



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:09 AM UTC

PDB ID : 5WS6 / pdb_00005ws6
Title : Native XFEL structure of Photosystem II (preflash two-flash dataset)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2016-12-05
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

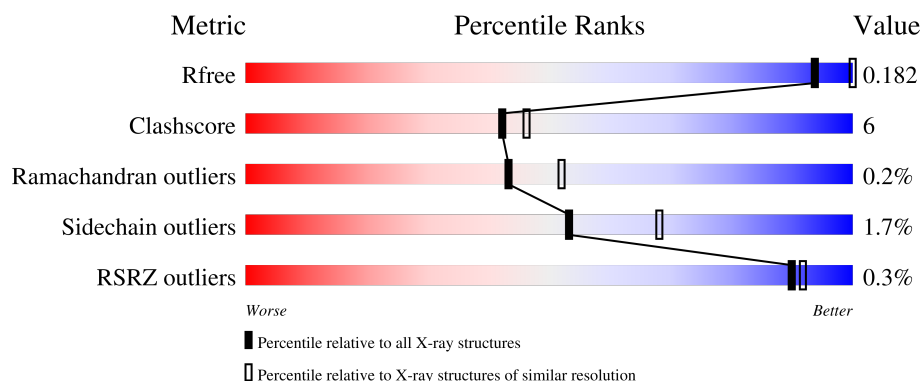
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



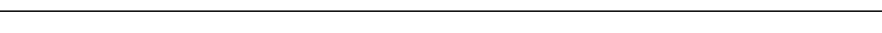
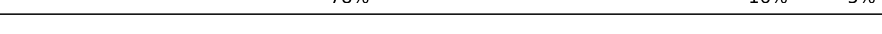
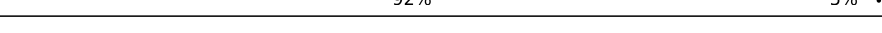
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	344	88% 10% .
1	a	344	84% 13% .
2	B	505	90% 10%
2	b	505	89% 10%
3	C	455	90% 9% .

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Mol	Chain	Length	Quality of chain
3	c	455	 88% 11%
4	D	342	 89% 10%
4	d	342	 88% 12%
5	E	84	 75% 21% .
5	e	84	 76% 18% 6%
6	F	44	 61% 16% 23%
6	f	44	 5% 66% 5% 30%
7	H	65	 2% 91% 6% . .
7	h	65	 2% 83% 15% .
8	I	38	 84% 16%
8	i	38	 3% 76% 24%
9	J	39	 77% 18% . .
9	j	39	 90% 10%
10	K	37	 76% 19% 5%
10	k	37	 78% 16% 5%
11	L	37	 92% 5% .
11	l	37	 86% 11% .
12	M	36	 78% 14% 8%
12	m	36	 81% 11% . 6%
13	O	244	 83% 16% .
13	o	244	 89% 10%
14	T	32	 3% 81% 9% . 6%
14	t	32	 3% 81% 6% 6% 6%
15	U	104	 82% 9% . 8%
15	u	104	 88% 5% . 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
24	CLA	A	404	X	-	-	-
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	350	X	-	-	-
24	CLA	a	403	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	b	601	X	-	-	-
24	CLA	b	602	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-
24	CLA	d	402	X	-	-	-

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

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 53280 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	29	0
			2850	1865	467	502	16			
1	a	334	Total	C	N	O	S	0	29	0
			2852	1867	466	503	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	8	0
			4007	2630	664	700	13			
2	b	504	Total	C	N	O	S	0	4	0
			3986	2618	661	694	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	10	0
			3542	2315	590	624	13			
3	c	455	Total	C	N	O	S	0	10	0
			3577	2340	595	629	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	3	0
			2748	1819	450	467	12			
4	d	341	Total	C	N	O	S	0	3	0
			2739	1814	449	464	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	1	0
			665	434	107	124			
5	e	79	Total	C	N	O	0	0	0
			648	424	105	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			514	344	84	84	2			
7	h	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			265	178	38	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	1
			2	2		

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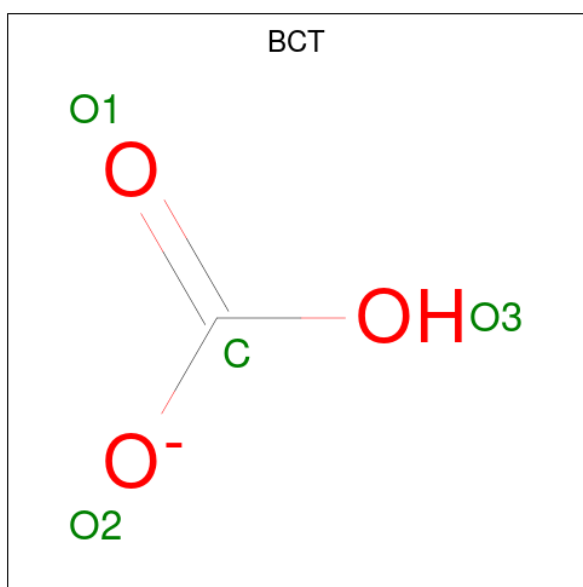
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	1
			2	2		

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

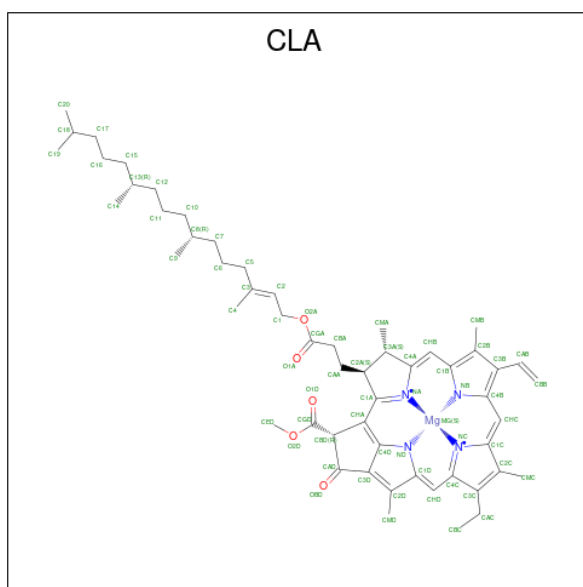
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	a	2	Total	Cl	0	0
			2	2		

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	1
			8	2	6		
23	a	1	Total	C	O	0	1
			8	2	6		

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).

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

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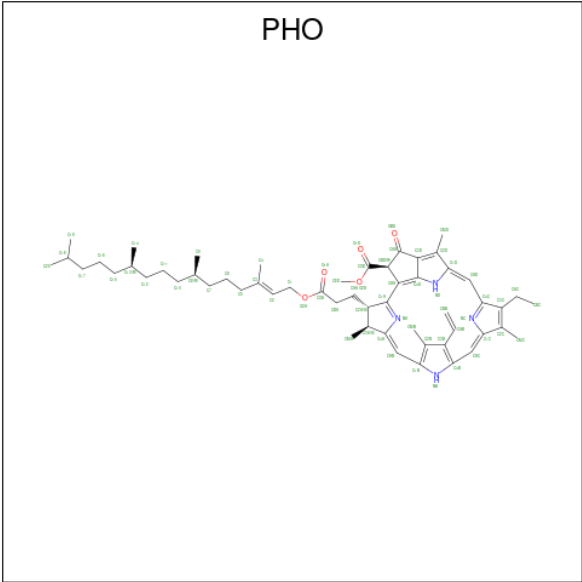
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

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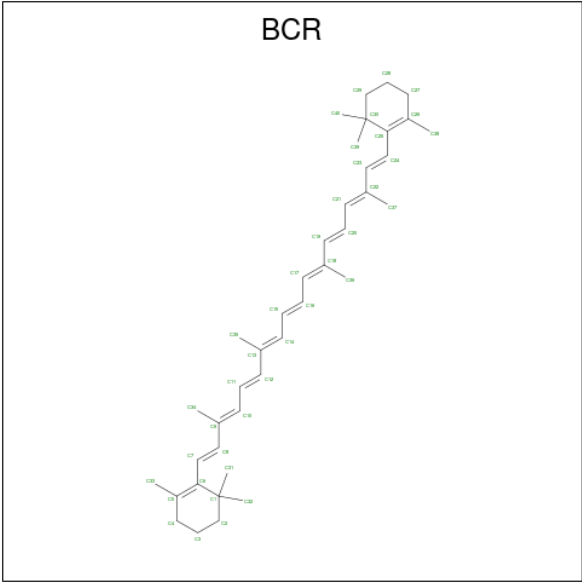
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



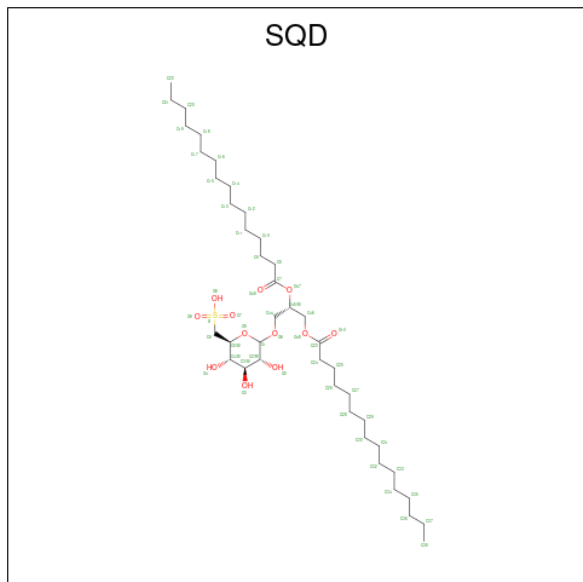
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



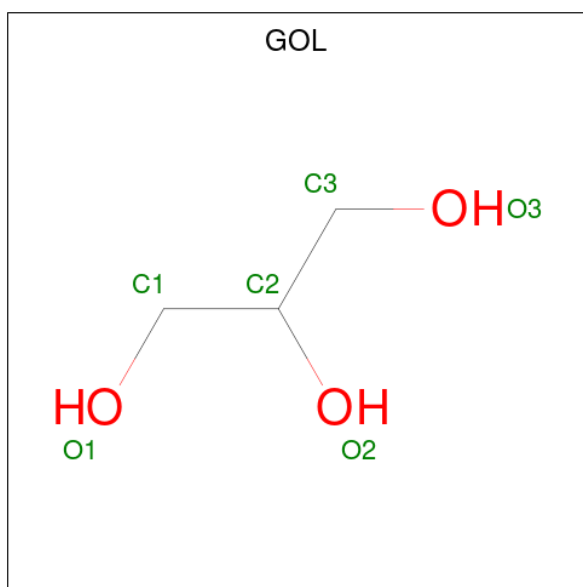
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	y	1	Total C 40 40	0	0

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



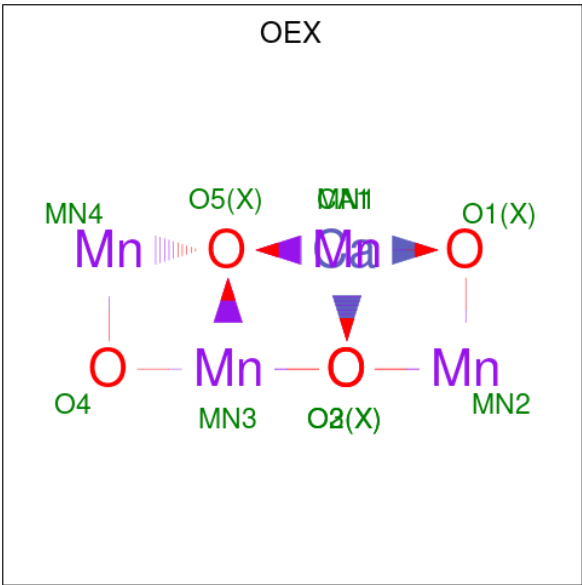
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			43	30	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0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

- Molecule 28 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



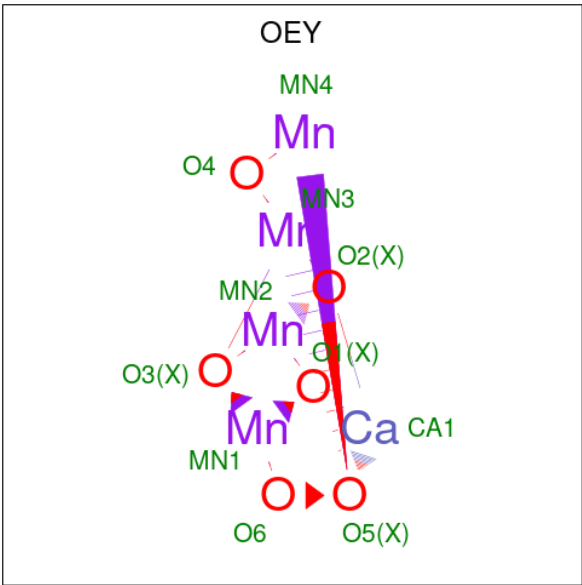
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28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

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



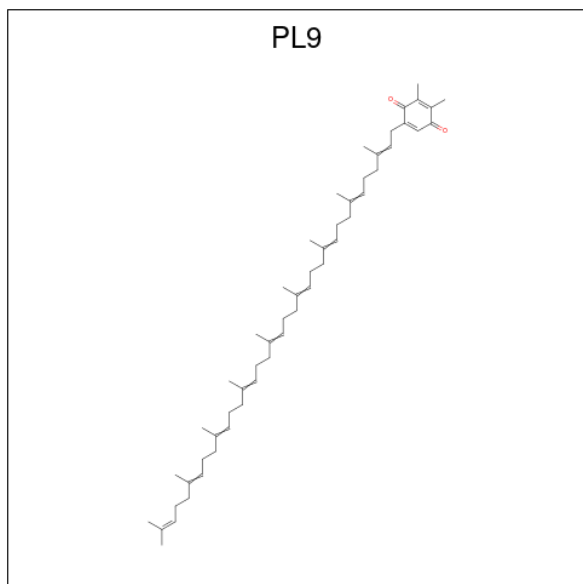
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 30 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
30	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 31 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
31	A	1	Total	C	O	0	1
			110	106	4		
31	D	1	Total	C	O	0	0
			55	53	2		
31	a	1	Total	C	O	0	1
			110	106	4		
31	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 32 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

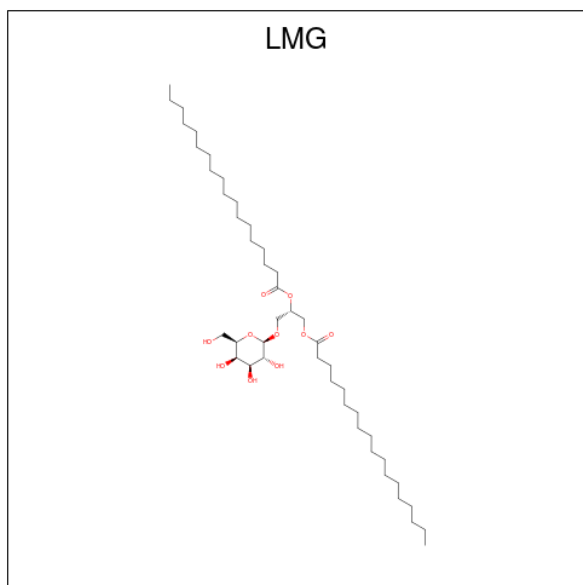
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			28	23	5		
32	B	1	Total	C	O	0	0
			33	28	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	I	1	Total	C	O	0	0
			40	35	5		
32	J	1	Total	C		0	0
			10	10			
32	K	1	Total	C	O	0	0
			34	29	5		

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

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



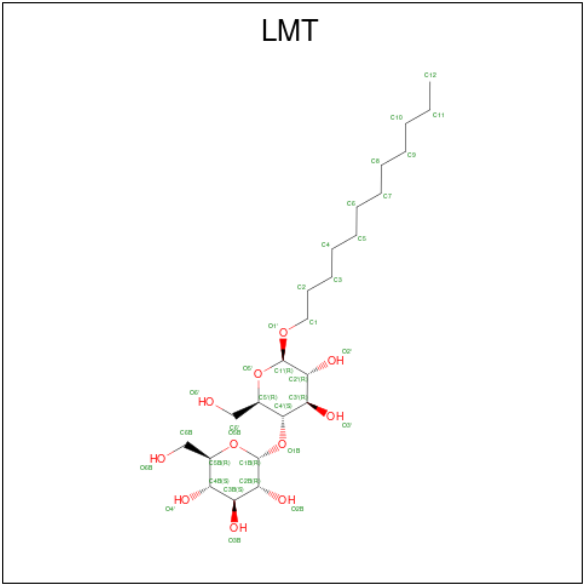
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total C O 51 41 10	0	0

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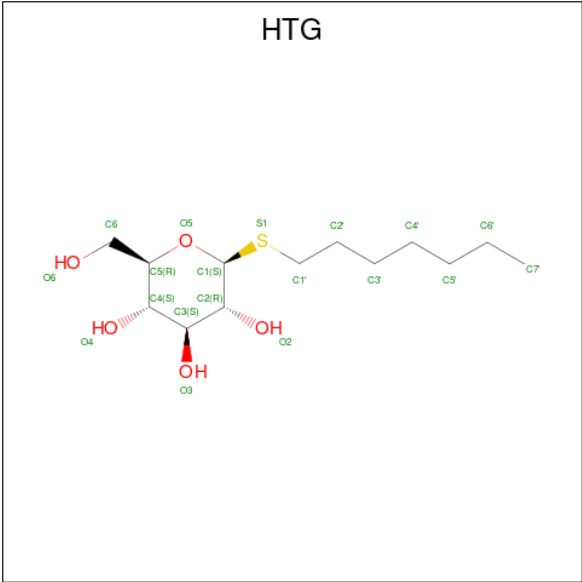
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	J	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total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

- Molecule 34 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



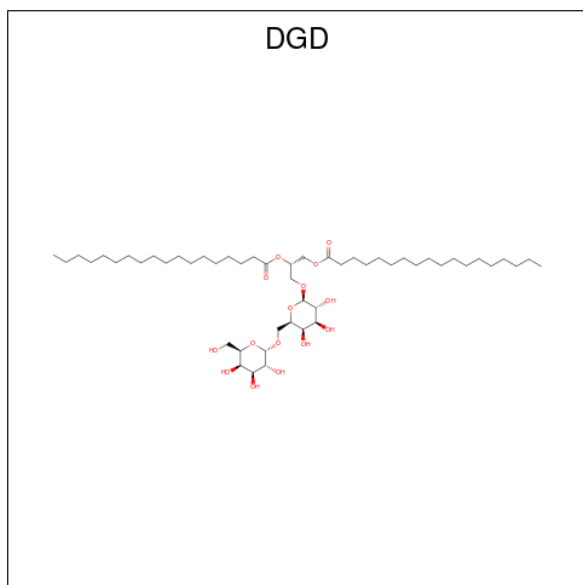
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			16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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	h	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

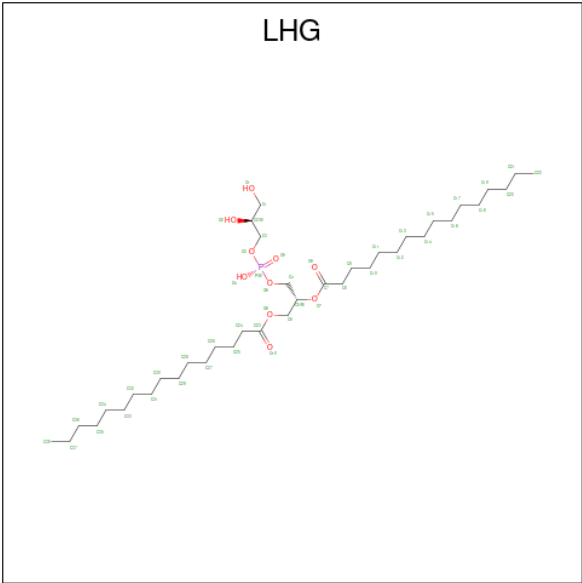


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	H	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15	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

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

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

- Molecule 38 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



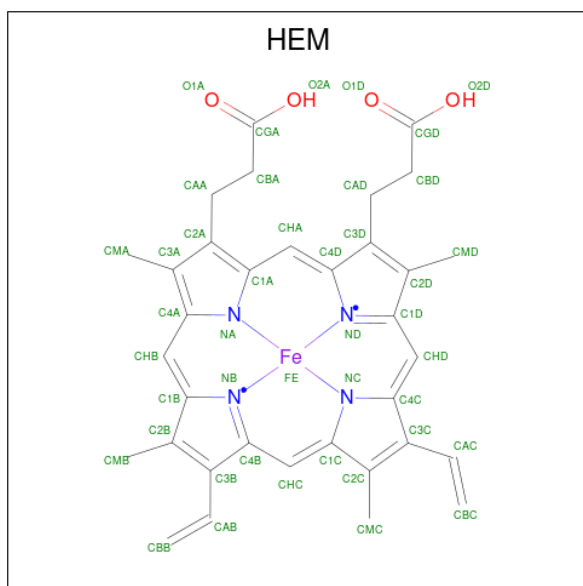
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	E	1	Total	C	O	P	0	0
			42	31	10	1		

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

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 40 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

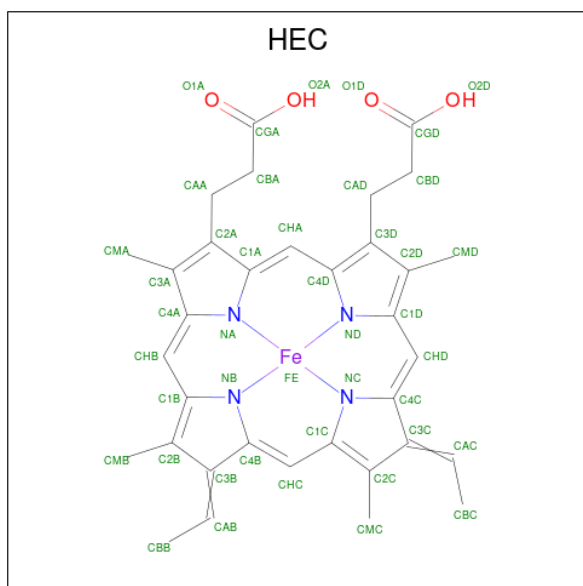
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	J	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	j	1	Total	Mg	0	0
			1	1		

- Molecule 41 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	A	125	Total	O	0	5
			130	130		
42	B	164	Total	O	0	0
			164	164		
42	C	147	Total	O	0	0
			147	147		
42	D	112	Total	O	0	0
			112	112		
42	E	14	Total	O	0	0
			14	14		
42	F	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	H	20	Total 20	O 20	0	0
42	I	6	Total 6	O 6	0	0
42	J	4	Total 4	O 4	0	0
42	K	7	Total 7	O 7	0	0
42	L	4	Total 4	O 4	0	0
42	M	7	Total 7	O 7	0	0
42	O	74	Total 74	O 74	0	0
42	T	8	Total 8	O 8	0	0
42	U	33	Total 33	O 33	0	0
42	V	65	Total 65	O 65	0	0
42	X	2	Total 2	O 2	0	0
42	Y	1	Total 1	O 1	0	0
42	a	128	Total 133	O 133	0	5
42	b	185	Total 185	O 185	0	0
42	c	122	Total 122	O 122	0	0
42	d	109	Total 109	O 109	0	0
42	e	7	Total 7	O 7	0	0
42	f	3	Total 3	O 3	0	0
42	h	14	Total 14	O 14	0	0
42	i	3	Total 3	O 3	0	0
42	j	2	Total 2	O 2	0	0

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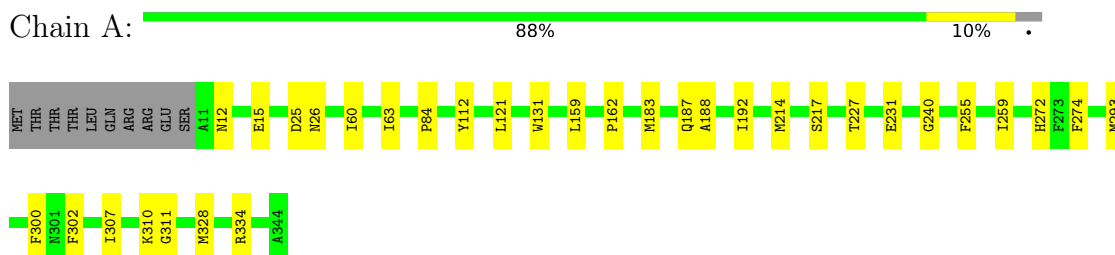
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	k	3	Total 3	O 3	0	0
42	l	6	Total 6	O 6	0	0
42	m	11	Total 11	O 11	0	0
42	o	78	Total 78	O 78	0	0
42	t	5	Total 5	O 5	0	0
42	u	47	Total 47	O 47	0	0
42	v	49	Total 49	O 49	0	0
42	x	4	Total 4	O 4	0	0
42	y	1	Total 1	O 1	0	0

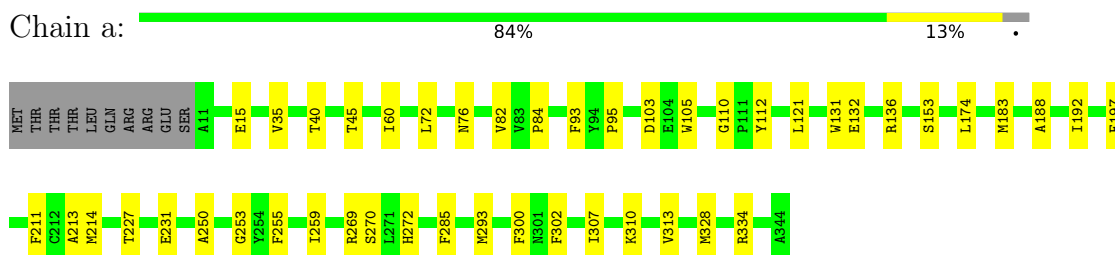
3 Residue-property plots [i](#)

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

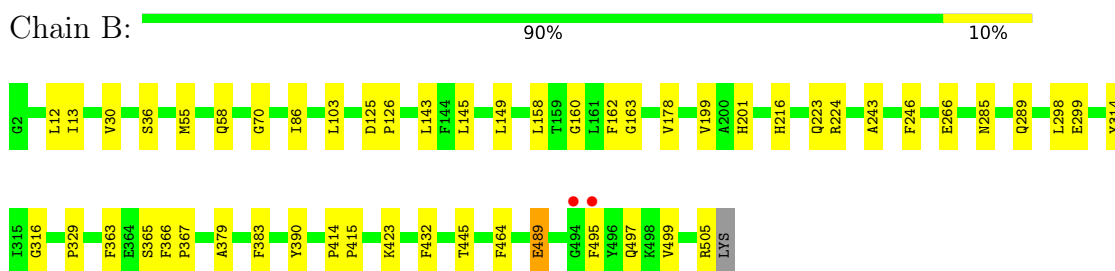
- Molecule 1: Photosystem II D1 protein



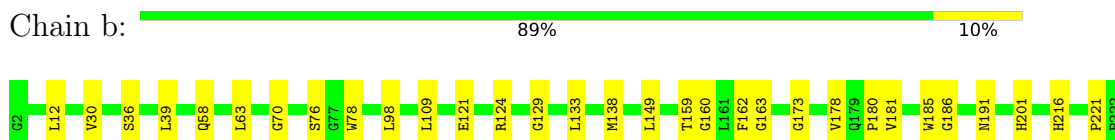
- Molecule 1: Photosystem II D1 protein



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein





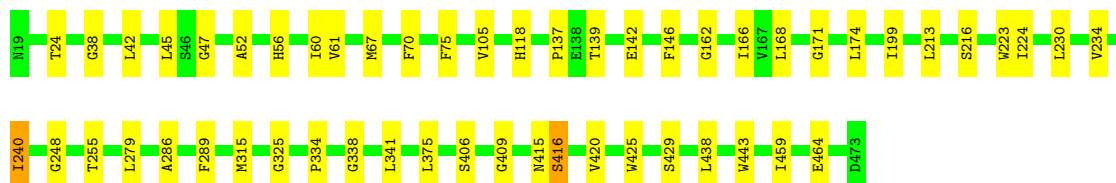
• Molecule 3: Photosystem II CP43 chlorophyll protein

Chain C: 90% 9%



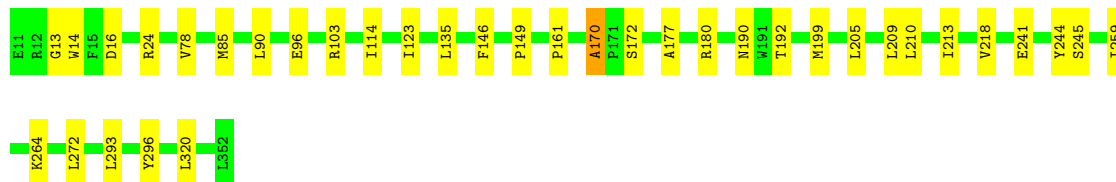
• Molecule 3: Photosystem II CP43 chlorophyll protein

Chain c: 88% 11%



• Molecule 4: Photosystem II D2 protein

Chain D: 89% 10%



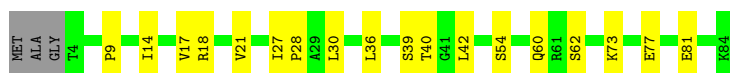
• Molecule 4: Photosystem II D2 protein

Chain d: 88% 12%

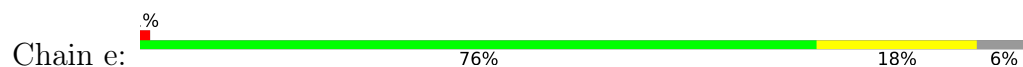


• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 75% 21%



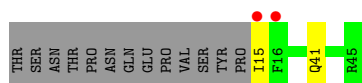
- Molecule 5: Cytochrome b559 subunit alpha



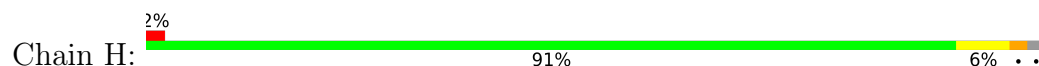
- Molecule 6: Cytochrome b559 subunit beta



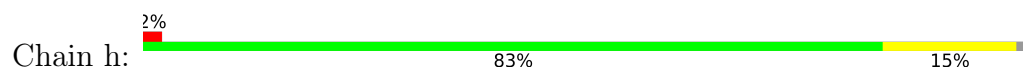
- Molecule 6: Cytochrome b559 subunit beta



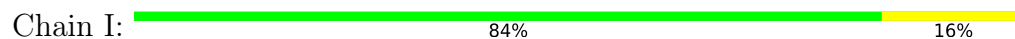
- Molecule 7: Photosystem II reaction center protein H



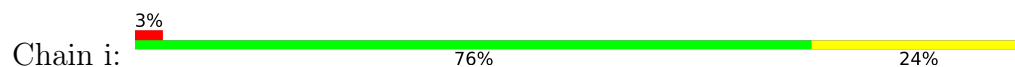
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I





- Molecule 9: Photosystem II reaction center protein J

Chain J: 77% 18% . .



- Molecule 9: Photosystem II reaction center protein J

Chain j: 90% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K: 76% 19% 5%



- Molecule 10: Photosystem II reaction center protein K

Chain k: 78% 16% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 92% 5% .



- Molecule 11: Photosystem II reaction center protein L

Chain l: 86% 11% .



- Molecule 12: Photosystem II reaction center protein M

Chain M: 78% 14% 8%



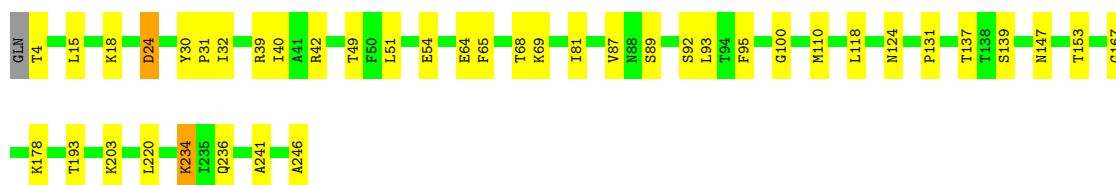
- Molecule 12: Photosystem II reaction center protein M

Chain m: 81% 11% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 83% 16%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 89% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 3% 81% 9% 6%



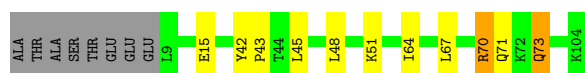
- Molecule 14: Photosystem II reaction center protein T

Chain t: 3% 81% 6% 6% 6%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 82% 9% 8%

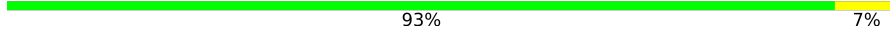


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  88% 5% • 7%



- Molecule 16: Cytochrome c-550

Chain V:  93% 7%



- Molecule 16: Cytochrome c-550

Chain v:  90% 9% •



- Molecule 17: Photosystem II reaction center protein X

Chain X:  90% 5% 5%



- Molecule 17: Photosystem II reaction center protein X

Chain x:  88% 8% 5%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  73% 20% • •

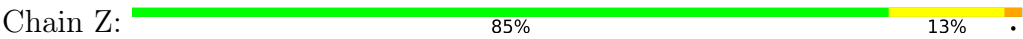


- Molecule 18: Photosystem II reaction center protein Ycf12

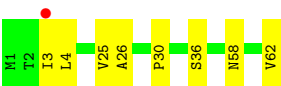
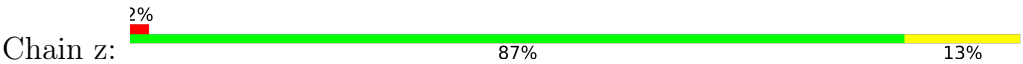
Chain y:  3% 80% 17% •



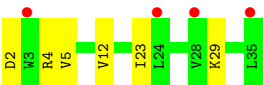
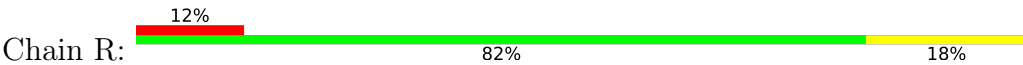
- Molecule 19: Photosystem II reaction center protein Z



● Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	124.96Å 230.22Å 286.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 20.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.35) 99.8 (20.00-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.129 , 0.175 0.140 , 0.182	Depositor DCC
R_{free} test set	17126 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 91.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53280	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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: OEY, SQD, MG, FE2, FME, LMT, DGD, UNL, CLA, CL, CA, HEM, GOL, OEX, BCR, BCT, PL9, HTG, PHO, LHG, HEC, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.57	0/2952	0.84	0/4019
1	a	0.52	0/2957	0.79	0/4027
2	B	0.53	0/4171	0.80	0/5683
2	b	0.51	0/4138	0.80	0/5640
3	C	0.52	0/3667	0.81	2/4992 (0.0%)
3	c	0.46	0/3703	0.79	0/5041
4	D	0.57	0/2847	0.82	2/3878 (0.1%)
4	d	0.52	0/2838	0.79	2/3866 (0.1%)
5	E	0.47	0/687	0.78	0/936
5	e	0.44	0/667	0.77	0/908
6	F	0.59	0/284	0.74	0/387
6	f	0.48	0/257	0.81	0/349
7	H	0.46	0/530	0.90	0/723
7	h	0.43	0/519	0.80	0/708
8	I	0.47	0/311	0.69	0/419
8	i	0.45	0/311	0.80	0/419
9	J	0.41	0/278	0.74	0/376
9	j	0.41	0/283	0.74	0/383
10	K	0.48	0/303	0.79	0/416
10	k	0.51	0/303	0.86	0/416
11	L	0.49	0/311	0.68	0/423
11	l	0.51	0/311	0.75	0/423
12	M	0.59	0/261	0.97	0/357
12	m	0.53	0/262	0.94	0/357
13	O	0.49	0/1935	0.80	0/2623
13	o	0.49	0/1910	0.81	2/2589 (0.1%)
14	T	0.59	0/257	0.74	0/349
14	t	0.54	0/257	0.78	0/349
15	U	0.48	0/776	0.77	0/1052
15	u	0.47	0/785	0.72	0/1064
16	V	0.49	0/1085	0.75	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.45	0/1085	0.77	0/1473
17	X	0.44	0/284	0.73	0/384
17	x	0.42	0/284	0.75	0/384
18	Y	0.41	0/216	0.77	0/289
18	y	0.41	0/216	0.81	0/289
19	Z	0.43	0/490	0.84	0/669
19	z	0.39	0/490	0.80	0/669
20	R	0.41	0/279	0.73	0/383
All	All	0.51	0/43500	0.80	8/59185 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	170	ALA	CA-C-N	-6.56	113.22	119.85
4	d	170	ALA	C-N-CA	-6.56	113.22	119.85
13	o	55	GLU	CA-C-N	6.29	126.05	119.76
13	o	55	GLU	C-N-CA	6.29	126.05	119.76
4	D	170	ALA	CA-C-N	-5.94	113.82	119.76
4	D	170	ALA	C-N-CA	-5.94	113.82	119.76
3	C	76	ILE	CA-C-N	5.45	125.79	119.47
3	C	76	ILE	C-N-CA	5.45	125.79	119.47

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	2850	0	2705	26	0
1	a	2852	0	2708	40	0
2	B	4007	0	3879	41	0
2	b	3986	0	3855	44	0
3	C	3542	0	3462	30	0
3	c	3577	0	3498	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2748	0	2650	30	0
4	d	2739	0	2644	30	0
5	E	665	0	653	13	0
5	e	648	0	634	16	0
6	F	275	0	282	7	0
6	f	250	0	261	1	0
7	H	514	0	542	4	0
7	h	506	0	529	10	0
8	I	314	0	328	4	0
8	i	314	0	328	4	0
9	J	272	0	279	6	0
9	j	277	0	284	3	0
10	K	293	0	305	7	0
10	k	293	0	305	5	0
11	L	301	0	315	2	0
11	l	301	0	315	3	0
12	M	265	0	286	3	0
12	m	269	0	288	7	0
13	O	1889	0	1871	23	0
13	o	1873	0	1852	14	0
14	T	258	0	261	4	0
14	t	258	0	261	3	0
15	U	765	0	767	6	0
15	u	774	0	773	4	0
16	V	1064	0	1073	5	0
16	v	1064	0	1073	10	0
17	X	281	0	312	2	0
17	x	281	0	312	4	0
18	Y	215	0	246	6	0
18	y	215	0	246	4	0
19	Z	479	0	516	4	0
19	z	479	0	516	3	0
20	R	273	0	305	6	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	8	0	0	0	0
23	a	8	0	0	0	0
24	A	260	0	288	14	0
24	B	1040	0	1152	37	0
24	C	845	0	936	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	D	130	0	144	6	0
24	a	260	0	288	14	0
24	b	1040	0	1152	39	0
24	c	845	0	936	50	0
24	d	130	0	144	7	0
25	A	128	0	148	6	0
25	a	128	0	148	5	0
26	A	40	0	56	2	0
26	B	120	0	168	7	0
26	C	80	0	112	6	0
26	D	40	0	56	3	0
26	H	40	0	56	3	0
26	K	40	0	56	1	0
26	T	40	0	56	6	0
26	Y	40	0	56	3	0
26	a	40	0	56	2	0
26	b	120	0	168	10	0
26	c	80	0	112	7	0
26	d	40	0	56	3	0
26	h	40	0	56	5	0
26	k	40	0	56	1	0
26	t	40	0	56	5	0
26	y	40	0	56	4	0
27	A	108	0	156	8	0
27	B	54	0	78	1	0
27	F	43	0	53	1	0
27	a	108	0	156	5	0
27	b	54	0	78	2	0
27	f	43	0	53	3	0
28	A	6	0	8	0	0
28	B	12	0	16	2	0
28	C	6	0	8	0	0
28	V	6	0	8	0	0
28	a	12	0	16	2	0
28	b	6	0	8	0	0
28	c	6	0	8	0	0
28	v	6	0	8	0	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	11	0	0	0	0
30	a	11	0	0	1	0
31	A	110	0	160	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	D	55	0	80	5	0
31	a	110	0	160	14	0
31	d	55	0	80	3	0
32	A	28	0	0	0	0
32	B	33	0	0	0	0
32	D	57	0	0	1	0
32	I	40	0	0	0	0
32	J	10	0	0	0	0
32	K	34	0	0	0	0
32	M	10	0	0	0	0
32	X	18	0	0	0	0
32	a	30	0	0	0	0
32	b	33	0	0	0	0
32	c	32	0	0	0	0
32	d	53	0	0	0	0
32	i	40	0	0	0	0
32	j	10	0	0	0	0
32	m	10	0	0	0	0
32	x	18	0	0	0	0
33	A	51	0	72	1	0
33	B	51	0	72	1	0
33	C	102	0	144	3	0
33	J	51	0	72	2	0
33	Z	37	0	44	5	0
33	a	51	0	72	3	0
33	b	51	0	72	1	0
33	c	102	0	144	2	0
33	j	51	0	72	4	0
33	z	39	0	48	2	0
34	A	35	0	46	2	0
34	B	60	0	81	3	0
34	E	35	0	46	1	0
34	I	35	0	46	1	0
34	M	70	0	92	3	0
34	a	70	0	92	4	0
34	b	50	0	70	0	0
34	e	35	0	46	1	0
34	m	35	0	46	1	0
34	t	26	0	35	1	0
35	B	76	0	104	5	0
35	C	38	0	52	2	0
35	D	16	0	17	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	V	11	0	10	0	0
35	b	76	0	104	7	0
35	c	38	0	52	0	0
35	h	16	0	17	0	0
36	C	186	0	246	4	0
36	H	62	0	82	2	0
36	c	186	0	246	6	0
36	h	62	0	82	0	0
37	C	1	0	0	0	0
37	O	1	0	0	0	0
37	V	1	0	0	0	0
37	b	1	0	0	0	0
37	c	2	0	0	0	0
37	o	1	0	0	0	0
37	v	1	0	0	0	0
38	D	147	0	222	10	0
38	E	42	0	57	6	0
38	L	49	0	74	2	0
38	a	42	0	57	3	0
38	d	147	0	222	12	0
38	l	49	0	74	2	0
39	E	43	0	30	2	0
39	e	43	0	30	4	0
40	J	1	0	0	0	0
40	j	1	0	0	0	0
41	V	43	0	30	0	0
41	v	43	0	30	0	0
42	A	130	0	0	1	0
42	B	164	0	0	2	0
42	C	147	0	0	1	0
42	D	112	0	0	1	0
42	E	14	0	0	1	0
42	F	4	0	0	0	0
42	H	20	0	0	0	0
42	I	6	0	0	1	0
42	J	4	0	0	0	0
42	K	7	0	0	0	0
42	L	4	0	0	0	0
42	M	7	0	0	0	0
42	O	74	0	0	1	0
42	T	8	0	0	0	0
42	U	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	V	65	0	0	0	0
42	X	2	0	0	0	0
42	Y	1	0	0	0	0
42	a	133	0	0	1	0
42	b	185	0	0	2	0
42	c	122	0	0	3	0
42	d	109	0	0	0	0
42	e	7	0	0	0	0
42	f	3	0	0	0	0
42	h	14	0	0	0	0
42	i	3	0	0	0	0
42	j	2	0	0	0	0
42	k	3	0	0	0	0
42	l	6	0	0	0	0
42	m	11	0	0	1	0
42	o	78	0	0	1	0
42	t	5	0	0	0	0
42	u	47	0	0	1	0
42	v	49	0	0	1	0
42	x	4	0	0	0	0
42	y	1	0	0	0	0
All	All	53280	0	52671	660	0

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

All (660) 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)
24:C:514:CLA:HBB1	26:C:515:BCR:H24C	1.35	1.05
24:B:604:CLA:H42	24:B:605:CLA:H2	1.47	0.95
13:o:124:ASN:HD22	13:o:147:ASN:HD22	1.19	0.89
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.54	0.88
5:e:67:THR:H	5:e:75:GLN:HE22	1.27	0.83
4:d:192:THR:HG23	24:d:402:CLA:HBC2	1.64	0.79
24:C:506:CLA:CMD	24:C:508:CLA:HAB	2.16	0.76
24:B:601:CLA:H12	24:B:601:CLA:H71	1.70	0.73
1:a:253:GLY:HA3	2:b:491:VAL:HG12	1.70	0.72
38:a:419:LHG:HC31	5:e:9:PRO:HA	1.72	0.72
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.71	0.72
3:c:279:LEU:HD22	24:c:511:CLA:HED2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:505:CLA:HBB1	24:c:514:CLA:H41	1.71	0.71
31:A:416[A]:PL9:H253	24:D:402:CLA:H141	1.72	0.70
24:A:405:CLA:HHC	24:A:405:CLA:HBB1	1.73	0.70
24:b:606:CLA:HHC	24:b:606:CLA:HBB1	1.74	0.69
33:Z:101:LMG:HO4	33:Z:101:LMG:HO5	1.39	0.69
31:a:414[A]:PL9:H28	38:a:419:LHG:H222	1.76	0.67
24:A:406:CLA:H152	31:A:416[B]:PL9:H252	1.77	0.67
8:I:37:LEU:O	42:I:201:HOH:O	2.12	0.67
1:A:121[B]:LEU:HD11	24:C:506:CLA:H122	1.75	0.67
24:B:614:CLA:H43	27:B:620:SQD:H111	1.76	0.67
24:c:506:CLA:H42	36:c:519:DGD:HB42	1.77	0.67
34:M:103:LMT:H11	12:m:6:LEU:HD11	1.77	0.67
38:d:406:LHG:H212	12:m:18:PRO:HG3	1.76	0.67
2:b:497:GLN:HB2	2:b:504:THR:HB	1.78	0.66
38:D:407:LHG:H132	38:D:407:LHG:H372	1.77	0.65
2:b:341:LYS:NZ	35:b:624:HTG:S1	2.61	0.65
33:A:418:LMG:H152	36:C:517:DGD:HA91	1.77	0.65
5:E:40:THR:HB	20:R:4:ARG:HG2	1.79	0.65
25:A:408:PHO:H3A	24:D:402:CLA:H142	1.77	0.65
24:b:603:CLA:C2D	24:b:605:CLA:H2	2.26	0.65
33:Z:101:LMG:O5	33:Z:101:LMG:O4	2.14	0.64
24:c:507:CLA:CMD	24:c:509:CLA:HAB	2.28	0.64
24:c:515:CLA:HBB1	26:c:516:BCR:H24C	1.78	0.64
25:a:406:PHO:HBC3	4:d:279:LEU:HD22	1.78	0.64
2:b:121:GLU:HG2	7:h:4:ARG:HG2	1.79	0.64
1:A:25:ASP:OD1	42:A:501:HOH:O	2.15	0.63
3:c:213[B]:LEU:HD11	26:c:517:BCR:H373	1.81	0.63
24:c:510:CLA:HBC3	24:c:512:CLA:H71	1.80	0.63
24:b:605:CLA:HHC	24:b:605:CLA:HBB1	1.79	0.63
3:C:286:ALA:HB2	24:C:503:CLA:HMD1	1.81	0.62
24:C:504:CLA:HHC	24:C:504:CLA:HBB1	1.81	0.62
27:a:409:SQD:H271	38:d:408:LHG:H141	1.79	0.62
33:C:521:LMG:H181	35:C:522:HTG:H6'2	1.80	0.62
10:K:15:TYR:OH	19:Z:58:ASN:ND2	2.32	0.62
24:c:503:CLA:C4D	24:c:505:CLA:H2	2.29	0.61
34:A:359:LMT:H71	2:b:39:LEU:HD13	1.83	0.61
3:c:438:LEU:HD11	24:c:507:CLA:HBB1	1.83	0.61
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.82	0.61
3:C:279:LEU:HD22	24:C:510:CLA:HED2	1.83	0.60
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.83	0.60
2:B:55:MET:HE3	28:B:627:GOL:H32	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:411:SQD:H251	38:D:407:LHG:H131	1.84	0.60
1:a:15:GLU:HB2	34:a:418:LMT:H6'2	1.84	0.60
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.84	0.60
2:b:12:LEU:HB2	24:b:612:CLA:HMC2	1.84	0.59
24:c:504:CLA:H61	24:c:514:CLA:H42	1.83	0.59
3:c:409[B]:GLY:O	42:c:601:HOH:O	2.15	0.59
3:C:406:SER:HA	3:C:420:VAL:HG23	1.85	0.59
35:B:623:HTG:H61	34:a:359:LMT:H6E	1.84	0.59
31:A:416[B]:PL9:H253	24:D:402:CLA:H141	1.84	0.59
10:k:21:LEU:HD13	18:y:24:MET:HE2	1.84	0.59
39:E:103:HEM:HAC	6:F:27:ALA:HB1	1.85	0.59
24:a:407:CLA:H152	24:c:508:CLA:H142	1.85	0.59
4:D:123:ILE:HD11	36:H:102:DGD:HAH2	1.84	0.59
3:c:286:ALA:HB2	24:c:504:CLA:HMD1	1.83	0.59
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.85	0.58
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.38	0.58
24:B:616:CLA:HHC	24:B:616:CLA:HBB1	1.85	0.58
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.83	0.58
3:C:325:GLY:O	15:U:51:LYS:NZ	2.35	0.58
1:a:214[B]:MET:HG2	31:a:414[B]:PL9:H103	1.84	0.58
3:c:168:LEU:HD21	24:c:511:CLA:H61	1.85	0.58
24:c:506:CLA:H151	24:c:510:CLA:H143	1.85	0.58
1:a:211[A]:PHE:CD2	31:a:414[A]:PL9:H101	2.39	0.58
2:b:224:ARG:NH1	4:d:16:ASP:OD2	2.36	0.58
24:c:513:CLA:H191	33:z:101:LMG:H242	1.85	0.58
24:A:409:CLA:H171	24:C:507:CLA:H142	1.86	0.58
1:a:211[B]:PHE:CD2	31:a:414[B]:PL9:H101	2.39	0.58
7:h:56:ASP:OD1	17:x:2:THR:OG1	2.15	0.58
24:B:613:CLA:H51	38:D:357:LHG:H361	1.85	0.57
24:C:514:CLA:H172	33:C:521:LMG:H402	1.86	0.57
13:O:32:ILE:HG13	13:O:93:LEU:HD11	1.85	0.57
24:C:509:CLA:HBC3	24:C:511:CLA:H71	1.86	0.57
24:B:616:CLA:HED2	24:B:616:CLA:H43	1.87	0.57
38:D:407:LHG:H112	38:D:407:LHG:H382	1.87	0.57
15:U:64:ILE:HB	15:U:67:LEU:HD11	1.87	0.57
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.85	0.57
13:O:42:ARG:O	13:O:241:ALA:HA	2.06	0.56
27:b:620:SQD:H462	27:b:620:SQD:H1	1.87	0.56
5:e:27:ILE:HD11	39:e:102:HEM:HBC2	1.88	0.56
1:A:227:THR:HB	1:A:231:GLU:HG3	1.87	0.56
13:O:68:THR:HG22	13:O:110[B]:MET:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:502:CLA:HHC	24:C:502:CLA:HBB1	1.86	0.56
3:C:95:LEU:HD13	24:C:503:CLA:H142	1.87	0.56
24:a:350:CLA:HHC	24:a:350:CLA:HBB1	1.87	0.56
1:a:227:THR:HB	1:a:231:GLU:HG3	1.87	0.56
30:a:413[B]:OEY:O4	42:a:502[B]:HOH:O	2.18	0.56
3:C:334:PRO:HA	13:O:153:THR:OG1	2.06	0.55
13:O:89:SER:N	42:O:402:HOH:O	2.35	0.55
31:D:405:PL9:H33	38:L:101:LHG:H222	1.88	0.55
5:e:60:GLN:HG3	5:e:62:SER:H	1.71	0.55
8:i:35:LYS:O	8:i:37:LEU:N	2.39	0.55
1:a:84:PRO:HA	1:a:112:TYR:CG	2.41	0.55
2:b:186:GLY:O	42:b:701:HOH:O	2.18	0.55
10:k:20:PRO:HB3	18:y:21:GLN:HG3	1.89	0.55
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.87	0.55
2:b:216:HIS:HE1	24:b:609:CLA:C1A	2.19	0.55
24:b:603:CLA:C3D	24:b:605:CLA:H2	2.37	0.55
10:k:15:TYR:OH	19:z:58:ASN:ND2	2.35	0.55
24:D:403:CLA:HHC	24:D:403:CLA:HBB1	1.89	0.55
24:c:515:CLA:HBB1	26:c:516:BCR:H371	1.89	0.55
24:C:506:CLA:HMD3	24:C:508:CLA:HAB	1.88	0.54
24:C:507:CLA:H62	34:I:101:LMT:H91	1.89	0.54
26:Y:101:BCR:H321	26:Y:101:BCR:HC8	1.88	0.54
24:A:406:CLA:H152	31:A:416[A]:PL9:H252	1.88	0.54
24:C:511:CLA:H192	24:C:511:CLA:HBC3	1.89	0.54
36:c:519:DGD:HB52	33:c:521:LMG:H362	1.90	0.54
2:B:216:HIS:HE1	24:B:609:CLA:C1A	2.21	0.54
38:E:101:LHG:O2	6:F:19:ARG:NH1	2.40	0.54
18:Y:23:THR:HB	18:Y:24:MET:HE2	1.90	0.54
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.07	0.54
24:B:602:CLA:HHC	24:B:602:CLA:HBB1	1.91	0.53
26:B:618:BCR:H363	26:t:102:BCR:H19C	1.91	0.53
3:c:409[A]:GLY:O	42:c:601:HOH:O	2.19	0.53
4:d:141:TYR:OH	38:d:406:LHG:O4	2.16	0.53
13:o:58:ASN:HD21	13:o:61:GLN:HB2	1.73	0.53
5:e:73:LYS:NZ	5:e:77:GLU:OE2	2.40	0.53
24:A:409:CLA:H193	24:C:507:CLA:H101	1.91	0.53
26:y:101:BCR:H321	26:y:101:BCR:HC8	1.89	0.53
24:d:403:CLA:H162	7:h:37:LEU:HD21	1.89	0.53
3:c:52:ALA:HB2	24:c:513:CLA:HMA2	1.91	0.53
1:a:214[A]:MET:HE2	1:a:255[A]:PHE:CE1	2.44	0.53
24:c:510:CLA:H203	36:c:519:DGD:HA92	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.90	0.53
5:e:56:TYR:O	16:v:1:ALA:N	2.34	0.53
1:A:84:PRO:HA	1:A:112:TYR:CG	2.43	0.52
4:D:14:TRP:CD1	35:D:410:HTG:H61	2.43	0.52
10:K:24:VAL:HG11	18:Y:25:ILE:HB	1.92	0.52
13:O:39:ARG:HB2	13:O:246:ALA:HB2	1.90	0.52
31:a:414[A]:PL9:H512	27:f:101:SQD:H292	1.90	0.52
4:D:192:THR:HG23	24:D:402:CLA:HBC2	1.92	0.52
25:a:405:PHO:HAB	4:d:205:LEU:HD13	1.90	0.52
10:k:16:ALA:O	10:k:19:ASP:HB2	2.09	0.52
2:B:36[A]:SER:OG	26:B:618:BCR:H362	2.09	0.52
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.92	0.52
3:c:146:PHE:HZ	24:c:514:CLA:HBB2	1.73	0.52
26:t:102:BCR:HC8	26:t:102:BCR:H321	1.91	0.52
16:v:85:GLU:OE2	42:v:301:HOH:O	2.19	0.52
13:O:193:THR:HG21	13:O:220:LEU:HD12	1.90	0.52
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.92	0.52
1:a:183:MET:HA	24:a:403:CLA:HMD1	1.92	0.52
24:c:514:CLA:O2D	24:c:515:CLA:HBB2	2.10	0.52
16:v:12:LEU:HD12	16:v:69:ILE:HB	1.91	0.52
3:C:148:GLY:O	3:C:156:LYS:NZ	2.39	0.52
10:K:20:PRO:HB3	18:Y:21:GLN:HG3	1.91	0.52
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.92	0.52
1:a:310:LYS:HD2	16:v:1:ALA:HB1	1.92	0.51
27:a:409:SQD:H141	38:d:408:LHG:H152	1.92	0.51
1:A:274[B]:PHE:HD1	27:A:411:SQD:H101	1.74	0.51
2:b:76[B]:SER:HG	2:b:78:TRP:CD1	2.28	0.51
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.46	0.51
38:d:408:LHG:H122	38:d:408:LHG:H381	1.91	0.51
2:b:162:PHE:O	24:b:606:CLA:HHD	2.11	0.51
5:E:18:ARG:H	9:J:2:SER:N	2.08	0.51
3:c:42:LEU:HD21	24:c:513:CLA:H2A	1.93	0.51
24:B:602:CLA:H101	24:B:609:CLA:H193	1.93	0.51
36:c:518:DGD:HG11	42:c:607:HOH:O	2.10	0.51
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.46	0.51
31:A:416[A]:PL9:H262	38:E:101:LHG:H223	1.93	0.50
4:D:13:GLY:HA3	35:D:410:HTG:H62	1.92	0.50
24:B:610:CLA:H122	24:B:615:CLA:HAA1	1.93	0.50
4:D:244:TYR:OH	4:D:264[B]:LYS:HE2	2.12	0.50
10:K:23:ASP:OD2	18:Y:21:GLN:NE2	2.45	0.50
13:O:24:ASP:HA	13:O:203:LYS:HE2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:507:CLA:H2	26:C:516:BCR:H10C	1.93	0.50
38:D:406:LHG:H322	14:T:21:ILE:HD11	1.93	0.50
1:a:72:LEU:HD11	34:a:359:LMT:H51	1.94	0.50
31:a:414[B]:PL9:H28	38:a:419:LHG:H222	1.93	0.50
24:b:607:CLA:H122	33:b:621:LMG:H242	1.93	0.50
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.93	0.50
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.93	0.50
3:c:67:MET:HE3	3:c:70:PHE:HB3	1.94	0.50
13:O:124:ASN:HD22	13:O:147:ASN:HD22	1.59	0.49
2:b:233:ASN:O	2:b:236:THR:HG22	2.12	0.49
13:o:40:ILE:HD12	13:o:95:PHE:CD1	2.46	0.49
34:M:101:LMT:H6D	11:l:9:PRO:HA	1.94	0.49
6:F:30:THR:HG21	33:J:101:LMG:H412	1.93	0.49
10:k:17:ILE:HD13	10:k:17:ILE:H	1.76	0.49
2:B:13:ILE:HG12	24:B:612:CLA:HAC2	1.95	0.49
2:b:30:VAL:HG12	24:b:605:CLA:HHD	1.93	0.49
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.95	0.49
24:c:503:CLA:C3D	24:c:505:CLA:H2	2.41	0.49
2:B:149:LEU:HD13	24:B:604:CLA:H171	1.95	0.49
13:O:51:LEU:HD12	13:O:234:LYS:HG2	1.94	0.49
14:T:2:GLU:H	14:T:2:GLU:CD	2.19	0.49
4:d:126:MET:HE3	4:d:143:ALA:O	2.13	0.49
3:C:41:ARG:NH1	24:C:512:CLA:HMD1	2.27	0.49
3:c:223:TRP:CG	3:c:224:ILE:H	2.31	0.49
5:e:26:THR:HB	39:e:102:HEM:HAB	1.94	0.49
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.48	0.49
3:C:443:TRP:CE2	24:C:509:CLA:HMD2	2.48	0.49
12:m:5:GLN:HB3	42:m:211:HOH:O	2.12	0.49
24:c:510:CLA:HBC2	38:d:408:LHG:H362	1.95	0.48
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.95	0.48
27:a:409:SQD:H383	26:y:101:BCR:H392	1.94	0.48
38:d:408:LHG:H122	38:d:408:LHG:C38	2.43	0.48
1:A:214[A]:MET:HE2	1:A:255[A]:PHE:CE1	2.48	0.48
24:a:404:CLA:HMB2	24:d:402:CLA:H122	1.95	0.48
38:d:407:LHG:HC62	11:l:15:THR:HG23	1.95	0.48
1:A:240:GLY:HA3	14:T:29:ILE:HG23	1.96	0.48
35:B:623:HTG:O5	28:a:410:GOL:H11	2.13	0.48
2:b:185:TRP:CD1	35:b:625:HTG:H2	2.48	0.48
5:e:8:ARG:HG3	5:e:9:PRO:HD2	1.95	0.48
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.94	0.48
34:M:103:LMT:O3'	34:M:103:LMT:O2B	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:614:CLA:H42	34:m:102:LMT:H62	1.95	0.48
2:b:461:LEU:HD21	4:d:284:ILE:HD11	1.96	0.48
13:o:40:ILE:HG12	13:o:243:ILE:HD13	1.96	0.48
31:A:416[A]:PL9:H171	31:A:416[A]:PL9:H151	1.52	0.48
1:a:334:ARG:HD3	4:d:320:LEU:HD13	1.94	0.48
33:c:521:LMG:H292	33:c:521:LMG:H152	1.96	0.48
1:A:26:ASN:OD1	27:A:413:SQD:O2	2.32	0.48
2:B:489:GLU:HB3	2:B:495:PHE:CG	2.49	0.48
4:D:85:MET:CE	4:D:96:GLU:HG2	2.43	0.48
24:A:404:CLA:CBD	24:A:405:CLA:HAC2	2.44	0.48
2:B:489:GLU:HB3	2:B:495:PHE:CD1	2.48	0.48
16:V:126:LEU:HB3	16:V:129:LYS:HB2	1.95	0.48
13:o:32:ILE:HG21	13:o:93:LEU:HD21	1.96	0.48
2:B:299:GLU:HG3	42:B:831:HOH:O	2.14	0.47
2:b:98:LEU:HB2	35:b:623:HTG:H7'1	1.95	0.47
12:m:12:ALA:HA	34:t:101:LMT:H123	1.95	0.47
4:D:199:MET:HG2	31:D:405:PL9:H321	1.96	0.47
1:A:183:MET:HA	24:A:404:CLA:HMD1	1.96	0.47
5:E:77:GLU:O	5:E:81:GLU:HG2	2.13	0.47
2:B:363:PHE:HB3	2:B:365:SER:O	2.15	0.47
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.49	0.47
3:c:174:LEU:HD22	24:c:504:CLA:H203	1.96	0.47
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.96	0.47
24:A:406:CLA:HED1	36:C:519:DGD:HAE2	1.95	0.47
24:a:403:CLA:HBB1	24:a:403:CLA:HMB3	1.96	0.47
2:b:413:ASP:O	2:b:417:VAL:HG23	2.15	0.47
24:a:403:CLA:H201	38:d:407:LHG:H161	1.97	0.47
2:b:124:ARG:HD2	2:b:129:GLY:O	2.15	0.47
2:b:245:VAL:HG22	24:b:612:CLA:H202	1.97	0.47
3:c:338:GLY:HA3	3:c:341:LEU:O	2.15	0.47
24:d:403:CLA:H142	24:d:403:CLA:H112	1.71	0.47
15:u:86:GLU:HG3	42:u:217:HOH:O	2.14	0.47
42:E:204:HOH:O	9:J:6:ARG:HG3	2.15	0.47
1:a:105:TRP:CE2	1:a:110:GLY:HA3	2.49	0.47
33:a:417:LMG:HC71	3:c:216:SER:HB2	1.96	0.47
6:F:15:ILE:HD13	20:R:23:ILE:HD11	1.97	0.47
24:b:614:CLA:H62	24:b:614:CLA:H41	1.50	0.47
2:b:201:HIS:HB2	24:b:602:CLA:C1B	2.45	0.47
2:b:341:LYS:HE2	42:b:704:HOH:O	2.14	0.47
24:b:606:CLA:H162	24:b:606:CLA:H122	1.62	0.47
3:c:429:SER:HA	36:c:519:DGD:HBW1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:416[B]:PL9:H262	38:E:101:LHG:H223	1.97	0.46
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.50	0.46
36:C:518:DGD:HAE2	36:C:518:DGD:HA81	1.68	0.46
3:c:334:PRO:HA	13:o:153:THR:OG1	2.14	0.46
3:c:406:SER:HA	3:c:420:VAL:HG23	1.97	0.46
24:c:507:CLA:HAA1	24:c:507:CLA:HBD	1.96	0.46
1:a:211[B]:PHE:HD2	31:a:414[B]:PL9:H101	1.77	0.46
24:b:601:CLA:H93	24:b:601:CLA:H111	1.83	0.46
36:c:519:DGD:HA81	36:c:519:DGD:HAF1	1.98	0.46
3:C:127:PHE:HZ	33:Z:101:LMG:H121	1.80	0.46
24:b:613:CLA:HBB1	24:b:613:CLA:HMB1	1.98	0.46
2:B:30:VAL:HG12	24:B:605:CLA:HHD	1.97	0.46
2:B:160:GLY:HA2	2:B:163:GLY:O	2.15	0.46
1:a:214[A]:MET:HG2	31:a:414[A]:PL9:H103	1.98	0.46
2:b:231:MET:HE2	24:b:610:CLA:HMC1	1.96	0.46
24:c:507:CLA:HMD3	24:c:509:CLA:HAB	1.97	0.46
24:A:404:CLA:H191	38:D:406:LHG:H332	1.98	0.46
2:B:58:GLN:C	2:B:329:PRO:HB3	2.39	0.46
24:C:502:CLA:C4D	24:C:504:CLA:H2	2.46	0.46
24:C:513:CLA:H101	24:C:514:CLA:H141	1.98	0.46
4:D:78:VAL:HG11	4:D:114:ILE:HD12	1.98	0.46
4:D:210:LEU:HA	4:D:213:ILE:HG22	1.98	0.46
24:C:505:CLA:H62	24:C:505:CLA:H41	1.75	0.46
1:a:214[B]:MET:HE2	1:a:255[B]:PHE:CE1	2.51	0.46
1:A:187:GLN:HB2	24:A:404:CLA:HAC2	1.96	0.46
34:B:622:LMT:H6E	4:D:16:ASP:OD2	2.15	0.46
3:C:42:LEU:HD21	24:C:512:CLA:H2A	1.98	0.46
24:a:404:CLA:H112	33:j:101:LMG:H231	1.98	0.46
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.81	0.46
2:B:145:LEU:HD22	24:B:604:CLA:H162	1.98	0.46
31:a:414[B]:PL9:H512	27:f:101:SQD:H292	1.98	0.46
26:b:619:BCR:H331	26:b:619:BCR:C8	2.46	0.46
35:b:624:HTG:H62	42:o:405:HOH:O	2.16	0.46
26:d:404:BCR:H383	33:j:101:LMG:H171	1.96	0.46
5:E:30:LEU:HD23	20:R:12:VAL:HG22	1.97	0.46
1:a:131:TRP:CH2	24:c:507:CLA:HAA2	2.51	0.46
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.51	0.46
24:b:605:CLA:HHC	24:b:605:CLA:CBB	2.46	0.46
24:C:509:CLA:H92	38:D:407:LHG:H371	1.98	0.45
38:D:406:LHG:HC62	11:L:15:THR:HG23	1.98	0.45
31:a:414[B]:PL9:H453	27:f:101:SQD:H271	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:605:CLA:HAA1	24:b:605:CLA:HBD	1.97	0.45
3:C:223:TRP:CG	3:C:224:ILE:H	2.34	0.45
24:b:611:CLA:HHC	24:b:611:CLA:HBB1	1.98	0.45
24:b:612:CLA:CMB	24:b:614:CLA:HBB1	2.46	0.45
27:A:411:SQD:H81	27:A:411:SQD:H112	1.66	0.45
19:z:26:ALA:HB1	19:z:36:SER:HB3	1.97	0.45
2:B:162:PHE:O	24:B:606:CLA:HHD	2.17	0.45
24:B:614:CLA:H62	24:B:614:CLA:H41	1.64	0.45
33:C:521:LMG:H152	35:C:522:HTG:H4'2	1.98	0.45
38:D:407:LHG:H332	38:D:407:LHG:H302	1.81	0.45
20:R:2:ASP:HB3	20:R:5:VAL:HG23	1.99	0.45
1:a:121[A]:LEU:HD21	24:a:407:CLA:HMB2	1.98	0.45
2:b:36:SER:OG	26:b:618:BCR:H362	2.15	0.45
24:c:509:CLA:H142	24:c:509:CLA:H112	1.74	0.45
24:d:403:CLA:H61	24:d:403:CLA:H41	1.44	0.45
26:t:102:BCR:H11C	26:t:102:BCR:H341	1.83	0.45
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.99	0.45
1:A:274[B]:PHE:CD1	27:A:411:SQD:H101	2.52	0.45
3:C:48:LYS:HD2	3:C:138:GLU:HG3	1.99	0.45
5:E:36:LEU:HA	5:E:39:SER:OG	2.16	0.45
20:R:29:LYS:HB3	20:R:29:LYS:HE2	1.76	0.45
24:b:605:CLA:H41	24:b:612:CLA:H161	1.99	0.45
4:d:83:ASN:ND2	4:d:166:SER:OG	2.50	0.45
13:o:92:SER:HB3	13:o:131:PRO:HA	1.98	0.45
31:D:405:PL9:C33	38:L:101:LHG:H222	2.45	0.45
31:a:414[A]:PL9:H322	31:a:414[A]:PL9:H301	1.86	0.45
26:K:102:BCR:H24C	26:K:102:BCR:H371	1.60	0.45
5:e:14:ILE:O	5:e:20:TRP:NE1	2.47	0.45
24:B:609:CLA:HMD1	7:H:27:THR:HB	1.98	0.45
3:C:95:LEU:HD21	24:C:502:CLA:OBD	2.17	0.45
2:b:58:GLN:C	2:b:329:PRO:HB3	2.42	0.45
26:b:617:BCR:H24C	26:b:617:BCR:H371	1.80	0.45
5:e:67:THR:N	5:e:75:GLN:HE22	2.06	0.45
24:B:602:CLA:H203	24:B:602:CLA:H162	1.70	0.45
24:B:605:CLA:H192	24:B:609:CLA:HBB2	1.99	0.45
26:B:619:BCR:H331	26:B:619:BCR:C8	2.47	0.45
3:C:464:GLU:OE2	4:D:245:SER:OG	2.34	0.45
24:a:404:CLA:H203	33:j:101:LMG:H412	1.98	0.45
24:b:613:CLA:H112	24:b:613:CLA:H151	1.62	0.45
16:v:61:LEU:HD23	16:v:61:LEU:HA	1.84	0.45
24:A:409:CLA:H171	24:C:507:CLA:H112	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:203:THR:O	3:C:235:GLY:HA3	2.17	0.44
7:H:43:LEU:HD12	7:H:43:LEU:HA	1.76	0.44
24:c:507:CLA:HMD2	24:c:509:CLA:HAB	1.99	0.44
4:d:186:GLN:HB2	24:d:402:CLA:HBC1	1.98	0.44
26:t:102:BCR:HC7	26:t:102:BCR:H331	1.49	0.44
1:A:300:PHE:HB3	1:A:302:PHE:CE1	2.52	0.44
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.99	0.44
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.99	0.44
26:D:404:BCR:H15C	26:D:404:BCR:H351	1.86	0.44
18:Y:22:LEU:HA	18:Y:25:ILE:HG22	1.99	0.44
24:c:512:CLA:HED2	24:c:512:CLA:H2	1.98	0.44
26:k:101:BCR:H371	26:k:101:BCR:H24C	1.64	0.44
35:B:624:HTG:H3	13:O:178:LYS:HE3	1.99	0.44
34:E:102:LMT:O3'	34:E:102:LMT:O2B	2.32	0.44
26:H:101:BCR:H24C	26:H:101:BCR:H371	1.72	0.44
13:O:92:SER:HB3	13:O:131:PRO:HA	1.98	0.44
24:a:403:CLA:CBD	24:a:350:CLA:HAC2	2.47	0.44
3:c:56:HIS:HB2	24:c:511:CLA:HMB1	2.00	0.44
26:c:516:BCR:H11C	26:c:516:BCR:H341	1.77	0.44
31:d:405:PL9:C33	38:l:101:LHG:H222	2.48	0.44
7:h:38:PHE:HB2	26:h:102:BCR:H10C	1.99	0.44
1:A:183:MET:HB3	24:A:404:CLA:HBC2	1.99	0.44
2:B:224:ARG:HD2	42:D:501:HOH:O	2.15	0.44
34:B:622:LMT:H5'	32:D:409:UNL:O9	2.17	0.44
1:a:76:ASN:HD22	28:a:416:GOL:H32	1.83	0.44
2:b:98:LEU:HD13	35:b:623:HTG:H7'1	1.98	0.44
26:b:619:BCR:H15C	26:b:619:BCR:H351	1.89	0.44
3:c:425:TRP:CD1	24:c:506:CLA:HMA3	2.52	0.44
3:c:443:TRP:CZ2	24:c:510:CLA:HMD1	2.52	0.44
8:i:2:GLU:O	8:i:6:ILE:HG12	2.17	0.44
24:B:613:CLA:HBB1	24:B:613:CLA:HMB1	1.98	0.44
24:C:502:CLA:C3D	24:C:504:CLA:H2	2.48	0.44
26:H:101:BCR:H331	26:H:101:BCR:C8	2.47	0.44
16:V:6:GLU:N	16:V:6:GLU:OE2	2.46	0.44
24:b:616:CLA:H62	24:b:616:CLA:H92	1.70	0.44
3:c:166:ILE:HG21	24:c:514:CLA:H171	2.00	0.44
9:j:17:GLY:HA3	26:y:101:BCR:H371	1.99	0.44
2:B:499:VAL:HG12	4:D:135:LEU:HB3	1.99	0.44
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.00	0.44
24:a:407:CLA:H172	24:c:508:CLA:H91	2.00	0.44
31:a:414[B]:PL9:H171	31:a:414[B]:PL9:H151	1.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:516:BCR:H15C	26:c:516:BCR:H351	1.78	0.44
4:d:244:TYR:OH	4:d:264[A]:LYS:HE2	2.18	0.44
24:d:403:CLA:H2	17:x:17:GLY:HA3	1.99	0.44
1:a:103:ASP:OD2	13:o:69:LYS:HE3	2.17	0.44
3:c:171:GLY:O	3:c:174:LEU:HB2	2.17	0.44
26:d:404:BCR:H15C	26:d:404:BCR:H351	1.81	0.44
12:m:5:GLN:HA	14:t:1:FME:HE1	2.00	0.44
2:B:143:LEU:HA	24:B:610:CLA:HED1	2.00	0.44
24:B:606:CLA:H151	24:B:616:CLA:H122	1.98	0.44
13:O:81:ILE:HA	13:O:100:GLY:HA3	2.00	0.44
25:a:405:PHO:ND	25:a:405:PHO:NC	2.66	0.44
3:c:199:ILE:HG21	3:c:234:VAL:HG21	1.99	0.44
4:d:55:VAL:O	4:d:66:SER:HB3	2.17	0.44
4:d:210:LEU:HA	4:d:213:ILE:HG22	1.99	0.44
31:d:405:PL9:H33	38:l:101:LHG:H222	2.00	0.44
8:i:17:LEU:HD22	8:i:21:PHE:HE2	1.82	0.44
34:A:359:LMT:H21	35:b:623:HTG:H1	2.00	0.43
3:C:276:LEU:HD23	24:C:510:CLA:HED1	2.00	0.43
5:E:14:ILE:HD12	9:J:12:VAL:HG11	2.00	0.43
1:a:82:VAL:HB	1:a:174:LEU:HB2	2.00	0.43
1:a:307[B]:ILE:HG22	1:a:313:VAL:HA	1.99	0.43
1:A:63:ILE:HB	3:C:335:THR:HG21	2.00	0.43
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.87	0.43
24:B:602:CLA:H92	36:H:102:DGD:HB71	1.99	0.43
3:C:60:ILE:HG22	24:C:504:CLA:HHD	1.99	0.43
36:C:517:DGD:HG11	42:C:601:HOH:O	2.18	0.43
31:D:405:PL9:H401	31:D:405:PL9:H422	1.54	0.43
1:a:270[B]:SER:HB2	27:a:409:SQD:O49	2.17	0.43
24:b:601:CLA:H72	24:b:601:CLA:H2	2.00	0.43
38:d:408:LHG:H331	38:d:408:LHG:H361	1.59	0.43
26:y:101:BCR:H15C	26:y:101:BCR:H351	1.86	0.43
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.53	0.43
3:C:213:LEU:HG	24:C:507:CLA:H202	2.00	0.43
26:T:101:BCR:H24C	26:T:101:BCR:H371	1.83	0.43
18:Y:39:LEU:HD23	18:Y:39:LEU:HA	1.85	0.43
19:Z:29:SER:HA	19:Z:30:PRO:HD3	1.87	0.43
27:a:409:SQD:H202	27:a:409:SQD:H171	1.81	0.43
26:h:102:BCR:H371	26:h:102:BCR:H24C	1.77	0.43
16:v:106:ASN:OD1	16:v:106:ASN:N	2.43	0.43
35:B:623:HTG:H1	34:a:359:LMT:H21	2.00	0.43
24:C:509:CLA:H142	24:C:509:CLA:H111	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:ARG:NH2	27:F:101:SQD:O4	2.51	0.43
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.18	0.43
13:O:30:TYR:HA	13:O:31:PRO:HD3	1.81	0.43
31:a:414[A]:PL9:H151	31:a:414[A]:PL9:H171	1.56	0.43
5:e:60:GLN:HE21	5:e:61:ARG:H	1.66	0.43
16:v:64:PRO:HD2	16:v:66:ARG:NH2	2.33	0.43
27:b:620:SQD:H62	11:l:7:ARG:NH1	2.33	0.43
3:c:325:GLY:O	15:u:51:LYS:NZ	2.46	0.43
4:d:85:MET:HE2	4:d:90:LEU:HD21	2.00	0.43
2:B:12:LEU:HB2	24:B:612:CLA:HMC2	2.00	0.43
3:c:38:GLY:HA3	24:c:513:CLA:HMD2	2.01	0.43
4:d:20:ASP:HB3	17:x:37:VAL:HG21	1.99	0.43
13:o:81:ILE:HG23	13:o:97:GLU:HG3	2.00	0.43
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.84	0.43
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.53	0.43
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.01	0.43
31:D:405:PL9:H28	31:D:405:PL9:H322	1.79	0.43
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.00	0.43
10:K:15:TYR:CE1	19:Z:5:PHE:HZ	2.37	0.43
15:U:48:LEU:HD23	15:U:48:LEU:HA	1.86	0.43
33:Z:101:LMG:H141	33:Z:101:LMG:H111	1.90	0.43
26:B:618:BCR:H15C	26:B:618:BCR:H351	1.86	0.43
12:M:18:PRO:O	12:M:21:PHE:HB3	2.18	0.43
13:O:137:THR:C	13:O:139:SER:H	2.25	0.43
26:T:101:BCR:H321	26:T:101:BCR:HC8	2.01	0.43
24:b:614:CLA:H162	24:b:614:CLA:H122	1.69	0.43
3:c:60:ILE:HG22	24:c:505:CLA:HHD	2.01	0.43
24:c:512:CLA:H61	24:c:512:CLA:H102	1.77	0.43
24:c:514:CLA:H92	24:c:514:CLA:H62	1.79	0.43
13:o:42:ARG:O	13:o:241:ALA:HA	2.19	0.43
25:A:407:PHO:HAB	4:D:205:LEU:HD13	2.01	0.43
2:B:103:LEU:HD21	24:B:605:CLA:HMC3	2.00	0.43
2:B:432:PHE:H	35:B:624:HTG:HO3	1.66	0.43
3:C:127:PHE:CE1	33:Z:101:LMG:H142	2.54	0.43
5:E:42:LEU:HA	20:R:4:ARG:NH2	2.34	0.43
3:c:61:VAL:HG12	3:c:118:HIS:O	2.19	0.43
24:c:512:CLA:H122	24:c:512:CLA:H161	1.79	0.43
24:c:514:CLA:HHC	24:c:514:CLA:HBB1	2.00	0.43
1:A:12:ASN:ND2	1:A:15:GLU:HB2	2.34	0.43
1:A:272[B]:HIS:CD2	4:D:218:VAL:HG21	2.54	0.43
24:B:615:CLA:H112	24:B:615:CLA:H152	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B:622:LMT:H62	34:B:622:LMT:H91	1.69	0.43
3:C:24:THR:HB	3:C:138:GLU:OE1	2.19	0.43
2:b:191:ASN:ND2	7:h:59:ASN:O	2.48	0.43
31:d:405:PL9:H322	31:d:405:PL9:H28	1.80	0.43
5:e:20:TRP:HZ2	9:j:12:VAL:HG13	1.84	0.43
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.54	0.42
38:D:357:LHG:H152	11:L:23:LEU:HD21	2.00	0.42
1:a:45:THR:HG23	24:a:350:CLA:H201	2.00	0.42
8:i:17:LEU:HD23	8:i:17:LEU:HA	1.82	0.42
24:B:606:CLA:H192	24:B:616:CLA:H101	2.01	0.42
24:B:614:CLA:H203	33:B:621:LMG:H421	2.00	0.42
15:U:70:ARG:HH21	15:U:73:GLN:HE21	1.66	0.42
19:Z:36:SER:O	19:Z:40:ILE:HG13	2.18	0.42
2:B:266:GLU:HB3	28:B:627:GOL:H12	2.02	0.42
3:C:230:LEU:HD23	3:C:230:LEU:HA	1.87	0.42
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.54	0.42
26:T:101:BCR:H19C	26:b:618:BCR:H363	2.02	0.42
1:a:121[B]:LEU:HD23	33:a:417:LMG:H212	2.00	0.42
24:b:613:CLA:H72	24:b:613:CLA:H111	1.73	0.42
3:c:213[A]:LEU:HG	24:c:508:CLA:H172	2.01	0.42
4:D:241:GLU:CD	4:D:241:GLU:H	2.27	0.42
4:D:293:LEU:HD12	4:D:293:LEU:HA	1.92	0.42
26:T:101:BCR:H331	26:T:101:BCR:HC7	1.56	0.42
13:o:234:LYS:HB2	13:o:234:LYS:HE2	1.68	0.42
26:t:102:BCR:H382	26:t:102:BCR:H23C	2.01	0.42
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.47	0.42
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.01	0.42
2:B:489:GLU:HG2	2:B:495:PHE:CE2	2.54	0.42
3:C:275:SER:HB3	24:C:510:CLA:HED3	2.00	0.42
9:J:7:ILE:HA	9:J:8:PRO:HD3	1.93	0.42
2:b:159:THR:HA	2:b:181:VAL:O	2.20	0.42
24:c:507:CLA:H72	24:c:507:CLA:H112	1.90	0.42
24:c:512:CLA:H111	24:c:512:CLA:H142	1.75	0.42
4:d:24:ARG:NH2	17:x:37:VAL:HG22	2.34	0.42
3:c:47:GLY:HA3	3:c:137:PRO:O	2.20	0.42
3:c:415:ASN:O	3:c:416[B]:SER:HB2	2.19	0.42
7:h:38:PHE:HB2	26:h:102:BCR:C10	2.49	0.42
33:j:101:LMG:H241	33:j:101:LMG:H191	2.01	0.42
31:A:416[B]:PL9:H151	31:A:416[B]:PL9:H171	1.59	0.42
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.54	0.42
3:C:146:PHE:HZ	24:C:513:CLA:HBB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:509:CLA:H122	24:C:509:CLA:H162	1.87	0.42
5:E:17:VAL:O	5:E:21:VAL:HG23	2.20	0.42
1:a:272[B]:HIS:CD2	4:d:218:VAL:HG21	2.54	0.42
3:c:45:LEU:HA	3:c:139:THR:HG22	2.01	0.42
3:c:459:ILE:HG21	3:c:464:GLU:HG3	2.01	0.42
2:B:216:HIS:CE1	24:B:609:CLA:NA	2.87	0.42
4:D:90:LEU:HA	4:D:90:LEU:HD23	1.82	0.42
39:E:103:HEM:CAC	6:F:27:ALA:HB1	2.50	0.42
26:H:101:BCR:H11C	26:H:101:BCR:H341	1.82	0.42
2:b:149:LEU:HG	24:b:606:CLA:HBB2	2.01	0.42
3:c:230:LEU:O	3:c:234:VAL:HG23	2.19	0.42
24:A:404:CLA:HBD	24:A:405:CLA:HAC2	2.02	0.42
24:C:502:CLA:H192	24:C:507:CLA:C1B	2.50	0.42
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.00	0.42
13:O:15:LEU:HD23	13:O:15:LEU:HA	1.82	0.42
1:a:60:ILE:HD12	1:a:84:PRO:HD2	2.01	0.42
1:a:188:ALA:HB2	1:a:328:MET:HB2	2.01	0.42
24:c:504:CLA:H102	24:c:505:CLA:CHB	2.50	0.42
1:A:307:ILE:CG2	1:A:311:GLY:HA2	2.50	0.42
1:A:310:LYS:HD2	16:V:1:ALA:HB1	2.01	0.42
2:B:445:THR:HA	42:B:707:HOH:O	2.18	0.42
26:B:618:BCR:H24C	26:B:618:BCR:H371	1.79	0.42
26:T:101:BCR:HC8	26:T:101:BCR:H311	2.01	0.42
1:a:93:PHE:CD1	1:a:95:PRO:HD3	2.54	0.42
24:b:613:CLA:H162	24:b:613:CLA:H141	1.75	0.42
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.55	0.42
1:A:214[B]:MET:HE2	1:A:255[B]:PHE:CE1	2.55	0.41
1:A:217:SER:HA	4:D:272:LEU:HD12	2.02	0.41
24:A:406:CLA:H191	38:E:101:LHG:H142	2.02	0.41
26:A:410:BCR:H24C	26:A:410:BCR:H371	1.74	0.41
27:A:411:SQD:H381	9:J:21:ILE:HD11	2.01	0.41
31:A:416[B]:PL9:H121	31:A:416[B]:PL9:HC8	1.79	0.41
13:O:234:LYS:HB2	13:O:234:LYS:HE2	1.86	0.41
25:a:406:PHO:ND	25:a:406:PHO:NC	2.69	0.41
24:a:350:CLA:H162	24:a:350:CLA:H203	1.85	0.41
2:b:221:PRO:HA	24:b:609:CLA:HED3	2.01	0.41
24:b:604:CLA:HAA1	24:b:604:CLA:HBD	2.02	0.41
24:b:614:CLA:H72	24:b:614:CLA:H112	1.78	0.41
26:b:619:BCR:HC7	26:b:619:BCR:H321	1.85	0.41
26:d:404:BCR:H11C	26:d:404:BCR:H341	1.93	0.41
3:C:433:LEU:HD13	24:C:503:CLA:CHC	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:504:CLA:HBB1	24:C:504:CLA:CHC	2.50	0.41
26:D:404:BCR:H20C	26:D:404:BCR:H361	1.89	0.41
5:E:60:GLN:HG2	5:E:62[B]:SER:H	1.86	0.41
10:K:17:ILE:H	10:K:17:ILE:HD13	1.85	0.41
10:K:25:LEU:HD22	26:Y:101:BCR:H332	2.01	0.41
16:V:26:TYR:OH	16:V:122:GLU:OE2	2.31	0.41
31:a:414[B]:PL9:HC8	31:a:414[B]:PL9:HC2	1.82	0.41
24:b:614:CLA:H101	26:b:617:BCR:H362	2.00	0.41
24:c:508:CLA:H162	24:c:508:CLA:H122	1.56	0.41
5:e:27:ILE:CD1	39:e:102:HEM:HBC2	2.49	0.41
7:h:43:LEU:HA	7:h:43:LEU:HD12	1.79	0.41
4:D:146:PHE:O	4:D:149:PRO:HD2	2.19	0.41
24:D:402:CLA:HAA2	24:D:402:CLA:HBD	2.01	0.41
26:D:404:BCR:H381	33:J:101:LMG:H231	2.03	0.41
26:T:101:BCR:H341	26:T:101:BCR:H11C	1.81	0.41
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.76	0.41
24:c:515:CLA:H111	24:c:515:CLA:H72	1.81	0.41
5:e:60:GLN:HE21	5:e:62:SER:H	1.67	0.41
16:v:57:GLU:H	16:v:57:GLU:CD	2.27	0.41
27:A:411:SQD:H122	27:A:411:SQD:H152	1.81	0.41
24:B:614:CLA:HAA1	24:B:614:CLA:HBD	2.01	0.41
26:C:515:BCR:H15C	26:C:515:BCR:H351	1.82	0.41
12:M:5:GLN:OE1	12:m:5:GLN:HG3	2.20	0.41
24:b:606:CLA:H192	24:b:606:CLA:H161	1.81	0.41
7:h:62:TRP:C	7:h:64:ALA:H	2.29	0.41
1:A:334:ARG:HD3	4:D:320:LEU:HD13	2.02	0.41
25:A:408:PHO:H72	25:A:408:PHO:H112	1.92	0.41
5:E:9:PRO:HA	38:E:101:LHG:HC31	2.03	0.41
26:Y:101:BCR:H15C	26:Y:101:BCR:H351	1.93	0.41
24:b:603:CLA:H3A	24:b:603:CLA:CGA	2.50	0.41
24:b:614:CLA:HAA1	24:b:614:CLA:HBD	2.02	0.41
26:b:617:BCR:H15C	26:b:617:BCR:H351	1.97	0.41
24:c:515:CLA:H171	26:c:516:BCR:H373	2.03	0.41
5:e:23:HIS:CD2	39:e:102:HEM:NC	2.89	0.41
13:o:83:GLY:HA2	13:o:98:GLU:HG3	2.03	0.41
1:A:131:TRP:CD2	1:A:131:TRP:C	2.96	0.41
1:A:159:LEU:C	1:A:162:PRO:HD2	2.45	0.41
13:O:49[A]:THR:OG1	13:O:236:GLN:HB2	2.20	0.41
26:a:408:BCR:H11C	26:a:408:BCR:H341	1.88	0.41
2:b:76[A]:SER:HB2	35:b:623:HTG:H2	2.02	0.41
33:z:101:LMG:H111	33:z:101:LMG:H142	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:616:CLA:H193	26:B:619:BCR:H331	2.02	0.41
24:C:514:CLA:HBB1	26:C:515:BCR:H371	2.01	0.41
4:D:24:ARG:HD3	17:X:37:VAL:HG22	2.02	0.41
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.55	0.41
8:I:18:LEU:HD23	8:I:18:LEU:HA	1.93	0.41
1:a:153:SER:HB3	24:a:403:CLA:H43	2.02	0.41
1:a:272[A]:HIS:CD2	4:d:218:VAL:HG21	2.56	0.41
2:b:413:ASP:HA	2:b:414:PRO:HD3	1.94	0.41
27:A:413:SQD:H261	2:b:109:LEU:HD13	2.03	0.41
26:B:619:BCR:H11C	26:B:619:BCR:H341	1.92	0.41
26:C:516:BCR:H15C	26:C:516:BCR:H351	1.88	0.41
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.03	0.41
8:I:33:LYS:HB3	8:I:34:ARG:H	1.67	0.41
16:V:41:HIS:HA	16:V:45:ILE:O	2.21	0.41
24:b:605:CLA:H192	24:b:609:CLA:HBB2	2.02	0.41
24:b:609:CLA:NC	26:h:102:BCR:H332	2.36	0.41
3:c:162:GLY:HA2	3:c:248:GLY:HA2	2.03	0.41
24:c:512:CLA:HBA1	24:c:512:CLA:H3A	1.78	0.41
25:A:408:PHO:NC	25:A:408:PHO:ND	2.68	0.41
3:C:262:ARG:HG2	8:I:38:GLU:HG2	2.02	0.41
24:C:506:CLA:HAA1	24:C:506:CLA:HBD	2.03	0.41
24:C:507:CLA:HBA1	24:C:507:CLA:H3A	1.79	0.41
5:E:60:GLN:HG2	5:E:62[A]:SER:H	1.86	0.41
13:O:54:GLU:HG2	13:O:64:GLU:O	2.21	0.41
25:a:406:PHO:H72	25:a:406:PHO:H112	1.85	0.41
2:b:133:LEU:HB3	2:b:138:MET:SD	2.60	0.41
24:c:506:CLA:H62	24:c:506:CLA:H41	1.85	0.41
4:d:261:PHE:CZ	38:d:407:LHG:HC81	2.55	0.41
4:d:343:GLU:HG2	16:v:135:VAL:HG11	2.01	0.41
26:h:102:BCR:C8	26:h:102:BCR:H331	2.50	0.41
13:o:51:LEU:HB3	13:o:65:PHE:HB3	2.02	0.41
15:u:17:LEU:HD23	15:u:17:LEU:HA	1.87	0.41
18:y:39:LEU:HD21	19:z:25:VAL:HA	2.02	0.41
2:B:201:HIS:HB2	24:B:602:CLA:CHB	2.51	0.41
2:B:285:ASN:O	2:B:289:GLN:HG2	2.21	0.41
2:B:464:PHE:HD2	24:B:611:CLA:HAC2	1.85	0.41
2:B:497:GLN:HE22	17:X:38:GLN:HB2	1.85	0.41
4:D:180:ARG:C	4:D:180:ARG:HD3	2.46	0.41
2:b:160:GLY:HA2	2:b:163:GLY:O	2.21	0.41
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.56	0.41
25:A:408:PHO:HBC2	25:A:408:PHO:HHD	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:612:CLA:HMB1	24:B:612:CLA:HBB1	2.03	0.40
13:O:124:ASN:ND2	13:O:147:ASN:HD22	2.18	0.40
1:a:40:THR:HG21	1:a:121[A]:LEU:HD23	2.02	0.40
1:a:269:ARG:NE	4:d:222:LEU:HD22	2.35	0.40
1:a:270[A]:SER:HA	4:d:232:PHE:CE2	2.57	0.40
26:a:408:BCR:H371	26:a:408:BCR:H24C	1.87	0.40
33:a:417:LMG:H242	24:c:507:CLA:H92	2.03	0.40
2:b:201:HIS:HB2	24:b:602:CLA:CHB	2.51	0.40
4:d:40:CYS:HB3	4:d:117:HIS:O	2.21	0.40
38:d:408:LHG:H332	38:d:408:LHG:H302	1.82	0.40
24:B:609:CLA:HBA1	24:B:609:CLA:H3A	1.86	0.40
4:D:209:LEU:HD23	4:D:209:LEU:C	2.46	0.40
15:U:42:TYR:HA	15:U:43:PRO:HA	1.86	0.40
1:a:300:PHE:HB3	1:a:302:PHE:CE1	2.56	0.40
14:t:20:ALA:O	14:t:24:ARG:HB3	2.21	0.40
24:B:613:CLA:H192	24:B:613:CLA:H161	1.75	0.40
18:y:30:ILE:HD12	18:y:30:ILE:HA	1.94	0.40
26:A:410:BCR:H15C	26:A:410:BCR:H351	1.88	0.40
2:B:423:LYS:HA	2:B:423:LYS:HD3	1.79	0.40
3:C:48:LYS:HG3	3:C:138:GLU:HG3	2.03	0.40
24:C:514:CLA:CBB	26:C:515:BCR:H371	2.51	0.40
38:E:101:LHG:H261	38:E:101:LHG:H291	1.82	0.40
1:a:132:GLU:O	1:a:136:ARG:HG2	2.22	0.40
1:a:197:PHE:HB3	1:a:285:PHE:O	2.21	0.40
1:a:213:ALA:HB2	4:d:275:PRO:HG2	2.03	0.40
3:c:375:LEU:HD23	3:c:375:LEU:HA	1.85	0.40
4:d:148:ALA:HB3	4:d:149:PRO:HD3	2.04	0.40
25:A:407:PHO:NC	25:A:407:PHO:ND	2.67	0.40
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.85	0.40
24:b:615:CLA:H72	26:b:619:BCR:C11	2.52	0.40
26:b:618:BCR:H351	26:b:618:BCR:H15C	1.86	0.40
26:c:517:BCR:H24C	26:c:517:BCR:H371	1.76	0.40
34:e:101:LMT:O3'	34:e:101:LMT:O2B	2.38	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	359/344 (104%)	355 (99%)	3 (1%)	1 (0%)	36	43
1	a	360/344 (105%)	355 (99%)	4 (1%)	1 (0%)	36	43
2	B	510/505 (101%)	506 (99%)	4 (1%)	0	100	100
2	b	506/505 (100%)	497 (98%)	9 (2%)	0	100	100
3	C	459/455 (101%)	447 (97%)	10 (2%)	2 (0%)	30	34
3	c	463/455 (102%)	449 (97%)	12 (3%)	2 (0%)	30	34
4	D	343/342 (100%)	333 (97%)	10 (3%)	0	100	100
4	d	342/342 (100%)	336 (98%)	6 (2%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
7	h	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	7	6
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4	2
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	246/244 (101%)	237 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	243/244 (100%)	238 (98%)	5 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	94/104 (90%)	92 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	27 (100%)	0	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	6
19	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	6
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5316/5384 (99%)	5202 (98%)	104 (2%)	10 (0%)	43	52

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
19	z	30	PRO
1	a	259	ILE
7	h	63	LYS
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	295/279 (106%)	295 (100%)	0	100	100
1	a	296/279 (106%)	295 (100%)	1 (0%)	86	92
2	B	410/403 (102%)	406 (99%)	4 (1%)	68	81
2	b	406/403 (101%)	398 (98%)	8 (2%)	48	63
3	C	360/356 (101%)	355 (99%)	5 (1%)	59	73
3	c	364/356 (102%)	358 (98%)	6 (2%)	55	70
4	D	280/277 (101%)	279 (100%)	1 (0%)	84	91
4	d	279/277 (101%)	279 (100%)	0	100	100
5	E	73/73 (100%)	72 (99%)	1 (1%)	59	73
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	24 (96%)	1 (4%)	28	37
7	H	55/54 (102%)	51 (93%)	4 (7%)	13	14
7	h	54/54 (100%)	54 (100%)	0	100	100
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	49
9	J	26/27 (96%)	24 (92%)	2 (8%)	12	13
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	39
10	K	30/30 (100%)	25 (83%)	5 (17%)	2	2
10	k	30/30 (100%)	26 (87%)	4 (13%)	4	3
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	34 (97%)	1 (3%)	37	49
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	33	44
13	O	211/207 (102%)	204 (97%)	7 (3%)	33	44
13	o	208/207 (100%)	207 (100%)	1 (0%)	81	89
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	39
14	t	26/28 (93%)	25 (96%)	1 (4%)	29	39
15	U	83/89 (93%)	80 (96%)	3 (4%)	31	41
15	u	84/89 (94%)	82 (98%)	2 (2%)	43	57
16	V	117/117 (100%)	116 (99%)	1 (1%)	70	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	v	117/117 (100%)	113 (97%)	4 (3%)	32	43
17	X	31/33 (94%)	31 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	20 (91%)	2 (9%)	9	9
18	y	22/23 (96%)	21 (96%)	1 (4%)	24	32
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18	22
19	z	52/52 (100%)	49 (94%)	3 (6%)	18	22
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4416/4403 (100%)	4341 (98%)	75 (2%)	53	68

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	86	ILE
2	B	223	GLN
2	B	489	GLU
2	B	505	ARG
3	C	78	GLU
3	C	142	GLU
3	C	289	PHE
3	C	315	MET
3	C	346	THR
4	D	259	ILE
5	E	54	SER
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	43	LEU
7	H	65	LEU
9	J	6	ARG
9	J	9	LEU
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
10	K	24	VAL
10	K	27	VAL
13	O	4	THR
13	O	18	LYS
13	O	24	ASP
13	O	69	LYS

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Mol	Chain	Res	Type
13	O	87	VAL
13	O	118	LEU
13	O	234	LYS
14	T	2	GLU
15	U	15	GLU
15	U	70	ARG
15	U	73	GLN
16	V	110	LYS
18	Y	25	ILE
18	Y	30	ILE
19	Z	3	ILE
19	Z	4	LEU
19	Z	20	VAL
1	a	35	VAL
2	b	63	LEU
2	b	223	GLN
2	b	245	VAL
2	b	287	ARG
2	b	298	LEU
2	b	352	GLU
2	b	485	GLU
2	b	491	VAL
3	c	24	THR
3	c	142	GLU
3	c	240	ILE
3	c	255	THR
3	c	289	PHE
3	c	315	MET
6	f	15	ILE
8	i	33	LYS
9	j	9	LEU
10	k	17	ILE
10	k	19	ASP
10	k	24	VAL
10	k	27	VAL
11	l	2	GLU
12	m	5	GLN
13	o	118	LEU
14	t	2	GLU
15	u	16	LYS
15	u	86	GLU
16	v	15	GLU

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Mol	Chain	Res	Type
16	v	81	THR
16	v	85	GLU
16	v	106	ASN
18	y	45	ASN
19	z	3	ILE
19	z	4	LEU
19	z	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	75	ASN
1	A	165	GLN
2	B	53	ASN
2	B	289	GLN
2	B	331	ASN
3	C	28	GLN
3	C	322	GLN
4	D	61	HIS
4	D	83	ASN
5	E	60	GLN
6	F	44	GLN
13	O	124	ASN
15	U	73	GLN
15	U	81	HIS
19	Z	58	ASN
1	a	165	GLN
2	b	53	ASN
2	b	223	GLN
2	b	289	GLN
3	c	44	ASN
3	c	201	ASN
4	d	83	ASN
5	e	60	GLN
5	e	75	GLN
6	f	44	GLN
13	o	124	ASN
15	u	78	ASN
15	u	81	HIS
19	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	m	1	12	8,9,10	0.60	0	8,9,11	1.22	0
12	FME	M	1	12	8,9,10	0.67	0	8,9,11	1.17	1 (12%)
14	FME	t	1	14	8,9,10	0.71	0	8,9,11	1.47	2 (25%)
8	FME	i	1	8	8,9,10	0.69	0	8,9,11	1.12	1 (12%)
8	FME	I	1	8	8,9,10	0.66	0	8,9,11	1.03	1 (12%)
14	FME	T	1	14	8,9,10	0.65	0	8,9,11	1.73	1 (12%)

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

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CB-CA-N	-3.36	104.40	110.52
14	t	1	FME	O-C-CA	-2.77	117.64	124.77
14	t	1	FME	C-CA-N	2.24	113.81	109.50
12	M	1	FME	O-C-CA	-2.13	119.30	124.77
8	I	1	FME	O-C-CA	-2.09	119.39	124.77
8	i	1	FME	O-C-CA	-2.06	119.46	124.77

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 227 ligands modelled in this entry, 18 are monoatomic and 18 are unknown - leaving 191 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
24	CLA	d	402	4	69,73,73	1.95	19 (27%)	82,113,113	2.62	33 (40%)
24	CLA	b	613	2	69,73,73	2.02	18 (26%)	82,113,113	2.64	29 (35%)
33	LMG	c	522	-	51,51,55	0.97	2 (3%)	59,59,63	1.14	6 (10%)
24	CLA	B	607	42	69,73,73	1.96	18 (26%)	82,113,113	2.75	31 (37%)
33	LMG	j	101	40	51,51,55	0.88	2 (3%)	59,59,63	1.14	5 (8%)
34	LMT	I	101	-	36,36,36	0.49	1 (2%)	47,47,47	1.09	3 (6%)
29	OEX	a	412[A]	1,42,3	0,15,15	-	-	-		
24	CLA	c	514	3	69,73,73	2.02	19 (27%)	82,113,113	2.74	34 (41%)
24	CLA	C	508	42	69,73,73	1.97	20 (28%)	82,113,113	2.59	31 (37%)
24	CLA	c	509	42	69,73,73	2.01	18 (26%)	82,113,113	2.69	30 (36%)
24	CLA	C	512	3	69,73,73	2.00	21 (30%)	82,113,113	2.60	29 (35%)
35	HTG	V	204	-	11,11,19	0.23	0	15,15,24	1.01	1 (6%)
24	CLA	c	510	3	69,73,73	2.01	20 (28%)	82,113,113	2.68	29 (35%)
27	SQD	b	620	-	52,54,54	0.97	2 (3%)	62,65,65	1.45	9 (14%)
26	BCR	c	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.76	12 (21%)
24	CLA	C	505	42	69,73,73	1.96	20 (28%)	82,113,113	2.71	35 (42%)
24	CLA	B	612	2	69,73,73	1.92	20 (28%)	82,113,113	2.72	31 (37%)
24	CLA	A	406	42	69,73,73	2.03	19 (27%)	82,113,113	2.72	34 (41%)
24	CLA	B	613	2	69,73,73	1.94	19 (27%)	82,113,113	2.71	32 (39%)
24	CLA	C	510	3	69,73,73	2.03	21 (30%)	82,113,113	2.68	31 (37%)
26	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.57	9 (16%)
27	SQD	F	101	-	41,43,54	1.10	2 (4%)	51,54,65	1.63	8 (15%)
28	GOL	c	502	-	5,5,5	0.42	0	5,5,5	0.32	0
34	LMT	B	630	-	25,25,36	0.43	0	30,30,47	0.72	1 (3%)
26	BCR	b	619	-	41,41,41	1.02	1 (2%)	56,56,56	1.66	12 (21%)
24	CLA	b	603	2	69,73,73	2.00	20 (28%)	82,113,113	2.75	32 (39%)
26	BCR	y	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.71	12 (21%)
24	CLA	c	512	3	69,73,73	2.00	20 (28%)	82,113,113	2.67	31 (37%)
27	SQD	B	620	-	52,54,54	0.96	2 (3%)	62,65,65	1.37	7 (11%)
38	LHG	a	419	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
39	HEM	e	102	5,6	50,50,50	1.53	8 (16%)	67,82,82	1.61	14 (20%)
35	HTG	D	410	-	16,16,19	0.99	2 (12%)	20,21,24	1.17	1 (5%)
33	LMG	J	101	40	51,51,55	0.89	3 (5%)	59,59,63	0.90	3 (5%)
24	CLA	c	504	3	69,73,73	1.95	20 (28%)	82,113,113	2.69	30 (36%)
33	LMG	a	417	-	51,51,55	0.92	2 (3%)	59,59,63	1.18	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMT	M	103	-	36,36,36	0.42	0	47,47,47	0.96	3 (6%)
24	CLA	c	511	3	69,73,73	2.06	20 (28%)	82,113,113	2.68	31 (37%)
34	LMT	a	359	-	36,36,36	0.51	1 (2%)	47,47,47	0.92	2 (4%)
24	CLA	c	506	42	69,73,73	2.00	21 (30%)	82,113,113	2.69	32 (39%)
38	LHG	D	406	-	48,48,48	0.90	3 (6%)	51,54,54	1.00	3 (5%)
23	BCT	a	420[B]	21	3,3,3	0.52	0	2,3,3	0.85	0
34	LMT	e	101	-	36,36,36	0.48	1 (2%)	47,47,47	0.81	1 (2%)
24	CLA	A	404	1	69,73,73	1.99	19 (27%)	82,113,113	2.76	30 (36%)
24	CLA	A	409	1	69,73,73	1.98	21 (30%)	82,113,113	2.78	33 (40%)
24	CLA	C	511	3	69,73,73	2.02	20 (28%)	82,113,113	2.74	32 (39%)
25	PHO	A	408	-	58,69,69	2.73	14 (24%)	55,99,99	3.19	18 (32%)
35	HTG	c	523	-	19,19,19	0.89	1 (5%)	23,24,24	1.21	1 (4%)
24	CLA	a	350	42	69,73,73	2.00	18 (26%)	82,113,113	2.75	30 (36%)
36	DGD	c	518	-	63,63,67	0.84	2 (3%)	77,77,81	1.10	4 (5%)
34	LMT	b	630	-	25,25,36	0.52	1 (4%)	30,30,47	0.86	0
24	CLA	a	403	1	69,73,73	1.99	19 (27%)	82,113,113	2.72	34 (41%)
34	LMT	A	359	-	36,36,36	0.56	1 (2%)	47,47,47	0.88	1 (2%)
24	CLA	b	604	2	69,73,73	1.96	17 (24%)	82,113,113	2.65	30 (36%)
24	CLA	B	611	2	69,73,73	1.94	20 (28%)	82,113,113	2.79	33 (40%)
24	CLA	b	605	2	69,73,73	1.94	19 (27%)	82,113,113	2.82	29 (35%)
36	DGD	C	519	-	63,63,67	0.82	3 (4%)	77,77,81	0.95	4 (5%)
24	CLA	b	602	2	69,73,73	2.03	20 (28%)	82,113,113	2.75	34 (41%)
34	LMT	m	102	-	36,36,36	0.42	0	47,47,47	0.88	1 (2%)
28	GOL	A	412	-	5,5,5	0.41	0	5,5,5	0.39	0
35	HTG	B	624	-	19,19,19	0.82	1 (5%)	23,24,24	1.24	1 (4%)
24	CLA	c	513	3	69,73,73	2.01	19 (27%)	82,113,113	2.70	31 (37%)
35	HTG	B	625	-	19,19,19	0.91	1 (5%)	23,24,24	1.43	3 (13%)
28	GOL	B	626	-	5,5,5	0.38	0	5,5,5	0.51	0
24	CLA	D	402	4	69,73,73	1.92	20 (28%)	82,113,113	2.77	32 (39%)
26	BCR	B	617	-	41,41,41	1.03	2 (4%)	56,56,56	1.55	10 (17%)
24	CLA	b	606	2	69,73,73	1.95	19 (27%)	82,113,113	2.74	33 (40%)
24	CLA	C	504	3	69,73,73	1.99	19 (27%)	82,113,113	2.70	28 (34%)
26	BCR	c	517	-	41,41,41	1.05	1 (2%)	56,56,56	1.66	12 (21%)
26	BCR	t	102	-	41,41,41	1.01	1 (2%)	56,56,56	1.74	14 (25%)
38	LHG	D	407	-	48,48,48	0.91	2 (4%)	51,54,54	1.00	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	HEC	v	203	16	46,50,50	1.79	10 (21%)	58,82,82	1.63	12 (20%)
31	PL9	A	416[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.89	19 (27%)
38	LHG	D	357	-	48,48,48	0.89	2 (4%)	51,54,54	1.22	5 (9%)
33	LMG	c	521	-	51,51,55	0.93	2 (3%)	59,59,63	1.08	5 (8%)
24	CLA	c	507	3	69,73,73	1.97	20 (28%)	82,113,113	2.58	28 (34%)
36	DGD	H	102	-	63,63,67	0.83	3 (4%)	77,77,81	0.94	4 (5%)
35	HTG	B	623	-	19,19,19	0.89	1 (5%)	23,24,24	1.34	4 (17%)
24	CLA	B	602	2	69,73,73	2.06	20 (28%)	82,113,113	2.71	34 (41%)
31	PL9	a	414[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.91	21 (30%)
33	LMG	C	521	-	51,51,55	1.00	3 (5%)	59,59,63	1.19	4 (6%)
24	CLA	B	605	2	69,73,73	1.99	19 (27%)	82,113,113	2.78	30 (36%)
24	CLA	b	611	2	69,73,73	1.98	19 (27%)	82,113,113	2.73	29 (35%)
34	LMT	E	102	-	36,36,36	0.48	0	47,47,47	0.83	0
24	CLA	B	606	2	69,73,73	1.92	19 (27%)	82,113,113	2.84	31 (37%)
36	DGD	h	103	-	63,63,67	0.86	3 (4%)	77,77,81	0.96	3 (3%)
25	PHO	a	405	-	58,69,69	2.72	15 (25%)	55,99,99	3.13	16 (29%)
34	LMT	M	101	-	36,36,36	0.50	0	47,47,47	1.10	3 (6%)
24	CLA	b	615	2	69,73,73	2.00	19 (27%)	82,113,113	2.69	31 (37%)
24	CLA	B	615	2	69,73,73	1.96	17 (24%)	82,113,113	2.74	32 (39%)
24	CLA	D	403	4	69,73,73	1.99	18 (26%)	82,113,113	2.73	33 (40%)
24	CLA	C	514	3	69,73,73	2.02	20 (28%)	82,113,113	2.67	30 (36%)
24	CLA	b	610	42	69,73,73	2.05	20 (28%)	82,113,113	2.73	31 (37%)
34	LMT	b	622	-	25,25,36	0.46	0	30,30,47	0.70	0
26	BCR	C	516	-	41,41,41	1.07	1 (2%)	56,56,56	1.63	12 (21%)
26	BCR	H	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.48	11 (19%)
35	HTG	h	101	-	16,16,19	1.05	2 (12%)	20,21,24	1.45	2 (10%)
24	CLA	b	601	42	69,73,73	2.06	20 (28%)	82,113,113	2.65	29 (35%)
25	PHO	A	407	-	58,69,69	2.65	14 (24%)	55,99,99	3.10	16 (29%)
35	HTG	b	628	-	19,19,19	0.83	1 (5%)	23,24,24	1.23	3 (13%)
24	CLA	B	601	42	69,73,73	2.04	19 (27%)	82,113,113	2.67	31 (37%)
26	BCR	B	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.51	14 (25%)
24	CLA	B	603	2	69,73,73	1.96	20 (28%)	82,113,113	2.83	32 (39%)
24	CLA	d	403	4	69,73,73	2.04	19 (27%)	82,113,113	2.75	34 (41%)
35	HTG	b	625	-	19,19,19	1.00	2 (10%)	23,24,24	1.57	3 (13%)
34	LMT	a	418	-	36,36,36	0.49	1 (2%)	47,47,47	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	a	407	1	69,73,73	1.99	20 (28%)	82,113,113	2.67	33 (40%)
31	PL9	D	405	-	55,55,55	0.69	2 (3%)	68,69,69	1.76	21 (30%)
33	LMG	B	621	-	51,51,55	0.90	2 (3%)	59,59,63	1.11	3 (5%)
31	PL9	a	414[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
33	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.10	4 (8%)
24	CLA	c	503	3	69,73,73	2.02	20 (28%)	82,113,113	2.66	31 (37%)
26	BCR	A	410	-	41,41,41	1.03	1 (2%)	56,56,56	1.64	11 (19%)
26	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.58	14 (25%)
35	HTG	C	522	-	19,19,19	0.92	1 (5%)	23,24,24	1.28	2 (8%)
38	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.12	5 (11%)
23	BCT	A	403[B]	21	3,3,3	0.55	0	2,3,3	0.82	0
24	CLA	b	614	2	69,73,73	1.94	20 (28%)	82,113,113	2.74	31 (37%)
38	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.09	4 (7%)
31	PL9	d	405	-	55,55,55	0.63	2 (3%)	68,69,69	1.71	17 (25%)
26	BCR	D	404	-	41,41,41	1.06	1 (2%)	56,56,56	1.87	16 (28%)
24	CLA	B	616	2	69,73,73	1.99	20 (28%)	82,113,113	2.72	31 (37%)
24	CLA	b	612	2	69,73,73	1.99	19 (27%)	82,113,113	2.59	30 (36%)
24	CLA	A	405	42	69,73,73	1.99	19 (27%)	82,113,113	2.80	32 (39%)
24	CLA	c	508	3	69,73,73	2.05	19 (27%)	82,113,113	2.58	32 (39%)
23	BCT	a	420[A]	21	3,3,3	0.53	0	2,3,3	0.95	0
30	OYE	a	413[B]	1,42,3	0,16,16	-	-	-	-	-
34	LMT	B	622	-	36,36,36	0.41	0	47,47,47	1.07	3 (6%)
24	CLA	b	608	2	69,73,73	2.01	20 (28%)	82,113,113	2.69	35 (42%)
27	SQD	f	101	-	41,43,54	1.10	2 (4%)	51,54,65	1.41	8 (15%)
39	HEM	E	103	5,6	50,50,50	1.55	8 (16%)	67,82,82	1.71	14 (20%)
36	DGD	C	517	-	63,63,67	0.81	2 (3%)	77,77,81	1.16	5 (6%)
24	CLA	b	616	2	69,73,73	1.99	19 (27%)	82,113,113	2.73	33 (40%)
28	GOL	v	202	-	5,5,5	0.38	0	5,5,5	0.31	0
24	CLA	b	609	2	69,73,73	1.99	21 (30%)	82,113,113	2.67	30 (36%)
27	SQD	A	413	-	52,54,54	0.95	2 (3%)	62,65,65	1.07	5 (8%)
24	CLA	C	506	3	69,73,73	1.98	20 (28%)	82,113,113	2.65	31 (37%)
35	HTG	b	623	-	19,19,19	0.95	1 (5%)	23,24,24	1.46	3 (13%)
28	GOL	a	410	-	5,5,5	0.37	0	5,5,5	0.37	0
38	LHG	d	407	-	48,48,48	0.89	3 (6%)	51,54,54	0.91	3 (5%)
24	CLA	B	614	2	69,73,73	1.93	20 (28%)	82,113,113	2.88	31 (37%)
35	HTG	C	523	-	19,19,19	0.97	1 (5%)	23,24,24	1.74	5 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	DGD	c	519	-	63,63,67	0.88	2 (3%)	77,77,81	0.95	4 (5%)
30	OEY	A	415[B]	1,42,3	0,16,16	-	-	-		
24	CLA	b	607	42	69,73,73	1.96	19 (27%)	82,113,113	2.72	30 (36%)
33	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.13	5 (8%)
24	CLA	B	608	2	69,73,73	1.96	19 (27%)	82,113,113	2.69	30 (36%)
26	BCR	h	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.49	10 (17%)
26	BCR	C	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.51	8 (14%)
24	CLA	C	507	3	69,73,73	2.01	21 (30%)	82,113,113	2.68	34 (41%)
24	CLA	C	513	3	69,73,73	2.02	20 (28%)	82,113,113	2.71	31 (37%)
28	GOL	a	416	-	5,5,5	0.37	0	5,5,5	0.68	0
33	LMG	A	418	-	51,51,55	0.91	2 (3%)	59,59,63	1.20	5 (8%)
38	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	1.13	5 (9%)
29	OEX	A	414[A]	1,42,3	0,15,15	-	-	-		
26	BCR	k	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.64	12 (21%)
24	CLA	C	502	3	69,73,73	1.98	21 (30%)	82,113,113	2.74	32 (39%)
35	HTG	B	628	-	19,19,19	0.88	2 (10%)	23,24,24	1.22	3 (13%)
31	PL9	A	416[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.02	24 (35%)
24	CLA	c	505	3	69,73,73	2.00	19 (27%)	82,113,113	2.63	29 (35%)
26	BCR	b	618	-	41,41,41	1.00	1 (2%)	56,56,56	1.45	15 (26%)
33	LMG	Z	101	-	37,37,55	1.00	3 (8%)	45,45,63	1.49	7 (15%)
26	BCR	d	404	-	41,41,41	1.16	2 (4%)	56,56,56	1.85	13 (23%)
24	CLA	B	604	2	69,73,73	1.95	19 (27%)	82,113,113	2.65	31 (37%)
38	LHG	d	406	-	48,48,48	0.90	3 (6%)	51,54,54	1.11	5 (9%)
26	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.77	14 (25%)
36	DGD	c	520	-	63,63,67	0.83	3 (4%)	77,77,81	1.09	4 (5%)
24	CLA	c	515	3	69,73,73	2.06	21 (30%)	82,113,113	2.71	32 (39%)
25	PHO	a	406	-	58,69,69	2.76	13 (22%)	55,99,99	3.01	17 (30%)
26	BCR	K	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.63	12 (21%)
27	SQD	a	411	-	52,54,54	0.99	3 (5%)	62,65,65	1.21	7 (11%)
36	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.02	6 (7%)
28	GOL	b	627	-	5,5,5	0.34	0	5,5,5	0.40	0
35	HTG	c	526	-	19,19,19	0.94	2 (10%)	23,24,24	1.37	3 (13%)
41	HEC	V	203	16	46,50,50	1.73	10 (21%)	58,82,82	1.73	11 (18%)
38	LHG	l	101	-	48,48,48	0.90	2 (4%)	51,54,54	1.12	4 (7%)
24	CLA	C	509	3	69,73,73	2.02	20 (28%)	82,113,113	2.63	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SQD	a	409	-	52,54,54	0.89	2 (3%)	62,65,65	1.76	12 (19%)
24	CLA	B	609	2	69,73,73	1.97	18 (26%)	82,113,113	2.71	29 (35%)
26	BCR	a	408	-	41,41,41	0.98	1 (2%)	56,56,56	1.57	12 (21%)
27	SQD	A	411	-	52,54,54	0.88	2 (3%)	62,65,65	1.78	12 (19%)
34	LMT	t	101	-	26,26,36	0.56	1 (3%)	31,31,47	1.15	2 (6%)
28	GOL	C	525	-	5,5,5	0.43	0	5,5,5	0.15	0
33	LMG	b	621	-	51,51,55	0.87	2 (3%)	59,59,63	1.28	5 (8%)
24	CLA	B	610	42	69,73,73	2.03	20 (28%)	82,113,113	2.69	32 (39%)
24	CLA	C	503	3	69,73,73	1.98	19 (27%)	82,113,113	2.65	30 (36%)
28	GOL	B	627	-	5,5,5	0.48	0	5,5,5	0.38	0
26	BCR	Y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.77	14 (25%)
35	HTG	b	624	-	19,19,19	0.93	1 (5%)	23,24,24	1.19	1 (4%)
23	BCT	A	403[A]	21	3,3,3	0.54	0	2,3,3	0.77	0
24	CLA	a	404	42	69,73,73	1.99	21 (30%)	82,113,113	2.71	31 (37%)
28	GOL	V	202	-	5,5,5	0.39	0	5,5,5	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	d	402	4	1/1/15/20	6/39/115/115	-
24	CLA	b	613	2	1/1/15/20	7/39/115/115	-
33	LMG	c	522	-	-	10/46/66/70	0/1/1/1
24	CLA	B	607	42	1/1/15/20	5/39/115/115	-
33	LMG	j	101	40	-	9/46/66/70	0/1/1/1
34	LMT	I	101	-	-	9/21/61/61	0/2/2/2
24	CLA	c	514	3	1/1/15/20	8/39/115/115	-
24	CLA	C	508	42	1/1/15/20	8/39/115/115	-
24	CLA	c	509	42	1/1/15/20	11/39/115/115	-
24	CLA	C	512	3	1/1/15/20	5/39/115/115	-
35	HTG	V	204	-	-	0/2/19/30	0/1/1/1
24	CLA	c	510	3	1/1/15/20	2/39/115/115	-
27	SQD	b	620	-	-	20/49/69/69	0/1/1/1
26	BCR	c	516	-	-	0/29/63/63	0/2/2/2
24	CLA	C	505	42	1/1/15/20	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	612	2	1/1/15/20	4/39/115/115	-
24	CLA	A	406	42	1/1/15/20	4/39/115/115	-
24	CLA	B	613	2	1/1/15/20	6/39/115/115	-
24	CLA	C	510	3	1/1/15/20	6/39/115/115	-
26	BCR	b	617	-	-	2/29/63/63	0/2/2/2
27	SQD	F	101	-	-	9/38/58/69	0/1/1/1
28	GOL	c	502	-	-	0/4/4/4	-
34	LMT	B	630	-	-	11/17/37/61	0/1/1/2
26	BCR	b	619	-	-	2/29/63/63	0/2/2/2
24	CLA	b	603	2	1/1/15/20	7/39/115/115	-
26	BCR	y	101	-	-	6/29/63/63	0/2/2/2
24	CLA	c	512	3	1/1/15/20	8/39/115/115	-
27	SQD	B	620	-	-	18/49/69/69	0/1/1/1
38	LHG	a	419	-	-	8/46/46/53	-
39	HEM	e	102	5,6	-	9/14/54/54	-
35	HTG	D	410	-	-	0/7/27/30	0/1/1/1
33	LMG	J	101	40	-	12/46/66/70	0/1/1/1
24	CLA	c	504	3	1/1/15/20	9/39/115/115	-
33	LMG	a	417	-	-	13/46/66/70	0/1/1/1
34	LMT	M	103	-	-	7/21/61/61	0/2/2/2
24	CLA	c	511	3	1/1/15/20	10/39/115/115	-
34	LMT	a	359	-	-	7/21/61/61	0/2/2/2
24	CLA	c	506	42	1/1/15/20	4/39/115/115	-
38	LHG	D	406	-	-	16/53/53/53	-
34	LMT	e	101	-	-	6/21/61/61	0/2/2/2
24	CLA	A	404	1	1/1/15/20	1/39/115/115	-
24	CLA	A	409	1	-	10/39/115/115	-
24	CLA	C	511	3	1/1/15/20	10/39/115/115	-
25	PHO	A	408	-	-	2/37/103/103	0/5/6/6
35	HTG	c	523	-	-	3/10/30/30	0/1/1/1
24	CLA	a	350	42	1/1/15/20	4/39/115/115	-
36	DGD	c	518	-	-	19/51/91/95	0/2/2/2
34	LMT	b	630	-	-	9/17/37/61	0/1/1/2
24	CLA	a	403	1	1/1/15/20	1/39/115/115	-
34	LMT	A	359	-	-	4/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	604	2	1/1/15/20	8/39/115/115	-
24	CLA	B	611	2	1/1/15/20	3/39/115/115	-
24	CLA	b	605	2	1/1/15/20	5/39/115/115	-
36	DGD	C	519	-	-	11/51/91/95	0/2/2/2
24	CLA	b	602	2	1/1/15/20	6/39/115/115	-
34	LMT	m	102	-	-	5/21/61/61	0/2/2/2
28	GOL	A	412	-	-	2/4/4/4	-
35	HTG	B	624	-	-	5/10/30/30	0/1/1/1
24	CLA	c	513	3	1/1/15/20	5/39/115/115	-
35	HTG	B	625	-	-	3/10/30/30	0/1/1/1
28	GOL	B	626	-	-	4/4/4/4	-
24	CLA	D	402	4	1/1/15/20	2/39/115/115	-
26	BCR	B	617	-	-	0/29/63/63	0/2/2/2
24	CLA	b	606	2	1/1/15/20	8/39/115/115	-
24	CLA	C	504	3	-	3/39/115/115	-
26	BCR	c	517	-	-	3/29/63/63	0/2/2/2
26	BCR	t	102	-	-	0/29/63/63	0/2/2/2
38	LHG	D	407	-	-	9/53/53/53	-
41	HEC	v	203	16	-	6/14/54/54	-
31	PL9	A	416[B]	-	-	18/53/73/73	0/1/1/1
38	LHG	D	357	-	-	14/53/53/53	-
33	LMG	c	521	-	-	8/46/66/70	0/1/1/1
24	CLA	c	507	3	1/1/15/20	4/39/115/115	-
36	DGD	H	102	-	-	15/51/91/95	0/2/2/2
35	HTG	B	623	-	-	2/10/30/30	0/1/1/1
24	CLA	B	602	2	1/1/15/20	4/39/115/115	-
31	PL9	a	414[B]	-	-	22/53/73/73	0/1/1/1
33	LMG	C	521	-	-	10/46/66/70	0/1/1/1
24	CLA	B	605	2	1/1/15/20	8/39/115/115	-
24	CLA	b	611	2	1/1/15/20	3/39/115/115	-
34	LMT	E	102	-	-	9/21/61/61	0/2/2/2
24	CLA	B	606	2	1/1/15/20	7/39/115/115	-
36	DGD	h	103	-	-	11/51/91/95	0/2/2/2
25	PHO	a	405	-	-	2/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMT	M	101	-	-	3/21/61/61	0/2/2/2
24	CLA	b	615	2	1/1/15/20	5/39/115/115	-
24	CLA	B	615	2	1/1/15/20	9/39/115/115	-
24	CLA	D	403	4	1/1/15/20	10/39/115/115	-
24	CLA	C	514	3	1/1/15/20	11/39/115/115	-
24	CLA	b	610	42	1/1/15/20	6/39/115/115	-
34	LMT	b	622	-	-	5/17/37/61	0/1/1/2
26	BCR	C	516	-	-	0/29/63/63	0/2/2/2
26	BCR	H	101	-	-	3/29/63/63	0/2/2/2
35	HTG	h	101	-	-	0/7/27/30	0/1/1/1
24	CLA	b	601	42	1/1/15/20	15/39/115/115	-
25	PHO	A	407	-	-	2/37/103/103	0/5/6/6
35	HTG	b	628	-	-	4/10/30/30	0/1/1/1
24	CLA	B	601	42	1/1/15/20	11/39/115/115	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	CLA	B	603	2	1/1/15/20	6/39/115/115	-
24	CLA	d	403	4	1/1/15/20	6/39/115/115	-
35	HTG	b	625	-	-	2/10/30/30	0/1/1/1
34	LMT	a	418	-	-	4/21/61/61	0/2/2/2
24	CLA	a	407	1	1/1/15/20	9/39/115/115	-
31	PL9	D	405	-	-	15/53/73/73	0/1/1/1
33	LMG	B	621	-	-	12/46/66/70	0/1/1/1
31	PL9	a	414[A]	-	-	16/53/73/73	0/1/1/1
33	LMG	z	101	-	-	6/34/54/70	0/1/1/1
24	CLA	c	503	3	1/1/15/20	3/39/115/115	-
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
38	LHG	E	101	-	-	15/46/46/53	-
24	CLA	b	614	2	1/1/15/20	11/39/115/115	-
38	LHG	L	101	-	-	13/53/53/53	-
31	PL9	d	405	-	-	10/53/73/73	0/1/1/1
26	BCR	D	404	-	-	5/29/63/63	0/2/2/2
24	CLA	B	616	2	1/1/15/20	7/39/115/115	-
24	CLA	b	612	2	1/1/15/20	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	405	42	1/1/15/20	3/39/115/115	-
24	CLA	c	508	3	1/1/15/20	9/39/115/115	-
34	LMT	B	622	-	-	8/21/61/61	0/2/2/2
24	CLA	b	608	2	-	2/39/115/115	-
27	SQD	f	101	-	-	14/38/58/69	0/1/1/1
39	HEM	E	103	5,6	-	6/14/54/54	-
36	DGD	C	517	-	-	16/51/91/95	0/2/2/2
24	CLA	b	616	2	1/1/15/20	12/39/115/115	-
28	GOL	v	202	-	-	2/4/4/4	-
24	CLA	b	609	2	1/1/15/20	5/39/115/115	-
27	SQD	A	413	-	-	7/49/69/69	0/1/1/1
24	CLA	C	506	3	1/1/15/20	9/39/115/115	-
35	HTG	b	623	-	-	6/10/30/30	0/1/1/1
28	GOL	a	410	-	-	4/4/4/4	-
38	LHG	d	407	-	-	15/53/53/53	-
24	CLA	B	614	2	1/1/15/20	11/39/115/115	-
35	HTG	C	523	-	-	1/10/30/30	0/1/1/1
36	DGD	c	519	-	-	11/51/91/95	0/2/2/2
33	LMG	C	520	-	-	14/46/66/70	0/1/1/1
24	CLA	b	607	42	1/1/15/20	3/39/115/115	-
24	CLA	B	608	2	-	4/39/115/115	-
26	BCR	h	102	-	-	2/29/63/63	0/2/2/2
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
24	CLA	C	507	3	1/1/15/20	10/39/115/115	-
24	CLA	C	513	3	1/1/15/20	8/39/115/115	-
28	GOL	a	416	-	-	3/4/4/4	-
33	LMG	A	418	-	-	10/46/66/70	0/1/1/1
38	LHG	d	408	-	-	11/53/53/53	-
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2
24	CLA	C	502	3	1/1/15/20	6/39/115/115	-
35	HTG	B	628	-	-	3/10/30/30	0/1/1/1
31	PL9	A	416[A]	-	-	16/53/73/73	0/1/1/1
24	CLA	c	505	3	1/1/15/20	0/39/115/115	-
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2
33	LMG	Z	101	-	-	11/31/51/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	d	404	-	-	6/29/63/63	0/2/2/2
24	CLA	B	604	2	1/1/15/20	10/39/115/115	-
38	LHG	d	406	-	-	7/53/53/53	-
26	BCR	T	101	-	-	2/29/63/63	0/2/2/2
36	DGD	c	520	-	-	11/51/91/95	0/2/2/2
24	CLA	c	515	3	1/1/15/20	7/39/115/115	-
25	PHO	a	406	-	-	2/37/103/103	0/5/6/6
26	BCR	K	102	-	-	2/29/63/63	0/2/2/2
27	SQD	a	411	-	-	15/49/69/69	0/1/1/1
36	DGD	C	518	-	-	9/51/91/95	0/2/2/2
28	GOL	b	627	-	-	2/4/4/4	-
35	HTG	c	526	-	-	1/10/30/30	0/1/1/1
41	HEC	V	203	16	-	6/14/54/54	-
38	LHG	l	101	-	-	16/53/53/53	-
24	CLA	C	509	3	1/1/15/20	2/39/115/115	-
27	SQD	a	409	-	-	12/49/69/69	0/1/1/1
24	CLA	B	609	2	1/1/15/20	4/39/115/115	-
26	BCR	a	408	-	-	0/29/63/63	0/2/2/2
27	SQD	A	411	-	-	15/49/69/69	0/1/1/1
34	LMT	t	101	-	-	5/17/38/61	0/1/1/2
28	GOL	C	525	-	-	2/4/4/4	-
33	LMG	b	621	-	-	10/46/66/70	0/1/1/1
24	CLA	B	610	42	1/1/15/20	7/39/115/115	-
24	CLA	C	503	3	1/1/15/20	10/39/115/115	-
28	GOL	B	627	-	-	2/4/4/4	-
26	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
35	HTG	b	624	-	-	3/10/30/30	0/1/1/1
24	CLA	a	404	42	-	6/39/115/115	-
28	GOL	V	202	-	-	2/4/4/4	-

