



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:38 AM UTC

PDB ID : 8IRF / pdb_00008irf
Title : XFEL structure of cyanobacterial photosystem II following two flashes (2F) with a 1-microsecond delay
Authors : Li, H.; Suga, M.; Shen, J.R.
Deposited on : 2023-03-17
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

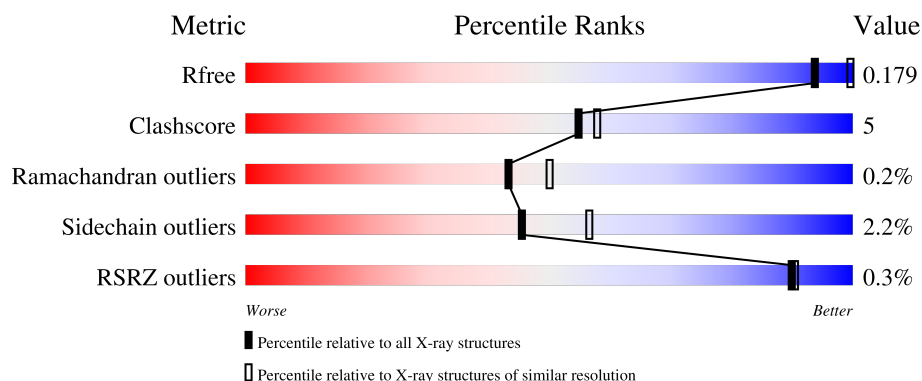
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



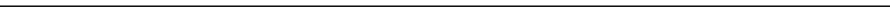
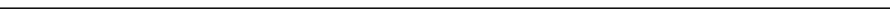
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	344	90% 7% 3%
1	a	344	88% 9% 3%
2	B	505	92% 8%
2	b	505	91% 9%
3	C	455	92% 7% 1%

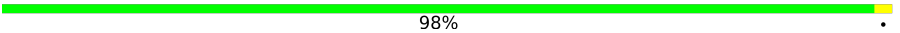
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Mol	Chain	Length	Quality of chain
3	c	455	 92% 7%
4	D	342	 91% 9%
4	d	342	 92% 8%
5	E	84	 77% 19% .
5	e	84	 2% 83% 11% 6%
6	F	44	 68% 9% 23%
6	f	44	 2% 61% 9% 30%
7	H	65	 2% 94% 5% .
7	h	65	 89% 9% .
8	I	38	 79% 21%
8	i	38	 3% 89% 8% .
9	J	39	 79% 15% . .
9	j	39	 92% 8%
10	K	37	 73% 22% 5%
10	k	37	 78% 16% 5%
11	L	37	 86% 11% .
11	l	37	 86% 11% .
12	M	36	 78% 11% . 8%
12	m	36	 78% 17% 6%
13	O	244	 86% 13%
13	o	244	 90% 9%
14	T	32	 78% 12% . 6%
14	t	32	 3% 78% 16% 6%
15	U	104	 84% 9% 8%
15	u	104	 90% . . 7%

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Mol	Chain	Length	Quality of chain
16	V	137	 98%
16	v	137	 91% 9%
17	X	40	 88% 8% 5%
17	x	40	 90% 5% 5%
18	Y	30	 83% 13% 3%
18	y	30	 70% 23% 7%
19	Z	62	 87% 11% 2%
19	z	62	 79% 21%
20	R	34	 76% 24% 6%

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[A]	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	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	402[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	405[A]	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	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402[A]	X	-	-	-
23	CLA	d	402[B]	X	-	-	-
23	CLA	d	403	X	-	-	-
27	GOL	A	418	-	-	X	-
27	GOL	D	412	-	X	-	-
27	GOL	a	419	-	-	X	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 62602 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	221	0
			4330	2830	716	759	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	20	0
			4146	2721	692	720	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	97	0
			4260	2788	713	741	18			
3	c	455	Total	C	N	O	S	0	100	0
			4308	2821	719	750	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	114	0
			3620	2387	596	622	15			
4	d	341	Total	C	N	O	S	0	116	0
			3628	2391	599	623	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	4	0
			807	513	134	160				

- 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).

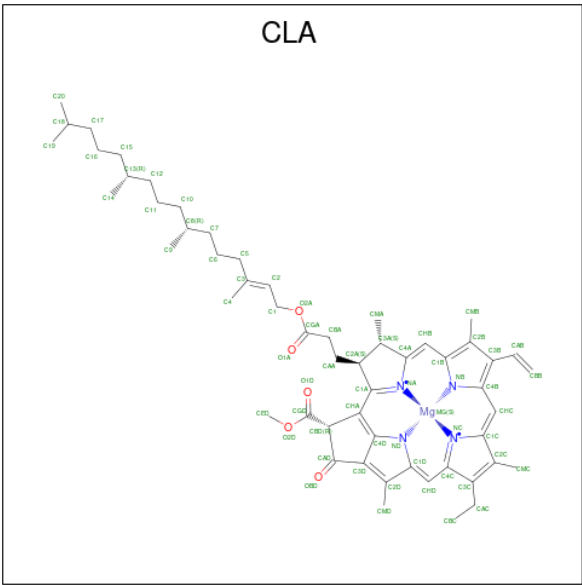
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		

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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		
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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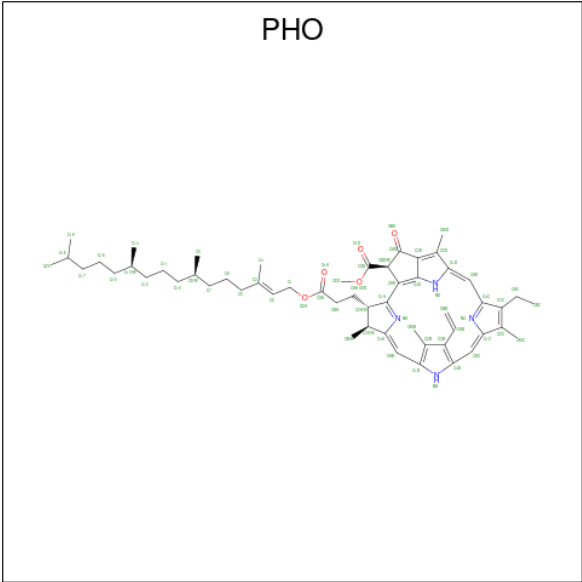
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23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 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

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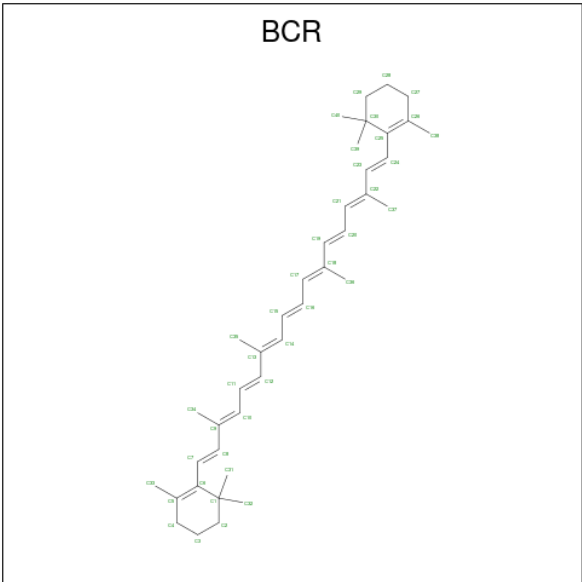
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



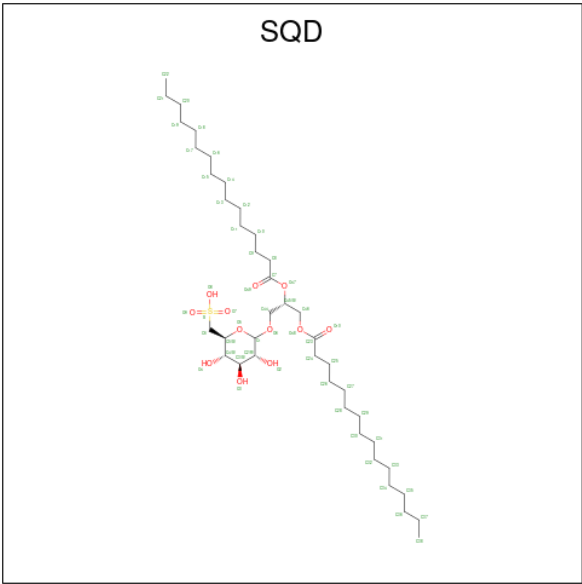
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		

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



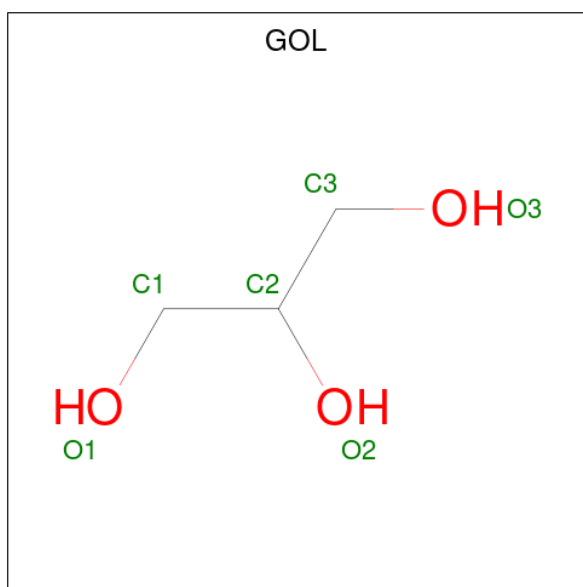
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total 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: C₄₁H₇₈O₁₂S).



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: C₃H₈O₃).



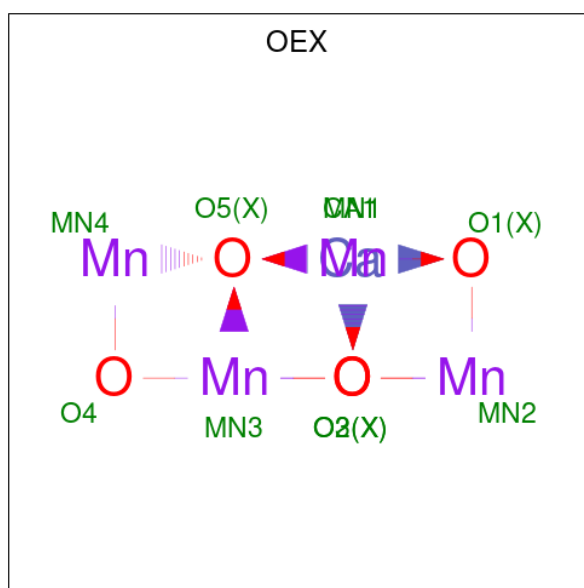
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	1
			12	6	6		
27	D	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27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

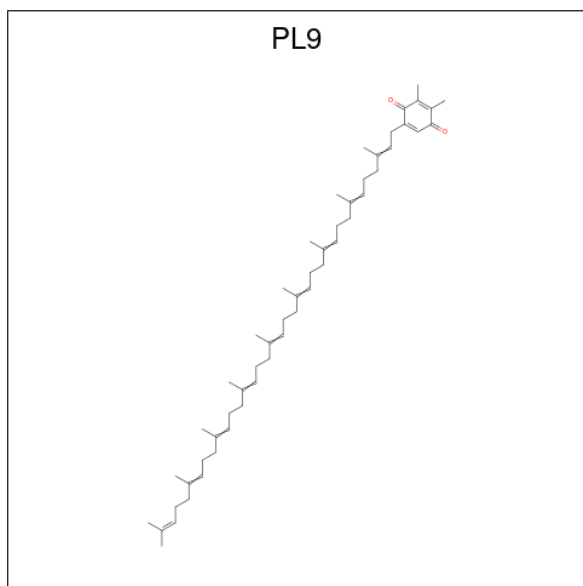
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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:).

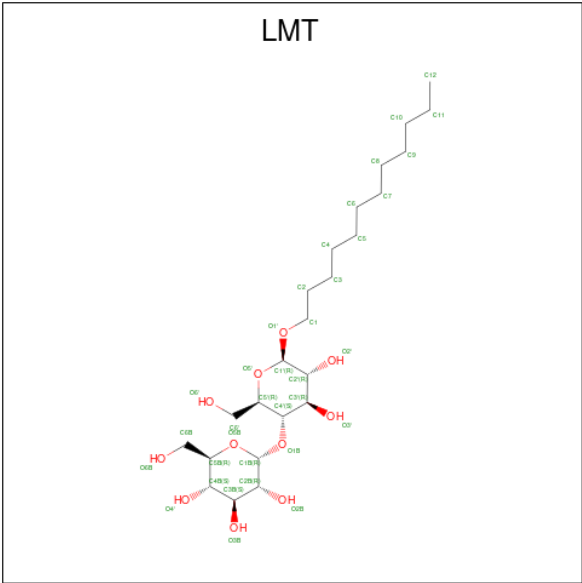
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	2	Total	C	O	0	0
			73	63	10		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	1
			68	58	10		
30	M	1	Total	C		0	0
			10	10			

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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	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: C₂₄H₄₆O₁₁).



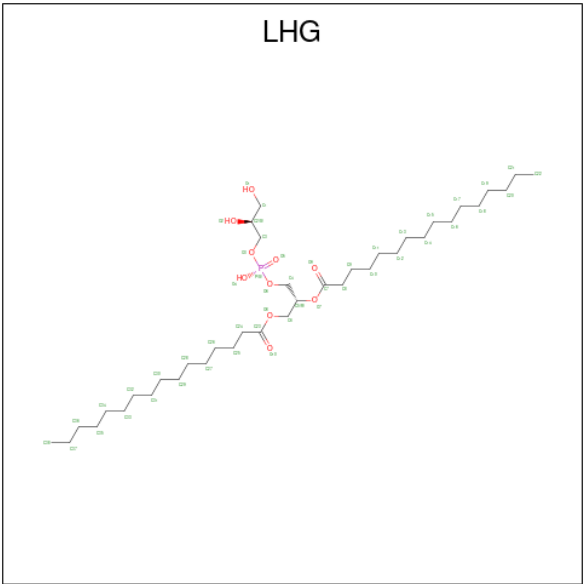
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			35	24	11		
31	A	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		

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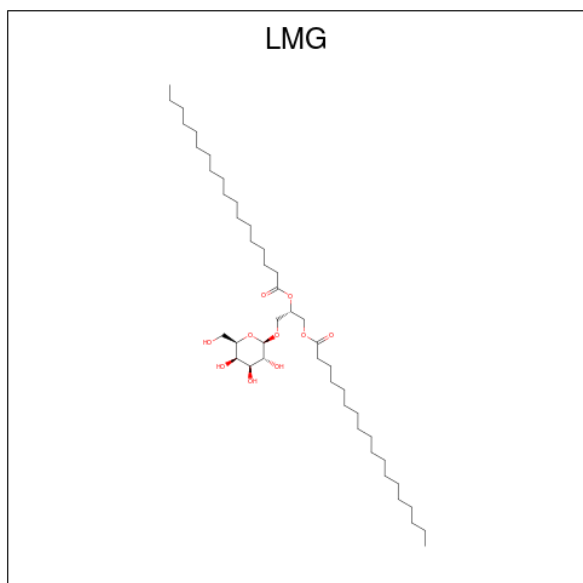
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			25	19	6		
31	F	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	a	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C	O	0	0
			25	19	6		
31	b	1	Total	C	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: $C_{45}H_{86}O_{10}$).



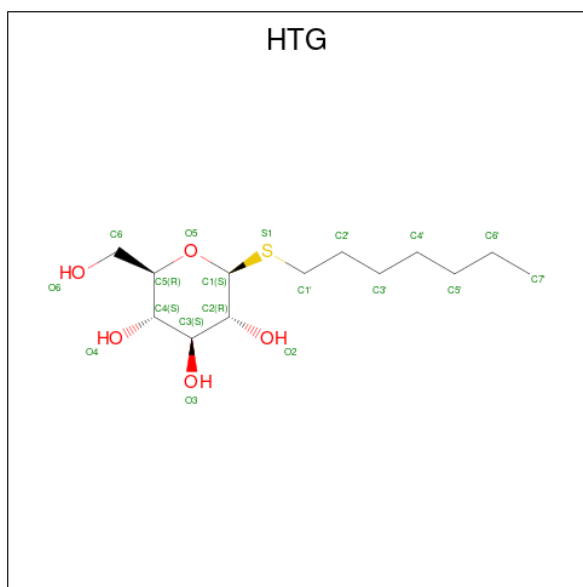
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		

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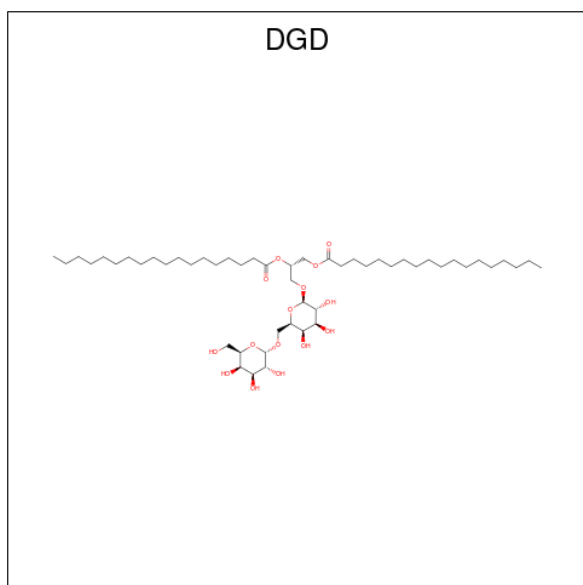
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	D	1	Total	C	O	0	0
			51	41	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	d	1	Total	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	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
34	o	1	Total C O S 19 13 5 1	0	0

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

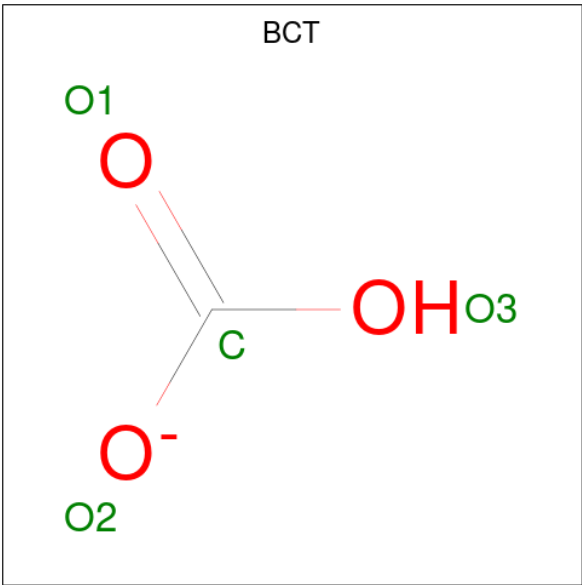


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 62 47 15	0	0
35	H	1	Total C O 62 47 15	0	0
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 62 47 15	0	0
35	h	1	Total C O 62 47 15	0	0

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

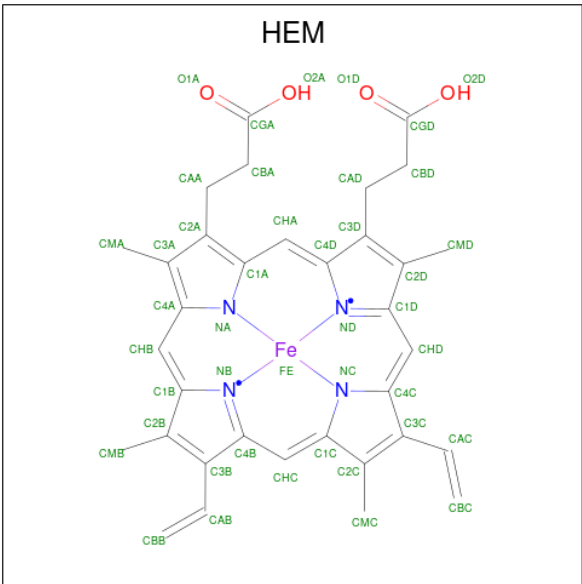
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total Ca 1 1	0	0
36	F	1	Total Ca 1 1	0	0
36	O	1	Total Ca 1 1	0	0
36	c	2	Total Ca 2 2	0	0
36	f	1	Total Ca 1 1	0	0
36	o	1	Total Ca 1 1	0	0

- 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	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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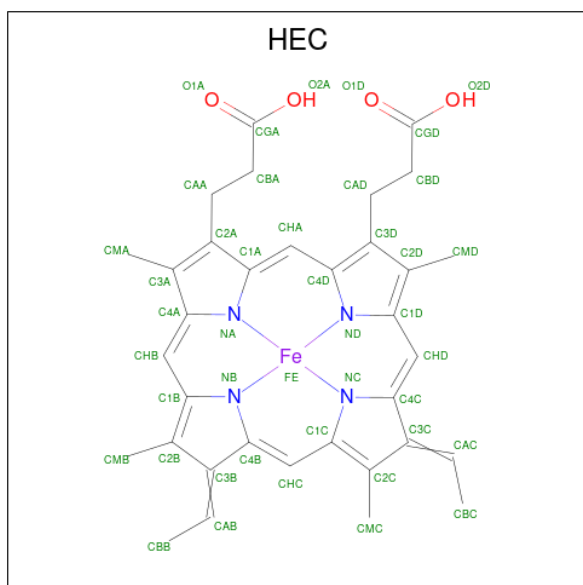
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	139	Total	O	0	84
			221	221		
41	B	192	Total	O	0	3
			195	195		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	C	167	Total 204	O 204	0	37
41	D	120	Total 155	O 155	0	35
41	E	19	Total 19	O 19	0	0
41	F	5	Total 5	O 5	0	0
41	H	22	Total 22	O 22	0	0
41	I	5	Total 5	O 5	0	0
41	J	6	Total 6	O 6	0	0
41	K	6	Total 6	O 6	0	0
41	L	8	Total 9	O 9	0	1
41	M	7	Total 7	O 7	0	0
41	O	101	Total 105	O 105	0	4
41	T	10	Total 13	O 13	0	3
41	U	46	Total 48	O 48	0	2
41	V	79	Total 81	O 81	0	2
41	X	7	Total 7	O 7	0	0
41	a	133	Total 212	O 212	0	81
41	b	199	Total 202	O 202	0	3
41	c	157	Total 190	O 190	0	33
41	d	120	Total 152	O 152	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	2	Total 2	O 2	0	0
41	k	3	Total 3	O 3	0	0
41	l	9	Total 10	O 10	0	1
41	m	11	Total 11	O 11	0	0
41	o	100	Total 105	O 105	0	5
41	t	7	Total 10	O 10	0	3
41	u	51	Total 52	O 52	0	1
41	v	55	Total 58	O 58	0	3
41	x	7	Total 7	O 7	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.

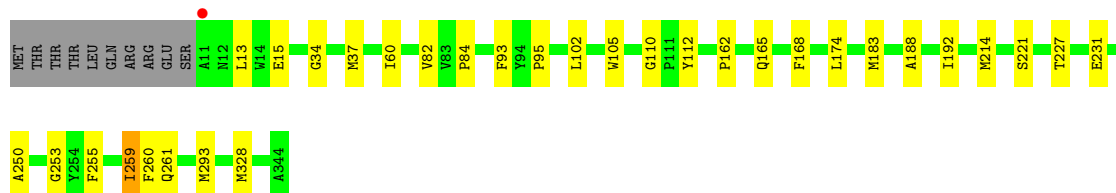
- Molecule 1: Photosystem II protein D1

Chain A: 



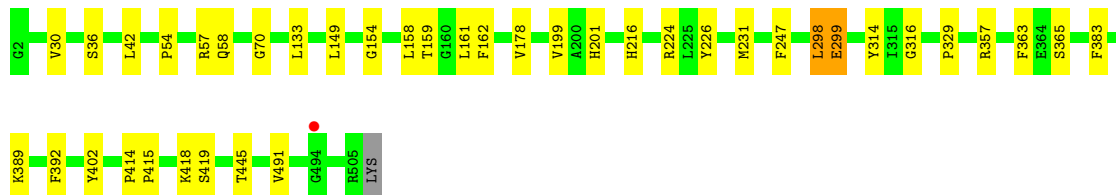
- Molecule 1: Photosystem II protein D1

Chain a: 



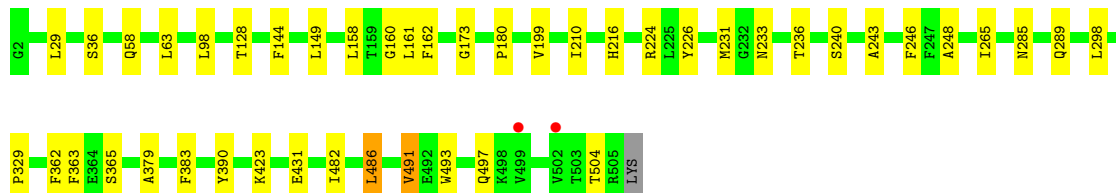
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 



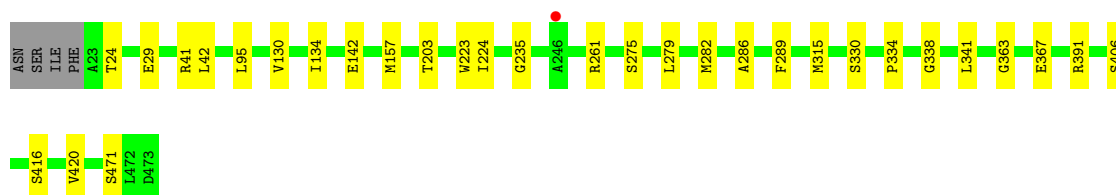
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 



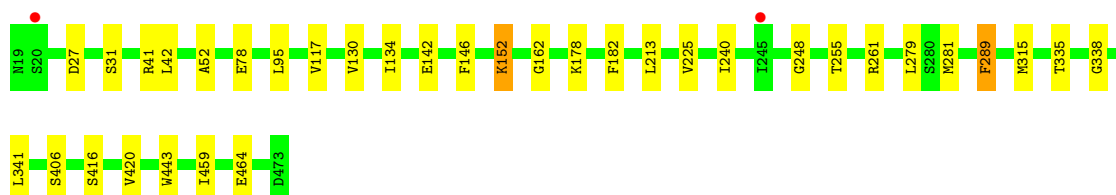
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  92% 7%



- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  92% 7%



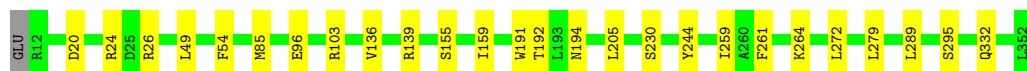
- Molecule 4: Photosystem II D2 protein

Chain D:  91% 9%



- Molecule 4: Photosystem II D2 protein

Chain d:  92% 8%



- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  77% 19%



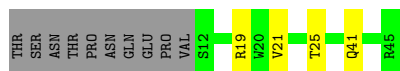
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  83% 11% 6%



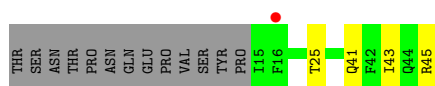
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 68% 9% 23%



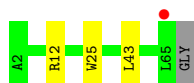
- Molecule 6: Cytochrome b559 subunit beta

Chain f: 2% 61% 9% 30%



- Molecule 7: Photosystem II reaction center protein H

Chain H: 2% 94% 5%



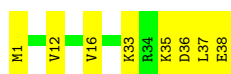
- Molecule 7: Photosystem II reaction center protein H

Chain h: 89% 9%



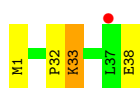
- Molecule 8: Photosystem II reaction center protein I

Chain I: 79% 21%



- Molecule 8: Photosystem II reaction center protein I

Chain i: 3% 89% 8%



- Molecule 9: Photosystem II reaction center protein J

Chain J: 79% 15%



- Molecule 9: Photosystem II reaction center protein J

Chain j: 92% 8%



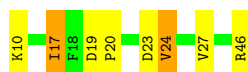
- Molecule 10: Photosystem II reaction center protein K

Chain K: 73% 22% 5%



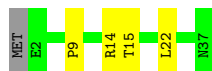
- Molecule 10: Photosystem II reaction center protein K

Chain k: 78% 16% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 86% 11% 3%



- Molecule 11: Photosystem II reaction center protein L

Chain l: 86% 11% 3%



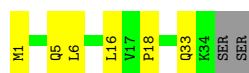
- Molecule 12: Photosystem II reaction center protein M

Chain M: 78% 11% 8% 3%



- Molecule 12: Photosystem II reaction center protein M

Chain m: 78% 17% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 86% 13%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 90% 9%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 78% 12% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 3% 78% 16% 6%



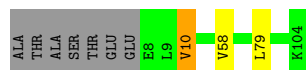
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 84% 9% 8%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 90% 7% 3%



- Molecule 16: Cytochrome c-550

Chain V: 98% 2%



- Molecule 16: Cytochrome c-550

Chain v: 91% 9%



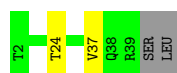
- Molecule 17: Photosystem II reaction center protein X

Chain X: 88% 8% 5%



- Molecule 17: Photosystem II reaction center protein X

Chain x: 90% 5% 5%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y: 3% 83% 13% .



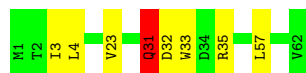
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y: 70% 23% . .



- Molecule 19: Photosystem II reaction center protein Z

Chain Z: 87% 11% .

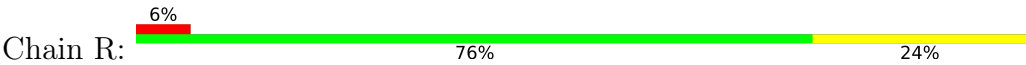


- Molecule 19: Photosystem II reaction center protein Z

Chain z: 79% 21%



● 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	125.77Å 231.76Å 288.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.25 19.99 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.25) 99.8 (19.99-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.26Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.140 , 0.177 0.141 , 0.179	Depositor DCC
R_{free} test set	19914 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	62602	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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: OEX, FE2, CLA, GOL, CL, BCR, LMT, UNL, CA, FME, SQD, MG, HEC, PHO, HEM, LMG, DGD, HTG, BCT, LHG, PL9

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	0.28	0/4478	0.44	0/6098
1	a	0.25	0/4470	0.41	0/6087
2	B	0.38	0/4293	0.52	0/5851
2	b	0.34	0/4285	0.51	0/5841
3	C	0.30	0/4404	0.44	0/5997
3	c	0.29	0/4459	0.44	0/6071
4	D	0.34	0/3741	0.47	0/5095
4	d	0.32	0/3749	0.46	0/5106
5	E	0.33	0/681	0.53	0/928
5	e	0.31	0/690	0.53	0/939
6	F	0.32	0/284	0.45	0/387
6	f	0.29	0/269	0.46	0/365
7	H	0.34	0/519	0.51	0/708
7	h	0.30	0/530	0.50	0/722
8	I	0.32	0/311	0.46	0/419
8	i	0.34	0/311	0.47	0/419
9	J	0.31	0/278	0.37	0/376
9	j	0.29	0/283	0.45	0/383
10	K	0.35	0/303	0.52	0/416
10	k	0.36	0/303	0.48	0/416
11	L	0.37	0/318	0.49	0/433
11	l	0.38	0/318	0.47	0/433
12	M	0.48	0/261	0.53	0/357
12	m	0.37	0/279	0.49	0/380
13	O	0.36	0/1991	0.52	0/2698
13	o	0.34	0/1966	0.52	0/2665
14	T	0.34	0/310	0.41	0/419
14	t	0.33	0/301	0.43	0/406
15	U	0.38	0/811	0.56	0/1095
15	u	0.37	0/818	0.57	0/1105
16	V	0.36	0/1142	0.51	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.31	0/1139	0.48	0/1542
17	X	0.25	0/292	0.38	0/395
17	x	0.25	0/284	0.40	0/384
18	Y	0.28	0/216	0.43	0/289
18	y	0.25	0/216	0.43	0/289
19	Z	0.40	1/490 (0.2%)	0.40	0/669
19	z	0.24	0/490	0.42	0/669
20	R	0.27	0/279	0.36	0/383
All	All	0.32	1/50562 (0.0%)	0.47	0/68780

