



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:51 AM UTC

PDB ID : 8IRA / pdb_00008ira
Title : XFEL structure of cyanobacterial photosystem II following one flash (1F) with a 200-microsecond delay
Authors : Li, H.; Suga, M.; Shen, J.R.
Deposited on : 2023-03-17
Resolution : 2.20 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

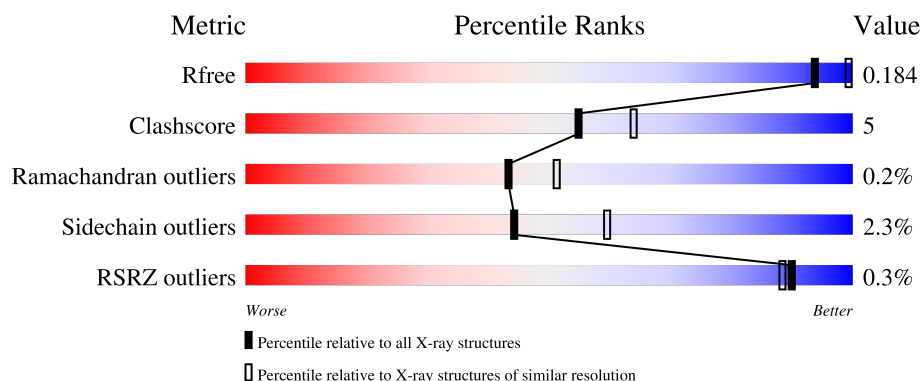
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



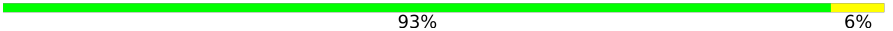
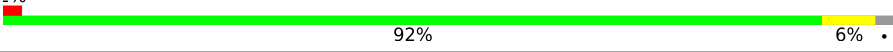
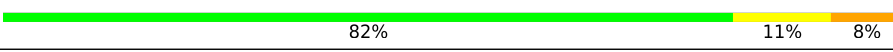
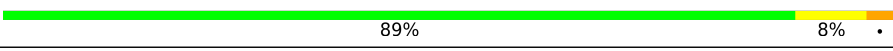
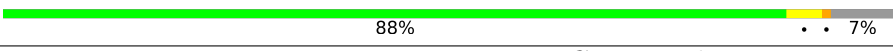
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	91% 6% .
1	a	344	89% 8% .
2	B	505	92% 7%
2	b	505	89% 10% .
3	C	455	91% 8% .

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Mol	Chain	Length	Quality of chain
3	c	455	 92% 8%
4	D	342	 90% 10%
4	d	342	 93% 6%
5	E	84	 % 81% 15% .
5	e	84	 % 87% 7% 6%
6	F	44	 64% 14% 23%
6	f	44	 2% 64% 7% 30%
7	H	65	 2% 92% 6% .
7	h	65	 2% 89% 9% .
8	I	38	 82% 11% 8%
8	i	38	 89% 8% .
9	J	39	 79% 15% . .
9	j	39	 92% 8%
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% 8% 6% 8%
12	m	36	 81% 11% . 6%
13	O	244	 83% 16%
13	o	244	 90% 9%
14	T	32	 81% 12% 6%
14	t	32	 3% 84% 9% 6%
15	U	104	 85% 8% 8%
15	u	104	 88% . . 7%

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404[A]	X	-	-	-
23	CLA	A	404[B]	X	-	-	-
23	CLA	A	405[B]	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	402[A]	X	-	-	-
23	CLA	D	402[B]	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	404[A]	X	-	-	-
23	CLA	a	404[B]	X	-	-	-
23	CLA	a	407	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	402[A]	X	-	-	-
23	CLA	d	402[B]	X	-	-	-
23	CLA	d	403[A]	X	-	-	-
23	CLA	d	403[B]	X	-	-	-
23	CLA	d	404	X	-	-	-
27	GOL	D	412	-	X	-	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 62674 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	222	0
			4338	2836	717	760	25			
1	a	334	Total	C	N	O	S	0	220	0
			4318	2821	715	757	25			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	22	0
			4166	2735	694	724	13			
2	b	504	Total	C	N	O	S	0	19	0
			4134	2718	687	716	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	99	0
			4272	2796	715	743	18			
3	c	455	Total	C	N	O	S	0	101	0
			4316	2827	720	751	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	expression tag	UNP D0VWR7
C	20	SER	-	expression tag	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	expression tag	UNP D0VWR7
C	22	PHE	-	expression tag	UNP D0VWR7
c	19	ASN	-	expression tag	UNP D0VWR7
c	20	SER	-	expression tag	UNP D0VWR7
c	21	ILE	-	expression tag	UNP D0VWR7
c	22	PHE	-	expression tag	UNP D0VWR7

- 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	115	0
			3625	2390	597	623	15			
4	d	341	Total	C	N	O	S	0	119	0
			3658	2412	605	626	15			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			662	432	107	123			
5	e	79	Total	C	N	O	0	2	0
			670	439	110	121			

- 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	1	0
			261	179	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			
7	h	64	Total	C	N	O	S	0	1	0
			517	345	85	85	2			

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	2	0
			311	207	49	55			
11	l	36	Total	C	N	O	0	2	0
			311	207	49	55			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	2	0
			286	190	43	52	1			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	10	0
			1958	1221	335	398	4			
13	o	243	Total	C	N	O	S	0	8	0
			1933	1207	330	392	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	6	0
			311	213	48	48	2			
14	t	30	Total	C	N	O	S	0	5	0
			302	208	47	45	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	4	0
			800	508	133	159				
15	u	97	Total	C	N	O		0	5	0
			815	519	135	161				

- 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	6	0
			1120	711	185	220	4			
16	v	137	Total	C	N	O	S	0	6	0
			1117	712	185	216	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	1	0
			289	194	46	49			
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) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

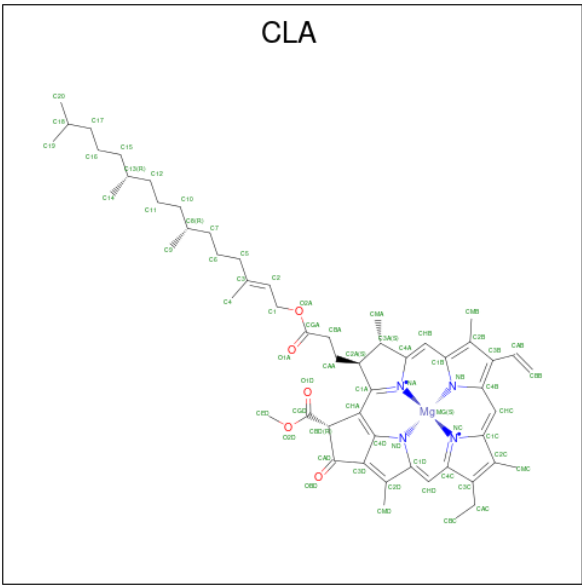
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	2	Total	Cl	0	2
			4	4		

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	A	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	A	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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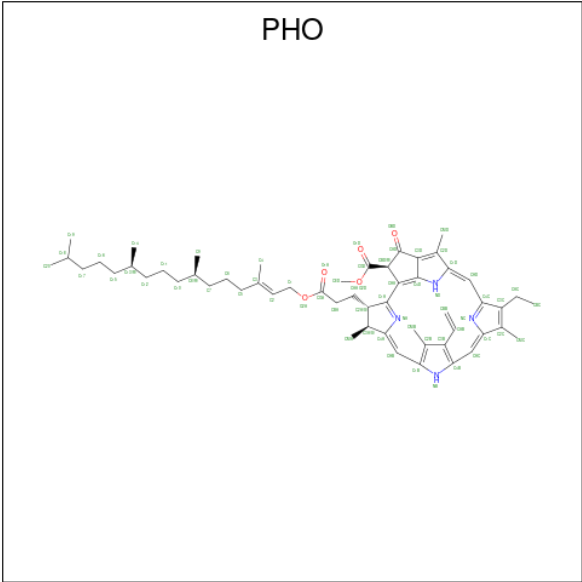
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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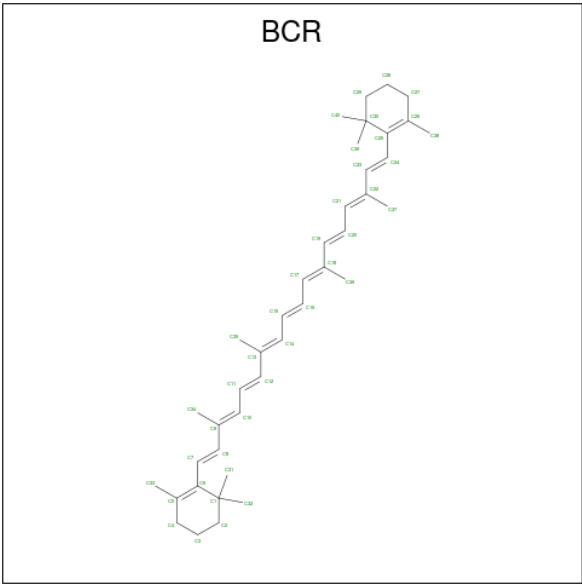
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	d	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



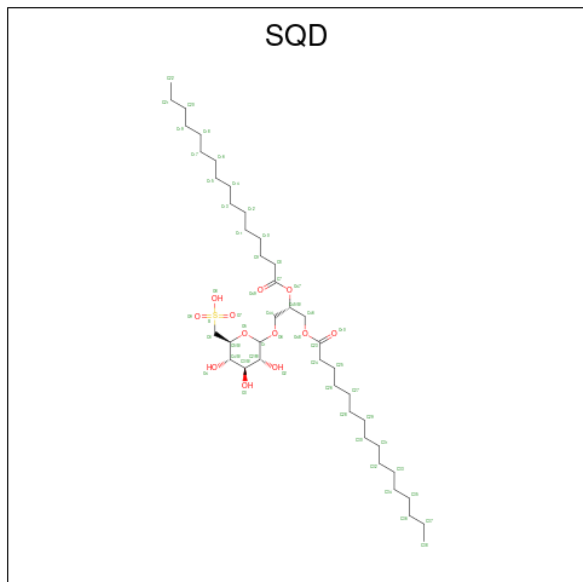
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		

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



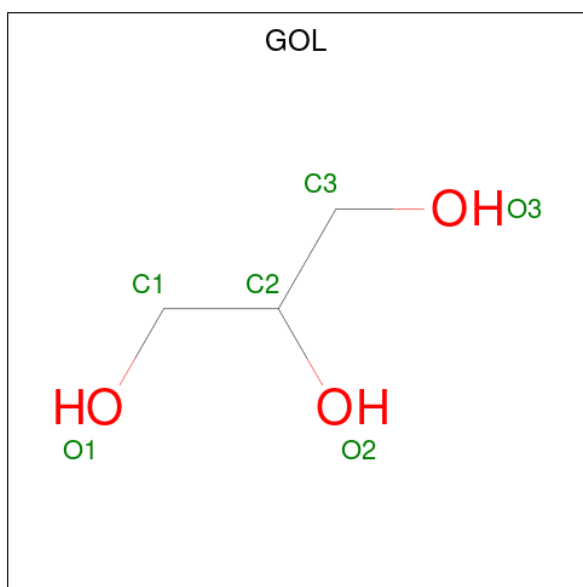
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

- Molecule 26 is 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
26	A	1	Total	C	O	S	0	1
			108	82	24	2		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			54	41	12	1		
26	F	1	Total	C	O	S	0	0
			43	30	12	1		
26	a	1	Total	C	O	S	0	1
			108	82	24	2		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	b	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

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



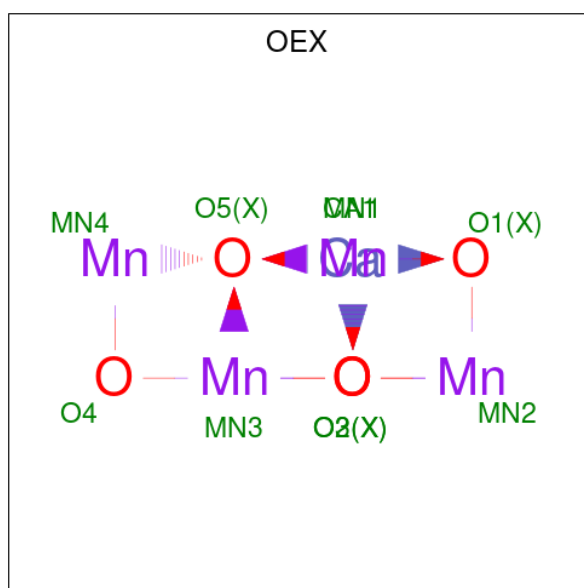
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	1
			12	6	6		
27	D	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	V	1	Total	C	O	0	1
			12	6	6		
27	a	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	c	1	Total	C	O	0	1
			12	6	6		
27	c	1	Total	C	O	0	0
			6	3	3		
27	d	1	Total	C	O	0	0
			6	3	3		
27	l	1	Total	C	O	0	1
			12	6	6		
27	o	1	Total	C	O	0	0
			6	3	3		
27	o	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	1
			12	6	6		

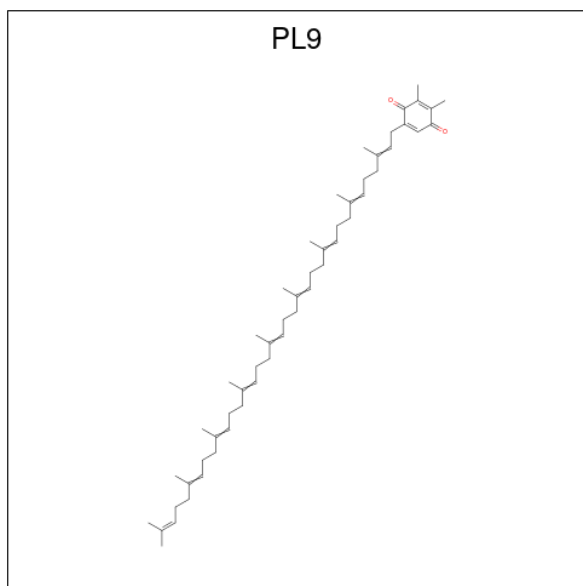
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	O	0	1
			20	2	8	10		
28	a	1	Total	Ca	Mn	O	0	1
			20	2	8	10		

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$)

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	1
			110	106	4		
29	D	1	Total	C	O	0	1
			110	106	4		
29	a	1	Total	C	O	0	1
			110	106	4		
29	d	1	Total	C	O	0	1
			110	106	4		

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

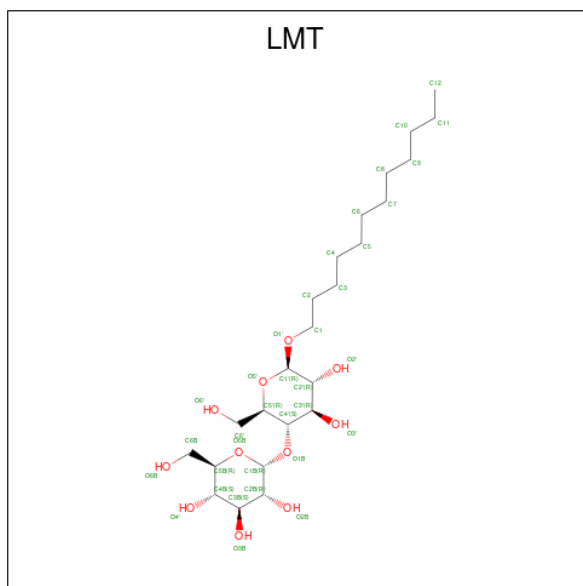
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	1
			68	58	10		
30	M	1	Total	C		0	0
			10	10			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	X	1	Total	C	O	0	0
			18	16	2		
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	1	Total	C	O	0	0
			33	28	5		
30	c	1	Total	C	O	0	1
			64	54	10		
30	d	2	Total	C	O	0	0
			53	47	6		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
			10	10			
30	x	1	Total	C	O	0	0
			18	16	2		

- Molecule 31 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



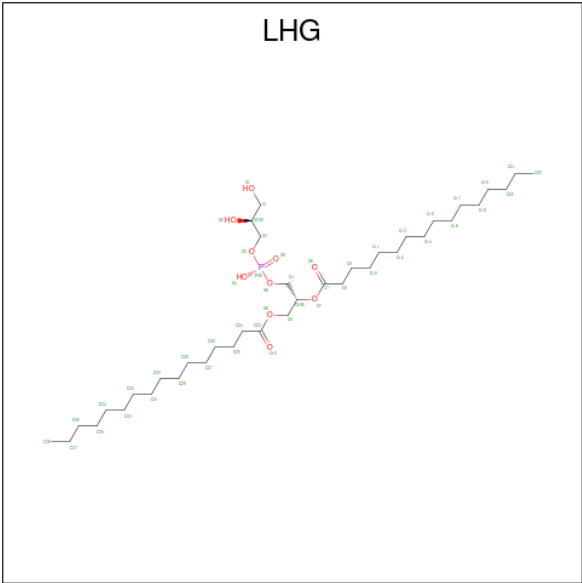
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total 35	C 24	O 11	0	0
31	A	1	Total 35	C 24	O 11	0	0

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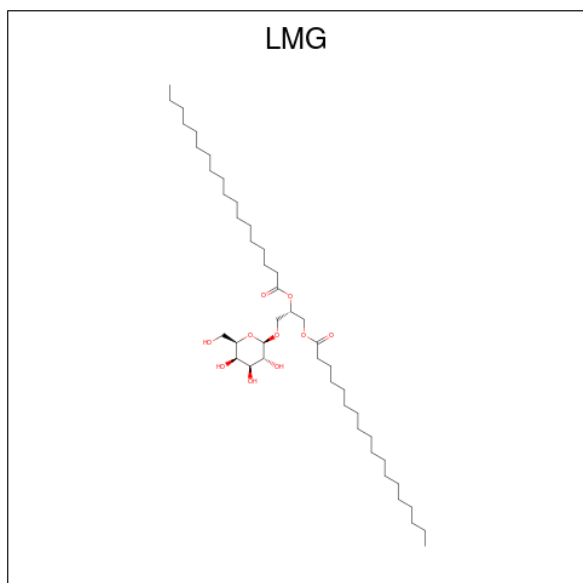
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			25	19	6		
31	F	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	T	1	Total	C	O	0	0
			35	24	11		
31	a	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C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

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	P	0	1
			98	76	20	2		
32	D	1	Total	C	O	P	0	1
			98	76	20	2		
32	D	1	Total	C	O	P	0	1
			98	76	20	2		
32	E	1	Total	C	O	P	0	1
			84	62	20	2		
32	L	1	Total	C	O	P	0	1
			98	76	20	2		
32	a	1	Total	C	O	P	0	1
			84	62	20	2		
32	b	1	Total	C	O	P	0	1
			98	76	20	2		
32	d	1	Total	C	O	P	0	1
			98	76	20	2		
32	d	1	Total	C	O	P	0	1
			98	76	20	2		
32	d	1	Total	C	O	P	0	1
			98	76	20	2		

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



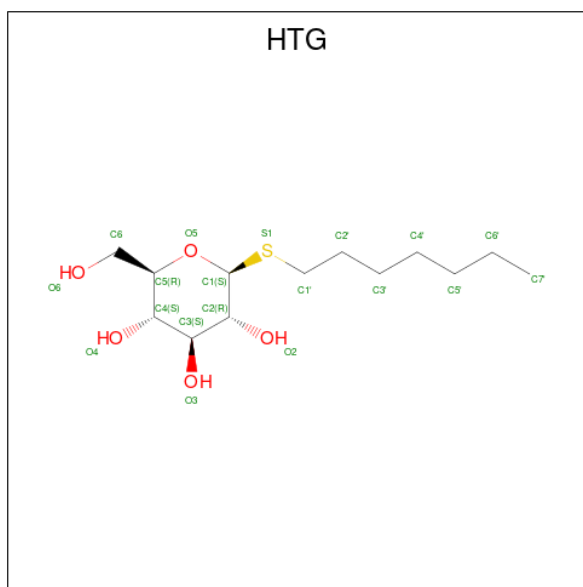
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		

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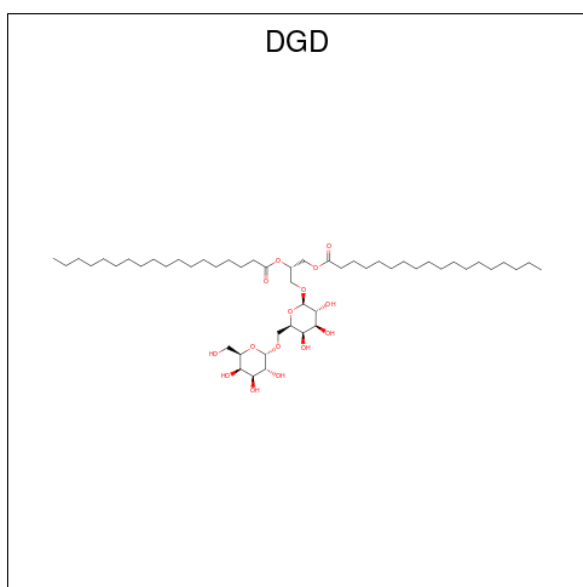
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	D	1	Total	C	O	0	0
			51	41	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	d	1	Total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

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



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

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

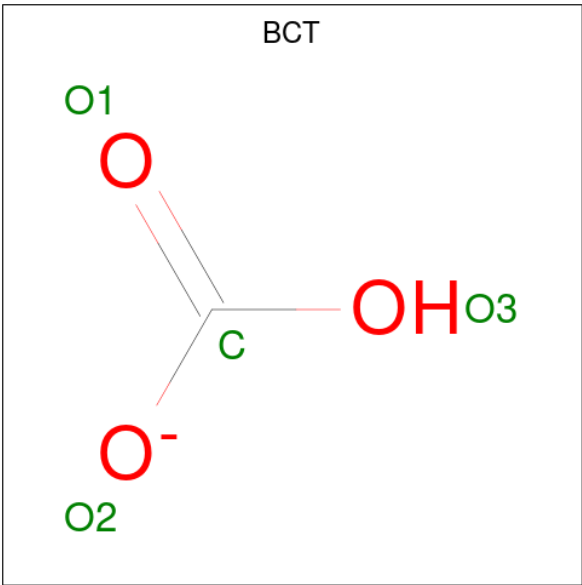


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 62 47 15	0	0
35	H	1	Total C O 62 47 15	0	0
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 62 47 15	0	0
35	h	1	Total C O 62 47 15	0	0

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

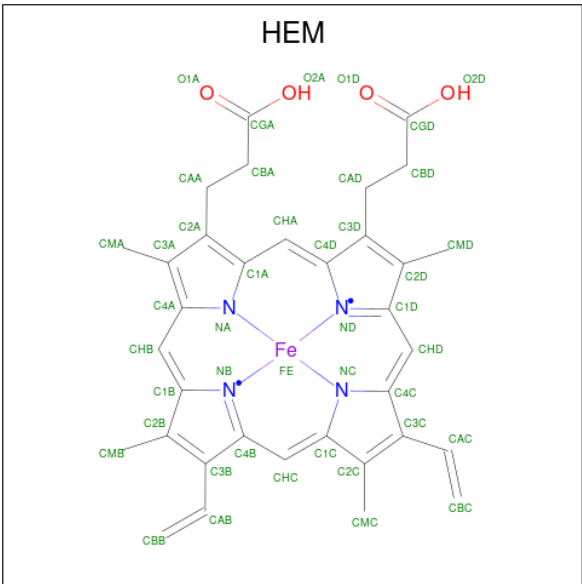
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total Ca 1 1	0	0
36	F	1	Total Ca 1 1	0	0
36	O	1	Total Ca 1 1	0	0
36	c	2	Total Ca 2 2	0	0
36	f	1	Total Ca 1 1	0	0
36	o	1	Total Ca 1 1	0	0

- Molecule 37 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	D	1	Total	C	O	0	1
			8	2	6		
37	d	1	Total	C	O	0	1
			8	2	6		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

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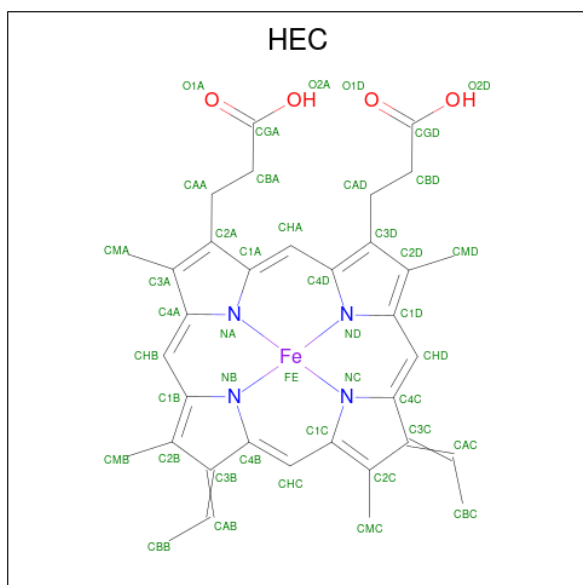
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	f	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

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

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	142	Total	O	0	86
			227	227		
41	B	187	Total	O	0	2
			189	189		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	C	169	Total 206	O 206	0	38
41	D	120	Total 155	O 155	0	35
41	E	17	Total 17	O 17	0	0
41	F	4	Total 4	O 4	0	0
41	H	22	Total 22	O 22	0	0
41	I	4	Total 4	O 4	0	0
41	J	6	Total 6	O 6	0	0
41	K	5	Total 5	O 5	0	0
41	L	9	Total 10	O 10	0	1
41	M	6	Total 6	O 6	0	0
41	O	104	Total 108	O 108	0	4
41	T	11	Total 14	O 14	0	3
41	U	47	Total 49	O 49	0	2
41	V	79	Total 80	O 80	0	1
41	X	7	Total 7	O 7	0	0
41	a	131	Total 211	O 211	0	81
41	b	201	Total 204	O 204	0	3
41	c	160	Total 193	O 193	0	34
41	d	117	Total 149	O 149	0	32
41	e	8	Total 8	O 8	0	0
41	f	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	h	17	Total 17	O 17	0	0
41	i	2	Total 2	O 2	0	0
41	j	1	Total 1	O 1	0	0
41	k	3	Total 3	O 3	0	0
41	l	8	Total 10	O 10	0	2
41	m	13	Total 13	O 13	0	0
41	o	99	Total 103	O 103	0	4
41	t	8	Total 11	O 11	0	3
41	u	51	Total 52	O 52	0	1
41	v	56	Total 58	O 58	0	2
41	x	6	Total 6	O 6	0	0
41	y	2	Total 2	O 2	0	0

3 Residue-property plots

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

- Molecule 1: Photosystem II protein D1

Chain A: 



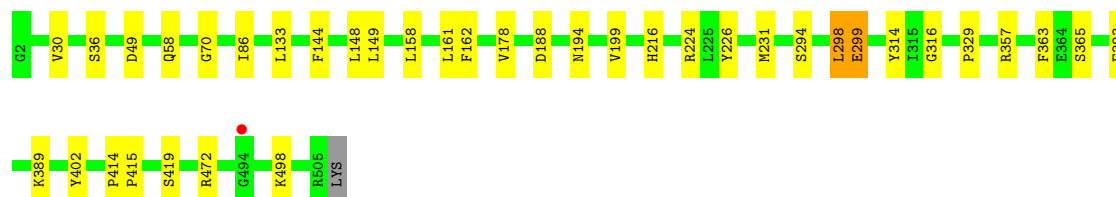
- Molecule 1: Photosystem II protein D1

Chain a: 



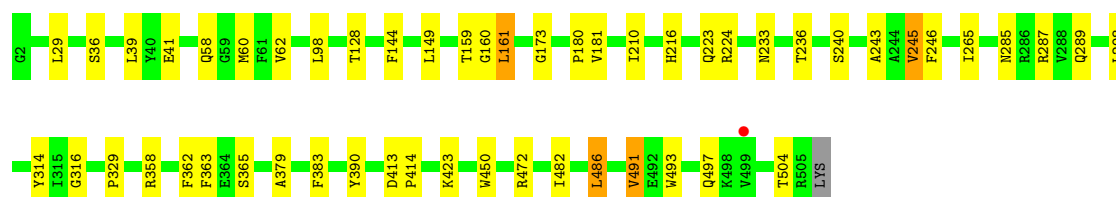
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 

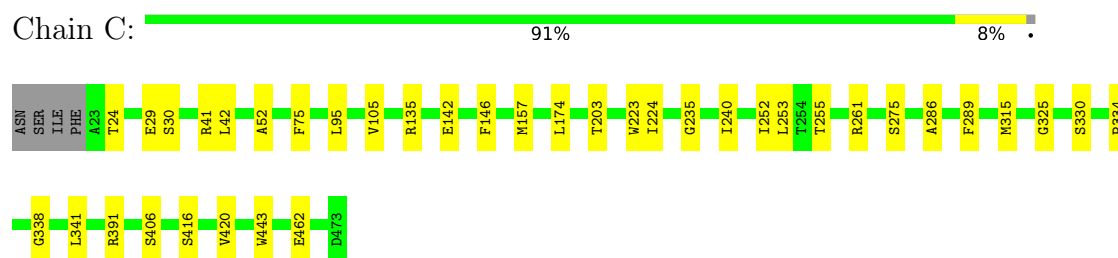


- Molecule 2: Photosystem II CP47 reaction center protein

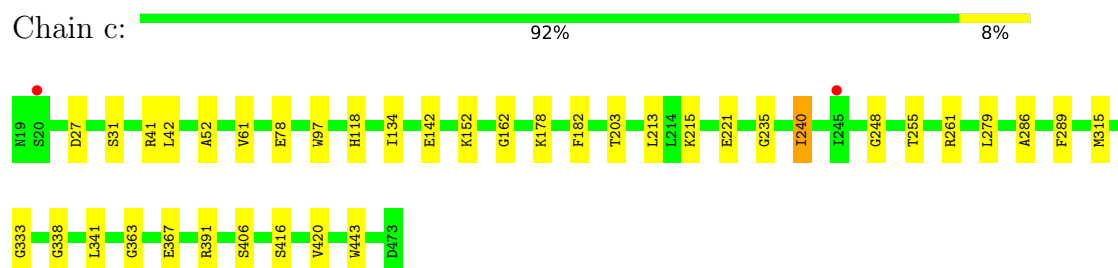
Chain b: 



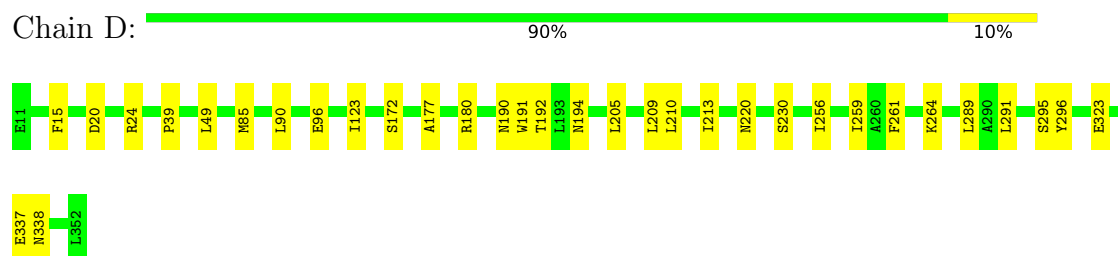
- Molecule 3: Photosystem II CP43 reaction center protein



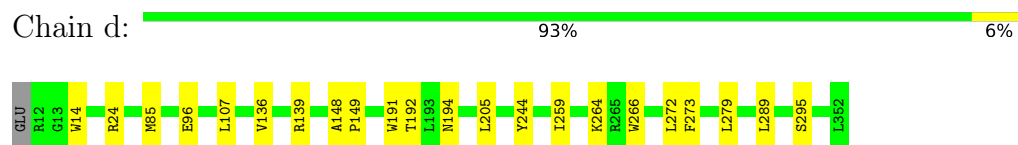
- Molecule 3: Photosystem II CP43 reaction center protein



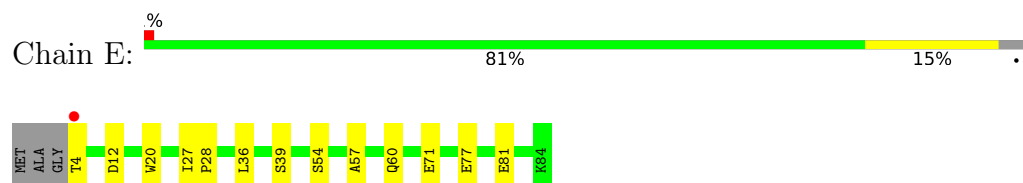
- Molecule 4: Photosystem II D2 protein



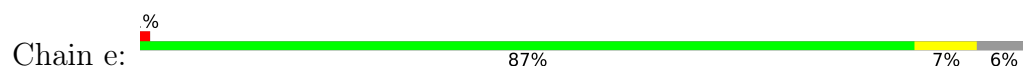
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha

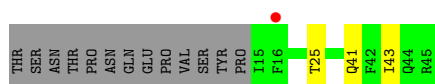




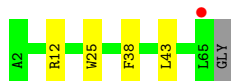
- Molecule 6: Cytochrome b559 subunit beta



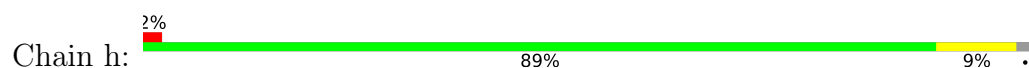
- Molecule 6: Cytochrome b559 subunit beta



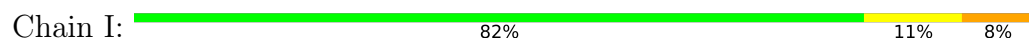
- Molecule 7: Photosystem II reaction center protein H



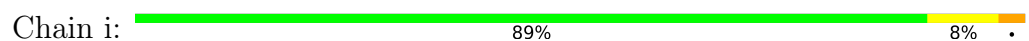
- Molecule 7: Photosystem II reaction center protein H



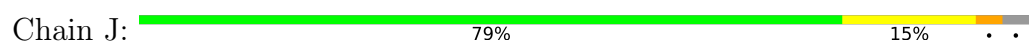
- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J





- Molecule 9: Photosystem II reaction center protein J

Chain j: 92% 8%



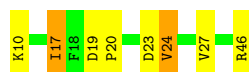
- Molecule 10: Photosystem II reaction center protein K

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% 8% 6% 8%



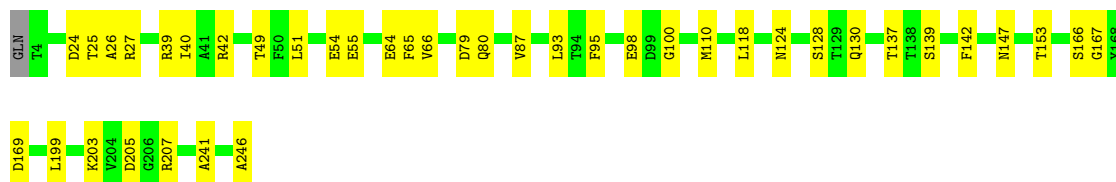
- Molecule 12: Photosystem II reaction center protein M

Chain m: 81% 11% . 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 83% 16%



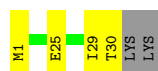
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 90% 9%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 81% 12% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 3% 84% 9% 6%



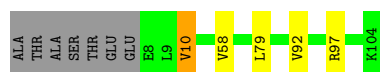
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 85% 8% 8%

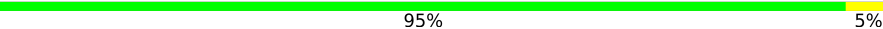


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 88% 7% 7%



- Molecule 16: Cytochrome c-550

Chain V:  95% 5%



- Molecule 16: Cytochrome c-550

Chain v:  91% 9%



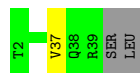
- Molecule 17: Photosystem II reaction center protein X

Chain X:  85% 10% 5%

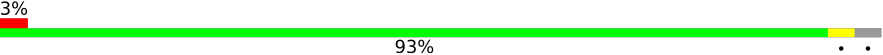


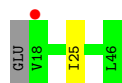
- Molecule 17: Photosystem II reaction center protein X

Chain x:  92% 5%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  3% 93%



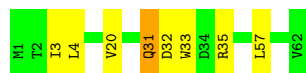
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  73% 23%

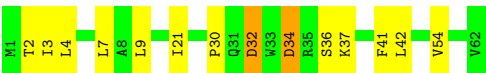
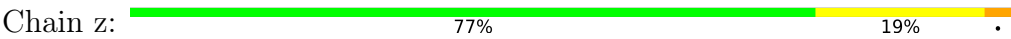


- Molecule 19: Photosystem II reaction center protein Z

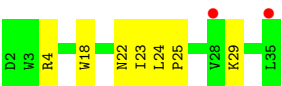
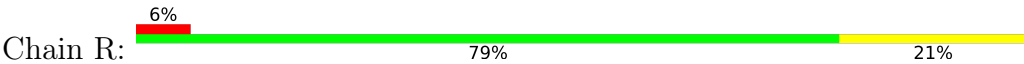
Chain Z:  87% 11%



- 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	125.75Å 231.60Å 288.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.20 19.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-2.20) 99.7 (19.98-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.19Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.142 , 0.178 0.154 , 0.184	Depositor DCC
R_{free} test set	21187 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	62674	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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: LHG, MG, FE2, CLA, CL, LMG, PHO, FME, LMT, DGD, CA, SQD, UNL, OEX, BCR, HTG, BCT, GOL, PL9, HEC, HEM

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	0.27	0/4478	0.44	0/6098
1	a	0.25	0/4457	0.42	0/6069
2	B	0.34	0/4314	0.49	0/5879
2	b	0.31	0/4285	0.48	0/5841
3	C	0.28	0/4416	0.42	0/6013
3	c	0.28	0/4467	0.42	0/6082
4	D	0.32	0/3746	0.47	0/5102
4	d	0.30	0/3780	0.45	0/5147
5	E	0.31	0/681	0.48	0/928
5	e	0.29	0/690	0.46	0/939
6	F	0.30	0/284	0.44	0/387
6	f	0.26	0/269	0.41	0/365
7	H	0.31	0/519	0.48	0/708
7	h	0.27	0/530	0.46	0/722
8	I	0.29	0/311	0.40	0/419
8	i	0.35	0/311	0.50	0/419
9	J	0.30	0/278	0.37	0/376
9	j	0.28	0/283	0.41	0/383
10	K	0.31	0/303	0.51	0/416
10	k	0.31	0/303	0.50	0/416
11	L	0.37	0/318	0.44	0/433
11	l	0.37	0/318	0.49	0/433
12	M	0.43	0/261	0.52	0/357
12	m	0.33	0/279	0.47	0/380
13	O	0.33	0/1991	0.51	0/2698
13	o	0.31	0/1966	0.50	0/2665
14	T	0.32	0/310	0.40	0/419
14	t	0.33	0/301	0.42	0/406
15	U	0.35	0/811	0.53	0/1095
15	u	0.34	0/826	0.53	0/1116
16	V	0.34	0/1142	0.48	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.30	0/1139	0.45	0/1542
17	X	0.23	0/292	0.37	0/395
17	x	0.23	0/284	0.36	0/384
18	Y	0.24	0/216	0.45	0/289
18	y	0.24	0/216	0.37	0/289
19	Z	0.21	0/490	0.35	0/669
19	z	0.21	0/490	0.33	0/669
20	R	0.24	0/279	0.35	0/383
All	All	0.30	0/50634	0.45	0/68876

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4338	0	4142	18	0
1	a	4318	0	4124	31	0
2	B	4166	0	3999	28	0
2	b	4134	0	3976	41	0
3	C	4272	0	4138	24	0
3	c	4316	0	4184	27	0
4	D	3625	0	3489	33	0
4	d	3658	0	3522	21	0
5	E	662	0	648	7	0
5	e	670	0	655	4	0
6	F	275	0	282	6	0
6	f	261	0	269	4	0
7	H	506	0	529	3	0
7	h	517	0	541	4	0
8	I	314	0	328	5	0
8	i	314	0	328	2	0
9	J	272	0	279	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	2	0
10	K	293	0	305	6	0
10	k	293	0	305	7	0
11	L	311	0	320	2	0
11	l	311	0	320	4	0
12	M	268	0	285	3	0
12	m	286	0	305	8	0
13	O	1958	0	1920	24	0
13	o	1933	0	1900	11	0
14	T	311	0	318	1	0
14	t	302	0	311	4	0
15	U	800	0	796	4	0
15	u	815	0	817	3	0
16	V	1120	0	1122	4	0
16	v	1117	0	1131	9	0
17	X	289	0	322	3	0
17	x	281	0	312	1	0
18	Y	215	0	246	1	0
18	y	215	0	246	4	0
19	Z	479	0	516	3	0
19	z	479	0	516	4	0
20	R	273	0	305	3	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	4	0	0	0	0
22	a	4	0	0	0	0
23	A	455	0	504	20	0
23	B	1040	0	1152	28	0
23	C	845	0	936	36	0
23	D	195	0	216	7	0
23	a	325	0	360	14	0
23	b	1040	0	1152	28	0
23	c	845	0	936	37	0
23	d	325	0	360	11	0
24	A	256	0	296	5	0
24	a	256	0	296	4	0
25	A	40	0	56	2	0
25	B	120	0	168	7	0
25	C	80	0	112	3	0
25	D	40	0	56	1	0
25	H	40	0	56	3	0
25	K	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	40	0	56	7	0
25	Y	40	0	56	2	0
25	a	40	0	56	0	0
25	b	120	0	168	9	0
25	c	80	0	112	5	0
25	d	40	0	56	0	0
25	h	40	0	56	4	0
25	k	40	0	56	2	0
25	t	40	0	56	5	0
25	y	40	0	56	2	0
26	A	162	0	232	4	0
26	B	54	0	78	2	0
26	F	43	0	53	2	0
26	a	162	0	233	11	0
26	b	54	0	78	4	0
26	f	43	0	53	0	0
27	A	12	0	15	2	0
27	B	18	0	24	1	0
27	C	12	0	16	0	0
27	D	6	0	7	2	0
27	O	12	0	16	4	0
27	V	12	0	16	0	0
27	a	12	0	16	5	0
27	b	12	0	16	2	0
27	c	18	0	24	0	0
27	d	6	0	8	0	0
27	l	12	0	16	2	0
27	o	12	0	16	0	0
27	v	12	0	16	3	0
28	A	20	0	0	0	0
28	a	20	0	0	0	0
29	A	110	0	160	21	0
29	D	110	0	160	0	0
29	a	110	0	160	9	0
29	d	110	0	160	0	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	D	57	0	0	0	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	K	68	0	0	0	0
30	M	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	X	18	0	0	0	0
30	a	30	0	0	0	0
30	b	33	0	0	0	0
30	c	64	0	0	0	0
30	d	53	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	70	0	92	2	0
31	B	95	0	127	2	0
31	F	35	0	46	0	0
31	M	35	0	46	1	0
31	T	35	0	46	1	0
31	a	35	0	46	1	0
31	b	50	0	70	1	0
31	e	35	0	46	1	0
31	m	35	0	46	2	0
31	t	26	0	35	2	0
32	A	98	0	148	2	0
32	D	196	0	296	13	0
32	E	84	0	114	8	0
32	L	98	0	148	0	0
32	a	84	0	114	9	0
32	b	98	0	148	1	0
32	d	294	0	444	26	0
33	B	51	0	72	1	0
33	C	153	0	216	4	0
33	D	51	0	72	0	0
33	Z	37	0	44	1	0
33	a	51	0	72	0	0
33	c	102	0	144	2	0
33	d	51	0	72	3	0
33	m	51	0	72	0	0
33	z	39	0	48	2	0
34	B	57	0	78	4	0
34	C	19	0	26	0	0
34	D	16	0	17	1	0
34	V	11	0	10	0	0
34	b	57	0	78	3	0
34	c	19	0	26	1	0
34	d	16	0	17	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	C	310	0	410	6	0
35	H	62	0	82	2	0
35	c	310	0	410	9	0
35	h	62	0	82	0	0
36	C	1	0	0	0	0
36	F	1	0	0	0	0
36	O	1	0	0	0	0
36	c	2	0	0	0	0
36	f	1	0	0	0	0
36	o	1	0	0	0	0
37	D	8	0	0	0	0
37	d	8	0	0	0	0
38	E	43	0	30	1	0
38	f	43	0	30	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	1	0
40	v	43	0	30	0	0
41	A	227	0	0	2	0
41	B	189	0	0	0	0
41	C	206	0	0	1	0
41	D	155	0	0	3	0
41	E	17	0	0	0	0
41	F	4	0	0	0	0
41	H	22	0	0	0	0
41	I	4	0	0	0	0
41	J	6	0	0	2	0
41	K	5	0	0	0	0
41	L	10	0	0	0	0
41	M	6	0	0	0	0
41	O	108	0	0	1	0
41	T	14	0	0	0	0
41	U	49	0	0	0	0
41	V	80	0	0	0	0
41	X	7	0	0	0	0
41	a	211	0	0	2	0
41	b	204	0	0	0	0
41	c	193	0	0	4	0
41	d	149	0	0	1	0
41	e	8	0	0	0	0
41	f	3	0	0	0	0
41	h	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	i	2	0	0	0	0
41	j	1	0	0	0	0
41	k	3	0	0	0	0
41	l	10	0	0	0	0
41	m	13	0	0	0	0
41	o	103	0	0	0	0
41	t	11	0	0	1	0
41	u	52	0	0	1	0
41	v	58	0	0	0	0
41	x	6	0	0	0	0
41	y	2	0	0	0	0
All	All	62674	0	61528	589	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (589) 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)
27:A:418:GOL:H11	12:M:1:FME:HG2	1.41	1.01
23:B:604:CLA:H42	23:B:605:CLA:H2	1.49	0.93
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.52	0.91
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.53	0.88
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.57	0.87
23:B:601:CLA:H12	23:B:601:CLA:H71	1.62	0.80
4:d:192[A]:THR:HG23	23:d:403[A]:CLA:HBC2	1.64	0.80
23:A:406[B]:CLA:H152	29:A:414[B]:PL9:H252	1.67	0.77
23:A:406[A]:CLA:H152	29:A:414[A]:PL9:H252	1.67	0.76
23:c:503:CLA:HBB1	23:c:512:CLA:H41	1.69	0.75
4:d:192[B]:THR:HG23	23:d:403[B]:CLA:HBC2	1.68	0.75
23:C:504:CLA:HBB1	23:C:513:CLA:H41	1.67	0.74
23:C:502:CLA:H193	23:C:508:CLA:HBB1	1.70	0.74
1:a:253[B]:GLY:HA3	2:b:491[B]:VAL:HG12	1.69	0.73
23:c:505:CLA:HHC	23:c:505:CLA:HBB1	1.71	0.73
23:d:402[B]:CLA:HHC	23:d:402[B]:CLA:HBB1	1.71	0.72
2:B:357[B]:ARG:NH2	4:D:337:GLU:O	2.22	0.72
23:b:606:CLA:H72	25:b:619:BCR:HC7	1.72	0.71
23:a:407:CLA:H192	23:c:505:CLA:H142	1.74	0.70
32:D:407[A]:LHG:H112	32:D:407[A]:LHG:H382	1.74	0.70
1:a:253[A]:GLY:HA3	2:b:491[A]:VAL:HG12	1.74	0.69
27:A:418:GOL:O2	41:A:501:HOH:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:279:LEU:HD22	23:c:509:CLA:HED2	1.74	0.69
23:C:514:CLA:H202	33:C:521:LMG:H402	1.75	0.69
32:D:407[B]:LHG:H382	32:D:407[B]:LHG:H112	1.76	0.67
23:B:615:CLA:H2	23:B:616:CLA:HBB2	1.76	0.67
23:C:507:CLA:H142	35:C:517[B]:DGD:HAF2	1.77	0.67
23:A:408:CLA:H193	23:C:507:CLA:H101	1.78	0.66
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.77	0.66
29:A:414[B]:PL9:H262	32:E:101[B]:LHG:H223	1.77	0.65
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	1.79	0.65
23:C:506:CLA:HHC	23:C:506:CLA:HBB1	1.79	0.64
1:A:102:LEU:HD12	34:b:625:HTG:H61	1.80	0.64
29:A:414[A]:PL9:H262	32:E:101[A]:LHG:H223	1.80	0.64
1:a:221[B]:SER:HB2	4:d:139[B]:ARG:O	1.99	0.63
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.80	0.63
23:a:407:CLA:H152	23:c:506:CLA:H142	1.80	0.63
10:k:23:ASP:OD2	18:y:21:GLN:NE2	2.32	0.63
3:C:286:ALA:HB2	23:C:503:CLA:HMD1	1.80	0.62
23:C:511:CLA:H192	23:C:511:CLA:HBC3	1.81	0.62
2:b:482[A]:ILE:HD12	2:b:486[A]:LEU:HD12	1.82	0.62
3:c:261:ARG:NH1	8:i:38:GLU:OE2	2.33	0.62
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.30	0.62
10:K:17:ILE:H	10:K:17:ILE:HD13	1.63	0.62
25:t:102:BCR:HC8	25:t:102:BCR:H321	1.82	0.62
15:U:86[B]:GLU:H	15:U:86[B]:GLU:CD	2.08	0.62
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.81	0.61
23:c:505:CLA:CMD	23:c:507:CLA:HAB	2.30	0.61
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.81	0.61
23:C:507:CLA:H142	35:C:517[A]:DGD:HAF2	1.81	0.61
12:M:33:GLN:HB2	12:m:33:GLN:HG3	1.81	0.61
23:b:601:CLA:H72	23:b:601:CLA:H2	1.81	0.61
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.83	0.61
2:B:226:TYR:HA	2:B:231:MET:HG3	1.81	0.60
3:c:213:LEU:HD13	23:c:506:CLA:H202	1.84	0.60
3:c:134[B]:ILE:HD13	23:c:511:CLA:H43	1.82	0.60
16:v:134[A]:LYS:HE2	27:v:202[A]:GOL:H32	1.83	0.60
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.84	0.59
33:z:101:LMG:H302	33:z:101:LMG:H141	1.84	0.59
1:a:334[B]:ARG:NH2	41:a:503[B]:HOH:O	2.35	0.59
19:z:32:ASP:O	19:z:36:SER:OG	2.18	0.59
29:A:414[B]:PL9:H253	23:D:402[B]:CLA:H141	1.84	0.59
25:y:101:BCR:H321	25:y:101:BCR:HC8	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:123:ILE:HD11	35:H:102:DGD:HAH2	1.85	0.58
23:d:402[A]:CLA:HHC	23:d:402[A]:CLA:HBB1	1.85	0.58
23:C:509:CLA:HBC3	23:C:511:CLA:H71	1.85	0.58
26:a:409[A]:SQD:H152	32:d:408[A]:LHG:H172	1.86	0.58
27:a:418:GOL:O3	14:t:2:GLU:OE1	2.22	0.58
13:O:169:ASP:OD1	27:O:303:GOL:H12	2.04	0.58
2:b:285:ASN:O	2:b:289:GLN:HG2	2.03	0.58
3:c:78:GLU:OE2	16:v:106:ASN:ND2	2.37	0.58
23:C:506:CLA:CMD	23:C:508:CLA:HAB	2.33	0.58
13:O:42:ARG:HH12	27:O:302:GOL:H12	1.68	0.58
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.86	0.57
25:b:619:BCR:H331	25:b:619:BCR:HC8	1.86	0.57
27:a:417:GOL:H32	12:m:1:FME:HG3	1.85	0.57
27:b:628:GOL:O3	27:b:628:GOL:O1	2.19	0.57
2:B:498:LYS:HE3	4:D:20:ASP:HA	1.86	0.57
31:A:417:LMT:H71	2:b:39:LEU:HD13	1.85	0.57
27:a:418:GOL:H11	12:m:1:FME:HE3	1.87	0.57
23:c:505:CLA:HMD1	23:c:507:CLA:HAB	1.87	0.56
1:a:221[A]:SER:HB2	4:d:139[A]:ARG:O	2.06	0.56
23:B:606:CLA:H202	26:a:410:SQD:H302	1.88	0.56
26:a:409[A]:SQD:H141	32:d:408[A]:LHG:H152	1.86	0.56
10:k:17:ILE:HD13	10:k:17:ILE:H	1.71	0.56
23:A:405[B]:CLA:HHC	23:A:405[B]:CLA:HBB1	1.88	0.56
25:T:102:BCR:H19C	25:b:618:BCR:H363	1.88	0.55
23:c:511:CLA:H191	33:z:101:LMG:H241	1.88	0.55
2:b:216:HIS:HE1	23:b:609:CLA:C1A	2.19	0.55
38:E:102:HEM:HAC	6:F:27:ALA:HB1	1.88	0.55
23:b:604:CLA:H42	23:b:605:CLA:H2	1.87	0.55
34:B:622:HTG:H4'1	31:B:630:LMT:H52	1.88	0.55
27:a:418:GOL:H31	12:m:1:FME:HG2	1.89	0.55
1:a:183[B]:MET:HA	23:a:404[B]:CLA:HMD1	1.90	0.54
23:a:405[A]:CLA:H191	32:a:419[A]:LHG:H111	1.88	0.54
4:D:192[B]:THR:HG23	23:D:402[B]:CLA:HBC2	1.89	0.54
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.42	0.54
2:b:482[B]:ILE:HD12	2:b:486[B]:LEU:HD12	1.90	0.54
1:a:183[A]:MET:HA	23:a:404[A]:CLA:HMD1	1.90	0.54
4:D:85:MET:CE	4:D:96:GLU:HG2	2.38	0.54
25:B:618:BCR:H363	25:t:102:BCR:H19C	1.90	0.53
26:F:102:SQD:H102	17:X:31:ILE:HD11	1.88	0.53
23:a:404[B]:CLA:H201	32:d:407[B]:LHG:H161	1.90	0.53
3:c:338[A]:GLY:HA3	3:c:341[A]:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:615:CLA:H2	23:B:616:CLA:CBB	2.38	0.53
25:b:619:BCR:H331	25:b:619:BCR:C8	2.39	0.53
32:d:407[B]:LHG:HC62	11:l:15[B]:THR:HG23	1.91	0.53
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.89	0.53
4:D:192[A]:THR:HG23	23:D:402[A]:CLA:HBC2	1.90	0.53
2:B:299:GLU:HG3	2:B:402:TYR:HD1	1.74	0.53
1:A:84[B]:PRO:HA	1:A:112[B]:TYR:CG	2.43	0.53
32:a:419[A]:LHG:HC31	5:e:9:PRO:HA	1.90	0.53
29:A:414[A]:PL9:H503	26:F:102:SQD:H341	1.91	0.53
23:a:407:CLA:H203	23:c:506:CLA:H101	1.91	0.53
25:C:515:BCR:H352	33:C:521:LMG:H352	1.91	0.52
23:B:609:CLA:HHC	23:B:609:CLA:HBB1	1.90	0.52
4:D:24:ARG:HD3	17:X:37:VAL:HG22	1.91	0.52
4:D:230[B]:SER:HB2	41:D:541:HOH:O	2.09	0.52
32:a:419[B]:LHG:HC31	5:e:9:PRO:HA	1.90	0.52
23:c:502:CLA:H61	23:c:512:CLA:H42	1.92	0.52
4:d:85:MET:CE	4:d:96:GLU:HG2	2.39	0.52
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.92	0.52
3:c:134[B]:ILE:HD11	23:c:511:CLA:H71	1.92	0.52
2:b:98:LEU:HB2	34:b:622:HTG:H7'1	1.92	0.51
1:a:84[A]:PRO:HA	1:a:112[A]:TYR:CG	2.45	0.51
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.23	0.51
23:C:502:CLA:C4D	23:C:504:CLA:H2	2.41	0.51
24:a:414[B]:PHO:HBC3	4:d:279:LEU:HD22	1.91	0.51
23:d:404:CLA:HHC	23:d:404:CLA:HBB1	1.93	0.51
23:c:501:CLA:C4D	23:c:503:CLA:H2	2.41	0.51
13:o:58:ASN:HD22	13:o:61:GLN:HG3	1.74	0.51
19:Z:32:ASP:OD2	19:Z:35:ARG:HB3	2.10	0.51
24:A:407[A]:PHO:HAB	4:D:205[A]:LEU:HD13	1.91	0.51
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.92	0.51
4:D:261[B]:PHE:CZ	32:D:406[B]:LHG:HC81	2.46	0.51
26:a:409[B]:SQD:H141	32:d:408[B]:LHG:H152	1.91	0.51
35:c:518:DGD:HBH2	32:d:408[B]:LHG:H211	1.93	0.51
27:l:801[A]:GOL:H32	14:t:25:GLU:HB2	1.91	0.51
1:A:84[A]:PRO:HA	1:A:112[A]:TYR:CG	2.46	0.51
6:F:21:VAL:O	6:F:25:THR:HG23	2.10	0.51
23:a:405[B]:CLA:H191	32:a:419[B]:LHG:H111	1.91	0.51
29:a:412[A]:PL9:H28	32:a:419[A]:LHG:H222	1.92	0.51
34:B:625:HTG:H61	1:a:102:LEU:HD12	1.92	0.51
2:B:383[B]:PHE:CZ	13:O:167:GLY:HA2	2.46	0.50
2:b:233:ASN:O	2:b:236:THR:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:42:LEU:HD21	23:c:511:CLA:H2A	1.93	0.50
3:c:338[B]:GLY:HA3	3:c:341[B]:LEU:O	2.11	0.50
29:A:414[A]:PL9:H253	23:D:402[A]:CLA:H141	1.92	0.50
13:O:124:ASN:OD1	13:O:147:ASN:ND2	2.43	0.50
24:a:406[B]:PHO:HAB	4:d:205[B]:LEU:HD13	1.93	0.50
32:d:407[A]:LHG:HC62	11:l:15[A]:THR:HG23	1.94	0.50
13:o:205:ASP:OD2	13:o:207:ARG:NH2	2.44	0.50
24:A:416[B]:PHO:H3A	23:D:402[B]:CLA:H142	1.94	0.50
25:h:101:BCR:H331	25:h:101:BCR:C8	2.42	0.50
27:O:303:GOL:O1	41:O:401:HOH:O	2.19	0.50
32:d:414[B]:LHG:H211	12:m:18:PRO:HG3	1.94	0.50
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.46	0.50
5:E:57:ALA:HB3	5:E:60:GLN:HG2	1.93	0.50
23:B:601:CLA:HHC	23:B:601:CLA:HBB1	1.94	0.50
3:C:252:ILE:HG22	3:C:253:LEU:HD23	1.94	0.50
5:E:77:GLU:O	5:E:81:GLU:HG2	2.12	0.50
10:K:24:VAL:HG13	18:Y:25:ILE:HD13	1.94	0.50
23:d:404:CLA:H162	7:h:37:LEU:HD21	1.94	0.50
13:O:25:THR:O	13:O:27:ARG:N	2.44	0.49
26:a:409[B]:SQD:H152	32:d:408[B]:LHG:H172	1.94	0.49
1:A:227[B]:THR:HB	1:A:231:GLU:HG3	1.94	0.49
23:C:502:CLA:C3D	23:C:504:CLA:H2	2.42	0.49
23:C:510:CLA:HMB1	23:C:510:CLA:HBB1	1.93	0.49
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.47	0.49
18:y:20:ALA:O	18:y:24:MET:HG2	2.13	0.49
3:C:203:THR:O	3:C:235:GLY:HA3	2.11	0.49
4:D:180:ARG:HD3	4:D:180:ARG:C	2.38	0.49
2:b:497:GLN:HB2	2:b:504:THR:HB	1.94	0.49
23:a:404[A]:CLA:H201	32:d:407[A]:LHG:H161	1.95	0.49
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.94	0.49
23:A:408:CLA:H151	23:C:507:CLA:H13	1.95	0.49
26:a:409[A]:SQD:H321	23:c:508:CLA:H102	1.95	0.49
8:I:35:LYS:O	8:I:37:LEU:N	2.46	0.48
9:j:6:ARG:NH1	9:j:6:ARG:HA	2.27	0.48
2:b:29:LEU:HD23	26:b:620:SQD:H201	1.95	0.48
23:B:613:CLA:H121	23:B:613:CLA:H162	1.64	0.48
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.95	0.48
32:d:408[A]:LHG:H331	32:d:408[A]:LHG:H361	1.55	0.48
33:d:412:LMG:H221	33:d:412:LMG:H191	1.57	0.48
3:C:42:LEU:HD21	23:C:512:CLA:H2A	1.95	0.48
23:C:502:CLA:HHC	23:C:502:CLA:HBB1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:245:VAL:HG22	23:b:612:CLA:H202	1.96	0.48
23:b:613:CLA:HBB1	23:b:613:CLA:HMB1	1.95	0.48
3:c:406:SER:HA	3:c:420[B]:VAL:HG23	1.96	0.48
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.94	0.48
9:J:2:SER:N	41:J:201:HOH:O	2.47	0.48
1:a:84[B]:PRO:HA	1:a:112[B]:TYR:CG	2.48	0.48
3:c:41:ARG:NH1	23:c:511:CLA:HMD1	2.28	0.48
32:D:407[A]:LHG:H382	32:D:407[A]:LHG:H132	1.96	0.48
5:E:57:ALA:H	5:E:60:GLN:HE21	1.60	0.48
10:K:26:PRO:O	10:K:29:PRO:HD2	2.14	0.48
1:a:227[B]:THR:HB	1:a:231:GLU:HG3	1.96	0.48
23:b:615:CLA:H61	23:b:615:CLA:H92	1.69	0.48
32:d:408[A]:LHG:C38	32:d:408[A]:LHG:H122	2.44	0.48
23:A:408:CLA:H18	23:C:506:CLA:H142	1.95	0.48
23:A:408:CLA:H41	23:A:408:CLA:H61	1.54	0.48
5:E:12:ASP:OD1	9:J:4:GLY:HA3	2.14	0.47
25:H:101:BCR:H24C	25:H:101:BCR:H371	1.70	0.47
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.14	0.47
23:A:404[B]:CLA:HBB1	23:A:404[B]:CLA:HMB3	1.96	0.47
23:A:405[A]:CLA:H203	23:A:405[A]:CLA:H162	1.74	0.47
3:C:95:LEU:HD21	23:C:502:CLA:OBD	2.14	0.47
3:C:275:SER:HB3	23:C:510:CLA:HED3	1.96	0.47
1:a:214[B]:MET:HB3	29:a:412[B]:PL9:H103	1.96	0.47
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.49	0.47
10:k:20:PRO:HB3	18:y:21:GLN:HG3	1.95	0.47
29:A:414[B]:PL9:H151	29:A:414[B]:PL9:H171	1.51	0.47
2:B:30:VAL:HG12	23:B:605:CLA:HHD	1.96	0.47
29:a:412[B]:PL9:H28	32:a:419[B]:LHG:H222	1.96	0.47
19:Z:4:LEU:HD22	19:Z:57:LEU:HD11	1.97	0.47
1:A:240[A]:GLY:HA3	14:T:29[A]:ILE:HG23	1.96	0.47
2:B:149:LEU:HG	23:B:606:CLA:HBB2	1.96	0.47
4:d:244[B]:TYR:OH	4:d:264[B]:LYS:HE3	2.13	0.47
32:A:419[B]:LHG:H361	23:B:613:CLA:H51	1.97	0.47
5:E:36:LEU:HA	5:E:39:SER:OG	2.15	0.47
25:H:101:BCR:C8	25:H:101:BCR:H331	2.45	0.47
1:a:160[A]:ILE:HD11	35:c:516[A]:DGD:HBT1	1.96	0.47
2:b:358:ARG:HB2	27:b:628:GOL:H31	1.96	0.47
12:m:5[B]:GLN:H	12:m:5[B]:GLN:NE2	2.12	0.47
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.95	0.47
2:b:36:SER:OG	25:b:618:BCR:H362	2.14	0.47
2:b:62:VAL:HB	23:b:605:CLA:HED3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:5[B]:GLN:H	12:m:5[B]:GLN:CD	2.20	0.47
26:A:410[A]:SQD:H152	26:A:410[A]:SQD:H122	1.54	0.47
15:u:10[A]:VAL:HG12	41:u:241:HOH:O	2.15	0.47
1:A:85[B]:SER:HA	1:A:109[B]:GLY:HA3	1.97	0.47
3:c:27:ASP:HB3	10:k:46:ARG:HG3	1.97	0.47
23:c:512:CLA:HMB2	23:c:512:CLA:H192	1.97	0.47
1:A:214[A]:MET:HE2	1:A:255[A]:PHE:CE1	2.49	0.47
3:C:261:ARG:NH1	8:I:38:GLU:OE2	2.47	0.47
25:T:102:BCR:HC7	25:T:102:BCR:H331	1.61	0.47
29:A:414[B]:PL9:H472	4:D:39:PRO:HD3	1.97	0.47
23:b:607:CLA:H91	23:b:607:CLA:H112	1.76	0.47
32:d:408[A]:LHG:H332	32:d:408[A]:LHG:H302	1.77	0.47
25:t:102:BCR:HC7	25:t:102:BCR:H331	1.56	0.47
31:B:631:LMT:H6E	31:t:101:LMT:H6D	1.97	0.46
26:a:409[B]:SQD:H321	23:c:508:CLA:H102	1.97	0.46
1:a:192[A]:ILE:HG13	1:a:293[A]:MET:HE1	1.97	0.46
32:d:408[B]:LHG:H122	32:d:408[B]:LHG:C38	2.45	0.46
13:O:205:ASP:OD1	13:O:207:ARG:HG3	2.16	0.46
29:a:412[B]:PL9:H351	6:f:25:THR:OG1	2.15	0.46
5:e:68:ASP:O	5:e:72:ALA:HB2	2.16	0.46
26:A:410[B]:SQD:H361	10:K:34:ALA:HA	1.98	0.46
4:D:323[A]:GLU:O	27:D:412:GOL:O2	2.33	0.46
29:a:412[A]:PL9:H151	29:a:412[A]:PL9:H171	1.57	0.46
23:B:614:CLA:H112	23:B:614:CLA:H71	1.56	0.46
23:b:611:CLA:H72	23:b:611:CLA:H112	1.83	0.46
3:C:223:TRP:CG	3:C:224:ILE:H	2.34	0.46
23:C:509:CLA:H142	23:C:509:CLA:H111	1.75	0.46
4:D:230[A]:SER:HB2	41:D:541:HOH:O	2.15	0.46
9:J:17:GLY:HA3	25:Y:101:BCR:H371	1.98	0.46
24:a:414[A]:PHO:HBC3	4:d:279:LEU:HD22	1.97	0.46
2:b:224:ARG:HH21	31:b:621:LMT:H1'	1.81	0.46
3:c:286:ALA:HB2	23:c:502:CLA:HMD1	1.97	0.46
3:C:334[A]:PRO:HA	13:O:153:THR:OG1	2.16	0.46
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.97	0.46
35:c:518:DGD:HBH2	32:d:408[A]:LHG:H211	1.98	0.46
23:B:610:CLA:H162	23:B:612:CLA:O1A	2.16	0.46
25:T:102:BCR:HC8	25:T:102:BCR:H311	1.97	0.46
23:C:505:CLA:H62	23:C:505:CLA:H41	1.72	0.46
3:c:182:PHE:HA	34:c:521:HTG:H61	1.98	0.46
1:A:231:GLU:HB3	41:A:637:HOH:O	2.15	0.46
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:504:CLA:H151	23:c:508:CLA:H143	1.98	0.46
23:c:508:CLA:H18	35:c:517[A]:DGD:HAT2	1.98	0.46
33:c:520:LMG:H232	33:c:520:LMG:H391	1.98	0.46
25:K:102:BCR:H24C	25:K:102:BCR:H371	1.68	0.45
23:d:402[A]:CLA:HBA1	23:d:402[A]:CLA:C4A	2.45	0.45
29:A:414[B]:PL9:HC8	29:A:414[B]:PL9:H121	1.74	0.45
2:B:383[A]:PHE:CZ	13:O:167:GLY:HA2	2.51	0.45
23:c:501:CLA:C3D	23:c:503:CLA:H2	2.46	0.45
13:o:58:ASN:C	13:o:60:ARG:H	2.23	0.45
2:B:36[B]:SER:OG	25:B:618:BCR:H362	2.17	0.45
23:C:511:CLA:H52	32:D:407[B]:LHG:H371	1.97	0.45
32:d:408[B]:LHG:H332	32:d:408[B]:LHG:H302	1.76	0.45
26:a:409[B]:SQD:H302	23:c:508:CLA:H71	1.97	0.45
29:a:412[B]:PL9:H171	29:a:412[B]:PL9:H151	1.55	0.45
2:B:144:PHE:CE2	2:B:148[A]:LEU:HD11	2.52	0.45
31:M:101:LMT:H6D	11:l:9:PRO:HA	1.99	0.45
23:b:614:CLA:H112	23:b:614:CLA:H72	1.65	0.45
1:A:82[B]:VAL:HB	1:A:174[B]:LEU:HB2	1.97	0.45
31:T:101:LMT:H112	31:T:101:LMT:H81	1.79	0.45
23:a:405[B]:CLA:H203	33:d:412:LMG:H412	1.98	0.45
26:b:620:SQD:H311	26:b:620:SQD:H341	1.64	0.45
3:c:391[B]:ARG:NH2	41:c:611:HOH:O	2.49	0.45
23:c:513:CLA:HBB1	25:c:514:BCR:H24C	1.99	0.45
32:D:407[B]:LHG:H382	32:D:407[B]:LHG:H132	1.99	0.45
13:O:142:PHE:HB2	13:O:199:LEU:HB2	1.98	0.45
25:T:102:BCR:HC8	25:T:102:BCR:H321	1.99	0.45
29:a:412[A]:PL9:H351	6:f:25:THR:OG1	2.17	0.45
27:a:417:GOL:H12	41:t:201:HOH:O	2.16	0.45
23:b:605:CLA:HBB1	23:b:605:CLA:CHC	2.38	0.45
32:d:408[B]:LHG:H331	32:d:408[B]:LHG:H361	1.60	0.45
23:A:405[B]:CLA:C4A	23:A:405[B]:CLA:HBA1	2.46	0.45
4:D:291:LEU:HD21	35:H:102:DGD:HBN1	1.99	0.45
4:D:323[B]:GLU:O	27:D:412:GOL:O2	2.34	0.45
25:T:102:BCR:H24C	25:T:102:BCR:H371	1.80	0.45
26:a:409[A]:SQD:H271	32:d:408[A]:LHG:H141	1.98	0.45
26:b:620:SQD:H462	26:b:620:SQD:H1	1.98	0.45
32:d:408[A]:LHG:H342	32:d:408[A]:LHG:H151	1.99	0.45
32:E:101[B]:LHG:O2	6:F:19:ARG:NH1	2.50	0.45
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.16	0.45
25:b:618:BCR:H24C	25:b:618:BCR:H371	1.83	0.45
25:C:516:BCR:H11C	25:C:516:BCR:H341	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:214[A]:MET:HE2	1:a:255[A]:PHE:CE1	2.52	0.45
2:B:188:ASP:OD2	2:B:194:ASN:ND2	2.39	0.44
23:C:507:CLA:H18	23:C:507:CLA:H152	1.45	0.44
32:E:101[B]:LHG:H291	32:E:101[B]:LHG:H261	1.74	0.44
15:u:92:VAL:HG12	15:u:97:ARG:HD2	1.98	0.44
23:C:506:CLA:HAA1	23:C:506:CLA:HBD	1.99	0.44
32:E:101[B]:LHG:H241	32:E:101[B]:LHG:HC61	1.83	0.44
8:I:36:ASP:OD1	8:I:36:ASP:N	2.50	0.44
1:a:131:TRP:CH2	23:c:505:CLA:HAA2	2.53	0.44
33:c:519:LMG:H181	10:k:27:VAL:HG11	1.98	0.44
4:d:24:ARG:NH1	17:x:37:VAL:HG22	2.32	0.44
10:k:24:VAL:HG21	18:y:25:ILE:HB	1.99	0.44
25:A:409:BCR:H24C	25:A:409:BCR:H371	1.71	0.44
31:A:420:LMT:O3'	31:A:420:LMT:H6'2	2.18	0.44
23:B:612:CLA:H61	23:B:612:CLA:H102	1.80	0.44
23:a:404[A]:CLA:H203	23:a:404[A]:CLA:H162	1.80	0.44
3:c:363:GLY:O	3:c:367:GLU:HG2	2.17	0.44
23:c:508:CLA:H18	35:c:517[B]:DGD:HAT2	2.00	0.44
26:A:410[B]:SQD:H122	26:A:410[B]:SQD:H152	1.66	0.44
4:D:261[A]:PHE:CZ	32:D:406[A]:LHG:HC81	2.52	0.44
6:F:15:ILE:HD13	20:R:23:ILE:HD11	1.99	0.44
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.99	0.44
3:c:203:THR:O	3:c:235:GLY:HA3	2.17	0.44
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.52	0.44
4:d:266[A]:TRP:CD1	32:d:407[A]:LHG:HC31	2.52	0.44
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.83	0.44
25:C:515:BCR:H24C	25:C:515:BCR:H371	1.82	0.44
35:C:518[A]:DGD:HAT1	35:C:519:DGD:HBE1	1.99	0.44
2:b:98:LEU:HB2	34:b:622:HTG:C7'	2.47	0.44
35:c:516[B]:DGD:HG11	41:c:603[B]:HOH:O	2.17	0.44
24:A:407[B]:PHO:HAB	4:D:205[B]:LEU:HD13	1.99	0.44
32:E:101[A]:LHG:H241	32:E:101[A]:LHG:HC61	1.85	0.44
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.45	0.44
1:a:105:TRP:CE2	1:a:110[A]:GLY:HA3	2.52	0.44
23:b:609:CLA:HMD1	7:h:27:THR:HB	1.99	0.44
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.99	0.44
20:R:18:TRP:O	20:R:22:ASN:ND2	2.43	0.44
19:z:37:LYS:HE2	19:z:41:PHE:HE2	1.83	0.44
1:A:133:LEU:HD23	4:D:256[B]:ILE:HG12	2.00	0.44
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.52	0.44
29:A:414[A]:PL9:H322	29:A:414[A]:PL9:H301	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:615:CLA:H91	23:B:615:CLA:H112	1.74	0.44
23:C:514:CLA:H161	33:C:521:LMG:H421	2.00	0.44
13:o:58:ASN:HB2	13:o:61:GLN:HG2	1.99	0.44
23:b:609:CLA:NC	25:h:101:BCR:H332	2.33	0.44
3:c:333[B]:GLY:HA3	41:c:730[B]:HOH:O	2.18	0.44
23:d:403[A]:CLA:HAA2	23:d:403[A]:CLA:HBD	2.00	0.44
13:O:130:GLN:H	13:O:130:GLN:CD	2.20	0.43
35:c:516[A]:DGD:HG11	41:c:603[A]:HOH:O	2.18	0.43
19:z:34:ASP:OD1	19:z:34:ASP:N	2.51	0.43
5:E:20:TRP:CD1	9:J:7:ILE:HD12	2.52	0.43
16:v:35:TYR:O	16:v:103:LYS:NZ	2.42	0.43
1:a:214[B]:MET:HE2	1:a:255[B]:PHE:CE1	2.54	0.43
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.53	0.43
23:b:605:CLA:H62	23:b:605:CLA:H41	1.63	0.43
25:c:514:BCR:H11C	25:c:514:BCR:H341	1.79	0.43
29:A:414[A]:PL9:H472	4:D:39:PRO:HD3	2.00	0.43
8:I:33:LYS:HB3	8:I:34:ARG:H	1.68	0.43
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.00	0.43
4:d:194:ASN:HA	4:d:295[B]:SER:OG	2.18	0.43
31:t:101:LMT:H112	31:t:101:LMT:H81	1.81	0.43
23:A:404[A]:CLA:H143	24:A:407[A]:PHO:H61	2.01	0.43
32:d:408[A]:LHG:H242	32:d:408[A]:LHG:H272	1.86	0.43
26:A:410[A]:SQD:H361	10:K:34:ALA:HA	2.01	0.43
3:C:443[A]:TRP:CE2	23:C:509:CLA:HMD2	2.54	0.43
4:D:264[B]:LYS:NZ	41:D:520[B]:HOH:O	2.50	0.43
32:D:406[A]:LHG:HC62	11:L:15[A]:THR:HG23	2.00	0.43
11:L:9:PRO:HA	31:m:103:LMT:H6D	2.00	0.43
26:a:409[B]:SQD:H271	32:d:408[B]:LHG:H141	1.99	0.43
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.81	0.43
31:e:101:LMT:H6'1	6:f:43:ILE:HG12	2.00	0.43
23:A:404[A]:CLA:HBB1	23:A:404[A]:CLA:HMB3	2.01	0.43
33:B:621:LMG:H112	33:B:621:LMG:H141	1.76	0.43
3:C:41:ARG:NH1	23:C:512:CLA:HMD1	2.33	0.43
35:C:517[A]:DGD:HG11	41:C:601[A]:HOH:O	2.18	0.43
2:b:144:PHE:CE1	2:b:210:ILE:HG23	2.53	0.43
10:k:19:ASP:HB3	10:k:20:PRO:HD3	2.01	0.43
26:B:620:SQD:H1	26:B:620:SQD:H462	2.00	0.43
3:C:52:ALA:HB2	23:C:512:CLA:HMA2	2.01	0.43
3:C:406:SER:HA	3:C:420[A]:VAL:HG23	2.00	0.43
4:D:261[B]:PHE:CE1	32:D:406[B]:LHG:HC81	2.54	0.43
3:c:97:TRP:CE2	3:c:178:LYS:HE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:d:402[B]:CLA:HHC	23:d:402[B]:CLA:CBB	2.46	0.43
13:o:92:SER:HB3	13:o:131:PRO:HA	1.99	0.43
23:A:405[A]:CLA:HHC	23:A:405[A]:CLA:HBB1	2.01	0.43
24:A:416[A]:PHO:H3A	23:D:402[A]:CLA:H142	1.99	0.43
2:B:363:PHE:HB3	2:B:365:SER:O	2.18	0.43
23:B:601:CLA:H192	23:B:601:CLA:H162	1.85	0.43
25:B:619:BCR:H371	25:B:619:BCR:H24C	1.74	0.43
23:b:602:CLA:HHC	23:b:602:CLA:HBB1	2.00	0.43
7:h:62:TRP:C	7:h:64:ALA:H	2.26	0.43
25:t:102:BCR:H382	25:t:102:BCR:H23C	2.01	0.43
29:A:414[B]:PL9:H322	29:A:414[B]:PL9:H301	1.77	0.43
34:B:623:HTG:H7'3	34:B:623:HTG:H4'2	1.85	0.43
3:C:157:MET:HE2	3:C:157:MET:HA	2.01	0.43
32:d:414[A]:LHG:H211	12:m:18:PRO:HG3	2.00	0.43
25:c:514:BCR:H15C	25:c:514:BCR:H351	1.82	0.42
19:Z:33:TRP:HZ2	33:Z:101:LMG:HC61	1.84	0.42
23:A:405[B]:CLA:H203	23:A:405[B]:CLA:H162	1.81	0.42
9:J:6:ARG:HG3	41:J:201:HOH:O	2.18	0.42
13:O:24:ASP:HA	13:O:203:LYS:HE2	2.02	0.42
25:T:102:BCR:H11C	25:T:102:BCR:H341	1.82	0.42
32:a:419[B]:LHG:H241	32:a:419[B]:LHG:HC61	1.88	0.42
2:b:491[A]:VAL:HG13	4:d:136[A]:VAL:HG13	2.02	0.42
23:b:616:CLA:H13	23:b:616:CLA:H102	1.84	0.42
1:A:227[A]:THR:HB	1:A:231:GLU:HG3	2.00	0.42
7:H:38:PHE:HB2	25:H:101:BCR:C10	2.49	0.42
15:U:45:LEU:HD21	15:U:71:GLN:HB3	2.01	0.42
1:a:105:TRP:CE2	1:a:110[B]:GLY:HA3	2.54	0.42
26:a:410:SQD:H1	41:a:622:HOH:O	2.19	0.42
32:a:419[A]:LHG:H241	32:a:419[A]:LHG:HC61	1.89	0.42
2:b:41:GLU:HB3	2:b:60:MET:SD	2.60	0.42
3:c:406:SER:HA	3:c:420[A]:VAL:HG23	2.02	0.42
23:c:509:CLA:H142	23:c:509:CLA:H112	1.83	0.42
1:A:131:TRP:CD2	1:A:131:TRP:C	2.96	0.42
23:B:614:CLA:H8	25:B:617:BCR:H362	2.01	0.42
23:C:510:CLA:H192	23:C:510:CLA:H162	1.83	0.42
23:C:511:CLA:H52	32:D:407[A]:LHG:H371	2.00	0.42
8:I:38:GLU:HG2	8:I:38:GLU:OXT	2.19	0.42
13:O:66:VAL:HG21	13:O:110:MET:HE3	2.01	0.42
23:a:407:CLA:H41	23:a:407:CLA:H61	1.90	0.42
29:A:414[A]:PL9:H171	29:A:414[A]:PL9:H151	1.53	0.42
2:b:161:LEU:HD12	2:b:161:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:491[B]:VAL:HG13	4:d:136[B]:VAL:HG13	2.02	0.42
4:d:148[B]:ALA:HB3	4:d:149[B]:PRO:HD3	2.01	0.42
16:v:134[B]:LYS:HE2	27:v:202[B]:GOL:H32	2.00	0.42
2:B:133:LEU:HB2	27:B:627:GOL:H31	2.02	0.42
3:C:338[A]:GLY:HA3	3:C:341[A]:LEU:O	2.20	0.42
4:D:15:PHE:H	34:D:410:HTG:H61	1.85	0.42
2:b:159:THR:HA	2:b:181:VAL:O	2.20	0.42
23:c:509:CLA:H43	23:c:509:CLA:H12	1.91	0.42
23:c:512:CLA:H121	23:c:513:CLA:H142	2.01	0.42
23:c:512:CLA:H142	23:c:512:CLA:H111	1.90	0.42
2:B:158:LEU:HB3	2:B:199:VAL:HG22	2.02	0.42
32:D:407[A]:LHG:H332	32:D:407[A]:LHG:H302	1.85	0.42
23:b:601:CLA:H92	25:h:101:BCR:H403	2.02	0.42
32:b:629[B]:LHG:H112	4:d:273[B]:PHE:CZ	2.55	0.42
25:c:515:BCR:H11C	25:c:515:BCR:H341	1.94	0.42
4:d:107:LEU:O	41:d:501:HOH:O	2.21	0.42
13:o:79:ASP:OD1	13:o:80:GLN:N	2.48	0.42
13:o:204:VAL:HG22	13:o:211:ILE:HG22	2.00	0.42
1:A:183[A]:MET:HA	23:A:404[A]:CLA:HMD1	2.01	0.42
32:A:419[A]:LHG:H361	23:B:613:CLA:H51	2.01	0.42
23:B:601:CLA:H72	23:B:601:CLA:C4D	2.49	0.42
25:B:617:BCR:H15C	25:B:617:BCR:H351	1.95	0.42
16:V:126:LEU:HB3	16:V:129:LYS:HB2	2.02	0.42
2:b:363:PHE:HB3	2:b:365:SER:O	2.20	0.42
25:b:617:BCR:H24C	25:b:617:BCR:H371	1.77	0.42
27:l:801[B]:GOL:H32	14:t:25:GLU:HB2	2.00	0.42
2:B:162:PHE:O	23:B:606:CLA:HHD	2.20	0.42
2:B:383[A]:PHE:O	13:O:166:SER:HA	2.20	0.42
3:C:174:LEU:HB3	23:C:503:CLA:H152	2.00	0.42
3:C:330:SER:HB3	13:O:100:GLY:O	2.19	0.42
13:O:42:ARG:O	13:O:241:ALA:HA	2.20	0.42
32:a:419[B]:LHG:H172	32:a:419[B]:LHG:H142	1.88	0.42
3:c:162:GLY:HA2	3:c:248:GLY:HA2	2.02	0.42
16:v:134[B]:LYS:HB3	27:v:202[B]:GOL:H32	2.02	0.42
23:A:405[A]:CLA:HBA1	23:A:405[A]:CLA:C4A	2.50	0.42
2:B:49:ASP:OD2	13:o:57:LYS:NZ	2.43	0.42
23:B:606:CLA:H122	23:B:606:CLA:H161	1.92	0.42
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.01	0.42
32:D:407[A]:LHG:H382	32:D:407[A]:LHG:C11	2.45	0.42
2:b:216:HIS:CE1	23:b:609:CLA:C1A	3.02	0.42
23:b:615:CLA:H91	23:b:615:CLA:H112	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:i:33:LYS:O	8:i:35:LYS:HG3	2.20	0.42
3:C:135:ARG:HA	3:C:135:ARG:HD2	1.95	0.41
23:C:504:CLA:CBB	23:C:513:CLA:H41	2.45	0.41
1:a:190[B]:HIS:ND1	1:a:298[B]:ASN:OD1	2.53	0.41
4:d:14:TRP:CD1	34:d:411:HTG:H61	2.54	0.41
13:o:216:GLU:CD	13:o:234:LYS:HD2	2.45	0.41
25:t:102:BCR:H371	25:t:102:BCR:H24C	1.87	0.41
23:A:404[A]:CLA:H192	23:A:404[A]:CLA:H161	1.80	0.41
25:B:618:BCR:H15C	25:B:618:BCR:H351	1.90	0.41
32:D:407[A]:LHG:H362	32:D:407[A]:LHG:H331	1.86	0.41
32:E:101[A]:LHG:O2	6:F:19:ARG:NH1	2.52	0.41
1:a:15:GLU:HB2	31:a:416:LMT:H6'2	2.02	0.41
23:b:605:CLA:HAA1	23:b:605:CLA:HBD	2.02	0.41
3:c:215:LYS:HD3	3:c:221:GLU:O	2.20	0.41
23:A:406[B]:CLA:HED1	35:C:519:DGD:HAE2	2.03	0.41
23:C:506:CLA:H93	23:C:506:CLA:H111	1.79	0.41
12:M:12:ALA:O	12:M:16[B]:LEU:HB2	2.21	0.41
1:a:261[A]:GLN:HG3	2:b:493[A]:TRP:CH2	2.56	0.41
3:c:61:VAL:HG12	3:c:118:HIS:O	2.20	0.41
23:c:512:CLA:HBA2	23:c:512:CLA:H3A	1.79	0.41
23:d:403[B]:CLA:HAA2	23:d:403[B]:CLA:HBD	2.02	0.41
25:k:101:BCR:H24C	25:k:101:BCR:H371	1.70	0.41
10:K:16:ALA:O	10:K:19:ASP:HB2	2.19	0.41
13:O:54:GLU:HG2	13:O:64:GLU:O	2.19	0.41
1:a:214[A]:MET:HB3	29:a:412[A]:PL9:H103	2.01	0.41
24:a:414[A]:PHO:H42	24:a:414[A]:PHO:H11	1.92	0.41
25:k:101:BCR:H15C	25:k:101:BCR:H351	1.92	0.41
13:O:93:LEU:O	13:O:128:SER:HA	2.20	0.41
13:O:169:ASP:H	27:O:303:GOL:H12	1.85	0.41
23:c:508:CLA:H122	23:c:508:CLA:H162	1.74	0.41
25:c:515:BCR:H24C	25:c:515:BCR:H371	1.89	0.41
4:d:148[A]:ALA:HB3	4:d:149[A]:PRO:HD3	2.03	0.41
23:d:404:CLA:H61	23:d:404:CLA:H41	1.69	0.41
32:d:408[A]:LHG:H142	32:d:408[A]:LHG:H372	2.03	0.41
29:A:414[B]:PL9:H221	29:A:414[B]:PL9:H201	1.87	0.41
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.02	0.41
13:O:39[A]:ARG:HB2	13:O:246:ALA:HB2	2.03	0.41
3:c:31:SER:CB	3:c:41:ARG:HG2	2.50	0.41
32:d:408[B]:LHG:H242	32:d:408[B]:LHG:H272	1.88	0.41
13:o:142:PHE:HB2	13:o:199:LEU:HB2	2.03	0.41
1:A:85[A]:SER:HA	1:A:109[A]:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:404[B]:CLA:CBD	23:A:405[B]:CLA:HAC2	2.50	0.41
2:B:58:GLN:C	2:B:329:PRO:HB3	2.46	0.41
2:B:86:ILE:H	2:B:86:ILE:HG13	1.77	0.41
25:B:618:BCR:C8	25:B:618:BCR:H331	2.50	0.41
13:O:79:ASP:OD1	13:O:80:GLN:N	2.47	0.41
2:b:383[B]:PHE:CZ	13:o:167:GLY:HA2	2.55	0.41
32:E:101[A]:LHG:H291	32:E:101[A]:LHG:H261	1.75	0.41
1:a:93[A]:PHE:CD2	1:a:95:PRO:HD3	2.55	0.41
2:b:58:GLN:C	2:b:329:PRO:HB3	2.45	0.41
23:b:603:CLA:H3A	23:b:603:CLA:CGA	2.51	0.41
11:l:14:ARG:HB3	14:t:25:GLU:HG3	2.03	0.41
1:A:214[B]:MET:HE2	1:A:255[B]:PHE:CE1	2.56	0.41
29:A:414[B]:PL9:HC8	29:A:414[B]:PL9:HC2	1.77	0.41
2:B:216:HIS:CE1	23:B:609:CLA:NA	2.88	0.41
2:B:383[B]:PHE:O	13:O:166:SER:HA	2.21	0.41
34:B:622:HTG:H6'2	34:B:622:HTG:H3'1	1.90	0.41
33:C:521:LMG:H331	33:C:521:LMG:H362	1.96	0.41
4:D:209[A]:LEU:C	4:D:209[A]:LEU:HD23	2.46	0.41
4:D:210[B]:LEU:HA	4:D:213[B]:ILE:HG22	2.02	0.41
1:a:160[B]:ILE:HD11	35:c:516[B]:DGD:HBT1	2.03	0.41
23:b:612:CLA:H122	23:b:612:CLA:H162	1.89	0.41
3:c:52:ALA:HB2	23:c:511:CLA:HMA1	2.03	0.41
23:c:512:CLA:H162	23:c:512:CLA:H122	1.79	0.41
25:h:101:BCR:H24C	25:h:101:BCR:H371	1.71	0.41
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.95	0.41
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.56	0.41
13:O:137:THR:C	13:O:139:SER:H	2.29	0.41
2:b:149[B]:LEU:HD11	23:b:604:CLA:H122	2.02	0.41
23:c:504:CLA:H62	35:c:518:DGD:HB62	2.03	0.41
25:y:101:BCR:H15C	25:y:101:BCR:H351	1.86	0.41
1:A:140[B]:ARG:HB2	4:D:220[B]:ASN:HA	2.02	0.40
1:A:243[A]:GLU:CD	1:A:243[A]:GLU:H	2.27	0.40
23:A:404[A]:CLA:CBD	23:A:405[A]:CLA:HAC2	2.51	0.40
29:A:414[B]:PL9:H451	17:X:28:LEU:HD11	2.03	0.40
23:C:513:CLA:H143	23:C:514:CLA:H142	2.02	0.40
23:D:402[B]:CLA:HAA2	23:D:402[B]:CLA:HBD	2.04	0.40
16:V:72:LEU:HA	16:V:72:LEU:HD23	1.90	0.40
1:a:217[B]:SER:O	1:a:221[B]:SER:HB3	2.20	0.40
2:b:216:HIS:CE1	23:b:609:CLA:NA	2.88	0.40
16:v:41:HIS:HA	16:v:45[B]:ILE:O	2.21	0.40
16:v:106:ASN:OD1	16:v:106:ASN:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:414[A]:PL9:H121	29:A:414[A]:PL9:HC8	1.78	0.40
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.88	0.40
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.03	0.40
23:B:615:CLA:H71	23:B:616:CLA:H172	2.03	0.40
26:B:620:SQD:H381	31:m:103:LMT:H121	2.03	0.40
3:C:325:GLY:O	15:U:51:LYS:NZ	2.36	0.40
4:D:194:ASN:HA	4:D:295[B]:SER:OG	2.20	0.40
25:T:102:BCR:H351	26:b:620:SQD:H211	2.02	0.40
23:a:405[A]:CLA:H203	33:d:412:LMG:H412	2.02	0.40
23:b:613:CLA:H72	23:b:613:CLA:H111	1.84	0.40
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.78	0.40
32:d:408[B]:LHG:H151	32:d:408[B]:LHG:H342	2.03	0.40
23:B:601:CLA:H72	23:B:601:CLA:C3D	2.51	0.40
3:C:406:SER:HA	3:C:420[B]:VAL:HG23	2.04	0.40
25:b:619:BCR:HC7	25:b:619:BCR:H311	1.71	0.40
1:A:192[B]:ILE:HG13	1:A:293[B]:MET:HE1	2.04	0.40
25:A:409:BCR:H15C	25:A:409:BCR:H351	1.90	0.40
29:A:414[A]:PL9:HC8	29:A:414[A]:PL9:HC2	1.71	0.40
3:C:146:PHE:HZ	23:C:513:CLA:HBB2	1.86	0.40
3:C:391[B]:ARG:HA	3:C:391[B]:ARG:HD3	1.85	0.40
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.57	0.40
1:a:227[A]:THR:HB	1:a:231:GLU:HG3	2.03	0.40
29:a:412[B]:PL9:H321	29:a:412[B]:PL9:H301	1.82	0.40
2:b:413:ASP:HA	2:b:414:PRO:HD3	1.95	0.40
2:b:450:TRP:HB3	23:b:607:CLA:HMB1	2.04	0.40
29:A:414[A]:PL9:H221	29:A:414[A]:PL9:H201	1.86	0.40
29:A:414[B]:PL9:H471	29:A:414[B]:PL9:H43	1.69	0.40
35:C:518[A]:DGD:HAE2	35:C:518[A]:DGD:HA81	1.86	0.40
4:D:49:LEU:HD13	25:D:404:BCR:C15	2.51	0.40
16:V:41:HIS:CD2	40:V:201:HEC:NB	2.89	0.40
23:a:404[B]:CLA:H203	23:a:404[B]:CLA:H162	1.86	0.40
25:b:619:BCR:H11C	25:b:619:BCR:H341	1.80	0.40
3:c:443[A]:TRP:CZ2	23:c:508:CLA:HMD1	2.56	0.40
20:R:24:LEU:N	20:R:25:PRO:HD2	2.36	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	553/344 (161%)	544 (98%)	7 (1%)	2 (0%)	30	34
1	a	551/344 (160%)	540 (98%)	9 (2%)	2 (0%)	30	34
2	B	524/505 (104%)	517 (99%)	7 (1%)	0	100	100
2	b	521/505 (103%)	507 (97%)	14 (3%)	0	100	100
3	C	548/455 (120%)	540 (98%)	7 (1%)	1 (0%)	43	51
3	c	554/455 (122%)	545 (98%)	8 (1%)	1 (0%)	43	51
4	D	454/342 (133%)	439 (97%)	15 (3%)	0	100	100
4	d	457/342 (134%)	446 (98%)	11 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	62 (100%)	0	0	100	100
7	h	63/65 (97%)	60 (95%)	2 (3%)	1 (2%)	7	6
8	I	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	4	2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
13	O	251/244 (103%)	242 (96%)	8 (3%)	1 (0%)	30	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	249/244 (102%)	244 (98%)	5 (2%)	0	100	100
14	T	33/32 (103%)	33 (100%)	0	0	100	100
14	t	32/32 (100%)	32 (100%)	0	0	100	100
15	U	97/104 (93%)	93 (96%)	4 (4%)	0	100	100
15	u	99/104 (95%)	94 (95%)	5 (5%)	0	100	100
16	V	140/137 (102%)	136 (97%)	4 (3%)	0	100	100
16	v	140/137 (102%)	135 (96%)	5 (4%)	0	100	100
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	24 (89%)	3 (11%)	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	5
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	5
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	6180/5384 (115%)	6042 (98%)	127 (2%)	11 (0%)	43	51

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	I	36	ASP
3	C	416	SER
13	O	26	ALA
3	c	416	SER
19	Z	31	GLN
19	z	30	PRO
7	h	63	LYS
1	a	259[A]	ILE
1	a	259[B]	ILE
1	A	259[A]	ILE
1	A	259[B]	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	444/279 (159%)	442 (100%)	2 (0%)	81	90
1	a	442/279 (158%)	441 (100%)	1 (0%)	87	94
2	B	423/403 (105%)	416 (98%)	7 (2%)	53	69
2	b	420/403 (104%)	407 (97%)	13 (3%)	35	48
3	C	431/356 (121%)	422 (98%)	9 (2%)	47	63
3	c	437/356 (123%)	430 (98%)	7 (2%)	55	71
4	D	368/277 (133%)	365 (99%)	3 (1%)	73	85
4	d	372/277 (134%)	368 (99%)	4 (1%)	65	79
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	36
5	e	72/73 (99%)	71 (99%)	1 (1%)	59	75
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	26 (100%)	0	100	100
7	H	54/54 (100%)	52 (96%)	2 (4%)	30	41
7	h	55/54 (102%)	55 (100%)	0	100	100
8	I	34/34 (100%)	32 (94%)	2 (6%)	18	22
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	51
9	J	26/27 (96%)	24 (92%)	2 (8%)	12	13
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	40
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	3
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	7
11	L	36/35 (103%)	36 (100%)	0	100	100
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	52
12	M	30/32 (94%)	27 (90%)	3 (10%)	7	7
12	m	32/32 (100%)	30 (94%)	2 (6%)	16	19
13	O	216/207 (104%)	210 (97%)	6 (3%)	38	52
13	o	213/207 (103%)	206 (97%)	7 (3%)	33	45
14	T	32/28 (114%)	28 (88%)	4 (12%)	4	4
14	t	31/28 (111%)	31 (100%)	0	100	100
15	U	86/89 (97%)	84 (98%)	2 (2%)	44	59
15	u	88/89 (99%)	86 (98%)	2 (2%)	44	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	123/117 (105%)	122 (99%)	1 (1%)	73	85
16	v	123/117 (105%)	120 (98%)	3 (2%)	43	58
17	X	32/33 (97%)	31 (97%)	1 (3%)	35	48
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	19 (86%)	3 (14%)	3	3
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18	22
19	z	52/52 (100%)	44 (85%)	8 (15%)	2	2
20	R	29/29 (100%)	27 (93%)	2 (7%)	14	16
All	All	5110/4403 (116%)	4997 (98%)	113 (2%)	44	61

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243[A]	GLU
1	A	243[B]	GLU
2	B	161	LEU
2	B	294	SER
2	B	298	LEU
2	B	299	GLU
2	B	389	LYS
2	B	419	SER
2	B	472	ARG
3	C	24	THR
3	C	29	GLU
3	C	30	SER
3	C	142	GLU
3	C	255	THR
3	C	289	PHE
3	C	315[A]	MET
3	C	315[B]	MET
3	C	462	GLU
4	D	259[A]	ILE
4	D	259[B]	ILE
4	D	338	ASN
5	E	4	THR
5	E	54	SER
5	E	71	GLU
7	H	12	ARG

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Mol	Chain	Res	Type
7	H	43	LEU
8	I	33	LYS
8	I	34	ARG
9	J	6	ARG
9	J	9	LEU
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
10	K	27	VAL
12	M	16[A]	LEU
12	M	16[B]	LEU
12	M	20	VAL
13	O	49	THR
13	O	55	GLU
13	O	87	VAL
13	O	98[A]	GLU
13	O	98[B]	GLU
13	O	118	LEU
14	T	25[A]	GLU
14	T	25[B]	GLU
14	T	30[A]	THR
14	T	30[B]	THR
15	U	10	VAL
15	U	70	ARG
16	V	15	GLU
17	X	14	LEU
1	a	13	LEU
2	b	128	THR
2	b	161	LEU
2	b	223	GLN
2	b	240	SER
2	b	245	VAL
2	b	287	ARG
2	b	298	LEU
2	b	362	PHE
2	b	472	ARG
2	b	486[A]	LEU
2	b	486[B]	LEU
2	b	491[A]	VAL
2	b	491[B]	VAL
3	c	142	GLU
3	c	152	LYS

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Mol	Chain	Res	Type
3	c	240	ILE
3	c	255	THR
3	c	289	PHE
3	c	315[A]	MET
3	c	315[B]	MET
4	d	259[A]	ILE
4	d	259[B]	ILE
4	d	272[A]	LEU
4	d	272[B]	LEU
5	e	71	GLU
8	i	33	LYS
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	24	VAL
11	l	2	GLU
12	m	16[A]	LEU
12	m	16[B]	LEU
13	o	25	THR
13	o	36	GLN
13	o	37	THR
13	o	58	ASN
13	o	69	LYS
13	o	118	LEU
13	o	194	LYS
15	u	10[A]	VAL
15	u	10[B]	VAL
16	v	15	GLU
16	v	24	LYS
16	v	85	GLU
18	y	18	VAL
18	y	19	ILE
18	y	45	ASN
19	Z	3	ILE
19	Z	20	VAL
19	Z	31	GLN
20	R	4	ARG
20	R	29	LYS
19	z	2	THR
19	z	3	ILE
19	z	4	LEU
19	z	7	LEU

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Mol	Chain	Res	Type
19	z	21	ILE
19	z	32	ASP
19	z	34	ASP
19	z	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	60	GLN
11	L	8	GLN
13	O	80	GLN
13	O	231	HIS
15	U	78	ASN
17	X	38	GLN
3	c	19	ASN
3	c	201	ASN
11	l	8	GLN
13	o	58	ASN
16	v	86	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	M	1	12	8,9,10	0.67	0	8,9,11	1.10	1 (12%)
14	FME	T	1	14	8,9,10	0.66	0	8,9,11	1.56	2 (25%)
8	FME	I	1	8	8,9,10	0.62	0	8,9,11	1.11	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	i	1	8	8,9,10	0.71	0	8,9,11	1.12	1 (12%)
12	FME	m	1	12	8,9,10	0.59	0	8,9,11	1.45	3 (37%)
14	FME	t	1	14	8,9,10	0.75	0	8,9,11	1.46	2 (25%)

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CB-CA-N	-2.89	105.26	110.52
12	m	1	FME	O1-CN-N	-2.62	118.54	125.32
14	t	1	FME	O-C-CA	-2.45	118.48	124.77
12	m	1	FME	CA-N-CN	-2.26	119.34	122.82
14	t	1	FME	CA-N-CN	-2.22	119.40	122.82
14	T	1	FME	CG-CB-CA	2.20	119.60	112.87
8	I	1	FME	O-C-CA	-2.13	119.28	124.77
8	i	1	FME	O-C-CA	-2.07	119.44	124.77
12	M	1	FME	O-C-CA	-2.05	119.49	124.77
12	m	1	FME	O-C-CA	-2.00	119.62	124.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
14	T	1	FME	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	1	FME	1	0
12	m	1	FME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 274 ligands modelled in this entry, 21 are monoatomic and 20 are unknown - leaving 233 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	$\# Z > 2$
26	SQD	B	620	-	52,54,54	1.03	3 (5%)	62,65,65	1.73	12 (19%)
29	PL9	A	414[B]	-	55,55,55	0.68	3 (5%)	68,69,69	2.01	25 (36%)
38	HEM	E	102	5,6	50,50,50	1.55	7 (14%)	67,82,82	1.77	16 (23%)
27	GOL	a	418	-	5,5,5	1.31	1 (20%)	5,5,5	1.10	1 (20%)
33	LMG	D	411	39	51,51,55	0.84	2 (3%)	59,59,63	1.00	4 (6%)
25	BCR	k	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.53	13 (23%)
23	CLA	c	510	-	69,73,73	2.01	20 (28%)	82,113,113	2.70	32 (39%)
27	GOL	V	203[A]	-	5,5,5	1.29	1 (20%)	5,5,5	0.97	0
32	LHG	D	406[A]	-	48,48,48	0.86	3 (6%)	51,54,54	1.00	4 (7%)
23	CLA	b	609	-	69,73,73	2.01	20 (28%)	82,113,113	2.70	35 (42%)
28	OEX	a	411[B]	41,1,3	0,15,15	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GOL	v	202[B]	-	5,5,5	1.19	0	5,5,5	0.93	0
32	LHG	d	408[A]	-	48,48,48	0.92	2 (4%)	51,54,54	1.00	3 (5%)
23	CLA	C	503	-	69,73,73	1.99	20 (28%)	82,113,113	2.64	30 (36%)
32	LHG	E	101[A]	-	41,41,48	1.07	2 (4%)	44,47,54	1.12	3 (6%)
27	GOL	c	526	-	5,5,5	1.07	0	5,5,5	1.07	0
37	BCT	d	401[B]	21	3,3,3	0.48	0	2,3,3	1.23	0
23	CLA	C	504	-	69,73,73	1.94	19 (27%)	82,113,113	2.77	30 (36%)
25	BCR	T	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.70	14 (25%)
32	LHG	d	407[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.09	4 (7%)
23	CLA	d	403[A]	-	69,73,73	1.92	19 (27%)	82,113,113	2.67	30 (36%)
27	GOL	B	624	-	5,5,5	0.76	0	5,5,5	1.19	1 (20%)
23	CLA	B	613	-	69,73,73	1.98	19 (27%)	82,113,113	2.65	32 (39%)
31	LMT	B	631	-	25,25,36	0.86	2 (8%)	30,30,47	1.17	3 (10%)
23	CLA	A	404[B]	-	69,73,73	2.00	20 (28%)	82,113,113	2.73	33 (40%)
23	CLA	c	501	-	69,73,73	1.98	20 (28%)	82,113,113	2.77	30 (36%)
23	CLA	c	506	-	69,73,73	2.02	20 (28%)	82,113,113	2.66	31 (37%)
27	GOL	O	303	-	5,5,5	1.01	0	5,5,5	1.19	1 (20%)
32	LHG	L	101[B]	-	48,48,48	0.93	3 (6%)	51,54,54	1.10	4 (7%)
33	LMG	B	621	-	51,51,55	0.92	2 (3%)	59,59,63	1.33	5 (8%)
24	PHO	A	416[A]	-	58,69,69	2.74	14 (24%)	55,99,99	2.91	17 (30%)
31	LMT	A	417	-	36,36,36	0.92	2 (5%)	47,47,47	0.99	1 (2%)
23	CLA	B	614	-	69,73,73	2.02	20 (28%)	82,113,113	2.79	33 (40%)
23	CLA	B	611	-	69,73,73	2.59	20 (28%)	82,113,113	3.62	33 (40%)
23	CLA	b	607	41	69,73,73	1.95	20 (28%)	82,113,113	2.65	31 (37%)
24	PHO	a	414[A]	-	58,69,69	2.76	13 (22%)	55,99,99	3.06	17 (30%)
25	BCR	b	618	-	41,41,41	1.02	1 (2%)	56,56,56	1.16	6 (10%)
23	CLA	d	402[A]	41	69,73,73	1.98	17 (24%)	82,113,113	2.66	30 (36%)
31	LMT	t	101	-	26,26,36	0.91	2 (7%)	31,31,47	1.37	2 (6%)
34	HTG	B	623	-	19,19,19	0.75	1 (5%)	23,24,24	1.32	2 (8%)
25	BCR	b	619	-	41,41,41	1.09	1 (2%)	56,56,56	1.37	6 (10%)
37	BCT	D	401[B]	21	3,3,3	0.50	0	2,3,3	1.05	0
23	CLA	B	602	-	69,73,73	2.07	20 (28%)	82,113,113	2.74	34 (41%)
23	CLA	C	507	-	69,73,73	2.01	21 (30%)	82,113,113	2.68	33 (40%)
27	GOL	B	627	-	5,5,5	1.05	0	5,5,5	1.14	1 (20%)
23	CLA	C	508	41	69,73,73	1.98	19 (27%)	82,113,113	2.68	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	D	403	-	69,73,73	2.07	18 (26%)	82,113,113	2.65	33 (40%)
26	SQD	b	620	-	52,54,54	0.99	2 (3%)	62,65,65	1.66	10 (16%)
27	GOL	a	417	-	5,5,5	1.05	0	5,5,5	1.09	1 (20%)
27	GOL	V	203[B]	-	5,5,5	1.16	0	5,5,5	0.96	0
32	LHG	D	406[B]	-	48,48,48	0.88	2 (4%)	51,54,54	0.94	3 (5%)
23	CLA	B	604	-	69,73,73	1.97	22 (31%)	82,113,113	2.58	31 (37%)
23	CLA	b	601	41	69,73,73	2.07	20 (28%)	82,113,113	2.65	30 (36%)
32	LHG	d	408[B]	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
32	LHG	E	101[B]	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	3 (6%)
33	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.51	8 (13%)
31	LMT	M	101	-	36,36,36	1.09	4 (11%)	47,47,47	1.19	4 (8%)
23	CLA	c	513	-	69,73,73	2.08	20 (28%)	82,113,113	2.71	30 (36%)
25	BCR	A	409	-	41,41,41	1.03	1 (2%)	56,56,56	1.43	7 (12%)
23	CLA	B	612	-	69,73,73	2.00	19 (27%)	82,113,113	2.68	32 (39%)
33	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.08	3 (6%)
25	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.43	12 (21%)
32	LHG	d	407[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.00	3 (5%)
23	CLA	b	608	-	69,73,73	1.96	19 (27%)	82,113,113	2.67	34 (41%)
23	CLA	d	403[B]	-	69,73,73	1.95	19 (27%)	82,113,113	2.72	29 (35%)
23	CLA	B	601	41	69,73,73	2.07	20 (28%)	82,113,113	2.69	29 (35%)
28	OEX	A	413[A]	41,1,3	0,15,15	-	-	-	-	-
23	CLA	c	505	-	69,73,73	2.01	18 (26%)	82,113,113	2.64	29 (35%)
31	LMT	B	630	-	36,36,36	0.99	3 (8%)	47,47,47	1.16	5 (10%)
23	CLA	C	512	3	69,73,73	2.00	20 (28%)	82,113,113	2.60	29 (35%)
29	PL9	d	406[A]	-	55,55,55	0.67	1 (1%)	68,69,69	1.62	15 (22%)
26	SQD	a	410	-	52,54,54	1.00	3 (5%)	62,65,65	1.18	7 (11%)
35	DGD	h	102	-	63,63,67	0.88	4 (6%)	77,77,81	1.08	6 (7%)
23	CLA	b	605	-	69,73,73	1.92	18 (26%)	82,113,113	2.82	31 (37%)
27	GOL	C	523[A]	-	5,5,5	1.24	0	5,5,5	0.89	0
23	CLA	B	610	41	69,73,73	2.05	19 (27%)	82,113,113	2.78	34 (41%)
27	GOL	b	624	-	5,5,5	1.29	1 (20%)	5,5,5	0.87	0
24	PHO	A	416[B]	-	58,69,69	2.74	11 (18%)	55,99,99	2.86	17 (30%)
34	HTG	C	522	-	19,19,19	0.80	1 (5%)	23,24,24	1.22	2 (8%)
23	CLA	c	508	-	69,73,73	2.10	20 (28%)	82,113,113	2.64	30 (36%)
24	PHO	a	414[B]	-	58,69,69	2.79	13 (22%)	55,99,99	2.94	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	DGD	C	517[A]	-	63,63,67	0.82	2 (3%)	77,77,81	1.21	9 (11%)
25	BCR	K	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.42	13 (23%)
23	CLA	C	509	-	69,73,73	2.01	18 (26%)	82,113,113	2.68	28 (34%)
23	CLA	b	616	-	69,73,73	1.96	19 (27%)	82,113,113	2.79	33 (40%)
23	CLA	d	402[B]	41	69,73,73	2.05	18 (26%)	82,113,113	2.70	35 (42%)
23	CLA	a	407	-	69,73,73	1.96	19 (27%)	82,113,113	2.88	33 (40%)
33	LMG	a	415	-	51,51,55	0.93	2 (3%)	59,59,63	1.21	6 (10%)
23	CLA	b	614	-	69,73,73	1.97	19 (27%)	82,113,113	2.78	33 (40%)
32	LHG	b	629[A]	-	48,48,48	0.86	3 (6%)	51,54,54	1.05	4 (7%)
35	DGD	c	517[A]	-	63,63,67	0.84	3 (4%)	77,77,81	0.98	5 (6%)
23	CLA	C	511	-	69,73,73	2.01	20 (28%)	82,113,113	2.80	33 (40%)
34	HTG	b	623	-	19,19,19	0.94	1 (5%)	23,24,24	1.57	2 (8%)
23	CLA	c	502	-	69,73,73	1.96	16 (23%)	82,113,113	2.64	28 (34%)
33	LMG	d	412	39	51,51,55	0.88	2 (3%)	59,59,63	1.13	4 (6%)
23	CLA	a	404[A]	-	69,73,73	1.94	19 (27%)	82,113,113	2.76	34 (41%)
23	CLA	b	602	-	69,73,73	2.07	19 (27%)	82,113,113	2.76	36 (43%)
27	GOL	l	801[A]	-	5,5,5	1.01	0	5,5,5	1.04	0
26	SQD	A	410[A]	-	52,54,54	0.86	2 (3%)	62,65,65	1.79	9 (14%)
33	LMG	Z	101	-	37,37,55	1.01	2 (5%)	45,45,63	1.45	6 (13%)
31	LMT	T	101	-	36,36,36	1.03	2 (5%)	47,47,47	1.04	2 (4%)
23	CLA	C	506	-	69,73,73	2.00	19 (27%)	82,113,113	2.66	32 (39%)
25	BCR	C	515	-	41,41,41	1.06	1 (2%)	56,56,56	1.36	7 (12%)
33	LMG	c	519	-	51,51,55	0.93	2 (3%)	59,59,63	1.11	4 (6%)
31	LMT	b	621	-	25,25,36	0.97	1 (4%)	30,30,47	1.21	2 (6%)
23	CLA	b	615	-	69,73,73	2.00	18 (26%)	82,113,113	2.67	31 (37%)
34	HTG	D	410	-	16,16,19	0.96	1 (6%)	20,21,24	1.26	1 (5%)
23	CLA	D	402[A]	-	69,73,73	1.96	18 (26%)	82,113,113	2.75	33 (40%)
25	BCR	t	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.58	11 (19%)
31	LMT	B	628	-	36,36,36	1.17	4 (11%)	47,47,47	1.38	6 (12%)
25	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.49	9 (16%)
28	OEX	A	413[B]	41,1,3	0,15,15	-	-	-	-	-
26	SQD	f	102	-	41,43,54	1.13	2 (4%)	51,54,65	1.53	10 (19%)
27	GOL	c	525[A]	-	5,5,5	0.99	0	5,5,5	1.02	0
29	PL9	d	406[B]	-	55,55,55	0.70	1 (1%)	68,69,69	1.60	17 (25%)
23	CLA	B	603	-	69,73,73	1.98	20 (28%)	82,113,113	2.81	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	A	412	-	52,54,54	0.98	2 (3%)	62,65,65	1.19	7 (11%)
27	GOL	C	523[B]	-	5,5,5	1.12	0	5,5,5	0.98	0
23	CLA	C	510	-	69,73,73	2.03	19 (27%)	82,113,113	2.71	31 (37%)
27	GOL	B	629	-	5,5,5	1.03	0	5,5,5	1.08	0
23	CLA	a	405[A]	41	69,73,73	1.94	19 (27%)	82,113,113	2.70	33 (40%)
34	HTG	B	625	-	19,19,19	0.88	2 (10%)	23,24,24	1.07	2 (8%)
34	HTG	d	411	-	16,16,19	0.88	1 (6%)	20,21,24	1.38	1 (5%)
35	DGD	C	517[B]	-	63,63,67	0.84	2 (3%)	77,77,81	1.11	7 (9%)
26	SQD	F	102	-	41,43,54	1.15	3 (7%)	51,54,65	2.14	14 (27%)
23	CLA	b	610	41	69,73,73	2.01	20 (28%)	82,113,113	2.71	35 (42%)
31	LMT	m	103	-	36,36,36	1.07	3 (8%)	47,47,47	1.13	3 (6%)
23	CLA	c	507	41	69,73,73	2.00	17 (24%)	82,113,113	2.77	30 (36%)
32	LHG	a	419[A]	-	41,41,48	1.04	2 (4%)	44,47,54	0.94	2 (4%)
32	LHG	b	629[B]	-	48,48,48	0.89	2 (4%)	51,54,54	1.03	4 (7%)
34	HTG	b	622	-	19,19,19	1.09	2 (10%)	23,24,24	1.90	7 (30%)
35	DGD	c	517[B]	-	63,63,67	0.87	2 (3%)	77,77,81	0.98	5 (6%)
33	LMG	C	521	-	51,51,55	1.07	3 (5%)	59,59,63	1.34	6 (10%)
34	HTG	c	521	-	19,19,19	0.86	1 (5%)	23,24,24	1.32	1 (4%)
34	HTG	V	202	-	11,11,19	0.29	0	15,15,24	1.15	1 (6%)
23	CLA	B	606	-	69,73,73	1.94	19 (27%)	82,113,113	2.80	33 (40%)
25	BCR	B	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.34	8 (14%)
35	DGD	c	518	-	63,63,67	0.87	3 (4%)	77,77,81	1.05	5 (6%)
23	CLA	a	404[B]	-	69,73,73	1.97	18 (26%)	82,113,113	2.73	35 (42%)
27	GOL	l	801[B]	-	5,5,5	0.92	0	5,5,5	1.04	0
40	HEC	v	201	16	46,50,50	1.94	5 (10%)	58,82,82	1.91	7 (12%)
26	SQD	A	410[B]	-	52,54,54	0.87	2 (3%)	62,65,65	1.75	10 (16%)
27	GOL	o	302	-	5,5,5	1.04	0	5,5,5	1.07	0
23	CLA	A	406[A]	41	69,73,73	1.97	18 (26%)	82,113,113	2.71	33 (40%)
32	LHG	d	414[A]	-	48,48,48	0.90	2 (4%)	51,54,54	1.14	5 (9%)
24	PHO	A	407[A]	-	58,69,69	2.70	13 (22%)	55,99,99	2.89	15 (27%)
27	GOL	D	412	-	5,5,5	1.49	2 (40%)	5,5,5	0.87	0
29	PL9	a	412[A]	-	55,55,55	0.67	2 (3%)	68,69,69	2.01	21 (30%)
23	CLA	D	402[B]	-	69,73,73	1.98	19 (27%)	82,113,113	2.74	33 (40%)
27	GOL	O	302	-	5,5,5	0.95	0	5,5,5	0.94	0
37	BCT	D	401[A]	21	3,3,3	0.43	0	2,3,3	1.83	0
35	DGD	C	519	-	63,63,67	0.87	3 (4%)	77,77,81	0.98	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	a	409[A]	-	52,54,54	0.89	2 (3%)	62,65,65	1.74	12 (19%)
23	CLA	B	607	41	69,73,73	1.94	19 (27%)	82,113,113	2.77	31 (37%)
25	BCR	Y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.79	13 (23%)
23	CLA	b	612	-	69,73,73	1.97	20 (28%)	82,113,113	2.71	31 (37%)
27	GOL	c	525[B]	-	5,5,5	1.08	0	5,5,5	0.95	0
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.40	6 (10%)
25	BCR	c	515	-	41,41,41	1.06	1 (2%)	56,56,56	1.45	13 (23%)
34	HTG	B	622	-	19,19,19	1.00	2 (10%)	23,24,24	1.49	5 (21%)
23	CLA	B	615	-	69,73,73	2.05	19 (27%)	82,113,113	2.69	31 (37%)
23	CLA	b	611	-	69,73,73	1.97	20 (28%)	82,113,113	2.77	32 (39%)
35	DGD	C	518[A]	-	63,63,67	0.89	3 (4%)	77,77,81	1.03	5 (6%)
35	DGD	c	516[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.12	6 (7%)
23	CLA	a	405[B]	41	69,73,73	1.99	20 (28%)	82,113,113	2.68	31 (37%)
23	CLA	b	603	-	69,73,73	1.99	18 (26%)	82,113,113	2.81	32 (39%)
23	CLA	B	605	-	69,73,73	1.99	19 (27%)	82,113,113	2.78	30 (36%)
33	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.24	6 (10%)
31	LMT	a	416	-	36,36,36	0.98	1 (2%)	47,47,47	1.04	1 (2%)
32	LHG	a	419[B]	-	41,41,48	1.03	2 (4%)	44,47,54	0.94	2 (4%)
23	CLA	d	404	-	69,73,73	2.02	19 (27%)	82,113,113	2.74	31 (37%)
31	LMT	A	420	-	36,36,36	1.02	2 (5%)	47,47,47	1.17	4 (8%)
32	LHG	D	407[A]	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	4 (7%)
34	HTG	b	625	-	19,19,19	0.95	2 (10%)	23,24,24	1.55	3 (13%)
23	CLA	A	405[A]	41	69,73,73	1.91	18 (26%)	82,113,113	2.74	36 (43%)
23	CLA	C	514	-	69,73,73	2.01	20 (28%)	82,113,113	2.70	31 (37%)
25	BCR	C	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.47	8 (14%)
23	CLA	c	509	-	69,73,73	1.99	17 (24%)	82,113,113	2.74	33 (40%)
27	GOL	b	628	-	5,5,5	0.56	0	5,5,5	1.45	1 (20%)
23	CLA	B	608	-	69,73,73	1.90	20 (28%)	82,113,113	2.68	34 (41%)
29	PL9	D	405[A]	-	55,55,55	0.64	2 (3%)	68,69,69	1.64	18 (26%)
23	CLA	C	502	-	69,73,73	1.97	20 (28%)	82,113,113	2.67	33 (40%)
32	LHG	A	419[A]	-	48,48,48	0.84	2 (4%)	51,54,54	1.33	6 (11%)
25	BCR	a	408	-	41,41,41	1.05	1 (2%)	56,56,56	1.29	8 (14%)
23	CLA	A	406[B]	41	69,73,73	2.02	19 (27%)	82,113,113	2.69	33 (40%)
32	LHG	d	414[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.09	5 (9%)
23	CLA	b	606	-	69,73,73	1.96	19 (27%)	82,113,113	2.76	33 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PHO	a	406[A]	-	58,69,69	2.73	11 (18%)	55,99,99	2.83	15 (27%)
23	CLA	c	511	3	69,73,73	2.04	20 (28%)	82,113,113	2.67	33 (40%)
24	PHO	A	407[B]	-	58,69,69	2.68	12 (20%)	55,99,99	2.99	15 (27%)
29	PL9	a	412[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.98	22 (32%)
29	PL9	A	414[A]	-	55,55,55	0.70	3 (5%)	68,69,69	2.11	27 (39%)
33	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.19	6 (10%)
23	CLA	C	513	-	69,73,73	2.02	20 (28%)	82,113,113	2.72	34 (41%)
23	CLA	b	604	-	69,73,73	1.98	19 (27%)	82,113,113	2.66	30 (36%)
23	CLA	B	609	-	69,73,73	1.99	18 (26%)	82,113,113	2.69	30 (36%)
26	SQD	a	409[B]	-	52,54,54	0.90	2 (3%)	62,65,65	1.62	12 (19%)
27	GOL	d	413	-	5,5,5	1.11	0	5,5,5	1.04	0
40	HEC	V	201	16	46,50,50	1.89	6 (13%)	58,82,82	1.85	10 (17%)
35	DGD	H	102	-	63,63,67	0.86	3 (4%)	77,77,81	1.05	6 (7%)
25	BCR	B	617	-	41,41,41	1.07	1 (2%)	56,56,56	1.33	6 (10%)
23	CLA	B	616	-	69,73,73	1.97	20 (28%)	82,113,113	2.76	29 (35%)
38	HEM	f	101	5,6	50,50,50	1.51	6 (12%)	67,82,82	1.63	12 (17%)
28	OEX	a	411[A]	41,1,3	0,15,15	-	-	-	-	-
23	CLA	c	503	-	69,73,73	2.02	19 (27%)	82,113,113	2.72	30 (36%)
27	GOL	v	202[A]	-	5,5,5	1.35	1 (20%)	5,5,5	0.77	0
25	BCR	D	404	-	41,41,41	1.13	1 (2%)	56,56,56	1.83	17 (30%)
27	GOL	A	418	-	5,5,5	1.69	2 (40%)	5,5,5	1.04	1 (20%)
23	CLA	c	504	41	69,73,73	2.04	21 (30%)	82,113,113	2.70	31 (37%)
31	LMT	e	101	-	36,36,36	1.00	3 (8%)	47,47,47	0.99	1 (2%)
35	DGD	C	518[B]	-	63,63,67	0.88	2 (3%)	77,77,81	1.08	5 (6%)
37	BCT	d	401[A]	21	3,3,3	0.46	0	2,3,3	1.59	0
27	GOL	A	411	-	5,5,5	1.19	0	5,5,5	0.81	0
35	DGD	c	516[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.01	3 (3%)
25	BCR	y	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.65	11 (19%)
23	CLA	A	408	-	69,73,73	1.98	20 (28%)	82,113,113	2.77	36 (43%)
23	CLA	b	613	-	69,73,73	1.96	19 (27%)	82,113,113	2.65	31 (37%)
25	BCR	c	514	-	41,41,41	1.00	1 (2%)	56,56,56	1.66	12 (21%)
31	LMT	F	101	-	36,36,36	1.05	1 (2%)	47,47,47	1.06	3 (6%)
32	LHG	D	407[B]	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	3 (5%)
31	LMT	b	627	-	25,25,36	0.88	0	30,30,47	1.11	3 (10%)
23	CLA	A	405[B]	41	69,73,73	2.02	18 (26%)	82,113,113	2.68	33 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	B	618	-	41,41,41	1.02	1 (2%)	56,56,56	1.32	6 (10%)
23	CLA	C	505	41	69,73,73	1.96	19 (27%)	82,113,113	2.63	29 (35%)
23	CLA	A	404[A]	-	69,73,73	1.97	19 (27%)	82,113,113	2.69	33 (40%)
25	BCR	d	405	-	41,41,41	1.16	2 (4%)	56,56,56	2.01	14 (25%)
33	LMG	c	520	-	51,51,55	1.00	2 (3%)	59,59,63	1.36	6 (10%)
29	PL9	D	405[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.68	17 (25%)
32	LHG	L	101[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.16	3 (5%)
32	LHG	A	419[B]	-	48,48,48	0.87	2 (4%)	51,54,54	1.19	5 (9%)
27	GOL	o	303	-	5,5,5	1.14	1 (20%)	5,5,5	1.16	0
24	PHO	a	406[B]	-	58,69,69	2.80	14 (24%)	55,99,99	2.86	16 (29%)
23	CLA	c	512	-	69,73,73	2.05	20 (28%)	82,113,113	2.70	32 (39%)

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
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
29	PL9	A	414[B]	-	-	17/53/73/73	0/1/1/1
38	HEM	E	102	5,6	-	4/14/54/54	-
27	GOL	a	418	-	-	0/4/4/4	-
33	LMG	D	411	39	-	7/46/66/70	0/1/1/1
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
23	CLA	c	510	-	1/1/15/20	11/39/115/115	-
27	GOL	V	203[A]	-	-	2/4/4/4	-
32	LHG	D	406[A]	-	-	16/53/53/53	-
23	CLA	b	609	-	1/1/15/20	2/39/115/115	-
27	GOL	v	202[B]	-	-	2/4/4/4	-
32	LHG	d	408[A]	-	-	11/53/53/53	-
23	CLA	C	503	-	-	9/39/115/115	-
32	LHG	E	101[A]	-	-	21/46/46/53	-
27	GOL	c	526	-	-	3/4/4/4	-
23	CLA	C	504	-	-	2/39/115/115	-
25	BCR	T	102	-	-	1/29/63/63	0/2/2/2
32	LHG	d	407[A]	-	-	12/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	d	403[A]	-	1/1/15/20	2/39/115/115	-
27	GOL	B	624	-	-	2/4/4/4	-
23	CLA	B	613	-	1/1/15/20	8/39/115/115	-
31	LMT	B	631	-	-	11/17/37/61	0/1/1/2
23	CLA	A	404[B]	-	1/1/15/20	4/39/115/115	-
23	CLA	c	501	-	1/1/15/20	4/39/115/115	-
23	CLA	c	506	-	1/1/15/20	6/39/115/115	-
27	GOL	O	303	-	-	2/4/4/4	-
32	LHG	L	101[B]	-	-	18/53/53/53	-
33	LMG	B	621	-	-	19/46/66/70	0/1/1/1
24	PHO	A	416[A]	-	-	1/37/103/103	0/5/6/6
31	LMT	A	417	-	-	8/21/61/61	0/2/2/2
23	CLA	B	614	-	1/1/15/20	12/39/115/115	-
23	CLA	B	611	-	1/1/15/20	2/39/115/115	-
23	CLA	b	607	41	1/1/15/20	3/39/115/115	-
24	PHO	a	414[A]	-	-	0/37/103/103	0/5/6/6
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	d	402[A]	41	1/1/15/20	4/39/115/115	-
31	LMT	t	101	-	-	8/17/38/61	0/1/1/2
34	HTG	B	623	-	-	4/10/30/30	0/1/1/1
25	BCR	b	619	-	-	2/29/63/63	0/2/2/2
23	CLA	B	602	-	1/1/15/20	8/39/115/115	-
23	CLA	C	507	-	1/1/15/20	11/39/115/115	-
27	GOL	B	627	-	-	1/4/4/4	-
23	CLA	C	508	41	1/1/15/20	8/39/115/115	-
23	CLA	D	403	-	1/1/15/20	14/39/115/115	-
26	SQD	b	620	-	-	19/49/69/69	0/1/1/1
27	GOL	a	417	-	-	2/4/4/4	-
27	GOL	V	203[B]	-	-	2/4/4/4	-
32	LHG	D	406[B]	-	-	16/53/53/53	-
23	CLA	B	604	-	1/1/15/20	3/39/115/115	-
23	CLA	b	601	41	1/1/15/20	17/39/115/115	-
32	LHG	d	408[B]	-	-	13/53/53/53	-
32	LHG	E	101[B]	-	-	22/46/46/53	-
33	LMG	C	501	-	-	13/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	M	101	-	-	4/21/61/61	0/2/2/2
23	CLA	c	513	-	1/1/15/20	12/39/115/115	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
23	CLA	B	612	-	1/1/15/20	5/39/115/115	-
33	LMG	z	101	-	-	9/34/54/70	0/1/1/1
25	BCR	h	101	-	-	0/29/63/63	0/2/2/2
32	LHG	d	407[B]	-	-	12/53/53/53	-
23	CLA	b	608	-	-	5/39/115/115	-
23	CLA	d	403[B]	-	1/1/15/20	4/39/115/115	-
23	CLA	B	601	41	1/1/15/20	12/39/115/115	-
23	CLA	c	505	-	1/1/15/20	6/39/115/115	-
31	LMT	B	630	-	-	12/21/61/61	0/2/2/2
23	CLA	C	512	3	1/1/15/20	3/39/115/115	-
29	PL9	d	406[A]	-	-	6/53/73/73	0/1/1/1
26	SQD	a	410	-	-	14/49/69/69	0/1/1/1
35	DGD	h	102	-	-	16/51/91/95	0/2/2/2
23	CLA	b	605	-	1/1/15/20	5/39/115/115	-
27	GOL	C	523[A]	-	-	0/4/4/4	-
23	CLA	B	610	41	1/1/15/20	7/39/115/115	-
27	GOL	b	624	-	-	2/4/4/4	-
24	PHO	A	416[B]	-	-	2/37/103/103	0/5/6/6
34	HTG	C	522	-	-	0/10/30/30	0/1/1/1
23	CLA	c	508	-	1/1/15/20	3/39/115/115	-
24	PHO	a	414[B]	-	-	1/37/103/103	0/5/6/6
35	DGD	C	517[A]	-	-	12/51/91/95	0/2/2/2
25	BCR	K	102	-	-	1/29/63/63	0/2/2/2
23	CLA	C	509	-	1/1/15/20	1/39/115/115	-
23	CLA	b	616	-	1/1/15/20	8/39/115/115	-
23	CLA	d	402[B]	41	1/1/15/20	2/39/115/115	-
23	CLA	a	407	-	1/1/15/20	10/39/115/115	-
33	LMG	a	415	-	-	12/46/66/70	0/1/1/1
23	CLA	b	614	-	1/1/15/20	12/39/115/115	-
32	LHG	b	629[A]	-	-	20/53/53/53	-
35	DGD	c	517[A]	-	-	17/51/91/95	0/2/2/2
23	CLA	C	511	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	HTG	b	623	-	-	5/10/30/30	0/1/1/1
23	CLA	c	502	-	1/1/15/20	5/39/115/115	-
33	LMG	d	412	39	-	11/46/66/70	0/1/1/1
23	CLA	a	404[A]	-	1/1/15/20	3/39/115/115	-
23	CLA	b	602	-	1/1/15/20	4/39/115/115	-
27	GOL	l	801[A]	-	-	1/4/4/4	-
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1
33	LMG	Z	101	-	-	10/31/51/70	0/1/1/1
31	LMT	T	101	-	-	10/21/61/61	0/2/2/2
23	CLA	C	506	-	1/1/15/20	6/39/115/115	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
33	LMG	c	519	-	-	12/46/66/70	0/1/1/1
31	LMT	b	621	-	-	8/17/37/61	0/1/1/2
23	CLA	b	615	-	1/1/15/20	7/39/115/115	-
34	HTG	D	410	-	-	3/7/27/30	0/1/1/1
23	CLA	D	402[A]	-	1/1/15/20	0/39/115/115	-
25	BCR	t	102	-	-	1/29/63/63	0/2/2/2
31	LMT	B	628	-	-	12/21/61/61	0/2/2/2
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
26	SQD	f	102	-	-	10/38/58/69	0/1/1/1
27	GOL	c	525[A]	-	-	0/4/4/4	-
29	PL9	d	406[B]	-	-	6/53/73/73	0/1/1/1
23	CLA	B	603	-	1/1/15/20	6/39/115/115	-
26	SQD	A	412	-	-	12/49/69/69	0/1/1/1
27	GOL	C	523[B]	-	-	0/4/4/4	-
23	CLA	C	510	-	1/1/15/20	6/39/115/115	-
27	GOL	B	629	-	-	4/4/4/4	-
23	CLA	a	405[A]	41	-	5/39/115/115	-
34	HTG	B	625	-	-	3/10/30/30	0/1/1/1
34	HTG	d	411	-	-	1/7/27/30	0/1/1/1
35	DGD	C	517[B]	-	-	15/51/91/95	0/2/2/2
26	SQD	F	102	-	-	14/38/58/69	0/1/1/1
23	CLA	b	610	41	1/1/15/20	4/39/115/115	-
31	LMT	m	103	-	-	4/21/61/61	0/2/2/2
23	CLA	c	507	41	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	a	419[A]	-	-	16/46/46/53	-
32	LHG	b	629[B]	-	-	18/53/53/53	-
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1
35	DGD	c	517[B]	-	-	17/51/91/95	0/2/2/2
33	LMG	C	521	-	-	14/46/66/70	0/1/1/1
34	HTG	c	521	-	-	2/10/30/30	0/1/1/1
34	HTG	V	202	-	-	0/2/19/30	0/1/1/1
23	CLA	B	606	-	1/1/15/20	7/39/115/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
35	DGD	c	518	-	-	10/51/91/95	0/2/2/2
23	CLA	a	404[B]	-	1/1/15/20	1/39/115/115	-
27	GOL	l	801[B]	-	-	2/4/4/4	-
40	HEC	v	201	16	-	6/14/54/54	-
26	SQD	A	410[B]	-	-	11/49/69/69	0/1/1/1
27	GOL	o	302	-	-	2/4/4/4	-
23	CLA	A	406[A]	41	-	7/39/115/115	-
32	LHG	d	414[A]	-	-	12/53/53/53	-
24	PHO	A	407[A]	-	-	1/37/103/103	0/5/6/6
27	GOL	D	412	-	-	4/4/4/4	-
29	PL9	a	412[A]	-	-	14/53/73/73	0/1/1/1
23	CLA	D	402[B]	-	1/1/15/20	2/39/115/115	-
27	GOL	O	302	-	-	2/4/4/4	-
35	DGD	C	519	-	-	16/51/91/95	0/2/2/2
26	SQD	a	409[A]	-	-	9/49/69/69	0/1/1/1
23	CLA	B	607	41	1/1/15/20	1/39/115/115	-
25	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
23	CLA	b	612	-	1/1/15/20	3/39/115/115	-
27	GOL	c	525[B]	-	-	0/4/4/4	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
23	CLA	B	615	-	1/1/15/20	8/39/115/115	-
23	CLA	b	611	-	1/1/15/20	2/39/115/115	-
35	DGD	C	518[A]	-	-	14/51/91/95	0/2/2/2
35	DGD	c	516[A]	-	-	20/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	405[B]	41	-	7/39/115/115	-
23	CLA	b	603	-	1/1/15/20	4/39/115/115	-
23	CLA	B	605	-	1/1/15/20	5/39/115/115	-
33	LMG	m	101	-	-	9/46/66/70	0/1/1/1
31	LMT	a	416	-	-	9/21/61/61	0/2/2/2
32	LHG	a	419[B]	-	-	16/46/46/53	-
23	CLA	d	404	-	1/1/15/20	8/39/115/115	-
31	LMT	A	420	-	-	15/21/61/61	0/2/2/2
32	LHG	D	407[A]	-	-	13/53/53/53	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
23	CLA	C	514	-	1/1/15/20	7/39/115/115	-
23	CLA	A	405[A]	41	-	2/39/115/115	-
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
23	CLA	c	509	-	1/1/15/20	15/39/115/115	-
27	GOL	b	628	-	-	0/4/4/4	-
23	CLA	B	608	-	-	4/39/115/115	-
29	PL9	D	405[A]	-	-	7/53/73/73	0/1/1/1
23	CLA	C	502	-	1/1/15/20	5/39/115/115	-
32	LHG	A	419[A]	-	-	10/53/53/53	-
25	BCR	a	408	-	-	0/29/63/63	0/2/2/2
23	CLA	A	406[B]	41	-	5/39/115/115	-
32	LHG	d	414[B]	-	-	11/53/53/53	-
23	CLA	b	606	-	1/1/15/20	11/39/115/115	-
24	PHO	a	406[A]	-	-	5/37/103/103	0/5/6/6
23	CLA	c	511	3	1/1/15/20	3/39/115/115	-
24	PHO	A	407[B]	-	-	0/37/103/103	0/5/6/6
29	PL9	a	412[B]	-	-	16/53/73/73	0/1/1/1
29	PL9	A	414[A]	-	-	15/53/73/73	0/1/1/1
33	LMG	C	520	-	-	10/46/66/70	0/1/1/1
23	CLA	C	513	-	1/1/15/20	7/39/115/115	-
23	CLA	b	604	-	1/1/15/20	11/39/115/115	-
23	CLA	B	609	-	1/1/15/20	0/39/115/115	-
26	SQD	a	409[B]	-	-	9/49/69/69	0/1/1/1
27	GOL	d	413	-	-	2/4/4/4	-
40	HEC	V	201	16	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	H	102	-	-	9/51/91/95	0/2/2/2
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	B	616	-	1/1/15/20	7/39/115/115	-
38	HEM	f	101	5,6	-	8/14/54/54	-
23	CLA	c	503	-	1/1/15/20	2/39/115/115	-
27	GOL	v	202[A]	-	-	1/4/4/4	-
25	BCR	D	404	-	-	4/29/63/63	0/2/2/2
27	GOL	A	418	-	-	1/4/4/4	-
23	CLA	c	504	41	1/1/15/20	6/39/115/115	-
31	LMT	e	101	-	-	14/21/61/61	0/2/2/2
35	DGD	C	518[B]	-	-	11/51/91/95	0/2/2/2
27	GOL	A	411	-	-	2/4/4/4	-
35	DGD	c	516[B]	-	-	19/51/91/95	0/2/2/2
25	BCR	y	101	-	-	5/29/63/63	0/2/2/2
23	CLA	A	408	-	1/1/15/20	8/39/115/115	-
23	CLA	b	613	-	1/1/15/20	5/39/115/115	-
25	BCR	c	514	-	-	0/29/63/63	0/2/2/2
31	LMT	F	101	-	-	8/21/61/61	0/2/2/2
32	LHG	D	407[B]	-	-	12/53/53/53	-
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
23	CLA	A	405[B]	41	1/1/15/20	2/39/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	C	505	41	1/1/15/20	8/39/115/115	-
23	CLA	A	404[A]	-	1/1/15/20	5/39/115/115	-
25	BCR	d	405	-	-	3/29/63/63	0/2/2/2
33	LMG	c	520	-	-	9/46/66/70	0/1/1/1
29	PL9	D	405[B]	-	-	8/53/73/73	0/1/1/1
32	LHG	L	101[A]	-	-	19/53/53/53	-
32	LHG	A	419[B]	-	-	13/53/53/53	-
27	GOL	o	303	-	-	2/4/4/4	-
24	PHO	a	406[B]	-	-	3/37/103/103	0/5/6/6
23	CLA	c	512	-	1/1/15/20	11/39/115/115	-