All (1608) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	406	PHO	C1D-C2D	8.98	1.49	1.39
25	a	405	PHO	C1B-C2B	8.89	1.49	1.39
25	a	405	PHO	C1D-C2D	8.73	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	406	PHO	C1B-C2B	8.63	1.49	1.39
25	A	408	PHO	C1B-C2B	8.38	1.48	1.39
25	A	407	PHO	C1B-C2B	8.34	1.48	1.39
25	A	408	PHO	C1D-C2D	8.32	1.48	1.39
25	A	408	PHO	C3B-C4B	8.06	1.49	1.41
25	A	407	PHO	C1D-C2D	7.97	1.48	1.39
25	a	406	PHO	C3B-C4B	7.73	1.49	1.41
25	a	405	PHO	C3B-C4B	7.54	1.49	1.41
25	A	407	PHO	C3B-C4B	7.30	1.48	1.41
25	a	405	PHO	C4D-CHA	6.87	1.49	1.39
25	A	407	PHO	C4D-CHA	6.80	1.49	1.39
25	A	408	PHO	C3B-C2B	6.62	1.49	1.40
25	a	405	PHO	C3B-C2B	6.43	1.49	1.40
25	A	407	PHO	C3B-C2B	6.36	1.49	1.40
25	A	408	PHO	C4D-CHA	6.33	1.49	1.39
25	a	406	PHO	C4D-CHA	6.31	1.49	1.39
25	a	406	PHO	C3B-C2B	6.18	1.48	1.40
24	B	610	CLA	C3C-C2C	5.67	1.49	1.36
25	a	406	PHO	C3D-C2D	5.65	1.49	1.39
24	C	513	CLA	C3C-C2C	5.47	1.48	1.36
24	b	613	CLA	C3C-C2C	5.46	1.48	1.36
24	b	615	CLA	C3C-C2C	5.44	1.48	1.36
25	A	408	PHO	C3D-C2D	5.43	1.48	1.39
24	b	610	CLA	C3C-C2C	5.41	1.48	1.36
24	a	350	CLA	C3C-C2C	5.41	1.48	1.36
24	b	603	CLA	C3C-C2C	5.41	1.48	1.36
24	c	514	CLA	C3C-C2C	5.40	1.48	1.36
26	d	404	BCR	C23-C22	-5.39	1.34	1.46
24	C	509	CLA	C3C-C2C	5.39	1.48	1.36
24	b	602	CLA	CHC-C1C	5.38	1.49	1.38
24	c	503	CLA	C3C-C2C	5.38	1.48	1.36
24	c	510	CLA	C3C-C2C	5.37	1.48	1.36
24	B	601	CLA	C3C-C2C	5.35	1.48	1.36
24	c	510	CLA	O2D-CGD	5.35	1.46	1.33
24	b	605	CLA	C3C-C2C	5.35	1.48	1.36
25	A	407	PHO	C3D-C2D	5.33	1.48	1.39
24	b	606	CLA	C3C-C2C	5.33	1.48	1.36
24	B	602	CLA	CHC-C1C	5.32	1.49	1.38
26	K	102	BCR	C23-C22	-5.31	1.34	1.46
39	e	102	HEM	FE-NB	5.31	2.11	1.94
24	B	616	CLA	C3C-C2C	5.31	1.48	1.36
24	b	602	CLA	C3C-C2C	5.30	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	C3C-C2C	5.29	1.48	1.36
24	b	611	CLA	C3C-C2C	5.28	1.48	1.36
24	c	508	CLA	C3C-C2C	5.28	1.48	1.36
24	C	510	CLA	C3C-C2C	5.27	1.48	1.36
26	B	619	BCR	C23-C22	-5.27	1.34	1.46
24	b	612	CLA	C3C-C2C	5.26	1.48	1.36
24	A	406	CLA	C3C-C2C	5.26	1.48	1.36
24	C	508	CLA	C3C-C2C	5.26	1.48	1.36
24	B	608	CLA	C3C-C2C	5.26	1.48	1.36
24	b	601	CLA	C3C-C2C	5.25	1.48	1.36
24	C	511	CLA	C3C-C2C	5.25	1.48	1.36
24	A	409	CLA	C3C-C2C	5.25	1.48	1.36
24	b	608	CLA	C3C-C2C	5.23	1.48	1.36
24	d	403	CLA	CHC-C1C	5.21	1.48	1.38
24	c	513	CLA	C3C-C2C	5.19	1.48	1.36
24	B	602	CLA	C3C-C2C	5.19	1.48	1.36
24	c	515	CLA	C3C-C2C	5.19	1.48	1.36
24	c	511	CLA	C3C-C2C	5.18	1.47	1.36
24	b	607	CLA	C3C-C2C	5.18	1.47	1.36
24	c	509	CLA	C3C-C2C	5.17	1.47	1.36
24	B	605	CLA	CHC-C1C	5.16	1.48	1.38
26	k	101	BCR	C23-C22	-5.16	1.34	1.46
26	C	516	BCR	C23-C22	-5.15	1.34	1.46
24	B	603	CLA	C3C-C2C	5.15	1.47	1.36
24	C	514	CLA	C3C-C2C	5.15	1.47	1.36
24	c	512	CLA	C3C-C2C	5.14	1.47	1.36
24	a	404	CLA	C3C-C2C	5.14	1.47	1.36
25	A	408	PHO	OBD-CAD	5.13	1.29	1.22
25	a	405	PHO	C3D-C2D	5.13	1.48	1.39
24	B	615	CLA	C3C-C2C	5.12	1.47	1.36
24	B	605	CLA	C3C-C2C	5.12	1.47	1.36
25	a	406	PHO	O2D-CGD	5.11	1.45	1.33
24	B	611	CLA	C3C-C2C	5.11	1.47	1.36
24	b	613	CLA	O2D-CGD	5.10	1.45	1.33
24	c	505	CLA	C3C-C2C	5.10	1.47	1.36
25	a	406	PHO	OBD-CAD	5.09	1.29	1.22
24	B	616	CLA	CHC-C1C	5.09	1.48	1.38
24	B	601	CLA	O2D-CGD	5.09	1.45	1.33
24	c	507	CLA	O2D-CGD	5.09	1.45	1.33
24	c	511	CLA	O2D-CGD	5.09	1.45	1.33
24	b	616	CLA	O2D-CGD	5.09	1.45	1.33
24	b	616	CLA	C3C-C2C	5.09	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	C3C-C2C	5.09	1.47	1.36
24	C	511	CLA	CHC-C1C	5.08	1.48	1.38
24	B	609	CLA	O2D-CGD	5.07	1.45	1.33
24	D	403	CLA	C3C-C2C	5.07	1.47	1.36
24	B	604	CLA	C3C-C2C	5.06	1.47	1.36
24	a	407	CLA	C3C-C2C	5.06	1.47	1.36
39	E	103	HEM	FE-NB	5.06	2.10	1.94
26	C	515	BCR	C23-C22	-5.04	1.35	1.46
24	C	509	CLA	C1D-ND	5.04	1.44	1.37
24	D	402	CLA	C3C-C2C	5.04	1.47	1.36
24	A	405	CLA	C3C-C2C	5.03	1.47	1.36
26	c	517	BCR	C23-C22	-5.03	1.35	1.46
24	c	508	CLA	O2D-CGD	5.03	1.45	1.33
24	C	507	CLA	O2D-CGD	5.03	1.45	1.33
24	c	504	CLA	C3C-C2C	5.03	1.47	1.36
24	C	512	CLA	O2D-CGD	5.03	1.45	1.33
24	B	607	CLA	C3C-C2C	5.02	1.47	1.36
24	C	504	CLA	C3C-C2C	5.02	1.47	1.36
26	c	516	BCR	C23-C22	-5.02	1.35	1.46
24	C	505	CLA	C3C-C2C	5.01	1.47	1.36
24	b	601	CLA	O2D-CGD	5.00	1.45	1.33
24	a	403	CLA	O2D-CGD	5.00	1.45	1.33
24	d	403	CLA	C3C-C2C	4.99	1.47	1.36
24	c	506	CLA	O2D-CGD	4.99	1.45	1.33
24	b	604	CLA	C3C-C2C	4.99	1.47	1.36
24	B	613	CLA	O2D-CGD	4.98	1.45	1.33
24	b	601	CLA	C1D-ND	4.98	1.44	1.37
24	C	507	CLA	C3C-C2C	4.98	1.47	1.36
24	D	403	CLA	CHC-C1C	4.98	1.48	1.38
24	a	350	CLA	O2D-CGD	4.98	1.45	1.33
26	t	102	BCR	C23-C22	-4.97	1.35	1.46
24	B	609	CLA	C3C-C2C	4.97	1.47	1.36
24	A	404	CLA	C3C-C2C	4.97	1.47	1.36
24	b	609	CLA	O2D-CGD	4.97	1.45	1.33
26	y	101	BCR	C23-C22	-4.97	1.35	1.46
24	A	406	CLA	O2D-CGD	4.96	1.45	1.33
24	B	614	CLA	C3C-C2C	4.96	1.47	1.36
24	C	513	CLA	CHC-C1C	4.95	1.48	1.38
24	c	513	CLA	C1D-ND	4.94	1.44	1.37
24	A	409	CLA	O2D-CGD	4.94	1.45	1.33
24	B	601	CLA	CHC-C1C	4.93	1.48	1.38
24	C	511	CLA	O2D-CGD	4.93	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	C3C-C2C	4.92	1.47	1.36
26	T	101	BCR	C23-C22	-4.91	1.35	1.46
24	c	506	CLA	C3C-C2C	4.91	1.47	1.36
24	C	506	CLA	C3C-C2C	4.91	1.47	1.36
24	C	506	CLA	CHC-C1C	4.90	1.48	1.38
24	B	605	CLA	O2D-CGD	4.90	1.45	1.33
24	B	602	CLA	C1D-ND	4.90	1.44	1.37
26	b	617	BCR	C23-C22	-4.90	1.35	1.46
24	b	616	CLA	CHC-C1C	4.89	1.48	1.38
24	a	403	CLA	C3C-C2C	4.89	1.47	1.36
24	c	504	CLA	O2D-CGD	4.88	1.45	1.33
24	A	406	CLA	CHC-C1C	4.87	1.48	1.38
24	b	610	CLA	CHC-C1C	4.87	1.48	1.38
26	A	410	BCR	C23-C22	-4.86	1.35	1.46
24	c	515	CLA	C1D-ND	4.86	1.44	1.37
26	D	404	BCR	C23-C22	-4.86	1.35	1.46
24	c	505	CLA	C1D-ND	4.85	1.44	1.37
24	C	505	CLA	O2D-CGD	4.85	1.45	1.33
24	D	403	CLA	O2D-CGD	4.84	1.45	1.33
24	b	605	CLA	O2D-CGD	4.84	1.45	1.33
24	C	503	CLA	O2D-CGD	4.84	1.45	1.33
24	C	514	CLA	C1D-ND	4.84	1.44	1.37
24	c	503	CLA	C1D-ND	4.84	1.44	1.37
24	c	514	CLA	CHC-C1C	4.83	1.48	1.38
24	c	515	CLA	O2D-CGD	4.83	1.45	1.33
24	b	614	CLA	C3C-C2C	4.83	1.47	1.36
24	B	602	CLA	O2D-CGD	4.83	1.45	1.33
24	b	602	CLA	O2D-CGD	4.83	1.45	1.33
24	C	503	CLA	CHC-C1C	4.82	1.48	1.38
24	b	604	CLA	CHC-C1C	4.82	1.48	1.38
24	B	610	CLA	CHC-C1C	4.82	1.48	1.38
24	b	615	CLA	C1D-ND	4.81	1.44	1.37
24	B	606	CLA	C3C-C2C	4.81	1.47	1.36
24	b	603	CLA	O2D-CGD	4.81	1.45	1.33
24	a	404	CLA	CHC-C1C	4.81	1.48	1.38
24	B	608	CLA	O2D-CGD	4.81	1.45	1.33
24	C	514	CLA	CHC-C1C	4.81	1.48	1.38
26	b	619	BCR	C23-C22	-4.80	1.35	1.46
24	A	405	CLA	CHC-C1C	4.80	1.48	1.38
24	c	509	CLA	O2D-CGD	4.79	1.45	1.33
24	d	402	CLA	C3C-C2C	4.79	1.47	1.36
24	C	502	CLA	CHC-C1C	4.79	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	512	CLA	O2D-CGD	4.78	1.45	1.33
24	B	605	CLA	C1D-ND	4.78	1.44	1.37
26	h	102	BCR	C23-C22	-4.78	1.35	1.46
25	A	407	PHO	O2D-CGD	4.77	1.45	1.33
24	c	505	CLA	CHC-C1C	4.77	1.48	1.38
24	b	608	CLA	O2D-CGD	4.77	1.44	1.33
24	b	616	CLA	C1D-ND	4.76	1.44	1.37
24	b	609	CLA	C3C-C2C	4.76	1.47	1.36
26	b	618	BCR	C23-C22	-4.76	1.35	1.46
24	B	615	CLA	C1D-ND	4.76	1.44	1.37
24	B	612	CLA	C3C-C2C	4.76	1.47	1.36
24	d	403	CLA	C1D-ND	4.76	1.44	1.37
24	B	604	CLA	CHC-C1C	4.75	1.48	1.38
24	C	506	CLA	O2D-CGD	4.75	1.44	1.33
24	c	503	CLA	CHC-C1C	4.75	1.48	1.38
24	B	615	CLA	O2D-CGD	4.75	1.44	1.33
24	c	512	CLA	C1D-ND	4.74	1.44	1.37
24	C	511	CLA	C1D-ND	4.74	1.44	1.37
24	c	510	CLA	CHC-C1C	4.73	1.48	1.38
24	a	350	CLA	CHC-C1C	4.73	1.48	1.38
24	c	514	CLA	O2D-CGD	4.72	1.44	1.33
24	C	514	CLA	O2D-CGD	4.72	1.44	1.33
24	A	405	CLA	C1D-ND	4.72	1.44	1.37
24	B	613	CLA	C3C-C2C	4.71	1.46	1.36
24	B	606	CLA	CHC-C1C	4.71	1.47	1.38
24	A	405	CLA	O2D-CGD	4.71	1.44	1.33
24	c	513	CLA	CHC-C1C	4.71	1.47	1.38
24	B	609	CLA	CHC-C1C	4.71	1.47	1.38
25	A	408	PHO	O2D-CGD	4.70	1.44	1.33
24	b	614	CLA	O2D-CGD	4.70	1.44	1.33
26	H	101	BCR	C23-C22	-4.70	1.35	1.46
24	b	612	CLA	O2D-CGD	4.69	1.44	1.33
24	b	611	CLA	O2D-CGD	4.69	1.44	1.33
24	C	504	CLA	C1D-ND	4.69	1.44	1.37
24	C	509	CLA	O2D-CGD	4.69	1.44	1.33
24	a	404	CLA	C1D-ND	4.68	1.44	1.37
24	C	513	CLA	C1D-ND	4.68	1.44	1.37
24	c	511	CLA	C1D-ND	4.68	1.44	1.37
24	b	615	CLA	CHC-C1C	4.67	1.47	1.38
24	C	507	CLA	CHD-C1D	4.67	1.47	1.38
24	c	508	CLA	C1D-ND	4.67	1.44	1.37
24	a	404	CLA	O2D-CGD	4.66	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	CHC-C1C	4.66	1.47	1.38
26	a	408	BCR	C23-C22	-4.65	1.36	1.46
24	C	512	CLA	C3C-C2C	4.65	1.46	1.36
24	c	503	CLA	O2D-CGD	4.65	1.44	1.33
24	a	407	CLA	O2D-CGD	4.65	1.44	1.33
24	c	505	CLA	O2D-CGD	4.65	1.44	1.33
24	b	611	CLA	CHC-C1C	4.64	1.47	1.38
24	d	402	CLA	O2D-CGD	4.64	1.44	1.33
24	C	513	CLA	O2D-CGD	4.64	1.44	1.33
24	D	402	CLA	O2D-CGD	4.64	1.44	1.33
24	C	504	CLA	CHC-C1C	4.64	1.47	1.38
24	B	611	CLA	C1D-ND	4.64	1.44	1.37
24	C	503	CLA	C1D-ND	4.64	1.44	1.37
24	C	510	CLA	O2D-CGD	4.64	1.44	1.33
24	b	604	CLA	C1D-ND	4.63	1.43	1.37
24	b	601	CLA	O2A-CGA	4.63	1.46	1.33
24	c	509	CLA	C1D-ND	4.62	1.43	1.37
24	A	404	CLA	CHC-C1C	4.62	1.47	1.38
24	a	407	CLA	CHC-C1C	4.62	1.47	1.38
24	c	513	CLA	O2D-CGD	4.62	1.44	1.33
24	b	603	CLA	CHC-C1C	4.62	1.47	1.38
24	d	402	CLA	CHC-C1C	4.61	1.47	1.38
24	c	508	CLA	CHC-C1C	4.61	1.47	1.38
26	Y	101	BCR	C23-C22	-4.61	1.36	1.46
24	C	509	CLA	CHC-C1C	4.61	1.47	1.38
24	c	511	CLA	CHC-C1C	4.61	1.47	1.38
24	c	509	CLA	CHC-C1C	4.60	1.47	1.38
24	b	607	CLA	O2D-CGD	4.60	1.44	1.33
24	C	510	CLA	CHC-C1C	4.60	1.47	1.38
24	A	406	CLA	C1D-ND	4.60	1.43	1.37
27	F	101	SQD	O47-C7	4.60	1.47	1.34
24	b	609	CLA	CHC-C1C	4.59	1.47	1.38
24	B	604	CLA	O2D-CGD	4.58	1.44	1.33
26	B	617	BCR	C23-C22	-4.58	1.36	1.46
24	B	612	CLA	O2D-CGD	4.58	1.44	1.33
24	b	615	CLA	O2D-CGD	4.57	1.44	1.33
24	A	404	CLA	C1D-ND	4.57	1.43	1.37
24	c	515	CLA	CHD-C1D	4.57	1.47	1.38
24	a	350	CLA	C1D-ND	4.57	1.43	1.37
24	c	504	CLA	C1D-ND	4.56	1.43	1.37
24	B	602	CLA	CHD-C1D	4.56	1.47	1.38
24	c	515	CLA	CHC-C1C	4.56	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	C1D-ND	4.56	1.43	1.37
24	b	613	CLA	C1D-ND	4.56	1.43	1.37
24	b	614	CLA	CHC-C1C	4.56	1.47	1.38
24	B	601	CLA	O2A-CGA	4.55	1.46	1.33
24	C	504	CLA	O2D-CGD	4.55	1.44	1.33
24	b	613	CLA	CHC-C1C	4.55	1.47	1.38
24	B	615	CLA	CHC-C1C	4.55	1.47	1.38
24	b	610	CLA	CHD-C1D	4.54	1.47	1.38
24	b	602	CLA	C1D-ND	4.54	1.43	1.37
24	c	507	CLA	CHC-C1C	4.54	1.47	1.38
24	B	601	CLA	C1D-ND	4.53	1.43	1.37
24	B	616	CLA	O2D-CGD	4.53	1.44	1.33
24	D	403	CLA	C1D-ND	4.53	1.43	1.37
24	c	508	CLA	CHD-C1D	4.53	1.47	1.38
24	c	512	CLA	CHC-C1C	4.51	1.47	1.38
24	B	610	CLA	O2D-CGD	4.51	1.44	1.33
24	C	507	CLA	C1D-ND	4.51	1.43	1.37
24	b	606	CLA	CHC-C1C	4.51	1.47	1.38
24	c	504	CLA	CHC-C1C	4.50	1.47	1.38
24	c	506	CLA	C1D-ND	4.50	1.43	1.37
24	A	404	CLA	O2D-CGD	4.50	1.44	1.33
24	B	611	CLA	CHC-C1C	4.49	1.47	1.38
24	b	608	CLA	CHC-C1C	4.49	1.47	1.38
33	z	101	LMG	O8-C28	4.49	1.46	1.33
24	c	509	CLA	CHD-C1D	4.49	1.47	1.38
24	C	510	CLA	CHD-C1D	4.49	1.47	1.38
24	C	505	CLA	CHC-C1C	4.47	1.47	1.38
24	B	603	CLA	O2D-CGD	4.47	1.44	1.33
24	C	508	CLA	O2D-CGD	4.46	1.44	1.33
24	B	610	CLA	C1D-ND	4.46	1.43	1.37
33	C	521	LMG	O8-C28	4.46	1.46	1.33
24	b	615	CLA	O2A-CGA	4.46	1.46	1.33
24	C	502	CLA	C1D-ND	4.45	1.43	1.37
24	B	614	CLA	CHC-C1C	4.45	1.47	1.38
25	a	405	PHO	O2D-CGD	4.44	1.44	1.33
26	B	618	BCR	C23-C22	-4.44	1.36	1.46
24	b	608	CLA	C1D-ND	4.44	1.43	1.37
24	B	611	CLA	O2D-CGD	4.44	1.44	1.33
24	c	505	CLA	CHD-C1D	4.43	1.47	1.38
24	A	409	CLA	CHC-C1C	4.43	1.47	1.38
27	a	411	SQD	O48-C23	4.42	1.46	1.33
24	b	612	CLA	CHD-C1D	4.41	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	O2D-CGD	4.41	1.44	1.33
24	d	403	CLA	CHD-C1D	4.41	1.47	1.38
24	C	510	CLA	C1D-ND	4.41	1.43	1.37
24	c	503	CLA	CHD-C1D	4.41	1.47	1.38
27	f	101	SQD	O47-C7	4.41	1.46	1.34
24	B	604	CLA	C1D-ND	4.40	1.43	1.37
24	b	606	CLA	C1D-ND	4.40	1.43	1.37
24	a	403	CLA	CHC-C1C	4.40	1.47	1.38
33	C	521	LMG	O7-C10	4.40	1.46	1.34
24	c	514	CLA	C1D-ND	4.39	1.43	1.37
24	B	603	CLA	CHC-C1C	4.39	1.47	1.38
24	b	610	CLA	O2D-CGD	4.39	1.44	1.33
24	B	613	CLA	CHC-C1C	4.38	1.47	1.38
24	b	605	CLA	C1D-ND	4.38	1.43	1.37
24	c	511	CLA	CHD-C1D	4.37	1.47	1.38
24	C	512	CLA	C1D-ND	4.37	1.43	1.37
24	B	607	CLA	CHC-C1C	4.37	1.47	1.38
24	B	608	CLA	CHC-C1C	4.37	1.47	1.38
24	b	601	CLA	CHC-C1C	4.37	1.47	1.38
25	a	405	PHO	OBD-CAD	4.37	1.28	1.22
24	B	603	CLA	C1D-ND	4.37	1.43	1.37
24	B	606	CLA	O2D-CGD	4.36	1.43	1.33
24	C	514	CLA	CHD-C1D	4.36	1.46	1.38
24	C	508	CLA	C1D-ND	4.35	1.43	1.37
33	c	522	LMG	O7-C10	4.35	1.46	1.34
24	C	508	CLA	CHC-C1C	4.35	1.47	1.38
24	b	610	CLA	CHC-C4B	4.35	1.49	1.39
24	b	611	CLA	C1D-ND	4.34	1.43	1.37
24	b	609	CLA	CHD-C1D	4.34	1.46	1.38
24	B	612	CLA	CHC-C1C	4.34	1.47	1.38
24	c	506	CLA	CHC-C1C	4.34	1.47	1.38
24	b	604	CLA	O2D-CGD	4.33	1.43	1.33
24	b	606	CLA	O2D-CGD	4.33	1.43	1.33
24	a	403	CLA	CHD-C1D	4.32	1.46	1.38
38	E	101	LHG	O8-C23	4.32	1.45	1.33
24	b	601	CLA	CHD-C1D	4.32	1.46	1.38
38	a	419	LHG	O8-C23	4.32	1.45	1.33
24	B	609	CLA	O2A-CGA	4.32	1.45	1.33
24	B	609	CLA	C1D-ND	4.31	1.43	1.37
33	c	521	LMG	O8-C28	4.31	1.45	1.33
33	c	522	LMG	O8-C28	4.31	1.45	1.33
41	v	203	HEC	CBC-CAC	-4.30	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	V	203	HEC	CAC-C3C	4.30	1.48	1.35
27	A	413	SQD	O48-C23	4.30	1.45	1.33
33	C	520	LMG	O8-C28	4.30	1.45	1.33
24	C	502	CLA	CHD-C1D	4.29	1.46	1.38
24	c	514	CLA	CHD-C1D	4.29	1.46	1.38
33	Z	101	LMG	O7-C10	4.29	1.46	1.34
24	b	609	CLA	C1D-ND	4.28	1.43	1.37
24	C	513	CLA	O2A-CGA	4.27	1.45	1.33
24	C	514	CLA	O2A-CGA	4.27	1.45	1.33
24	B	607	CLA	O2D-CGD	4.27	1.43	1.33
24	A	409	CLA	C1D-ND	4.27	1.43	1.37
24	d	403	CLA	O2A-CGA	4.26	1.45	1.33
33	B	621	LMG	O8-C28	4.26	1.45	1.33
24	c	515	CLA	O2A-CGA	4.25	1.45	1.33
24	a	407	CLA	CHD-C1D	4.25	1.46	1.38
24	c	514	CLA	O2A-CGA	4.25	1.45	1.33
24	a	350	CLA	O2A-CGA	4.25	1.45	1.33
24	C	513	CLA	CHD-C1D	4.24	1.46	1.38
41	v	203	HEC	CAC-C3C	4.24	1.48	1.35
24	b	603	CLA	C1D-ND	4.24	1.43	1.37
24	B	607	CLA	C1D-ND	4.24	1.43	1.37
24	c	509	CLA	CHD-C4C	4.23	1.48	1.39
24	C	512	CLA	O2A-CGA	4.23	1.45	1.33
24	c	511	CLA	O2A-CGA	4.23	1.45	1.33
24	b	602	CLA	CHD-C1D	4.22	1.46	1.38
41	v	203	HEC	CBB-CAB	-4.22	1.33	1.49
24	c	513	CLA	O2A-CGA	4.22	1.45	1.33
38	a	419	LHG	O7-C7	4.20	1.46	1.34
24	d	403	CLA	O2D-CGD	4.20	1.43	1.33
24	b	614	CLA	O2A-CGA	4.20	1.45	1.33
24	b	607	CLA	CHC-C1C	4.20	1.46	1.38
24	a	407	CLA	O2A-CGA	4.20	1.45	1.33
27	B	620	SQD	O48-C23	4.20	1.45	1.33
24	C	502	CLA	O2D-CGD	4.20	1.43	1.33
27	b	620	SQD	O47-C7	4.20	1.46	1.34
24	c	509	CLA	O2A-CGA	4.19	1.45	1.33
24	B	608	CLA	C1D-ND	4.19	1.43	1.37
24	A	405	CLA	O2A-CGA	4.19	1.45	1.33
27	f	101	SQD	O48-C23	4.19	1.45	1.33
24	A	406	CLA	CHD-C4C	4.18	1.48	1.39
24	b	610	CLA	C1D-ND	4.18	1.43	1.37
24	C	502	CLA	O2A-CGA	4.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	403	CLA	C1D-ND	4.17	1.43	1.37
24	C	511	CLA	CHD-C1D	4.17	1.46	1.38
24	c	503	CLA	O2A-CGA	4.17	1.45	1.33
24	c	510	CLA	O2A-CGA	4.17	1.45	1.33
27	A	411	SQD	O48-C23	4.17	1.45	1.33
24	b	612	CLA	C1D-ND	4.16	1.43	1.37
27	B	620	SQD	O47-C7	4.16	1.46	1.34
33	a	417	LMG	O8-C28	4.16	1.45	1.33
24	B	614	CLA	C1D-ND	4.16	1.43	1.37
36	h	103	DGD	O1G-C1A	4.16	1.45	1.33
38	d	408	LHG	O7-C7	4.16	1.46	1.34
36	c	519	DGD	O1G-C1A	4.16	1.45	1.33
24	b	607	CLA	CHD-C1D	4.16	1.46	1.38
24	d	403	CLA	CHC-C4B	4.16	1.48	1.39
39	E	103	HEM	FE-NC	4.15	2.08	1.95
24	c	512	CLA	CHD-C1D	4.15	1.46	1.38
33	b	621	LMG	O8-C28	4.15	1.45	1.33
24	C	508	CLA	O2A-CGA	4.15	1.45	1.33
27	A	413	SQD	O47-C7	4.15	1.46	1.34
24	B	606	CLA	C1D-ND	4.15	1.43	1.37
24	C	512	CLA	C3D-C2D	4.15	1.50	1.39
24	b	602	CLA	O2A-CGA	4.14	1.45	1.33
41	v	203	HEC	CAB-C3B	4.14	1.48	1.35
24	b	613	CLA	C3D-C2D	4.14	1.50	1.39
27	b	620	SQD	O48-C23	4.14	1.45	1.33
24	C	509	CLA	O2A-CGA	4.13	1.45	1.33
24	C	506	CLA	CHD-C1D	4.13	1.46	1.38
24	c	508	CLA	CHD-C4C	4.13	1.48	1.39
24	D	402	CLA	CHC-C1C	4.13	1.46	1.38
24	a	404	CLA	CHD-C1D	4.13	1.46	1.38
33	A	418	LMG	O8-C28	4.13	1.45	1.33
24	c	506	CLA	CHD-C1D	4.12	1.46	1.38
24	A	405	CLA	C3D-C2D	4.12	1.50	1.39
24	B	615	CLA	O2A-CGA	4.12	1.45	1.33
41	V	203	HEC	CBC-CAC	-4.12	1.34	1.49
38	l	101	LHG	O8-C23	4.12	1.45	1.33
24	b	601	CLA	C3D-C2D	4.11	1.50	1.39
24	C	510	CLA	CHD-C4C	4.11	1.48	1.39
24	c	508	CLA	C3D-C2D	4.11	1.50	1.39
24	b	608	CLA	O2A-CGA	4.11	1.45	1.33
24	B	609	CLA	CHD-C1D	4.11	1.46	1.38
33	C	520	LMG	O7-C10	4.11	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	O2A-CGA	4.10	1.45	1.33
24	b	611	CLA	O2A-CGA	4.10	1.45	1.33
24	C	507	CLA	CHC-C1C	4.10	1.46	1.38
24	b	606	CLA	O2A-CGA	4.10	1.45	1.33
24	b	611	CLA	CHD-C1D	4.10	1.46	1.38
24	B	604	CLA	CHB-C1B	4.10	1.48	1.39
24	B	601	CLA	CHD-C1D	4.09	1.46	1.38
24	C	505	CLA	CHD-C1D	4.09	1.46	1.38
41	V	203	HEC	CBB-CAB	-4.09	1.34	1.49
24	b	607	CLA	C1D-ND	4.09	1.43	1.37
38	L	101	LHG	O8-C23	4.09	1.45	1.33
24	C	506	CLA	C1D-ND	4.09	1.43	1.37
24	C	512	CLA	CHD-C1D	4.09	1.46	1.38
24	a	403	CLA	CHD-C4C	4.08	1.48	1.39
36	c	518	DGD	O1G-C1A	4.08	1.45	1.33
24	A	406	CLA	CHD-C1D	4.08	1.46	1.38
24	C	508	CLA	CHD-C1D	4.08	1.46	1.38
24	C	509	CLA	C3D-C2D	4.08	1.50	1.39
24	B	607	CLA	O2A-CGA	4.08	1.45	1.33
24	b	616	CLA	O2A-CGA	4.07	1.45	1.33
24	d	403	CLA	CHD-C4C	4.07	1.48	1.39
24	c	515	CLA	CHD-C4C	4.07	1.48	1.39
24	a	350	CLA	C3D-C2D	4.07	1.50	1.39
24	C	503	CLA	O2A-CGA	4.07	1.45	1.33
24	b	615	CLA	CHD-C1D	4.07	1.46	1.38
24	C	503	CLA	CHD-C1D	4.06	1.46	1.38
24	B	602	CLA	CHD-C4C	4.06	1.48	1.39
24	C	509	CLA	CHD-C1D	4.06	1.46	1.38
27	a	411	SQD	O47-C7	4.06	1.45	1.34
41	V	203	HEC	CAB-C3B	4.06	1.48	1.35
24	b	602	CLA	CHD-C4C	4.06	1.48	1.39
24	A	409	CLA	O2A-CGA	4.06	1.45	1.33
24	c	506	CLA	O2A-CGA	4.05	1.45	1.33
24	B	603	CLA	CHD-C1D	4.05	1.46	1.38
24	B	612	CLA	CHD-C1D	4.05	1.46	1.38
25	a	406	PHO	O2A-CGA	4.05	1.45	1.33
24	C	505	CLA	C1D-ND	4.04	1.43	1.37
36	c	520	DGD	O1G-C1A	4.04	1.45	1.33
24	b	602	CLA	CHC-C4B	4.04	1.48	1.39
24	b	605	CLA	CHC-C1C	4.04	1.46	1.38
24	B	610	CLA	C3D-C2D	4.04	1.50	1.39
24	C	514	CLA	CHD-C4C	4.04	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	O2A-CGA	4.03	1.45	1.33
24	c	512	CLA	CHD-C4C	4.03	1.48	1.39
24	B	613	CLA	C1D-ND	4.03	1.43	1.37
33	a	417	LMG	O7-C10	4.03	1.45	1.34
24	C	507	CLA	CHD-C4C	4.03	1.48	1.39
36	C	518	DGD	O1G-C1A	4.03	1.45	1.33
24	B	606	CLA	O2A-CGA	4.03	1.45	1.33
24	A	405	CLA	CHC-C4B	4.03	1.48	1.39
24	b	609	CLA	O2A-CGA	4.03	1.45	1.33
33	A	418	LMG	O7-C10	4.03	1.45	1.34
27	F	101	SQD	O48-C23	4.02	1.45	1.33
24	B	616	CLA	CHD-C1D	4.02	1.46	1.38
33	z	101	LMG	O7-C10	4.02	1.45	1.34
24	b	604	CLA	CHD-C1D	4.02	1.46	1.38
24	A	406	CLA	C3D-C2D	4.01	1.49	1.39
24	B	610	CLA	OBD-CAD	4.01	1.29	1.22
24	C	504	CLA	CHD-C1D	4.01	1.46	1.38
27	a	409	SQD	O48-C23	4.01	1.45	1.33
24	c	513	CLA	CHB-C1B	4.01	1.48	1.39
24	c	510	CLA	C3D-C2D	4.00	1.49	1.39
24	c	507	CLA	O2A-CGA	4.00	1.45	1.33
24	B	608	CLA	CHD-C1D	4.00	1.46	1.38
24	b	608	CLA	CHD-C1D	4.00	1.46	1.38
24	c	514	CLA	C3D-C2D	4.00	1.49	1.39
36	C	519	DGD	O1G-C1A	4.00	1.45	1.33
24	c	515	CLA	C3D-C2D	4.00	1.49	1.39
24	C	504	CLA	CHD-C4C	4.00	1.48	1.39
24	D	403	CLA	CHD-C1D	4.00	1.46	1.38
24	a	404	CLA	C3D-C2D	3.99	1.49	1.39
24	C	514	CLA	C3D-C2D	3.99	1.49	1.39
33	c	521	LMG	O7-C10	3.99	1.45	1.34
24	c	510	CLA	C1D-ND	3.99	1.43	1.37
24	b	606	CLA	CHD-C1D	3.98	1.46	1.38
24	b	601	CLA	CHD-C4C	3.98	1.48	1.39
24	a	404	CLA	CHD-C4C	3.98	1.48	1.39
24	c	512	CLA	CHB-C1B	3.98	1.48	1.39
24	c	503	CLA	CHD-C4C	3.98	1.48	1.39
24	a	407	CLA	C1D-ND	3.98	1.43	1.37
24	b	612	CLA	CHC-C1C	3.98	1.46	1.38
24	c	506	CLA	OBD-CAD	3.98	1.29	1.22
24	A	404	CLA	CHD-C1D	3.98	1.46	1.38
38	E	101	LHG	O7-C7	3.98	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	O2A-CGA	3.97	1.44	1.33
24	d	402	CLA	O2A-CGA	3.97	1.44	1.33
24	B	609	CLA	C3D-C2D	3.97	1.49	1.39
24	b	603	CLA	CHD-C1D	3.97	1.46	1.38
24	b	607	CLA	O2A-CGA	3.97	1.44	1.33
24	B	602	CLA	C3D-C2D	3.97	1.49	1.39
24	b	612	CLA	CHB-C1B	3.97	1.48	1.39
24	C	502	CLA	CHC-C4B	3.97	1.48	1.39
24	B	613	CLA	O2A-CGA	3.96	1.44	1.33
24	c	508	CLA	O2A-CGA	3.96	1.44	1.33
24	B	612	CLA	CHB-C1B	3.96	1.48	1.39
39	e	102	HEM	FE-NC	3.96	2.08	1.95
33	j	101	LMG	O8-C28	3.96	1.44	1.33
24	C	508	CLA	C3D-C2D	3.96	1.49	1.39
24	B	603	CLA	O2A-CGA	3.96	1.44	1.33
24	B	607	CLA	CHD-C4C	3.96	1.48	1.39
24	B	610	CLA	CHD-C1D	3.96	1.46	1.38
24	a	407	CLA	C3D-C2D	3.95	1.49	1.39
24	B	611	CLA	CHD-C1D	3.95	1.46	1.38
24	B	613	CLA	CHD-C1D	3.95	1.46	1.38
24	c	507	CLA	CHD-C1D	3.95	1.46	1.38
24	C	511	CLA	CHD-C4C	3.95	1.48	1.39
24	D	403	CLA	CHC-C4B	3.94	1.48	1.39
24	c	505	CLA	O2A-CGA	3.94	1.44	1.33
24	c	511	CLA	C3D-C2D	3.94	1.49	1.39
33	j	101	LMG	O7-C10	3.94	1.45	1.34
24	B	602	CLA	CHC-C4B	3.94	1.48	1.39
27	a	409	SQD	O47-C7	3.94	1.45	1.34
24	a	404	CLA	O2A-CGA	3.94	1.44	1.33
24	B	607	CLA	CHD-C1D	3.94	1.46	1.38
24	b	612	CLA	O2A-CGA	3.94	1.44	1.33
24	b	616	CLA	CHD-C1D	3.94	1.46	1.38
24	b	603	CLA	OBD-CAD	3.94	1.29	1.22
24	A	409	CLA	CHD-C1D	3.94	1.46	1.38
25	A	407	PHO	OBD-CAD	3.94	1.27	1.22
24	C	511	CLA	O2A-CGA	3.93	1.44	1.33
24	c	504	CLA	O2A-CGA	3.93	1.44	1.33
38	D	407	LHG	O8-C23	3.93	1.44	1.33
24	B	610	CLA	CHC-C4B	3.93	1.48	1.39
24	b	607	CLA	C1B-NB	-3.92	1.32	1.37
24	c	505	CLA	CHD-C4C	3.92	1.48	1.39
24	b	615	CLA	CHD-C4C	3.92	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	C1B-NB	-3.92	1.32	1.37
24	B	616	CLA	C3D-C2D	3.92	1.49	1.39
36	H	102	DGD	O1G-C1A	3.92	1.44	1.33
24	B	601	CLA	C3D-C2D	3.91	1.49	1.39
36	h	103	DGD	O2G-C1B	3.91	1.45	1.34
24	B	601	CLA	CHC-C4B	3.91	1.48	1.39
24	b	609	CLA	CHB-C1B	3.91	1.48	1.39
24	C	513	CLA	C3D-C2D	3.90	1.49	1.39
24	c	503	CLA	C3D-C2D	3.90	1.49	1.39
24	b	604	CLA	O2A-CGA	3.90	1.44	1.33
24	c	504	CLA	CHD-C1D	3.90	1.46	1.38
24	B	605	CLA	C3D-C2D	3.90	1.49	1.39
24	b	608	CLA	C3D-C2D	3.90	1.49	1.39
24	d	403	CLA	C3D-C2D	3.89	1.49	1.39
24	A	404	CLA	CHC-C4B	3.89	1.48	1.39
24	B	615	CLA	C3D-C2D	3.89	1.49	1.39
24	C	512	CLA	CHD-C4C	3.89	1.48	1.39
24	C	509	CLA	CHB-C1B	3.89	1.48	1.39
24	d	402	CLA	CHC-C4B	3.89	1.48	1.39
24	c	511	CLA	CHD-C4C	3.89	1.48	1.39
24	B	610	CLA	CHB-C1B	3.89	1.48	1.39
24	b	604	CLA	CHD-C4C	3.89	1.48	1.39
24	B	608	CLA	O2A-CGA	3.89	1.44	1.33
24	b	610	CLA	CHD-C4C	3.89	1.48	1.39
24	c	507	CLA	CHC-C4B	3.88	1.48	1.39
24	d	402	CLA	CHD-C1D	3.88	1.46	1.38
24	b	614	CLA	C1D-ND	3.88	1.43	1.37
33	B	621	LMG	O7-C10	3.88	1.45	1.34
24	C	510	CLA	OBD-CAD	3.88	1.29	1.22
24	D	402	CLA	O2A-CGA	3.88	1.44	1.33
24	a	407	CLA	C1B-NB	-3.88	1.32	1.37
24	c	513	CLA	CHD-C4C	3.88	1.48	1.39
24	c	506	CLA	C3D-C2D	3.88	1.49	1.39
24	b	613	CLA	CHD-C1D	3.88	1.46	1.38
24	B	611	CLA	C3D-C2D	3.88	1.49	1.39
24	C	511	CLA	CHB-C1B	3.88	1.48	1.39
24	a	350	CLA	CHD-C1D	3.87	1.46	1.38
24	C	510	CLA	O2A-CGA	3.87	1.44	1.33
33	J	101	LMG	O8-C28	3.87	1.44	1.33
24	c	514	CLA	CHD-C4C	3.87	1.48	1.39
24	C	506	CLA	CHD-C4C	3.86	1.48	1.39
38	d	408	LHG	O8-C23	3.86	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	C3D-C2D	3.86	1.49	1.39
36	C	517	DGD	O2G-C1B	3.86	1.45	1.34
24	C	502	CLA	CHD-C4C	3.86	1.48	1.39
24	b	609	CLA	CHD-C4C	3.86	1.48	1.39
24	c	508	CLA	OBD-CAD	3.86	1.29	1.22
38	D	357	LHG	O8-C23	3.86	1.44	1.33
24	c	511	CLA	CHB-C1B	3.86	1.48	1.39
24	c	507	CLA	CHB-C1B	3.85	1.48	1.39
24	C	506	CLA	CHB-C1B	3.85	1.48	1.39
24	c	509	CLA	C3D-C2D	3.85	1.49	1.39
24	b	611	CLA	CHC-C4B	3.84	1.48	1.39
24	A	409	CLA	CHD-C4C	3.84	1.48	1.39
24	b	614	CLA	C3D-C2D	3.84	1.49	1.39
24	C	506	CLA	O2A-CGA	3.84	1.44	1.33
24	c	514	CLA	CHC-C4B	3.84	1.48	1.39
25	A	407	PHO	O2A-CGA	3.84	1.44	1.33
24	b	613	CLA	CHC-C4B	3.84	1.48	1.39
24	C	513	CLA	CHD-C4C	3.84	1.47	1.39
24	d	402	CLA	C1B-NB	-3.84	1.32	1.37
24	b	616	CLA	C3D-C2D	3.83	1.49	1.39
24	b	614	CLA	CHD-C1D	3.83	1.45	1.38
24	B	615	CLA	CHD-C1D	3.83	1.45	1.38
24	C	503	CLA	CHD-C4C	3.83	1.47	1.39
24	B	605	CLA	CHC-C4B	3.83	1.48	1.39
24	B	608	CLA	C3D-C2D	3.83	1.49	1.39
24	B	605	CLA	CHB-C1B	3.83	1.48	1.39
24	B	613	CLA	C3D-C2D	3.83	1.49	1.39
36	C	518	DGD	O2G-C1B	3.82	1.45	1.34
38	d	406	LHG	O8-C23	3.82	1.44	1.33
24	b	602	CLA	C3D-C2D	3.82	1.49	1.39
24	d	402	CLA	C3D-C2D	3.81	1.49	1.39
24	b	603	CLA	O2A-CGA	3.81	1.44	1.33
24	b	615	CLA	C3D-C2D	3.81	1.49	1.39
24	b	608	CLA	CHD-C4C	3.81	1.47	1.39
24	c	513	CLA	OBD-CAD	3.81	1.29	1.22
24	c	510	CLA	CHD-C1D	3.81	1.45	1.38
24	c	512	CLA	O2A-CGA	3.81	1.44	1.33
24	B	603	CLA	CHD-C4C	3.81	1.47	1.39
36	c	518	DGD	O2G-C1B	3.81	1.45	1.34
24	C	505	CLA	CHB-C1B	3.80	1.47	1.39
38	l	101	LHG	O7-C7	3.80	1.45	1.34
24	B	615	CLA	CHC-C4B	3.80	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	CHB-C1B	3.80	1.47	1.39
24	D	403	CLA	O2A-CGA	3.80	1.44	1.33
24	B	614	CLA	CHD-C4C	3.79	1.47	1.39
24	b	612	CLA	C3D-C2D	3.79	1.49	1.39
24	B	614	CLA	O2A-CGA	3.79	1.44	1.33
24	C	505	CLA	O2A-CGA	3.79	1.44	1.33
24	A	409	CLA	C3D-C2D	3.79	1.49	1.39
24	b	605	CLA	CHD-C1D	3.78	1.45	1.38
38	D	407	LHG	O7-C7	3.78	1.45	1.34
24	a	403	CLA	C3D-C2D	3.78	1.49	1.39
24	b	611	CLA	C3D-C2D	3.78	1.49	1.39
24	C	513	CLA	CHC-C4B	3.78	1.47	1.39
24	C	504	CLA	O2A-CGA	3.78	1.44	1.33
24	B	604	CLA	CHD-C1D	3.78	1.45	1.38
24	a	350	CLA	CHC-C4B	3.77	1.47	1.39
24	b	603	CLA	C3D-C2D	3.77	1.49	1.39
24	B	606	CLA	C3D-C2D	3.77	1.49	1.39
24	B	603	CLA	CHC-C4B	3.76	1.47	1.39
24	a	350	CLA	CHD-C4C	3.76	1.47	1.39
24	B	610	CLA	CHD-C4C	3.76	1.47	1.39
24	b	612	CLA	C1B-NB	-3.76	1.32	1.37
24	D	403	CLA	CHD-C4C	3.76	1.47	1.39
24	B	608	CLA	CHB-C1B	3.75	1.47	1.39
24	C	508	CLA	CHD-C4C	3.75	1.47	1.39
24	D	402	CLA	CHD-C4C	3.75	1.47	1.39
38	d	407	LHG	O8-C23	3.75	1.44	1.33
24	c	513	CLA	C3D-C2D	3.75	1.49	1.39
24	b	609	CLA	OBD-CAD	3.75	1.28	1.22
24	c	513	CLA	CHD-C1D	3.75	1.45	1.38
24	A	404	CLA	C3D-C2D	3.74	1.49	1.39
24	b	606	CLA	C3D-C2D	3.74	1.49	1.39
24	B	605	CLA	CHD-C1D	3.74	1.45	1.38
24	A	406	CLA	O2A-CGA	3.74	1.44	1.33
24	b	607	CLA	CHB-C1B	3.74	1.47	1.39
24	B	605	CLA	O2A-CGA	3.74	1.44	1.33
24	b	605	CLA	CHB-C1B	3.74	1.47	1.39
24	c	505	CLA	C3D-C2D	3.74	1.49	1.39
24	d	402	CLA	CHB-C1B	3.74	1.47	1.39
24	c	508	CLA	CHB-C1B	3.73	1.47	1.39
24	c	505	CLA	CHC-C4B	3.73	1.47	1.39
33	J	101	LMG	O7-C10	3.73	1.44	1.34
36	c	519	DGD	O2G-C1B	3.72	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	O2A-CGA	3.72	1.44	1.33
24	D	403	CLA	C3D-C2D	3.72	1.49	1.39
24	C	505	CLA	CHD-C4C	3.72	1.47	1.39
24	b	605	CLA	O2A-CGA	3.72	1.44	1.33
24	B	602	CLA	O2A-CGA	3.72	1.44	1.33
24	c	506	CLA	CHD-C4C	3.72	1.47	1.39
24	D	402	CLA	CHD-C1D	3.72	1.45	1.38
24	C	510	CLA	C3D-C2D	3.72	1.49	1.39
24	b	614	CLA	CHD-C4C	3.72	1.47	1.39
38	L	101	LHG	O7-C7	3.72	1.44	1.34
24	b	611	CLA	CHD-C4C	3.72	1.47	1.39
24	b	611	CLA	CHB-C1B	3.71	1.47	1.39
24	a	407	CLA	CHD-C4C	3.71	1.47	1.39
24	b	613	CLA	CHD-C4C	3.71	1.47	1.39
24	C	502	CLA	C3D-C2D	3.71	1.49	1.39
24	c	509	CLA	OBD-CAD	3.71	1.28	1.22
24	b	606	CLA	CHD-C4C	3.71	1.47	1.39
24	D	403	CLA	CHB-C1B	3.71	1.47	1.39
24	b	615	CLA	OBD-CAD	3.71	1.28	1.22
24	B	609	CLA	C1B-NB	-3.70	1.33	1.37
24	B	607	CLA	OBD-CAD	3.70	1.28	1.22
24	b	608	CLA	OBD-CAD	3.70	1.28	1.22
24	b	612	CLA	CHD-C4C	3.70	1.47	1.39
24	b	610	CLA	CHB-C1B	3.70	1.47	1.39
24	c	503	CLA	CHC-C4B	3.70	1.47	1.39
24	B	612	CLA	C3D-C2D	3.70	1.49	1.39
24	b	605	CLA	C3D-C2D	3.69	1.49	1.39
24	b	609	CLA	C3D-C2D	3.69	1.49	1.39
24	b	612	CLA	CHC-C4B	3.69	1.47	1.39
24	C	511	CLA	CHC-C4B	3.69	1.47	1.39
24	c	510	CLA	CHC-C4B	3.69	1.47	1.39
24	A	404	CLA	CHD-C4C	3.69	1.47	1.39
24	b	604	CLA	C3D-C2D	3.69	1.49	1.39
24	c	504	CLA	CHD-C4C	3.68	1.47	1.39
24	c	504	CLA	CHB-C1B	3.68	1.47	1.39
36	c	520	DGD	O2G-C1B	3.68	1.44	1.34
24	C	505	CLA	C3D-C2D	3.68	1.49	1.39
24	c	512	CLA	C3D-C2D	3.68	1.49	1.39
38	D	406	LHG	O7-C7	3.68	1.44	1.34
24	B	604	CLA	O2A-CGA	3.68	1.44	1.33
24	b	614	CLA	CHB-C1B	3.68	1.47	1.39
24	b	605	CLA	CHD-C4C	3.68	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	514	CLA	CHB-C1B	3.68	1.47	1.39
24	c	509	CLA	CHC-C4B	3.67	1.47	1.39
24	B	611	CLA	CHB-C1B	3.67	1.47	1.39
24	c	511	CLA	C1B-NB	-3.67	1.33	1.37
36	C	517	DGD	O1G-C1A	3.67	1.44	1.33
24	C	508	CLA	CHC-C4B	3.67	1.47	1.39
24	a	404	CLA	OBD-CAD	3.66	1.28	1.22
24	c	510	CLA	OBD-CAD	3.66	1.28	1.22
24	B	610	CLA	O2A-CGA	3.66	1.44	1.33
24	B	604	CLA	CHD-C4C	3.66	1.47	1.39
24	C	512	CLA	CHB-C1B	3.66	1.47	1.39
24	d	403	CLA	OBD-CAD	3.65	1.28	1.22
24	B	615	CLA	OBD-CAD	3.65	1.28	1.22
24	C	513	CLA	OBD-CAD	3.65	1.28	1.22
24	B	607	CLA	CHB-C1B	3.64	1.47	1.39
24	B	601	CLA	CHD-C4C	3.64	1.47	1.39
24	B	614	CLA	C4B-NB	-3.64	1.33	1.37
38	D	357	LHG	O7-C7	3.64	1.44	1.34
24	c	508	CLA	CHC-C4B	3.64	1.47	1.39
24	B	609	CLA	CHD-C4C	3.64	1.47	1.39
24	C	504	CLA	C3D-C2D	3.64	1.48	1.39
24	b	607	CLA	C3D-C2D	3.64	1.48	1.39
24	B	616	CLA	CHD-C4C	3.64	1.47	1.39
24	C	509	CLA	CHD-C4C	3.64	1.47	1.39
24	c	510	CLA	CHD-C4C	3.64	1.47	1.39
24	b	610	CLA	C1B-NB	-3.64	1.33	1.37
24	C	502	CLA	CHB-C1B	3.64	1.47	1.39
24	b	604	CLA	CHB-C1B	3.63	1.47	1.39
24	B	611	CLA	CHD-C4C	3.63	1.47	1.39
24	C	507	CLA	C3D-C2D	3.63	1.48	1.39
24	c	503	CLA	CHB-C1B	3.63	1.47	1.39
24	B	614	CLA	CHC-C4B	3.63	1.47	1.39
24	C	503	CLA	OBD-CAD	3.63	1.28	1.22
24	B	613	CLA	CHB-C1B	3.62	1.47	1.39
24	B	613	CLA	CHD-C4C	3.62	1.47	1.39
24	A	406	CLA	CHC-C4B	3.62	1.47	1.39
24	a	404	CLA	CHB-C1B	3.62	1.47	1.39
24	b	613	CLA	C4B-NB	-3.62	1.33	1.37
24	c	504	CLA	C3D-C2D	3.62	1.48	1.39
24	b	601	CLA	OBD-CAD	3.61	1.28	1.22
38	D	406	LHG	O8-C23	3.61	1.43	1.33
35	b	623	HTG	C1'-S1	-3.61	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	CHC-C4B	3.61	1.47	1.39
24	A	409	CLA	CHB-C1B	3.61	1.47	1.39
24	b	604	CLA	CHC-C4B	3.60	1.47	1.39
24	a	403	CLA	O2A-CGA	3.60	1.43	1.33
24	B	616	CLA	CHC-C4B	3.60	1.47	1.39
24	c	513	CLA	CHC-C4B	3.60	1.47	1.39
36	C	519	DGD	O2G-C1B	3.60	1.44	1.34
24	B	603	CLA	C3D-C2D	3.60	1.48	1.39
24	c	506	CLA	CHB-C1B	3.60	1.47	1.39
24	b	601	CLA	CHB-C1B	3.59	1.47	1.39
38	d	406	LHG	O7-C7	3.59	1.44	1.34
24	A	405	CLA	CHB-C1B	3.59	1.47	1.39
24	b	608	CLA	CHB-C1B	3.59	1.47	1.39
24	c	514	CLA	OBD-CAD	3.58	1.28	1.22
24	C	504	CLA	CHC-C4B	3.58	1.47	1.39
24	C	514	CLA	OBD-CAD	3.58	1.28	1.22
24	B	606	CLA	CHD-C1D	3.58	1.45	1.38
24	b	613	CLA	CHB-C1B	3.58	1.47	1.39
24	A	405	CLA	CHD-C1D	3.58	1.45	1.38
24	B	612	CLA	C1B-NB	-3.58	1.33	1.37
24	A	406	CLA	OBD-CAD	3.58	1.28	1.22
24	C	509	CLA	OBD-CAD	3.58	1.28	1.22
24	c	510	CLA	CHB-C1B	3.58	1.47	1.39
24	b	603	CLA	CHD-C4C	3.58	1.47	1.39
24	C	510	CLA	CHC-C4B	3.58	1.47	1.39
24	b	610	CLA	O2A-CGA	3.58	1.43	1.33
24	b	610	CLA	OBD-CAD	3.57	1.28	1.22
24	B	607	CLA	C3D-C2D	3.57	1.48	1.39
38	d	407	LHG	O7-C7	3.57	1.44	1.34
24	D	402	CLA	CHB-C1B	3.57	1.47	1.39
24	A	404	CLA	C1B-NB	-3.57	1.33	1.37
24	B	616	CLA	OBD-CAD	3.56	1.28	1.22
24	B	611	CLA	OBD-CAD	3.56	1.28	1.22
24	b	616	CLA	CHD-C4C	3.56	1.47	1.39
24	b	603	CLA	CHC-C4B	3.56	1.47	1.39
24	B	614	CLA	C3D-C2D	3.55	1.48	1.39
24	a	350	CLA	C1B-NB	-3.55	1.33	1.37
24	a	403	CLA	CHB-C1B	3.55	1.47	1.39
24	B	609	CLA	CHC-C4B	3.55	1.47	1.39
24	C	506	CLA	CHC-C4B	3.55	1.47	1.39
24	c	507	CLA	CHD-C4C	3.55	1.47	1.39
24	c	505	CLA	CHB-C1B	3.55	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	402	CLA	CHD-C4C	3.55	1.47	1.39
24	B	605	CLA	CHD-C4C	3.55	1.47	1.39
24	B	604	CLA	OBD-CAD	3.55	1.28	1.22
24	C	512	CLA	OBD-CAD	3.55	1.28	1.22
24	d	402	CLA	C1D-ND	3.54	1.42	1.37
24	b	608	CLA	CHC-C4B	3.54	1.47	1.39
24	B	606	CLA	CHC-C4B	3.54	1.47	1.39
24	C	511	CLA	C3D-C2D	3.54	1.48	1.39
35	b	625	HTG	C1'-S1	-3.54	1.76	1.81
24	B	612	CLA	C1D-ND	3.54	1.42	1.37
24	c	515	CLA	CHC-C4B	3.53	1.47	1.39
24	b	606	CLA	CHC-C4B	3.53	1.47	1.39
27	A	411	SQD	O47-C7	3.53	1.44	1.34
24	b	614	CLA	CHC-C4B	3.53	1.47	1.39
24	B	601	CLA	OBD-CAD	3.52	1.28	1.22
24	D	403	CLA	OBD-CAD	3.52	1.28	1.22
24	d	403	CLA	CHB-C1B	3.52	1.47	1.39
24	A	404	CLA	OBD-CAD	3.52	1.28	1.22
24	A	405	CLA	C1B-NB	-3.52	1.33	1.37
24	b	616	CLA	C1B-NB	-3.52	1.33	1.37
24	b	601	CLA	CHC-C4B	3.52	1.47	1.39
24	B	609	CLA	CHB-C1B	3.52	1.47	1.39
24	B	616	CLA	CHB-C1B	3.51	1.47	1.39
24	C	503	CLA	CHB-C1B	3.51	1.47	1.39
24	D	402	CLA	C1D-ND	3.51	1.42	1.37
24	C	508	CLA	CHB-C1B	3.50	1.47	1.39
24	A	406	CLA	C1B-NB	-3.50	1.33	1.37
24	c	515	CLA	CHB-C1B	3.50	1.47	1.39
24	D	402	CLA	C3D-C2D	3.50	1.48	1.39
24	b	615	CLA	CHC-C4B	3.50	1.47	1.39
33	b	621	LMG	O7-C10	3.50	1.44	1.34
24	B	604	CLA	CHC-C4B	3.50	1.47	1.39
24	B	606	CLA	C1B-NB	-3.50	1.33	1.37
24	B	611	CLA	O2A-CGA	3.50	1.43	1.33
24	c	507	CLA	C1D-ND	3.48	1.42	1.37
24	B	612	CLA	CHC-C4B	3.48	1.47	1.39
24	B	608	CLA	CHD-C4C	3.48	1.47	1.39
24	c	512	CLA	OBD-CAD	3.48	1.28	1.22
24	b	616	CLA	CHC-C4B	3.47	1.47	1.39
24	b	602	CLA	CHB-C1B	3.47	1.47	1.39
24	C	507	CLA	C1B-NB	-3.47	1.33	1.37
36	H	102	DGD	O2G-C1B	3.47	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	C1B-NB	-3.47	1.33	1.37
24	C	508	CLA	OBD-CAD	3.47	1.28	1.22
24	B	607	CLA	CHC-C4B	3.47	1.47	1.39
24	B	614	CLA	CHB-C1B	3.47	1.47	1.39
24	A	404	CLA	O2A-CGA	3.46	1.43	1.33
24	c	515	CLA	OBD-CAD	3.46	1.28	1.22
24	c	507	CLA	C3D-C2D	3.46	1.48	1.39
24	C	514	CLA	CHC-C4B	3.46	1.47	1.39
24	b	607	CLA	CHD-C4C	3.46	1.47	1.39
24	b	614	CLA	OBD-CAD	3.46	1.28	1.22
24	B	606	CLA	CHD-C4C	3.45	1.47	1.39
24	c	512	CLA	CHC-C4B	3.45	1.47	1.39
24	c	515	CLA	C4B-NB	-3.45	1.33	1.37
25	A	408	PHO	CHA-CBD	-3.44	1.47	1.51
24	C	507	CLA	CHC-C4B	3.44	1.47	1.39
24	C	504	CLA	OBD-CAD	3.44	1.28	1.22
24	D	402	CLA	C1B-NB	-3.44	1.33	1.37
24	C	512	CLA	CHC-C4B	3.44	1.47	1.39
24	B	615	CLA	CHD-C4C	3.44	1.47	1.39
24	A	405	CLA	CHD-C4C	3.44	1.47	1.39
24	c	509	CLA	CHB-C1B	3.43	1.47	1.39
35	B	623	HTG	C1'-S1	-3.43	1.76	1.81
24	C	504	CLA	CHB-C1B	3.43	1.47	1.39
24	B	602	CLA	OBD-CAD	3.43	1.28	1.22
24	b	608	CLA	C4B-NB	-3.43	1.33	1.37
24	C	507	CLA	CHB-C1B	3.43	1.47	1.39
24	c	503	CLA	OBD-CAD	3.43	1.28	1.22
24	a	407	CLA	CHC-C4B	3.43	1.47	1.39
24	c	511	CLA	CHC-C4B	3.42	1.47	1.39
24	D	402	CLA	C4B-NB	-3.42	1.33	1.37
24	B	612	CLA	CHD-C4C	3.42	1.47	1.39
25	A	408	PHO	O2A-CGA	3.42	1.43	1.33
25	a	405	PHO	O2A-CGA	3.42	1.43	1.33
24	a	407	CLA	CHB-C1B	3.42	1.47	1.39
24	a	350	CLA	OBD-CAD	3.42	1.28	1.22
24	b	602	CLA	OBD-CAD	3.42	1.28	1.22
24	B	601	CLA	CHB-C1B	3.42	1.47	1.39
24	b	605	CLA	CHC-C4B	3.42	1.47	1.39
24	B	604	CLA	C3D-C2D	3.42	1.48	1.39
24	C	509	CLA	CHC-C4B	3.42	1.47	1.39
24	B	613	CLA	CHC-C4B	3.41	1.47	1.39
24	C	502	CLA	OBD-CAD	3.41	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	511	CLA	OBD-CAD	3.41	1.28	1.22
24	C	511	CLA	OBD-CAD	3.40	1.28	1.22
24	B	615	CLA	CHB-C1B	3.40	1.47	1.39
24	C	505	CLA	CHC-C4B	3.40	1.47	1.39
24	b	610	CLA	C3D-C2D	3.39	1.48	1.39
35	h	101	HTG	C1'-S1	-3.39	1.76	1.81
24	b	604	CLA	OBD-CAD	3.38	1.28	1.22
24	c	506	CLA	CHC-C4B	3.38	1.47	1.39
24	A	406	CLA	CHB-C1B	3.37	1.47	1.39
24	a	403	CLA	C4B-NB	-3.37	1.33	1.37
24	B	606	CLA	CHB-C1B	3.37	1.47	1.39
24	B	611	CLA	C4B-NB	-3.37	1.33	1.37
25	A	407	PHO	CHA-CBD	-3.37	1.47	1.51
24	c	514	CLA	CHB-C1B	3.36	1.47	1.39
24	a	403	CLA	OBD-CAD	3.36	1.28	1.22
39	E	103	HEM	C1B-NB	-3.36	1.34	1.40
24	B	612	CLA	OBD-CAD	3.35	1.28	1.22
24	B	613	CLA	C1B-NB	-3.35	1.33	1.37
24	c	509	CLA	C1B-NB	-3.35	1.33	1.37
24	b	616	CLA	CHB-C1B	3.35	1.46	1.39
24	B	614	CLA	CHD-C1D	3.34	1.44	1.38
24	b	609	CLA	CHC-C4B	3.34	1.46	1.39
24	B	613	CLA	OBD-CAD	3.33	1.28	1.22
24	b	603	CLA	CHB-C1B	3.33	1.46	1.39
35	C	523	HTG	C1'-S1	-3.33	1.76	1.81
24	C	506	CLA	C1B-NB	-3.32	1.33	1.37
24	C	513	CLA	CHB-C1B	3.32	1.46	1.39
24	A	404	CLA	CHB-C1B	3.32	1.46	1.39
24	c	506	CLA	C1B-NB	-3.31	1.33	1.37
24	B	608	CLA	CHC-C4B	3.31	1.46	1.39
24	b	608	CLA	C1B-NB	-3.30	1.33	1.37
24	c	505	CLA	OBD-CAD	3.30	1.28	1.22
24	b	607	CLA	OBD-CAD	3.30	1.28	1.22
24	B	602	CLA	CHB-C1B	3.29	1.46	1.39
35	c	526	HTG	C1'-S1	-3.29	1.76	1.81
24	a	350	CLA	CHB-C1B	3.29	1.46	1.39
24	B	603	CLA	CHB-C1B	3.29	1.46	1.39
24	b	610	CLA	C4B-NB	-3.29	1.33	1.37
24	d	402	CLA	OBD-CAD	3.29	1.28	1.22
35	b	624	HTG	C1'-S1	-3.29	1.76	1.81
24	A	409	CLA	C4B-NB	-3.29	1.33	1.37
24	a	404	CLA	CHC-C4B	3.29	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	C4B-NB	-3.28	1.33	1.37
24	a	403	CLA	C1B-NB	-3.27	1.33	1.37
24	C	506	CLA	OBD-CAD	3.27	1.28	1.22
24	b	615	CLA	C1B-NB	-3.27	1.33	1.37
24	B	608	CLA	C4B-NB	-3.27	1.33	1.37
24	b	615	CLA	CHB-C1B	3.27	1.46	1.39
24	C	507	CLA	OBD-CAD	3.26	1.28	1.22
24	c	507	CLA	OBD-CAD	3.25	1.28	1.22
24	C	506	CLA	C3D-C2D	3.25	1.47	1.39
24	a	404	CLA	C1B-NB	-3.25	1.33	1.37
39	E	103	HEM	C4D-ND	-3.25	1.34	1.40
24	A	409	CLA	OBD-CAD	3.25	1.28	1.22
24	b	611	CLA	C1B-NB	-3.25	1.33	1.37
24	b	605	CLA	OBD-CAD	3.25	1.28	1.22
24	c	504	CLA	C1B-NB	-3.24	1.33	1.37
24	C	507	CLA	C4B-NB	-3.24	1.33	1.37
24	c	504	CLA	CHC-C4B	3.24	1.46	1.39
24	A	409	CLA	C1B-NB	-3.23	1.33	1.37
24	B	602	CLA	C1B-NB	-3.23	1.33	1.37
24	A	409	CLA	CHC-C4B	3.23	1.46	1.39
24	b	616	CLA	OBD-CAD	3.23	1.28	1.22
24	c	504	CLA	OBD-CAD	3.23	1.28	1.22
24	b	603	CLA	C1B-NB	-3.23	1.33	1.37
24	c	507	CLA	C4B-NB	-3.23	1.33	1.37
24	b	609	CLA	C1B-NB	-3.22	1.33	1.37
24	b	605	CLA	C1B-NB	-3.22	1.33	1.37
24	C	511	CLA	C1B-NB	-3.20	1.33	1.37
24	B	603	CLA	C1B-NB	-3.20	1.33	1.37
24	b	613	CLA	C1B-NB	-3.20	1.33	1.37
24	B	603	CLA	OBD-CAD	3.20	1.28	1.22
24	c	514	CLA	C1B-NB	-3.19	1.33	1.37
24	c	511	CLA	C4B-NB	-3.19	1.33	1.37
24	b	601	CLA	C4B-NB	-3.19	1.33	1.37
24	C	505	CLA	OBD-CAD	3.19	1.28	1.22
24	A	405	CLA	OBD-CAD	3.18	1.28	1.22
24	B	608	CLA	OBD-CAD	3.18	1.28	1.22
24	D	403	CLA	C1B-NB	-3.18	1.33	1.37
24	B	601	CLA	C1B-NB	-3.18	1.33	1.37
35	B	625	HTG	C1'-S1	-3.17	1.77	1.81
24	B	608	CLA	C1B-NB	-3.16	1.33	1.37
24	B	615	CLA	C1B-NB	-3.15	1.33	1.37
35	C	522	HTG	C1'-S1	-3.15	1.77	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	C1B-NB	-3.14	1.33	1.37
24	c	506	CLA	C4B-NB	-3.14	1.33	1.37
24	C	505	CLA	C4B-NB	-3.14	1.33	1.37
24	b	607	CLA	C4B-NB	-3.14	1.33	1.37
41	V	203	HEC	C4D-ND	-3.14	1.33	1.39
24	C	512	CLA	C4B-NB	-3.13	1.33	1.37
24	C	505	CLA	C1B-NB	-3.13	1.33	1.37
24	c	515	CLA	C1B-NB	-3.12	1.33	1.37
41	v	203	HEC	C1D-ND	-3.12	1.33	1.39
24	B	611	CLA	CHC-C4B	3.12	1.46	1.39
39	e	102	HEM	C1B-NB	-3.12	1.34	1.40
24	C	504	CLA	C1B-NB	-3.11	1.33	1.37
24	b	613	CLA	OBD-CAD	3.11	1.27	1.22
24	B	614	CLA	OBD-CAD	3.10	1.27	1.22
35	c	523	HTG	C1'-S1	-3.09	1.77	1.81
24	B	613	CLA	C4B-NB	-3.09	1.33	1.37
24	B	615	CLA	C4B-NB	-3.09	1.33	1.37
24	B	604	CLA	C1B-NB	-3.08	1.33	1.37
24	b	607	CLA	CHC-C4B	3.08	1.46	1.39
24	B	614	CLA	C1B-NB	-3.08	1.33	1.37
24	C	508	CLA	C1B-NB	-3.07	1.33	1.37
24	b	601	CLA	C1B-NB	-3.07	1.33	1.37
24	b	611	CLA	OBD-CAD	3.07	1.27	1.22
24	C	513	CLA	C1B-NB	-3.07	1.33	1.37
24	b	606	CLA	CHB-C1B	3.06	1.46	1.39
24	d	402	CLA	C4B-NB	-3.05	1.33	1.37
24	C	506	CLA	C1C-C2C	3.05	1.50	1.44
39	e	102	HEM	C4D-ND	-3.04	1.35	1.40
24	B	610	CLA	C1B-NB	-3.04	1.33	1.37
24	c	513	CLA	C1B-C2B	3.03	1.50	1.43
24	c	504	CLA	C4B-NB	-3.02	1.33	1.37
24	B	607	CLA	C1B-NB	-3.02	1.33	1.37
24	a	403	CLA	CHC-C4B	3.02	1.46	1.39
41	v	203	HEC	C4D-ND	-3.01	1.33	1.39
24	C	505	CLA	C1B-C2B	3.01	1.50	1.43
24	a	407	CLA	C4B-NB	-3.00	1.33	1.37
24	B	607	CLA	C4B-NB	-3.00	1.33	1.37
24	b	607	CLA	C1B-C2B	3.00	1.50	1.43
41	v	203	HEC	C1B-NB	-2.99	1.34	1.39
24	a	407	CLA	OBD-CAD	2.99	1.27	1.22
24	b	604	CLA	C1B-NB	-2.99	1.33	1.37
24	B	609	CLA	OBD-CAD	2.98	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	C4B-NB	-2.98	1.33	1.37
24	c	510	CLA	C1B-NB	-2.97	1.34	1.37
24	c	513	CLA	C1B-NB	-2.97	1.34	1.37
24	c	503	CLA	C4B-NB	-2.96	1.34	1.37
24	B	616	CLA	C1B-NB	-2.96	1.34	1.37
35	D	410	HTG	C1'-S1	-2.96	1.77	1.81
35	B	628	HTG	C1'-S1	-2.96	1.77	1.81
24	B	604	CLA	C1B-C2B	2.96	1.50	1.43
24	c	507	CLA	C1B-NB	-2.95	1.34	1.37
24	c	512	CLA	C4B-NB	-2.95	1.34	1.37
24	D	402	CLA	CHC-C4B	2.95	1.46	1.39
24	D	402	CLA	OBD-CAD	2.95	1.27	1.22
24	B	606	CLA	OBD-CAD	2.95	1.27	1.22
24	b	603	CLA	C4B-NB	-2.95	1.34	1.37
41	V	203	HEC	C1B-NB	-2.95	1.34	1.39
24	b	614	CLA	C1B-C2B	2.94	1.50	1.43
24	B	605	CLA	C1B-NB	-2.94	1.34	1.37
24	C	508	CLA	C4B-NB	-2.94	1.34	1.37
24	B	607	CLA	C4D-CHA	2.93	1.48	1.38
24	C	509	CLA	C4B-NB	-2.93	1.34	1.37
24	b	612	CLA	OBD-CAD	2.93	1.27	1.22
24	c	512	CLA	C1B-C2B	2.93	1.50	1.43
24	c	510	CLA	C4B-NB	-2.93	1.34	1.37
24	C	506	CLA	C4B-NB	-2.92	1.34	1.37
24	c	511	CLA	C1B-C2B	2.92	1.50	1.43
24	C	510	CLA	C4B-NB	-2.91	1.34	1.37
24	c	505	CLA	C1B-NB	-2.91	1.34	1.37
24	B	610	CLA	C4B-NB	-2.91	1.34	1.37
31	a	414[A]	PL9	C6-C5	2.90	1.49	1.35
24	d	403	CLA	C1B-NB	-2.90	1.34	1.37
24	A	404	CLA	C4B-NB	-2.90	1.34	1.37
24	C	504	CLA	C4B-NB	-2.89	1.34	1.37
24	B	607	CLA	C1B-C2B	2.89	1.49	1.43
24	B	605	CLA	C1B-C2B	2.89	1.49	1.43
31	A	416[A]	PL9	C6-C5	2.88	1.49	1.35
24	B	606	CLA	C4B-NB	-2.87	1.34	1.37
24	b	610	CLA	C3D-C4D	-2.87	1.37	1.44
24	c	507	CLA	C1C-C2C	2.87	1.50	1.44
24	b	606	CLA	OBD-CAD	2.85	1.27	1.22
24	b	614	CLA	C1B-NB	-2.85	1.34	1.37
24	C	512	CLA	C1B-C2B	2.85	1.49	1.43
24	C	502	CLA	C1B-NB	-2.85	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	C1B-NB	-2.85	1.34	1.37
24	b	613	CLA	C4D-CHA	2.85	1.48	1.38
24	d	403	CLA	C3B-C4B	2.84	1.51	1.42
24	c	511	CLA	C4D-CHA	2.84	1.48	1.38
24	b	605	CLA	C1B-C2B	2.84	1.49	1.43
35	B	624	HTG	C1'-S1	-2.83	1.77	1.81
24	C	503	CLA	C4B-NB	-2.83	1.34	1.37
24	D	403	CLA	C1B-C2B	2.83	1.49	1.43
31	a	414[B]	PL9	C6-C5	2.83	1.49	1.35
24	B	603	CLA	C4B-NB	-2.82	1.34	1.37
24	B	601	CLA	C4B-NB	-2.81	1.34	1.37
24	c	509	CLA	C4D-CHA	2.81	1.48	1.38
41	V	203	HEC	C1D-ND	-2.81	1.34	1.39
24	A	406	CLA	C4B-NB	-2.80	1.34	1.37
24	b	615	CLA	C1B-C2B	2.80	1.49	1.43
31	A	416[B]	PL9	C6-C5	2.80	1.49	1.35
24	b	604	CLA	C1B-C2B	2.79	1.49	1.43
24	B	602	CLA	C1C-C2C	2.79	1.50	1.44
24	B	605	CLA	OBD-CAD	2.79	1.27	1.22
24	b	605	CLA	C4B-NB	-2.78	1.34	1.37
24	b	601	CLA	C1B-C2B	2.78	1.49	1.43
24	b	602	CLA	C1C-C2C	2.78	1.50	1.44
24	B	612	CLA	C1B-C2B	2.78	1.49	1.43
24	C	514	CLA	C1B-NB	-2.77	1.34	1.37
41	V	203	HEC	C4B-NB	-2.76	1.34	1.39
24	C	506	CLA	C1B-C2B	2.76	1.49	1.43
24	c	514	CLA	C4B-NB	-2.76	1.34	1.37
24	C	503	CLA	C1B-C2B	2.75	1.49	1.43
24	b	604	CLA	C4D-CHA	2.75	1.47	1.38
24	C	507	CLA	C4D-CHA	2.75	1.47	1.38
24	C	514	CLA	C1B-C2B	2.75	1.49	1.43
24	b	606	CLA	C4B-NB	-2.75	1.34	1.37
24	C	512	CLA	C4D-CHA	2.75	1.47	1.38
24	C	508	CLA	C4D-CHA	2.75	1.47	1.38
24	A	405	CLA	C1C-C2C	2.75	1.50	1.44
24	C	508	CLA	C1B-C2B	2.75	1.49	1.43
24	b	603	CLA	C1C-C2C	2.75	1.50	1.44
24	C	507	CLA	C4C-C3C	2.75	1.49	1.45
35	b	628	HTG	C1'-S1	-2.75	1.77	1.81
24	c	509	CLA	C1B-C2B	2.74	1.49	1.43
24	A	405	CLA	C4D-CHA	2.74	1.47	1.38
24	B	613	CLA	C4C-C3C	2.74	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	405	PL9	C6-C5	2.74	1.48	1.35
24	C	511	CLA	C4B-NB	-2.74	1.34	1.37
24	C	511	CLA	C4D-CHA	2.74	1.47	1.38
24	c	504	CLA	C1B-C2B	2.73	1.49	1.43
24	B	616	CLA	C4D-CHA	2.73	1.47	1.38
24	B	611	CLA	C1B-C2B	2.73	1.49	1.43
24	b	609	CLA	C4D-CHA	2.72	1.47	1.38
24	c	508	CLA	C4B-NB	-2.72	1.34	1.37
24	d	403	CLA	C4B-NB	-2.72	1.34	1.37
24	a	404	CLA	C4B-NB	-2.72	1.34	1.37
24	C	511	CLA	C1B-C2B	2.72	1.49	1.43
24	c	505	CLA	C1B-C2B	2.72	1.49	1.43
24	C	504	CLA	C4C-C3C	2.72	1.49	1.45
24	C	514	CLA	C4B-NB	-2.71	1.34	1.37
24	c	514	CLA	C4D-CHA	2.71	1.47	1.38
24	D	402	CLA	C3D-C4D	-2.71	1.38	1.44
24	c	511	CLA	C4C-C3C	2.71	1.49	1.45
31	d	405	PL9	C6-C5	2.71	1.48	1.35
39	e	102	HEM	C1C-C2C	-2.71	1.40	1.45
24	b	612	CLA	C4D-CHA	2.70	1.47	1.38
24	B	605	CLA	C3B-C4B	2.70	1.50	1.42
24	B	604	CLA	C4D-CHA	2.70	1.47	1.38
24	b	610	CLA	C4D-CHA	2.70	1.47	1.38
24	b	601	CLA	C4D-CHA	2.69	1.47	1.38
24	B	613	CLA	C4D-CHA	2.69	1.47	1.38
24	C	513	CLA	C1C-C2C	2.69	1.50	1.44
25	a	406	PHO	C4B-NB	-2.69	1.33	1.38
24	A	404	CLA	C1C-C2C	2.69	1.50	1.44
24	c	512	CLA	C4D-CHA	2.68	1.47	1.38
24	b	611	CLA	C3B-C4B	2.68	1.50	1.42
24	a	403	CLA	C3D-C4D	-2.68	1.38	1.44
24	C	510	CLA	C4D-CHA	2.68	1.47	1.38
24	c	513	CLA	C4B-NB	-2.68	1.34	1.37
24	c	513	CLA	C4D-CHA	2.68	1.47	1.38
24	b	613	CLA	C1C-C2C	2.68	1.50	1.44
24	a	403	CLA	C4D-CHA	2.67	1.47	1.38
24	B	606	CLA	C1C-C2C	2.67	1.49	1.44
24	b	602	CLA	C1B-NB	-2.67	1.34	1.37
24	c	509	CLA	C4B-NB	-2.66	1.34	1.37
24	c	507	CLA	C1B-C2B	2.66	1.49	1.43
24	b	603	CLA	C1B-C2B	2.66	1.49	1.43
24	D	402	CLA	C1B-C2B	2.66	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	CLA	C4C-C3C	2.66	1.49	1.45
24	c	503	CLA	C1B-NB	-2.66	1.34	1.37
24	C	502	CLA	C4D-CHA	2.66	1.47	1.38
24	C	510	CLA	C1C-C2C	2.66	1.49	1.44
24	B	603	CLA	C4D-CHA	2.65	1.47	1.38
24	B	605	CLA	C1C-C2C	2.65	1.49	1.44
24	c	506	CLA	C1B-C2B	2.65	1.49	1.43
24	b	612	CLA	C1B-C2B	2.65	1.49	1.43
24	b	616	CLA	C4D-CHA	2.65	1.47	1.38
24	B	607	CLA	C1C-C2C	2.65	1.49	1.44
24	B	610	CLA	C4D-CHA	2.65	1.47	1.38
24	B	613	CLA	C1C-C2C	2.64	1.49	1.44
24	B	616	CLA	C3B-C4B	2.64	1.50	1.42
24	D	403	CLA	C3B-C4B	2.64	1.50	1.42
24	A	409	CLA	C1B-C2B	2.64	1.49	1.43
24	b	608	CLA	C4D-CHA	2.64	1.47	1.38
24	c	512	CLA	C1B-NB	-2.64	1.34	1.37
24	C	506	CLA	C3D-C4D	-2.64	1.38	1.44
24	C	513	CLA	C4D-CHA	2.64	1.47	1.38
24	B	608	CLA	C1B-C2B	2.64	1.49	1.43
33	Z	101	LMG	O8-C28	2.63	1.46	1.33
24	c	507	CLA	C4D-CHA	2.63	1.47	1.38
24	C	502	CLA	C3B-C4B	2.63	1.50	1.42
24	B	615	CLA	C1B-C2B	2.63	1.49	1.43
24	C	510	CLA	C3B-C2B	2.63	1.50	1.41
24	B	601	CLA	C1C-C2C	2.63	1.49	1.44
24	A	406	CLA	C1B-C2B	2.63	1.49	1.43
24	c	503	CLA	C4D-CHA	2.63	1.47	1.38
24	C	504	CLA	C4D-CHA	2.63	1.47	1.38
24	c	508	CLA	C4D-CHA	2.63	1.47	1.38
24	A	409	CLA	C4D-CHA	2.63	1.47	1.38
24	C	509	CLA	C1B-NB	-2.62	1.34	1.37
24	B	602	CLA	C4D-CHA	2.62	1.47	1.38
24	a	407	CLA	C4D-CHA	2.62	1.47	1.38
24	c	510	CLA	C4D-CHA	2.62	1.47	1.38
25	A	408	PHO	C3A-C2A	-2.62	1.52	1.54
24	B	606	CLA	C4D-CHA	2.62	1.47	1.38
24	C	509	CLA	C1B-C2B	2.62	1.49	1.43
24	C	504	CLA	C3B-C4B	2.62	1.50	1.42
24	a	403	CLA	C1B-C2B	2.62	1.49	1.43
24	a	407	CLA	C1B-C2B	2.62	1.49	1.43
24	C	514	CLA	C1C-C2C	2.62	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	C4D-CHA	2.61	1.47	1.38
24	b	606	CLA	C4D-CHA	2.61	1.47	1.38
25	A	407	PHO	C4B-NB	-2.61	1.33	1.38
24	B	608	CLA	C4D-CHA	2.61	1.47	1.38
24	A	404	CLA	C4D-CHA	2.61	1.47	1.38
24	c	507	CLA	C3D-C4D	-2.61	1.38	1.44
24	B	609	CLA	C1B-C2B	2.61	1.49	1.43
24	a	350	CLA	C4D-CHA	2.61	1.47	1.38
24	B	601	CLA	C4D-CHA	2.61	1.47	1.38
24	b	611	CLA	C4D-CHA	2.61	1.47	1.38
24	b	615	CLA	C4D-CHA	2.61	1.47	1.38
24	C	510	CLA	C1B-C2B	2.60	1.49	1.43
24	B	614	CLA	C4D-CHA	2.60	1.47	1.38
24	b	606	CLA	C3B-C4B	2.60	1.50	1.42
24	C	505	CLA	C4D-CHA	2.60	1.47	1.38
24	A	404	CLA	C4C-C3C	2.60	1.49	1.45
24	D	402	CLA	C4D-CHA	2.60	1.47	1.38
24	A	406	CLA	C3B-C4B	2.59	1.50	1.42
24	B	615	CLA	C4D-CHA	2.59	1.47	1.38
24	b	616	CLA	C3B-C4B	2.59	1.50	1.42
24	c	514	CLA	C3B-C4B	2.58	1.50	1.42
24	C	512	CLA	C1B-NB	-2.58	1.34	1.37
24	B	607	CLA	C4C-C3C	2.58	1.49	1.45
24	B	614	CLA	C4C-C3C	2.58	1.49	1.45
24	c	515	CLA	C4C-C3C	2.58	1.49	1.45
24	c	505	CLA	C4B-NB	-2.58	1.34	1.37
24	C	510	CLA	C4C-C3C	2.58	1.49	1.45
24	b	604	CLA	C1C-C2C	2.58	1.49	1.44
24	C	514	CLA	C4D-CHA	2.58	1.47	1.38
24	B	602	CLA	C4C-C3C	2.58	1.49	1.45
24	B	603	CLA	C3D-C4D	-2.58	1.38	1.44
24	B	603	CLA	C1C-C2C	2.58	1.49	1.44
24	b	610	CLA	C4C-C3C	2.58	1.49	1.45
24	B	611	CLA	C4D-CHA	2.58	1.47	1.38
24	c	510	CLA	C1B-C2B	2.58	1.49	1.43
24	C	513	CLA	C4B-NB	-2.57	1.34	1.37
24	d	402	CLA	C3D-C4D	-2.57	1.38	1.44
24	C	504	CLA	C1B-C2B	2.57	1.49	1.43
24	a	404	CLA	C1B-C2B	2.56	1.49	1.43
25	a	405	PHO	CHA-CBD	-2.56	1.48	1.51
24	B	605	CLA	C4D-CHA	2.56	1.47	1.38
24	b	602	CLA	C3B-C4B	2.56	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	601	CLA	C3B-C4B	2.56	1.50	1.42
24	c	505	CLA	C4D-CHA	2.55	1.47	1.38
24	C	511	CLA	C3D-C4D	-2.55	1.38	1.44
24	C	507	CLA	C3D-C4D	-2.55	1.38	1.44
24	c	504	CLA	C4D-CHA	2.55	1.47	1.38
24	B	609	CLA	C4D-CHA	2.55	1.47	1.38
41	v	203	HEC	C4B-NB	-2.54	1.34	1.39
24	D	403	CLA	C1C-C2C	2.54	1.49	1.44
24	b	616	CLA	C1B-C2B	2.54	1.49	1.43
24	B	606	CLA	C3B-C4B	2.54	1.50	1.42
24	A	404	CLA	C1B-C2B	2.53	1.49	1.43
24	C	511	CLA	C1C-C2C	2.53	1.49	1.44
34	A	359	LMT	O1'-C1'	2.53	1.44	1.40
24	d	402	CLA	C1B-C2B	2.53	1.49	1.43
24	c	515	CLA	C1C-C2C	2.53	1.49	1.44
24	B	615	CLA	C1C-C2C	2.52	1.49	1.44
25	a	405	PHO	C1D-ND	-2.52	1.34	1.38
24	b	605	CLA	C4D-CHA	2.52	1.47	1.38
24	B	609	CLA	C1C-C2C	2.51	1.49	1.44
24	C	506	CLA	C4D-CHA	2.51	1.47	1.38
24	c	514	CLA	C1B-C2B	2.51	1.49	1.43
24	C	512	CLA	C1C-C2C	2.51	1.49	1.44
24	b	614	CLA	C4D-CHA	2.51	1.47	1.38
24	B	604	CLA	C1C-C2C	2.51	1.49	1.44
24	C	509	CLA	C4D-CHA	2.50	1.47	1.38
25	a	405	PHO	CBD-CGD	-2.50	1.49	1.52
24	b	612	CLA	C4C-C3C	2.50	1.49	1.45
24	c	505	CLA	C4C-C3C	2.50	1.49	1.45
24	C	503	CLA	C3B-C4B	2.50	1.50	1.42
24	C	502	CLA	C1B-C2B	2.50	1.49	1.43
24	A	405	CLA	C3B-C4B	2.50	1.50	1.42
24	b	602	CLA	C4D-CHA	2.50	1.47	1.38
24	B	610	CLA	C1B-C2B	2.50	1.49	1.43
24	a	407	CLA	C1C-C2C	2.49	1.49	1.44
24	b	613	CLA	C1B-C2B	2.49	1.49	1.43
24	C	503	CLA	C4D-CHA	2.49	1.46	1.38
25	a	405	PHO	C4B-NB	-2.49	1.34	1.38
24	C	508	CLA	C1C-C2C	2.49	1.49	1.44
24	B	602	CLA	C3B-C4B	2.49	1.50	1.42
39	E	103	HEM	C1C-C2C	-2.49	1.40	1.45
24	a	404	CLA	C4D-CHA	2.49	1.46	1.38
24	B	613	CLA	C3B-C2B	2.48	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	402	CLA	C4D-CHA	2.48	1.46	1.38
24	d	403	CLA	C1B-C2B	2.48	1.49	1.43
24	B	604	CLA	C4B-NB	-2.48	1.34	1.37
24	c	515	CLA	C4D-CHA	2.48	1.46	1.38
24	B	616	CLA	C1B-C2B	2.48	1.49	1.43
24	C	513	CLA	C1B-C2B	2.48	1.49	1.43
24	c	506	CLA	C4D-CHA	2.48	1.46	1.38
24	d	403	CLA	C1C-C2C	2.48	1.49	1.44
24	b	610	CLA	C1C-C2C	2.48	1.49	1.44
24	c	515	CLA	C1B-C2B	2.48	1.48	1.43
24	b	608	CLA	C1B-C2B	2.48	1.48	1.43
24	c	510	CLA	C1C-C2C	2.48	1.49	1.44
24	b	609	CLA	C4C-C3C	2.47	1.49	1.45
24	b	614	CLA	C4B-NB	-2.47	1.34	1.37
24	B	602	CLA	C3D-C4D	-2.47	1.38	1.44
24	C	503	CLA	C3D-C4D	-2.47	1.38	1.44
24	A	405	CLA	C1B-C2B	2.47	1.48	1.43
24	B	614	CLA	C1C-C2C	2.47	1.49	1.44
24	B	610	CLA	C3D-C4D	-2.47	1.38	1.44
24	C	505	CLA	C1C-C2C	2.47	1.49	1.44
24	c	508	CLA	C1B-C2B	2.47	1.48	1.43
24	b	614	CLA	C1C-C2C	2.47	1.49	1.44
24	A	406	CLA	C3D-C4D	-2.47	1.38	1.44
24	c	506	CLA	C1C-C2C	2.47	1.49	1.44
24	b	609	CLA	C1B-C2B	2.46	1.48	1.43
24	b	603	CLA	C4C-C3C	2.46	1.49	1.45
24	B	612	CLA	C4D-CHA	2.46	1.46	1.38
24	B	605	CLA	C4B-NB	-2.46	1.34	1.37
24	A	406	CLA	C4D-CHA	2.46	1.46	1.38
24	B	614	CLA	C3D-C4D	-2.46	1.38	1.44
24	c	503	CLA	C3B-C4B	2.46	1.49	1.42
24	b	603	CLA	C3B-C4B	2.45	1.49	1.42
24	C	503	CLA	C1B-NB	-2.45	1.34	1.37
24	c	512	CLA	C3D-C4D	-2.45	1.38	1.44
24	C	502	CLA	C1C-C2C	2.45	1.49	1.44
25	a	406	PHO	C1B-NB	-2.45	1.34	1.38
24	B	610	CLA	C3B-C4B	2.45	1.49	1.42
39	e	102	HEM	C1D-ND	-2.45	1.34	1.38
24	A	404	CLA	C3D-C4D	-2.45	1.38	1.44
25	a	406	PHO	CHA-CBD	-2.45	1.48	1.51
24	B	612	CLA	C3B-C2B	2.45	1.49	1.41
24	b	616	CLA	C3D-C4D	-2.45	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	CLA	C3D-C4D	-2.44	1.38	1.44
24	A	406	CLA	C1C-C2C	2.44	1.49	1.44
24	c	505	CLA	C3B-C4B	2.43	1.49	1.42
24	c	513	CLA	C1C-C2C	2.43	1.49	1.44
24	b	612	CLA	C3D-C4D	-2.42	1.38	1.44
24	b	615	CLA	C4B-NB	-2.42	1.34	1.37
24	d	403	CLA	C4D-CHA	2.42	1.46	1.38
24	B	601	CLA	C1B-C2B	2.42	1.48	1.43
24	A	404	CLA	C3B-C2B	2.42	1.49	1.41
24	A	405	CLA	C4B-NB	-2.42	1.34	1.37
24	C	513	CLA	C3B-C4B	2.42	1.49	1.42
24	b	615	CLA	C4C-C3C	2.42	1.49	1.45
25	a	406	PHO	C3A-C2A	-2.42	1.52	1.54
24	C	509	CLA	C3B-C2B	2.42	1.49	1.41
24	c	503	CLA	C1B-C2B	2.42	1.48	1.43
24	c	515	CLA	C3B-C4B	2.42	1.49	1.42
24	C	509	CLA	C1C-C2C	2.41	1.49	1.44
24	a	350	CLA	C1B-C2B	2.41	1.48	1.43
24	b	607	CLA	C4C-C3C	2.41	1.49	1.45
24	B	606	CLA	C3D-C4D	-2.41	1.38	1.44
24	C	505	CLA	C3D-C4D	-2.41	1.38	1.44
24	c	506	CLA	C4C-C3C	2.41	1.49	1.45
24	B	614	CLA	C1B-C2B	2.41	1.48	1.43
24	C	502	CLA	C3D-C4D	-2.40	1.38	1.44
25	a	405	PHO	C3A-C2A	-2.40	1.52	1.54
24	c	510	CLA	C4C-C3C	2.40	1.49	1.45
24	C	512	CLA	C3B-C2B	2.40	1.49	1.41
24	B	611	CLA	C3D-C4D	-2.40	1.38	1.44
24	a	407	CLA	C3D-C4D	-2.40	1.38	1.44
24	C	509	CLA	C4C-C3C	2.39	1.49	1.45
24	b	610	CLA	C3B-C2B	2.39	1.49	1.41
24	b	608	CLA	C1C-C2C	2.39	1.49	1.44
24	b	607	CLA	C1C-C2C	2.39	1.49	1.44
24	B	609	CLA	C3B-C4B	2.39	1.49	1.42
24	b	616	CLA	C4B-NB	-2.38	1.34	1.37
24	c	510	CLA	C3B-C4B	2.38	1.49	1.42
24	B	606	CLA	C1B-C2B	2.38	1.48	1.43
24	C	505	CLA	C4C-C3C	2.38	1.49	1.45
24	C	508	CLA	C3D-C4D	-2.38	1.38	1.44
24	C	512	CLA	C4C-C3C	2.37	1.49	1.45
24	a	350	CLA	C3B-C4B	2.37	1.49	1.42
24	a	407	CLA	C3B-C4B	2.37	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	CLA	C1C-C2C	2.37	1.49	1.44
24	b	603	CLA	C4D-CHA	2.37	1.46	1.38
24	C	506	CLA	C4C-C3C	2.37	1.49	1.45
24	c	508	CLA	C4C-C3C	2.37	1.49	1.45
24	b	608	CLA	C3D-C4D	-2.37	1.38	1.44
24	D	403	CLA	C4D-CHA	2.37	1.46	1.38
24	B	601	CLA	C3D-C4D	-2.37	1.38	1.44
24	B	603	CLA	C1B-C2B	2.37	1.48	1.43
24	b	611	CLA	C1C-C2C	2.37	1.49	1.44
24	b	609	CLA	C4B-NB	-2.36	1.34	1.37
24	b	612	CLA	C1C-C2C	2.36	1.49	1.44
31	D	405	PL9	C2-C3	2.36	1.40	1.34
24	b	614	CLA	C3D-C4D	-2.36	1.38	1.44
24	c	503	CLA	C4C-C3C	2.36	1.49	1.45
24	B	603	CLA	C3B-C4B	2.36	1.49	1.42
24	A	409	CLA	C1C-NC	-2.36	1.34	1.37
24	B	616	CLA	C3D-C4D	-2.36	1.38	1.44
26	B	619	BCR	C30-C25	-2.36	1.50	1.53
24	b	611	CLA	C1B-C2B	2.36	1.48	1.43
24	b	606	CLA	C3D-C4D	-2.36	1.38	1.44
24	c	511	CLA	C3D-C4D	-2.35	1.38	1.44
24	a	350	CLA	C4B-NB	-2.35	1.34	1.37
24	b	606	CLA	C1C-C2C	2.34	1.49	1.44
24	b	606	CLA	C1B-C2B	2.34	1.48	1.43
26	B	617	BCR	C1-C6	-2.34	1.50	1.53
24	b	601	CLA	C3B-C4B	2.34	1.49	1.42
24	a	403	CLA	C3B-C2B	2.34	1.49	1.41
24	b	612	CLA	C3B-C2B	2.33	1.49	1.41
25	A	408	PHO	C3D-C4D	-2.33	1.38	1.41
24	B	603	CLA	C3B-C2B	2.33	1.49	1.41
24	B	610	CLA	C1C-C2C	2.33	1.49	1.44
24	c	505	CLA	C1C-C2C	2.33	1.49	1.44
24	C	505	CLA	C3B-C4B	2.33	1.49	1.42
24	c	506	CLA	C3B-C2B	2.33	1.49	1.41
24	C	507	CLA	C1B-C2B	2.33	1.48	1.43
24	c	512	CLA	C4C-C3C	2.32	1.49	1.45
24	a	404	CLA	C3B-C4B	2.32	1.49	1.42
24	c	510	CLA	C3D-C4D	-2.32	1.39	1.44
24	C	512	CLA	C3B-C4B	2.32	1.49	1.42
24	D	403	CLA	C3D-C4D	-2.32	1.39	1.44
38	d	406	LHG	O7-C5	-2.32	1.41	1.46
39	E	103	HEM	C1D-ND	-2.31	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	403	CLA	C4C-C3C	2.31	1.49	1.45
36	C	519	DGD	O2G-C2G	-2.31	1.41	1.46
24	b	609	CLA	C1C-C2C	2.31	1.49	1.44
24	b	605	CLA	C4C-C3C	2.31	1.49	1.45
24	B	605	CLA	C3D-C4D	-2.31	1.39	1.44
24	b	613	CLA	C3B-C2B	2.30	1.48	1.41
24	B	616	CLA	C1C-C2C	2.30	1.49	1.44
24	B	613	CLA	C1B-C2B	2.30	1.48	1.43
24	C	502	CLA	C4B-NB	-2.30	1.34	1.37
24	b	602	CLA	C1B-C2B	2.30	1.48	1.43
24	B	608	CLA	C3D-C4D	-2.30	1.39	1.44
24	b	602	CLA	C3D-C4D	-2.30	1.39	1.44
24	B	615	CLA	C3B-C4B	2.30	1.49	1.42
24	c	503	CLA	C1C-C2C	2.30	1.49	1.44
24	C	514	CLA	C3B-C4B	2.30	1.49	1.42
24	B	602	CLA	C4B-NB	-2.29	1.34	1.37
25	A	408	PHO	C4B-NB	-2.29	1.34	1.38
24	c	515	CLA	C3D-C4D	-2.29	1.39	1.44
24	c	512	CLA	C1C-C2C	2.29	1.49	1.44
38	D	406	LHG	O7-C5	-2.29	1.41	1.46
24	a	407	CLA	C4C-C3C	2.29	1.48	1.45
24	c	509	CLA	C1C-C2C	2.28	1.49	1.44
24	b	615	CLA	C3B-C4B	2.28	1.49	1.42
24	c	504	CLA	C1C-C2C	2.28	1.49	1.44
24	b	608	CLA	C3B-C4B	2.27	1.49	1.42
24	b	609	CLA	C3D-C4D	-2.27	1.39	1.44
24	B	609	CLA	C3D-C4D	-2.27	1.39	1.44
24	D	402	CLA	C3B-C2B	2.27	1.48	1.41
24	B	612	CLA	C1C-NC	-2.27	1.34	1.37
24	B	608	CLA	C3B-C2B	2.27	1.48	1.41
35	D	410	HTG	C1-S1	-2.27	1.76	1.80
24	c	510	CLA	C3B-C2B	2.27	1.48	1.41
24	b	610	CLA	C3B-C4B	2.27	1.49	1.42
24	B	612	CLA	C1C-C2C	2.26	1.49	1.44
24	C	510	CLA	C3D-C4D	-2.26	1.39	1.44
24	C	502	CLA	C4C-C3C	2.26	1.48	1.45
24	c	504	CLA	C3D-C4D	-2.26	1.39	1.44
24	c	511	CLA	C3B-C4B	2.26	1.49	1.42
24	c	508	CLA	C3D-C4D	-2.26	1.39	1.44
24	b	614	CLA	C3B-C4B	2.25	1.49	1.42
24	C	505	CLA	C3B-C2B	2.25	1.48	1.41
24	d	402	CLA	C1C-C2C	2.25	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	C1C-C2C	2.24	1.49	1.44
24	d	403	CLA	C3D-C4D	-2.24	1.39	1.44
24	B	603	CLA	C4C-C3C	2.24	1.48	1.45
24	B	614	CLA	C3B-C2B	2.24	1.48	1.41
24	c	514	CLA	C1C-C2C	2.24	1.49	1.44
24	d	402	CLA	C4C-C3C	2.24	1.48	1.45
24	c	503	CLA	C3D-C4D	-2.24	1.39	1.44
24	b	611	CLA	C3D-C4D	-2.23	1.39	1.44
24	c	507	CLA	C4C-C3C	2.23	1.48	1.45
24	c	509	CLA	C3D-C4D	-2.23	1.39	1.44
24	C	506	CLA	C3B-C4B	2.23	1.49	1.42
24	B	612	CLA	C4C-C3C	2.23	1.48	1.45
24	b	605	CLA	C3D-C4D	-2.23	1.39	1.44
24	C	503	CLA	C3B-C2B	2.23	1.48	1.41
24	a	404	CLA	C1C-C2C	2.23	1.49	1.44
24	A	409	CLA	C1C-C2C	2.23	1.49	1.44
39	e	102	HEM	C3B-C4B	2.23	1.49	1.44
24	b	601	CLA	C3D-C4D	-2.22	1.39	1.44
24	B	608	CLA	C1C-C2C	2.22	1.49	1.44
24	b	608	CLA	C4C-C3C	2.22	1.48	1.45
24	C	514	CLA	C3D-C4D	-2.22	1.39	1.44
24	b	601	CLA	C3B-C2B	2.22	1.48	1.41
24	c	507	CLA	C3B-C4B	2.22	1.49	1.42
24	B	608	CLA	C3B-C4B	2.22	1.49	1.42
24	b	605	CLA	C3B-C4B	2.21	1.49	1.42
24	c	512	CLA	C3B-C4B	2.21	1.49	1.42
24	b	601	CLA	C1C-NC	-2.21	1.34	1.37
35	B	628	HTG	C1-S1	-2.21	1.77	1.80
24	c	514	CLA	C4C-C3C	2.20	1.48	1.45
24	c	513	CLA	C4C-C3C	2.20	1.48	1.45
24	b	614	CLA	C4C-C3C	2.20	1.48	1.45
41	v	203	HEC	C4A-C3A	-2.20	1.41	1.45
34	t	101	LMT	O1'-C1'	2.19	1.43	1.40
34	a	359	LMT	O1'-C1'	2.19	1.43	1.40
24	C	511	CLA	C4C-C3C	2.19	1.48	1.45
24	c	514	CLA	C3D-C4D	-2.19	1.39	1.44
24	D	403	CLA	C4B-NB	-2.19	1.35	1.37
24	c	506	CLA	C3D-C4D	-2.19	1.39	1.44
24	c	512	CLA	C3B-C2B	2.19	1.48	1.41
24	C	507	CLA	C1D-C2D	2.19	1.49	1.45
24	B	607	CLA	C3B-C4B	2.19	1.49	1.42
24	A	406	CLA	C4C-C3C	2.19	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	611	CLA	C4C-C3C	2.18	1.48	1.45
24	B	616	CLA	C4B-NB	-2.18	1.35	1.37
24	c	511	CLA	C1C-C2C	2.18	1.48	1.44
24	C	502	CLA	C3B-C2B	2.18	1.48	1.41
24	d	402	CLA	C3B-C2B	2.18	1.48	1.41
36	H	102	DGD	O5D-C1E	2.18	1.43	1.40
24	c	505	CLA	C3D-C4D	-2.18	1.39	1.44
24	c	511	CLA	C3B-C2B	2.17	1.48	1.41
24	A	405	CLA	C3D-C4D	-2.17	1.39	1.44
24	c	515	CLA	C1D-C2D	2.17	1.49	1.45
24	B	602	CLA	C1B-C2B	2.17	1.48	1.43
25	A	407	PHO	C1D-ND	-2.17	1.34	1.38
24	a	404	CLA	C4C-C3C	2.16	1.48	1.45
24	c	513	CLA	C3B-C2B	2.16	1.48	1.41
24	b	614	CLA	C3B-C2B	2.16	1.48	1.41
24	b	602	CLA	C4B-NB	-2.16	1.35	1.37
24	A	409	CLA	C3B-C4B	2.16	1.49	1.42
24	c	509	CLA	C1D-C2D	2.16	1.49	1.45
24	a	403	CLA	C1C-C2C	2.16	1.48	1.44
24	b	602	CLA	C4C-C3C	2.16	1.48	1.45
24	C	512	CLA	C3D-C4D	-2.16	1.39	1.44
26	d	404	BCR	C30-C25	-2.16	1.51	1.53
24	a	350	CLA	C1C-C2C	2.16	1.48	1.44
33	C	521	LMG	O1-C1	2.16	1.43	1.40
24	C	510	CLA	C3B-C4B	2.15	1.49	1.42
24	C	513	CLA	C4C-C3C	2.15	1.48	1.45
25	a	405	PHO	C1B-NB	-2.15	1.34	1.38
24	b	603	CLA	C3D-C4D	-2.15	1.39	1.44
24	C	513	CLA	C3D-C4D	-2.14	1.39	1.44
24	B	612	CLA	C3D-C4D	-2.14	1.39	1.44
34	a	418	LMT	O1'-C1'	2.14	1.43	1.40
31	a	414[A]	PL9	C2-C3	2.14	1.40	1.34
31	a	414[B]	PL9	C2-C3	2.14	1.40	1.34
24	B	604	CLA	C3D-C4D	-2.14	1.39	1.44
24	b	616	CLA	C1C-C2C	2.14	1.48	1.44
33	Z	101	LMG	O1-C1	2.14	1.43	1.40
24	A	405	CLA	C3B-C2B	2.14	1.48	1.41
24	b	606	CLA	C3B-C2B	2.14	1.48	1.41
24	b	615	CLA	C3D-C4D	-2.13	1.39	1.44
24	B	611	CLA	C3B-C2B	2.13	1.48	1.41
24	b	604	CLA	C3B-C4B	2.13	1.49	1.42
24	a	404	CLA	C3D-C4D	-2.13	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	416[B]	PL9	C2-C3	2.13	1.40	1.34
24	C	511	CLA	C3B-C2B	2.13	1.48	1.41
24	C	509	CLA	C3D-C4D	-2.13	1.39	1.44
24	b	615	CLA	C1D-C2D	2.13	1.49	1.45
24	b	601	CLA	C1C-C2C	2.13	1.48	1.44
24	A	409	CLA	C3B-C2B	2.13	1.48	1.41
24	B	604	CLA	C3B-C2B	2.13	1.48	1.41
24	B	616	CLA	C3B-C2B	2.13	1.48	1.41
24	b	603	CLA	C3B-C2B	2.12	1.48	1.41
24	b	602	CLA	C3B-C2B	2.12	1.48	1.41
24	b	611	CLA	C4B-NB	-2.11	1.35	1.37
24	B	601	CLA	C3B-C2B	2.11	1.48	1.41
24	c	508	CLA	C3B-C4B	2.11	1.48	1.42
36	h	103	DGD	O5D-C1E	2.11	1.43	1.40
24	b	608	CLA	C3B-C2B	2.11	1.48	1.41
38	d	407	LHG	O7-C5	-2.11	1.41	1.46
34	b	630	LMT	O1'-C1'	2.11	1.43	1.40
24	C	514	CLA	C4C-C3C	2.11	1.48	1.45
24	C	508	CLA	C4C-C3C	2.10	1.48	1.45
36	c	520	DGD	O2G-C2G	-2.10	1.41	1.46
35	h	101	HTG	C1-S1	-2.10	1.77	1.80
24	c	504	CLA	C3B-C4B	2.10	1.48	1.42
24	B	611	CLA	C1C-C2C	2.10	1.48	1.44
24	d	403	CLA	C1D-C2D	2.09	1.49	1.45
24	b	605	CLA	C1D-C2D	2.09	1.49	1.45
24	C	506	CLA	C3B-C2B	2.09	1.48	1.41
24	c	504	CLA	C3B-C2B	2.09	1.48	1.41
39	e	102	HEM	C3C-C4C	-2.09	1.42	1.46
24	B	611	CLA	C1C-NC	-2.09	1.34	1.37
41	V	203	HEC	C1A-C2A	-2.09	1.41	1.45
24	b	616	CLA	C1C-NC	-2.09	1.34	1.37
24	C	514	CLA	C3B-C2B	2.09	1.48	1.41
31	d	405	PL9	C2-C3	2.08	1.39	1.34
24	D	402	CLA	C1C-NC	-2.08	1.34	1.37
41	V	203	HEC	C4A-C3A	-2.08	1.41	1.45
24	C	502	CLA	C1D-C2D	2.08	1.49	1.45
24	c	503	CLA	C3B-C2B	2.08	1.48	1.41
24	B	614	CLA	C3B-C4B	2.07	1.48	1.42
39	E	103	HEM	C3C-C4C	-2.07	1.42	1.46
41	v	203	HEC	C1A-C2A	-2.07	1.41	1.45
24	C	503	CLA	C1C-C2C	2.07	1.48	1.44
24	b	609	CLA	C3B-C2B	2.07	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	C3B-C2B	2.06	1.48	1.41
34	I	101	LMT	O1'-C1'	2.06	1.43	1.40
24	A	409	CLA	C4C-C3C	2.06	1.48	1.45
25	A	408	PHO	C1D-ND	-2.06	1.34	1.38
24	B	616	CLA	C1C-NC	-2.05	1.34	1.37
24	C	511	CLA	C3B-C4B	2.05	1.48	1.42
24	C	512	CLA	C1C-NC	-2.05	1.34	1.37
24	C	508	CLA	C3B-C2B	2.05	1.48	1.41
24	B	611	CLA	C3B-C4B	2.05	1.48	1.42
24	B	605	CLA	C4C-C3C	2.05	1.48	1.45
24	B	613	CLA	C3D-C4D	-2.05	1.39	1.44
25	A	407	PHO	CBD-CGD	-2.05	1.49	1.52
24	C	507	CLA	C3B-C2B	2.05	1.48	1.41
24	c	513	CLA	C3B-C4B	2.05	1.48	1.42
24	a	407	CLA	C3B-C2B	2.04	1.48	1.41
24	c	504	CLA	C4C-C3C	2.04	1.48	1.45
35	b	625	HTG	C1-S1	-2.04	1.77	1.80
24	c	507	CLA	C3B-C2B	2.04	1.48	1.41
34	e	101	LMT	O1'-C1'	2.04	1.43	1.40
24	b	610	CLA	C1B-C2B	2.04	1.47	1.43
24	C	507	CLA	C1C-C2C	2.04	1.48	1.44
24	c	508	CLA	C3B-C2B	2.04	1.48	1.41
24	C	509	CLA	C1C-NC	-2.03	1.34	1.37
31	A	416[A]	PL9	C2-C3	2.03	1.39	1.34
24	b	607	CLA	C1C-NC	-2.03	1.34	1.37
35	c	526	HTG	C1-S1	-2.03	1.77	1.80
24	b	604	CLA	C3D-C4D	-2.03	1.39	1.44
24	C	507	CLA	C3B-C4B	2.03	1.48	1.42
24	C	508	CLA	C3B-C4B	2.03	1.48	1.42
24	a	350	CLA	C3D-C4D	-2.03	1.39	1.44
24	B	606	CLA	C3B-C2B	2.02	1.48	1.41
39	E	103	HEM	C4B-NB	-2.02	1.34	1.38
24	C	513	CLA	C3B-C2B	2.02	1.48	1.41
24	B	609	CLA	C4C-C3C	2.02	1.48	1.45
24	c	515	CLA	C3B-C2B	2.02	1.48	1.41
27	a	411	SQD	O6-C1	2.02	1.43	1.40
24	B	602	CLA	CHB-C4A	-2.02	1.32	1.37
24	c	506	CLA	C3B-C4B	2.02	1.48	1.42
24	C	510	CLA	C1D-C2D	2.01	1.49	1.45
25	A	407	PHO	C3D-C4D	-2.01	1.38	1.41
24	b	613	CLA	C4C-C3C	2.01	1.48	1.45
24	c	506	CLA	C1D-C2D	2.01	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	101	LMG	O7-C8	-2.01	1.41	1.46
24	a	404	CLA	C1C-NC	-2.01	1.34	1.37
24	b	607	CLA	C3B-C2B	2.01	1.47	1.41
24	a	404	CLA	C3B-C2B	2.00	1.47	1.41
24	B	604	CLA	C3B-C4B	2.00	1.48	1.42
24	b	609	CLA	C3B-C4B	2.00	1.48	1.42
24	C	504	CLA	C3D-C4D	-2.00	1.39	1.44
24	B	610	CLA	C4C-C3C	2.00	1.48	1.45
24	b	609	CLA	C1D-C2D	2.00	1.49	1.45