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	23	VAL	CA-CB	6.96	1.58	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	22	0
1	a	4330	0	4132	36	0
2	B	4146	0	3983	31	0
2	b	4134	0	3976	39	0
3	C	4260	0	4123	19	0
3	c	4308	0	4171	28	0
4	D	3620	0	3484	32	0
4	d	3628	0	3490	21	0
5	E	662	0	648	11	0
5	e	670	0	655	7	0
6	F	275	0	282	4	0
6	f	261	0	269	5	0
7	H	506	0	529	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	h	517	0	541	6	0
8	I	314	0	328	4	0
8	i	314	0	328	2	0
9	J	272	0	279	6	0
9	j	277	0	284	2	0
10	K	293	0	305	6	0
10	k	293	0	305	8	0
11	L	311	0	320	4	0
11	l	311	0	320	4	0
12	M	268	0	285	4	0
12	m	286	0	305	9	0
13	O	1958	0	1920	18	0
13	o	1933	0	1900	11	0
14	T	311	0	318	3	0
14	t	302	0	311	5	0
15	U	800	0	796	4	0
15	u	807	0	805	2	0
16	V	1120	0	1122	2	0
16	v	1117	0	1131	10	0
17	X	289	0	322	2	0
17	x	281	0	312	2	0
18	Y	215	0	246	3	0
18	y	215	0	246	6	0
19	Z	479	0	516	5	0
19	z	479	0	516	3	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	17	0
23	B	1040	0	1152	30	0
23	C	845	0	936	29	0
23	D	195	0	216	7	0
23	a	455	0	504	23	0
23	b	1040	0	1152	26	0
23	c	845	0	936	34	0
23	d	195	0	216	6	0
24	A	256	0	296	6	0
24	a	256	0	296	4	0
25	A	40	0	56	2	0
25	B	120	0	168	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	C	80	0	112	1	0
25	D	40	0	56	1	0
25	H	40	0	56	2	0
25	K	40	0	56	0	0
25	T	40	0	56	6	0
25	Y	40	0	56	2	0
25	a	40	0	56	1	0
25	b	120	0	168	10	0
25	c	80	0	112	3	0
25	d	40	0	56	2	0
25	h	40	0	56	5	0
25	k	40	0	56	2	0
25	t	40	0	56	6	0
25	y	40	0	56	3	0
26	A	162	0	234	4	0
26	B	54	0	78	1	0
26	F	43	0	53	1	0
26	a	162	0	233	8	0
26	b	54	0	78	2	0
26	f	43	0	53	0	0
27	A	12	0	15	4	0
27	B	18	0	24	4	0
27	C	12	0	16	0	0
27	D	6	0	7	3	0
27	O	12	0	16	2	0
27	V	12	0	16	0	0
27	a	12	0	16	6	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	4	0
28	A	20	0	0	0	0
28	a	20	0	0	0	0
29	A	110	0	160	19	0
29	D	110	0	160	1	0
29	a	110	0	160	9	0
29	d	110	0	160	0	0
30	A	28	0	0	0	0
30	B	73	0	0	0	0
30	D	57	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	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	126	4	0
31	F	35	0	46	0	0
31	M	70	0	92	2	0
31	a	35	0	46	1	0
31	b	50	0	70	2	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	9	0
32	E	84	0	114	6	0
32	L	98	0	148	1	0
32	a	84	0	114	9	0
32	b	98	0	148	0	0
32	d	294	0	444	25	0
33	B	51	0	72	1	0
33	C	153	0	216	3	0
33	D	51	0	72	0	0
33	Z	37	0	44	2	0
33	a	51	0	72	0	0
33	c	102	0	144	3	0
33	d	51	0	72	3	0
33	m	51	0	72	0	0
33	z	39	0	48	2	0
34	B	38	0	52	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	c	19	0	26	1	0
34	d	16	0	17	0	0
34	o	19	0	26	3	0
35	C	310	0	410	5	0
35	H	62	0	82	1	0
35	c	310	0	410	12	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	F	43	0	30	1	0
38	f	43	0	30	1	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	221	0	0	1	0
41	B	195	0	0	2	0
41	C	204	0	0	0	0
41	D	155	0	0	3	0
41	E	19	0	0	1	0
41	F	5	0	0	0	0
41	H	22	0	0	0	0
41	I	5	0	0	0	0
41	J	6	0	0	0	0
41	K	6	0	0	0	0
41	L	9	0	0	0	0
41	M	7	0	0	0	0
41	O	105	0	0	0	0
41	T	13	0	0	0	0
41	U	48	0	0	0	0
41	V	81	0	0	0	0
41	X	7	0	0	0	0
41	a	212	0	0	2	0
41	b	202	0	0	1	0
41	c	190	0	0	4	0
41	d	152	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	e	8	0	0	0	0
41	f	3	0	0	1	0
41	h	17	0	0	0	0
41	i	2	0	0	0	0
41	j	2	0	0	0	0
41	k	3	0	0	0	0
41	l	10	0	0	0	0
41	m	11	0	0	0	0
41	o	105	0	0	0	0
41	t	10	0	0	0	0
41	u	52	0	0	1	0
41	v	58	0	0	0	0
41	x	7	0	0	0	0
41	y	2	0	0	0	0
All	All	62602	0	61444	588	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 (588) 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	1.43	1.00
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.48	0.96
23:B:604:CLA:H42	23:B:605:CLA:H2	1.49	0.94
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.51	0.93
23:B:601:CLA:H12	23:B:601:CLA:H71	1.61	0.82
23:c:503:CLA:HBB1	23:c:512:CLA:H41	1.60	0.81
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.65	0.78
4:d:192[A]:THR:HG23	23:d:402[A]:CLA:HBC2	1.66	0.77
23:A:406[A]:CLA:H152	29:A:414[A]:PL9:H252	1.67	0.76
4:d:192[B]:THR:HG23	23:d:402[B]:CLA:HBC2	1.67	0.76
23:C:506:CLA:HHC	23:C:506:CLA:HBB1	1.68	0.76
23:A:406[B]:CLA:H152	29:A:414[B]:PL9:H252	1.68	0.75
23:C:502:CLA:H193	23:C:508:CLA:HBB1	1.69	0.75
1:a:253[B]:GLY:HA3	2:b:491[B]:VAL:HG12	1.70	0.74
23:a:408:CLA:H192	23:c:505:CLA:H142	1.73	0.69
1:a:253[A]:GLY:HA3	2:b:491[A]:VAL:HG12	1.75	0.69
23:a:408:CLA:H152	23:c:506:CLA:H142	1.73	0.69
3:c:213:LEU:HD13	23:c:506:CLA:H202	1.74	0.68
27:A:418:GOL:O2	41:A:501:HOH:O	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:D:407[A]:LHG:H112	32:D:407[A]:LHG:H382	1.76	0.68
23:c:502:CLA:H61	23:c:512:CLA:H42	1.75	0.67
23:C:511:CLA:H192	23:C:511:CLA:HBC3	1.77	0.67
23:a:405[B]:CLA:HHC	23:a:405[B]:CLA:HBB1	1.77	0.67
23:c:505:CLA:CMD	23:c:507:CLA:HAB	2.25	0.66
23:C:506:CLA:CMD	23:C:508:CLA:HAB	2.25	0.66
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.78	0.66
2:b:98:LEU:HB2	34:b:622:HTG:H7'1	1.77	0.66
23:C:514:CLA:H202	33:C:521:LMG:H402	1.77	0.66
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.78	0.65
25:y:101:BCR:H321	25:y:101:BCR:HC8	1.78	0.65
23:B:615:CLA:H2	23:B:616:CLA:HBB2	1.78	0.65
31:B:631:LMT:H6E	31:t:101:LMT:H6D	1.77	0.65
25:b:619:BCR:H331	25:b:619:BCR:HC8	1.78	0.65
27:a:419:GOL:O2	41:a:501:HOH:O	2.13	0.65
23:a:405[A]:CLA:HHC	23:a:405[A]:CLA:HBB1	1.80	0.64
23:C:507:CLA:H142	35:C:517[B]:DGD:HAF2	1.79	0.64
2:B:357[B]:ARG:NH2	4:D:337:GLU:O	2.31	0.64
2:b:482[A]:ILE:HD12	2:b:486[A]:LEU:HD12	1.80	0.64
33:z:101:LMG:H302	33:z:101:LMG:H141	1.79	0.64
25:t:102:BCR:HC8	25:t:102:BCR:H321	1.80	0.63
29:A:414[A]:PL9:H262	32:E:101[A]:LHG:H223	1.80	0.63
27:b:628:GOL:HO1	27:b:628:GOL:HO3	1.46	0.63
23:c:505:CLA:HHC	23:c:505:CLA:HBB1	1.80	0.63
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	1.81	0.63
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.79	0.62
1:a:221[B]:SER:HB2	4:d:139[B]:ARG:O	1.99	0.62
3:c:134[B]:ILE:HD13	23:c:511:CLA:H43	1.82	0.62
26:a:410[A]:SQD:H152	32:d:407[A]:LHG:H172	1.82	0.62
2:B:226:TYR:HA	2:B:231:MET:HG3	1.81	0.62
4:D:192[B]:THR:HG23	23:D:402[B]:CLA:HBC2	1.81	0.62
1:A:192[B]:ILE:HG13	1:A:293[B]:MET:HE1	1.82	0.61
23:A:406[B]:CLA:HHC	23:A:406[B]:CLA:HBB1	1.82	0.61
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.82	0.61
23:b:601:CLA:H72	23:b:601:CLA:H2	1.83	0.61
32:D:407[B]:LHG:H382	32:D:407[B]:LHG:H112	1.82	0.61
3:c:261:ARG:NH1	8:i:38:GLU:OE2	2.32	0.61
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.83	0.61
23:C:507:CLA:H142	35:C:517[A]:DGD:HAF2	1.81	0.60
10:K:17:ILE:H	10:K:17:ILE:HD13	1.64	0.60
23:A:408:CLA:H193	23:C:507:CLA:H101	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:511:CLA:H191	33:z:101:LMG:H241	1.83	0.60
27:a:418:GOL:H32	12:m:1:FME:HG3	1.82	0.60
23:A:404[B]:CLA:HBB1	23:D:402[B]:CLA:C4B	2.08	0.60
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.82	0.60
1:a:214[B]:MET:HB3	29:a:413[B]:PL9:H103	1.84	0.60
23:b:606:CLA:H72	25:b:619:BCR:HC7	1.83	0.60
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.84	0.60
23:c:505:CLA:HMD1	23:c:507:CLA:HAB	1.83	0.59
3:c:279:LEU:HD22	23:c:509:CLA:HED2	1.84	0.59
26:a:410[A]:SQD:H141	32:d:407[A]:LHG:H152	1.84	0.59
27:a:419:GOL:H31	12:m:1:FME:HG2	1.84	0.59
27:a:419:GOL:O3	14:t:2:GLU:OE1	2.21	0.59
23:c:513:CLA:HBB1	25:c:514:BCR:H24C	1.83	0.58
26:F:103:SQD:H102	17:X:31:ILE:HD11	1.85	0.58
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.85	0.58
23:c:501:CLA:C4D	23:c:503:CLA:H2	2.33	0.58
13:O:169:ASP:OD1	27:O:303:GOL:H12	2.04	0.58
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.85	0.58
15:U:86[B]:GLU:H	15:U:86[B]:GLU:CD	2.12	0.57
3:c:78:GLU:OE2	16:v:106:ASN:ND2	2.37	0.57
4:D:192[A]:THR:HG23	23:D:402[A]:CLA:HBC2	1.87	0.57
1:a:15:GLU:HB2	31:a:417:LMT:H6'2	1.87	0.57
26:a:410[B]:SQD:H141	32:d:407[B]:LHG:H152	1.85	0.57
27:b:628:GOL:O3	27:b:628:GOL:O1	2.19	0.57
10:k:17:ILE:HD13	10:k:17:ILE:H	1.69	0.57
29:A:414[B]:PL9:H262	32:E:101[B]:LHG:H223	1.87	0.57
23:C:509:CLA:HBC3	23:C:511:CLA:H71	1.86	0.57
23:a:406[A]:CLA:H191	32:a:420[A]:LHG:H111	1.85	0.57
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.87	0.57
35:c:518:DGD:HBH2	32:d:407[A]:LHG:H211	1.87	0.56
32:d:406[B]:LHG:HC62	11:l:15[B]:THR:HG23	1.87	0.56
1:A:85[B]:SER:HA	1:A:109[B]:GLY:HA3	1.88	0.56
35:c:516[A]:DGD:HG11	41:c:606[A]:HOH:O	2.06	0.56
20:R:18:TRP:O	20:R:22:ASN:ND2	2.37	0.56
23:B:609:CLA:HHC	23:B:609:CLA:HBB1	1.87	0.56
2:b:285:ASN:O	2:b:289:GLN:HG2	2.06	0.55
19:Z:32:ASP:OD2	19:Z:35:ARG:HB3	2.07	0.55
3:C:157:MET:HE2	3:C:157:MET:HA	1.89	0.55
2:b:233:ASN:O	2:b:236:THR:HG22	2.07	0.55
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.89	0.55
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:261:ARG:NH1	8:I:38:GLU:OE2	2.39	0.55
4:D:24:ARG:HD3	17:X:37:VAL:HG22	1.89	0.55
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.88	0.55
27:a:419:GOL:H11	12:m:1:FME:HE3	1.89	0.55
13:o:205:ASP:OD2	13:o:207:ARG:NH2	2.40	0.54
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.43	0.54
1:a:183[A]:MET:HA	23:a:404[A]:CLA:HMD1	1.89	0.54
3:c:27:ASP:HB3	10:k:46:ARG:HG3	1.90	0.54
16:v:134[A]:LYS:HE2	27:v:202[A]:GOL:H32	1.88	0.54
24:a:415[A]:PHO:HBC3	4:d:279:LEU:HD22	1.88	0.54
32:D:407[A]:LHG:H382	32:D:407[A]:LHG:H132	1.89	0.54
5:E:30:LEU:HD23	20:R:12:VAL:HG22	1.89	0.54
1:a:84[B]:PRO:HA	1:a:112[B]:TYR:CG	2.42	0.54
1:a:183[B]:MET:HA	23:a:404[B]:CLA:HMD1	1.89	0.54
23:b:609:CLA:HHC	23:b:609:CLA:HBB1	1.88	0.54
3:c:42:LEU:HD21	23:c:511:CLA:H2A	1.89	0.54
12:M:33:GLN:HB2	12:m:33:GLN:HG3	1.90	0.54
33:c:520:LMG:H232	33:c:520:LMG:H391	1.89	0.54
23:C:504:CLA:HBB1	23:C:513:CLA:H41	1.90	0.54
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.42	0.54
25:b:619:BCR:H331	25:b:619:BCR:C8	2.38	0.54
26:a:410[B]:SQD:H152	32:d:407[B]:LHG:H172	1.90	0.54
2:b:216:HIS:HE1	23:b:609:CLA:C1A	2.20	0.54
10:k:23:ASP:OD2	18:y:21:GLN:NE2	2.40	0.54
29:A:414[A]:PL9:H253	23:D:402[A]:CLA:H141	1.89	0.54
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.43	0.54
13:O:42:ARG:HH12	27:O:302:GOL:H12	1.73	0.53
23:B:615:CLA:H2	23:B:616:CLA:CBB	2.38	0.53
23:a:406[B]:CLA:H191	32:a:420[B]:LHG:H111	1.89	0.53
1:a:192[A]:ILE:HG13	1:a:293[A]:MET:HE1	1.90	0.53
4:D:85:MET:CE	4:D:96:GLU:HG2	2.38	0.53
24:A:416[B]:PHO:H3A	23:D:402[B]:CLA:H142	1.91	0.53
31:e:101:LMT:H6'1	6:f:43:ILE:HG12	1.90	0.53
1:a:192[B]:ILE:HG13	1:a:293[B]:MET:HE1	1.91	0.53
1:A:227[B]:THR:HB	1:A:231:GLU:HG3	1.91	0.53
19:z:32:ASP:O	19:z:36:SER:OG	2.17	0.52
2:b:149[B]:LEU:HD11	23:b:604:CLA:H122	1.90	0.52
23:C:502:CLA:C4D	23:C:504:CLA:H2	2.40	0.52
25:C:515:BCR:H352	33:C:521:LMG:H352	1.91	0.52
1:a:165[B]:GLN:OE1	41:a:519[B]:HOH:O	2.18	0.52
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:502:CLA:C3D	23:C:504:CLA:H2	2.40	0.52
4:D:323[A]:GLU:O	27:D:412:GOL:O2	2.28	0.52
3:c:338[A]:GLY:HA3	3:c:341[A]:LEU:O	2.10	0.52
1:A:84[A]:PRO:HA	1:A:112[A]:TYR:CG	2.44	0.52
27:A:418:GOL:H31	12:M:1:FME:HE3	1.90	0.52
8:I:35:LYS:O	8:I:37:LEU:N	2.43	0.52
41:E:201:HOH:O	9:J:6:ARG:HG3	2.10	0.51
2:b:482[B]:ILE:HD12	2:b:486[B]:LEU:HD12	1.92	0.51
23:c:501:CLA:C3D	23:c:503:CLA:H2	2.40	0.51
3:C:203:THR:O	3:C:235:GLY:HA3	2.10	0.51
26:b:620:SQD:H462	26:b:620:SQD:H1	1.91	0.51
3:c:134[B]:ILE:HD11	23:c:511:CLA:H71	1.92	0.51
24:A:407[B]:PHO:HAB	4:D:205[B]:LEU:HD13	1.91	0.51
27:l:801[A]:GOL:H32	14:t:25:GLU:HB2	1.93	0.51
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.92	0.51
13:O:66:VAL:HG21	13:O:110:MET:HE3	1.92	0.50
35:c:518:DGD:HBH2	32:d:407[B]:LHG:H211	1.94	0.50
23:A:405[B]:CLA:HHC	23:A:405[B]:CLA:HBB1	1.94	0.50
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.46	0.50
32:D:407[B]:LHG:H382	32:D:407[B]:LHG:H132	1.93	0.50
26:B:620:SQD:H1	26:B:620:SQD:H462	1.92	0.50
2:B:36[B]:SER:OG	25:B:618:BCR:H362	2.12	0.50
23:B:606:CLA:H202	26:a:411:SQD:H302	1.93	0.50
23:A:408:CLA:H18	23:C:506:CLA:H142	1.93	0.50
3:c:338[B]:GLY:HA3	3:c:341[B]:LEU:O	2.12	0.50
23:B:612:CLA:HBB1	23:B:612:CLA:HMB1	1.93	0.50
13:O:25:THR:O	13:O:27:ARG:N	2.45	0.50
13:O:42:ARG:O	13:O:241:ALA:HA	2.12	0.49
29:A:414[B]:PL9:H253	23:D:402[B]:CLA:H141	1.93	0.49
1:a:221[A]:SER:HB2	4:d:139[A]:ARG:O	2.12	0.49
4:d:244[B]:TYR:OH	4:d:264[B]:LYS:HE3	2.11	0.49
13:o:204:VAL:HG22	13:o:211:ILE:HG22	1.93	0.49
32:a:420[A]:LHG:HC31	5:e:9:PRO:HA	1.92	0.49
4:D:123:ILE:HD11	35:H:102:DGD:HAH2	1.95	0.49
23:a:404[A]:CLA:H201	32:d:406[A]:LHG:H161	1.95	0.49
3:c:335[B]:THR:OG1	41:c:601[B]:HOH:O	2.18	0.49
1:A:102:LEU:HD12	34:b:625:HTG:H61	1.94	0.49
1:A:227[A]:THR:HB	1:A:231:GLU:HG3	1.93	0.49
3:C:95:LEU:HD21	23:C:502:CLA:OBD	2.12	0.49
5:E:12:ASP:OD1	9:J:4:GLY:HA3	2.13	0.49
32:d:407[B]:LHG:H342	32:d:407[B]:LHG:H151	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:261[B]:PHE:CZ	32:D:406[B]:LHG:HC81	2.48	0.49
2:b:36:SER:OG	25:b:618:BCR:H362	2.12	0.49
2:b:98:LEU:HB2	34:b:622:HTG:C7'	2.42	0.49
32:d:406[A]:LHG:HC62	11:l:15[A]:THR:HG23	1.95	0.49
3:c:182:PHE:HA	34:c:521:HTG:H61	1.94	0.49
32:d:413[B]:LHG:H211	12:m:18:PRO:HG3	1.94	0.49
29:a:413[A]:PL9:H351	6:f:25:THR:OG1	2.13	0.48
26:a:410[B]:SQD:H271	32:d:407[B]:LHG:H141	1.93	0.48
24:A:416[A]:PHO:H3A	23:D:402[A]:CLA:H142	1.94	0.48
32:d:407[A]:LHG:H122	32:d:407[A]:LHG:C38	2.44	0.48
2:b:29:LEU:HD23	26:b:620:SQD:H201	1.95	0.48
13:o:43:LEU:HB3	13:o:81:ILE:HB	1.95	0.48
19:z:37:LYS:HE2	19:z:41:PHE:HE2	1.78	0.48
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.94	0.48
24:a:407[B]:PHO:HAB	4:d:205[B]:LEU:HD13	1.95	0.48
25:t:102:BCR:HC7	25:t:102:BCR:H331	1.62	0.48
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.96	0.48
10:k:24:VAL:HG22	18:y:25:ILE:HD13	1.95	0.48
3:c:152:LYS:HD2	41:c:741:HOH:O	2.12	0.48
23:C:504:CLA:HBB1	23:C:504:CLA:HHC	1.96	0.48
32:D:406[A]:LHG:HC62	11:L:15[A]:THR:HG23	1.96	0.48
13:O:205:ASP:OD1	13:O:207:ARG:HG3	2.14	0.47
2:b:144:PHE:CE1	2:b:210:ILE:HG23	2.49	0.47
2:b:497:GLN:HB2	2:b:504:THR:HB	1.96	0.47
11:l:20:GLY:O	11:l:24:ILE:HG12	2.13	0.47
33:d:411:LMG:H221	33:d:411:LMG:H191	1.58	0.47
1:A:84[B]:PRO:HA	1:A:112[B]:TYR:CG	2.49	0.47
3:C:286:ALA:HB2	23:C:503:CLA:HMD2	1.96	0.47
25:d:404:BCR:H331	25:d:404:BCR:C8	2.45	0.47
13:o:58:ASN:HB2	13:o:61:GLN:HG2	1.96	0.47
2:B:299:GLU:HG3	2:B:402:TYR:HD1	1.78	0.47
1:a:84[A]:PRO:HA	1:a:112[A]:TYR:CG	2.49	0.47
1:a:214[A]:MET:HE2	1:a:255[A]:PHE:CE1	2.50	0.47
4:d:85:MET:CE	4:d:96:GLU:HG2	2.43	0.47
32:d:407[A]:LHG:H342	32:d:407[A]:LHG:H151	1.97	0.47
10:k:19:ASP:HB3	10:k:20:PRO:HD3	1.97	0.47
13:o:216:GLU:CD	13:o:234:LYS:HD2	2.39	0.47
29:A:414[A]:PL9:H472	4:D:39:PRO:HD3	1.97	0.47
13:O:51:LEU:HB3	13:O:65:PHE:HB3	1.97	0.47
23:a:406[A]:CLA:H203	33:d:411:LMG:H412	1.96	0.47
1:A:272[B]:HIS:CD2	4:D:218[B]:VAL:HG21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:418:GOL:H12	14:T:2:GLU:OE1	2.13	0.47
23:B:602:CLA:H203	23:B:602:CLA:H162	1.63	0.47
5:E:77:GLU:O	5:E:81:GLU:HG2	2.14	0.47
32:d:407[A]:LHG:H302	32:d:407[A]:LHG:H332	1.67	0.47
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.15	0.47
25:h:101:BCR:C8	25:h:101:BCR:H331	2.45	0.47
2:B:133:LEU:HB2	27:B:626:GOL:H31	1.97	0.47
24:a:415[B]:PHO:HBC3	4:d:279:LEU:HD22	1.96	0.47
5:e:68:ASP:O	5:e:72:ALA:HB2	2.14	0.47
1:A:231:GLU:HB3	41:B:882:HOH:O	2.15	0.47
29:a:413[A]:PL9:H171	29:a:413[A]:PL9:H151	1.58	0.47
29:a:413[B]:PL9:H171	29:a:413[B]:PL9:H151	1.54	0.47
3:c:178:LYS:HA	3:c:182:PHE:HB2	1.97	0.47
3:c:443[B]:TRP:CE2	23:c:508:CLA:HMD2	2.50	0.47
3:C:406:SER:HA	3:C:420[A]:VAL:HG23	1.98	0.46
3:C:406:SER:HA	3:C:420[B]:VAL:HG23	1.98	0.46
23:c:508:CLA:H18	35:c:517[A]:DGD:HAT2	1.97	0.46
19:Z:4:LEU:HD22	19:Z:57:LEU:HD11	1.97	0.46
1:A:192[A]:ILE:HG13	1:A:293[A]:MET:HE1	1.97	0.46
2:B:357[A]:ARG:HH12	27:B:623:GOL:H32	1.80	0.46
23:a:404[B]:CLA:HBB1	23:d:402[B]:CLA:C4B	2.19	0.46
13:o:58:ASN:C	13:o:60:ARG:H	2.22	0.46
31:t:101:LMT:H81	31:t:101:LMT:H112	1.56	0.46
3:C:279:LEU:HA	3:C:282:MET:HE3	1.97	0.46
1:a:34:GLY:HA2	1:a:37:MET:HB3	1.97	0.46
25:t:102:BCR:H382	25:t:102:BCR:H23C	1.98	0.46
23:a:405[A]:CLA:HBA1	23:a:405[A]:CLA:C4A	2.45	0.46
32:a:420[B]:LHG:HC31	5:e:9:PRO:HA	1.96	0.46
2:b:383[A]:PHE:CZ	13:o:167:GLY:HA2	2.50	0.46
23:b:601:CLA:H92	25:h:101:BCR:H403	1.96	0.46
16:v:41:HIS:HA	16:v:45[B]:ILE:O	2.15	0.46
25:H:101:BCR:H331	25:H:101:BCR:C8	2.45	0.46
23:a:406[B]:CLA:H203	33:d:411:LMG:H412	1.97	0.46
26:a:410[A]:SQD:H271	32:d:407[A]:LHG:H141	1.97	0.46
3:C:334[B]:PRO:HA	13:O:153:THR:OG1	2.16	0.46
5:E:27:ILE:HD11	38:F:102:HEM:HBC2	1.98	0.46
2:B:363:PHE:HB3	2:B:365:SER:O	2.16	0.46
18:y:20:ALA:O	18:y:24:MET:HG2	2.16	0.46
2:B:357[A]:ARG:HH12	27:B:623:GOL:C3	2.28	0.46
23:B:615:CLA:HHC	23:B:615:CLA:HBB1	1.98	0.46
18:Y:23:THR:HB	18:Y:24:MET:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:d:407[A]:LHG:H331	32:d:407[A]:LHG:H361	1.46	0.46
3:C:41:ARG:NH1	23:C:512:CLA:HMD1	2.31	0.46
23:C:511:CLA:H152	23:C:511:CLA:H112	1.66	0.46
4:D:180:ARG:HD3	4:D:180:ARG:C	2.41	0.46
29:A:414[B]:PL9:H151	29:A:414[B]:PL9:H171	1.53	0.46
2:B:30:VAL:HG12	23:B:605:CLA:HHD	1.98	0.46
23:C:507:CLA:H152	23:C:507:CLA:H18	1.51	0.45
5:E:20:TRP:CD1	9:J:7:ILE:HD12	2.51	0.45
25:T:101:BCR:H24C	25:T:101:BCR:H371	1.82	0.45
4:d:332[A]:GLN:NE2	41:d:505:HOH:O	2.48	0.45
16:V:126:LEU:HB3	16:V:129:LYS:HB2	1.98	0.45
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.98	0.45
2:b:248:ALA:HA	23:b:603:CLA:H42	1.98	0.45
25:b:618:BCR:H371	25:b:618:BCR:H24C	1.81	0.45
31:M:101:LMT:H6D	11:l:9:PRO:HA	1.98	0.45
25:T:101:BCR:H331	25:T:101:BCR:HC7	1.60	0.45
2:b:363:PHE:HB3	2:b:365:SER:O	2.17	0.45
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.98	0.45
4:d:24:ARG:NH1	17:x:37:VAL:HG22	2.31	0.45
19:Z:31:GLN:CD	19:Z:31:GLN:H	2.24	0.45
2:B:58:GLN:C	2:B:329:PRO:HB3	2.41	0.45
25:T:101:BCR:H311	25:T:101:BCR:HC8	1.98	0.45
23:a:404[B]:CLA:H203	23:a:404[B]:CLA:H162	1.82	0.45
23:b:612:CLA:HBB1	23:b:612:CLA:HMB1	1.99	0.45
2:B:149:LEU:HG	23:B:606:CLA:HBB2	1.98	0.45
2:B:247:PHE:CE2	23:B:602:CLA:H102	2.52	0.45
4:D:261[A]:PHE:CZ	32:D:406[A]:LHG:HC81	2.52	0.45
2:B:383:PHE:O	13:O:166:SER:HA	2.17	0.45
2:b:224:ARG:HH21	31:b:621:LMT:H1'	1.82	0.45
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.51	0.45
25:A:409:BCR:H24C	25:A:409:BCR:H371	1.63	0.45
32:A:419[B]:LHG:H171	23:B:613:CLA:H141	1.99	0.45
4:D:230[B]:SER:HB2	41:D:529:HOH:O	2.17	0.45
4:D:317[B]:LYS:NZ	41:D:510[B]:HOH:O	2.48	0.45
23:a:408:CLA:H203	23:c:506:CLA:H101	1.99	0.45
32:d:407[A]:LHG:H372	32:d:407[A]:LHG:H142	1.97	0.45
7:h:43:LEU:O	7:h:47:GLU:HG3	2.17	0.45
1:A:133:LEU:HD23	4:D:256[A]:ILE:HG12	1.99	0.45
23:A:404[B]:CLA:HBD	23:A:405[B]:CLA:HAC2	1.99	0.45
25:B:619:BCR:H24C	25:B:619:BCR:H371	1.76	0.45
31:B:627:LMT:H62	31:B:627:LMT:H91	1.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:5[B]:GLN:CD	12:m:5[B]:GLN:H	2.23	0.45
23:A:404[B]:CLA:H143	24:A:407[B]:PHO:H61	1.98	0.45
35:C:518[B]:DGD:HAT1	35:C:519:DGD:HBE1	1.99	0.45
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.52	0.45
1:a:105:TRP:CE2	1:a:110[A]:GLY:HA3	2.51	0.45
25:a:409:BCR:H24C	25:a:409:BCR:H371	1.79	0.45
3:c:225:VAL:HG13	3:c:289:PHE:HA	1.98	0.45
23:c:508:CLA:H18	35:c:517[B]:DGD:HAT2	1.99	0.45
3:C:223:TRP:CG	3:C:224:ILE:H	2.35	0.45
32:E:101[A]:LHG:H241	32:E:101[A]:LHG:HC61	1.83	0.45
10:k:24:VAL:HG21	18:y:25:ILE:HB	1.99	0.45
13:O:54:GLU:HG2	13:O:64:GLU:O	2.17	0.44
29:a:413[B]:PL9:H28	32:a:420[B]:LHG:H222	1.98	0.44
32:a:420[B]:LHG:H241	32:a:420[B]:LHG:HC61	1.87	0.44
3:c:406:SER:HA	3:c:420[B]:VAL:HG23	1.99	0.44
12:m:5[B]:GLN:H	12:m:5[B]:GLN:NE2	2.15	0.44
1:A:334[B]:ARG:HD3	4:D:320[B]:LEU:HD13	1.99	0.44
4:D:230[A]:SER:HB2	41:D:529:HOH:O	2.16	0.44
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.99	0.44
23:b:605:CLA:H41	23:b:605:CLA:H62	1.63	0.44
4:d:261[B]:PHE:CZ	32:d:406[B]:LHG:HC81	2.52	0.44
32:d:407[B]:LHG:C38	32:d:407[B]:LHG:H122	2.47	0.44
7:h:38:PHE:HB2	25:h:101:BCR:C10	2.46	0.44
19:Z:33:TRP:HZ2	33:Z:101:LMG:HC61	1.83	0.44
20:R:8:VAL:O	20:R:11:PRO:HD2	2.17	0.44
29:A:414[A]:PL9:H151	29:A:414[A]:PL9:H171	1.55	0.44
29:A:414[A]:PL9:H301	29:A:414[A]:PL9:H322	1.76	0.44
23:B:601:CLA:H72	23:B:601:CLA:C4D	2.47	0.44
2:B:158:LEU:HB3	2:B:199:VAL:HG22	2.00	0.44
8:I:38:GLU:HG2	8:I:38:GLU:OXT	2.17	0.44
35:c:517[A]:DGD:HAT1	35:c:518:DGD:HBF2	2.00	0.44
32:d:407[B]:LHG:H331	32:d:407[B]:LHG:H361	1.62	0.44
23:A:404[B]:CLA:CBD	23:A:405[B]:CLA:HAC2	2.48	0.44
4:D:194:ASN:HA	4:D:295[B]:SER:OG	2.17	0.44
13:O:58:ASN:HD21	13:O:61:GLN:HG3	1.81	0.44
13:o:58:ASN:HD22	13:o:61:GLN:HG3	1.82	0.44
29:A:414[B]:PL9:H43	29:A:414[B]:PL9:H471	1.59	0.44
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.87	0.44
4:D:103:ARG:HG3	5:E:73:LYS:HG3	2.00	0.44
10:K:26:PRO:O	10:K:29:PRO:HD2	2.18	0.44
13:O:130:GLN:H	13:O:130:GLN:CD	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:214[A]:MET:HB3	29:a:413[A]:PL9:H103	1.98	0.44
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.52	0.44
23:c:512:CLA:H142	23:c:512:CLA:H111	1.89	0.44
4:d:194:ASN:HA	4:d:295[B]:SER:OG	2.18	0.44
31:A:420:LMT:O3'	31:A:420:LMT:H6'2	2.18	0.44
23:B:604:CLA:HMD1	23:B:612:CLA:H203	1.99	0.44
4:D:327:ALA:HB2	27:D:412:GOL:H2	1.99	0.44
5:E:9:PRO:HA	32:E:101[A]:LHG:HC31	1.99	0.44
23:a:404[B]:CLA:H201	32:d:406[B]:LHG:H161	1.99	0.44
25:b:619:BCR:HC7	25:b:619:BCR:H311	1.68	0.44
14:t:2:GLU:HG2	14:t:3:THR:N	2.33	0.44
23:b:609:CLA:HMD1	7:h:27:THR:HB	2.00	0.44
3:c:281:MET:HE3	3:c:281:MET:HB2	1.79	0.44
25:B:618:BCR:H363	25:t:102:BCR:H19C	1.99	0.44
1:a:214[B]:MET:HE2	1:a:255[B]:PHE:CE1	2.52	0.44
25:A:409:BCR:H15C	25:A:409:BCR:H351	1.88	0.43
31:B:629:LMT:H21	34:o:301:HTG:H1	1.99	0.43
29:a:413[A]:PL9:H28	32:a:420[A]:LHG:H222	1.99	0.43
23:c:509:CLA:H112	23:c:509:CLA:H142	1.80	0.43
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.17	0.43
13:O:39[B]:ARG:NH1	13:O:244:GLU:OE2	2.42	0.43
25:T:101:BCR:H19C	25:b:618:BCR:H363	2.00	0.43
1:a:227[A]:THR:HB	1:a:231:GLU:HG3	2.00	0.43
1:a:259[A]:ILE:HG22	1:a:260[A]:PHE:CD1	2.53	0.43
23:b:614:CLA:H112	23:b:614:CLA:H72	1.62	0.43
3:c:406:SER:HA	3:c:420[A]:VAL:HG23	2.00	0.43
35:c:516[B]:DGD:HG11	41:c:606[B]:HOH:O	2.18	0.43
7:h:38:PHE:HB2	25:h:101:BCR:H10C	2.01	0.43
4:d:20:ASP:O	4:d:24:ARG:HG2	2.19	0.43
25:T:101:BCR:HC8	25:T:101:BCR:H321	2.01	0.43
1:a:261[B]:GLN:HG3	2:b:493[B]:TRP:CH2	2.54	0.43
2:b:160:GLY:HA3	2:b:180:PRO:HB3	2.00	0.43
29:A:414[A]:PL9:HC2	29:A:414[A]:PL9:HC8	1.71	0.43
29:A:414[A]:PL9:H221	29:A:414[A]:PL9:H201	1.88	0.43
31:B:629:LMT:H52	34:o:301:HTG:H4'1	2.00	0.43
3:C:130:VAL:O	3:C:134:ILE:HG12	2.18	0.43
23:C:509:CLA:HBC2	32:D:407[A]:LHG:H351	2.01	0.43
29:D:405[A]:PL9:H401	29:D:405[A]:PL9:H422	1.75	0.43
1:a:60[B]:ILE:HD12	1:a:84[B]:PRO:HD2	2.01	0.43
23:a:405[B]:CLA:HBB1	23:a:405[B]:CLA:CHC	2.46	0.43
7:h:25:TRP:O	7:h:26:GLY:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:LEU:HD21	23:C:512:CLA:H2A	2.01	0.43
3:C:275:SER:HB3	23:C:510:CLA:HED3	2.00	0.43
26:a:410[A]:SQD:H321	23:c:508:CLA:H102	2.00	0.43
29:a:413[B]:PL9:H351	6:f:25:THR:OG1	2.18	0.43
23:c:506:CLA:H3A	23:c:506:CLA:HBA1	1.83	0.43
35:c:517[B]:DGD:HA81	35:c:517[B]:DGD:HAF1	1.99	0.43
26:A:410[B]:SQD:H122	26:A:410[B]:SQD:H152	1.65	0.43
2:B:162:PHE:O	23:B:606:CLA:HHD	2.19	0.43
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.54	0.43
3:C:363:GLY:O	3:C:367:GLU:HG2	2.19	0.43
25:T:101:BCR:H11C	25:T:101:BCR:H341	1.81	0.43
16:V:57:GLU:CD	16:V:57:GLU:H	2.26	0.43
23:b:615:CLA:H112	23:b:615:CLA:H91	1.73	0.43
26:A:410[A]:SQD:H122	26:A:410[A]:SQD:H152	1.52	0.43
23:c:512:CLA:HMB2	23:c:512:CLA:H192	2.01	0.43
16:v:134[B]:LYS:HE2	27:v:202[B]:GOL:H32	2.01	0.43
18:y:30:ILE:HD12	18:y:30:ILE:HA	1.90	0.43
1:A:82[B]:VAL:HB	1:A:174[B]:LEU:HB2	2.00	0.43
29:A:414[B]:PL9:H121	29:A:414[B]:PL9:HC8	1.65	0.43
13:O:137:THR:C	13:O:139:SER:H	2.27	0.43
29:a:413[A]:PL9:H503	17:x:24:THR:OG1	2.19	0.43
3:c:443[A]:TRP:CE2	23:c:508:CLA:HMD2	2.53	0.43
29:A:414[B]:PL9:HC8	29:A:414[B]:PL9:HC2	1.85	0.43
16:v:134[B]:LYS:HB3	27:v:202[B]:GOL:H32	2.01	0.43
23:A:408:CLA:H41	23:A:408:CLA:H61	1.56	0.42
3:C:391[B]:ARG:HA	3:C:391[B]:ARG:HD3	1.82	0.42
4:D:209[A]:LEU:C	4:D:209[A]:LEU:HD23	2.44	0.42
11:L:22:LEU:HD23	32:L:101[B]:LHG:H172	2.00	0.42
1:a:261[A]:GLN:HG3	2:b:493[A]:TRP:CH2	2.54	0.42
23:a:405[B]:CLA:HHC	23:a:405[B]:CLA:CBB	2.46	0.42
24:A:407[A]:PHO:HAB	4:D:205[A]:LEU:HD13	2.00	0.42
23:C:505:CLA:H62	23:C:505:CLA:H41	1.69	0.42
4:D:209[B]:LEU:HD23	4:D:209[B]:LEU:C	2.43	0.42
32:E:101[A]:LHG:O2	6:F:19:ARG:NH1	2.52	0.42
3:C:279:LEU:HD22	23:C:510:CLA:HED2	2.01	0.42
23:A:405[A]:CLA:H203	23:A:405[A]:CLA:H162	1.76	0.42
29:A:414[B]:PL9:H221	29:A:414[B]:PL9:H201	1.88	0.42
23:B:601:CLA:HHC	23:B:601:CLA:HBB1	2.01	0.42
33:B:621:LMG:H112	33:B:621:LMG:H141	1.80	0.42
23:c:504:CLA:ND	35:c:517[A]:DGD:HB32	2.35	0.42
33:c:519:LMG:H181	10:k:27:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:6:ARG:NH1	9:j:6:ARG:HA	2.34	0.42
1:A:15:GLU:HG2	31:A:420:LMT:O3B	2.19	0.42
1:A:82[A]:VAL:HB	1:A:174[A]:LEU:HB2	2.01	0.42
26:A:410[B]:SQD:H361	10:K:34:ALA:HA	2.02	0.42
29:A:414[B]:PL9:H322	29:A:414[B]:PL9:H301	1.74	0.42
25:k:101:BCR:C12	25:y:101:BCR:H333	2.50	0.42
16:v:45[B]:ILE:HD13	27:v:202[B]:GOL:H11	2.01	0.42
23:B:613:CLA:H162	23:B:613:CLA:H121	1.70	0.42
25:B:619:BCR:H20C	25:B:619:BCR:H361	1.95	0.42
27:B:628:GOL:H12	34:o:301:HTG:O5	2.20	0.42
4:D:323[B]:GLU:O	27:D:412:GOL:O2	2.38	0.42
25:k:101:BCR:H15C	25:k:101:BCR:H351	1.93	0.42
12:m:6:LEU:HD23	12:m:6:LEU:HA	1.88	0.42
23:A:404[A]:CLA:HBB1	23:A:404[A]:CLA:HMB3	2.02	0.42
34:B:622:HTG:H7'3	34:B:622:HTG:H4'2	1.74	0.42
23:C:506:CLA:HAA1	23:C:506:CLA:HBD	2.02	0.42
33:C:521:LMG:H331	33:C:521:LMG:H362	1.94	0.42
5:E:18:ARG:H	9:J:2:SER:N	2.17	0.42
2:b:224:ARG:HH21	31:b:621:LMT:H11	1.83	0.42
3:c:130:VAL:O	3:c:134[A]:ILE:HG12	2.20	0.42
23:d:403:CLA:H41	23:d:403:CLA:H61	1.59	0.42
5:e:26:THR:HB	38:f:101:HEM:HAB	2.02	0.42
1:A:183[A]:MET:HA	23:A:404[A]:CLA:HMD1	2.01	0.42
23:A:405[B]:CLA:C4A	23:A:405[B]:CLA:HBA1	2.48	0.42
2:B:42:LEU:HD23	2:B:42:LEU:HA	1.90	0.42
23:C:503:CLA:H141	23:C:503:CLA:H161	1.83	0.42
32:D:407[A]:LHG:H302	32:D:407[A]:LHG:H332	1.81	0.42
25:b:619:BCR:H15C	25:b:619:BCR:H351	1.89	0.42
32:A:419[A]:LHG:H171	23:B:613:CLA:H141	2.01	0.42
5:E:57:ALA:H	5:E:60:GLN:HE21	1.66	0.42
1:a:93[A]:PHE:CD2	1:a:95:PRO:HD3	2.55	0.42
2:b:226:TYR:HA	2:b:231:MET:HG3	2.01	0.42
1:A:243[A]:GLU:CD	1:A:243[A]:GLU:H	2.27	0.41
24:A:416[B]:PHO:HBC2	24:A:416[B]:PHO:HHD	2.02	0.41
23:B:614:CLA:H71	23:B:614:CLA:H112	1.46	0.41
25:b:617:BCR:H24C	25:b:617:BCR:H371	1.76	0.41
35:c:517[B]:DGD:HAT1	35:c:518:DGD:HBF2	2.02	0.41
15:u:10[A]:VAL:HG12	41:u:242:HOH:O	2.20	0.41
16:v:41:HIS:HA	16:v:45[A]:ILE:O	2.20	0.41
23:A:405[B]:CLA:H162	23:A:405[B]:CLA:H203	1.81	0.41
23:B:603:CLA:H61	23:B:603:CLA:H102	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:338[B]:GLY:HA3	3:C:341[B]:LEU:O	2.20	0.41
23:C:509:CLA:H142	23:C:509:CLA:H111	1.88	0.41
8:I:12:VAL:O	8:I:16:VAL:HG23	2.19	0.41
31:M:103:LMT:H112	31:M:103:LMT:H81	1.73	0.41
15:U:53:ALA:HB1	15:U:54:PRO:HA	2.02	0.41
23:a:405[B]:CLA:C4A	23:a:405[B]:CLA:HBA1	2.50	0.41
13:o:153:THR:HA	13:o:190:PHE:HE2	1.85	0.41
25:t:102:BCR:H11C	25:t:102:BCR:H341	1.89	0.41
16:v:126:LEU:HB3	16:v:129:LYS:HB2	2.01	0.41
1:A:133:LEU:HD23	4:D:256[B]:ILE:HG12	2.00	0.41
23:B:615:CLA:H172	23:B:615:CLA:H13	1.89	0.41
25:H:101:BCR:H24C	25:H:101:BCR:H371	1.77	0.41
23:a:405[B]:CLA:H203	23:a:405[B]:CLA:H162	1.86	0.41
32:a:420[A]:LHG:H241	32:a:420[A]:LHG:HC61	1.90	0.41
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.82	0.41
23:b:611:CLA:H193	23:b:611:CLA:H162	1.88	0.41
23:c:512:CLA:H3A	23:c:512:CLA:HBA2	1.78	0.41
10:K:24:VAL:HG13	18:Y:25:ILE:HD13	2.01	0.41
27:a:419:GOL:C3	12:m:1:FME:HG2	2.48	0.41
2:b:58:GLN:C	2:b:329:PRO:HB3	2.45	0.41
2:b:162:PHE:O	23:b:606:CLA:HHD	2.20	0.41
23:b:607:CLA:H91	23:b:607:CLA:H112	1.55	0.41
23:b:616:CLA:HHC	23:b:616:CLA:HBB1	2.02	0.41
23:c:504:CLA:H151	23:c:508:CLA:H143	2.02	0.41
23:c:509:CLA:H91	23:c:509:CLA:H111	1.82	0.41
19:Z:57:LEU:HD23	19:Z:57:LEU:HA	1.82	0.41
23:a:405[A]:CLA:HHC	23:a:405[A]:CLA:CBB	2.48	0.41
23:b:606:CLA:H18	23:b:616:CLA:H93	2.01	0.41
23:b:616:CLA:H13	23:b:616:CLA:H102	1.94	0.41
16:v:117:GLY:O	16:v:121:VAL:HG23	2.20	0.41
29:A:414[A]:PL9:H43	29:A:414[A]:PL9:H471	1.69	0.41
2:B:216:HIS:CE1	23:B:609:CLA:NA	2.89	0.41
23:C:504:CLA:CBB	23:C:513:CLA:H41	2.51	0.41
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.03	0.41
6:F:21:VAL:O	6:F:25:THR:HG23	2.20	0.41
10:K:23:ASP:OD2	18:Y:21:GLN:NE2	2.52	0.41
1:a:93[B]:PHE:CD2	1:a:95:PRO:HD3	2.55	0.41
32:d:407[A]:LHG:H131	32:d:407[A]:LHG:H102	1.91	0.41
27:l:801[B]:GOL:H32	14:t:25:GLU:HB2	2.01	0.41
2:B:392:PHE:CD2	2:B:418:LYS:HG2	2.56	0.41
23:B:614:CLA:HAA1	23:B:614:CLA:HBD	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:15:PHE:H	34:D:410:HTG:H61	1.86	0.41
5:E:56:TYR:HA	5:E:60:GLN:HE21	1.85	0.41
1:a:82[B]:VAL:HB	1:a:174[B]:LEU:HB2	2.02	0.41
3:c:31:SER:CB	3:c:41:ARG:HG2	2.50	0.41
4:d:155:SER:HA	4:d:159:ILE:HB	2.02	0.41
23:d:402[B]:CLA:HAA2	23:d:402[B]:CLA:HBD	2.02	0.41
34:B:624:HTG:H61	1:a:102:LEU:HD12	2.03	0.41
10:K:16:ALA:O	10:K:19:ASP:HB2	2.21	0.41
1:a:105:TRP:CE2	1:a:110[B]:GLY:HA3	2.55	0.41
1:a:259[B]:ILE:HG22	1:a:260[B]:PHE:CD1	2.56	0.41
23:b:603:CLA:H3A	23:b:603:CLA:CGA	2.51	0.41
3:c:52:ALA:HB2	23:c:511:CLA:HMA2	2.01	0.41
25:c:514:BCR:H11C	25:c:514:BCR:H341	1.79	0.41
10:k:20:PRO:HB3	18:y:21:GLN:HG3	2.03	0.41
2:B:491[A]:VAL:HG12	4:D:136[A]:VAL:HG13	2.03	0.41
23:B:614:CLA:H192	14:t:8:PHE:CE1	2.55	0.41
23:C:506:CLA:H111	23:C:506:CLA:H93	1.68	0.41
35:C:518[A]:DGD:HAE2	35:C:518[A]:DGD:HA81	1.91	0.41
11:L:9:PRO:HA	31:m:103:LMT:H6D	2.03	0.41
1:a:162[A]:PRO:HB3	1:a:168[A]:PHE:HA	2.03	0.41
24:a:407[B]:PHO:ND	24:a:407[B]:PHO:NC	2.69	0.41
2:b:158:LEU:HB3	2:b:199:VAL:HG22	2.03	0.41
23:b:609:CLA:NC	25:h:101:BCR:H332	2.36	0.41
23:b:610:CLA:HHC	23:b:610:CLA:HBB1	2.02	0.41
23:b:615:CLA:H111	23:b:615:CLA:H152	1.91	0.41
25:b:618:BCR:H15C	25:b:618:BCR:H351	1.80	0.41
23:c:504:CLA:H62	35:c:518:DGD:HB62	2.03	0.41
25:c:514:BCR:H15C	25:c:514:BCR:H351	1.77	0.41
6:f:45:ARG:HG2	41:f:201:HOH:O	2.20	0.41
8:i:32:PRO:C	8:i:33:LYS:HD2	2.46	0.41
1:A:13:LEU:HD12	1:A:13:LEU:HA	1.83	0.41
29:A:414[A]:PL9:HC8	29:A:414[A]:PL9:H121	1.79	0.41
2:B:154:GLY:O	2:B:159:THR:HG23	2.20	0.41
2:B:201:HIS:HB2	23:B:602:CLA:C1B	2.51	0.41
25:B:617:BCR:H24C	25:B:617:BCR:H371	1.85	0.41
25:D:404:BCR:H11C	25:D:404:BCR:H341	1.98	0.41
12:M:32:GLN:HG2	31:m:103:LMT:H6'2	2.03	0.41
2:b:491[B]:VAL:HG13	4:d:136[B]:VAL:HG13	2.03	0.41
4:d:54:PHE:HB3	5:e:47:PHE:CD2	2.55	0.41
13:o:92:SER:HB3	13:o:131:PRO:HA	2.02	0.41
25:t:102:BCR:H371	25:t:102:BCR:H24C	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:445:THR:HA	41:B:704:HOH:O	2.20	0.40
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.02	0.40
9:J:17:GLY:HA3	25:Y:101:BCR:H371	2.03	0.40
1:a:261[B]:GLN:HG3	2:b:493[B]:TRP:CZ3	2.56	0.40
32:a:420[A]:LHG:H142	32:a:420[A]:LHG:H172	1.83	0.40
2:b:216:HIS:CE1	23:b:609:CLA:NA	2.88	0.40
3:c:95:LEU:HD21	23:c:501:CLA:OBD	2.21	0.40
26:A:412:SQD:H222	26:A:412:SQD:H192	1.88	0.40
3:c:146:PHE:HZ	23:c:512:CLA:HBB2	1.86	0.40
32:d:407[A]:LHG:H242	32:d:407[A]:LHG:H272	1.92	0.40
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.03	0.40
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.03	0.40
23:a:404[B]:CLA:HAA2	23:a:404[B]:CLA:HBD	2.04	0.40
3:c:117:VAL:HG12	33:c:520:LMG:H221	2.04	0.40
4:d:49:LEU:HD13	25:d:404:BCR:C15	2.50	0.40
25:y:101:BCR:H15C	25:y:101:BCR:H351	1.94	0.40
1:A:162[B]:PRO:HB3	1:A:168[B]:PHE:HA	2.03	0.40
32:E:101[B]:LHG:O2	6:F:19:ARG:NH1	2.54	0.40
11:L:14:ARG:HB3	14:T:25[A]:GLU:HG2	2.04	0.40
1:a:261[A]:GLN:HG3	2:b:493[A]:TRP:CZ3	2.55	0.40
2:b:431:GLU:OE2	41:b:701:HOH:O	2.22	0.40
23:b:604:CLA:H192	23:b:604:CLA:H162	1.92	0.40
3:c:459[B]:ILE:HG21	3:c:464[B]:GLU:HG3	2.02	0.40
35:c:517[A]:DGD:HBF2	35:c:517[A]:DGD:HBE1	1.91	0.40
33:Z:101:LMG:H141	33:Z:101:LMG:H111	1.88	0.40
1:A:131:TRP:CD2	1:A:131:TRP:C	2.98	0.40
1:A:240[B]:GLY:HA3	14:T:29[B]:ILE:HG23	2.04	0.40
23:A:406[B]:CLA:HED1	35:C:519:DGD:HAE2	2.03	0.40
3:C:330:SER:HB3	13:O:100:GLY:O	2.20	0.40
23:a:406[B]:CLA:HMB2	23:d:402[B]:CLA:H122	2.03	0.40
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.56	0.40
23:b:611:CLA:H72	23:b:611:CLA:H112	1.74	0.40
32:d:407[B]:LHG:H242	32:d:407[B]:LHG:H272	1.94	0.40
13:o:142:PHE:HB2	13:o:199:LEU:HB2	2.03	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	31
1	a	552/344 (160%)	545 (99%)	5 (1%)	2 (0%)	30	31
2	B	522/505 (103%)	514 (98%)	8 (2%)	0	100	100
2	b	521/505 (103%)	508 (98%)	13 (2%)	0	100	100
3	C	546/455 (120%)	539 (99%)	6 (1%)	1 (0%)	43	50
3	c	553/455 (122%)	542 (98%)	10 (2%)	1 (0%)	43	50
4	D	453/342 (132%)	438 (97%)	15 (3%)	0	100	100
4	d	454/342 (133%)	442 (97%)	12 (3%)	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%)	60 (97%)	2 (3%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	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	31

