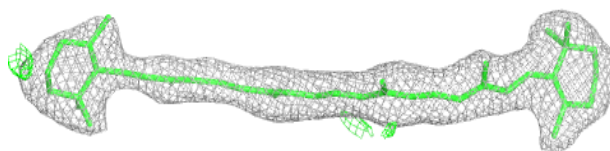
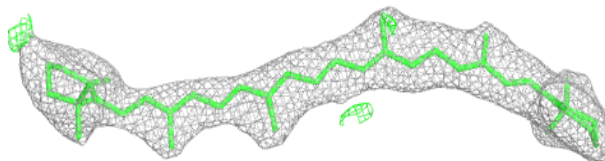
**Electron density around BCR D 405:**

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

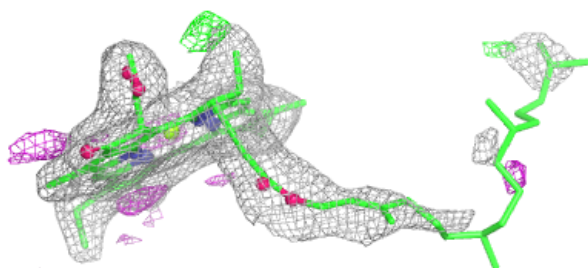
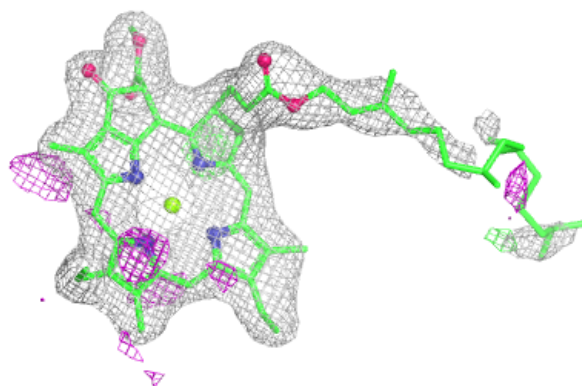


Electron density around BCR H 101:

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

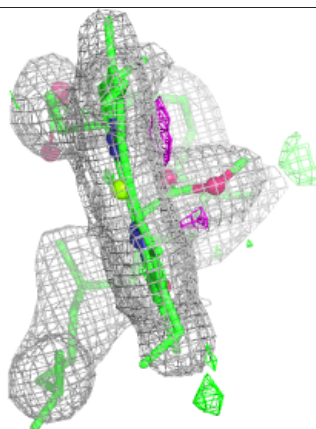
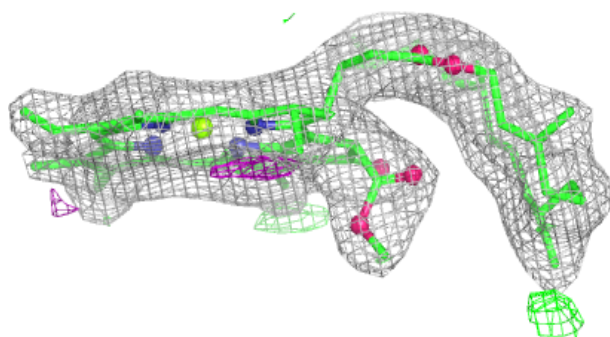
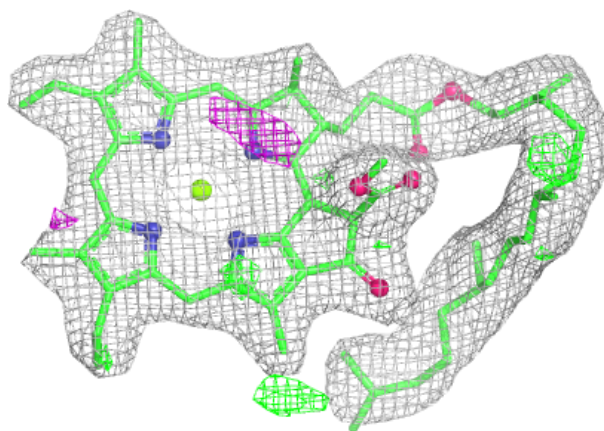
**Electron density around CLA a 408:**

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

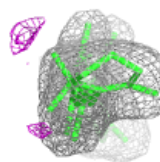
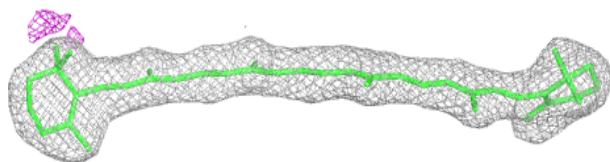
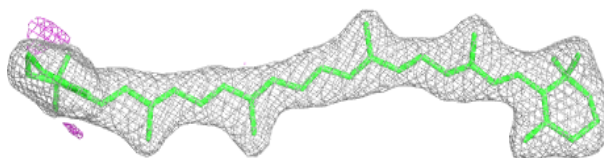


Electron density around CLA B 610:

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

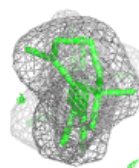
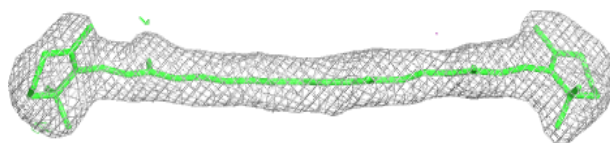
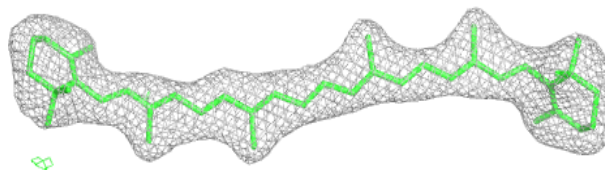
**Electron density around BCR b 617:**

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

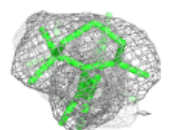
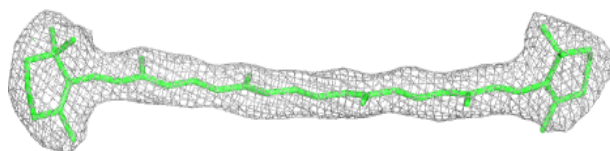
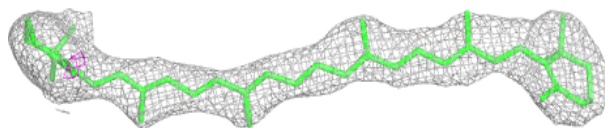


Electron density around BCR b 618:

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

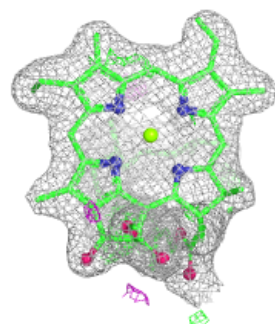
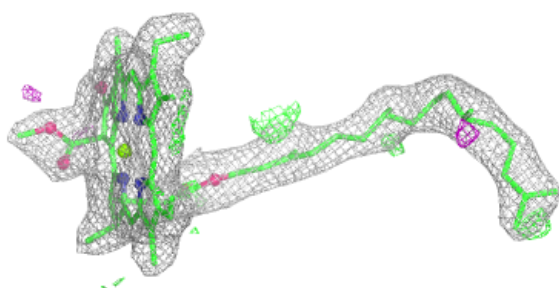
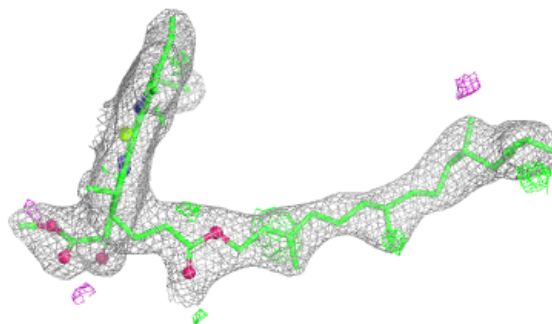
**Electron density around BCR c 516:**

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

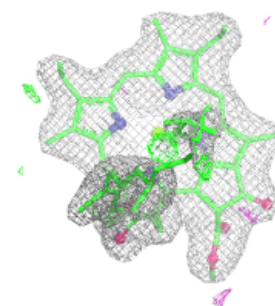
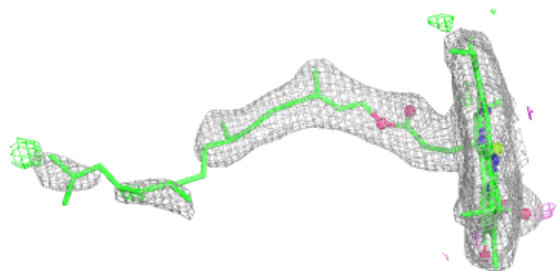
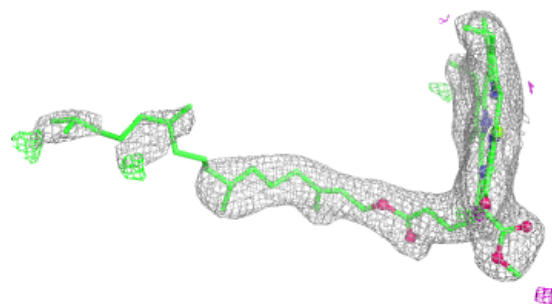


Electron density around CLA b 605:

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

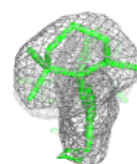
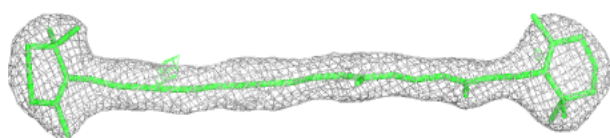
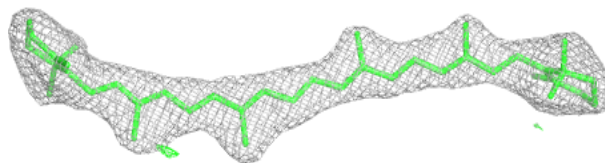
**Electron density around CLA b 606:**

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

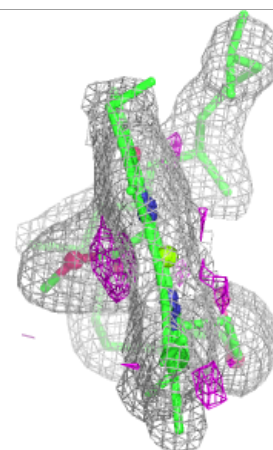
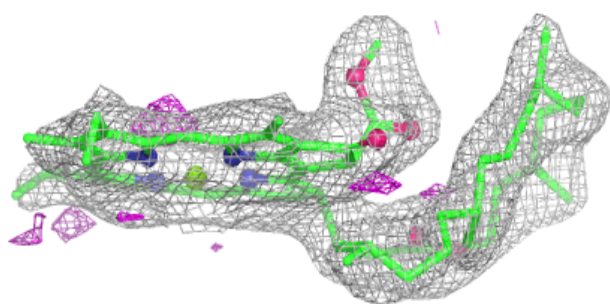
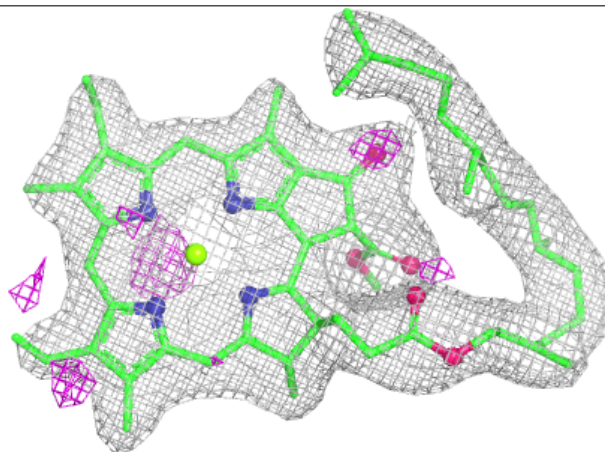


Electron density around BCR c 517:

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

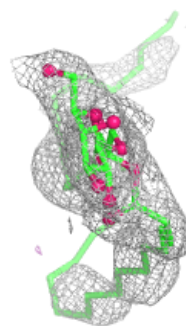
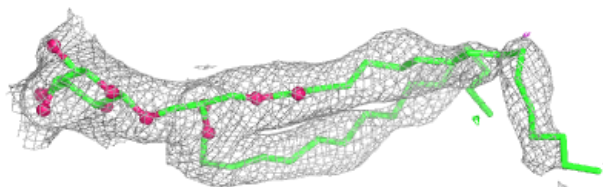
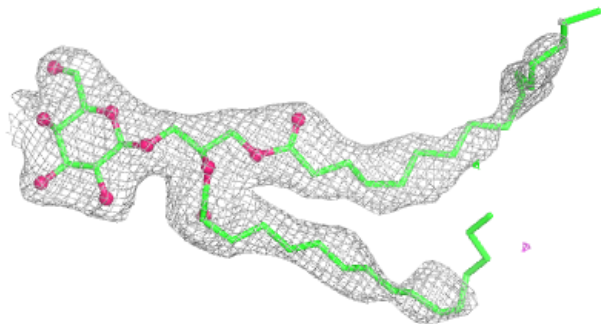
**Electron density around CLA b 610:**

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

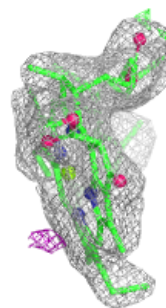
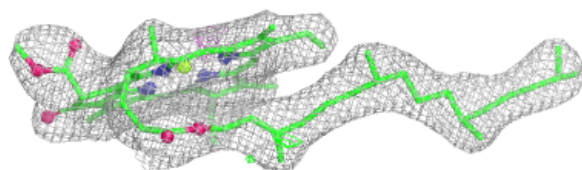
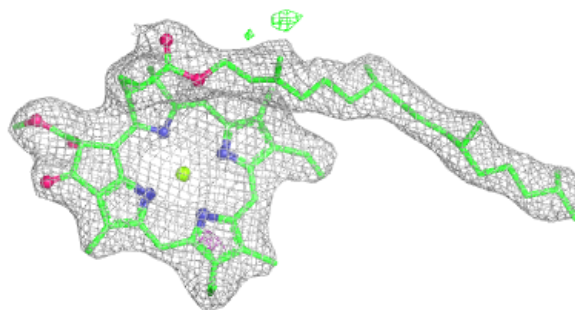


Electron density around LMG d 412:

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

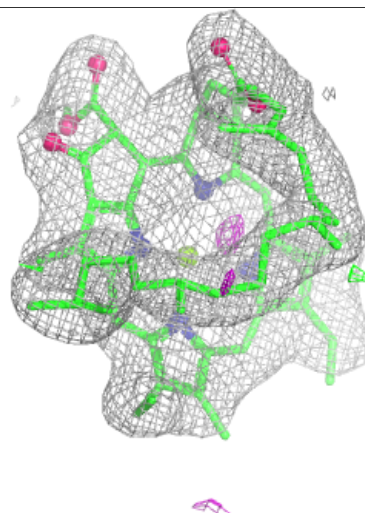
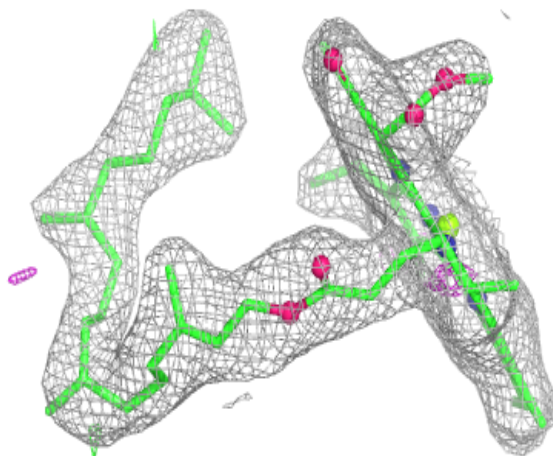
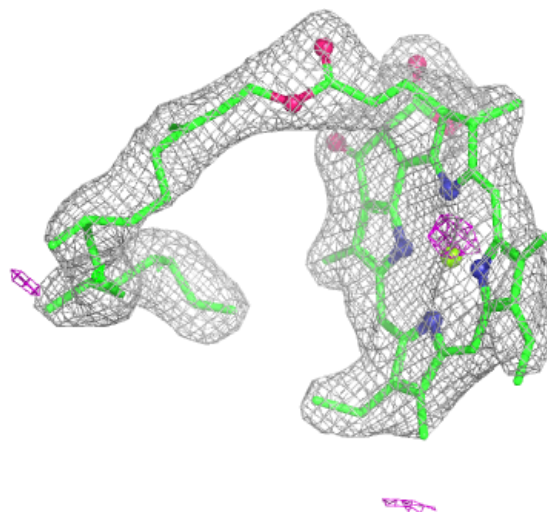
**Electron density around CLA C 503:**

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



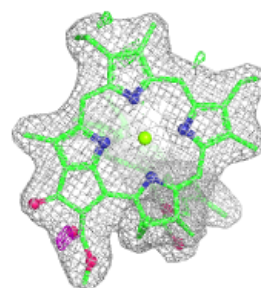
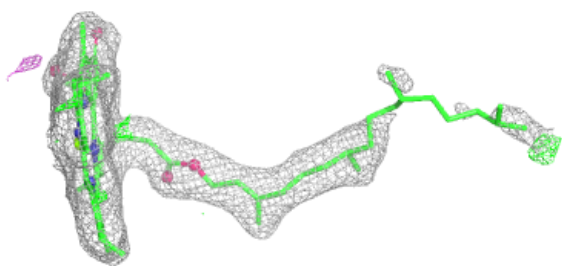
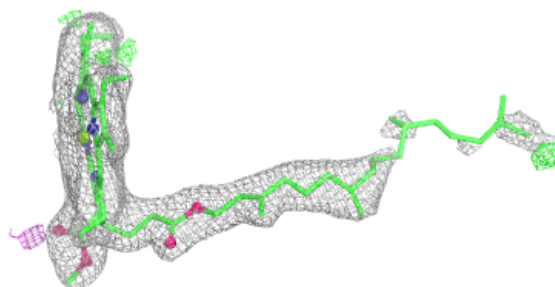
Electron density around CLA C 505:

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

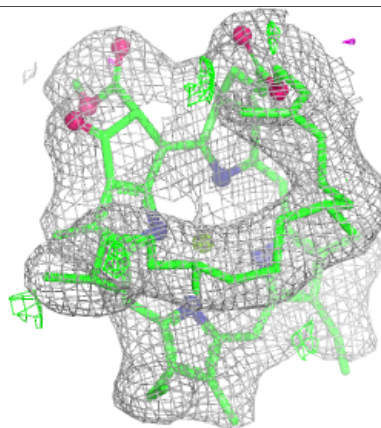
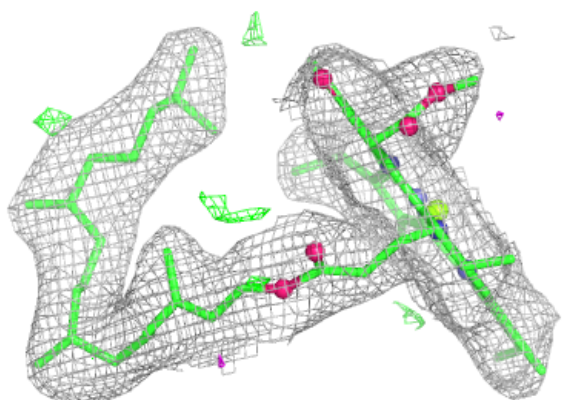
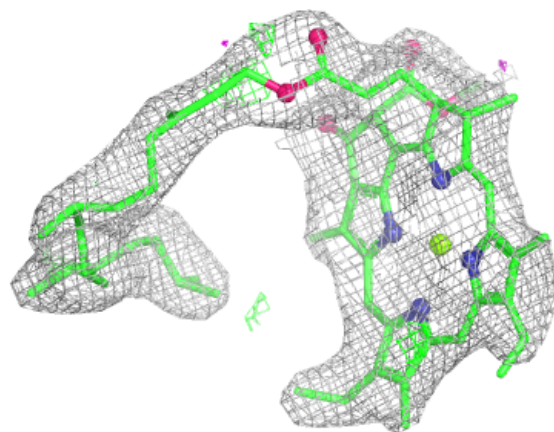


Electron density around CLA B 606:

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

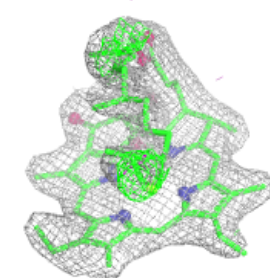
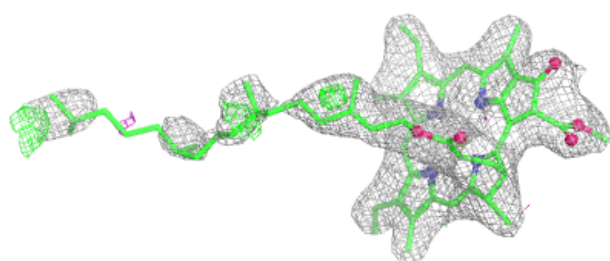
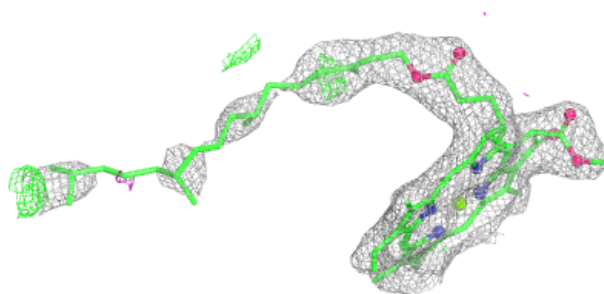
**Electron density around CLA c 505:**

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

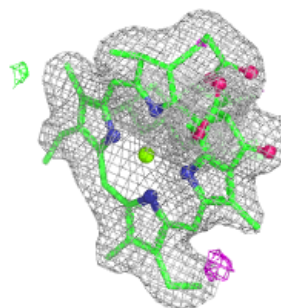
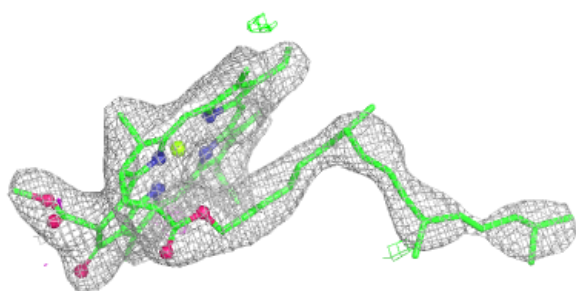
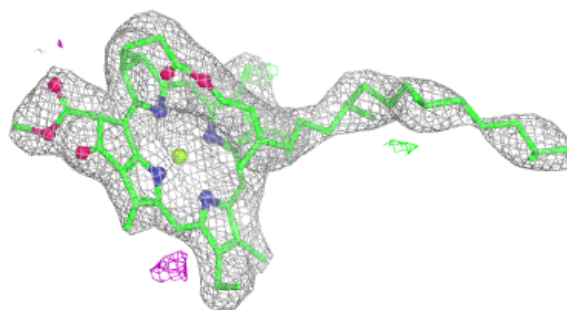


Electron density around CLA c 506:

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

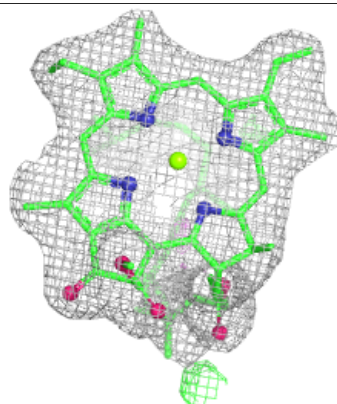
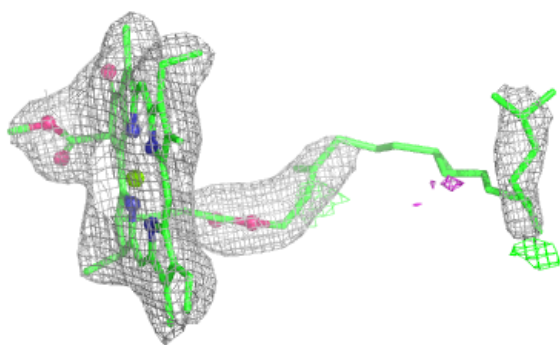
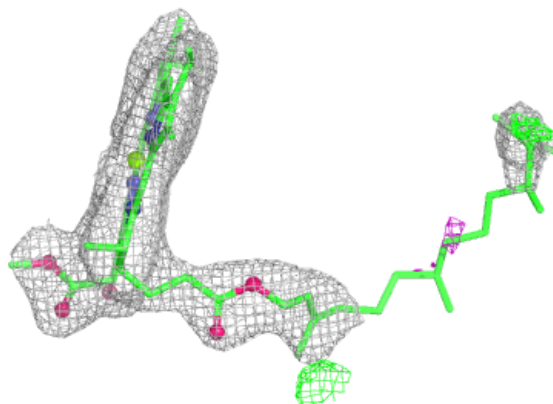
**Electron density around CLA c 507:**

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

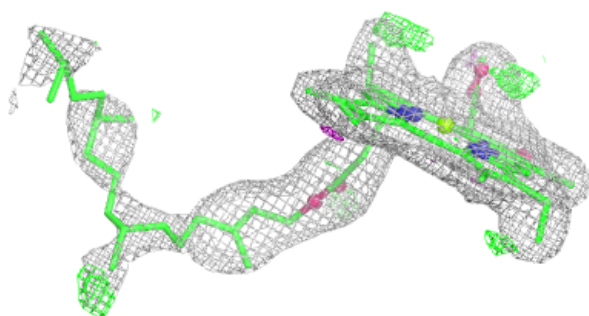
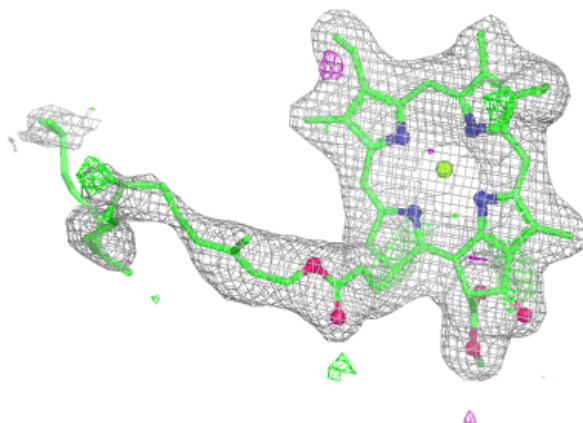


Electron density around CLA c 508:

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

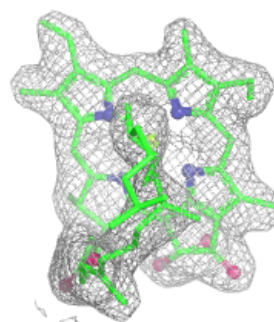
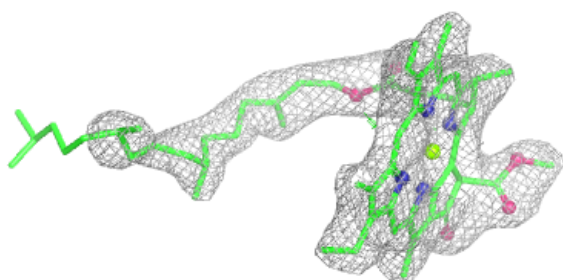
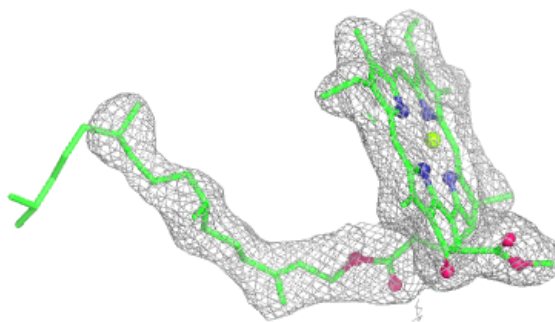
**Electron density around CLA A 408:**

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



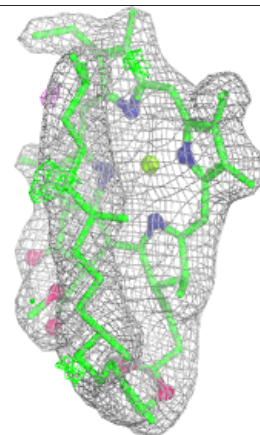
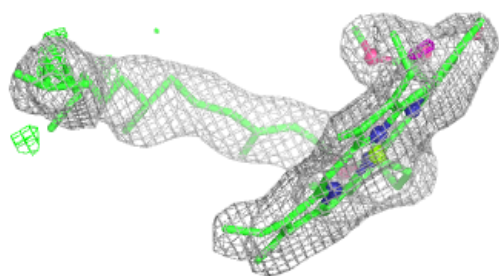
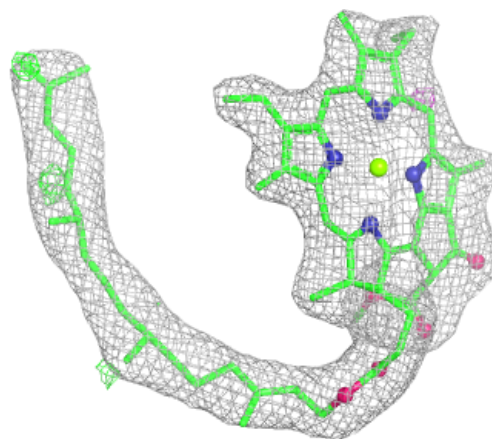
Electron density around CLA c 510:

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



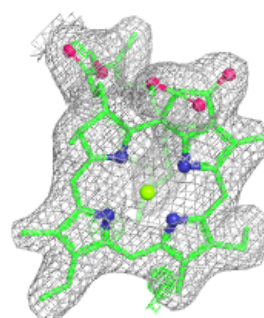
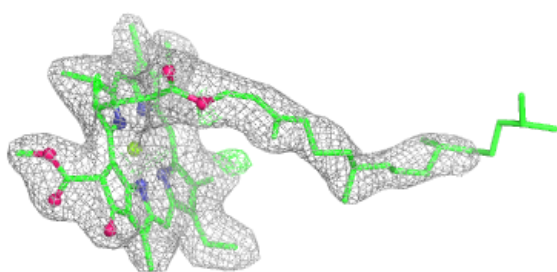
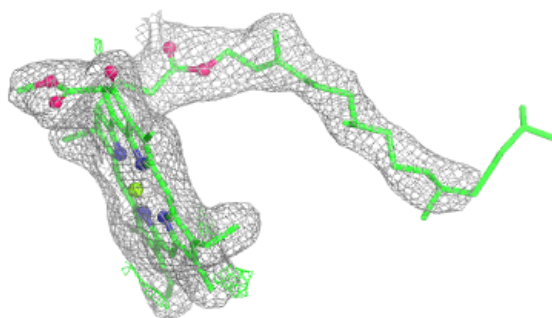
Electron density around CLA C 509:

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

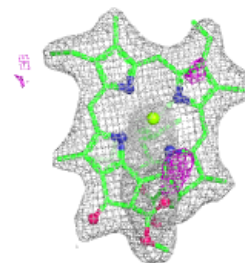
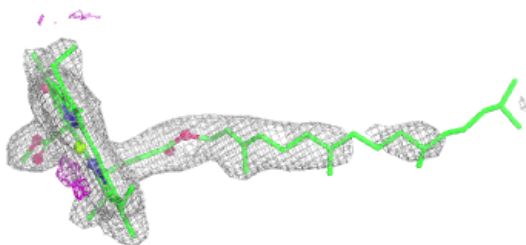
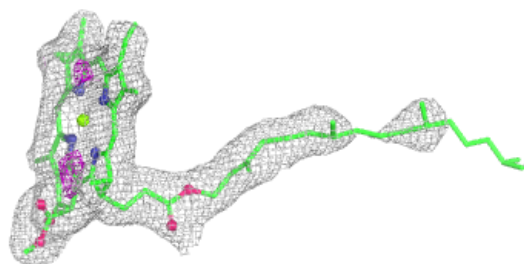


Electron density around CLA C 510:

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

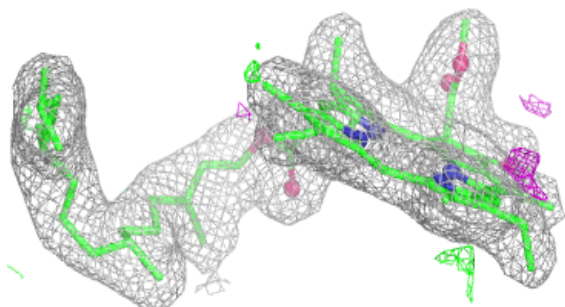
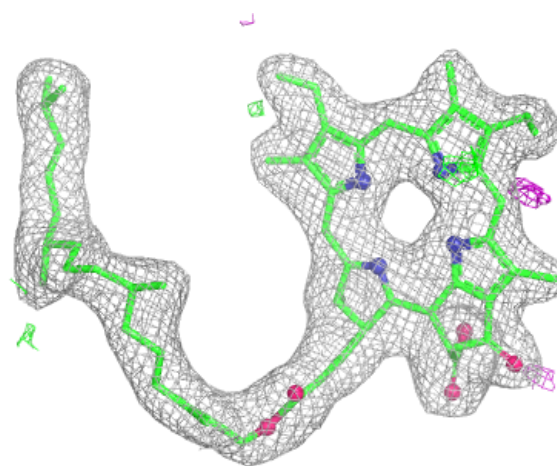
**Electron density around CLA d 403:**

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



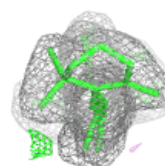
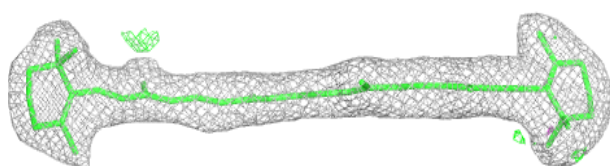
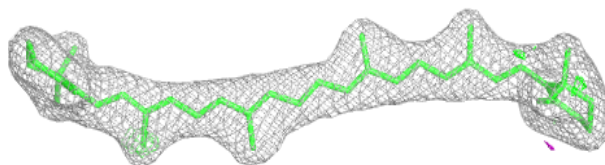
Electron density around PHO A 415:

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

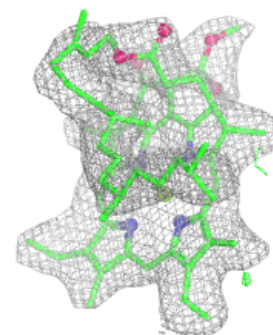
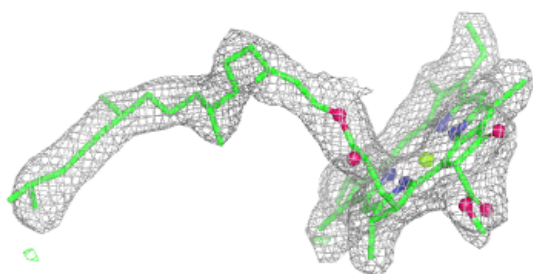
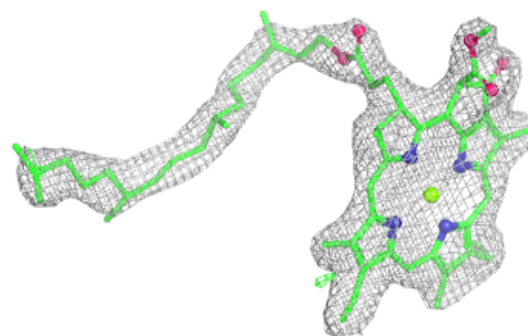


Electron density around BCR A 409:

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

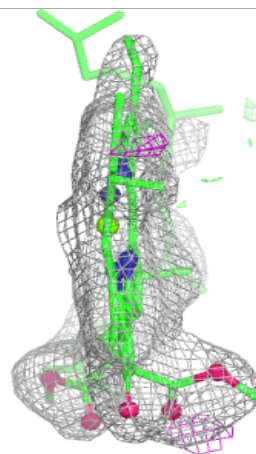
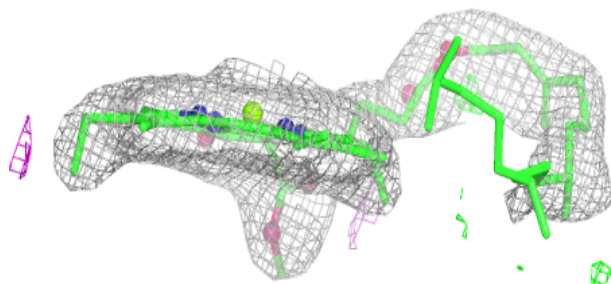
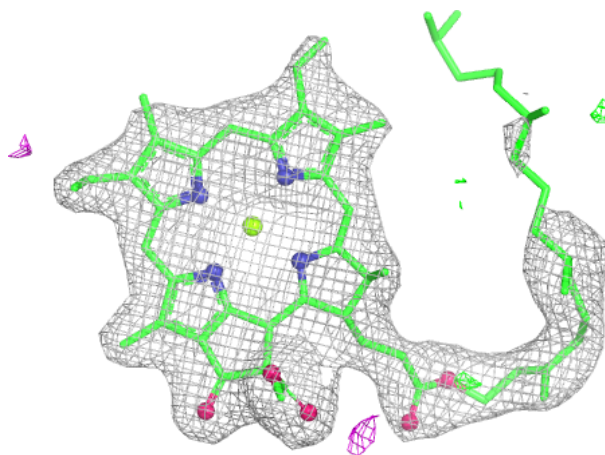
**Electron density around CLA C 513:**

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



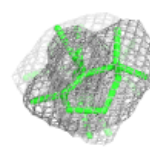
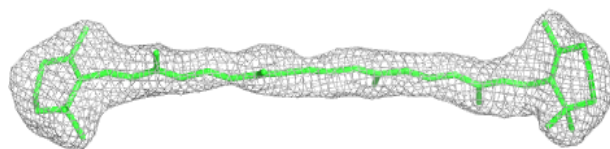
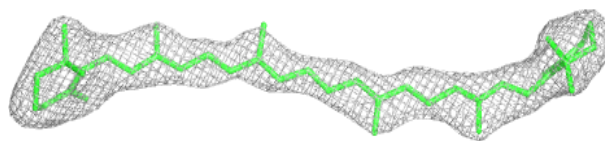
Electron density around CLA C 514:

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



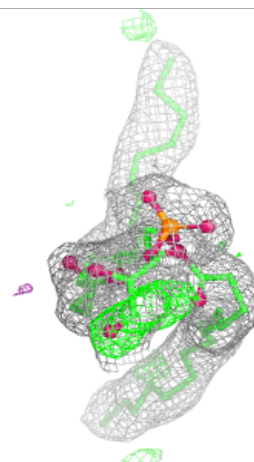
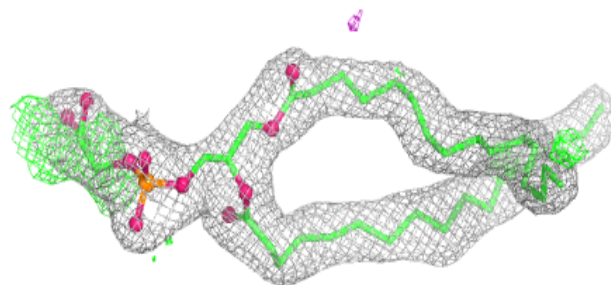
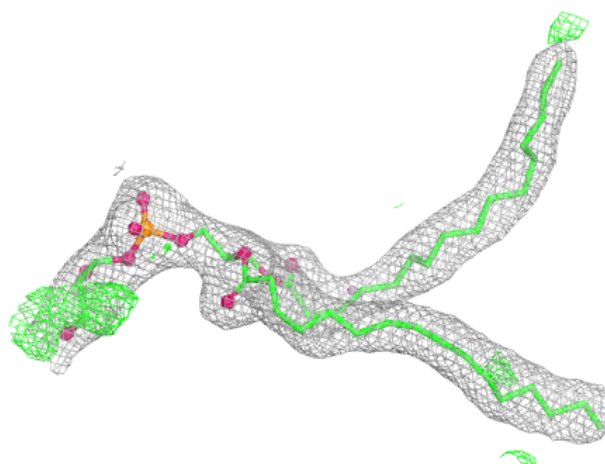
Electron density around BCR C 516:

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



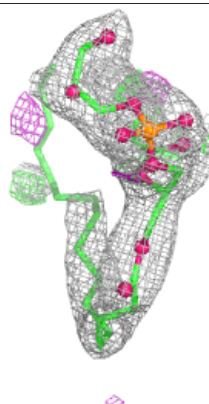
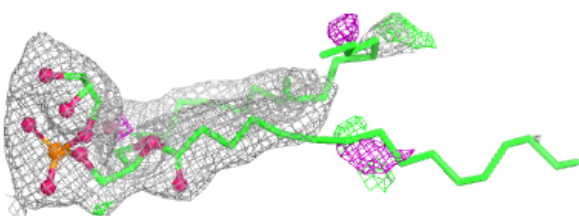
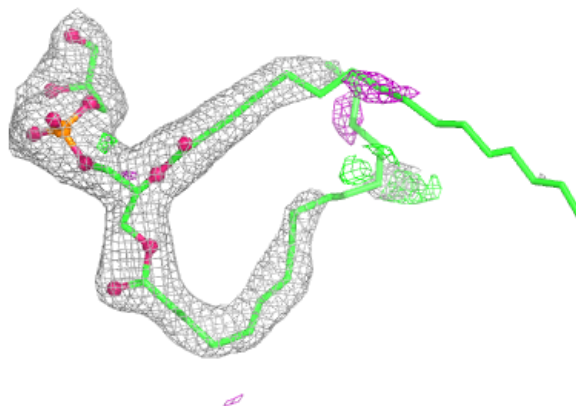
Electron density around LHG D 407:

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

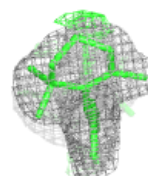
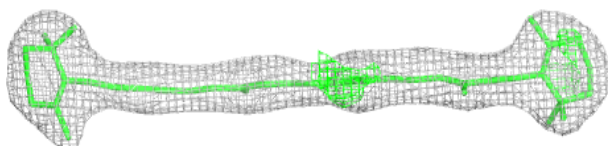
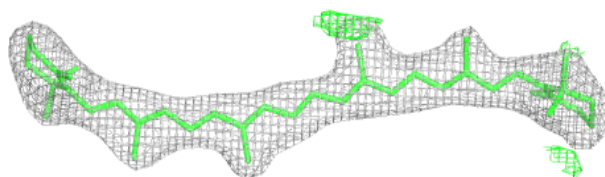


Electron density around LHG D 408:

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

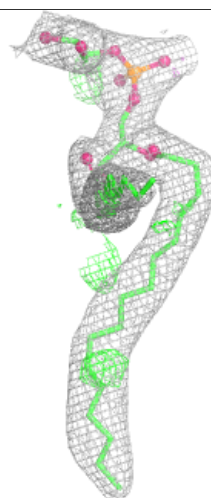
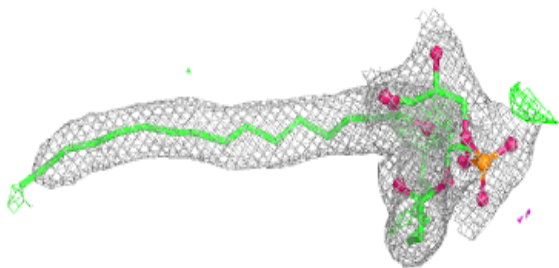
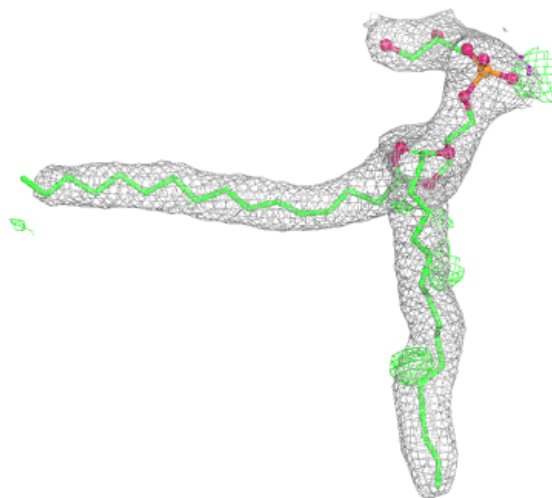
**Electron density around BCR C 517:**

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



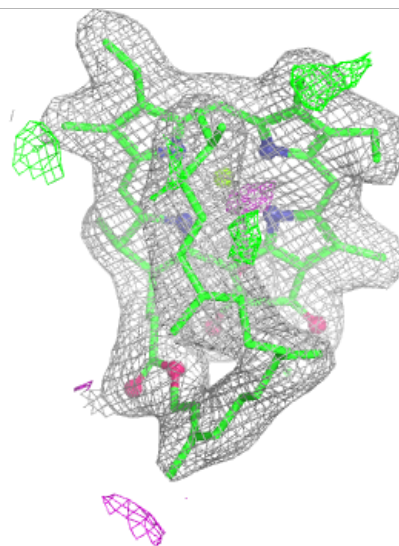
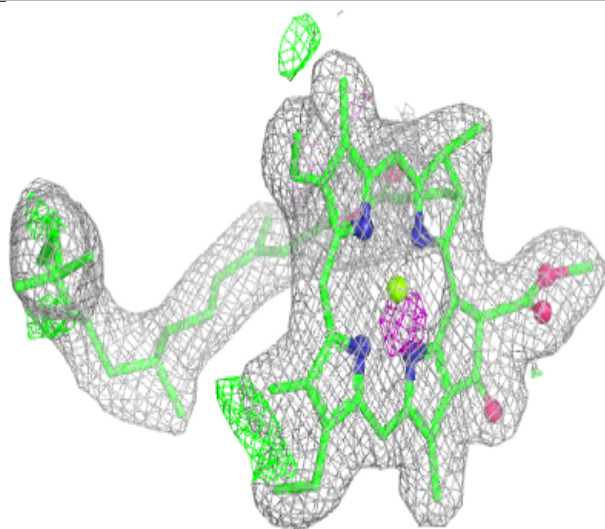
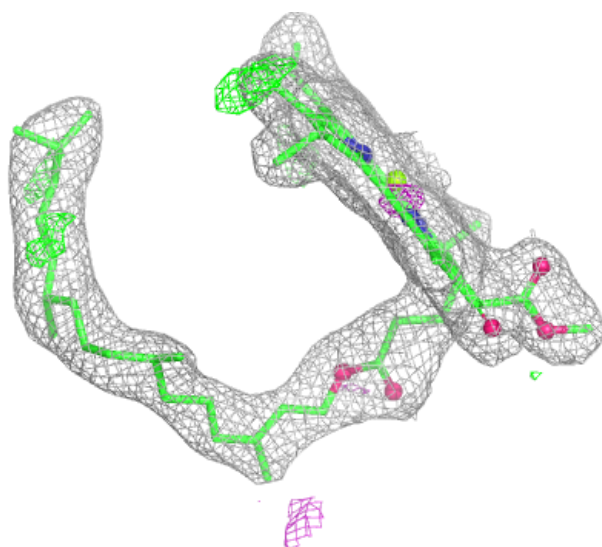
Electron density around LHG L 101:

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



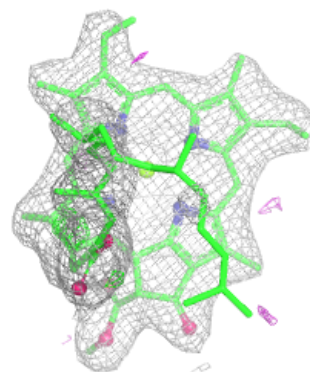
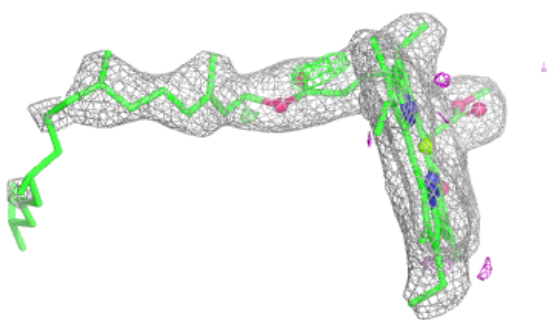
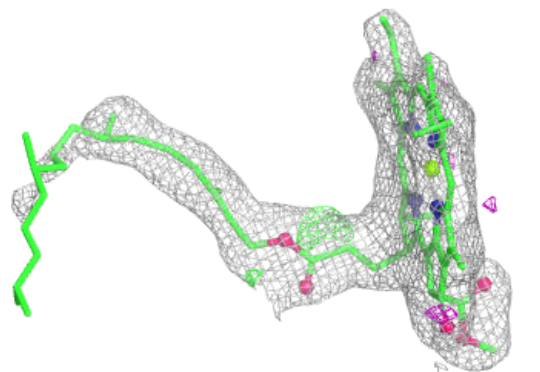
Electron density around CLA B 611:

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

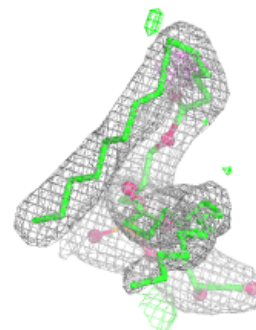
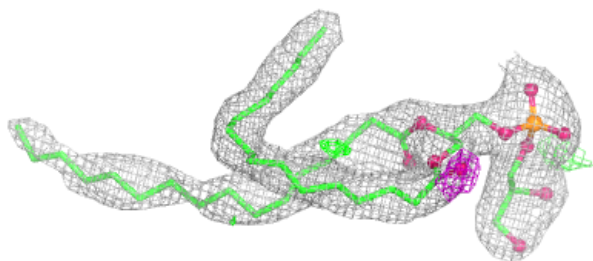
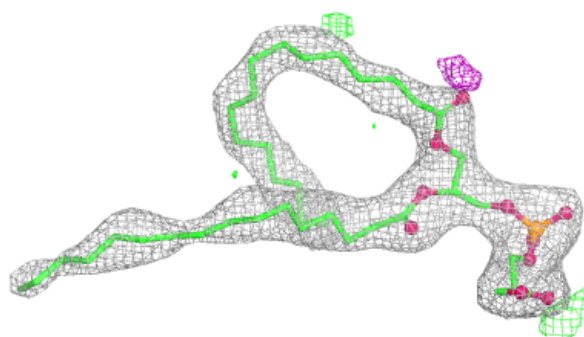


Electron density around CLA D 404:

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

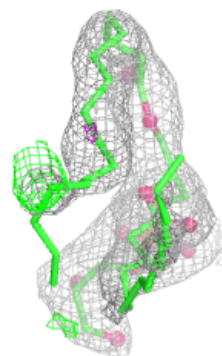
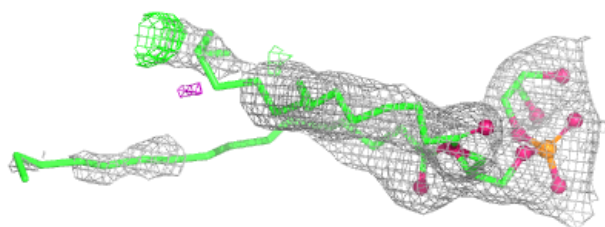
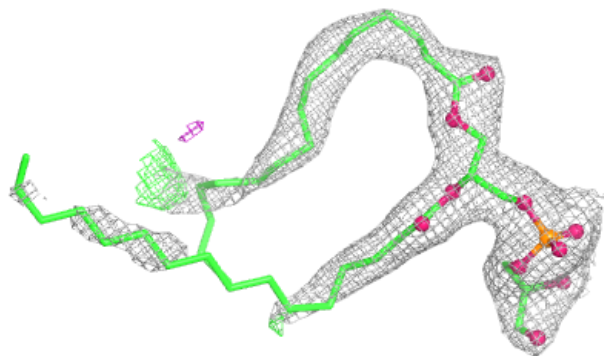
**Electron density around LHG d 406:**

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

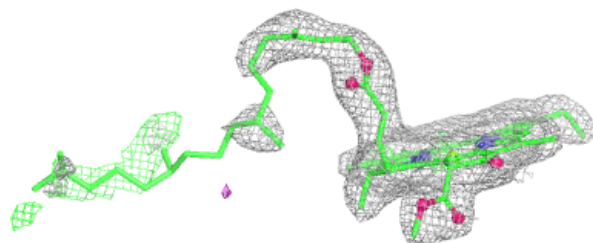
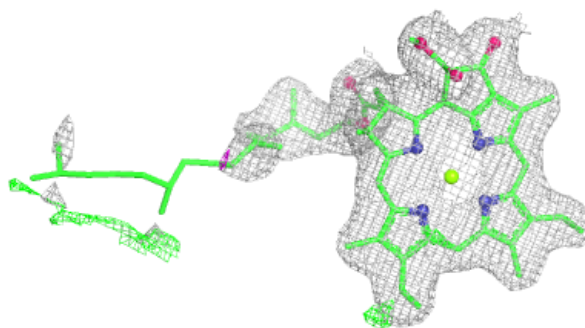


Electron density around LHG d 408:

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

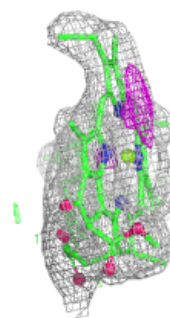
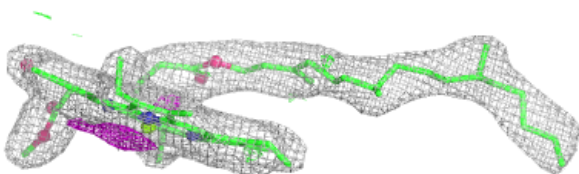
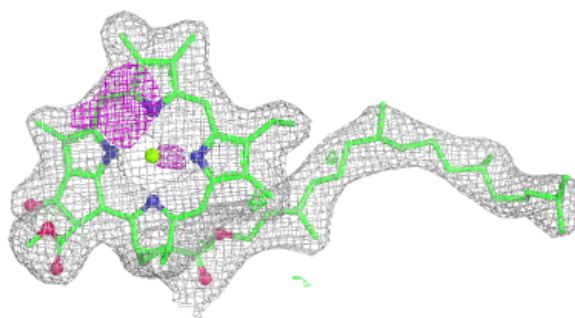
**Electron density around CLA a 406:**

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

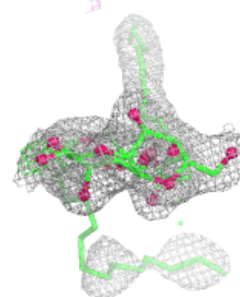
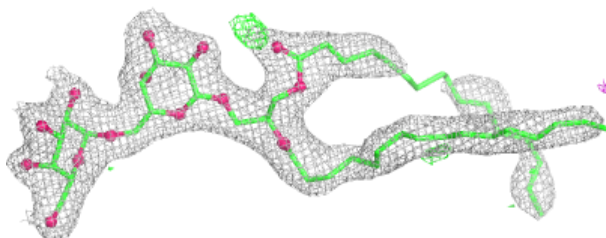
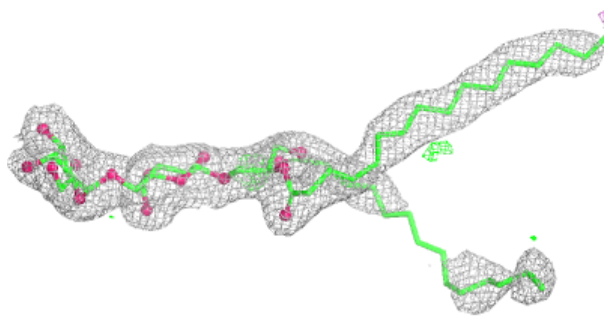


Electron density around CLA B 603:

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

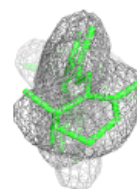
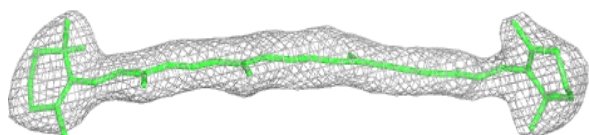
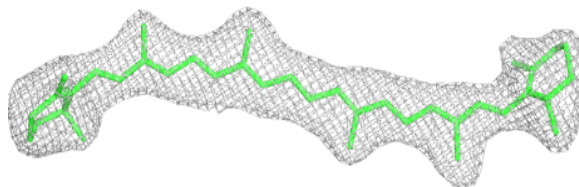
**Electron density around DGD C 518:**

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

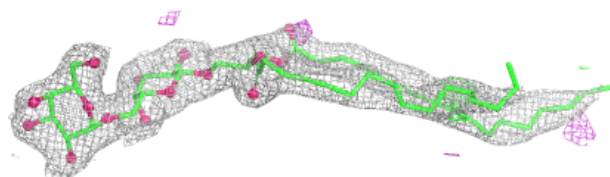
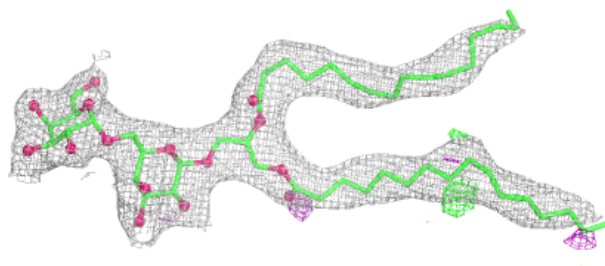


Electron density around BCR Y 101:

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

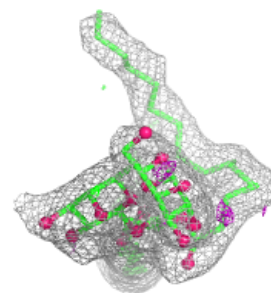
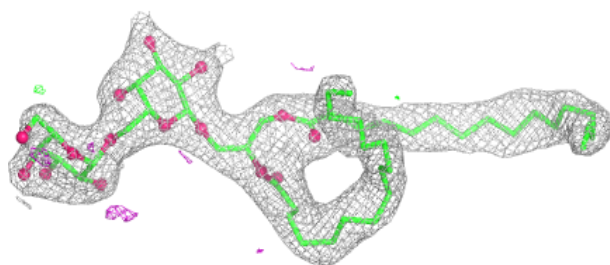
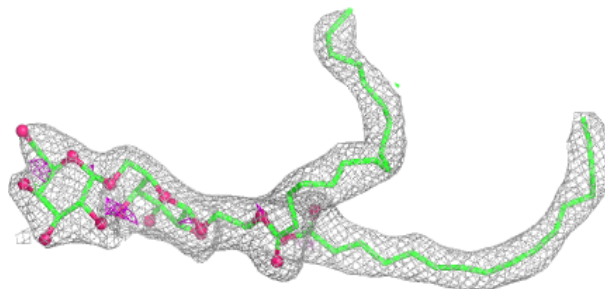
**Electron density around DGD C 520:**

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

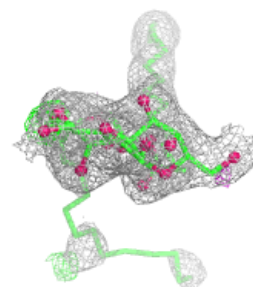
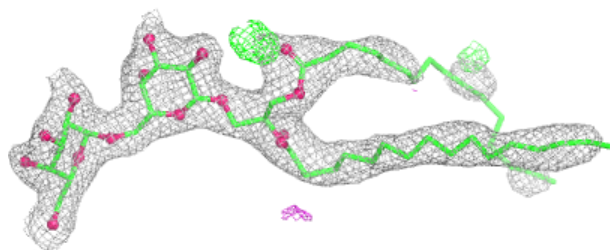
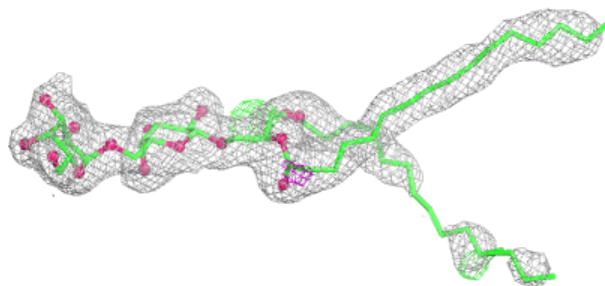


Electron density around DGD H 102:

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

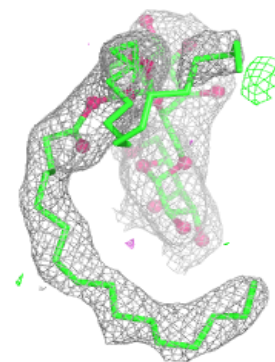
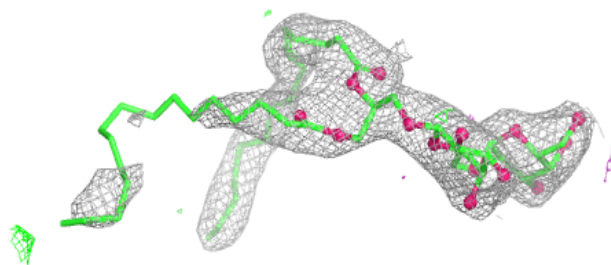
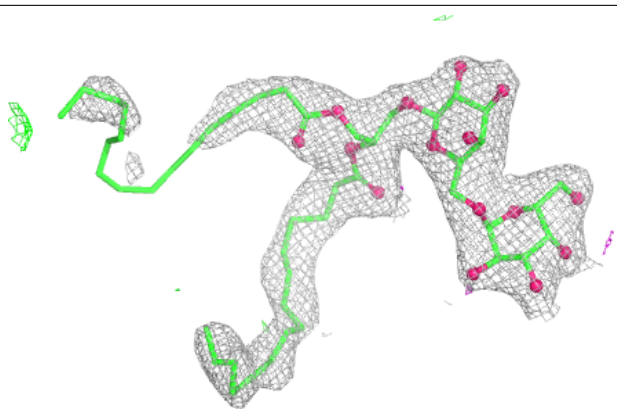
**Electron density around DGD c 518:**

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

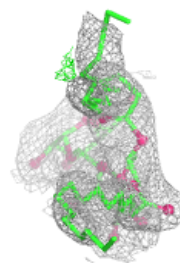
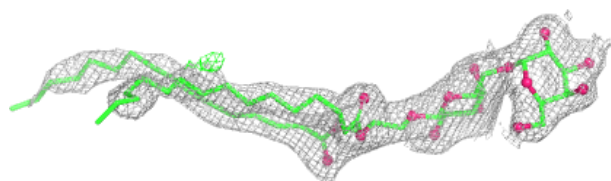
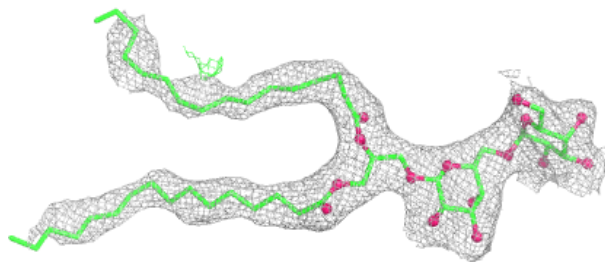


Electron density around DGD c 519:

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

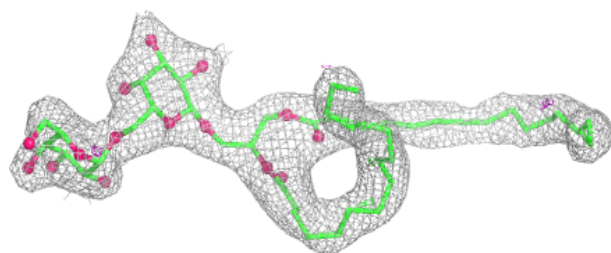
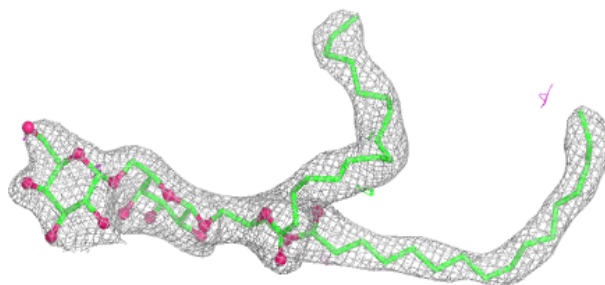
**Electron density around DGD c 520:**

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

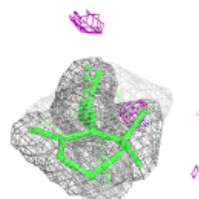
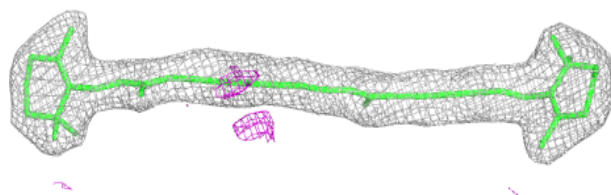
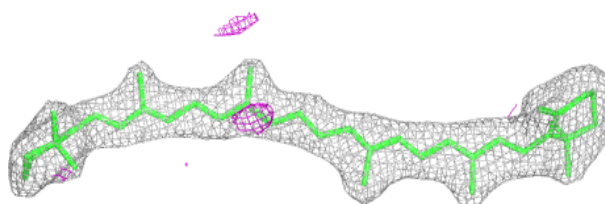


Electron density around DGD h 103:

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

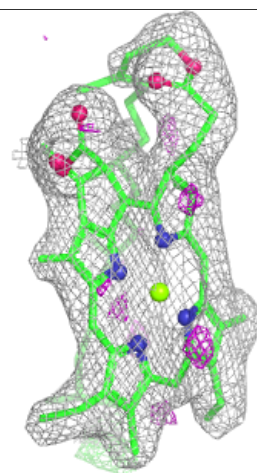
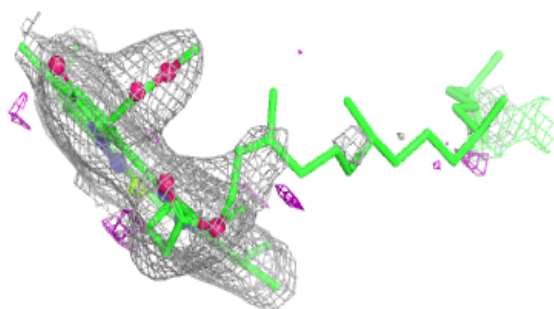
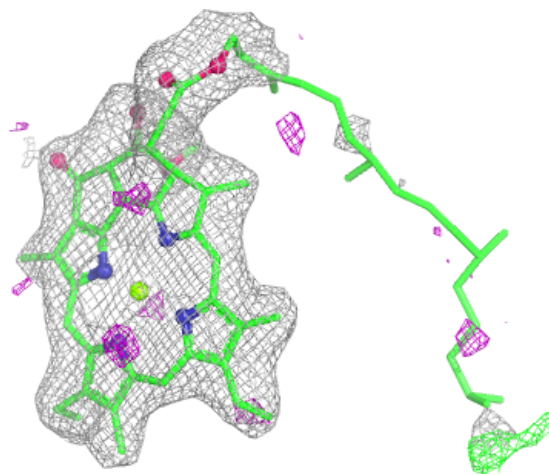
**Electron density around BCR a 409:**

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



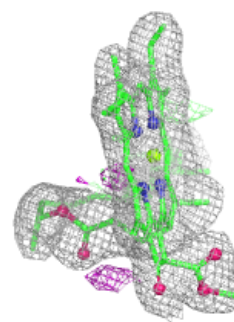
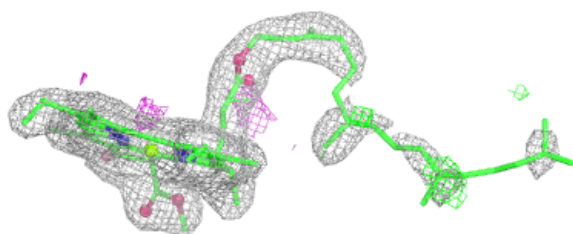
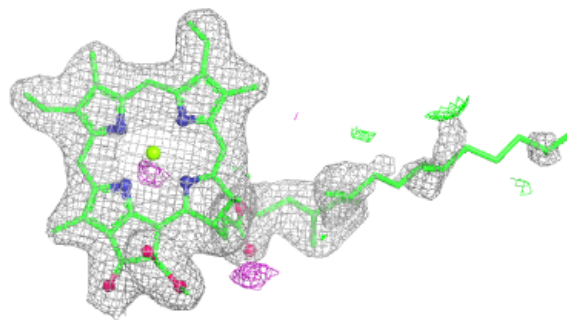
Electron density around CLA B 616:

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



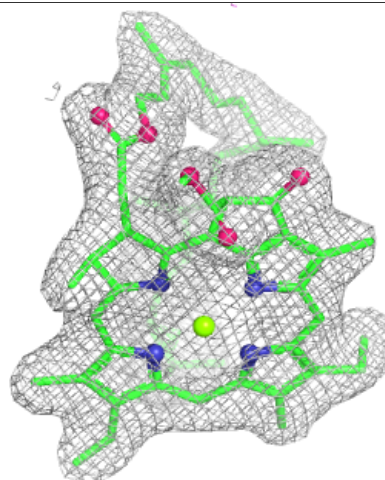
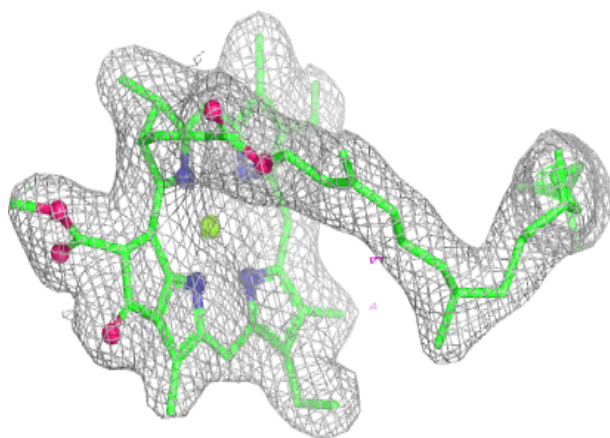
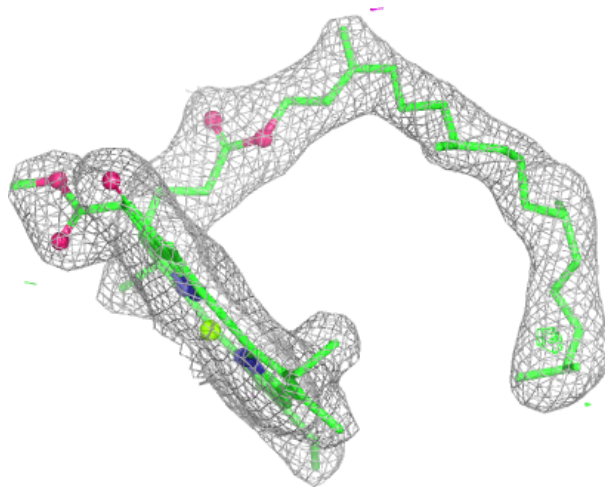
Electron density around CLA A 406:

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



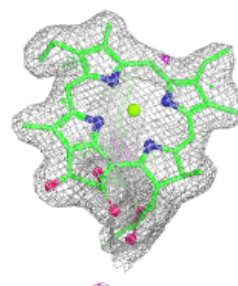
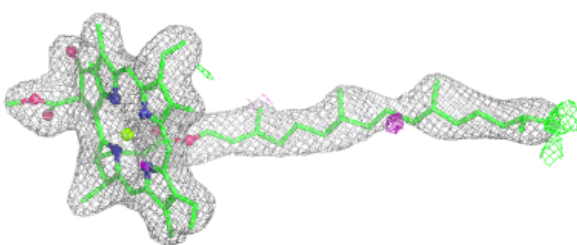
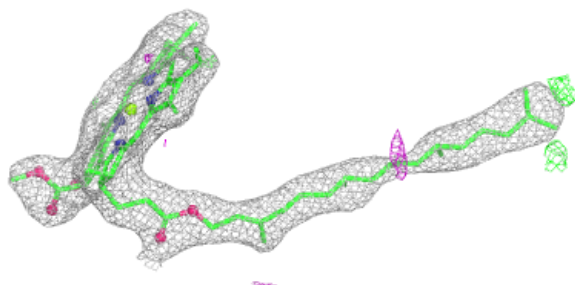
Electron density around CLA b 611:

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

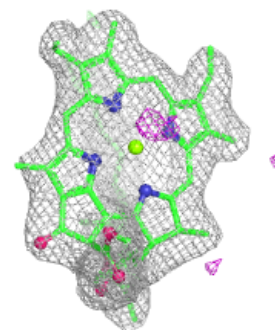
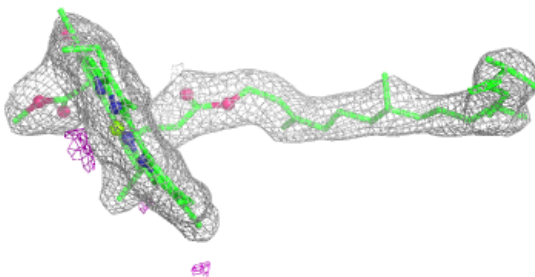
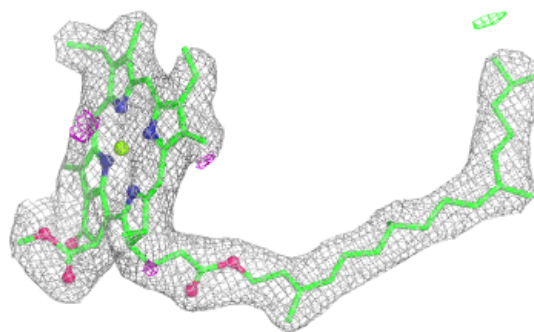


Electron density around CLA B 607:

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

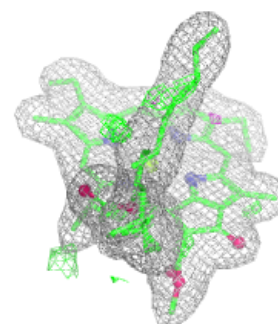
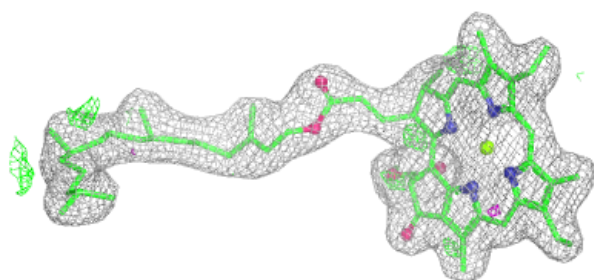
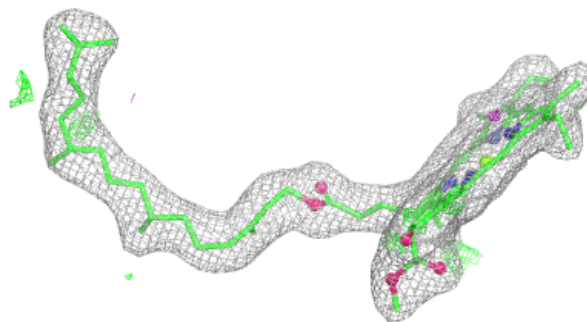
**Electron density around CLA B 609:**

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

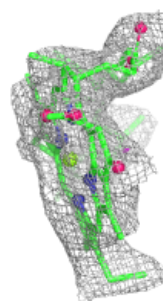
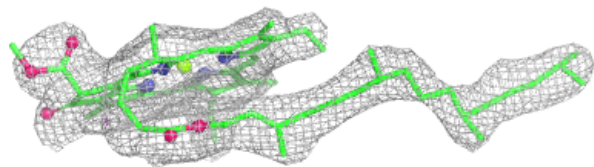
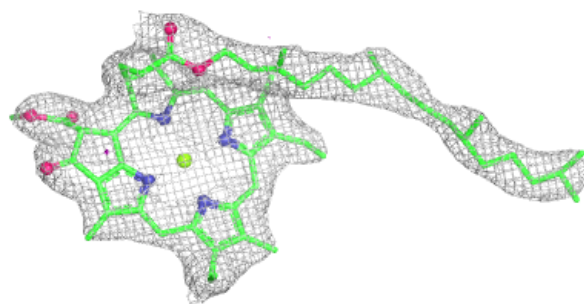


Electron density around CLA D 403:

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

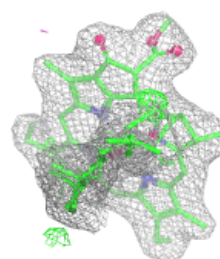
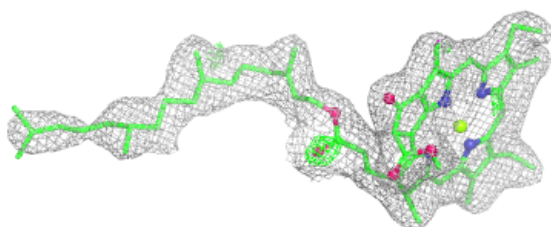
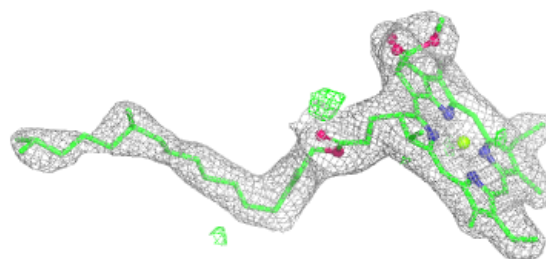
**Electron density around CLA c 503:**

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

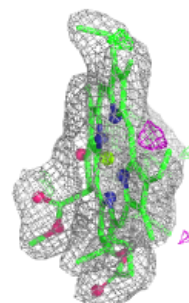
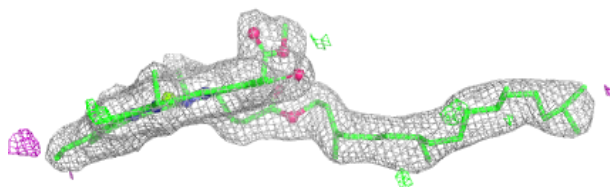
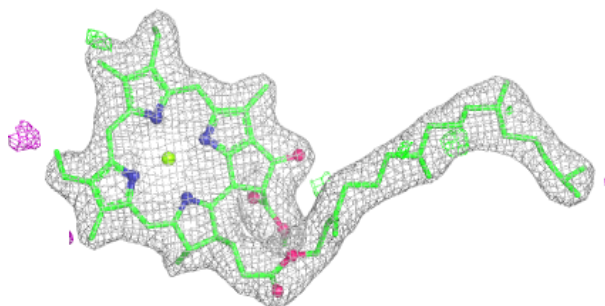


Electron density around CLA c 504:

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

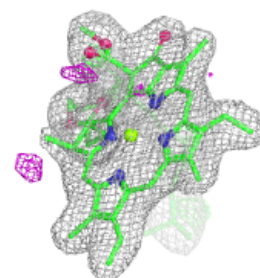
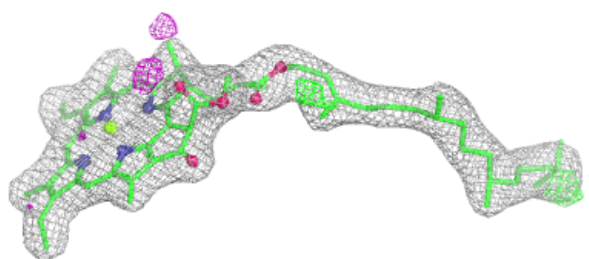
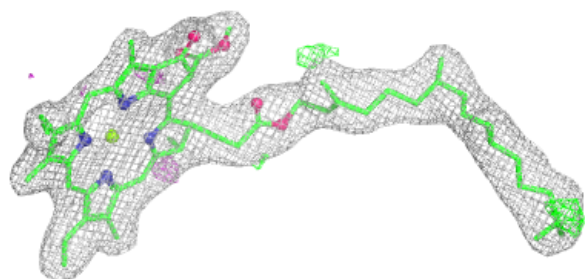
**Electron density around CLA B 602:**

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



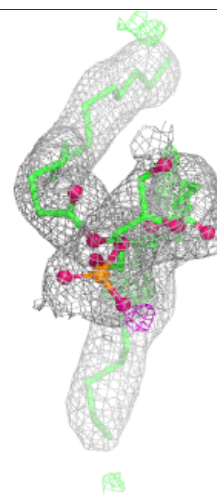
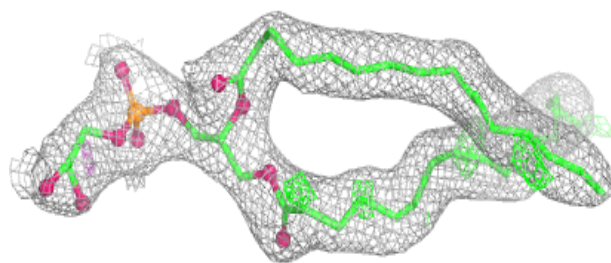
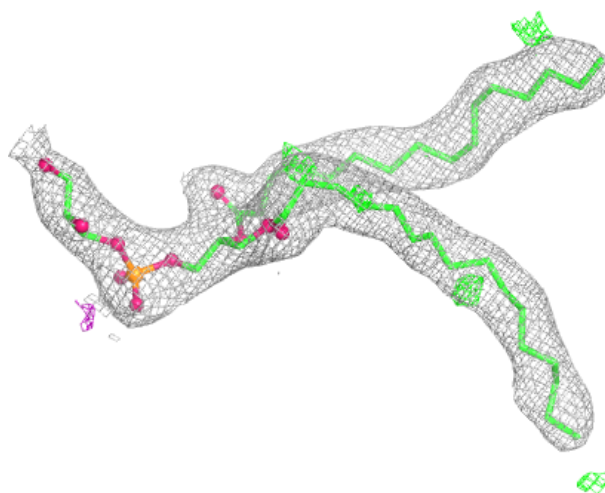
Electron density around CLA a 404:

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



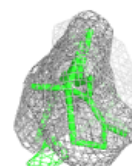
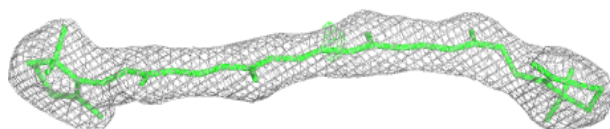
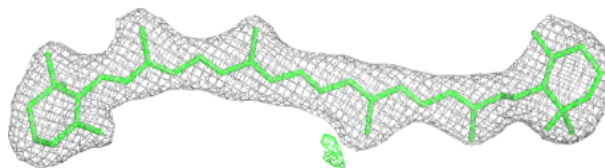
Electron density around LHG d 407:

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

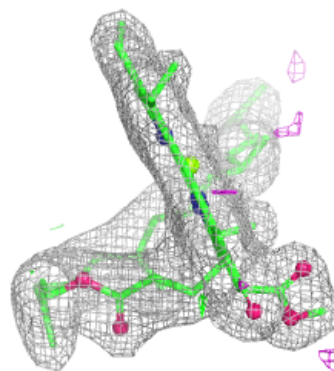
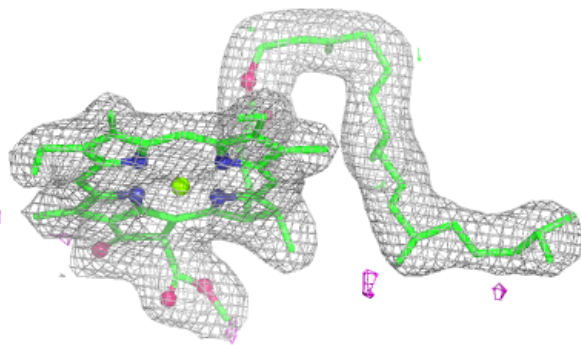
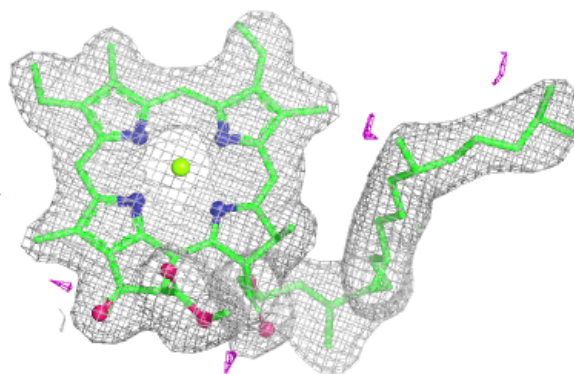


Electron density around BCR b 619:

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

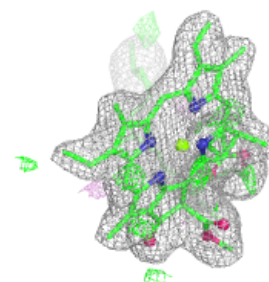
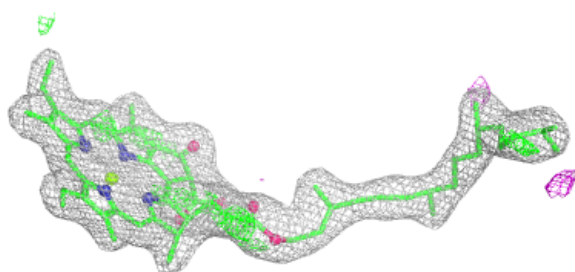
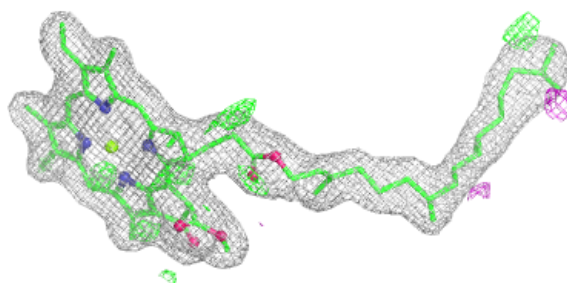
**Electron density around CLA a 405:**

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



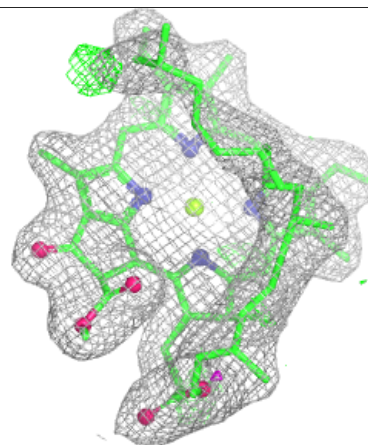
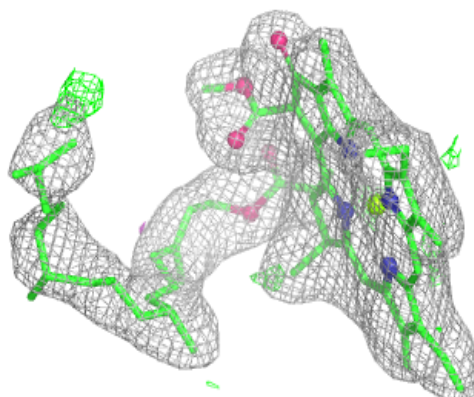
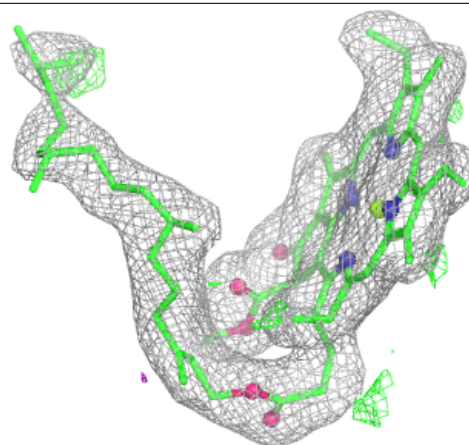
Electron density around CLA A 404:

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



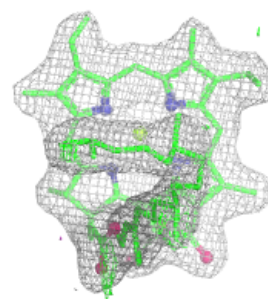
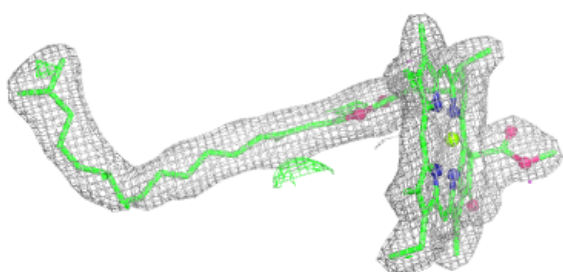
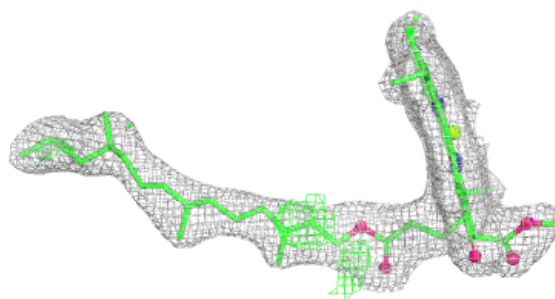
Electron density around CLA B 613:

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

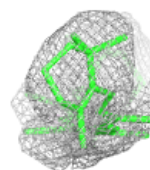
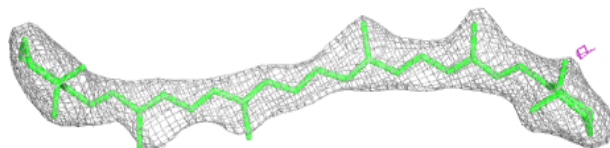
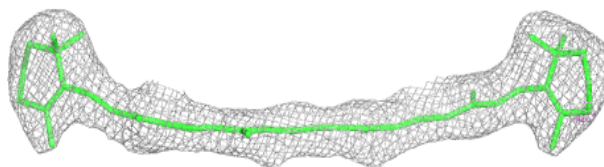


Electron density around CLA B 605:

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

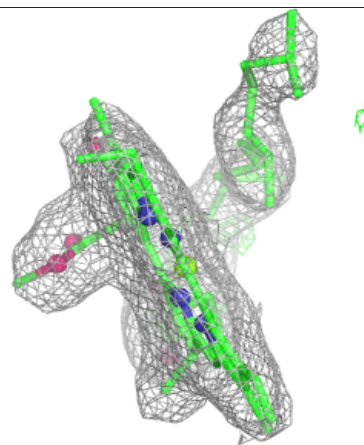
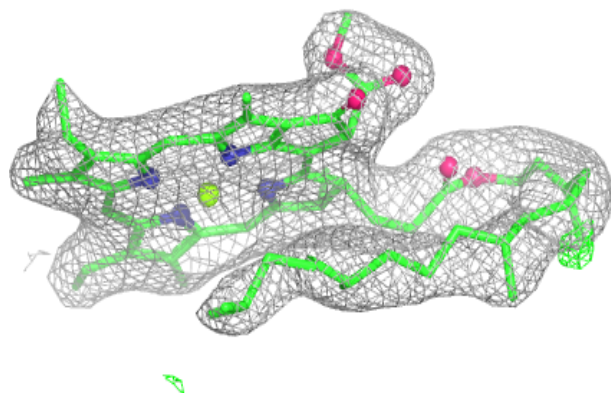
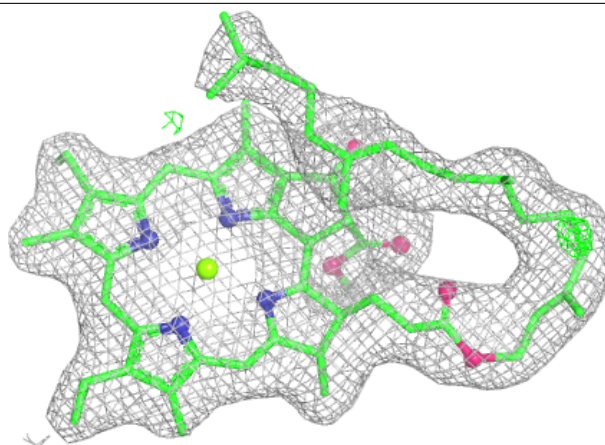
**Electron density around BCR k 101:**

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



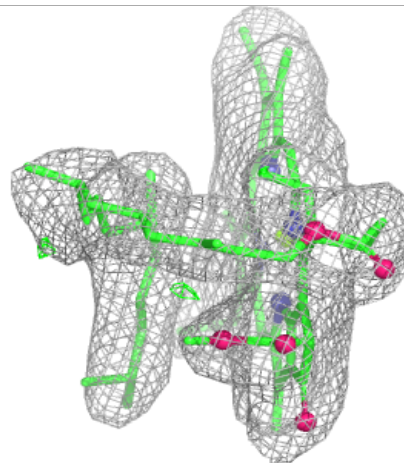
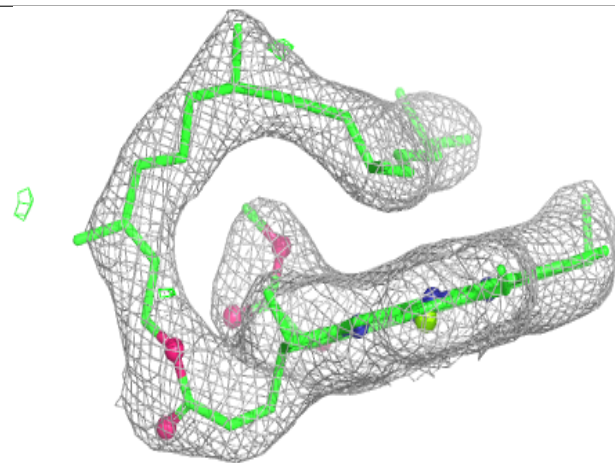
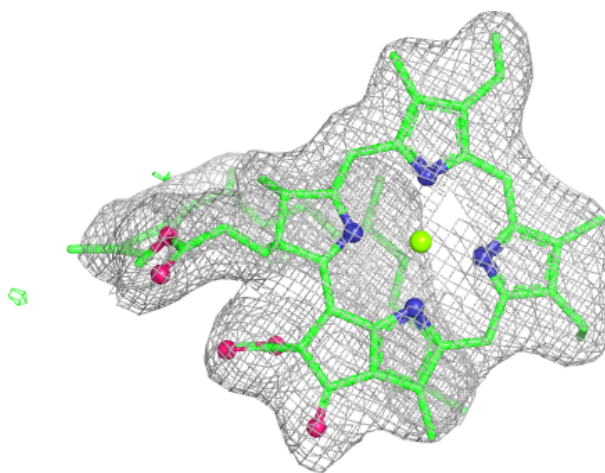
Electron density around CLA c 511:

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



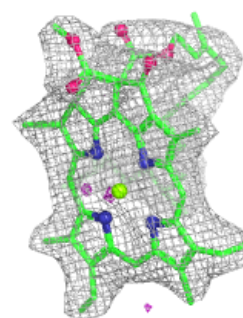
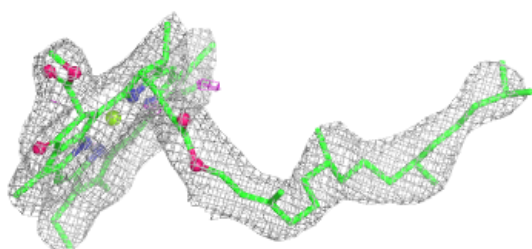
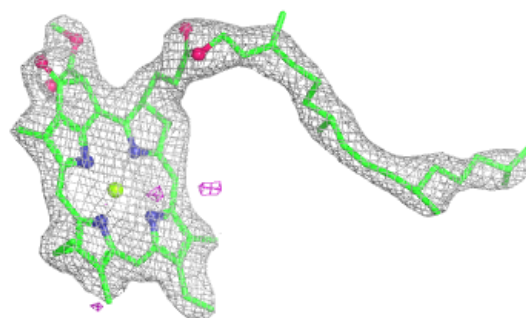
Electron density around CLA c 512:

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

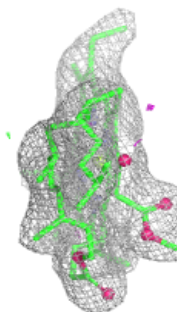
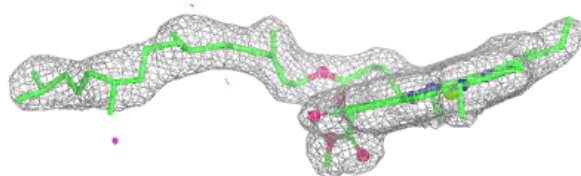
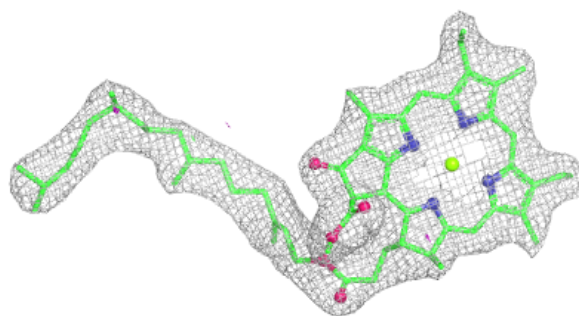


Electron density around CLA c 513:

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

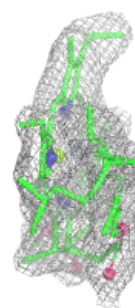
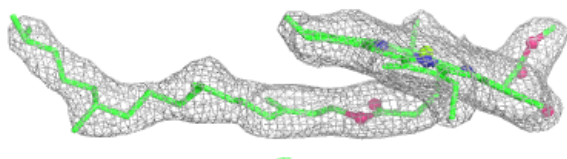
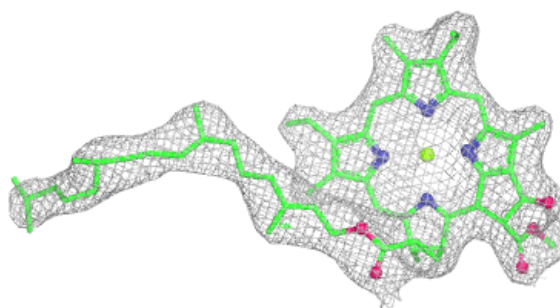
**Electron density around CLA b 602:**

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

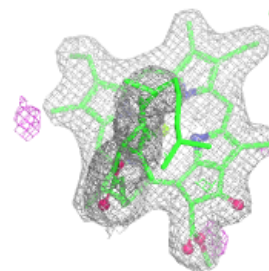
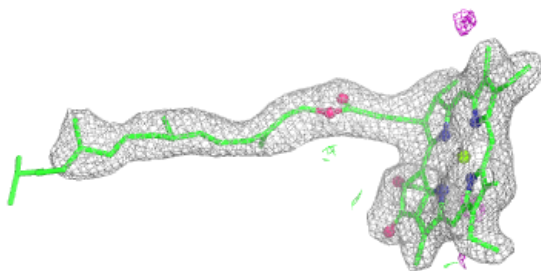
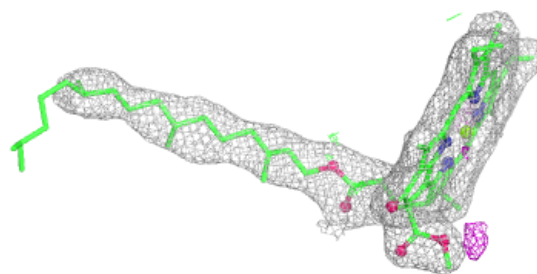


Electron density around CLA b 603:

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

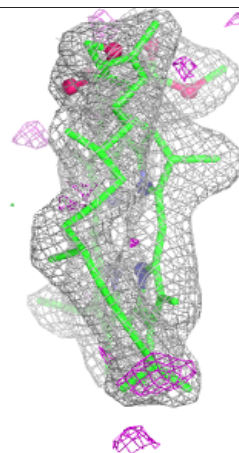
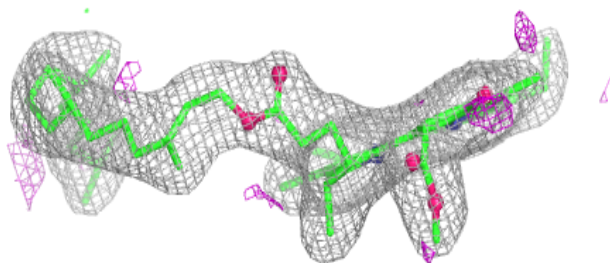
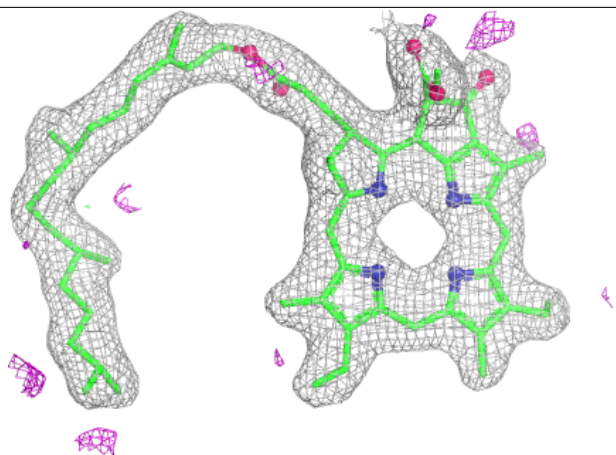
**Electron density around CLA b 604:**

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



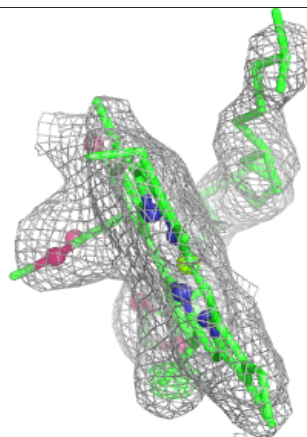
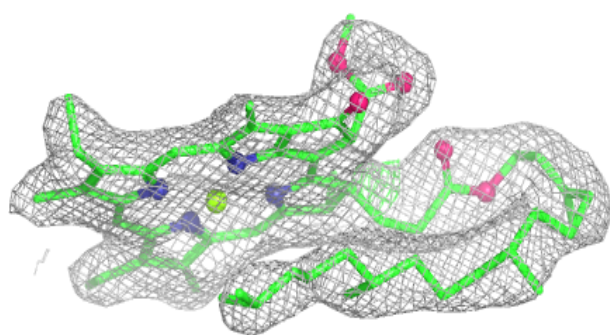
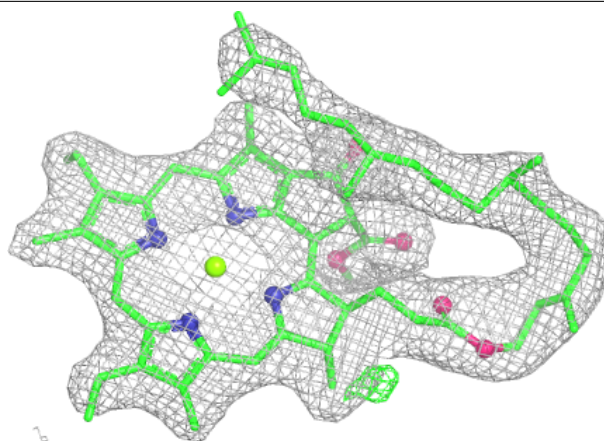
Electron density around PHO A 407:

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



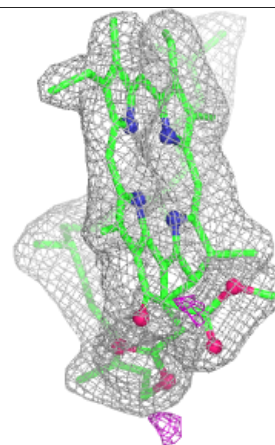
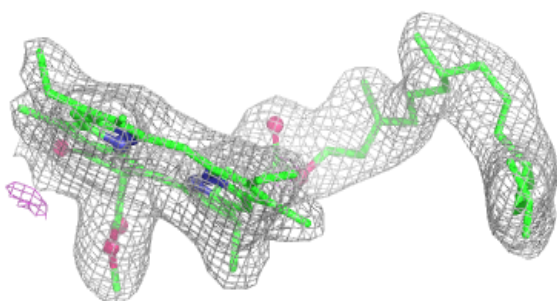
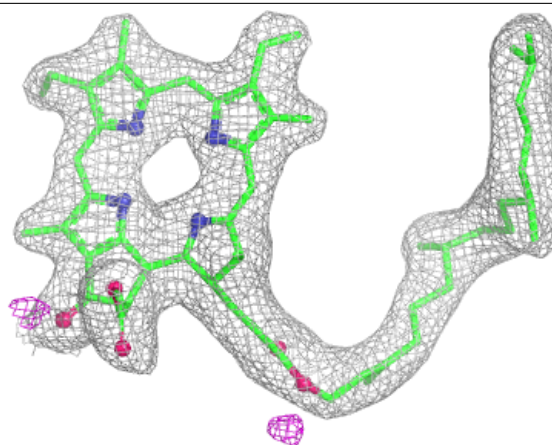
Electron density around CLA C 511:

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



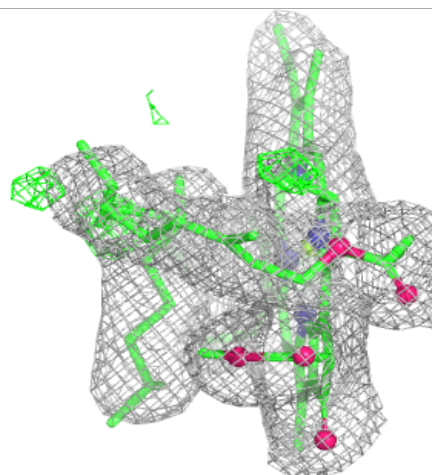
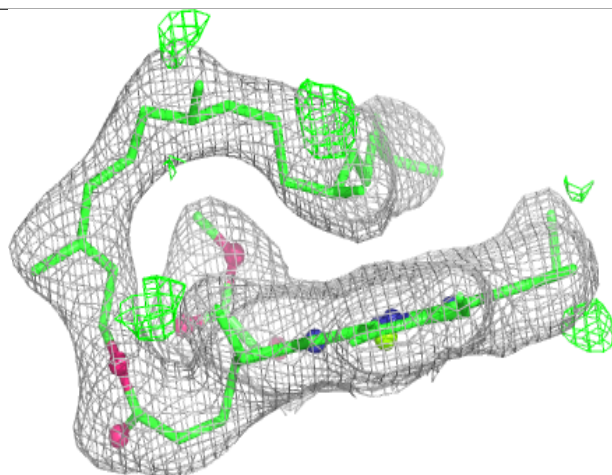
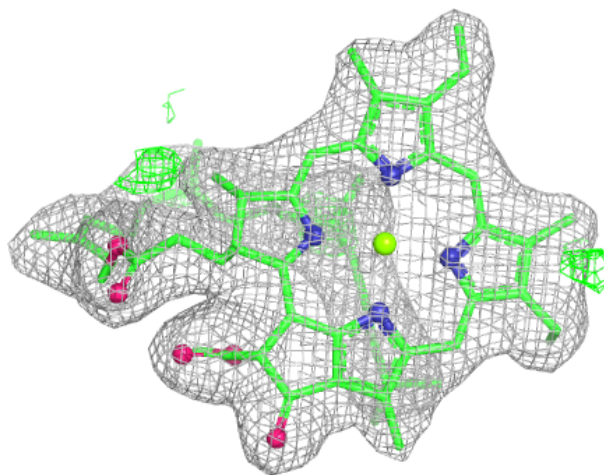
Electron density around PHO a 417:

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



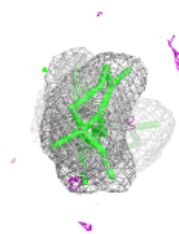
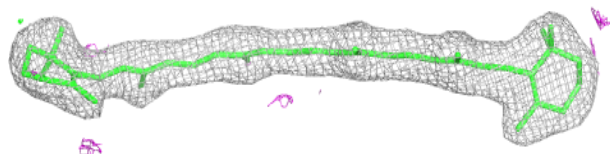
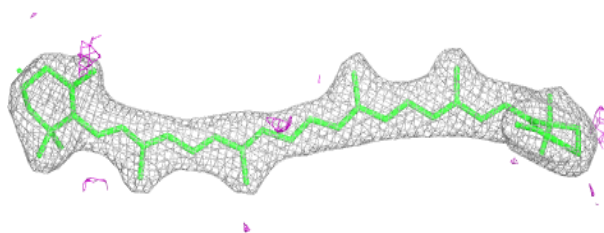
Electron density around CLA C 512:

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

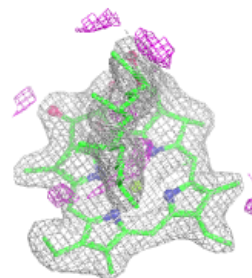
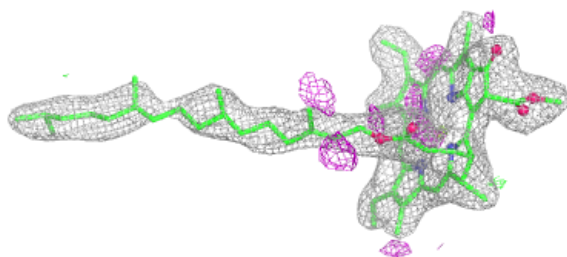
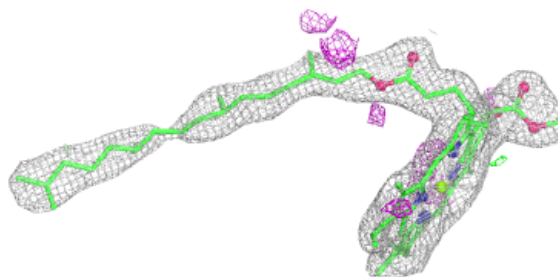


Electron density around BCR B 617:

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

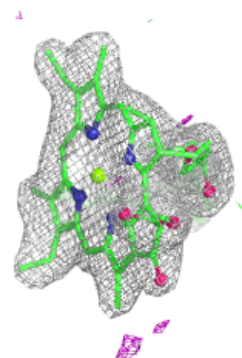
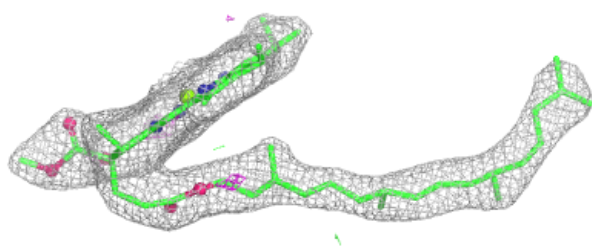
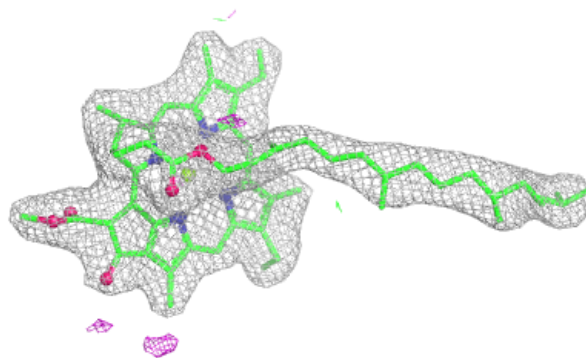
**Electron density around CLA b 607:**

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

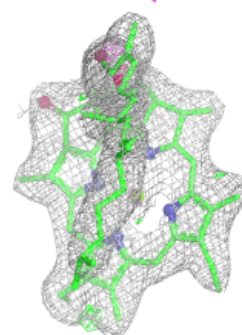
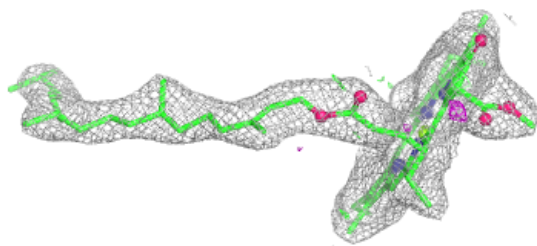
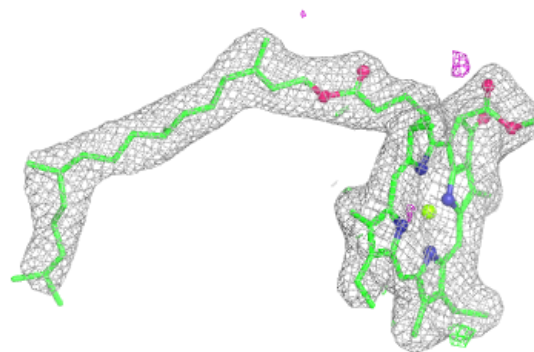


Electron density around CLA b 608:

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

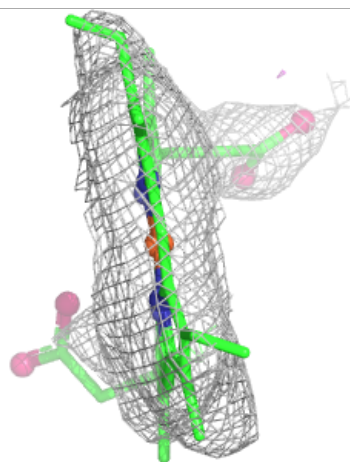
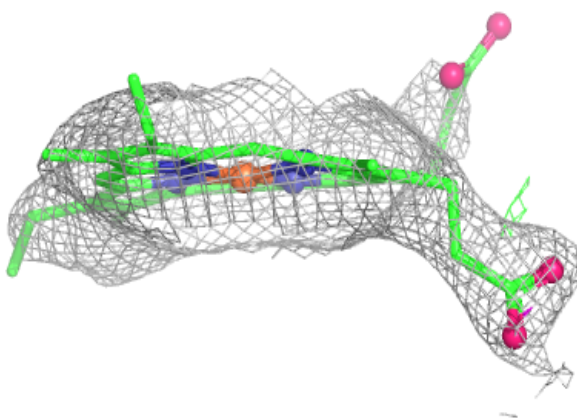
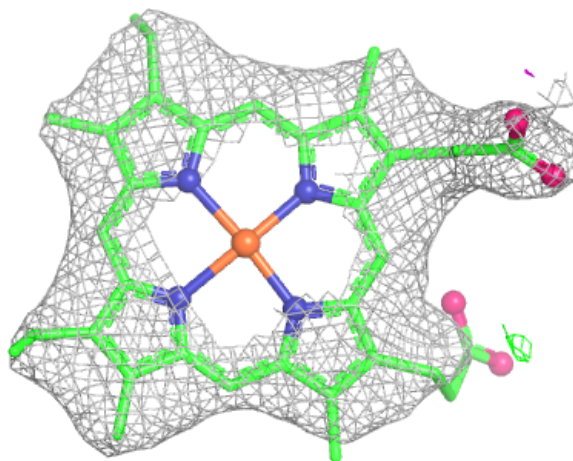
**Electron density around CLA b 609:**

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



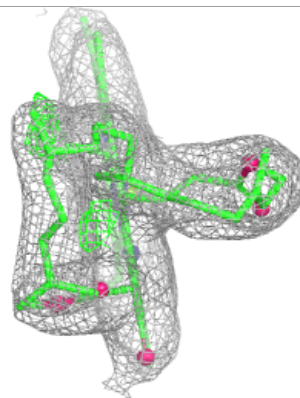
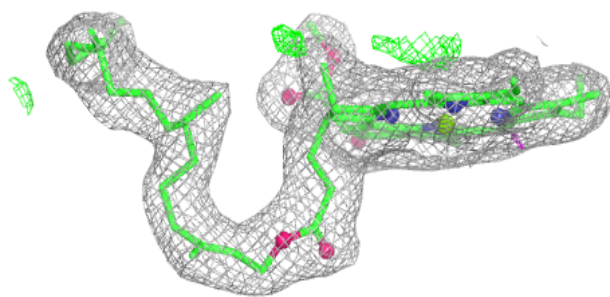
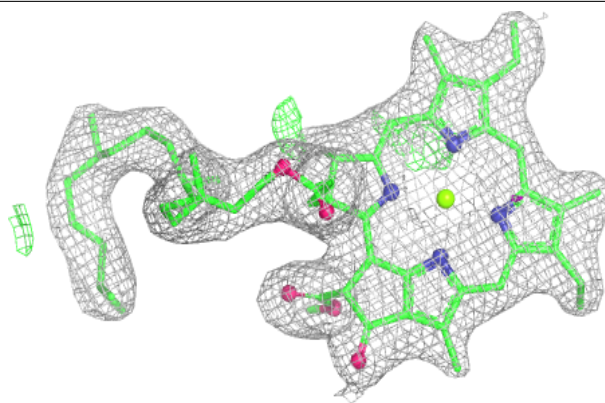
Electron density around HEC e 102:

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

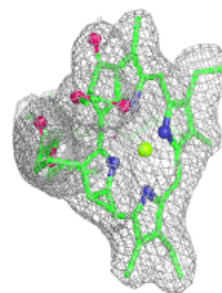
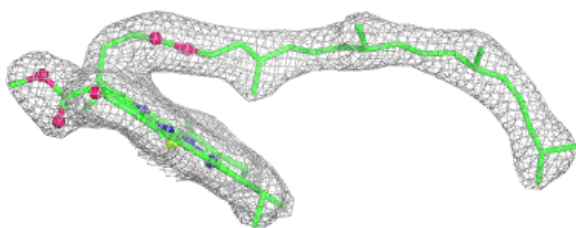
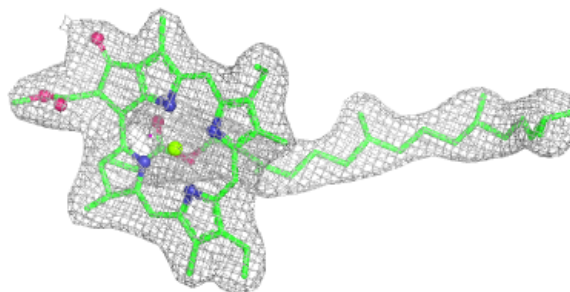


Electron density around CLA B 612:

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

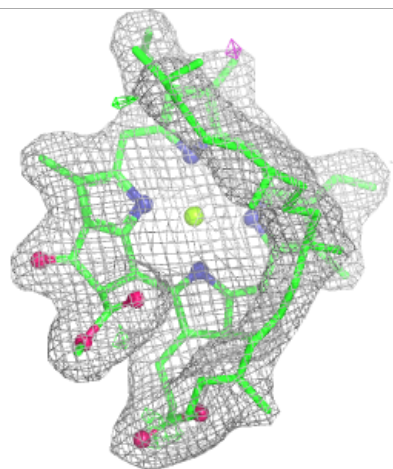
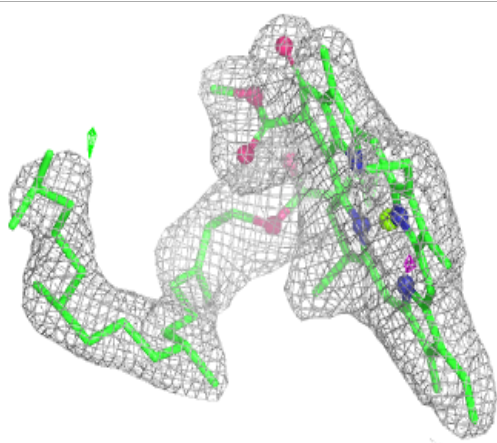
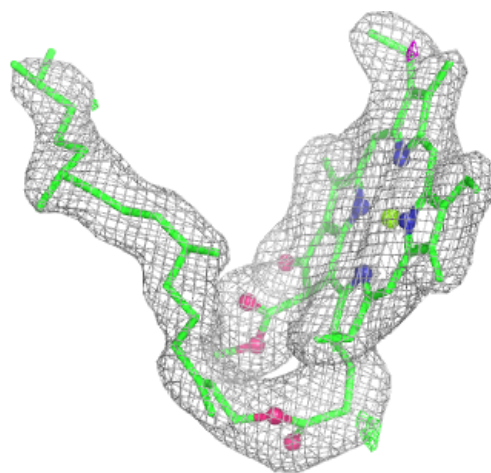
**Electron density around CLA B 608:**

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



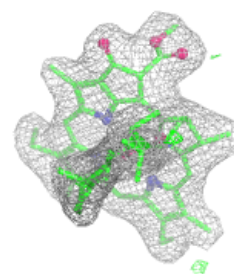
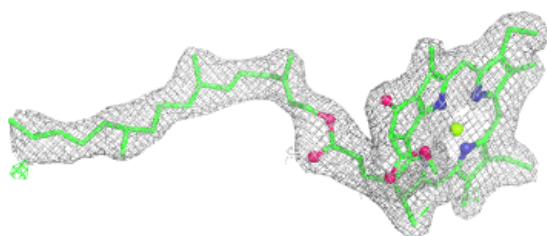
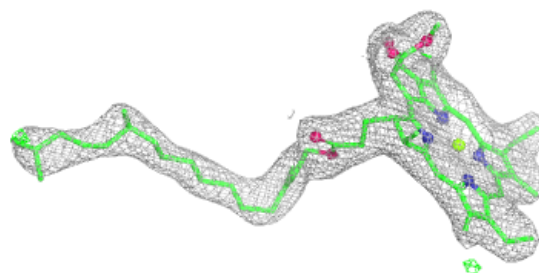
Electron density around CLA b 613:

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



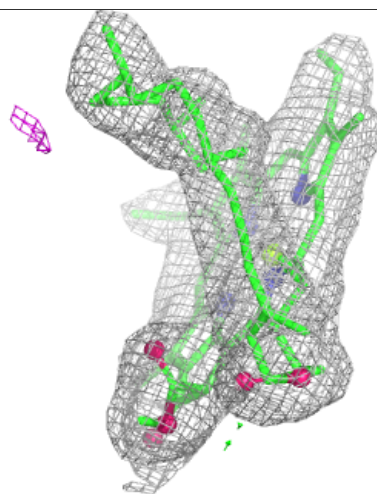
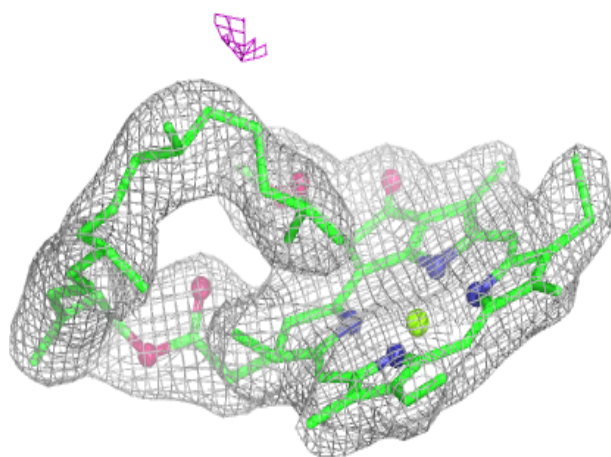
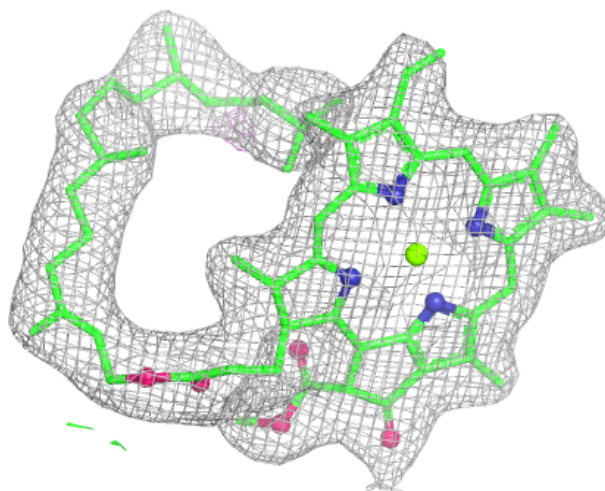
Electron density around CLA C 504:

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



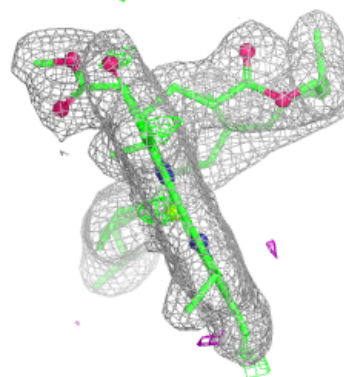
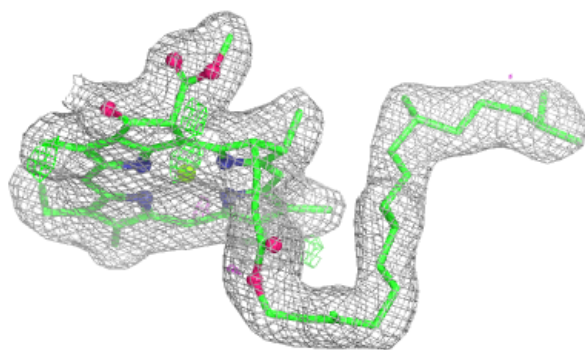
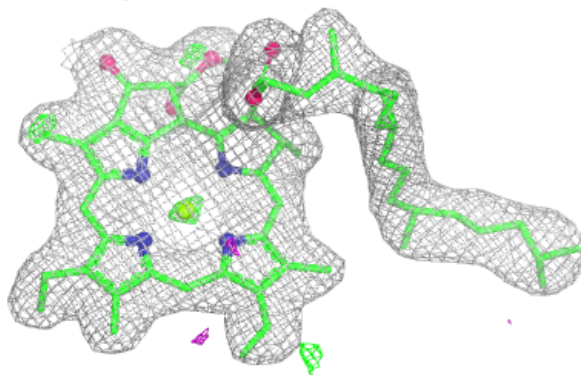
Electron density around CLA b 615:

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



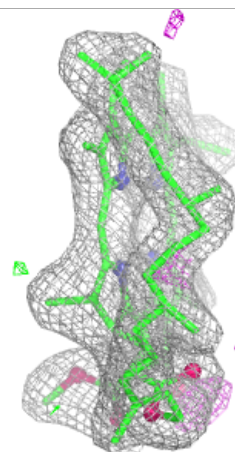
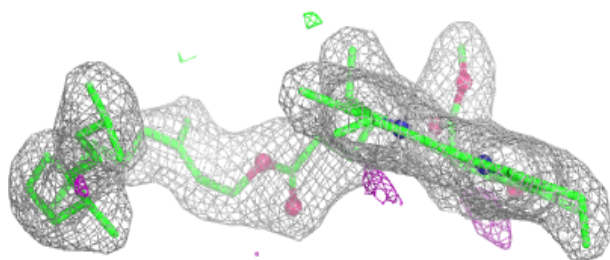
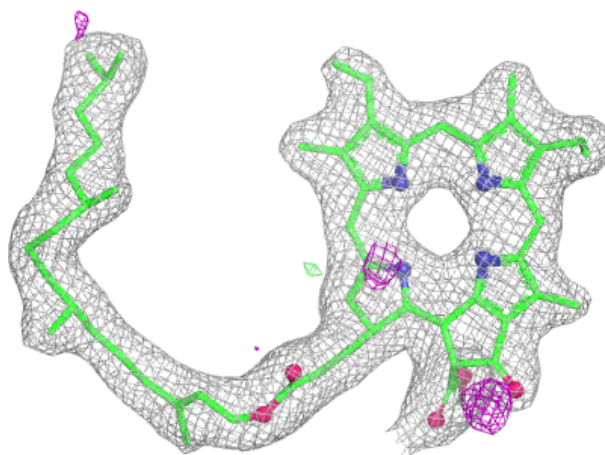
Electron density around CLA A 405:

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



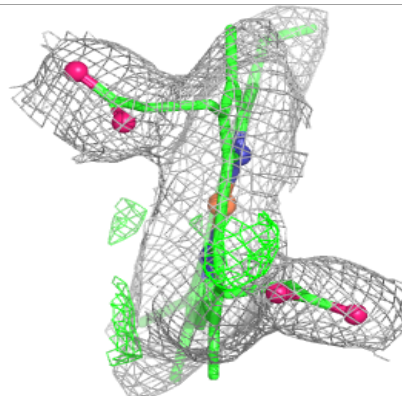
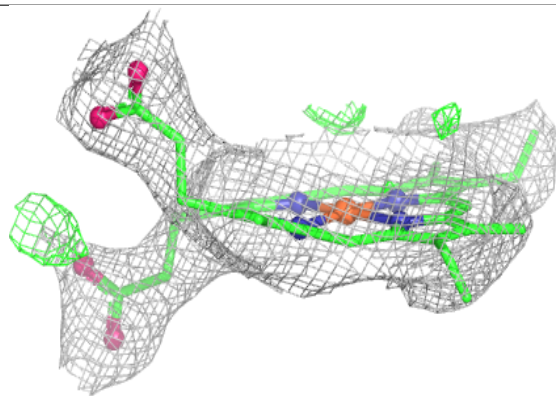
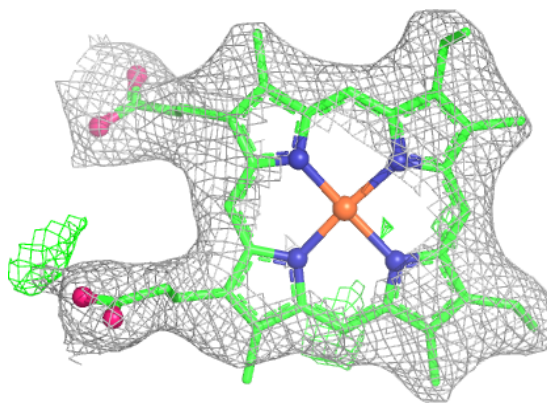
Electron density around PHO a 407:

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



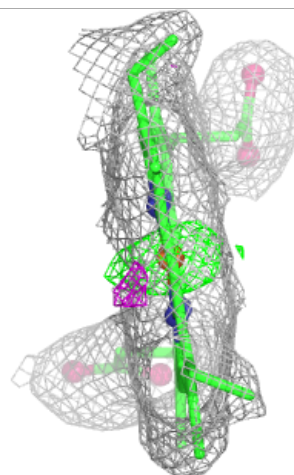
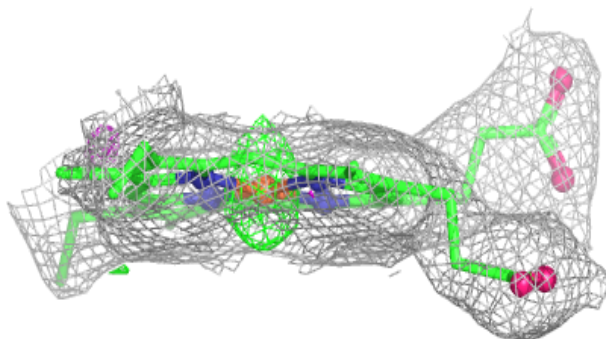
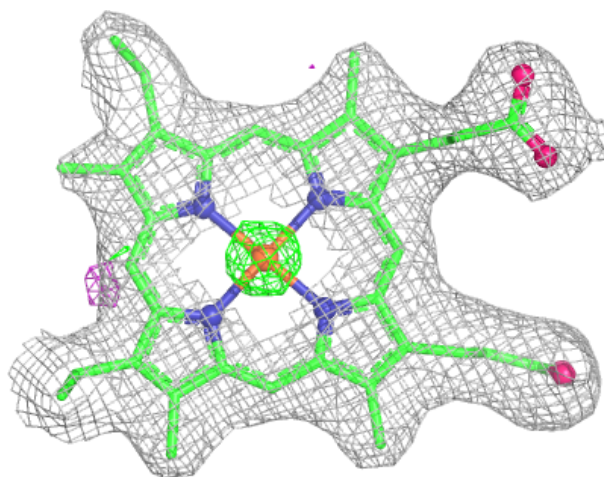
Electron density around HEC E 103:

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



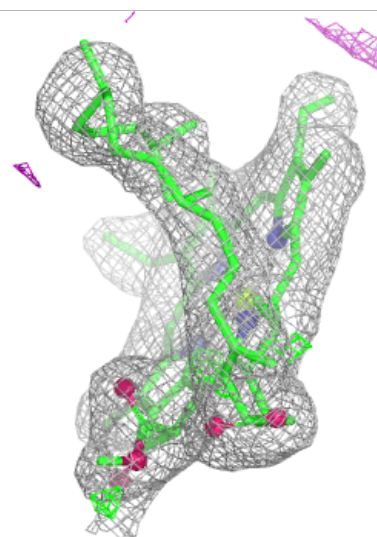
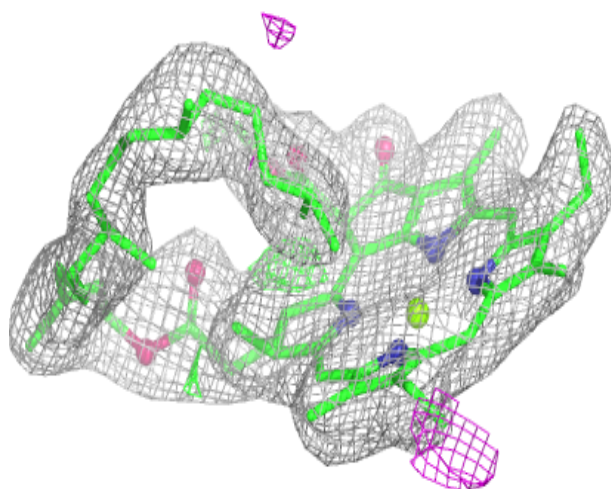
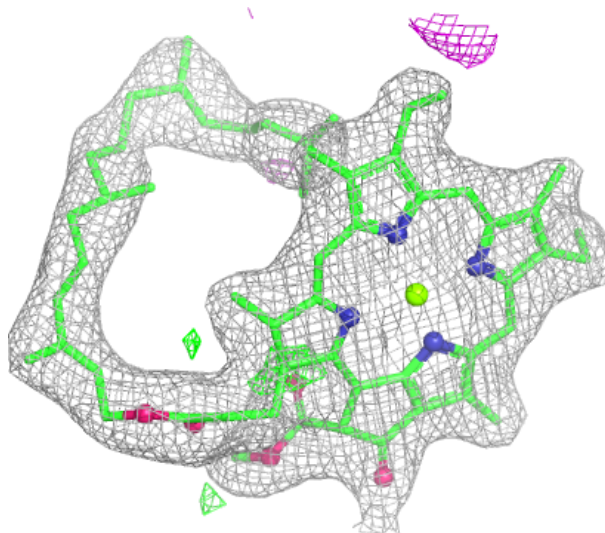
Electron density around HEC V 201:

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



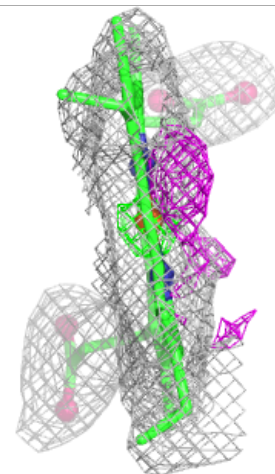
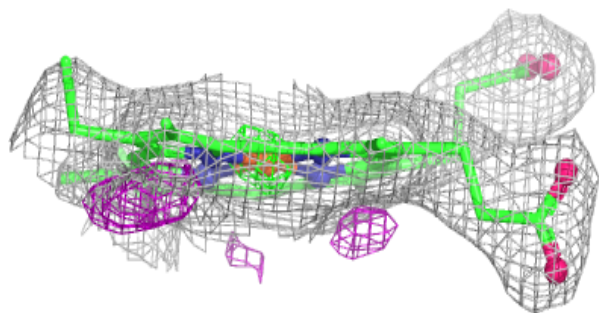
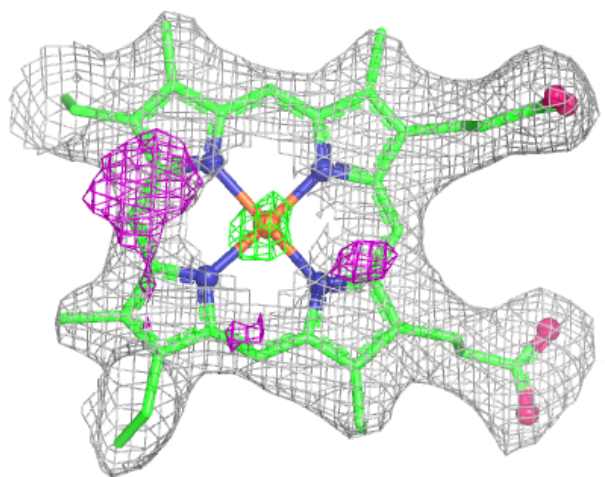
Electron density around CLA B 615:

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



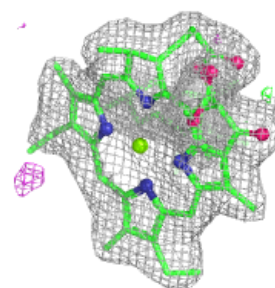
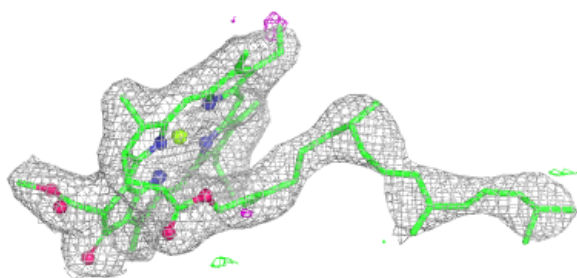
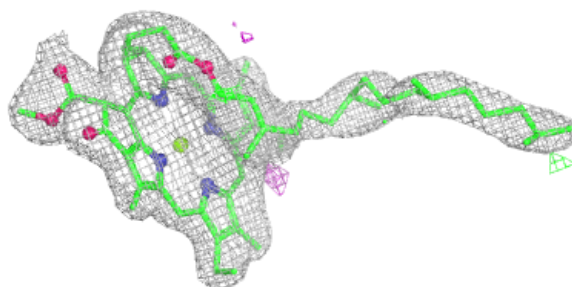
Electron density around HEC v 202:

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

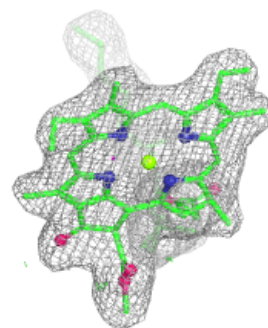
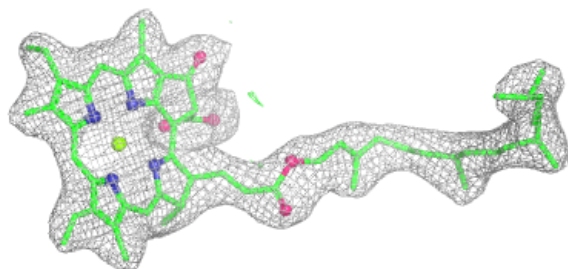
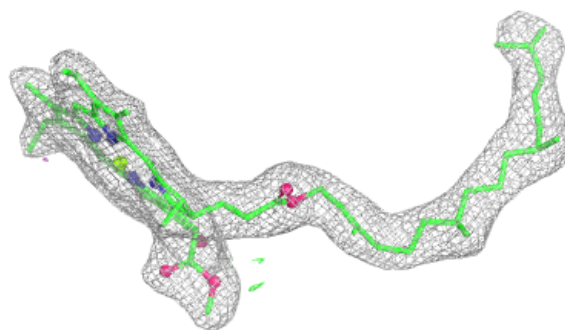


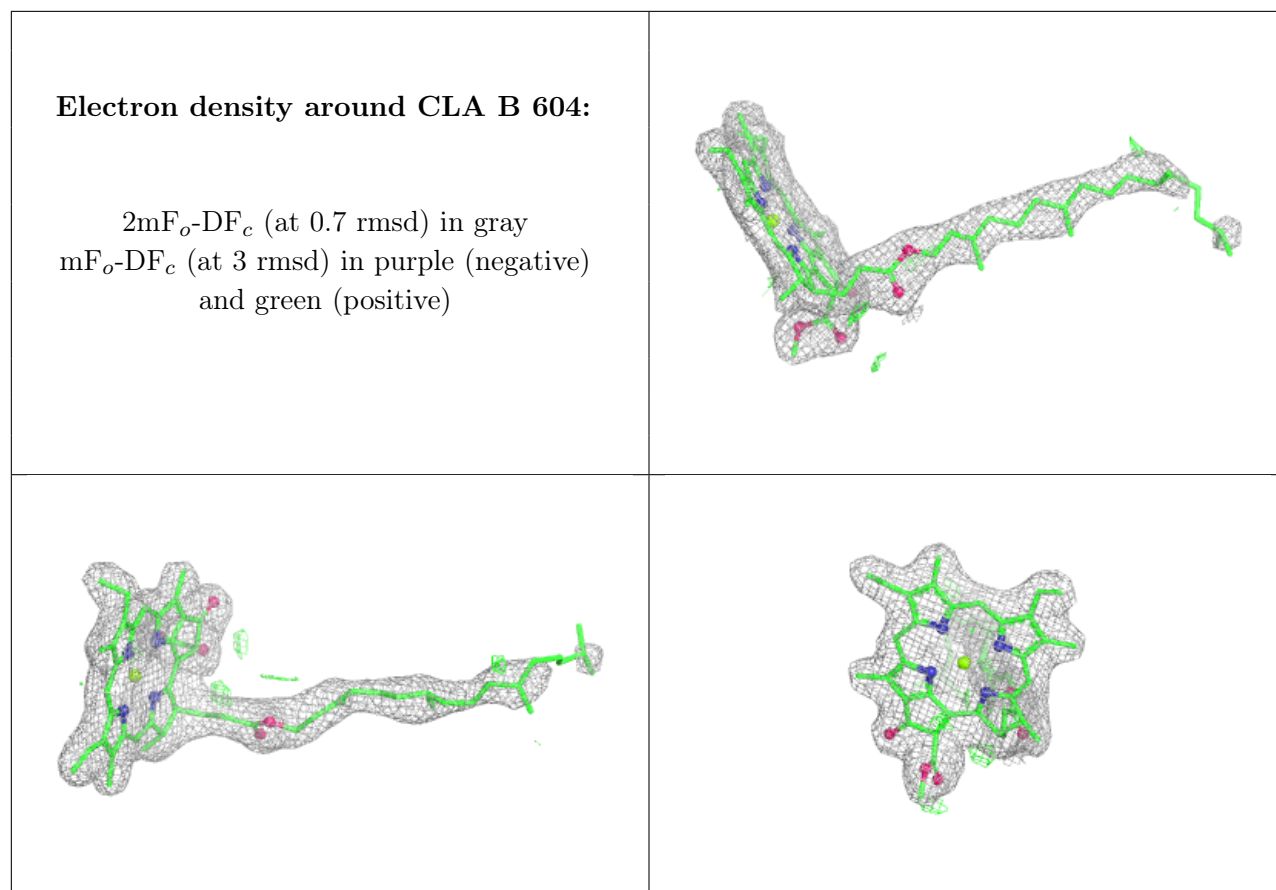
Electron density around CLA C 507:

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

**Electron density around CLA 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.