All (1837) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	406[B]	PHO	C1B-C2B	9.35	1.49	1.39
24	A	407[A]	PHO	C1D-C2D	9.27	1.49	1.39
24	A	407[B]	PHO	C1D-C2D	9.24	1.49	1.39
24	a	414[B]	PHO	C1D-C2D	9.22	1.49	1.39
24	a	406[A]	PHO	C1B-C2B	9.11	1.49	1.39
24	a	406[B]	PHO	C1D-C2D	9.04	1.49	1.39
24	a	414[A]	PHO	C1B-C2B	8.92	1.49	1.39
24	A	416[A]	PHO	C1D-C2D	8.86	1.49	1.39
24	a	414[B]	PHO	C1B-C2B	8.80	1.49	1.39
24	a	414[A]	PHO	C1D-C2D	8.73	1.49	1.39
24	A	407[B]	PHO	C1B-C2B	8.72	1.49	1.39
24	a	406[A]	PHO	C1D-C2D	8.59	1.48	1.39
24	A	416[B]	PHO	C1B-C2B	8.52	1.48	1.39
24	A	407[A]	PHO	C1B-C2B	8.44	1.48	1.39
24	A	416[A]	PHO	C1B-C2B	8.41	1.48	1.39
24	A	416[B]	PHO	C1D-C2D	8.30	1.48	1.39
24	A	416[B]	PHO	C3B-C4B	8.10	1.49	1.41
24	a	414[A]	PHO	C3B-C4B	8.05	1.49	1.41
24	a	406[B]	PHO	C3B-C4B	7.90	1.49	1.41
24	a	414[B]	PHO	C3B-C4B	7.75	1.49	1.41
23	B	611	CLA	CMB-C2B	7.54	1.66	1.50
24	A	416[A]	PHO	C3B-C4B	7.47	1.49	1.41
24	a	406[A]	PHO	C3B-C4B	7.36	1.49	1.41
24	A	407[A]	PHO	C3B-C4B	7.26	1.48	1.41
24	A	407[B]	PHO	C3B-C4B	7.13	1.48	1.41
40	V	201	HEC	CAC-C3C	7.08	1.58	1.35
40	v	201	HEC	CAC-C3C	6.98	1.57	1.35
23	B	611	CLA	C1B-C2B	6.91	1.59	1.43
24	A	416[A]	PHO	C4D-CHA	6.82	1.49	1.39
24	A	407[A]	PHO	C4D-CHA	6.81	1.49	1.39
24	a	406[A]	PHO	C4D-CHA	6.79	1.49	1.39
24	a	414[B]	PHO	C4D-CHA	6.71	1.49	1.39
24	A	416[B]	PHO	C4D-CHA	6.68	1.49	1.39
24	a	406[B]	PHO	C4D-CHA	6.61	1.49	1.39
24	A	416[B]	PHO	C3B-C2B	6.60	1.49	1.40
24	a	414[A]	PHO	C4D-CHA	6.52	1.49	1.39
24	a	406[A]	PHO	C3B-C2B	6.52	1.49	1.40
40	v	201	HEC	CAB-C3B	6.52	1.56	1.35
24	A	407[B]	PHO	C4D-CHA	6.35	1.49	1.39
24	A	407[A]	PHO	C3B-C2B	6.34	1.49	1.40
24	A	416[A]	PHO	C3B-C2B	6.26	1.48	1.40
24	a	406[B]	PHO	C3B-C2B	6.22	1.48	1.40
24	a	414[B]	PHO	C3B-C2B	6.10	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	414[A]	PHO	C3B-C2B	6.05	1.48	1.40
40	V	201	HEC	CAB-C3B	6.04	1.54	1.35
23	B	611	CLA	C1D-ND	6.02	1.45	1.37
24	A	407[B]	PHO	C3B-C2B	6.02	1.48	1.40
23	B	611	CLA	CHC-C1C	6.01	1.50	1.38
23	B	610	CLA	C3C-C2C	5.84	1.49	1.36
23	B	611	CLA	C3C-C2C	5.70	1.49	1.36
24	a	406[B]	PHO	C3D-C2D	5.70	1.49	1.39
40	v	201	HEC	C3D-C2D	5.66	1.53	1.38
24	a	414[B]	PHO	C3D-C2D	5.60	1.49	1.39
23	d	402[B]	CLA	C3C-C2C	5.59	1.48	1.36
23	D	403	CLA	C3C-C2C	5.58	1.48	1.36
24	a	406[A]	PHO	C3D-C2D	5.56	1.49	1.39
24	A	416[B]	PHO	C3D-C2D	5.54	1.49	1.39
24	a	414[B]	PHO	OBD-CAD	5.49	1.29	1.22
23	C	509	CLA	C3C-C2C	5.48	1.48	1.36
23	c	512	CLA	C3C-C2C	5.45	1.48	1.36
23	c	508	CLA	C3C-C2C	5.44	1.48	1.36
23	C	504	CLA	C3C-C2C	5.43	1.48	1.36
23	B	616	CLA	C3C-C2C	5.43	1.48	1.36
24	a	414[A]	PHO	C3D-C2D	5.42	1.48	1.39
23	d	404	CLA	C3C-C2C	5.41	1.48	1.36
23	b	607	CLA	C3C-C2C	5.40	1.48	1.36
23	c	509	CLA	C3C-C2C	5.40	1.48	1.36
24	A	416[A]	PHO	C3D-C2D	5.39	1.48	1.39
23	C	511	CLA	C1D-ND	5.38	1.44	1.37
24	A	416[B]	PHO	OBD-CAD	5.35	1.29	1.22
23	A	404[A]	CLA	C3C-C2C	5.35	1.48	1.36
23	c	505	CLA	C3C-C2C	5.34	1.48	1.36
23	C	511	CLA	C3C-C2C	5.33	1.48	1.36
23	C	508	CLA	C3C-C2C	5.32	1.48	1.36
23	A	406[B]	CLA	C3C-C2C	5.32	1.48	1.36
23	b	603	CLA	C3C-C2C	5.32	1.48	1.36
23	b	606	CLA	C3C-C2C	5.32	1.48	1.36
23	A	404[B]	CLA	C3C-C2C	5.32	1.48	1.36
23	C	513	CLA	C3C-C2C	5.31	1.48	1.36
23	C	510	CLA	C3C-C2C	5.30	1.48	1.36
23	b	615	CLA	C3C-C2C	5.30	1.48	1.36
23	c	513	CLA	C3C-C2C	5.30	1.48	1.36
23	D	402[B]	CLA	C3C-C2C	5.29	1.48	1.36
23	b	610	CLA	C3C-C2C	5.29	1.48	1.36
23	B	613	CLA	O2D-CGD	5.29	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	CHC-C1C	5.27	1.49	1.38
24	a	406[B]	PHO	OBD-CAD	5.27	1.29	1.22
23	c	503	CLA	C3C-C2C	5.26	1.48	1.36
23	d	402[A]	CLA	C3C-C2C	5.26	1.48	1.36
23	d	402[B]	CLA	O2D-CGD	5.25	1.46	1.33
23	b	602	CLA	C3C-C2C	5.24	1.48	1.36
23	a	405[A]	CLA	C3C-C2C	5.24	1.48	1.36
23	b	601	CLA	C3C-C2C	5.24	1.48	1.36
23	c	504	CLA	C3C-C2C	5.22	1.48	1.36
23	c	509	CLA	O2D-CGD	5.22	1.46	1.33
23	c	512	CLA	CHC-C1C	5.21	1.48	1.38
23	C	509	CLA	O2D-CGD	5.20	1.46	1.33
23	B	612	CLA	CHC-C1C	5.20	1.48	1.38
25	C	515	BCR	C23-C22	-5.19	1.34	1.46
23	b	614	CLA	C3C-C2C	5.19	1.48	1.36
23	b	612	CLA	C3C-C2C	5.18	1.47	1.36
23	c	502	CLA	C3C-C2C	5.18	1.47	1.36
23	b	605	CLA	C3C-C2C	5.17	1.47	1.36
23	c	513	CLA	C1D-ND	5.16	1.44	1.37
24	a	414[A]	PHO	OBD-CAD	5.16	1.29	1.22
23	B	601	CLA	C3C-C2C	5.16	1.47	1.36
23	d	403[A]	CLA	C3C-C2C	5.14	1.47	1.36
40	V	201	HEC	C3D-C2D	5.14	1.52	1.38
23	B	602	CLA	C1D-ND	5.13	1.44	1.37
23	c	508	CLA	O2D-CGD	5.13	1.45	1.33
23	c	504	CLA	O2D-CGD	5.13	1.45	1.33
23	D	402[A]	CLA	C3C-C2C	5.13	1.47	1.36
23	d	403[B]	CLA	C3C-C2C	5.13	1.47	1.36
23	B	601	CLA	O2A-CGA	5.12	1.48	1.33
25	k	101	BCR	C23-C22	-5.12	1.35	1.46
23	a	404[A]	CLA	C3C-C2C	5.12	1.47	1.36
23	b	602	CLA	CHC-C1C	5.12	1.48	1.38
24	A	407[B]	PHO	C3D-C2D	5.12	1.48	1.39
23	C	514	CLA	C3C-C2C	5.11	1.47	1.36
23	a	407	CLA	C3C-C2C	5.11	1.47	1.36
23	C	512	CLA	O2D-CGD	5.11	1.45	1.33
23	B	609	CLA	C3C-C2C	5.10	1.47	1.36
23	b	609	CLA	O2D-CGD	5.10	1.45	1.33
23	B	601	CLA	O2D-CGD	5.10	1.45	1.33
23	c	510	CLA	O2D-CGD	5.10	1.45	1.33
23	c	510	CLA	C3C-C2C	5.10	1.47	1.36
23	B	605	CLA	C3C-C2C	5.10	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	O2D-CGD	5.09	1.45	1.33
23	a	405[B]	CLA	C3C-C2C	5.09	1.47	1.36
23	c	508	CLA	CHC-C1C	5.09	1.48	1.38
23	A	408	CLA	C3C-C2C	5.09	1.47	1.36
23	b	614	CLA	CHC-C1C	5.08	1.48	1.38
23	B	604	CLA	C3C-C2C	5.08	1.47	1.36
23	B	609	CLA	CHC-C1C	5.08	1.48	1.38
23	A	406[B]	CLA	CHC-C1C	5.08	1.48	1.38
23	B	606	CLA	C3C-C2C	5.08	1.47	1.36
23	B	614	CLA	C3C-C2C	5.08	1.47	1.36
23	c	501	CLA	C3C-C2C	5.08	1.47	1.36
23	B	601	CLA	CHC-C1C	5.07	1.48	1.38
23	c	505	CLA	CHC-C1C	5.05	1.48	1.38
23	B	603	CLA	C3C-C2C	5.05	1.47	1.36
25	d	405	BCR	C23-C22	-5.04	1.35	1.46
24	a	414[B]	PHO	O2D-CGD	5.04	1.45	1.33
23	B	612	CLA	C3C-C2C	5.03	1.47	1.36
23	B	615	CLA	O2D-CGD	5.03	1.45	1.33
23	a	404[B]	CLA	C3C-C2C	5.02	1.47	1.36
23	b	601	CLA	C1D-ND	5.02	1.44	1.37
23	b	611	CLA	C3C-C2C	5.02	1.47	1.36
24	A	416[B]	PHO	O2D-CGD	5.02	1.45	1.33
23	c	511	CLA	C3C-C2C	5.01	1.47	1.36
38	f	101	HEM	FE-NB	5.01	2.10	1.94
24	A	407[A]	PHO	C3D-C2D	5.00	1.48	1.39
23	b	613	CLA	CHC-C1C	5.00	1.48	1.38
23	a	407	CLA	O2D-CGD	5.00	1.45	1.33
23	C	507	CLA	C3C-C2C	5.00	1.47	1.36
23	A	405[B]	CLA	C3C-C2C	4.99	1.47	1.36
23	B	610	CLA	C1D-ND	4.98	1.44	1.37
23	D	403	CLA	C1D-ND	4.98	1.44	1.37
23	d	404	CLA	CHC-C1C	4.98	1.48	1.38
24	a	406[A]	PHO	O2D-CGD	4.98	1.45	1.33
25	B	619	BCR	C23-C22	-4.98	1.35	1.46
23	C	505	CLA	C3C-C2C	4.97	1.47	1.36
23	d	404	CLA	C1D-ND	4.97	1.44	1.37
23	b	616	CLA	C3C-C2C	4.97	1.47	1.36
24	A	407[B]	PHO	O2D-CGD	4.97	1.45	1.33
23	c	508	CLA	C1D-ND	4.96	1.44	1.37
23	C	507	CLA	O2D-CGD	4.96	1.45	1.33
23	c	506	CLA	C3C-C2C	4.96	1.47	1.36
23	C	503	CLA	C1D-ND	4.96	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	CHC-C1C	4.96	1.48	1.38
23	A	406[A]	CLA	C3C-C2C	4.96	1.47	1.36
23	B	602	CLA	C3C-C2C	4.96	1.47	1.36
23	C	502	CLA	C3C-C2C	4.96	1.47	1.36
23	a	407	CLA	CHC-C1C	4.96	1.48	1.38
23	B	608	CLA	C3C-C2C	4.95	1.47	1.36
23	B	613	CLA	CHC-C1C	4.95	1.48	1.38
23	b	605	CLA	O2D-CGD	4.95	1.45	1.33
23	B	613	CLA	C3C-C2C	4.95	1.47	1.36
23	d	402[A]	CLA	O2D-CGD	4.93	1.45	1.33
23	B	615	CLA	CHC-C1C	4.93	1.48	1.38
23	c	513	CLA	O2D-CGD	4.92	1.45	1.33
23	B	604	CLA	O2D-CGD	4.91	1.45	1.33
23	B	603	CLA	C1D-ND	4.91	1.44	1.37
23	A	404[B]	CLA	O2D-CGD	4.91	1.45	1.33
25	y	101	BCR	C23-C22	-4.91	1.35	1.46
23	A	405[B]	CLA	O2D-CGD	4.90	1.45	1.33
24	a	414[A]	PHO	O2D-CGD	4.90	1.45	1.33
23	C	502	CLA	CHC-C1C	4.90	1.48	1.38
38	E	102	HEM	FE-NB	4.90	2.10	1.94
23	B	615	CLA	C3C-C2C	4.90	1.47	1.36
23	B	606	CLA	CHC-C1C	4.90	1.48	1.38
24	a	406[B]	PHO	O2D-CGD	4.89	1.45	1.33
23	A	405[B]	CLA	CHC-C1C	4.89	1.48	1.38
23	A	406[B]	CLA	O2D-CGD	4.89	1.45	1.33
23	B	611	CLA	CHC-C4B	4.89	1.50	1.39
23	a	405[B]	CLA	CHC-C1C	4.88	1.48	1.38
23	c	507	CLA	C3C-C2C	4.88	1.47	1.36
25	D	404	BCR	C23-C22	-4.88	1.35	1.46
23	D	402[B]	CLA	O2D-CGD	4.88	1.45	1.33
23	D	403	CLA	O2D-CGD	4.88	1.45	1.33
23	c	510	CLA	C1D-ND	4.88	1.44	1.37
23	C	514	CLA	O2D-CGD	4.87	1.45	1.33
23	c	512	CLA	C1D-ND	4.87	1.44	1.37
23	b	602	CLA	O2D-CGD	4.87	1.45	1.33
23	b	608	CLA	C3C-C2C	4.87	1.47	1.36
23	b	609	CLA	CHC-C1C	4.86	1.48	1.38
24	A	416[A]	PHO	O2D-CGD	4.86	1.45	1.33
23	b	610	CLA	O2D-CGD	4.86	1.45	1.33
23	c	503	CLA	CHC-C1C	4.86	1.48	1.38
25	c	515	BCR	C23-C22	-4.86	1.35	1.46
23	b	614	CLA	O2D-CGD	4.85	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	CHC-C1C	4.85	1.48	1.38
23	b	609	CLA	C3C-C2C	4.85	1.47	1.36
23	b	613	CLA	C3C-C2C	4.85	1.47	1.36
23	c	501	CLA	CHC-C1C	4.85	1.48	1.38
23	C	505	CLA	O2D-CGD	4.85	1.45	1.33
24	A	407[A]	PHO	O2D-CGD	4.85	1.45	1.33
23	A	406[A]	CLA	O2D-CGD	4.85	1.45	1.33
23	c	511	CLA	O2D-CGD	4.85	1.45	1.33
23	b	604	CLA	C3C-C2C	4.84	1.47	1.36
23	B	611	CLA	O2D-CGD	4.84	1.45	1.33
23	D	403	CLA	CHC-C1C	4.84	1.48	1.38
23	c	506	CLA	C1D-ND	4.84	1.44	1.37
23	C	503	CLA	C3C-C2C	4.84	1.47	1.36
23	d	402[B]	CLA	C1D-ND	4.83	1.44	1.37
23	C	512	CLA	CHC-C1C	4.83	1.48	1.38
23	c	506	CLA	O2D-CGD	4.82	1.45	1.33
26	F	102	SQD	O47-C7	4.82	1.47	1.34
23	B	602	CLA	CHC-C1C	4.82	1.48	1.38
23	C	506	CLA	CHC-C1C	4.81	1.48	1.38
23	C	503	CLA	O2D-CGD	4.81	1.45	1.33
23	B	607	CLA	C3C-C2C	4.80	1.47	1.36
23	A	406[A]	CLA	CHC-C1C	4.80	1.48	1.38
23	c	507	CLA	CHC-C1C	4.79	1.48	1.38
23	C	504	CLA	CHC-C1C	4.79	1.48	1.38
23	C	510	CLA	O2D-CGD	4.79	1.45	1.33
23	B	610	CLA	CHC-C1C	4.78	1.48	1.38
23	A	405[A]	CLA	C3C-C2C	4.78	1.47	1.36
23	d	402[A]	CLA	C1D-ND	4.77	1.44	1.37
23	b	603	CLA	CHC-C1C	4.76	1.48	1.38
23	B	609	CLA	O2D-CGD	4.76	1.44	1.33
23	B	601	CLA	C1D-ND	4.76	1.44	1.37
23	C	506	CLA	C3C-C2C	4.76	1.47	1.36
23	B	605	CLA	C1D-ND	4.76	1.44	1.37
23	b	601	CLA	O2A-CGA	4.76	1.47	1.33
23	c	503	CLA	C1D-ND	4.76	1.44	1.37
25	K	102	BCR	C23-C22	-4.75	1.35	1.46
24	A	407[B]	PHO	OBD-CAD	4.75	1.28	1.22
23	b	601	CLA	O2D-CGD	4.75	1.44	1.33
23	D	402[A]	CLA	O2D-CGD	4.75	1.44	1.33
25	C	516	BCR	C23-C22	-4.75	1.35	1.46
23	c	504	CLA	CHC-C1C	4.75	1.48	1.38
23	C	508	CLA	CHC-C1C	4.74	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	O2D-CGD	4.74	1.44	1.33
23	C	511	CLA	O2D-CGD	4.74	1.44	1.33
23	b	602	CLA	CHD-C1D	4.73	1.47	1.38
23	B	615	CLA	CHD-C1D	4.73	1.47	1.38
23	b	611	CLA	O2D-CGD	4.72	1.44	1.33
23	d	403[B]	CLA	O2D-CGD	4.72	1.44	1.33
23	b	615	CLA	O2D-CGD	4.72	1.44	1.33
23	c	511	CLA	C1D-ND	4.72	1.44	1.37
23	a	404[B]	CLA	C1D-ND	4.70	1.44	1.37
23	b	604	CLA	CHC-C1C	4.70	1.47	1.38
23	b	616	CLA	CHC-C1C	4.70	1.47	1.38
25	B	617	BCR	C23-C22	-4.70	1.35	1.46
23	a	405[B]	CLA	O2D-CGD	4.70	1.44	1.33
23	B	615	CLA	C1D-ND	4.70	1.44	1.37
23	c	511	CLA	CHC-C1C	4.69	1.47	1.38
23	b	613	CLA	O2D-CGD	4.69	1.44	1.33
23	A	404[B]	CLA	CHC-C1C	4.69	1.47	1.38
23	C	506	CLA	O2D-CGD	4.69	1.44	1.33
23	b	616	CLA	C1D-ND	4.69	1.44	1.37
23	A	404[A]	CLA	O2D-CGD	4.68	1.44	1.33
23	c	501	CLA	C1D-ND	4.68	1.44	1.37
23	c	502	CLA	O2D-CGD	4.68	1.44	1.33
23	B	616	CLA	O2D-CGD	4.68	1.44	1.33
23	B	605	CLA	O2D-CGD	4.68	1.44	1.33
23	c	507	CLA	C1D-ND	4.68	1.44	1.37
23	A	408	CLA	O2D-CGD	4.67	1.44	1.33
23	c	513	CLA	CHC-C1C	4.67	1.47	1.38
23	a	405[A]	CLA	CHC-C1C	4.66	1.47	1.38
23	b	616	CLA	O2D-CGD	4.66	1.44	1.33
25	b	619	BCR	C23-C22	-4.66	1.36	1.46
25	T	102	BCR	C23-C22	-4.66	1.36	1.46
25	A	409	BCR	C23-C22	-4.65	1.36	1.46
33	c	520	LMG	O7-C10	4.65	1.47	1.34
23	c	507	CLA	O2D-CGD	4.64	1.44	1.33
24	a	406[A]	PHO	OBD-CAD	4.64	1.28	1.22
23	A	405[A]	CLA	CHC-C1C	4.63	1.47	1.38
23	A	405[B]	CLA	C1D-ND	4.63	1.43	1.37
23	b	602	CLA	C1D-ND	4.62	1.43	1.37
25	H	101	BCR	C23-C22	-4.62	1.36	1.46
23	C	506	CLA	C1D-ND	4.62	1.43	1.37
23	b	615	CLA	CHC-C1C	4.62	1.47	1.38
23	B	614	CLA	C1D-ND	4.62	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	C1D-ND	4.62	1.43	1.37
23	C	514	CLA	C1D-ND	4.62	1.43	1.37
23	d	403[A]	CLA	O2D-CGD	4.62	1.44	1.33
23	C	508	CLA	C1D-ND	4.61	1.43	1.37
33	C	521	LMG	O7-C10	4.60	1.47	1.34
24	A	416[A]	PHO	OBD-CAD	4.60	1.28	1.22
23	c	512	CLA	O2D-CGD	4.59	1.44	1.33
23	C	514	CLA	CHC-C1C	4.59	1.47	1.38
23	b	608	CLA	O2D-CGD	4.59	1.44	1.33
23	B	605	CLA	CHC-C1C	4.59	1.47	1.38
23	b	601	CLA	CHC-C1C	4.59	1.47	1.38
25	b	617	BCR	C23-C22	-4.58	1.36	1.46
23	b	606	CLA	O2D-CGD	4.58	1.44	1.33
25	t	102	BCR	C23-C22	-4.58	1.36	1.46
23	b	611	CLA	CHC-C1C	4.58	1.47	1.38
26	B	620	SQD	O47-C7	4.58	1.47	1.34
23	b	612	CLA	O2D-CGD	4.57	1.44	1.33
23	b	612	CLA	CHC-C1C	4.57	1.47	1.38
23	B	602	CLA	O2D-CGD	4.56	1.44	1.33
23	B	610	CLA	O2D-CGD	4.56	1.44	1.33
23	B	616	CLA	CHC-C1C	4.55	1.47	1.38
23	c	506	CLA	CHC-C1C	4.55	1.47	1.38
25	c	514	BCR	C23-C22	-4.55	1.36	1.46
23	a	404[B]	CLA	O2D-CGD	4.55	1.44	1.33
23	A	404[B]	CLA	C1D-ND	4.54	1.43	1.37
23	C	511	CLA	CHC-C1C	4.54	1.47	1.38
23	B	604	CLA	CHC-C1C	4.53	1.47	1.38
23	b	614	CLA	C1D-ND	4.53	1.43	1.37
23	c	505	CLA	O2D-CGD	4.52	1.44	1.33
23	b	604	CLA	C1D-ND	4.52	1.43	1.37
26	f	102	SQD	O47-C7	4.52	1.47	1.34
23	C	512	CLA	C3C-C2C	4.52	1.46	1.36
23	C	502	CLA	C1D-ND	4.50	1.43	1.37
23	b	608	CLA	CHC-C1C	4.50	1.47	1.38
23	c	504	CLA	C1D-ND	4.50	1.43	1.37
33	C	521	LMG	O8-C28	4.50	1.46	1.33
23	a	404[A]	CLA	O2D-CGD	4.49	1.44	1.33
23	B	606	CLA	C1D-ND	4.49	1.43	1.37
23	B	606	CLA	O2D-CGD	4.49	1.44	1.33
32	E	101[B]	LHG	O8-C23	4.49	1.46	1.33
32	E	101[A]	LHG	O8-C23	4.48	1.46	1.33
23	B	611	CLA	C4B-NB	-4.48	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402[A]	CLA	CHC-C1C	4.48	1.47	1.38
23	C	513	CLA	O2D-CGD	4.48	1.44	1.33
26	A	412	SQD	O48-C23	4.48	1.46	1.33
23	b	611	CLA	O2A-CGA	4.48	1.46	1.33
23	C	507	CLA	CHD-C1D	4.48	1.47	1.38
23	d	402[B]	CLA	CHC-C1C	4.47	1.47	1.38
23	b	607	CLA	O2D-CGD	4.47	1.44	1.33
23	C	503	CLA	CHC-C1C	4.47	1.47	1.38
23	c	513	CLA	CHD-C1D	4.46	1.47	1.38
23	b	601	CLA	CHD-C1D	4.46	1.47	1.38
25	b	618	BCR	C23-C22	-4.46	1.36	1.46
23	c	512	CLA	O2A-CGA	4.45	1.46	1.33
23	D	402[B]	CLA	CHC-C1C	4.45	1.47	1.38
23	a	405[A]	CLA	O2D-CGD	4.45	1.44	1.33
25	Y	101	BCR	C23-C22	-4.45	1.36	1.46
25	a	408	BCR	C23-C22	-4.45	1.36	1.46
25	h	101	BCR	C23-C22	-4.45	1.36	1.46
23	D	403	CLA	CHD-C1D	4.44	1.47	1.38
23	B	603	CLA	O2D-CGD	4.44	1.44	1.33
23	a	404[A]	CLA	CHC-C1C	4.44	1.47	1.38
23	b	607	CLA	CHC-C1C	4.43	1.47	1.38
23	d	402[A]	CLA	C3D-C2D	4.43	1.51	1.39
23	B	604	CLA	CHD-C1D	4.43	1.47	1.38
33	z	101	LMG	O8-C28	4.43	1.46	1.33
23	a	405[B]	CLA	C1D-ND	4.42	1.43	1.37
23	b	605	CLA	CHC-C1C	4.42	1.47	1.38
23	C	509	CLA	CHC-C1C	4.42	1.47	1.38
24	A	407[A]	PHO	OBD-CAD	4.41	1.28	1.22
33	B	621	LMG	O8-C28	4.41	1.46	1.33
23	B	612	CLA	CHB-C1B	4.41	1.49	1.39
23	C	502	CLA	CHD-C1D	4.40	1.47	1.38
32	a	419[A]	LHG	O8-C23	4.40	1.46	1.33
23	C	509	CLA	C1D-ND	4.40	1.43	1.37
23	c	511	CLA	CHD-C1D	4.40	1.47	1.38
38	E	102	HEM	FE-NC	4.40	2.09	1.95
23	b	605	CLA	C1D-ND	4.40	1.43	1.37
23	A	404[A]	CLA	CHC-C1C	4.39	1.47	1.38
23	C	505	CLA	CHC-C1C	4.39	1.47	1.38
23	C	508	CLA	O2A-CGA	4.38	1.46	1.33
26	b	620	SQD	O47-C7	4.38	1.46	1.34
23	B	603	CLA	CHC-C1C	4.38	1.47	1.38
23	C	510	CLA	CHC-C1C	4.38	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	O2A-CGA	4.38	1.46	1.33
23	a	404[B]	CLA	CHC-C1C	4.37	1.47	1.38
23	B	602	CLA	CHD-C1D	4.37	1.46	1.38
26	a	410	SQD	O48-C23	4.37	1.46	1.33
23	B	605	CLA	CHC-C4B	4.37	1.49	1.39
23	B	609	CLA	CHD-C1D	4.37	1.46	1.38
23	B	608	CLA	CHD-C1D	4.37	1.46	1.38
23	B	613	CLA	C1D-ND	4.36	1.43	1.37
23	a	407	CLA	O2A-CGA	4.36	1.46	1.33
23	b	609	CLA	CHD-C1D	4.36	1.46	1.38
23	A	408	CLA	O2A-CGA	4.36	1.46	1.33
23	c	502	CLA	C1D-ND	4.35	1.43	1.37
23	c	513	CLA	O2A-CGA	4.35	1.46	1.33
23	b	609	CLA	C1D-ND	4.35	1.43	1.37
32	a	419[B]	LHG	O8-C23	4.35	1.46	1.33
23	B	607	CLA	CHC-C1C	4.35	1.47	1.38
23	b	606	CLA	C1D-ND	4.35	1.43	1.37
23	d	402[B]	CLA	C3D-C2D	4.34	1.50	1.39
23	C	504	CLA	O2D-CGD	4.34	1.43	1.33
23	c	508	CLA	CHD-C1D	4.33	1.46	1.38
23	C	505	CLA	C1D-ND	4.33	1.43	1.37
23	c	510	CLA	CHC-C1C	4.33	1.47	1.38
23	B	615	CLA	C3D-C2D	4.33	1.50	1.39
23	C	508	CLA	O2D-CGD	4.32	1.43	1.33
23	b	613	CLA	C1D-ND	4.32	1.43	1.37
23	D	402[A]	CLA	CHC-C1C	4.32	1.47	1.38
23	B	614	CLA	C4B-NB	-4.32	1.32	1.37
32	d	408[A]	LHG	O8-C23	4.32	1.45	1.33
23	b	615	CLA	C1D-ND	4.31	1.43	1.37
33	C	520	LMG	O8-C28	4.31	1.45	1.33
23	C	506	CLA	CHD-C1D	4.31	1.46	1.38
23	A	405[A]	CLA	O2D-CGD	4.30	1.43	1.33
23	C	502	CLA	O2A-CGA	4.30	1.45	1.33
23	a	404[B]	CLA	CHD-C1D	4.29	1.46	1.38
23	b	604	CLA	CHC-C4B	4.29	1.49	1.39
38	f	101	HEM	FE-NC	4.29	2.09	1.95
23	D	402[B]	CLA	O2A-CGA	4.29	1.45	1.33
23	c	502	CLA	CHC-C1C	4.28	1.47	1.38
23	B	614	CLA	CHB-C1B	4.28	1.49	1.39
23	d	404	CLA	O2D-CGD	4.28	1.43	1.33
23	a	405[B]	CLA	O2A-CGA	4.27	1.45	1.33
23	A	408	CLA	CHC-C1C	4.27	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	CHD-C1D	4.27	1.46	1.38
33	c	519	LMG	O7-C10	4.27	1.46	1.34
32	d	408[B]	LHG	O8-C23	4.27	1.45	1.33
23	B	609	CLA	O2A-CGA	4.27	1.45	1.33
23	B	611	CLA	CHD-C1D	4.26	1.46	1.38
23	c	506	CLA	O2A-CGA	4.26	1.45	1.33
23	a	404[A]	CLA	C1D-ND	4.26	1.43	1.37
23	d	404	CLA	O2A-CGA	4.26	1.45	1.33
26	B	620	SQD	O48-C23	4.26	1.45	1.33
26	f	102	SQD	O48-C23	4.25	1.45	1.33
23	C	509	CLA	O2A-CGA	4.25	1.45	1.33
23	c	509	CLA	C1D-ND	4.25	1.43	1.37
23	A	405[B]	CLA	O2A-CGA	4.25	1.45	1.33
23	b	603	CLA	C1D-ND	4.24	1.43	1.37
23	B	614	CLA	CHC-C1C	4.24	1.47	1.38
23	C	514	CLA	O2A-CGA	4.24	1.45	1.33
26	b	620	SQD	O48-C23	4.24	1.45	1.33
23	A	404[B]	CLA	CHD-C1D	4.24	1.46	1.38
23	C	510	CLA	C1D-ND	4.24	1.43	1.37
33	c	520	LMG	O8-C28	4.23	1.45	1.33
23	D	402[A]	CLA	O2A-CGA	4.23	1.45	1.33
23	b	611	CLA	C1D-ND	4.22	1.43	1.37
23	B	607	CLA	O2D-CGD	4.22	1.43	1.33
23	c	511	CLA	O2A-CGA	4.22	1.45	1.33
23	b	604	CLA	O2D-CGD	4.22	1.43	1.33
23	C	509	CLA	OBD-CAD	4.22	1.29	1.22
23	B	612	CLA	C1B-NB	-4.22	1.32	1.37
23	C	514	CLA	CHD-C1D	4.22	1.46	1.38
23	d	402[B]	CLA	CHD-C1D	4.21	1.46	1.38
23	C	510	CLA	CHD-C1D	4.21	1.46	1.38
33	Z	101	LMG	O7-C10	4.21	1.46	1.34
23	d	404	CLA	CHD-C1D	4.21	1.46	1.38
23	b	602	CLA	CHD-C4C	4.21	1.48	1.39
23	d	403[A]	CLA	CHC-C1C	4.21	1.46	1.38
23	C	508	CLA	CHD-C1D	4.20	1.46	1.38
23	A	406[B]	CLA	CHD-C1D	4.20	1.46	1.38
23	b	610	CLA	C1D-ND	4.20	1.43	1.37
33	m	101	LMG	O8-C28	4.20	1.45	1.33
32	E	101[A]	LHG	O7-C7	4.19	1.46	1.34
23	c	506	CLA	CHD-C1D	4.18	1.46	1.38
23	a	404[B]	CLA	CHD-C4C	4.18	1.48	1.39
25	B	618	BCR	C23-C22	-4.18	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406[B]	CLA	C1D-ND	4.18	1.43	1.37
23	b	601	CLA	CHD-C4C	4.18	1.48	1.39
23	b	608	CLA	O2A-CGA	4.17	1.45	1.33
23	C	513	CLA	CHC-C4B	4.17	1.48	1.39
32	E	101[B]	LHG	O7-C7	4.16	1.46	1.34
35	c	518	DGD	O1G-C1A	4.16	1.45	1.33
23	b	602	CLA	CHC-C4B	4.16	1.48	1.39
23	b	610	CLA	CHD-C1D	4.16	1.46	1.38
23	A	408	CLA	CHD-C4C	4.16	1.48	1.39
23	b	601	CLA	C3D-C2D	4.16	1.50	1.39
23	C	513	CLA	CHD-C1D	4.16	1.46	1.38
23	c	503	CLA	CHD-C1D	4.16	1.46	1.38
33	c	519	LMG	O8-C28	4.16	1.45	1.33
23	D	402[B]	CLA	C1D-ND	4.16	1.43	1.37
23	c	507	CLA	CHD-C1D	4.16	1.46	1.38
23	b	612	CLA	CHB-C1B	4.15	1.48	1.39
23	c	502	CLA	CHD-C1D	4.15	1.46	1.38
23	c	508	CLA	C3D-C2D	4.15	1.50	1.39
23	A	406[A]	CLA	CHD-C1D	4.15	1.46	1.38
23	C	512	CLA	O2A-CGA	4.15	1.45	1.33
23	C	509	CLA	C3D-C2D	4.14	1.50	1.39
32	a	419[B]	LHG	O7-C7	4.14	1.46	1.34
23	C	507	CLA	C1D-ND	4.14	1.43	1.37
23	b	609	CLA	OBD-CAD	4.14	1.29	1.22
32	a	419[A]	LHG	O7-C7	4.13	1.46	1.34
23	c	505	CLA	CHD-C1D	4.13	1.46	1.38
33	a	415	LMG	O7-C10	4.13	1.46	1.34
23	c	503	CLA	O2D-CGD	4.13	1.43	1.33
23	b	608	CLA	CHD-C1D	4.13	1.46	1.38
23	a	405[A]	CLA	O2A-CGA	4.13	1.45	1.33
23	b	603	CLA	CHD-C1D	4.13	1.46	1.38
23	A	406[B]	CLA	O2A-CGA	4.13	1.45	1.33
23	B	608	CLA	C1D-ND	4.12	1.43	1.37
35	c	517[B]	DGD	O1G-C1A	4.12	1.45	1.33
23	b	615	CLA	CHD-C1D	4.12	1.46	1.38
23	C	507	CLA	CHD-C4C	4.12	1.48	1.39
23	b	612	CLA	C1D-ND	4.12	1.43	1.37
23	b	604	CLA	CHD-C1D	4.12	1.46	1.38
23	B	613	CLA	C3D-C2D	4.12	1.50	1.39
23	B	611	CLA	O2A-CGA	4.12	1.45	1.33
23	c	504	CLA	CHD-C1D	4.12	1.46	1.38
32	D	407[B]	LHG	O8-C23	4.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	C1D-ND	4.11	1.43	1.37
23	b	610	CLA	CHB-C1B	4.11	1.48	1.39
23	C	510	CLA	C3D-C2D	4.11	1.50	1.39
23	d	403[B]	CLA	CHC-C1C	4.11	1.46	1.38
23	d	403[A]	CLA	CHB-C1B	4.11	1.48	1.39
23	B	611	CLA	C3B-C2B	4.11	1.55	1.41
23	C	511	CLA	CHD-C4C	4.11	1.48	1.39
23	d	403[B]	CLA	O2A-CGA	4.11	1.45	1.33
23	A	405[A]	CLA	C3D-C2D	4.10	1.50	1.39
23	d	402[B]	CLA	O2A-CGA	4.10	1.45	1.33
23	c	503	CLA	CHC-C4B	4.10	1.48	1.39
35	c	516[B]	DGD	O2G-C1B	4.10	1.45	1.34
23	A	408	CLA	C1D-ND	4.10	1.43	1.37
23	B	614	CLA	O2A-CGA	4.10	1.45	1.33
23	B	609	CLA	C1D-ND	4.09	1.43	1.37
23	B	610	CLA	OBD-CAD	4.09	1.29	1.22
23	C	503	CLA	C3D-C2D	4.09	1.50	1.39
23	d	402[A]	CLA	O2A-CGA	4.09	1.45	1.33
35	c	516[A]	DGD	O2G-C1B	4.09	1.45	1.34
23	B	606	CLA	CHD-C1D	4.09	1.46	1.38
23	B	602	CLA	O2A-CGA	4.09	1.45	1.33
33	z	101	LMG	O7-C10	4.09	1.45	1.34
35	h	102	DGD	O2G-C1B	4.09	1.45	1.34
23	b	615	CLA	O2A-CGA	4.09	1.45	1.33
35	C	517[B]	DGD	O2G-C1B	4.09	1.45	1.34
23	C	513	CLA	O2A-CGA	4.08	1.45	1.33
23	B	601	CLA	CHD-C1D	4.08	1.46	1.38
23	c	504	CLA	C3D-C2D	4.08	1.50	1.39
26	a	409[B]	SQD	O48-C23	4.08	1.45	1.33
23	A	405[B]	CLA	CHD-C1D	4.08	1.46	1.38
23	C	503	CLA	CHD-C1D	4.08	1.46	1.38
23	b	613	CLA	C3D-C2D	4.07	1.50	1.39
23	B	601	CLA	CHC-C4B	4.07	1.48	1.39
23	B	607	CLA	C1B-NB	-4.07	1.32	1.37
23	C	512	CLA	C1D-ND	4.07	1.43	1.37
23	B	611	CLA	CHB-C1B	4.07	1.48	1.39
26	a	409[A]	SQD	O47-C7	4.07	1.45	1.34
23	c	505	CLA	C1D-ND	4.07	1.43	1.37
24	A	416[B]	PHO	O2A-CGA	4.07	1.45	1.33
23	d	404	CLA	CHC-C4B	4.06	1.48	1.39
32	L	101[B]	LHG	O8-C23	4.06	1.45	1.33
23	c	507	CLA	O2A-CGA	4.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405[B]	CLA	C3D-C2D	4.06	1.50	1.39
35	C	517[A]	DGD	O2G-C1B	4.06	1.45	1.34
23	d	403[A]	CLA	O2A-CGA	4.06	1.45	1.33
26	a	409[B]	SQD	O47-C7	4.06	1.45	1.34
23	B	610	CLA	CHB-C1B	4.06	1.48	1.39
23	b	614	CLA	CHD-C1D	4.05	1.46	1.38
23	D	402[A]	CLA	CHB-C1B	4.05	1.48	1.39
23	c	506	CLA	CHD-C4C	4.05	1.48	1.39
33	C	501	LMG	O7-C10	4.05	1.45	1.34
23	C	507	CLA	CHC-C1C	4.05	1.46	1.38
23	c	505	CLA	CHC-C4B	4.04	1.48	1.39
23	c	509	CLA	C1B-NB	-4.03	1.32	1.37
26	a	410	SQD	O47-C7	4.03	1.45	1.34
33	a	415	LMG	O8-C28	4.03	1.45	1.33
26	A	412	SQD	O47-C7	4.03	1.45	1.34
23	c	503	CLA	CHD-C4C	4.03	1.48	1.39
23	c	512	CLA	C3D-C2D	4.03	1.50	1.39
23	d	403[B]	CLA	CHB-C1B	4.03	1.48	1.39
23	B	615	CLA	CHD-C4C	4.03	1.48	1.39
23	C	506	CLA	CHB-C1B	4.03	1.48	1.39
23	c	502	CLA	O2A-CGA	4.02	1.45	1.33
23	C	512	CLA	CHB-C1B	4.02	1.48	1.39
23	A	404[B]	CLA	CHD-C4C	4.01	1.48	1.39
23	C	507	CLA	O2A-CGA	4.01	1.45	1.33
23	b	615	CLA	CHD-C4C	4.01	1.48	1.39
23	d	402[B]	CLA	CHD-C4C	4.01	1.48	1.39
23	c	503	CLA	CHB-C1B	4.01	1.48	1.39
23	b	606	CLA	CHD-C1D	4.01	1.46	1.38
23	b	609	CLA	CHB-C1B	4.01	1.48	1.39
23	c	513	CLA	CHD-C4C	4.01	1.48	1.39
33	C	501	LMG	O8-C28	4.00	1.45	1.33
23	b	612	CLA	OBD-CAD	4.00	1.29	1.22
23	A	404[A]	CLA	CHD-C1D	4.00	1.46	1.38
23	c	512	CLA	CHD-C4C	4.00	1.48	1.39
32	d	414[B]	LHG	O8-C23	4.00	1.45	1.33
23	C	502	CLA	CHC-C4B	4.00	1.48	1.39
23	b	616	CLA	O2A-CGA	4.00	1.45	1.33
23	c	506	CLA	C3D-C2D	4.00	1.49	1.39
23	c	510	CLA	CHB-C1B	4.00	1.48	1.39
23	B	615	CLA	O2A-CGA	4.00	1.45	1.33
23	b	614	CLA	CHC-C4B	3.99	1.48	1.39
23	c	511	CLA	CHB-C1B	3.99	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	C3D-C2D	3.99	1.49	1.39
23	B	602	CLA	C3D-C2D	3.99	1.49	1.39
23	a	405[B]	CLA	C3D-C2D	3.99	1.49	1.39
23	c	507	CLA	CHD-C4C	3.99	1.48	1.39
23	D	403	CLA	CHC-C4B	3.99	1.48	1.39
23	D	403	CLA	C3D-C2D	3.99	1.49	1.39
26	a	409[A]	SQD	O48-C23	3.99	1.45	1.33
32	D	407[A]	LHG	O7-C7	3.98	1.45	1.34
23	C	505	CLA	CHB-C1B	3.98	1.48	1.39
23	a	404[A]	CLA	CHD-C4C	3.98	1.48	1.39
23	c	503	CLA	O2A-CGA	3.98	1.45	1.33
23	c	501	CLA	O2D-CGD	3.98	1.43	1.33
23	B	615	CLA	OBD-CAD	3.98	1.29	1.22
23	B	610	CLA	CHD-C1D	3.98	1.46	1.38
23	c	509	CLA	CHC-C1C	3.97	1.46	1.38
23	B	609	CLA	C3D-C2D	3.97	1.49	1.39
23	A	408	CLA	CHD-C1D	3.97	1.46	1.38
23	c	504	CLA	O2A-CGA	3.97	1.44	1.33
23	c	501	CLA	CHD-C1D	3.97	1.46	1.38
23	A	406[B]	CLA	C3D-C2D	3.97	1.49	1.39
35	C	518[B]	DGD	O1G-C1A	3.97	1.44	1.33
23	B	616	CLA	C3D-C2D	3.97	1.49	1.39
23	C	502	CLA	O2D-CGD	3.97	1.43	1.33
23	C	514	CLA	C3D-C2D	3.96	1.49	1.39
23	c	501	CLA	C3D-C2D	3.96	1.49	1.39
23	c	501	CLA	CHB-C1B	3.96	1.48	1.39
23	B	608	CLA	O2D-CGD	3.96	1.43	1.33
23	B	602	CLA	CHD-C4C	3.96	1.48	1.39
23	b	615	CLA	C3D-C2D	3.96	1.49	1.39
23	b	610	CLA	CHC-C4B	3.96	1.48	1.39
23	B	614	CLA	CHD-C4C	3.96	1.48	1.39
23	c	502	CLA	C3D-C2D	3.96	1.49	1.39
23	c	508	CLA	OBD-CAD	3.96	1.29	1.22
23	C	507	CLA	C3D-C2D	3.96	1.49	1.39
33	d	412	LMG	O8-C28	3.96	1.44	1.33
23	C	512	CLA	CHD-C1D	3.96	1.46	1.38
23	a	404[A]	CLA	CHD-C1D	3.96	1.46	1.38
23	c	511	CLA	OBD-CAD	3.96	1.29	1.22
32	L	101[B]	LHG	O7-C7	3.95	1.45	1.34
23	B	602	CLA	CHB-C1B	3.95	1.48	1.39
23	B	612	CLA	O2D-CGD	3.95	1.42	1.33
23	B	609	CLA	CHC-C4B	3.95	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	410[B]	SQD	O48-C23	3.95	1.44	1.33
23	A	408	CLA	C3D-C2D	3.95	1.49	1.39
23	a	405[A]	CLA	C3D-C2D	3.95	1.49	1.39
23	C	503	CLA	CHC-C4B	3.95	1.48	1.39
23	c	507	CLA	OBD-CAD	3.94	1.29	1.22
23	D	402[B]	CLA	CHD-C1D	3.94	1.46	1.38
23	b	608	CLA	C1D-ND	3.94	1.43	1.37
23	D	402[A]	CLA	C1D-ND	3.94	1.43	1.37
23	c	513	CLA	C3D-C2D	3.93	1.49	1.39
26	F	102	SQD	O48-C23	3.93	1.44	1.33
35	C	519	DGD	O1G-C1A	3.93	1.44	1.33
23	D	403	CLA	CHB-C1B	3.93	1.48	1.39
23	c	501	CLA	CHD-C4C	3.93	1.48	1.39
23	B	607	CLA	CHB-C1B	3.93	1.48	1.39
23	C	503	CLA	O2A-CGA	3.93	1.44	1.33
23	B	616	CLA	C1D-ND	3.93	1.43	1.37
23	c	508	CLA	CHD-C4C	3.93	1.48	1.39
23	b	607	CLA	CHD-C1D	3.92	1.46	1.38
23	B	607	CLA	CHC-C4B	3.92	1.48	1.39
23	c	506	CLA	CHB-C1B	3.92	1.48	1.39
23	B	608	CLA	CHC-C1C	3.92	1.46	1.38
23	c	509	CLA	CHB-C1B	3.92	1.48	1.39
23	D	402[A]	CLA	CHD-C4C	3.92	1.48	1.39
23	B	616	CLA	O2A-CGA	3.92	1.44	1.33
23	C	511	CLA	O2A-CGA	3.92	1.44	1.33
23	c	502	CLA	CHD-C4C	3.92	1.48	1.39
23	B	616	CLA	CHB-C1B	3.91	1.48	1.39
32	D	407[A]	LHG	O8-C23	3.91	1.44	1.33
33	C	520	LMG	O7-C10	3.91	1.45	1.34
23	b	606	CLA	O2A-CGA	3.91	1.44	1.33
23	B	611	CLA	OBD-CAD	3.91	1.29	1.22
23	B	613	CLA	OBD-CAD	3.91	1.29	1.22
23	C	504	CLA	CHD-C4C	3.91	1.48	1.39
23	C	513	CLA	C3D-C2D	3.90	1.49	1.39
23	c	510	CLA	O2A-CGA	3.90	1.44	1.33
23	B	603	CLA	C3D-C2D	3.90	1.49	1.39
23	C	510	CLA	C4B-NB	-3.90	1.32	1.37
23	b	608	CLA	C3D-C2D	3.90	1.49	1.39
23	A	404[A]	CLA	C1D-ND	3.89	1.43	1.37
23	b	605	CLA	CHB-C1B	3.89	1.48	1.39
23	D	402[A]	CLA	CHD-C1D	3.89	1.46	1.38
23	A	406[B]	CLA	CHD-C4C	3.89	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406[A]	CLA	C3D-C2D	3.89	1.49	1.39
23	C	506	CLA	CHD-C4C	3.89	1.48	1.39
23	b	607	CLA	C3D-C2D	3.89	1.49	1.39
23	B	604	CLA	CHB-C1B	3.89	1.48	1.39
23	D	402[B]	CLA	CHD-C4C	3.88	1.48	1.39
23	b	604	CLA	C3D-C2D	3.88	1.49	1.39
23	c	505	CLA	CHB-C1B	3.88	1.48	1.39
23	c	507	CLA	C3D-C2D	3.88	1.49	1.39
23	A	405[B]	CLA	CHC-C4B	3.88	1.48	1.39
23	C	504	CLA	O2A-CGA	3.88	1.44	1.33
23	c	511	CLA	C3D-C2D	3.88	1.49	1.39
23	C	510	CLA	CHD-C4C	3.88	1.48	1.39
23	C	514	CLA	CHD-C4C	3.88	1.48	1.39
23	B	605	CLA	O2A-CGA	3.88	1.44	1.33
24	a	414[B]	PHO	O2A-CGA	3.88	1.44	1.33
23	c	505	CLA	C3D-C2D	3.87	1.49	1.39
23	B	611	CLA	C3D-C2D	3.87	1.49	1.39
23	c	509	CLA	O2A-CGA	3.87	1.44	1.33
23	c	508	CLA	CHB-C1B	3.87	1.48	1.39
23	C	512	CLA	C3D-C2D	3.87	1.49	1.39
24	A	407[B]	PHO	O2A-CGA	3.87	1.44	1.33
23	c	509	CLA	CHD-C1D	3.87	1.46	1.38
24	A	416[A]	PHO	O2A-CGA	3.86	1.44	1.33
23	B	603	CLA	CHB-C1B	3.86	1.48	1.39
23	c	508	CLA	CHC-C4B	3.86	1.48	1.39
23	B	615	CLA	CHB-C1B	3.86	1.48	1.39
35	c	516[B]	DGD	O1G-C1A	3.86	1.44	1.33
23	b	603	CLA	CHC-C4B	3.86	1.48	1.39
33	B	621	LMG	O7-C10	3.86	1.45	1.34
35	C	518[B]	DGD	O2G-C1B	3.86	1.45	1.34
23	c	510	CLA	C3D-C2D	3.86	1.49	1.39
23	d	404	CLA	C3D-C2D	3.86	1.49	1.39
26	A	410[A]	SQD	O48-C23	3.85	1.44	1.33
23	C	504	CLA	CHC-C4B	3.85	1.48	1.39
35	C	518[A]	DGD	O2G-C1B	3.85	1.45	1.34
35	H	102	DGD	O1G-C1A	3.85	1.44	1.33
23	B	606	CLA	CHB-C1B	3.85	1.48	1.39
32	b	629[B]	LHG	O7-C7	3.85	1.45	1.34
32	L	101[A]	LHG	O8-C23	3.85	1.44	1.33
23	c	507	CLA	CHC-C4B	3.85	1.48	1.39
23	B	608	CLA	C3D-C2D	3.84	1.49	1.39
23	C	510	CLA	O2A-CGA	3.84	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	CHB-C1B	3.84	1.48	1.39
32	d	407[B]	LHG	O7-C7	3.84	1.45	1.34
23	C	514	CLA	CHB-C1B	3.84	1.48	1.39
35	c	517[A]	DGD	O1G-C1A	3.84	1.44	1.33
23	A	405[A]	CLA	O2A-CGA	3.84	1.44	1.33
23	a	407	CLA	CHC-C4B	3.84	1.48	1.39
23	b	605	CLA	CHD-C4C	3.84	1.47	1.39
23	b	602	CLA	O2A-CGA	3.84	1.44	1.33
23	c	510	CLA	CHD-C1D	3.84	1.45	1.38
24	a	414[A]	PHO	O2A-CGA	3.84	1.44	1.33
23	c	513	CLA	CHB-C1B	3.83	1.48	1.39
23	A	405[B]	CLA	CHD-C4C	3.83	1.47	1.39
23	B	605	CLA	C3D-C2D	3.83	1.49	1.39
23	B	605	CLA	CHD-C4C	3.83	1.47	1.39
23	b	611	CLA	CHB-C1B	3.83	1.48	1.39
23	B	610	CLA	C3D-C2D	3.83	1.49	1.39
23	a	405[A]	CLA	C1D-ND	3.83	1.42	1.37
23	c	501	CLA	O2A-CGA	3.83	1.44	1.33
23	c	512	CLA	CHC-C4B	3.82	1.48	1.39
23	d	403[B]	CLA	C1D-ND	3.82	1.42	1.37
32	L	101[A]	LHG	O7-C7	3.82	1.45	1.34
32	D	406[B]	LHG	O7-C7	3.82	1.45	1.34
23	c	510	CLA	CHD-C4C	3.82	1.47	1.39
23	C	506	CLA	CHC-C4B	3.82	1.48	1.39
23	B	601	CLA	CHD-C4C	3.82	1.47	1.39
23	B	613	CLA	CHB-C1B	3.82	1.48	1.39
32	b	629[B]	LHG	O8-C23	3.81	1.44	1.33
23	b	612	CLA	CHC-C4B	3.81	1.48	1.39
32	D	407[B]	LHG	O7-C7	3.81	1.45	1.34
23	B	606	CLA	CHC-C4B	3.81	1.48	1.39
35	C	517[B]	DGD	O1G-C1A	3.81	1.44	1.33
23	b	616	CLA	CHD-C1D	3.81	1.45	1.38
23	c	501	CLA	CHC-C4B	3.81	1.48	1.39
23	b	613	CLA	O2A-CGA	3.81	1.44	1.33
23	b	615	CLA	CHC-C4B	3.81	1.48	1.39
23	c	505	CLA	CHD-C4C	3.81	1.47	1.39
23	C	504	CLA	CHD-C1D	3.81	1.45	1.38
23	B	602	CLA	CHC-C4B	3.81	1.48	1.39
23	b	609	CLA	CHD-C4C	3.81	1.47	1.39
23	A	406[A]	CLA	O2A-CGA	3.81	1.44	1.33
33	d	412	LMG	O7-C10	3.81	1.45	1.34
23	C	510	CLA	OBD-CAD	3.80	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	CHD-C4C	3.80	1.47	1.39
23	b	604	CLA	CHD-C4C	3.80	1.47	1.39
23	C	512	CLA	CHD-C4C	3.80	1.47	1.39
23	b	610	CLA	C3D-C2D	3.80	1.49	1.39
23	B	603	CLA	CHC-C4B	3.80	1.47	1.39
23	A	406[A]	CLA	CHC-C4B	3.79	1.47	1.39
23	b	610	CLA	CHD-C4C	3.79	1.47	1.39
23	b	602	CLA	C3D-C2D	3.79	1.49	1.39
23	c	511	CLA	CHD-C4C	3.79	1.47	1.39
35	c	517[B]	DGD	O2G-C1B	3.78	1.45	1.34
32	d	408[B]	LHG	O7-C7	3.78	1.45	1.34
23	b	613	CLA	CHB-C1B	3.78	1.47	1.39
23	A	405[A]	CLA	CHB-C1B	3.78	1.47	1.39
23	b	608	CLA	OBD-CAD	3.78	1.29	1.22
23	d	403[A]	CLA	CHD-C1D	3.78	1.45	1.38
23	b	611	CLA	CHD-C1D	3.77	1.45	1.38
23	B	616	CLA	CHC-C4B	3.77	1.47	1.39
23	d	402[A]	CLA	OBD-CAD	3.77	1.29	1.22
23	c	505	CLA	OBD-CAD	3.77	1.29	1.22
23	C	502	CLA	CHD-C4C	3.77	1.47	1.39
23	d	402[A]	CLA	CHD-C1D	3.77	1.45	1.38
23	B	604	CLA	CHD-C4C	3.77	1.47	1.39
35	h	102	DGD	O1G-C1A	3.77	1.44	1.33
23	a	405[B]	CLA	CHD-C1D	3.77	1.45	1.38
23	B	604	CLA	OBD-CAD	3.77	1.29	1.22
23	d	402[B]	CLA	OBD-CAD	3.76	1.29	1.22
23	D	403	CLA	CHD-C4C	3.76	1.47	1.39
23	c	502	CLA	CHB-C1B	3.76	1.47	1.39
23	A	404[A]	CLA	CHD-C4C	3.76	1.47	1.39
23	b	608	CLA	CHB-C1B	3.76	1.47	1.39
32	d	414[A]	LHG	O8-C23	3.75	1.44	1.33
23	A	406[B]	CLA	OBD-CAD	3.75	1.28	1.22
23	b	614	CLA	CHD-C4C	3.75	1.47	1.39
23	C	509	CLA	CHD-C1D	3.75	1.45	1.38
23	B	607	CLA	CHD-C1D	3.75	1.45	1.38
23	a	405[A]	CLA	CHB-C1B	3.75	1.47	1.39
23	C	503	CLA	CHB-C1B	3.75	1.47	1.39
23	B	604	CLA	O2A-CGA	3.75	1.44	1.33
23	C	513	CLA	CHD-C4C	3.75	1.47	1.39
23	a	405[B]	CLA	OBD-CAD	3.75	1.28	1.22
23	b	616	CLA	CHC-C4B	3.74	1.47	1.39
23	d	404	CLA	OBD-CAD	3.74	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	CHB-C1B	3.74	1.47	1.39
23	b	603	CLA	CHD-C4C	3.74	1.47	1.39
23	A	406[A]	CLA	OBD-CAD	3.74	1.28	1.22
23	b	613	CLA	CHC-C4B	3.74	1.47	1.39
23	B	607	CLA	CHD-C4C	3.73	1.47	1.39
23	c	504	CLA	CHD-C4C	3.73	1.47	1.39
23	b	605	CLA	C3D-C2D	3.73	1.49	1.39
23	b	616	CLA	C3D-C2D	3.73	1.49	1.39
23	d	403[B]	CLA	CHD-C4C	3.73	1.47	1.39
23	B	609	CLA	CHD-C4C	3.73	1.47	1.39
23	b	609	CLA	CHC-C4B	3.73	1.47	1.39
23	a	407	CLA	C1D-ND	3.73	1.42	1.37
23	b	612	CLA	CHD-C1D	3.72	1.45	1.38
32	d	407[A]	LHG	O7-C7	3.72	1.44	1.34
33	m	101	LMG	O7-C10	3.72	1.44	1.34
35	C	518[A]	DGD	O1G-C1A	3.72	1.44	1.33
23	B	612	CLA	O2A-CGA	3.72	1.44	1.33
32	d	407[B]	LHG	O8-C23	3.71	1.44	1.33
23	c	512	CLA	OBD-CAD	3.71	1.28	1.22
23	a	404[A]	CLA	C3D-C2D	3.71	1.49	1.39
23	b	615	CLA	OBD-CAD	3.71	1.28	1.22
23	b	615	CLA	CHB-C1B	3.71	1.47	1.39
23	C	502	CLA	C3D-C2D	3.71	1.49	1.39
23	D	402[B]	CLA	CHB-C1B	3.71	1.47	1.39
23	A	406[B]	CLA	CHC-C4B	3.71	1.47	1.39
23	b	605	CLA	CHD-C1D	3.71	1.45	1.38
23	A	406[A]	CLA	C1D-ND	3.71	1.42	1.37
32	A	419[B]	LHG	O7-C7	3.70	1.44	1.34
23	D	403	CLA	O2A-CGA	3.70	1.44	1.33
23	b	607	CLA	CHC-C4B	3.70	1.47	1.39
32	A	419[B]	LHG	O8-C23	3.70	1.44	1.33
23	c	505	CLA	O2A-CGA	3.70	1.44	1.33
23	b	614	CLA	C3D-C2D	3.70	1.49	1.39
23	b	604	CLA	CHB-C1B	3.70	1.47	1.39
23	B	603	CLA	CHD-C4C	3.70	1.47	1.39
23	C	505	CLA	CHD-C4C	3.70	1.47	1.39
23	b	614	CLA	CHB-C1B	3.70	1.47	1.39
23	C	503	CLA	CHD-C4C	3.69	1.47	1.39
35	C	519	DGD	O2G-C1B	3.69	1.44	1.34
23	b	611	CLA	CHC-C4B	3.69	1.47	1.39
23	A	406[A]	CLA	CHD-C4C	3.69	1.47	1.39
23	A	404[B]	CLA	C3D-C2D	3.69	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	CHC-C4B	3.69	1.47	1.39
23	b	603	CLA	O2A-CGA	3.69	1.44	1.33
23	A	405[A]	CLA	CHD-C1D	3.69	1.45	1.38
23	B	612	CLA	CHD-C1D	3.69	1.45	1.38
23	a	404[A]	CLA	CHB-C1B	3.69	1.47	1.39
23	B	601	CLA	C3D-C2D	3.69	1.49	1.39
23	b	601	CLA	OBD-CAD	3.69	1.28	1.22
23	c	510	CLA	CHC-C4B	3.69	1.47	1.39
26	A	410[A]	SQD	O47-C7	3.68	1.44	1.34
23	A	404[A]	CLA	C3D-C2D	3.68	1.49	1.39
23	a	405[A]	CLA	OBD-CAD	3.68	1.28	1.22
23	d	403[A]	CLA	C1B-NB	-3.68	1.33	1.37
23	B	603	CLA	O2A-CGA	3.68	1.44	1.33
23	C	504	CLA	CHB-C1B	3.68	1.47	1.39
32	d	414[B]	LHG	O7-C7	3.68	1.44	1.34
23	C	509	CLA	CHB-C1B	3.67	1.47	1.39
23	a	405[B]	CLA	CHB-C1B	3.67	1.47	1.39
23	C	508	CLA	C3D-C2D	3.67	1.49	1.39
23	a	404[B]	CLA	C3D-C2D	3.67	1.49	1.39
33	D	411	LMG	O8-C28	3.67	1.44	1.33
23	d	404	CLA	CHB-C1B	3.67	1.47	1.39
23	b	607	CLA	CHD-C4C	3.67	1.47	1.39
23	C	511	CLA	CHD-C1D	3.67	1.45	1.38
23	B	603	CLA	OBD-CAD	3.66	1.28	1.22
23	B	612	CLA	C4B-NB	-3.66	1.33	1.37
32	d	408[A]	LHG	O7-C7	3.66	1.44	1.34
23	a	404[B]	CLA	O2A-CGA	3.66	1.44	1.33
23	c	509	CLA	C3D-C2D	3.66	1.49	1.39
23	a	404[B]	CLA	OBD-CAD	3.66	1.28	1.22
23	a	404[B]	CLA	CHB-C1B	3.66	1.47	1.39
23	C	511	CLA	CHB-C1B	3.66	1.47	1.39
23	B	606	CLA	C3D-C2D	3.65	1.49	1.39
23	B	608	CLA	CHB-C1B	3.65	1.47	1.39
23	b	606	CLA	C3D-C2D	3.65	1.49	1.39
23	C	508	CLA	CHC-C4B	3.65	1.47	1.39
23	C	511	CLA	C3D-C2D	3.65	1.48	1.39
24	A	407[A]	PHO	O2A-CGA	3.65	1.44	1.33
23	B	611	CLA	C1C-C2C	3.65	1.51	1.44
23	c	509	CLA	CHD-C4C	3.64	1.47	1.39
23	C	506	CLA	O2A-CGA	3.64	1.44	1.33
23	b	608	CLA	CHD-C4C	3.64	1.47	1.39
23	d	402[A]	CLA	CHD-C4C	3.64	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	C3D-C2D	3.64	1.48	1.39
23	c	506	CLA	CHC-C4B	3.64	1.47	1.39
23	b	604	CLA	OBD-CAD	3.63	1.28	1.22
23	B	609	CLA	CHB-C1B	3.63	1.47	1.39
23	b	612	CLA	C3D-C2D	3.63	1.48	1.39
23	C	506	CLA	C3D-C2D	3.63	1.48	1.39
23	A	408	CLA	CHC-C4B	3.63	1.47	1.39
23	A	405[B]	CLA	CHB-C1B	3.63	1.47	1.39
23	c	512	CLA	CHB-C1B	3.63	1.47	1.39
23	C	505	CLA	CHD-C1D	3.63	1.45	1.38
23	b	601	CLA	CHC-C4B	3.63	1.47	1.39
23	C	507	CLA	OBD-CAD	3.63	1.28	1.22
23	b	602	CLA	OBD-CAD	3.63	1.28	1.22
23	B	603	CLA	CHD-C1D	3.63	1.45	1.38
35	c	516[A]	DGD	O1G-C1A	3.62	1.43	1.33
23	C	505	CLA	CHC-C4B	3.62	1.47	1.39
23	b	613	CLA	C1B-NB	-3.62	1.33	1.37
23	b	616	CLA	CHD-C4C	3.62	1.47	1.39
32	b	629[A]	LHG	O7-C7	3.62	1.44	1.34
23	b	607	CLA	C1D-ND	3.62	1.42	1.37
23	B	613	CLA	CHD-C1D	3.62	1.45	1.38
23	a	404[A]	CLA	OBD-CAD	3.62	1.28	1.22
23	b	606	CLA	CHC-C4B	3.61	1.47	1.39
23	b	607	CLA	CHB-C1B	3.61	1.47	1.39
23	B	611	CLA	CHD-C4C	3.61	1.47	1.39
23	D	403	CLA	OBD-CAD	3.61	1.28	1.22
23	a	405[A]	CLA	CHD-C4C	3.61	1.47	1.39
23	b	609	CLA	C3D-C2D	3.60	1.48	1.39
23	B	610	CLA	CHC-C4B	3.60	1.47	1.39
23	B	605	CLA	CHD-C1D	3.60	1.45	1.38
32	D	406[A]	LHG	O7-C7	3.60	1.44	1.34
23	b	609	CLA	O2A-CGA	3.60	1.43	1.33
23	d	403[A]	CLA	C3D-C2D	3.60	1.48	1.39
23	b	613	CLA	CHD-C1D	3.60	1.45	1.38
23	B	606	CLA	O2A-CGA	3.60	1.43	1.33
32	D	406[B]	LHG	O8-C23	3.60	1.43	1.33
26	A	410[B]	SQD	O47-C7	3.60	1.44	1.34
23	b	616	CLA	CHB-C1B	3.59	1.47	1.39
23	d	403[A]	CLA	CHD-C4C	3.59	1.47	1.39
23	D	402[B]	CLA	C3D-C2D	3.59	1.48	1.39
23	B	601	CLA	CHB-C1B	3.59	1.47	1.39
23	d	403[B]	CLA	CHD-C1D	3.59	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	CHD-C4C	3.59	1.47	1.39
23	a	407	CLA	CHB-C1B	3.59	1.47	1.39
23	C	508	CLA	CHD-C4C	3.59	1.47	1.39
23	b	605	CLA	CHC-C4B	3.59	1.47	1.39
23	B	612	CLA	C3D-C2D	3.58	1.48	1.39
23	A	404[B]	CLA	CHB-C1B	3.58	1.47	1.39
23	B	607	CLA	OBD-CAD	3.58	1.28	1.22
23	A	405[A]	CLA	C1D-ND	3.58	1.42	1.37
23	A	405[A]	CLA	CHD-C4C	3.58	1.47	1.39
23	A	404[B]	CLA	O2A-CGA	3.58	1.43	1.33
23	d	403[B]	CLA	C3D-C2D	3.58	1.48	1.39
23	B	604	CLA	C1D-ND	3.58	1.42	1.37
23	b	603	CLA	C3D-C2D	3.57	1.48	1.39
23	a	405[B]	CLA	CHD-C4C	3.57	1.47	1.39
23	b	606	CLA	CHD-C4C	3.57	1.47	1.39
23	a	404[B]	CLA	CHC-C4B	3.57	1.47	1.39
23	A	408	CLA	C1B-NB	-3.56	1.33	1.37
23	C	507	CLA	C4B-NB	-3.56	1.33	1.37
24	a	406[B]	PHO	O2A-CGA	3.56	1.43	1.33
35	C	517[A]	DGD	O1G-C1A	3.56	1.43	1.33
35	c	518	DGD	O2G-C1B	3.56	1.44	1.34
23	c	509	CLA	C4B-NB	-3.55	1.33	1.37
23	A	405[A]	CLA	CHC-C4B	3.55	1.47	1.39
23	b	614	CLA	O2A-CGA	3.55	1.43	1.33
23	A	404[A]	CLA	CHB-C1B	3.55	1.47	1.39
23	d	403[B]	CLA	CHC-C4B	3.55	1.47	1.39
23	D	402[A]	CLA	C1B-NB	-3.54	1.33	1.37
23	b	603	CLA	CHB-C1B	3.54	1.47	1.39
23	A	405[B]	CLA	OBD-CAD	3.54	1.28	1.22
23	A	404[B]	CLA	CHC-C4B	3.54	1.47	1.39
35	c	517[A]	DGD	O2G-C1B	3.54	1.44	1.34
23	b	603	CLA	OBD-CAD	3.54	1.28	1.22
23	C	513	CLA	OBD-CAD	3.54	1.28	1.22
32	d	407[A]	LHG	O8-C23	3.54	1.43	1.33
23	C	510	CLA	CHB-C1B	3.53	1.47	1.39
32	D	406[A]	LHG	O8-C23	3.53	1.43	1.33
23	a	407	CLA	CHD-C1D	3.53	1.45	1.38
23	B	603	CLA	C1B-NB	-3.53	1.33	1.37
23	C	514	CLA	OBD-CAD	3.53	1.28	1.22
33	D	411	LMG	O7-C10	3.53	1.44	1.34
23	a	405[B]	CLA	CHC-C4B	3.53	1.47	1.39
23	B	616	CLA	CHD-C1D	3.53	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	419[A]	LHG	O8-C23	3.53	1.43	1.33
23	b	610	CLA	OBD-CAD	3.52	1.28	1.22
23	B	614	CLA	CHD-C1D	3.52	1.45	1.38
23	b	606	CLA	CHB-C1B	3.52	1.47	1.39
23	B	608	CLA	CHD-C4C	3.52	1.47	1.39
23	b	607	CLA	C1B-NB	-3.52	1.33	1.37
23	b	612	CLA	O2A-CGA	3.51	1.43	1.33
23	a	405[A]	CLA	CHD-C1D	3.51	1.45	1.38
23	c	504	CLA	CHC-C4B	3.51	1.47	1.39
23	C	507	CLA	CHB-C1B	3.51	1.47	1.39
23	C	508	CLA	CHB-C1B	3.51	1.47	1.39
23	B	602	CLA	C1B-NB	-3.51	1.33	1.37
23	b	615	CLA	C1B-NB	-3.51	1.33	1.37
23	c	503	CLA	C3D-C2D	3.51	1.48	1.39
32	d	414[A]	LHG	O7-C7	3.50	1.44	1.34
23	B	613	CLA	CHC-C4B	3.50	1.47	1.39
23	A	404[A]	CLA	C4B-NB	-3.50	1.33	1.37
32	A	419[A]	LHG	O7-C7	3.50	1.44	1.34
32	b	629[A]	LHG	O8-C23	3.50	1.43	1.33
23	d	403[B]	CLA	C1B-NB	-3.50	1.33	1.37
23	A	406[A]	CLA	C1B-NB	-3.49	1.33	1.37
23	B	612	CLA	CHC-C4B	3.49	1.47	1.39
23	d	402[B]	CLA	CHB-C1B	3.49	1.47	1.39
23	D	402[B]	CLA	OBD-CAD	3.49	1.28	1.22
38	E	102	HEM	C1B-NB	-3.49	1.34	1.40
23	c	502	CLA	OBD-CAD	3.48	1.28	1.22
23	D	402[A]	CLA	C3D-C2D	3.48	1.48	1.39
23	A	405[A]	CLA	C1B-NB	-3.48	1.33	1.37
23	c	509	CLA	OBD-CAD	3.48	1.28	1.22
23	B	613	CLA	CHD-C4C	3.48	1.47	1.39
23	b	607	CLA	O2A-CGA	3.48	1.43	1.33
23	d	402[A]	CLA	CHB-C1B	3.47	1.47	1.39
23	B	607	CLA	O2A-CGA	3.47	1.43	1.33
23	C	504	CLA	C3D-C2D	3.47	1.48	1.39
23	c	511	CLA	CHC-C4B	3.47	1.47	1.39
38	f	101	HEM	C4D-ND	-3.47	1.34	1.40
23	d	402[A]	CLA	CHC-C4B	3.46	1.47	1.39
23	c	506	CLA	OBD-CAD	3.46	1.28	1.22
23	c	513	CLA	CHC-C4B	3.45	1.47	1.39
23	C	503	CLA	OBD-CAD	3.45	1.28	1.22
23	C	509	CLA	CHD-C4C	3.45	1.47	1.39
23	B	606	CLA	CHD-C4C	3.45	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	C1B-NB	-3.44	1.33	1.37
23	B	604	CLA	CHC-C4B	3.44	1.47	1.39
23	B	608	CLA	O2A-CGA	3.44	1.43	1.33
23	d	404	CLA	CHD-C4C	3.44	1.47	1.39
23	B	601	CLA	OBD-CAD	3.44	1.28	1.22
23	B	610	CLA	O2A-CGA	3.43	1.43	1.33
23	A	406[A]	CLA	CHB-C1B	3.42	1.47	1.39
23	B	615	CLA	CHC-C4B	3.42	1.47	1.39
23	C	513	CLA	CHB-C1B	3.42	1.47	1.39
23	C	505	CLA	O2A-CGA	3.42	1.43	1.33
23	d	403[A]	CLA	CHC-C4B	3.42	1.47	1.39
23	B	614	CLA	C3D-C2D	3.41	1.48	1.39
23	d	403[A]	CLA	OBD-CAD	3.41	1.28	1.22
23	b	616	CLA	OBD-CAD	3.41	1.28	1.22
34	B	622	HTG	C1'-S1	-3.41	1.76	1.81
23	C	505	CLA	OBD-CAD	3.41	1.28	1.22
23	B	607	CLA	C1D-ND	3.41	1.42	1.37
23	C	502	CLA	CHB-C1B	3.41	1.47	1.39
23	C	505	CLA	C1B-NB	-3.41	1.33	1.37
23	B	612	CLA	CHD-C4C	3.40	1.46	1.39
23	C	510	CLA	CHC-C4B	3.40	1.47	1.39
23	b	601	CLA	CHB-C1B	3.40	1.47	1.39
23	B	602	CLA	OBD-CAD	3.40	1.28	1.22
23	c	513	CLA	OBD-CAD	3.40	1.28	1.22
24	a	406[A]	PHO	O2A-CGA	3.40	1.43	1.33
23	b	604	CLA	O2A-CGA	3.39	1.43	1.33
23	A	405[B]	CLA	C1B-NB	-3.39	1.33	1.37
23	b	605	CLA	O2A-CGA	3.39	1.43	1.33
23	c	502	CLA	CHC-C4B	3.38	1.47	1.39
35	H	102	DGD	O2G-C1B	3.37	1.43	1.34
23	c	504	CLA	C1B-NB	-3.37	1.33	1.37
23	C	514	CLA	CHC-C4B	3.37	1.47	1.39
23	a	407	CLA	C1B-NB	-3.36	1.33	1.37
23	A	406[B]	CLA	CHB-C1B	3.36	1.47	1.39
23	B	614	CLA	CHC-C4B	3.36	1.47	1.39
23	c	504	CLA	CHB-C1B	3.36	1.47	1.39
23	d	403[B]	CLA	OBD-CAD	3.36	1.28	1.22
23	a	404[A]	CLA	CHC-C4B	3.36	1.46	1.39
34	b	622	HTG	C1'-S1	-3.36	1.76	1.81
23	a	407	CLA	CHD-C4C	3.35	1.46	1.39
23	B	612	CLA	C1D-ND	3.34	1.42	1.37
38	f	101	HEM	C1B-NB	-3.34	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404[A]	CLA	OBD-CAD	3.34	1.28	1.22
23	c	510	CLA	OBD-CAD	3.33	1.28	1.22
23	D	402[A]	CLA	CHC-C4B	3.33	1.46	1.39
23	D	402[B]	CLA	CHC-C4B	3.33	1.46	1.39
23	C	511	CLA	CHC-C4B	3.32	1.46	1.39
23	B	613	CLA	O2A-CGA	3.31	1.43	1.33
23	b	602	CLA	CHB-C1B	3.31	1.46	1.39
23	C	509	CLA	CHC-C4B	3.31	1.46	1.39
23	c	505	CLA	C1B-NB	-3.31	1.33	1.37
23	b	606	CLA	OBD-CAD	3.31	1.28	1.22
23	C	504	CLA	OBD-CAD	3.30	1.28	1.22
23	B	609	CLA	OBD-CAD	3.29	1.28	1.22
23	b	613	CLA	CHD-C4C	3.29	1.46	1.39
23	b	608	CLA	C1B-NB	-3.28	1.33	1.37
23	C	511	CLA	C4B-NB	-3.28	1.33	1.37
23	B	607	CLA	C3D-C2D	3.27	1.47	1.39
23	b	608	CLA	CHC-C4B	3.27	1.46	1.39
23	d	402[B]	CLA	C1B-NB	-3.27	1.33	1.37
23	D	402[A]	CLA	OBD-CAD	3.26	1.28	1.22
34	b	623	HTG	C1'-S1	-3.26	1.76	1.81
23	d	402[B]	CLA	CHC-C4B	3.24	1.46	1.39
23	b	606	CLA	C1B-NB	-3.24	1.33	1.37
23	C	511	CLA	OBD-CAD	3.24	1.28	1.22
23	C	511	CLA	C1B-NB	-3.24	1.33	1.37
23	b	605	CLA	OBD-CAD	3.24	1.28	1.22
23	B	614	CLA	C1B-NB	-3.24	1.33	1.37
23	B	606	CLA	OBD-CAD	3.24	1.28	1.22
23	c	513	CLA	C4B-NB	-3.23	1.33	1.37
23	a	405[A]	CLA	CHC-C4B	3.23	1.46	1.39
23	D	403	CLA	C1B-NB	-3.23	1.33	1.37
24	A	416[A]	PHO	CHA-CBD	-3.23	1.47	1.51
23	B	616	CLA	C4B-NB	-3.23	1.33	1.37
23	b	612	CLA	CHD-C4C	3.22	1.46	1.39
23	A	404[B]	CLA	OBD-CAD	3.22	1.28	1.22
23	C	508	CLA	C4B-NB	-3.22	1.33	1.37
23	B	609	CLA	C1B-NB	-3.22	1.33	1.37
23	B	616	CLA	OBD-CAD	3.21	1.28	1.22
23	d	402[A]	CLA	C1B-NB	-3.20	1.33	1.37
23	C	506	CLA	C1B-C2B	3.20	1.50	1.43
23	A	404[A]	CLA	O2A-CGA	3.20	1.42	1.33
23	B	613	CLA	C1B-NB	-3.20	1.33	1.37
23	D	402[B]	CLA	C1B-NB	-3.19	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	OBD-CAD	3.19	1.28	1.22
23	b	607	CLA	C1B-C2B	3.19	1.50	1.43
23	b	614	CLA	C1B-NB	-3.19	1.33	1.37
23	B	616	CLA	CHD-C4C	3.18	1.46	1.39
23	C	502	CLA	OBD-CAD	3.18	1.28	1.22
23	b	612	CLA	C1B-C2B	3.18	1.50	1.43
23	C	507	CLA	C1B-NB	-3.17	1.33	1.37
23	b	610	CLA	O2A-CGA	3.17	1.42	1.33
23	c	510	CLA	C1B-NB	-3.17	1.33	1.37
23	B	611	CLA	C3B-C4B	3.17	1.51	1.42
23	B	604	CLA	C1B-C2B	3.15	1.50	1.43
23	A	404[A]	CLA	CHC-C4B	3.15	1.46	1.39
23	a	404[A]	CLA	C1B-NB	-3.15	1.33	1.37
23	B	602	CLA	C1C-C2C	3.15	1.50	1.44
23	c	511	CLA	C1B-C2B	3.14	1.50	1.43
23	B	608	CLA	OBD-CAD	3.14	1.27	1.22
23	b	612	CLA	C1B-NB	-3.14	1.33	1.37
23	C	512	CLA	C4D-CHA	3.14	1.49	1.38
23	B	612	CLA	C1C-C2C	3.13	1.50	1.44
23	c	501	CLA	OBD-CAD	3.13	1.27	1.22
23	c	502	CLA	C1B-NB	-3.13	1.33	1.37
38	E	102	HEM	C4D-ND	-3.13	1.34	1.40
23	a	407	CLA	C1B-C2B	3.13	1.50	1.43
23	C	510	CLA	C1B-NB	-3.13	1.33	1.37
23	C	512	CLA	C4B-NB	-3.12	1.33	1.37
23	C	508	CLA	OBD-CAD	3.12	1.27	1.22
23	A	405[A]	CLA	OBD-CAD	3.12	1.27	1.22
23	b	601	CLA	C1B-NB	-3.12	1.33	1.37
23	B	612	CLA	OBD-CAD	3.11	1.27	1.22
23	D	402[B]	CLA	C4B-NB	-3.11	1.33	1.37
23	B	614	CLA	OBD-CAD	3.10	1.27	1.22
23	C	514	CLA	C1B-NB	-3.09	1.33	1.37
23	b	611	CLA	C1B-C2B	3.09	1.50	1.43
23	A	404[B]	CLA	C4B-NB	-3.09	1.33	1.37
23	c	509	CLA	C1B-C2B	3.08	1.50	1.43
23	a	404[A]	CLA	O2A-CGA	3.08	1.42	1.33
23	c	503	CLA	C1B-NB	-3.07	1.33	1.37
23	C	502	CLA	C1B-NB	-3.07	1.33	1.37
23	c	513	CLA	C1B-NB	-3.06	1.33	1.37
24	A	407[A]	PHO	CBD-CGD	-3.06	1.48	1.52
23	C	514	CLA	C4B-NB	-3.05	1.33	1.37
23	B	604	CLA	C3D-C2D	3.05	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	OBD-CAD	3.05	1.27	1.22
23	b	604	CLA	C1B-NB	-3.05	1.33	1.37
23	a	407	CLA	C3D-C2D	3.04	1.47	1.39
23	a	407	CLA	C4B-NB	-3.04	1.33	1.37
23	c	504	CLA	C4B-NB	-3.04	1.33	1.37
23	C	512	CLA	OBD-CAD	3.03	1.27	1.22
23	b	611	CLA	OBD-CAD	3.03	1.27	1.22
23	B	602	CLA	C1B-C2B	3.03	1.50	1.43
23	B	605	CLA	OBD-CAD	3.03	1.27	1.22
23	A	408	CLA	OBD-CAD	3.03	1.27	1.22
23	D	402[A]	CLA	C4B-NB	-3.03	1.33	1.37
23	c	506	CLA	C1B-NB	-3.03	1.33	1.37
23	B	616	CLA	C1B-C2B	3.02	1.50	1.43
23	a	404[A]	CLA	C4B-NB	-3.02	1.33	1.37
23	c	506	CLA	C4B-NB	-3.02	1.33	1.37
23	b	604	CLA	C1B-C2B	3.02	1.50	1.43
23	a	404[B]	CLA	C4B-NB	-3.02	1.33	1.37
23	d	403[B]	CLA	C4B-NB	-3.02	1.33	1.37
23	A	406[B]	CLA	C3B-C4B	3.01	1.51	1.42
23	b	616	CLA	C1B-NB	-3.01	1.33	1.37
23	b	602	CLA	C1B-NB	-3.01	1.33	1.37
23	d	403[A]	CLA	C1D-ND	3.01	1.41	1.37
23	c	513	CLA	C1B-C2B	3.00	1.50	1.43
23	A	404[A]	CLA	C4C-C3C	3.00	1.50	1.45
23	A	408	CLA	C4D-CHA	3.00	1.48	1.38
23	C	505	CLA	C4D-CHA	3.00	1.48	1.38
23	C	513	CLA	C1B-NB	-2.99	1.33	1.37
23	B	615	CLA	C1B-C2B	2.99	1.50	1.43
23	A	408	CLA	CHB-C1B	2.98	1.46	1.39
23	C	507	CLA	CHC-C4B	2.98	1.46	1.39
23	B	604	CLA	C1B-NB	-2.97	1.34	1.37
23	c	508	CLA	C1B-C2B	2.97	1.50	1.43
23	a	407	CLA	OBD-CAD	2.97	1.27	1.22
34	B	625	HTG	C1'-S1	-2.97	1.77	1.81
23	A	406[B]	CLA	C1B-NB	-2.97	1.34	1.37
23	b	614	CLA	C1B-C2B	2.96	1.50	1.43
23	c	504	CLA	C1B-C2B	2.96	1.50	1.43
23	C	508	CLA	C4D-CHA	2.96	1.48	1.38
23	C	506	CLA	C1B-NB	-2.96	1.34	1.37
23	A	404[A]	CLA	C1B-NB	-2.95	1.34	1.37
23	a	405[A]	CLA	C1B-NB	-2.95	1.34	1.37
29	A	414[A]	PL9	C6-C5	2.94	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	C1C-C2C	2.94	1.50	1.44
29	A	414[B]	PL9	C6-C5	2.94	1.49	1.35
23	a	405[B]	CLA	C1B-NB	-2.93	1.34	1.37
29	a	412[A]	PL9	C6-C5	2.93	1.49	1.35
23	b	614	CLA	OBD-CAD	2.93	1.27	1.22
23	b	613	CLA	C4B-NB	-2.93	1.34	1.37
23	b	613	CLA	C1B-C2B	2.93	1.50	1.43
23	c	507	CLA	C4B-NB	-2.93	1.34	1.37
23	B	604	CLA	C4D-CHA	2.93	1.48	1.38
23	C	512	CLA	C1B-C2B	2.92	1.50	1.43
27	A	418	GOL	O2-C2	-2.92	1.34	1.43
35	H	102	DGD	O5D-C1E	2.92	1.45	1.40
23	B	607	CLA	C1B-C2B	2.92	1.50	1.43
23	d	402[B]	CLA	C1B-C2B	2.92	1.50	1.43
23	c	509	CLA	CHC-C4B	2.91	1.46	1.39
23	B	608	CLA	C4B-NB	-2.91	1.34	1.37
23	b	605	CLA	C1B-NB	-2.91	1.34	1.37
23	c	505	CLA	C1B-C2B	2.91	1.50	1.43
34	D	410	HTG	C1'-S1	-2.91	1.77	1.81
23	c	505	CLA	C4C-C3C	2.91	1.50	1.45
23	B	613	CLA	C4B-NB	-2.91	1.34	1.37
23	a	407	CLA	C1C-C2C	2.90	1.50	1.44
23	A	404[B]	CLA	C1B-NB	-2.90	1.34	1.37
29	a	412[B]	PL9	C6-C5	2.90	1.49	1.35
23	D	402[A]	CLA	C1B-C2B	2.90	1.49	1.43
23	B	607	CLA	C4D-CHA	2.89	1.48	1.38
23	B	614	CLA	C1B-C2B	2.89	1.49	1.43
23	C	506	CLA	C4D-CHA	2.89	1.48	1.38
34	d	411	HTG	C1'-S1	-2.89	1.77	1.81
23	B	608	CLA	CHC-C4B	2.88	1.45	1.39
23	C	507	CLA	C1B-C2B	2.88	1.49	1.43
23	A	408	CLA	C1B-C2B	2.88	1.49	1.43
23	b	612	CLA	C4B-NB	-2.88	1.34	1.37
23	c	502	CLA	C4B-NB	-2.88	1.34	1.37
23	c	510	CLA	C1B-C2B	2.87	1.49	1.43
23	C	509	CLA	C4B-NB	-2.87	1.34	1.37
23	B	612	CLA	C4D-CHA	2.86	1.48	1.38
23	b	611	CLA	C4B-NB	-2.86	1.34	1.37
23	b	604	CLA	C4D-CHA	2.86	1.48	1.38
23	C	504	CLA	C1B-NB	-2.86	1.34	1.37
23	C	513	CLA	C1C-C2C	2.86	1.50	1.44
34	c	521	HTG	C1'-S1	-2.86	1.77	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	403[A]	CLA	C4B-NB	-2.86	1.34	1.37
23	b	602	CLA	C1C-C2C	2.85	1.50	1.44
23	B	612	CLA	C1B-C2B	2.85	1.49	1.43
23	b	601	CLA	C4B-NB	-2.85	1.34	1.37
23	B	614	CLA	C3D-C4D	-2.85	1.37	1.44
23	d	403[B]	CLA	C1B-C2B	2.84	1.49	1.43
23	B	608	CLA	C1B-NB	-2.84	1.34	1.37
23	b	612	CLA	C1C-C2C	2.84	1.50	1.44
23	B	615	CLA	C4D-CHA	2.84	1.48	1.38
23	C	514	CLA	C1B-C2B	2.84	1.49	1.43
34	b	625	HTG	C1'-S1	-2.83	1.77	1.81
23	c	503	CLA	C1B-C2B	2.83	1.49	1.43
23	C	503	CLA	C1B-C2B	2.83	1.49	1.43
23	A	406[A]	CLA	C4D-CHA	2.83	1.48	1.38
23	c	510	CLA	C1C-C2C	2.83	1.50	1.44
23	b	613	CLA	C4D-CHA	2.82	1.48	1.38
23	B	605	CLA	C1B-C2B	2.82	1.49	1.43
23	B	608	CLA	C1B-C2B	2.82	1.49	1.43
23	c	503	CLA	C1C-C2C	2.82	1.50	1.44
23	b	610	CLA	C4D-CHA	2.82	1.48	1.38
23	A	404[A]	CLA	C1B-C2B	2.82	1.49	1.43
23	D	402[A]	CLA	C4D-CHA	2.81	1.48	1.38
23	a	405[B]	CLA	C4B-NB	-2.81	1.34	1.37
23	c	507	CLA	C1B-C2B	2.81	1.49	1.43
23	c	510	CLA	C4D-CHA	2.81	1.48	1.38
23	A	405[B]	CLA	C1C-C2C	2.80	1.50	1.44
23	B	606	CLA	C1C-C2C	2.80	1.50	1.44
33	Z	101	LMG	O8-C28	2.80	1.46	1.33
23	B	611	CLA	C4D-CHA	2.80	1.48	1.38
23	B	601	CLA	C1B-NB	-2.80	1.34	1.37
23	B	611	CLA	MG-NB	2.80	2.11	2.05
23	a	404[B]	CLA	C1B-NB	-2.80	1.34	1.37
23	C	502	CLA	C4D-CHA	2.80	1.48	1.38
23	c	512	CLA	C4D-CHA	2.80	1.48	1.38
23	b	608	CLA	C4D-CHA	2.79	1.47	1.38
23	d	402[A]	CLA	C1B-C2B	2.79	1.49	1.43
23	A	405[A]	CLA	C4D-CHA	2.78	1.47	1.38
23	b	609	CLA	C4D-CHA	2.78	1.47	1.38
23	c	507	CLA	C4D-CHA	2.78	1.47	1.38
23	B	603	CLA	C4B-NB	-2.78	1.34	1.37
23	b	607	CLA	C4D-CHA	2.78	1.47	1.38
23	B	614	CLA	C4D-CHA	2.77	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	519	DGD	O2G-C2G	-2.77	1.40	1.46
23	b	613	CLA	OBD-CAD	2.76	1.27	1.22
23	c	508	CLA	C4C-C3C	2.76	1.49	1.45
23	b	610	CLA	C1B-NB	-2.76	1.34	1.37
23	C	505	CLA	C1B-C2B	2.76	1.49	1.43
23	D	402[B]	CLA	C1B-C2B	2.76	1.49	1.43
23	B	615	CLA	C1C-C2C	2.75	1.50	1.44
23	d	404	CLA	C1C-C2C	2.75	1.50	1.44
23	c	503	CLA	OBD-CAD	2.75	1.27	1.22
23	D	403	CLA	C4C-C3C	2.75	1.49	1.45
23	b	615	CLA	C1B-C2B	2.75	1.49	1.43
23	b	610	CLA	C1B-C2B	2.75	1.49	1.43
23	b	611	CLA	C1B-NB	-2.75	1.34	1.37
23	A	406[A]	CLA	C4B-NB	-2.74	1.34	1.37
23	c	511	CLA	C4D-CHA	2.74	1.47	1.38
23	c	501	CLA	C1C-C2C	2.74	1.50	1.44
23	a	405[A]	CLA	C1B-C2B	2.74	1.49	1.43
23	C	507	CLA	C4C-C3C	2.74	1.49	1.45
23	c	503	CLA	C4B-NB	-2.74	1.34	1.37
23	B	605	CLA	C3D-C4D	-2.74	1.38	1.44
23	C	510	CLA	C1B-C2B	2.73	1.49	1.43
23	C	511	CLA	C1B-C2B	2.73	1.49	1.43
23	b	616	CLA	C1B-C2B	2.73	1.49	1.43
23	c	508	CLA	C1C-C2C	2.73	1.50	1.44
23	b	602	CLA	C3B-C4B	2.73	1.50	1.42
23	c	501	CLA	C4D-CHA	2.73	1.47	1.38
23	a	405[B]	CLA	C4D-CHA	2.73	1.47	1.38
23	B	609	CLA	C3B-C4B	2.73	1.50	1.42
23	b	615	CLA	C4D-CHA	2.73	1.47	1.38
23	C	512	CLA	C1C-C2C	2.72	1.50	1.44
23	B	605	CLA	C1B-NB	-2.72	1.34	1.37
23	c	506	CLA	C1B-C2B	2.72	1.49	1.43
23	b	606	CLA	C4D-CHA	2.72	1.47	1.38
23	a	404[A]	CLA	C1B-C2B	2.72	1.49	1.43
23	C	503	CLA	C4B-NB	-2.72	1.34	1.37
23	a	405[A]	CLA	C4D-CHA	2.72	1.47	1.38
23	B	610	CLA	C4D-CHA	2.72	1.47	1.38
23	d	403[A]	CLA	C1B-C2B	2.71	1.49	1.43
23	c	504	CLA	C4D-CHA	2.71	1.47	1.38
23	C	509	CLA	C1B-C2B	2.71	1.49	1.43
23	A	405[B]	CLA	C4D-CHA	2.71	1.47	1.38
23	d	402[B]	CLA	C4D-CHA	2.71	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	C4D-CHA	2.71	1.47	1.38
23	B	616	CLA	C1C-C2C	2.71	1.50	1.44
23	C	507	CLA	C4D-CHA	2.71	1.47	1.38
23	b	608	CLA	C4B-NB	-2.71	1.34	1.37
23	c	507	CLA	C1B-NB	-2.70	1.34	1.37
23	A	404[B]	CLA	C4C-C3C	2.70	1.49	1.45
23	B	601	CLA	C4B-NB	-2.70	1.34	1.37
24	a	414[A]	PHO	C3A-C2A	-2.70	1.52	1.54
23	D	403	CLA	C1B-C2B	2.70	1.49	1.43
23	b	611	CLA	C4C-C3C	2.70	1.49	1.45
23	B	609	CLA	C1C-C2C	2.70	1.50	1.44
23	B	613	CLA	C4D-CHA	2.70	1.47	1.38
23	B	610	CLA	C4B-NB	-2.69	1.34	1.37
29	D	405[B]	PL9	C6-C5	2.69	1.48	1.35
23	b	609	CLA	C1B-NB	-2.69	1.34	1.37
23	c	502	CLA	C1B-C2B	2.69	1.49	1.43
23	b	611	CLA	C4D-CHA	2.69	1.47	1.38
23	A	404[B]	CLA	C1B-C2B	2.69	1.49	1.43
23	a	405[B]	CLA	C1C-C2C	2.69	1.50	1.44
23	b	614	CLA	C3D-C4D	-2.68	1.38	1.44
23	c	503	CLA	C4D-CHA	2.68	1.47	1.38
23	B	602	CLA	C3D-C4D	-2.68	1.38	1.44
23	A	405[A]	CLA	C1B-C2B	2.68	1.49	1.43
23	B	602	CLA	C4D-CHA	2.68	1.47	1.38
23	B	606	CLA	C4D-CHA	2.68	1.47	1.38
23	b	603	CLA	C1B-C2B	2.68	1.49	1.43
34	b	625	HTG	C1-S1	-2.67	1.76	1.80
23	B	613	CLA	C1B-C2B	2.67	1.49	1.43
23	C	514	CLA	C4D-CHA	2.67	1.47	1.38
23	B	605	CLA	C4B-NB	-2.67	1.34	1.37
23	b	605	CLA	C1B-C2B	2.67	1.49	1.43
23	b	610	CLA	C4C-C3C	2.67	1.49	1.45
23	c	508	CLA	C4D-CHA	2.67	1.47	1.38
23	c	503	CLA	C3B-C4B	2.67	1.50	1.42
23	b	607	CLA	C4B-NB	-2.67	1.34	1.37
23	A	404[A]	CLA	C4D-CHA	2.66	1.47	1.38
23	c	505	CLA	C1C-C2C	2.66	1.49	1.44
23	B	605	CLA	C4D-CHA	2.66	1.47	1.38
23	B	609	CLA	C4D-CHA	2.66	1.47	1.38
23	c	502	CLA	C4D-CHA	2.66	1.47	1.38
23	c	509	CLA	C4D-CHA	2.66	1.47	1.38
23	a	404[B]	CLA	C1B-C2B	2.66	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	C1B-NB	-2.66	1.34	1.37
23	b	616	CLA	C1C-C2C	2.66	1.49	1.44
29	d	406[B]	PL9	C6-C5	2.65	1.48	1.35
23	D	403	CLA	C3B-C4B	2.65	1.50	1.42
23	c	511	CLA	C1C-C2C	2.65	1.49	1.44
23	c	505	CLA	C4D-CHA	2.65	1.47	1.38
23	b	607	CLA	OBD-CAD	2.65	1.27	1.22
23	d	403[B]	CLA	C4D-CHA	2.65	1.47	1.38
23	a	405[B]	CLA	C1B-C2B	2.64	1.49	1.43
23	C	506	CLA	C4C-C3C	2.64	1.49	1.45
23	a	404[B]	CLA	C4D-CHA	2.64	1.47	1.38
23	B	607	CLA	C1C-C2C	2.64	1.49	1.44
23	C	502	CLA	C3B-C4B	2.64	1.50	1.42
23	B	603	CLA	C1B-C2B	2.64	1.49	1.43
23	B	606	CLA	C1B-C2B	2.64	1.49	1.43
23	C	510	CLA	C4D-CHA	2.64	1.47	1.38
23	b	603	CLA	C1B-NB	-2.63	1.34	1.37
23	b	602	CLA	C4C-C3C	2.63	1.49	1.45
23	b	604	CLA	C1C-C2C	2.63	1.49	1.44
23	A	404[B]	CLA	C4D-CHA	2.63	1.47	1.38
23	C	506	CLA	C1C-C2C	2.62	1.49	1.44
23	B	612	CLA	C3B-C2B	2.62	1.50	1.41
23	B	606	CLA	C1B-NB	-2.62	1.34	1.37
23	c	504	CLA	C1C-C2C	2.62	1.49	1.44
23	a	405[A]	CLA	C1C-C2C	2.62	1.49	1.44
23	C	511	CLA	C4D-CHA	2.62	1.47	1.38
23	A	405[A]	CLA	C4B-NB	-2.62	1.34	1.37
23	b	606	CLA	C4B-NB	-2.62	1.34	1.37
23	C	513	CLA	C3B-C4B	2.61	1.50	1.42
23	B	605	CLA	C3B-C4B	2.61	1.50	1.42
23	c	510	CLA	C4B-NB	-2.61	1.34	1.37
23	A	406[B]	CLA	C4D-CHA	2.61	1.47	1.38
23	D	402[B]	CLA	C4D-CHA	2.61	1.47	1.38
23	C	503	CLA	C1C-C2C	2.61	1.49	1.44
23	B	601	CLA	C1B-C2B	2.61	1.49	1.43
23	C	509	CLA	C3B-C2B	2.61	1.50	1.41
23	b	601	CLA	C4D-CHA	2.61	1.47	1.38
23	A	405[B]	CLA	C3B-C4B	2.61	1.50	1.42
23	B	601	CLA	C3B-C4B	2.61	1.50	1.42
23	B	615	CLA	C1B-NB	-2.61	1.34	1.37
23	C	502	CLA	C1B-C2B	2.60	1.49	1.43
23	b	603	CLA	C4B-NB	-2.60	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	C1C-C2C	2.60	1.49	1.44
23	c	501	CLA	C3D-C4D	-2.60	1.38	1.44
23	B	610	CLA	C1B-C2B	2.60	1.49	1.43
23	C	513	CLA	C4D-CHA	2.60	1.47	1.38
23	b	605	CLA	C4B-NB	-2.60	1.34	1.37
23	A	408	CLA	C3D-C4D	-2.60	1.38	1.44
23	B	601	CLA	C1C-C2C	2.59	1.49	1.44
23	d	403[A]	CLA	C4C-C3C	2.59	1.49	1.45
23	C	505	CLA	C1C-C2C	2.59	1.49	1.44
34	C	522	HTG	C1'-S1	-2.59	1.77	1.81
27	a	418	GOL	C1-C2	2.59	1.61	1.51
23	C	512	CLA	C3B-C2B	2.59	1.49	1.41
23	B	607	CLA	C4B-NB	-2.59	1.34	1.37
33	C	521	LMG	O1-C1	2.58	1.44	1.40
23	B	601	CLA	C4D-CHA	2.58	1.47	1.38
23	B	616	CLA	C4D-CHA	2.58	1.47	1.38
23	c	511	CLA	C1B-NB	-2.58	1.34	1.37
23	A	405[A]	CLA	C3B-C4B	2.58	1.50	1.42
23	d	403[B]	CLA	C4C-C3C	2.58	1.49	1.45
23	b	609	CLA	C3B-C4B	2.58	1.50	1.42
23	C	509	CLA	C1B-NB	-2.58	1.34	1.37
23	b	613	CLA	C4C-C3C	2.57	1.49	1.45
23	c	505	CLA	C3B-C4B	2.57	1.50	1.42
23	b	610	CLA	C1C-C2C	2.57	1.49	1.44
23	C	509	CLA	C4D-CHA	2.57	1.47	1.38
23	a	404[A]	CLA	C4D-CHA	2.57	1.47	1.38
23	d	402[A]	CLA	C4D-CHA	2.57	1.47	1.38
23	b	605	CLA	C4D-CHA	2.57	1.47	1.38
23	c	501	CLA	C1B-C2B	2.56	1.49	1.43
24	A	407[B]	PHO	CHA-CBD	-2.56	1.48	1.51
24	A	416[B]	PHO	CHA-CBD	-2.56	1.48	1.51
23	c	513	CLA	C4D-CHA	2.56	1.47	1.38
23	B	603	CLA	C4D-CHA	2.56	1.47	1.38
23	d	404	CLA	C1B-NB	-2.55	1.34	1.37
23	A	405[B]	CLA	C1B-C2B	2.55	1.49	1.43
23	b	609	CLA	C1B-C2B	2.55	1.49	1.43
23	b	616	CLA	C4D-CHA	2.55	1.47	1.38
40	V	201	HEC	CMB-C2B	2.55	1.56	1.50
23	A	406[B]	CLA	C4B-NB	-2.55	1.34	1.37
23	b	608	CLA	C1B-C2B	2.54	1.49	1.43
25	B	619	BCR	C30-C25	-2.54	1.50	1.53
23	b	612	CLA	C4D-CHA	2.54	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	501	CLA	C4B-NB	-2.53	1.34	1.37
23	a	404[A]	CLA	C4C-C3C	2.53	1.49	1.45
23	b	603	CLA	C4D-CHA	2.53	1.47	1.38
23	C	505	CLA	C4B-NB	-2.53	1.34	1.37
27	b	624	GOL	C3-C2	2.53	1.61	1.51
23	c	510	CLA	C4C-C3C	2.53	1.49	1.45
23	C	508	CLA	C1B-C2B	2.53	1.49	1.43
24	a	406[A]	PHO	CBD-CGD	-2.52	1.49	1.52
23	c	501	CLA	C1B-NB	-2.52	1.34	1.37
23	d	404	CLA	C4D-CHA	2.52	1.47	1.38
23	a	407	CLA	C4D-CHA	2.52	1.47	1.38
23	c	512	CLA	C4B-NB	-2.52	1.34	1.37
23	A	406[A]	CLA	C3B-C4B	2.52	1.50	1.42
38	f	101	HEM	C1D-ND	-2.52	1.33	1.38
23	c	512	CLA	C1B-C2B	2.52	1.49	1.43
23	a	404[B]	CLA	C4C-C3C	2.52	1.49	1.45
23	B	616	CLA	C1B-NB	-2.52	1.34	1.37
23	a	405[A]	CLA	C4B-NB	-2.52	1.34	1.37
34	b	622	HTG	O5-C1	2.51	1.46	1.42
23	c	503	CLA	C3D-C4D	-2.51	1.38	1.44
29	d	406[A]	PL9	C6-C5	2.51	1.47	1.35
23	b	603	CLA	C1C-C2C	2.51	1.49	1.44
23	c	512	CLA	C3B-C4B	2.50	1.50	1.42
23	B	608	CLA	C3B-C2B	2.50	1.49	1.41
23	A	406[A]	CLA	C1B-C2B	2.50	1.49	1.43
23	b	607	CLA	C1C-C2C	2.50	1.49	1.44
38	E	102	HEM	C1C-C2C	-2.50	1.40	1.45
23	c	506	CLA	C4D-CHA	2.50	1.47	1.38
23	d	404	CLA	C3B-C4B	2.50	1.50	1.42
23	B	609	CLA	C1B-C2B	2.50	1.49	1.43
23	b	606	CLA	C3D-C4D	-2.49	1.38	1.44
23	C	504	CLA	C4D-CHA	2.49	1.47	1.38
29	D	405[A]	PL9	C6-C5	2.49	1.47	1.35
23	C	502	CLA	C1C-C2C	2.49	1.49	1.44
24	A	416[A]	PHO	C3A-C2A	-2.49	1.52	1.54
23	B	602	CLA	C4C-C3C	2.49	1.49	1.45
23	c	506	CLA	C4C-C3C	2.48	1.49	1.45
23	C	511	CLA	C3D-C4D	-2.48	1.38	1.44
23	c	513	CLA	C1C-C2C	2.48	1.49	1.44
31	B	628	LMT	C3'-C2'	2.47	1.58	1.52
35	c	518	DGD	O2G-C2G	-2.47	1.40	1.46
23	B	611	CLA	C3D-C4D	-2.47	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	408	CLA	C4B-NB	-2.47	1.34	1.37
24	a	406[B]	PHO	C4B-NB	-2.47	1.34	1.38
23	b	601	CLA	C3B-C4B	2.47	1.49	1.42
23	B	616	CLA	C3B-C2B	2.47	1.49	1.41
23	B	612	CLA	C4C-C3C	2.47	1.49	1.45
23	d	403[A]	CLA	C4D-CHA	2.47	1.46	1.38
23	b	603	CLA	C3B-C4B	2.47	1.49	1.42
23	b	616	CLA	C3B-C4B	2.46	1.49	1.42
23	a	405[B]	CLA	C3B-C4B	2.46	1.49	1.42
24	A	416[A]	PHO	C3D-C4D	-2.46	1.37	1.41
23	B	610	CLA	C3B-C4B	2.46	1.49	1.42
23	d	404	CLA	C1B-C2B	2.46	1.48	1.43
31	t	101	LMT	O3'-C3'	-2.46	1.36	1.43
23	a	405[A]	CLA	C3B-C4B	2.46	1.49	1.42
23	a	405[A]	CLA	C3D-C4D	-2.46	1.38	1.44
23	C	511	CLA	C1C-C2C	2.45	1.49	1.44
23	b	602	CLA	C3D-C4D	-2.45	1.38	1.44
23	C	510	CLA	C1C-C2C	2.45	1.49	1.44
23	c	504	CLA	C4C-C3C	2.44	1.49	1.45
23	c	513	CLA	C4C-C3C	2.44	1.49	1.45
23	C	504	CLA	C1B-C2B	2.44	1.48	1.43
23	b	608	CLA	C3B-C2B	2.44	1.49	1.41
23	b	602	CLA	C4D-CHA	2.44	1.46	1.38
24	A	407[B]	PHO	CBD-CGD	-2.44	1.49	1.52
23	C	508	CLA	C1C-C2C	2.44	1.49	1.44
23	c	511	CLA	C4B-NB	-2.44	1.34	1.37
23	B	610	CLA	C3D-C4D	-2.44	1.38	1.44
31	M	101	LMT	O2B-C2B	-2.43	1.36	1.43
23	C	503	CLA	C4D-CHA	2.43	1.46	1.38
23	b	613	CLA	C1C-C2C	2.43	1.49	1.44
23	D	402[B]	CLA	C3D-C4D	-2.43	1.38	1.44
23	C	513	CLA	C3D-C4D	-2.43	1.38	1.44
23	b	603	CLA	C3B-C2B	2.43	1.49	1.41
23	c	509	CLA	C4C-C3C	2.42	1.49	1.45
23	C	512	CLA	C4C-C3C	2.42	1.49	1.45
23	d	402[B]	CLA	C4B-NB	-2.42	1.34	1.37
23	c	502	CLA	C3B-C2B	2.42	1.49	1.41
23	d	402[B]	CLA	C3B-C4B	2.42	1.49	1.42
23	b	614	CLA	C4D-CHA	2.42	1.46	1.38
23	b	611	CLA	C1C-C2C	2.42	1.49	1.44
23	b	615	CLA	C4C-C3C	2.42	1.49	1.45
23	B	610	CLA	C4C-C3C	2.42	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	C3D-C4D	-2.41	1.38	1.44
23	B	603	CLA	C3B-C2B	2.41	1.49	1.41
23	b	606	CLA	C1C-C2C	2.41	1.49	1.44
23	c	508	CLA	C4B-NB	-2.41	1.34	1.37
23	C	504	CLA	C3B-C4B	2.41	1.49	1.42
23	b	601	CLA	C4C-C3C	2.41	1.49	1.45
23	C	510	CLA	C3B-C2B	2.41	1.49	1.41
23	D	402[A]	CLA	C3D-C4D	-2.41	1.38	1.44
23	B	615	CLA	C3B-C4B	2.41	1.49	1.42
23	C	506	CLA	C4B-NB	-2.40	1.34	1.37
23	C	508	CLA	C1B-NB	-2.40	1.34	1.37
23	b	610	CLA	C3B-C4B	2.40	1.49	1.42
23	A	404[A]	CLA	C1C-C2C	2.40	1.49	1.44
23	A	406[B]	CLA	C1C-C2C	2.40	1.49	1.44
23	D	402[B]	CLA	C4C-C3C	2.40	1.49	1.45
23	c	504	CLA	C3B-C2B	2.40	1.49	1.41
23	b	601	CLA	C1C-C2C	2.40	1.49	1.44
23	A	408	CLA	C3B-C2B	2.40	1.49	1.41
25	d	405	BCR	C30-C25	-2.40	1.50	1.53
31	A	420	LMT	O3'-C3'	-2.39	1.37	1.43
23	A	406[B]	CLA	C1B-C2B	2.39	1.48	1.43
23	d	402[A]	CLA	C3B-C4B	2.38	1.49	1.42
23	c	511	CLA	C3B-C2B	2.38	1.49	1.41
23	B	608	CLA	C1C-NC	-2.38	1.34	1.37
23	C	510	CLA	C4C-C3C	2.38	1.49	1.45
23	B	613	CLA	C3B-C2B	2.38	1.49	1.41
23	B	606	CLA	C3D-C4D	-2.38	1.38	1.44
23	C	506	CLA	C3B-C4B	2.38	1.49	1.42
23	b	610	CLA	C3D-C4D	-2.38	1.38	1.44
31	m	103	LMT	C3'-C2'	2.37	1.58	1.52
23	b	615	CLA	C3D-C4D	-2.37	1.38	1.44
23	A	405[B]	CLA	C4B-NB	-2.37	1.34	1.37
23	d	404	CLA	C4B-NB	-2.37	1.34	1.37
23	C	511	CLA	C4C-C3C	2.37	1.49	1.45
23	C	507	CLA	C3D-C4D	-2.37	1.38	1.44
31	b	621	LMT	C3'-C2'	2.37	1.58	1.52
24	a	414[B]	PHO	C3A-C2A	-2.37	1.52	1.54
23	C	514	CLA	C1C-C2C	2.37	1.49	1.44
23	b	606	CLA	C3B-C4B	2.36	1.49	1.42
23	b	612	CLA	C3B-C4B	2.36	1.49	1.42
23	c	512	CLA	C1C-C2C	2.36	1.49	1.44
23	B	608	CLA	C3D-C4D	-2.36	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	C1B-C2B	2.36	1.48	1.43
23	b	607	CLA	C4C-C3C	2.36	1.49	1.45
23	A	405[A]	CLA	C3D-C4D	-2.36	1.38	1.44
23	B	607	CLA	C3B-C2B	2.35	1.49	1.41
23	C	504	CLA	C1C-C2C	2.35	1.49	1.44
31	e	101	LMT	O3'-C3'	-2.35	1.37	1.43
23	C	502	CLA	C3D-C4D	-2.35	1.38	1.44
23	A	406[B]	CLA	C4C-C3C	2.35	1.49	1.45
24	A	416[A]	PHO	C4B-NB	-2.35	1.34	1.38
23	B	609	CLA	C3D-C4D	-2.35	1.38	1.44
24	A	416[B]	PHO	C4B-NB	-2.35	1.34	1.38
23	C	503	CLA	C3B-C2B	2.35	1.49	1.41
23	C	514	CLA	C3B-C2B	2.34	1.49	1.41
23	B	604	CLA	C3D-C4D	-2.34	1.38	1.44
23	a	404[A]	CLA	C3B-C2B	2.34	1.49	1.41
23	A	404[A]	CLA	C3B-C2B	2.34	1.49	1.41
23	b	601	CLA	C3B-C2B	2.34	1.49	1.41
23	c	507	CLA	C3D-C4D	-2.33	1.38	1.44
23	B	602	CLA	C4B-NB	-2.33	1.34	1.37
26	F	102	SQD	O6-C1	2.33	1.44	1.40
23	B	608	CLA	C4C-C3C	2.33	1.49	1.45
23	C	508	CLA	C4C-C3C	2.33	1.49	1.45
23	C	514	CLA	C3D-C4D	-2.33	1.39	1.44
23	D	403	CLA	C4D-CHA	2.33	1.46	1.38
23	c	501	CLA	C3B-C4B	2.32	1.49	1.42
23	b	609	CLA	C1C-NC	-2.32	1.34	1.37
23	B	605	CLA	C1C-C2C	2.32	1.49	1.44
23	d	403[B]	CLA	C3D-C4D	-2.32	1.39	1.44
23	A	405[A]	CLA	C1C-C2C	2.32	1.49	1.44
23	A	406[A]	CLA	C1C-C2C	2.32	1.49	1.44
23	B	604	CLA	C4C-C3C	2.32	1.49	1.45
23	d	403[A]	CLA	C3D-C4D	-2.32	1.39	1.44
23	C	503	CLA	C3D-C4D	-2.32	1.39	1.44
23	b	602	CLA	C1B-C2B	2.31	1.48	1.43
23	C	505	CLA	C3D-C4D	-2.31	1.39	1.44
23	b	614	CLA	C1C-C2C	2.31	1.49	1.44
23	C	510	CLA	C3B-C4B	2.31	1.49	1.42
23	a	404[B]	CLA	C3B-C2B	2.31	1.49	1.41
29	D	405[B]	PL9	C2-C3	2.31	1.40	1.34
23	c	501	CLA	C4C-C3C	2.31	1.49	1.45
23	b	609	CLA	C1C-C2C	2.31	1.49	1.44
23	a	407	CLA	C3B-C4B	2.31	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	C1B-NB	-2.31	1.34	1.37
23	d	403[B]	CLA	C1C-C2C	2.31	1.49	1.44
23	b	609	CLA	C4B-NB	-2.31	1.34	1.37
23	b	604	CLA	C3B-C2B	2.30	1.48	1.41
38	f	101	HEM	C1C-C2C	-2.30	1.40	1.45
23	B	610	CLA	C1C-C2C	2.30	1.49	1.44
23	C	504	CLA	C3D-C4D	-2.30	1.39	1.44
23	b	607	CLA	C3D-C4D	-2.30	1.39	1.44
23	C	513	CLA	C4B-NB	-2.30	1.34	1.37
29	a	412[A]	PL9	C2-C3	2.30	1.40	1.34
23	b	616	CLA	C3B-C2B	2.30	1.48	1.41
23	C	505	CLA	C3B-C2B	2.30	1.48	1.41
23	c	504	CLA	C1C-NC	-2.29	1.34	1.37
23	B	603	CLA	C4C-C3C	2.29	1.48	1.45
40	v	201	HEC	CMD-C2D	2.29	1.55	1.50
23	A	404[B]	CLA	C3B-C2B	2.29	1.48	1.41
23	b	612	CLA	C3B-C2B	2.29	1.48	1.41
31	B	628	LMT	O3'-C3'	-2.29	1.37	1.43
23	B	616	CLA	C1C-NC	-2.29	1.34	1.37
23	c	508	CLA	C1B-NB	-2.28	1.34	1.37
24	A	416[A]	PHO	C1D-ND	-2.28	1.34	1.38
23	b	616	CLA	C3D-C4D	-2.28	1.39	1.44
23	b	610	CLA	C3B-C2B	2.28	1.48	1.41
23	B	606	CLA	C3B-C4B	2.28	1.49	1.42
24	a	414[B]	PHO	C1B-NB	-2.28	1.34	1.38
23	A	404[B]	CLA	C3D-C4D	-2.28	1.39	1.44
23	B	613	CLA	C4C-C3C	2.28	1.48	1.45
31	m	103	LMT	O2B-C2B	-2.27	1.37	1.43
31	F	101	LMT	O3'-C3'	-2.27	1.37	1.43
23	c	513	CLA	C3B-C4B	2.27	1.49	1.42
23	C	504	CLA	C4B-NB	-2.27	1.34	1.37
23	C	502	CLA	C4C-C3C	2.27	1.48	1.45
31	B	630	LMT	O2'-C2'	-2.27	1.37	1.43
23	c	513	CLA	C3D-C4D	-2.27	1.39	1.44
23	C	507	CLA	C1C-C2C	2.27	1.49	1.44
23	B	604	CLA	C4B-NB	-2.27	1.34	1.37
23	b	609	CLA	C3D-C4D	-2.27	1.39	1.44
31	B	630	LMT	O2B-C2B	-2.27	1.37	1.43
23	c	511	CLA	C4C-C3C	2.26	1.48	1.45
31	A	420	LMT	O2'-C2'	-2.26	1.37	1.43
23	b	606	CLA	C1B-C2B	2.26	1.48	1.43
27	D	412	GOL	O2-C2	-2.26	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	C4B-NB	-2.26	1.34	1.37
23	D	402[B]	CLA	C1C-C2C	2.26	1.49	1.44
23	c	510	CLA	C3D-C4D	-2.26	1.39	1.44
31	T	101	LMT	O3'-C3'	-2.26	1.37	1.43
23	c	512	CLA	C4C-C3C	2.26	1.48	1.45
23	B	614	CLA	C4C-C3C	2.26	1.48	1.45
23	A	406[A]	CLA	C3D-C4D	-2.26	1.39	1.44
24	a	406[B]	PHO	CBD-CGD	-2.26	1.49	1.52
23	c	506	CLA	C3B-C4B	2.26	1.49	1.42
23	b	612	CLA	C3D-C4D	-2.26	1.39	1.44
35	C	518[A]	DGD	O5D-C1E	2.26	1.44	1.40
27	A	418	GOL	C3-C2	2.25	1.60	1.51
23	c	508	CLA	C3B-C4B	2.25	1.49	1.42
23	A	404[B]	CLA	C1C-C2C	2.25	1.49	1.44
31	a	416	LMT	O3'-C3'	-2.25	1.37	1.43
31	B	631	LMT	O3'-C3'	-2.25	1.37	1.43
23	c	512	CLA	C3D-C4D	-2.25	1.39	1.44
23	C	506	CLA	C3D-C4D	-2.25	1.39	1.44
31	M	101	LMT	O3'-C3'	-2.24	1.37	1.43
23	b	614	CLA	C3B-C4B	2.24	1.49	1.42
23	c	504	CLA	C3D-C4D	-2.24	1.39	1.44
23	D	402[A]	CLA	C4C-C3C	2.24	1.48	1.45
23	b	605	CLA	C3D-C4D	-2.24	1.39	1.44
23	b	604	CLA	C3B-C4B	2.24	1.49	1.42
23	a	407	CLA	C4C-C3C	2.23	1.48	1.45
23	b	610	CLA	C4B-NB	-2.23	1.34	1.37
23	b	605	CLA	C1C-C2C	2.23	1.49	1.44
23	C	507	CLA	C3B-C2B	2.23	1.48	1.41
23	C	512	CLA	C3B-C4B	2.23	1.49	1.42
31	M	101	LMT	O2'-C2'	-2.23	1.37	1.43
24	a	406[A]	PHO	C4B-NB	-2.22	1.34	1.38
23	B	603	CLA	C1C-C2C	2.22	1.49	1.44
23	a	407	CLA	C3B-C2B	2.22	1.48	1.41
23	c	508	CLA	C3B-C2B	2.22	1.48	1.41
23	C	505	CLA	C4C-C3C	2.22	1.48	1.45
31	A	417	LMT	O2'-C2'	-2.22	1.37	1.43
23	c	510	CLA	C3B-C2B	2.22	1.48	1.41
23	d	403[A]	CLA	C1C-C2C	2.22	1.49	1.44
35	h	102	DGD	O5D-C1E	2.22	1.43	1.40
34	B	623	HTG	C1'-S1	-2.22	1.78	1.81
31	t	101	LMT	O2'-C2'	-2.22	1.37	1.43
23	B	615	CLA	C4B-NB	-2.21	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	414[A]	PHO	C4B-NB	-2.21	1.34	1.38
23	c	511	CLA	MG-NA	2.21	2.11	2.06
23	D	402[B]	CLA	C3B-C2B	2.21	1.48	1.41
29	a	412[B]	PL9	C2-C3	2.21	1.40	1.34
27	D	412	GOL	C3-C2	2.21	1.60	1.51
23	b	611	CLA	C3B-C2B	2.21	1.48	1.41
23	C	512	CLA	C3D-C4D	-2.21	1.39	1.44
23	D	402[A]	CLA	C3B-C2B	2.21	1.48	1.41
23	b	615	CLA	C4B-NB	-2.21	1.35	1.37
24	A	407[A]	PHO	C4B-NB	-2.21	1.34	1.38
23	b	613	CLA	C3B-C2B	2.21	1.48	1.41
34	B	625	HTG	C1-S1	-2.21	1.77	1.80
29	A	414[A]	PL9	C2-C1	-2.21	1.39	1.44
23	c	506	CLA	C3B-C2B	2.20	1.48	1.41
23	A	408	CLA	C4C-C3C	2.20	1.48	1.45
23	C	507	CLA	C1D-C2D	2.20	1.49	1.45
23	C	511	CLA	C3B-C2B	2.20	1.48	1.41
24	A	407[B]	PHO	C4B-NB	-2.20	1.34	1.38
23	b	614	CLA	C3B-C2B	2.19	1.48	1.41
27	o	303	GOL	C1-C2	2.19	1.60	1.51
23	C	503	CLA	C4C-C3C	2.19	1.48	1.45
23	B	602	CLA	C3B-C2B	2.19	1.48	1.41
23	C	504	CLA	C4C-C3C	2.19	1.48	1.45
23	c	506	CLA	C3D-C4D	-2.19	1.39	1.44
23	B	615	CLA	MG-NA	2.19	2.11	2.06
24	a	414[B]	PHO	CHA-CBD	-2.19	1.49	1.51
24	a	406[B]	PHO	C1B-NB	-2.19	1.34	1.38
23	b	608	CLA	C3B-C4B	2.18	1.49	1.42
23	a	405[B]	CLA	C3D-C4D	-2.18	1.39	1.44
23	C	502	CLA	C4B-NB	-2.18	1.35	1.37
31	B	628	LMT	O5'-C5'	-2.18	1.39	1.44
23	b	607	CLA	C3B-C2B	2.18	1.48	1.41
24	A	407[A]	PHO	C1B-NB	-2.18	1.34	1.38
23	c	503	CLA	C4C-C3C	2.17	1.48	1.45
24	a	414[A]	PHO	CBD-CGD	-2.17	1.49	1.52
23	B	616	CLA	C3B-C4B	2.17	1.49	1.42
23	b	611	CLA	C3D-C4D	-2.17	1.39	1.44
23	a	404[A]	CLA	C1C-C2C	2.17	1.48	1.44
24	a	414[B]	PHO	C4B-NB	-2.17	1.34	1.38
23	B	601	CLA	C3D-C4D	-2.17	1.39	1.44
23	B	602	CLA	C3B-C4B	2.17	1.49	1.42
23	C	512	CLA	C1B-NB	-2.16	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	C4C-C3C	2.16	1.48	1.45
23	b	613	CLA	C3B-C4B	2.16	1.49	1.42
23	d	402[B]	CLA	C1C-NC	-2.16	1.34	1.37
23	B	601	CLA	C3B-C2B	2.16	1.48	1.41
23	c	509	CLA	C3B-C2B	2.16	1.48	1.41
32	b	629[A]	LHG	O7-C5	-2.16	1.41	1.46
23	B	614	CLA	C1C-C2C	2.15	1.48	1.44
23	B	604	CLA	C3B-C2B	2.15	1.48	1.41
23	B	612	CLA	C3D-C4D	-2.15	1.39	1.44
24	A	407[A]	PHO	C1D-ND	-2.14	1.34	1.38
31	m	103	LMT	O3'-C3'	-2.14	1.37	1.43
23	b	605	CLA	C3B-C4B	2.14	1.49	1.42
27	V	203[A]	GOL	C1-C2	2.14	1.59	1.51
23	A	408	CLA	C1C-C2C	2.14	1.48	1.44
26	a	410	SQD	O6-C1	2.14	1.43	1.40
23	c	510	CLA	C3B-C4B	2.14	1.49	1.42
29	D	405[A]	PL9	C2-C3	2.14	1.40	1.34
23	a	405[B]	CLA	C4C-C3C	2.13	1.48	1.45
31	B	630	LMT	O3'-C3'	-2.13	1.37	1.43
23	b	601	CLA	C1B-C2B	2.13	1.48	1.43
23	B	605	CLA	C4C-C3C	2.13	1.48	1.45
23	d	402[B]	CLA	C3D-C4D	-2.13	1.39	1.44
23	b	608	CLA	C1C-C2C	2.12	1.48	1.44
31	A	417	LMT	O3'-C3'	-2.12	1.37	1.43
23	B	616	CLA	C3D-C4D	-2.12	1.39	1.44
23	d	404	CLA	C3D-C4D	-2.12	1.39	1.44
23	B	607	CLA	C3D-C4D	-2.12	1.39	1.44
23	c	513	CLA	C3B-C2B	2.12	1.48	1.41
23	d	402[A]	CLA	C4B-NB	-2.12	1.35	1.37
23	B	606	CLA	C4C-C3C	2.12	1.48	1.45
23	B	604	CLA	C3B-C4B	2.12	1.48	1.42
23	C	503	CLA	C3B-C4B	2.12	1.48	1.42
23	B	604	CLA	C1A-CHA	2.12	1.51	1.43
29	A	414[B]	PL9	C2-C3	2.12	1.39	1.34
23	a	405[A]	CLA	C4C-C3C	2.12	1.48	1.45
23	c	511	CLA	C3B-C4B	2.11	1.48	1.42
24	a	414[A]	PHO	C1B-NB	-2.11	1.34	1.38
23	d	403[B]	CLA	C3B-C2B	2.11	1.48	1.41
23	A	405[B]	CLA	C3D-C4D	-2.11	1.39	1.44
23	c	504	CLA	C3B-C4B	2.10	1.48	1.42
23	B	613	CLA	C1C-C2C	2.10	1.48	1.44
23	D	403	CLA	C4B-NB	-2.10	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	C3B-C2B	2.10	1.48	1.41
25	y	101	BCR	C30-C25	-2.10	1.51	1.53
34	B	622	HTG	O5-C1	2.10	1.45	1.42
23	A	404[B]	CLA	C3B-C4B	2.10	1.48	1.42
24	a	406[B]	PHO	C3A-C2A	-2.10	1.52	1.54
35	c	517[A]	DGD	O2G-C2G	-2.10	1.41	1.46
23	B	601	CLA	C4C-C3C	2.09	1.48	1.45
32	L	101[B]	LHG	O7-C5	-2.09	1.41	1.46
23	B	614	CLA	C3B-C4B	2.09	1.48	1.42
26	B	620	SQD	O6-C1	2.09	1.43	1.40
27	v	202[A]	GOL	C3-C2	2.09	1.59	1.51
23	d	404	CLA	C3B-C2B	2.09	1.48	1.41
23	a	404[B]	CLA	C3D-C4D	-2.09	1.39	1.44
23	d	403[A]	CLA	C3B-C2B	2.09	1.48	1.41
23	B	615	CLA	C3D-C4D	-2.09	1.39	1.44
38	E	102	HEM	C3C-C4C	-2.08	1.42	1.46
23	A	406[B]	CLA	C3D-C4D	-2.07	1.39	1.44
23	a	404[A]	CLA	C3B-C4B	2.07	1.48	1.42
23	B	609	CLA	C4C-C3C	2.07	1.48	1.45
23	C	509	CLA	C1C-C2C	2.07	1.48	1.44
23	c	508	CLA	C3D-C4D	-2.07	1.39	1.44
23	b	615	CLA	C3B-C4B	2.07	1.48	1.42
23	C	502	CLA	C3B-C2B	2.07	1.48	1.41
23	C	508	CLA	C3D-C4D	-2.07	1.39	1.44
23	c	506	CLA	C1C-C2C	2.07	1.48	1.44
23	B	604	CLA	C1C-C2C	2.07	1.48	1.44
23	B	608	CLA	C3B-C4B	2.06	1.48	1.42
31	T	101	LMT	O3B-C3B	-2.06	1.37	1.43
24	a	406[B]	PHO	C1D-ND	-2.06	1.34	1.38
23	B	607	CLA	C4C-C3C	2.06	1.48	1.45
29	A	414[B]	PL9	C2-C1	-2.06	1.39	1.44
23	c	505	CLA	C3D-C4D	-2.06	1.39	1.44
23	A	408	CLA	C3B-C4B	2.06	1.48	1.42
23	c	501	CLA	C1C-NC	-2.05	1.34	1.37
23	C	513	CLA	C3B-C2B	2.05	1.48	1.41
35	h	102	DGD	O2G-C2G	-2.05	1.41	1.46
23	B	606	CLA	C3B-C2B	2.05	1.48	1.41
23	b	601	CLA	C1D-C2D	2.05	1.49	1.45
23	b	614	CLA	C4C-C3C	2.04	1.48	1.45
23	d	402[A]	CLA	C1C-C2C	2.04	1.48	1.44
23	b	606	CLA	C3B-C2B	2.04	1.48	1.41
40	v	201	HEC	C3B-C2B	-2.04	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	C3B-C2B	2.04	1.48	1.41
23	b	611	CLA	C3B-C4B	2.04	1.48	1.42
23	b	612	CLA	C4C-C3C	2.03	1.48	1.45
23	A	404[A]	CLA	C3D-C4D	-2.03	1.39	1.44
31	e	101	LMT	O2'-C2'	-2.03	1.37	1.43
32	D	406[A]	LHG	O7-C5	-2.03	1.41	1.46
23	C	514	CLA	C1C-NC	-2.03	1.34	1.37
23	b	604	CLA	C4C-C3C	2.03	1.48	1.45
23	B	613	CLA	C1A-CHA	2.02	1.51	1.43
31	B	628	LMT	O4'-C4B	-2.02	1.37	1.43
23	B	614	CLA	C3B-C2B	2.02	1.48	1.41
40	V	201	HEC	CMD-C2D	2.02	1.54	1.50
23	B	604	CLA	MG-NA	2.02	2.11	2.06
23	a	405[B]	CLA	C3B-C2B	2.02	1.48	1.41
23	b	607	CLA	CBD-CAD	-2.02	1.47	1.56
23	b	604	CLA	C1A-CHA	2.02	1.51	1.43
29	A	414[A]	PL9	C2-C3	2.02	1.39	1.34
23	B	603	CLA	C3D-C4D	-2.02	1.39	1.44
23	C	513	CLA	C4C-C3C	2.01	1.48	1.45
23	C	508	CLA	C3B-C2B	2.01	1.47	1.41
31	M	101	LMT	O1'-C1'	-2.01	1.36	1.40
38	E	102	HEM	C3B-C4B	2.01	1.48	1.44
23	b	616	CLA	C1C-NC	-2.01	1.34	1.37
31	B	631	LMT	O2'-C2'	-2.01	1.38	1.43
40	V	201	HEC	CMC-C2C	2.01	1.54	1.50
31	e	101	LMT	O2B-C2B	-2.01	1.38	1.43
23	C	511	CLA	C3B-C4B	2.01	1.48	1.42
23	C	514	CLA	C3B-C4B	2.01	1.48	1.42
23	B	603	CLA	C3B-C4B	2.00	1.48	1.42
23	C	507	CLA	C3B-C4B	2.00	1.48	1.42