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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%)	92 (95%)	5 (5%)	0	100	100
15	u	98/104 (94%)	94 (96%)	4 (4%)	0	100	100
16	V	140/137 (102%)	134 (96%)	6 (4%)	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	3
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	3
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	6171/5384 (115%)	6031 (98%)	130 (2%)	10 (0%)	43	50

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	I	36	ASP
19	Z	31	GLN
3	C	416	SER
13	O	26	ALA
3	c	416	SER
19	z	30	PRO
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%)	440 (99%)	4 (1%)	70	79
1	a	443/279 (159%)	442 (100%)	1 (0%)	87	92
2	B	421/403 (104%)	416 (99%)	5 (1%)	63	74
2	b	420/403 (104%)	410 (98%)	10 (2%)	43	54
3	C	430/356 (121%)	423 (98%)	7 (2%)	55	66
3	c	436/356 (122%)	429 (98%)	7 (2%)	55	66
4	D	368/277 (133%)	365 (99%)	3 (1%)	73	80
4	d	369/277 (133%)	362 (98%)	7 (2%)	50	61
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	31
5	e	72/73 (99%)	71 (99%)	1 (1%)	59	70
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	37
7	h	55/54 (102%)	55 (100%)	0	100	100
8	I	34/34 (100%)	33 (97%)	1 (3%)	37	47
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	47
9	J	26/27 (96%)	24 (92%)	2 (8%)	12	10
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	36
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	2
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	5
11	L	36/35 (103%)	36 (100%)	0	100	100
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	30/32 (94%)	27 (90%)	3 (10%)	7	5
12	m	32/32 (100%)	30 (94%)	2 (6%)	16	16
13	O	216/207 (104%)	208 (96%)	8 (4%)	30	37
13	o	213/207 (103%)	206 (97%)	7 (3%)	33	42
14	T	32/28 (114%)	28 (88%)	4 (12%)	4	3
14	t	31/28 (111%)	31 (100%)	0	100	100
15	U	86/89 (97%)	84 (98%)	2 (2%)	44	55
15	u	87/89 (98%)	85 (98%)	2 (2%)	44	55
16	V	123/117 (105%)	123 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	v	123/117 (105%)	120 (98%)	3 (2%)	43	54
17	X	32/33 (97%)	31 (97%)	1 (3%)	35	44
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%)	18 (82%)	4 (18%)	2	0
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29	36
19	z	52/52 (100%)	46 (88%)	6 (12%)	5	3
20	R	29/29 (100%)	26 (90%)	3 (10%)	7	5
All	All	5103/4403 (116%)	4994 (98%)	109 (2%)	45	58

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243[A]	GLU
1	A	243[B]	GLU
1	A	244[A]	GLU
1	A	244[B]	GLU
2	B	161	LEU
2	B	298	LEU
2	B	299	GLU
2	B	389	LYS
2	B	419	SER
3	C	24	THR
3	C	29	GLU
3	C	142	GLU
3	C	289	PHE
3	C	315[A]	MET
3	C	315[B]	MET
3	C	471	SER
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
7	H	43	LEU
8	I	33	LYS
9	J	6	ARG

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Mol	Chain	Res	Type
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	4	THR
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
13	O	180	GLU
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
17	X	14	LEU
1	a	13	LEU
2	b	63	LEU
2	b	128	THR
2	b	161	LEU
2	b	240	SER
2	b	298	LEU
2	b	362	PHE
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
3	c	240	ILE
3	c	255	THR
3	c	289	PHE
3	c	315[A]	MET
3	c	315[B]	MET
4	d	26	ARG

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Mol	Chain	Res	Type
4	d	230[A]	SER
4	d	230[B]	SER
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
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	30	ILE
18	y	45	ASN
19	Z	3	ILE
19	Z	31	GLN
20	R	4	ARG
20	R	6	LEU
20	R	29	LYS
19	z	2	THR
19	z	3	ILE
19	z	4	LEU
19	z	7	LEU
19	z	20	VAL
19	z	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13)

such sidechains are listed below:

Mol	Chain	Res	Type
2	B	394	GLN
3	C	44	ASN
3	C	322	GLN
5	E	60	GLN
13	O	231	HIS
15	U	78	ASN
2	b	331	ASN
3	c	201	ASN
11	l	8	GLN
13	o	58	ASN
15	u	78	ASN
16	v	86	GLN
19	Z	31	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	$\# Z > 2$
14	FME	T	1	14	8,9,10	0.63	0	8,9,11	1.75	2 (25%)
12	FME	M	1	12	8,9,10	0.58	0	8,9,11	1.39	3 (37%)
8	FME	I	1	8	8,9,10	0.65	0	8,9,11	1.15	1 (12%)
8	FME	i	1	8	8,9,10	0.69	0	8,9,11	1.30	2 (25%)
14	FME	t	1	14	8,9,10	0.75	0	8,9,11	1.49	2 (25%)
12	FME	m	1	12	8,9,10	0.53	0	8,9,11	1.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-3.03	116.97	124.77
14	T	1	FME	CB-CA-N	-2.83	105.36	110.52
14	T	1	FME	CG-CB-CA	2.67	121.04	112.87
12	M	1	FME	O-C-CA	-2.51	118.31	124.77
8	I	1	FME	O-C-CA	-2.45	118.47	124.77
8	i	1	FME	CA-N-CN	-2.13	119.55	122.82
14	t	1	FME	CA-N-CN	-2.08	119.62	122.82
12	M	1	FME	CA-N-CN	-2.07	119.64	122.82
8	i	1	FME	O-C-CA	-2.02	119.57	124.77
12	M	1	FME	O1-CN-N	-2.00	120.14	125.32

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	1	FME	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	4	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
23	CLA	B	607	41	69,73,73	1.94	19 (27%)	82,113,113	2.69	33 (40%)
23	CLA	a	408	-	69,73,73	1.94	19 (27%)	82,113,113	2.77	31 (37%)
27	GOL	b	624	-	5,5,5	1.21	1 (20%)	5,5,5	0.91	0
27	GOL	o	303	-	5,5,5	1.30	0	5,5,5	0.86	0
23	CLA	A	408	-	69,73,73	1.94	19 (27%)	82,113,113	2.76	34 (41%)
23	CLA	B	601	41	69,73,73	2.04	21 (30%)	82,113,113	2.72	31 (37%)
25	BCR	H	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.50	7 (12%)
27	GOL	d	412	-	5,5,5	1.13	1 (20%)	5,5,5	1.13	0
31	LMT	F	101	-	36,36,36	1.03	1 (2%)	47,47,47	1.08	4 (8%)
28	OEX	A	413[B]	1,41,3	0,15,15	-	-	-	-	-
23	CLA	c	506	-	69,73,73	1.99	20 (28%)	82,113,113	2.68	31 (37%)
23	CLA	C	503	-	69,73,73	2.00	19 (27%)	82,113,113	2.54	30 (36%)
23	CLA	A	406[A]	41	69,73,73	2.01	19 (27%)	82,113,113	2.69	33 (40%)
35	DGD	C	519	-	63,63,67	0.86	3 (4%)	77,77,81	1.05	3 (3%)
27	GOL	C	523[A]	-	5,5,5	1.16	0	5,5,5	0.94	0
31	LMT	B	631	-	25,25,36	0.87	1 (4%)	30,30,47	1.16	3 (10%)
34	HTG	o	301	-	19,19,19	1.04	2 (10%)	23,24,24	1.60	5 (21%)
23	CLA	C	509	-	69,73,73	2.06	19 (27%)	82,113,113	2.63	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	a	410[A]	-	52,54,54	0.89	2 (3%)	62,65,65	1.80	11 (17%)
32	LHG	d	406[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.06	4 (7%)
23	CLA	d	403	-	69,73,73	2.00	19 (27%)	82,113,113	2.64	33 (40%)
23	CLA	b	612	-	69,73,73	1.99	19 (27%)	82,113,113	2.61	31 (37%)
23	CLA	D	402[B]	-	69,73,73	2.01	19 (27%)	82,113,113	2.72	31 (37%)
26	SQD	B	620	-	52,54,54	1.02	3 (5%)	62,65,65	1.73	12 (19%)
23	CLA	b	601	41	69,73,73	2.07	19 (27%)	82,113,113	2.69	30 (36%)
32	LHG	D	407[A]	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	4 (7%)
32	LHG	E	101[A]	-	41,41,48	1.08	2 (4%)	44,47,54	1.12	3 (6%)
27	GOL	B	623	-	5,5,5	0.90	0	5,5,5	1.32	1 (20%)
31	LMT	B	629	-	36,36,36	1.00	2 (5%)	47,47,47	1.17	3 (6%)
32	LHG	b	629[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.02	2 (3%)
24	PHO	a	407[B]	-	58,69,69	2.70	11 (18%)	55,99,99	2.82	19 (34%)
23	CLA	c	507	41	69,73,73	2.03	19 (27%)	82,113,113	2.72	31 (37%)
23	CLA	B	608	-	69,73,73	1.88	19 (27%)	82,113,113	2.68	35 (42%)
34	HTG	V	202	-	11,11,19	0.36	0	15,15,24	1.24	1 (6%)
34	HTG	c	521	-	19,19,19	0.87	1 (5%)	23,24,24	1.35	1 (4%)
24	PHO	a	415[B]	-	58,69,69	2.79	13 (22%)	55,99,99	2.96	16 (29%)
29	PL9	a	413[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.96	22 (32%)
38	HEM	f	101	6,5	50,50,50	1.50	6 (12%)	67,82,82	1.69	13 (19%)
33	LMG	d	411	39	51,51,55	0.87	2 (3%)	59,59,63	1.17	4 (6%)
23	CLA	A	405[B]	41	69,73,73	1.99	20 (28%)	82,113,113	2.66	35 (42%)
23	CLA	b	610	41	69,73,73	2.00	19 (27%)	82,113,113	2.77	33 (40%)
33	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.55	9 (15%)
37	BCT	d	401[A]	21	3,3,3	0.49	0	2,3,3	1.49	0
25	BCR	a	409	-	41,41,41	1.09	1 (2%)	56,56,56	1.33	9 (16%)
27	GOL	l	801[A]	-	5,5,5	0.98	0	5,5,5	1.05	1 (20%)
23	CLA	c	513	-	69,73,73	2.10	21 (30%)	82,113,113	2.69	30 (36%)
32	LHG	d	407[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.00	3 (5%)
23	CLA	C	507	-	69,73,73	2.01	21 (30%)	82,113,113	2.69	32 (39%)
24	PHO	A	407[B]	-	58,69,69	2.72	14 (24%)	55,99,99	2.91	17 (30%)
25	BCR	B	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.30	6 (10%)
35	DGD	c	517[A]	-	63,63,67	0.85	3 (4%)	77,77,81	0.98	4 (5%)
23	CLA	a	404[A]	-	69,73,73	1.97	19 (27%)	82,113,113	2.75	34 (41%)
23	CLA	B	610	41	69,73,73	2.05	19 (27%)	82,113,113	2.75	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LHG	A	419[B]	-	48,48,48	0.89	2 (4%)	51,54,54	1.19	5 (9%)
27	GOL	v	202[A]	-	5,5,5	1.26	0	5,5,5	0.88	0
33	LMG	c	519	-	51,51,55	0.91	2 (3%)	59,59,63	1.16	5 (8%)
37	BCT	D	401[A]	21	3,3,3	0.55	0	2,3,3	1.29	0
23	CLA	a	406[A]	41	69,73,73	1.96	19 (27%)	82,113,113	2.67	32 (39%)
34	HTG	C	522	-	19,19,19	0.80	1 (5%)	23,24,24	1.28	2 (8%)
23	CLA	b	606	-	69,73,73	1.97	19 (27%)	82,113,113	2.79	31 (37%)
27	GOL	V	203[B]	-	5,5,5	1.06	0	5,5,5	1.06	0
23	CLA	d	402[B]	-	69,73,73	1.98	19 (27%)	82,113,113	2.64	29 (35%)
40	HEC	V	201	16	46,50,50	1.93	7 (15%)	58,82,82	1.86	9 (15%)
33	LMG	Z	101	-	37,37,55	1.03	2 (5%)	45,45,63	1.47	7 (15%)
35	DGD	C	518[A]	-	63,63,67	0.91	3 (4%)	77,77,81	1.04	5 (6%)
23	CLA	b	614	-	69,73,73	2.00	20 (28%)	82,113,113	2.77	33 (40%)
23	CLA	c	503	-	69,73,73	2.07	20 (28%)	82,113,113	2.67	29 (35%)
31	LMT	A	420	-	36,36,36	1.01	2 (5%)	47,47,47	1.17	4 (8%)
32	LHG	a	420[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.94	2 (4%)
35	DGD	H	102	-	63,63,67	0.88	4 (6%)	77,77,81	1.15	9 (11%)
23	CLA	c	505	-	69,73,73	2.01	18 (26%)	82,113,113	2.64	28 (34%)
27	GOL	c	525[A]	-	5,5,5	1.04	0	5,5,5	1.05	0
27	GOL	D	412	-	5,5,5	1.60	2 (40%)	5,5,5	0.86	0
31	LMT	M	103	-	36,36,36	1.06	3 (8%)	47,47,47	1.08	2 (4%)
33	LMG	C	521	-	51,51,55	1.09	3 (5%)	59,59,63	1.36	6 (10%)
23	CLA	b	602	-	69,73,73	2.05	19 (27%)	82,113,113	2.86	36 (43%)
32	LHG	d	413[B]	-	48,48,48	0.93	2 (4%)	51,54,54	1.05	5 (9%)
23	CLA	b	603	-	69,73,73	1.92	20 (28%)	82,113,113	2.77	30 (36%)
25	BCR	C	516	-	41,41,41	1.07	1 (2%)	56,56,56	1.29	7 (12%)
29	PL9	A	414[B]	-	55,55,55	0.66	2 (3%)	68,69,69	2.01	26 (38%)
27	GOL	a	419	-	5,5,5	1.39	1 (20%)	5,5,5	0.99	0
35	DGD	C	517[B]	-	63,63,67	0.85	2 (3%)	77,77,81	1.07	6 (7%)
23	CLA	B	604	-	69,73,73	1.99	21 (30%)	82,113,113	2.58	32 (39%)
23	CLA	c	510	-	69,73,73	1.99	19 (27%)	82,113,113	2.75	32 (39%)
23	CLA	C	505	41	69,73,73	1.92	19 (27%)	82,113,113	2.67	26 (31%)
27	GOL	a	418	-	5,5,5	1.28	1 (20%)	5,5,5	1.03	0
25	BCR	B	617	-	41,41,41	1.10	1 (2%)	56,56,56	1.36	8 (14%)
23	CLA	B	615	-	69,73,73	1.99	18 (26%)	82,113,113	2.75	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	A	410[B]	-	52,54,54	0.87	2 (3%)	62,65,65	1.69	9 (14%)
23	CLA	b	613	-	69,73,73	1.95	18 (26%)	82,113,113	2.68	33 (40%)
23	CLA	b	605	-	69,73,73	1.95	20 (28%)	82,113,113	2.88	28 (34%)
25	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.40	5 (8%)
25	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.56	11 (19%)
23	CLA	A	406[B]	41	69,73,73	2.05	18 (26%)	82,113,113	2.68	34 (41%)
27	GOL	B	628	-	5,5,5	1.00	0	5,5,5	1.00	0
27	GOL	C	523[B]	-	5,5,5	1.18	0	5,5,5	0.86	0
23	CLA	C	504	-	69,73,73	1.97	19 (27%)	82,113,113	2.66	28 (34%)
33	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	3 (5%)
23	CLA	B	611	-	69,73,73	2.52	21 (30%)	82,113,113	3.62	32 (39%)
32	LHG	b	629[A]	-	48,48,48	0.84	3 (6%)	51,54,54	1.05	4 (7%)
33	LMG	B	621	-	51,51,55	0.89	2 (3%)	59,59,63	1.40	9 (15%)
25	BCR	c	514	-	41,41,41	1.00	1 (2%)	56,56,56	1.66	14 (25%)
29	PL9	D	405[A]	-	55,55,55	0.65	1 (1%)	68,69,69	1.61	17 (25%)
26	SQD	a	410[B]	-	52,54,54	0.90	2 (3%)	62,65,65	1.56	10 (16%)
32	LHG	d	406[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.11	4 (7%)
23	CLA	B	613	-	69,73,73	2.02	20 (28%)	82,113,113	2.63	31 (37%)
23	CLA	A	404[A]	-	69,73,73	1.98	19 (27%)	82,113,113	2.74	31 (37%)
32	LHG	D	407[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
23	CLA	B	609	-	69,73,73	2.03	17 (24%)	82,113,113	2.69	32 (39%)
32	LHG	E	101[B]	-	41,41,48	1.06	2 (4%)	44,47,54	1.12	4 (9%)
25	BCR	T	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.63	12 (21%)
25	BCR	b	618	-	41,41,41	1.01	1 (2%)	56,56,56	1.29	7 (12%)
23	CLA	a	405[A]	41	69,73,73	2.01	17 (24%)	82,113,113	2.72	31 (37%)
23	CLA	b	616	-	69,73,73	1.97	19 (27%)	82,113,113	2.77	33 (40%)
24	PHO	A	416[B]	-	58,69,69	2.83	14 (24%)	55,99,99	2.83	17 (30%)
35	DGD	c	516[A]	-	63,63,67	0.86	2 (3%)	77,77,81	1.10	8 (10%)
29	PL9	d	405[A]	-	55,55,55	0.72	1 (1%)	68,69,69	1.61	17 (25%)
23	CLA	B	614	-	69,73,73	2.02	21 (30%)	82,113,113	2.84	31 (37%)
25	BCR	Y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.76	15 (26%)
32	LHG	d	407[A]	-	48,48,48	0.92	2 (4%)	51,54,54	1.02	3 (5%)
23	CLA	B	612	-	69,73,73	1.95	20 (28%)	82,113,113	2.62	32 (39%)
27	GOL	A	418	-	5,5,5	1.73	2 (40%)	5,5,5	0.90	0
32	LHG	D	406[B]	-	48,48,48	0.89	2 (4%)	51,54,54	0.99	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HTG	b	622	-	19,19,19	1.15	3 (15%)	23,24,24	2.05	7 (30%)
37	BCT	d	401[B]	21	3,3,3	0.50	0	2,3,3	1.10	0
23	CLA	D	403	-	69,73,73	2.08	17 (24%)	82,113,113	2.72	33 (40%)
31	LMT	m	103	-	36,36,36	1.04	2 (5%)	47,47,47	1.14	4 (8%)
26	SQD	A	412	-	52,54,54	1.01	2 (3%)	62,65,65	1.22	8 (12%)
27	GOL	c	526	-	5,5,5	1.20	0	5,5,5	1.01	0
32	LHG	L	101[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.15	4 (7%)
31	LMT	A	417	-	36,36,36	0.89	0	47,47,47	1.07	2 (4%)
33	LMG	D	411	39	51,51,55	0.85	2 (3%)	59,59,63	1.14	4 (6%)
33	LMG	a	416	-	51,51,55	0.94	2 (3%)	59,59,63	1.24	5 (8%)
25	BCR	d	404	-	41,41,41	1.18	2 (4%)	56,56,56	1.96	17 (30%)
23	CLA	a	404[B]	-	69,73,73	2.04	19 (27%)	82,113,113	2.78	33 (40%)
27	GOL	b	628	-	5,5,5	0.42	0	5,5,5	1.46	1 (20%)
31	LMT	a	417	-	36,36,36	0.94	0	47,47,47	1.06	2 (4%)
23	CLA	d	402[A]	-	69,73,73	1.94	19 (27%)	82,113,113	2.64	33 (40%)
23	CLA	c	509	-	69,73,73	2.02	20 (28%)	82,113,113	2.69	31 (37%)
26	SQD	F	103	-	41,43,54	1.18	3 (7%)	51,54,65	2.16	15 (29%)
32	LHG	L	101[A]	-	48,48,48	0.89	3 (6%)	51,54,54	1.16	4 (7%)
27	GOL	v	202[B]	-	5,5,5	1.16	0	5,5,5	0.91	0
33	LMG	c	520	-	51,51,55	1.02	2 (3%)	59,59,63	1.36	6 (10%)
34	HTG	D	410	-	16,16,19	0.89	1 (6%)	20,21,24	1.38	1 (5%)
38	HEM	F	102	6,5	50,50,50	1.56	8 (16%)	67,82,82	1.80	17 (25%)
28	OEX	a	412[B]	1,41,3	0,15,15	-	-	-	-	-
37	BCT	D	401[B]	21	3,3,3	0.53	0	2,3,3	1.06	0
23	CLA	a	406[B]	41	69,73,73	1.99	19 (27%)	82,113,113	2.73	32 (39%)
23	CLA	C	513	-	69,73,73	2.02	19 (27%)	82,113,113	2.73	35 (42%)
28	OEX	A	413[A]	1,41,3	0,15,15	-	-	-	-	-
23	CLA	C	512	3	69,73,73	1.99	21 (30%)	82,113,113	2.53	29 (35%)
31	LMT	t	101	-	26,26,36	0.89	1 (3%)	31,31,47	1.38	2 (6%)
23	CLA	c	502	-	69,73,73	1.95	17 (24%)	82,113,113	2.62	30 (36%)
23	CLA	c	501	-	69,73,73	2.03	19 (27%)	82,113,113	2.66	30 (36%)
25	BCR	b	619	-	41,41,41	1.10	1 (2%)	56,56,56	1.44	9 (16%)
23	CLA	c	508	-	69,73,73	2.10	20 (28%)	82,113,113	2.66	31 (37%)
34	HTG	b	625	-	19,19,19	0.92	2 (10%)	23,24,24	1.43	3 (13%)
25	BCR	D	404	-	41,41,41	1.13	1 (2%)	56,56,56	1.92	16 (28%)
23	CLA	C	514	-	69,73,73	2.02	18 (26%)	82,113,113	2.68	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GOL	A	411	-	5,5,5	1.22	0	5,5,5	0.72	0
32	LHG	d	413[A]	-	48,48,48	0.89	3 (6%)	51,54,54	1.13	4 (7%)
35	DGD	C	518[B]	-	63,63,67	0.88	3 (4%)	77,77,81	1.02	5 (6%)
35	DGD	c	518	-	63,63,67	0.87	4 (6%)	77,77,81	1.05	3 (3%)
23	CLA	b	608	-	69,73,73	1.95	20 (28%)	82,113,113	2.72	36 (43%)
23	CLA	D	402[A]	-	69,73,73	1.98	19 (27%)	82,113,113	2.74	34 (41%)
29	PL9	A	414[A]	-	55,55,55	0.71	3 (5%)	68,69,69	2.05	25 (36%)
23	CLA	b	604	-	69,73,73	2.00	20 (28%)	82,113,113	2.56	30 (36%)
25	BCR	t	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.56	10 (17%)
23	CLA	C	510	-	69,73,73	2.00	20 (28%)	82,113,113	2.65	29 (35%)
25	BCR	c	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.37	10 (17%)
27	GOL	c	525[B]	-	5,5,5	0.98	0	5,5,5	1.08	0
31	LMT	b	627	-	25,25,36	0.88	0	30,30,47	1.11	2 (6%)
27	GOL	B	626	-	5,5,5	1.15	0	5,5,5	1.03	0
33	LMG	m	101	-	51,51,55	0.88	2 (3%)	59,59,63	1.36	6 (10%)
24	PHO	a	407[A]	-	58,69,69	2.77	13 (22%)	55,99,99	2.94	14 (25%)
23	CLA	C	502	-	69,73,73	1.93	19 (27%)	82,113,113	2.75	33 (40%)
25	BCR	b	617	-	41,41,41	1.09	2 (4%)	56,56,56	1.46	7 (12%)
25	BCR	A	409	-	41,41,41	1.04	1 (2%)	56,56,56	1.40	7 (12%)
35	DGD	c	517[B]	-	63,63,67	0.87	2 (3%)	77,77,81	0.97	6 (7%)
23	CLA	b	615	-	69,73,73	2.00	19 (27%)	82,113,113	2.66	35 (42%)
24	PHO	a	415[A]	-	58,69,69	2.79	14 (24%)	55,99,99	3.05	17 (30%)
23	CLA	C	506	-	69,73,73	2.00	19 (27%)	82,113,113	2.69	29 (35%)
26	SQD	A	410[A]	-	52,54,54	0.86	2 (3%)	62,65,65	1.85	10 (16%)
29	PL9	a	413[A]	-	55,55,55	0.68	2 (3%)	68,69,69	2.03	23 (33%)
31	LMT	e	101	-	36,36,36	0.98	1 (2%)	47,47,47	1.00	1 (2%)
23	CLA	A	405[A]	41	69,73,73	2.00	18 (26%)	82,113,113	2.70	35 (42%)
23	CLA	B	602	-	69,73,73	2.05	20 (28%)	82,113,113	2.74	34 (41%)
23	CLA	c	504	41	69,73,73	2.04	20 (28%)	82,113,113	2.63	33 (40%)
23	CLA	B	603	-	69,73,73	1.99	19 (27%)	82,113,113	2.77	32 (39%)
23	CLA	c	511	3	69,73,73	2.05	21 (30%)	82,113,113	2.73	33 (40%)
27	GOL	O	302	-	5,5,5	1.00	0	5,5,5	0.94	0
27	GOL	O	303	-	5,5,5	0.89	0	5,5,5	1.19	0
24	PHO	A	407[A]	-	58,69,69	2.66	12 (20%)	55,99,99	2.93	14 (25%)
25	BCR	y	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.63	11 (19%)
23	CLA	b	609	-	69,73,73	2.03	20 (28%)	82,113,113	2.70	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LHG	A	419[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.29	6 (11%)
27	GOL	l	801[B]	-	5,5,5	0.90	0	5,5,5	1.08	0
34	HTG	B	624	-	19,19,19	1.06	2 (10%)	23,24,24	1.05	0
23	CLA	B	616	-	69,73,73	1.98	19 (27%)	82,113,113	2.74	30 (36%)
24	PHO	A	416[A]	-	58,69,69	2.81	14 (24%)	55,99,99	2.93	16 (29%)
23	CLA	B	605	-	69,73,73	1.99	18 (26%)	82,113,113	2.96	33 (40%)
29	PL9	D	405[B]	-	55,55,55	0.62	2 (3%)	68,69,69	1.67	16 (23%)
27	GOL	V	203[A]	-	5,5,5	1.41	1 (20%)	5,5,5	0.86	0
23	CLA	A	404[B]	-	69,73,73	2.07	20 (28%)	82,113,113	2.70	34 (41%)
26	SQD	f	102	-	41,43,54	1.15	2 (4%)	51,54,65	1.48	9 (17%)
27	GOL	o	304	-	5,5,5	1.18	1 (20%)	5,5,5	1.24	1 (20%)
23	CLA	b	607	41	69,73,73	1.93	20 (28%)	82,113,113	2.55	31 (37%)
25	BCR	C	515	-	41,41,41	1.05	1 (2%)	56,56,56	1.48	6 (10%)
32	LHG	D	406[A]	-	48,48,48	0.88	3 (6%)	51,54,54	1.02	3 (5%)
23	CLA	C	508	41	69,73,73	1.93	20 (28%)	82,113,113	2.68	28 (34%)
40	HEC	v	201	16	46,50,50	1.95	5 (10%)	58,82,82	1.90	8 (13%)
23	CLA	a	405[B]	41	69,73,73	2.04	18 (26%)	82,113,113	2.65	31 (37%)
32	LHG	a	420[A]	-	41,41,48	1.06	2 (4%)	44,47,54	0.93	2 (4%)
35	DGD	h	102	-	63,63,67	0.88	3 (4%)	77,77,81	1.14	6 (7%)
35	DGD	c	516[B]	-	63,63,67	0.85	2 (3%)	77,77,81	1.09	5 (6%)
29	PL9	d	405[B]	-	55,55,55	0.69	2 (3%)	68,69,69	1.63	15 (22%)
31	LMT	B	627	-	36,36,36	1.14	3 (8%)	47,47,47	1.42	7 (14%)
31	LMT	M	101	-	36,36,36	1.13	4 (11%)	47,47,47	1.26	5 (10%)
34	HTG	d	410	-	16,16,19	0.91	1 (6%)	20,21,24	1.33	1 (5%)
26	SQD	b	620	-	52,54,54	1.00	3 (5%)	62,65,65	1.67	9 (14%)
31	LMT	b	621	-	25,25,36	0.96	1 (4%)	30,30,47	1.27	3 (10%)
35	DGD	C	517[A]	-	63,63,67	0.84	2 (3%)	77,77,81	1.20	6 (7%)
23	CLA	B	606	-	69,73,73	1.94	19 (27%)	82,113,113	2.90	32 (39%)
28	OEX	a	412[A]	1,41,3	0,15,15	-	-	-	-	-
33	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.09	4 (8%)
23	CLA	c	512	-	69,73,73	2.04	19 (27%)	82,113,113	2.70	33 (40%)
26	SQD	a	411	-	52,54,54	1.01	2 (3%)	62,65,65	1.18	8 (12%)
25	BCR	K	102	-	41,41,41	1.09	1 (2%)	56,56,56	1.43	11 (19%)
23	CLA	C	511	-	69,73,73	2.00	20 (28%)	82,113,113	2.83	32 (39%)
34	HTG	b	623	-	19,19,19	0.99	1 (5%)	23,24,24	1.72	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	611	-	69,73,73	1.91	20 (28%)	82,113,113	2.81	30 (36%)
34	HTG	B	622	-	19,19,19	0.77	1 (5%)	23,24,24	1.29	1 (4%)
25	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.49	13 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	607	41	1/1/15/20	1/39/115/115	-
23	CLA	a	408	-	1/1/15/20	9/39/115/115	-
27	GOL	b	624	-	-	2/4/4/4	-
27	GOL	o	303	-	-	2/4/4/4	-
23	CLA	A	408	-	1/1/15/20	8/39/115/115	-
23	CLA	B	601	41	1/1/15/20	13/39/115/115	-
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
27	GOL	d	412	-	-	2/4/4/4	-
31	LMT	F	101	-	-	8/21/61/61	0/2/2/2
23	CLA	c	506	-	1/1/15/20	6/39/115/115	-
23	CLA	C	503	-	1/1/15/20	7/39/115/115	-
23	CLA	A	406[A]	41	-	5/39/115/115	-
35	DGD	C	519	-	-	18/51/91/95	0/2/2/2
27	GOL	C	523[A]	-	-	0/4/4/4	-
31	LMT	B	631	-	-	11/17/37/61	0/1/1/2
34	HTG	o	301	-	-	3/10/30/30	0/1/1/1
23	CLA	C	509	-	1/1/15/20	3/39/115/115	-
26	SQD	a	410[A]	-	-	9/49/69/69	0/1/1/1
32	LHG	d	406[A]	-	-	12/53/53/53	-
23	CLA	d	403	-	1/1/15/20	8/39/115/115	-
23	CLA	b	612	-	1/1/15/20	5/39/115/115	-
23	CLA	D	402[B]	-	1/1/15/20	2/39/115/115	-
26	SQD	B	620	-	-	14/49/69/69	0/1/1/1
23	CLA	b	601	41	1/1/15/20	16/39/115/115	-
32	LHG	D	407[A]	-	-	13/53/53/53	-
32	LHG	E	101[A]	-	-	21/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	B	623	-	-	4/4/4/4	-
31	LMT	B	629	-	-	11/21/61/61	0/2/2/2
32	LHG	b	629[B]	-	-	17/53/53/53	-
24	PHO	a	407[B]	-	-	4/37/103/103	0/5/6/6
23	CLA	c	507	41	1/1/15/20	9/39/115/115	-
23	CLA	B	608	-	-	4/39/115/115	-
34	HTG	V	202	-	-	0/2/19/30	0/1/1/1
34	HTG	c	521	-	-	1/10/30/30	0/1/1/1
24	PHO	a	415[B]	-	-	1/37/103/103	0/5/6/6
29	PL9	a	413[B]	-	-	14/53/73/73	0/1/1/1
38	HEM	f	101	6,5	-	8/14/54/54	-
33	LMG	d	411	39	-	11/46/66/70	0/1/1/1
23	CLA	A	405[B]	41	1/1/15/20	3/39/115/115	-
23	CLA	b	610	41	1/1/15/20	4/39/115/115	-
33	LMG	C	501	-	-	13/46/66/70	0/1/1/1
25	BCR	a	409	-	-	0/29/63/63	0/2/2/2
27	GOL	l	801[A]	-	-	2/4/4/4	-
23	CLA	c	513	-	1/1/15/20	12/39/115/115	-
32	LHG	d	407[B]	-	-	10/53/53/53	-
23	CLA	C	507	-	1/1/15/20	11/39/115/115	-
24	PHO	A	407[B]	-	-	1/37/103/103	0/5/6/6
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
35	DGD	c	517[A]	-	-	16/51/91/95	0/2/2/2
23	CLA	a	404[A]	-	1/1/15/20	4/39/115/115	-
23	CLA	B	610	41	1/1/15/20	8/39/115/115	-
32	LHG	A	419[B]	-	-	9/53/53/53	-
27	GOL	v	202[A]	-	-	2/4/4/4	-
33	LMG	c	519	-	-	12/46/66/70	0/1/1/1
23	CLA	a	406[A]	41	-	6/39/115/115	-
34	HTG	C	522	-	-	0/10/30/30	0/1/1/1
23	CLA	b	606	-	1/1/15/20	12/39/115/115	-
27	GOL	V	203[B]	-	-	2/4/4/4	-
23	CLA	d	402[B]	-	1/1/15/20	5/39/115/115	-
40	HEC	V	201	16	-	6/14/54/54	-
33	LMG	Z	101	-	-	11/31/51/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	C	518[A]	-	-	12/51/91/95	0/2/2/2
23	CLA	b	614	-	1/1/15/20	11/39/115/115	-
23	CLA	c	503	-	1/1/15/20	1/39/115/115	-
31	LMT	A	420	-	-	16/21/61/61	0/2/2/2
32	LHG	a	420[B]	-	-	16/46/46/53	-
35	DGD	H	102	-	-	10/51/91/95	0/2/2/2
23	CLA	c	505	-	1/1/15/20	6/39/115/115	-
27	GOL	c	525[A]	-	-	0/4/4/4	-
27	GOL	D	412	-	-	4/4/4/4	-
31	LMT	M	103	-	-	8/21/61/61	0/2/2/2
33	LMG	C	521	-	-	15/46/66/70	0/1/1/1
23	CLA	b	602	-	1/1/15/20	5/39/115/115	-
32	LHG	d	413[B]	-	-	10/53/53/53	-
23	CLA	b	603	-	1/1/15/20	6/39/115/115	-
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
29	PL9	A	414[B]	-	-	13/53/73/73	0/1/1/1
27	GOL	a	419	-	-	0/4/4/4	-
35	DGD	C	517[B]	-	-	15/51/91/95	0/2/2/2
23	CLA	B	604	-	1/1/15/20	4/39/115/115	-
23	CLA	c	510	-	1/1/15/20	10/39/115/115	-
23	CLA	C	505	41	1/1/15/20	7/39/115/115	-
27	GOL	a	418	-	-	2/4/4/4	-
25	BCR	B	617	-	-	1/29/63/63	0/2/2/2
23	CLA	B	615	-	1/1/15/20	6/39/115/115	-
26	SQD	A	410[B]	-	-	12/49/69/69	0/1/1/1
23	CLA	b	613	-	1/1/15/20	5/39/115/115	-
23	CLA	b	605	-	1/1/15/20	6/39/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
25	BCR	h	101	-	-	0/29/63/63	0/2/2/2
23	CLA	A	406[B]	41	-	4/39/115/115	-
27	GOL	B	628	-	-	4/4/4/4	-
27	GOL	C	523[B]	-	-	0/4/4/4	-
23	CLA	C	504	-	1/1/15/20	3/39/115/115	-
33	LMG	C	520	-	-	15/46/66/70	0/1/1/1
23	CLA	B	611	-	1/1/15/20	2/39/115/115	-
32	LHG	b	629[A]	-	-	15/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	B	621	-	-	19/46/66/70	0/1/1/1
25	BCR	c	514	-	-	0/29/63/63	0/2/2/2
29	PL9	D	405[A]	-	-	6/53/73/73	0/1/1/1
26	SQD	a	410[B]	-	-	10/49/69/69	0/1/1/1
32	LHG	d	406[B]	-	-	16/53/53/53	-
23	CLA	B	613	-	1/1/15/20	7/39/115/115	-
23	CLA	A	404[A]	-	1/1/15/20	3/39/115/115	-
32	LHG	D	407[B]	-	-	12/53/53/53	-
23	CLA	B	609	-	1/1/15/20	1/39/115/115	-
32	LHG	E	101[B]	-	-	20/46/46/53	-
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	a	405[A]	41	1/1/15/20	4/39/115/115	-
23	CLA	b	616	-	1/1/15/20	9/39/115/115	-
24	PHO	A	416[B]	-	-	1/37/103/103	0/5/6/6
35	DGD	c	516[A]	-	-	17/51/91/95	0/2/2/2
29	PL9	d	405[A]	-	-	6/53/73/73	0/1/1/1
23	CLA	B	614	-	1/1/15/20	13/39/115/115	-
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
32	LHG	d	407[A]	-	-	12/53/53/53	-
23	CLA	B	612	-	1/1/15/20	3/39/115/115	-
27	GOL	A	418	-	-	1/4/4/4	-
32	LHG	D	406[B]	-	-	17/53/53/53	-
34	HTG	b	622	-	-	4/10/30/30	0/1/1/1
23	CLA	D	403	-	1/1/15/20	13/39/115/115	-
31	LMT	m	103	-	-	4/21/61/61	0/2/2/2
26	SQD	A	412	-	-	14/49/69/69	0/1/1/1
27	GOL	c	526	-	-	3/4/4/4	-
32	LHG	L	101[B]	-	-	18/53/53/53	-
31	LMT	A	417	-	-	7/21/61/61	0/2/2/2
33	LMG	D	411	39	-	10/46/66/70	0/1/1/1
33	LMG	a	416	-	-	14/46/66/70	0/1/1/1
25	BCR	d	404	-	-	3/29/63/63	0/2/2/2
23	CLA	a	404[B]	-	1/1/15/20	6/39/115/115	-
27	GOL	b	628	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	a	417	-	-	10/21/61/61	0/2/2/2
23	CLA	d	402[A]	-	1/1/15/20	4/39/115/115	-
23	CLA	c	509	-	1/1/15/20	14/39/115/115	-
26	SQD	F	103	-	-	15/38/58/69	0/1/1/1
32	LHG	L	101[A]	-	-	20/53/53/53	-
27	GOL	v	202[B]	-	-	2/4/4/4	-
33	LMG	c	520	-	-	11/46/66/70	0/1/1/1
34	HTG	D	410	-	-	3/7/27/30	0/1/1/1
38	HEM	F	102	6,5	-	8/14/54/54	-
23	CLA	a	406[B]	41	-	5/39/115/115	-
23	CLA	C	513	-	1/1/15/20	9/39/115/115	-
23	CLA	C	512	3	1/1/15/20	3/39/115/115	-
31	LMT	t	101	-	-	9/17/38/61	0/1/1/2
23	CLA	c	502	-	1/1/15/20	6/39/115/115	-
23	CLA	c	501	-	1/1/15/20	2/39/115/115	-
25	BCR	b	619	-	-	6/29/63/63	0/2/2/2
23	CLA	c	508	-	1/1/15/20	3/39/115/115	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
25	BCR	D	404	-	-	4/29/63/63	0/2/2/2
23	CLA	C	514	-	1/1/15/20	7/39/115/115	-
27	GOL	A	411	-	-	2/4/4/4	-
32	LHG	d	413[A]	-	-	15/53/53/53	-
35	DGD	C	518[B]	-	-	12/51/91/95	0/2/2/2
35	DGD	c	518	-	-	8/51/91/95	0/2/2/2
23	CLA	b	608	-	-	6/39/115/115	-
23	CLA	D	402[A]	-	1/1/15/20	2/39/115/115	-
29	PL9	A	414[A]	-	-	14/53/73/73	0/1/1/1
23	CLA	b	604	-	1/1/15/20	10/39/115/115	-
25	BCR	t	102	-	-	1/29/63/63	0/2/2/2
23	CLA	C	510	-	1/1/15/20	6/39/115/115	-
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
27	GOL	c	525[B]	-	-	0/4/4/4	-
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
27	GOL	B	626	-	-	2/4/4/4	-
33	LMG	m	101	-	-	12/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	a	407[A]	-	-	6/37/103/103	0/5/6/6
23	CLA	C	502	-	1/1/15/20	5/39/115/115	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
35	DGD	c	517[B]	-	-	14/51/91/95	0/2/2/2
23	CLA	b	615	-	1/1/15/20	8/39/115/115	-
24	PHO	a	415[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	C	506	-	1/1/15/20	7/39/115/115	-
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1
29	PL9	a	413[A]	-	-	14/53/73/73	0/1/1/1
31	LMT	e	101	-	-	15/21/61/61	0/2/2/2
23	CLA	A	405[A]	41	1/1/15/20	1/39/115/115	-
23	CLA	B	602	-	1/1/15/20	10/39/115/115	-
23	CLA	c	504	41	1/1/15/20	8/39/115/115	-
23	CLA	B	603	-	1/1/15/20	5/39/115/115	-
23	CLA	c	511	3	1/1/15/20	5/39/115/115	-
27	GOL	O	302	-	-	2/4/4/4	-
27	GOL	O	303	-	-	2/4/4/4	-
24	PHO	A	407[A]	-	-	0/37/103/103	0/5/6/6
25	BCR	y	101	-	-	3/29/63/63	0/2/2/2
23	CLA	b	609	-	1/1/15/20	0/39/115/115	-
32	LHG	A	419[A]	-	-	14/53/53/53	-
27	GOL	l	801[B]	-	-	2/4/4/4	-
34	HTG	B	624	-	-	4/10/30/30	0/1/1/1
23	CLA	B	616	-	1/1/15/20	7/39/115/115	-
24	PHO	A	416[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	B	605	-	1/1/15/20	4/39/115/115	-
29	PL9	D	405[B]	-	-	8/53/73/73	0/1/1/1
27	GOL	V	203[A]	-	-	2/4/4/4	-
23	CLA	A	404[B]	-	1/1/15/20	7/39/115/115	-
26	SQD	f	102	-	-	13/38/58/69	0/1/1/1
27	GOL	o	304	-	-	2/4/4/4	-
23	CLA	b	607	41	1/1/15/20	1/39/115/115	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
32	LHG	D	406[A]	-	-	17/53/53/53	-
23	CLA	C	508	41	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	HEC	v	201	16	-	6/14/54/54	-
23	CLA	a	405[B]	41	1/1/15/20	2/39/115/115	-
32	LHG	a	420[A]	-	-	16/46/46/53	-
35	DGD	h	102	-	-	11/51/91/95	0/2/2/2
35	DGD	c	516[B]	-	-	17/51/91/95	0/2/2/2
29	PL9	d	405[B]	-	-	7/53/73/73	0/1/1/1
31	LMT	B	627	-	-	12/21/61/61	0/2/2/2
31	LMT	M	101	-	-	5/21/61/61	0/2/2/2
34	HTG	d	410	-	-	1/7/27/30	0/1/1/1
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
31	LMT	b	621	-	-	8/17/37/61	0/1/1/2
35	DGD	C	517[A]	-	-	15/51/91/95	0/2/2/2
23	CLA	B	606	-	1/1/15/20	5/39/115/115	-
33	LMG	z	101	-	-	9/34/54/70	0/1/1/1
23	CLA	c	512	-	1/1/15/20	13/39/115/115	-
26	SQD	a	411	-	-	15/49/69/69	0/1/1/1
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
23	CLA	C	511	-	1/1/15/20	13/39/115/115	-
34	HTG	b	623	-	-	5/10/30/30	0/1/1/1
23	CLA	b	611	-	1/1/15/20	3/39/115/115	-
34	HTG	B	622	-	-	2/10/30/30	0/1/1/1
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2