All (2957) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	405	PHO	C2D-C1D-ND	11.98	118.09	109.43
25	A	407	PHO	C2D-C1D-ND	11.89	118.02	109.43
25	A	408	PHO	C2D-C1D-ND	11.80	117.96	109.43
25	a	406	PHO	C2D-C1D-ND	10.47	117.00	109.43
25	a	405	PHO	O2D-CGD-CBD	10.45	122.43	110.95
24	a	404	CLA	C1D-ND-C4D	-10.20	99.15	106.31
24	b	605	CLA	C1D-ND-C4D	-10.11	99.22	106.31
24	c	513	CLA	C1D-ND-C4D	-10.07	99.24	106.31
24	B	614	CLA	C1D-ND-C4D	-10.05	99.26	106.31
24	a	350	CLA	C1D-ND-C4D	-9.93	99.34	106.31
24	D	403	CLA	C1D-ND-C4D	-9.91	99.36	106.31
24	A	409	CLA	C1D-ND-C4D	-9.91	99.36	106.31
24	A	405	CLA	C1D-ND-C4D	-9.89	99.37	106.31
24	B	615	CLA	C1D-ND-C4D	-9.87	99.38	106.31
24	C	504	CLA	C1D-ND-C4D	-9.87	99.39	106.31
24	B	607	CLA	C1D-ND-C4D	-9.87	99.39	106.31
24	C	502	CLA	C1D-ND-C4D	-9.84	99.41	106.31
24	c	506	CLA	C1D-ND-C4D	-9.76	99.47	106.31
24	d	403	CLA	C1D-ND-C4D	-9.72	99.49	106.31
24	C	514	CLA	C1D-ND-C4D	-9.72	99.49	106.31
24	c	504	CLA	C1D-ND-C4D	-9.72	99.49	106.31
24	B	609	CLA	C1D-ND-C4D	-9.70	99.51	106.31
24	b	607	CLA	C1D-ND-C4D	-9.68	99.52	106.31
24	B	612	CLA	C1D-ND-C4D	-9.67	99.53	106.31
24	c	505	CLA	C1D-ND-C4D	-9.57	99.60	106.31
24	B	605	CLA	C1D-ND-C4D	-9.56	99.61	106.31
25	a	406	PHO	O2D-CGD-CBD	9.49	121.37	110.95
24	c	515	CLA	C1D-ND-C4D	-9.49	99.65	106.31
24	b	602	CLA	C1D-ND-C4D	-9.47	99.67	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	C1D-ND-C4D	-9.46	99.68	106.31
24	B	606	CLA	C1D-ND-C4D	-9.45	99.68	106.31
24	A	406	CLA	C1D-ND-C4D	-9.42	99.70	106.31
24	B	613	CLA	C1D-ND-C4D	-9.40	99.72	106.31
24	b	611	CLA	C1D-ND-C4D	-9.38	99.73	106.31
24	C	505	CLA	C1D-ND-C4D	-9.38	99.73	106.31
24	B	608	CLA	C1D-ND-C4D	-9.37	99.73	106.31
24	b	615	CLA	C1D-ND-C4D	-9.35	99.75	106.31
24	D	402	CLA	C1D-ND-C4D	-9.35	99.75	106.31
24	b	603	CLA	C1D-ND-C4D	-9.35	99.75	106.31
24	c	503	CLA	C1D-ND-C4D	-9.34	99.76	106.31
24	C	510	CLA	C1D-ND-C4D	-9.33	99.76	106.31
24	b	610	CLA	C1D-ND-C4D	-9.28	99.80	106.31
24	c	510	CLA	C1D-ND-C4D	-9.28	99.80	106.31
24	B	601	CLA	C1D-ND-C4D	-9.26	99.81	106.31
24	b	608	CLA	C1D-ND-C4D	-9.23	99.84	106.31
25	A	408	PHO	O2D-CGD-CBD	9.19	121.05	110.95
24	B	616	CLA	C1D-ND-C4D	-9.17	99.88	106.31
24	C	511	CLA	C1D-ND-C4D	-9.15	99.89	106.31
24	C	503	CLA	C1D-ND-C4D	-9.10	99.93	106.31
24	B	611	CLA	C1D-ND-C4D	-9.08	99.94	106.31
24	c	514	CLA	C1D-ND-C4D	-9.07	99.95	106.31
24	b	609	CLA	C1D-ND-C4D	-9.06	99.95	106.31
24	C	512	CLA	C1D-ND-C4D	-9.00	100.00	106.31
24	B	603	CLA	C1D-ND-C4D	-8.96	100.02	106.31
24	B	610	CLA	C1D-ND-C4D	-8.95	100.03	106.31
24	B	604	CLA	C1D-ND-C4D	-8.91	100.06	106.31
24	C	513	CLA	C1D-ND-C4D	-8.90	100.07	106.31
24	b	601	CLA	C1D-ND-C4D	-8.89	100.07	106.31
24	b	606	CLA	C1D-ND-C4D	-8.88	100.08	106.31
24	C	509	CLA	C1D-ND-C4D	-8.82	100.13	106.31
24	c	511	CLA	C1D-ND-C4D	-8.80	100.14	106.31
24	c	509	CLA	C1D-ND-C4D	-8.79	100.15	106.31
24	c	508	CLA	C1D-ND-C4D	-8.77	100.16	106.31
24	c	507	CLA	C1D-ND-C4D	-8.76	100.16	106.31
24	A	404	CLA	C1D-ND-C4D	-8.74	100.18	106.31
24	d	402	CLA	C1D-ND-C4D	-8.71	100.20	106.31
24	b	613	CLA	C1D-ND-C4D	-8.70	100.21	106.31
24	b	604	CLA	C1D-ND-C4D	-8.62	100.26	106.31
25	A	407	PHO	C3B-C4B-NB	8.61	113.08	107.46
24	C	506	CLA	C1D-ND-C4D	-8.58	100.29	106.31
24	B	602	CLA	C1D-ND-C4D	-8.53	100.32	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	403	CLA	C1D-ND-C4D	-8.50	100.35	106.31
24	b	616	CLA	C1D-ND-C4D	-8.50	100.35	106.31
24	c	512	CLA	C1D-ND-C4D	-8.44	100.39	106.31
24	b	612	CLA	C1D-ND-C4D	-8.43	100.39	106.31
24	C	508	CLA	C1D-ND-C4D	-8.43	100.40	106.31
24	C	507	CLA	C1D-ND-C4D	-8.26	100.52	106.31
25	a	405	PHO	C3B-C4B-NB	8.17	112.79	107.46
25	A	407	PHO	O2D-CGD-CBD	8.17	119.92	110.95
24	B	602	CLA	C4A-NA-C1A	-8.14	102.97	106.68
25	A	408	PHO	C3B-C4B-NB	8.03	112.70	107.46
24	a	407	CLA	C1D-ND-C4D	-7.98	100.71	106.31
25	A	407	PHO	C2B-C1B-NB	7.29	114.70	109.43
24	c	509	CLA	CMD-C2D-C1D	7.27	137.53	124.73
25	A	408	PHO	C2B-C1B-NB	7.23	114.66	109.43
24	b	616	CLA	C4A-NA-C1A	-7.22	103.39	106.68
24	C	504	CLA	C4A-NA-C1A	-7.20	103.39	106.68
24	B	606	CLA	C4A-NA-C1A	-7.19	103.40	106.68
24	C	507	CLA	CMD-C2D-C1D	7.17	137.36	124.73
24	b	611	CLA	C4A-NA-C1A	-7.16	103.41	106.68
25	a	406	PHO	C3B-C4B-NB	7.14	112.12	107.46
25	a	405	PHO	C2B-C1B-NB	7.11	114.57	109.43
24	A	405	CLA	CHD-C4C-C3C	-7.09	114.44	124.77
24	B	615	CLA	CHD-C4C-C3C	-7.04	114.51	124.77
24	A	405	CLA	C2D-C1D-ND	7.03	117.08	110.13
24	b	615	CLA	CMD-C2D-C1D	7.00	137.05	124.73
24	A	404	CLA	CMD-C2D-C1D	6.98	137.02	124.73
24	C	506	CLA	CMD-C2D-C1D	6.98	137.01	124.73
24	C	511	CLA	CMD-C2D-C1D	6.98	137.01	124.73
24	B	616	CLA	C4A-NA-C1A	-6.97	103.50	106.68
24	b	602	CLA	C4A-NA-C1A	-6.97	103.50	106.68
24	B	605	CLA	CHD-C4C-C3C	-6.96	114.62	124.77
24	D	402	CLA	CMD-C2D-C1D	6.94	136.96	124.73
24	A	404	CLA	C4A-NA-C1A	-6.91	103.53	106.68
24	B	614	CLA	CMD-C2D-C1D	6.89	136.86	124.73
24	B	606	CLA	CHD-C4C-C3C	-6.86	114.77	124.77
24	b	606	CLA	C4A-NA-C1A	-6.86	103.55	106.68
24	b	607	CLA	C2D-C1D-ND	6.86	116.91	110.13
24	B	614	CLA	C2D-C1D-ND	6.77	116.83	110.13
24	B	602	CLA	CMD-C2D-C1D	6.77	136.64	124.73
24	b	610	CLA	CMD-C2D-C1D	6.75	136.62	124.73
24	B	615	CLA	C2D-C1D-ND	6.72	116.78	110.13
24	c	512	CLA	CMD-C2D-C1D	6.70	136.53	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	O2D-CGD-CBD	6.69	122.93	111.23
24	B	609	CLA	C2D-C1D-ND	6.69	116.75	110.13
24	B	604	CLA	CHD-C4C-C3C	-6.68	115.04	124.77
24	B	607	CLA	C2D-C1D-ND	6.67	116.73	110.13
24	B	603	CLA	CMD-C2D-C1D	6.63	136.41	124.73
24	B	616	CLA	CHD-C4C-C3C	-6.63	115.11	124.77
24	B	606	CLA	C2D-C1D-ND	6.62	116.68	110.13
24	c	503	CLA	CMD-C2D-C1D	6.61	136.37	124.73
24	b	605	CLA	CMD-C2D-C1D	6.60	136.35	124.73
27	A	411	SQD	O6-C1-C2	6.60	118.29	108.27
24	b	602	CLA	CMD-C2D-C1D	6.56	136.28	124.73
24	b	613	CLA	CHD-C4C-C3C	-6.56	115.21	124.77
25	a	406	PHO	C2B-C1B-NB	6.53	114.15	109.43
24	B	601	CLA	CHD-C4C-C3C	-6.53	115.25	124.77
24	c	510	CLA	C2D-C1D-ND	6.53	116.59	110.13
24	C	510	CLA	CMD-C2D-C1D	6.53	136.23	124.73
24	B	616	CLA	O2D-CGD-CBD	6.53	122.64	111.23
24	b	616	CLA	CHD-C4C-C3C	-6.52	115.27	124.77
24	B	606	CLA	CMD-C2D-C1D	6.52	136.21	124.73
24	B	609	CLA	CHD-C4C-C3C	-6.51	115.28	124.77
24	B	611	CLA	CHD-C4C-C3C	-6.51	115.29	124.77
24	C	504	CLA	CMD-C2D-C1D	6.50	136.17	124.73
24	a	350	CLA	CHD-C4C-C3C	-6.49	115.31	124.77
24	a	404	CLA	C2D-C1D-ND	6.49	116.55	110.13
24	B	611	CLA	C2D-C1D-ND	6.47	116.53	110.13
24	a	350	CLA	C2D-C1D-ND	6.46	116.52	110.13
24	B	612	CLA	O2D-CGD-CBD	6.46	122.52	111.23
24	c	507	CLA	CHD-C4C-C3C	-6.46	115.36	124.77
24	A	409	CLA	C2D-C1D-ND	6.45	116.51	110.13
24	c	513	CLA	C2D-C1D-ND	6.44	116.50	110.13
24	C	513	CLA	CHD-C4C-C3C	-6.44	115.38	124.77
24	b	607	CLA	CMD-C2D-C1D	6.44	136.07	124.73
24	c	515	CLA	CMD-C2D-C1D	6.43	136.05	124.73
24	B	605	CLA	C2D-C1D-ND	6.42	116.48	110.13
24	c	513	CLA	CHD-C4C-C3C	-6.41	115.43	124.77
24	B	603	CLA	O2D-CGD-CBD	6.40	122.42	111.23
24	d	403	CLA	CMD-C2D-C1D	6.40	136.00	124.73
24	C	502	CLA	CMD-C2D-C1D	6.40	135.99	124.73
24	b	605	CLA	C2D-C1D-ND	6.40	116.46	110.13
24	D	403	CLA	C2D-C1D-ND	6.39	116.45	110.13
24	b	613	CLA	C2D-C1D-ND	6.39	116.45	110.13
24	c	506	CLA	CMD-C2D-C1D	6.39	135.99	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	407	CLA	C4A-NA-C1A	-6.39	103.76	106.68
24	c	514	CLA	O2D-CGD-CBD	6.39	122.40	111.23
24	C	506	CLA	CHD-C4C-C3C	-6.36	115.50	124.77
24	D	403	CLA	CHD-C4C-C3C	-6.35	115.51	124.77
24	B	608	CLA	CHD-C4C-C3C	-6.34	115.54	124.77
24	b	603	CLA	C4A-NA-C1A	-6.33	103.79	106.68
24	c	509	CLA	O2D-CGD-CBD	6.33	122.29	111.23
24	D	402	CLA	C2D-C1D-ND	6.32	116.39	110.13
24	B	613	CLA	C2D-C1D-ND	6.32	116.38	110.13
24	C	511	CLA	CHD-C4C-C3C	-6.31	115.58	124.77
24	b	609	CLA	CMD-C2D-C1D	6.30	135.82	124.73
24	C	505	CLA	C2D-C1D-ND	6.30	116.36	110.13
24	b	614	CLA	C2D-C1D-ND	6.29	116.35	110.13
24	b	605	CLA	CHD-C4C-C3C	-6.28	115.61	124.77
24	c	504	CLA	CHD-C4C-C3C	-6.28	115.61	124.77
24	b	609	CLA	C4A-NA-C1A	-6.28	103.81	106.68
24	b	601	CLA	CHD-C4C-C3C	-6.28	115.62	124.77
24	b	614	CLA	O2D-CGD-CBD	6.27	122.19	111.23
24	D	403	CLA	CMD-C2D-C1D	6.27	135.76	124.73
24	b	604	CLA	C4A-NA-C1A	-6.26	103.82	106.68
24	c	513	CLA	CMD-C2D-C1D	6.26	135.75	124.73
24	C	513	CLA	O2D-CGD-CBD	6.26	122.17	111.23
24	C	503	CLA	CHD-C4C-C3C	-6.24	115.68	124.77
24	b	606	CLA	CMD-C2D-C1D	6.24	135.71	124.73
24	B	611	CLA	C4A-NA-C1A	-6.23	103.83	106.68
24	B	608	CLA	C2D-C1D-ND	6.23	116.30	110.13
24	B	610	CLA	CHD-C4C-C3C	-6.23	115.69	124.77
24	b	611	CLA	CMD-C2D-C1D	6.22	135.69	124.73
24	B	603	CLA	CHD-C4C-C3C	-6.22	115.70	124.77
24	c	504	CLA	C2D-C1D-ND	6.22	116.28	110.13
24	b	606	CLA	CHD-C4C-C3C	-6.20	115.73	124.77
24	b	611	CLA	CHD-C4C-C3C	-6.20	115.73	124.77
24	c	510	CLA	CHD-C4C-C3C	-6.20	115.73	124.77
24	B	607	CLA	CMD-C2D-C1D	6.20	135.64	124.73
24	b	606	CLA	C2D-C1D-ND	6.20	116.26	110.13
24	B	612	CLA	C2D-C1D-ND	6.18	116.24	110.13
24	b	616	CLA	CMD-C2D-C1D	6.18	135.61	124.73
24	B	616	CLA	CMD-C2D-C1D	6.16	135.58	124.73
24	B	615	CLA	CMD-C2D-C1D	6.16	135.57	124.73
24	B	614	CLA	O2D-CGD-CBD	6.16	121.99	111.23
24	b	604	CLA	CHD-C4C-C3C	-6.15	115.80	124.77
24	B	603	CLA	C4A-NA-C1A	-6.15	103.87	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	404	CLA	CHD-C4C-C3C	-6.15	115.81	124.77
24	C	504	CLA	C2D-C1D-ND	6.15	116.21	110.13
24	b	608	CLA	CMD-C2D-C1D	6.13	135.53	124.73
24	C	508	CLA	O2D-CGD-CBD	6.13	121.95	111.23
25	A	408	PHO	C4D-ND-C1D	-6.13	101.52	108.87
24	A	409	CLA	CMD-C2D-C1D	6.13	135.51	124.73
24	c	511	CLA	CMD-C2D-C1D	6.12	135.51	124.73
24	B	611	CLA	CMD-C2D-C1D	6.12	135.51	124.73
24	b	608	CLA	C2D-C1D-ND	6.12	116.18	110.13
24	D	402	CLA	C4A-NA-C1A	-6.12	103.89	106.68
24	B	612	CLA	CHD-C4C-C3C	-6.12	115.86	124.77
24	c	506	CLA	C2D-C1D-ND	6.11	116.17	110.13
24	b	602	CLA	CHD-C4C-C3C	-6.11	115.86	124.77
24	B	616	CLA	C2D-C1D-ND	6.10	116.16	110.13
24	b	601	CLA	CMD-C2D-C1D	6.10	135.46	124.73
24	b	612	CLA	C4A-NA-C1A	-6.09	103.90	106.68
24	A	406	CLA	CMD-C2D-C1D	6.09	135.45	124.73
24	b	604	CLA	CMD-C2D-C1D	6.09	135.45	124.73
24	C	513	CLA	C4A-NA-C1A	-6.08	103.91	106.68
24	C	505	CLA	CMD-C2D-C1D	6.07	135.42	124.73
24	c	505	CLA	CMD-C2D-C1D	6.07	135.41	124.73
24	B	609	CLA	CMD-C2D-C1D	6.07	135.41	124.73
24	d	403	CLA	C4A-NA-C1A	-6.06	103.91	106.68
25	a	405	PHO	C4D-ND-C1D	-6.06	101.61	108.87
24	B	610	CLA	C2D-C1D-ND	6.05	116.11	110.13
24	B	601	CLA	CMD-C2D-C1D	6.03	135.35	124.73
24	b	603	CLA	CHD-C4C-C3C	-6.03	115.98	124.77
24	b	608	CLA	CHD-C4C-C3C	-6.03	115.98	124.77
24	C	508	CLA	CMD-C2D-C1D	6.02	135.34	124.73
24	C	509	CLA	CHD-C4C-C3C	-6.02	115.99	124.77
24	b	616	CLA	O2D-CGD-CBD	6.01	121.73	111.23
24	B	610	CLA	CMD-C2D-C1D	5.99	135.27	124.73
24	C	514	CLA	C2D-C1D-ND	5.99	116.05	110.13
24	B	601	CLA	C2D-C1D-ND	5.98	116.05	110.13
24	c	505	CLA	C2D-C1D-ND	5.98	116.05	110.13
24	b	601	CLA	O2D-CGD-CBD	5.98	121.68	111.23
24	C	502	CLA	CHD-C4C-C3C	-5.96	116.09	124.77
24	c	505	CLA	C4A-NA-C1A	-5.95	103.96	106.68
24	b	603	CLA	O2D-CGD-CBD	5.95	121.64	111.23
24	b	611	CLA	C2D-C1D-ND	5.95	116.01	110.13
24	B	601	CLA	O2D-CGD-CBD	5.94	121.61	111.23
24	a	403	CLA	CMD-C2D-C1D	5.94	135.19	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	C4A-NA-C1A	-5.92	103.98	106.68
24	b	613	CLA	C4A-NA-C1A	-5.92	103.98	106.68
24	A	409	CLA	CHD-C4C-C3C	-5.92	116.14	124.77
24	b	607	CLA	CHD-C4C-C3C	-5.92	116.15	124.77
24	C	514	CLA	CMD-C2D-C1D	5.91	135.14	124.73
24	c	510	CLA	O2D-CGD-CBD	5.91	121.56	111.23
24	B	614	CLA	CHD-C4C-C3C	-5.91	116.16	124.77
24	c	503	CLA	O2D-CGD-CBD	5.90	121.54	111.23
24	A	406	CLA	CHD-C4C-C3C	-5.90	116.17	124.77
24	b	604	CLA	O2D-CGD-CBD	5.89	121.53	111.23
24	c	503	CLA	C2D-C1D-ND	5.89	115.96	110.13
24	b	614	CLA	CHD-C4C-C3C	-5.89	116.19	124.77
24	b	603	CLA	C2D-C1D-ND	5.87	115.94	110.13
24	C	503	CLA	CMD-C2D-C1D	5.86	135.06	124.73
25	A	407	PHO	C4D-ND-C1D	-5.86	101.85	108.87
24	A	404	CLA	CHD-C4C-C3C	-5.85	116.24	124.77
24	b	615	CLA	C2D-C1D-ND	5.85	115.91	110.13
24	C	508	CLA	CHD-C4C-C3C	-5.84	116.25	124.77
24	b	616	CLA	C2D-C1D-ND	5.84	115.91	110.13
24	C	514	CLA	CHD-C4C-C3C	-5.84	116.26	124.77
24	c	504	CLA	CMD-C2D-C1D	5.84	135.00	124.73
24	d	403	CLA	C2D-C1D-ND	5.83	115.90	110.13
24	C	502	CLA	C4A-NA-C1A	-5.83	104.02	106.68
24	c	505	CLA	CHD-C4C-C3C	-5.83	116.27	124.77
24	c	515	CLA	C4A-NA-C1A	-5.83	104.02	106.68
24	c	509	CLA	CHD-C4C-C3C	-5.82	116.28	124.77
24	b	614	CLA	CMD-C2D-C1D	5.82	134.98	124.73
24	A	406	CLA	C2D-C1D-ND	5.82	115.89	110.13
24	C	503	CLA	C2D-C1D-ND	5.82	115.89	110.13
24	a	350	CLA	CMD-C2D-C1D	5.82	134.97	124.73
24	c	514	CLA	C4A-NA-C1A	-5.81	104.03	106.68
24	b	605	CLA	C4A-NA-C1A	-5.81	104.03	106.68
24	c	514	CLA	CHD-C4C-C3C	-5.81	116.30	124.77
24	B	613	CLA	CMD-C2D-C1D	5.81	134.96	124.73
24	C	502	CLA	O2D-CGD-CBD	5.81	121.38	111.23
24	B	604	CLA	C2D-C1D-ND	5.80	115.87	110.13
24	C	502	CLA	C2D-C1D-ND	5.80	115.87	110.13
24	d	402	CLA	CHD-C4C-C3C	-5.80	116.31	124.77
24	B	605	CLA	CMD-C2D-C1D	5.80	134.95	124.73
24	B	604	CLA	CMD-C2D-C1D	5.80	134.94	124.73
24	C	511	CLA	C4A-NA-C1A	-5.80	104.03	106.68
24	c	508	CLA	CMD-C2D-C1D	5.80	134.94	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	508	CLA	C2D-C1D-ND	5.79	115.86	110.13
24	c	514	CLA	C2D-C1D-ND	5.79	115.86	110.13
24	c	514	CLA	C2B-C1B-NB	5.78	116.32	110.33
24	C	512	CLA	CHD-C4C-C3C	-5.78	116.35	124.77
24	d	403	CLA	CHD-C4C-C3C	-5.78	116.35	124.77
27	a	409	SQD	O6-C1-C2	5.78	117.04	108.27
24	b	602	CLA	C2D-C1D-ND	5.77	115.84	110.13
24	b	602	CLA	O2D-CGD-CBD	5.77	121.32	111.23
24	C	512	CLA	C2D-C1D-ND	5.75	115.82	110.13
26	D	404	BCR	C7-C8-C9	-5.74	117.74	126.23
24	B	602	CLA	CHD-C4C-C3C	-5.74	116.41	124.77
24	b	611	CLA	O2D-CGD-CBD	5.73	121.25	111.23
24	C	510	CLA	CHD-C4C-C3C	-5.72	116.44	124.77
24	d	402	CLA	C2D-C1D-ND	5.69	115.76	110.13
24	D	402	CLA	C2C-C1C-NC	5.68	115.95	109.98
24	C	511	CLA	O2D-CGD-CBD	5.68	121.16	111.23
24	C	506	CLA	O2D-CGD-CBD	5.68	121.15	111.23
24	b	612	CLA	CHD-C4C-C3C	-5.67	116.51	124.77
24	b	604	CLA	C2D-C1D-ND	5.66	115.73	110.13
24	b	609	CLA	CHD-C4C-C3C	-5.66	116.52	124.77
24	b	610	CLA	CHD-C4C-C3C	-5.66	116.52	124.77
24	b	610	CLA	O2D-CGD-CBD	5.65	121.11	111.23
24	b	601	CLA	C2D-C1D-ND	5.65	115.72	110.13
24	b	615	CLA	C4A-NA-C1A	-5.65	104.10	106.68
24	c	515	CLA	C2D-C1D-ND	5.65	115.71	110.13
24	C	509	CLA	O2D-CGD-CBD	5.65	121.10	111.23
24	C	513	CLA	C2D-C1D-ND	5.63	115.70	110.13
24	A	409	CLA	C4A-NA-C1A	-5.63	104.11	106.68
24	a	403	CLA	C2C-C1C-NC	5.63	115.89	109.98
24	c	512	CLA	CHD-C4C-C3C	-5.63	116.57	124.77
24	C	507	CLA	C2C-C1C-NC	5.63	115.89	109.98
24	C	510	CLA	C2D-C1D-ND	5.63	115.69	110.13
24	C	507	CLA	C4A-NA-C1A	-5.62	104.11	106.68
24	c	507	CLA	O2D-CGD-CBD	5.62	121.05	111.23
25	A	408	PHO	C1-C2-C3	-5.61	117.00	126.20
24	B	607	CLA	CHD-C4C-C3C	-5.61	116.59	124.77
27	F	101	SQD	O47-C7-C8	5.61	123.61	111.48
35	b	625	HTG	C1'-S1-C1	5.61	112.56	100.45
24	B	604	CLA	O2D-CGD-CBD	5.61	121.03	111.23
24	c	507	CLA	CMD-C2D-C1D	5.60	134.59	124.73
24	a	403	CLA	C4A-NA-C1A	-5.60	104.12	106.68
24	a	404	CLA	CMD-C2D-C1D	5.60	134.59	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	O2D-CGD-CBD	5.60	121.02	111.23
24	b	609	CLA	C2D-C1D-ND	5.60	115.67	110.13
24	a	407	CLA	CHD-C4C-C3C	-5.60	116.61	124.77
24	B	607	CLA	C2C-C1C-NC	5.59	115.86	109.98
24	B	604	CLA	C1-C2-C3	-5.59	117.03	126.20
25	a	406	PHO	C4D-ND-C1D	-5.59	102.18	108.87
24	c	506	CLA	CHD-C4C-C3C	-5.59	116.63	124.77
24	C	509	CLA	C2D-C1D-ND	5.58	115.65	110.13
24	d	402	CLA	CMD-C2D-C1D	5.56	134.52	124.73
24	b	606	CLA	O2D-CGD-CBD	5.55	120.93	111.23
24	c	509	CLA	C2D-C1D-ND	5.53	115.60	110.13
24	C	509	CLA	CMD-C2D-C1D	5.53	134.46	124.73
24	c	508	CLA	C2D-C1D-ND	5.52	115.59	110.13
24	b	615	CLA	CHD-C4C-C3C	-5.52	116.73	124.77
24	B	609	CLA	C4A-NA-C1A	-5.52	104.16	106.68
24	B	603	CLA	C2D-C1D-ND	5.51	115.58	110.13
24	B	614	CLA	C3B-C2B-C1B	-5.51	100.67	107.17
24	B	608	CLA	CMD-C2D-C1D	5.51	134.43	124.73
25	a	406	PHO	C3D-C4D-ND	5.50	114.76	107.71
24	c	507	CLA	C2D-C1D-ND	5.49	115.56	110.13
24	C	513	CLA	CMD-C2D-C1D	5.49	134.40	124.73
24	b	603	CLA	CMD-C2D-C1D	5.49	134.39	124.73
24	C	512	CLA	CMD-C2D-C1D	5.49	134.39	124.73
25	a	406	PHO	C1-C2-C3	-5.47	117.23	126.20
24	c	511	CLA	C2D-C1D-ND	5.47	115.54	110.13
24	C	511	CLA	C2D-C1D-ND	5.47	115.54	110.13
27	b	620	SQD	O6-C1-C2	5.46	116.57	108.27
24	a	407	CLA	C2D-C1D-ND	5.46	115.53	110.13
24	C	510	CLA	O2D-CGD-CBD	5.46	120.77	111.23
24	B	610	CLA	O2D-CGD-CBD	5.45	120.76	111.23
26	Y	101	BCR	C33-C5-C6	-5.44	118.55	124.48
24	c	503	CLA	CHD-C4C-C3C	-5.43	116.86	124.77
24	b	614	CLA	C4A-NA-C1A	-5.43	104.20	106.68
24	B	613	CLA	C1-C2-C3	-5.40	117.35	126.20
24	b	605	CLA	O2D-CGD-CBD	5.39	120.66	111.23
24	C	504	CLA	CHD-C4C-C3C	-5.39	116.91	124.77
24	B	613	CLA	CHD-C4C-C3C	-5.39	116.92	124.77
25	A	408	PHO	C3D-C4D-ND	5.38	114.60	107.71
24	c	514	CLA	CMD-C2D-C1D	5.36	134.17	124.73
24	B	615	CLA	C4A-NA-C1A	-5.36	104.23	106.68
24	A	404	CLA	C2D-C1D-ND	5.35	115.42	110.13
24	B	614	CLA	C3D-C2D-C1D	-5.35	98.53	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	514	CLA	C3B-C2B-C1B	-5.34	100.87	107.17
27	a	409	SQD	O47-C7-C8	5.34	123.03	111.48
25	a	405	PHO	C3D-C4D-ND	5.33	114.55	107.71
24	d	403	CLA	O2D-CGD-CBD	5.33	120.55	111.23
24	c	511	CLA	C1-C2-C3	-5.33	117.46	126.20
24	A	406	CLA	C4A-NA-C1A	-5.33	104.25	106.68
24	B	605	CLA	O2D-CGD-CBD	5.33	120.54	111.23
24	A	405	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
24	d	403	CLA	C2B-C1B-NB	5.32	115.84	110.33
24	A	405	CLA	CMD-C2D-C1D	5.31	134.07	124.73
24	c	515	CLA	CHD-C4C-C3C	-5.30	117.05	124.77
24	B	614	CLA	C2B-C1B-NB	5.29	115.81	110.33
24	c	504	CLA	O2D-CGD-CBD	5.29	120.48	111.23
24	b	606	CLA	C2B-C1B-NB	5.27	115.79	110.33
31	A	416[A]	PL9	C7-C8-C9	-5.25	117.78	126.83
24	c	511	CLA	C4A-NA-C1A	-5.25	104.28	106.68
24	C	505	CLA	C2C-C1C-NC	5.24	115.49	109.98
24	b	607	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
24	C	505	CLA	CHD-C4C-C3C	-5.24	117.14	124.77
24	b	610	CLA	C2D-C1D-ND	5.23	115.30	110.13
24	c	508	CLA	CHD-C4C-C3C	-5.23	117.15	124.77
24	B	609	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
24	a	350	CLA	C4A-NA-C1A	-5.23	104.30	106.68
24	B	607	CLA	O2D-CGD-CBD	5.22	120.36	111.23
24	C	509	CLA	C2C-C1C-NC	5.22	115.46	109.98
27	F	101	SQD	O6-C1-C2	5.21	116.19	108.27
24	c	510	CLA	C2C-C1C-NC	5.21	115.45	109.98
24	B	611	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
24	b	613	CLA	C3B-C2B-C1B	-5.20	101.04	107.17
27	f	101	SQD	O47-C7-C8	5.20	122.73	111.48
24	c	515	CLA	C2B-C1B-NB	5.20	115.72	110.33
24	B	605	CLA	C4A-NA-C1A	-5.19	104.31	106.68
24	b	612	CLA	CMD-C2D-C1D	5.18	133.86	124.73
24	c	508	CLA	C2C-C1C-NC	5.18	115.42	109.98
24	b	610	CLA	C3B-C2B-C1B	-5.17	101.07	107.17
24	D	402	CLA	CHD-C4C-C3C	-5.17	117.23	124.77
24	C	504	CLA	C2B-C1B-NB	5.17	115.69	110.33
24	b	610	CLA	C1-C2-C3	-5.17	117.73	126.20
24	a	407	CLA	O2D-CGD-CBD	5.16	120.26	111.23
26	b	617	BCR	C7-C8-C9	-5.16	118.60	126.23
24	B	613	CLA	C2C-C1C-NC	5.16	115.41	109.98
24	b	612	CLA	C2D-C1D-ND	5.16	115.23	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	C2D-C1D-ND	5.15	115.23	110.13
24	c	512	CLA	C4A-NA-C1A	-5.15	104.33	106.68
24	B	614	CLA	C2C-C1C-NC	5.15	115.39	109.98
24	A	405	CLA	O2D-CGD-CBD	5.14	120.22	111.23
24	b	612	CLA	C2C-C1C-NC	5.13	115.37	109.98
24	c	509	CLA	C4A-NA-C1A	-5.13	104.34	106.68
24	c	510	CLA	CMD-C2D-C1D	5.13	133.76	124.73
35	C	523	HTG	C1-O5-C5	5.13	121.76	112.56
24	c	511	CLA	O2D-CGD-CBD	5.13	120.19	111.23
24	c	515	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
35	B	625	HTG	C1'-S1-C1	5.12	111.51	100.45
24	a	407	CLA	CMD-C2D-C1D	5.12	133.74	124.73
24	b	613	CLA	CMD-C2D-C1D	5.12	133.74	124.73
24	b	607	CLA	C4A-NA-C1A	-5.11	104.35	106.68
24	C	512	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
24	B	606	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
24	C	503	CLA	O2D-CGD-CBD	5.10	120.14	111.23
24	c	511	CLA	CHD-C4C-C3C	-5.09	117.34	124.77
41	V	203	HEC	CHC-C4B-NB	5.09	130.00	124.45
24	d	403	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
24	C	503	CLA	C4A-NA-C1A	-5.09	104.36	106.68
25	A	407	PHO	C3D-C4D-ND	5.08	114.21	107.71
24	b	606	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
24	D	402	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
24	B	611	CLA	O2D-CGD-CBD	5.04	120.04	111.23
24	b	601	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
41	V	203	HEC	CBB-CAB-C3B	-5.04	117.36	127.43
24	B	607	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
24	a	403	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
24	B	605	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
24	b	605	CLA	C2C-C1C-NC	5.03	115.27	109.98
24	b	607	CLA	C2C-C1C-NC	5.03	115.26	109.98
24	b	609	CLA	C2C-C1C-NC	5.03	115.26	109.98
24	B	601	CLA	C2B-C1B-NB	5.03	115.54	110.33
24	B	602	CLA	C2D-C1D-ND	5.02	115.10	110.13
24	A	405	CLA	C4A-NA-C1A	-5.02	104.39	106.68
24	c	503	CLA	C4A-NA-C1A	-5.02	104.39	106.68
26	y	101	BCR	C33-C5-C6	-5.01	119.01	124.48
24	B	615	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
24	C	513	CLA	C2B-C1B-NB	5.01	115.52	110.33
24	c	509	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
24	b	601	CLA	C4A-NA-C1A	-5.00	104.40	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	505	CLA	C2C-C1C-NC	5.00	115.23	109.98
24	c	513	CLA	O2D-CGD-CBD	5.00	119.96	111.23
24	B	612	CLA	C1-C2-C3	-4.98	118.03	126.20
24	b	615	CLA	C2C-C1C-NC	4.98	115.22	109.98
24	d	402	CLA	C2C-C1C-NC	4.96	115.20	109.98
24	a	403	CLA	CHD-C4C-C3C	-4.96	117.54	124.77
24	a	404	CLA	C3D-C4D-ND	4.96	118.05	109.99
24	b	605	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
24	C	513	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
24	D	403	CLA	C4A-NA-C1A	-4.95	104.42	106.68
24	A	406	CLA	C2B-C1B-NB	4.95	115.45	110.33
24	A	404	CLA	C3B-C2B-C1B	-4.94	101.34	107.17
24	C	507	CLA	C2D-C1D-ND	4.94	115.02	110.13
31	a	414[B]	PL9	C7-C3-C4	4.94	120.98	116.91
24	D	402	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
24	C	505	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
24	c	510	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
24	C	514	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
24	a	404	CLA	C4A-NA-C1A	-4.92	104.43	106.68
24	b	613	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
24	c	512	CLA	C2C-C1C-NC	4.92	115.15	109.98
24	b	616	CLA	C3D-C2D-C1D	-4.91	99.12	105.83
24	B	615	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
24	C	503	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
24	c	513	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
24	D	403	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
24	A	406	CLA	O2D-CGD-CBD	4.91	119.81	111.23
24	b	608	CLA	O2D-CGD-CBD	4.91	119.81	111.23
24	c	506	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
24	c	507	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
24	A	404	CLA	CAA-C2A-C3A	-4.89	99.77	113.00
24	B	603	CLA	C2C-C1C-NC	4.89	115.12	109.98
24	B	606	CLA	C2B-C1B-NB	4.89	115.40	110.33
24	B	607	CLA	C1C-C2C-C3C	-4.89	101.84	106.98
24	b	609	CLA	O2D-CGD-CBD	4.89	119.77	111.23
24	c	504	CLA	C2C-C1C-NC	4.89	115.11	109.98
35	h	101	HTG	C1'-S1-C1	4.88	110.99	100.45
24	B	610	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
24	A	409	CLA	C2B-C1B-NB	4.88	115.38	110.33
24	C	504	CLA	C2C-C1C-NC	4.88	115.10	109.98
24	A	409	CLA	C3D-C2D-C1D	-4.88	99.18	105.83
24	A	404	CLA	C2C-C1C-NC	4.88	115.10	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	409	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
24	C	506	CLA	C2D-C1D-ND	4.87	114.95	110.13
24	B	612	CLA	C2C-C1C-NC	4.87	115.10	109.98
24	a	404	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
24	C	507	CLA	CHD-C4C-C3C	-4.87	117.68	124.77
24	b	613	CLA	C2C-C1C-NC	4.86	115.09	109.98
24	d	403	CLA	C3D-C4D-ND	4.86	117.89	109.99
24	B	601	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
26	t	102	BCR	C33-C5-C6	-4.86	119.18	124.48
24	B	613	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
24	C	508	CLA	C2C-C1C-NC	4.85	115.08	109.98
24	C	507	CLA	O2D-CGD-CBD	4.85	119.71	111.23
24	c	506	CLA	O2D-CGD-CBD	4.85	119.70	111.23
24	A	406	CLA	C3B-C2B-C1B	-4.85	101.46	107.17
24	a	403	CLA	C2B-C1B-NB	4.84	115.35	110.33
24	C	510	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
24	c	507	CLA	C4A-NA-C1A	-4.84	104.47	106.68
24	a	407	CLA	C2B-C1B-NB	4.84	115.34	110.33
24	a	403	CLA	C2D-C1D-ND	4.84	114.91	110.13
24	a	404	CLA	C2B-C1B-NB	4.83	115.34	110.33
24	B	608	CLA	C2C-C1C-NC	4.83	115.06	109.98
24	b	614	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
24	B	602	CLA	C2B-C1B-NB	4.83	115.33	110.33
24	c	507	CLA	C3C-C4C-NC	4.82	116.61	110.43
24	c	504	CLA	C4A-NA-C1A	-4.82	104.48	106.68
24	b	605	CLA	C3D-C4D-ND	4.82	117.82	109.99
24	B	616	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
24	C	504	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
24	b	612	CLA	O2D-CGD-CBD	4.81	119.64	111.23
24	c	513	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
24	c	512	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
24	c	515	CLA	C3D-C4D-ND	4.80	117.79	109.99
24	C	511	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
24	B	616	CLA	C2B-C1B-NB	4.80	115.30	110.33
24	D	402	CLA	CHD-C1D-ND	-4.80	118.05	124.80
24	B	608	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
24	b	615	CLA	C2B-C1B-NB	4.80	115.30	110.33
24	A	409	CLA	C2C-C1C-NC	4.80	115.02	109.98
24	b	604	CLA	C2C-C1C-NC	4.79	115.01	109.98
24	D	403	CLA	O2D-CGD-CBD	4.79	119.60	111.23
24	c	515	CLA	C2C-C1C-NC	4.79	115.01	109.98
24	b	608	CLA	C3D-C2D-C1D	-4.78	99.30	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	506	CLA	C2C-C1C-NC	4.78	115.00	109.98
24	b	610	CLA	C4A-NA-C1A	-4.77	104.50	106.68
24	b	608	CLA	C4A-NA-C1A	-4.77	104.50	106.68
24	c	506	CLA	C3D-C4D-ND	4.77	117.74	109.99
24	C	512	CLA	C2B-C1B-NB	4.77	115.27	110.33
26	H	101	BCR	C11-C10-C9	-4.77	120.59	127.28
27	b	620	SQD	O47-C7-C8	4.77	121.79	111.48
24	a	403	CLA	C3B-C4B-NB	4.76	114.78	110.53
24	a	350	CLA	C3D-C4D-ND	4.76	117.73	109.99
24	C	508	CLA	C3B-C2B-C1B	-4.76	101.56	107.17
24	b	601	CLA	C2B-C1B-NB	4.76	115.26	110.33
24	c	511	CLA	C3B-C2B-C1B	-4.76	101.56	107.17
24	c	509	CLA	CHD-C1D-ND	-4.75	118.11	124.80
24	C	502	CLA	C3D-C4D-ND	4.75	117.71	109.99
24	B	601	CLA	C4A-NA-C1A	-4.75	104.51	106.68
24	B	602	CLA	C3B-C2B-C1B	-4.75	101.58	107.17
24	A	406	CLA	C3D-C4D-ND	4.74	117.70	109.99
24	b	602	CLA	C2B-C1B-NB	4.74	115.25	110.33
24	b	610	CLA	C2B-C1B-NB	4.74	115.24	110.33
24	b	616	CLA	C2B-C1B-NB	4.74	115.24	110.33
24	b	602	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
24	c	504	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
24	B	608	CLA	C2B-C1B-NB	4.74	115.24	110.33
24	c	511	CLA	C2C-C1C-NC	4.74	114.96	109.98
26	d	404	BCR	C15-C14-C13	-4.73	120.64	127.28
24	C	510	CLA	C2C-C1C-NC	4.73	114.95	109.98
24	B	612	CLA	C3D-C4D-ND	4.73	117.67	109.99
24	b	614	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
24	c	508	CLA	C4A-NA-C1A	-4.73	104.52	106.68
24	C	514	CLA	C2B-C1B-NB	4.73	115.23	110.33
24	C	505	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
24	b	603	CLA	C2C-C1C-NC	4.72	114.94	109.98
35	b	624	HTG	C1'-S1-C1	4.72	110.65	100.45
24	B	606	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
24	a	403	CLA	CAA-C2A-C3A	-4.72	100.26	113.00
24	B	611	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
24	B	611	CLA	C2C-C1C-NC	4.71	114.93	109.98
24	C	514	CLA	C3D-C4D-ND	4.71	117.65	109.99
26	c	517	BCR	C7-C8-C9	-4.71	119.26	126.23
24	b	603	CLA	C2B-C1B-NB	4.71	115.21	110.33
24	b	606	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
33	j	101	LMG	O7-C10-C11	4.70	121.65	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	604	CLA	C2C-C1C-NC	4.70	114.92	109.98
24	B	608	CLA	O2D-CGD-CBD	4.70	119.45	111.23
24	C	514	CLA	O2D-CGD-CBD	4.70	119.44	111.23
24	c	507	CLA	C2C-C1C-NC	4.70	114.92	109.98
24	b	615	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
24	c	503	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
24	a	403	CLA	C1C-C2C-C3C	-4.69	102.05	106.98
24	D	403	CLA	C2B-C1B-NB	4.68	115.18	110.33
24	B	603	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
24	a	350	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
24	b	608	CLA	C2C-C1C-NC	4.68	114.89	109.98
24	b	602	CLA	C3D-C4D-ND	4.67	117.59	109.99
24	b	615	CLA	C3B-C2B-C1B	-4.67	101.66	107.17
24	b	605	CLA	CHD-C1D-ND	-4.67	118.23	124.80
24	C	502	CLA	C2B-C1B-NB	4.67	115.17	110.33
24	C	512	CLA	C2C-C1C-NC	4.67	114.89	109.98
24	B	606	CLA	CHD-C1D-ND	-4.67	118.23	124.80
24	c	510	CLA	C2B-C1B-NB	4.67	115.17	110.33
24	B	613	CLA	CAC-C3C-C4C	4.67	130.86	124.79
24	c	510	CLA	C3B-C2B-C1B	-4.66	101.67	107.17
24	c	506	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
39	E	103	HEM	CHC-C4B-NB	4.66	129.44	124.42
24	a	404	CLA	C3B-C2B-C1B	-4.66	101.68	107.17
24	B	601	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
24	c	505	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
24	B	609	CLA	C2C-C1C-NC	4.65	114.87	109.98
24	c	512	CLA	C2B-C1B-NB	4.65	115.15	110.33
24	C	508	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
24	B	615	CLA	C2B-C1B-NB	4.65	115.14	110.33
24	c	506	CLA	C2B-C1B-NB	4.65	115.14	110.33
24	b	608	CLA	C3B-C2B-C1B	-4.64	101.69	107.17
24	C	509	CLA	C4A-NA-C1A	-4.64	104.56	106.68
24	B	608	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
41	v	203	HEC	CHC-C4B-NB	4.64	129.51	124.45
24	B	610	CLA	C4A-NA-C1A	-4.64	104.56	106.68
24	C	510	CLA	C4A-NA-C1A	-4.64	104.56	106.68
24	C	504	CLA	C3D-C4D-ND	4.64	117.53	109.99
24	c	511	CLA	C2B-C1B-NB	4.64	115.13	110.33
24	c	504	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
24	c	503	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
35	D	410	HTG	C1'-S1-C1	4.63	110.44	100.45
24	c	505	CLA	C2B-C1B-NB	4.62	115.12	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	C3D-C4D-ND	4.62	117.50	109.99
24	d	402	CLA	O2D-CGD-CBD	4.62	119.31	111.23
24	A	409	CLA	C3D-C4D-ND	4.62	117.50	109.99
24	b	603	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
24	b	605	CLA	C3B-C2B-C1B	-4.62	101.73	107.17
24	c	509	CLA	C2C-C1C-NC	4.61	114.83	109.98
24	B	613	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
24	B	611	CLA	C1-C2-C3	-4.61	118.65	126.20
24	b	611	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
24	c	506	CLA	CHD-C1D-ND	-4.60	118.32	124.80
24	C	504	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
24	A	409	CLA	O2D-CGD-CBD	4.60	119.27	111.23
24	A	404	CLA	C2B-C1B-NB	4.60	115.10	110.33
24	b	614	CLA	C2C-C1C-NC	4.60	114.81	109.98
24	B	603	CLA	C2B-C1B-NB	4.60	115.09	110.33
24	b	602	CLA	CHD-C1D-ND	-4.60	118.33	124.80
24	a	407	CLA	C2C-C1C-NC	4.59	114.81	109.98
24	a	350	CLA	C2B-C1B-NB	4.59	115.09	110.33
24	B	604	CLA	C3C-C4C-NC	4.59	116.31	110.43
33	Z	101	LMG	O7-C10-C11	4.59	121.41	111.48
24	C	506	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
31	D	405	PL9	C37-C38-C39	-4.59	117.12	127.62
24	C	503	CLA	C2C-C1C-NC	4.59	114.80	109.98
24	d	402	CLA	C4A-NA-C1A	-4.59	104.59	106.68
24	B	612	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
33	A	418	LMG	O7-C10-C11	4.58	121.39	111.48
24	b	610	CLA	C2C-C1C-NC	4.58	114.79	109.98
24	B	612	CLA	C3C-C4C-NC	4.58	116.29	110.43
24	C	510	CLA	C3D-C4D-ND	4.58	117.42	109.99
24	C	512	CLA	O2D-CGD-CBD	4.57	119.23	111.23
24	b	607	CLA	CHD-C1D-ND	-4.57	118.37	124.80
24	B	602	CLA	O2D-CGD-CBD	4.57	119.22	111.23
24	A	406	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
24	c	505	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
24	C	511	CLA	C1-C2-C3	-4.57	118.71	126.20
24	c	509	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
24	b	603	CLA	C3D-C4D-ND	4.57	117.41	109.99
24	c	503	CLA	C2B-C1B-NB	4.57	115.06	110.33
24	b	613	CLA	C2B-C1B-NB	4.56	115.06	110.33
24	b	601	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
24	b	614	CLA	C3D-C4D-ND	4.56	117.40	109.99
24	c	505	CLA	C1D-CHD-C4C	-4.55	116.34	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	C2B-C1B-NB	4.55	115.05	110.33
24	D	403	CLA	C3D-C4D-ND	4.55	117.38	109.99
24	c	505	CLA	C3D-C4D-ND	4.55	117.38	109.99
24	B	605	CLA	C2B-C1B-NB	4.55	115.04	110.33
24	B	615	CLA	O2D-CGD-CBD	4.55	119.18	111.23
24	C	505	CLA	C2B-C1B-NB	4.54	115.04	110.33
24	d	403	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
24	C	512	CLA	C3D-C4D-ND	4.54	117.36	109.99
24	B	607	CLA	C3D-C4D-ND	4.54	117.36	109.99
24	C	503	CLA	C2B-C1B-NB	4.54	115.03	110.33
24	A	405	CLA	C3B-C2B-C1B	-4.53	101.82	107.17
24	b	601	CLA	C2C-C1C-NC	4.53	114.74	109.98
24	c	508	CLA	C3D-C4D-ND	4.53	117.36	109.99
24	B	612	CLA	CMD-C2D-C1D	4.53	132.70	124.73
24	C	514	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	B	614	CLA	CHD-C1D-ND	-4.53	118.43	124.80
24	B	609	CLA	C3D-C4D-ND	4.52	117.34	109.99
24	c	504	CLA	C3D-C4D-ND	4.52	117.34	109.99
24	B	610	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
31	a	414[A]	PL9	C7-C3-C4	4.52	120.63	116.91
24	a	403	CLA	C3D-C4D-ND	4.51	117.33	109.99
24	c	513	CLA	C3D-C4D-ND	4.51	117.33	109.99
27	a	409	SQD	C1-O5-C5	-4.51	104.91	113.72
24	d	402	CLA	C3B-C2B-C1B	-4.51	101.85	107.17
24	a	407	CLA	C3B-C2B-C1B	-4.51	101.85	107.17
24	b	608	CLA	C2B-C1B-NB	4.51	115.00	110.33
24	D	402	CLA	C1-C2-C3	-4.51	118.81	126.20
24	b	609	CLA	C3D-C4D-ND	4.51	117.32	109.99
24	C	503	CLA	C1-C2-C3	-4.51	118.81	126.20
24	A	405	CLA	C2B-C1B-NB	4.50	114.99	110.33
24	C	503	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
24	b	615	CLA	C3D-C4D-ND	4.50	117.30	109.99
24	C	510	CLA	C1-C2-C3	-4.50	118.83	126.20
24	C	502	CLA	C3B-C2B-C1B	-4.50	101.87	107.17
24	b	611	CLA	C3D-C4D-ND	4.50	117.29	109.99
24	C	502	CLA	C2C-C1C-NC	4.49	114.69	109.98
24	c	514	CLA	C3D-C4D-ND	4.48	117.27	109.99
24	C	511	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
24	b	602	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
24	A	406	CLA	CHD-C1D-ND	-4.48	118.50	124.80
24	c	515	CLA	O2D-CGD-CBD	4.48	119.06	111.23
24	c	515	CLA	C3D-C2D-C1D	-4.48	99.72	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	507	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
24	C	507	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
24	d	403	CLA	CHD-C1D-ND	-4.47	118.51	124.80
24	b	609	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
24	C	506	CLA	C2C-C1C-NC	4.47	114.67	109.98
24	C	507	CLA	C1C-C2C-C3C	-4.47	102.28	106.98
24	d	402	CLA	C3D-C4D-ND	4.47	117.25	109.99
26	T	101	BCR	C15-C16-C17	-4.47	114.38	123.52
24	c	512	CLA	C1-C2-C3	-4.47	118.88	126.20
24	B	610	CLA	C2B-C1B-NB	4.47	114.96	110.33
24	c	515	CLA	CHD-C1D-ND	-4.46	118.52	124.80
24	D	402	CLA	C1C-C2C-C3C	-4.46	102.29	106.98
24	b	604	CLA	C1-C2-C3	-4.46	118.89	126.20
24	b	614	CLA	C2B-C1B-NB	4.46	114.95	110.33
24	c	514	CLA	C2C-C1C-NC	4.46	114.67	109.98
24	b	611	CLA	C1-C2-C3	-4.46	118.89	126.20
24	c	503	CLA	C3D-C4D-ND	4.46	117.23	109.99
24	C	509	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
24	C	509	CLA	C3D-C4D-ND	4.45	117.22	109.99
35	B	624	HTG	C1'-S1-C1	4.45	110.05	100.45
24	c	510	CLA	C3D-C4D-ND	4.45	117.21	109.99
24	C	507	CLA	C2B-C1B-NB	4.45	114.94	110.33
24	C	511	CLA	C2B-C1B-NB	4.44	114.93	110.33
24	b	606	CLA	C2C-C1C-NC	4.44	114.64	109.98
24	c	503	CLA	CHD-C1D-ND	-4.44	118.56	124.80
24	a	350	CLA	CHD-C1D-ND	-4.44	118.56	124.80
24	B	602	CLA	C3D-C4D-ND	4.43	117.20	109.99
24	D	403	CLA	C3B-C2B-C1B	-4.43	101.94	107.17
24	C	514	CLA	C4A-NA-C1A	-4.43	104.66	106.68
24	a	404	CLA	CHD-C1D-ND	-4.43	118.57	124.80
24	c	503	CLA	C2C-C1C-NC	4.43	114.63	109.98
24	B	613	CLA	C3D-C4D-ND	4.43	117.18	109.99
24	B	605	CLA	C1D-CHD-C4C	-4.42	116.61	126.02
24	B	601	CLA	C3D-C4D-ND	4.42	117.18	109.99
24	a	407	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
24	a	404	CLA	C2C-C1C-NC	4.42	114.62	109.98
24	C	504	CLA	CHD-C1D-ND	-4.42	118.58	124.80
24	C	506	CLA	C3C-C4C-NC	4.42	116.09	110.43
24	B	609	CLA	CHD-C1D-ND	-4.42	118.58	124.80
24	c	510	CLA	C1C-C2C-C3C	-4.42	102.34	106.98
24	B	608	CLA	C3D-C4D-ND	4.42	117.16	109.99
24	B	605	CLA	C3D-C4D-ND	4.41	117.16	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	508	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
24	B	610	CLA	C2C-C1C-NC	4.41	114.61	109.98
24	B	605	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
27	A	411	SQD	C1-O5-C5	-4.41	105.11	113.72
24	B	616	CLA	C3B-C2B-C1B	-4.40	101.98	107.17
26	b	617	BCR	C33-C5-C6	-4.40	119.68	124.48
27	B	620	SQD	O6-C1-C2	4.40	114.96	108.27
24	C	502	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
24	B	614	CLA	C4A-NA-C1A	-4.40	104.67	106.68
24	C	507	CLA	CHD-C1D-ND	-4.40	118.61	124.80
24	C	509	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
24	B	615	CLA	C3D-C4D-ND	4.40	117.13	109.99
24	C	511	CLA	C3D-C4D-ND	4.39	117.13	109.99
24	C	509	CLA	C3C-C4C-NC	4.39	116.06	110.43
24	b	601	CLA	C3D-C4D-ND	4.39	117.13	109.99
27	A	411	SQD	O47-C7-C8	4.39	120.98	111.48
26	d	404	BCR	C38-C26-C25	-4.39	119.69	124.48
24	A	404	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
33	C	520	LMG	O7-C10-C11	4.38	120.97	111.48
24	b	603	CLA	C1D-CHD-C4C	-4.38	116.70	126.02
24	B	614	CLA	C3D-C4D-ND	4.38	117.11	109.99
24	B	613	CLA	C2B-C1B-NB	4.38	114.87	110.33
24	b	605	CLA	C2B-C1B-NB	4.38	114.87	110.33
24	C	510	CLA	C2B-C1B-NB	4.38	114.87	110.33
24	B	615	CLA	C1D-CHD-C4C	-4.38	116.71	126.02
24	A	405	CLA	C3D-C4D-ND	4.38	117.11	109.99
24	b	615	CLA	CHD-C1D-ND	-4.38	118.64	124.80
31	A	416[B]	PL9	C7-C3-C4	4.38	120.52	116.91
24	c	512	CLA	O2D-CGD-CBD	4.38	118.88	111.23
24	a	403	CLA	C1D-CHD-C4C	-4.37	116.72	126.02
24	C	505	CLA	C3D-C4D-ND	4.37	117.09	109.99
24	b	611	CLA	C2B-C1B-NB	4.37	114.85	110.33
24	B	609	CLA	C3C-C4C-NC	4.36	116.02	110.43
27	B	620	SQD	O47-C7-C8	4.36	120.92	111.48
24	b	607	CLA	C3D-C4D-ND	4.36	117.08	109.99
24	C	511	CLA	C2C-C1C-NC	4.36	114.56	109.98
24	c	513	CLA	CHD-C1D-ND	-4.36	118.67	124.80
24	B	614	CLA	C1C-C2C-C3C	-4.36	102.40	106.98
24	d	402	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
24	B	611	CLA	C1D-CHD-C4C	-4.35	116.77	126.02
24	B	609	CLA	O2D-CGD-CBD	4.35	118.83	111.23
24	D	402	CLA	C3D-C4D-ND	4.34	117.05	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	C1D-CHD-C4C	-4.34	116.79	126.02
24	B	607	CLA	CHD-C1D-ND	-4.34	118.69	124.80
24	C	513	CLA	C3D-C4D-ND	4.34	117.05	109.99
24	c	511	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
24	c	511	CLA	C3D-C4D-ND	4.34	117.04	109.99
24	B	614	CLA	O2D-CGD-O1D	-4.33	115.41	123.85
24	b	604	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
35	c	523	HTG	C1'-S1-C1	4.33	109.80	100.45
24	C	510	CLA	C3D-C2D-C1D	-4.33	99.93	105.83
24	C	502	CLA	CHD-C1D-ND	-4.32	118.72	124.80
24	b	608	CLA	C3D-C4D-ND	4.32	117.01	109.99
24	c	507	CLA	C3D-C4D-ND	4.32	117.01	109.99
24	C	512	CLA	C3D-C2D-C1D	-4.32	99.94	105.83
24	C	503	CLA	C3D-C4D-ND	4.32	117.01	109.99
26	K	102	BCR	C24-C23-C22	-4.31	119.85	126.23
24	C	513	CLA	C3D-C2D-C1D	-4.31	99.94	105.83
24	c	514	CLA	C3D-C2D-C1D	-4.31	99.94	105.83
24	A	404	CLA	C3D-C4D-ND	4.31	116.99	109.99
24	B	606	CLA	C3C-C4C-NC	4.31	115.95	110.43
24	B	603	CLA	C3D-C4D-ND	4.31	116.99	109.99
24	B	610	CLA	C3D-C4D-ND	4.31	116.99	109.99
26	B	617	BCR	C7-C8-C9	-4.31	119.86	126.23
24	B	605	CLA	C3C-C4C-NC	4.30	115.94	110.43
24	b	610	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
24	B	616	CLA	C3D-C4D-ND	4.30	116.98	109.99
24	b	612	CLA	C3B-C2B-C1B	-4.29	102.11	107.17
24	B	603	CLA	C3D-C2D-C1D	-4.29	99.97	105.83
24	b	616	CLA	C3B-C2B-C1B	-4.29	102.11	107.17
24	B	611	CLA	C3B-C4B-NB	4.29	114.36	110.53
38	E	101	LHG	O7-C7-C8	4.29	120.76	111.48
24	c	505	CLA	O2D-CGD-CBD	4.29	118.73	111.23
24	b	616	CLA	C1D-CHD-C4C	-4.28	116.92	126.02
24	d	402	CLA	C3C-C4C-NC	4.28	115.92	110.43
24	b	604	CLA	C3C-C4C-NC	4.28	115.91	110.43
24	D	402	CLA	C2B-C1B-NB	4.28	114.76	110.33
24	b	607	CLA	C3B-C4B-NB	4.27	114.35	110.53
24	B	615	CLA	C3C-C4C-NC	4.27	115.90	110.43
24	c	512	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
24	a	350	CLA	C3B-C2B-C1B	-4.27	102.13	107.17
24	A	409	CLA	CHD-C1D-ND	-4.27	118.79	124.80
24	B	602	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
24	b	611	CLA	CHD-C1D-ND	-4.27	118.79	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	613	CLA	C4A-NA-C1A	-4.27	104.73	106.68
24	c	509	CLA	C3D-C4D-ND	4.27	116.92	109.99
35	c	526	HTG	C1'-S1-C1	4.27	109.66	100.45
24	C	514	CLA	CHD-C1D-ND	-4.26	118.80	124.80
24	b	607	CLA	O2D-CGD-CBD	4.26	118.68	111.23
24	B	607	CLA	C4A-NA-C1A	-4.26	104.73	106.68
24	c	509	CLA	C2B-C1B-NB	4.26	114.74	110.33
24	c	509	CLA	C1C-C2C-C3C	-4.25	102.51	106.98
24	C	505	CLA	C1C-C2C-C3C	-4.25	102.52	106.98
24	b	601	CLA	C1D-CHD-C4C	-4.24	117.00	126.02
24	c	513	CLA	C2B-C1B-NB	4.24	114.72	110.33
24	b	612	CLA	C3D-C4D-ND	4.24	116.88	109.99
35	C	522	HTG	C1'-S1-C1	4.24	109.60	100.45
24	C	514	CLA	C2C-C1C-NC	4.24	114.43	109.98
26	c	516	BCR	C15-C14-C13	-4.24	121.33	127.28
24	b	608	CLA	C1-C2-C3	-4.23	119.27	126.20
24	B	604	CLA	C3B-C2B-C1B	-4.23	102.19	107.17
24	b	603	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
24	c	504	CLA	C2B-C1B-NB	4.22	114.70	110.33
24	b	613	CLA	C3C-C4C-NC	4.22	115.83	110.43
24	B	605	CLA	C4-C3-C5	4.22	122.55	115.23
24	B	604	CLA	C3D-C2D-C1D	-4.22	100.08	105.83
26	k	101	BCR	C29-C30-C25	4.22	116.56	110.44
24	B	607	CLA	CMB-C2B-C1B	4.21	131.84	125.42
24	C	510	CLA	CHD-C1D-ND	-4.21	118.88	124.80
39	e	102	HEM	CHC-C4B-NB	4.21	128.95	124.42
24	C	507	CLA	C3D-C4D-ND	4.20	116.82	109.99
24	A	405	CLA	C1D-CHD-C4C	-4.20	117.09	126.02
24	D	403	CLA	CHD-C1D-ND	-4.19	118.90	124.80
24	b	606	CLA	CHD-C1D-ND	-4.19	118.90	124.80
24	C	512	CLA	CAC-C3C-C4C	4.19	130.24	124.79
24	b	611	CLA	C2C-C1C-NC	4.19	114.38	109.98
27	A	411	SQD	C1-C2-C3	-4.19	101.20	110.01
24	C	502	CLA	O2D-CGD-O1D	-4.18	115.70	123.85
24	a	350	CLA	O2D-CGD-CBD	4.18	118.54	111.23
24	C	506	CLA	C3D-C4D-ND	4.18	116.78	109.99
24	B	605	CLA	C2C-C1C-NC	4.17	114.37	109.98
24	c	512	CLA	C3B-C4B-NB	4.17	114.26	110.53
24	C	511	CLA	C1D-CHD-C4C	-4.17	117.16	126.02
24	a	350	CLA	C2C-C1C-NC	4.17	114.36	109.98
24	b	608	CLA	CHD-C1D-ND	-4.17	118.94	124.80
24	B	603	CLA	C1C-C2C-C3C	-4.16	102.60	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	C3D-C4D-ND	4.16	116.75	109.99
24	c	512	CLA	C1C-C2C-C3C	-4.16	102.60	106.98
24	B	601	CLA	C1D-CHD-C4C	-4.16	117.19	126.02
24	c	513	CLA	C2C-C1C-NC	4.15	114.35	109.98
24	B	604	CLA	C1D-CHD-C4C	-4.15	117.19	126.02
24	a	404	CLA	O2D-CGD-CBD	4.15	118.49	111.23
31	a	414[B]	PL9	C7-C3-C2	-4.15	118.50	123.39
24	B	607	CLA	C3B-C2B-C1B	-4.15	102.28	107.17
26	B	617	BCR	C33-C5-C6	-4.15	119.96	124.48
24	b	612	CLA	C3B-C4B-NB	4.14	114.23	110.53
33	C	521	LMG	O7-C10-C11	4.14	120.44	111.48
24	C	506	CLA	C2B-C1B-NB	4.14	114.61	110.33
24	B	612	CLA	C3D-C2D-C1D	-4.14	100.19	105.83
24	b	607	CLA	C3C-C4C-NC	4.13	115.73	110.43
24	b	612	CLA	C1D-CHD-C4C	-4.13	117.24	126.02
24	C	505	CLA	C3B-C4B-NB	4.13	114.21	110.53
24	C	513	CLA	C2C-C1C-NC	4.12	114.31	109.98
24	B	603	CLA	C4-C3-C5	4.12	122.38	115.23
24	A	406	CLA	C1-C2-C3	-4.12	119.45	126.20
24	B	606	CLA	C3D-C4D-ND	4.12	116.68	109.99
24	c	508	CLA	C2B-C1B-NB	4.11	114.59	110.33
24	c	506	CLA	C1C-C2C-C3C	-4.11	102.66	106.98
24	b	609	CLA	C1-C2-C3	-4.10	119.47	126.20
31	A	416[B]	PL9	C7-C3-C2	-4.10	118.56	123.39
26	C	515	BCR	C7-C8-C9	-4.09	120.18	126.23
24	A	404	CLA	C1D-CHD-C4C	-4.09	117.32	126.02
31	a	414[A]	PL9	C32-C33-C34	-4.09	118.26	127.62
24	c	506	CLA	C4A-NA-C1A	-4.09	104.81	106.68
24	A	409	CLA	C1-C2-C3	-4.09	119.50	126.20
24	C	509	CLA	C1D-CHD-C4C	-4.09	117.34	126.02
24	b	603	CLA	C3C-C4C-NC	4.08	115.66	110.43
24	C	512	CLA	C4A-NA-C1A	-4.08	104.82	106.68
24	b	614	CLA	C3C-C4C-NC	4.08	115.66	110.43
24	B	615	CLA	C2C-C1C-NC	4.08	114.27	109.98
24	C	505	CLA	CHD-C1D-ND	-4.08	119.06	124.80
26	c	516	BCR	C11-C10-C9	-4.08	121.56	127.28
39	E	103	HEM	CAD-CBD-CGD	4.08	124.48	113.67
24	B	615	CLA	CHD-C1D-ND	-4.08	119.06	124.80
24	a	407	CLA	C3D-C4D-ND	4.07	116.61	109.99
24	A	404	CLA	O2A-CGA-CBA	4.07	124.24	111.83
24	b	614	CLA	CHD-C1D-ND	-4.07	119.08	124.80
24	b	613	CLA	C3D-C4D-ND	4.07	116.60	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	404	BCR	C24-C23-C22	-4.07	120.22	126.23
24	B	612	CLA	C4A-NA-C1A	-4.06	104.83	106.68
24	B	615	CLA	CMB-C2B-C1B	4.06	131.60	125.42
24	B	606	CLA	C1D-CHD-C4C	-4.06	117.39	126.02
26	K	102	BCR	C3-C4-C5	-4.06	106.82	114.06
24	A	405	CLA	CHD-C1D-ND	-4.06	119.09	124.80
24	a	350	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
24	b	607	CLA	C3B-C2B-C1B	-4.06	102.39	107.17
24	c	507	CLA	CMB-C2B-C1B	4.06	131.60	125.42
24	c	507	CLA	C2B-C1B-NB	4.06	114.53	110.33
24	A	405	CLA	C2C-C1C-NC	4.06	114.24	109.98
24	B	616	CLA	CHD-C1D-ND	-4.05	119.10	124.80
24	B	602	CLA	C2C-C1C-NC	4.05	114.23	109.98
24	A	406	CLA	CMB-C2B-C1B	4.05	131.58	125.42
24	B	602	CLA	CHD-C1D-ND	-4.04	119.11	124.80
24	b	613	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
24	c	508	CLA	C3B-C4B-NB	4.04	114.13	110.53
31	A	416[A]	PL9	C37-C38-C39	-4.04	118.38	127.62
24	c	503	CLA	O2D-CGD-O1D	-4.03	116.00	123.85
24	b	616	CLA	C3C-C4C-NC	4.03	115.60	110.43
24	A	406	CLA	C2C-C1C-NC	4.03	114.21	109.98
24	d	402	CLA	C2B-C1B-NB	4.03	114.50	110.33
24	A	409	CLA	C3B-C4B-NB	4.03	114.12	110.53
24	b	610	CLA	O2A-CGA-CBA	4.02	124.11	111.83
24	b	604	CLA	C3D-C4D-ND	4.02	116.53	109.99
26	D	404	BCR	C38-C26-C25	-4.02	120.09	124.48
24	C	508	CLA	C1D-CHD-C4C	-4.02	117.47	126.02
24	B	616	CLA	C3C-C4C-NC	4.02	115.58	110.43
24	C	509	CLA	C1-C2-C3	-4.02	119.62	126.20
24	c	511	CLA	C3B-C4B-NB	4.02	114.11	110.53
24	D	403	CLA	C3C-C4C-NC	4.01	115.57	110.43
24	A	404	CLA	CHD-C1D-ND	-4.01	119.15	124.80
24	a	350	CLA	C1D-CHD-C4C	-4.01	117.49	126.02
24	B	612	CLA	C3B-C4B-NB	4.01	114.11	110.53
24	C	513	CLA	C3C-C4C-NC	4.01	115.56	110.43
24	b	609	CLA	CHD-C1D-ND	-4.01	119.16	124.80
24	C	508	CLA	C3C-C4C-NC	4.01	115.56	110.43
24	c	508	CLA	CHD-C1D-ND	-4.01	119.16	124.80
31	A	416[A]	PL9	C7-C3-C2	-4.01	118.67	123.39
24	B	606	CLA	O2D-CGD-O1D	-4.00	116.05	123.85
24	b	612	CLA	C1-C2-C3	-4.00	119.64	126.20
24	B	604	CLA	C3D-C4D-ND	4.00	116.49	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	414[A]	PL9	C7-C3-C2	-4.00	118.67	123.39
26	c	516	BCR	C20-C21-C22	-4.00	121.67	127.28
24	b	606	CLA	C3D-C4D-ND	4.00	116.49	109.99
41	v	203	HEC	CBB-CAB-C3B	-4.00	119.44	127.43
24	c	508	CLA	C1C-C2C-C3C	-4.00	102.78	106.98
24	b	605	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
24	B	603	CLA	C1D-CHD-C4C	-3.99	117.54	126.02
24	b	612	CLA	C3C-C4C-NC	3.99	115.54	110.43
24	c	508	CLA	O2D-CGD-CBD	3.99	118.20	111.23
38	D	357	LHG	O7-C7-C8	3.99	120.11	111.48
24	c	507	CLA	C3D-C2D-C1D	-3.99	100.39	105.83
24	c	510	CLA	C4A-NA-C1A	-3.98	104.86	106.68
24	b	606	CLA	C1D-CHD-C4C	-3.98	117.55	126.02
24	a	407	CLA	C1D-CHD-C4C	-3.98	117.56	126.02
24	c	504	CLA	C1C-C2C-C3C	-3.98	102.79	106.98
24	B	612	CLA	C2B-C1B-NB	3.98	114.45	110.33
24	c	504	CLA	CHD-C1D-ND	-3.97	119.21	124.80
24	B	611	CLA	C3D-C4D-ND	3.97	116.44	109.99
24	C	502	CLA	C1D-CHD-C4C	-3.97	117.58	126.02
24	B	609	CLA	C2B-C1B-NB	3.97	114.44	110.33
24	c	510	CLA	C3C-C4C-NC	3.96	115.51	110.43
24	B	611	CLA	C3C-C4C-NC	3.96	115.50	110.43
31	A	416[B]	PL9	C7-C8-C9	-3.96	120.01	126.83
24	B	608	CLA	C3C-C4C-NC	3.96	115.50	110.43
24	B	616	CLA	C1D-CHD-C4C	-3.96	117.60	126.02
38	d	408	LHG	O7-C7-C8	3.96	120.05	111.48
31	a	414[A]	PL9	C22-C23-C24	-3.96	118.57	127.62
24	c	508	CLA	C1-C2-C3	-3.95	119.72	126.20
34	I	101	LMT	C1'-O5'-C5'	3.95	121.44	113.72
24	c	512	CLA	CHD-C1D-ND	-3.95	119.24	124.80
24	c	513	CLA	C4A-NA-C1A	-3.95	104.88	106.68
24	b	604	CLA	CMB-C2B-C1B	3.95	131.43	125.42
24	C	503	CLA	C1D-CHD-C4C	-3.95	117.63	126.02
24	c	511	CLA	CAC-C3C-C4C	3.95	129.92	124.79
24	C	504	CLA	C1D-CHD-C4C	-3.94	117.64	126.02
24	A	405	CLA	C1C-C2C-C3C	-3.94	102.83	106.98
24	b	615	CLA	O2D-CGD-CBD	3.94	118.12	111.23
24	D	402	CLA	C3B-C4B-NB	3.94	114.05	110.53
24	B	608	CLA	C3B-C4B-NB	3.94	114.05	110.53
24	C	514	CLA	C3C-C4C-NC	3.94	115.47	110.43
24	C	514	CLA	C1-C2-C3	-3.93	119.75	126.20
24	d	402	CLA	C1-C2-C3	-3.93	119.75	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	C1D-CHD-C4C	-3.93	117.66	126.02
24	c	507	CLA	C1D-CHD-C4C	-3.93	117.66	126.02
24	c	514	CLA	C1D-CHD-C4C	-3.93	117.66	126.02
24	a	350	CLA	CBC-CAC-C3C	-3.93	101.76	112.42
24	C	511	CLA	CHD-C1D-ND	-3.93	119.27	124.80
35	C	523	HTG	C1'-S1-C1	3.93	108.94	100.45
33	c	522	LMG	O7-C10-C11	3.93	119.98	111.48
24	b	606	CLA	C3C-C4C-NC	3.93	115.46	110.43
24	B	608	CLA	C1C-C2C-C3C	-3.93	102.85	106.98
24	B	612	CLA	O2D-CGD-O1D	-3.93	116.20	123.85
24	c	512	CLA	C1D-CHD-C4C	-3.93	117.67	126.02
33	c	521	LMG	O7-C10-C11	3.92	119.97	111.48
24	D	402	CLA	O2D-CGD-CBD	3.92	118.09	111.23
24	b	601	CLA	CHD-C1D-ND	-3.92	119.29	124.80
24	B	613	CLA	C1C-C2C-C3C	-3.92	102.86	106.98
24	A	405	CLA	CMC-C2C-C1C	3.92	131.15	125.03
24	C	508	CLA	C2B-C1B-NB	3.91	114.38	110.33
24	B	608	CLA	C4A-NA-C1A	-3.91	104.90	106.68
24	C	508	CLA	C3D-C4D-ND	3.90	116.33	109.99
24	B	608	CLA	C1D-CHD-C4C	-3.90	117.73	126.02
24	B	611	CLA	O2D-CGD-O1D	-3.90	116.26	123.85
24	C	509	CLA	C2B-C1B-NB	3.90	114.37	110.33
24	b	616	CLA	C3D-C4D-ND	3.90	116.32	109.99
24	A	404	CLA	C3C-C4C-NC	3.90	115.42	110.43
24	c	515	CLA	C1D-CHD-C4C	-3.90	117.74	126.02
24	B	613	CLA	C3C-C4C-NC	3.90	115.42	110.43
35	b	623	HTG	C1-O5-C5	3.89	119.54	112.56
24	c	508	CLA	C3B-C2B-C1B	-3.89	102.58	107.17
26	T	101	BCR	C11-C10-C9	-3.89	121.83	127.28
24	a	403	CLA	C3D-C2D-C1D	-3.89	100.53	105.83
33	a	417	LMG	O7-C10-C11	3.88	119.88	111.48
24	c	505	CLA	C3C-C4C-NC	3.88	115.40	110.43
24	b	605	CLA	O2D-CGD-O1D	-3.88	116.29	123.85
24	b	612	CLA	C3D-C2D-C1D	-3.88	100.53	105.83
24	b	608	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
26	b	619	BCR	C15-C14-C13	-3.88	121.84	127.28
24	c	505	CLA	CHD-C1D-ND	-3.87	119.35	124.80
31	D	405	PL9	C42-C43-C44	-3.87	118.76	127.62
24	C	512	CLA	CHD-C1D-ND	-3.87	119.36	124.80
24	a	404	CLA	C1D-CHD-C4C	-3.87	117.80	126.02
27	a	409	SQD	C45-O47-C7	-3.87	108.54	117.80
24	B	606	CLA	C2C-C1C-NC	3.87	114.04	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	407	CLA	C3C-C4C-NC	3.86	115.38	110.43
24	c	508	CLA	C1D-CHD-C4C	-3.86	117.82	126.02
24	B	610	CLA	C3C-C4C-NC	3.86	115.37	110.43
39	e	102	HEM	CHD-C4C-NC	3.86	128.65	124.45
26	C	515	BCR	C15-C14-C13	-3.86	121.87	127.28
24	B	603	CLA	C3C-C4C-NC	3.86	115.37	110.43
24	B	608	CLA	CHD-C1D-ND	-3.86	119.38	124.80
24	b	614	CLA	O2D-CGD-O1D	-3.85	116.35	123.85
24	A	405	CLA	C3C-C4C-NC	3.85	115.36	110.43
24	c	511	CLA	C1D-CHD-C4C	-3.85	117.84	126.02
24	C	503	CLA	C3C-C4C-NC	3.85	115.36	110.43
24	c	506	CLA	C3B-C4B-NB	3.85	113.97	110.53
24	b	613	CLA	C1D-CHD-C4C	-3.85	117.84	126.02
24	B	613	CLA	C3B-C4B-NB	3.85	113.96	110.53
24	B	604	CLA	C1C-C2C-C3C	-3.84	102.94	106.98
24	C	508	CLA	C4A-NA-C1A	-3.84	104.93	106.68
26	K	102	BCR	C7-C8-C9	-3.84	120.55	126.23
24	B	601	CLA	C3C-C4C-NC	3.84	115.35	110.43
24	B	613	CLA	CMC-C2C-C1C	3.83	131.02	125.03
31	a	414[A]	PL9	C7-C8-C9	-3.83	120.23	126.83
24	A	405	CLA	CHD-C4C-NC	3.83	130.17	124.23
24	b	604	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
24	C	508	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
26	y	101	BCR	C38-C26-C25	-3.83	120.31	124.48
24	A	409	CLA	C3C-C4C-NC	3.82	115.33	110.43
24	c	504	CLA	C1D-CHD-C4C	-3.82	117.90	126.02
24	B	603	CLA	CHD-C1D-ND	-3.82	119.43	124.80
26	t	102	BCR	C11-C10-C9	-3.82	121.92	127.28
24	B	614	CLA	C1D-CHD-C4C	-3.81	117.91	126.02
36	C	517	DGD	O2G-C1B-C2B	3.81	119.73	111.48
24	C	503	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
24	b	610	CLA	C3C-C4C-NC	3.81	115.31	110.43
24	b	611	CLA	C3C-C4C-NC	3.81	115.31	110.43
24	b	616	CLA	C2C-C1C-NC	3.81	113.98	109.98
24	B	601	CLA	C2C-C1C-NC	3.81	113.98	109.98
24	C	512	CLA	C3C-C4C-NC	3.81	115.31	110.43
24	b	605	CLA	C1D-CHD-C4C	-3.80	117.93	126.02
26	A	410	BCR	C15-C14-C13	-3.80	121.94	127.28
24	B	612	CLA	C1D-CHD-C4C	-3.80	117.94	126.02
24	c	514	CLA	C1-C2-C3	-3.80	119.97	126.20
24	a	407	CLA	CAA-C2A-C3A	-3.80	102.74	113.00
24	C	513	CLA	C1-C2-C3	-3.80	119.97	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	604	CLA	C3B-C2B-C1B	-3.80	102.69	107.17
24	b	611	CLA	C1D-CHD-C4C	-3.79	117.95	126.02
31	A	416[A]	PL9	C32-C33-C34	-3.79	118.94	127.62
24	C	506	CLA	C3D-C2D-C1D	-3.79	100.66	105.83
24	B	601	CLA	CHD-C1D-ND	-3.79	119.47	124.80
24	C	508	CLA	CHD-C1D-ND	-3.79	119.47	124.80
33	B	621	LMG	O7-C10-C11	3.79	119.67	111.48
24	b	612	CLA	C2B-C1B-NB	3.79	114.25	110.33
24	a	407	CLA	C3B-C4B-NB	3.78	113.91	110.53
24	B	610	CLA	CHD-C1D-ND	-3.78	119.48	124.80
39	E	103	HEM	CHD-C4C-NC	3.78	128.57	124.45
24	A	409	CLA	C1D-CHD-C4C	-3.78	117.98	126.02
24	c	510	CLA	C1D-CHD-C4C	-3.78	117.98	126.02
24	a	407	CLA	C4-C3-C5	3.78	121.79	115.23
25	A	407	PHO	CMA-C3A-C4A	-3.78	106.47	114.61
24	A	405	CLA	CBC-CAC-C3C	-3.78	102.18	112.42
24	C	512	CLA	C1D-CHD-C4C	-3.77	118.00	126.02
24	b	609	CLA	C3B-C2B-C1B	-3.77	102.72	107.17
24	b	615	CLA	C1D-CHD-C4C	-3.77	118.00	126.02
24	B	605	CLA	CMB-C2B-C1B	3.77	131.16	125.42
24	B	602	CLA	C3C-C4C-NC	3.77	115.26	110.43
24	B	607	CLA	C2B-C1B-NB	3.77	114.23	110.33
24	B	611	CLA	C1C-C2C-C3C	-3.77	103.02	106.98
27	a	409	SQD	C1-C2-C3	-3.77	102.08	110.01
24	b	602	CLA	C3C-C4C-NC	3.77	115.25	110.43
24	b	603	CLA	C1C-C2C-C3C	-3.76	103.02	106.98
36	c	518	DGD	O2G-C1B-C2B	3.76	119.62	111.48
24	C	514	CLA	C1D-CHD-C4C	-3.76	118.03	126.02
24	B	613	CLA	CHD-C1D-ND	-3.76	119.51	124.80
24	C	510	CLA	C3C-C4C-NC	3.76	115.25	110.43
26	C	516	BCR	C11-C10-C9	-3.76	122.01	127.28
24	B	605	CLA	O2D-CGD-O1D	-3.76	116.53	123.85
24	C	505	CLA	C1D-CHD-C4C	-3.75	118.04	126.02
24	c	511	CLA	CHD-C1D-ND	-3.75	119.52	124.80
24	c	514	CLA	CHD-C1D-ND	-3.75	119.52	124.80
24	c	513	CLA	C1-C2-C3	-3.75	120.05	126.20
24	b	610	CLA	C1D-CHD-C4C	-3.75	118.05	126.02
24	b	610	CLA	CHD-C1D-ND	-3.74	119.53	124.80
24	D	402	CLA	C3C-C4C-NC	3.74	115.22	110.43
33	b	621	LMG	O7-C10-C11	3.74	119.57	111.48
24	b	609	CLA	C3C-C4C-NC	3.74	115.22	110.43
24	c	504	CLA	C3C-C4C-NC	3.74	115.22	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	509	CLA	O2D-CGD-O1D	-3.74	116.57	123.85
24	C	508	CLA	O2D-CGD-O1D	-3.73	116.58	123.85
24	d	402	CLA	C1D-CHD-C4C	-3.73	118.08	126.02
24	b	609	CLA	C1C-C2C-C3C	-3.73	103.05	106.98
24	b	608	CLA	C3C-C4C-NC	3.73	115.21	110.43
26	h	102	BCR	C7-C8-C9	-3.73	120.72	126.23
24	b	611	CLA	C3B-C2B-C1B	-3.73	102.77	107.17
24	b	613	CLA	C1-C2-C3	-3.73	120.09	126.20
26	C	516	BCR	C7-C8-C9	-3.73	120.72	126.23
24	b	603	CLA	CHD-C1D-ND	-3.73	119.56	124.80
24	B	610	CLA	C1D-CHD-C4C	-3.73	118.10	126.02
27	a	411	SQD	O47-C7-C8	3.72	119.53	111.48
24	B	607	CLA	C3B-C4B-NB	3.72	113.85	110.53
24	B	612	CLA	C4C-C3C-C2C	-3.72	101.48	106.89
24	b	604	CLA	C1D-CHD-C4C	-3.72	118.12	126.02
24	b	604	CLA	CHD-C1D-ND	-3.72	119.57	124.80
24	a	404	CLA	C1-C2-C3	-3.71	120.11	126.20
24	D	403	CLA	C2C-C1C-NC	3.71	113.88	109.98
24	b	609	CLA	CAC-C3C-C4C	3.71	129.62	124.79
24	b	614	CLA	C1D-CHD-C4C	-3.71	118.13	126.02
24	c	514	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
24	c	503	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
26	b	619	BCR	C7-C8-C9	-3.71	120.75	126.23
24	B	611	CLA	CHD-C1D-ND	-3.71	119.58	124.80
24	C	502	CLA	C1C-C2C-C3C	-3.70	103.08	106.98
24	c	513	CLA	C1D-CHD-C4C	-3.70	118.15	126.02
31	a	414[A]	PL9	C37-C38-C39	-3.70	119.15	127.62
26	k	101	BCR	C20-C21-C22	-3.70	122.09	127.28
24	c	510	CLA	CHD-C1D-ND	-3.70	119.60	124.80
24	a	350	CLA	CHD-C4C-NC	3.70	129.97	124.23
24	c	509	CLA	CMB-C2B-C1B	3.70	131.05	125.42
31	a	414[B]	PL9	C27-C28-C29	-3.70	119.16	127.62
25	A	407	PHO	CBC-CAC-C3C	-3.70	107.58	112.87
24	b	614	CLA	CAC-C3C-C4C	3.69	129.60	124.79
24	B	605	CLA	CHD-C1D-ND	-3.69	119.60	124.80
26	Y	101	BCR	C16-C17-C18	-3.69	122.10	127.28
24	B	604	CLA	C4A-NA-C1A	-3.69	105.00	106.68
26	B	618	BCR	C29-C30-C25	3.69	115.80	110.44
24	c	504	CLA	C1-C2-C3	-3.69	120.16	126.20
24	B	602	CLA	C1D-CHD-C4C	-3.68	118.19	126.02
24	C	503	CLA	CHD-C1D-ND	-3.68	119.62	124.80
24	d	403	CLA	O2D-CGD-O1D	-3.68	116.68	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	C2C-C1C-NC	3.68	113.85	109.98
24	D	403	CLA	C1D-CHD-C4C	-3.68	118.19	126.02
31	a	414[B]	PL9	C32-C33-C34	-3.68	119.20	127.62
26	a	408	BCR	C7-C8-C9	-3.68	120.79	126.23
24	b	602	CLA	C2C-C1C-NC	3.68	113.84	109.98
24	A	409	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
24	C	511	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
24	c	515	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
24	B	605	CLA	O2A-CGA-O1A	-3.67	114.45	123.63
31	d	405	PL9	C42-C43-C44	-3.67	119.23	127.62
24	A	406	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
24	C	503	CLA	CMB-C2B-C1B	3.66	131.00	125.42
24	b	615	CLA	CMB-C2B-C1B	3.66	131.00	125.42
24	c	513	CLA	C3C-C4C-NC	3.66	115.12	110.43
24	C	507	CLA	C3B-C4B-NB	3.66	113.80	110.53
24	C	512	CLA	C3B-C4B-NB	3.66	113.80	110.53
24	C	505	CLA	C3C-C4C-NC	3.66	115.11	110.43
24	C	513	CLA	CHD-C1D-ND	-3.66	119.66	124.80
24	B	603	CLA	O2D-CGD-O1D	-3.65	116.74	123.85
25	A	408	PHO	O2D-CGD-O1D	-3.65	116.74	123.85
24	c	507	CLA	C4C-C3C-C2C	-3.65	101.58	106.89
24	b	609	CLA	C1D-CHD-C4C	-3.65	118.27	126.02
27	f	101	SQD	C1-O5-C5	3.65	120.84	113.72
24	b	606	CLA	C1C-C2C-C3C	-3.64	103.15	106.98
24	A	404	CLA	C1C-C2C-C3C	-3.64	103.15	106.98
24	C	509	CLA	C3B-C4B-NB	3.64	113.78	110.53
24	b	603	CLA	CAA-C2A-C3A	-3.64	103.17	113.00
24	A	405	CLA	CAA-C2A-C3A	-3.63	103.18	113.00
24	B	602	CLA	CAA-C2A-C3A	-3.63	103.18	113.00
26	h	102	BCR	C16-C17-C18	-3.63	122.19	127.28
24	a	407	CLA	CMA-C3A-C2A	-3.63	99.95	113.98
24	d	403	CLA	C1D-CHD-C4C	-3.63	118.31	126.02
24	b	607	CLA	C1C-C2C-C3C	-3.62	103.17	106.98
24	c	508	CLA	C4B-C3B-C2B	-3.62	102.80	107.30
41	V	203	HEC	CHA-C1A-NA	3.62	128.39	124.45
24	C	505	CLA	C1-C2-C3	-3.61	120.28	126.20
24	B	614	CLA	C3C-C4C-NC	3.61	115.06	110.43
25	A	408	PHO	C1A-C2A-C3A	-3.61	99.40	102.84
31	A	416[A]	PL9	C17-C18-C19	-3.61	119.36	127.62
41	v	203	HEC	CHA-C1A-NA	3.61	128.38	124.45
24	a	407	CLA	C1C-C2C-C3C	-3.61	103.19	106.98
24	B	610	CLA	C1C-C2C-C3C	-3.60	103.19	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	C3C-C4C-NC	3.60	115.05	110.43
26	d	404	BCR	C24-C23-C22	-3.60	120.91	126.23
24	b	615	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
39	E	103	HEM	C1B-NB-C4B	3.60	109.47	105.21
24	c	509	CLA	C1D-CHD-C4C	-3.60	118.37	126.02
24	a	403	CLA	O2D-CGD-CBD	3.60	117.52	111.23
24	b	613	CLA	O2D-CGD-CBD	3.59	117.51	111.23
24	B	612	CLA	CAC-C3C-C4C	3.59	129.47	124.79
24	C	506	CLA	CMB-C2B-C1B	3.59	130.89	125.42
38	l	101	LHG	O7-C7-C8	3.59	119.25	111.48
24	a	403	CLA	CHD-C1D-ND	-3.59	119.75	124.80
24	a	407	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
24	C	504	CLA	C3C-C4C-NC	3.59	115.02	110.43
24	b	608	CLA	C1D-CHD-C4C	-3.59	118.40	126.02
25	a	406	PHO	C4-C3-C5	3.58	121.45	115.23
24	B	616	CLA	C4C-C3C-C2C	-3.58	101.68	106.89
24	b	607	CLA	C1D-CHD-C4C	-3.58	118.41	126.02
24	c	503	CLA	C1D-CHD-C4C	-3.58	118.41	126.02
24	D	403	CLA	CMB-C2B-C1B	3.58	130.87	125.42
31	a	414[B]	PL9	C42-C43-C44	-3.58	119.43	127.62
38	L	101	LHG	O7-C7-C8	3.58	119.22	111.48
24	B	609	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
24	C	512	CLA	CMC-C2C-C1C	3.57	130.61	125.03
24	B	610	CLA	O2A-CGA-CBA	3.57	122.72	111.83
24	C	506	CLA	CHD-C1D-ND	-3.57	119.78	124.80
24	B	613	CLA	O2D-CGD-CBD	3.57	117.47	111.23
31	d	405	PL9	C37-C38-C39	-3.57	119.46	127.62
24	a	404	CLA	C3C-C4C-NC	3.57	115.00	110.43
24	b	606	CLA	O2D-CGD-O1D	-3.56	116.91	123.85
24	B	604	CLA	O2A-CGA-O1A	-3.56	114.72	123.63
24	C	510	CLA	C1C-C2C-C3C	-3.56	103.23	106.98
31	A	416[A]	PL9	C10-C9-C11	3.56	121.41	115.23
24	B	607	CLA	C3C-C4C-NC	3.56	114.99	110.43
24	b	601	CLA	C3C-C4C-NC	3.56	114.99	110.43
26	B	617	BCR	C16-C17-C18	-3.56	122.29	127.28
24	d	403	CLA	C1-C2-C3	-3.56	120.37	126.20
24	C	504	CLA	C1-C2-C3	-3.56	120.37	126.20
24	a	404	CLA	C1C-C2C-C3C	-3.55	103.24	106.98
26	D	404	BCR	C15-C14-C13	-3.55	122.29	127.28
24	A	404	CLA	CAC-C3C-C4C	3.55	129.41	124.79
24	b	615	CLA	C3C-C4C-NC	3.55	114.98	110.43
31	a	414[A]	PL9	C15-C14-C16	3.55	121.39	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	506	CLA	C1D-CHD-C4C	-3.55	118.48	126.02
39	e	102	HEM	CHA-C4D-ND	3.55	128.76	124.37
24	C	509	CLA	C4C-C3C-C2C	-3.55	101.73	106.89
31	a	414[B]	PL9	C37-C38-C39	-3.55	119.51	127.62
24	b	612	CLA	C1C-C2C-C3C	-3.54	103.25	106.98
24	C	510	CLA	C1D-CHD-C4C	-3.54	118.49	126.02
31	A	416[A]	PL9	C27-C28-C29	-3.54	119.52	127.62
24	b	616	CLA	CHD-C1D-ND	-3.54	119.82	124.80
24	b	612	CLA	C4B-C3B-C2B	-3.54	102.90	107.30
24	c	510	CLA	C1-C2-C3	-3.54	120.40	126.20
24	B	604	CLA	C2B-C1B-NB	3.54	114.00	110.33
24	b	616	CLA	C4C-C3C-C2C	-3.53	101.75	106.89
24	B	608	CLA	C1-C2-C3	-3.53	120.41	126.20
24	d	402	CLA	C3B-C4B-NB	3.53	113.68	110.53
24	c	515	CLA	CAC-C3C-C4C	3.53	129.38	124.79
35	B	628	HTG	C1'-S1-C1	3.53	108.07	100.45
24	C	509	CLA	C1C-C2C-C3C	-3.53	103.27	106.98
24	B	606	CLA	CMC-C2C-C1C	3.53	130.55	125.03
31	a	414[A]	PL9	C42-C43-C44	-3.53	119.55	127.62
24	B	609	CLA	C3B-C2B-C1B	-3.53	103.01	107.17
24	a	350	CLA	C1-C2-C3	-3.53	120.42	126.20
25	A	407	PHO	C1A-C2A-C3A	-3.53	99.48	102.84
24	C	511	CLA	C3C-C4C-NC	3.52	114.94	110.43
24	C	504	CLA	C4-C3-C5	3.52	121.34	115.23
35	C	523	HTG	O5-C5-C4	3.52	116.04	109.70
24	B	616	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
24	c	515	CLA	C3C-C4C-NC	3.52	114.94	110.43
24	A	406	CLA	CAA-C2A-C3A	-3.52	103.50	113.00
24	B	609	CLA	C4B-C3B-C2B	-3.52	102.93	107.30
24	B	610	CLA	CAA-C2A-C3A	-3.51	103.50	113.00
24	b	615	CLA	C3B-C4B-NB	3.51	113.67	110.53
24	A	404	CLA	O2A-CGA-O1A	-3.51	114.84	123.63
24	d	402	CLA	CHD-C1D-ND	-3.51	119.87	124.80
24	C	504	CLA	C1C-C2C-C3C	-3.51	103.29	106.98
24	b	613	CLA	C3B-C4B-NB	3.51	113.66	110.53
24	C	511	CLA	C4-C3-C5	3.50	121.31	115.23
31	A	416[B]	PL9	C17-C18-C19	-3.50	119.61	127.62
24	b	614	CLA	CMC-C2C-C1C	3.50	130.50	125.03
24	b	614	CLA	C1-C2-C3	-3.50	120.46	126.20
24	B	607	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
24	b	603	CLA	C3B-C4B-NB	3.50	113.65	110.53
24	a	404	CLA	CAA-C2A-C3A	-3.50	103.55	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
34	M	101	LMT	O1'-C1'-C2'	3.49	113.58	108.27
24	b	601	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
24	b	609	CLA	C2B-C1B-NB	3.49	113.95	110.33
24	c	511	CLA	C1C-C2C-C3C	-3.49	103.31	106.98
24	b	602	CLA	C1D-CHD-C4C	-3.48	118.62	126.02
33	b	621	LMG	O8-C28-C29	3.48	122.44	111.83
25	A	407	PHO	O1D-CGD-CBD	-3.47	119.45	124.72
24	c	505	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
24	b	604	CLA	C2B-C1B-NB	3.47	113.92	110.33
24	D	403	CLA	CAC-C3C-C4C	3.47	129.30	124.79
26	A	410	BCR	C33-C5-C6	-3.47	120.70	124.48
24	B	614	CLA	C3B-C4B-NB	3.47	113.62	110.53
24	b	607	CLA	C4B-C3B-C2B	-3.46	103.00	107.30
26	A	410	BCR	C16-C17-C18	-3.46	122.42	127.28
24	B	609	CLA	C1D-CHD-C4C	-3.46	118.67	126.02
24	A	406	CLA	C1D-CHD-C4C	-3.46	118.67	126.02
24	d	402	CLA	CAC-C3C-C4C	3.46	129.29	124.79
26	b	618	BCR	C15-C14-C13	-3.46	122.43	127.28
26	c	516	BCR	C16-C17-C18	-3.46	122.43	127.28
24	b	610	CLA	C1C-C2C-C3C	-3.46	103.34	106.98
31	a	414[B]	PL9	C22-C23-C24	-3.45	119.72	127.62
24	b	616	CLA	O2A-CGA-CBA	3.45	122.36	111.83
24	b	602	CLA	CAA-C2A-C3A	-3.45	103.67	113.00
24	B	615	CLA	CHD-C4C-NC	3.45	129.58	124.23
24	B	610	CLA	CMA-C3A-C4A	-3.45	102.50	111.77
24	B	613	CLA	C1D-CHD-C4C	-3.45	118.69	126.02
24	C	507	CLA	CAC-C3C-C4C	3.45	129.28	124.79
38	D	407	LHG	O7-C7-C8	3.45	118.94	111.48
24	d	402	CLA	C1C-C2C-C3C	-3.45	103.36	106.98
24	b	611	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
24	b	605	CLA	C3C-C4C-NC	3.44	114.84	110.43
26	t	102	BCR	C7-C8-C9	-3.44	121.15	126.23
24	c	510	CLA	C3B-C4B-NB	3.44	113.60	110.53
26	B	618	BCR	C15-C14-C13	-3.44	122.45	127.28
24	C	505	CLA	C4A-NA-C1A	-3.44	105.11	106.68
39	E	103	HEM	CBD-CAD-C3D	-3.43	103.04	112.53
24	c	514	CLA	C3C-C4C-NC	3.43	114.83	110.43
31	A	416[B]	PL9	C42-C43-C44	-3.43	119.76	127.62
24	c	515	CLA	C1-C2-C3	-3.43	120.58	126.20
24	b	601	CLA	C1C-C2C-C3C	-3.43	103.37	106.98
24	b	605	CLA	CHD-C4C-NC	3.43	129.55	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	605	CLA	C4C-C3C-C2C	-3.43	101.90	106.89
33	A	418	LMG	C7-O1-C1	-3.43	106.45	113.80
26	a	408	BCR	C20-C21-C22	-3.43	122.47	127.28
24	A	404	CLA	C3B-C4B-NB	3.42	113.59	110.53
24	a	407	CLA	CAC-C3C-C4C	3.42	129.24	124.79
24	C	507	CLA	C1D-CHD-C4C	-3.42	118.75	126.02
24	b	605	CLA	C3B-C4B-NB	3.42	113.58	110.53
24	B	606	CLA	C1C-C2C-C3C	-3.41	103.39	106.98
24	b	613	CLA	CHD-C1D-ND	-3.41	120.00	124.80
24	b	608	CLA	C3B-C4B-NB	3.41	113.57	110.53
31	a	414[A]	PL9	C27-C28-C29	-3.41	119.83	127.62
33	C	520	LMG	O8-C28-C29	3.41	122.22	111.83
31	a	414[B]	PL9	C17-C18-C19	-3.40	119.83	127.62
24	c	503	CLA	C3C-C4C-NC	3.40	114.79	110.43
34	I	101	LMT	O1B-C4'-C3'	3.40	115.87	107.23
24	b	614	CLA	C1C-C2C-C3C	-3.40	103.41	106.98
24	d	403	CLA	C2C-C1C-NC	3.40	113.55	109.98
24	c	505	CLA	CMB-C2B-C1B	3.39	130.59	125.42
26	C	515	BCR	C33-C5-C6	-3.39	120.78	124.48
24	A	404	CLA	CMC-C2C-C1C	3.39	130.34	125.03
24	B	607	CLA	C1D-CHD-C4C	-3.39	118.81	126.02
26	k	101	BCR	C24-C23-C22	-3.39	121.22	126.23
35	c	526	HTG	C1-O5-C5	3.39	118.64	112.56
24	a	407	CLA	C4B-C3B-C2B	-3.39	103.09	107.30
24	d	402	CLA	C4-C3-C5	3.39	121.11	115.23
24	d	403	CLA	CMC-C2C-C1C	3.39	130.32	125.03
24	C	511	CLA	CHD-C4C-NC	3.38	129.47	124.23
31	a	414[A]	PL9	C30-C29-C31	3.38	121.10	115.23
31	A	416[B]	PL9	C37-C38-C39	-3.38	119.89	127.62
26	C	516	BCR	C33-C5-C6	-3.38	120.80	124.48
24	c	504	CLA	C3B-C4B-NB	3.38	113.55	110.53
27	A	411	SQD	O9-S-C6	3.38	111.80	106.76
33	Z	101	LMG	C1-C2-C3	3.37	117.11	110.01
24	B	603	CLA	O2A-CGA-O1A	-3.37	115.19	123.63
24	C	507	CLA	CBC-CAC-C3C	-3.37	103.28	112.42
24	C	505	CLA	CAC-C3C-C4C	3.37	129.18	124.79
24	b	601	CLA	C4-C3-C5	3.37	121.08	115.23
24	b	601	CLA	C3B-C4B-NB	3.37	113.54	110.53
24	b	611	CLA	C4B-C3B-C2B	-3.37	103.11	107.30
24	C	506	CLA	C4C-C3C-C2C	-3.37	101.99	106.89
31	A	416[B]	PL9	C32-C33-C34	-3.37	119.92	127.62
24	c	513	CLA	CHD-C4C-NC	3.36	129.45	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	CMB-C2B-C1B	3.36	130.54	125.42
24	C	507	CLA	C1-C2-C3	-3.36	120.69	126.20
24	a	404	CLA	C3B-C4B-NB	3.36	113.53	110.53
31	d	405	PL9	C10-C9-C11	3.36	121.06	115.23
24	B	605	CLA	CHD-C4C-NC	3.36	129.44	124.23
36	c	520	DGD	O2G-C1B-C2B	3.36	118.74	111.48
24	C	512	CLA	C1C-C2C-C3C	-3.35	103.45	106.98
24	a	350	CLA	C3C-C4C-NC	3.35	114.73	110.43
24	c	503	CLA	C1-C2-C3	-3.35	120.71	126.20
24	d	403	CLA	CAC-C3C-C4C	3.35	129.15	124.79
24	c	512	CLA	CBC-CAC-C3C	-3.35	103.34	112.42
26	Y	101	BCR	C15-C14-C13	-3.35	122.58	127.28
24	b	607	CLA	C4C-C3C-C2C	-3.34	102.03	106.89
26	T	101	BCR	C33-C5-C6	-3.34	120.84	124.48
38	l	101	LHG	O8-C23-C24	3.34	122.03	111.83
33	z	101	LMG	O7-C10-C11	3.34	118.71	111.48
26	h	102	BCR	C38-C26-C25	-3.34	120.84	124.48
26	T	101	BCR	C7-C8-C9	-3.34	121.30	126.23
24	B	601	CLA	CHD-C4C-NC	3.33	129.40	124.23
24	c	514	CLA	C4-C3-C5	3.33	121.01	115.23
24	B	615	CLA	C1C-C2C-C3C	-3.33	103.48	106.98
24	B	602	CLA	C1-C2-C3	-3.33	120.74	126.20
39	E	103	HEM	CHB-C1B-NB	3.33	128.48	124.37
24	C	510	CLA	C3B-C4B-NB	3.33	113.50	110.53
24	b	601	CLA	CHD-C4C-NC	3.33	129.39	124.23
24	b	610	CLA	O2A-CGA-O1A	-3.33	115.31	123.63
36	C	518	DGD	O2G-C1B-C2B	3.33	118.68	111.48
36	c	519	DGD	O2G-C1B-C2B	3.33	118.68	111.48
24	B	604	CLA	C3B-C4B-NB	3.32	113.50	110.53
38	D	357	LHG	O8-C23-C24	3.32	121.97	111.83
26	y	101	BCR	C15-C14-C13	-3.32	122.62	127.28
24	C	508	CLA	CMB-C2B-C1B	3.32	130.48	125.42
33	B	621	LMG	O8-C28-C29	3.32	121.96	111.83
24	b	605	CLA	C4-C3-C5	3.31	120.98	115.23
24	a	403	CLA	CHC-C1C-C2C	-3.31	117.53	126.95
24	b	612	CLA	C4-C3-C5	3.31	120.98	115.23
24	D	403	CLA	CMC-C2C-C1C	3.31	130.21	125.03
26	c	517	BCR	C21-C20-C19	-3.31	113.61	123.20
24	C	507	CLA	CHC-C1C-C2C	-3.31	117.55	126.95
24	B	602	CLA	CAC-C3C-C4C	3.31	129.09	124.79
38	d	406	LHG	O7-C7-C8	3.30	118.63	111.48
26	A	410	BCR	C11-C10-C9	-3.30	122.65	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	408	BCR	C11-C10-C9	-3.30	122.65	127.28
26	b	619	BCR	C2-C1-C6	3.30	115.23	110.44
24	c	506	CLA	C3C-C4C-NC	3.30	114.66	110.43
24	B	614	CLA	C4-C3-C5	3.30	120.95	115.23
24	d	402	CLA	C4C-C3C-C2C	-3.30	102.09	106.89
24	c	511	CLA	C3C-C4C-NC	3.30	114.65	110.43
24	A	406	CLA	C3C-C4C-NC	3.30	114.65	110.43
24	B	609	CLA	C1-O2A-CGA	3.29	124.62	116.65
39	e	102	HEM	CHB-C1B-NB	3.29	128.44	124.37
24	C	511	CLA	C3B-C4B-NB	3.29	113.47	110.53
24	c	513	CLA	C3B-C4B-NB	3.29	113.47	110.53
24	B	614	CLA	CMC-C2C-C1C	3.29	130.17	125.03
24	b	607	CLA	C2B-C1B-NB	3.29	113.74	110.33
24	C	507	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
24	c	513	CLA	C1C-C2C-C3C	-3.28	103.53	106.98
24	B	616	CLA	CHD-C4C-NC	3.28	129.31	124.23
24	b	612	CLA	CAC-C3C-C4C	3.27	129.05	124.79
24	c	515	CLA	C3B-C4B-NB	3.27	113.45	110.53
24	a	350	CLA	CAA-C2A-C3A	-3.27	104.15	113.00
25	a	406	PHO	O2D-CGD-O1D	-3.27	117.48	123.85
24	c	511	CLA	C4B-C3B-C2B	-3.27	103.23	107.30
24	d	402	CLA	O2A-CGA-CBA	3.27	121.81	111.83
24	c	514	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
24	C	506	CLA	C1C-C2C-C3C	-3.27	103.54	106.98
24	B	612	CLA	C4B-C3B-C2B	-3.27	103.24	107.30
24	b	604	CLA	O2A-CGA-CBA	3.27	121.79	111.83
24	d	403	CLA	C3C-C4C-NC	3.27	114.61	110.43
24	c	512	CLA	C4-C3-C5	3.26	120.89	115.23
24	b	602	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
24	B	606	CLA	CHD-C4C-NC	3.26	129.28	124.23
24	C	514	CLA	C4C-C3C-C2C	-3.26	102.15	106.89
24	A	409	CLA	CAA-C2A-C3A	-3.26	104.19	113.00
24	C	514	CLA	CAC-C3C-C4C	3.26	129.03	124.79
24	C	513	CLA	C1C-C2C-C3C	-3.26	103.56	106.98
24	b	605	CLA	O2A-CGA-O1A	-3.26	115.48	123.63
24	b	612	CLA	CHD-C1D-ND	-3.26	120.22	124.80
24	c	504	CLA	CMB-C2B-C1B	3.25	130.37	125.42
24	B	609	CLA	C3B-C4B-NB	3.25	113.43	110.53
24	c	508	CLA	CHC-C1C-C2C	-3.25	117.71	126.95
24	D	403	CLA	C4C-C3C-C2C	-3.25	102.17	106.89
27	A	411	SQD	C44-O6-C1	-3.25	106.84	113.80
24	b	612	CLA	C4C-C3C-C2C	-3.24	102.17	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	C4C-C3C-C2C	-3.24	102.17	106.89
24	c	507	CLA	CAC-C3C-C4C	3.24	129.01	124.79
24	a	407	CLA	CHD-C1D-ND	-3.24	120.24	124.80
36	h	103	DGD	O1G-C1A-C2A	3.24	121.71	111.83
24	a	403	CLA	CAC-C3C-C4C	3.24	129.00	124.79
24	C	514	CLA	CMB-C2B-C1B	3.24	130.35	125.42
24	A	405	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
24	a	403	CLA	C1-C2-C3	-3.23	120.90	126.20
24	b	611	CLA	C4C-C3C-C2C	-3.23	102.19	106.89
24	b	603	CLA	O2A-CGA-CBA	3.23	121.69	111.83
24	c	513	CLA	C4-C3-C5	3.23	120.84	115.23
31	A	416[A]	PL9	C15-C14-C16	3.23	120.83	115.23
24	B	603	CLA	CBC-CAC-C3C	-3.23	103.67	112.42
24	B	603	CLA	O2A-CGA-CBA	3.23	121.67	111.83
24	C	505	CLA	C4B-C3B-C2B	-3.23	103.29	107.30
24	c	509	CLA	CHD-C4C-NC	3.22	129.23	124.23
24	C	514	CLA	C1C-C2C-C3C	-3.22	103.59	106.98
26	d	404	BCR	C7-C8-C9	-3.22	121.47	126.23
24	c	508	CLA	C3C-C4C-NC	3.22	114.56	110.43
24	A	409	CLA	C4C-C3C-C2C	-3.22	102.20	106.89
24	B	610	CLA	C4C-C3C-C2C	-3.22	102.20	106.89
26	k	101	BCR	C15-C14-C13	-3.22	122.76	127.28
26	b	619	BCR	C38-C26-C25	-3.22	120.97	124.48
24	b	615	CLA	CHC-C1C-C2C	-3.22	117.81	126.95
27	A	413	SQD	O47-C7-C8	3.22	118.44	111.48
26	B	619	BCR	C24-C23-C22	-3.22	121.48	126.23
24	a	403	CLA	C4B-C3B-C2B	-3.21	103.31	107.30
24	b	611	CLA	C1C-C2C-C3C	-3.21	103.60	106.98
24	c	505	CLA	C3B-C4B-NB	3.21	113.40	110.53
26	D	404	BCR	C28-C27-C26	-3.21	108.34	114.06
24	B	611	CLA	CHD-C4C-NC	3.21	129.20	124.23
38	d	406	LHG	O8-C23-O10	-3.20	115.61	123.63
24	b	614	CLA	C3B-C4B-NB	3.20	113.39	110.53
25	a	405	PHO	O1D-CGD-CBD	-3.20	119.87	124.72
24	b	605	CLA	CMB-C2B-C1B	3.20	130.29	125.42
24	c	507	CLA	C1C-C2C-C3C	-3.20	103.61	106.98
24	C	514	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
24	B	604	CLA	CMB-C2B-C1B	3.20	130.29	125.42
24	C	512	CLA	C1-C2-C3	-3.20	120.96	126.20
24	C	509	CLA	CHD-C1D-ND	-3.20	120.30	124.80
24	B	612	CLA	CHD-C1D-ND	-3.20	120.30	124.80
24	B	602	CLA	C4C-C3C-C2C	-3.20	102.24	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	612	CLA	C4-C3-C5	3.20	120.77	115.23
24	c	514	CLA	CMB-C2B-C1B	3.20	130.28	125.42
36	C	517	DGD	C3G-C2G-C1G	-3.19	104.34	111.78
26	D	404	BCR	C10-C11-C12	-3.19	113.95	123.20
24	a	404	CLA	CHD-C4C-NC	3.19	129.18	124.23
24	B	609	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
24	b	609	CLA	C4B-C3B-C2B	-3.19	103.33	107.30
26	b	619	BCR	C10-C11-C12	-3.19	113.95	123.20
24	c	512	CLA	C3C-C4C-NC	3.19	114.51	110.43
33	c	521	LMG	O8-C28-C29	3.19	121.55	111.83
31	d	405	PL9	C45-C44-C46	3.19	120.76	115.23
24	B	601	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
24	c	504	CLA	CHD-C4C-NC	3.18	129.17	124.23
24	c	506	CLA	CMC-C2C-C1C	3.18	130.01	125.03
24	B	611	CLA	C4B-C3B-C2B	-3.18	103.34	107.30
24	a	403	CLA	O2A-CGA-CBA	3.18	121.53	111.83
24	b	610	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
26	T	101	BCR	C12-C13-C14	-3.18	114.01	119.01
24	b	603	CLA	O2A-CGA-O1A	-3.18	115.68	123.63
33	C	521	LMG	C3-C4-C5	3.18	115.99	110.23
31	a	414[A]	PL9	C17-C18-C19	-3.18	120.35	127.62
34	t	101	LMT	C1'-O5'-C5'	3.18	119.92	113.72
24	b	602	CLA	C1C-C2C-C3C	-3.17	103.64	106.98
38	D	357	LHG	C5-O7-C7	-3.17	110.20	117.80
24	B	615	CLA	C4C-C3C-C2C	-3.17	102.27	106.89
26	c	517	BCR	C33-C5-C6	-3.17	121.02	124.48
38	D	357	LHG	O8-C23-O10	-3.17	115.69	123.63
24	C	507	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
38	d	406	LHG	O8-C23-C24	3.17	121.50	111.83
24	C	504	CLA	O2D-CGD-CBD	3.17	116.77	111.23
27	a	409	SQD	O8-S-C6	3.17	112.09	105.97
36	c	518	DGD	C2G-O2G-C1B	-3.17	110.22	117.80
24	A	406	CLA	CHD-C4C-NC	3.17	129.14	124.23
24	b	606	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
24	b	616	CLA	CHD-C4C-NC	3.16	129.14	124.23
24	C	514	CLA	C3B-C4B-NB	3.16	113.35	110.53
27	B	620	SQD	O7-S-C6	3.16	111.48	106.76
24	B	601	CLA	C1C-C2C-C3C	-3.16	103.66	106.98
24	B	601	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
24	c	509	CLA	C4-C3-C5	3.16	120.71	115.23
24	B	608	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
24	B	601	CLA	O2A-CGA-CBA	3.16	121.47	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	405	PHO	O2D-CGD-O1D	-3.16	117.70	123.85
24	c	509	CLA	C3C-C4C-NC	3.15	114.47	110.43
24	C	510	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
24	b	615	CLA	C4C-C3C-C2C	-3.15	102.30	106.89
24	b	616	CLA	C4B-C3B-C2B	-3.15	103.38	107.30
24	B	608	CLA	CMA-C3A-C4A	-3.15	103.30	111.77
24	C	510	CLA	C4C-C3C-C2C	-3.15	102.31	106.89
24	B	615	CLA	CMC-C2C-C1C	3.15	129.96	125.03
27	B	620	SQD	O48-C23-C24	3.15	121.43	111.83
24	B	604	CLA	C4C-C3C-C2C	-3.15	102.31	106.89
24	c	505	CLA	C4C-C3C-C2C	-3.15	102.31	106.89
24	B	602	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
33	c	522	LMG	O6-C5-C4	3.14	115.36	109.70
24	b	609	CLA	C3B-C4B-NB	3.14	113.33	110.53
24	B	604	CLA	O2A-CGA-CBA	3.14	121.41	111.83
24	C	504	CLA	C3B-C4B-NB	3.14	113.33	110.53
24	D	403	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
33	C	521	LMG	O6-C5-C4	3.13	115.35	109.70
24	B	614	CLA	O2A-CGA-O1A	-3.13	115.80	123.63
24	b	614	CLA	C4C-C3C-C2C	-3.13	102.34	106.89
26	A	410	BCR	C38-C26-C25	-3.13	121.07	124.48
24	d	402	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
24	c	508	CLA	C4-C3-C5	3.12	120.65	115.23
24	B	612	CLA	C1C-C2C-C3C	-3.12	103.70	106.98
24	b	603	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
24	b	613	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
24	B	605	CLA	C1C-C2C-C3C	-3.12	103.70	106.98
24	B	606	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
24	B	603	CLA	CAA-C2A-C3A	-3.12	104.58	113.00
36	C	518	DGD	O1G-C1A-C2A	3.12	121.33	111.83
24	b	602	CLA	C4C-C3C-C2C	-3.12	102.36	106.89
24	C	513	CLA	CHD-C4C-NC	3.11	129.06	124.23
24	C	510	CLA	CAC-C3C-C4C	3.11	128.84	124.79
24	a	403	CLA	C3C-C4C-NC	3.11	114.41	110.43
24	b	601	CLA	C4C-C3C-C2C	-3.11	102.37	106.89
24	b	603	CLA	C4B-C3B-C2B	-3.11	103.44	107.30
24	A	406	CLA	O2A-CGA-CBA	3.11	121.30	111.83
39	e	102	HEM	CAD-CBD-CGD	3.10	121.89	113.67
25	a	405	PHO	CMA-C3A-C4A	-3.10	107.93	114.61
24	d	403	CLA	CHD-C4C-NC	3.10	129.03	124.23
24	C	512	CLA	C4C-C3C-C2C	-3.10	102.38	106.89
24	C	504	CLA	CHC-C1C-C2C	-3.10	118.14	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	416[B]	PL9	C27-C28-C29	-3.10	120.54	127.62
24	C	503	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
24	a	403	CLA	CAA-C2A-C1A	-3.10	101.83	111.97
24	B	607	CLA	C4B-C3B-C2B	-3.09	103.45	107.30
33	a	417	LMG	O6-C5-C4	3.09	115.27	109.70
24	D	402	CLA	CHC-C1C-C2C	-3.09	118.16	126.95
24	c	504	CLA	CBC-CAC-C3C	-3.09	104.04	112.42
24	b	605	CLA	CHC-C1C-C2C	-3.09	118.17	126.95
24	c	508	CLA	CAA-C2A-C3A	-3.09	104.65	113.00
26	c	517	BCR	C38-C26-C25	-3.09	121.11	124.48
24	a	350	CLA	C4B-C3B-C2B	-3.09	103.46	107.30
24	c	507	CLA	CMC-C2C-C1C	3.09	129.86	125.03
31	A	416[A]	PL9	C42-C43-C44	-3.09	120.56	127.62
24	A	406	CLA	CMA-C3A-C2A	-3.09	102.05	113.98
24	b	613	CLA	O2A-CGA-CBA	3.08	121.24	111.83
24	d	402	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
24	b	612	CLA	CHC-C1C-C2C	-3.08	118.19	126.95
26	D	404	BCR	C37-C22-C23	3.08	122.79	118.09
31	A	416[A]	PL9	C22-C23-C24	-3.08	120.58	127.62
24	B	613	CLA	C4-C3-C5	3.08	120.57	115.23
41	V	203	HEC	CHD-C4C-NC	3.08	127.81	124.45
24	c	504	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
24	B	604	CLA	CHD-C1D-ND	-3.08	120.47	124.80
34	M	103	LMT	O5'-C5'-C4'	3.07	116.08	109.72
27	a	409	SQD	O47-C7-O49	-3.07	116.52	123.70
24	c	511	CLA	CHC-C1C-C2C	-3.07	118.21	126.95
27	A	413	SQD	O48-C23-C24	3.07	121.20	111.83
24	c	512	CLA	O2A-CGA-CBA	3.07	121.20	111.83
24	b	603	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
24	A	409	CLA	C4B-C3B-C2B	-3.07	103.48	107.30
26	K	102	BCR	C20-C21-C22	-3.07	122.97	127.28
31	d	405	PL9	C12-C13-C14	-3.07	120.60	127.62
24	b	609	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
26	T	101	BCR	C21-C20-C19	-3.07	114.31	123.20
24	b	616	CLA	C3B-C4B-NB	3.07	113.27	110.53
24	b	612	CLA	O2A-CGA-CBA	3.07	121.19	111.83
25	a	405	PHO	C1A-C2A-C3A	-3.07	99.92	102.84
24	b	604	CLA	C4C-C3C-C2C	-3.07	102.43	106.89
24	a	407	CLA	C1-C2-C3	-3.06	121.18	126.20
24	C	507	CLA	C3C-C4C-NC	3.06	114.35	110.43
24	B	607	CLA	CMC-C2C-C1C	3.06	129.82	125.03
24	C	502	CLA	C1-C2-C3	-3.06	121.18	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	e	102	HEM	C1B-NB-C4B	3.06	108.83	105.21
31	A	416[B]	PL9	C10-C9-C8	-3.06	115.78	123.63
24	b	606	CLA	C4C-C3C-C2C	-3.05	102.44	106.89
41	v	203	HEC	CHD-C4C-NC	3.05	127.78	124.45
31	A	416[A]	PL9	C35-C34-C36	3.05	120.53	115.23
24	c	513	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
27	A	411	SQD	O48-C23-C24	3.05	121.14	111.83
25	a	406	PHO	C1A-C2A-C3A	-3.05	99.93	102.84
24	C	504	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
24	B	608	CLA	CHD-C4C-NC	3.05	128.96	124.23
24	b	613	CLA	CHD-C4C-NC	3.05	128.96	124.23
24	C	509	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
24	b	611	CLA	CHD-C4C-NC	3.05	128.96	124.23
24	b	608	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
24	B	601	CLA	C1-C2-C3	-3.05	121.20	126.20
24	B	614	CLA	CHC-C1C-C2C	-3.05	118.29	126.95
24	a	407	CLA	C4C-C3C-C2C	-3.05	102.46	106.89
24	B	603	CLA	C5-C3-C2	-3.05	114.33	121.17
24	a	404	CLA	C4C-C3C-C2C	-3.04	102.46	106.89
24	C	506	CLA	CMC-C2C-C1C	3.04	129.79	125.03
24	c	515	CLA	CAA-C2A-C3A	-3.04	104.78	113.00
24	D	403	CLA	C1C-C2C-C3C	-3.04	103.78	106.98
24	C	503	CLA	CHD-C4C-NC	3.04	128.94	124.23
24	b	609	CLA	CBC-CAC-C3C	-3.04	104.18	112.42
24	c	510	CLA	C4B-C3B-C2B	-3.04	103.53	107.30
24	B	610	CLA	CHD-C4C-NC	3.04	128.94	124.23
25	A	408	PHO	C4-C3-C5	3.04	120.50	115.23
24	C	508	CLA	C4C-C3C-C2C	-3.03	102.47	106.89
24	A	406	CLA	O2A-CGA-O1A	-3.03	116.04	123.63
24	B	608	CLA	O2A-CGA-O1A	-3.03	116.04	123.63
24	B	611	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
24	c	506	CLA	C4B-C3B-C2B	-3.03	103.53	107.30
24	C	508	CLA	C4-C3-C5	3.03	120.49	115.23
26	k	101	BCR	C10-C11-C12	-3.03	114.41	123.20
24	B	602	CLA	C1C-C2C-C3C	-3.03	103.79	106.98
24	D	403	CLA	C3B-C4B-NB	3.03	113.23	110.53
24	b	610	CLA	CAC-C3C-C4C	3.03	128.73	124.79
24	B	603	CLA	CHD-C4C-NC	3.03	128.93	124.23
31	A	416[A]	PL9	C7-C3-C4	3.03	119.40	116.91
24	c	506	CLA	CAC-C3C-C4C	3.03	128.73	124.79
24	B	607	CLA	CBC-CAC-C3C	-3.03	104.21	112.42
24	B	605	CLA	C3B-C4B-NB	3.03	113.23	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	605	CLA	C2A-C1A-CHA	-3.03	118.62	123.87
24	b	604	CLA	C3B-C4B-NB	3.02	113.23	110.53
33	J	101	LMG	O7-C10-C11	3.02	118.02	111.48
24	c	512	CLA	CHD-C4C-NC	3.02	128.92	124.23
24	c	512	CLA	CHC-C1C-C2C	-3.02	118.36	126.95
24	c	507	CLA	CHD-C1D-ND	-3.02	120.55	124.80
24	b	615	CLA	C4-C3-C5	3.02	120.47	115.23
24	a	350	CLA	C3B-C4B-NB	3.02	113.22	110.53
31	a	414[A]	PL9	C10-C9-C11	3.01	120.46	115.23
24	B	613	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
24	b	608	CLA	O2A-CGA-CBA	3.01	121.02	111.83
24	D	403	CLA	CHD-C4C-NC	3.01	128.90	124.23
38	D	407	LHG	O8-C23-O10	-3.01	116.10	123.63
24	C	511	CLA	O2A-CGA-CBA	3.01	121.00	111.83
24	B	608	CLA	C4C-C3C-C2C	-3.01	102.52	106.89
31	A	416[B]	PL9	C22-C23-C24	-3.00	120.75	127.62
26	Y	101	BCR	C28-C27-C26	-3.00	108.70	114.06
26	t	102	BCR	C37-C22-C23	3.00	122.68	118.09
26	b	618	BCR	C29-C30-C25	3.00	114.80	110.44
26	t	102	BCR	C1-C6-C7	3.00	123.79	115.65
24	C	504	CLA	CMB-C2B-C1B	3.00	129.99	125.42
35	b	628	HTG	C1-O5-C5	3.00	117.94	112.56
24	b	602	CLA	C2A-C1A-CHA	-3.00	118.66	123.87
25	A	408	PHO	CMB-C2B-C3B	3.00	130.68	124.68
24	b	602	CLA	CHD-C4C-NC	3.00	128.88	124.23
24	c	503	CLA	CAC-C3C-C4C	3.00	128.69	124.79
24	C	506	CLA	C3B-C4B-NB	3.00	113.20	110.53
24	b	606	CLA	C3B-C4B-NB	3.00	113.20	110.53
24	C	513	CLA	O2A-CGA-CBA	2.99	120.97	111.83
24	C	503	CLA	CBC-CAC-C3C	-2.99	104.30	112.42
24	A	409	CLA	C4-C3-C5	2.99	120.42	115.23
24	A	406	CLA	C2A-C1A-CHA	-2.99	118.67	123.87
31	d	405	PL9	C40-C39-C41	2.99	120.42	115.23
36	C	517	DGD	O3G-C3G-C2G	-2.99	103.54	110.82
24	c	514	CLA	CHD-C4C-NC	2.99	128.87	124.23
24	A	404	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
27	a	411	SQD	O7-S-C6	2.99	111.22	106.76
24	c	509	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
38	D	407	LHG	O8-C23-C24	2.99	120.95	111.83
24	C	502	CLA	CHD-C4C-NC	2.99	128.87	124.23
24	c	515	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
24	B	614	CLA	CAC-C3C-C4C	2.99	128.67	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	E	101	LHG	O8-C23-C24	2.98	120.94	111.83
24	c	512	CLA	C4B-C3B-C2B	-2.98	103.59	107.30
33	z	101	LMG	O8-C28-C29	2.98	120.93	111.83
26	B	619	BCR	C38-C26-C25	-2.98	121.23	124.48
24	b	608	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
24	B	616	CLA	CMB-C2B-C1B	2.98	129.96	125.42
27	a	411	SQD	O48-C23-C24	2.98	120.93	111.83
39	E	103	HEM	CHD-C1D-ND	2.98	127.63	124.42
24	D	402	CLA	CMB-C2B-C1B	2.98	129.96	125.42
26	H	101	BCR	C38-C26-C25	-2.98	121.23	124.48
24	c	505	CLA	CAC-C3C-C4C	2.98	128.67	124.79
27	a	409	SQD	O48-C23-C24	2.98	120.92	111.83
26	C	516	BCR	C38-C26-C25	-2.98	121.23	124.48
24	C	504	CLA	CAC-C3C-C4C	2.97	128.66	124.79
24	b	604	CLA	C4B-C3B-C2B	-2.97	103.61	107.30
24	b	606	CLA	C4-C3-C5	2.97	120.38	115.23
31	D	405	PL9	C32-C33-C34	-2.97	120.84	127.62
24	b	609	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
24	b	616	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
26	d	404	BCR	C33-C5-C6	-2.96	121.26	124.48
24	b	610	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
24	A	404	CLA	C4B-C3B-C2B	-2.96	103.63	107.30
24	C	510	CLA	C4B-C3B-C2B	-2.96	103.63	107.30
24	b	614	CLA	CMB-C2B-C1B	2.95	129.92	125.42
24	B	602	CLA	CMB-C2B-C1B	2.95	129.92	125.42
24	b	606	CLA	CHD-C4C-NC	2.95	128.81	124.23
24	a	407	CLA	O2A-CGA-CBA	2.95	120.83	111.83
24	b	608	CLA	CHD-C4C-NC	2.95	128.81	124.23
24	d	403	CLA	C1C-C2C-C3C	-2.95	103.88	106.98
24	c	510	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
24	b	611	CLA	C3B-C4B-NB	2.95	113.16	110.53
24	b	604	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
24	b	615	CLA	C11-C10-C8	-2.94	106.18	115.97
24	d	403	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
24	B	607	CLA	C1-C2-C3	-2.94	121.38	126.20
24	c	505	CLA	C4-C3-C5	2.94	120.33	115.23
24	B	606	CLA	C4-C3-C5	2.94	120.33	115.23
25	A	408	PHO	C6-C5-C3	-2.94	106.31	113.47
24	c	511	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
24	b	611	CLA	CHC-C1C-C2C	-2.94	118.60	126.95
31	D	405	PL9	C12-C13-C14	-2.94	120.90	127.62
24	b	610	CLA	C4-C3-C5	2.94	120.33	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	405	PL9	C40-C39-C41	2.94	120.33	115.23
24	c	509	CLA	CMC-C2C-C1C	2.94	129.62	125.03
24	C	513	CLA	CMB-C2B-C1B	2.93	129.89	125.42
24	b	605	CLA	C1-C2-C3	-2.93	121.39	126.20
24	c	513	CLA	O2A-CGA-CBA	2.93	120.78	111.83
24	B	616	CLA	C4B-C3B-C2B	-2.93	103.65	107.30
38	d	408	LHG	O8-C23-C24	2.93	120.78	111.83
26	t	102	BCR	C7-C6-C5	-2.93	114.80	121.56
24	C	512	CLA	C4-C3-C5	2.93	120.31	115.23
36	c	520	DGD	O3G-C3G-C2G	-2.93	103.69	110.82
24	b	613	CLA	C4-C3-C5	2.93	120.31	115.23
24	C	505	CLA	CHC-C1C-C2C	-2.93	118.62	126.95
24	B	614	CLA	CHD-C4C-NC	2.93	128.77	124.23
24	B	608	CLA	CHC-C1C-C2C	-2.93	118.63	126.95
24	d	403	CLA	CAA-C2A-C3A	-2.92	105.10	113.00
24	c	514	CLA	O2A-CGA-CBA	2.92	120.75	111.83
24	D	403	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
24	A	405	CLA	C1-C2-C3	-2.92	121.41	126.20
24	C	510	CLA	O2A-CGA-CBA	2.92	120.74	111.83
24	c	510	CLA	CHD-C4C-NC	2.92	128.76	124.23
24	A	406	CLA	CMC-C2C-C1C	2.92	129.59	125.03
24	C	507	CLA	O2A-CGA-CBA	2.92	120.73	111.83
24	C	506	CLA	C4-C3-C5	2.92	120.29	115.23
24	C	510	CLA	CMC-C2C-C1C	2.92	129.59	125.03
24	A	404	CLA	CAA-C2A-C1A	-2.92	102.41	111.97
24	B	613	CLA	C7-C6-C5	-2.92	105.49	113.26
24	B	604	CLA	C4B-C3B-C2B	-2.92	103.68	107.30
24	D	402	CLA	C4B-C3B-C2B	-2.92	103.68	107.30
24	b	607	CLA	CHC-C1C-C2C	-2.91	118.67	126.95
24	C	507	CLA	CAA-C2A-C3A	-2.91	105.13	113.00
24	b	605	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
24	c	510	CLA	CHC-C1C-C2C	-2.91	118.67	126.95
24	C	502	CLA	C4C-C3C-C2C	-2.91	102.66	106.89
24	B	614	CLA	O2A-CGA-CBA	2.91	120.70	111.83
24	D	403	CLA	CAA-C2A-C3A	-2.91	105.15	113.00
26	A	410	BCR	C24-C23-C22	-2.91	121.94	126.23
24	C	503	CLA	O2A-CGA-CBA	2.90	120.69	111.83
33	c	522	LMG	O8-C28-C29	2.90	120.68	111.83
24	a	404	CLA	C4B-C3B-C2B	-2.90	103.69	107.30
24	a	404	CLA	C4-C3-C5	2.90	120.26	115.23
24	b	607	CLA	C4-C3-C5	2.90	120.26	115.23
31	A	416[A]	PL9	C20-C19-C21	2.90	120.26	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	503	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
31	A	416[B]	PL9	C12-C13-C14	-2.90	121.00	127.62
24	B	613	CLA	O2A-CGA-CBA	2.90	120.67	111.83
35	b	623	HTG	C1'-S1-C1	2.89	106.70	100.45
24	B	603	CLA	C2A-C1A-CHA	-2.89	118.85	123.87
24	B	610	CLA	C3B-C4B-NB	2.89	113.11	110.53
38	a	419	LHG	O7-C7-C8	2.89	117.74	111.48
24	b	616	CLA	CMB-C2B-C1B	2.89	129.82	125.42
24	c	506	CLA	CHD-C4C-NC	2.89	128.71	124.23
24	B	603	CLA	CMC-C2C-C1C	2.89	129.55	125.03
24	B	603	CLA	C4B-C3B-C2B	-2.89	103.71	107.30
24	c	504	CLA	O2A-CGA-O1A	-2.89	116.41	123.63
24	b	610	CLA	CAA-C2A-C3A	-2.88	105.20	113.00
36	C	517	DGD	C2G-O2G-C1B	-2.88	110.89	117.80
26	T	101	BCR	C16-C17-C18	-2.88	123.24	127.28
24	c	504	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
24	B	607	CLA	CHC-C1C-C2C	-2.88	118.77	126.95
26	K	102	BCR	C11-C10-C9	-2.88	123.25	127.28
24	C	502	CLA	C4-C3-C5	2.87	120.22	115.23
24	b	612	CLA	C2A-C1A-CHA	-2.87	118.88	123.87
24	B	609	CLA	CHD-C4C-NC	2.87	128.69	124.23
24	c	515	CLA	CMC-C2C-C1C	2.87	129.52	125.03
24	C	503	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
24	c	513	CLA	CMB-C2B-C1B	2.87	129.79	125.42
24	c	503	CLA	CHC-C1C-C2C	-2.87	118.79	126.95
24	b	602	CLA	CMB-C2B-C1B	2.87	129.79	125.42
24	d	403	CLA	C1-O2A-CGA	2.87	123.59	116.65
24	c	514	CLA	C4C-C3C-C2C	-2.87	102.72	106.89
24	C	505	CLA	CBC-CAC-C3C	-2.87	104.65	112.42
31	D	405	PL9	C45-C44-C46	2.87	120.20	115.23
24	a	407	CLA	CMC-C2C-C1C	2.86	129.51	125.03
24	b	609	CLA	CMC-C2C-C1C	2.86	129.51	125.03
24	B	614	CLA	CBC-CAC-C3C	-2.86	104.66	112.42
24	C	509	CLA	C2A-C1A-CHA	-2.86	118.90	123.87
26	b	617	BCR	C29-C30-C25	2.86	114.60	110.44
26	d	404	BCR	C28-C27-C26	-2.86	108.95	114.06
24	b	607	CLA	CMB-C2B-C1B	2.86	129.78	125.42
26	b	619	BCR	C3-C4-C5	-2.86	108.95	114.06
41	V	203	HEC	CHA-C4D-ND	2.86	129.05	123.86
24	C	514	CLA	C2A-C1A-CHA	-2.86	118.90	123.87
24	c	503	CLA	C3B-C4B-NB	2.86	113.08	110.53
24	b	614	CLA	O2A-CGA-CBA	2.85	120.54	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	402	CLA	CMC-C2C-C1C	2.85	129.49	125.03
24	a	404	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
26	B	618	BCR	C37-C22-C23	2.85	122.45	118.09
31	a	414[B]	PL9	C35-C34-C36	2.85	120.18	115.23
24	B	604	CLA	CHD-C4C-NC	2.85	128.65	124.23
24	B	610	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
24	c	504	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
24	C	502	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
36	c	520	DGD	O1G-C1A-C2A	2.85	120.52	111.83
24	A	409	CLA	CMA-C3A-C2A	-2.85	102.97	113.98
24	b	609	CLA	CHC-C1C-C2C	-2.85	118.86	126.95
24	C	507	CLA	O2A-CGA-O1A	-2.85	116.51	123.63
24	C	505	CLA	CMC-C2C-C1C	2.85	129.48	125.03
25	A	407	PHO	C4A-C3A-C2A	-2.84	100.13	102.84
24	b	601	CLA	CMB-C2B-C1B	2.84	129.75	125.42
24	a	403	CLA	C2A-C1A-CHA	-2.84	118.93	123.87
24	b	615	CLA	C4B-C3B-C2B	-2.84	103.77	107.30
24	D	402	CLA	C4C-C3C-C2C	-2.84	102.75	106.89
24	C	509	CLA	CAC-C3C-C4C	2.84	128.49	124.79
24	B	611	CLA	CHC-C1C-C2C	-2.84	118.87	126.95
24	b	606	CLA	CHC-C1C-C2C	-2.84	118.89	126.95
24	c	505	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
35	V	204	HTG	C1-O5-C5	2.84	115.99	112.19
24	c	506	CLA	CHC-C1C-C2C	-2.84	118.89	126.95
24	B	615	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
24	A	405	CLA	CMA-C3A-C2A	-2.83	103.03	113.98
26	B	617	BCR	C15-C14-C13	-2.83	123.30	127.28
24	D	402	CLA	C1D-CHD-C4C	-2.83	120.00	126.02
24	C	514	CLA	CMC-C2C-C1C	2.83	129.46	125.03
24	a	350	CLA	CHC-C1C-C2C	-2.83	118.91	126.95
24	c	504	CLA	CHC-C1C-C2C	-2.83	118.91	126.95
24	c	514	CLA	CHC-C1C-C2C	-2.83	118.91	126.95
24	B	608	CLA	O2A-CGA-CBA	2.83	120.45	111.83
24	A	409	CLA	CHC-C1C-C2C	-2.83	118.92	126.95
26	B	617	BCR	C29-C30-C25	2.83	114.54	110.44
24	c	509	CLA	CHC-C1C-C2C	-2.82	118.92	126.95
26	c	516	BCR	C38-C26-C25	-2.82	121.40	124.48
24	b	608	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
24	B	605	CLA	C4B-C3B-C2B	-2.82	103.79	107.30
24	B	613	CLA	C4C-C3C-C2C	-2.82	102.78	106.89
24	B	616	CLA	C3B-C4B-NB	2.82	113.05	110.53
24	b	605	CLA	C4B-C3B-C2B	-2.82	103.79	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	601	CLA	CMC-C2C-C1C	2.82	129.44	125.03
24	b	601	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
24	c	514	CLA	C3B-C4B-NB	2.82	113.05	110.53
24	C	512	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
24	B	603	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
26	y	101	BCR	C37-C22-C23	2.82	122.39	118.09
24	d	403	CLA	CMB-C2B-C1B	2.82	129.71	125.42
24	C	509	CLA	CHC-C1C-C2C	-2.82	118.95	126.95
31	A	416[B]	PL9	C53-C6-C1	2.81	121.03	115.28
24	C	508	CLA	CHC-C1C-C2C	-2.81	118.96	126.95
24	c	506	CLA	C2A-C1A-CHA	-2.81	118.99	123.87
24	c	509	CLA	C3B-C4B-NB	2.81	113.04	110.53
24	C	506	CLA	CAC-C3C-C4C	2.81	128.44	124.79
24	C	502	CLA	CMB-C2B-C1B	2.80	129.69	125.42
24	C	511	CLA	CBC-CAC-C3C	-2.80	104.82	112.42
24	C	507	CLA	C4-C3-C5	2.80	120.09	115.23
24	b	616	CLA	C1-C2-C3	-2.80	121.61	126.20
26	c	516	BCR	C28-C27-C26	-2.80	109.06	114.06
24	b	612	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
24	C	513	CLA	C4-C3-C5	2.80	120.09	115.23
24	c	510	CLA	C4C-C3C-C2C	-2.80	102.82	106.89
24	b	614	CLA	C2A-C1A-CHA	-2.80	119.01	123.87
24	B	604	CLA	CMC-C2C-C1C	2.80	129.41	125.03
24	b	607	CLA	CAC-C3C-C4C	2.80	128.43	124.79
24	a	350	CLA	C2A-C1A-CHA	-2.80	119.02	123.87
33	b	621	LMG	C8-O7-C10	-2.80	111.11	117.80
26	a	408	BCR	C38-C26-C25	-2.79	121.44	124.48
24	B	610	CLA	CHC-C1C-C2C	-2.79	119.01	126.95
24	A	406	CLA	C4C-C3C-C2C	-2.79	102.83	106.89
24	C	502	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
24	C	506	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
31	D	405	PL9	C53-C6-C1	2.79	121.00	115.28
24	B	607	CLA	C4-C3-C5	2.79	120.07	115.23
26	y	101	BCR	C10-C11-C12	-2.79	115.11	123.20
24	C	510	CLA	O2A-CGA-O1A	-2.79	116.65	123.63
24	b	613	CLA	O2A-CGA-O1A	-2.79	116.65	123.63
24	c	505	CLA	CHC-C1C-C2C	-2.79	119.02	126.95
24	B	606	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
24	c	504	CLA	O2A-CGA-CBA	2.79	120.34	111.83
24	c	511	CLA	C1-O2A-CGA	2.79	123.40	116.65
24	D	403	CLA	CBC-CAC-C3C	-2.79	104.86	112.42
24	B	611	CLA	CBC-CAC-C3C	-2.79	104.87	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
24	A	405	CLA	C4B-C3B-C2B	-2.79	103.84	107.30
38	d	408	LHG	O8-C23-O10	-2.78	116.66	123.63
24	B	603	CLA	C3B-C4B-NB	2.78	113.01	110.53
24	c	505	CLA	C4B-C3B-C2B	-2.78	103.84	107.30
24	B	611	CLA	CMC-C2C-C1C	2.78	129.38	125.03
26	C	516	BCR	C15-C14-C13	-2.78	123.38	127.28
26	b	619	BCR	C37-C22-C23	2.78	122.33	118.09
31	a	414[B]	PL9	C7-C8-C9	-2.78	122.05	126.83
24	B	606	CLA	CBC-CAC-C3C	-2.78	104.89	112.42
26	B	618	BCR	C28-C27-C26	-2.78	109.10	114.06
24	C	506	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
24	B	612	CLA	C2A-C1A-CHA	-2.78	119.05	123.87
24	C	506	CLA	C1-C2-C3	-2.78	121.65	126.20
24	C	512	CLA	C4B-C3B-C2B	-2.77	103.85	107.30
24	c	514	CLA	CMA-C3A-C4A	-2.77	104.32	111.77
24	b	614	CLA	CHC-C1C-C2C	-2.77	119.07	126.95
24	A	409	CLA	CHD-C4C-NC	2.77	128.53	124.23
33	C	521	LMG	O8-C28-C29	2.77	120.29	111.83
26	t	102	BCR	C35-C13-C12	2.77	122.32	118.09
31	a	414[A]	PL9	C35-C34-C36	2.77	120.04	115.23
33	z	101	LMG	C8-O7-C10	-2.77	111.17	117.80
31	A	416[B]	PL9	C25-C24-C26	2.76	120.03	115.23
24	c	511	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
24	C	503	CLA	C3B-C4B-NB	2.76	113.00	110.53
24	b	611	CLA	CMB-C2B-C1B	2.76	129.63	125.42
33	j	101	LMG	O8-C28-O10	-2.76	116.72	123.63
24	C	504	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
24	b	609	CLA	CMB-C2B-C1B	2.76	129.62	125.42
24	c	513	CLA	CHC-C1C-C2C	-2.76	119.10	126.95
26	C	515	BCR	C16-C17-C18	-2.76	123.41	127.28
24	B	609	CLA	CHC-C1C-C2C	-2.76	119.11	126.95
24	D	403	CLA	C4-C3-C5	2.76	120.02	115.23
24	b	601	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
24	D	402	CLA	CAC-C3C-C4C	2.76	128.38	124.79
39	e	102	HEM	CHD-C1D-ND	2.76	127.39	124.42
24	c	511	CLA	O2A-CGA-CBA	2.75	120.23	111.83
26	A	410	BCR	C8-C7-C6	-2.75	119.64	127.00
24	D	402	CLA	O2A-CGA-CBA	2.75	120.23	111.83
24	b	605	CLA	CED-O2D-CGD	2.75	122.16	115.92
24	a	407	CLA	CHC-C1C-C2C	-2.75	119.13	126.95
24	C	512	CLA	CHC-C1C-C2C	-2.75	119.13	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	511	CLA	C4-C3-C5	2.75	120.00	115.23
24	C	505	CLA	CMB-C2B-C1B	2.75	129.60	125.42
24	B	610	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
26	d	404	BCR	C29-C30-C25	2.75	114.43	110.44
31	a	414[A]	PL9	C25-C24-C26	2.75	120.00	115.23
41	V	203	HEC	C4B-NB-C1B	2.75	110.30	105.82
24	c	504	CLA	CMC-C2C-C1C	2.75	129.33	125.03
31	d	405	PL9	C22-C23-C24	-2.75	121.34	127.62
24	b	604	CLA	CMC-C2C-C1C	2.75	129.33	125.03
33	j	101	LMG	C8-O7-C10	-2.75	111.22	117.80
24	B	609	CLA	O2A-CGA-CBA	2.75	120.21	111.83
24	B	614	CLA	C1-C2-C3	-2.75	121.70	126.20
24	a	403	CLA	C4-C3-C5	2.75	119.99	115.23
24	C	511	CLA	C4C-C3C-C2C	-2.74	102.90	106.89
24	c	508	CLA	CBC-CAC-C3C	-2.74	104.98	112.42
24	D	402	CLA	O2A-CGA-O1A	-2.74	116.77	123.63
24	D	402	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
24	B	610	CLA	CAA-CBA-CGA	-2.74	105.42	113.21
26	b	618	BCR	C28-C27-C26	-2.74	109.17	114.06
24	b	601	CLA	CBC-CAC-C3C	-2.74	104.99	112.42
24	b	607	CLA	CAA-C2A-C3A	-2.74	105.59	113.00
26	d	404	BCR	C40-C30-C25	-2.74	105.94	110.24
31	D	405	PL9	C27-C28-C29	-2.74	121.35	127.62
26	h	102	BCR	C10-C11-C12	-2.74	115.26	123.20
31	A	416[A]	PL9	C30-C29-C31	2.74	119.98	115.23
24	c	515	CLA	C2A-C1A-CHA	-2.74	119.11	123.87
26	k	101	BCR	C11-C10-C9	-2.74	123.44	127.28
26	Y	101	BCR	C38-C26-C25	-2.74	121.50	124.48
24	b	615	CLA	CAC-C3C-C4C	2.74	128.35	124.79
24	b	608	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
24	b	603	CLA	CMB-C2B-C1B	2.74	129.58	125.42
26	D	404	BCR	C33-C5-C6	-2.73	121.50	124.48
24	B	612	CLA	CHC-C1C-C2C	-2.73	119.18	126.95
24	A	405	CLA	C4-C3-C5	2.73	119.97	115.23
26	T	101	BCR	C35-C13-C12	2.73	122.26	118.09
24	d	403	CLA	C2A-C1A-CHA	-2.73	119.12	123.87
24	a	350	CLA	CMB-C2B-C1B	2.73	129.57	125.42
24	C	513	CLA	O1D-CGD-CBD	-2.73	119.14	124.52
24	C	511	CLA	CHC-C1C-C2C	-2.73	119.20	126.95
24	B	615	CLA	C3B-C4B-NB	2.73	112.96	110.53
26	Y	101	BCR	C10-C11-C12	-2.73	115.30	123.20
24	c	510	CLA	C4-C3-C5	2.72	119.96	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	603	CLA	C2A-C1A-CHA	-2.72	119.14	123.87
24	b	610	CLA	CMC-C2C-C1C	2.72	129.29	125.03
31	D	405	PL9	C17-C18-C19	-2.72	121.40	127.62
24	b	616	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
24	C	505	CLA	C4-C3-C5	2.72	119.94	115.23
27	B	620	SQD	C3-C4-C5	2.71	115.15	110.23
24	B	616	CLA	O2A-CGA-CBA	2.71	120.11	111.83
24	B	611	CLA	O2A-CGA-O1A	-2.71	116.84	123.63
36	H	102	DGD	O1G-C1A-C2A	2.71	120.10	111.83
35	b	628	HTG	C1'-S1-C1	2.71	106.30	100.45
27	b	620	SQD	C3-C4-C5	2.71	115.14	110.23
24	c	512	CLA	CMC-C2C-C1C	2.71	129.26	125.03
26	H	101	BCR	C16-C17-C18	-2.71	123.48	127.28
24	B	613	CLA	CHC-C1C-C2C	-2.71	119.25	126.95
24	c	508	CLA	C4C-C3C-C2C	-2.71	102.95	106.89
36	C	518	DGD	O1G-C1A-O1A	-2.71	116.86	123.63
24	b	610	CLA	CHC-C1C-C2C	-2.71	119.26	126.95
24	b	603	CLA	CHC-C1C-C2C	-2.70	119.26	126.95
24	C	511	CLA	C4B-C3B-C2B	-2.70	103.94	107.30
36	C	519	DGD	O1G-C1A-C2A	2.70	120.07	111.83
24	B	601	CLA	C3B-C4B-NB	2.70	112.94	110.53
24	B	607	CLA	CHD-C4C-NC	2.70	128.42	124.23
24	B	601	CLA	C4B-C3B-C2B	-2.70	103.94	107.30
26	d	404	BCR	C21-C20-C19	-2.70	115.38	123.20
24	b	606	CLA	CAA-C2A-C3A	-2.70	105.71	113.00
24	c	515	CLA	CHC-C1C-C2C	-2.70	119.28	126.95
24	B	614	CLA	C2A-C1A-CHA	-2.70	119.19	123.87
24	A	406	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
24	c	503	CLA	C4B-C3B-C2B	-2.69	103.95	107.30
31	a	414[A]	PL9	C40-C39-C41	2.69	119.90	115.23
27	F	101	SQD	C3-C4-C5	2.69	115.11	110.23
24	C	506	CLA	CHD-C4C-NC	2.69	128.40	124.23
24	B	606	CLA	O2A-CGA-CBA	2.69	120.04	111.83
24	c	515	CLA	C4B-C3B-C2B	-2.69	103.96	107.30
26	B	618	BCR	C7-C8-C9	-2.69	122.26	126.23
26	D	404	BCR	C29-C30-C25	2.69	114.34	110.44
24	C	505	CLA	C4C-C3C-C2C	-2.69	102.98	106.89
24	C	503	CLA	CHC-C1C-C2C	-2.69	119.31	126.95
36	H	102	DGD	O2G-C1B-C2B	2.69	117.30	111.48
26	y	101	BCR	C21-C20-C19	-2.68	115.42	123.20
24	B	613	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
24	b	616	CLA	CBC-CAC-C3C	-2.68	105.14	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	PHO	C4D-CHA-CBD	2.68	109.74	108.45
26	c	517	BCR	C11-C10-C9	-2.68	123.52	127.28
24	b	611	CLA	C2A-C1A-CHA	-2.68	119.22	123.87
24	D	402	CLA	C4-C3-C5	2.68	119.88	115.23
24	b	602	CLA	CMC-C2C-C1C	2.68	129.22	125.03
24	C	514	CLA	C4-C3-C5	2.68	119.88	115.23
31	A	416[A]	PL9	C25-C24-C26	2.68	119.88	115.23
25	a	406	PHO	C4A-C3A-C2A	-2.68	100.29	102.84
24	D	403	CLA	C2A-C1A-CHA	-2.68	119.22	123.87
26	b	619	BCR	C31-C1-C6	-2.68	106.05	110.24
33	b	621	LMG	O8-C28-O10	-2.68	116.93	123.63
35	B	628	HTG	C1-O5-C5	2.68	117.36	112.56
24	A	404	CLA	C2A-C1A-CHA	-2.67	119.23	123.87
24	b	611	CLA	O2A-CGA-CBA	2.67	119.99	111.83
27	a	411	SQD	C1-O5-C5	2.67	118.94	113.72
24	A	405	CLA	C4C-C3C-C2C	-2.67	103.00	106.89
24	C	513	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
24	c	503	CLA	O2A-CGA-CBA	2.67	119.97	111.83
24	b	608	CLA	CMA-C3A-C4A	-2.67	104.60	111.77
24	B	603	CLA	C4C-C3C-C2C	-2.67	103.01	106.89
27	f	101	SQD	O48-C23-C24	2.67	119.97	111.83
24	b	603	CLA	C4-C3-C5	2.66	119.85	115.23
26	c	517	BCR	C20-C21-C22	-2.66	123.54	127.28
24	D	403	CLA	C1-C2-C3	-2.66	121.84	126.20
24	A	409	CLA	C2A-C1A-CHA	-2.66	119.25	123.87
24	C	510	CLA	CHC-C1C-C2C	-2.66	119.38	126.95
24	c	503	CLA	CHD-C4C-NC	2.66	128.36	124.23
26	D	404	BCR	C16-C17-C18	-2.66	123.55	127.28
24	C	508	CLA	C3B-C4B-NB	2.66	112.91	110.53
24	c	512	CLA	O2A-CGA-O1A	-2.66	116.97	123.63
33	c	521	LMG	C8-O7-C10	-2.66	111.43	117.80
24	B	616	CLA	CHC-C1C-C2C	-2.66	119.39	126.95
26	C	516	BCR	C15-C16-C17	-2.66	118.08	123.52
24	b	603	CLA	CHD-C4C-NC	2.66	128.35	124.23
24	c	503	CLA	CBC-CAC-C3C	-2.66	105.21	112.42
26	b	619	BCR	C16-C17-C18	-2.66	123.55	127.28
26	H	101	BCR	C2-C1-C6	2.65	114.29	110.44
24	C	512	CLA	CHD-C4C-NC	2.65	128.34	124.23
24	A	409	CLA	O2A-CGA-CBA	2.65	119.92	111.83
24	b	604	CLA	O2A-CGA-O1A	-2.65	117.00	123.63
24	b	613	CLA	C4B-C3B-C2B	-2.65	104.01	107.30
24	b	616	CLA	CHC-C1C-C2C	-2.65	119.42	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	604	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
26	T	101	BCR	C3-C4-C5	-2.65	109.33	114.06
24	C	513	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
24	c	508	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
24	b	611	CLA	O2A-CGA-O1A	-2.65	117.01	123.63
35	b	625	HTG	O5-C1-C2	2.64	113.96	110.32
24	c	508	CLA	O2A-CGA-CBA	2.64	119.90	111.83
24	d	402	CLA	O2A-CGA-O1A	-2.64	117.01	123.63
24	B	602	CLA	CHD-C4C-NC	2.64	128.33	124.23
24	B	607	CLA	CAA-C2A-C3A	-2.64	105.86	113.00
26	k	101	BCR	C7-C8-C9	-2.64	122.33	126.23
24	d	402	CLA	CHC-C1C-C2C	-2.64	119.45	126.95
24	C	502	CLA	CBC-CAC-C3C	-2.64	105.26	112.42
24	c	514	CLA	CBC-CAC-C3C	-2.64	105.27	112.42
24	c	508	CLA	CAC-C3C-C4C	2.64	128.22	124.79
24	c	505	CLA	CHD-C4C-NC	2.64	128.32	124.23
24	B	616	CLA	C1C-C2C-C3C	-2.64	104.21	106.98
24	C	513	CLA	CBA-CAA-C2A	-2.64	105.95	113.79
26	B	618	BCR	C24-C23-C22	-2.64	122.33	126.23
24	b	616	CLA	OBD-CAD-C3D	-2.64	122.25	128.42
24	C	510	CLA	CHD-C4C-NC	2.63	128.31	124.23
24	c	507	CLA	O2A-CGA-CBA	2.63	119.85	111.83
24	B	610	CLA	C1-C2-C3	-2.63	121.89	126.20
24	A	404	CLA	CHD-C4C-NC	2.63	128.31	124.23
24	B	603	CLA	C7-C6-C5	-2.63	106.26	113.26
24	c	506	CLA	CMB-C2B-C1B	2.63	129.42	125.42
26	T	101	BCR	C2-C1-C6	2.62	114.25	110.44
38	D	406	LHG	O8-C23-O10	-2.62	117.06	123.63
24	C	508	CLA	C1-C2-C3	-2.62	121.90	126.20
31	a	414[B]	PL9	C40-C39-C41	2.62	119.78	115.23
24	b	612	CLA	O2A-CGA-O1A	-2.62	117.07	123.63
24	b	615	CLA	CHD-C4C-NC	2.62	128.29	124.23
26	B	619	BCR	C21-C20-C19	-2.62	115.61	123.20
24	C	502	CLA	C2A-C1A-CHA	-2.62	119.32	123.87
24	c	508	CLA	CHD-C4C-NC	2.62	128.29	124.23
25	A	407	PHO	CMB-C2B-C3B	2.62	129.92	124.68
26	Y	101	BCR	C37-C22-C23	2.62	122.09	118.09
26	a	408	BCR	C29-C30-C25	2.62	114.24	110.44
24	b	607	CLA	CBC-CAC-C3C	-2.61	105.33	112.42
24	B	606	CLA	C3B-C4B-NB	2.61	112.86	110.53
33	Z	101	LMG	O6-C1-C2	2.61	115.74	110.37
24	b	604	CLA	CHD-C4C-NC	2.61	128.28	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	j	101	LMG	O8-C28-C29	2.61	119.80	111.83
33	c	522	LMG	C3-C4-C5	2.61	114.97	110.23
24	C	502	CLA	C3B-C4B-NB	2.61	112.86	110.53
24	c	508	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
41	V	203	HEC	CHB-C1B-NB	2.61	128.59	123.86
24	C	507	CLA	CMB-C2B-C1B	2.61	129.39	125.42
24	a	403	CLA	C17-C16-C15	-2.61	101.59	113.28
24	c	506	CLA	C4C-C3C-C2C	-2.61	103.09	106.89
36	C	519	DGD	O2G-C1B-C2B	2.61	117.12	111.48
24	C	505	CLA	C2A-C1A-CHA	-2.61	119.34	123.87
24	A	404	CLA	CHC-C1C-C2C	-2.61	119.54	126.95
24	B	613	CLA	CHB-C4A-NA	2.60	128.16	124.40
35	B	623	HTG	C1-O5-C5	2.60	117.23	112.56
24	B	601	CLA	CMB-C2B-C1B	2.60	129.38	125.42
24	b	603	CLA	CMC-C2C-C1C	2.60	129.10	125.03
24	C	507	CLA	C2A-C1A-CHA	-2.60	119.35	123.87
24	C	514	CLA	CHD-C4C-NC	2.60	128.27	124.23
24	B	608	CLA	CHB-C4A-NA	2.60	128.16	124.40
24	c	515	CLA	O2A-CGA-CBA	2.60	119.77	111.83
27	F	101	SQD	O48-C23-C24	2.60	119.77	111.83
26	c	516	BCR	C33-C5-C6	-2.60	121.65	124.48
24	b	613	CLA	CHC-C1C-C2C	-2.60	119.56	126.95
24	a	350	CLA	C4C-C3C-C2C	-2.60	103.11	106.89
24	B	602	CLA	CHC-C1C-C2C	-2.60	119.56	126.95
24	C	505	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
24	A	404	CLA	CAA-CBA-CGA	-2.60	105.83	113.21
24	C	509	CLA	O2A-CGA-CBA	2.60	119.75	111.83
24	b	614	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
24	B	605	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
24	c	507	CLA	C1-C2-C3	-2.60	121.94	126.20
24	C	514	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
31	D	405	PL9	C25-C24-C26	2.60	119.73	115.23
24	a	350	CLA	O2A-CGA-CBA	2.60	119.75	111.83
24	b	609	CLA	CHD-C4C-NC	2.59	128.25	124.23
26	B	619	BCR	C3-C4-C5	-2.59	109.43	114.06
24	C	513	CLA	C3B-C4B-NB	2.59	112.84	110.53
35	B	625	HTG	O5-C1-C2	2.59	113.89	110.32
24	B	611	CLA	OBD-CAD-C3D	-2.59	122.36	128.42
24	a	404	CLA	O2A-CGA-CBA	2.59	119.74	111.83
24	c	507	CLA	C4-C3-C5	2.59	119.72	115.23
24	d	402	CLA	CAA-C2A-C3A	-2.59	106.00	113.00
33	Z	101	LMG	C3-C4-C5	2.59	114.92	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	102	BCR	C10-C11-C12	-2.58	115.71	123.20
39	e	102	HEM	C3B-C4B-NB	-2.58	107.61	109.47
24	b	616	CLA	C4-C3-C5	2.58	119.71	115.23
24	C	502	CLA	O2A-CGA-CBA	2.58	119.71	111.83
35	C	522	HTG	C1-O5-C5	2.58	117.19	112.56
38	l	101	LHG	O8-C23-O10	-2.58	117.17	123.63
41	v	203	HEC	C2A-C1A-NA	-2.58	107.83	110.32
24	b	607	CLA	O2A-CGA-O1A	-2.58	117.18	123.63
24	c	515	CLA	C4-C3-C5	2.58	119.70	115.23
26	b	618	BCR	C24-C23-C22	-2.57	122.43	126.23
24	B	611	CLA	C2A-C1A-CHA	-2.57	119.41	123.87
27	f	101	SQD	O47-C7-O49	-2.57	117.70	123.70
36	c	519	DGD	O1G-C1A-C2A	2.57	119.66	111.83
24	C	509	CLA	C4-C3-C5	2.57	119.68	115.23
26	H	101	BCR	C3-C4-C5	-2.56	109.48	114.06
24	B	614	CLA	C4C-C3C-C2C	-2.56	103.16	106.89
26	B	619	BCR	C7-C8-C9	-2.56	122.44	126.23
31	D	405	PL9	C22-C23-C24	-2.56	121.76	127.62
26	Y	101	BCR	C29-C30-C25	2.56	114.16	110.44
26	d	404	BCR	C16-C17-C18	-2.56	123.69	127.28
36	c	518	DGD	O3G-C3G-C2G	-2.56	104.59	110.82
24	C	512	CLA	O2A-CGA-CBA	2.56	119.64	111.83
24	A	406	CLA	C4B-C3B-C2B	-2.56	104.12	107.30
26	c	517	BCR	C24-C23-C22	-2.56	122.45	126.23
24	b	608	CLA	CMC-C2C-C1C	2.56	129.03	125.03
26	C	516	BCR	C37-C22-C23	2.56	121.99	118.09
24	b	616	CLA	CAC-C3C-C4C	2.56	128.12	124.79
26	B	618	BCR	C33-C5-C6	-2.56	121.70	124.48
24	C	502	CLA	C1-O2A-CGA	2.55	122.83	116.65
24	B	612	CLA	CMC-C2C-C1C	2.55	129.03	125.03
38	D	406	LHG	O7-C7-C8	2.55	117.01	111.48
38	a	419	LHG	O8-C23-C24	2.55	119.62	111.83
24	a	403	CLA	CMA-C3A-C2A	-2.55	104.11	113.98
24	B	615	CLA	O2A-CGA-CBA	2.55	119.62	111.83
24	A	406	CLA	C3B-C4B-NB	2.55	112.81	110.53
24	c	503	CLA	CMB-C2B-C1B	2.55	129.30	125.42
24	b	607	CLA	C2A-C1A-CHA	-2.55	119.44	123.87
27	F	101	SQD	O47-C7-O49	-2.55	117.75	123.70
41	v	203	HEC	CHB-C1B-NB	2.55	128.48	123.86
24	C	508	CLA	CHD-C4C-NC	2.55	128.18	124.23
24	C	511	CLA	CMC-C2C-C1C	2.55	129.02	125.03
24	b	615	CLA	O2A-CGA-CBA	2.55	119.60	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	515	CLA	CMB-C2B-C1B	2.54	129.29	125.42
24	a	403	CLA	CMC-C2C-C1C	2.54	129.01	125.03
31	d	405	PL9	C17-C18-C19	-2.54	121.81	127.62
24	C	514	CLA	O2A-CGA-CBA	2.54	119.58	111.83
24	A	409	CLA	CMB-C2B-C1B	2.54	129.29	125.42
24	b	606	CLA	CMC-C2C-C1C	2.54	129.00	125.03
33	A	418	LMG	O1-C1-C2	2.54	112.13	108.27
24	c	514	CLA	CHB-C4A-NA	2.54	128.06	124.40
24	d	403	CLA	O2A-CGA-CBA	2.54	119.57	111.83
26	C	515	BCR	C11-C10-C9	-2.54	123.72	127.28
26	c	516	BCR	C24-C23-C22	-2.54	122.48	126.23
33	Z	101	LMG	C9-C8-C7	-2.54	105.87	111.78
26	B	617	BCR	C31-C1-C6	-2.54	106.27	110.24
27	F	101	SQD	O8-S-C6	2.54	110.87	105.97
24	B	613	CLA	C2A-C1A-CHA	-2.54	119.47	123.87
24	b	610	CLA	CHD-C4C-NC	2.54	128.16	124.23
24	C	514	CLA	C4B-C3B-C2B	-2.53	104.15	107.30
27	f	101	SQD	O5-C1-C2	2.53	115.57	110.37
26	t	102	BCR	C21-C20-C19	-2.53	115.87	123.20
33	Z	101	LMG	C4-C3-C2	2.53	115.27	110.83
26	y	101	BCR	C40-C30-C25	-2.53	106.28	110.24
24	B	614	CLA	C4B-C3B-C2B	-2.53	104.16	107.30
24	b	614	CLA	CHD-C4C-NC	2.53	128.15	124.23
26	y	101	BCR	C35-C13-C12	2.52	121.94	118.09
26	a	408	BCR	C33-C5-C6	-2.52	121.73	124.48
24	C	511	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
38	L	101	LHG	O8-C23-C24	2.52	119.53	111.83
24	b	616	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
33	A	418	LMG	O8-C28-C29	2.52	119.52	111.83
24	a	403	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
26	T	101	BCR	C1-C6-C7	2.52	122.49	115.65
24	A	409	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
39	E	103	HEM	CHA-C4D-ND	2.52	127.48	124.37
31	d	405	PL9	C25-C24-C26	2.52	119.60	115.23
24	A	409	CLA	CMA-C3A-C4A	-2.52	105.00	111.77
24	C	502	CLA	CAC-C3C-C4C	2.52	128.07	124.79
27	b	620	SQD	O48-C23-C24	2.52	119.51	111.83
24	A	405	CLA	O2A-CGA-O1A	-2.52	117.34	123.63
24	b	605	CLA	CBC-CAC-C3C	-2.52	105.60	112.42
33	a	417	LMG	C3-C4-C5	2.51	114.79	110.23
24	c	507	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
24	c	513	CLA	C4B-C3B-C2B	-2.51	104.18	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	405	PL9	C10-C9-C11	2.51	119.59	115.23
26	C	516	BCR	C21-C20-C19	-2.51	115.92	123.20
26	b	619	BCR	C21-C20-C19	-2.51	115.92	123.20
24	b	607	CLA	CHD-C4C-NC	2.51	128.12	124.23
39	e	102	HEM	C4C-NC-C1C	2.51	109.91	105.82
39	e	102	HEM	C4D-ND-C1D	2.51	108.18	105.21
24	b	602	CLA	C1-O2A-CGA	2.51	122.72	116.65
24	c	513	CLA	CBC-CAC-C3C	-2.51	105.62	112.42
24	B	604	CLA	CHC-C1C-C2C	-2.50	119.83	126.95
26	b	618	BCR	C16-C17-C18	-2.50	123.77	127.28
31	a	414[B]	PL9	C53-C6-C1	2.50	120.40	115.28
27	b	620	SQD	C1-O5-C5	-2.50	108.84	113.72
38	d	406	LHG	C5-O7-C7	-2.50	111.82	117.80
25	a	405	PHO	O2A-CGA-CBA	2.50	119.45	111.83
24	B	601	CLA	C4-C3-C5	2.50	119.56	115.23
24	b	602	CLA	C11-C10-C8	-2.50	107.67	115.97
24	B	604	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
41	v	203	HEC	C4B-NB-C1B	2.49	109.89	105.82
31	A	416[A]	PL9	C45-C44-C46	2.49	119.55	115.23
24	b	606	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
24	C	508	CLA	CMC-C2C-C1C	2.49	128.93	125.03
24	D	403	CLA	CHC-C1C-C2C	-2.49	119.87	126.95
24	B	601	CLA	CAC-C3C-C4C	2.49	128.03	124.79
24	A	409	CLA	CBC-CAC-C3C	-2.49	105.67	112.42
24	B	605	CLA	C2A-C1A-CHA	-2.49	119.55	123.87
35	B	623	HTG	O2-C2-C3	-2.49	104.51	110.38
26	C	516	BCR	C3-C4-C5	-2.49	109.62	114.06
24	C	508	CLA	O2A-CGA-CBA	2.49	119.42	111.83
24	b	602	CLA	CMA-C3A-C2A	-2.49	104.37	113.98
26	c	517	BCR	C15-C14-C13	-2.49	123.79	127.28
24	c	506	CLA	O2A-CGA-CBA	2.49	119.42	111.83
24	C	514	CLA	CAA-C2A-C3A	-2.49	106.28	113.00
24	B	602	CLA	CED-O2D-CGD	2.48	121.55	115.92
36	h	103	DGD	O2G-C1B-C2B	2.48	116.85	111.48
24	B	601	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
24	c	511	CLA	CBC-CAC-C3C	-2.48	105.69	112.42
31	d	405	PL9	C32-C33-C34	-2.48	121.95	127.62
27	A	411	SQD	O48-C23-O10	-2.48	117.43	123.63
31	A	416[B]	PL9	C47-C48-C49	-2.48	119.38	127.64
24	A	406	CLA	CHC-C1C-C2C	-2.48	119.91	126.95
31	d	405	PL9	C27-C28-C29	-2.48	121.96	127.62
26	d	404	BCR	C37-C22-C23	2.48	121.87	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	CAC-C3C-C4C	2.47	128.01	124.79
24	C	507	CLA	C4C-C3C-C2C	-2.47	103.29	106.89
24	C	504	CLA	CHD-C4C-NC	2.47	128.07	124.23
26	K	102	BCR	C2-C1-C6	2.47	114.03	110.44
35	b	628	HTG	O5-C5-C4	2.47	114.15	109.70
24	d	402	CLA	C2A-C1A-CHA	-2.47	119.58	123.87
24	B	609	CLA	CBC-CAC-C3C	-2.47	105.73	112.42
24	C	506	CLA	CHC-C1C-C2C	-2.47	119.93	126.95
41	V	203	HEC	C2A-C1A-NA	-2.47	107.94	110.32
24	c	506	CLA	CBC-CAC-C3C	-2.47	105.73	112.42
36	h	103	DGD	O1G-C1A-O1A	-2.47	117.45	123.63
31	A	416[A]	PL9	C53-C6-C1	2.47	120.33	115.28
24	B	605	CLA	O2A-CGA-CBA	2.47	119.36	111.83
31	a	414[B]	PL9	C15-C14-C16	2.47	119.51	115.23
24	D	402	CLA	C2A-C1A-CHA	-2.47	119.59	123.87
24	C	503	CLA	C4B-C3B-C2B	-2.47	104.24	107.30
24	a	407	CLA	O2A-CGA-O1A	-2.46	117.46	123.63
24	B	610	CLA	CMB-C2B-C1B	2.46	129.17	125.42
26	b	617	BCR	C24-C23-C22	-2.46	122.59	126.23
24	C	507	CLA	CMC-C2C-C1C	2.46	128.88	125.03
27	a	411	SQD	O5-C5-C4	2.46	114.14	109.70
24	c	509	CLA	O1D-CGD-CBD	-2.46	119.67	124.52
24	c	509	CLA	CBC-CAC-C3C	-2.46	105.76	112.42
24	c	510	CLA	O2A-CGA-CBA	2.46	119.33	111.83
39	E	103	HEM	C3B-C4B-NB	-2.46	107.70	109.47
26	C	516	BCR	C16-C17-C18	-2.46	123.83	127.28
25	A	407	PHO	C1-C2-C3	-2.46	122.17	126.20
24	B	604	CLA	C4-C3-C5	2.45	119.49	115.23
41	v	203	HEC	CBC-CAC-C3C	-2.45	122.53	127.43
24	b	601	CLA	O2A-CGA-CBA	2.45	119.32	111.83
25	A	408	PHO	OBD-CAD-C3D	-2.45	124.07	127.89
24	c	507	CLA	CHD-C4C-NC	2.45	128.03	124.23
24	c	510	CLA	C2A-C1A-CHA	-2.45	119.61	123.87
26	B	619	BCR	C16-C15-C14	-2.45	118.50	123.52
26	H	101	BCR	C7-C8-C9	-2.45	122.61	126.23
24	a	403	CLA	CHD-C4C-NC	2.45	128.03	124.23
24	a	350	CLA	CMA-C3A-C2A	-2.45	104.52	113.98
24	b	602	CLA	CAC-C3C-C4C	2.45	127.97	124.79
24	B	602	CLA	C2A-C1A-CHA	-2.44	119.62	123.87
26	y	101	BCR	C16-C15-C14	-2.44	118.52	123.52
26	H	101	BCR	C16-C15-C14	-2.44	118.52	123.52
24	b	602	CLA	C4-C3-C5	2.44	119.47	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	404	CLA	O2D-CGD-CBD	2.44	115.50	111.23
24	a	407	CLA	CHD-C4C-NC	2.44	128.01	124.23
24	c	515	CLA	CHD-C4C-NC	2.44	128.01	124.23
24	C	504	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
24	C	511	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
24	C	512	CLA	CMB-C2B-C1B	2.44	129.13	125.42
33	a	417	LMG	C8-O7-C10	-2.44	111.96	117.80
24	c	512	CLA	C4C-C3C-C2C	-2.44	103.34	106.89
26	b	619	BCR	C24-C23-C22	-2.44	122.63	126.23
24	C	513	CLA	C4B-C3B-C2B	-2.44	104.27	107.30
24	b	602	CLA	CHC-C1C-C2C	-2.44	120.02	126.95
25	a	406	PHO	CMB-C2B-C3B	2.44	129.55	124.68
38	d	406	LHG	O7-C7-O9	-2.44	118.01	123.70
24	C	503	CLA	CMC-C2C-C1C	2.44	128.84	125.03
26	b	617	BCR	C36-C18-C19	2.44	121.81	118.09
38	d	407	LHG	O7-C7-C8	2.44	116.75	111.48
38	d	407	LHG	O8-C23-O10	-2.43	117.54	123.63
39	E	103	HEM	CHA-C1A-NA	2.43	128.27	123.86
24	c	511	CLA	CHD-C4C-NC	2.43	128.00	124.23
31	a	414[A]	PL9	C45-C44-C46	2.43	119.44	115.23
24	a	404	CLA	CMB-C2B-C1B	2.43	129.12	125.42
24	b	602	CLA	C1-C2-C3	-2.43	122.22	126.20
24	A	405	CLA	O2A-CGA-CBA	2.43	119.23	111.83
24	c	510	CLA	CAA-C2A-C3A	-2.42	106.45	113.00
27	F	101	SQD	C44-O6-C1	-2.42	108.60	113.80
24	B	607	CLA	C4C-C3C-C2C	-2.42	103.36	106.89
24	C	502	CLA	CMC-C2C-C1C	2.42	128.82	125.03
26	D	404	BCR	C30-C25-C24	2.42	122.22	115.65
24	b	615	CLA	CBC-CAC-C3C	-2.42	105.85	112.42
24	B	615	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
24	b	601	CLA	CAA-C2A-C3A	-2.42	106.45	113.00
24	a	407	CLA	CMB-C2B-C1B	2.42	129.10	125.42
24	B	612	CLA	O2A-CGA-CBA	2.42	119.22	111.83
27	B	620	SQD	O48-C23-O10	-2.42	117.57	123.63
24	b	608	CLA	CMB-C2B-C1B	2.42	129.10	125.42
24	b	609	CLA	O2A-CGA-CBA	2.42	119.21	111.83
24	b	606	CLA	O2A-CGA-CBA	2.42	119.21	111.83
26	B	619	BCR	C34-C9-C8	2.42	121.78	118.09
26	H	101	BCR	C24-C23-C22	-2.42	122.66	126.23
24	B	616	CLA	C1-O2A-CGA	2.41	122.50	116.65
24	B	611	CLA	CMB-C2B-C1B	2.41	129.09	125.42
24	c	504	CLA	C2A-C1A-CHA	-2.41	119.68	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	617	BCR	C15-C16-C17	-2.41	118.59	123.52
31	a	414[A]	PL9	C20-C19-C21	2.41	119.41	115.23
24	C	507	CLA	CHD-C4C-NC	2.41	127.97	124.23
41	V	203	HEC	CBC-CAC-C3C	-2.41	122.62	127.43
24	B	609	CLA	C1-C2-C3	-2.41	122.25	126.20
26	c	516	BCR	C21-C20-C19	-2.41	116.22	123.20
27	A	413	SQD	O48-C23-O10	-2.41	117.61	123.63
26	Y	101	BCR	C21-C20-C19	-2.41	116.23	123.20
24	B	615	CLA	CBC-CAC-C3C	-2.40	105.90	112.42
24	a	407	CLA	CBC-CAC-C3C	-2.40	105.91	112.42
24	b	608	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
24	B	609	CLA	CMC-C2C-C1C	2.40	128.79	125.03
31	a	414[B]	PL9	C12-C13-C14	-2.40	122.13	127.62
24	c	508	CLA	C2A-C1A-CHA	-2.40	119.70	123.87
25	a	405	PHO	CMB-C2B-C3B	2.40	129.48	124.68
26	B	617	BCR	C11-C10-C9	-2.40	123.92	127.28
35	b	623	HTG	O5-C5-C4	2.40	114.02	109.70
24	B	602	CLA	CMC-C2C-C1C	2.40	128.78	125.03
24	B	609	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
36	c	519	DGD	C2G-O2G-C1B	-2.40	112.06	117.80
27	f	101	SQD	O5-C5-C4	2.40	114.02	109.70
34	I	101	LMT	O5'-C5'-C4'	2.40	114.67	109.72
24	b	612	CLA	CHD-C4C-NC	2.39	127.94	124.23
26	a	408	BCR	C37-C22-C23	2.39	121.74	118.09
24	C	503	CLA	C4-C3-C5	2.39	119.38	115.23
26	T	101	BCR	C7-C6-C5	-2.39	116.04	121.56
33	J	101	LMG	O8-C28-C29	2.39	119.13	111.83
31	a	414[B]	PL9	C30-C29-C31	2.39	119.38	115.23
24	C	509	CLA	CHD-C4C-NC	2.39	127.94	124.23
24	B	616	CLA	CAC-C3C-C4C	2.39	127.90	124.79
24	B	607	CLA	C2A-C1A-CHA	-2.39	119.72	123.87
38	D	406	LHG	O8-C23-C24	2.39	119.12	111.83
24	C	503	CLA	C2A-C1A-CHA	-2.39	119.72	123.87
24	c	513	CLA	CMC-C2C-C1C	2.39	128.77	125.03
24	D	403	CLA	O2A-CGA-CBA	2.39	119.11	111.83
24	b	610	CLA	C4B-C3B-C2B	-2.39	104.33	107.30
24	B	615	CLA	CHC-C1C-C2C	-2.39	120.16	126.95
24	b	605	CLA	O2A-CGA-CBA	2.39	119.11	111.83
24	C	508	CLA	C4B-C3B-C2B	-2.39	104.33	107.30
24	A	404	CLA	CMA-C3A-C2A	-2.39	104.75	113.98
26	k	101	BCR	C16-C17-C18	-2.39	123.93	127.28
33	C	520	LMG	O8-C28-O10	-2.39	117.66	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	CBC-CAC-C3C	-2.39	105.95	112.42
38	D	357	LHG	O7-C7-O9	-2.38	118.13	123.70
24	b	614	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
26	K	102	BCR	C15-C14-C13	-2.38	123.94	127.28
24	b	613	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
24	B	608	CLA	CMC-C2C-C1C	2.38	128.75	125.03
31	A	416[B]	PL9	C20-C19-C21	2.38	119.36	115.23
24	B	605	CLA	C7-C6-C5	-2.38	106.92	113.26
26	A	410	BCR	C20-C21-C22	-2.38	123.94	127.28
24	c	509	CLA	C1-C2-C3	-2.38	122.30	126.20
27	b	620	SQD	C44-O6-C1	-2.38	108.70	113.80
24	C	511	CLA	C2A-C1A-CHA	-2.38	119.74	123.87
24	b	601	CLA	C2A-C1A-CHA	-2.38	119.74	123.87
26	b	618	BCR	C38-C26-C25	-2.38	121.89	124.48
24	B	606	CLA	C2A-C1A-CHA	-2.38	119.74	123.87
24	B	612	CLA	C11-C12-C13	-2.37	108.08	115.97
35	h	101	HTG	C1-O5-C5	2.37	116.82	112.56
24	A	405	CLA	CMB-C2B-C1B	2.37	129.03	125.42
24	B	602	CLA	CHB-C1B-C2B	-2.37	120.54	127.43
25	a	405	PHO	CBA-CAA-C2A	-2.37	106.79	113.78
26	c	516	BCR	C37-C22-C21	-2.37	118.97	122.82
24	c	507	CLA	CHC-C1C-C2C	-2.37	120.21	126.95
24	C	511	CLA	CMB-C2B-C1B	2.37	129.03	125.42
31	A	416[A]	PL9	C40-C39-C41	2.37	119.34	115.23
26	K	102	BCR	C36-C18-C19	2.37	121.71	118.09
31	A	416[A]	PL9	C37-C36-C34	-2.37	105.34	113.19
24	B	615	CLA	CED-O2D-CGD	2.36	121.28	115.92
24	B	606	CLA	CHB-C1B-C2B	-2.36	120.56	127.43
24	a	404	CLA	CBC-CAC-C3C	-2.36	106.01	112.42
31	A	416[B]	PL9	C40-C39-C41	2.36	119.33	115.23
25	a	406	PHO	O1D-CGD-CBD	-2.36	121.14	124.72
26	d	404	BCR	C16-C15-C14	-2.36	118.69	123.52
26	B	619	BCR	C10-C11-C12	-2.36	116.36	123.20
24	A	409	CLA	CAC-C3C-C4C	2.36	127.86	124.79
26	a	408	BCR	C15-C16-C17	-2.36	118.69	123.52
26	B	619	BCR	C20-C21-C22	-2.36	123.97	127.28
33	C	520	LMG	O6-C5-C6	2.36	112.29	106.44
24	d	403	CLA	CBC-CAC-C3C	-2.36	106.02	112.42
24	b	615	CLA	C11-C12-C13	-2.36	108.13	115.97
24	c	503	CLA	CMC-C2C-C1C	2.36	128.72	125.03
24	C	508	CLA	C6-C7-C8	-2.36	108.13	115.97
26	t	102	BCR	C15-C16-C17	-2.35	118.70	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	M	103	LMT	C1'-O5'-C5'	2.35	118.32	113.72
26	B	618	BCR	C10-C11-C12	-2.35	116.38	123.20
33	j	101	LMG	O7-C10-O9	-2.35	118.20	123.70
24	a	404	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
24	D	402	CLA	CMC-C2C-C1C	2.35	128.71	125.03
24	B	611	CLA	CAC-C3C-C4C	2.35	127.85	124.79
24	C	508	CLA	CAC-C3C-C4C	2.35	127.85	124.79
41	V	203	HEC	CHD-C1D-ND	2.35	128.12	123.86
31	D	405	PL9	C40-C39-C38	-2.35	117.59	123.63
24	c	506	CLA	C4-C3-C5	2.35	119.31	115.23
24	c	504	CLA	CAC-C3C-C4C	2.35	127.84	124.79
24	B	601	CLA	C2A-C1A-CHA	-2.35	119.80	123.87
24	C	509	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
24	B	610	CLA	C2A-C1A-CHA	-2.35	119.80	123.87
24	c	509	CLA	O2A-CGA-CBA	2.34	118.98	111.83
24	c	514	CLA	C4B-C3B-C2B	-2.34	104.39	107.30
24	A	406	CLA	C4-C3-C5	2.34	119.29	115.23
24	C	511	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
31	A	416[A]	PL9	C2-C3-C4	2.34	121.92	118.78
24	B	610	CLA	CHB-C4A-NA	2.34	127.78	124.40
24	c	515	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
24	B	615	CLA	C4-C3-C5	2.34	119.29	115.23
34	M	101	LMT	O1B-C1B-C2B	2.34	113.84	108.09
24	C	506	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
24	b	610	CLA	C2A-C1A-CHA	-2.34	119.81	123.87
36	C	518	DGD	C2G-O2G-C1B	-2.33	112.21	117.80
24	B	611	CLA	O2A-CGA-CBA	2.33	118.95	111.83
24	B	612	CLA	CHD-C4C-NC	2.33	127.85	124.23
24	b	606	CLA	C1-C2-C3	-2.33	122.38	126.20
26	h	102	BCR	C37-C22-C21	-2.33	119.04	122.82
26	t	102	BCR	C10-C11-C12	-2.33	116.44	123.20
24	c	512	CLA	CMB-C2B-C1B	2.33	128.97	125.42
38	d	407	LHG	O8-C23-C24	2.33	118.93	111.83
24	B	615	CLA	CAC-C3C-C4C	2.33	127.82	124.79
27	a	409	SQD	O48-C23-O10	-2.33	117.81	123.63
26	b	618	BCR	C2-C1-C6	2.33	113.82	110.44
24	a	404	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
24	a	350	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
24	A	405	CLA	C3B-C4B-NB	2.33	112.61	110.53
24	b	604	CLA	C2A-C1A-CHA	-2.33	119.83	123.87
24	c	514	CLA	CBA-CAA-C2A	-2.32	106.88	113.79
24	D	403	CLA	CMA-C3A-C2A	-2.32	105.00	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	O2A-CGA-CBA	2.32	118.91	111.83
26	Y	101	BCR	C40-C30-C25	-2.32	106.60	110.24
24	C	504	CLA	O2A-CGA-CBA	2.32	118.91	111.83
31	D	405	PL9	C20-C19-C21	2.32	119.26	115.23
24	B	604	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
24	B	613	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
24	B	615	CLA	C4B-C3B-C2B	-2.32	104.42	107.30
26	B	618	BCR	C2-C1-C6	2.32	113.81	110.44
24	b	606	CLA	CHB-C1B-C2B	-2.32	120.70	127.43
34	M	101	LMT	C1-O1'-C1'	-2.32	109.72	113.68
35	C	523	HTG	O5-C1-C2	2.32	113.51	110.32
24	c	503	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
24	d	403	CLA	C4B-C3B-C2B	-2.31	104.42	107.30
24	d	402	CLA	CBC-CAC-C3C	-2.31	106.15	112.42
26	C	515	BCR	C37-C22-C23	2.31	121.62	118.09
25	a	405	PHO	C4A-C3A-C2A	-2.31	100.64	102.84
26	c	517	BCR	C15-C16-C17	-2.31	118.79	123.52
31	D	405	PL9	C7-C8-C9	-2.31	122.85	126.83
24	A	405	CLA	CHC-C1C-C2C	-2.31	120.38	126.95
26	a	408	BCR	C37-C22-C21	-2.31	119.08	122.82
31	a	414[A]	PL9	C53-C6-C1	2.31	120.00	115.28
25	A	408	PHO	O2A-CGA-O1A	-2.31	117.86	123.63
24	a	350	CLA	CED-O2D-CGD	2.31	121.14	115.92
24	a	404	CLA	C2A-C1A-CHA	-2.30	119.87	123.87
26	b	619	BCR	C16-C15-C14	-2.30	118.81	123.52
26	k	101	BCR	C15-C16-C17	-2.30	118.81	123.52
24	B	616	CLA	C4-C3-C5	2.30	119.23	115.23
24	c	513	CLA	CAA-CBA-CGA	-2.30	106.67	113.21
24	d	403	CLA	CHC-C1C-C2C	-2.30	120.41	126.95
24	c	507	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
24	c	506	CLA	C1-O2A-CGA	2.30	122.22	116.65
31	a	414[A]	PL9	C47-C48-C49	-2.30	119.97	127.64
24	c	512	CLA	C2A-C1A-CHA	-2.30	119.87	123.87
24	B	607	CLA	C1-O2A-CGA	2.30	122.21	116.65
34	B	622	LMT	O5'-C5'-C4'	2.30	114.47	109.72
27	A	411	SQD	O9-S-O7	-2.30	106.35	113.82
27	A	411	SQD	O47-C7-O49	-2.30	118.33	123.70
24	b	606	CLA	C6-C7-C8	-2.30	108.33	115.97
34	B	630	LMT	C1-O1'-C1'	-2.30	109.76	113.68
24	c	507	CLA	C3B-C4B-NB	2.30	112.58	110.53
35	B	623	HTG	O5-C1-C2	2.29	113.48	110.32
24	B	606	CLA	O2A-CGA-O1A	-2.29	117.89	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	H	102	DGD	C2G-O2G-C1B	-2.29	112.31	117.80
24	B	606	CLA	CHC-C1C-C2C	-2.29	120.43	126.95
26	c	516	BCR	C7-C8-C9	-2.29	122.84	126.23
24	a	407	CLA	C2A-C1A-CHA	-2.29	119.89	123.87
26	h	102	BCR	C35-C13-C12	2.29	121.59	118.09
25	A	408	PHO	C4A-C3A-C2A	-2.29	100.66	102.84
36	H	102	DGD	O1G-C1A-O1A	-2.29	117.90	123.63
26	y	101	BCR	C11-C10-C9	-2.29	124.07	127.28
26	a	408	BCR	C10-C11-C12	-2.29	116.57	123.20
24	b	602	CLA	O2A-CGA-CBA	2.29	118.81	111.83
26	h	102	BCR	C16-C15-C14	-2.29	118.84	123.52
24	c	503	CLA	C4-C3-C5	2.29	119.20	115.23
24	c	511	CLA	CMC-C2C-C1C	2.29	128.61	125.03
26	K	102	BCR	C29-C30-C25	2.29	113.76	110.44
25	a	405	PHO	O2A-CGA-O1A	-2.29	117.91	123.63
26	h	102	BCR	C20-C21-C22	-2.29	124.07	127.28
24	B	610	CLA	CMA-C3A-C2A	-2.29	105.15	113.98
25	A	407	PHO	O2A-CGA-CBA	2.28	118.80	111.83
24	d	402	CLA	CHD-C4C-NC	2.28	127.77	124.23
24	B	608	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
24	C	510	CLA	C4-C3-C5	2.28	119.19	115.23
24	b	604	CLA	C4-C3-C5	2.28	119.19	115.23
24	D	403	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
25	A	407	PHO	CBA-CAA-C2A	-2.28	107.06	113.78
27	B	620	SQD	O47-C7-O49	-2.28	118.38	123.70
31	d	405	PL9	C35-C34-C36	2.28	119.18	115.23
24	d	402	CLA	CHB-C4A-NA	2.28	127.69	124.40
26	y	101	BCR	C23-C24-C25	-2.28	120.91	127.00
24	C	511	CLA	C4-C3-C2	-2.28	117.78	123.63
24	B	601	CLA	CBC-CAC-C3C	-2.28	106.25	112.42
36	c	519	DGD	O1G-C1A-O1A	-2.28	117.94	123.63
24	c	509	CLA	C4C-C3C-C2C	-2.27	103.58	106.89
24	C	510	CLA	C2A-C1A-CHA	-2.27	119.92	123.87
24	b	609	CLA	C4-C3-C5	2.27	119.17	115.23
24	c	513	CLA	CAC-C3C-C4C	2.27	127.74	124.79
24	D	402	CLA	CMA-C3A-C4A	-2.27	105.68	111.77
34	m	102	LMT	C1-O1'-C1'	-2.27	109.81	113.68
31	d	405	PL9	C20-C19-C18	-2.27	117.80	123.63
25	A	408	PHO	O2A-CGA-CBA	2.27	118.75	111.83
26	H	101	BCR	C31-C1-C6	-2.27	106.69	110.24
26	t	102	BCR	C36-C18-C19	2.27	121.55	118.09
24	B	605	CLA	CMC-C2C-C1C	2.27	128.57	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	619	BCR	C39-C30-C25	-2.27	106.69	110.24
24	c	514	CLA	CAA-C2A-C3A	-2.26	106.88	113.00
24	C	505	CLA	CHD-C4C-NC	2.26	127.74	124.23
24	c	505	CLA	CMC-C2C-C1C	2.26	128.57	125.03
26	T	101	BCR	C15-C14-C13	2.26	130.45	127.28
41	v	203	HEC	O2A-CGA-CBA	2.26	121.14	114.00
41	v	203	HEC	O2D-CGD-CBD	2.26	121.14	114.00
24	B	612	CLA	C6-C5-C3	-2.26	107.97	113.47
24	C	505	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
26	Y	101	BCR	C34-C9-C8	2.26	121.53	118.09
33	J	101	LMG	O8-C28-O10	-2.26	117.99	123.63
33	c	522	LMG	O8-C28-O10	-2.26	117.99	123.63
24	b	601	CLA	C1-O2A-CGA	2.25	122.11	116.65
27	A	411	SQD	C45-O47-C7	-2.25	112.40	117.80
26	B	618	BCR	C21-C20-C19	-2.25	116.67	123.20
24	b	606	CLA	C2A-C1A-CHA	-2.25	119.95	123.87
27	b	620	SQD	C1-C2-C3	-2.25	105.27	110.01
24	b	602	CLA	C4B-C3B-C2B	-2.25	104.50	107.30
24	B	608	CLA	C4-C3-C5	2.25	119.14	115.23
24	b	603	CLA	CAC-C3C-C4C	2.25	127.72	124.79
24	c	506	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
24	b	616	CLA	C2A-C1A-CHA	-2.25	119.96	123.87
24	b	615	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
26	A	410	BCR	C10-C11-C12	-2.25	116.69	123.20
25	a	406	PHO	CMA-C3A-C4A	-2.25	109.77	114.61
24	c	505	CLA	O2A-CGA-CBA	2.24	118.68	111.83
27	F	101	SQD	O7-S-C6	2.24	110.11	106.76
24	B	605	CLA	C1-C2-C3	-2.24	122.52	126.20
26	C	515	BCR	C20-C21-C22	-2.24	124.13	127.28
25	A	408	PHO	CMA-C3A-C4A	-2.24	109.78	114.61
25	a	406	PHO	O2A-CGA-CBA	2.24	118.67	111.83
36	C	519	DGD	O3G-C3G-C2G	-2.24	105.36	110.82
34	a	359	LMT	O5'-C5'-C4'	2.24	114.36	109.72
35	c	526	HTG	O5-C5-C4	2.24	113.73	109.70
33	c	521	LMG	O7-C10-O9	-2.24	118.47	123.70
24	c	510	CLA	CMC-C2C-C1C	2.24	128.53	125.03
24	A	405	CLA	C2A-C1A-CHA	-2.24	119.98	123.87
24	b	608	CLA	C6-C7-C8	-2.24	108.53	115.97
26	A	410	BCR	C31-C1-C6	-2.24	106.74	110.24
31	A	416[A]	PL9	C51-C49-C50	2.24	119.73	114.59
24	c	507	CLA	C4B-C3B-C2B	-2.24	104.52	107.30
24	B	605	CLA	CAA-C2A-C3A	-2.23	106.96	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	503	CLA	C2A-C1A-CHA	-2.23	119.99	123.87
24	b	604	CLA	C6-C7-C8	-2.23	108.54	115.97
26	B	618	BCR	C38-C26-C25	-2.23	122.05	124.48
24	b	602	CLA	C11-C12-C13	-2.23	108.54	115.97
24	d	403	CLA	C4-C3-C5	2.23	119.11	115.23
24	B	602	CLA	O2A-CGA-CBA	2.23	118.64	111.83
31	A	416[A]	PL9	C12-C13-C14	-2.23	122.51	127.62
24	C	508	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
26	b	617	BCR	C16-C17-C18	-2.23	124.15	127.28
24	a	403	CLA	C4C-C3C-C2C	-2.23	103.64	106.89
24	D	402	CLA	CAA-C2A-C3A	-2.23	106.97	113.00
24	c	514	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
26	D	404	BCR	C40-C30-C25	-2.23	106.75	110.24
24	c	512	CLA	O1D-CGD-CBD	-2.22	120.13	124.52
31	A	416[A]	PL9	C47-C48-C49	-2.22	120.22	127.64
24	b	612	CLA	CMC-C2C-C1C	2.22	128.51	125.03
24	B	608	CLA	C2A-C1A-CHA	-2.22	120.01	123.87
24	B	616	CLA	C2A-C1A-CHA	-2.22	120.01	123.87
24	B	610	CLA	C6-C7-C8	-2.22	108.57	115.97
27	a	409	SQD	O9-S-C6	2.22	110.07	106.76
24	B	603	CLA	CHB-C1B-C2B	-2.22	120.98	127.43
24	a	403	CLA	CAA-CBA-CGA	-2.22	106.90	113.21
26	k	101	BCR	C39-C30-C25	-2.22	106.76	110.24
24	C	510	CLA	C16-C15-C13	-2.22	108.58	115.97
24	B	611	CLA	C4-C3-C5	2.22	119.08	115.23
31	d	405	PL9	C7-C8-C9	-2.22	123.01	126.83
26	c	517	BCR	C3-C4-C5	-2.22	110.10	114.06
26	t	102	BCR	C3-C4-C5	-2.22	110.10	114.06
25	a	406	PHO	CBA-CAA-C2A	-2.22	107.24	113.78
24	d	403	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
24	B	602	CLA	CMA-C3A-C2A	-2.22	105.41	113.98
24	c	511	CLA	CAA-C2A-C3A	-2.22	107.01	113.00
26	B	618	BCR	C3-C4-C5	-2.22	110.10	114.06
26	b	618	BCR	C21-C20-C19	-2.22	116.78	123.20
24	c	509	CLA	C4B-C3B-C2B	-2.22	104.55	107.30
33	Z	101	LMG	C1-O6-C5	2.22	118.05	113.72
31	a	414[B]	PL9	C47-C48-C49	-2.22	120.25	127.64
26	K	102	BCR	C38-C26-C25	-2.22	122.07	124.48
31	a	414[A]	PL9	C51-C49-C50	2.22	119.69	114.59
24	B	602	CLA	C11-C12-C13	-2.22	108.60	115.97
24	b	608	CLA	CBC-CAC-C3C	-2.21	106.42	112.42
24	B	602	CLA	C4B-C3B-C2B	-2.21	104.55	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	414[B]	PL9	C10-C9-C11	2.21	119.07	115.23
26	B	617	BCR	C21-C20-C19	-2.21	116.79	123.20
24	D	402	CLA	CBC-CAC-C3C	-2.21	106.42	112.42
24	c	511	CLA	C2A-C1A-CHA	-2.21	120.03	123.87
24	B	613	CLA	CHD-C4C-NC	2.21	127.66	124.23
31	D	405	PL9	C2-C1-C6	2.21	121.62	119.00
24	b	607	CLA	C1-C2-C3	-2.21	122.58	126.20
24	b	608	CLA	C2A-C1A-CHA	-2.21	120.04	123.87
26	K	102	BCR	C16-C17-C18	-2.21	124.18	127.28
26	D	404	BCR	C21-C20-C19	-2.21	116.81	123.20
24	b	602	CLA	CHB-C1B-C2B	-2.21	121.03	127.43
24	b	607	CLA	C6-C7-C8	-2.20	108.64	115.97
26	B	619	BCR	C11-C10-C9	-2.20	124.19	127.28
24	B	604	CLA	C6-C7-C8	-2.20	108.64	115.97
24	c	514	CLA	CMC-C2C-C1C	2.20	128.47	125.03
24	d	402	CLA	CMB-C2B-C1B	2.20	128.77	125.42
27	f	101	SQD	C4-C3-C2	-2.20	106.97	110.83
24	b	616	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
26	D	404	BCR	C15-C16-C17	-2.20	119.02	123.52
26	B	618	BCR	C15-C16-C17	-2.20	119.02	123.52
26	b	618	BCR	C37-C22-C23	2.20	121.44	118.09
24	C	505	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
26	D	404	BCR	C3-C4-C5	-2.20	110.14	114.06
24	C	508	CLA	C1-O2A-CGA	2.20	121.97	116.65
24	b	614	CLA	C4-C3-C5	2.20	119.04	115.23
31	D	405	PL9	C42-C41-C39	-2.20	105.91	113.19
24	c	512	CLA	CMA-C3A-C4A	-2.19	105.87	111.77
31	d	405	PL9	C40-C39-C38	-2.19	117.99	123.63
24	c	511	CLA	CMB-C2B-C1B	2.19	128.76	125.42
26	D	404	BCR	C24-C25-C26	-2.19	116.51	121.56
24	B	613	CLA	CMA-C3A-C4A	-2.19	105.88	111.77
34	e	101	LMT	O5'-C5'-C4'	2.19	114.25	109.72
27	A	413	SQD	O8-S-C6	2.19	110.20	105.97
38	E	101	LHG	O8-C23-O10	-2.19	118.15	123.63
24	B	606	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
24	b	607	CLA	O2A-CGA-CBA	2.19	118.50	111.83
36	C	517	DGD	O1G-C1A-O1A	-2.19	118.16	123.63
24	c	515	CLA	CED-O2D-CGD	2.18	120.87	115.92
38	E	101	LHG	C5-O7-C7	-2.18	112.57	117.80
26	b	618	BCR	C10-C11-C12	-2.18	116.88	123.20
24	c	505	CLA	C1-C2-C3	-2.18	122.62	126.20
26	b	618	BCR	C11-C10-C9	-2.18	124.22	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	622	LMT	C1-O1'-C1'	-2.18	109.96	113.68
39	E	103	HEM	O2A-CGA-CBA	2.18	120.88	114.00
26	C	515	BCR	C21-C20-C19	-2.18	116.89	123.20
24	c	508	CLA	CHB-C4A-NA	2.18	127.54	124.40
26	A	410	BCR	C40-C30-C25	-2.18	106.83	110.24
35	B	625	HTG	C1-C2-C3	2.18	114.80	110.55
36	C	518	DGD	C3G-O3G-C1D	-2.18	109.13	113.80
24	c	506	CLA	CAA-C2A-C3A	-2.17	107.12	113.00
24	b	613	CLA	C2A-C1A-CHA	-2.17	120.10	123.87
24	C	505	CLA	CED-O2D-CGD	2.17	120.84	115.92
24	B	608	CLA	CBC-CAC-C3C	-2.17	106.53	112.42
36	c	518	DGD	O1G-C1A-C2A	2.17	118.46	111.83
38	d	408	LHG	C6-C5-C4	-2.17	106.72	111.78
26	B	619	BCR	C2-C3-C4	-2.17	106.50	111.28
24	d	403	CLA	C3B-C4B-NB	2.17	112.47	110.53
24	a	403	CLA	CBC-CAC-C3C	-2.17	106.54	112.42
26	Y	101	BCR	C16-C15-C14	-2.17	119.08	123.52
26	c	517	BCR	C29-C30-C25	2.17	113.59	110.44
26	k	101	BCR	C2-C1-C6	2.17	113.59	110.44
31	a	414[B]	PL9	C25-C24-C26	2.17	118.99	115.23
24	b	611	CLA	CAA-C2A-C3A	-2.16	107.15	113.00
24	b	606	CLA	CBC-CAC-C3C	-2.16	106.56	112.42
27	a	409	SQD	O4-C4-C3	-2.16	105.28	110.38
24	A	406	CLA	CMA-C3A-C4A	-2.16	105.97	111.77
24	A	406	CLA	CAC-C3C-C4C	2.16	127.60	124.79
27	A	413	SQD	O6-C44-C45	-2.16	105.57	110.82
33	a	417	LMG	O8-C28-C29	2.16	118.41	111.83
24	b	614	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
24	C	509	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
24	D	403	CLA	CMA-C3A-C4A	-2.15	105.99	111.77
33	B	621	LMG	O8-C28-O10	-2.15	118.25	123.63
31	D	405	PL9	C45-C44-C43	-2.15	118.10	123.63
41	v	203	HEC	CHD-C1D-ND	2.15	127.76	123.86
26	B	618	BCR	C37-C22-C21	-2.15	119.34	122.82
24	B	602	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
24	b	606	CLA	OBD-CAD-C3D	-2.15	123.40	128.42
36	C	518	DGD	O6E-C5E-C6E	2.15	111.76	106.44
26	b	617	BCR	C20-C21-C22	-2.15	124.27	127.28
26	t	102	BCR	C23-C22-C21	-2.15	115.63	119.01
24	B	612	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
24	B	603	CLA	C16-C15-C13	-2.14	108.84	115.97
24	b	609	CLA	CMA-C3A-C4A	-2.14	106.02	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	504	CLA	C4-C3-C5	2.14	118.95	115.23
24	B	607	CLA	CAC-C3C-C4C	2.14	127.58	124.79
24	b	604	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
24	A	409	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
26	b	618	BCR	C39-C30-C25	-2.14	106.89	110.24
24	c	508	CLA	CMB-C2B-C1B	2.14	128.68	125.42
24	B	602	CLA	CMA-C3A-C4A	-2.14	106.03	111.77
26	Y	101	BCR	C36-C18-C19	2.14	121.35	118.09
24	C	502	CLA	C11-C12-C13	-2.14	108.86	115.97
33	b	621	LMG	O1-C1-C2	-2.14	105.03	108.27
24	D	402	CLA	CHD-C4C-NC	2.13	127.54	124.23
34	a	359	LMT	C1B-O5B-C5B	2.13	117.88	113.72
24	B	609	CLA	C7-C6-C5	-2.13	107.58	113.26
33	A	418	LMG	C8-O7-C10	-2.13	112.70	117.80
24	b	601	CLA	CMC-C2C-C1C	2.13	128.36	125.03
24	c	506	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
24	d	403	CLA	CHB-C1B-C2B	-2.13	121.25	127.43
35	b	625	HTG	C1-O5-C5	2.13	116.38	112.56
38	E	101	LHG	O7-C7-O9	-2.12	118.74	123.70
26	h	102	BCR	C36-C18-C19	2.12	121.33	118.09
24	c	510	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
41	v	203	HEC	CBA-CAA-C2A	-2.12	106.66	112.53
39	E	103	HEM	O2D-CGD-CBD	2.12	120.71	114.00
34	t	101	LMT	C3'-C4'-C5'	-2.12	106.22	110.93
24	C	513	CLA	CBC-CAC-C3C	-2.12	106.67	112.42
24	C	507	CLA	OBD-CAD-C3D	-2.12	123.46	128.42
33	z	101	LMG	C7-O1-C1	-2.12	109.25	113.80
31	A	416[B]	PL9	C35-C34-C33	-2.12	118.18	123.63
24	C	507	CLA	CGD-CBD-CAD	-2.12	103.98	110.85
26	t	102	BCR	C12-C13-C14	-2.12	115.68	119.01
31	a	414[A]	PL9	C12-C13-C14	-2.12	122.78	127.62
33	c	521	LMG	O8-C28-O10	-2.12	118.34	123.63
24	c	505	CLA	C2A-C1A-CHA	-2.12	120.20	123.87
24	C	502	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
24	B	616	CLA	CHB-C1B-C2B	-2.11	121.29	127.43
24	C	505	CLA	OBD-CAD-C3D	-2.11	123.48	128.42
24	c	508	CLA	CGD-CBD-CAD	-2.11	104.01	110.85
26	B	619	BCR	C2-C1-C6	2.11	113.50	110.44
24	b	615	CLA	C2A-C1A-CHA	-2.11	120.21	123.87
39	e	102	HEM	CBD-CAD-C3D	-2.11	106.70	112.53
26	b	618	BCR	C8-C7-C6	-2.11	121.37	127.00
24	B	616	CLA	O1D-CGD-CBD	-2.11	120.36	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	405	PHO	C1-C2-C3	-2.11	122.75	126.20
24	C	506	CLA	C11-C10-C8	-2.10	108.97	115.97
24	c	509	CLA	CMD-C2D-C3D	-2.10	122.87	127.69
33	a	417	LMG	C30-C29-C28	-2.10	105.99	113.69
24	b	613	CLA	CAC-C3C-C2C	2.10	131.42	127.56
26	B	617	BCR	C37-C22-C23	2.10	121.30	118.09
24	C	506	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
24	c	506	CLA	CHB-C4A-NA	2.10	127.43	124.40
24	C	505	CLA	C1-O2A-CGA	2.10	121.73	116.65
38	L	101	LHG	C6-C5-C4	-2.10	106.89	111.78
24	a	350	CLA	CAA-CBA-CGA	2.10	119.17	113.21
24	b	608	CLA	C11-C10-C8	-2.10	108.99	115.97
35	B	628	HTG	O5-C5-C4	2.10	113.48	109.70
26	C	516	BCR	C2-C1-C6	2.10	113.48	110.44
31	a	414[B]	PL9	C51-C49-C50	2.10	119.41	114.59
24	C	505	CLA	O2A-CGA-CBA	2.10	118.23	111.83
24	b	613	CLA	CMC-C2C-C1C	2.09	128.31	125.03
26	B	617	BCR	C38-C26-C25	-2.09	122.20	124.48
24	b	608	CLA	OBD-CAD-C3D	-2.09	123.52	128.42
26	C	516	BCR	C36-C18-C19	2.09	121.29	118.09
24	d	403	CLA	C11-C10-C8	-2.09	109.01	115.97
24	a	404	CLA	CAC-C3C-C4C	2.09	127.51	124.79
26	k	101	BCR	C36-C18-C19	2.09	121.28	118.09
24	B	609	CLA	C2A-C1A-CHA	-2.09	120.24	123.87
27	a	411	SQD	C3-C4-C5	2.09	114.02	110.23
24	B	616	CLA	CHA-C1A-NA	-2.09	121.66	126.39
39	e	102	HEM	CHA-C1A-NA	2.09	127.65	123.86
24	B	606	CLA	CAC-C3C-C4C	2.09	127.51	124.79
24	C	513	CLA	CHB-C1B-C2B	-2.09	121.37	127.43
41	V	203	HEC	CBD-CAD-C3D	-2.09	106.76	112.53
24	b	603	CLA	CHB-C1B-C2B	-2.09	121.37	127.43
24	C	512	CLA	C2A-C1A-CHA	-2.09	120.25	123.87
24	b	615	CLA	C1-O2A-CGA	2.08	121.69	116.65
24	C	507	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
24	C	513	CLA	CHB-C4A-NA	2.08	127.41	124.40
24	C	514	CLA	CBC-CAC-C3C	-2.08	106.78	112.42
26	c	517	BCR	C37-C22-C23	2.08	121.27	118.09
24	b	611	CLA	CAC-C3C-C4C	2.08	127.50	124.79
24	B	607	CLA	O2A-CGA-CBA	2.08	118.18	111.83
39	E	103	HEM	C4D-ND-C1D	2.08	107.67	105.21
24	b	611	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
24	d	402	CLA	CMA-C3A-C4A	-2.08	106.19	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	612	CLA	C11-C12-C13	-2.08	109.06	115.97
24	C	506	CLA	CHA-C1A-NA	-2.08	121.69	126.39
24	B	601	CLA	CAA-C2A-C3A	-2.08	107.39	113.00
24	B	614	CLA	CHB-C4A-NA	2.08	127.39	124.40
36	C	519	DGD	O1G-C1A-O1A	-2.08	118.44	123.63
26	h	102	BCR	C24-C23-C22	-2.07	123.17	126.23
31	A	416[B]	PL9	C35-C34-C36	2.07	118.83	115.23
35	C	523	HTG	C3-C4-C5	2.07	113.99	110.23
39	E	103	HEM	CMD-C2D-C1D	2.07	128.27	125.03
24	A	406	CLA	CHB-C4A-NA	2.07	127.39	124.40
35	B	623	HTG	C1-C2-C3	2.07	114.60	110.55
24	C	504	CLA	CHB-C1B-C2B	-2.07	121.42	127.43
24	b	613	CLA	CED-O2D-CGD	2.07	120.61	115.92
24	C	508	CLA	CBC-CAC-C3C	-2.07	106.81	112.42
39	e	102	HEM	CHB-C1B-C2B	-2.07	121.07	126.95
24	B	613	CLA	CED-O2D-CGD	2.07	120.60	115.92
26	d	404	BCR	C38-C26-C27	2.07	118.00	113.60
24	C	512	CLA	CBC-CAC-C3C	-2.07	106.82	112.42
24	b	615	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
24	B	615	CLA	C2A-C1A-CHA	-2.06	120.28	123.87
26	b	618	BCR	C33-C5-C6	-2.06	122.23	124.48
24	b	614	CLA	CBC-CAC-C3C	-2.06	106.83	112.42
33	c	522	LMG	C9-C8-C7	-2.06	106.98	111.78
38	L	101	LHG	O8-C23-O10	-2.06	118.47	123.63
24	b	603	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
24	c	513	CLA	C2A-C1A-CHA	-2.06	120.29	123.87
24	B	604	CLA	C2A-C1A-CHA	-2.06	120.29	123.87
26	H	101	BCR	C2-C3-C4	-2.06	106.75	111.28
26	Y	101	BCR	C1-C6-C7	2.06	121.23	115.65
24	b	606	CLA	CAC-C3C-C4C	2.06	127.47	124.79
24	a	403	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
24	c	514	CLA	CHA-C1A-NA	-2.06	121.74	126.39
27	A	411	SQD	C3-C4-C5	2.05	113.96	110.23
31	d	405	PL9	C47-C48-C49	-2.05	120.79	127.64
24	a	404	CLA	CMC-C2C-C1C	2.05	128.24	125.03
24	c	509	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
34	M	103	LMT	O1B-C1B-C2B	2.05	113.14	108.09
26	b	618	BCR	C7-C8-C9	-2.05	123.20	126.23
38	d	408	LHG	C5-O7-C7	-2.05	112.89	117.80
24	C	513	CLA	CMC-C2C-C1C	2.05	128.24	125.03
24	B	611	CLA	CAA-C2A-C3A	-2.05	107.46	113.00
26	c	516	BCR	C37-C22-C23	2.05	121.22	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	617	BCR	C11-C10-C9	-2.05	124.41	127.28
24	C	509	CLA	CMB-C2B-C1B	2.05	128.54	125.42
24	A	404	CLA	CBC-CAC-C3C	-2.05	106.87	112.42
31	D	405	PL9	C15-C14-C16	2.05	118.78	115.23
34	B	622	LMT	O1B-C4'-C3'	2.04	112.43	107.23
39	e	102	HEM	CHA-C4D-C3D	-2.04	121.46	125.23
24	B	604	CLA	C11-C12-C13	-2.04	109.17	115.97
24	B	601	CLA	CHB-C4A-NA	2.04	127.35	124.40
24	c	515	CLA	C11-C10-C8	-2.04	109.18	115.97
24	c	515	CLA	CBC-CAC-C3C	-2.04	106.89	112.42
25	A	407	PHO	C1-O2A-CGA	2.04	121.59	116.65
26	T	101	BCR	C16-C15-C14	2.04	127.69	123.52
24	C	503	CLA	CAC-C3C-C4C	2.04	127.44	124.79
24	C	510	CLA	CAA-C2A-C3A	-2.04	107.49	113.00
27	b	620	SQD	O7-S-C6	2.04	109.80	106.76
24	c	503	CLA	CHB-C1B-C2B	-2.04	121.51	127.43
24	C	510	CLA	CBC-CAC-C3C	-2.04	106.90	112.42
24	b	610	CLA	CMA-C3A-C2A	-2.03	106.12	113.98
26	B	619	BCR	C15-C14-C13	-2.03	124.43	127.28
24	A	409	CLA	CHB-C4A-NA	2.03	127.33	124.40
24	B	616	CLA	CMC-C2C-C1C	2.03	128.21	125.03
24	C	503	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
24	B	602	CLA	C4-C3-C5	2.03	118.75	115.23
38	l	101	LHG	O7-C7-O9	-2.03	118.96	123.70
24	B	606	CLA	C1-C2-C3	-2.03	122.87	126.20
24	c	513	CLA	C11-C10-C8	-2.03	109.22	115.97
24	b	609	CLA	C2A-C1A-CHA	-2.03	120.35	123.87
24	B	614	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
24	B	612	CLA	CMA-C3A-C2A	-2.02	106.15	113.98
27	a	411	SQD	O48-C23-O10	-2.02	118.56	123.63
33	C	520	LMG	O7-C10-O9	-2.02	118.97	123.70
25	a	406	PHO	C4-C3-C2	-2.02	118.43	123.63
27	a	409	SQD	C44-O6-C1	-2.02	109.46	113.80
24	C	511	CLA	CAC-C3C-C4C	2.02	127.42	124.79
24	c	505	CLA	CBC-CAC-C3C	-2.02	106.94	112.42
24	b	603	CLA	CMA-C3A-C2A	-2.02	106.17	113.98
31	D	405	PL9	C30-C29-C28	-2.02	118.44	123.63
24	a	407	CLA	OBD-CAD-C3D	-2.02	123.69	128.42
31	A	416[B]	PL9	C15-C14-C16	2.02	118.74	115.23
24	C	509	CLA	CHB-C4A-NA	2.02	127.32	124.40
31	a	414[B]	PL9	C25-C24-C23	-2.02	118.44	123.63
24	C	504	CLA	CHA-C1A-NA	-2.02	121.82	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	408	BCR	C3-C4-C5	-2.02	110.46	114.06
24	b	608	CLA	CAC-C3C-C4C	2.02	127.42	124.79
31	a	414[A]	PL9	C10-C9-C8	-2.02	118.45	123.63
24	c	514	CLA	CHB-C1B-C2B	-2.02	121.57	127.43
31	A	416[A]	PL9	C47-C46-C44	-2.02	106.51	113.19
24	A	405	CLA	CAA-CBA-CGA	2.02	118.93	113.21
27	f	101	SQD	O7-S-C6	2.01	109.76	106.76
24	C	505	CLA	CHB-C4A-NA	2.01	127.31	124.40
24	b	616	CLA	CHB-C1B-C2B	-2.01	121.58	127.43
24	b	602	CLA	CAA-CBA-CGA	-2.01	107.49	113.21
27	b	620	SQD	O47-C7-O49	-2.01	119.00	123.70
24	b	616	CLA	CHA-C1A-NA	-2.01	121.83	126.39
24	b	610	CLA	C4-C3-C2	-2.01	118.46	123.63
24	C	509	CLA	CMA-C3A-C2A	-2.01	106.21	113.98
24	B	615	CLA	CHB-C4A-NA	2.01	127.30	124.40
24	b	608	CLA	CMA-C3A-C2A	-2.01	106.22	113.98
24	b	610	CLA	CMB-C2B-C1B	2.01	128.47	125.42
24	B	615	CLA	CHA-C1A-NA	-2.01	121.85	126.39
34	A	359	LMT	O1B-C1B-C2B	2.01	113.02	108.09
31	D	405	PL9	C25-C24-C23	-2.00	118.48	123.63
24	b	612	CLA	CAA-C2A-C3A	-2.00	107.58	113.00
26	a	408	BCR	C24-C23-C22	-2.00	123.27	126.23
31	a	414[B]	PL9	C30-C29-C28	-2.00	118.48	123.63
36	c	520	DGD	O2G-C1B-O1B	-2.00	119.02	123.70
26	y	101	BCR	C1-C6-C7	2.00	121.08	115.65
31	d	405	PL9	C15-C14-C16	2.00	118.70	115.23
24	B	611	CLA	C11-C12-C13	-2.00	109.31	115.97
24	b	608	CLA	C11-C12-C13	-2.00	109.31	115.97
26	H	101	BCR	C29-C30-C25	2.00	113.35	110.44
24	c	510	CLA	CBC-CAC-C3C	-2.00	107.00	112.42