All (3416) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C3B-C2B-C1B	-13.94	90.73	107.17
24	a	414[A]	PHO	C2D-C1D-ND	11.51	117.75	109.43
23	a	407	CLA	C1D-ND-C4D	-11.46	98.27	106.31
24	A	407[B]	PHO	C2D-C1D-ND	11.33	117.62	109.43
23	B	611	CLA	C1D-ND-C4D	-11.27	98.40	106.31
23	B	611	CLA	C2B-C1B-NB	11.11	121.85	110.33
24	A	407[A]	PHO	C2D-C1D-ND	11.05	117.42	109.43
24	a	406[A]	PHO	C2D-C1D-ND	10.84	117.26	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	414[B]	PHO	C2D-C1D-ND	10.79	117.23	109.43
23	B	612	CLA	C1D-ND-C4D	-10.69	98.81	106.31
24	A	416[B]	PHO	C2D-C1D-ND	10.69	117.16	109.43
24	a	406[B]	PHO	C2D-C1D-ND	10.53	117.04	109.43
23	C	504	CLA	C1D-ND-C4D	-10.42	99.00	106.31
24	A	416[A]	PHO	C2D-C1D-ND	10.38	116.93	109.43
40	v	201	HEC	CBB-CAB-C3B	-10.17	107.10	127.43
23	b	605	CLA	C1D-ND-C4D	-10.16	99.18	106.31
23	b	603	CLA	C1D-ND-C4D	-10.12	99.21	106.31
23	A	406[B]	CLA	C1D-ND-C4D	-10.07	99.25	106.31
23	a	405[B]	CLA	C1D-ND-C4D	-9.95	99.33	106.31
23	c	503	CLA	C1D-ND-C4D	-9.94	99.34	106.31
23	d	404	CLA	C1D-ND-C4D	-9.92	99.35	106.31
23	c	511	CLA	C1D-ND-C4D	-9.83	99.41	106.31
23	a	405[A]	CLA	C1D-ND-C4D	-9.78	99.45	106.31
23	B	606	CLA	C1D-ND-C4D	-9.75	99.47	106.31
23	B	607	CLA	C1D-ND-C4D	-9.72	99.49	106.31
23	B	601	CLA	C1D-ND-C4D	-9.70	99.51	106.31
23	C	514	CLA	C1D-ND-C4D	-9.68	99.52	106.31
23	d	403[B]	CLA	C1D-ND-C4D	-9.67	99.53	106.31
23	C	511	CLA	C1D-ND-C4D	-9.58	99.59	106.31
23	B	609	CLA	C1D-ND-C4D	-9.57	99.59	106.31
23	c	509	CLA	C1D-ND-C4D	-9.53	99.62	106.31
23	B	605	CLA	C1D-ND-C4D	-9.52	99.63	106.31
23	c	501	CLA	C1D-ND-C4D	-9.50	99.64	106.31
23	A	406[A]	CLA	C1D-ND-C4D	-9.49	99.65	106.31
23	B	616	CLA	C1D-ND-C4D	-9.45	99.68	106.31
23	a	404[B]	CLA	C1D-ND-C4D	-9.45	99.68	106.31
23	b	611	CLA	C1D-ND-C4D	-9.44	99.69	106.31
23	B	603	CLA	C1D-ND-C4D	-9.43	99.70	106.31
23	c	513	CLA	C1D-ND-C4D	-9.43	99.70	106.31
23	b	615	CLA	C1D-ND-C4D	-9.36	99.75	106.31
23	B	614	CLA	C1D-ND-C4D	-9.32	99.77	106.31
23	C	502	CLA	C1D-ND-C4D	-9.32	99.77	106.31
23	b	612	CLA	C1D-ND-C4D	-9.31	99.78	106.31
23	b	609	CLA	C1D-ND-C4D	-9.28	99.80	106.31
23	B	610	CLA	C1D-ND-C4D	-9.26	99.82	106.31
23	A	405[B]	CLA	C1D-ND-C4D	-9.25	99.82	106.31
23	B	615	CLA	C1D-ND-C4D	-9.23	99.83	106.31
23	D	402[A]	CLA	C1D-ND-C4D	-9.22	99.84	106.31
23	A	408	CLA	C1D-ND-C4D	-9.20	99.86	106.31
23	b	614	CLA	C1D-ND-C4D	-9.19	99.86	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	C1D-ND-C4D	-9.19	99.87	106.31
23	c	505	CLA	C1D-ND-C4D	-9.18	99.87	106.31
23	c	504	CLA	C1D-ND-C4D	-9.17	99.88	106.31
23	b	616	CLA	C1D-ND-C4D	-9.15	99.89	106.31
24	a	406[B]	PHO	O2D-CGD-CBD	9.14	121.00	110.95
23	A	405[A]	CLA	C1D-ND-C4D	-9.14	99.90	106.31
23	d	403[A]	CLA	C1D-ND-C4D	-9.11	99.92	106.31
23	b	608	CLA	C1D-ND-C4D	-9.07	99.95	106.31
23	C	506	CLA	C1D-ND-C4D	-9.07	99.95	106.31
23	D	402[B]	CLA	C1D-ND-C4D	-9.06	99.95	106.31
23	b	602	CLA	C1D-ND-C4D	-9.06	99.95	106.31
23	a	404[A]	CLA	C1D-ND-C4D	-9.05	99.96	106.31
23	B	608	CLA	C1D-ND-C4D	-8.98	100.01	106.31
23	c	506	CLA	C1D-ND-C4D	-8.94	100.04	106.31
23	C	505	CLA	C1D-ND-C4D	-8.93	100.05	106.31
23	C	509	CLA	C1D-ND-C4D	-8.92	100.06	106.31
23	c	502	CLA	C1D-ND-C4D	-8.91	100.06	106.31
24	A	407[B]	PHO	O2D-CGD-CBD	8.90	120.73	110.95
23	c	507	CLA	C1D-ND-C4D	-8.87	100.08	106.31
23	b	610	CLA	C1D-ND-C4D	-8.86	100.09	106.31
23	b	606	CLA	C1D-ND-C4D	-8.85	100.10	106.31
23	B	613	CLA	C1D-ND-C4D	-8.80	100.14	106.31
23	b	601	CLA	C1D-ND-C4D	-8.79	100.15	106.31
23	b	607	CLA	C1D-ND-C4D	-8.79	100.15	106.31
23	D	403	CLA	C1D-ND-C4D	-8.78	100.15	106.31
23	C	513	CLA	C1D-ND-C4D	-8.77	100.16	106.31
23	B	602	CLA	C1D-ND-C4D	-8.77	100.16	106.31
23	d	402[B]	CLA	C1D-ND-C4D	-8.76	100.17	106.31
23	c	512	CLA	C1D-ND-C4D	-8.75	100.17	106.31
23	d	402[A]	CLA	C1D-ND-C4D	-8.74	100.18	106.31
23	A	404[B]	CLA	C1D-ND-C4D	-8.73	100.19	106.31
23	c	508	CLA	C1D-ND-C4D	-8.72	100.20	106.31
23	C	512	CLA	C1D-ND-C4D	-8.71	100.20	106.31
23	C	507	CLA	C1D-ND-C4D	-8.71	100.20	106.31
23	C	508	CLA	C1D-ND-C4D	-8.68	100.22	106.31
24	A	407[B]	PHO	C3B-C4B-NB	8.64	113.10	107.46
24	A	416[A]	PHO	O2D-CGD-CBD	8.55	120.34	110.95
40	V	201	HEC	CBB-CAB-C3B	-8.54	110.36	127.43
23	C	503	CLA	C1D-ND-C4D	-8.50	100.35	106.31
23	b	613	CLA	C1D-ND-C4D	-8.38	100.43	106.31
24	a	414[A]	PHO	O2D-CGD-CBD	8.36	120.13	110.95
24	a	406[A]	PHO	O2D-CGD-CBD	8.30	120.07	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	C1D-ND-C4D	-8.23	100.53	106.31
24	A	407[A]	PHO	C3B-C4B-NB	8.22	112.82	107.46
24	A	416[B]	PHO	O2D-CGD-CBD	8.21	119.97	110.95
24	a	414[B]	PHO	O2D-CGD-CBD	8.17	119.92	110.95
23	c	510	CLA	C1D-ND-C4D	-8.11	100.62	106.31
24	A	407[A]	PHO	O2D-CGD-CBD	8.01	119.75	110.95
24	a	406[A]	PHO	C3B-C4B-NB	8.00	112.68	107.46
23	b	602	CLA	C4A-NA-C1A	-7.96	103.05	106.68
23	a	407	CLA	C2D-C1D-ND	7.95	117.99	110.13
24	a	414[B]	PHO	C3B-C4B-NB	7.86	112.58	107.46
23	A	404[A]	CLA	C1D-ND-C4D	-7.76	100.87	106.31
23	B	604	CLA	C1D-ND-C4D	-7.74	100.88	106.31
23	C	511	CLA	CMD-C2D-C1D	7.73	138.34	124.73
23	B	611	CLA	CMB-C2B-C1B	7.72	137.18	125.42
24	a	414[A]	PHO	C3B-C4B-NB	7.69	112.47	107.46
23	B	616	CLA	O2D-CGD-CBD	7.62	124.55	111.23
23	B	611	CLA	CHD-C4C-C3C	-7.56	113.74	124.77
26	F	102	SQD	O6-C1-C2	7.49	119.65	108.27
23	c	501	CLA	CMD-C2D-C1D	7.47	137.88	124.73
23	B	611	CLA	CHB-C1B-NB	-7.41	112.94	124.05
24	a	406[B]	PHO	C3B-C4B-NB	7.33	112.24	107.46
23	B	615	CLA	C4A-NA-C1A	-7.26	103.37	106.68
23	c	507	CLA	O2D-CGD-CBD	7.22	123.86	111.23
23	b	616	CLA	O2D-CGD-CBD	7.20	123.81	111.23
23	B	603	CLA	O2D-CGD-CBD	7.18	123.79	111.23
23	B	606	CLA	CMD-C2D-C1D	7.17	137.36	124.73
23	b	606	CLA	C4A-NA-C1A	-7.11	103.43	106.68
23	c	507	CLA	CMD-C2D-C1D	7.11	137.25	124.73
23	a	407	CLA	CHD-C4C-C3C	-7.11	114.41	124.77
23	d	404	CLA	CMD-C2D-C1D	7.03	137.10	124.73
23	B	611	CLA	C2D-C1D-ND	7.02	117.08	110.13
23	A	404[B]	CLA	C4A-NA-C1A	-7.00	103.48	106.68
23	C	513	CLA	C4A-NA-C1A	-6.96	103.50	106.68
23	B	612	CLA	C2D-C1D-ND	6.94	116.99	110.13
24	A	416[A]	PHO	C2B-C1B-NB	6.94	114.44	109.43
23	B	605	CLA	CHD-C4C-C3C	-6.93	114.66	124.77
24	a	414[A]	PHO	C2B-C1B-NB	6.93	114.44	109.43
23	B	614	CLA	CMD-C2D-C1D	6.90	136.88	124.73
23	B	609	CLA	C4A-NA-C1A	-6.89	103.54	106.68
23	C	504	CLA	C2D-C1D-ND	6.87	116.92	110.13
23	B	616	CLA	CHD-C4C-C3C	-6.87	114.76	124.77
23	C	504	CLA	C4A-NA-C1A	-6.85	103.56	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	CHD-C4C-C3C	-6.83	114.82	124.77
23	B	607	CLA	C2D-C1D-ND	6.81	116.87	110.13
24	A	416[A]	PHO	C3B-C4B-NB	6.78	111.89	107.46
24	A	416[B]	PHO	C2B-C1B-NB	6.78	114.33	109.43
23	B	606	CLA	C2D-C1D-ND	6.78	116.84	110.13
23	C	513	CLA	CHD-C4C-C3C	-6.75	114.93	124.77
23	B	616	CLA	C2D-C1D-ND	6.75	116.81	110.13
23	b	605	CLA	CHD-C4C-C3C	-6.75	114.93	124.77
23	A	405[A]	CLA	C2D-C1D-ND	6.74	116.79	110.13
23	b	611	CLA	C2D-C1D-ND	6.70	116.76	110.13
23	b	606	CLA	CMD-C2D-C1D	6.70	136.52	124.73
23	B	610	CLA	O2D-CGD-CBD	6.70	122.94	111.23
24	a	414[B]	PHO	C2B-C1B-NB	6.69	114.27	109.43
23	D	402[B]	CLA	CMD-C2D-C1D	6.69	136.51	124.73
23	C	505	CLA	C2D-C1D-ND	6.68	116.74	110.13
23	b	612	CLA	CHD-C4C-C3C	-6.67	115.04	124.77
23	b	603	CLA	C4A-NA-C1A	-6.67	103.64	106.68
23	b	606	CLA	CHD-C4C-C3C	-6.67	115.05	124.77
23	C	504	CLA	CHD-C4C-C3C	-6.66	115.06	124.77
23	B	605	CLA	CMD-C2D-C1D	6.66	136.45	124.73
23	b	601	CLA	O2D-CGD-CBD	6.64	122.83	111.23
23	c	513	CLA	CMD-C2D-C1D	6.62	136.38	124.73
23	b	605	CLA	C2D-C1D-ND	6.62	116.68	110.13
23	A	404[A]	CLA	CMD-C2D-C1D	6.62	136.38	124.73
23	B	613	CLA	C2D-C1D-ND	6.58	116.64	110.13
23	a	405[B]	CLA	C2D-C1D-ND	6.58	116.64	110.13
23	B	611	CLA	CMD-C2D-C1D	6.56	136.29	124.73
23	C	504	CLA	CMD-C2D-C1D	6.56	136.28	124.73
23	a	405[A]	CLA	C2D-C1D-ND	6.54	116.60	110.13
23	b	613	CLA	C2D-C1D-ND	6.54	116.60	110.13
23	b	601	CLA	C4A-NA-C1A	-6.50	103.71	106.68
23	c	506	CLA	CMD-C2D-C1D	6.50	136.17	124.73
23	A	408	CLA	C2D-C1D-ND	6.49	116.55	110.13
23	b	614	CLA	C2D-C1D-ND	6.49	116.55	110.13
23	A	406[B]	CLA	C2D-C1D-ND	6.49	116.55	110.13
23	C	508	CLA	CMD-C2D-C1D	6.48	136.14	124.73
23	c	503	CLA	CHD-C4C-C3C	-6.47	115.33	124.77
23	b	609	CLA	CHD-C4C-C3C	-6.47	115.34	124.77
23	D	402[A]	CLA	CMD-C2D-C1D	6.46	136.10	124.73
23	c	503	CLA	C2D-C1D-ND	6.45	116.51	110.13
23	B	612	CLA	CHD-C4C-C3C	-6.45	115.37	124.77
23	b	615	CLA	C4A-NA-C1A	-6.44	103.74	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	CHD-C4C-C3C	-6.44	115.39	124.77
23	B	601	CLA	CHD-C4C-C3C	-6.44	115.39	124.77
23	d	404	CLA	C2D-C1D-ND	6.43	116.49	110.13
23	b	610	CLA	CHD-C4C-C3C	-6.42	115.42	124.77
23	A	404[B]	CLA	CMD-C2D-C1D	6.41	136.01	124.73
23	c	510	CLA	CMD-C2D-C1D	6.40	136.00	124.73
23	B	609	CLA	CHD-C4C-C3C	-6.39	115.46	124.77
23	A	406[A]	CLA	C2D-C1D-ND	6.39	116.45	110.13
23	c	509	CLA	C2D-C1D-ND	6.38	116.44	110.13
23	B	609	CLA	C2D-C1D-ND	6.37	116.43	110.13
23	D	402[A]	CLA	C4A-NA-C1A	-6.37	103.77	106.68
23	b	613	CLA	CHD-C4C-C3C	-6.35	115.51	124.77
23	B	603	CLA	C2D-C1D-ND	6.35	116.41	110.13
23	a	405[A]	CLA	CHD-C4C-C3C	-6.34	115.52	124.77
23	C	509	CLA	C2D-C1D-ND	6.34	116.40	110.13
23	b	611	CLA	CMD-C2D-C1D	6.33	135.88	124.73
23	b	603	CLA	CHD-C4C-C3C	-6.33	115.54	124.77
23	c	503	CLA	C4A-NA-C1A	-6.33	103.79	106.68
23	B	601	CLA	CMD-C2D-C1D	6.33	135.88	124.73
23	B	615	CLA	C2D-C1D-ND	6.33	116.39	110.13
23	b	602	CLA	CMD-C2D-C1D	6.33	135.87	124.73
23	d	402[A]	CLA	C2D-C1D-ND	6.33	116.39	110.13
23	B	615	CLA	CHD-C4C-C3C	-6.31	115.57	124.77
23	c	511	CLA	CHD-C4C-C3C	-6.31	115.57	124.77
23	c	503	CLA	CMD-C2D-C1D	6.31	135.83	124.73
24	a	406[B]	PHO	C2B-C1B-NB	6.30	113.99	109.43
23	c	511	CLA	C2D-C1D-ND	6.30	116.36	110.13
23	C	509	CLA	CHD-C4C-C3C	-6.30	115.59	124.77
23	D	402[A]	CLA	C2D-C1D-ND	6.29	116.35	110.13
23	b	614	CLA	O2D-CGD-CBD	6.29	122.22	111.23
23	c	508	CLA	C2D-C1D-ND	6.29	116.35	110.13
23	A	405[B]	CLA	CHD-C4C-C3C	-6.29	115.61	124.77
23	c	502	CLA	C2D-C1D-ND	6.28	116.34	110.13
23	C	508	CLA	O2D-CGD-CBD	6.28	122.20	111.23
23	b	605	CLA	CMD-C2D-C1D	6.27	135.77	124.73
23	b	601	CLA	CMD-C2D-C1D	6.27	135.77	124.73
26	A	410[B]	SQD	O6-C1-C2	6.27	117.79	108.27
23	C	502	CLA	C4A-NA-C1A	-6.26	103.82	106.68
23	C	514	CLA	C2D-C1D-ND	6.26	116.32	110.13
24	a	406[A]	PHO	C2B-C1B-NB	6.26	113.95	109.43
23	D	403	CLA	C4A-NA-C1A	-6.25	103.83	106.68
23	b	611	CLA	CHD-C4C-C3C	-6.25	115.66	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402[B]	CLA	CHD-C4C-C3C	-6.25	115.66	124.77
26	B	620	SQD	O6-C1-C2	6.25	117.77	108.27
26	F	102	SQD	O47-C7-C8	6.25	124.99	111.48
23	A	408	CLA	CMD-C2D-C1D	6.25	135.73	124.73
23	b	603	CLA	C2D-C1D-ND	6.24	116.31	110.13
23	B	610	CLA	C2D-C1D-ND	6.23	116.29	110.13
23	c	509	CLA	C1-C2-C3	-6.23	115.99	126.20
26	A	410[A]	SQD	O6-C1-C2	6.22	117.72	108.27
23	b	614	CLA	CMD-C2D-C1D	6.22	135.69	124.73
23	d	402[A]	CLA	CHD-C4C-C3C	-6.22	115.70	124.77
23	B	609	CLA	CMD-C2D-C1D	6.21	135.67	124.73
23	b	614	CLA	CHD-C4C-C3C	-6.21	115.72	124.77
23	d	404	CLA	CHD-C4C-C3C	-6.20	115.73	124.77
23	b	616	CLA	C2D-C1D-ND	6.20	116.26	110.13
23	c	510	CLA	CHD-C4C-C3C	-6.19	115.74	124.77
23	b	616	CLA	C4A-NA-C1A	-6.19	103.85	106.68
23	B	602	CLA	CHD-C4C-C3C	-6.19	115.75	124.77
24	A	416[B]	PHO	C3B-C4B-NB	6.18	111.50	107.46
23	B	606	CLA	C4A-NA-C1A	-6.18	103.86	106.68
23	D	402[B]	CLA	C4A-NA-C1A	-6.18	103.86	106.68
23	B	601	CLA	C2D-C1D-ND	6.18	116.24	110.13
23	B	605	CLA	C2D-C1D-ND	6.18	116.24	110.13
23	c	505	CLA	O2D-CGD-CBD	6.18	122.03	111.23
23	C	506	CLA	CMD-C2D-C1D	6.18	135.60	124.73
23	b	609	CLA	CMD-C2D-C1D	6.17	135.59	124.73
23	C	507	CLA	CMD-C2D-C1D	6.16	135.58	124.73
23	B	614	CLA	C2D-C1D-ND	6.16	116.22	110.13
23	B	610	CLA	CMD-C2D-C1D	6.16	135.57	124.73
23	a	405[B]	CLA	CHD-C4C-C3C	-6.16	115.80	124.77
23	C	508	CLA	CHD-C4C-C3C	-6.16	115.80	124.77
23	B	603	CLA	CHD-C4C-C3C	-6.15	115.80	124.77
23	C	510	CLA	C2D-C1D-ND	6.15	116.21	110.13
23	b	615	CLA	C2D-C1D-ND	6.14	116.20	110.13
23	c	512	CLA	CMD-C2D-C1D	6.14	135.53	124.73
23	B	602	CLA	CMD-C2D-C1D	6.13	135.51	124.73
23	b	607	CLA	C2D-C1D-ND	6.12	116.19	110.13
23	d	403[B]	CLA	CMD-C2D-C1D	6.12	135.51	124.73
23	A	405[B]	CLA	C2D-C1D-ND	6.12	116.19	110.13
23	c	504	CLA	C2D-C1D-ND	6.12	116.18	110.13
23	c	501	CLA	C2D-C1D-ND	6.12	116.18	110.13
23	B	601	CLA	O2D-CGD-CBD	6.11	121.91	111.23
24	A	407[A]	PHO	C2B-C1B-NB	6.10	113.84	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404[B]	CLA	CMD-C2D-C1D	6.10	135.47	124.73
24	A	407[B]	PHO	C2B-C1B-NB	6.10	113.84	109.43
23	C	512	CLA	C2D-C1D-ND	6.10	116.16	110.13
23	b	604	CLA	O2D-CGD-CBD	6.09	121.88	111.23
24	A	407[B]	PHO	C4D-ND-C1D	-6.09	101.57	108.87
23	b	615	CLA	CMD-C2D-C1D	6.09	135.45	124.73
23	C	512	CLA	CHD-C4C-C3C	-6.08	115.90	124.77
23	B	610	CLA	CHD-C4C-C3C	-6.08	115.91	124.77
23	B	608	CLA	C2D-C1D-ND	6.08	116.14	110.13
23	d	403[B]	CLA	CHD-C4C-C3C	-6.07	115.92	124.77
23	c	504	CLA	CMD-C2D-C1D	6.07	135.42	124.73
23	c	512	CLA	C4A-NA-C1A	-6.07	103.91	106.68
34	b	623	HTG	C1'-S1-C1	6.06	113.55	100.45
23	b	610	CLA	C2D-C1D-ND	6.05	116.11	110.13
24	a	414[A]	PHO	C4D-ND-C1D	-6.05	101.62	108.87
23	c	512	CLA	O2D-CGD-CBD	6.05	121.80	111.23
23	a	404[A]	CLA	C4A-NA-C1A	-6.04	103.92	106.68
23	d	403[B]	CLA	C2D-C1D-ND	6.04	116.10	110.13
23	b	609	CLA	C4A-NA-C1A	-6.04	103.92	106.68
23	C	502	CLA	CMD-C2D-C1D	6.03	135.34	124.73
23	C	502	CLA	O2D-CGD-CBD	6.01	121.74	111.23
23	c	508	CLA	CHD-C4C-C3C	-6.01	116.00	124.77
23	A	408	CLA	CHD-C4C-C3C	-6.01	116.01	124.77
23	c	501	CLA	CHD-C4C-C3C	-6.01	116.01	124.77
23	C	505	CLA	CMD-C2D-C1D	6.01	135.31	124.73
23	c	505	CLA	CHD-C4C-C3C	-6.00	116.02	124.77
23	b	616	CLA	CMD-C2D-C1D	6.00	135.29	124.73
23	C	511	CLA	C2D-C1D-ND	6.00	116.06	110.13
23	b	611	CLA	O2D-CGD-CBD	5.99	121.70	111.23
23	A	406[A]	CLA	CHD-C4C-C3C	-5.99	116.05	124.77
23	d	402[B]	CLA	C2D-C1D-ND	5.98	116.05	110.13
23	C	506	CLA	CHD-C4C-C3C	-5.98	116.05	124.77
23	c	502	CLA	CHD-C4C-C3C	-5.98	116.05	124.77
23	B	614	CLA	O2D-CGD-CBD	5.98	121.68	111.23
23	a	404[A]	CLA	C2D-C1D-ND	5.96	116.02	110.13
23	C	503	CLA	CHD-C4C-C3C	-5.95	116.09	124.77
23	b	612	CLA	C2D-C1D-ND	5.95	116.01	110.13
23	D	402[B]	CLA	C2D-C1D-ND	5.94	116.00	110.13
23	C	511	CLA	CHD-C4C-C3C	-5.92	116.14	124.77
23	c	506	CLA	C2D-C1D-ND	5.92	115.99	110.13
23	B	606	CLA	O2D-CGD-CBD	5.92	121.58	111.23
23	c	504	CLA	CHD-C4C-C3C	-5.92	116.14	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	C1-C2-C3	-5.92	116.50	126.20
23	D	403	CLA	C2D-C1D-ND	5.91	115.98	110.13
23	A	406[B]	CLA	CMD-C2D-C1D	5.91	135.14	124.73
23	b	608	CLA	C2D-C1D-ND	5.91	115.97	110.13
23	c	505	CLA	C2D-C1D-ND	5.90	115.97	110.13
23	A	405[A]	CLA	CHD-C4C-C3C	-5.89	116.18	124.77
23	C	514	CLA	CMD-C2D-C1D	5.89	135.10	124.73
23	C	502	CLA	C2D-C1D-ND	5.89	115.95	110.13
23	C	507	CLA	C2C-C1C-NC	5.88	116.16	109.98
23	d	403[A]	CLA	C4A-NA-C1A	-5.88	104.00	106.68
23	d	403[A]	CLA	C2D-C1D-ND	5.88	115.94	110.13
23	C	508	CLA	C2D-C1D-ND	5.87	115.94	110.13
23	D	403	CLA	CHD-C4C-C3C	-5.87	116.22	124.77
23	b	604	CLA	CMD-C2D-C1D	5.86	135.04	124.73
23	c	513	CLA	C2D-C1D-ND	5.85	115.92	110.13
23	d	403[B]	CLA	C2C-C1C-NC	5.85	116.13	109.98
24	A	407[A]	PHO	C4D-ND-C1D	-5.85	101.86	108.87
23	c	507	CLA	CHD-C4C-C3C	-5.84	116.26	124.77
23	B	604	CLA	C2C-C1C-NC	5.83	116.11	109.98
23	B	607	CLA	CMD-C2D-C1D	5.83	135.00	124.73
23	b	603	CLA	CMD-C2D-C1D	5.81	134.96	124.73
23	B	602	CLA	O2D-CGD-CBD	5.81	121.39	111.23
23	d	402[B]	CLA	CMD-C2D-C1D	5.80	134.95	124.73
23	b	606	CLA	C2D-C1D-ND	5.80	115.87	110.13
23	d	403[A]	CLA	C2C-C1C-NC	5.80	116.07	109.98
23	C	512	CLA	CMD-C2D-C1D	5.80	134.94	124.73
23	b	609	CLA	C2D-C1D-ND	5.79	115.86	110.13
23	B	614	CLA	CHD-C4C-C3C	-5.79	116.33	124.77
23	B	602	CLA	C4A-NA-C1A	-5.78	104.04	106.68
23	c	502	CLA	C2C-C1C-NC	5.78	116.05	109.98
23	c	509	CLA	CHD-C4C-C3C	-5.77	116.36	124.77
23	b	601	CLA	CHD-C4C-C3C	-5.77	116.36	124.77
25	Y	101	BCR	C33-C5-C6	-5.77	118.19	124.48
23	B	607	CLA	CHD-C4C-C3C	-5.77	116.36	124.77
23	C	510	CLA	C4A-NA-C1A	-5.77	104.05	106.68
23	C	514	CLA	CHD-C4C-C3C	-5.76	116.37	124.77
23	b	604	CLA	C2D-C1D-ND	5.76	115.83	110.13
23	c	507	CLA	C2D-C1D-ND	5.76	115.83	110.13
23	C	505	CLA	CHD-C4C-C3C	-5.76	116.37	124.77
23	B	608	CLA	CHD-C4C-C3C	-5.76	116.38	124.77
24	a	414[A]	PHO	C1-C2-C3	-5.76	116.76	126.20
26	a	409[A]	SQD	O6-C1-C2	5.76	117.02	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	CMD-C2D-C1D	5.75	134.86	124.73
23	c	501	CLA	O2D-CGD-CBD	5.75	121.28	111.23
23	a	404[A]	CLA	CMD-C2D-C1D	5.74	134.84	124.73
23	A	404[A]	CLA	C4A-NA-C1A	-5.74	104.06	106.68
23	c	511	CLA	CMD-C2D-C1D	5.74	134.83	124.73
23	D	403	CLA	CMD-C2D-C1D	5.73	134.82	124.73
23	C	502	CLA	CHD-C4C-C3C	-5.73	116.42	124.77
23	C	503	CLA	C2D-C1D-ND	5.73	115.80	110.13
23	c	509	CLA	CMD-C2D-C1D	5.73	134.81	124.73
23	c	510	CLA	C4A-NA-C1A	-5.72	104.07	106.68
29	A	414[A]	PL9	C7-C8-C9	-5.71	116.99	126.83
23	b	615	CLA	CHD-C4C-C3C	-5.71	116.44	124.77
23	b	604	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
23	c	506	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
23	b	608	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
23	B	604	CLA	O2D-CGD-CBD	5.70	121.19	111.23
23	C	511	CLA	O2D-CGD-CBD	5.69	121.18	111.23
23	C	509	CLA	C2C-C1C-NC	5.69	115.96	109.98
23	B	604	CLA	CMD-C2D-C1D	5.68	134.73	124.73
23	A	406[B]	CLA	CHD-C4C-C3C	-5.68	116.49	124.77
23	b	607	CLA	CMD-C2D-C1D	5.68	134.73	124.73
23	C	503	CLA	CMD-C2D-C1D	5.68	134.72	124.73
23	b	605	CLA	O2D-CGD-CBD	5.67	121.15	111.23
23	B	604	CLA	CHD-C4C-C3C	-5.67	116.50	124.77
23	b	610	CLA	CMD-C2D-C1D	5.67	134.71	124.73
23	c	512	CLA	CHD-C4C-C3C	-5.66	116.51	124.77
23	c	513	CLA	CHD-C4C-C3C	-5.65	116.54	124.77
23	c	504	CLA	C4A-NA-C1A	-5.65	104.10	106.68
23	B	613	CLA	CHD-C4C-C3C	-5.64	116.55	124.77
23	C	513	CLA	C2D-C1D-ND	5.64	115.70	110.13
23	B	603	CLA	CMD-C2D-C1D	5.63	134.65	124.73
23	d	403[A]	CLA	CMD-C2D-C1D	5.63	134.65	124.73
23	c	508	CLA	CMD-C2D-C1D	5.63	134.64	124.73
26	b	620	SQD	O6-C1-C2	5.63	116.82	108.27
25	D	404	BCR	C7-C8-C9	-5.62	117.92	126.23
23	C	510	CLA	CHD-C4C-C3C	-5.62	116.58	124.77
23	B	611	CLA	O2D-CGD-CBD	5.62	121.05	111.23
26	A	410[A]	SQD	C1-O5-C5	-5.61	102.77	113.72
23	d	402[A]	CLA	C4A-NA-C1A	-5.60	104.12	106.68
23	c	512	CLA	C2D-C1D-ND	5.60	115.67	110.13
23	B	605	CLA	C4A-NA-C1A	-5.60	104.13	106.68
23	B	611	CLA	C3D-C2D-C1D	-5.60	98.19	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	CLA	C4A-NA-C1A	-5.59	104.13	106.68
23	A	405[B]	CLA	CMD-C2D-C1D	5.59	134.57	124.73
23	A	404[A]	CLA	C2D-C1D-ND	5.59	115.66	110.13
24	a	414[B]	PHO	C4D-ND-C1D	-5.59	102.18	108.87
23	C	505	CLA	C2C-C1C-NC	5.58	115.85	109.98
23	A	406[A]	CLA	C4A-NA-C1A	-5.58	104.13	106.68
23	a	404[B]	CLA	C2D-C1D-ND	5.58	115.65	110.13
24	A	416[B]	PHO	C4D-ND-C1D	-5.58	102.19	108.87
23	D	402[A]	CLA	C2C-C1C-NC	5.57	115.84	109.98
23	A	406[B]	CLA	C4A-NA-C1A	-5.57	104.14	106.68
23	a	404[A]	CLA	C2C-C1C-NC	5.57	115.83	109.98
23	b	610	CLA	O2D-CGD-CBD	5.56	120.94	111.23
23	d	403[A]	CLA	CHD-C4C-C3C	-5.55	116.69	124.77
23	D	402[B]	CLA	CHD-C4C-C3C	-5.54	116.69	124.77
23	B	602	CLA	C2D-C1D-ND	5.54	115.61	110.13
23	D	402[A]	CLA	CHD-C4C-C3C	-5.53	116.71	124.77
23	B	615	CLA	CMD-C2D-C1D	5.52	134.45	124.73
25	t	102	BCR	C33-C5-C6	-5.52	118.46	124.48
23	a	404[B]	CLA	C2C-C1C-NC	5.52	115.78	109.98
23	c	510	CLA	C2D-C1D-ND	5.52	115.59	110.13
24	A	407[A]	PHO	C3D-C4D-ND	5.51	114.77	107.71
24	A	407[B]	PHO	C3D-C4D-ND	5.51	114.77	107.71
23	d	404	CLA	O2D-CGD-CBD	5.50	120.85	111.23
23	b	607	CLA	CHD-C4C-C3C	-5.50	116.75	124.77
23	b	613	CLA	C2C-C1C-NC	5.49	115.75	109.98
23	C	506	CLA	C2D-C1D-ND	5.49	115.56	110.13
26	F	102	SQD	C1-O5-C5	-5.49	103.00	113.72
24	A	416[A]	PHO	C4D-ND-C1D	-5.48	102.30	108.87
23	C	510	CLA	C3B-C2B-C1B	-5.48	100.71	107.17
23	a	405[B]	CLA	CMD-C2D-C1D	5.48	134.38	124.73
23	b	602	CLA	CHD-C4C-C3C	-5.48	116.79	124.77
23	A	405[A]	CLA	O2D-CGD-CBD	5.46	120.78	111.23
24	a	406[B]	PHO	C4D-ND-C1D	-5.46	102.33	108.87
23	C	505	CLA	C3D-C2D-C1D	-5.46	98.39	105.83
23	b	607	CLA	C2C-C1C-NC	5.45	115.71	109.98
23	C	513	CLA	O2D-CGD-CBD	5.45	120.75	111.23
23	a	407	CLA	C3D-C2D-C1D	-5.45	98.40	105.83
23	B	606	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
23	b	611	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
23	b	601	CLA	C2D-C1D-ND	5.43	115.50	110.13
23	b	612	CLA	CMD-C2D-C1D	5.43	134.29	124.73
26	a	409[B]	SQD	O6-C1-C2	5.43	116.51	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	406[A]	PHO	C4D-ND-C1D	-5.42	102.38	108.87
24	a	414[A]	PHO	C3D-C4D-ND	5.42	114.66	107.71
23	A	404[A]	CLA	C2C-C1C-NC	5.41	115.67	109.98
23	a	405[A]	CLA	C4A-NA-C1A	-5.41	104.21	106.68
23	A	404[B]	CLA	CHD-C4C-C3C	-5.41	116.89	124.77
23	C	507	CLA	C2D-C1D-ND	5.41	115.48	110.13
23	D	402[B]	CLA	C2C-C1C-NC	5.40	115.66	109.98
23	c	507	CLA	C4A-NA-C1A	-5.39	104.22	106.68
23	a	404[A]	CLA	CHD-C4C-C3C	-5.38	116.92	124.77
23	b	602	CLA	O2D-CGD-CBD	5.38	120.64	111.23
23	C	510	CLA	CMD-C2D-C1D	5.38	134.20	124.73
23	b	604	CLA	C1-C2-C3	-5.38	117.39	126.20
23	b	611	CLA	C2C-C1C-NC	5.38	115.63	109.98
23	C	503	CLA	O2D-CGD-CBD	5.37	120.62	111.23
23	C	506	CLA	O2D-CGD-CBD	5.37	120.61	111.23
23	b	604	CLA	C2C-C1C-NC	5.36	115.61	109.98
23	A	408	CLA	C3D-C2D-C1D	-5.36	98.52	105.83
24	a	406[B]	PHO	C3D-C4D-ND	5.34	114.56	107.71
23	b	613	CLA	CMD-C2D-C1D	5.34	134.13	124.73
23	a	405[A]	CLA	CMD-C2D-C1D	5.33	134.12	124.73
23	C	508	CLA	C4A-NA-C1A	-5.33	104.25	106.68
23	C	512	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
23	b	614	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
23	b	605	CLA	C4A-NA-C1A	-5.32	104.25	106.68
23	B	607	CLA	C2C-C1C-NC	5.31	115.56	109.98
34	c	521	HTG	C1'-S1-C1	5.31	111.91	100.45
23	b	602	CLA	C2D-C1D-ND	5.29	115.36	110.13
24	a	414[B]	PHO	C3D-C4D-ND	5.29	114.48	107.71
23	B	614	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
23	c	512	CLA	C2B-C1B-NB	5.26	115.78	110.33
23	C	509	CLA	CMD-C2D-C1D	5.26	133.99	124.73
23	c	505	CLA	C4A-NA-C1A	-5.26	104.28	106.68
23	a	404[B]	CLA	CHD-C4C-C3C	-5.26	117.11	124.77
23	c	512	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
23	c	502	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
23	b	606	CLA	O2D-CGD-CBD	5.25	120.41	111.23
23	A	404[B]	CLA	C2D-C1D-ND	5.25	115.32	110.13
23	c	505	CLA	CMD-C2D-C1D	5.25	133.97	124.73
23	B	616	CLA	C3C-C4C-NC	5.24	117.15	110.43
23	d	402[B]	CLA	C2C-C1C-NC	5.24	115.49	109.98
23	c	509	CLA	C2C-C1C-NC	5.23	115.48	109.98
24	A	416[A]	PHO	C3D-C4D-ND	5.23	114.42	107.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	620	SQD	O47-C7-C8	5.23	122.79	111.48
23	B	607	CLA	C4A-NA-C1A	-5.22	104.30	106.68
23	a	405[B]	CLA	C4A-NA-C1A	-5.21	104.30	106.68
23	A	406[B]	CLA	C2B-C1B-NB	5.20	115.72	110.33
26	a	409[A]	SQD	O47-C7-C8	5.20	122.73	111.48
26	A	410[A]	SQD	C1-C2-C3	-5.20	99.07	110.01
23	b	613	CLA	C4A-NA-C1A	-5.19	104.31	106.68
23	A	405[A]	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	d	402[A]	CLA	CMD-C2D-C1D	5.18	133.85	124.73
23	B	605	CLA	C3D-C2D-C1D	-5.18	98.77	105.83
23	b	608	CLA	C4A-NA-C1A	-5.17	104.32	106.68
23	b	603	CLA	O2D-CGD-CBD	5.17	120.27	111.23
23	c	506	CLA	C2C-C1C-NC	5.17	115.41	109.98
23	b	604	CLA	C4A-NA-C1A	-5.17	104.32	106.68
23	c	503	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
23	A	404[B]	CLA	C2C-C1C-NC	5.16	115.40	109.98
23	c	504	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
23	d	402[B]	CLA	O2D-CGD-CBD	5.15	120.24	111.23
23	c	508	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
38	f	101	HEM	CHC-C4B-NB	5.15	129.96	124.42
23	C	506	CLA	C2C-C1C-NC	5.14	115.39	109.98
23	b	610	CLA	C1-C2-C3	-5.14	117.77	126.20
23	a	407	CLA	O2D-CGD-CBD	5.14	120.22	111.23
23	b	605	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
23	C	503	CLA	C2C-C1C-NC	5.14	115.38	109.98
23	c	504	CLA	O2D-CGD-CBD	5.14	120.21	111.23
23	C	508	CLA	C3B-C2B-C1B	-5.14	101.12	107.17
23	c	502	CLA	O2D-CGD-CBD	5.13	120.20	111.23
24	A	416[B]	PHO	C3D-C4D-ND	5.12	114.28	107.71
23	D	402[A]	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
24	A	416[B]	PHO	C1-C2-C3	-5.12	117.81	126.20
25	d	405	BCR	C7-C8-C9	-5.12	118.66	126.23
23	B	614	CLA	C2C-C1C-NC	5.12	115.36	109.98
23	A	406[A]	CLA	CMD-C2D-C1D	5.12	133.74	124.73
23	c	508	CLA	C2C-C1C-NC	5.11	115.35	109.98
23	B	610	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
23	C	503	CLA	C4A-NA-C1A	-5.10	104.35	106.68
23	B	612	CLA	CMD-C2D-C1D	5.10	133.71	124.73
23	b	613	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
23	B	605	CLA	O2D-CGD-CBD	5.10	120.14	111.23
23	b	608	CLA	C2C-C1C-NC	5.10	115.33	109.98
23	b	615	CLA	C2C-C1C-NC	5.09	115.33	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	CMD-C2D-C1D	5.09	133.69	124.73
23	a	407	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
23	B	614	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
23	c	501	CLA	O2D-CGD-O1D	-5.08	113.95	123.85
23	C	511	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
23	A	408	CLA	C2B-C1B-NB	5.08	115.59	110.33
26	b	620	SQD	O47-C7-C8	5.08	122.46	111.48
23	c	501	CLA	C4A-NA-C1A	-5.08	104.36	106.68
23	a	407	CLA	CMD-C2D-C1D	5.08	133.67	124.73
24	a	414[B]	PHO	C1-C2-C3	-5.08	117.88	126.20
23	B	607	CLA	O2D-CGD-CBD	5.07	120.10	111.23
23	A	408	CLA	C2C-C1C-NC	5.07	115.31	109.98
23	A	406[B]	CLA	C3D-C4D-ND	5.07	118.23	109.99
23	B	612	CLA	O2D-CGD-CBD	5.07	120.09	111.23
23	A	404[B]	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
23	b	606	CLA	C2B-C1B-NB	5.05	115.56	110.33
23	b	607	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	c	501	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
23	B	608	CLA	O2D-CGD-CBD	5.03	120.03	111.23
23	C	510	CLA	C2B-C1B-NB	5.03	115.55	110.33
23	C	508	CLA	C2C-C1C-NC	5.03	115.27	109.98
23	C	507	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
23	B	608	CLA	C2C-C1C-NC	5.02	115.25	109.98
23	C	509	CLA	O2D-CGD-CBD	5.01	119.99	111.23
23	A	404[A]	CLA	C3B-C2B-C1B	-5.01	101.27	107.17
25	d	405	BCR	C15-C14-C13	-5.01	120.25	127.28
23	C	504	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
23	B	607	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
23	C	510	CLA	C2C-C1C-NC	5.00	115.23	109.98
23	B	613	CLA	CMD-C2D-C1D	5.00	133.53	124.73
23	B	613	CLA	C2C-C1C-NC	4.99	115.23	109.98
23	B	608	CLA	CMD-C2D-C1D	4.99	133.52	124.73
23	C	507	CLA	CHD-C4C-C3C	-4.99	117.49	124.77
23	d	404	CLA	C2B-C1B-NB	4.99	115.50	110.33
23	d	402[A]	CLA	C2C-C1C-NC	4.99	115.22	109.98
23	b	611	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
23	B	613	CLA	C3D-C2D-C1D	-4.99	99.03	105.83
23	A	408	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
23	d	404	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
34	D	410	HTG	C1'-S1-C1	4.97	111.19	100.45
24	a	406[A]	PHO	C3D-C4D-ND	4.97	114.08	107.71
23	c	513	CLA	C4A-NA-C1A	-4.97	104.41	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	C3D-C2D-C1D	-4.97	99.04	105.83
23	b	602	CLA	C2B-C1B-NB	4.97	115.48	110.33
23	B	603	CLA	C4A-NA-C1A	-4.97	104.41	106.68
23	A	405[A]	CLA	C2C-C1C-NC	4.96	115.19	109.98
23	b	610	CLA	C4A-NA-C1A	-4.95	104.42	106.68
23	B	614	CLA	C4A-NA-C1A	-4.94	104.42	106.68
23	c	507	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
23	B	604	CLA	C2D-C1D-ND	4.94	115.01	110.13
23	c	502	CLA	C1C-C2C-C3C	-4.94	101.79	106.98
23	C	514	CLA	C3B-C2B-C1B	-4.93	101.35	107.17
23	b	609	CLA	O2D-CGD-CBD	4.93	119.85	111.23
29	A	414[B]	PL9	C7-C8-C9	-4.93	118.34	126.83
26	f	102	SQD	O47-C7-C8	4.93	122.14	111.48
23	d	404	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
23	C	513	CLA	C2B-C1B-NB	4.92	115.43	110.33
23	C	507	CLA	C1C-C2C-C3C	-4.92	101.81	106.98
23	B	603	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
23	a	405[A]	CLA	C3D-C2D-C1D	-4.91	99.12	105.83
23	B	616	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
23	B	608	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
23	C	511	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
23	B	604	CLA	C1-C2-C3	-4.90	118.17	126.20
23	C	503	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
23	B	616	CLA	C4A-NA-C1A	-4.90	104.44	106.68
23	c	509	CLA	O2D-CGD-CBD	4.90	119.79	111.23
23	b	605	CLA	C2C-C1C-NC	4.89	115.12	109.98
23	c	510	CLA	C2C-C1C-NC	4.89	115.12	109.98
40	v	201	HEC	CBC-CAC-C3C	-4.89	117.65	127.43
23	d	402[A]	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	c	506	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	c	501	CLA	CHD-C1D-ND	-4.88	117.93	124.80
23	B	601	CLA	C3B-C2B-C1B	-4.88	101.42	107.17
23	B	607	CLA	C1C-C2C-C3C	-4.87	101.85	106.98
24	A	416[A]	PHO	C1-C2-C3	-4.87	118.22	126.20
23	c	513	CLA	C2C-C1C-NC	4.87	115.09	109.98
23	B	601	CLA	C2B-C1B-NB	4.86	115.37	110.33
23	B	609	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	A	405[B]	CLA	O2D-CGD-CBD	4.86	119.72	111.23
23	c	504	CLA	C3D-C2D-C1D	-4.86	99.21	105.83
23	b	601	CLA	C2B-C1B-NB	4.85	115.35	110.33
25	H	101	BCR	C38-C26-C25	-4.85	119.20	124.48
23	c	513	CLA	C3B-C2B-C1B	-4.84	101.46	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406[A]	CLA	O2D-CGD-CBD	4.84	119.69	111.23
23	a	404[B]	CLA	C4A-NA-C1A	-4.84	104.47	106.68
23	A	404[A]	CLA	CHD-C4C-C3C	-4.83	117.73	124.77
33	d	412	LMG	O7-C10-C11	4.83	121.94	111.48
23	b	614	CLA	C4A-NA-C1A	-4.83	104.47	106.68
23	c	511	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
23	b	613	CLA	C3C-C4C-NC	4.83	116.61	110.43
23	C	513	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
23	C	512	CLA	O2D-CGD-CBD	4.82	119.67	111.23
23	a	405[B]	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
23	B	613	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
23	D	402[B]	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
23	a	405[A]	CLA	C3D-C4D-ND	4.81	117.81	109.99
23	b	613	CLA	C1-C2-C3	-4.81	118.31	126.20
23	c	506	CLA	C4A-NA-C1A	-4.81	104.48	106.68
23	b	612	CLA	C3C-C4C-NC	4.81	116.59	110.43
23	C	506	CLA	C4A-NA-C1A	-4.81	104.48	106.68
23	a	405[B]	CLA	O2D-CGD-CBD	4.81	119.63	111.23
23	c	510	CLA	C1-C2-C3	-4.81	118.32	126.20
23	b	605	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
23	B	611	CLA	C3D-C4D-ND	4.80	117.79	109.99
23	c	505	CLA	C2C-C1C-NC	4.80	115.02	109.98
23	D	403	CLA	O2D-CGD-CBD	4.80	119.61	111.23
23	b	603	CLA	C3D-C4D-ND	4.79	117.78	109.99
23	c	503	CLA	O2D-CGD-CBD	4.79	119.61	111.23
23	C	509	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
23	c	508	CLA	C3B-C2B-C1B	-4.79	101.53	107.17
23	c	509	CLA	C3B-C2B-C1B	-4.79	101.53	107.17
23	d	402[B]	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
23	A	404[B]	CLA	C2B-C1B-NB	4.78	115.29	110.33
23	b	614	CLA	C2B-C1B-NB	4.78	115.29	110.33
23	C	508	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
23	d	404	CLA	C4A-NA-C1A	-4.78	104.50	106.68
23	a	404[B]	CLA	C3B-C2B-C1B	-4.78	101.54	107.17
23	B	615	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	C	511	CLA	C2C-C1C-NC	4.78	115.00	109.98
23	b	603	CLA	C2B-C1B-NB	4.77	115.28	110.33
23	B	608	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
23	A	405[B]	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
23	B	616	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
33	C	501	LMG	C7-O1-C1	-4.77	103.58	113.80
23	b	605	CLA	C3D-C4D-ND	4.76	117.73	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
23	C	514	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
34	b	622	HTG	C1-O5-C5	4.76	121.10	112.56
26	a	409[B]	SQD	O47-C7-C8	4.76	121.78	111.48
23	c	502	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
23	b	606	CLA	C3B-C2B-C1B	-4.76	101.56	107.17
23	C	514	CLA	O2D-CGD-CBD	4.75	119.53	111.23
23	B	606	CLA	CHD-C1D-ND	-4.75	118.12	124.80
23	C	504	CLA	O2D-CGD-CBD	4.75	119.53	111.23
23	c	508	CLA	C4A-NA-C1A	-4.75	104.51	106.68
23	B	612	CLA	C3C-C4C-NC	4.75	116.51	110.43
23	b	612	CLA	O2D-CGD-CBD	4.74	119.53	111.23
23	A	406[A]	CLA	C2C-C1C-NC	4.74	114.97	109.98
23	D	403	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	C	503	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	b	601	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
23	C	510	CLA	O2D-CGD-CBD	4.74	119.51	111.23
23	c	507	CLA	C2C-C1C-NC	4.74	114.96	109.98
23	A	406[B]	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
23	D	402[B]	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
23	A	405[A]	CLA	C1C-C2C-C3C	-4.73	102.00	106.98
23	b	615	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
23	b	612	CLA	C2C-C1C-NC	4.73	114.95	109.98
23	b	610	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
23	B	603	CLA	C2C-C1C-NC	4.72	114.94	109.98
23	a	405[B]	CLA	C3D-C4D-ND	4.72	117.67	109.99
23	C	514	CLA	C2C-C1C-NC	4.72	114.94	109.98
23	b	605	CLA	O2D-CGD-O1D	-4.72	114.66	123.85
23	A	405[A]	CLA	C4A-NA-C1A	-4.72	104.53	106.68
23	c	502	CLA	C2B-C1B-NB	4.71	115.21	110.33
23	A	404[A]	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	c	507	CLA	CHD-C1D-ND	-4.71	118.18	124.80
23	c	513	CLA	O2D-CGD-CBD	4.70	119.45	111.23
34	d	411	HTG	C1'-S1-C1	4.70	110.60	100.45
23	b	614	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
23	c	513	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	C	512	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	A	406[B]	CLA	CHD-C1D-ND	-4.69	118.20	124.80
23	C	511	CLA	C2B-C1B-NB	4.69	115.19	110.33
23	A	406[A]	CLA	C3D-C4D-ND	4.69	117.61	109.99
23	B	602	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
23	B	601	CLA	C3D-C2D-C1D	-4.68	99.44	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
23	B	610	CLA	C2C-C1C-NC	4.68	114.90	109.98
23	b	602	CLA	C3D-C4D-ND	4.68	117.59	109.99
31	t	101	LMT	C3'-C4'-C5'	-4.67	100.57	110.93
23	a	405[A]	CLA	O2D-CGD-CBD	4.67	119.40	111.23
23	b	603	CLA	C3B-C2B-C1B	-4.67	101.66	107.17
23	B	604	CLA	C3C-C4C-NC	4.67	116.41	110.43
29	A	414[A]	PL9	C7-C3-C2	-4.67	117.89	123.39
23	d	403[B]	CLA	C3D-C4D-ND	4.67	117.57	109.99
23	C	505	CLA	O2D-CGD-CBD	4.66	119.38	111.23
38	E	102	HEM	CHC-C4B-NB	4.66	129.44	124.42
23	b	607	CLA	C4A-NA-C1A	-4.66	104.55	106.68
23	A	405[B]	CLA	C2C-C1C-NC	4.66	114.88	109.98
25	y	101	BCR	C33-C5-C6	-4.66	119.40	124.48
23	C	512	CLA	C4A-NA-C1A	-4.66	104.55	106.68
23	B	610	CLA	O2A-CGA-CBA	4.66	126.03	111.83
23	B	612	CLA	C3D-C4D-ND	4.65	117.55	109.99
26	A	410[B]	SQD	C1-O5-C5	-4.65	104.63	113.72
23	b	602	CLA	C3B-C2B-C1B	-4.65	101.68	107.17
23	D	402[A]	CLA	O2D-CGD-CBD	4.65	119.36	111.23
23	C	510	CLA	C1-C2-C3	-4.65	118.58	126.20
23	a	407	CLA	C2C-C1C-NC	4.65	114.86	109.98
23	B	611	CLA	CMC-C2C-C1C	4.64	132.29	125.03
23	c	510	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
23	c	507	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
23	a	407	CLA	C3C-C4C-NC	4.63	116.36	110.43
23	B	602	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
23	C	507	CLA	C2B-C1B-NB	4.63	115.13	110.33
23	d	403[B]	CLA	C4A-NA-C1A	-4.63	104.57	106.68
23	D	402[B]	CLA	C1-C2-C3	-4.63	118.62	126.20
23	A	406[A]	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
33	B	621	LMG	O7-C10-C11	4.62	121.48	111.48
23	c	513	CLA	C2B-C1B-NB	4.62	115.12	110.33
26	b	620	SQD	C1-O5-C5	-4.62	104.69	113.72
23	b	607	CLA	O2D-CGD-CBD	4.62	119.30	111.23
23	C	507	CLA	C3D-C4D-ND	4.62	117.49	109.99
23	C	504	CLA	C3B-C2B-C1B	-4.61	101.73	107.17
23	B	609	CLA	C3D-C4D-ND	4.61	117.48	109.99
23	a	405[B]	CLA	C3B-C2B-C1B	-4.61	101.73	107.17
23	a	404[B]	CLA	C3D-C4D-ND	4.61	117.48	109.99
23	b	608	CLA	C1C-C2C-C3C	-4.61	102.13	106.98
23	c	504	CLA	C2B-C1B-NB	4.60	115.10	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	C2C-C1C-NC	4.60	114.81	109.98
23	C	502	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
23	d	403[B]	CLA	C1C-C2C-C3C	-4.60	102.14	106.98
23	d	404	CLA	CHD-C1D-ND	-4.60	118.33	124.80
23	a	404[A]	CLA	C3B-C2B-C1B	-4.60	101.75	107.17
23	b	607	CLA	C3C-C4C-NC	4.59	116.32	110.43
23	c	508	CLA	O2D-CGD-CBD	4.59	119.26	111.23
23	b	611	CLA	C2B-C1B-NB	4.59	115.09	110.33
23	b	603	CLA	C1D-CHD-C4C	-4.59	116.26	126.02
23	c	504	CLA	C2C-C1C-NC	4.59	114.80	109.98
23	a	404[A]	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	c	510	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	c	511	CLA	C3D-C4D-ND	4.58	117.43	109.99
23	b	610	CLA	C2C-C1C-NC	4.58	114.79	109.98
23	a	407	CLA	C3D-C4D-ND	4.58	117.42	109.99
23	c	509	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
23	C	509	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
23	D	402[B]	CLA	O2D-CGD-CBD	4.57	119.22	111.23
38	E	102	HEM	CAD-CBD-CGD	4.57	125.79	113.67
23	d	403[A]	CLA	C3D-C4D-ND	4.57	117.42	109.99
23	B	605	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
23	b	608	CLA	C3D-C4D-ND	4.57	117.41	109.99
23	b	604	CLA	C1C-C2C-C3C	-4.57	102.18	106.98
23	B	609	CLA	CHD-C1D-ND	-4.56	118.38	124.80
23	A	404[A]	CLA	C2B-C1B-NB	4.56	115.06	110.33
23	C	504	CLA	C3D-C4D-ND	4.56	117.40	109.99
23	C	514	CLA	C2B-C1B-NB	4.56	115.06	110.33
23	c	511	CLA	C2C-C1C-NC	4.56	114.77	109.98
23	c	510	CLA	O2D-CGD-CBD	4.56	119.20	111.23
23	b	609	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
23	D	403	CLA	C2B-C1B-NB	4.55	115.04	110.33
23	B	612	CLA	C3B-C2B-C1B	-4.55	101.81	107.17
23	a	405[B]	CLA	C2B-C1B-NB	4.55	115.04	110.33
23	d	402[B]	CLA	C2B-C1B-NB	4.55	115.04	110.33
23	B	602	CLA	C2C-C1C-NC	4.55	114.76	109.98
23	C	507	CLA	O2D-CGD-CBD	4.55	119.18	111.23
23	b	601	CLA	C3D-C4D-ND	4.54	117.37	109.99
23	a	404[B]	CLA	C2B-C1B-NB	4.54	115.04	110.33
23	A	405[A]	CLA	CMD-C2D-C1D	4.54	132.73	124.73
23	c	501	CLA	C3B-C2B-C1B	-4.54	101.82	107.17
23	b	607	CLA	C3B-C4B-NB	4.54	114.58	110.53
23	c	504	CLA	CHD-C1D-ND	-4.54	118.42	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	C3D-C4D-ND	4.54	117.36	109.99
23	B	610	CLA	C4A-NA-C1A	-4.53	104.61	106.68
23	d	404	CLA	C3D-C4D-ND	4.53	117.35	109.99
23	c	511	CLA	O2D-CGD-CBD	4.53	119.15	111.23
29	a	412[B]	PL9	C32-C33-C34	-4.53	117.27	127.62
23	b	608	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
23	c	511	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
23	C	509	CLA	C3C-C4C-NC	4.52	116.22	110.43
26	A	410[B]	SQD	C1-C2-C3	-4.52	100.51	110.01
23	c	512	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
23	c	505	CLA	C3C-C4C-NC	4.52	116.21	110.43
23	C	514	CLA	C3D-C4D-ND	4.51	117.32	109.99
23	C	513	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
23	d	402[A]	CLA	C1C-C2C-C3C	-4.51	102.24	106.98
23	D	402[A]	CLA	C3B-C2B-C1B	-4.51	101.86	107.17
29	A	414[A]	PL9	C32-C33-C34	-4.50	117.31	127.62
23	B	603	CLA	O2D-CGD-O1D	-4.50	115.08	123.85
23	c	503	CLA	C2B-C1B-NB	4.50	115.00	110.33
23	B	616	CLA	C2C-C1C-NC	4.50	114.71	109.98
23	A	406[A]	CLA	C2B-C1B-NB	4.50	114.99	110.33
23	b	604	CLA	C3D-C2D-C1D	-4.50	99.70	105.83
29	A	414[B]	PL9	C32-C33-C34	-4.50	117.33	127.62
23	b	608	CLA	O2D-CGD-CBD	4.49	119.09	111.23
23	c	506	CLA	C1-C2-C3	-4.49	118.83	126.20
23	d	402[B]	CLA	C1C-C2C-C3C	-4.49	102.26	106.98
23	b	607	CLA	C3B-C2B-C1B	-4.49	101.88	107.17
23	B	605	CLA	C2C-C1C-NC	4.49	114.70	109.98
23	c	503	CLA	C3B-C2B-C1B	-4.49	101.88	107.17
23	c	509	CLA	C3B-C4B-NB	4.49	114.53	110.53
23	c	501	CLA	C3D-C4D-ND	4.48	117.28	109.99
23	d	402[A]	CLA	O2D-CGD-CBD	4.48	119.07	111.23
23	c	505	CLA	C3D-C4D-ND	4.48	117.28	109.99
23	B	616	CLA	O2D-CGD-O1D	-4.48	115.12	123.85
23	C	507	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	B	608	CLA	C4A-NA-C1A	-4.48	104.64	106.68
23	c	513	CLA	C3D-C4D-ND	4.47	117.26	109.99
29	a	412[A]	PL9	C7-C8-C9	-4.47	119.13	126.83
25	c	514	BCR	C11-C10-C9	-4.47	121.01	127.28
23	c	501	CLA	C2B-C1B-NB	4.47	114.96	110.33
23	C	506	CLA	CMB-C2B-C1B	4.47	132.22	125.42
23	b	607	CLA	C3D-C4D-ND	4.47	117.25	109.99
23	A	404[A]	CLA	C3B-C4B-NB	4.47	114.52	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	403[A]	CLA	C1C-C2C-C3C	-4.47	102.28	106.98
40	V	201	HEC	CBC-CAC-C3C	-4.47	118.51	127.43
23	B	609	CLA	C2B-C1B-NB	4.46	114.95	110.33
23	C	510	CLA	C3D-C4D-ND	4.46	117.24	109.99
23	B	615	CLA	CMB-C2B-C1B	4.46	132.21	125.42
23	C	504	CLA	C2B-C1B-NB	4.46	114.95	110.33
25	C	516	BCR	C7-C8-C9	-4.45	119.65	126.23
23	B	613	CLA	C2B-C1B-NB	4.45	114.94	110.33
23	C	505	CLA	C1C-C2C-C3C	-4.45	102.30	106.98
23	C	507	CLA	C4A-NA-C1A	-4.45	104.65	106.68
23	A	405[B]	CLA	C3D-C4D-ND	4.45	117.22	109.99
23	b	610	CLA	C3C-C4C-NC	4.45	116.13	110.43
23	B	602	CLA	C2B-C1B-NB	4.45	114.94	110.33
23	B	608	CLA	C2B-C1B-NB	4.44	114.94	110.33
23	B	615	CLA	C2C-C1C-NC	4.44	114.65	109.98
23	c	505	CLA	C2B-C1B-NB	4.44	114.93	110.33
23	c	502	CLA	C4A-NA-C1A	-4.44	104.65	106.68
23	B	603	CLA	C2B-C1B-NB	4.44	114.93	110.33
23	a	407	CLA	C2B-C1B-NB	4.44	114.93	110.33
23	c	504	CLA	C3D-C4D-ND	4.44	117.20	109.99
23	c	510	CLA	C2B-C1B-NB	4.44	114.93	110.33
23	B	605	CLA	C3D-C4D-ND	4.44	117.20	109.99
23	C	507	CLA	CHD-C1D-ND	-4.44	118.56	124.80
23	B	615	CLA	C3D-C4D-ND	4.44	117.20	109.99
23	b	609	CLA	C3D-C4D-ND	4.43	117.19	109.99
23	a	404[A]	CLA	C2B-C1B-NB	4.43	114.92	110.33
23	C	502	CLA	C2B-C1B-NB	4.43	114.92	110.33
23	C	502	CLA	O2D-CGD-O1D	-4.43	115.23	123.85
23	c	508	CLA	C2B-C1B-NB	4.43	114.92	110.33
23	c	506	CLA	C3D-C4D-ND	4.42	117.18	109.99
23	C	506	CLA	C3B-C2B-C1B	-4.42	101.96	107.17
23	A	405[B]	CLA	C2B-C1B-NB	4.42	114.91	110.33
23	C	514	CLA	CHD-C1D-ND	-4.42	118.58	124.80
33	c	520	LMG	O6-C5-C4	4.41	117.65	109.70
23	c	506	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
23	C	512	CLA	C2B-C1B-NB	4.41	114.90	110.33
23	B	609	CLA	C2C-C1C-NC	4.40	114.61	109.98
23	C	502	CLA	C3D-C4D-ND	4.40	117.14	109.99
23	B	601	CLA	C3D-C4D-ND	4.40	117.14	109.99
23	d	403[B]	CLA	C3B-C2B-C1B	-4.40	101.99	107.17
23	a	405[A]	CLA	C2C-C1C-NC	4.39	114.60	109.98
23	c	513	CLA	C1D-CHD-C4C	-4.39	116.69	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	C4A-NA-C1A	-4.39	104.68	106.68
33	C	501	LMG	O7-C10-C11	4.39	120.97	111.48
23	B	611	CLA	C3C-C4C-NC	4.38	116.05	110.43
23	C	510	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
26	f	102	SQD	C1-O5-C5	4.38	122.28	113.72
23	B	612	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
23	b	615	CLA	C2B-C1B-NB	4.38	114.87	110.33
34	B	623	HTG	C1'-S1-C1	4.38	109.91	100.45
23	c	507	CLA	C1C-C2C-C3C	-4.38	102.37	106.98
23	c	503	CLA	C1D-CHD-C4C	-4.38	116.71	126.02
23	b	609	CLA	C2C-C1C-NC	4.38	114.58	109.98
23	C	514	CLA	C4A-NA-C1A	-4.38	104.68	106.68
23	d	402[B]	CLA	C3D-C4D-ND	4.37	117.10	109.99
23	a	404[B]	CLA	C3B-C4B-NB	4.37	114.44	110.53
23	b	616	CLA	C1D-CHD-C4C	-4.37	116.73	126.02
23	b	605	CLA	C2B-C1B-NB	4.37	114.86	110.33
23	b	602	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
23	A	404[B]	CLA	C3D-C4D-ND	4.37	117.09	109.99
23	b	603	CLA	C2C-C1C-NC	4.37	114.57	109.98
23	D	402[B]	CLA	CHD-C1D-ND	-4.37	118.66	124.80
23	a	405[A]	CLA	CHD-C1D-ND	-4.37	118.66	124.80
23	C	506	CLA	C3D-C4D-ND	4.36	117.08	109.99
23	B	606	CLA	C2C-C1C-NC	4.36	114.56	109.98
25	T	102	BCR	C15-C16-C17	-4.36	114.60	123.52
23	C	511	CLA	C3D-C4D-ND	4.36	117.07	109.99
23	c	503	CLA	C2C-C1C-NC	4.36	114.56	109.98
29	a	412[A]	PL9	C7-C3-C2	-4.36	118.25	123.39
23	B	603	CLA	C3D-C4D-ND	4.35	117.06	109.99
23	C	507	CLA	C3B-C4B-NB	4.35	114.42	110.53
23	a	404[A]	CLA	C3D-C4D-ND	4.35	117.06	109.99
23	b	601	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
29	D	405[B]	PL9	C42-C43-C44	-4.35	117.67	127.62
23	B	616	CLA	C3D-C4D-ND	4.35	117.06	109.99
23	c	503	CLA	C3D-C4D-ND	4.35	117.05	109.99
23	A	404[A]	CLA	C1C-C2C-C3C	-4.34	102.41	106.98
23	a	405[A]	CLA	C2B-C1B-NB	4.34	114.83	110.33
23	A	405[B]	CLA	C1C-C2C-C3C	-4.34	102.41	106.98
23	c	507	CLA	CMB-C2B-C1B	4.34	132.02	125.42
23	d	403[B]	CLA	CHD-C1D-ND	-4.33	118.70	124.80
23	B	616	CLA	CMD-C2D-C1D	4.33	132.36	124.73
23	A	406[B]	CLA	C3B-C2B-C1B	-4.33	102.06	107.17
23	c	512	CLA	C1-C2-C3	-4.33	119.11	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	CMC-C2C-C1C	4.33	131.80	125.03
23	b	615	CLA	C3B-C2B-C1B	-4.33	102.07	107.17
23	b	601	CLA	C2C-C1C-NC	4.33	114.53	109.98
23	C	508	CLA	C1D-CHD-C4C	-4.32	116.83	126.02
23	a	405[A]	CLA	C3B-C2B-C1B	-4.32	102.07	107.17
32	E	101[A]	LHG	O7-C7-C8	4.32	120.82	111.48
23	C	509	CLA	C3B-C4B-NB	4.32	114.38	110.53
23	b	613	CLA	C3B-C2B-C1B	-4.32	102.08	107.17
23	a	404[A]	CLA	CAA-C2A-C3A	-4.31	101.34	113.00
23	b	611	CLA	C3D-C4D-ND	4.31	117.00	109.99
23	C	506	CLA	C3C-C4C-NC	4.31	115.95	110.43
33	a	415	LMG	O7-C10-C11	4.31	120.81	111.48
23	c	509	CLA	C3D-C4D-ND	4.31	116.99	109.99
23	a	405[B]	CLA	CHD-C1D-ND	-4.31	118.74	124.80
23	a	404[A]	CLA	C1C-C2C-C3C	-4.31	102.45	106.98
25	d	405	BCR	C40-C30-C25	-4.31	103.49	110.24
23	d	403[B]	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
23	b	609	CLA	C3C-C4C-NC	4.30	115.94	110.43
23	c	506	CLA	CHD-C1D-ND	-4.30	118.75	124.80
23	C	504	CLA	CHD-C1D-ND	-4.30	118.75	124.80
25	B	618	BCR	C29-C30-C25	4.30	116.69	110.44
23	C	513	CLA	C1D-CHD-C4C	-4.30	116.89	126.02
23	d	402[B]	CLA	C3B-C2B-C1B	-4.30	102.11	107.17
29	a	412[B]	PL9	C7-C3-C4	4.30	120.45	116.91
34	C	522	HTG	C1'-S1-C1	4.30	109.73	100.45
23	c	506	CLA	C2B-C1B-NB	4.29	114.78	110.33
23	C	509	CLA	C3D-C4D-ND	4.29	116.97	109.99
23	C	505	CLA	C3C-C4C-NC	4.29	115.93	110.43
23	A	404[B]	CLA	CHD-C1D-ND	-4.29	118.77	124.80
23	A	404[B]	CLA	C1C-C2C-C3C	-4.29	102.47	106.98
23	B	607	CLA	CHD-C1D-ND	-4.29	118.77	124.80
23	B	611	CLA	C4A-NA-C1A	-4.29	104.72	106.68
29	a	412[A]	PL9	C7-C3-C4	4.28	120.44	116.91
23	c	502	CLA	C3D-C4D-ND	4.28	116.95	109.99
23	B	608	CLA	C3D-C4D-ND	4.28	116.94	109.99
23	a	404[B]	CLA	C1D-CHD-C4C	-4.28	116.93	126.02
23	B	615	CLA	C3B-C2B-C1B	-4.28	102.13	107.17
23	c	511	CLA	C2B-C1B-NB	4.27	114.76	110.33
23	A	408	CLA	C3D-C4D-ND	4.27	116.93	109.99
23	D	402[A]	CLA	CHD-C1D-ND	-4.27	118.79	124.80
23	c	501	CLA	C2C-C1C-NC	4.27	114.47	109.98
23	D	402[B]	CLA	C3D-C4D-ND	4.27	116.93	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	C	501	LMG	O1-C1-C2	4.27	114.75	108.27
23	b	605	CLA	CHD-C1D-ND	-4.27	118.80	124.80
23	c	502	CLA	C1D-CHD-C4C	-4.26	116.96	126.02
23	b	604	CLA	C3C-C4C-NC	4.26	115.89	110.43
23	d	403[B]	CLA	O2D-CGD-CBD	4.26	118.68	111.23
23	B	614	CLA	C2B-C1B-NB	4.26	114.74	110.33
23	B	607	CLA	C3D-C4D-ND	4.26	116.91	109.99
23	C	513	CLA	C3D-C4D-ND	4.26	116.91	109.99
23	b	606	CLA	CHD-C1D-ND	-4.26	118.81	124.80
23	d	402[A]	CLA	C3D-C4D-ND	4.25	116.90	109.99
23	b	606	CLA	C1D-CHD-C4C	-4.25	116.98	126.02
23	C	509	CLA	C2B-C1B-NB	4.25	114.73	110.33
23	a	404[A]	CLA	C1D-CHD-C4C	-4.25	116.98	126.02
23	b	614	CLA	C2C-C1C-NC	4.25	114.44	109.98
23	c	505	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
23	c	509	CLA	C2B-C1B-NB	4.25	114.73	110.33
23	D	402[A]	CLA	C1-C2-C3	-4.24	119.25	126.20
23	B	602	CLA	C3D-C4D-ND	4.24	116.88	109.99
23	b	606	CLA	C2C-C1C-NC	4.24	114.44	109.98
23	A	405[A]	CLA	C2B-C1B-NB	4.24	114.72	110.33
23	c	502	CLA	CMD-C2D-C1D	4.24	132.19	124.73
23	a	404[A]	CLA	C3B-C4B-NB	4.24	114.31	110.53
25	b	617	BCR	C33-C5-C6	-4.23	119.86	124.48
23	C	506	CLA	C3D-C2D-C1D	-4.23	100.05	105.83
25	d	405	BCR	C29-C30-C25	4.23	116.59	110.44
23	A	405[A]	CLA	C3D-C4D-ND	4.23	116.87	109.99
23	c	513	CLA	CHD-C1D-ND	-4.23	118.85	124.80
23	C	502	CLA	C2C-C1C-NC	4.23	114.43	109.98
34	b	625	HTG	C1-O5-C5	4.23	120.15	112.56
23	C	509	CLA	C1-C2-C3	-4.23	119.27	126.20
23	A	404[B]	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
23	b	603	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
23	B	604	CLA	C3B-C2B-C1B	-4.22	102.19	107.17
23	d	402[A]	CLA	C2B-C1B-NB	4.22	114.71	110.33
23	B	614	CLA	C1-C2-C3	-4.22	119.29	126.20
23	D	403	CLA	C3D-C4D-ND	4.21	116.84	109.99
23	A	404[A]	CLA	CAA-C2A-C3A	-4.21	101.61	113.00
23	A	405[A]	CLA	CAA-C2A-C3A	-4.21	101.61	113.00
23	A	404[B]	CLA	CAA-C2A-C3A	-4.21	101.61	113.00
23	b	610	CLA	C3B-C2B-C1B	-4.21	102.21	107.17
23	B	615	CLA	C1D-CHD-C4C	-4.21	117.07	126.02
33	Z	101	LMG	O7-C10-C11	4.21	120.59	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C1D-CHD-C4C	-4.21	117.07	126.02
23	b	611	CLA	C3B-C4B-NB	4.21	114.29	110.53
23	B	610	CLA	C3D-C4D-ND	4.21	116.82	109.99
23	D	403	CLA	C3B-C2B-C1B	-4.20	102.21	107.17
23	d	403[A]	CLA	O2D-CGD-CBD	4.20	118.58	111.23
23	a	407	CLA	C1D-CHD-C4C	-4.20	117.08	126.02
23	C	511	CLA	CHD-C1D-ND	-4.20	118.89	124.80
23	D	402[A]	CLA	C3D-C4D-ND	4.20	116.82	109.99
23	C	503	CLA	C2B-C1B-NB	4.20	114.68	110.33
23	B	610	CLA	CAA-C2A-C3A	-4.20	101.65	113.00
23	c	512	CLA	C3D-C4D-ND	4.20	116.81	109.99
23	b	607	CLA	C1C-C2C-C3C	-4.20	102.56	106.98
23	c	505	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
23	b	602	CLA	CHD-C1D-ND	-4.20	118.90	124.80
23	b	616	CLA	O2D-CGD-O1D	-4.20	115.68	123.85
23	d	403[A]	CLA	C3C-C4C-NC	4.19	115.80	110.43
23	A	408	CLA	C3B-C4B-NB	4.19	114.27	110.53
23	B	613	CLA	O2D-CGD-CBD	4.19	118.56	111.23
23	B	606	CLA	C3C-C4C-NC	4.19	115.80	110.43
23	b	612	CLA	C3B-C4B-NB	4.19	114.27	110.53
23	b	610	CLA	O2A-CGA-CBA	4.19	124.61	111.83
23	B	609	CLA	C3C-C4C-NC	4.19	115.80	110.43
23	B	605	CLA	C2B-C1B-NB	4.19	114.67	110.33
23	B	606	CLA	C3D-C4D-ND	4.19	116.79	109.99
29	A	414[B]	PL9	C7-C3-C2	-4.19	118.45	123.39
23	c	511	CLA	C4A-NA-C1A	-4.18	104.77	106.68
23	b	612	CLA	C3D-C4D-ND	4.18	116.79	109.99
23	a	404[B]	CLA	C1C-C2C-C3C	-4.18	102.58	106.98
23	b	610	CLA	C3D-C4D-ND	4.18	116.78	109.99
23	c	508	CLA	C3C-C4C-NC	4.18	115.79	110.43
23	c	503	CLA	C3C-C4C-NC	4.18	115.79	110.43
23	A	406[B]	CLA	C2C-C1C-NC	4.18	114.37	109.98
23	b	612	CLA	C4A-NA-C1A	-4.18	104.77	106.68
25	Y	101	BCR	C16-C17-C18	-4.18	121.42	127.28
23	A	404[B]	CLA	C1D-CHD-C4C	-4.18	117.14	126.02
29	a	412[B]	PL9	C7-C3-C2	-4.18	118.47	123.39
23	A	406[A]	CLA	C1C-C2C-C3C	-4.18	102.59	106.98
23	B	615	CLA	C2B-C1B-NB	4.17	114.66	110.33
23	C	502	CLA	C3B-C2B-C1B	-4.17	102.25	107.17
29	d	406[B]	PL9	C7-C8-C9	-4.17	119.65	126.83
23	A	406[B]	CLA	O2D-CGD-CBD	4.17	118.52	111.23
23	b	608	CLA	C2B-C1B-NB	4.17	114.65	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402[B]	CLA	C1D-CHD-C4C	-4.17	117.16	126.02
25	b	617	BCR	C7-C8-C9	-4.16	120.08	126.23
23	D	402[A]	CLA	C1C-C2C-C3C	-4.16	102.60	106.98
23	B	608	CLA	C3C-C4C-NC	4.16	115.76	110.43
23	B	616	CLA	C2B-C1B-NB	4.16	114.64	110.33
24	A	407[B]	PHO	C1A-C2A-C3A	-4.16	98.89	102.84
23	c	509	CLA	C1C-C2C-C3C	-4.15	102.61	106.98
23	d	403[B]	CLA	C3B-C4B-NB	4.15	114.24	110.53
23	B	616	CLA	C4C-C3C-C2C	-4.15	100.84	106.89
26	a	409[A]	SQD	C1-C2-C3	-4.15	101.27	110.01
23	C	511	CLA	C3B-C4B-NB	4.15	114.24	110.53
23	b	612	CLA	C3B-C2B-C1B	-4.15	102.28	107.17
23	b	611	CLA	C1C-C2C-C3C	-4.15	102.61	106.98
23	B	605	CLA	CHD-C1D-ND	-4.15	118.97	124.80
23	c	508	CLA	C3D-C4D-ND	4.14	116.72	109.99
23	C	505	CLA	C3B-C2B-C1B	-4.14	102.29	107.17
23	B	601	CLA	C2C-C1C-NC	4.14	114.33	109.98
23	B	614	CLA	C1D-CHD-C4C	-4.13	117.23	126.02
23	D	402[B]	CLA	C1C-C2C-C3C	-4.13	102.63	106.98
23	b	616	CLA	C3D-C4D-ND	4.13	116.70	109.99
23	C	504	CLA	C3C-C4C-NC	4.13	115.72	110.43
23	C	503	CLA	C3D-C4D-ND	4.13	116.70	109.99
23	b	616	CLA	C2B-C1B-NB	4.13	114.61	110.33
23	B	606	CLA	O2D-CGD-O1D	-4.13	115.81	123.85
23	A	408	CLA	CHD-C1D-ND	-4.13	119.00	124.80
23	C	503	CLA	C1C-C2C-C3C	-4.13	102.64	106.98
23	a	404[B]	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
23	b	607	CLA	CHD-C1D-ND	-4.12	119.00	124.80
29	d	406[A]	PL9	C42-C43-C44	-4.12	118.19	127.62
23	B	604	CLA	C4A-NA-C1A	-4.12	104.80	106.68
23	B	616	CLA	C3B-C4B-NB	4.12	114.21	110.53
23	b	609	CLA	C2B-C1B-NB	4.12	114.60	110.33
23	b	608	CLA	C3B-C2B-C1B	-4.12	102.31	107.17
35	C	518[B]	DGD	O2G-C1B-C2B	4.11	120.38	111.48
23	b	616	CLA	C3C-C4C-NC	4.11	115.70	110.43
23	B	607	CLA	C3B-C2B-C1B	-4.11	102.32	107.17
23	d	403[A]	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
23	b	614	CLA	O2D-CGD-O1D	-4.11	115.84	123.85
26	a	409[A]	SQD	C1-O5-C5	-4.11	105.69	113.72
23	B	601	CLA	CHD-C1D-ND	-4.11	119.02	124.80
32	E	101[B]	LHG	O7-C7-C8	4.11	120.37	111.48
33	C	521	LMG	O6-C5-C4	4.11	117.10	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
29	a	412[B]	PL9	C7-C8-C9	-4.10	119.76	126.83
23	B	610	CLA	C2B-C1B-NB	4.10	114.58	110.33
23	c	504	CLA	C1-O2A-CGA	4.10	126.58	116.65
23	b	608	CLA	CMC-C2C-C1C	4.10	131.44	125.03
23	D	403	CLA	C2C-C1C-NC	4.10	114.29	109.98
23	C	509	CLA	C4A-NA-C1A	-4.10	104.81	106.68
23	b	602	CLA	C2C-C1C-NC	4.10	114.29	109.98
23	d	403[A]	CLA	C3B-C2B-C1B	-4.10	102.34	107.17
23	c	507	CLA	C3D-C4D-ND	4.10	116.65	109.99
23	c	513	CLA	C3B-C4B-NB	4.10	114.19	110.53
23	B	604	CLA	C1D-CHD-C4C	-4.09	117.32	126.02
23	C	511	CLA	C1-C2-C3	-4.09	119.49	126.20
23	d	402[A]	CLA	C3B-C2B-C1B	-4.09	102.34	107.17
23	C	508	CLA	C3C-C4C-NC	4.09	115.67	110.43
23	B	605	CLA	C1D-CHD-C4C	-4.09	117.33	126.02
23	A	406[A]	CLA	CHD-C1D-ND	-4.09	119.05	124.80
23	C	513	CLA	C1-C2-C3	-4.09	119.50	126.20
23	b	605	CLA	C3C-C4C-NC	4.09	115.66	110.43
23	b	611	CLA	CHD-C1D-ND	-4.08	119.06	124.80
29	a	412[A]	PL9	C32-C33-C34	-4.08	118.28	127.62
23	b	604	CLA	C3B-C2B-C1B	-4.08	102.36	107.17
23	b	616	CLA	C3B-C2B-C1B	-4.08	102.36	107.17
29	A	414[B]	PL9	C37-C38-C39	-4.07	118.30	127.62
23	b	609	CLA	C1-C2-C3	-4.07	119.52	126.20
23	D	403	CLA	CMB-C2B-C1B	4.07	131.62	125.42
23	c	506	CLA	O2D-CGD-CBD	4.07	118.35	111.23
35	C	517[A]	DGD	O2G-C1B-C2B	4.07	120.29	111.48
33	c	520	LMG	O7-C10-C11	4.07	120.28	111.48
33	C	521	LMG	O7-C10-C11	4.07	120.28	111.48
23	a	404[B]	CLA	CAA-C2A-C3A	-4.06	102.02	113.00
23	B	613	CLA	C3C-C4C-NC	4.06	115.63	110.43
23	C	509	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
23	b	606	CLA	C3D-C4D-ND	4.06	116.58	109.99
23	C	503	CLA	O2D-CGD-O1D	-4.06	115.95	123.85
23	C	504	CLA	C2C-C1C-NC	4.06	114.24	109.98
23	C	512	CLA	C3D-C4D-ND	4.05	116.58	109.99
23	C	503	CLA	C3C-C4C-NC	4.05	115.62	110.43
23	B	612	CLA	C2C-C1C-NC	4.05	114.24	109.98
23	d	402[A]	CLA	C1D-CHD-C4C	-4.05	117.41	126.02
23	d	403[B]	CLA	C2B-C1B-NB	4.05	114.53	110.33
23	A	406[A]	CLA	C3B-C2B-C1B	-4.05	102.39	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	CHD-C1D-ND	-4.05	119.10	124.80
23	A	405[B]	CLA	CHD-C1D-ND	-4.05	119.11	124.80
23	B	602	CLA	CMC-C2C-C1C	4.05	131.36	125.03
23	B	612	CLA	CHD-C1D-ND	-4.04	119.11	124.80
23	c	505	CLA	O2D-CGD-O1D	-4.04	115.97	123.85
23	b	607	CLA	C2B-C1B-NB	4.04	114.52	110.33
23	A	404[A]	CLA	CHD-C1D-ND	-4.04	119.11	124.80
23	b	601	CLA	CHD-C1D-ND	-4.04	119.11	124.80
23	b	610	CLA	C1D-CHD-C4C	-4.04	117.43	126.02
23	b	614	CLA	C3D-C4D-ND	4.04	116.55	109.99
23	c	510	CLA	C1D-CHD-C4C	-4.04	117.44	126.02
23	C	512	CLA	C1D-CHD-C4C	-4.04	117.44	126.02
23	b	611	CLA	C3C-C4C-NC	4.03	115.60	110.43
23	C	512	CLA	C3C-C4C-NC	4.03	115.60	110.43
23	A	408	CLA	O2D-CGD-CBD	4.03	118.28	111.23
23	B	610	CLA	C3B-C2B-C1B	-4.03	102.42	107.17
23	c	510	CLA	C3C-C4C-NC	4.03	115.59	110.43
23	A	405[B]	CLA	C4A-NA-C1A	-4.02	104.84	106.68
23	b	616	CLA	O2A-CGA-CBA	4.02	124.11	111.83
23	B	604	CLA	C1C-C2C-C3C	-4.02	102.76	106.98
23	D	402[B]	CLA	C3C-C4C-NC	4.01	115.57	110.43
23	B	615	CLA	C3C-C4C-NC	4.01	115.57	110.43
23	A	405[A]	CLA	C3B-C2B-C1B	-4.01	102.44	107.17
23	b	603	CLA	CHD-C1D-ND	-4.01	119.16	124.80
23	B	607	CLA	C3C-C4C-NC	4.01	115.57	110.43
23	C	510	CLA	CHD-C1D-ND	-4.01	119.16	124.80
23	A	405[B]	CLA	C3B-C2B-C1B	-4.01	102.45	107.17
25	d	405	BCR	C16-C17-C18	-4.01	121.66	127.28
23	B	613	CLA	C3D-C4D-ND	4.01	116.50	109.99
23	d	402[A]	CLA	CAA-C2A-C3A	-4.00	102.19	113.00
23	b	613	CLA	C2B-C1B-NB	4.00	114.47	110.33
23	c	509	CLA	C1D-CHD-C4C	-4.00	117.52	126.02
23	C	504	CLA	C1D-CHD-C4C	-3.99	117.53	126.02
23	C	506	CLA	C2B-C1B-NB	3.99	114.47	110.33
23	C	514	CLA	C3B-C4B-NB	3.99	114.09	110.53
23	b	608	CLA	C3B-C4B-NB	3.99	114.09	110.53
23	d	403[B]	CLA	C3C-C4C-NC	3.99	115.55	110.43
23	b	615	CLA	C1D-CHD-C4C	-3.99	117.54	126.02
23	b	601	CLA	C1D-CHD-C4C	-3.99	117.55	126.02
23	b	603	CLA	C3C-C4C-NC	3.99	115.54	110.43
23	a	405[B]	CLA	C2C-C1C-NC	3.98	114.17	109.98
23	C	513	CLA	C3C-C4C-NC	3.98	115.53	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	C1D-CHD-C4C	-3.98	117.55	126.02
23	C	511	CLA	C4A-NA-C1A	-3.98	104.86	106.68
23	C	511	CLA	C1D-CHD-C4C	-3.98	117.56	126.02
23	B	603	CLA	CHD-C1D-ND	-3.98	119.20	124.80
23	B	606	CLA	C3B-C2B-C1B	-3.97	102.48	107.17
23	B	613	CLA	C3B-C4B-NB	3.97	114.08	110.53
23	D	403	CLA	C3C-C4C-NC	3.97	115.52	110.43
23	B	610	CLA	C1C-C2C-C3C	-3.97	102.81	106.98
23	C	502	CLA	C1D-CHD-C4C	-3.97	117.59	126.02
23	C	511	CLA	C1C-C2C-C3C	-3.97	102.81	106.98
23	B	602	CLA	C3C-C4C-NC	3.96	115.51	110.43
23	b	604	CLA	C3D-C4D-ND	3.96	116.42	109.99
23	b	605	CLA	C1D-CHD-C4C	-3.96	117.61	126.02
23	B	609	CLA	O2D-CGD-CBD	3.96	118.15	111.23
23	B	601	CLA	C1D-CHD-C4C	-3.96	117.61	126.02
23	C	505	CLA	C3D-C4D-ND	3.96	116.42	109.99
23	b	604	CLA	C2B-C1B-NB	3.96	114.43	110.33
23	B	601	CLA	C3C-C4C-NC	3.95	115.50	110.43
23	D	402[B]	CLA	C2B-C1B-NB	3.95	114.43	110.33
23	b	609	CLA	C3B-C2B-C1B	-3.95	102.51	107.17
23	C	508	CLA	C3D-C4D-ND	3.95	116.41	109.99
23	c	511	CLA	C1D-CHD-C4C	-3.95	117.63	126.02
23	a	405[A]	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
23	A	404[B]	CLA	O2D-CGD-CBD	3.95	118.13	111.23
23	A	408	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
23	c	506	CLA	C3B-C4B-NB	3.95	114.05	110.53
23	b	604	CLA	CHD-C1D-ND	-3.95	119.25	124.80
23	B	603	CLA	C3C-C4C-NC	3.95	115.48	110.43
23	c	511	CLA	CHD-C1D-ND	-3.94	119.25	124.80
23	A	405[B]	CLA	CAA-C2A-C3A	-3.94	102.34	113.00
33	C	520	LMG	O7-C10-C11	3.94	120.01	111.48
23	C	508	CLA	C2B-C1B-NB	3.94	114.42	110.33
23	C	510	CLA	C1C-C2C-C3C	-3.94	102.83	106.98
31	B	628	LMT	C1'-O5'-C5'	-3.94	106.02	113.72
23	c	511	CLA	C3C-C4C-NC	3.94	115.47	110.43
23	B	602	CLA	C1D-CHD-C4C	-3.93	117.66	126.02
32	A	419[A]	LHG	O8-C23-O10	-3.93	113.79	123.63
23	B	602	CLA	O2D-CGD-O1D	-3.93	116.20	123.85
33	c	520	LMG	C3-C4-C5	3.93	117.35	110.23
23	C	508	CLA	CHD-C1D-ND	-3.93	119.28	124.80
23	B	605	CLA	C3C-C4C-NC	3.93	115.46	110.43
23	b	614	CLA	C1D-CHD-C4C	-3.93	117.68	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405[B]	CLA	C1D-CHD-C4C	-3.92	117.69	126.02
23	B	613	CLA	C4A-NA-C1A	-3.92	104.89	106.68
35	C	517[B]	DGD	O2G-C1B-C2B	3.91	119.95	111.48
23	B	615	CLA	CHD-C1D-ND	-3.91	119.29	124.80
23	b	613	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
23	a	404[B]	CLA	CHD-C1D-ND	-3.90	119.31	124.80
23	b	608	CLA	C1-C2-C3	-3.90	119.81	126.20
23	d	402[B]	CLA	CHD-C1D-ND	-3.90	119.31	124.80
23	c	501	CLA	CMB-C2B-C1B	3.89	131.35	125.42
23	d	402[B]	CLA	CMB-C2B-C1B	3.89	131.35	125.42
23	c	512	CLA	CHD-C1D-ND	-3.89	119.33	124.80
25	T	102	BCR	C16-C17-C18	-3.89	121.82	127.28
26	B	620	SQD	C3-C4-C5	3.89	117.28	110.23
23	A	408	CLA	C3C-C4C-NC	3.89	115.41	110.43
23	D	402[A]	CLA	C3C-C4C-NC	3.89	115.41	110.43
23	B	613	CLA	C1C-C2C-C3C	-3.89	102.89	106.98
23	B	614	CLA	C3D-C4D-ND	3.88	116.30	109.99
23	B	607	CLA	O2D-CGD-O1D	-3.88	116.29	123.85
23	b	613	CLA	C3B-C4B-NB	3.88	114.00	110.53
23	d	402[B]	CLA	C3B-C4B-NB	3.88	114.00	110.53
23	b	612	CLA	CMC-C2C-C1C	3.88	131.10	125.03
23	b	612	CLA	CAC-C3C-C4C	3.88	129.84	124.79
23	c	503	CLA	CHD-C1D-ND	-3.88	119.34	124.80
23	a	407	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
26	A	410[B]	SQD	C44-O6-C1	-3.88	105.48	113.80
35	c	516[A]	DGD	O2G-C1B-C2B	3.88	119.87	111.48
23	d	403[A]	CLA	CHD-C1D-ND	-3.88	119.35	124.80
23	B	610	CLA	C3C-C4C-NC	3.87	115.39	110.43
23	B	616	CLA	C1D-CHD-C4C	-3.87	117.79	126.02
23	c	506	CLA	C1C-C2C-C3C	-3.87	102.91	106.98
26	A	412	SQD	O47-C7-C8	3.87	119.85	111.48
23	C	506	CLA	C1-C2-C3	-3.87	119.86	126.20
24	A	407[A]	PHO	C1A-C2A-C3A	-3.87	99.16	102.84
23	C	506	CLA	C1D-CHD-C4C	-3.87	117.80	126.02
23	c	508	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
23	b	603	CLA	CAA-C2A-C3A	-3.86	102.56	113.00
23	b	606	CLA	C3C-C4C-NC	3.86	115.38	110.43
23	B	614	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
23	b	606	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
23	A	405[A]	CLA	CHD-C1D-ND	-3.86	119.37	124.80
33	m	101	LMG	O7-C10-C11	3.86	119.83	111.48
25	H	101	BCR	C16-C17-C18	-3.86	121.87	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404[A]	CLA	C3D-C4D-ND	3.85	116.25	109.99
23	b	603	CLA	O2D-CGD-O1D	-3.85	116.35	123.85
23	C	505	CLA	C3B-C4B-NB	3.85	113.97	110.53
23	B	611	CLA	CHD-C4C-NC	3.85	130.20	124.23
40	V	201	HEC	C4D-ND-C1D	3.85	112.10	105.82
23	C	502	CLA	CHD-C1D-ND	-3.85	119.38	124.80
23	d	403[A]	CLA	C1-C2-C3	-3.85	119.89	126.20
23	B	614	CLA	O2D-CGD-O1D	-3.85	116.35	123.85
23	b	615	CLA	CHD-C1D-ND	-3.85	119.39	124.80
23	B	605	CLA	CMB-C2B-C1B	3.84	131.27	125.42
29	A	414[A]	PL9	C37-C38-C39	-3.84	118.82	127.62
23	B	614	CLA	C3B-C4B-NB	3.84	113.96	110.53
23	c	513	CLA	C3C-C4C-NC	3.84	115.34	110.43
23	C	510	CLA	C3C-C4C-NC	3.83	115.34	110.43
23	B	605	CLA	C4-C3-C5	3.83	121.88	115.23
23	d	402[B]	CLA	C4A-NA-C1A	-3.83	104.93	106.68
23	a	405[A]	CLA	C3C-C4C-NC	3.83	115.34	110.43
23	C	513	CLA	C2C-C1C-NC	3.83	114.01	109.98
23	b	602	CLA	C1-C2-C3	-3.83	119.92	126.20
23	A	405[A]	CLA	CBC-CAC-C3C	-3.83	102.04	112.42
23	b	609	CLA	CHD-C1D-ND	-3.83	119.41	124.80
23	c	501	CLA	C3C-C4C-NC	3.83	115.33	110.43
23	C	514	CLA	C3C-C4C-NC	3.83	115.33	110.43
23	b	612	CLA	C2B-C1B-NB	3.82	114.29	110.33
23	c	512	CLA	C1D-CHD-C4C	-3.82	117.90	126.02
23	D	403	CLA	C1D-CHD-C4C	-3.82	117.91	126.02
23	c	507	CLA	C2B-C1B-NB	3.82	114.28	110.33
29	A	414[A]	PL9	C7-C3-C4	3.82	120.05	116.91
23	B	614	CLA	CHD-C1D-ND	-3.81	119.44	124.80
23	C	514	CLA	C1C-C2C-C3C	-3.81	102.98	106.98
23	B	608	CLA	C3B-C4B-NB	3.80	113.92	110.53
23	b	613	CLA	O2D-CGD-CBD	3.80	117.87	111.23
24	A	416[A]	PHO	C1A-C2A-C3A	-3.80	99.22	102.84
23	d	402[A]	CLA	CHD-C1D-ND	-3.80	119.46	124.80
23	d	404	CLA	C3C-C4C-NC	3.80	115.29	110.43
32	A	419[A]	LHG	O7-C7-C8	3.80	119.69	111.48
23	C	503	CLA	C1-C2-C3	-3.79	119.98	126.20
23	c	504	CLA	C3C-C4C-NC	3.79	115.29	110.43
33	c	519	LMG	O7-C10-C11	3.79	119.68	111.48
23	A	405[A]	CLA	CMC-C2C-C1C	3.79	130.95	125.03
23	c	502	CLA	O2D-CGD-O1D	-3.79	116.48	123.85
40	V	201	HEC	CBD-CAD-C3D	-3.78	102.08	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	C2B-C1B-NB	3.78	114.25	110.33
23	B	606	CLA	C1D-CHD-C4C	-3.78	117.99	126.02
23	b	609	CLA	C1D-CHD-C4C	-3.78	117.99	126.02
24	a	414[B]	PHO	C4-C3-C5	3.78	121.78	115.23
23	b	606	CLA	C4-C3-C5	3.77	121.78	115.23
23	a	405[B]	CLA	C3C-C4C-NC	3.77	115.26	110.43
23	b	604	CLA	C3B-C4B-NB	3.77	113.90	110.53
23	d	402[A]	CLA	CMB-C2B-C1B	3.77	131.16	125.42
23	b	610	CLA	C2B-C1B-NB	3.77	114.23	110.33
23	c	507	CLA	O2D-CGD-O1D	-3.77	116.51	123.85
23	A	406[A]	CLA	C1D-CHD-C4C	-3.77	118.01	126.02
23	b	616	CLA	C2C-C1C-NC	3.77	113.94	109.98
23	B	607	CLA	CBC-CAC-C3C	-3.77	102.21	112.42
23	B	609	CLA	C3B-C2B-C1B	-3.77	102.73	107.17
23	d	404	CLA	C2C-C1C-NC	3.77	113.94	109.98
26	A	410[B]	SQD	O47-C7-C8	3.77	119.63	111.48
23	b	602	CLA	C3C-C4C-NC	3.76	115.25	110.43
23	D	402[A]	CLA	C3B-C4B-NB	3.76	113.89	110.53
23	c	510	CLA	C3B-C4B-NB	3.76	113.89	110.53
23	B	610	CLA	CHD-C1D-ND	-3.76	119.51	124.80
33	Z	101	LMG	C1-C2-C3	3.76	117.92	110.01
23	A	404[B]	CLA	C3B-C4B-NB	3.75	113.88	110.53
35	c	517[B]	DGD	O2G-C1B-C2B	3.75	119.60	111.48
23	b	608	CLA	C1D-CHD-C4C	-3.75	118.06	126.02
26	a	410	SQD	O47-C7-C8	3.74	119.58	111.48
23	C	508	CLA	C1C-C2C-C3C	-3.74	103.04	106.98
38	E	102	HEM	CHD-C4C-NC	3.74	128.52	124.45
23	B	604	CLA	C3D-C2D-C1D	-3.74	100.73	105.83
26	A	410[A]	SQD	O47-C7-C8	3.74	119.56	111.48
23	B	608	CLA	O2D-CGD-O1D	-3.73	116.58	123.85
23	b	614	CLA	CHD-C1D-ND	-3.73	119.55	124.80
23	c	511	CLA	C3B-C4B-NB	3.73	113.86	110.53
23	B	608	CLA	CAC-C3C-C4C	3.73	129.64	124.79
23	c	512	CLA	C2C-C1C-NC	3.73	113.90	109.98
29	d	406[B]	PL9	C42-C43-C44	-3.73	119.09	127.62
23	a	404[B]	CLA	O2D-CGD-CBD	3.72	117.74	111.23
23	C	503	CLA	CHD-C1D-ND	-3.72	119.56	124.80
23	c	510	CLA	C3D-C4D-ND	3.72	116.04	109.99
23	B	612	CLA	C4C-C3C-C2C	-3.72	101.48	106.89
23	B	611	CLA	CHD-C1D-ND	-3.72	119.57	124.80
25	b	619	BCR	C24-C23-C22	-3.72	120.74	126.23
23	B	606	CLA	C1C-C2C-C3C	-3.71	103.07	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	C1C-C2C-C3C	-3.71	103.07	106.98
23	a	404[A]	CLA	O2A-CGA-O1A	-3.71	114.34	123.63
29	a	412[A]	PL9	C27-C28-C29	-3.71	119.13	127.62
23	B	604	CLA	C2B-C1B-NB	3.71	114.17	110.33
23	C	505	CLA	C2B-C1B-NB	3.71	114.17	110.33
23	b	615	CLA	CMB-C2B-C1B	3.71	131.06	125.42
23	d	403[A]	CLA	C3B-C4B-NB	3.71	113.84	110.53
23	b	610	CLA	C4C-C3C-C2C	-3.71	101.50	106.89
23	c	504	CLA	C1C-C2C-C3C	-3.70	103.08	106.98
23	a	404[A]	CLA	CHD-C1D-ND	-3.70	119.59	124.80
23	D	402[A]	CLA	C2B-C1B-NB	3.70	114.17	110.33
23	B	603	CLA	CAA-C2A-C3A	-3.70	103.00	113.00
25	T	102	BCR	C11-C10-C9	-3.70	122.09	127.28
23	B	607	CLA	C3B-C4B-NB	3.70	113.83	110.53
23	B	610	CLA	O2D-CGD-O1D	-3.70	116.66	123.85
23	b	613	CLA	C3D-C4D-ND	3.69	115.99	109.99
23	c	510	CLA	C1C-C2C-C3C	-3.69	103.09	106.98
38	f	101	HEM	CHD-C1D-ND	3.69	128.40	124.42
23	B	612	CLA	O2D-CGD-O1D	-3.69	116.66	123.85
23	c	508	CLA	C1D-CHD-C4C	-3.69	118.17	126.02
25	c	515	BCR	C7-C8-C9	-3.69	120.77	126.23
33	B	621	LMG	O8-C28-C29	3.69	123.09	111.83
35	C	518[A]	DGD	O2G-C1B-C2B	3.69	119.46	111.48
23	b	612	CLA	C1D-CHD-C4C	-3.69	118.18	126.02
23	b	615	CLA	C3C-C4C-NC	3.68	115.15	110.43
23	C	512	CLA	CAC-C3C-C4C	3.68	129.58	124.79
29	A	414[A]	PL9	C22-C23-C24	-3.68	119.19	127.62
23	b	611	CLA	C4A-NA-C1A	-3.68	105.00	106.68
23	b	614	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
32	L	101[A]	LHG	O7-C7-C8	3.68	119.43	111.48
23	D	403	CLA	CHD-C1D-ND	-3.68	119.63	124.80
32	d	414[B]	LHG	O7-C7-C8	3.67	119.43	111.48
23	c	504	CLA	C1D-CHD-C4C	-3.67	118.21	126.02
23	d	402[B]	CLA	CAA-C2A-C3A	-3.67	103.07	113.00
26	A	410[B]	SQD	O9-S-C6	3.67	112.24	106.76
23	B	610	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
23	B	604	CLA	C3B-C4B-NB	3.67	113.80	110.53
24	a	414[A]	PHO	C4-C3-C5	3.67	121.59	115.23
23	b	614	CLA	C1-C2-C3	-3.67	120.19	126.20
23	B	603	CLA	C3B-C4B-NB	3.67	113.80	110.53
25	B	617	BCR	C7-C8-C9	-3.67	120.81	126.23
23	A	406[A]	CLA	C3C-C4C-NC	3.67	115.13	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	C3B-C4B-NB	3.67	113.80	110.53
23	B	615	CLA	O2D-CGD-CBD	3.66	117.64	111.23
23	d	402[A]	CLA	C3C-C4C-NC	3.66	115.12	110.43
23	b	605	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
23	b	608	CLA	C4B-C3B-C2B	-3.66	102.75	107.30
23	C	514	CLA	C1D-CHD-C4C	-3.66	118.25	126.02
23	B	613	CLA	CHD-C1D-ND	-3.65	119.66	124.80
23	A	405[A]	CLA	C1D-CHD-C4C	-3.65	118.25	126.02
23	B	603	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
23	B	604	CLA	C3D-C4D-ND	3.65	115.92	109.99
23	b	611	CLA	C1-C2-C3	-3.65	120.22	126.20
29	a	412[A]	PL9	C15-C14-C16	3.65	121.56	115.23
23	b	612	CLA	C4-C3-C5	3.65	121.56	115.23
23	B	609	CLA	C1C-C2C-C3C	-3.65	103.15	106.98
23	c	501	CLA	C1C-C2C-C3C	-3.65	103.15	106.98
23	B	602	CLA	C3B-C4B-NB	3.65	113.78	110.53
25	b	619	BCR	C11-C10-C9	-3.64	122.17	127.28
23	A	406[A]	CLA	CMB-C2B-C1B	3.64	130.97	125.42
23	b	608	CLA	CHD-C1D-ND	-3.64	119.68	124.80
23	B	605	CLA	CHD-C4C-NC	3.64	129.88	124.23
29	D	405[A]	PL9	C42-C43-C44	-3.64	119.29	127.62
23	A	406[B]	CLA	C1C-C2C-C3C	-3.64	103.15	106.98
23	c	509	CLA	CHD-C1D-ND	-3.64	119.68	124.80
23	C	506	CLA	C1C-C2C-C3C	-3.64	103.16	106.98
23	b	612	CLA	C1-C2-C3	-3.63	120.24	126.20
23	B	611	CLA	C4C-C3C-C2C	-3.63	101.60	106.89
23	b	603	CLA	C3B-C4B-NB	3.63	113.77	110.53
23	b	616	CLA	CHD-C1D-ND	-3.63	119.69	124.80
23	C	513	CLA	C4-C3-C5	3.63	121.53	115.23
23	A	408	CLA	CAA-C2A-C3A	-3.63	103.19	113.00
25	B	617	BCR	C33-C5-C6	-3.63	120.52	124.48
23	B	615	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
25	d	405	BCR	C38-C26-C25	-3.63	120.53	124.48
23	B	608	CLA	CHD-C1D-ND	-3.63	119.70	124.80
25	y	101	BCR	C38-C26-C25	-3.62	120.53	124.48
23	A	404[A]	CLA	O2D-CGD-CBD	3.61	117.54	111.23
23	b	606	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
23	d	403[B]	CLA	C1D-CHD-C4C	-3.61	118.34	126.02
26	a	409[B]	SQD	C1-O5-C5	-3.61	106.67	113.72
23	c	505	CLA	CHD-C1D-ND	-3.61	119.72	124.80
23	A	408	CLA	C1D-CHD-C4C	-3.61	118.35	126.02
23	A	404[A]	CLA	O2A-CGA-CBA	3.61	122.83	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	402[B]	CLA	C3B-C4B-NB	3.61	113.75	110.53
23	A	405[A]	CLA	O2D-CGD-O1D	-3.61	116.83	123.85
23	c	505	CLA	CAC-C3C-C4C	3.60	129.48	124.79
26	a	409[A]	SQD	C44-O6-C1	-3.59	106.09	113.80
23	B	602	CLA	C1C-C2C-C3C	-3.59	103.20	106.98
38	E	102	HEM	C1B-NB-C4B	3.59	109.46	105.21
23	d	403[A]	CLA	O2A-CGA-CBA	3.59	122.77	111.83
23	B	610	CLA	CMB-C2B-C1B	3.59	130.88	125.42
32	L	101[B]	LHG	O7-C7-C8	3.59	119.24	111.48
23	b	609	CLA	C4C-C3C-C2C	-3.58	101.67	106.89
23	c	503	CLA	CMB-C2B-C1B	3.58	130.87	125.42
25	C	515	BCR	C33-C5-C6	-3.58	120.58	124.48
23	B	610	CLA	O2A-CGA-O1A	-3.58	114.68	123.63
32	A	419[B]	LHG	O7-C7-C8	3.58	119.22	111.48
23	B	608	CLA	C4C-C3C-C2C	-3.58	101.69	106.89
23	B	612	CLA	CAC-C3C-C4C	3.58	129.44	124.79
23	b	602	CLA	CAA-C2A-C3A	-3.57	103.34	113.00
23	d	402[B]	CLA	C3C-C4C-NC	3.57	115.01	110.43
23	d	403[A]	CLA	C2B-C1B-NB	3.57	114.03	110.33
23	B	602	CLA	CHD-C1D-ND	-3.57	119.78	124.80
23	b	612	CLA	C4B-C3B-C2B	-3.57	102.86	107.30
23	a	404[A]	CLA	C3C-C4C-NC	3.57	115.00	110.43
23	b	612	CLA	C4C-C3C-C2C	-3.57	101.69	106.89
23	a	407	CLA	CHD-C1D-ND	-3.57	119.78	124.80
23	c	505	CLA	C4C-C3C-C2C	-3.57	101.70	106.89
25	Y	101	BCR	C15-C14-C13	-3.57	122.28	127.28
25	D	404	BCR	C29-C30-C25	3.57	115.62	110.44
23	A	404[A]	CLA	C3C-C4C-NC	3.57	115.00	110.43
23	b	602	CLA	O2D-CGD-O1D	-3.56	116.91	123.85
23	B	608	CLA	C1D-CHD-C4C	-3.56	118.45	126.02
23	b	601	CLA	O2D-CGD-O1D	-3.56	116.91	123.85
23	B	608	CLA	C1-C2-C3	-3.56	120.36	126.20
23	C	507	CLA	C1-C2-C3	-3.56	120.36	126.20
32	d	408[B]	LHG	O7-C7-C8	3.56	119.18	111.48
29	a	412[B]	PL9	C15-C14-C16	3.56	121.40	115.23
23	c	513	CLA	C1C-C2C-C3C	-3.56	103.24	106.98
23	C	502	CLA	C3C-C4C-NC	3.56	114.99	110.43
34	V	202	HTG	C1-O5-C5	3.55	116.95	112.19
23	a	407	CLA	CMC-C2C-C1C	3.55	130.58	125.03
23	a	404[A]	CLA	O2D-CGD-CBD	3.55	117.43	111.23
33	Z	101	LMG	O6-C1-C2	3.55	117.66	110.37
23	A	404[A]	CLA	C1D-CHD-C4C	-3.54	118.49	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	C3B-C4B-NB	3.54	113.69	110.53
29	a	412[B]	PL9	C27-C28-C29	-3.54	119.52	127.62
23	C	510	CLA	C3B-C4B-NB	3.54	113.69	110.53
23	c	501	CLA	C1-C2-C3	-3.54	120.40	126.20
23	A	405[B]	CLA	C3C-C4C-NC	3.54	114.96	110.43
23	a	404[A]	CLA	O2A-CGA-CBA	3.54	122.61	111.83
34	b	625	HTG	O5-C5-C4	3.53	116.07	109.70
23	c	508	CLA	C1-C2-C3	-3.53	120.41	126.20
23	c	503	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
23	c	511	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
23	b	612	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
23	B	612	CLA	CMC-C2C-C1C	3.53	130.55	125.03
23	C	506	CLA	CHD-C1D-ND	-3.53	119.84	124.80
23	b	614	CLA	C3C-C4C-NC	3.53	114.95	110.43
23	a	405[A]	CLA	C1D-CHD-C4C	-3.53	118.53	126.02
24	A	416[A]	PHO	C4D-CHA-CBD	3.52	110.14	108.45
23	A	408	CLA	C1-C2-C3	-3.52	120.43	126.20
25	A	409	BCR	C24-C23-C22	-3.52	121.03	126.23
23	C	504	CLA	C1-C2-C3	-3.52	120.44	126.20
23	C	509	CLA	C1D-CHD-C4C	-3.51	118.56	126.02
23	a	405[B]	CLA	C1C-C2C-C3C	-3.51	103.29	106.98
23	b	615	CLA	C3B-C4B-NB	3.51	113.66	110.53
23	A	406[A]	CLA	O2A-CGA-O1A	-3.51	114.85	123.63
23	C	513	CLA	CHD-C1D-ND	-3.51	119.87	124.80
34	b	622	HTG	C1'-S1-C1	3.51	108.02	100.45
24	A	416[B]	PHO	C1A-C2A-C3A	-3.50	99.51	102.84
23	c	508	CLA	CHD-C1D-ND	-3.50	119.87	124.80
23	A	406[B]	CLA	C3C-C4C-NC	3.50	114.91	110.43
23	c	506	CLA	C3C-C4C-NC	3.50	114.91	110.43
25	K	102	BCR	C7-C8-C9	-3.50	121.06	126.23
23	b	605	CLA	CMB-C2B-C1B	3.49	130.74	125.42
23	B	605	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
23	C	512	CLA	CHD-C1D-ND	-3.48	119.90	124.80
23	c	506	CLA	C1D-CHD-C4C	-3.48	118.61	126.02
23	A	405[A]	CLA	C3C-C4C-NC	3.48	114.89	110.43
23	a	405[B]	CLA	C1D-CHD-C4C	-3.48	118.62	126.02
23	c	508	CLA	C3B-C4B-NB	3.48	113.64	110.53
23	C	508	CLA	CMB-C2B-C1B	3.48	130.72	125.42
24	A	407[A]	PHO	CMA-C3A-C4A	-3.48	107.11	114.61
23	b	608	CLA	CAC-C3C-C4C	3.48	129.32	124.79
25	c	514	BCR	C15-C14-C13	-3.48	122.40	127.28
23	c	507	CLA	C3C-C4C-NC	3.48	114.88	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	403[B]	CLA	C1-C2-C3	-3.48	120.50	126.20
23	B	607	CLA	C4B-C3B-C2B	-3.47	102.98	107.30
23	B	607	CLA	CMC-C2C-C1C	3.47	130.46	125.03
23	C	503	CLA	C1D-CHD-C4C	-3.47	118.64	126.02
23	b	602	CLA	C1D-CHD-C4C	-3.47	118.64	126.02
23	b	603	CLA	C2A-C1A-CHA	-3.47	117.84	123.87
29	a	412[B]	PL9	C37-C38-C39	-3.47	119.68	127.62
26	A	410[A]	SQD	C44-O6-C1	-3.47	106.36	113.80
23	b	601	CLA	C3C-C4C-NC	3.47	114.88	110.43
23	b	613	CLA	CHD-C1D-ND	-3.46	119.93	124.80
23	C	508	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
29	d	406[A]	PL9	C40-C39-C41	3.46	121.23	115.23
23	c	502	CLA	C3C-C4C-NC	3.46	114.86	110.43
23	c	510	CLA	CMC-C2C-C1C	3.46	130.44	125.03
25	k	101	BCR	C29-C30-C25	3.46	115.46	110.44
23	c	503	CLA	C1-C2-C3	-3.46	120.53	126.20
23	d	404	CLA	C1C-C2C-C3C	-3.46	103.34	106.98
23	C	509	CLA	CHD-C1D-ND	-3.46	119.94	124.80
26	B	620	SQD	C1-O5-C5	-3.45	106.97	113.72
23	C	505	CLA	C1-O2A-CGA	3.45	125.01	116.65
40	v	201	HEC	C4D-ND-C1D	3.45	111.44	105.82
38	E	102	HEM	CBD-CAD-C3D	-3.44	103.01	112.53
23	b	606	CLA	CHD-C4C-NC	3.44	129.57	124.23
25	C	515	BCR	C7-C8-C9	-3.44	121.15	126.23
23	c	511	CLA	C1C-C2C-C3C	-3.44	103.37	106.98
23	C	509	CLA	C4C-C3C-C2C	-3.44	101.89	106.89
29	A	414[B]	PL9	C22-C23-C24	-3.43	119.76	127.62
23	b	611	CLA	C1D-CHD-C4C	-3.43	118.72	126.02
25	k	101	BCR	C7-C8-C9	-3.43	121.16	126.23
32	b	629[B]	LHG	O7-C7-C8	3.43	118.90	111.48
23	A	406[B]	CLA	CAA-C2A-C3A	-3.43	103.73	113.00
23	A	406[A]	CLA	C3B-C4B-NB	3.43	113.59	110.53
29	A	414[A]	PL9	C15-C14-C16	3.43	121.18	115.23
32	A	419[B]	LHG	O8-C23-O10	-3.43	115.06	123.63
23	c	512	CLA	O2D-CGD-O1D	-3.43	117.18	123.85
23	B	607	CLA	C2B-C1B-NB	3.42	113.88	110.33
23	C	513	CLA	CHD-C4C-NC	3.42	129.54	124.23
23	a	407	CLA	CAA-C2A-C3A	-3.42	103.75	113.00
23	c	508	CLA	CMB-C2B-C1B	3.42	130.63	125.42
23	C	512	CLA	CMC-C2C-C1C	3.42	130.38	125.03
23	C	504	CLA	C4C-C3C-C2C	-3.42	101.92	106.89
23	b	612	CLA	C1C-C2C-C3C	-3.42	103.39	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	C	521	LMG	C3-C4-C5	3.41	116.42	110.23
23	b	615	CLA	O2D-CGD-CBD	3.41	117.19	111.23
23	b	612	CLA	C2A-C1A-CHA	-3.41	117.95	123.87
23	C	505	CLA	C1D-CHD-C4C	-3.41	118.77	126.02
23	b	610	CLA	O2A-CGA-O1A	-3.41	115.10	123.63
23	B	602	CLA	CAA-C2A-C3A	-3.41	103.80	113.00
23	b	603	CLA	C1C-C2C-C3C	-3.40	103.40	106.98
23	b	613	CLA	C4C-C3C-C2C	-3.40	101.94	106.89
23	C	510	CLA	C1D-CHD-C4C	-3.40	118.79	126.02
23	b	613	CLA	C1D-CHD-C4C	-3.40	118.80	126.02
29	a	412[A]	PL9	C30-C29-C31	3.40	121.13	115.23
23	b	601	CLA	C1C-C2C-C3C	-3.40	103.41	106.98
23	B	613	CLA	C4-C3-C5	3.40	121.13	115.23
23	a	405[A]	CLA	C1-C2-C3	-3.39	120.64	126.20
23	b	616	CLA	C4C-C3C-C2C	-3.39	101.95	106.89
23	b	613	CLA	C4B-C3B-C2B	-3.39	103.09	107.30
25	d	405	BCR	C10-C11-C12	-3.39	113.39	123.20
23	b	616	CLA	CHD-C4C-NC	3.39	129.48	124.23
23	C	503	CLA	CMB-C2B-C1B	3.38	130.57	125.42
23	b	608	CLA	C3C-C4C-NC	3.38	114.76	110.43
23	c	509	CLA	C3C-C4C-NC	3.38	114.76	110.43
23	A	405[A]	CLA	C4B-C3B-C2B	-3.38	103.10	107.30
23	C	507	CLA	C1D-CHD-C4C	-3.37	118.85	126.02
35	c	517[A]	DGD	O2G-C1B-C2B	3.37	118.77	111.48
25	y	101	BCR	C24-C23-C22	-3.37	121.25	126.23
23	a	404[A]	CLA	C4B-C3B-C2B	-3.37	103.11	107.30
23	A	404[B]	CLA	C3C-C4C-NC	3.37	114.74	110.43
23	B	614	CLA	C3C-C4C-NC	3.36	114.74	110.43
23	c	509	CLA	C4B-C3B-C2B	-3.36	103.12	107.30
23	d	403[A]	CLA	C1D-CHD-C4C	-3.36	118.87	126.02
25	C	516	BCR	C33-C5-C6	-3.36	120.82	124.48
23	C	514	CLA	C1-C2-C3	-3.36	120.69	126.20
23	a	404[B]	CLA	CHC-C1C-C2C	-3.36	117.40	126.95
33	z	101	LMG	O7-C10-C11	3.35	118.74	111.48
29	D	405[A]	PL9	C53-C6-C1	3.35	122.15	115.28
23	A	405[B]	CLA	CHD-C4C-NC	3.35	129.43	124.23
23	C	506	CLA	CAC-C3C-C4C	3.35	129.15	124.79
23	B	605	CLA	C1C-C2C-C3C	-3.35	103.46	106.98
23	C	512	CLA	C1-O2A-CGA	3.35	124.75	116.65
25	h	101	BCR	C38-C26-C25	-3.35	120.83	124.48
23	B	611	CLA	C2A-C1A-CHA	-3.35	118.06	123.87
23	c	510	CLA	CHD-C1D-ND	-3.35	120.09	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405[B]	CLA	C4B-C3B-C2B	-3.34	103.14	107.30
23	C	505	CLA	C4B-C3B-C2B	-3.34	103.14	107.30
32	d	414[B]	LHG	O8-C23-C24	3.34	122.03	111.83
32	d	414[A]	LHG	O8-C23-O10	-3.34	115.27	123.63
25	D	404	BCR	C10-C11-C12	-3.34	113.52	123.20
23	C	507	CLA	CBC-CAC-C3C	-3.34	103.37	112.42
33	C	520	LMG	O8-C28-C29	3.34	122.02	111.83
23	C	504	CLA	C4-C3-C5	3.34	121.02	115.23
23	A	405[A]	CLA	C3B-C4B-NB	3.34	113.51	110.53
23	B	604	CLA	C4C-C3C-C2C	-3.34	102.03	106.89
23	a	404[A]	CLA	C1-C2-C3	-3.34	120.73	126.20
23	b	602	CLA	CMB-C2B-C1B	3.34	130.50	125.42
29	a	412[A]	PL9	C17-C18-C19	-3.34	119.99	127.62
23	B	615	CLA	CMC-C2C-C1C	3.34	130.25	125.03
29	A	414[B]	PL9	C7-C3-C4	3.34	119.66	116.91
23	c	503	CLA	C1C-C2C-C3C	-3.33	103.47	106.98
32	d	414[A]	LHG	O8-C23-C24	3.33	122.00	111.83
23	A	406[A]	CLA	C4B-C3B-C2B	-3.33	103.16	107.30
23	b	609	CLA	CAC-C3C-C4C	3.33	129.12	124.79
23	b	605	CLA	CHD-C4C-NC	3.33	129.40	124.23
29	a	412[A]	PL9	C35-C34-C36	3.33	121.01	115.23
29	A	414[A]	PL9	C27-C28-C29	-3.33	120.01	127.62
23	B	616	CLA	CAC-C3C-C4C	3.33	129.12	124.79
25	y	101	BCR	C15-C14-C13	-3.33	122.61	127.28
23	A	404[B]	CLA	O2A-CGA-CBA	3.33	121.97	111.83
23	C	509	CLA	C4B-C3B-C2B	-3.33	103.17	107.30
23	B	607	CLA	C4-C3-C5	3.32	121.00	115.23
23	B	615	CLA	C3B-C4B-NB	3.32	113.50	110.53
25	K	102	BCR	C38-C26-C25	-3.32	120.86	124.48
23	b	604	CLA	C4B-C3B-C2B	-3.32	103.17	107.30
24	a	406[B]	PHO	CMA-C3A-C4A	-3.32	107.45	114.61
23	B	603	CLA	CAC-C3C-C4C	3.32	129.11	124.79
23	B	607	CLA	O2A-CGA-O1A	-3.32	115.32	123.63
25	T	102	BCR	C12-C13-C14	-3.32	113.79	119.01
23	C	502	CLA	CAC-C3C-C4C	3.32	129.11	124.79
23	c	505	CLA	C1D-CHD-C4C	-3.32	118.97	126.02
23	B	612	CLA	C4A-NA-C1A	-3.32	105.17	106.68
23	b	607	CLA	C4B-C3B-C2B	-3.32	103.18	107.30
23	d	404	CLA	C1D-CHD-C4C	-3.31	118.98	126.02
23	C	512	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
23	B	613	CLA	O2A-CGA-O1A	-3.31	115.34	123.63
23	c	502	CLA	C3B-C4B-NB	3.31	113.48	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	C1C-C2C-C3C	-3.31	103.50	106.98
23	a	404[B]	CLA	CAC-C3C-C4C	3.31	129.09	124.79
29	D	405[A]	PL9	C25-C24-C26	3.31	120.97	115.23
23	B	614	CLA	CAC-C3C-C4C	3.31	129.09	124.79
23	b	616	CLA	O2A-CGA-O1A	-3.30	115.36	123.63
23	c	506	CLA	C4B-C3B-C2B	-3.30	103.19	107.30
26	F	102	SQD	C1-C2-C3	-3.30	103.07	110.01
23	c	509	CLA	CHC-C1C-C2C	-3.30	117.57	126.95
23	b	604	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
23	c	510	CLA	C4-C3-C5	3.30	120.95	115.23
23	A	406[B]	CLA	C1D-CHD-C4C	-3.30	119.01	126.02
23	B	608	CLA	C1C-C2C-C3C	-3.30	103.51	106.98
29	D	405[A]	PL9	C17-C18-C19	-3.30	120.08	127.62
23	c	512	CLA	O2A-CGA-CBA	3.29	121.88	111.83
23	c	507	CLA	C1D-CHD-C4C	-3.29	119.02	126.02
23	d	404	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
23	D	403	CLA	C4C-C3C-C2C	-3.29	102.10	106.89
23	d	402[B]	CLA	CHD-C4C-NC	3.29	129.33	124.23
23	c	507	CLA	C4-C3-C5	3.29	120.94	115.23
23	c	505	CLA	C1C-C2C-C3C	-3.29	103.52	106.98
23	c	502	CLA	CHC-C1C-C2C	-3.29	117.60	126.95
23	A	404[A]	CLA	C1-C2-C3	-3.29	120.81	126.20
23	c	502	CLA	CBC-CAC-C3C	-3.29	103.50	112.42
32	d	408[A]	LHG	O7-C7-C8	3.29	118.59	111.48
33	C	521	LMG	O8-C28-C29	3.29	121.86	111.83
23	b	614	CLA	CHD-C4C-NC	3.29	129.33	124.23
23	c	512	CLA	C4-C3-C5	3.28	120.93	115.23
29	D	405[B]	PL9	C53-C6-C1	3.28	122.00	115.28
23	B	606	CLA	CMC-C2C-C1C	3.28	130.16	125.03
23	c	503	CLA	CMC-C2C-C1C	3.28	130.16	125.03
23	B	611	CLA	CHB-C4A-NA	3.28	129.14	124.40
25	D	404	BCR	C37-C22-C23	3.28	123.10	118.09
23	b	607	CLA	C4C-C3C-C2C	-3.28	102.12	106.89
23	B	613	CLA	O2A-CGA-CBA	3.28	121.83	111.83
23	d	403[B]	CLA	C4B-C3B-C2B	-3.28	103.22	107.30
23	C	511	CLA	C3C-C4C-NC	3.28	114.63	110.43
23	D	403	CLA	C1C-C2C-C3C	-3.28	103.53	106.98
23	B	601	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
23	a	404[B]	CLA	C3C-C4C-NC	3.28	114.63	110.43
23	d	403[A]	CLA	C4B-C3B-C2B	-3.27	103.23	107.30
23	a	404[B]	CLA	O2A-CGA-CBA	3.27	121.81	111.83
25	D	404	BCR	C38-C26-C25	-3.27	120.92	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	CAC-C3C-C4C	3.27	129.04	124.79
26	F	102	SQD	O8-S-C6	3.27	112.28	105.97
35	h	102	DGD	O2G-C1B-C2B	3.27	118.55	111.48
32	A	419[A]	LHG	O8-C23-C24	3.26	121.79	111.83
23	c	507	CLA	CBC-CAC-C3C	-3.26	103.58	112.42
23	C	513	CLA	C1C-C2C-C3C	-3.26	103.55	106.98
23	C	508	CLA	C4C-C3C-C2C	-3.26	102.15	106.89
23	d	402[B]	CLA	C4B-C3B-C2B	-3.25	103.25	107.30
33	a	415	LMG	C7-O1-C1	-3.25	106.82	113.80
23	C	512	CLA	C1C-C2C-C3C	-3.25	103.56	106.98
23	B	605	CLA	C1-C2-C3	-3.25	120.87	126.20
23	B	609	CLA	C1D-CHD-C4C	-3.25	119.11	126.02
23	C	507	CLA	CHC-C1C-C2C	-3.25	117.71	126.95
23	B	601	CLA	C4C-C3C-C2C	-3.25	102.16	106.89
34	b	622	HTG	O2-C2-C1	3.25	116.07	110.30
31	b	627	LMT	C3'-C4'-C5'	-3.25	103.73	110.93
23	C	505	CLA	C4A-NA-C1A	-3.25	105.20	106.68
32	d	414[A]	LHG	O7-C7-C8	3.24	118.50	111.48
23	c	513	CLA	CMB-C2B-C1B	3.24	130.36	125.42
23	c	512	CLA	C1C-C2C-C3C	-3.24	103.57	106.98
32	A	419[A]	LHG	C5-O7-C7	-3.24	110.03	117.80
24	A	407[B]	PHO	CMA-C3A-C4A	-3.24	107.62	114.61
29	A	414[B]	PL9	C27-C28-C29	-3.24	120.21	127.62
23	a	407	CLA	C4A-NA-C1A	-3.24	105.20	106.68
29	A	414[B]	PL9	C15-C14-C16	3.24	120.85	115.23
23	b	613	CLA	O2A-CGA-O1A	-3.24	115.53	123.63
24	A	407[A]	PHO	O1D-CGD-CBD	-3.24	119.81	124.72
23	d	402[A]	CLA	C3B-C4B-NB	3.24	113.42	110.53
34	b	622	HTG	O5-C5-C4	3.23	115.52	109.70
23	b	612	CLA	CHD-C1D-ND	-3.23	120.26	124.80
23	c	502	CLA	CHD-C1D-ND	-3.23	120.26	124.80
23	a	407	CLA	CHD-C4C-NC	3.22	129.23	124.23
23	B	612	CLA	C1D-CHD-C4C	-3.22	119.17	126.02
23	C	511	CLA	CHD-C4C-NC	3.22	129.23	124.23
23	b	612	CLA	O2A-CGA-O1A	-3.22	115.57	123.63
23	c	509	CLA	O2A-CGA-CBA	3.22	121.66	111.83
24	a	414[A]	PHO	C4A-C3A-C2A	-3.22	99.77	102.84
23	C	503	CLA	CAC-C3C-C4C	3.22	128.98	124.79
23	B	614	CLA	CMC-C2C-C1C	3.22	130.06	125.03
35	c	516[B]	DGD	O2G-C1B-C2B	3.22	118.44	111.48
23	b	611	CLA	CHC-C1C-C2C	-3.22	117.80	126.95
23	C	504	CLA	CHD-C4C-NC	3.22	129.22	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	C4B-C3B-C2B	-3.22	103.30	107.30
23	A	405[B]	CLA	CBC-CAC-C3C	-3.22	103.70	112.42
23	B	602	CLA	CAC-C3C-C4C	3.21	128.97	124.79
23	A	404[A]	CLA	O2A-CGA-O1A	-3.21	115.59	123.63
23	C	511	CLA	C4-C3-C5	3.21	120.81	115.23
23	C	502	CLA	C1C-C2C-C3C	-3.21	103.60	106.98
23	c	512	CLA	CMB-C2B-C1B	3.21	130.31	125.42
23	c	506	CLA	CAC-C3C-C4C	3.21	128.97	124.79
23	c	506	CLA	CHC-C1C-C2C	-3.21	117.82	126.95
23	A	405[B]	CLA	CMC-C2C-C1C	3.21	130.05	125.03
23	D	403	CLA	CAC-C3C-C4C	3.21	128.96	124.79
23	c	504	CLA	C4C-C3C-C2C	-3.21	102.22	106.89
23	c	512	CLA	C3C-C4C-NC	3.21	114.54	110.43
23	D	402[B]	CLA	O2A-CGA-CBA	3.20	121.60	111.83
23	B	606	CLA	O2A-CGA-O1A	-3.20	115.62	123.63
23	A	405[B]	CLA	C3B-C4B-NB	3.20	113.39	110.53
23	B	605	CLA	O2A-CGA-O1A	-3.20	115.62	123.63
23	D	402[A]	CLA	C1D-CHD-C4C	-3.20	119.22	126.02
23	A	406[A]	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
23	a	404[A]	CLA	CHC-C1C-C2C	-3.20	117.86	126.95
23	c	511	CLA	CMC-C2C-C1C	3.20	130.03	125.03
23	d	403[B]	CLA	O2A-CGA-CBA	3.20	121.58	111.83
29	a	412[B]	PL9	C30-C29-C31	3.19	120.77	115.23
23	C	511	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
23	a	404[A]	CLA	CAA-C2A-C1A	-3.19	101.52	111.97
23	C	506	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
23	B	609	CLA	C4B-C3B-C2B	-3.19	103.34	107.30
23	b	611	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
23	b	602	CLA	CAC-C3C-C4C	3.19	128.94	124.79
38	E	102	HEM	CHD-C1D-ND	3.19	127.85	124.42
23	b	602	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
23	c	513	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
23	b	604	CLA	CMC-C2C-C1C	3.18	130.01	125.03
23	d	402[A]	CLA	CHD-C4C-NC	3.18	129.17	124.23
23	b	603	CLA	CMA-C3A-C2A	-3.18	101.68	113.98
23	C	509	CLA	CHC-C1C-C2C	-3.18	117.91	126.95
23	b	603	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
29	A	414[B]	PL9	C17-C18-C19	-3.18	120.35	127.62
23	C	504	CLA	CMB-C2B-C1B	3.18	130.26	125.42
26	f	102	SQD	O5-C1-C2	3.18	116.90	110.37
23	B	610	CLA	CAA-CBA-CGA	-3.18	104.19	113.21
23	B	611	CLA	O2D-CGD-O1D	-3.18	117.67	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	C4C-C3C-C2C	-3.17	102.27	106.89
23	B	603	CLA	O2A-CGA-O1A	-3.17	115.69	123.63
29	D	405[B]	PL9	C27-C28-C29	-3.17	120.36	127.62
23	b	605	CLA	C2A-C1A-CHA	-3.17	118.36	123.87
23	b	609	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
38	f	101	HEM	CHA-C4D-ND	3.17	128.28	124.37
23	B	603	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
23	D	402[A]	CLA	O2A-CGA-CBA	3.16	121.48	111.83
29	d	406[A]	PL9	C37-C38-C39	-3.16	120.38	127.62
23	a	405[A]	CLA	CHD-C4C-NC	3.16	129.13	124.23
23	C	506	CLA	C3B-C4B-NB	3.16	113.35	110.53
25	c	514	BCR	C16-C17-C18	-3.16	122.85	127.28
23	c	505	CLA	CMB-C2B-C1B	3.16	130.23	125.42
23	A	408	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
23	C	506	CLA	CMC-C2C-C1C	3.16	129.97	125.03
25	D	404	BCR	C28-C27-C26	-3.16	108.42	114.06
23	D	402[B]	CLA	C1D-CHD-C4C	-3.16	119.31	126.02
23	B	610	CLA	C4C-C3C-C2C	-3.16	102.30	106.89
23	a	407	CLA	C4C-C3C-C2C	-3.16	102.30	106.89
29	d	406[B]	PL9	C10-C9-C11	3.16	120.70	115.23
23	a	405[A]	CLA	C3B-C4B-NB	3.15	113.34	110.53
29	a	412[A]	PL9	C42-C43-C44	-3.15	120.41	127.62
23	C	513	CLA	O2A-CGA-CBA	3.15	121.45	111.83
23	c	503	CLA	C4C-C3C-C2C	-3.15	102.30	106.89
29	d	406[B]	PL9	C37-C38-C39	-3.15	120.41	127.62
23	D	403	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
23	B	601	CLA	CHD-C4C-NC	3.15	129.11	124.23
33	m	101	LMG	O8-C28-C29	3.15	121.43	111.83
23	b	610	CLA	CHD-C1D-ND	-3.15	120.37	124.80
23	a	405[B]	CLA	CMC-C2C-C1C	3.15	129.95	125.03
26	b	620	SQD	C3-C4-C5	3.15	115.94	110.23
23	C	511	CLA	CHC-C1C-C2C	-3.15	118.01	126.95
23	d	403[A]	CLA	O2D-CGD-O1D	-3.15	117.73	123.85
26	F	102	SQD	C44-O6-C1	-3.14	107.05	113.80
35	h	102	DGD	O1G-C1A-O1A	-3.14	115.77	123.63
23	A	406[A]	CLA	O2A-CGA-CBA	3.14	121.42	111.83
23	b	614	CLA	CMC-C2C-C1C	3.14	129.94	125.03
25	K	102	BCR	C24-C23-C22	-3.14	121.59	126.23
24	a	406[B]	PHO	O1D-CGD-CBD	-3.14	119.97	124.72
23	B	614	CLA	O2A-CGA-CBA	3.14	121.39	111.83
23	d	402[B]	CLA	CHC-C1C-C2C	-3.13	118.04	126.95
25	b	617	BCR	C29-C30-C25	3.13	114.99	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	C3B-C4B-NB	3.13	113.33	110.53
23	C	512	CLA	C4C-C3C-C2C	-3.13	102.33	106.89
23	A	404[A]	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
23	B	610	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
23	c	502	CLA	CHD-C4C-NC	3.13	129.09	124.23
23	B	615	CLA	C11-C10-C8	-3.13	105.56	115.97
29	D	405[B]	PL9	C10-C9-C11	3.13	120.66	115.23
23	b	604	CLA	C1D-CHD-C4C	-3.13	119.37	126.02
23	a	407	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
38	f	101	HEM	CHD-C4C-NC	3.13	127.86	124.45
35	h	102	DGD	O1G-C1A-C2A	3.13	121.36	111.83
23	d	403[B]	CLA	CHC-C1C-C2C	-3.12	118.07	126.95
23	a	407	CLA	C3B-C4B-NB	3.12	113.32	110.53
31	B	628	LMT	C4B-C3B-C2B	3.12	116.31	110.83
23	A	408	CLA	O2A-CGA-CBA	3.12	121.35	111.83
33	c	520	LMG	C9-C8-C7	-3.12	104.51	111.78
23	d	403[B]	CLA	C4-C3-C5	3.12	120.65	115.23
23	b	615	CLA	CHC-C1C-C2C	-3.12	118.08	126.95
23	C	507	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
25	H	101	BCR	C24-C23-C22	-3.12	121.62	126.23
29	a	412[B]	PL9	C42-C43-C44	-3.12	120.48	127.62
23	A	405[A]	CLA	CMB-C2B-C1B	3.12	130.17	125.42
23	C	503	CLA	C3B-C4B-NB	3.12	113.31	110.53
23	b	604	CLA	CMB-C2B-C1B	3.12	130.17	125.42
23	A	406[B]	CLA	C4B-C3B-C2B	-3.11	103.43	107.30
26	a	409[B]	SQD	C1-C2-C3	-3.11	103.46	110.01
25	h	101	BCR	C7-C8-C9	-3.11	121.63	126.23
23	b	616	CLA	CBC-CAC-C3C	-3.11	103.99	112.42
24	a	406[A]	PHO	O1D-CGD-CBD	-3.11	120.01	124.72
23	b	603	CLA	C4B-C3B-C2B	-3.11	103.44	107.30
26	a	409[B]	SQD	C45-O47-C7	-3.11	110.36	117.80
23	a	404[B]	CLA	C4B-C3B-C2B	-3.11	103.44	107.30
26	a	410	SQD	O48-C23-C24	3.11	121.31	111.83
23	c	501	CLA	C4C-C3C-C2C	-3.11	102.37	106.89
29	A	414[B]	PL9	C20-C19-C21	3.11	120.62	115.23
23	B	605	CLA	C4C-C3C-C2C	-3.10	102.37	106.89
23	c	511	CLA	C4C-C3C-C2C	-3.10	102.37	106.89
23	a	405[B]	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
26	B	620	SQD	O48-C23-C24	3.10	121.30	111.83
25	k	101	BCR	C20-C21-C22	-3.10	122.93	127.28
23	c	513	CLA	O2A-CGA-CBA	3.10	121.29	111.83
23	b	612	CLA	O2A-CGA-CBA	3.10	121.29	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	404	CLA	C4-C3-C5	3.10	120.61	115.23
23	b	602	CLA	C1C-C2C-C3C	-3.10	103.72	106.98
29	a	412[A]	PL9	C25-C24-C26	3.10	120.61	115.23
24	A	407[B]	PHO	O1D-CGD-CBD	-3.10	120.03	124.72
23	B	612	CLA	C4B-C3B-C2B	-3.10	103.45	107.30
26	a	409[B]	SQD	C44-O6-C1	-3.10	107.16	113.80
29	a	412[B]	PL9	C25-C24-C26	3.09	120.60	115.23
34	B	622	HTG	C1'-S1-C1	3.09	107.13	100.45
32	D	407[A]	LHG	O8-C23-C24	3.09	121.27	111.83
29	a	412[B]	PL9	C22-C23-C24	-3.09	120.54	127.62
32	D	407[B]	LHG	O7-C7-C8	3.09	118.17	111.48
23	C	509	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
32	b	629[A]	LHG	O7-C7-C8	3.09	118.16	111.48
38	f	101	HEM	C1B-NB-C4B	3.09	108.86	105.21
23	B	603	CLA	C4C-C3C-C2C	-3.09	102.40	106.89
26	a	409[A]	SQD	C45-O47-C7	-3.08	110.42	117.80
23	B	616	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
32	E	101[A]	LHG	O8-C23-C24	3.08	121.23	111.83
24	A	416[A]	PHO	C4-C3-C5	3.08	120.58	115.23
29	a	412[B]	PL9	C17-C18-C19	-3.08	120.57	127.62
23	C	507	CLA	C3C-C4C-NC	3.08	114.37	110.43
23	d	403[A]	CLA	C2A-C1A-CHA	-3.07	118.53	123.87
23	d	403[A]	CLA	O2A-CGA-O1A	-3.07	115.94	123.63
29	A	414[A]	PL9	C17-C18-C19	-3.07	120.59	127.62
23	C	504	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
29	d	406[A]	PL9	C22-C23-C24	-3.07	120.60	127.62
23	b	609	CLA	C3B-C4B-NB	3.07	113.27	110.53
25	C	516	BCR	C29-C30-C25	3.07	114.89	110.44
23	d	402[B]	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
23	c	511	CLA	CAC-C3C-C4C	3.07	128.78	124.79
23	B	609	CLA	CMC-C2C-C1C	3.06	129.82	125.03
23	C	503	CLA	CMC-C2C-C1C	3.06	129.82	125.03
25	Y	101	BCR	C36-C18-C19	3.06	122.77	118.09
23	d	402[A]	CLA	CMA-C3A-C2A	-3.06	102.14	113.98
23	b	615	CLA	C4-C3-C5	3.06	120.54	115.23
29	d	406[A]	PL9	C27-C28-C29	-3.06	120.61	127.62
23	C	511	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
23	d	404	CLA	CHD-C4C-NC	3.06	128.98	124.23
25	b	619	BCR	C38-C26-C25	-3.06	121.14	124.48
23	B	603	CLA	O2A-CGA-CBA	3.06	121.16	111.83
23	B	612	CLA	C1C-C2C-C3C	-3.06	103.76	106.98
23	C	507	CLA	C4B-C3B-C2B	-3.06	103.50	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	501	CLA	C1D-CHD-C4C	-3.06	119.52	126.02
23	b	616	CLA	CMB-C2B-C1B	3.06	130.07	125.42
25	t	102	BCR	C15-C16-C17	-3.06	117.27	123.52
23	c	508	CLA	O2A-CGA-CBA	3.05	121.15	111.83
23	C	512	CLA	C3B-C4B-NB	3.05	113.26	110.53
23	c	509	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
23	b	606	CLA	CAA-C2A-C3A	-3.05	104.75	113.00
29	a	412[A]	PL9	C22-C23-C24	-3.05	120.64	127.62
23	c	511	CLA	C4-C3-C5	3.05	120.52	115.23
25	A	409	BCR	C40-C30-C25	-3.05	105.46	110.24
23	B	608	CLA	O2A-CGA-O1A	-3.05	116.00	123.63
23	c	511	CLA	CHD-C4C-NC	3.05	128.96	124.23
23	C	502	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
23	C	510	CLA	CAC-C3C-C4C	3.05	128.75	124.79
23	a	407	CLA	O2A-CGA-CBA	3.05	121.12	111.83
23	B	604	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
23	d	403[A]	CLA	C4C-C3C-C2C	-3.04	102.46	106.89
23	b	607	CLA	CHC-C1C-C2C	-3.04	118.30	126.95
32	E	101[B]	LHG	O8-C23-C24	3.04	121.11	111.83
23	c	512	CLA	CHD-C4C-NC	3.04	128.95	124.23
23	c	513	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
23	A	406[A]	CLA	CAA-C2A-C3A	-3.04	104.78	113.00
23	D	402[A]	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
23	C	513	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
23	a	405[B]	CLA	CHD-C4C-NC	3.04	128.94	124.23
23	C	510	CLA	CMC-C2C-C1C	3.04	129.78	125.03
23	B	613	CLA	C4B-C3B-C2B	-3.04	103.53	107.30
29	D	405[A]	PL9	C10-C9-C11	3.03	120.50	115.23
23	B	613	CLA	C4C-C3C-C2C	-3.03	102.47	106.89
32	d	407[B]	LHG	O7-C7-C8	3.03	118.04	111.48
23	d	404	CLA	CAA-C2A-C3A	-3.03	104.81	113.00
23	c	510	CLA	O2A-CGA-CBA	3.03	121.08	111.83
29	D	405[B]	PL9	C25-C24-C26	3.03	120.49	115.23
23	A	404[B]	CLA	CHC-C1C-C2C	-3.03	118.34	126.95
23	B	608	CLA	CHC-C1C-C2C	-3.03	118.34	126.95
23	c	510	CLA	C4B-C3B-C2B	-3.03	103.53	107.30
23	b	607	CLA	C1D-CHD-C4C	-3.03	119.58	126.02
23	B	607	CLA	CAA-C2A-C3A	-3.03	104.81	113.00
23	b	615	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
23	A	405[A]	CLA	CHD-C4C-NC	3.03	128.93	124.23
23	b	603	CLA	CHD-C4C-NC	3.03	128.93	124.23
23	C	510	CLA	C4C-C3C-C2C	-3.03	102.49	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414[A]	PL9	C10-C9-C11	3.03	120.48	115.23
23	c	513	CLA	CAC-C3C-C4C	3.03	128.73	124.79
23	b	613	CLA	CHC-C1C-C2C	-3.02	118.35	126.95
23	a	404[B]	CLA	CAA-C2A-C1A	-3.02	102.07	111.97
25	d	405	BCR	C21-C20-C19	-3.02	114.44	123.20
25	C	516	BCR	C11-C10-C9	-3.02	123.04	127.28
23	B	610	CLA	C3B-C4B-NB	3.02	113.23	110.53
23	d	403[B]	CLA	CAA-C2A-C3A	-3.02	104.83	113.00
23	d	404	CLA	C4C-C3C-C2C	-3.02	102.49	106.89
23	c	501	CLA	C3B-C4B-NB	3.02	113.22	110.53
23	B	613	CLA	C1D-CHD-C4C	-3.02	119.60	126.02
26	A	410[A]	SQD	O48-C23-C24	3.02	121.04	111.83
23	b	610	CLA	CAA-C2A-C3A	-3.02	104.84	113.00
26	A	412	SQD	O48-C23-C24	3.02	121.03	111.83
32	d	414[B]	LHG	O8-C23-O10	-3.02	116.08	123.63
23	B	603	CLA	CHC-C1C-C2C	-3.02	118.38	126.95
23	A	408	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
23	D	402[A]	CLA	CAC-C3C-C4C	3.02	128.71	124.79
23	B	602	CLA	C4B-C3B-C2B	-3.02	103.55	107.30
23	A	406[B]	CLA	CMB-C2B-C1B	3.02	130.01	125.42
23	A	404[A]	CLA	CAA-C2A-C1A	-3.01	102.09	111.97
23	B	614	CLA	O2A-CGA-O1A	-3.01	116.09	123.63
32	A	419[B]	LHG	C5-O7-C7	-3.01	110.58	117.80
23	B	612	CLA	C2B-C1B-NB	3.01	113.45	110.33
23	B	607	CLA	C1D-CHD-C4C	-3.01	119.62	126.02
23	a	405[B]	CLA	C3B-C4B-NB	3.01	113.22	110.53
26	a	409[A]	SQD	O9-S-C6	3.01	111.25	106.76
23	B	614	CLA	CHD-C4C-NC	3.01	128.90	124.23
23	B	616	CLA	C1-O2A-CGA	3.01	123.94	116.65
29	a	412[A]	PL9	C10-C9-C11	3.01	120.45	115.23
32	d	407[A]	LHG	O7-C7-C8	3.01	117.99	111.48
31	A	417	LMT	O5B-C5B-C4B	3.01	115.12	109.70
25	A	409	BCR	C15-C14-C13	-3.01	123.06	127.28
23	d	402[A]	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
23	b	613	CLA	O2A-CGA-CBA	3.01	121.00	111.83
23	b	605	CLA	C4C-C3C-C2C	-3.00	102.52	106.89
23	c	509	CLA	CHD-C4C-NC	3.00	128.88	124.23
23	b	610	CLA	C1C-C2C-C3C	-3.00	103.82	106.98
23	A	406[B]	CLA	O2A-CGA-CBA	3.00	120.98	111.83
24	a	414[B]	PHO	C4A-C3A-C2A	-3.00	99.99	102.84
23	b	609	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
23	a	405[B]	CLA	C1-C2-C3	-3.00	121.28	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404[A]	CLA	CHC-C1C-C2C	-3.00	118.43	126.95
29	D	405[A]	PL9	C51-C49-C50	3.00	121.49	114.59
29	a	412[A]	PL9	C37-C38-C39	-3.00	120.77	127.62
26	F	102	SQD	O7-S-C6	2.99	111.23	106.76
23	d	404	CLA	CMB-C2B-C1B	2.99	129.98	125.42
23	D	402[B]	CLA	C4C-C3C-C2C	-2.99	102.53	106.89
32	A	419[B]	LHG	O8-C23-C24	2.99	120.96	111.83
23	B	604	CLA	CHC-C1C-C2C	-2.99	118.44	126.95
23	c	503	CLA	CHD-C4C-NC	2.99	128.87	124.23
23	B	615	CLA	CHD-C4C-NC	2.99	128.86	124.23
29	d	406[A]	PL9	C10-C9-C11	2.98	120.41	115.23
23	b	611	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
23	b	601	CLA	C4-C3-C5	2.98	120.41	115.23
23	a	404[A]	CLA	C4-C3-C5	2.98	120.41	115.23
35	C	517[B]	DGD	O6D-C1D-O3G	-2.98	103.00	110.04
23	c	507	CLA	CHD-C4C-NC	2.98	128.85	124.23
32	a	419[B]	LHG	O7-C7-C8	2.98	117.93	111.48
23	b	602	CLA	CMC-C2C-C1C	2.98	129.69	125.03
24	a	406[A]	PHO	O2A-CGA-CBA	2.98	120.92	111.83
23	a	404[B]	CLA	C1-C2-C3	-2.98	121.32	126.20
23	b	609	CLA	CBC-CAC-C3C	-2.98	104.35	112.42
25	A	409	BCR	C38-C26-C25	-2.98	121.24	124.48
23	a	405[A]	CLA	CMC-C2C-C1C	2.98	129.68	125.03
32	D	406[A]	LHG	O8-C23-O10	-2.97	116.19	123.63
23	C	514	CLA	C4B-C3B-C2B	-2.97	103.61	107.30
23	b	601	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
29	A	414[A]	PL9	C20-C19-C21	2.97	120.38	115.23
23	d	402[A]	CLA	CBC-CAC-C3C	-2.97	104.38	112.42
23	B	606	CLA	O2A-CGA-CBA	2.97	120.88	111.83
23	A	406[A]	CLA	CHD-C4C-NC	2.96	128.83	124.23
23	d	402[A]	CLA	CHC-C1C-C2C	-2.96	118.53	126.95
23	B	612	CLA	C11-C12-C13	-2.96	106.12	115.97
23	c	510	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
23	A	404[B]	CLA	C2A-C1A-CHA	-2.96	118.73	123.87
32	b	629[A]	LHG	O8-C23-C24	2.96	120.84	111.83
23	d	403[A]	CLA	C4-C3-C5	2.95	120.36	115.23
23	b	608	CLA	CBC-CAC-C3C	-2.95	104.41	112.42
23	B	608	CLA	C4B-C3B-C2B	-2.95	103.63	107.30
23	A	406[B]	CLA	C3B-C4B-NB	2.95	113.17	110.53
29	a	412[B]	PL9	C35-C34-C36	2.95	120.35	115.23
23	B	609	CLA	CBC-CAC-C3C	-2.95	104.42	112.42
23	C	510	CLA	C16-C15-C13	-2.95	106.15	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
23	B	616	CLA	C1C-C2C-C3C	-2.95	103.88	106.98
23	b	605	CLA	CHC-C1C-C2C	-2.95	118.56	126.95
38	E	102	HEM	CBA-CAA-C2A	-2.95	104.38	112.53
32	D	407[A]	LHG	O8-C23-O10	-2.95	116.25	123.63
23	c	513	CLA	CAA-C2A-C3A	-2.95	105.04	113.00
24	A	416[B]	PHO	O2D-CGD-O1D	-2.95	118.11	123.85
23	b	607	CLA	CAA-C2A-C3A	-2.95	105.04	113.00
23	B	606	CLA	CHD-C4C-NC	2.95	128.80	124.23
23	A	406[B]	CLA	O2A-CGA-O1A	-2.95	116.26	123.63
23	b	615	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
23	B	611	CLA	C1-C2-C3	-2.94	121.37	126.20
26	f	102	SQD	C4-C3-C2	-2.94	105.66	110.83
25	B	619	BCR	C24-C23-C22	-2.94	121.88	126.23
34	B	622	HTG	O5-C1-C2	2.94	114.37	110.32
23	A	406[B]	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
23	B	604	CLA	CAC-C3C-C4C	2.94	128.62	124.79
23	C	505	CLA	CHC-C1C-C2C	-2.94	118.59	126.95
23	C	510	CLA	O2A-CGA-CBA	2.94	120.80	111.83
23	B	615	CLA	C4-C3-C5	2.94	120.33	115.23
23	C	513	CLA	CMC-C2C-C1C	2.94	129.62	125.03
23	A	404[B]	CLA	C1-C2-C3	-2.94	121.39	126.20
23	b	608	CLA	CHC-C1C-C2C	-2.94	118.60	126.95
23	b	608	CLA	CHD-C4C-NC	2.93	128.78	124.23
32	a	419[A]	LHG	O7-C7-C8	2.93	117.83	111.48
26	B	620	SQD	O7-S-C6	2.93	111.13	106.76
23	c	509	CLA	C4A-NA-C1A	-2.93	105.34	106.68
26	A	410[B]	SQD	O48-C23-C24	2.93	120.77	111.83
29	A	414[B]	PL9	C30-C29-C31	2.93	120.31	115.23
23	b	614	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
23	B	616	CLA	CHD-C1D-ND	-2.93	120.68	124.80
23	B	609	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
23	C	502	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
23	C	504	CLA	O2A-CGA-O1A	-2.93	116.31	123.63
23	b	601	CLA	CHD-C4C-NC	2.93	128.77	124.23
23	A	408	CLA	CHC-C1C-C2C	-2.93	118.64	126.95
23	A	404[A]	CLA	C4C-C3C-C2C	-2.92	102.63	106.89
23	B	605	CLA	CMC-C2C-C1C	2.92	129.60	125.03
23	A	405[B]	CLA	C1-C2-C3	-2.92	121.41	126.20
23	a	404[A]	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
32	D	407[B]	LHG	O8-C23-C24	2.92	120.74	111.83
23	b	614	CLA	CMB-C2B-C1B	2.92	129.87	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405[B]	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
33	z	101	LMG	O8-C28-C29	2.92	120.74	111.83
23	b	606	CLA	C1-C2-C3	-2.92	121.42	126.20
23	C	514	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
23	D	402[B]	CLA	CHC-C1C-C2C	-2.92	118.66	126.95
31	A	420	LMT	O5B-C5B-C4B	2.92	114.95	109.70
23	A	406[A]	CLA	C1-C2-C3	-2.92	121.42	126.20
23	a	404[B]	CLA	O2A-CGA-O1A	-2.91	116.34	123.63
23	b	614	CLA	CBC-CAC-C3C	-2.91	104.52	112.42
25	y	101	BCR	C10-C11-C12	-2.91	114.76	123.20
23	D	402[B]	CLA	CMB-C2B-C1B	2.91	129.85	125.42
23	B	609	CLA	CHD-C4C-NC	2.91	128.75	124.23
23	B	609	CLA	CMB-C2B-C1B	2.91	129.85	125.42
23	b	611	CLA	CHD-C4C-NC	2.91	128.75	124.23
33	c	519	LMG	O8-C28-C29	2.91	120.71	111.83
23	B	602	CLA	CHD-C4C-NC	2.91	128.74	124.23
23	C	511	CLA	O2A-CGA-CBA	2.91	120.71	111.83
23	D	402[A]	CLA	O2A-CGA-O1A	-2.91	116.35	123.63
25	D	404	BCR	C40-C30-C25	-2.91	105.68	110.24
23	a	405[B]	CLA	CAA-C2A-C3A	-2.91	105.14	113.00
23	B	604	CLA	O2A-CGA-O1A	-2.91	116.36	123.63
23	b	614	CLA	O2A-CGA-O1A	-2.91	116.36	123.63
25	A	409	BCR	C16-C17-C18	-2.90	123.20	127.28
25	C	515	BCR	C15-C14-C13	-2.90	123.21	127.28
23	c	511	CLA	O2A-CGA-CBA	2.90	120.69	111.83
23	a	405[A]	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
25	T	102	BCR	C35-C13-C12	2.90	122.52	118.09
23	D	403	CLA	C4B-C3B-C2B	-2.90	103.70	107.30
31	b	621	LMT	C1'-O5'-C5'	-2.90	108.06	113.72
23	C	506	CLA	C4-C3-C5	2.90	120.25	115.23
23	C	514	CLA	CBC-CAC-C3C	-2.89	104.57	112.42
23	A	405[A]	CLA	CHC-C1C-C2C	-2.89	118.72	126.95
23	D	402[A]	CLA	CHC-C1C-C2C	-2.89	118.72	126.95
23	b	609	CLA	CHD-C4C-NC	2.89	128.72	124.23
23	D	402[B]	CLA	CAC-C3C-C4C	2.89	128.55	124.79
25	t	102	BCR	C21-C20-C19	-2.89	114.83	123.20
23	D	402[A]	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
23	B	603	CLA	CHD-C4C-NC	2.89	128.71	124.23
23	b	616	CLA	CAC-C3C-C4C	2.88	128.54	124.79
23	a	405[A]	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
24	a	414[A]	PHO	CMB-C2B-C3B	2.88	130.44	124.68
23	a	407	CLA	C4-C3-C5	2.88	120.23	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	C3B-C4B-NB	2.88	113.10	110.53
25	D	404	BCR	C15-C14-C13	-2.88	123.24	127.28
23	B	610	CLA	CHD-C4C-NC	2.88	128.70	124.23
23	c	505	CLA	C3B-C4B-NB	2.88	113.10	110.53
23	C	503	CLA	CHC-C1C-C2C	-2.88	118.77	126.95
23	C	513	CLA	CMB-C2B-C1B	2.88	129.80	125.42
26	a	409[A]	SQD	O47-C7-O49	-2.88	116.98	123.70
29	A	414[A]	PL9	C30-C29-C31	2.88	120.22	115.23
23	b	609	CLA	C1C-C2C-C3C	-2.88	103.96	106.98
23	B	615	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
35	C	517[B]	DGD	C2G-O2G-C1B	-2.87	110.92	117.80
23	C	504	CLA	C1C-C2C-C3C	-2.87	103.96	106.98
23	b	602	CLA	CMA-C3A-C4A	-2.87	104.05	111.77
23	B	609	CLA	O2A-CGA-CBA	2.87	120.58	111.83
23	B	602	CLA	C4C-C3C-C2C	-2.87	102.72	106.89
23	B	606	CLA	C4C-C3C-C2C	-2.87	102.72	106.89
23	C	514	CLA	CMC-C2C-C1C	2.87	129.51	125.03
23	C	505	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
23	c	505	CLA	C4B-C3B-C2B	-2.87	103.74	107.30
29	D	405[B]	PL9	C17-C18-C19	-2.87	121.07	127.62
25	D	404	BCR	C16-C17-C18	-2.86	123.26	127.28
23	a	405[A]	CLA	CMB-C2B-C1B	2.86	129.78	125.42
23	C	506	CLA	CHC-C1C-C2C	-2.86	118.81	126.95
24	a	406[B]	PHO	C1A-C2A-C3A	-2.86	100.12	102.84
23	D	403	CLA	C4-C3-C5	2.86	120.19	115.23
23	c	510	CLA	CHD-C4C-NC	2.86	128.67	124.23
24	a	406[A]	PHO	CMA-C3A-C4A	-2.86	108.45	114.61
23	c	505	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
23	c	508	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
23	B	604	CLA	C6-C5-C3	-2.85	106.51	113.47
23	b	614	CLA	CHC-C1C-C2C	-2.85	118.83	126.95
23	b	605	CLA	O2A-CGA-O1A	-2.85	116.49	123.63
23	B	601	CLA	O2A-CGA-CBA	2.85	120.53	111.83
31	a	416	LMT	C3'-C4'-C5'	-2.85	104.61	110.93
23	A	405[B]	CLA	CMB-C2B-C1B	2.85	129.76	125.42
24	a	406[A]	PHO	C1A-C2A-C3A	-2.85	100.13	102.84
29	d	406[B]	PL9	C40-C39-C41	2.85	120.17	115.23
23	c	501	CLA	CHD-C4C-NC	2.85	128.65	124.23
23	c	506	CLA	C4C-C3C-C2C	-2.85	102.75	106.89
23	b	604	CLA	CHC-C1C-C2C	-2.85	118.86	126.95
23	c	506	CLA	CHD-C4C-NC	2.84	128.64	124.23
25	T	102	BCR	C33-C5-C6	-2.84	121.38	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	f	101	HEM	CBD-CAD-C3D	-2.84	104.67	112.53
23	D	402[B]	CLA	CAA-C2A-C3A	-2.84	105.32	113.00
23	C	507	CLA	C4-C3-C5	2.84	120.16	115.23
23	b	601	CLA	CAC-C3C-C4C	2.84	128.49	124.79
23	A	404[A]	CLA	CAA-CBA-CGA	-2.84	105.14	113.21
25	A	409	BCR	C31-C1-C6	-2.84	105.79	110.24
23	C	502	CLA	C3B-C4B-NB	2.84	113.07	110.53
23	B	613	CLA	CMC-C2C-C1C	2.84	129.47	125.03
23	b	616	CLA	C1C-C2C-C3C	-2.84	103.99	106.98
23	c	509	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
23	A	405[A]	CLA	C4-C3-C5	2.84	120.16	115.23
23	b	607	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
23	d	403[B]	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
23	D	402[A]	CLA	CAA-C2A-C3A	-2.84	105.33	113.00
23	B	614	CLA	CHC-C1C-C2C	-2.84	118.88	126.95
23	c	513	CLA	CHC-C1C-C2C	-2.84	118.88	126.95
23	b	601	CLA	CHC-C1C-C2C	-2.84	118.88	126.95
25	B	619	BCR	C29-C30-C25	2.84	114.56	110.44
23	C	514	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
29	a	412[B]	PL9	C10-C9-C11	2.83	120.15	115.23
23	C	508	CLA	C1-C2-C3	-2.83	121.55	126.20
23	c	505	CLA	C1-C2-C3	-2.83	121.55	126.20
23	b	603	CLA	C4-C3-C5	2.83	120.14	115.23
23	b	602	CLA	C2A-C1A-CHA	-2.83	118.95	123.87
25	k	101	BCR	C38-C26-C25	-2.83	121.39	124.48
33	c	520	LMG	O8-C28-C29	2.83	120.47	111.83
23	B	613	CLA	CAC-C3C-C4C	2.83	128.47	124.79
23	C	505	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
23	b	610	CLA	CMB-C2B-C1B	2.83	129.73	125.42
32	d	408[A]	LHG	O8-C23-C24	2.83	120.46	111.83
23	b	615	CLA	O2A-CGA-O1A	-2.83	116.55	123.63
23	C	511	CLA	O2A-CGA-O1A	-2.83	116.56	123.63
23	B	601	CLA	CMB-C2B-C1B	2.83	129.72	125.42
25	Y	101	BCR	C38-C26-C25	-2.83	121.40	124.48
23	c	510	CLA	O2A-CGA-O1A	-2.82	116.56	123.63
23	B	607	CLA	C2A-C1A-CHA	-2.82	118.97	123.87
23	B	610	CLA	CHC-C1C-C2C	-2.82	118.92	126.95
26	f	102	SQD	O48-C23-C24	2.82	120.44	111.83
23	c	507	CLA	O2A-CGA-CBA	2.82	120.44	111.83
23	b	606	CLA	C3B-C4B-NB	2.82	113.05	110.53
23	b	610	CLA	C4B-C3B-C2B	-2.82	103.80	107.30
23	A	405[B]	CLA	C4-C3-C5	2.82	120.12	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414[B]	PL9	C10-C9-C11	2.82	120.12	115.23
23	B	614	CLA	C4B-C3B-C2B	-2.82	103.80	107.30
26	F	102	SQD	O48-C23-C24	2.82	120.42	111.83
23	C	502	CLA	CMB-C2B-C1B	2.82	129.71	125.42
23	b	601	CLA	C4B-C3B-C2B	-2.81	103.80	107.30
23	B	606	CLA	C4B-C3B-C2B	-2.81	103.80	107.30
23	A	406[B]	CLA	CHD-C4C-NC	2.81	128.59	124.23
23	C	502	CLA	CHD-C4C-NC	2.81	128.59	124.23
23	d	402[B]	CLA	O2A-CGA-CBA	2.81	120.41	111.83
23	c	502	CLA	C1-C2-C3	-2.81	121.59	126.20
33	Z	101	LMG	C4-C3-C2	2.81	115.77	110.83
35	C	519	DGD	O1G-C1A-C2A	2.81	120.41	111.83
23	B	604	CLA	CMB-C2B-C1B	2.81	129.70	125.42
24	A	416[B]	PHO	C4-C3-C5	2.81	120.11	115.23
23	C	510	CLA	O2A-CGA-O1A	-2.81	116.60	123.63
33	a	415	LMG	C8-O7-C10	-2.81	111.07	117.80
23	A	404[B]	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
32	A	419[A]	LHG	O7-C7-O9	-2.81	117.13	123.70
23	B	611	CLA	C3B-C4B-NB	2.81	113.04	110.53
23	d	403[A]	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
35	C	517[A]	DGD	C2G-O2G-C1B	-2.81	111.07	117.80
23	b	611	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
23	C	514	CLA	C2A-C1A-CHA	-2.81	119.00	123.87
23	D	403	CLA	C3B-C4B-NB	2.81	113.04	110.53
23	C	508	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
23	b	606	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
23	C	507	CLA	CMC-C2C-C1C	2.80	129.41	125.03
31	B	628	LMT	C2'-C3'-C4'	2.80	116.04	109.68
23	A	408	CLA	CHD-C4C-NC	2.80	128.57	124.23
23	B	611	CLA	C4B-C3B-C2B	2.80	110.78	107.30
26	B	620	SQD	C4-C3-C2	2.80	115.75	110.83
23	A	406[A]	CLA	CHC-C1C-C2C	-2.80	118.99	126.95
23	A	404[B]	CLA	CAA-C2A-C1A	-2.80	102.80	111.97
23	B	603	CLA	C4-C3-C5	2.80	120.09	115.23
23	c	512	CLA	CAC-C3C-C4C	2.80	128.43	124.79
23	c	508	CLA	CAA-C2A-C3A	-2.80	105.44	113.00
23	c	504	CLA	CHD-C4C-NC	2.80	128.57	124.23
29	D	405[A]	PL9	C37-C38-C39	-2.80	121.22	127.62
23	D	402[B]	CLA	O2A-CGA-O1A	-2.80	116.63	123.63
38	E	102	HEM	CHB-C1B-NB	2.80	127.83	124.37
23	b	615	CLA	C11-C10-C8	-2.80	106.67	115.97
23	D	403	CLA	CAA-C2A-C3A	-2.80	105.44	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	C4B-C3B-C2B	-2.80	103.83	107.30
23	c	502	CLA	CMC-C2C-C1C	2.79	129.40	125.03
31	M	101	LMT	C1'-O5'-C5'	-2.79	108.26	113.72
25	C	515	BCR	C38-C26-C25	-2.79	121.44	124.48
23	C	511	CLA	CAC-C3C-C4C	2.79	128.42	124.79
25	k	101	BCR	C39-C30-C25	-2.79	105.86	110.24
23	c	512	CLA	C4C-C3C-C2C	-2.79	102.83	106.89
23	c	509	CLA	C4-C3-C5	2.79	120.07	115.23
23	b	608	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	D	402[B]	CLA	C4B-C3B-C2B	-2.79	103.84	107.30
23	B	614	CLA	C2A-C1A-CHA	-2.79	119.03	123.87
23	C	514	CLA	O2A-CGA-CBA	2.79	120.33	111.83
23	A	405[B]	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
23	B	603	CLA	CMC-C2C-C1C	2.78	129.38	125.03
32	D	407[A]	LHG	O7-C7-C8	2.78	117.50	111.48
29	A	414[B]	PL9	C12-C13-C14	-2.78	121.25	127.62
23	B	602	CLA	C2A-C1A-CHA	-2.78	119.04	123.87
35	H	102	DGD	O1G-C1A-C2A	2.78	120.32	111.83
31	M	101	LMT	C3'-C4'-C5'	-2.78	104.76	110.93
23	b	607	CLA	C4-C3-C5	2.78	120.06	115.23
26	a	409[B]	SQD	O9-S-C6	2.78	110.91	106.76
23	c	513	CLA	C1-C2-C3	-2.78	121.64	126.20
29	D	405[B]	PL9	C37-C38-C39	-2.78	121.26	127.62
23	b	609	CLA	O2A-CGA-O1A	-2.78	116.67	123.63
23	B	615	CLA	C6-C7-C8	-2.78	106.73	115.97
23	A	408	CLA	CBC-CAC-C3C	-2.78	104.89	112.42
32	a	419[A]	LHG	O8-C23-C24	2.78	120.30	111.83
23	c	505	CLA	CMC-C2C-C1C	2.78	129.37	125.03
24	a	414[A]	PHO	O1D-CGD-CBD	-2.78	120.51	124.72
35	c	518	DGD	O3G-C1D-C2D	-2.78	104.06	108.27
23	d	404	CLA	C2A-C1A-CHA	-2.78	119.05	123.87
25	a	408	BCR	C38-C26-C25	-2.78	121.45	124.48
25	b	618	BCR	C15-C14-C13	-2.78	123.39	127.28
23	a	405[A]	CLA	CAA-C2A-C3A	-2.78	105.50	113.00
23	d	403[B]	CLA	CHD-C4C-NC	2.77	128.53	124.23
23	A	406[A]	CLA	CBC-CAC-C3C	-2.77	104.90	112.42
23	B	614	CLA	C4C-C3C-C2C	-2.77	102.85	106.89
23	b	601	CLA	C1-O2A-CGA	2.77	123.36	116.65
23	C	508	CLA	CHD-C4C-NC	2.77	128.53	124.23
25	d	405	BCR	C33-C5-C6	-2.77	121.46	124.48
23	c	504	CLA	CHC-C1C-C2C	-2.77	119.07	126.95
29	d	406[A]	PL9	C53-C6-C1	2.77	120.95	115.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	514	CLA	CAC-C3C-C4C	2.77	128.40	124.79
23	B	606	CLA	C3B-C4B-NB	2.77	113.00	110.53
23	C	502	CLA	CMC-C2C-C1C	2.77	129.36	125.03
29	A	414[B]	PL9	C40-C39-C41	2.77	120.03	115.23
33	C	501	LMG	O6-C1-O1	-2.77	103.50	110.04
23	C	513	CLA	O2A-CGA-O1A	-2.77	116.71	123.63
33	c	519	LMG	O1-C7-C8	-2.77	104.09	110.82
29	D	405[A]	PL9	C42-C41-C39	-2.76	104.03	113.19
23	D	403	CLA	CHC-C1C-C2C	-2.76	119.09	126.95
25	c	514	BCR	C37-C22-C21	-2.76	118.34	122.82
23	c	501	CLA	CHC-C1C-C2C	-2.76	119.10	126.95
23	c	510	CLA	CHC-C1C-C2C	-2.76	119.10	126.95
23	c	503	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
23	b	609	CLA	CHC-C1C-C2C	-2.76	119.10	126.95
23	a	405[B]	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
23	C	509	CLA	O2A-CGA-CBA	2.76	120.25	111.83
35	c	516[A]	DGD	O3G-C3G-C2G	-2.76	104.11	110.82
23	C	507	CLA	CAC-C3C-C4C	2.76	128.38	124.79
23	a	404[B]	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
23	c	507	CLA	C1-C2-C3	-2.76	121.68	126.20
25	D	404	BCR	C3-C4-C5	-2.75	109.14	114.06
23	C	510	CLA	C4B-C3B-C2B	-2.75	103.88	107.30
23	C	512	CLA	CHD-C4C-NC	2.75	128.50	124.23
33	C	501	LMG	C6-C5-C4	2.75	119.78	113.02
32	b	629[B]	LHG	O8-C23-C24	2.75	120.22	111.83
23	C	505	CLA	CMC-C2C-C1C	2.75	129.33	125.03
25	B	617	BCR	C16-C17-C18	-2.75	123.42	127.28
23	C	512	CLA	C4-C3-C5	2.75	120.00	115.23
33	C	501	LMG	C8-O7-C10	-2.75	111.22	117.80
23	c	504	CLA	C2A-C1A-CHA	-2.75	119.10	123.87
31	B	630	LMT	O1'-C1'-C2'	2.75	112.44	108.27
23	c	511	CLA	C4B-C3B-C2B	-2.75	103.89	107.30
23	d	404	CLA	CBC-CAC-C3C	-2.75	104.98	112.42
25	c	514	BCR	C20-C21-C22	-2.75	123.43	127.28
35	c	518	DGD	O2G-C1B-C2B	2.75	117.42	111.48
23	A	405[B]	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
23	B	615	CLA	C4B-C3B-C2B	-2.74	103.89	107.30
23	A	406[B]	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
23	A	404[A]	CLA	CAC-C3C-C4C	2.74	128.36	124.79
23	a	407	CLA	CMA-C3A-C2A	-2.74	103.38	113.98
23	a	404[B]	CLA	C4-C3-C5	2.74	119.99	115.23
40	v	201	HEC	CMC-C2C-C1C	-2.74	121.25	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	H	101	BCR	C31-C1-C6	-2.74	105.95	110.24
23	d	402[A]	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
31	B	631	LMT	C3'-C4'-C5'	-2.74	104.86	110.93
35	C	517[A]	DGD	O3G-C3G-C2G	-2.74	104.16	110.82
23	d	402[B]	CLA	C4C-C3C-C2C	-2.74	102.91	106.89
23	b	610	CLA	C4-C3-C5	2.74	119.98	115.23
35	C	518[A]	DGD	O1G-C1A-O1A	-2.74	116.78	123.63
25	T	102	BCR	C15-C14-C13	2.74	131.12	127.28
23	d	403[A]	CLA	CAA-C2A-C3A	-2.74	105.61	113.00
23	b	615	CLA	O2A-CGA-CBA	2.73	120.17	111.83
23	C	514	CLA	CHC-C1C-C2C	-2.73	119.18	126.95
25	c	515	BCR	C15-C14-C13	-2.73	123.44	127.28
23	c	512	CLA	CHC-C1C-C2C	-2.73	119.18	126.95
25	k	101	BCR	C24-C23-C22	-2.73	122.19	126.23
25	h	101	BCR	C33-C5-C6	-2.73	121.50	124.48
23	B	616	CLA	O2A-CGA-CBA	2.73	120.16	111.83
23	A	406[A]	CLA	C2A-C1A-CHA	-2.73	119.13	123.87
23	A	404[A]	CLA	C2A-C1A-CHA	-2.73	119.13	123.87
23	B	601	CLA	C1-O2A-CGA	2.73	123.25	116.65
32	D	406[B]	LHG	O7-C7-C8	2.73	117.38	111.48
29	d	406[B]	PL9	C22-C23-C24	-2.73	121.38	127.62
23	a	405[B]	CLA	C4-C3-C5	2.73	119.96	115.23
23	B	612	CLA	C2A-C1A-CHA	-2.73	119.14	123.87
23	C	507	CLA	C2A-C1A-CHA	-2.73	119.14	123.87
25	B	618	BCR	C2-C1-C6	2.73	114.40	110.44
23	a	405[A]	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
23	b	610	CLA	CHD-C4C-NC	2.72	128.46	124.23
23	b	607	CLA	CMB-C2B-C1B	2.72	129.56	125.42
23	b	606	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
23	c	511	CLA	CMB-C2B-C1B	2.72	129.56	125.42
23	B	616	CLA	C2A-C1A-CHA	-2.72	119.15	123.87
26	a	410	SQD	C3-C4-C5	2.72	115.16	110.23
23	b	607	CLA	CAC-C3C-C4C	2.71	128.32	124.79
23	c	509	CLA	C1-O2A-CGA	2.71	123.22	116.65
29	A	414[A]	PL9	C10-C9-C8	-2.71	116.66	123.63
35	c	516[A]	DGD	C3G-C2G-C1G	-2.71	105.46	111.78
25	h	101	BCR	C16-C17-C18	-2.71	123.47	127.28
25	B	619	BCR	C21-C20-C19	-2.71	115.34	123.20
32	D	406[A]	LHG	O8-C23-C24	2.71	120.09	111.83
29	A	414[B]	PL9	C42-C43-C44	-2.71	121.42	127.62
23	C	502	CLA	CHC-C1C-C2C	-2.71	119.25	126.95
23	b	610	CLA	CAA-CBA-CGA	-2.70	105.53	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	620	SQD	O9-S-C6	2.70	110.79	106.76
23	a	404[B]	CLA	C2A-C1A-CHA	-2.70	119.17	123.87
31	B	628	LMT	O1'-C1'-C2'	2.70	112.38	108.27
23	C	511	CLA	C4C-C3C-C2C	-2.70	102.96	106.89
23	a	404[B]	CLA	CMA-C3A-C4A	-2.70	104.51	111.77
23	c	513	CLA	C2A-C1A-CHA	-2.70	119.18	123.87
23	C	510	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
25	H	101	BCR	C10-C11-C12	-2.70	115.37	123.20
29	D	405[A]	PL9	C2-C1-C6	2.70	122.21	119.00
23	B	613	CLA	CHC-C1C-C2C	-2.70	119.28	126.95
34	B	622	HTG	C1-O5-C5	2.70	117.40	112.56
23	a	405[B]	CLA	CMB-C2B-C1B	2.70	129.53	125.42
25	c	514	BCR	C28-C27-C26	-2.70	109.24	114.06
23	c	511	CLA	CHC-C1C-C2C	-2.70	119.28	126.95
32	L	101[A]	LHG	O8-C23-C24	2.70	120.06	111.83
23	A	408	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
32	d	408[B]	LHG	O8-C23-C24	2.70	120.05	111.83
23	c	506	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
23	b	603	CLA	O2A-CGA-CBA	2.69	120.05	111.83
23	a	405[A]	CLA	CHC-C1C-C2C	-2.69	119.29	126.95
23	d	402[A]	CLA	O2A-CGA-CBA	2.69	120.05	111.83
26	A	410[A]	SQD	O48-C23-O10	-2.69	116.89	123.63
23	b	615	CLA	CHD-C4C-NC	2.69	128.41	124.23
23	A	405[A]	CLA	CMA-C3A-C2A	-2.69	103.58	113.98
23	D	402[B]	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
23	b	611	CLA	O2A-CGA-CBA	2.69	120.04	111.83
23	c	501	CLA	CAC-C3C-C4C	2.69	128.29	124.79
23	c	505	CLA	O2A-CGA-CBA	2.69	120.03	111.83
29	A	414[A]	PL9	C40-C39-C41	2.69	119.90	115.23
24	a	406[B]	PHO	O2A-CGA-CBA	2.69	120.03	111.83
23	A	405[A]	CLA	CAC-C3C-C4C	2.69	128.29	124.79
32	L	101[B]	LHG	O8-C23-C24	2.69	120.03	111.83
23	a	404[A]	CLA	C4C-C3C-C2C	-2.69	102.98	106.89
23	C	513	CLA	CBC-CAC-C3C	-2.69	105.14	112.42
23	c	504	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
32	a	419[B]	LHG	O8-C23-C24	2.69	120.02	111.83
23	B	612	CLA	O2A-CGA-CBA	2.68	120.02	111.83
25	d	405	BCR	C28-C27-C26	-2.68	109.27	114.06
23	b	606	CLA	C4C-C3C-C2C	-2.68	102.99	106.89
23	c	501	CLA	O2A-CGA-O1A	-2.68	116.92	123.63
35	c	518	DGD	O1G-C1A-C2A	2.68	120.02	111.83
23	D	403	CLA	CMA-C3A-C2A	-2.68	103.62	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	C	520	LMG	O1-C1-C2	-2.68	104.20	108.27
23	b	614	CLA	C2A-C1A-CHA	-2.68	119.22	123.87
25	T	102	BCR	C2-C1-C6	2.68	114.33	110.44
23	b	614	CLA	C4C-C3C-C2C	-2.68	103.00	106.89
25	c	515	BCR	C21-C20-C19	-2.68	115.45	123.20
23	C	503	CLA	C4C-C3C-C2C	-2.67	103.00	106.89
29	D	405[B]	PL9	C51-C49-C50	2.67	120.74	114.59
23	A	404[B]	CLA	O2A-CGA-O1A	-2.67	116.94	123.63
23	C	510	CLA	CHC-C1C-C2C	-2.67	119.35	126.95
27	b	628	GOL	C3-C2-C1	-2.67	102.00	111.80
23	A	404[B]	CLA	C4C-C3C-C2C	-2.67	103.00	106.89
23	c	501	CLA	CMC-C2C-C1C	2.67	129.21	125.03
24	a	406[B]	PHO	O2A-CGA-O1A	-2.67	116.95	123.63
23	A	406[A]	CLA	CMA-C3A-C2A	-2.67	103.66	113.98
38	f	101	HEM	CAD-CBD-CGD	2.67	120.75	113.67
33	D	411	LMG	O8-C28-O10	-2.67	116.95	123.63
23	b	609	CLA	O2A-CGA-CBA	2.67	119.97	111.83
26	a	410	SQD	C1-O5-C5	2.67	118.93	113.72
23	b	616	CLA	CHC-C1C-C2C	-2.67	119.37	126.95
23	C	506	CLA	C4B-C3B-C2B	-2.67	103.99	107.30
23	c	502	CLA	CMB-C2B-C1B	2.67	129.48	125.42
23	b	612	CLA	CHD-C4C-NC	2.67	128.37	124.23
23	b	610	CLA	CMA-C3A-C4A	-2.66	104.61	111.77
23	B	609	CLA	CHC-C1C-C2C	-2.66	119.38	126.95
23	a	404[A]	CLA	CAC-C3C-C4C	2.66	128.25	124.79
23	B	605	CLA	C2A-C1A-CHA	-2.66	119.25	123.87
29	D	405[B]	PL9	C7-C8-C9	-2.66	122.25	126.83
23	A	404[B]	CLA	CHD-C4C-NC	2.66	128.35	124.23
23	b	605	CLA	C3B-C4B-NB	2.66	112.90	110.53
26	b	620	SQD	O7-S-C6	2.66	110.72	106.76
23	B	609	CLA	O2A-CGA-O1A	-2.65	116.99	123.63
23	B	601	CLA	C3B-C4B-NB	2.65	112.90	110.53
31	T	101	LMT	C3'-C4'-C5'	-2.65	105.05	110.93
23	B	608	CLA	CMA-C3A-C4A	-2.65	104.64	111.77
23	D	402[B]	CLA	C2A-C1A-CHA	-2.65	119.26	123.87
24	A	416[B]	PHO	C4D-CHA-CBD	2.65	109.73	108.45
25	t	102	BCR	C11-C10-C9	-2.65	123.56	127.28
23	a	405[B]	CLA	O2A-CGA-CBA	2.65	119.92	111.83
25	Y	101	BCR	C24-C23-C22	-2.65	122.31	126.23
23	c	502	CLA	O2A-CGA-CBA	2.65	119.92	111.83
23	B	601	CLA	CMC-C2C-C1C	2.65	129.18	125.03
24	A	416[A]	PHO	O2D-CGD-O1D	-2.65	118.69	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	514	CLA	CAA-C2A-C3A	-2.65	105.84	113.00
23	A	408	CLA	CMA-C3A-C2A	-2.65	103.74	113.98
29	D	405[B]	PL9	C45-C44-C46	2.65	119.82	115.23
23	B	615	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
23	C	509	CLA	CAC-C3C-C4C	2.64	128.23	124.79
23	A	406[B]	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
40	v	201	HEC	CBD-CAD-C3D	-2.64	105.23	112.53
24	a	414[A]	PHO	CBA-CAA-C2A	-2.64	105.99	113.78
23	C	507	CLA	CAA-C2A-C3A	-2.64	105.87	113.00
24	a	414[B]	PHO	CBA-CAA-C2A	-2.64	106.01	113.78
23	A	406[A]	CLA	C4C-C3C-C2C	-2.64	103.05	106.89
23	b	612	CLA	C4D-CHA-C1A	-2.64	118.10	121.24
35	C	518[B]	DGD	O1G-C1A-C2A	2.64	119.87	111.83
23	b	613	CLA	C4-C3-C5	2.63	119.80	115.23
23	B	609	CLA	C3B-C4B-NB	2.63	112.88	110.53
26	F	102	SQD	O47-C7-O49	-2.63	117.55	123.70
33	D	411	LMG	O8-C28-C29	2.63	119.86	111.83
23	D	402[A]	CLA	CMC-C2C-C1C	2.63	129.15	125.03
23	C	502	CLA	CBC-CAC-C3C	-2.63	105.30	112.42
23	A	406[B]	CLA	C2A-C1A-CHA	-2.63	119.31	123.87
23	A	405[A]	CLA	OBD-CAD-C3D	-2.63	122.28	128.42
31	m	103	LMT	C3'-C4'-C5'	-2.63	105.11	110.93
23	b	608	CLA	C11-C12-C13	-2.62	107.24	115.97
23	B	614	CLA	OBD-CAD-C3D	-2.62	122.28	128.42
23	C	514	CLA	CHD-C4C-NC	2.62	128.30	124.23
23	C	508	CLA	O2A-CGA-CBA	2.62	119.83	111.83
23	B	608	CLA	CHB-C4A-NA	2.62	128.19	124.40
35	H	102	DGD	O1G-C1A-O1A	-2.62	117.07	123.63
33	C	520	LMG	O8-C28-O10	-2.62	117.07	123.63
23	A	404[A]	CLA	CMA-C3A-C2A	-2.62	103.85	113.98
29	a	412[B]	PL9	C40-C39-C41	2.62	119.78	115.23
33	B	621	LMG	O8-C28-O10	-2.62	117.08	123.63
23	A	406[A]	CLA	CMC-C2C-C1C	2.62	129.12	125.03
23	B	608	CLA	CMC-C2C-C1C	2.62	129.12	125.03
29	a	412[A]	PL9	C53-C6-C1	2.62	120.64	115.28
23	a	407	CLA	C4B-C3B-C2B	-2.62	104.05	107.30
23	c	512	CLA	CMC-C2C-C1C	2.61	129.12	125.03
23	C	503	CLA	C4-C3-C5	2.61	119.76	115.23
23	c	506	CLA	CMB-C2B-C1B	2.61	129.40	125.42
23	C	503	CLA	CHD-C4C-NC	2.61	128.28	124.23
26	f	102	SQD	O47-C7-O49	-2.61	117.60	123.70
23	a	404[A]	CLA	C2A-C1A-CHA	-2.61	119.34	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	102	BCR	C33-C5-C6	-2.61	121.64	124.48
26	F	102	SQD	O8-S-O7	-2.61	104.87	111.40
23	b	603	CLA	CHC-C1C-C2C	-2.61	119.53	126.95
23	c	508	CLA	CAC-C3C-C4C	2.61	128.19	124.79
38	E	102	HEM	CHA-C4D-ND	2.61	127.59	124.37
24	A	407[A]	PHO	O2A-CGA-CBA	2.61	119.78	111.83
23	A	405[B]	CLA	C2A-C1A-CHA	-2.61	119.34	123.87
32	D	406[A]	LHG	O7-C7-C8	2.61	117.12	111.48
23	D	403	CLA	O2A-CGA-O1A	-2.61	117.11	123.63
23	b	606	CLA	CBC-CAC-C3C	-2.60	105.37	112.42
23	c	508	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
23	D	403	CLA	CHD-C4C-NC	2.60	128.26	124.23
23	a	404[B]	CLA	CHD-C4C-NC	2.60	128.26	124.23
23	B	612	CLA	C3B-C4B-NB	2.60	112.85	110.53
26	a	409[B]	SQD	O47-C7-O49	-2.60	117.63	123.70
23	c	501	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
32	D	407[B]	LHG	O8-C23-O10	-2.60	117.13	123.63
35	c	516[A]	DGD	O1G-C1A-O1A	-2.60	117.13	123.63
23	a	407	CLA	CMB-C2B-C1B	2.60	129.37	125.42
23	D	403	CLA	O2A-CGA-CBA	2.60	119.75	111.83
23	A	408	CLA	CMC-C2C-C1C	2.60	129.09	125.03
23	B	613	CLA	CMA-C3A-C4A	-2.59	104.80	111.77
23	b	614	CLA	O2A-CGA-CBA	2.59	119.74	111.83
29	d	406[A]	PL9	C17-C18-C19	-2.59	121.69	127.62
29	D	405[A]	PL9	C40-C39-C41	2.59	119.72	115.23
24	a	414[B]	PHO	CMB-C2B-C3B	2.59	129.86	124.68
29	d	406[B]	PL9	C27-C28-C29	-2.59	121.70	127.62
23	B	611	CLA	O2A-CGA-O1A	-2.59	117.15	123.63
23	b	610	CLA	C3B-C4B-NB	2.59	112.84	110.53
23	B	612	CLA	C1-C2-C3	-2.59	121.96	126.20
23	D	402[A]	CLA	C2A-C1A-CHA	-2.59	119.38	123.87
23	C	505	CLA	CBC-CAC-C3C	-2.59	105.41	112.42
23	a	405[A]	CLA	O2A-CGA-CBA	2.59	119.72	111.83
23	A	408	CLA	CAC-C3C-C4C	2.58	128.15	124.79
31	m	103	LMT	C1'-O5'-C5'	-2.58	108.68	113.72
23	B	608	CLA	C11-C12-C13	-2.58	107.39	115.97
23	C	504	CLA	O2A-CGA-CBA	2.58	119.70	111.83
23	D	402[A]	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
23	B	615	CLA	CHC-C1C-C2C	-2.58	119.62	126.95
23	B	608	CLA	CBC-CAC-C3C	-2.58	105.43	112.42
23	A	406[A]	CLA	C4-C3-C5	2.58	119.70	115.23
23	b	605	CLA	C4-C3-C5	2.58	119.70	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	CAC-C3C-C4C	2.58	128.14	124.79
23	C	503	CLA	C2A-C1A-CHA	-2.57	119.40	123.87
23	B	604	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
23	d	402[B]	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
23	a	404[A]	CLA	CMA-C3A-C4A	-2.57	104.87	111.77
38	f	101	HEM	C4D-ND-C1D	2.57	108.25	105.21
23	b	604	CLA	C4C-C3C-C2C	-2.57	103.15	106.89
23	B	606	CLA	CHC-C1C-C2C	-2.57	119.65	126.95
23	b	606	CLA	CMC-C2C-C1C	2.57	129.05	125.03
23	D	403	CLA	C2A-C1A-CHA	-2.57	119.41	123.87
23	c	511	CLA	CBC-CAC-C3C	-2.57	105.46	112.42
23	b	610	CLA	CHC-C1C-C2C	-2.57	119.65	126.95
32	d	407[B]	LHG	O8-C23-C24	2.57	119.66	111.83
23	C	507	CLA	O2A-CGA-O1A	-2.57	117.21	123.63
38	f	101	HEM	CHB-C1B-NB	2.57	127.54	124.37
23	c	508	CLA	CHD-C4C-NC	2.56	128.21	124.23
31	F	101	LMT	C1'-O5'-C5'	-2.56	108.71	113.72
23	b	616	CLA	CMC-C2C-C1C	2.56	129.04	125.03
23	A	404[B]	CLA	CAA-CBA-CGA	-2.56	105.93	113.21
25	Y	101	BCR	C10-C11-C12	-2.56	115.77	123.20
23	B	601	CLA	C4B-C3B-C2B	-2.56	104.12	107.30
23	B	609	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
23	b	611	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
31	A	420	LMT	O5'-C5'-C6'	2.56	112.78	106.44
25	B	619	BCR	C7-C8-C9	-2.56	122.45	126.23
23	a	405[B]	CLA	CAC-C3C-C4C	2.56	128.12	124.79
23	c	503	CLA	CAC-C3C-C4C	2.56	128.12	124.79
29	D	405[A]	PL9	C27-C28-C29	-2.56	121.77	127.62
23	c	507	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
23	B	606	CLA	C2A-C1A-CHA	-2.56	119.43	123.87
34	b	622	HTG	O2-C2-C3	-2.56	104.35	110.38
23	c	508	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
24	A	407[B]	PHO	CBC-CAC-C3C	-2.55	109.22	112.87
35	C	518[B]	DGD	O1G-C1A-O1A	-2.55	117.24	123.63
23	C	509	CLA	CHD-C4C-NC	2.55	128.19	124.23
23	A	405[A]	CLA	C2A-C1A-CHA	-2.55	119.44	123.87
25	c	515	BCR	C37-C22-C23	2.55	121.99	118.09
23	c	507	CLA	CAC-C3C-C4C	2.55	128.11	124.79
31	m	103	LMT	C3B-C4B-C5B	-2.55	105.61	110.23
23	A	405[B]	CLA	CED-O2D-CGD	2.55	121.70	115.92
23	C	505	CLA	CAC-C3C-C4C	2.55	128.10	124.79
23	B	603	CLA	CMA-C3A-C2A	-2.55	104.14	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	408	BCR	C29-C30-C25	2.55	114.14	110.44
23	a	405[A]	CLA	C2A-C1A-CHA	-2.55	119.45	123.87
24	a	406[B]	PHO	C1-C2-C3	-2.55	122.03	126.20
26	B	620	SQD	O5-C1-C2	-2.54	105.14	110.37
23	a	405[A]	CLA	O2A-CGA-O1A	-2.54	117.26	123.63
29	a	412[A]	PL9	C47-C48-C49	-2.54	119.16	127.64
23	B	608	CLA	O2A-CGA-CBA	2.54	119.59	111.83
35	c	517[B]	DGD	C2G-O2G-C1B	-2.54	111.71	117.80
40	v	201	HEC	CHA-C1A-NA	2.54	127.22	124.45
23	a	405[B]	CLA	C2A-C1A-CHA	-2.54	119.46	123.87
35	c	517[B]	DGD	O1G-C1A-C2A	2.54	119.57	111.83
25	H	101	BCR	C7-C8-C9	-2.53	122.48	126.23
23	d	402[A]	CLA	C2A-C1A-CHA	-2.53	119.47	123.87
29	D	405[B]	PL9	C22-C23-C24	-2.53	121.82	127.62
26	a	409[B]	SQD	O48-C23-C24	2.53	119.56	111.83
26	f	102	SQD	O5-C5-C4	2.53	114.26	109.70
23	c	502	CLA	C4B-C3B-C2B	-2.53	104.15	107.30
24	A	407[B]	PHO	O2A-CGA-CBA	2.53	119.56	111.83
25	k	101	BCR	C15-C14-C13	-2.53	123.73	127.28
23	b	608	CLA	O2A-CGA-CBA	2.53	119.55	111.83
23	C	506	CLA	O2A-CGA-CBA	2.53	119.55	111.83
23	c	504	CLA	CMB-C2B-C1B	2.53	129.27	125.42
29	d	406[B]	PL9	C17-C18-C19	-2.53	121.84	127.62
29	a	412[B]	PL9	C20-C19-C21	2.53	119.62	115.23
25	B	618	BCR	C15-C14-C13	-2.53	123.73	127.28
24	a	414[B]	PHO	O2D-CGD-O1D	-2.53	118.93	123.85
23	c	507	CLA	C3B-C4B-NB	2.53	112.78	110.53
25	A	409	BCR	C33-C5-C6	-2.53	121.73	124.48
40	V	201	HEC	CHA-C1A-NA	2.53	127.20	124.45
23	a	405[B]	CLA	O2A-CGA-O1A	-2.52	117.31	123.63
23	c	503	CLA	C2A-C1A-CHA	-2.52	119.49	123.87
23	C	505	CLA	C4-C3-C5	2.52	119.61	115.23
25	T	102	BCR	C21-C20-C19	-2.52	115.90	123.20
29	a	412[B]	PL9	C47-C48-C49	-2.52	119.24	127.64
23	C	506	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
23	C	504	CLA	C2A-C1A-CHA	-2.52	119.49	123.87
23	B	602	CLA	C1-C2-C3	-2.52	122.07	126.20
26	A	412	SQD	O8-S-C6	2.52	110.83	105.97
31	A	420	LMT	O1'-C1'-C2'	2.52	112.09	108.27
23	B	610	CLA	CMA-C3A-C2A	-2.52	104.26	113.98
23	c	509	CLA	CAC-C3C-C4C	2.51	128.06	124.79
23	B	607	CLA	CHC-C1C-C2C	-2.51	119.80	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414[A]	PL9	C42-C43-C44	-2.51	121.87	127.62
23	C	507	CLA	CHD-C4C-NC	2.51	128.13	124.23
33	C	520	LMG	C8-O7-C10	-2.51	111.78	117.80
23	d	403[B]	CLA	O2A-CGA-O1A	-2.51	117.34	123.63
24	A	407[A]	PHO	O2A-CGA-O1A	-2.51	117.34	123.63
23	c	506	CLA	CAA-C2A-C3A	-2.51	106.22	113.00
23	C	504	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
23	c	513	CLA	CHD-C4C-NC	2.50	128.12	124.23
23	C	507	CLA	O2A-CGA-CBA	2.50	119.47	111.83
23	D	402[B]	CLA	C4-C3-C5	2.50	119.57	115.23
23	d	403[B]	CLA	C2A-C1A-CHA	-2.50	119.52	123.87
23	b	601	CLA	C3B-C4B-NB	2.50	112.77	110.53
23	B	601	CLA	CHC-C1C-C2C	-2.50	119.84	126.95
23	B	612	CLA	CHD-C4C-NC	2.50	128.11	124.23
23	A	404[B]	CLA	CAC-C3C-C4C	2.50	128.04	124.79
24	A	416[A]	PHO	CMA-C3A-C4A	-2.50	109.23	114.61
23	B	604	CLA	O2A-CGA-CBA	2.50	119.45	111.83
24	A	416[B]	PHO	O2A-CGA-CBA	2.50	119.45	111.83
32	d	407[A]	LHG	O8-C23-O10	-2.50	117.38	123.63
25	y	101	BCR	C40-C30-C25	-2.50	106.33	110.24
23	c	501	CLA	O2A-CGA-CBA	2.50	119.45	111.83
23	c	506	CLA	C4-C3-C5	2.50	119.56	115.23
26	a	410	SQD	O7-S-C6	2.50	110.48	106.76
23	B	608	CLA	CAA-C2A-C3A	-2.50	106.25	113.00
23	a	405[B]	CLA	CHC-C1C-C2C	-2.50	119.85	126.95
23	b	605	CLA	C1-C2-C3	-2.50	122.11	126.20
23	C	508	CLA	CBC-CAC-C3C	-2.50	105.66	112.42
23	c	507	CLA	O1D-CGD-CBD	-2.50	119.60	124.52
25	k	101	BCR	C2-C1-C6	2.49	114.06	110.44
23	B	603	CLA	C2A-C1A-CHA	-2.49	119.54	123.87
23	B	616	CLA	CHC-C1C-C2C	-2.49	119.86	126.95
23	b	614	CLA	CAC-C3C-C4C	2.49	128.03	124.79
23	B	604	CLA	CHD-C1D-ND	-2.49	121.30	124.80
23	c	513	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
23	B	616	CLA	CHD-C4C-NC	2.49	128.09	124.23
31	B	630	LMT	O5'-C5'-C6'	2.49	112.60	106.44
38	E	102	HEM	O2D-CGD-CBD	2.49	121.86	114.00
32	D	406[B]	LHG	O8-C23-O10	-2.49	117.41	123.63
23	D	402[B]	CLA	CMC-C2C-C1C	2.49	128.92	125.03
23	b	612	CLA	CHC-C1C-C2C	-2.49	119.88	126.95
25	a	408	BCR	C33-C5-C6	-2.49	121.77	124.48
23	b	612	CLA	OBD-CAD-C3D	-2.48	122.61	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404[B]	CLA	C4C-C3C-C2C	-2.48	103.28	106.89
23	B	605	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
23	C	504	CLA	CMC-C2C-C1C	2.48	128.91	125.03
31	T	101	LMT	C1'-O5'-C5'	-2.48	108.88	113.72
23	b	603	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
26	B	620	SQD	O48-C23-O10	-2.48	117.42	123.63
23	B	606	CLA	C4-C3-C5	2.48	119.53	115.23
23	C	510	CLA	CHD-C4C-NC	2.48	128.08	124.23
24	A	416[A]	PHO	O1D-CGD-CBD	-2.48	120.96	124.72
23	B	612	CLA	O2A-CGA-O1A	-2.48	117.43	123.63
24	a	406[B]	PHO	CMC-C2C-C1C	2.48	129.19	124.73
23	b	604	CLA	C6-C5-C3	-2.48	107.43	113.47
29	A	414[A]	PL9	C35-C34-C36	2.48	119.53	115.23
23	A	405[A]	CLA	O2A-CGA-O1A	-2.48	117.44	123.63
23	B	607	CLA	CHD-C4C-NC	2.48	128.07	124.23
24	A	407[B]	PHO	C1-C2-C3	-2.47	122.14	126.20
23	B	604	CLA	C11-C12-C13	-2.47	107.74	115.97
23	C	508	CLA	C4-C3-C5	2.47	119.52	115.23
25	d	405	BCR	C39-C30-C25	-2.47	106.36	110.24
24	a	406[B]	PHO	O2D-CGD-O1D	-2.47	119.03	123.85
23	B	601	CLA	CAC-C3C-C4C	2.47	128.00	124.79
25	t	102	BCR	C10-C11-C12	-2.47	116.04	123.20
23	C	502	CLA	O2A-CGA-CBA	2.47	119.36	111.83
23	b	605	CLA	CMC-C2C-C1C	2.47	128.89	125.03
29	A	414[A]	PL9	C53-C6-C1	2.47	120.33	115.28
26	A	410[A]	SQD	O9-S-C6	2.47	110.44	106.76
23	A	404[B]	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
29	d	406[A]	PL9	C36-C34-C33	-2.47	115.63	121.17
23	c	506	CLA	C2A-C1A-CHA	-2.47	119.59	123.87
23	B	602	CLA	CMB-C2B-C1B	2.47	129.18	125.42
24	a	406[A]	PHO	O2A-CGA-O1A	-2.47	117.46	123.63
23	d	402[B]	CLA	C2A-C1A-CHA	-2.47	119.59	123.87
29	D	405[A]	PL9	C22-C23-C24	-2.47	121.98	127.62
23	C	502	CLA	C2A-C1A-CHA	-2.46	119.59	123.87
25	K	102	BCR	C39-C30-C25	-2.46	106.38	110.24
23	B	614	CLA	CBC-CAC-C3C	-2.46	105.74	112.42
23	C	511	CLA	C2A-C1A-CHA	-2.46	119.59	123.87
25	y	101	BCR	C21-C20-C19	-2.46	116.07	123.20
23	a	404[A]	CLA	CHD-C4C-NC	2.46	128.05	124.23
23	C	510	CLA	C11-C12-C13	-2.46	107.80	115.97
23	d	403[B]	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
23	B	602	CLA	CHC-C1C-C2C	-2.46	119.97	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	V	201	HEC	CMD-C2D-C1D	2.45	129.16	125.42
31	B	631	LMT	O1'-C1'-C2'	2.45	112.00	108.27
33	C	521	LMG	C9-C8-C7	-2.45	106.06	111.78
25	Y	101	BCR	C34-C9-C8	2.45	121.84	118.09
25	k	101	BCR	C3-C4-C5	-2.45	109.68	114.06
29	d	406[A]	PL9	C47-C48-C49	-2.45	119.47	127.64
23	d	402[A]	CLA	C4C-C3C-C2C	-2.45	103.32	106.89
23	C	505	CLA	CAA-C2A-C3A	-2.45	106.37	113.00
23	B	602	CLA	C11-C12-C13	-2.45	107.82	115.97
23	C	509	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
23	a	404[B]	CLA	CMC-C2C-C1C	2.45	128.86	125.03
29	D	405[B]	PL9	C40-C39-C41	2.45	119.48	115.23
23	b	613	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
23	B	602	CLA	CAA-CBA-CGA	-2.45	106.25	113.21
23	A	405[A]	CLA	CMA-C3A-C4A	-2.45	105.19	111.77
25	t	102	BCR	C1-C6-C7	2.45	122.29	115.65
23	C	503	CLA	C4B-C3B-C2B	-2.45	104.26	107.30
23	c	506	CLA	CMC-C2C-C1C	2.45	128.86	125.03
25	Y	101	BCR	C36-C18-C17	-2.45	118.85	122.82
23	c	504	CLA	C1-C2-C3	-2.44	122.19	126.20
23	c	505	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
26	A	410[B]	SQD	O9-S-O7	-2.44	105.88	113.82
23	d	402[A]	CLA	C1-O2A-CGA	2.44	122.56	116.65
23	A	406[B]	CLA	CBC-CAC-C3C	-2.44	105.81	112.42
40	v	201	HEC	C2A-C1A-NA	-2.44	107.97	110.32
23	a	404[A]	CLA	CMC-C2C-C1C	2.44	128.84	125.03
23	B	606	CLA	CMB-C2B-C1B	2.43	129.13	125.42
23	c	508	CLA	CMC-C2C-C1C	2.43	128.84	125.03
25	H	101	BCR	C16-C15-C14	-2.43	118.54	123.52
33	m	101	LMG	C8-O7-C10	-2.43	111.97	117.80
23	B	602	CLA	CMA-C3A-C2A	-2.43	104.58	113.98
23	B	607	CLA	C4C-C3C-C2C	-2.43	103.35	106.89
23	b	609	CLA	CMB-C2B-C1B	2.43	129.12	125.42
23	b	602	CLA	C11-C12-C13	-2.43	107.88	115.97
34	B	625	HTG	O5-C5-C4	2.43	114.08	109.70
32	A	419[B]	LHG	O7-C7-O9	-2.43	118.03	123.70
23	b	601	CLA	C2A-C1A-CHA	-2.43	119.65	123.87
23	B	604	CLA	C6-C7-C8	-2.43	107.89	115.97
26	A	412	SQD	C4-C3-C2	-2.43	106.57	110.83
23	c	510	CLA	C4-C3-C2	-2.43	117.39	123.63
33	D	411	LMG	O7-C10-C11	2.43	116.73	111.48
23	b	606	CLA	O2A-CGA-O1A	-2.43	117.55	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	V	201	HEC	C2A-C1A-NA	-2.43	107.98	110.32
23	b	616	CLA	C1-C2-C3	-2.43	122.22	126.20
23	C	506	CLA	CHD-C4C-NC	2.43	127.99	124.23
35	C	518[B]	DGD	C2G-O2G-C1B	-2.42	111.99	117.80
23	b	614	CLA	CAA-C2A-C3A	-2.42	106.45	113.00
23	C	513	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
23	c	507	CLA	CHC-C1C-C2C	-2.42	120.07	126.95
35	C	518[A]	DGD	O1G-C1A-C2A	2.42	119.21	111.83
35	c	517[A]	DGD	O1G-C1A-C2A	2.42	119.21	111.83
23	d	404	CLA	CHC-C1C-C2C	-2.42	120.07	126.95
32	d	407[B]	LHG	O8-C23-O10	-2.42	117.58	123.63
32	d	407[A]	LHG	O8-C23-C24	2.42	119.21	111.83
24	A	407[A]	PHO	C1-C2-C3	-2.42	122.24	126.20
25	Y	101	BCR	C37-C22-C23	2.42	121.78	118.09
23	A	404[B]	CLA	CMC-C2C-C1C	2.42	128.81	125.03
25	T	102	BCR	C3-C4-C5	-2.42	109.75	114.06
32	L	101[A]	LHG	O8-C23-O10	-2.42	117.59	123.63
23	b	611	CLA	C2A-C1A-CHA	-2.41	119.68	123.87
23	C	507	CLA	CMB-C2B-C1B	2.41	129.10	125.42
23	B	604	CLA	CMC-C2C-C1C	2.41	128.81	125.03
32	D	406[B]	LHG	O8-C23-C24	2.41	119.20	111.83
23	b	610	CLA	CAC-C3C-C4C	2.41	127.93	124.79
23	c	509	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
23	B	613	CLA	CBC-CAC-C3C	-2.41	105.88	112.42
23	b	609	CLA	CMC-C2C-C1C	2.41	128.80	125.03
25	B	618	BCR	C38-C26-C25	-2.41	121.85	124.48
23	c	511	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
23	a	404[A]	CLA	CMA-C3A-C2A	-2.41	104.66	113.98
25	C	516	BCR	C32-C1-C6	-2.41	106.46	110.24
23	b	608	CLA	CAA-C2A-C3A	-2.41	106.48	113.00
25	d	405	BCR	C40-C30-C39	2.41	115.54	108.63
23	C	514	CLA	C4-C3-C5	2.41	119.41	115.23
23	c	505	CLA	C4-C3-C5	2.41	119.41	115.23
23	B	613	CLA	CHB-C4A-NA	2.41	127.88	124.40
25	C	515	BCR	C24-C23-C22	-2.41	122.67	126.23
23	B	606	CLA	C7-C6-C5	-2.41	106.84	113.26
26	a	409[A]	SQD	O48-C23-C24	2.41	119.17	111.83
25	c	514	BCR	C38-C26-C25	-2.41	121.86	124.48
23	b	611	CLA	CMB-C2B-C1B	2.41	129.08	125.42
29	a	412[B]	PL9	C45-C44-C46	2.41	119.40	115.23
33	B	621	LMG	O1-C7-C8	-2.40	104.97	110.82
23	c	513	CLA	O2D-CGD-O1D	-2.40	119.17	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	CED-O2D-CGD	2.40	121.37	115.92
23	C	511	CLA	CBC-CAC-C3C	-2.40	105.91	112.42
25	D	404	BCR	C21-C20-C19	-2.40	116.24	123.20
23	c	506	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
26	b	620	SQD	O8-S-C6	2.40	110.61	105.97
25	K	102	BCR	C2-C1-C6	2.40	113.93	110.44
23	b	602	CLA	CHD-C4C-NC	2.40	127.95	124.23
40	V	201	HEC	CAD-CBD-CGD	-2.40	107.30	113.67
25	c	515	BCR	C38-C26-C25	-2.40	121.86	124.48
25	b	617	BCR	C32-C1-C6	-2.40	106.48	110.24
29	D	405[B]	PL9	C12-C13-C14	-2.40	122.13	127.62
29	a	412[A]	PL9	C40-C39-C41	2.40	119.39	115.23
23	B	602	CLA	CMA-C3A-C4A	-2.40	105.33	111.77
25	c	515	BCR	C2-C1-C6	2.40	113.92	110.44
23	B	607	CLA	O2A-CGA-CBA	2.39	119.14	111.83
29	a	412[A]	PL9	C20-C19-C21	2.39	119.38	115.23
23	C	512	CLA	CHC-C1C-C2C	-2.39	120.15	126.95
23	C	513	CLA	CHC-C1C-C2C	-2.39	120.15	126.95
35	c	516[B]	DGD	C3G-C2G-C1G	-2.39	106.21	111.78
35	c	516[A]	DGD	C2G-O2G-C1B	-2.39	112.07	117.80
23	a	407	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
38	E	102	HEM	O2A-CGA-CBA	2.39	121.55	114.00
29	A	414[A]	PL9	C35-C34-C33	-2.39	117.49	123.63
23	b	613	CLA	CAC-C3C-C4C	2.39	127.90	124.79
23	C	508	CLA	C3B-C4B-NB	2.39	112.66	110.53
23	C	511	CLA	CMC-C2C-C1C	2.39	128.76	125.03
23	A	404[B]	CLA	C4-C3-C5	2.39	119.37	115.23
23	b	603	CLA	C7-C6-C5	-2.39	106.90	113.26
23	D	402[B]	CLA	CBC-CAC-C3C	-2.39	105.95	112.42
23	b	607	CLA	C2A-C1A-CHA	-2.38	119.73	123.87
23	c	508	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
25	h	101	BCR	C36-C18-C17	-2.38	118.95	122.82
23	c	511	CLA	C2A-C1A-CHA	-2.38	119.73	123.87
23	d	402[A]	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
25	c	515	BCR	C32-C1-C6	-2.38	106.51	110.24
23	A	405[B]	CLA	C4C-C3C-C2C	-2.38	103.42	106.89
33	d	412	LMG	O7-C10-O9	-2.38	118.14	123.70
23	B	610	CLA	C2A-C1A-CHA	-2.38	119.73	123.87
23	b	605	CLA	CAC-C3C-C4C	2.38	127.89	124.79
23	d	402[B]	CLA	CBC-CAC-C3C	-2.38	105.97	112.42
23	c	504	CLA	CAC-C3C-C4C	2.38	127.88	124.79
25	a	408	BCR	C7-C8-C9	-2.38	122.72	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C1C-C2C-C3C	-2.38	104.48	106.98
25	B	617	BCR	C31-C1-C6	-2.38	106.52	110.24
25	h	101	BCR	C34-C9-C8	2.38	121.72	118.09
23	C	507	CLA	CGD-CBD-CAD	-2.38	103.16	110.85
29	A	414[A]	PL9	C2-C3-C4	2.38	121.97	118.78
23	b	606	CLA	CMB-C2B-C1B	2.37	129.03	125.42
23	B	608	CLA	CMA-C3A-C2A	-2.37	104.82	113.98
23	C	504	CLA	CAC-C3C-C4C	2.37	127.87	124.79
23	b	602	CLA	CHC-C1C-C2C	-2.37	120.21	126.95
25	k	101	BCR	C34-C9-C8	2.37	121.71	118.09
23	b	602	CLA	CHB-C1B-C2B	-2.37	120.55	127.43
23	d	404	CLA	C3B-C4B-NB	2.37	112.64	110.53
24	A	407[B]	PHO	O2D-CGD-O1D	-2.37	119.24	123.85
23	b	610	CLA	CMC-C2C-C1C	2.37	128.73	125.03
26	F	102	SQD	O5-C1-O6	2.37	115.64	110.04
26	b	620	SQD	C1-C2-C3	-2.37	105.03	110.01
23	B	615	CLA	CAC-C3C-C4C	2.37	127.87	124.79
23	d	402[B]	CLA	CMA-C3A-C2A	-2.37	104.84	113.98
23	d	404	CLA	CMA-C3A-C2A	-2.36	104.84	113.98
23	c	501	CLA	CBC-CAC-C3C	-2.36	106.02	112.42
25	B	618	BCR	C37-C22-C23	2.36	121.69	118.09
23	C	506	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
24	a	414[B]	PHO	O1D-CGD-CBD	-2.36	121.14	124.72
23	c	506	CLA	O2A-CGA-CBA	2.36	119.03	111.83
25	b	618	BCR	C8-C7-C6	-2.36	120.69	127.00
23	c	512	CLA	C3B-C4B-NB	2.36	112.64	110.53
25	h	101	BCR	C16-C15-C14	-2.36	118.69	123.52
23	b	611	CLA	C7-C6-C5	-2.36	106.98	113.26
23	A	408	CLA	C4-C3-C5	2.36	119.32	115.23
23	b	601	CLA	O2A-CGA-CBA	2.36	119.02	111.83
23	c	508	CLA	C4-C3-C5	2.36	119.32	115.23
33	c	520	LMG	O8-C28-O10	-2.36	117.73	123.63
23	C	509	CLA	C2A-C1A-CHA	-2.36	119.78	123.87
35	C	518[A]	DGD	O6E-C5E-C6E	2.36	112.28	106.44
29	A	414[A]	PL9	C37-C36-C34	-2.36	105.38	113.19
23	c	504	CLA	O2A-CGA-O1A	-2.36	117.74	123.63
29	a	412[A]	PL9	C10-C9-C8	-2.35	117.58	123.63
23	C	514	CLA	CMB-C2B-C1B	2.35	129.00	125.42
23	C	512	CLA	O2A-CGA-CBA	2.35	119.01	111.83
23	b	613	CLA	CHD-C4C-NC	2.35	127.88	124.23
23	D	402[A]	CLA	CHD-C4C-NC	2.35	127.88	124.23
25	h	101	BCR	C24-C23-C22	-2.35	122.76	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	CMA-C3A-C2A	-2.35	104.90	113.98
31	B	630	LMT	O5'-C5'-C4'	2.35	114.58	109.72
35	H	102	DGD	O2G-C1B-C2B	2.35	116.56	111.48
23	b	611	CLA	CMC-C2C-C1C	2.35	128.70	125.03
24	A	407[A]	PHO	CMB-C2B-C3B	2.35	129.37	124.68
26	F	102	SQD	O5-C1-C2	-2.35	105.55	110.37
34	B	622	HTG	C2'-C1'-S1	-2.35	104.46	112.36
29	D	405[B]	PL9	C20-C19-C21	2.35	119.30	115.23
29	a	412[B]	PL9	C53-C6-C1	2.35	120.08	115.28
23	B	608	CLA	CHD-C4C-NC	2.35	127.87	124.23
23	B	611	CLA	CAC-C3C-C4C	2.34	127.84	124.79
35	C	519	DGD	O2G-C1B-C2B	2.34	116.55	111.48
23	B	611	CLA	CMB-C2B-C3B	2.34	132.06	126.55
23	b	606	CLA	CHB-C1B-C2B	-2.34	120.62	127.43
23	d	404	CLA	CMC-C2C-C1C	2.34	128.69	125.03
35	C	517[B]	DGD	O3G-C3G-C2G	-2.34	105.12	110.82
25	t	102	BCR	C28-C27-C26	-2.34	109.88	114.06
23	c	501	CLA	C4-C3-C5	2.34	119.29	115.23
23	B	616	CLA	CBC-CAC-C3C	-2.34	106.08	112.42
26	a	409[B]	SQD	O8-S-C6	2.34	110.49	105.97
25	a	408	BCR	C40-C30-C25	-2.34	106.58	110.24
32	d	414[A]	LHG	O7-C7-O9	-2.34	118.24	123.70
23	d	404	CLA	O2A-CGA-CBA	2.34	118.96	111.83
23	C	512	CLA	C4B-C3B-C2B	-2.34	104.40	107.30
23	b	608	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
26	F	102	SQD	O48-C23-O10	-2.34	117.78	123.63
23	C	503	CLA	O2A-CGA-CBA	2.34	118.96	111.83
33	c	519	LMG	C8-O7-C10	-2.33	112.21	117.80
23	a	407	CLA	C2A-C1A-CHA	-2.33	119.82	123.87
23	a	407	CLA	CHC-C1C-C2C	-2.33	120.32	126.95
25	k	101	BCR	C10-C11-C12	-2.33	116.44	123.20
23	C	505	CLA	OBD-CAD-C3D	-2.33	122.97	128.42
25	B	619	BCR	C38-C26-C25	-2.33	121.94	124.48
23	b	607	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
34	b	622	HTG	O5-C1-C2	2.33	113.53	110.32
23	a	407	CLA	CAC-C3C-C4C	2.33	127.82	124.79
24	A	416[B]	PHO	CMB-C2B-C3B	2.33	129.34	124.68
25	K	102	BCR	C20-C21-C22	-2.33	124.01	127.28
25	Y	101	BCR	C15-C16-C17	-2.33	118.76	123.52
29	D	405[A]	PL9	C45-C44-C46	2.33	119.27	115.23
29	d	406[B]	PL9	C45-C44-C46	2.33	119.27	115.23
23	C	502	CLA	O2A-CGA-O1A	-2.33	117.81	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	420	LMT	O5'-C5'-C4'	2.33	114.53	109.72
29	A	414[B]	PL9	C45-C44-C46	2.32	119.26	115.23
23	b	602	CLA	C4B-C3B-C2B	-2.32	104.41	107.30
24	a	406[A]	PHO	CMB-C2B-C3B	2.32	129.33	124.68
23	c	504	CLA	CAA-C2A-C3A	-2.32	106.72	113.00
32	d	408[A]	LHG	O8-C23-O10	-2.32	117.82	123.63
23	a	405[A]	CLA	CBC-CAC-C3C	-2.32	106.12	112.42
29	A	414[B]	PL9	C47-C48-C49	-2.32	119.90	127.64
29	A	414[A]	PL9	C2-C1-C6	2.32	121.76	119.00
23	b	604	CLA	O2A-CGA-CBA	2.32	118.91	111.83
23	c	503	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
25	b	618	BCR	C37-C22-C23	2.32	121.63	118.09
23	c	512	CLA	CHB-C4A-NA	2.32	127.75	124.40
23	C	513	CLA	C4B-C3B-C2B	-2.32	104.42	107.30
29	d	406[A]	PL9	C7-C8-C9	-2.32	122.84	126.83
23	d	402[B]	CLA	CAA-CBA-CGA	2.32	119.79	113.21
25	Y	101	BCR	C28-C27-C26	-2.32	109.92	114.06
23	A	404[A]	CLA	CMA-C3A-C4A	-2.32	105.54	111.77
23	b	608	CLA	C2A-C1A-CHA	-2.32	119.85	123.87
29	A	414[A]	PL9	C47-C48-C49	-2.32	119.92	127.64
25	k	101	BCR	C11-C10-C9	-2.32	124.03	127.28
32	d	414[B]	LHG	C5-O7-C7	-2.31	112.26	117.80
29	A	414[B]	PL9	C2-C3-C4	2.31	121.89	118.78
23	b	601	CLA	CMC-C2C-C1C	2.31	128.65	125.03
32	d	414[B]	LHG	O7-C7-O9	-2.31	118.30	123.70
31	B	628	LMT	C1B-C2B-C3B	2.31	114.88	110.01
33	Z	101	LMG	C9-C8-C7	-2.31	106.39	111.78
40	V	201	HEC	C3D-C4D-ND	-2.31	107.59	110.15
25	B	618	BCR	C11-C10-C9	-2.31	124.04	127.28
23	A	406[B]	CLA	C4-C3-C5	2.31	119.24	115.23
23	B	613	CLA	CHD-C4C-NC	2.31	127.81	124.23
23	B	604	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
25	t	102	BCR	C7-C6-C5	-2.31	116.24	121.56
23	c	507	CLA	C4C-C3C-C2C	-2.31	103.53	106.89
23	b	616	CLA	C4-C3-C5	2.31	119.23	115.23
23	b	613	CLA	CED-O2D-CGD	2.31	121.15	115.92
26	b	620	SQD	O48-C23-C24	2.31	118.87	111.83
24	a	414[A]	PHO	O2D-CGD-O1D	-2.31	119.36	123.85
29	A	414[B]	PL9	C10-C9-C8	-2.31	117.70	123.63
29	a	412[A]	PL9	C35-C34-C33	-2.31	117.70	123.63
31	F	101	LMT	C3B-C4B-C5B	-2.31	106.05	110.23
23	B	605	CLA	O2A-CGA-CBA	2.30	118.86	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	101	BCR	C16-C15-C14	-2.30	118.80	123.52
23	d	402[B]	CLA	C1-C2-C3	-2.30	122.42	126.20
29	d	406[B]	PL9	C20-C19-C21	2.30	119.23	115.23
23	B	605	CLA	CBC-CAC-C3C	-2.30	106.18	112.42
26	a	410	SQD	O48-C23-O10	-2.30	117.87	123.63
29	A	414[A]	PL9	C45-C44-C46	2.30	119.22	115.23
29	A	414[B]	PL9	C37-C36-C34	-2.30	105.56	113.19
29	a	412[A]	PL9	C45-C44-C46	2.30	119.22	115.23
25	T	102	BCR	C1-C6-C7	2.30	121.89	115.65
23	D	402[B]	CLA	CED-O2D-CGD	2.30	121.13	115.92
23	B	614	CLA	CAA-C2A-C3A	-2.30	106.79	113.00
23	B	609	CLA	CAC-C3C-C4C	2.29	127.77	124.79
23	b	611	CLA	OBD-CAD-C3D	-2.29	123.06	128.42
32	b	629[A]	LHG	O8-C23-O10	-2.29	117.90	123.63
23	b	607	CLA	CBC-CAC-C3C	-2.29	106.21	112.42
32	d	407[A]	LHG	C6-C5-C4	-2.29	106.44	111.78
25	t	102	BCR	C20-C21-C22	-2.29	124.07	127.28
31	B	631	LMT	O5'-C5'-C4'	2.29	114.46	109.72
31	e	101	LMT	O1'-C1'-C2'	2.29	111.75	108.27
33	a	415	LMG	O8-C28-C29	2.29	118.81	111.83
25	c	514	BCR	C36-C18-C19	2.29	121.58	118.09
33	d	412	LMG	O8-C28-C29	2.29	118.81	111.83
25	b	617	BCR	C11-C10-C9	-2.29	124.07	127.28
23	b	603	CLA	CBC-CAC-C3C	-2.29	106.22	112.42
23	C	510	CLA	C2A-C1A-CHA	-2.29	119.90	123.87
38	E	102	HEM	C4B-C3B-C2B	-2.29	105.18	107.28
25	c	514	BCR	C33-C5-C6	-2.29	121.99	124.48
26	a	409[A]	SQD	O9-S-O7	-2.29	106.39	113.82
23	B	612	CLA	CHC-C1C-C2C	-2.29	120.45	126.95
23	B	615	CLA	C2A-C1A-CHA	-2.28	119.90	123.87
38	E	102	HEM	C4C-NC-C1C	2.28	109.55	105.82
24	A	416[A]	PHO	O2A-CGA-CBA	2.28	118.80	111.83
23	C	503	CLA	CBC-CAC-C3C	-2.28	106.23	112.42
23	a	407	CLA	CHB-C4A-NA	2.28	127.69	124.40
23	B	614	CLA	C4-C3-C5	2.28	119.19	115.23
23	b	615	CLA	CAC-C3C-C4C	2.28	127.76	124.79
23	B	612	CLA	C7-C6-C5	-2.28	107.18	113.26
29	d	406[B]	PL9	C53-C6-C1	2.28	119.95	115.28
23	b	601	CLA	CHB-C1B-C2B	-2.28	120.81	127.43
23	c	503	CLA	CHC-C1C-C2C	-2.28	120.47	126.95
26	A	412	SQD	O6-C44-C45	-2.28	105.28	110.82
23	c	505	CLA	CHD-C4C-NC	2.28	127.76	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	CAC-C3C-C4C	2.28	127.75	124.79
23	c	504	CLA	CMC-C2C-C1C	2.28	128.59	125.03
23	b	605	CLA	C4B-C3B-C2B	-2.28	104.47	107.30
23	a	407	CLA	CBC-CAC-C3C	-2.28	106.25	112.42
23	B	611	CLA	C11-C12-C13	-2.27	108.41	115.97
23	B	606	CLA	CBC-CAC-C3C	-2.27	106.26	112.42
26	A	412	SQD	C1-C2-C3	-2.27	105.23	110.01
23	a	405[A]	CLA	C4-C3-C5	2.27	119.17	115.23
24	A	416[A]	PHO	C6-C5-C3	-2.27	107.94	113.47
25	c	515	BCR	C16-C17-C18	-2.27	124.09	127.28
29	A	414[B]	PL9	C35-C34-C36	2.27	119.17	115.23
23	C	512	CLA	CMB-C2B-C1B	2.27	128.88	125.42
23	d	402[B]	CLA	CHB-C4A-NA	2.27	127.67	124.40
23	c	503	CLA	O2A-CGA-CBA	2.27	118.75	111.83
23	c	510	CLA	C11-C10-C8	-2.27	108.43	115.97
23	A	408	CLA	CHB-C4A-NA	2.27	127.67	124.40
23	C	507	CLA	C4C-C3C-C2C	-2.27	103.59	106.89
23	b	607	CLA	C1-C2-C3	-2.27	122.49	126.20
32	L	101[B]	LHG	O8-C23-O10	-2.26	117.96	123.63
33	C	501	LMG	O8-C28-C29	2.26	118.74	111.83
23	b	608	CLA	C11-C10-C8	-2.26	108.44	115.97
29	d	406[B]	PL9	C12-C13-C14	-2.26	122.44	127.62
23	C	511	CLA	CHB-C4A-NA	2.26	127.67	124.40
26	a	410	SQD	O5-C5-C4	2.26	113.78	109.70
23	b	608	CLA	C4C-C3C-C2C	-2.26	103.60	106.89
26	F	102	SQD	C46-C45-C44	-2.26	106.51	111.78
25	T	102	BCR	C39-C30-C25	-2.26	106.70	110.24
25	c	515	BCR	C11-C10-C9	-2.26	124.11	127.28
32	A	419[A]	LHG	O4-P-O5	2.26	122.95	112.44
23	B	609	CLA	C2A-C1A-CHA	-2.26	119.95	123.87
23	B	607	CLA	CED-O2D-CGD	2.26	121.04	115.92
23	D	402[B]	CLA	CHD-C4C-NC	2.26	127.73	124.23
26	A	410[A]	SQD	O9-S-O7	-2.26	106.48	113.82
26	f	102	SQD	O48-C23-O10	-2.26	117.98	123.63
23	d	402[B]	CLA	CAC-C3C-C2C	2.26	131.70	127.56
23	c	509	CLA	CMB-C2B-C1B	2.26	128.85	125.42
23	D	403	CLA	CMA-C3A-C4A	-2.25	105.71	111.77
23	C	513	CLA	C2A-C1A-CHA	-2.25	119.96	123.87
23	b	615	CLA	C6-C7-C8	-2.25	108.48	115.97
23	A	406[B]	CLA	C1-C2-C3	-2.25	122.51	126.20
29	D	405[B]	PL9	C42-C41-C39	-2.25	105.72	113.19
23	C	507	CLA	CHB-C4A-NA	2.25	127.65	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	502	CLA	C4C-C3C-C2C	-2.25	103.62	106.89
23	d	403[A]	CLA	CMC-C2C-C1C	2.25	128.55	125.03
23	A	404[B]	CLA	CMA-C3A-C2A	-2.25	105.30	113.98
35	C	517[A]	DGD	C3G-C2G-C1G	-2.25	106.55	111.78
23	C	504	CLA	C4B-C3B-C2B	-2.24	104.51	107.30
23	C	513	CLA	O1D-CGD-CBD	-2.24	120.09	124.52
24	a	414[A]	PHO	CED-O2D-CGD	2.24	121.00	115.92
23	A	404[A]	CLA	CMC-C2C-C1C	2.24	128.54	125.03
25	k	101	BCR	C36-C18-C19	2.24	121.52	118.09
23	c	511	CLA	C1-C2-C3	-2.24	122.52	126.20
25	c	515	BCR	C29-C30-C25	2.24	113.70	110.44
23	d	404	CLA	C4B-C3B-C2B	-2.24	104.51	107.30
23	c	513	CLA	C4-C3-C5	2.24	119.12	115.23
23	c	505	CLA	CMA-C3A-C4A	-2.24	105.75	111.77
35	c	517[A]	DGD	C2G-O2G-C1B	-2.24	112.43	117.80
23	b	609	CLA	C4-C3-C5	2.24	119.11	115.23
23	C	505	CLA	CHD-C4C-NC	2.24	127.70	124.23
25	C	515	BCR	C16-C17-C18	-2.24	124.14	127.28
23	C	502	CLA	C1-O2A-CGA	2.24	122.06	116.65
23	D	403	CLA	CMC-C2C-C1C	2.24	128.53	125.03
23	b	608	CLA	CMA-C3A-C4A	-2.23	105.77	111.77
23	C	506	CLA	CBC-CAC-C3C	-2.23	106.36	112.42
24	a	414[A]	PHO	C4-C3-C2	-2.23	117.89	123.63
27	O	303	GOL	C3-C2-C1	-2.23	103.61	111.80
26	A	410[B]	SQD	O48-C23-O10	-2.23	118.05	123.63
23	a	404[A]	CLA	C7-C6-C5	-2.23	107.32	113.26
29	A	414[B]	PL9	C25-C24-C26	2.23	119.10	115.23
26	b	620	SQD	O5-C1-C2	-2.23	105.79	110.37
23	c	509	CLA	C2A-C1A-CHA	-2.23	120.00	123.87
38	E	102	HEM	CHA-C1A-NA	2.23	127.90	123.86
23	b	602	CLA	C4-C3-C5	2.23	119.09	115.23
23	C	506	CLA	O1D-CGD-CBD	-2.23	120.13	124.52
27	A	418	GOL	C3-C2-C1	-2.22	103.64	111.80
34	b	623	HTG	O5-C1-C2	2.22	113.38	110.32
23	b	612	CLA	CMA-C3A-C2A	-2.22	105.40	113.98
23	B	615	CLA	CHA-C1A-NA	-2.22	121.36	126.39
23	C	508	CLA	C6-C7-C8	-2.22	108.59	115.97
40	V	201	HEC	C1D-C2D-C3D	-2.22	104.28	106.82
23	C	513	CLA	CMA-C3A-C4A	-2.22	105.81	111.77
25	B	619	BCR	C10-C11-C12	-2.22	116.77	123.20
23	A	405[B]	CLA	CHB-C4A-NA	2.22	127.60	124.40
23	C	509	CLA	C4-C3-C5	2.22	119.08	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	C1-C2-C3	-2.22	122.56	126.20
23	b	615	CLA	CHA-C1A-NA	-2.22	121.37	126.39
26	A	412	SQD	O48-C23-O10	-2.22	118.09	123.63
23	B	611	CLA	C2C-C1C-NC	2.22	112.31	109.98
23	D	402[A]	CLA	C4-C3-C5	2.22	119.07	115.23
23	b	613	CLA	C2A-C1A-CHA	-2.22	120.02	123.87
23	c	501	CLA	C2A-C1A-CHA	-2.22	120.02	123.87
23	b	604	CLA	CHD-C4C-NC	2.21	127.66	124.23
35	C	518[B]	DGD	O2G-C1B-O1B	-2.21	118.53	123.70
35	C	518[A]	DGD	C2G-O2G-C1B	-2.21	112.50	117.80
25	b	617	BCR	C8-C7-C6	-2.21	121.09	127.00
25	D	404	BCR	C31-C1-C6	-2.21	106.77	110.24
23	a	404[B]	CLA	CHB-C4A-NA	2.21	127.59	124.40
29	A	414[A]	PL9	C12-C13-C14	-2.21	122.56	127.62
33	C	520	LMG	O7-C10-O9	-2.21	118.53	123.70
25	c	515	BCR	C33-C5-C6	-2.21	122.07	124.48
23	b	602	CLA	CMA-C3A-C2A	-2.21	105.44	113.98
23	a	405[A]	CLA	CAC-C3C-C4C	2.21	127.67	124.79
23	D	403	CLA	CED-O2D-CGD	2.21	120.92	115.92
23	B	604	CLA	C4-C3-C5	2.21	119.06	115.23
31	b	621	LMT	C2'-C3'-C4'	2.21	114.69	109.68
23	A	405[A]	CLA	O2A-CGA-CBA	2.21	118.56	111.83
23	A	408	CLA	OBD-CAD-C3D	-2.21	123.26	128.42
23	A	405[B]	CLA	CMA-C3A-C2A	-2.21	105.45	113.98
29	D	405[A]	PL9	C20-C19-C21	2.20	119.05	115.23
23	A	405[A]	CLA	CHB-C4A-NA	2.20	127.58	124.40
23	b	601	CLA	CAA-C2A-C3A	-2.20	107.05	113.00
25	C	516	BCR	C39-C30-C25	-2.20	106.79	110.24
29	d	406[A]	PL9	C2-C1-C6	2.20	121.62	119.00
35	C	517[A]	DGD	O5D-C6D-C5D	-2.20	104.46	109.42
23	B	601	CLA	CHB-C4A-NA	2.20	127.58	124.40
23	b	611	CLA	CBC-CAC-C3C	-2.20	106.46	112.42
23	A	408	CLA	CMB-C2B-C1B	2.20	128.77	125.42
35	c	518	DGD	O3G-C3G-C2G	-2.20	105.47	110.82
23	B	605	CLA	OBD-CAD-C3D	-2.20	123.28	128.42
35	H	102	DGD	O6E-C5E-C6E	2.20	111.89	106.44
25	D	404	BCR	C15-C16-C17	-2.20	119.03	123.52
27	B	627	GOL	C3-C2-C1	-2.19	103.75	111.80
29	d	406[A]	PL9	C12-C13-C14	-2.19	122.60	127.62
23	b	606	CLA	O2A-CGA-CBA	2.19	118.53	111.83
29	A	414[B]	PL9	C51-C49-C50	2.19	119.64	114.59
26	a	409[B]	SQD	C3-C4-C5	2.19	114.21	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	C7-C6-C5	-2.19	107.42	113.26
35	H	102	DGD	C3E-C4E-C5E	-2.19	106.25	110.23
23	B	614	CLA	CMA-C3A-C2A	-2.19	105.51	113.98
25	c	514	BCR	C29-C30-C25	2.19	113.62	110.44
23	B	612	CLA	C4-C3-C5	2.19	119.03	115.23
23	C	502	CLA	C4-C3-C5	2.19	119.03	115.23
31	M	101	LMT	C3B-C4B-C5B	-2.19	106.26	110.23
23	D	402[A]	CLA	CED-O2D-CGD	2.19	120.88	115.92
25	T	102	BCR	C7-C8-C9	-2.19	123.00	126.23
23	d	403[A]	CLA	CAC-C3C-C4C	2.19	127.64	124.79
29	A	414[B]	PL9	C53-C6-C1	2.19	119.76	115.28
23	B	601	CLA	C2A-C1A-CHA	-2.19	120.08	123.87
31	B	630	LMT	O5B-C5B-C4B	2.18	113.64	109.70
23	b	608	CLA	CMA-C3A-C2A	-2.18	105.54	113.98
35	c	517[A]	DGD	O4E-C4E-C3E	-2.18	105.23	110.38
25	t	102	BCR	C7-C8-C9	-2.18	123.00	126.23
23	C	514	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
35	c	516[A]	DGD	O6D-C1D-O3G	-2.18	104.89	110.04
34	C	522	HTG	C1-O5-C5	2.18	116.47	112.56
23	c	502	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
26	b	620	SQD	O47-C7-O49	-2.18	118.61	123.70
25	b	618	BCR	C29-C30-C25	2.18	113.60	110.44
27	B	624	GOL	C3-C2-C1	-2.18	103.81	111.80
29	a	412[B]	PL9	C10-C9-C8	-2.18	118.03	123.63
23	b	611	CLA	CAC-C3C-C4C	2.18	127.62	124.79
25	h	101	BCR	C36-C18-C19	2.18	121.42	118.09
23	c	508	CLA	C2A-C1A-CHA	-2.18	120.09	123.87
24	a	414[B]	PHO	O2A-CGA-CBA	2.18	118.47	111.83
25	T	102	BCR	C7-C6-C5	-2.18	116.54	121.56
35	C	517[B]	DGD	O1G-C1A-O1A	-2.18	118.19	123.63
25	y	101	BCR	C1-C6-C7	2.17	121.55	115.65
23	B	605	CLA	C4B-C3B-C2B	-2.17	104.60	107.30
25	D	404	BCR	C30-C25-C24	2.17	121.55	115.65
26	B	620	SQD	C44-O6-C1	-2.17	109.14	113.80
26	f	102	SQD	O8-S-C6	2.17	110.17	105.97
25	B	619	BCR	C34-C9-C8	2.17	121.41	118.09
24	A	407[B]	PHO	C4-C3-C5	2.17	119.00	115.23
23	c	511	CLA	C11-C10-C8	-2.17	108.75	115.97
32	b	629[A]	LHG	O7-C7-O9	-2.17	118.63	123.70
23	b	615	CLA	C2A-C1A-CHA	-2.17	120.10	123.87
25	C	516	BCR	C3-C4-C5	-2.17	110.19	114.06
26	a	409[B]	SQD	O9-S-O7	-2.17	106.77	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	C4-C3-C2	-2.17	118.06	123.63
23	B	616	CLA	CMC-C2C-C1C	2.17	128.42	125.03
23	B	612	CLA	CMA-C3A-C2A	-2.17	105.61	113.98
25	K	102	BCR	C3-C4-C5	-2.17	110.19	114.06
23	C	513	CLA	C4-C3-C2	-2.17	118.06	123.63
31	B	630	LMT	C3B-C4B-C5B	-2.17	106.31	110.23
26	A	410[B]	SQD	O47-C7-O49	-2.17	118.64	123.70
32	E	101[A]	LHG	O7-C7-O9	-2.17	118.64	123.70
25	B	619	BCR	C2-C1-C6	2.17	113.58	110.44
23	b	601	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
23	C	503	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
25	C	516	BCR	C2-C1-C6	2.16	113.58	110.44
23	c	512	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
23	B	616	CLA	C4-C3-C2	-2.16	118.07	123.63
23	C	511	CLA	CMB-C2B-C1B	2.16	128.71	125.42
33	m	101	LMG	O8-C28-O10	-2.16	118.22	123.63
23	D	403	CLA	C1-C2-C3	-2.16	122.66	126.20
23	A	405[A]	CLA	C4C-C3C-C2C	-2.16	103.75	106.89
29	D	405[A]	PL9	C12-C13-C14	-2.16	122.68	127.62
23	B	610	CLA	CHB-C4A-NA	2.16	127.52	124.40
31	B	628	LMT	O1B-C4'-C5'	-2.16	103.81	109.48
35	C	517[A]	DGD	O1G-C1A-O1A	-2.16	118.22	123.63
23	b	606	CLA	C2A-C1A-CHA	-2.16	120.12	123.87
35	c	517[A]	DGD	O1G-C1A-O1A	-2.16	118.23	123.63
23	C	512	CLA	CBC-CAC-C3C	-2.16	106.57	112.42
24	A	407[B]	PHO	O2A-CGA-O1A	-2.16	118.23	123.63
25	B	617	BCR	C15-C14-C13	-2.16	124.25	127.28
23	C	506	CLA	CHA-C1A-NA	-2.16	121.50	126.39
23	b	613	CLA	CMC-C2C-C1C	2.16	128.41	125.03
23	B	611	CLA	O2A-CGA-CBA	2.16	118.41	111.83
23	d	402[B]	CLA	C4-C3-C5	2.16	118.97	115.23
29	D	405[B]	PL9	C30-C29-C31	2.16	118.97	115.23
31	t	101	LMT	C1-O1'-C1'	2.16	117.36	113.68
35	C	517[A]	DGD	O6D-C1D-O3G	-2.16	104.95	110.04
33	Z	101	LMG	C1-O6-C5	2.16	117.93	113.72
34	B	623	HTG	C1-C2-C3	2.15	114.76	110.55
29	D	405[B]	PL9	C47-C48-C49	-2.15	120.46	127.64
23	C	502	CLA	OBD-CAD-C3D	-2.15	123.38	128.42
23	c	510	CLA	OBD-CAD-C3D	-2.15	123.38	128.42
24	A	416[B]	PHO	CMA-C3A-C4A	-2.15	109.97	114.61
23	B	606	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
24	A	416[B]	PHO	OBD-CAD-C3D	-2.15	124.53	127.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	617	BCR	C11-C10-C9	-2.15	124.26	127.28
23	a	405[B]	CLA	CBC-CAC-C3C	-2.15	106.59	112.42
23	a	404[B]	CLA	C7-C6-C5	-2.15	107.53	113.26
23	C	502	CLA	C1-C2-C3	-2.15	122.67	126.20
23	C	510	CLA	C4-C3-C5	2.15	118.96	115.23
23	C	511	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
23	b	610	CLA	C4-C3-C2	-2.15	118.11	123.63
23	A	406[B]	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
23	b	611	CLA	CHB-C4A-NA	2.15	127.50	124.40
35	C	517[B]	DGD	O1G-C1A-C2A	2.15	118.38	111.83
23	b	607	CLA	CAA-CBA-CGA	2.14	119.30	113.21
33	z	101	LMG	C8-O7-C10	-2.14	112.67	117.80
23	c	503	CLA	C4-C3-C5	2.14	118.95	115.23
23	B	605	CLA	C3B-C4B-NB	2.14	112.44	110.53
25	Y	101	BCR	C1-C6-C7	2.14	121.46	115.65
23	a	404[B]	CLA	CMA-C3A-C2A	-2.14	105.71	113.98
23	b	607	CLA	C1-O2A-CGA	2.14	121.83	116.65
23	b	610	CLA	CMA-C3A-C2A	-2.14	105.71	113.98
24	a	406[A]	PHO	CBA-CAA-C2A	-2.14	107.47	113.78
32	b	629[B]	LHG	O8-C23-O10	-2.14	118.28	123.63
32	L	101[B]	LHG	O4-P-O5	2.14	122.40	112.44
23	A	406[B]	CLA	CMC-C2C-C1C	2.14	128.38	125.03
23	b	606	CLA	C1-O2A-CGA	2.14	121.83	116.65
35	C	519	DGD	O3G-C3G-C2G	-2.14	105.62	110.82
23	C	509	CLA	CAA-C2A-C3A	-2.14	107.22	113.00
29	d	406[B]	PL9	C7-C3-C2	-2.14	120.87	123.39
23	A	406[B]	CLA	CAC-C3C-C4C	2.13	127.57	124.79
23	c	510	CLA	CAA-C2A-C3A	-2.13	107.23	113.00
38	E	102	HEM	C3B-C4B-NB	-2.13	107.94	109.47
23	b	602	CLA	CAA-CBA-CGA	-2.13	107.16	113.21
35	C	517[B]	DGD	C3G-C2G-C1G	-2.13	106.82	111.78
38	f	101	HEM	C4C-NC-C1C	2.13	109.29	105.82
23	b	604	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
23	B	608	CLA	C11-C10-C8	-2.13	108.89	115.97
32	d	408[B]	LHG	O8-C23-O10	-2.13	118.31	123.63
32	D	407[A]	LHG	O4-P-O5	2.13	122.34	112.44
23	b	609	CLA	CHA-C1A-NA	-2.13	121.57	126.39
32	E	101[B]	LHG	O7-C7-O9	-2.13	118.73	123.70
23	B	610	CLA	C4-C3-C5	2.13	118.92	115.23
23	B	616	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
27	a	418	GOL	C3-C2-C1	-2.13	104.00	111.80
23	d	404	CLA	CHB-C4A-NA	2.13	127.47	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	514	BCR	C37-C22-C23	2.12	121.33	118.09
23	A	408	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
24	a	414[A]	PHO	C1A-C2A-C3A	-2.12	100.82	102.84
23	c	509	CLA	C4-C3-C2	-2.12	118.17	123.63
25	h	101	BCR	C10-C11-C12	-2.12	117.05	123.20
33	a	415	LMG	O6-C5-C4	2.12	113.53	109.70
23	B	602	CLA	C4-C3-C5	2.12	118.91	115.23
38	E	102	HEM	CMD-C2D-C1D	2.12	128.35	125.03
23	c	507	CLA	C2A-C1A-CHA	-2.12	120.18	123.87
23	C	508	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
25	D	404	BCR	C29-C28-C27	-2.12	106.61	111.28
25	b	618	BCR	C37-C22-C21	-2.12	119.38	122.82
23	A	408	CLA	C11-C12-C13	-2.12	108.92	115.97
23	a	407	CLA	OBD-CAD-C3D	-2.12	123.46	128.42
23	B	609	CLA	C16-C15-C13	-2.12	108.92	115.97
23	b	614	CLA	C4-C3-C5	2.12	118.90	115.23
23	b	602	CLA	C11-C10-C8	-2.12	108.93	115.97
35	c	517[B]	DGD	O2G-C1B-O1B	-2.12	118.76	123.70
29	D	405[A]	PL9	O2-C1-C6	-2.12	117.11	120.48
23	b	615	CLA	O2D-CGD-O1D	-2.12	119.73	123.85
23	b	609	CLA	C7-C6-C5	-2.12	107.62	113.26
23	A	405[B]	CLA	CAC-C3C-C4C	2.12	127.54	124.79
29	A	414[A]	PL9	C51-C49-C50	2.11	119.46	114.59
23	B	615	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
29	d	406[B]	PL9	C51-C49-C50	2.11	119.45	114.59
23	C	512	CLA	C1-C2-C3	-2.11	122.73	126.20
23	B	607	CLA	CAA-CBA-CGA	2.11	119.21	113.21
23	C	513	CLA	CHB-C1B-C2B	-2.11	121.29	127.43
23	B	610	CLA	C1-C2-C3	-2.11	122.74	126.20
23	b	606	CLA	OBD-CAD-C3D	-2.11	123.48	128.42
23	c	511	CLA	C1-O2A-CGA	2.11	121.76	116.65
25	b	619	BCR	C28-C27-C26	-2.11	110.29	114.06
23	c	513	CLA	CMC-C2C-C1C	2.11	128.33	125.03
23	B	607	CLA	OBD-CAD-C3D	-2.11	123.49	128.42
23	c	506	CLA	C1-O2A-CGA	2.11	121.75	116.65
23	a	404[A]	CLA	CMB-C2B-C3B	2.11	131.51	126.55
24	A	407[A]	PHO	CBA-CAA-C2A	-2.11	107.57	113.78
23	B	610	CLA	CMC-C2C-C1C	2.11	128.33	125.03
33	D	411	LMG	O1-C1-C2	-2.11	105.07	108.27
23	b	608	CLA	C4-C3-C5	2.11	118.88	115.23
29	d	406[A]	PL9	C35-C34-C36	2.11	118.88	115.23
23	b	602	CLA	O2A-CGA-CBA	2.10	118.25	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C4-C3-C2	-2.10	118.22	123.63
24	a	414[A]	PHO	O2A-CGA-CBA	2.10	118.25	111.83
23	B	606	CLA	CHB-C1B-C2B	-2.10	121.32	127.43
31	M	101	LMT	O5B-C5B-C6B	2.10	111.65	106.44
23	c	502	CLA	CAC-C3C-C4C	2.10	127.53	124.79
24	A	416[A]	PHO	CMB-C2B-C3B	2.10	128.88	124.68
23	d	403[A]	CLA	CHD-C4C-NC	2.10	127.49	124.23
23	b	609	CLA	C16-C15-C13	-2.10	108.99	115.97
23	A	405[B]	CLA	O2A-CGA-CBA	2.10	118.24	111.83
23	c	510	CLA	CED-O2D-CGD	2.10	120.68	115.92
29	A	414[A]	PL9	C25-C24-C26	2.10	118.87	115.23
25	d	405	BCR	C29-C28-C27	-2.10	106.67	111.28
29	d	406[A]	PL9	C51-C49-C50	2.10	119.42	114.59
23	c	512	CLA	CBC-CAC-C3C	-2.10	106.73	112.42
23	b	605	CLA	CHB-C4A-NA	2.10	127.43	124.40
38	f	101	HEM	CHA-C1A-NA	2.10	127.66	123.86
24	A	416[B]	PHO	C6-C5-C3	-2.10	108.36	113.47
23	b	605	CLA	C1-O2A-CGA	2.10	121.72	116.65
23	b	604	CLA	C4-C3-C5	2.10	118.86	115.23
25	h	101	BCR	C11-C10-C9	-2.09	124.34	127.28
23	c	509	CLA	CBC-CAC-C3C	-2.09	106.74	112.42
23	b	603	CLA	CMB-C2B-C1B	2.09	128.61	125.42
35	h	102	DGD	O3G-C1D-C2D	2.09	111.45	108.27
29	A	414[A]	PL9	O1-C4-C3	-2.09	118.52	120.73
23	B	611	CLA	OBD-CAD-C3D	-2.09	123.53	128.42
23	C	505	CLA	C1-C2-C3	-2.09	122.77	126.20
23	C	508	CLA	CAC-C3C-C4C	2.09	127.51	124.79
25	H	101	BCR	C33-C5-C6	-2.09	122.20	124.48
33	C	521	LMG	O1-C1-C2	2.09	111.45	108.27
23	A	404[A]	CLA	C7-C6-C5	-2.09	107.69	113.26
24	a	414[B]	PHO	C7-C6-C5	-2.09	107.69	113.26
23	A	405[A]	CLA	C1-C2-C3	-2.09	122.77	126.20
29	a	412[B]	PL9	C35-C34-C33	-2.09	118.26	123.63
33	m	101	LMG	C3-C4-C5	2.09	114.02	110.23
23	b	603	CLA	CHB-C1B-C2B	-2.09	121.36	127.43
23	b	603	CLA	CMC-C2C-C1C	2.09	128.30	125.03
23	c	504	CLA	O2A-CGA-CBA	2.09	118.20	111.83
25	b	618	BCR	C33-C5-C6	-2.09	122.21	124.48
34	B	622	HTG	O2-C2-C3	-2.09	105.45	110.38
25	h	101	BCR	C37-C22-C21	-2.09	119.43	122.82
23	B	606	CLA	OBD-CAD-C3D	-2.09	123.54	128.42
25	t	102	BCR	C16-C15-C14	2.09	127.79	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	402[B]	CLA	OBD-CAD-C3D	-2.09	123.54	128.42
31	b	627	LMT	O1'-C1'-C2'	2.09	111.44	108.27
25	c	514	BCR	C21-C20-C19	-2.09	117.16	123.20
23	b	610	CLA	C2A-C1A-CHA	-2.08	120.25	123.87
25	H	101	BCR	C36-C18-C17	-2.08	119.44	122.82
23	B	610	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
23	c	512	CLA	C4B-C3B-C2B	-2.08	104.71	107.30
23	b	609	CLA	CAA-C2A-C3A	-2.08	107.37	113.00
23	b	616	CLA	CHA-C1A-NA	-2.08	121.68	126.39
25	D	404	BCR	C20-C21-C22	-2.08	124.36	127.28
26	a	409[A]	SQD	O7-S-C6	2.08	109.86	106.76
23	b	602	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
27	a	417	GOL	C3-C2-C1	-2.08	104.17	111.80
23	A	406[B]	CLA	CHB-C4A-NA	2.08	127.40	124.40
23	C	508	CLA	CHA-C1A-NA	-2.08	121.69	126.39
25	b	619	BCR	C21-C20-C19	-2.08	117.19	123.20
23	B	608	CLA	C4-C3-C5	2.08	118.83	115.23
23	c	511	CLA	CMA-C3A-C4A	2.07	117.35	111.77
23	B	611	CLA	CMA-C3A-C2A	-2.07	105.98	113.98
25	D	404	BCR	C37-C22-C21	-2.07	119.46	122.82
25	a	408	BCR	C8-C7-C6	-2.07	121.47	127.00
24	a	406[A]	PHO	CBC-CAC-C3C	-2.07	109.91	112.87
23	c	504	CLA	CBC-CAC-C3C	-2.07	106.81	112.42
33	C	501	LMG	O7-C10-O9	-2.07	118.87	123.70
23	c	509	CLA	CHB-C1B-NB	-2.07	120.95	124.05
23	b	610	CLA	CHB-C4A-NA	2.07	127.38	124.40
35	h	102	DGD	O4D-C4D-C3D	-2.07	105.51	110.38
29	a	412[B]	PL9	C51-C49-C50	2.06	119.34	114.59
23	b	605	CLA	OBD-CAD-C3D	-2.06	123.59	128.42
35	C	517[A]	DGD	O1G-C1A-C2A	2.06	118.13	111.83
33	d	412	LMG	O8-C28-O10	-2.06	118.47	123.63
26	a	409[A]	SQD	O48-C23-O10	-2.06	118.47	123.63
25	K	102	BCR	C11-C10-C9	-2.06	124.39	127.28
34	b	622	HTG	C6-C5-C4	-2.06	107.96	113.02
23	b	609	CLA	CGD-CBD-CAD	-2.06	104.17	110.85
23	D	402[A]	CLA	CMB-C2B-C1B	2.06	128.56	125.42
23	d	403[B]	CLA	CMB-C2B-C1B	2.06	128.56	125.42
25	y	101	BCR	C11-C10-C9	-2.06	124.39	127.28
23	c	503	CLA	OBD-CAD-C3D	-2.06	123.60	128.42
25	y	101	BCR	C32-C1-C6	-2.06	107.01	110.24
23	b	616	CLA	C11-C12-C13	-2.06	109.13	115.97
25	C	515	BCR	C21-C20-C19	-2.06	117.24	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	CHA-C1A-NA	-2.05	121.74	126.39
29	A	414[B]	PL9	C35-C34-C33	-2.05	118.35	123.63
23	C	506	CLA	C11-C10-C8	-2.05	109.14	115.97
25	b	619	BCR	C16-C15-C14	-2.05	119.32	123.52
23	B	613	CLA	C7-C6-C5	-2.05	107.80	113.26
33	B	621	LMG	C12-C11-C10	-2.05	106.18	113.69
25	K	102	BCR	C21-C20-C19	-2.05	117.26	123.20
23	A	406[A]	CLA	CMA-C3A-C4A	-2.05	106.26	111.77
35	c	517[B]	DGD	O1G-C1A-O1A	-2.05	118.50	123.63
34	B	625	HTG	C1'-S1-C1	2.05	104.88	100.45
25	d	405	BCR	C36-C18-C17	-2.05	119.50	122.82
23	D	402[A]	CLA	CMA-C3A-C2A	-2.05	106.06	113.98
23	b	607	CLA	CMA-C3A-C2A	-2.05	106.07	113.98
23	c	510	CLA	C2A-C1A-CHA	-2.05	120.32	123.87
23	d	402[A]	CLA	CAA-CBA-CGA	2.04	119.01	113.21
23	d	403[A]	CLA	CBC-CAC-C3C	-2.04	106.88	112.42
23	b	609	CLA	CMA-C3A-C4A	-2.04	106.28	111.77
25	K	102	BCR	C29-C30-C25	2.04	113.41	110.44
23	C	510	CLA	CMB-C2B-C1B	2.04	128.53	125.42
32	D	406[A]	LHG	O4-P-O5	2.04	121.95	112.44
23	b	613	CLA	C16-C15-C13	-2.04	109.18	115.97
29	D	405[A]	PL9	C25-C24-C23	-2.04	118.38	123.63
23	A	404[B]	CLA	CHB-C1B-C2B	-2.04	121.50	127.43
31	F	101	LMT	O1'-C1'-C2'	2.04	111.37	108.27
23	d	402[B]	CLA	CED-O2D-CGD	2.04	120.55	115.92
33	a	415	LMG	O7-C10-O9	-2.04	118.93	123.70
23	A	404[A]	CLA	CHB-C4A-NA	2.04	127.34	124.40
23	D	402[A]	CLA	CBC-CAC-C3C	-2.04	106.89	112.42
23	d	404	CLA	C1-O2A-CGA	2.04	121.59	116.65
23	c	512	CLA	CMA-C3A-C4A	-2.04	106.29	111.77
24	a	414[B]	PHO	C4-C3-C2	-2.04	118.39	123.63
23	b	614	CLA	OBD-CAD-C3D	-2.04	123.65	128.42
23	C	504	CLA	CBC-CAC-C3C	-2.04	106.90	112.42
23	c	509	CLA	O2A-C1-C2	2.04	115.95	108.11
32	d	414[A]	LHG	C5-O7-C7	-2.04	112.92	117.80
25	a	408	BCR	C24-C23-C22	-2.04	123.22	126.23
23	b	613	CLA	CMA-C3A-C4A	-2.04	106.30	111.77
23	B	612	CLA	CAA-C2A-C3A	-2.03	107.50	113.00
23	b	616	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
23	b	616	CLA	C2A-C1A-CHA	-2.03	120.34	123.87
23	A	404[A]	CLA	C4-C3-C5	2.03	118.75	115.23
35	c	518	DGD	O2G-C1B-O1B	-2.03	118.96	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	CMB-C2B-C1B	2.03	128.51	125.42
23	A	408	CLA	CMA-C3A-C4A	-2.03	106.32	111.77
23	C	502	CLA	C11-C12-C13	-2.03	109.23	115.97
29	D	405[A]	PL9	C30-C29-C31	2.03	118.75	115.23
24	a	406[A]	PHO	O2D-CGD-O1D	-2.03	119.90	123.85
23	a	405[A]	CLA	CAA-CBA-CGA	2.02	118.96	113.21
31	b	627	LMT	C1'-O5'-C5'	-2.02	109.77	113.72
23	C	513	CLA	CHB-C4A-NA	2.02	127.32	124.40
23	a	405[A]	CLA	CMA-C3A-C2A	-2.02	106.16	113.98
35	C	517[A]	DGD	C3E-C4E-C5E	2.02	113.90	110.23
33	m	101	LMG	O1-C7-C8	-2.02	105.90	110.82
25	K	102	BCR	C36-C18-C19	2.02	121.18	118.09
23	d	403[B]	CLA	CBC-CAC-C3C	-2.02	106.94	112.42
25	c	515	BCR	C20-C21-C22	-2.02	124.44	127.28
35	c	516[B]	DGD	O1G-C1A-O1A	-2.02	118.57	123.63
35	h	102	DGD	C3B-C2B-C1B	-2.02	106.29	113.69
23	b	602	CLA	CHB-C4A-NA	2.02	127.32	124.40
23	B	613	CLA	C2A-C1A-CHA	-2.02	120.36	123.87
24	A	416[A]	PHO	CED-O2D-CGD	2.02	120.49	115.92
35	H	102	DGD	O3G-C3G-C2G	-2.02	105.91	110.82
23	B	601	CLA	CAA-C2A-C3A	-2.02	107.55	113.00
23	B	602	CLA	OBD-CAD-C3D	-2.02	123.70	128.42
24	a	406[B]	PHO	C4-C3-C5	2.02	118.73	115.23
34	b	625	HTG	C1-C2-C3	-2.02	106.61	110.55
25	c	515	BCR	C37-C22-C21	-2.01	119.55	122.82
23	C	504	CLA	C3B-C4B-NB	2.01	112.33	110.53
26	f	102	SQD	C44-O6-C1	-2.01	109.48	113.80
23	A	405[A]	CLA	C4D-C3D-CAD	-2.01	105.92	108.11
38	f	101	HEM	CMD-C2D-C1D	2.01	128.18	125.03
23	A	406[A]	CLA	CHB-C4A-NA	2.01	127.30	124.40
23	b	604	CLA	C2A-C1A-CHA	-2.01	120.38	123.87
23	A	408	CLA	C2A-C1A-CHA	-2.01	120.38	123.87
23	B	602	CLA	CHB-C4A-NA	2.01	127.30	124.40
29	d	406[B]	PL9	C47-C48-C49	-2.01	120.94	127.64
32	b	629[B]	LHG	O4-P-O5	2.01	121.79	112.44
24	A	416[B]	PHO	CED-O2D-CGD	2.01	120.47	115.92
25	a	408	BCR	C37-C22-C21	-2.01	119.56	122.82
23	B	610	CLA	CAC-C3C-C4C	2.01	127.40	124.79
29	d	406[B]	PL9	C35-C34-C36	2.01	118.71	115.23
29	d	406[B]	PL9	C25-C24-C26	2.00	118.71	115.23
24	A	407[A]	PHO	C4-C3-C5	2.00	118.70	115.23
25	K	102	BCR	C10-C11-C12	-2.00	117.40	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	CHA-C1A-NA	-2.00	121.86	126.39
23	d	402[B]	CLA	C1-O2A-CGA	2.00	121.49	116.65
23	a	404[B]	CLA	CMB-C2B-C3B	2.00	131.26	126.55
24	a	406[B]	PHO	CAC-C3C-C4C	2.00	129.17	124.03
23	B	609	CLA	C7-C6-C5	-2.00	107.93	113.26
26	B	620	SQD	O47-C7-O49	-2.00	119.03	123.70

All (69) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404[A]	CLA	ND
23	A	404[B]	CLA	ND
23	A	405[B]	CLA	ND
23	A	408	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	609	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	502	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	C	514	CLA	ND
23	D	402[A]	CLA	ND
23	D	402[B]	CLA	ND

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Mol	Chain	Res	Type	Atom
23	D	403	CLA	ND
23	a	404[A]	CLA	ND
23	a	404[B]	CLA	ND
23	a	407	CLA	ND
23	b	601	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	c	501	CLA	ND
23	c	502	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	d	402[A]	CLA	ND
23	d	402[B]	CLA	ND
23	d	403[A]	CLA	ND
23	d	403[B]	CLA	ND
23	d	404	CLA	ND