All (1845) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407[A]	PHO	C1B-C2B	9.37	1.49	1.39
24	A	407[B]	PHO	C1D-C2D	9.27	1.49	1.39
24	a	415[B]	PHO	C1B-C2B	9.15	1.49	1.39
24	A	416[B]	PHO	C1B-C2B	9.08	1.49	1.39
24	A	407[A]	PHO	C1D-C2D	9.05	1.49	1.39
24	a	415[B]	PHO	C1D-C2D	9.04	1.49	1.39
24	a	407[B]	PHO	C1D-C2D	8.98	1.49	1.39
24	a	415[A]	PHO	C1B-C2B	8.84	1.49	1.39
24	A	416[A]	PHO	C1B-C2B	8.80	1.49	1.39
24	a	415[A]	PHO	C1D-C2D	8.76	1.49	1.39
24	A	416[B]	PHO	C1D-C2D	8.72	1.49	1.39
24	A	416[A]	PHO	C1D-C2D	8.67	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407[A]	PHO	C1B-C2B	8.59	1.48	1.39
24	a	407[A]	PHO	C1D-C2D	8.55	1.48	1.39
24	A	407[B]	PHO	C1B-C2B	8.40	1.48	1.39
24	a	407[B]	PHO	C1B-C2B	8.29	1.48	1.39
24	a	415[A]	PHO	C3B-C4B	8.28	1.49	1.41
24	A	416[B]	PHO	C3B-C4B	8.10	1.49	1.41
24	A	416[A]	PHO	C3B-C4B	8.05	1.49	1.41
24	a	407[A]	PHO	C3B-C4B	7.53	1.49	1.41
24	a	415[B]	PHO	C3B-C4B	7.48	1.49	1.41
24	a	407[B]	PHO	C3B-C4B	7.35	1.48	1.41
23	B	611	CLA	CMB-C2B	7.33	1.65	1.50
24	A	407[B]	PHO	C3B-C4B	7.21	1.48	1.41
40	V	201	HEC	CAC-C3C	7.18	1.58	1.35
23	B	611	CLA	C1B-C2B	7.09	1.59	1.43
24	A	407[B]	PHO	C4D-CHA	7.01	1.50	1.39
24	a	407[A]	PHO	C4D-CHA	7.01	1.50	1.39
24	A	407[A]	PHO	C3B-C4B	6.95	1.48	1.41
40	v	201	HEC	CAC-C3C	6.87	1.57	1.35
24	a	407[B]	PHO	C4D-CHA	6.83	1.49	1.39
24	A	416[B]	PHO	C3B-C2B	6.81	1.49	1.40
40	v	201	HEC	CAB-C3B	6.72	1.56	1.35
24	A	416[A]	PHO	C4D-CHA	6.72	1.49	1.39
24	A	416[B]	PHO	C4D-CHA	6.63	1.49	1.39
24	A	407[A]	PHO	C4D-CHA	6.57	1.49	1.39
24	a	407[A]	PHO	C3B-C2B	6.55	1.49	1.40
24	a	415[B]	PHO	C4D-CHA	6.52	1.49	1.39
24	a	415[A]	PHO	C4D-CHA	6.48	1.49	1.39
40	V	201	HEC	CAB-C3B	6.38	1.55	1.35
24	a	415[B]	PHO	C3B-C2B	6.30	1.48	1.40
24	a	407[B]	PHO	C3B-C2B	6.29	1.48	1.40
24	A	407[A]	PHO	C3B-C2B	6.28	1.48	1.40
24	A	416[A]	PHO	C3B-C2B	6.09	1.48	1.40
24	A	407[B]	PHO	C3B-C2B	6.09	1.48	1.40
24	a	415[A]	PHO	C3B-C2B	6.02	1.48	1.40
40	v	201	HEC	C3D-C2D	5.83	1.54	1.38
23	B	611	CLA	CHC-C1C	5.77	1.50	1.38
23	B	611	CLA	C1D-ND	5.77	1.45	1.37
23	C	513	CLA	C3C-C2C	5.68	1.49	1.36
23	B	611	CLA	C3C-C2C	5.68	1.49	1.36
23	c	508	CLA	O2D-CGD	5.66	1.47	1.33
24	a	415[A]	PHO	OBD-CAD	5.65	1.29	1.22
23	B	610	CLA	C3C-C2C	5.65	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407[B]	PHO	C3D-C2D	5.64	1.49	1.39
23	B	605	CLA	C3C-C2C	5.63	1.48	1.36
24	A	416[A]	PHO	OBD-CAD	5.63	1.29	1.22
24	a	415[B]	PHO	C3D-C2D	5.62	1.49	1.39
24	a	415[A]	PHO	C3D-C2D	5.62	1.49	1.39
24	a	407[A]	PHO	C3D-C2D	5.61	1.49	1.39
24	A	416[B]	PHO	C3D-C2D	5.59	1.49	1.39
23	C	504	CLA	C3C-C2C	5.53	1.48	1.36
23	a	405[A]	CLA	C3C-C2C	5.48	1.48	1.36
23	a	404[B]	CLA	C3C-C2C	5.48	1.48	1.36
24	A	416[A]	PHO	C3D-C2D	5.48	1.49	1.39
23	a	406[B]	CLA	C3C-C2C	5.46	1.48	1.36
23	b	609	CLA	O2D-CGD	5.42	1.46	1.33
23	b	615	CLA	C3C-C2C	5.41	1.48	1.36
24	a	415[B]	PHO	OBD-CAD	5.40	1.29	1.22
23	c	505	CLA	C3C-C2C	5.39	1.48	1.36
23	D	402[B]	CLA	C3C-C2C	5.39	1.48	1.36
23	a	405[B]	CLA	C3C-C2C	5.38	1.48	1.36
23	D	403	CLA	C3C-C2C	5.36	1.48	1.36
23	b	610	CLA	CHC-C1C	5.36	1.49	1.38
23	d	403	CLA	C3C-C2C	5.35	1.48	1.36
23	b	612	CLA	C3C-C2C	5.34	1.48	1.36
23	D	403	CLA	C1D-ND	5.34	1.44	1.37
23	A	404[B]	CLA	C3C-C2C	5.34	1.48	1.36
23	A	404[A]	CLA	C3C-C2C	5.33	1.48	1.36
23	c	503	CLA	C3C-C2C	5.33	1.48	1.36
23	a	405[B]	CLA	C1D-ND	5.32	1.44	1.37
23	A	406[B]	CLA	C3C-C2C	5.32	1.48	1.36
23	b	605	CLA	C3C-C2C	5.32	1.48	1.36
23	c	511	CLA	C1D-ND	5.32	1.44	1.37
23	C	511	CLA	C1D-ND	5.30	1.44	1.37
23	c	512	CLA	C3C-C2C	5.29	1.48	1.36
23	C	513	CLA	CHC-C1C	5.29	1.49	1.38
23	c	510	CLA	O2D-CGD	5.28	1.46	1.33
23	A	406[B]	CLA	CHC-C1C	5.28	1.49	1.38
23	C	506	CLA	CHC-C1C	5.26	1.49	1.38
23	b	603	CLA	C3C-C2C	5.25	1.48	1.36
23	b	601	CLA	C3C-C2C	5.24	1.48	1.36
24	A	416[B]	PHO	OBD-CAD	5.23	1.29	1.22
23	d	402[B]	CLA	C3C-C2C	5.22	1.48	1.36
23	a	406[A]	CLA	C3C-C2C	5.21	1.48	1.36
23	c	513	CLA	C1D-ND	5.21	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	402[A]	CLA	C3C-C2C	5.21	1.48	1.36
23	B	601	CLA	C3C-C2C	5.21	1.48	1.36
23	b	610	CLA	C3C-C2C	5.20	1.48	1.36
23	a	408	CLA	CHC-C1C	5.19	1.48	1.38
23	c	513	CLA	C3C-C2C	5.19	1.48	1.36
23	A	408	CLA	C3C-C2C	5.19	1.48	1.36
24	a	407[A]	PHO	O2D-CGD	5.19	1.46	1.33
23	c	504	CLA	O2D-CGD	5.18	1.46	1.33
23	b	606	CLA	C3C-C2C	5.18	1.47	1.36
23	C	510	CLA	C3C-C2C	5.18	1.47	1.36
25	d	404	BCR	C23-C22	-5.18	1.34	1.46
23	C	509	CLA	C3C-C2C	5.17	1.47	1.36
23	B	609	CLA	CHC-C1C	5.16	1.48	1.38
23	B	613	CLA	CHC-C1C	5.16	1.48	1.38
23	c	505	CLA	CHC-C1C	5.16	1.48	1.38
23	c	510	CLA	C1D-ND	5.16	1.44	1.37
23	B	604	CLA	C3C-C2C	5.15	1.47	1.36
23	b	614	CLA	C3C-C2C	5.15	1.47	1.36
23	b	607	CLA	C3C-C2C	5.15	1.47	1.36
23	b	605	CLA	O2D-CGD	5.15	1.45	1.33
23	A	404[B]	CLA	C1D-ND	5.15	1.44	1.37
23	b	616	CLA	C3C-C2C	5.15	1.47	1.36
23	c	508	CLA	C3C-C2C	5.15	1.47	1.36
23	B	603	CLA	C3C-C2C	5.14	1.47	1.36
23	b	601	CLA	C1D-ND	5.14	1.44	1.37
23	c	503	CLA	CHC-C1C	5.14	1.48	1.38
23	B	601	CLA	O2A-CGA	5.14	1.48	1.33
23	c	509	CLA	O2D-CGD	5.13	1.45	1.33
23	c	509	CLA	C3C-C2C	5.12	1.47	1.36
23	B	602	CLA	C3C-C2C	5.12	1.47	1.36
23	c	501	CLA	CHC-C1C	5.11	1.48	1.38
23	B	606	CLA	CHC-C1C	5.11	1.48	1.38
23	B	616	CLA	C3C-C2C	5.11	1.47	1.36
23	C	511	CLA	C3C-C2C	5.11	1.47	1.36
23	b	615	CLA	CHC-C1C	5.10	1.48	1.38
23	C	508	CLA	C3C-C2C	5.10	1.47	1.36
23	c	506	CLA	O2D-CGD	5.10	1.45	1.33
23	C	509	CLA	O2D-CGD	5.09	1.45	1.33
23	A	405[A]	CLA	O2D-CGD	5.09	1.45	1.33
23	b	609	CLA	CHC-C1C	5.08	1.48	1.38
23	c	508	CLA	C1D-ND	5.08	1.44	1.37
23	b	604	CLA	C3C-C2C	5.07	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	V	201	HEC	C3D-C2D	5.07	1.52	1.38
23	c	504	CLA	C1D-ND	5.07	1.44	1.37
25	K	102	BCR	C23-C22	-5.07	1.35	1.46
23	b	613	CLA	CHC-C1C	5.06	1.48	1.38
23	B	609	CLA	C3C-C2C	5.06	1.47	1.36
23	B	606	CLA	C3C-C2C	5.05	1.47	1.36
23	A	406[A]	CLA	C3C-C2C	5.04	1.47	1.36
23	D	403	CLA	CHC-C1C	5.04	1.48	1.38
23	A	406[A]	CLA	CHC-C1C	5.03	1.48	1.38
38	F	102	HEM	FE-NB	5.03	2.10	1.94
23	C	512	CLA	O2D-CGD	5.03	1.45	1.33
23	c	501	CLA	C3C-C2C	5.02	1.47	1.36
23	D	402[B]	CLA	O2D-CGD	5.02	1.45	1.33
23	a	405[B]	CLA	O2D-CGD	5.01	1.45	1.33
23	a	405[A]	CLA	C1D-ND	5.01	1.44	1.37
23	B	614	CLA	C3C-C2C	5.01	1.47	1.36
23	A	404[B]	CLA	CHC-C1C	5.01	1.48	1.38
23	c	502	CLA	C3C-C2C	5.00	1.47	1.36
23	b	603	CLA	O2D-CGD	5.00	1.45	1.33
23	d	402[A]	CLA	C3C-C2C	5.00	1.47	1.36
23	a	406[B]	CLA	O2D-CGD	4.99	1.45	1.33
23	b	602	CLA	CHC-C1C	4.99	1.48	1.38
23	B	614	CLA	C1D-ND	4.99	1.44	1.37
23	c	511	CLA	C3C-C2C	4.98	1.47	1.36
23	A	405[B]	CLA	C3C-C2C	4.98	1.47	1.36
23	c	504	CLA	C3C-C2C	4.98	1.47	1.36
25	C	515	BCR	C23-C22	-4.98	1.35	1.46
23	A	408	CLA	O2D-CGD	4.97	1.45	1.33
23	C	506	CLA	C3C-C2C	4.96	1.47	1.36
23	C	507	CLA	O2D-CGD	4.96	1.45	1.33
23	C	502	CLA	CHC-C1C	4.96	1.48	1.38
23	C	505	CLA	C3C-C2C	4.96	1.47	1.36
25	k	101	BCR	C23-C22	-4.96	1.35	1.46
23	A	406[B]	CLA	O2D-CGD	4.95	1.45	1.33
23	a	404[B]	CLA	CHC-C1C	4.95	1.48	1.38
23	B	610	CLA	O2D-CGD	4.95	1.45	1.33
38	f	101	HEM	FE-NB	4.95	2.10	1.94
23	c	512	CLA	CHC-C1C	4.95	1.48	1.38
24	A	416[B]	PHO	O2D-CGD	4.94	1.45	1.33
23	a	408	CLA	C3C-C2C	4.94	1.47	1.36
24	A	407[B]	PHO	C3D-C2D	4.94	1.48	1.39
23	c	506	CLA	C3C-C2C	4.93	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	C3C-C2C	4.93	1.47	1.36
23	a	404[A]	CLA	C3C-C2C	4.93	1.47	1.36
23	b	602	CLA	C3C-C2C	4.93	1.47	1.36
23	B	613	CLA	O2D-CGD	4.93	1.45	1.33
23	C	507	CLA	C3C-C2C	4.93	1.47	1.36
23	c	501	CLA	C1D-ND	4.92	1.44	1.37
24	a	415[B]	PHO	O2D-CGD	4.92	1.45	1.33
23	C	508	CLA	CHC-C1C	4.91	1.48	1.38
23	b	601	CLA	O2A-CGA	4.91	1.47	1.33
23	c	513	CLA	O2D-CGD	4.91	1.45	1.33
24	A	407[A]	PHO	C3D-C2D	4.91	1.48	1.39
26	F	103	SQD	O47-C7	4.91	1.48	1.34
23	A	405[B]	CLA	O2D-CGD	4.91	1.45	1.33
23	a	404[B]	CLA	C1D-ND	4.91	1.44	1.37
23	a	405[A]	CLA	O2D-CGD	4.90	1.45	1.33
24	A	407[B]	PHO	OBD-CAD	4.90	1.28	1.22
24	A	416[A]	PHO	O2D-CGD	4.90	1.45	1.33
23	B	613	CLA	C3C-C2C	4.90	1.47	1.36
23	C	509	CLA	C1D-ND	4.89	1.44	1.37
24	a	407[B]	PHO	O2D-CGD	4.88	1.45	1.33
23	B	616	CLA	CHC-C1C	4.87	1.48	1.38
23	d	403	CLA	C1D-ND	4.87	1.44	1.37
23	A	405[A]	CLA	C3C-C2C	4.87	1.47	1.36
23	C	503	CLA	C1D-ND	4.86	1.44	1.37
23	c	507	CLA	O2D-CGD	4.86	1.45	1.33
24	A	407[A]	PHO	O2D-CGD	4.86	1.45	1.33
23	B	601	CLA	O2D-CGD	4.86	1.45	1.33
23	C	514	CLA	C3C-C2C	4.86	1.47	1.36
23	b	602	CLA	O2D-CGD	4.85	1.45	1.33
23	b	609	CLA	C3C-C2C	4.85	1.47	1.36
23	C	513	CLA	C1D-ND	4.85	1.44	1.37
23	B	604	CLA	CHC-C1C	4.85	1.48	1.38
25	B	619	BCR	C23-C22	-4.84	1.35	1.46
23	C	502	CLA	C3C-C2C	4.84	1.47	1.36
33	c	520	LMG	O7-C10	4.84	1.48	1.34
24	A	407[B]	PHO	O2D-CGD	4.84	1.45	1.33
23	B	605	CLA	O2D-CGD	4.84	1.45	1.33
23	D	402[A]	CLA	O2D-CGD	4.83	1.45	1.33
23	a	406[B]	CLA	CHC-C1C	4.83	1.48	1.38
23	d	403	CLA	CHC-C1C	4.83	1.48	1.38
23	a	404[B]	CLA	O2D-CGD	4.81	1.45	1.33
23	C	503	CLA	O2D-CGD	4.81	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	CHC-C1C	4.81	1.48	1.38
23	B	615	CLA	C3C-C2C	4.80	1.47	1.36
23	B	611	CLA	O2D-CGD	4.80	1.45	1.33
23	B	601	CLA	CHC-C1C	4.79	1.48	1.38
24	a	415[A]	PHO	O2D-CGD	4.79	1.45	1.33
23	c	507	CLA	C3C-C2C	4.79	1.47	1.36
23	b	606	CLA	CHC-C1C	4.79	1.48	1.38
23	B	608	CLA	C3C-C2C	4.79	1.47	1.36
23	C	511	CLA	CHC-C1C	4.79	1.48	1.38
23	C	514	CLA	O2D-CGD	4.78	1.45	1.33
23	b	616	CLA	CHC-C1C	4.78	1.48	1.38
23	B	612	CLA	C1B-NB	-4.78	1.31	1.37
23	A	404[B]	CLA	O2D-CGD	4.77	1.45	1.33
25	B	617	BCR	C23-C22	-4.77	1.35	1.46
23	B	615	CLA	CHD-C1D	4.77	1.47	1.38
23	b	613	CLA	C1D-ND	4.77	1.44	1.37
23	C	504	CLA	CHC-C1C	4.76	1.48	1.38
23	B	602	CLA	C1D-ND	4.76	1.44	1.37
23	b	601	CLA	O2D-CGD	4.76	1.44	1.33
23	A	405[B]	CLA	CHC-C1C	4.76	1.48	1.38
23	C	510	CLA	O2D-CGD	4.75	1.44	1.33
23	c	503	CLA	CHD-C1D	4.75	1.47	1.38
23	B	602	CLA	O2D-CGD	4.74	1.44	1.33
25	D	404	BCR	C23-C22	-4.74	1.35	1.46
23	c	512	CLA	C1D-ND	4.74	1.44	1.37
23	a	404[A]	CLA	C1D-ND	4.74	1.44	1.37
23	c	508	CLA	CHC-C1C	4.74	1.48	1.38
23	A	404[A]	CLA	C1D-ND	4.74	1.44	1.37
25	T	101	BCR	C23-C22	-4.74	1.35	1.46
23	c	503	CLA	C1D-ND	4.73	1.44	1.37
23	B	611	CLA	CHC-C4B	4.73	1.50	1.39
23	B	607	CLA	C3C-C2C	4.73	1.47	1.36
23	b	601	CLA	CHC-C1C	4.73	1.48	1.38
23	B	602	CLA	CHC-C1C	4.72	1.47	1.38
23	a	404[A]	CLA	CHC-C1C	4.72	1.47	1.38
23	A	404[A]	CLA	O2D-CGD	4.72	1.44	1.33
23	B	612	CLA	CHC-C1C	4.72	1.47	1.38
23	C	514	CLA	CHC-C1C	4.72	1.47	1.38
23	C	505	CLA	O2D-CGD	4.72	1.44	1.33
25	b	619	BCR	C23-C22	-4.72	1.35	1.46
23	b	604	CLA	CHC-C1C	4.72	1.47	1.38
23	B	604	CLA	CHD-C1D	4.72	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	O2D-CGD	4.72	1.44	1.33
23	c	513	CLA	CHC-C1C	4.71	1.47	1.38
23	B	606	CLA	O2D-CGD	4.71	1.44	1.33
23	D	403	CLA	O2D-CGD	4.71	1.44	1.33
23	B	615	CLA	CHC-C1C	4.71	1.47	1.38
23	c	510	CLA	C3C-C2C	4.71	1.46	1.36
23	B	613	CLA	C1D-ND	4.71	1.44	1.37
23	b	610	CLA	O2D-CGD	4.70	1.44	1.33
23	A	405[A]	CLA	CHC-C1C	4.69	1.47	1.38
23	b	613	CLA	C3C-C2C	4.69	1.46	1.36
23	B	604	CLA	O2D-CGD	4.69	1.44	1.33
23	a	406[A]	CLA	CHC-C1C	4.69	1.47	1.38
23	b	611	CLA	C3C-C2C	4.69	1.46	1.36
23	A	406[B]	CLA	C1D-ND	4.68	1.44	1.37
23	B	609	CLA	O2D-CGD	4.68	1.44	1.33
23	A	406[A]	CLA	O2D-CGD	4.68	1.44	1.33
33	C	521	LMG	O7-C10	4.68	1.47	1.34
23	b	608	CLA	O2D-CGD	4.68	1.44	1.33
23	B	603	CLA	O2D-CGD	4.68	1.44	1.33
25	A	409	BCR	C23-C22	-4.67	1.35	1.46
23	b	608	CLA	C3C-C2C	4.67	1.46	1.36
23	c	506	CLA	C1D-ND	4.67	1.44	1.37
23	D	402[B]	CLA	CHC-C1C	4.66	1.47	1.38
23	B	615	CLA	O2D-CGD	4.66	1.44	1.33
23	B	612	CLA	C3C-C2C	4.66	1.46	1.36
23	c	511	CLA	O2D-CGD	4.66	1.44	1.33
25	C	516	BCR	C23-C22	-4.66	1.36	1.46
26	a	411	SQD	O48-C23	4.65	1.46	1.33
23	b	614	CLA	O2D-CGD	4.65	1.44	1.33
24	a	407[B]	PHO	OBD-CAD	4.65	1.28	1.22
23	b	614	CLA	CHC-C1C	4.64	1.47	1.38
23	c	511	CLA	CHC-C1C	4.64	1.47	1.38
23	b	616	CLA	O2D-CGD	4.64	1.44	1.33
23	d	402[B]	CLA	O2D-CGD	4.63	1.44	1.33
23	B	610	CLA	C1D-ND	4.63	1.43	1.37
23	B	609	CLA	CHD-C1D	4.62	1.47	1.38
23	b	602	CLA	CHD-C1D	4.62	1.47	1.38
23	D	402[A]	CLA	CHC-C1C	4.62	1.47	1.38
23	B	605	CLA	C1D-ND	4.61	1.43	1.37
25	t	102	BCR	C23-C22	-4.61	1.36	1.46
23	a	406[A]	CLA	O2D-CGD	4.60	1.44	1.33
23	B	605	CLA	CHC-C1C	4.60	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	408	CLA	O2D-CGD	4.59	1.44	1.33
33	C	521	LMG	O8-C28	4.59	1.46	1.33
32	E	101[A]	LHG	O8-C23	4.58	1.46	1.33
23	b	615	CLA	O2D-CGD	4.58	1.44	1.33
25	y	101	BCR	C23-C22	-4.58	1.36	1.46
26	f	102	SQD	O47-C7	4.57	1.47	1.34
23	B	609	CLA	C1D-ND	4.57	1.43	1.37
23	B	607	CLA	CHC-C1C	4.57	1.47	1.38
23	C	506	CLA	O2D-CGD	4.57	1.44	1.33
23	b	605	CLA	C1D-ND	4.56	1.43	1.37
23	A	404[A]	CLA	CHC-C1C	4.56	1.47	1.38
23	a	405[B]	CLA	CHC-C1C	4.56	1.47	1.38
25	b	617	BCR	C23-C22	-4.55	1.36	1.46
23	B	610	CLA	CHC-C1C	4.55	1.47	1.38
23	B	606	CLA	C1D-ND	4.55	1.43	1.37
23	C	511	CLA	O2D-CGD	4.54	1.44	1.33
23	d	402[A]	CLA	O2D-CGD	4.54	1.44	1.33
23	C	514	CLA	C1D-ND	4.54	1.43	1.37
23	b	603	CLA	CHC-C1C	4.54	1.47	1.38
23	c	507	CLA	C1D-ND	4.54	1.43	1.37
23	B	603	CLA	C1D-ND	4.54	1.43	1.37
23	B	611	CLA	C3B-C2B	4.53	1.56	1.41
26	B	620	SQD	O47-C7	4.53	1.47	1.34
23	a	405[A]	CLA	CHC-C1C	4.52	1.47	1.38
25	c	515	BCR	C23-C22	-4.52	1.36	1.46
23	b	607	CLA	CHC-C1C	4.51	1.47	1.38
23	C	506	CLA	C1D-ND	4.51	1.43	1.37
32	a	420[A]	LHG	O8-C23	4.51	1.46	1.33
23	C	507	CLA	CHD-C1D	4.51	1.47	1.38
25	h	101	BCR	C23-C22	-4.51	1.36	1.46
23	B	616	CLA	O2D-CGD	4.51	1.44	1.33
25	c	514	BCR	C23-C22	-4.50	1.36	1.46
23	c	513	CLA	O2A-CGA	4.50	1.46	1.33
23	C	503	CLA	CHD-C1D	4.49	1.47	1.38
23	C	509	CLA	OBD-CAD	4.49	1.30	1.22
23	c	504	CLA	CHC-C1C	4.49	1.47	1.38
23	c	513	CLA	CHD-C1D	4.48	1.47	1.38
23	b	611	CLA	CHC-C1C	4.48	1.47	1.38
23	c	509	CLA	C1D-ND	4.48	1.43	1.37
23	D	402[B]	CLA	O2A-CGA	4.48	1.46	1.33
23	c	502	CLA	O2D-CGD	4.47	1.44	1.33
23	c	512	CLA	O2D-CGD	4.47	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	E	101[B]	LHG	O8-C23	4.47	1.46	1.33
23	b	614	CLA	CHD-C1D	4.46	1.47	1.38
23	B	601	CLA	C1D-ND	4.46	1.43	1.37
23	B	614	CLA	O2D-CGD	4.46	1.44	1.33
23	B	614	CLA	CHC-C1C	4.46	1.47	1.38
23	B	610	CLA	OBD-CAD	4.46	1.30	1.22
23	b	616	CLA	C1D-ND	4.46	1.43	1.37
23	c	507	CLA	CHD-C1D	4.46	1.47	1.38
23	C	502	CLA	C1D-ND	4.45	1.43	1.37
23	b	604	CLA	O2D-CGD	4.45	1.44	1.33
23	C	512	CLA	CHC-C1C	4.45	1.47	1.38
23	b	608	CLA	CHC-C1C	4.45	1.47	1.38
23	c	510	CLA	CHC-C1C	4.45	1.47	1.38
23	b	606	CLA	O2D-CGD	4.44	1.44	1.33
23	b	604	CLA	CHD-C1D	4.44	1.47	1.38
25	Y	101	BCR	C23-C22	-4.44	1.36	1.46
23	b	607	CLA	CHD-C1D	4.44	1.47	1.38
23	C	513	CLA	O2D-CGD	4.44	1.44	1.33
33	z	101	LMG	O8-C28	4.43	1.46	1.33
23	b	604	CLA	C1D-ND	4.43	1.43	1.37
23	D	403	CLA	CHD-C1D	4.43	1.47	1.38
23	C	514	CLA	O2A-CGA	4.42	1.46	1.33
23	C	509	CLA	CHC-C1C	4.42	1.47	1.38
23	C	510	CLA	CHC-C1C	4.42	1.47	1.38
23	b	612	CLA	O2D-CGD	4.42	1.44	1.33
23	C	504	CLA	O2D-CGD	4.41	1.44	1.33
24	A	407[A]	PHO	OBD-CAD	4.41	1.28	1.22
23	b	606	CLA	C1D-ND	4.40	1.43	1.37
23	c	505	CLA	O2D-CGD	4.40	1.44	1.33
23	d	403	CLA	C3D-C2D	4.40	1.51	1.39
23	c	512	CLA	CHD-C1D	4.40	1.47	1.38
23	c	508	CLA	CHB-C1B	4.39	1.49	1.39
23	B	612	CLA	CHB-C1B	4.39	1.49	1.39
23	B	603	CLA	CHC-C1C	4.39	1.47	1.38
26	A	412	SQD	O48-C23	4.39	1.46	1.33
23	A	408	CLA	O2A-CGA	4.39	1.46	1.33
23	c	511	CLA	CHB-C1B	4.38	1.49	1.39
23	C	512	CLA	C3C-C2C	4.38	1.46	1.36
23	C	503	CLA	C3D-C2D	4.38	1.50	1.39
23	b	602	CLA	CHD-C4C	4.37	1.49	1.39
23	C	505	CLA	CHC-C1C	4.37	1.47	1.38
25	b	618	BCR	C23-C22	-4.37	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	C1D-ND	4.37	1.43	1.37
23	b	602	CLA	CHC-C4B	4.37	1.49	1.39
23	b	610	CLA	CHD-C1D	4.37	1.46	1.38
23	b	601	CLA	CHD-C1D	4.36	1.46	1.38
32	a	420[B]	LHG	O8-C23	4.36	1.46	1.33
23	a	405[A]	CLA	C3D-C2D	4.36	1.50	1.39
23	c	512	CLA	O2A-CGA	4.36	1.46	1.33
23	a	408	CLA	O2A-CGA	4.35	1.46	1.33
23	c	506	CLA	CHC-C1C	4.35	1.47	1.38
25	a	409	BCR	C23-C22	-4.35	1.36	1.46
23	B	608	CLA	C1D-ND	4.35	1.43	1.37
23	d	403	CLA	O2A-CGA	4.34	1.46	1.33
23	A	405[B]	CLA	C1D-ND	4.34	1.43	1.37
23	b	614	CLA	C1D-ND	4.34	1.43	1.37
26	b	620	SQD	O47-C7	4.34	1.46	1.34
23	a	404[A]	CLA	O2D-CGD	4.34	1.43	1.33
23	C	510	CLA	C1D-ND	4.33	1.43	1.37
23	d	403	CLA	O2D-CGD	4.32	1.43	1.33
23	d	402[B]	CLA	O2A-CGA	4.32	1.45	1.33
23	C	511	CLA	CHD-C4C	4.31	1.49	1.39
23	c	510	CLA	CHB-C1B	4.31	1.49	1.39
26	A	412	SQD	O47-C7	4.31	1.46	1.34
23	C	510	CLA	CHD-C1D	4.31	1.46	1.38
26	b	620	SQD	O48-C23	4.30	1.45	1.33
23	c	505	CLA	CHC-C4B	4.30	1.49	1.39
23	b	611	CLA	O2D-CGD	4.30	1.43	1.33
23	c	504	CLA	C3D-C2D	4.29	1.50	1.39
32	a	420[A]	LHG	O7-C7	4.28	1.46	1.34
23	C	509	CLA	C3D-C2D	4.28	1.50	1.39
23	d	402[A]	CLA	CHC-C1C	4.28	1.47	1.38
23	a	404[B]	CLA	CHD-C1D	4.28	1.46	1.38
23	B	615	CLA	C1D-ND	4.27	1.43	1.37
23	C	508	CLA	O2D-CGD	4.27	1.43	1.33
26	f	102	SQD	O48-C23	4.27	1.45	1.33
23	B	613	CLA	CHD-C1D	4.27	1.46	1.38
23	b	611	CLA	O2A-CGA	4.27	1.45	1.33
23	B	614	CLA	C4B-NB	-4.27	1.32	1.37
23	C	504	CLA	C1D-ND	4.26	1.43	1.37
23	a	405[B]	CLA	C3D-C2D	4.26	1.50	1.39
23	A	404[B]	CLA	CHD-C1D	4.26	1.46	1.38
23	D	402[B]	CLA	C1D-ND	4.26	1.43	1.37
23	d	402[B]	CLA	CHC-C1C	4.26	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	408	CLA	CHC-C1C	4.25	1.47	1.38
23	C	514	CLA	CHD-C1D	4.25	1.46	1.38
33	Z	101	LMG	O7-C10	4.25	1.46	1.34
23	b	601	CLA	C3D-C2D	4.25	1.50	1.39
23	b	602	CLA	C1D-ND	4.25	1.43	1.37
25	H	101	BCR	C23-C22	-4.25	1.36	1.46
23	c	507	CLA	O2A-CGA	4.24	1.45	1.33
23	b	609	CLA	C1D-ND	4.24	1.43	1.37
23	b	605	CLA	CHC-C1C	4.24	1.47	1.38
23	C	507	CLA	CHC-C1C	4.23	1.47	1.38
23	B	605	CLA	CHC-C4B	4.22	1.48	1.39
23	B	615	CLA	O2A-CGA	4.22	1.45	1.33
32	E	101[A]	LHG	O7-C7	4.22	1.46	1.34
23	c	503	CLA	CHD-C4C	4.22	1.48	1.39
23	c	503	CLA	O2A-CGA	4.21	1.45	1.33
23	B	610	CLA	C3D-C2D	4.21	1.50	1.39
23	A	406[B]	CLA	CHD-C1D	4.21	1.46	1.38
23	B	608	CLA	C3D-C2D	4.21	1.50	1.39
32	d	407[A]	LHG	O8-C23	4.20	1.45	1.33
33	B	621	LMG	O8-C28	4.20	1.45	1.33
23	D	402[B]	CLA	CHD-C1D	4.20	1.46	1.38
23	c	501	CLA	CHD-C1D	4.20	1.46	1.38
23	c	511	CLA	CHD-C1D	4.20	1.46	1.38
23	A	405[A]	CLA	C1D-ND	4.20	1.43	1.37
23	B	607	CLA	O2D-CGD	4.20	1.43	1.33
23	C	505	CLA	C1D-ND	4.19	1.43	1.37
26	B	620	SQD	O48-C23	4.19	1.45	1.33