All (65) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	404	CLA	ND
24	A	405	CLA	ND
24	A	406	CLA	ND
24	B	601	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND

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Mol	Chain	Res	Type	Atom
24	B	606	CLA	ND
24	B	607	CLA	ND
24	B	609	CLA	ND
24	B	610	CLA	ND
24	B	611	CLA	ND
24	B	612	CLA	ND
24	B	613	CLA	ND
24	B	614	CLA	ND
24	B	615	CLA	ND
24	B	616	CLA	ND
24	C	502	CLA	ND
24	C	503	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	507	CLA	ND
24	C	508	CLA	ND
24	C	509	CLA	ND
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	C	514	CLA	ND
24	D	402	CLA	ND
24	D	403	CLA	ND
24	a	403	CLA	ND
24	a	407	CLA	ND
24	a	350	CLA	ND
24	b	601	CLA	ND
24	b	602	CLA	ND
24	b	603	CLA	ND
24	b	604	CLA	ND
24	b	605	CLA	ND
24	b	606	CLA	ND
24	b	607	CLA	ND
24	b	609	CLA	ND
24	b	610	CLA	ND
24	b	611	CLA	ND
24	b	612	CLA	ND
24	b	613	CLA	ND
24	b	614	CLA	ND
24	b	615	CLA	ND
24	b	616	CLA	ND

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Mol	Chain	Res	Type	Atom
24	c	503	CLA	ND
24	c	504	CLA	ND
24	c	505	CLA	ND
24	c	506	CLA	ND
24	c	507	CLA	ND
24	c	508	CLA	ND
24	c	509	CLA	ND
24	c	510	CLA	ND
24	c	511	CLA	ND
24	c	512	CLA	ND
24	c	513	CLA	ND
24	c	514	CLA	ND
24	c	515	CLA	ND
24	d	402	CLA	ND
24	d	403	CLA	ND

All (1226) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	601	CLA	CAD-CBD-CGD-O2D
24	B	603	CLA	C2B-C3B-CAB-CBB
24	B	603	CLA	C4B-C3B-CAB-CBB
24	B	614	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	C2B-C3B-CAB-CBB
24	C	503	CLA	C4B-C3B-CAB-CBB
24	C	506	CLA	C2B-C3B-CAB-CBB
24	C	506	CLA	C4B-C3B-CAB-CBB
24	C	508	CLA	C2B-C3B-CAB-CBB
24	C	508	CLA	C4B-C3B-CAB-CBB
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	C	510	CLA	CHA-CBD-CGD-O2D
24	C	514	CLA	C2B-C3B-CAB-CBB
24	C	514	CLA	C4B-C3B-CAB-CBB
24	b	603	CLA	C2B-C3B-CAB-CBB
24	b	603	CLA	C4B-C3B-CAB-CBB
24	b	604	CLA	C2B-C3B-CAB-CBB
24	b	604	CLA	C4B-C3B-CAB-CBB
24	b	614	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	c	504	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
24	c	511	CLA	C2-C1-O2A-CGA
24	c	511	CLA	CHA-CBD-CGD-O1D
24	c	511	CLA	CHA-CBD-CGD-O2D
26	D	404	BCR	C21-C22-C23-C24
26	D	404	BCR	C37-C22-C23-C24
26	H	101	BCR	C7-C8-C9-C10
26	H	101	BCR	C7-C8-C9-C34
26	T	101	BCR	C13-C14-C15-C16
26	Y	101	BCR	C1-C6-C7-C8
26	Y	101	BCR	C5-C6-C7-C8
26	d	404	BCR	C7-C8-C9-C10
26	d	404	BCR	C21-C22-C23-C24
26	d	404	BCR	C37-C22-C23-C24
26	y	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
26	y	101	BCR	C21-C22-C23-C24
27	A	413	SQD	O6-C44-C45-O47
27	B	620	SQD	O49-C7-O47-C45
27	F	101	SQD	O49-C7-O47-C45
27	F	101	SQD	C8-C7-O47-C45
27	a	411	SQD	O6-C44-C45-O47
27	a	411	SQD	C5-C6-S-O7
27	a	411	SQD	C5-C6-S-O8
27	a	411	SQD	C5-C6-S-O9
27	b	620	SQD	O49-C7-O47-C45
27	f	101	SQD	O6-C44-C45-O47
27	f	101	SQD	O49-C7-O47-C45
27	f	101	SQD	C8-C7-O47-C45
28	A	412	GOL	O1-C1-C2-C3
28	B	626	GOL	O1-C1-C2-C3
28	B	627	GOL	C1-C2-C3-O3
28	B	627	GOL	O2-C2-C3-O3
28	C	525	GOL	O1-C1-C2-C3
28	V	202	GOL	O1-C1-C2-O2
28	V	202	GOL	O1-C1-C2-C3
28	a	410	GOL	O1-C1-C2-C3
28	a	410	GOL	C1-C2-C3-O3
28	a	416	GOL	O1-C1-C2-O2
28	a	416	GOL	O1-C1-C2-C3
28	v	202	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	A	416[A]	PL9	C20-C19-C21-C22
31	A	416[B]	PL9	C7-C8-C9-C11
31	D	405	PL9	C32-C33-C34-C36
31	D	405	PL9	C42-C43-C44-C45
31	a	414[B]	PL9	C7-C8-C9-C10
31	a	414[B]	PL9	C7-C8-C9-C11
31	a	414[B]	PL9	C17-C18-C19-C20
31	a	414[B]	PL9	C22-C23-C24-C25
31	a	414[B]	PL9	C25-C24-C26-C27
33	Z	101	LMG	O9-C10-O7-C8
33	Z	101	LMG	C11-C10-O7-C8
33	c	522	LMG	C11-C10-O7-C8
33	z	101	LMG	C11-C10-O7-C8
34	A	359	LMT	C2'-C1'-O1'-C1
34	A	359	LMT	O5'-C1'-O1'-C1
34	B	630	LMT	O5'-C1'-O1'-C1
34	I	101	LMT	O5'-C1'-O1'-C1
34	M	103	LMT	C2'-C1'-O1'-C1
34	M	103	LMT	O5'-C1'-O1'-C1
34	a	418	LMT	C2'-C1'-O1'-C1
34	a	418	LMT	O5'-C1'-O1'-C1
34	a	359	LMT	C2'-C1'-O1'-C1
34	a	359	LMT	O5'-C1'-O1'-C1
34	b	622	LMT	O5'-C1'-O1'-C1
34	b	630	LMT	O5'-C1'-O1'-C1
34	t	101	LMT	O5'-C1'-O1'-C1
35	B	624	HTG	C2'-C1'-S1-C1
35	B	625	HTG	O5-C1-S1-C1'
35	b	624	HTG	O5-C1-S1-C1'
38	D	406	LHG	O2-C2-C3-O3
38	D	406	LHG	C3-O3-P-O4
38	D	406	LHG	C3-O3-P-O6
38	D	406	LHG	C4-O6-P-O3
38	D	406	LHG	C4-O6-P-O4
38	E	101	LHG	C3-O3-P-O4
38	E	101	LHG	C3-O3-P-O5
38	E	101	LHG	C3-O3-P-O6
38	E	101	LHG	O10-C23-O8-C6
38	E	101	LHG	C24-C23-O8-C6
38	L	101	LHG	C4-O6-P-O3
38	L	101	LHG	C4-O6-P-O4
38	a	419	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
38	d	407	LHG	C3-O3-P-O4
38	d	407	LHG	C3-O3-P-O6
38	d	407	LHG	C4-O6-P-O3
38	d	407	LHG	C4-O6-P-O4
38	d	407	LHG	C4-O6-P-O5
38	l	101	LHG	C4-O6-P-O3
38	l	101	LHG	C4-O6-P-O4
38	l	101	LHG	C4-O6-P-O5
39	E	103	HEM	C2C-C3C-CAC-CBC
39	E	103	HEM	C4C-C3C-CAC-CBC
39	e	102	HEM	C2C-C3C-CAC-CBC
39	e	102	HEM	C4C-C3C-CAC-CBC
41	V	203	HEC	C2B-C3B-CAB-CBB
41	V	203	HEC	C4B-C3B-CAB-CBB
41	V	203	HEC	C2C-C3C-CAC-CBC
41	V	203	HEC	C4C-C3C-CAC-CBC
41	v	203	HEC	C2B-C3B-CAB-CBB
41	v	203	HEC	C4B-C3B-CAB-CBB
41	v	203	HEC	C2C-C3C-CAC-CBC
41	v	203	HEC	C4C-C3C-CAC-CBC
34	I	101	LMT	C3'-C4'-O1B-C1B
38	a	419	LHG	O10-C23-O8-C6
38	a	419	LHG	C24-C23-O8-C6
33	A	418	LMG	O9-C10-O7-C8
33	c	522	LMG	O9-C10-O7-C8
33	z	101	LMG	O9-C10-O7-C8
24	B	604	CLA	C3-C5-C6-C7
24	c	508	CLA	C3-C5-C6-C7
24	c	514	CLA	C3-C5-C6-C7
24	d	403	CLA	C3-C5-C6-C7
24	C	514	CLA	CBD-CGD-O2D-CED
24	c	513	CLA	CBD-CGD-O2D-CED
27	B	620	SQD	C8-C7-O47-C45
27	b	620	SQD	C8-C7-O47-C45
24	B	603	CLA	C4-C3-C5-C6
24	B	614	CLA	C4-C3-C5-C6
24	C	505	CLA	C4-C3-C5-C6
24	b	603	CLA	C4-C3-C5-C6
24	c	506	CLA	C4-C3-C5-C6
31	A	416[B]	PL9	C15-C14-C16-C17
31	A	416[B]	PL9	C20-C19-C21-C22
31	A	416[B]	PL9	C25-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
31	D	405	PL9	C40-C39-C41-C42
31	a	414[A]	PL9	C25-C24-C26-C27
31	a	414[B]	PL9	C15-C14-C16-C17
24	B	603	CLA	C2-C3-C5-C6
24	B	614	CLA	C2-C3-C5-C6
24	C	505	CLA	C2-C3-C5-C6
24	b	603	CLA	C2-C3-C5-C6
24	c	506	CLA	C2-C3-C5-C6
31	A	416[A]	PL9	C18-C19-C21-C22
31	D	405	PL9	C38-C39-C41-C42
24	A	409	CLA	C3-C5-C6-C7
24	b	616	CLA	C3-C5-C6-C7
31	A	416[B]	PL9	C27-C28-C29-C30
31	D	405	PL9	C42-C43-C44-C46
34	E	102	LMT	O5'-C5'-C6'-O6'
35	c	523	HTG	O5-C5-C6-O6
24	B	614	CLA	C3-C5-C6-C7
24	C	502	CLA	CBD-CGD-O2D-CED
38	d	407	LHG	O2-C2-C3-O3
35	c	523	HTG	C4-C5-C6-O6
27	A	411	SQD	C8-C7-O47-C45
33	A	418	LMG	C11-C10-O7-C8
34	I	101	LMT	O5B-C5B-C6B-O6B
24	B	616	CLA	C3-C5-C6-C7
24	B	605	CLA	C4-C3-C5-C6
24	C	508	CLA	C4-C3-C5-C6
24	b	605	CLA	C4-C3-C5-C6
24	c	509	CLA	C4-C3-C5-C6
24	d	403	CLA	C4-C3-C5-C6
31	a	414[A]	PL9	C15-C14-C16-C17
31	a	414[A]	PL9	C30-C29-C31-C32
24	B	605	CLA	C2-C3-C5-C6
24	C	508	CLA	C2-C3-C5-C6
24	b	605	CLA	C2-C3-C5-C6
24	b	614	CLA	C2-C3-C5-C6
24	c	509	CLA	C2-C3-C5-C6
24	d	403	CLA	C2-C3-C5-C6
31	A	416[B]	PL9	C13-C14-C16-C17
31	A	416[B]	PL9	C18-C19-C21-C22
31	a	414[A]	PL9	C13-C14-C16-C17
31	a	414[B]	PL9	C13-C14-C16-C17
33	c	522	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
33	z	101	LMG	O6-C5-C6-O5
31	A	416[A]	PL9	C9-C11-C12-C13
31	A	416[A]	PL9	C14-C16-C17-C18
31	a	414[A]	PL9	C14-C16-C17-C18
34	E	102	LMT	C4'-C5'-C6'-O6'
24	C	504	CLA	CBD-CGD-O2D-CED
33	C	521	LMG	O6-C5-C6-O5
27	B	620	SQD	O5-C1-O6-C44
34	E	102	LMT	O5'-C1'-O1'-C1
34	e	101	LMT	O5'-C1'-O1'-C1
35	B	625	HTG	O5-C5-C6-O6
24	c	503	CLA	CBD-CGD-O2D-CED
33	a	417	LMG	O6-C5-C6-O5
31	a	414[B]	PL9	C27-C28-C29-C30
34	B	622	LMT	O5B-C5B-C6B-O6B
24	a	407	CLA	CBA-CGA-O2A-C1
24	c	511	CLA	CBA-CGA-O2A-C1
33	C	521	LMG	C4-C5-C6-O5
34	B	622	LMT	C4B-C5B-C6B-O6B
24	b	614	CLA	C4-C3-C5-C6
31	A	416[A]	PL9	C15-C14-C16-C17
31	A	416[A]	PL9	C13-C14-C16-C17
31	a	414[A]	PL9	C23-C24-C26-C27
31	a	414[A]	PL9	C28-C29-C31-C32
24	B	605	CLA	C6-C7-C8-C9
24	B	616	CLA	C6-C7-C8-C9
24	C	503	CLA	C14-C13-C15-C16
24	b	610	CLA	C11-C12-C13-C14
24	c	504	CLA	C14-C13-C15-C16
24	c	508	CLA	C6-C7-C8-C9
24	C	514	CLA	O1D-CGD-O2D-CED
34	B	630	LMT	C2'-C1'-O1'-C1
34	E	102	LMT	C2'-C1'-O1'-C1
34	I	101	LMT	C2'-C1'-O1'-C1
34	b	630	LMT	C2'-C1'-O1'-C1
34	e	101	LMT	C2'-C1'-O1'-C1
26	d	404	BCR	C7-C8-C9-C34
26	y	101	BCR	C37-C22-C23-C24
24	c	511	CLA	O1A-CGA-O2A-C1
27	A	411	SQD	O49-C7-O47-C45
24	B	601	CLA	CBA-CGA-O2A-C1
24	b	601	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
24	B	601	CLA	C5-C6-C7-C8
24	B	601	CLA	C10-C11-C12-C13
24	B	614	CLA	C10-C11-C12-C13
24	b	611	CLA	C15-C16-C17-C18
28	v	202	GOL	O1-C1-C2-O2
24	b	614	CLA	C3-C5-C6-C7
24	C	511	CLA	CBA-CGA-O2A-C1
36	C	518	DGD	C1A-C2A-C3A-C4A
31	D	405	PL9	C47-C48-C49-C51
31	A	416[A]	PL9	C44-C46-C47-C48
31	a	414[B]	PL9	C24-C26-C27-C28
31	d	405	PL9	C39-C41-C42-C43
34	I	101	LMT	O1'-C1-C2-C3
24	B	615	CLA	C8-C10-C11-C12
24	b	608	CLA	C13-C15-C16-C17
24	a	407	CLA	O1A-CGA-O2A-C1
24	A	409	CLA	C5-C6-C7-C8
24	B	614	CLA	C5-C6-C7-C8
24	C	508	CLA	C5-C6-C7-C8
33	Z	101	LMG	O6-C5-C6-O5
24	b	606	CLA	C2A-CAA-CBA-CGA
24	B	601	CLA	C15-C16-C17-C18
24	B	613	CLA	C15-C16-C17-C18
24	c	513	CLA	O1D-CGD-O2D-CED
34	M	103	LMT	O1'-C1-C2-C3
34	B	622	LMT	C5'-C4'-O1B-C1B
24	B	606	CLA	C13-C15-C16-C17
24	C	511	CLA	C5-C6-C7-C8
24	b	605	CLA	C8-C10-C11-C12
24	b	606	CLA	C10-C11-C12-C13
24	b	614	CLA	C13-C15-C16-C17
24	b	616	CLA	C5-C6-C7-C8
33	b	621	LMG	C30-C31-C32-C33
24	B	603	CLA	CBD-CGD-O2D-CED
34	I	101	LMT	C4B-C5B-C6B-O6B
34	b	630	LMT	C4'-C5'-C6'-O6'
31	D	405	PL9	C37-C38-C39-C40
24	C	511	CLA	O1A-CGA-O2A-C1
34	b	630	LMT	O5'-C5'-C6'-O6'
24	B	615	CLA	C5-C6-C7-C8
24	C	502	CLA	C15-C16-C17-C18
24	b	602	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
34	B	630	LMT	C4'-C5'-C6'-O6'
24	B	601	CLA	O1A-CGA-O2A-C1
35	b	623	HTG	S1-C1'-C2'-C3'
35	b	623	HTG	O5-C5-C6-O6
24	C	513	CLA	C3-C5-C6-C7
34	B	622	LMT	C3'-C4'-O1B-C1B
38	D	406	LHG	C1-C2-C3-O3
38	d	407	LHG	C1-C2-C3-O3
24	B	606	CLA	C2A-CAA-CBA-CGA
24	d	403	CLA	CBA-CGA-O2A-C1
24	B	602	CLA	C13-C15-C16-C17
24	B	604	CLA	C13-C15-C16-C17
24	B	614	CLA	C8-C10-C11-C12
24	C	507	CLA	C13-C15-C16-C17
24	c	509	CLA	C8-C10-C11-C12
34	M	103	LMT	O5'-C5'-C6'-O6'
24	B	616	CLA	C10-C11-C12-C13
24	C	507	CLA	C8-C10-C11-C12
24	c	512	CLA	C10-C11-C12-C13
34	B	622	LMT	O5'-C5'-C6'-O6'
33	C	520	LMG	C11-C10-O7-C8
33	C	520	LMG	O9-C10-O7-C8
33	Z	101	LMG	C2-C1-O1-C7
34	b	622	LMT	C2'-C1'-O1'-C1
34	m	102	LMT	C2'-C1'-O1'-C1
36	C	518	DGD	C2E-C1E-O5D-C6D
24	B	606	CLA	C10-C11-C12-C13
31	a	414[A]	PL9	C9-C11-C12-C13
34	B	630	LMT	O5'-C5'-C6'-O6'
33	z	101	LMG	C4-C5-C6-O5
38	L	101	LHG	C23-C24-C25-C26
38	E	101	LHG	C11-C10-C9-C8
28	B	626	GOL	C1-C2-C3-O3
28	b	627	GOL	O1-C1-C2-C3
38	D	357	LHG	O1-C1-C2-C3
27	A	411	SQD	C11-C10-C9-C8
24	C	514	CLA	C16-C17-C18-C20
24	C	502	CLA	O1D-CGD-O2D-CED
24	d	403	CLA	O1A-CGA-O2A-C1
33	b	621	LMG	C11-C10-O7-C8
31	A	416[B]	PL9	C23-C24-C26-C27
35	c	523	HTG	S1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
24	B	610	CLA	C16-C17-C18-C19
24	B	615	CLA	C16-C17-C18-C20
24	a	407	CLA	C16-C17-C18-C20
24	b	615	CLA	C16-C17-C18-C19
35	B	624	HTG	C2'-C3'-C4'-C5'
38	E	101	LHG	C24-C25-C26-C27
35	B	625	HTG	C4-C5-C6-O6
33	J	101	LMG	C19-C20-C21-C22
36	C	517	DGD	CAA-CBA-CCA-CDA
36	H	102	DGD	CBB-CCB-CDB-CEB
36	c	520	DGD	C8A-C9A-CAA-CBA
38	L	101	LHG	C12-C13-C14-C15
24	A	405	CLA	C15-C16-C17-C18
33	B	621	LMG	C36-C37-C38-C39
38	D	357	LHG	C32-C33-C34-C35
36	c	518	DGD	O6D-C5D-C6D-O5D
33	C	521	LMG	C16-C17-C18-C19
28	A	412	GOL	O1-C1-C2-O2
28	B	626	GOL	O1-C1-C2-O2
28	C	525	GOL	O1-C1-C2-O2
28	a	410	GOL	O1-C1-C2-O2
28	a	410	GOL	O2-C2-C3-O3
34	b	630	LMT	C2-C1-O1'-C1'
38	D	357	LHG	O1-C1-C2-O2
27	b	620	SQD	C27-C28-C29-C30
33	c	522	LMG	C32-C33-C34-C35
36	c	519	DGD	C7A-C8A-C9A-CAA
38	d	408	LHG	C27-C28-C29-C30
24	C	513	CLA	C4B-C3B-CAB-CBB
33	Z	101	LMG	C10-C11-C12-C13
24	C	514	CLA	C16-C17-C18-C19
24	c	504	CLA	C16-C17-C18-C20
24	b	610	CLA	C2A-CAA-CBA-CGA
27	b	620	SQD	C14-C15-C16-C17
24	B	610	CLA	C13-C15-C16-C17
24	c	508	CLA	C10-C11-C12-C13
34	a	359	LMT	C3-C4-C5-C6
24	A	409	CLA	C12-C13-C15-C16
27	a	409	SQD	C11-C12-C13-C14
33	A	418	LMG	C18-C19-C20-C21
24	D	403	CLA	C4-C3-C5-C6
24	C	504	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
33	A	418	LMG	C37-C38-C39-C40
24	b	606	CLA	C13-C15-C16-C17
24	c	515	CLA	C10-C11-C12-C13
24	c	503	CLA	O1D-CGD-O2D-CED
34	A	359	LMT	O1'-C1-C2-C3
36	C	517	DGD	O6D-C5D-C6D-O5D
36	h	103	DGD	C9A-CAA-CBA-CCA
27	a	411	SQD	C24-C25-C26-C27
33	b	621	LMG	C38-C39-C40-C41
24	c	514	CLA	CBA-CGA-O2A-C1
38	d	408	LHG	C24-C23-O8-C6
38	a	419	LHG	C4-C5-C6-O8
33	A	418	LMG	C29-C30-C31-C32
34	B	630	LMT	C5-C6-C7-C8
36	c	519	DGD	C1B-C2B-C3B-C4B
27	A	411	SQD	C9-C10-C11-C12
34	a	359	LMT	C6-C7-C8-C9
38	d	407	LHG	C30-C31-C32-C33
36	C	517	DGD	C5B-C6B-C7B-C8B
36	c	519	DGD	CAA-CBA-CCA-CDA
36	H	102	DGD	CBA-CCA-CDA-CEA
34	I	101	LMT	C1-C2-C3-C4
33	j	101	LMG	C21-C22-C23-C24
34	M	101	LMT	C3-C4-C5-C6
31	a	414[B]	PL9	C37-C38-C39-C40
24	B	610	CLA	C16-C17-C18-C20
24	C	513	CLA	C2B-C3B-CAB-CBB
24	c	504	CLA	C2B-C3B-CAB-CBB
26	D	404	BCR	C23-C24-C25-C30
33	Z	101	LMG	C19-C20-C21-C22
38	l	101	LHG	C14-C15-C16-C17
24	a	407	CLA	C3-C5-C6-C7
27	F	101	SQD	C32-C33-C34-C35
35	b	623	HTG	C2'-C3'-C4'-C5'
24	b	611	CLA	C8-C10-C11-C12
27	A	413	SQD	C26-C27-C28-C29
33	C	521	LMG	C15-C16-C17-C18
38	d	408	LHG	O10-C23-O8-C6
31	a	414[A]	PL9	C4-C3-C7-C8
27	a	409	SQD	C13-C14-C15-C16
36	H	102	DGD	CAB-CBB-CCB-CDB
38	D	406	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
33	b	621	LMG	O9-C10-O7-C8
38	l	101	LHG	C27-C28-C29-C30
31	d	405	PL9	C32-C33-C34-C36
24	c	514	CLA	C10-C11-C12-C13
24	D	403	CLA	C2-C3-C5-C6
27	a	411	SQD	C25-C26-C27-C28
36	h	103	DGD	C5B-C6B-C7B-C8B
38	L	101	LHG	C14-C15-C16-C17
38	L	101	LHG	C25-C26-C27-C28
24	C	513	CLA	CBA-CGA-O2A-C1
24	C	513	CLA	C6-C7-C8-C9
24	b	616	CLA	C6-C7-C8-C9
27	b	620	SQD	C18-C19-C20-C21
33	C	521	LMG	C12-C13-C14-C15
36	C	517	DGD	C3B-C4B-C5B-C6B
34	m	102	LMT	O5'-C1'-O1'-C1
36	C	518	DGD	O6E-C1E-O5D-C6D
36	c	518	DGD	O6E-C1E-O5D-C6D
36	c	519	DGD	O6E-C1E-O5D-C6D
33	c	521	LMG	C33-C34-C35-C36
36	c	518	DGD	CBB-CCB-CDB-CEB
34	t	101	LMT	C2'-C1'-O1'-C1
24	c	509	CLA	C5-C6-C7-C8
33	j	101	LMG	C29-C30-C31-C32
38	a	419	LHG	C26-C27-C28-C29
31	A	416[B]	PL9	C47-C48-C49-C51
24	c	504	CLA	C15-C16-C17-C18
24	b	601	CLA	CBA-CGA-O2A-C1
33	B	621	LMG	C11-C10-O7-C8
33	a	417	LMG	C11-C10-O7-C8
34	B	630	LMT	C3'-C4'-O1B-C1B
34	m	102	LMT	O5'-C5'-C6'-O6'
33	J	101	LMG	C35-C36-C37-C38
38	L	101	LHG	C17-C18-C19-C20
38	D	406	LHG	C28-C29-C30-C31
36	h	103	DGD	CAA-CBA-CCA-CDA
27	F	101	SQD	C23-C24-C25-C26
33	C	520	LMG	C17-C18-C19-C20
24	C	510	CLA	C3-C5-C6-C7
24	c	515	CLA	C3-C5-C6-C7
24	B	615	CLA	C16-C17-C18-C19
24	b	615	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
34	a	418	LMT	C6-C7-C8-C9
24	B	604	CLA	C4-C3-C5-C6
31	A	416[A]	PL9	C25-C24-C26-C27
39	e	102	HEM	C2B-C3B-CAB-CBB
33	a	417	LMG	C34-C35-C36-C37
33	b	621	LMG	C35-C36-C37-C38
24	C	509	CLA	C10-C11-C12-C13
27	A	411	SQD	C15-C16-C17-C18
33	B	621	LMG	O9-C10-O7-C8
31	A	416[B]	PL9	C29-C31-C32-C33
31	d	405	PL9	C34-C36-C37-C38
24	a	407	CLA	C16-C17-C18-C19
24	c	504	CLA	C16-C17-C18-C19
36	C	518	DGD	C7B-C8B-C9B-CAB
36	H	102	DGD	CCA-CDA-CEA-CFA
38	L	101	LHG	C13-C14-C15-C16
36	c	518	DGD	C4D-C5D-C6D-O5D
27	B	620	SQD	C11-C12-C13-C14
27	B	620	SQD	C31-C32-C33-C34
24	b	601	CLA	C13-C15-C16-C17
27	B	620	SQD	C26-C27-C28-C29
27	a	411	SQD	C10-C11-C12-C13
27	F	101	SQD	C30-C31-C32-C33
36	C	517	DGD	C4B-C5B-C6B-C7B
38	D	406	LHG	C16-C17-C18-C19
33	J	101	LMG	O6-C5-C6-O5
34	a	359	LMT	C2-C3-C4-C5
33	C	520	LMG	C30-C31-C32-C33
35	C	523	HTG	O5-C5-C6-O6
35	b	628	HTG	O5-C5-C6-O6
24	c	508	CLA	C15-C16-C17-C18
27	F	101	SQD	C24-C25-C26-C27
27	a	409	SQD	C9-C10-C11-C12
27	a	409	SQD	C27-C28-C29-C30
36	c	518	DGD	C9A-CAA-CBA-CCA
24	C	511	CLA	C2-C3-C5-C6
31	D	405	PL9	C43-C44-C46-C47
38	d	407	LHG	C16-C17-C18-C19
24	C	512	CLA	CBD-CGD-O2D-CED
24	b	613	CLA	CBD-CGD-O2D-CED
24	c	513	CLA	CBA-CGA-O2A-C1
36	C	517	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
35	B	624	HTG	C1'-C2'-C3'-C4'
24	b	606	CLA	C15-C16-C17-C18
33	b	621	LMG	C39-C40-C41-C42
24	C	513	CLA	O1A-CGA-O2A-C1
24	c	514	CLA	O1A-CGA-O2A-C1
24	C	503	CLA	C3-C5-C6-C7
27	f	101	SQD	C26-C27-C28-C29
33	B	621	LMG	C17-C18-C19-C20
33	C	521	LMG	C33-C34-C35-C36
27	a	409	SQD	C30-C31-C32-C33
24	c	513	CLA	O1A-CGA-O2A-C1
27	b	620	SQD	C13-C14-C15-C16
34	I	101	LMT	O5'-C5'-C6'-O6'
24	b	601	CLA	C3-C5-C6-C7
24	B	615	CLA	C11-C12-C13-C15
24	D	403	CLA	C11-C10-C8-C7
24	a	404	CLA	C11-C12-C13-C15
24	b	601	CLA	C6-C7-C8-C10
27	A	411	SQD	C18-C19-C20-C21
38	D	407	LHG	C29-C30-C31-C32
31	A	416[A]	PL9	C12-C11-C9-C10
24	c	507	CLA	C2-C3-C5-C6
31	A	416[A]	PL9	C12-C11-C9-C8
24	b	601	CLA	O1A-CGA-O2A-C1
35	b	625	HTG	O5-C5-C6-O6
34	t	101	LMT	O1'-C1-C2-C3
24	B	616	CLA	C14-C13-C15-C16
24	C	505	CLA	C14-C13-C15-C16
24	C	506	CLA	C14-C13-C15-C16
24	D	403	CLA	C11-C10-C8-C9
24	b	601	CLA	C6-C7-C8-C9
35	B	623	HTG	C3'-C4'-C5'-C6'
36	C	517	DGD	O6E-C5E-C6E-O5E
36	c	519	DGD	C2E-C1E-O5D-C6D
27	b	620	SQD	C12-C13-C14-C15
27	B	620	SQD	C44-C45-C46-O48
27	b	620	SQD	C44-C45-C46-O48
27	f	101	SQD	O6-C44-C45-C46
38	E	101	LHG	C4-C5-C6-O8
33	B	621	LMG	C18-C19-C20-C21
34	b	630	LMT	C3-C4-C5-C6
24	A	409	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	C	519	DGD	C2A-C1A-O1G-C1G
36	c	518	DGD	C2A-C1A-O1G-C1G
35	B	628	HTG	O5-C5-C6-O6
36	c	518	DGD	O6E-C5E-C6E-O5E
34	E	102	LMT	O1'-C1-C2-C3
27	B	620	SQD	C34-C35-C36-C37
34	B	630	LMT	C11-C10-C9-C8
34	b	630	LMT	C4-C5-C6-C7
35	c	526	HTG	O5-C5-C6-O6
38	D	357	LHG	C25-C26-C27-C28
24	C	511	CLA	C4-C3-C5-C6
31	d	405	PL9	C15-C14-C16-C17
31	D	405	PL9	C13-C14-C16-C17
31	d	405	PL9	C28-C29-C31-C32
26	K	102	BCR	C7-C8-C9-C34
26	b	619	BCR	C37-C22-C23-C24
33	a	417	LMG	O9-C10-O7-C8
33	a	417	LMG	C4-C5-C6-O5
33	j	101	LMG	O6-C5-C6-O5
38	l	101	LHG	C34-C35-C36-C37
36	C	519	DGD	CCB-CDB-CEB-CFB
36	C	518	DGD	CCB-CDB-CEB-CFB
31	a	414[B]	PL9	C32-C33-C34-C35
27	F	101	SQD	C29-C30-C31-C32
36	c	518	DGD	CAA-CBA-CCA-CDA
38	d	407	LHG	C13-C14-C15-C16
27	b	620	SQD	C24-C25-C26-C27
36	c	519	DGD	C2B-C3B-C4B-C5B
36	c	520	DGD	C2A-C1A-O1G-C1G
33	C	520	LMG	C37-C38-C39-C40
24	c	507	CLA	C4-C3-C5-C6
31	A	416[B]	PL9	C12-C11-C9-C8
27	A	411	SQD	C16-C17-C18-C19
33	B	621	LMG	C33-C34-C35-C36
27	f	101	SQD	C25-C26-C27-C28
33	C	521	LMG	C17-C18-C19-C20
27	A	411	SQD	O6-C44-C45-O47
34	e	101	LMT	C4-C5-C6-C7
36	c	518	DGD	C5A-C6A-C7A-C8A
36	C	518	DGD	CDA-CEA-CFA-CGA
38	D	357	LHG	C16-C17-C18-C19
36	c	520	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
36	C	519	DGD	O1A-C1A-O1G-C1G
38	D	357	LHG	C23-C24-C25-C26
25	A	408	PHO	C2C-C3C-CAC-CBC
36	c	518	DGD	C7B-C8B-C9B-CAB
24	a	350	CLA	C15-C16-C17-C18
24	A	409	CLA	O1A-CGA-O2A-C1
27	b	620	SQD	C26-C27-C28-C29
31	D	405	PL9	C45-C44-C46-C47
31	a	414[B]	PL9	C20-C19-C21-C22
35	b	628	HTG	C4'-C5'-C6'-C7'
24	B	609	CLA	C2-C3-C5-C6
34	M	101	LMT	C2-C3-C4-C5
33	c	521	LMG	C35-C36-C37-C38
35	B	628	HTG	C2'-C3'-C4'-C5'
28	B	626	GOL	O2-C2-C3-O3
34	t	101	LMT	C2-C1-O1'-C1'
24	B	606	CLA	C11-C10-C8-C9
24	C	514	CLA	C11-C10-C8-C9
24	a	404	CLA	C11-C12-C13-C14
38	D	357	LHG	C11-C12-C13-C14
38	a	419	LHG	C11-C12-C13-C14
38	d	406	LHG	C25-C26-C27-C28
24	C	505	CLA	C4B-C3B-CAB-CBB
24	D	402	CLA	C4B-C3B-CAB-CBB
36	c	519	DGD	C7B-C8B-C9B-CAB
38	D	357	LHG	C24-C25-C26-C27
35	B	628	HTG	C4'-C5'-C6'-C7'
38	l	101	LHG	C12-C13-C14-C15
36	c	518	DGD	C2E-C1E-O5D-C6D
33	J	101	LMG	C36-C37-C38-C39
24	A	406	CLA	C12-C13-C15-C16
24	B	606	CLA	C11-C10-C8-C7
24	B	615	CLA	C12-C13-C15-C16
24	B	616	CLA	C12-C13-C15-C16
24	C	505	CLA	C12-C13-C15-C16
24	C	506	CLA	C12-C13-C15-C16
24	C	514	CLA	C11-C10-C8-C7
24	a	407	CLA	C11-C10-C8-C7
24	b	603	CLA	C11-C10-C8-C7
24	c	515	CLA	C12-C13-C15-C16
24	b	610	CLA	C15-C16-C17-C18
34	M	101	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	B	609	CLA	C3A-C2A-CAA-CBA
24	b	609	CLA	C3A-C2A-CAA-CBA
24	c	512	CLA	C4-C3-C5-C6
31	A	416[A]	PL9	C45-C44-C46-C47
31	d	405	PL9	C45-C44-C46-C47
24	b	601	CLA	CAA-CBA-CGA-O2A
31	d	405	PL9	C13-C14-C16-C17
34	B	630	LMT	C3-C4-C5-C6
36	c	518	DGD	O1A-C1A-O1G-C1G
24	a	350	CLA	C13-C15-C16-C17
36	c	520	DGD	C2B-C3B-C4B-C5B
34	E	102	LMT	C3-C4-C5-C6
36	c	520	DGD	O1A-C1A-O1G-C1G
36	C	519	DGD	C8B-C9B-CAB-CBB
36	H	102	DGD	C7B-C8B-C9B-CAB
36	c	518	DGD	C4B-C5B-C6B-C7B
33	j	101	LMG	C38-C39-C40-C41
27	A	411	SQD	O6-C44-C45-C46
27	A	413	SQD	O6-C44-C45-C46
27	a	411	SQD	O6-C44-C45-C46
24	b	607	CLA	C3-C5-C6-C7
38	L	101	LHG	C16-C17-C18-C19
35	b	623	HTG	C1'-C2'-C3'-C4'
33	B	621	LMG	O8-C28-C29-C30
31	A	416[A]	PL9	C43-C44-C46-C47
31	d	405	PL9	C43-C44-C46-C47
38	d	408	LHG	C25-C26-C27-C28
27	f	101	SQD	C35-C36-C37-C38
26	D	404	BCR	C23-C24-C25-C26
26	b	617	BCR	C1-C6-C7-C8
26	d	404	BCR	C23-C24-C25-C30
33	J	101	LMG	C16-C17-C18-C19
38	d	406	LHG	C24-C25-C26-C27
39	e	102	HEM	C2A-CAA-CBA-CGA
33	J	101	LMG	C34-C35-C36-C37
38	l	101	LHG	C13-C14-C15-C16
36	H	102	DGD	O2G-C1B-C2B-C3B
27	f	101	SQD	O47-C45-C46-O48
33	A	418	LMG	O1-C7-C8-O7
33	a	417	LMG	O7-C8-C9-O8
38	L	101	LHG	C24-C25-C26-C27
31	A	416[A]	PL9	C4-C3-C7-C8

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Mol	Chain	Res	Type	Atoms
33	j	101	LMG	C19-C20-C21-C22
34	M	103	LMT	O5B-C1B-O1B-C4'
24	B	609	CLA	C4-C3-C5-C6
27	A	411	SQD	C12-C13-C14-C15
24	c	512	CLA	C2-C3-C5-C6
24	C	511	CLA	C16-C17-C18-C19
33	b	621	LMG	C37-C38-C39-C40
24	B	614	CLA	C14-C13-C15-C16
24	B	615	CLA	C14-C13-C15-C16
24	d	402	CLA	C11-C12-C13-C14
24	B	601	CLA	CAA-CBA-CGA-O2A
34	e	101	LMT	C3-C4-C5-C6
33	c	522	LMG	C4-C5-C6-O5
36	c	518	DGD	CDB-CEB-CFB-CGB
38	D	406	LHG	C9-C10-C11-C12
31	A	416[B]	PL9	C9-C11-C12-C13
31	a	414[B]	PL9	C14-C16-C17-C18
36	C	519	DGD	O6E-C5E-C6E-O5E
27	f	101	SQD	C29-C30-C31-C32
24	b	601	CLA	C8-C10-C11-C12
24	b	602	CLA	C13-C15-C16-C17
24	c	511	CLA	C3-C5-C6-C7
36	h	103	DGD	O2G-C1B-C2B-C3B
31	D	405	PL9	C28-C29-C31-C32
24	B	605	CLA	C13-C15-C16-C17
34	B	622	LMT	C6-C7-C8-C9
38	d	406	LHG	C33-C34-C35-C36
35	B	624	HTG	C4-C5-C6-O6
24	C	506	CLA	C10-C11-C12-C13
33	b	621	LMG	C14-C15-C16-C17
38	E	101	LHG	C10-C11-C12-C13
38	l	101	LHG	O6-C4-C5-C6
34	e	101	LMT	C2B-C1B-O1B-C4'
36	C	517	DGD	C8A-C9A-CAA-CBA
24	b	613	CLA	C5-C6-C7-C8
33	c	522	LMG	C30-C31-C32-C33
38	D	406	LHG	C26-C27-C28-C29
24	B	604	CLA	C6-C7-C8-C10
24	B	614	CLA	C12-C13-C15-C16
24	C	507	CLA	C6-C7-C8-C10
24	b	615	CLA	C12-C13-C15-C16
24	d	402	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
33	Z	101	LMG	C29-C28-O8-C9
24	A	404	CLA	C13-C15-C16-C17
24	B	612	CLA	C10-C11-C12-C13
24	c	508	CLA	C13-C15-C16-C17
24	c	514	CLA	C15-C16-C17-C18
24	b	616	CLA	CBA-CGA-O2A-C1
36	c	518	DGD	CAB-CBB-CCB-CDB
36	C	518	DGD	C5D-C6D-O5D-C1E
36	c	519	DGD	C5D-C6D-O5D-C1E
24	B	602	CLA	C15-C16-C17-C18
24	C	511	CLA	C8-C10-C11-C12
24	b	601	CLA	C4-C3-C5-C6
31	A	416[B]	PL9	C43-C44-C46-C47
39	E	103	HEM	C2B-C3B-CAB-CBB
36	c	519	DGD	C9A-CAA-CBA-CCA
38	E	101	LHG	C25-C26-C27-C28
28	a	416	GOL	C1-C2-C3-O3
34	M	103	LMT	C2B-C1B-O1B-C4'
25	a	405	PHO	O2A-C1-C2-C3
27	B	620	SQD	C46-C45-O47-C7
27	f	101	SQD	C31-C32-C33-C34
24	c	512	CLA	CBA-CGA-O2A-C1
36	H	102	DGD	CDB-CEB-CFB-CGB
24	b	612	CLA	C10-C11-C12-C13
38	l	101	LHG	O6-C4-C5-O7
33	c	521	LMG	C31-C32-C33-C34
33	z	101	LMG	O6-C1-O1-C7
27	f	101	SQD	C44-C45-C46-O48
33	a	417	LMG	C7-C8-C9-O8
36	H	102	DGD	O1G-C1G-C2G-C3G
39	e	102	HEM	C4B-C3B-CAB-CBB
36	c	518	DGD	CCB-CDB-CEB-CFB
31	a	414[A]	PL9	C12-C11-C9-C10
31	a	414[B]	PL9	C47-C48-C49-C51
24	B	603	CLA	O1D-CGD-O2D-CED
34	b	630	LMT	C6-C7-C8-C9
38	D	406	LHG	C14-C15-C16-C17
33	a	417	LMG	O8-C28-C29-C30
24	b	616	CLA	O1A-CGA-O2A-C1
24	c	512	CLA	O1A-CGA-O2A-C1
27	a	411	SQD	C27-C28-C29-C30
33	C	520	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
24	B	605	CLA	C8-C10-C11-C12
36	h	103	DGD	CBA-CCA-CDA-CEA
33	C	521	LMG	C38-C39-C40-C41
24	C	507	CLA	C16-C17-C18-C20
36	C	519	DGD	CBA-CCA-CDA-CEA
34	b	622	LMT	C3'-C4'-O1B-C1B
38	l	101	LHG	C16-C17-C18-C19
24	b	601	CLA	C2-C3-C5-C6
24	D	403	CLA	C8-C10-C11-C12
38	E	101	LHG	C14-C15-C16-C17
38	D	357	LHG	C12-C13-C14-C15
24	D	403	CLA	C3-C5-C6-C7
33	B	621	LMG	C14-C15-C16-C17
36	C	519	DGD	O6D-C5D-C6D-O5D
24	C	511	CLA	C16-C17-C18-C20
24	B	606	CLA	C4B-C3B-CAB-CBB
24	C	502	CLA	C1A-C2A-CAA-CBA
24	a	404	CLA	C4B-C3B-CAB-CBB
24	c	507	CLA	C4B-C3B-CAB-CBB
24	c	509	CLA	C4B-C3B-CAB-CBB
27	a	411	SQD	C24-C23-O48-C46
27	b	620	SQD	C24-C23-O48-C46
26	K	102	BCR	C7-C8-C9-C10
33	a	417	LMG	C20-C21-C22-C23
27	a	411	SQD	O10-C23-O48-C46
27	A	413	SQD	C15-C16-C17-C18
24	C	508	CLA	C13-C15-C16-C17
33	C	520	LMG	O7-C10-C11-C12
27	B	620	SQD	C11-C10-C9-C8
24	B	604	CLA	C11-C12-C13-C15
24	B	610	CLA	C12-C13-C15-C16
24	B	616	CLA	C6-C7-C8-C10
27	B	620	SQD	C30-C31-C32-C33
38	d	408	LHG	C28-C29-C30-C31
38	D	407	LHG	C2-C3-O3-P
38	d	408	LHG	C2-C3-O3-P
33	C	520	LMG	C14-C15-C16-C17
24	C	506	CLA	C4-C3-C5-C6
24	B	604	CLA	C6-C7-C8-C9
24	C	507	CLA	C6-C7-C8-C9
24	b	615	CLA	C14-C13-C15-C16
26	c	517	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
36	H	102	DGD	C7A-C8A-C9A-CAA
24	B	609	CLA	C13-C15-C16-C17
38	d	408	LHG	C33-C34-C35-C36
24	c	510	CLA	C5-C6-C7-C8
24	C	512	CLA	O1D-CGD-O2D-CED
36	C	519	DGD	CDA-CEA-CFA-CGA
27	a	411	SQD	C31-C32-C33-C34
27	B	620	SQD	O47-C45-C46-O48
36	H	102	DGD	O1G-C1G-C2G-O2G
38	E	101	LHG	O7-C5-C6-O8
38	a	419	LHG	O7-C5-C6-O8
27	F	101	SQD	C27-C28-C29-C30
38	d	406	LHG	C32-C33-C34-C35
38	a	419	LHG	C24-C25-C26-C27
33	A	418	LMG	O1-C7-C8-C9
24	B	615	CLA	C4-C3-C5-C6
35	B	623	HTG	C2'-C3'-C4'-C5'
24	B	607	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	b	601	CLA	CAD-CBD-CGD-O2D
24	c	504	CLA	CAD-CBD-CGD-O2D
38	D	407	LHG	C24-C23-O8-C6
24	A	405	CLA	C13-C15-C16-C17
24	B	608	CLA	C13-C15-C16-C17
24	c	509	CLA	C2A-CAA-CBA-CGA
27	b	620	SQD	O10-C23-O48-C46
38	D	407	LHG	O10-C23-O8-C6
36	c	520	DGD	C3B-C4B-C5B-C6B
24	B	601	CLA	CAD-CBD-CGD-O1D
24	B	605	CLA	CAD-CBD-CGD-O1D
24	B	607	CLA	CAD-CBD-CGD-O1D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O1D
24	b	601	CLA	CAD-CBD-CGD-O1D
24	b	605	CLA	CAD-CBD-CGD-O1D
24	b	609	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D
24	c	514	CLA	CHA-CBD-CGD-O1D
24	c	514	CLA	CHA-CBD-CGD-O2D
38	D	406	LHG	C4-O6-P-O5
38	E	101	LHG	C4-O6-P-O5
38	L	101	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
34	e	101	LMT	O5B-C1B-O1B-C4'
33	C	521	LMG	C35-C36-C37-C38
24	D	402	CLA	C2B-C3B-CAB-CBB
27	a	411	SQD	C12-C13-C14-C15
24	C	506	CLA	C2-C3-C5-C6
31	A	416[A]	PL9	C23-C24-C26-C27
31	a	414[A]	PL9	C12-C11-C9-C8
24	B	611	CLA	C8-C10-C11-C12
26	c	517	BCR	C7-C8-C9-C34
34	m	102	LMT	C7-C8-C9-C10
36	C	519	DGD	C9A-CAA-CBA-CCA
33	c	521	LMG	C29-C30-C31-C32
27	B	620	SQD	C16-C17-C18-C19
34	b	622	LMT	C4-C5-C6-C7
28	b	627	GOL	O1-C1-C2-O2
36	C	517	DGD	C2A-C3A-C4A-C5A
36	H	102	DGD	C9B-CAB-CBB-CCB
27	B	620	SQD	C7-C8-C9-C10
27	b	620	SQD	C46-C45-O47-C7
31	A	416[B]	PL9	C14-C16-C17-C18
24	d	403	CLA	C10-C11-C12-C13
24	b	610	CLA	C16-C17-C18-C19
27	b	620	SQD	C11-C10-C9-C8
24	A	406	CLA	C14-C13-C15-C16
24	B	610	CLA	C14-C13-C15-C16
24	a	407	CLA	C11-C10-C8-C9
24	b	603	CLA	C11-C10-C8-C9
24	c	506	CLA	C14-C13-C15-C16
24	c	515	CLA	C14-C13-C15-C16
24	C	503	CLA	C12-C13-C15-C16
24	b	606	CLA	C12-C13-C15-C16
24	c	506	CLA	C12-C13-C15-C16
24	c	508	CLA	C6-C7-C8-C10
35	b	628	HTG	C3'-C4'-C5'-C6'
36	C	517	DGD	CAB-CBB-CCB-CDB
24	C	512	CLA	O1A-CGA-O2A-C1
27	b	620	SQD	O5-C1-O6-C44
33	c	521	LMG	C21-C22-C23-C24
24	b	613	CLA	O1D-CGD-O2D-CED
34	E	102	LMT	C2B-C1B-O1B-C4'
27	a	409	SQD	C16-C17-C18-C19
36	h	103	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
33	B	621	LMG	C29-C30-C31-C32
27	b	620	SQD	O47-C45-C46-O48
36	C	517	DGD	C7A-C8A-C9A-CAA
33	j	101	LMG	C28-C29-C30-C31
33	Z	101	LMG	C4-C5-C6-O5
36	C	517	DGD	CBB-CCB-CDB-CEB
34	E	102	LMT	O5B-C1B-O1B-C4'
33	c	522	LMG	C29-C30-C31-C32
38	d	406	LHG	C13-C14-C15-C16
38	D	407	LHG	C13-C14-C15-C16
24	B	616	CLA	C2-C1-O2A-CGA
35	b	624	HTG	C4-C5-C6-O6
35	b	625	HTG	C1'-C2'-C3'-C4'
24	c	511	CLA	C13-C15-C16-C17
33	C	520	LMG	C34-C35-C36-C37
38	D	407	LHG	C27-C28-C29-C30
36	c	518	DGD	C5D-C6D-O5D-C1E
24	C	502	CLA	C2A-CAA-CBA-CGA
24	B	608	CLA	C16-C17-C18-C20
33	a	417	LMG	C10-C11-C12-C13
33	J	101	LMG	C30-C31-C32-C33
36	H	102	DGD	C5B-C6B-C7B-C8B
24	C	509	CLA	C13-C15-C16-C17
36	h	103	DGD	CDB-CEB-CFB-CGB
34	a	359	LMT	C5-C6-C7-C8
33	C	521	LMG	C18-C19-C20-C21
24	C	512	CLA	CBA-CGA-O2A-C1
24	b	602	CLA	C4B-C3B-CAB-CBB
35	b	628	HTG	C1'-C2'-C3'-C4'
36	H	102	DGD	C4E-C5E-C6E-O5E
24	c	512	CLA	C15-C16-C17-C18
31	a	414[A]	PL9	C45-C44-C46-C47
24	B	615	CLA	C2-C3-C5-C6
31	a	414[B]	PL9	C43-C44-C46-C47
38	E	101	LHG	C15-C16-C17-C18
33	A	418	LMG	C30-C31-C32-C33
38	d	407	LHG	C26-C27-C28-C29
39	E	103	HEM	C4B-C3B-CAB-CBB
34	A	359	LMT	O5B-C5B-C6B-O6B
33	A	418	LMG	O8-C28-C29-C30
24	b	614	CLA	C6-C7-C8-C10
24	c	504	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
38	l	101	LHG	C35-C36-C37-C38
24	b	610	CLA	C16-C17-C18-C20
38	d	408	LHG	C9-C10-C11-C12
24	C	512	CLA	C3-C5-C6-C7
27	a	409	SQD	O6-C44-C45-O47
36	h	103	DGD	O1G-C1G-C2G-O2G
31	D	405	PL9	C32-C33-C34-C35
24	B	607	CLA	C3-C5-C6-C7
34	B	630	LMT	C4-C5-C6-C7
24	B	608	CLA	C2-C1-O2A-CGA
36	c	519	DGD	CCA-CDA-CEA-CFA
24	C	507	CLA	C5-C6-C7-C8
33	j	101	LMG	C11-C12-C13-C14
24	C	503	CLA	O1D-CGD-O2D-CED
38	E	101	LHG	C7-C8-C9-C10
34	t	101	LMT	C5-C6-C7-C8
31	a	414[A]	PL9	C20-C19-C21-C22
31	a	414[A]	PL9	C43-C44-C46-C47
24	C	507	CLA	C16-C17-C18-C19
24	a	404	CLA	C16-C17-C18-C20
24	D	403	CLA	C10-C11-C12-C13
31	a	414[A]	PL9	C2-C3-C7-C8
41	v	203	HEC	CAD-CBD-CGD-O1D
27	A	411	SQD	C30-C31-C32-C33
34	a	418	LMT	C5-C6-C7-C8
34	b	630	LMT	C11-C10-C9-C8
24	B	610	CLA	C11-C12-C13-C14
24	b	602	CLA	C6-C7-C8-C9
24	b	609	CLA	C6-C7-C8-C9
24	b	614	CLA	C6-C7-C8-C9
24	c	510	CLA	C6-C7-C8-C9
24	c	511	CLA	C14-C13-C15-C16
27	a	409	SQD	C10-C11-C12-C13
34	I	101	LMT	C4-C5-C6-C7
38	D	357	LHG	C17-C18-C19-C20
27	a	409	SQD	C35-C36-C37-C38
33	c	521	LMG	C4-C5-C6-O5
36	c	520	DGD	C1A-C2A-C3A-C4A
41	v	203	HEC	CAD-CBD-CGD-O2D
33	c	522	LMG	C12-C13-C14-C15
36	H	102	DGD	O1B-C1B-C2B-C3B
24	A	406	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	B	611	CLA	C16-C17-C18-C20
25	a	406	PHO	C8-C10-C11-C12
24	B	606	CLA	C2B-C3B-CAB-CBB
24	B	607	CLA	C2B-C3B-CAB-CBB
24	C	505	CLA	C2B-C3B-CAB-CBB
24	a	404	CLA	C2B-C3B-CAB-CBB
24	b	602	CLA	C2B-C3B-CAB-CBB
24	c	507	CLA	C2B-C3B-CAB-CBB
24	c	509	CLA	C2B-C3B-CAB-CBB
26	b	617	BCR	C5-C6-C7-C8
26	d	404	BCR	C23-C24-C25-C26
26	h	102	BCR	C23-C24-C25-C30
26	y	101	BCR	C23-C24-C25-C30
34	B	622	LMT	C4'-C5'-C6'-O6'
39	e	102	HEM	CAA-CBA-CGA-O2A
27	a	409	SQD	C26-C27-C28-C29
24	C	514	CLA	C3-C5-C6-C7
24	b	616	CLA	C4-C3-C5-C6
33	j	101	LMG	C16-C17-C18-C19
24	B	604	CLA	C2-C3-C5-C6
31	a	414[B]	PL9	C18-C19-C21-C22
38	D	406	LHG	C33-C34-C35-C36
39	E	103	HEM	CAD-CBD-CGD-O1D
24	C	502	CLA	C12-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C15
24	b	614	CLA	C12-C13-C15-C16
24	b	616	CLA	C11-C12-C13-C15
24	c	508	CLA	C12-C13-C15-C16
24	c	509	CLA	C12-C13-C15-C16
31	a	414[B]	PL9	C4-C3-C7-C8
38	d	407	LHG	C9-C10-C11-C12
24	C	503	CLA	CBD-CGD-O2D-CED
34	B	630	LMT	C7-C8-C9-C10
35	B	624	HTG	C4'-C5'-C6'-C7'
31	a	414[A]	PL9	C18-C19-C21-C22
38	d	408	LHG	C32-C33-C34-C35
33	z	101	LMG	C10-C11-C12-C13
36	c	520	DGD	C7B-C8B-C9B-CAB
24	A	409	CLA	C6-C7-C8-C9
24	b	606	CLA	C11-C10-C8-C9
35	b	624	HTG	C3'-C4'-C5'-C6'
24	B	604	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
24	A	409	CLA	C4-C3-C5-C6
24	c	515	CLA	C4-C3-C5-C6
31	A	416[A]	PL9	C30-C29-C31-C32
31	A	416[B]	PL9	C45-C44-C46-C47
31	a	414[B]	PL9	C35-C34-C36-C37
31	D	405	PL9	C18-C19-C21-C22
36	c	520	DGD	CAB-CBB-CCB-CDB
36	C	517	DGD	C2E-C1E-O5D-C6D
24	b	614	CLA	C15-C16-C17-C18
36	c	518	DGD	C2A-C3A-C4A-C5A
38	D	407	LHG	C12-C13-C14-C15
39	e	102	HEM	CAA-CBA-CGA-O1A
27	b	620	SQD	C9-C10-C11-C12
24	B	602	CLA	C2A-CAA-CBA-CGA
24	a	403	CLA	C2A-CAA-CBA-CGA
39	E	103	HEM	CAD-CBD-CGD-O2D
31	A	416[B]	PL9	C40-C39-C41-C42
31	D	405	PL9	C30-C29-C31-C32
27	A	413	SQD	C32-C33-C34-C35
26	H	101	BCR	C9-C10-C11-C12
24	B	607	CLA	C4B-C3B-CAB-CBB
24	a	407	CLA	C4B-C3B-CAB-CBB
24	d	402	CLA	C4B-C3B-CAB-CBB
36	C	517	DGD	C9A-CAA-CBA-CCA
24	b	601	CLA	CAA-CBA-CGA-O1A
33	B	621	LMG	O10-C28-C29-C30
36	C	519	DGD	C9B-CAB-CBB-CCB
38	D	357	LHG	C29-C30-C31-C32
24	C	503	CLA	C10-C11-C12-C13
24	b	613	CLA	C8-C10-C11-C12
36	h	103	DGD	C6A-C7A-C8A-C9A
38	d	407	LHG	C25-C26-C27-C28
31	D	405	PL9	C15-C14-C16-C17
33	A	418	LMG	C12-C13-C14-C15
33	Z	101	LMG	O10-C28-O8-C9
24	b	602	CLA	C10-C11-C12-C13
41	V	203	HEC	CAD-CBD-CGD-O1D
24	A	409	CLA	C2-C3-C5-C6
24	b	616	CLA	C2-C3-C5-C6
24	A	409	CLA	C6-C7-C8-C10
35	b	623	HTG	C3'-C4'-C5'-C6'
24	b	603	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
38	l	101	LHG	C32-C33-C34-C35
26	b	619	BCR	C21-C22-C23-C24
34	m	102	LMT	C4'-C5'-C6'-O6'
27	B	620	SQD	C5-C6-S-O8
33	J	101	LMG	C8-C7-O1-C1
36	C	517	DGD	C5D-C6D-O5D-C1E
34	B	630	LMT	C2-C3-C4-C5
24	A	409	CLA	C2-C1-O2A-CGA
24	B	613	CLA	C16-C17-C18-C19
24	B	601	CLA	C3A-C2A-CAA-CBA
24	C	507	CLA	C3A-C2A-CAA-CBA
41	V	203	HEC	CAD-CBD-CGD-O2D
38	D	357	LHG	C9-C10-C11-C12
34	b	622	LMT	C6-C7-C8-C9
25	A	407	PHO	O2A-C1-C2-C3
24	b	604	CLA	C2C-C3C-CAC-CBC
38	d	407	LHG	C28-C29-C30-C31
36	c	520	DGD	CCB-CDB-CEB-CFB
38	d	408	LHG	C30-C31-C32-C33
33	B	621	LMG	C15-C16-C17-C18
38	D	407	LHG	C33-C34-C35-C36
24	C	504	CLA	C8-C10-C11-C12
24	C	513	CLA	C10-C11-C12-C13
24	b	611	CLA	C13-C15-C16-C17
24	D	403	CLA	O1A-CGA-O2A-C1
36	C	517	DGD	O6E-C1E-O5D-C6D
36	h	103	DGD	O1G-C1G-C2G-C3G
24	b	606	CLA	C8-C10-C11-C12
33	B	621	LMG	C32-C33-C34-C35
33	j	101	LMG	C36-C37-C38-C39
24	C	510	CLA	C8-C10-C11-C12
26	k	101	BCR	C9-C10-C11-C12
33	C	520	LMG	C29-C30-C31-C32
33	J	101	LMG	C37-C38-C39-C40
24	B	613	CLA	CAA-CBA-CGA-O2A
27	b	620	SQD	O48-C23-C24-C25
33	c	522	LMG	O10-C28-O8-C9
24	b	604	CLA	C13-C15-C16-C17
24	B	604	CLA	C11-C12-C13-C14
24	B	611	CLA	C16-C17-C18-C19
24	A	405	CLA	C2C-C3C-CAC-CBC
24	C	511	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
39	e	102	HEM	CAD-CBD-CGD-O1D
24	b	613	CLA	CAA-CBA-CGA-O2A
31	a	414[B]	PL9	C12-C11-C9-C8
24	B	613	CLA	C11-C10-C8-C7
24	b	606	CLA	C11-C10-C8-C7
24	b	610	CLA	C11-C12-C13-C15
24	b	616	CLA	C12-C13-C15-C16
24	c	511	CLA	C12-C13-C15-C16
24	C	507	CLA	C3-C5-C6-C7
24	b	607	CLA	C2B-C3B-CAB-CBB
24	d	402	CLA	C2B-C3B-CAB-CBB
26	h	102	BCR	C23-C24-C25-C26
26	y	101	BCR	C23-C24-C25-C26
27	A	413	SQD	C17-C18-C19-C20
24	C	510	CLA	C2-C1-O2A-CGA
24	b	613	CLA	C2-C1-O2A-CGA
24	c	513	CLA	C2-C1-O2A-CGA
24	d	402	CLA	C2-C1-O2A-CGA
34	B	622	LMT	C5-C6-C7-C8
24	a	350	CLA	C2C-C3C-CAC-CBC
36	C	518	DGD	C8A-C9A-CAA-CBA
24	B	601	CLA	C2A-CAA-CBA-CGA
24	c	503	CLA	C2A-CAA-CBA-CGA
35	b	623	HTG	C4-C5-C6-O6
24	B	601	CLA	CAA-CBA-CGA-O1A
24	A	406	CLA	C13-C15-C16-C17
27	a	411	SQD	C34-C35-C36-C37
24	B	608	CLA	C16-C17-C18-C19
31	A	416[B]	PL9	C4-C3-C7-C8
36	C	519	DGD	C7B-C8B-C9B-CAB
38	L	101	LHG	O7-C7-C8-C9
38	l	101	LHG	O7-C7-C8-C9
24	B	604	CLA	C4C-C3C-CAC-CBC
33	J	101	LMG	C12-C13-C14-C15
24	c	508	CLA	C4-C3-C5-C6
31	A	416[B]	PL9	C12-C13-C14-C16
33	a	417	LMG	C37-C38-C39-C40
24	c	512	CLA	CAA-CBA-CGA-O2A
27	a	411	SQD	C13-C14-C15-C16
33	C	520	LMG	C36-C37-C38-C39
24	b	616	CLA	C11-C12-C13-C14
24	c	509	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	c	511	CLA	C11-C10-C8-C9
33	C	520	LMG	O1-C7-C8-C9
25	a	406	PHO	C2C-C3C-CAC-CBC
34	E	102	LMT	C5-C6-C7-C8
24	a	407	CLA	C15-C16-C17-C18
24	b	607	CLA	C4B-C3B-CAB-CBB
24	c	515	CLA	C1A-C2A-CAA-CBA
24	c	515	CLA	C4B-C3B-CAB-CBB
38	d	407	LHG	C14-C15-C16-C17
24	B	602	CLA	C4-C3-C5-C6
33	b	621	LMG	C21-C22-C23-C24
27	F	101	SQD	O5-C1-O6-C44
33	Z	101	LMG	O6-C1-O1-C7
31	a	414[B]	PL9	C36-C37-C38-C39
26	D	404	BCR	C7-C8-C9-C10
27	A	411	SQD	O47-C7-C8-C9
33	J	101	LMG	O7-C10-C11-C12
33	c	521	LMG	O7-C10-C11-C12
38	d	406	LHG	O10-C23-O8-C6
38	d	406	LHG	C27-C28-C29-C30
24	b	605	CLA	C13-C15-C16-C17
27	B	620	SQD	C5-C6-S-O7
27	B	620	SQD	C5-C6-S-O9
31	a	414[B]	PL9	C26-C27-C28-C29
36	H	102	DGD	CDA-CEA-CFA-CGA
36	h	103	DGD	O1B-C1B-C2B-C3B
27	A	411	SQD	C34-C35-C36-C37
24	B	613	CLA	C2-C1-O2A-CGA
24	C	514	CLA	C2-C1-O2A-CGA
24	b	612	CLA	CAA-CBA-CGA-O2A
27	f	101	SQD	O47-C7-C8-C9
24	C	507	CLA	C12-C13-C15-C16
24	D	403	CLA	C12-C13-C15-C16
24	a	350	CLA	C6-C7-C8-C10
24	b	604	CLA	C11-C12-C13-C15
24	b	604	CLA	C12-C13-C15-C16
24	c	508	CLA	C11-C12-C13-C15
33	c	522	LMG	C29-C28-O8-C9
38	D	406	LHG	C34-C35-C36-C37
34	M	103	LMT	C11-C10-C9-C8
38	D	406	LHG	C25-C26-C27-C28
34	a	359	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
38	D	357	LHG	C33-C34-C35-C36
39	e	102	HEM	CAD-CBD-CGD-O2D
36	c	520	DGD	C8B-C9B-CAB-CBB
24	B	610	CLA	C2A-CAA-CBA-CGA
24	B	614	CLA	C2A-CAA-CBA-CGA
24	b	604	CLA	C4C-C3C-CAC-CBC
31	a	414[B]	PL9	C45-C44-C46-C47
24	b	612	CLA	C13-C15-C16-C17
31	d	405	PL9	C18-C19-C21-C22
25	a	405	PHO	C8-C10-C11-C12
38	l	101	LHG	C17-C18-C19-C20
33	C	520	LMG	O9-C10-C11-C12
27	a	409	SQD	C15-C16-C17-C18
33	Z	101	LMG	C15-C16-C17-C18
27	B	620	SQD	O10-C23-O48-C46
38	L	101	LHG	O9-C7-C8-C9
24	C	506	CLA	C11-C12-C13-C14
33	a	417	LMG	O10-C28-C29-C30
36	c	518	DGD	C6A-C7A-C8A-C9A
38	D	407	LHG	C9-C10-C11-C12
26	T	101	BCR	C15-C16-C17-C18
27	A	413	SQD	C25-C26-C27-C28
24	C	510	CLA	C10-C11-C12-C13
24	b	613	CLA	CAA-CBA-CGA-O1A
27	b	620	SQD	O10-C23-C24-C25
38	l	101	LHG	O9-C7-C8-C9
24	D	403	CLA	CBA-CGA-O2A-C1
24	b	609	CLA	C2-C3-C5-C6
33	C	520	LMG	C16-C17-C18-C19
24	B	612	CLA	C13-C15-C16-C17
25	A	407	PHO	C10-C11-C12-C13
24	C	514	CLA	O1A-CGA-O2A-C1
24	d	402	CLA	CAA-CBA-CGA-O2A
24	b	604	CLA	C16-C17-C18-C20
24	B	605	CLA	C5-C6-C7-C8
26	c	517	BCR	C7-C8-C9-C10
33	b	621	LMG	C22-C23-C24-C25
36	c	519	DGD	C2G-C3G-O3G-C1D
24	B	613	CLA	CAA-CBA-CGA-O1A
24	C	511	CLA	CAA-CBA-CGA-O1A
33	c	521	LMG	O9-C10-C11-C12
24	B	612	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
33	a	417	LMG	C30-C31-C32-C33
27	a	409	SQD	O6-C44-C45-C46
24	c	512	CLA	CAA-CBA-CGA-O1A
27	A	411	SQD	O49-C7-C8-C9
31	A	416[A]	PL9	C35-C34-C36-C37
31	d	405	PL9	C11-C12-C13-C14
27	b	620	SQD	C19-C20-C21-C22
24	B	605	CLA	CAD-CBD-CGD-O2D
24	b	609	CLA	CAD-CBD-CGD-O2D
24	b	616	CLA	CAD-CBD-CGD-O2D
25	A	408	PHO	CAD-CBD-CGD-O2D
38	d	408	LHG	O8-C23-C24-C25
27	f	101	SQD	O49-C7-C8-C9
24	b	601	CLA	C10-C11-C12-C13
27	A	411	SQD	C14-C15-C16-C17
24	C	513	CLA	C2-C1-O2A-CGA
24	b	608	CLA	C2-C1-O2A-CGA
24	b	614	CLA	C2-C1-O2A-CGA
24	c	514	CLA	CAA-CBA-CGA-O2A
36	C	518	DGD	O2G-C1B-C2B-C3B
24	b	615	CLA	C10-C11-C12-C13
24	b	616	CLA	C10-C11-C12-C13
24	a	404	CLA	C16-C17-C18-C19
33	J	101	LMG	O9-C10-C11-C12
27	f	101	SQD	C28-C29-C30-C31
24	B	612	CLA	CAA-CBA-CGA-O1A
38	D	357	LHG	C30-C31-C32-C33

There are no ring outliers.

154 monomers are involved in 383 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	d	402	CLA	3	0
24	b	613	CLA	4	0
33	j	101	LMG	4	0
34	I	101	LMT	1	0
24	c	514	CLA	7	0
24	C	508	CLA	2	0
24	c	509	CLA	4	0
24	C	512	CLA	2	0
24	c	510	CLA	5	0
27	b	620	SQD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	516	BCR	5	0
24	C	505	CLA	1	0
24	B	612	CLA	3	0
24	A	406	CLA	4	0
24	B	613	CLA	3	0
24	C	510	CLA	3	0
26	b	617	BCR	3	0
27	F	101	SQD	1	0
26	b	619	BCR	4	0
24	b	603	CLA	3	0
26	y	101	BCR	4	0
24	c	512	CLA	6	0
27	B	620	SQD	1	0
38	a	419	LHG	3	0
39	e	102	HEM	4	0
35	D	410	HTG	2	0
33	J	101	LMG	2	0
24	c	504	CLA	4	0
33	a	417	LMG	3	0
34	M	103	LMT	2	0
24	c	511	CLA	3	0
34	a	359	LMT	3	0
24	c	506	CLA	4	0
38	D	406	LHG	3	0
34	e	101	LMT	1	0
24	A	404	CLA	6	0
24	A	409	CLA	3	0
24	C	511	CLA	2	0
25	A	408	PHO	4	0
24	a	350	CLA	4	0
36	c	518	DGD	1	0
24	a	403	CLA	5	0
34	A	359	LMT	2	0
24	b	604	CLA	1	0
24	B	611	CLA	1	0
24	b	605	CLA	8	0
36	C	519	DGD	1	0
24	b	602	CLA	2	0
34	m	102	LMT	1	0
35	B	624	HTG	2	0
24	c	513	CLA	4	0
24	D	402	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	606	CLA	5	0
24	C	504	CLA	5	0
26	c	517	BCR	2	0
26	t	102	BCR	5	0
38	D	407	LHG	5	0
31	A	416[B]	PL9	5	0
38	D	357	LHG	2	0
33	c	521	LMG	2	0
24	c	507	CLA	8	0
36	H	102	DGD	2	0
35	B	623	HTG	3	0
24	B	602	CLA	5	0
31	a	414[B]	PL9	8	0
33	C	521	LMG	3	0
24	B	605	CLA	4	0
24	b	611	CLA	1	0
34	E	102	LMT	1	0
24	B	606	CLA	3	0
25	a	405	PHO	2	0
34	M	101	LMT	1	0
24	b	615	CLA	1	0
24	B	615	CLA	2	0
24	D	403	CLA	1	0
24	C	514	CLA	5	0
24	b	610	CLA	1	0
26	C	516	BCR	2	0
26	H	101	BCR	3	0
24	b	601	CLA	2	0
25	A	407	PHO	2	0
24	B	601	CLA	1	0
26	B	619	BCR	3	0
24	d	403	CLA	4	0
35	b	625	HTG	1	0
34	a	418	LMT	1	0
24	a	407	CLA	3	0
31	D	405	PL9	5	0
33	B	621	LMG	1	0
31	a	414[A]	PL9	6	0
33	z	101	LMG	2	0
24	c	503	CLA	2	0
26	A	410	BCR	2	0
26	B	618	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	C	522	HTG	2	0
38	E	101	LHG	6	0
24	b	614	CLA	6	0
38	L	101	LHG	2	0
31	d	405	PL9	3	0
26	D	404	BCR	3	0
24	B	616	CLA	5	0
24	b	612	CLA	4	0
24	A	405	CLA	3	0
24	c	508	CLA	4	0
30	a	413[B]	OEY	1	0
34	B	622	LMT	3	0
27	f	101	SQD	3	0
39	E	103	HEM	2	0
36	C	517	DGD	2	0
24	b	616	CLA	1	0
24	b	609	CLA	4	0
27	A	413	SQD	2	0
24	C	506	CLA	4	0
35	b	623	HTG	4	0
28	a	410	GOL	1	0
38	d	407	LHG	3	0
24	B	614	CLA	5	0
36	c	519	DGD	5	0
24	b	607	CLA	1	0
26	h	102	BCR	5	0
26	C	515	BCR	4	0
24	C	507	CLA	8	0
24	C	513	CLA	2	0
28	a	416	GOL	1	0
33	A	418	LMG	1	0
38	d	408	LHG	7	0
26	k	101	BCR	1	0
24	C	502	CLA	5	0
31	A	416[A]	PL9	4	0
24	c	505	CLA	5	0
26	b	618	BCR	3	0
33	Z	101	LMG	5	0
26	d	404	BCR	3	0
24	B	604	CLA	3	0
38	d	406	LHG	2	0
26	T	101	BCR	6	0

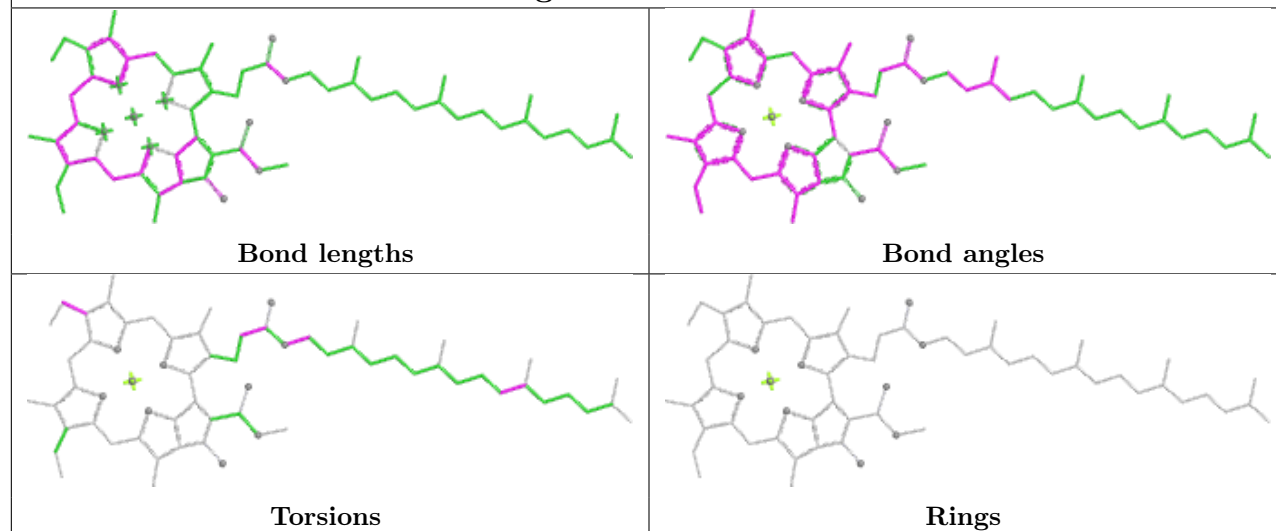
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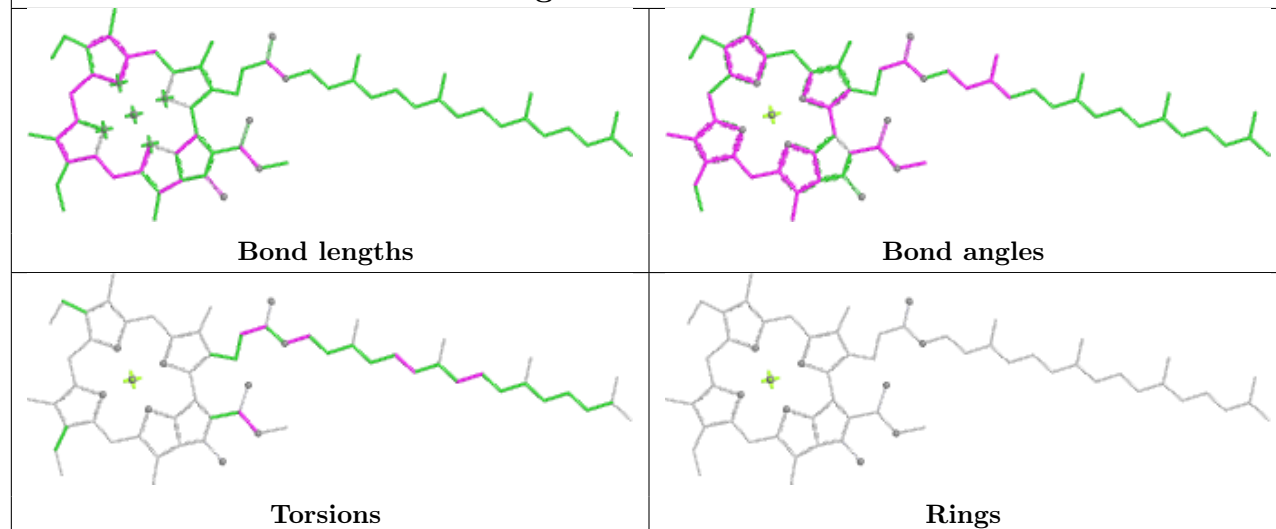
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	515	CLA	5	0
25	a	406	PHO	3	0
26	K	102	BCR	1	0
36	C	518	DGD	1	0
38	l	101	LHG	2	0
24	C	509	CLA	5	0
27	a	409	SQD	5	0
24	B	609	CLA	6	0
26	a	408	BCR	2	0
27	A	411	SQD	6	0
34	t	101	LMT	1	0
33	b	621	LMG	1	0
24	B	610	CLA	2	0
24	C	503	CLA	3	0
28	B	627	GOL	2	0
26	Y	101	BCR	3	0
35	b	624	HTG	2	0
24	a	404	CLA	3	0

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

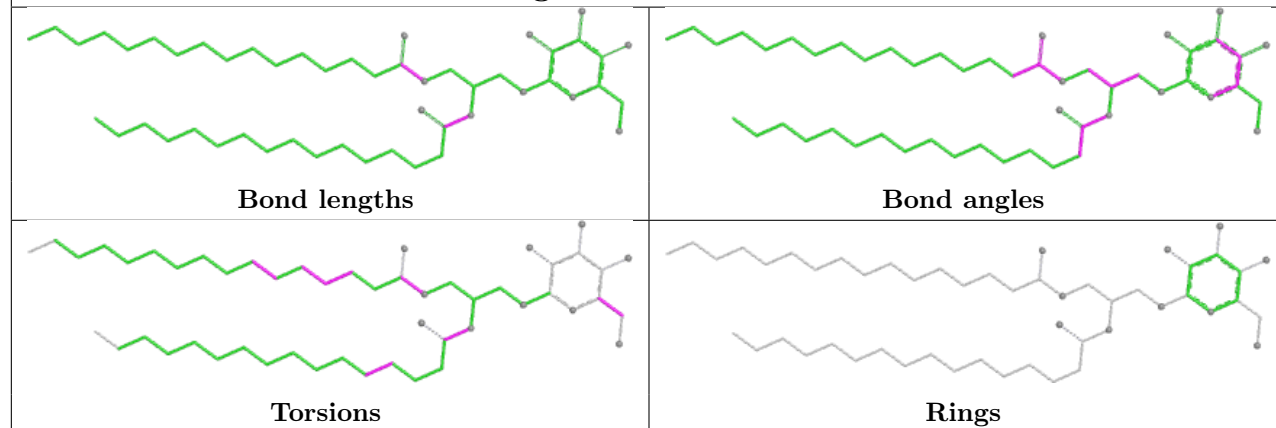
Ligand CLA d 402

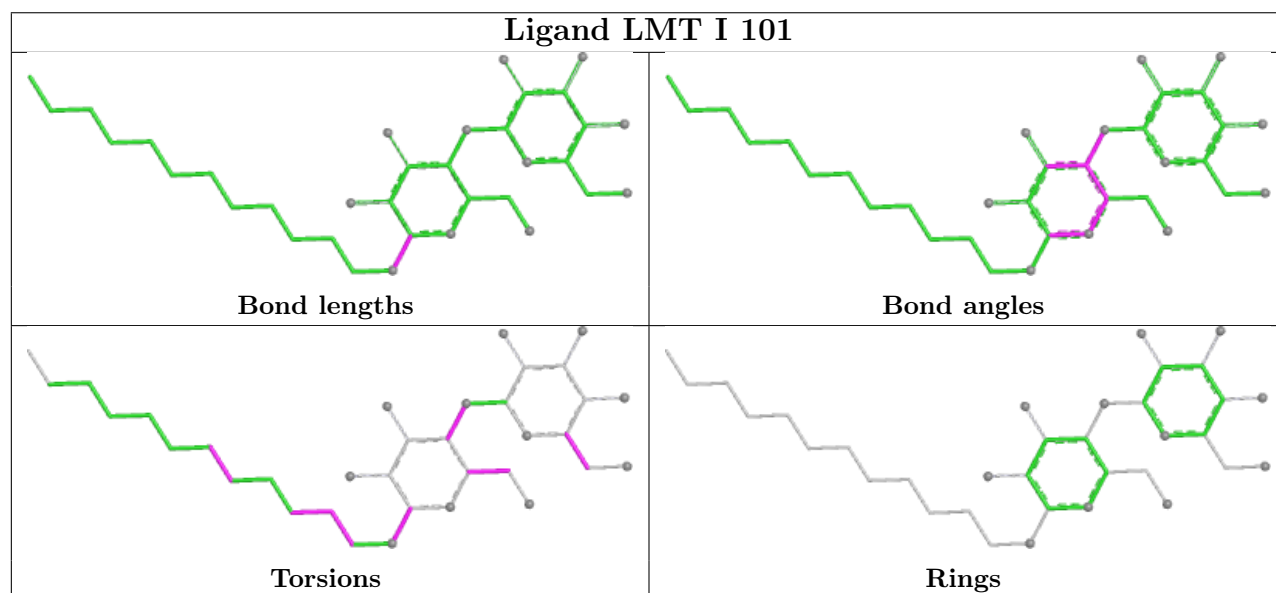
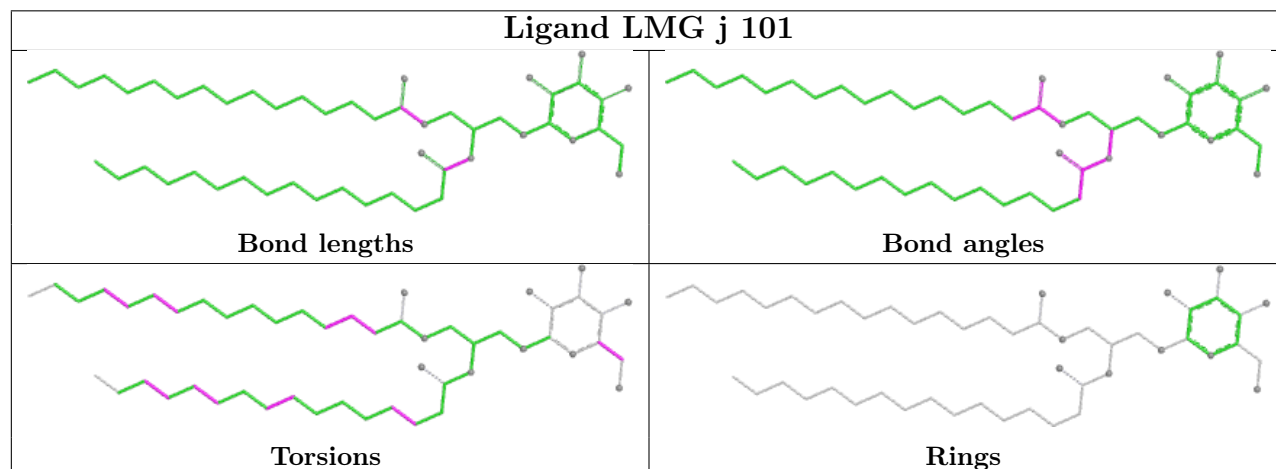
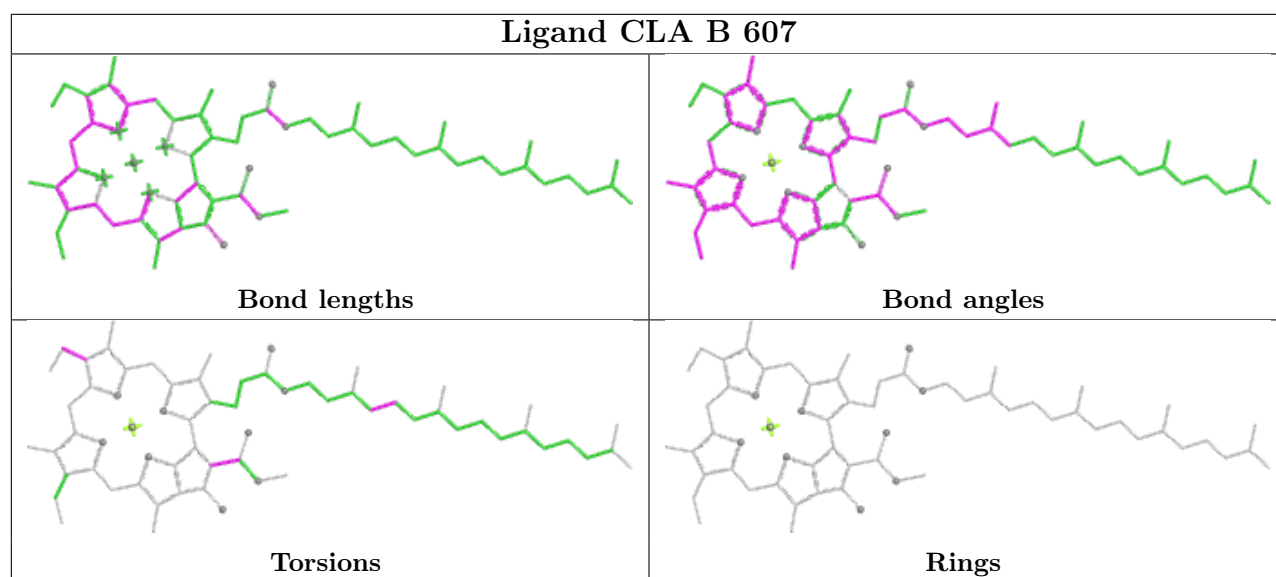


Ligand CLA b 613

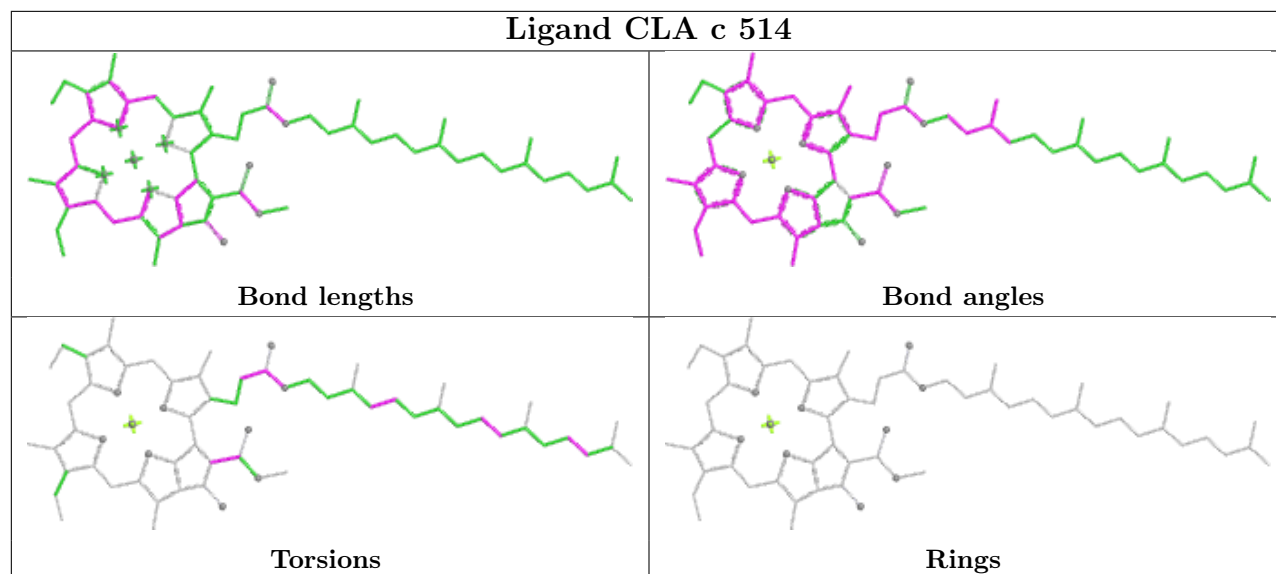


Ligand LMG c 522

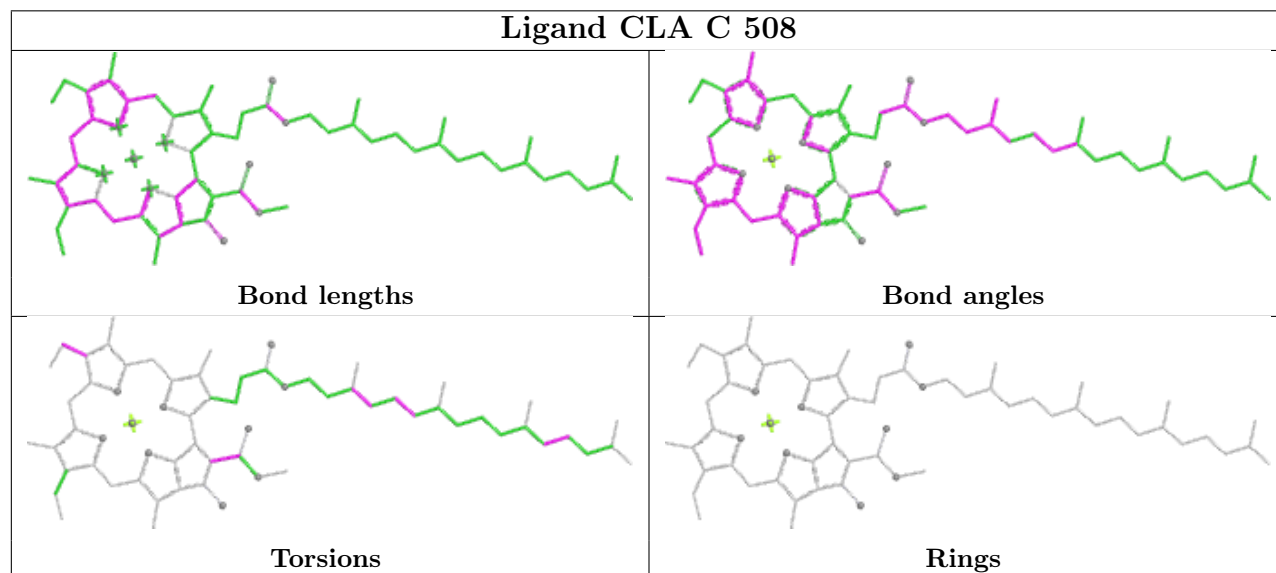




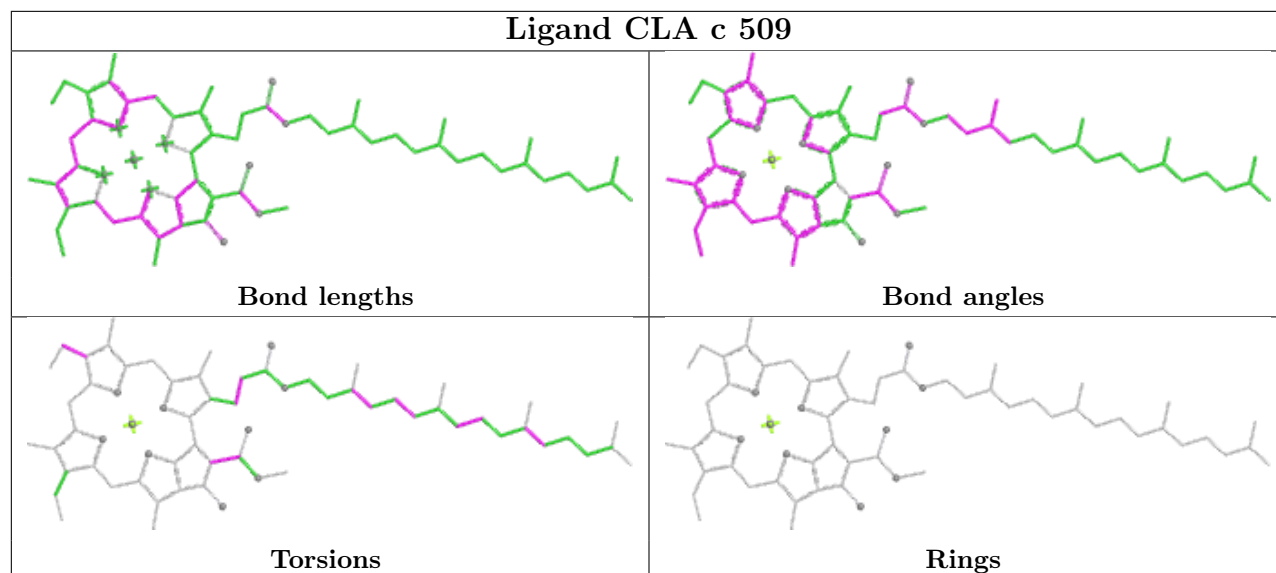
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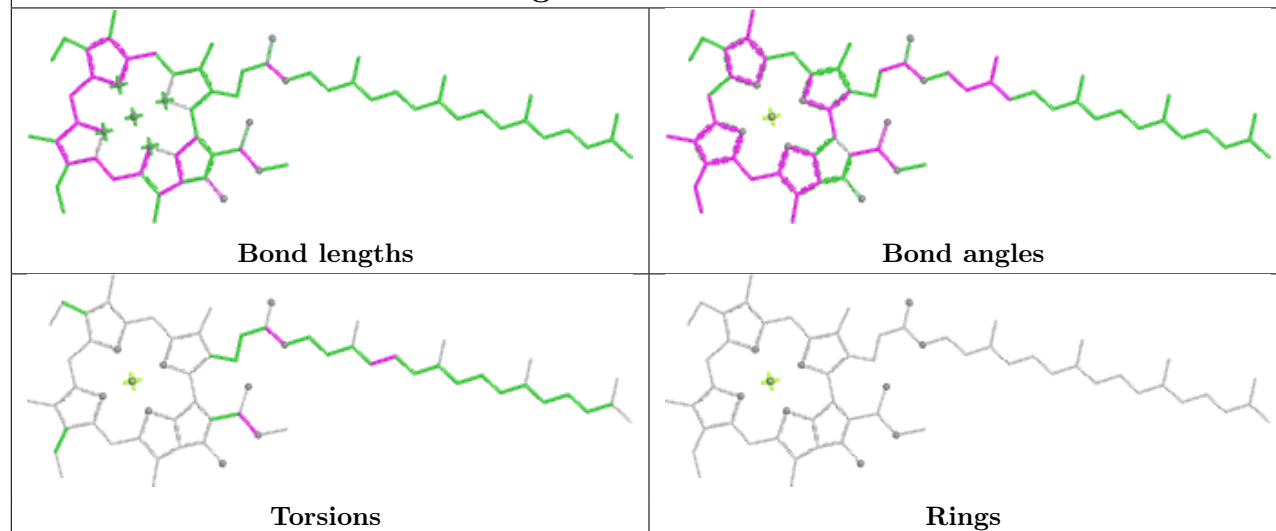
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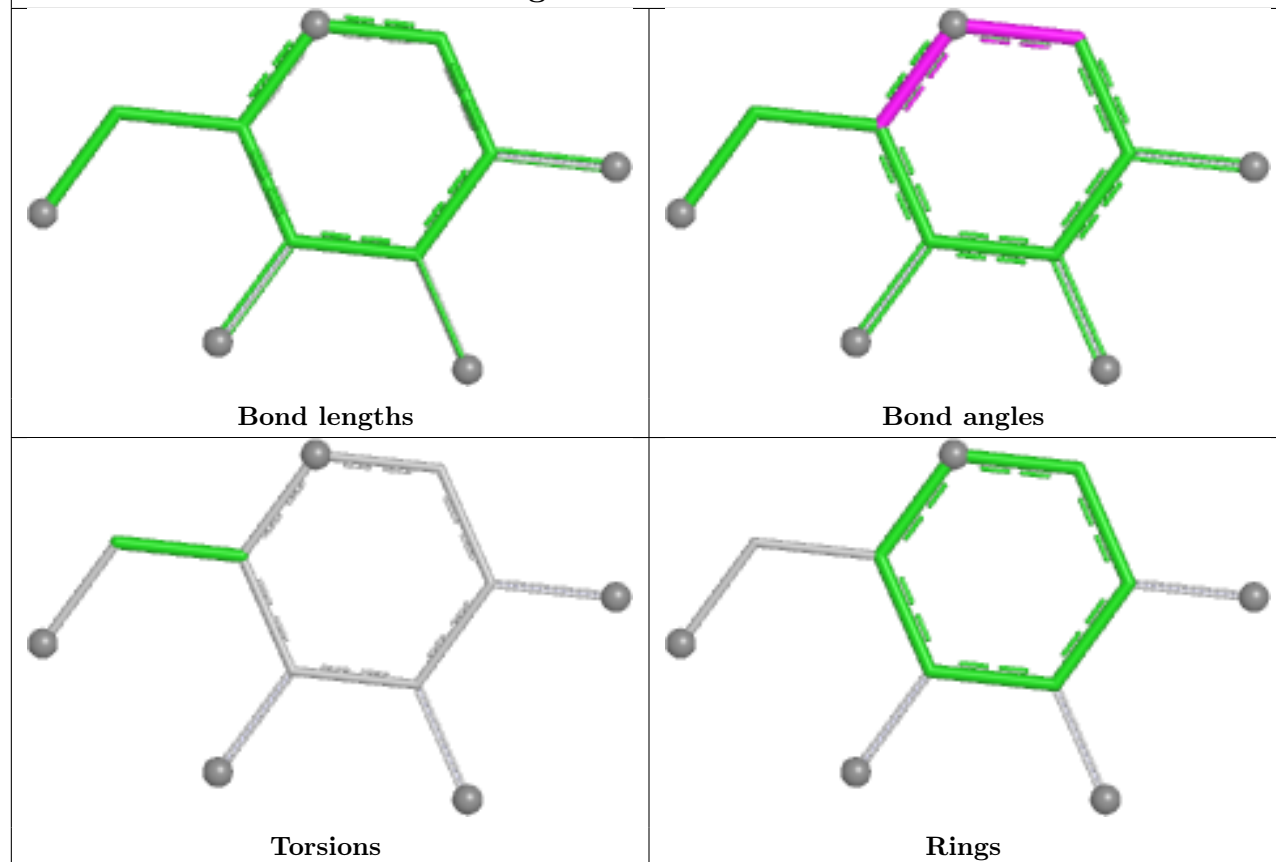
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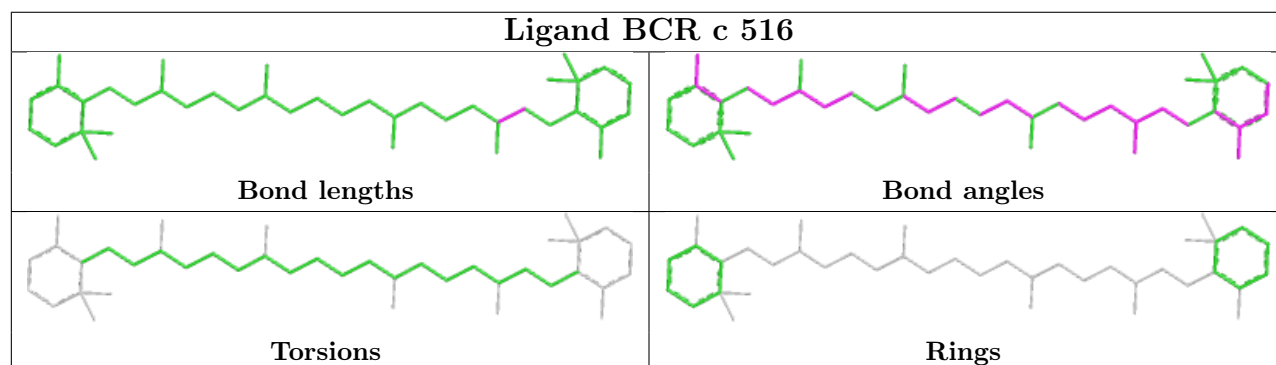
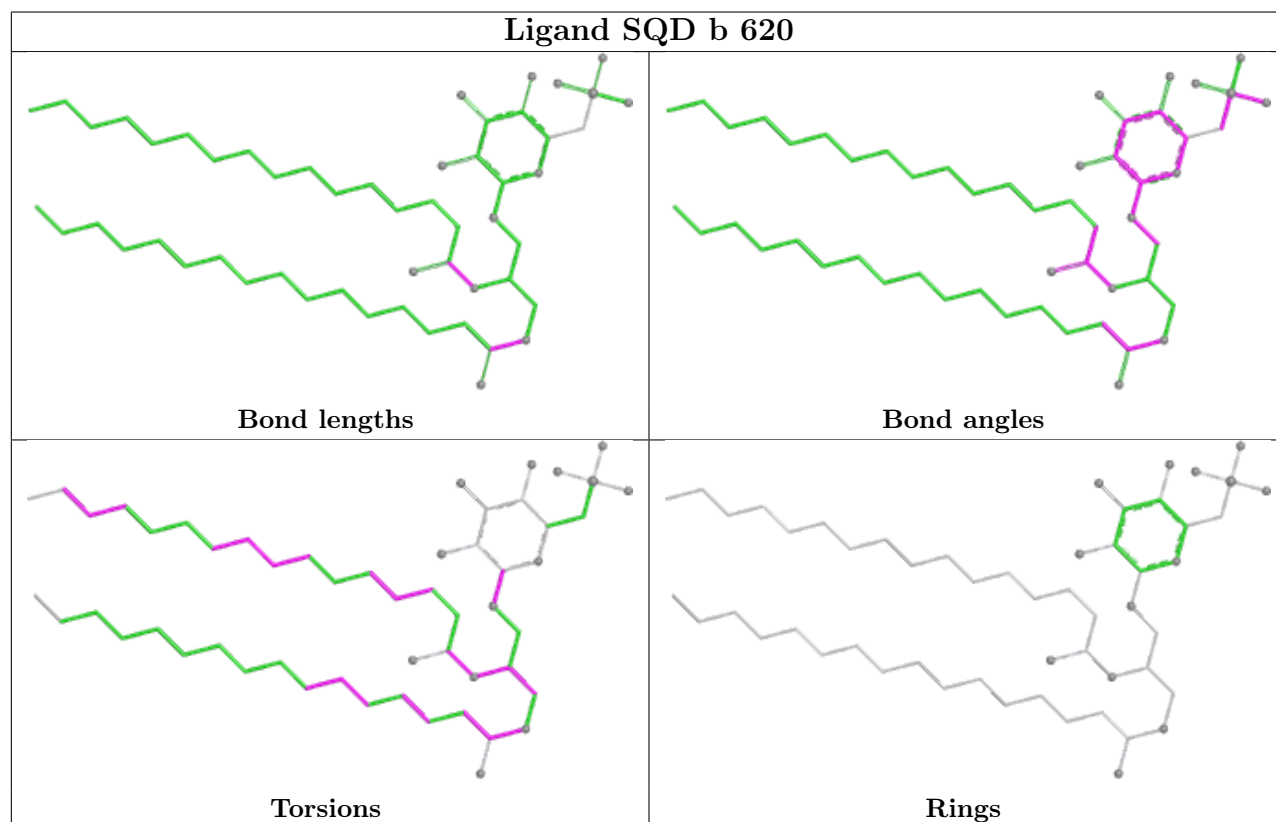
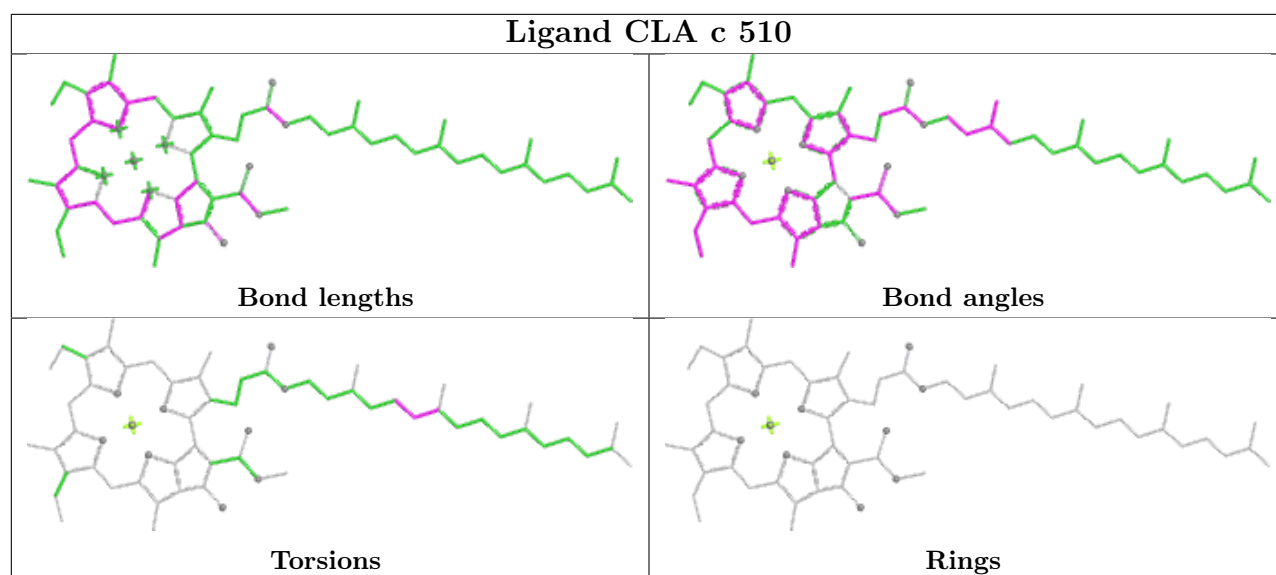


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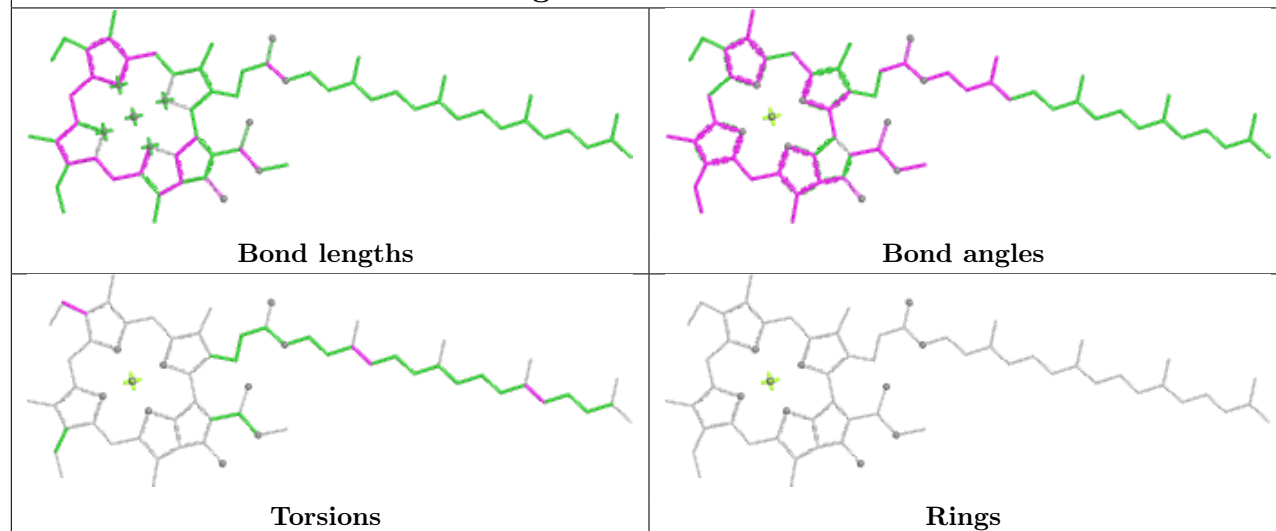


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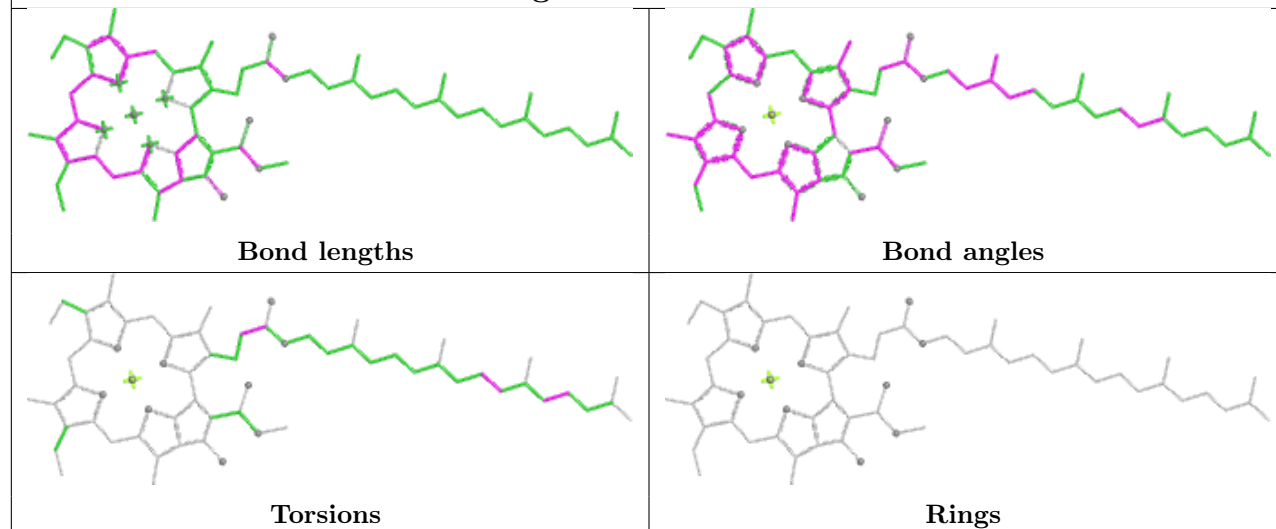




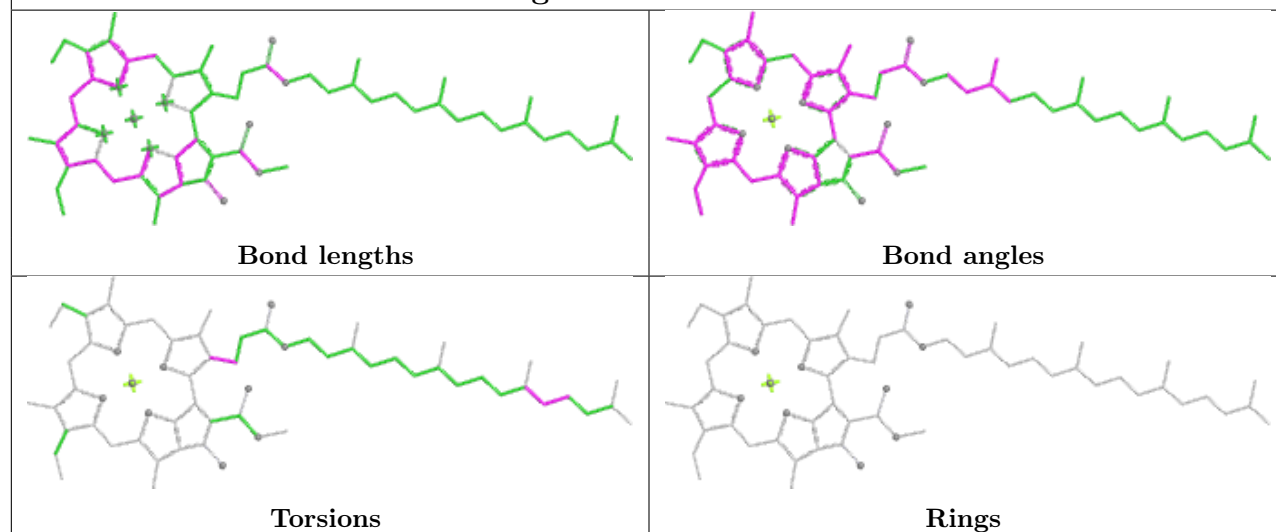
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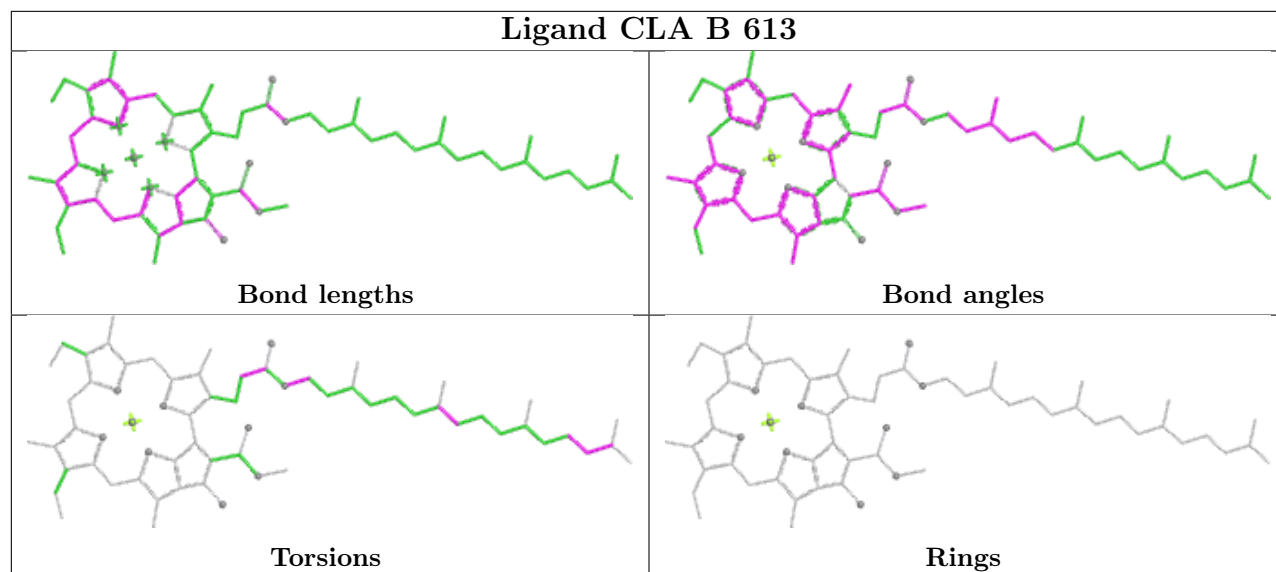
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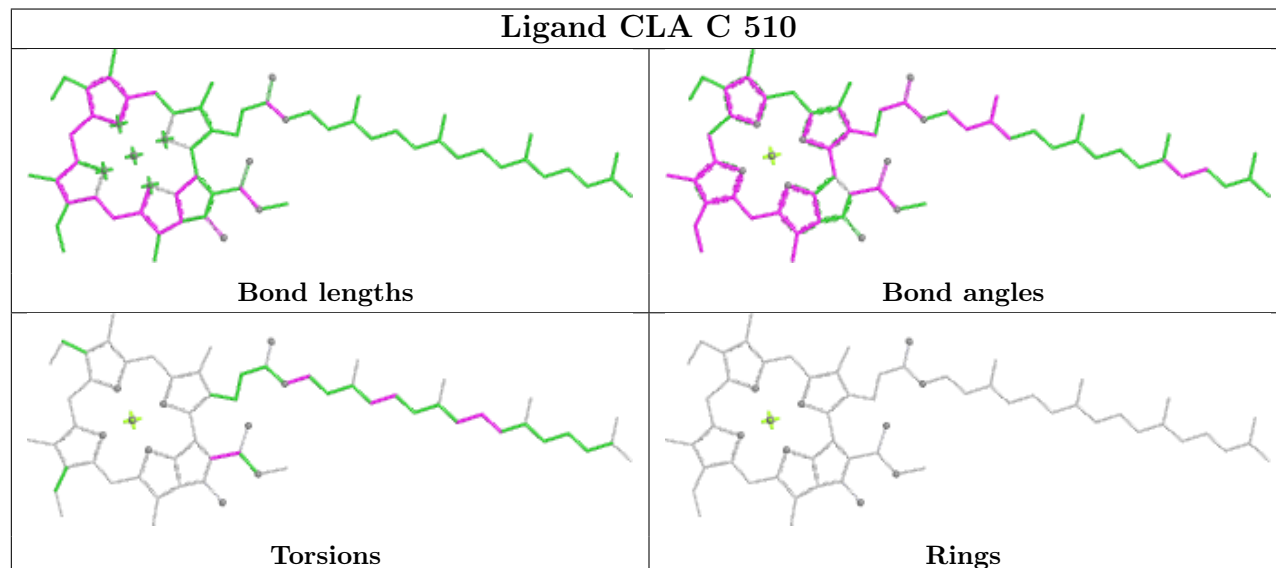
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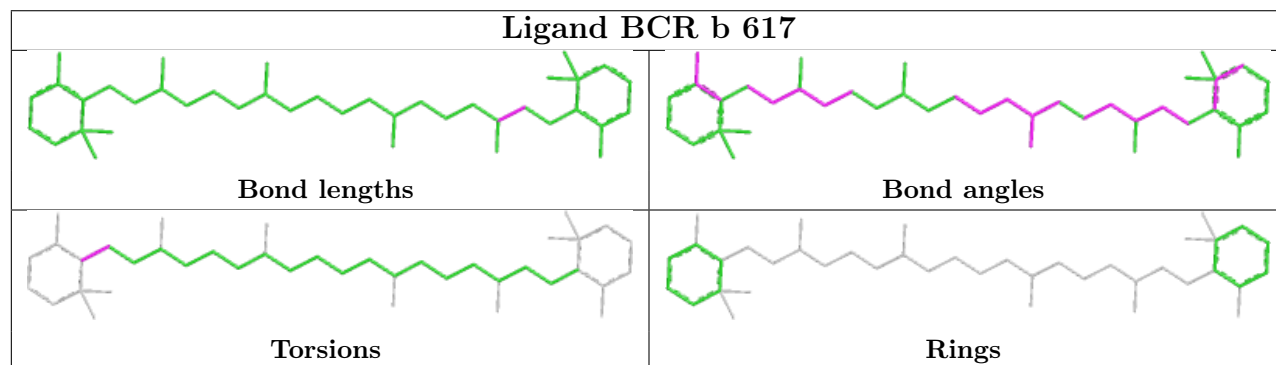
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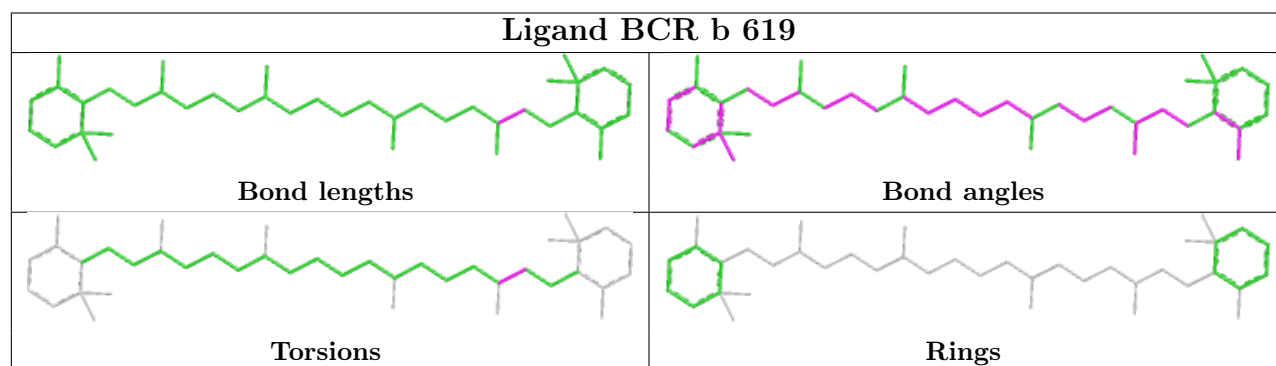
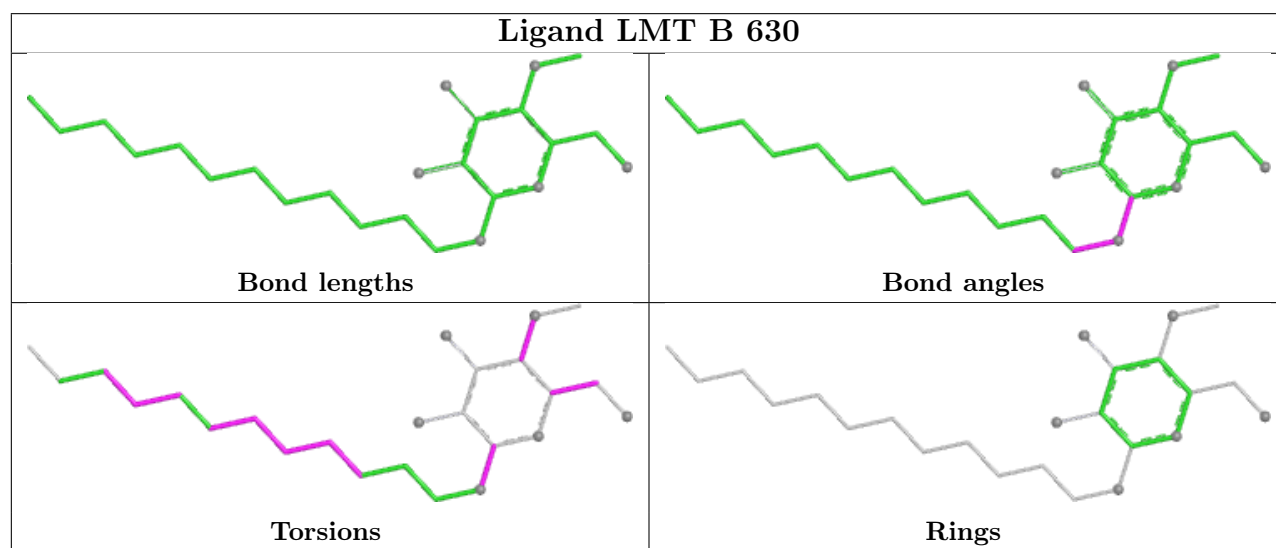
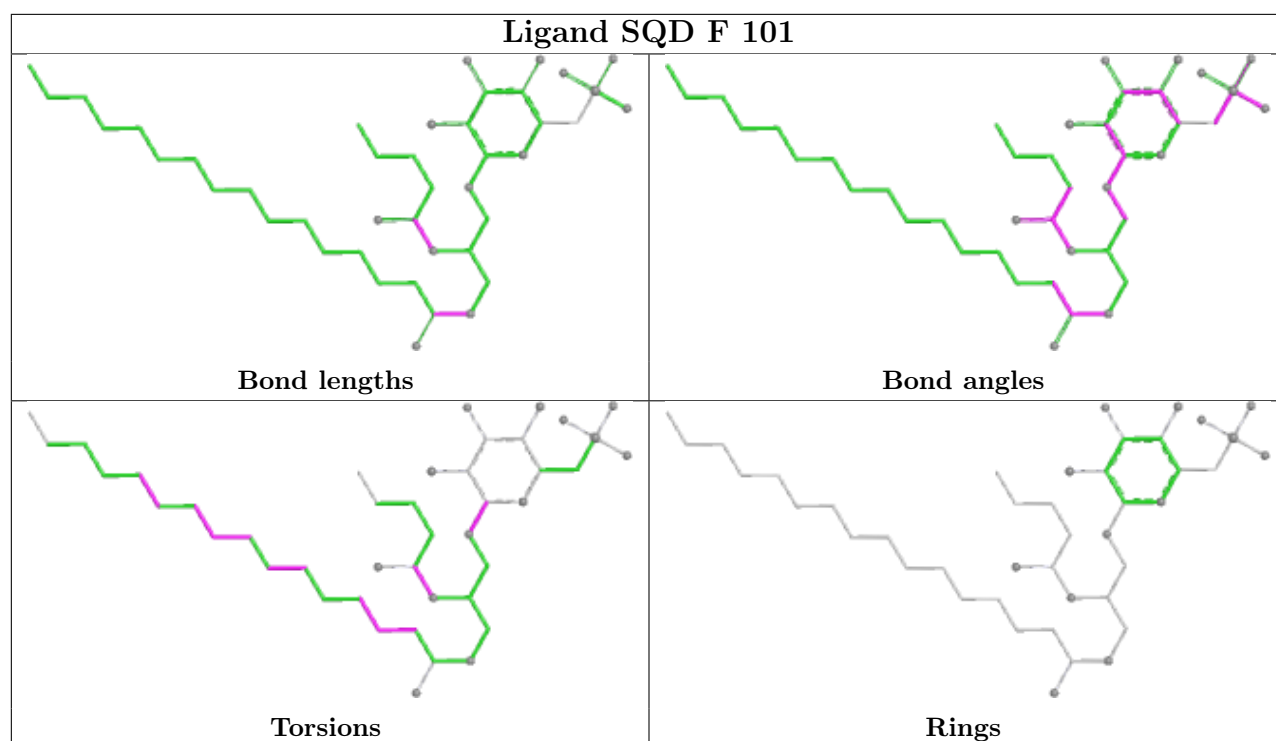