All (1566) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	614	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	C14-C13-C15-C16
23	C	508	CLA	C4B-C3B-CAB-CBB
23	C	508	CLA	CHA-CBD-CGD-O2D
23	a	407	CLA	C4-C3-C5-C6
23	b	601	CLA	C11-C10-C8-C9
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	507	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O2D
23	c	509	CLA	C2-C1-O2A-CGA
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	509	CLA	C11-C10-C8-C9
23	c	513	CLA	C2B-C3B-CAB-CBB
23	c	513	CLA	C4B-C3B-CAB-CBB
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	Y	101	BCR	C21-C22-C23-C24
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
26	A	410[A]	SQD	O49-C7-O47-C45
26	A	410[B]	SQD	O49-C7-O47-C45
26	A	412	SQD	O6-C44-C45-O47
26	B	620	SQD	O49-C7-O47-C45
26	F	102	SQD	O49-C7-O47-C45
26	F	102	SQD	C8-C7-O47-C45
26	a	410	SQD	O6-C44-C45-O47
26	a	410	SQD	C5-C6-S-O7
26	a	410	SQD	C5-C6-S-O8
26	a	410	SQD	C5-C6-S-O9
26	b	620	SQD	C8-C7-O47-C45
26	f	102	SQD	O6-C44-C45-O47
26	f	102	SQD	O49-C7-O47-C45
26	f	102	SQD	C8-C7-O47-C45
27	A	411	GOL	O1-C1-C2-O2
27	A	411	GOL	O1-C1-C2-C3
27	B	624	GOL	C1-C2-C3-O3
27	B	629	GOL	O1-C1-C2-C3
27	D	412	GOL	C1-C2-C3-O3
27	V	203[A]	GOL	C1-C2-C3-O3
27	V	203[B]	GOL	C1-C2-C3-O3
27	b	624	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
27	c	526	GOL	C1-C2-C3-O3
27	o	302	GOL	C1-C2-C3-O3
27	o	303	GOL	C1-C2-C3-O3
29	a	412[A]	PL9	C25-C24-C26-C27
31	A	420	LMT	O5'-C1'-O1'-C1
31	B	630	LMT	C2'-C1'-O1'-C1
31	B	631	LMT	O5'-C1'-O1'-C1
31	B	631	LMT	C2-C1-O1'-C1'
31	F	101	LMT	C2'-C1'-O1'-C1
31	F	101	LMT	O5'-C1'-O1'-C1
31	b	627	LMT	C2'-C1'-O1'-C1
31	b	627	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	O5'-C1'-O1'-C1
32	D	406[A]	LHG	O2-C2-C3-O3
32	D	406[A]	LHG	C3-O3-P-O4
32	D	406[A]	LHG	C3-O3-P-O5
32	D	406[A]	LHG	C3-O3-P-O6
32	D	406[A]	LHG	C4-O6-P-O4
32	D	406[B]	LHG	C3-O3-P-O4
32	D	406[B]	LHG	C3-O3-P-O5
32	D	406[B]	LHG	C3-O3-P-O6
32	D	406[B]	LHG	C4-O6-P-O3
32	D	406[B]	LHG	C4-O6-P-O4
32	D	406[B]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C3-O3-P-O4
32	E	101[A]	LHG	C3-O3-P-O5
32	E	101[A]	LHG	C3-O3-P-O6
32	E	101[A]	LHG	C4-O6-P-O3
32	E	101[A]	LHG	O10-C23-O8-C6
32	E	101[A]	LHG	C24-C23-O8-C6
32	E	101[B]	LHG	C3-O3-P-O4
32	E	101[B]	LHG	C3-O3-P-O5
32	E	101[B]	LHG	C3-O3-P-O6
32	E	101[B]	LHG	C4-O6-P-O3
32	E	101[B]	LHG	O10-C23-O8-C6
32	E	101[B]	LHG	C24-C23-O8-C6
32	L	101[A]	LHG	C4-O6-P-O3
32	L	101[A]	LHG	C4-O6-P-O4
32	L	101[A]	LHG	C4-O6-P-O5
32	L	101[B]	LHG	C4-O6-P-O3
32	L	101[B]	LHG	C4-O6-P-O4
32	L	101[B]	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
32	a	419[A]	LHG	C3-O3-P-O4
32	a	419[A]	LHG	C3-O3-P-O6
32	a	419[A]	LHG	C4-O6-P-O3
32	a	419[A]	LHG	C4-O6-P-O5
32	a	419[A]	LHG	O10-C23-O8-C6
32	a	419[A]	LHG	C24-C23-O8-C6
32	a	419[B]	LHG	C3-O3-P-O4
32	a	419[B]	LHG	C3-O3-P-O6
32	a	419[B]	LHG	C4-O6-P-O3
32	a	419[B]	LHG	C4-O6-P-O5
32	a	419[B]	LHG	O10-C23-O8-C6
32	a	419[B]	LHG	C24-C23-O8-C6
32	b	629[A]	LHG	C4-O6-P-O3
32	b	629[A]	LHG	C4-O6-P-O4
32	b	629[A]	LHG	C4-O6-P-O5
32	b	629[B]	LHG	C4-O6-P-O3
32	b	629[B]	LHG	C4-O6-P-O4
32	b	629[B]	LHG	C4-O6-P-O5
32	d	407[A]	LHG	C3-O3-P-O5
32	d	407[A]	LHG	C3-O3-P-O6
32	d	407[A]	LHG	C4-O6-P-O4
32	d	407[B]	LHG	C3-O3-P-O4
32	d	407[B]	LHG	C3-O3-P-O5
32	d	407[B]	LHG	C3-O3-P-O6
32	d	407[B]	LHG	C4-O6-P-O3
32	d	407[B]	LHG	C4-O6-P-O4
32	d	414[A]	LHG	C3-O3-P-O5
33	C	521	LMG	C11-C10-O7-C8
33	c	520	LMG	O9-C10-O7-C8
33	c	520	LMG	C11-C10-O7-C8
33	Z	101	LMG	O9-C10-O7-C8
33	Z	101	LMG	C11-C10-O7-C8
33	z	101	LMG	O6-C1-O1-C7
34	B	623	HTG	C2'-C1'-S1-C1
34	b	623	HTG	O5-C1-S1-C1'
38	E	102	HEM	C2C-C3C-CAC-CBC
38	E	102	HEM	C4C-C3C-CAC-CBC
40	V	201	HEC	C2B-C3B-CAB-CBB
40	V	201	HEC	C4B-C3B-CAB-CBB
40	V	201	HEC	C2C-C3C-CAC-CBC
40	V	201	HEC	C4C-C3C-CAC-CBC
40	v	201	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
40	v	201	HEC	C4B-C3B-CAB-CBB
40	v	201	HEC	C2C-C3C-CAC-CBC
40	v	201	HEC	C4C-C3C-CAC-CBC
31	A	420	LMT	O5B-C1B-O1B-C4'
31	B	630	LMT	C4'-C5'-C6'-O6'
26	b	620	SQD	O49-C7-O47-C45
23	D	403	CLA	C3-C5-C6-C7
23	c	512	CLA	C3-C5-C6-C7
23	d	404	CLA	C3-C5-C6-C7
31	m	103	LMT	C4B-C5B-C6B-O6B
26	A	410[A]	SQD	C8-C7-O47-C45
26	A	410[B]	SQD	C8-C7-O47-C45
26	B	620	SQD	C8-C7-O47-C45
23	A	408	CLA	C4-C3-C5-C6
23	D	403	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
23	d	404	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C15-C14-C16-C17
29	A	414[B]	PL9	C15-C14-C16-C17
29	A	414[B]	PL9	C30-C29-C31-C32
29	a	412[B]	PL9	C25-C24-C26-C27
23	a	407	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	d	404	CLA	C2-C3-C5-C6
23	B	614	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
23	b	616	CLA	C3-C5-C6-C7
31	B	630	LMT	O5B-C5B-C6B-O6B
31	a	416	LMT	O5B-C5B-C6B-O6B
31	m	103	LMT	O5B-C5B-C6B-O6B
34	D	410	HTG	O5-C5-C6-O6
31	T	101	LMT	C4B-C5B-C6B-O6B
25	T	102	BCR	C13-C14-C15-C16
33	C	521	LMG	O9-C10-O7-C8
31	F	101	LMT	O5'-C5'-C6'-O6'
31	B	628	LMT	C4'-C5'-C6'-O6'
23	A	408	CLA	C3-C5-C6-C7
32	D	406[B]	LHG	O2-C2-C3-O3
32	E	101[A]	LHG	O2-C2-C3-O3
32	d	407[A]	LHG	O2-C2-C3-O3
32	d	407[B]	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
31	T	101	LMT	O5'-C5'-C6'-O6'
33	c	520	LMG	C4-C5-C6-O5
33	z	101	LMG	C11-C10-O7-C8
33	C	521	LMG	O6-C5-C6-O5
34	b	625	HTG	O5-C5-C6-O6
31	b	621	LMT	O5'-C5'-C6'-O6'
31	b	627	LMT	O5'-C5'-C6'-O6'
34	b	625	HTG	S1-C1'-C2'-C3'
23	B	605	CLA	C4-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
23	C	508	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
29	a	412[A]	PL9	C30-C29-C31-C32
29	a	412[B]	PL9	C15-C14-C16-C17
29	a	412[B]	PL9	C30-C29-C31-C32
23	A	408	CLA	C2-C3-C5-C6
23	B	605	CLA	C2-C3-C5-C6
23	C	508	CLA	C2-C3-C5-C6
23	D	403	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C13-C14-C16-C17
29	A	414[A]	PL9	C18-C19-C21-C22
29	A	414[B]	PL9	C13-C14-C16-C17
29	a	412[A]	PL9	C13-C14-C16-C17
29	a	412[A]	PL9	C28-C29-C31-C32
29	a	412[B]	PL9	C13-C14-C16-C17
29	a	412[B]	PL9	C28-C29-C31-C32
31	B	628	LMT	O5'-C5'-C6'-O6'
29	A	414[A]	PL9	C9-C11-C12-C13
29	A	414[A]	PL9	C14-C16-C17-C18
29	A	414[B]	PL9	C9-C11-C12-C13
29	A	414[B]	PL9	C14-C16-C17-C18
29	D	405[A]	PL9	C39-C41-C42-C43
29	a	412[A]	PL9	C9-C11-C12-C13
29	a	412[A]	PL9	C14-C16-C17-C18
29	a	412[B]	PL9	C9-C11-C12-C13
29	a	412[B]	PL9	C14-C16-C17-C18
31	a	416	LMT	C4B-C5B-C6B-O6B
34	D	410	HTG	C4-C5-C6-O6
31	B	630	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
31	T	101	LMT	C4'-C5'-C6'-O6'
26	B	620	SQD	O5-C1-O6-C44
31	A	417	LMT	O5'-C1'-O1'-C1
31	e	101	LMT	O5'-C1'-O1'-C1
31	A	420	LMT	O5'-C5'-C6'-O6'
31	F	101	LMT	C4'-C5'-C6'-O6'
23	C	502	CLA	CBD-CGD-O2D-CED
23	C	504	CLA	CBD-CGD-O2D-CED
23	c	510	CLA	CBD-CGD-O2D-CED
31	B	628	LMT	O5B-C5B-C6B-O6B
31	A	420	LMT	O5B-C5B-C6B-O6B
31	B	630	LMT	O5'-C5'-C6'-O6'
31	B	631	LMT	O5'-C5'-C6'-O6'
31	T	101	LMT	O5B-C5B-C6B-O6B
31	B	628	LMT	C6-C7-C8-C9
23	D	403	CLA	CBD-CGD-O2D-CED
32	d	407[A]	LHG	C1-C2-C3-O3
23	c	509	CLA	CBA-CGA-O2A-C1
31	t	101	LMT	O5'-C5'-C6'-O6'
33	c	520	LMG	O6-C5-C6-O5
35	C	519	DGD	C6B-C7B-C8B-C9B
31	A	420	LMT	C4B-C5B-C6B-O6B
31	e	101	LMT	C4'-C5'-C6'-O6'
29	A	414[A]	PL9	C20-C19-C21-C22
29	A	414[B]	PL9	C20-C19-C21-C22
29	a	412[A]	PL9	C15-C14-C16-C17
23	C	505	CLA	C2-C3-C5-C6
23	c	507	CLA	C2-C3-C5-C6
29	A	414[B]	PL9	C18-C19-C21-C22
29	a	412[A]	PL9	C23-C24-C26-C27
29	a	412[B]	PL9	C23-C24-C26-C27
23	B	613	CLA	C11-C12-C13-C14
23	C	503	CLA	C14-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C9
23	b	616	CLA	C6-C7-C8-C9
23	c	504	CLA	C11-C12-C13-C14
26	F	102	SQD	C2-C1-O6-C44
31	A	417	LMT	C2'-C1'-O1'-C1
31	A	420	LMT	C2'-C1'-O1'-C1
25	Y	101	BCR	C37-C22-C23-C24
25	b	619	BCR	C7-C8-C9-C34
34	D	410	HTG	S1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
34	b	622	HTG	S1-C1'-C2'-C3'
25	b	619	BCR	C7-C8-C9-C10
31	b	627	LMT	C4'-C5'-C6'-O6'
26	F	102	SQD	C23-C24-C25-C26
31	e	101	LMT	O5B-C5B-C6B-O6B
31	B	628	LMT	C5'-C4'-O1B-C1B
23	a	407	CLA	CBA-CGA-O2A-C1
31	B	628	LMT	C4B-C5B-C6B-O6B
31	A	420	LMT	C5'-C4'-O1B-C1B
27	B	624	GOL	O2-C2-C3-O3
27	V	203[A]	GOL	O2-C2-C3-O3
31	B	631	LMT	C4'-C5'-C6'-O6'
33	B	621	LMG	C39-C40-C41-C42
23	A	408	CLA	C12-C13-C15-C16
23	C	511	CLA	C11-C12-C13-C15
23	b	614	CLA	C12-C13-C15-C16
31	A	417	LMT	O5B-C5B-C6B-O6B
33	z	101	LMG	O9-C10-O7-C8
29	A	414[A]	PL9	C44-C46-C47-C48
29	A	414[B]	PL9	C44-C46-C47-C48
29	D	405[B]	PL9	C39-C41-C42-C43
29	d	406[A]	PL9	C39-C41-C42-C43
29	d	406[B]	PL9	C39-C41-C42-C43
31	b	621	LMT	C4'-C5'-C6'-O6'
23	b	601	CLA	C10-C11-C12-C13
31	A	420	LMT	C4'-C5'-C6'-O6'
32	D	407[A]	LHG	C33-C34-C35-C36
35	c	517[B]	DGD	C1B-C2B-C3B-C4B
23	c	509	CLA	O1A-CGA-O2A-C1
23	B	602	CLA	C13-C15-C16-C17
23	B	614	CLA	C8-C10-C11-C12
23	b	604	CLA	C8-C10-C11-C12
23	c	512	CLA	C15-C16-C17-C18
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
31	A	420	LMT	O1'-C1-C2-C3
23	C	508	CLA	C5-C6-C7-C8
23	D	403	CLA	C10-C11-C12-C13
23	b	605	CLA	C8-C10-C11-C12
23	b	614	CLA	C8-C10-C11-C12
35	c	517[A]	DGD	C1B-C2B-C3B-C4B
23	c	509	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	F	102	SQD	O5-C1-O6-C44
31	B	630	LMT	O5'-C1'-O1'-C1
31	b	621	LMT	O5'-C1'-O1'-C1
23	A	408	CLA	C5-C6-C7-C8
33	Z	101	LMG	C10-C11-C12-C13
23	B	606	CLA	C10-C11-C12-C13
23	b	611	CLA	C15-C16-C17-C18
31	a	416	LMT	O1'-C1-C2-C3
23	a	407	CLA	O1A-CGA-O2A-C1
34	B	625	HTG	S1-C1'-C2'-C3'
32	E	101[A]	LHG	C23-C24-C25-C26
23	B	601	CLA	C5-C6-C7-C8
23	B	601	CLA	C10-C11-C12-C13
23	b	606	CLA	C10-C11-C12-C13
26	B	620	SQD	C30-C31-C32-C33
33	d	412	LMG	C10-C11-C12-C13
32	D	406[A]	LHG	C1-C2-C3-O3
32	D	406[B]	LHG	C1-C2-C3-O3
32	d	407[B]	LHG	C1-C2-C3-O3
34	b	623	HTG	C1'-C2'-C3'-C4'
23	B	615	CLA	C5-C6-C7-C8
23	C	503	CLA	C13-C15-C16-C17
23	b	604	CLA	C5-C6-C7-C8
23	b	606	CLA	C15-C16-C17-C18
23	c	513	CLA	C10-C11-C12-C13
23	c	512	CLA	CBD-CGD-O2D-CED
26	B	620	SQD	C7-C8-C9-C10
23	B	614	CLA	C10-C11-C12-C13
23	C	513	CLA	C10-C11-C12-C13
31	A	417	LMT	O1'-C1-C2-C3
34	B	625	HTG	O5-C5-C6-O6
31	B	631	LMT	O1'-C1-C2-C3
35	C	519	DGD	C2B-C3B-C4B-C5B
34	d	411	HTG	S1-C1'-C2'-C3'
23	C	509	CLA	C10-C11-C12-C13
23	a	404[A]	CLA	C15-C16-C17-C18
23	a	404[B]	CLA	C15-C16-C17-C18
23	b	606	CLA	C13-C15-C16-C17
31	e	101	LMT	O5'-C5'-C6'-O6'
31	B	631	LMT	C2'-C1'-O1'-C1
31	b	621	LMT	C2'-C1'-O1'-C1
31	e	101	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
35	C	518[A]	DGD	C2E-C1E-O5D-C6D
35	C	518[B]	DGD	C2E-C1E-O5D-C6D
33	c	519	LMG	C4-C5-C6-O5
32	E	101[B]	LHG	O2-C2-C3-O3
23	a	407	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C20
31	a	416	LMT	O5'-C5'-C6'-O6'
32	D	407[B]	LHG	C33-C34-C35-C36
35	C	517[B]	DGD	O6D-C5D-C6D-O5D
27	B	629	GOL	C1-C2-C3-O3
27	D	412	GOL	O1-C1-C2-C3
27	O	302	GOL	O1-C1-C2-C3
27	O	303	GOL	O1-C1-C2-C3
27	a	417	GOL	O1-C1-C2-C3
27	d	413	GOL	O1-C1-C2-C3
27	l	801[B]	GOL	O1-C1-C2-C3
27	v	202[B]	GOL	O1-C1-C2-C3
32	A	419[B]	LHG	O1-C1-C2-C3
26	A	410[A]	SQD	C7-C8-C9-C10
32	E	101[B]	LHG	C23-C24-C25-C26
23	C	510	CLA	CBD-CGD-O2D-CED
34	b	625	HTG	C4-C5-C6-O6
23	d	404	CLA	C16-C17-C18-C20
33	B	621	LMG	C15-C16-C17-C18
26	b	620	SQD	C31-C32-C33-C34
35	C	518[B]	DGD	O6E-C1E-O5D-C6D
33	B	621	LMG	C11-C10-O7-C8
34	B	622	HTG	C1'-C2'-C3'-C4'
29	A	414[B]	PL9	C28-C29-C31-C32
31	a	416	LMT	C4'-C5'-C6'-O6'
23	b	601	CLA	C2-C1-O2A-CGA
23	B	615	CLA	C16-C17-C18-C19
23	a	407	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C19
23	c	508	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C19
31	A	420	LMT	C1-C2-C3-C4
26	F	102	SQD	C30-C31-C32-C33
32	D	406[B]	LHG	C16-C17-C18-C19
32	L	101[B]	LHG	C12-C13-C14-C15
26	A	410[A]	SQD	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	A	420	LMT	C3-C4-C5-C6
32	L	101[A]	LHG	C12-C13-C14-C15
32	b	629[B]	LHG	C14-C15-C16-C17
32	d	407[B]	LHG	C34-C35-C36-C37
32	d	414[A]	LHG	C16-C17-C18-C19
33	C	521	LMG	C18-C19-C20-C21
33	D	411	LMG	C19-C20-C21-C22
33	a	415	LMG	C30-C31-C32-C33
35	c	517[A]	DGD	CAA-CBA-CCA-CDA
23	b	611	CLA	C8-C10-C11-C12
26	A	410[B]	SQD	C15-C16-C17-C18
33	B	621	LMG	C34-C35-C36-C37
35	c	516[B]	DGD	C2B-C3B-C4B-C5B
35	c	517[B]	DGD	C9A-CAA-CBA-CCA
35	c	517[B]	DGD	CAA-CBA-CCA-CDA
35	c	516[A]	DGD	C2A-C1A-O1G-C1G
35	c	516[A]	DGD	O6D-C5D-C6D-O5D
35	c	516[B]	DGD	O6D-C5D-C6D-O5D
31	a	416	LMT	C1-C2-C3-C4
32	L	101[A]	LHG	C17-C18-C19-C20
33	B	621	LMG	O9-C10-O7-C8
27	B	629	GOL	O1-C1-C2-O2
27	D	412	GOL	O1-C1-C2-O2
27	D	412	GOL	O2-C2-C3-O3
27	O	302	GOL	O1-C1-C2-O2
27	V	203[B]	GOL	O2-C2-C3-O3
27	b	624	GOL	O2-C2-C3-O3
27	c	526	GOL	O2-C2-C3-O3
27	o	302	GOL	O2-C2-C3-O3
27	v	202[B]	GOL	O1-C1-C2-O2
31	T	101	LMT	C2-C1-O1'-C1'
31	t	101	LMT	C2-C1-O1'-C1'
32	d	414[B]	LHG	C16-C17-C18-C19
33	a	415	LMG	C34-C35-C36-C37
23	D	402[B]	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C4B-C3B-CAB-CBB
23	c	507	CLA	C4B-C3B-CAB-CBB
35	c	517[A]	DGD	C9A-CAA-CBA-CCA
23	B	603	CLA	C16-C17-C18-C19
23	B	603	CLA	C16-C17-C18-C20
23	B	615	CLA	C16-C17-C18-C20
23	b	602	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	b	602	CLA	C16-C17-C18-C20
31	b	627	LMT	C7-C8-C9-C10
34	b	622	HTG	C2'-C3'-C4'-C5'
33	m	101	LMG	C11-C10-O7-C8
34	b	622	HTG	O5-C5-C6-O6
23	B	614	CLA	C11-C10-C8-C7
23	b	606	CLA	C12-C13-C15-C16
26	f	102	SQD	C32-C33-C34-C35
32	D	407[B]	LHG	C32-C33-C34-C35
35	C	518[A]	DGD	CCB-CDB-CEB-CFB
35	H	102	DGD	C5B-C6B-C7B-C8B
35	h	102	DGD	C6B-C7B-C8B-C9B
31	t	101	LMT	C4-C5-C6-C7
33	C	520	LMG	C16-C17-C18-C19
35	C	518[B]	DGD	CCB-CDB-CEB-CFB
35	c	516[A]	DGD	C2B-C3B-C4B-C5B
35	c	517[B]	DGD	CBA-CCA-CDA-CEA
23	B	602	CLA	C15-C16-C17-C18
23	C	507	CLA	C5-C6-C7-C8
23	C	511	CLA	C10-C11-C12-C13
32	D	407[A]	LHG	C32-C33-C34-C35
23	c	508	CLA	C16-C17-C18-C20
23	d	404	CLA	C16-C17-C18-C19
32	L	101[A]	LHG	C25-C26-C27-C28
32	L	101[B]	LHG	C15-C16-C17-C18
32	b	629[B]	LHG	C16-C17-C18-C19
35	h	102	DGD	C9A-CAA-CBA-CCA
32	A	419[B]	LHG	C12-C13-C14-C15
32	L	101[B]	LHG	C25-C26-C27-C28
32	a	419[B]	LHG	C26-C27-C28-C29
32	d	414[A]	LHG	C32-C33-C34-C35
35	c	516[B]	DGD	C2A-C1A-O1G-C1G
31	t	101	LMT	O1'-C1-C2-C3
33	C	501	LMG	C17-C18-C19-C20
33	C	521	LMG	C17-C18-C19-C20
33	D	411	LMG	C35-C36-C37-C38
33	m	101	LMG	C35-C36-C37-C38
34	B	623	HTG	C3'-C4'-C5'-C6'
23	C	510	CLA	C3-C5-C6-C7
33	c	519	LMG	C10-C11-C12-C13
32	a	419[A]	LHG	C26-C27-C28-C29
32	d	407[A]	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
35	C	517[A]	DGD	C4B-C5B-C6B-C7B
35	C	517[A]	DGD	C5B-C6B-C7B-C8B
35	C	517[B]	DGD	C5B-C6B-C7B-C8B
35	c	516[A]	DGD	C9A-CAA-CBA-CCA
31	B	628	LMT	C3'-C4'-O1B-C1B
26	b	620	SQD	C18-C19-C20-C21
31	b	627	LMT	C3-C4-C5-C6
32	b	629[A]	LHG	C14-C15-C16-C17
23	c	506	CLA	C15-C16-C17-C18
33	C	501	LMG	C36-C37-C38-C39
23	b	606	CLA	C16-C17-C18-C20
23	d	403[B]	CLA	C16-C17-C18-C20
31	A	420	LMT	C3'-C4'-O1B-C1B
23	C	508	CLA	C2B-C3B-CAB-CBB
23	a	405[A]	CLA	C2B-C3B-CAB-CBB
23	c	507	CLA	C2B-C3B-CAB-CBB
26	a	410	SQD	C31-C32-C33-C34
26	A	410[A]	SQD	C12-C13-C14-C15
26	F	102	SQD	C24-C25-C26-C27
32	b	629[A]	LHG	C16-C17-C18-C19
23	C	504	CLA	O1D-CGD-O2D-CED
23	c	510	CLA	O1D-CGD-O2D-CED
31	e	101	LMT	C4-C5-C6-C7
31	e	101	LMT	C5-C6-C7-C8
32	A	419[A]	LHG	C12-C13-C14-C15
32	L	101[A]	LHG	C15-C16-C17-C18
33	m	101	LMG	C38-C39-C40-C41
23	b	610	CLA	C2A-CAA-CBA-CGA
33	C	501	LMG	C12-C13-C14-C15
33	D	411	LMG	C12-C13-C14-C15
32	L	101[B]	LHG	C13-C14-C15-C16
35	c	516[B]	DGD	C9A-CAA-CBA-CCA
33	m	101	LMG	O9-C10-O7-C8
31	b	621	LMT	C3'-C4'-O1B-C1B
29	A	414[A]	PL9	C30-C29-C31-C32
32	D	406[A]	LHG	C16-C17-C18-C19
32	E	101[A]	LHG	C24-C25-C26-C27
23	B	614	CLA	C5-C6-C7-C8
32	A	419[B]	LHG	C34-C35-C36-C37
35	c	516[B]	DGD	C5A-C6A-C7A-C8A
35	c	517[A]	DGD	CBA-CCA-CDA-CEA
35	h	102	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
35	h	102	DGD	C7B-C8B-C9B-CAB
23	c	512	CLA	CBA-CGA-O2A-C1
23	c	513	CLA	C6-C7-C8-C9
32	A	419[A]	LHG	C34-C35-C36-C37
33	c	519	LMG	C33-C34-C35-C36
23	A	404[B]	CLA	C13-C15-C16-C17
31	B	628	LMT	C5-C6-C7-C8
31	B	630	LMT	C2-C3-C4-C5
32	D	407[A]	LHG	C15-C16-C17-C18
33	D	411	LMG	C30-C31-C32-C33
35	c	516[A]	DGD	C5A-C6A-C7A-C8A
35	C	518[A]	DGD	O6E-C1E-O5D-C6D
35	C	517[B]	DGD	C4D-C5D-C6D-O5D
33	C	501	LMG	C19-C20-C21-C22
33	C	521	LMG	C19-C20-C21-C22
35	c	518	DGD	CBB-CCB-CDB-CEB
31	t	101	LMT	C2'-C1'-O1'-C1
35	c	516[A]	DGD	O1A-C1A-O1G-C1G
35	c	517[A]	DGD	CBB-CCB-CDB-CEB
26	A	410[B]	SQD	C7-C8-C9-C10
33	C	521	LMG	C13-C14-C15-C16
26	F	102	SQD	C29-C30-C31-C32
35	C	517[B]	DGD	C4B-C5B-C6B-C7B
23	b	614	CLA	C16-C17-C18-C19
26	b	620	SQD	C27-C28-C29-C30
32	d	414[A]	LHG	C29-C30-C31-C32
34	b	622	HTG	C3'-C4'-C5'-C6'
35	c	516[A]	DGD	C7A-C8A-C9A-CAA
25	d	405	BCR	C7-C8-C9-C34
31	B	631	LMT	C4-C5-C6-C7
23	B	607	CLA	C3-C5-C6-C7
23	B	610	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C20
23	d	403[B]	CLA	C16-C17-C18-C19
29	A	414[A]	PL9	C45-C44-C46-C47
29	d	406[A]	PL9	C13-C14-C16-C17
32	L	101[A]	LHG	C13-C14-C15-C16
32	d	407[A]	LHG	C34-C35-C36-C37
32	d	408[B]	LHG	C27-C28-C29-C30
23	B	603	CLA	C13-C15-C16-C17
26	A	412	SQD	C26-C27-C28-C29
32	E	101[B]	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
33	c	519	LMG	C31-C32-C33-C34
33	m	101	LMG	C39-C40-C41-C42
35	c	516[B]	DGD	O1A-C1A-O1G-C1G
23	C	503	CLA	C15-C16-C17-C18
32	d	414[B]	LHG	C32-C33-C34-C35
31	B	628	LMT	C1-C2-C3-C4
32	D	407[A]	LHG	C29-C30-C31-C32
32	d	408[A]	LHG	C27-C28-C29-C30
31	B	630	LMT	C5-C6-C7-C8
31	B	631	LMT	C11-C10-C9-C8
35	C	517[A]	DGD	O6E-C5E-C6E-O5E
33	C	501	LMG	C10-C11-C12-C13
33	a	415	LMG	C10-C11-C12-C13
23	B	601	CLA	C15-C16-C17-C18
31	B	630	LMT	C6-C7-C8-C9
33	c	519	LMG	C34-C35-C36-C37
33	Z	101	LMG	O6-C5-C6-O5
26	A	410[A]	SQD	O6-C44-C45-O47
26	A	410[B]	SQD	O6-C44-C45-O47
31	t	101	LMT	C4'-C5'-C6'-O6'
35	H	102	DGD	CCB-CDB-CEB-CFB
34	b	623	HTG	O5-C5-C6-O6
32	L	101[B]	LHG	C17-C18-C19-C20
31	B	631	LMT	C3-C4-C5-C6
33	d	412	LMG	C29-C30-C31-C32
23	B	616	CLA	C2-C1-O2A-CGA
23	C	510	CLA	C2-C1-O2A-CGA
33	d	412	LMG	O6-C5-C6-O5
31	M	101	LMT	C3-C4-C5-C6
33	B	621	LMG	C17-C18-C19-C20
31	b	627	LMT	C5-C6-C7-C8
23	C	511	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C12-C11-C9-C8
29	D	405[A]	PL9	C13-C14-C16-C17
31	e	101	LMT	C1-C2-C3-C4
26	f	102	SQD	C25-C26-C27-C28
35	c	516[A]	DGD	CAA-CBA-CCA-CDA
23	B	610	CLA	C2A-CAA-CBA-CGA
26	a	410	SQD	C25-C26-C27-C28
32	b	629[B]	LHG	C12-C13-C14-C15
26	a	409[B]	SQD	C12-C13-C14-C15
26	b	620	SQD	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
23	d	403[A]	CLA	C16-C17-C18-C20
27	B	629	GOL	O2-C2-C3-O3
27	d	413	GOL	O1-C1-C2-O2
27	o	303	GOL	O2-C2-C3-O3
23	b	607	CLA	C3-C5-C6-C7
26	B	620	SQD	C11-C10-C9-C8
35	c	516[A]	DGD	C4D-C5D-C6D-O5D
35	c	516[B]	DGD	C4D-C5D-C6D-O5D
35	c	517[B]	DGD	C2B-C3B-C4B-C5B
23	A	405[A]	CLA	C1A-C2A-CAA-CBA
23	B	611	CLA	C1A-C2A-CAA-CBA
23	B	608	CLA	C13-C15-C16-C17
35	c	517[B]	DGD	O6E-C1E-O5D-C6D
35	C	517[A]	DGD	C8A-C9A-CAA-CBA
35	H	102	DGD	C9B-CAB-CBB-CCB
26	A	410[B]	SQD	C11-C10-C9-C8
35	C	517[B]	DGD	C8A-C9A-CAA-CBA
23	c	512	CLA	O1A-CGA-O2A-C1
23	d	402[B]	CLA	C2C-C3C-CAC-CBC
26	A	412	SQD	C17-C18-C19-C20
32	D	407[B]	LHG	C15-C16-C17-C18
35	c	516[B]	DGD	CAA-CBA-CCA-CDA
35	c	517[A]	DGD	C6A-C7A-C8A-C9A
35	C	517[B]	DGD	C9A-CAA-CBA-CCA
23	B	613	CLA	C11-C10-C8-C7
23	B	614	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C7
23	C	514	CLA	C11-C12-C13-C15
23	D	403	CLA	C12-C13-C15-C16
23	b	601	CLA	C11-C10-C8-C7
23	c	504	CLA	C11-C12-C13-C15
23	c	505	CLA	C11-C12-C13-C15
23	c	512	CLA	C12-C13-C15-C16
32	d	408[B]	LHG	C29-C30-C31-C32
33	a	415	LMG	C21-C22-C23-C24
23	B	610	CLA	C16-C17-C18-C19
23	A	406[B]	CLA	C13-C15-C16-C17
23	A	406[A]	CLA	C13-C15-C16-C17
23	b	601	CLA	C8-C10-C11-C12
23	c	505	CLA	C2-C3-C5-C6
29	A	414[B]	PL9	C12-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
29	D	405[B]	PL9	C13-C14-C16-C17
32	D	406[A]	LHG	C13-C14-C15-C16
23	b	614	CLA	C10-C11-C12-C13
23	B	614	CLA	C14-C13-C15-C16
31	T	101	LMT	C7-C8-C9-C10
23	A	404[A]	CLA	C13-C15-C16-C17
23	C	502	CLA	O1D-CGD-O2D-CED
26	b	620	SQD	C14-C15-C16-C17
32	d	408[A]	LHG	C25-C26-C27-C28
23	C	512	CLA	C8-C10-C11-C12
33	z	101	LMG	C10-C11-C12-C13
26	A	410[A]	SQD	O6-C44-C45-C46
26	A	410[B]	SQD	O6-C44-C45-C46
26	A	412	SQD	O6-C44-C45-C46
26	B	620	SQD	C44-C45-C46-O48
26	a	409[A]	SQD	O6-C44-C45-C46
26	b	620	SQD	C44-C45-C46-O48
26	f	102	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
32	E	101[B]	LHG	C4-C5-C6-O8
33	a	415	LMG	C7-C8-C9-O8
32	d	414[B]	LHG	C29-C30-C31-C32
23	D	403	CLA	O1D-CGD-O2D-CED
33	C	501	LMG	C13-C14-C15-C16
23	c	511	CLA	C8-C10-C11-C12
23	C	513	CLA	CBA-CGA-O2A-C1
26	b	620	SQD	C24-C23-O48-C46
33	D	411	LMG	O6-C5-C6-O5
35	C	517[B]	DGD	O6E-C5E-C6E-O5E
35	c	516[A]	DGD	O6E-C5E-C6E-O5E
26	A	412	SQD	C27-C28-C29-C30
26	a	409[A]	SQD	C9-C10-C11-C12
32	d	408[B]	LHG	C25-C26-C27-C28
33	C	520	LMG	C17-C18-C19-C20
32	E	101[A]	LHG	C25-C26-C27-C28
35	h	102	DGD	CAA-CBA-CCA-CDA
31	b	627	LMT	C1-C2-C3-C4
23	c	505	CLA	C4-C3-C5-C6
23	C	511	CLA	C2-C3-C5-C6
29	d	406[B]	PL9	C13-C14-C16-C17
23	A	405[A]	CLA	C15-C16-C17-C18
23	C	507	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	b	610	CLA	C15-C16-C17-C18
23	d	403[A]	CLA	C16-C17-C18-C19
33	m	101	LMG	C37-C38-C39-C40
33	z	101	LMG	C19-C20-C21-C22
35	C	517[A]	DGD	C9A-CAA-CBA-CCA
35	c	516[B]	DGD	O6E-C5E-C6E-O5E
25	y	101	BCR	C21-C22-C23-C24
23	c	512	CLA	C10-C11-C12-C13
26	B	620	SQD	C34-C35-C36-C37
32	D	407[B]	LHG	C17-C18-C19-C20
35	C	517[A]	DGD	C3B-C4B-C5B-C6B
35	h	102	DGD	C3B-C4B-C5B-C6B
23	B	601	CLA	C2A-CAA-CBA-CGA
33	D	411	LMG	C36-C37-C38-C39
35	c	517[A]	DGD	C2B-C3B-C4B-C5B
26	A	410[B]	SQD	C12-C13-C14-C15
31	m	103	LMT	C7-C8-C9-C10
32	E	101[B]	LHG	C25-C26-C27-C28
32	b	629[A]	LHG	C13-C14-C15-C16
35	c	517[B]	DGD	C6A-C7A-C8A-C9A
23	C	511	CLA	CBA-CGA-O2A-C1
32	D	407[B]	LHG	C24-C23-O8-C6
26	b	620	SQD	C46-C45-O47-C7
23	d	402[A]	CLA	C2C-C3C-CAC-CBC
26	b	620	SQD	C26-C27-C28-C29
32	D	407[A]	LHG	C17-C18-C19-C20
35	c	517[B]	DGD	C4A-C5A-C6A-C7A
35	C	517[A]	DGD	O6D-C5D-C6D-O5D
23	b	604	CLA	C15-C16-C17-C18
33	a	415	LMG	C35-C36-C37-C38
32	b	629[B]	LHG	C27-C28-C29-C30
32	d	414[B]	LHG	C24-C25-C26-C27
23	C	506	CLA	C2-C3-C5-C6
26	a	409[A]	SQD	C12-C13-C14-C15
31	A	420	LMT	C4-C5-C6-C7
35	C	518[B]	DGD	CDA-CEA-CFA-CGA
24	A	416[B]	PHO	C2C-C3C-CAC-CBC
32	d	408[A]	LHG	C34-C35-C36-C37
35	c	517[A]	DGD	C4A-C5A-C6A-C7A
35	C	518[A]	DGD	CDA-CEA-CFA-CGA
32	D	407[B]	LHG	C29-C30-C31-C32
33	d	412	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
31	b	621	LMT	C11-C10-C9-C8
32	D	406[B]	LHG	C12-C13-C14-C15
33	C	520	LMG	C36-C37-C38-C39
23	B	612	CLA	C10-C11-C12-C13
33	a	415	LMG	C29-C30-C31-C32
23	C	511	CLA	O1A-CGA-O2A-C1
31	a	416	LMT	C9-C10-C11-C12
32	d	414[B]	LHG	C25-C26-C27-C28
35	h	102	DGD	CAB-CBB-CCB-CDB
31	a	416	LMT	C2-C3-C4-C5
35	c	518	DGD	CBA-CCA-CDA-CEA
35	C	519	DGD	CAA-CBA-CCA-CDA
23	A	405[B]	CLA	C15-C16-C17-C18
32	d	408[A]	LHG	C29-C30-C31-C32
34	B	622	HTG	C2'-C3'-C4'-C5'
23	B	613	CLA	C13-C15-C16-C17
23	b	601	CLA	C13-C15-C16-C17
29	D	405[B]	PL9	C15-C14-C16-C17
29	a	412[B]	PL9	C12-C11-C9-C10
29	d	406[A]	PL9	C45-C44-C46-C47
23	B	601	CLA	CBA-CGA-O2A-C1
34	b	623	HTG	S1-C1'-C2'-C3'
33	C	501	LMG	C18-C19-C20-C21
32	d	414[A]	LHG	C33-C34-C35-C36
35	C	518[B]	DGD	C5B-C6B-C7B-C8B
35	H	102	DGD	C7A-C8A-C9A-CAA
31	B	628	LMT	C2-C1-O1'-C1'
31	b	627	LMT	C2-C1-O1'-C1'
23	B	602	CLA	C6-C7-C8-C9
23	B	610	CLA	C14-C13-C15-C16
23	C	505	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	C	514	CLA	C6-C7-C8-C9
23	C	514	CLA	C11-C10-C8-C9
23	b	601	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C12-C13-C14
26	a	409[B]	SQD	C9-C10-C11-C12
23	A	406[A]	CLA	C4B-C3B-CAB-CBB
23	B	602	CLA	C4B-C3B-CAB-CBB
23	a	405[A]	CLA	C4B-C3B-CAB-CBB
35	h	102	DGD	CDB-CEB-CFB-CGB
26	b	620	SQD	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
32	D	406[A]	LHG	C12-C13-C14-C15
33	C	520	LMG	C37-C38-C39-C40
26	A	412	SQD	C2-C1-O6-C44
35	c	517[B]	DGD	C2E-C1E-O5D-C6D
31	t	101	LMT	C7-C8-C9-C10
32	D	406[B]	LHG	C10-C11-C12-C13
35	h	102	DGD	C9B-CAB-CBB-CCB
32	b	629[A]	LHG	O6-C4-C5-C6
32	D	407[B]	LHG	C13-C14-C15-C16
32	d	408[B]	LHG	C28-C29-C30-C31
35	h	102	DGD	CBA-CCA-CDA-CEA
23	A	406[A]	CLA	C12-C13-C15-C16
23	A	406[B]	CLA	C12-C13-C15-C16
23	B	610	CLA	C12-C13-C15-C16
23	C	503	CLA	C12-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
23	b	601	CLA	C6-C7-C8-C10
23	c	506	CLA	C11-C10-C8-C7
23	c	509	CLA	C11-C10-C8-C7
23	c	510	CLA	C11-C10-C8-C7
23	B	608	CLA	C16-C17-C18-C20
31	M	101	LMT	O1'-C1-C2-C3
23	C	513	CLA	O1A-CGA-O2A-C1
31	a	416	LMT	C3-C4-C5-C6
33	C	520	LMG	C34-C35-C36-C37
23	c	506	CLA	C3A-C2A-CAA-CBA
29	a	412[A]	PL9	C12-C11-C9-C10
23	c	512	CLA	C13-C15-C16-C17
33	C	521	LMG	C35-C36-C37-C38
33	C	501	LMG	C11-C12-C13-C14
26	b	620	SQD	O10-C23-O48-C46
23	b	601	CLA	CBA-CGA-O2A-C1
33	c	520	LMG	C29-C28-O8-C9
32	d	408[A]	LHG	C28-C29-C30-C31
25	y	101	BCR	C37-C22-C23-C24
32	D	407[B]	LHG	O10-C23-O8-C6
26	a	410	SQD	C16-C17-C18-C19
31	e	101	LMT	C4B-C5B-C6B-O6B
31	M	101	LMT	O5'-C5'-C6'-O6'
23	b	613	CLA	CBD-CGD-O2D-CED
33	m	101	LMG	C14-C15-C16-C17
35	c	517[A]	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
32	b	629[A]	LHG	C27-C28-C29-C30
35	C	517[B]	DGD	CCA-CDA-CEA-CFA
32	a	419[A]	LHG	C4-C5-C6-O8
32	a	419[B]	LHG	C4-C5-C6-O8
34	c	521	HTG	C4'-C5'-C6'-C7'
35	C	518[A]	DGD	C5B-C6B-C7B-C8B
23	C	507	CLA	C16-C17-C18-C20
32	D	407[A]	LHG	C13-C14-C15-C16
32	d	408[A]	LHG	C9-C10-C11-C12
32	D	406[A]	LHG	C10-C11-C12-C13
32	d	407[A]	LHG	C13-C14-C15-C16
23	C	506	CLA	C4-C3-C5-C6
23	c	513	CLA	C4-C3-C5-C6
29	A	414[B]	PL9	C45-C44-C46-C47
29	D	405[A]	PL9	C43-C44-C46-C47
32	A	419[A]	LHG	C26-C27-C28-C29
32	E	101[A]	LHG	O6-C4-C5-O7
26	F	102	SQD	C34-C35-C36-C37
32	L	101[B]	LHG	C24-C25-C26-C27
35	C	517[A]	DGD	C7A-C8A-C9A-CAA
25	B	617	BCR	C1-C6-C7-C8
25	b	617	BCR	C1-C6-C7-C8
23	c	506	CLA	C13-C15-C16-C17
23	C	514	CLA	CBD-CGD-O2D-CED
23	c	501	CLA	CBD-CGD-O2D-CED
33	Z	101	LMG	C19-C20-C21-C22
35	c	516[B]	DGD	C7A-C8A-C9A-CAA
23	B	608	CLA	C16-C17-C18-C19
26	a	409[A]	SQD	O6-C44-C45-O47
26	a	409[B]	SQD	O6-C44-C45-O47
26	b	620	SQD	O47-C45-C46-O48
26	f	102	SQD	O47-C45-C46-O48
33	B	621	LMG	C32-C33-C34-C35
29	A	414[B]	PL9	C4-C3-C7-C8
35	C	519	DGD	CDB-CEB-CFB-CGB
35	C	518[B]	DGD	C1A-C2A-C3A-C4A
29	d	406[A]	PL9	C15-C14-C16-C17
29	d	406[B]	PL9	C15-C14-C16-C17
32	a	419[A]	LHG	C10-C11-C12-C13
32	b	629[A]	LHG	C12-C13-C14-C15
35	C	517[B]	DGD	C7A-C8A-C9A-CAA
35	H	102	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
24	a	406[B]	PHO	C2-C3-C5-C6
29	A	414[A]	PL9	C43-C44-C46-C47
32	L	101[A]	LHG	C24-C25-C26-C27
32	L	101[A]	LHG	C11-C12-C13-C14
32	d	414[B]	LHG	C33-C34-C35-C36
33	C	501	LMG	C29-C30-C31-C32
35	c	517[A]	DGD	C5A-C6A-C7A-C8A
33	c	519	LMG	C28-C29-C30-C31
23	c	512	CLA	O1D-CGD-O2D-CED
31	F	101	LMT	C4-C5-C6-C7
23	B	601	CLA	O1A-CGA-O2A-C1
23	c	513	CLA	CBD-CGD-O2D-CED
23	C	511	CLA	C14-C13-C15-C16
23	D	403	CLA	C14-C13-C15-C16
31	b	621	LMT	C3-C4-C5-C6
35	C	519	DGD	C8A-C9A-CAA-CBA
32	d	408[B]	LHG	C9-C10-C11-C12
23	b	606	CLA	C16-C17-C18-C19
26	a	409[A]	SQD	C34-C35-C36-C37
32	b	629[A]	LHG	C31-C32-C33-C34
29	a	412[A]	PL9	C24-C26-C27-C28
35	c	517[B]	DGD	C5A-C6A-C7A-C8A
32	E	101[A]	LHG	C17-C18-C19-C20
35	c	518	DGD	C2B-C3B-C4B-C5B
23	c	507	CLA	C5-C6-C7-C8
27	O	303	GOL	O1-C1-C2-O2
27	c	526	GOL	O1-C1-C2-O2
32	A	419[B]	LHG	O1-C1-C2-O2
32	d	408[B]	LHG	C24-C23-O8-C6
25	t	102	BCR	C13-C14-C15-C16
33	B	621	LMG	O8-C28-C29-C30
23	A	406[A]	CLA	C16-C17-C18-C20
32	D	407[B]	LHG	C10-C11-C12-C13
26	B	620	SQD	C24-C25-C26-C27
35	C	518[A]	DGD	C8B-C9B-CAB-CBB
23	B	601	CLA	C13-C15-C16-C17
31	B	630	LMT	C3-C4-C5-C6
32	D	406[B]	LHG	C13-C14-C15-C16
32	D	407[A]	LHG	C10-C11-C12-C13
33	C	521	LMG	C4-C5-C6-O5
35	C	518[A]	DGD	C8A-C9A-CAA-CBA
32	E	101[A]	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
32	d	408[B]	LHG	O10-C23-O8-C6
23	C	511	CLA	C13-C15-C16-C17
32	b	629[B]	LHG	C13-C14-C15-C16
32	d	408[B]	LHG	C34-C35-C36-C37
23	B	602	CLA	C11-C12-C13-C15
23	C	507	CLA	C6-C7-C8-C10
23	C	511	CLA	C12-C13-C15-C16
23	a	407	CLA	C11-C10-C8-C7
23	b	604	CLA	C6-C7-C8-C10
23	c	509	CLA	C6-C7-C8-C10
32	a	419[A]	LHG	C7-C8-C9-C10
32	a	419[B]	LHG	C23-C24-C25-C26
35	H	102	DGD	CAB-CBB-CCB-CDB
33	C	520	LMG	C29-C30-C31-C32
23	B	613	CLA	C15-C16-C17-C18
25	D	404	BCR	C21-C22-C23-C24
25	d	405	BCR	C7-C8-C9-C10
26	A	412	SQD	C24-C23-O48-C46
35	c	518	DGD	C2A-C1A-O1G-C1G
31	e	101	LMT	C9-C10-C11-C12
35	C	518[A]	DGD	C2G-C3G-O3G-C1D
35	c	517[A]	DGD	C2G-C3G-O3G-C1D
35	c	517[A]	DGD	C5D-C6D-O5D-C1E
35	c	517[B]	DGD	C5D-C6D-O5D-C1E
23	b	615	CLA	C10-C11-C12-C13
32	d	414[A]	LHG	C25-C26-C27-C28
23	A	406[B]	CLA	C16-C17-C18-C20
23	c	510	CLA	C4-C3-C5-C6
24	a	406[B]	PHO	C4-C3-C5-C6
29	D	405[A]	PL9	C15-C14-C16-C17
29	D	405[A]	PL9	C45-C44-C46-C47
33	c	520	LMG	O10-C28-O8-C9
38	f	101	HEM	C2B-C3B-CAB-CBB
32	E	101[B]	LHG	C13-C14-C15-C16
34	B	625	HTG	C4'-C5'-C6'-C7'
27	B	627	GOL	C1-C2-C3-O3
32	A	419[B]	LHG	C26-C27-C28-C29
35	c	517[B]	DGD	CBB-CCB-CDB-CEB
24	a	406[A]	PHO	O2A-C1-C2-C3
26	B	620	SQD	C46-C45-O47-C7
26	A	412	SQD	C30-C31-C32-C33
32	a	419[B]	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	b	601	CLA	O1A-CGA-O2A-C1
23	c	511	CLA	O1A-CGA-O2A-C1
35	c	518	DGD	O1A-C1A-O1G-C1G
23	C	513	CLA	C3-C5-C6-C7
23	c	511	CLA	CBA-CGA-O2A-C1
32	D	407[B]	LHG	C27-C28-C29-C30
32	E	101[B]	LHG	O6-C4-C5-O7
32	b	629[A]	LHG	O6-C4-C5-O7
26	F	102	SQD	C32-C33-C34-C35
32	L	101[A]	LHG	C11-C10-C9-C8
32	d	414[A]	LHG	C24-C25-C26-C27
26	A	412	SQD	O5-C1-O6-C44
26	a	410	SQD	O6-C44-C45-C46
32	E	101[A]	LHG	C4-C5-C6-O8
33	z	101	LMG	C14-C15-C16-C17
32	b	629[A]	LHG	C34-C35-C36-C37
35	C	517[A]	DGD	C4D-C5D-C6D-O5D
31	A	420	LMT	C5-C6-C7-C8
35	C	517[A]	DGD	CCA-CDA-CEA-CFA
32	b	629[A]	LHG	C9-C10-C11-C12
26	F	102	SQD	O47-C45-C46-O48
32	a	419[A]	LHG	O7-C5-C6-O8
33	a	415	LMG	O7-C8-C9-O8
35	h	102	DGD	O1G-C1G-C2G-O2G
23	C	507	CLA	C6-C7-C8-C9
23	C	513	CLA	C6-C7-C8-C9
23	c	509	CLA	C6-C7-C8-C9
23	c	512	CLA	C6-C7-C8-C9
32	E	101[A]	LHG	C13-C14-C15-C16
32	d	407[B]	LHG	C11-C10-C9-C8
26	a	409[A]	SQD	C27-C28-C29-C30
33	c	519	LMG	C29-C30-C31-C32
23	B	606	CLA	C8-C10-C11-C12
23	B	615	CLA	C10-C11-C12-C13
31	b	627	LMT	C6-C7-C8-C9
23	C	510	CLA	O1D-CGD-O2D-CED
32	d	407[B]	LHG	C13-C14-C15-C16
35	C	518[A]	DGD	C7A-C8A-C9A-CAA
23	c	509	CLA	C8-C10-C11-C12
32	D	406[A]	LHG	C34-C35-C36-C37
23	b	601	CLA	CAA-CBA-CGA-O2A
23	b	604	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	a	409[B]	SQD	C34-C35-C36-C37
23	b	601	CLA	C4-C3-C5-C6
29	d	406[B]	PL9	C45-C44-C46-C47
29	a	412[B]	PL9	C12-C11-C9-C8
33	C	520	LMG	C31-C32-C33-C34
32	d	408[A]	LHG	C24-C23-O8-C6
32	L	101[B]	LHG	C23-C24-C25-C26
33	B	621	LMG	C36-C37-C38-C39
23	b	601	CLA	C3-C5-C6-C7
33	c	519	LMG	O6-C5-C6-O5
35	C	517[B]	DGD	C3B-C4B-C5B-C6B
27	a	417	GOL	O1-C1-C2-O2
31	A	420	LMT	C2-C1-O1'-C1'
29	a	412[B]	PL9	C24-C26-C27-C28
23	a	405[B]	CLA	C4B-C3B-CAB-CBB
23	b	606	CLA	C4B-C3B-CAB-CBB
23	c	501	CLA	C4B-C3B-CAB-CBB
23	d	402[A]	CLA	C1A-C2A-CAA-CBA
23	b	602	CLA	C10-C11-C12-C13
33	C	501	LMG	C39-C40-C41-C42
26	a	409[A]	SQD	C35-C36-C37-C38
23	b	604	CLA	C13-C15-C16-C17
23	a	404[A]	CLA	C2C-C3C-CAC-CBC
31	b	621	LMT	C7-C8-C9-C10
31	e	101	LMT	C3-C4-C5-C6
33	Z	101	LMG	C11-C12-C13-C14
35	C	518[B]	DGD	C8B-C9B-CAB-CBB
33	C	521	LMG	C12-C13-C14-C15
31	F	101	LMT	C6-C7-C8-C9
32	A	419[A]	LHG	C32-C33-C34-C35
32	L	101[B]	LHG	C27-C28-C29-C30
32	d	414[B]	LHG	C34-C35-C36-C37
23	B	616	CLA	C12-C13-C15-C16
23	b	601	CLA	C11-C12-C13-C15
23	b	603	CLA	C11-C10-C8-C7
23	b	608	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C10
23	c	505	CLA	C12-C13-C15-C16
23	d	403[B]	CLA	C11-C12-C13-C15
23	A	404[B]	CLA	C16-C17-C18-C19
32	d	408[A]	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
35	H	102	DGD	O2G-C1B-C2B-C3B
32	D	407[A]	LHG	C24-C23-O8-C6
35	C	519	DGD	CBA-CCA-CDA-CEA
23	b	608	CLA	C13-C15-C16-C17
26	A	412	SQD	O10-C23-O48-C46
32	D	407[A]	LHG	O10-C23-O8-C6
35	c	517[A]	DGD	C1A-C2A-C3A-C4A
32	D	407[B]	LHG	C2-C3-O3-P
23	c	506	CLA	C10-C11-C12-C13
26	A	410[A]	SQD	C18-C19-C20-C21
23	A	406[A]	CLA	C14-C13-C15-C16
23	a	407	CLA	C11-C10-C8-C9
23	b	601	CLA	C11-C12-C13-C14
23	b	615	CLA	C14-C13-C15-C16
23	c	506	CLA	C11-C10-C8-C9
23	c	510	CLA	C11-C10-C8-C9
23	d	404	CLA	C11-C12-C13-C14
32	d	414[A]	LHG	C27-C28-C29-C30
35	c	516[A]	DGD	CCB-CDB-CEB-CFB
32	E	101[A]	LHG	O7-C5-C6-O8
32	a	419[B]	LHG	O7-C5-C6-O8
32	D	406[B]	LHG	C34-C35-C36-C37
23	C	507	CLA	C16-C17-C18-C19
35	h	102	DGD	C6A-C7A-C8A-C9A
26	a	409[B]	SQD	O6-C44-C45-C46
33	C	501	LMG	C7-C8-C9-O8
29	a	412[A]	PL9	C12-C11-C9-C8
32	a	419[A]	LHG	C23-C24-C25-C26
23	B	601	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	509	CLA	C15-C16-C17-C18
26	A	410[A]	SQD	C34-C35-C36-C37
32	D	406[B]	LHG	C26-C27-C28-C29
32	L	101[B]	LHG	C11-C10-C9-C8
35	c	516[A]	DGD	C8B-C9B-CAB-CBB
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	C	510	CLA	CHA-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O1D
32	D	406[A]	LHG	C4-O6-P-O3
32	D	406[A]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C4-O6-P-O5
32	E	101[B]	LHG	C4-O6-P-O5
32	a	419[A]	LHG	C4-O6-P-O4
32	a	419[B]	LHG	C4-O6-P-O4
32	d	407[A]	LHG	C3-O3-P-O4
32	d	407[B]	LHG	C4-O6-P-O5
32	d	414[B]	LHG	C3-O3-P-O5
26	a	409[B]	SQD	C35-C36-C37-C38
35	C	519	DGD	CAB-CBB-CCB-CDB
24	a	406[A]	PHO	C8-C10-C11-C12
29	A	414[B]	PL9	C25-C24-C26-C27
23	A	406[A]	CLA	C2B-C3B-CAB-CBB
23	D	402[B]	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
23	b	609	CLA	C2-C3-C5-C6
23	c	510	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C28-C29-C31-C32
32	D	407[A]	LHG	C2-C3-O3-P
32	d	408[A]	LHG	C2-C3-O3-P
32	d	408[B]	LHG	C2-C3-O3-P
35	c	517[B]	DGD	C1A-C2A-C3A-C4A
23	B	601	CLA	CAA-CBA-CGA-O2A
32	b	629[B]	LHG	C34-C35-C36-C37
35	c	517[B]	DGD	C9B-CAB-CBB-CCB
26	a	409[A]	SQD	C11-C12-C13-C14
27	l	801[B]	GOL	O1-C1-C2-O2
31	T	101	LMT	C3-C4-C5-C6
35	C	517[B]	DGD	C2A-C3A-C4A-C5A
29	D	405[B]	PL9	C4-C3-C7-C8
29	a	412[A]	PL9	C4-C3-C7-C8
29	a	412[B]	PL9	C4-C3-C7-C8
35	C	518[A]	DGD	C1A-C2A-C3A-C4A
23	d	402[B]	CLA	C4C-C3C-CAC-CBC
31	B	628	LMT	C9-C10-C11-C12
23	b	601	CLA	C2-C3-C5-C6
32	b	629[B]	LHG	C25-C26-C27-C28
35	C	519	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
33	B	621	LMG	C20-C21-C22-C23
32	E	101[B]	LHG	O6-C4-C5-C6
32	L	101[A]	LHG	O6-C4-C5-C6
32	b	629[B]	LHG	O6-C4-C5-C6
23	A	406[B]	CLA	C14-C13-C15-C16
23	B	602	CLA	C11-C12-C13-C14
23	b	603	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C10-C8-C9
23	b	614	CLA	C14-C13-C15-C16
23	b	606	CLA	C11-C10-C8-C7
23	c	510	CLA	C12-C13-C15-C16
32	E	101[A]	LHG	C1-C2-C3-O3
32	L	101[A]	LHG	O6-C4-C5-O7
35	c	516[A]	DGD	O6E-C1E-O5D-C6D
33	m	101	LMG	C11-C12-C13-C14
23	D	403	CLA	O1A-CGA-O2A-C1
34	B	622	HTG	C3'-C4'-C5'-C6'
35	h	102	DGD	CDA-CEA-CFA-CGA
31	b	627	LMT	O1'-C1-C2-C3
34	b	622	HTG	C1'-C2'-C3'-C4'
35	c	517[A]	DGD	C2E-C1E-O5D-C6D
24	a	406[A]	PHO	C4-C3-C5-C6
26	A	410[A]	SQD	C16-C17-C18-C19
33	C	521	LMG	C20-C21-C22-C23
35	c	517[B]	DGD	C7B-C8B-C9B-CAB
31	B	631	LMT	C1-C2-C3-C4
32	d	407[A]	LHG	O10-C23-O8-C6
32	d	414[A]	LHG	C34-C35-C36-C37
26	B	620	SQD	O47-C45-C46-O48
32	E	101[B]	LHG	O7-C5-C6-O8
34	B	623	HTG	C4'-C5'-C6'-C7'
23	b	615	CLA	C5-C6-C7-C8
23	b	616	CLA	O1A-CGA-O2A-C1
32	d	408[A]	LHG	C32-C33-C34-C35
35	H	102	DGD	C6A-C7A-C8A-C9A
32	d	407[A]	LHG	C24-C23-O8-C6
26	A	410[B]	SQD	C16-C17-C18-C19
33	a	415	LMG	O8-C28-C29-C30
33	z	101	LMG	C13-C14-C15-C16
26	a	410	SQD	O10-C23-O48-C46
29	D	405[B]	PL9	C45-C44-C46-C47
26	A	412	SQD	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
35	h	102	DGD	O1G-C1G-C2G-C3G
23	C	512	CLA	C3-C5-C6-C7
23	B	605	CLA	C5-C6-C7-C8
35	C	517[A]	DGD	C6A-C7A-C8A-C9A
25	D	404	BCR	C37-C22-C23-C24
23	c	510	CLA	O1A-CGA-O2A-C1
35	C	518[B]	DGD	C2G-C3G-O3G-C1D
35	c	516[B]	DGD	C5D-C6D-O5D-C1E
25	K	102	BCR	C19-C20-C21-C22
33	d	412	LMG	C11-C12-C13-C14
32	D	406[B]	LHG	C11-C10-C9-C8
23	b	609	CLA	C4-C3-C5-C6
33	B	621	LMG	O6-C5-C6-O5
24	a	406[A]	PHO	C2-C3-C5-C6
38	f	101	HEM	C2C-C3C-CAC-CBC
26	a	410	SQD	C24-C23-O48-C46
26	B	620	SQD	C29-C30-C31-C32
32	a	419[B]	LHG	C7-C8-C9-C10
23	d	402[A]	CLA	C4C-C3C-CAC-CBC
32	L	101[A]	LHG	C26-C27-C28-C29
31	F	101	LMT	C2-C1-O1'-C1'
32	d	414[A]	LHG	C1-C2-C3-O3
35	C	517[B]	DGD	C6A-C7A-C8A-C9A
23	B	614	CLA	C11-C10-C8-C9
23	C	511	CLA	C11-C12-C13-C14
23	b	608	CLA	C14-C13-C15-C16
23	b	610	CLA	C11-C12-C13-C14
23	c	505	CLA	C14-C13-C15-C16
23	d	403[B]	CLA	C11-C12-C13-C14
23	b	613	CLA	O1D-CGD-O2D-CED
23	b	616	CLA	CBA-CGA-O2A-C1
35	c	518	DGD	O6D-C5D-C6D-O5D
32	L	101[A]	LHG	C27-C28-C29-C30
23	b	616	CLA	C4-C3-C5-C6
29	a	412[B]	PL9	C45-C44-C46-C47
29	a	412[B]	PL9	C43-C44-C46-C47
29	d	406[A]	PL9	C43-C44-C46-C47
33	B	621	LMG	C37-C38-C39-C40
38	f	101	HEM	C4B-C3B-CAB-CBB
38	f	101	HEM	C4C-C3C-CAC-CBC
23	D	403	CLA	C11-C10-C8-C7
23	b	615	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	a	406[B]	PHO	C8-C10-C11-C12
26	a	410	SQD	C26-C27-C28-C29
32	A	419[B]	LHG	C32-C33-C34-C35
31	F	101	LMT	C2-C3-C4-C5
23	D	403	CLA	CBA-CGA-O2A-C1
23	a	404[A]	CLA	C4C-C3C-CAC-CBC
35	c	516[B]	DGD	CAB-CBB-CCB-CDB
32	D	407[A]	LHG	C27-C28-C29-C30
32	E	101[B]	LHG	C17-C18-C19-C20
32	d	408[A]	LHG	C33-C34-C35-C36
23	C	507	CLA	C3A-C2A-CAA-CBA
29	a	412[A]	PL9	C45-C44-C46-C47
23	b	605	CLA	C13-C15-C16-C17
29	D	405[B]	PL9	C43-C44-C46-C47
33	C	521	LMG	C10-C11-C12-C13
26	a	410	SQD	C24-C25-C26-C27
26	b	620	SQD	C30-C31-C32-C33
31	e	101	LMT	C2-C3-C4-C5
35	c	516[A]	DGD	C4B-C5B-C6B-C7B
35	c	516[B]	DGD	C8B-C9B-CAB-CBB
26	A	412	SQD	C7-C8-C9-C10
23	d	402[A]	CLA	C15-C16-C17-C18
33	d	412	LMG	C18-C19-C20-C21
35	C	518[B]	DGD	C8A-C9A-CAA-CBA
23	A	405[B]	CLA	C2C-C3C-CAC-CBC
32	A	419[B]	LHG	C17-C18-C19-C20
26	A	410[A]	SQD	C11-C10-C9-C8
23	A	408	CLA	C16-C17-C18-C19
23	D	403	CLA	C8-C10-C11-C12
33	C	520	LMG	C30-C31-C32-C33
32	A	419[B]	LHG	C18-C19-C20-C21
33	c	519	LMG	C32-C33-C34-C35
29	D	405[A]	PL9	C35-C34-C36-C37
29	a	412[A]	PL9	C43-C44-C46-C47
29	d	406[B]	PL9	C43-C44-C46-C47
35	C	518[B]	DGD	C7A-C8A-C9A-CAA
32	b	629[B]	LHG	C28-C29-C30-C31
32	a	419[A]	LHG	C24-C25-C26-C27
33	c	519	LMG	C30-C31-C32-C33
33	d	412	LMG	C19-C20-C21-C22
23	B	606	CLA	C11-C10-C8-C9
23	D	403	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	a	405[A]	CLA	C11-C12-C13-C14
23	a	405[B]	CLA	C14-C13-C15-C16
35	C	519	DGD	C7A-C8A-C9A-CAA
27	l	801[A]	GOL	O1-C1-C2-C3
27	v	202[A]	GOL	O1-C1-C2-C3
32	b	629[A]	LHG	C25-C26-C27-C28
32	d	414[B]	LHG	C13-C14-C15-C16
33	a	415	LMG	C33-C34-C35-C36
23	c	510	CLA	CBA-CGA-O2A-C1
32	D	406[A]	LHG	C11-C10-C9-C8
35	C	519	DGD	C8B-C9B-CAB-CBB
35	h	102	DGD	C4E-C5E-C6E-O5E
23	C	502	CLA	C16-C17-C18-C20
33	a	415	LMG	C13-C14-C15-C16
23	b	616	CLA	C2-C3-C5-C6
27	A	418	GOL	O2-C2-C3-O3
33	z	101	LMG	O7-C10-C11-C12
23	B	604	CLA	C1A-C2A-CAA-CBA
23	a	405[B]	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	C1A-C2A-CAA-CBA
23	A	404[A]	CLA	C2C-C3C-CAC-CBC
23	C	505	CLA	C2B-C3B-CAB-CBB
23	a	405[B]	CLA	C2B-C3B-CAB-CBB
23	b	606	CLA	C2B-C3B-CAB-CBB
23	c	501	CLA	C2B-C3B-CAB-CBB
25	B	617	BCR	C5-C6-C7-C8
25	D	404	BCR	C23-C24-C25-C30
25	b	617	BCR	C5-C6-C7-C8
26	A	410[A]	SQD	C13-C14-C15-C16
26	b	620	SQD	C11-C10-C9-C8
32	A	419[A]	LHG	C18-C19-C20-C21
23	A	406[A]	CLA	C16-C17-C18-C19
23	c	501	CLA	O1D-CGD-O2D-CED
40	V	201	HEC	CAD-CBD-CGD-O1D
23	c	513	CLA	O1D-CGD-O2D-CED
33	d	412	LMG	C38-C39-C40-C41
35	c	517[A]	DGD	C7B-C8B-C9B-CAB
32	d	414[B]	LHG	C27-C28-C29-C30
32	b	629[A]	LHG	C17-C18-C19-C20
23	B	601	CLA	C11-C12-C13-C15
23	B	606	CLA	C11-C10-C8-C7
29	A	414[B]	PL9	C39-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
23	A	404[B]	CLA	C2A-CAA-CBA-CGA
33	C	501	LMG	O7-C8-C9-O8
35	H	102	DGD	O1G-C1G-C2G-O2G
29	A	414[A]	PL9	C4-C3-C7-C8
26	F	102	SQD	C24-C23-O48-C46
31	A	417	LMT	C7-C8-C9-C10
38	E	102	HEM	CAD-CBD-CGD-O1D
26	A	410[B]	SQD	C34-C35-C36-C37
32	D	406[A]	LHG	C26-C27-C28-C29
40	v	201	HEC	CAD-CBD-CGD-O2D
29	D	405[B]	PL9	C35-C34-C36-C37
32	d	407[A]	LHG	C16-C17-C18-C19
23	A	406[B]	CLA	C16-C17-C18-C19
40	V	201	HEC	CAD-CBD-CGD-O2D
31	M	101	LMT	C2-C3-C4-C5
35	c	516[B]	DGD	C4B-C5B-C6B-C7B
34	b	623	HTG	C4'-C5'-C6'-C7'
35	c	517[A]	DGD	O6E-C1E-O5D-C6D
29	a	412[B]	PL9	C35-C34-C36-C37
40	v	201	HEC	CAD-CBD-CGD-O1D
23	c	513	CLA	C2-C3-C5-C6
29	A	414[B]	PL9	C23-C24-C26-C27
23	B	610	CLA	C13-C15-C16-C17
35	c	517[B]	DGD	CDA-CEA-CFA-CGA
23	B	612	CLA	CBA-CGA-O2A-C1
35	c	516[A]	DGD	C2E-C1E-O5D-C6D
23	d	404	CLA	O1A-CGA-O2A-C1
38	E	102	HEM	CAD-CBD-CGD-O2D
38	f	101	HEM	CAA-CBA-CGA-O2A
26	B	620	SQD	C33-C34-C35-C36
32	L	101[A]	LHG	C23-C24-C25-C26
23	c	507	CLA	C2A-CAA-CBA-CGA
32	d	408[B]	LHG	C33-C34-C35-C36
32	A	419[A]	LHG	C29-C30-C31-C32
32	b	629[B]	LHG	O6-C4-C5-O7
23	C	514	CLA	O1D-CGD-O2D-CED
23	B	603	CLA	C4-C3-C5-C6
23	c	504	CLA	C4-C3-C5-C6
26	a	409[B]	SQD	C10-C11-C12-C13
23	c	502	CLA	C16-C17-C18-C19
31	T	101	LMT	C1-C2-C3-C4
26	F	102	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
23	A	404[A]	CLA	C16-C17-C18-C19
33	C	501	LMG	C20-C21-C22-C23
24	A	416[B]	PHO	CHA-CBD-CGD-O1D
23	C	512	CLA	O1A-CGA-O2A-C1
33	a	415	LMG	C31-C32-C33-C34
35	c	518	DGD	CDA-CEA-CFA-CGA
32	a	419[B]	LHG	C24-C25-C26-C27
35	c	518	DGD	O6E-C5E-C6E-O5E
33	D	411	LMG	C34-C35-C36-C37
23	b	604	CLA	C2C-C3C-CAC-CBC
32	L	101[B]	LHG	O6-C4-C5-C6
29	A	414[A]	PL9	C25-C24-C26-C27
23	B	606	CLA	C15-C16-C17-C18
35	c	516[A]	DGD	CAB-CBB-CCB-CDB
32	d	408[B]	LHG	C32-C33-C34-C35
35	c	518	DGD	C7B-C8B-C9B-CAB
23	B	604	CLA	C2C-C3C-CAC-CBC
33	C	520	LMG	C11-C12-C13-C14
23	a	405[B]	CLA	C11-C12-C13-C14
23	b	614	CLA	C11-C12-C13-C14
23	c	502	CLA	C11-C12-C13-C14
23	c	504	CLA	C14-C13-C15-C16
33	C	521	LMG	C8-C7-O1-C1
35	C	518[A]	DGD	C5D-C6D-O5D-C1E
35	c	516[A]	DGD	C5D-C6D-O5D-C1E
23	C	507	CLA	C2-C1-O2A-CGA
23	C	514	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C16-C17-C18-C20
32	A	419[A]	LHG	C35-C36-C37-C38
38	f	101	HEM	CAA-CBA-CGA-O1A
32	b	629[A]	LHG	C10-C11-C12-C13
26	f	102	SQD	C26-C27-C28-C29
33	Z	101	LMG	C2-C1-O1-C7
35	C	517[B]	DGD	C2E-C1E-O5D-C6D
31	B	631	LMT	C6-C7-C8-C9
23	c	509	CLA	C10-C11-C12-C13
32	L	101[A]	LHG	C16-C17-C18-C19
35	h	102	DGD	O2G-C1B-C2B-C3B
23	C	502	CLA	C2A-CAA-CBA-CGA
33	Z	101	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
23	A	404[A]	CLA	C15-C16-C17-C18
23	B	612	CLA	O1A-CGA-O2A-C1
23	C	503	CLA	C16-C17-C18-C19
35	C	517[B]	DGD	O6E-C1E-O5D-C6D
32	L	101[B]	LHG	C32-C33-C34-C35
33	B	621	LMG	C30-C31-C32-C33
35	C	519	DGD	C3B-C4B-C5B-C6B
32	d	408[B]	LHG	C10-C11-C12-C13
35	c	517[A]	DGD	C9B-CAB-CBB-CCB
26	F	102	SQD	C44-C45-C46-O48
29	A	414[A]	PL9	C39-C41-C42-C43
23	C	511	CLA	C8-C10-C11-C12
23	B	616	CLA	C16-C17-C18-C20
26	a	409[B]	SQD	C27-C28-C29-C30
35	C	519	DGD	O1A-C1A-O1G-C1G
31	B	628	LMT	C7-C8-C9-C10
32	D	407[A]	LHG	C28-C29-C30-C31
32	L	101[B]	LHG	C10-C11-C12-C13
32	b	629[A]	LHG	C30-C31-C32-C33
32	b	629[B]	LHG	C9-C10-C11-C12
32	A	419[B]	LHG	O8-C23-C24-C25
33	C	521	LMG	C38-C39-C40-C41
34	B	623	HTG	S1-C1'-C2'-C3'
23	B	614	CLA	C6-C7-C8-C9
23	B	616	CLA	C6-C7-C8-C9
23	B	616	CLA	C14-C13-C15-C16
23	D	403	CLA	C6-C7-C8-C9
23	a	405[A]	CLA	C14-C13-C15-C16
33	d	412	LMG	C16-C17-C18-C19
23	C	503	CLA	C3-C5-C6-C7
23	b	616	CLA	C5-C6-C7-C8
23	C	513	CLA	CAA-CBA-CGA-O2A
32	A	419[A]	LHG	O8-C23-C24-C25
32	A	419[B]	LHG	C35-C36-C37-C38
23	B	615	CLA	C11-C12-C13-C15
23	C	507	CLA	C12-C13-C15-C16
23	a	405[A]	CLA	C11-C12-C13-C15
23	a	405[B]	CLA	C11-C12-C13-C15
23	b	607	CLA	C12-C13-C15-C16
23	c	502	CLA	C11-C12-C13-C15
23	c	508	CLA	C12-C13-C15-C16
23	B	602	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	b	613	CLA	C2B-C3B-CAB-CBB
25	D	404	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C30
25	Y	101	BCR	C23-C24-C25-C26
25	Y	101	BCR	C23-C24-C25-C30
25	y	101	BCR	C23-C24-C25-C30
33	m	101	LMG	C30-C31-C32-C33
23	B	613	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
26	b	620	SQD	C16-C17-C18-C19
31	T	101	LMT	O1'-C1-C2-C3
26	b	620	SQD	C33-C34-C35-C36
23	B	611	CLA	C8-C10-C11-C12
33	B	621	LMG	O6-C1-O1-C7
23	B	606	CLA	C16-C17-C18-C19
32	b	629[B]	LHG	C32-C33-C34-C35
33	Z	101	LMG	O7-C10-C11-C12
38	f	101	HEM	CAD-CBD-CGD-O1D
32	A	419[B]	LHG	C9-C10-C11-C12
34	B	622	HTG	C2'-C1'-S1-C1
34	c	521	HTG	C2'-C1'-S1-C1
35	C	519	DGD	CDA-CEA-CFA-CGA
23	A	404[A]	CLA	C4C-C3C-CAC-CBC
32	d	414[A]	LHG	C13-C14-C15-C16
33	d	412	LMG	C40-C41-C42-C43
23	B	613	CLA	CAA-CBA-CGA-O2A
32	L	101[A]	LHG	O7-C7-C8-C9
32	A	419[A]	LHG	C17-C18-C19-C20
35	C	518[A]	DGD	CAB-CBB-CCB-CDB
31	A	417	LMT	C9-C10-C11-C12
33	c	520	LMG	C39-C40-C41-C42
32	a	419[A]	LHG	O8-C23-C24-C25
32	b	629[A]	LHG	O7-C7-C8-C9
33	B	621	LMG	C14-C15-C16-C17
33	B	621	LMG	O10-C28-C29-C30
23	B	604	CLA	C4C-C3C-CAC-CBC
23	B	615	CLA	C4-C3-C5-C6
31	e	101	LMT	O1'-C1-C2-C3
35	c	516[B]	DGD	C1A-C2A-C3A-C4A
32	E	101[B]	LHG	C12-C13-C14-C15
33	c	519	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	a	412[B]	PL9	C33-C34-C36-C37
35	c	518	DGD	C6A-C7A-C8A-C9A
23	B	616	CLA	C16-C17-C18-C19
32	L	101[B]	LHG	C26-C27-C28-C29
32	d	414[B]	LHG	C18-C19-C20-C21
31	m	103	LMT	C2-C1-O1'-C1'
23	a	407	CLA	C15-C16-C17-C18
23	A	408	CLA	C11-C12-C13-C14
33	B	621	LMG	C21-C22-C23-C24
32	L	101[B]	LHG	O7-C7-C8-C9
32	b	629[B]	LHG	O7-C7-C8-C9
33	B	621	LMG	O1-C7-C8-C9
24	a	414[B]	PHO	C2C-C3C-CAC-CBC
23	B	610	CLA	C4B-C3B-CAB-CBB
23	C	502	CLA	C1A-C2A-CAA-CBA
23	C	505	CLA	C4B-C3B-CAB-CBB
32	d	414[A]	LHG	C18-C19-C20-C21
32	b	629[A]	LHG	C24-C25-C26-C27
23	C	507	CLA	C4-C3-C5-C6
29	A	414[B]	PL9	C12-C11-C9-C10
29	D	405[A]	PL9	C40-C39-C41-C42
35	c	516[B]	DGD	O6E-C1E-O5D-C6D
32	E	101[B]	LHG	O7-C7-C8-C9
35	C	519	DGD	O1G-C1A-C2A-C3A
33	c	520	LMG	C32-C33-C34-C35
33	c	520	LMG	O1-C7-C8-O7
25	d	405	BCR	C21-C22-C23-C24
23	A	404[B]	CLA	C15-C16-C17-C18
23	b	612	CLA	C10-C11-C12-C13
23	C	511	CLA	CAA-CBA-CGA-O2A
33	B	621	LMG	C29-C30-C31-C32
23	c	503	CLA	C8-C10-C11-C12
23	c	507	CLA	C8-C10-C11-C12
23	c	510	CLA	CAA-CBA-CGA-O2A
23	a	407	CLA	C8-C10-C11-C12
23	b	612	CLA	C8-C10-C11-C12
32	A	419[B]	LHG	C11-C12-C13-C14
23	c	503	CLA	C4-C3-C5-C6
26	a	409[B]	SQD	C11-C12-C13-C14
23	A	408	CLA	C2-C1-O2A-CGA
23	B	608	CLA	C2-C1-O2A-CGA
23	c	513	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
23	B	613	CLA	C11-C12-C13-C15
23	B	615	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	c	504	CLA	C12-C13-C15-C16
23	c	513	CLA	C12-C13-C15-C16
23	d	404	CLA	CBA-CGA-O2A-C1
33	d	412	LMG	C28-C29-C30-C31
32	D	407[B]	LHG	C28-C29-C30-C31
32	a	419[B]	LHG	O8-C23-C24-C25
32	D	406[B]	LHG	C28-C29-C30-C31
35	C	519	DGD	C9A-CAA-CBA-CCA
23	B	612	CLA	C8-C10-C11-C12
23	b	610	CLA	C13-C15-C16-C17
23	B	603	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C2A-CAA-CBA-CGA
23	C	503	CLA	C16-C17-C18-C20
29	D	405[B]	PL9	C11-C12-C13-C14
35	c	516[B]	DGD	CDB-CEB-CFB-CGB
31	T	101	LMT	C4-C5-C6-C7
32	b	629[B]	LHG	C31-C32-C33-C34
38	f	101	HEM	CAD-CBD-CGD-O2D
32	E	101[A]	LHG	O7-C7-C8-C9
35	c	516[A]	DGD	O2G-C1B-C2B-C3B
26	a	410	SQD	C18-C19-C20-C21
26	a	409[A]	SQD	C10-C11-C12-C13
33	Z	101	LMG	O9-C10-C11-C12
35	c	516[B]	DGD	C7B-C8B-C9B-CAB
23	b	613	CLA	CAA-CBA-CGA-O2A
29	A	414[B]	PL9	C46-C47-C48-C49
32	b	629[A]	LHG	O9-C7-C8-C9
31	A	417	LMT	C2B-C1B-O1B-C4'
23	b	602	CLA	C2A-CAA-CBA-CGA
23	B	601	CLA	C11-C12-C13-C14
23	B	615	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	a	405[B]	CLA	C6-C7-C8-C9
23	b	607	CLA	C14-C13-C15-C16
23	c	513	CLA	C14-C13-C15-C16
32	A	419[B]	LHG	O10-C23-C24-C25
23	C	513	CLA	CAA-CBA-CGA-O1A
33	c	519	LMG	O9-C10-C11-C12
24	A	416[A]	PHO	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
35	C	518[A]	DGD	C3A-C4A-C5A-C6A
23	B	603	CLA	C2-C3-C5-C6
23	B	602	CLA	C8-C10-C11-C12
26	f	102	SQD	O5-C5-C6-S
32	A	419[A]	LHG	O10-C23-C24-C25
32	a	419[A]	LHG	O10-C23-C24-C25
31	B	630	LMT	C1-C2-C3-C4
23	B	612	CLA	CAA-CBA-CGA-O2A
32	D	406[A]	LHG	C28-C29-C30-C31
23	B	613	CLA	CAA-CBA-CGA-O1A
23	b	601	CLA	CAA-CBA-CGA-O1A
32	a	419[B]	LHG	O10-C23-C24-C25
26	a	410	SQD	C45-C44-O6-C1
35	C	517[A]	DGD	C5D-C6D-O5D-C1E
35	C	517[B]	DGD	C5D-C6D-O5D-C1E
31	e	101	LMT	C2B-C1B-O1B-C4'
32	E	101[B]	LHG	O9-C7-C8-C9
23	b	612	CLA	CAA-CBA-CGA-O2A
32	E	101[B]	LHG	O8-C23-C24-C25
23	C	508	CLA	C2A-CAA-CBA-CGA
32	E	101[A]	LHG	C11-C10-C9-C8
33	C	520	LMG	O1-C7-C8-C9
33	z	101	LMG	C20-C21-C22-C23
35	C	519	DGD	O1A-C1A-C2A-C3A
29	d	406[A]	PL9	C11-C12-C13-C14
32	L	101[A]	LHG	O9-C7-C8-C9
32	b	629[B]	LHG	O9-C7-C8-C9
23	B	605	CLA	CAD-CBD-CGD-O2D
23	C	505	CLA	CAD-CBD-CGD-O2D
23	b	605	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O2D
24	A	407[A]	PHO	CAD-CBD-CGD-O2D
24	a	406[A]	PHO	CAD-CBD-CGD-O2D
35	c	516[B]	DGD	CBA-CCA-CDA-CEA
32	L	101[B]	LHG	O9-C7-C8-C9
31	B	630	LMT	C7-C8-C9-C10
23	c	512	CLA	CAA-CBA-CGA-O2A
35	c	516[A]	DGD	C1A-C2A-C3A-C4A
35	c	516[A]	DGD	CBA-CCA-CDA-CEA
23	c	510	CLA	CAA-CBA-CGA-O1A
23	b	604	CLA	C4C-C3C-CAC-CBC
26	b	620	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
32	D	407[A]	LHG	O8-C23-C24-C25
35	C	518[B]	DGD	O2G-C1B-C2B-C3B
29	d	406[B]	PL9	C28-C29-C31-C32
26	A	410[B]	SQD	C18-C19-C20-C21
32	E	101[B]	LHG	C11-C10-C9-C8
35	c	517[B]	DGD	O6D-C5D-C6D-O5D
32	E	101[A]	LHG	O8-C23-C24-C25
32	d	408[B]	LHG	O8-C23-C24-C25
35	C	518[A]	DGD	O2G-C1B-C2B-C3B
31	A	417	LMT	C4B-C5B-C6B-O6B
32	d	407[B]	LHG	C16-C17-C18-C19

There are no ring outliers.

175 monomers are involved in 370 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	620	SQD	2	0
29	A	414[B]	PL9	11	0
38	E	102	HEM	1	0
27	a	418	GOL	3	0
25	k	101	BCR	2	0
32	D	406[A]	LHG	2	0
23	b	609	CLA	5	0
27	v	202[B]	GOL	2	0
32	d	408[A]	LHG	10	0
23	C	503	CLA	2	0
32	E	101[A]	LHG	4	0
23	C	504	CLA	4	0
25	T	102	BCR	7	0
32	d	407[A]	LHG	3	0
23	d	403[A]	CLA	2	0
23	B	613	CLA	4	0
31	B	631	LMT	1	0
23	A	404[B]	CLA	2	0
23	c	501	CLA	2	0
23	c	506	CLA	3	0
27	O	303	GOL	3	0
33	B	621	LMG	1	0
24	A	416[A]	PHO	1	0
31	A	417	LMT	1	0
23	B	614	CLA	2	0
23	b	607	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	a	414[A]	PHO	2	0
25	b	618	BCR	3	0
23	d	402[A]	CLA	2	0
31	t	101	LMT	2	0
34	B	623	HTG	1	0
25	b	619	BCR	5	0
23	C	507	CLA	5	0
27	B	627	GOL	1	0
23	C	508	CLA	2	0
26	b	620	SQD	4	0
27	a	417	GOL	2	0
32	D	406[B]	LHG	2	0
23	B	604	CLA	1	0
23	b	601	CLA	2	0
32	d	408[B]	LHG	9	0
32	E	101[B]	LHG	4	0
31	M	101	LMT	1	0
23	c	513	CLA	2	0
25	A	409	BCR	2	0
23	B	612	CLA	2	0
33	z	101	LMG	2	0
25	h	101	BCR	4	0
32	d	407[B]	LHG	2	0
23	d	403[B]	CLA	2	0
23	B	601	CLA	5	0
23	c	505	CLA	5	0
31	B	630	LMT	1	0
23	C	512	CLA	3	0
26	a	410	SQD	2	0
23	b	605	CLA	6	0
23	B	610	CLA	1	0
24	A	416[B]	PHO	1	0
23	c	508	CLA	8	0
24	a	414[B]	PHO	1	0
35	C	517[A]	DGD	2	0
25	K	102	BCR	1	0
23	C	509	CLA	3	0
23	b	616	CLA	1	0
23	d	402[B]	CLA	2	0
23	a	407	CLA	4	0
23	b	614	CLA	1	0
35	c	517[A]	DGD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	511	CLA	4	0
23	c	502	CLA	2	0
33	d	412	LMG	3	0
23	a	404[A]	CLA	3	0
23	b	602	CLA	1	0
27	l	801[A]	GOL	1	0
26	A	410[A]	SQD	2	0
33	Z	101	LMG	1	0
31	T	101	LMT	1	0
23	C	506	CLA	5	0
25	C	515	BCR	2	0
33	c	519	LMG	1	0
31	b	621	LMT	1	0
23	b	615	CLA	2	0
34	D	410	HTG	1	0
23	D	402[A]	CLA	3	0
25	t	102	BCR	5	0
25	H	101	BCR	3	0
23	C	510	CLA	3	0
23	a	405[A]	CLA	2	0
34	B	625	HTG	1	0
34	d	411	HTG	1	0
35	C	517[B]	DGD	1	0
26	F	102	SQD	2	0
31	m	103	LMT	2	0
23	c	507	CLA	2	0
32	a	419[A]	LHG	4	0
32	b	629[B]	LHG	1	0
34	b	622	HTG	2	0
35	c	517[B]	DGD	1	0
33	C	521	LMG	4	0
34	c	521	HTG	1	0
23	B	606	CLA	4	0
25	B	619	BCR	1	0
35	c	518	DGD	3	0
23	a	404[B]	CLA	3	0
27	l	801[B]	GOL	1	0
26	A	410[B]	SQD	2	0
23	A	406[A]	CLA	1	0
32	d	414[A]	LHG	1	0
24	A	407[A]	PHO	2	0
27	D	412	GOL	2	0

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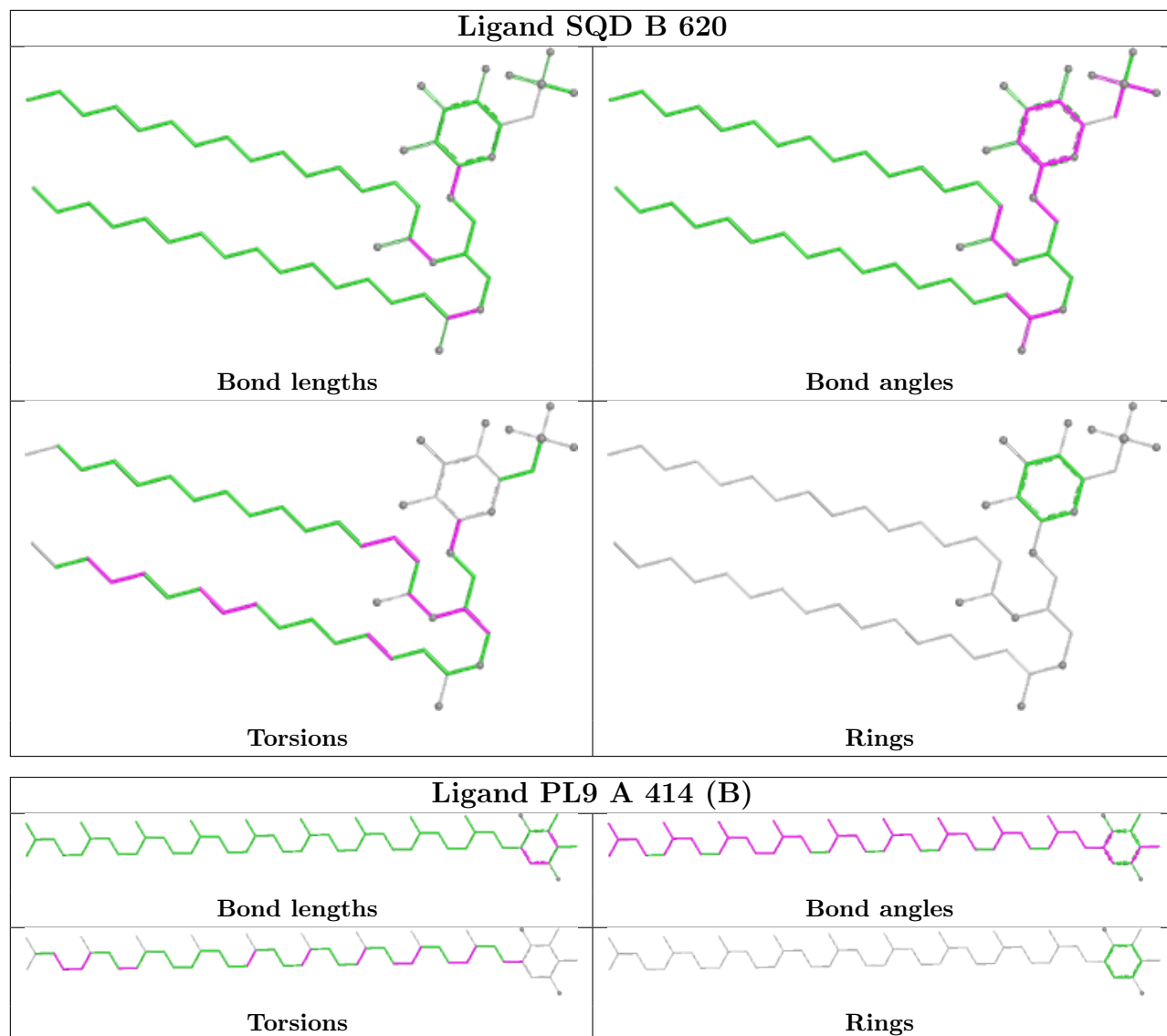
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29	a	412[A]	PL9	4	0
23	D	402[B]	CLA	4	0
27	O	302	GOL	1	0
35	C	519	DGD	2	0
26	a	409[A]	SQD	4	0
25	Y	101	BCR	2	0
23	b	612	CLA	2	0
25	b	617	BCR	1	0
25	c	515	BCR	2	0
34	B	622	HTG	2	0
23	B	615	CLA	4	0
23	b	611	CLA	1	0
35	C	518[A]	DGD	2	0
35	c	516[A]	DGD	2	0
23	a	405[B]	CLA	2	0
23	b	603	CLA	1	0
23	B	605	CLA	3	0
31	a	416	LMT	1	0
32	a	419[B]	LHG	5	0
23	d	404	CLA	3	0
31	A	420	LMT	1	0
32	D	407[A]	LHG	6	0
34	b	625	HTG	1	0
23	A	405[A]	CLA	4	0
23	C	514	CLA	3	0
25	C	516	BCR	1	0
23	c	509	CLA	3	0
27	b	628	GOL	2	0
23	C	502	CLA	5	0
32	A	419[A]	LHG	1	0
23	A	406[B]	CLA	2	0
32	d	414[B]	LHG	1	0
23	b	606	CLA	1	0
23	c	511	CLA	6	0
24	A	407[B]	PHO	1	0
29	a	412[B]	PL9	5	0
29	A	414[A]	PL9	10	0
23	C	513	CLA	4	0
23	b	604	CLA	2	0
23	B	609	CLA	3	0
26	a	409[B]	SQD	5	0
40	V	201	HEC	1	0

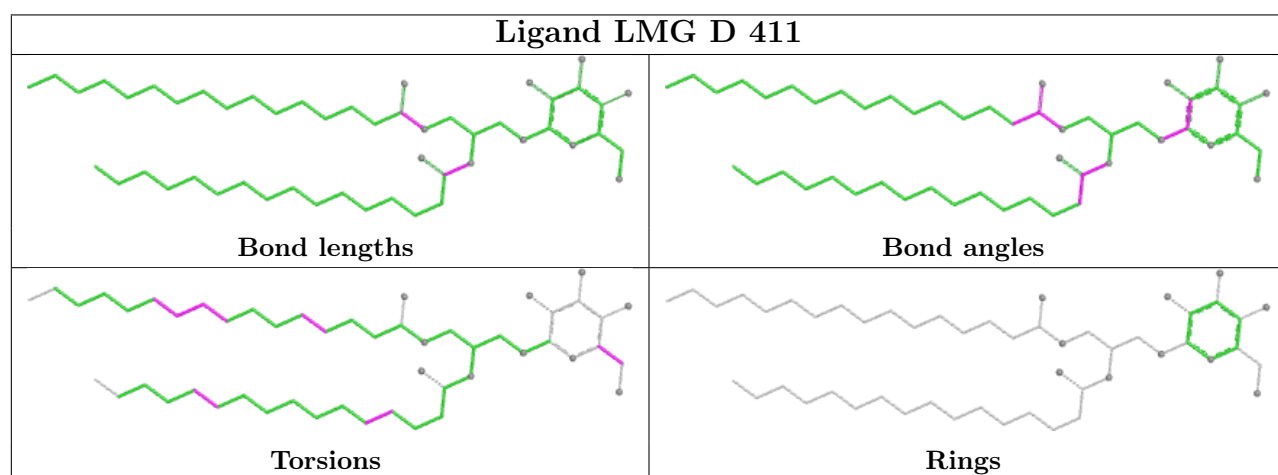
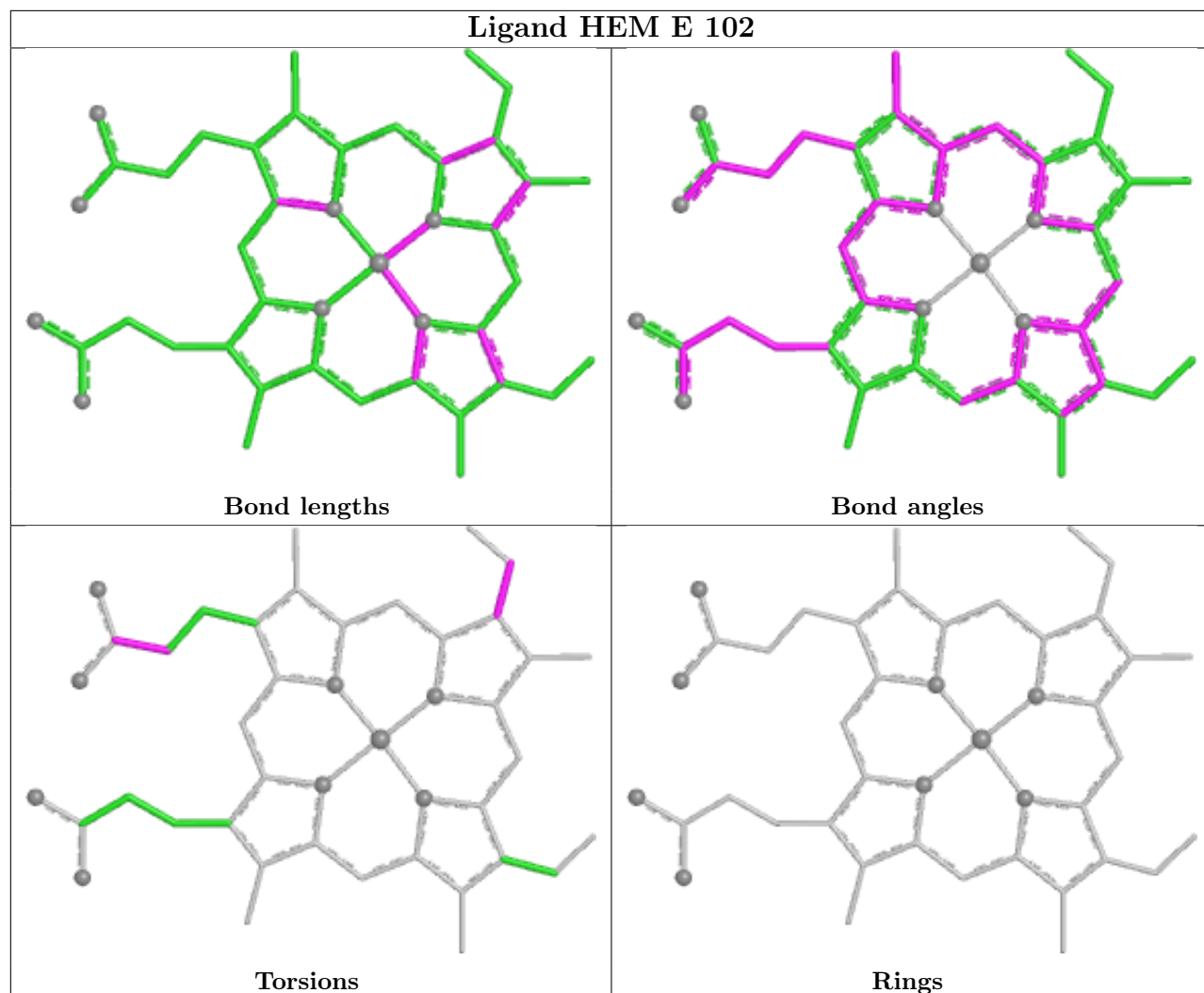
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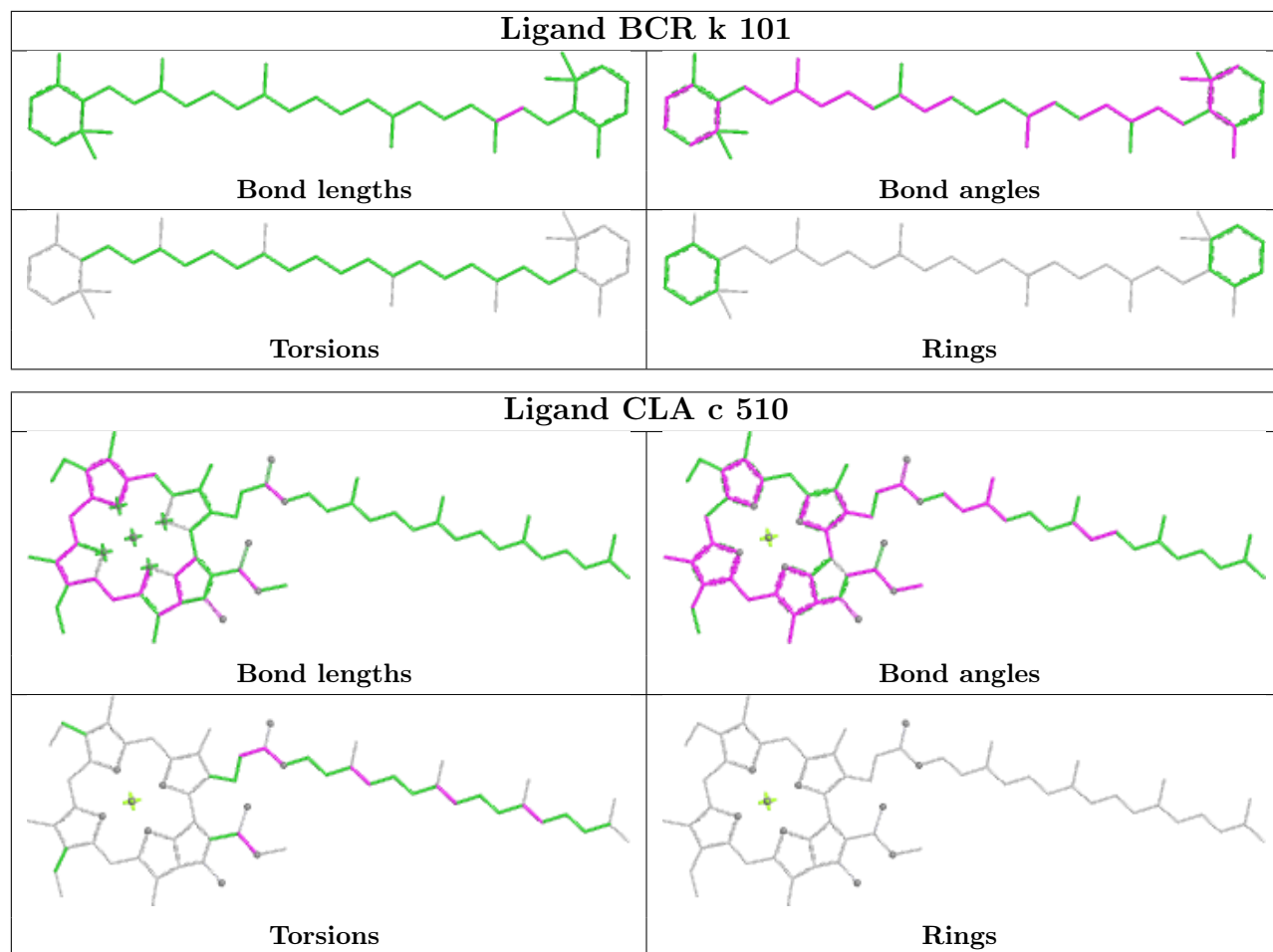
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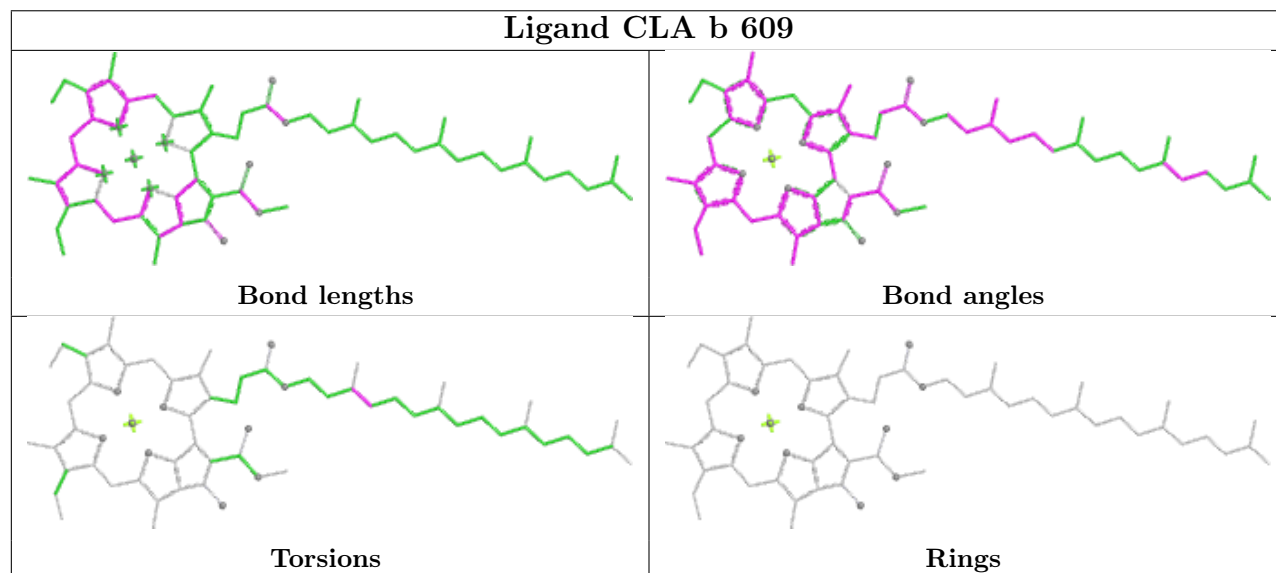
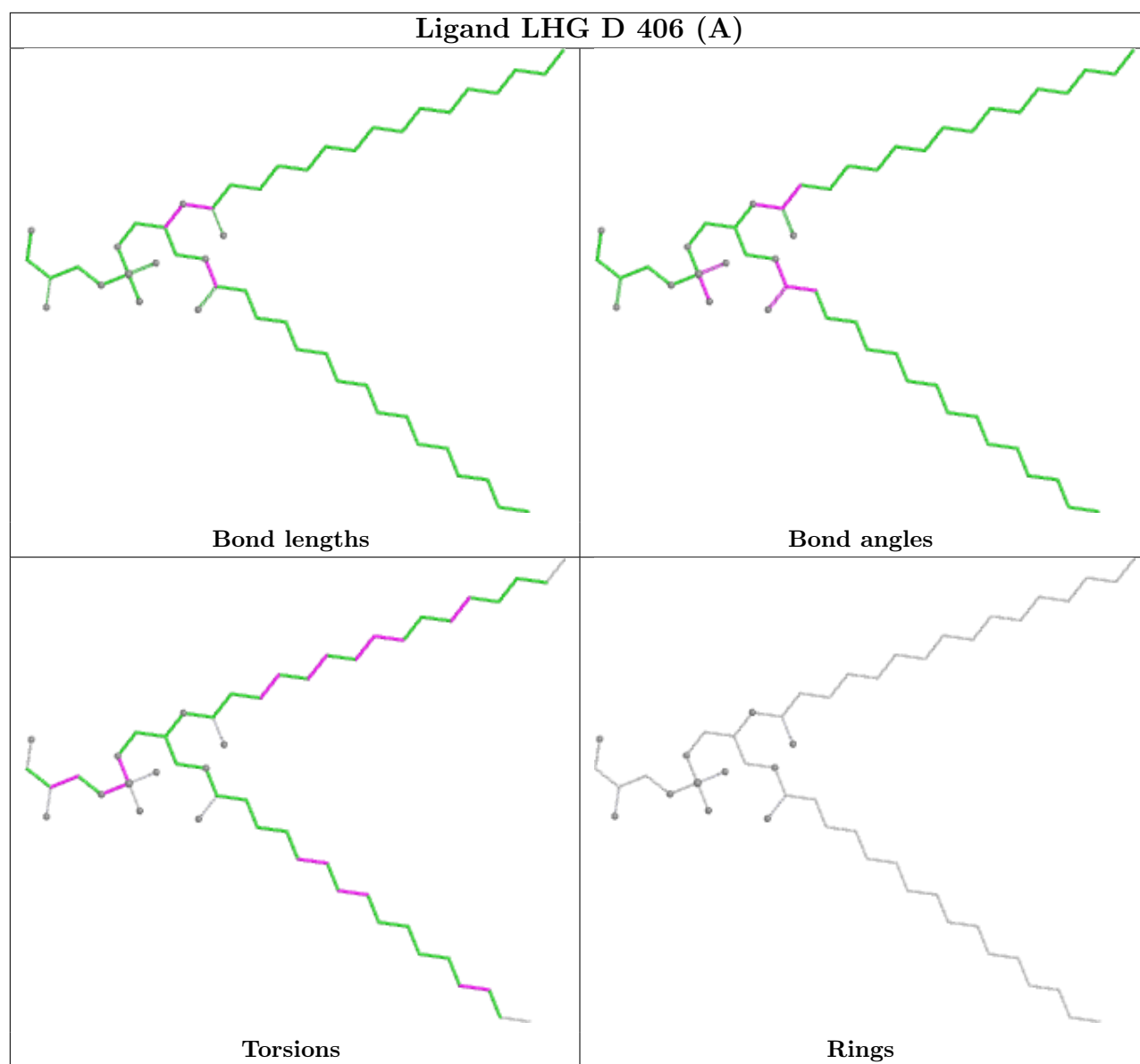
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	H	102	DGD	2	0
25	B	617	BCR	2	0
23	B	616	CLA	4	0
23	c	503	CLA	3	0
27	v	202[A]	GOL	1	0
25	D	404	BCR	1	0
27	A	418	GOL	2	0
23	c	504	CLA	2	0
31	e	101	LMT	1	0
35	c	516[B]	DGD	2	0
25	y	101	BCR	2	0
23	A	408	CLA	4	0
23	b	613	CLA	2	0
25	c	514	BCR	3	0
32	D	407[B]	LHG	3	0
23	A	405[B]	CLA	4	0
25	B	618	BCR	4	0
23	C	505	CLA	1	0
23	A	404[A]	CLA	5	0
33	c	520	LMG	1	0
32	A	419[B]	LHG	1	0
24	a	406[B]	PHO	1	0
23	c	512	CLA	7	0

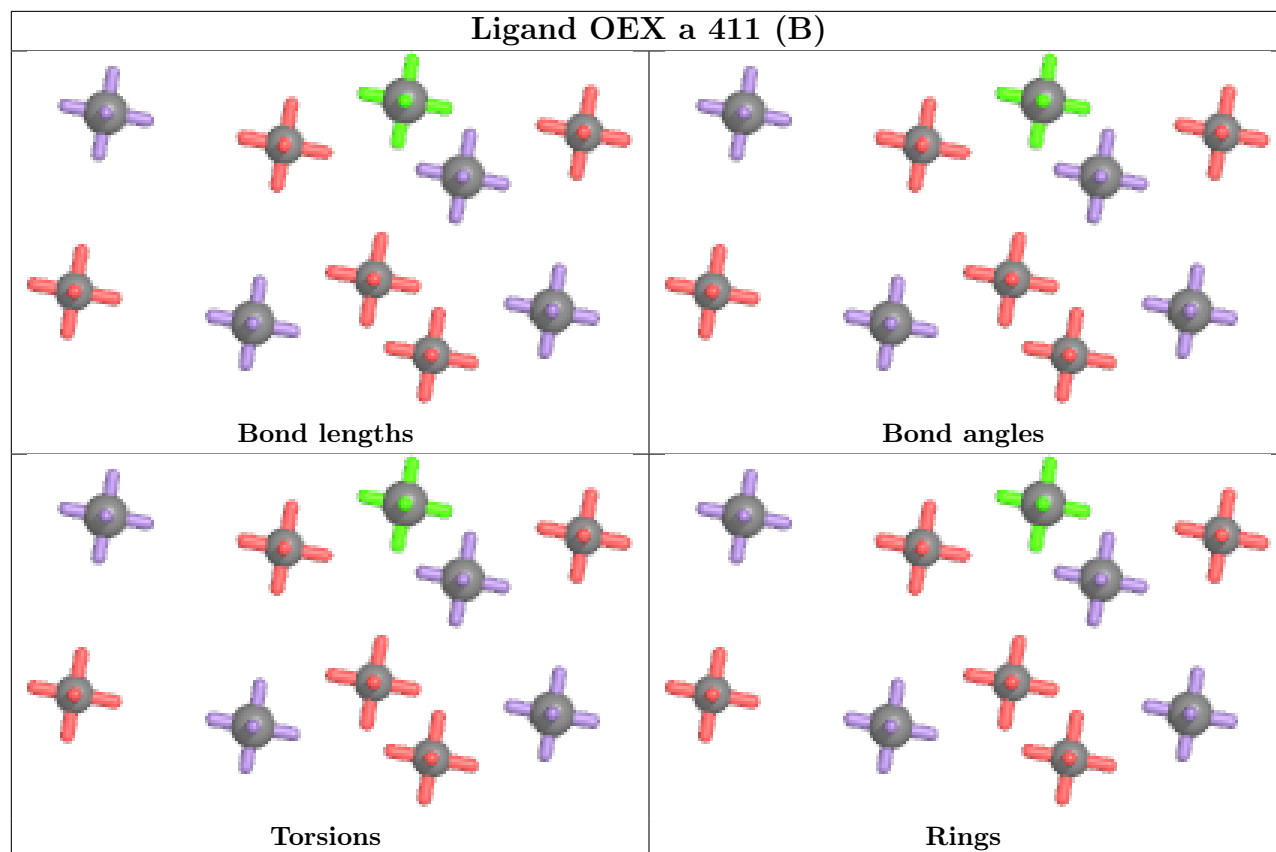
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

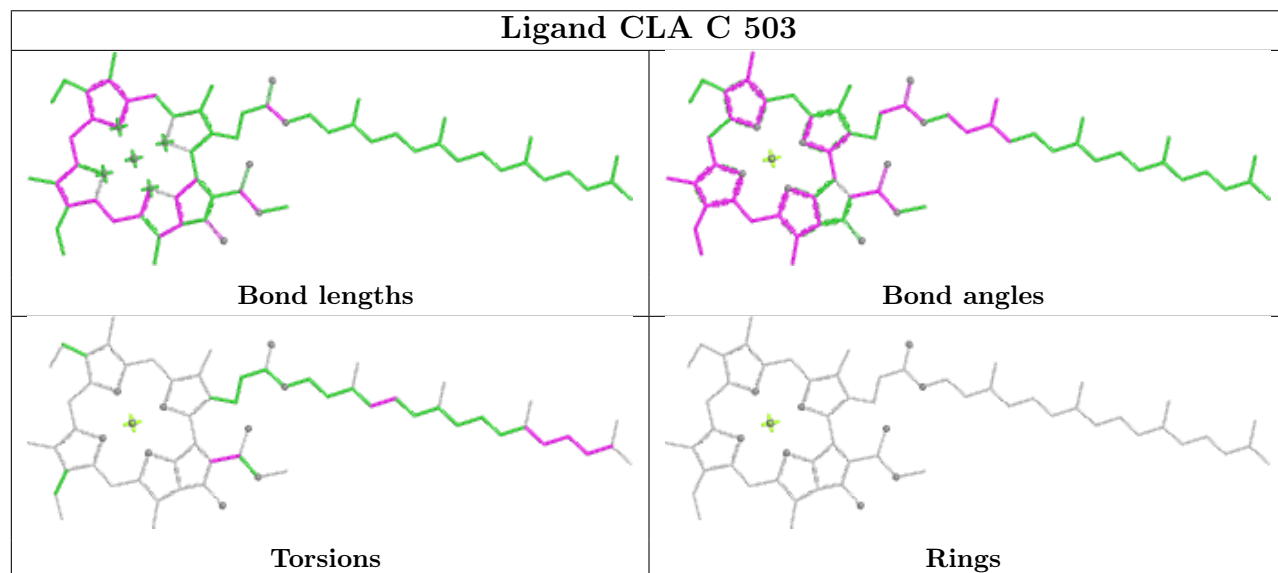
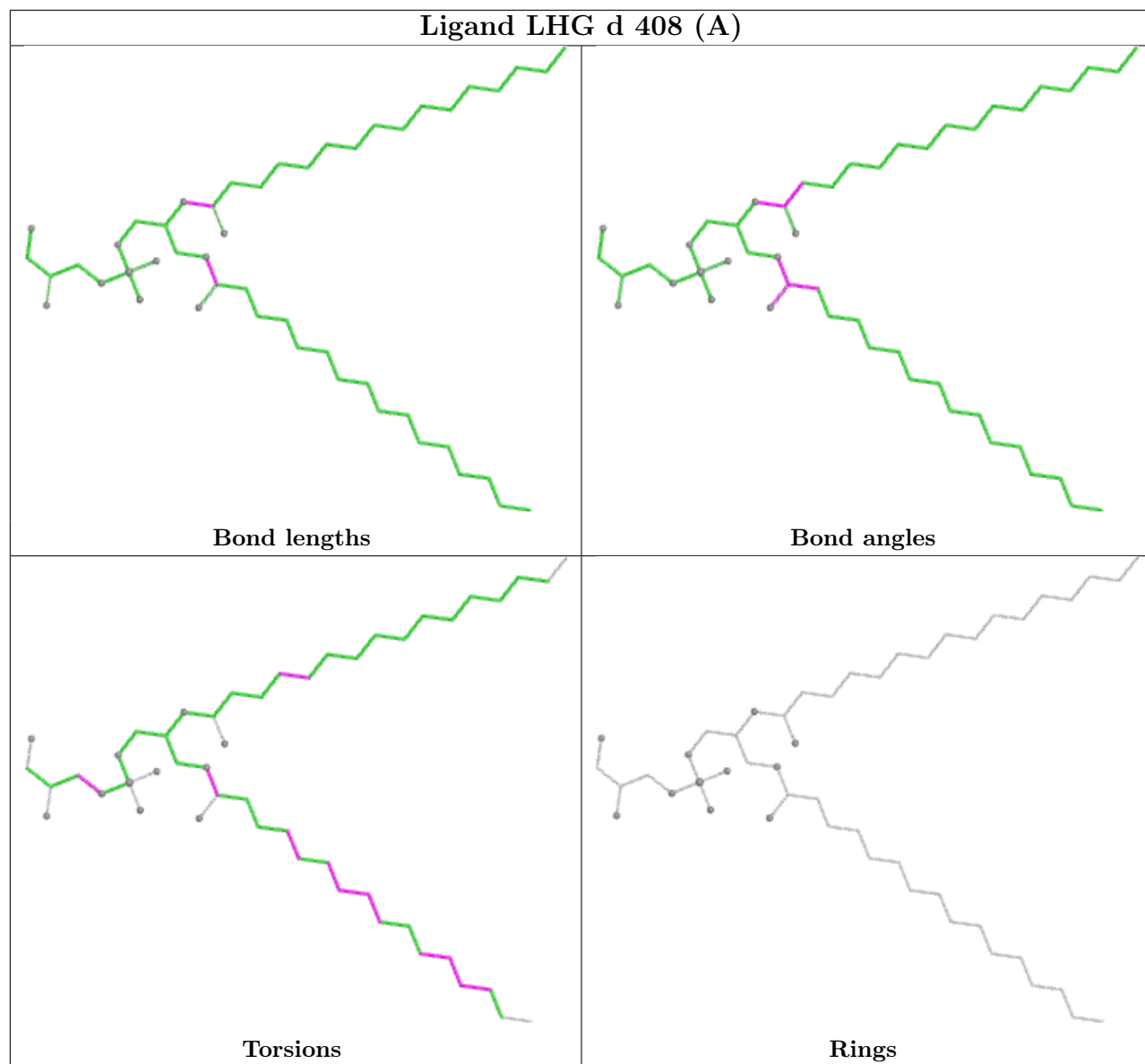


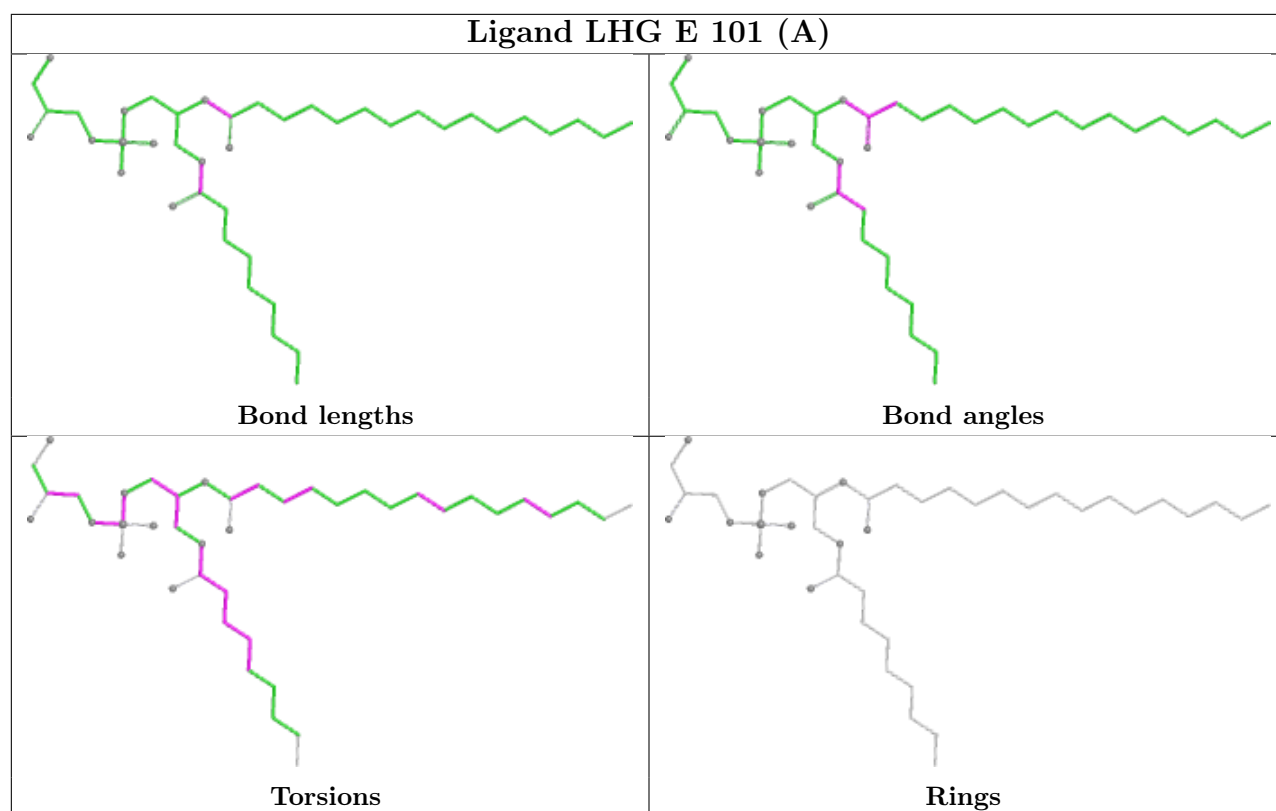


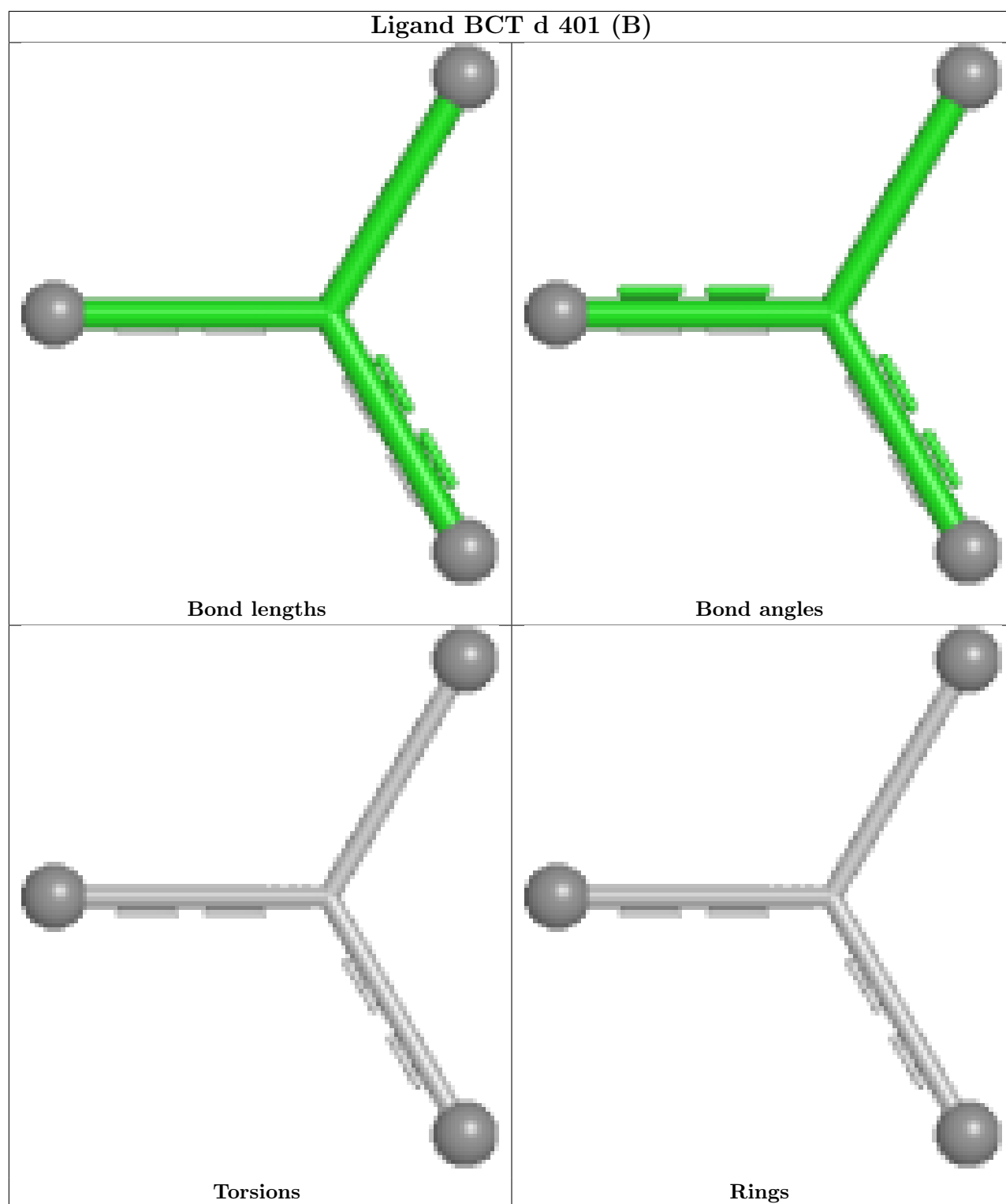


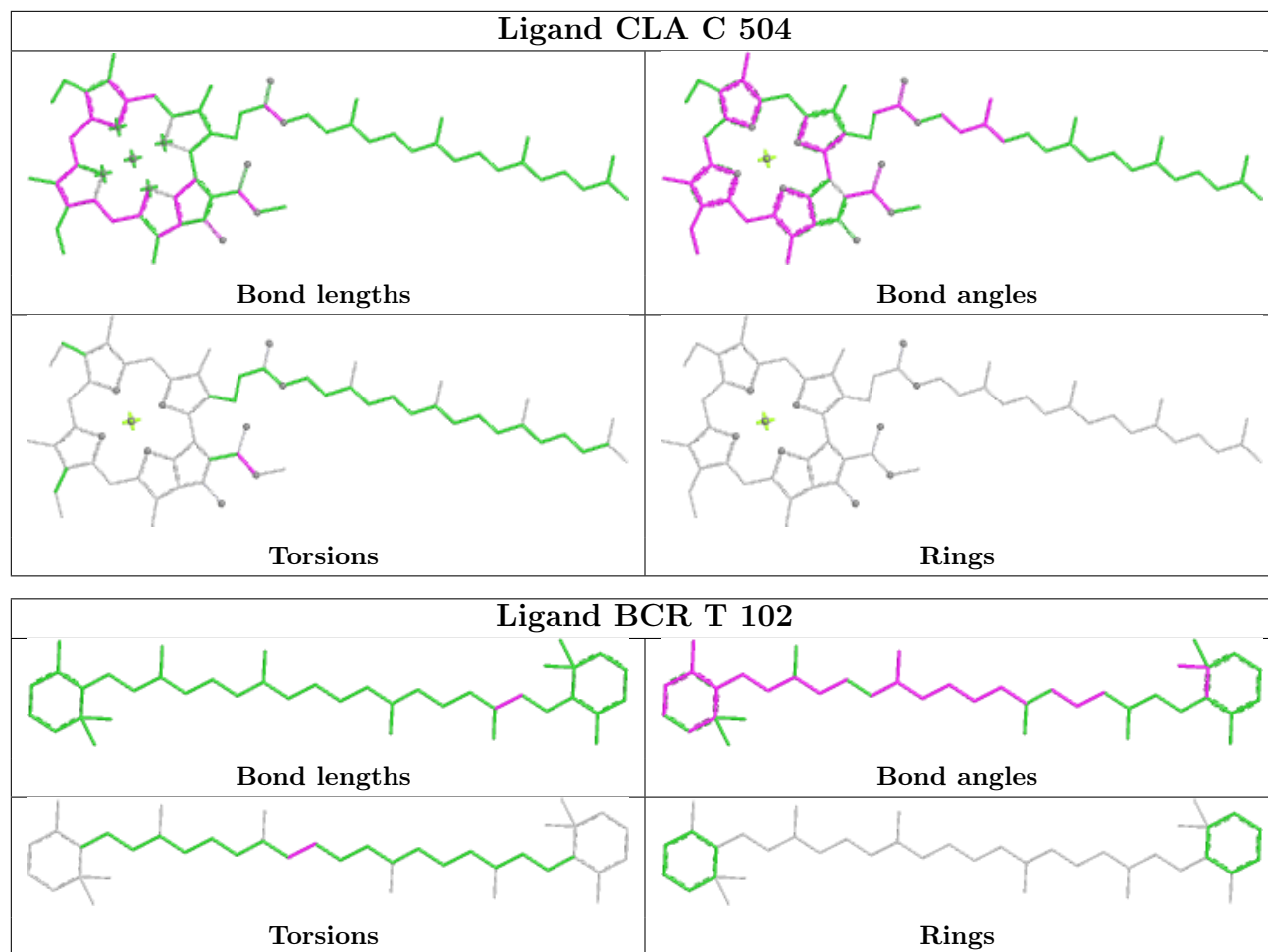


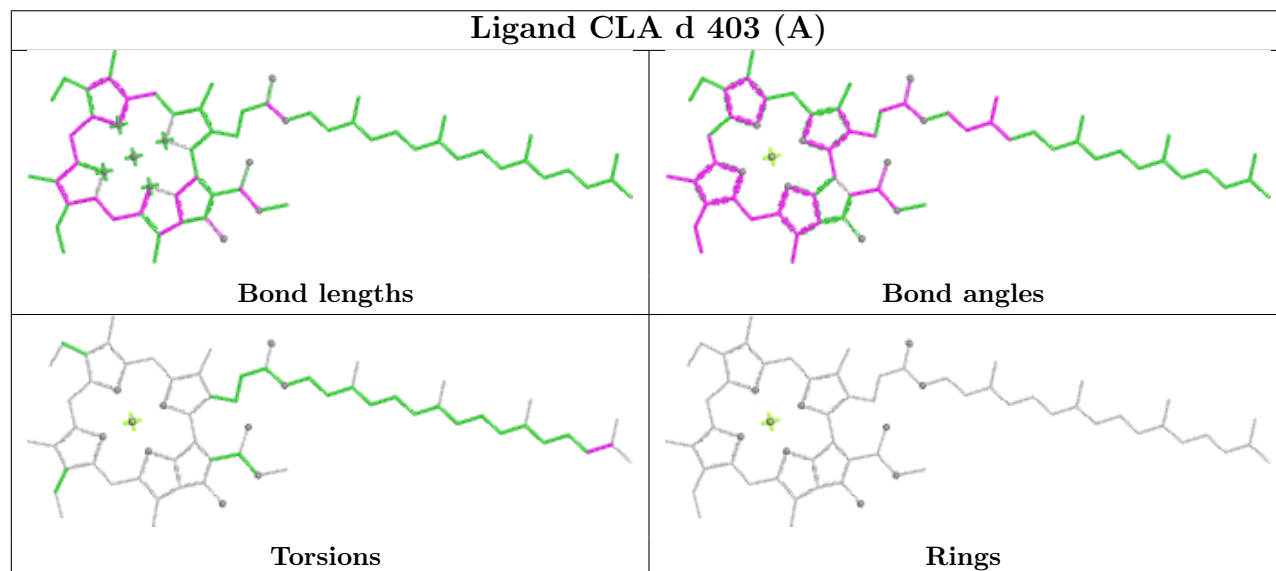
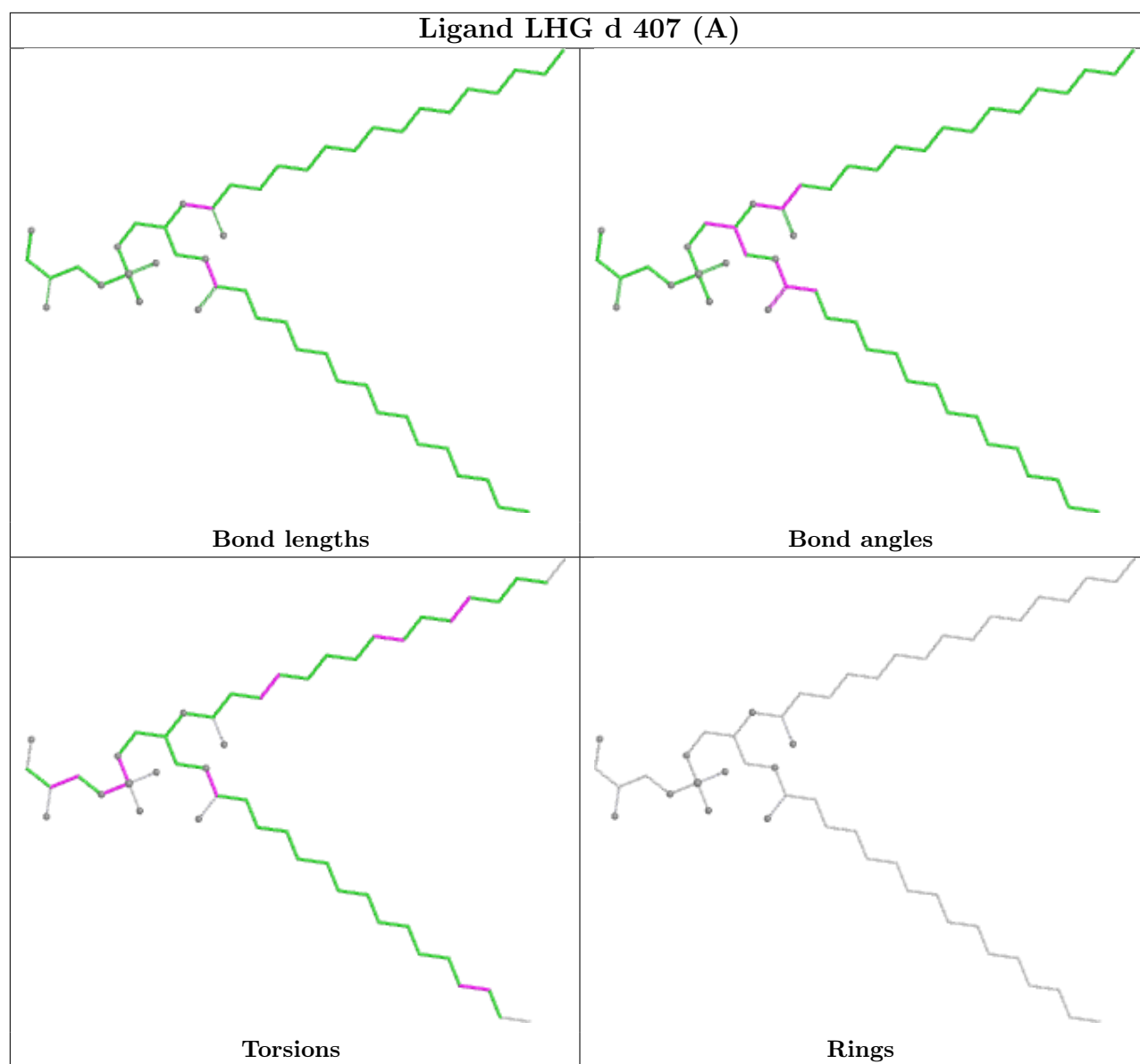




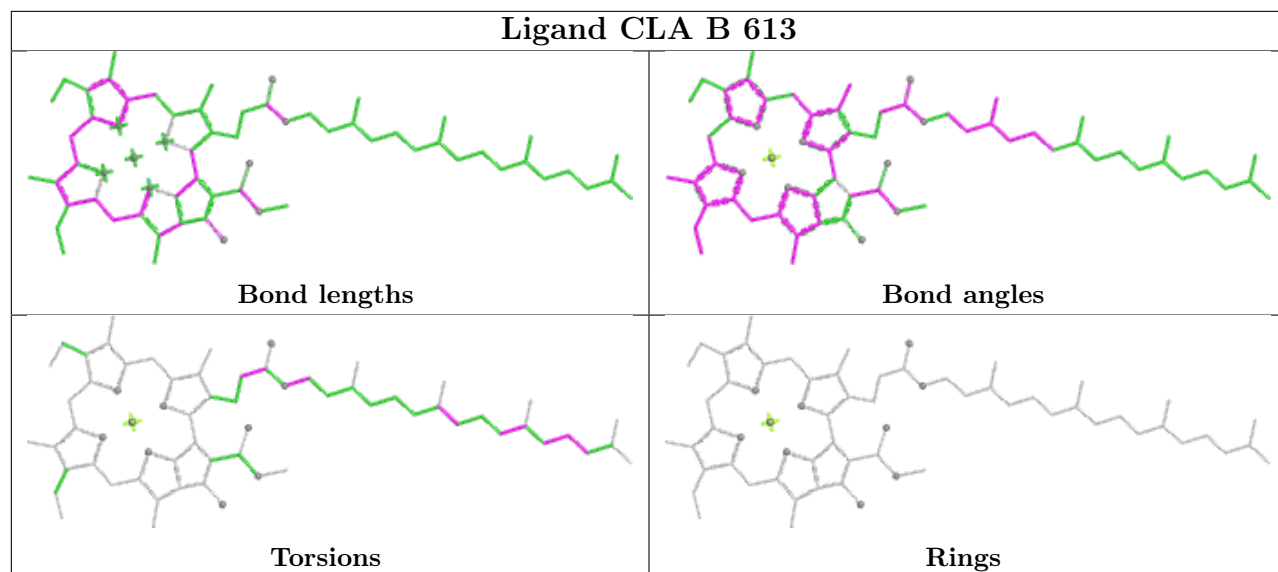




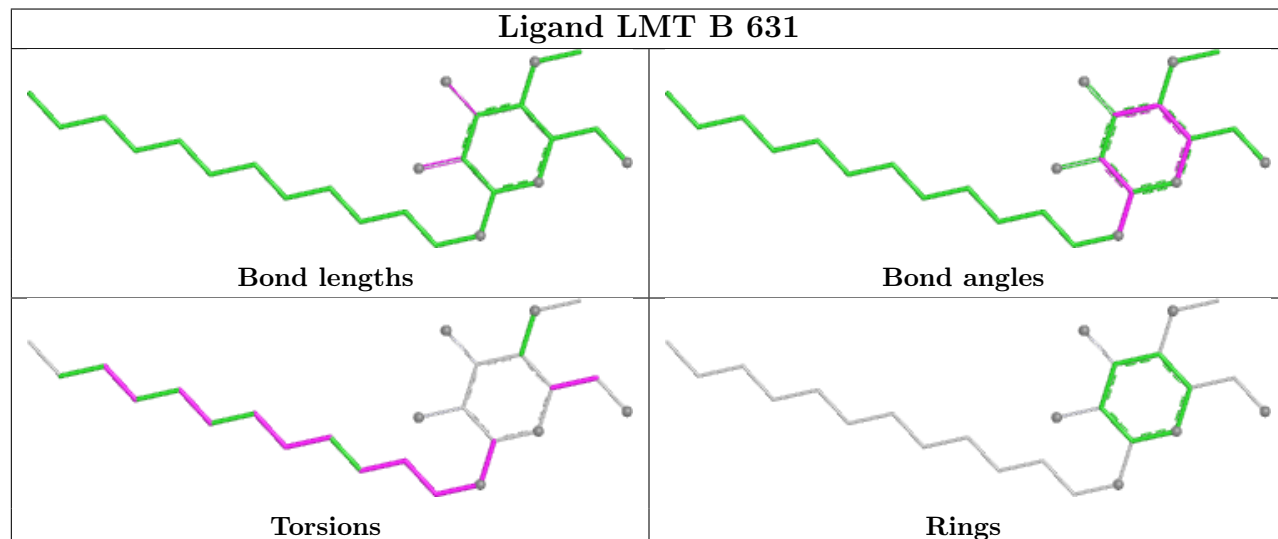




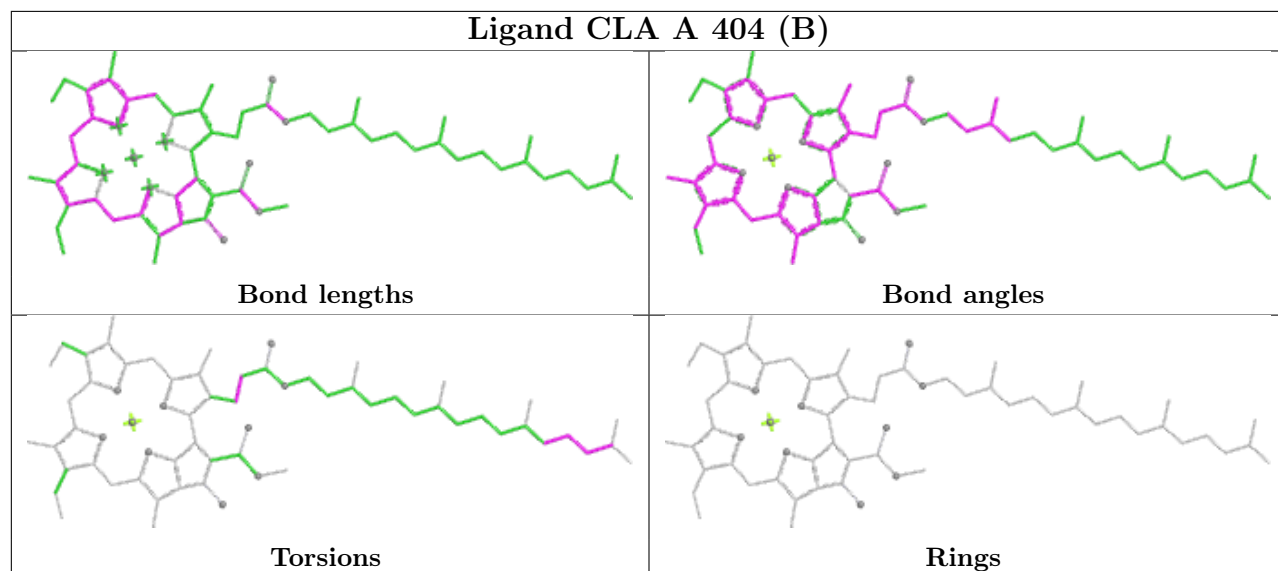
Ligand CLA B 613



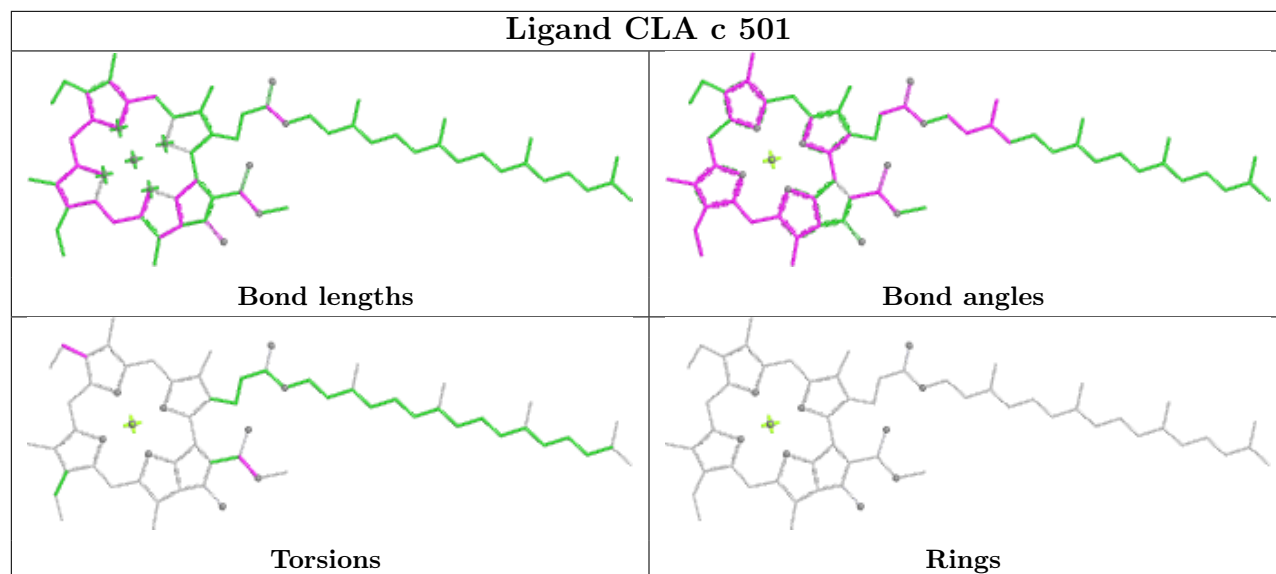
Ligand LMT B 631



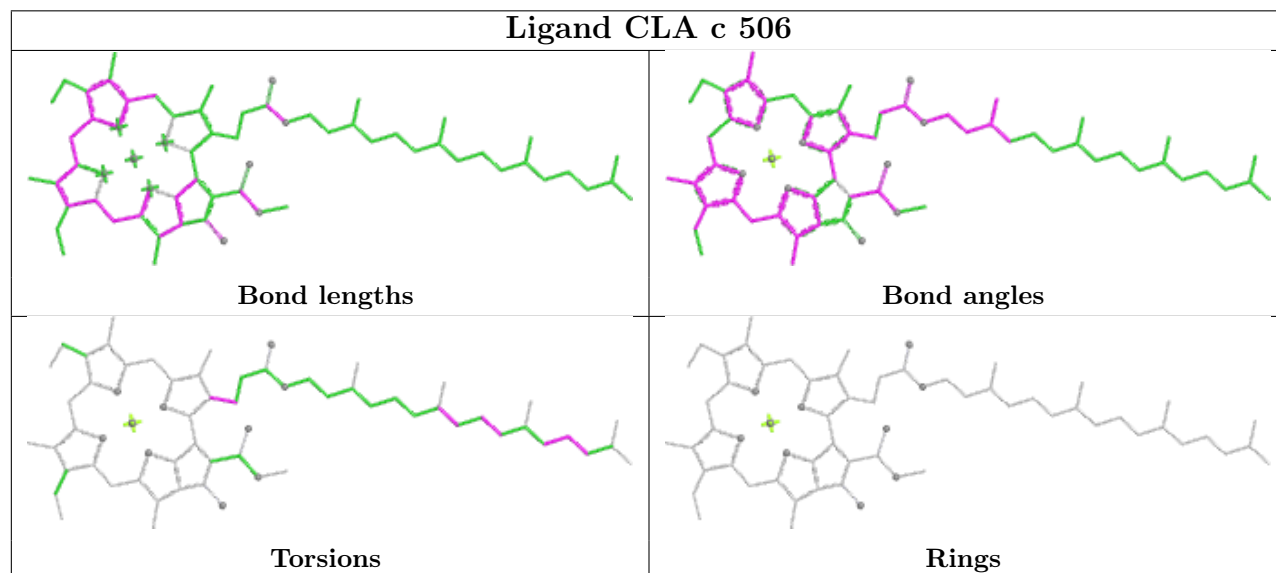
Ligand CLA A 404 (B)



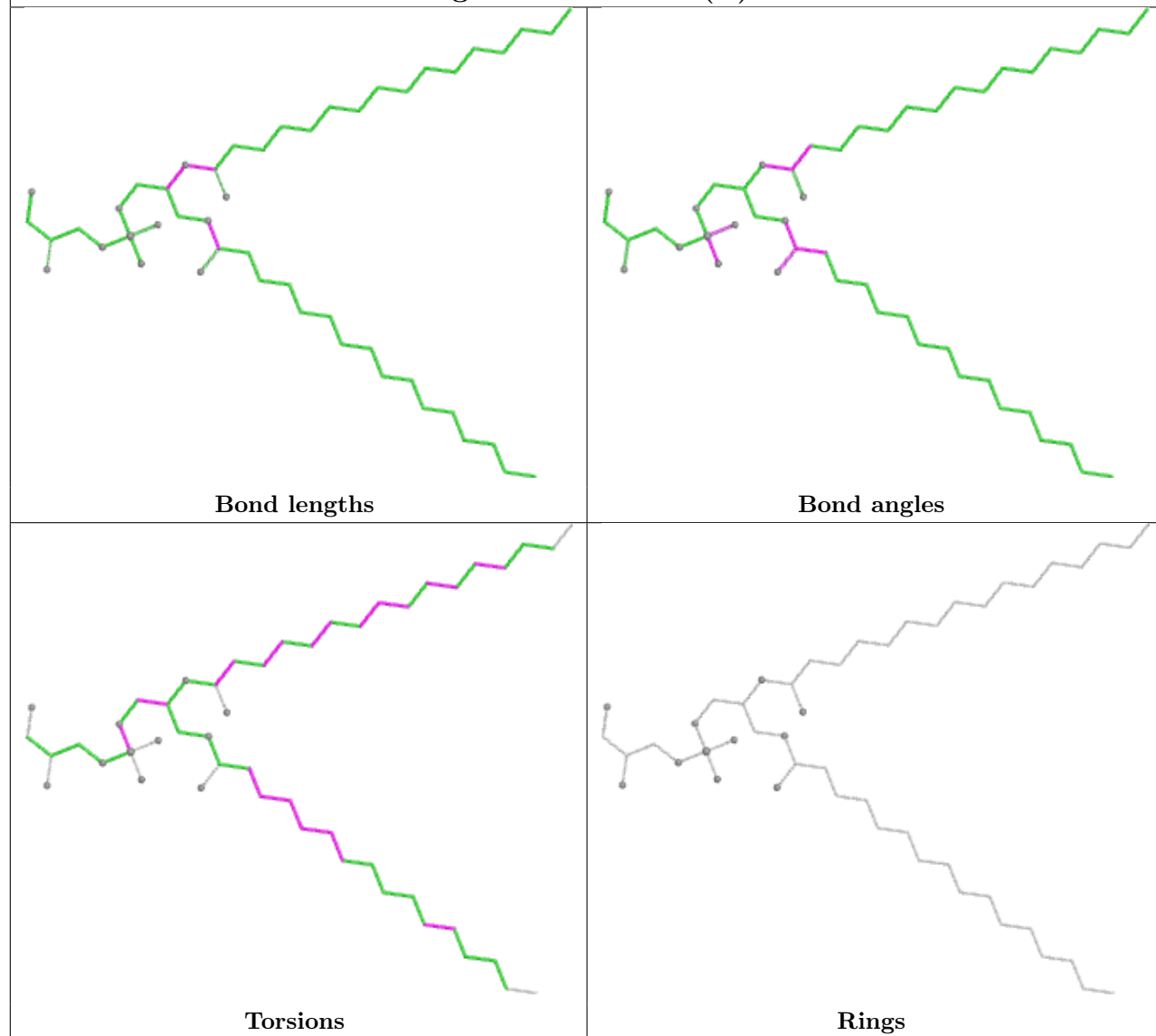
Ligand CLA c 501



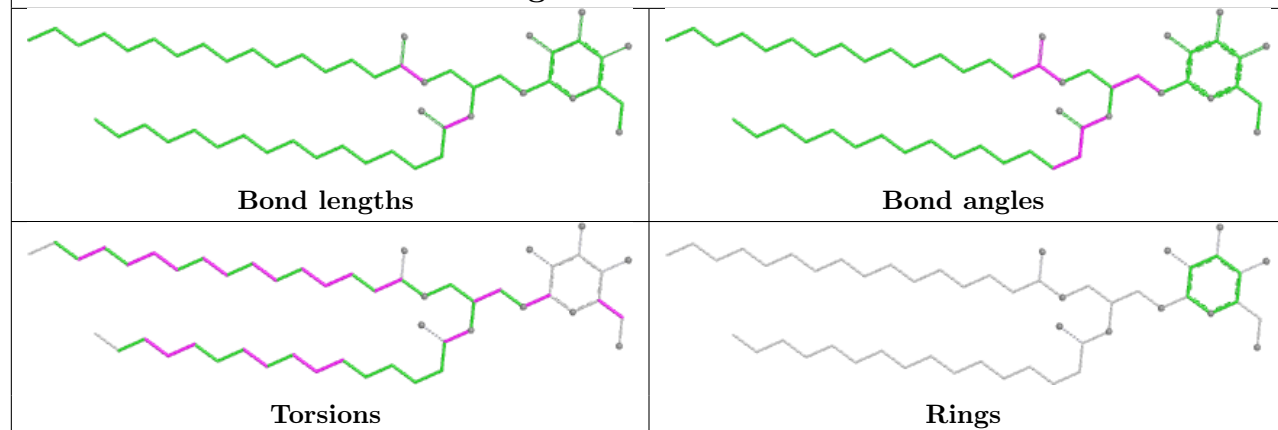
Ligand CLA c 506



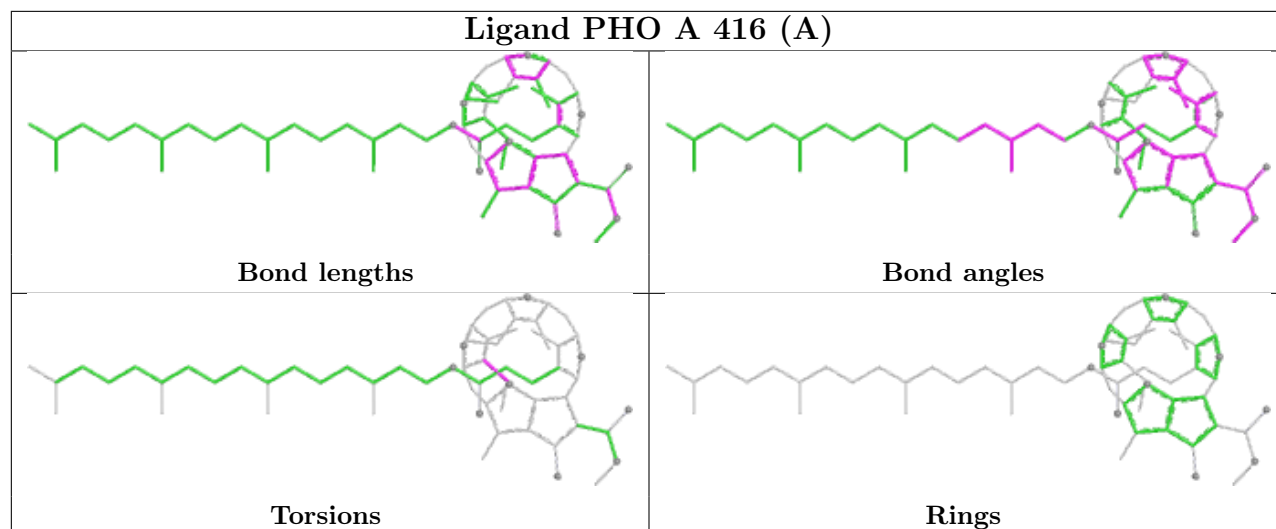
Ligand LHG L 101 (B)



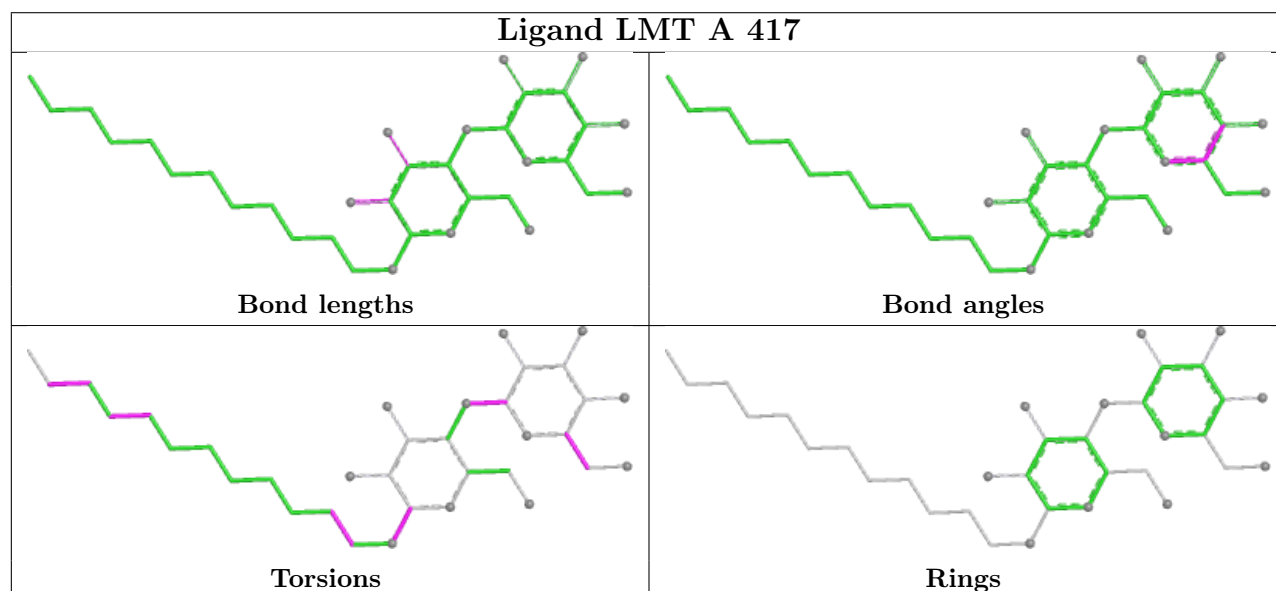
Ligand LMG B 621



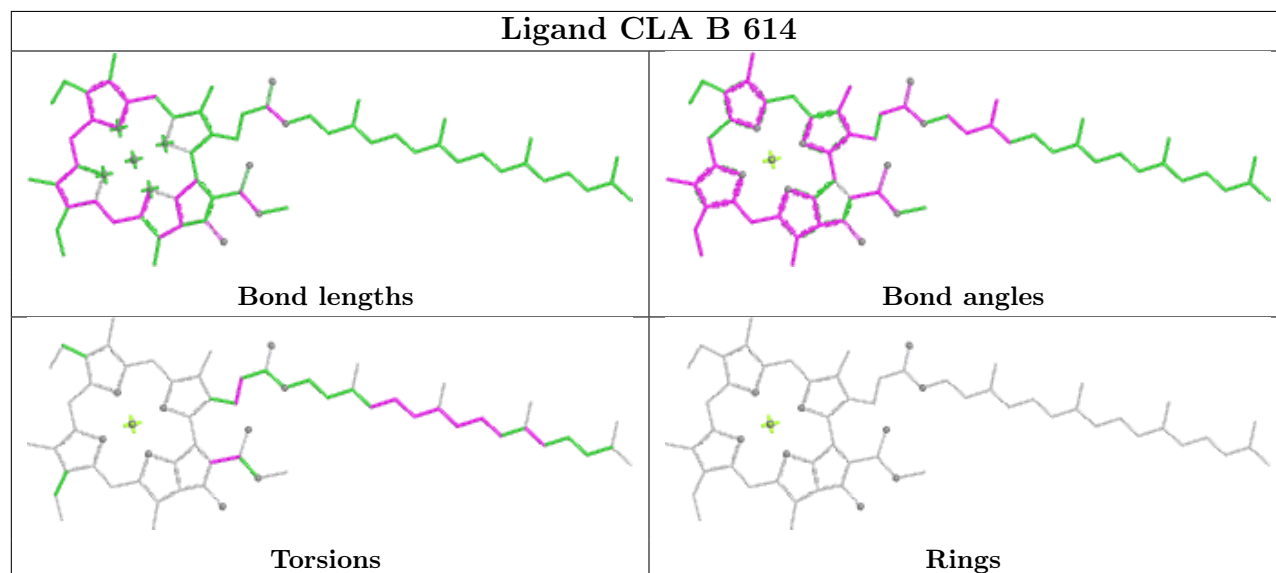
Ligand PHO A 416 (A)



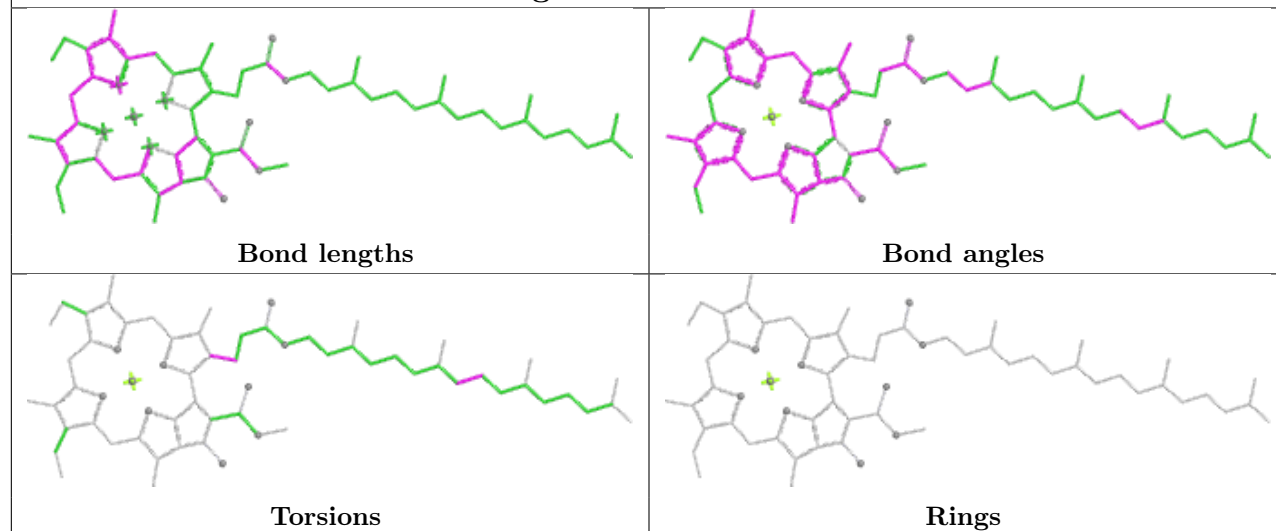
Ligand LMT A 417



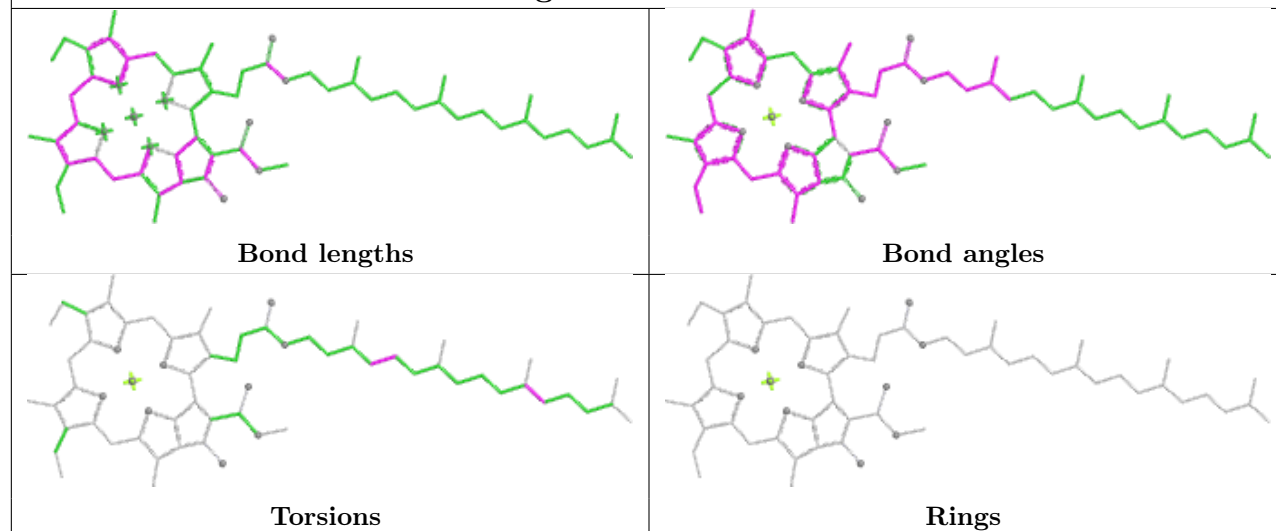
Ligand CLA B 614



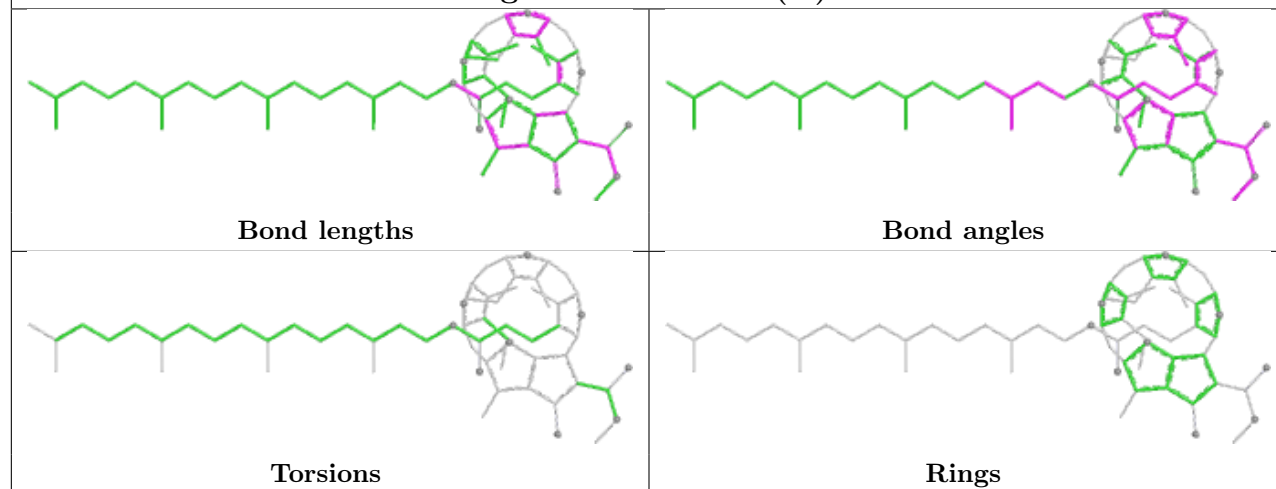
Ligand CLA B 611



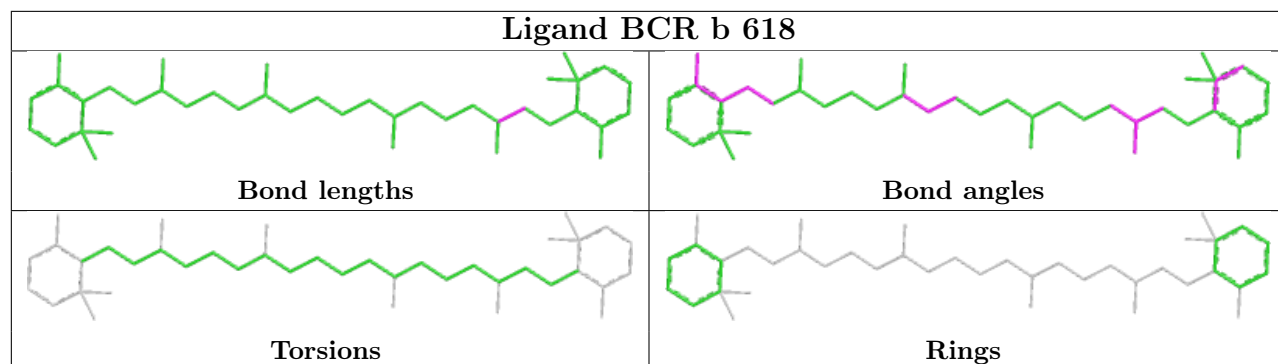
Ligand CLA b 607



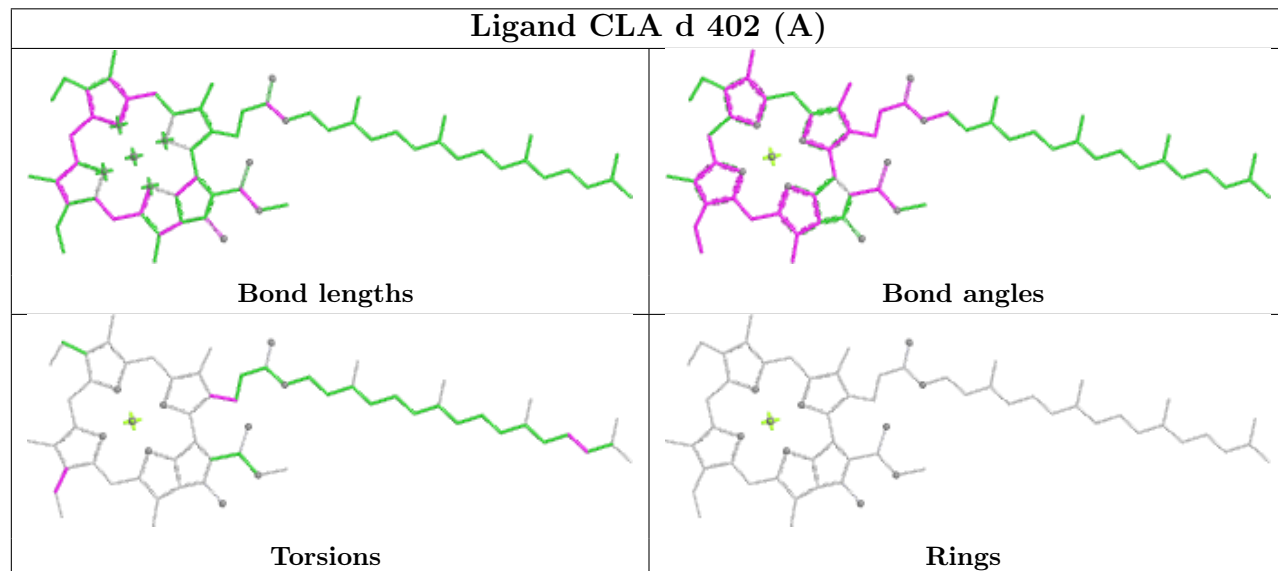
Ligand PHO a 414 (A)



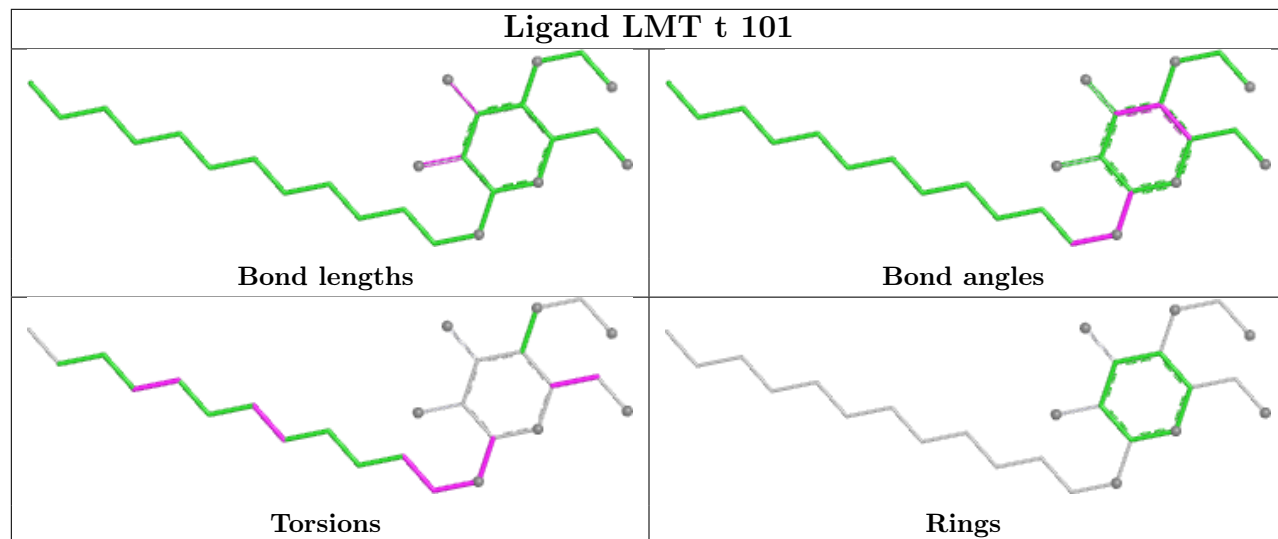
Ligand BCR b 618

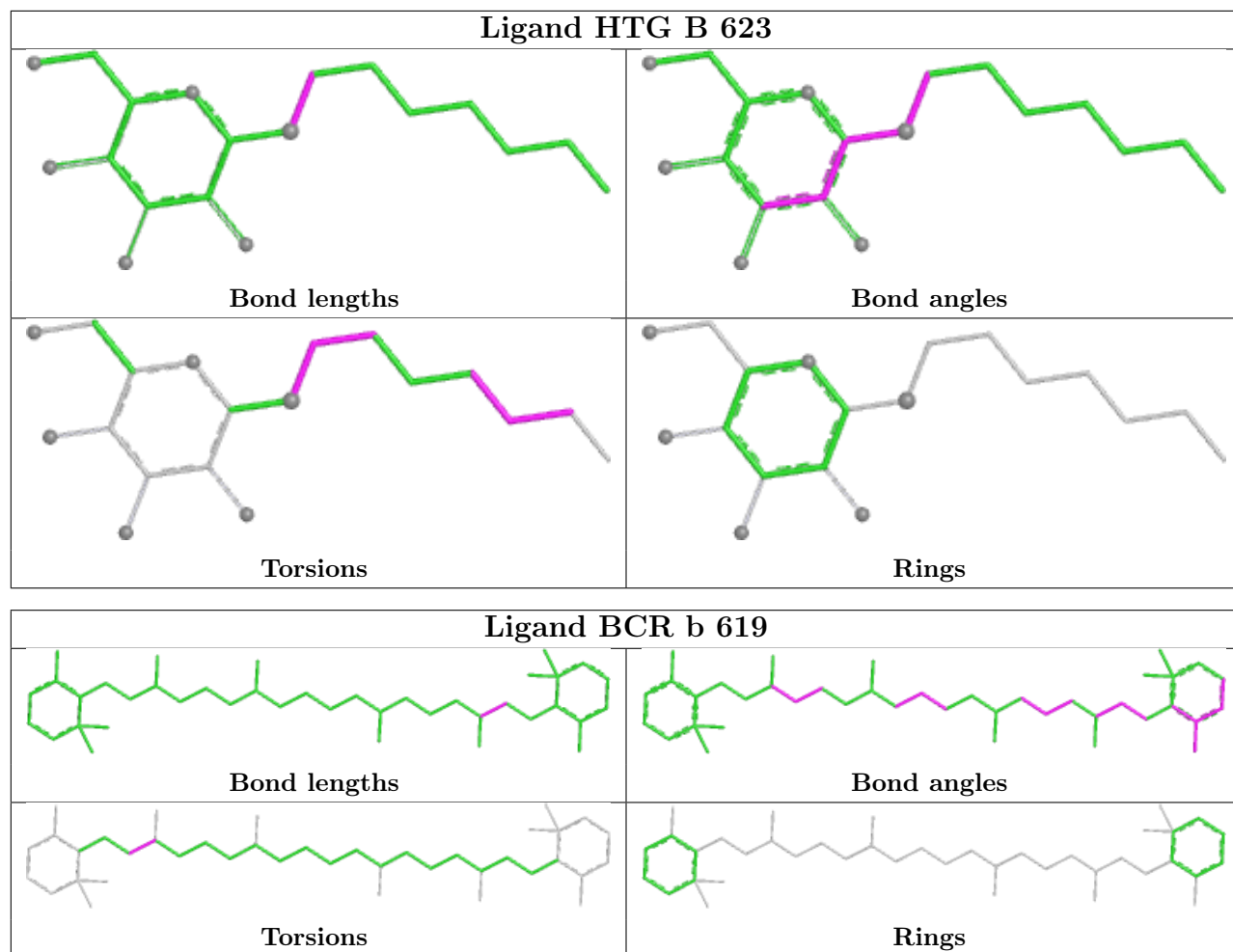


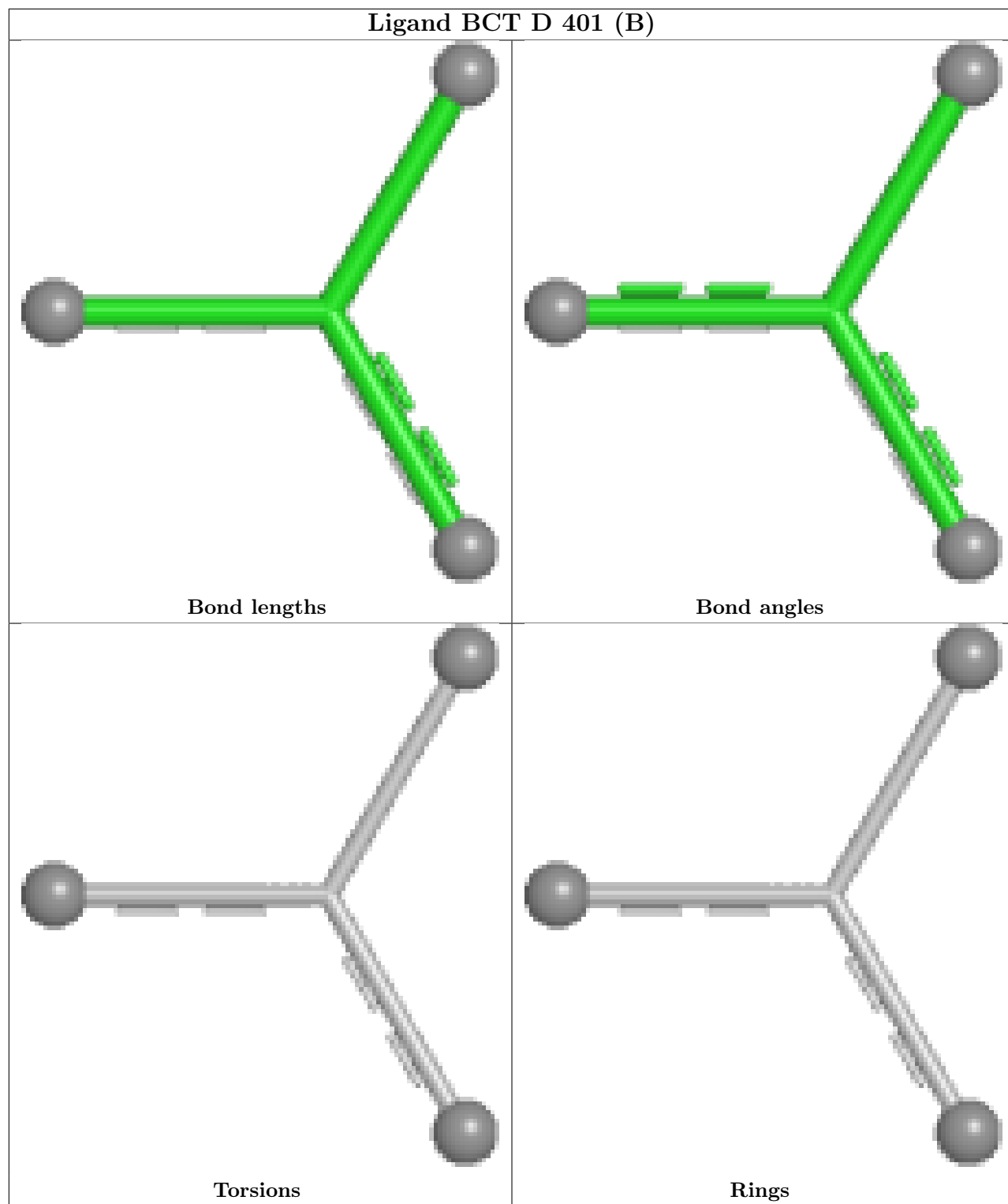
Ligand CLA d 402 (A)



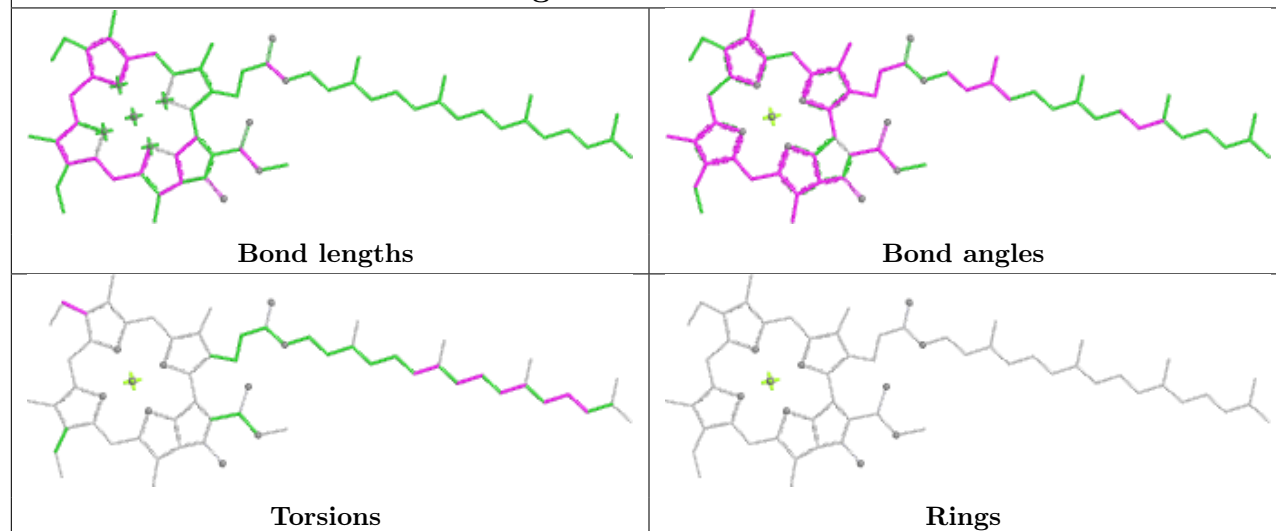
Ligand LMT t 101



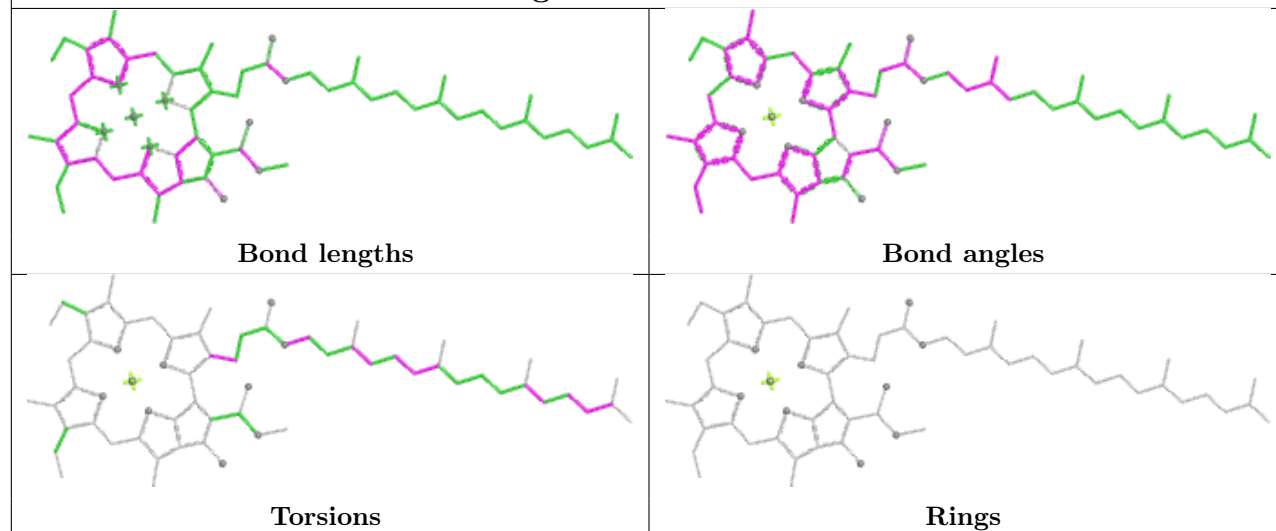




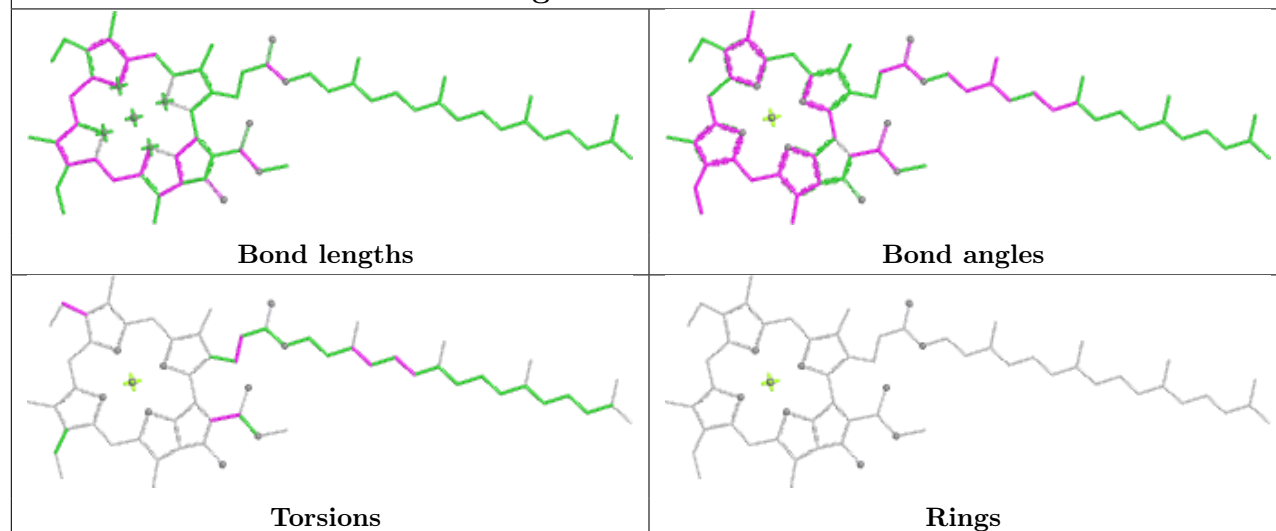
Ligand CLA B 602

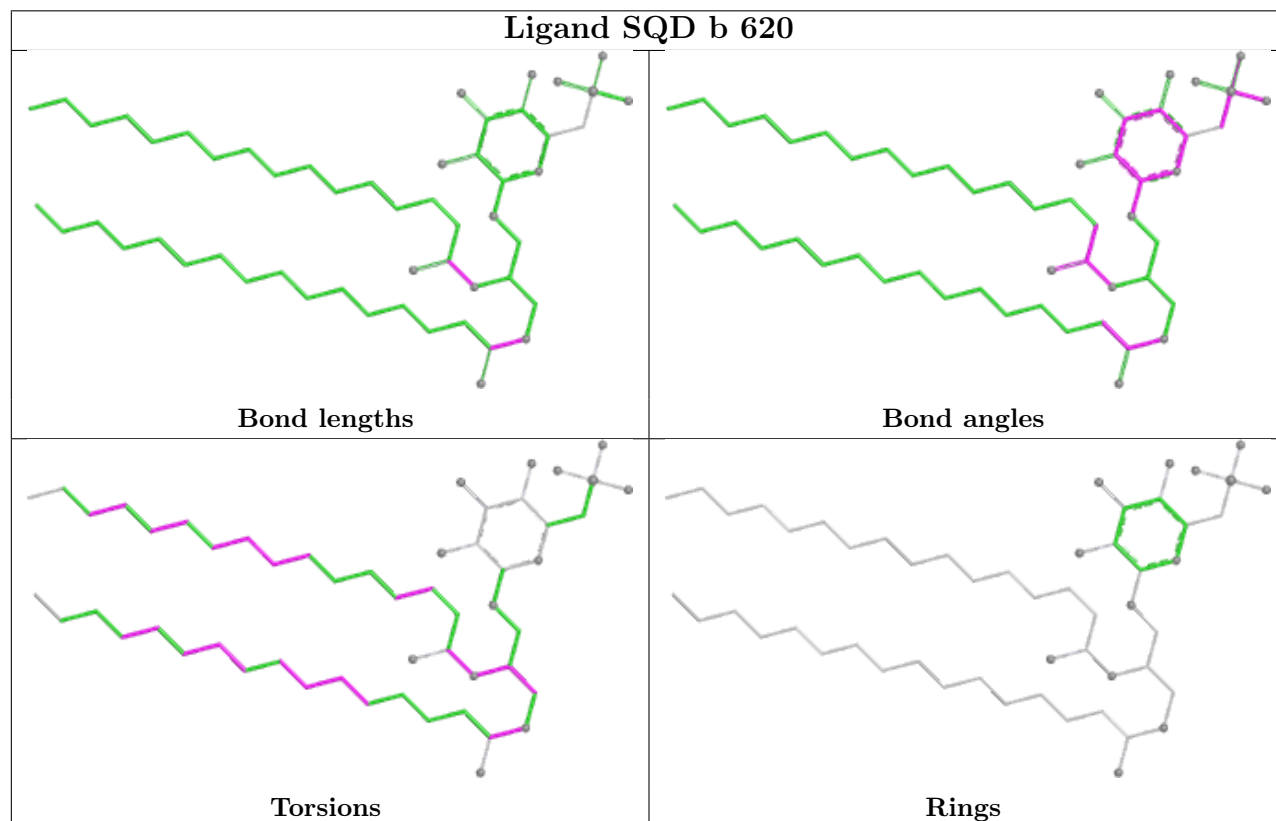
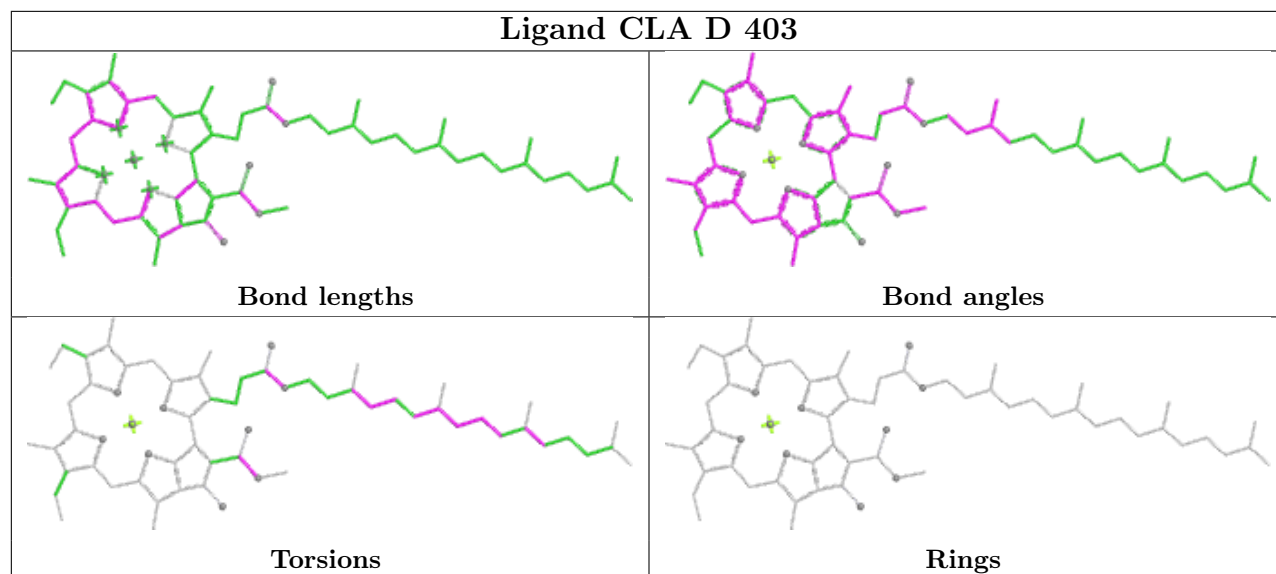


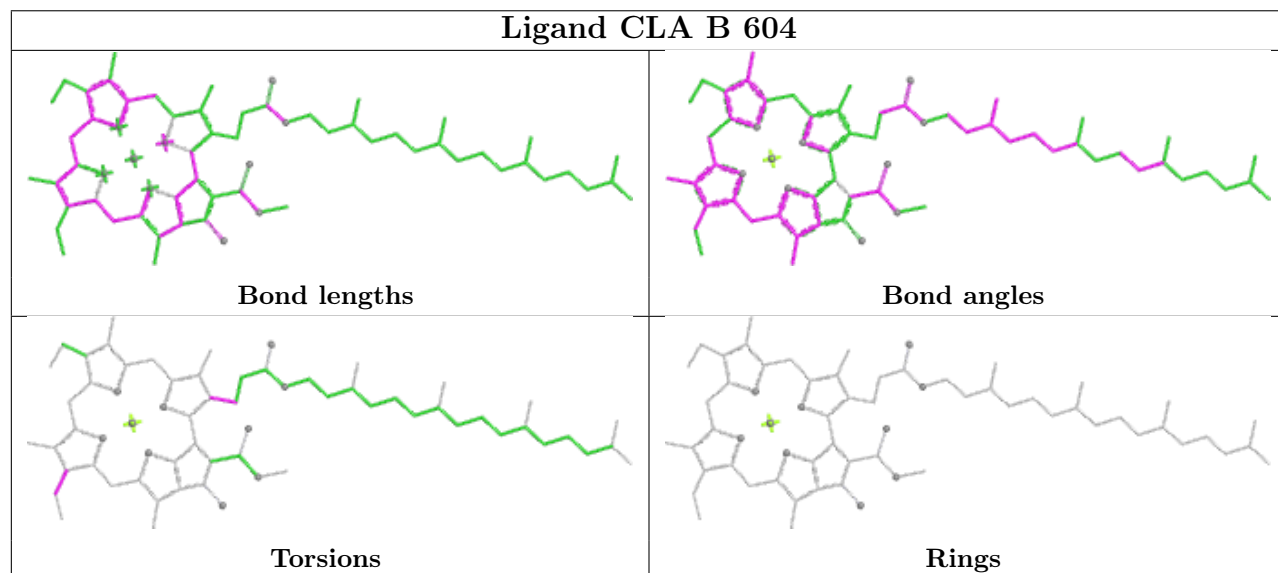
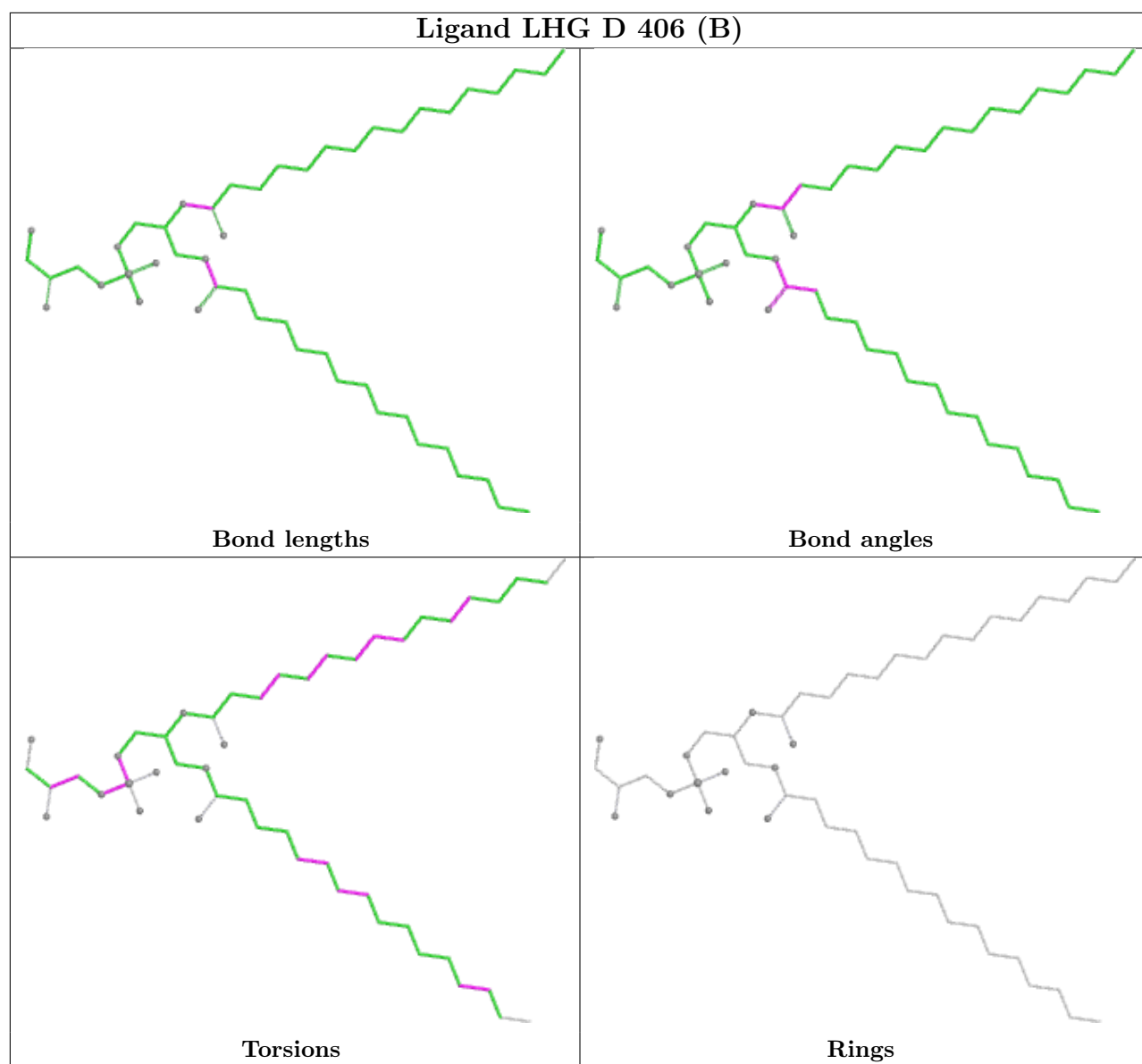
Ligand CLA C 507

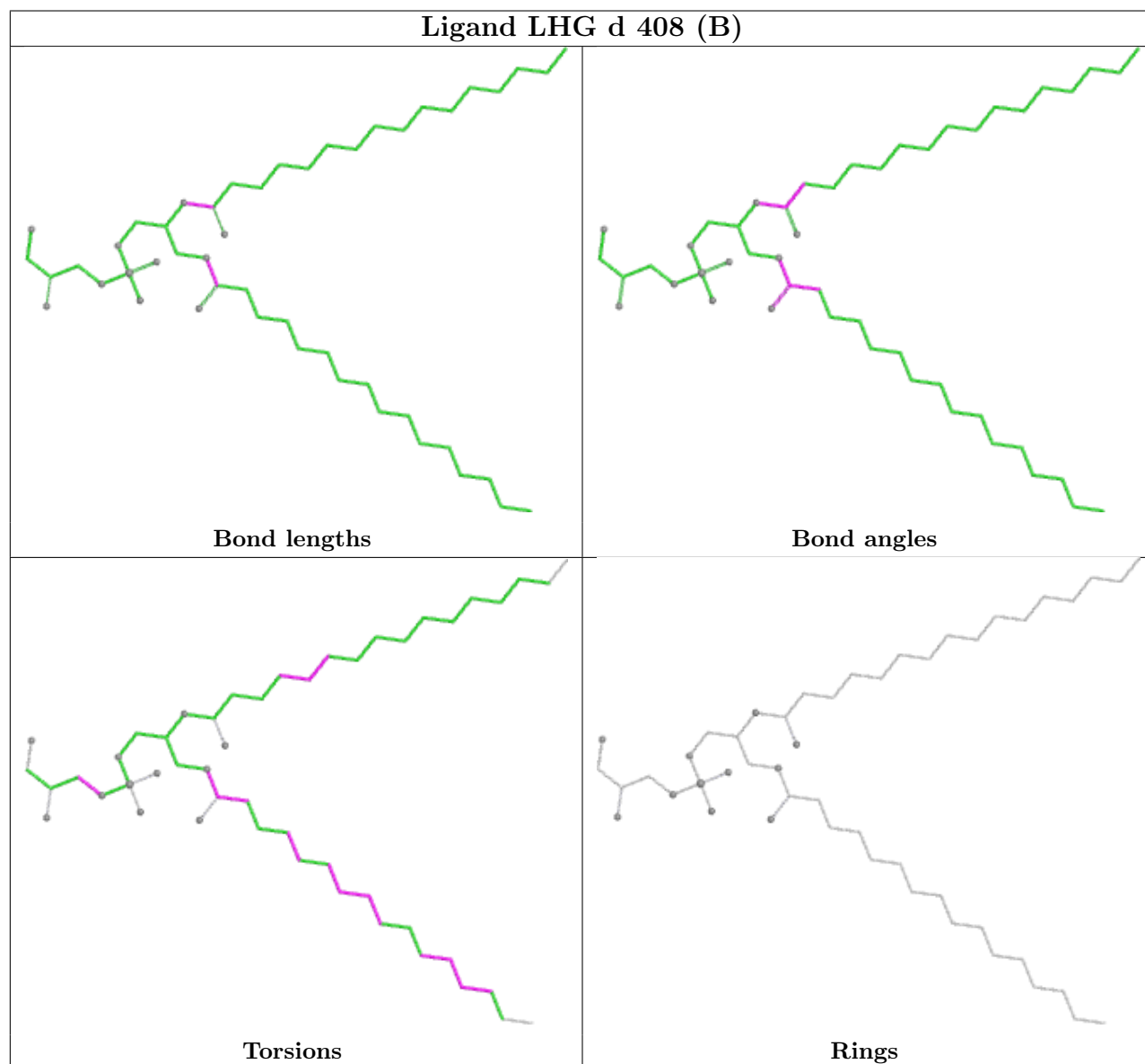
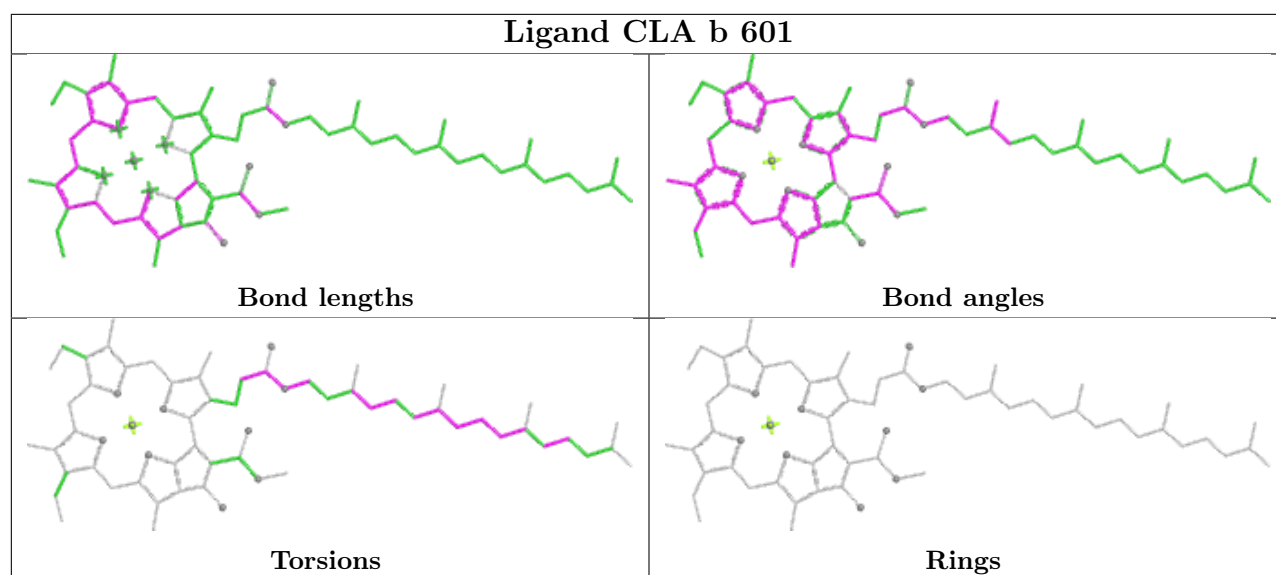