23	A	404[B]	CLA	CHD-C4C	4.19	1.48	1.39
23	c	502	CLA	C1D-ND	4.19	1.43	1.37
33	a	416	LMG	O8-C28	4.19	1.45	1.33
23	B	611	CLA	C4B-NB	-4.19	1.32	1.37
35	c	518	DGD	O1G-C1A	4.19	1.45	1.33
23	b	608	CLA	CHD-C1D	4.19	1.46	1.38
32	E	101[B]	LHG	O7-C7	4.19	1.46	1.34
23	D	402[A]	CLA	O2A-CGA	4.19	1.45	1.33
23	D	403	CLA	CHB-C1B	4.19	1.48	1.39
23	b	607	CLA	C1B-NB	-4.19	1.32	1.37
23	b	612	CLA	CHC-C1C	4.19	1.46	1.38
33	C	520	LMG	O8-C28	4.18	1.45	1.33
38	f	101	HEM	FE-NC	4.18	2.09	1.95
23	a	406[B]	CLA	O2A-CGA	4.18	1.45	1.33
33	c	520	LMG	O8-C28	4.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	O2A-CGA	4.17	1.45	1.33
38	F	102	HEM	FE-NC	4.17	2.08	1.95
32	a	420[B]	LHG	O7-C7	4.17	1.46	1.34
32	d	407[B]	LHG	O8-C23	4.17	1.45	1.33
26	F	103	SQD	O48-C23	4.17	1.45	1.33
33	m	101	LMG	O8-C28	4.17	1.45	1.33
23	B	609	CLA	O2A-CGA	4.16	1.45	1.33
23	C	507	CLA	C1D-ND	4.16	1.43	1.37
23	b	604	CLA	CHD-C4C	4.16	1.48	1.39
23	C	503	CLA	CHC-C1C	4.16	1.46	1.38
23	D	402[A]	CLA	CHD-C1D	4.16	1.46	1.38
23	A	405[A]	CLA	C3D-C2D	4.15	1.50	1.39
23	c	511	CLA	O2A-CGA	4.15	1.45	1.33
23	c	508	CLA	C3D-C2D	4.15	1.50	1.39
33	c	519	LMG	O7-C10	4.15	1.46	1.34
33	C	520	LMG	O7-C10	4.15	1.46	1.34
23	A	408	CLA	CHD-C1D	4.14	1.46	1.38
23	D	403	CLA	C3D-C2D	4.14	1.50	1.39
26	a	410[B]	SQD	O47-C7	4.14	1.46	1.34
23	a	405[B]	CLA	O2A-CGA	4.14	1.45	1.33
23	c	502	CLA	C3D-C2D	4.14	1.50	1.39
23	c	503	CLA	CHC-C4B	4.14	1.48	1.39
23	C	509	CLA	CHB-C1B	4.14	1.48	1.39
23	C	506	CLA	CHD-C1D	4.14	1.46	1.38
23	c	502	CLA	CHC-C1C	4.13	1.46	1.38
23	a	406[A]	CLA	C1D-ND	4.13	1.43	1.37
35	C	517[A]	DGD	O2G-C1B	4.13	1.46	1.34
24	a	407[A]	PHO	OBD-CAD	4.13	1.27	1.22
23	A	405[B]	CLA	O2A-CGA	4.13	1.45	1.33
23	C	502	CLA	CHD-C1D	4.13	1.46	1.38
23	B	602	CLA	CHD-C4C	4.13	1.48	1.39
23	C	507	CLA	O2A-CGA	4.13	1.45	1.33
23	a	405[A]	CLA	O2A-CGA	4.13	1.45	1.33
23	a	404[A]	CLA	CHD-C4C	4.12	1.48	1.39
23	c	507	CLA	CHD-C4C	4.12	1.48	1.39
23	b	614	CLA	C3D-C2D	4.12	1.50	1.39
23	c	508	CLA	CHD-C1D	4.12	1.46	1.38
23	c	509	CLA	CHD-C4C	4.12	1.48	1.39
23	B	602	CLA	CHB-C1B	4.12	1.48	1.39
23	A	406[A]	CLA	C1B-NB	-4.11	1.32	1.37
23	C	512	CLA	CHB-C1B	4.11	1.48	1.39
23	c	512	CLA	CHC-C4B	4.11	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	CHB-C1B	4.11	1.48	1.39
23	C	512	CLA	CHD-C1D	4.11	1.46	1.38
23	c	505	CLA	CHD-C1D	4.11	1.46	1.38
23	B	608	CLA	CHB-C1B	4.11	1.48	1.39
23	b	609	CLA	CHB-C1B	4.10	1.48	1.39
23	C	512	CLA	O2A-CGA	4.10	1.45	1.33
23	d	403	CLA	CHD-C1D	4.10	1.46	1.38
23	c	513	CLA	CHD-C4C	4.10	1.48	1.39
23	B	611	CLA	CHB-C1B	4.10	1.48	1.39
23	c	508	CLA	O2A-CGA	4.10	1.45	1.33
23	a	404[B]	CLA	CHD-C4C	4.10	1.48	1.39
23	C	513	CLA	C3D-C2D	4.09	1.50	1.39
23	c	509	CLA	CHD-C1D	4.09	1.46	1.38
23	b	616	CLA	CHD-C1D	4.08	1.46	1.38
23	a	404[A]	CLA	CHD-C1D	4.08	1.46	1.38
23	A	405[A]	CLA	O2A-CGA	4.08	1.45	1.33
23	b	612	CLA	C1D-ND	4.08	1.43	1.37
23	C	504	CLA	CHD-C4C	4.08	1.48	1.39
23	b	610	CLA	CHB-C1B	4.08	1.48	1.39
33	z	101	LMG	O7-C10	4.08	1.45	1.34
23	a	406[B]	CLA	C1D-ND	4.08	1.43	1.37
23	C	514	CLA	C3D-C2D	4.07	1.50	1.39
23	A	406[A]	CLA	CHD-C1D	4.07	1.46	1.38
35	C	517[B]	DGD	O2G-C1B	4.07	1.45	1.34
32	D	407[B]	LHG	O7-C7	4.07	1.45	1.34
23	C	512	CLA	C1D-ND	4.07	1.43	1.37
35	C	519	DGD	O1G-C1A	4.06	1.45	1.33
23	b	608	CLA	OBD-CAD	4.06	1.29	1.22
23	c	506	CLA	CHD-C1D	4.06	1.46	1.38
23	A	406[B]	CLA	C3D-C2D	4.06	1.50	1.39
23	B	604	CLA	CHD-C4C	4.06	1.48	1.39
23	c	501	CLA	C3D-C2D	4.06	1.50	1.39
23	B	601	CLA	CHC-C4B	4.06	1.48	1.39
23	C	509	CLA	O2A-CGA	4.06	1.45	1.33
23	A	405[B]	CLA	CHD-C1D	4.06	1.46	1.38
23	C	503	CLA	O2A-CGA	4.06	1.45	1.33
23	B	614	CLA	CHB-C1B	4.06	1.48	1.39
33	a	416	LMG	O7-C10	4.05	1.45	1.34
23	B	604	CLA	CHB-C1B	4.05	1.48	1.39
26	a	410[A]	SQD	O47-C7	4.05	1.45	1.34
23	B	607	CLA	OBD-CAD	4.05	1.29	1.22
23	B	602	CLA	CHD-C1D	4.05	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	CHD-C1D	4.05	1.46	1.38
23	C	513	CLA	CHD-C1D	4.04	1.46	1.38
23	B	609	CLA	C3D-C2D	4.04	1.50	1.39
23	c	512	CLA	CHB-C1B	4.04	1.48	1.39
23	c	502	CLA	CHD-C4C	4.04	1.48	1.39
23	c	502	CLA	CHD-C1D	4.04	1.46	1.38
23	B	614	CLA	CHD-C4C	4.04	1.48	1.39
23	D	402[B]	CLA	CHD-C4C	4.04	1.48	1.39
32	d	413[B]	LHG	O8-C23	4.03	1.45	1.33
23	c	506	CLA	CHB-C1B	4.03	1.48	1.39
23	b	615	CLA	O2A-CGA	4.03	1.45	1.33
23	B	603	CLA	C3D-C2D	4.03	1.50	1.39
23	a	405[B]	CLA	CHD-C1D	4.03	1.46	1.38
23	B	606	CLA	CHD-C1D	4.03	1.46	1.38
23	B	602	CLA	C3D-C2D	4.03	1.50	1.39
24	A	416[A]	PHO	O2A-CGA	4.03	1.45	1.33
33	C	501	LMG	O7-C10	4.02	1.45	1.34
23	D	402[A]	CLA	CHB-C1B	4.02	1.48	1.39
23	b	612	CLA	CHC-C4B	4.02	1.48	1.39
23	C	508	CLA	O2A-CGA	4.02	1.45	1.33
23	b	612	CLA	CHD-C1D	4.02	1.46	1.38
23	d	402[B]	CLA	CHB-C1B	4.01	1.48	1.39
23	b	609	CLA	CHD-C1D	4.01	1.46	1.38
35	h	102	DGD	O2G-C1B	4.01	1.45	1.34
35	c	517[B]	DGD	O1G-C1A	4.01	1.45	1.33
23	a	406[A]	CLA	C3D-C2D	4.01	1.49	1.39
23	a	404[A]	CLA	CHB-C1B	4.01	1.48	1.39
35	c	517[A]	DGD	O1G-C1A	4.01	1.45	1.33
23	b	603	CLA	CHD-C1D	4.01	1.46	1.38
32	L	101[B]	LHG	O8-C23	4.01	1.45	1.33
23	b	607	CLA	O2D-CGD	4.01	1.43	1.33
23	c	501	CLA	CHC-C4B	4.00	1.48	1.39
23	B	613	CLA	OBD-CAD	4.00	1.29	1.22
23	b	616	CLA	O2A-CGA	4.00	1.45	1.33
26	a	410[B]	SQD	O48-C23	4.00	1.45	1.33
23	B	616	CLA	CHB-C1B	4.00	1.48	1.39
23	A	406[A]	CLA	C3D-C2D	4.00	1.49	1.39
23	c	509	CLA	C1B-NB	-4.00	1.32	1.37
23	c	503	CLA	O2D-CGD	3.99	1.43	1.33
23	b	601	CLA	CHD-C4C	3.99	1.48	1.39
23	c	506	CLA	C3D-C2D	3.99	1.49	1.39
23	d	402[B]	CLA	CHD-C1D	3.99	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402[A]	CLA	CHB-C1B	3.99	1.48	1.39
23	d	402[B]	CLA	C1D-ND	3.99	1.43	1.37
23	c	501	CLA	CHD-C4C	3.99	1.48	1.39
23	C	513	CLA	O2A-CGA	3.99	1.45	1.33
33	C	501	LMG	O8-C28	3.98	1.45	1.33
26	A	410[B]	SQD	O48-C23	3.98	1.45	1.33
24	A	407[B]	PHO	O2A-CGA	3.98	1.45	1.33
33	c	519	LMG	O8-C28	3.98	1.44	1.33
23	D	403	CLA	CHD-C4C	3.98	1.48	1.39
26	a	410[A]	SQD	O48-C23	3.98	1.44	1.33
23	b	612	CLA	C3D-C2D	3.98	1.49	1.39
23	b	609	CLA	OBD-CAD	3.98	1.29	1.22
23	b	615	CLA	C3D-C2D	3.97	1.49	1.39
23	C	504	CLA	CHC-C4B	3.97	1.48	1.39
23	B	615	CLA	OBD-CAD	3.97	1.29	1.22
23	b	613	CLA	CHC-C4B	3.97	1.48	1.39
23	C	510	CLA	C3D-C2D	3.97	1.49	1.39
35	c	516[B]	DGD	O2G-C1B	3.97	1.45	1.34
23	a	406[A]	CLA	O2A-CGA	3.97	1.44	1.33
23	d	402[A]	CLA	O2A-CGA	3.96	1.44	1.33
23	B	612	CLA	CHD-C1D	3.96	1.46	1.38
23	c	512	CLA	CHD-C4C	3.96	1.48	1.39
23	c	506	CLA	CHD-C4C	3.96	1.48	1.39
23	b	602	CLA	C3D-C2D	3.96	1.49	1.39
23	B	608	CLA	O2D-CGD	3.96	1.43	1.33
23	c	510	CLA	CHC-C4B	3.96	1.48	1.39
23	B	607	CLA	C1B-NB	-3.95	1.32	1.37
23	B	603	CLA	CHB-C1B	3.95	1.48	1.39
32	b	629[B]	LHG	O7-C7	3.95	1.45	1.34
23	A	406[A]	CLA	OBD-CAD	3.95	1.29	1.22
23	B	613	CLA	C3D-C2D	3.95	1.49	1.39
23	a	406[B]	CLA	C3D-C2D	3.95	1.49	1.39
23	c	503	CLA	CHB-C1B	3.95	1.48	1.39
32	d	406[B]	LHG	O7-C7	3.94	1.45	1.34
23	c	508	CLA	CHD-C4C	3.94	1.48	1.39
23	c	501	CLA	O2D-CGD	3.94	1.42	1.33
23	A	405[A]	CLA	CHD-C1D	3.94	1.46	1.38
23	C	512	CLA	C3D-C2D	3.94	1.49	1.39
23	c	505	CLA	C1D-ND	3.94	1.43	1.37
23	b	610	CLA	OBD-CAD	3.94	1.29	1.22
23	b	605	CLA	CHD-C4C	3.94	1.48	1.39
23	c	512	CLA	C3D-C2D	3.94	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	509	CLA	CHB-C1B	3.93	1.48	1.39
23	C	506	CLA	CHB-C1B	3.93	1.48	1.39
32	b	629[B]	LHG	O8-C23	3.93	1.44	1.33
23	c	501	CLA	CHB-C1B	3.93	1.48	1.39
32	D	406[B]	LHG	O7-C7	3.92	1.45	1.34
23	C	506	CLA	CHD-C4C	3.92	1.48	1.39
32	L	101[A]	LHG	O8-C23	3.92	1.44	1.33
23	C	508	CLA	CHD-C1D	3.92	1.46	1.38
23	a	405[B]	CLA	CHD-C4C	3.92	1.48	1.39
35	C	517[B]	DGD	O1G-C1A	3.92	1.44	1.33
23	D	402[A]	CLA	C1D-ND	3.92	1.43	1.37
23	C	514	CLA	CHB-C1B	3.92	1.48	1.39
23	B	609	CLA	CHC-C4B	3.92	1.48	1.39
23	C	513	CLA	CHC-C4B	3.92	1.48	1.39
35	C	518[B]	DGD	O2G-C1B	3.92	1.45	1.34
23	B	608	CLA	CHD-C4C	3.91	1.48	1.39
32	D	407[A]	LHG	O8-C23	3.91	1.44	1.33
23	b	609	CLA	O2A-CGA	3.91	1.44	1.33
35	c	516[B]	DGD	O1G-C1A	3.91	1.44	1.33
23	B	616	CLA	C3D-C2D	3.91	1.49	1.39
23	c	507	CLA	C3D-C2D	3.91	1.49	1.39
23	B	616	CLA	O2A-CGA	3.91	1.44	1.33
23	a	405[A]	CLA	C1B-NB	-3.90	1.32	1.37
23	c	502	CLA	O2A-CGA	3.90	1.44	1.33
23	C	514	CLA	CHD-C4C	3.90	1.48	1.39
32	d	406[A]	LHG	O7-C7	3.90	1.45	1.34
23	B	601	CLA	CHD-C1D	3.90	1.46	1.38
23	b	611	CLA	CHD-C1D	3.90	1.46	1.38
23	B	611	CLA	C1C-C2C	3.90	1.52	1.44
23	B	615	CLA	CHD-C4C	3.89	1.48	1.39
23	d	402[A]	CLA	CHD-C1D	3.89	1.46	1.38
23	A	405[B]	CLA	C3D-C2D	3.89	1.49	1.39
23	B	609	CLA	CHD-C4C	3.89	1.48	1.39
23	a	404[B]	CLA	O2A-CGA	3.89	1.44	1.33
32	D	407[A]	LHG	O7-C7	3.89	1.45	1.34
23	b	605	CLA	CHD-C1D	3.89	1.46	1.38
23	C	510	CLA	OBD-CAD	3.89	1.29	1.22
23	b	615	CLA	OBD-CAD	3.89	1.29	1.22
23	C	505	CLA	CHB-C1B	3.89	1.48	1.39
23	B	607	CLA	CHB-C1B	3.89	1.48	1.39
23	C	502	CLA	O2D-CGD	3.89	1.42	1.33
23	c	507	CLA	CHC-C4B	3.89	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	416[B]	PHO	O2A-CGA	3.89	1.44	1.33
23	b	613	CLA	CHB-C1B	3.89	1.48	1.39
23	b	613	CLA	C1B-NB	-3.89	1.32	1.37
23	C	507	CLA	CHD-C4C	3.88	1.48	1.39
23	b	616	CLA	CHC-C4B	3.88	1.48	1.39
23	c	501	CLA	O2A-CGA	3.88	1.44	1.33
23	D	403	CLA	CHC-C4B	3.88	1.48	1.39
23	b	608	CLA	C3D-C2D	3.87	1.49	1.39
23	b	603	CLA	CHC-C4B	3.87	1.48	1.39
23	b	614	CLA	CHB-C1B	3.87	1.48	1.39
23	B	615	CLA	CHB-C1B	3.87	1.48	1.39
32	d	407[B]	LHG	O7-C7	3.87	1.45	1.34
23	B	608	CLA	CHC-C1C	3.86	1.46	1.38
23	a	406[B]	CLA	CHD-C1D	3.86	1.45	1.38
23	C	511	CLA	CHB-C1B	3.86	1.48	1.39
23	A	406[B]	CLA	O2A-CGA	3.86	1.44	1.33
23	B	613	CLA	CHB-C1B	3.86	1.48	1.39
23	c	510	CLA	C3D-C2D	3.86	1.49	1.39
23	A	404[A]	CLA	C3D-C2D	3.86	1.49	1.39
23	C	505	CLA	C3D-C2D	3.85	1.49	1.39
23	b	608	CLA	O2A-CGA	3.85	1.44	1.33
23	c	511	CLA	CHD-C4C	3.85	1.48	1.39
24	a	415[A]	PHO	O2A-CGA	3.85	1.44	1.33
32	L	101[B]	LHG	O7-C7	3.85	1.45	1.34
23	C	508	CLA	C1D-ND	3.85	1.42	1.37
23	b	610	CLA	C3D-C2D	3.85	1.49	1.39
23	A	406[B]	CLA	CHD-C4C	3.85	1.48	1.39
35	C	518[A]	DGD	O2G-C1B	3.85	1.45	1.34
23	C	504	CLA	CHD-C1D	3.84	1.45	1.38
23	b	605	CLA	C1B-NB	-3.84	1.32	1.37
23	b	604	CLA	CHC-C4B	3.84	1.48	1.39
23	a	405[A]	CLA	OBD-CAD	3.84	1.29	1.22
23	B	611	CLA	OBD-CAD	3.84	1.29	1.22
23	b	611	CLA	CHB-C1B	3.84	1.48	1.39
23	B	607	CLA	CHD-C1D	3.84	1.45	1.38
23	B	610	CLA	CHD-C1D	3.84	1.45	1.38
32	D	407[B]	LHG	O8-C23	3.84	1.44	1.33
23	c	505	CLA	OBD-CAD	3.83	1.29	1.22
23	c	505	CLA	CHD-C4C	3.83	1.47	1.39
25	B	618	BCR	C23-C22	-3.83	1.37	1.46
33	d	411	LMG	O8-C28	3.83	1.44	1.33
23	c	513	CLA	C3D-C2D	3.83	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	h	102	DGD	O1G-C1A	3.83	1.44	1.33
23	b	604	CLA	C3D-C2D	3.83	1.49	1.39
23	b	615	CLA	CHD-C1D	3.83	1.45	1.38
23	B	605	CLA	CHB-C1B	3.82	1.48	1.39
23	B	612	CLA	O2D-CGD	3.82	1.42	1.33
23	b	603	CLA	C1D-ND	3.82	1.42	1.37
23	c	513	CLA	CHB-C1B	3.82	1.48	1.39
23	b	607	CLA	C3D-C2D	3.82	1.49	1.39
35	C	518[B]	DGD	O1G-C1A	3.82	1.44	1.33
23	C	512	CLA	CHD-C4C	3.81	1.47	1.39
23	A	405[A]	CLA	CHD-C4C	3.81	1.47	1.39
35	c	516[A]	DGD	O2G-C1B	3.81	1.45	1.34
24	a	415[B]	PHO	O2A-CGA	3.81	1.44	1.33
23	a	406[A]	CLA	CHD-C4C	3.81	1.47	1.39
23	A	404[B]	CLA	CHC-C4B	3.81	1.48	1.39
23	a	406[B]	CLA	OBD-CAD	3.80	1.29	1.22
23	c	504	CLA	CHB-C1B	3.80	1.47	1.39
23	C	502	CLA	CHD-C4C	3.80	1.47	1.39
32	d	413[B]	LHG	O7-C7	3.80	1.45	1.34
23	c	509	CLA	C3D-C2D	3.80	1.49	1.39
35	C	518[A]	DGD	O1G-C1A	3.80	1.44	1.33
23	b	612	CLA	OBD-CAD	3.79	1.29	1.22
23	A	404[A]	CLA	CHB-C1B	3.79	1.47	1.39
23	B	614	CLA	O2A-CGA	3.79	1.44	1.33
23	B	604	CLA	OBD-CAD	3.79	1.29	1.22
23	B	608	CLA	CHD-C1D	3.79	1.45	1.38
35	c	516[A]	DGD	O1G-C1A	3.79	1.44	1.33
26	a	411	SQD	O47-C7	3.78	1.45	1.34
23	B	616	CLA	CHD-C1D	3.78	1.45	1.38
23	C	506	CLA	O2A-CGA	3.78	1.44	1.33
35	c	517[B]	DGD	O2G-C1B	3.78	1.45	1.34
23	B	603	CLA	CHC-C4B	3.78	1.47	1.39
23	c	510	CLA	O2A-CGA	3.78	1.44	1.33
23	b	611	CLA	CHC-C4B	3.78	1.47	1.39
24	A	407[A]	PHO	O2A-CGA	3.77	1.44	1.33
23	a	408	CLA	CHB-C1B	3.77	1.47	1.39
23	c	505	CLA	CHB-C1B	3.77	1.47	1.39
23	A	406[A]	CLA	C1D-ND	3.77	1.42	1.37
32	A	419[B]	LHG	O7-C7	3.77	1.44	1.34
26	A	410[A]	SQD	O48-C23	3.76	1.44	1.33
23	b	603	CLA	C3D-C2D	3.76	1.49	1.39
33	m	101	LMG	O7-C10	3.76	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	d	411	LMG	O7-C10	3.76	1.44	1.34
23	A	405[A]	CLA	CHC-C4B	3.76	1.47	1.39
24	A	416[A]	PHO	CHA-CBD	-3.76	1.47	1.51
23	c	504	CLA	CHD-C1D	3.76	1.45	1.38
23	C	507	CLA	CHB-C1B	3.76	1.47	1.39
23	A	406[B]	CLA	CHC-C4B	3.76	1.47	1.39
23	B	606	CLA	CHB-C1B	3.76	1.47	1.39
23	c	509	CLA	CHC-C1C	3.76	1.46	1.38
23	B	611	CLA	O2A-CGA	3.76	1.44	1.33
23	b	606	CLA	CHB-C1B	3.75	1.47	1.39
33	B	621	LMG	O7-C10	3.75	1.44	1.34
23	a	406[B]	CLA	CHD-C4C	3.75	1.47	1.39
23	c	511	CLA	C3D-C2D	3.75	1.49	1.39
23	A	408	CLA	CHD-C4C	3.75	1.47	1.39
23	C	507	CLA	C3D-C2D	3.75	1.49	1.39
23	D	402[B]	CLA	CHB-C1B	3.75	1.47	1.39
23	C	502	CLA	O2A-CGA	3.75	1.44	1.33
33	D	411	LMG	O7-C10	3.75	1.44	1.34
23	C	513	CLA	CHD-C4C	3.75	1.47	1.39
23	A	408	CLA	C3D-C2D	3.74	1.49	1.39
32	A	419[B]	LHG	O8-C23	3.74	1.44	1.33
23	C	504	CLA	C3D-C2D	3.74	1.49	1.39
23	a	404[A]	CLA	OBD-CAD	3.74	1.28	1.22
23	B	604	CLA	C1D-ND	3.74	1.42	1.37
23	B	606	CLA	CHC-C4B	3.74	1.47	1.39
23	A	406[A]	CLA	O2A-CGA	3.74	1.44	1.33
23	b	616	CLA	C3D-C2D	3.74	1.49	1.39
23	c	507	CLA	CHB-C1B	3.73	1.47	1.39
23	B	602	CLA	CHC-C4B	3.73	1.47	1.39
23	B	601	CLA	C3D-C2D	3.73	1.49	1.39
23	A	405[B]	CLA	CHD-C4C	3.73	1.47	1.39
23	b	606	CLA	C3D-C2D	3.73	1.49	1.39
23	A	406[A]	CLA	CHD-C4C	3.73	1.47	1.39
23	a	405[B]	CLA	OBD-CAD	3.72	1.28	1.22
23	b	608	CLA	C4B-NB	-3.72	1.33	1.37
23	a	404[A]	CLA	C3D-C2D	3.72	1.49	1.39
23	B	610	CLA	CHD-C4C	3.72	1.47	1.39
23	c	510	CLA	CHD-C4C	3.72	1.47	1.39
23	c	509	CLA	O2A-CGA	3.72	1.44	1.33
23	d	402[B]	CLA	CHD-C4C	3.72	1.47	1.39
23	b	610	CLA	C1D-ND	3.71	1.42	1.37
23	C	511	CLA	O2A-CGA	3.71	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	CHD-C1D	3.71	1.45	1.38
23	B	614	CLA	CHC-C4B	3.71	1.47	1.39
23	B	605	CLA	CHD-C1D	3.71	1.45	1.38
23	B	616	CLA	C1D-ND	3.71	1.42	1.37
23	b	608	CLA	CHD-C4C	3.71	1.47	1.39
23	b	609	CLA	CHD-C4C	3.71	1.47	1.39
23	c	512	CLA	OBD-CAD	3.71	1.28	1.22
23	c	508	CLA	OBD-CAD	3.70	1.28	1.22
23	b	615	CLA	CHB-C1B	3.70	1.47	1.39
23	B	605	CLA	O2A-CGA	3.70	1.44	1.33
23	a	404[B]	CLA	CHC-C4B	3.70	1.47	1.39
23	B	610	CLA	CHB-C1B	3.70	1.47	1.39
23	B	603	CLA	O2A-CGA	3.70	1.44	1.33
23	b	615	CLA	CHC-C4B	3.70	1.47	1.39
23	A	405[B]	CLA	CHC-C4B	3.70	1.47	1.39
23	C	502	CLA	CHB-C1B	3.69	1.47	1.39
26	A	410[B]	SQD	O47-C7	3.69	1.44	1.34
23	C	510	CLA	CHB-C1B	3.69	1.47	1.39
23	A	404[A]	CLA	CHD-C4C	3.69	1.47	1.39
32	D	406[B]	LHG	O8-C23	3.69	1.44	1.33
24	a	407[B]	PHO	O2A-CGA	3.69	1.44	1.33
23	B	605	CLA	CHD-C4C	3.69	1.47	1.39
23	C	509	CLA	CHD-C4C	3.69	1.47	1.39
23	b	614	CLA	CHC-C4B	3.69	1.47	1.39
32	L	101[A]	LHG	O7-C7	3.69	1.44	1.34
26	A	410[A]	SQD	O47-C7	3.68	1.44	1.34
23	B	602	CLA	O2A-CGA	3.68	1.44	1.33
23	B	602	CLA	OBD-CAD	3.68	1.28	1.22
23	D	403	CLA	OBD-CAD	3.68	1.28	1.22
23	C	512	CLA	C4B-NB	-3.68	1.33	1.37
34	B	624	HTG	C1'-S1	-3.68	1.76	1.81
23	A	404[B]	CLA	C3D-C2D	3.68	1.49	1.39
32	d	407[A]	LHG	O7-C7	3.68	1.44	1.34
23	a	404[B]	CLA	OBD-CAD	3.68	1.28	1.22
23	d	403	CLA	CHC-C4B	3.68	1.47	1.39
23	d	403	CLA	CHB-C1B	3.68	1.47	1.39
23	B	611	CLA	CHD-C4C	3.68	1.47	1.39
23	b	613	CLA	C3D-C2D	3.67	1.49	1.39
23	c	507	CLA	OBD-CAD	3.67	1.28	1.22
23	C	503	CLA	CHC-C4B	3.67	1.47	1.39
23	D	402[A]	CLA	CHD-C4C	3.67	1.47	1.39
23	C	510	CLA	O2A-CGA	3.67	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	CHC-C4B	3.67	1.47	1.39
23	A	404[A]	CLA	CHD-C1D	3.67	1.45	1.38
32	D	406[A]	LHG	O7-C7	3.67	1.44	1.34
23	b	602	CLA	O2A-CGA	3.67	1.44	1.33
23	b	614	CLA	CHD-C4C	3.66	1.47	1.39
23	a	408	CLA	CHC-C4B	3.66	1.47	1.39
23	b	610	CLA	CHC-C4B	3.66	1.47	1.39
23	b	607	CLA	C1D-ND	3.66	1.42	1.37
23	a	406[B]	CLA	CHC-C4B	3.66	1.47	1.39
23	b	612	CLA	O2A-CGA	3.66	1.44	1.33
23	b	604	CLA	CHB-C1B	3.66	1.47	1.39
23	b	614	CLA	O2A-CGA	3.66	1.44	1.33
23	d	402[B]	CLA	C3D-C2D	3.66	1.49	1.39
35	C	517[A]	DGD	O1G-C1A	3.66	1.44	1.33
23	d	403	CLA	CHD-C4C	3.66	1.47	1.39
23	C	504	CLA	CHB-C1B	3.65	1.47	1.39
23	B	609	CLA	CHB-C1B	3.65	1.47	1.39
23	b	609	CLA	C3D-C2D	3.65	1.49	1.39
32	d	413[A]	LHG	O8-C23	3.65	1.44	1.33
23	b	608	CLA	CHB-C1B	3.65	1.47	1.39
23	A	405[A]	CLA	CHB-C1B	3.65	1.47	1.39
23	C	510	CLA	CHD-C4C	3.64	1.47	1.39
23	a	405[B]	CLA	CHB-C1B	3.64	1.47	1.39
23	B	616	CLA	C4B-NB	-3.64	1.33	1.37
23	c	505	CLA	C3D-C2D	3.64	1.48	1.39
23	B	601	CLA	OBD-CAD	3.64	1.28	1.22
23	C	506	CLA	CHC-C4B	3.64	1.47	1.39
23	A	406[A]	CLA	CHC-C4B	3.64	1.47	1.39
23	A	404[B]	CLA	C1B-NB	-3.64	1.33	1.37
23	b	616	CLA	CHD-C4C	3.63	1.47	1.39
35	H	102	DGD	O1G-C1A	3.63	1.43	1.33
23	d	402[A]	CLA	CHD-C4C	3.62	1.47	1.39
23	D	402[B]	CLA	C3D-C2D	3.62	1.48	1.39
23	b	615	CLA	CHD-C4C	3.62	1.47	1.39
23	a	405[A]	CLA	CHD-C1D	3.62	1.45	1.38
23	a	408	CLA	CHD-C4C	3.62	1.47	1.39
23	c	502	CLA	CHB-C1B	3.62	1.47	1.39
23	C	511	CLA	CHD-C1D	3.62	1.45	1.38
23	C	505	CLA	O2A-CGA	3.62	1.43	1.33
23	A	406[B]	CLA	CHB-C1B	3.62	1.47	1.39
23	b	613	CLA	O2A-CGA	3.62	1.43	1.33
23	b	602	CLA	OBD-CAD	3.61	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	OBD-CAD	3.61	1.28	1.22
23	B	611	CLA	CHD-C1D	3.61	1.45	1.38
23	A	405[B]	CLA	C1B-NB	-3.61	1.33	1.37
23	c	505	CLA	O2A-CGA	3.61	1.43	1.33
23	d	402[A]	CLA	OBD-CAD	3.61	1.28	1.22
32	b	629[A]	LHG	O7-C7	3.61	1.44	1.34
32	D	406[A]	LHG	O8-C23	3.61	1.43	1.33
23	B	601	CLA	CHB-C1B	3.60	1.47	1.39
23	C	508	CLA	CHC-C4B	3.60	1.47	1.39
23	B	612	CLA	C3D-C2D	3.60	1.48	1.39
23	B	609	CLA	OBD-CAD	3.60	1.28	1.22
23	C	503	CLA	CHB-C1B	3.60	1.47	1.39
23	b	613	CLA	CHD-C1D	3.60	1.45	1.38
23	A	406[A]	CLA	CHB-C1B	3.60	1.47	1.39
32	A	419[A]	LHG	O7-C7	3.60	1.44	1.34
23	B	603	CLA	CHD-C1D	3.60	1.45	1.38
23	b	612	CLA	C4B-NB	-3.60	1.33	1.37
23	D	402[A]	CLA	C3D-C2D	3.60	1.48	1.39
23	b	605	CLA	CHB-C1B	3.60	1.47	1.39
23	C	503	CLA	CHD-C4C	3.60	1.47	1.39
23	C	502	CLA	C3D-C2D	3.59	1.48	1.39
23	c	508	CLA	CHC-C4B	3.59	1.47	1.39
23	C	507	CLA	OBD-CAD	3.59	1.28	1.22
23	c	504	CLA	O2A-CGA	3.59	1.43	1.33
23	B	610	CLA	C1B-NB	-3.59	1.33	1.37
32	d	406[A]	LHG	O8-C23	3.58	1.43	1.33
23	a	406[A]	CLA	CHD-C1D	3.58	1.45	1.38