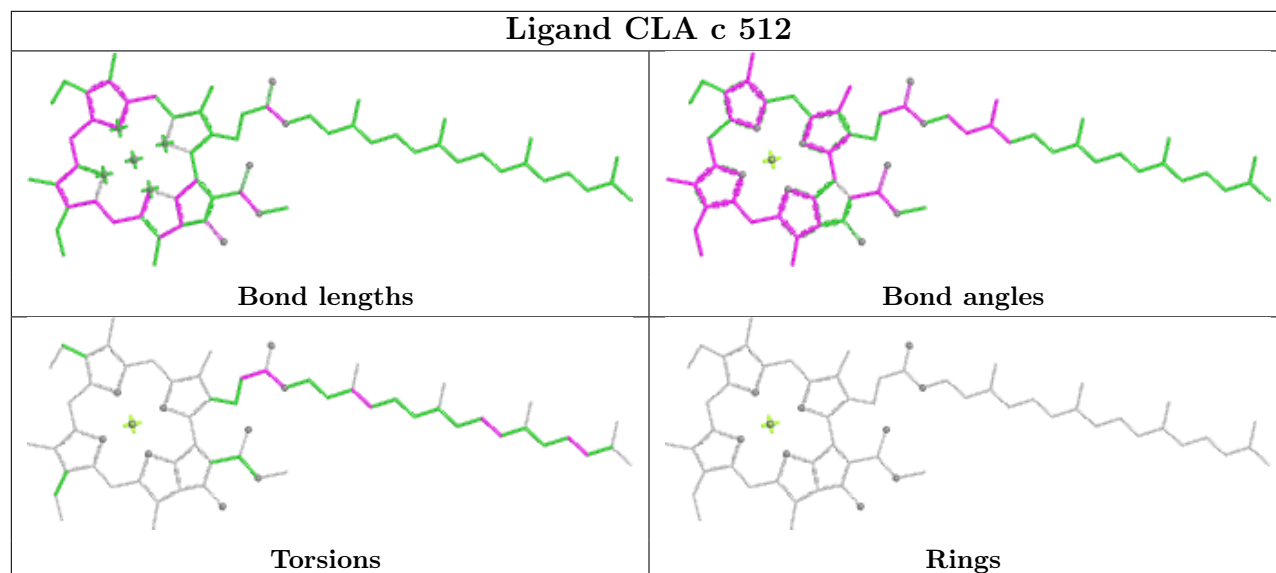
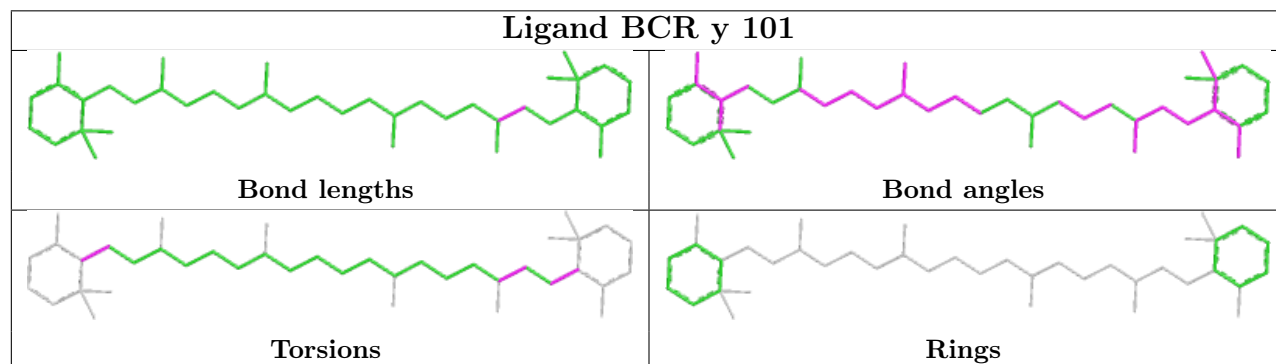
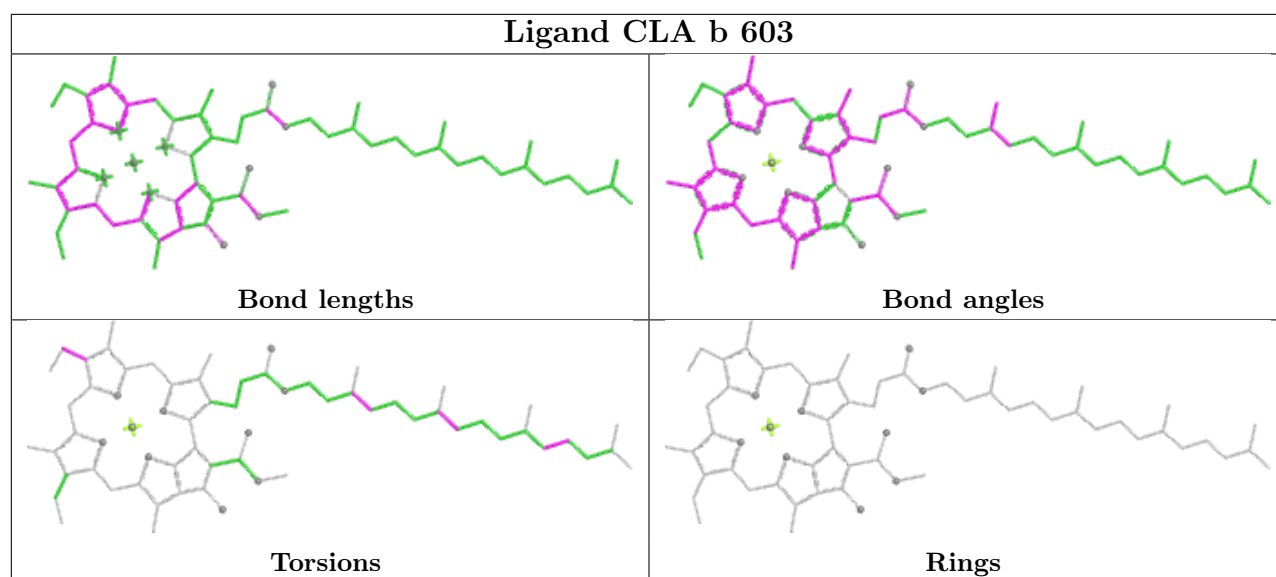
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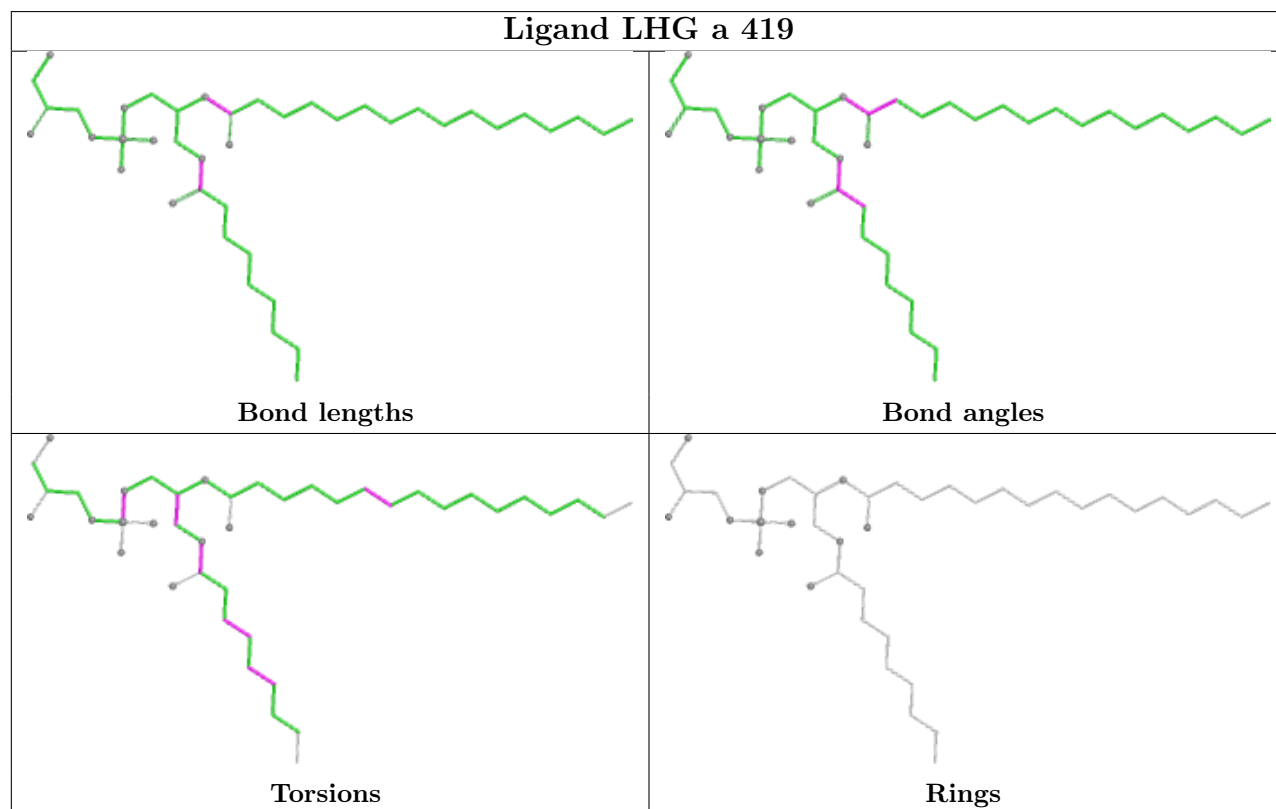
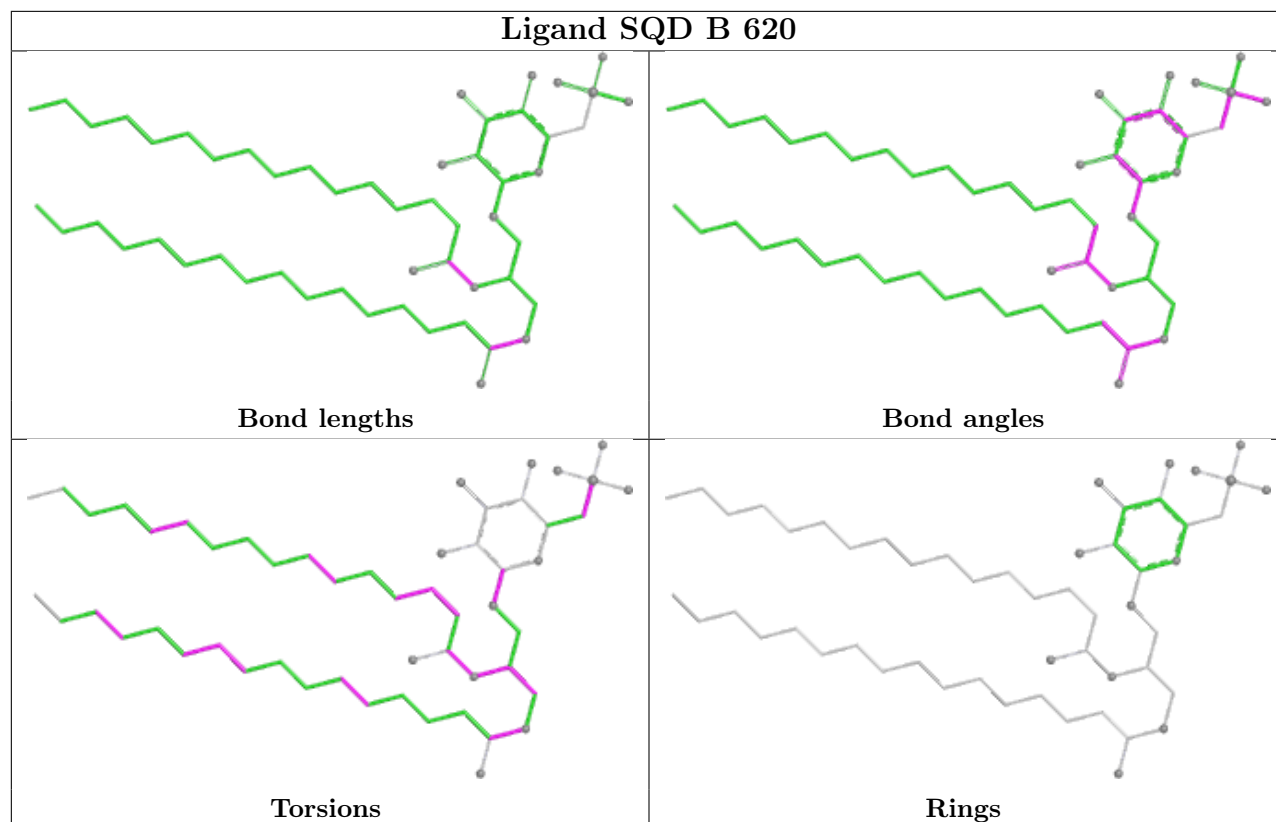


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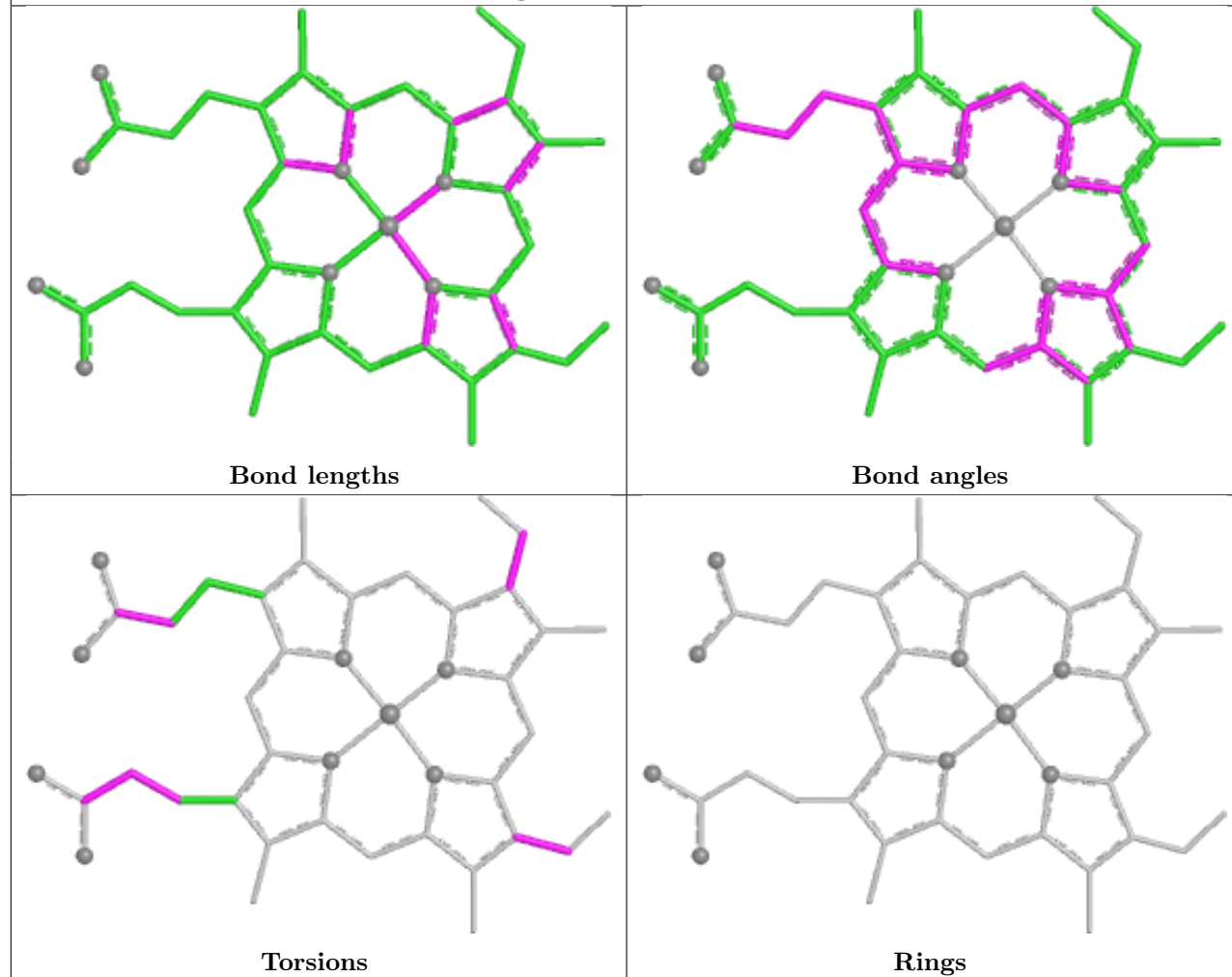


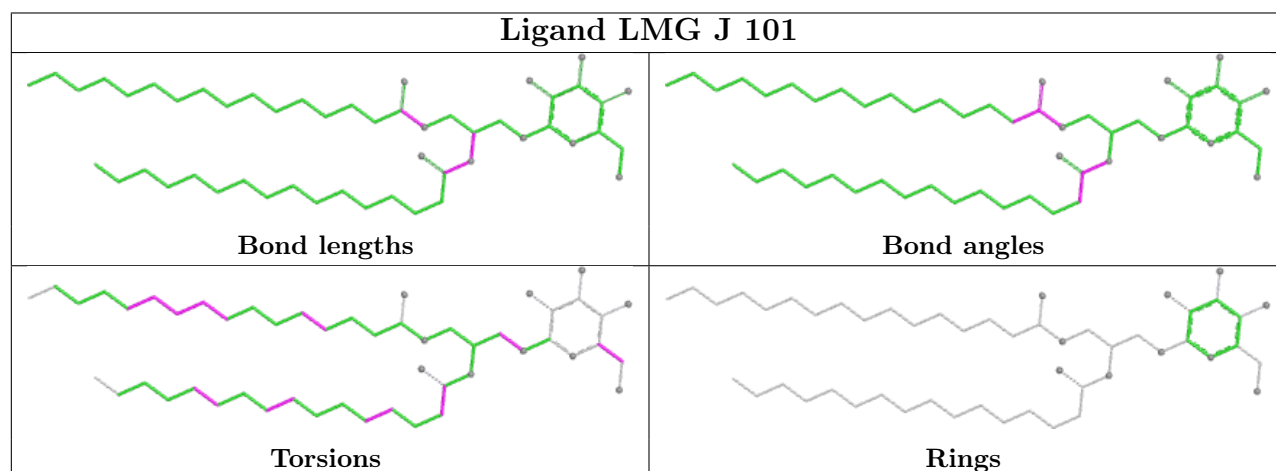
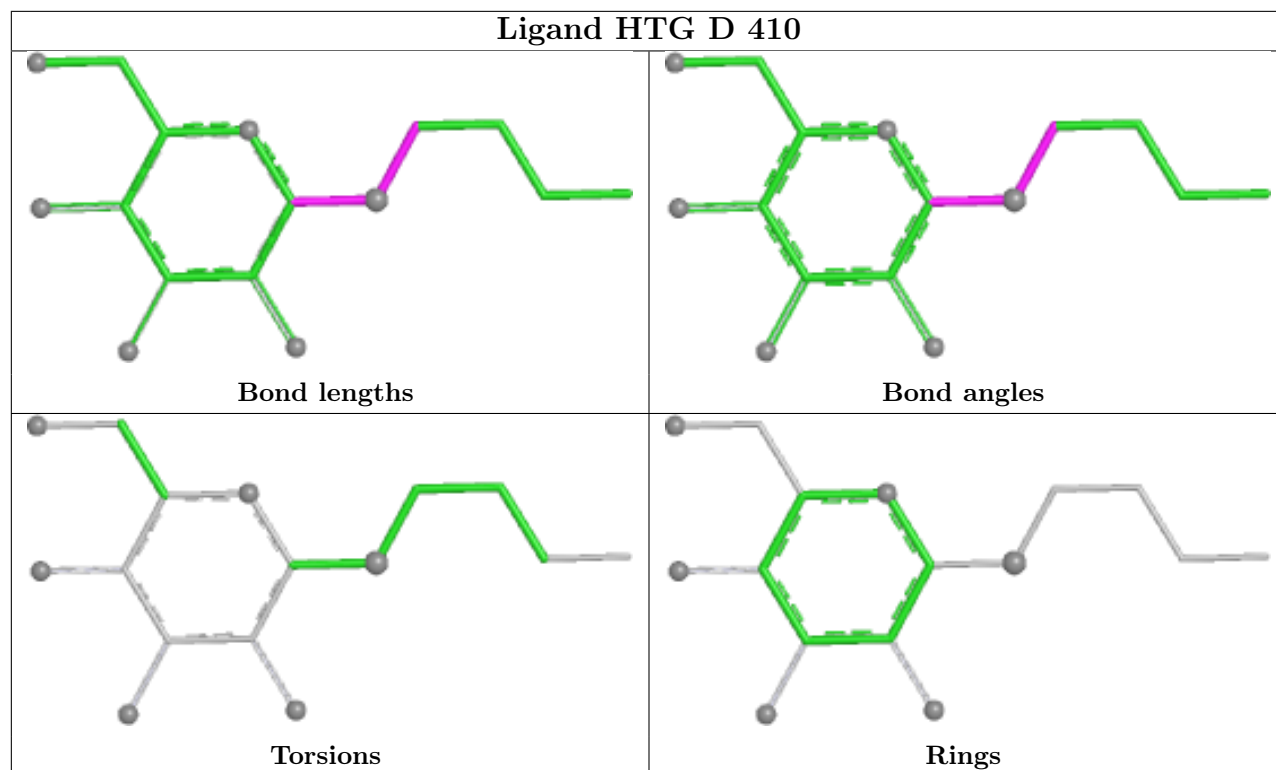


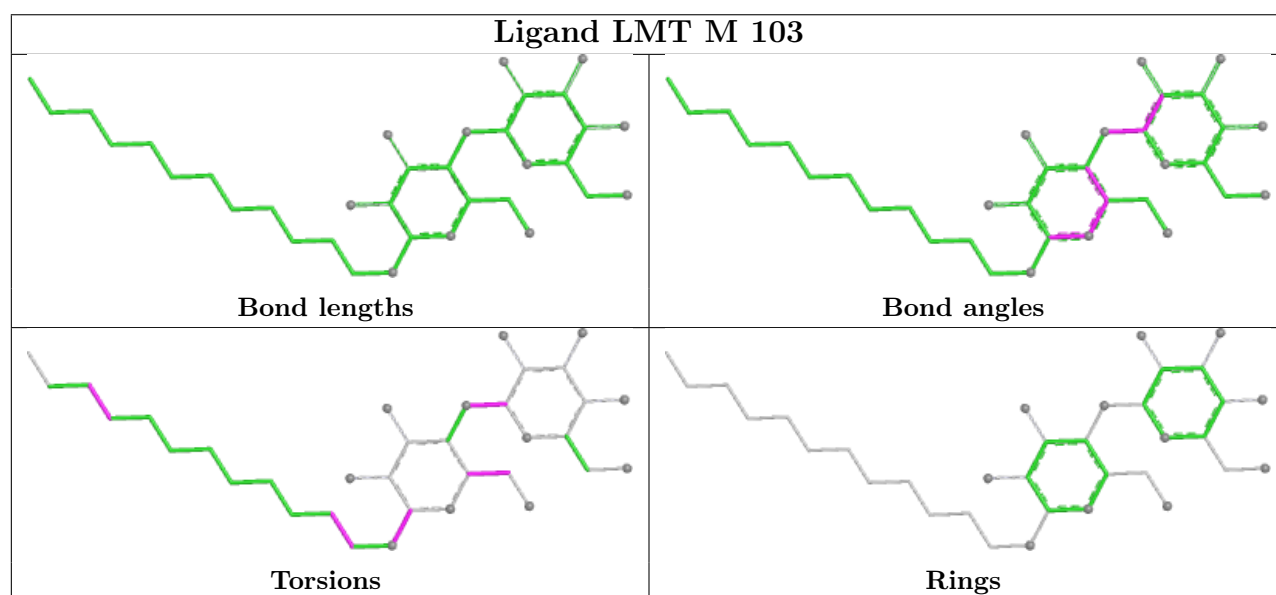
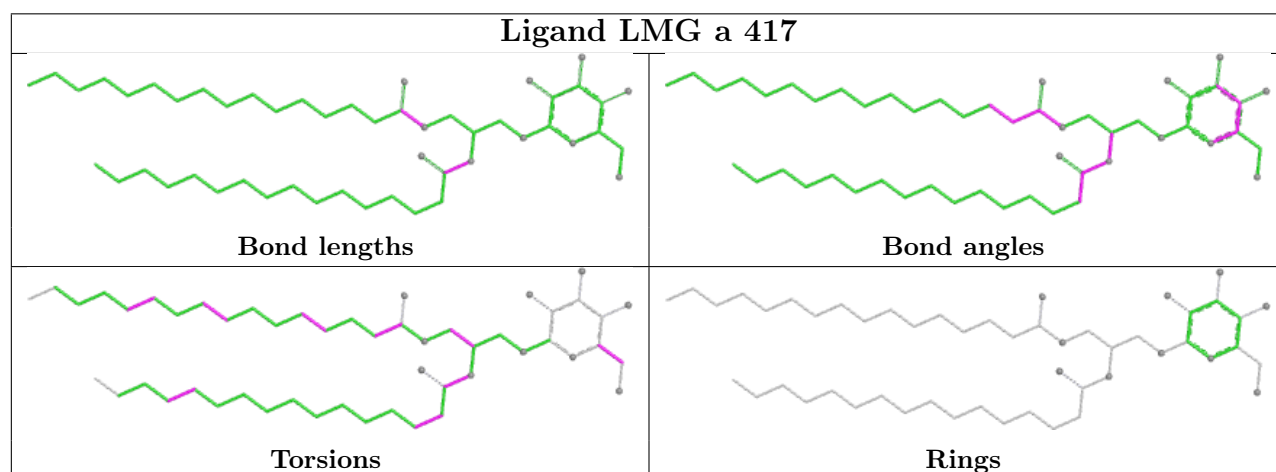
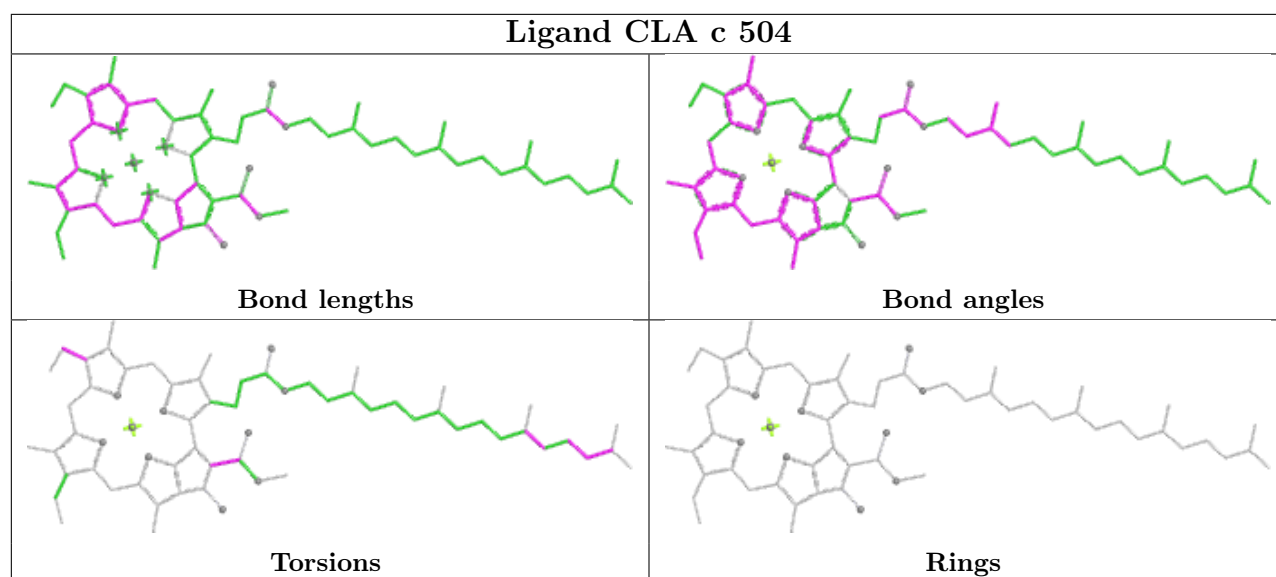




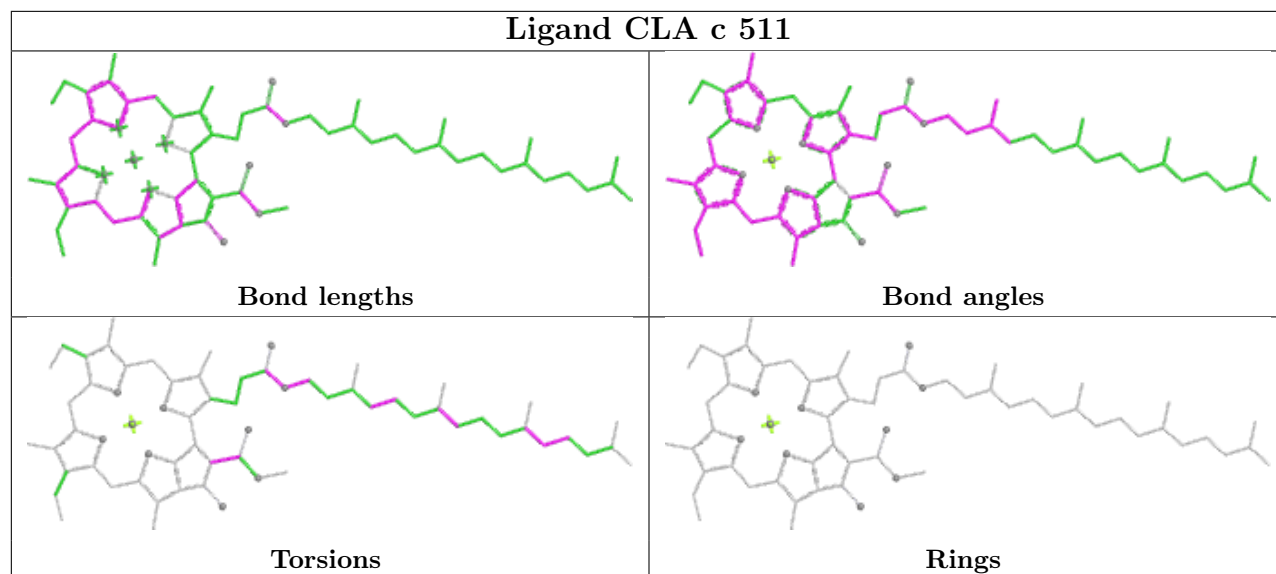
Ligand HEM e 102



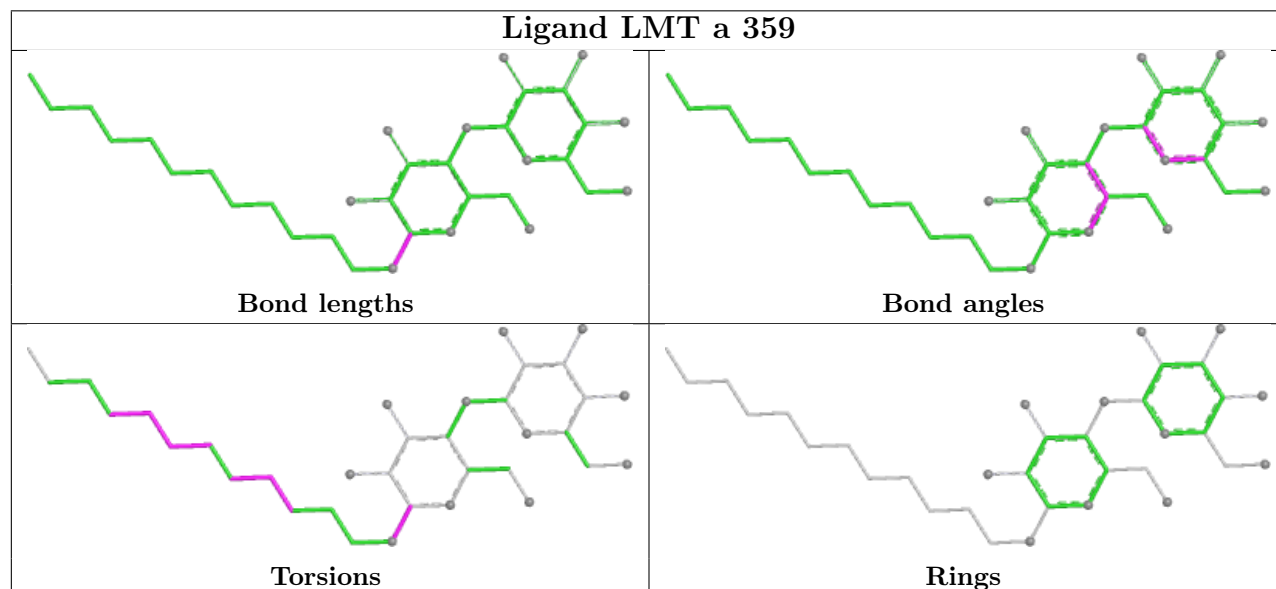




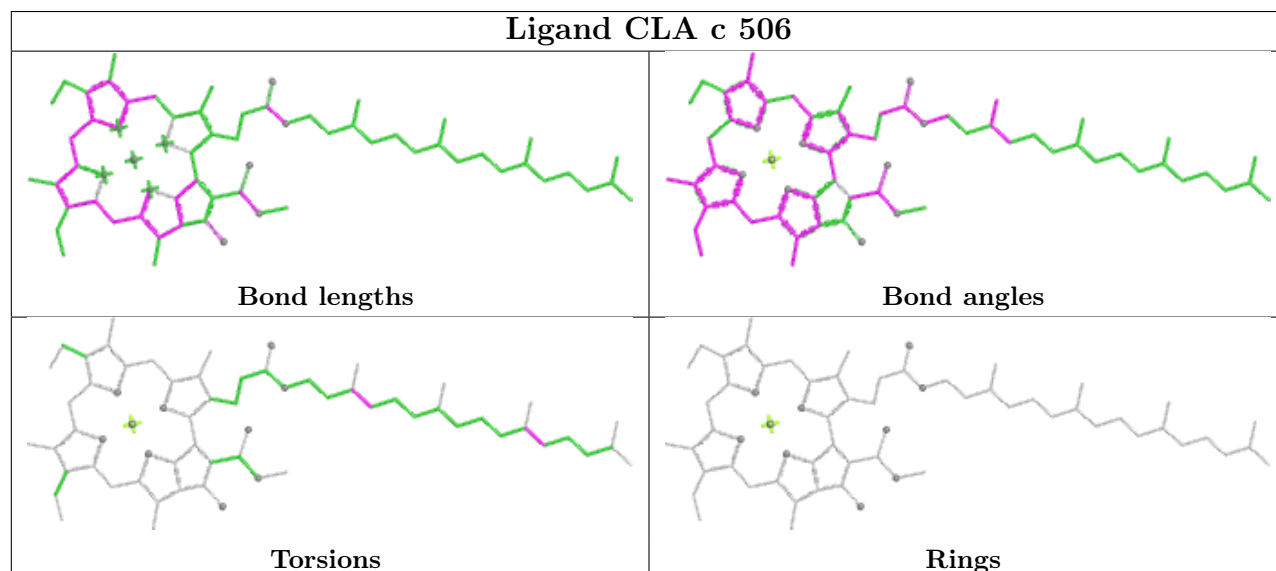
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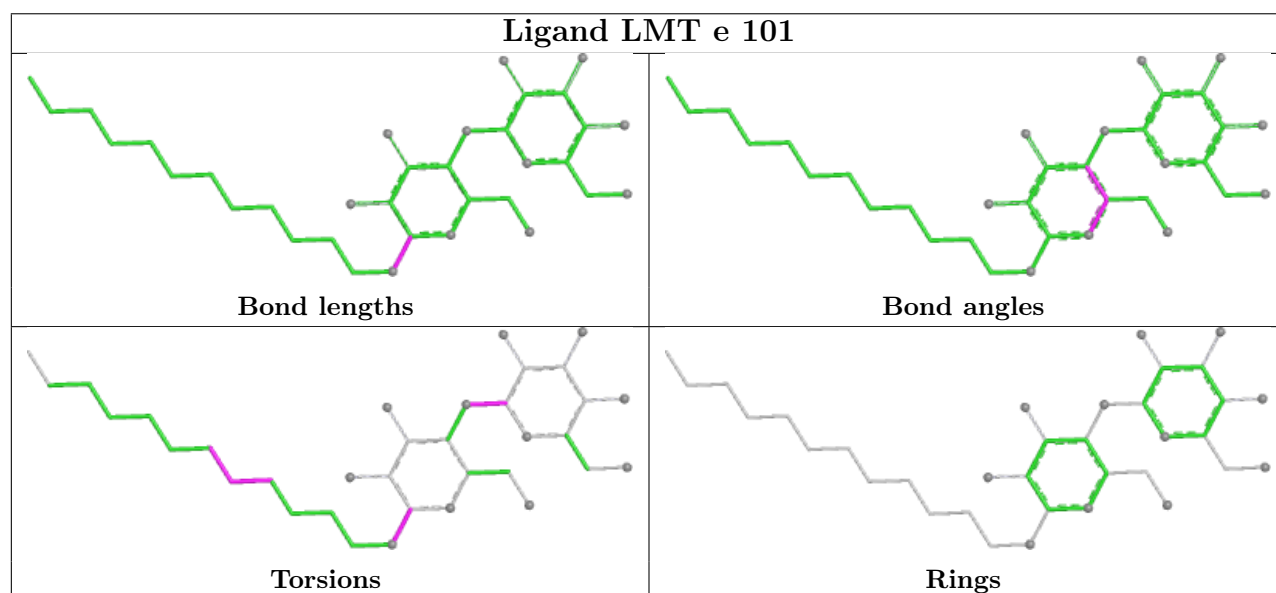
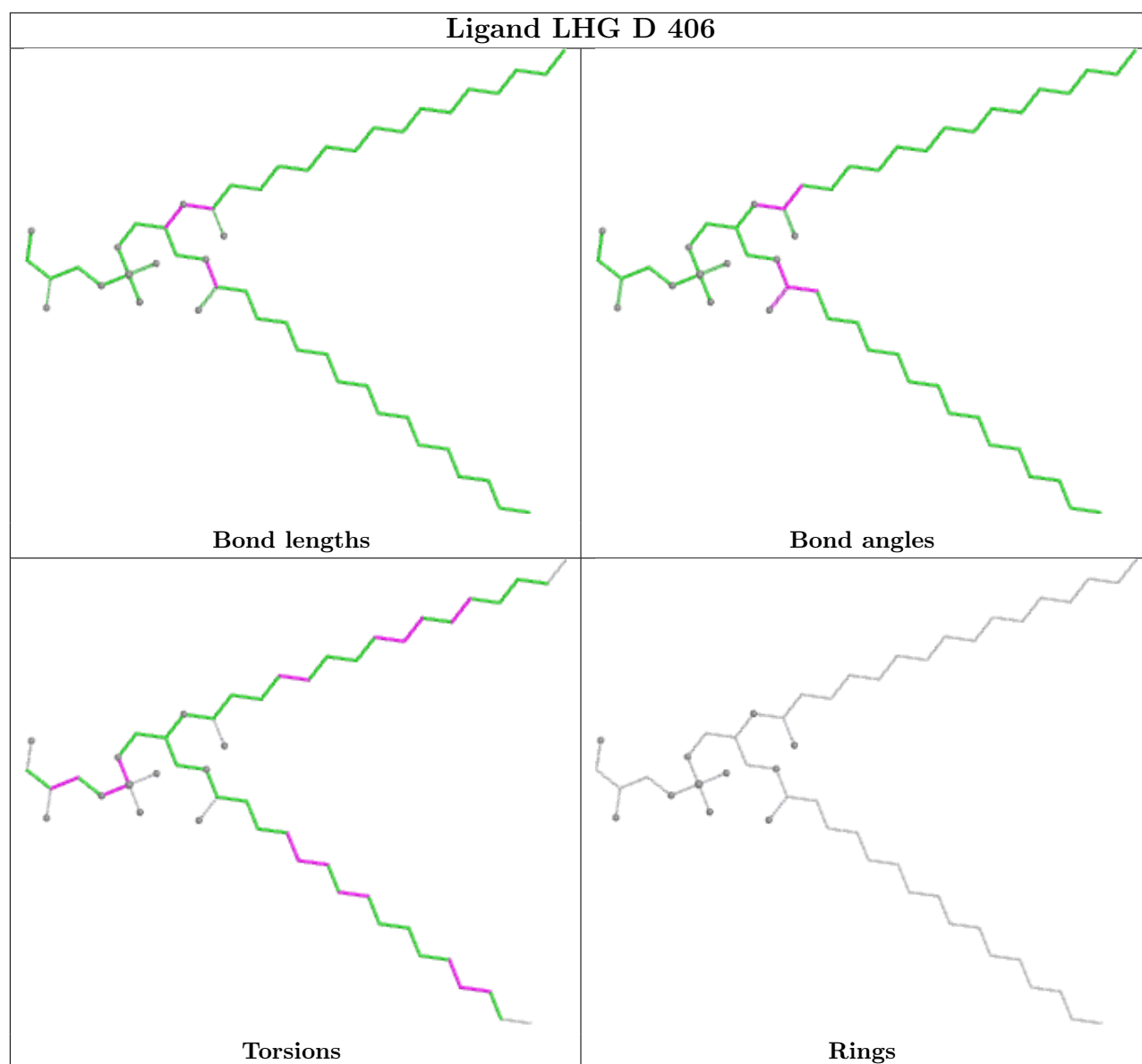


Ligand LMT a 359

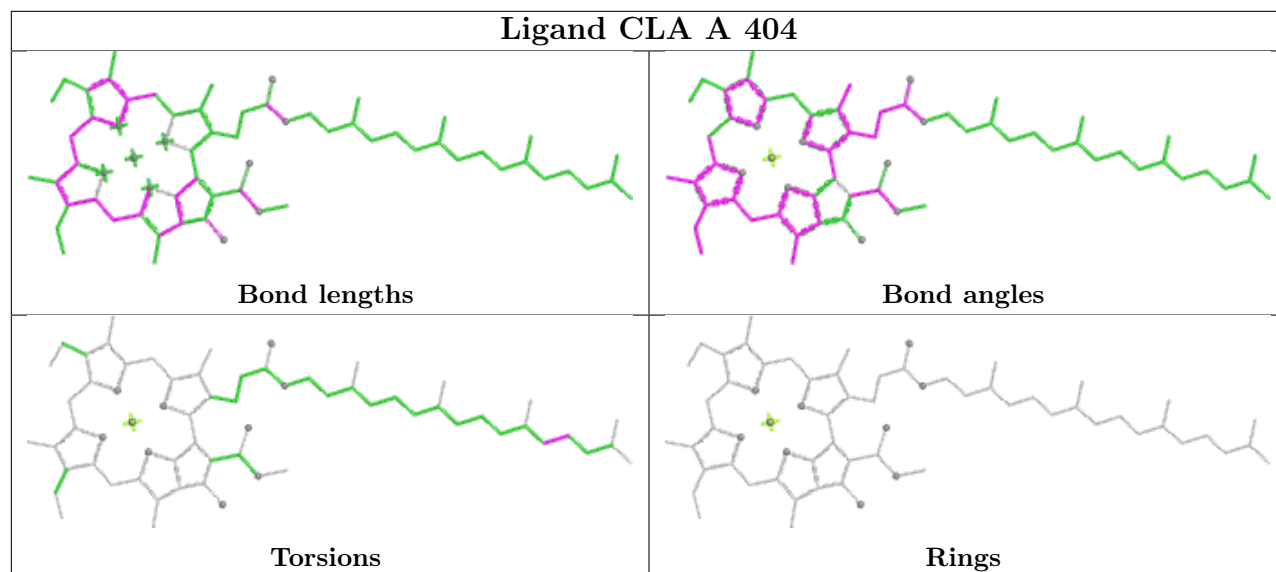


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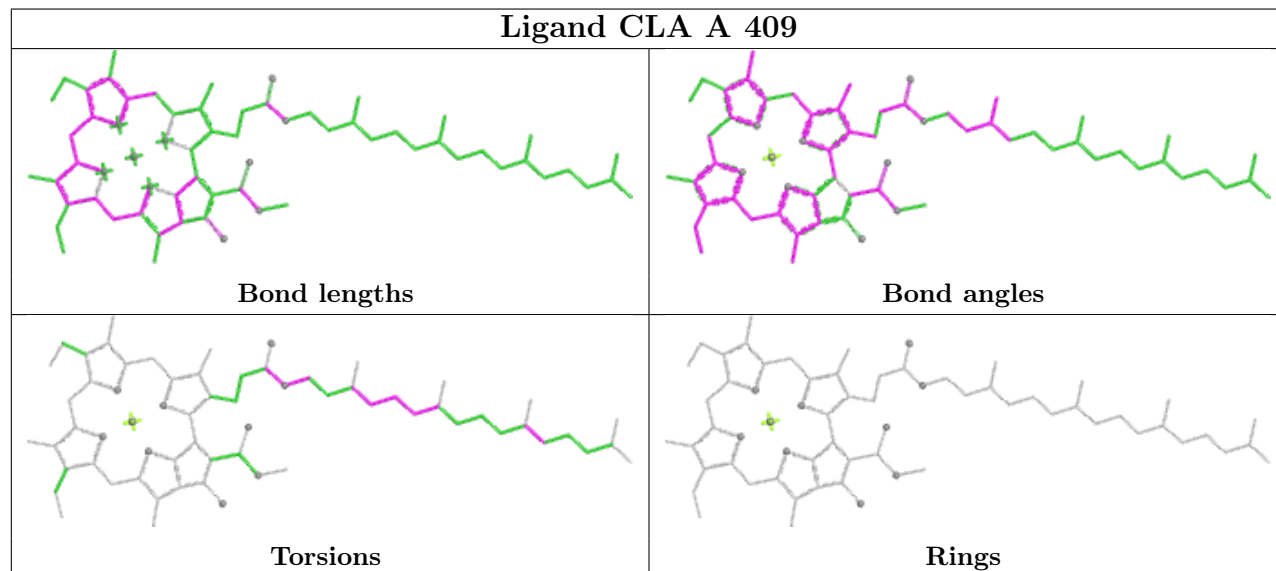




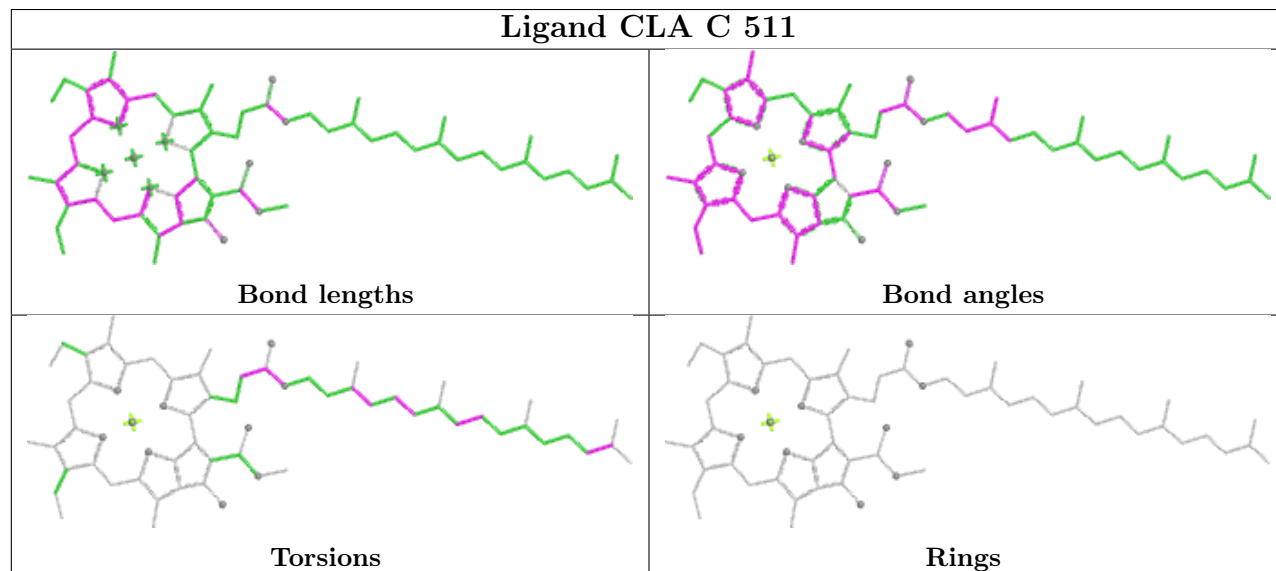
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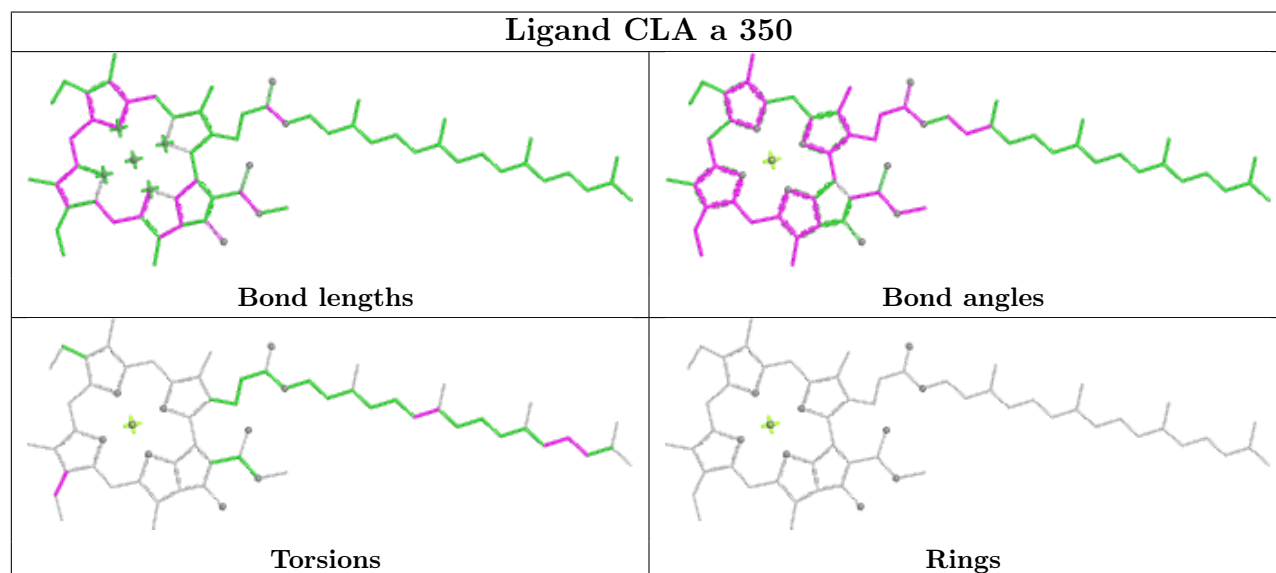
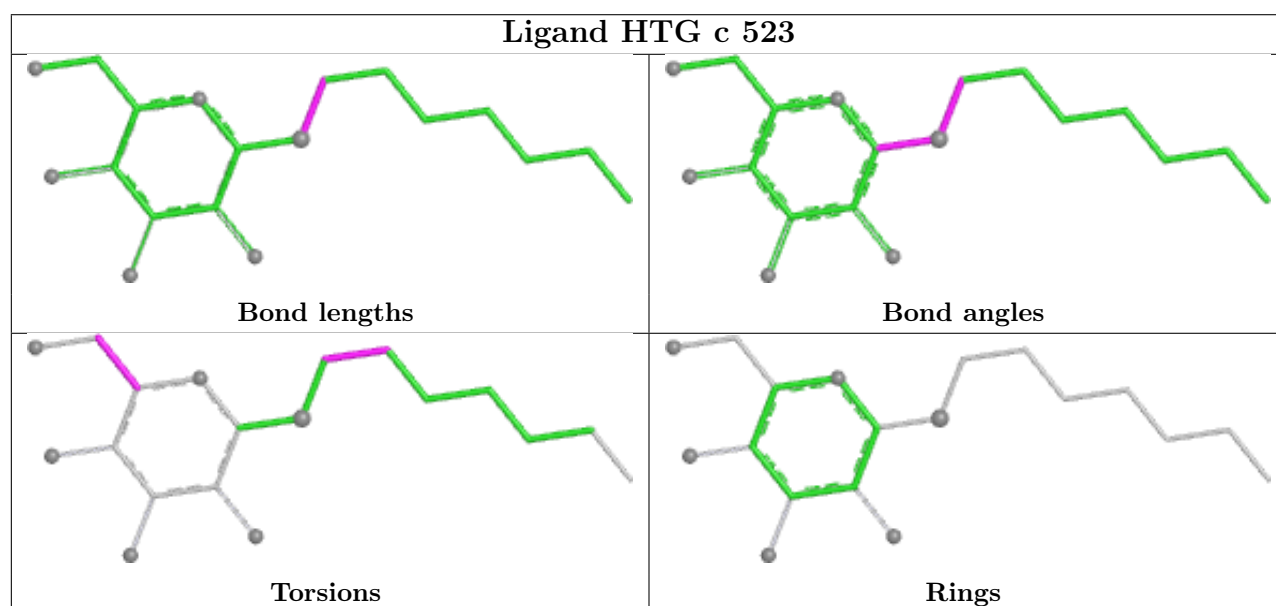
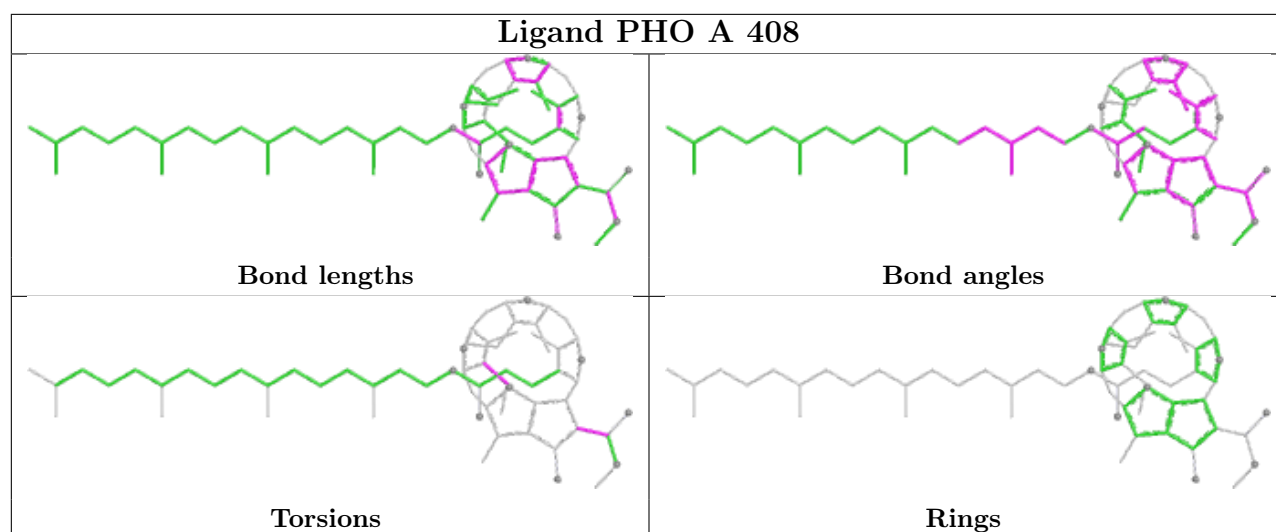


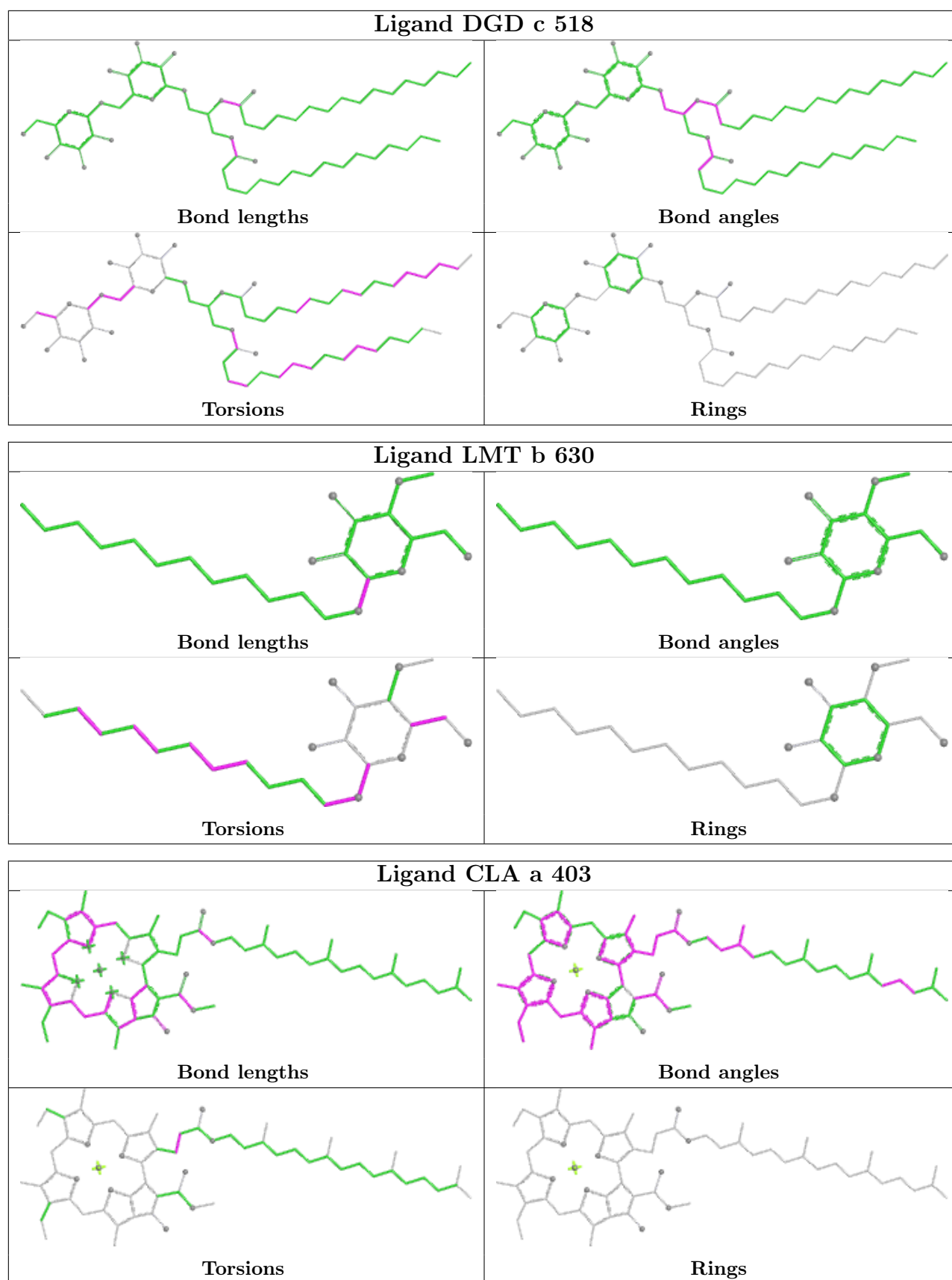
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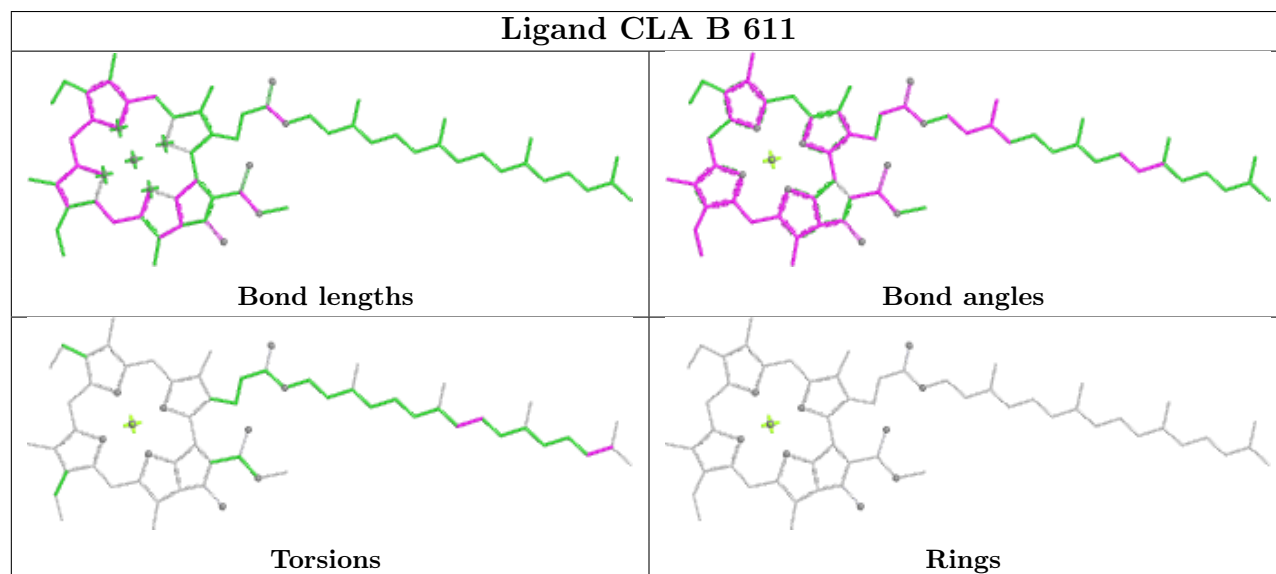
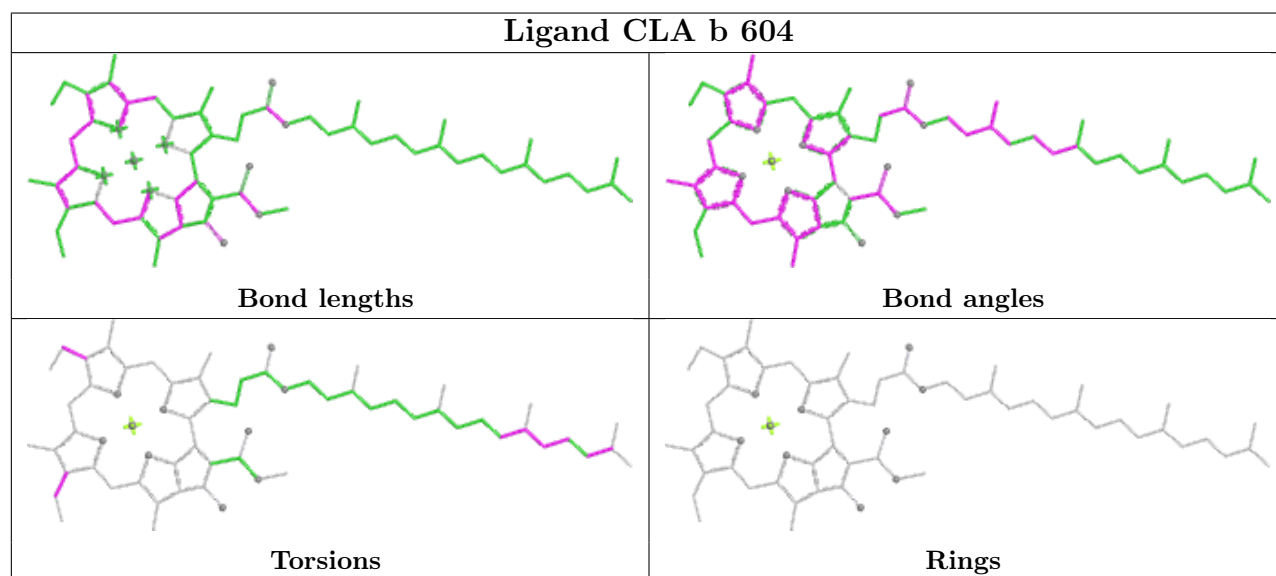
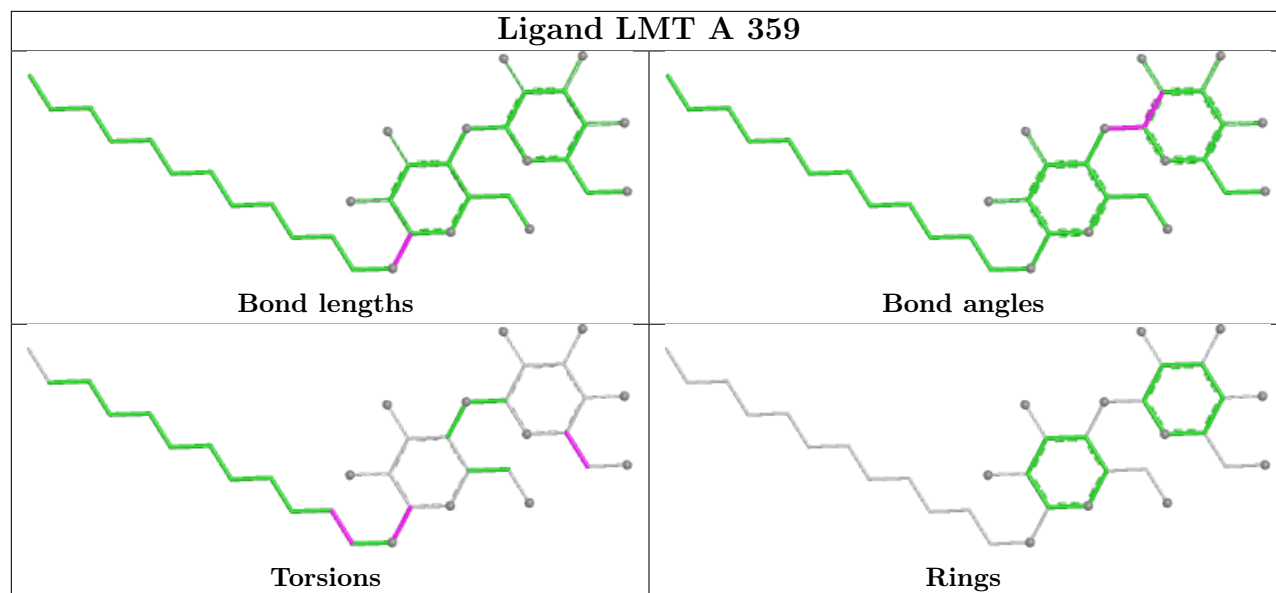


Ligand CLA C 511

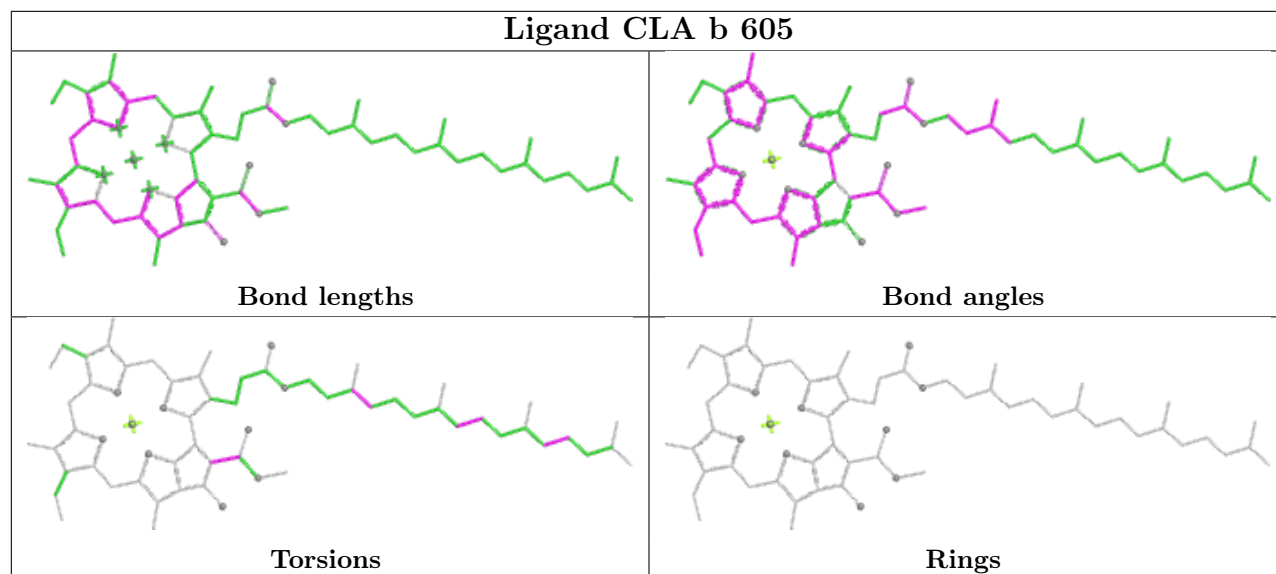




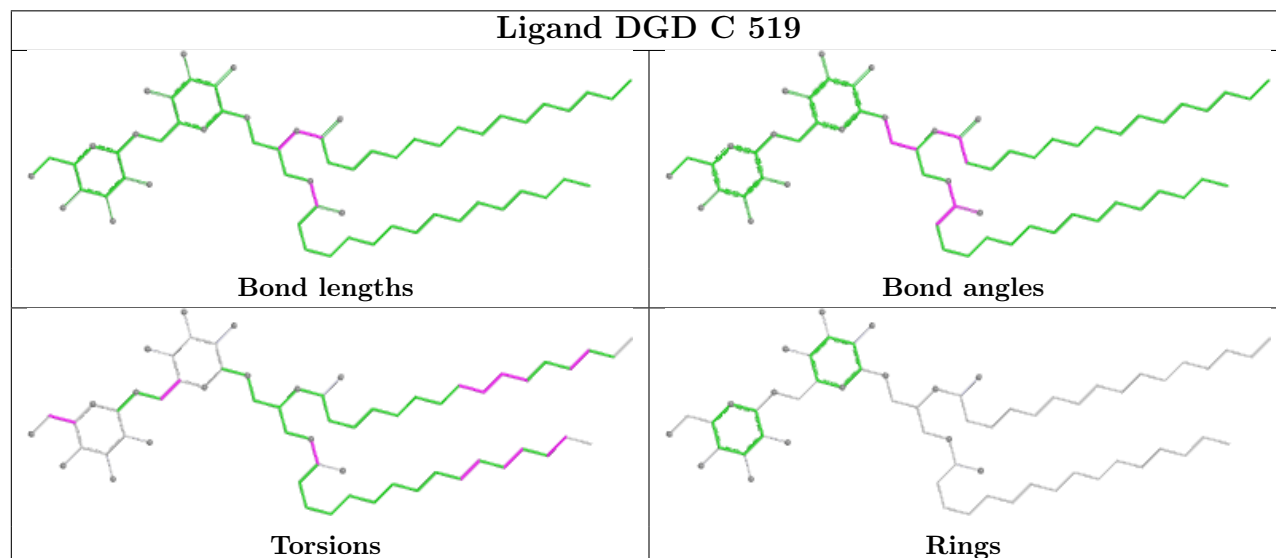




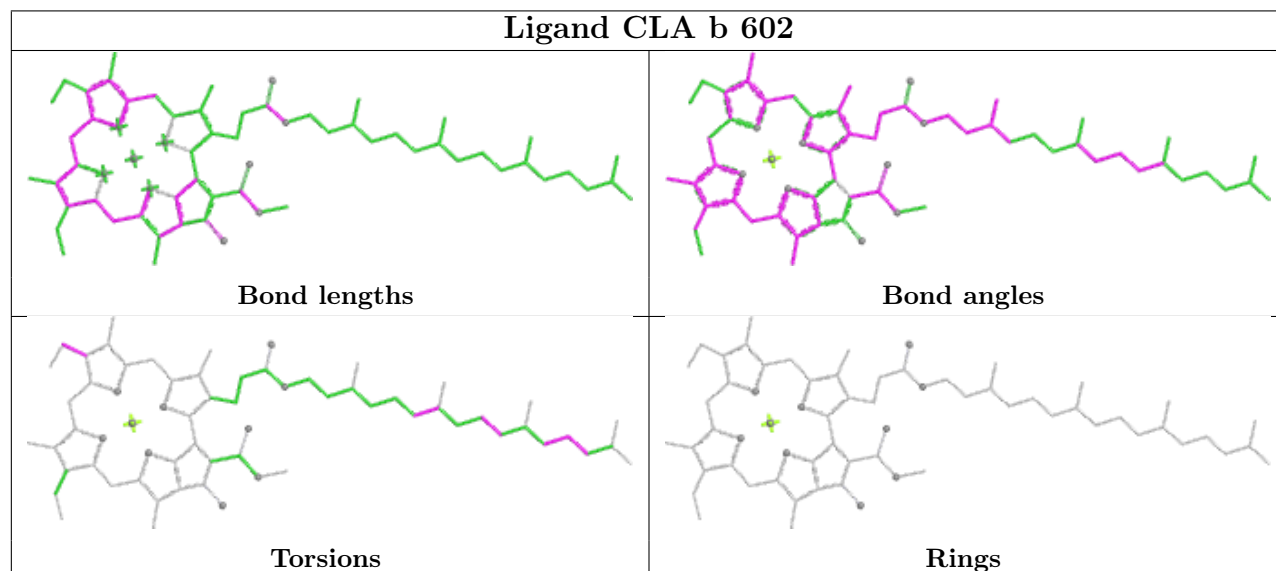
Ligand CLA b 605

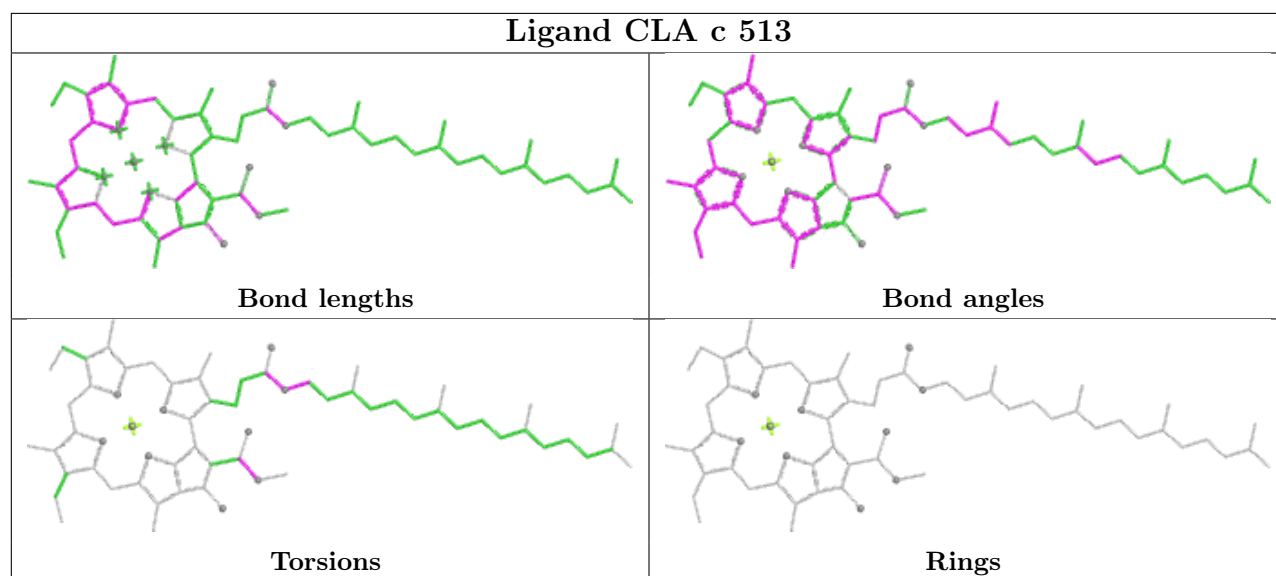
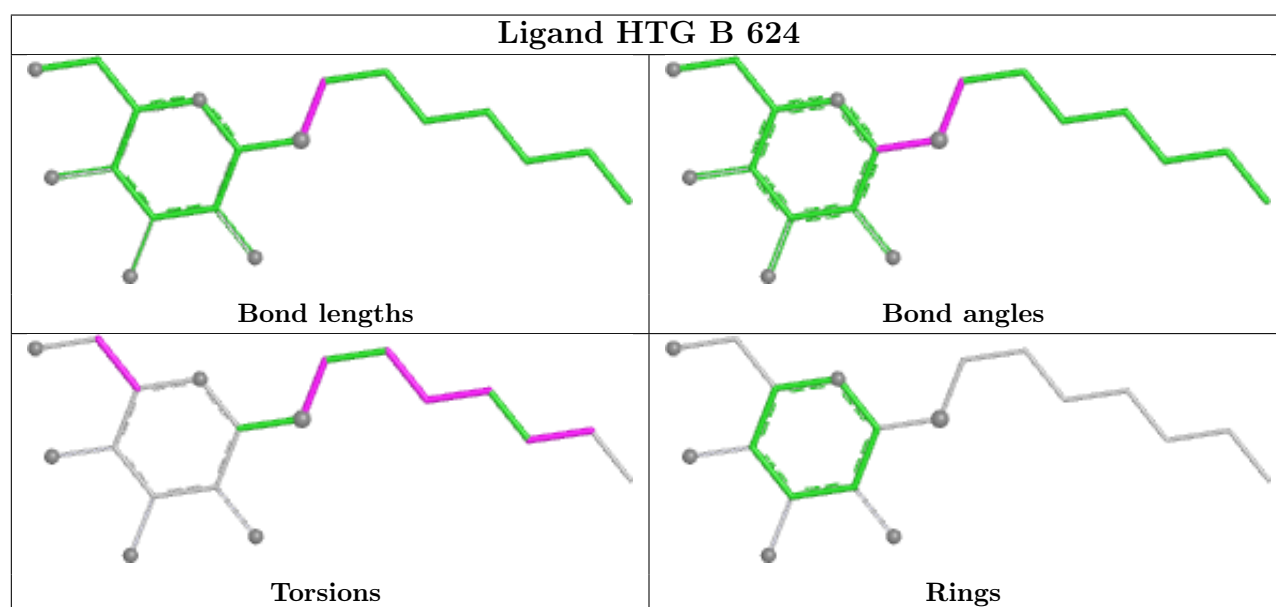
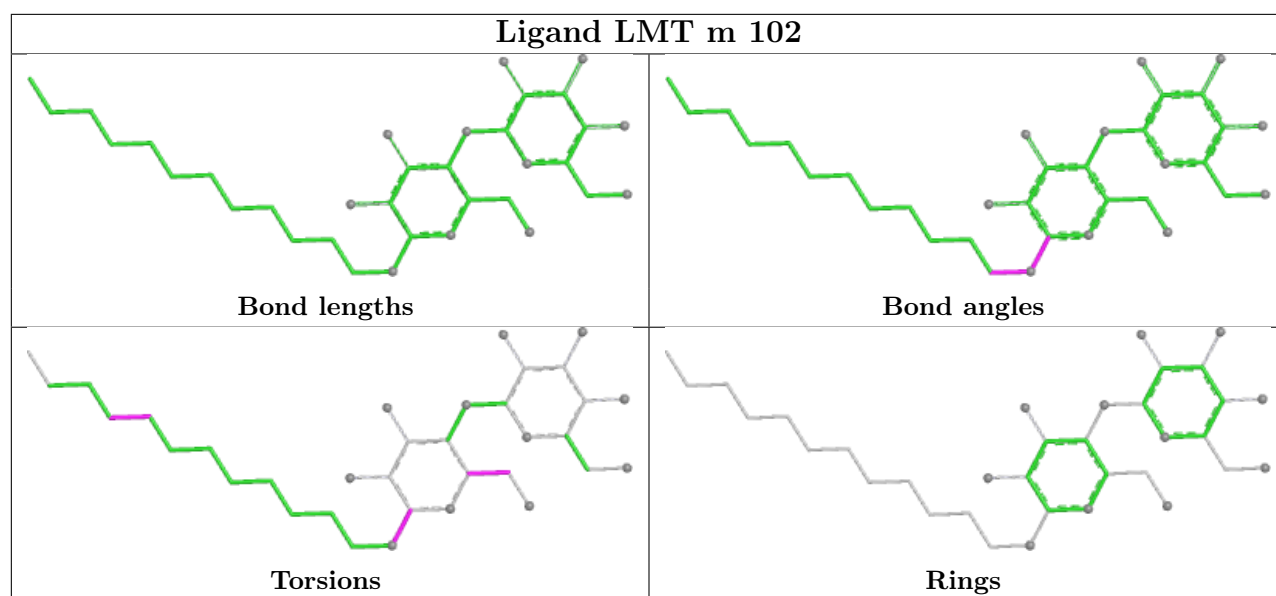


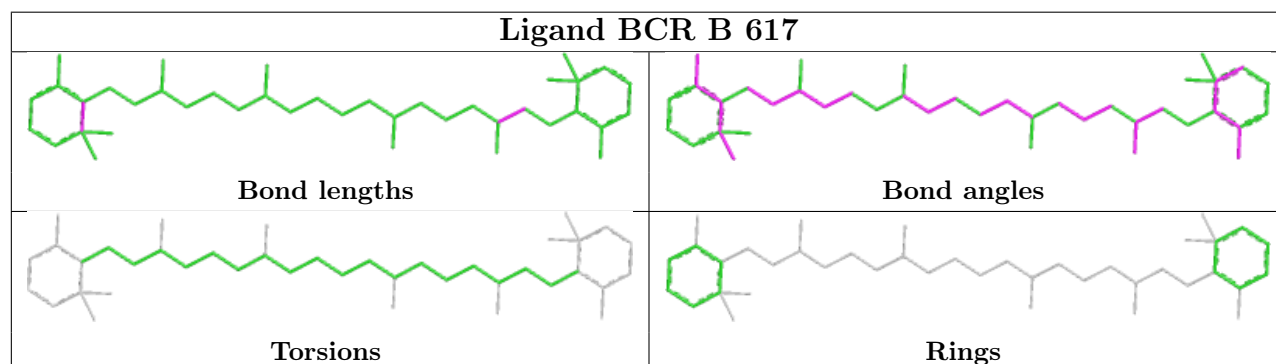
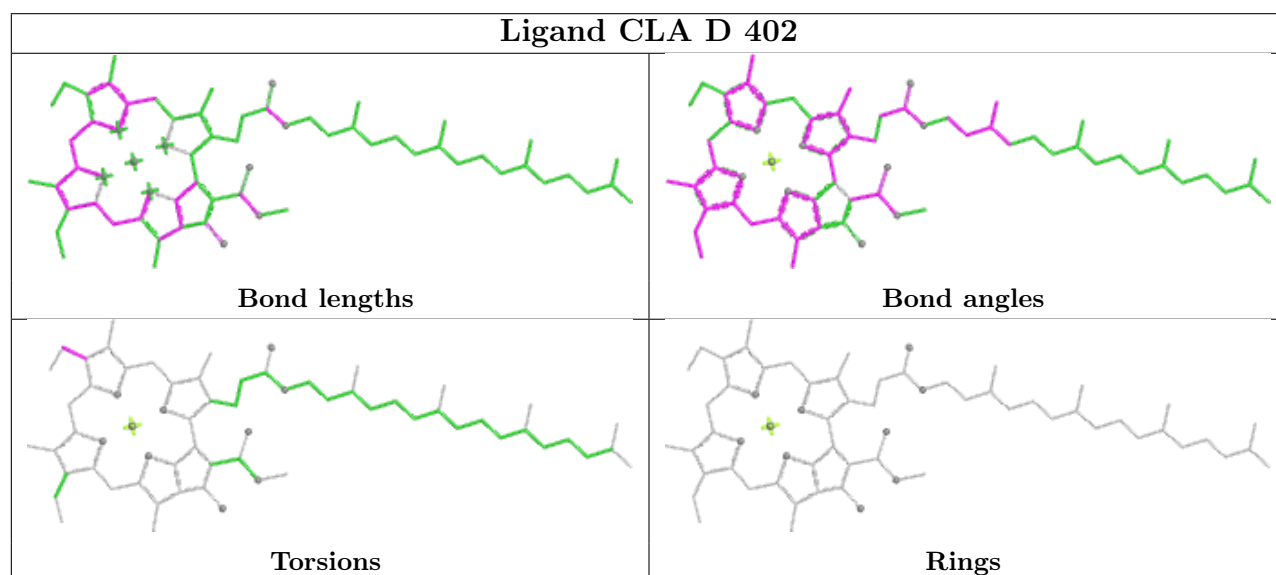
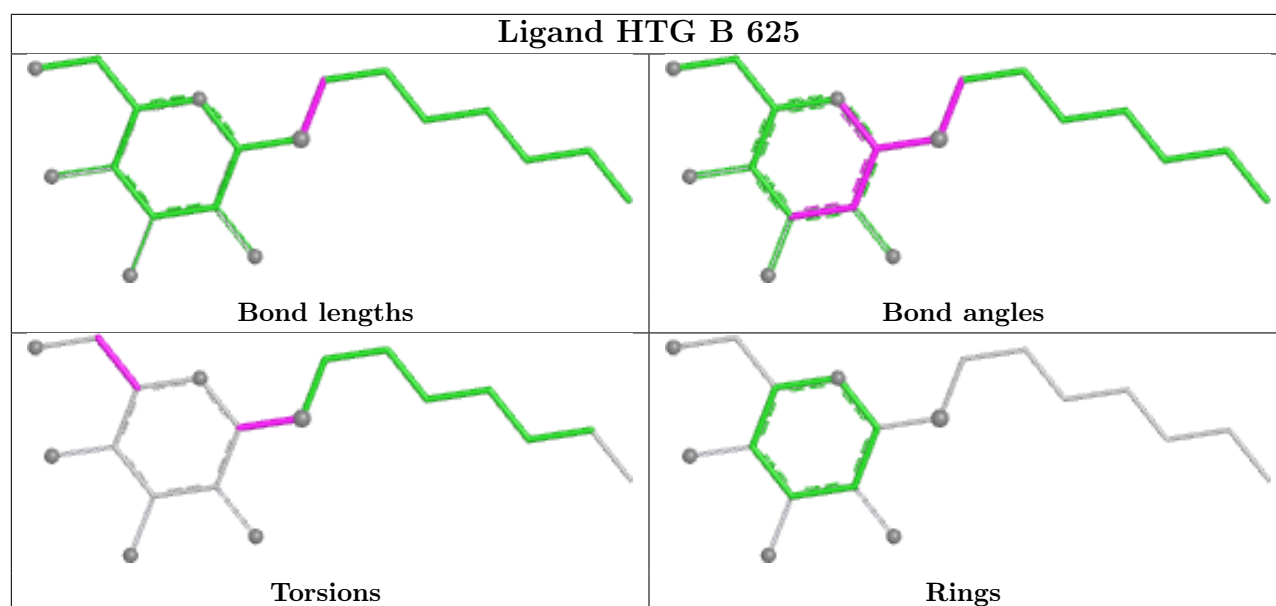
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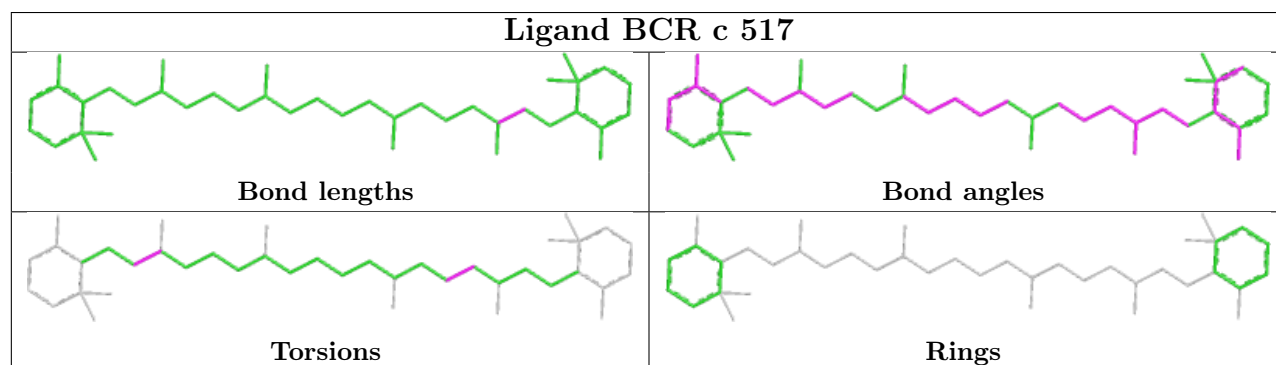
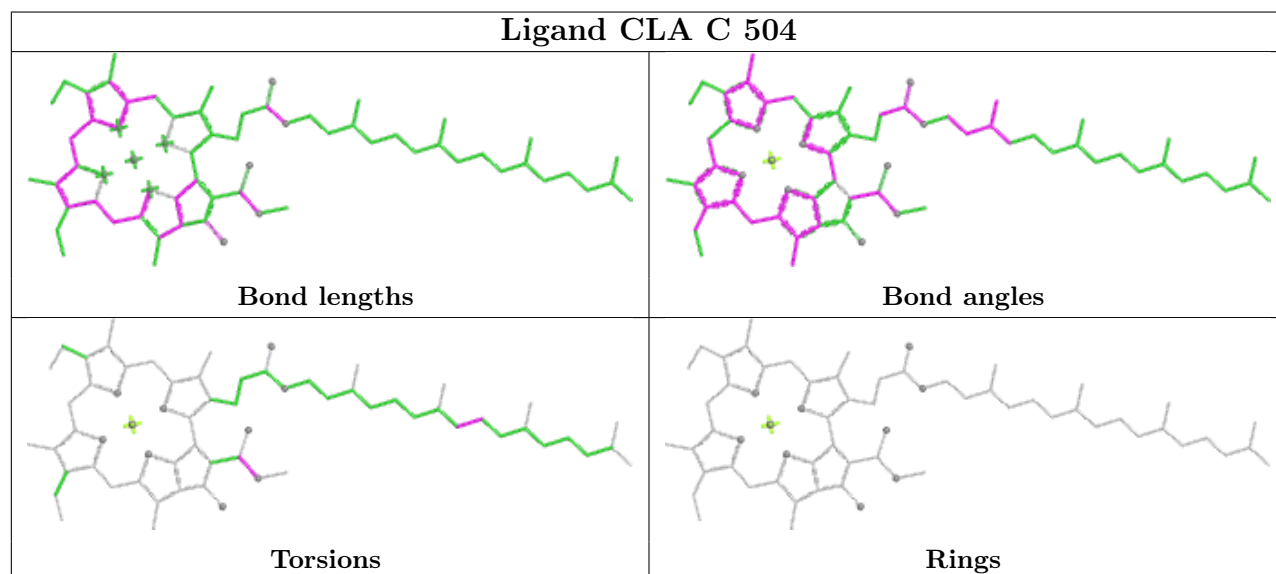
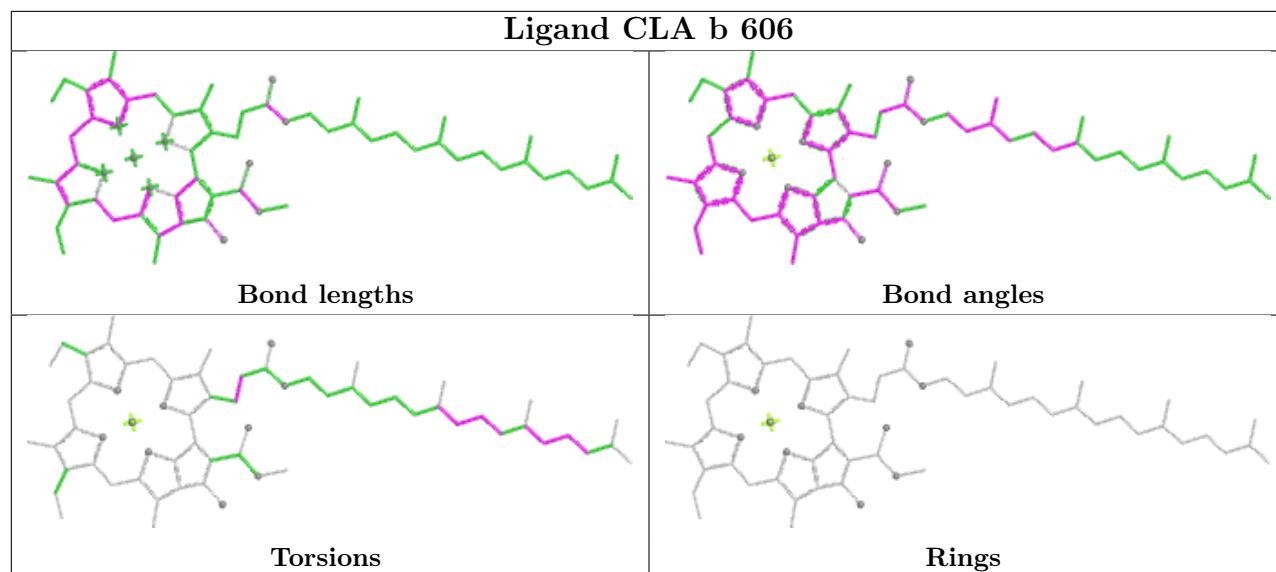


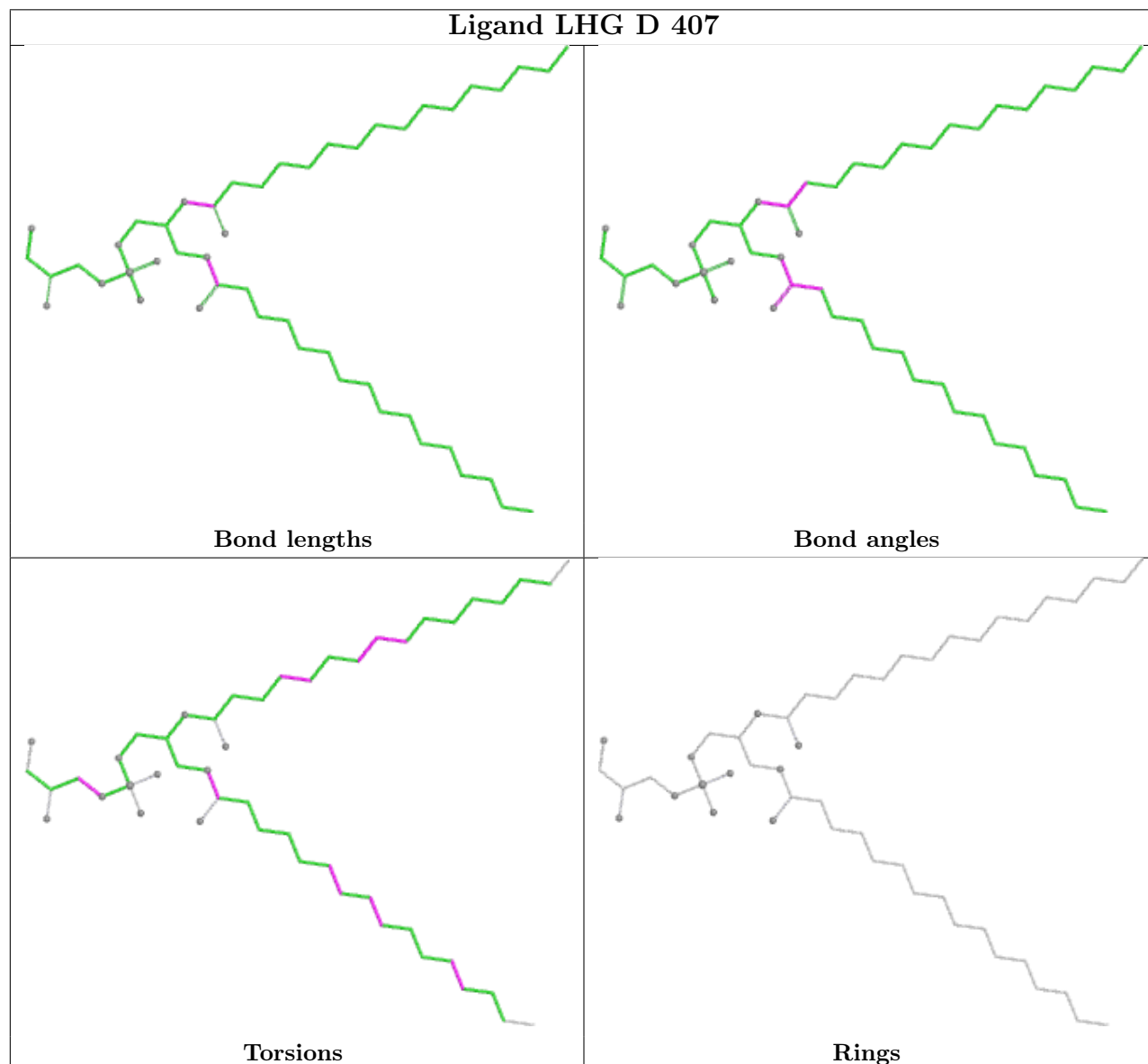
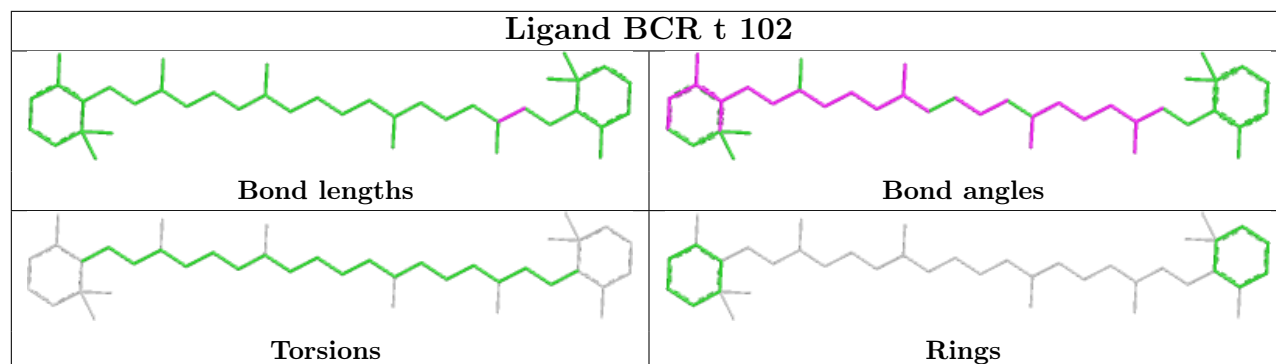
Ligand CLA b 602



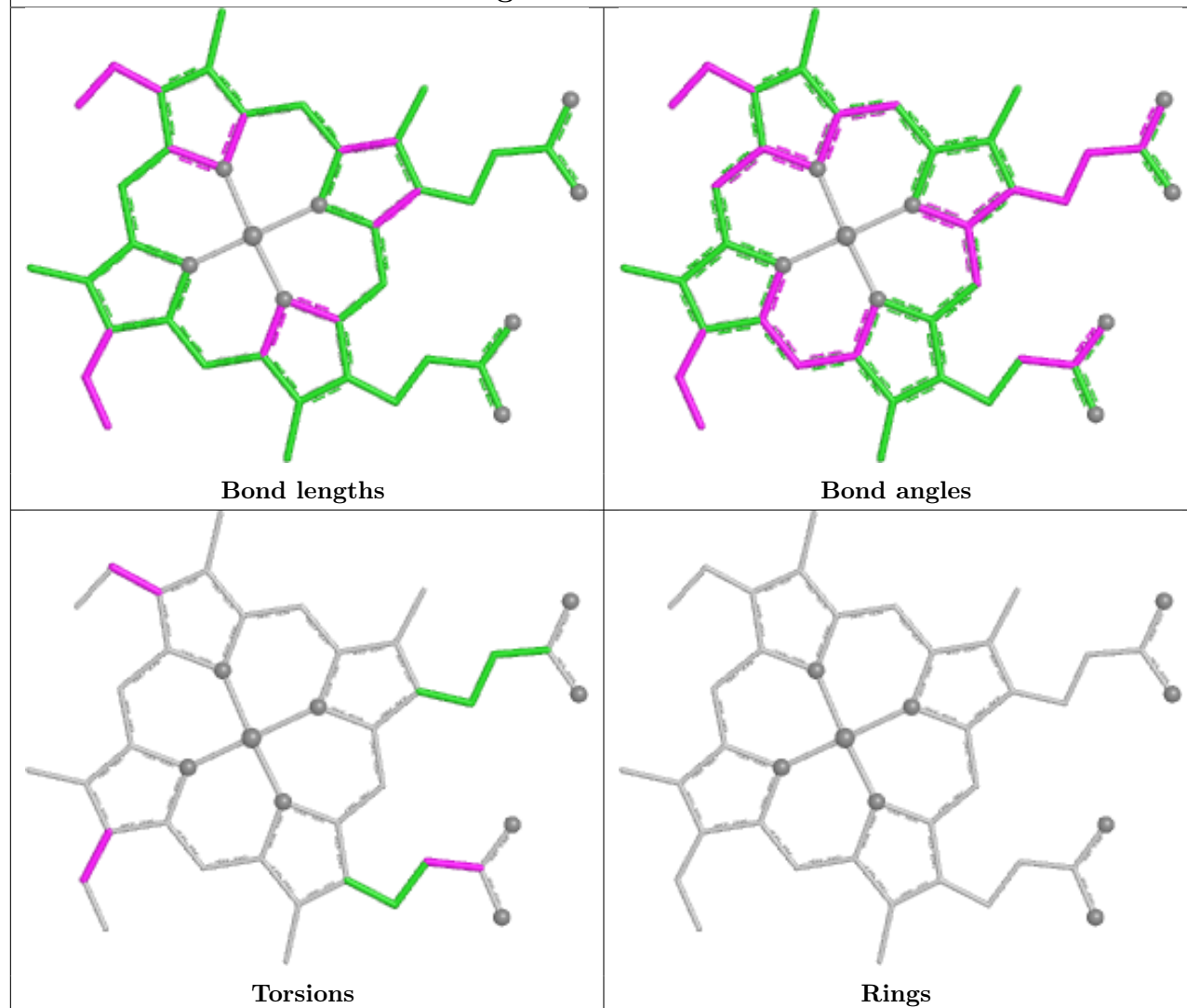




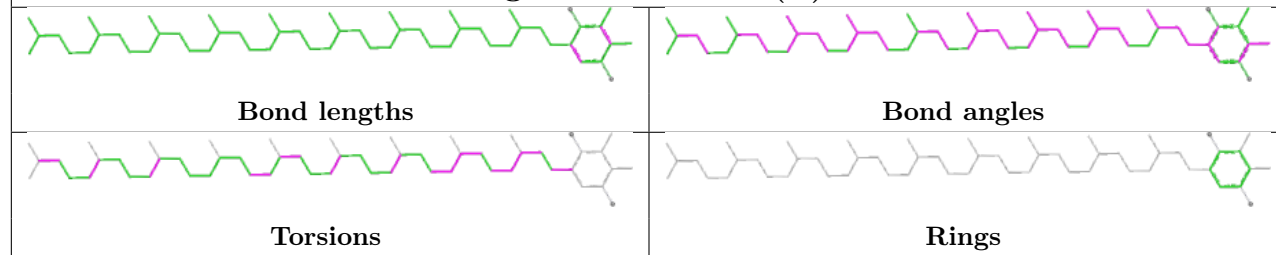


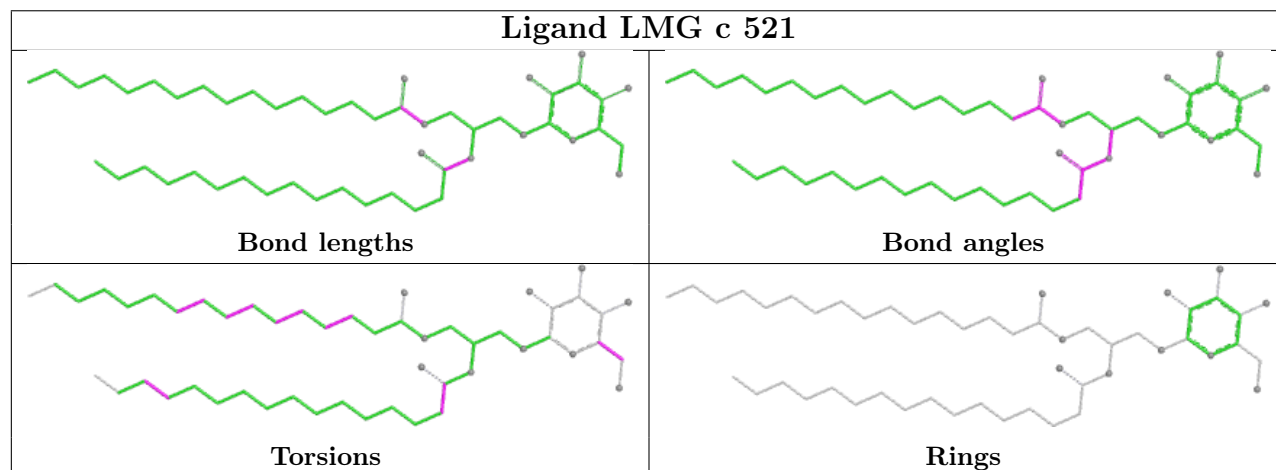
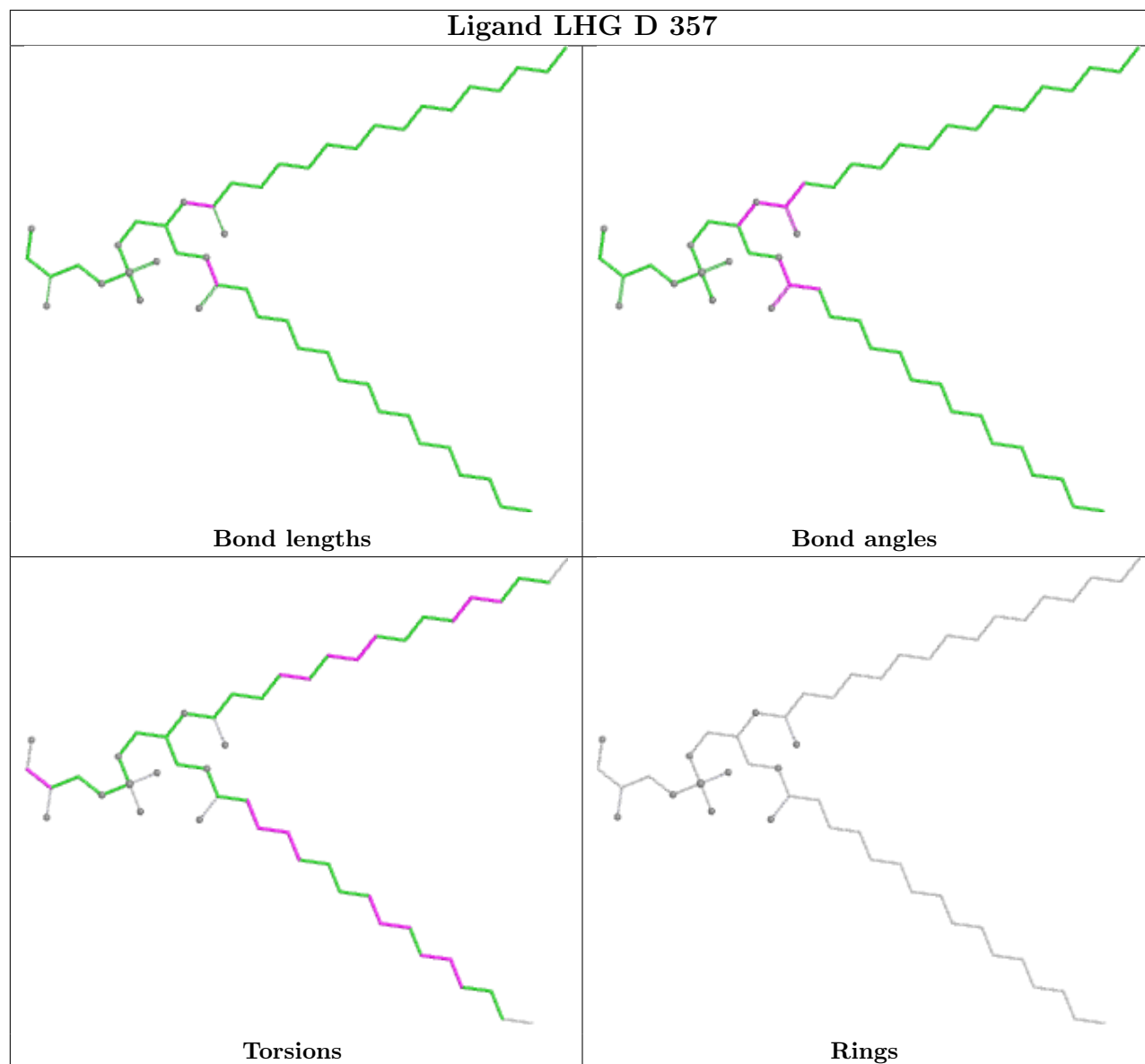


Ligand HEC v 203

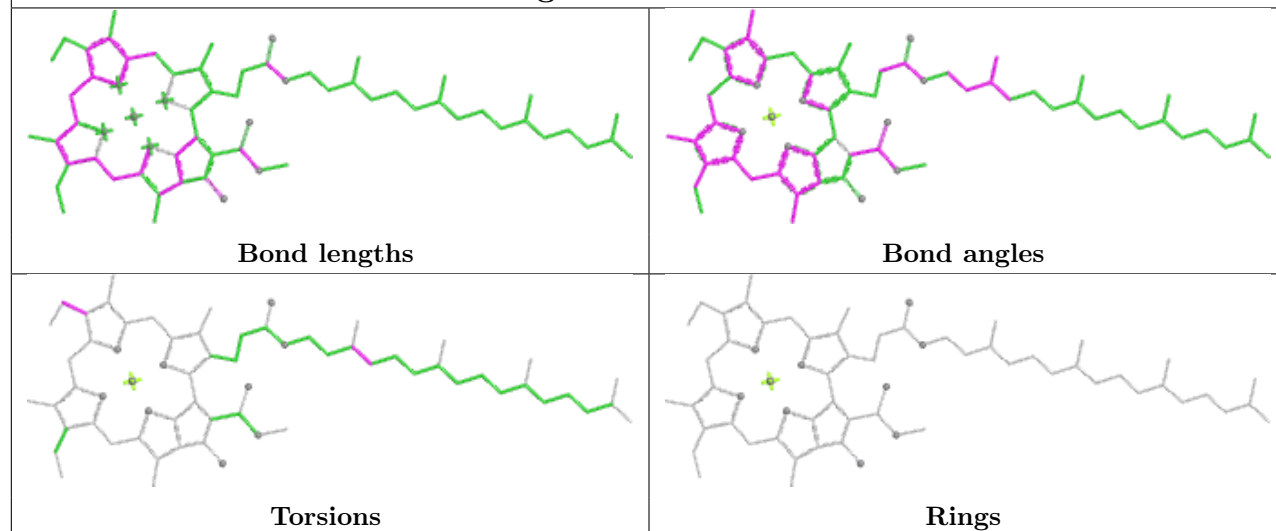


Ligand PL9 A 416 (B)

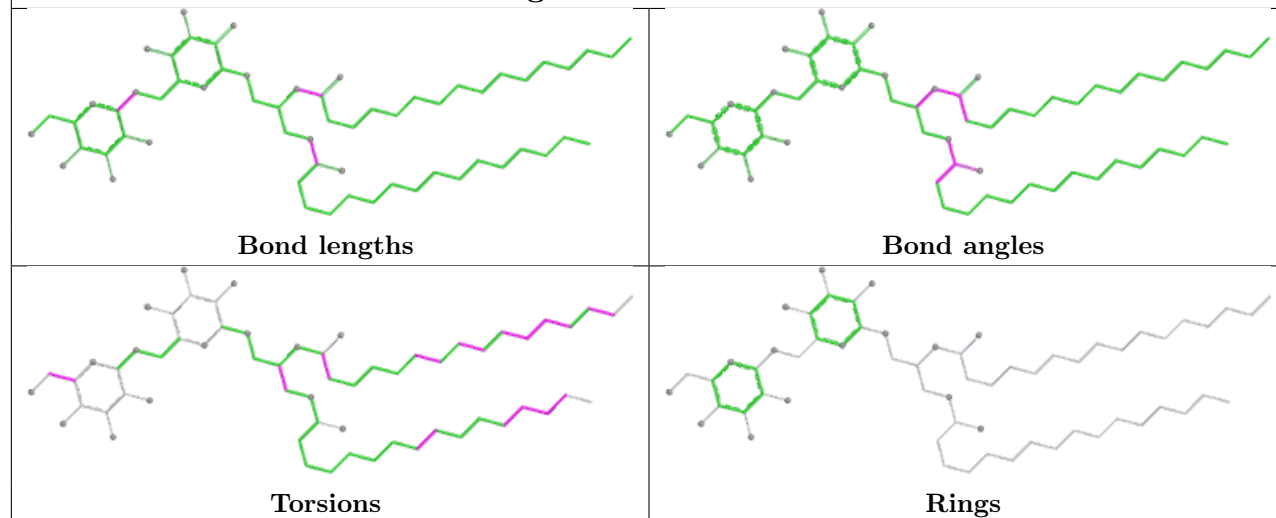




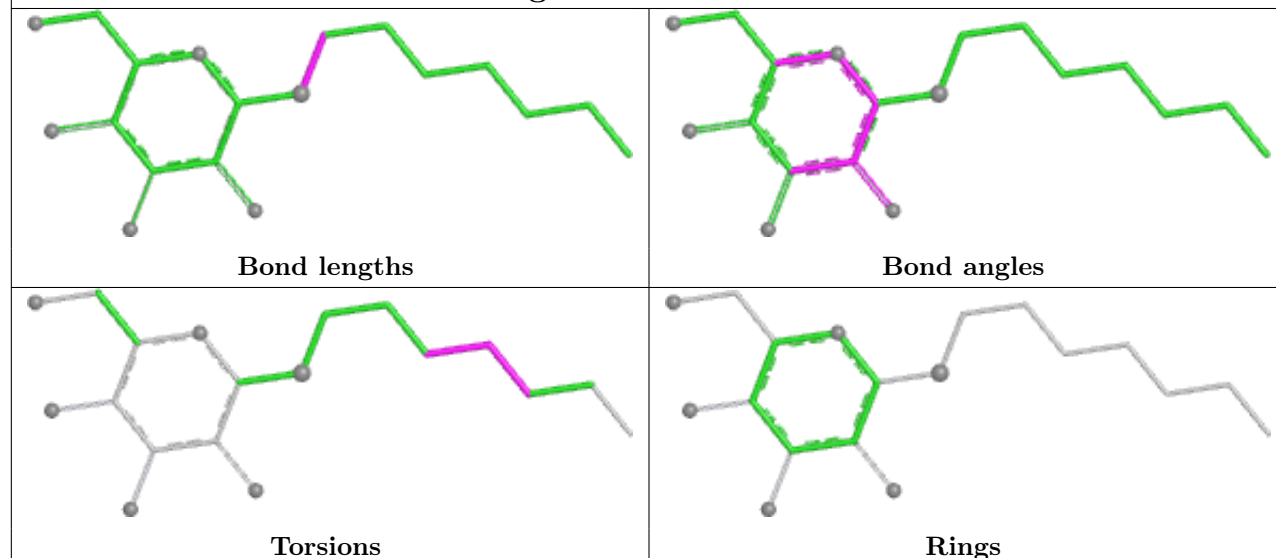
Ligand CLA c 507

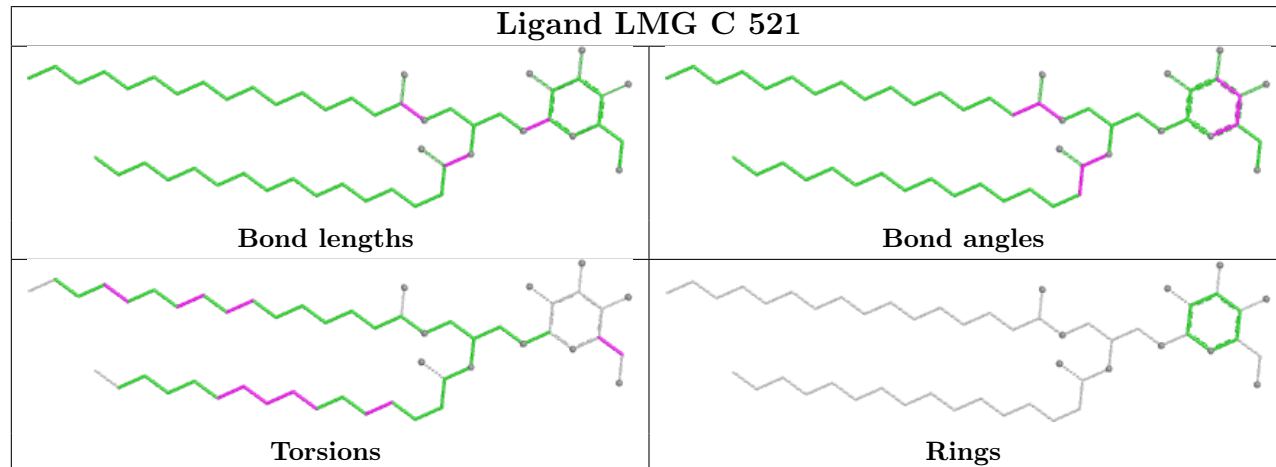
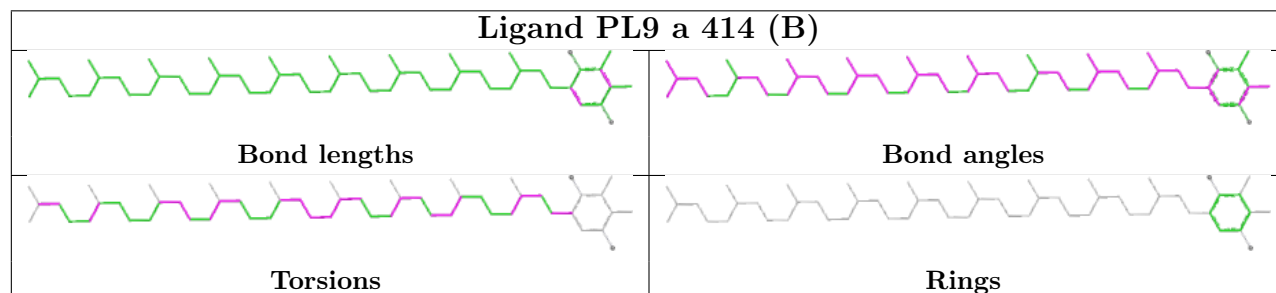
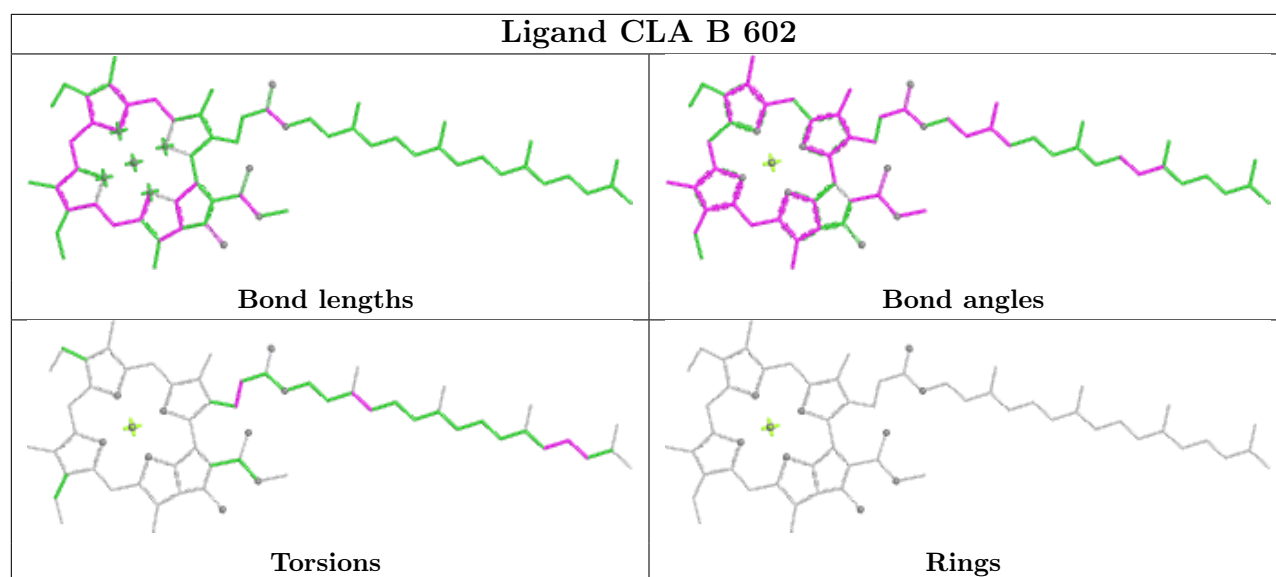


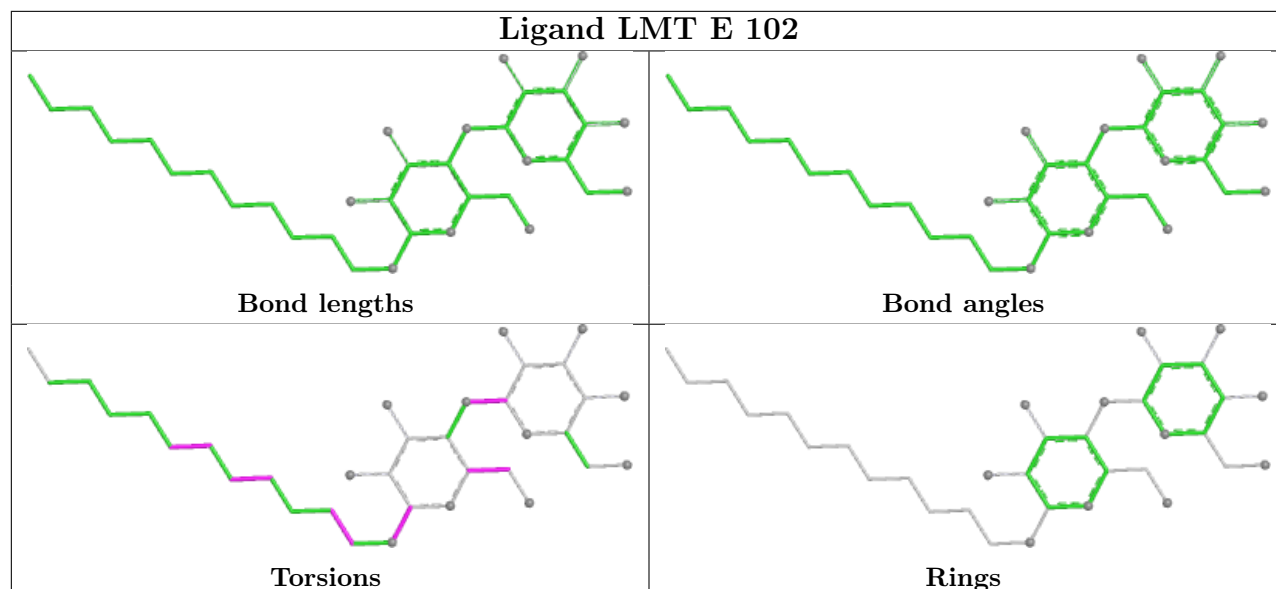
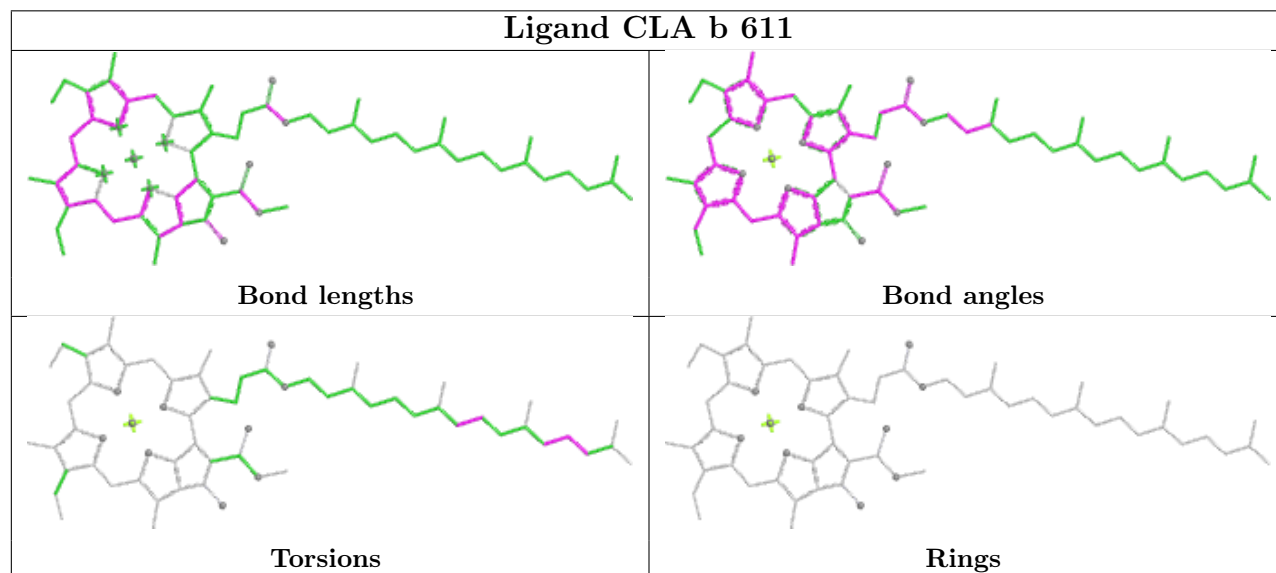
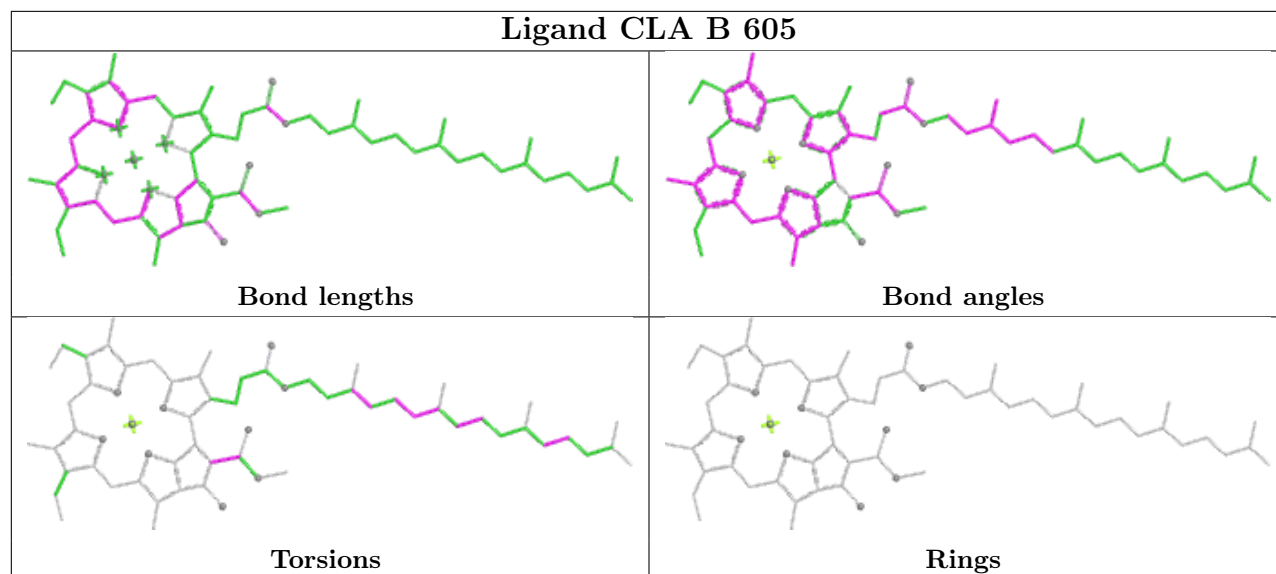
Ligand DGD H 102



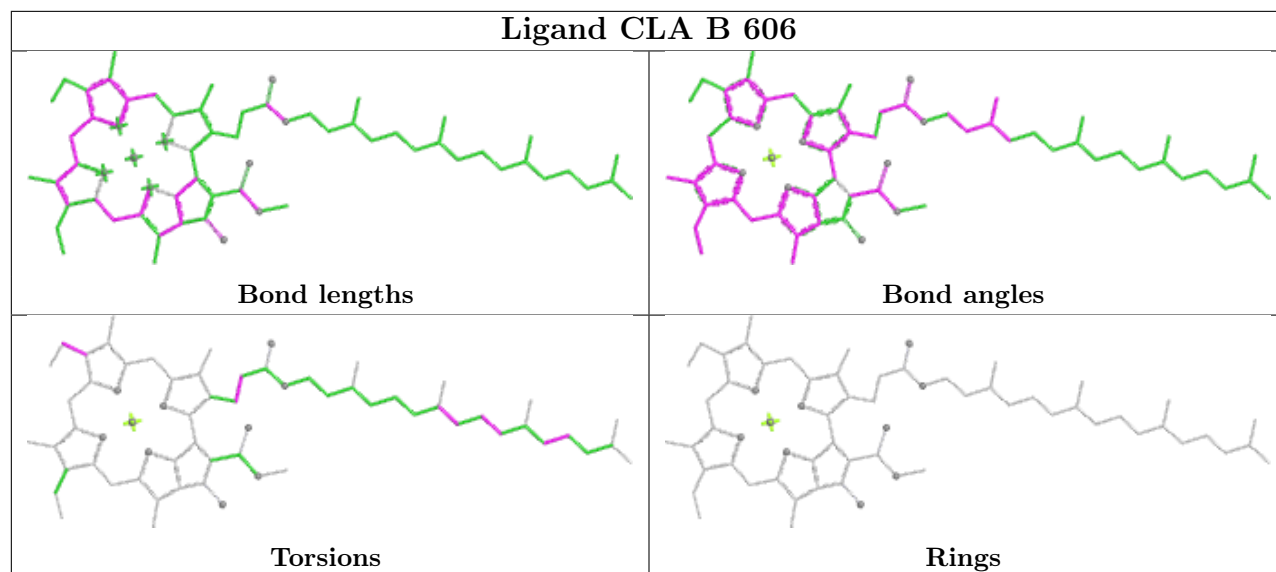
Ligand HTG B 623



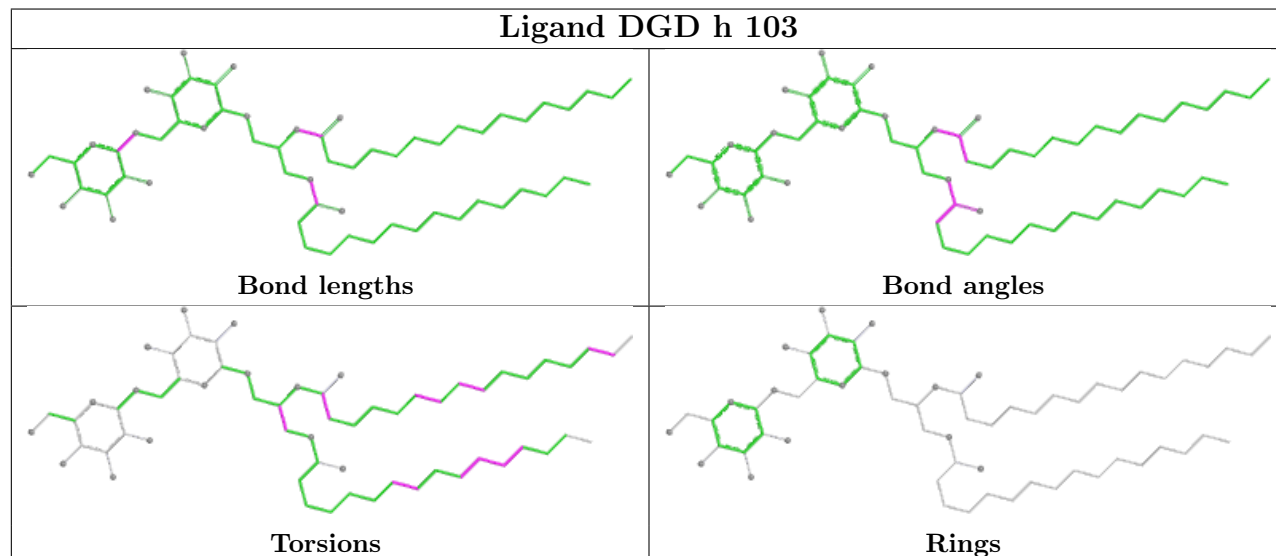




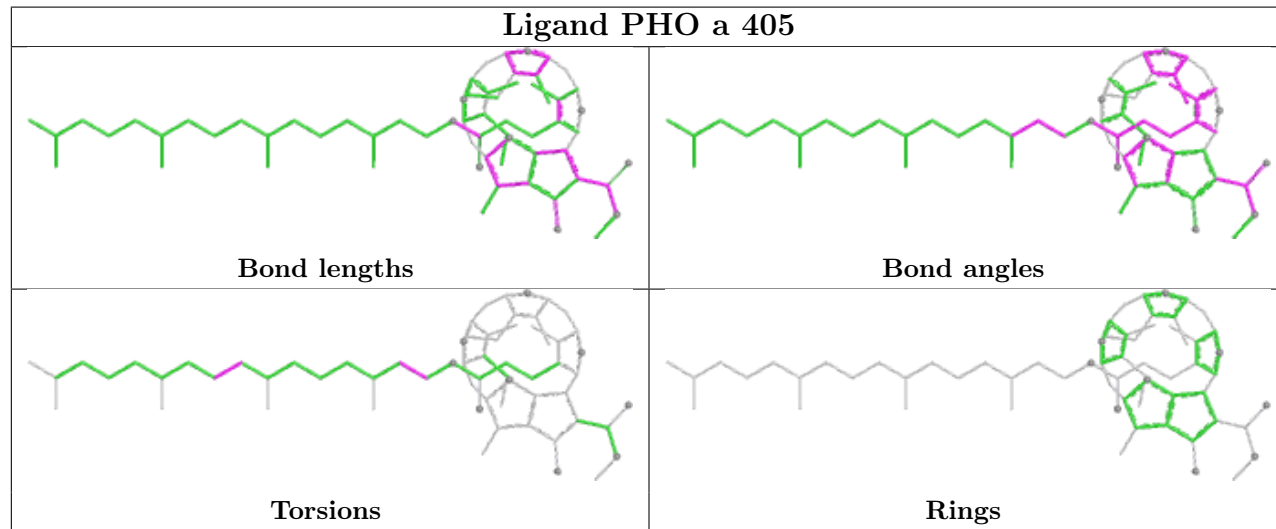
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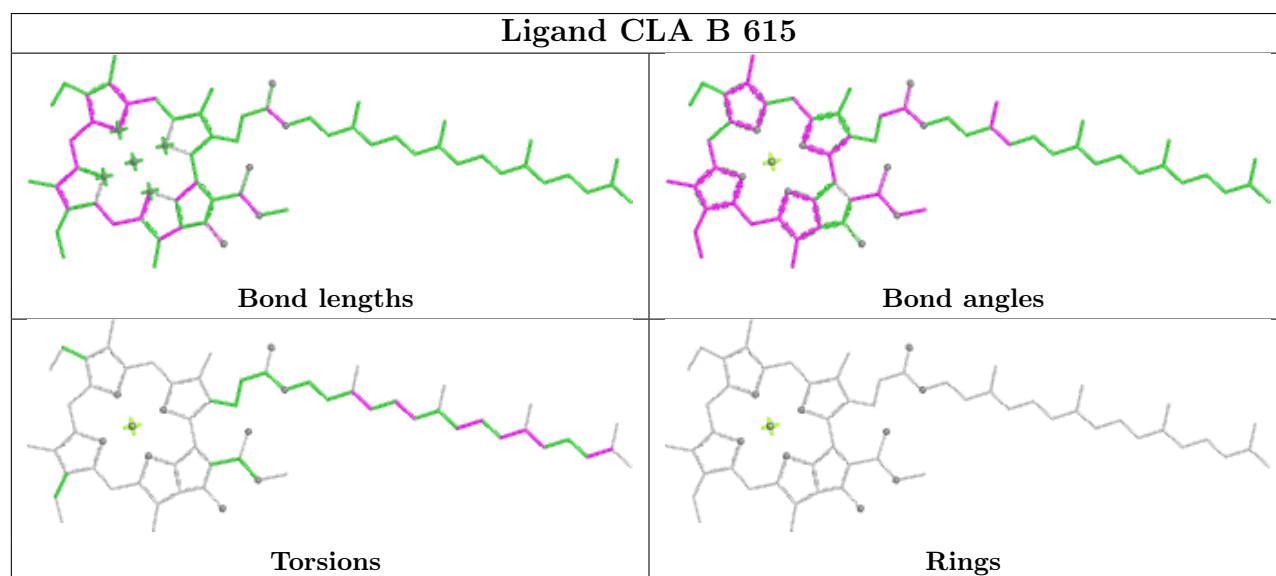
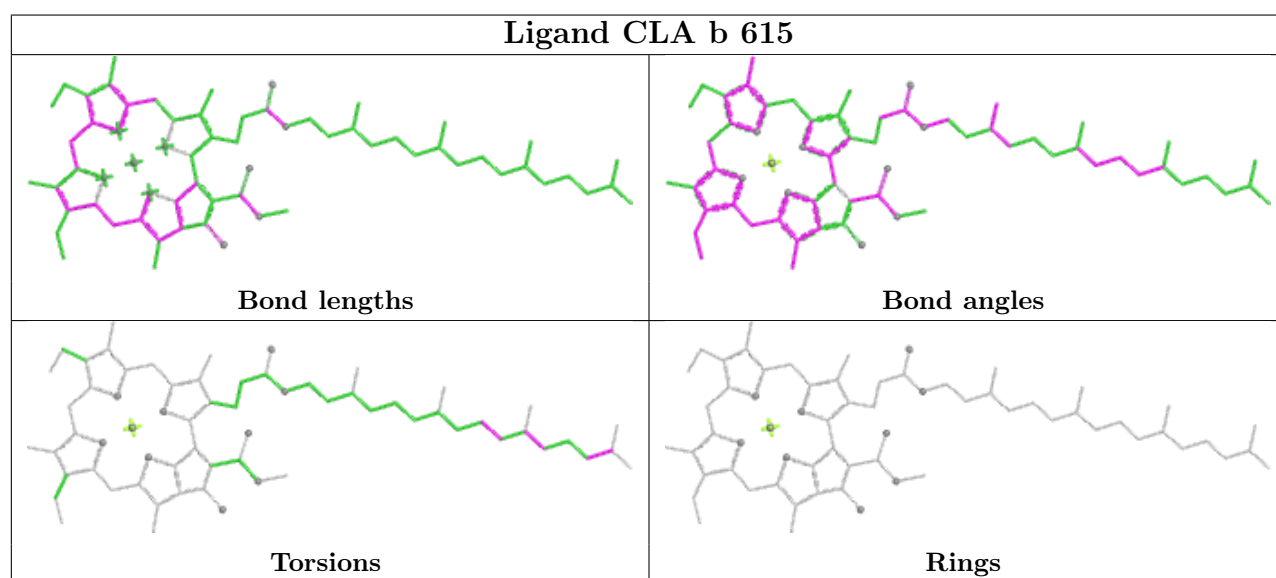
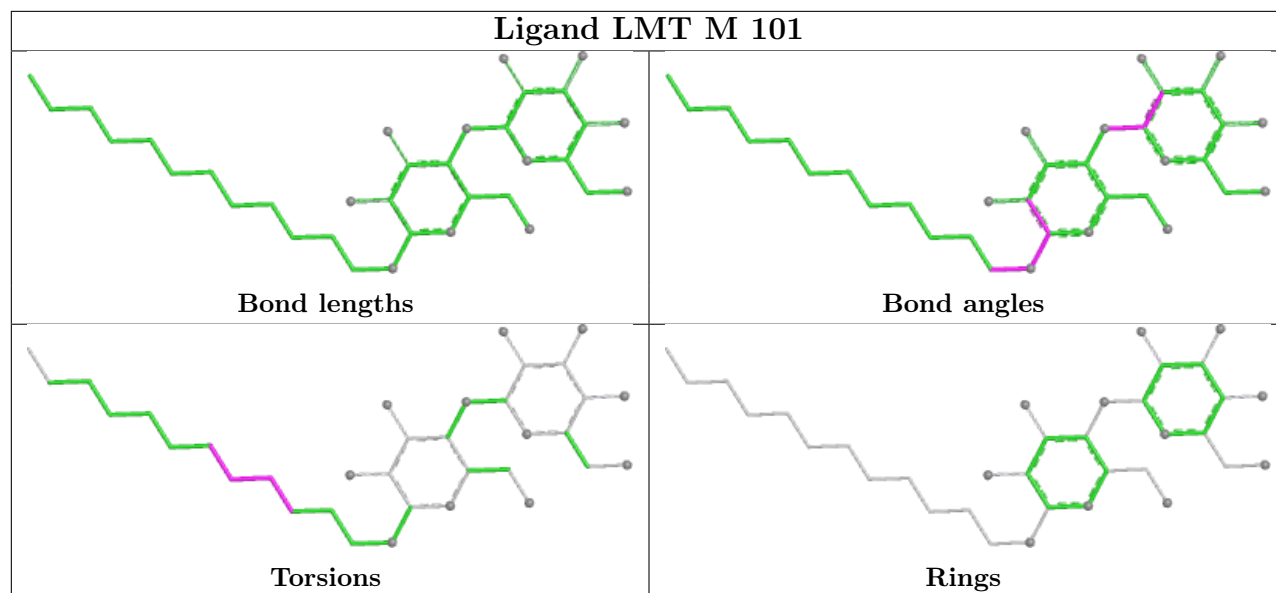


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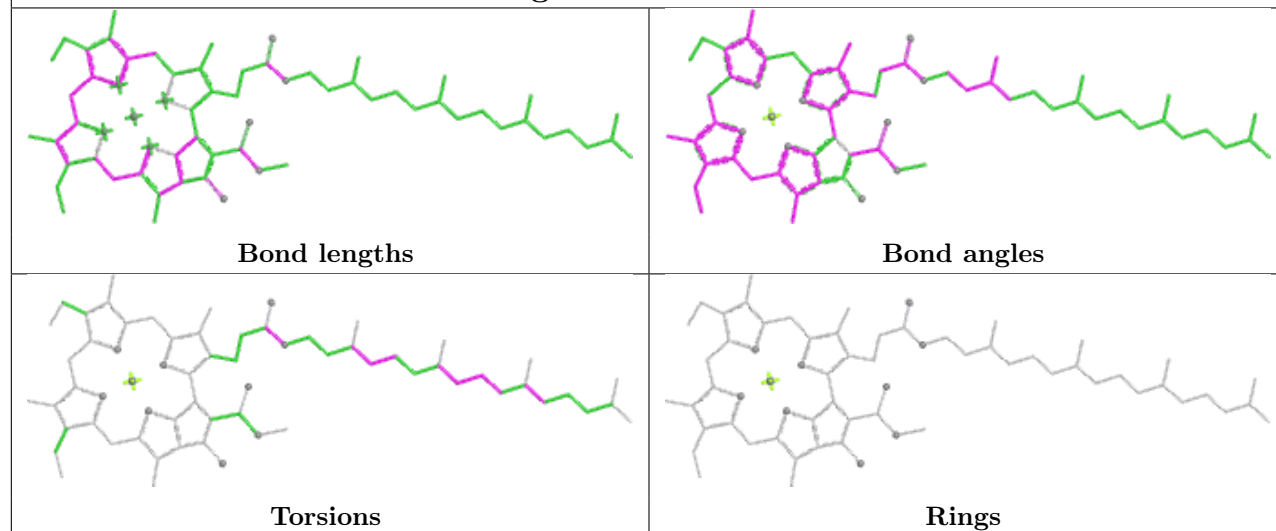


Ligand PHO a 405

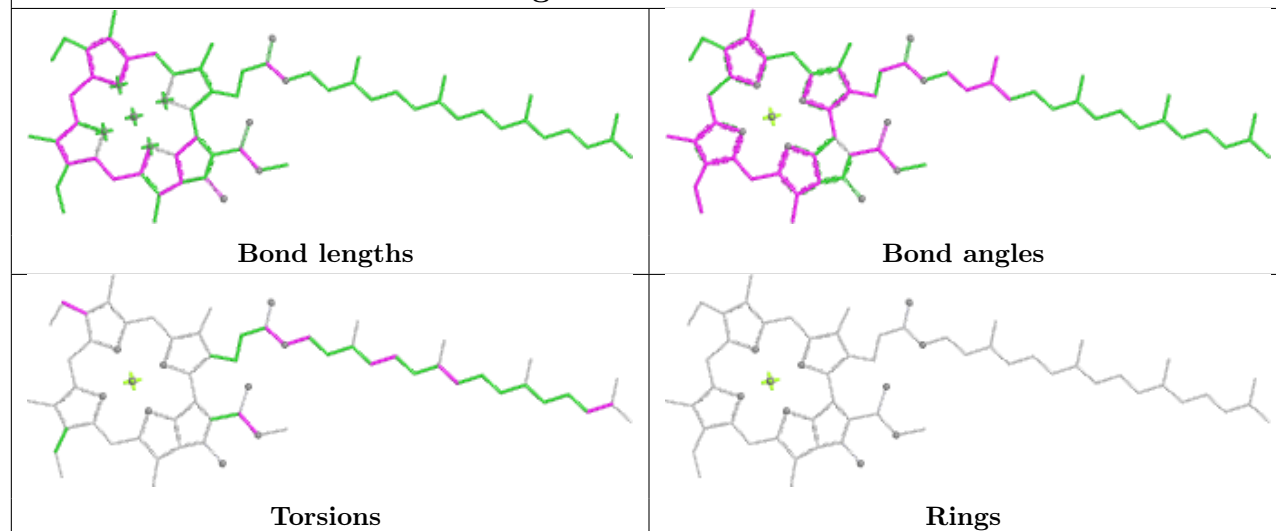




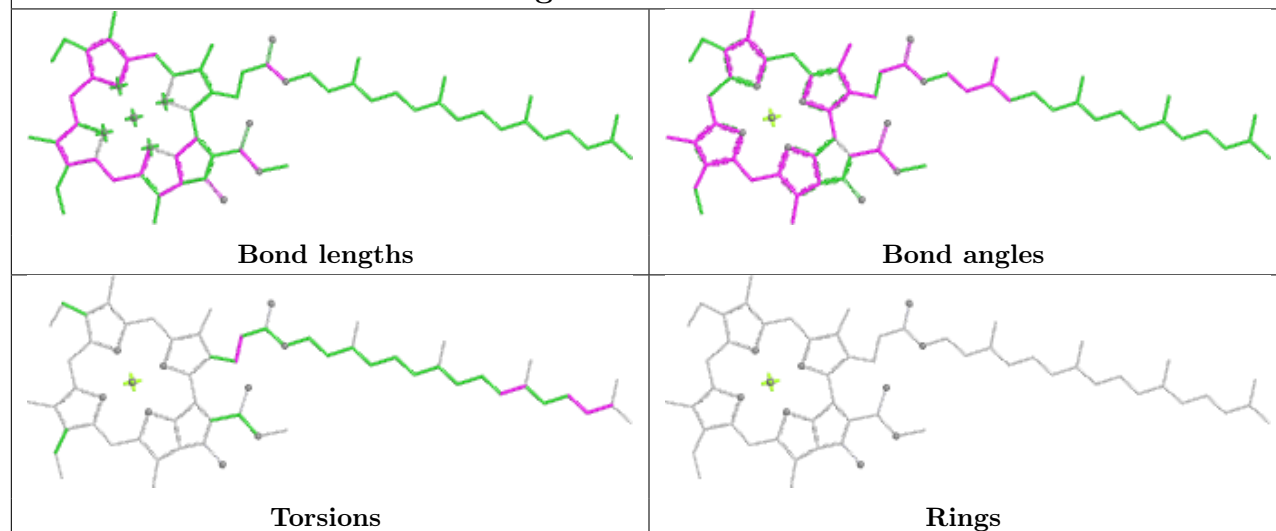
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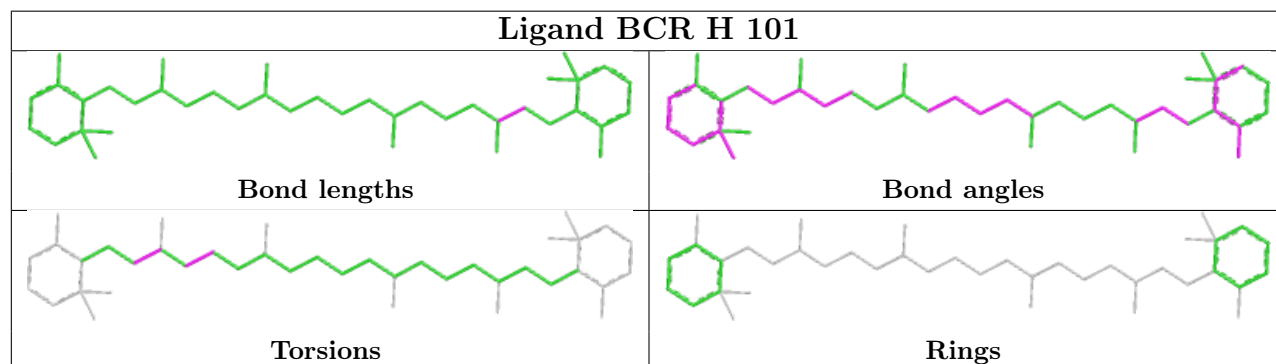
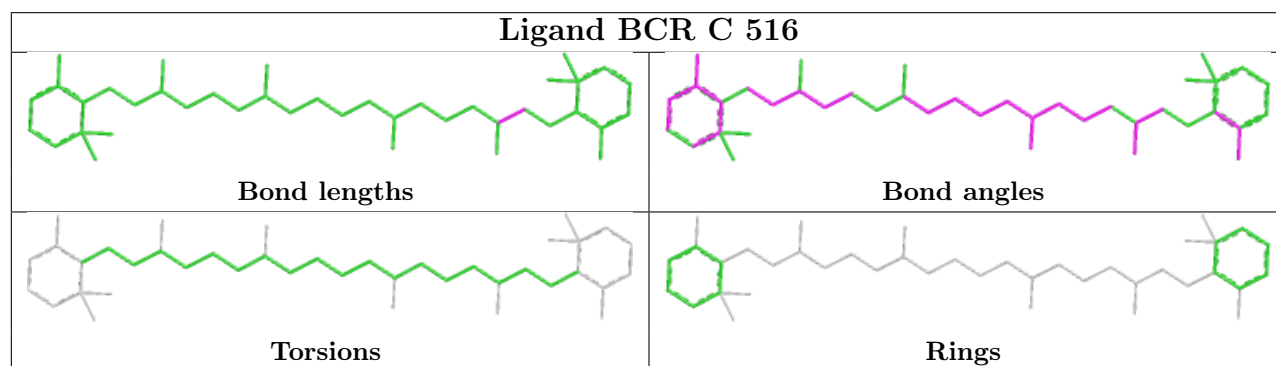
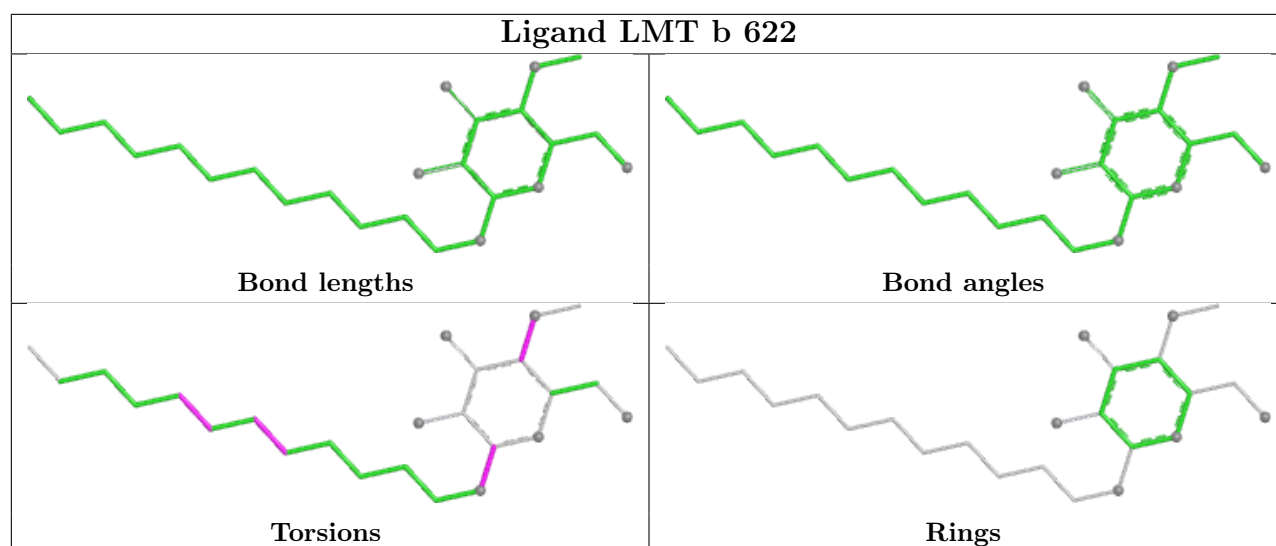