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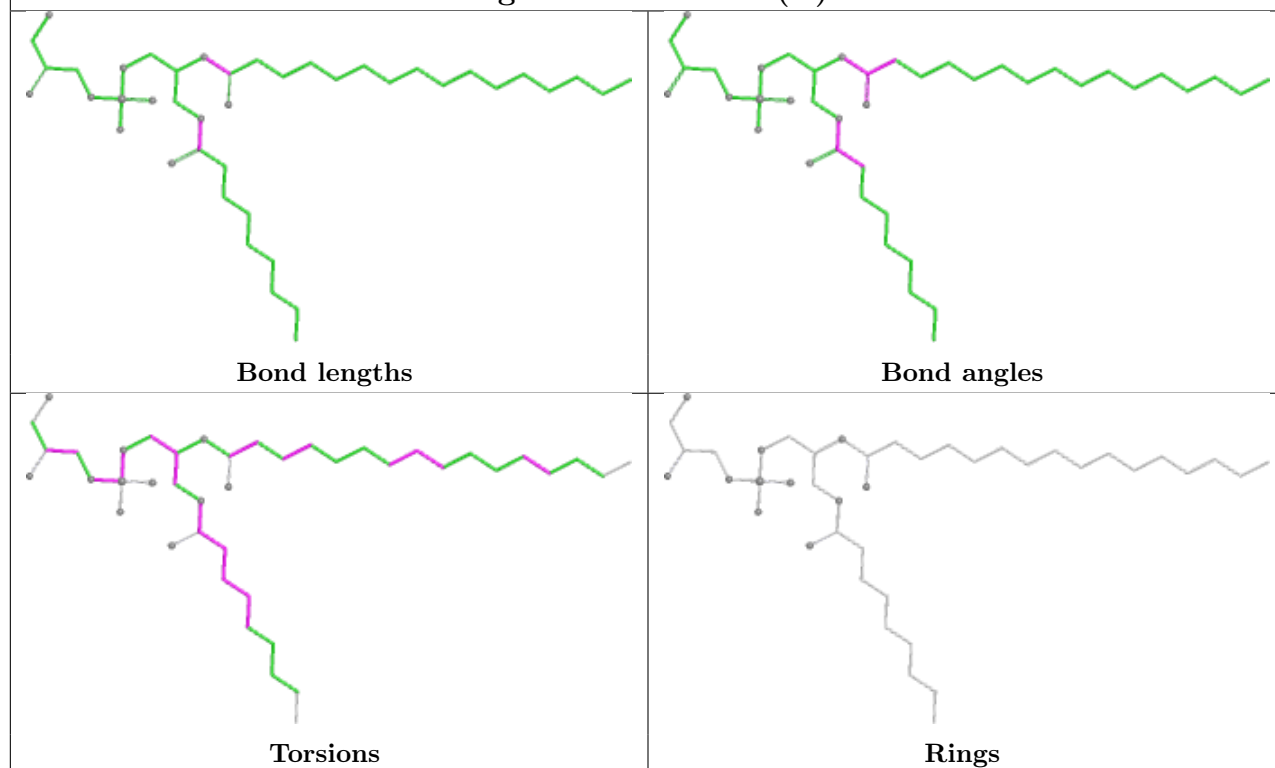




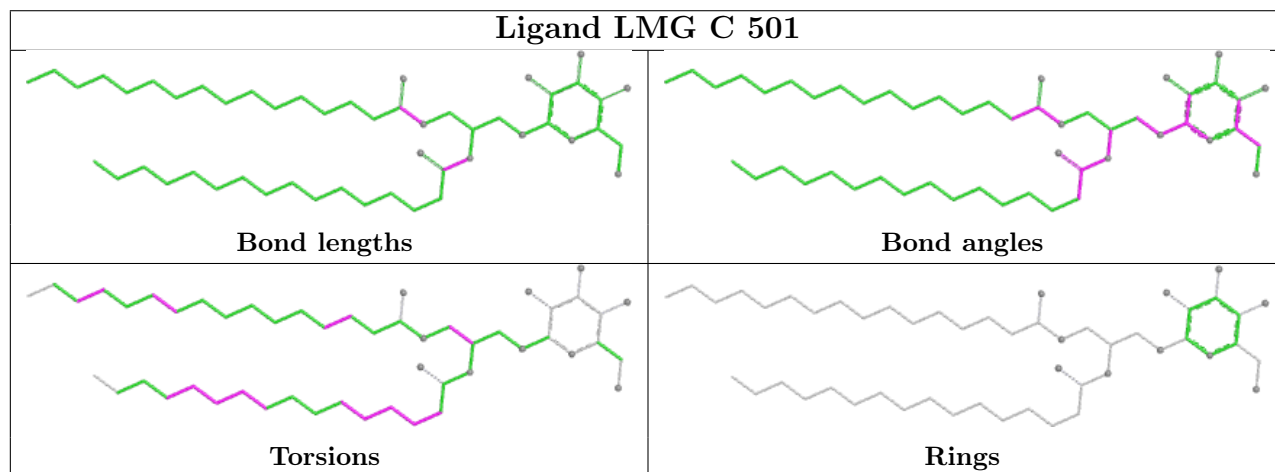


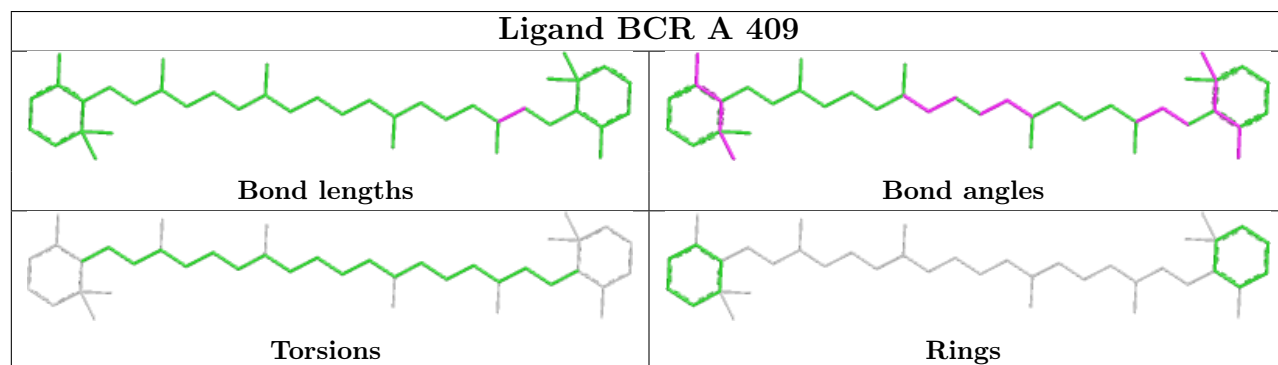
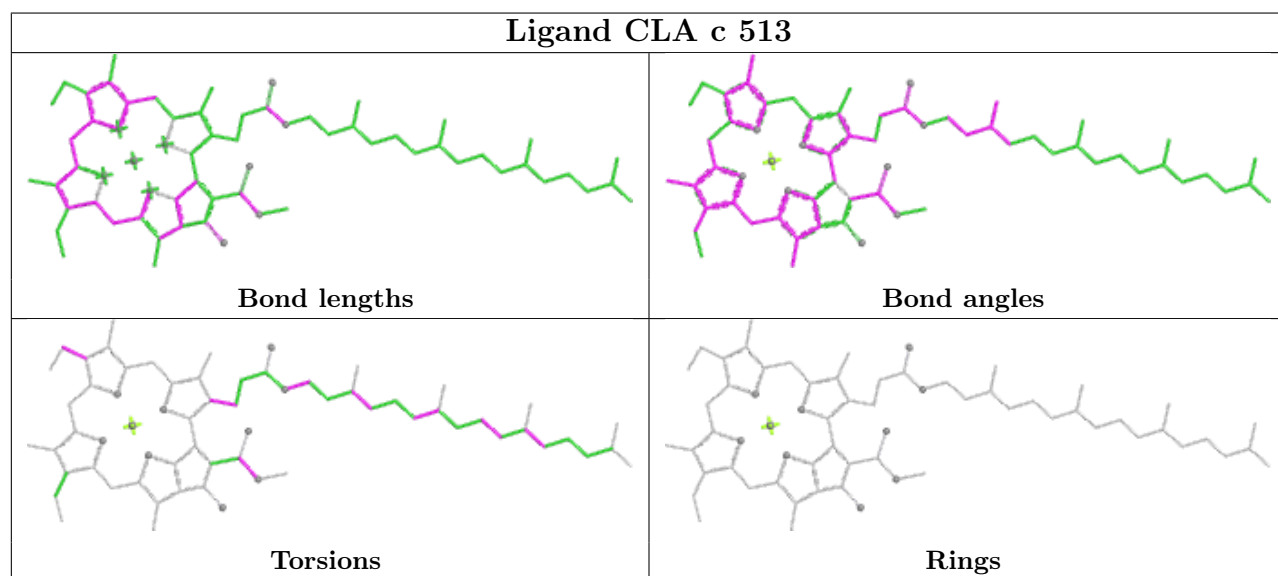
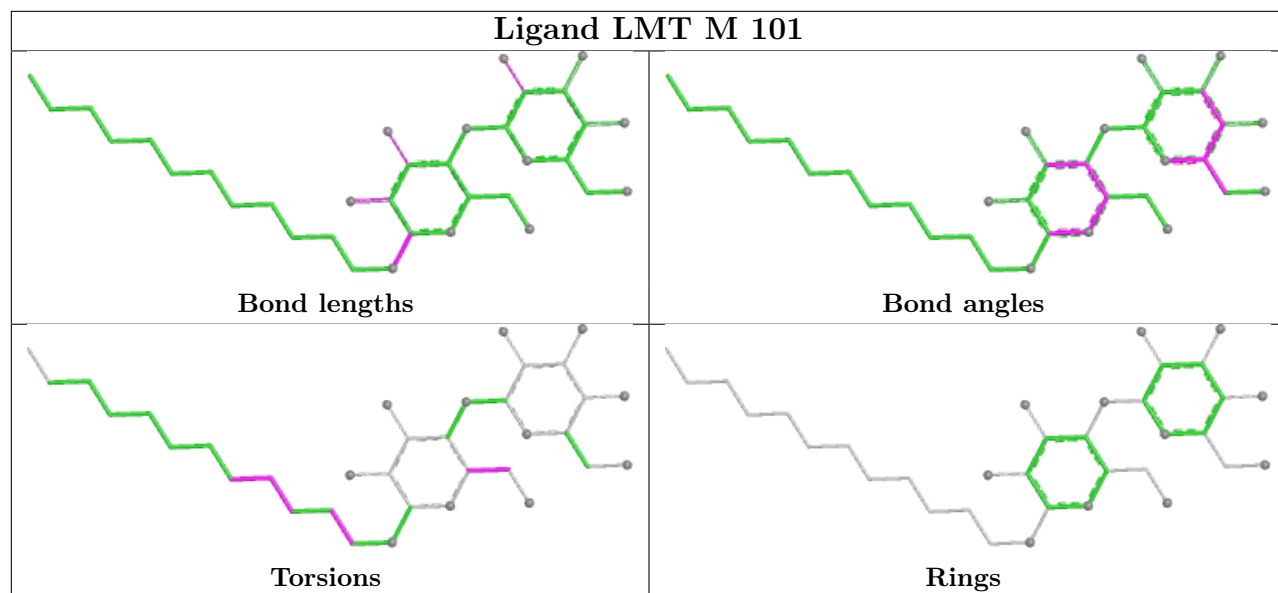


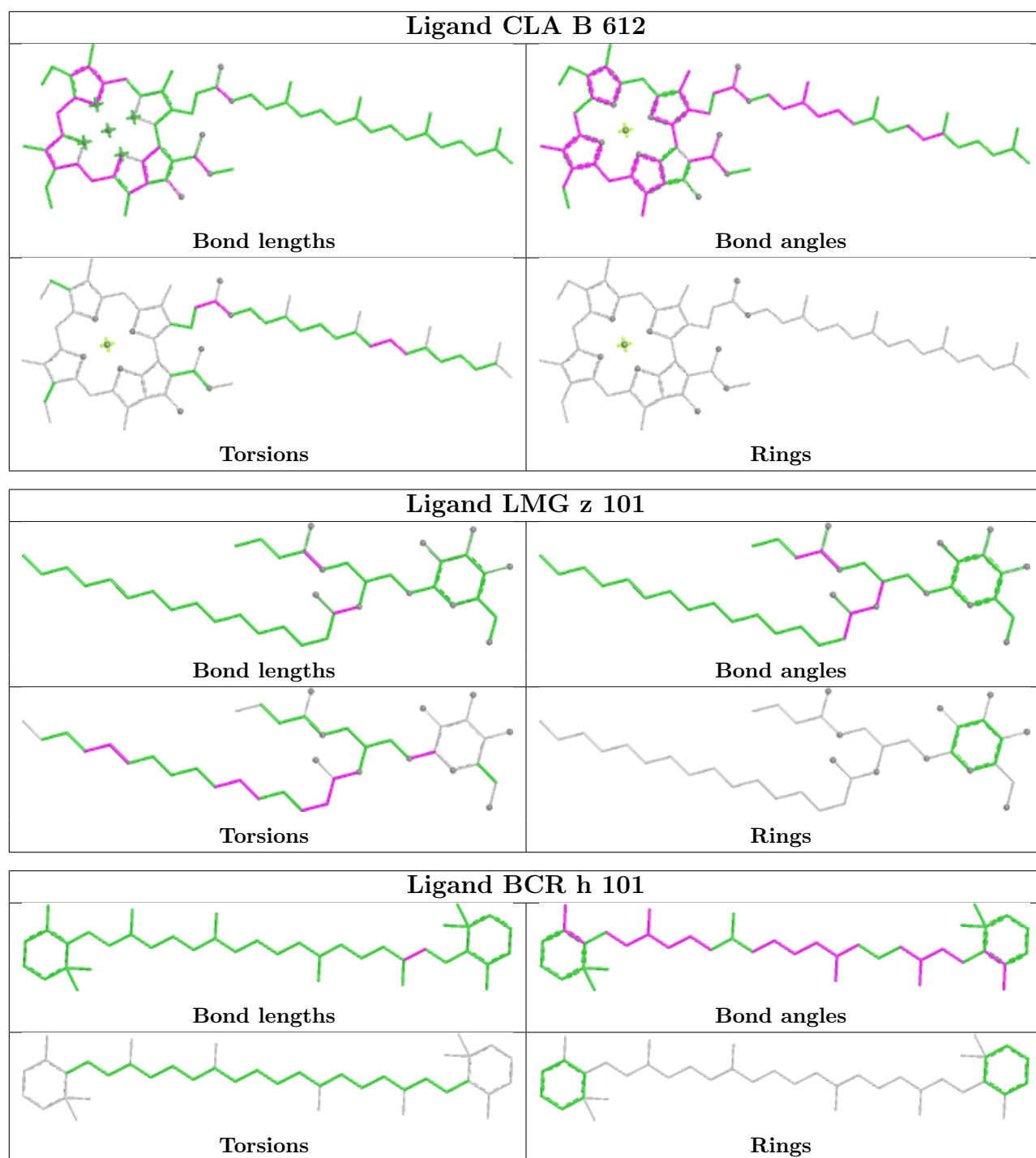
Ligand LHG E 101 (B)



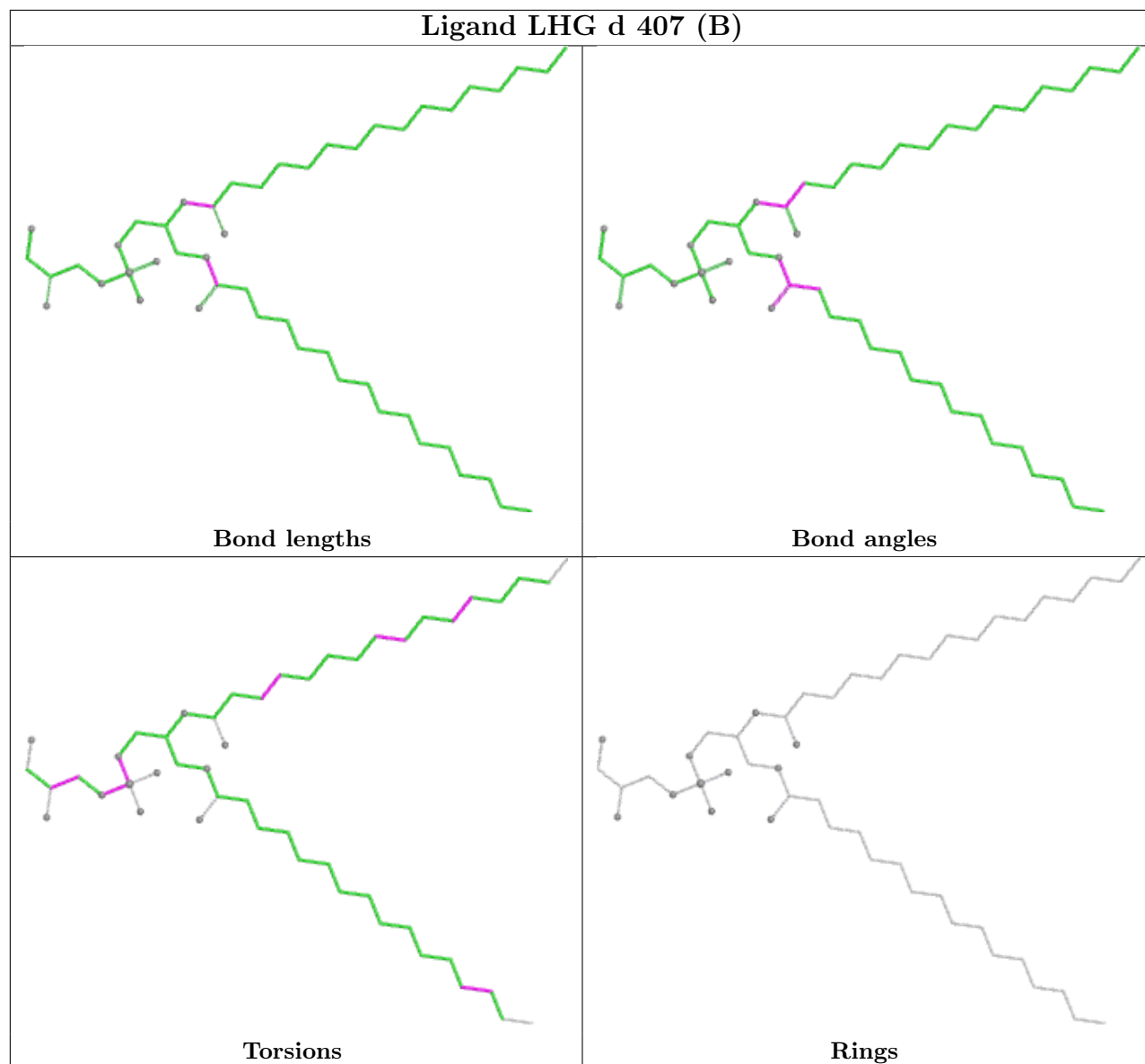
Ligand LMG C 501



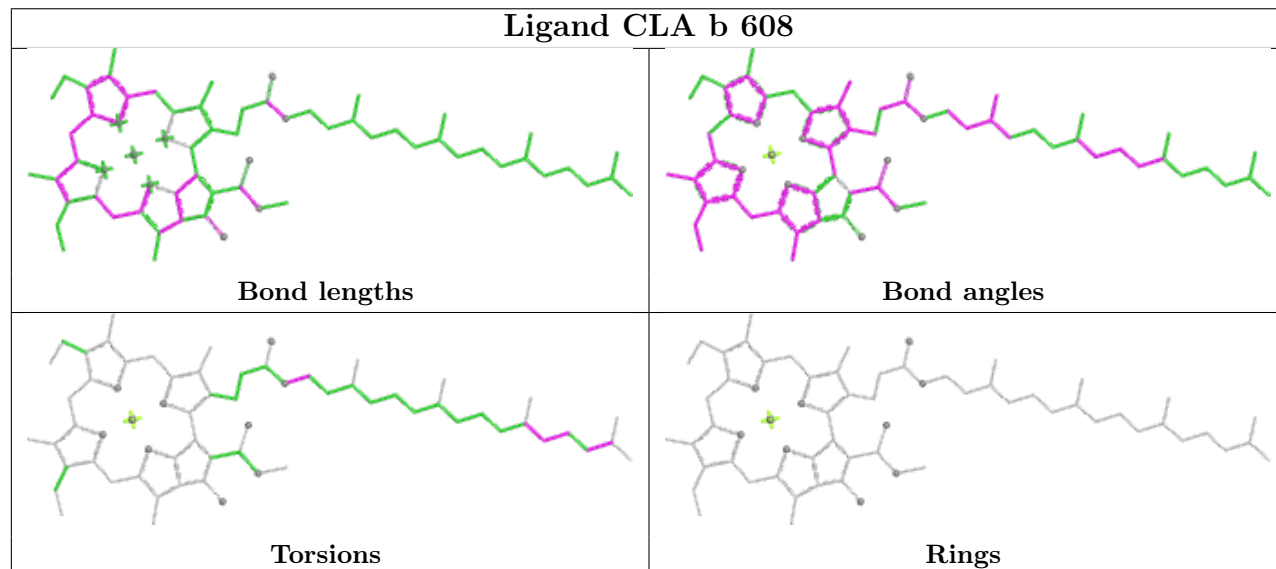


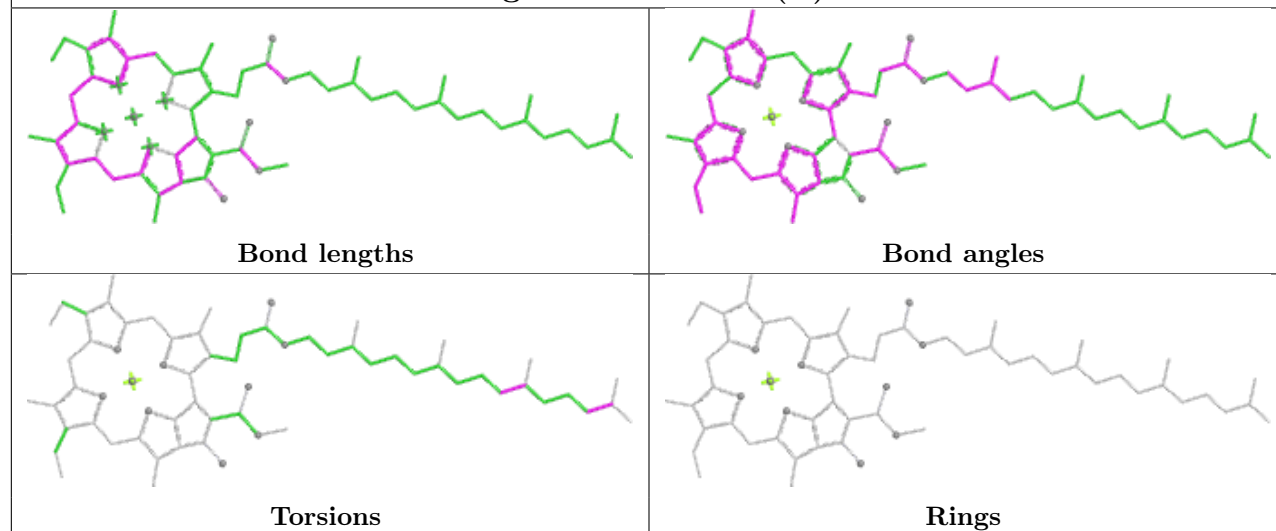
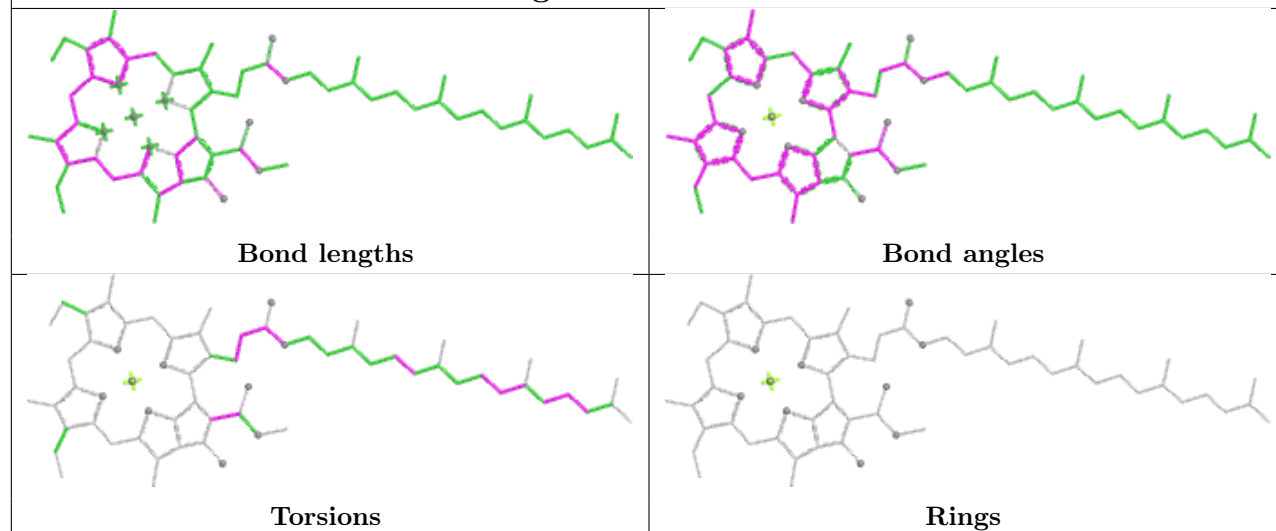


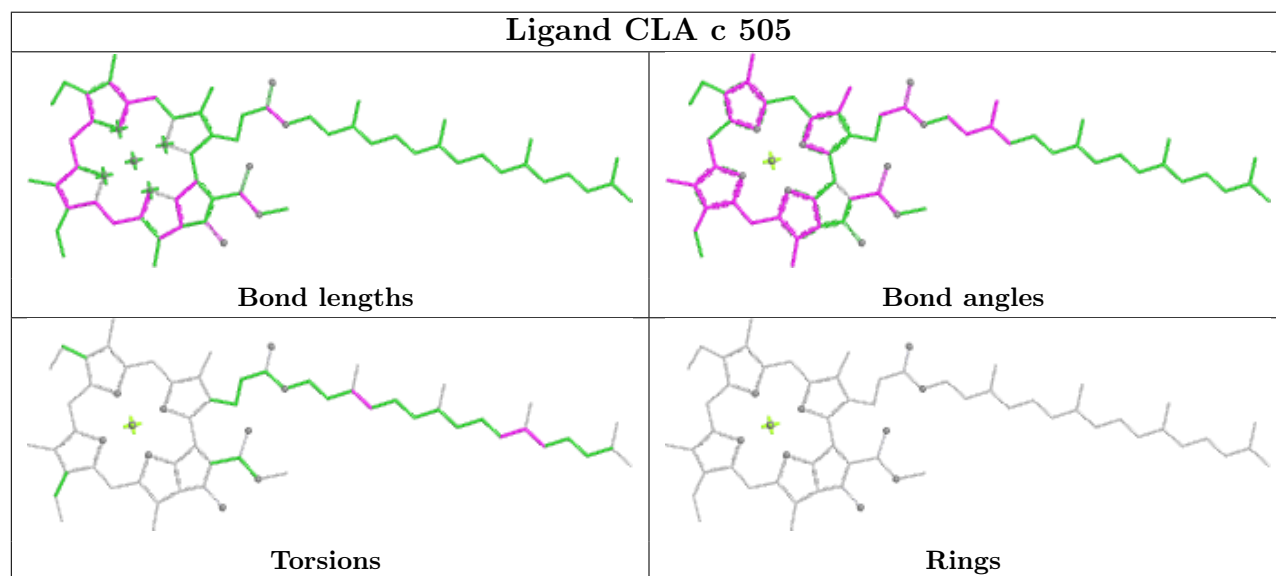
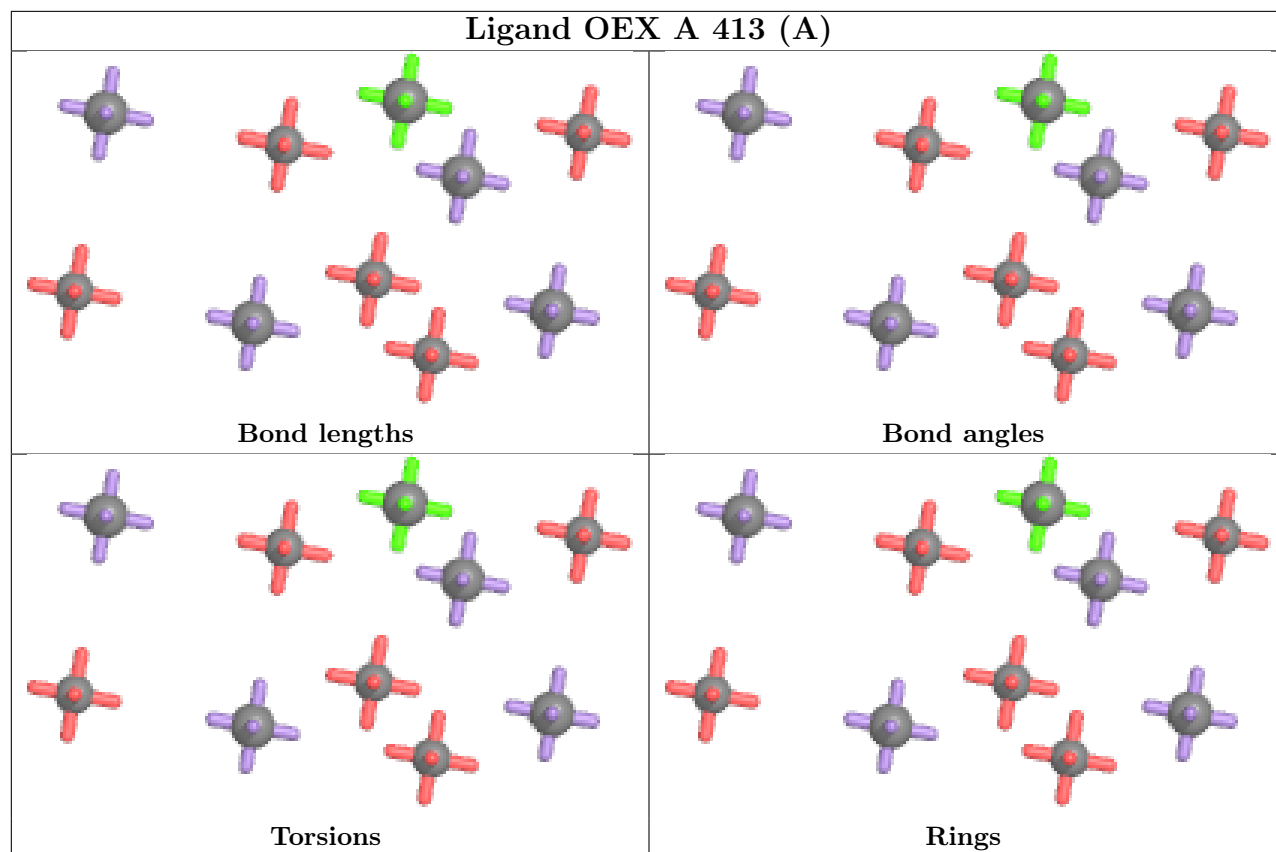
Ligand LHG d 407 (B)

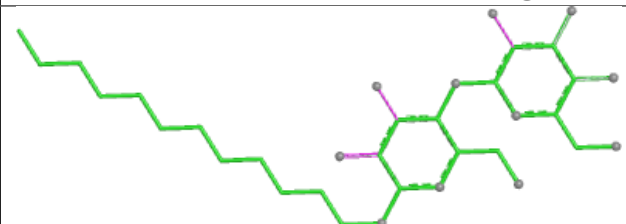
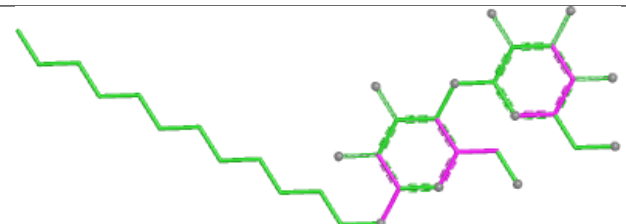
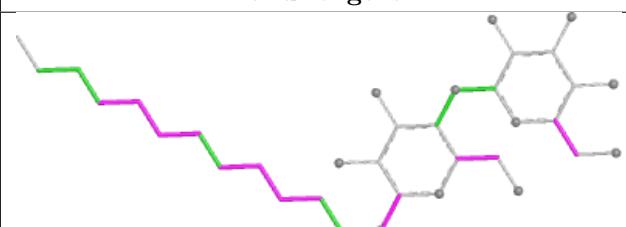
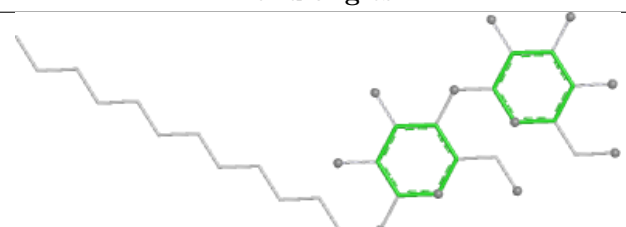
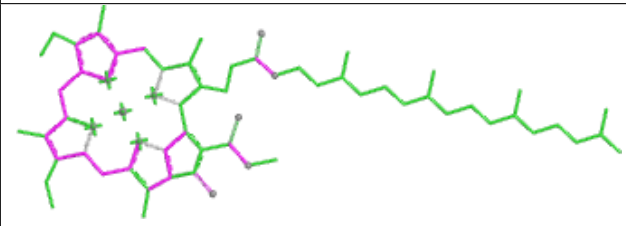
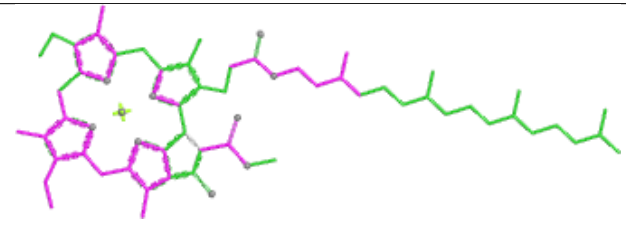
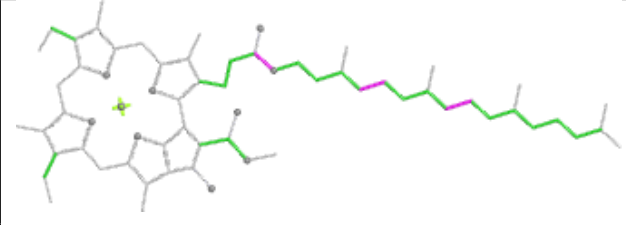
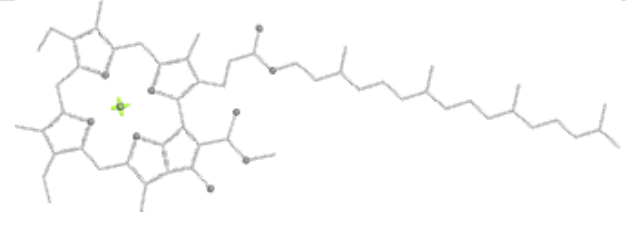
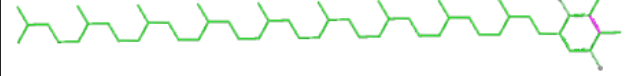
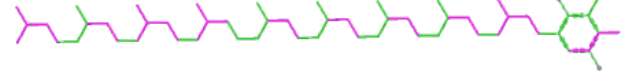
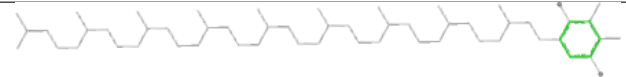


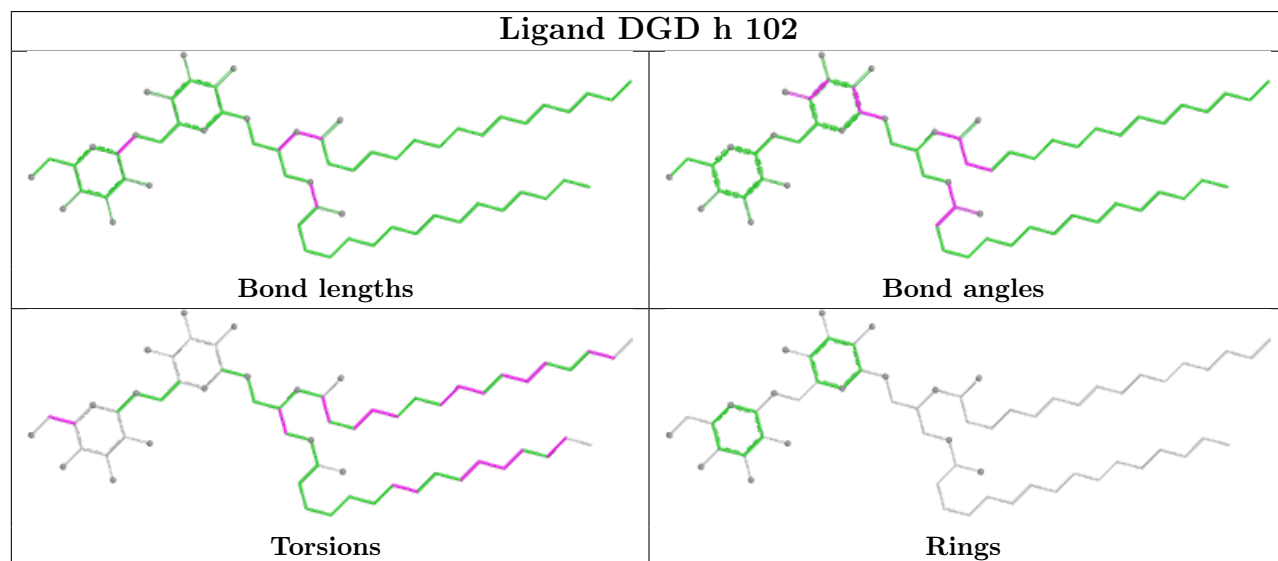
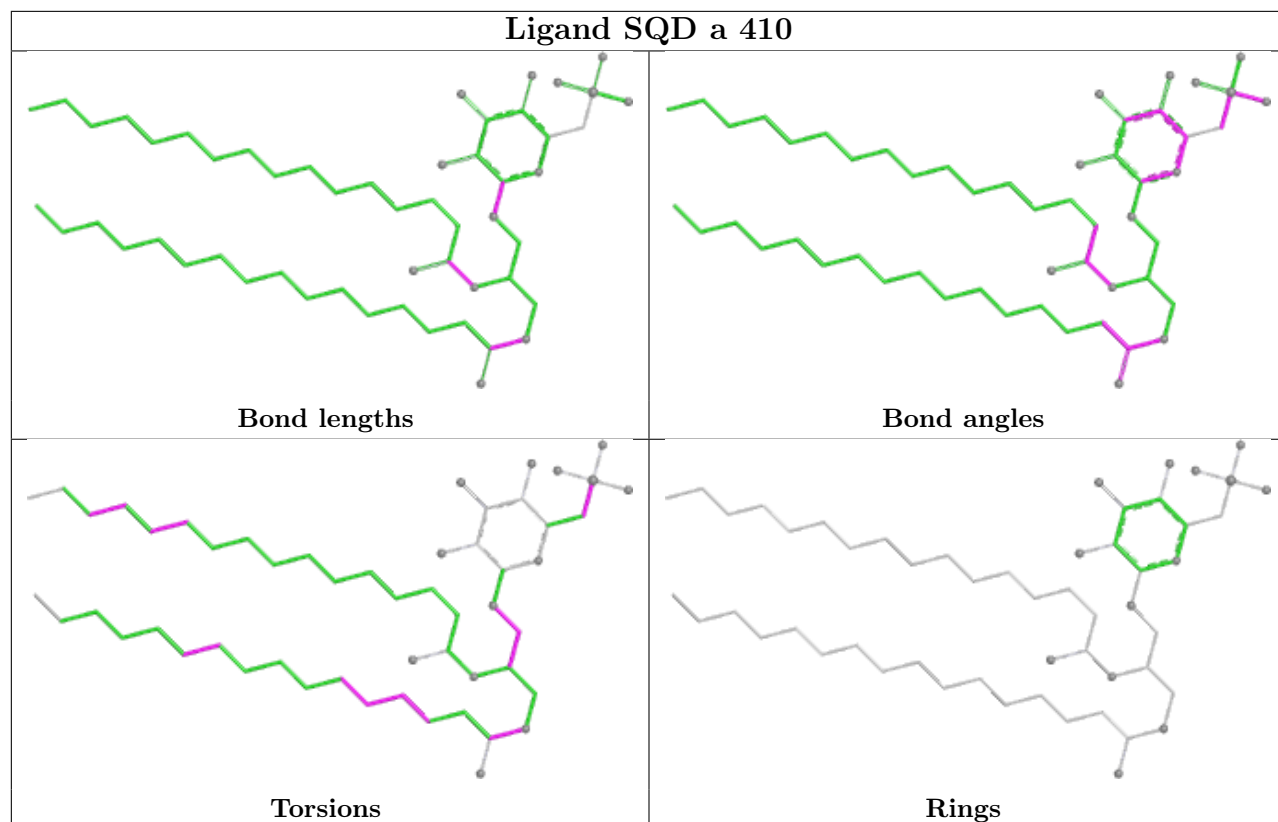
Ligand CLA b 608



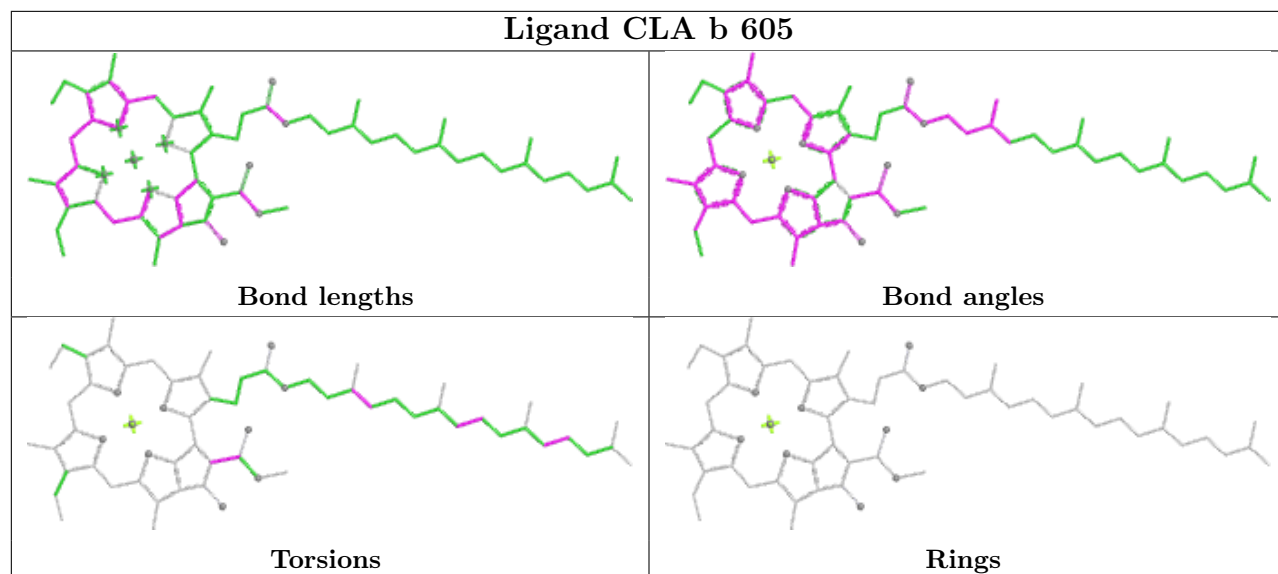
Ligand CLA d 403 (B)**Ligand CLA B 601**



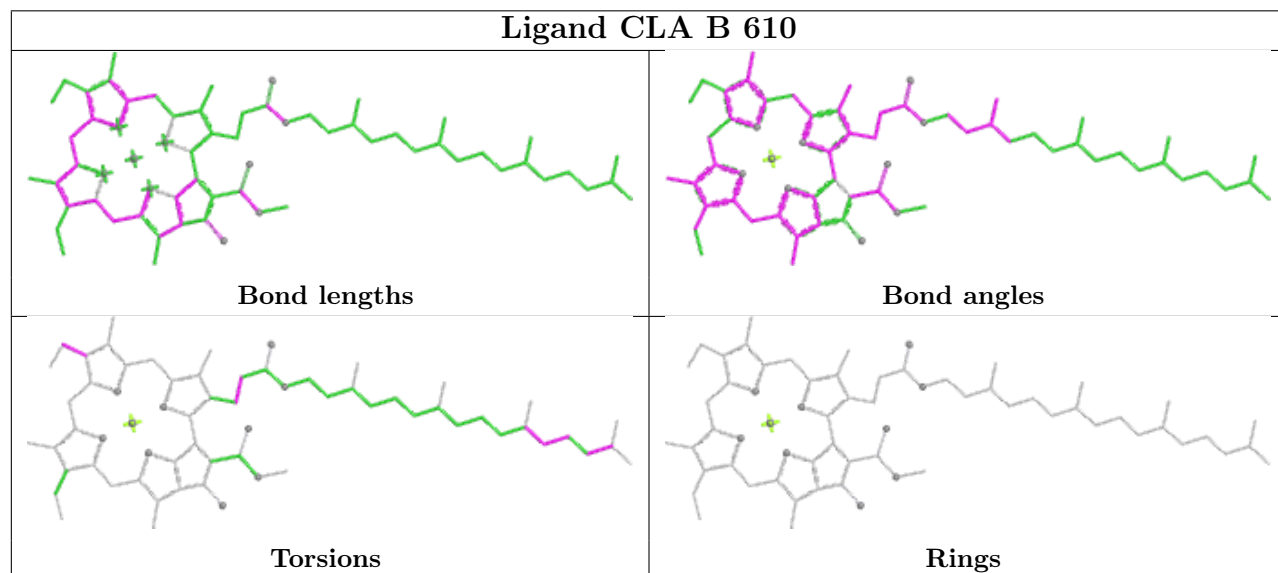
Ligand LMT B 630	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 512	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 d 406 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings



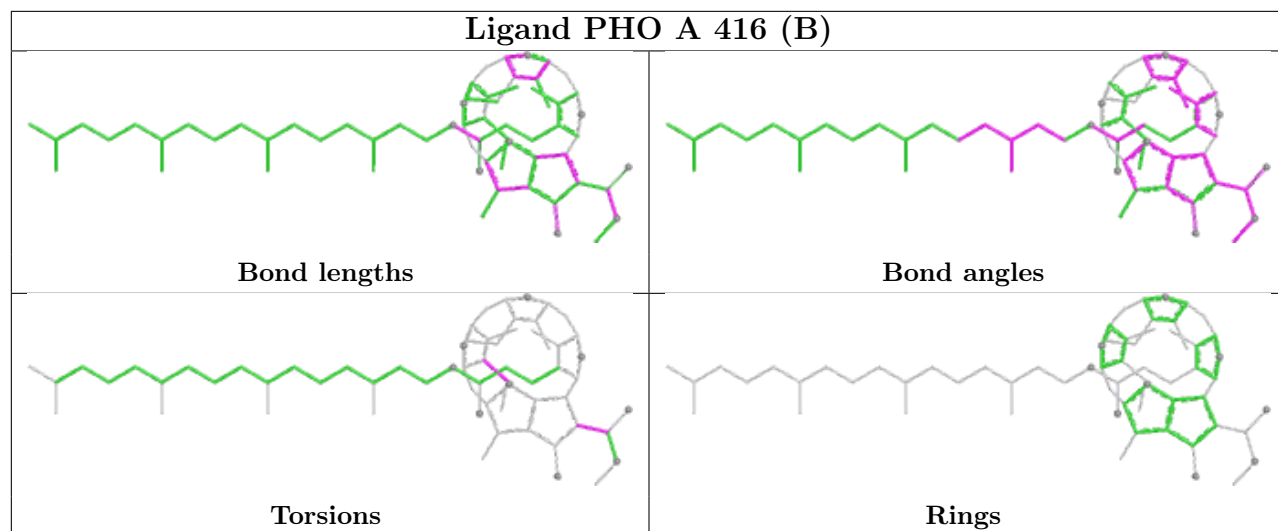
Ligand CLA b 605

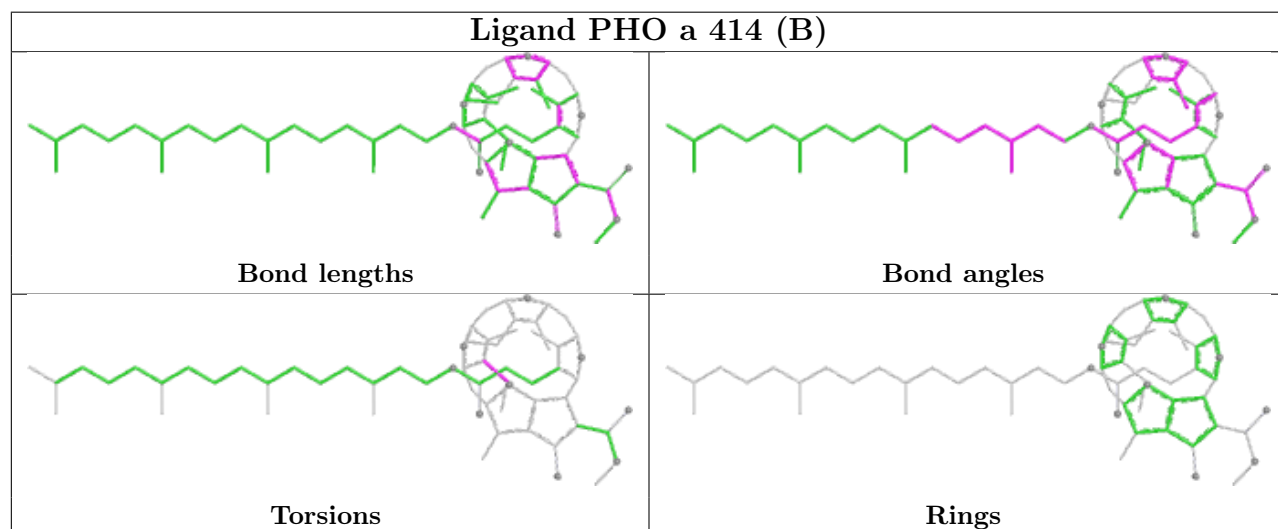
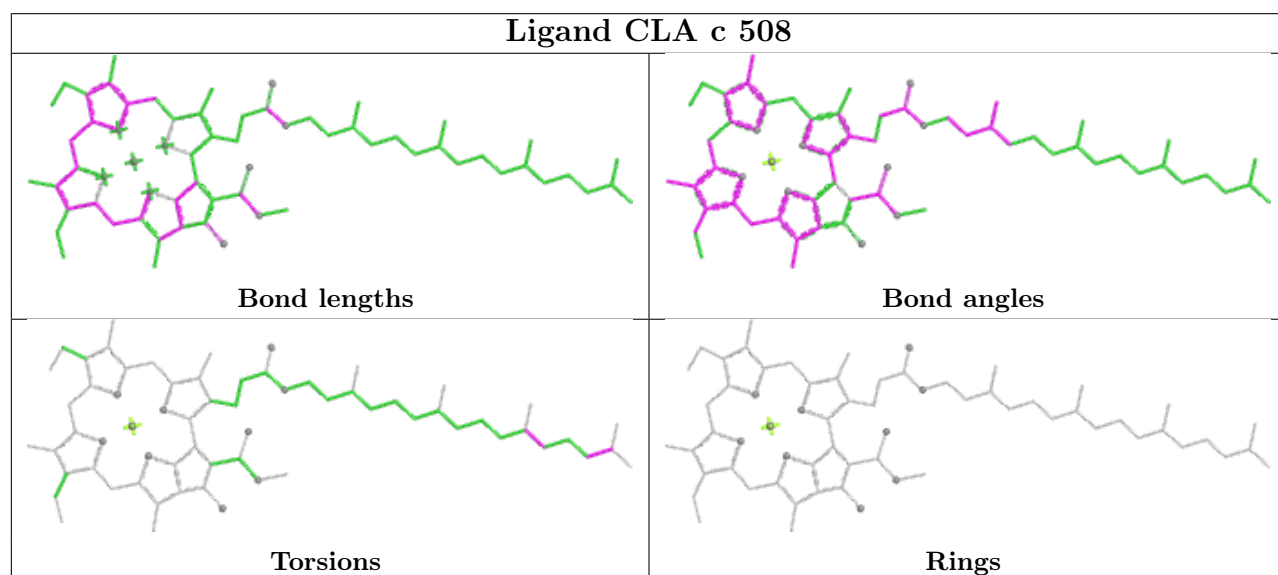
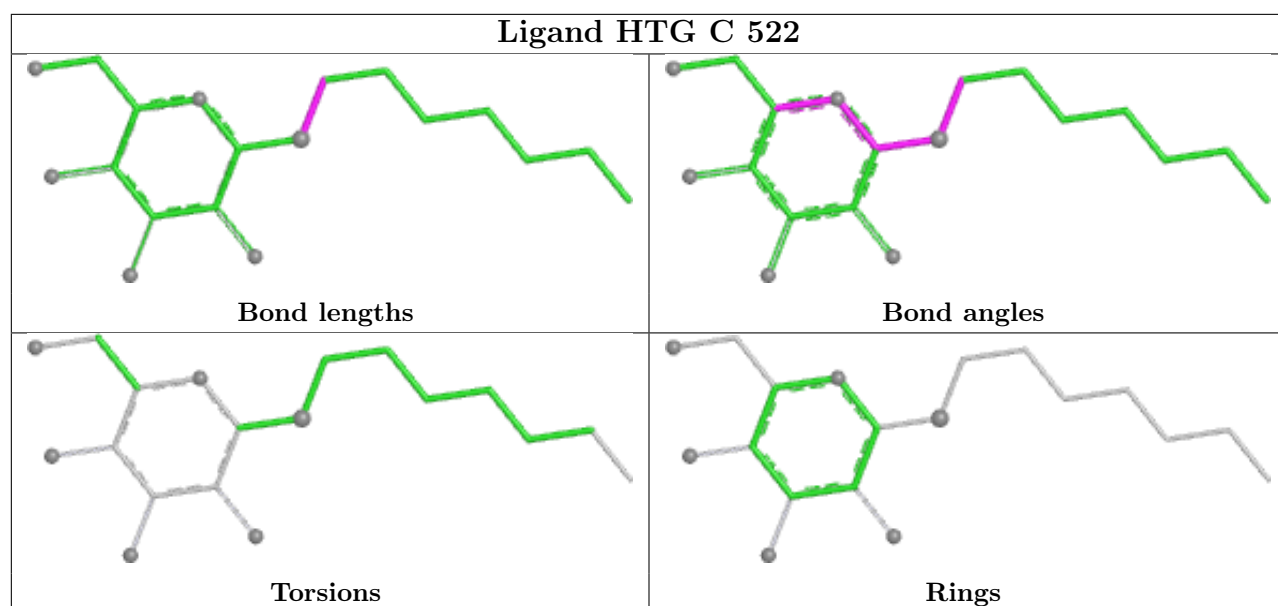


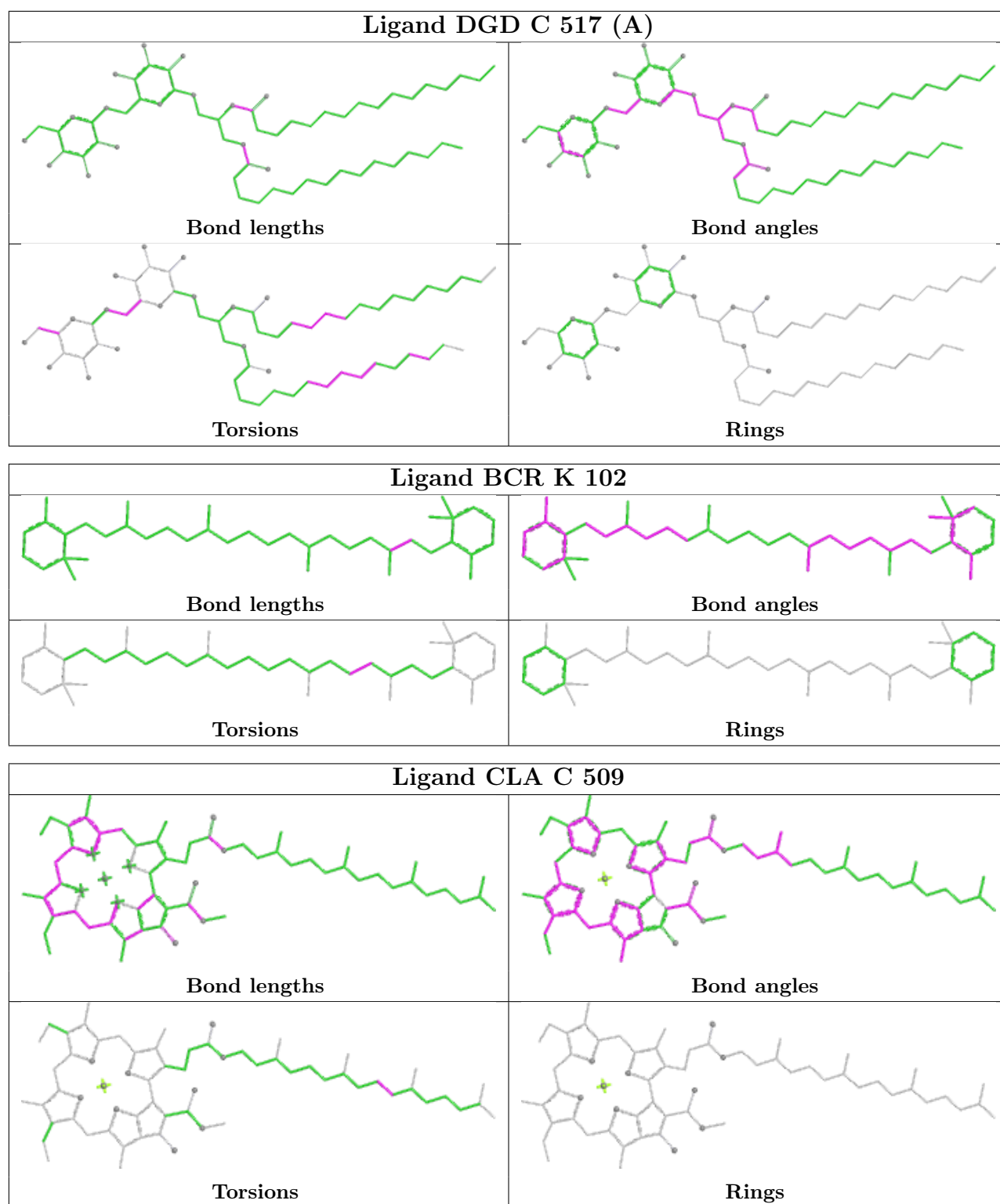
Ligand CLA B 610



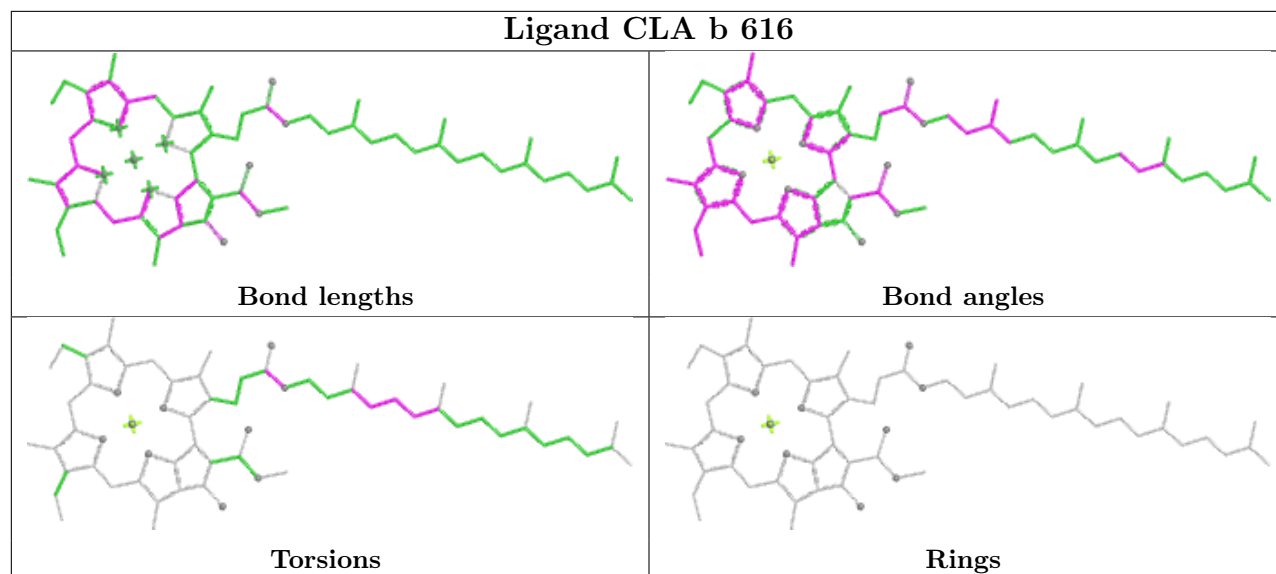
Ligand PHO A 416 (B)



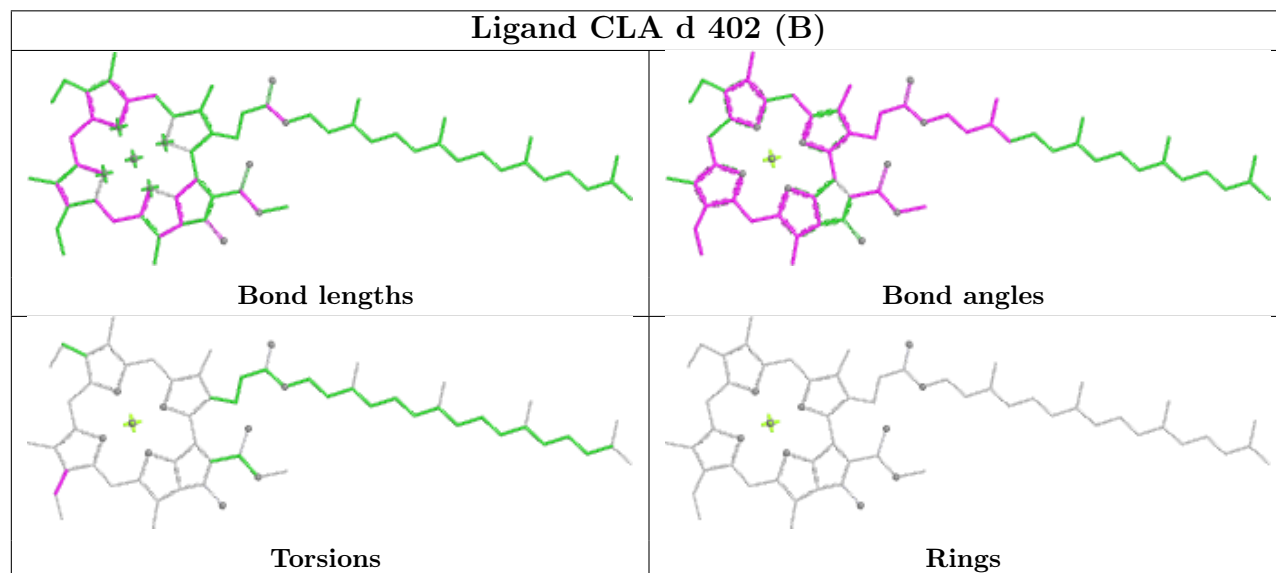




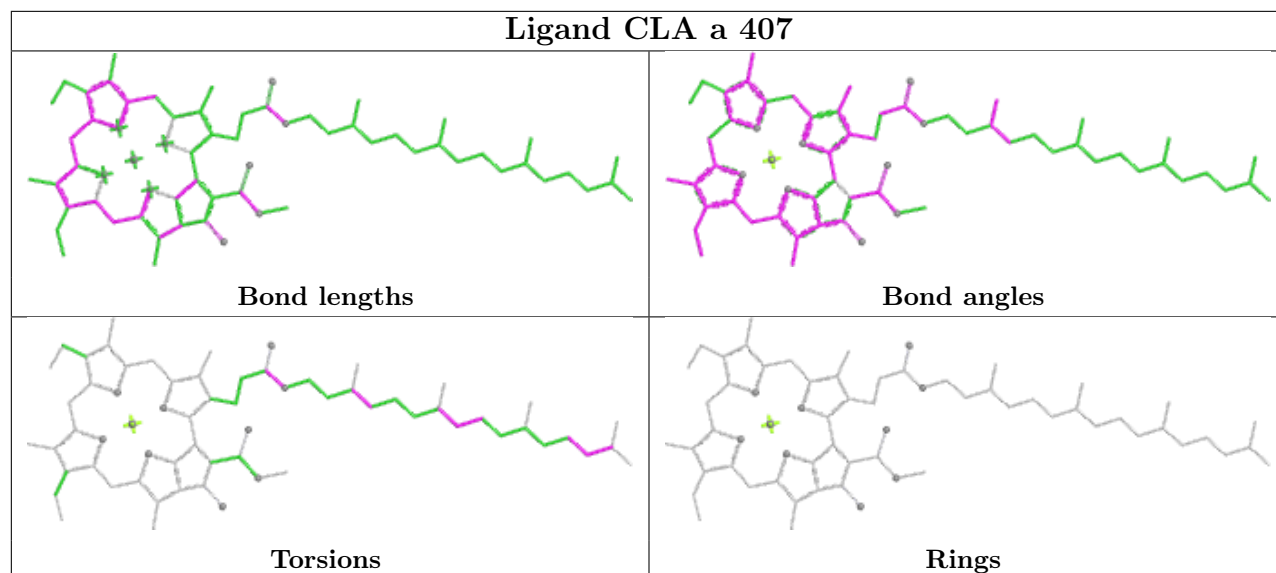
Ligand CLA b 616

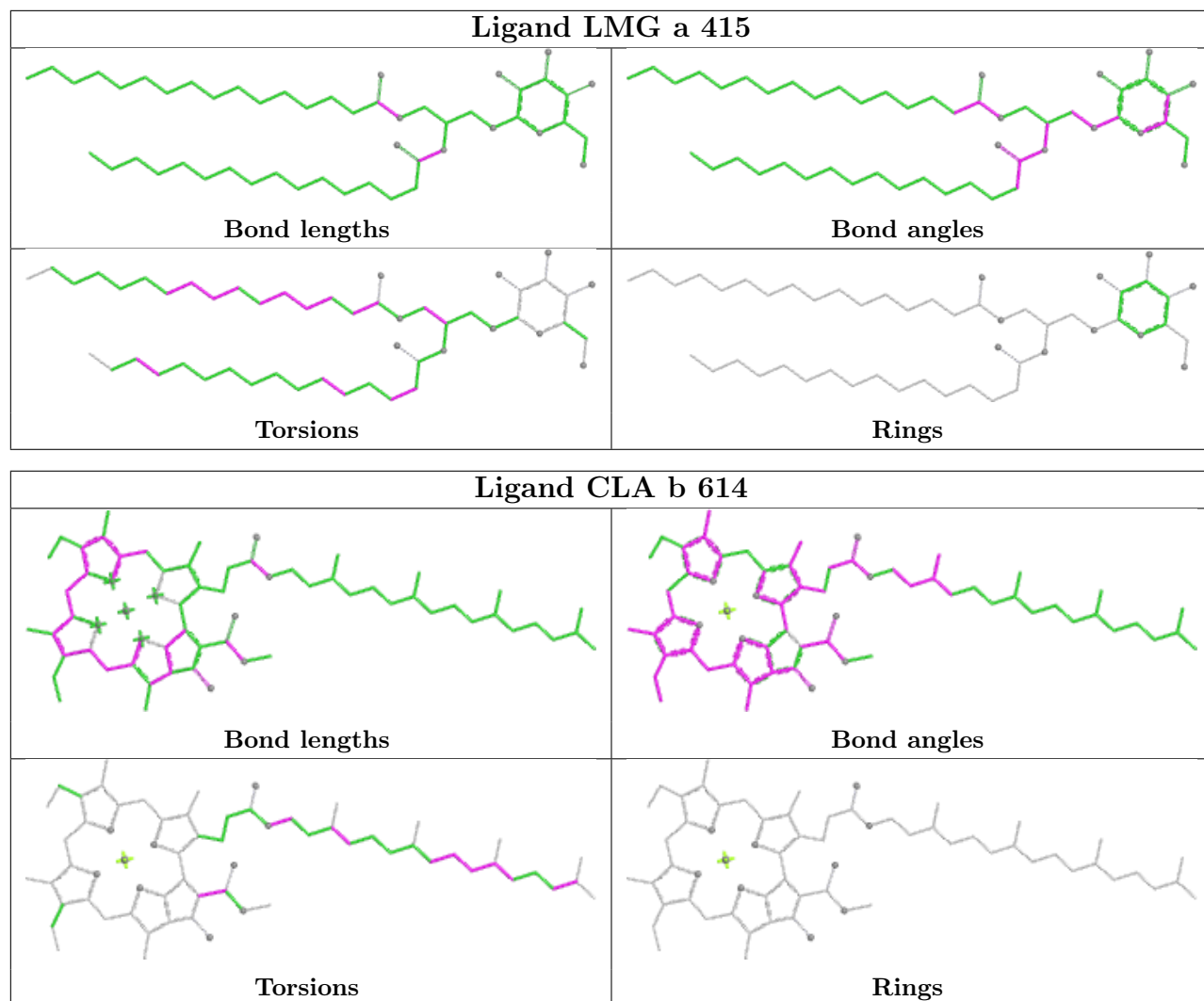


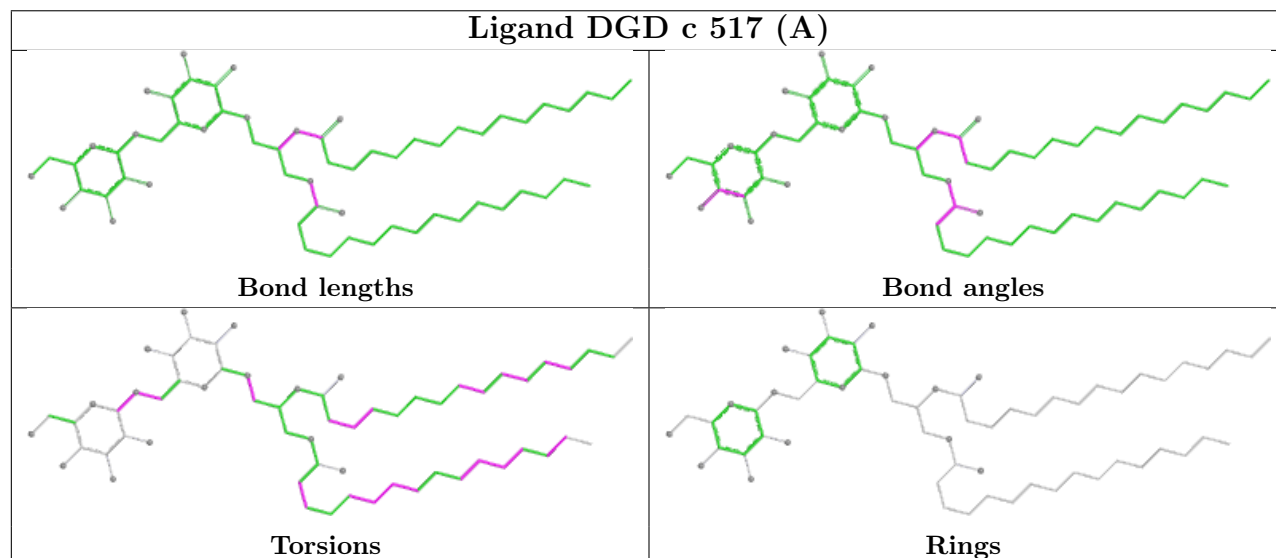
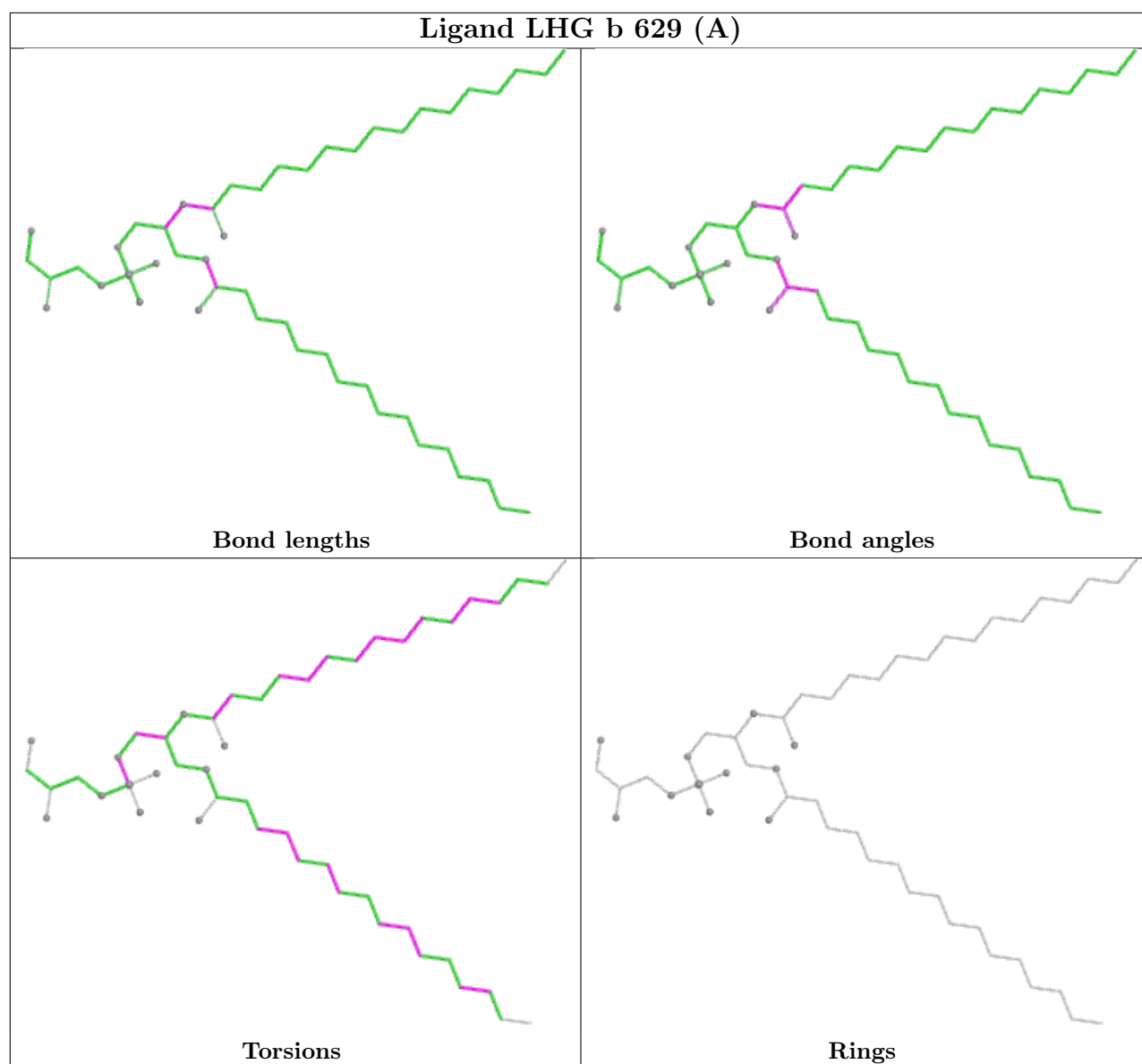
Ligand CLA d 402 (B)



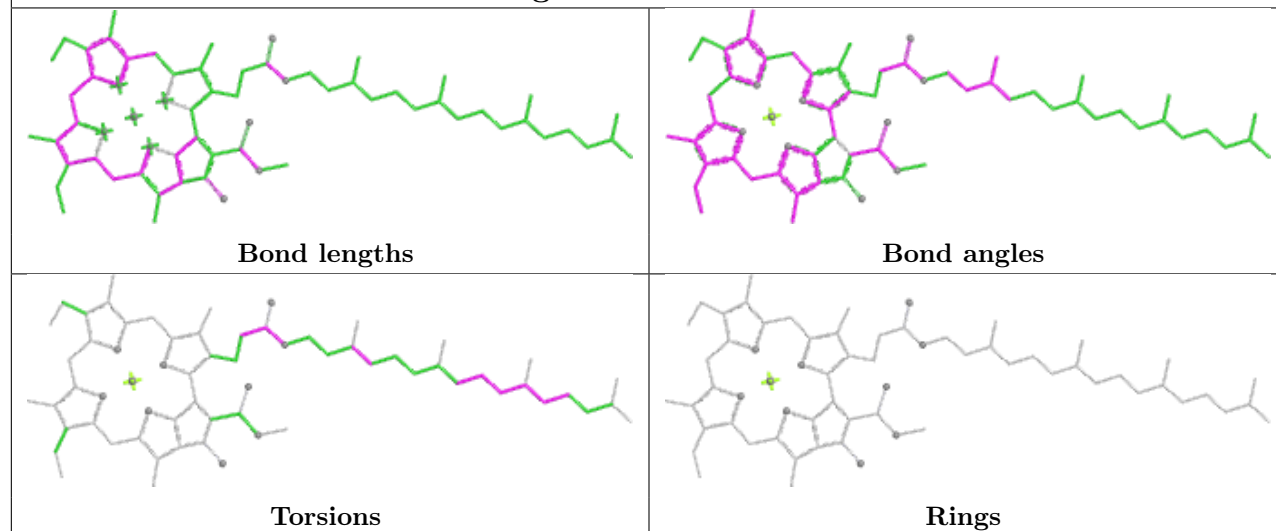
Ligand CLA a 407



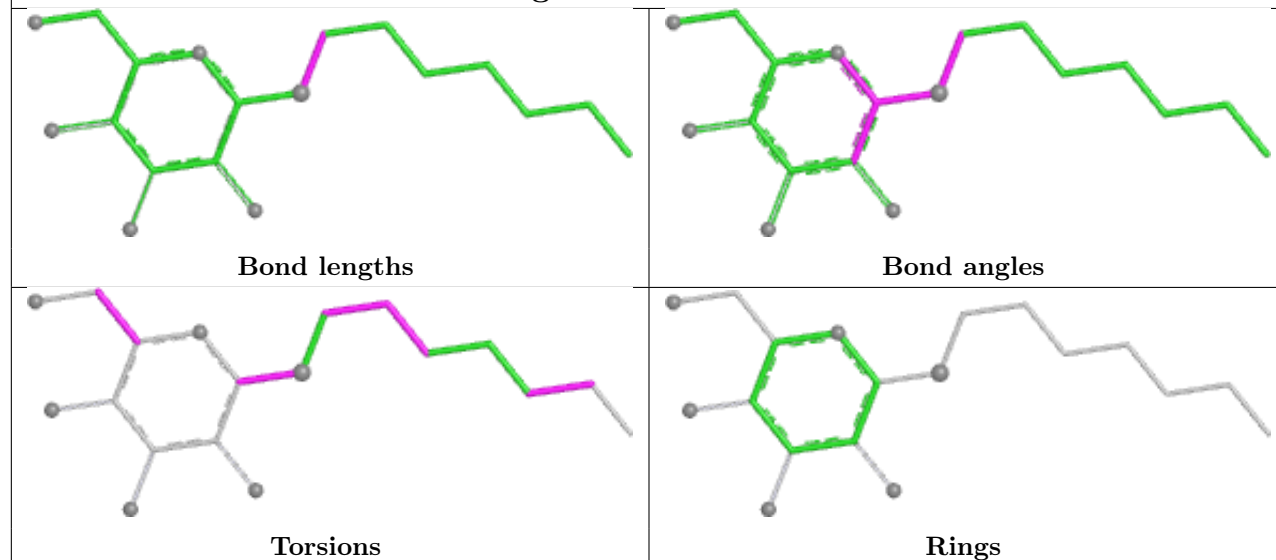




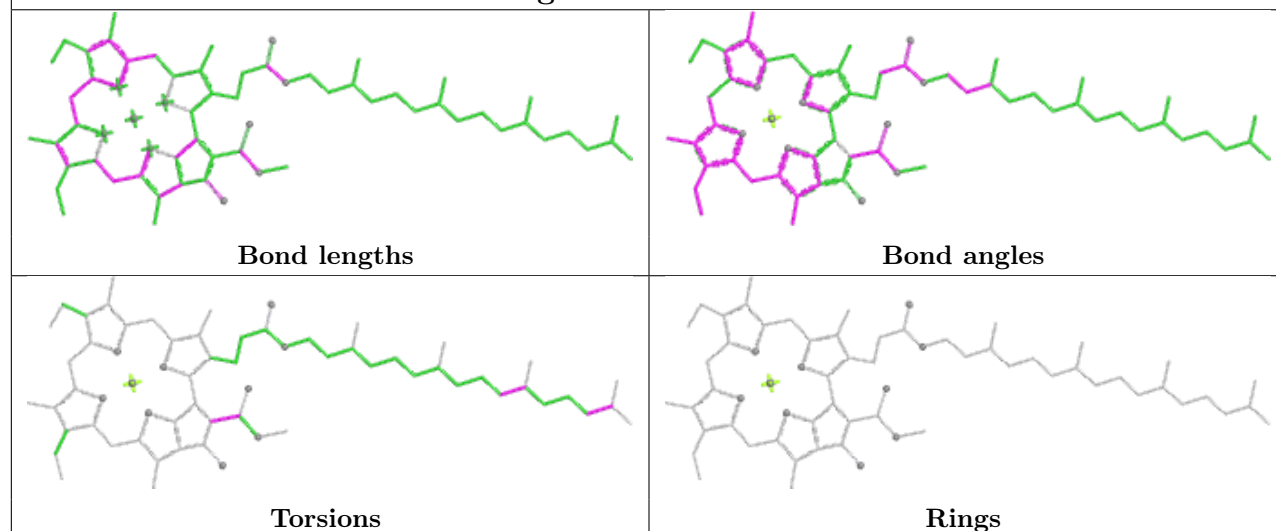
Ligand CLA C 511

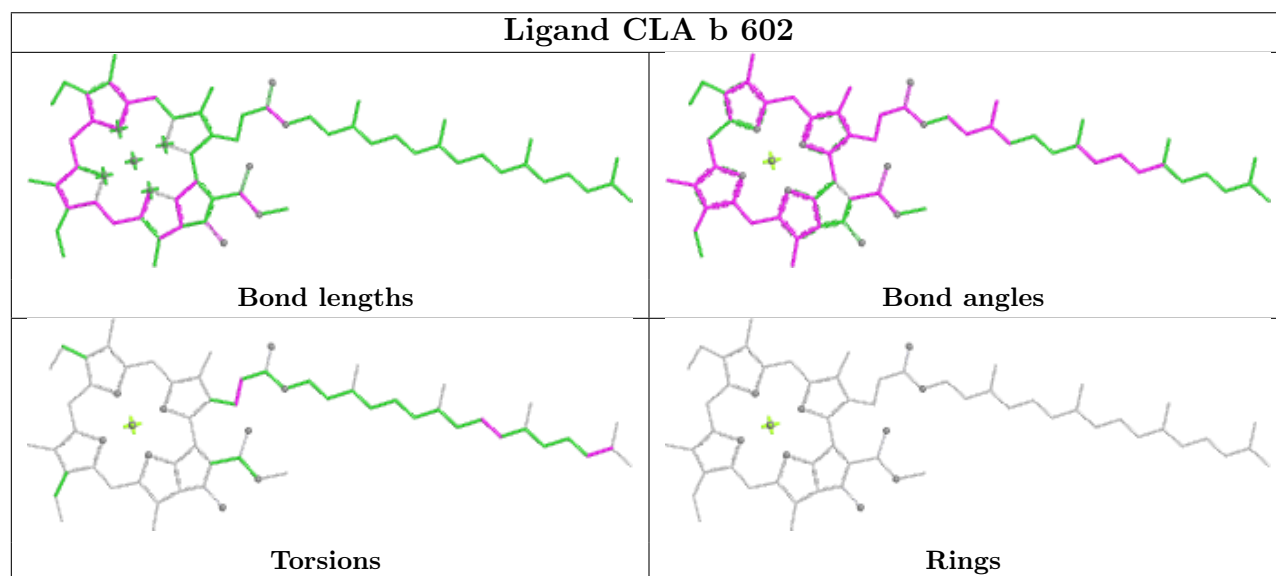
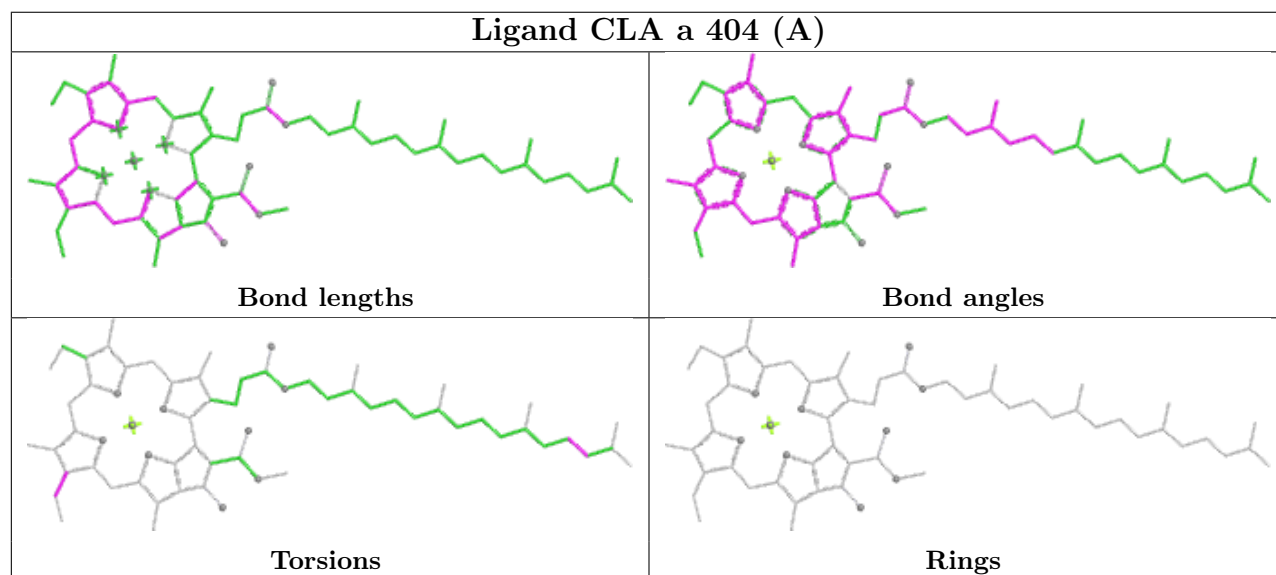
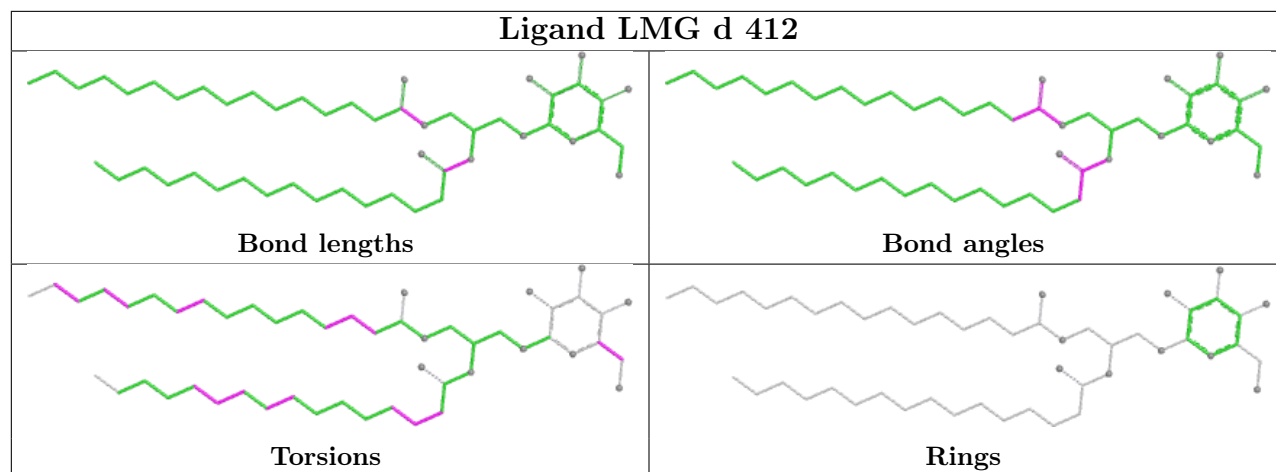


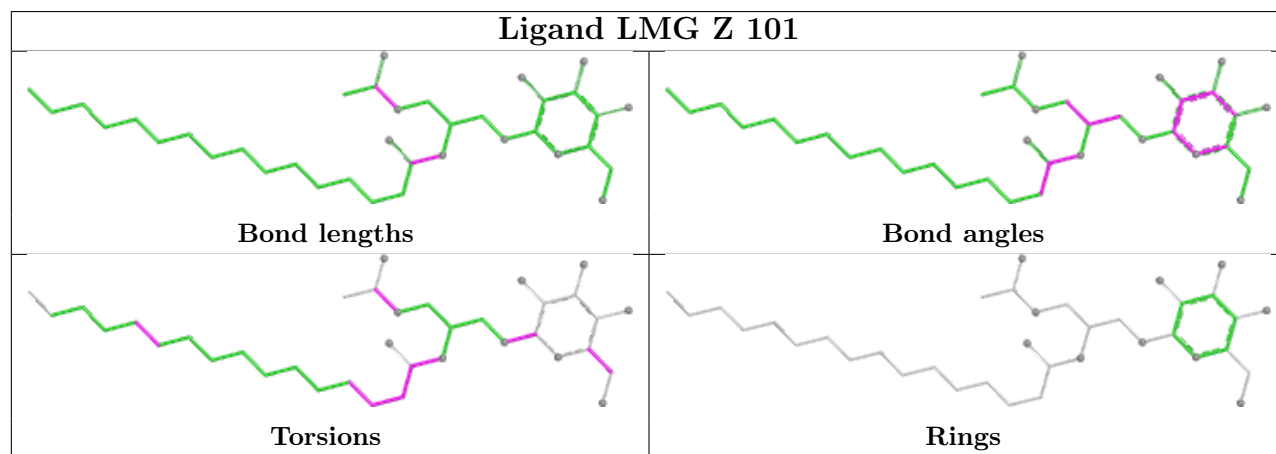
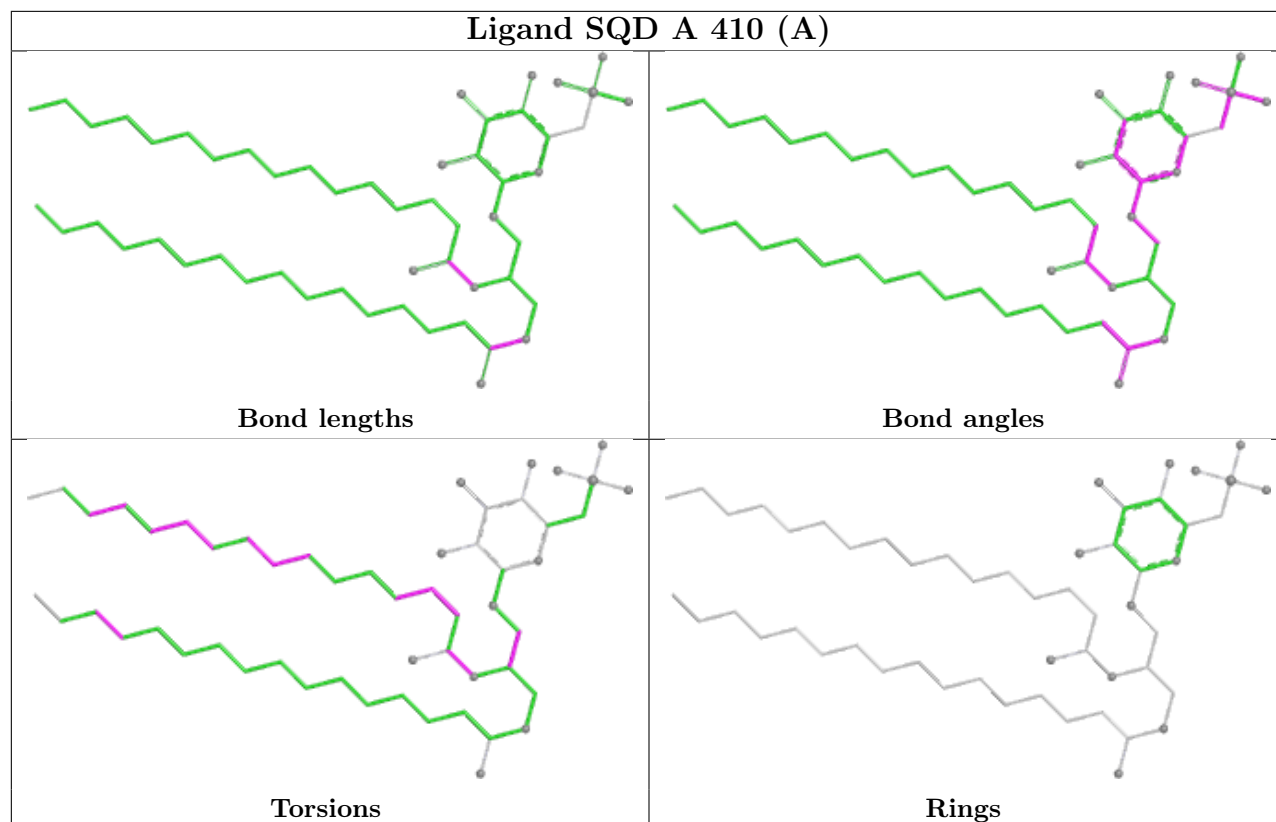
Ligand HTG b 623

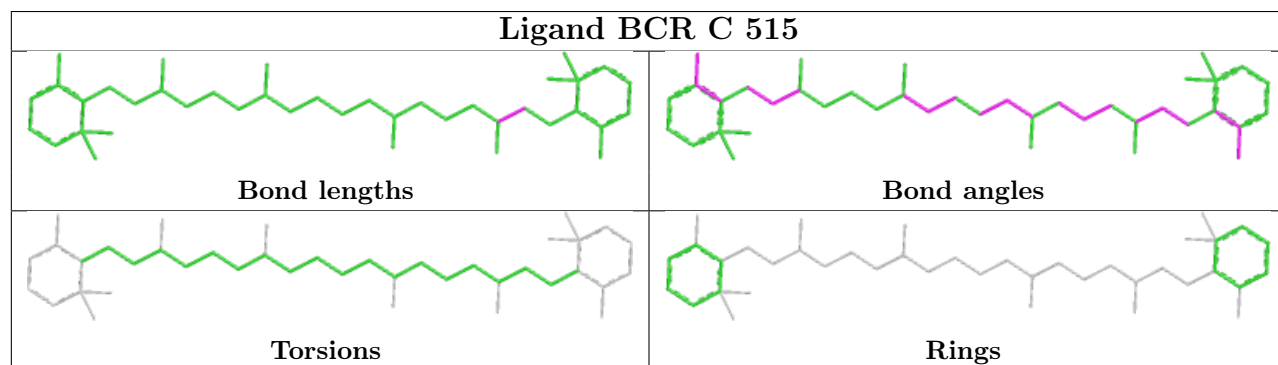
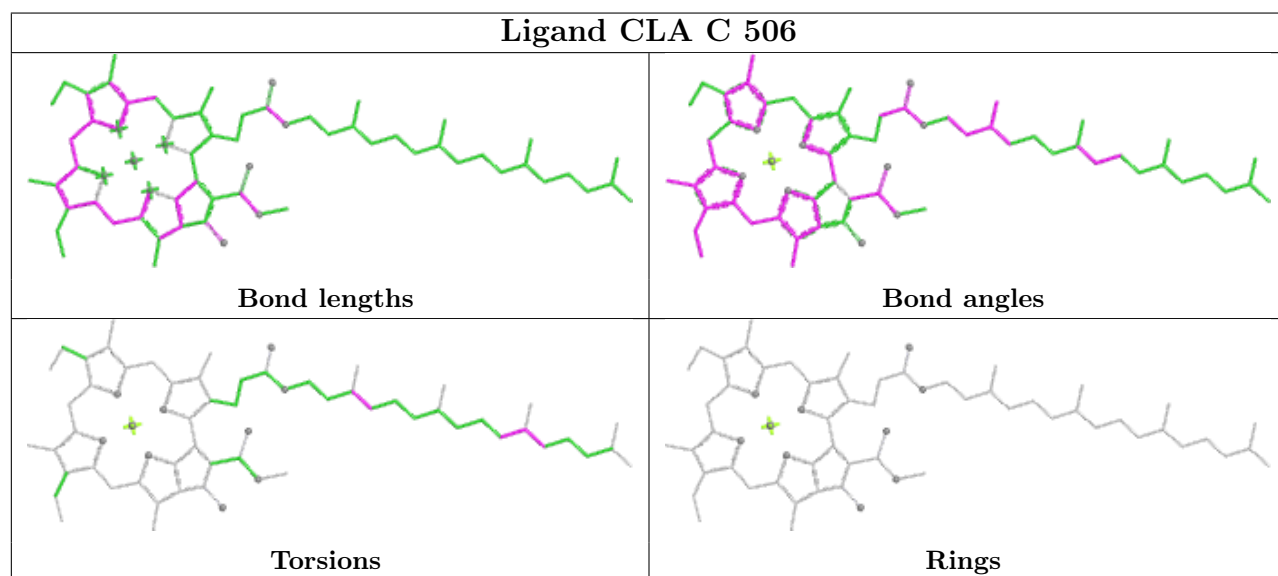
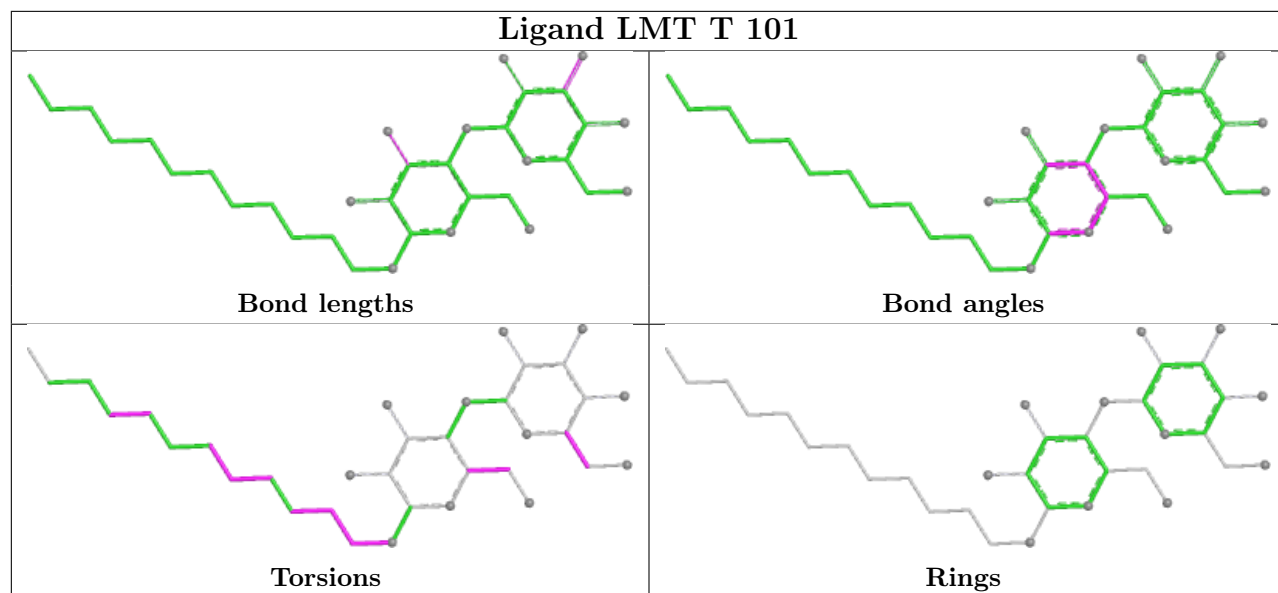


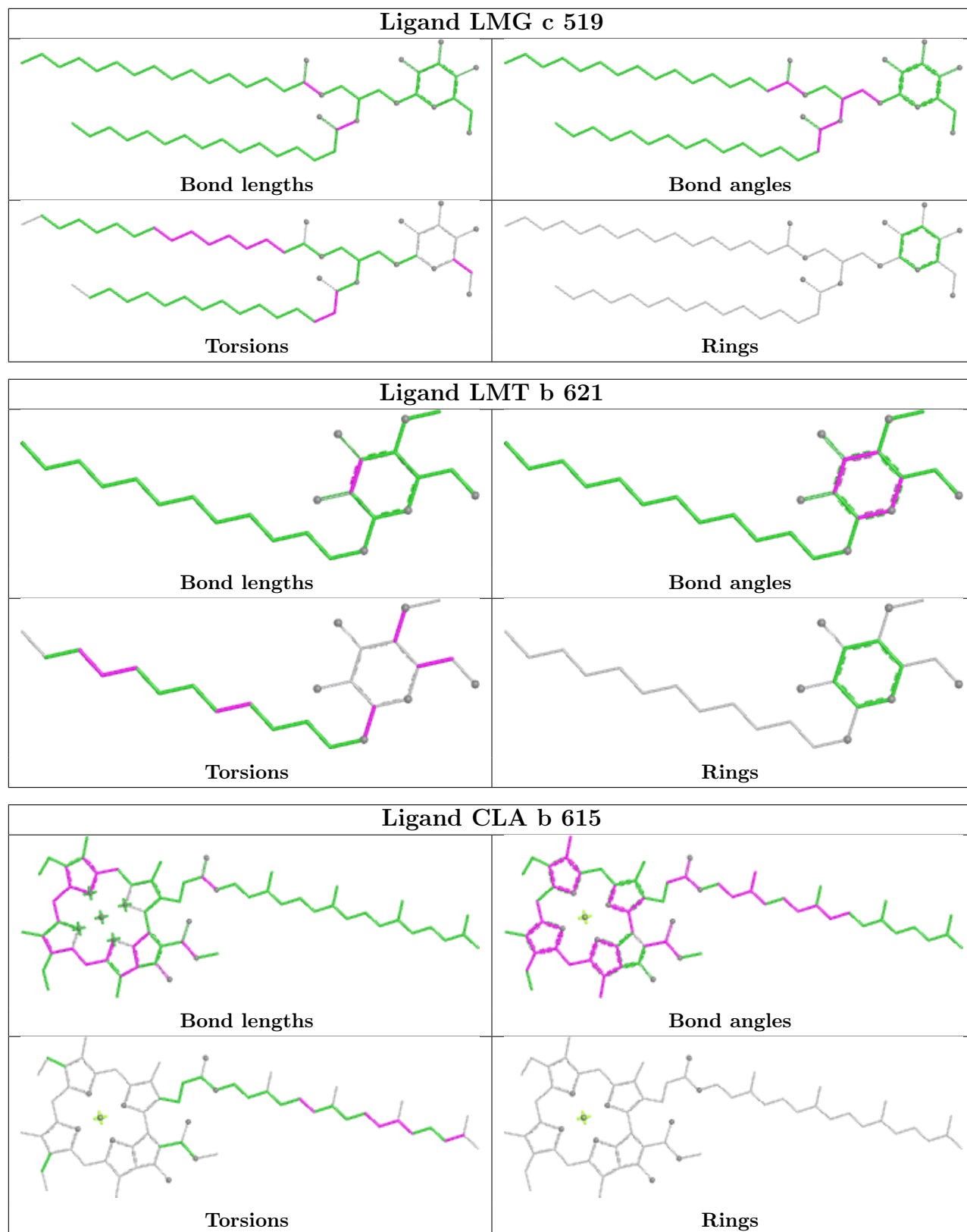
Ligand CLA c 502

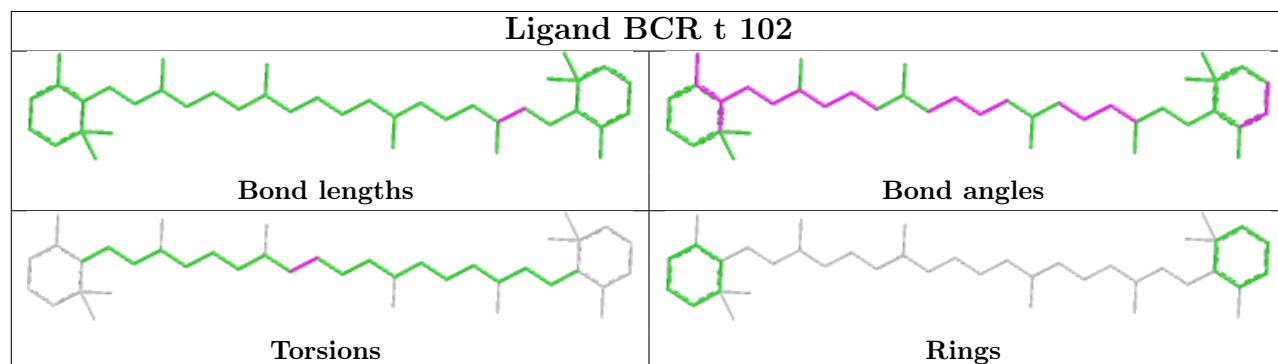
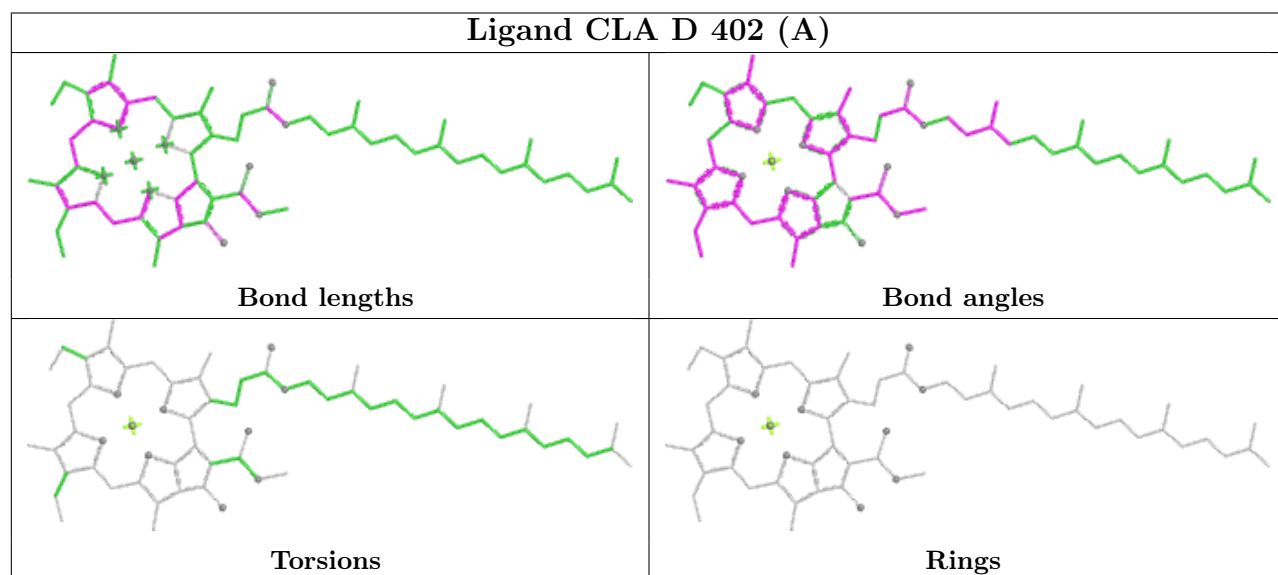
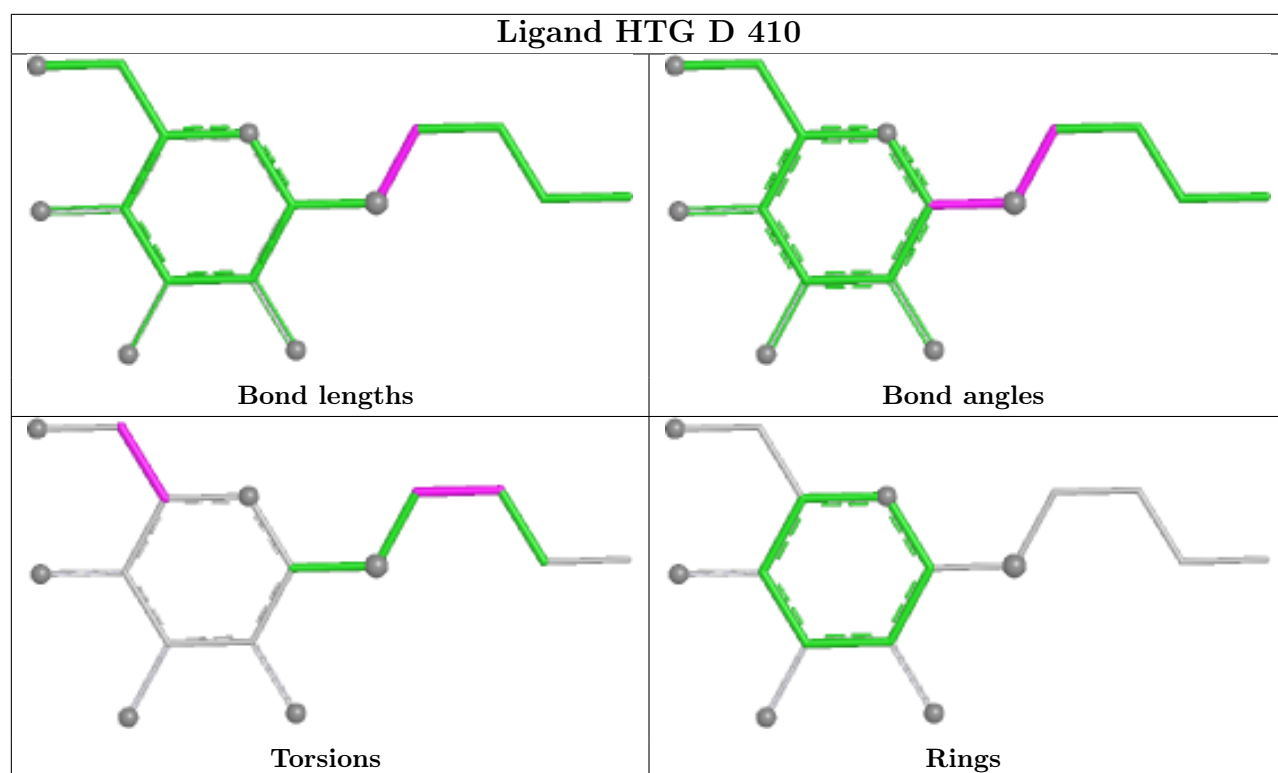


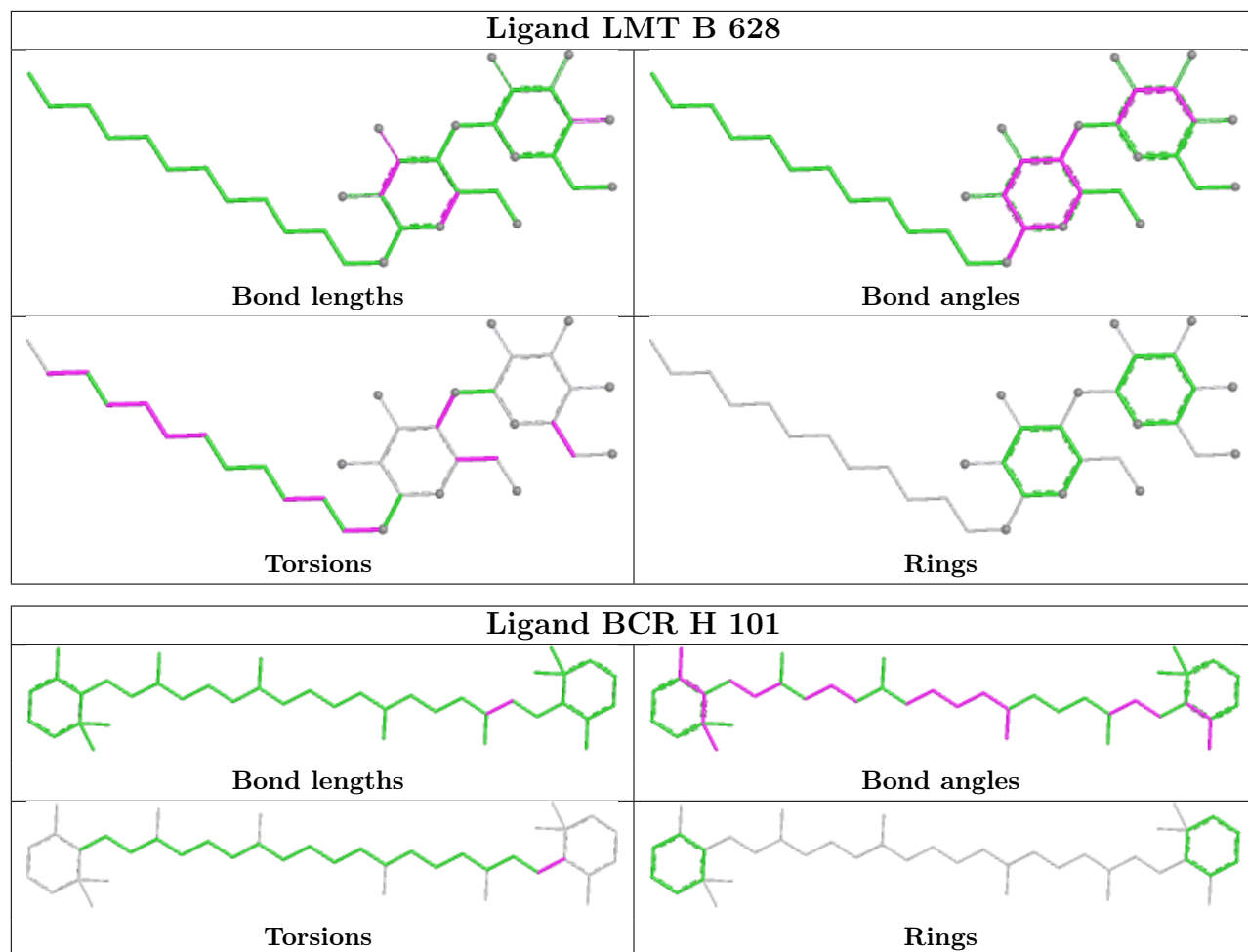


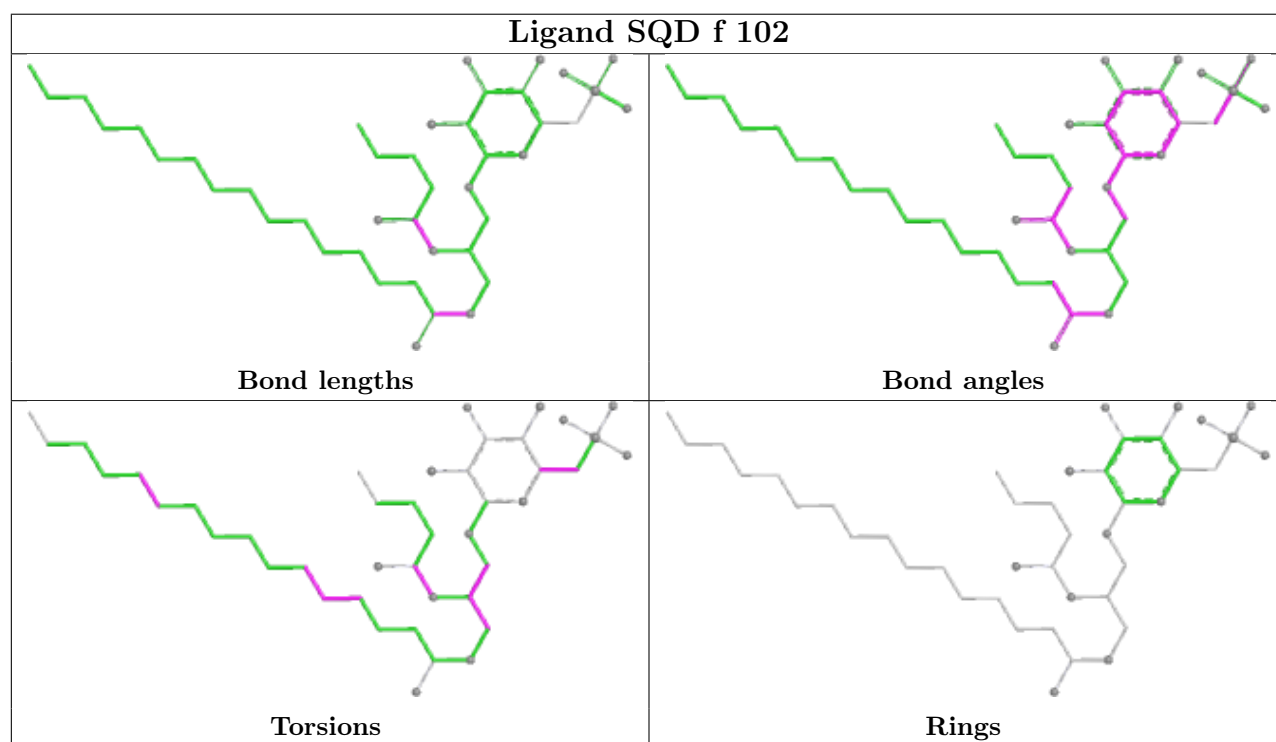
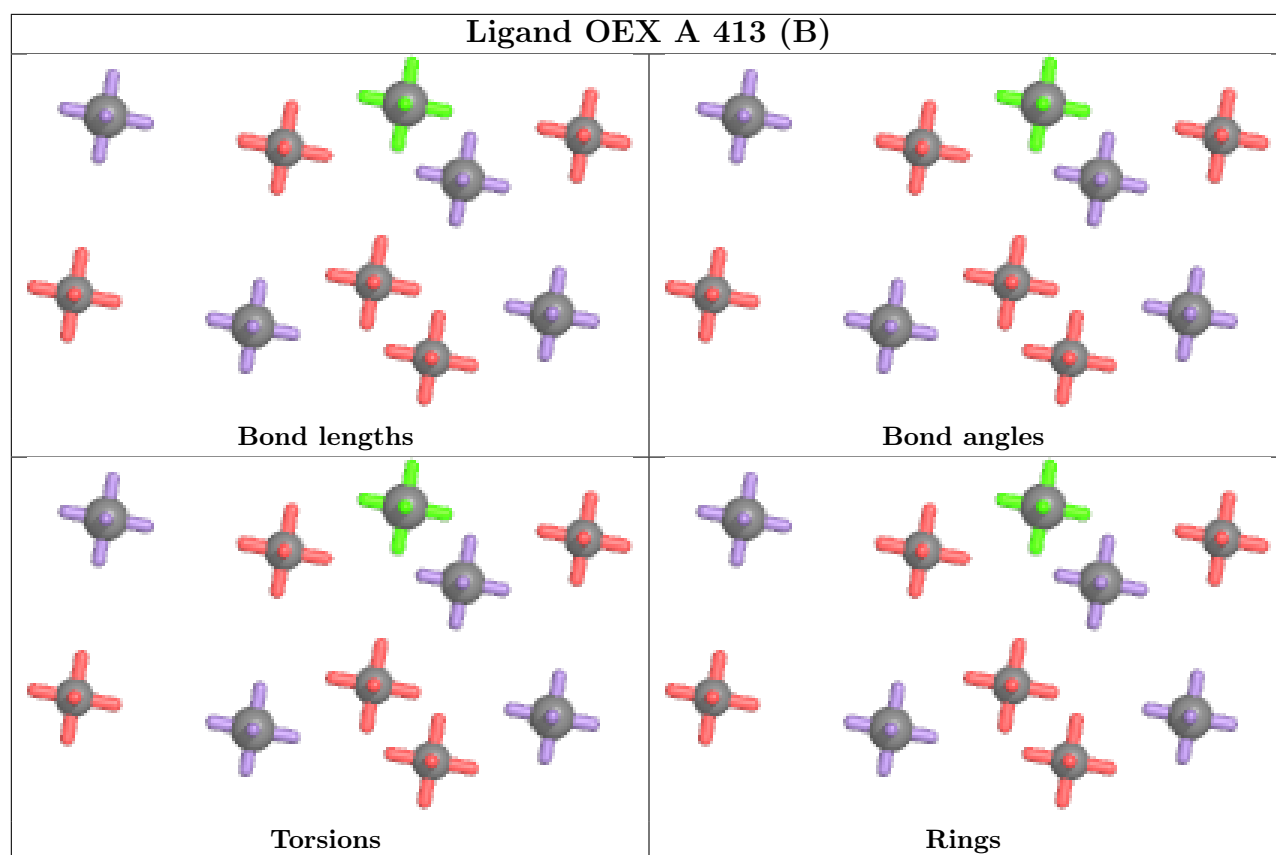


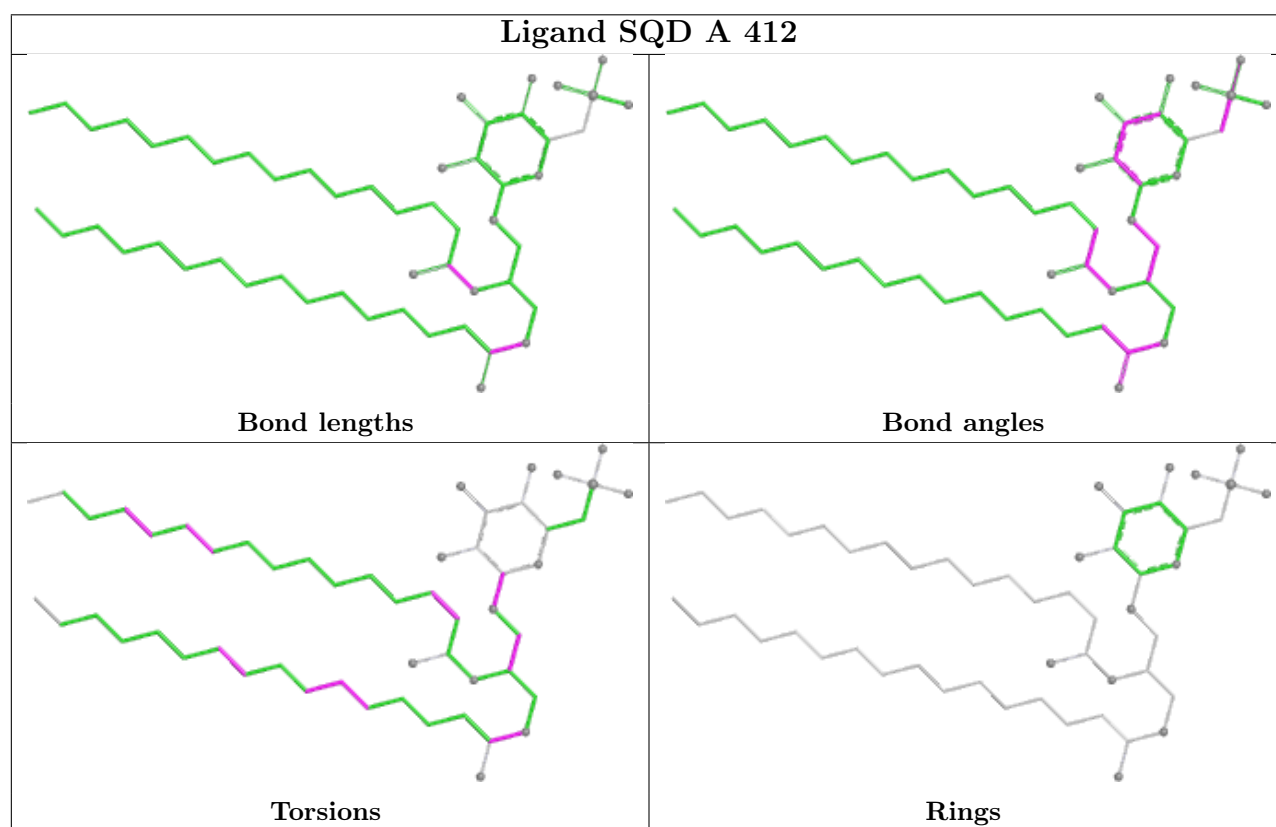
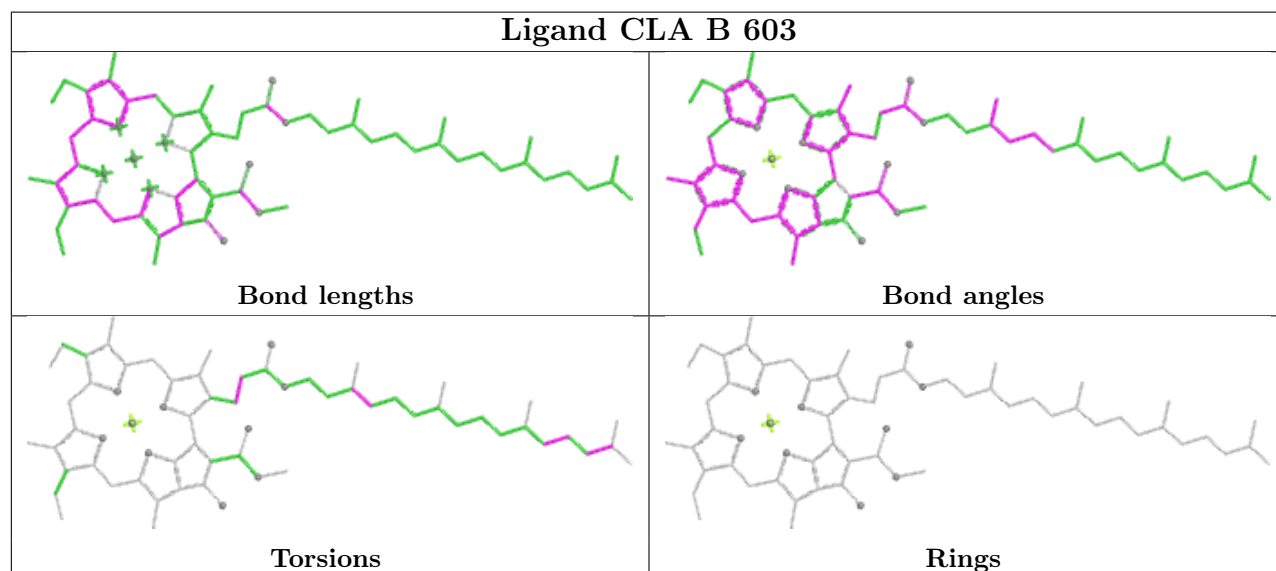
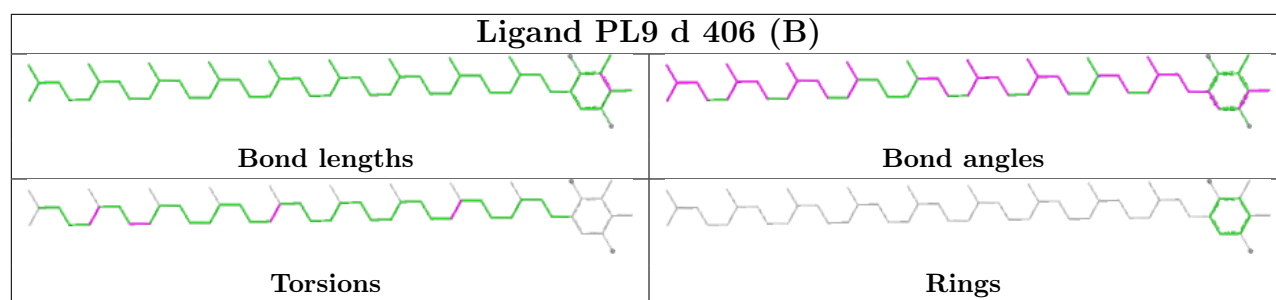




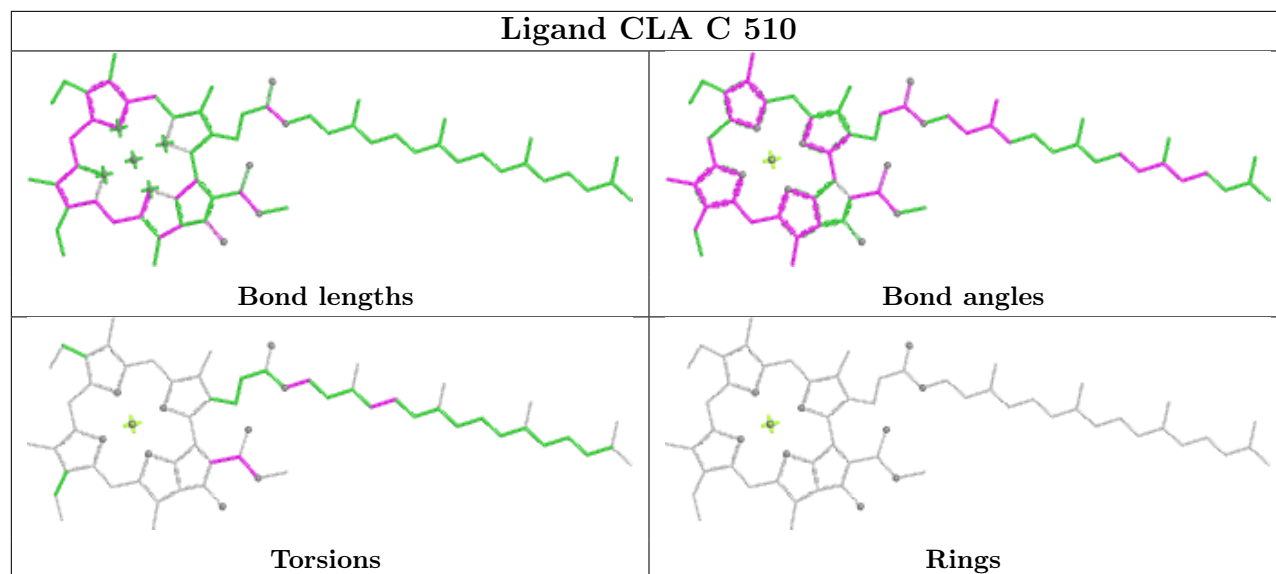




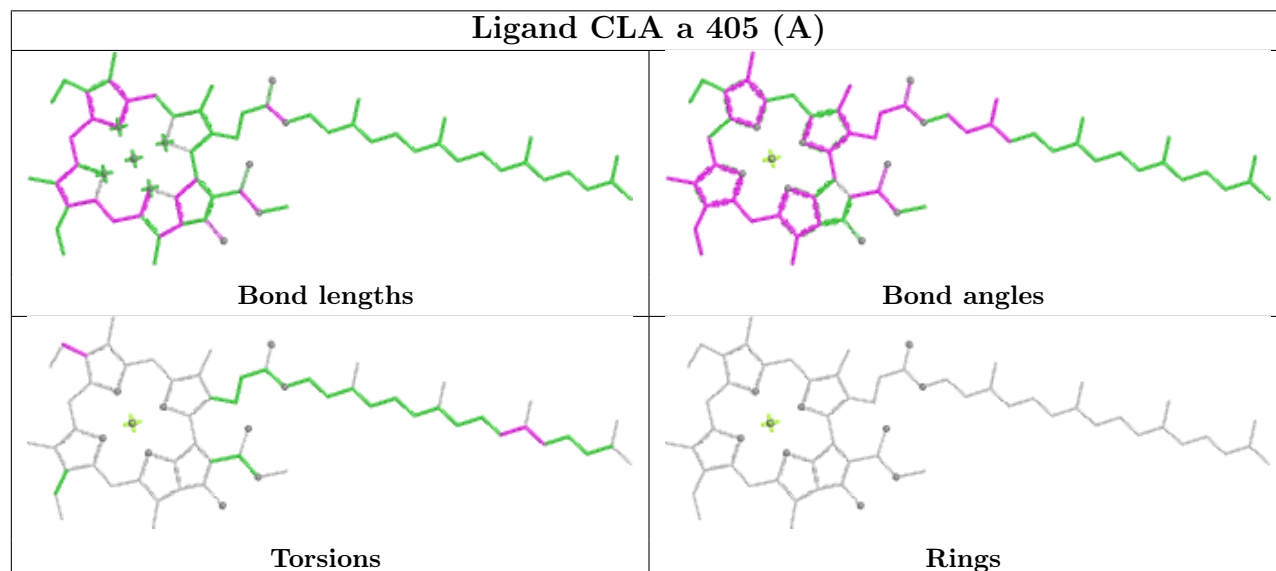




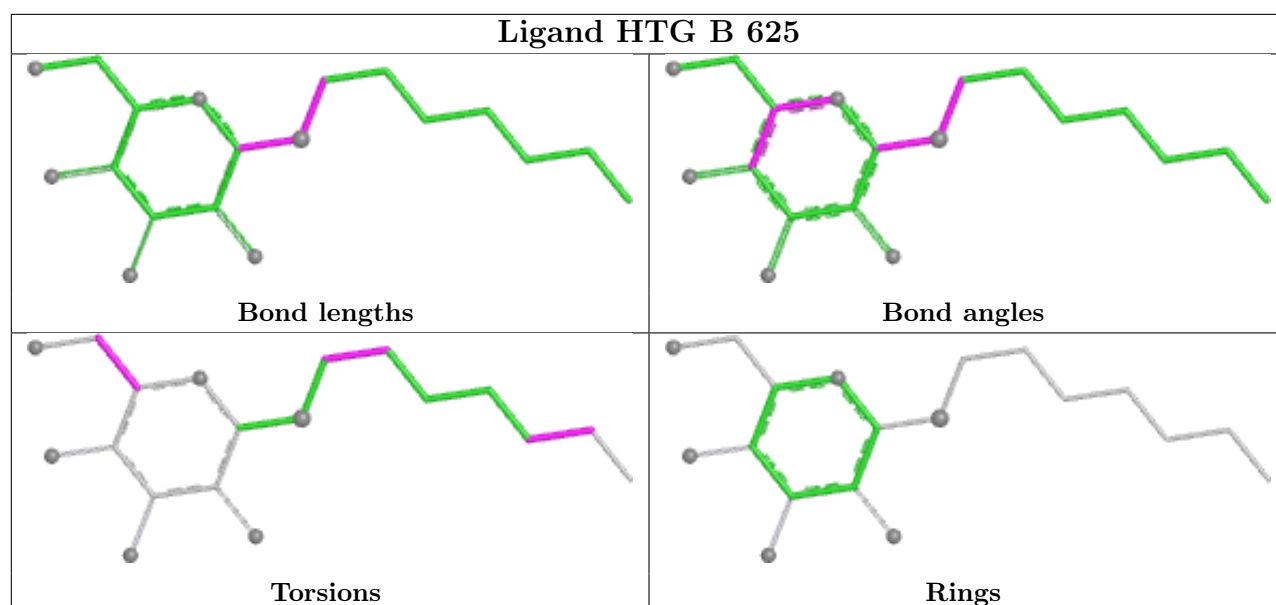
Ligand CLA C 510

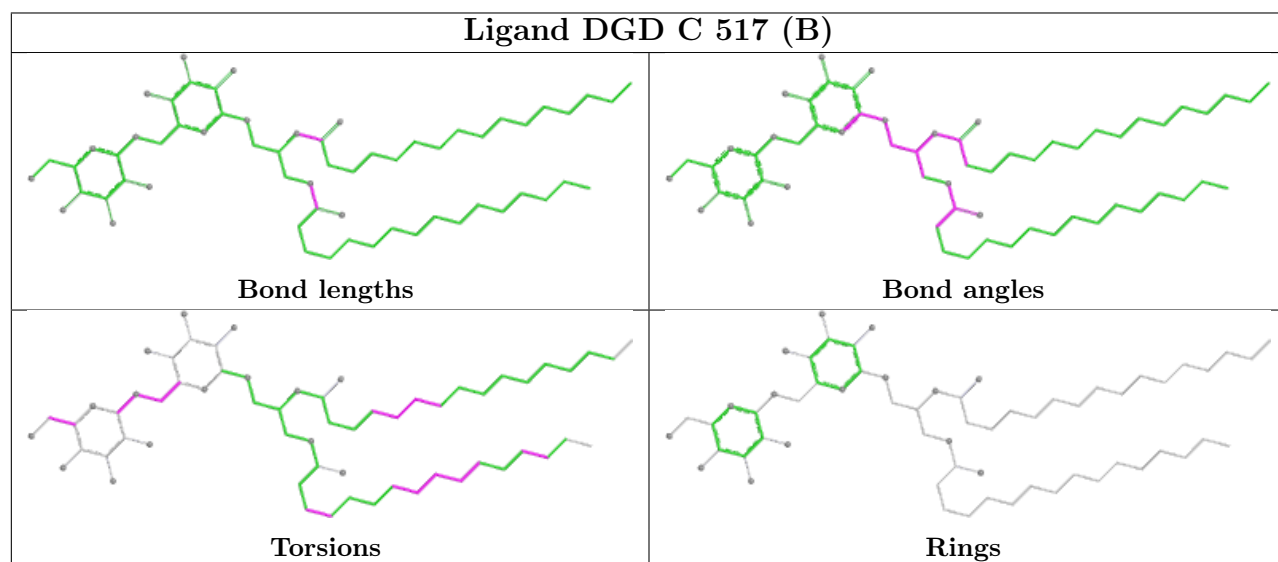
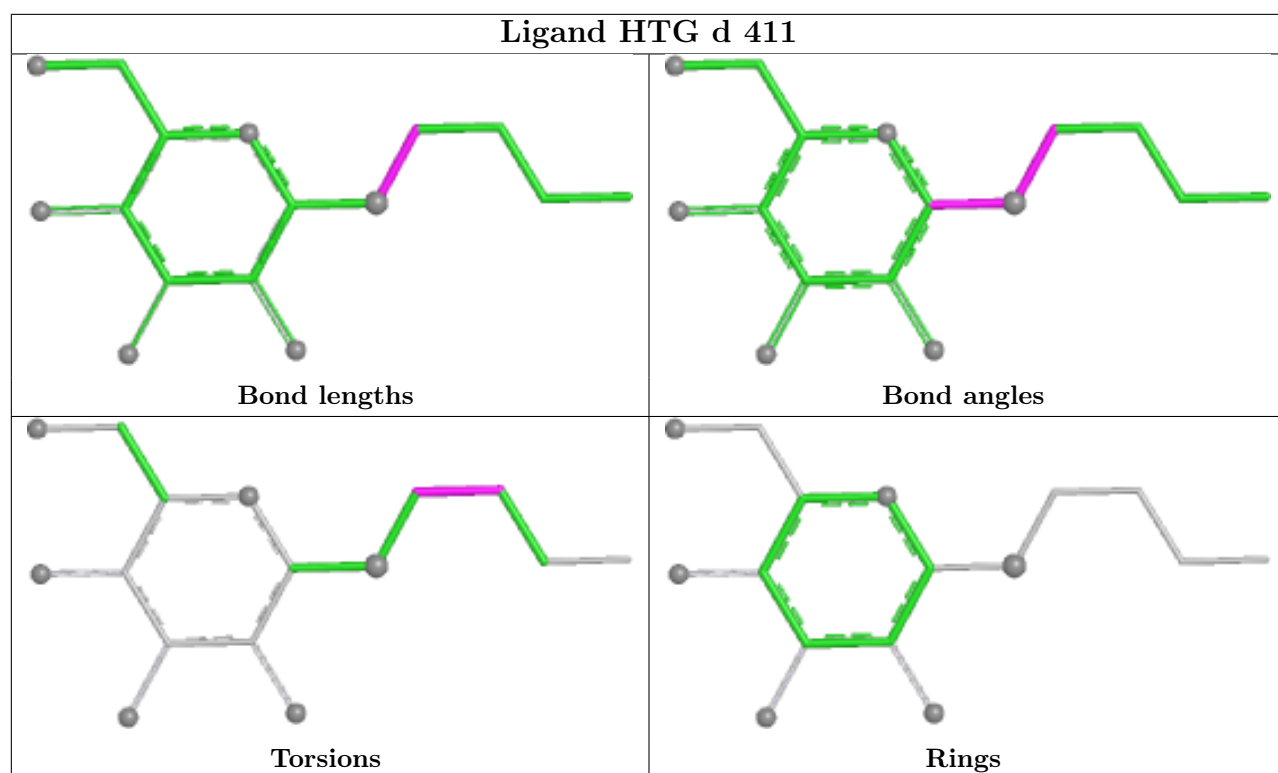


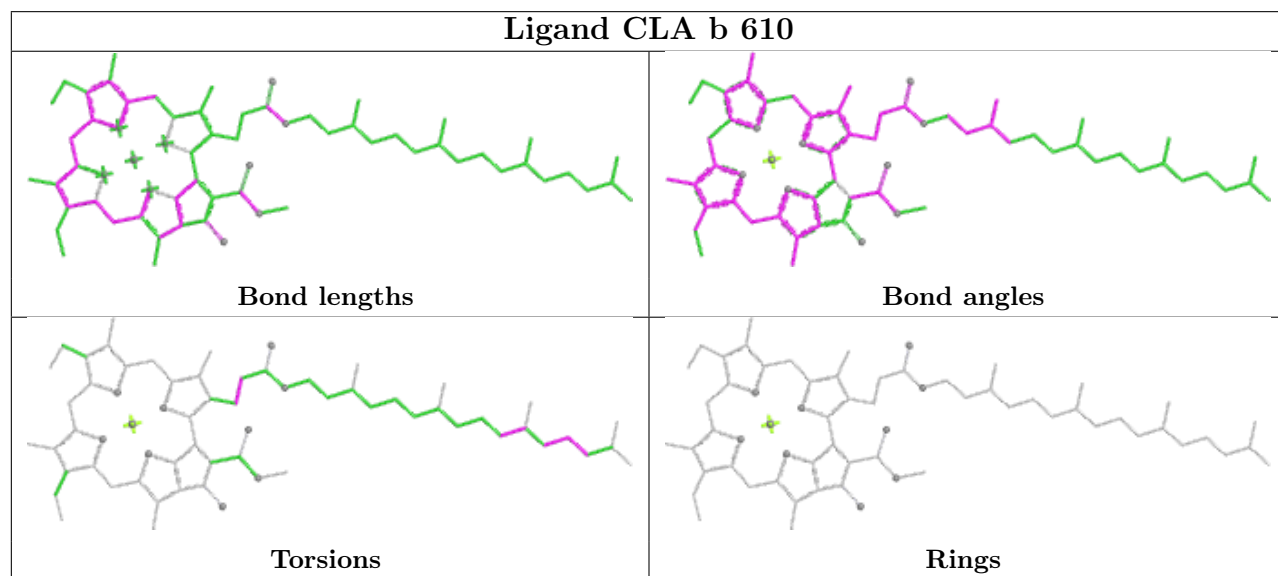
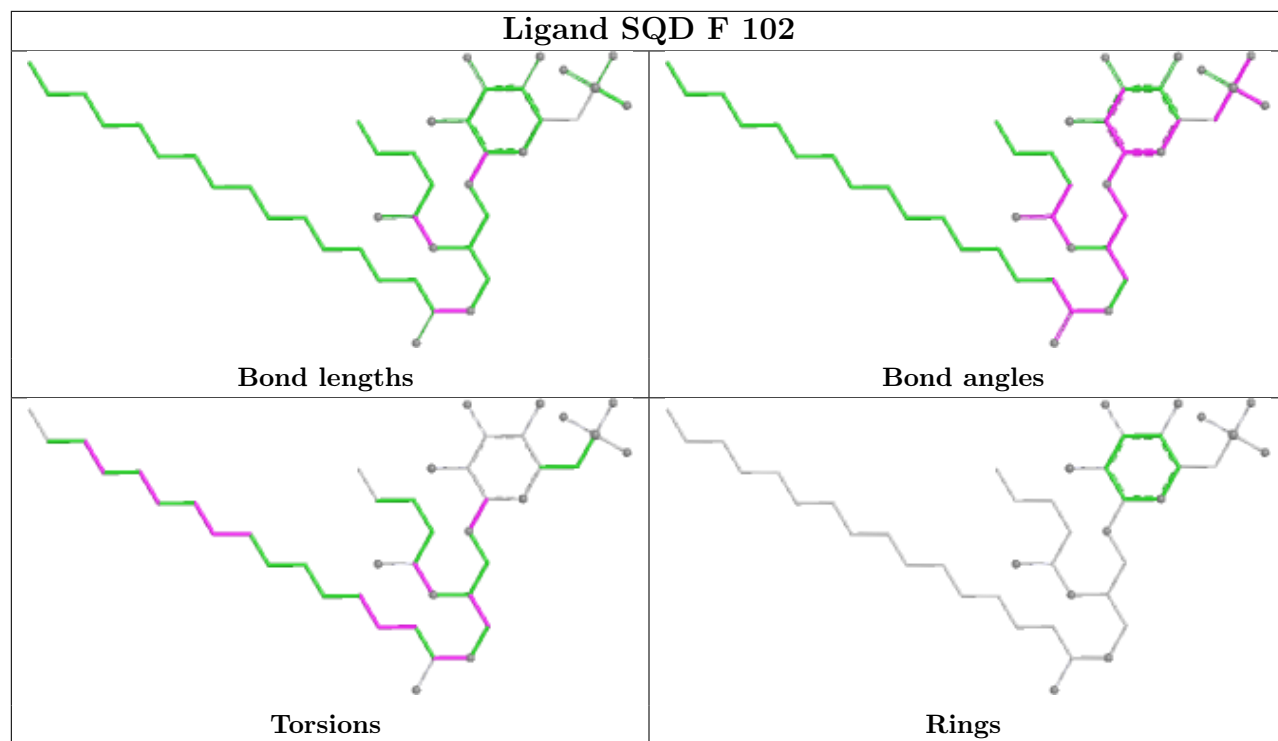
Ligand CLA a 405 (A)

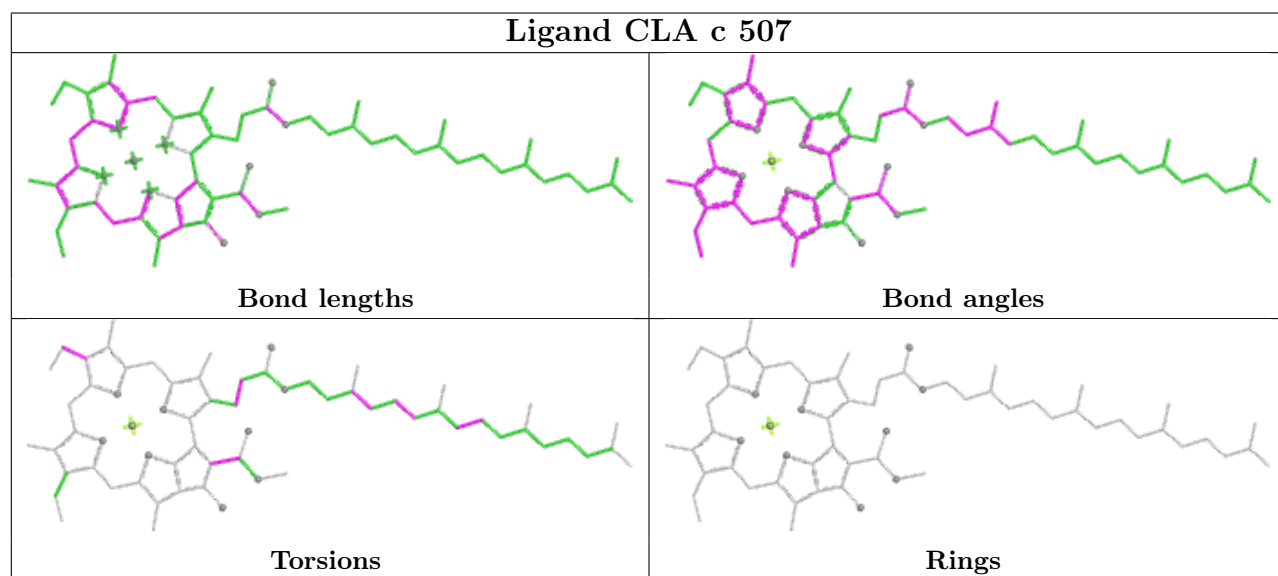
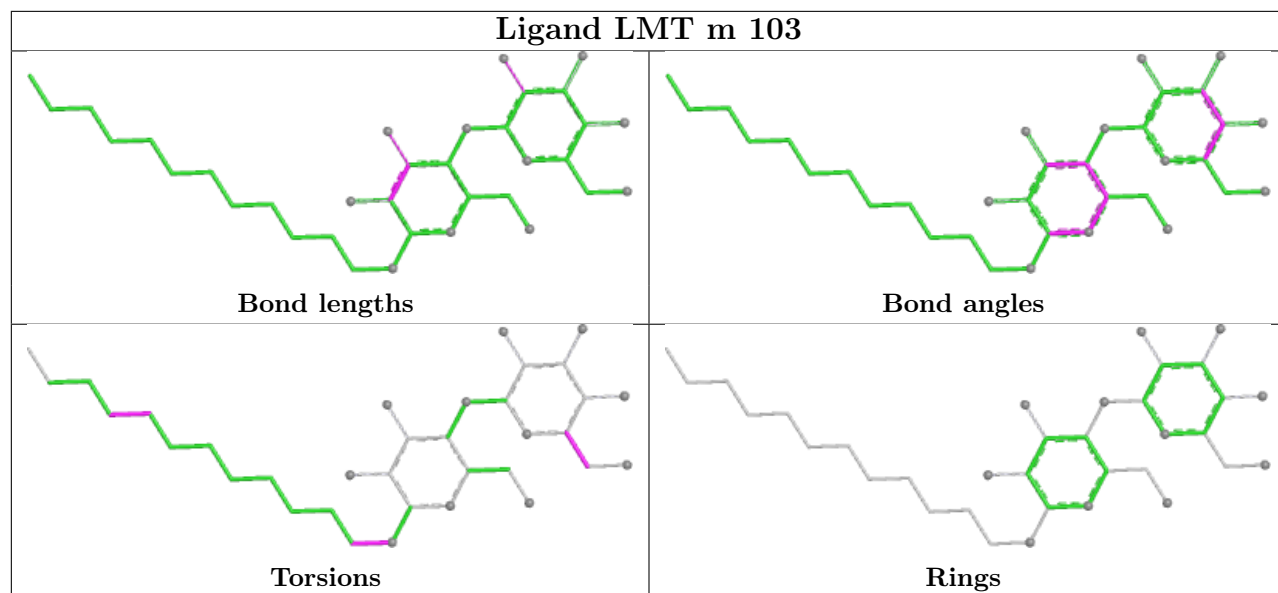


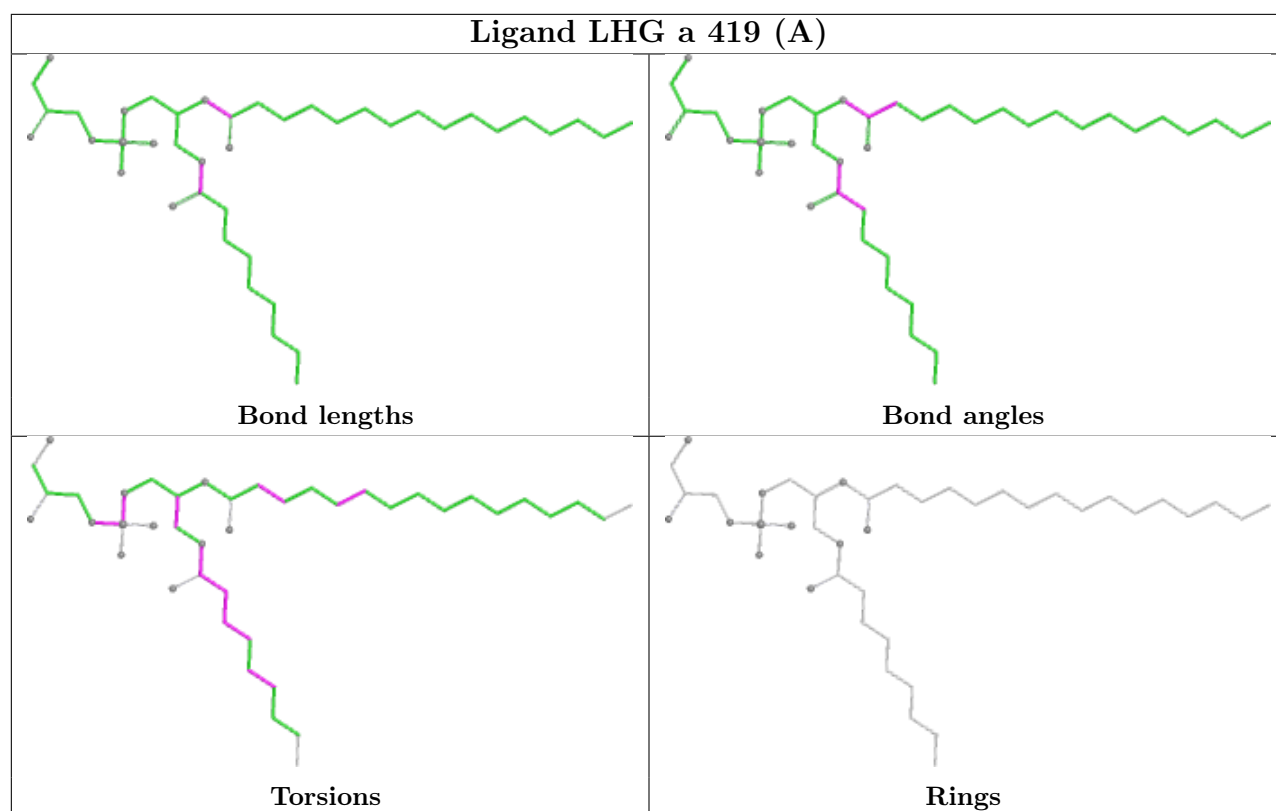
Ligand HTG B 625

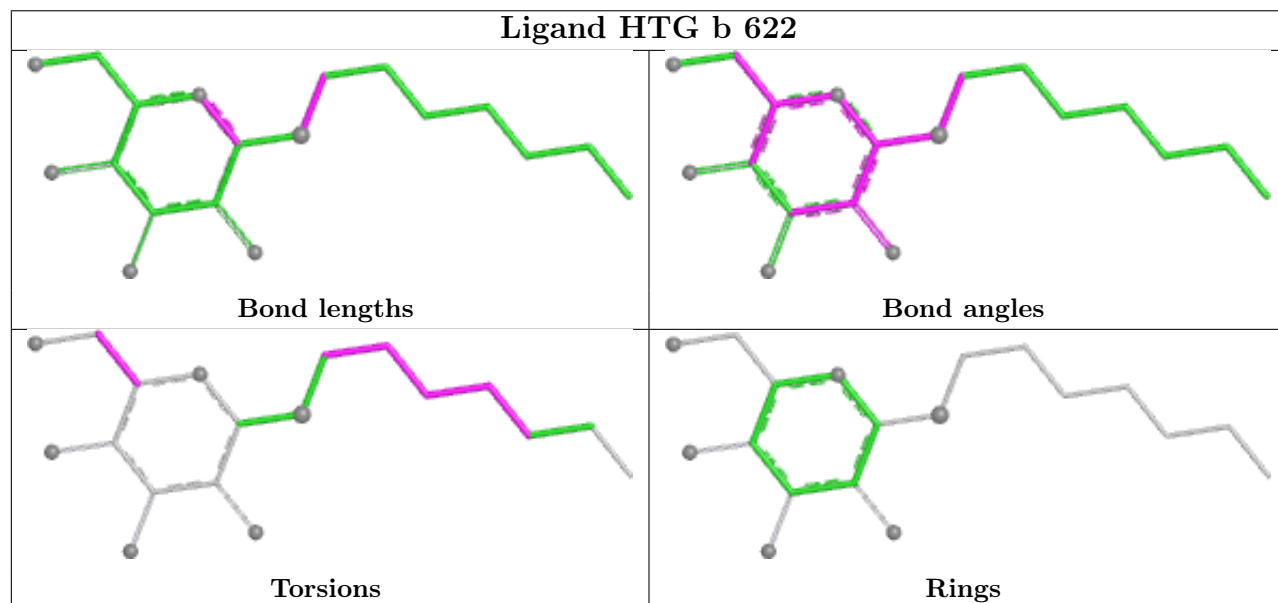
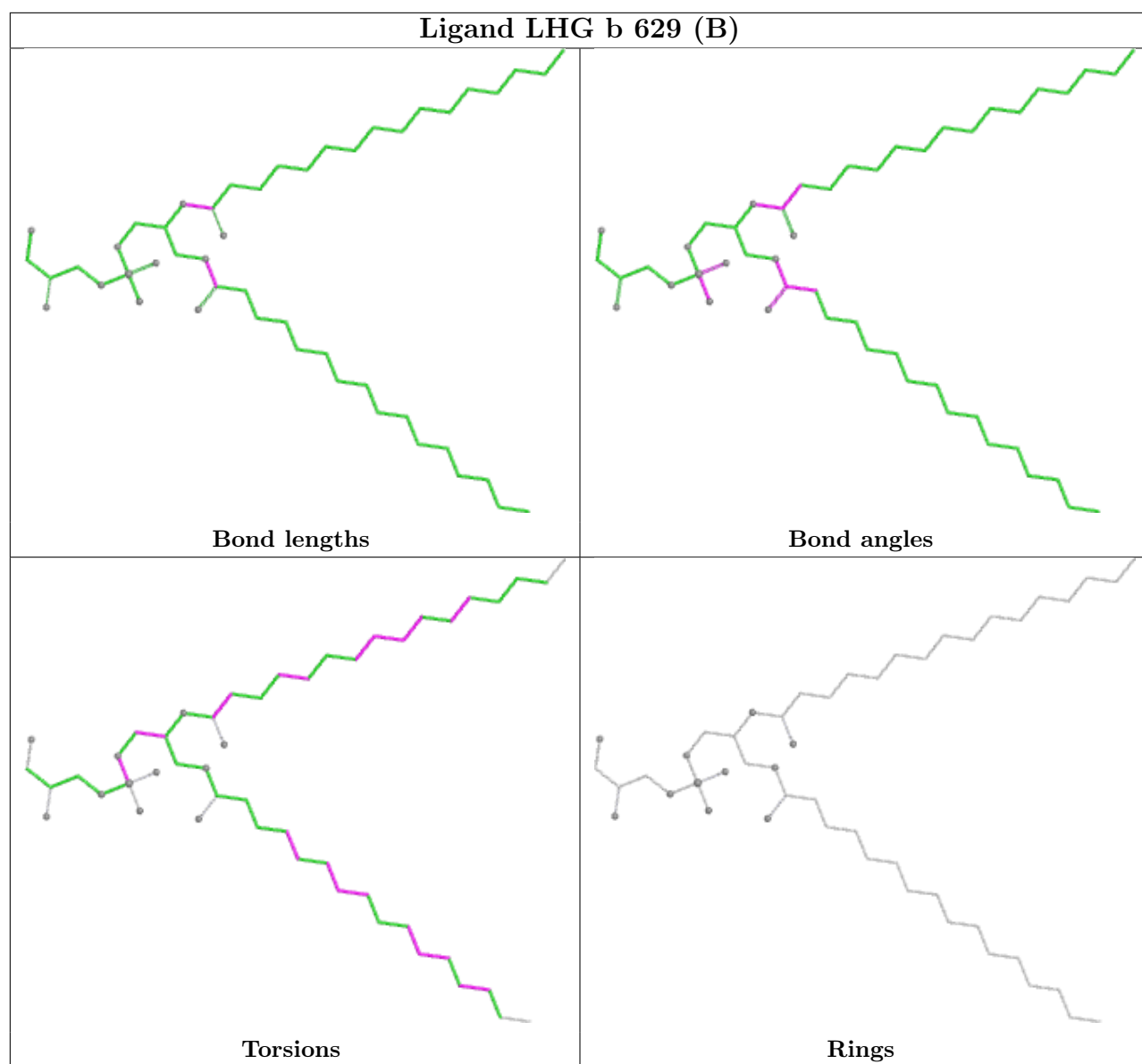


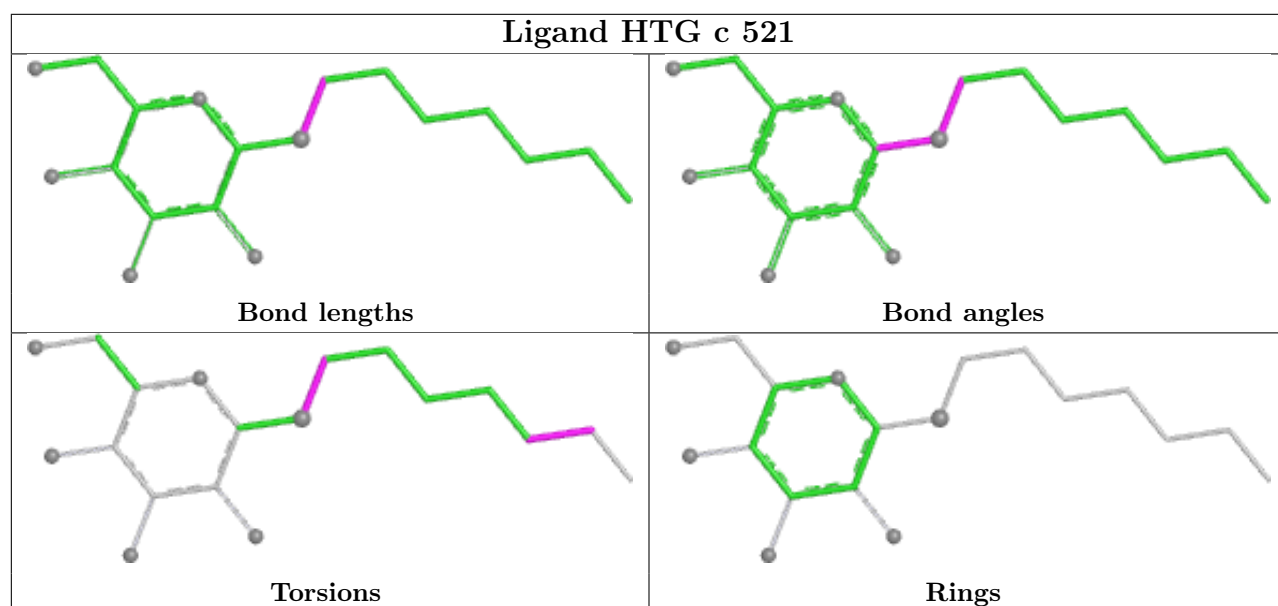
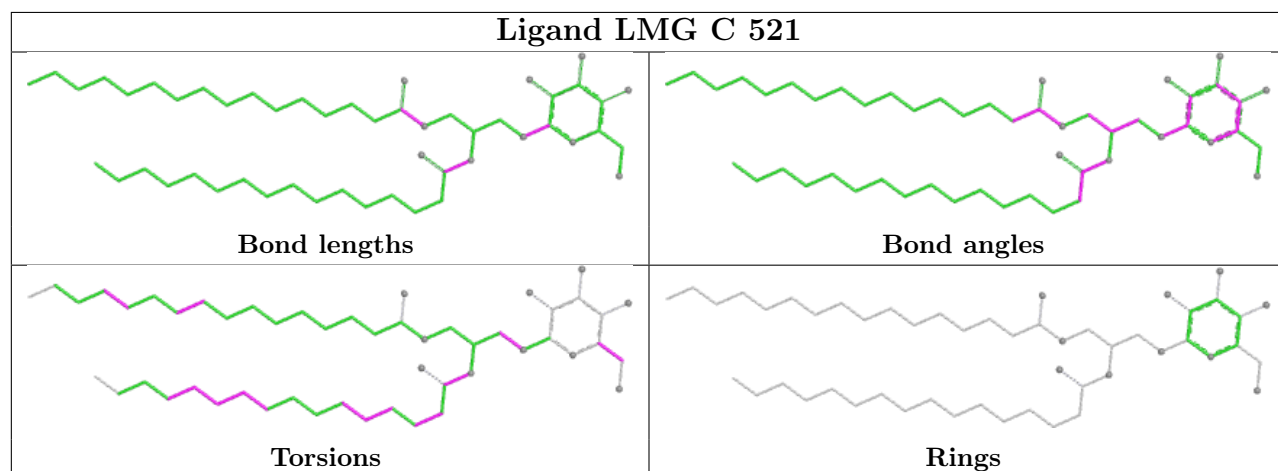
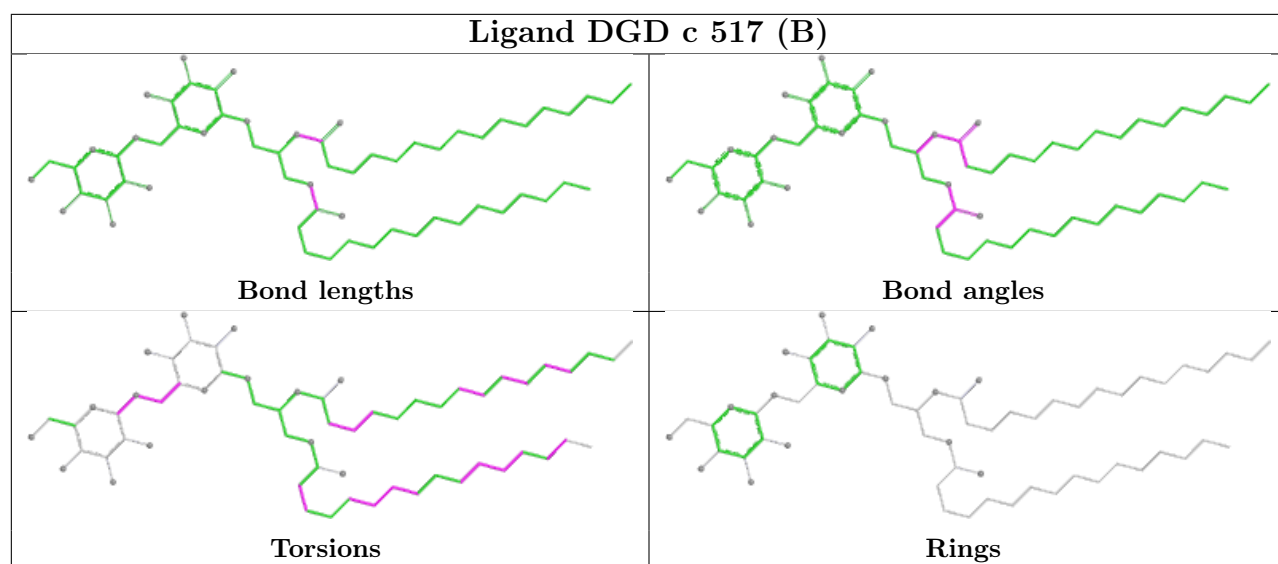


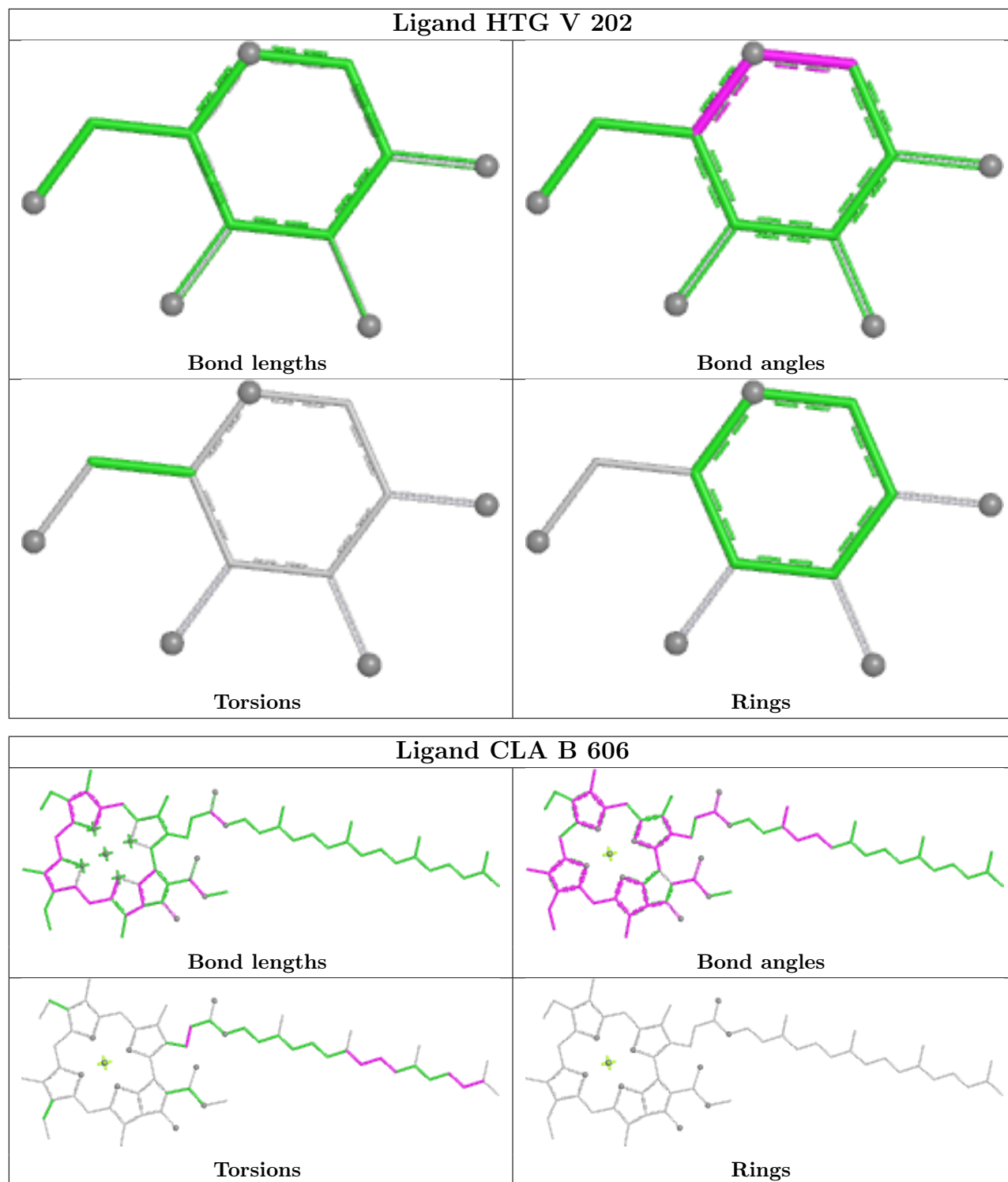


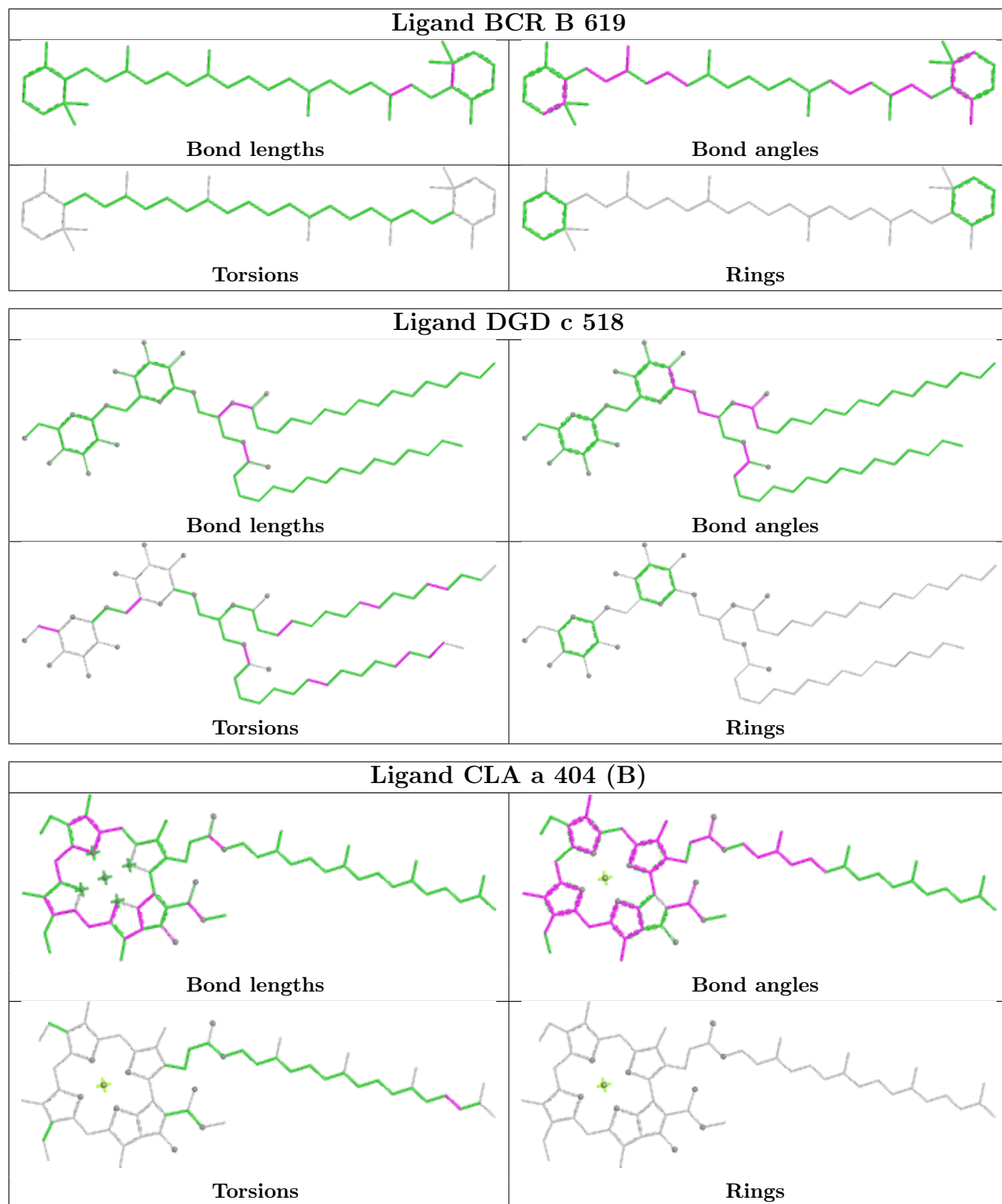




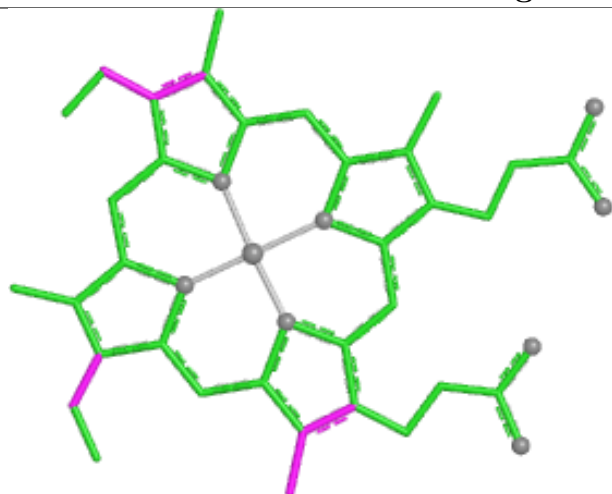




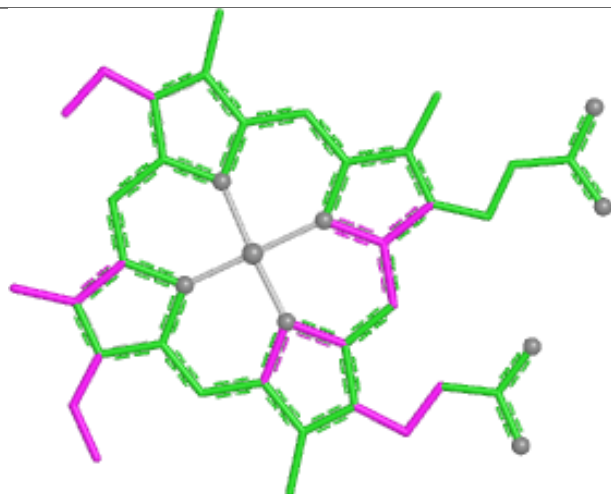




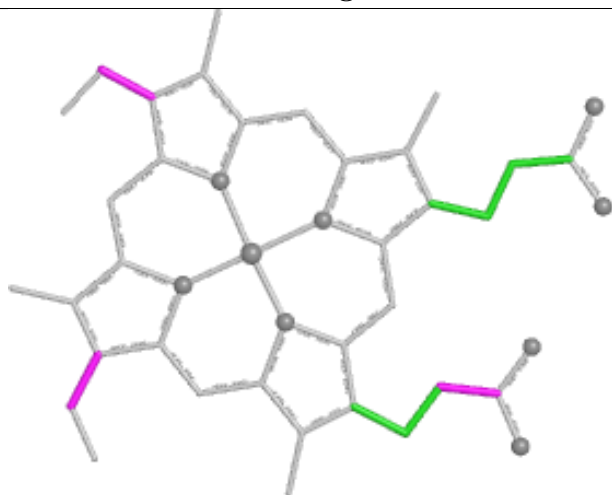
Ligand HEC v 201



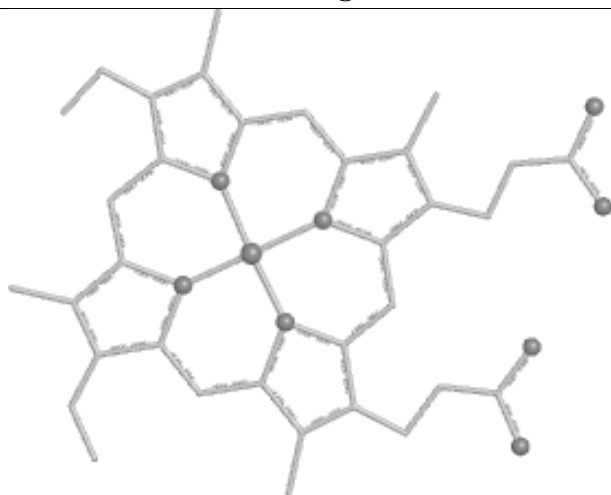
Bond lengths



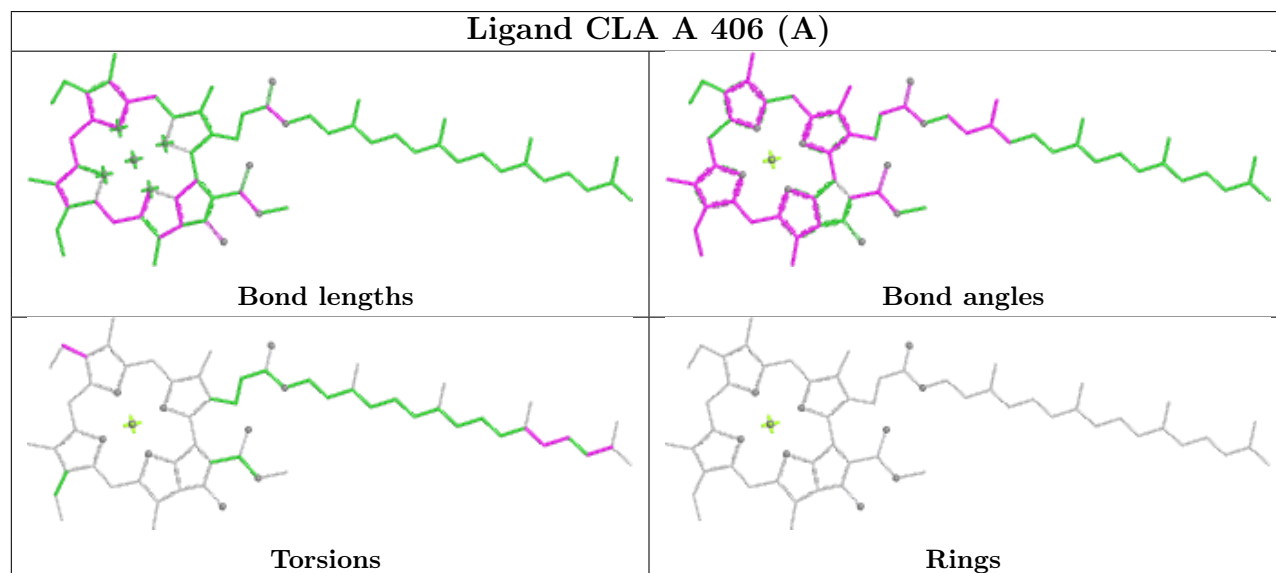
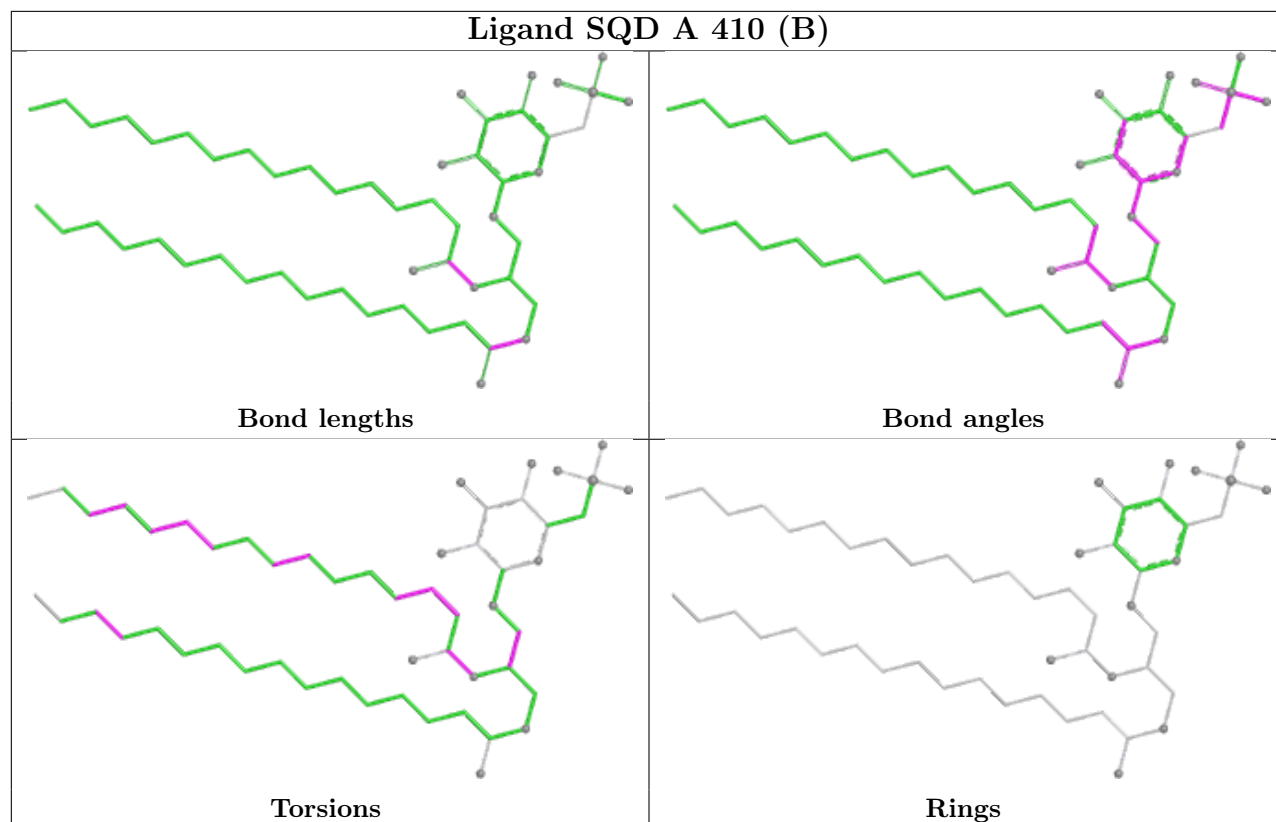
Bond angles