23	B	610	CLA	CHC-C4B	3.58	1.47	1.39
23	d	402[A]	CLA	C3D-C2D	3.58	1.48	1.39
23	b	605	CLA	CHC-C4B	3.58	1.47	1.39
23	B	607	CLA	CHD-C4C	3.58	1.47	1.39
23	C	509	CLA	CHC-C4B	3.58	1.47	1.39
23	A	404[B]	CLA	O2A-CGA	3.58	1.43	1.33
23	B	601	CLA	CHD-C4C	3.58	1.47	1.39
23	C	504	CLA	O2A-CGA	3.58	1.43	1.33
23	C	508	CLA	C3D-C2D	3.58	1.48	1.39
23	b	611	CLA	C1D-ND	3.57	1.42	1.37
23	B	603	CLA	CHD-C4C	3.57	1.47	1.39
23	C	509	CLA	CHD-C1D	3.57	1.45	1.38
23	A	404[B]	CLA	CHB-C1B	3.57	1.47	1.39
23	B	606	CLA	CHD-C4C	3.56	1.47	1.39
23	b	601	CLA	CHB-C1B	3.56	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402[B]	CLA	C4B-NB	-3.56	1.33	1.37
23	b	607	CLA	CHB-C1B	3.56	1.47	1.39
23	b	606	CLA	CHC-C4B	3.56	1.47	1.39
23	A	405[B]	CLA	OBD-CAD	3.56	1.28	1.22
23	a	404[B]	CLA	C3D-C2D	3.56	1.48	1.39
23	D	402[B]	CLA	OBD-CAD	3.56	1.28	1.22
23	b	610	CLA	CHD-C4C	3.55	1.47	1.39
23	b	606	CLA	CHD-C4C	3.55	1.47	1.39
23	B	606	CLA	C3D-C2D	3.55	1.48	1.39
23	a	404[A]	CLA	CHC-C4B	3.55	1.47	1.39
23	a	404[B]	CLA	CHB-C1B	3.55	1.47	1.39
23	a	406[A]	CLA	CHB-C1B	3.55	1.47	1.39
23	a	405[A]	CLA	CHD-C4C	3.55	1.47	1.39
23	A	406[B]	CLA	OBD-CAD	3.55	1.28	1.22
23	B	605	CLA	C3D-C2D	3.54	1.48	1.39
23	C	512	CLA	CHC-C4B	3.54	1.47	1.39
23	B	616	CLA	CHC-C4B	3.54	1.47	1.39
35	c	517[A]	DGD	O2G-C1B	3.54	1.44	1.34
23	b	604	CLA	OBD-CAD	3.53	1.28	1.22
23	b	614	CLA	OBD-CAD	3.53	1.28	1.22
23	B	603	CLA	C1B-NB	-3.53	1.33	1.37
23	C	511	CLA	C3D-C2D	3.53	1.48	1.39
23	C	507	CLA	C4B-NB	-3.52	1.33	1.37
23	B	616	CLA	CHD-C4C	3.52	1.47	1.39
23	B	604	CLA	O2A-CGA	3.52	1.43	1.33
23	c	502	CLA	OBD-CAD	3.52	1.28	1.22
23	c	513	CLA	CHC-C4B	3.52	1.47	1.39
35	C	519	DGD	O2G-C1B	3.52	1.44	1.34
32	d	406[B]	LHG	O8-C23	3.51	1.43	1.33
23	C	513	CLA	OBD-CAD	3.51	1.28	1.22
34	b	623	HTG	C1'-S1	-3.51	1.76	1.81
32	d	413[A]	LHG	O7-C7	3.51	1.44	1.34
23	B	607	CLA	O2A-CGA	3.51	1.43	1.33
23	c	513	CLA	OBD-CAD	3.50	1.28	1.22
23	b	608	CLA	C1D-ND	3.50	1.42	1.37
23	c	502	CLA	CHC-C4B	3.50	1.47	1.39
32	A	419[A]	LHG	O8-C23	3.50	1.43	1.33
23	c	504	CLA	C1B-NB	-3.50	1.33	1.37
23	b	606	CLA	O2A-CGA	3.50	1.43	1.33
23	B	613	CLA	CHC-C4B	3.50	1.47	1.39
23	a	406[A]	CLA	OBD-CAD	3.50	1.28	1.22
23	D	402[A]	CLA	CHC-C4B	3.49	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	C3D-C2D	3.49	1.48	1.39
23	B	614	CLA	C3D-C2D	3.49	1.48	1.39
23	C	505	CLA	CHD-C4C	3.49	1.47	1.39
23	c	509	CLA	OBD-CAD	3.48	1.28	1.22
23	b	608	CLA	CHC-C4B	3.48	1.47	1.39
23	b	601	CLA	CHC-C4B	3.48	1.47	1.39
23	B	607	CLA	CHC-C4B	3.48	1.47	1.39
23	D	403	CLA	O2A-CGA	3.48	1.43	1.33
23	c	504	CLA	CHD-C4C	3.48	1.47	1.39
23	a	405[A]	CLA	CHB-C1B	3.47	1.47	1.39
23	B	610	CLA	O2A-CGA	3.47	1.43	1.33
23	B	607	CLA	C1D-ND	3.46	1.42	1.37
23	d	402[B]	CLA	OBD-CAD	3.46	1.28	1.22
33	D	411	LMG	O8-C28	3.46	1.43	1.33
23	A	404[B]	CLA	OBD-CAD	3.45	1.28	1.22
23	c	510	CLA	CHD-C1D	3.45	1.45	1.38
23	B	612	CLA	C1D-ND	3.45	1.42	1.37
23	b	609	CLA	CHC-C4B	3.45	1.47	1.39
23	C	503	CLA	OBD-CAD	3.44	1.28	1.22
23	B	613	CLA	C1B-NB	-3.44	1.33	1.37
23	a	404[B]	CLA	C1B-NB	-3.43	1.33	1.37
23	c	511	CLA	CHC-C4B	3.43	1.47	1.39
23	b	601	CLA	OBD-CAD	3.43	1.28	1.22
23	b	605	CLA	C3D-C2D	3.43	1.48	1.39
23	C	504	CLA	OBD-CAD	3.43	1.28	1.22
23	B	612	CLA	CHC-C4B	3.43	1.47	1.39
23	C	514	CLA	OBD-CAD	3.43	1.28	1.22
23	c	504	CLA	CHC-C4B	3.42	1.47	1.39
38	f	101	HEM	C4D-ND	-3.42	1.34	1.40
23	A	408	CLA	C1D-ND	3.42	1.42	1.37
23	c	501	CLA	OBD-CAD	3.41	1.28	1.22
23	C	511	CLA	OBD-CAD	3.41	1.28	1.22
38	F	102	HEM	C4D-ND	-3.41	1.34	1.40
23	B	613	CLA	CHD-C4C	3.40	1.46	1.39
23	B	612	CLA	C4B-NB	-3.40	1.33	1.37
23	C	510	CLA	C4B-NB	-3.40	1.33	1.37
23	C	506	CLA	C1B-C2B	3.40	1.51	1.43
23	b	602	CLA	CHB-C1B	3.40	1.47	1.39
23	b	603	CLA	CHD-C4C	3.40	1.46	1.39
32	b	629[A]	LHG	O8-C23	3.40	1.43	1.33
23	B	607	CLA	C3D-C2D	3.39	1.48	1.39
35	H	102	DGD	O2G-C1B	3.39	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404[A]	CLA	C4B-NB	-3.39	1.33	1.37
23	C	510	CLA	CHC-C4B	3.39	1.47	1.39
23	a	408	CLA	CHD-C1D	3.39	1.45	1.38
23	B	615	CLA	CHC-C4B	3.38	1.47	1.39
23	B	606	CLA	O2A-CGA	3.38	1.43	1.33
23	B	615	CLA	C3D-C2D	3.38	1.48	1.39
23	b	613	CLA	CHD-C4C	3.38	1.46	1.39
23	C	505	CLA	CHC-C4B	3.37	1.47	1.39
23	d	402[A]	CLA	CHC-C4B	3.37	1.47	1.39
23	B	612	CLA	O2A-CGA	3.37	1.43	1.33
23	C	508	CLA	CHD-C4C	3.37	1.46	1.39
23	b	606	CLA	OBD-CAD	3.37	1.28	1.22
23	C	502	CLA	C1B-NB	-3.37	1.33	1.37
23	B	608	CLA	O2A-CGA	3.37	1.43	1.33
35	c	518	DGD	O2G-C1B	3.37	1.43	1.34
23	A	405[B]	CLA	CHB-C1B	3.36	1.47	1.39
23	b	611	CLA	C3D-C2D	3.36	1.48	1.39
23	a	405[B]	CLA	CHC-C4B	3.36	1.47	1.39
23	c	506	CLA	CHC-C4B	3.36	1.47	1.39
23	b	604	CLA	O2A-CGA	3.36	1.43	1.33
23	b	611	CLA	C1B-NB	-3.36	1.33	1.37
23	A	405[A]	CLA	OBD-CAD	3.36	1.28	1.22
24	a	407[A]	PHO	O2A-CGA	3.36	1.43	1.33
23	B	611	CLA	C3D-C2D	3.35	1.48	1.39
23	a	405[B]	CLA	C1B-NB	-3.35	1.33	1.37
23	C	508	CLA	CHB-C1B	3.34	1.46	1.39
23	C	508	CLA	OBD-CAD	3.34	1.28	1.22
23	B	613	CLA	O2A-CGA	3.34	1.43	1.33
38	f	101	HEM	C1B-NB	-3.34	1.34	1.40
23	C	506	CLA	OBD-CAD	3.34	1.28	1.22
23	B	603	CLA	OBD-CAD	3.33	1.28	1.22
23	c	513	CLA	C1B-NB	-3.33	1.33	1.37
23	A	404[A]	CLA	OBD-CAD	3.33	1.28	1.22
34	b	622	HTG	C1'-S1	-3.33	1.76	1.81
23	d	402[A]	CLA	C1D-ND	3.32	1.42	1.37
23	b	614	CLA	C1B-NB	-3.32	1.33	1.37
23	c	503	CLA	C3D-C2D	3.32	1.48	1.39
23	b	616	CLA	CHB-C1B	3.32	1.46	1.39
23	b	607	CLA	CHD-C4C	3.32	1.46	1.39
23	A	405[A]	CLA	C1B-NB	-3.32	1.33	1.37
23	b	612	CLA	CHD-C4C	3.32	1.46	1.39
23	C	513	CLA	CHB-C1B	3.31	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	CHC-C4B	3.31	1.46	1.39
23	b	605	CLA	OBD-CAD	3.31	1.28	1.22
23	C	511	CLA	C4B-NB	-3.31	1.33	1.37
23	b	616	CLA	OBD-CAD	3.30	1.28	1.22
23	b	603	CLA	OBD-CAD	3.29	1.28	1.22
23	D	402[B]	CLA	CHC-C4B	3.29	1.46	1.39
23	D	403	CLA	C1B-NB	-3.29	1.33	1.37
23	d	402[B]	CLA	CHC-C4B	3.28	1.46	1.39
23	A	404[A]	CLA	O2A-CGA	3.28	1.42	1.33
23	b	603	CLA	CHB-C1B	3.28	1.46	1.39
23	a	408	CLA	C1D-ND	3.28	1.42	1.37
23	c	509	CLA	C4B-NB	-3.28	1.33	1.37
23	B	608	CLA	CHC-C4B	3.27	1.46	1.39
23	A	408	CLA	OBD-CAD	3.26	1.28	1.22
23	a	406[A]	CLA	CHC-C4B	3.26	1.46	1.39
23	C	503	CLA	C4B-NB	-3.26	1.33	1.37
34	o	301	HTG	C1'-S1	-3.26	1.76	1.81
23	c	511	CLA	C1B-C2B	3.25	1.50	1.43
23	b	611	CLA	CHD-C4C	3.25	1.46	1.39
23	d	402[A]	CLA	C1B-NB	-3.25	1.33	1.37
23	D	402[A]	CLA	OBD-CAD	3.24	1.28	1.22
23	C	514	CLA	C1B-NB	-3.24	1.33	1.37
23	B	614	CLA	CHD-C1D	3.24	1.44	1.38
23	c	509	CLA	C1B-C2B	3.24	1.50	1.43
23	b	602	CLA	C1B-NB	-3.23	1.33	1.37
23	a	405[A]	CLA	CHC-C4B	3.23	1.46	1.39
23	b	612	CLA	C1B-C2B	3.23	1.50	1.43
23	a	406[B]	CLA	CHB-C1B	3.22	1.46	1.39
23	B	612	CLA	CHD-C4C	3.22	1.46	1.39
23	c	506	CLA	OBD-CAD	3.21	1.28	1.22
23	b	610	CLA	C1B-NB	-3.21	1.33	1.37
23	b	603	CLA	O2A-CGA	3.21	1.42	1.33
23	B	616	CLA	C1B-C2B	3.21	1.50	1.43
23	b	604	CLA	C1B-NB	-3.21	1.33	1.37
23	a	408	CLA	C3D-C2D	3.21	1.47	1.39
23	C	507	CLA	CHC-C4B	3.20	1.46	1.39
23	C	514	CLA	CHC-C4B	3.20	1.46	1.39
23	a	404[A]	CLA	O2A-CGA	3.19	1.42	1.33
23	B	602	CLA	C1B-NB	-3.19	1.33	1.37
23	c	504	CLA	OBD-CAD	3.19	1.28	1.22
23	b	607	CLA	C1B-C2B	3.19	1.50	1.43
38	F	102	HEM	C1B-NB	-3.18	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	C1B-NB	-3.17	1.33	1.37
23	B	606	CLA	OBD-CAD	3.16	1.27	1.22
23	C	505	CLA	OBD-CAD	3.16	1.27	1.22
23	a	408	CLA	OBD-CAD	3.15	1.27	1.22
23	A	408	CLA	C1B-NB	-3.14	1.33	1.37
23	b	604	CLA	C4D-CHA	3.14	1.49	1.38
23	B	609	CLA	C1B-NB	-3.14	1.33	1.37
23	b	601	CLA	C1B-NB	-3.13	1.33	1.37
23	B	612	CLA	C1C-C2C	3.13	1.50	1.44
23	C	514	CLA	C4B-NB	-3.12	1.33	1.37
23	c	507	CLA	C4B-NB	-3.12	1.33	1.37
23	c	506	CLA	C1B-NB	-3.12	1.33	1.37
23	C	511	CLA	C1B-C2B	3.11	1.50	1.43
23	A	406[B]	CLA	C1B-NB	-3.11	1.33	1.37
23	b	604	CLA	C1B-C2B	3.10	1.50	1.43
23	C	508	CLA	C1B-NB	-3.09	1.33	1.37
23	B	604	CLA	C3D-C2D	3.09	1.47	1.39
23	c	509	CLA	CHC-C4B	3.09	1.46	1.39
23	c	513	CLA	C4B-NB	-3.09	1.33	1.37
23	C	511	CLA	CHC-C4B	3.09	1.46	1.39
23	B	603	CLA	C4B-NB	-3.08	1.33	1.37
23	B	605	CLA	C1B-C2B	3.08	1.50	1.43
23	b	607	CLA	CHC-C4B	3.08	1.46	1.39
23	d	403	CLA	OBD-CAD	3.08	1.27	1.22
23	c	501	CLA	C1C-C2C	3.08	1.50	1.44
23	B	607	CLA	C4D-CHA	3.07	1.48	1.38
23	b	605	CLA	O2A-CGA	3.07	1.42	1.33
23	C	506	CLA	C1B-NB	-3.07	1.33	1.37
23	B	613	CLA	C1B-C2B	3.07	1.50	1.43
23	B	614	CLA	OBD-CAD	3.06	1.27	1.22
23	b	610	CLA	O2A-CGA	3.06	1.42	1.33
23	C	508	CLA	C4B-NB	-3.06	1.33	1.37
23	c	504	CLA	C4C-C3C	3.06	1.50	1.45
23	A	408	CLA	CHB-C1B	3.06	1.46	1.39
23	c	504	CLA	C1B-C2B	3.05	1.50	1.43
23	C	512	CLA	C4D-CHA	3.05	1.48	1.38
23	D	402[A]	CLA	C1B-NB	-3.05	1.33	1.37
23	b	615	CLA	C1B-NB	-3.05	1.33	1.37
23	B	602	CLA	C1B-C2B	3.05	1.50	1.43
23	c	502	CLA	C4B-NB	-3.05	1.33	1.37
23	D	403	CLA	C1C-C2C	3.03	1.50	1.44
23	B	612	CLA	C1B-C2B	3.03	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406[A]	CLA	C1B-C2B	3.03	1.50	1.43
23	D	402[B]	CLA	C4B-NB	-3.03	1.33	1.37
23	c	513	CLA	C1B-C2B	3.02	1.50	1.43
23	A	408	CLA	C1B-C2B	3.02	1.50	1.43
23	c	502	CLA	C1B-C2B	3.01	1.50	1.43
23	A	404[A]	CLA	CHC-C4B	3.01	1.46	1.39
23	C	510	CLA	C1B-NB	-3.00	1.33	1.37
23	C	505	CLA	C1B-NB	-3.00	1.33	1.37
23	B	615	CLA	C1B-NB	-3.00	1.33	1.37
23	B	616	CLA	C4D-CHA	3.00	1.48	1.38
23	a	406[B]	CLA	C4B-NB	-2.99	1.33	1.37
29	A	414[A]	PL9	C6-C5	2.99	1.49	1.35
24	A	407[A]	PHO	CBD-CGD	-2.99	1.48	1.52
23	B	604	CLA	C1B-C2B	2.99	1.50	1.43
23	B	608	CLA	C4B-NB	-2.98	1.33	1.37
23	C	507	CLA	C1B-NB	-2.97	1.34	1.37
23	A	404[B]	CLA	C4C-C3C	2.97	1.50	1.45
23	B	602	CLA	C1C-C2C	2.95	1.50	1.44
23	A	404[A]	CLA	C1B-NB	-2.95	1.34	1.37
23	c	505	CLA	C1B-NB	-2.95	1.34	1.37
23	d	402[A]	CLA	C4B-NB	-2.95	1.34	1.37
23	C	503	CLA	C1B-C2B	2.95	1.50	1.43
23	c	510	CLA	OBD-CAD	2.94	1.27	1.22
23	B	615	CLA	C1B-C2B	2.94	1.50	1.43
23	D	403	CLA	C1B-C2B	2.94	1.50	1.43
23	B	605	CLA	C4B-NB	-2.94	1.34	1.37
23	B	605	CLA	C1C-C2C	2.94	1.50	1.44
23	C	514	CLA	C1B-C2B	2.94	1.50	1.43
23	B	613	CLA	C1C-C2C	2.94	1.50	1.44
23	C	508	CLA	C4D-CHA	2.93	1.48	1.38
23	C	513	CLA	C1C-C2C	2.93	1.50	1.44
23	b	611	CLA	OBD-CAD	2.93	1.27	1.22
23	C	502	CLA	OBD-CAD	2.93	1.27	1.22
23	c	508	CLA	C4D-CHA	2.93	1.48	1.38
23	a	406[B]	CLA	C1B-NB	-2.93	1.34	1.37
23	B	614	CLA	C1B-C2B	2.93	1.50	1.43
23	c	510	CLA	C4D-CHA	2.92	1.48	1.38
29	a	413[A]	PL9	C6-C5	2.92	1.49	1.35
23	a	404[A]	CLA	C1B-NB	-2.92	1.34	1.37
23	b	602	CLA	C1C-C2C	2.91	1.50	1.44
29	a	413[B]	PL9	C6-C5	2.91	1.49	1.35
23	a	404[A]	CLA	C4B-NB	-2.91	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	C4B-NB	-2.91	1.34	1.37
23	B	612	CLA	C4D-CHA	2.91	1.48	1.38
23	b	609	CLA	C1B-NB	-2.91	1.34	1.37
23	B	607	CLA	C1B-C2B	2.91	1.50	1.43
23	b	603	CLA	C1B-C2B	2.91	1.50	1.43
24	a	415[B]	PHO	C3A-C2A	-2.91	1.52	1.54
23	c	508	CLA	C1B-C2B	2.91	1.49	1.43
23	a	406[A]	CLA	C1B-NB	-2.91	1.34	1.37
34	d	410	HTG	C1'-S1	-2.91	1.77	1.81
23	d	402[B]	CLA	C1B-NB	-2.90	1.34	1.37
23	A	406[B]	CLA	C3B-C4B	2.90	1.51	1.42
23	c	503	CLA	C1B-NB	-2.90	1.34	1.37
23	B	616	CLA	OBD-CAD	2.90	1.27	1.22
29	A	414[B]	PL9	C6-C5	2.90	1.49	1.35
23	B	614	CLA	C4D-CHA	2.89	1.48	1.38
23	D	403	CLA	C4C-C3C	2.89	1.49	1.45
23	c	507	CLA	C1B-C2B	2.89	1.49	1.43
23	a	408	CLA	C1B-C2B	2.88	1.49	1.43
23	A	404[A]	CLA	C4C-C3C	2.88	1.49	1.45
23	b	611	CLA	C4C-C3C	2.88	1.49	1.45
23	B	610	CLA	C4D-CHA	2.88	1.48	1.38
23	c	509	CLA	C4D-CHA	2.88	1.48	1.38
23	b	607	CLA	C4C-C3C	2.88	1.49	1.45
23	a	408	CLA	C1C-C2C	2.87	1.50	1.44
24	A	416[B]	PHO	CHA-CBD	-2.87	1.48	1.51
23	b	609	CLA	C4D-CHA	2.87	1.48	1.38
23	c	507	CLA	C1B-NB	-2.86	1.34	1.37
23	b	614	CLA	C4D-CHA	2.86	1.48	1.38
23	D	402[A]	CLA	C1B-C2B	2.86	1.49	1.43
23	c	511	CLA	C4D-CHA	2.85	1.48	1.38
23	c	510	CLA	C1B-NB	-2.85	1.34	1.37
23	C	505	CLA	C4D-CHA	2.85	1.48	1.38
23	c	507	CLA	C4D-CHA	2.85	1.48	1.38
33	Z	101	LMG	O8-C28	2.85	1.47	1.33
23	C	506	CLA	C4D-CHA	2.84	1.48	1.38
23	c	503	CLA	C1B-C2B	2.84	1.49	1.43
23	C	505	CLA	C1B-C2B	2.84	1.49	1.43
23	D	402[B]	CLA	C1B-NB	-2.84	1.34	1.37
23	a	408	CLA	C4B-NB	-2.84	1.34	1.37
23	c	503	CLA	C1C-C2C	2.84	1.50	1.44
23	d	402[A]	CLA	C4C-C3C	2.84	1.49	1.45
23	A	408	CLA	CHC-C4B	2.83	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	C3B-C4B	2.83	1.51	1.42
23	c	512	CLA	C1B-NB	-2.83	1.34	1.37
23	A	404[A]	CLA	C1B-C2B	2.83	1.49	1.43
23	C	502	CLA	C1B-C2B	2.82	1.49	1.43
23	c	503	CLA	OBD-CAD	2.82	1.27	1.22
23	c	501	CLA	C4D-CHA	2.82	1.48	1.38
23	b	610	CLA	C4D-CHA	2.82	1.48	1.38
23	b	614	CLA	C1B-C2B	2.81	1.49	1.43
23	C	507	CLA	C4C-C3C	2.81	1.49	1.45
23	c	510	CLA	C1B-C2B	2.81	1.49	1.43
23	b	608	CLA	C1B-NB	-2.81	1.34	1.37
23	b	615	CLA	C4D-CHA	2.81	1.48	1.38
23	B	605	CLA	C1B-NB	-2.81	1.34	1.37
23	c	505	CLA	C1C-C2C	2.80	1.50	1.44
23	c	503	CLA	C4D-CHA	2.80	1.48	1.38
23	B	609	CLA	C3B-C4B	2.79	1.50	1.42
23	a	406[A]	CLA	C1C-C2C	2.79	1.50	1.44
23	c	512	CLA	C1B-C2B	2.79	1.49	1.43
23	C	511	CLA	C1B-NB	-2.79	1.34	1.37
23	A	405[A]	CLA	C4D-CHA	2.79	1.48	1.38
24	a	407[A]	PHO	CBD-CGD	-2.79	1.49	1.52
23	D	402[B]	CLA	C1B-C2B	2.79	1.49	1.43
23	c	510	CLA	C1C-C2C	2.79	1.50	1.44
23	C	509	CLA	C4B-NB	-2.79	1.34	1.37
23	c	505	CLA	C1B-C2B	2.79	1.49	1.43
27	A	418	GOL	O2-C2	-2.78	1.35	1.43
23	b	607	CLA	O2A-CGA	2.78	1.41	1.33
35	C	519	DGD	O2G-C2G	-2.78	1.40	1.46
23	c	503	CLA	C4B-NB	-2.78	1.34	1.37
23	b	608	CLA	C4D-CHA	2.77	1.47	1.38
23	a	406[A]	CLA	C4D-CHA	2.77	1.47	1.38
23	B	604	CLA	C4D-CHA	2.77	1.47	1.38
23	c	504	CLA	C1C-C2C	2.77	1.50	1.44
23	b	606	CLA	C4D-CHA	2.77	1.47	1.38
23	C	509	CLA	C1B-C2B	2.76	1.49	1.43
23	b	614	CLA	C4B-NB	-2.76	1.34	1.37
23	B	604	CLA	C4C-C3C	2.76	1.49	1.45
34	b	625	HTG	C1-S1	-2.76	1.76	1.80
23	b	611	CLA	C4B-NB	-2.76	1.34	1.37
23	c	501	CLA	C1B-NB	-2.76	1.34	1.37
23	C	502	CLA	C4D-CHA	2.76	1.47	1.38
23	A	405[A]	CLA	C1B-C2B	2.76	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	C4D-CHA	2.76	1.47	1.38
23	B	608	CLA	C1B-C2B	2.75	1.49	1.43
23	C	507	CLA	C1B-C2B	2.75	1.49	1.43
23	B	601	CLA	C1C-C2C	2.75	1.50	1.44
23	B	601	CLA	C4B-NB	-2.75	1.34	1.37
23	A	404[B]	CLA	C4D-CHA	2.75	1.47	1.38
23	B	609	CLA	C1B-C2B	2.75	1.49	1.43
23	c	506	CLA	C4D-CHA	2.74	1.47	1.38
23	D	402[A]	CLA	C4B-NB	-2.74	1.34	1.37
23	B	608	CLA	OBD-CAD	2.73	1.27	1.22
23	C	510	CLA	C1C-C2C	2.73	1.50	1.44
35	H	102	DGD	O5D-C1E	2.73	1.44	1.40
23	a	406[A]	CLA	C1B-C2B	2.73	1.49	1.43
23	c	512	CLA	C4D-CHA	2.73	1.47	1.38
23	B	606	CLA	C1C-C2C	2.73	1.50	1.44
23	b	601	CLA	C4B-NB	-2.73	1.34	1.37
23	C	506	CLA	C4C-C3C	2.73	1.49	1.45
23	a	405[A]	CLA	C1B-C2B	2.73	1.49	1.43
23	b	613	CLA	C4B-NB	-2.73	1.34	1.37
23	c	504	CLA	C4B-NB	-2.73	1.34	1.37
23	B	605	CLA	OBD-CAD	2.72	1.27	1.22
23	b	606	CLA	C1B-C2B	2.72	1.49	1.43
23	c	505	CLA	C4C-C3C	2.72	1.49	1.45
23	B	615	CLA	C1C-C2C	2.72	1.50	1.44
23	c	507	CLA	C1C-C2C	2.72	1.50	1.44
23	a	408	CLA	C4D-CHA	2.71	1.47	1.38
23	A	406[A]	CLA	C3B-C4B	2.71	1.50	1.42
23	D	402[A]	CLA	C4D-CHA	2.71	1.47	1.38
33	C	521	LMG	O1-C1	2.71	1.44	1.40
23	B	610	CLA	C4B-NB	-2.71	1.34	1.37
23	C	513	CLA	C3B-C4B	2.71	1.50	1.42
23	C	512	CLA	C4C-C3C	2.71	1.49	1.45
23	B	608	CLA	C4D-CHA	2.71	1.47	1.38
23	B	616	CLA	C1B-NB	-2.70	1.34	1.37
23	c	505	CLA	C4D-CHA	2.70	1.47	1.38
23	C	509	CLA	C4D-CHA	2.70	1.47	1.38
24	A	416[B]	PHO	C3D-C4D	-2.70	1.37	1.41
27	a	419	GOL	C1-C2	2.70	1.62	1.51
23	d	402[A]	CLA	C4D-CHA	2.70	1.47	1.38
23	b	607	CLA	OBD-CAD	2.70	1.27	1.22
23	b	613	CLA	C1B-C2B	2.69	1.49	1.43
23	c	506	CLA	C1B-C2B	2.69	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C4D-CHA	2.68	1.47	1.38
23	b	605	CLA	C4D-CHA	2.68	1.47	1.38
23	C	509	CLA	C3B-C2B	2.68	1.50	1.41
23	c	503	CLA	C3B-C4B	2.68	1.50	1.42
23	b	612	CLA	C1B-NB	-2.68	1.34	1.37
23	C	514	CLA	C4D-CHA	2.68	1.47	1.38
23	b	613	CLA	C4D-CHA	2.68	1.47	1.38
23	b	610	CLA	C4C-C3C	2.68	1.49	1.45
23	b	616	CLA	C1B-NB	-2.68	1.34	1.37
23	C	502	CLA	C3B-C4B	2.68	1.50	1.42
23	A	406[A]	CLA	C4D-CHA	2.67	1.47	1.38
23	A	406[B]	CLA	C4B-NB	-2.67	1.34	1.37
34	c	521	HTG	C1'-S1	-2.67	1.77	1.81
24	a	415[A]	PHO	C3A-C2A	-2.67	1.52	1.54
23	c	508	CLA	C4C-C3C	2.67	1.49	1.45
23	b	607	CLA	C4D-CHA	2.67	1.47	1.38
23	A	405[B]	CLA	C4D-CHA	2.67	1.47	1.38
23	b	616	CLA	C4D-CHA	2.66	1.47	1.38
23	a	406[B]	CLA	C4D-CHA	2.66	1.47	1.38
23	b	611	CLA	C1B-C2B	2.66	1.49	1.43
23	a	405[B]	CLA	C4D-CHA	2.66	1.47	1.38
23	B	606	CLA	C1B-C2B	2.66	1.49	1.43
23	B	614	CLA	C1B-NB	-2.66	1.34	1.37
23	B	612	CLA	OBD-CAD	2.66	1.27	1.22
23	b	615	CLA	C1B-C2B	2.66	1.49	1.43
29	D	405[A]	PL9	C6-C5	2.66	1.48	1.35
23	c	501	CLA	C1B-C2B	2.66	1.49	1.43
31	B	627	LMT	C3'-C2'	2.65	1.59	1.52
23	c	504	CLA	C4D-CHA	2.65	1.47	1.38
23	B	606	CLA	C4D-CHA	2.65	1.47	1.38
23	d	402[B]	CLA	C1B-C2B	2.65	1.49	1.43
23	B	613	CLA	C4D-CHA	2.65	1.47	1.38
23	A	405[B]	CLA	C1B-C2B	2.65	1.49	1.43
23	a	408	CLA	C3B-C4B	2.65	1.50	1.42
23	a	404[A]	CLA	C4D-CHA	2.65	1.47	1.38
23	b	602	CLA	C3B-C4B	2.65	1.50	1.42
23	A	408	CLA	C4D-CHA	2.65	1.47	1.38
23	b	610	CLA	C3D-C4D	-2.64	1.38	1.44
23	B	614	CLA	C3D-C4D	-2.64	1.38	1.44
23	c	505	CLA	C3B-C4B	2.64	1.50	1.42
23	b	609	CLA	C1C-NC	-2.64	1.33	1.37
23	C	504	CLA	C4B-NB	-2.64	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404[A]	CLA	C4D-CHA	2.64	1.47	1.38
23	D	403	CLA	C3B-C4B	2.63	1.50	1.42
23	a	404[B]	CLA	C4D-CHA	2.63	1.47	1.38
23	d	403	CLA	C4D-CHA	2.63	1.47	1.38
34	D	410	HTG	C1'-S1	-2.63	1.77	1.81
23	a	406[A]	CLA	C4B-NB	-2.63	1.34	1.37
23	C	509	CLA	C4C-C3C	2.63	1.49	1.45
23	A	405[A]	CLA	C1C-C2C	2.62	1.49	1.44
23	b	610	CLA	C1B-C2B	2.62	1.49	1.43
23	c	503	CLA	C3D-C4D	-2.62	1.38	1.44
23	b	601	CLA	C4D-CHA	2.62	1.47	1.38
23	a	405[A]	CLA	C4D-CHA	2.61	1.47	1.38
23	b	611	CLA	C1C-C2C	2.61	1.49	1.44
34	C	522	HTG	C1'-S1	-2.61	1.77	1.81
23	a	405[A]	CLA	C4B-NB	-2.61	1.34	1.37
23	b	603	CLA	C4D-CHA	2.61	1.47	1.38
23	B	610	CLA	C4C-C3C	2.61	1.49	1.45
23	C	511	CLA	C4D-CHA	2.61	1.47	1.38
23	a	404[B]	CLA	C3B-C4B	2.61	1.50	1.42
23	C	512	CLA	C1C-C2C	2.61	1.49	1.44
23	B	605	CLA	C4D-CHA	2.61	1.47	1.38
23	c	513	CLA	C4C-C3C	2.61	1.49	1.45
23	B	601	CLA	C3B-C4B	2.60	1.50	1.42
23	c	511	CLA	C4B-NB	-2.60	1.34	1.37
24	A	416[A]	PHO	C3D-C4D	-2.60	1.37	1.41
23	B	616	CLA	C1C-NC	-2.60	1.33	1.37
23	A	405[A]	CLA	C4B-NB	-2.60	1.34	1.37
24	A	407[B]	PHO	CBD-CGD	-2.60	1.49	1.52