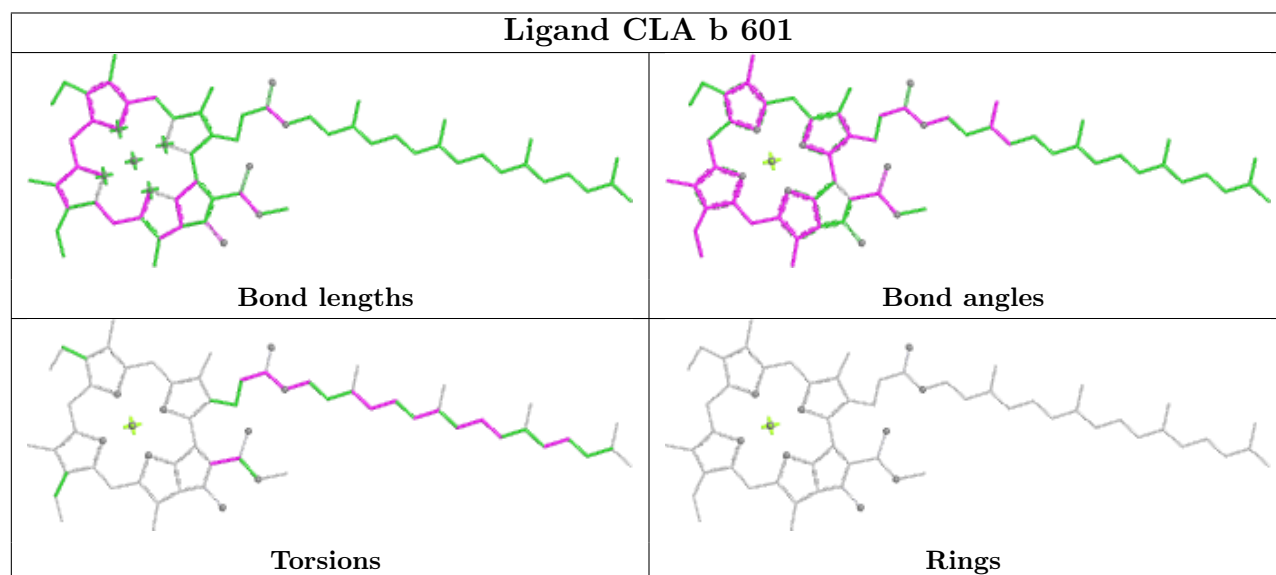
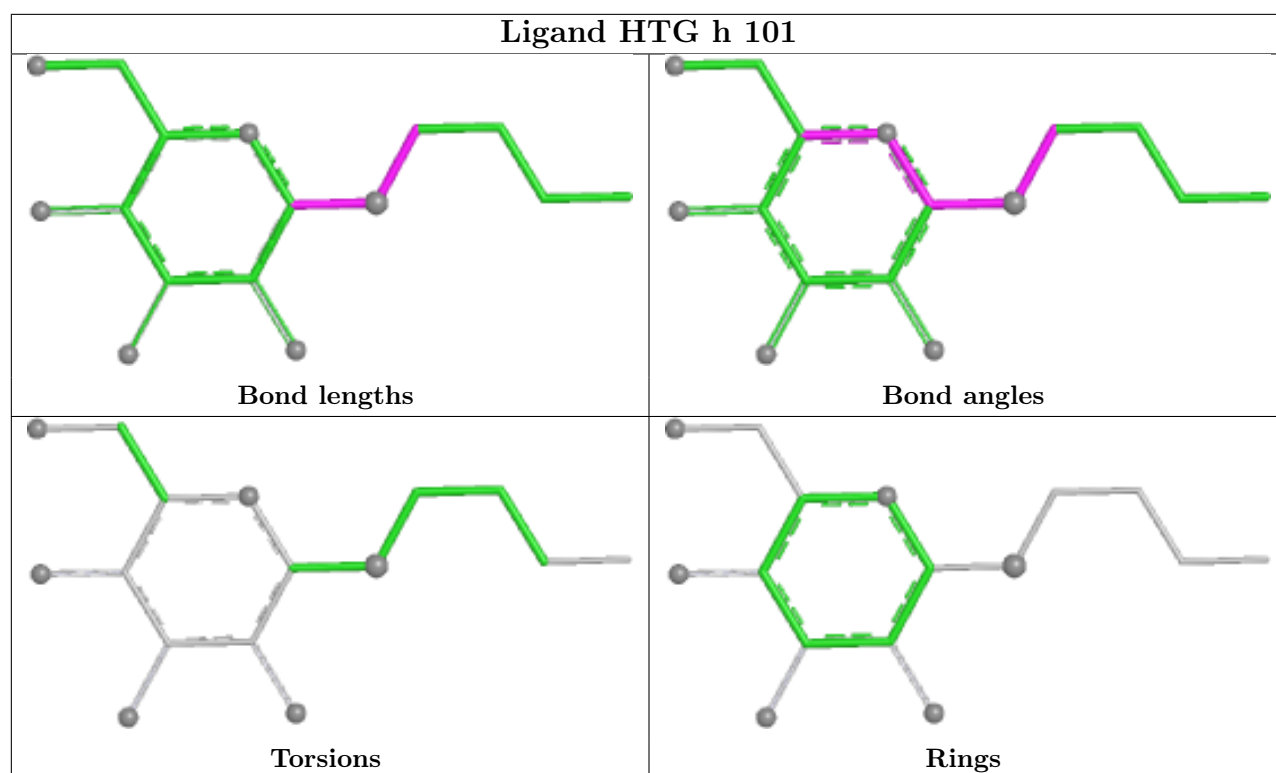
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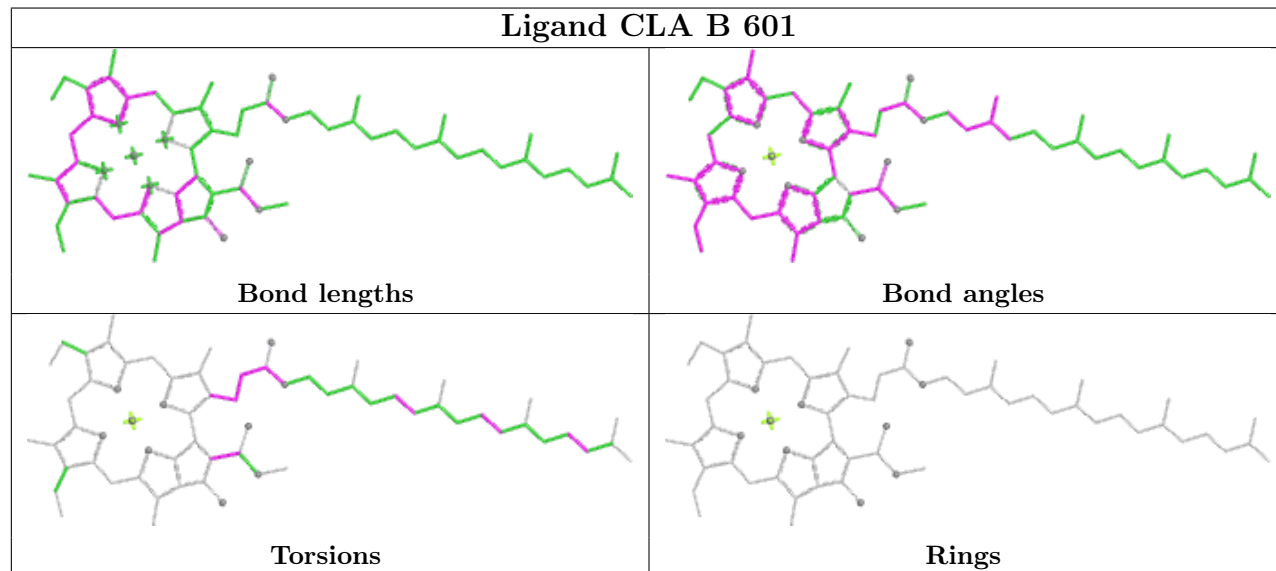
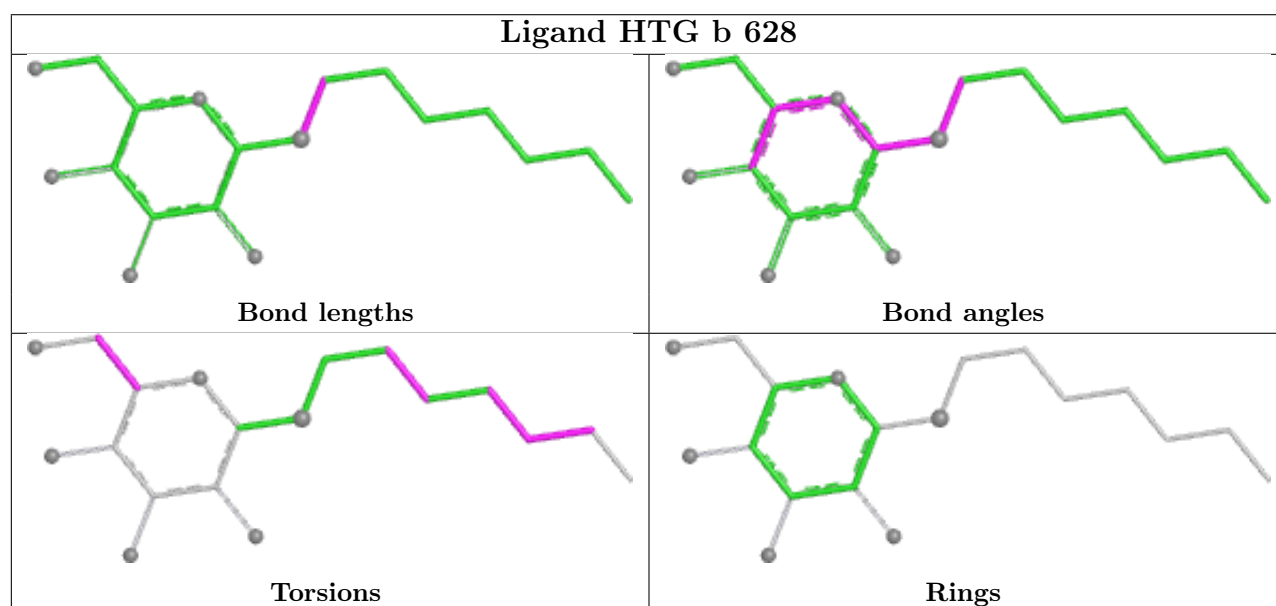
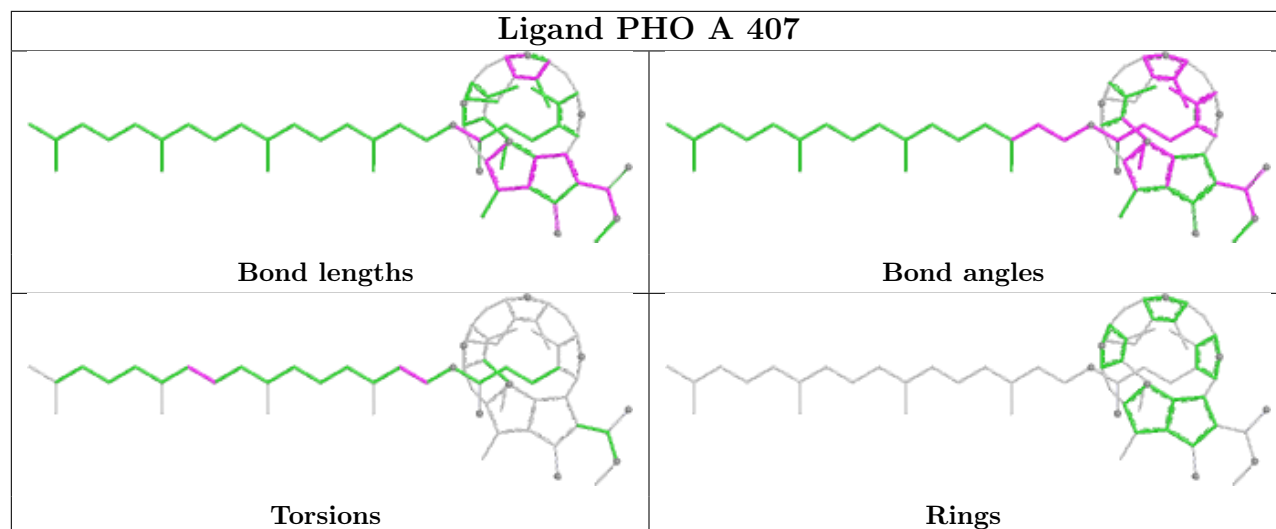


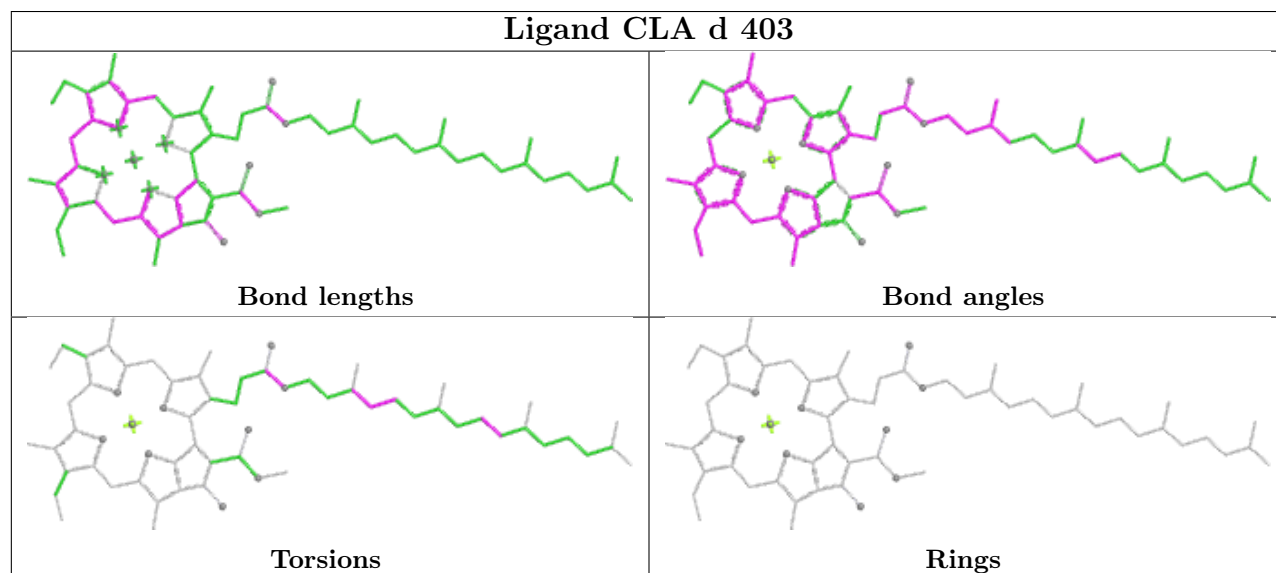
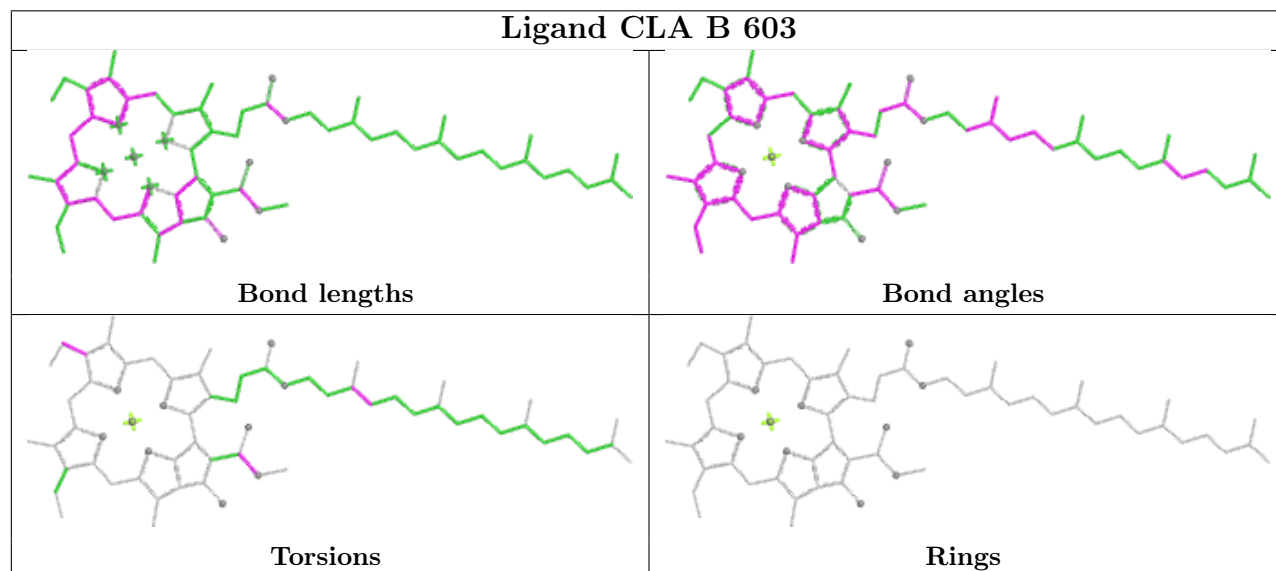
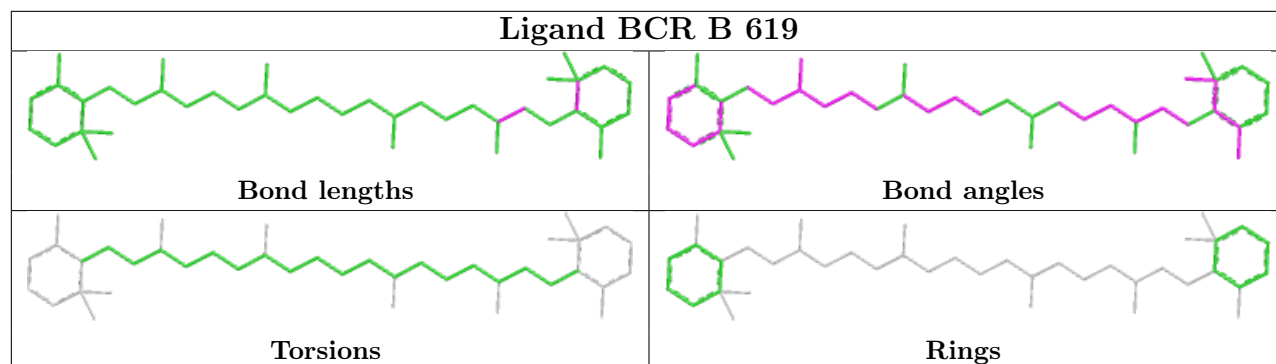
Ligand CLA b 610

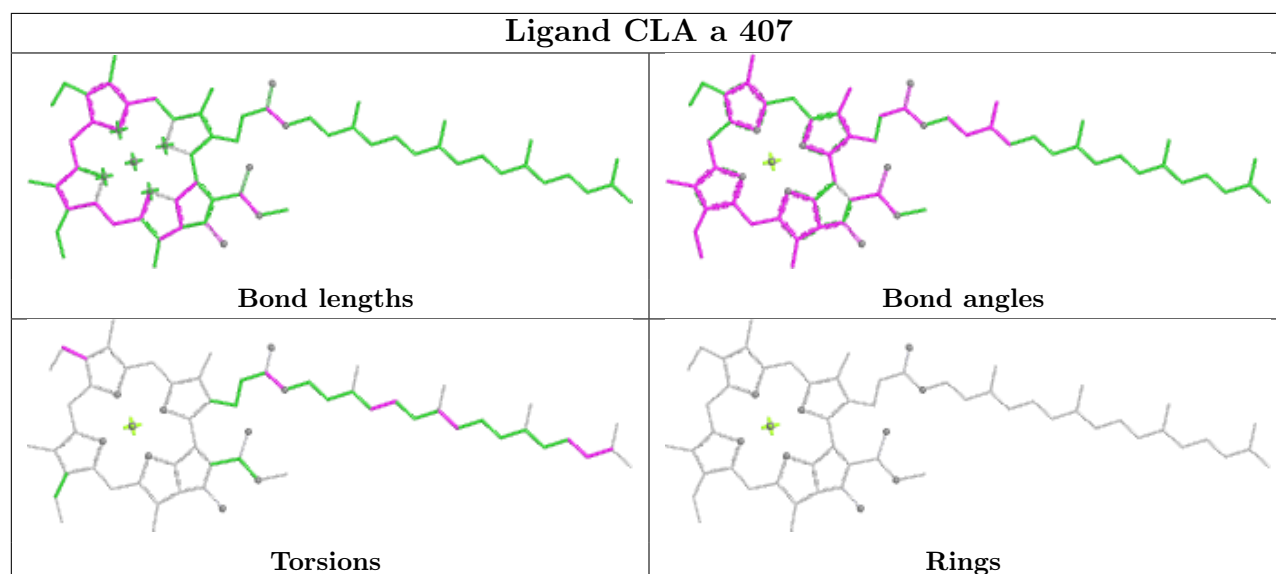
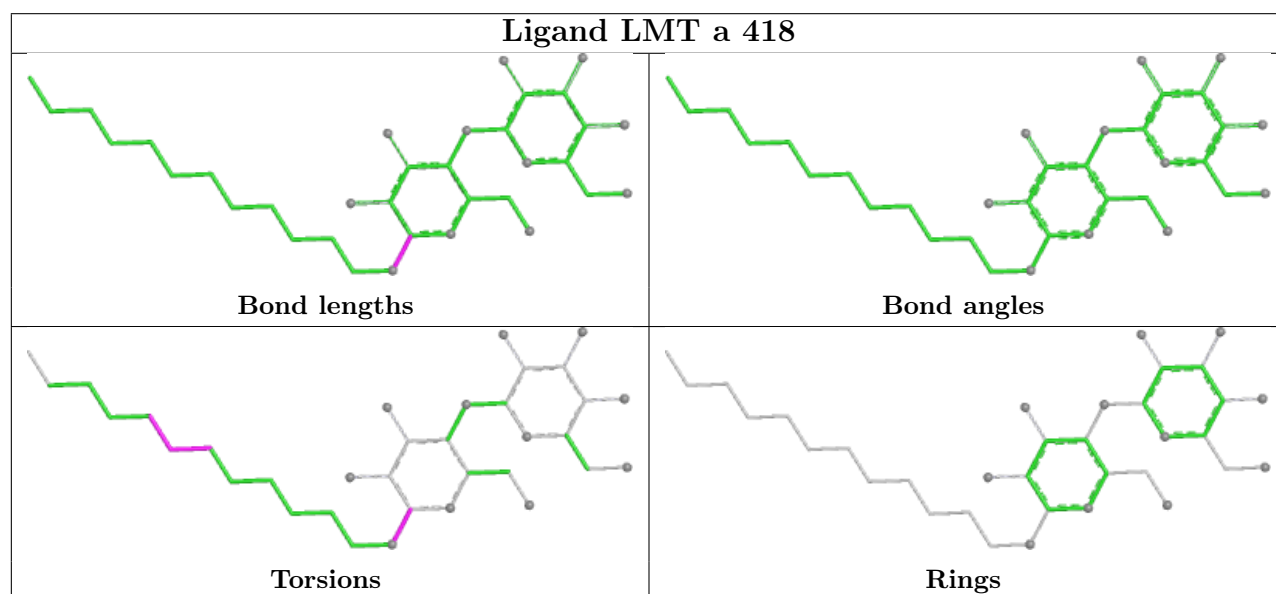
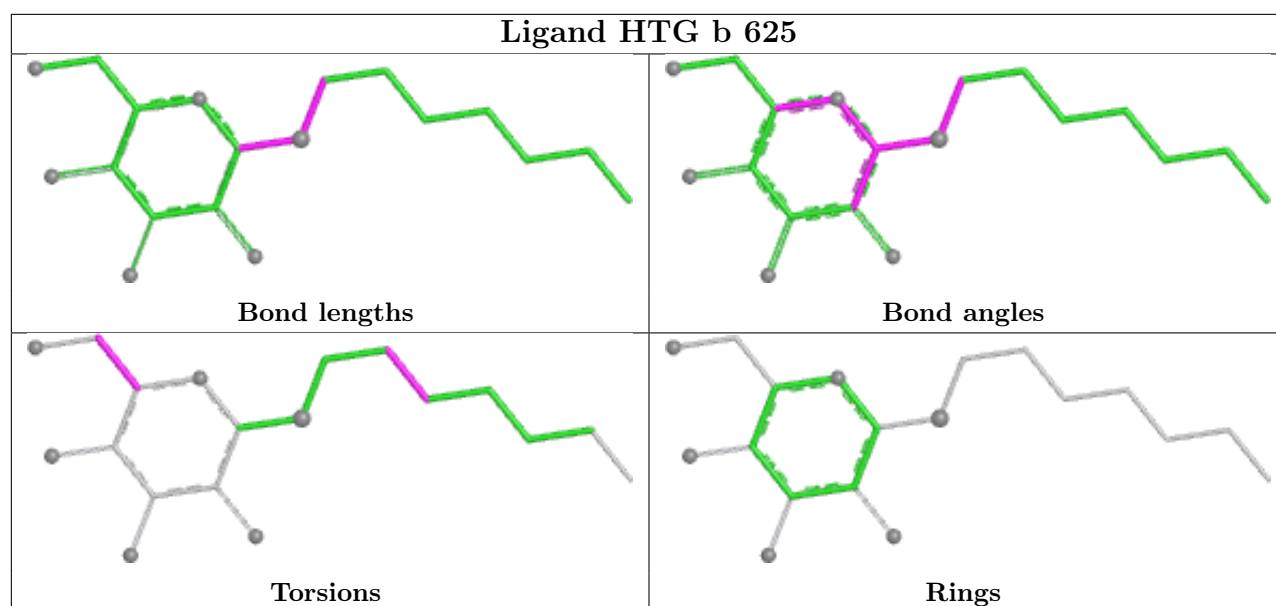


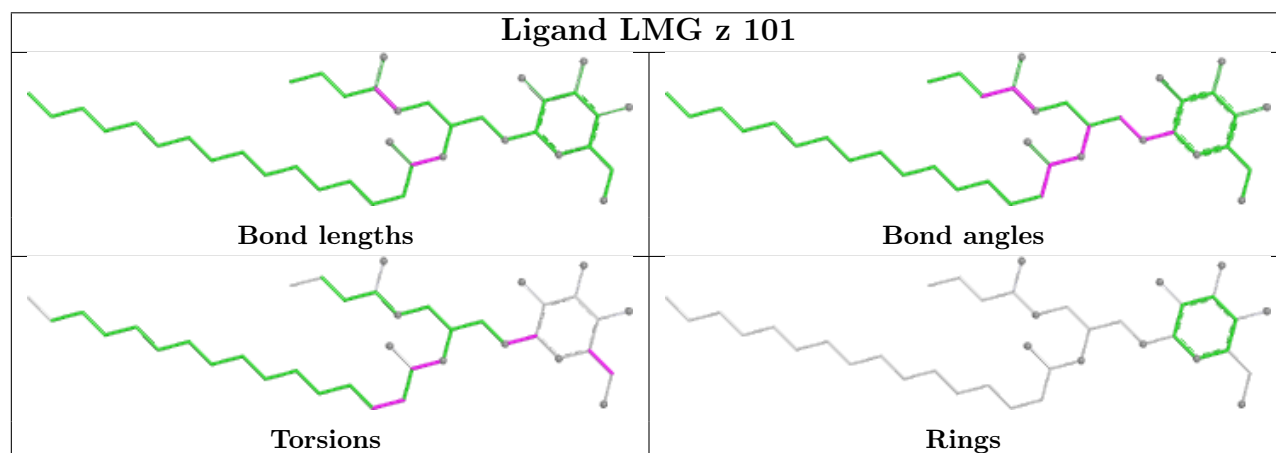
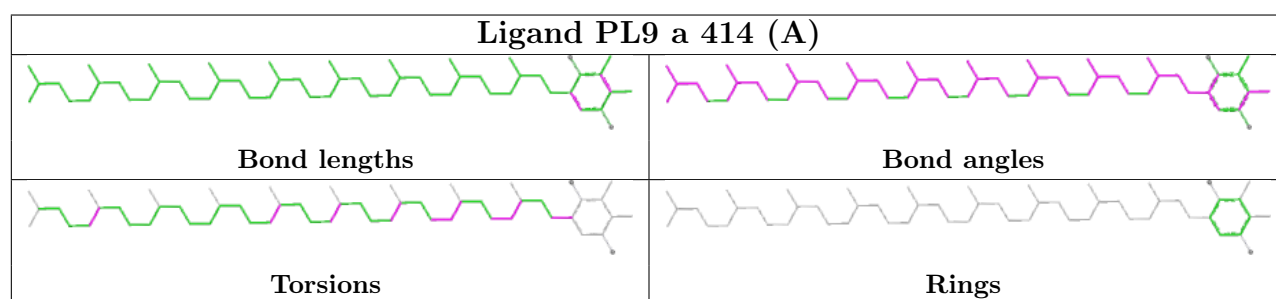
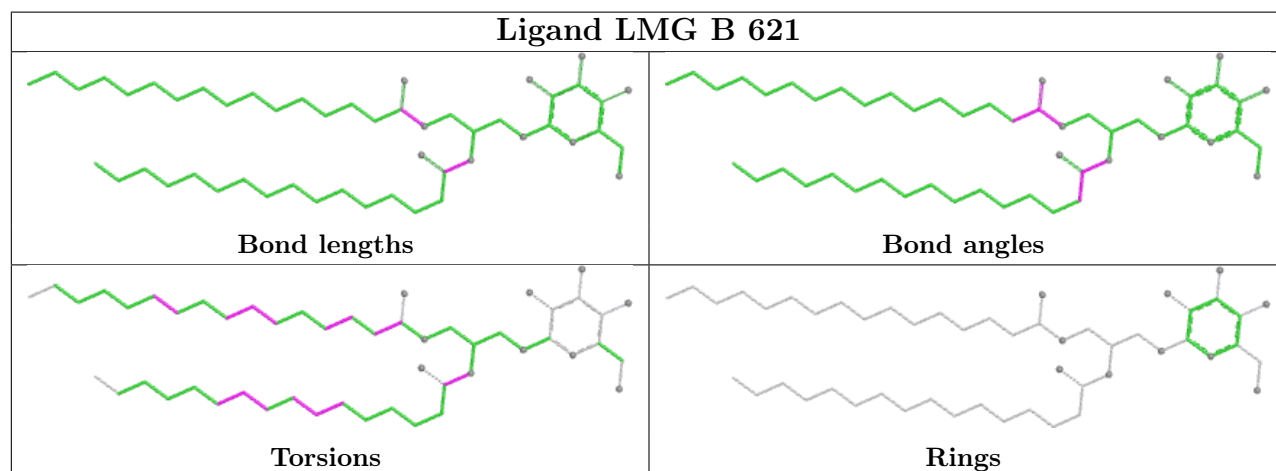
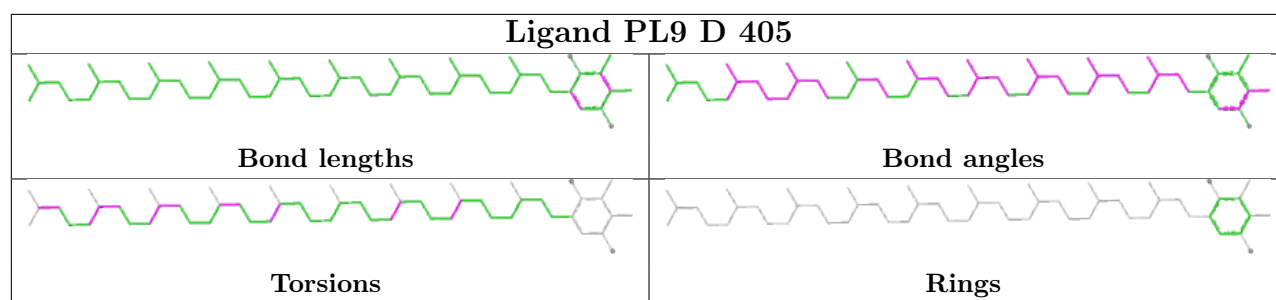


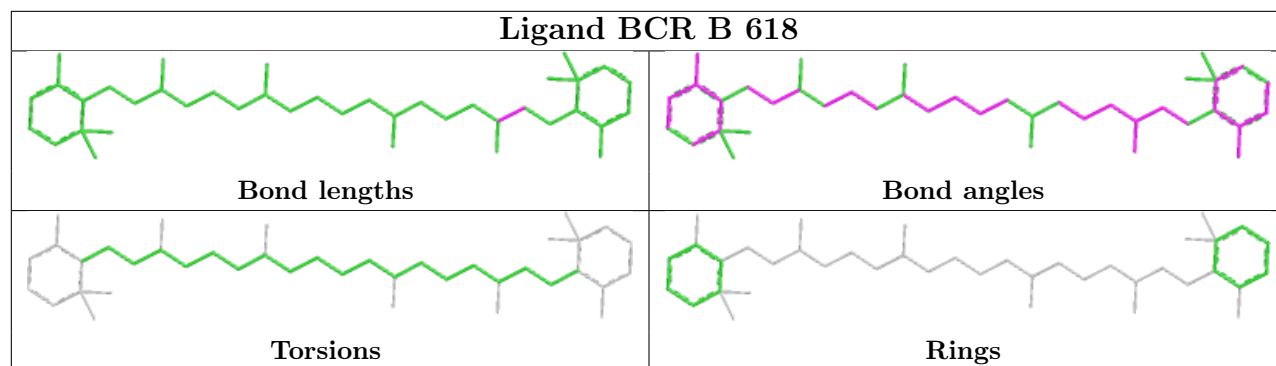
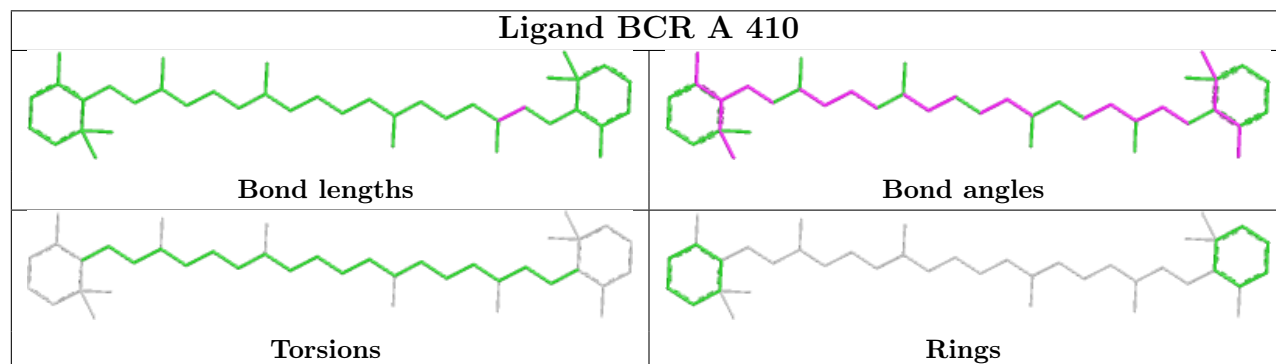
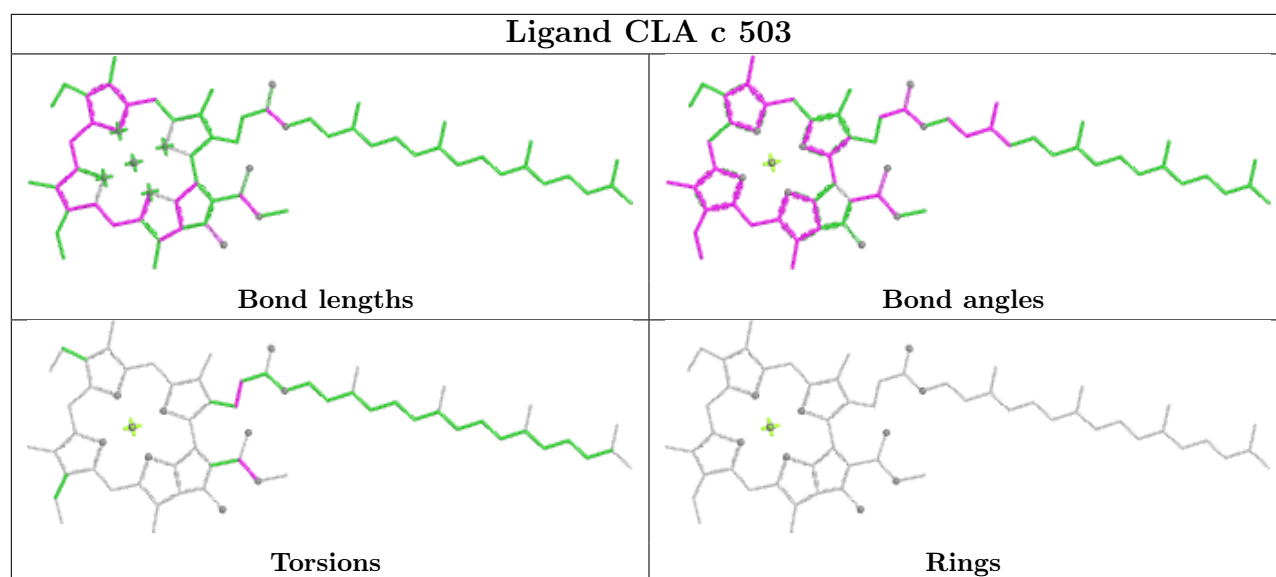


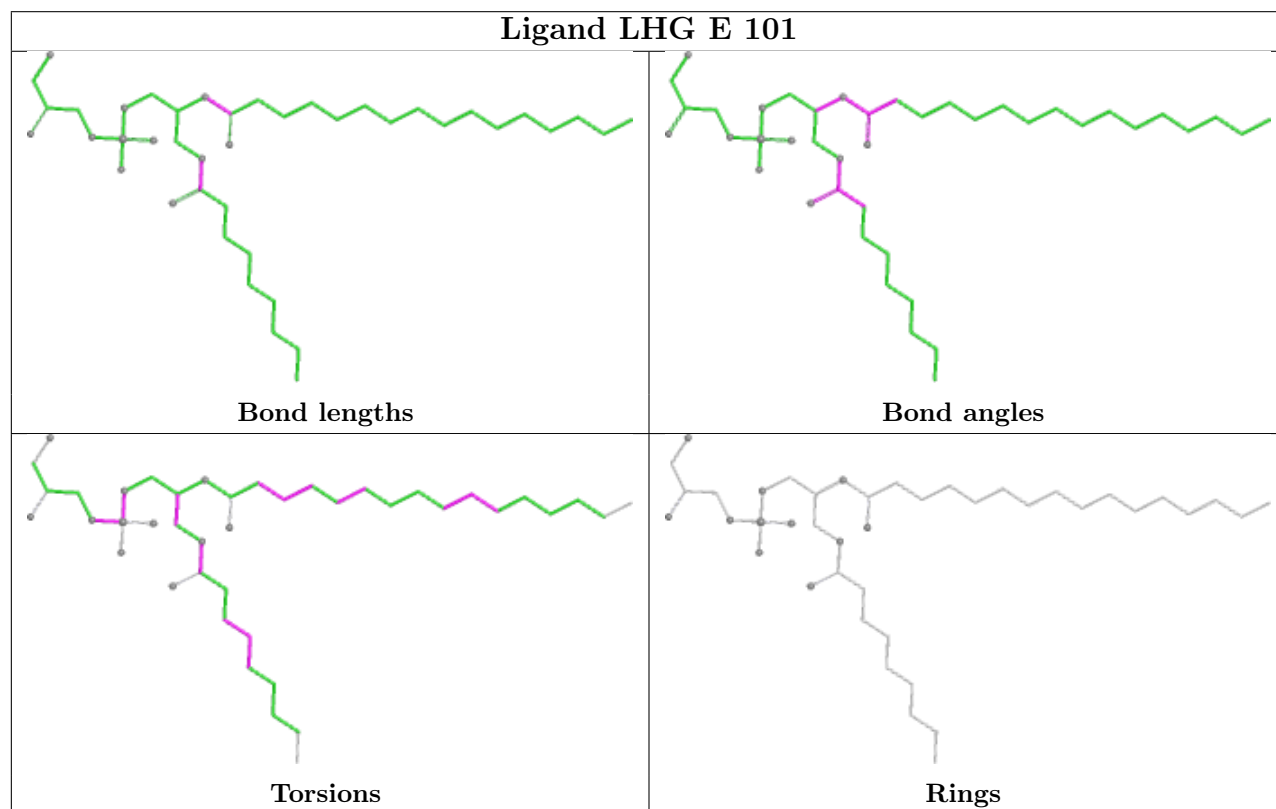
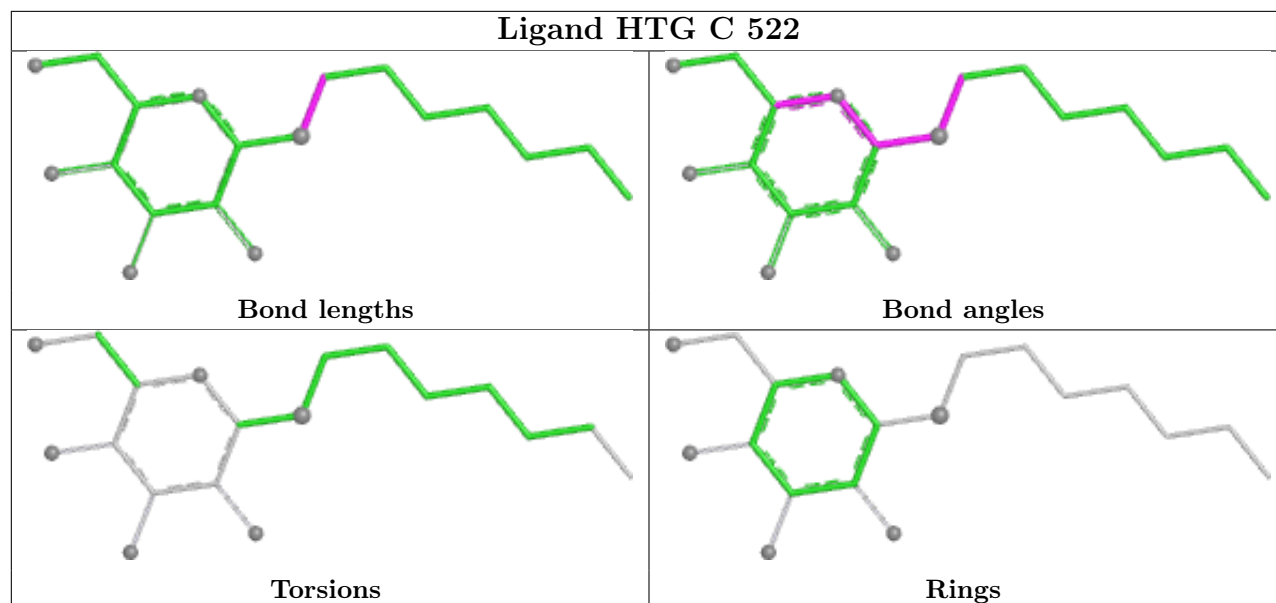


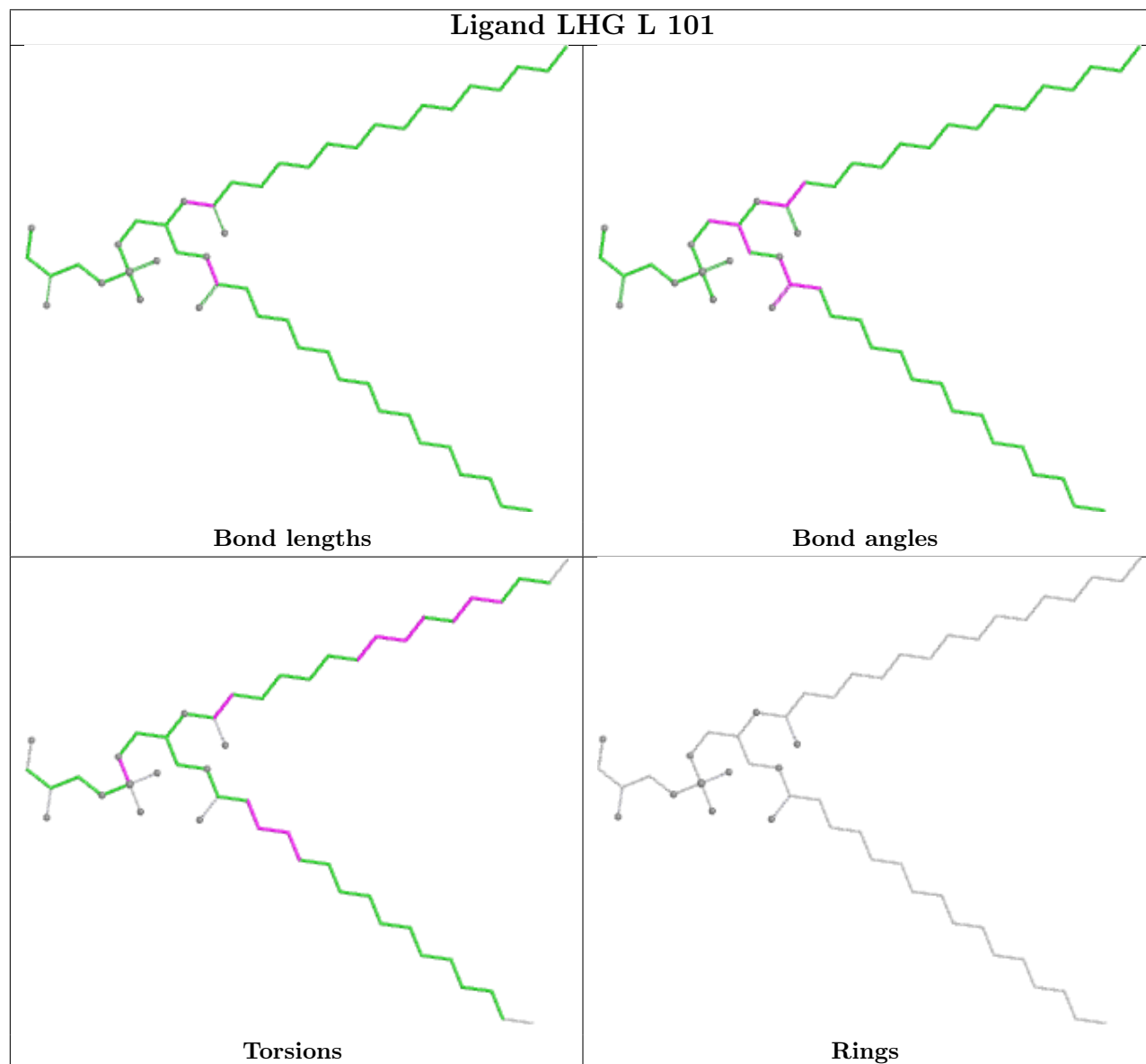
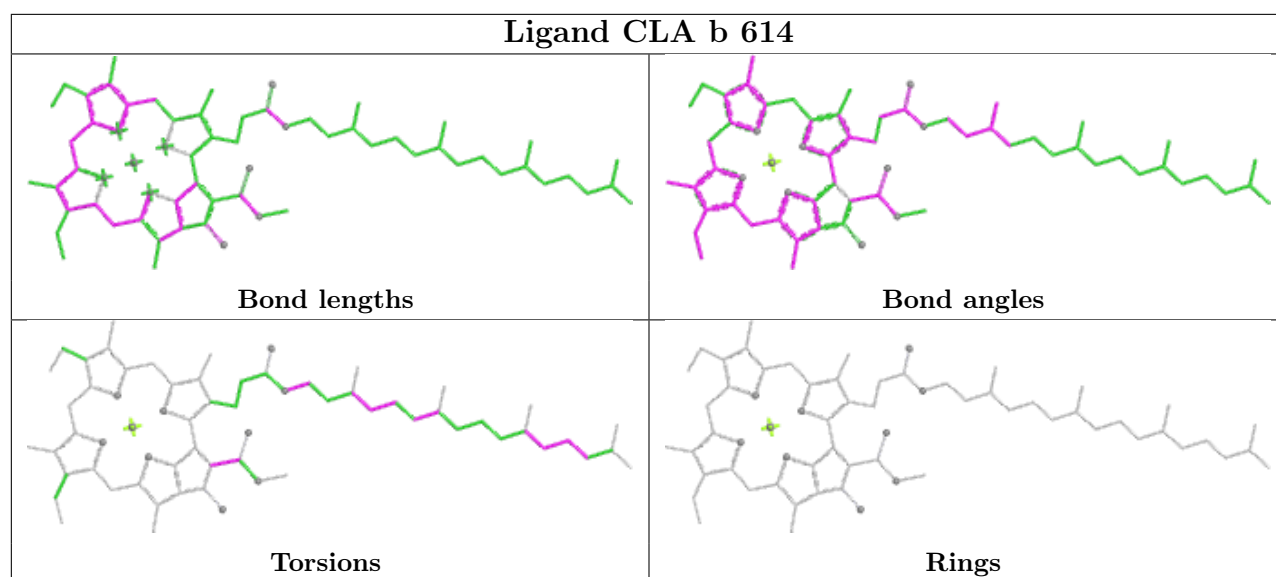


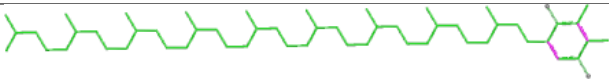
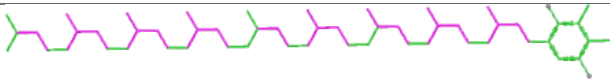
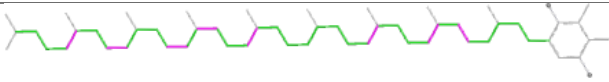
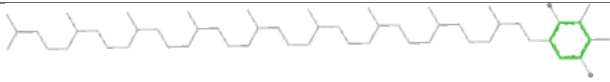


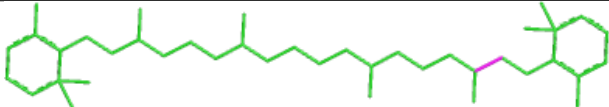
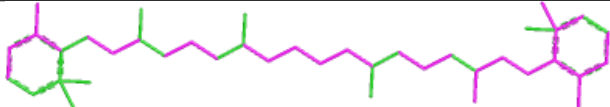
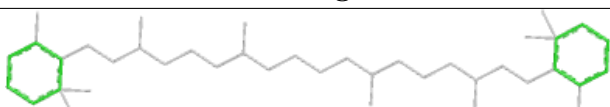


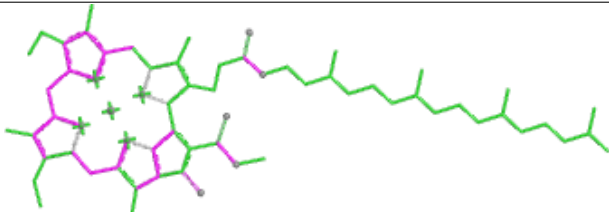
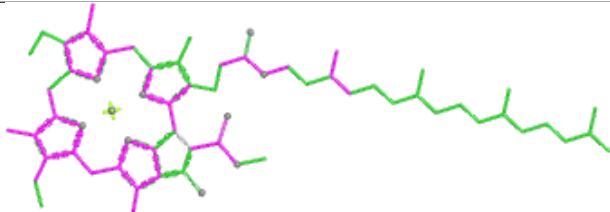
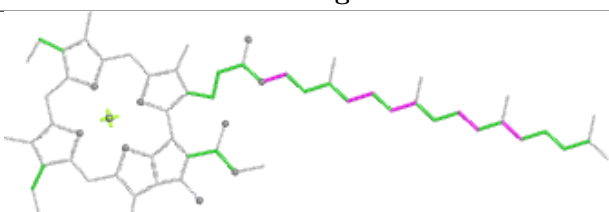
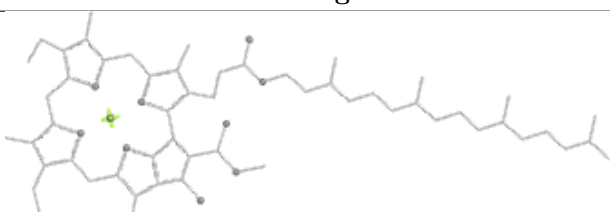




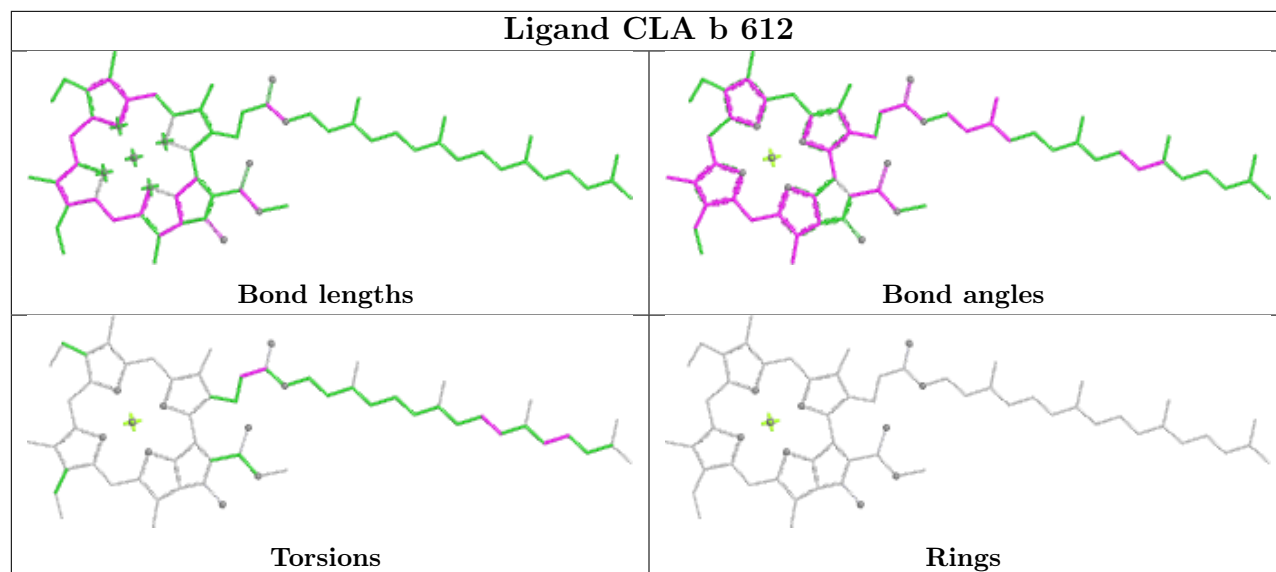


Ligand PL9 d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

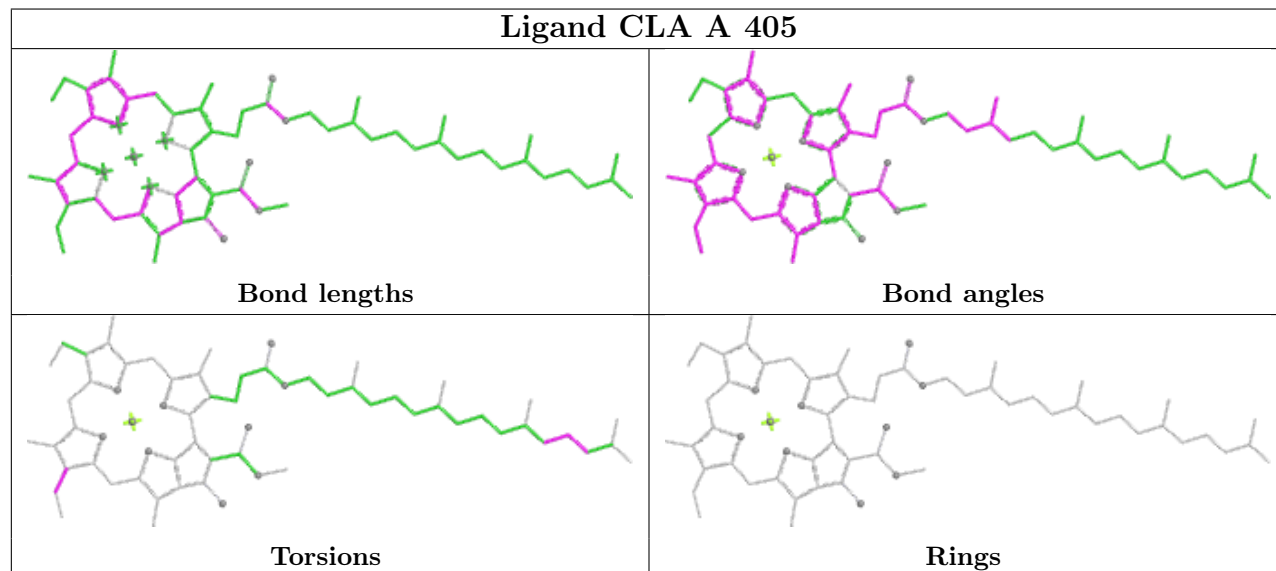
Ligand BCR D 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

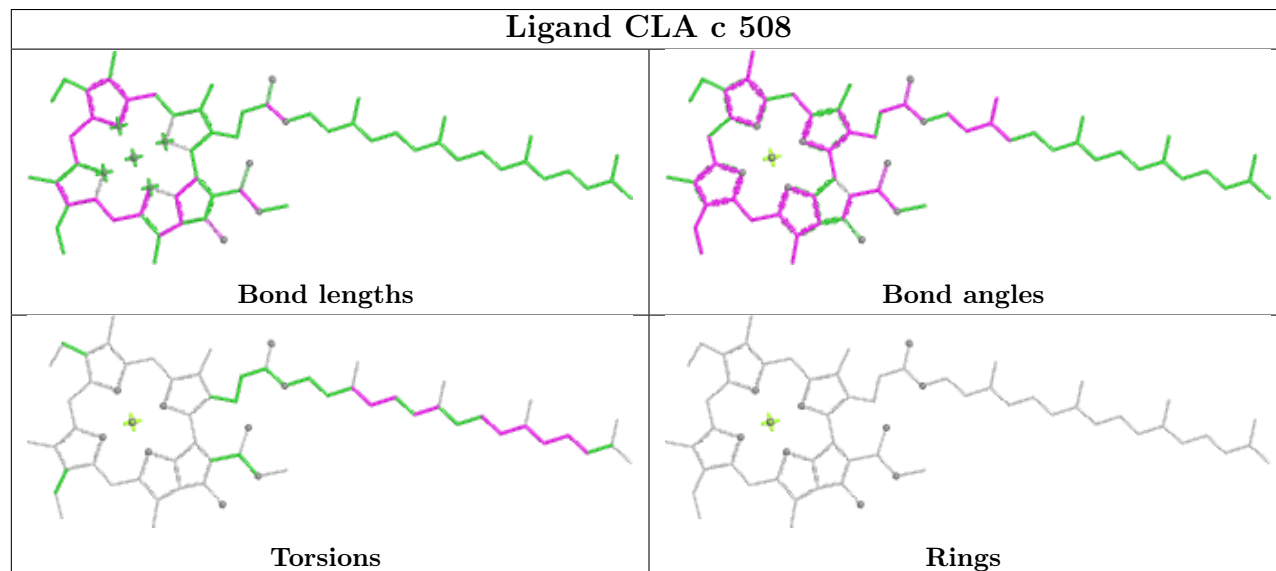
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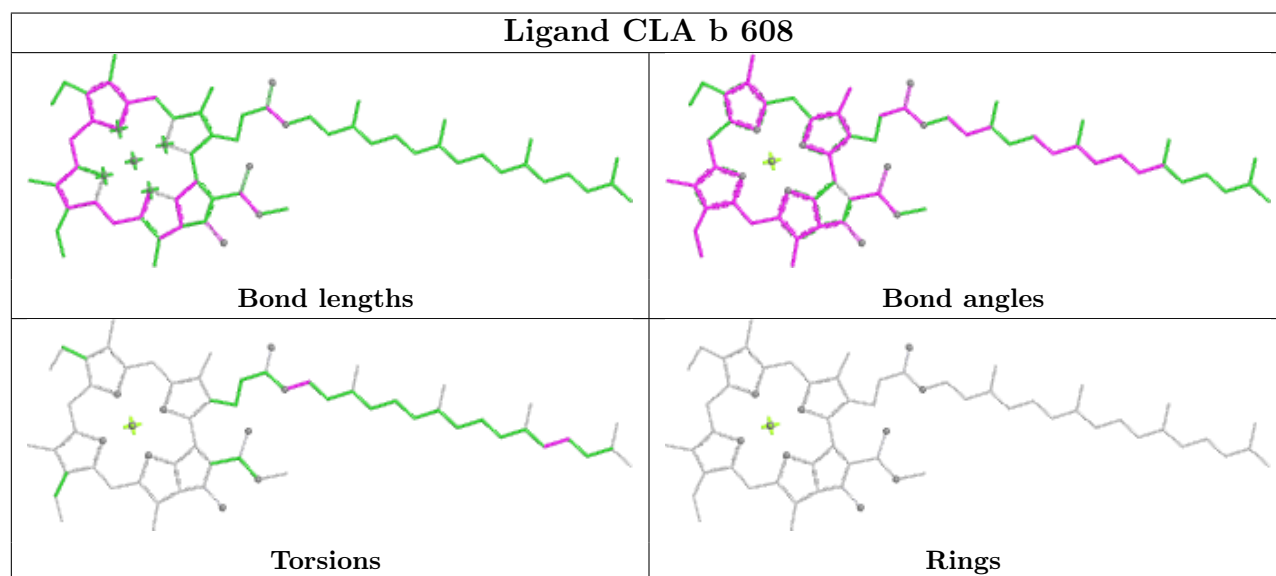
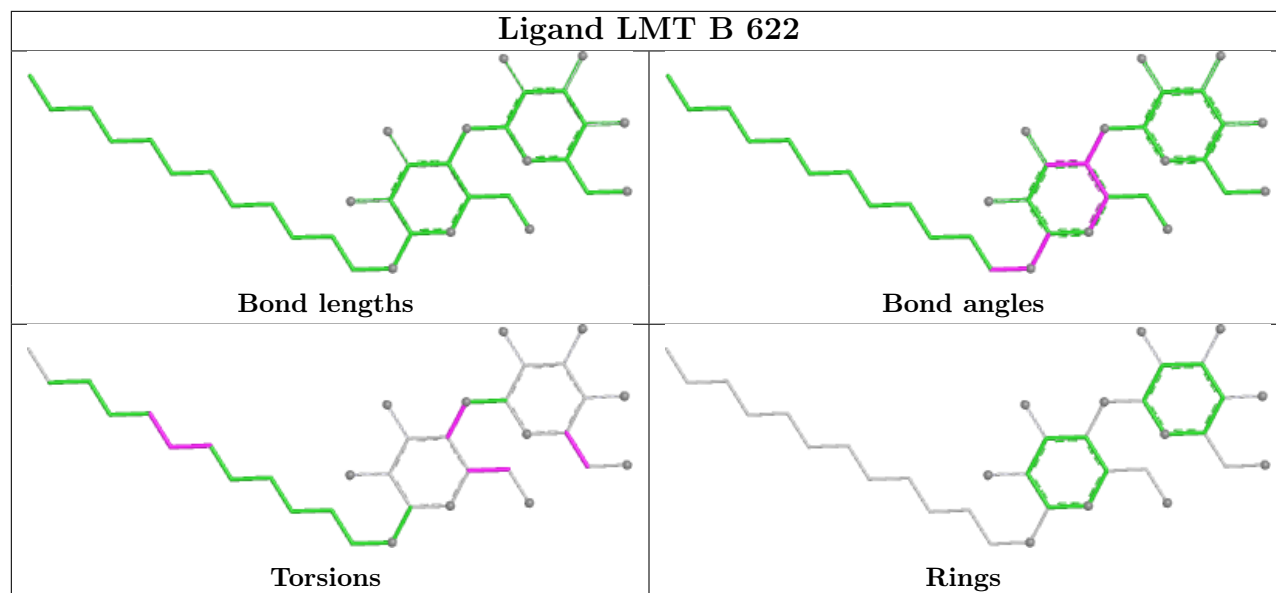


Ligand CLA A 405

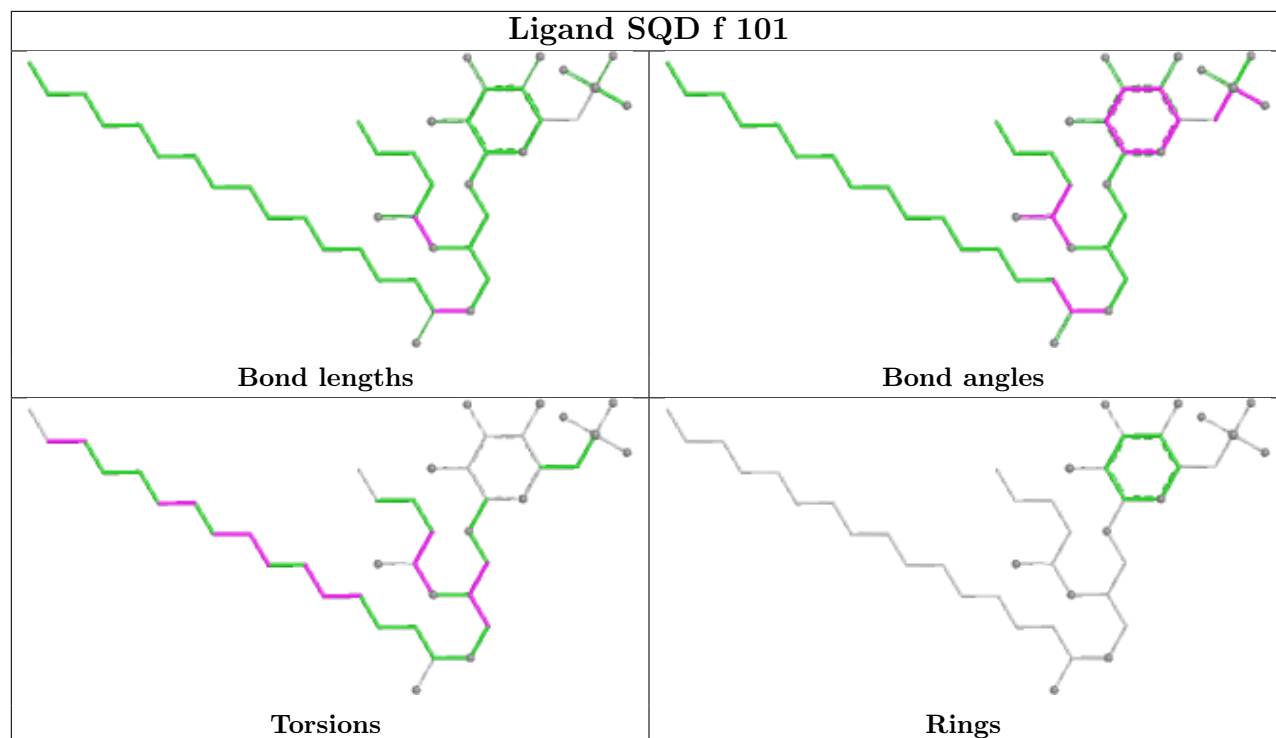


Ligand CLA c 508

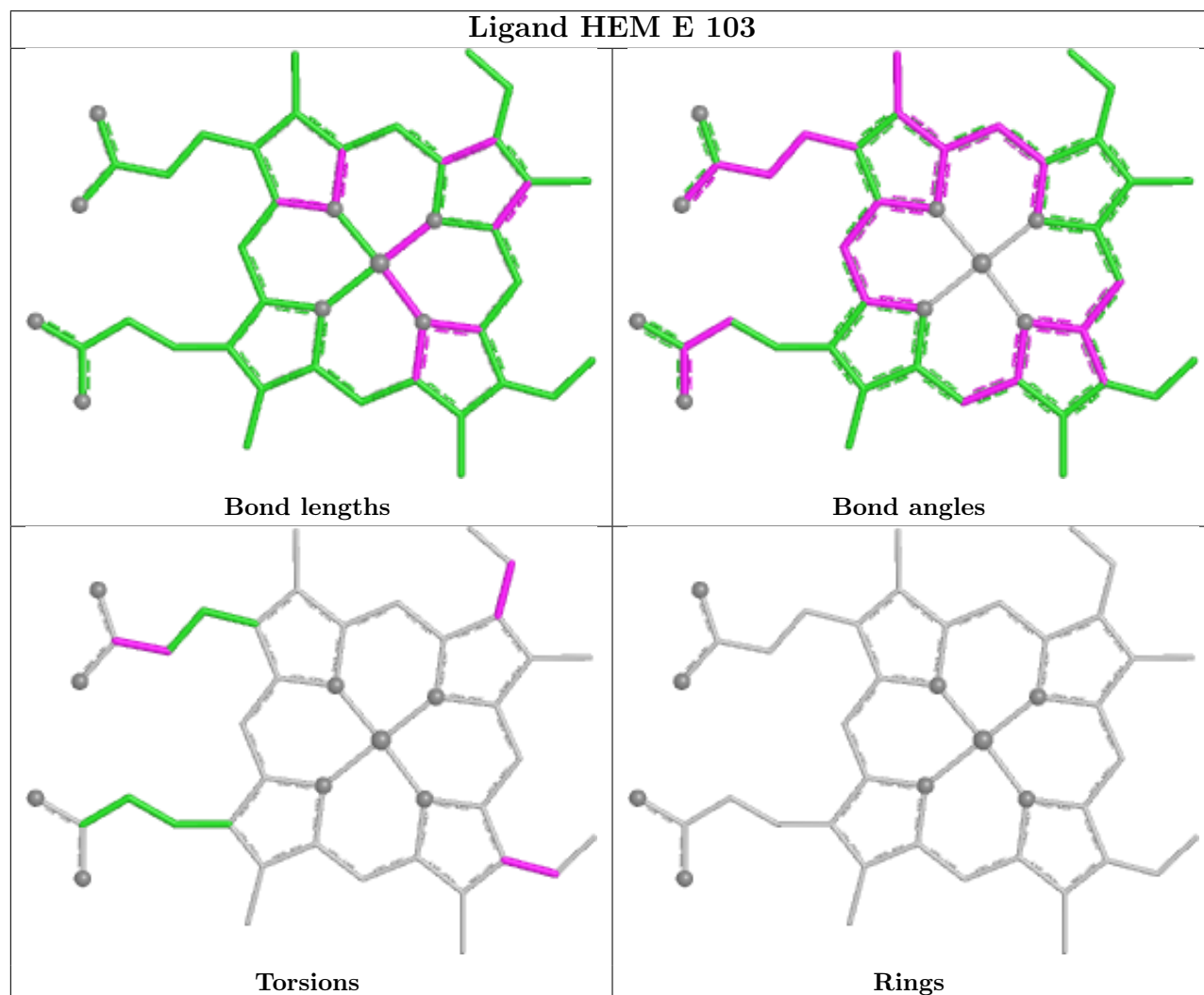


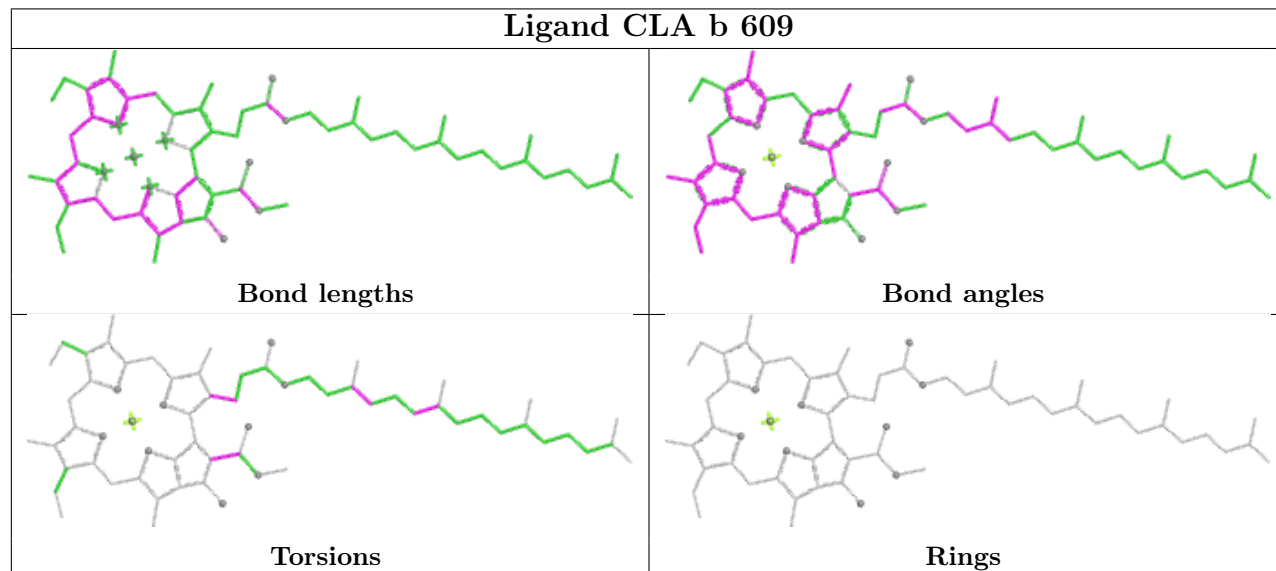
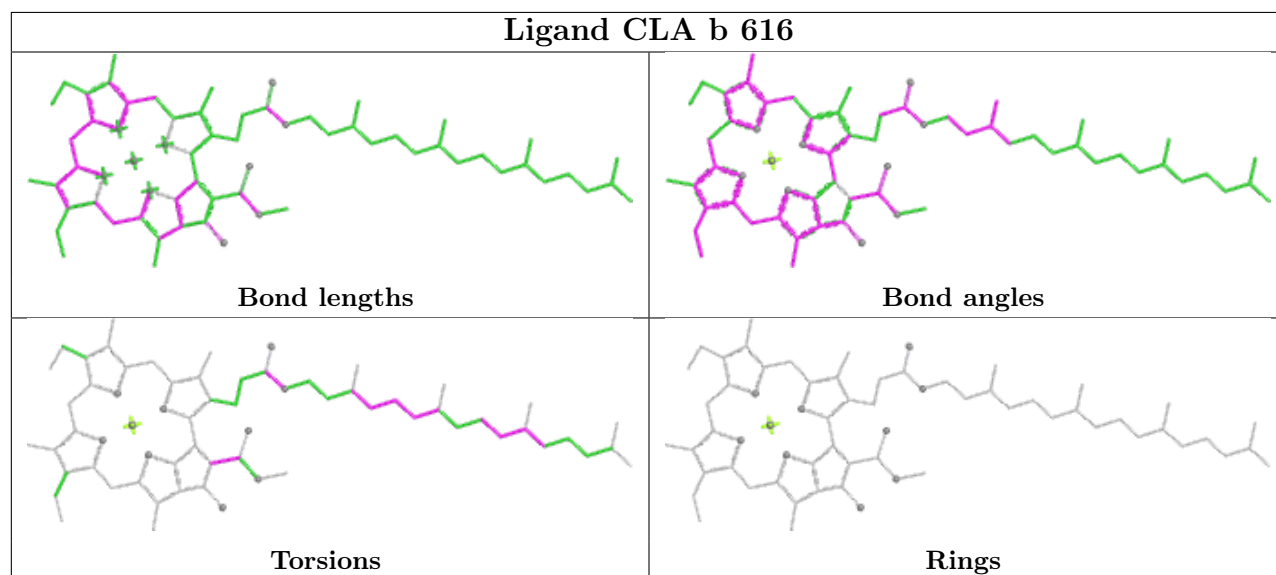
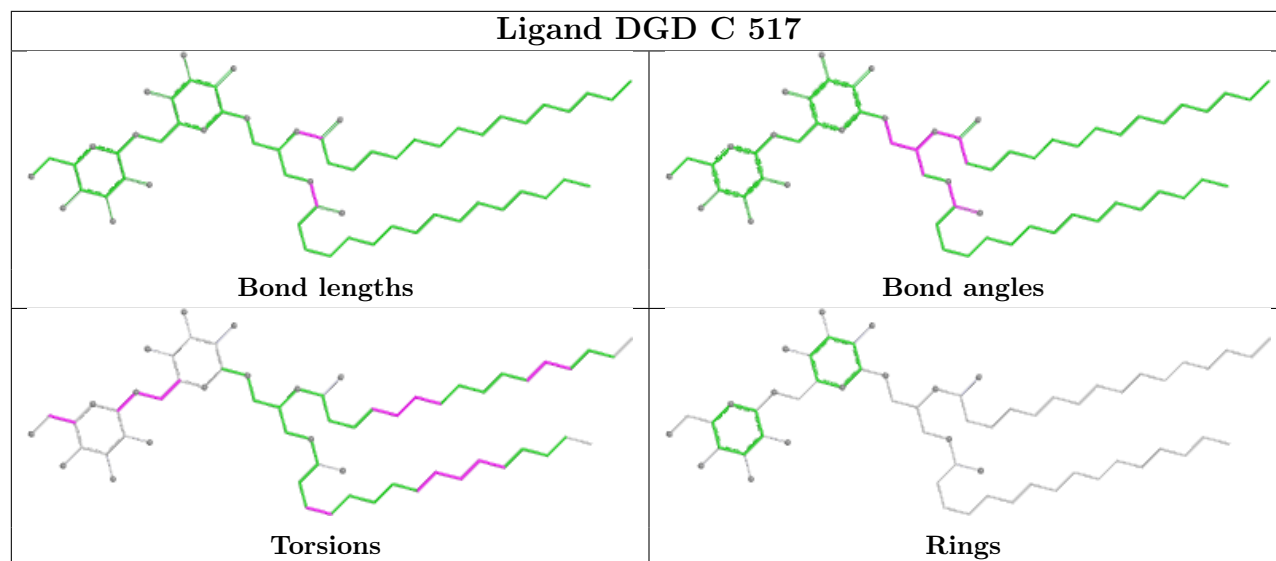


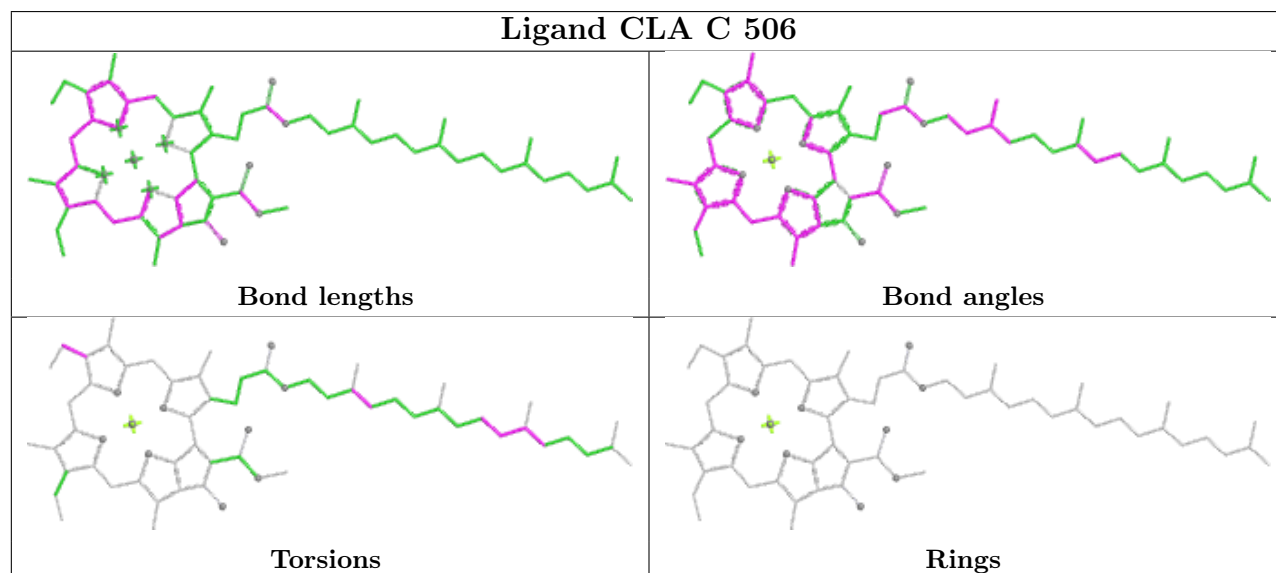
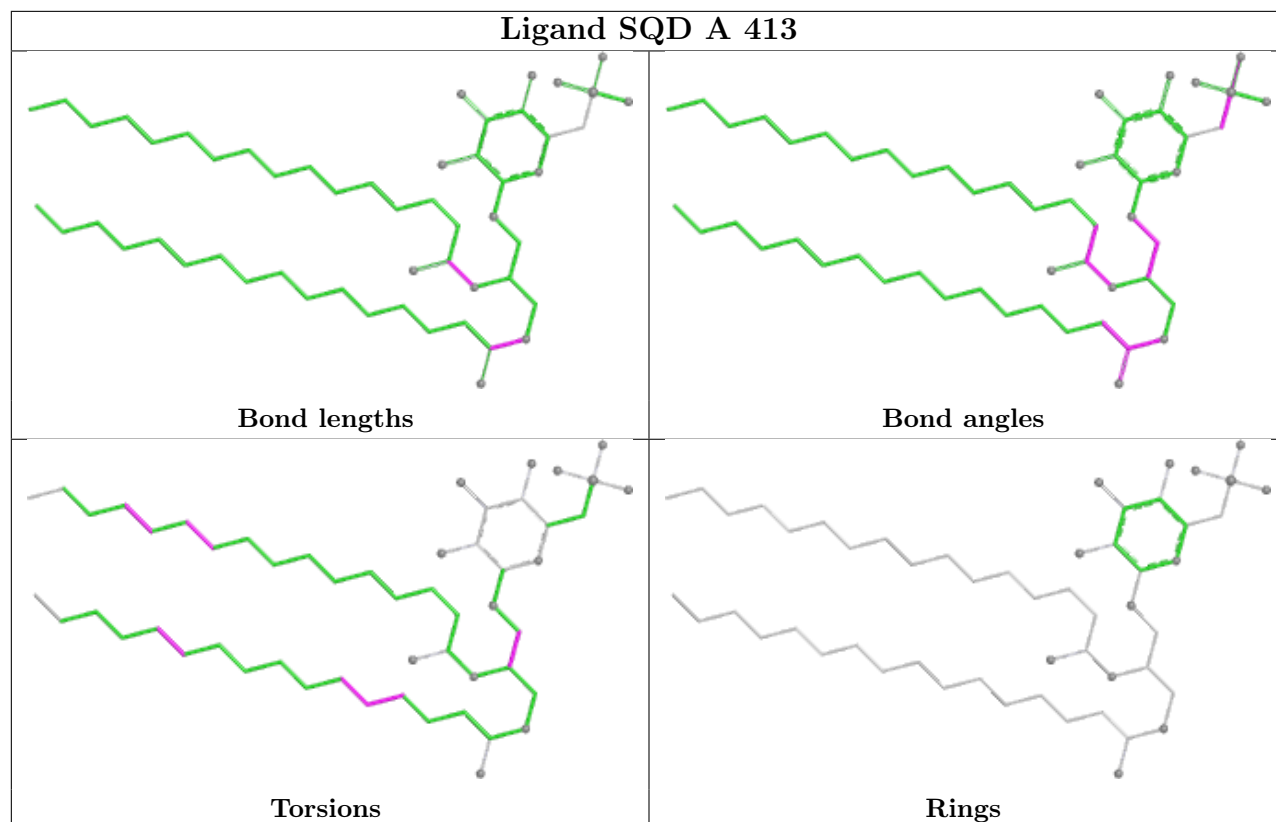
Ligand SQD f 101

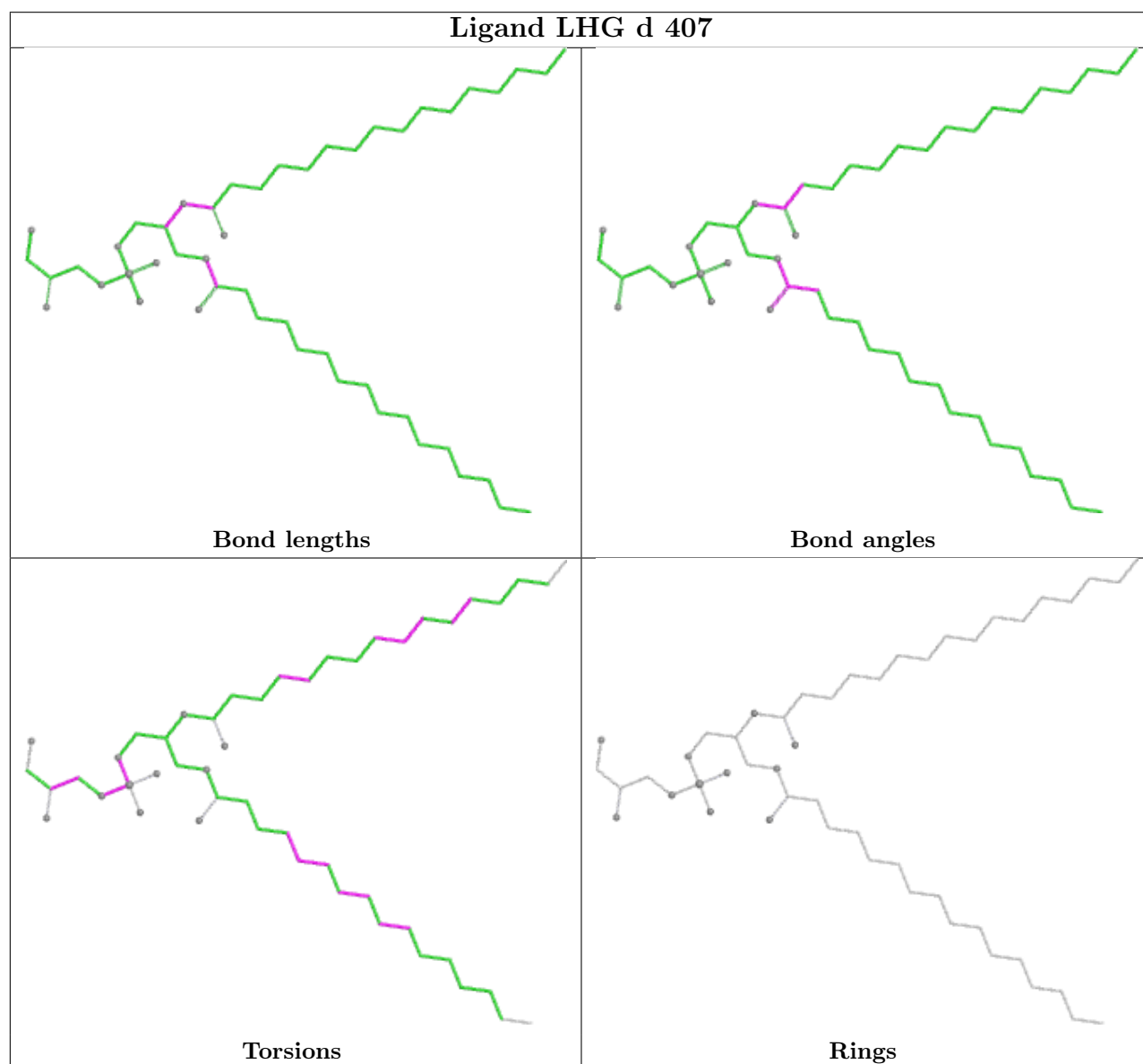
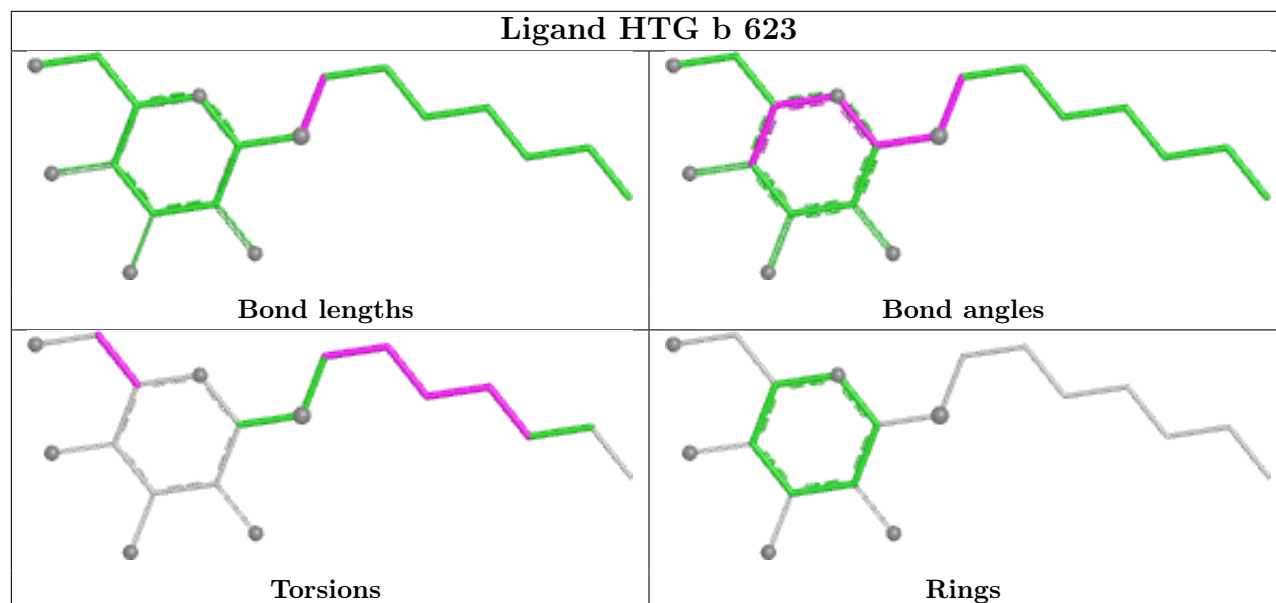


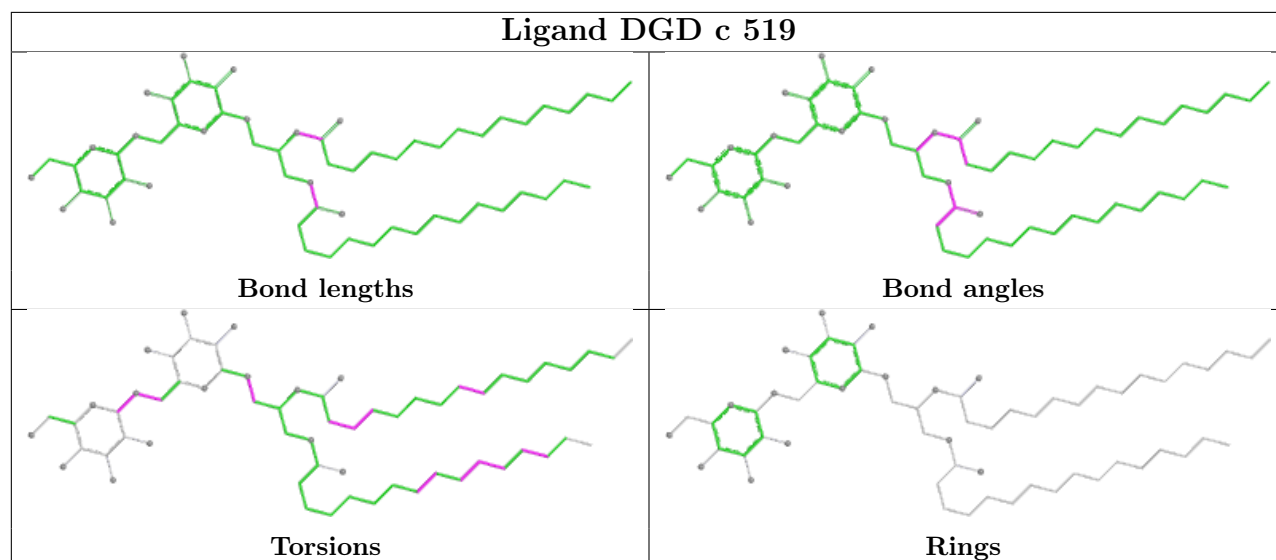
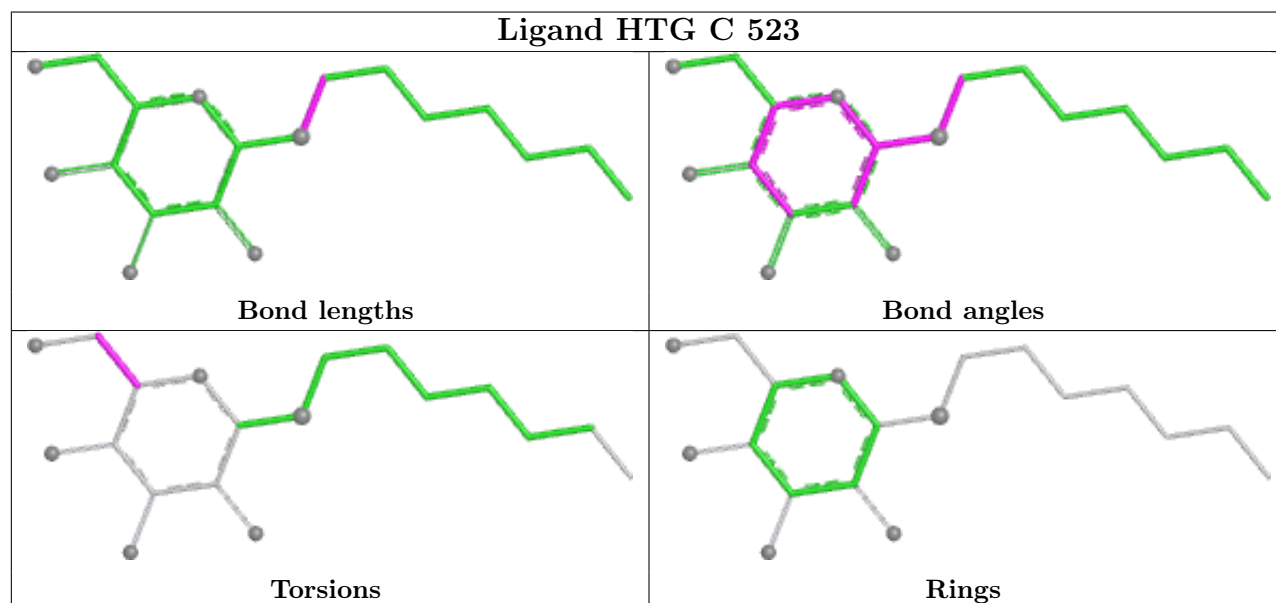
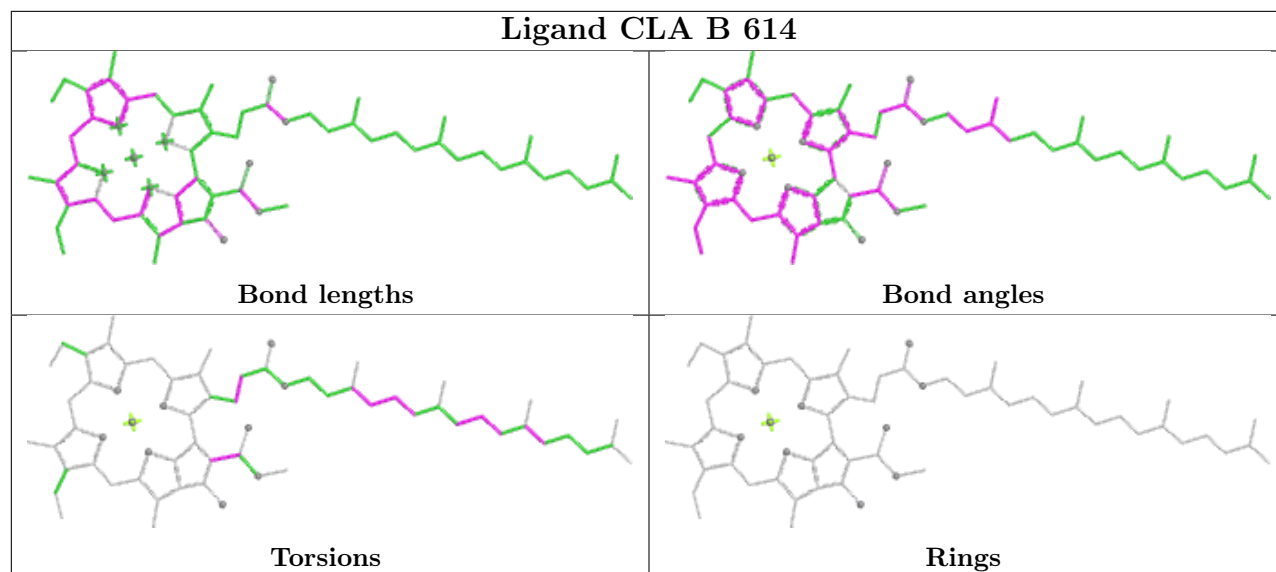
Ligand HEM E 103



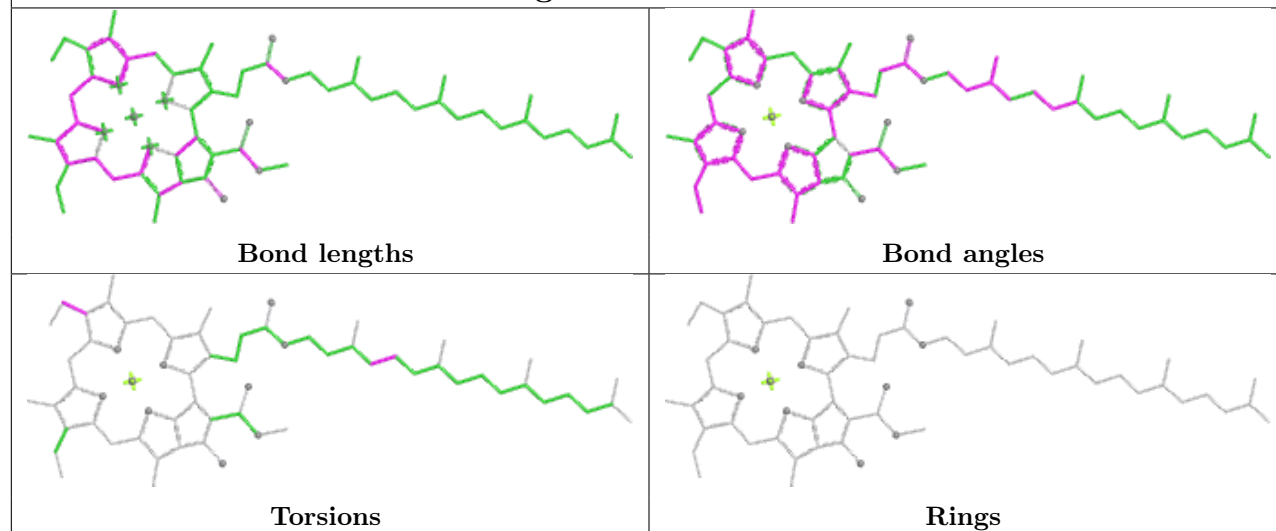




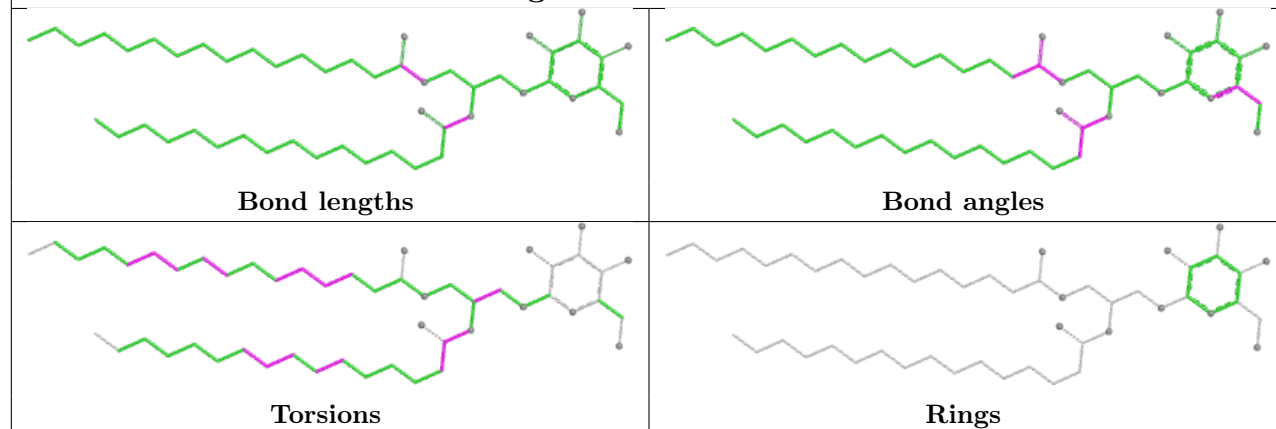




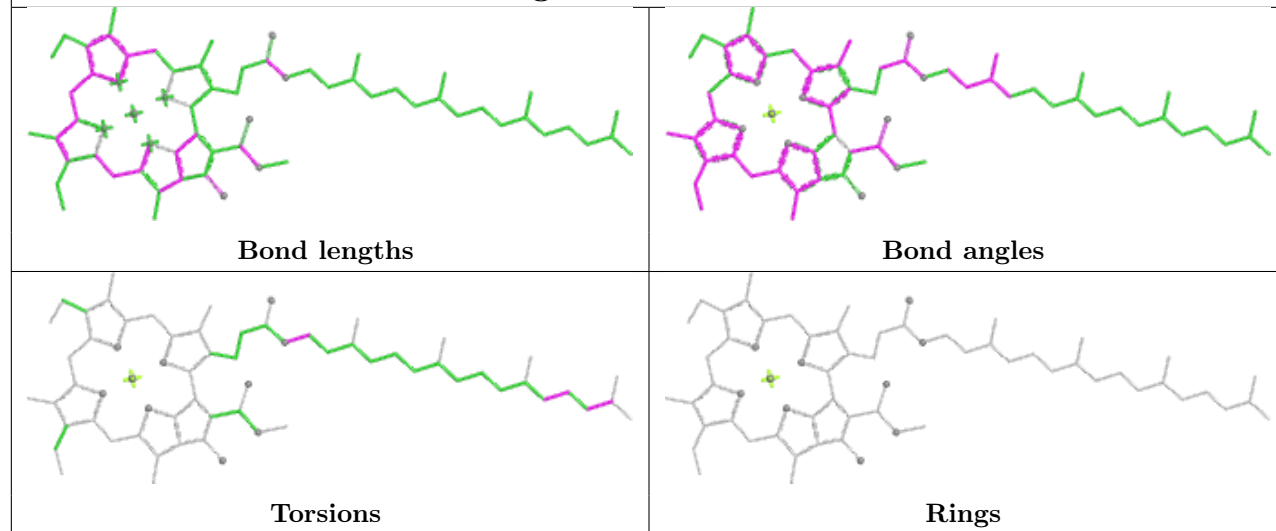
Ligand CLA b 607

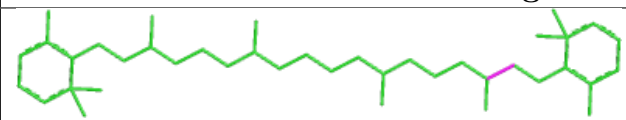
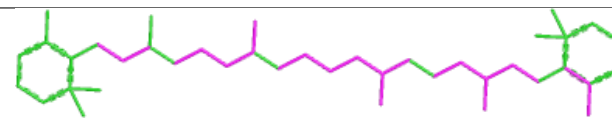
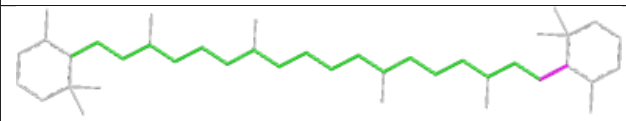
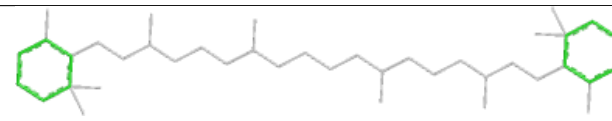


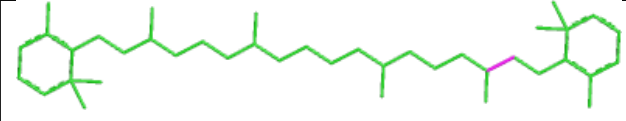
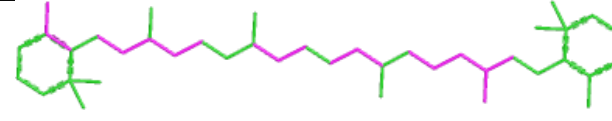
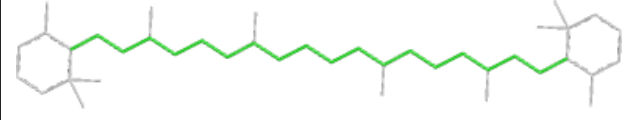
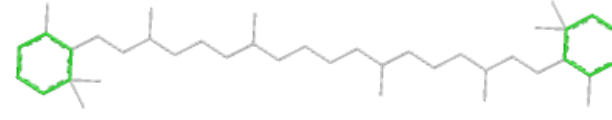
Ligand LMG C 520

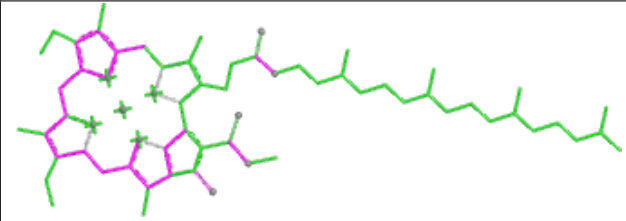
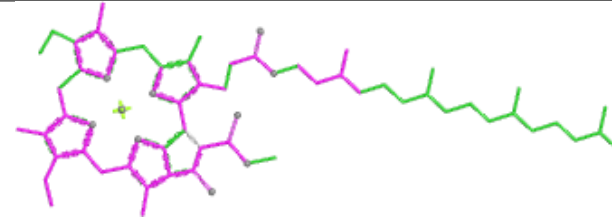
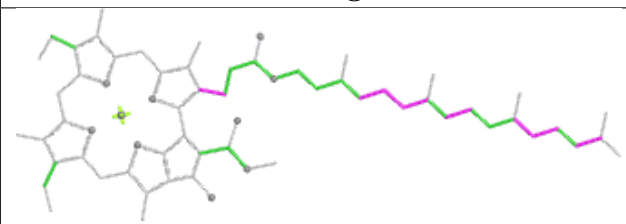
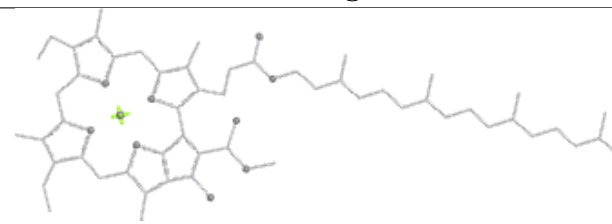


Ligand CLA B 608

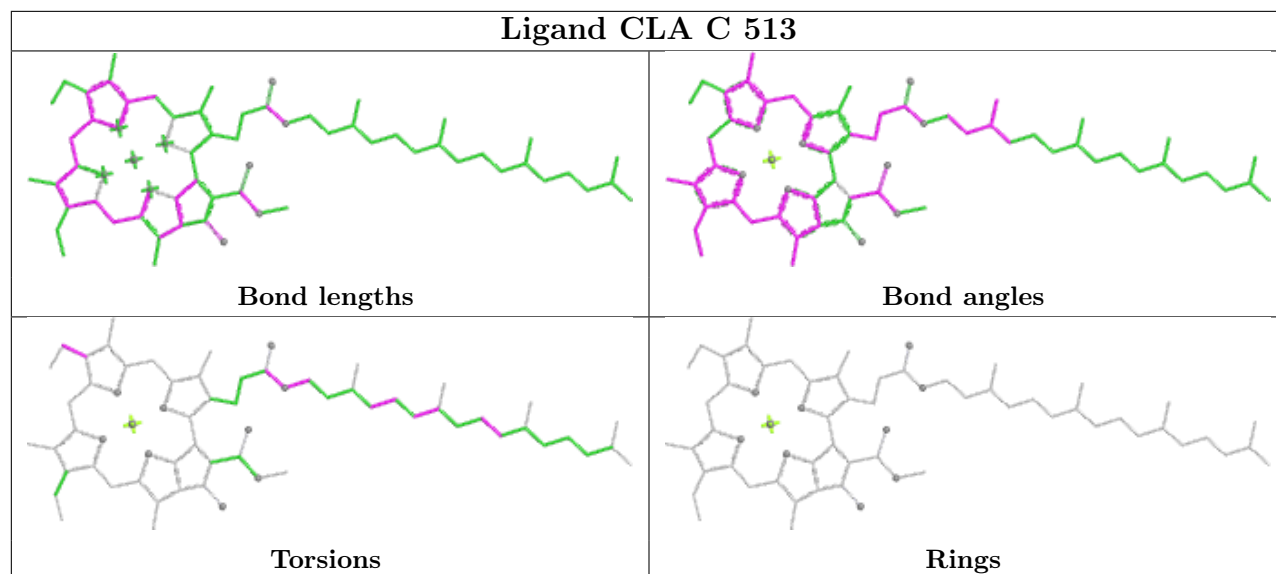


Ligand BCR h 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

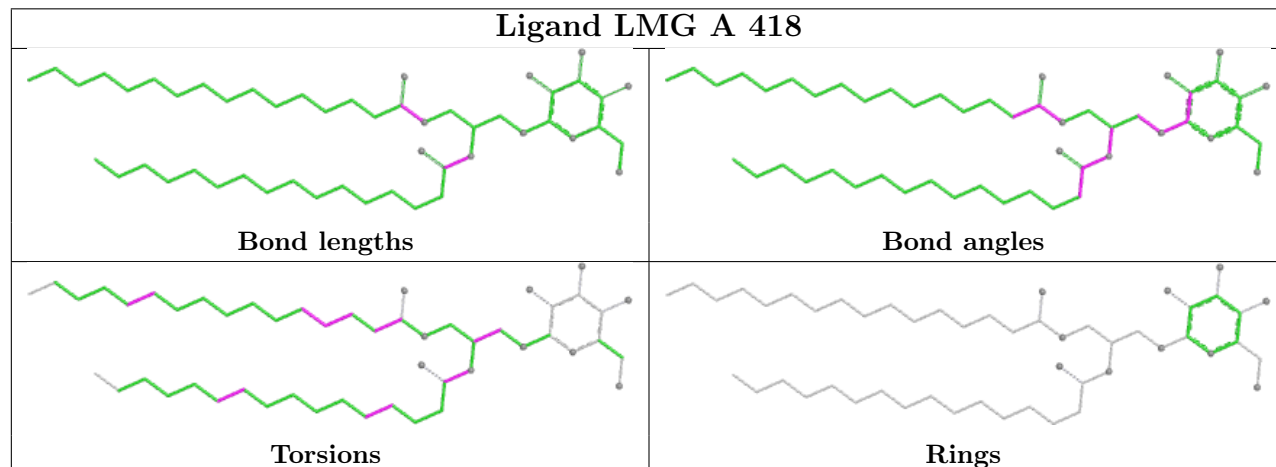
Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

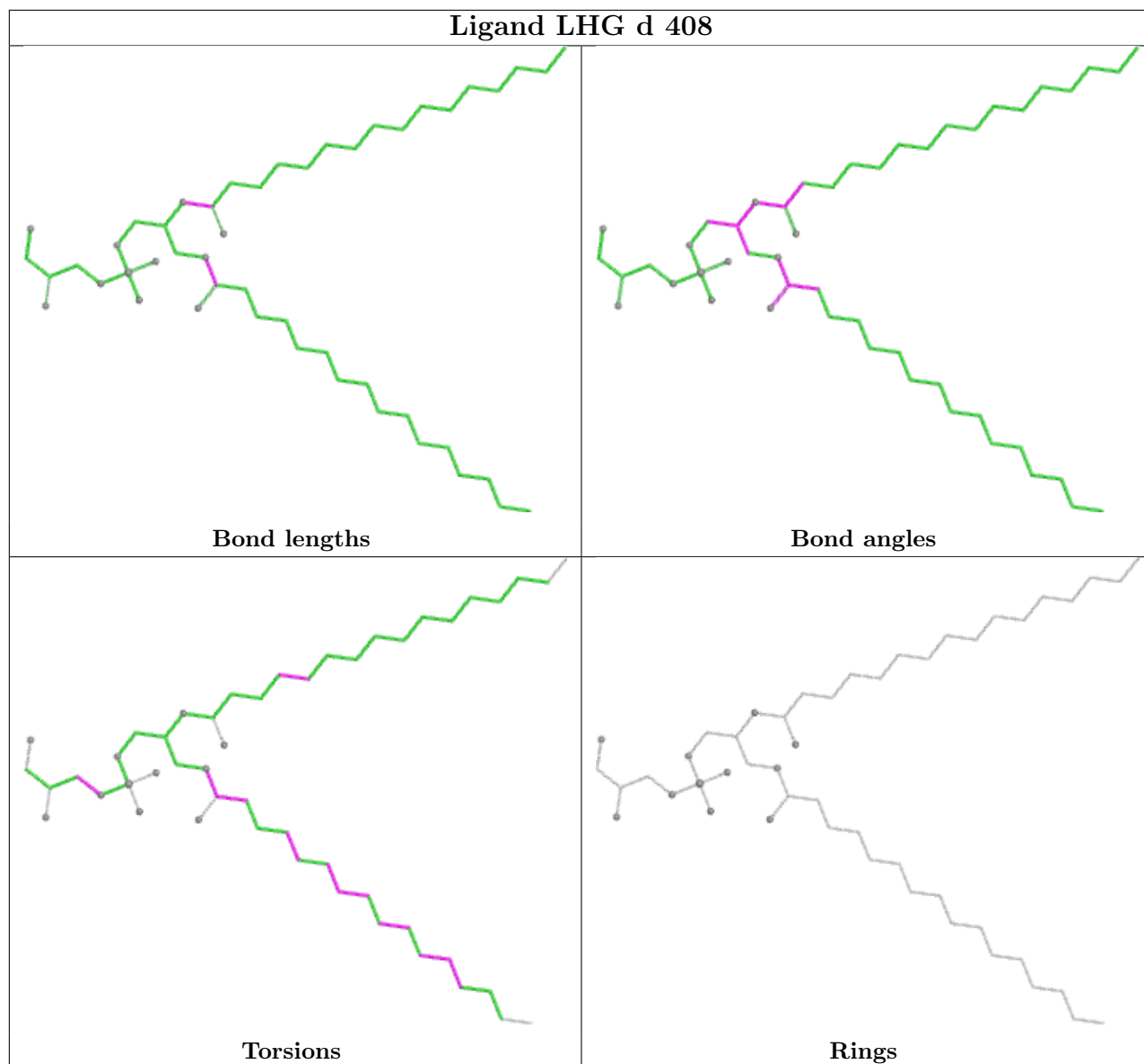
Ligand CLA C 513



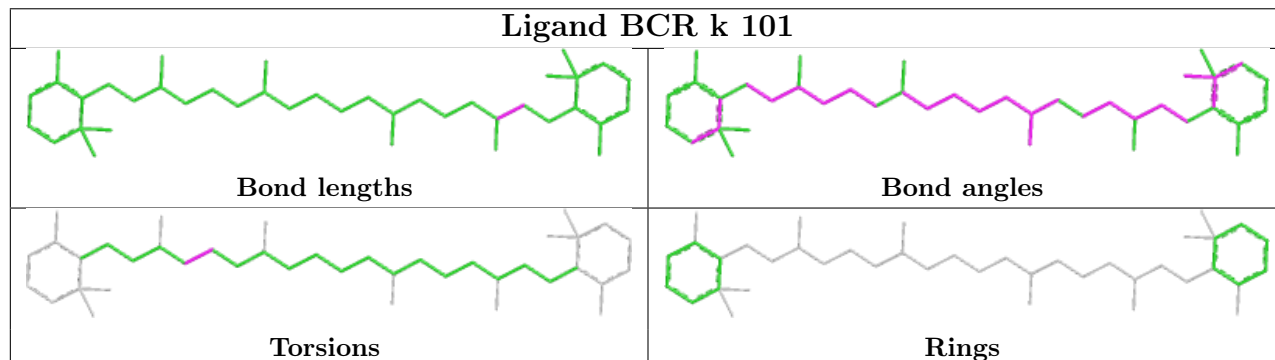
Ligand LMG A 418

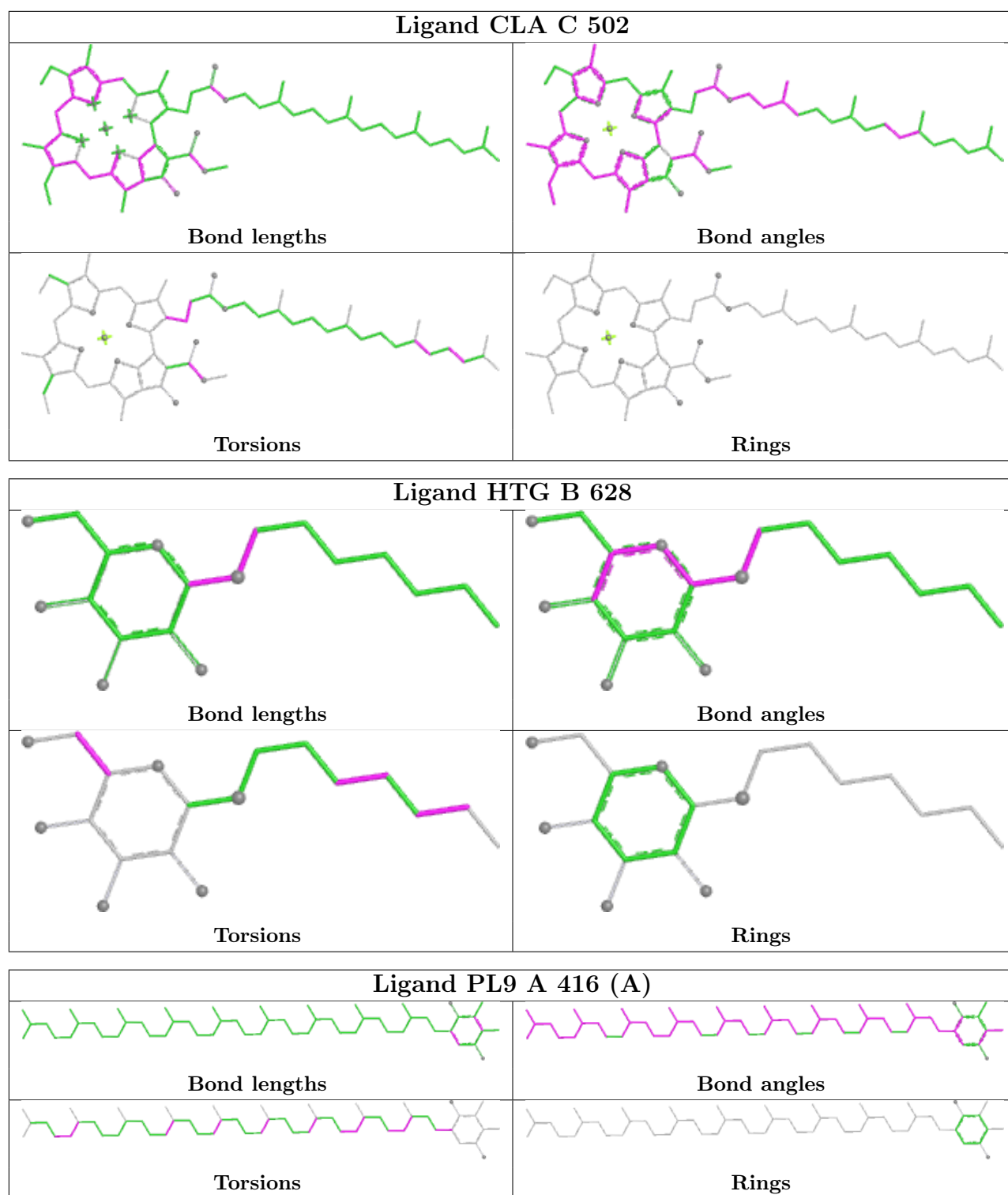


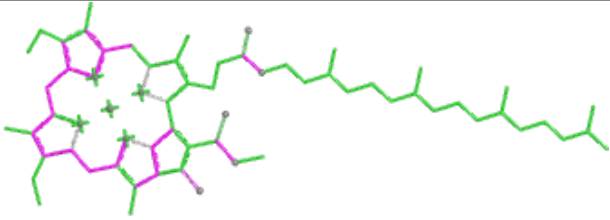
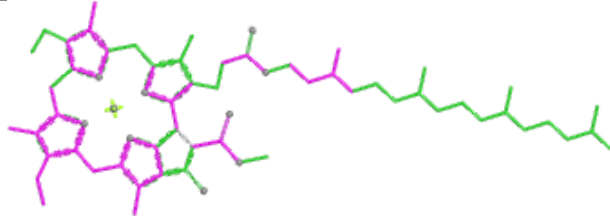
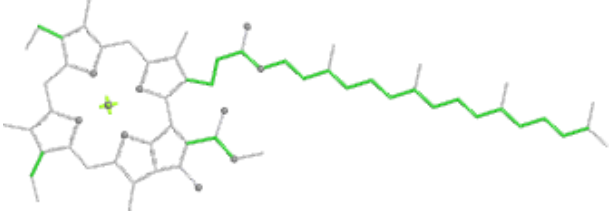
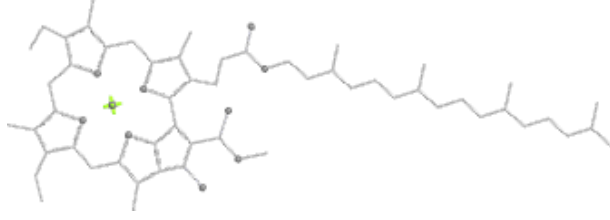
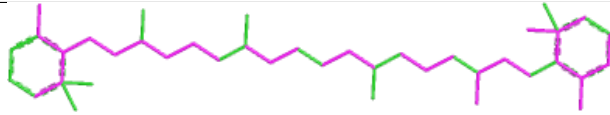
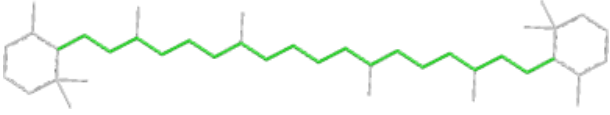
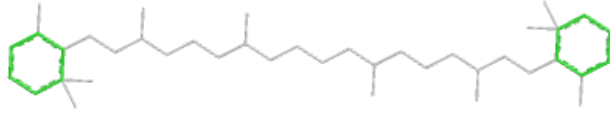
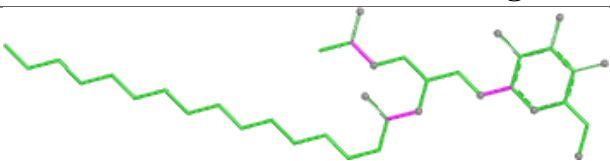
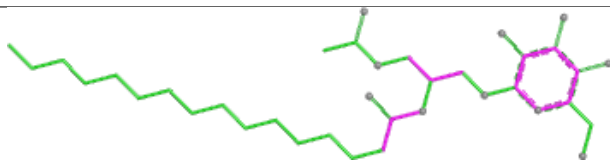
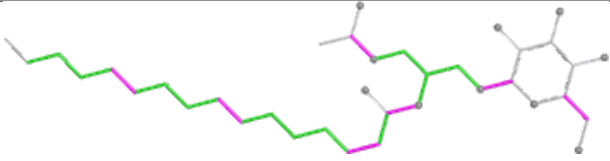
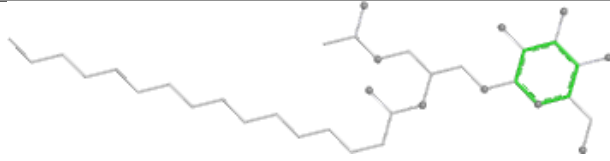
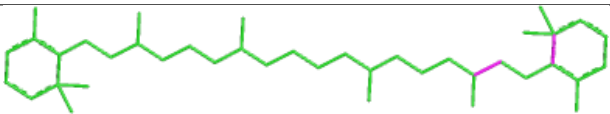
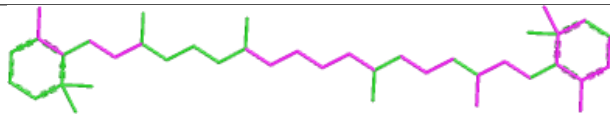
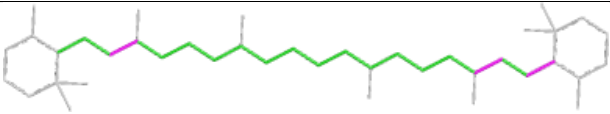
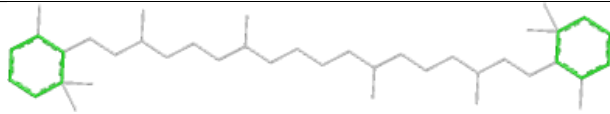
Ligand LHG d 408

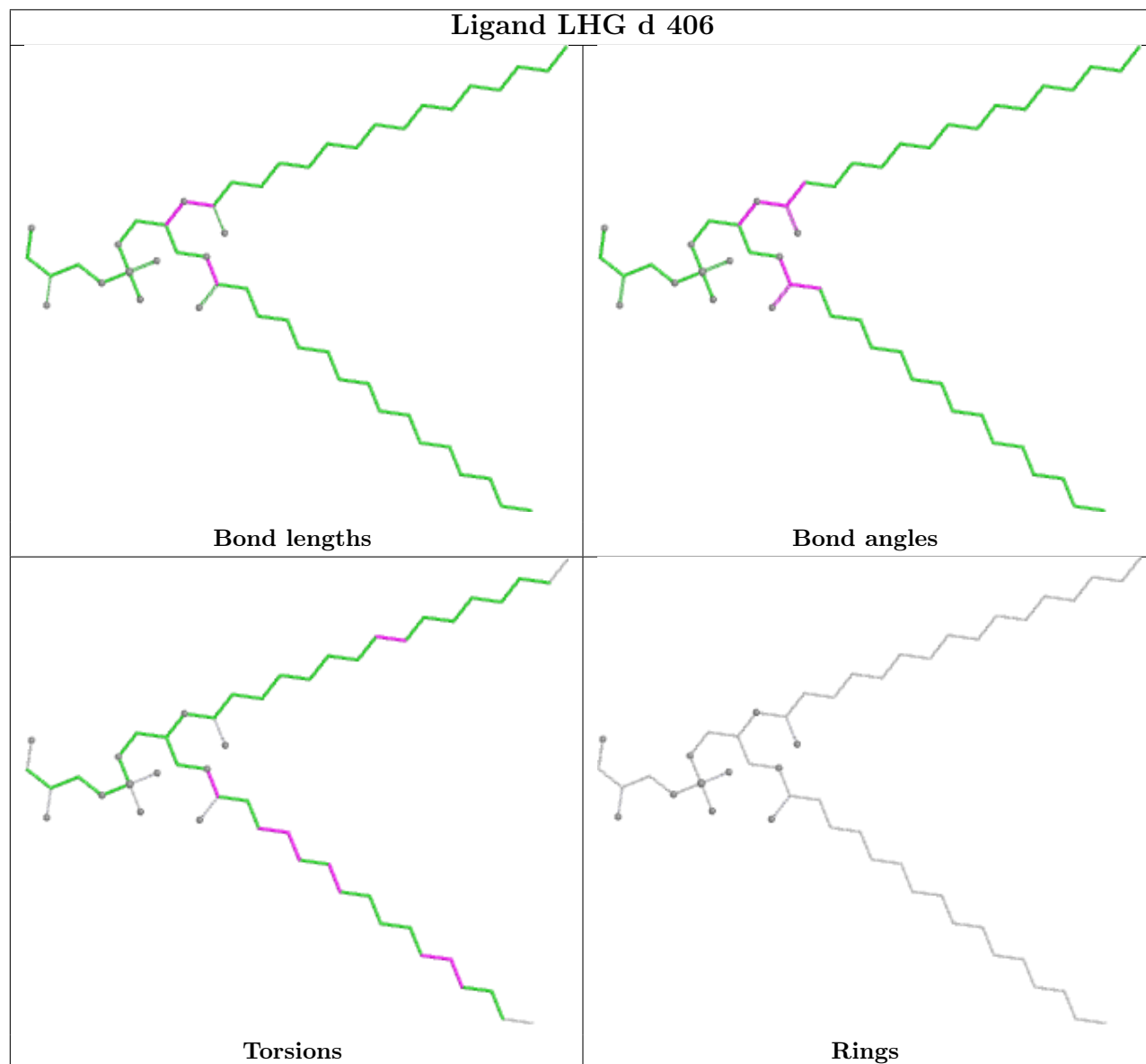
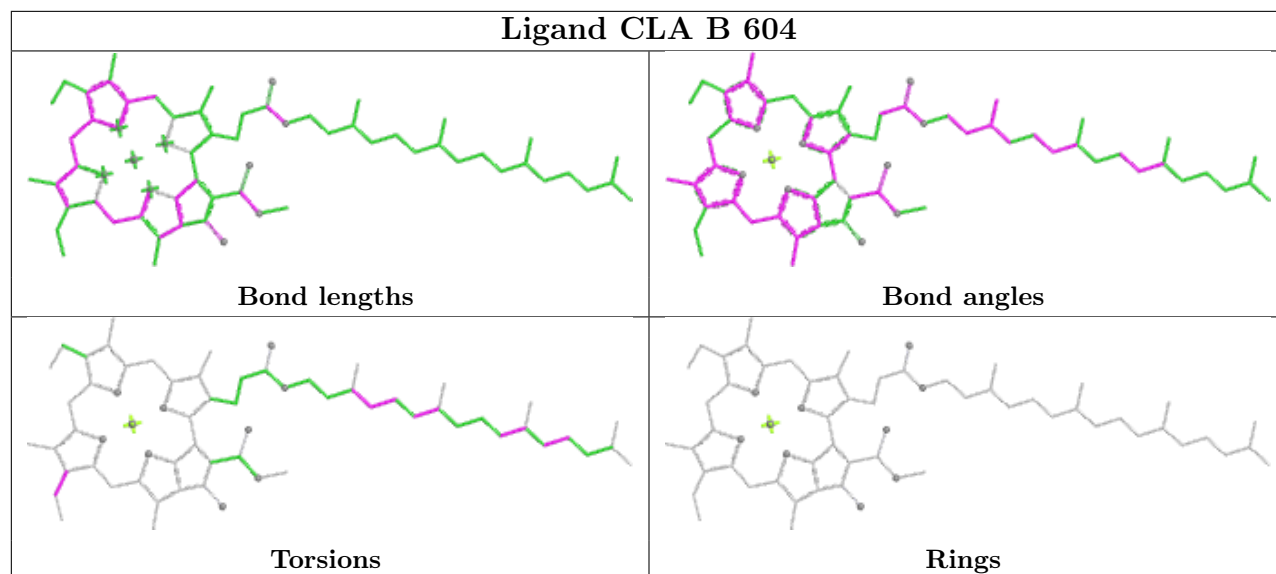


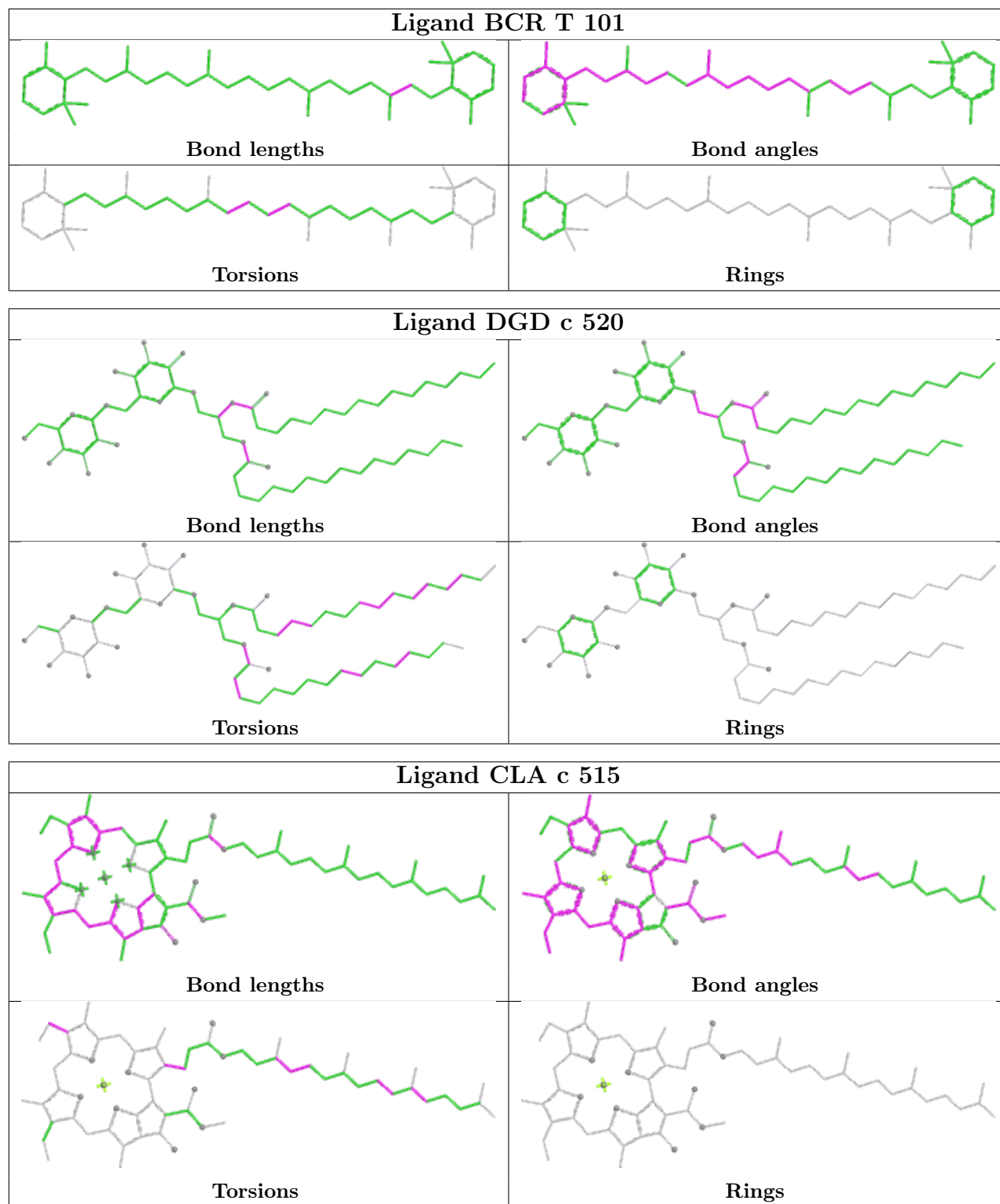
Ligand BCR k 101

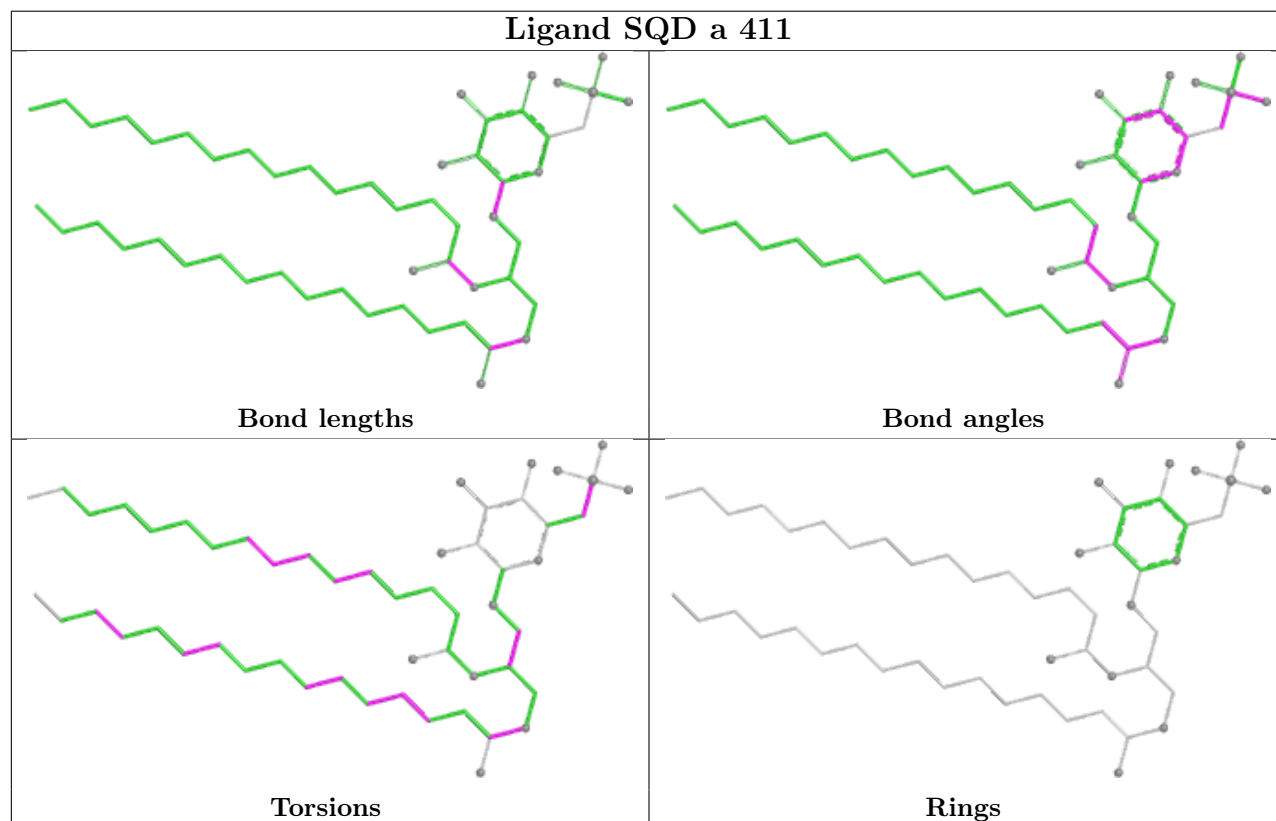
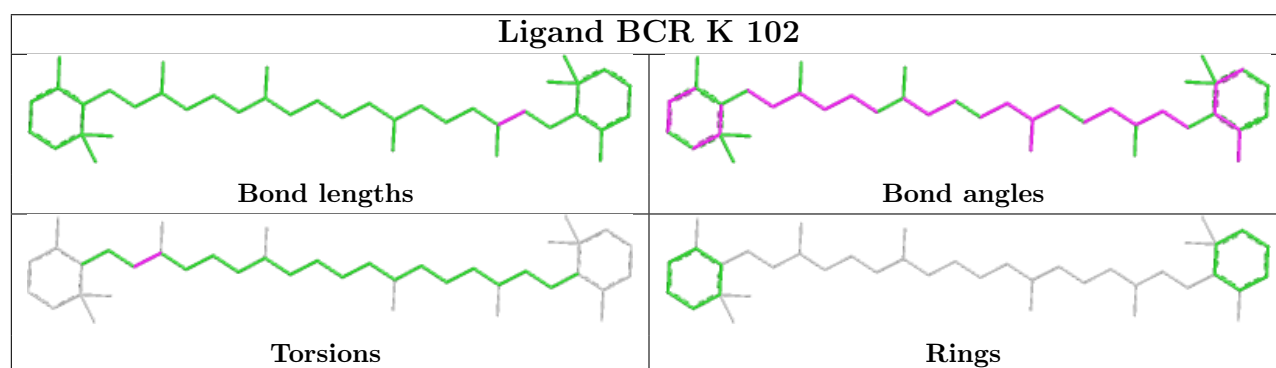
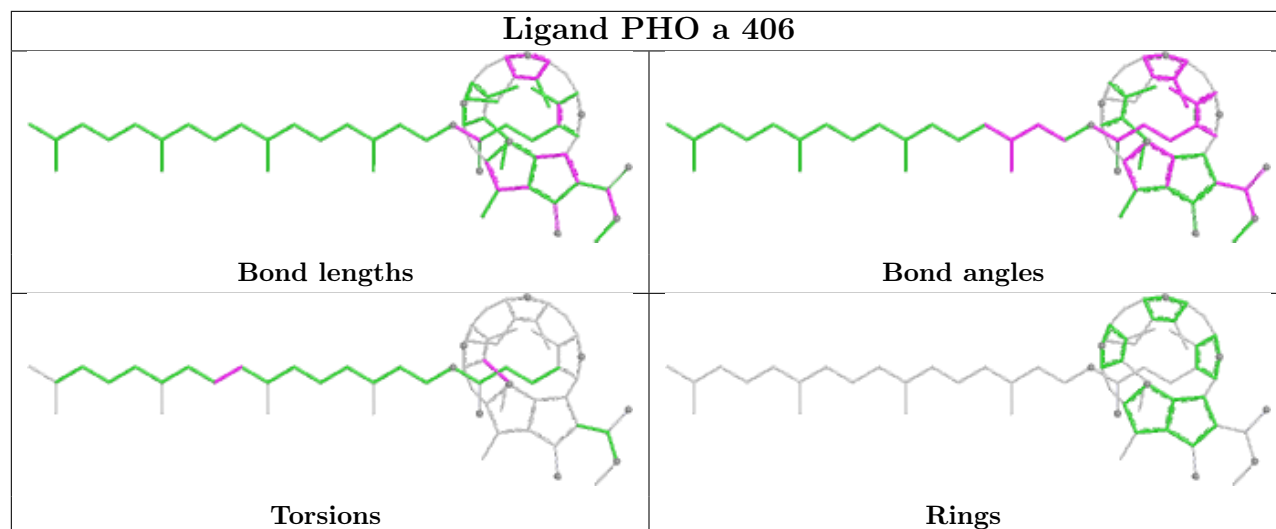


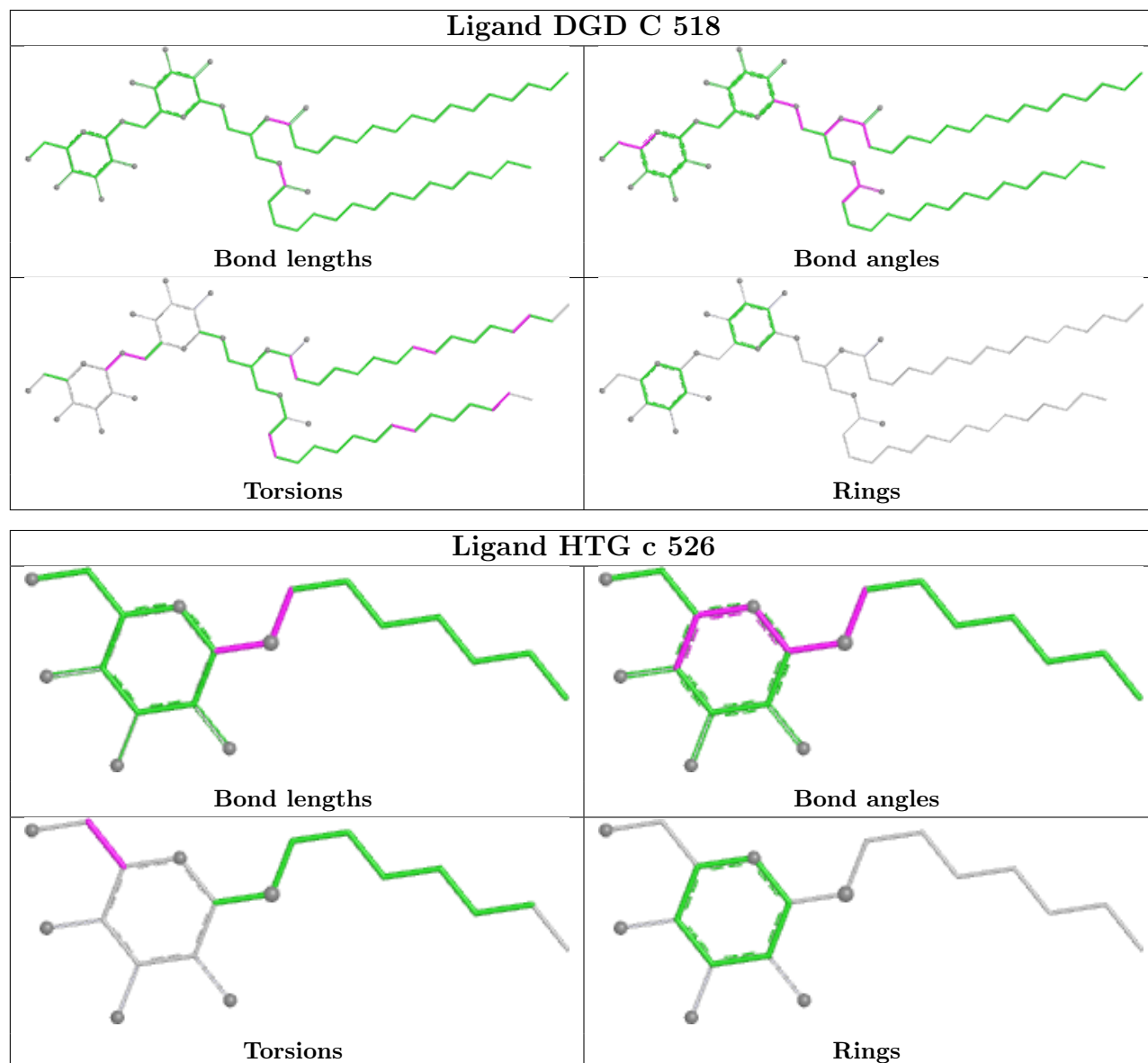


Ligand CLA c 505	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG Z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR d 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

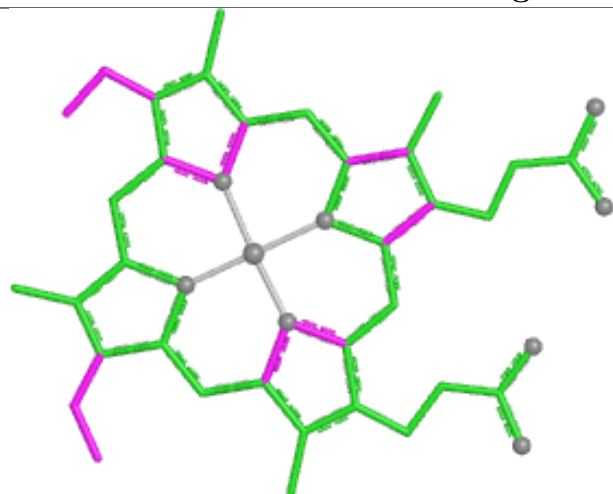




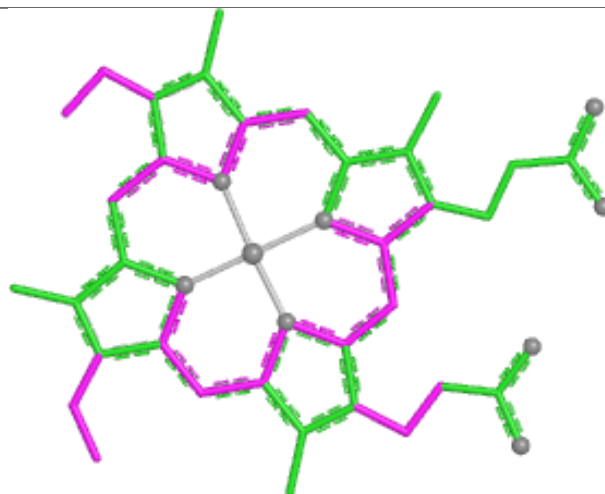




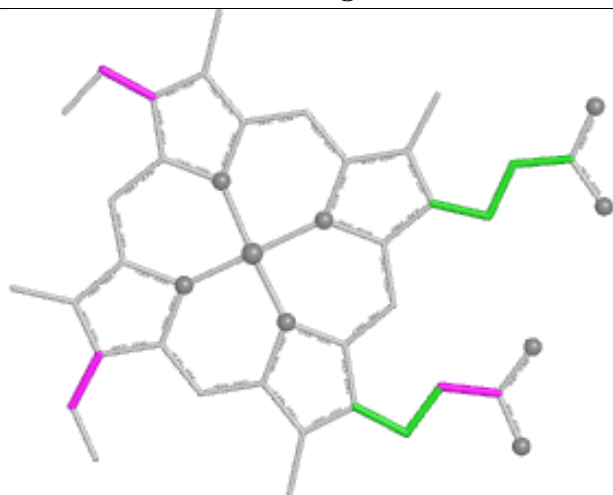
Ligand HEC V 203



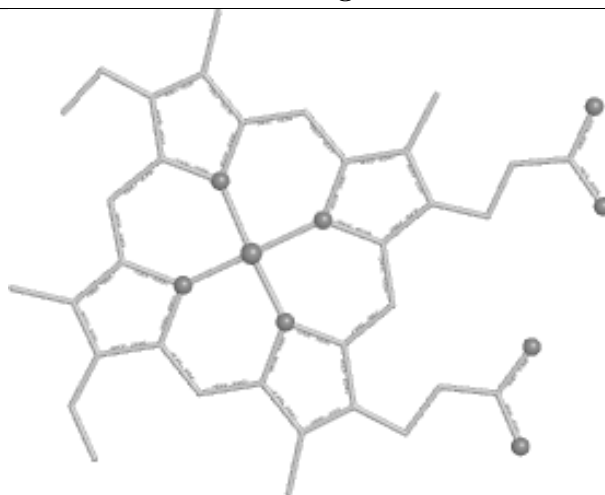
Bond lengths



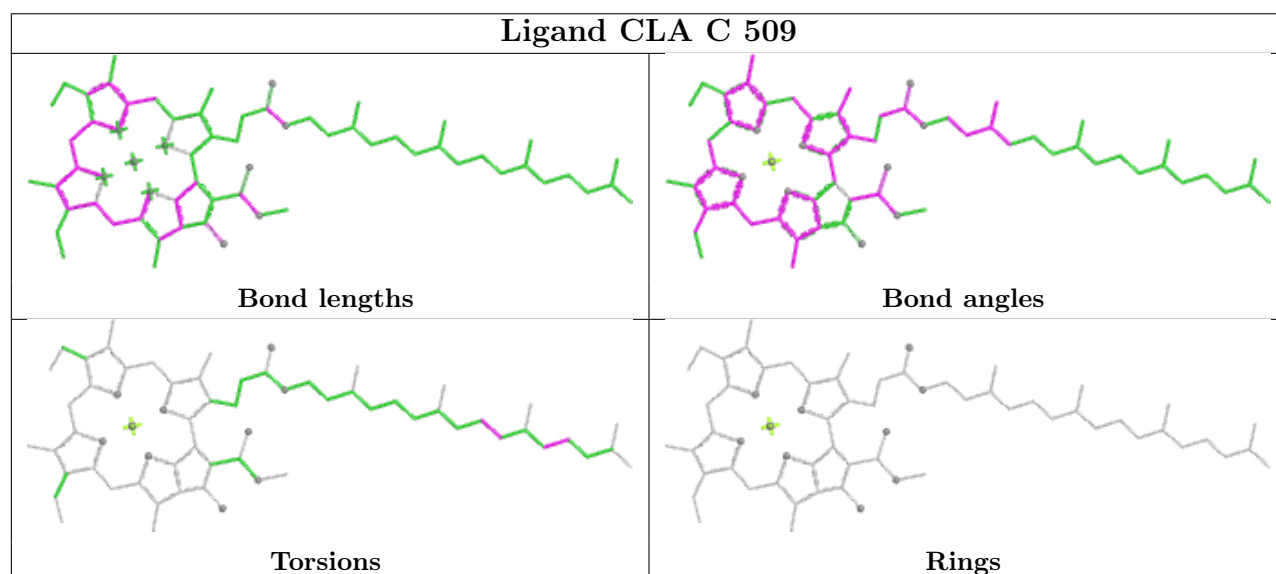
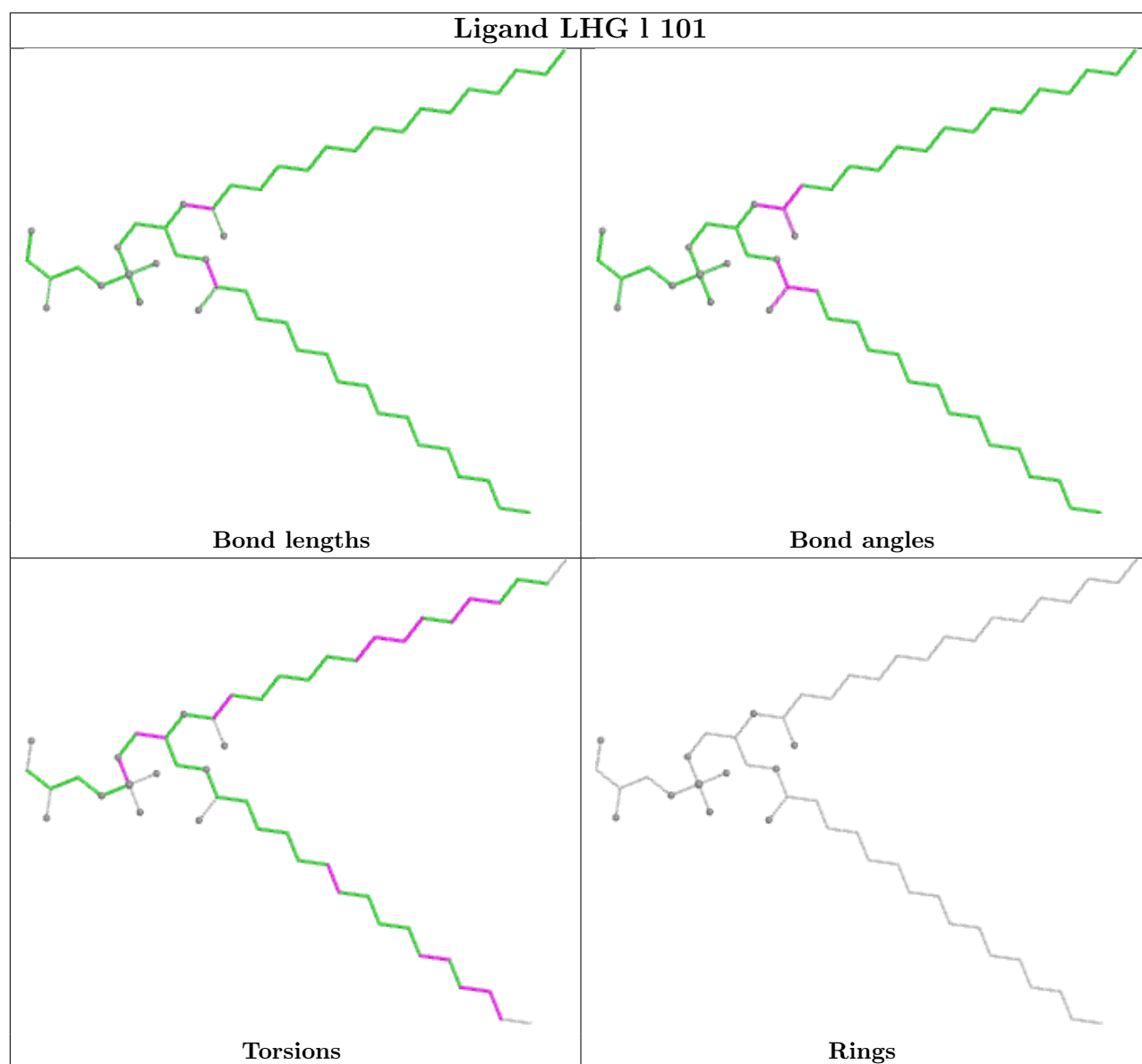
Bond angles