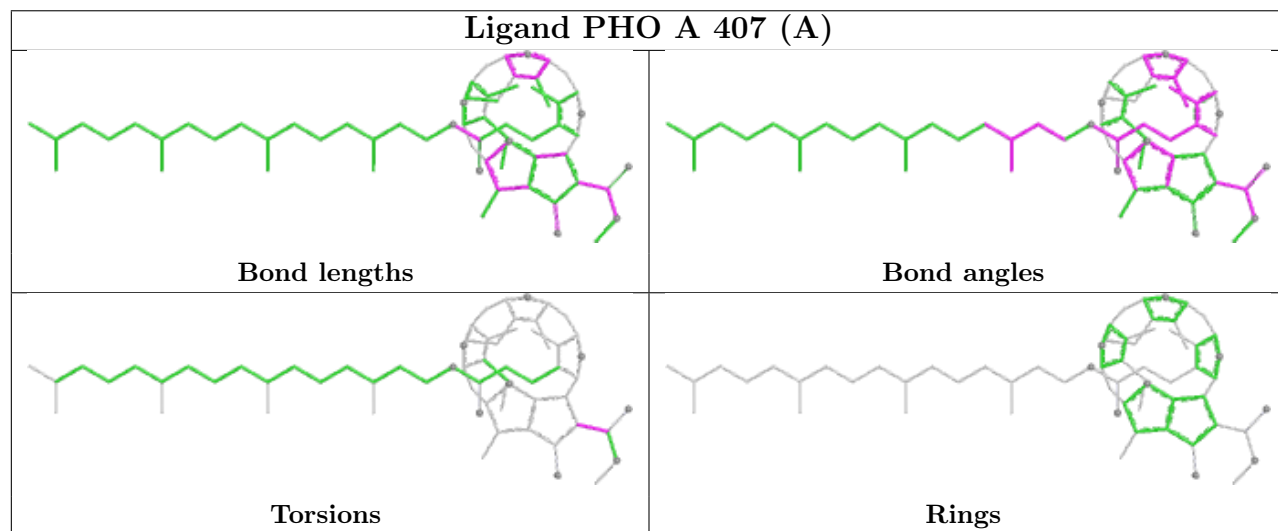
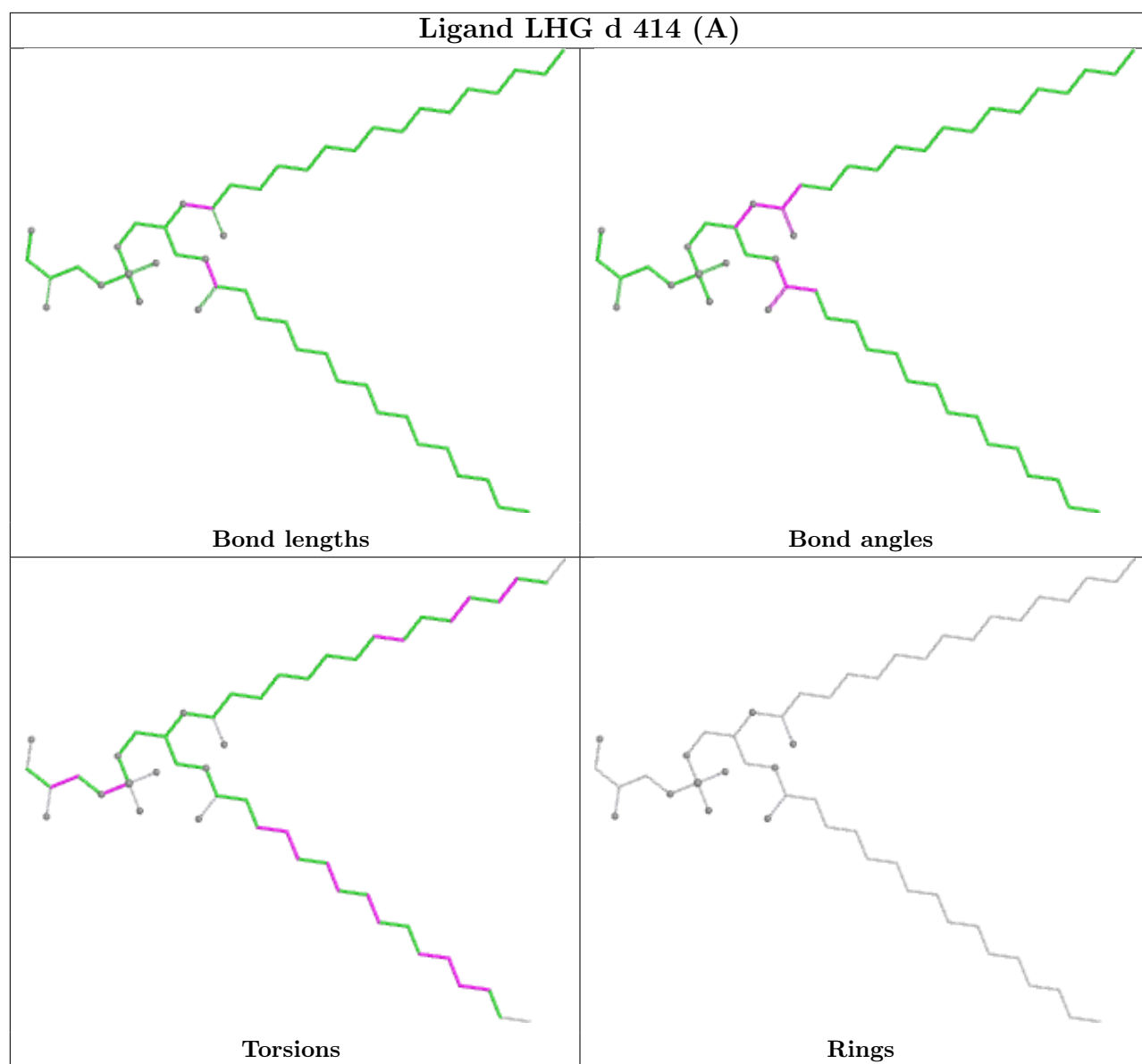


Torsions

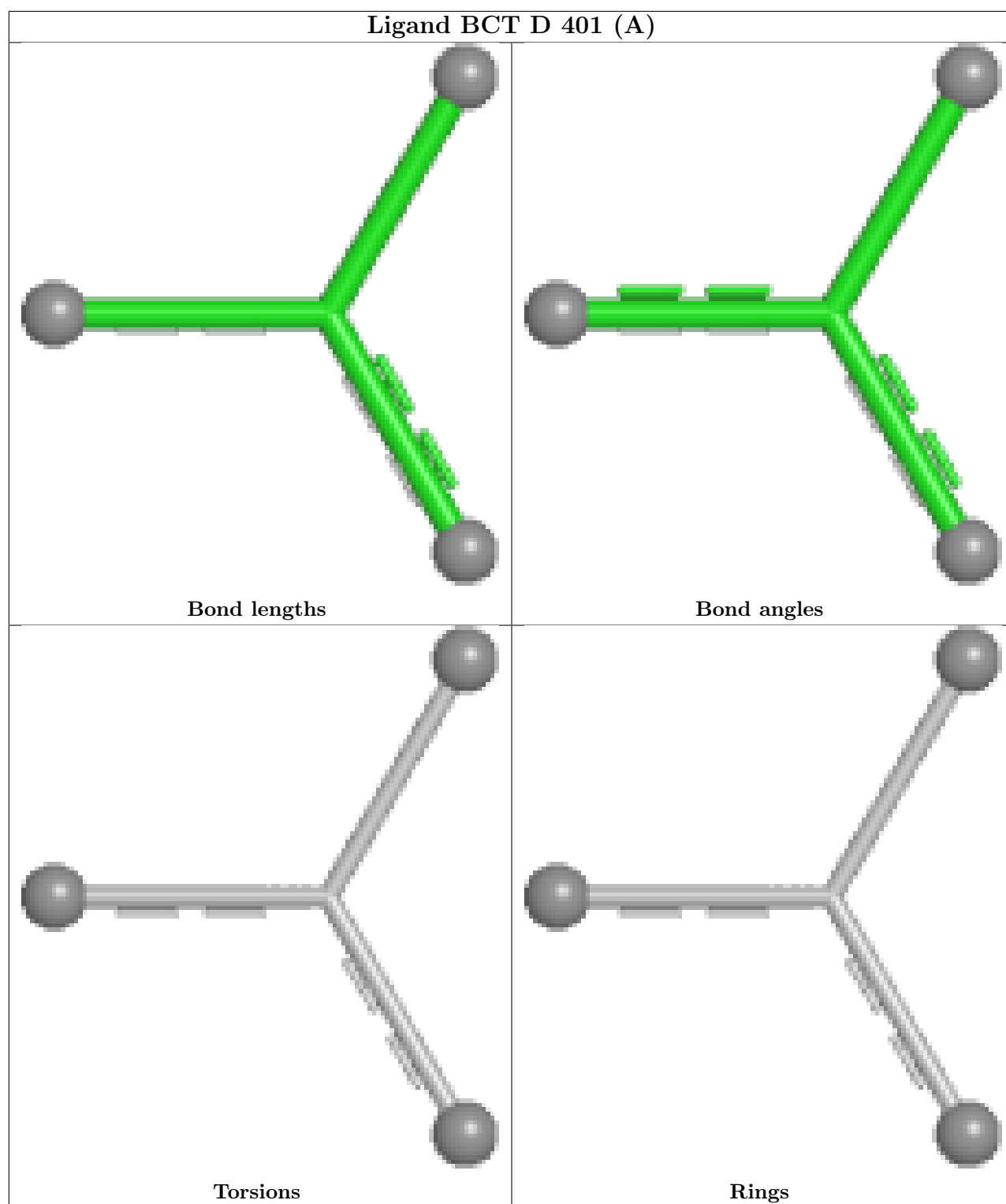


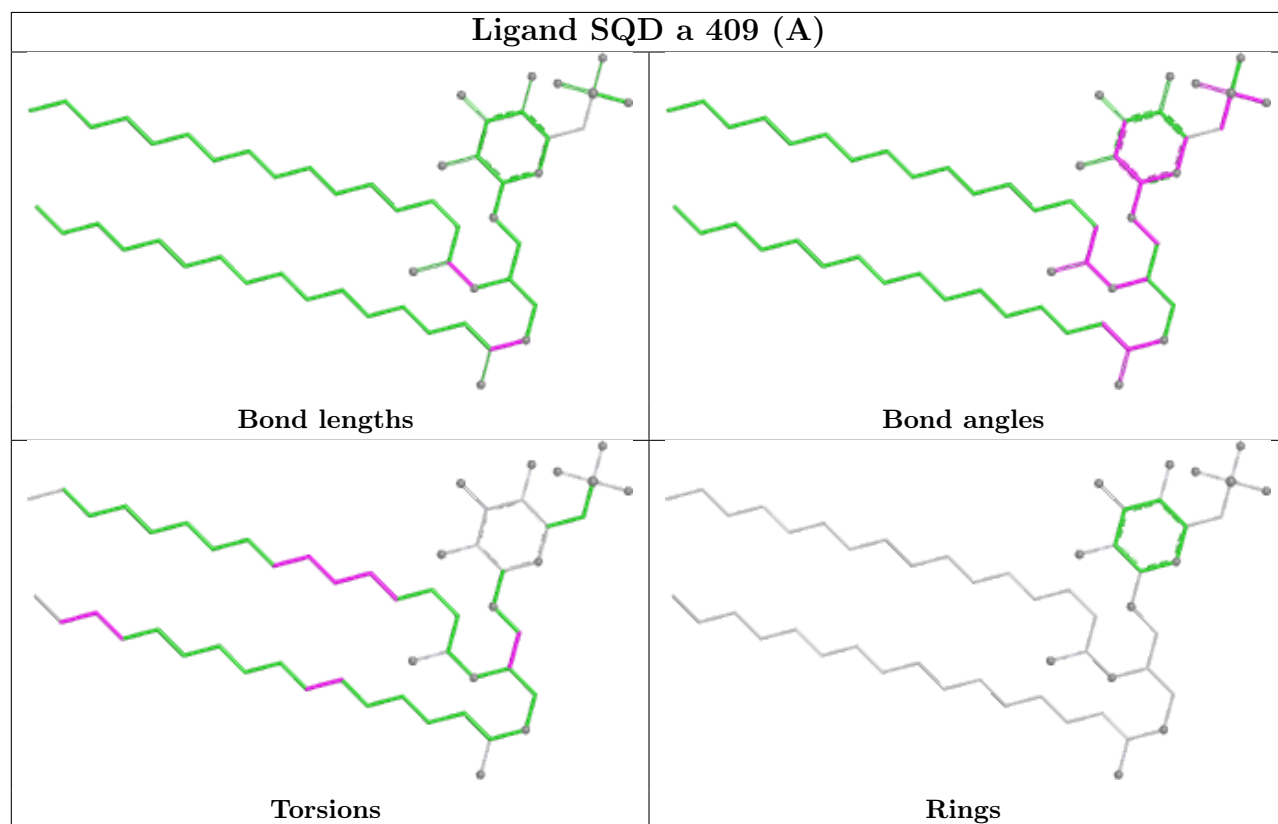
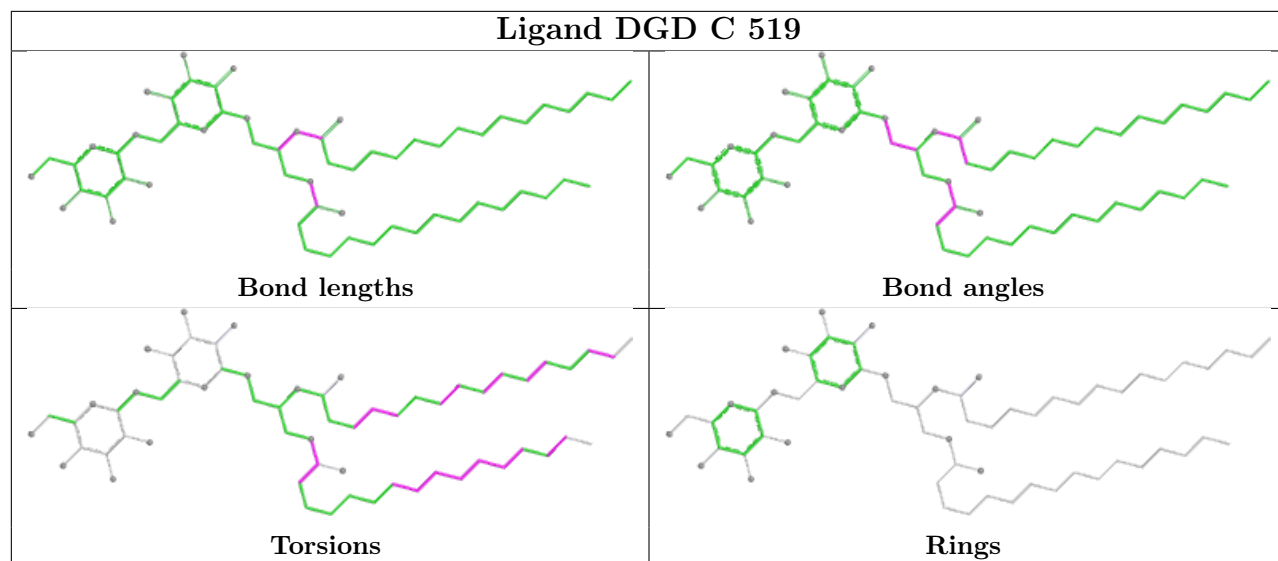
Rings

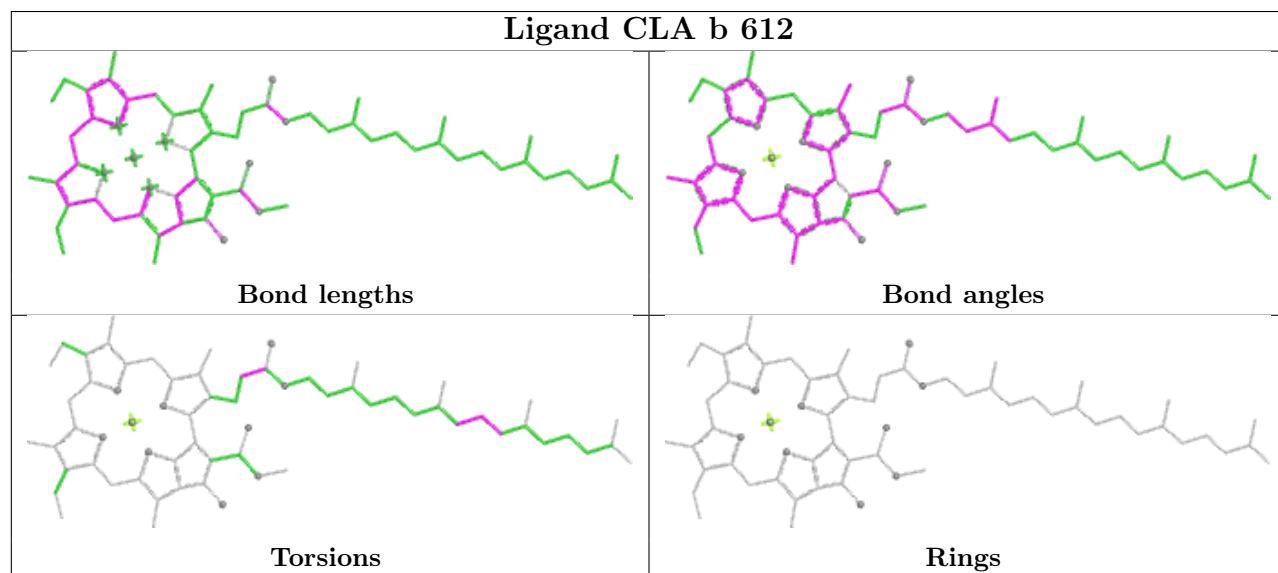
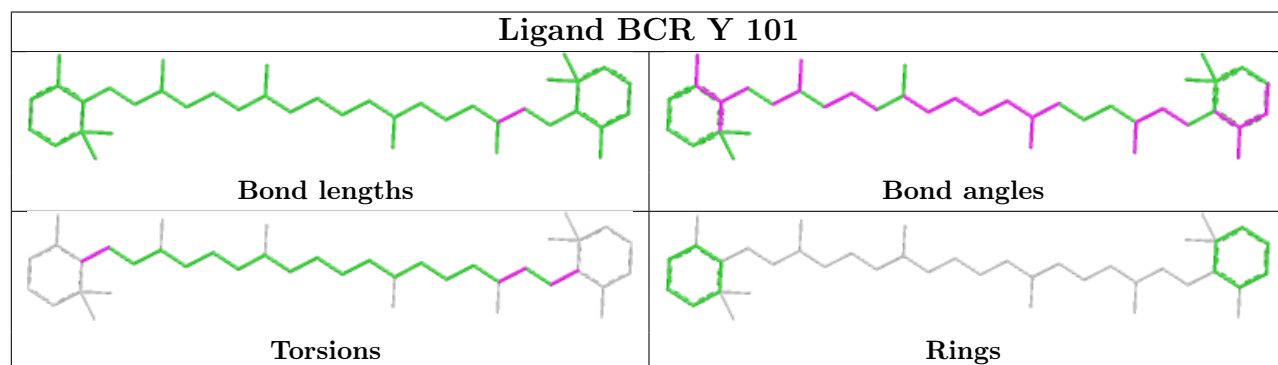
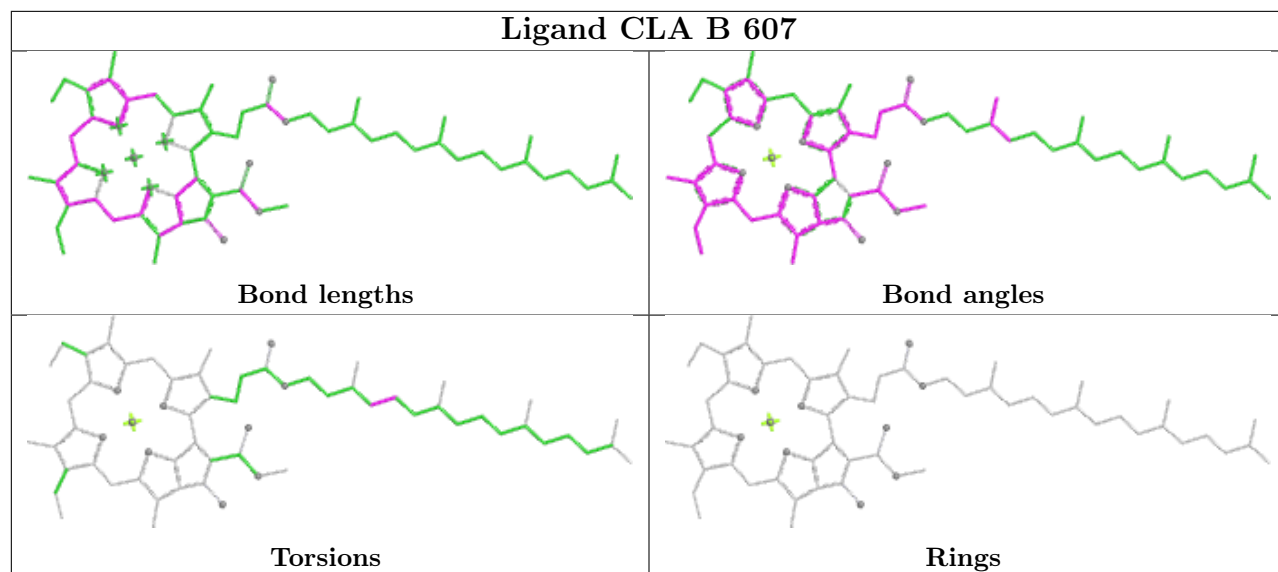


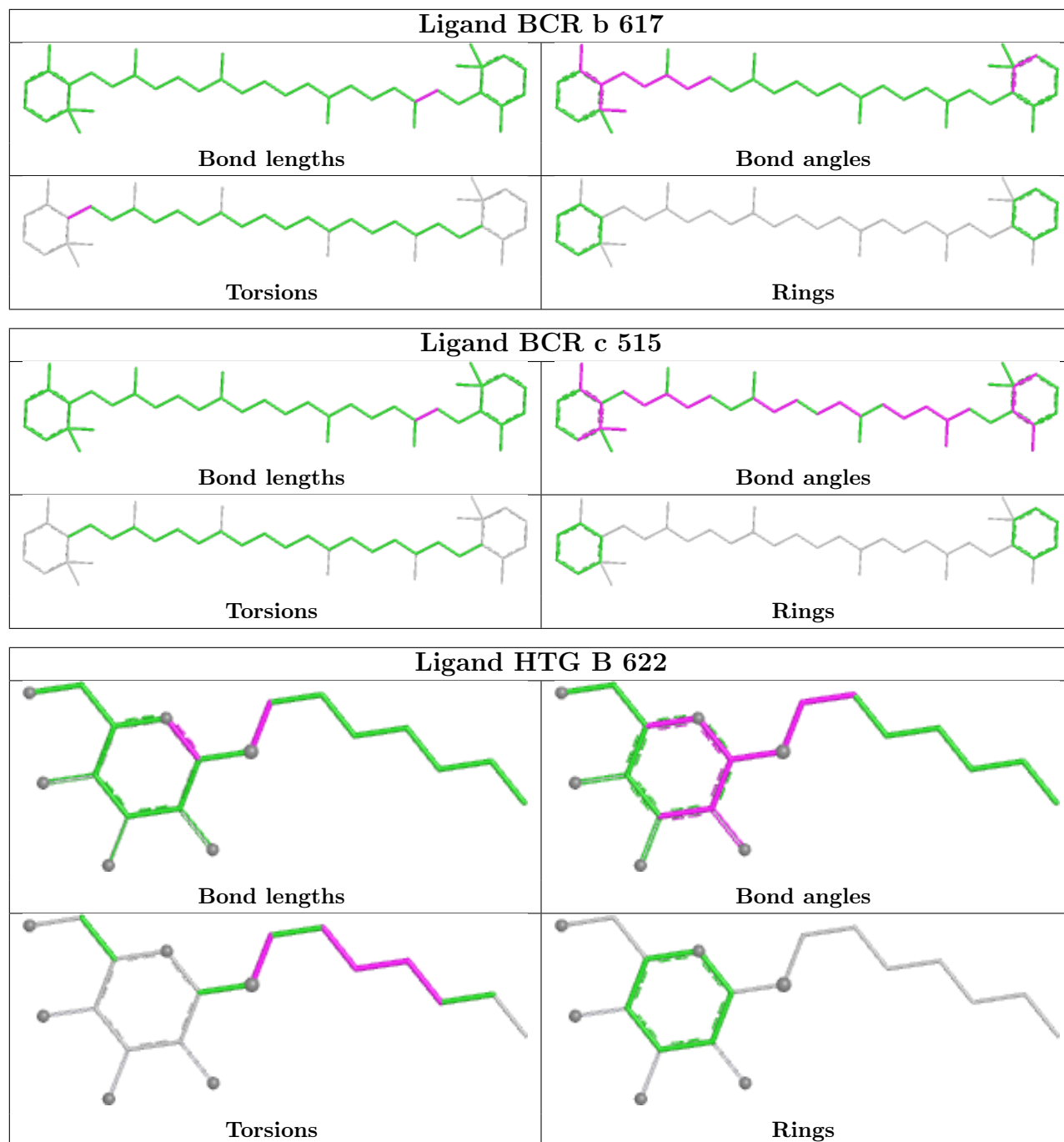


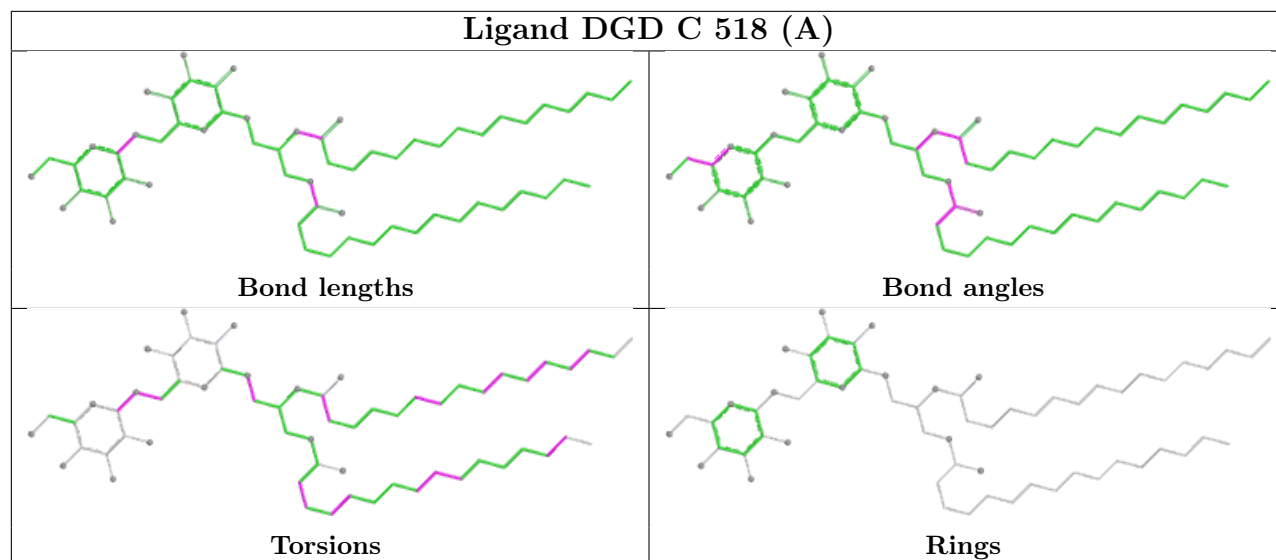
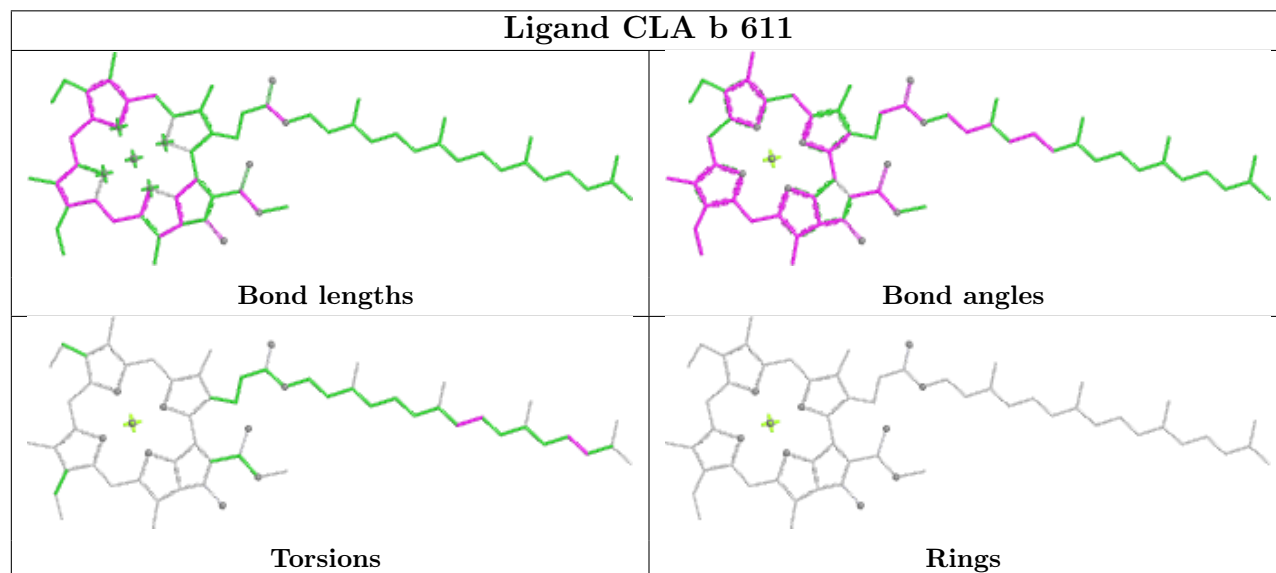
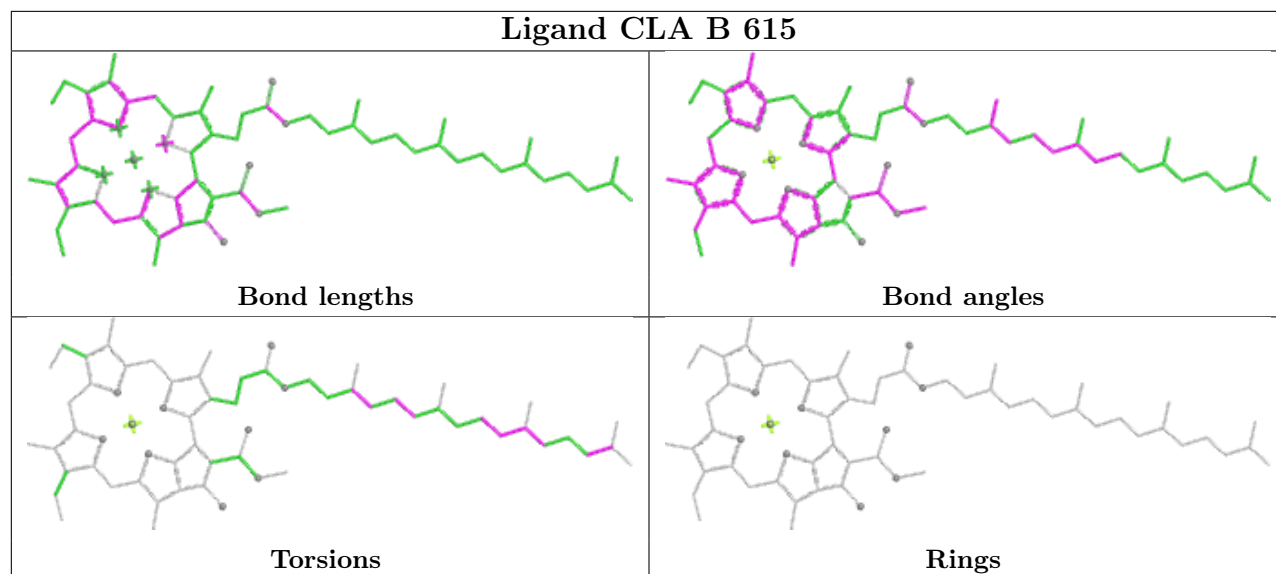
Ligand PL9 a 412 (A)	
Bond lengths	Bond angles
Torsions	Rings
Ligand CLA D 402 (B)	
Bond lengths	Bond angles
Torsions	Rings

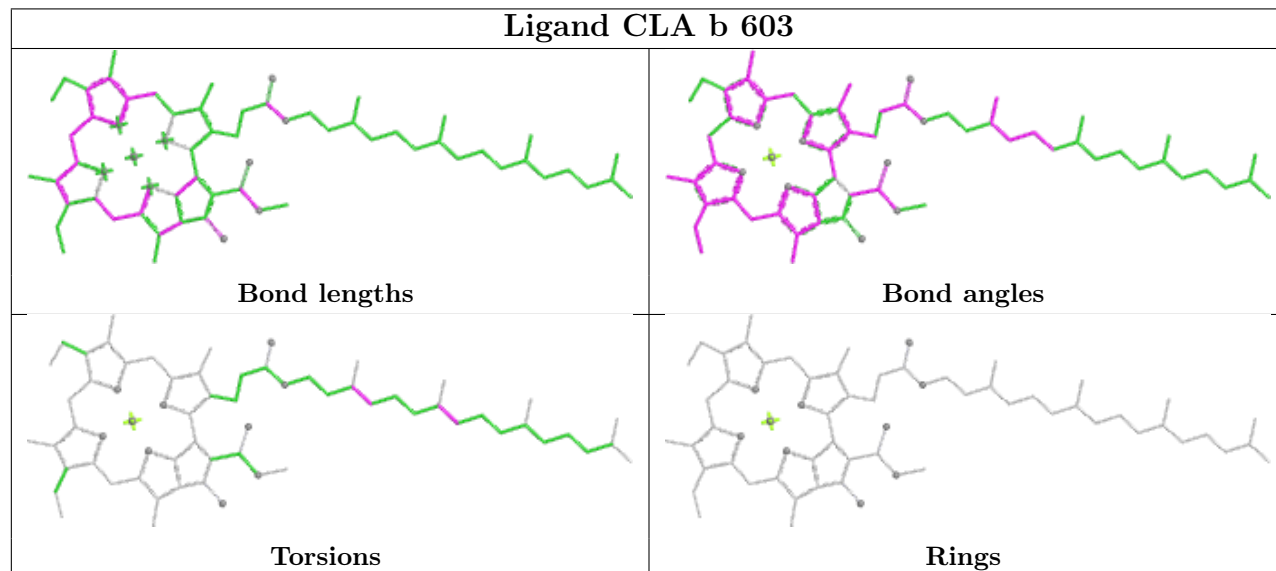
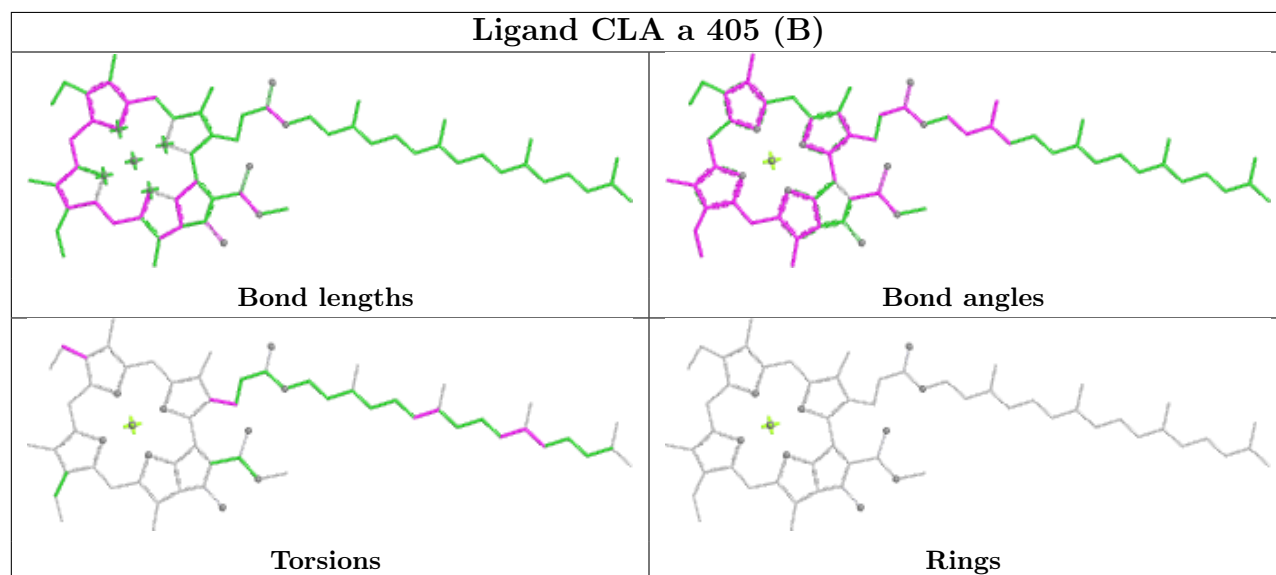
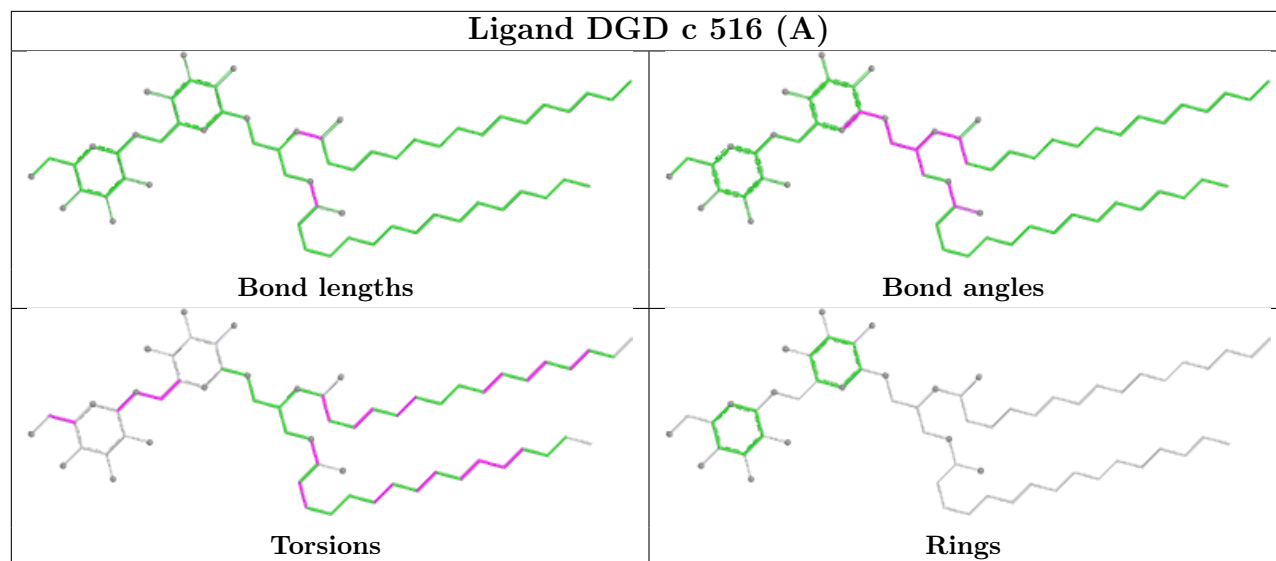


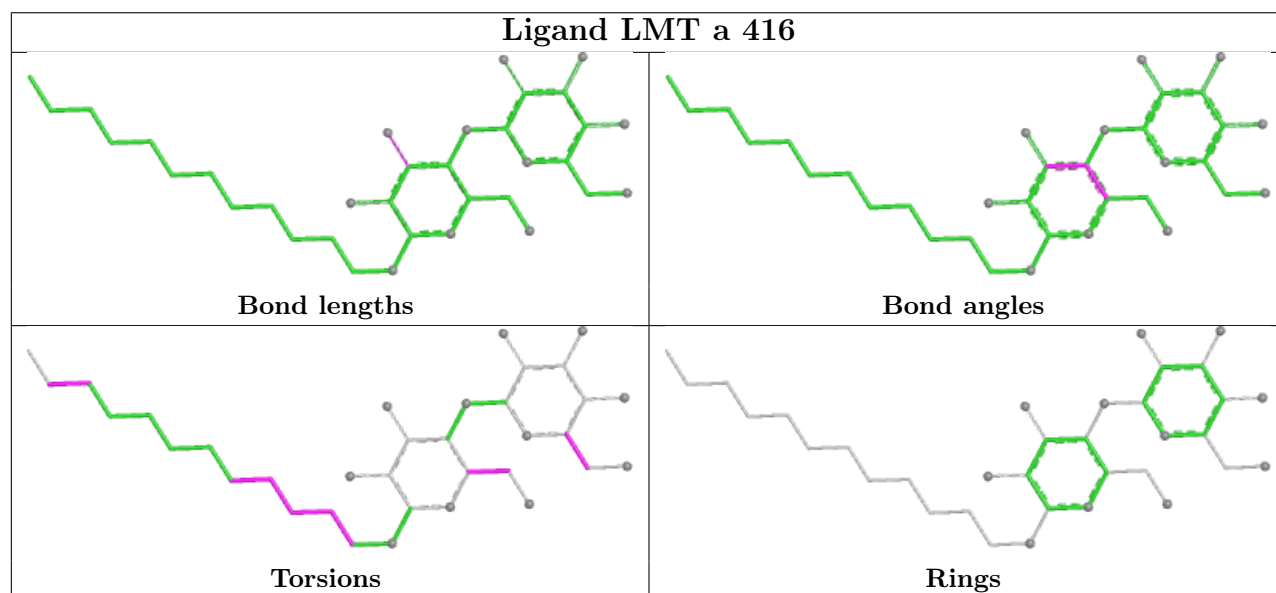
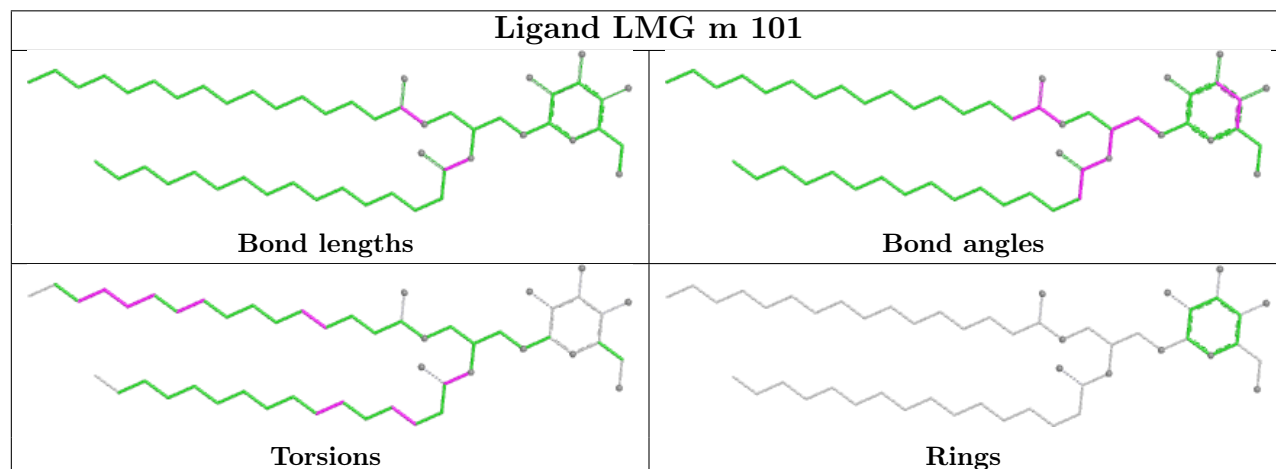
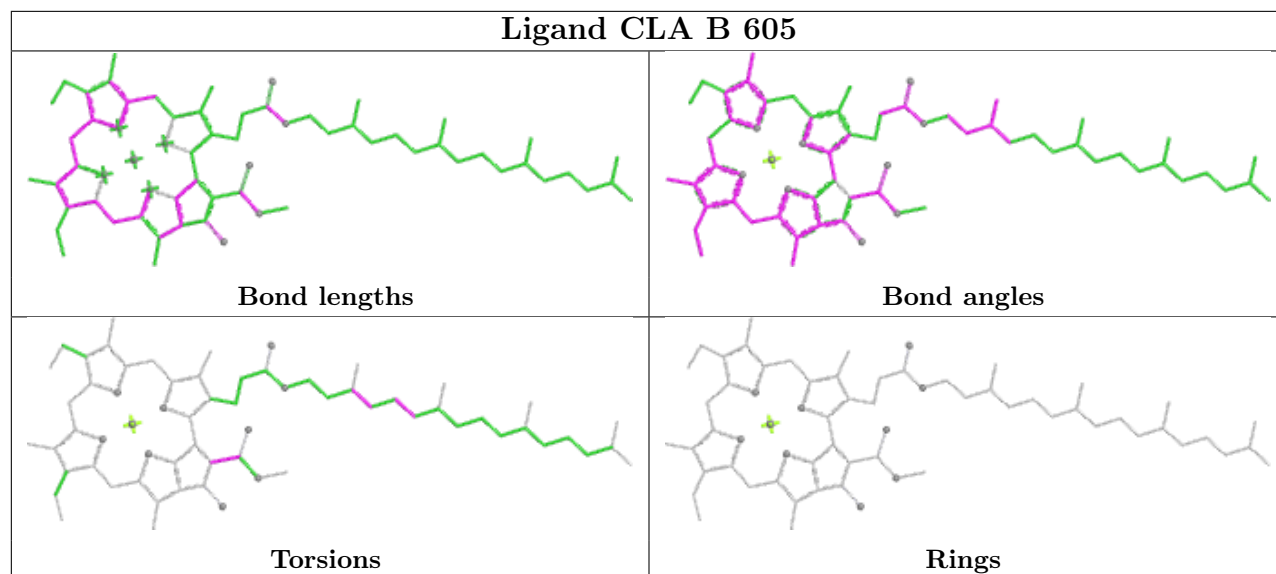


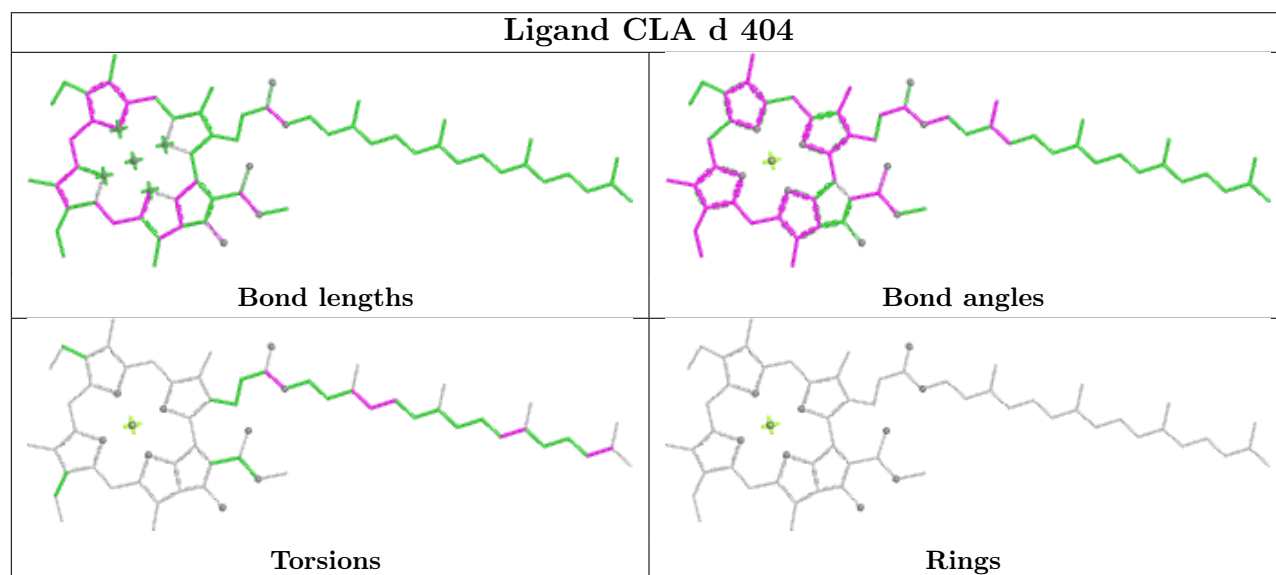
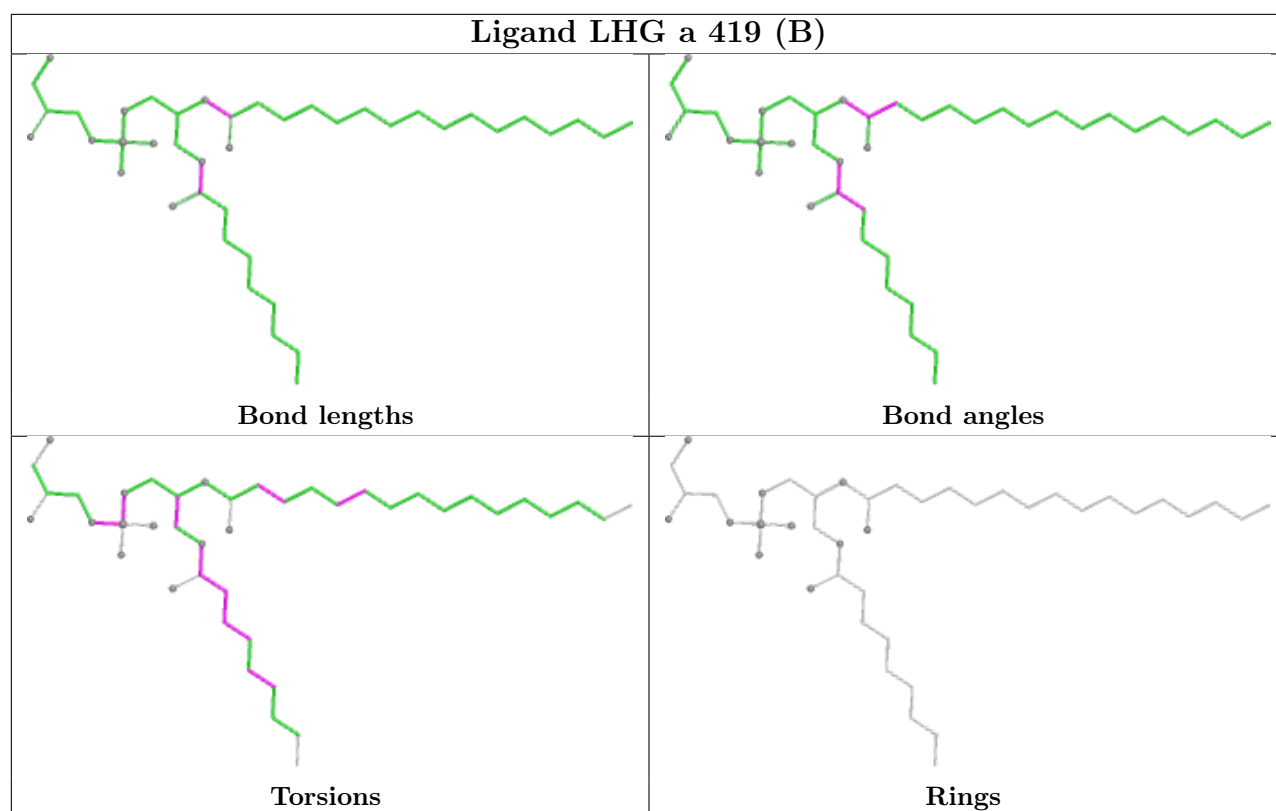


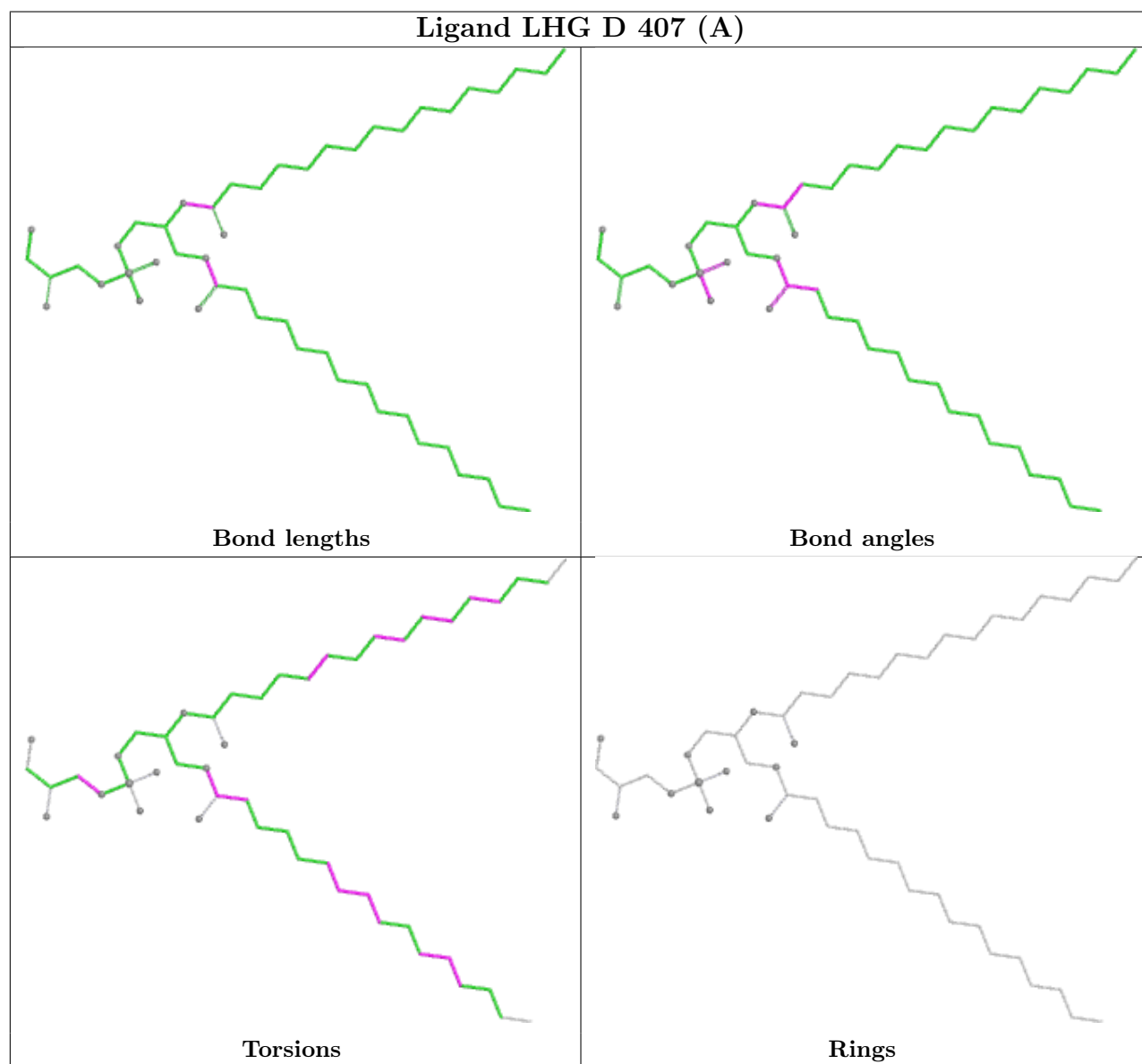
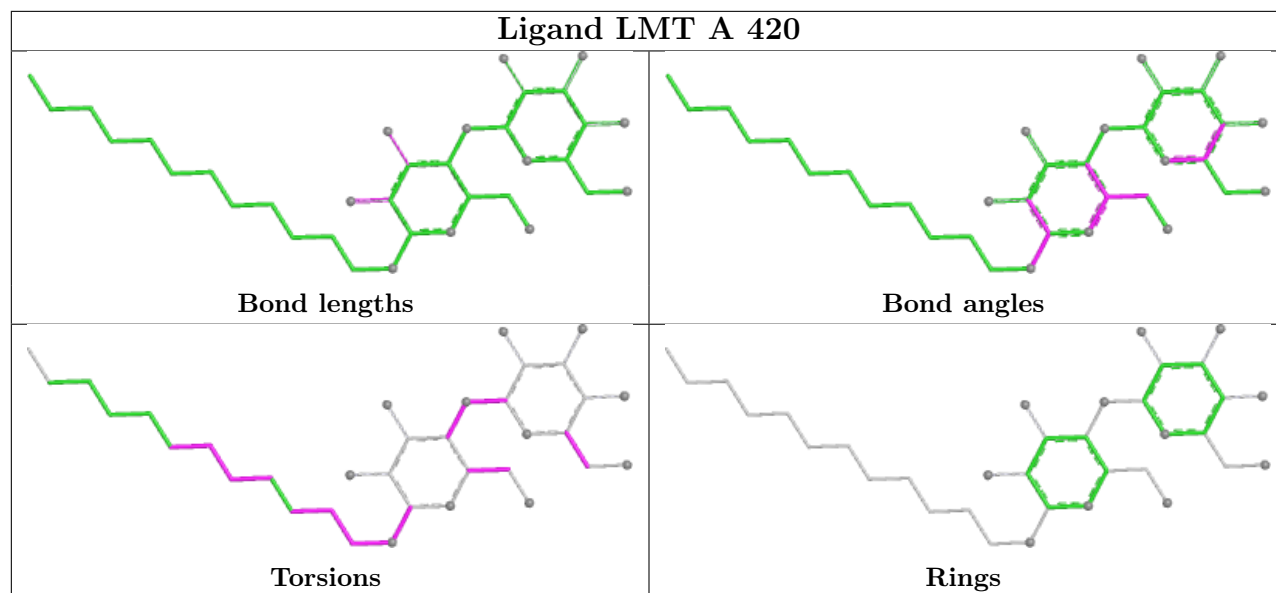


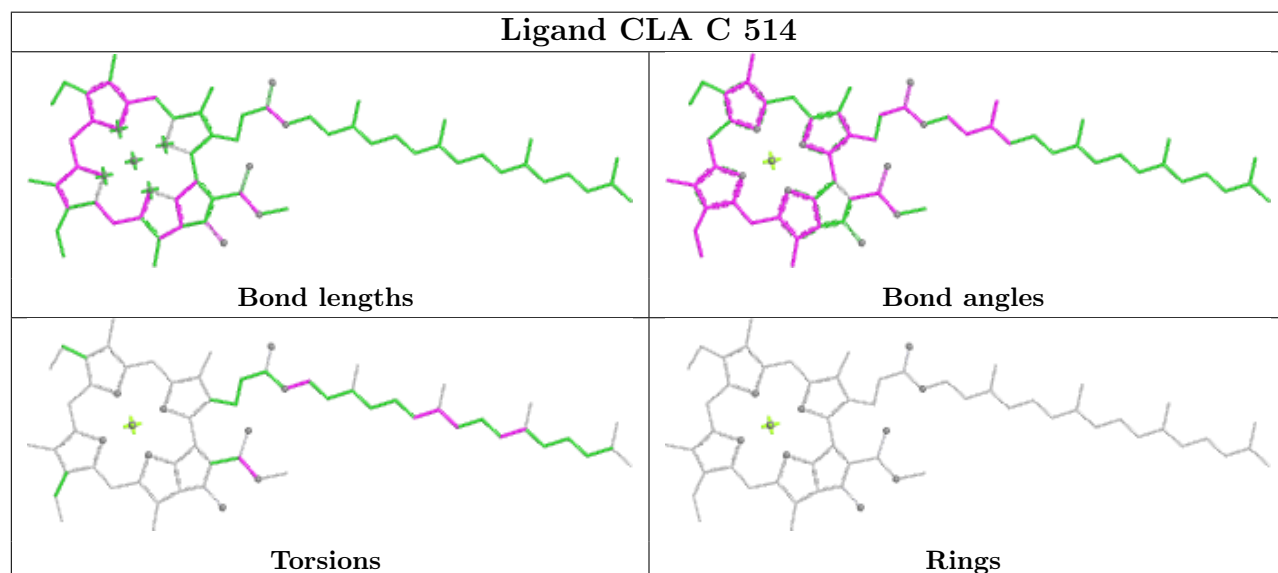
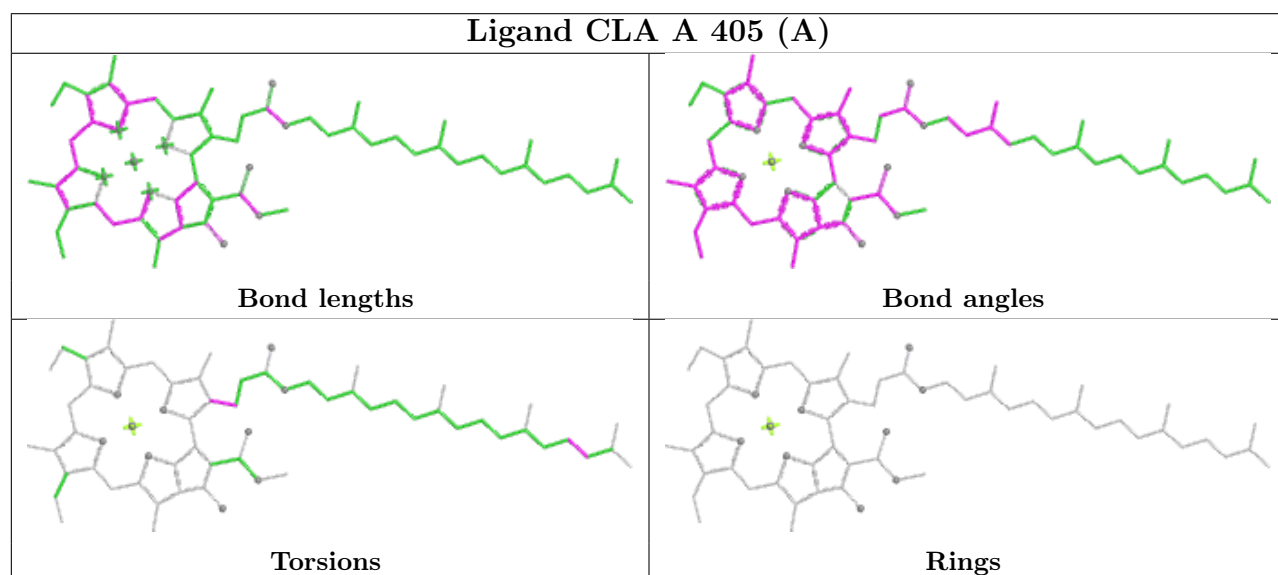
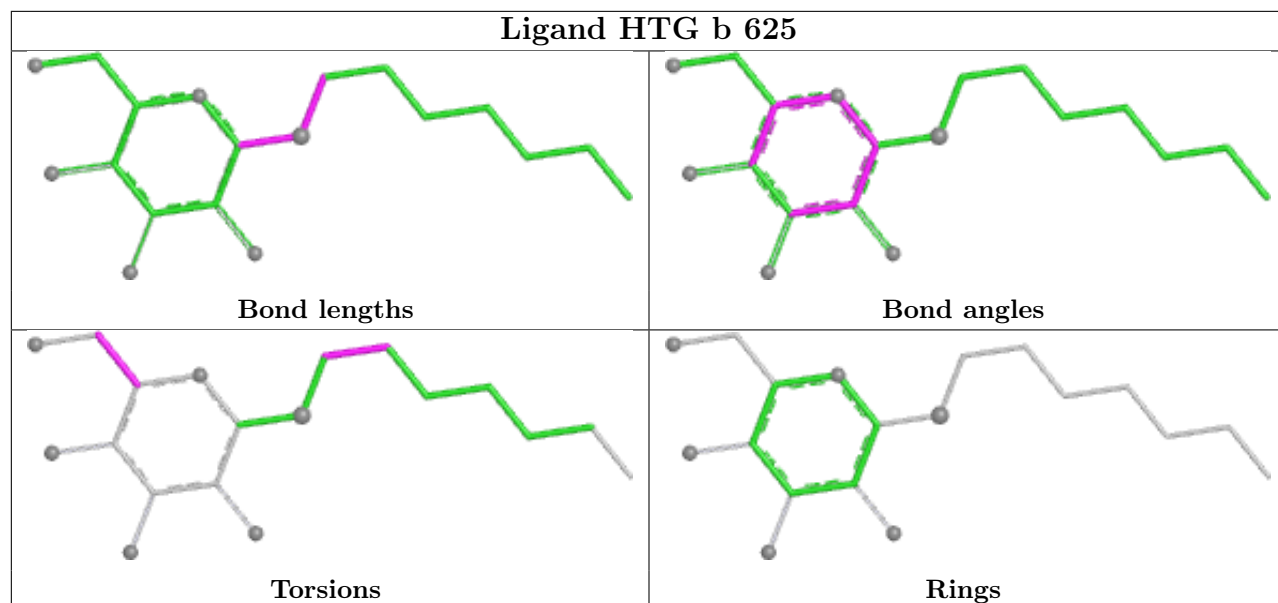


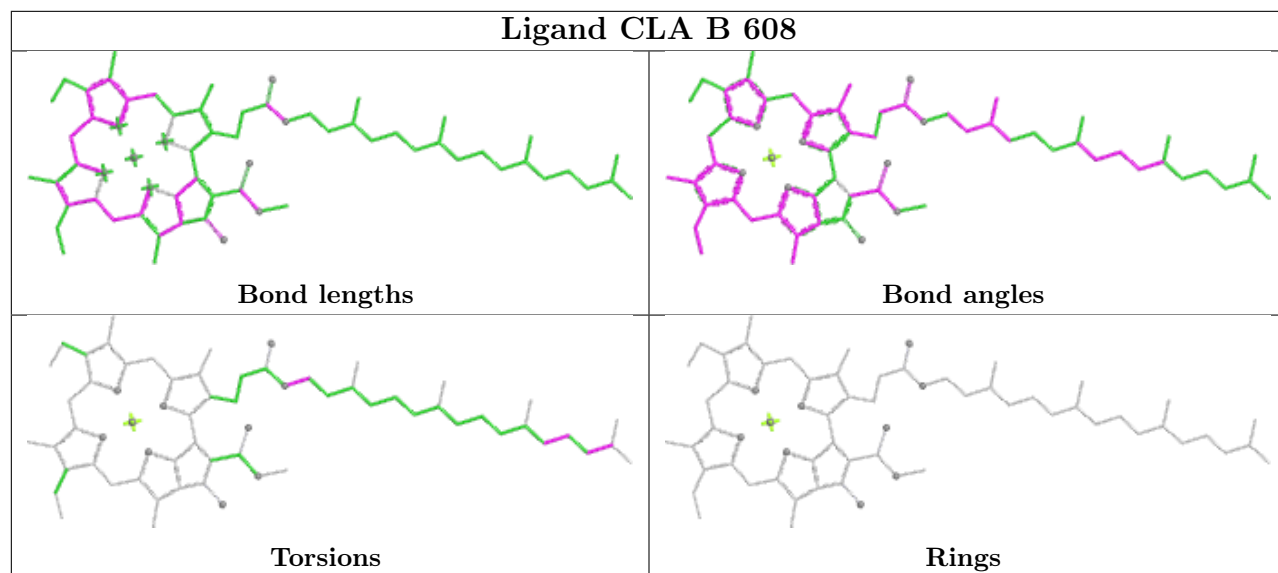
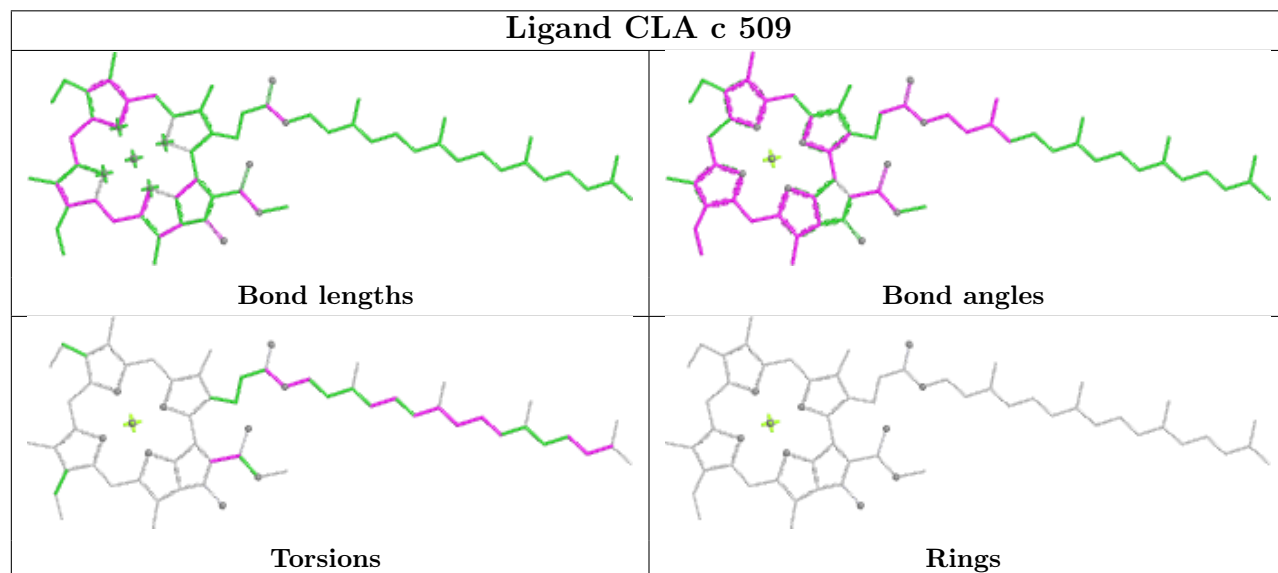
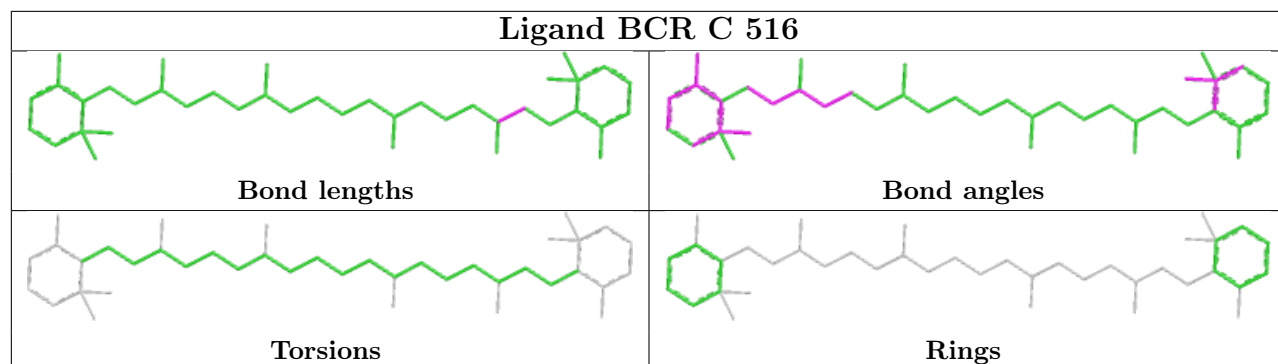


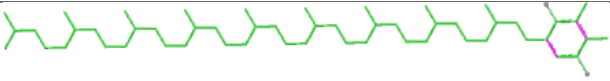
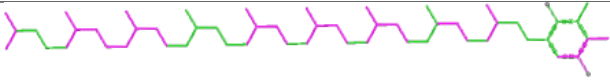
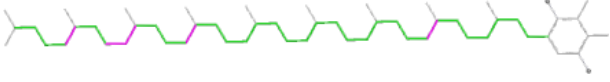
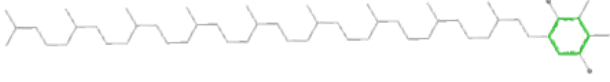


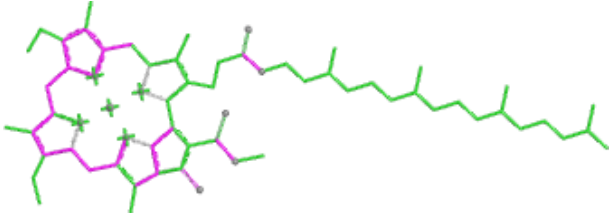
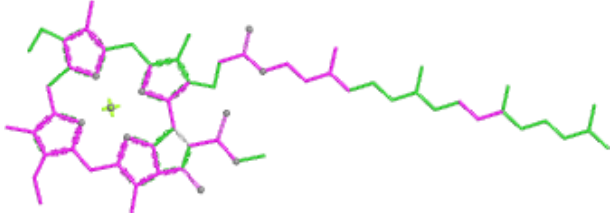
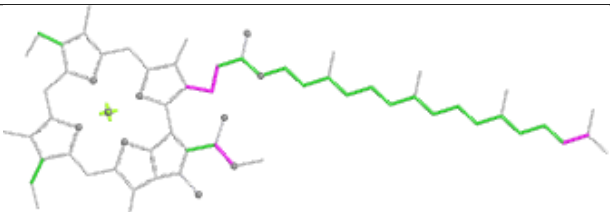
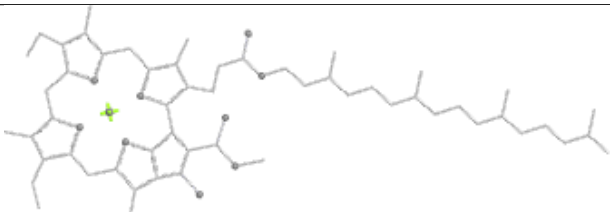




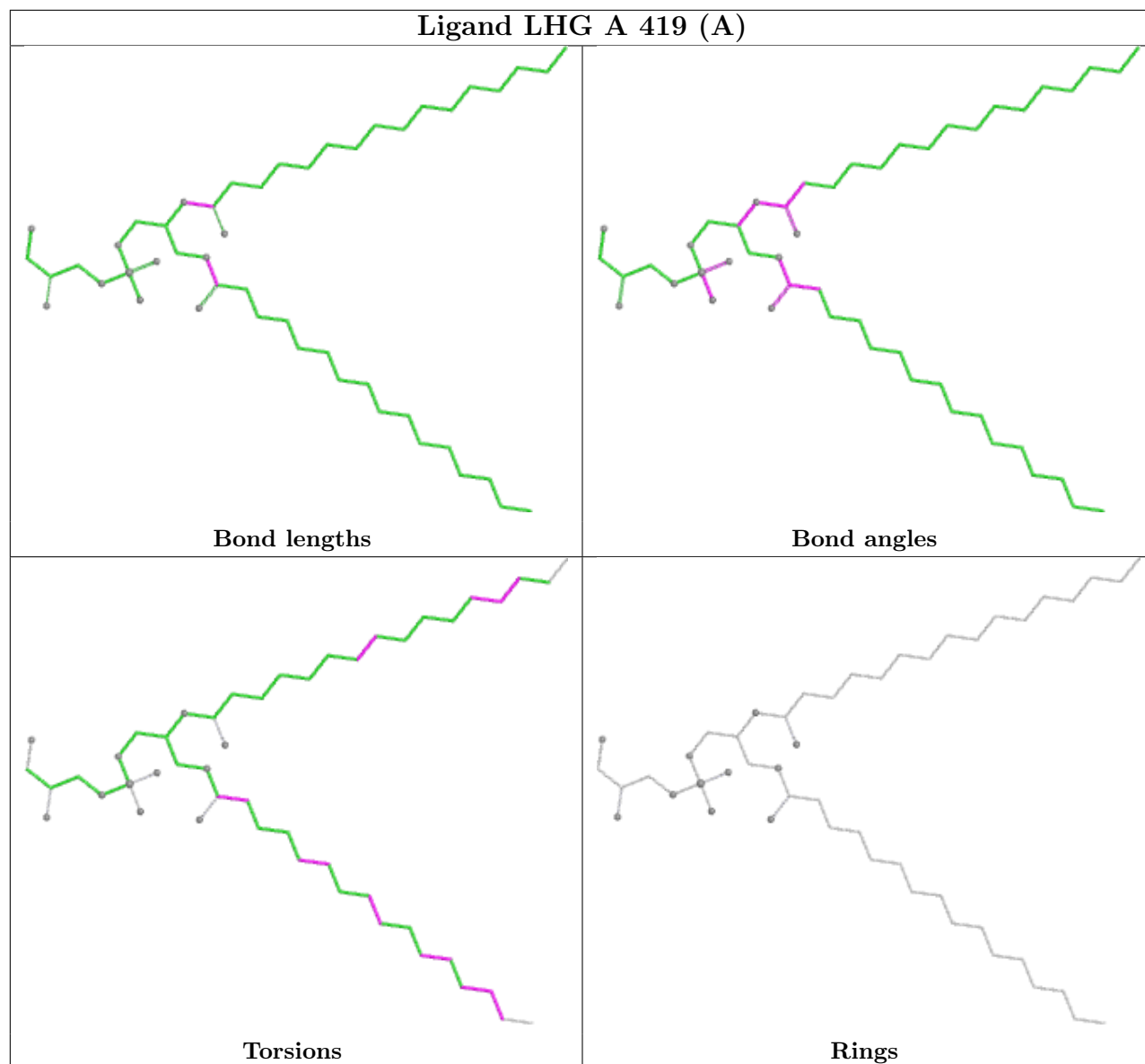




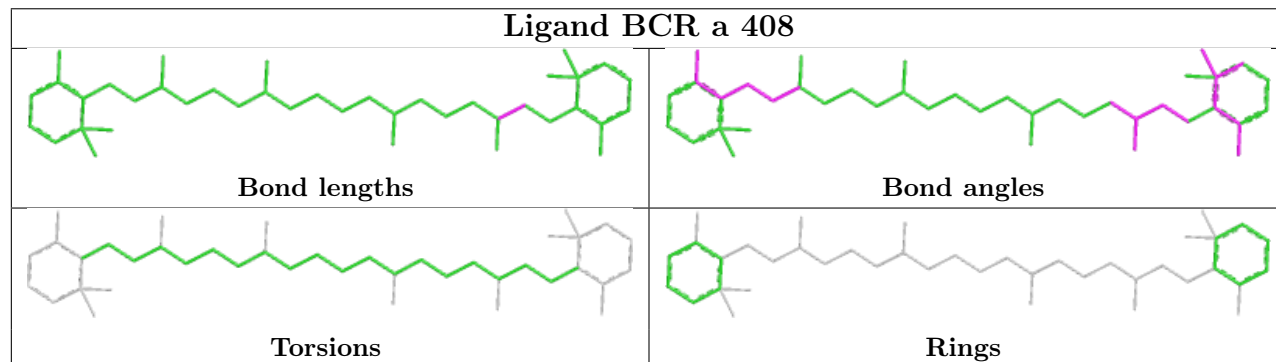
Ligand PL9 D 405 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

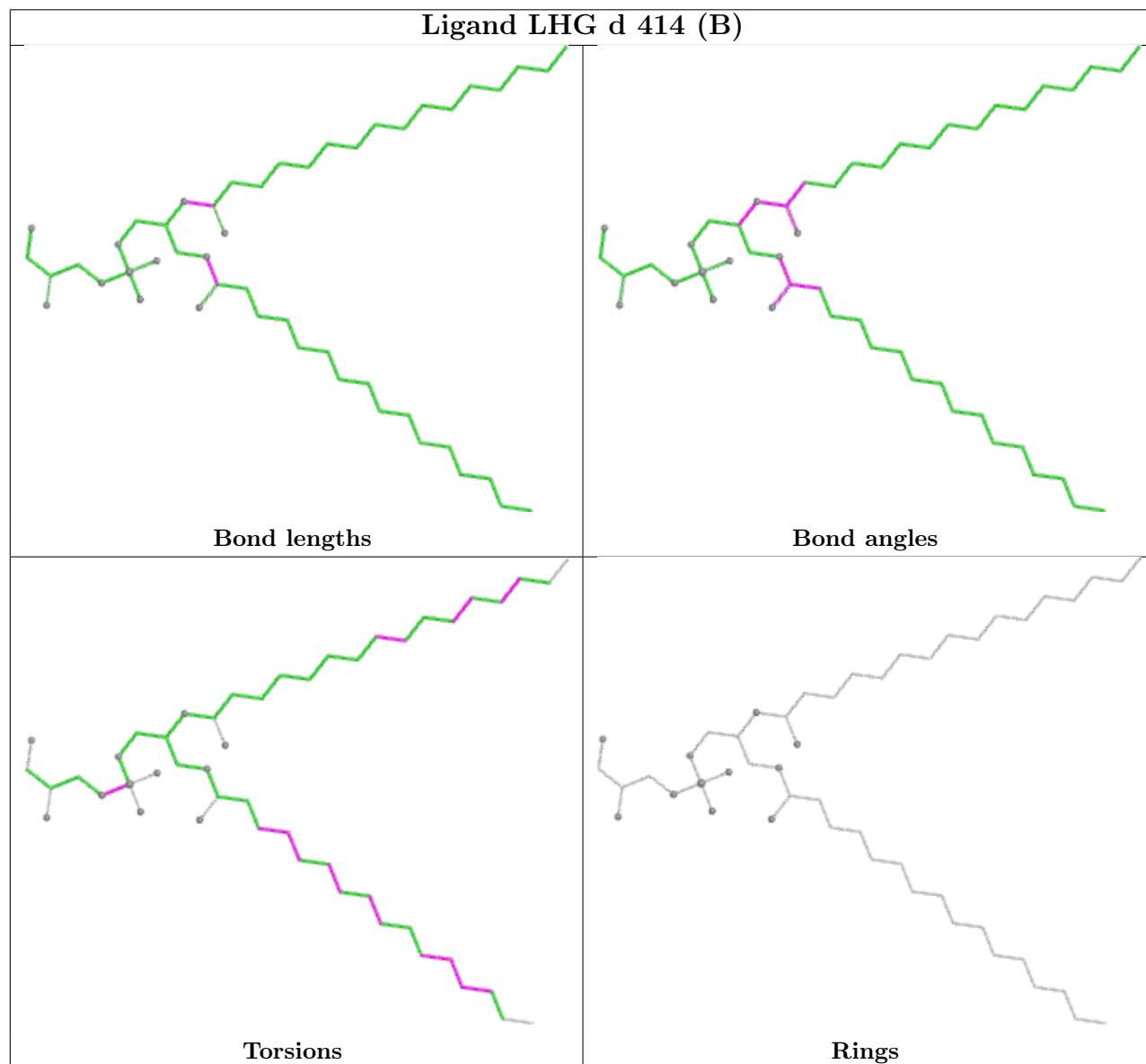
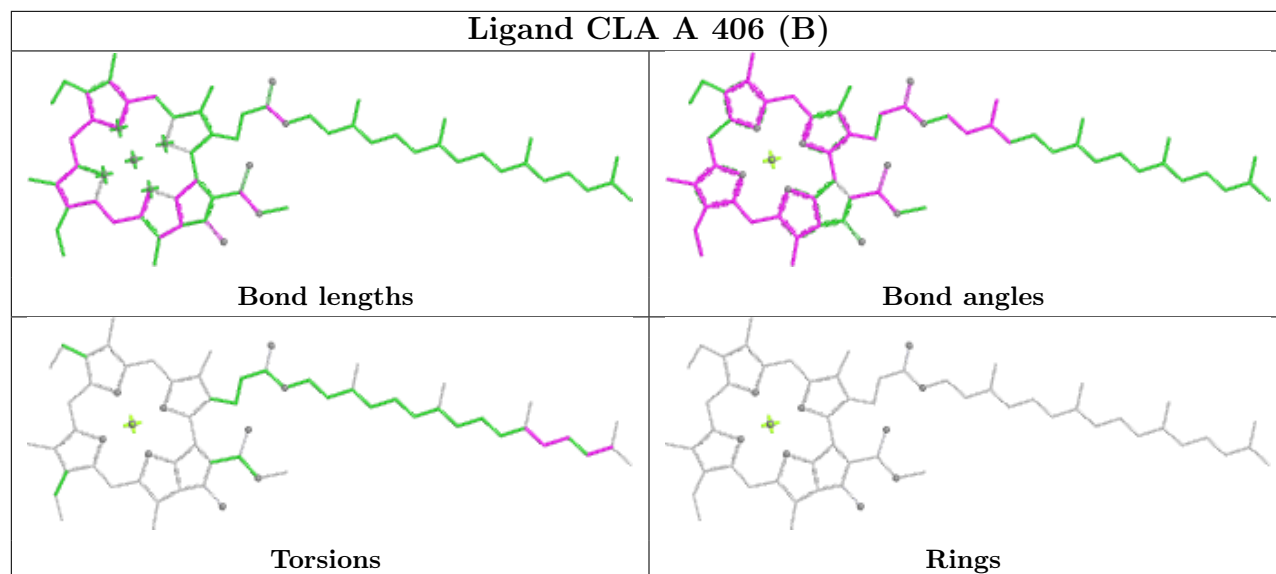
Ligand CLA C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG A 419 (A)

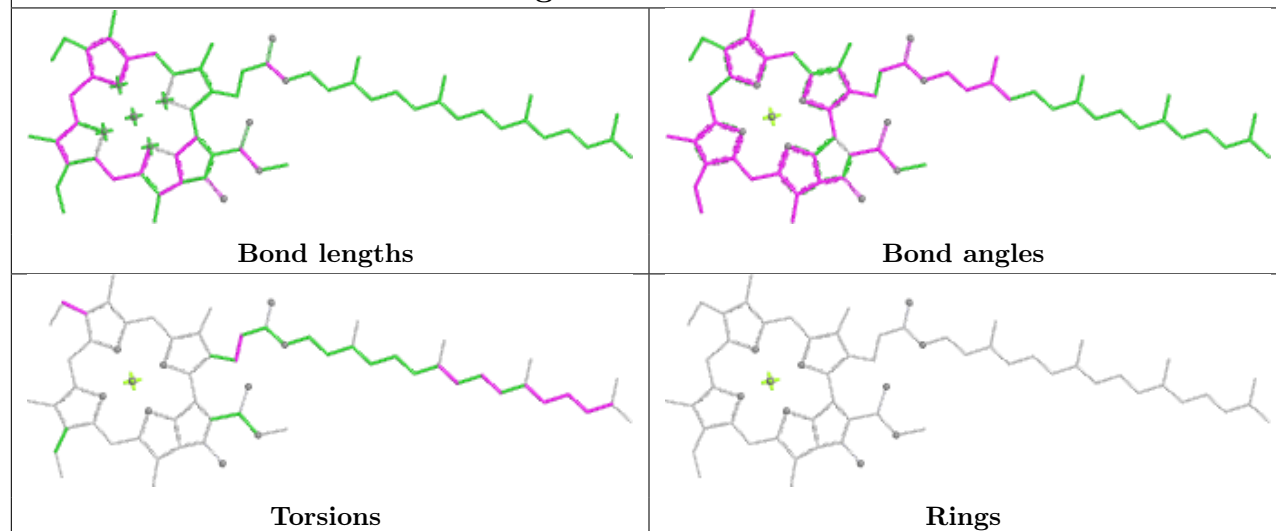


Ligand BCR a 408

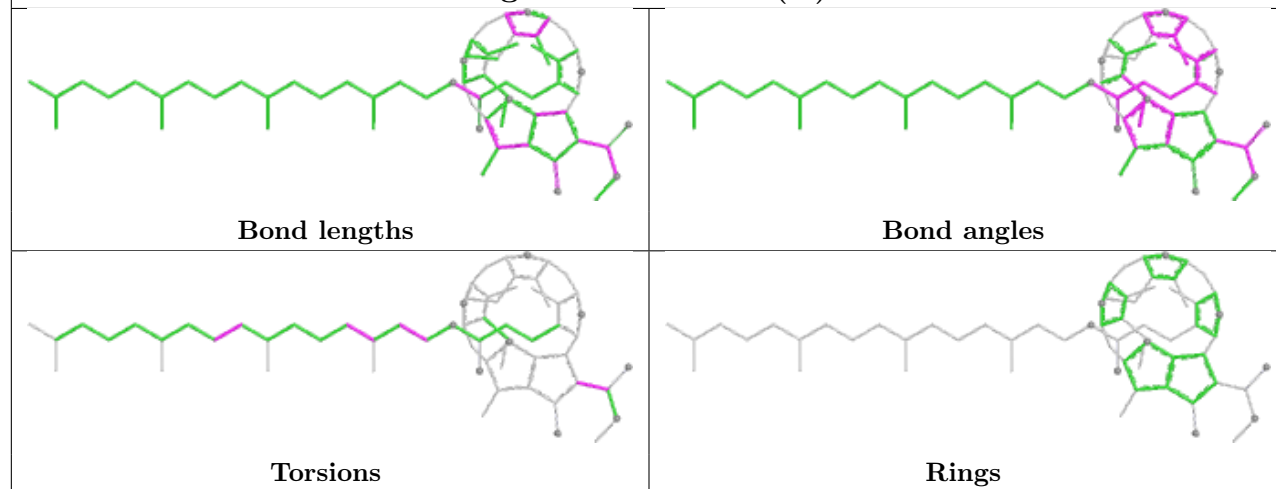




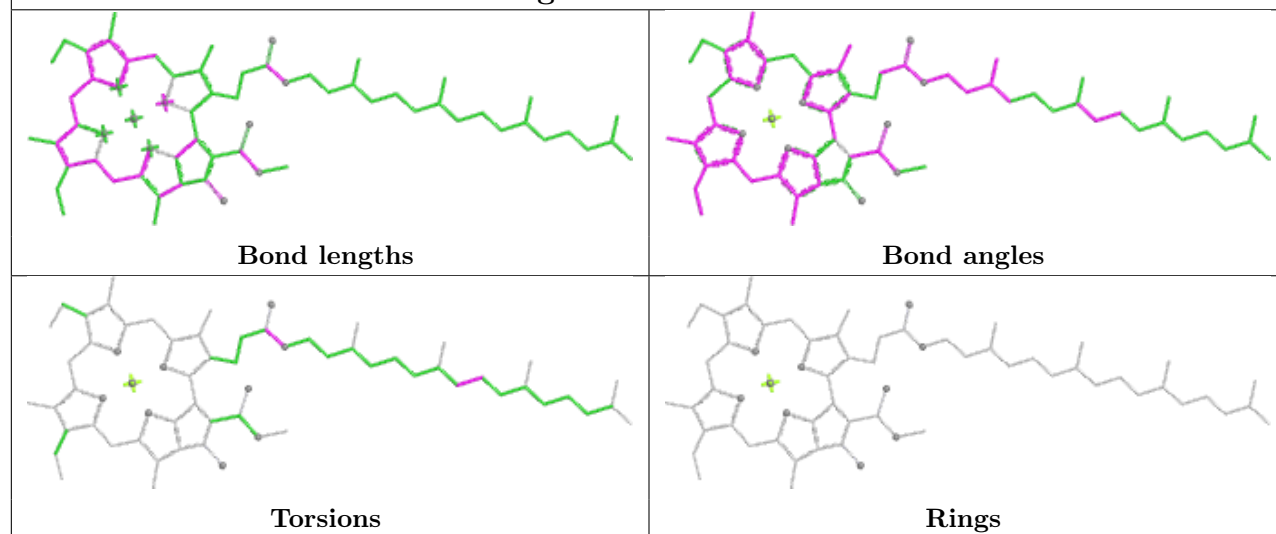
Ligand CLA b 606

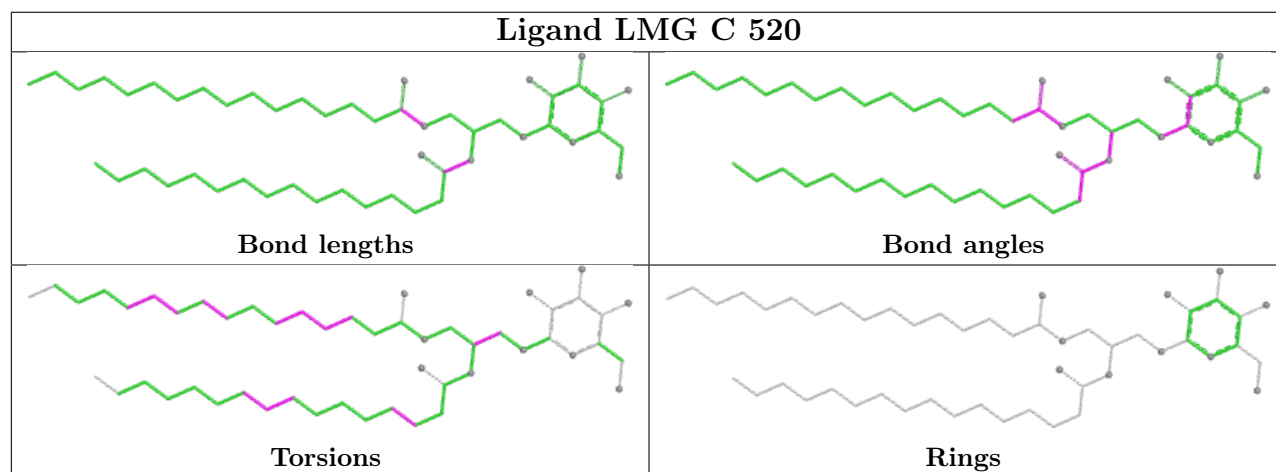
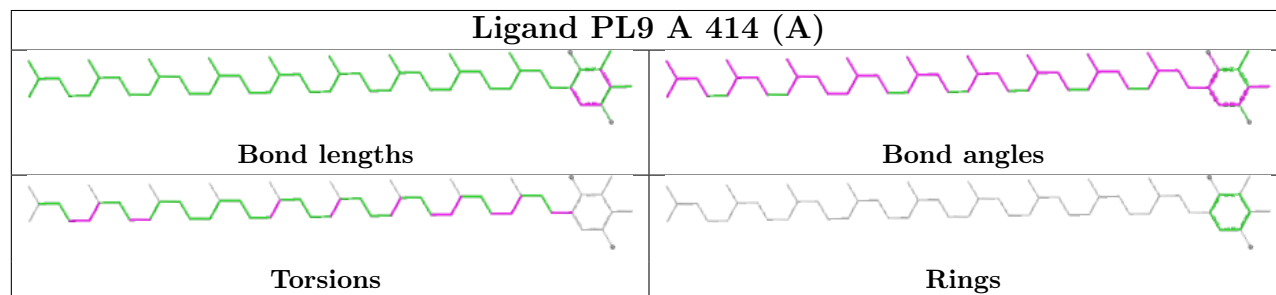
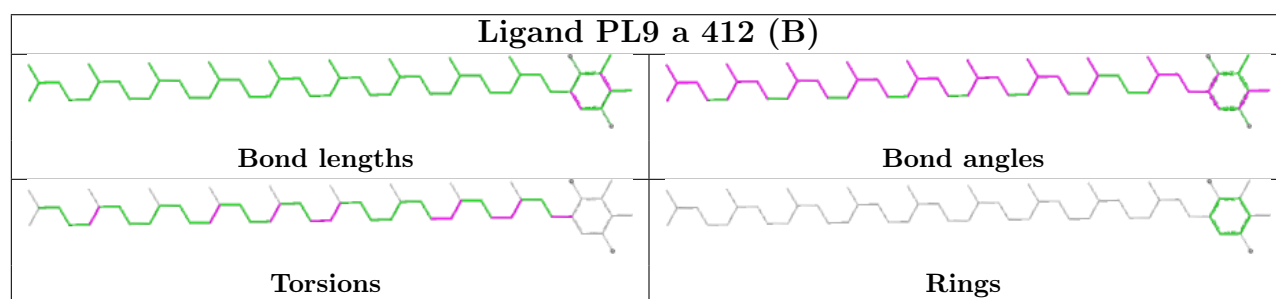
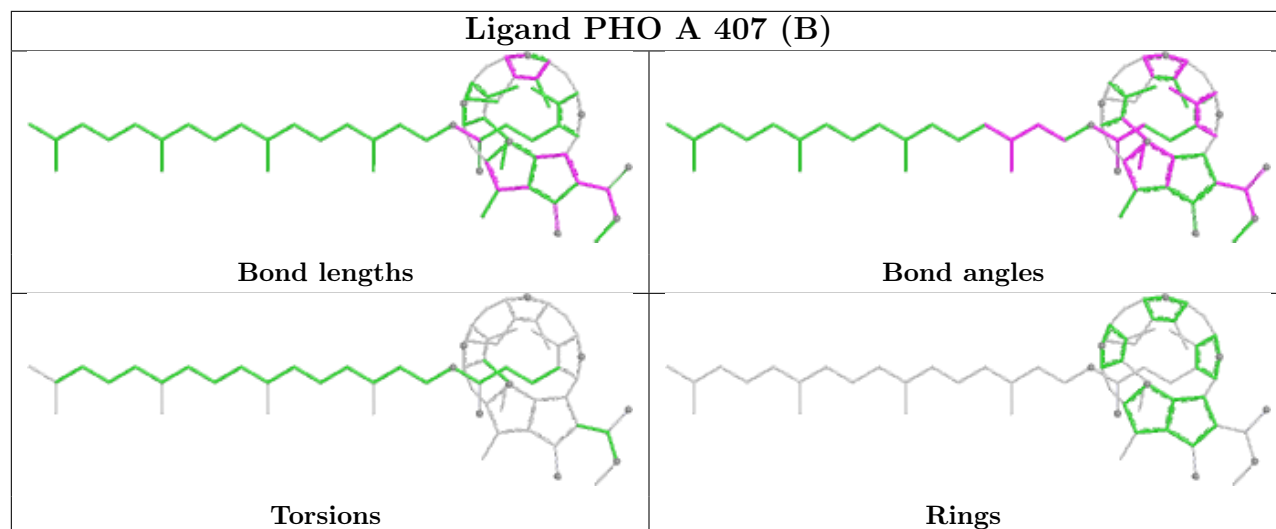


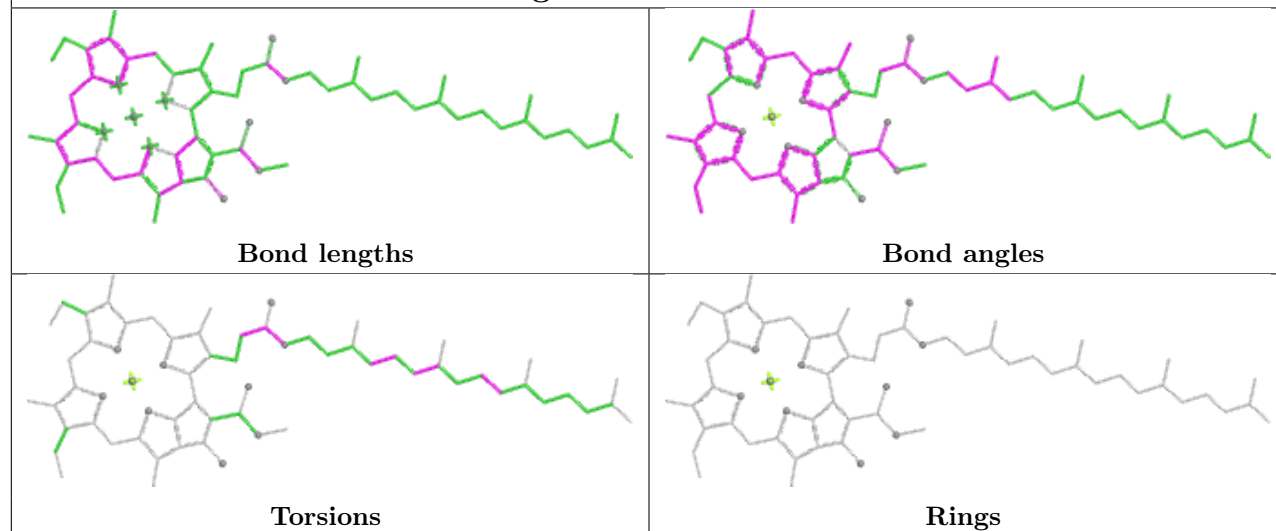
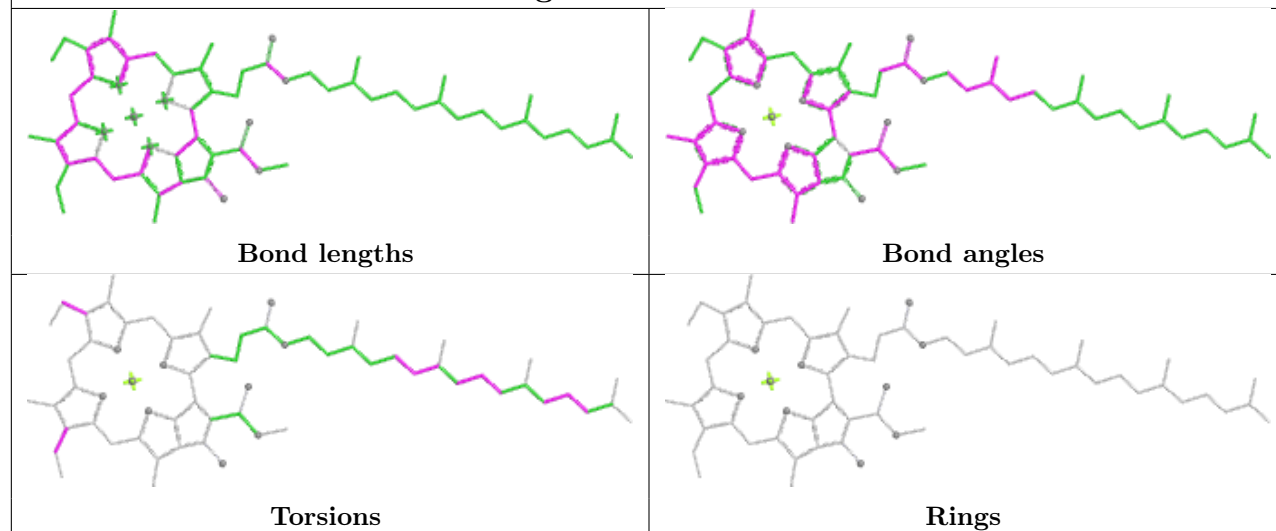
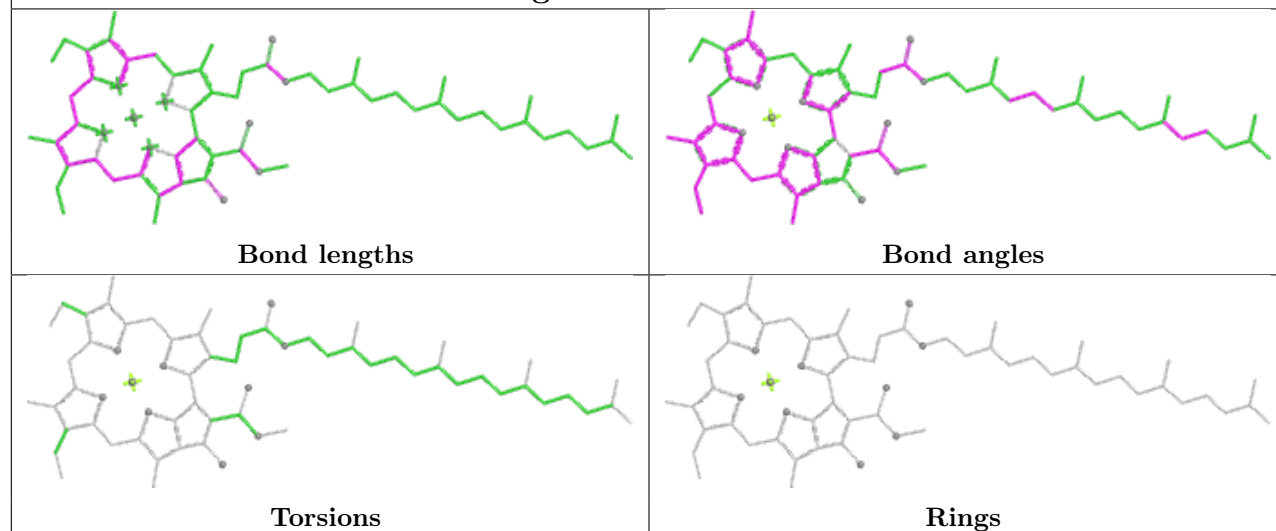
Ligand PHO a 406 (A)

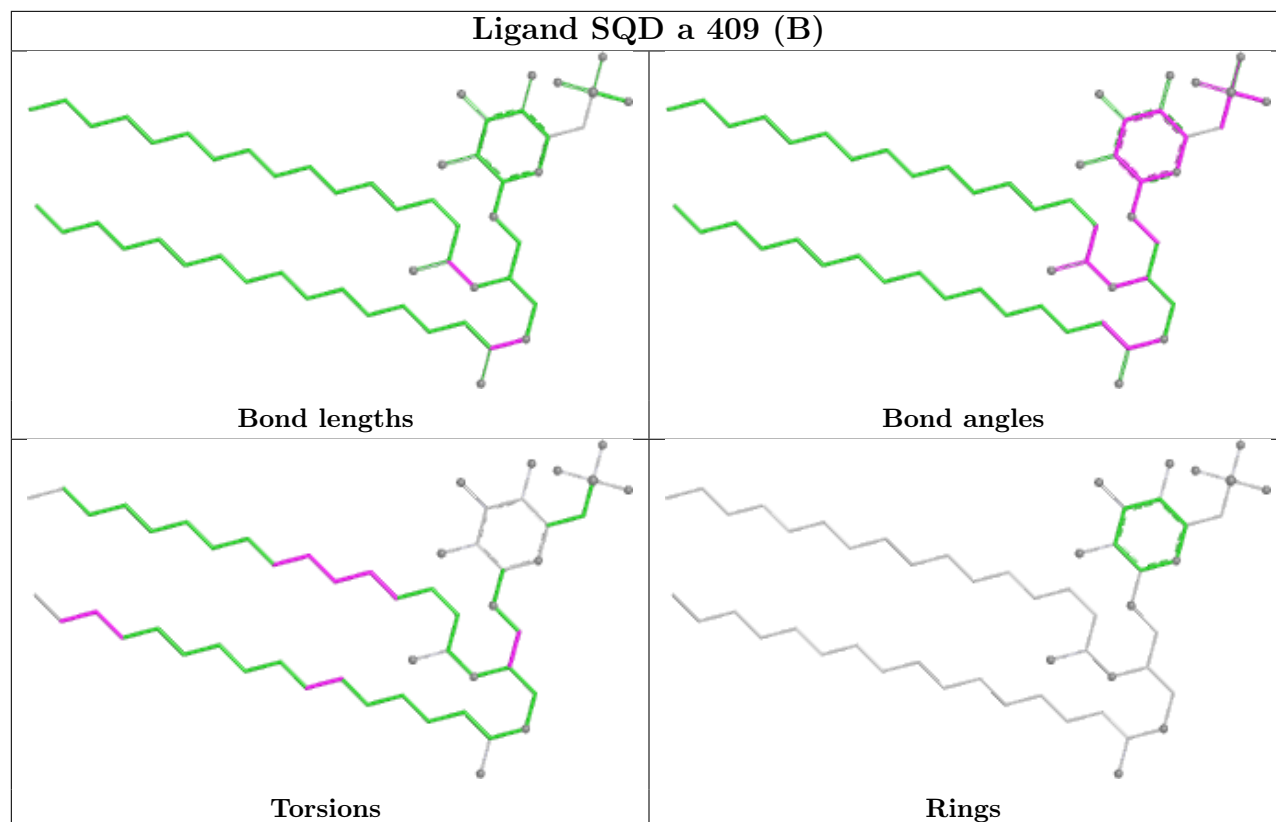


Ligand CLA c 511

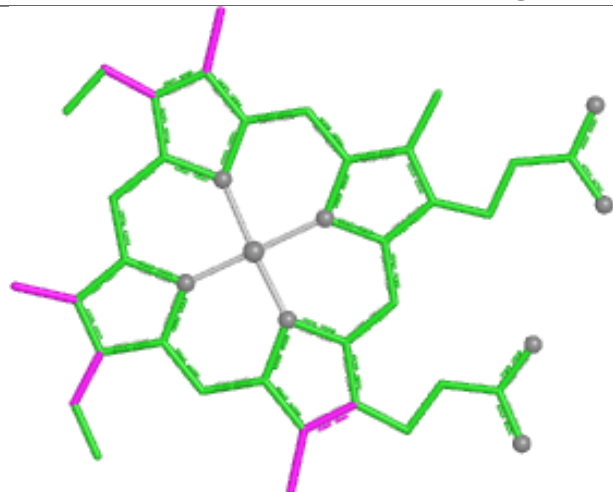




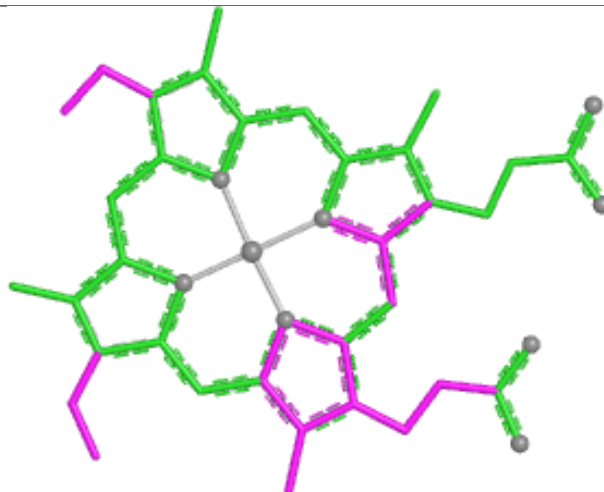
Ligand CLA C 513**Ligand CLA b 604****Ligand CLA B 609**



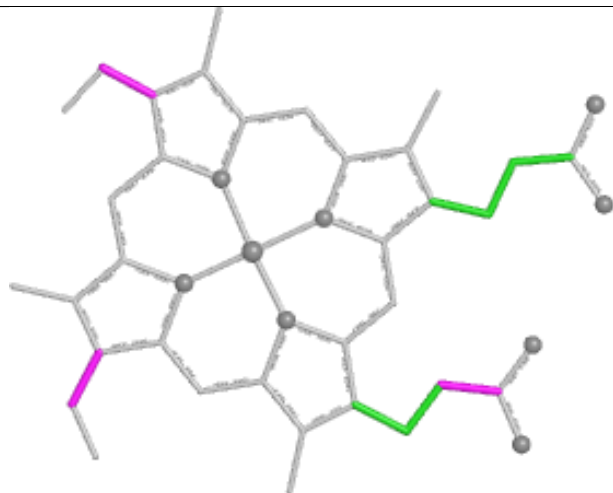
Ligand HEC V 201



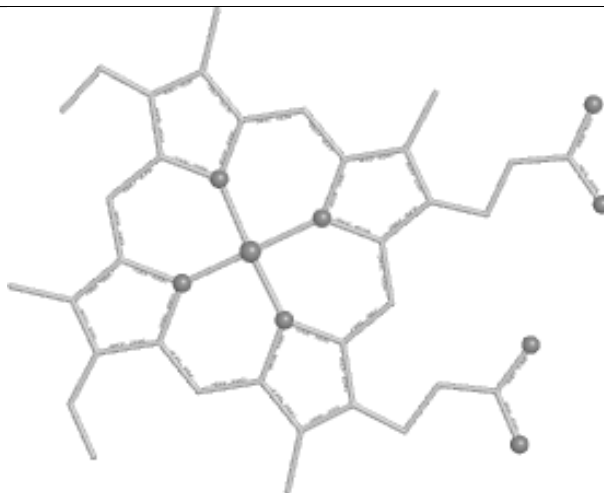
Bond lengths



Bond angles

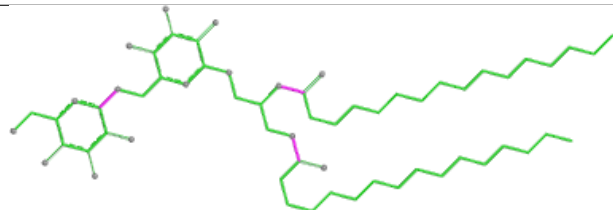


Torsions

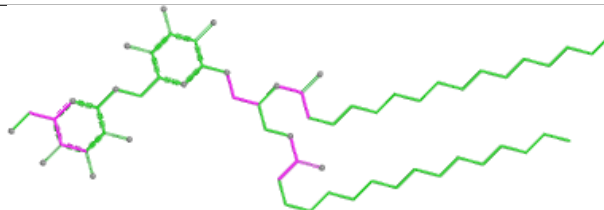


Rings

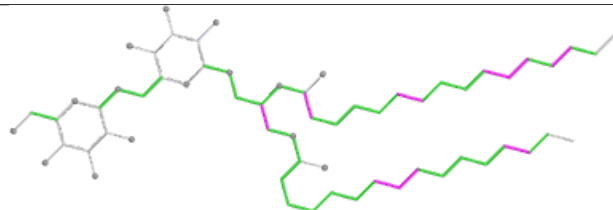
Ligand DGD H 102



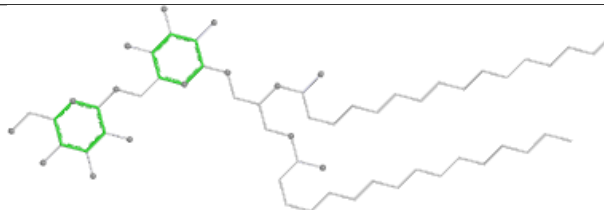
Bond lengths



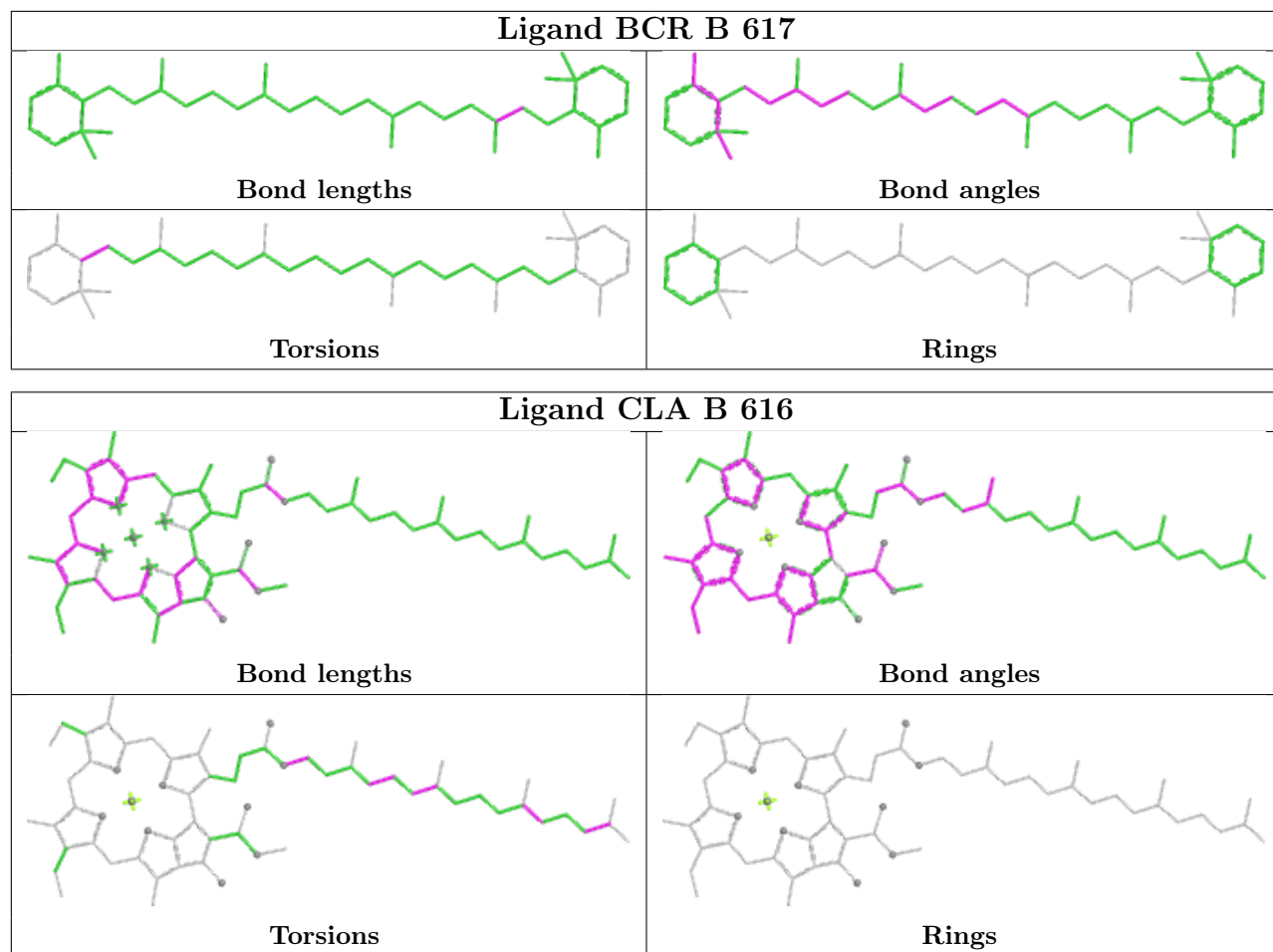
Bond angles



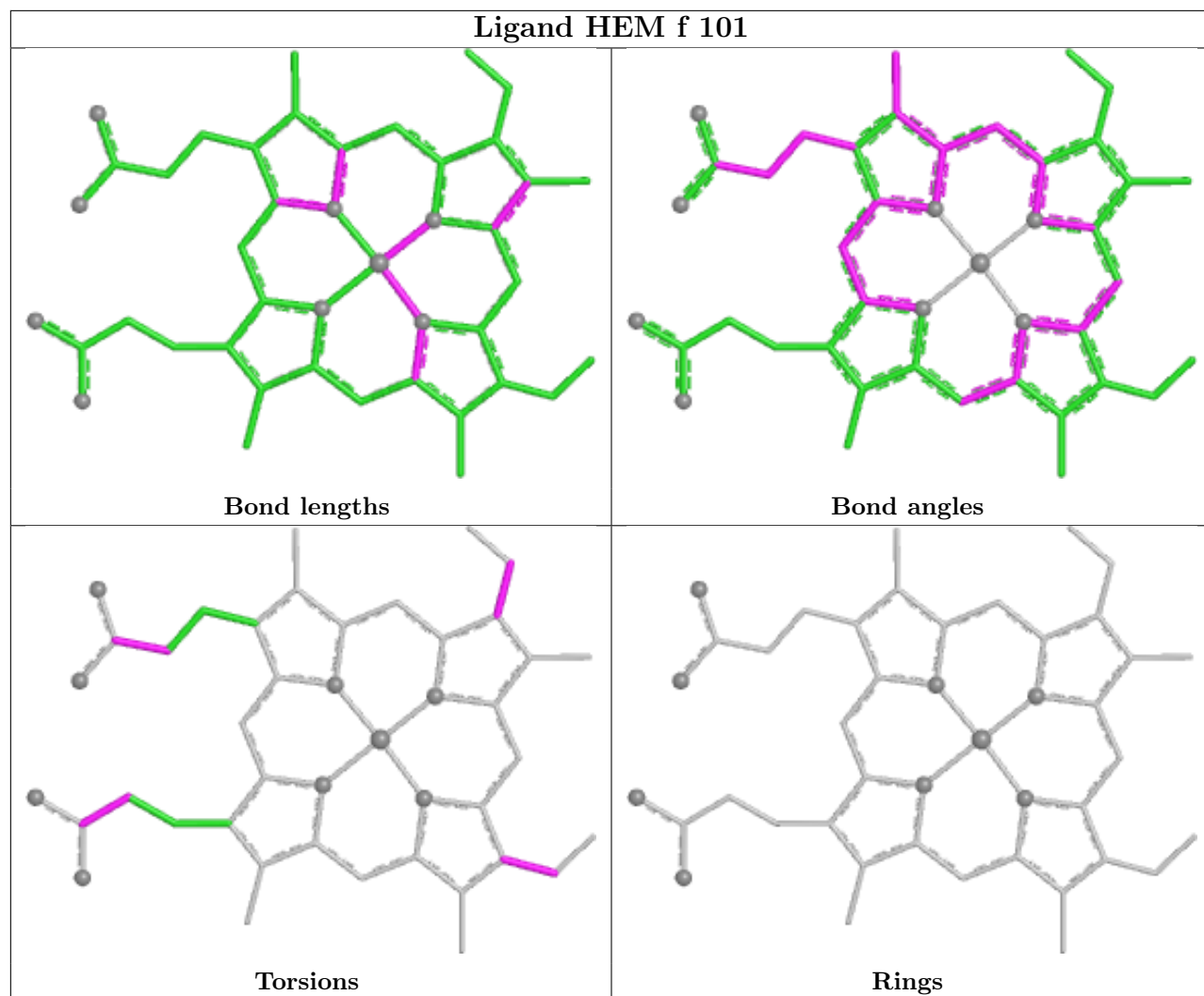
Torsions

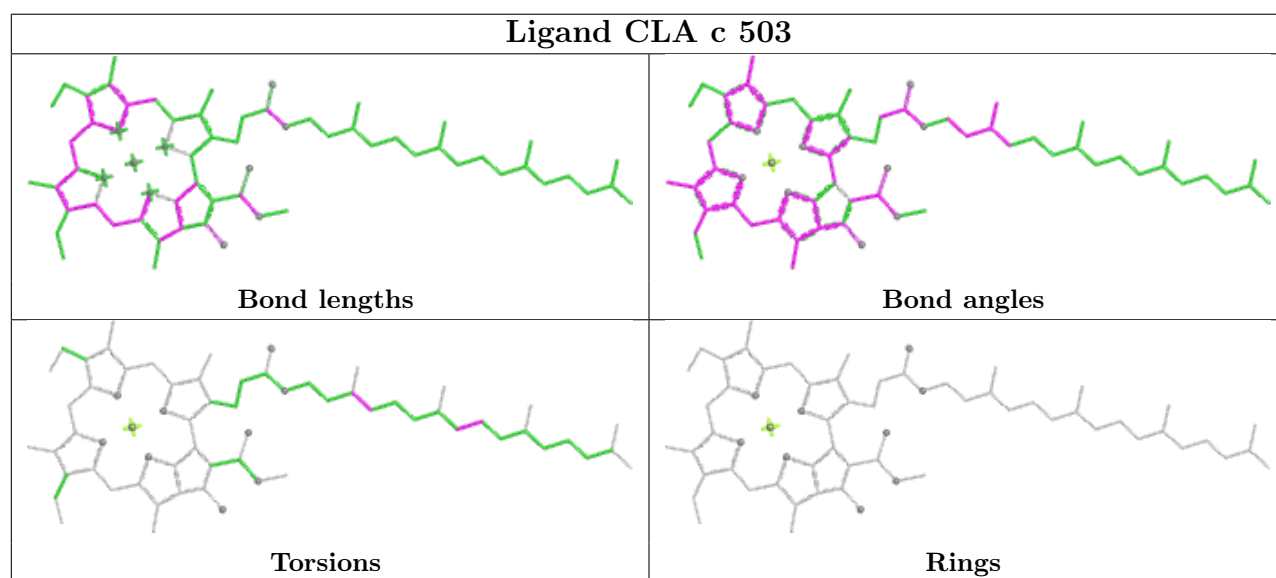
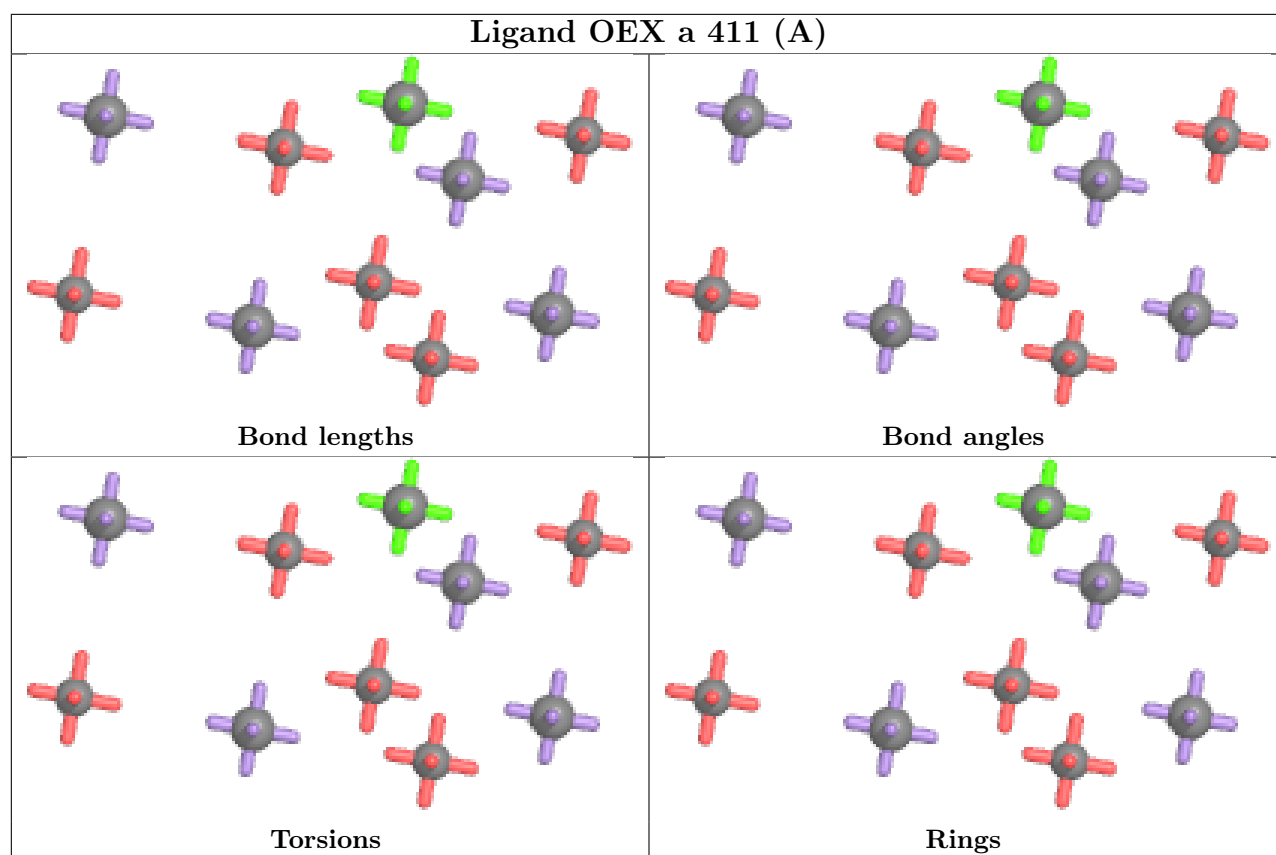


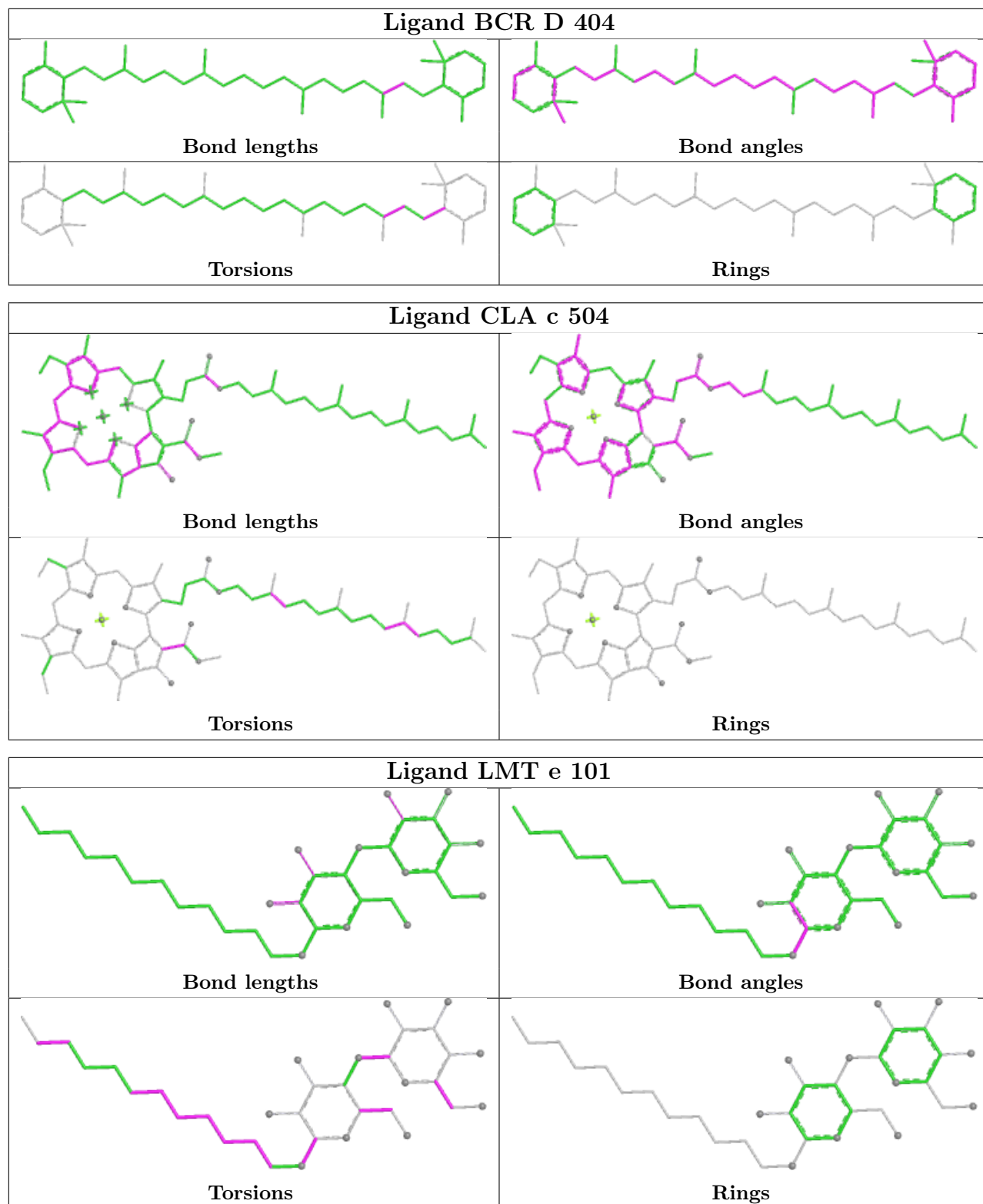
Rings

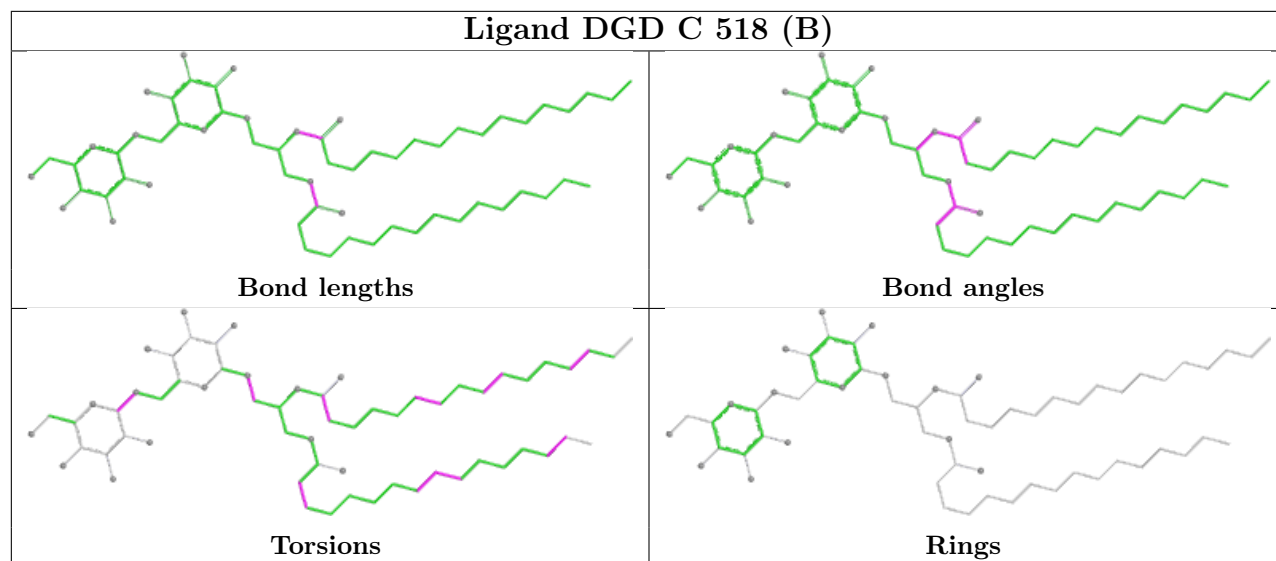


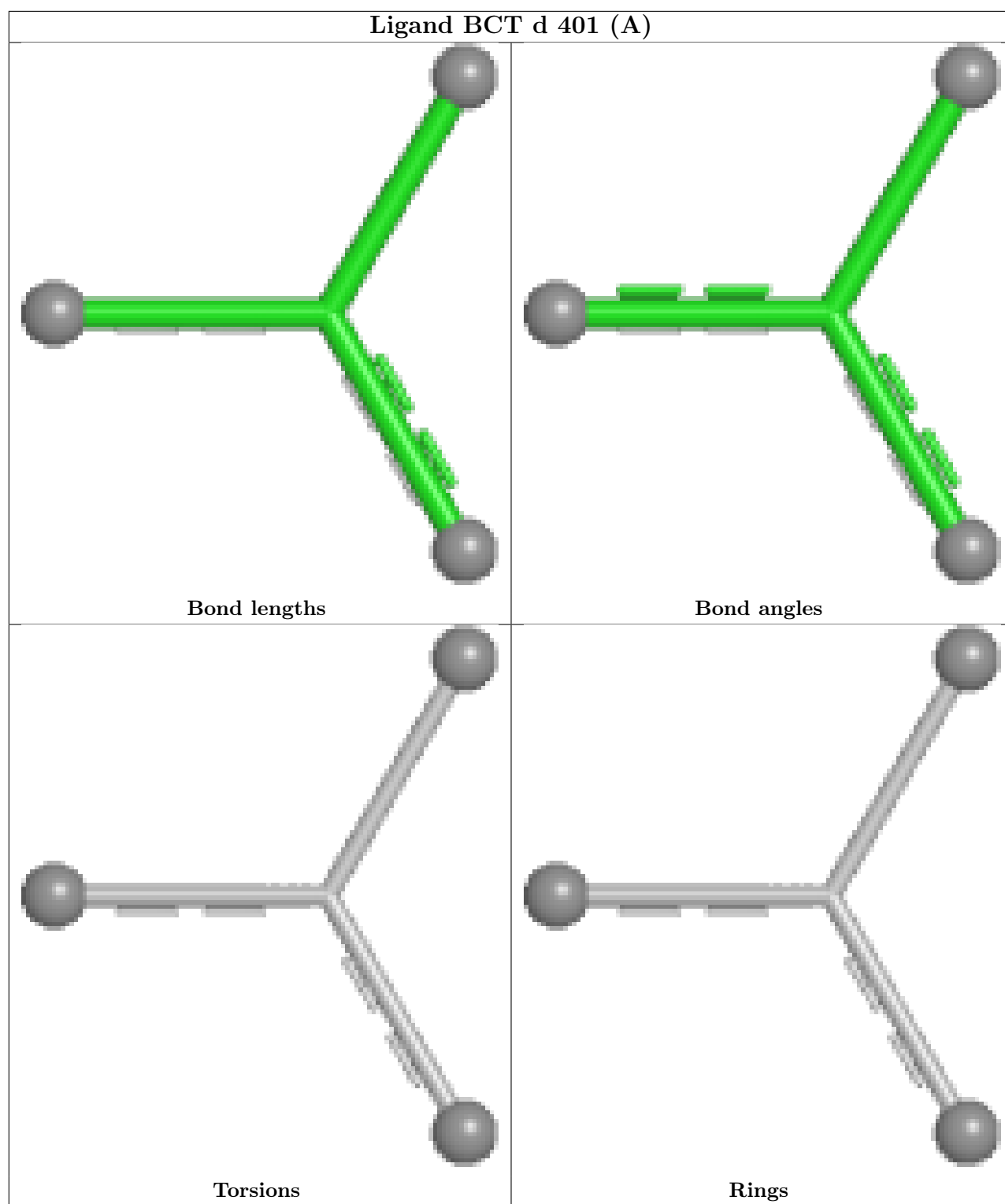
Ligand HEM f 101

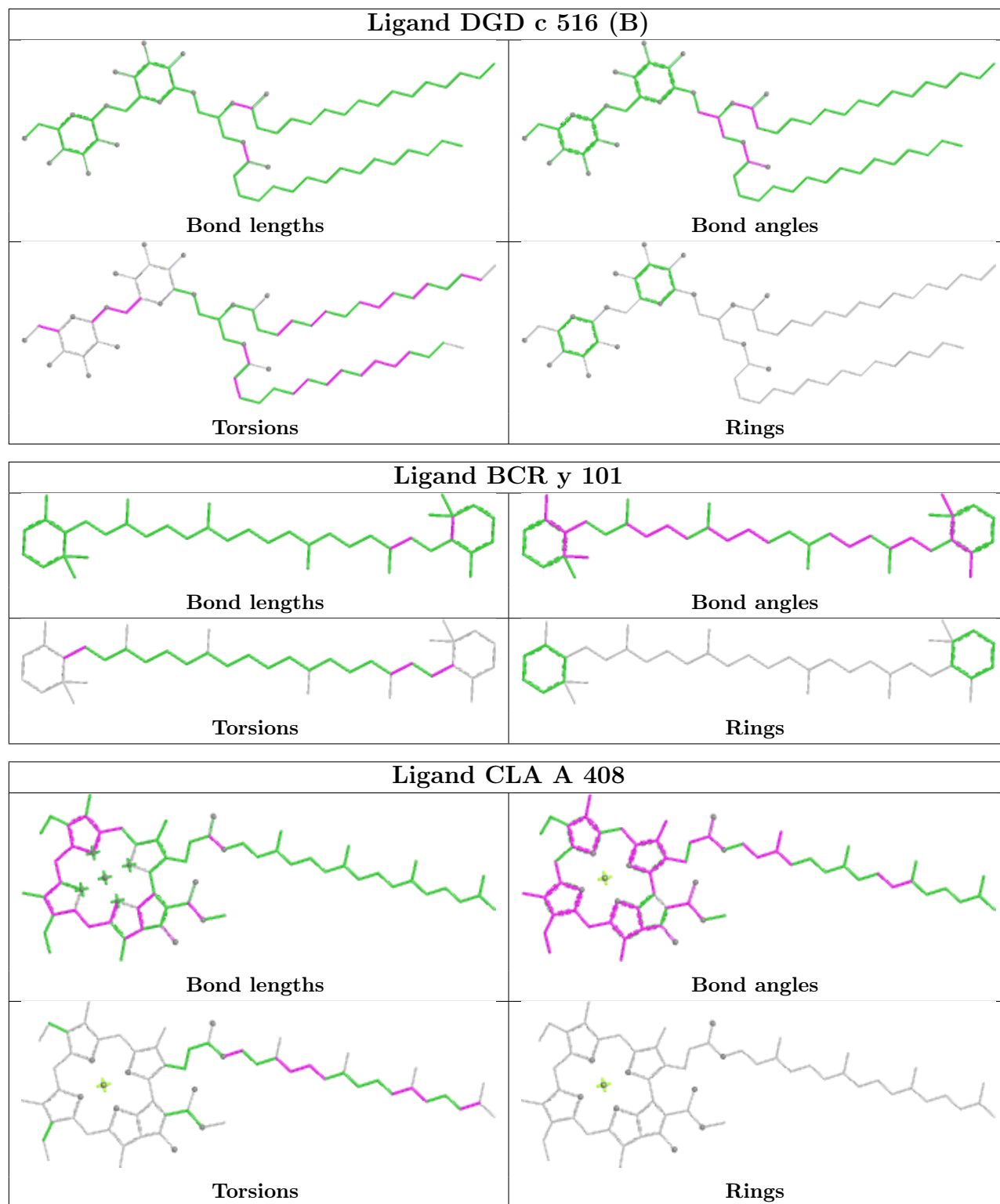


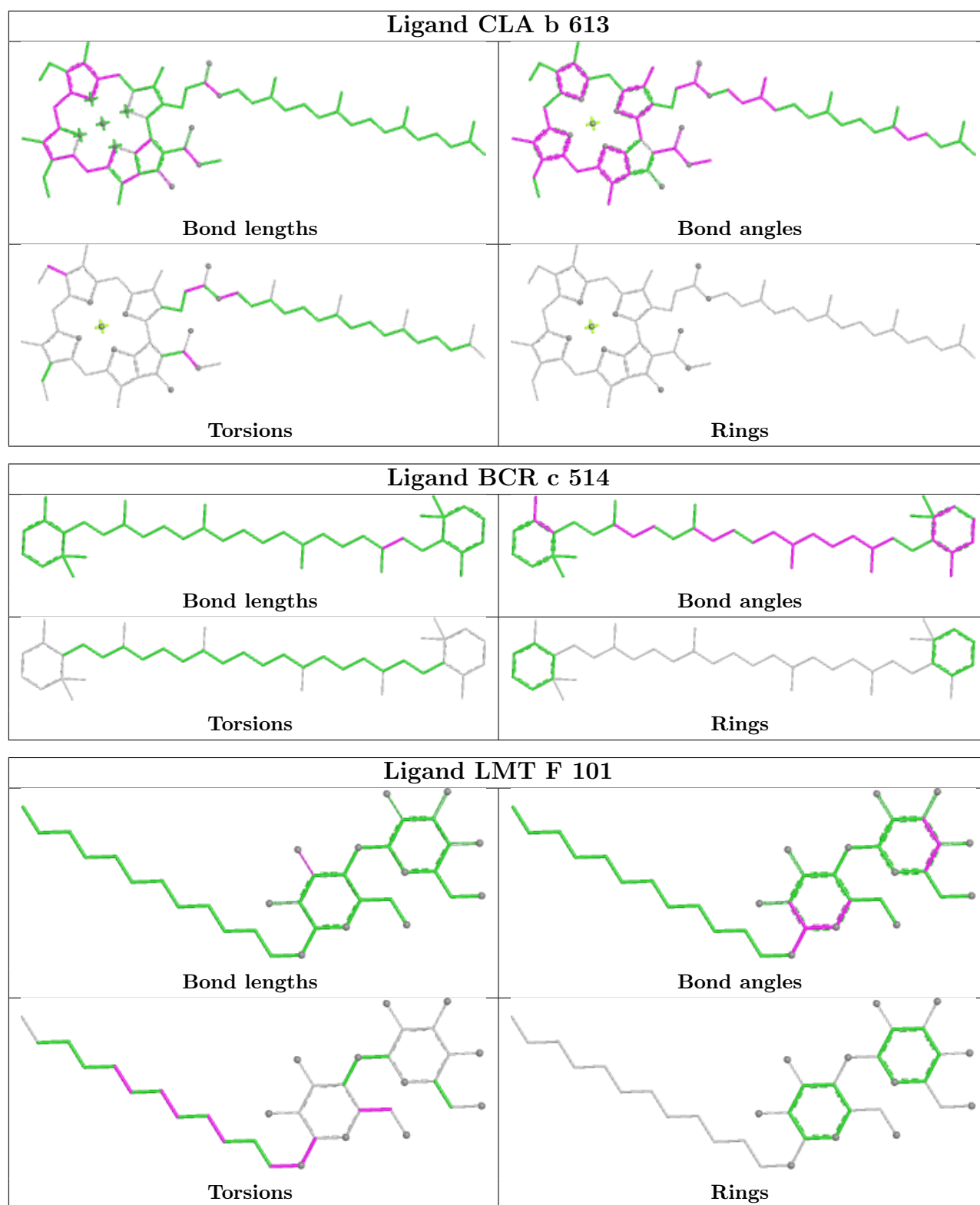


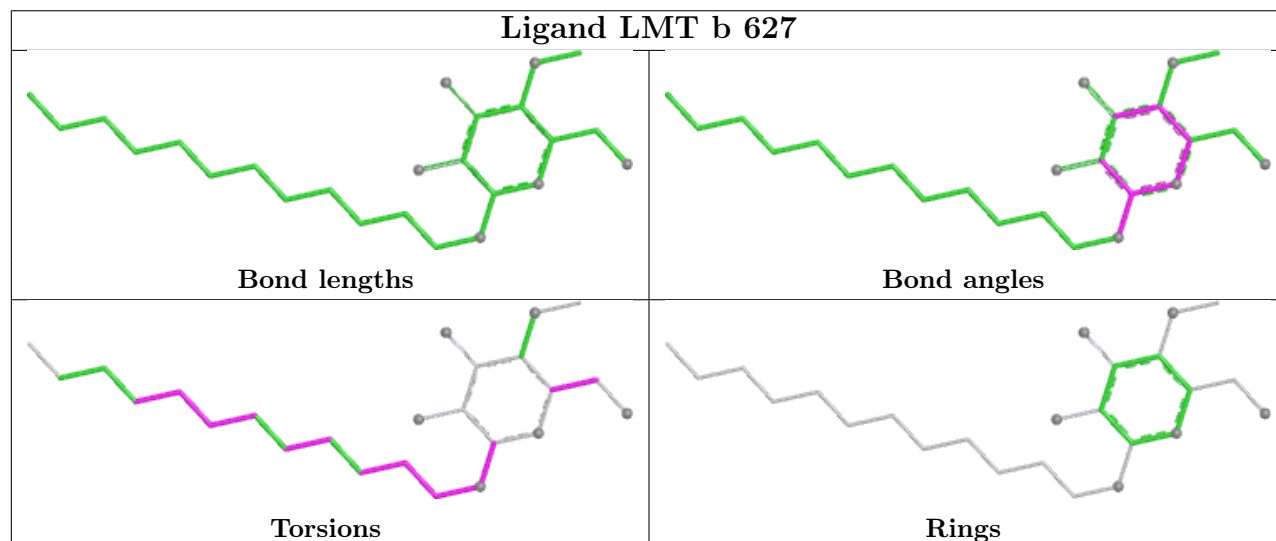
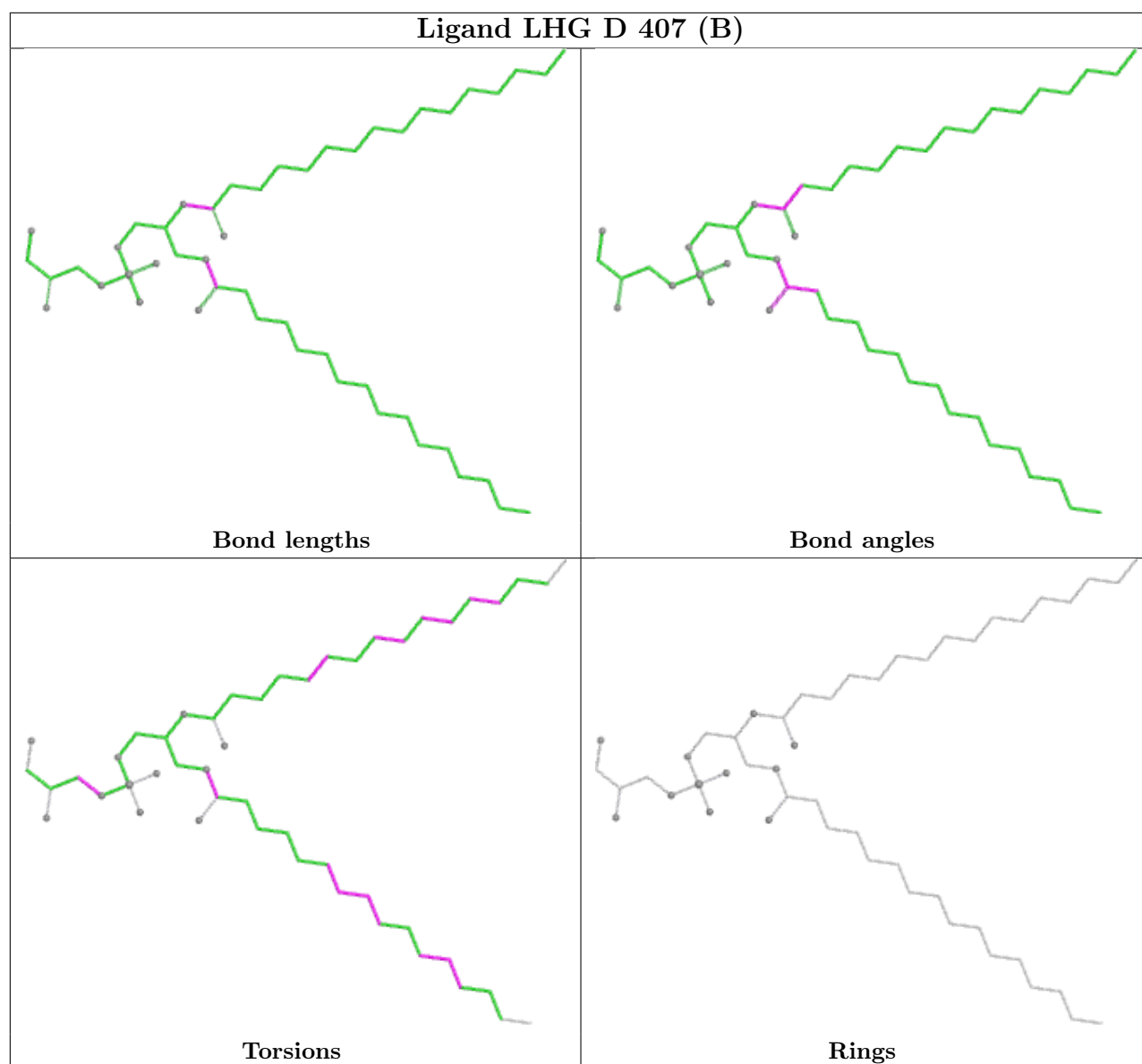




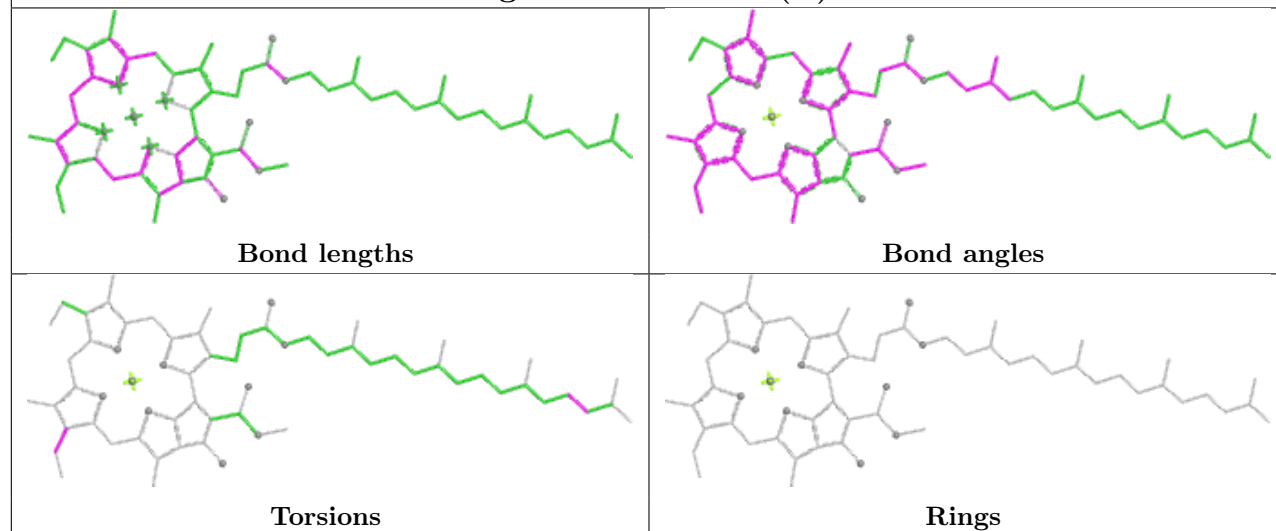




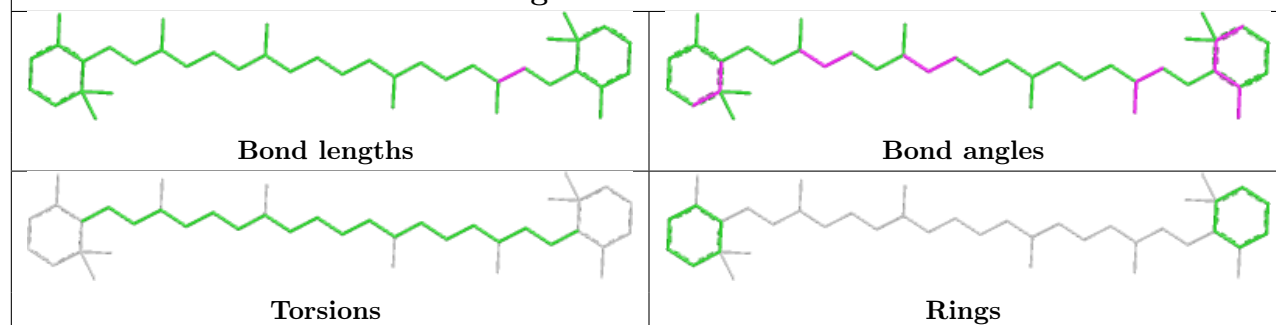




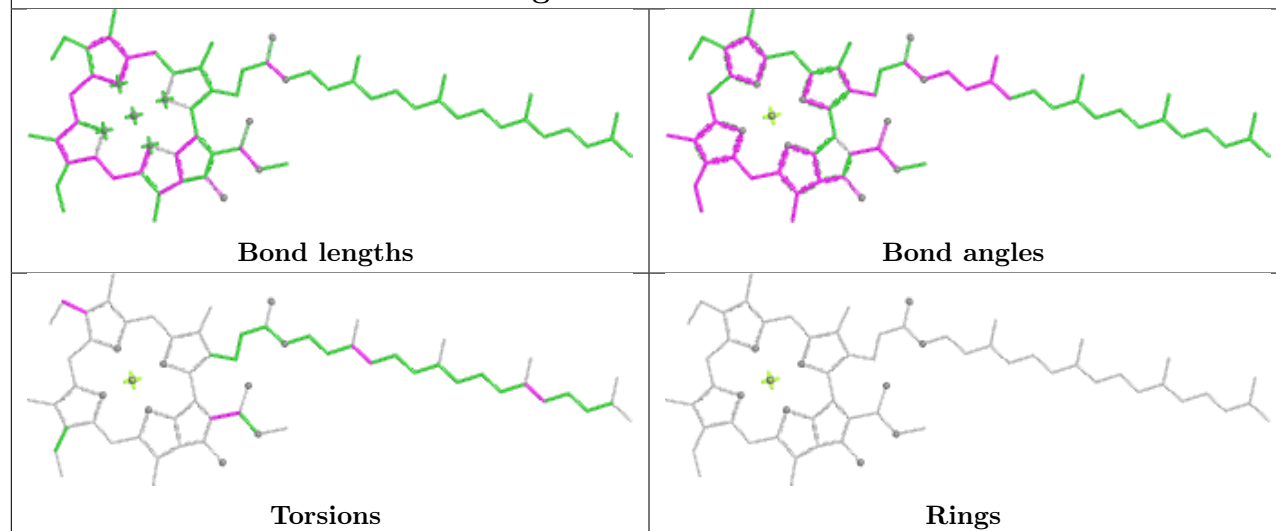
Ligand CLA A 405 (B)

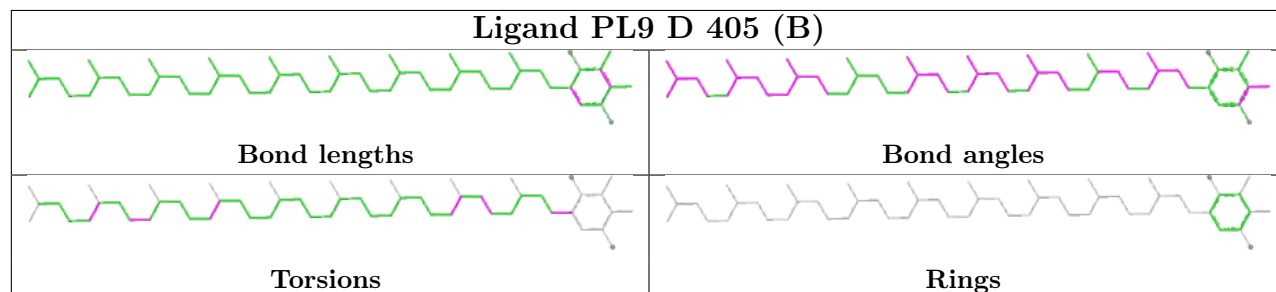
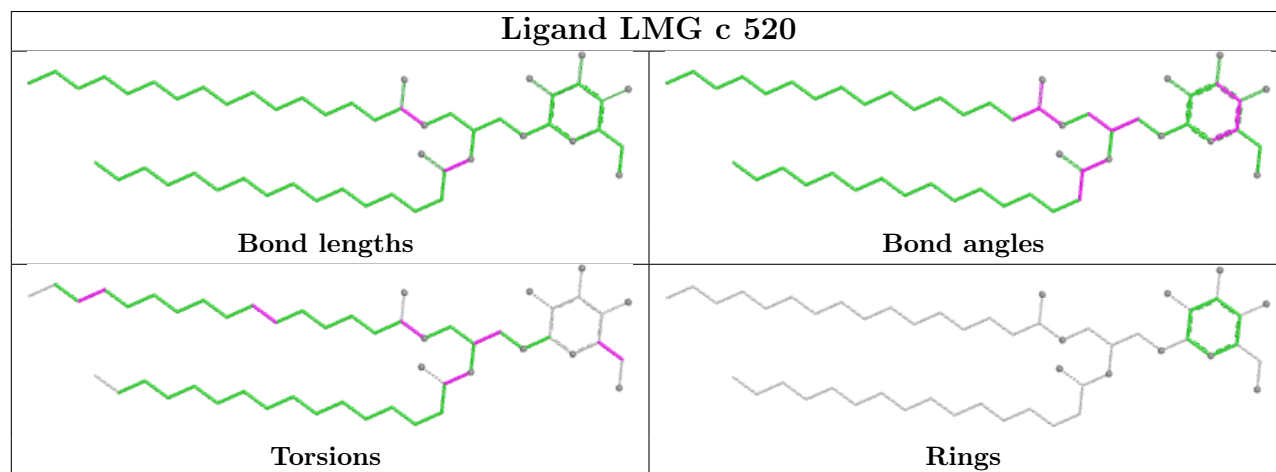
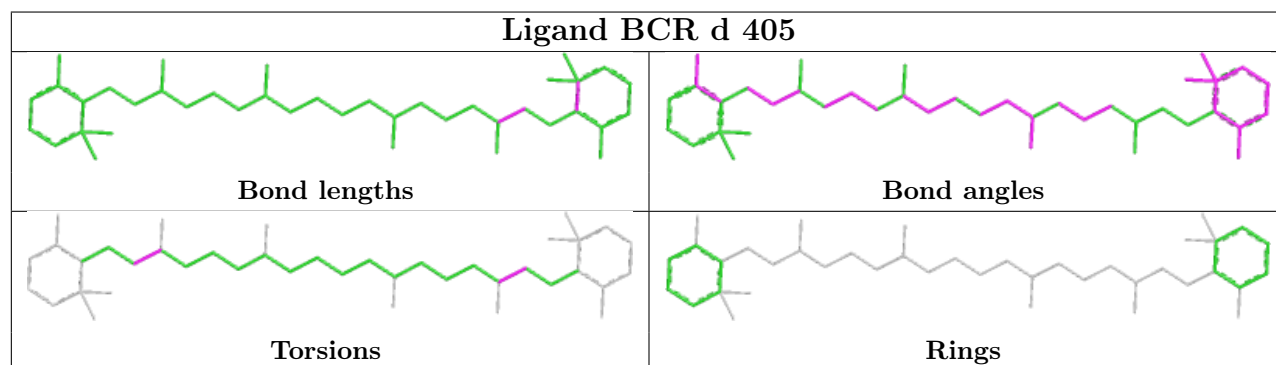
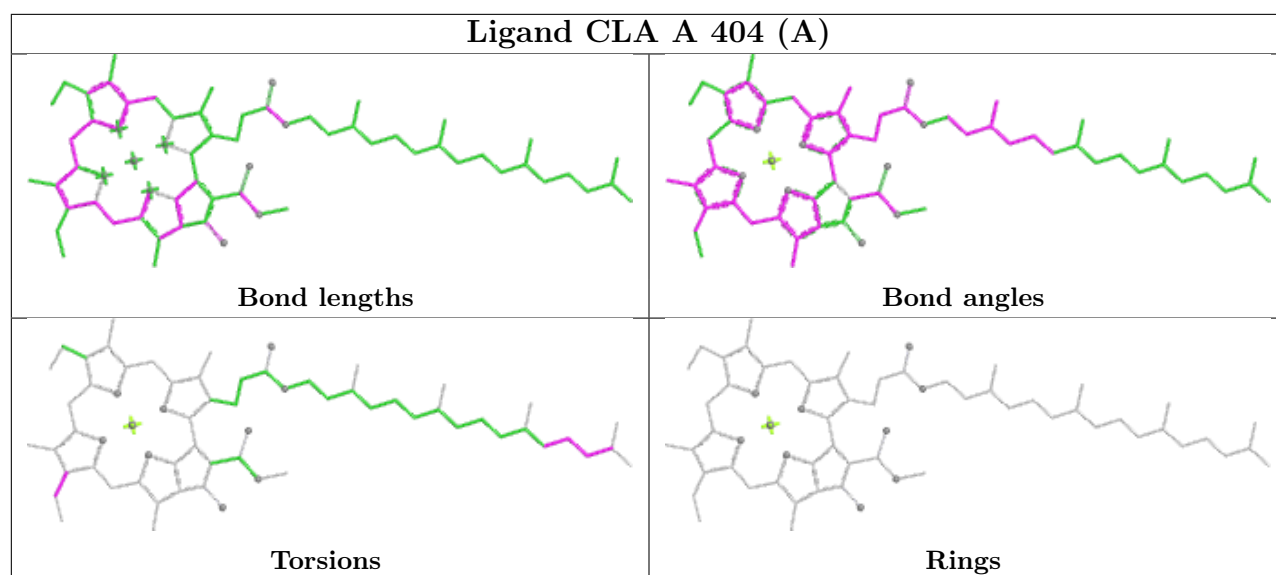


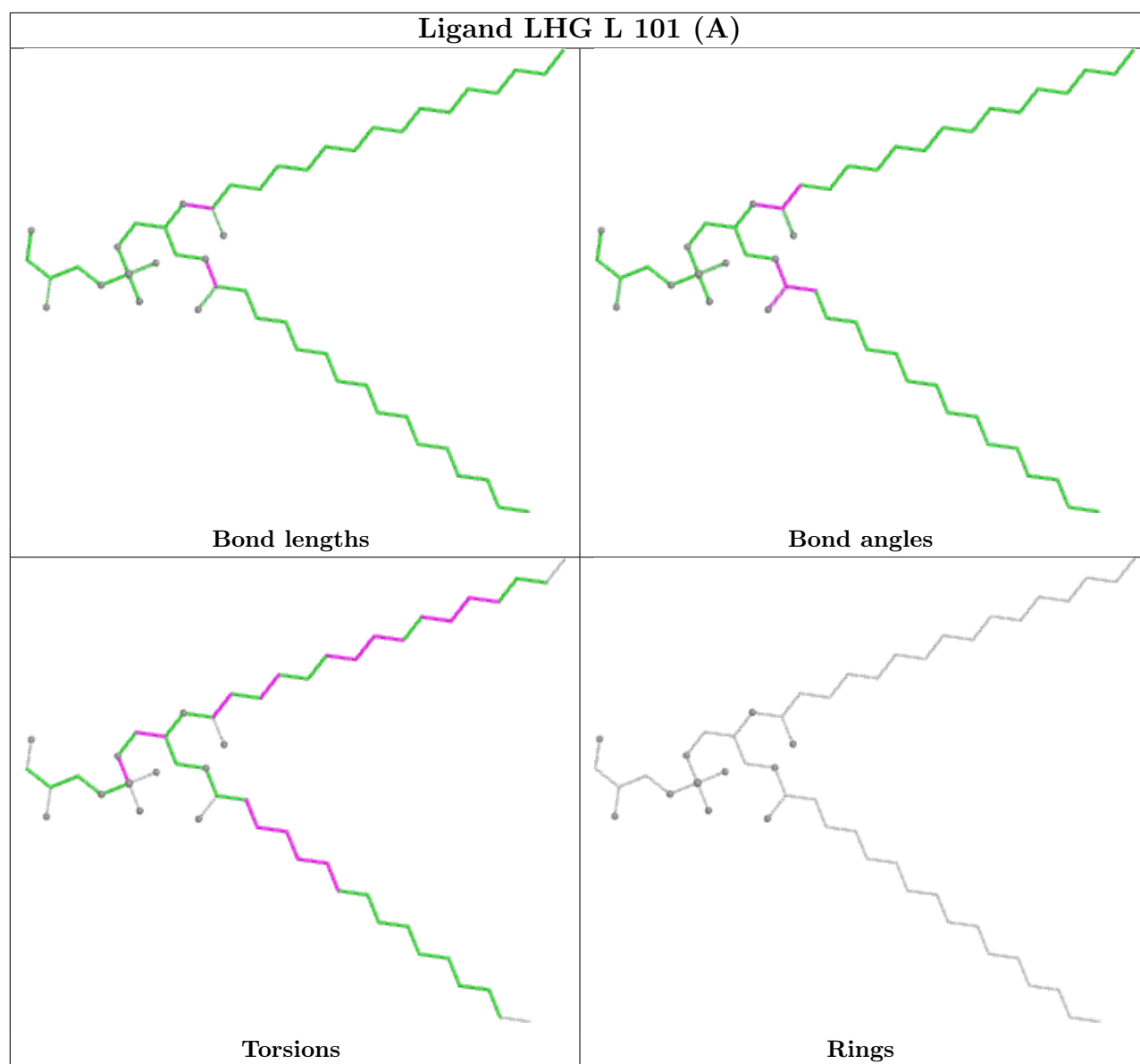
Ligand BCR B 618



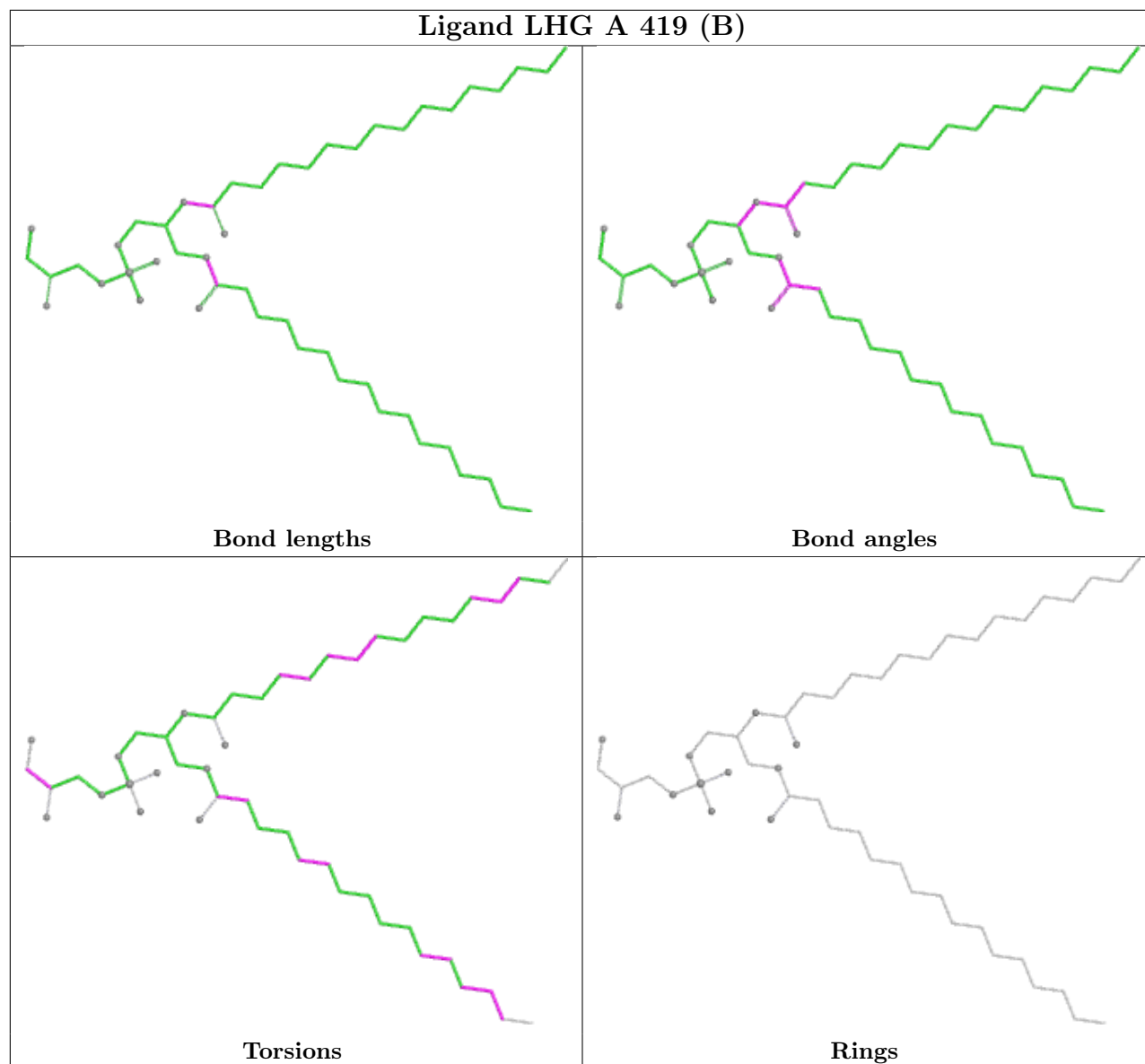
Ligand CLA C 505



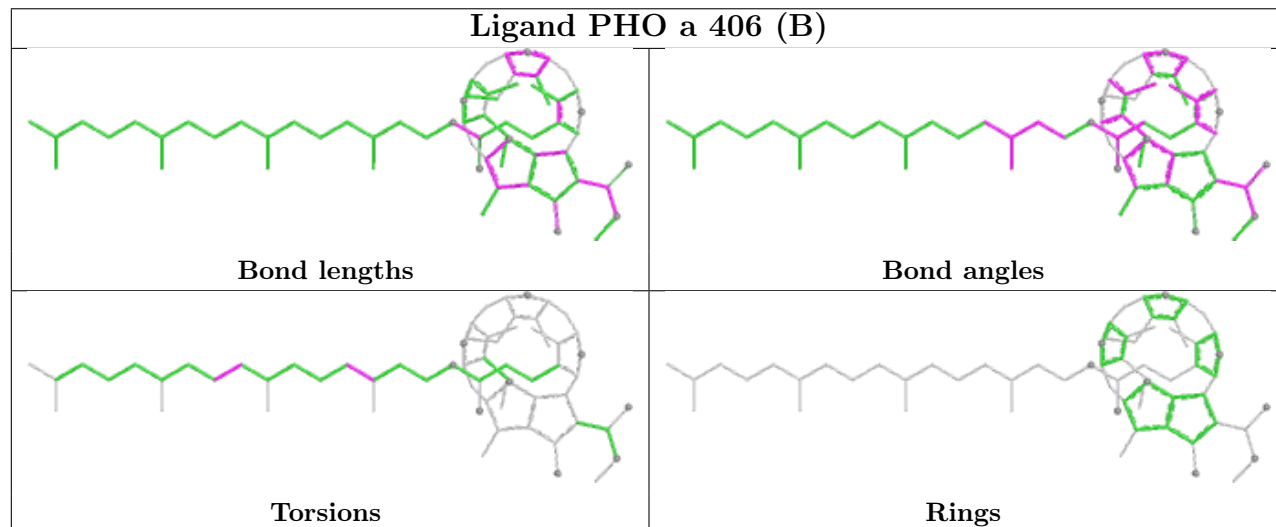


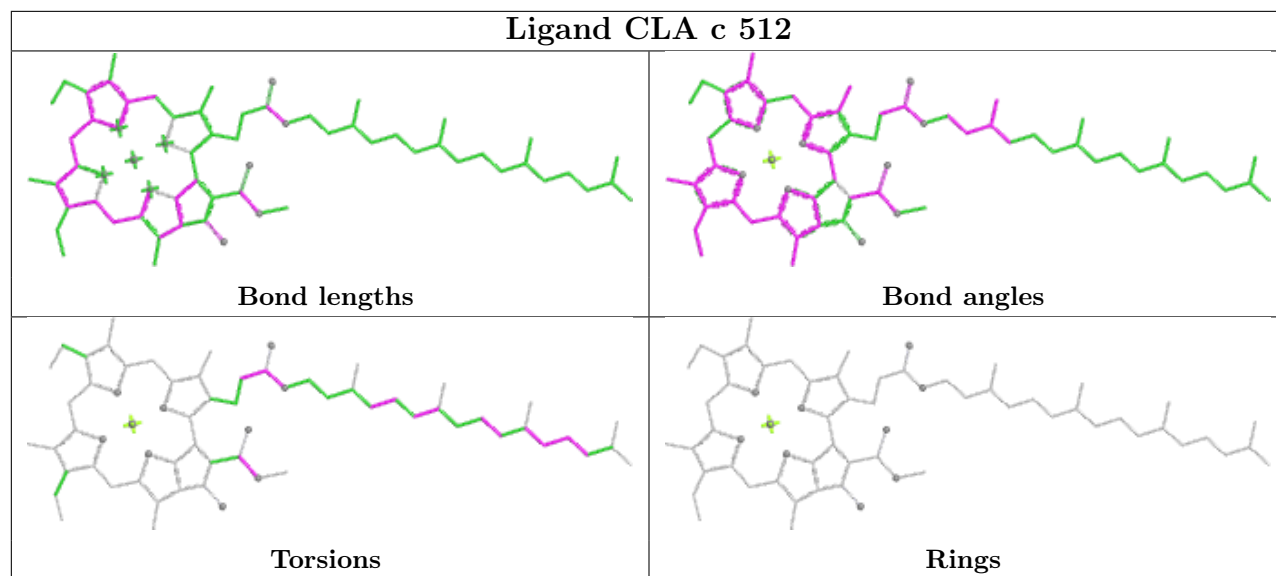


Ligand LHG A 419 (B)



Ligand PHO a 406 (B)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.57	1 (0%) 90 88	20, 26, 58, 126	222 (66%)
1	a	334/344 (97%)	-0.51	1 (0%) 90 88	22, 29, 65, 132	220 (65%)
2	B	504/505 (99%)	-0.43	1 (0%) 91 90	23, 54, 81, 116	22 (4%)
2	b	504/505 (99%)	-0.36	1 (0%) 91 90	24, 57, 94, 167	19 (3%)
3	C	451/455 (99%)	-0.50	0 100 100	23, 59, 79, 163	99 (21%)
3	c	455/455 (100%)	-0.39	2 (0%) 88 87	24, 65, 85, 134	101 (22%)
4	D	342/342 (100%)	-0.57	0 100 100	20, 46, 65, 141	115 (33%)
4	d	341/342 (99%)	-0.56	0 100 100	22, 51, 72, 133	119 (34%)
5	E	81/84 (96%)	-0.30	1 (1%) 76 74	53, 70, 102, 166	0
5	e	79/84 (94%)	-0.24	1 (1%) 75 73	32, 76, 116, 153	2 (2%)
6	F	34/44 (77%)	-0.54	0 100 100	54, 62, 84, 115	0
6	f	31/44 (70%)	-0.45	1 (3%) 50 47	54, 66, 95, 156	1 (3%)
7	H	64/65 (98%)	-0.15	1 (1%) 70 67	51, 63, 86, 111	0
7	h	64/65 (98%)	-0.29	1 (1%) 70 67	38, 69, 94, 113	1 (1%)
8	I	37/38 (97%)	-0.20	0 100 100	57, 63, 124, 169	0
8	i	37/38 (97%)	-0.22	0 100 100	54, 64, 122, 146	0
9	J	38/39 (97%)	-0.29	0 100 100	52, 69, 117, 183	0
9	j	39/39 (100%)	-0.29	0 100 100	59, 77, 129, 165	0
10	K	37/37 (100%)	-0.61	0 100 100	60, 68, 88, 105	0
10	k	37/37 (100%)	-0.49	0 100 100	68, 74, 95, 113	0
11	L	36/37 (97%)	-0.55	0 100 100	23, 47, 103, 147	2 (5%)
11	l	36/37 (97%)	-0.52	0 100 100	24, 48, 100, 124	2 (5%)
12	M	32/36 (88%)	-0.58	0 100 100	27, 49, 77, 136	1 (3%)
12	m	33/36 (91%)	-0.46	0 100 100	25, 49, 70, 153	2 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.43	0 100 100	22, 64, 120, 188	10 (4%)
13	o	243/244 (99%)	-0.38	0 100 100	23, 66, 124, 171	8 (3%)
14	T	29/32 (90%)	-0.57	0 100 100	26, 47, 57, 65	6 (20%)
14	t	29/32 (90%)	-0.56	1 (3%) 48 45	27, 49, 63, 74	5 (17%)
15	U	96/104 (92%)	-0.56	0 100 100	26, 59, 92, 102	4 (4%)
15	u	97/104 (93%)	-0.55	0 100 100	29, 62, 83, 137	5 (5%)
16	V	137/137 (100%)	-0.62	0 100 100	24, 57, 83, 109	6 (4%)
16	v	137/137 (100%)	-0.54	0 100 100	27, 71, 102, 138	6 (4%)
17	X	38/40 (95%)	-0.28	0 100 100	35, 71, 90, 114	1 (2%)
17	x	38/40 (95%)	0.04	0 100 100	64, 77, 119, 164	0
18	Y	29/30 (96%)	0.01	1 (3%) 48 45	67, 84, 127, 131	0
18	y	29/30 (96%)	-0.16	0 100 100	75, 92, 112, 119	0
19	Z	62/62 (100%)	-0.28	0 100 100	67, 80, 132, 162	0
19	z	62/62 (100%)	0.14	0 100 100	80, 94, 140, 206	0
20	R	34/34 (100%)	0.47	2 (5%) 28 25	79, 101, 130, 137	0
All	All	5283/5384 (98%)	-0.44	15 (0%) 90 88	20, 58, 99, 206	979 (18%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	3.9
5	e	79[A]	PHE	3.8
6	f	16[A]	PHE	2.6
1	a	11	ALA	2.5
5	E	4	THR	2.5
3	c	20	SER	2.5
1	A	11	ALA	2.5
14	t	30[A]	THR	2.4
2	B	494	GLY	2.3
3	c	245[A]	ILE	2.3
20	R	28	VAL	2.2
7	h	65	LEU	2.2
18	Y	18	VAL	2.2
20	R	35	LEU	2.1
2	b	499	VAL	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.94	0.08	45,55,64,72	0
8	FME	I	1	10/11	0.95	0.07	58,69,79,82	0
12	FME	m	1	10/11	0.96	0.07	53,63,88,122	0
14	FME	t	1	10/11	0.96	0.07	44,51,65,75	0
8	FME	i	1	10/11	0.97	0.07	53,68,77,90	0
12	FME	M	1	10/11	0.98	0.06	52,60,89,108	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
27	GOL	a	417	6/6	0.63	0.15	78,98,110,112	0
31	LMT	A	417	35/35	0.67	0.15	65,116,144,148	0
31	LMT	B	630	35/35	0.67	0.15	66,117,148,156	0
31	LMT	F	101	35/35	0.69	0.15	102,138,184,189	0
30	UNL	j	101	10/-	0.70	0.18	80,93,103,106	0
30	UNL	I	101	40/-	0.71	0.16	73,111,158,166	0
30	UNL	a	413	30/-	0.71	0.12	93,119,146,161	0
30	UNL	A	415	28/-	0.71	0.15	93,117,135,155	0
34	HTG	B	623	19/19	0.71	0.17	67,93,117,125	0
30	UNL	J	101	10/-	0.72	0.24	72,81,90,95	0
30	UNL	m	102	10/-	0.72	0.21	73,77,96,102	0
30	UNL	K	101[A]	34/-	0.74	0.14	88,115,128,132	34
30	UNL	K	101[B]	34/-	0.74	0.14	88,115,128,133	34
31	LMT	A	420	35/35	0.74	0.13	100,135,156,170	0
34	HTG	C	522	19/19	0.74	0.13	112,130,148,148	0
31	LMT	a	416	35/35	0.75	0.13	109,138,152,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LMT	e	101	35/35	0.76	0.13	110,151,197,199	0
30	UNL	M	102	10/-	0.77	0.16	69,78,93,96	0
26	SQD	f	102	43/54	0.77	0.13	90,133,179,195	0
30	UNL	i	101	40/-	0.78	0.14	73,110,160,171	0
30	UNL	b	626	33/-	0.79	0.13	68,97,161,173	0
30	UNL	c	524[A]	32/-	0.79	0.15	98,113,127,139	32
31	LMT	b	621	25/35	0.79	0.13	84,112,164,173	0
30	UNL	c	524[B]	32/-	0.79	0.15	98,113,127,139	32
33	LMG	C	521	51/55	0.79	0.11	63,117,164,179	0
30	UNL	d	410	36/-	0.79	0.12	65,93,136,146	0
27	GOL	o	302	6/6	0.79	0.17	84,102,112,116	0
34	HTG	D	410	16/19	0.79	0.12	84,104,134,149	0
27	GOL	d	413	6/6	0.80	0.14	55,75,76,91	0
30	UNL	D	409	40/-	0.80	0.13	67,94,139,151	0
36	CA	F	103	1/1	0.81	0.24	127,127,127,127	0
30	UNL	B	626	33/-	0.82	0.15	54,117,145,149	0
34	HTG	V	202	11/19	0.82	0.10	83,111,123,130	0
34	HTG	b	623	19/19	0.82	0.11	84,135,161,168	0
34	HTG	c	521	19/19	0.82	0.10	105,125,141,151	0
31	LMT	B	628	35/35	0.82	0.12	67,102,138,150	0
32	LHG	a	419[B]	42/49	0.83	0.11	94,140,157,165	42
26	SQD	a	410	54/54	0.83	0.11	67,97,136,154	0
27	GOL	o	303	6/6	0.83	0.14	82,91,102,110	0
27	GOL	v	202[A]	6/6	0.83	0.13	65,79,85,86	6
27	GOL	v	202[B]	6/6	0.83	0.13	65,79,85,87	6
27	GOL	a	418	6/6	0.83	0.15	58,78,84,88	0
27	GOL	b	624	6/6	0.83	0.15	88,95,107,111	0
27	GOL	O	303	6/6	0.83	0.13	82,95,107,108	0
32	LHG	a	419[A]	42/49	0.83	0.11	94,140,157,165	42
27	GOL	l	801[B]	6/6	0.84	0.19	73,105,107,111	6
31	LMT	B	631	25/35	0.84	0.12	63,87,150,170	0
27	GOL	B	627	6/6	0.84	0.13	71,88,97,112	0
34	HTG	d	411	16/19	0.84	0.11	89,122,140,154	0
27	GOL	l	801[A]	6/6	0.84	0.19	73,104,107,111	6
33	LMG	c	520	51/55	0.85	0.10	73,135,172,190	0
33	LMG	z	101	39/55	0.85	0.13	78,132,153,170	0
29	PL9	A	414[A]	55/55	0.85	0.15	74,100,115,120	55
29	PL9	A	414[B]	55/55	0.85	0.15	74,100,115,120	55
31	LMT	T	101	35/35	0.85	0.11	77,131,185,192	0
36	CA	f	103	1/1	0.85	0.10	120,120,120,120	0
27	GOL	A	411	6/6	0.86	0.12	64,81,85,91	0
34	HTG	b	622	19/19	0.86	0.12	58,80,121,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	LMG	Z	101	37/55	0.86	0.14	72,123,151,171	0
31	LMT	t	101	26/35	0.86	0.12	78,105,148,163	0
29	PL9	a	412[A]	55/55	0.86	0.15	82,109,121,129	55
29	PL9	a	412[B]	55/55	0.86	0.15	82,109,121,129	55
26	SQD	A	412	54/54	0.86	0.11	65,90,140,150	0
31	LMT	M	101	35/35	0.87	0.10	63,96,120,125	0
31	LMT	m	103	35/35	0.87	0.10	66,90,109,125	0
27	GOL	B	629	6/6	0.87	0.13	74,79,93,97	0
34	HTG	B	622	19/19	0.87	0.13	61,87,121,126	0
27	GOL	O	302	6/6	0.87	0.08	77,86,99,113	0
27	GOL	c	526	6/6	0.87	0.16	102,111,120,127	0
31	LMT	b	627	25/35	0.87	0.12	59,100,155,167	0
27	GOL	A	418	6/6	0.88	0.15	51,82,88,93	0
26	SQD	F	102	43/54	0.88	0.12	69,107,131,145	0
23	CLA	b	601	65/65	0.88	0.11	59,84,128,166	0
27	GOL	D	412	6/6	0.88	0.12	51,68,73,94	0
26	SQD	b	620	54/54	0.89	0.10	65,96,118,130	0
32	LHG	E	101[A]	42/49	0.89	0.12	76,106,118,123	42
32	LHG	E	101[B]	42/49	0.89	0.12	76,106,118,124	42
26	SQD	B	620	54/54	0.89	0.10	66,93,135,146	0
30	UNL	D	408	17/-	0.89	0.11	62,78,99,122	0
36	CA	o	301	1/1	0.89	0.07	103,103,103,103	0
27	GOL	V	203[B]	6/6	0.90	0.13	60,70,77,77	6
23	CLA	c	513	65/65	0.90	0.10	66,93,129,148	0
23	CLA	B	601	65/65	0.90	0.10	57,78,114,156	0
33	LMG	C	501	51/55	0.90	0.10	68,90,118,136	0
27	GOL	V	203[A]	6/6	0.90	0.13	60,70,77,77	6
33	LMG	a	415	51/55	0.91	0.09	71,96,115,119	0
33	LMG	c	519	51/55	0.91	0.10	62,91,136,161	0
27	GOL	B	624	6/6	0.91	0.09	70,73,86,91	0
33	LMG	m	101	51/55	0.91	0.09	63,76,98,115	0
34	HTG	B	625	19/19	0.91	0.08	68,82,98,105	0
30	UNL	d	409	17/-	0.92	0.10	69,79,114,116	0
33	LMG	D	411	51/55	0.92	0.10	50,72,124,138	0
23	CLA	b	616	65/65	0.92	0.09	48,62,133,146	0
33	LMG	C	520	51/55	0.92	0.09	55,85,123,134	0
34	HTG	b	625	19/19	0.92	0.08	68,79,97,110	0
37	BCT	d	401[A]	4/4	0.92	0.09	59,61,69,78	4
37	BCT	d	401[B]	4/4	0.92	0.09	60,61,69,80	4
25	BCR	t	102	40/40	0.93	0.07	44,59,80,89	0
26	SQD	A	410[A]	54/54	0.93	0.09	57,81,115,119	54
26	SQD	A	410[B]	54/54	0.93	0.09	57,81,115,119	54

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	B	603	65/65	0.93	0.09	43,54,73,83	0
23	CLA	C	507	65/65	0.93	0.08	53,71,125,144	0
33	LMG	d	412	51/55	0.93	0.09	54,72,124,155	0
23	CLA	c	506	65/65	0.93	0.09	54,72,126,142	0
26	SQD	a	409[A]	54/54	0.93	0.10	61,83,121,123	54
26	SQD	a	409[B]	54/54	0.93	0.10	61,83,121,123	54
23	CLA	c	512	65/65	0.93	0.09	60,81,126,140	0
23	CLA	C	514	65/65	0.93	0.08	59,83,115,120	0
23	CLA	d	404	65/65	0.93	0.09	52,67,130,157	0
25	BCR	B	619	40/40	0.93	0.09	47,60,90,101	0
25	BCR	D	404	40/40	0.93	0.09	44,62,108,115	0
32	LHG	A	419[A]	49/49	0.93	0.10	50,66,89,93	49
32	LHG	A	419[B]	49/49	0.93	0.10	50,66,89,93	49
32	LHG	D	407[A]	49/49	0.93	0.09	49,61,110,113	49
32	LHG	D	407[B]	49/49	0.93	0.09	49,61,110,114	49
25	BCR	H	101	40/40	0.93	0.09	53,68,90,93	0
25	BCR	T	102	40/40	0.93	0.07	45,57,73,86	0
35	DGD	C	518[A]	62/66	0.93	0.08	49,63,114,118	62
35	DGD	C	518[B]	62/66	0.93	0.08	49,63,114,118	62
25	BCR	a	408	40/40	0.93	0.07	45,53,67,69	0
27	GOL	C	523[A]	6/6	0.93	0.11	59,62,67,72	6
33	LMG	B	621	51/55	0.93	0.08	55,72,95,116	0
27	GOL	C	523[B]	6/6	0.93	0.11	59,63,67,72	6
25	BCR	d	405	40/40	0.93	0.08	51,69,109,113	0
32	LHG	d	414[B]	49/49	0.94	0.09	51,69,82,94	49
23	CLA	D	403	65/65	0.94	0.09	47,60,132,138	0
23	CLA	a	407	65/65	0.94	0.10	42,57,141,161	0
25	BCR	K	102	40/40	0.94	0.09	56,65,76,82	0
23	CLA	B	614	65/65	0.94	0.08	39,50,104,118	0
25	BCR	Y	101	40/40	0.94	0.08	54,65,84,92	0
29	PL9	D	405[A]	55/55	0.94	0.07	38,50,57,72	55
29	PL9	D	405[B]	55/55	0.94	0.07	38,50,58,72	55
23	CLA	b	606	65/65	0.94	0.08	43,58,117,132	0
25	BCR	b	619	40/40	0.94	0.08	48,64,90,95	0
25	BCR	c	514	40/40	0.94	0.09	71,83,93,98	0
23	CLA	b	614	65/65	0.94	0.07	42,53,102,117	0
25	BCR	h	101	40/40	0.94	0.09	55,70,91,97	0
23	CLA	B	616	65/65	0.94	0.09	48,59,132,147	0
25	BCR	y	101	40/40	0.94	0.08	59,71,89,100	0
23	CLA	c	504	65/65	0.94	0.07	53,64,107,142	0
23	CLA	C	505	65/65	0.94	0.08	42,58,106,131	0
23	CLA	c	507	65/65	0.94	0.10	50,67,85,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	A	408	65/65	0.94	0.09	43,54,128,149	0
30	UNL	X	101	18/-	0.94	0.11	64,73,112,112	0
27	GOL	b	628	6/6	0.94	0.07	78,88,92,92	0
23	CLA	C	508	65/65	0.94	0.09	47,61,83,93	0
23	CLA	C	513	65/65	0.94	0.09	54,72,117,136	0
25	BCR	A	409	40/40	0.94	0.07	40,52,67,71	0
25	BCR	B	618	40/40	0.94	0.06	43,55,73,80	0
23	CLA	B	606	65/65	0.94	0.09	44,56,114,130	0
35	DGD	C	519	62/66	0.94	0.08	45,61,103,122	0
35	DGD	H	102	62/66	0.94	0.09	47,63,75,90	0
35	DGD	c	516[A]	62/66	0.94	0.08	48,64,103,113	62
35	DGD	c	516[B]	62/66	0.94	0.08	47,64,103,114	62
35	DGD	c	517[A]	62/66	0.94	0.08	56,69,123,138	62
35	DGD	c	517[B]	62/66	0.94	0.08	56,69,123,139	62
35	DGD	c	518	62/66	0.94	0.08	50,67,106,131	0
35	DGD	h	102	62/66	0.94	0.08	52,65,79,82	0
32	LHG	b	629[A]	49/49	0.94	0.08	51,60,72,95	49
32	LHG	b	629[B]	49/49	0.94	0.08	51,60,72,95	49
32	LHG	d	408[A]	49/49	0.94	0.09	52,64,117,134	49
32	LHG	d	408[B]	49/49	0.94	0.09	52,64,117,134	49
32	LHG	d	414[A]	49/49	0.94	0.09	51,69,81,93	49
23	CLA	c	508	65/65	0.95	0.07	46,63,133,152	0
23	CLA	C	509	65/65	0.95	0.07	47,56,122,147	0
23	CLA	C	502	65/65	0.95	0.07	49,60,74,81	0
25	BCR	b	617	40/40	0.95	0.06	43,53,64,69	0
25	BCR	b	618	40/40	0.95	0.07	47,57,76,94	0
23	CLA	b	612	65/65	0.95	0.08	41,54,65,76	0
24	PHO	A	416[A]	64/64	0.95	0.07	39,51,56,63	64
25	BCR	c	515	40/40	0.95	0.07	57,65,78,86	0
24	PHO	A	416[B]	64/64	0.95	0.07	38,51,56,64	64
24	PHO	a	414[A]	64/64	0.95	0.07	44,56,64,72	64
32	LHG	d	407[A]	49/49	0.95	0.08	49,57,72,79	49
32	LHG	d	407[B]	49/49	0.95	0.08	49,58,72,79	49
35	DGD	C	517[A]	62/66	0.95	0.07	47,57,103,109	62
35	DGD	C	517[B]	62/66	0.95	0.07	47,57,103,109	62
30	UNL	x	101	18/-	0.95	0.11	68,84,140,141	0
25	BCR	k	101	40/40	0.95	0.09	59,75,85,87	0
24	PHO	a	414[B]	64/64	0.95	0.07	44,56,64,72	64
23	CLA	B	611	65/65	0.95	0.07	38,46,65,74	0
29	PL9	d	406[A]	55/55	0.95	0.07	41,52,63,72	55
29	PL9	d	406[B]	55/55	0.95	0.07	40,52,63,72	55
23	CLA	B	609	65/65	0.95	0.07	47,59,72,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	c	501	65/65	0.95	0.08	55,67,80,93	0
25	BCR	C	515	40/40	0.95	0.07	55,75,91,93	0
25	BCR	C	516	40/40	0.95	0.07	51,61,76,90	0
23	CLA	a	405[A]	65/65	0.95	0.07	43,55,126,133	65
23	CLA	a	405[B]	65/65	0.95	0.07	42,55,126,133	65
27	GOL	c	525[A]	6/6	0.95	0.08	65,72,77,77	6
37	BCT	D	401[A]	4/4	0.95	0.08	54,55,61,68	4
37	BCT	D	401[B]	4/4	0.95	0.08	54,55,62,69	4
27	GOL	c	525[B]	6/6	0.95	0.08	65,73,77,78	6
23	CLA	B	610	65/65	0.95	0.09	42,55,68,84	0
23	CLA	b	607	65/65	0.96	0.07	38,48,81,94	0
23	CLA	b	609	65/65	0.96	0.07	49,65,77,90	0
23	CLA	b	611	65/65	0.96	0.07	41,51,72,81	0
23	CLA	C	506	65/65	0.96	0.07	46,60,96,109	0
23	CLA	b	613	65/65	0.96	0.06	43,50,88,108	0
23	CLA	B	607	65/65	0.96	0.07	38,48,72,85	0
23	CLA	b	615	65/65	0.96	0.06	48,59,83,95	0
23	CLA	A	406[A]	65/65	0.96	0.06	41,48,114,125	65
32	LHG	D	406[A]	49/49	0.96	0.08	46,57,70,80	49
32	LHG	D	406[B]	49/49	0.96	0.08	46,57,71,80	49
23	CLA	A	406[B]	65/65	0.96	0.06	41,48,114,125	65
23	CLA	c	503	65/65	0.96	0.07	49,70,86,93	0
23	CLA	C	510	65/65	0.96	0.08	50,59,83,94	0
23	CLA	c	505	65/65	0.96	0.07	51,64,92,97	0
32	LHG	L	101[A]	49/49	0.96	0.07	49,58,71,94	49
32	LHG	L	101[B]	49/49	0.96	0.07	48,58,71,94	49
23	CLA	C	512	65/65	0.96	0.07	49,64,80,84	0
22	CL	a	402[A]	1/1	0.96	0.06	50,50,50,50	1
23	CLA	B	613	65/65	0.96	0.06	39,48,100,109	0
23	CLA	c	509	65/65	0.96	0.08	46,62,90,101	0
23	CLA	c	511	65/65	0.96	0.08	56,68,87,107	0
22	CL	a	402[B]	1/1	0.96	0.06	50,50,50,50	1
23	CLA	B	615	65/65	0.96	0.06	45,55,78,96	0
23	CLA	B	602	65/65	0.96	0.07	46,56,74,88	0
23	CLA	A	404[A]	65/65	0.96	0.07	37,45,63,71	65
23	CLA	C	504	65/65	0.96	0.06	46,62,72,88	0
24	PHO	a	406[A]	64/64	0.96	0.06	43,50,55,60	64
36	CA	C	524	1/1	0.96	0.05	72,72,72,72	0
24	PHO	a	406[B]	64/64	0.96	0.06	43,50,56,60	64
36	CA	O	301	1/1	0.96	0.04	104,104,104,104	0
36	CA	c	522	1/1	0.96	0.10	73,73,73,73	0
23	CLA	b	602	65/65	0.96	0.07	47,61,80,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	b	603	65/65	0.96	0.07	43,56,80,101	0
23	CLA	b	604	65/65	0.96	0.07	42,52,106,121	0
25	BCR	B	617	40/40	0.96	0.06	42,55,65,69	0
23	CLA	b	605	65/65	0.96	0.08	38,52,73,83	0
23	CLA	A	404[B]	65/65	0.96	0.07	37,45,63,71	65
23	CLA	A	405[A]	65/65	0.97	0.06	37,45,58,74	65
23	CLA	A	405[B]	65/65	0.97	0.06	37,45,58,75	65
23	CLA	c	502	65/65	0.97	0.07	46,60,92,112	0
23	CLA	B	608	65/65	0.97	0.05	40,50,69,83	0
23	CLA	C	511	65/65	0.97	0.06	48,59,81,89	0
22	CL	a	403[A]	1/1	0.97	0.07	54,54,54,54	1
23	CLA	C	503	65/65	0.97	0.06	43,55,84,91	0
22	CL	a	403[B]	1/1	0.97	0.07	54,54,54,54	1
23	CLA	D	402[A]	65/65	0.97	0.07	36,45,69,80	65
23	CLA	b	608	65/65	0.97	0.06	41,57,79,95	0
23	CLA	c	510	65/65	0.97	0.06	51,62,80,95	0
23	CLA	D	402[B]	65/65	0.97	0.07	36,45,69,80	65
23	CLA	b	610	65/65	0.97	0.07	46,57,68,71	0
23	CLA	B	604	65/65	0.97	0.06	37,49,118,134	0
23	CLA	d	402[A]	65/65	0.97	0.05	40,46,64,73	65
23	CLA	d	402[B]	65/65	0.97	0.05	40,46,64,73	65
23	CLA	d	403[A]	65/65	0.97	0.06	38,48,76,95	65
23	CLA	d	403[B]	65/65	0.97	0.06	37,48,76,95	65
23	CLA	a	404[A]	65/65	0.97	0.07	41,46,64,77	65
24	PHO	A	407[A]	64/64	0.97	0.05	38,47,53,59	64
24	PHO	A	407[B]	64/64	0.97	0.05	38,47,53,60	64
23	CLA	a	404[B]	65/65	0.97	0.07	41,46,65,78	65
23	CLA	B	612	65/65	0.97	0.06	38,50,63,72	0
23	CLA	B	605	65/65	0.97	0.06	39,49,69,86	0
22	CL	A	402[B]	1/1	0.98	0.05	44,44,44,44	1
22	CL	A	403[A]	1/1	0.98	0.04	49,49,49,49	1
22	CL	A	403[B]	1/1	0.98	0.04	49,49,49,49	1
21	FE2	a	401[A]	1/1	0.98	0.04	55,55,55,55	1
21	FE2	a	401[B]	1/1	0.98	0.04	55,55,55,55	1
22	CL	A	402[A]	1/1	0.98	0.05	44,44,44,44	1
38	HEM	E	102	43/43	0.98	0.07	53,69,82,94	0
38	HEM	f	101	43/43	0.98	0.08	61,80,114,135	0
40	HEC	V	201	43/43	0.98	0.06	40,51,58,62	0
40	HEC	v	201	43/43	0.98	0.07	50,62,67,75	0
28	OEX	A	413[A]	10/10	0.99	0.03	42,44,48,50	10
28	OEX	A	413[B]	10/10	0.99	0.03	42,45,49,50	10
28	OEX	a	411[A]	10/10	0.99	0.03	48,51,52,56	10

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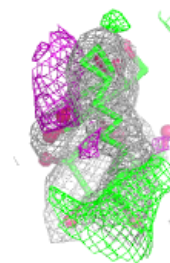
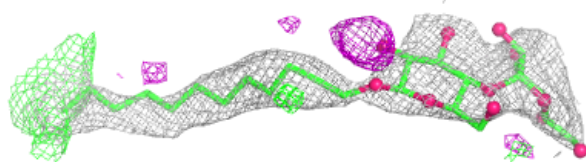
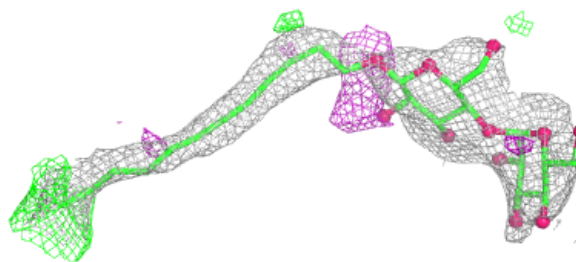
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	CA	c	523	1/1	0.99	0.03	77,77,77,77	0
28	OEX	a	411[B]	10/10	0.99	0.03	48,50,52,54	10
39	MG	J	102	1/1	0.99	0.03	57,57,57,57	0
39	MG	j	102	1/1	0.99	0.06	62,62,62,62	0
21	FE2	A	401[A]	1/1	0.99	0.02	51,51,51,51	1
21	FE2	A	401[B]	1/1	0.99	0.02	51,51,51,51	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.