23	C	502	CLA	C1C-C2C	2.59	1.49	1.44
35	c	518	DGD	O2G-C2G	-2.59	1.40	1.46
29	d	405[B]	PL9	C6-C5	2.59	1.48	1.35
29	D	405[B]	PL9	C6-C5	2.59	1.48	1.35
23	b	607	CLA	C4B-NB	-2.59	1.34	1.37
23	C	512	CLA	C1B-C2B	2.59	1.49	1.43
23	b	602	CLA	C3D-C4D	-2.59	1.38	1.44
23	C	513	CLA	C4D-CHA	2.58	1.47	1.38
23	a	404[B]	CLA	C1B-C2B	2.58	1.49	1.43
34	b	625	HTG	C1'-S1	-2.58	1.77	1.81
23	B	615	CLA	C4D-CHA	2.58	1.47	1.38
23	B	601	CLA	C1B-NB	-2.58	1.34	1.37
23	d	402[A]	CLA	C1B-C2B	2.57	1.49	1.43
23	A	408	CLA	C3D-C4D	-2.57	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	502	CLA	C3B-C2B	2.57	1.49	1.41
23	A	406[B]	CLA	C4D-CHA	2.57	1.47	1.38
23	c	509	CLA	C4C-C3C	2.57	1.49	1.45
23	b	609	CLA	C3B-C4B	2.56	1.50	1.42
31	b	621	LMT	C3'-C2'	2.56	1.59	1.52
23	a	405[B]	CLA	C1B-C2B	2.56	1.49	1.43
23	D	402[B]	CLA	C4D-CHA	2.56	1.47	1.38
23	b	602	CLA	C4D-CHA	2.56	1.47	1.38
23	B	602	CLA	C4B-NB	-2.56	1.34	1.37
23	A	405[A]	CLA	C3B-C4B	2.56	1.50	1.42
23	A	405[B]	CLA	C3B-C4B	2.55	1.50	1.42
23	B	605	CLA	C3B-C4B	2.55	1.50	1.42
23	d	403	CLA	C3B-C4B	2.55	1.50	1.42
34	b	622	HTG	O5-C1	2.55	1.46	1.42
23	c	513	CLA	C4D-CHA	2.55	1.47	1.38
23	c	508	CLA	C1C-C2C	2.55	1.49	1.44
23	b	611	CLA	C4D-CHA	2.55	1.47	1.38
23	B	609	CLA	C1C-C2C	2.55	1.49	1.44
23	C	514	CLA	C1C-C2C	2.55	1.49	1.44
23	c	513	CLA	C1C-C2C	2.54	1.49	1.44
23	B	612	CLA	C3B-C2B	2.54	1.49	1.41
23	b	609	CLA	C4B-NB	-2.54	1.34	1.37
23	b	616	CLA	C1C-C2C	2.54	1.49	1.44
23	C	512	CLA	OBD-CAD	2.54	1.26	1.22
23	d	403	CLA	C1C-C2C	2.54	1.49	1.44
23	A	408	CLA	C4B-NB	-2.54	1.34	1.37
23	b	606	CLA	C3D-C4D	-2.54	1.38	1.44
23	b	613	CLA	OBD-CAD	2.54	1.26	1.22
23	B	601	CLA	C4D-CHA	2.54	1.47	1.38
34	B	624	HTG	C1-S1	-2.54	1.76	1.80
23	c	506	CLA	C4C-C3C	2.54	1.49	1.45
23	C	510	CLA	C4D-CHA	2.54	1.47	1.38
23	a	408	CLA	C4C-C3C	2.53	1.49	1.45
23	B	610	CLA	C1C-C2C	2.53	1.49	1.44
23	a	404[A]	CLA	C1B-C2B	2.53	1.49	1.43
38	F	102	HEM	C1C-C2C	-2.53	1.40	1.45
23	B	609	CLA	C4D-CHA	2.53	1.47	1.38
23	b	606	CLA	C3B-C4B	2.53	1.50	1.42
23	a	408	CLA	C1B-NB	-2.53	1.34	1.37
23	C	504	CLA	C3D-C4D	-2.53	1.38	1.44
23	A	405[B]	CLA	C4B-NB	-2.53	1.34	1.37
23	C	513	CLA	C1B-NB	-2.53	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402[B]	CLA	C4C-C3C	2.53	1.49	1.45
23	B	611	CLA	MG-NB	2.52	2.10	2.05
23	B	602	CLA	C4D-CHA	2.52	1.47	1.38
24	A	416[B]	PHO	C4B-NB	-2.52	1.34	1.38
23	b	601	CLA	C1C-C2C	2.52	1.49	1.44
23	c	511	CLA	C1C-C2C	2.52	1.49	1.44
23	C	511	CLA	C4C-C3C	2.52	1.49	1.45
23	A	405[B]	CLA	C3D-C4D	-2.52	1.38	1.44
23	B	604	CLA	C1B-NB	-2.52	1.34	1.37
23	d	402[B]	CLA	C4D-CHA	2.51	1.47	1.38
38	f	101	HEM	C1D-ND	-2.51	1.33	1.38
23	C	512	CLA	C3D-C4D	-2.51	1.38	1.44
23	b	616	CLA	C3B-C4B	2.51	1.50	1.42
23	B	613	CLA	C4C-C3C	2.51	1.49	1.45
24	A	416[A]	PHO	C3A-C2A	-2.51	1.52	1.54
23	C	503	CLA	C1C-C2C	2.51	1.49	1.44
27	o	304	GOL	C1-C2	2.51	1.61	1.51
23	c	501	CLA	C3D-C4D	-2.51	1.38	1.44
23	B	606	CLA	C1B-NB	-2.51	1.34	1.37
35	h	102	DGD	O5D-C1E	2.51	1.44	1.40
23	b	603	CLA	C1C-C2C	2.51	1.49	1.44
24	a	407[B]	PHO	C4B-NB	-2.51	1.34	1.38
23	B	602	CLA	C4C-C3C	2.51	1.49	1.45
23	b	606	CLA	C1C-C2C	2.50	1.49	1.44
23	c	510	CLA	C4B-NB	-2.50	1.34	1.37
23	B	613	CLA	C4B-NB	-2.50	1.34	1.37
23	C	508	CLA	C1C-C2C	2.50	1.49	1.44
23	b	605	CLA	C1B-C2B	2.50	1.49	1.43
23	B	616	CLA	C3B-C2B	2.50	1.49	1.41
23	A	406[B]	CLA	C1B-C2B	2.50	1.49	1.43
23	a	405[B]	CLA	C4B-NB	-2.50	1.34	1.37
23	c	506	CLA	C4B-NB	-2.50	1.34	1.37
24	a	415[A]	PHO	C4B-NB	-2.50	1.34	1.38
23	B	603	CLA	C1C-C2C	2.50	1.49	1.44
23	C	504	CLA	C3B-C4B	2.49	1.50	1.42
23	B	614	CLA	C1C-C2C	2.49	1.49	1.44
23	C	508	CLA	C1B-C2B	2.49	1.49	1.43
23	A	404[B]	CLA	C1B-C2B	2.49	1.49	1.43
23	A	404[B]	CLA	C3B-C4B	2.49	1.50	1.42
27	D	412	GOL	O2-C2	-2.49	1.36	1.43
23	b	613	CLA	C1C-C2C	2.49	1.49	1.44
23	c	501	CLA	C4C-C3C	2.49	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407[A]	PHO	C4B-NB	-2.48	1.34	1.38
23	d	403	CLA	C1B-NB	-2.48	1.34	1.37
23	b	609	CLA	C1B-C2B	2.48	1.49	1.43
23	B	605	CLA	C3D-C4D	-2.48	1.38	1.44
29	d	405[A]	PL9	C6-C5	2.48	1.47	1.35
31	B	629	LMT	O2'-C2'	-2.48	1.36	1.43
23	B	601	CLA	C1B-C2B	2.48	1.48	1.43
23	B	608	CLA	C1B-NB	-2.48	1.34	1.37
23	C	503	CLA	C4D-CHA	2.47	1.46	1.38
23	C	514	CLA	C3B-C2B	2.47	1.49	1.41
24	A	416[A]	PHO	C4B-NB	-2.47	1.34	1.38
23	B	611	CLA	C4D-CHA	2.47	1.46	1.38
23	b	616	CLA	C4B-NB	-2.47	1.34	1.37
23	c	512	CLA	C3B-C4B	2.47	1.49	1.42
23	b	612	CLA	C3B-C2B	2.47	1.49	1.41
31	t	101	LMT	O3'-C3'	-2.47	1.36	1.43
23	B	610	CLA	C3D-C4D	-2.46	1.38	1.44
23	d	402[A]	CLA	C3D-C4D	-2.46	1.38	1.44
23	b	605	CLA	C1C-C2C	2.46	1.49	1.44
23	B	604	CLA	C1A-CHA	2.46	1.53	1.43
23	b	603	CLA	C3B-C2B	2.46	1.49	1.41
23	C	504	CLA	C4D-CHA	2.46	1.46	1.38
23	d	402[A]	CLA	C1C-C2C	2.45	1.49	1.44
23	b	612	CLA	C4C-C3C	2.45	1.49	1.45
23	B	603	CLA	C1B-C2B	2.45	1.48	1.43
23	b	603	CLA	C4B-NB	-2.45	1.34	1.37
23	A	406[A]	CLA	C4B-NB	-2.44	1.34	1.37
23	D	402[A]	CLA	C3D-C4D	-2.44	1.38	1.44
23	D	402[B]	CLA	C3D-C4D	-2.44	1.38	1.44
23	C	506	CLA	C3B-C4B	2.44	1.49	1.42
23	A	406[B]	CLA	C1C-C2C	2.44	1.49	1.44
23	C	509	CLA	C1C-C2C	2.44	1.49	1.44
23	B	604	CLA	C1C-C2C	2.44	1.49	1.44
38	f	101	HEM	C1C-C2C	-2.43	1.40	1.45
23	d	403	CLA	C1B-C2B	2.43	1.48	1.43
23	a	406[B]	CLA	C1B-C2B	2.43	1.48	1.43
23	B	616	CLA	C3D-C4D	-2.42	1.38	1.44
23	c	511	CLA	C3B-C2B	2.42	1.49	1.41
23	b	616	CLA	C3D-C4D	-2.42	1.38	1.44
23	C	504	CLA	C1B-C2B	2.42	1.48	1.43
23	b	612	CLA	C1C-C2C	2.41	1.49	1.44
23	c	509	CLA	C1C-C2C	2.41	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C3D-C4D	-2.41	1.38	1.44
23	b	610	CLA	C3B-C4B	2.41	1.49	1.42
23	c	507	CLA	C1D-C2D	2.41	1.50	1.45
23	D	403	CLA	C4D-CHA	2.41	1.46	1.38
23	b	609	CLA	C3D-C4D	-2.41	1.38	1.44
23	a	406[A]	CLA	C3B-C4B	2.41	1.49	1.42
24	A	416[B]	PHO	C3A-C2A	-2.40	1.52	1.54
23	b	601	CLA	C3B-C4B	2.40	1.49	1.42
23	C	510	CLA	C3B-C2B	2.40	1.49	1.41
23	D	402[A]	CLA	C3B-C2B	2.40	1.49	1.41
23	c	502	CLA	C4D-CHA	2.40	1.46	1.38
23	B	603	CLA	C3B-C2B	2.40	1.49	1.41
23	a	406[B]	CLA	C3B-C4B	2.40	1.49	1.42
26	F	103	SQD	O6-C1	2.40	1.44	1.40
23	C	510	CLA	C1B-C2B	2.39	1.48	1.43
23	a	404[A]	CLA	C4C-C3C	2.39	1.49	1.45
34	o	301	HTG	O5-C1	2.39	1.46	1.42
23	C	511	CLA	C1C-C2C	2.39	1.49	1.44
23	b	616	CLA	C1B-C2B	2.39	1.48	1.43
23	C	513	CLA	C1B-C2B	2.39	1.48	1.43
23	C	506	CLA	C3D-C4D	-2.39	1.38	1.44
23	b	605	CLA	C3D-C4D	-2.38	1.38	1.44
23	b	608	CLA	C3B-C4B	2.38	1.49	1.42
23	c	511	CLA	C1B-NB	-2.38	1.34	1.37
23	C	510	CLA	C4C-C3C	2.38	1.49	1.45
23	a	406[A]	CLA	C3D-C4D	-2.38	1.38	1.44
23	B	606	CLA	C3B-C4B	2.38	1.49	1.42
23	a	404[A]	CLA	C1C-C2C	2.38	1.49	1.44
31	m	103	LMT	C3'-C2'	2.38	1.58	1.52
23	b	604	CLA	C4B-NB	-2.38	1.34	1.37
23	C	507	CLA	C3D-C4D	-2.37	1.38	1.44
23	c	503	CLA	C4C-C3C	2.37	1.49	1.45
23	D	402[A]	CLA	C1C-C2C	2.37	1.49	1.44
23	b	615	CLA	C4C-C3C	2.37	1.49	1.45
23	B	615	CLA	C3B-C4B	2.37	1.49	1.42
23	b	603	CLA	C3B-C4B	2.37	1.49	1.42
31	M	101	LMT	O1'-C1'	-2.37	1.36	1.40
23	b	603	CLA	C1B-NB	-2.37	1.34	1.37
23	C	514	CLA	C3D-C4D	-2.37	1.38	1.44
23	b	615	CLA	C4B-NB	-2.37	1.34	1.37
23	c	512	CLA	C1C-C2C	2.37	1.49	1.44
23	d	403	CLA	C4B-NB	-2.36	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	C1C-C2C	2.36	1.49	1.44
23	c	513	CLA	C3B-C4B	2.36	1.49	1.42
23	C	512	CLA	C3B-C2B	2.36	1.49	1.41
23	c	508	CLA	C3B-C2B	2.36	1.49	1.41
23	B	606	CLA	C3D-C4D	-2.36	1.38	1.44
24	A	407[B]	PHO	C4B-NB	-2.36	1.34	1.38
23	C	505	CLA	C4C-C3C	2.35	1.49	1.45
23	b	601	CLA	C3B-C2B	2.35	1.49	1.41
23	B	602	CLA	C3B-C2B	2.35	1.49	1.41
23	C	505	CLA	C3B-C2B	2.35	1.49	1.41
23	b	601	CLA	C1B-C2B	2.35	1.48	1.43
23	B	616	CLA	C1C-C2C	2.35	1.49	1.44
38	F	102	HEM	C3C-C4C	-2.35	1.41	1.46
24	a	415[B]	PHO	C4B-NB	-2.35	1.34	1.38
24	A	416[B]	PHO	C1D-ND	-2.34	1.34	1.38
25	d	404	BCR	C30-C25	-2.34	1.50	1.53
27	A	418	GOL	C3-C2	2.34	1.60	1.51
23	b	602	CLA	C4C-C3C	2.34	1.49	1.45
24	a	407[A]	PHO	C1D-ND	-2.34	1.34	1.38
23	b	615	CLA	C3B-C4B	2.33	1.49	1.42
23	B	610	CLA	C1B-C2B	2.33	1.48	1.43
23	b	614	CLA	C4C-C3C	2.33	1.49	1.45
34	B	622	HTG	C1'-S1	-2.33	1.78	1.81
23	a	405[B]	CLA	C3B-C4B	2.33	1.49	1.42
23	b	612	CLA	C3D-C4D	-2.33	1.38	1.44
23	C	505	CLA	C4B-NB	-2.33	1.34	1.37
23	A	404[A]	CLA	C1C-C2C	2.33	1.49	1.44
23	a	404[B]	CLA	C1C-C2C	2.32	1.49	1.44
38	F	102	HEM	C3B-C4B	2.32	1.49	1.44
23	b	607	CLA	C1C-C2C	2.32	1.49	1.44
31	A	420	LMT	O3'-C3'	-2.32	1.37	1.43
23	B	614	CLA	C4C-C3C	2.32	1.49	1.45
23	b	604	CLA	MG-NA	2.32	2.11	2.06
23	b	612	CLA	C4D-CHA	2.32	1.46	1.38
23	a	406[B]	CLA	C1C-C2C	2.32	1.49	1.44
23	b	606	CLA	C3B-C2B	2.32	1.49	1.41
23	A	404[B]	CLA	C1C-C2C	2.31	1.49	1.44
23	c	502	CLA	C1B-NB	-2.31	1.34	1.37
23	a	406[B]	CLA	C3D-C4D	-2.31	1.39	1.44
23	d	402[B]	CLA	C3D-C4D	-2.31	1.39	1.44
23	D	402[B]	CLA	C3B-C2B	2.31	1.48	1.41
27	b	624	GOL	C3-C2	2.31	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	C3D-C4D	-2.30	1.39	1.44
23	A	406[A]	CLA	C1C-C2C	2.30	1.49	1.44
23	C	504	CLA	C1C-C2C	2.30	1.49	1.44
23	A	408	CLA	C3B-C4B	2.30	1.49	1.42
23	C	506	CLA	C1C-C2C	2.30	1.49	1.44
23	C	502	CLA	C3D-C4D	-2.29	1.39	1.44
23	A	408	CLA	C3B-C2B	2.29	1.48	1.41
23	b	611	CLA	C3D-C4D	-2.29	1.39	1.44
23	b	602	CLA	C4B-NB	-2.29	1.34	1.37
23	C	507	CLA	C1C-C2C	2.29	1.49	1.44
23	a	405[A]	CLA	C3B-C4B	2.29	1.49	1.42
23	c	513	CLA	C1D-C2D	2.28	1.49	1.45
31	B	631	LMT	O3'-C3'	-2.28	1.37	1.43
23	D	402[B]	CLA	C4C-C3C	2.28	1.48	1.45
24	a	407[B]	PHO	C3A-C2A	-2.28	1.52	1.54
23	A	408	CLA	C1C-NC	-2.28	1.34	1.37
23	b	614	CLA	C3D-C4D	-2.28	1.39	1.44
23	B	608	CLA	C3B-C2B	2.28	1.48	1.41
23	A	404[B]	CLA	C3B-C2B	2.28	1.48	1.41
23	c	506	CLA	C3B-C2B	2.28	1.48	1.41
31	M	103	LMT	O3'-C3'	-2.28	1.37	1.43
23	b	608	CLA	C3B-C2B	2.28	1.48	1.41
23	b	611	CLA	C3B-C2B	2.28	1.48	1.41
23	a	404[B]	CLA	C4C-C3C	2.28	1.48	1.45
23	a	406[B]	CLA	C4C-C3C	2.27	1.48	1.45
35	C	518[A]	DGD	O5D-C1E	2.27	1.44	1.40
23	C	510	CLA	C3B-C4B	2.27	1.49	1.42
23	B	610	CLA	C3B-C4B	2.27	1.49	1.42
23	d	402[B]	CLA	C3B-C2B	2.27	1.48	1.41
23	c	508	CLA	C4B-NB	-2.27	1.34	1.37
23	B	607	CLA	C1C-C2C	2.27	1.49	1.44
23	b	615	CLA	C3D-C4D	-2.27	1.39	1.44
23	B	607	CLA	C3D-C4D	-2.27	1.39	1.44
23	A	405[A]	CLA	C3D-C4D	-2.26	1.39	1.44
24	A	416[A]	PHO	C1D-ND	-2.26	1.34	1.38
23	B	614	CLA	C1C-NC	-2.26	1.34	1.37
23	B	604	CLA	C3D-C4D	-2.26	1.39	1.44
23	B	601	CLA	C3D-C4D	-2.26	1.39	1.44
23	C	509	CLA	C1B-NB	-2.26	1.34	1.37
23	b	604	CLA	C3B-C4B	2.26	1.49	1.42
23	C	511	CLA	C3B-C2B	2.26	1.48	1.41
23	c	504	CLA	C1C-NC	-2.25	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407[B]	PHO	C1D-ND	-2.25	1.34	1.38
23	C	513	CLA	C3D-C4D	-2.25	1.39	1.44
23	c	508	CLA	C1B-NB	-2.25	1.34	1.37
23	b	605	CLA	C4C-C3C	2.24	1.48	1.45
23	b	607	CLA	C3D-C4D	-2.24	1.39	1.44
23	c	510	CLA	C3B-C4B	2.24	1.49	1.42
31	M	101	LMT	O2'-C2'	-2.24	1.37	1.43
23	B	601	CLA	C3B-C2B	2.24	1.48	1.41
23	C	504	CLA	C1B-NB	-2.23	1.34	1.37
23	c	501	CLA	C3B-C4B	2.23	1.49	1.42
23	c	512	CLA	C4B-NB	-2.23	1.34	1.37
23	c	513	CLA	C3D-C4D	-2.23	1.39	1.44
23	A	405[B]	CLA	C4C-C3C	2.23	1.48	1.45
31	F	101	LMT	O3'-C3'	-2.23	1.37	1.43
23	C	503	CLA	C3B-C2B	2.23	1.48	1.41
23	b	608	CLA	C1B-C2B	2.22	1.48	1.43
29	a	413[A]	PL9	C2-C3	2.22	1.40	1.34
23	c	511	CLA	C4C-C3C	2.22	1.48	1.45
23	C	505	CLA	C1C-C2C	2.22	1.49	1.44
23	C	508	CLA	C4C-C3C	2.22	1.48	1.45
23	A	404[A]	CLA	C3B-C2B	2.22	1.48	1.41
31	e	101	LMT	O3'-C3'	-2.22	1.37	1.43
24	A	407[B]	PHO	CHA-CBD	-2.21	1.49	1.51
23	D	402[A]	CLA	C4C-C3C	2.21	1.48	1.45
35	H	102	DGD	O2G-C2G	-2.21	1.41	1.46
23	C	512	CLA	C3B-C4B	2.21	1.49	1.42
23	B	608	CLA	C4C-C3C	2.21	1.48	1.45
27	D	412	GOL	C3-C2	2.21	1.60	1.51
23	b	614	CLA	C3B-C2B	2.21	1.48	1.41
35	c	517[A]	DGD	O2G-C2G	-2.21	1.41	1.46
23	C	512	CLA	C1B-NB	-2.20	1.35	1.37
40	V	201	HEC	CMD-C2D	2.20	1.55	1.50
29	a	413[B]	PL9	C2-C3	2.20	1.40	1.34
23	B	606	CLA	C3B-C2B	2.20	1.48	1.41
23	B	612	CLA	C1C-NC	-2.20	1.34	1.37
23	c	504	CLA	C3B-C2B	2.20	1.48	1.41
23	A	404[B]	CLA	C3D-C4D	-2.20	1.39	1.44
35	c	518	DGD	O5D-C1E	2.20	1.43	1.40
23	B	608	CLA	C3D-C4D	-2.19	1.39	1.44
23	B	613	CLA	C3B-C2B	2.19	1.48	1.41
23	c	506	CLA	C3D-C4D	-2.19	1.39	1.44
23	B	604	CLA	C4B-NB	-2.19	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	C3D-C4D	-2.19	1.39	1.44
23	B	604	CLA	C3B-C4B	2.19	1.49	1.42
27	d	412	GOL	O2-C2	-2.19	1.37	1.43
23	c	502	CLA	C1C-C2C	2.18	1.49	1.44
35	C	518[B]	DGD	O5D-C1E	2.18	1.43	1.40
23	C	502	CLA	C4C-C3C	2.18	1.48	1.45
23	c	510	CLA	C3B-C2B	2.18	1.48	1.41
31	M	101	LMT	O2B-C2B	-2.18	1.37	1.43
23	c	509	CLA	C3B-C2B	2.18	1.48	1.41
23	C	505	CLA	C3D-C4D	-2.18	1.39	1.44
31	m	103	LMT	O3'-C3'	-2.18	1.37	1.43
23	a	404[A]	CLA	C3B-C2B	2.18	1.48	1.41
23	C	503	CLA	C3D-C4D	-2.17	1.39	1.44
23	B	607	CLA	C4C-C3C	2.17	1.48	1.45
23	b	604	CLA	C1C-C2C	2.17	1.48	1.44
31	M	103	LMT	O2'-C2'	-2.17	1.37	1.43
25	B	619	BCR	C30-C25	-2.17	1.51	1.53
23	B	613	CLA	C3D-C4D	-2.17	1.39	1.44
23	c	504	CLA	C3D-C4D	-2.16	1.39	1.44
40	V	201	HEC	CMC-C2C	2.16	1.55	1.50
24	a	415[A]	PHO	C1B-NB	-2.16	1.34	1.38
29	d	405[B]	PL9	C2-C3	2.16	1.40	1.34
23	b	614	CLA	C1C-C2C	2.16	1.48	1.44
23	b	608	CLA	C3D-C4D	-2.16	1.39	1.44
23	c	509	CLA	C3D-C4D	-2.16	1.39	1.44
23	b	616	CLA	C3B-C2B	2.16	1.48	1.41
23	b	610	CLA	C1C-C2C	2.16	1.48	1.44
23	c	508	CLA	C3B-C4B	2.15	1.49	1.42
40	V	201	HEC	CMA-C3A	2.15	1.55	1.50
23	a	408	CLA	C3B-C2B	2.15	1.48	1.41
31	M	101	LMT	O3'-C3'	-2.15	1.37	1.43
23	B	604	CLA	MG-NA	2.15	2.11	2.06
23	a	404[B]	CLA	C3B-C2B	2.15	1.48	1.41
23	C	509	CLA	C1A-CHA	2.15	1.51	1.43
23	C	511	CLA	C1D-C2D	2.15	1.49	1.45
23	B	602	CLA	C3B-C4B	2.15	1.49	1.42
23	B	611	CLA	C1D-C2D	2.15	1.49	1.45
23	C	507	CLA	C3B-C2B	2.15	1.48	1.41
23	c	511	CLA	MG-NA	2.15	2.11	2.06
23	c	507	CLA	C4C-C3C	2.14	1.48	1.45
23	B	614	CLA	C3B-C4B	2.14	1.49	1.42
23	b	603	CLA	C4C-C3C	2.14	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	C3D-C4D	-2.14	1.39	1.44
23	c	508	CLA	C3D-C4D	-2.14	1.39	1.44
23	C	503	CLA	C1B-NB	-2.14	1.35	1.37
23	C	513	CLA	C3B-C2B	2.14	1.48	1.41
23	B	614	CLA	C3B-C2B	2.13	1.48	1.41
23	B	612	CLA	C4C-C3C	2.13	1.48	1.45
23	D	402[B]	CLA	C1C-C2C	2.13	1.48	1.44
23	a	406[A]	CLA	C4C-C3C	2.13	1.48	1.45
23	C	507	CLA	C1D-C2D	2.13	1.49	1.45
23	A	406[A]	CLA	C3D-C4D	-2.12	1.39	1.44
24	A	407[A]	PHO	C1B-NB	-2.12	1.34	1.38
23	A	405[B]	CLA	C1C-C2C	2.12	1.48	1.44
25	b	617	BCR	C19-C18	2.12	1.50	1.46
23	A	406[B]	CLA	C3D-C4D	-2.12	1.39	1.44
23	a	404[B]	CLA	C4B-NB	-2.12	1.35	1.37
32	d	413[A]	LHG	O7-C5	-2.12	1.41	1.46
23	c	509	CLA	C1C-NC	-2.12	1.34	1.37
23	A	404[B]	CLA	C4B-NB	-2.12	1.35	1.37
23	d	403	CLA	C4C-C3C	2.12	1.48	1.45
24	a	415[B]	PHO	C1B-NB	-2.12	1.34	1.38
29	A	414[A]	PL9	C2-C1	-2.12	1.39	1.44
23	c	507	CLA	C3D-C4D	-2.11	1.39	1.44
23	b	608	CLA	C1C-C2C	2.11	1.48	1.44
23	a	404[A]	CLA	C3D-C4D	-2.11	1.39	1.44
23	b	602	CLA	C1B-C2B	2.11	1.48	1.43
23	c	511	CLA	C1D-C2D	2.11	1.49	1.45
23	b	607	CLA	C3B-C2B	2.11	1.48	1.41
29	D	405[B]	PL9	C2-C3	2.11	1.39	1.34
23	b	613	CLA	C4C-C3C	2.10	1.48	1.45
23	d	402[A]	CLA	C3B-C2B	2.10	1.48	1.41
23	C	504	CLA	C4C-C3C	2.10	1.48	1.45
23	C	513	CLA	C4B-NB	-2.10	1.35	1.37
40	v	201	HEC	C3B-C2B	-2.10	1.34	1.41
23	b	604	CLA	C3B-C2B	2.10	1.48	1.41
31	B	629	LMT	O2B-C2B	-2.09	1.37	1.43
23	d	402[B]	CLA	C1C-C2C	2.09	1.48	1.44
23	c	505	CLA	C4B-NB	-2.09	1.35	1.37
23	B	603	CLA	C3B-C4B	2.09	1.48	1.42
31	B	627	LMT	O3'-C3'	-2.09	1.37	1.43
23	d	403	CLA	C3D-C4D	-2.09	1.39	1.44
23	C	503	CLA	C3B-C4B	2.09	1.48	1.42
29	A	414[B]	PL9	C2-C3	2.09	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	C3D-C4D	-2.09	1.39	1.44
24	a	415[B]	PHO	C1D-ND	-2.09	1.34	1.38
32	D	406[A]	LHG	O7-C5	-2.08	1.41	1.46
23	B	606	CLA	MG-NA	2.08	2.11	2.06
23	b	606	CLA	C4B-NB	-2.08	1.35	1.37
31	M	103	LMT	O1'-C1'	-2.08	1.36	1.40
23	b	603	CLA	C3D-C4D	-2.08	1.39	1.44
23	c	501	CLA	C1C-NC	-2.08	1.34	1.37
23	b	614	CLA	CHB-C4A	-2.08	1.32	1.37
23	b	605	CLA	C4B-NB	-2.08	1.35	1.37
24	A	407[A]	PHO	C4B-NB	-2.08	1.34	1.38
23	A	405[B]	CLA	C3B-C2B	2.07	1.48	1.41
23	b	611	CLA	C3B-C4B	2.07	1.48	1.42
23	A	406[A]	CLA	C1C-NC	-2.07	1.34	1.37
23	B	608	CLA	C3B-C4B	2.06	1.48	1.42
23	B	601	CLA	C1C-NC	-2.06	1.34	1.37
23	B	601	CLA	C4C-C3C	2.06	1.48	1.45
23	c	513	CLA	C3B-C2B	2.06	1.48	1.41
23	C	507	CLA	C3B-C4B	2.06	1.48	1.42
23	b	613	CLA	C3B-C2B	2.06	1.48	1.41
23	B	612	CLA	C3D-C4D	-2.06	1.39	1.44
23	c	510	CLA	C3D-C4D	-2.06	1.39	1.44
23	B	607	CLA	C3B-C2B	2.06	1.48	1.41
34	b	622	HTG	C1-C2	2.05	1.56	1.53
23	b	607	CLA	CBD-CAD	-2.05	1.47	1.56
23	B	611	CLA	C3D-C4D	-2.05	1.39	1.44
40	V	201	HEC	CMB-C2B	2.05	1.55	1.50
31	B	627	LMT	O5'-C5'	-2.05	1.39	1.44
23	b	601	CLA	C4C-C3C	2.05	1.48	1.45
23	C	502	CLA	C3B-C2B	2.05	1.48	1.41
23	b	610	CLA	C3B-C2B	2.05	1.48	1.41
29	A	414[A]	PL9	C2-C3	2.05	1.39	1.34
23	A	404[A]	CLA	C3D-C4D	-2.04	1.39	1.44
32	b	629[A]	LHG	O7-C5	-2.04	1.41	1.46
23	C	510	CLA	C1C-NC	-2.04	1.34	1.37
27	V	203[A]	GOL	C1-C2	2.04	1.59	1.51
24	A	407[B]	PHO	C3A-C2A	-2.04	1.53	1.54
38	F	102	HEM	C4B-NB	-2.04	1.34	1.38
23	a	405[A]	CLA	C1C-C2C	2.04	1.48	1.44
23	c	511	CLA	C3B-C4B	2.04	1.48	1.42
24	a	407[A]	PHO	CHA-CBD	-2.03	1.49	1.51
31	A	420	LMT	O2'-C2'	-2.03	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	C3B-C2B	2.03	1.48	1.41
23	B	615	CLA	MG-NA	2.03	2.11	2.06
23	c	503	CLA	MG-NA	2.03	2.11	2.06
23	b	608	CLA	C4C-C3C	2.03	1.48	1.45
23	b	605	CLA	C3B-C4B	2.03	1.48	1.42
27	a	418	GOL	C1-C2	2.03	1.59	1.51
23	B	603	CLA	C1C-NC	-2.03	1.34	1.37
24	a	415[A]	PHO	C1D-ND	-2.03	1.35	1.38
32	L	101[A]	LHG	O7-C5	-2.02	1.41	1.46
26	b	620	SQD	O6-C1	2.02	1.43	1.40
23	a	405[B]	CLA	C3D-C4D	-2.02	1.39	1.44
23	b	615	CLA	C1C-C2C	2.02	1.48	1.44
40	v	201	HEC	CMC-C2C	2.02	1.54	1.50
23	C	506	CLA	C4B-NB	-2.02	1.35	1.37
23	c	506	CLA	C3B-C4B	2.02	1.48	1.42
23	B	613	CLA	C1A-CHA	2.02	1.51	1.43
23	C	508	CLA	C1D-C2D	2.02	1.49	1.45
23	b	605	CLA	O2A-C1	-2.01	1.40	1.46
23	B	615	CLA	C3D-C4D	-2.01	1.39	1.44
23	a	405[B]	CLA	C1C-C2C	2.01	1.48	1.44
23	c	512	CLA	C3B-C2B	2.01	1.47	1.41
23	C	508	CLA	C3B-C2B	2.01	1.47	1.41
23	b	604	CLA	C3D-C4D	-2.01	1.39	1.44
23	c	506	CLA	C1C-C2C	2.00	1.48	1.44
26	B	620	SQD	O6-C1	2.00	1.43	1.40
23	C	512	CLA	C1A-CHA	2.00	1.51	1.43
24	a	415[A]	PHO	CHA-CBD	-2.00	1.49	1.51