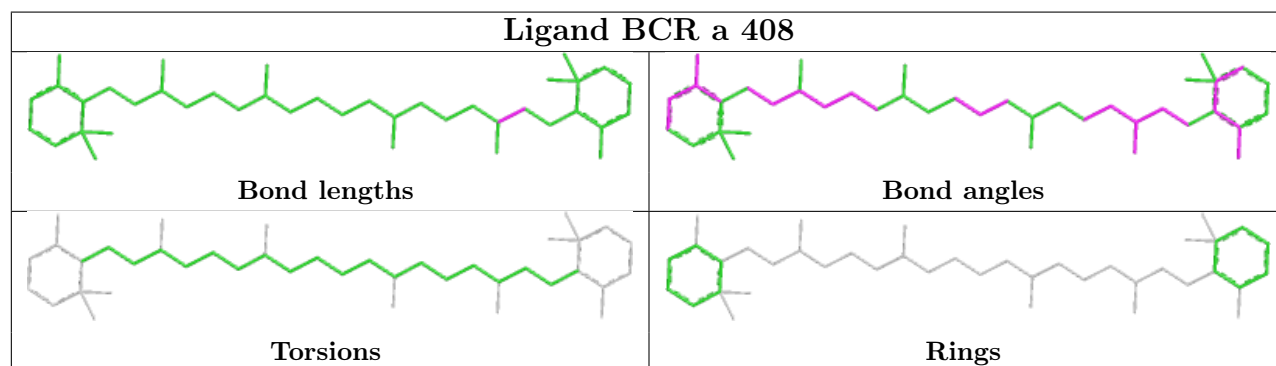
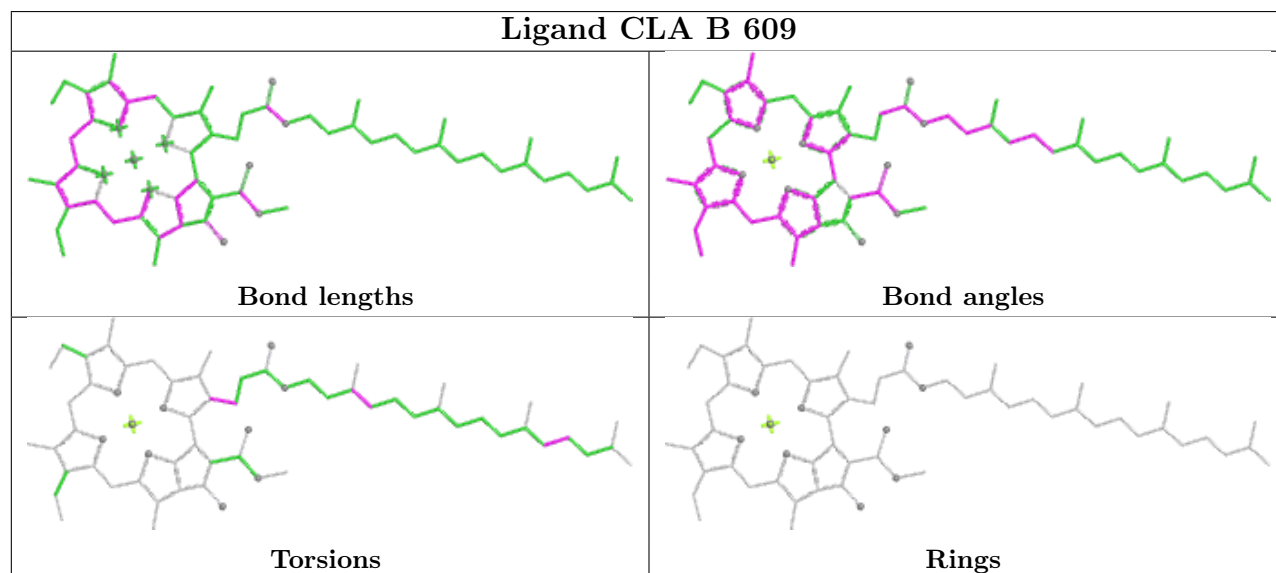
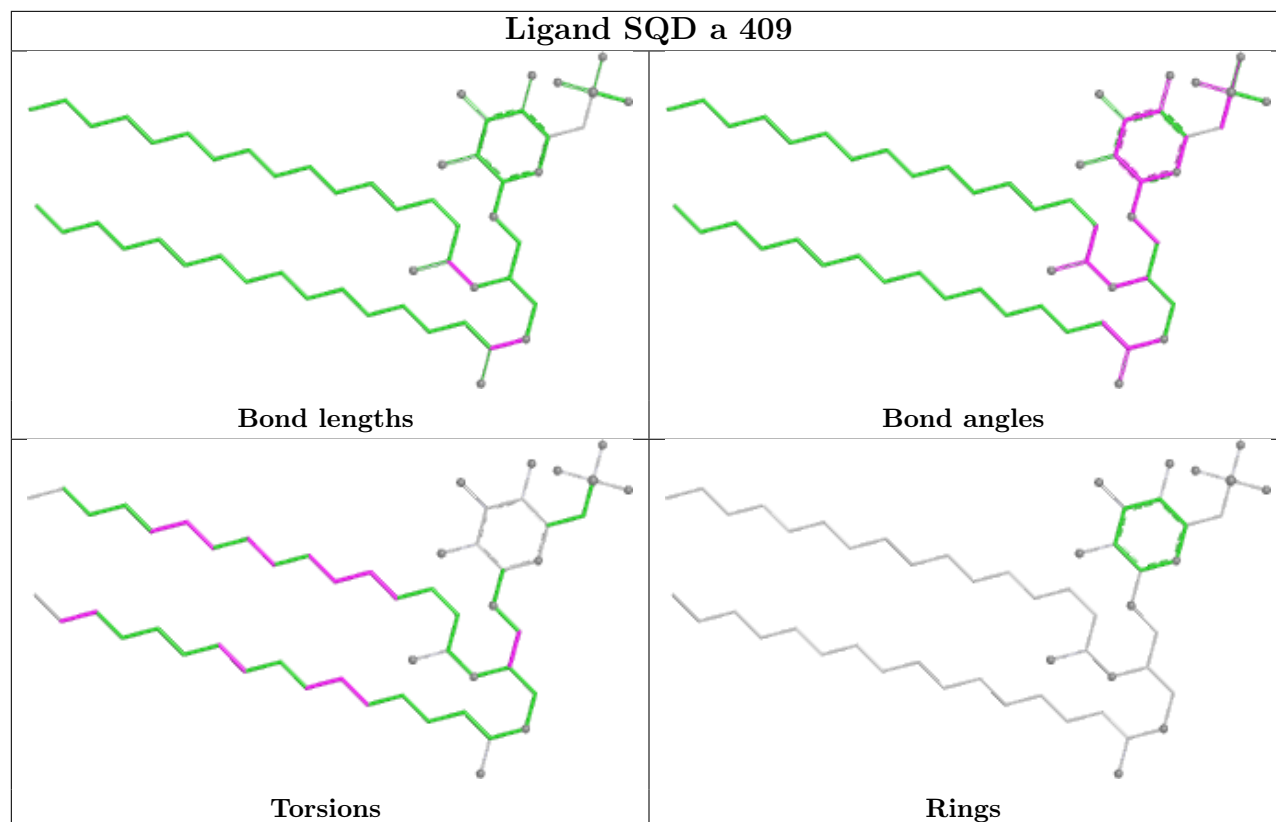


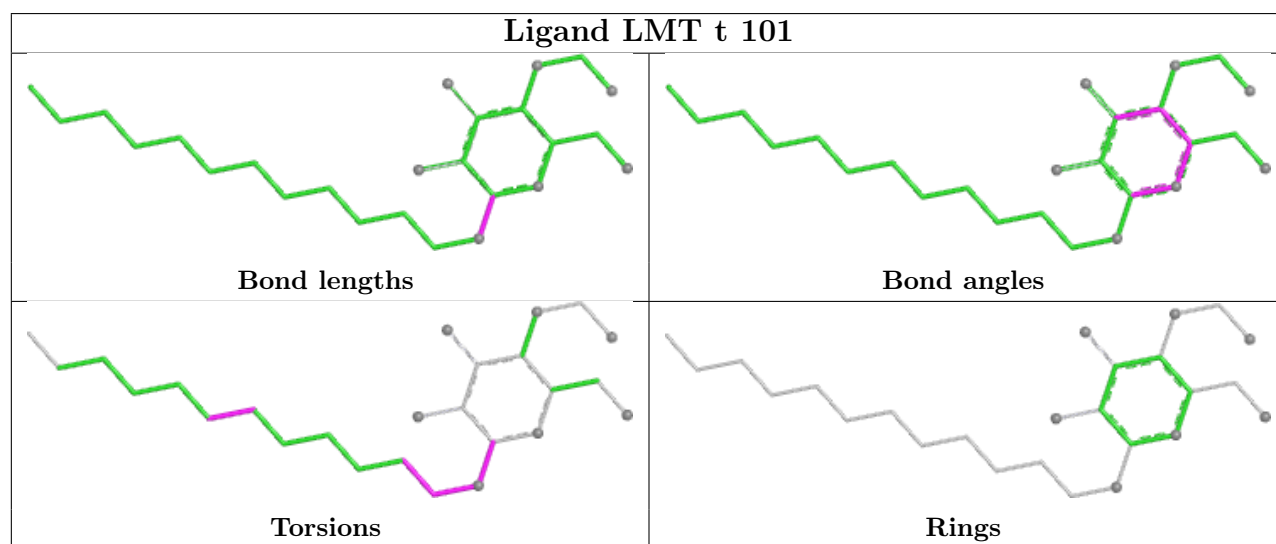
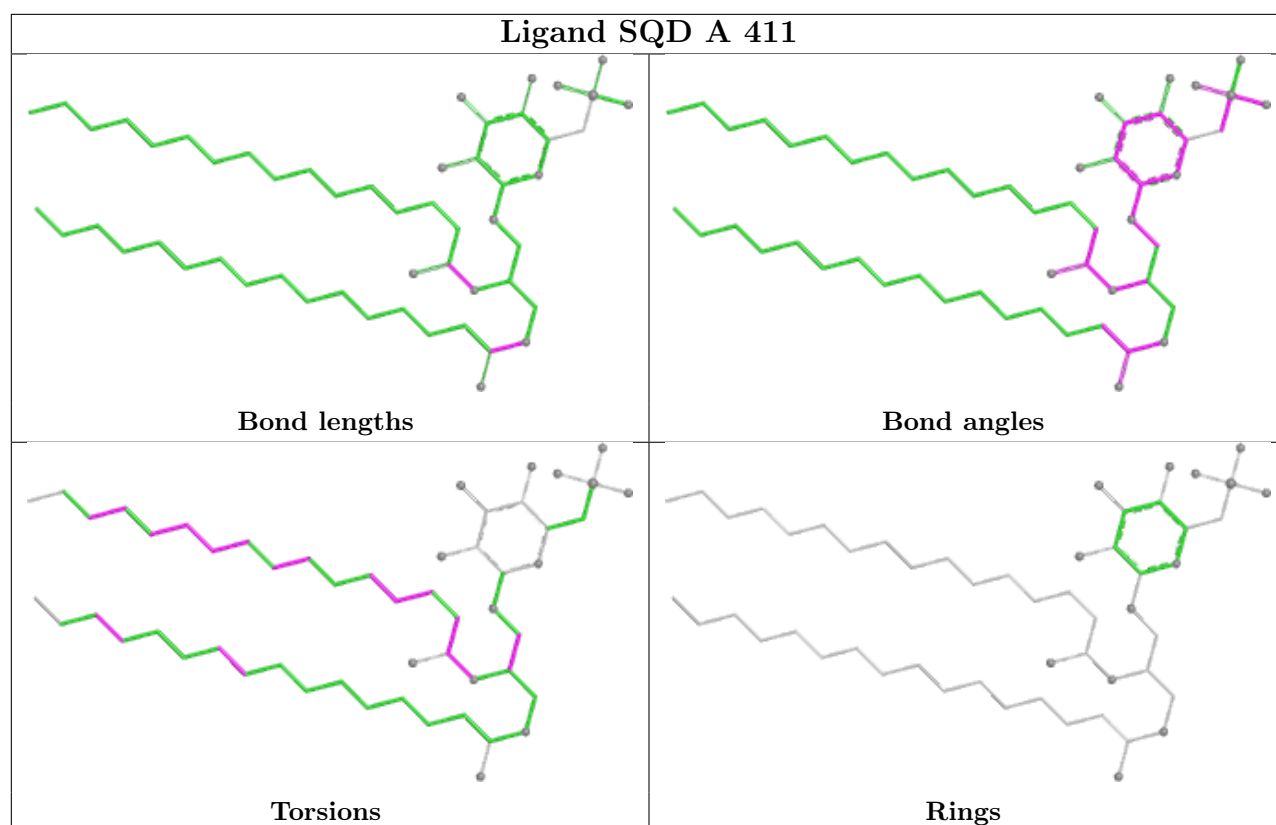
Torsions

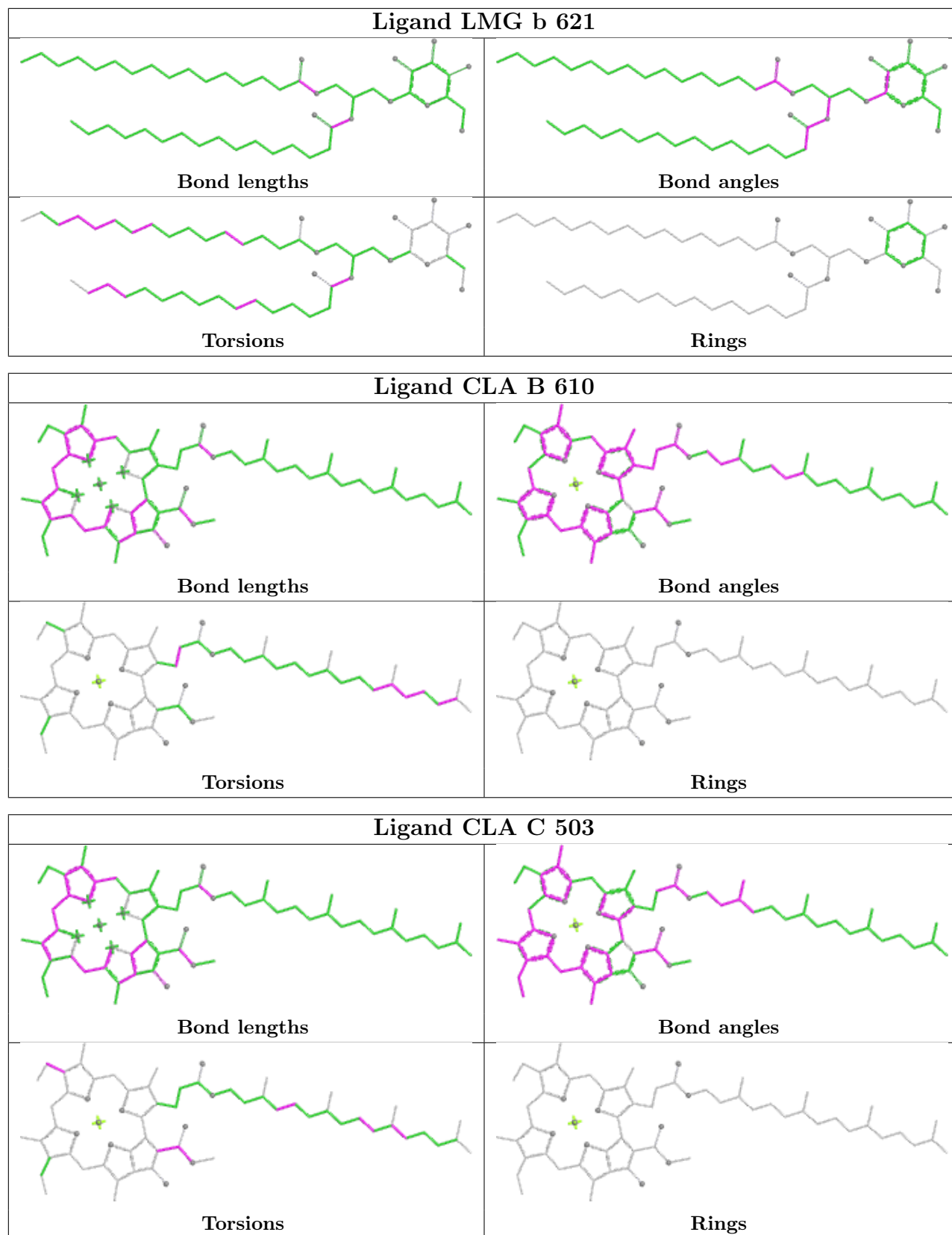


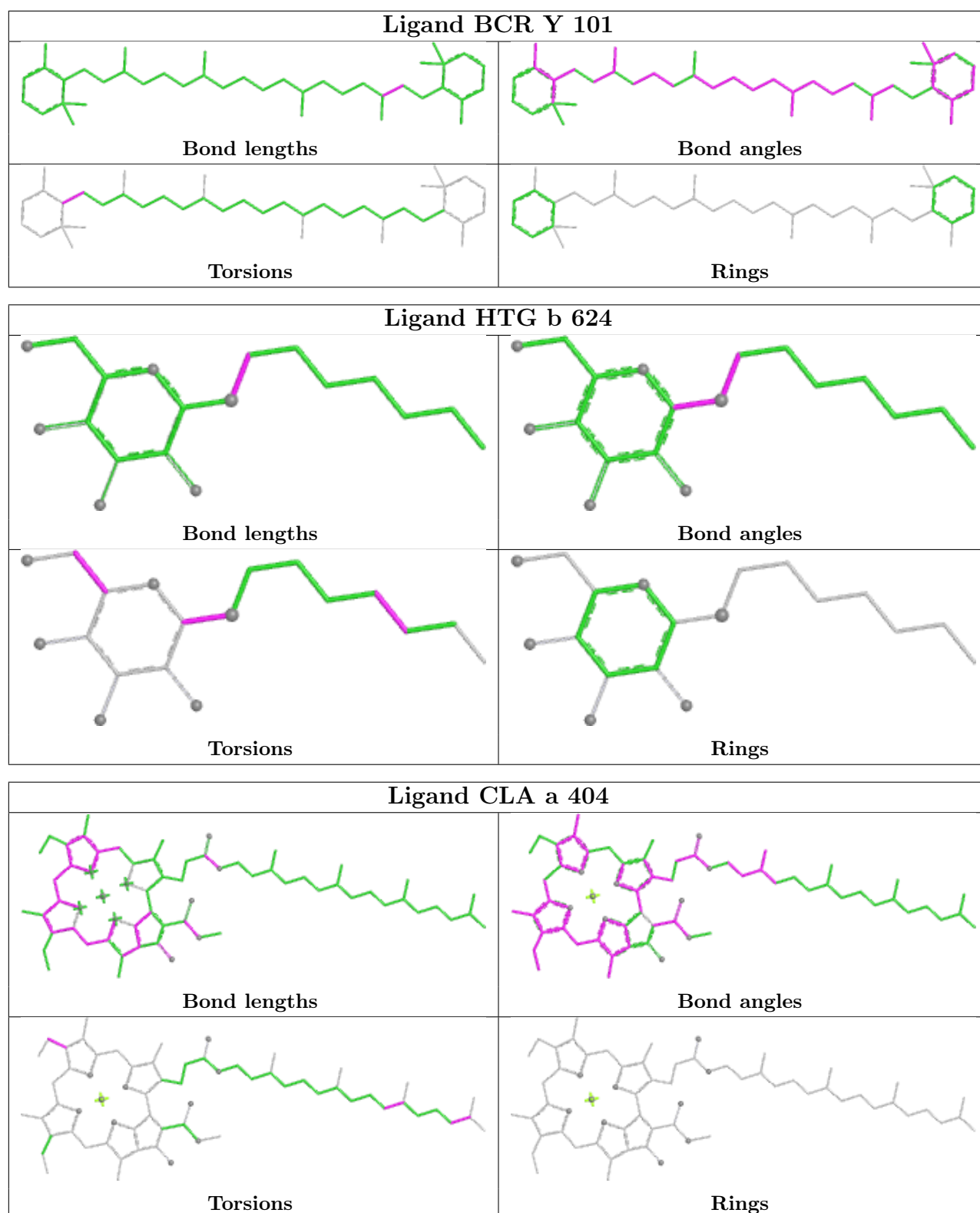
Rings











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.68	0 100 100	22, 47, 68, 120	29 (8%)
1	a	334/344 (97%)	-0.62	0 100 100	23, 51, 82, 120	29 (8%)
2	B	504/505 (99%)	-0.60	2 (0%) 88 91	30, 53, 83, 128	8 (1%)
2	b	504/505 (99%)	-0.53	2 (0%) 88 91	35, 57, 97, 149	4 (0%)
3	C	451/455 (99%)	-0.59	0 100 100	23, 59, 80, 142	10 (2%)
3	c	455/455 (100%)	-0.48	0 100 100	26, 67, 89, 129	10 (2%)
4	D	342/342 (100%)	-0.73	0 100 100	23, 49, 68, 139	3 (0%)
4	d	341/342 (99%)	-0.67	0 100 100	24, 55, 78, 147	3 (0%)
5	E	81/84 (96%)	-0.23	0 100 100	53, 70, 100, 151	1 (1%)
5	e	79/84 (94%)	-0.12	1 (1%) 75 79	62, 78, 122, 140	0
6	F	34/44 (77%)	-0.46	0 100 100	52, 63, 90, 117	0
6	f	31/44 (70%)	-0.22	2 (6%) 25 28	62, 68, 100, 140	0
7	H	64/65 (98%)	-0.44	1 (1%) 70 76	33, 62, 81, 129	1 (1%)
7	h	64/65 (98%)	-0.37	1 (1%) 70 76	58, 69, 95, 147	0
8	I	37/38 (97%)	-0.30	0 100 100	55, 62, 127, 147	0
8	i	37/38 (97%)	-0.24	1 (2%) 56 63	57, 66, 123, 138	0
9	J	38/39 (97%)	-0.20	0 100 100	51, 71, 129, 175	0
9	j	39/39 (100%)	0.00	0 100 100	56, 80, 149, 175	0
10	K	37/37 (100%)	-0.43	0 100 100	60, 67, 89, 101	0
10	k	37/37 (100%)	-0.34	0 100 100	70, 77, 101, 117	0
11	L	36/37 (97%)	-0.60	0 100 100	27, 47, 109, 162	1 (2%)
11	l	36/37 (97%)	-0.64	0 100 100	28, 48, 103, 152	1 (2%)
12	M	32/36 (88%)	-0.55	0 100 100	28, 49, 74, 134	1 (3%)
12	m	33/36 (91%)	-0.58	0 100 100	43, 50, 86, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.47	0 100 100	36, 63, 115, 176	5 (2%)
13	o	243/244 (99%)	-0.44	0 100 100	34, 65, 121, 161	2 (0%)
14	T	29/32 (90%)	-0.65	1 (3%) 48 55	42, 49, 81, 115	0
14	t	29/32 (90%)	-0.64	1 (3%) 48 55	43, 50, 81, 130	0
15	U	96/104 (92%)	-0.62	0 100 100	47, 60, 90, 101	0
15	u	97/104 (93%)	-0.62	0 100 100	51, 62, 84, 121	0
16	V	137/137 (100%)	-0.66	0 100 100	46, 57, 82, 112	0
16	v	137/137 (100%)	-0.48	0 100 100	52, 71, 104, 137	0
17	X	38/40 (95%)	-0.23	0 100 100	59, 71, 96, 126	0
17	x	38/40 (95%)	0.00	0 100 100	65, 78, 117, 154	0
18	Y	29/30 (96%)	0.27	0 100 100	73, 87, 140, 155	0
18	y	29/30 (96%)	0.18	1 (3%) 48 55	79, 97, 126, 136	0
19	Z	62/62 (100%)	-0.11	0 100 100	67, 84, 131, 173	0
19	z	62/62 (100%)	0.31	1 (1%) 70 76	83, 99, 148, 185	0
20	R	34/34 (100%)	1.17	4 (11%) 9 10	97, 125, 149, 154	0
All	All	5283/5384 (98%)	-0.51	18 (0%) 90 92	22, 59, 104, 185	108 (2%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	5.1
7	h	65	LEU	4.4
2	b	502	VAL	3.2
14	t	30	THR	2.7
2	B	494	GLY	2.7
20	R	28	VAL	2.6
14	T	30	THR	2.6
20	R	24	LEU	2.5
8	i	37	LEU	2.4
2	B	495	PHE	2.3
5	e	79	PHE	2.3
2	b	495	PHE	2.2
6	f	15	ILE	2.2
18	y	18	VAL	2.2
19	z	3	ILE	2.1
20	R	35	LEU	2.1
6	f	16	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
20	R	3	TRP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.96	0.08	44,50,74,88	0
12	FME	m	1	10/11	0.96	0.08	47,60,91,103	0
12	FME	M	1	10/11	0.97	0.09	34,56,91,100	0
14	FME	t	1	10/11	0.97	0.07	43,51,75,84	0
8	FME	i	1	10/11	0.98	0.06	59,64,77,78	0
8	FME	I	1	10/11	0.98	0.06	46,65,76,76	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(Å ²)	Q<0.9
35	HTG	c	523	19/19	0.74	0.14	118,144,148,169	0
34	LMT	e	101	35/35	0.75	0.15	121,166,181,186	0
34	LMT	a	418	35/35	0.78	0.15	113,136,151,151	0
32	UNL	i	101	40/-	0.78	0.15	77,109,164,165	0
35	HTG	C	522	19/19	0.78	0.14	112,123,133,150	0
34	LMT	A	359	35/35	0.78	0.15	73,134,144,148	0
35	HTG	c	526	19/19	0.78	0.13	114,161,170,200	0
34	LMT	E	102	35/35	0.79	0.15	119,145,171,173	0
32	UNL	a	415	30/-	0.79	0.16	98,115,136,146	0
32	UNL	K	101	34/-	0.80	0.14	83,119,134,150	0
27	SQD	f	101	43/54	0.80	0.14	118,136,170,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	UNL	A	417	28/-	0.80	0.16	98,110,128,144	0
32	UNL	j	102	10/-	0.80	0.15	87,106,117,118	0
32	UNL	m	101	10/-	0.80	0.12	69,78,80,84	0
32	UNL	J	102	10/-	0.80	0.16	77,81,99,104	0
32	UNL	c	527	32/-	0.81	0.15	93,125,140,143	0
35	HTG	b	624	19/19	0.81	0.18	114,128,145,170	0
34	LMT	a	359	35/35	0.81	0.15	65,144,151,154	0
34	LMT	I	101	35/35	0.81	0.14	110,145,160,162	0
37	CA	b	626	1/1	0.81	0.08	151,151,151,151	0
32	UNL	I	102	40/-	0.82	0.15	66,113,156,158	0
38	LHG	a	419	42/49	0.82	0.11	78,141,167,179	0
33	LMG	C	521	51/55	0.83	0.13	68,121,155,157	0
35	HTG	B	624	19/19	0.83	0.16	71,103,114,115	0
34	LMT	b	622	25/35	0.84	0.12	88,117,159,160	0
35	HTG	B	625	19/19	0.84	0.13	82,167,178,238	0
32	UNL	b	629	33/-	0.84	0.14	72,108,162,162	0
35	HTG	h	101	16/19	0.84	0.14	98,133,140,163	0
35	HTG	C	523	19/19	0.84	0.12	84,153,166,186	0
35	HTG	D	410	16/19	0.84	0.12	82,121,136,138	0
35	HTG	b	625	19/19	0.85	0.13	91,138,154,196	0
32	UNL	D	409	40/-	0.85	0.12	67,93,136,140	0
31	PL9	A	416[A]	55/55	0.86	0.14	66,93,107,111	55
34	LMT	M	103	35/35	0.86	0.11	68,146,169,171	0
33	LMG	c	522	51/55	0.86	0.11	80,127,154,158	0
31	PL9	A	416[B]	55/55	0.86	0.14	66,93,108,113	55
34	LMT	B	622	35/35	0.86	0.13	78,125,142,144	0
32	UNL	d	410	36/-	0.86	0.12	73,100,136,140	0
33	LMG	Z	101	37/55	0.87	0.13	77,129,150,151	0
33	LMG	z	101	39/55	0.88	0.12	84,133,148,153	0
28	GOL	a	410	6/6	0.88	0.12	79,81,90,95	0
34	LMT	t	101	26/35	0.88	0.11	71,110,152,153	0
27	SQD	a	411	54/54	0.88	0.10	72,95,139,149	0
38	LHG	E	101	42/49	0.88	0.11	72,118,132,132	0
27	SQD	F	101	43/54	0.88	0.12	81,114,134,137	0
35	HTG	V	204	11/19	0.89	0.12	104,117,122,125	0
28	GOL	c	502	6/6	0.89	0.19	68,70,71,75	0
32	UNL	B	629	33/-	0.89	0.12	57,103,166,173	0
35	HTG	B	623	19/19	0.89	0.12	70,88,128,128	0
28	GOL	v	202	6/6	0.89	0.11	75,86,94,96	0
33	LMG	A	418	51/55	0.89	0.11	61,97,118,121	0
32	UNL	M	102	10/-	0.89	0.09	62,72,86,92	0
34	LMT	B	630	25/35	0.89	0.12	54,89,147,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	LMT	b	630	25/35	0.89	0.12	57,81,151,153	0
28	GOL	B	627	6/6	0.90	0.14	58,77,85,87	0
27	SQD	B	620	54/54	0.90	0.10	65,93,132,134	0
28	GOL	a	416	6/6	0.90	0.21	55,82,84,86	0
28	GOL	b	627	6/6	0.90	0.12	97,106,113,116	0
27	SQD	b	620	54/54	0.90	0.10	68,93,144,152	0
27	SQD	A	413	54/54	0.90	0.10	63,91,128,137	0
28	GOL	A	412	6/6	0.91	0.12	80,82,86,98	0
24	CLA	B	601	65/65	0.91	0.10	53,77,112,132	0
33	LMG	a	417	51/55	0.91	0.10	76,100,122,129	0
24	CLA	c	515	65/65	0.91	0.10	70,91,134,138	0
37	CA	V	201	1/1	0.91	0.14	141,141,141,141	0
34	LMT	m	102	35/35	0.91	0.11	63,95,117,121	0
37	CA	v	201	1/1	0.91	0.13	123,123,123,123	0
31	PL9	a	414[A]	55/55	0.91	0.16	97,107,120,124	55
31	PL9	a	414[B]	55/55	0.91	0.16	97,107,120,124	55
34	LMT	M	101	35/35	0.92	0.10	61,99,123,126	0
24	CLA	b	601	65/65	0.92	0.10	58,85,115,130	0
33	LMG	c	521	51/55	0.92	0.09	68,101,145,156	0
33	LMG	C	520	51/55	0.92	0.09	56,90,127,140	0
35	HTG	b	623	19/19	0.92	0.11	68,88,130,131	0
28	GOL	V	202	6/6	0.93	0.11	64,74,85,92	0
24	CLA	c	514	65/65	0.93	0.09	59,80,123,128	0
35	HTG	B	628	19/19	0.93	0.08	65,80,89,95	0
24	CLA	C	514	65/65	0.93	0.09	60,81,122,127	0
28	GOL	C	525	6/6	0.93	0.12	66,73,76,78	0
32	UNL	D	408	17/-	0.93	0.09	66,85,107,110	0
26	BCR	d	404	40/40	0.94	0.08	53,67,96,98	0
24	CLA	C	507	65/65	0.94	0.09	53,69,137,141	0
37	CA	O	301	1/1	0.94	0.07	119,119,119,119	0
24	CLA	C	513	65/65	0.94	0.08	60,73,118,123	0
26	BCR	C	515	40/40	0.94	0.08	63,75,82,85	0
27	SQD	a	409	54/54	0.94	0.09	63,85,127,131	0
33	LMG	b	621	51/55	0.94	0.09	53,74,105,124	0
26	BCR	D	404	40/40	0.94	0.08	46,61,94,95	0
24	CLA	c	506	65/65	0.95	0.07	51,66,116,125	0
24	CLA	c	508	65/65	0.95	0.08	60,72,120,133	0
33	LMG	J	101	51/55	0.95	0.08	48,73,119,126	0
24	CLA	c	509	65/65	0.95	0.08	56,70,86,92	0
24	CLA	C	509	65/65	0.95	0.07	44,57,115,131	0
24	CLA	B	614	65/65	0.95	0.08	38,49,103,113	0
24	CLA	d	403	65/65	0.95	0.08	46,64,132,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	C	505	65/65	0.95	0.07	42,56,103,113	0
33	LMG	j	101	51/55	0.95	0.08	60,70,121,138	0
24	CLA	B	606	65/65	0.95	0.08	41,52,104,114	0
26	BCR	K	102	40/40	0.95	0.07	56,67,74,81	0
32	UNL	X	101	18/-	0.95	0.09	57,76,100,100	0
26	BCR	Y	101	40/40	0.95	0.07	57,68,74,81	0
35	HTG	b	628	19/19	0.95	0.08	61,82,106,112	0
24	CLA	b	606	65/65	0.95	0.08	45,58,114,129	0
26	BCR	h	102	40/40	0.95	0.07	56,70,80,81	0
26	BCR	t	102	40/40	0.95	0.07	45,60,76,80	0
36	DGD	C	518	62/66	0.95	0.08	48,67,127,131	0
36	DGD	c	519	62/66	0.95	0.08	56,73,136,145	0
26	BCR	y	101	40/40	0.95	0.08	58,74,88,88	0
27	SQD	A	411	54/54	0.95	0.08	55,86,123,126	0
24	CLA	b	614	65/65	0.95	0.07	41,49,116,120	0
37	CA	o	301	1/1	0.95	0.06	108,108,108,108	0
32	UNL	x	101	18/-	0.95	0.09	70,85,105,106	0
38	LHG	D	407	49/49	0.95	0.09	53,61,120,125	0
24	CLA	b	616	65/65	0.95	0.09	50,60,124,127	0
33	LMG	B	621	51/55	0.95	0.08	53,72,94,108	0
38	LHG	d	406	49/49	0.95	0.08	50,66,90,106	0
38	LHG	d	408	49/49	0.95	0.09	53,68,121,125	0
28	GOL	B	626	6/6	0.96	0.10	85,88,90,95	0
26	BCR	A	410	40/40	0.96	0.06	42,51,61,62	0
26	BCR	B	618	40/40	0.96	0.06	44,57,70,77	0
26	BCR	B	619	40/40	0.96	0.06	45,57,80,87	0
24	CLA	C	504	65/65	0.96	0.07	47,58,76,85	0
24	CLA	b	607	65/65	0.96	0.07	35,49,77,87	0
26	BCR	H	101	40/40	0.96	0.06	50,65,77,82	0
24	CLA	b	609	65/65	0.96	0.07	50,61,83,99	0
26	BCR	T	101	40/40	0.96	0.06	46,57,68,72	0
24	CLA	B	602	65/65	0.96	0.07	45,55,80,84	0
26	BCR	b	617	40/40	0.96	0.06	45,52,63,63	0
26	BCR	b	618	40/40	0.96	0.06	44,60,73,75	0
26	BCR	c	516	40/40	0.96	0.07	77,86,93,96	0
24	CLA	b	615	65/65	0.96	0.07	46,59,81,86	0
24	CLA	B	616	65/65	0.96	0.10	45,58,147,153	0
26	BCR	k	101	40/40	0.96	0.07	58,73,84,90	0
36	DGD	C	517	62/66	0.96	0.07	43,63,104,106	0
24	CLA	c	505	65/65	0.96	0.06	58,67,77,83	0
36	DGD	C	519	62/66	0.96	0.07	43,60,94,116	0
36	DGD	c	518	62/66	0.96	0.07	49,67,95,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	D	403	65/65	0.96	0.08	44,58,139,144	0
36	DGD	c	520	62/66	0.96	0.07	55,64,100,116	0
24	CLA	c	507	65/65	0.96	0.07	49,61,91,95	0
24	CLA	a	404	65/65	0.96	0.07	42,53,126,133	0
24	CLA	a	407	65/65	0.96	0.09	44,57,134,140	0
24	CLA	c	510	65/65	0.96	0.07	53,63,141,145	0
24	CLA	c	511	65/65	0.96	0.08	51,69,82,89	0
24	CLA	c	513	65/65	0.96	0.07	57,71,91,97	0
38	LHG	D	357	49/49	0.96	0.07	49,64,86,102	0
24	CLA	C	508	65/65	0.96	0.07	49,60,80,82	0
32	UNL	d	409	17/-	0.96	0.07	68,83,111,114	0
24	CLA	b	602	65/65	0.96	0.07	51,62,79,88	0
24	CLA	b	604	65/65	0.96	0.07	37,50,122,128	0
38	LHG	l	101	49/49	0.96	0.07	50,60,74,91	0
39	HEM	e	102	43/43	0.96	0.09	67,93,128,137	0
24	CLA	a	403	65/65	0.97	0.06	36,48,69,86	0
26	BCR	B	617	40/40	0.97	0.05	44,52,59,65	0
31	PL9	D	405	55/55	0.97	0.06	37,49,62,78	0
24	CLA	B	609	65/65	0.97	0.06	47,57,73,80	0
24	CLA	B	610	65/65	0.97	0.07	43,53,64,80	0
31	PL9	d	405	55/55	0.97	0.06	41,50,66,85	0
24	CLA	a	350	65/65	0.97	0.05	36,46,63,77	0
26	BCR	C	516	40/40	0.97	0.06	53,62,72,81	0
24	CLA	B	611	65/65	0.97	0.06	37,47,63,73	0
24	CLA	B	612	65/65	0.97	0.05	35,47,57,74	0
24	CLA	b	603	65/65	0.97	0.06	46,56,85,92	0
24	CLA	B	613	65/65	0.97	0.06	37,47,94,103	0
24	CLA	b	605	65/65	0.97	0.06	43,52,70,74	0
26	BCR	a	408	40/40	0.97	0.05	42,52,65,68	0
24	CLA	A	406	65/65	0.97	0.06	36,47,110,116	0
24	CLA	B	615	65/65	0.97	0.06	37,52,74,83	0
26	BCR	b	619	40/40	0.97	0.06	51,62,81,84	0
24	CLA	b	608	65/65	0.97	0.05	46,58,81,84	0
26	BCR	c	517	40/40	0.97	0.06	56,67,80,81	0
24	CLA	A	409	65/65	0.97	0.08	42,53,136,144	0
24	CLA	b	610	65/65	0.97	0.07	47,58,73,75	0
24	CLA	b	611	65/65	0.97	0.06	41,52,73,82	0
24	CLA	b	612	65/65	0.97	0.06	43,54,64,75	0
24	CLA	C	502	65/65	0.97	0.06	48,59,73,83	0
24	CLA	C	503	65/65	0.97	0.06	47,55,78,95	0
23	BCT	A	403[A]	4/4	0.97	0.06	58,60,60,69	4
36	DGD	H	102	62/66	0.97	0.07	46,63,76,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	c	503	65/65	0.97	0.07	56,66,79,86	0
24	CLA	c	504	65/65	0.97	0.06	45,65,86,89	0
23	BCT	A	403[B]	4/4	0.97	0.06	55,61,62,78	4
36	DGD	h	103	62/66	0.97	0.07	52,66,78,86	0
24	CLA	C	506	65/65	0.97	0.06	49,57,92,100	0
24	CLA	B	603	65/65	0.97	0.06	42,52,69,76	0
24	CLA	B	604	65/65	0.97	0.07	34,46,123,127	0
24	CLA	B	605	65/65	0.97	0.06	39,48,65,68	0
24	CLA	C	510	65/65	0.97	0.07	49,60,81,91	0
38	LHG	D	406	49/49	0.97	0.07	47,57,76,93	0
24	CLA	C	511	65/65	0.97	0.06	49,61,74,88	0
24	CLA	c	512	65/65	0.97	0.07	50,65,81,92	0
24	CLA	C	512	65/65	0.97	0.06	52,63,79,86	0
38	LHG	L	101	49/49	0.97	0.06	45,55,67,96	0
24	CLA	A	404	65/65	0.97	0.06	36,43,66,80	0
24	CLA	B	607	65/65	0.97	0.06	32,45,71,78	0
38	LHG	d	407	49/49	0.97	0.06	48,59,73,85	0
24	CLA	B	608	65/65	0.97	0.05	41,54,68,71	0
25	PHO	A	408	64/64	0.97	0.06	37,49,57,60	0
39	HEM	E	103	43/43	0.97	0.07	60,70,80,93	0
25	PHO	a	406	64/64	0.97	0.06	41,55,63,65	0
24	CLA	b	613	65/65	0.98	0.05	42,49,101,106	0
24	CLA	A	405	65/65	0.98	0.05	34,45,54,63	0
24	CLA	d	402	65/65	0.98	0.05	39,48,74,86	0
22	CL	a	347	1/1	0.98	0.09	53,53,53,53	0
37	CA	c	524	1/1	0.98	0.09	78,78,78,78	0
37	CA	c	525	1/1	0.98	0.04	92,92,92,92	0
25	PHO	A	407	64/64	0.98	0.05	35,45,54,58	0
24	CLA	D	402	65/65	0.98	0.05	31,45,68,82	0
25	PHO	a	405	64/64	0.98	0.05	41,49,56,64	0
22	CL	A	347	1/1	0.98	0.06	49,49,49,49	0
40	MG	j	103	1/1	0.98	0.04	64,64,64,64	0
41	HEC	V	203	43/43	0.98	0.05	39,52,58,60	0
41	HEC	v	203	43/43	0.98	0.06	51,64,72,78	0
21	FE2	A	401[A]	1/1	0.99	0.04	62,62,62,62	1
23	BCT	a	420[A]	4/4	0.99	0.05	58,63,63,68	4
23	BCT	a	420[B]	4/4	0.99	0.05	54,63,64,72	4
29	OEX	A	414[A]	10/10	0.99	0.05	44,48,55,59	10
29	OEX	a	412[A]	10/10	0.99	0.05	50,55,61,74	10
30	OXY	A	415[B]	11/11	0.99	0.05	43,49,55,56	11
30	OXY	a	413[B]	11/11	0.99	0.05	50,54,58,74	11
22	CL	a	402	1/1	0.99	0.02	51,51,51,51	0

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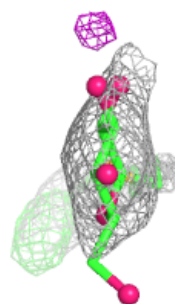
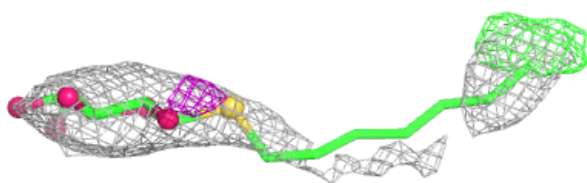
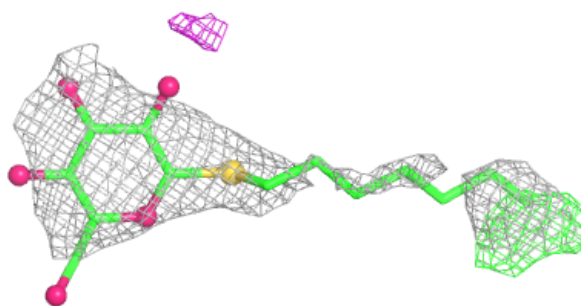
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
40	MG	J	103	1/1	0.99	0.06	61,61,61,61	0
21	FE2	A	401[B]	1/1	0.99	0.04	60,60,60,60	1
22	CL	A	402	1/1	0.99	0.04	44,44,44,44	0
37	CA	C	524	1/1	0.99	0.10	72,72,72,72	0
21	FE2	a	401[B]	1/1	1.00	0.05	60,60,60,60	1
21	FE2	a	401[A]	1/1	1.00	0.05	60,60,60,60	1

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

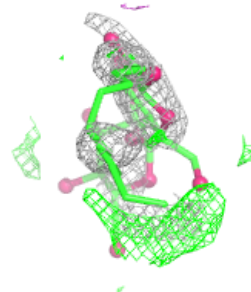
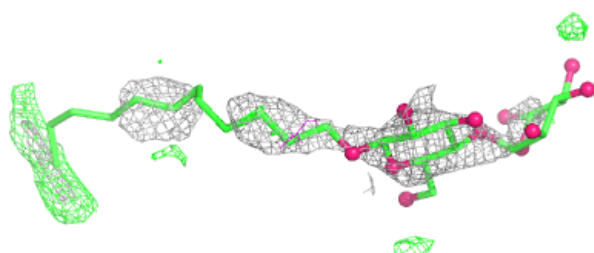
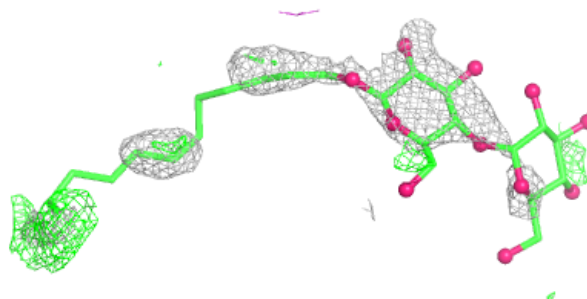
Electron density around HTG c 523:

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

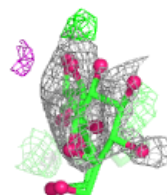
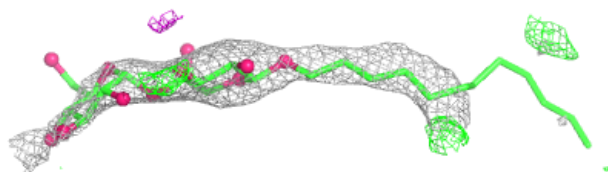
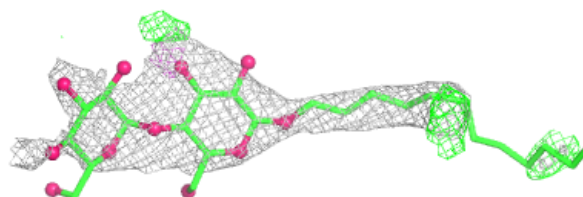


Electron density around LMT e 101:

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

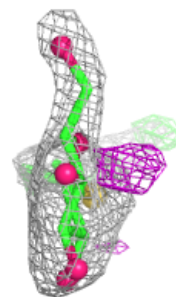
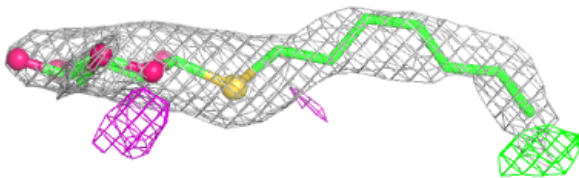
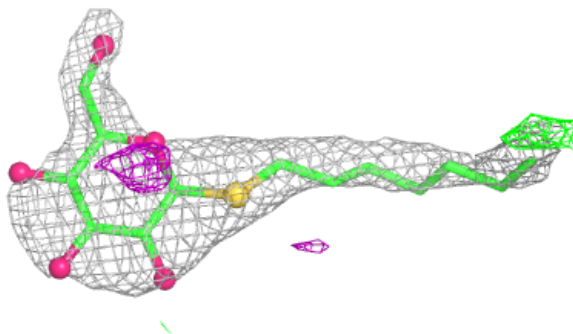
**Electron density around LMT a 418:**

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

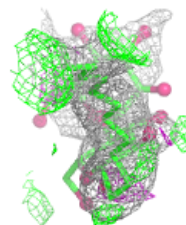
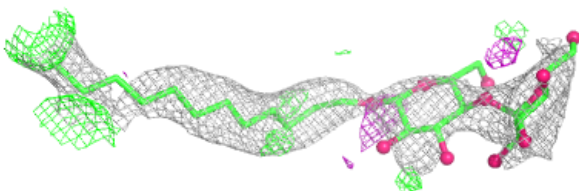
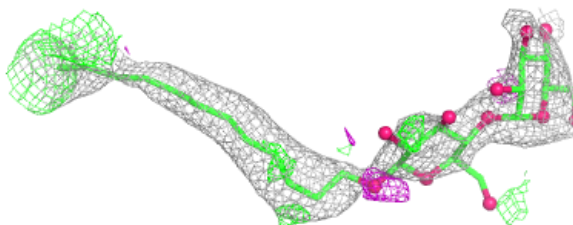


Electron density around HTG C 522:

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

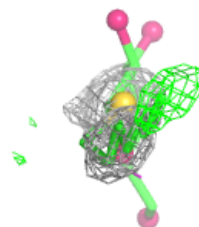
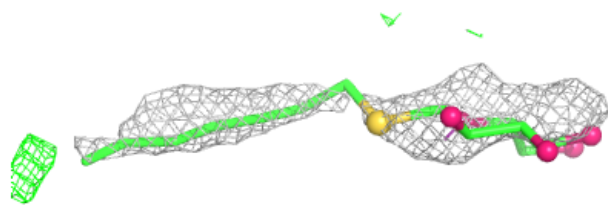
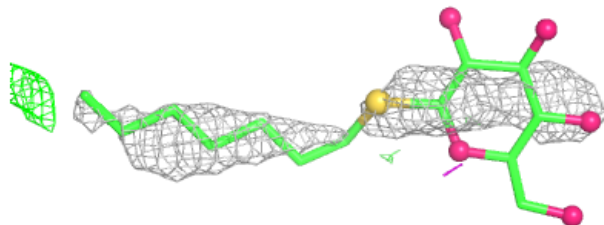
**Electron density around LMT A 359:**

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

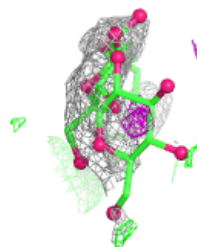
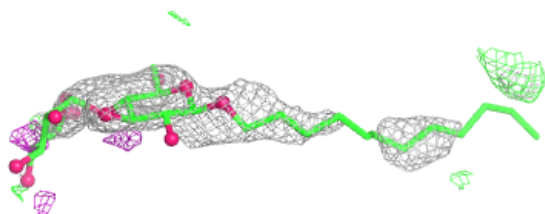
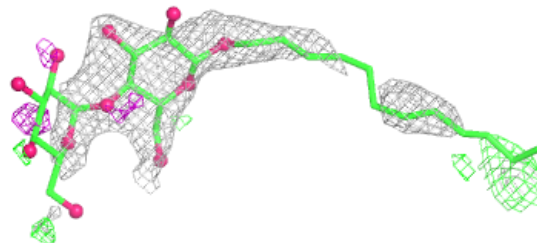


Electron density around HTG c 526:

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

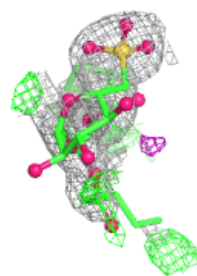
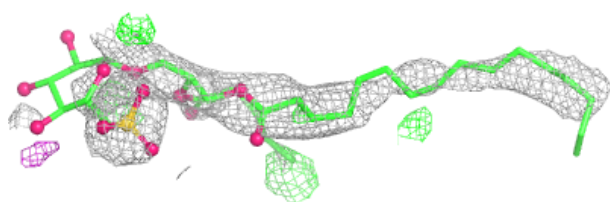
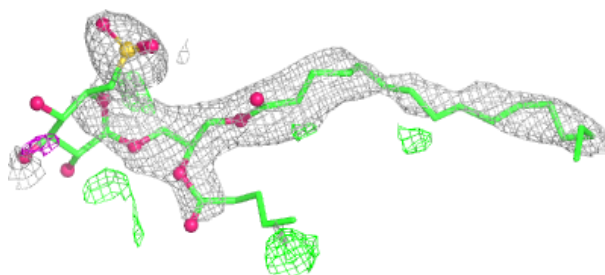
**Electron density around LMT E 102:**

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

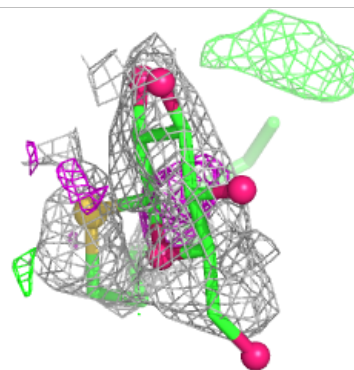
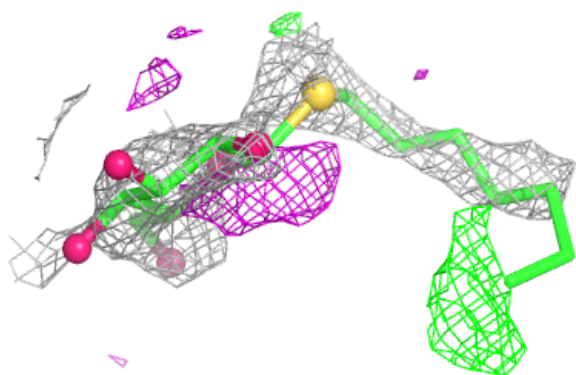
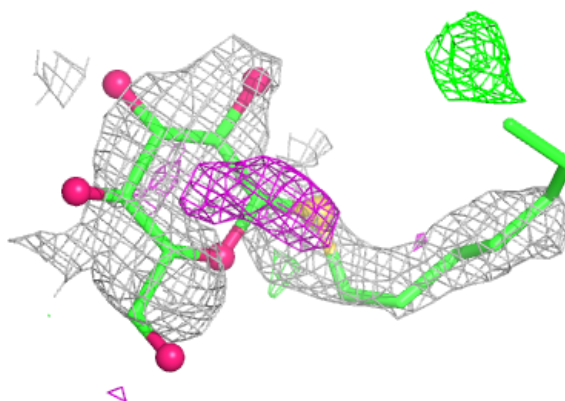


Electron density around SQD f 101:

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

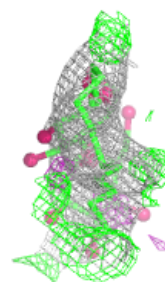
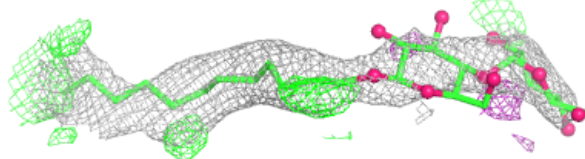
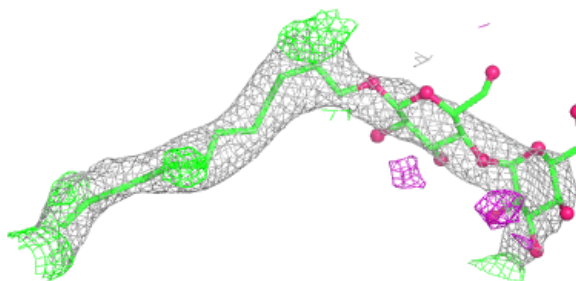
**Electron density around HTG b 624:**

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

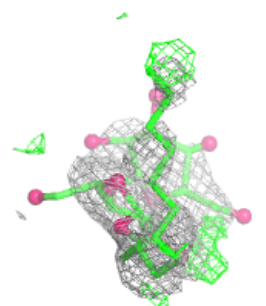
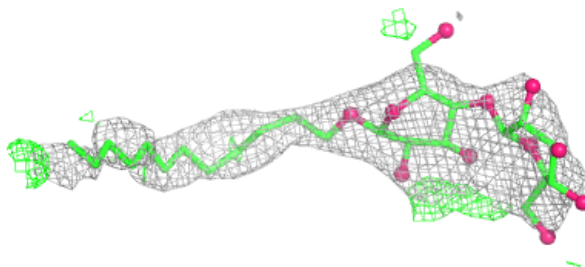
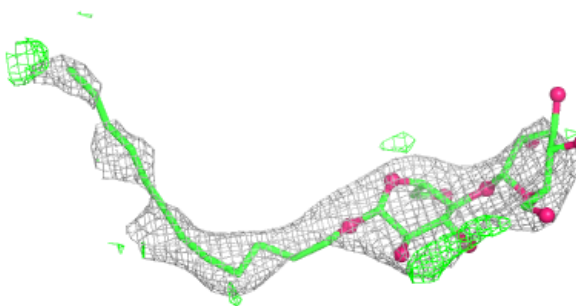


Electron density around LMT a 359:

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

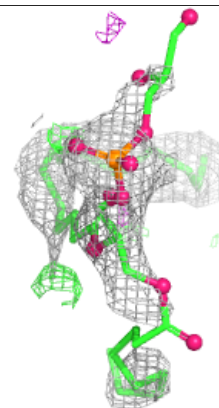
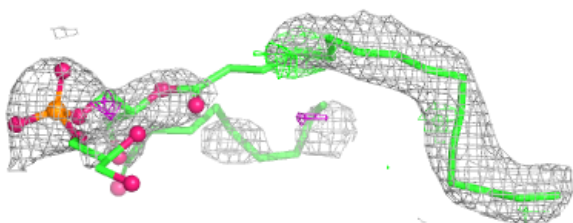
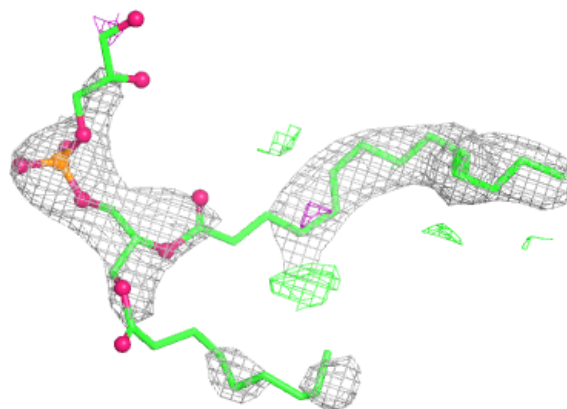
**Electron density around LMT I 101:**

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

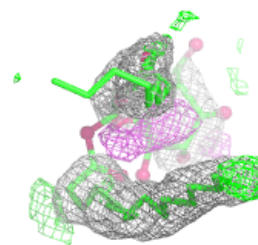
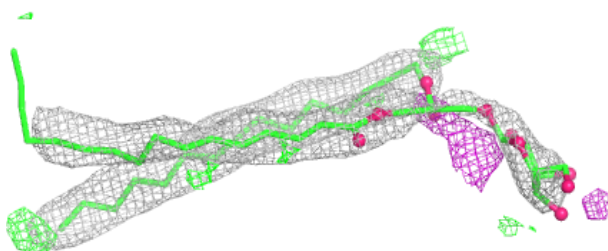
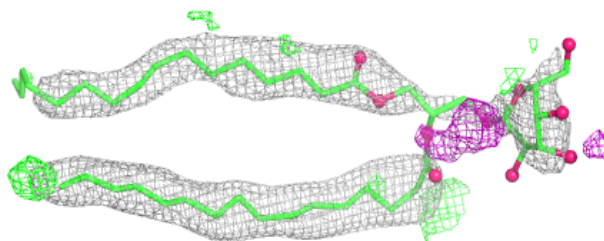


Electron density around LHG a 419:

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

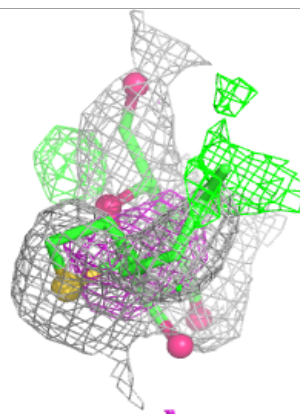
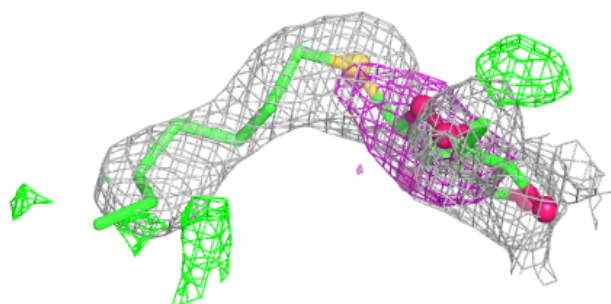
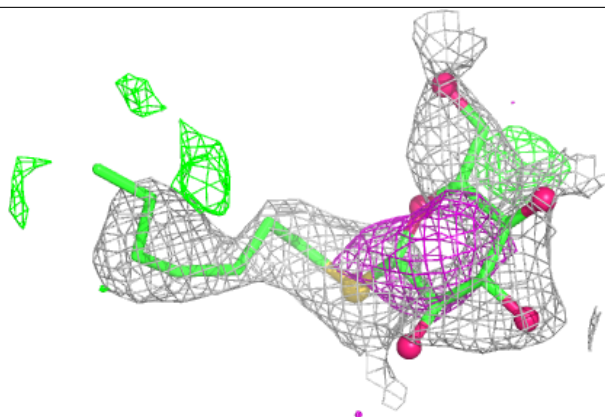
**Electron density around LMG C 521:**

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

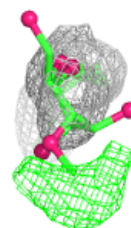
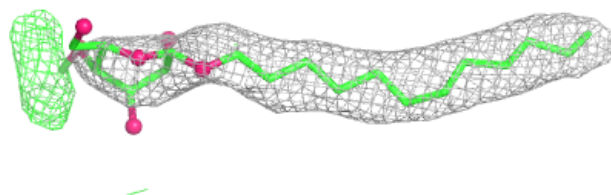
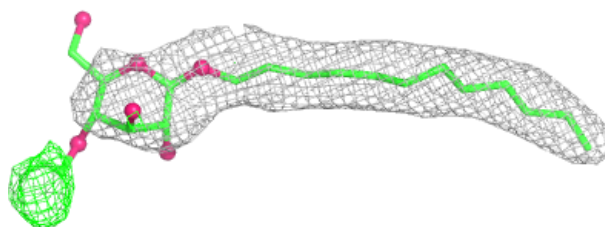


Electron density around HTG B 624:

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

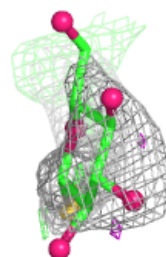
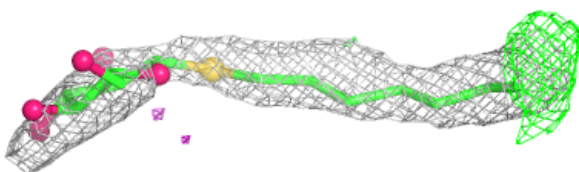
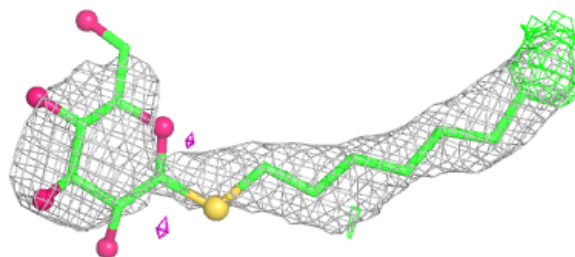
**Electron density around LMT b 622:**

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

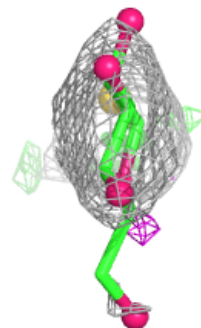
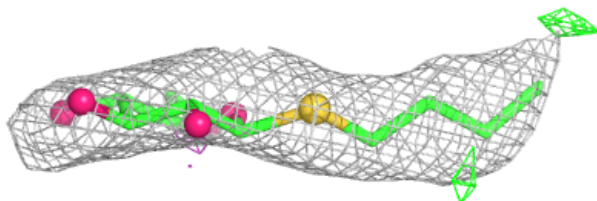
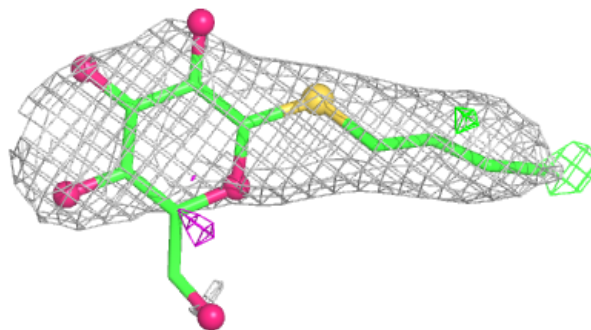


Electron density around HTG B 625:

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

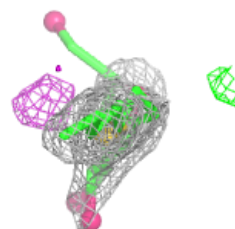
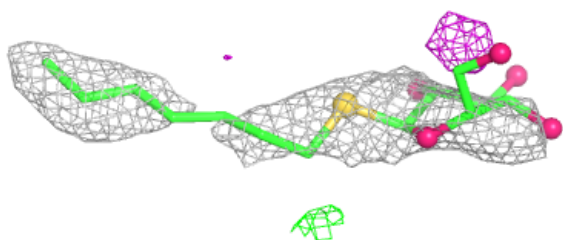
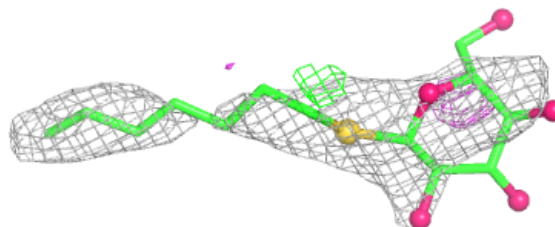
**Electron density around HTG h 101:**

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

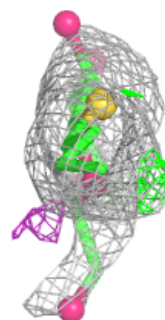
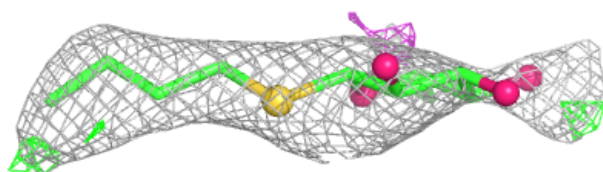
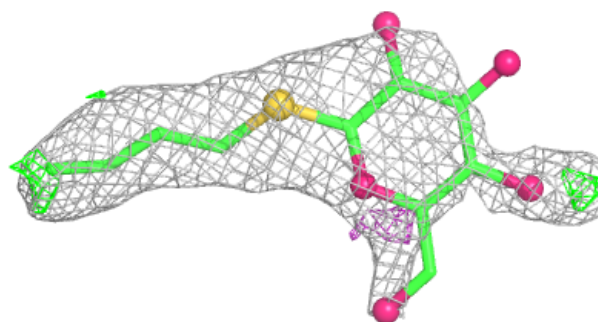


Electron density around HTG C 523:

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

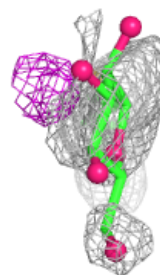
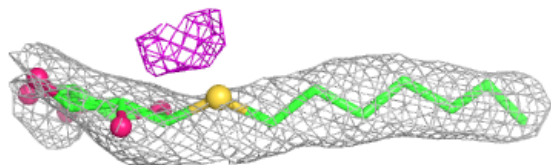
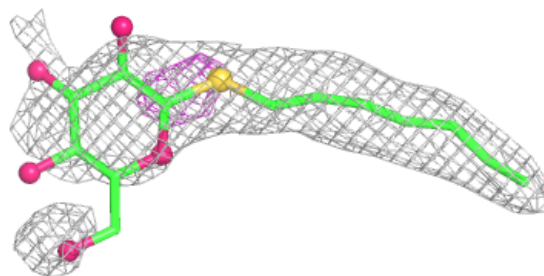
**Electron density around HTG D 410:**

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

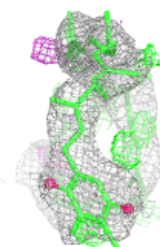
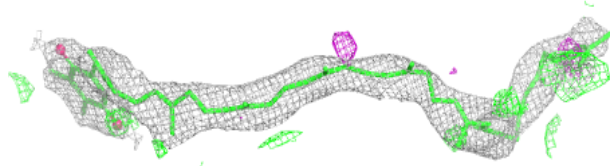
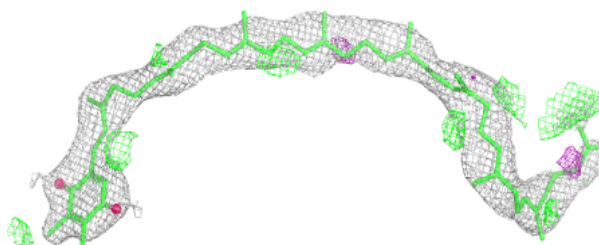


Electron density around HTG b 625:

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

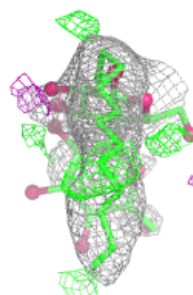
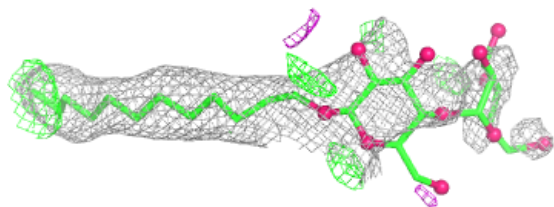
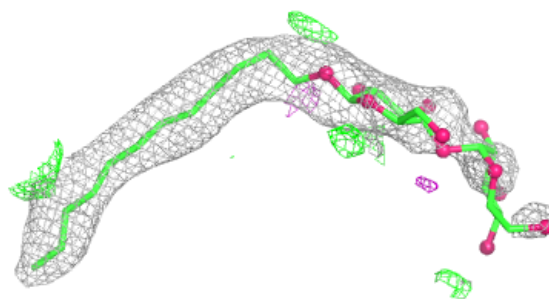
**Electron density around PL9 A 416 (A):**

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

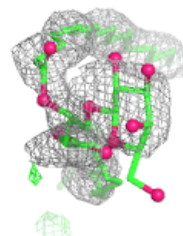
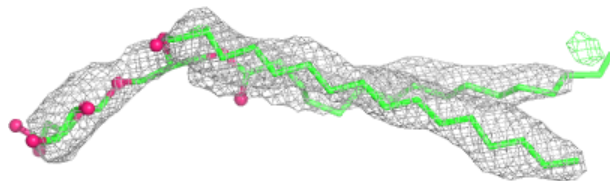
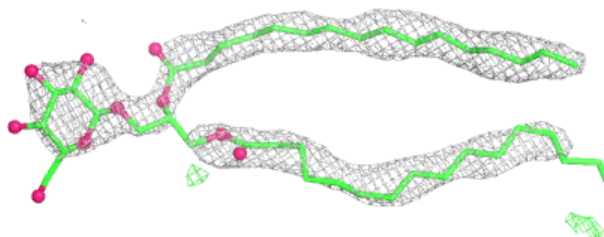


Electron density around LMT M 103:

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

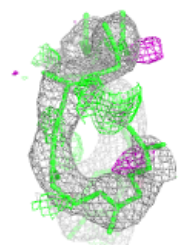
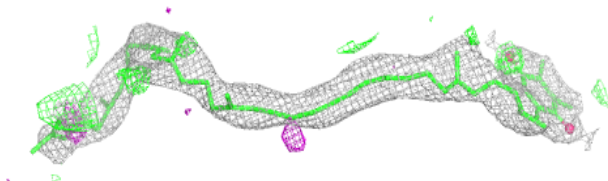
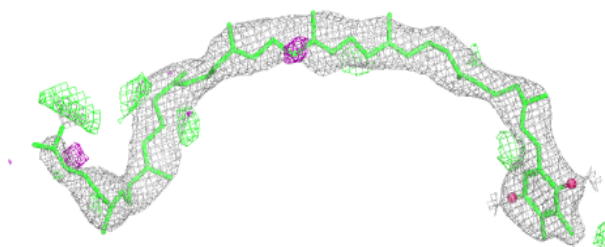
**Electron density around LMG c 522:**

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

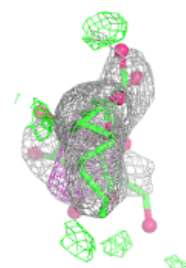
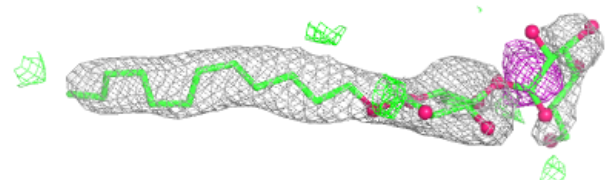
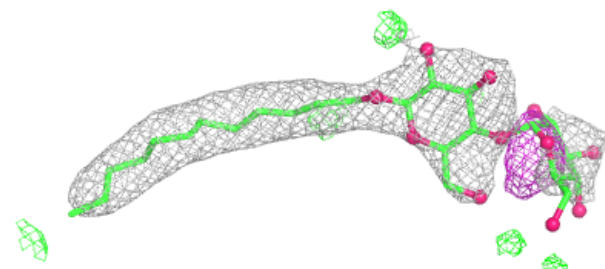


Electron density around PL9 A 416 (B):

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

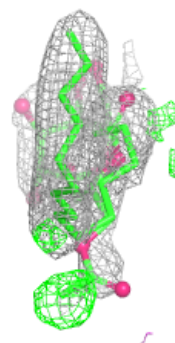
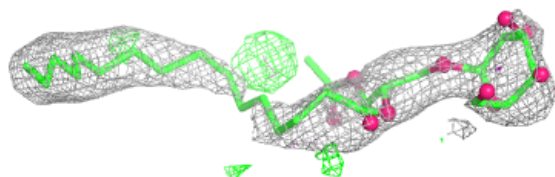
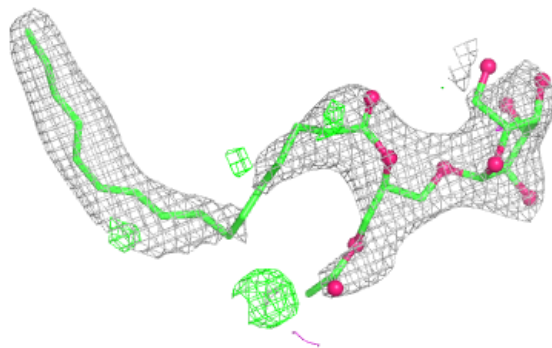
**Electron density around LMT B 622:**

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

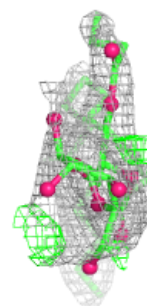
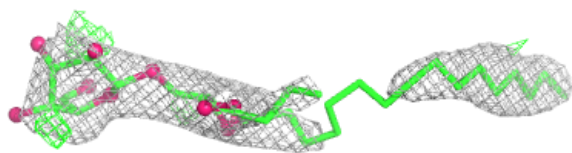
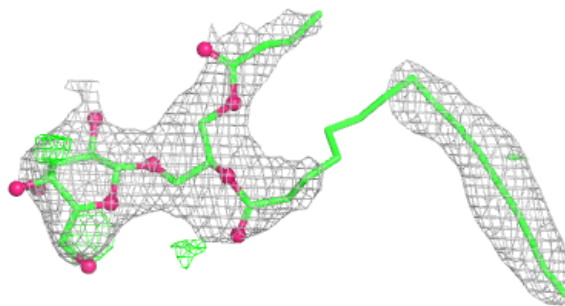


Electron density around LMG Z 101:

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

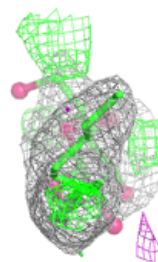
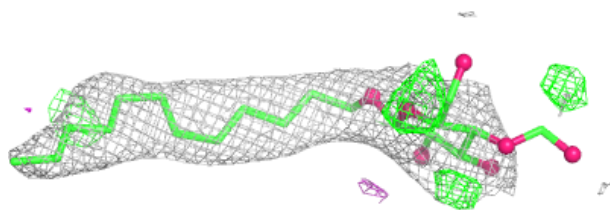
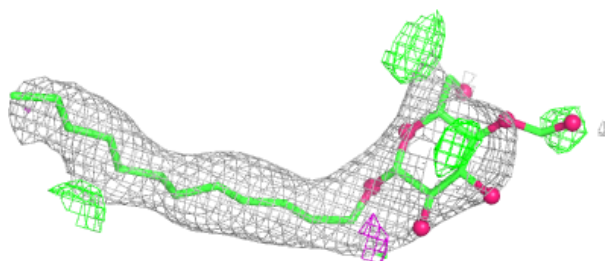
**Electron density around LMG z 101:**

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

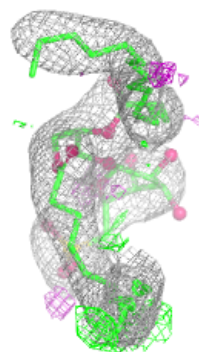
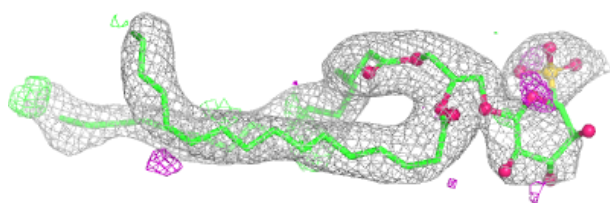
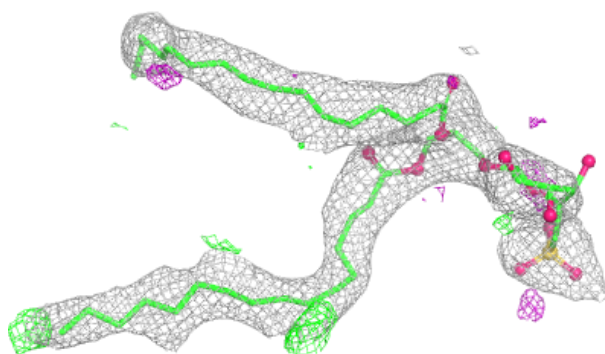


Electron density around LMT t 101:

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

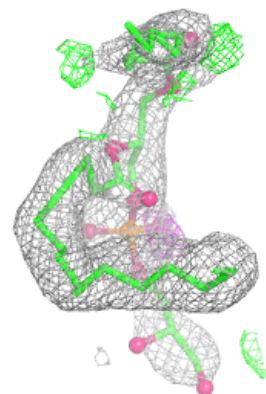
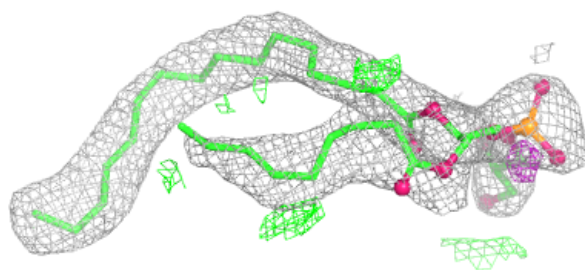
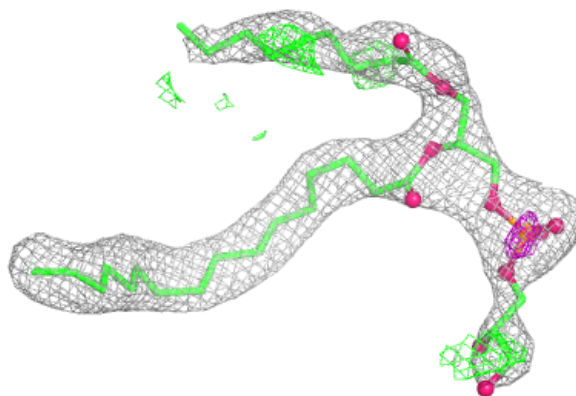
**Electron density around SQD a 411:**

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

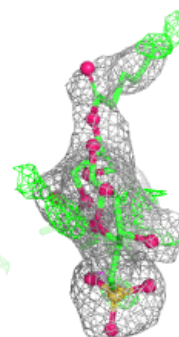
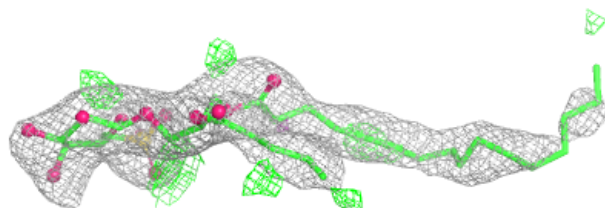
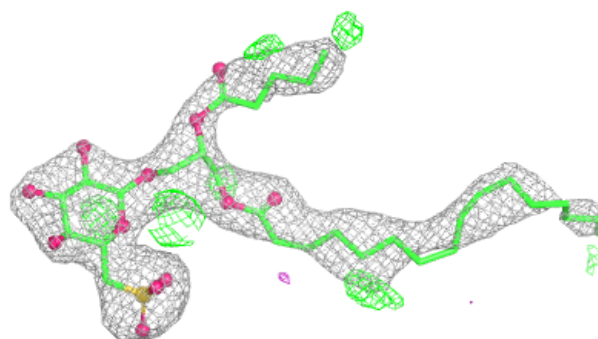


Electron density around LHG E 101:

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

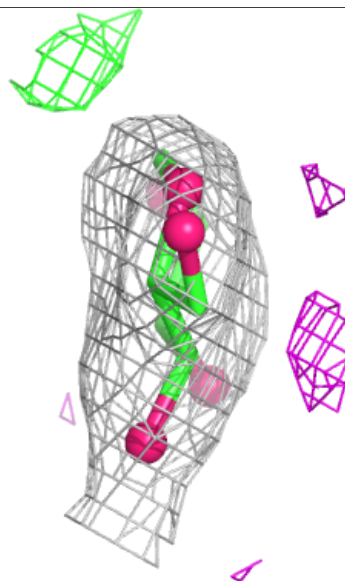
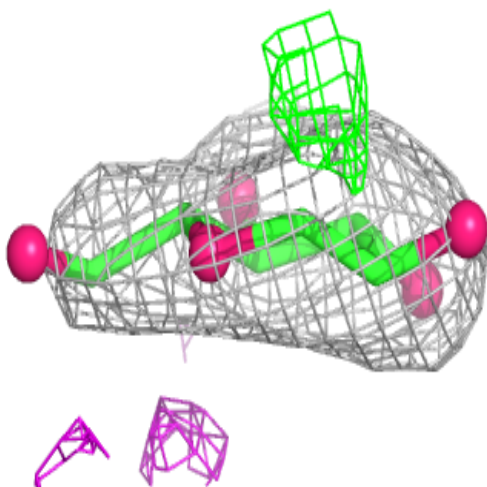
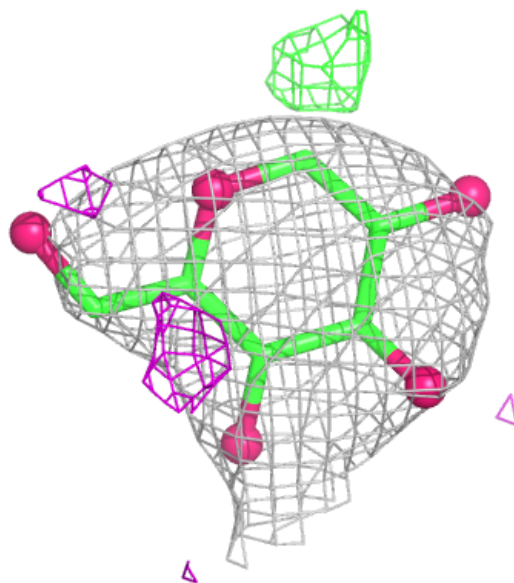
**Electron density around SQD F 101:**

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



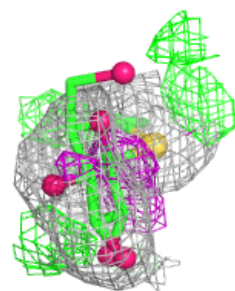
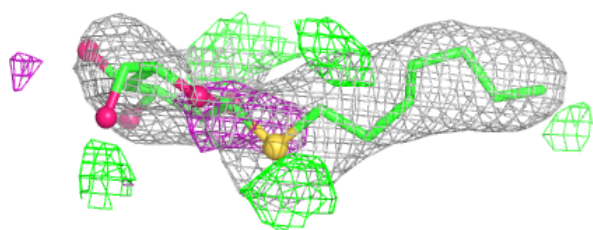
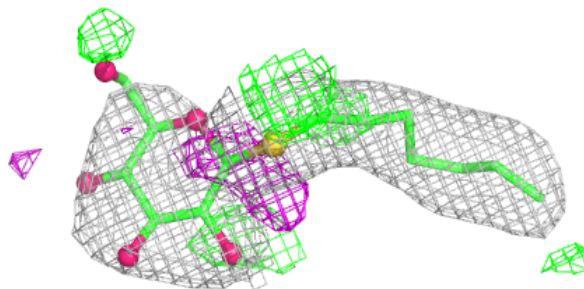
Electron density around HTG V 204:

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

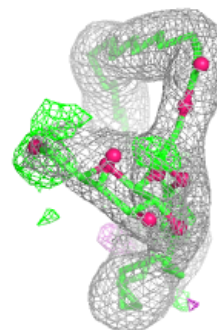
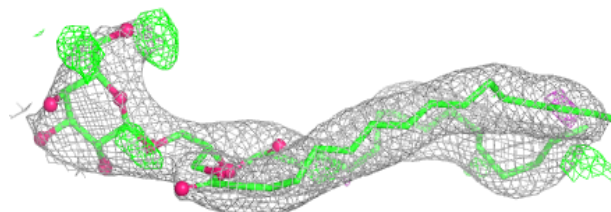
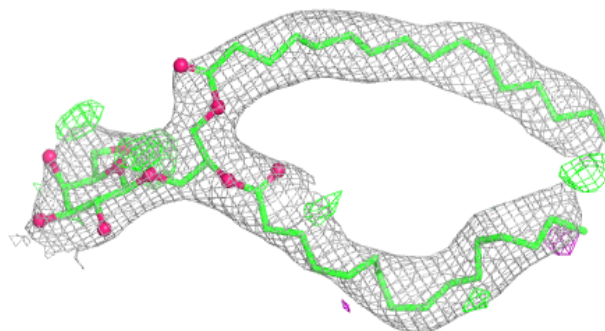


Electron density around HTG B 623:

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

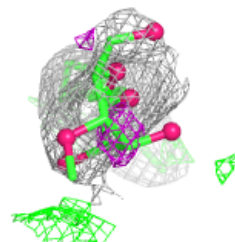
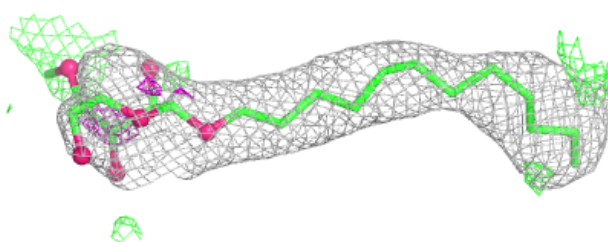
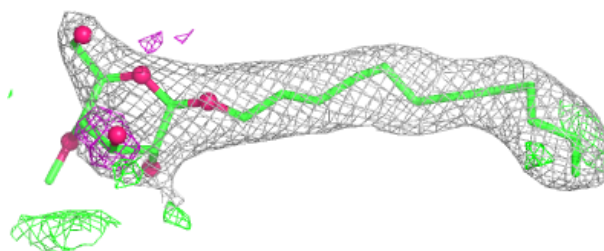
**Electron density around LMG A 418:**

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

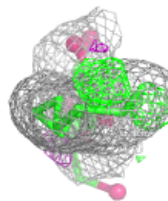
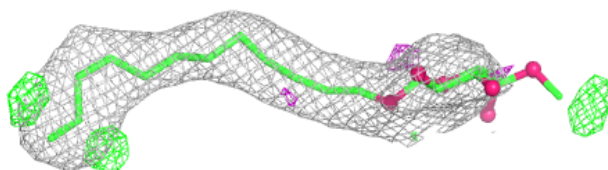
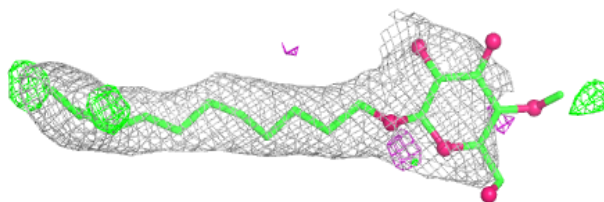


Electron density around LMT B 630:

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

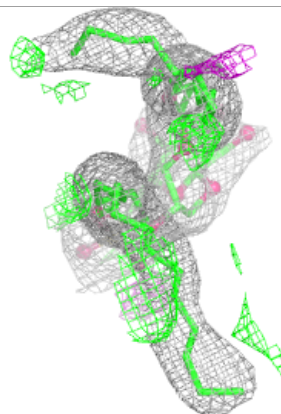
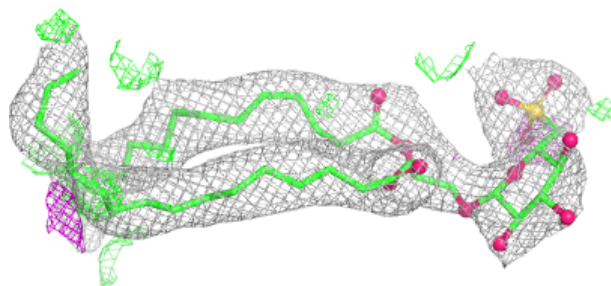
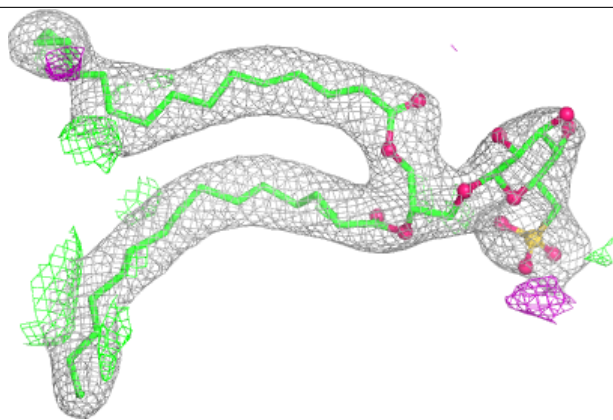
**Electron density around LMT b 630:**

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

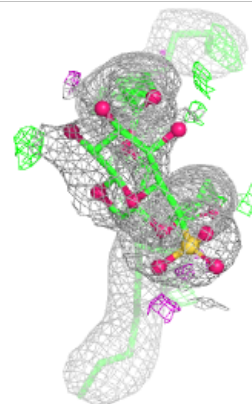
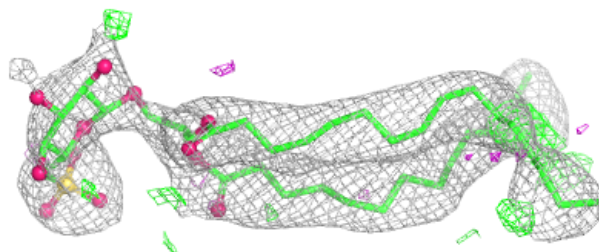
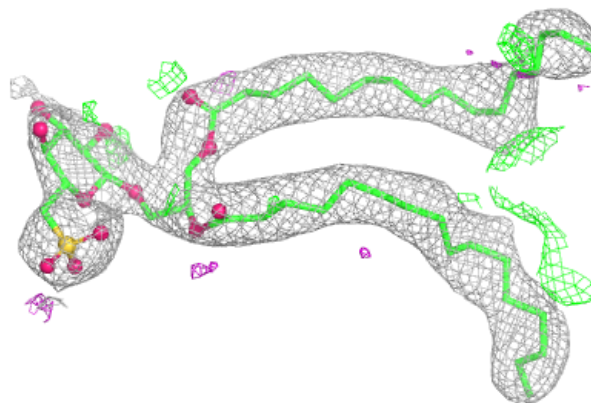


Electron density around SQD B 620:

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

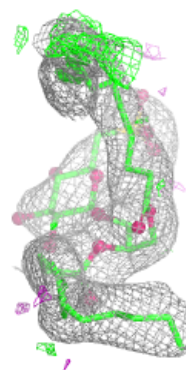
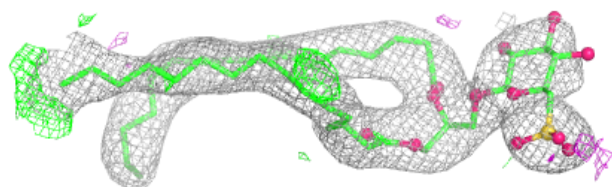
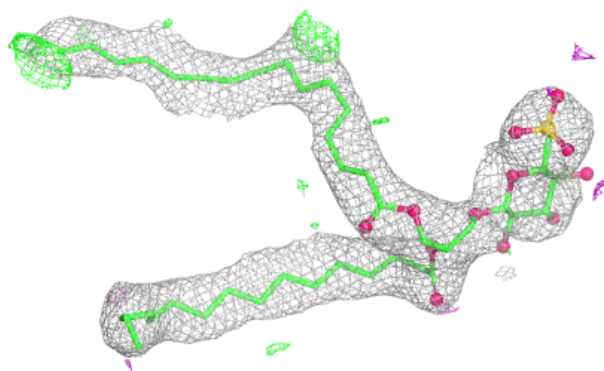
**Electron density around SQD b 620:**

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

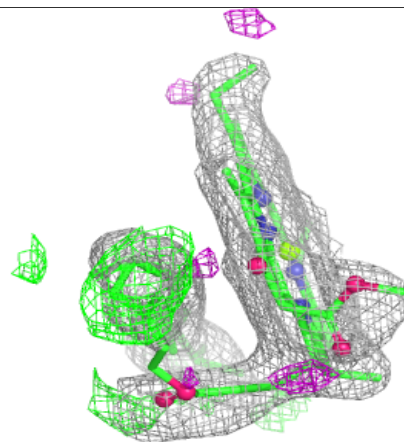
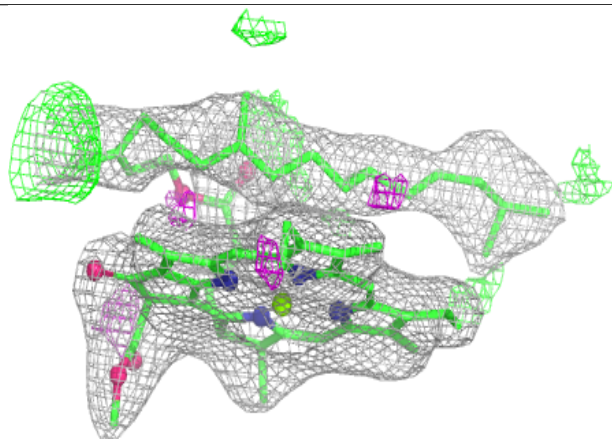
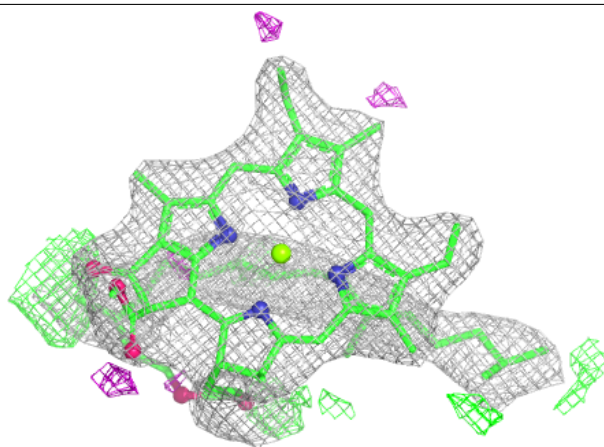


Electron density around SQD A 413:

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

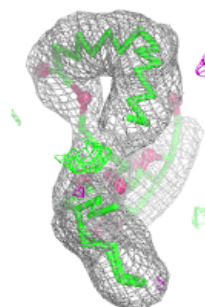
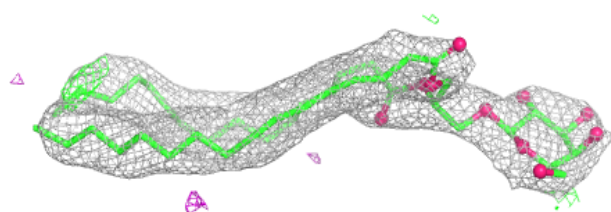
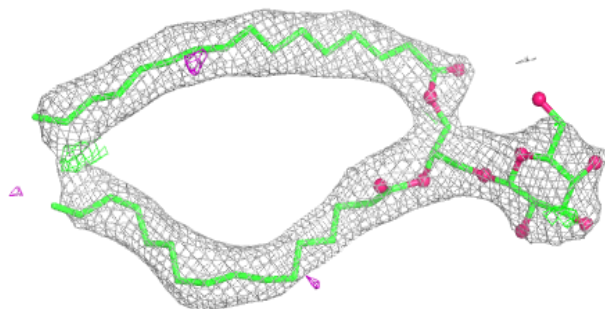
**Electron density around CLA B 601:**

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

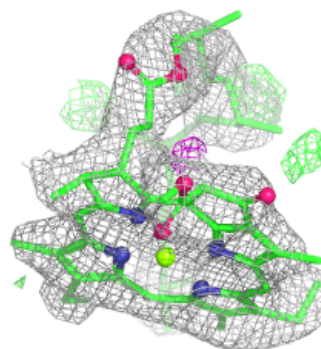
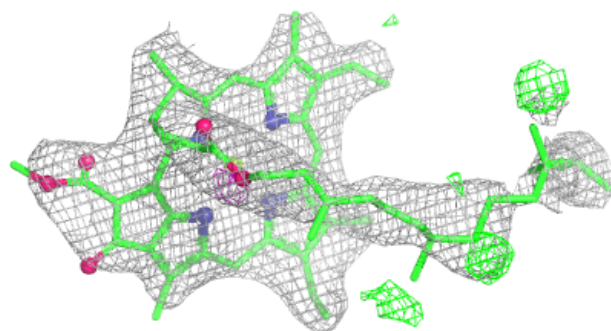
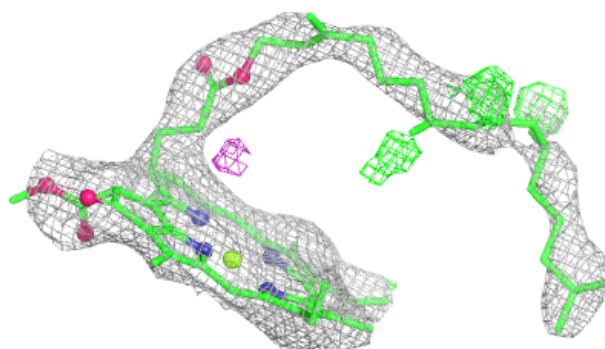


Electron density around LMG a 417:

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

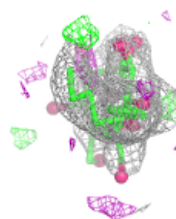
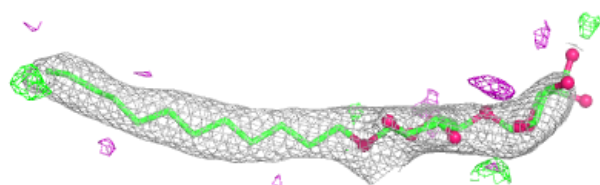
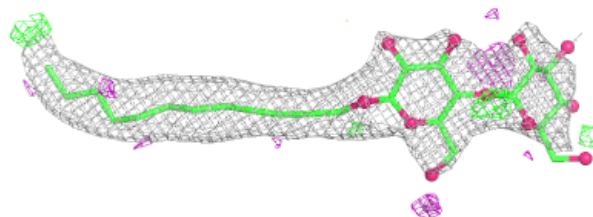
**Electron density around CLA c 515:**

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

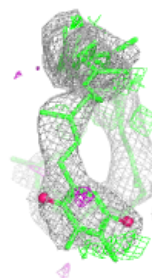
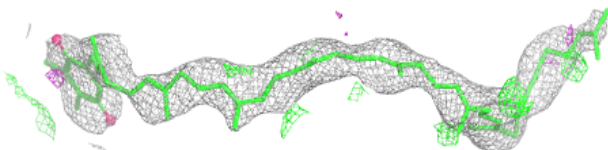
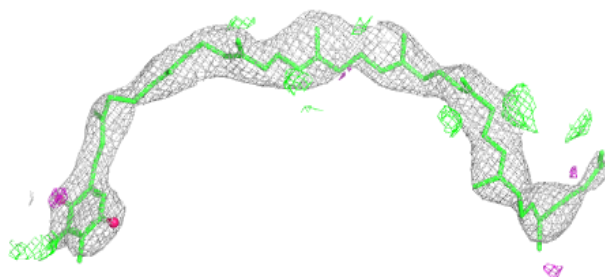


Electron density around LMT m 102:

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

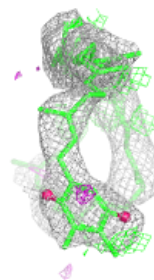
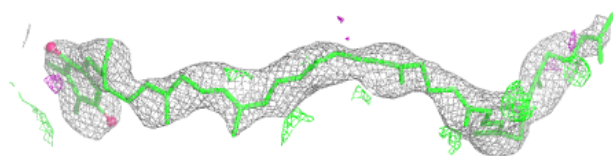
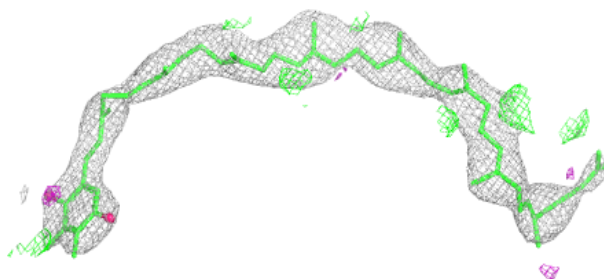
**Electron density around PL9 a 414 (A):**

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

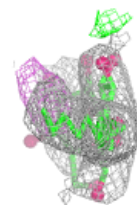
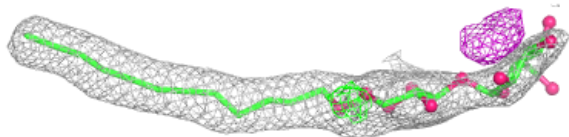
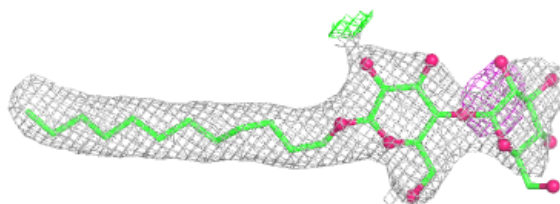


Electron density around PL9 a 414 (B):

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

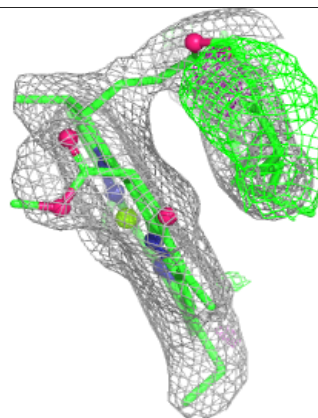
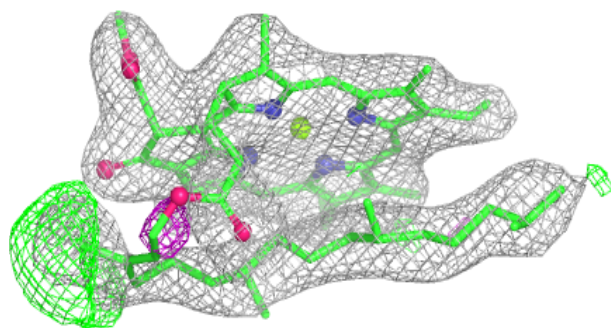
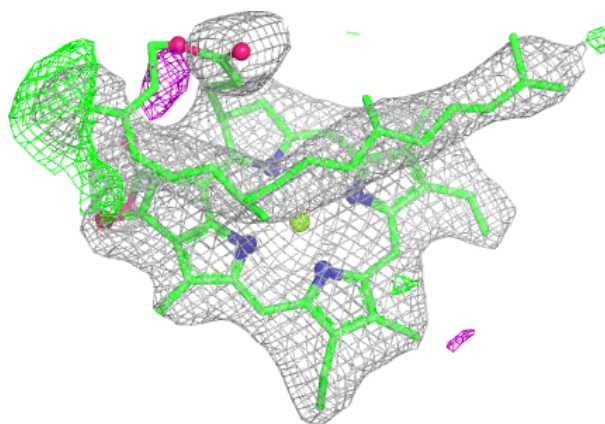
**Electron density around LMT M 101:**

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



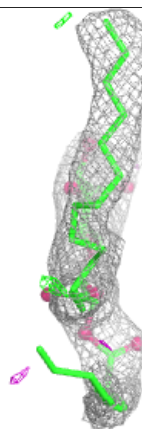
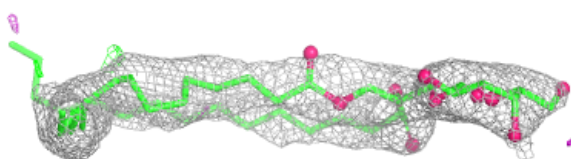
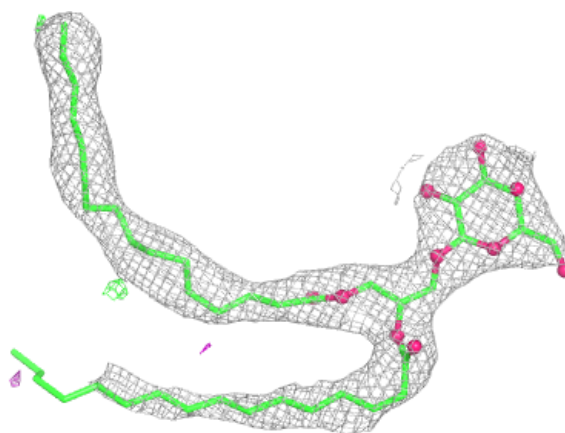
Electron density around CLA b 601:

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



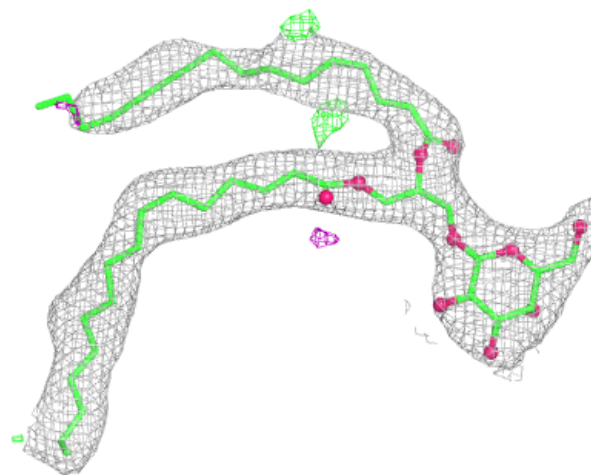
Electron density around LMG c 521:

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



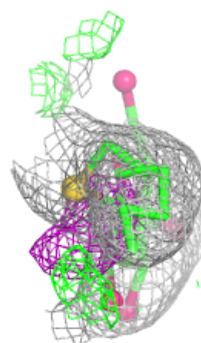
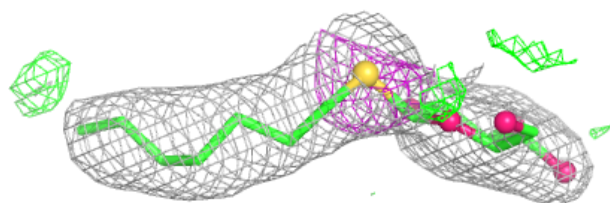
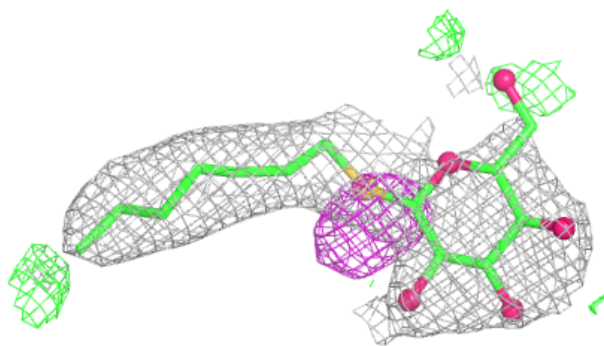
Electron density around LMG C 520:

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



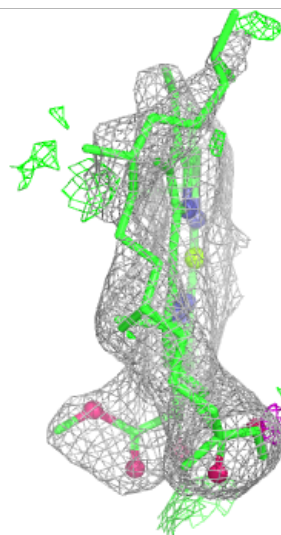
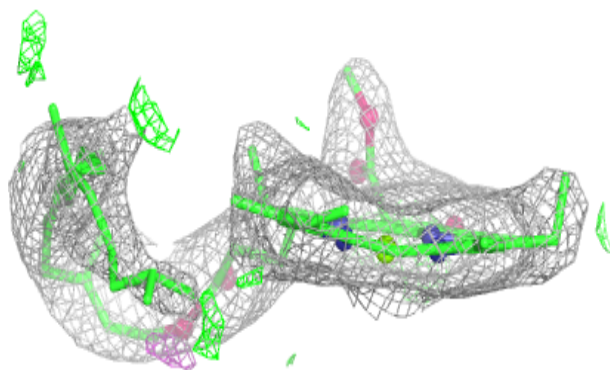
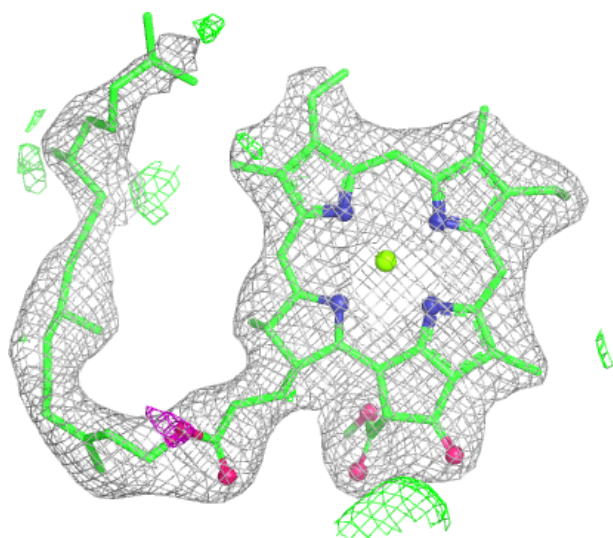
Electron density around HTG b 623:

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



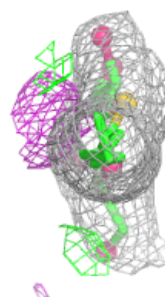
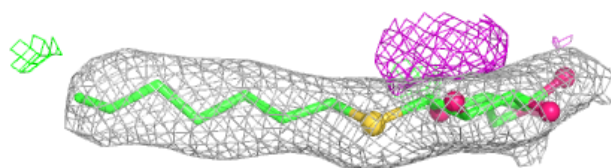
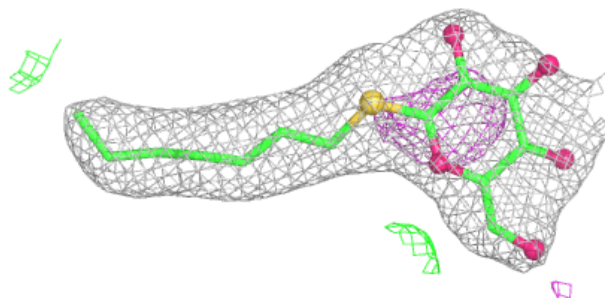
Electron density around CLA c 514:

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

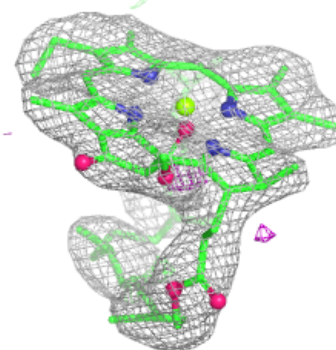
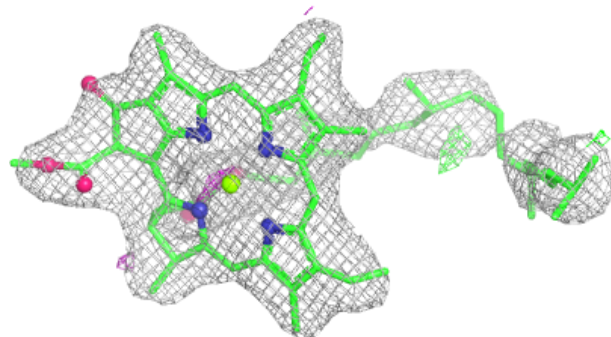
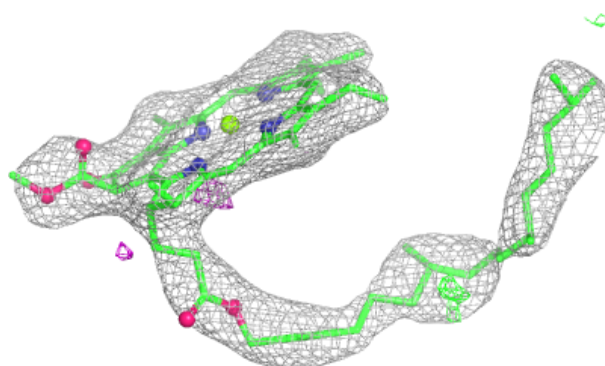


Electron density around HTG B 628:

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

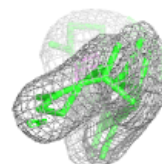
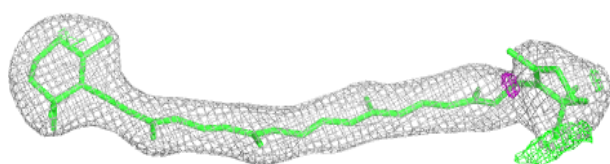
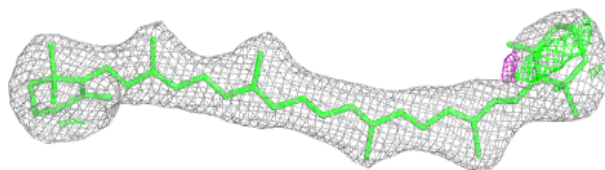
**Electron density around CLA C 514:**

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

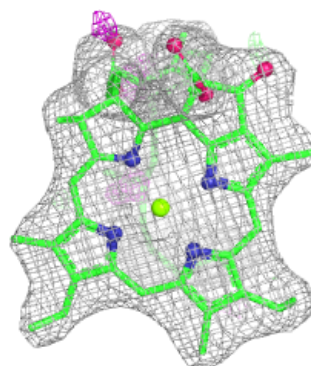
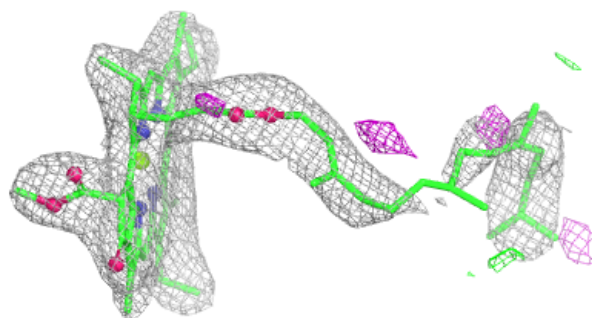
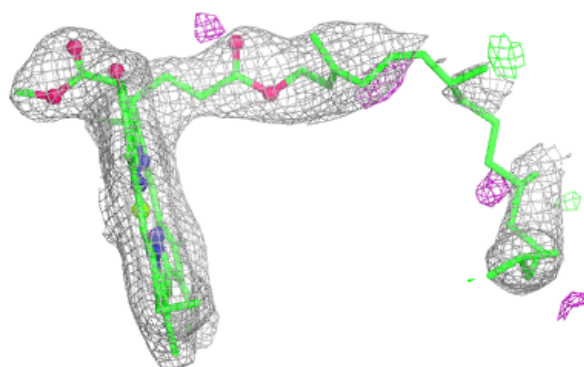


Electron density around BCR d 404:

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

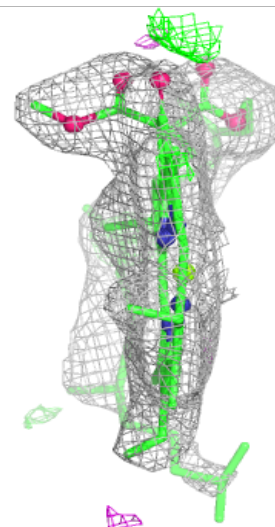
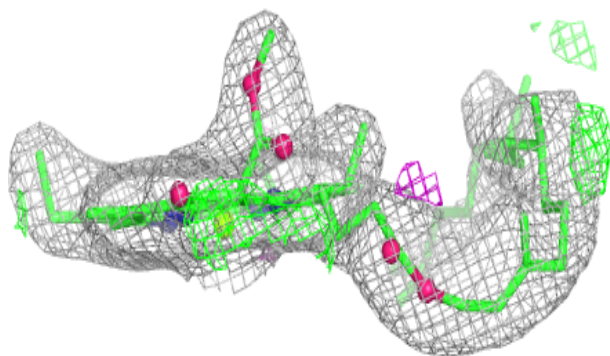
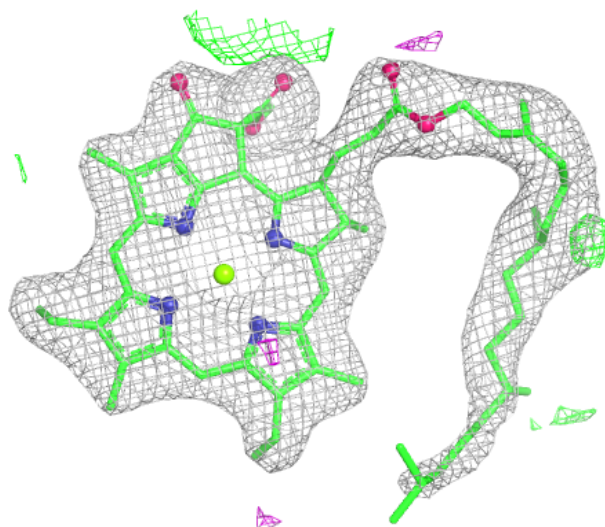
**Electron density around CLA C 507:**

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



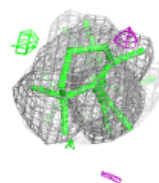
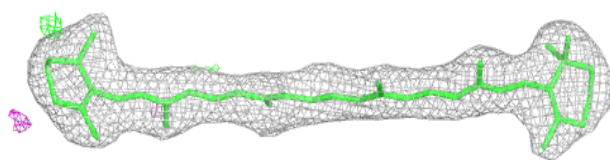
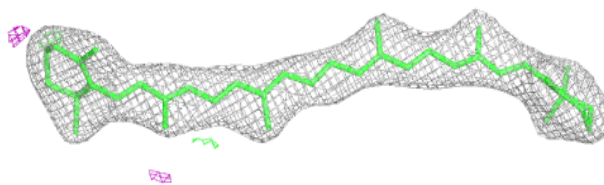
Electron density around CLA C 513:

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



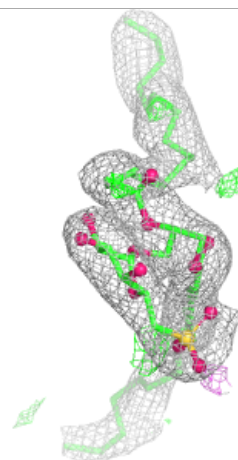
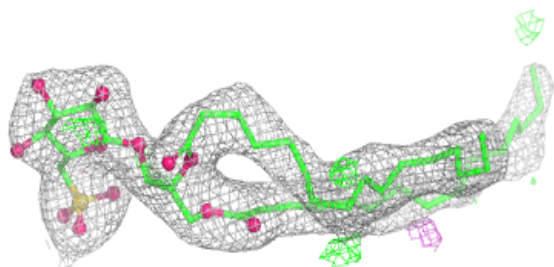
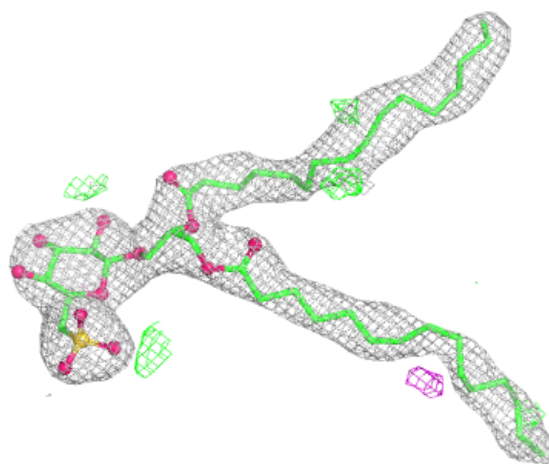
Electron density around BCR C 515:

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



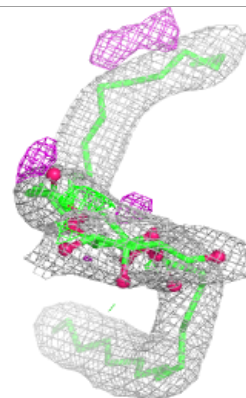
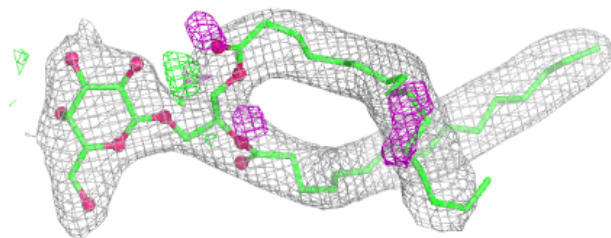
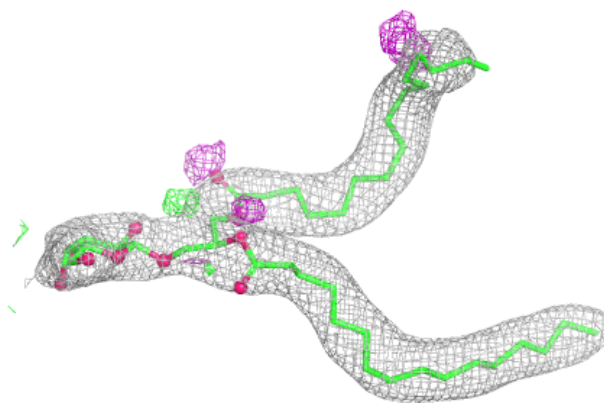
Electron density around SQD a 409:

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

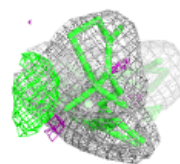
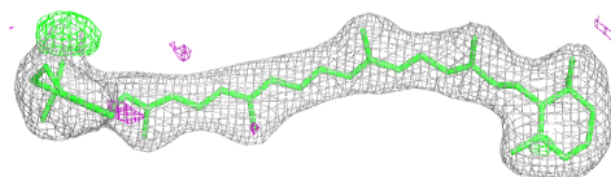
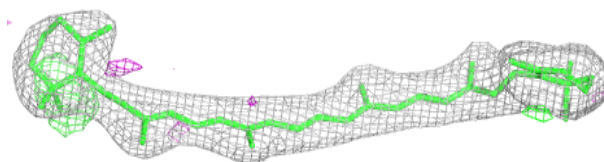


Electron density around LMG b 621:

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

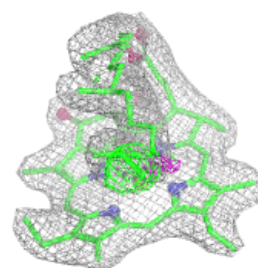
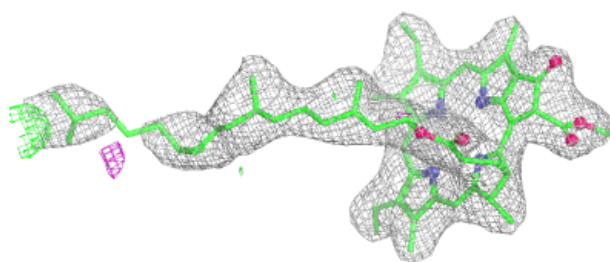
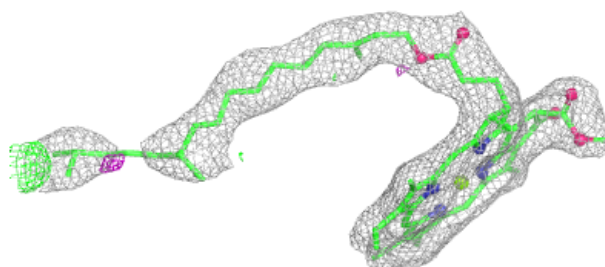
**Electron density around BCR D 404:**

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

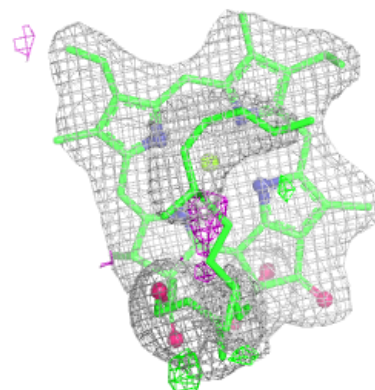
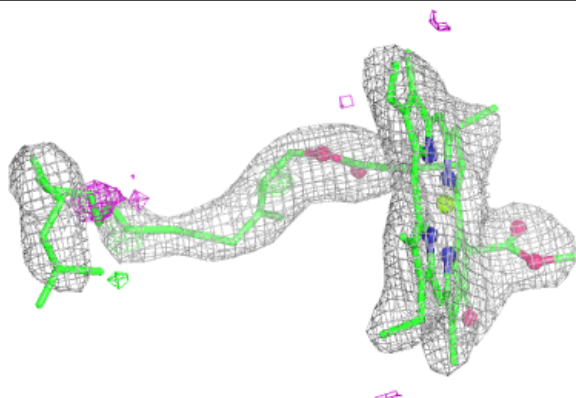
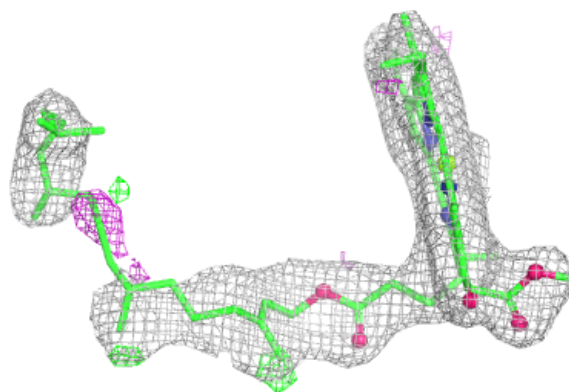


Electron density around CLA c 506:

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

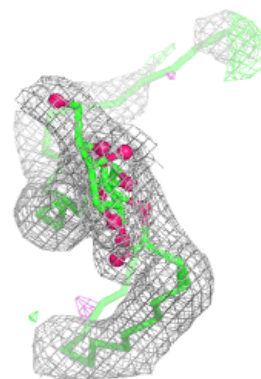
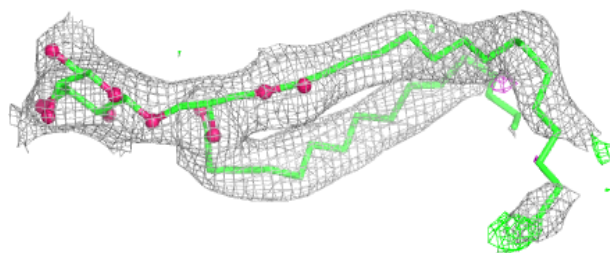
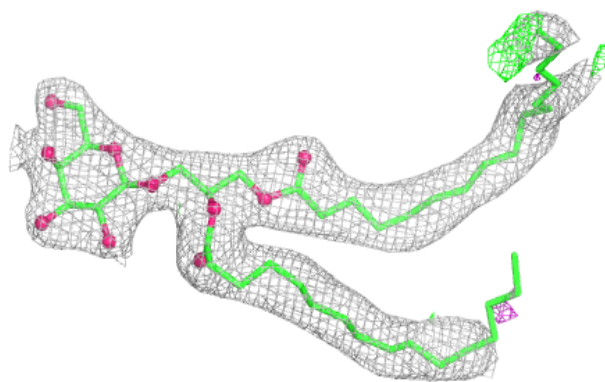
**Electron density around CLA c 508:**

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



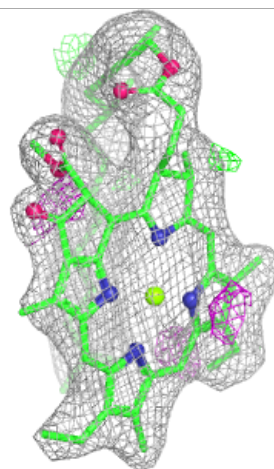
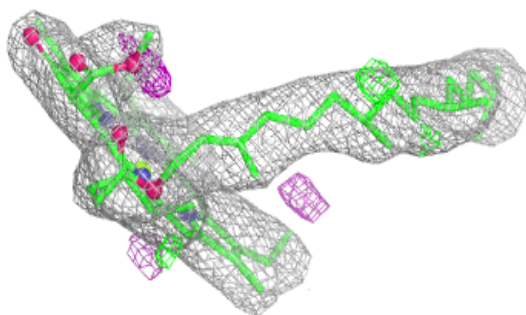
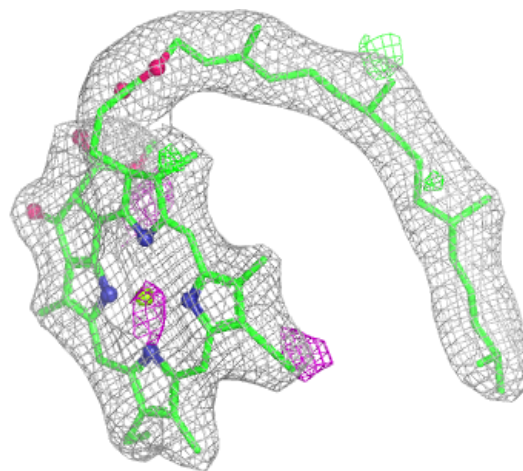
Electron density around LMG J 101:

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



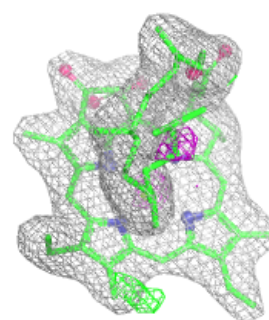
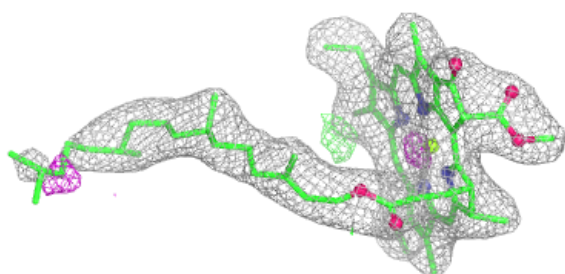
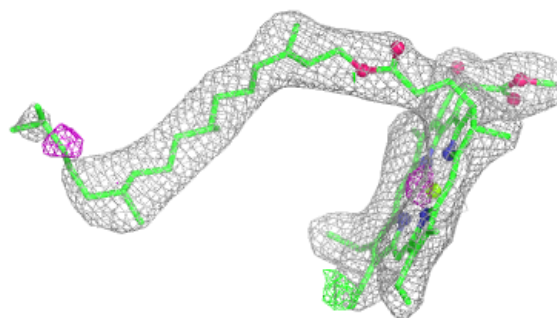
Electron density around CLA c 509:

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

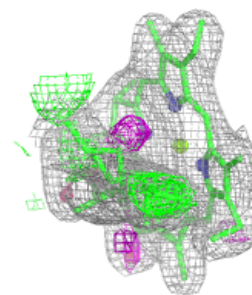
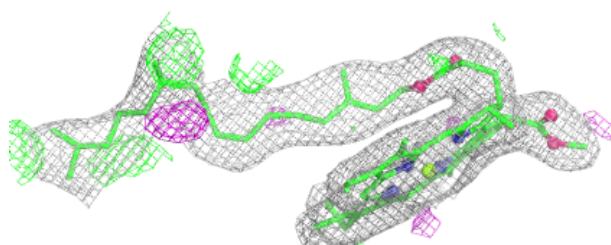
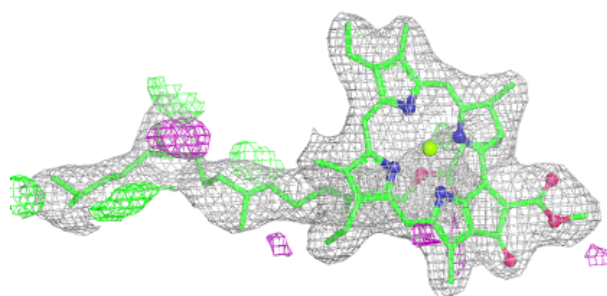


Electron density around CLA C 509:

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

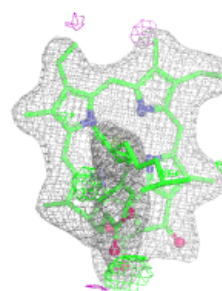
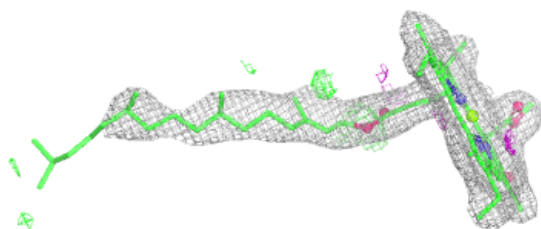
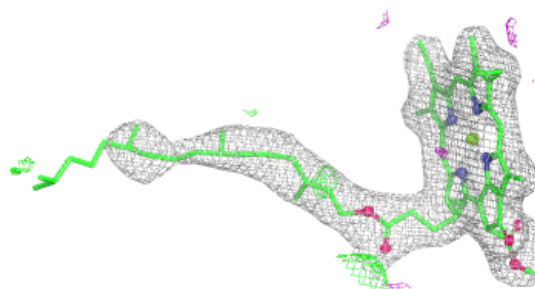
**Electron density around CLA B 614:**

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

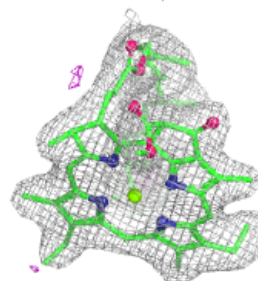
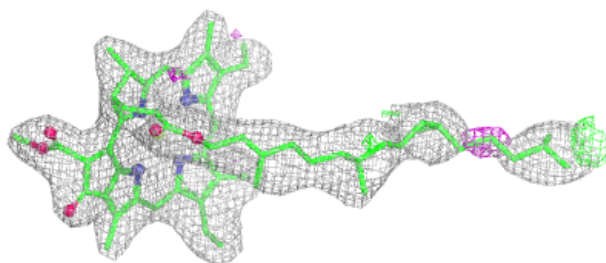
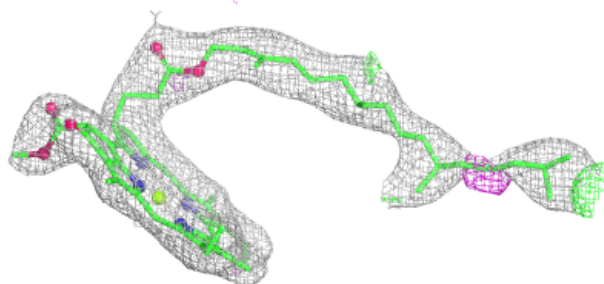


Electron density around CLA d 403:

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

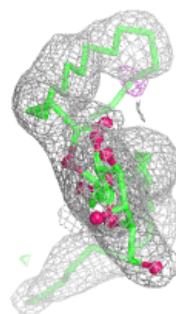
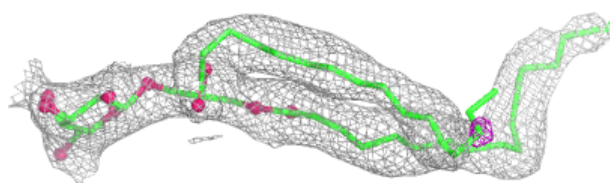
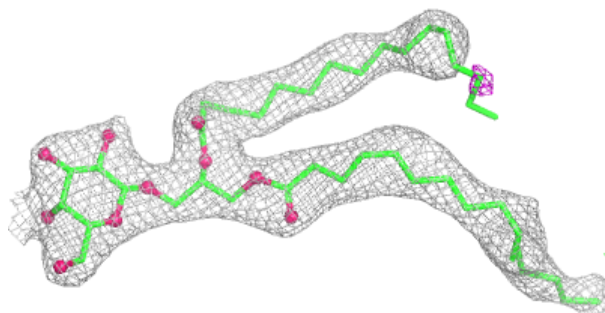
**Electron density around CLA C 505:**

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

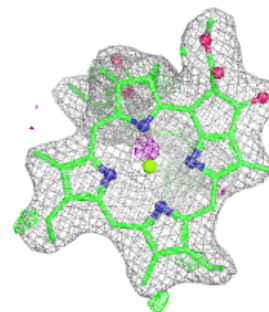
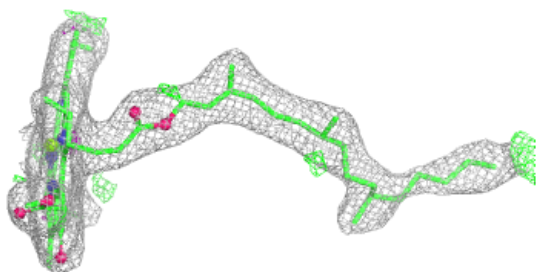
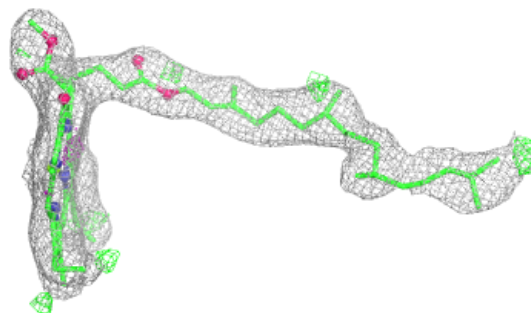


Electron density around LMG j 101:

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

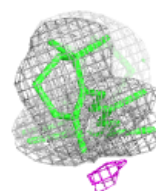
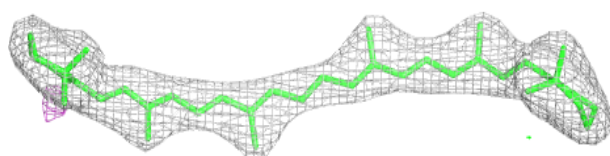
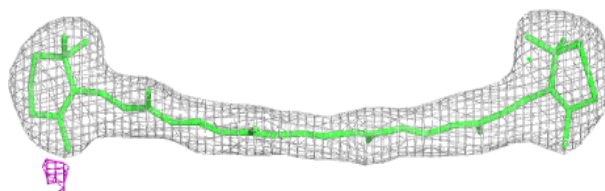
**Electron density around CLA B 606:**

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

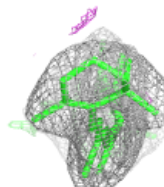
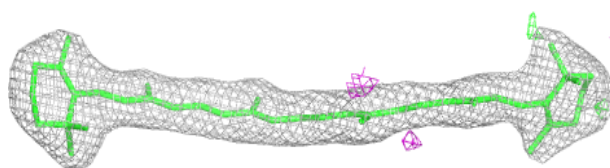
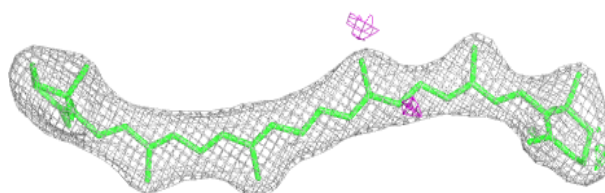


Electron density around BCR K 102:

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

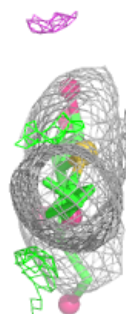
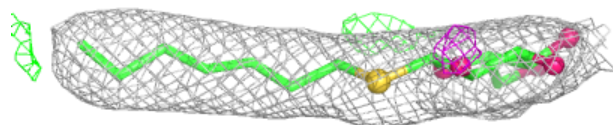
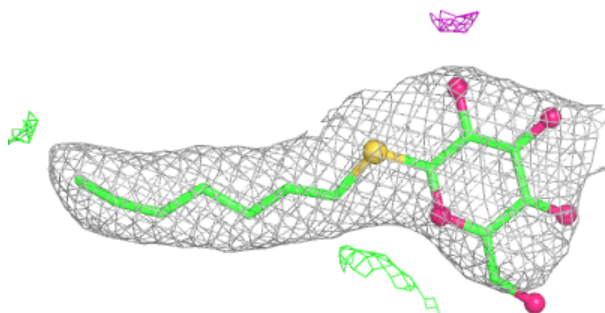
**Electron density around BCR Y 101:**

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

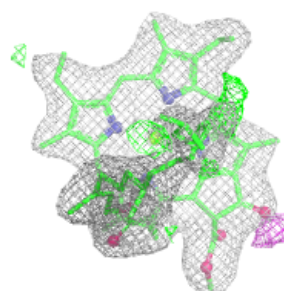
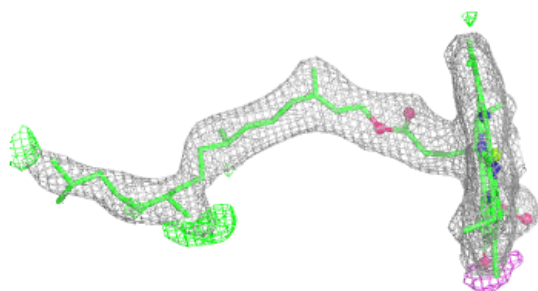
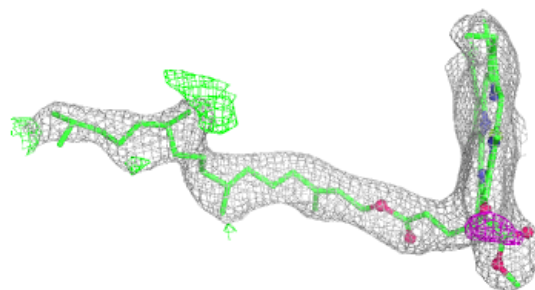


Electron density around HTG b 628:

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

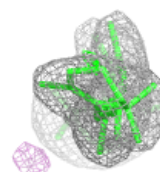
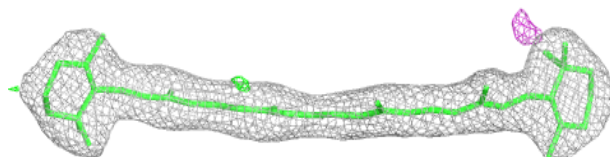
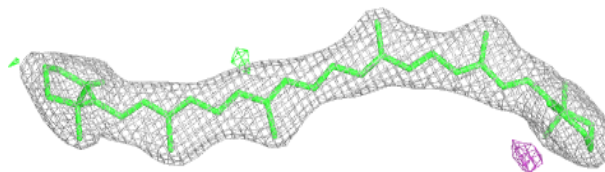
**Electron density around CLA b 606:**

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

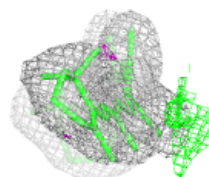
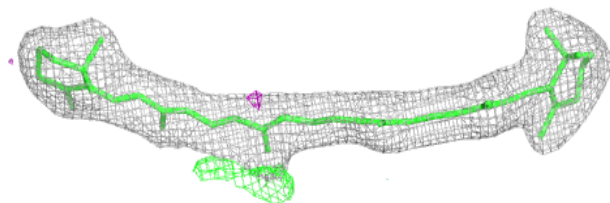
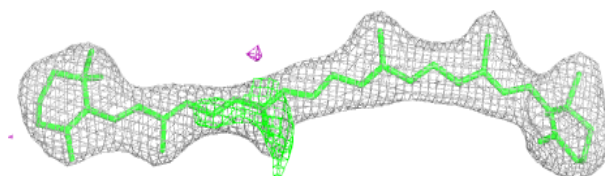


Electron density around BCR h 102:

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

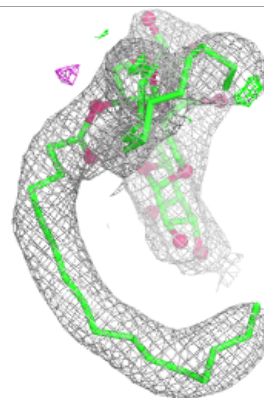
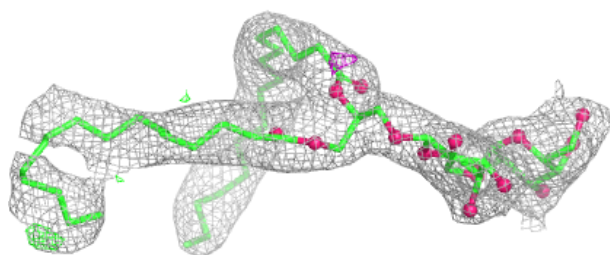
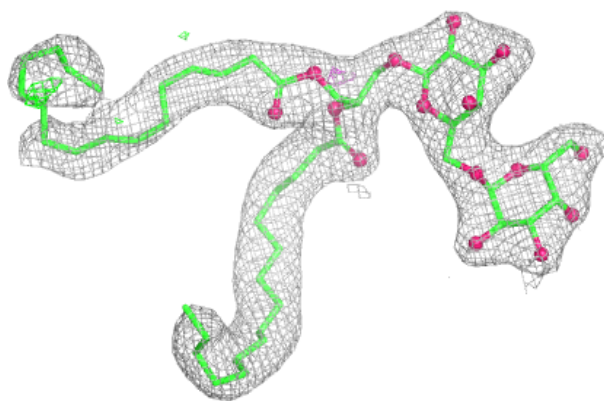
**Electron density around BCR t 102:**