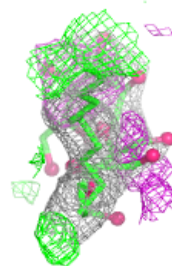
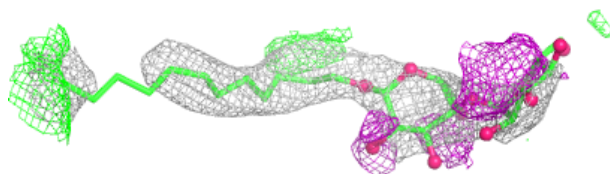
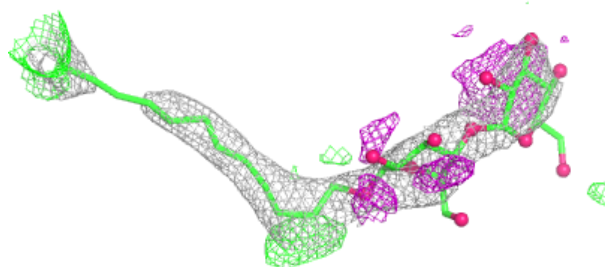
Electron density around LMT A 417:

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

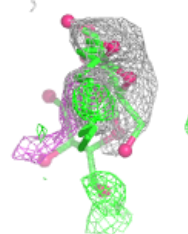
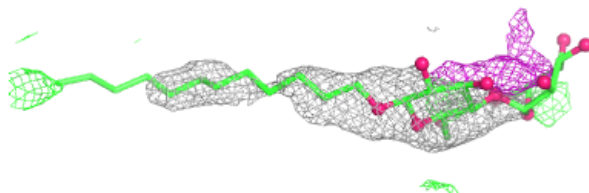
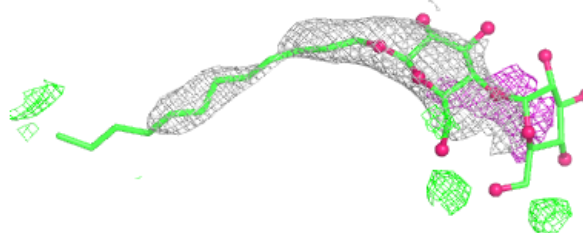


Electron density around LMT B 630:

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

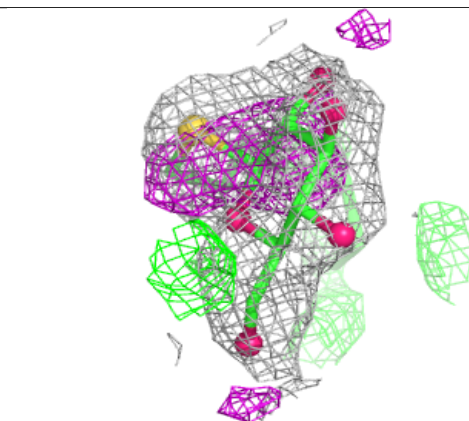
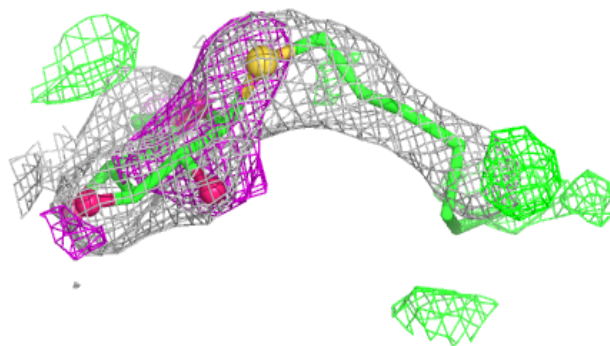
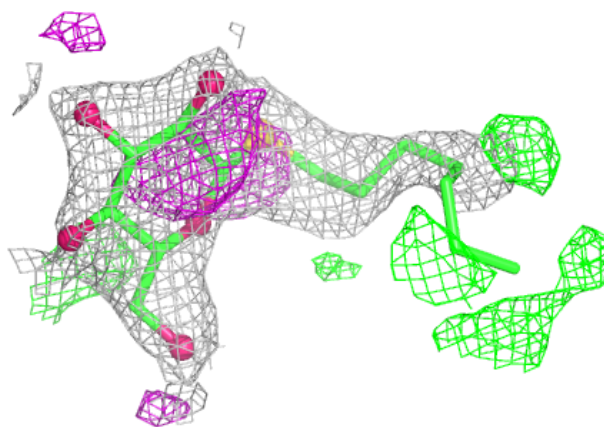
**Electron density around LMT F 101:**

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

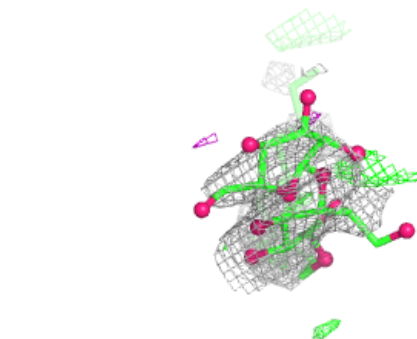
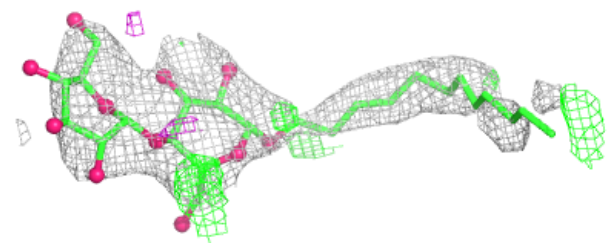
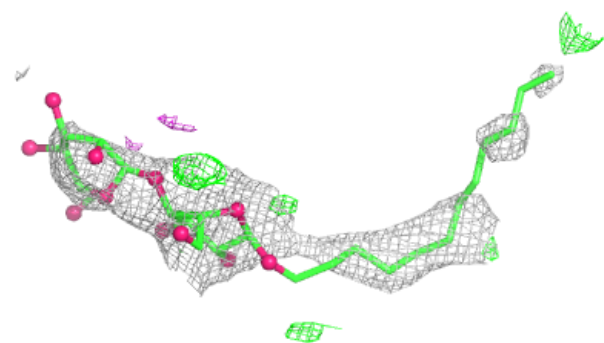


Electron density around HTG B 623:

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

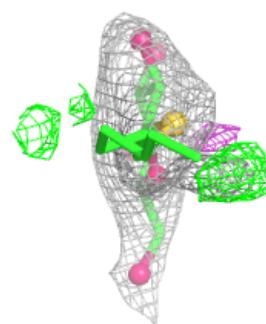
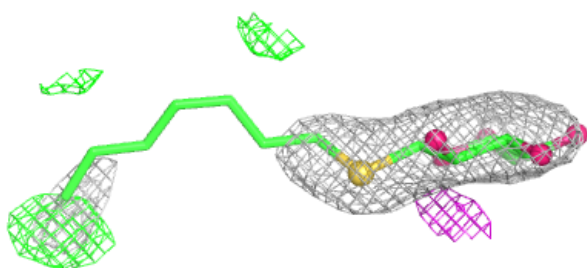
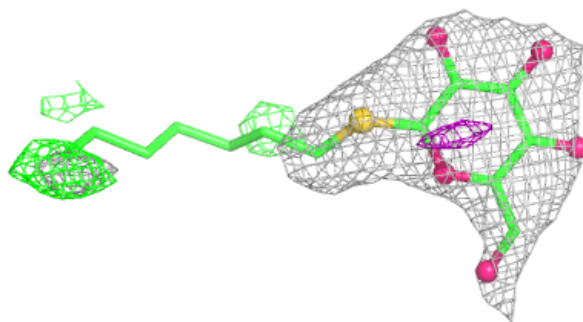
**Electron density around LMT A 420:**

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

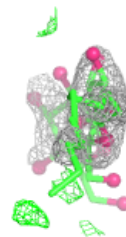
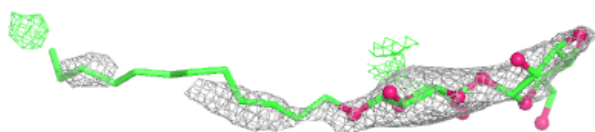
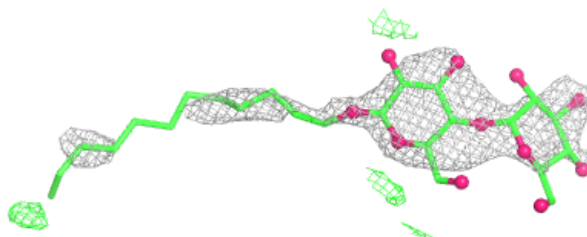


Electron density around HTG C 522:

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

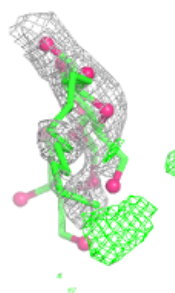
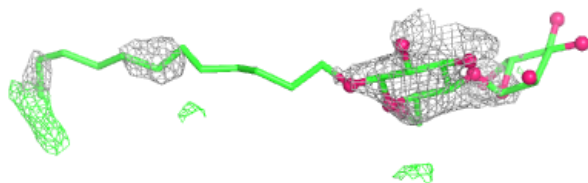
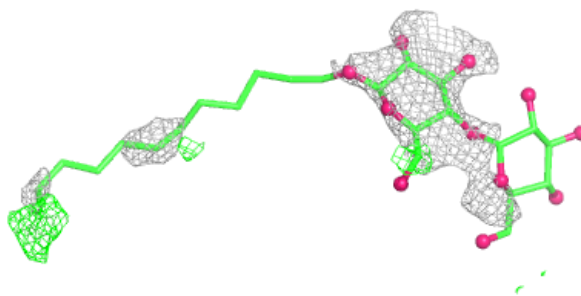
**Electron density around LMT a 416:**

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

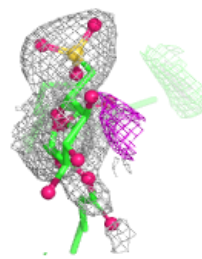
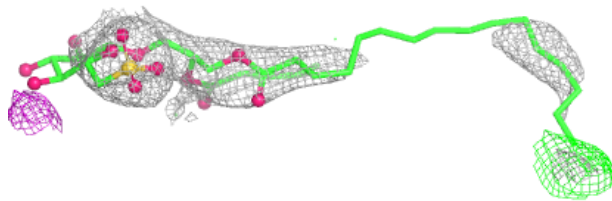
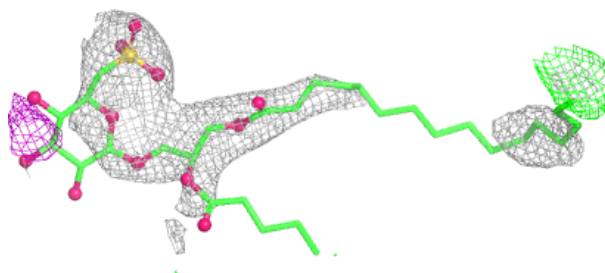


Electron density around LMT e 101:

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

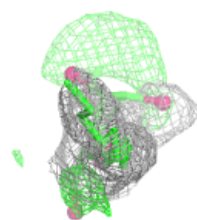
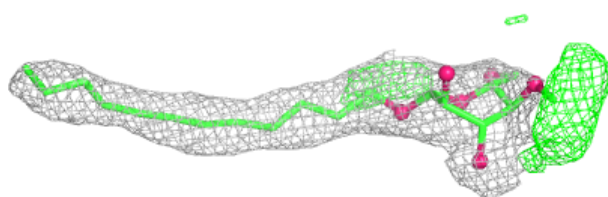
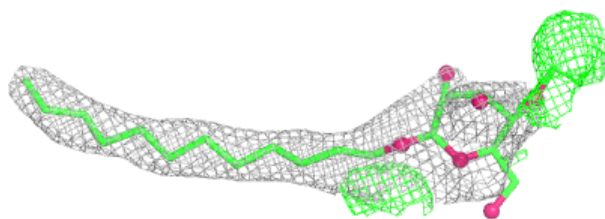
**Electron density around SQD f 102:**

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

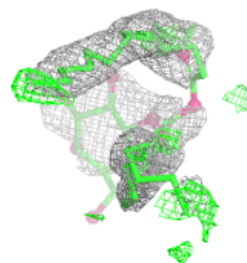
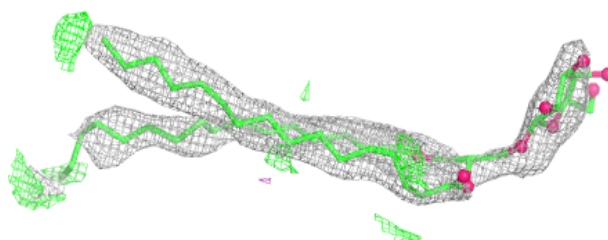
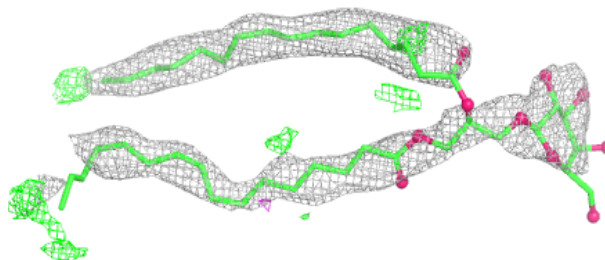


Electron density around LMT b 621:

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

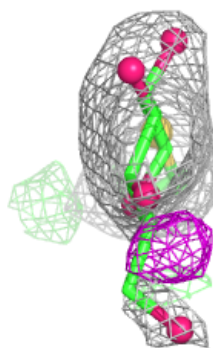
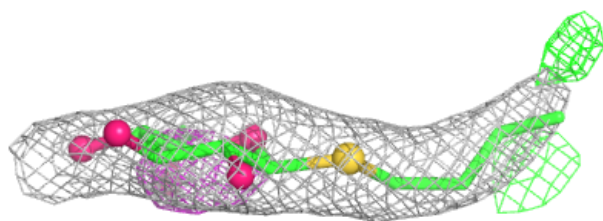
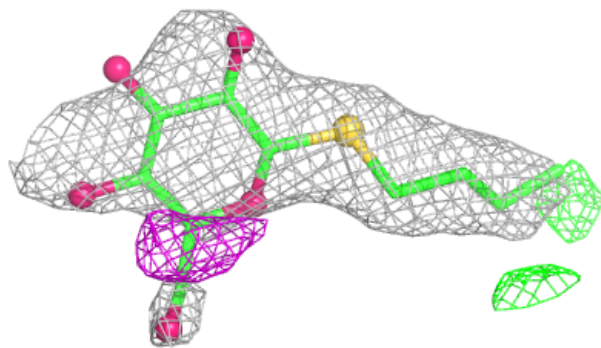
**Electron density around LMG C 521:**

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



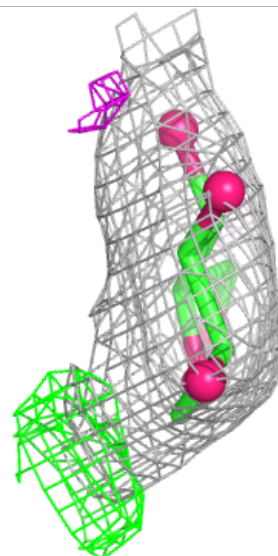
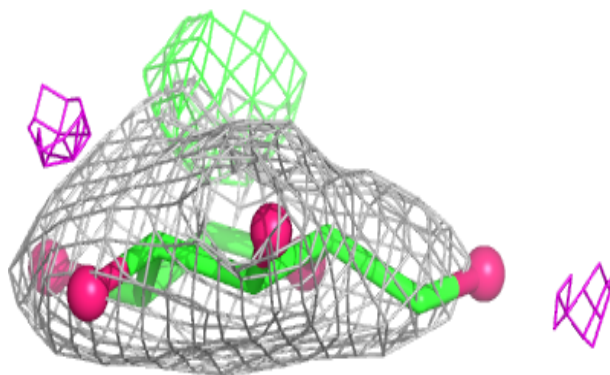
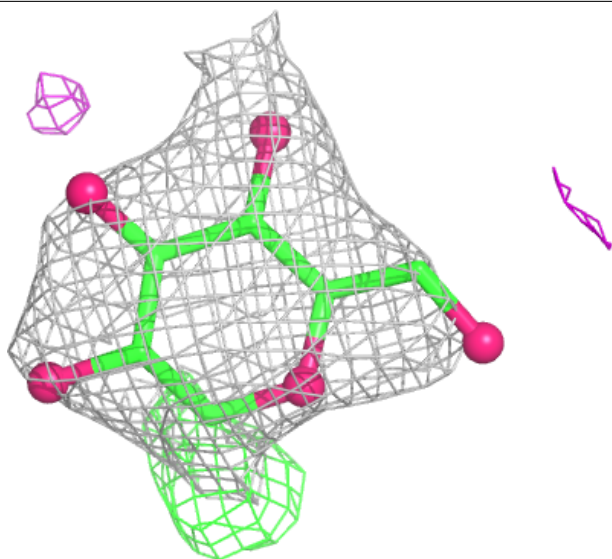
Electron density around HTG D 410:

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



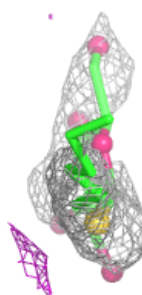
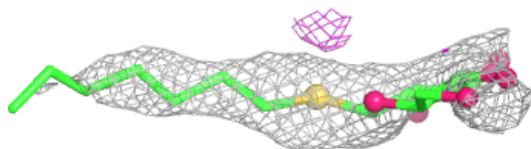
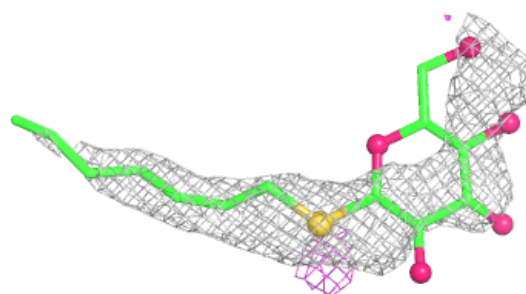
Electron density around HTG V 202:

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

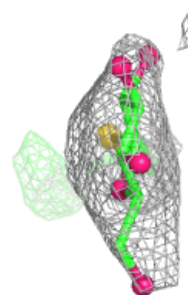
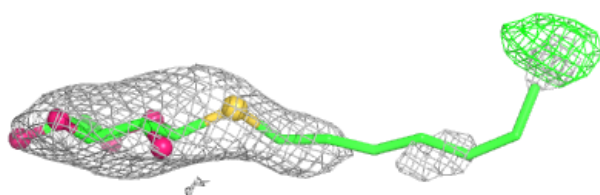
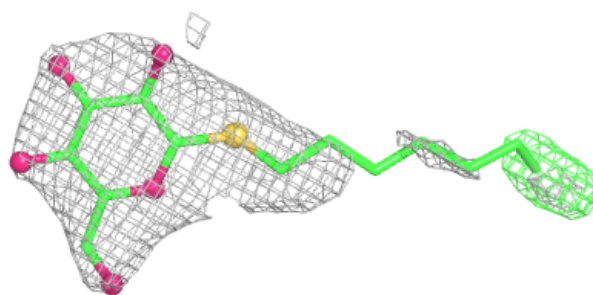


Electron density around HTG b 623:

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

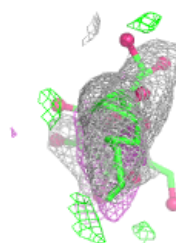
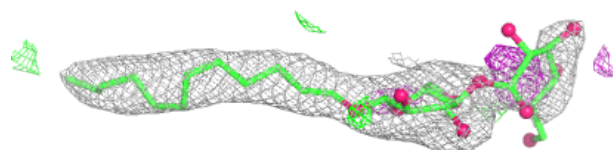
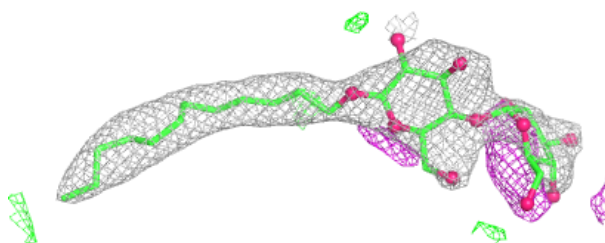
**Electron density around HTG c 521:**

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

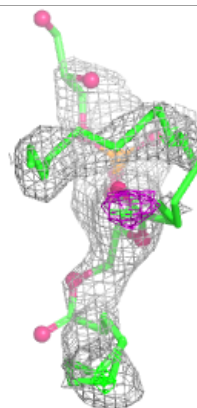
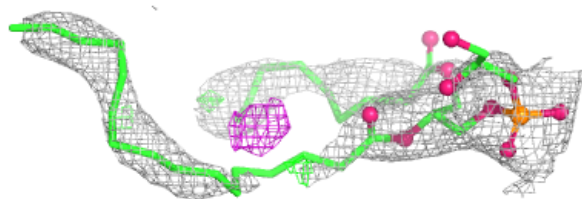
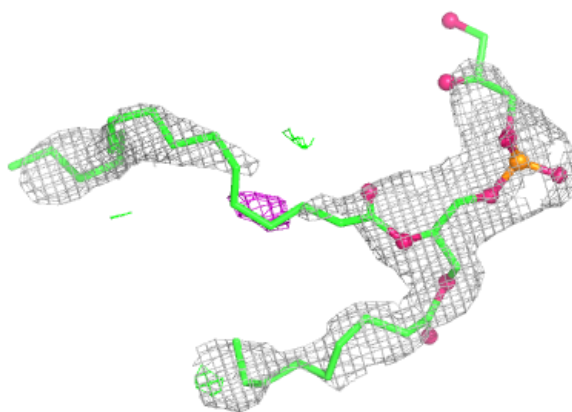


Electron density around LMT B 628:

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

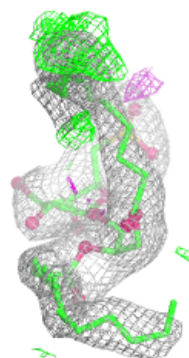
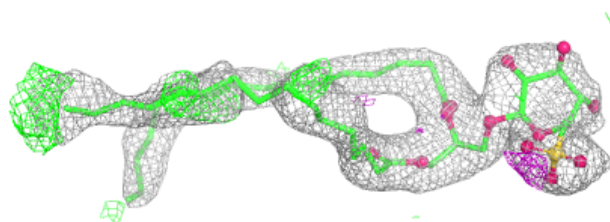
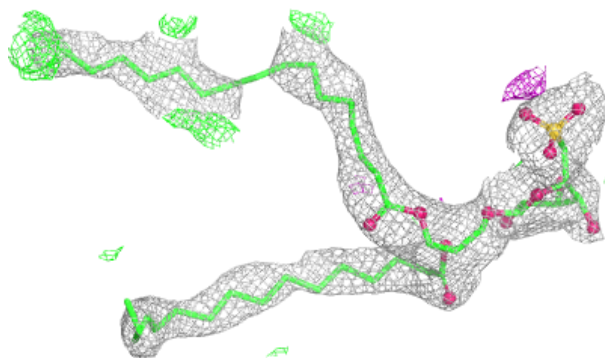
**Electron density around LHG a 419 (B):**

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

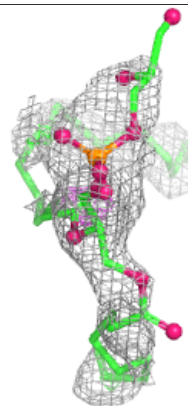
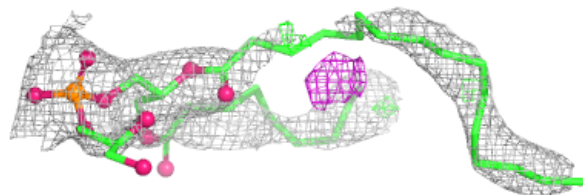
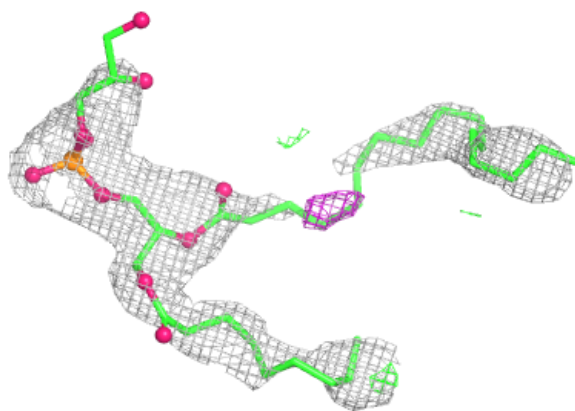


Electron density around SQD a 410:

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

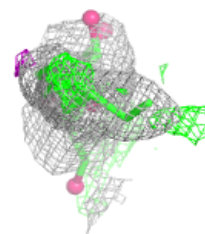
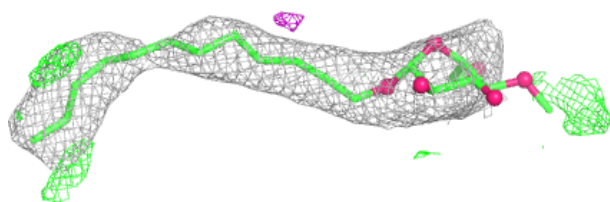
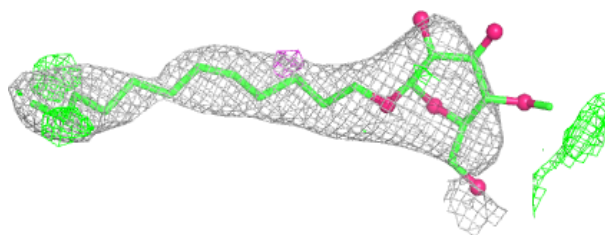
**Electron density around LHG a 419 (A):**

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

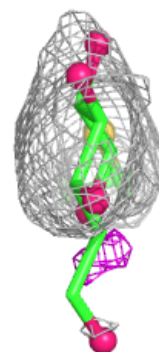
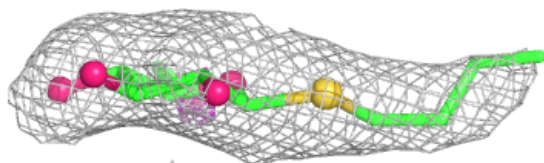
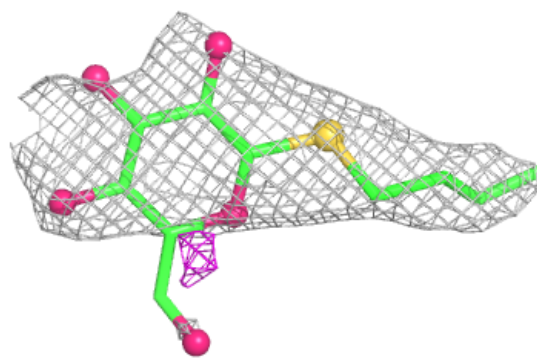


Electron density around LMT B 631:

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

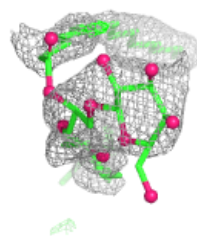
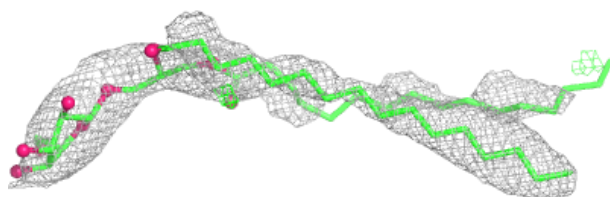
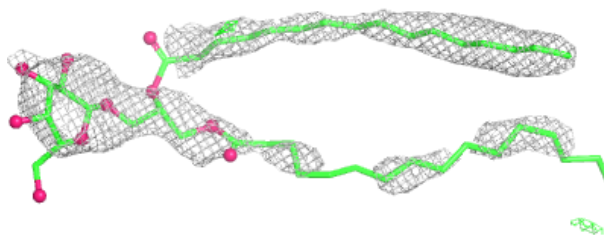
**Electron density around HTG d 411:**

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

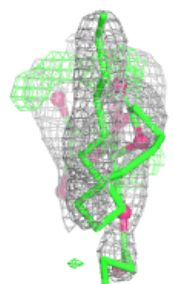
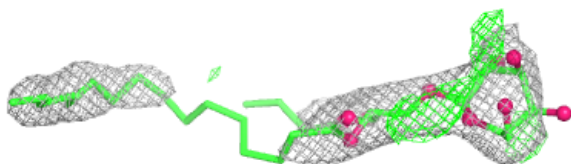
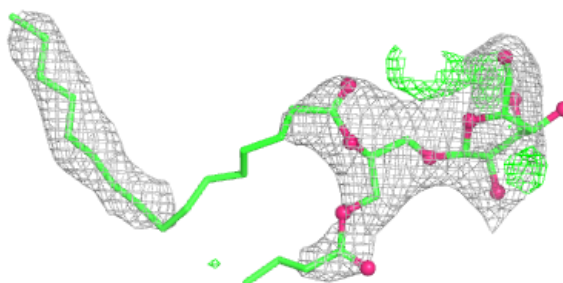


Electron density around LMG c 520:

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

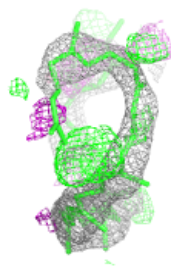
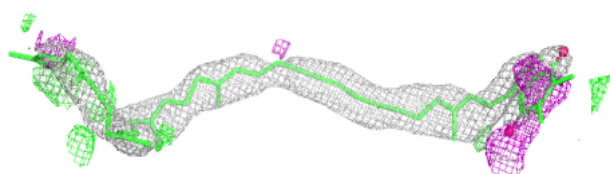
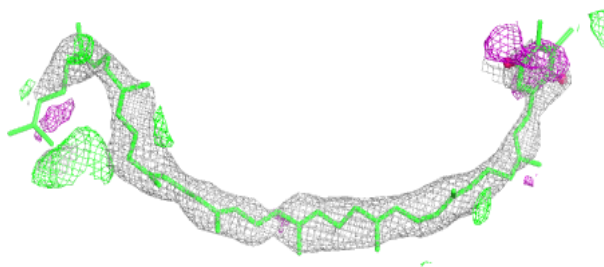
**Electron density around LMG z 101:**

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

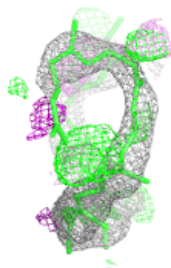
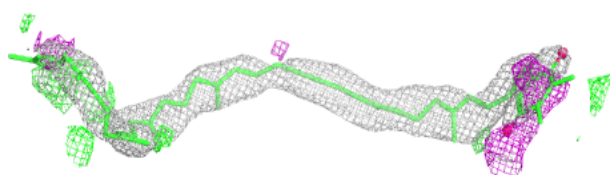
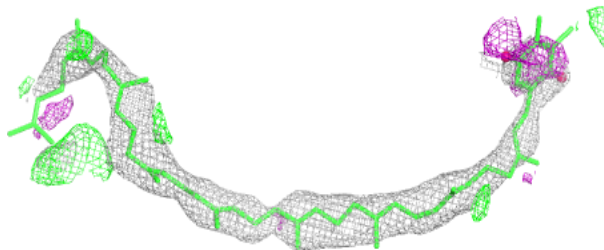


Electron density around PL9 A 414 (A):

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

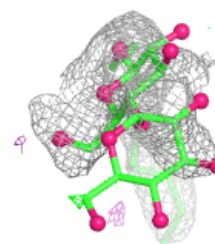
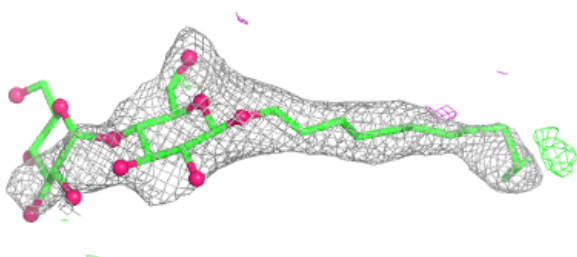
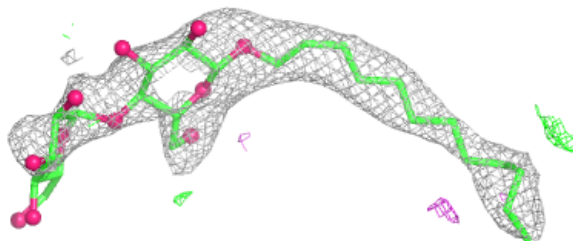
**Electron density around PL9 A 414 (B):**

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

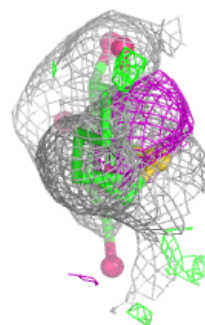
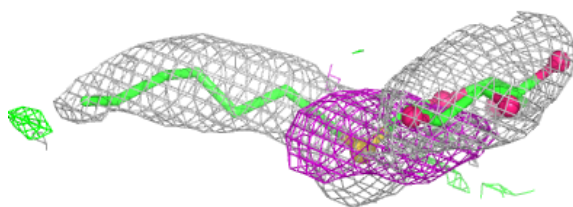
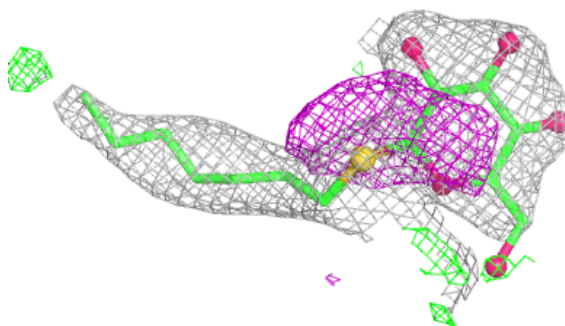


Electron density around LMT T 101:

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

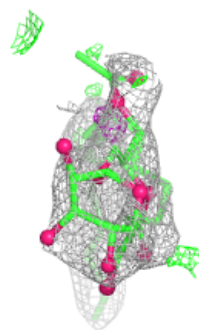
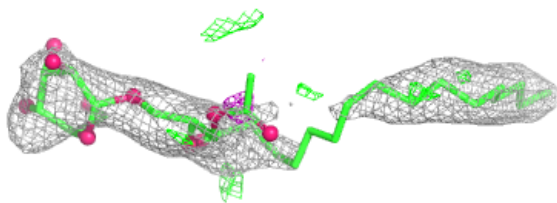
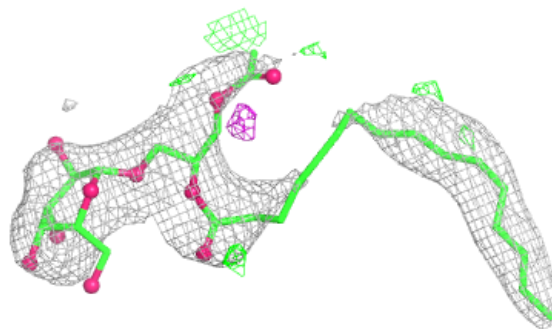
**Electron density around HTG b 622:**

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

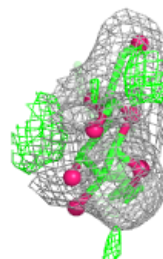
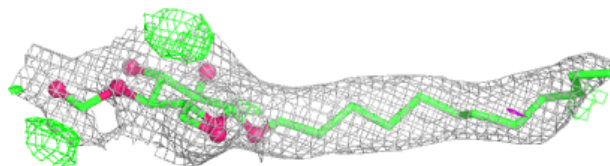
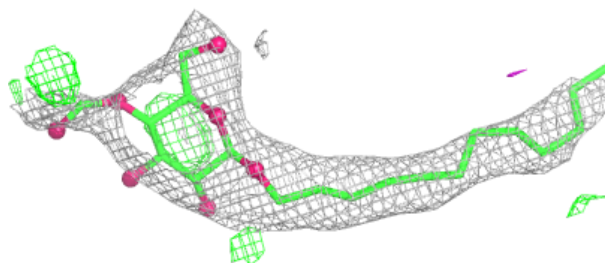


Electron density around LMG Z 101:

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

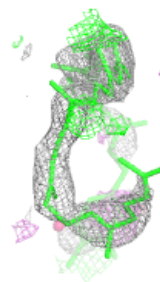
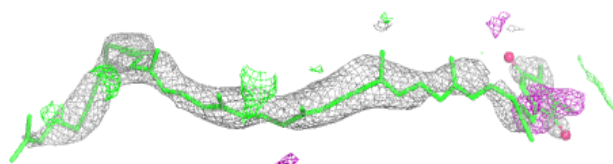
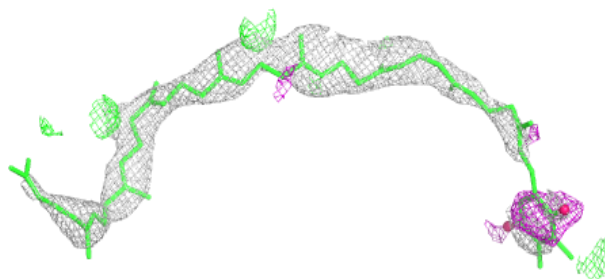
**Electron density around LMT t 101:**

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

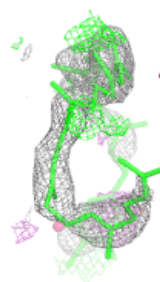
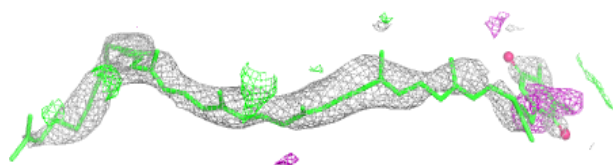
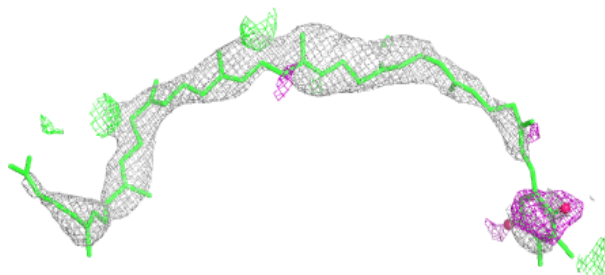


Electron density around PL9 a 412 (A):

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

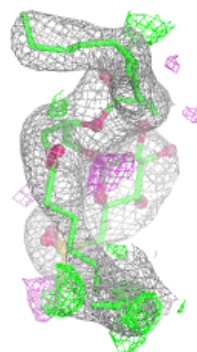
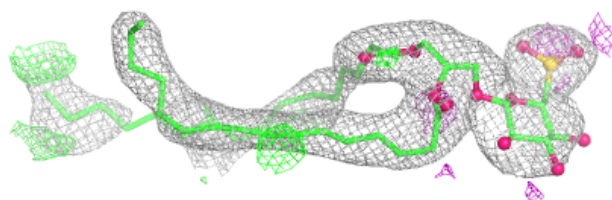
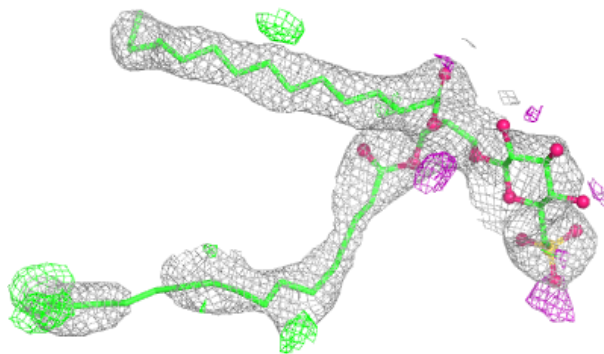
**Electron density around PL9 a 412 (B):**

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

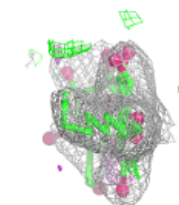
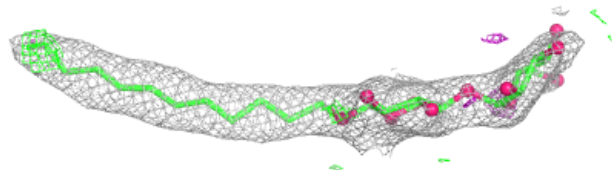
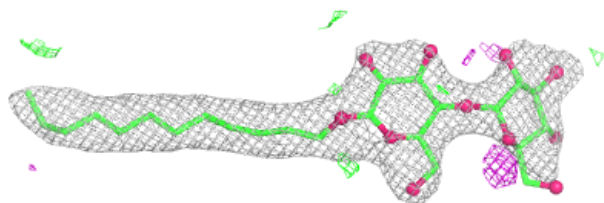


Electron density around SQD A 412:

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

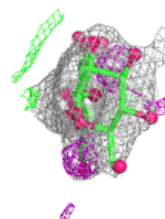
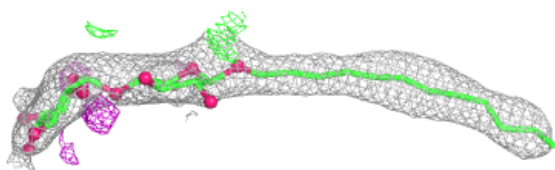
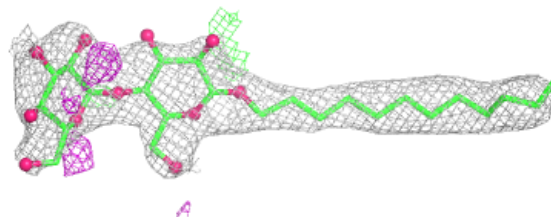
**Electron density around LMT M 101:**

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

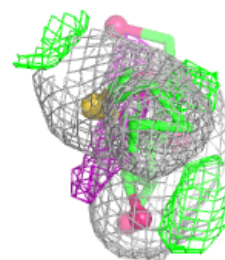
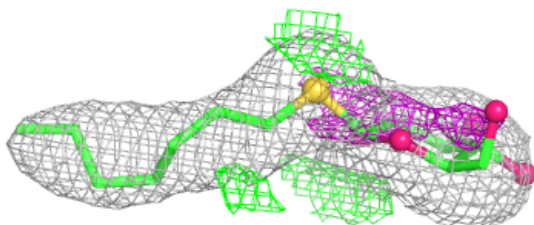
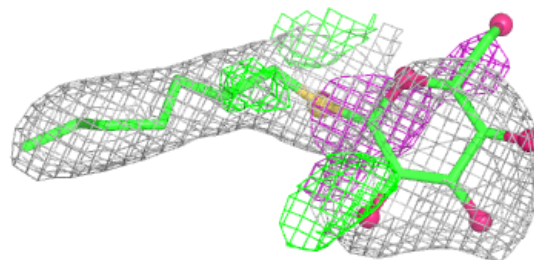


Electron density around LMT m 103:

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

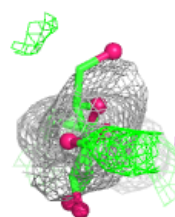
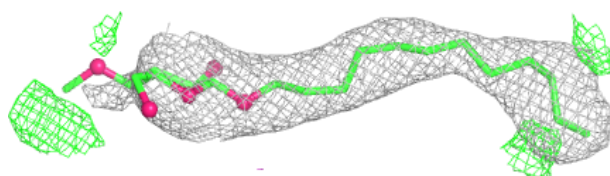
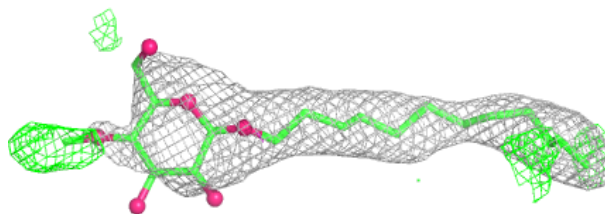
**Electron density around HTG B 622:**

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

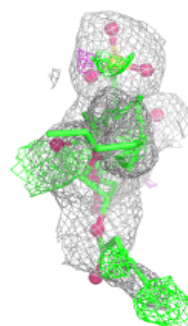
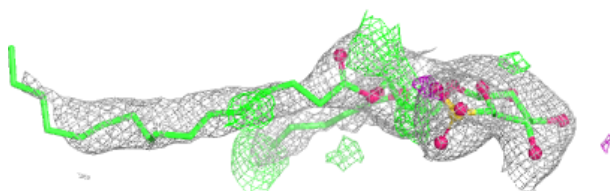
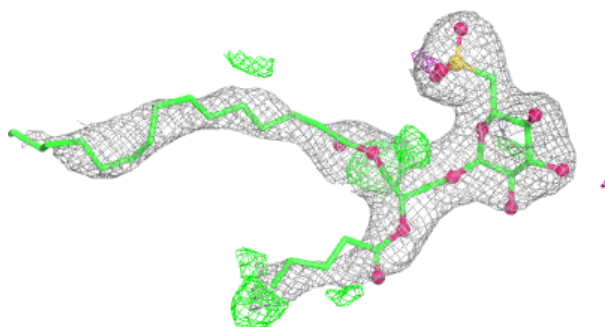


Electron density around LMT b 627:

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

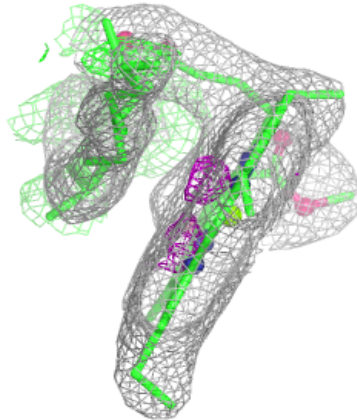
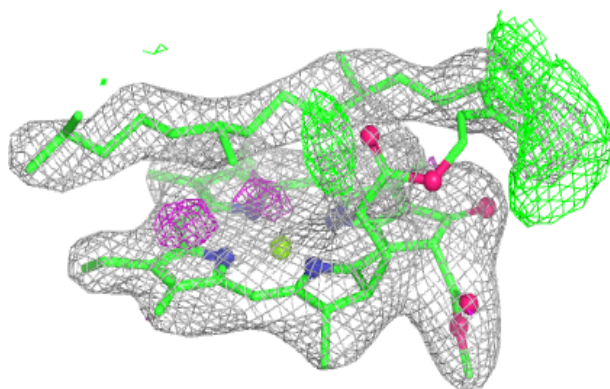
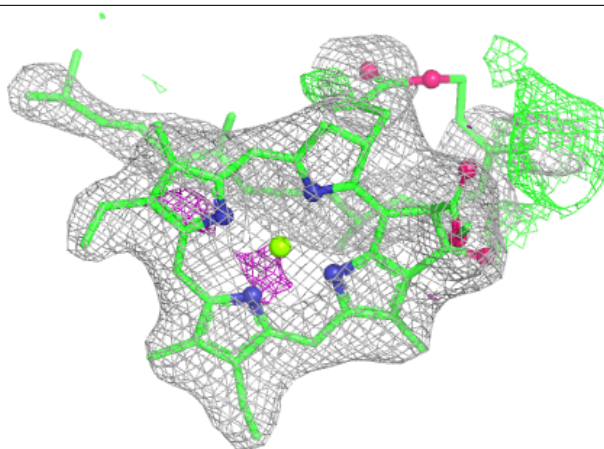
**Electron density around SQD F 102:**

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

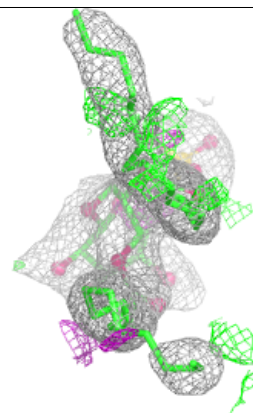
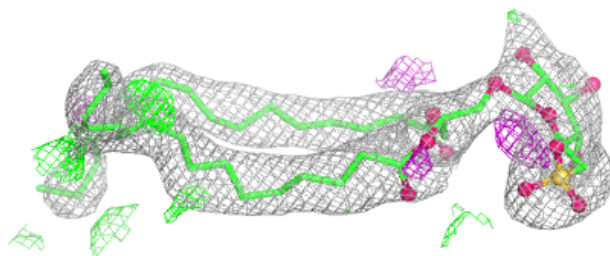
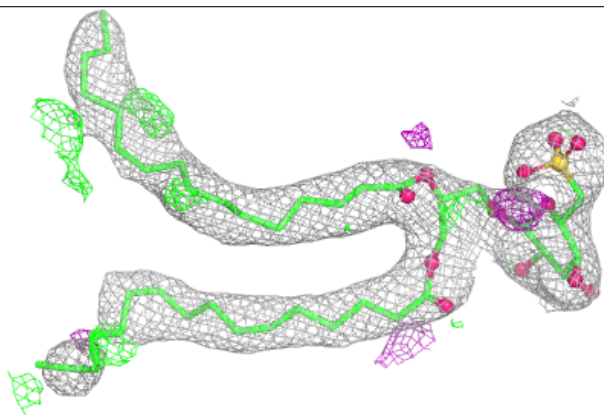


Electron density around CLA b 601:

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

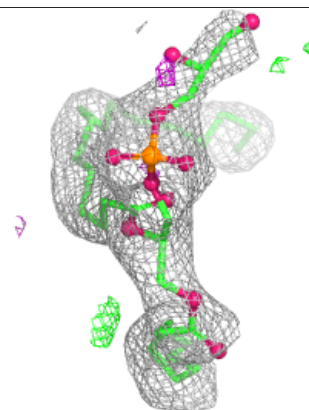
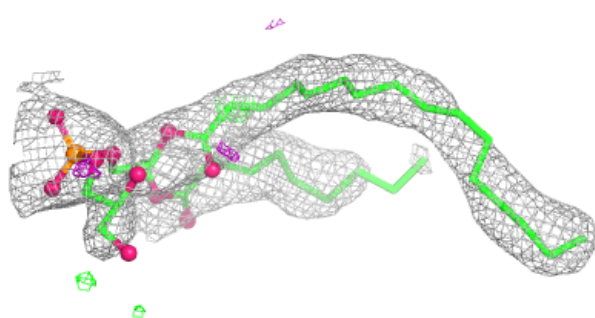
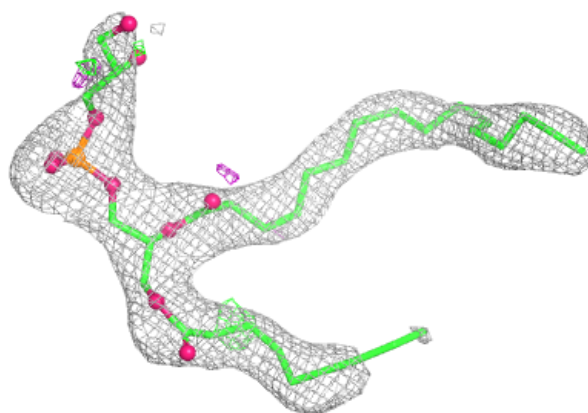
**Electron density around SQD b 620:**

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

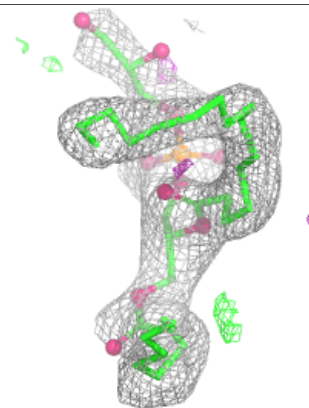
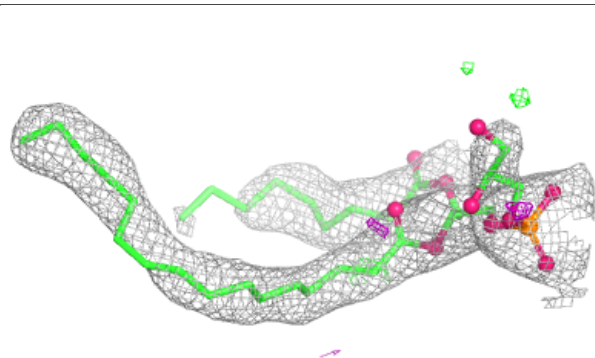
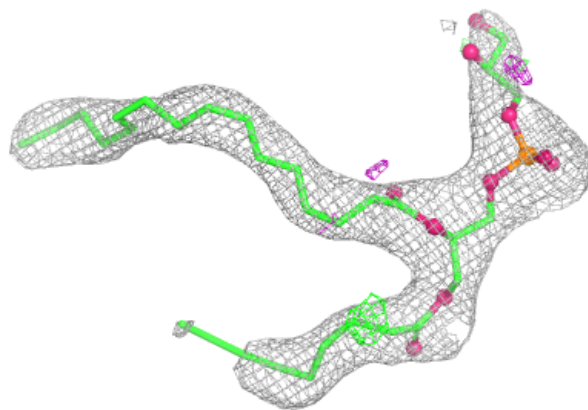


Electron density around LHG E 101 (A):

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

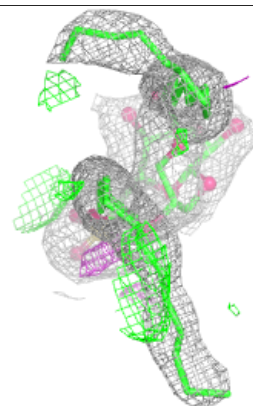
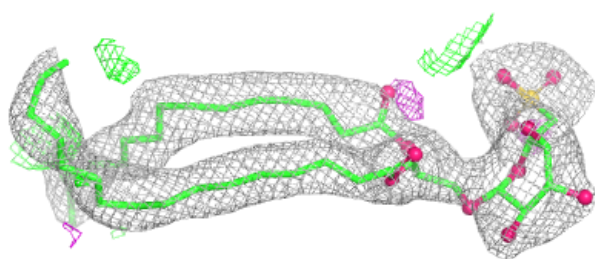
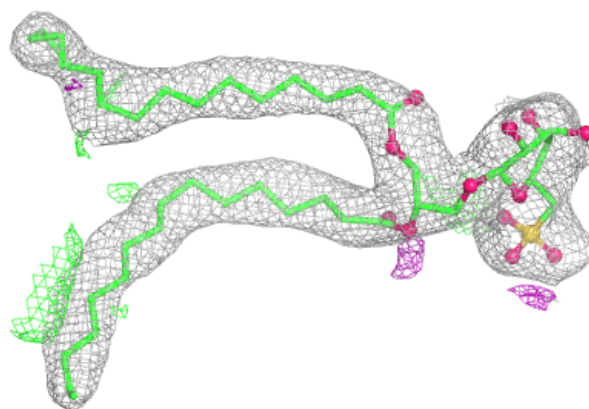
**Electron density around LHG E 101 (B):**

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

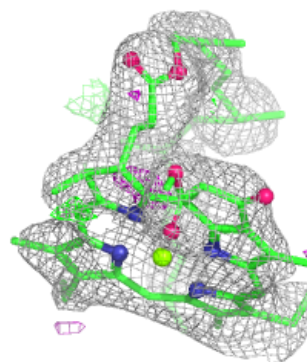
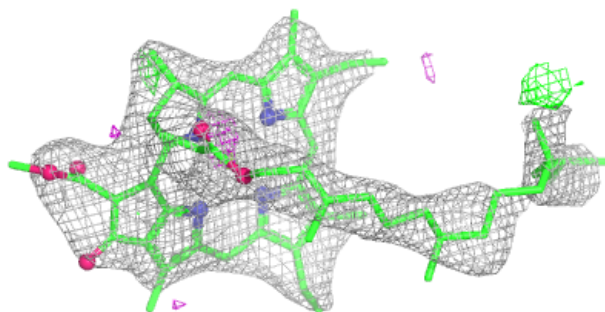
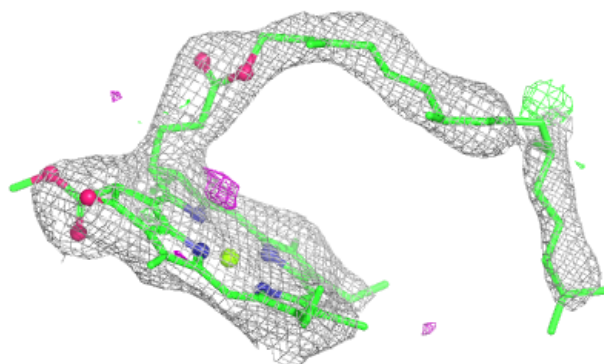


Electron density around SQD B 620:

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

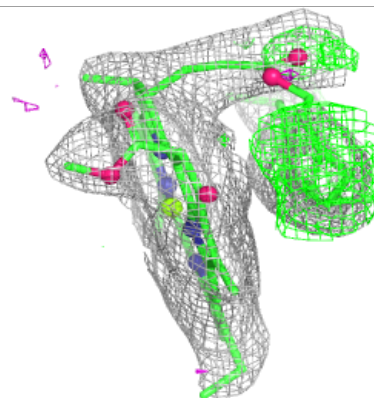
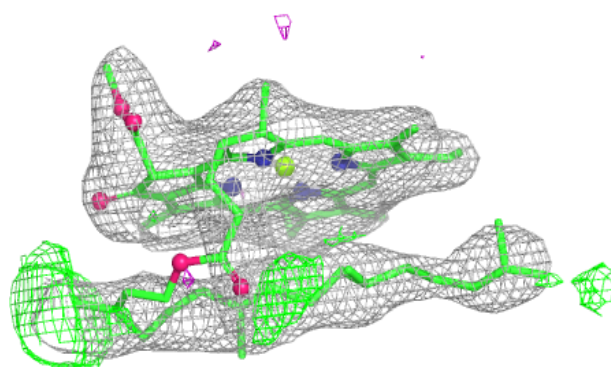
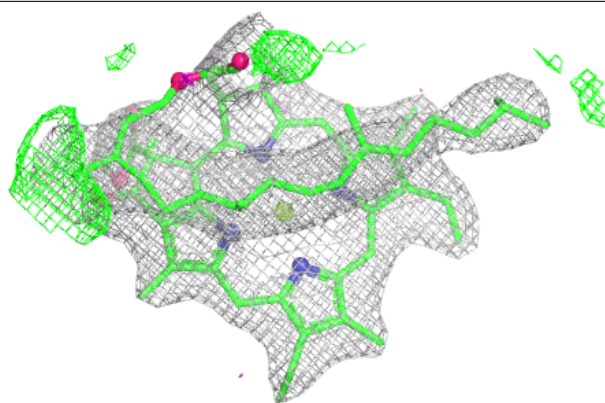
**Electron density around CLA c 513:**

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

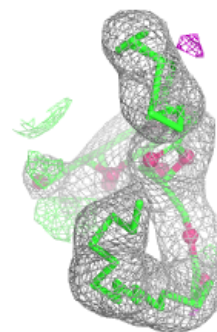
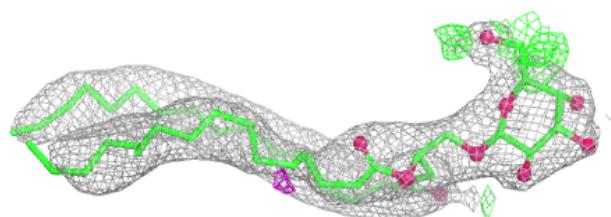
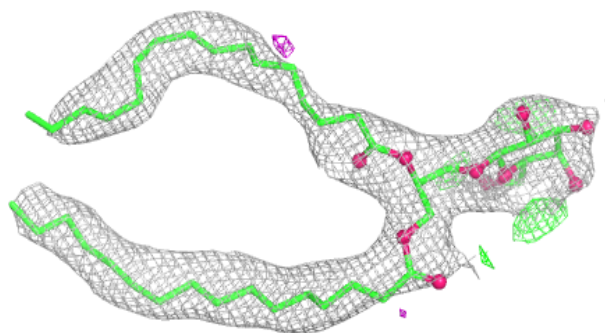


Electron density around CLA B 601:

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

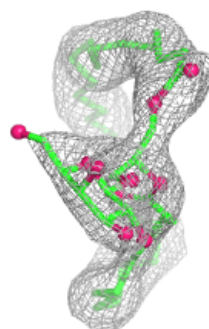
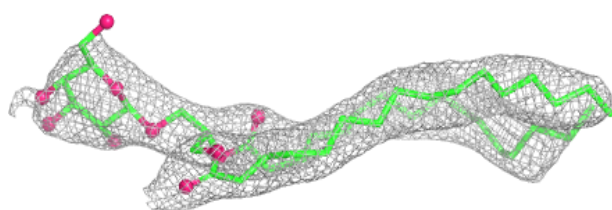
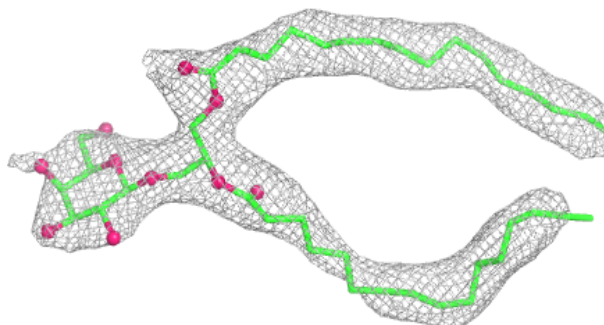
**Electron density around LMG C 501:**

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

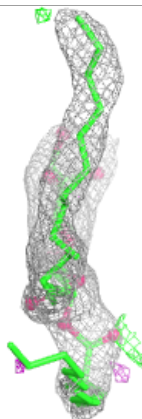
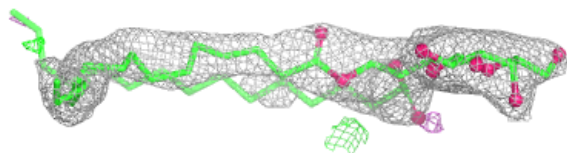
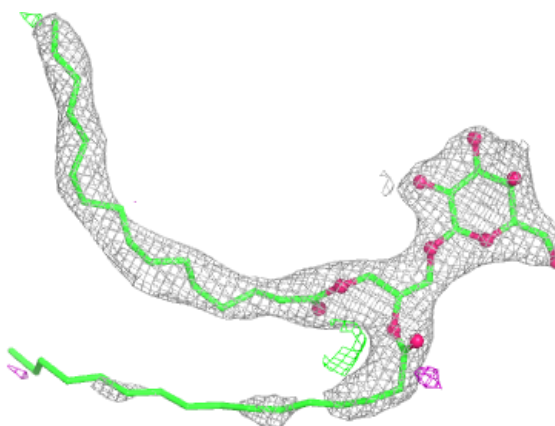


Electron density around LMG a 415:

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

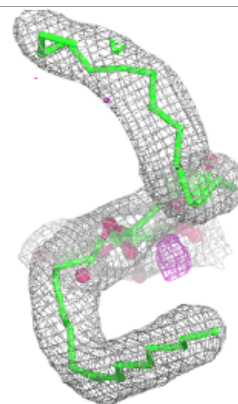
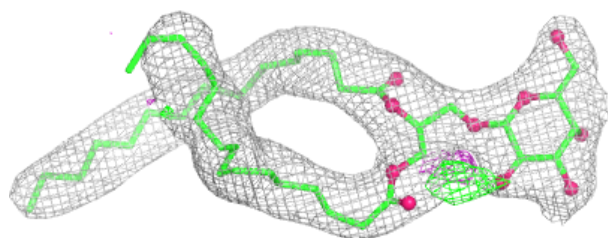
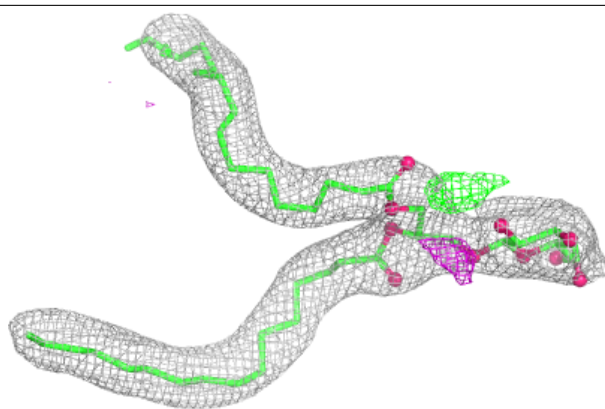
**Electron density around LMG c 519:**

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

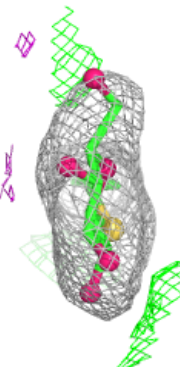
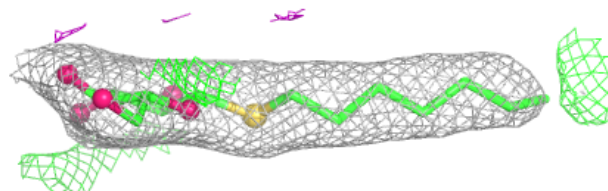
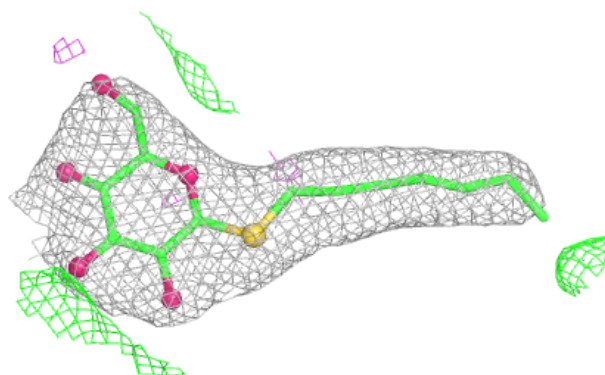


Electron density around LMG m 101:

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

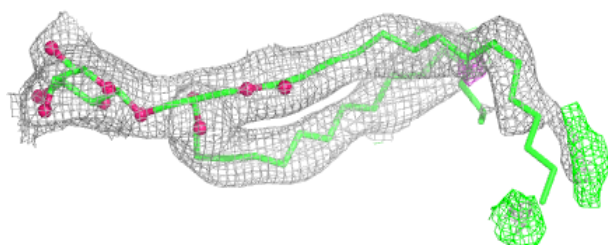
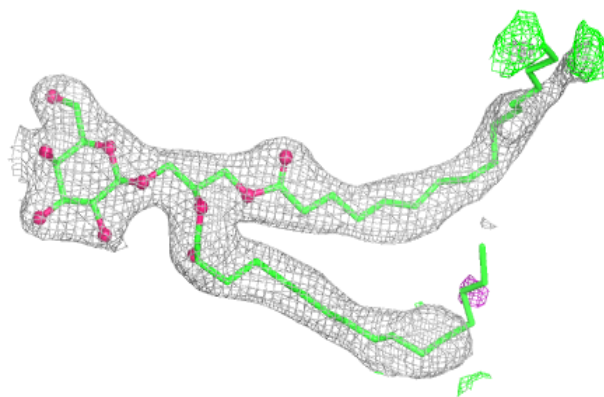
**Electron density around HTG B 625:**

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



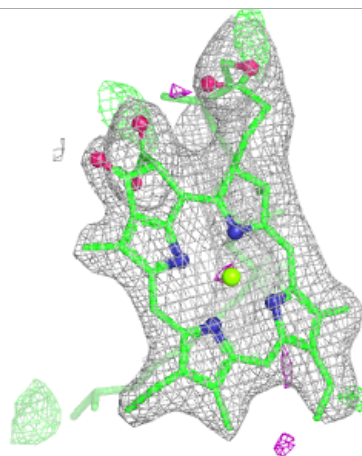
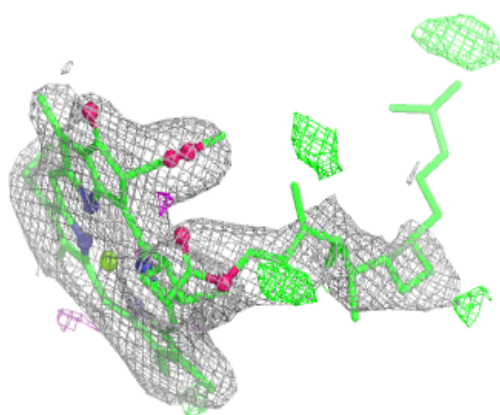
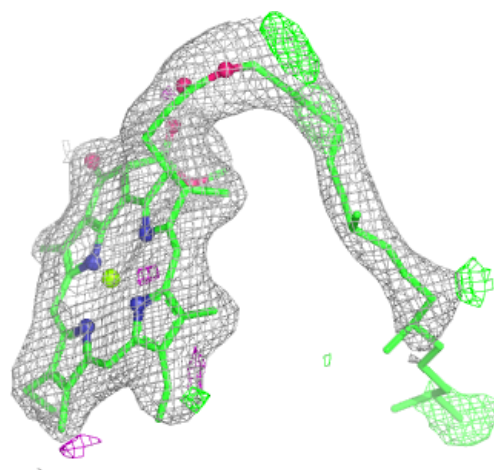
Electron density around LMG D 411:

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



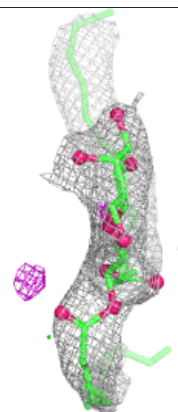
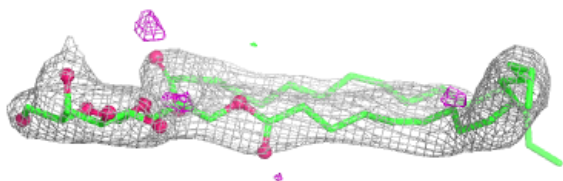
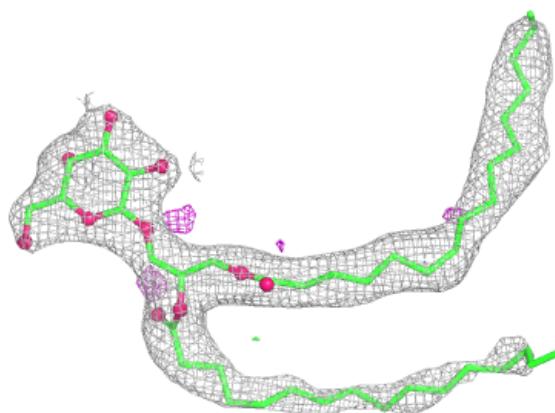
Electron density around CLA b 616:

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

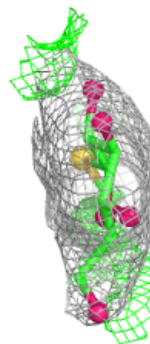
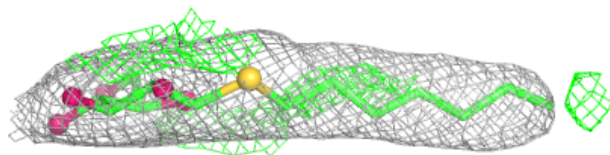
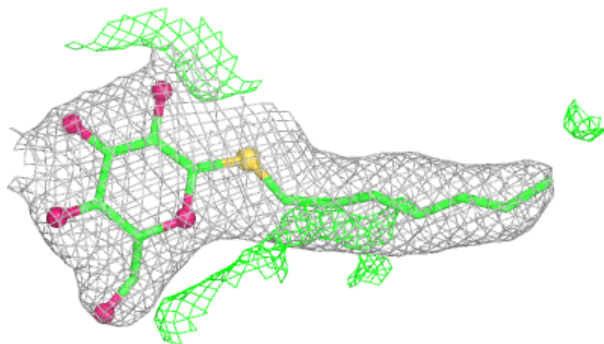


Electron density around LMG C 520:

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

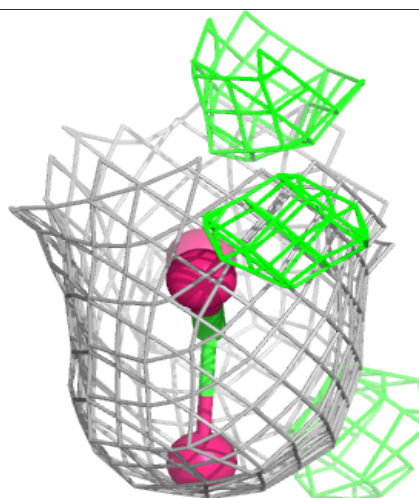
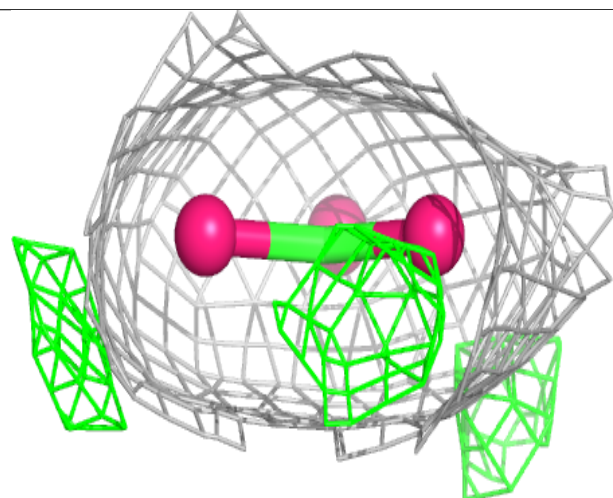
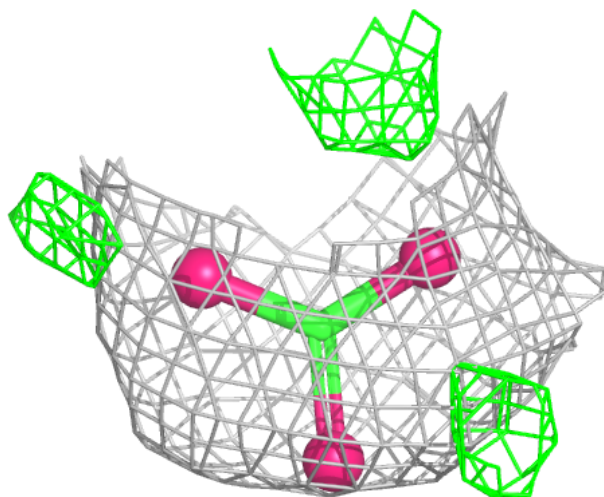
**Electron density around HTG b 625:**

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



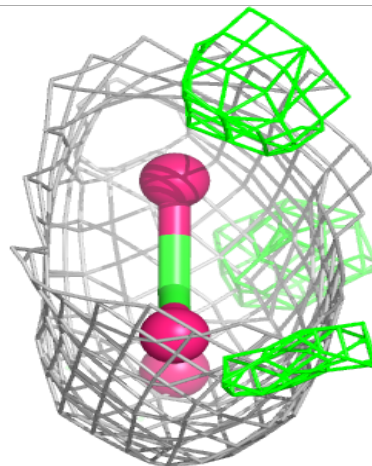
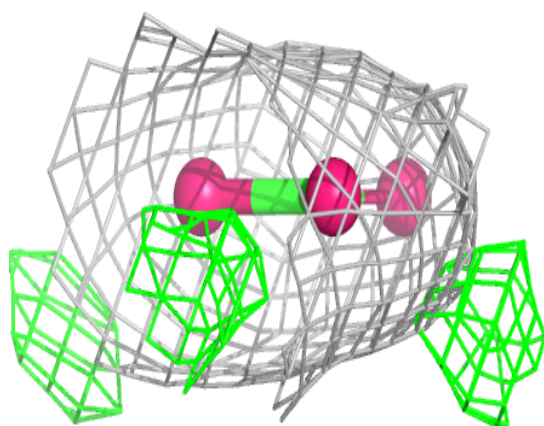
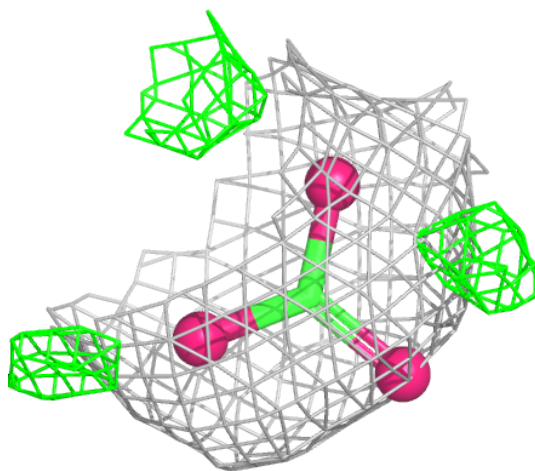
Electron density around BCT d 401 (A):

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



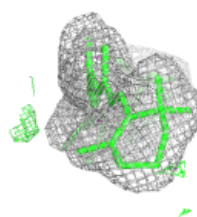
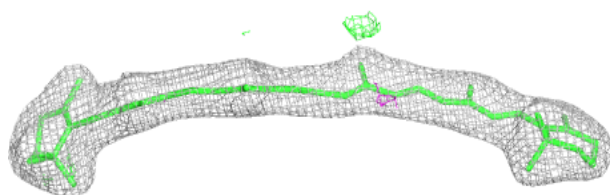
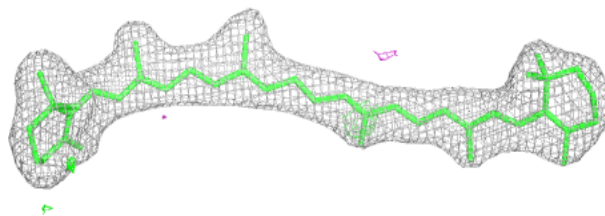
Electron density around BCT d 401 (B):

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

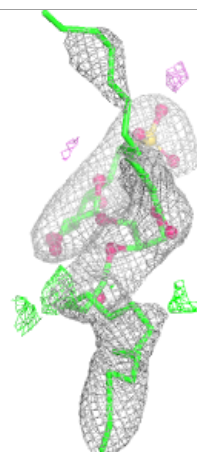
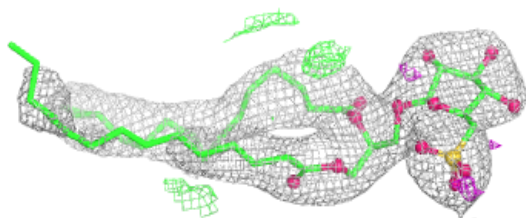
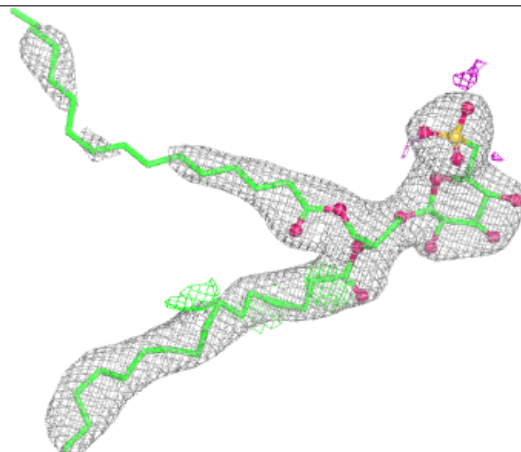


Electron density around BCR t 102:

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

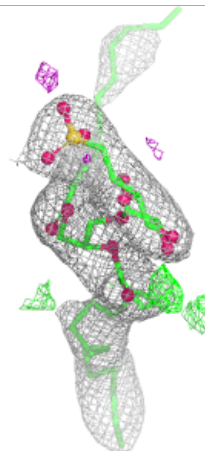
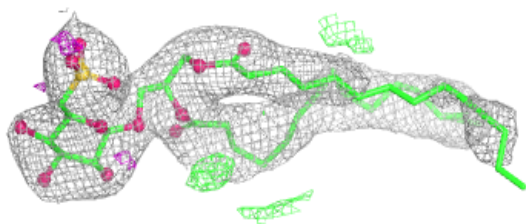
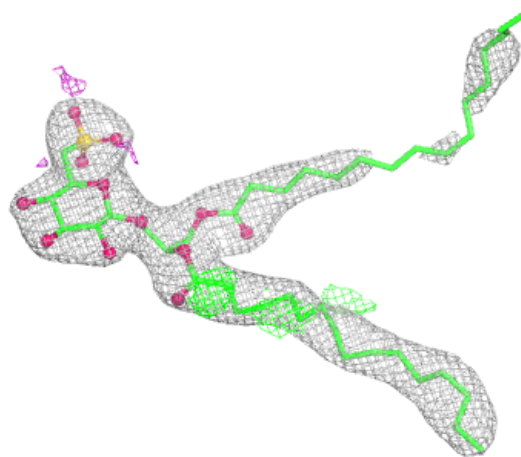
**Electron density around SQD A 410 (A):**

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



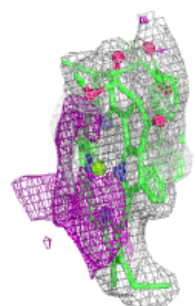
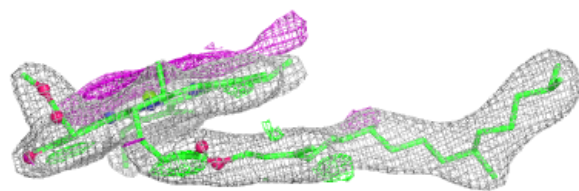
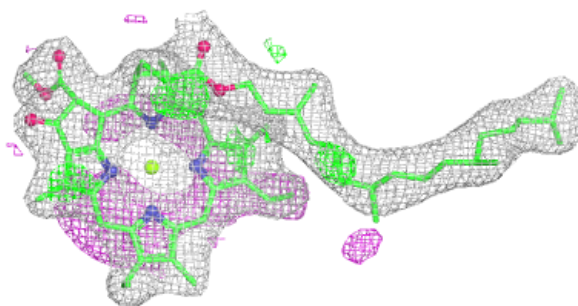
Electron density around SQD A 410 (B):

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

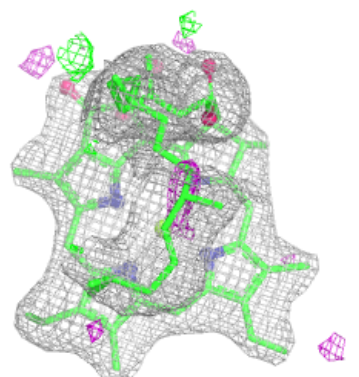
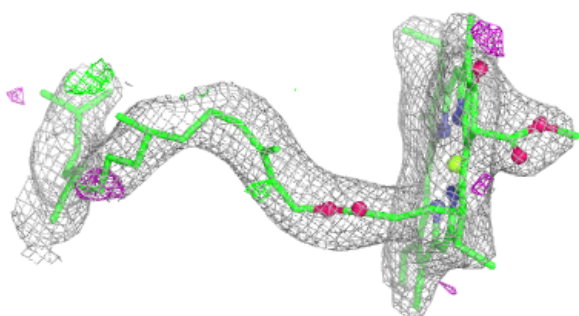
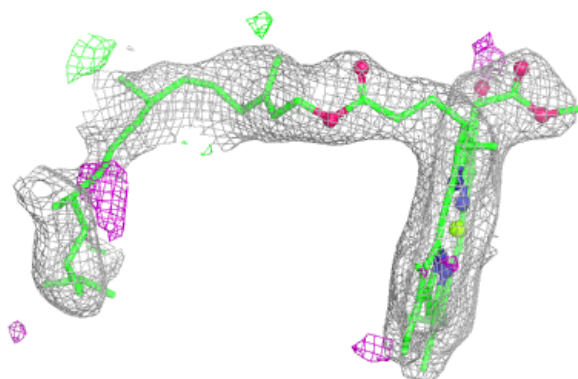


Electron density around CLA B 603:

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

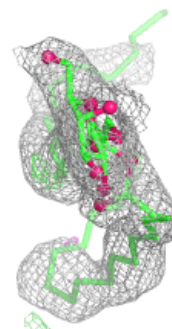
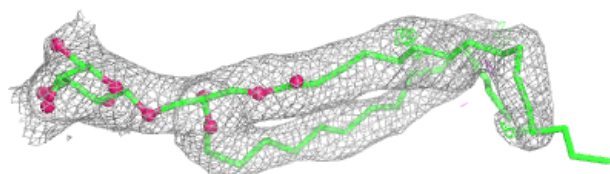
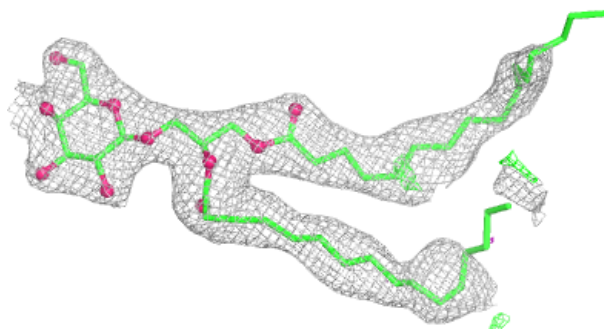
**Electron density around CLA C 507:**

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

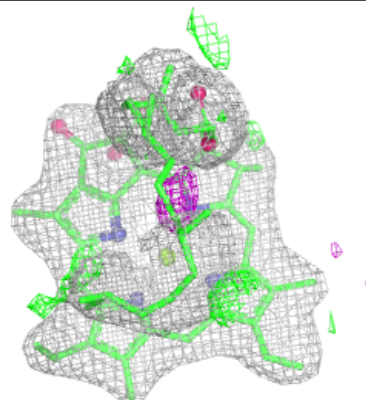
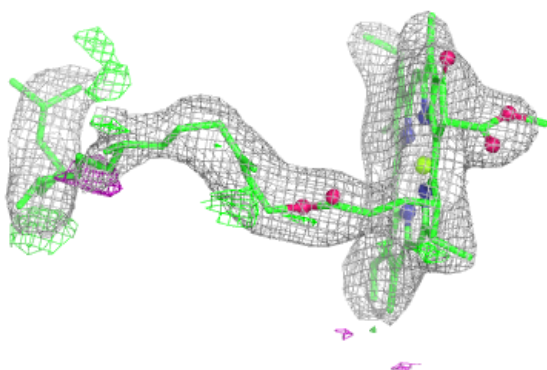
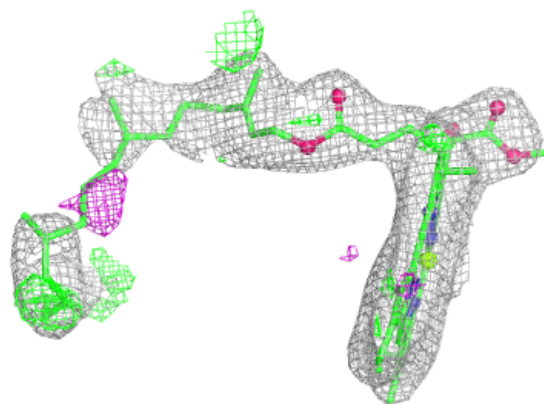


Electron density around LMG d 412:

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

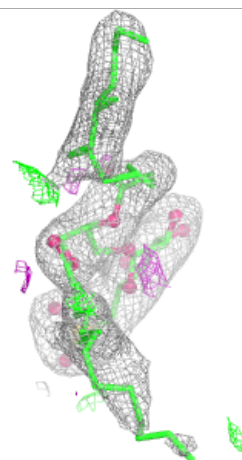
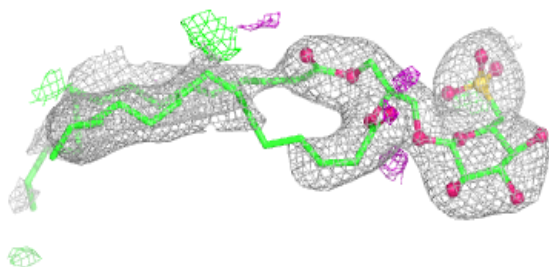
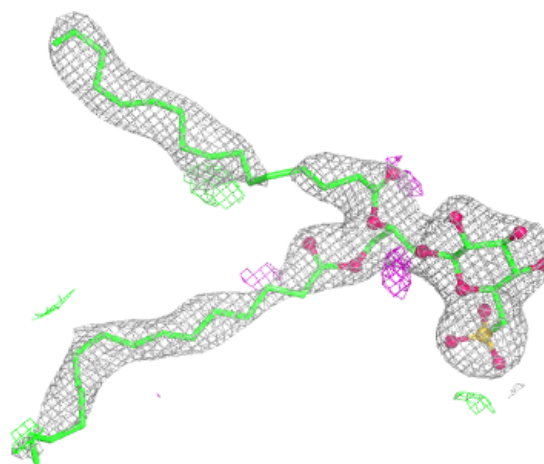
**Electron density around CLA c 506:**

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



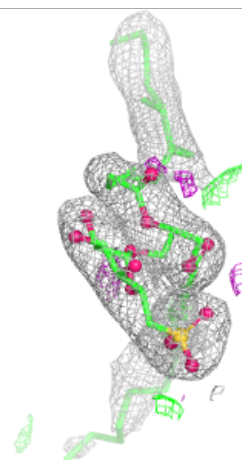
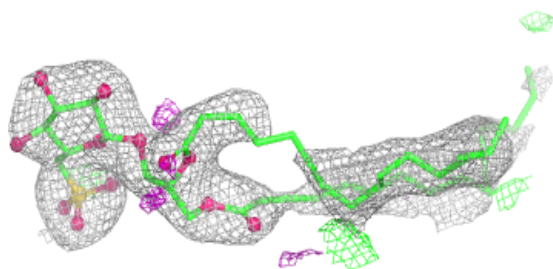
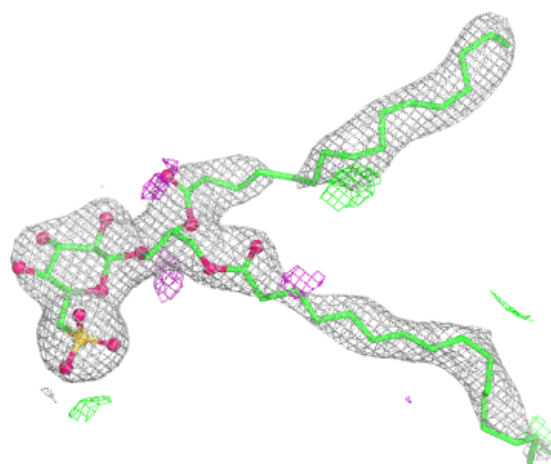
Electron density around SQD a 409 (A):

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



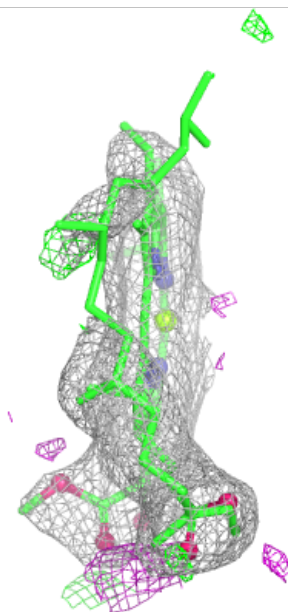
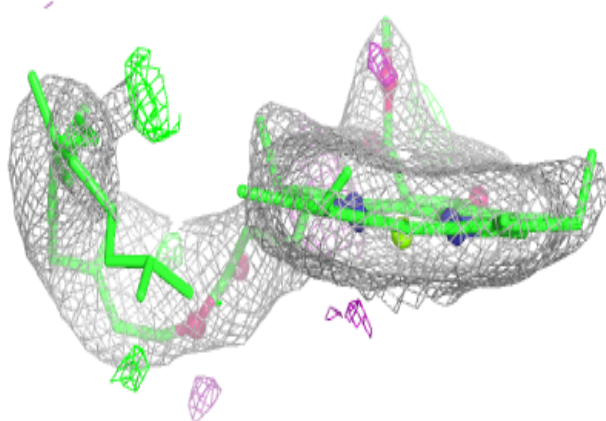
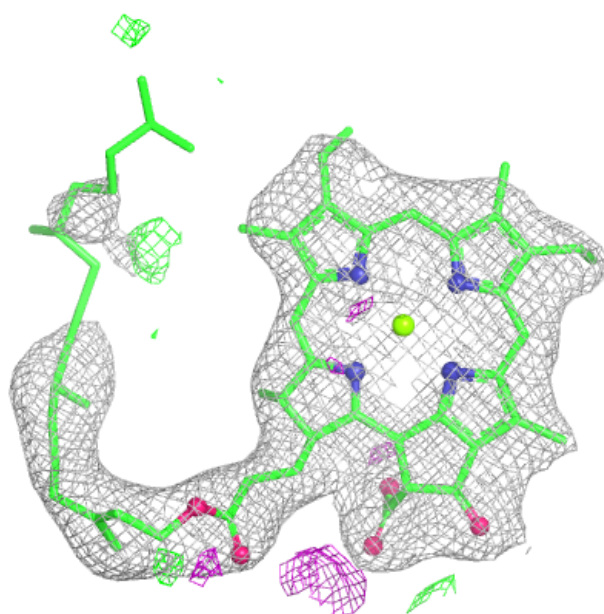
Electron density around SQD a 409 (B):

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



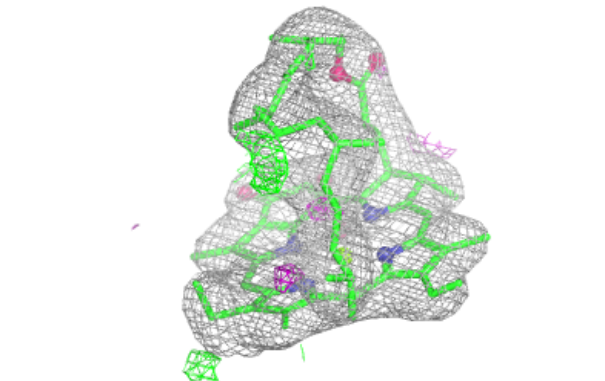
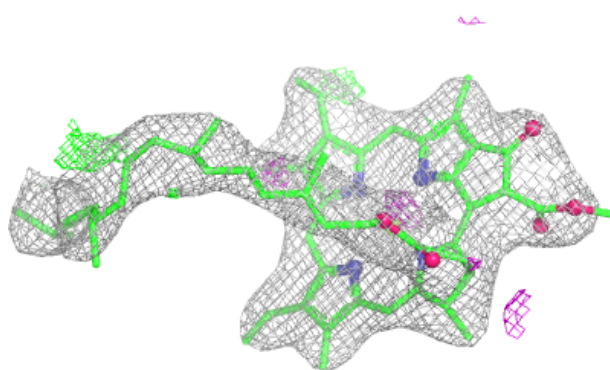
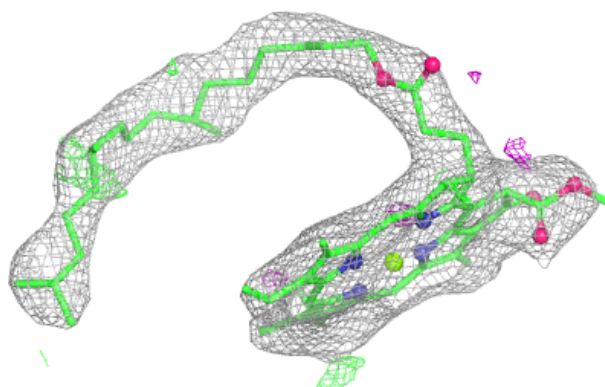
Electron density around CLA c 512:

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

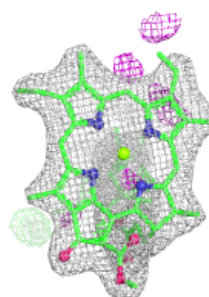
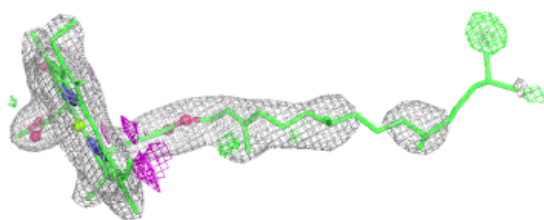
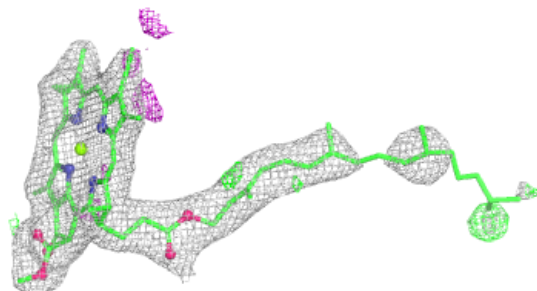


Electron density around CLA C 514:

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

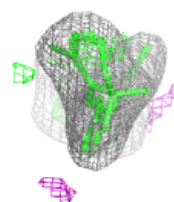
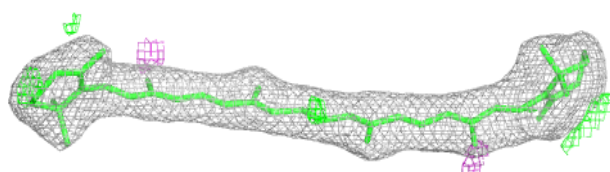
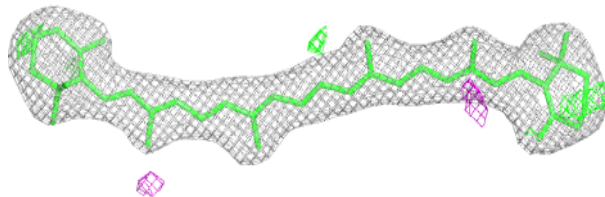
**Electron density around CLA d 404:**

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

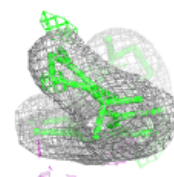
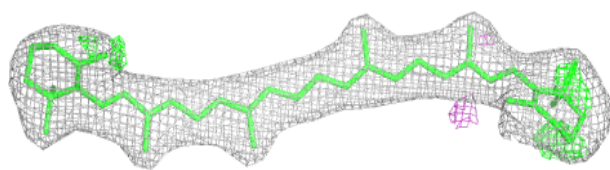
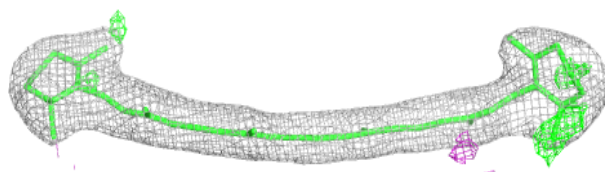


Electron density around BCR B 619:

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

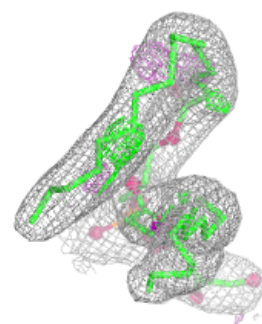
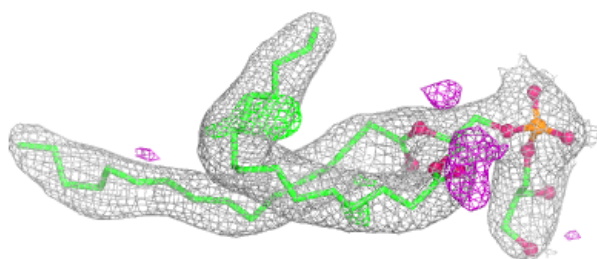
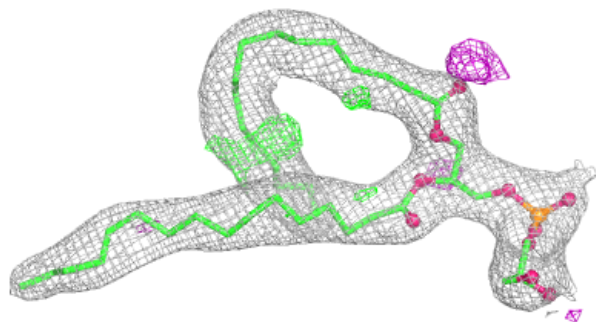
**Electron density around BCR D 404:**

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

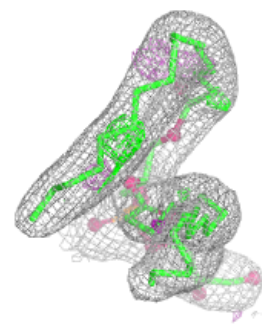
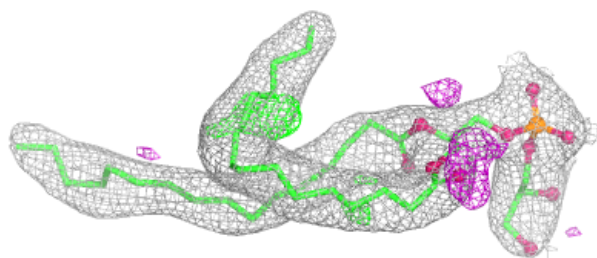
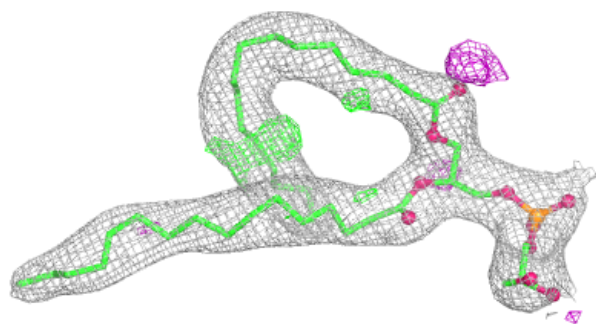


Electron density around LHG A 419 (A):

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

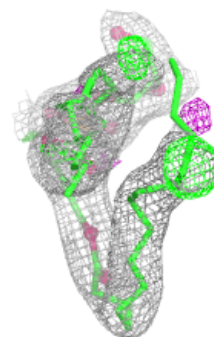
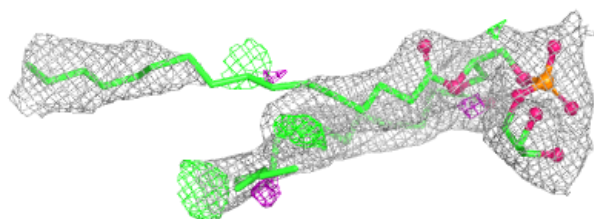
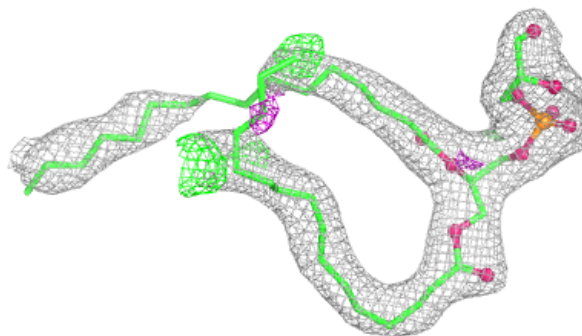
**Electron density around LHG A 419 (B):**

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

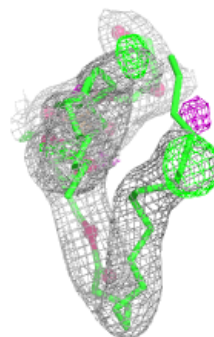
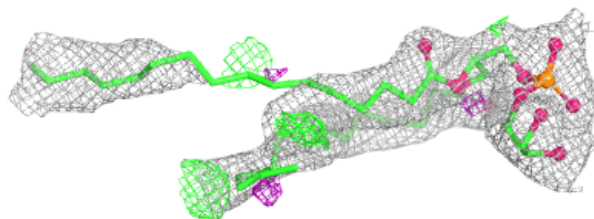
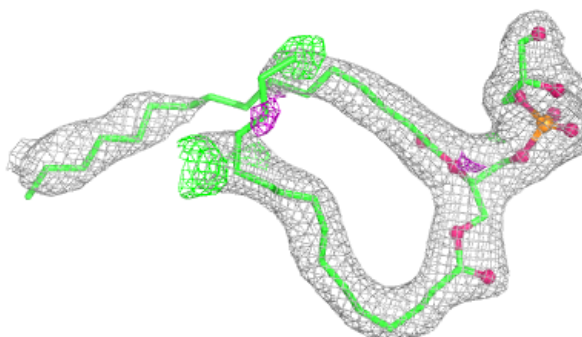


Electron density around LHG D 407 (A):

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

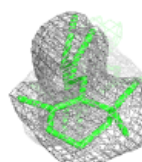
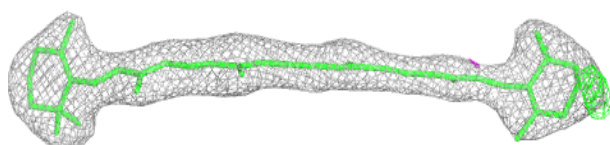
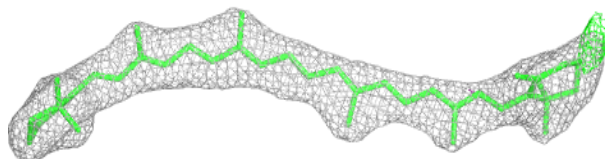
**Electron density around LHG D 407 (B):**

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

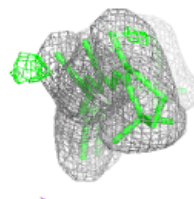
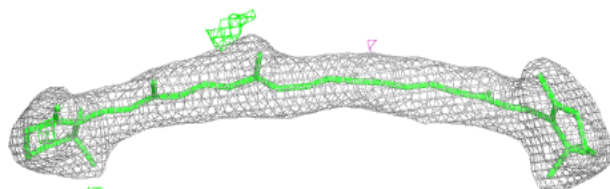
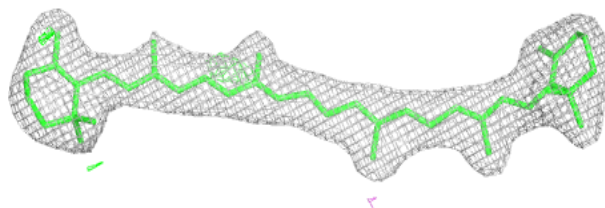


Electron density around BCR H 101:

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

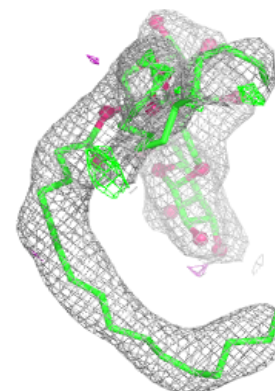
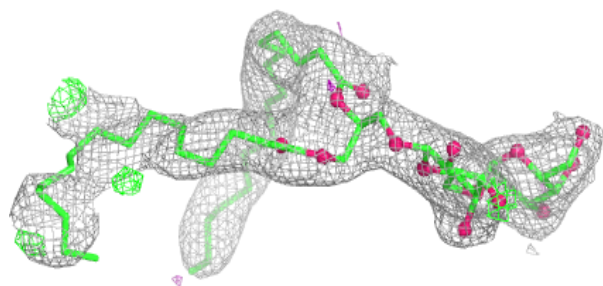
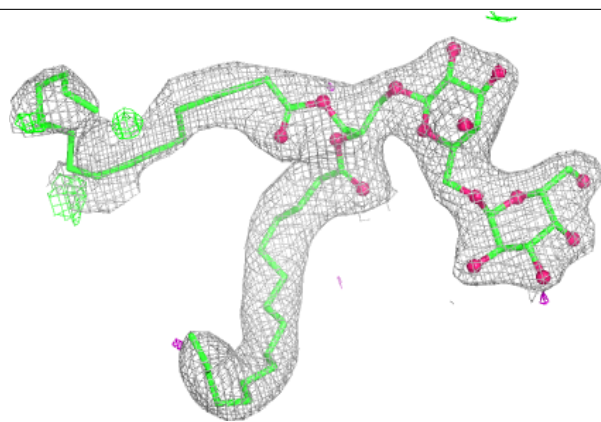
**Electron density around BCR T 102:**

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

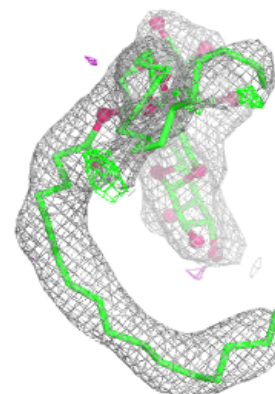
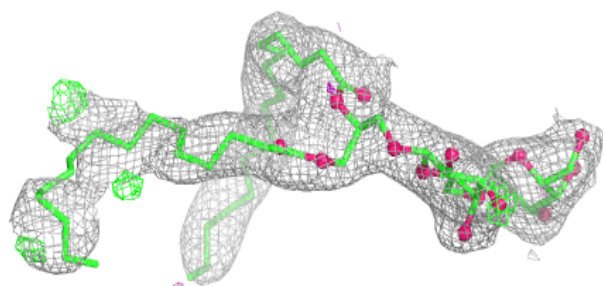
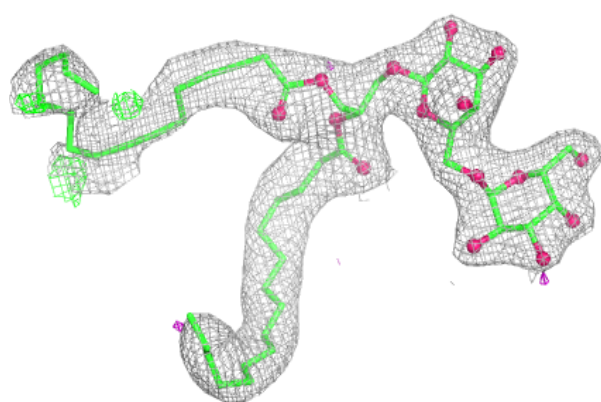


Electron density around DGD C 518 (A):

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

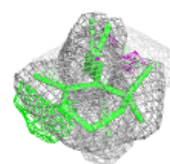
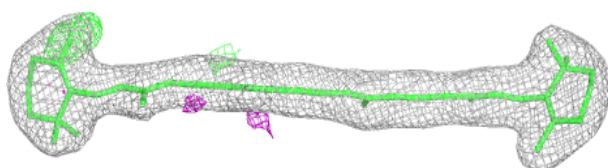
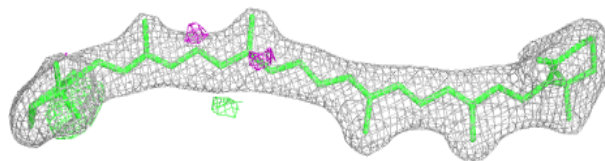
**Electron density around DGD C 518 (B):**

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

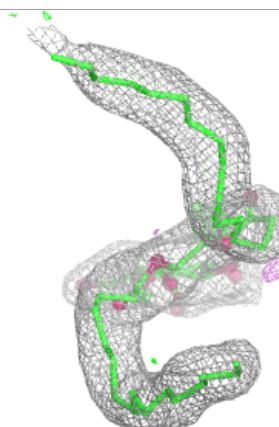
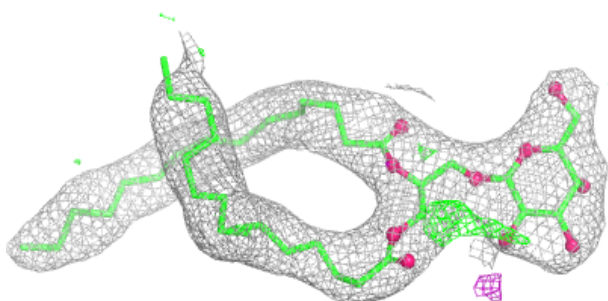
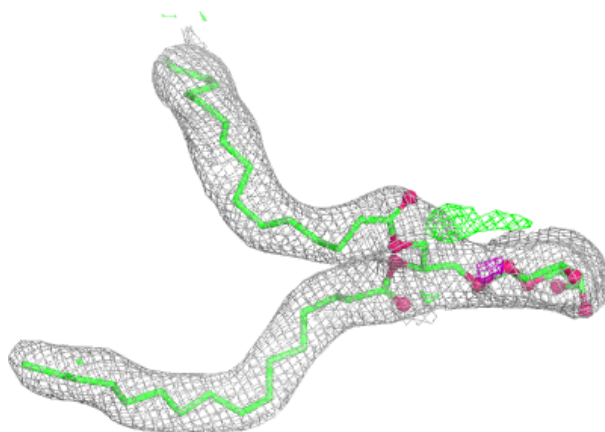


Electron density around BCR a 408:

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

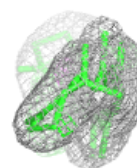
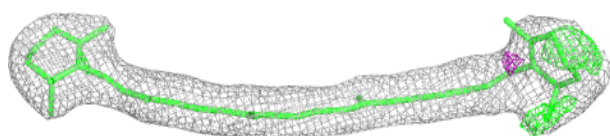
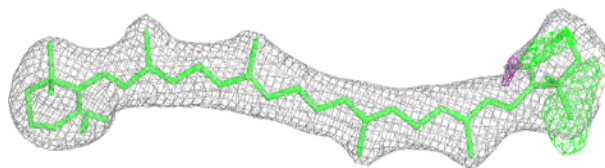
**Electron density around LMG B 621:**

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

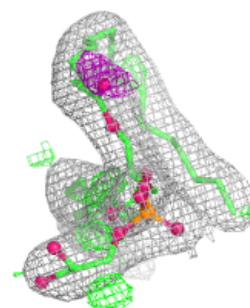
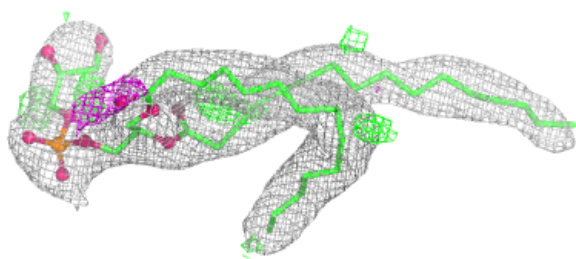
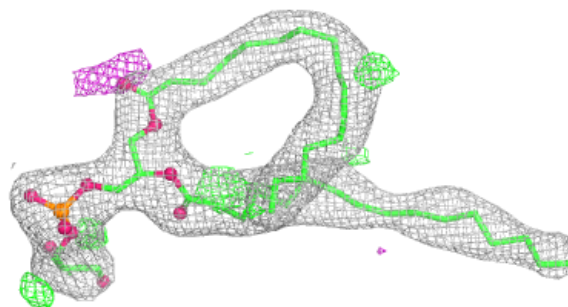


Electron density around BCR d 405:

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

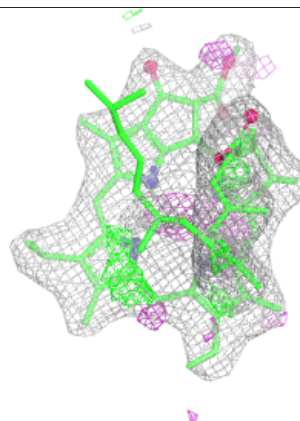
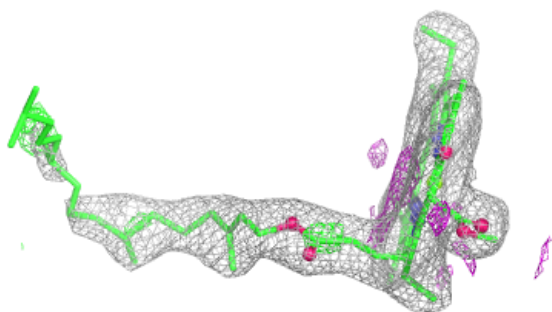
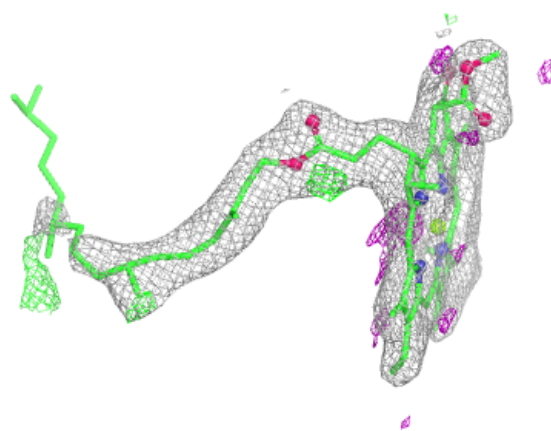
**Electron density around LHG d 414 (B):**

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

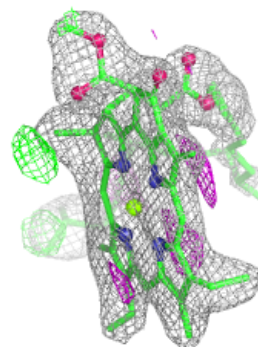
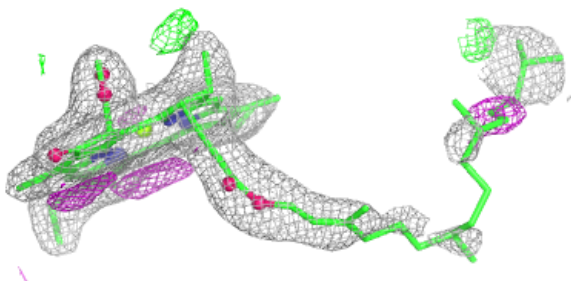
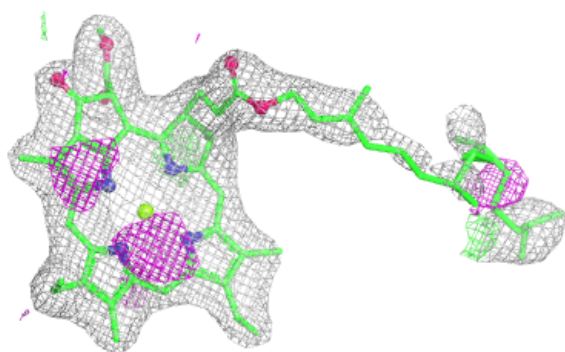


Electron density around CLA D 403:

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

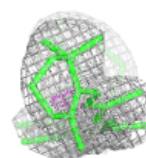
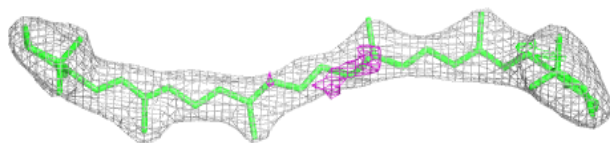
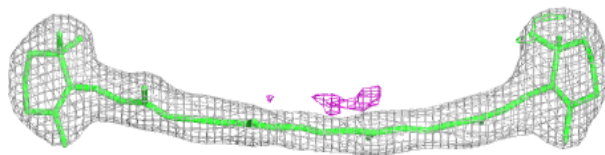
**Electron density around CLA a 407:**

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

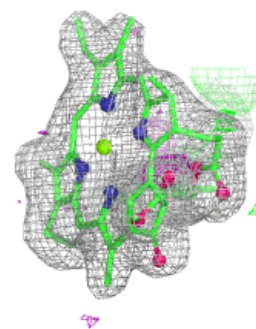
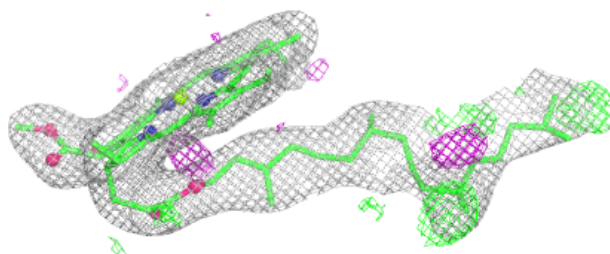
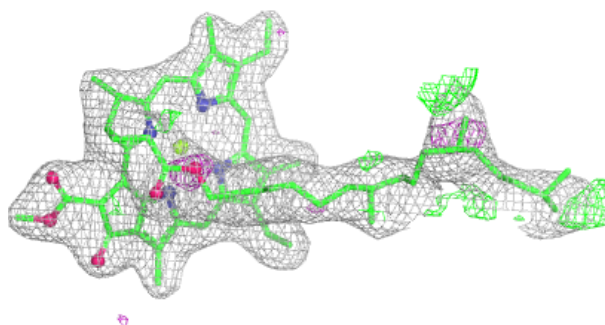


Electron density around BCR K 102:

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

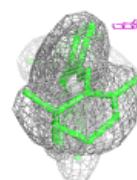
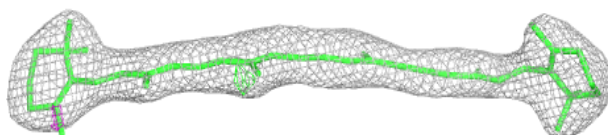
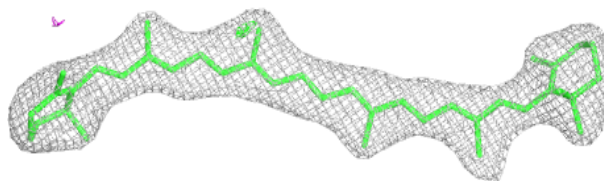
**Electron density around CLA B 614:**

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

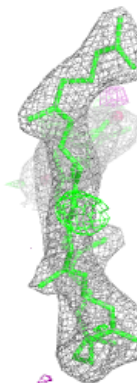
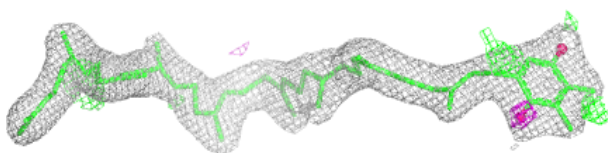
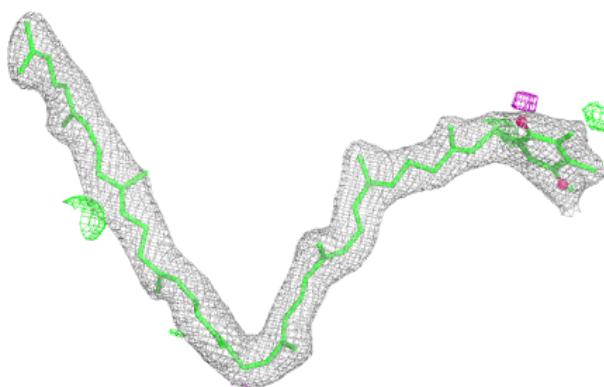


Electron density around BCR Y 101:

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

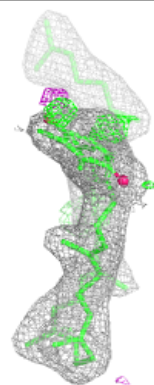
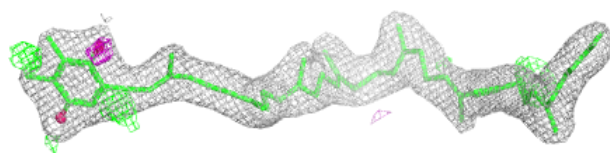
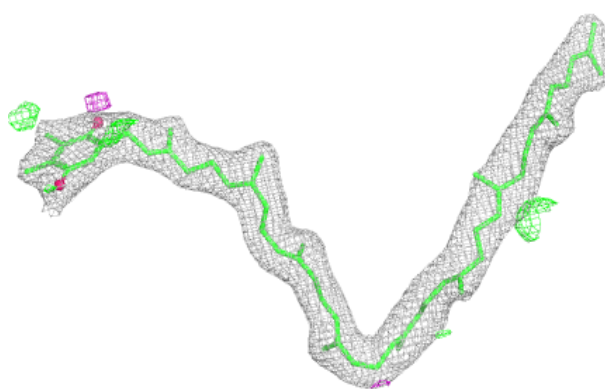
**Electron density around PL9 D 405 (A):**

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

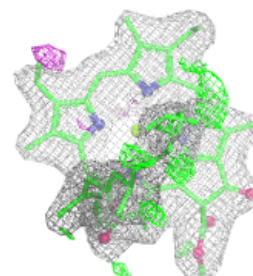
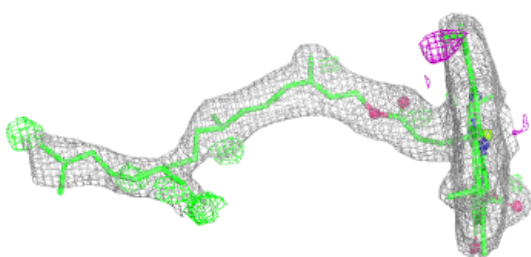
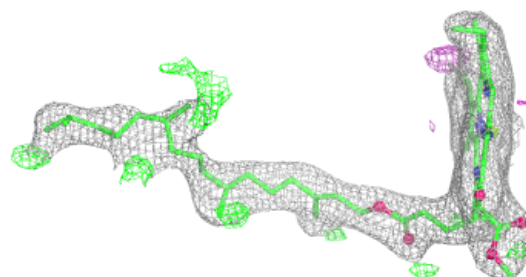


Electron density around PL9 D 405 (B):

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

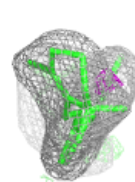
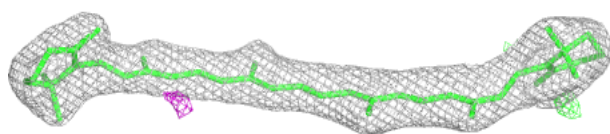
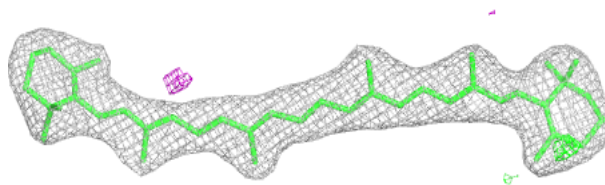
**Electron density around CLA b 606:**

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

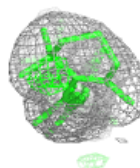
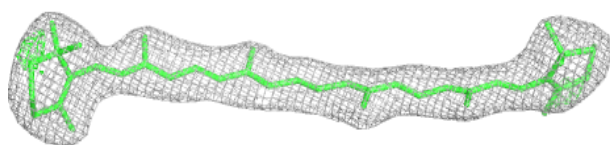
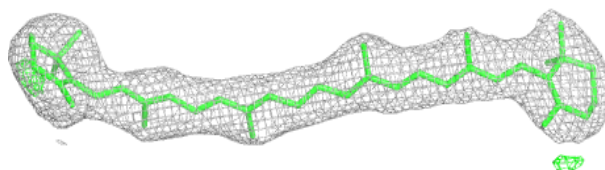


Electron density around BCR b 619:

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

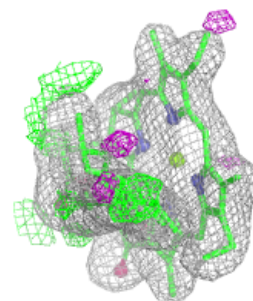
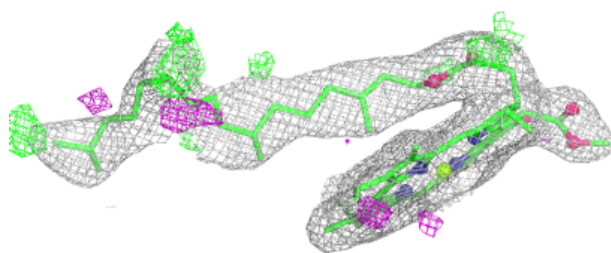
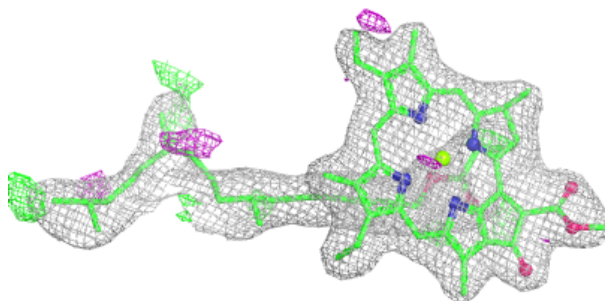
**Electron density around BCR c 514:**

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

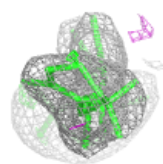
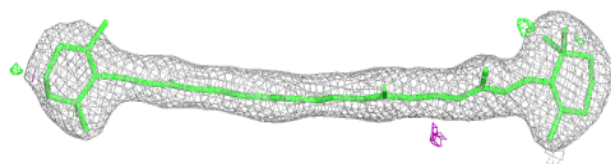
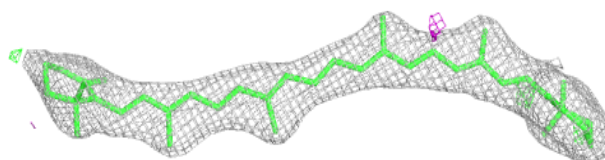


Electron density around CLA b 614:

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

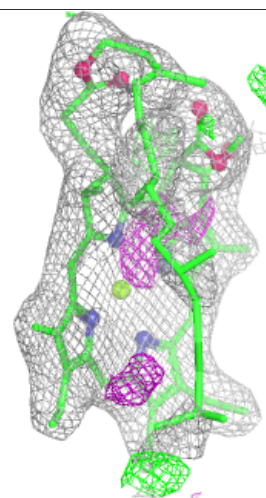
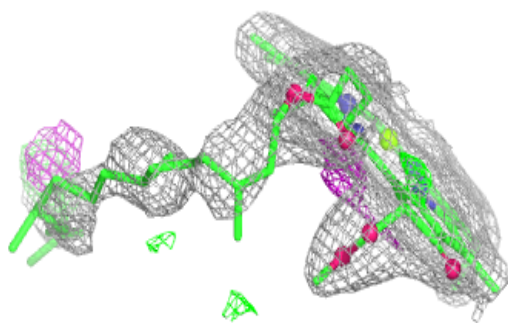
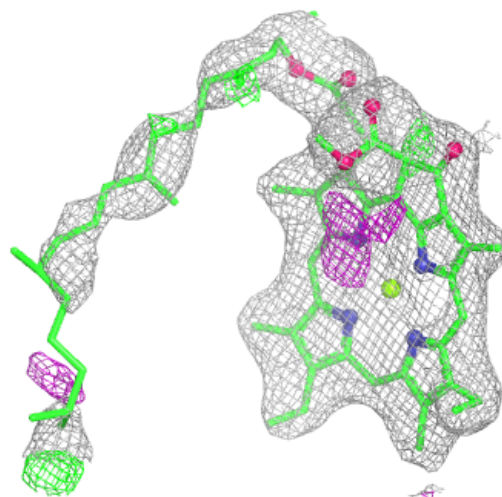
**Electron density around BCR h 101:**

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



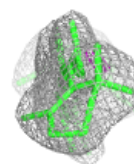
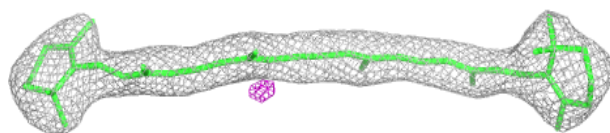
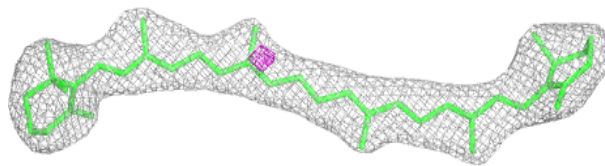
Electron density around CLA B 616:

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

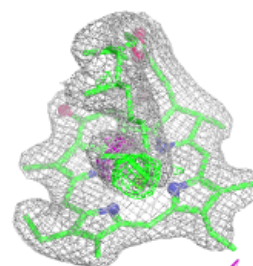
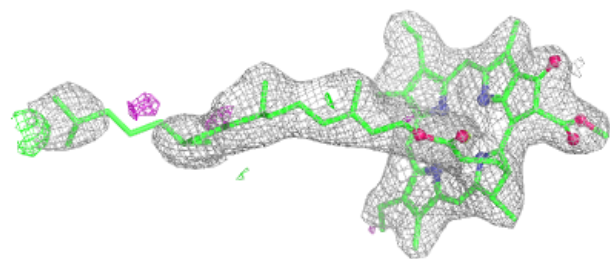
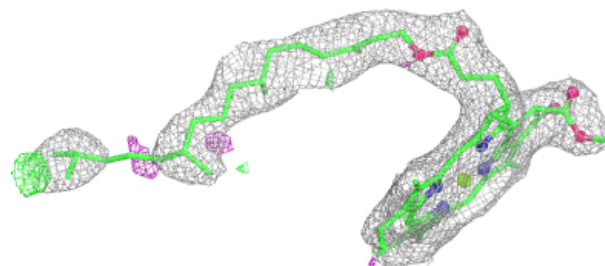


Electron density around BCR y 101:

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

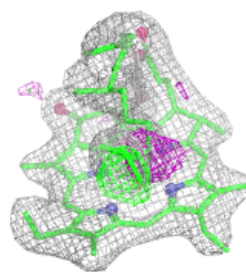
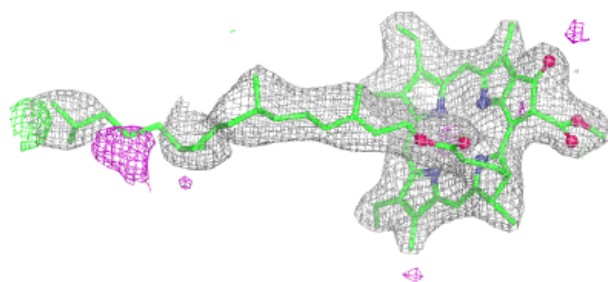
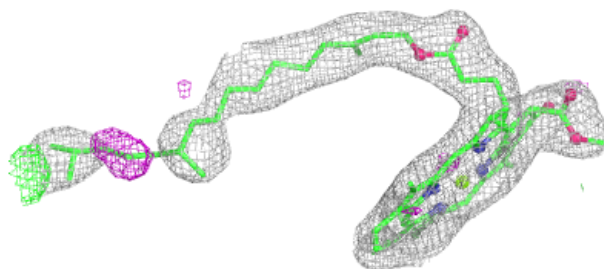
**Electron density around CLA c 504:**

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



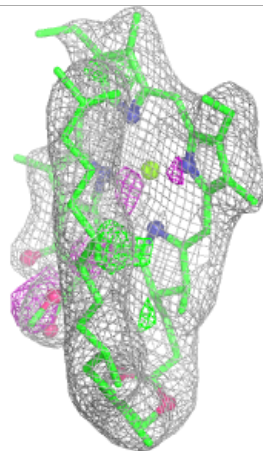
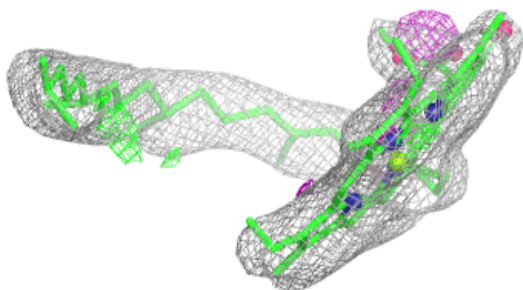
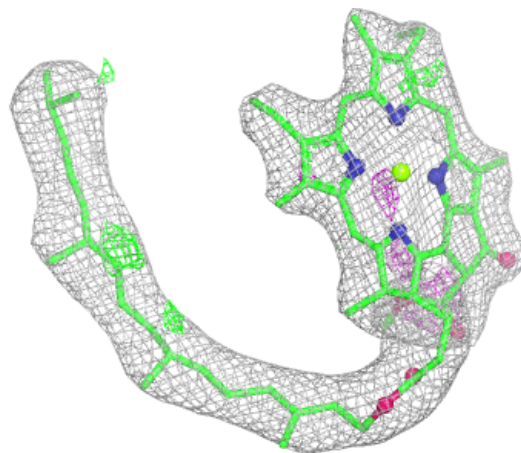
Electron density around CLA C 505:

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



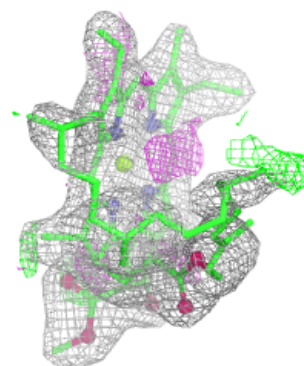
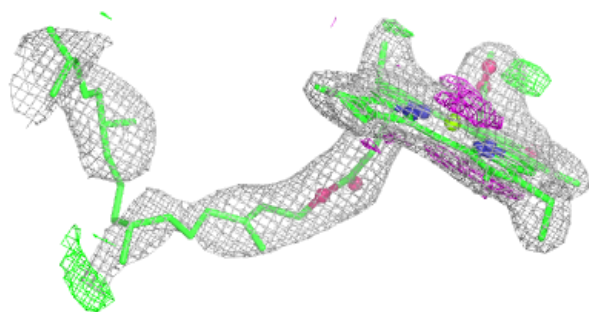
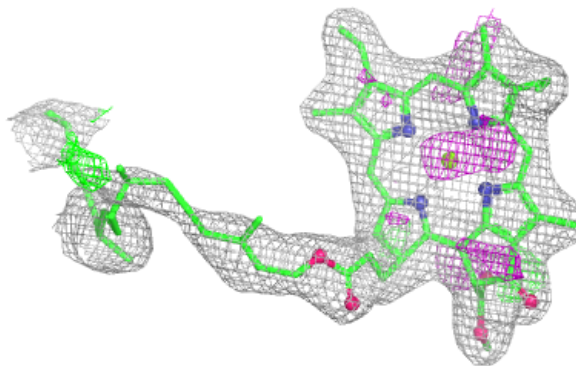
Electron density around CLA c 507:

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

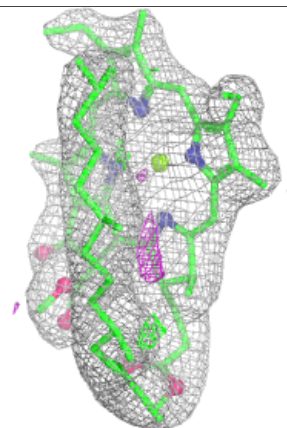
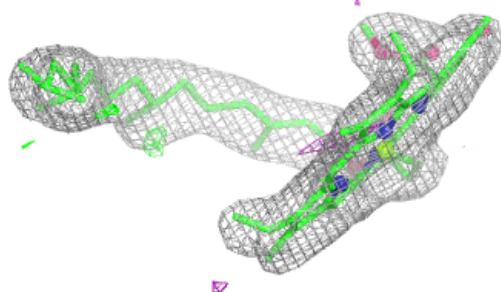
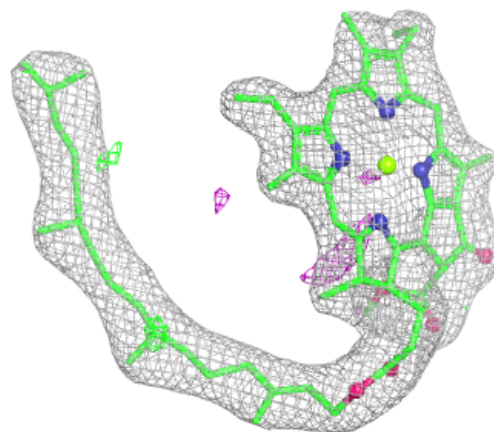


Electron density around CLA A 408:

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

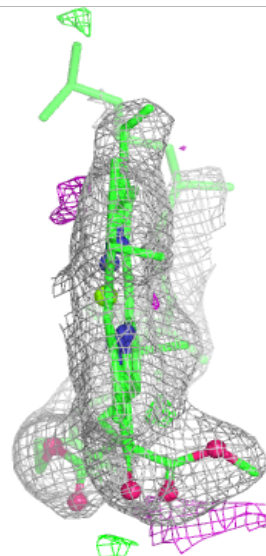
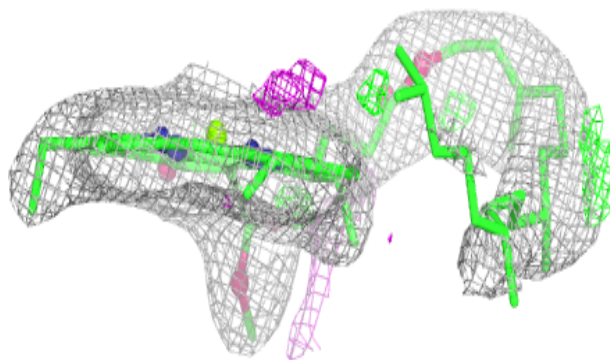
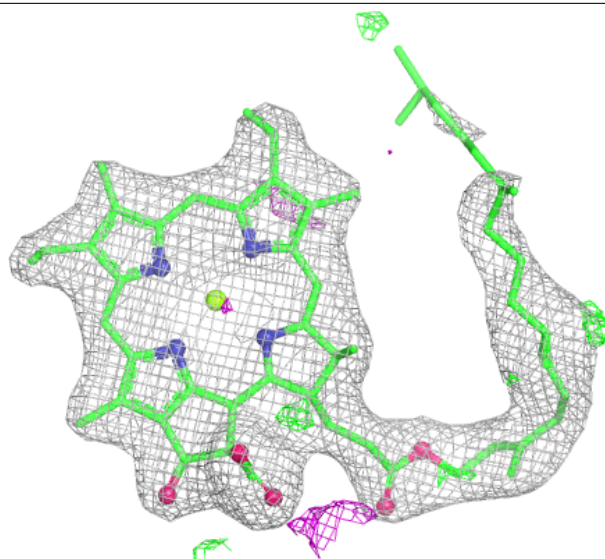
**Electron density around CLA C 508:**

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



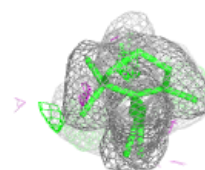
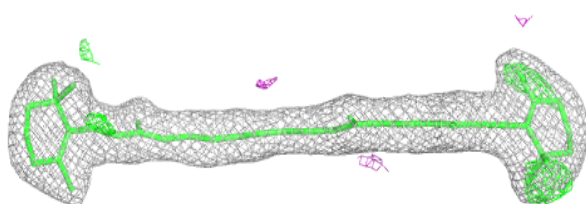
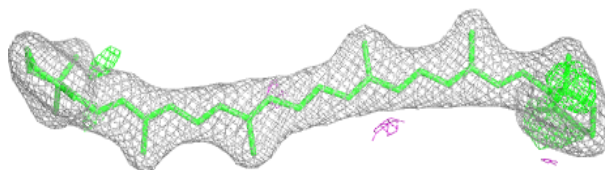
Electron density around CLA C 513:

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

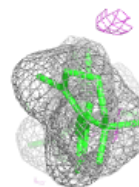
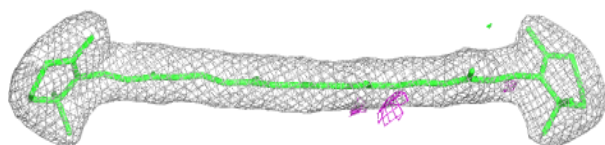
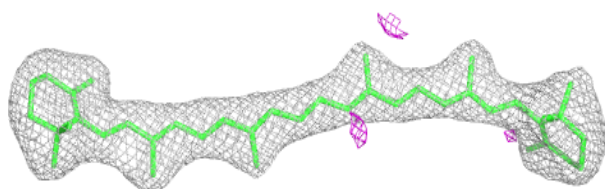


Electron density around BCR A 409:

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

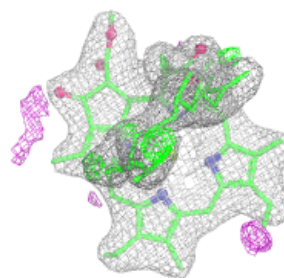
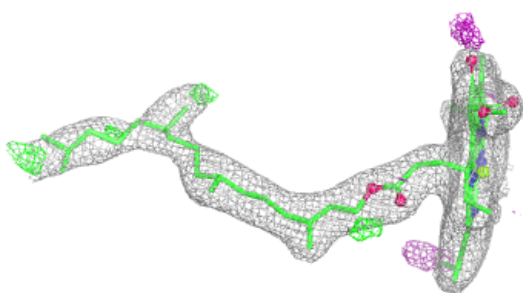
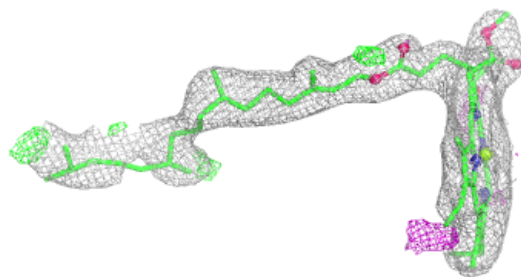
**Electron density around BCR B 618:**

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

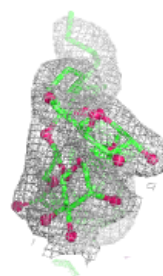
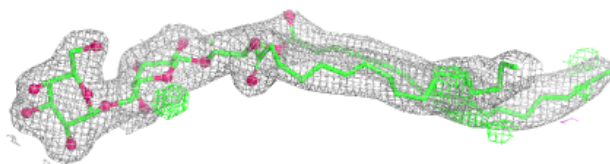
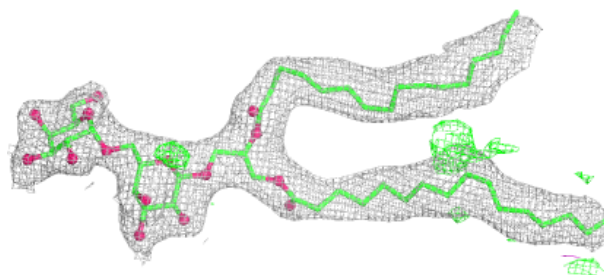


Electron density around CLA B 606:

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

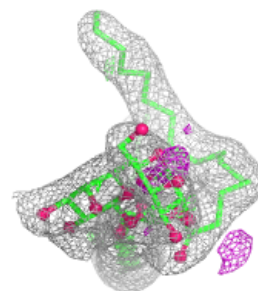
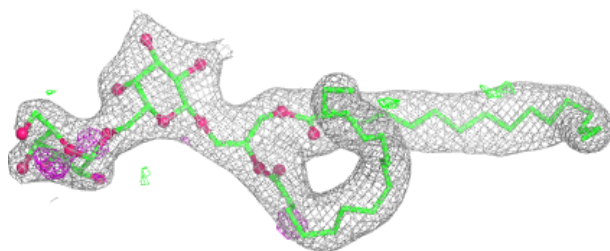
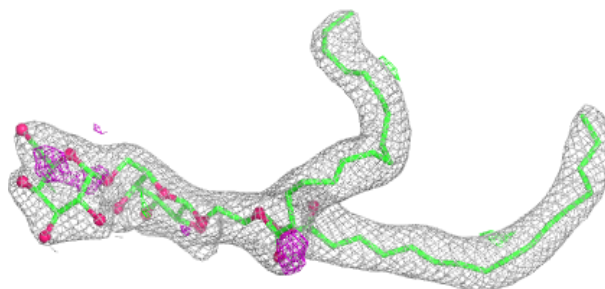
**Electron density around DGD C 519:**

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

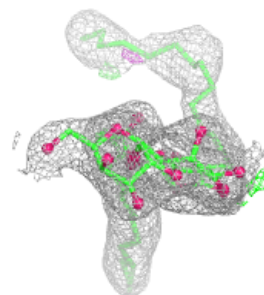
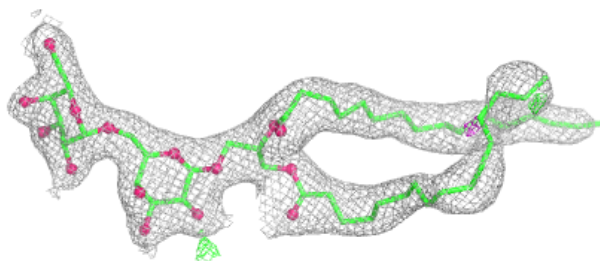
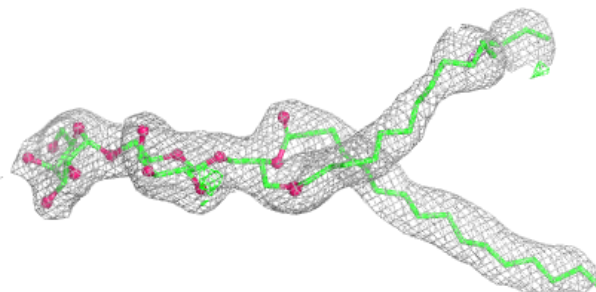


Electron density around DGD H 102:

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

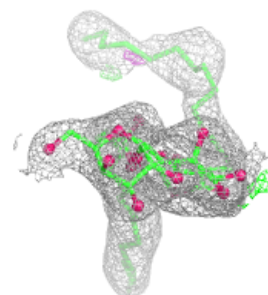
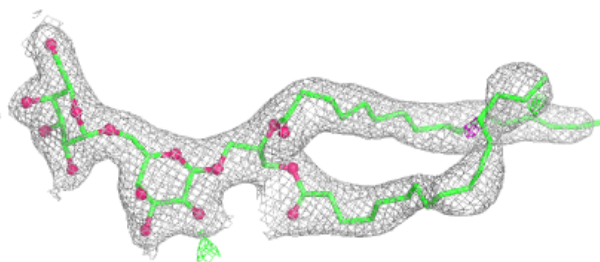
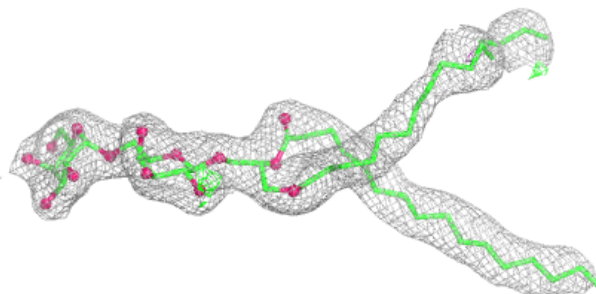
**Electron density around DGD c 516 (A):**

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

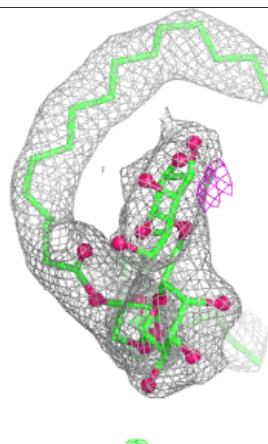
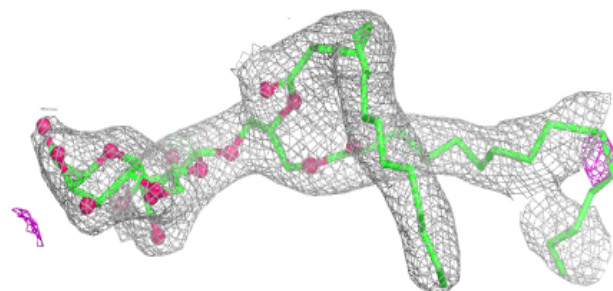
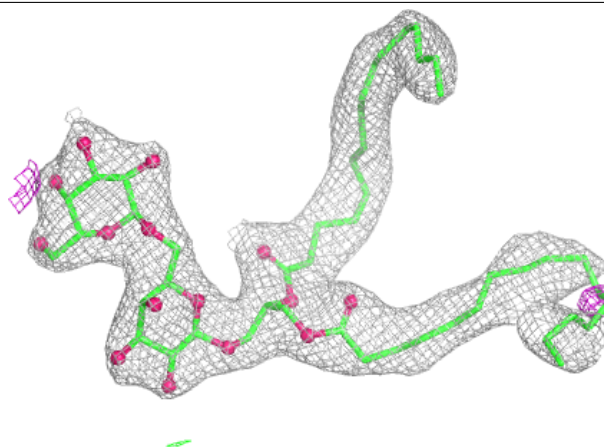


Electron density around DGD c 516 (B):

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

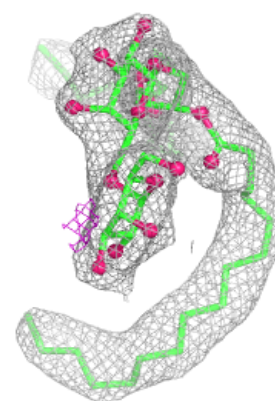
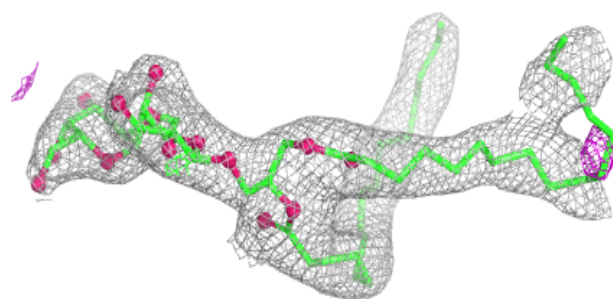
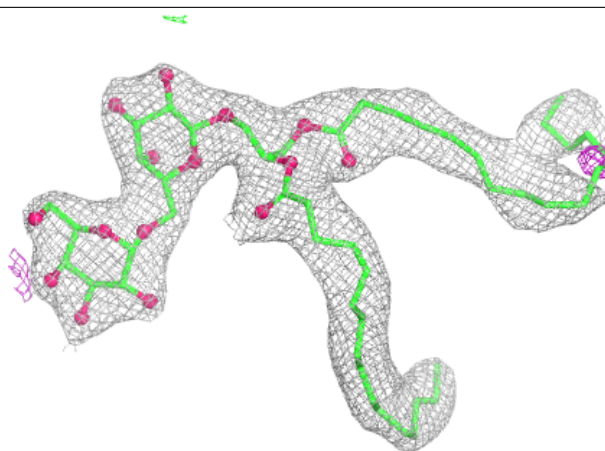
**Electron density around DGD c 517 (A):**

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

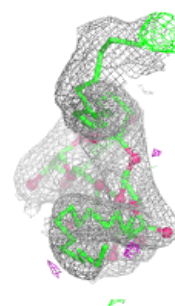
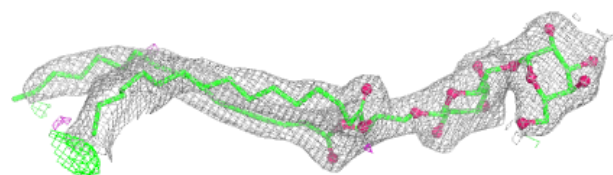
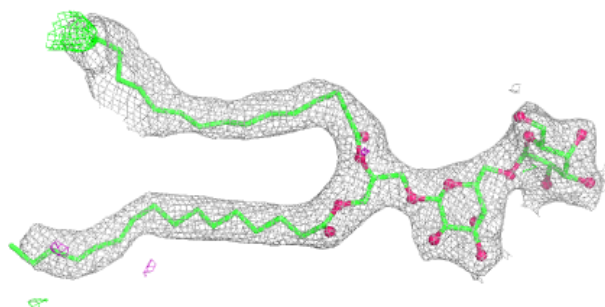


Electron density around DGD c 517 (B):

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

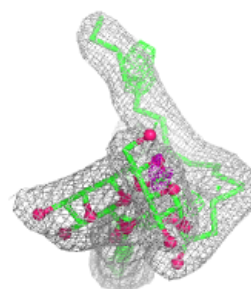
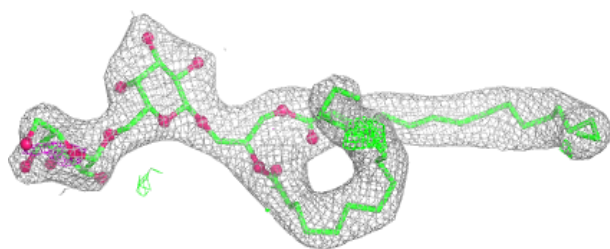
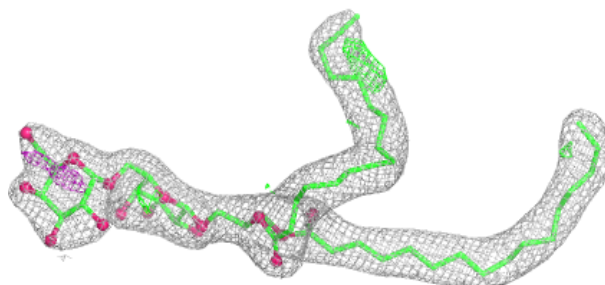
**Electron density around DGD c 518:**

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



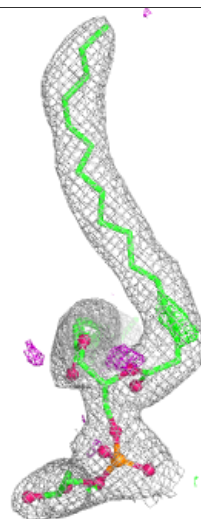
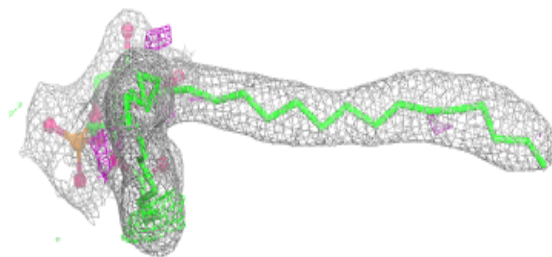
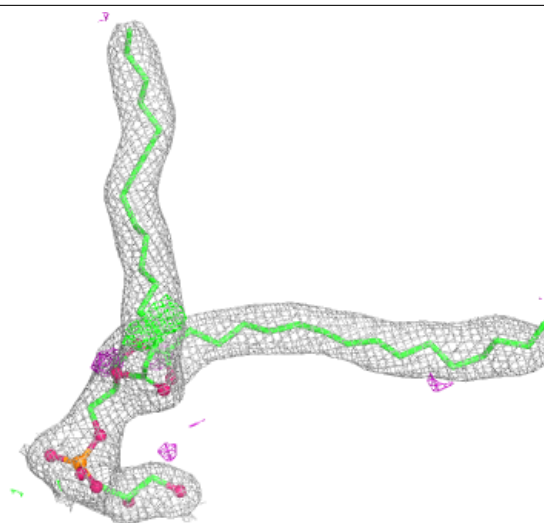
Electron density around DGD h 102:

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



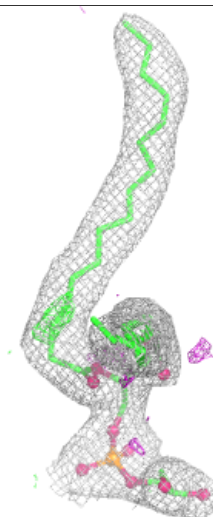
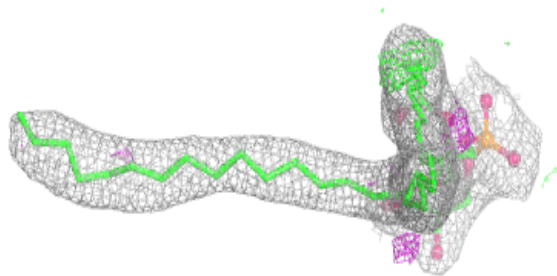
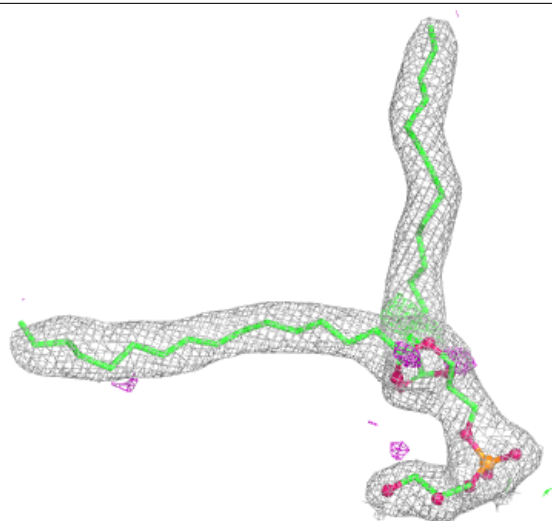
Electron density around LHG b 629 (A):

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



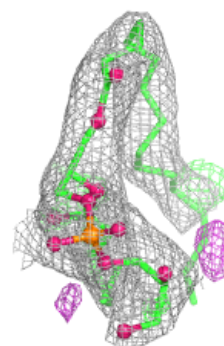
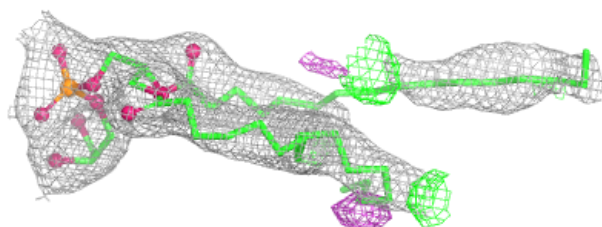
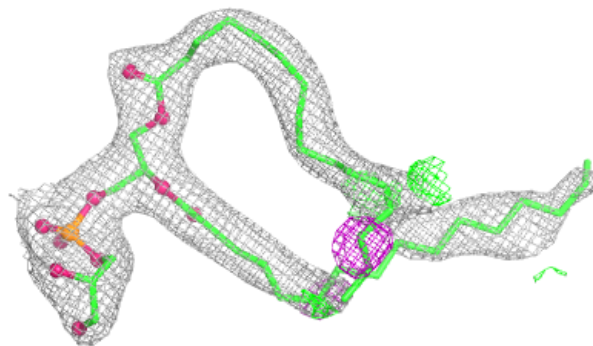
Electron density around LHG b 629 (B):

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

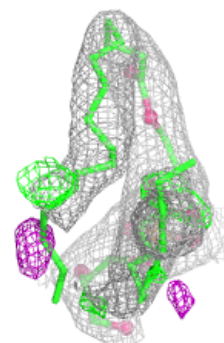
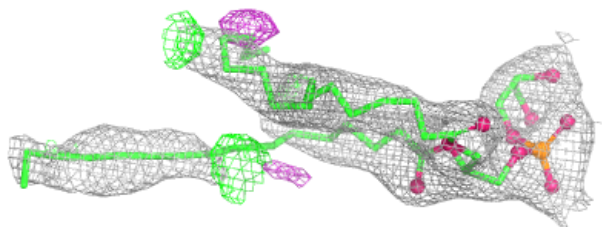
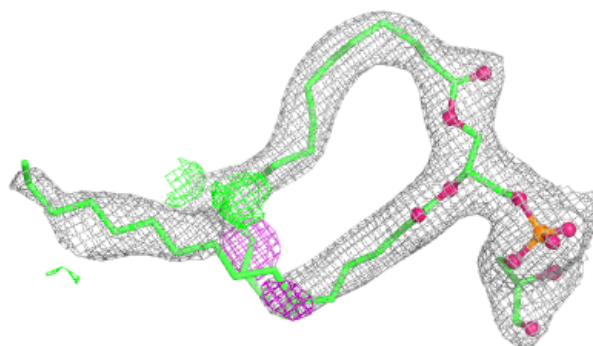


Electron density around LHG d 408 (A):

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

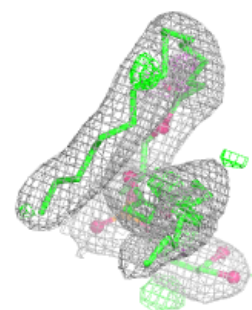
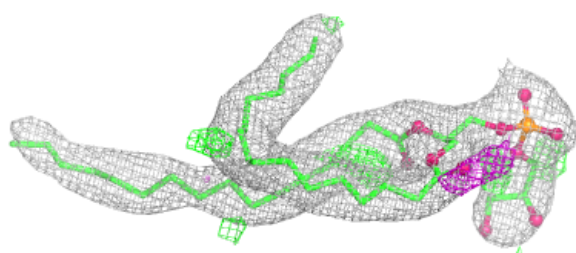
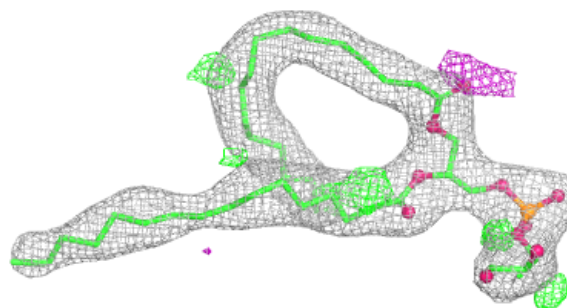
**Electron density around LHG d 408 (B):**

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

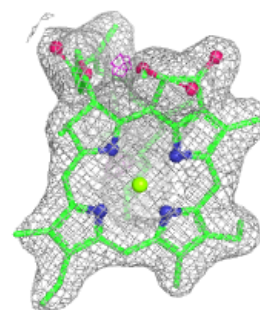
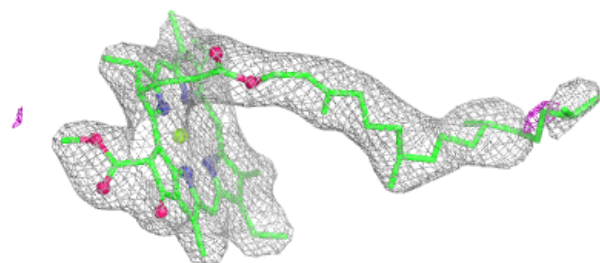
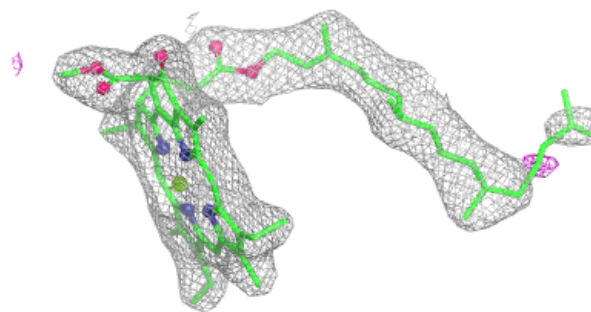


Electron density around LHG d 414 (A):

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

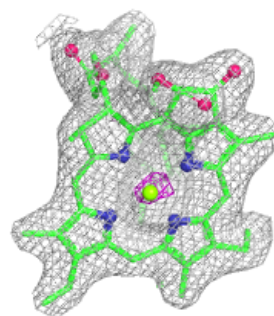
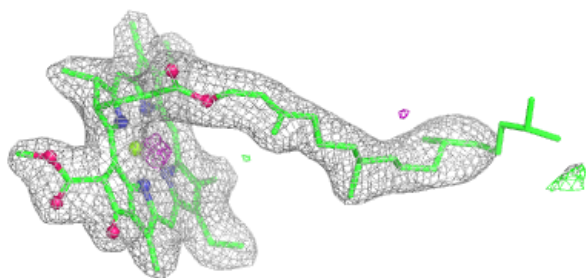
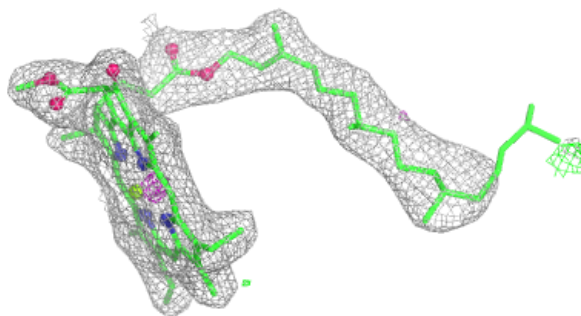
**Electron density around CLA c 508:**

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

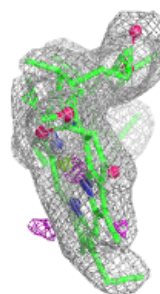
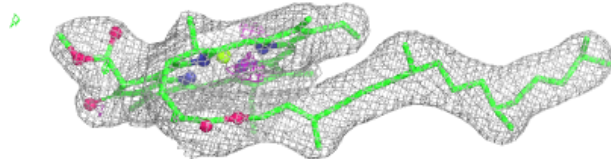
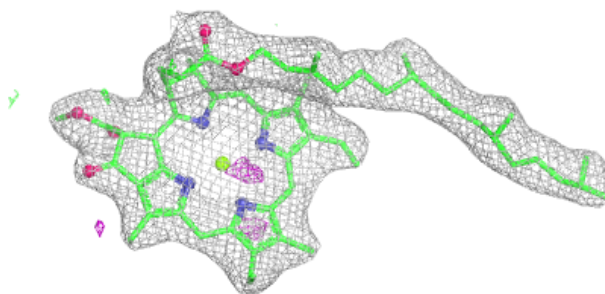


Electron density around CLA C 509:

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

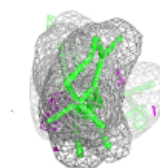
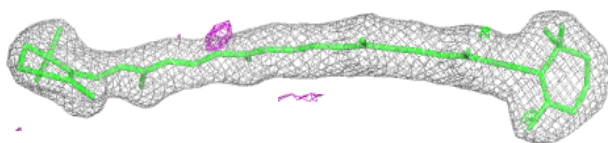
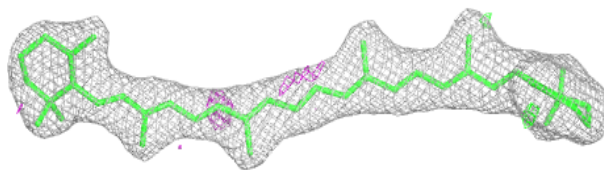
**Electron density around CLA C 502:**

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

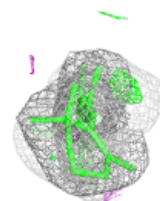
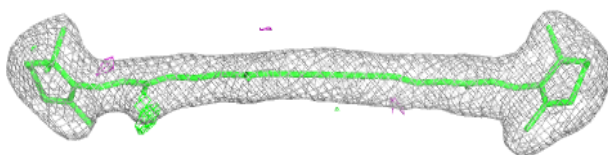
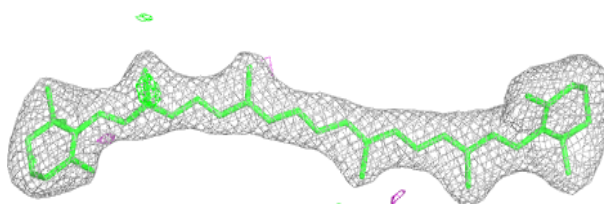


Electron density around BCR b 617:

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

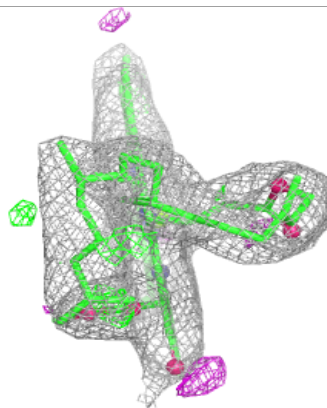
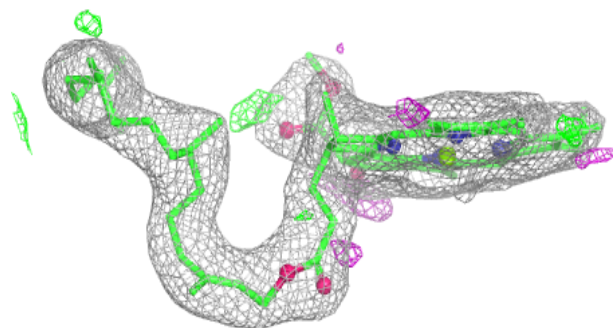
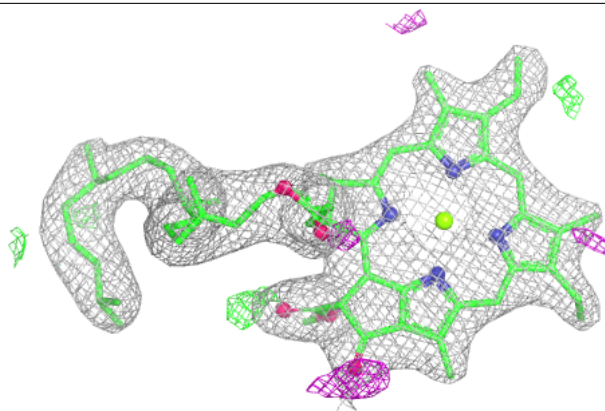
**Electron density around BCR b 618:**

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



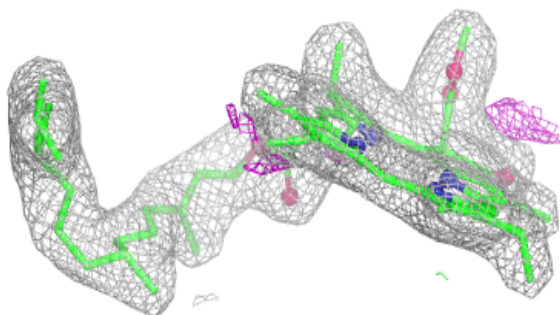
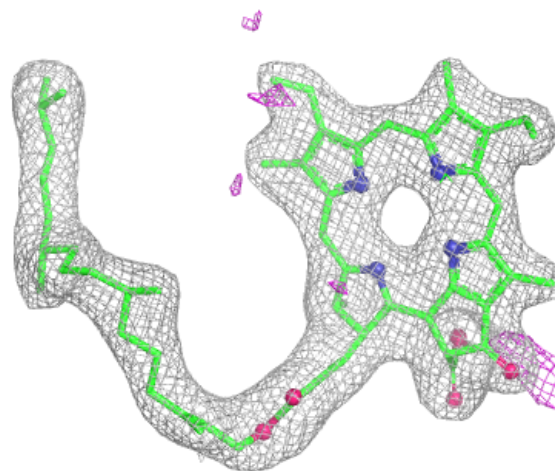
Electron density around CLA b 612:

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



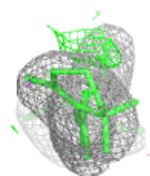
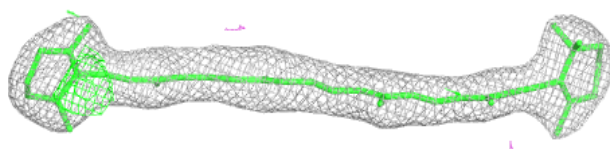
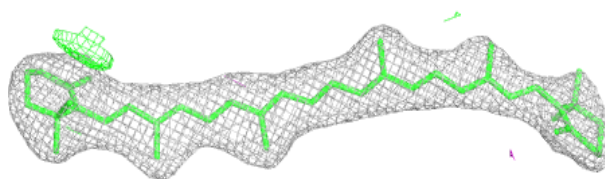
Electron density around PHO A 416 (A):