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

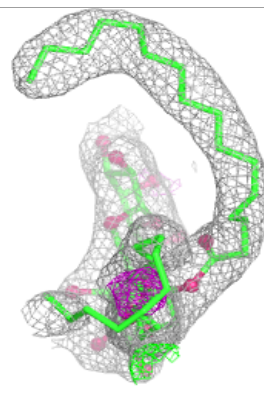
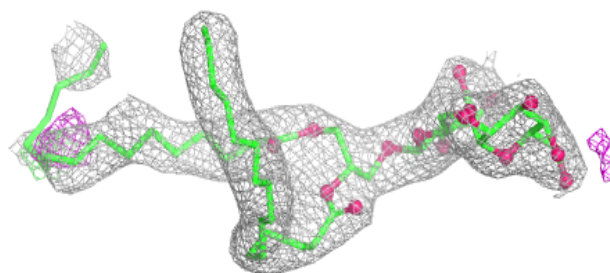
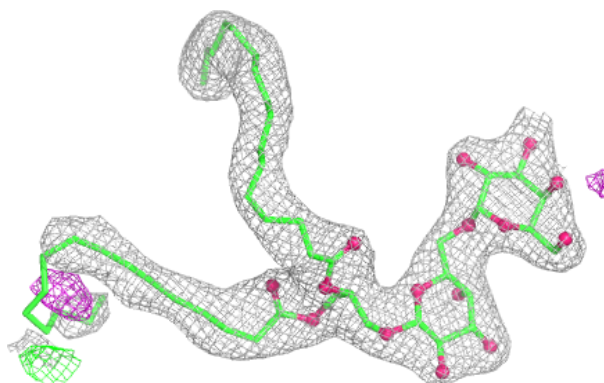


Electron density around DGD C 518:

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

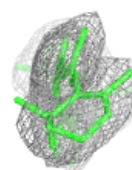
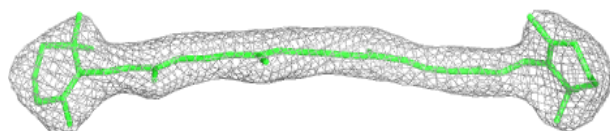
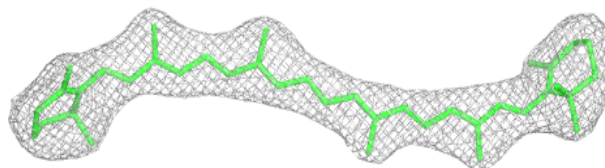
**Electron density around DGD c 519:**

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

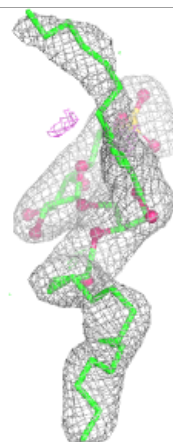
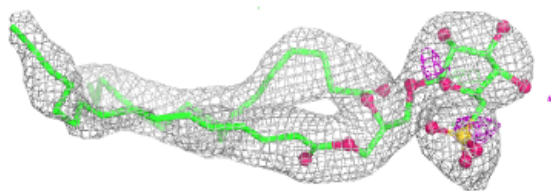
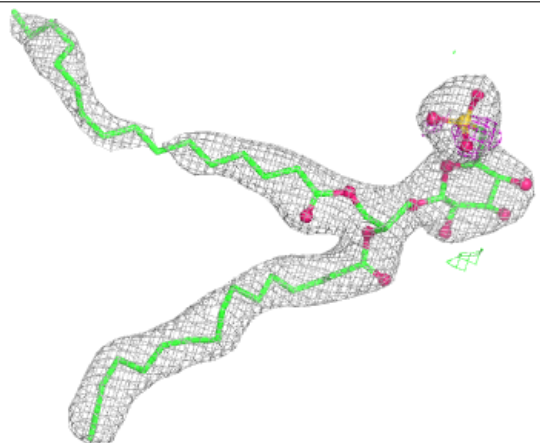


Electron density around BCR y 101:

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

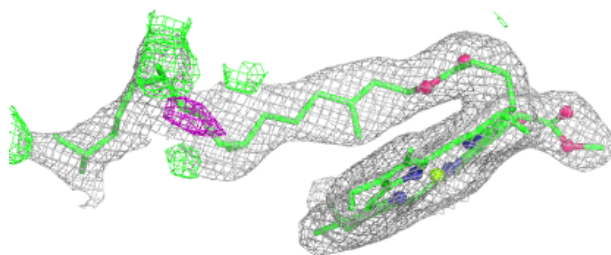
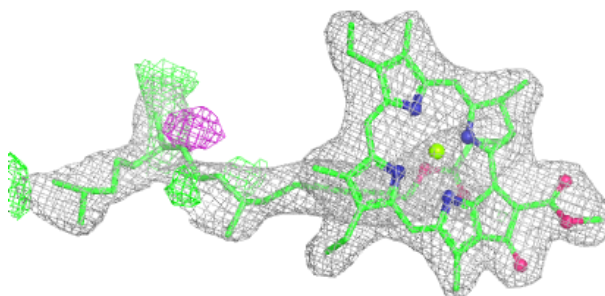
**Electron density around SQD A 411:**

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

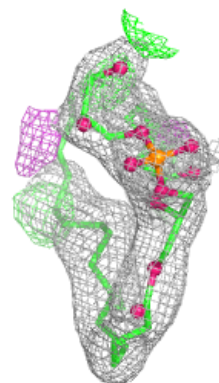
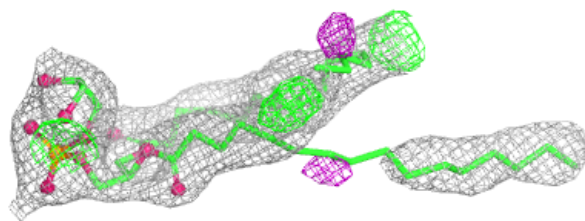
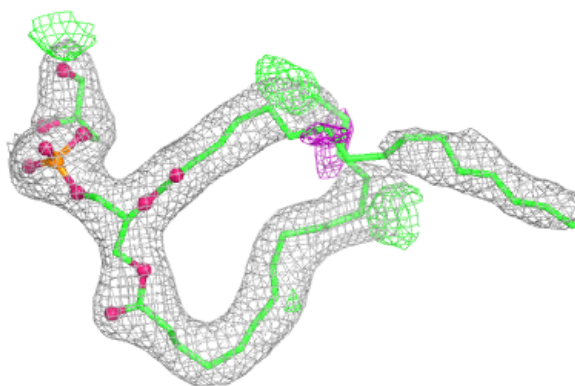


Electron density around CLA b 614:

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

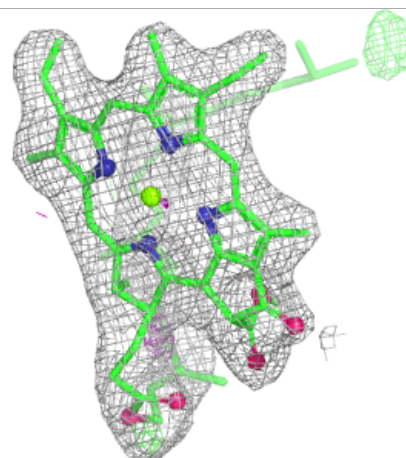
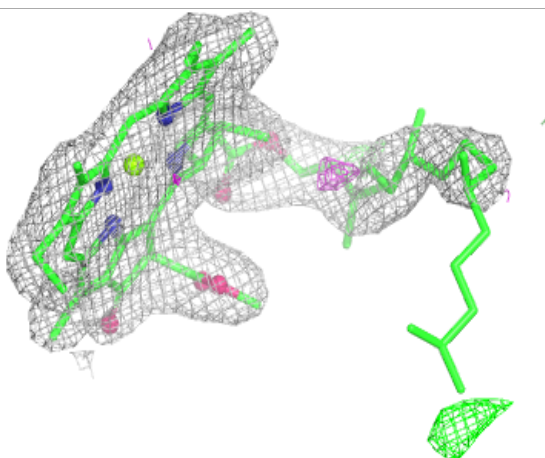
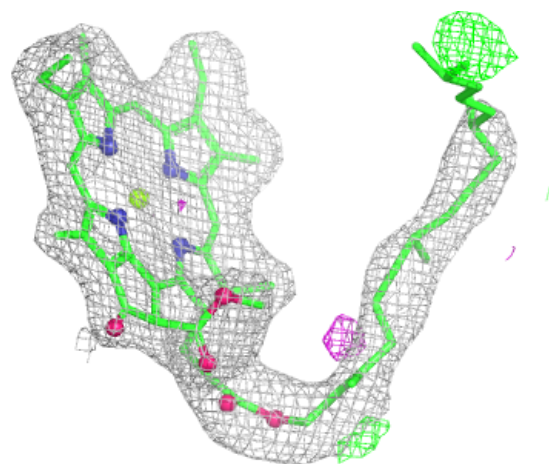
**Electron density around LHG D 407:**

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



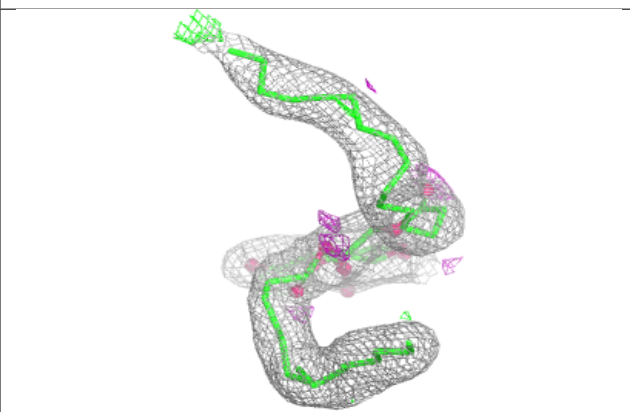
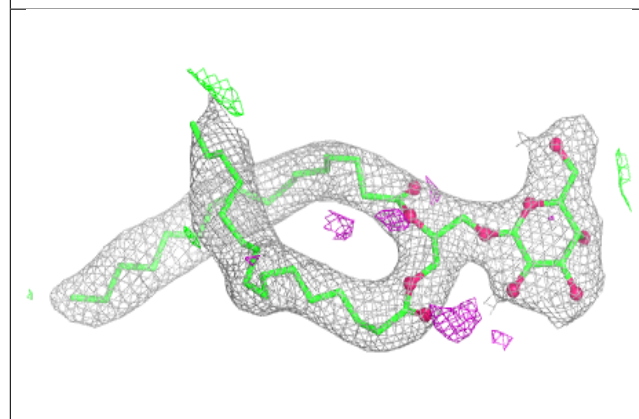
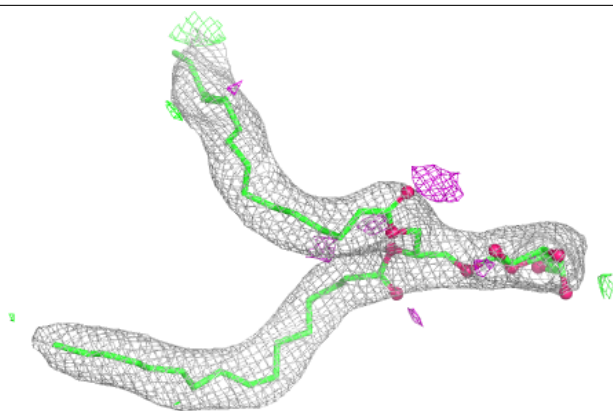
Electron density around CLA b 616:

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

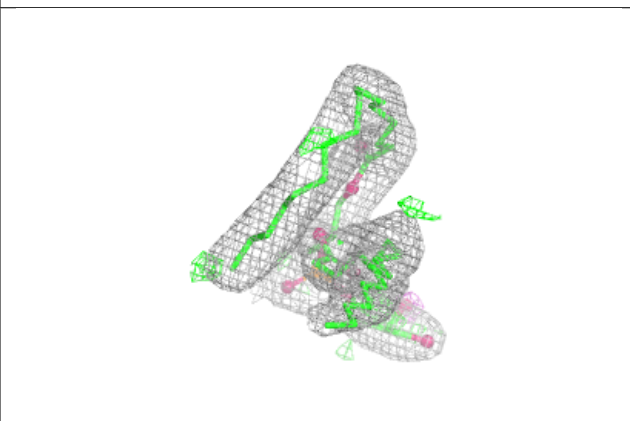
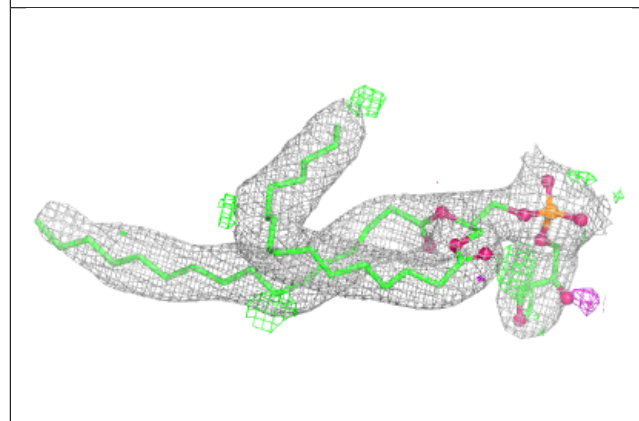
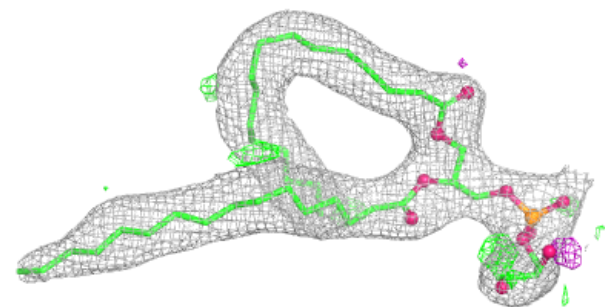


Electron density around LMG B 621:

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

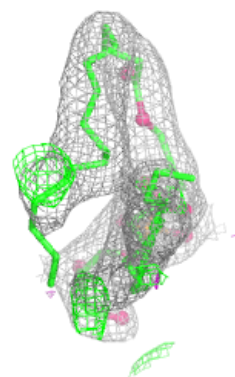
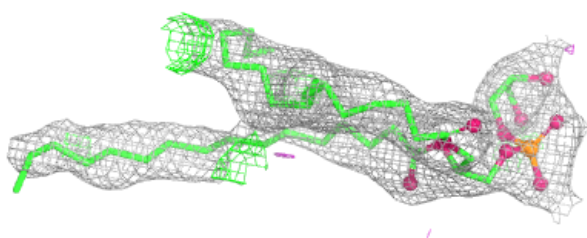
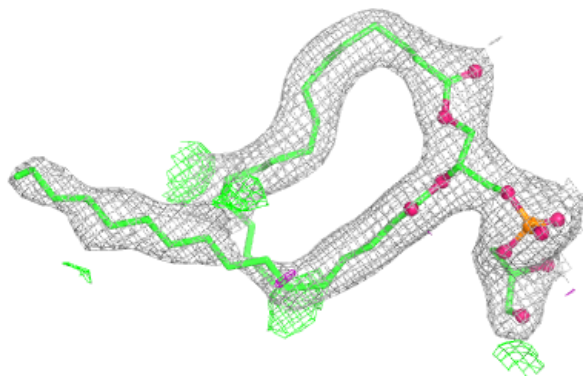
**Electron density around LHG d 406:**

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

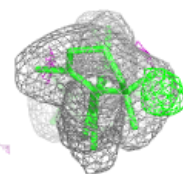
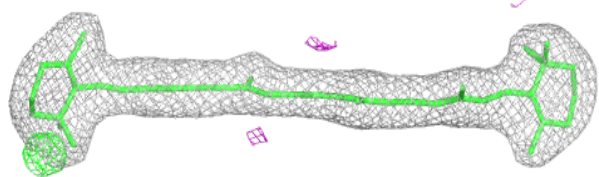
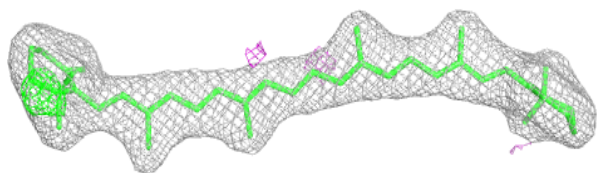


Electron density around LHG d 408:

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

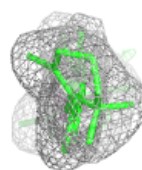
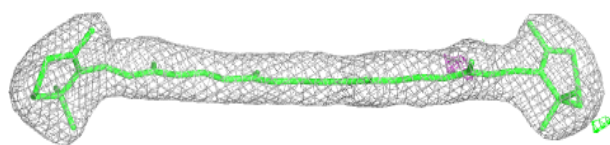
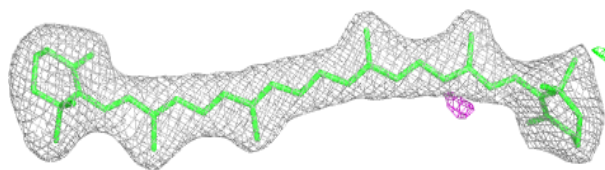
**Electron density around BCR A 410:**

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

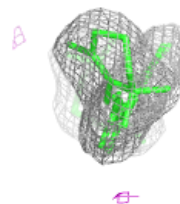
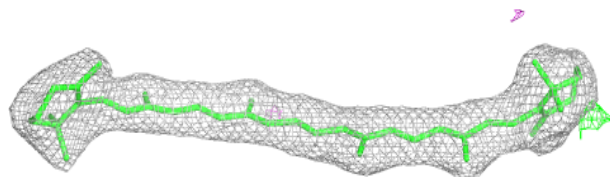
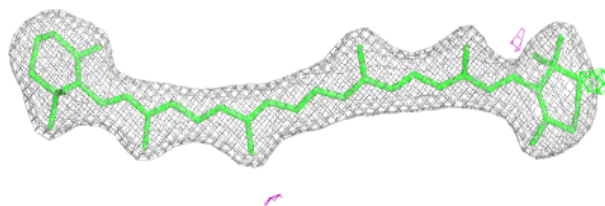


Electron density around BCR B 618:

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

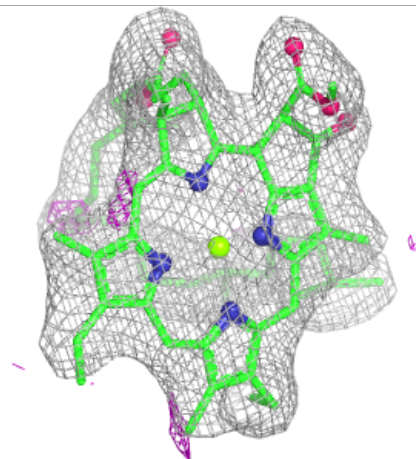
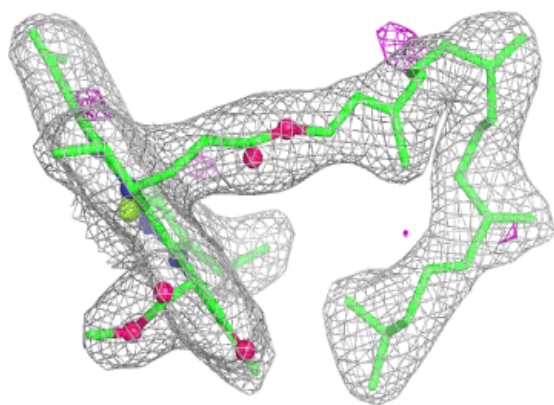
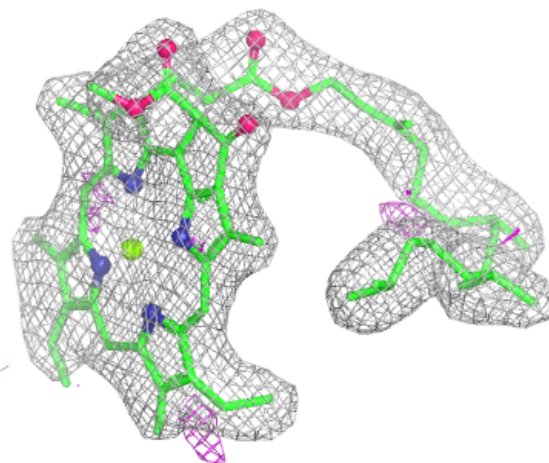
**Electron density around BCR B 619:**

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



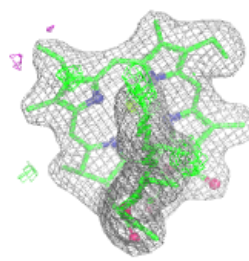
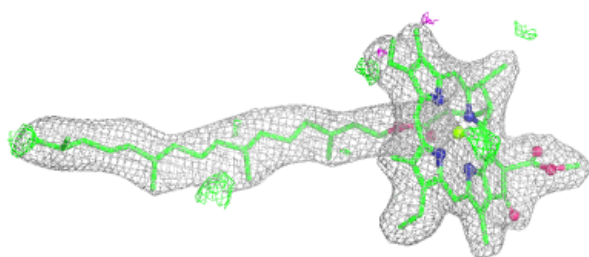
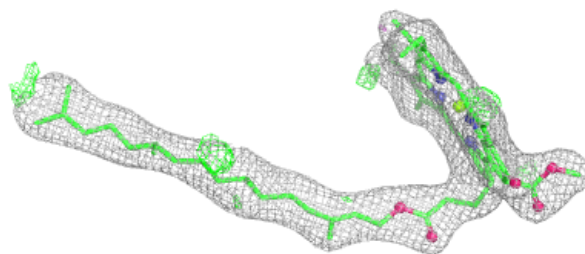
Electron density around CLA C 504:

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

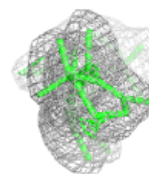
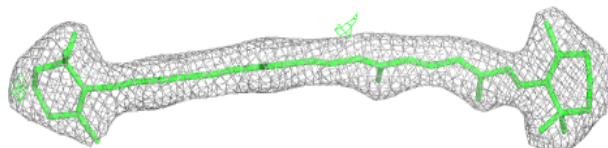
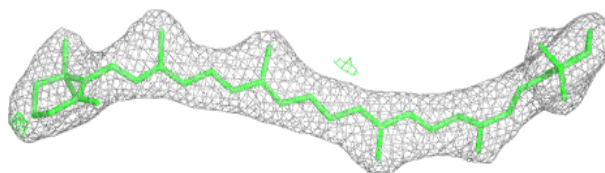


Electron density around CLA b 607:

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

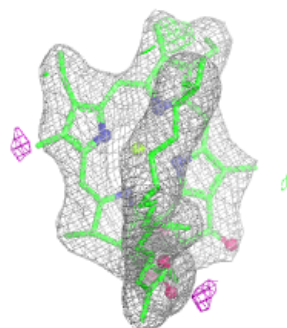
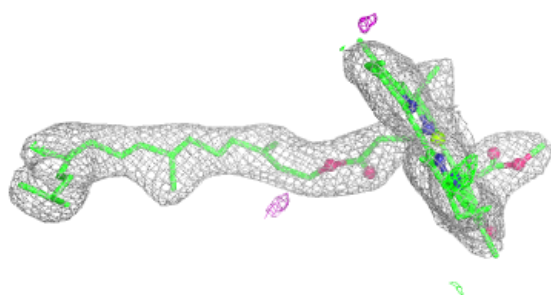
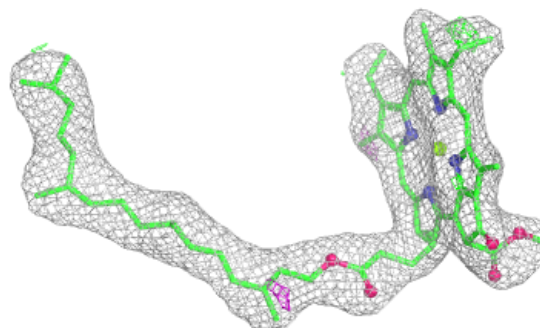
**Electron density around BCR H 101:**

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

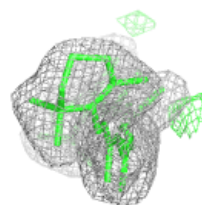
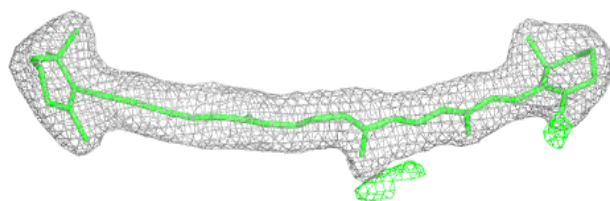
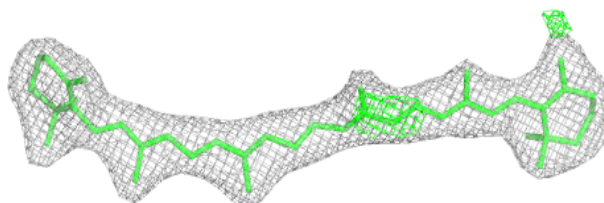


Electron density around CLA b 609:

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

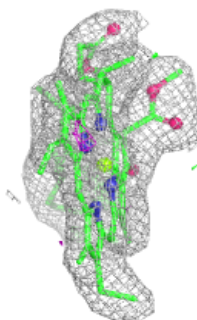
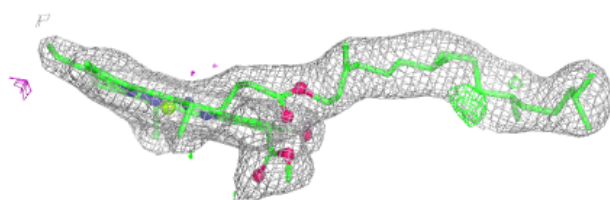
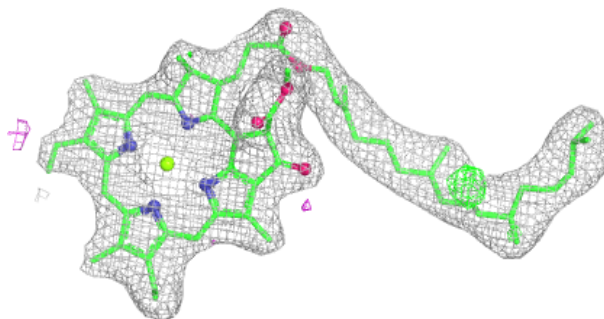
**Electron density around BCR T 101:**

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

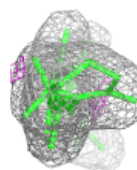
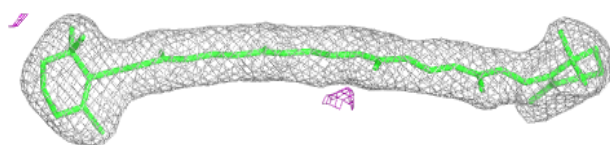
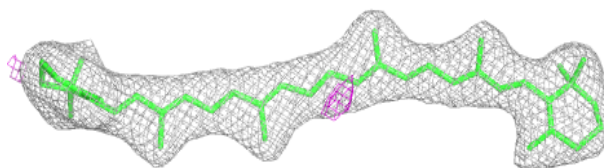


Electron density around CLA B 602:

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

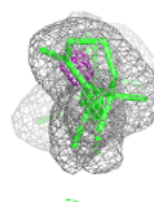
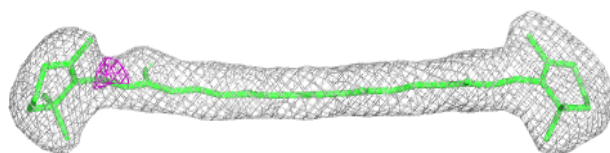
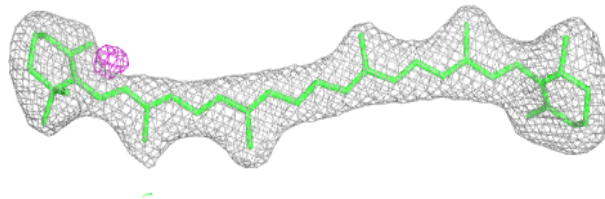
**Electron density around BCR b 617:**

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

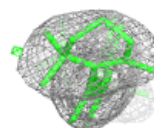
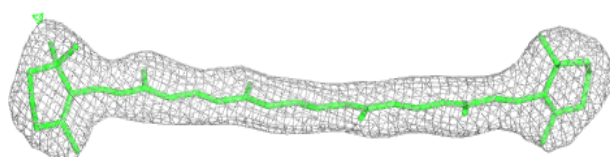
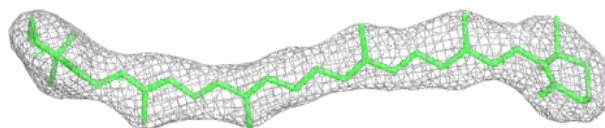


Electron density around BCR b 618:

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

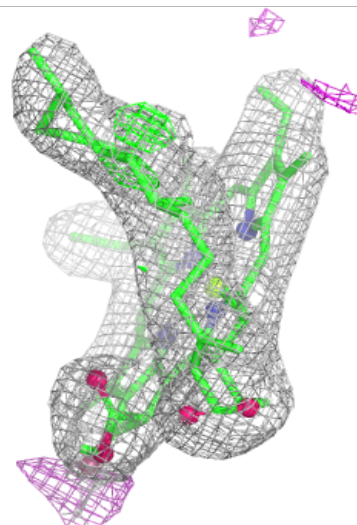
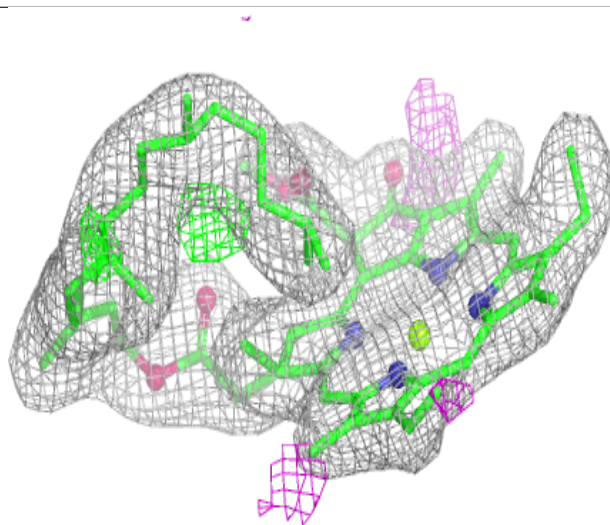
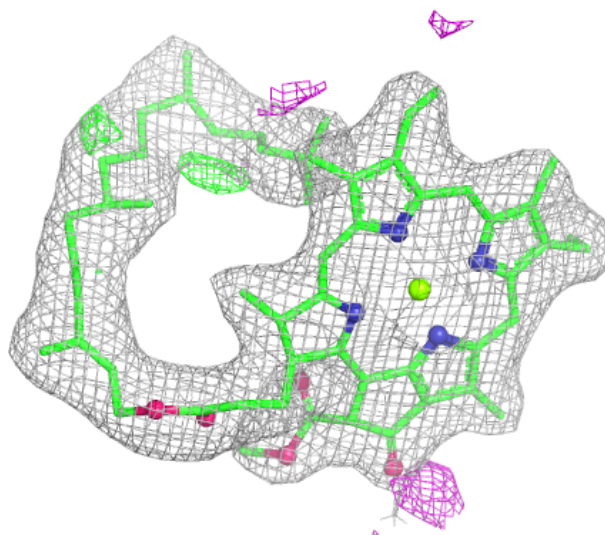
**Electron density around BCR c 516:**

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



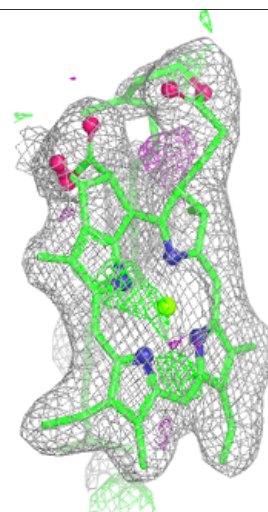
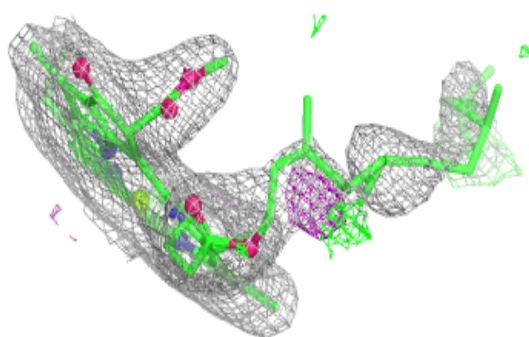
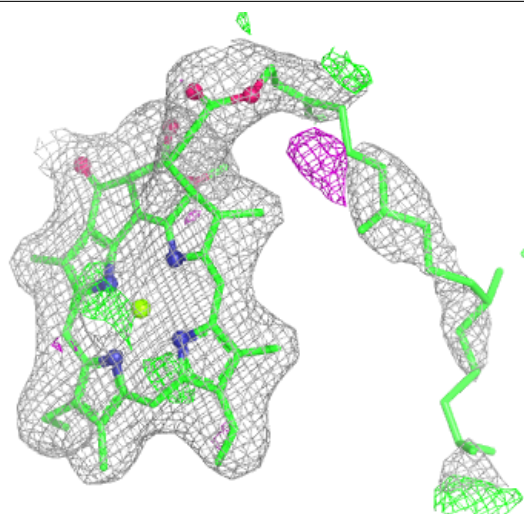
Electron density around CLA b 615:

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



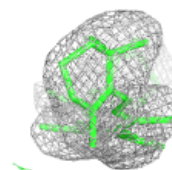
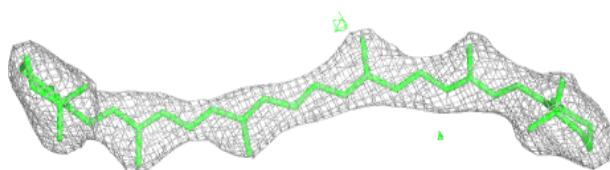
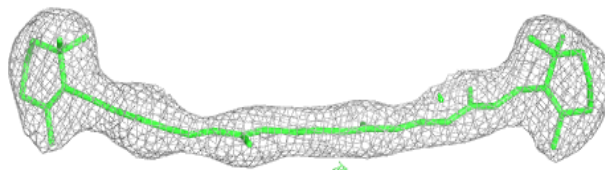
Electron density around CLA B 616:

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

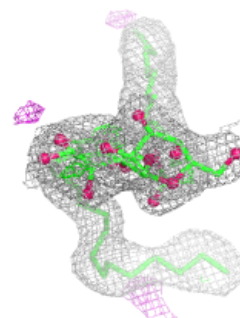
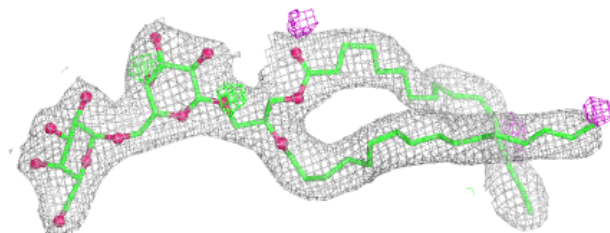
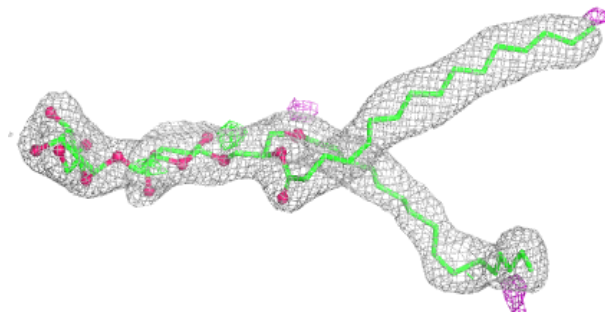


Electron density around BCR k 101:

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

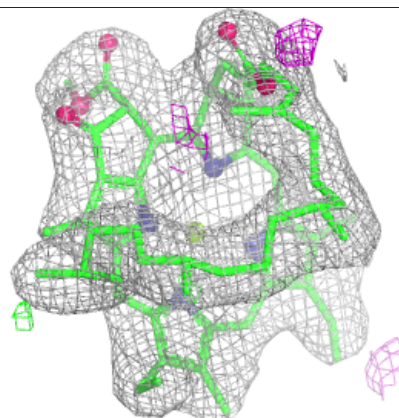
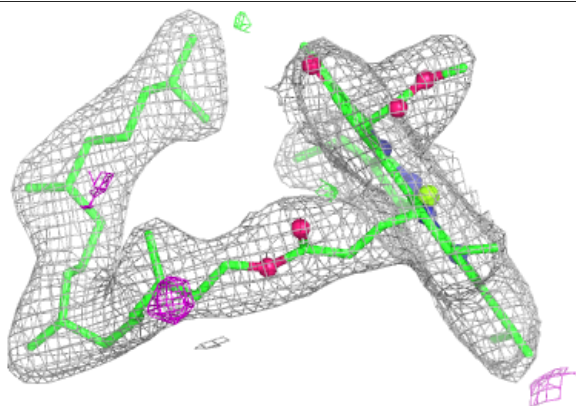
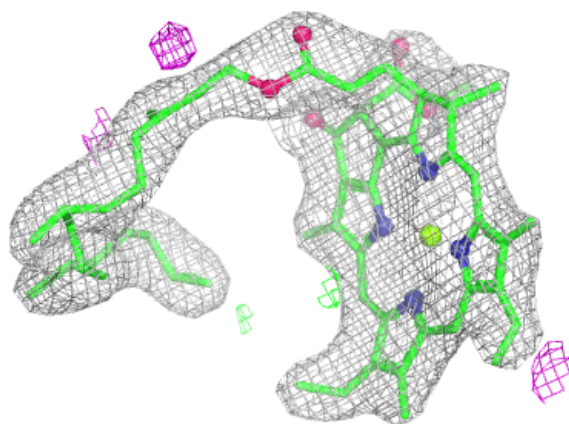
**Electron density around DGD C 517:**

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

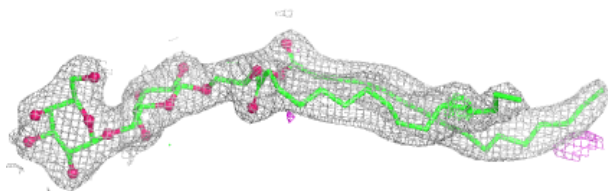
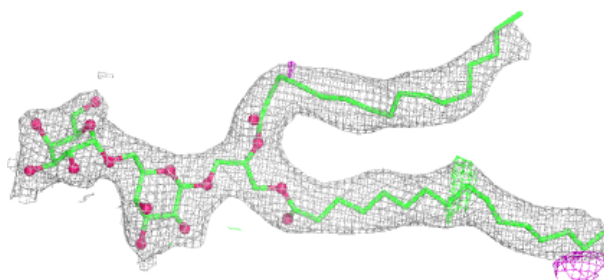


Electron density around CLA c 505:

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

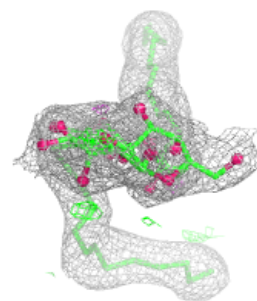
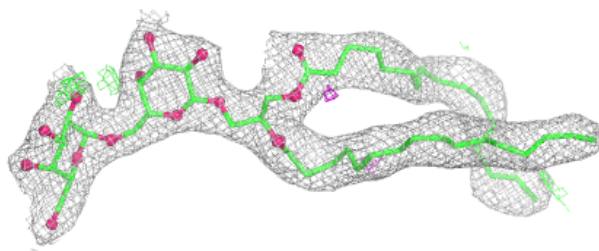
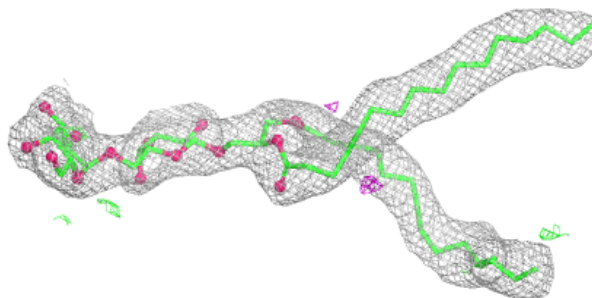
**Electron density around DGD C 519:**

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

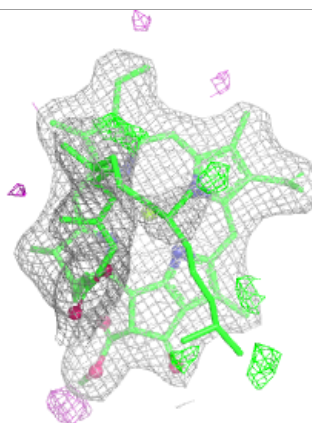
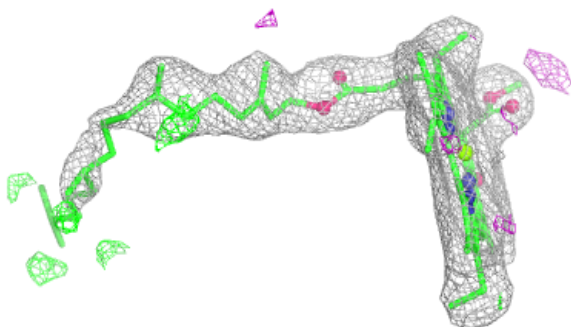
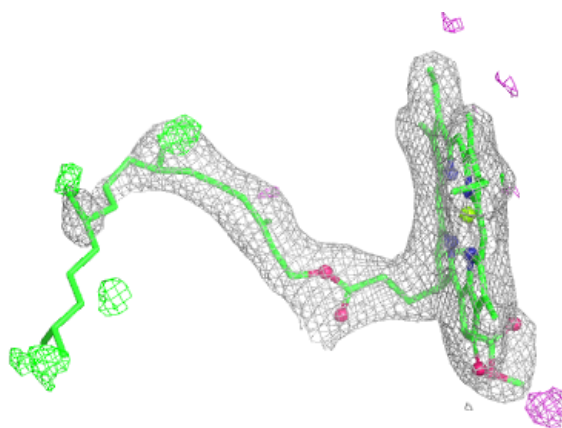


Electron density around DGD c 518:

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

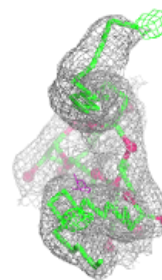
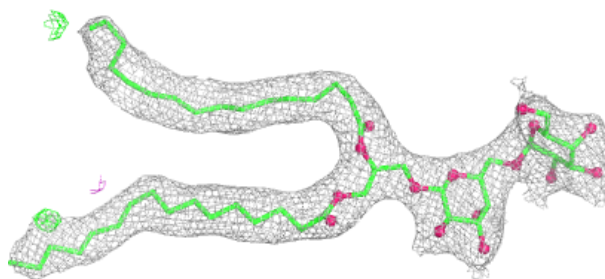
**Electron density around CLA D 403:**

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

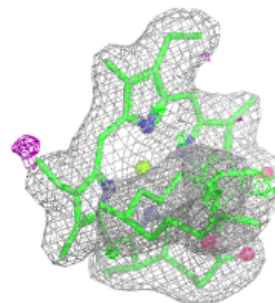
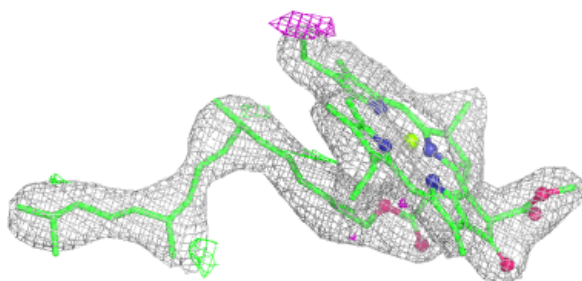
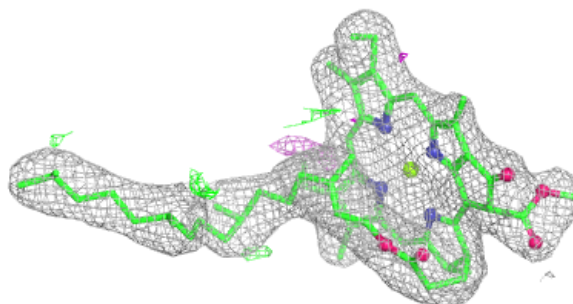


Electron density around DGD c 520:

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

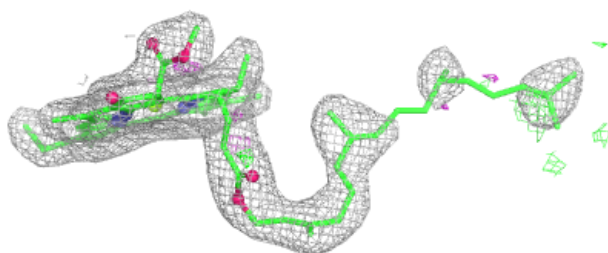
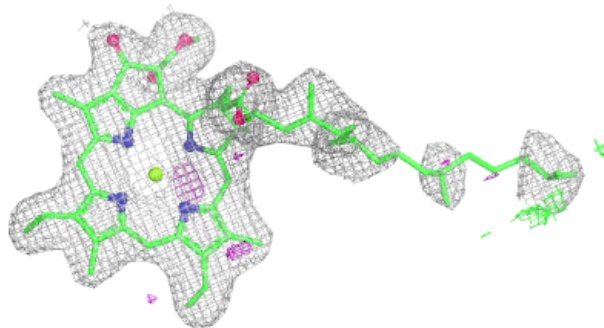
**Electron density around CLA c 507:**

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

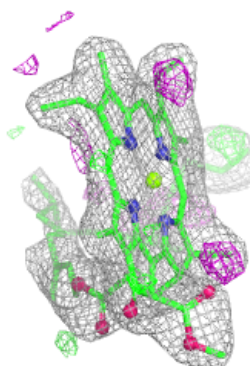
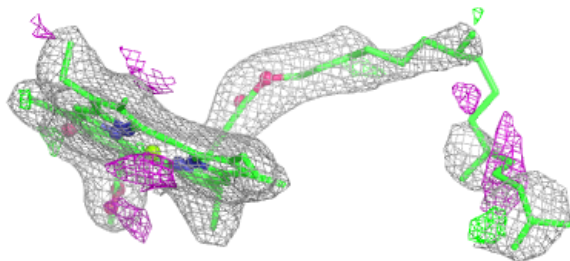
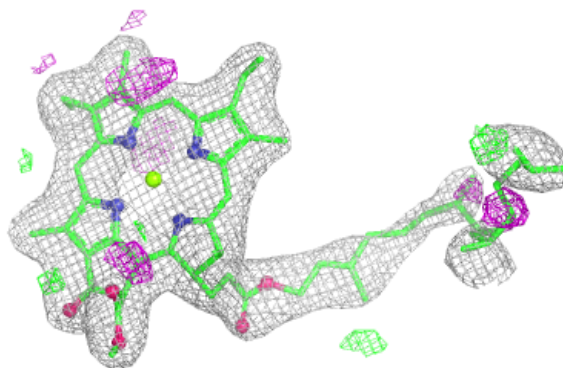


Electron density around CLA a 404:

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

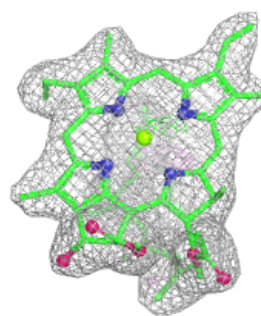
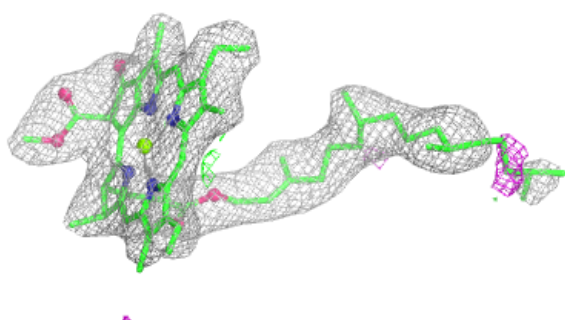
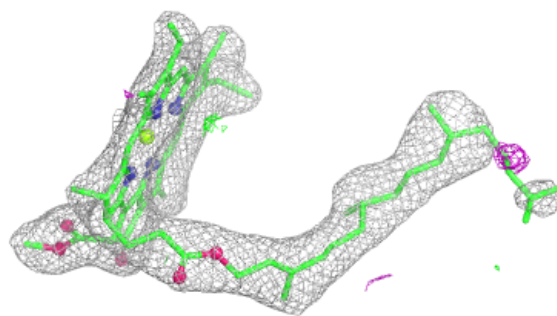
**Electron density around CLA a 407:**

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



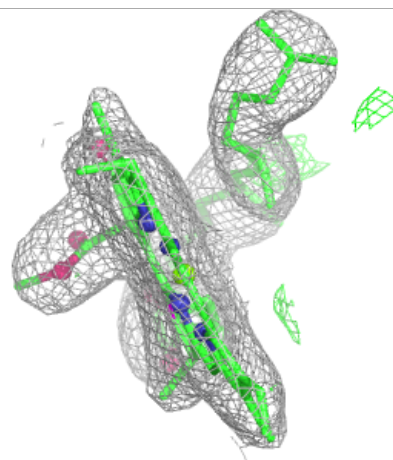
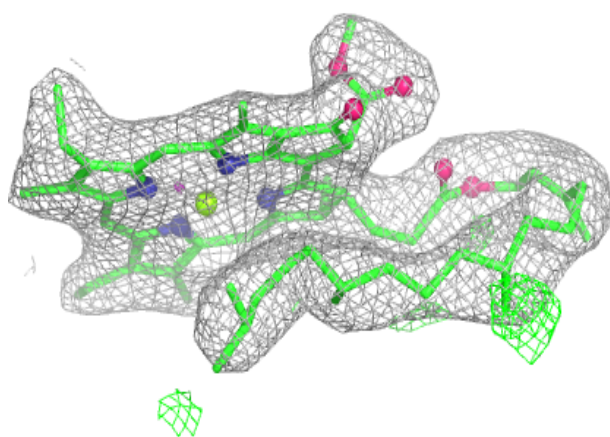
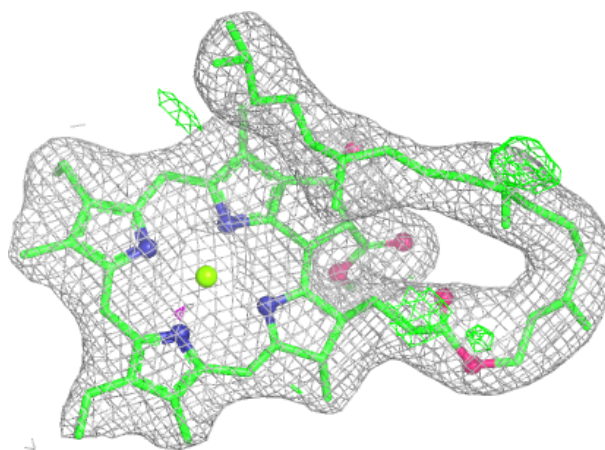
Electron density around CLA c 510:

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



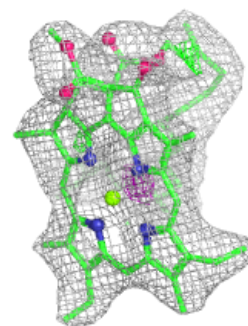
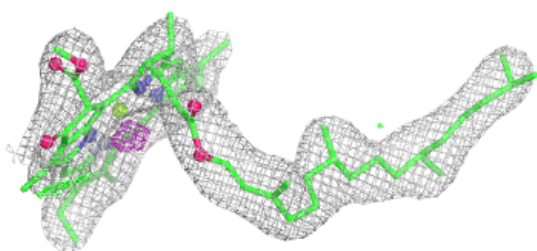
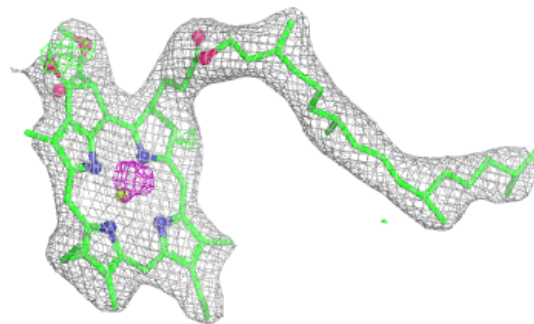
Electron density around CLA c 511:

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

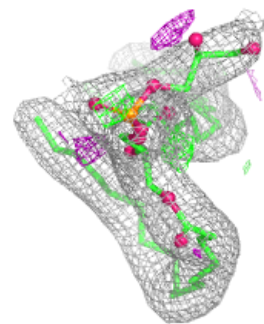
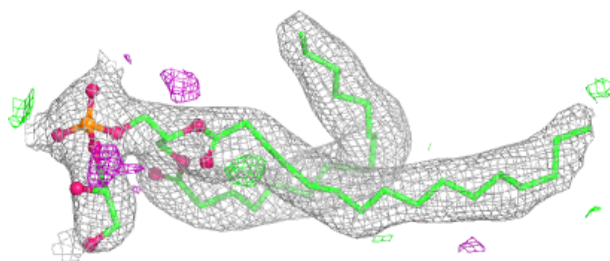
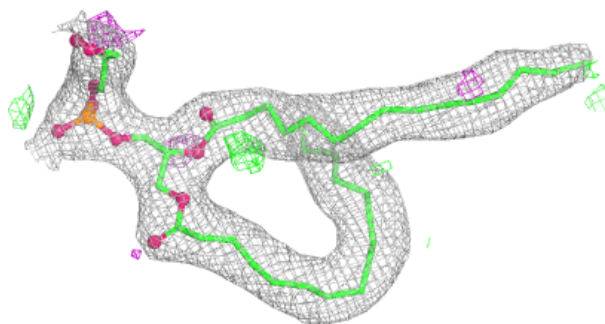


Electron density around CLA c 513:

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

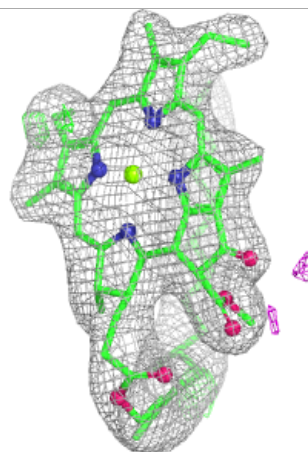
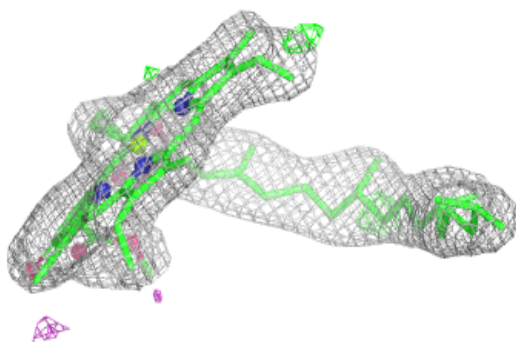
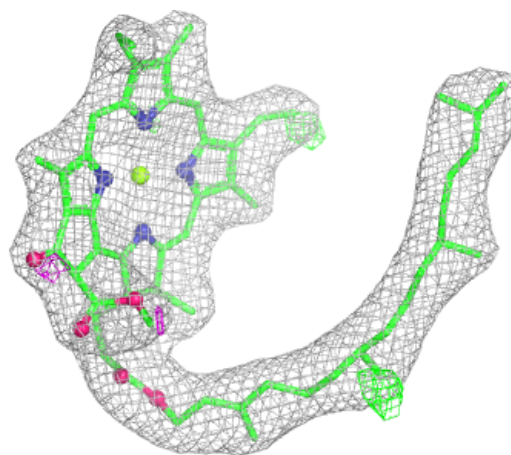
**Electron density around LHG D 357:**

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



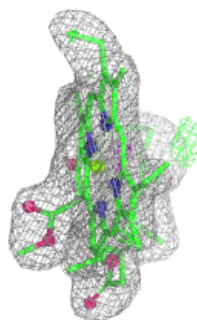
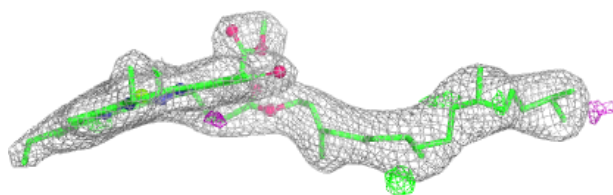
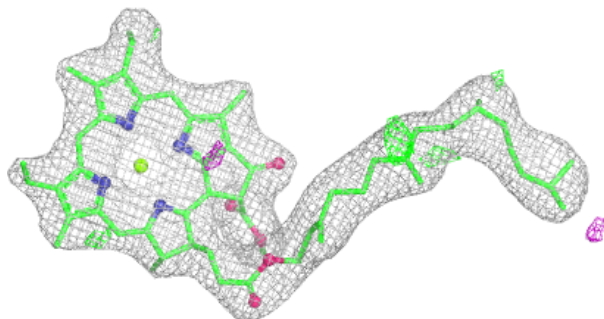
Electron density around CLA C 508:

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

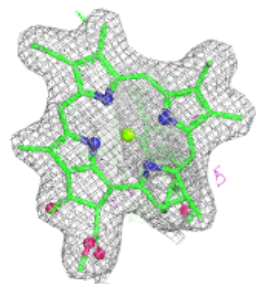
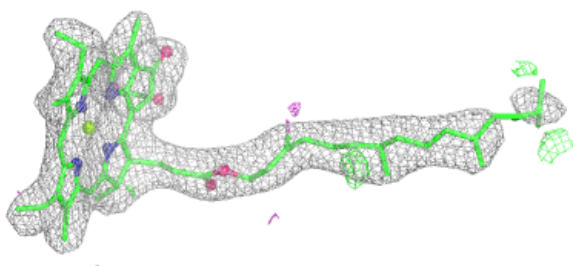
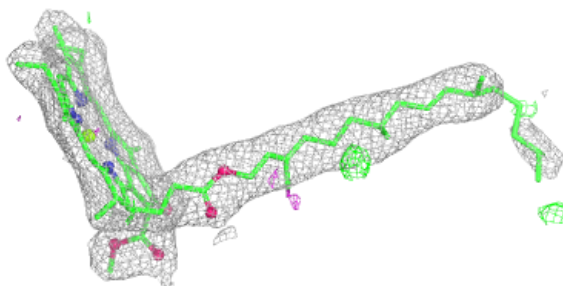


Electron density around CLA b 602:

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

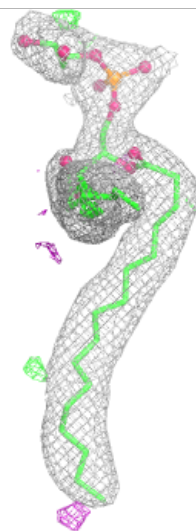
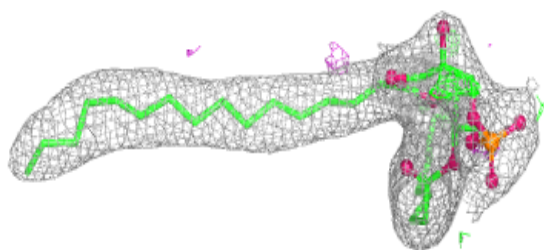
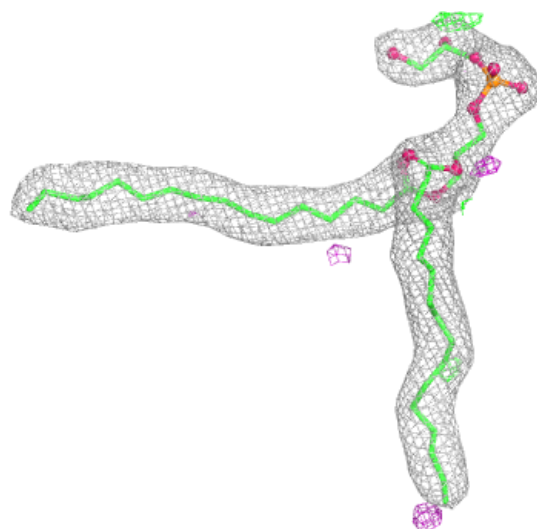
**Electron density around CLA b 604:**

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



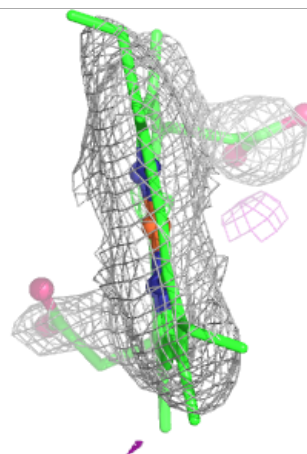
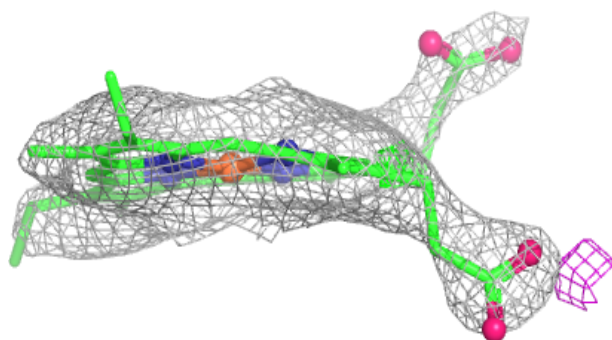
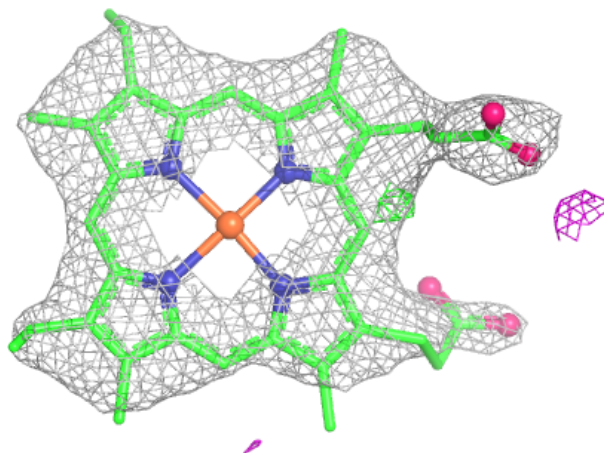
Electron density around LHG 1 101:

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



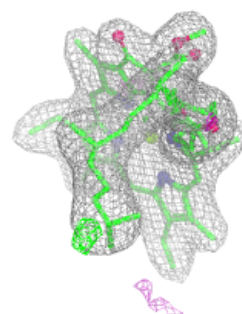
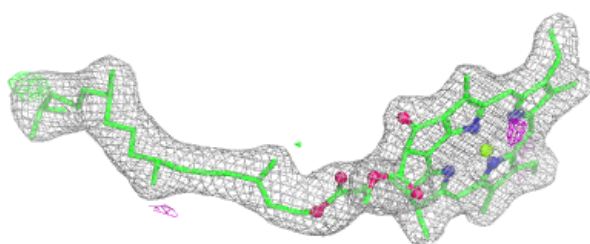
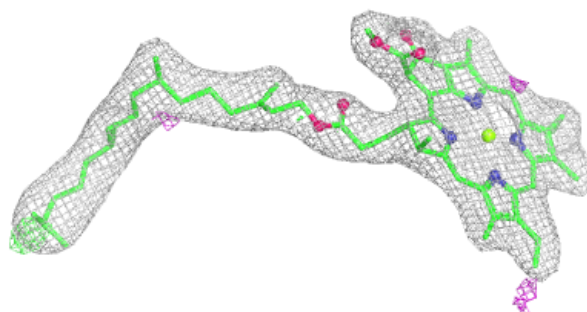
Electron density around HEM e 102:

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

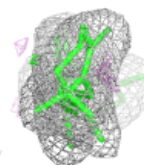
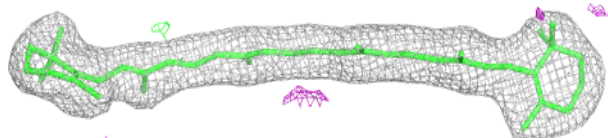
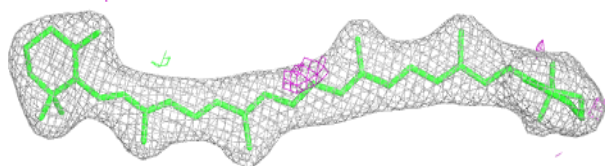


Electron density around CLA a 403:

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

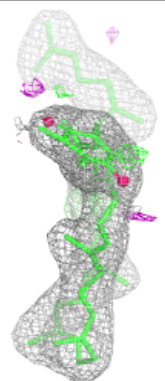
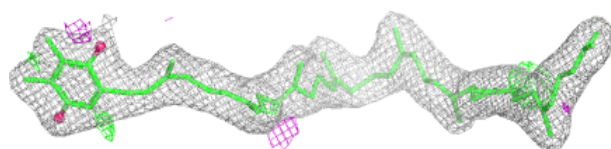
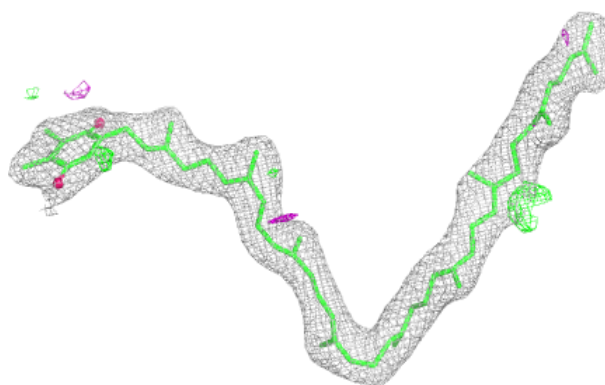
**Electron density around BCR B 617:**

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

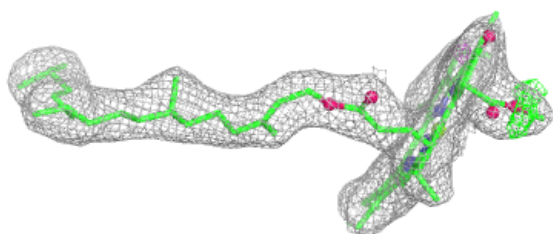
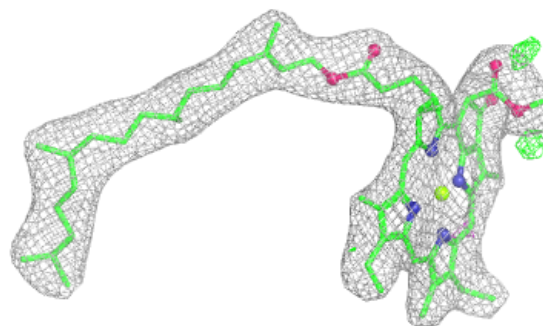


Electron density around PL9 D 405:

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

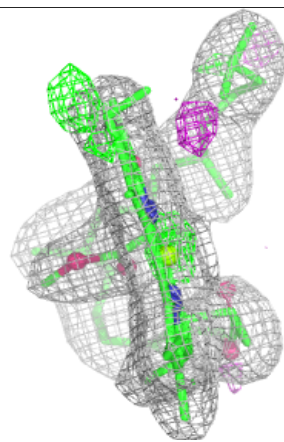
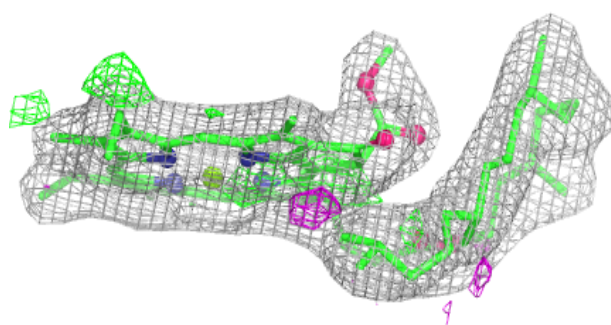
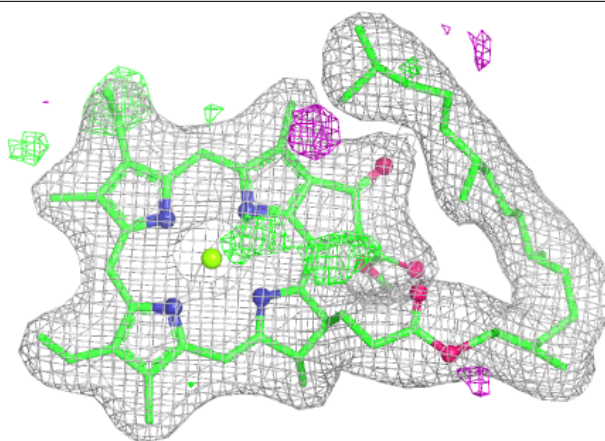
**Electron density around CLA B 609:**

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

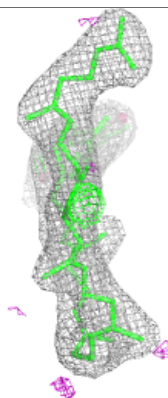
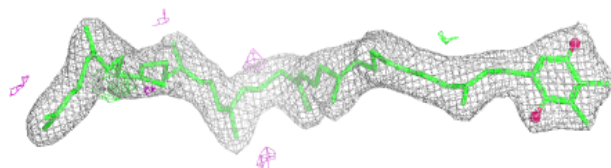
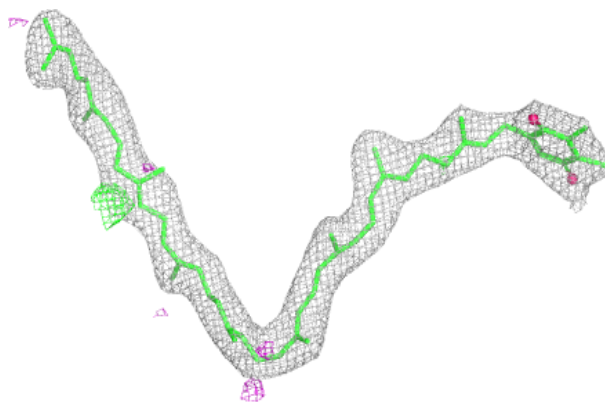


Electron density around CLA B 610:

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

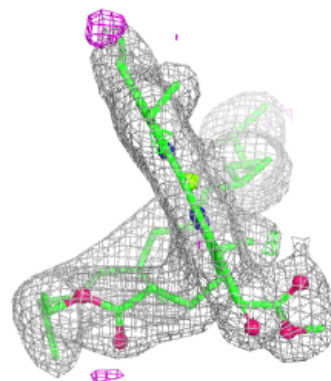
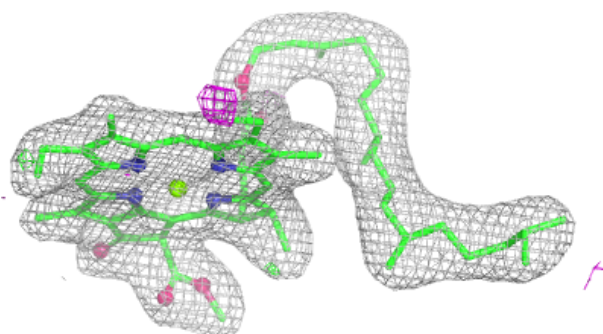
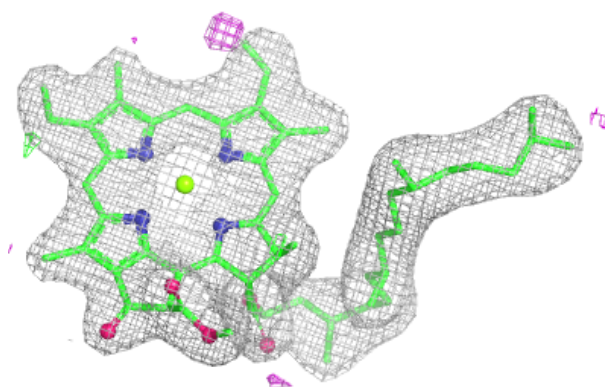
**Electron density around PL9 d 405:**

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

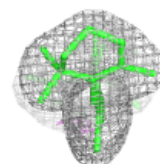
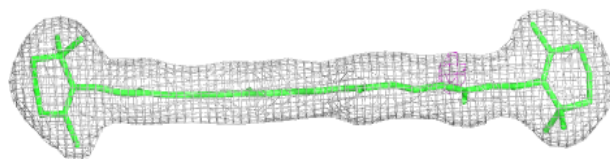
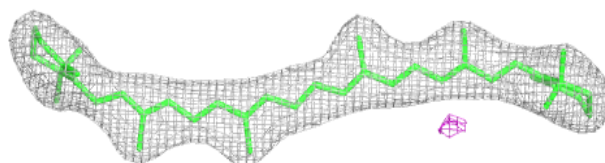


Electron density around CLA a 350:

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

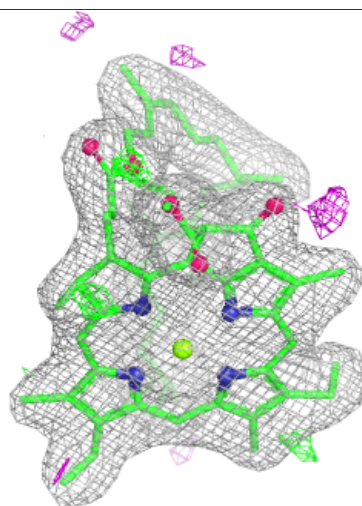
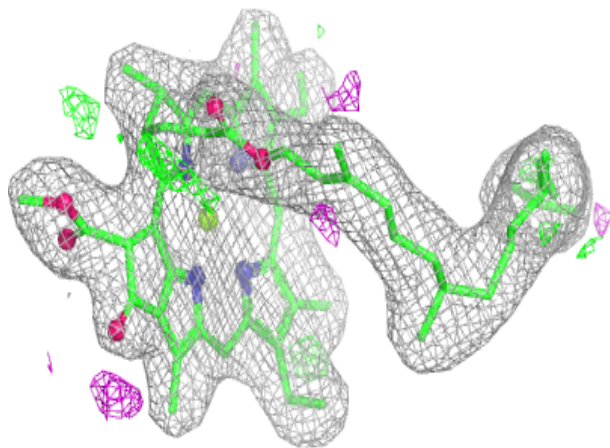
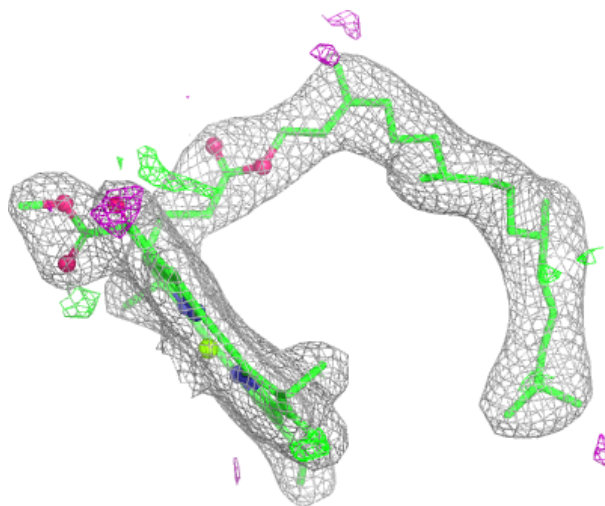
**Electron density around BCR C 516:**

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



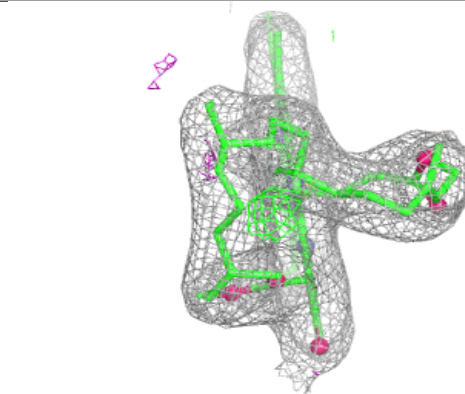
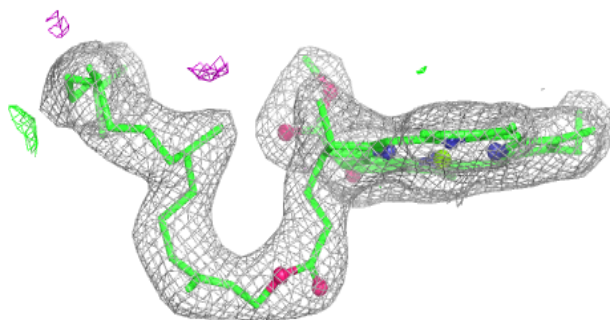
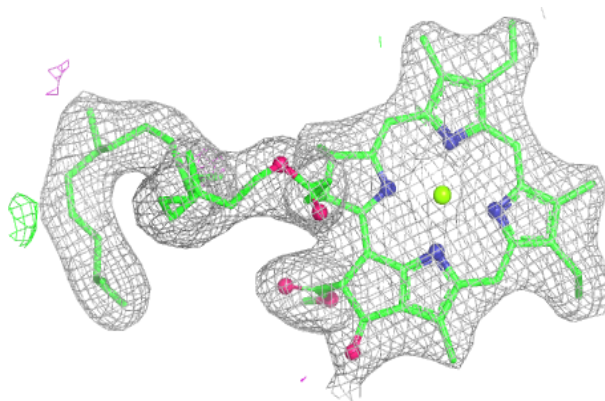
Electron density around CLA B 611:

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

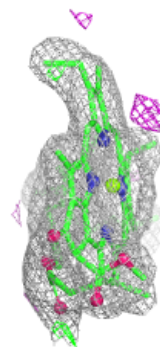
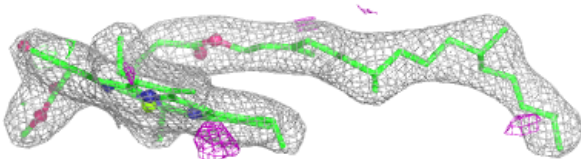
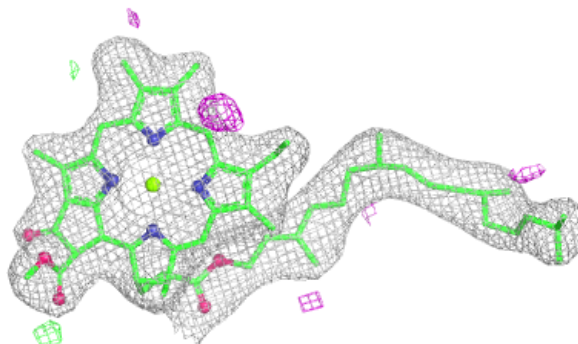


Electron density around CLA B 612:

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

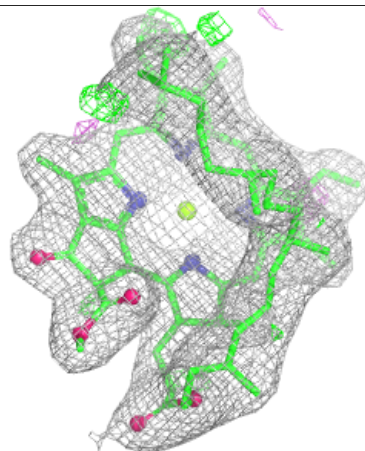
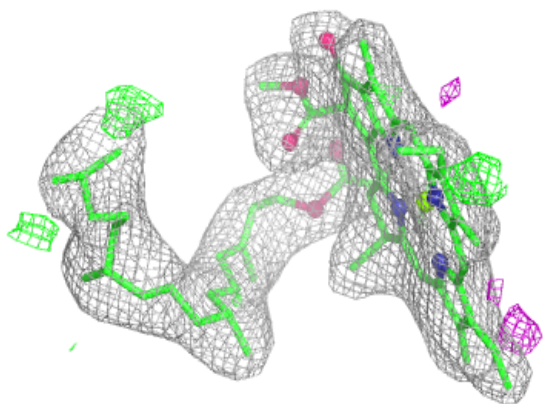
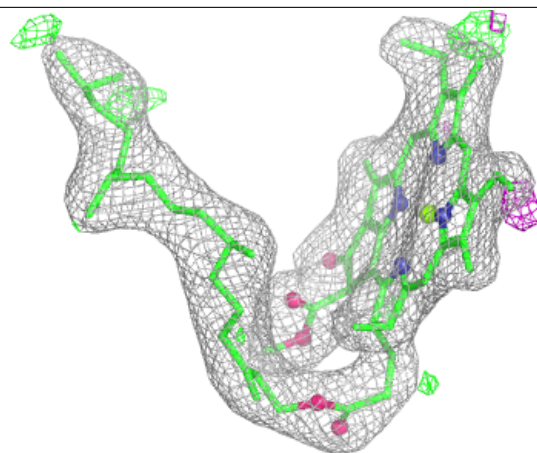
**Electron density around CLA b 603:**

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



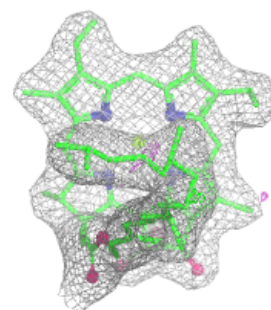
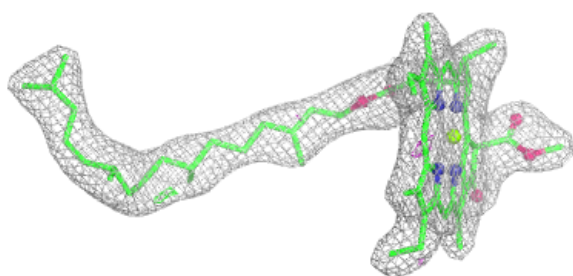
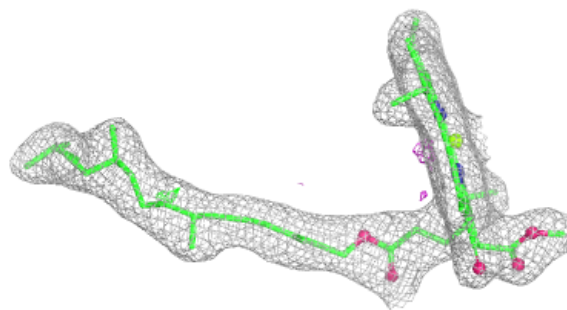
Electron density around CLA B 613:

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

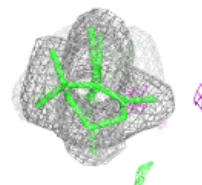
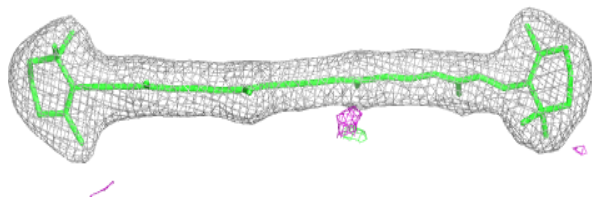
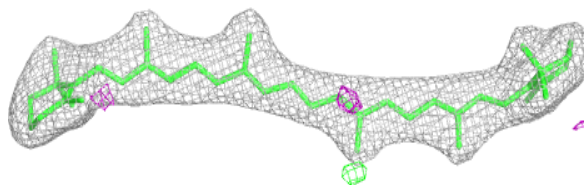


Electron density around CLA b 605:

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

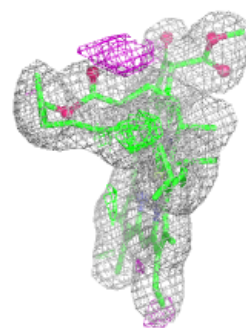
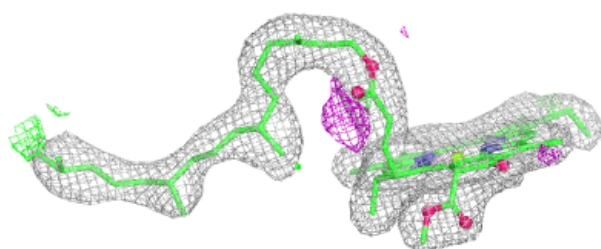
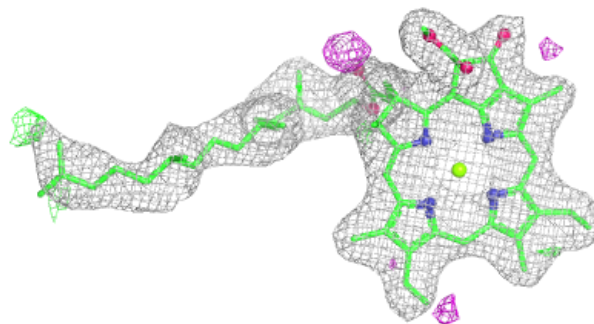
**Electron density around BCR a 408:**

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



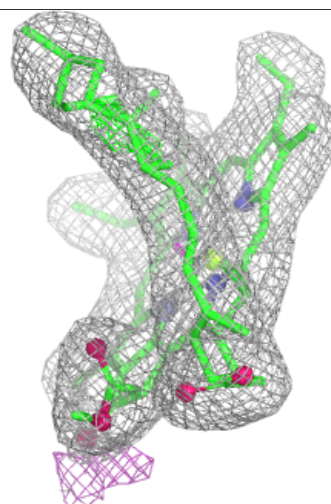
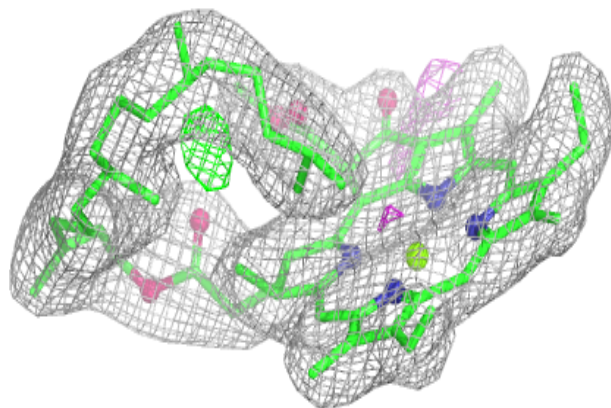
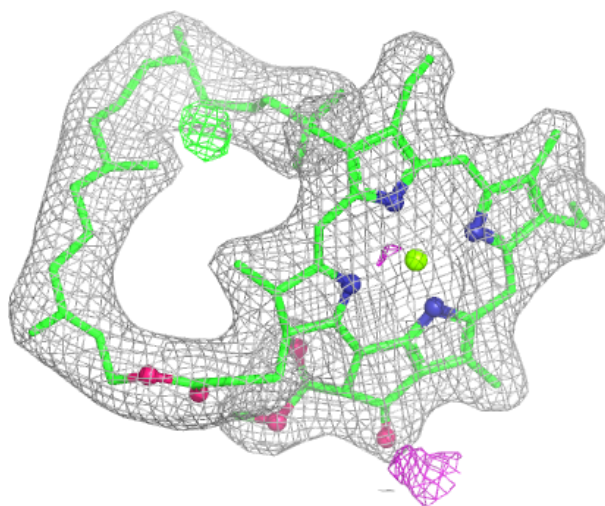
Electron density around CLA A 406:

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



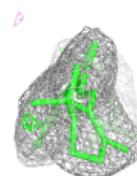
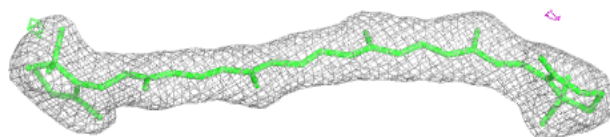
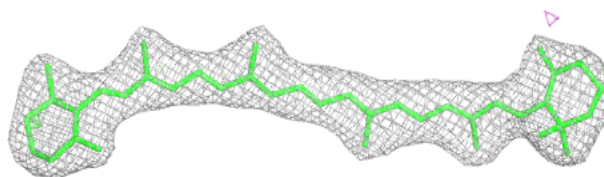
Electron density around CLA B 615:

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

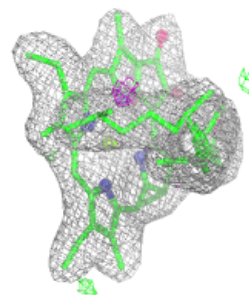
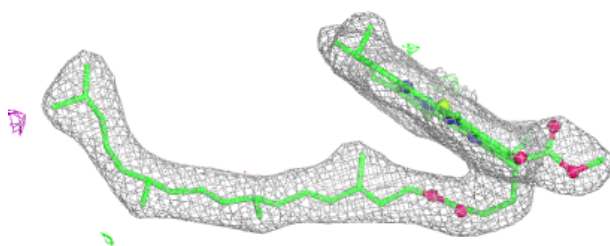
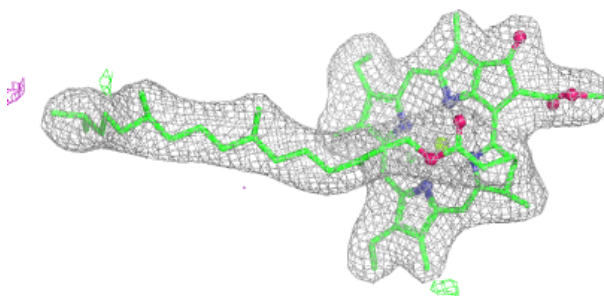


Electron density around BCR b 619:

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

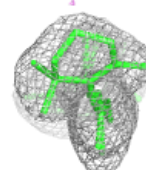
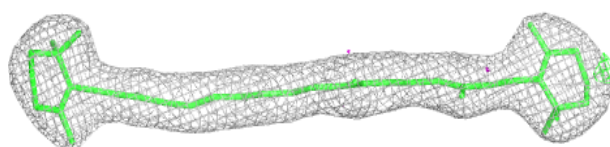
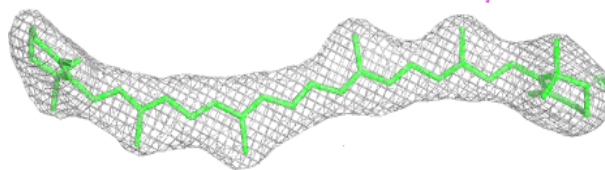
**Electron density around CLA b 608:**

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

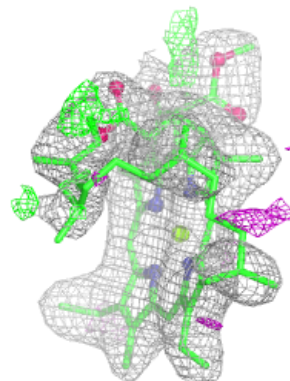
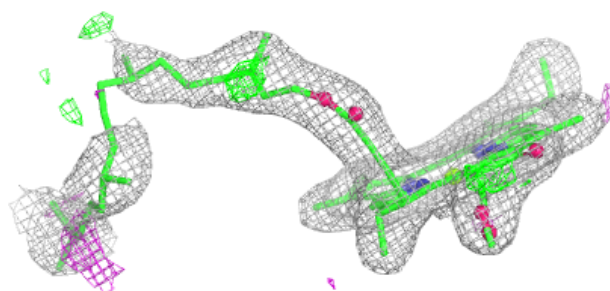
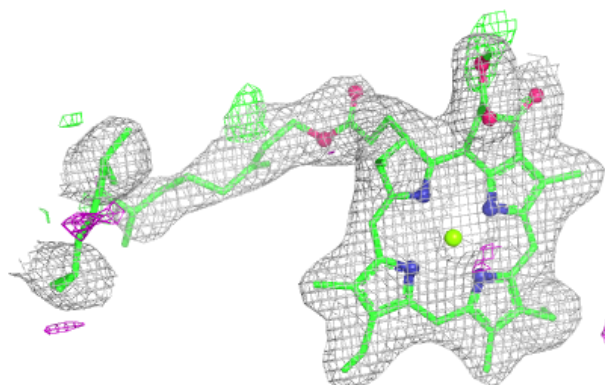


Electron density around BCR c 517:

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

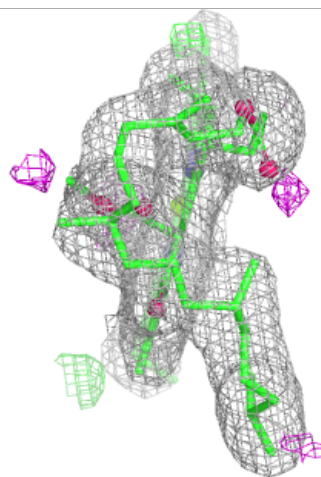
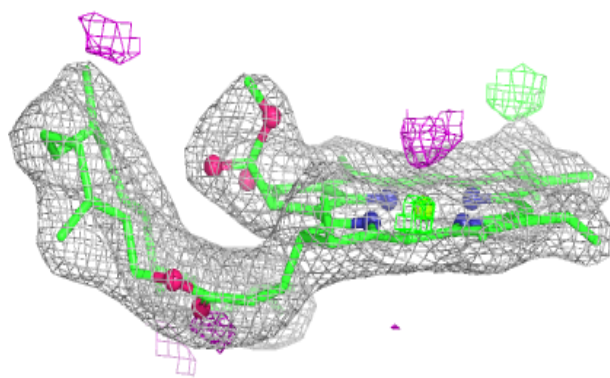
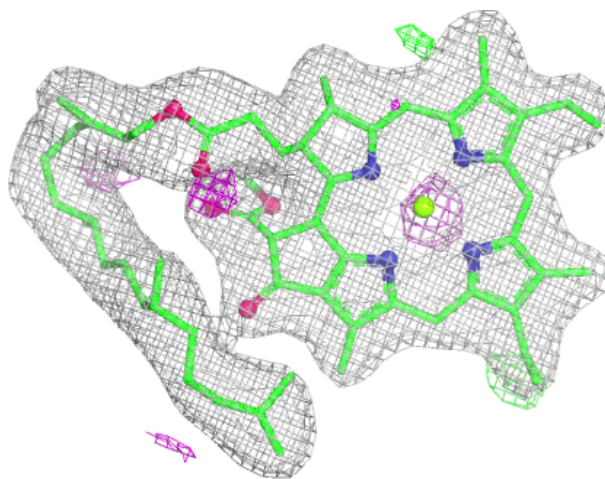
**Electron density around CLA A 409:**

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



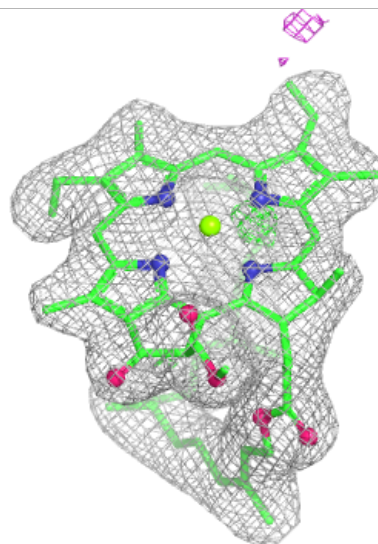
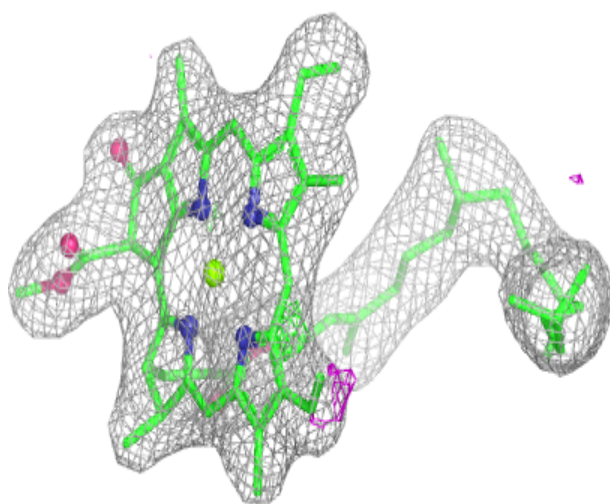
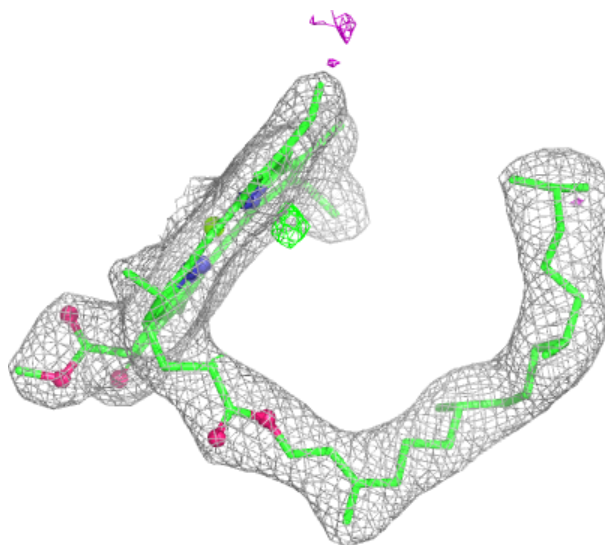
Electron density around CLA b 610:

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



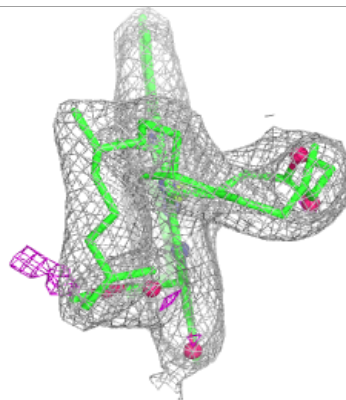
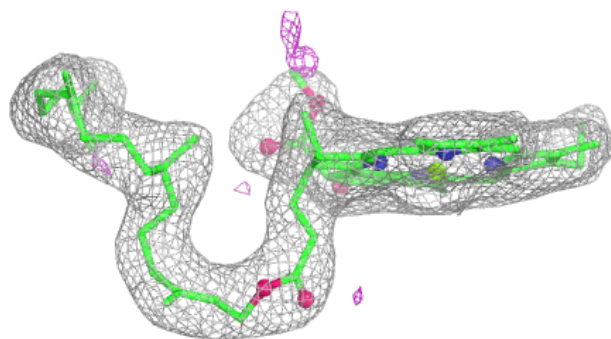
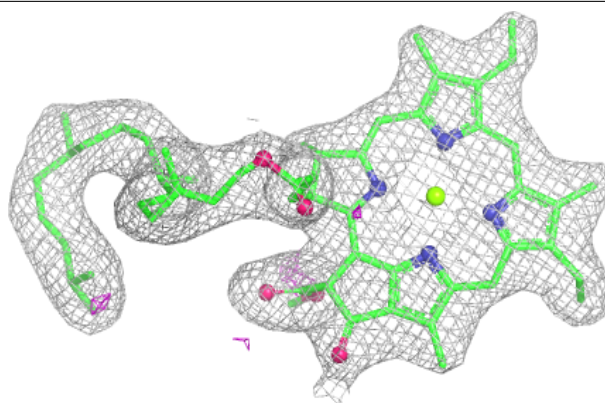
Electron density around CLA b 611:

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

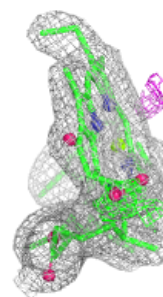
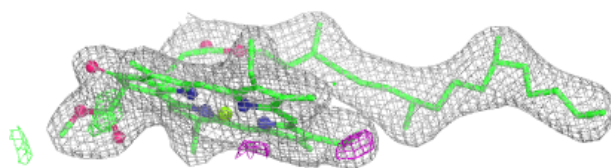
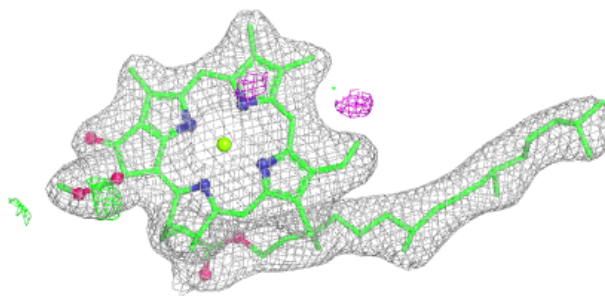


Electron density around CLA b 612:

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

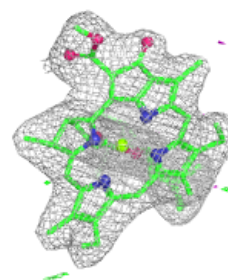
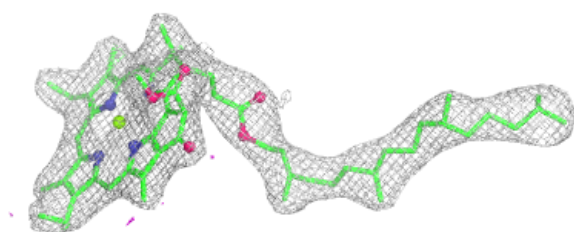
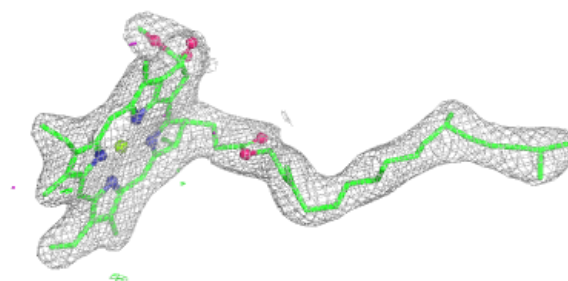
**Electron density around CLA C 502:**

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

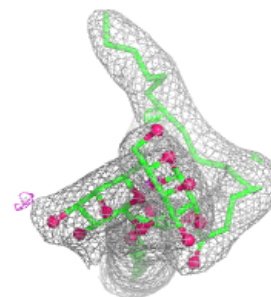
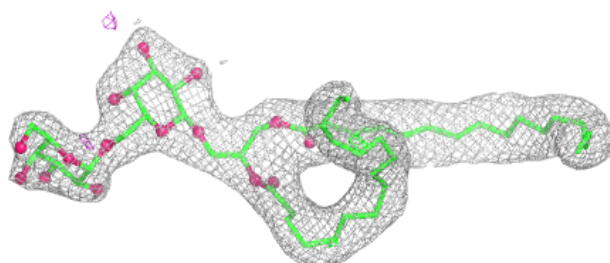
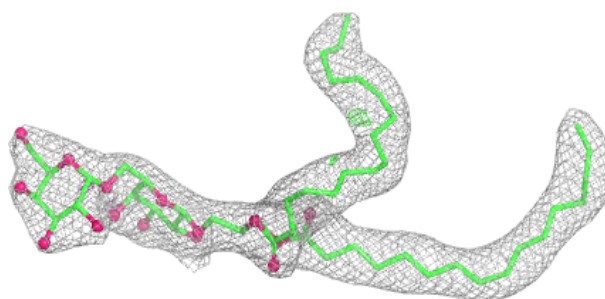


Electron density around CLA C 503:

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

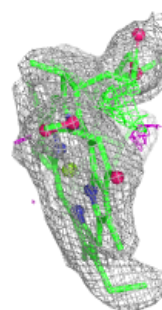
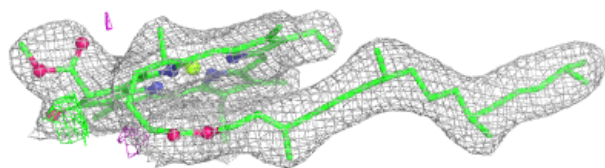
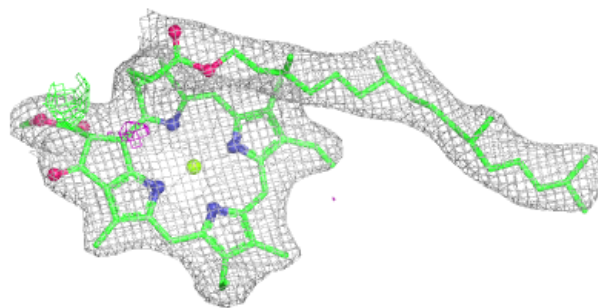
**Electron density around DGD H 102:**

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

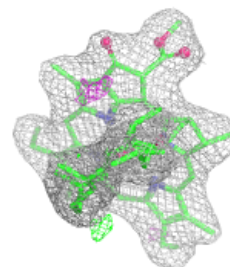
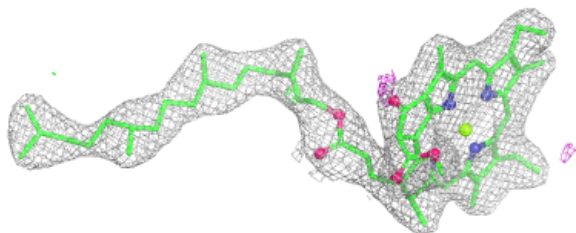
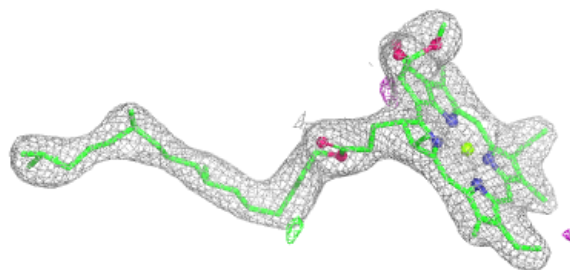


Electron density around CLA c 503:

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

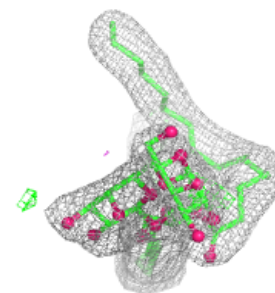
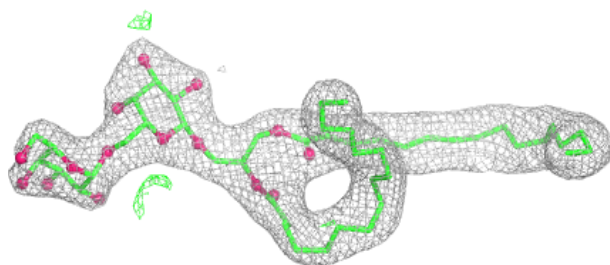
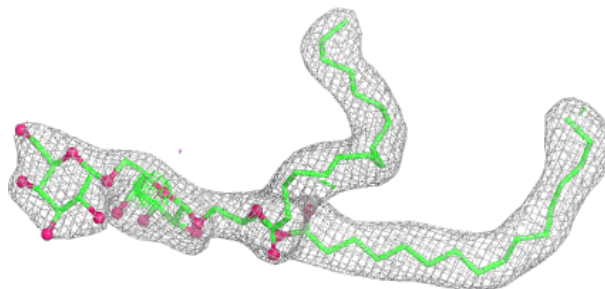
**Electron density around CLA c 504:**

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

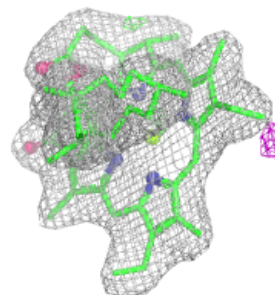
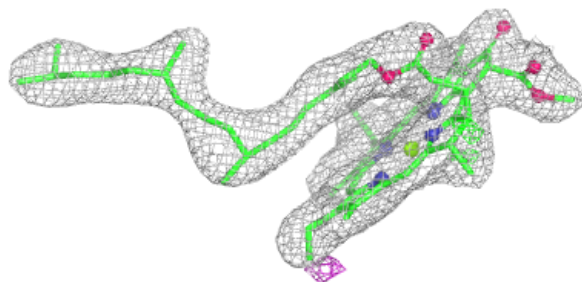
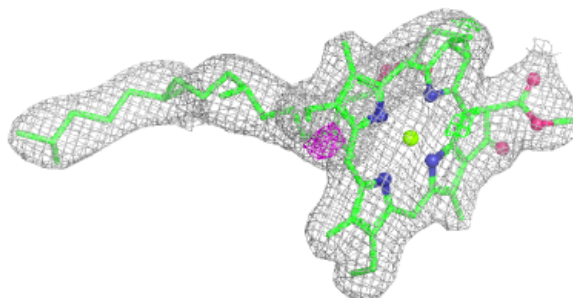


Electron density around DGD h 103:

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

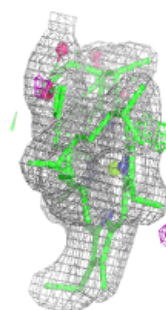
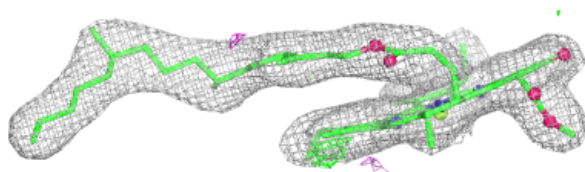
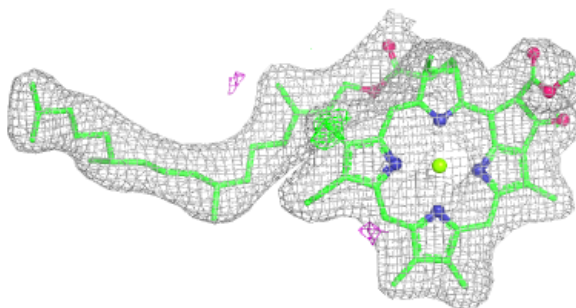
**Electron density around CLA C 506:**

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

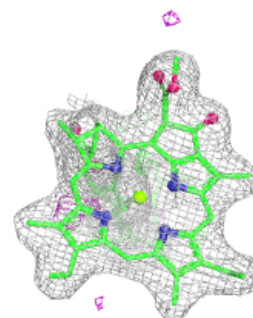
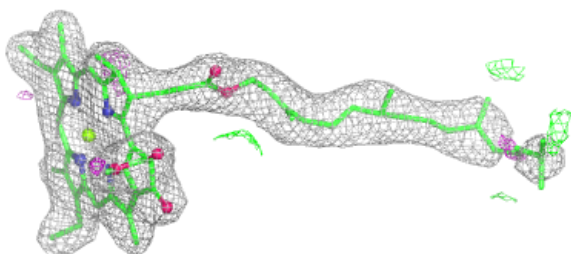
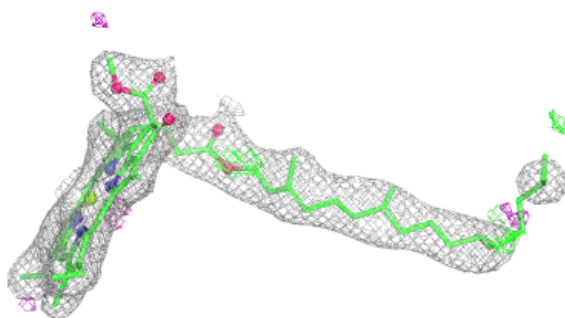


Electron density around CLA B 603:

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

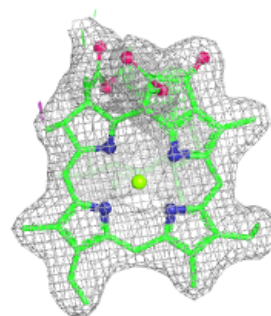
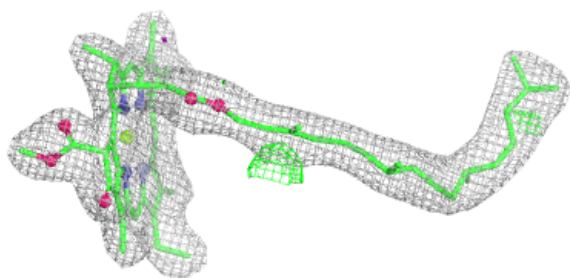
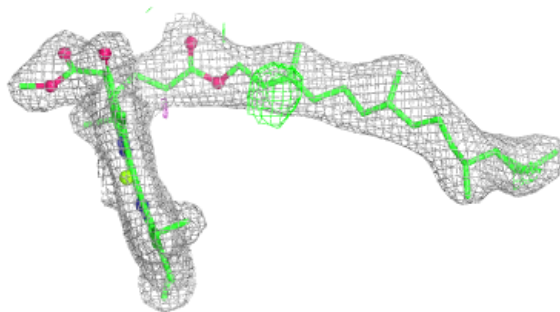
**Electron density around CLA B 604:**

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



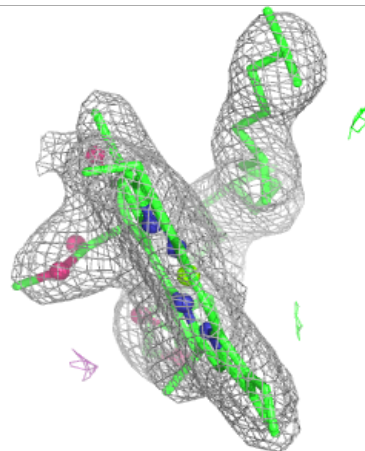
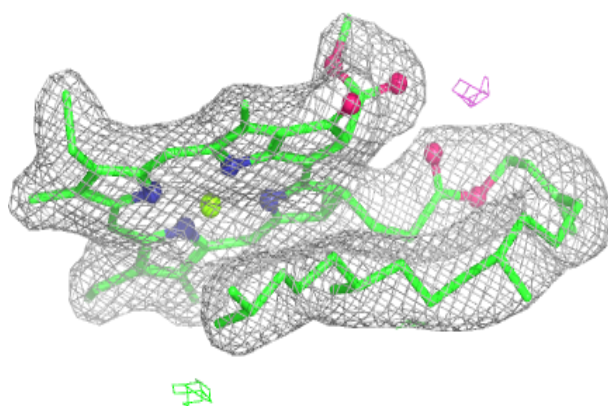
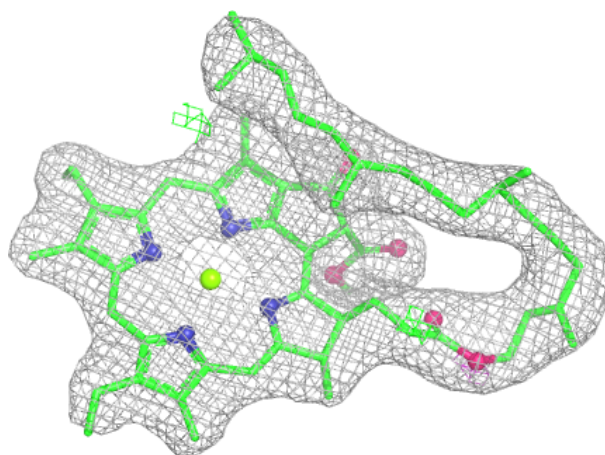
Electron density around CLA B 605:

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



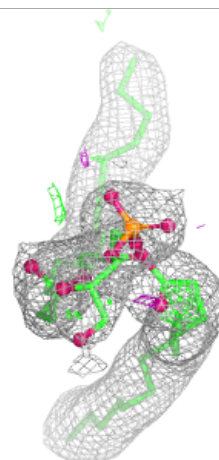
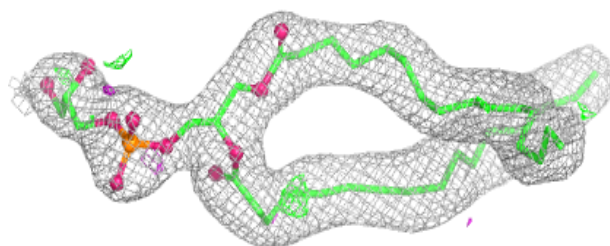
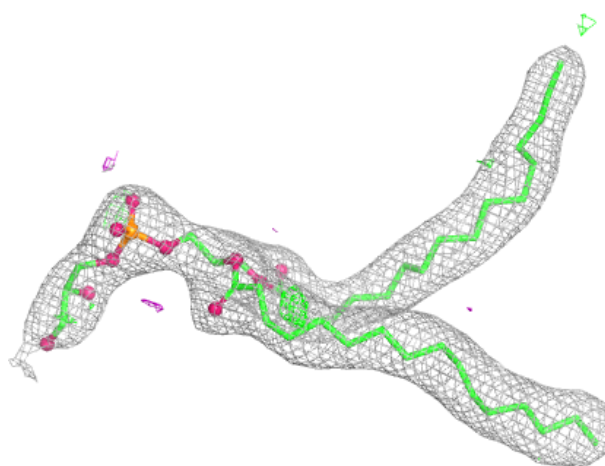
Electron density around CLA C 510:

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



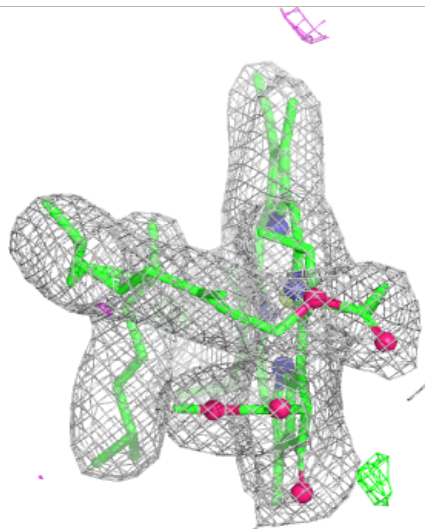
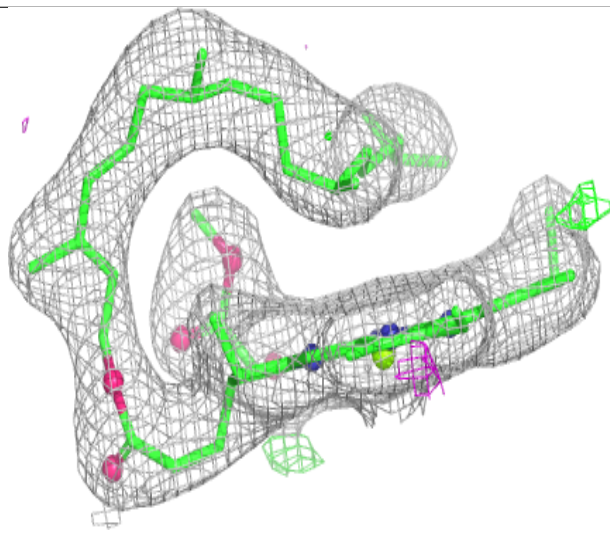
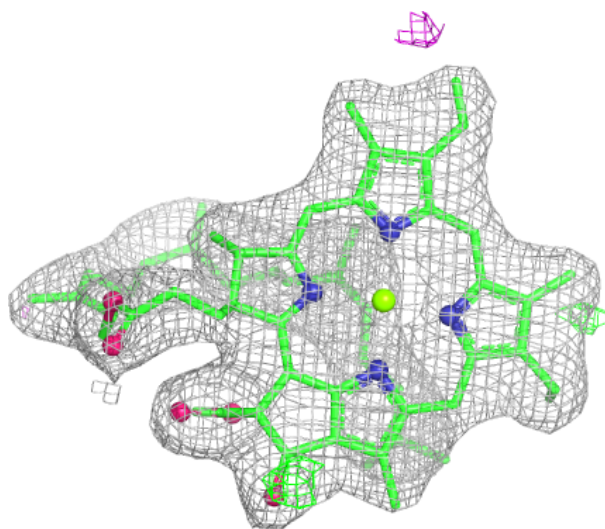
Electron density around LHG D 406:

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



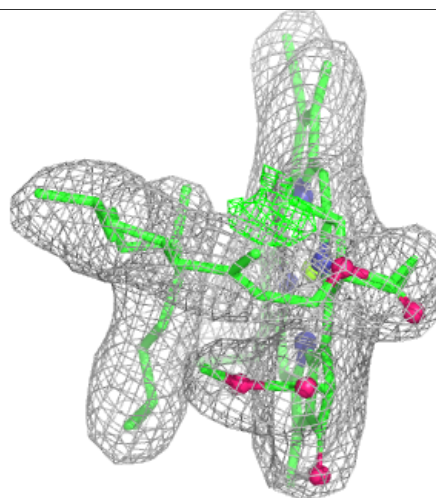
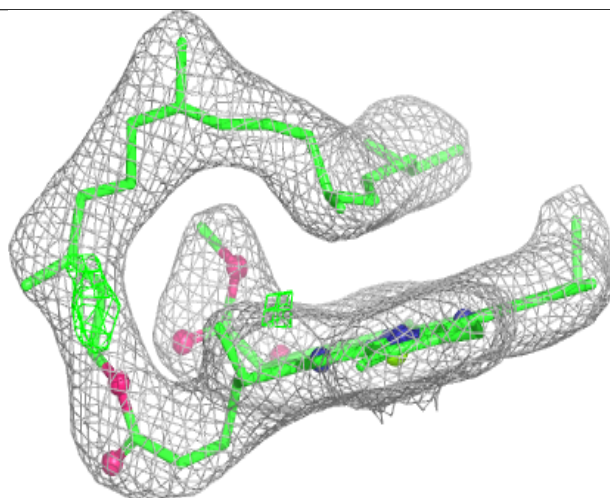
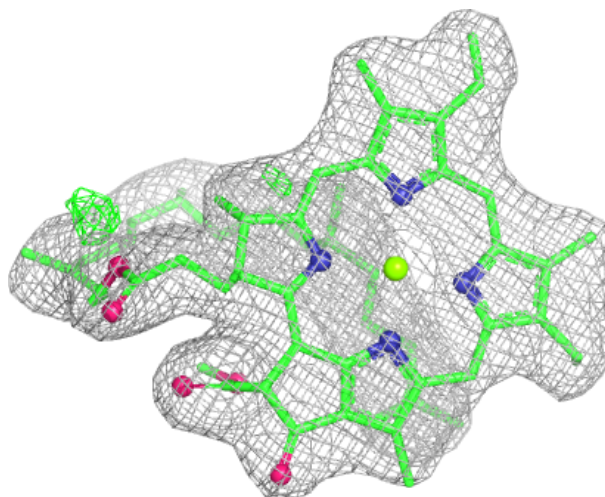
Electron density around CLA C 511:

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



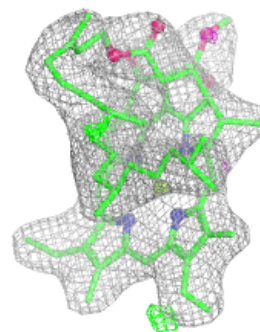
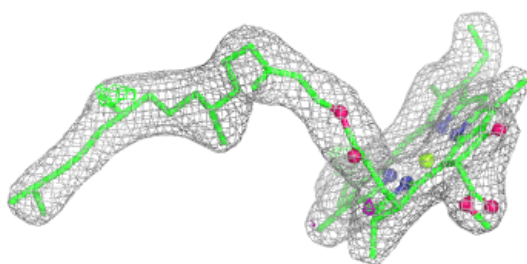
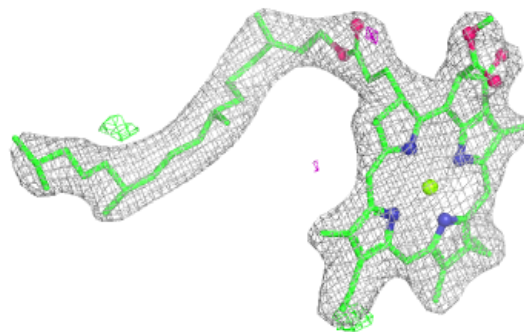
Electron density around CLA c 512:

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



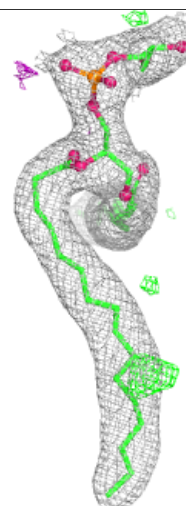
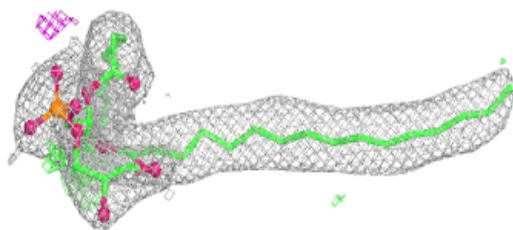
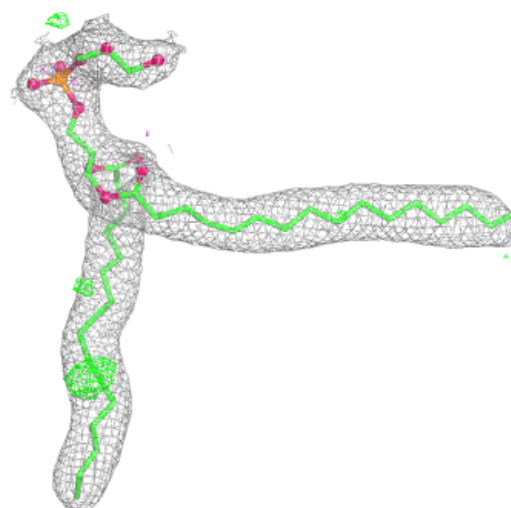
Electron density around CLA C 512:

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



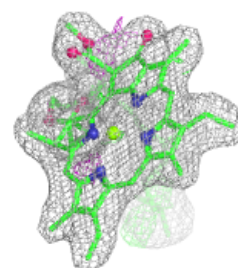
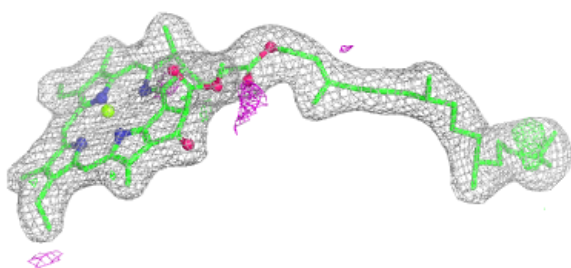
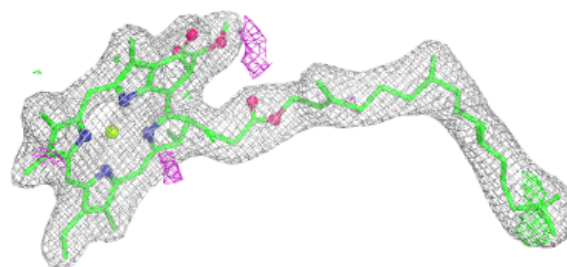
Electron density around LHG L 101:

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

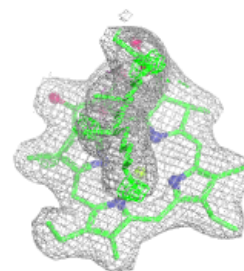
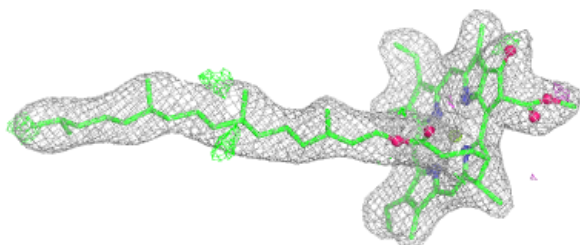
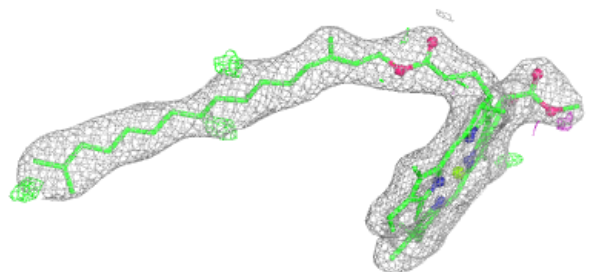


Electron density around CLA A 404:

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

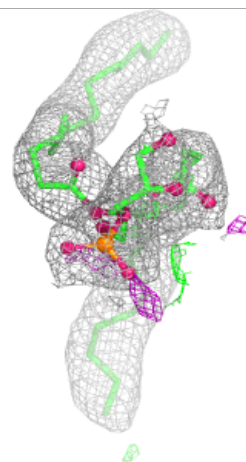
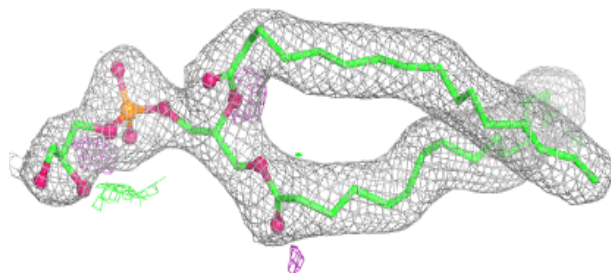
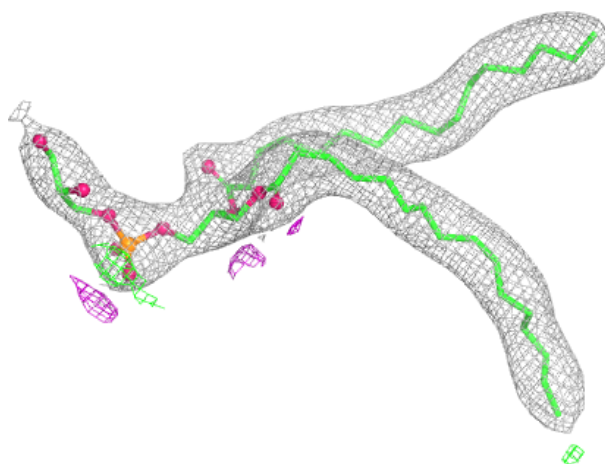
**Electron density around CLA B 607:**

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



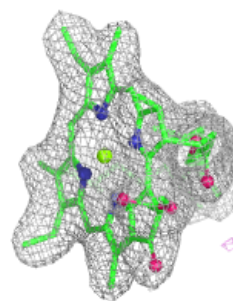
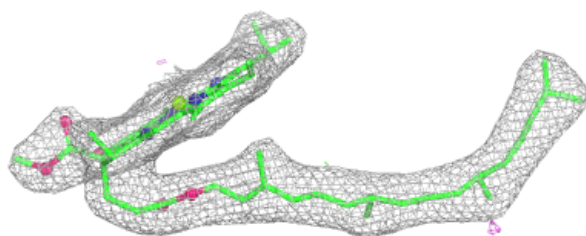
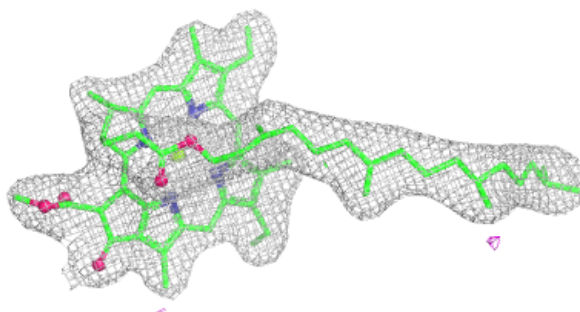
Electron density around LHG d 407:

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

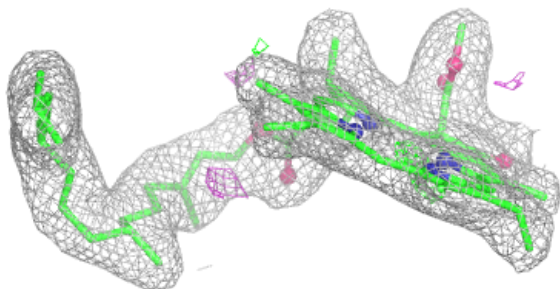
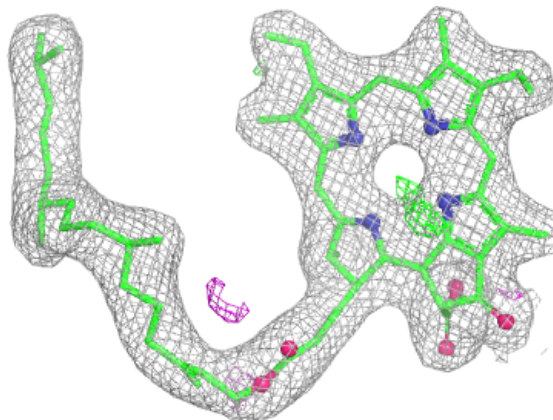


Electron density around CLA B 608:

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

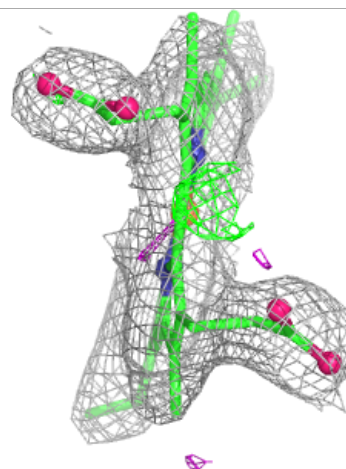
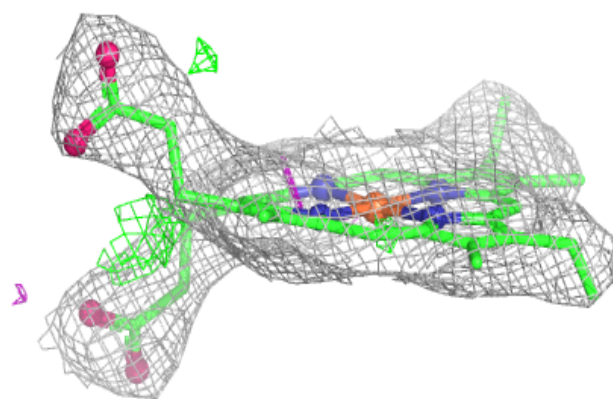
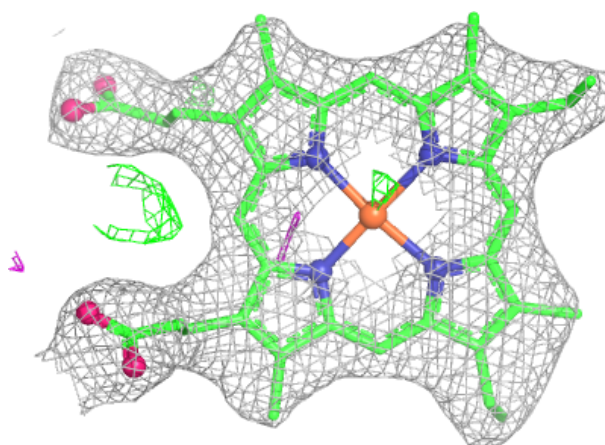
**Electron density around PHO A 408:**

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



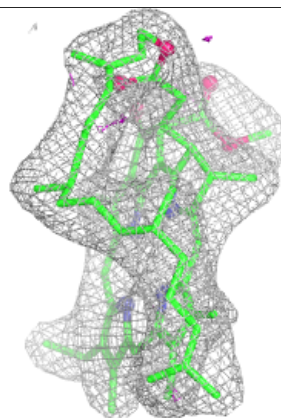
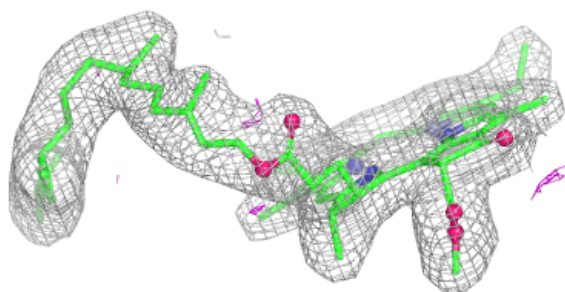
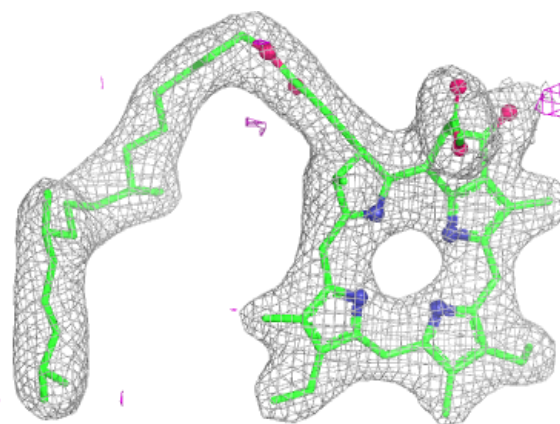
Electron density around HEM E 103:

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



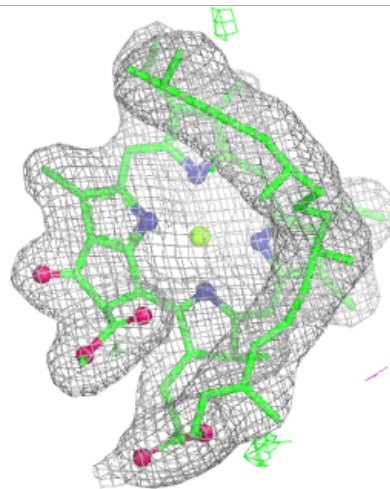
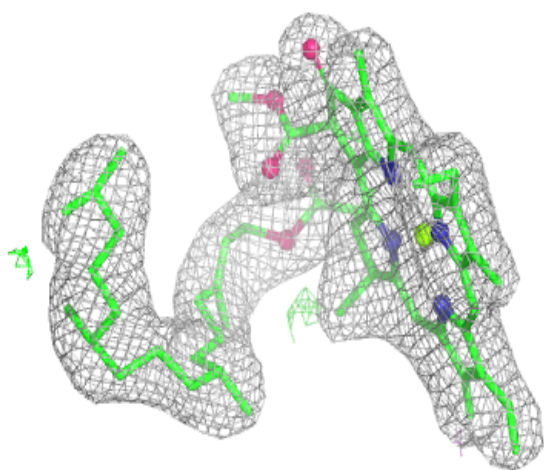
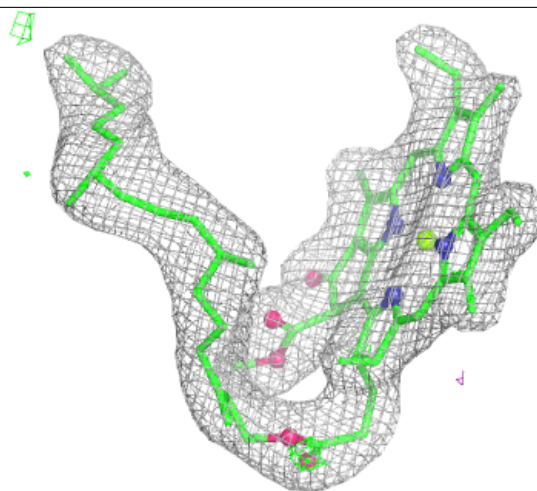
Electron density around PHO a 406:

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



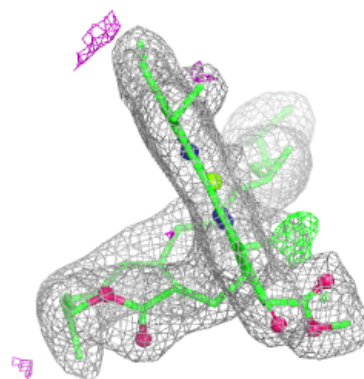
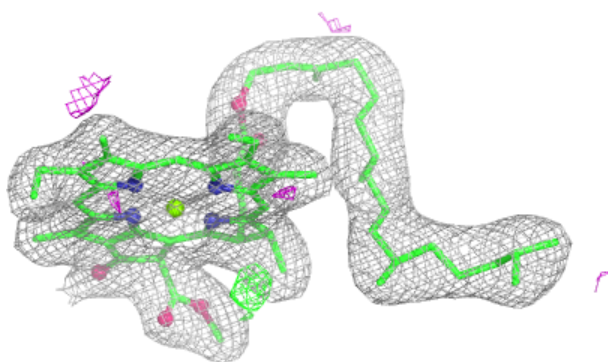
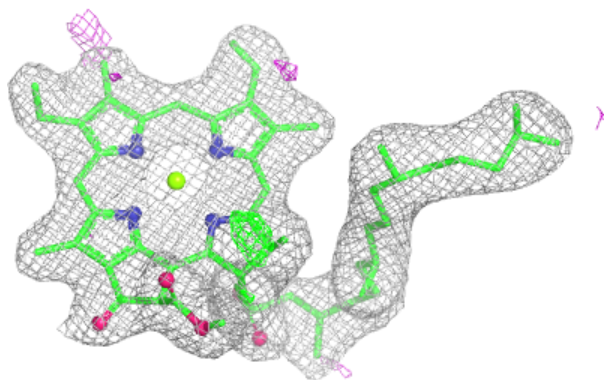
Electron density around CLA b 613:

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

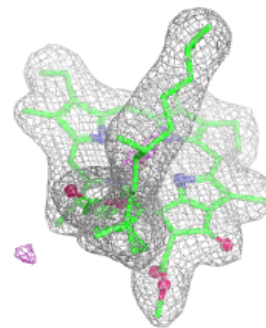
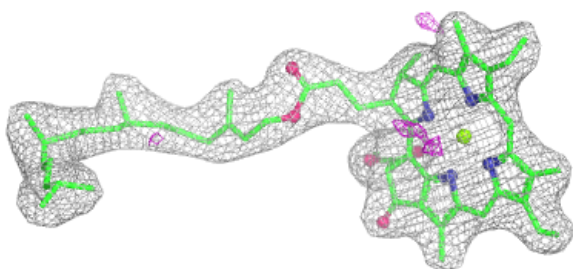
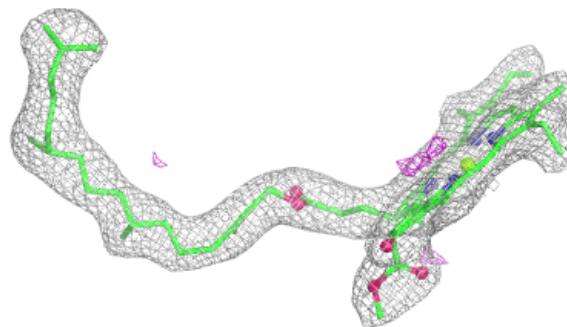


Electron density around CLA A 405:

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

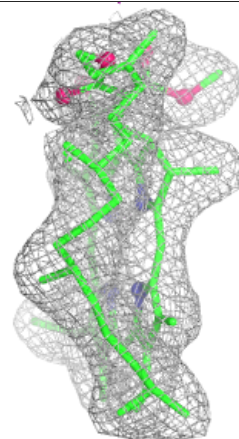
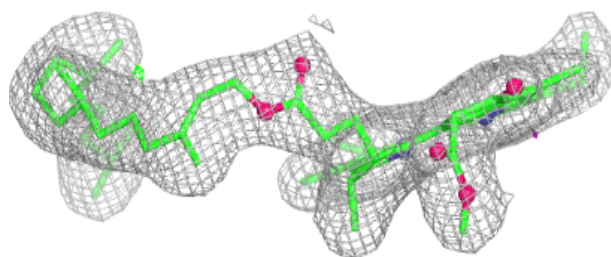
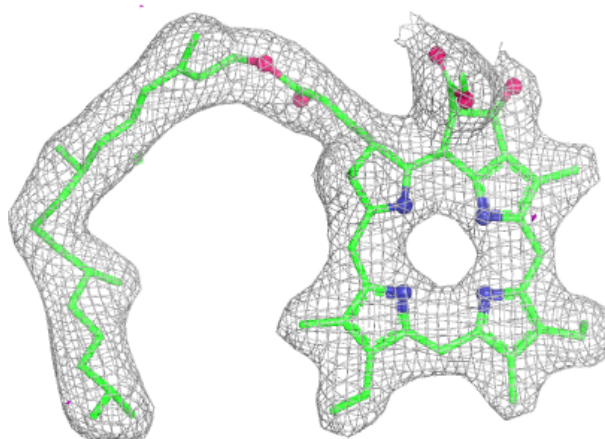
**Electron density around CLA d 402:**

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



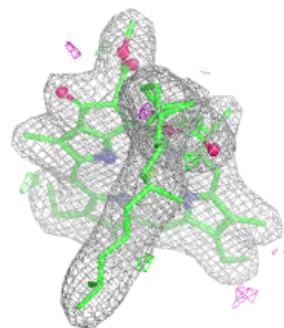
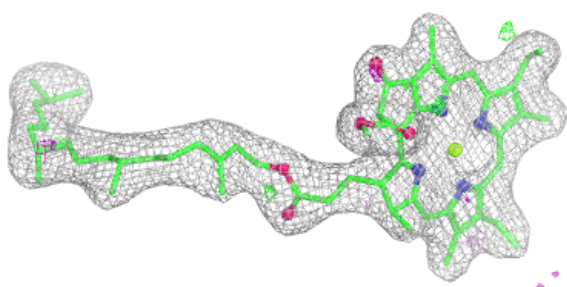
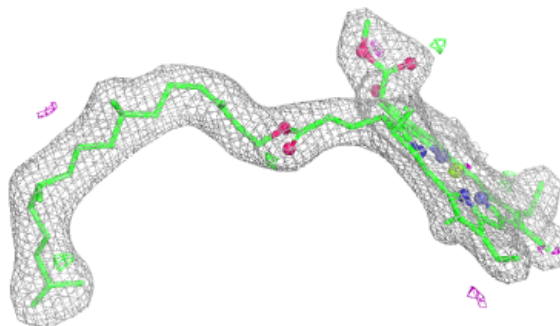
Electron density around PHO A 407:

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



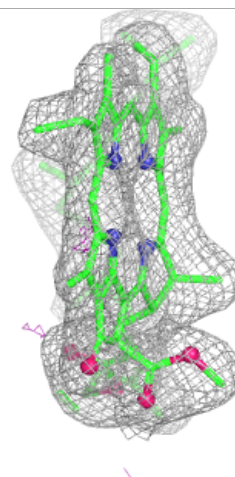
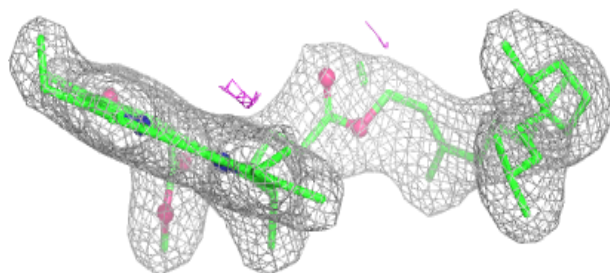
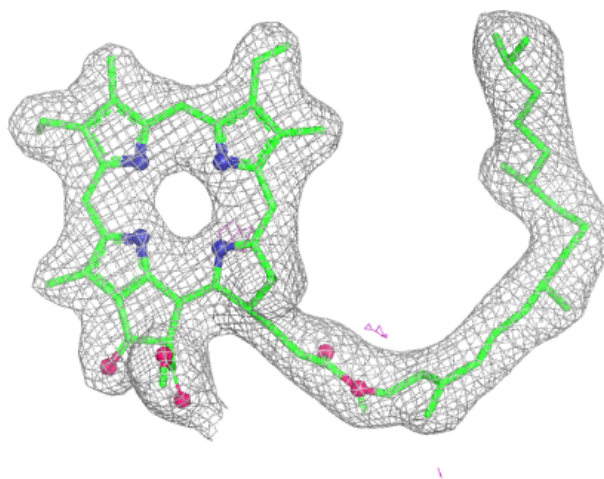
Electron density around CLA D 402:

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



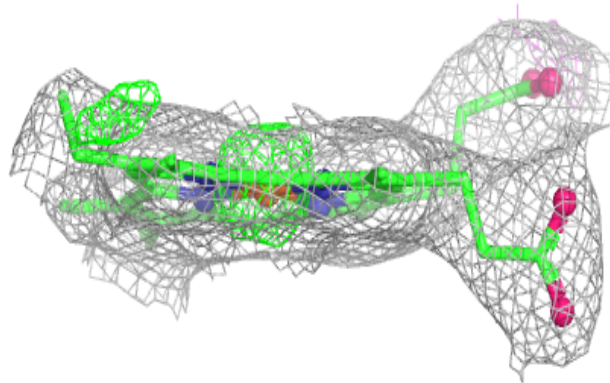
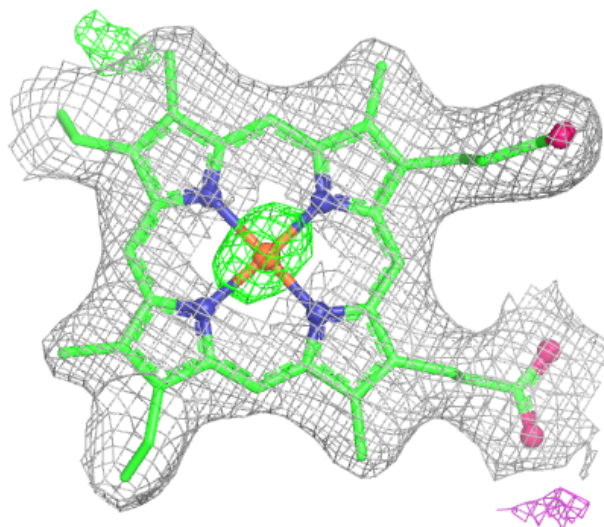
Electron density around PHO a 405:

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



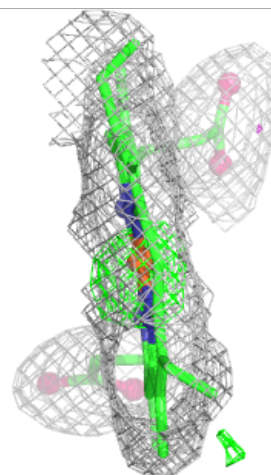
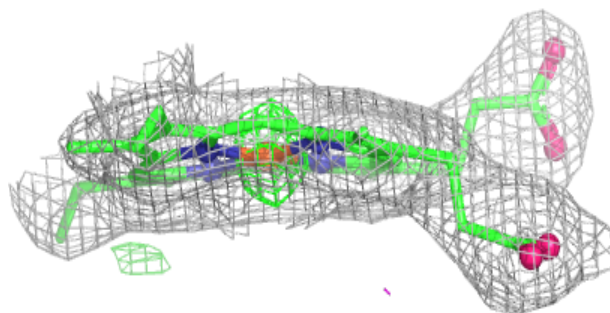
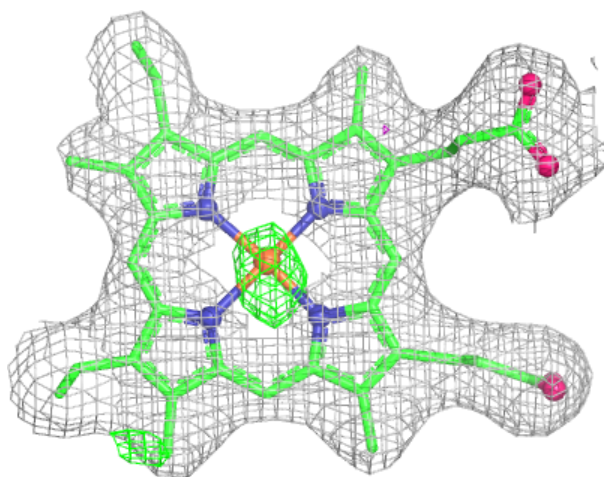
Electron density around HEC V 203:

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



Electron density around HEC v 203:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.