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



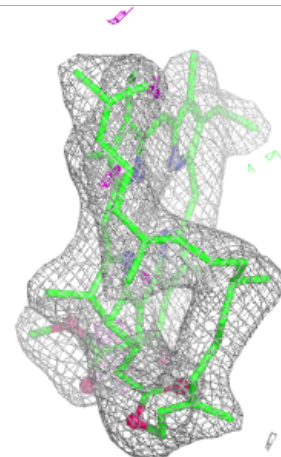
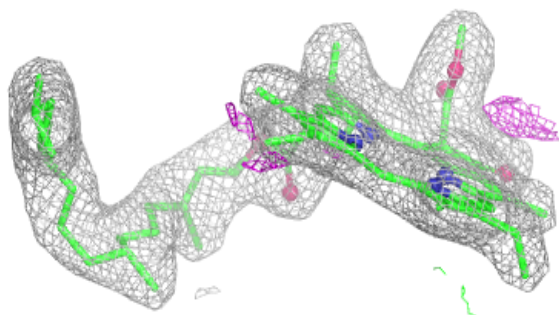
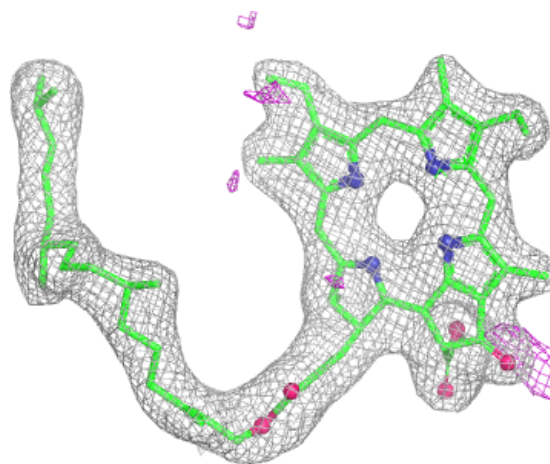
Electron density around BCR c 515:

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



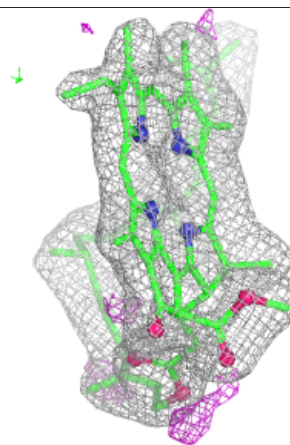
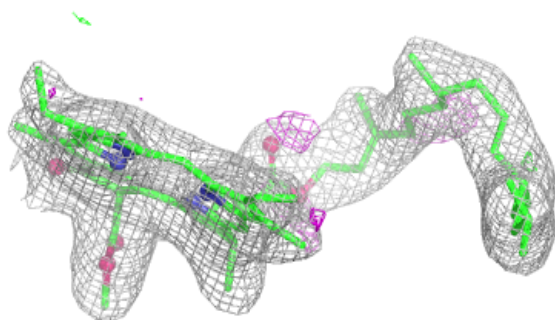
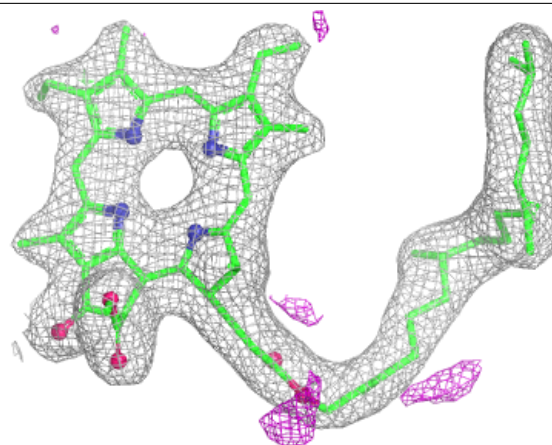
Electron density around PHO A 416 (B):

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



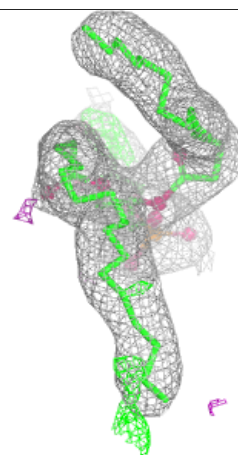
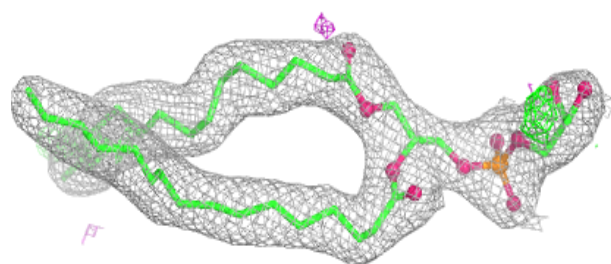
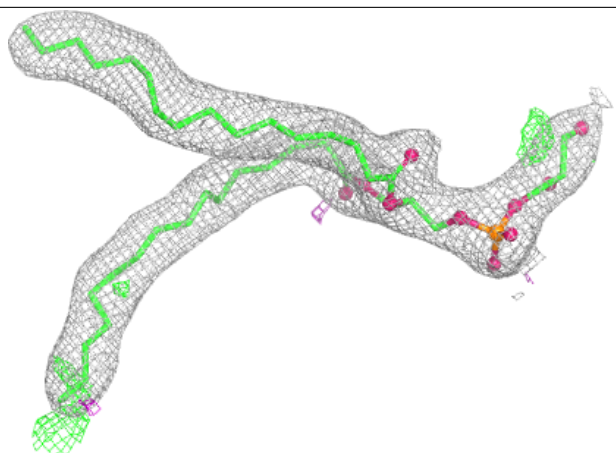
Electron density around PHO a 414 (A):

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



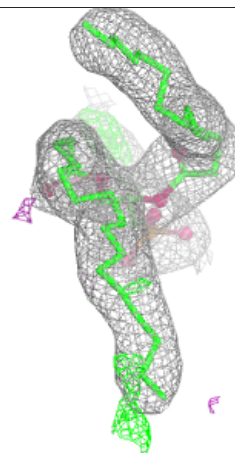
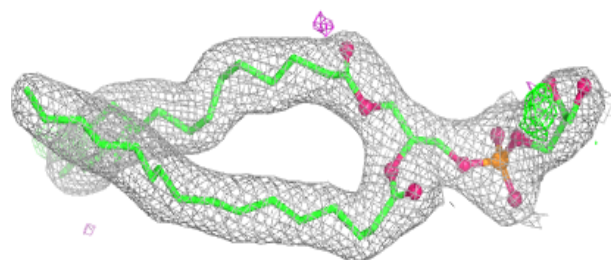
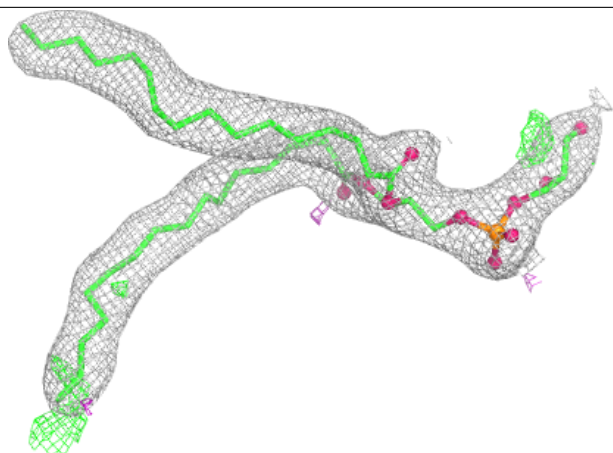
Electron density around LHG d 407 (A):

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

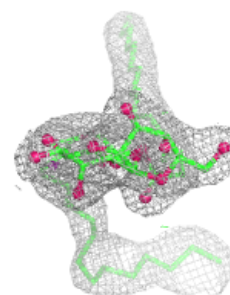
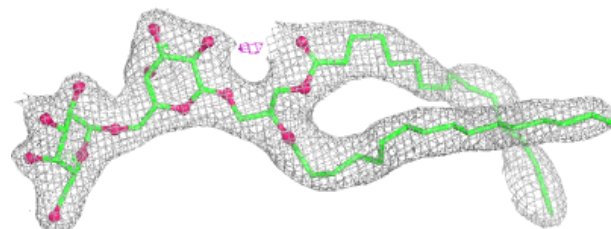
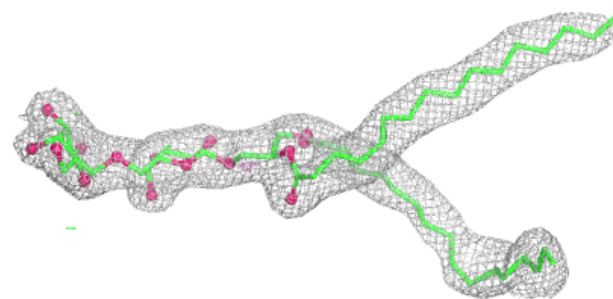


Electron density around LHG d 407 (B):

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

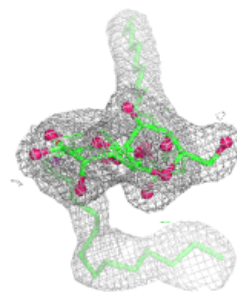
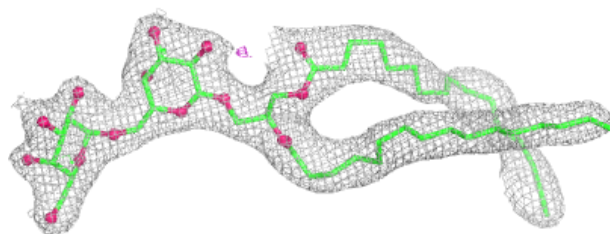
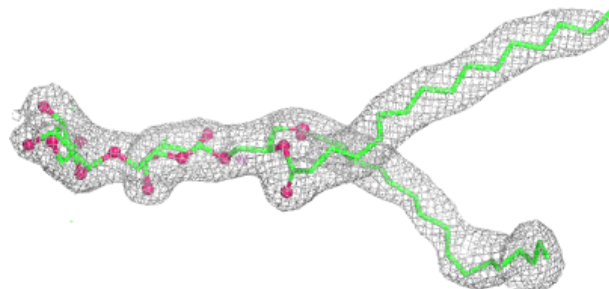
**Electron density around DGD C 517 (A):**

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

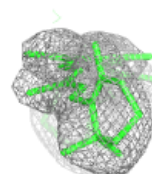
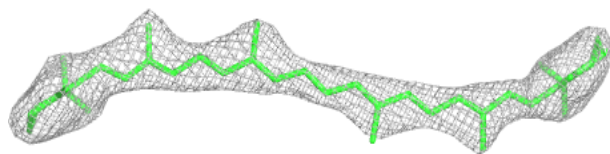
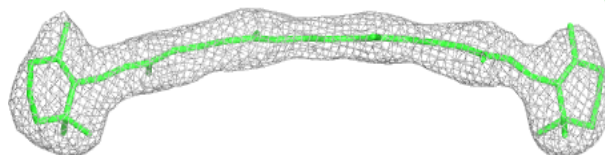


Electron density around DGD C 517 (B):

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

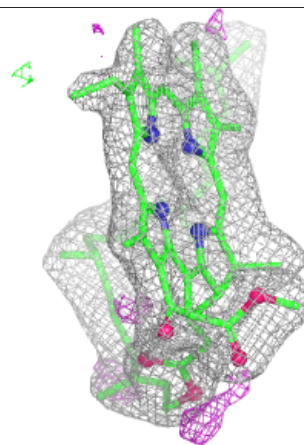
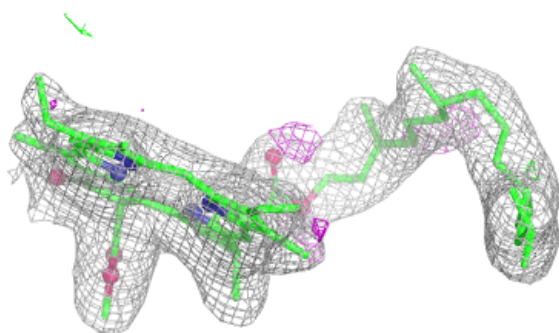
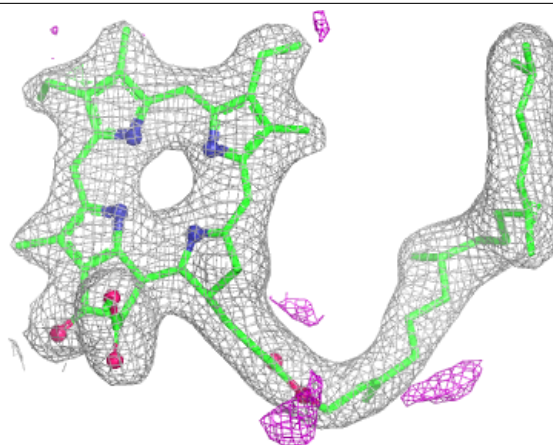
**Electron density around BCR k 101:**

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



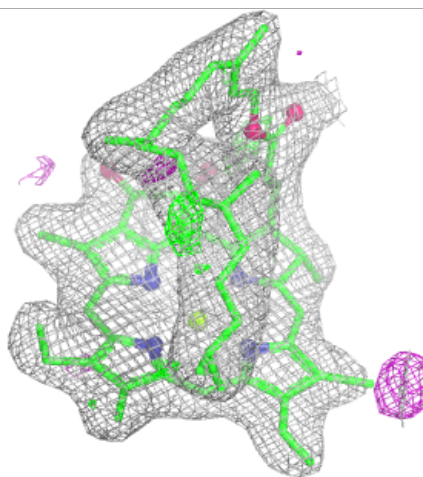
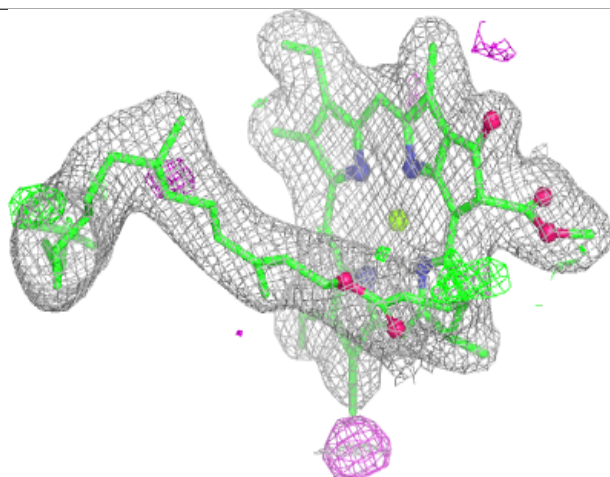
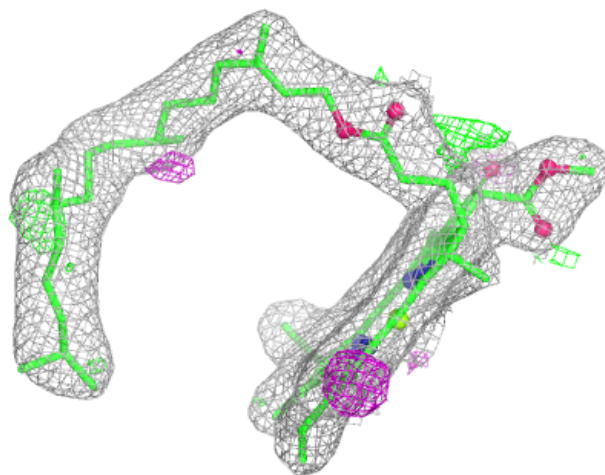
Electron density around PHO a 414 (B):

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



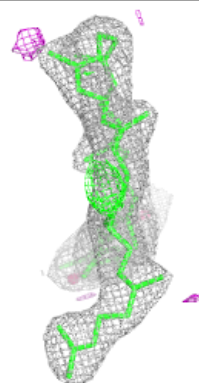
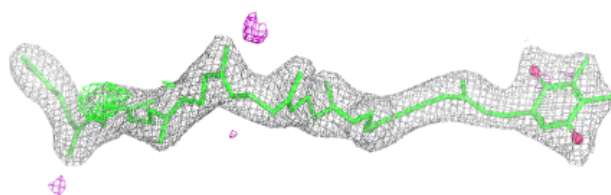
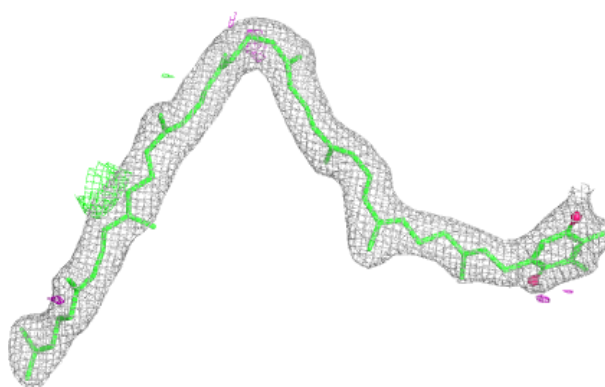
Electron density around CLA B 611:

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

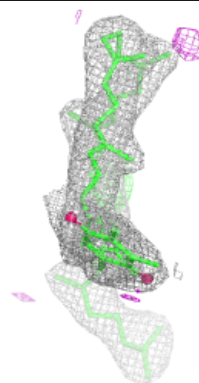
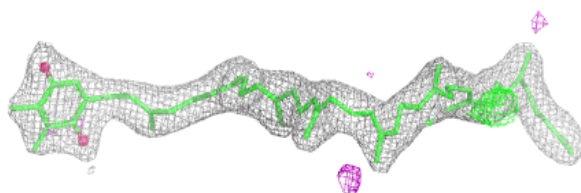
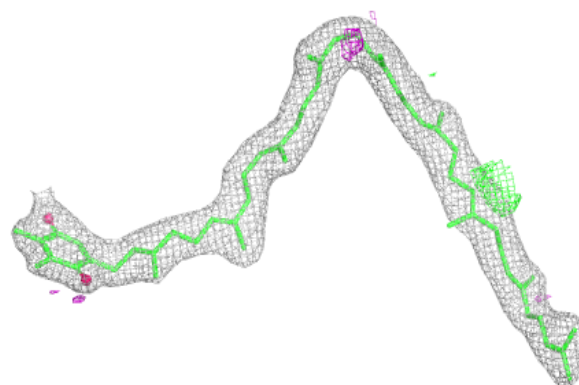


Electron density around PL9 d 406 (A):

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

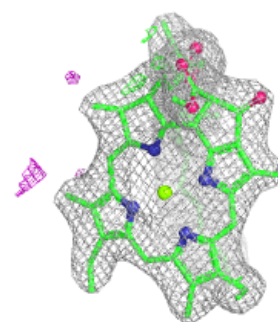
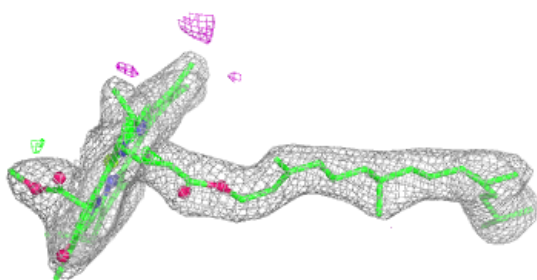
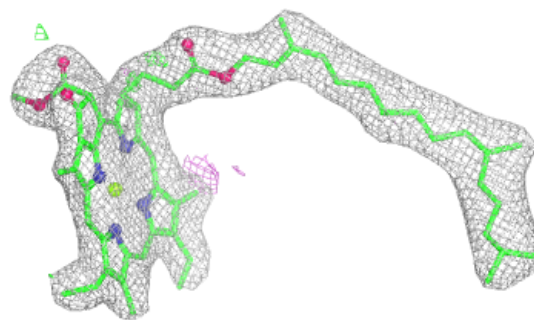
**Electron density around PL9 d 406 (B):**

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

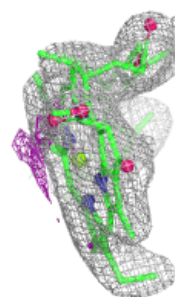
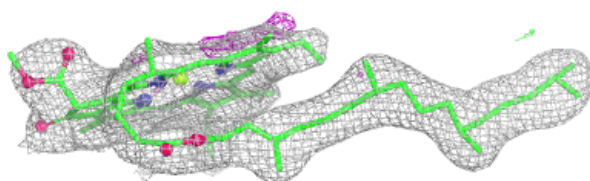
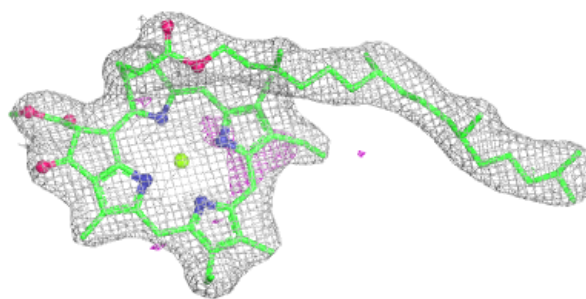


Electron density around CLA B 609:

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

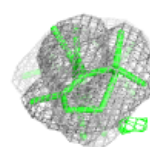
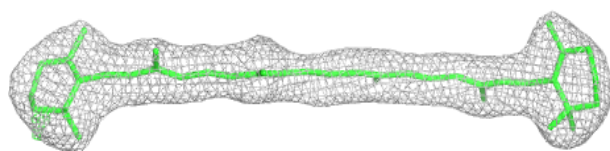
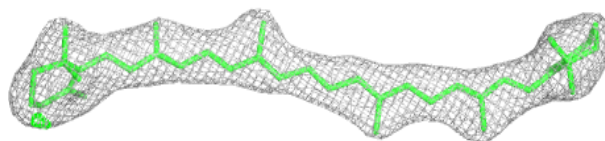
**Electron density around CLA c 501:**

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

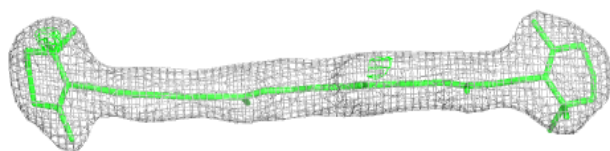
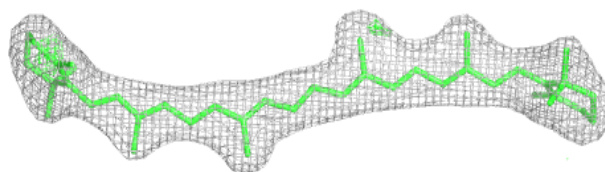


Electron density around BCR C 515:

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

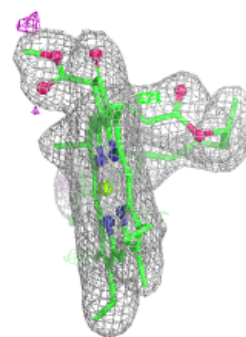
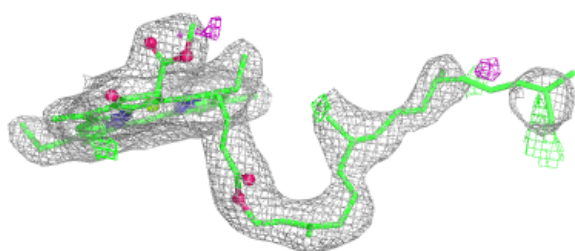
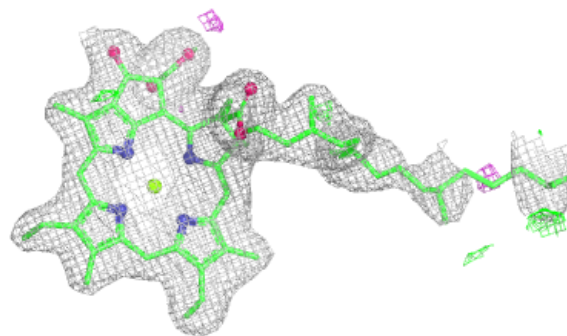
**Electron density around BCR C 516:**

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

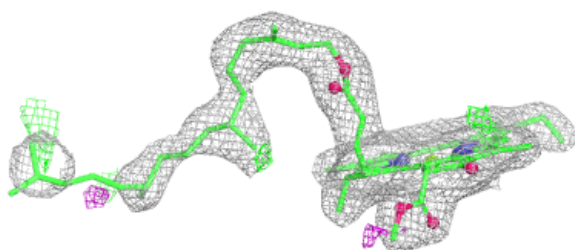
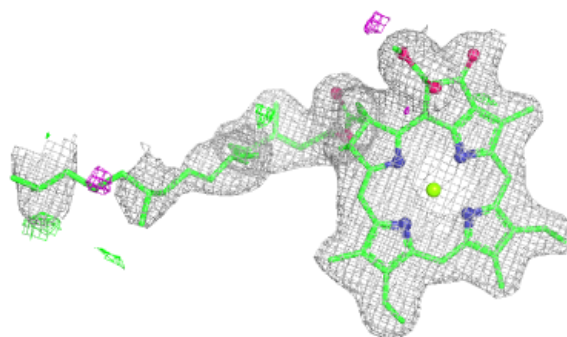


Electron density around CLA a 405 (A):

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

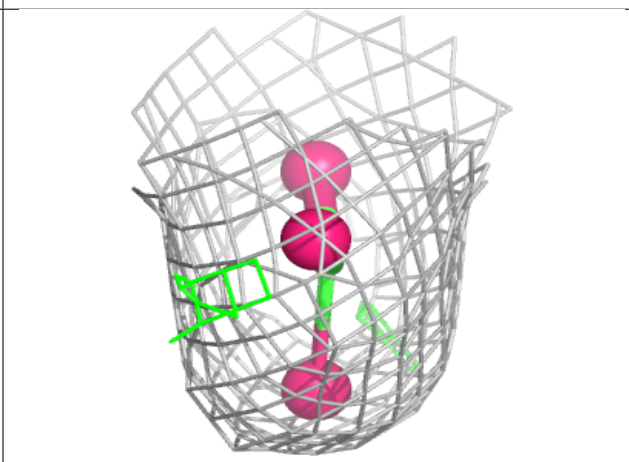
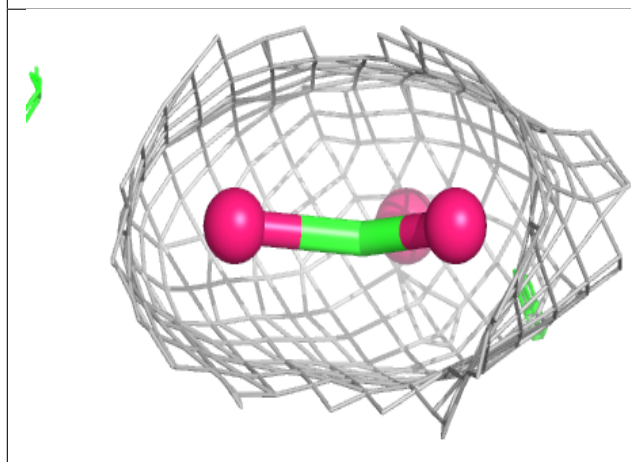
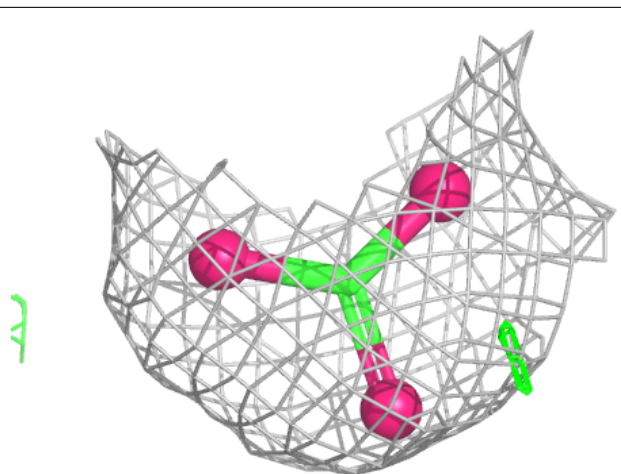
**Electron density around CLA a 405 (B):**

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



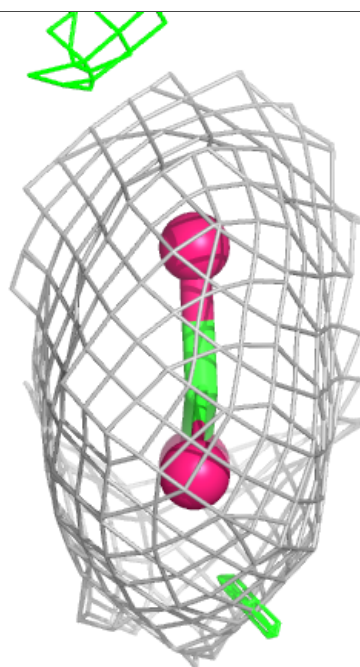
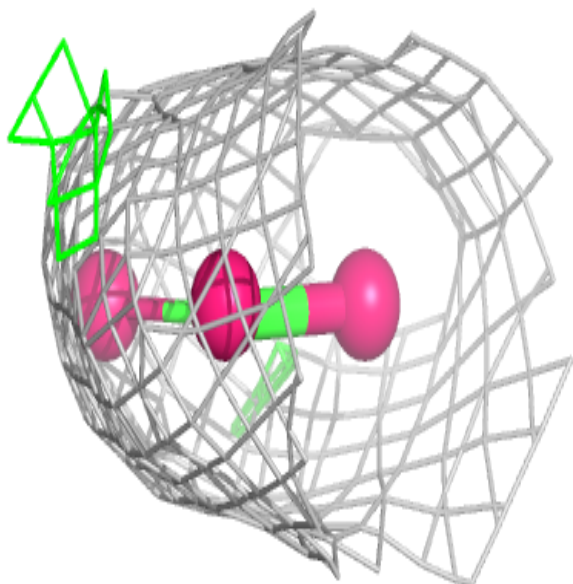
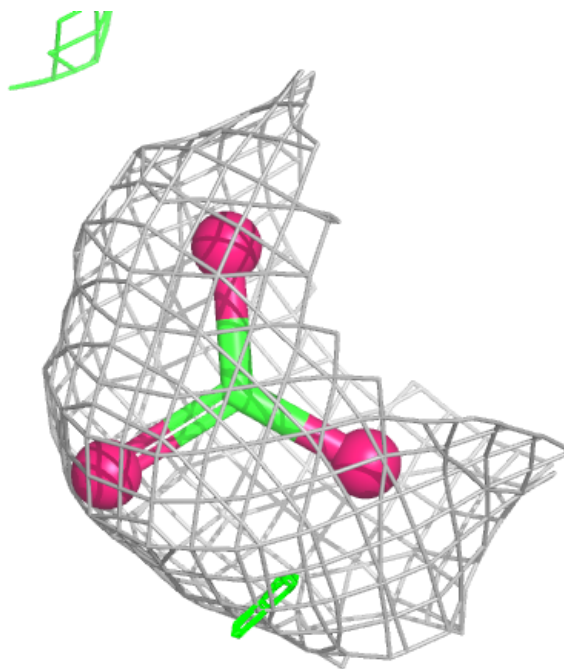
Electron density around BCT D 401 (A):

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



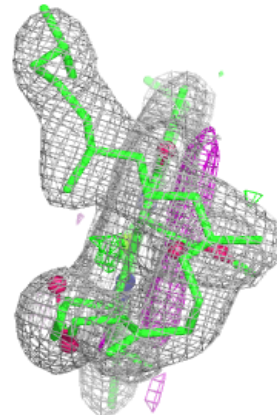
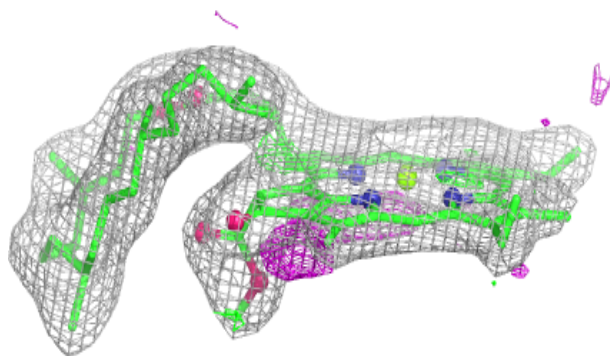
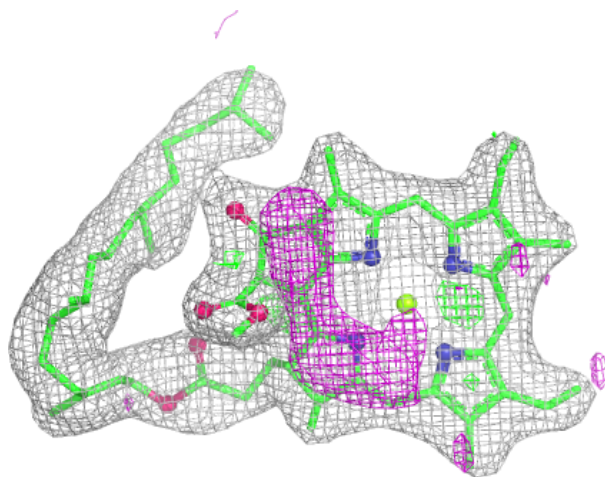
Electron density around BCT D 401 (B):

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



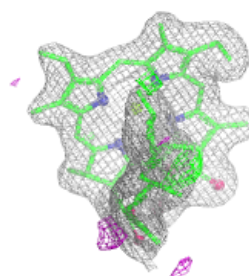
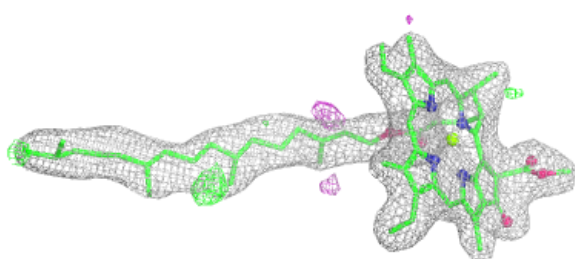
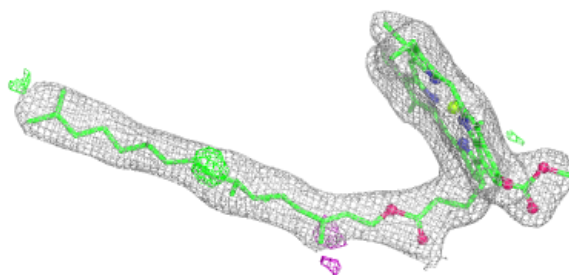
Electron density around CLA B 610:

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

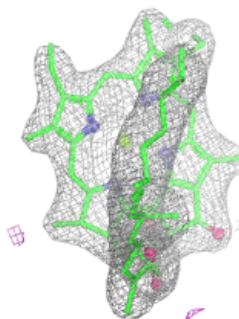
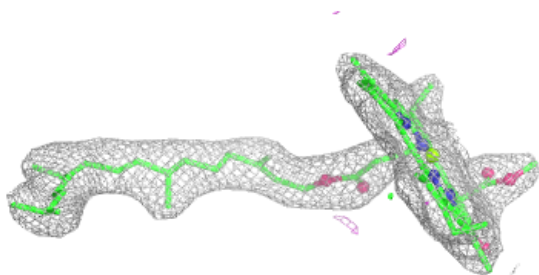
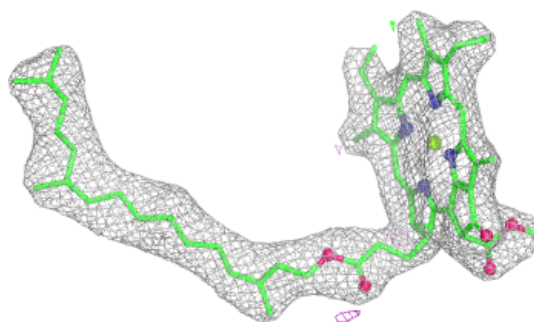


Electron density around CLA b 607:

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

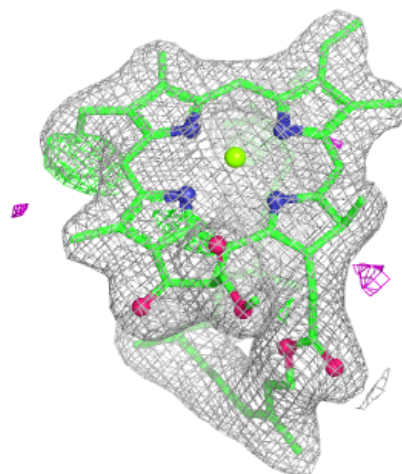
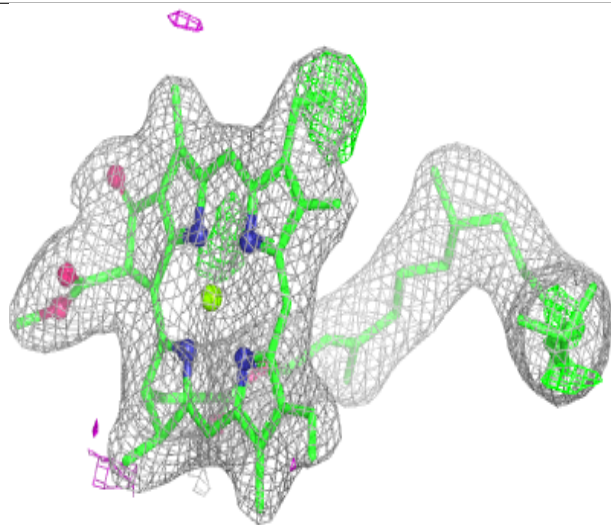
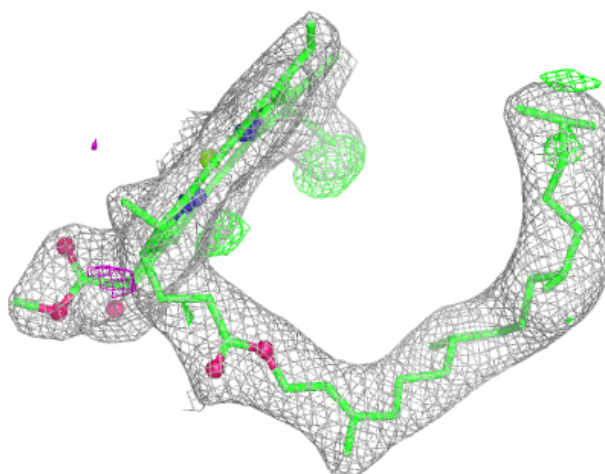
**Electron density around CLA b 609:**

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



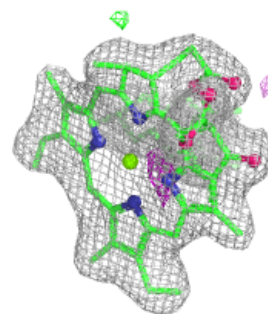
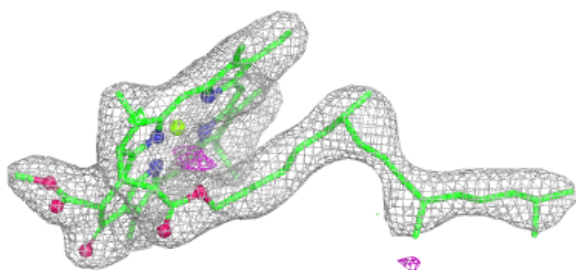
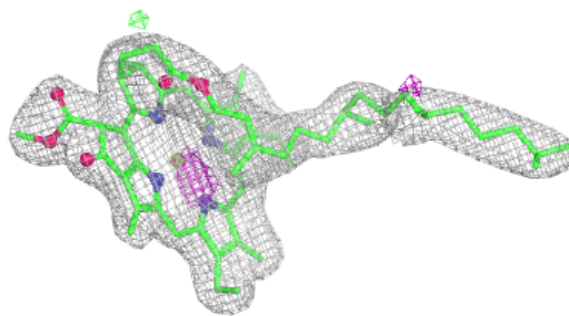
Electron density around CLA b 611:

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



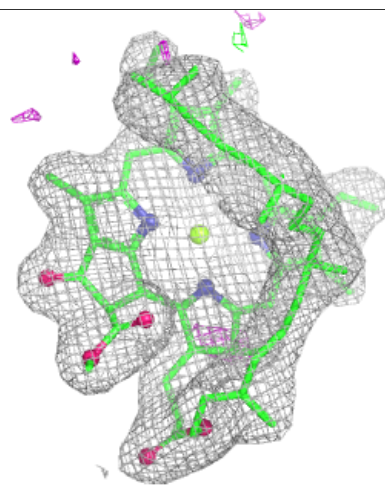
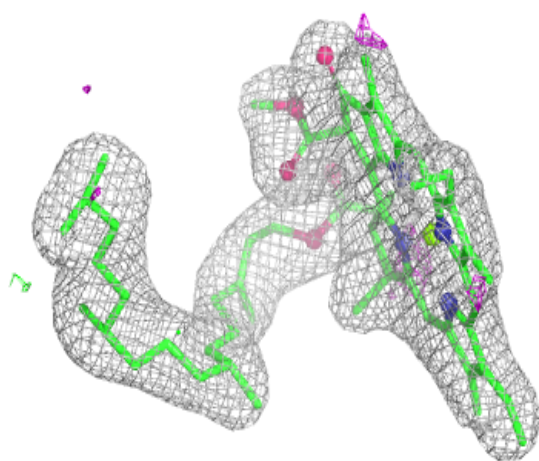
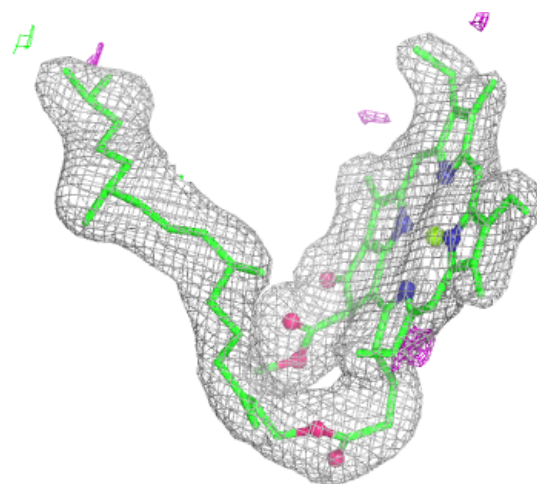
Electron density around CLA C 506:

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



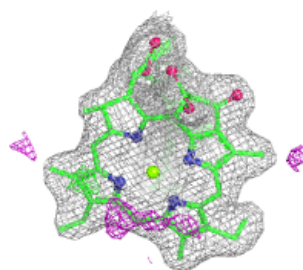
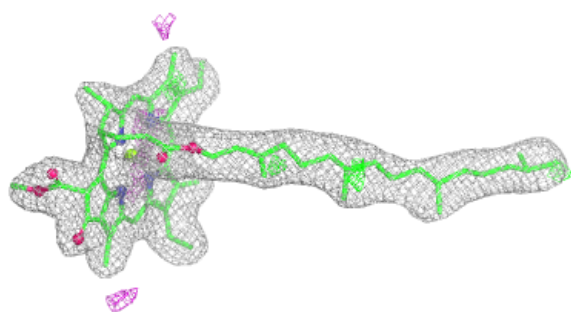
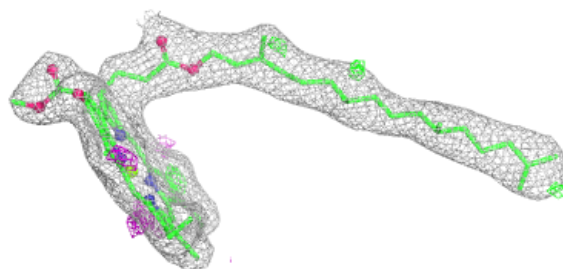
Electron density around CLA b 613:

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



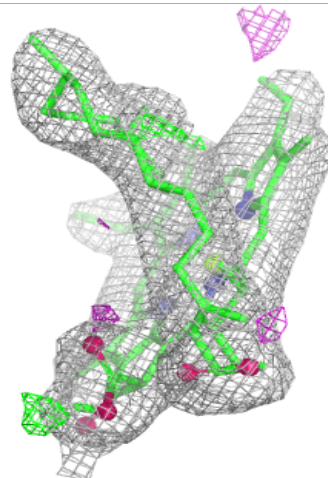
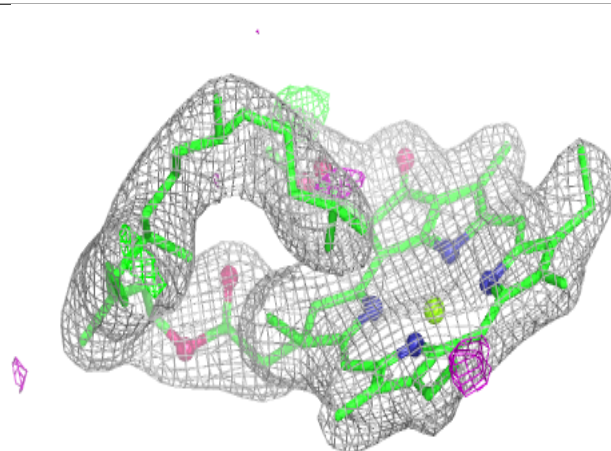
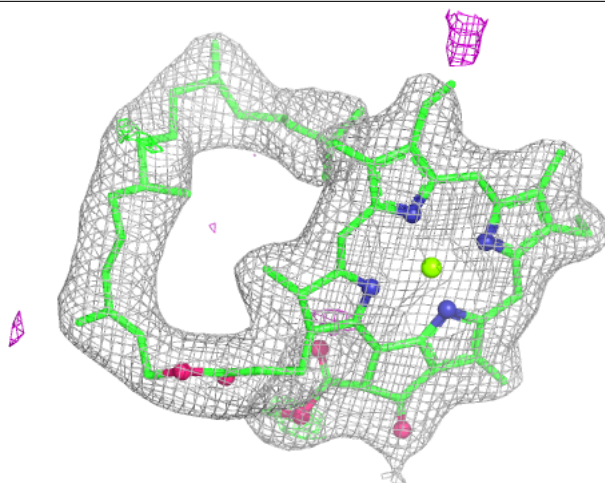
Electron density around CLA B 607:

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



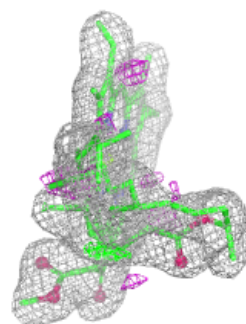
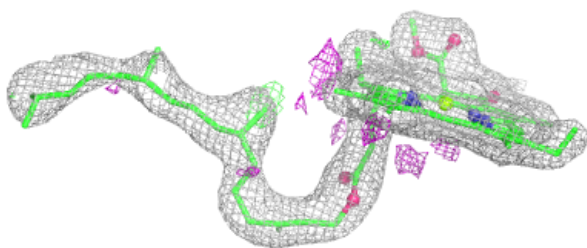
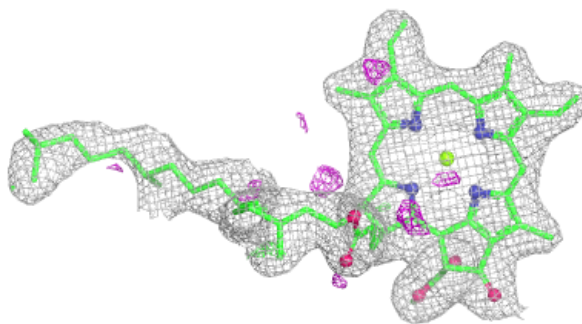
Electron density around CLA b 615:

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



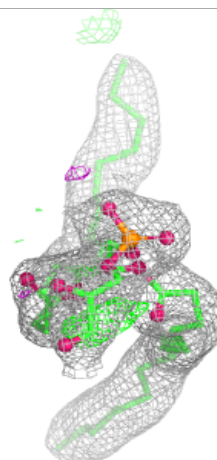
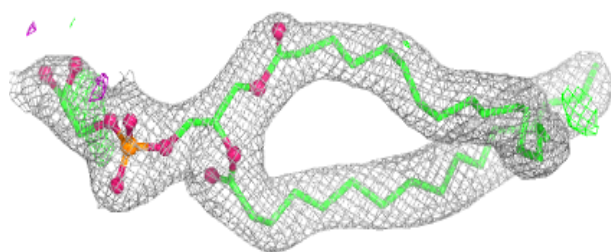
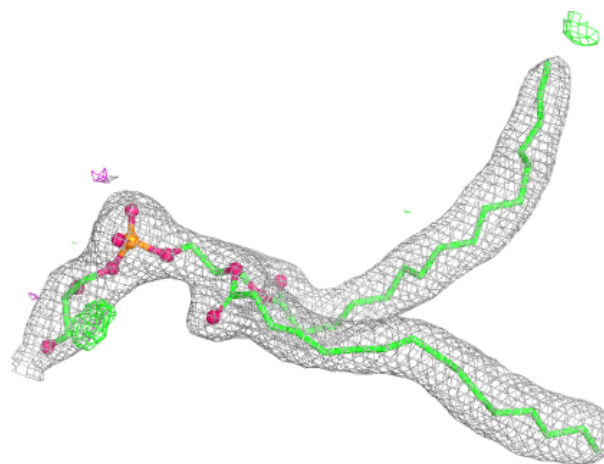
Electron density around CLA A 406 (A):

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



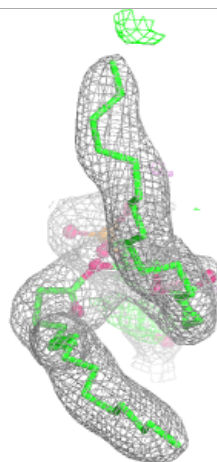
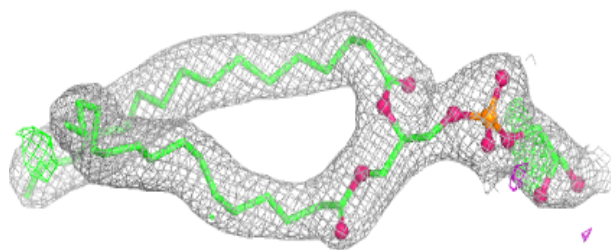
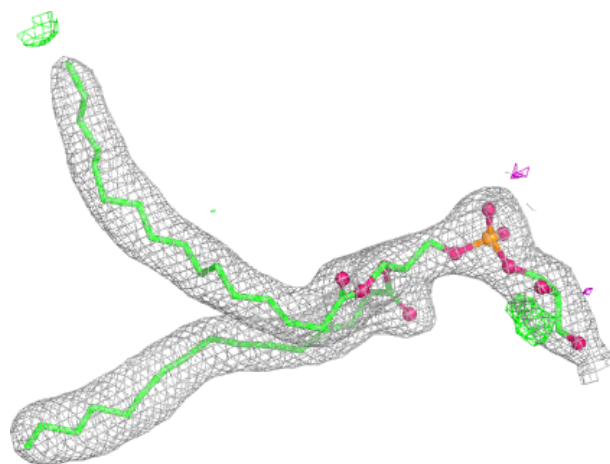
Electron density around LHG D 406 (A):

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



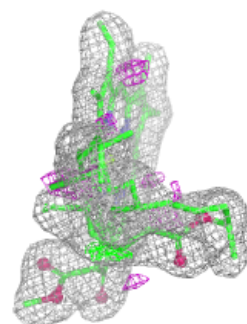
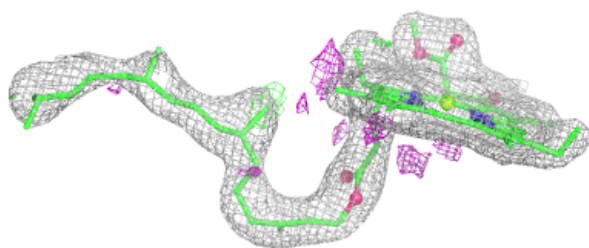
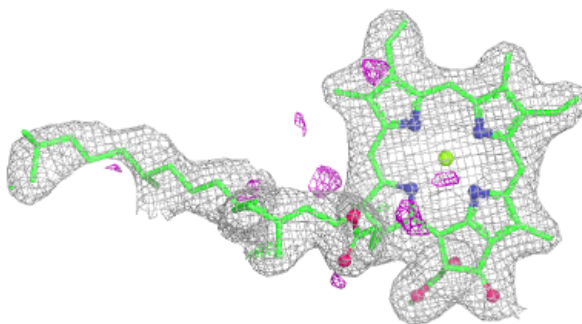
Electron density around LHG D 406 (B):

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



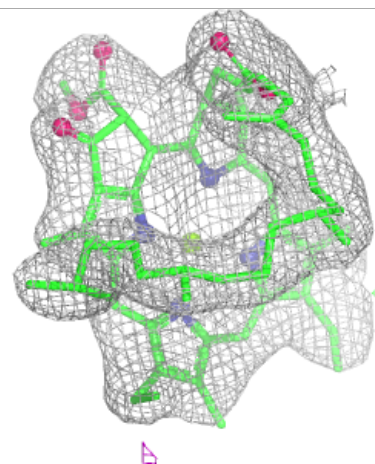
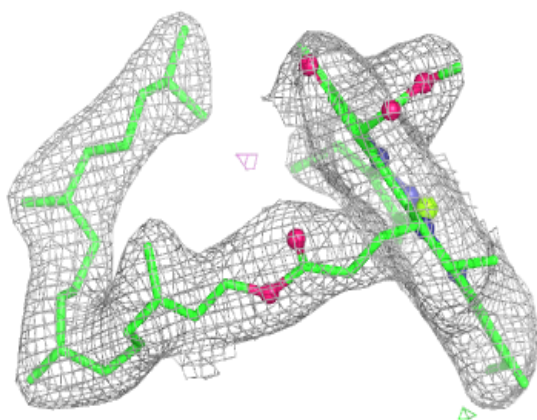
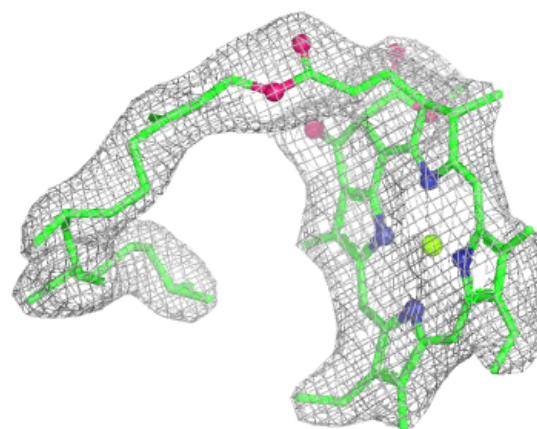
Electron density around CLA A 406 (B):

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



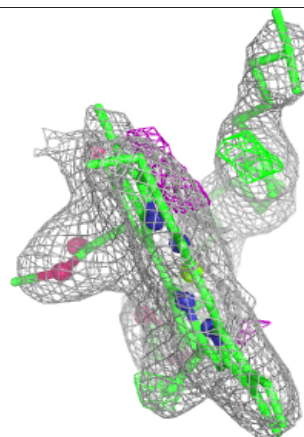
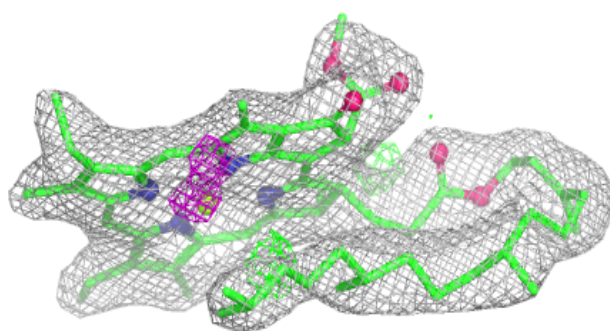
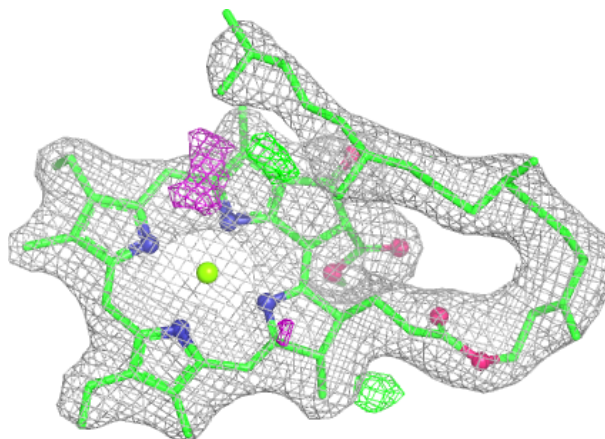
Electron density around CLA c 503:

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



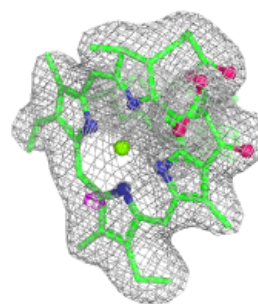
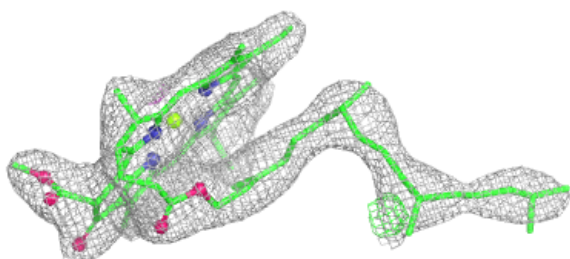
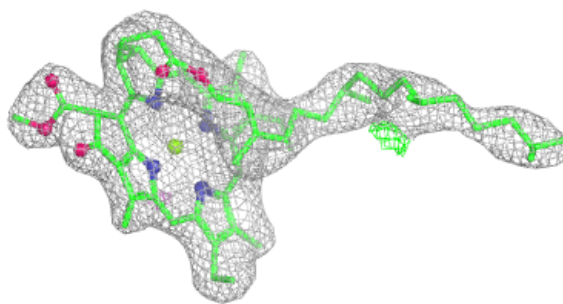
Electron density around CLA C 510:

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



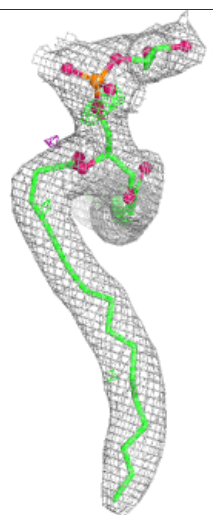
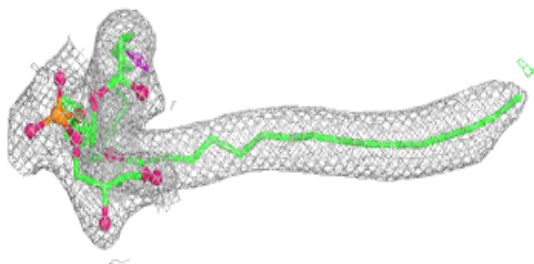
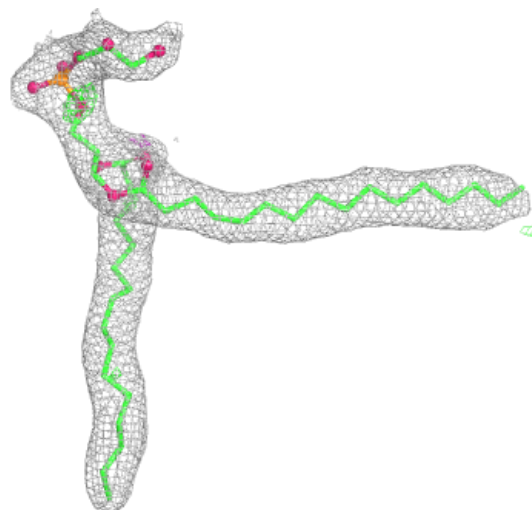
Electron density around CLA c 505:

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



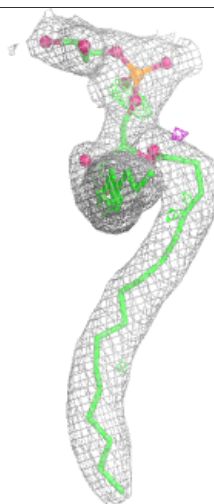
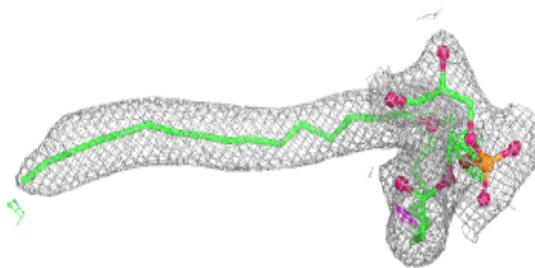
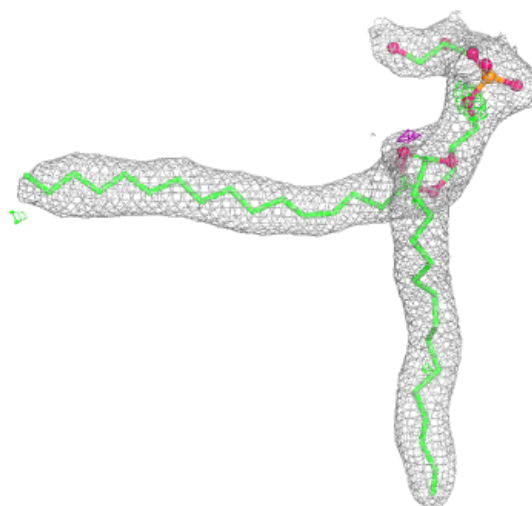
Electron density around LHG L 101 (A):

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



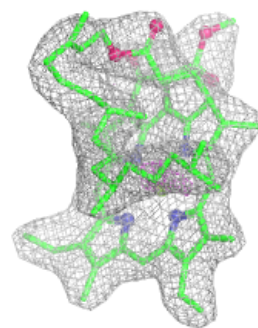
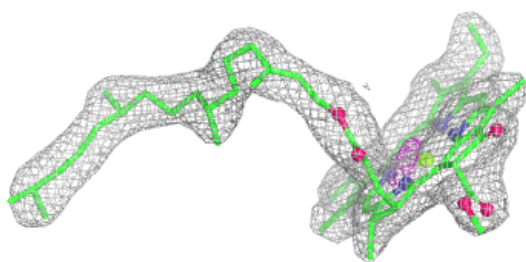
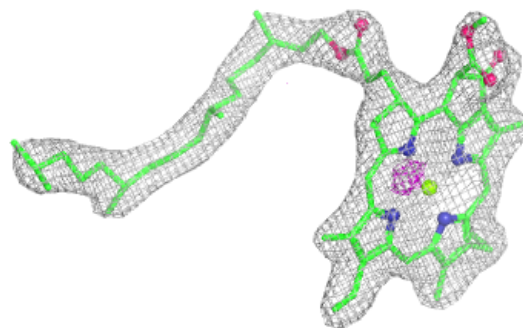
Electron density around LHG L 101 (B):

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



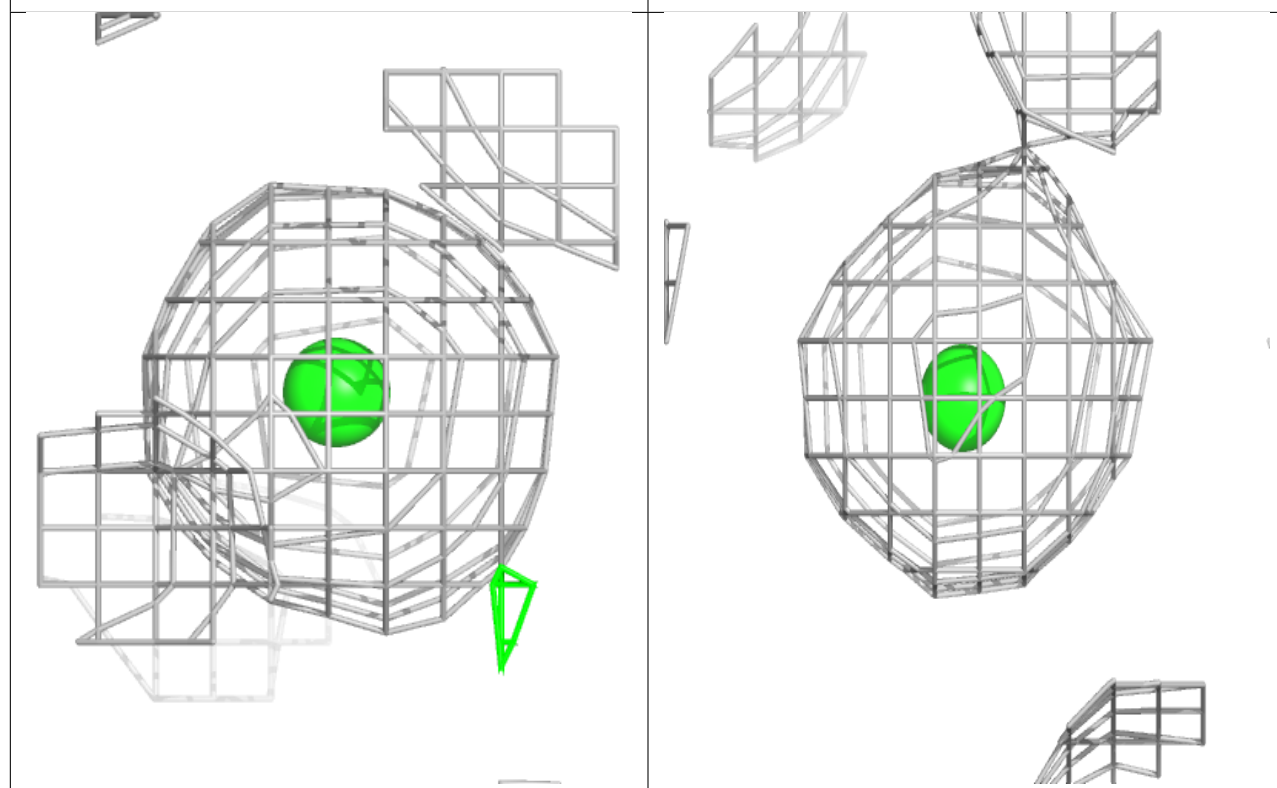
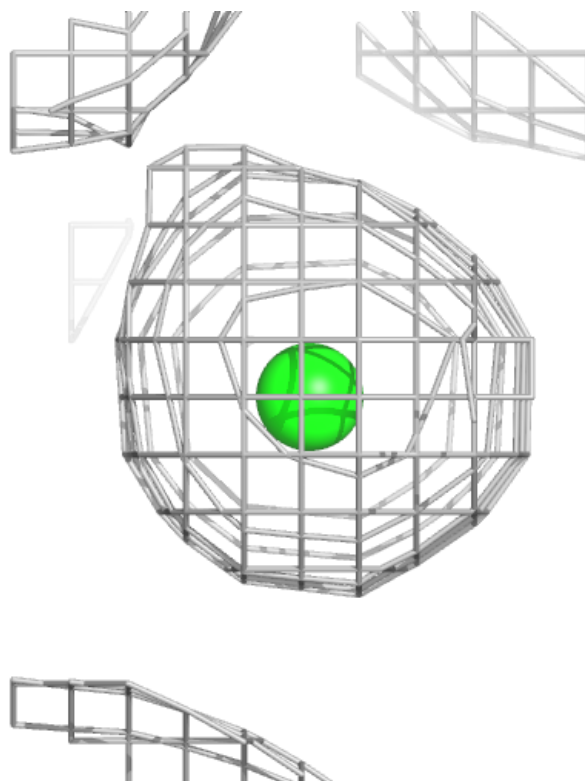
Electron density around CLA C 512:

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



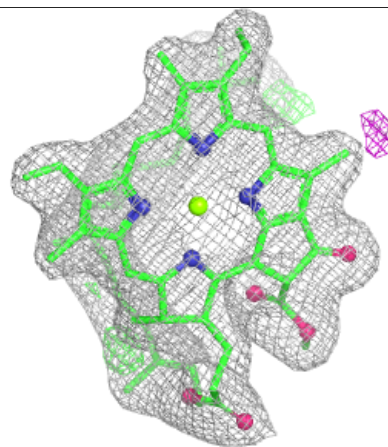
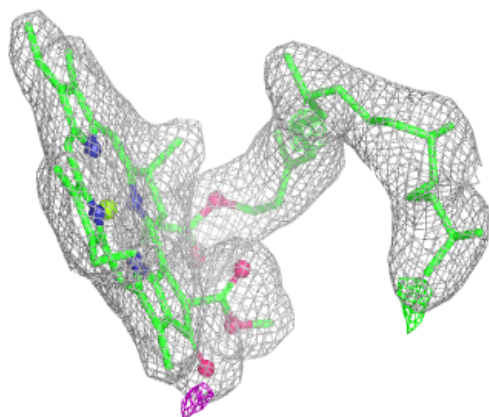
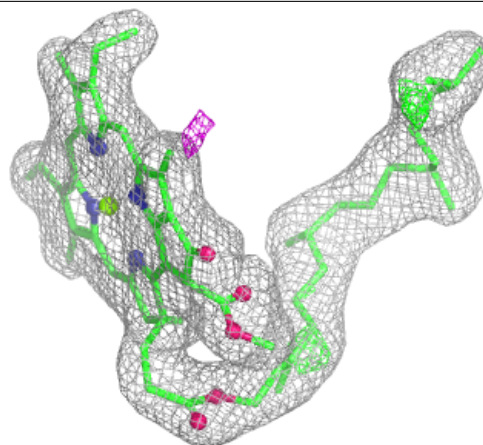
Electron density around CL a 402 (A):

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



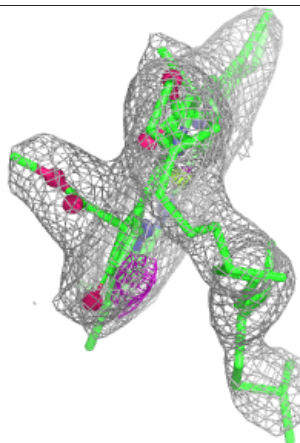
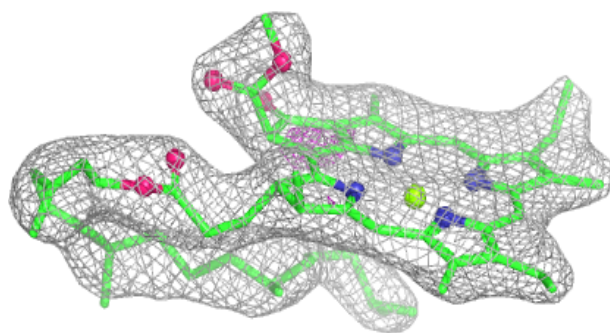
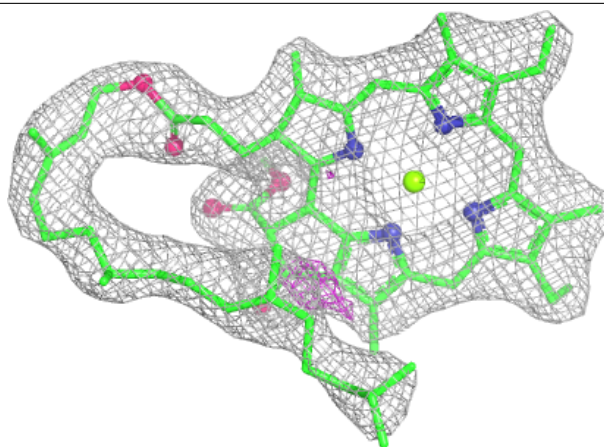
Electron density around CLA B 613:

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



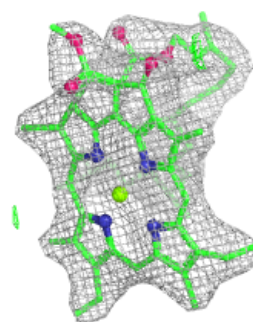
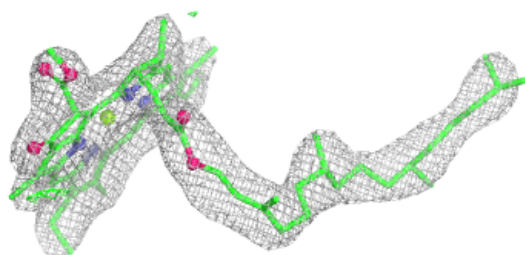
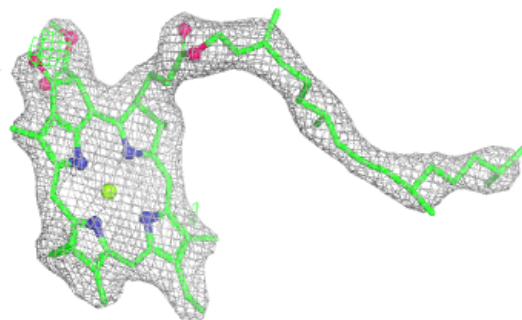
Electron density around CLA c 509:

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



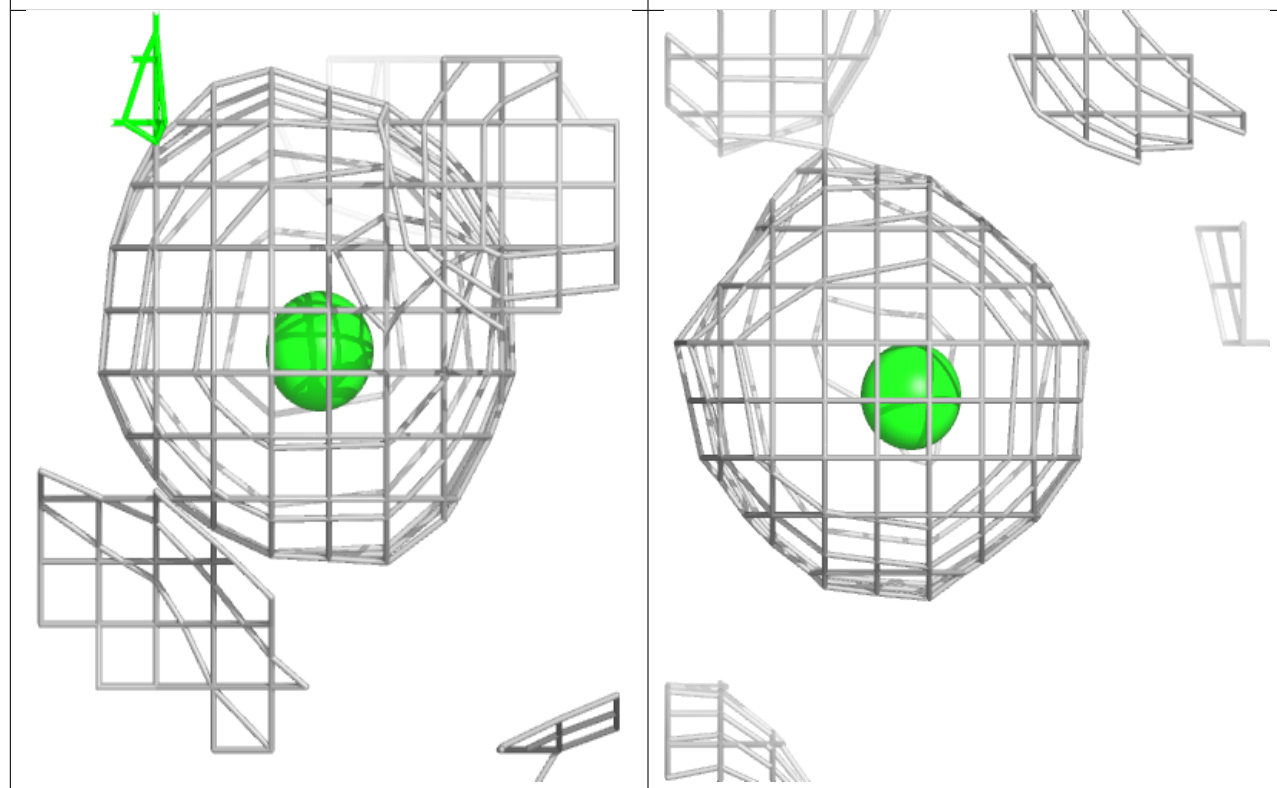
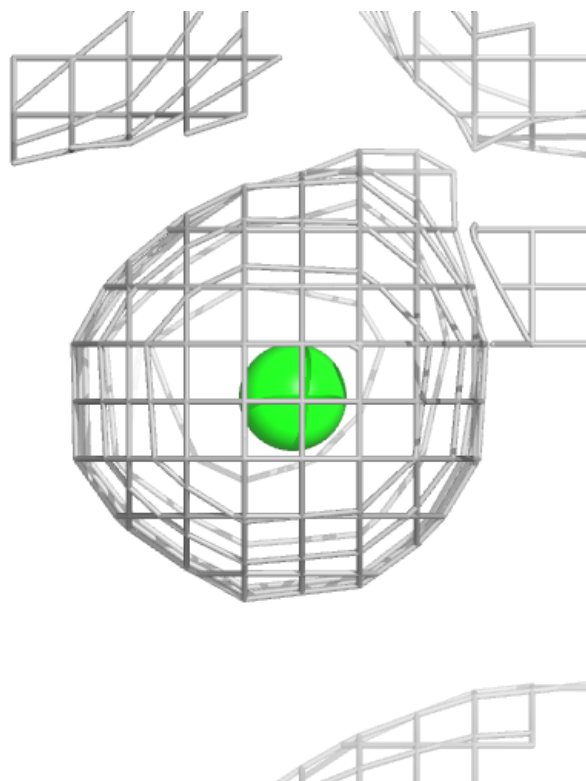
Electron density around CLA c 511:

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



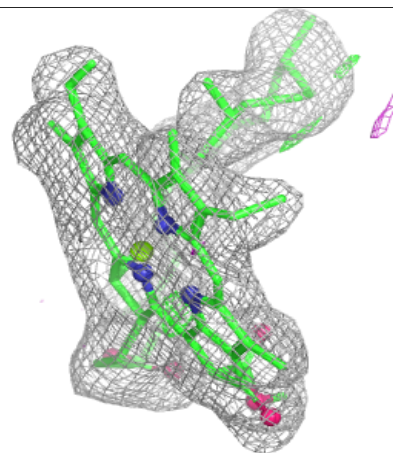
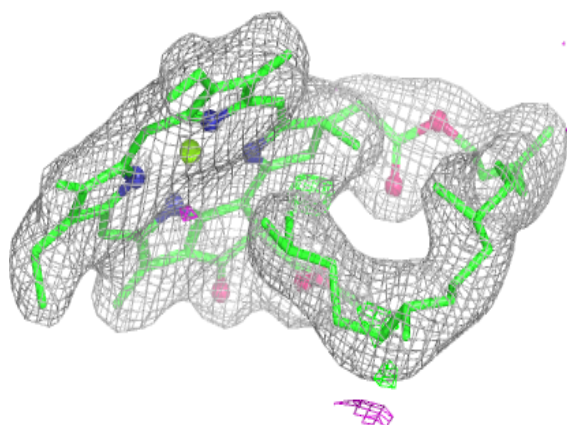
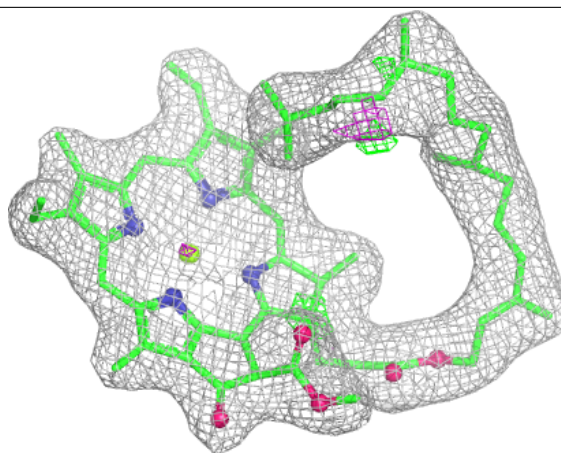
Electron density around CL a 402 (B):

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

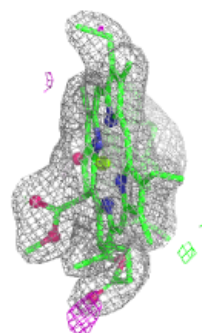
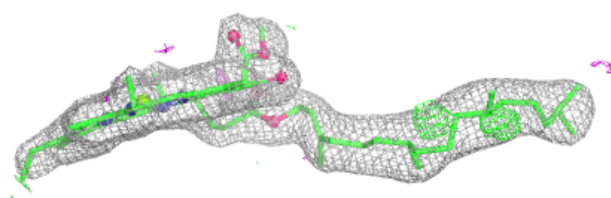
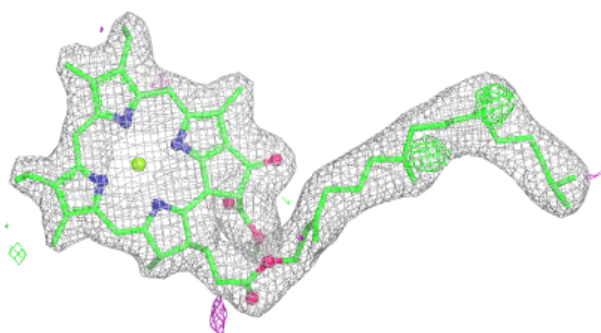


Electron density around CLA B 615:

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

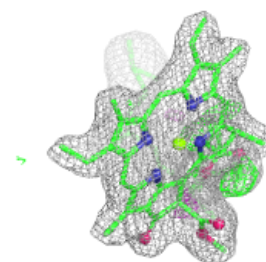
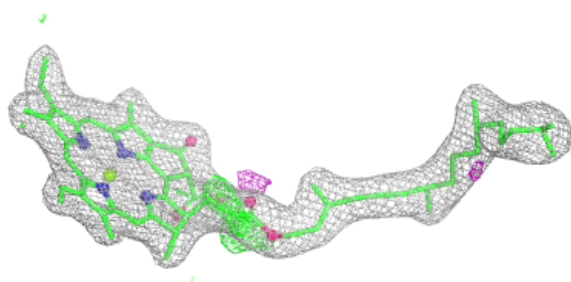
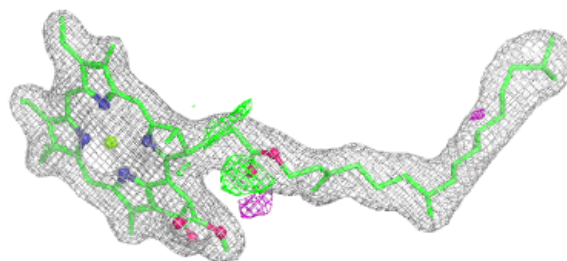
**Electron density around CLA B 602:**

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



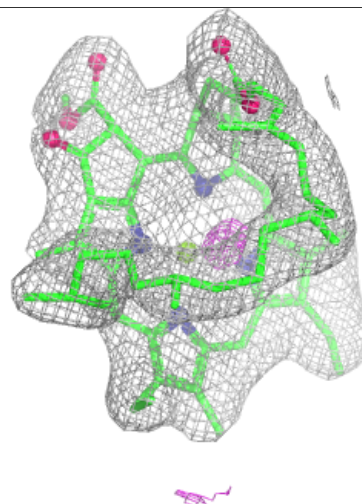
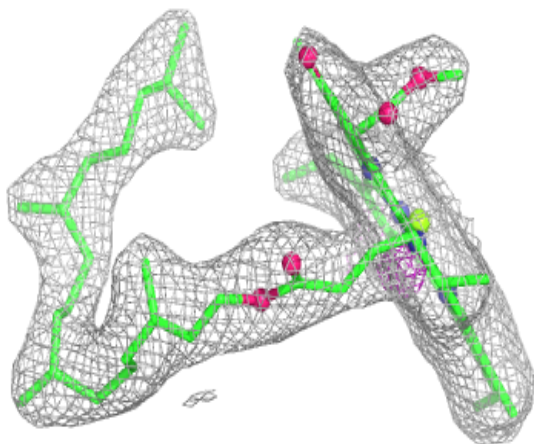
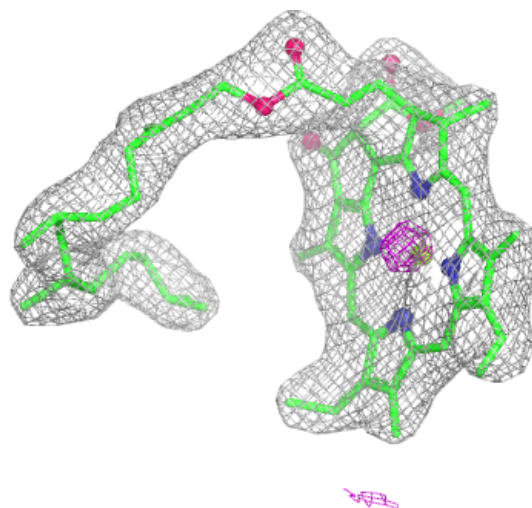
Electron density around CLA A 404 (A):

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



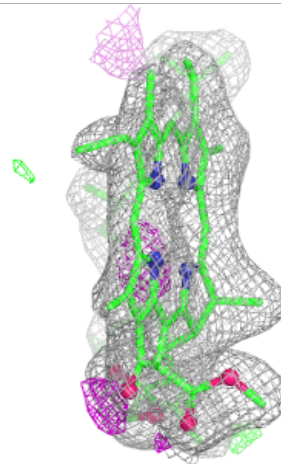
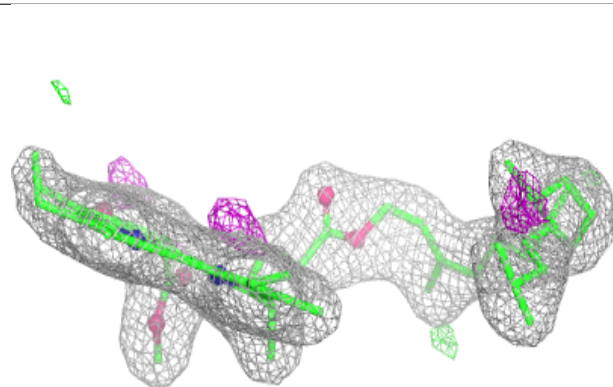
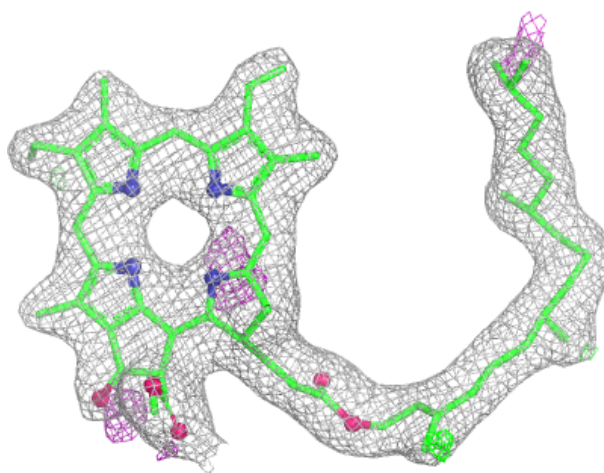
Electron density around CLA C 504:

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



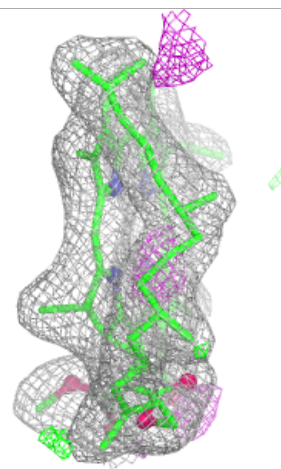
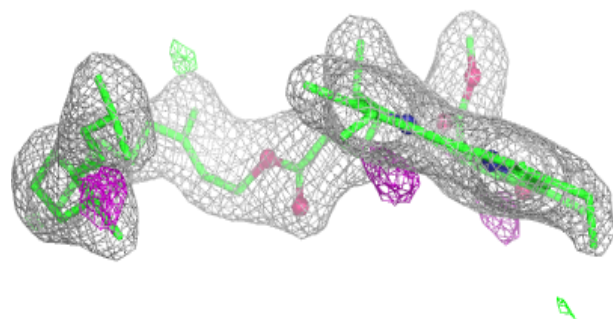
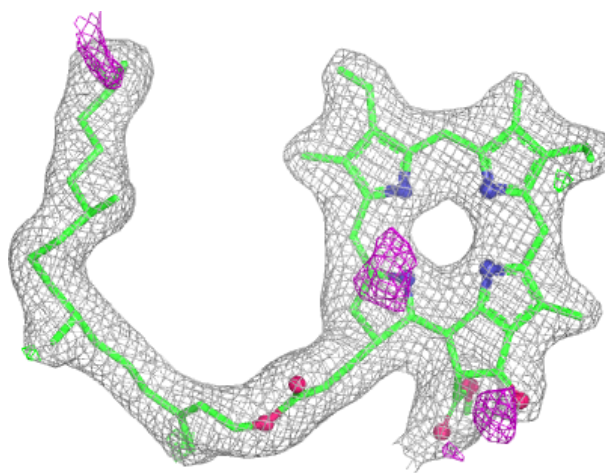
Electron density around PHO a 406 (A):

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



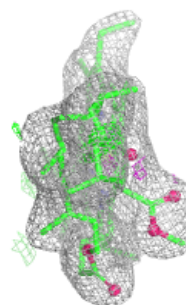
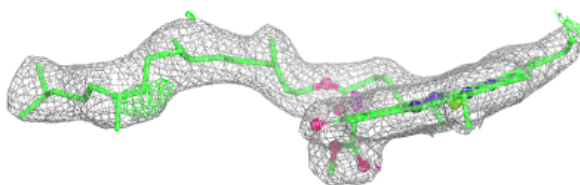
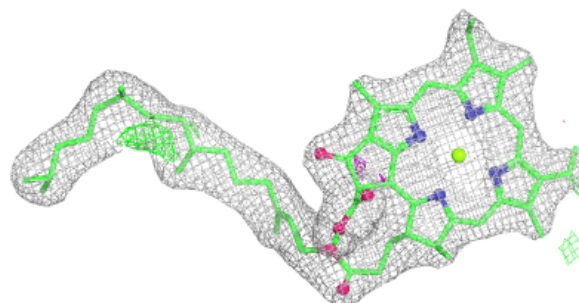
Electron density around PHO a 406 (B):

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

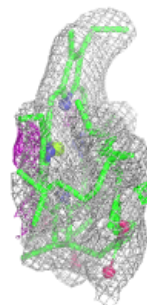
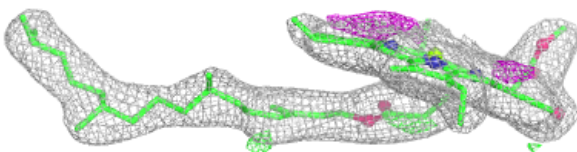
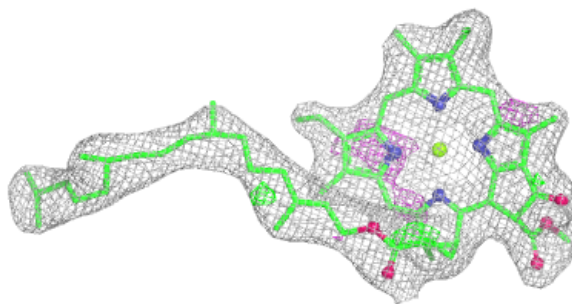


Electron density around CLA b 602:

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

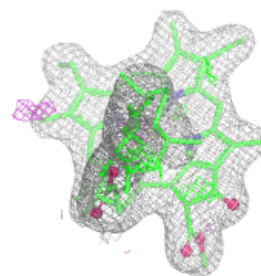
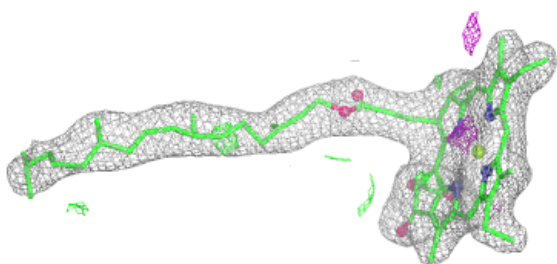
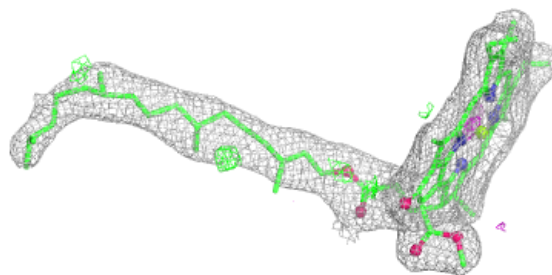
**Electron density around CLA b 603:**

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

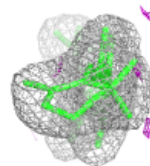
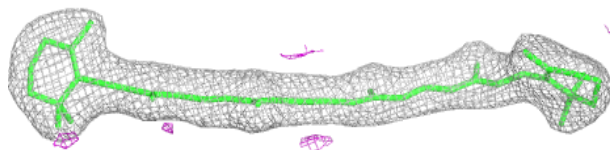
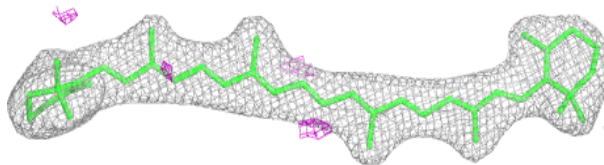


Electron density around CLA b 604:

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

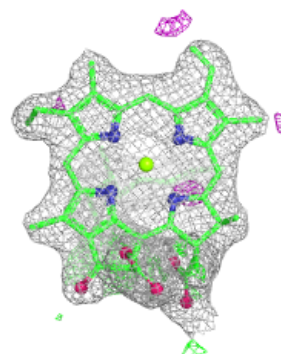
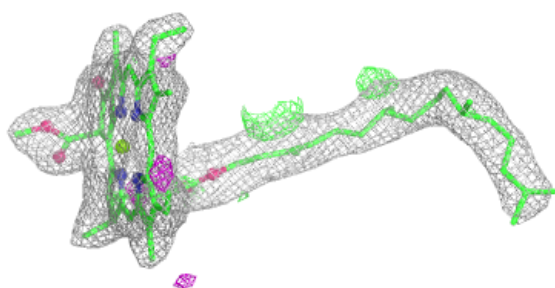
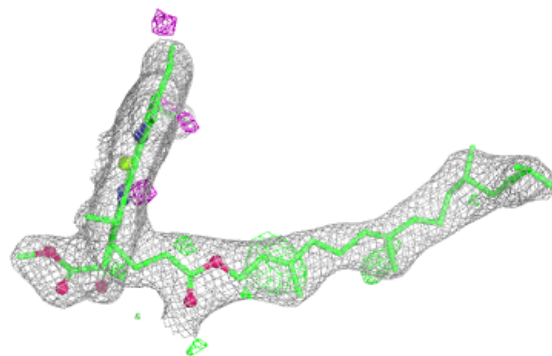
**Electron density around BCR B 617:**

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

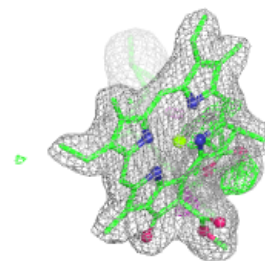
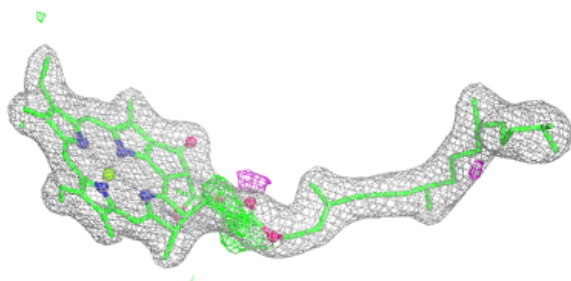
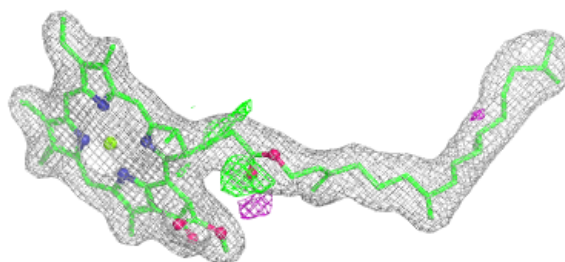


Electron density around CLA b 605:

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

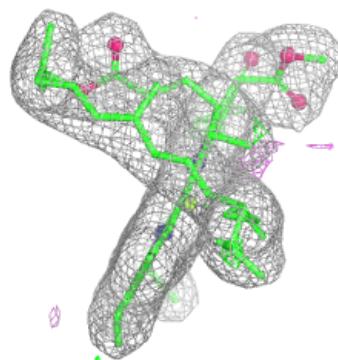
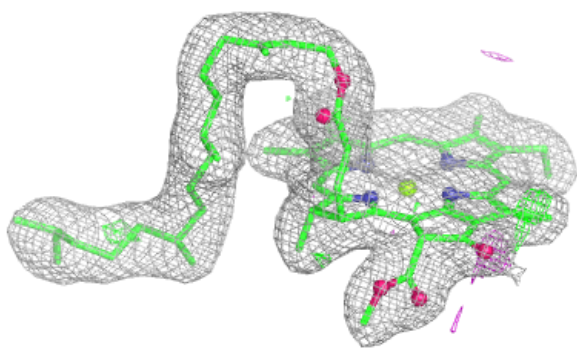
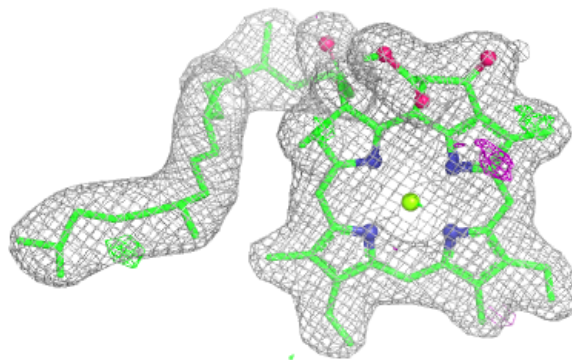
**Electron density around CLA A 404 (B):**

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

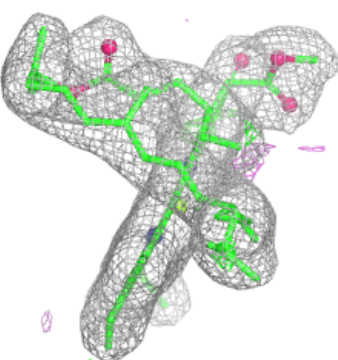
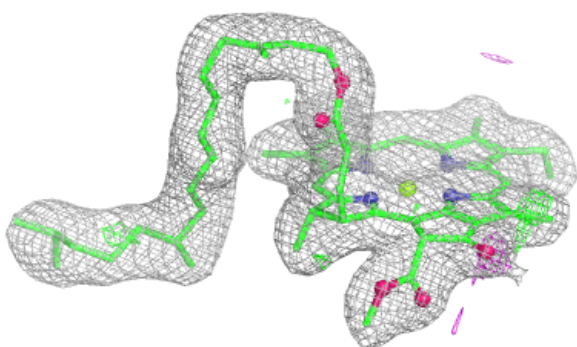
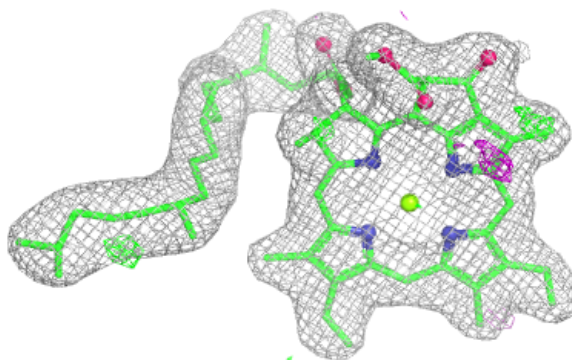


Electron density around CLA A 405 (A):

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

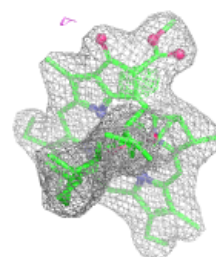
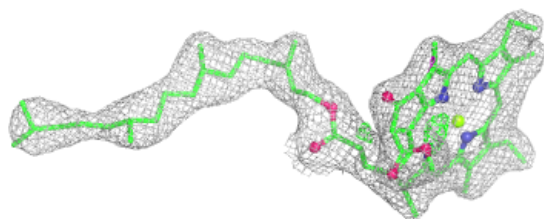
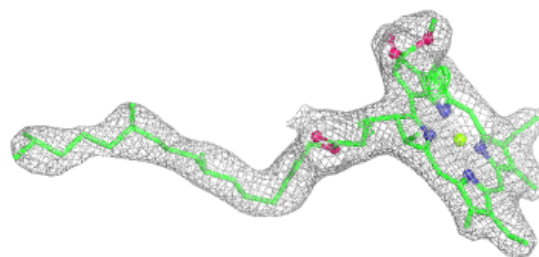
**Electron density around CLA A 405 (B):**

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

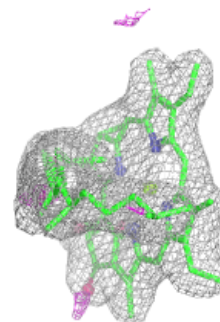
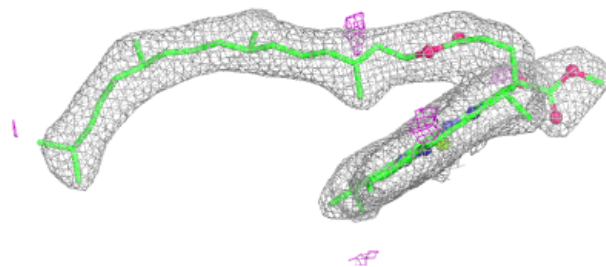
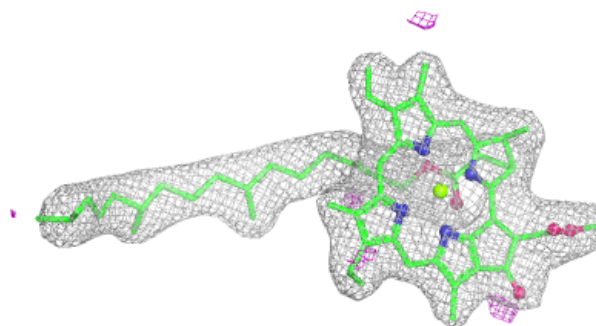


Electron density around CLA c 502:

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

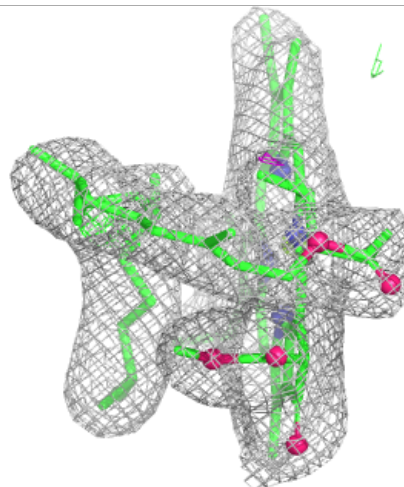
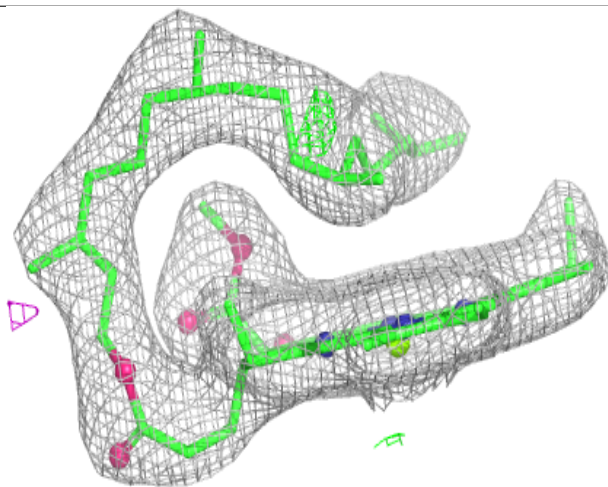
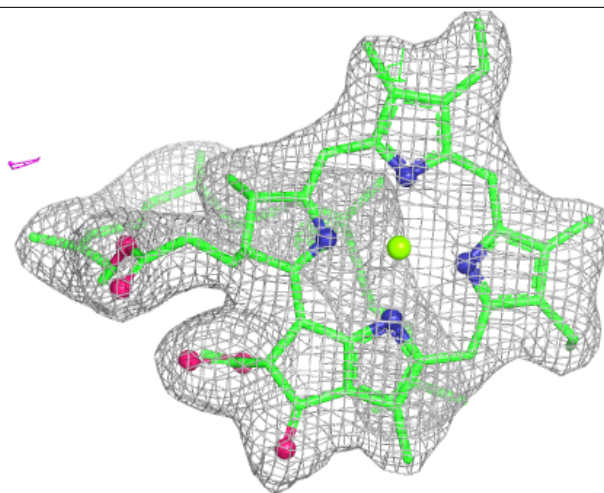
**Electron density around CLA B 608:**

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



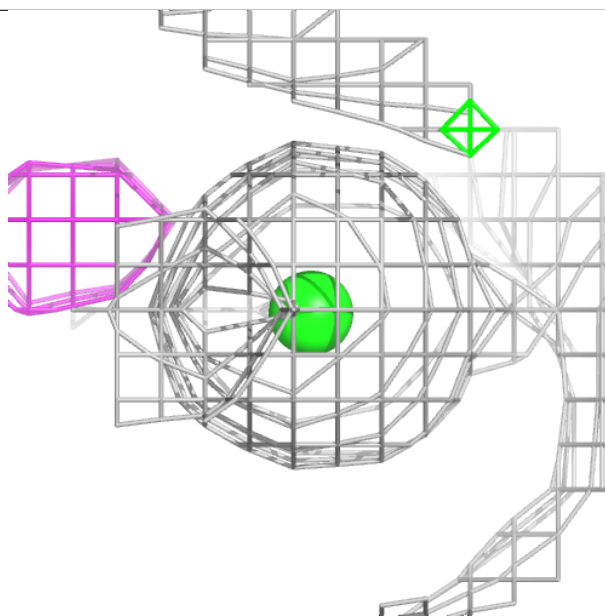
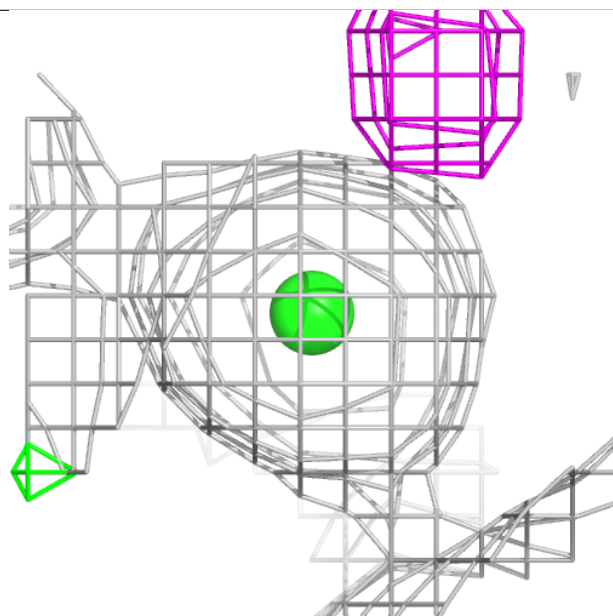
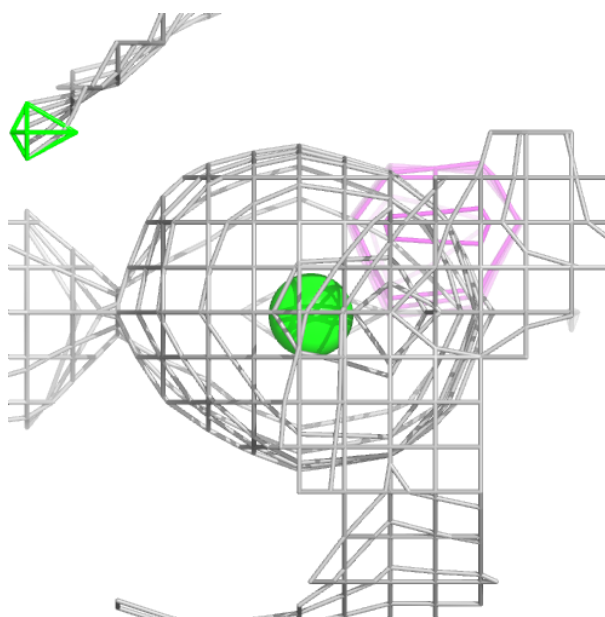
Electron density around CLA C 511:

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



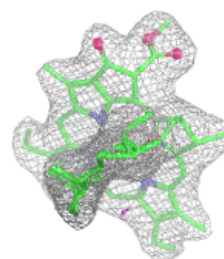
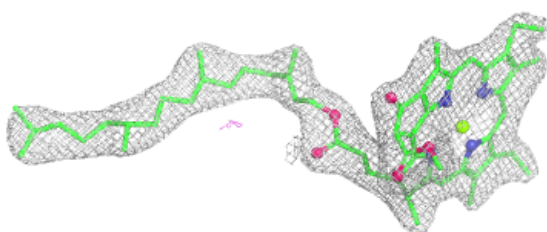
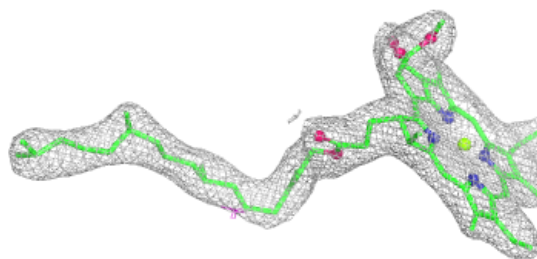
Electron density around CL a 403 (A):

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



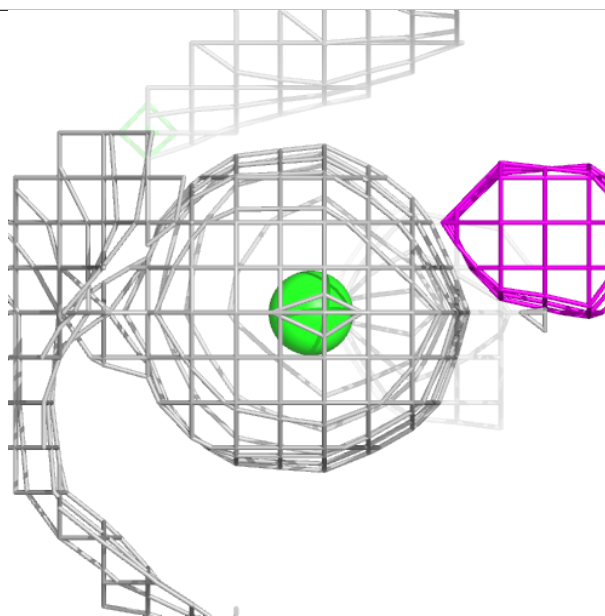
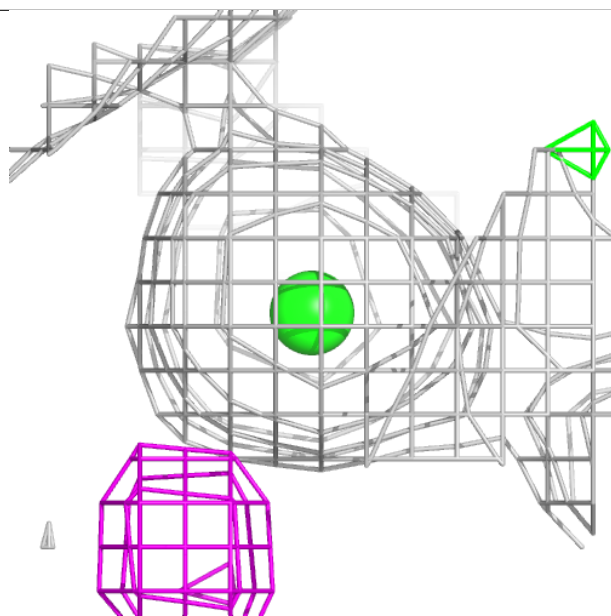
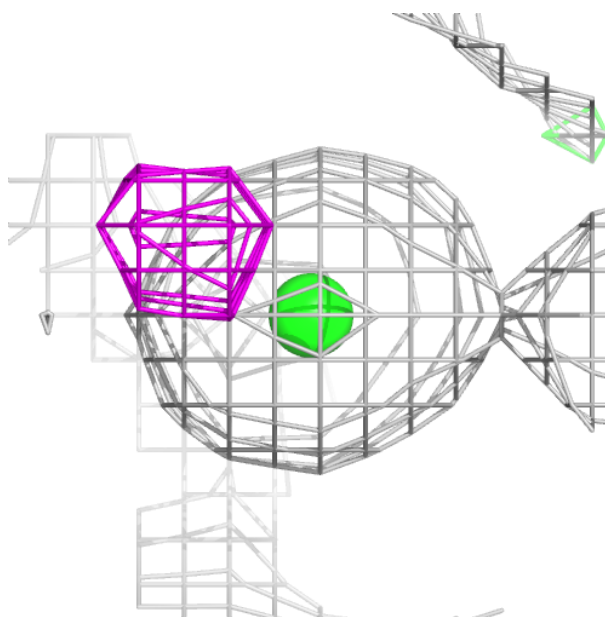
Electron density around CLA C 503:

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



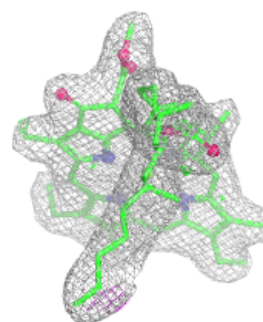
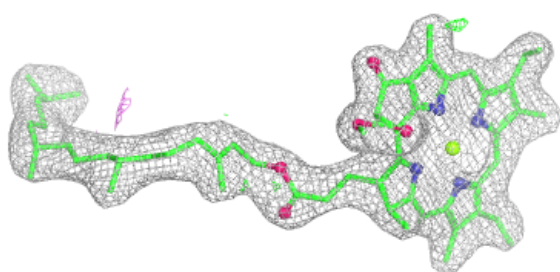
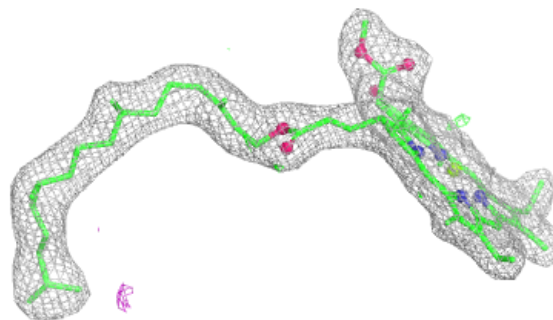
Electron density around CL a 403 (B):

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

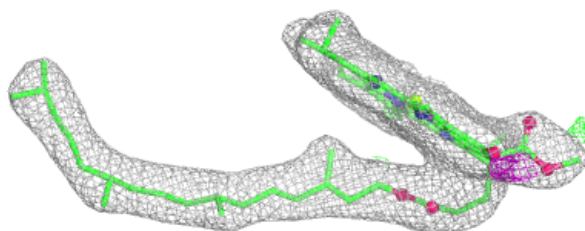
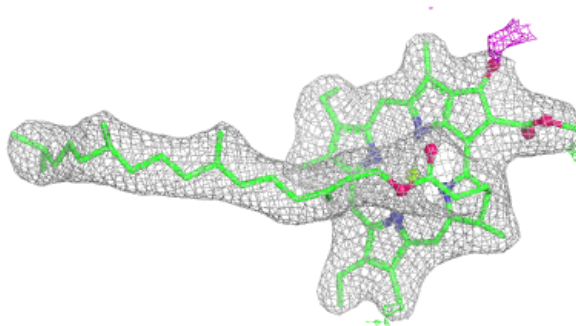


Electron density around CLA D 402 (A):

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

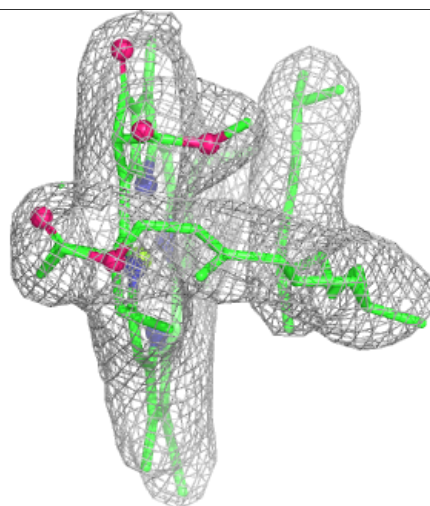
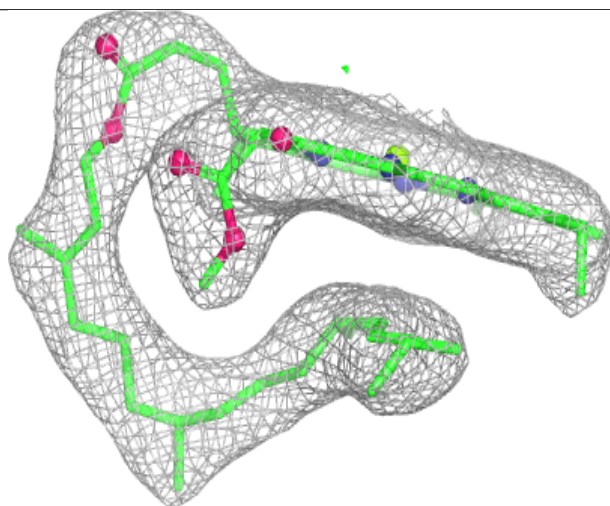
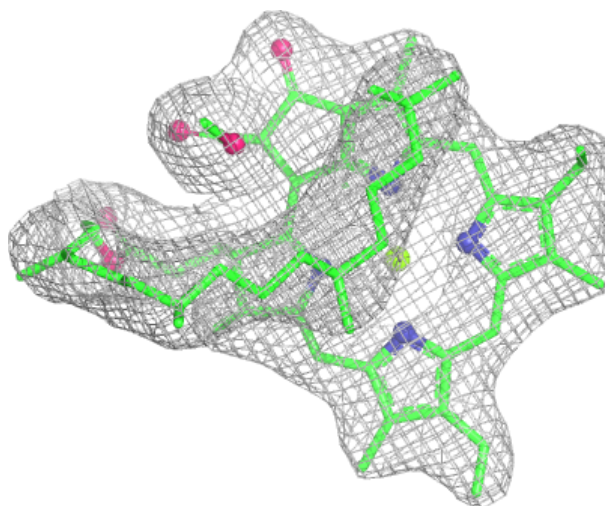
**Electron density around CLA b 608:**

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



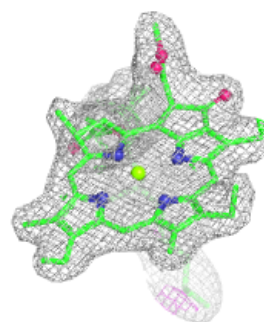
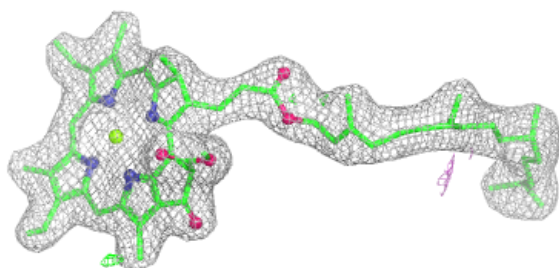
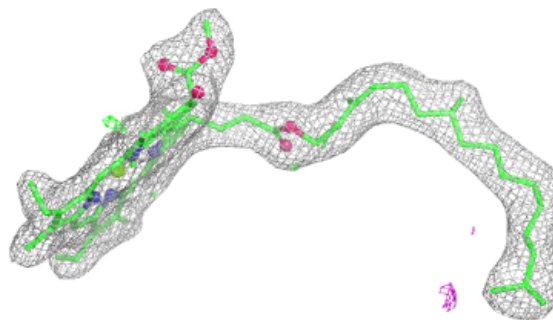
Electron density around CLA c 510:

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

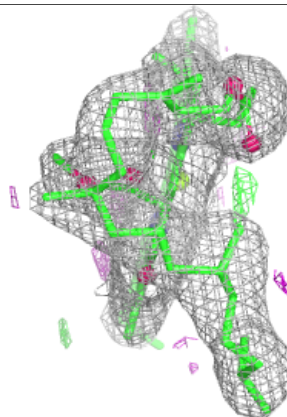
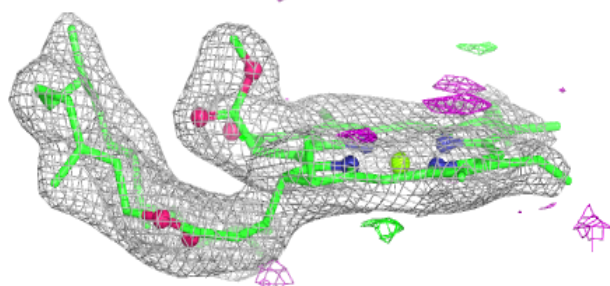
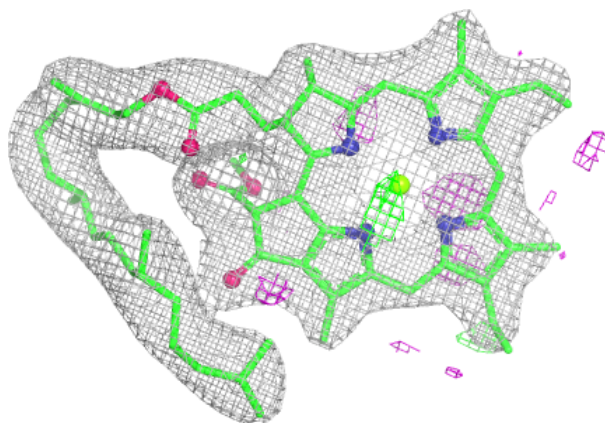


Electron density around CLA D 402 (B):

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

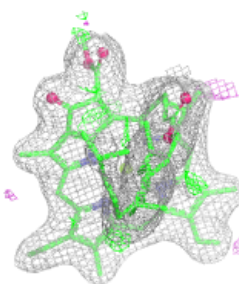
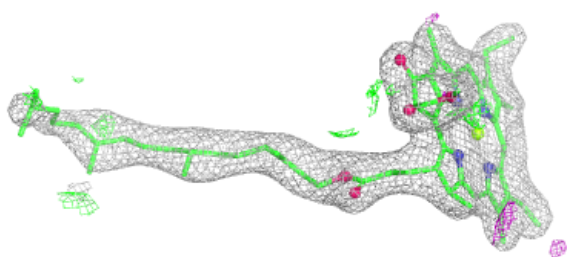
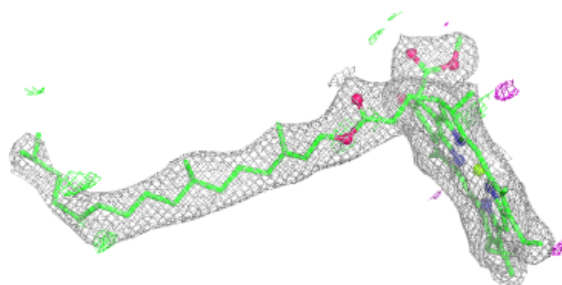
**Electron density around CLA b 610:**

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

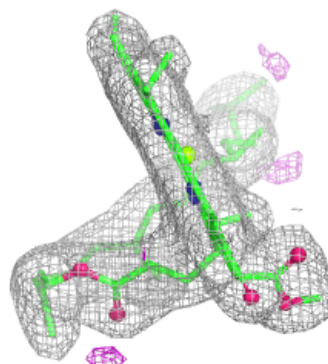
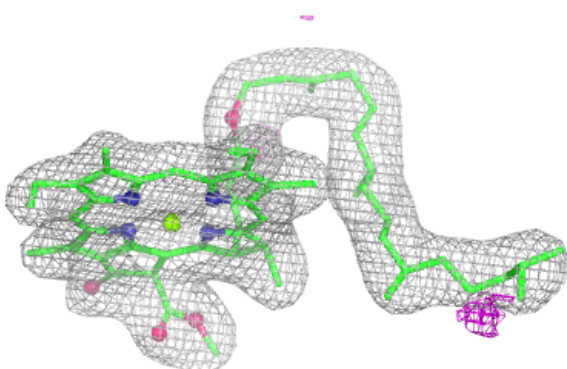
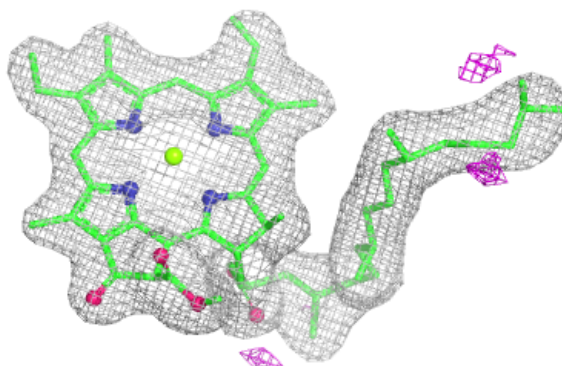


Electron density around CLA B 604:

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

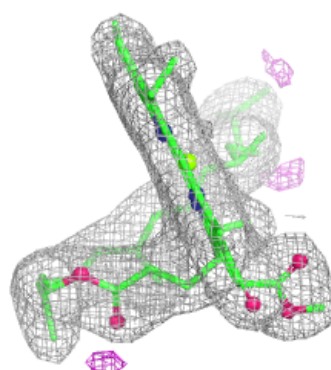
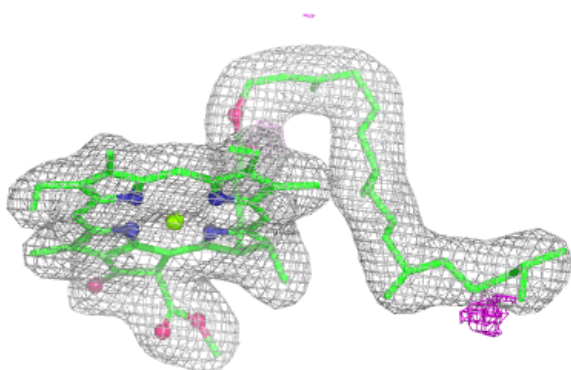
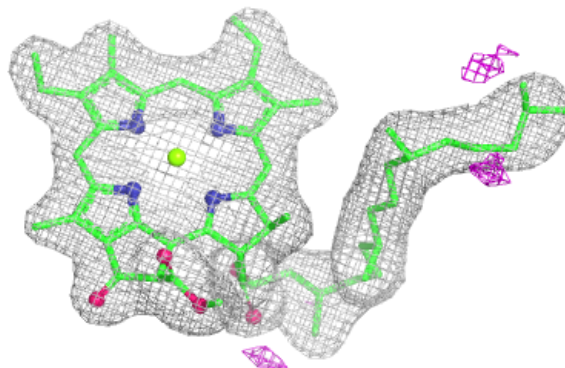
**Electron density around CLA d 402 (A):**

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

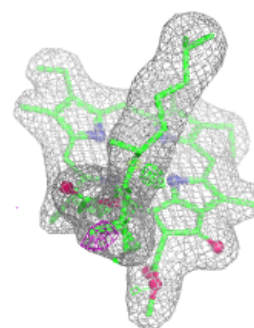
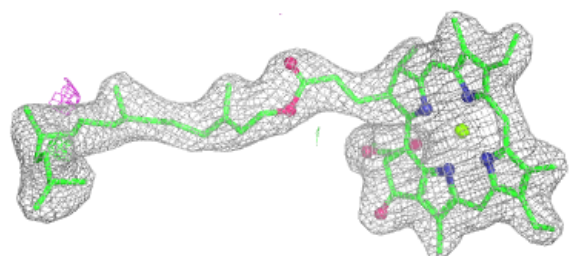
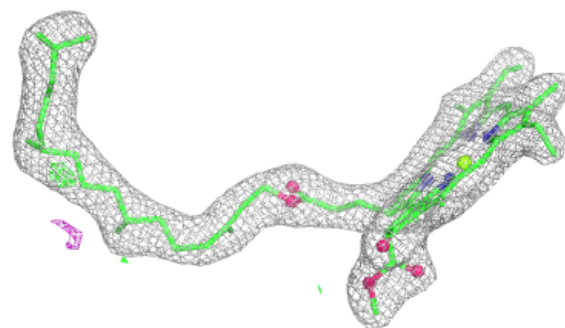


Electron density around CLA d 402 (B):

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

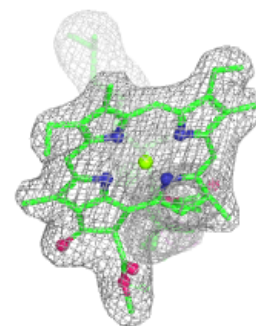
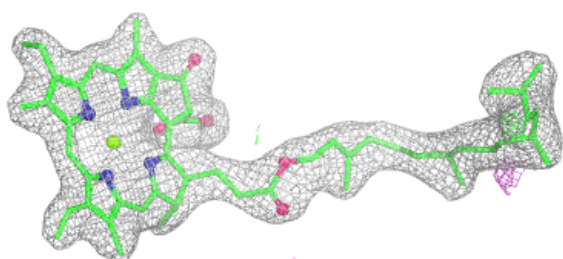
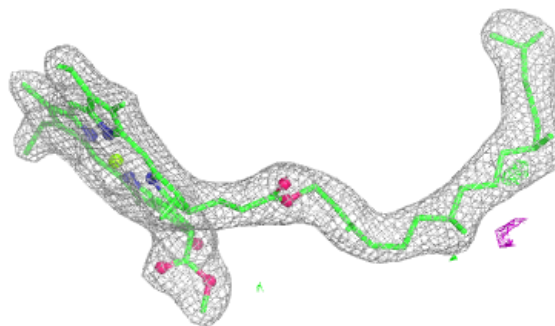
**Electron density around CLA d 403 (A):**

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

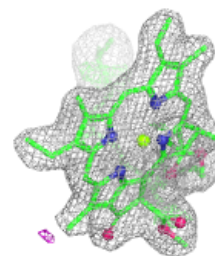
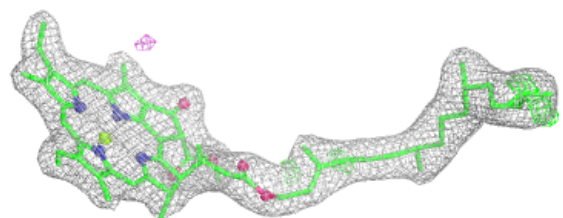
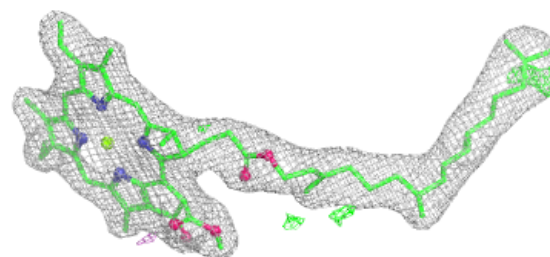


Electron density around CLA d 403 (B):

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

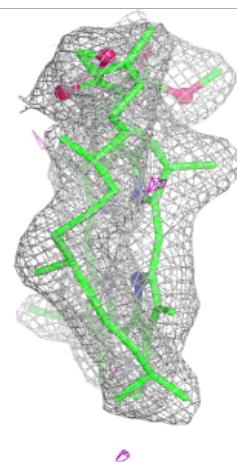
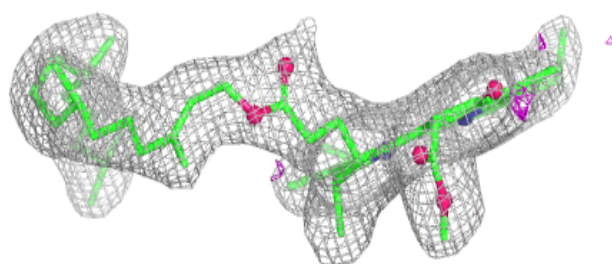
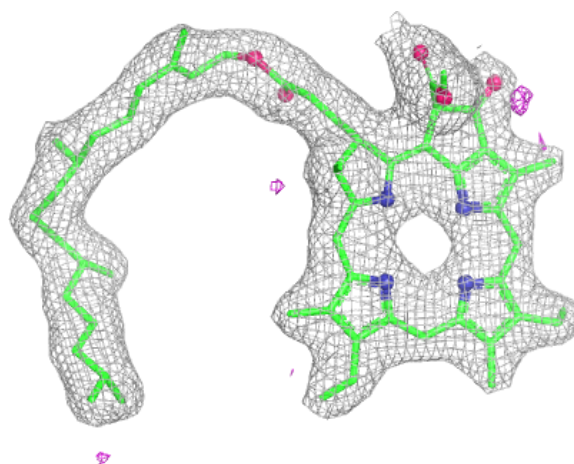
**Electron density around CLA a 404 (A):**

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



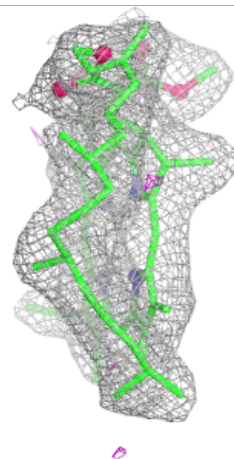
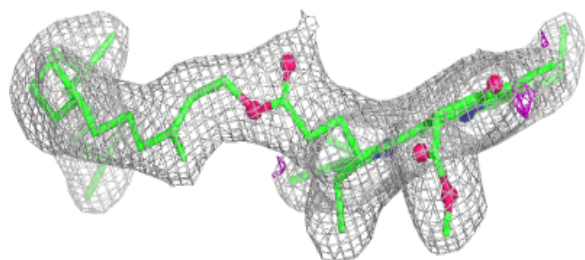
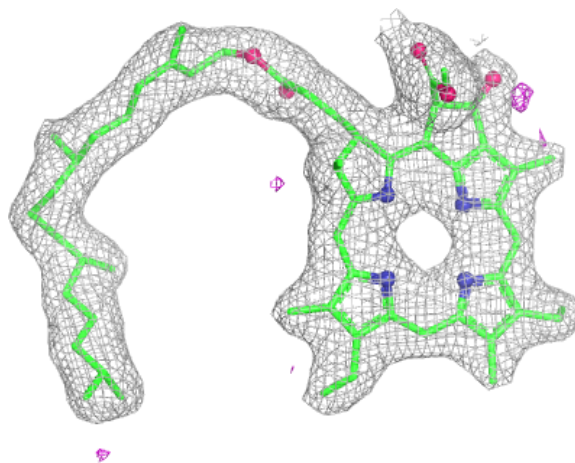
Electron density around PHO A 407 (A):

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



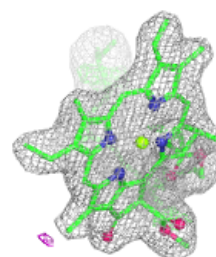
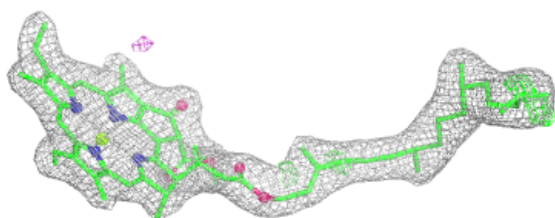
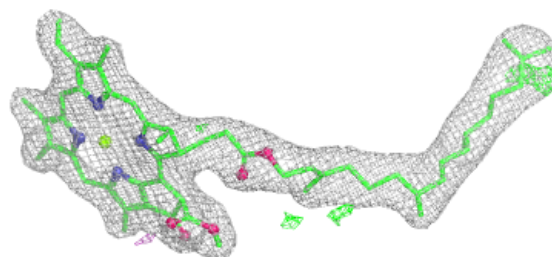
Electron density around PHO A 407 (B):

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

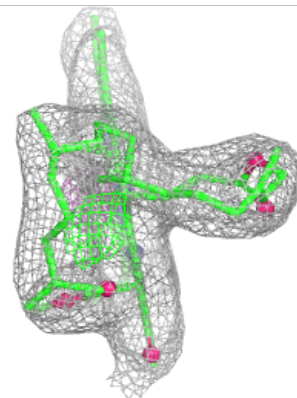
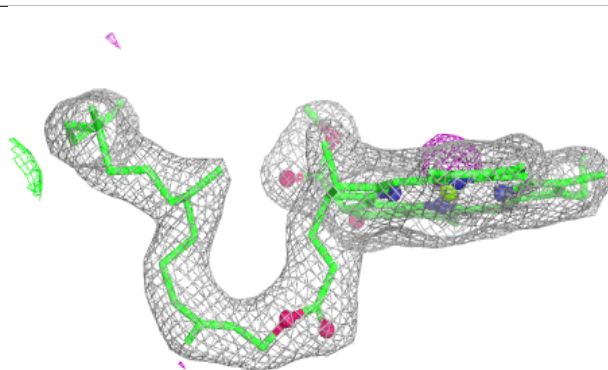
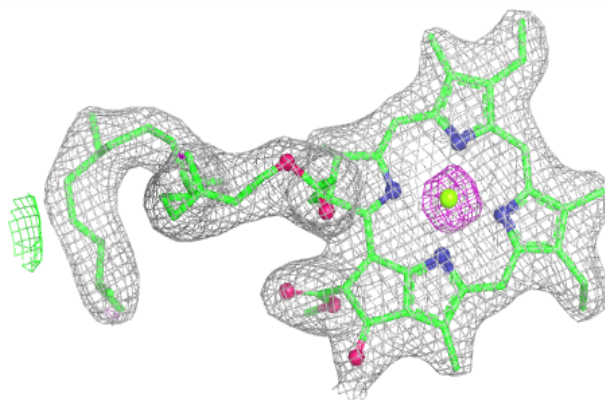


Electron density around CLA a 404 (B):

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

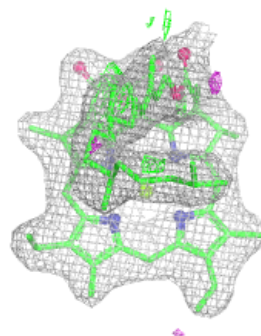
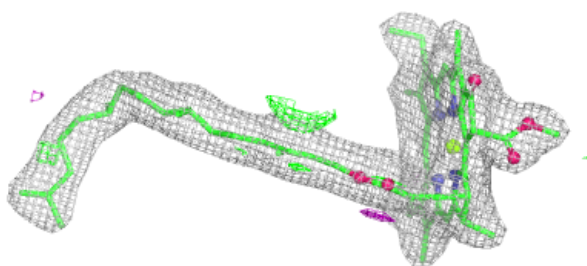
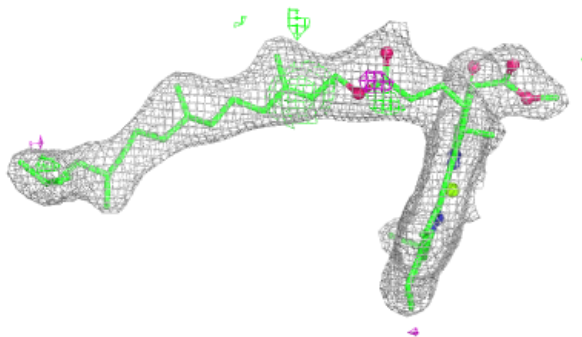
**Electron density around CLA B 612:**

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



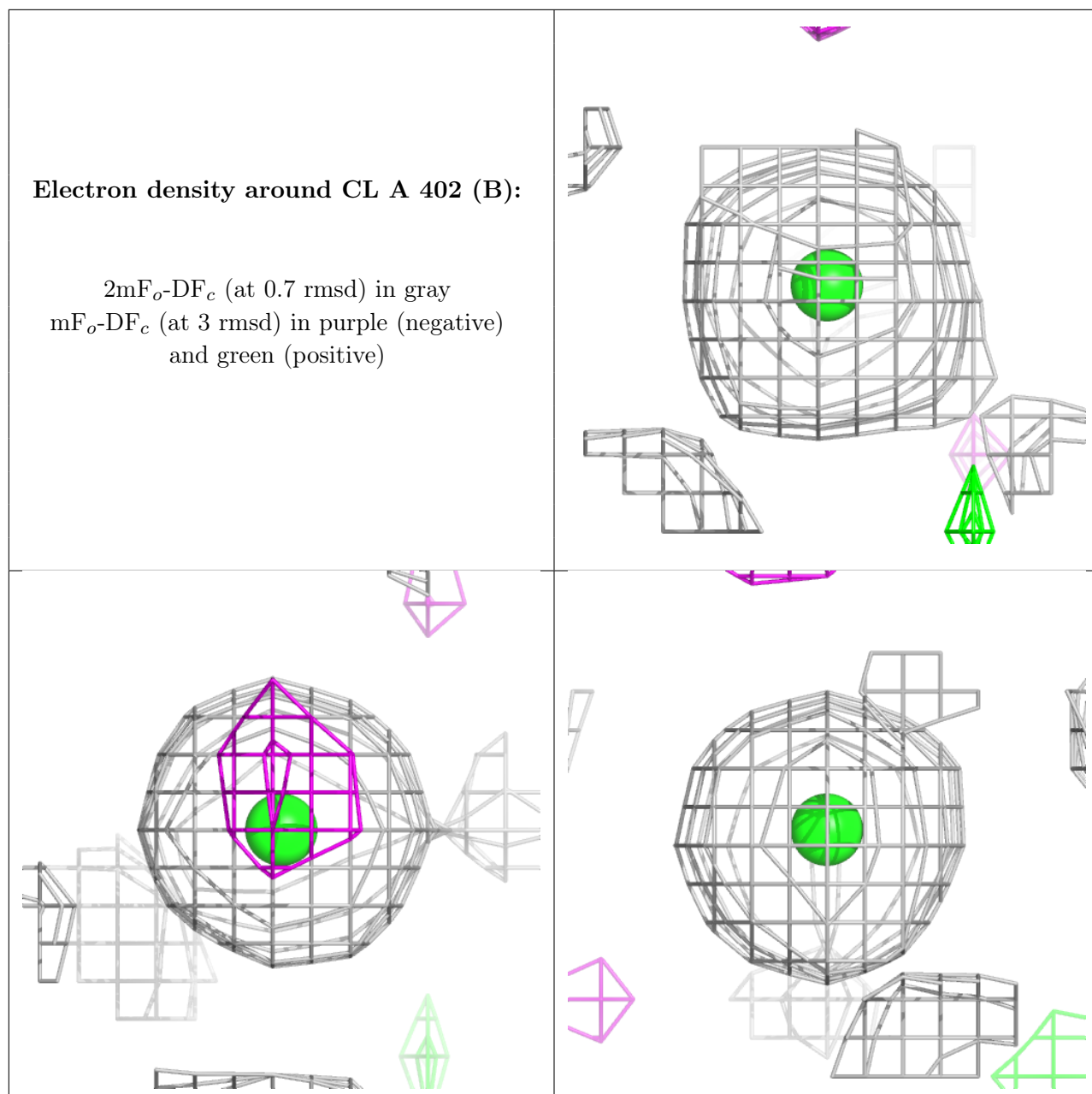
Electron density around CLA B 605:

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



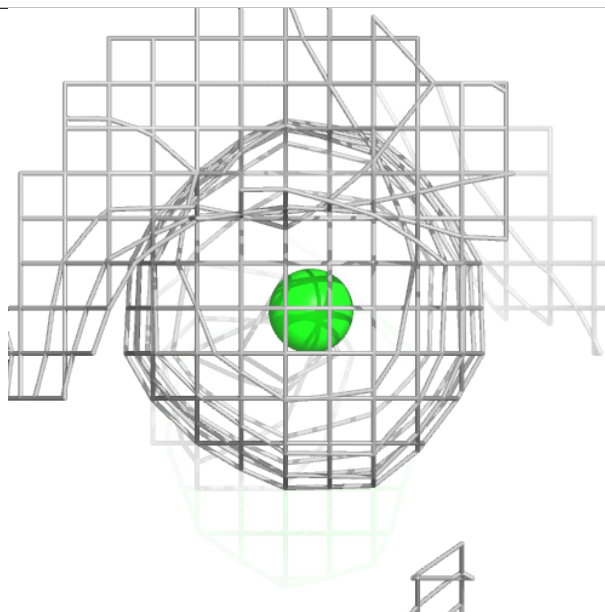
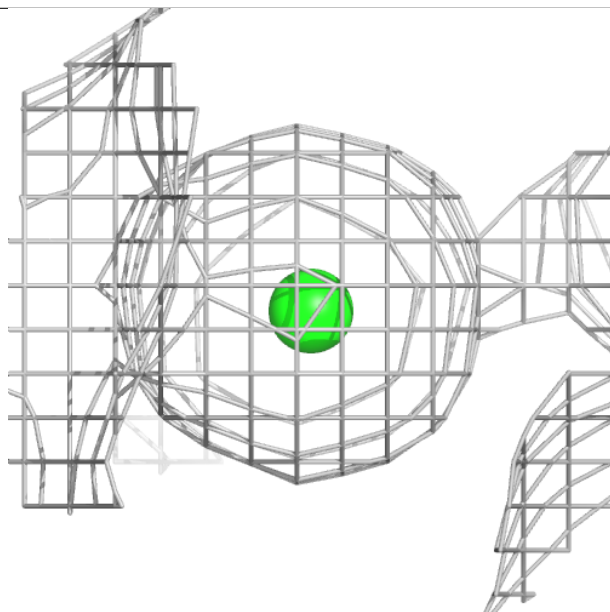
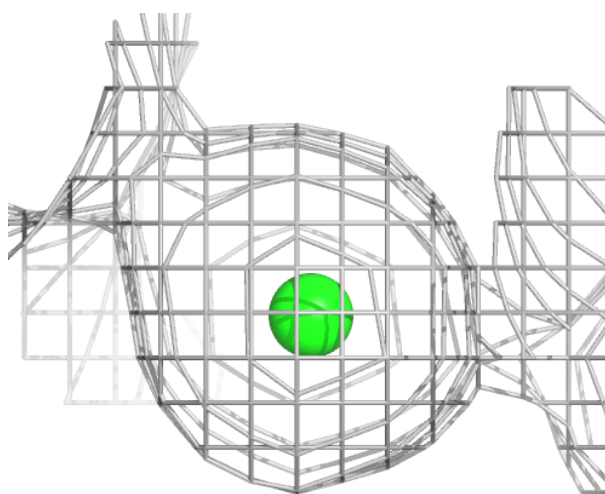
Electron density around CL A 402 (B):

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



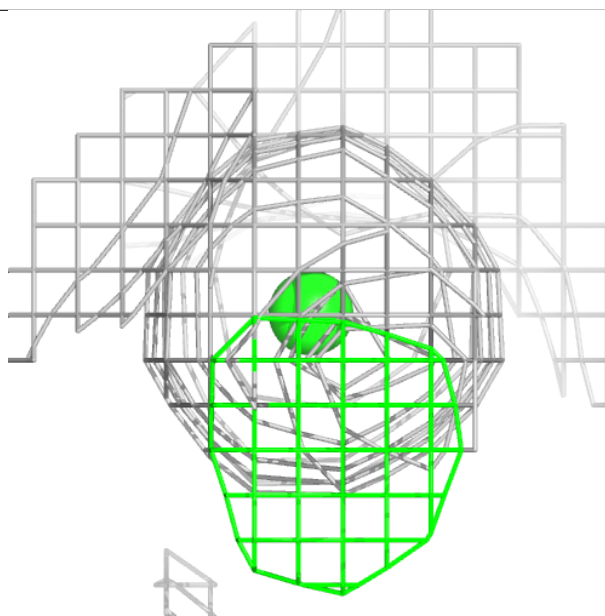
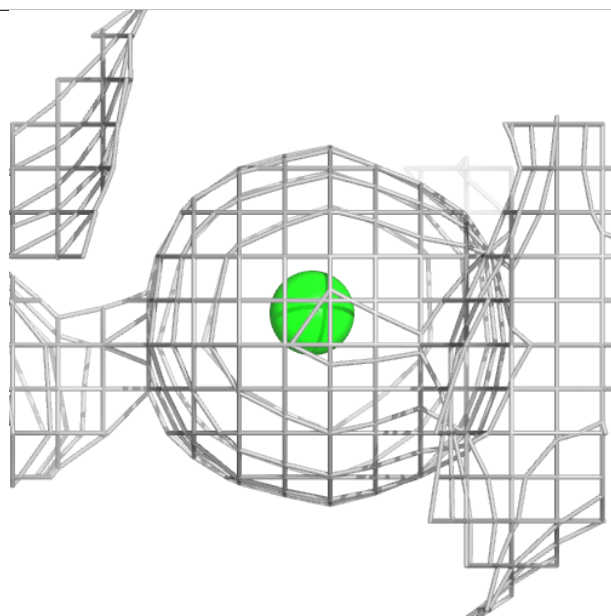
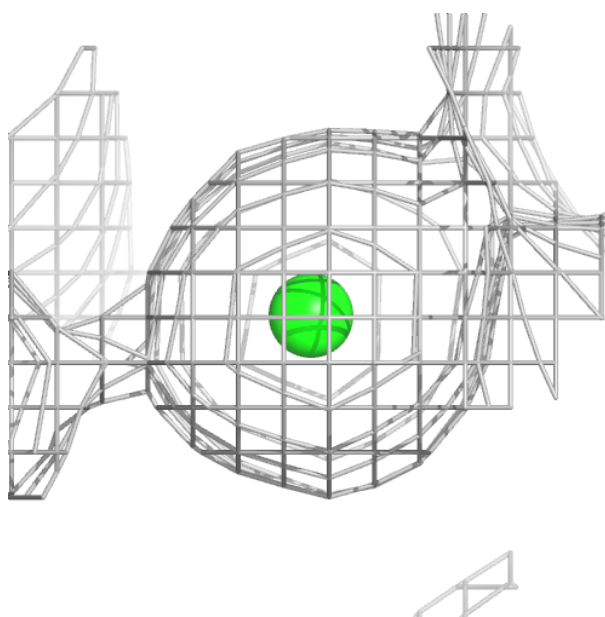
Electron density around CL A 403 (A):

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



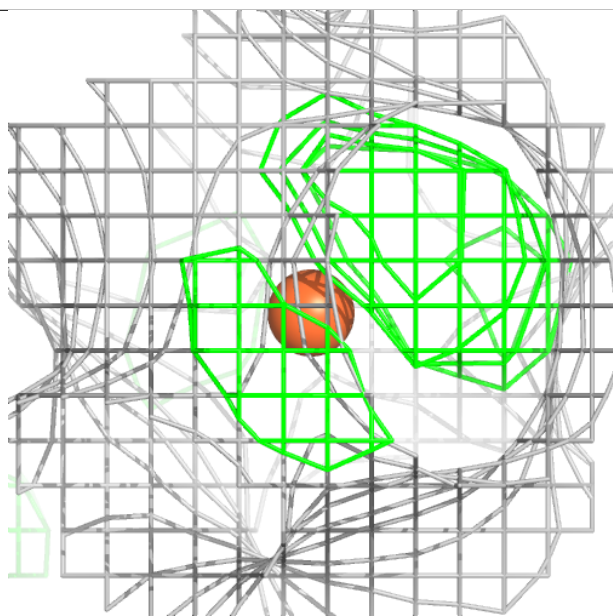
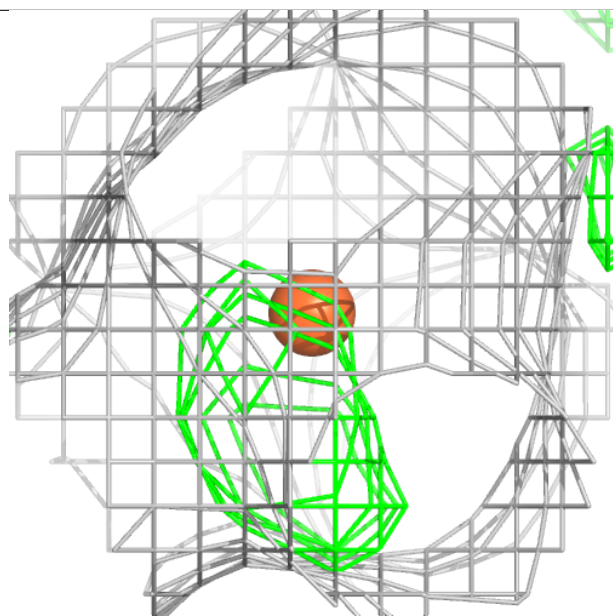
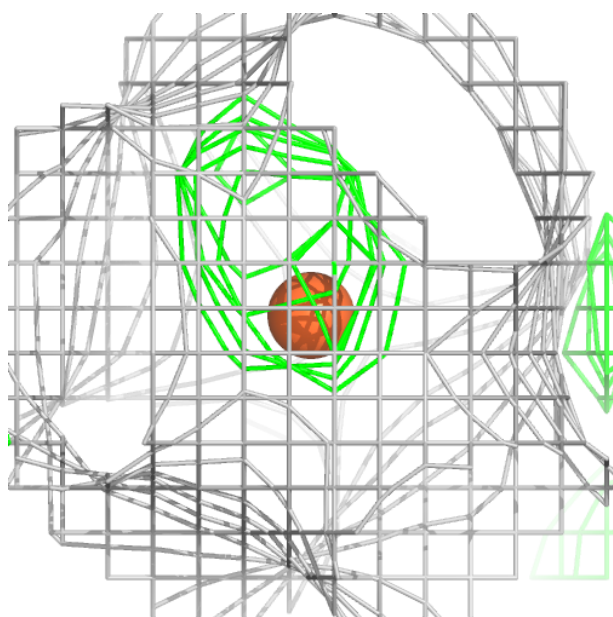
Electron density around CL A 403 (B):

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



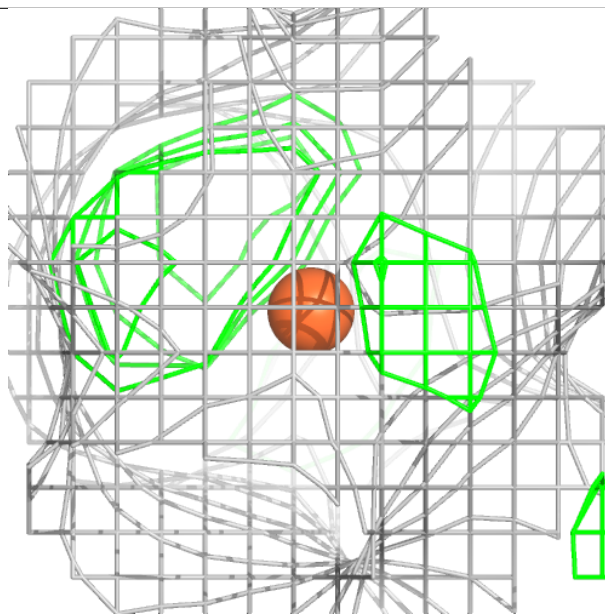
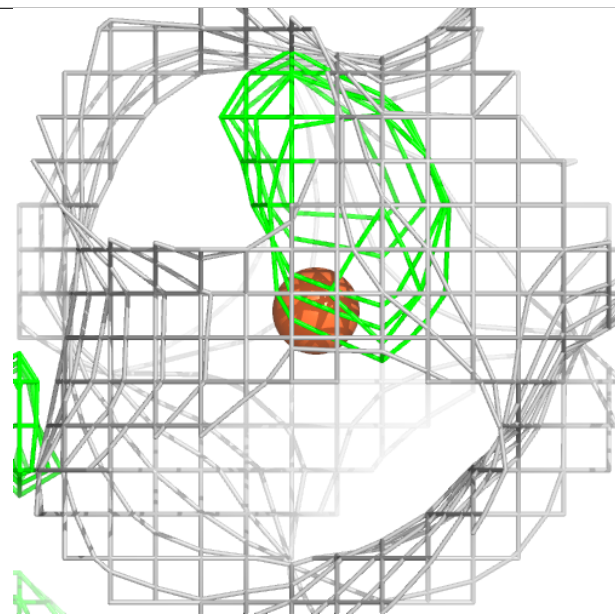
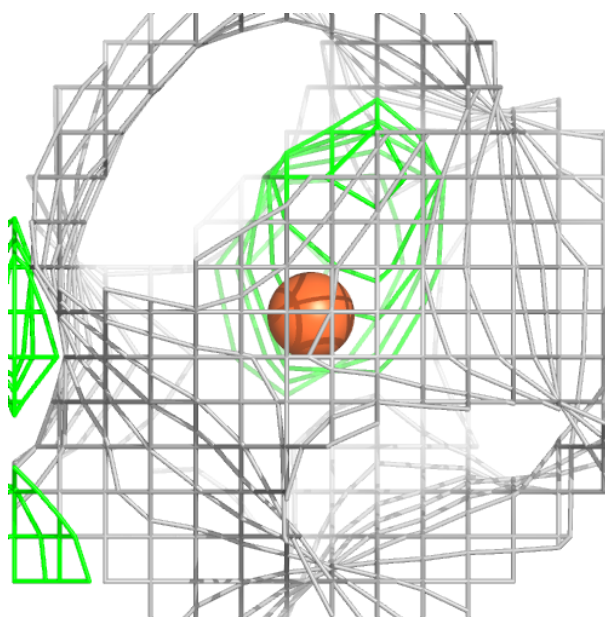
Electron density around FE2 a 401 (A):

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



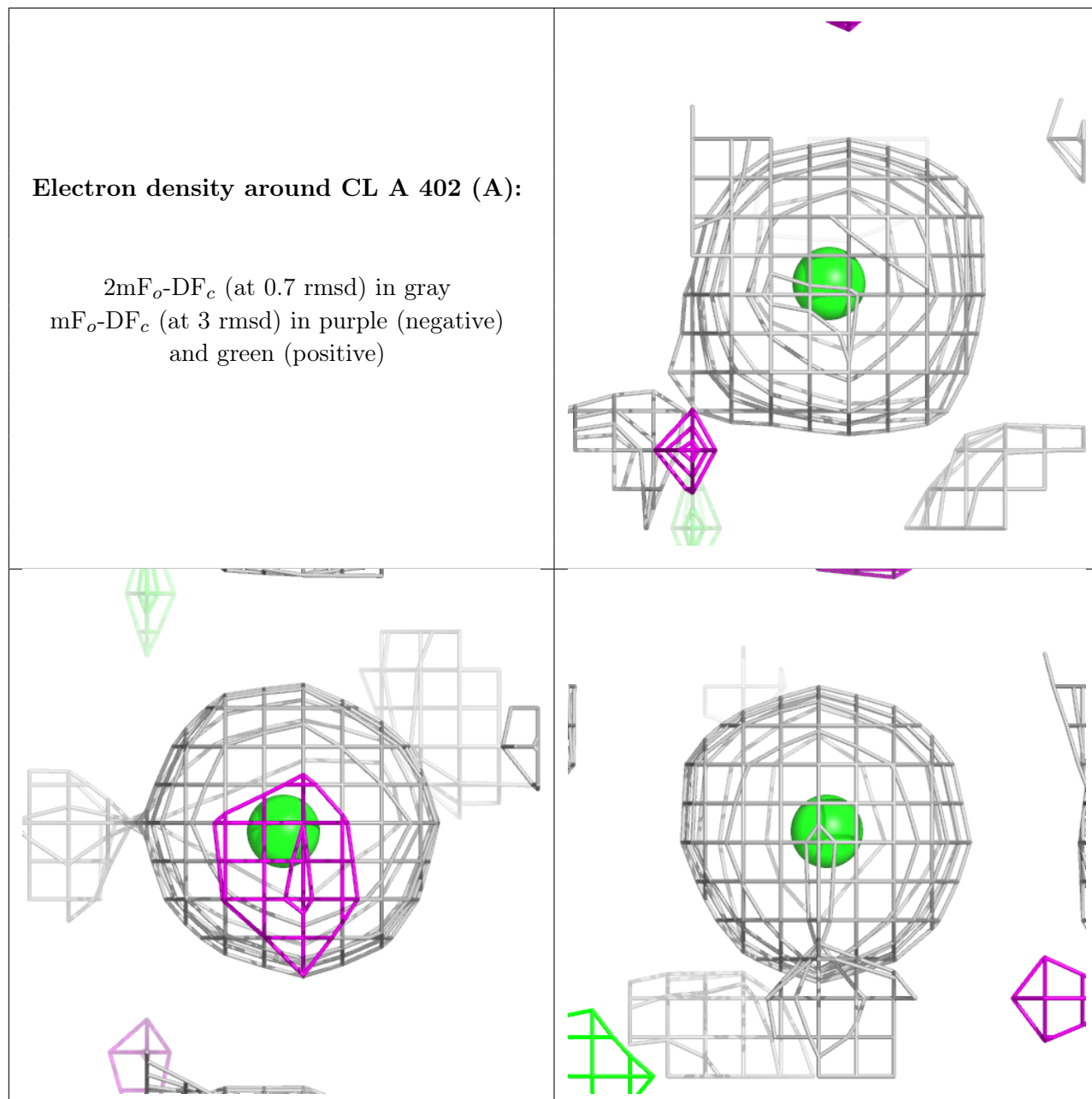
Electron density around FE2 a 401 (B):

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



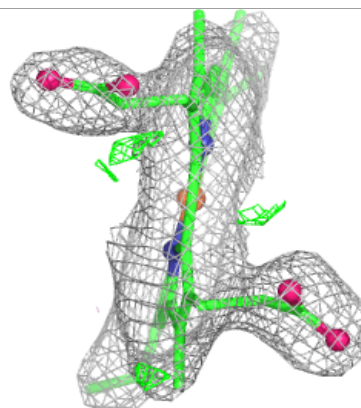
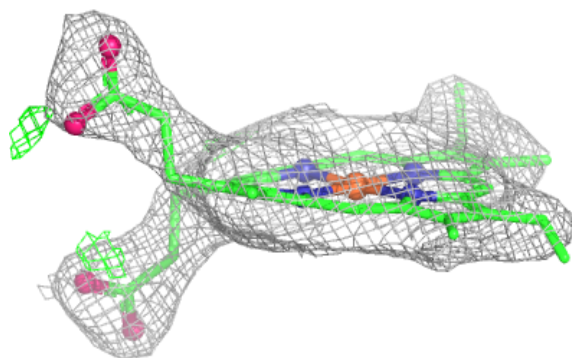
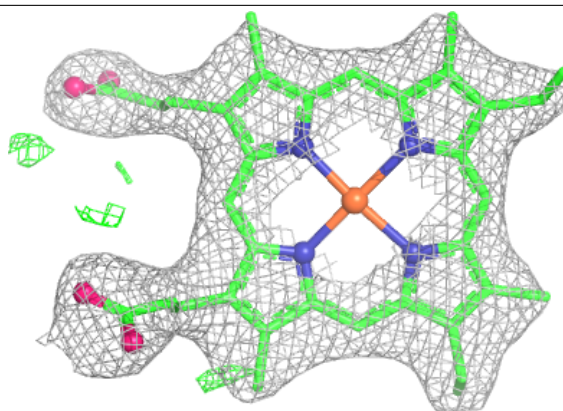
Electron density around CL A 402 (A):

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



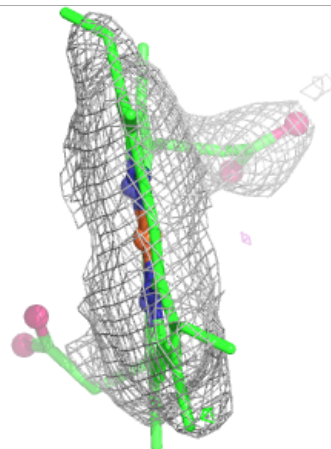
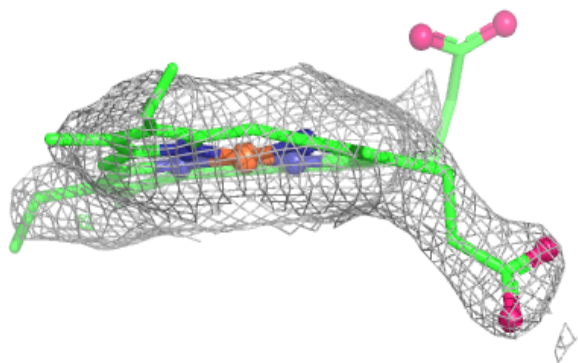
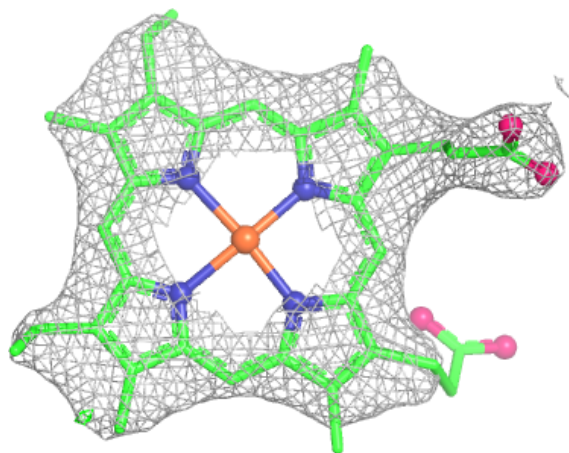
Electron density around HEM E 102:

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



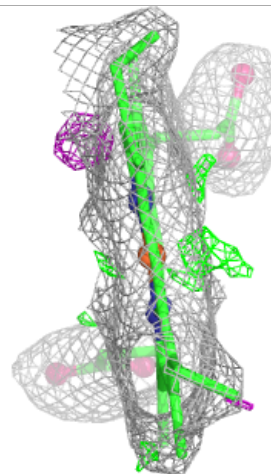
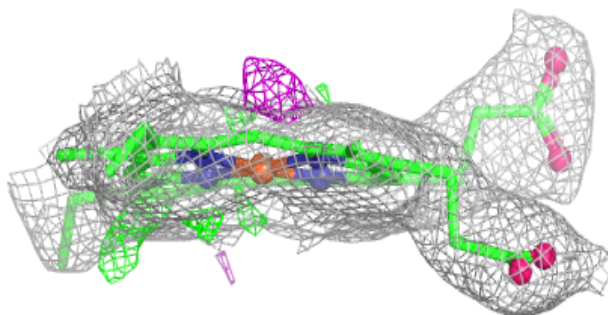
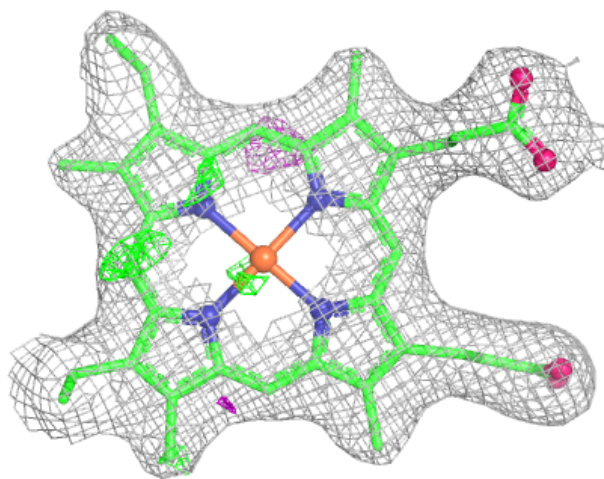
Electron density around HEM f 101:

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



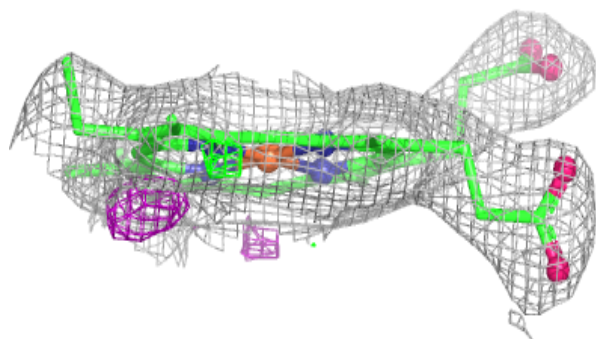
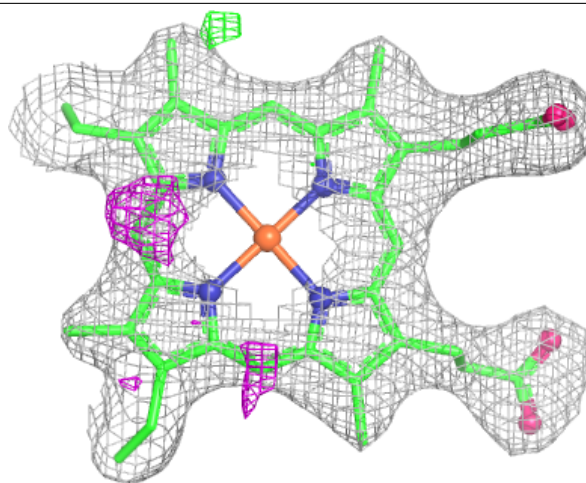
Electron density around HEC V 201:

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



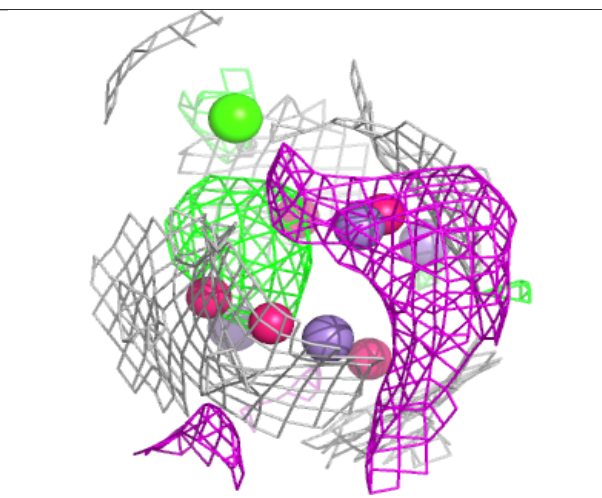
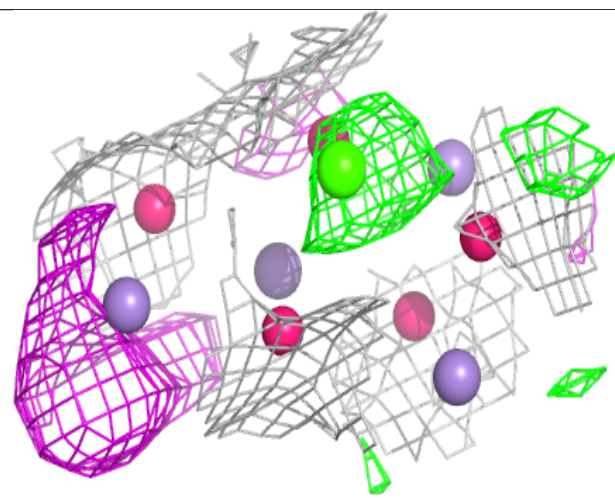
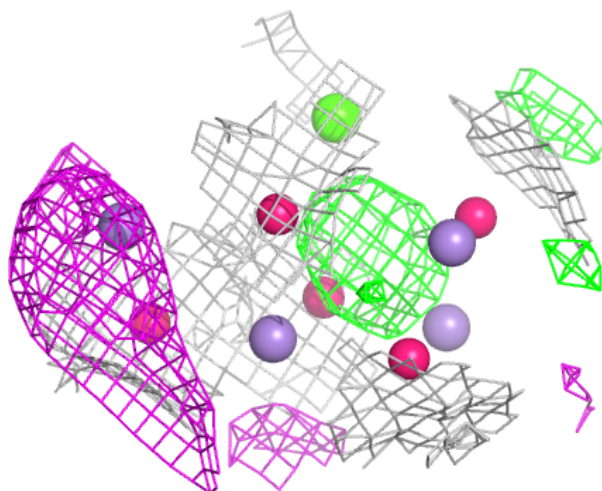
Electron density around HEC v 201:

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



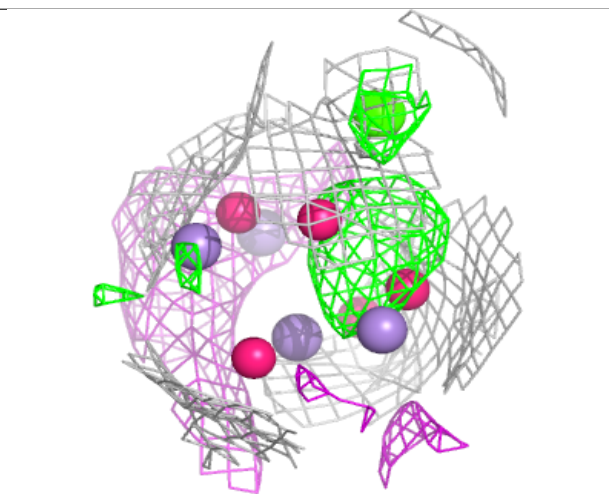
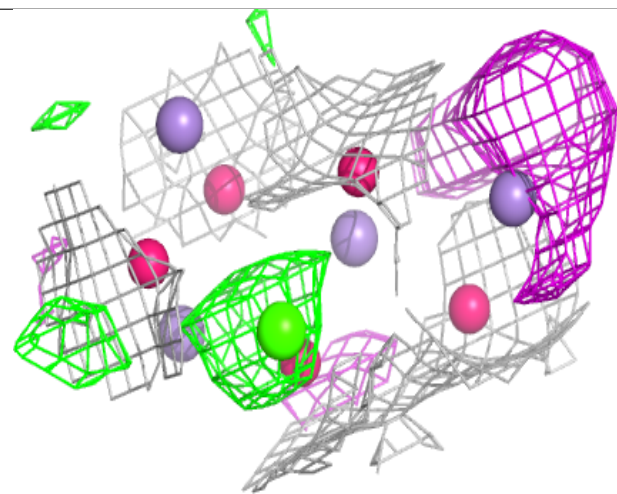
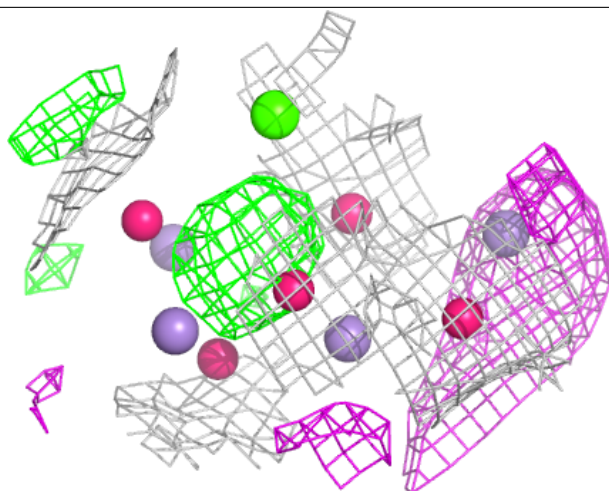
Electron density around OEX A 413 (A):

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



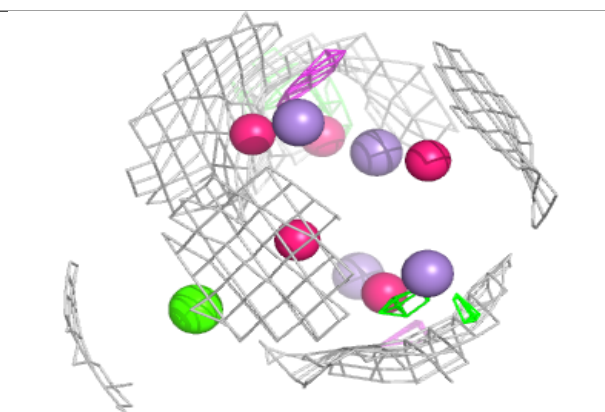
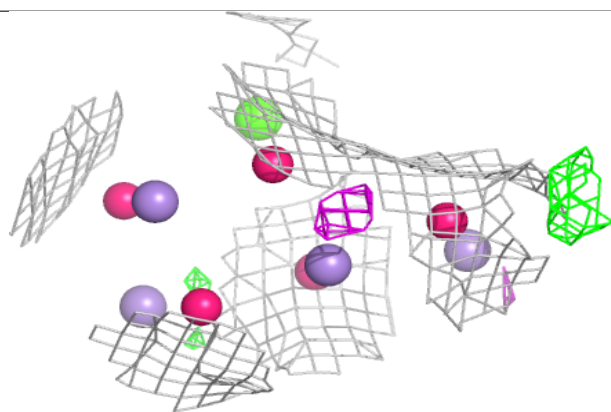
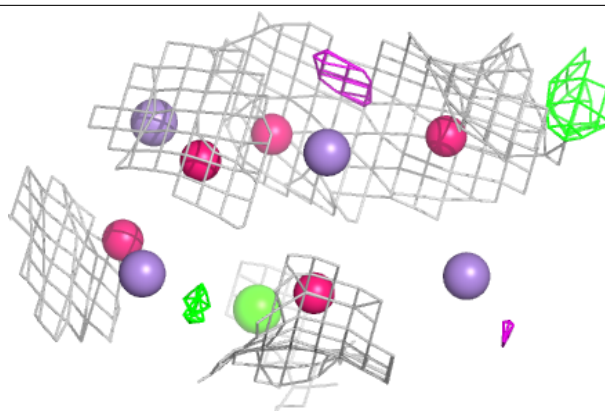
Electron density around OEX A 413 (B):

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

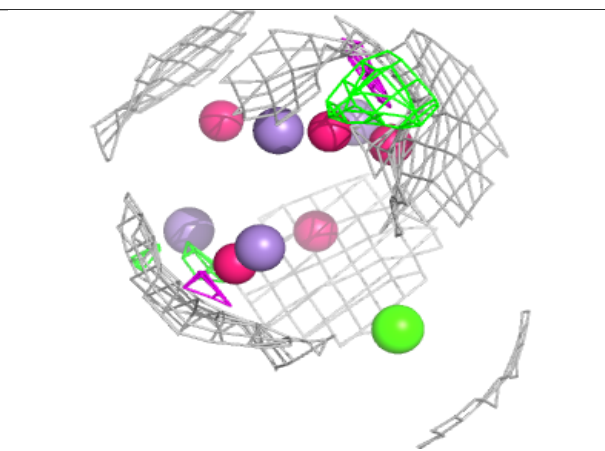
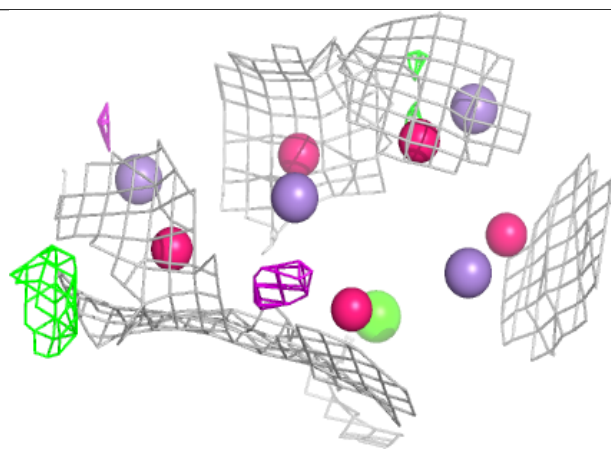
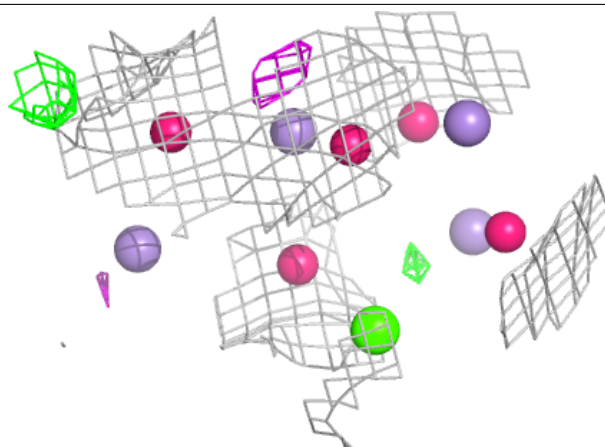


Electron density around OEX a 411 (A):

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

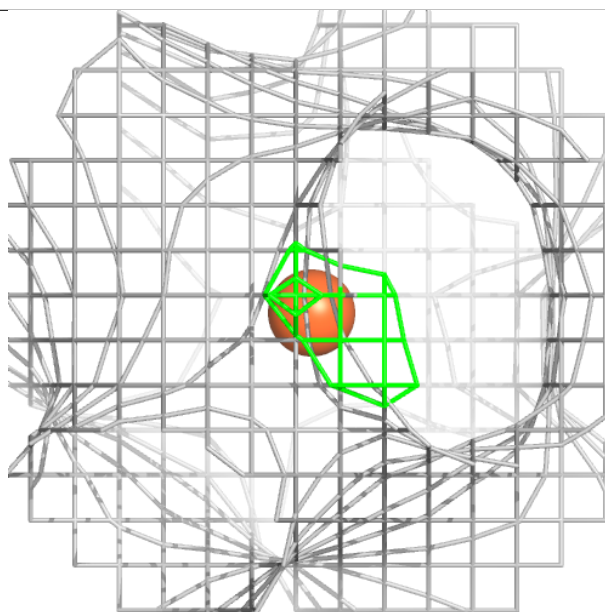
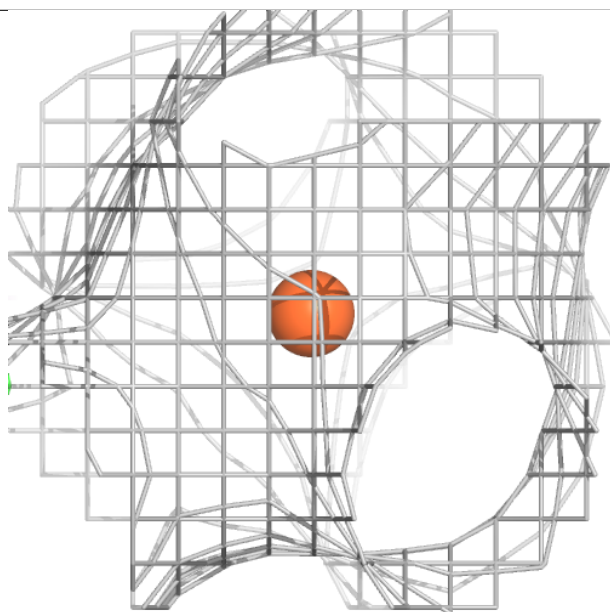
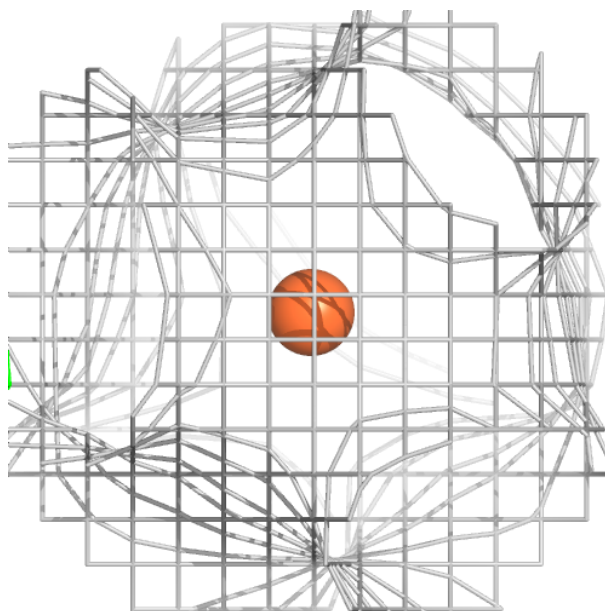
**Electron density around OEX a 411 (B):**

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



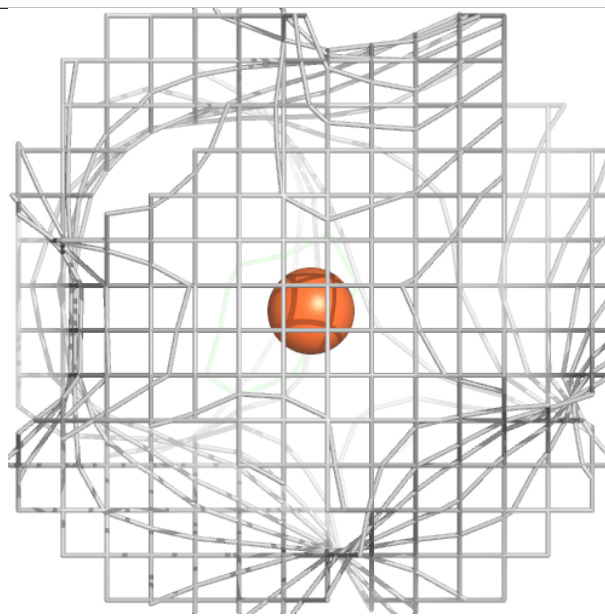
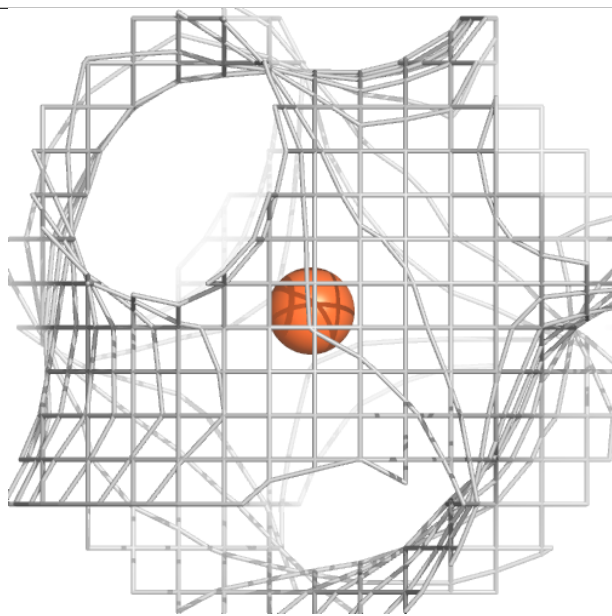
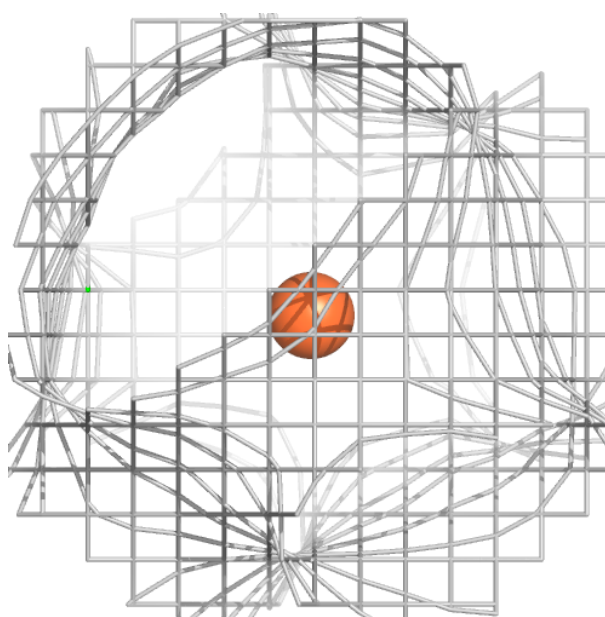
Electron density around FE2 A 401 (A):

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



Electron density around FE2 A 401 (B):

$2mF_o-DF_c$ (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.