All (3412) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C3B-C2B-C1B	-13.97	90.70	107.17
23	B	611	CLA	C1D-ND-C4D	-12.13	97.80	106.31
24	A	407[A]	PHO	C2D-C1D-ND	11.49	117.73	109.43
24	a	415[A]	PHO	C2D-C1D-ND	10.99	117.38	109.43
24	a	415[B]	PHO	C2D-C1D-ND	10.94	117.34	109.43
24	A	407[B]	PHO	C2D-C1D-ND	10.88	117.30	109.43
24	a	407[A]	PHO	C2D-C1D-ND	10.81	117.24	109.43
23	a	408	CLA	C1D-ND-C4D	-10.59	98.88	106.31
24	A	416[A]	PHO	C2D-C1D-ND	10.58	117.08	109.43
23	B	615	CLA	C1D-ND-C4D	-10.58	98.89	106.31
24	a	407[B]	PHO	C2D-C1D-ND	10.52	117.03	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C2B-C1B-NB	10.42	121.13	110.33
23	a	404[B]	CLA	C1D-ND-C4D	-10.25	99.12	106.31
23	b	605	CLA	C1D-ND-C4D	-10.23	99.13	106.31
24	A	416[B]	PHO	C2D-C1D-ND	10.22	116.82	109.43
23	B	605	CLA	C1D-ND-C4D	-10.20	99.16	106.31
23	c	511	CLA	C1D-ND-C4D	-10.16	99.18	106.31
23	b	611	CLA	C1D-ND-C4D	-10.15	99.19	106.31
23	B	601	CLA	C1D-ND-C4D	-10.14	99.20	106.31
23	B	606	CLA	C1D-ND-C4D	-10.01	99.29	106.31
23	b	603	CLA	C1D-ND-C4D	-9.97	99.32	106.31
23	a	406[B]	CLA	C1D-ND-C4D	-9.89	99.38	106.31
23	C	511	CLA	C1D-ND-C4D	-9.85	99.40	106.31
40	v	201	HEC	CBB-CAB-C3B	-9.78	107.88	127.43
23	c	505	CLA	C1D-ND-C4D	-9.70	99.50	106.31
23	C	504	CLA	C1D-ND-C4D	-9.66	99.53	106.31
40	V	201	HEC	CBB-CAB-C3B	-9.58	108.29	127.43
23	A	406[B]	CLA	C1D-ND-C4D	-9.55	99.61	106.31
23	B	607	CLA	C1D-ND-C4D	-9.55	99.61	106.31
23	c	513	CLA	C1D-ND-C4D	-9.55	99.61	106.31
23	B	614	CLA	C1D-ND-C4D	-9.55	99.61	106.31
23	c	503	CLA	C1D-ND-C4D	-9.54	99.62	106.31
23	C	505	CLA	C1D-ND-C4D	-9.53	99.63	106.31
23	B	612	CLA	C1D-ND-C4D	-9.49	99.65	106.31
24	a	407[A]	PHO	O2D-CGD-CBD	9.43	121.31	110.95
23	b	614	CLA	C1D-ND-C4D	-9.42	99.70	106.31
23	d	403	CLA	C1D-ND-C4D	-9.41	99.71	106.31
23	C	502	CLA	C1D-ND-C4D	-9.38	99.73	106.31
23	b	608	CLA	C1D-ND-C4D	-9.37	99.74	106.31
23	b	609	CLA	C1D-ND-C4D	-9.37	99.74	106.31
23	b	601	CLA	C1D-ND-C4D	-9.34	99.76	106.31
23	D	402[B]	CLA	C1D-ND-C4D	-9.31	99.78	106.31
23	c	501	CLA	C1D-ND-C4D	-9.30	99.79	106.31
23	b	602	CLA	C1D-ND-C4D	-9.29	99.80	106.31
23	b	610	CLA	C1D-ND-C4D	-9.28	99.80	106.31
23	C	513	CLA	C1D-ND-C4D	-9.27	99.81	106.31
23	a	406[A]	CLA	C1D-ND-C4D	-9.26	99.82	106.31
23	D	403	CLA	C1D-ND-C4D	-9.25	99.82	106.31
23	D	402[A]	CLA	C1D-ND-C4D	-9.24	99.83	106.31
23	C	514	CLA	C1D-ND-C4D	-9.22	99.84	106.31
23	B	603	CLA	C1D-ND-C4D	-9.20	99.86	106.31
23	A	408	CLA	C1D-ND-C4D	-9.18	99.87	106.31
23	B	602	CLA	C1D-ND-C4D	-9.18	99.87	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402[B]	CLA	C1D-ND-C4D	-9.18	99.87	106.31
23	d	402[A]	CLA	C1D-ND-C4D	-9.17	99.88	106.31
23	C	506	CLA	C1D-ND-C4D	-9.17	99.88	106.31
23	A	406[A]	CLA	C1D-ND-C4D	-9.16	99.89	106.31
23	A	405[B]	CLA	C1D-ND-C4D	-9.15	99.89	106.31
23	c	506	CLA	C1D-ND-C4D	-9.15	99.90	106.31
23	b	615	CLA	C1D-ND-C4D	-9.13	99.90	106.31
23	a	405[A]	CLA	C1D-ND-C4D	-9.12	99.91	106.31
24	a	415[A]	PHO	O2D-CGD-CBD	9.07	120.91	110.95
23	A	405[A]	CLA	C1D-ND-C4D	-8.99	100.01	106.31
23	B	613	CLA	C1D-ND-C4D	-8.94	100.04	106.31
23	B	609	CLA	C1D-ND-C4D	-8.92	100.05	106.31
23	a	404[A]	CLA	C1D-ND-C4D	-8.91	100.06	106.31
23	c	512	CLA	C1D-ND-C4D	-8.89	100.07	106.31
23	C	510	CLA	C1D-ND-C4D	-8.87	100.08	106.31
23	C	507	CLA	C1D-ND-C4D	-8.83	100.12	106.31
23	c	502	CLA	C1D-ND-C4D	-8.83	100.12	106.31
23	A	404[B]	CLA	C1D-ND-C4D	-8.82	100.12	106.31
23	c	510	CLA	C1D-ND-C4D	-8.81	100.13	106.31
23	B	608	CLA	C1D-ND-C4D	-8.81	100.13	106.31
23	c	504	CLA	C1D-ND-C4D	-8.78	100.15	106.31
23	a	405[B]	CLA	C1D-ND-C4D	-8.77	100.16	106.31
24	A	407[A]	PHO	C3B-C4B-NB	8.75	113.17	107.46
23	b	606	CLA	C1D-ND-C4D	-8.75	100.18	106.31
23	C	509	CLA	C1D-ND-C4D	-8.72	100.19	106.31
23	b	612	CLA	C1D-ND-C4D	-8.68	100.22	106.31
23	c	508	CLA	C1D-ND-C4D	-8.66	100.23	106.31
23	b	613	CLA	C1D-ND-C4D	-8.66	100.24	106.31
24	A	416[A]	PHO	O2D-CGD-CBD	8.64	120.44	110.95
23	B	616	CLA	C1D-ND-C4D	-8.63	100.26	106.31
23	b	616	CLA	C1D-ND-C4D	-8.61	100.27	106.31
23	b	602	CLA	C4A-NA-C1A	-8.60	102.75	106.68
23	c	509	CLA	C1D-ND-C4D	-8.60	100.28	106.31
24	a	415[B]	PHO	O2D-CGD-CBD	8.58	120.37	110.95
23	A	404[A]	CLA	C1D-ND-C4D	-8.57	100.30	106.31
24	a	407[B]	PHO	O2D-CGD-CBD	8.55	120.34	110.95
23	C	508	CLA	C1D-ND-C4D	-8.48	100.36	106.31
23	B	610	CLA	C1D-ND-C4D	-8.39	100.42	106.31
23	c	507	CLA	C1D-ND-C4D	-8.37	100.44	106.31
24	A	407[B]	PHO	C3B-C4B-NB	8.37	112.92	107.46
24	A	407[B]	PHO	O2D-CGD-CBD	8.35	120.12	110.95
24	A	416[B]	PHO	O2D-CGD-CBD	8.18	119.93	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	C1D-ND-C4D	-8.16	100.59	106.31
23	C	503	CLA	C1D-ND-C4D	-8.15	100.59	106.31
24	a	407[A]	PHO	C3B-C4B-NB	8.10	112.75	107.46
23	B	604	CLA	C1D-ND-C4D	-8.02	100.68	106.31
23	B	606	CLA	CMD-C2D-C1D	7.94	138.72	124.73
24	a	415[A]	PHO	C3B-C4B-NB	7.89	112.61	107.46
23	B	605	CLA	CHD-C4C-C3C	-7.88	113.29	124.77
23	B	609	CLA	C4A-NA-C1A	-7.75	103.14	106.68
23	B	611	CLA	CHD-C4C-C3C	-7.64	113.63	124.77
23	B	611	CLA	CMB-C2B-C1B	7.64	137.06	125.42
24	A	416[A]	PHO	C3B-C4B-NB	7.61	112.43	107.46
24	a	407[B]	PHO	C3B-C4B-NB	7.61	112.42	107.46
26	F	103	SQD	O6-C1-C2	7.59	119.81	108.27
23	C	504	CLA	C4A-NA-C1A	-7.58	103.22	106.68
23	C	511	CLA	CMD-C2D-C1D	7.56	138.04	124.73
23	C	512	CLA	C1D-ND-C4D	-7.50	101.05	106.31
24	a	415[B]	PHO	C3B-C4B-NB	7.47	112.33	107.46
23	B	611	CLA	C2D-C1D-ND	7.40	117.45	110.13
23	b	604	CLA	C1D-ND-C4D	-7.39	101.13	106.31
23	c	507	CLA	O2D-CGD-CBD	7.36	124.10	111.23
23	D	402[B]	CLA	C4A-NA-C1A	-7.30	103.35	106.68
24	A	416[A]	PHO	C2B-C1B-NB	7.26	114.68	109.43
23	c	503	CLA	C4A-NA-C1A	-7.26	103.37	106.68
24	A	407[A]	PHO	O2D-CGD-CBD	7.23	118.89	110.95
23	B	606	CLA	C4A-NA-C1A	-7.17	103.41	106.68
23	b	606	CLA	C4A-NA-C1A	-7.15	103.42	106.68
23	b	616	CLA	C4A-NA-C1A	-7.13	103.42	106.68
23	B	605	CLA	C2D-C1D-ND	7.08	117.13	110.13
23	B	616	CLA	O2D-CGD-CBD	7.07	123.60	111.23
23	D	402[A]	CLA	C4A-NA-C1A	-7.05	103.46	106.68
23	b	611	CLA	C2D-C1D-ND	7.04	117.09	110.13
23	b	601	CLA	O2D-CGD-CBD	7.03	123.53	111.23
23	C	513	CLA	CHD-C4C-C3C	-7.03	114.53	124.77
23	D	403	CLA	C4A-NA-C1A	-7.01	103.48	106.68
23	a	408	CLA	C2D-C1D-ND	7.01	117.06	110.13
23	C	508	CLA	O2D-CGD-CBD	6.96	123.40	111.23
23	b	616	CLA	O2D-CGD-CBD	6.96	123.40	111.23
24	A	416[B]	PHO	C3B-C4B-NB	6.95	111.99	107.46
23	C	505	CLA	C2D-C1D-ND	6.93	116.99	110.13
23	B	611	CLA	CHB-C1B-NB	-6.93	113.66	124.05
23	c	503	CLA	CMD-C2D-C1D	6.88	136.85	124.73
23	B	611	CLA	CMD-C2D-C1D	6.87	136.82	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	605	CLA	CHD-C4C-C3C	-6.87	114.76	124.77
23	B	614	CLA	CMD-C2D-C1D	6.86	136.81	124.73
23	B	615	CLA	C4A-NA-C1A	-6.85	103.55	106.68
23	b	614	CLA	C2D-C1D-ND	6.83	116.88	110.13
23	B	605	CLA	CMD-C2D-C1D	6.82	136.74	124.73
23	b	606	CLA	CHD-C4C-C3C	-6.81	114.84	124.77
23	b	615	CLA	C4A-NA-C1A	-6.81	103.57	106.68
23	c	507	CLA	CMD-C2D-C1D	6.79	136.69	124.73
23	b	605	CLA	CMD-C2D-C1D	6.79	136.68	124.73
23	B	606	CLA	C2D-C1D-ND	6.76	116.82	110.13
23	C	502	CLA	O2D-CGD-CBD	6.75	123.04	111.23
24	a	415[A]	PHO	C2B-C1B-NB	6.74	114.30	109.43
23	c	513	CLA	CMD-C2D-C1D	6.74	136.60	124.73
23	B	615	CLA	C2D-C1D-ND	6.73	116.79	110.13
23	c	501	CLA	CMD-C2D-C1D	6.72	136.56	124.73
23	c	511	CLA	CHD-C4C-C3C	-6.72	114.98	124.77
23	B	603	CLA	O2D-CGD-CBD	6.71	122.97	111.23
23	A	404[A]	CLA	CMD-C2D-C1D	6.70	136.53	124.73
23	b	616	CLA	CHD-C4C-C3C	-6.69	115.02	124.77
23	b	605	CLA	C2D-C1D-ND	6.69	116.75	110.13
23	B	616	CLA	CHD-C4C-C3C	-6.68	115.03	124.77
23	B	614	CLA	C2D-C1D-ND	6.66	116.72	110.13
23	B	606	CLA	CHD-C4C-C3C	-6.66	115.06	124.77
23	b	613	CLA	C2D-C1D-ND	6.66	116.71	110.13
26	A	410[A]	SQD	O6-C1-C2	6.64	118.36	108.27
24	a	407[B]	PHO	C2B-C1B-NB	6.63	114.22	109.43
23	B	610	CLA	O2D-CGD-CBD	6.62	122.80	111.23
23	a	405[A]	CLA	CHD-C4C-C3C	-6.62	115.12	124.77
23	C	508	CLA	CMD-C2D-C1D	6.61	136.38	124.73
23	b	609	CLA	CHD-C4C-C3C	-6.61	115.13	124.77
23	b	613	CLA	CHD-C4C-C3C	-6.61	115.13	124.77
23	B	606	CLA	O2D-CGD-CBD	6.61	122.78	111.23
24	a	415[B]	PHO	C2B-C1B-NB	6.60	114.20	109.43
23	A	404[B]	CLA	CMD-C2D-C1D	6.60	136.35	124.73
23	d	403	CLA	C2D-C1D-ND	6.57	116.62	110.13
23	b	611	CLA	CHD-C4C-C3C	-6.56	115.20	124.77
23	c	511	CLA	C2D-C1D-ND	6.56	116.62	110.13
23	C	511	CLA	O2D-CGD-CBD	6.56	122.69	111.23
23	b	610	CLA	CHD-C4C-C3C	-6.53	115.25	124.77
23	c	510	CLA	CHD-C4C-C3C	-6.53	115.25	124.77
23	C	507	CLA	CMD-C2D-C1D	6.53	136.24	124.73
23	A	408	CLA	C2D-C1D-ND	6.53	116.59	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405[A]	CLA	C2D-C1D-ND	6.50	116.56	110.13
23	b	603	CLA	C2D-C1D-ND	6.49	116.55	110.13
23	B	607	CLA	C2D-C1D-ND	6.48	116.54	110.13
23	B	601	CLA	CHD-C4C-C3C	-6.48	115.33	124.77
23	c	509	CLA	C1-C2-C3	-6.46	115.61	126.20
23	D	402[B]	CLA	CMD-C2D-C1D	6.45	136.09	124.73
23	B	608	CLA	C2D-C1D-ND	6.45	116.51	110.13
23	B	601	CLA	C2D-C1D-ND	6.45	116.50	110.13
34	b	623	HTG	C1'-S1-C1	6.44	114.35	100.45
23	b	601	CLA	C4A-NA-C1A	-6.43	103.75	106.68
23	b	606	CLA	CMD-C2D-C1D	6.43	136.05	124.73
23	C	506	CLA	CMD-C2D-C1D	6.43	136.05	124.73
23	a	406[A]	CLA	C2D-C1D-ND	6.42	116.48	110.13
23	a	404[B]	CLA	CMD-C2D-C1D	6.42	136.03	124.73
23	a	406[B]	CLA	C2D-C1D-ND	6.41	116.47	110.13
23	a	406[A]	CLA	CHD-C4C-C3C	-6.41	115.43	124.77
23	b	611	CLA	CMD-C2D-C1D	6.39	135.97	124.73
24	A	407[B]	PHO	C2B-C1B-NB	6.38	114.04	109.43
23	B	603	CLA	CHD-C4C-C3C	-6.37	115.48	124.77
25	D	404	BCR	C7-C8-C9	-6.36	116.83	126.23
23	a	405[B]	CLA	CHD-C4C-C3C	-6.34	115.52	124.77
24	a	407[A]	PHO	C2B-C1B-NB	6.33	114.01	109.43
23	B	603	CLA	C2D-C1D-ND	6.33	116.39	110.13
26	F	103	SQD	O47-C7-C8	6.32	125.14	111.48
23	a	404[B]	CLA	C2D-C1D-ND	6.31	116.37	110.13
23	B	609	CLA	CHD-C4C-C3C	-6.31	115.57	124.77
23	c	508	CLA	C2D-C1D-ND	6.31	116.37	110.13
23	b	602	CLA	O2D-CGD-CBD	6.31	122.26	111.23
23	D	402[A]	CLA	C2D-C1D-ND	6.30	116.37	110.13
23	B	612	CLA	C2D-C1D-ND	6.30	116.36	110.13
23	B	614	CLA	CHD-C4C-C3C	-6.29	115.60	124.77
23	A	404[A]	CLA	C4A-NA-C1A	-6.29	103.81	106.68
23	c	510	CLA	CMD-C2D-C1D	6.29	135.80	124.73
24	A	407[A]	PHO	C4D-ND-C1D	-6.28	101.35	108.87
23	c	505	CLA	CHD-C4C-C3C	-6.28	115.62	124.77
23	c	506	CLA	CMD-C2D-C1D	6.28	135.78	124.73
24	A	416[B]	PHO	C2B-C1B-NB	6.27	113.97	109.43
23	B	612	CLA	CHD-C4C-C3C	-6.27	115.64	124.77
23	B	601	CLA	CMD-C2D-C1D	6.24	135.72	124.73
23	B	610	CLA	C2D-C1D-ND	6.23	116.29	110.13
23	B	601	CLA	O2D-CGD-CBD	6.22	122.11	111.23
23	c	506	CLA	C2D-C1D-ND	6.20	116.26	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	O2D-CGD-CBD	6.19	122.06	111.23
23	b	609	CLA	CMD-C2D-C1D	6.17	135.60	124.73
23	c	511	CLA	CMD-C2D-C1D	6.16	135.58	124.73
23	A	405[B]	CLA	C2D-C1D-ND	6.16	116.22	110.13
23	C	510	CLA	CHD-C4C-C3C	-6.16	115.80	124.77
23	B	616	CLA	C2D-C1D-ND	6.15	116.22	110.13
23	b	603	CLA	CHD-C4C-C3C	-6.15	115.80	124.77
23	c	512	CLA	CHD-C4C-C3C	-6.15	115.81	124.77
23	C	514	CLA	C2D-C1D-ND	6.15	116.21	110.13
23	C	504	CLA	C2D-C1D-ND	6.14	116.20	110.13
23	c	505	CLA	C2D-C1D-ND	6.14	116.20	110.13
23	B	602	CLA	O2D-CGD-CBD	6.14	121.96	111.23
23	A	406[B]	CLA	C2D-C1D-ND	6.13	116.19	110.13
23	b	615	CLA	CHD-C4C-C3C	-6.12	115.85	124.77
23	A	405[A]	CLA	C2D-C1D-ND	6.12	116.18	110.13
23	B	613	CLA	C2D-C1D-ND	6.12	116.18	110.13
23	C	510	CLA	C2D-C1D-ND	6.12	116.18	110.13
23	a	408	CLA	CHD-C4C-C3C	-6.12	115.86	124.77
23	b	610	CLA	O2D-CGD-CBD	6.11	121.92	111.23
23	b	605	CLA	O2D-CGD-CBD	6.11	121.91	111.23
23	A	408	CLA	CMD-C2D-C1D	6.10	135.48	124.73
23	b	601	CLA	CHD-C4C-C3C	-6.10	115.88	124.77
23	c	502	CLA	C2D-C1D-ND	6.10	116.16	110.13
23	D	402[A]	CLA	CMD-C2D-C1D	6.10	135.47	124.73
23	a	406[B]	CLA	CMD-C2D-C1D	6.09	135.46	124.73
23	C	513	CLA	C2D-C1D-ND	6.09	116.16	110.13
23	b	615	CLA	C2D-C1D-ND	6.09	116.16	110.13
23	C	509	CLA	C2D-C1D-ND	6.09	116.15	110.13
23	C	513	CLA	C4A-NA-C1A	-6.09	103.90	106.68
23	C	510	CLA	CMD-C2D-C1D	6.09	135.44	124.73
25	Y	101	BCR	C33-C5-C6	-6.08	117.85	124.48
23	B	609	CLA	CMD-C2D-C1D	6.08	135.43	124.73
23	c	504	CLA	C2D-C1D-ND	6.08	116.14	110.13
23	C	504	CLA	CMD-C2D-C1D	6.07	135.42	124.73
23	B	615	CLA	CHD-C4C-C3C	-6.07	115.92	124.77
23	a	404[A]	CLA	CMD-C2D-C1D	6.07	135.41	124.73
23	c	512	CLA	C4A-NA-C1A	-6.07	103.91	106.68
23	C	514	CLA	CHD-C4C-C3C	-6.07	115.93	124.77
23	c	510	CLA	C4A-NA-C1A	-6.06	103.91	106.68
23	C	509	CLA	CHD-C4C-C3C	-6.06	115.93	124.77
23	C	506	CLA	CHD-C4C-C3C	-6.05	115.95	124.77
23	A	406[A]	CLA	C2D-C1D-ND	6.05	116.11	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	403	CLA	CHD-C4C-C3C	-6.05	115.95	124.77
26	A	410[B]	SQD	O6-C1-C2	6.05	117.46	108.27
23	c	508	CLA	CHD-C4C-C3C	-6.04	115.97	124.77
23	B	610	CLA	CMD-C2D-C1D	6.04	135.36	124.73
23	b	614	CLA	CHD-C4C-C3C	-6.04	115.97	124.77
23	d	402[B]	CLA	CMD-C2D-C1D	6.03	135.35	124.73
23	a	404[A]	CLA	C4A-NA-C1A	-6.03	103.93	106.68
23	c	504	CLA	CHD-C4C-C3C	-6.03	115.99	124.77
23	b	610	CLA	C2D-C1D-ND	6.02	116.09	110.13
23	a	406[A]	CLA	C4A-NA-C1A	-6.02	103.93	106.68
23	A	408	CLA	CHD-C4C-C3C	-6.02	116.00	124.77
23	C	502	CLA	C2D-C1D-ND	6.01	116.08	110.13
23	b	608	CLA	C2D-C1D-ND	6.01	116.07	110.13
23	D	403	CLA	C2D-C1D-ND	6.00	116.07	110.13
24	A	407[A]	PHO	C2B-C1B-NB	6.00	113.77	109.43
23	B	613	CLA	CHD-C4C-C3C	-5.99	116.03	124.77
23	b	602	CLA	CHD-C4C-C3C	-5.99	116.03	124.77
23	C	502	CLA	C4A-NA-C1A	-5.99	103.95	106.68
23	b	616	CLA	CMD-C2D-C1D	5.98	135.26	124.73
23	C	512	CLA	CHD-C4C-C3C	-5.96	116.08	124.77
23	c	512	CLA	O2D-CGD-CBD	5.96	121.65	111.23
23	A	405[B]	CLA	CMD-C2D-C1D	5.96	135.22	124.73
23	A	406[B]	CLA	CHD-C4C-C3C	-5.95	116.10	124.77
23	b	601	CLA	CMD-C2D-C1D	5.94	135.19	124.73
23	a	404[B]	CLA	CHD-C4C-C3C	-5.93	116.12	124.77
23	a	405[A]	CLA	CMD-C2D-C1D	5.93	135.16	124.73
23	b	613	CLA	CMD-C2D-C1D	5.92	135.15	124.73
23	b	610	CLA	CMD-C2D-C1D	5.92	135.15	124.73
23	B	602	CLA	CHD-C4C-C3C	-5.92	116.15	124.77
23	C	504	CLA	CHD-C4C-C3C	-5.91	116.15	124.77
23	a	406[B]	CLA	CHD-C4C-C3C	-5.91	116.16	124.77
23	d	402[B]	CLA	C4A-NA-C1A	-5.90	103.98	106.68
23	D	402[B]	CLA	C2D-C1D-ND	5.90	115.97	110.13
23	c	501	CLA	CHD-C4C-C3C	-5.90	116.18	124.77
23	B	605	CLA	O2D-CGD-CBD	5.89	121.52	111.23
23	A	406[A]	CLA	CMD-C2D-C1D	5.89	135.10	124.73
23	A	405[B]	CLA	CHD-C4C-C3C	-5.89	116.19	124.77
23	c	505	CLA	O2D-CGD-CBD	5.88	121.51	111.23
23	b	612	CLA	CHD-C4C-C3C	-5.88	116.20	124.77
23	C	509	CLA	C2C-C1C-NC	5.88	116.15	109.98
23	a	405[B]	CLA	C2D-C1D-ND	5.88	115.94	110.13
23	C	503	CLA	CHD-C4C-C3C	-5.87	116.21	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	410[A]	SQD	O6-C1-C2	5.87	117.19	108.27
23	A	406[B]	CLA	CMD-C2D-C1D	5.87	135.07	124.73
23	C	507	CLA	C2C-C1C-NC	5.87	116.15	109.98
23	c	510	CLA	C2D-C1D-ND	5.87	115.93	110.13
23	c	503	CLA	CHD-C4C-C3C	-5.87	116.22	124.77
23	a	408	CLA	O2D-CGD-CBD	5.87	121.48	111.23
23	A	404[B]	CLA	CHD-C4C-C3C	-5.86	116.23	124.77
23	c	503	CLA	C2D-C1D-ND	5.85	115.92	110.13
23	B	602	CLA	C2D-C1D-ND	5.85	115.91	110.13
23	A	406[A]	CLA	CHD-C4C-C3C	-5.85	116.25	124.77
26	B	620	SQD	O6-C1-C2	5.84	117.14	108.27
24	a	415[B]	PHO	C4D-ND-C1D	-5.84	101.88	108.87
23	c	502	CLA	CHD-C4C-C3C	-5.83	116.27	124.77
23	b	609	CLA	C2D-C1D-ND	5.83	115.90	110.13
23	d	403	CLA	CHD-C4C-C3C	-5.83	116.28	124.77
24	A	407[B]	PHO	C4D-ND-C1D	-5.82	101.90	108.87
23	B	614	CLA	O2D-CGD-CBD	5.82	121.40	111.23
23	b	601	CLA	C2D-C1D-ND	5.80	115.87	110.13
23	c	509	CLA	CMD-C2D-C1D	5.80	134.95	124.73
23	B	604	CLA	CMD-C2D-C1D	5.80	134.94	124.73
23	d	402[A]	CLA	C2D-C1D-ND	5.80	115.87	110.13
23	c	501	CLA	C2D-C1D-ND	5.79	115.85	110.13
24	a	415[A]	PHO	C1-C2-C3	-5.78	116.72	126.20
23	C	508	CLA	C2D-C1D-ND	5.78	115.85	110.13
23	B	610	CLA	CHD-C4C-C3C	-5.78	116.34	124.77
23	d	402[A]	CLA	C2C-C1C-NC	5.78	116.05	109.98
23	c	513	CLA	C2D-C1D-ND	5.77	115.84	110.13
23	B	614	CLA	C3D-C2D-C1D	-5.77	97.95	105.83
23	A	405[A]	CLA	CHD-C4C-C3C	-5.77	116.36	124.77
23	A	406[A]	CLA	C4A-NA-C1A	-5.77	104.05	106.68
23	b	607	CLA	C2D-C1D-ND	5.77	115.83	110.13
23	c	512	CLA	C2D-C1D-ND	5.76	115.83	110.13
23	b	611	CLA	O2D-CGD-CBD	5.76	121.31	111.23
23	c	507	CLA	C4A-NA-C1A	-5.75	104.05	106.68
23	b	615	CLA	CMD-C2D-C1D	5.75	134.85	124.73
24	a	415[A]	PHO	C4D-ND-C1D	-5.74	101.99	108.87
23	b	616	CLA	C2D-C1D-ND	5.74	115.81	110.13
23	C	505	CLA	CMD-C2D-C1D	5.73	134.82	124.73
23	B	603	CLA	CMD-C2D-C1D	5.73	134.82	124.73
23	b	607	CLA	C2C-C1C-NC	5.72	115.99	109.98
23	B	616	CLA	C4A-NA-C1A	-5.72	104.07	106.68
23	B	604	CLA	CHD-C4C-C3C	-5.72	116.44	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	O2D-CGD-CBD	5.71	121.21	111.23
23	C	502	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
23	B	604	CLA	C2C-C1C-NC	5.71	115.98	109.98
23	B	608	CLA	O2D-CGD-CBD	5.70	121.20	111.23
23	b	604	CLA	C1-C2-C3	-5.70	116.86	126.20
23	C	505	CLA	C2C-C1C-NC	5.69	115.95	109.98
26	A	410[A]	SQD	C1-O5-C5	-5.69	102.61	113.72
24	A	407[A]	PHO	C3D-C4D-ND	5.69	115.00	107.71
23	C	502	CLA	CMD-C2D-C1D	5.68	134.74	124.73
23	b	603	CLA	C4A-NA-C1A	-5.67	104.09	106.68
23	B	607	CLA	CHD-C4C-C3C	-5.67	116.51	124.77
23	C	514	CLA	CMD-C2D-C1D	5.67	134.71	124.73
23	A	404[A]	CLA	C2D-C1D-ND	5.67	115.73	110.13
23	c	509	CLA	CHD-C4C-C3C	-5.66	116.52	124.77
23	C	511	CLA	CHD-C4C-C3C	-5.66	116.52	124.77
23	b	608	CLA	O2D-CGD-CBD	5.66	121.12	111.23
23	b	607	CLA	CMD-C2D-C1D	5.65	134.68	124.73
23	B	605	CLA	C3D-C2D-C1D	-5.65	98.12	105.83
23	B	613	CLA	C1-C2-C3	-5.63	116.98	126.20
23	b	614	CLA	O2D-CGD-CBD	5.62	121.06	111.23
23	d	402[B]	CLA	C2D-C1D-ND	5.61	115.68	110.13
23	C	508	CLA	CHD-C4C-C3C	-5.61	116.59	124.77
23	C	506	CLA	O2D-CGD-CBD	5.61	121.04	111.23
23	c	508	CLA	C4A-NA-C1A	-5.61	104.12	106.68
23	C	511	CLA	C2D-C1D-ND	5.61	115.67	110.13
23	d	402[B]	CLA	C2C-C1C-NC	5.58	115.85	109.98
23	c	506	CLA	CHD-C4C-C3C	-5.58	116.64	124.77
26	B	620	SQD	O47-C7-C8	5.58	123.55	111.48
23	B	609	CLA	C2D-C1D-ND	5.57	115.64	110.13
23	B	611	CLA	C3D-C2D-C1D	-5.57	98.23	105.83
23	a	405[B]	CLA	CMD-C2D-C1D	5.57	134.54	124.73
23	D	403	CLA	CMD-C2D-C1D	5.57	134.53	124.73
24	a	415[B]	PHO	C3D-C4D-ND	5.56	114.84	107.71
23	b	608	CLA	CHD-C4C-C3C	-5.56	116.67	124.77
23	D	402[A]	CLA	CHD-C4C-C3C	-5.54	116.70	124.77
23	b	604	CLA	C2C-C1C-NC	5.53	115.80	109.98
23	C	505	CLA	O2D-CGD-CBD	5.53	120.90	111.23
34	b	622	HTG	C1-O5-C5	5.53	122.48	112.56
23	a	404[A]	CLA	C2C-C1C-NC	5.53	115.79	109.98
24	a	415[A]	PHO	C3D-C4D-ND	5.52	114.79	107.71
23	b	602	CLA	C2D-C1D-ND	5.52	115.59	110.13
23	b	606	CLA	C2D-C1D-ND	5.52	115.59	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	C4A-NA-C1A	-5.51	104.16	106.68
23	b	603	CLA	O2D-CGD-CBD	5.51	120.87	111.23
23	c	507	CLA	CHD-C4C-C3C	-5.51	116.74	124.77
23	B	612	CLA	O2D-CGD-CBD	5.51	120.86	111.23
23	a	404[A]	CLA	CHD-C4C-C3C	-5.51	116.74	124.77
23	c	502	CLA	C2C-C1C-NC	5.50	115.76	109.98
23	b	603	CLA	CMD-C2D-C1D	5.50	134.41	124.73
23	d	402[A]	CLA	CHD-C4C-C3C	-5.49	116.76	124.77
24	A	416[A]	PHO	C4D-ND-C1D	-5.49	102.29	108.87
23	D	402[B]	CLA	CHD-C4C-C3C	-5.48	116.78	124.77
23	c	508	CLA	C2C-C1C-NC	5.48	115.74	109.98
23	a	406[A]	CLA	CMD-C2D-C1D	5.48	134.38	124.73
23	c	513	CLA	CHD-C4C-C3C	-5.48	116.78	124.77
23	b	612	CLA	CMD-C2D-C1D	5.47	134.36	124.73
23	d	403	CLA	CMD-C2D-C1D	5.47	134.36	124.73
23	C	508	CLA	C4A-NA-C1A	-5.46	104.19	106.68
23	a	406[B]	CLA	C4A-NA-C1A	-5.46	104.19	106.68
34	c	521	HTG	C1'-S1-C1	5.46	112.24	100.45
23	B	608	CLA	CHD-C4C-C3C	-5.46	116.82	124.77
23	B	605	CLA	C4A-NA-C1A	-5.45	104.19	106.68
23	C	503	CLA	CMD-C2D-C1D	5.45	134.32	124.73
23	B	604	CLA	O2D-CGD-CBD	5.44	120.73	111.23
23	C	505	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
23	C	506	CLA	C2D-C1D-ND	5.43	115.50	110.13
23	d	402[A]	CLA	CMD-C2D-C1D	5.43	134.30	124.73
23	a	404[A]	CLA	C2D-C1D-ND	5.43	115.50	110.13
23	C	507	CLA	C2D-C1D-ND	5.42	115.50	110.13
23	A	404[B]	CLA	C2D-C1D-ND	5.42	115.49	110.13
23	c	505	CLA	C4A-NA-C1A	-5.42	104.20	106.68
23	a	404[B]	CLA	C4A-NA-C1A	-5.42	104.21	106.68
23	b	605	CLA	C3D-C2D-C1D	-5.41	98.44	105.83
23	B	614	CLA	C2C-C1C-NC	5.41	115.67	109.98
25	t	102	BCR	C33-C5-C6	-5.41	118.58	124.48
23	B	607	CLA	O2D-CGD-CBD	5.40	120.67	111.23
23	b	608	CLA	C4A-NA-C1A	-5.40	104.22	106.68
23	B	604	CLA	C1-C2-C3	-5.39	117.36	126.20
23	b	611	CLA	C3D-C2D-C1D	-5.39	98.47	105.83
23	B	606	CLA	C3D-C2D-C1D	-5.39	98.47	105.83
23	c	506	CLA	C2C-C1C-NC	5.39	115.64	109.98
23	C	503	CLA	C2D-C1D-ND	5.39	115.46	110.13
23	c	509	CLA	C2D-C1D-ND	5.39	115.46	110.13
23	C	511	CLA	C2C-C1C-NC	5.39	115.64	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405[B]	CLA	C2C-C1C-NC	5.38	115.63	109.98
23	b	611	CLA	C4A-NA-C1A	-5.37	104.23	106.68
23	b	612	CLA	C2D-C1D-ND	5.36	115.44	110.13
23	d	402[B]	CLA	CHD-C4C-C3C	-5.36	116.95	124.77
23	c	508	CLA	CMD-C2D-C1D	5.36	134.17	124.73
24	A	407[B]	PHO	C3D-C4D-ND	5.36	114.58	107.71
23	B	611	CLA	O2D-CGD-CBD	5.36	120.60	111.23
23	c	505	CLA	CMD-C2D-C1D	5.36	134.17	124.73
23	c	507	CLA	C2D-C1D-ND	5.36	115.43	110.13
23	B	602	CLA	C4A-NA-C1A	-5.35	104.24	106.68
23	b	602	CLA	CMD-C2D-C1D	5.34	134.14	124.73
26	b	620	SQD	O6-C1-C2	5.34	116.39	108.27
23	B	615	CLA	CMD-C2D-C1D	5.33	134.12	124.73
24	A	416[B]	PHO	C4D-ND-C1D	-5.33	102.48	108.87
23	B	607	CLA	C4A-NA-C1A	-5.33	104.25	106.68
24	a	407[B]	PHO	C4D-ND-C1D	-5.33	102.49	108.87
33	C	501	LMG	C7-O1-C1	-5.32	102.38	113.80
23	C	508	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
23	C	513	CLA	O2D-CGD-CBD	5.32	120.53	111.23
24	a	415[B]	PHO	C1-C2-C3	-5.32	117.48	126.20
23	b	613	CLA	C3D-C2D-C1D	-5.31	98.59	105.83
26	A	410[A]	SQD	C1-C2-C3	-5.30	98.86	110.01
23	C	503	CLA	C3B-C2B-C1B	-5.30	100.93	107.17
34	D	410	HTG	C1'-S1-C1	5.29	111.87	100.45
23	b	602	CLA	C2B-C1B-NB	5.28	115.81	110.33
24	A	416[A]	PHO	C3D-C4D-ND	5.28	114.48	107.71
23	c	502	CLA	O2D-CGD-CBD	5.28	120.46	111.23
23	c	508	CLA	C3D-C2D-C1D	-5.28	98.63	105.83
23	b	610	CLA	C1-C2-C3	-5.26	117.58	126.20
23	c	512	CLA	CMD-C2D-C1D	5.25	133.98	124.73
23	c	506	CLA	C4A-NA-C1A	-5.25	104.28	106.68
23	b	614	CLA	C3B-C2B-C1B	-5.25	100.98	107.17
23	C	512	CLA	C2D-C1D-ND	5.25	115.32	110.13
23	A	405[A]	CLA	C4A-NA-C1A	-5.24	104.29	106.68
23	c	501	CLA	C4A-NA-C1A	-5.24	104.29	106.68
23	D	402[A]	CLA	C2C-C1C-NC	5.23	115.48	109.98
23	c	504	CLA	CMD-C2D-C1D	5.23	133.94	124.73
23	B	606	CLA	CHD-C1D-ND	-5.23	117.44	124.80
23	A	408	CLA	C2C-C1C-NC	5.23	115.47	109.98
23	c	502	CLA	C3B-C2B-C1B	-5.23	101.01	107.17
23	C	513	CLA	CMD-C2D-C1D	5.22	133.92	124.73
25	A	409	BCR	C24-C23-C22	-5.22	118.51	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	C2C-C1C-NC	5.21	115.46	109.98
23	C	512	CLA	CMD-C2D-C1D	5.21	133.90	124.73
23	c	513	CLA	C4A-NA-C1A	-5.20	104.31	106.68
23	B	602	CLA	CMD-C2D-C1D	5.20	133.89	124.73
23	A	404[A]	CLA	C2C-C1C-NC	5.20	115.44	109.98
23	A	404[B]	CLA	C4A-NA-C1A	-5.19	104.31	106.68
23	C	507	CLA	CHD-C4C-C3C	-5.19	117.21	124.77
23	A	406[B]	CLA	C4A-NA-C1A	-5.18	104.31	106.68
26	b	620	SQD	O47-C7-C8	5.18	122.69	111.48
23	C	512	CLA	C3B-C2B-C1B	-5.17	101.07	107.17
23	D	403	CLA	O2D-CGD-CBD	5.17	120.27	111.23
23	b	604	CLA	CHD-C4C-C3C	-5.17	117.23	124.77
24	a	407[A]	PHO	C4D-ND-C1D	-5.17	102.68	108.87
23	C	513	CLA	C2B-C1B-NB	5.16	115.68	110.33
24	A	416[B]	PHO	C3D-C4D-ND	5.16	114.32	107.71
23	B	613	CLA	CMD-C2D-C1D	5.15	133.81	124.73
23	c	504	CLA	O2D-CGD-CBD	5.15	120.24	111.23
23	c	507	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
23	A	408	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
26	b	620	SQD	C1-O5-C5	-5.13	103.69	113.72
23	A	404[A]	CLA	CHD-C4C-C3C	-5.13	117.30	124.77
23	D	402[B]	CLA	C2C-C1C-NC	5.13	115.37	109.98
23	B	616	CLA	C3C-C4C-NC	5.12	116.99	110.43
23	b	606	CLA	C2B-C1B-NB	5.12	115.63	110.33
23	d	403	CLA	O2D-CGD-CBD	5.12	120.17	111.23
23	c	512	CLA	C3B-C2B-C1B	-5.11	101.14	107.17
23	B	608	CLA	C2C-C1C-NC	5.11	115.35	109.98
23	B	612	CLA	CMD-C2D-C1D	5.11	133.73	124.73
29	A	414[B]	PL9	C7-C8-C9	-5.11	118.02	126.83
23	A	405[A]	CLA	O2D-CGD-CBD	5.11	120.17	111.23
23	b	606	CLA	O2D-CGD-CBD	5.11	120.16	111.23
23	B	614	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
23	c	509	CLA	C2C-C1C-NC	5.11	115.35	109.98
23	C	503	CLA	C2C-C1C-NC	5.11	115.34	109.98
23	b	605	CLA	C4A-NA-C1A	-5.10	104.35	106.68
23	b	614	CLA	CMD-C2D-C1D	5.10	133.71	124.73
23	B	607	CLA	C2C-C1C-NC	5.10	115.34	109.98
23	c	510	CLA	O2D-CGD-CBD	5.10	120.14	111.23
23	C	510	CLA	C4A-NA-C1A	-5.09	104.36	106.68
38	f	101	HEM	CHC-C4B-NB	5.08	129.89	124.42
23	B	608	CLA	CMD-C2D-C1D	5.08	133.67	124.73
23	C	514	CLA	C3B-C2B-C1B	-5.08	101.18	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405[A]	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
26	a	410[A]	SQD	O47-C7-C8	5.07	122.45	111.48
23	a	406[B]	CLA	O2D-CGD-CBD	5.07	120.09	111.23
23	b	609	CLA	C1-C2-C3	-5.07	117.89	126.20
23	B	611	CLA	CMC-C2C-C1C	5.07	132.95	125.03
23	b	604	CLA	C2D-C1D-ND	5.07	115.14	110.13
23	D	402[A]	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
23	b	604	CLA	CMD-C2D-C1D	5.06	133.64	124.73
23	B	610	CLA	C3D-C2D-C1D	-5.05	98.93	105.83
23	b	611	CLA	C2C-C1C-NC	5.05	115.29	109.98
23	A	408	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
23	A	405[B]	CLA	C3D-C2D-C1D	-5.05	98.95	105.83
23	c	501	CLA	O2D-CGD-CBD	5.03	120.03	111.23
23	C	512	CLA	C2C-C1C-NC	5.03	115.26	109.98
23	d	403	CLA	C2B-C1B-NB	5.03	115.54	110.33
26	F	103	SQD	C1-O5-C5	-5.02	103.91	113.72
23	A	408	CLA	C2B-C1B-NB	5.02	115.53	110.33
23	a	404[B]	CLA	C2B-C1B-NB	5.01	115.53	110.33
23	b	604	CLA	C4A-NA-C1A	-5.01	104.39	106.68
34	B	622	HTG	C1'-S1-C1	5.01	111.27	100.45
23	c	512	CLA	C2B-C1B-NB	5.01	115.52	110.33
23	b	614	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
23	B	616	CLA	C2C-C1C-NC	5.01	115.24	109.98
23	a	406[B]	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
23	d	403	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
23	A	404[B]	CLA	C2C-C1C-NC	5.00	115.23	109.98
23	B	602	CLA	C2C-C1C-NC	5.00	115.23	109.98
23	B	608	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
23	A	405[B]	CLA	C2C-C1C-NC	4.99	115.23	109.98
23	a	405[B]	CLA	O2D-CGD-CBD	4.99	119.96	111.23
23	C	514	CLA	C4A-NA-C1A	-4.98	104.41	106.68
23	B	611	CLA	C3D-C4D-ND	4.98	118.09	109.99
23	C	513	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
23	b	607	CLA	CHD-C4C-C3C	-4.98	117.52	124.77
23	a	406[B]	CLA	C2B-C1B-NB	4.97	115.48	110.33
23	b	613	CLA	C4A-NA-C1A	-4.97	104.41	106.68
23	b	602	CLA	C3B-C2B-C1B	-4.97	101.32	107.17
23	a	406[A]	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
23	C	510	CLA	C2C-C1C-NC	4.96	115.19	109.98
23	B	610	CLA	O2A-CGA-CBA	4.96	126.96	111.83
23	B	601	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
23	c	506	CLA	C3D-C2D-C1D	-4.96	99.07	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	v	201	HEC	CBC-CAC-C3C	-4.95	117.53	127.43
23	C	506	CLA	C2C-C1C-NC	4.95	115.18	109.98
26	a	410[A]	SQD	C1-O5-C5	-4.95	104.05	113.72
25	b	617	BCR	C7-C8-C9	-4.95	118.91	126.23
26	a	410[B]	SQD	O47-C7-C8	4.95	122.19	111.48
23	C	506	CLA	C4A-NA-C1A	-4.94	104.42	106.68
24	a	407[A]	PHO	C3D-C4D-ND	4.94	114.04	107.71
23	A	405[A]	CLA	C2C-C1C-NC	4.93	115.17	109.98
23	a	408	CLA	C4A-NA-C1A	-4.93	104.43	106.68
23	C	505	CLA	CHD-C4C-C3C	-4.93	117.58	124.77
23	C	511	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
23	c	507	CLA	C2C-C1C-NC	4.91	115.14	109.98
24	a	407[B]	PHO	C3D-C4D-ND	4.91	114.00	107.71
23	c	502	CLA	C1C-C2C-C3C	-4.91	101.82	106.98
23	c	511	CLA	C3D-C2D-C1D	-4.91	99.14	105.83
23	B	616	CLA	C3B-C2B-C1B	-4.91	101.39	107.17
23	b	616	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
23	a	405[A]	CLA	C2C-C1C-NC	4.90	115.13	109.98
23	a	408	CLA	C2C-C1C-NC	4.90	115.12	109.98
23	B	612	CLA	C3C-C4C-NC	4.90	116.70	110.43
23	b	605	CLA	CHD-C1D-ND	-4.90	117.91	124.80
23	c	503	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
23	c	509	CLA	O2D-CGD-CBD	4.89	119.78	111.23
23	B	616	CLA	CMD-C2D-C1D	4.89	133.34	124.73
23	c	508	CLA	O2D-CGD-CBD	4.89	119.77	111.23
23	C	509	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
23	b	613	CLA	C2C-C1C-NC	4.89	115.11	109.98
23	B	613	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
23	b	608	CLA	C2B-C1B-NB	4.87	115.38	110.33
23	B	616	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
23	b	602	CLA	C3D-C4D-ND	4.87	117.90	109.99
23	C	511	CLA	C3D-C4D-ND	4.86	117.89	109.99
23	C	506	CLA	CMB-C2B-C1B	4.86	132.82	125.42
23	c	509	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
23	B	604	CLA	C2D-C1D-ND	4.86	114.93	110.13
23	C	514	CLA	C2C-C1C-NC	4.85	115.08	109.98
23	C	502	CLA	O2D-CGD-O1D	-4.85	114.41	123.85
23	B	601	CLA	C2B-C1B-NB	4.85	115.35	110.33
23	A	404[B]	CLA	C1D-CHD-C4C	-4.85	115.72	126.02
23	C	510	CLA	O2D-CGD-CBD	4.84	119.70	111.23
33	B	621	LMG	O7-C10-C11	4.84	121.96	111.48
23	b	608	CLA	CMD-C2D-C1D	4.84	133.26	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	C1-C2-C3	-4.84	118.27	126.20
23	b	604	CLA	C1C-C2C-C3C	-4.84	101.89	106.98
23	b	614	CLA	C2B-C1B-NB	4.84	115.34	110.33
29	a	413[A]	PL9	C7-C8-C9	-4.84	118.50	126.83
26	f	102	SQD	O47-C7-C8	4.83	121.94	111.48
23	a	404[A]	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
26	A	410[B]	SQD	C1-O5-C5	-4.83	104.29	113.72
23	c	502	CLA	C4A-NA-C1A	-4.83	104.48	106.68
23	B	603	CLA	C3D-C2D-C1D	-4.83	99.25	105.83
23	C	507	CLA	C3B-C2B-C1B	-4.82	101.48	107.17
23	D	403	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
23	b	614	CLA	C2C-C1C-NC	4.82	115.05	109.98
23	c	510	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
23	B	605	CLA	C3C-C4C-NC	4.82	116.60	110.43
23	C	507	CLA	O2D-CGD-CBD	4.81	119.64	111.23
23	c	504	CLA	C2C-C1C-NC	4.81	115.04	109.98
23	B	615	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
23	B	605	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
38	F	102	HEM	CAD-CBD-CGD	4.80	126.41	113.67
29	A	414[A]	PL9	C7-C8-C9	-4.80	118.56	126.83
23	A	408	CLA	C4A-NA-C1A	-4.80	104.49	106.68
23	C	505	CLA	C1C-C2C-C3C	-4.79	101.94	106.98
23	c	504	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
23	c	504	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
23	b	607	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
23	A	405[A]	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	a	406[B]	CLA	C3D-C4D-ND	4.78	117.76	109.99
23	A	405[B]	CLA	O2D-CGD-CBD	4.78	119.58	111.23
23	C	514	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	b	603	CLA	C3D-C4D-ND	4.77	117.75	109.99
23	A	406[B]	CLA	C2B-C1B-NB	4.77	115.28	110.33
23	a	408	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
23	A	406[A]	CLA	C2B-C1B-NB	4.77	115.27	110.33
23	C	504	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
23	A	405[A]	CLA	CMD-C2D-C1D	4.77	133.12	124.73
23	c	513	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
25	y	101	BCR	C33-C5-C6	-4.77	119.28	124.48
23	B	608	CLA	C4A-NA-C1A	-4.77	104.50	106.68
23	b	608	CLA	C3B-C2B-C1B	-4.76	101.55	107.17
23	a	408	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
23	B	615	CLA	C3D-C4D-ND	4.76	117.73	109.99
23	d	402[A]	CLA	C4A-NA-C1A	-4.76	104.51	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	C3B-C2B-C1B	-4.76	101.56	107.17
25	H	101	BCR	C38-C26-C25	-4.75	119.30	124.48
23	B	601	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	C	502	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	d	403	CLA	C3B-C2B-C1B	-4.75	101.57	107.17
23	C	511	CLA	C1C-C2C-C3C	-4.75	101.99	106.98
23	a	408	CLA	C3D-C4D-ND	4.75	117.70	109.99
23	a	405[B]	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
31	t	101	LMT	C3'-C4'-C5'	-4.74	100.42	110.93
23	A	406[B]	CLA	C3D-C4D-ND	4.74	117.69	109.99
23	c	513	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	C	508	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
23	b	603	CLA	C2C-C1C-NC	4.73	114.95	109.98
23	D	402[B]	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
23	a	405[A]	CLA	O2D-CGD-CBD	4.73	119.49	111.23
23	b	605	CLA	C2C-C1C-NC	4.73	114.95	109.98
23	c	513	CLA	C2B-C1B-NB	4.72	115.22	110.33
23	C	507	CLA	C1C-C2C-C3C	-4.72	102.01	106.98
23	C	513	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
23	a	405[B]	CLA	C1C-C2C-C3C	-4.72	102.02	106.98
23	B	607	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
23	c	501	CLA	O2D-CGD-O1D	-4.71	114.67	123.85
23	c	501	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
23	c	505	CLA	C3C-C4C-NC	4.71	116.46	110.43
23	b	601	CLA	C3D-C4D-ND	4.71	117.64	109.99
23	C	509	CLA	C3C-C4C-NC	4.70	116.46	110.43
23	b	615	CLA	C2C-C1C-NC	4.70	114.92	109.98
23	c	513	CLA	C2C-C1C-NC	4.70	114.91	109.98
23	B	602	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
23	B	607	CLA	CMD-C2D-C1D	4.69	132.99	124.73
23	A	404[A]	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
23	A	406[B]	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	a	404[B]	CLA	C3D-C4D-ND	4.69	117.61	109.99
23	a	408	CLA	CMD-C2D-C1D	4.69	132.99	124.73
23	b	605	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
23	d	402[B]	CLA	O2D-CGD-CBD	4.69	119.42	111.23
23	a	404[B]	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
23	a	406[B]	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
23	B	609	CLA	C2C-C1C-NC	4.68	114.90	109.98
23	c	510	CLA	C2B-C1B-NB	4.68	115.17	110.33
23	B	601	CLA	C3D-C4D-ND	4.67	117.58	109.99
23	A	406[B]	CLA	O2D-CGD-CBD	4.67	119.40	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402[B]	CLA	C3B-C2B-C1B	-4.67	101.67	107.17
23	C	507	CLA	C4A-NA-C1A	-4.66	104.55	106.68
23	C	512	CLA	C4A-NA-C1A	-4.66	104.55	106.68
23	A	406[A]	CLA	C3D-C4D-ND	4.66	117.56	109.99
23	B	616	CLA	O2D-CGD-O1D	-4.66	114.78	123.85
23	D	402[B]	CLA	C1-C2-C3	-4.66	118.56	126.20
23	b	608	CLA	C3D-C4D-ND	4.66	117.56	109.99
26	a	410[B]	SQD	O6-C1-C2	4.66	115.35	108.27
23	b	606	CLA	C3B-C2B-C1B	-4.66	101.68	107.17
23	d	402[B]	CLA	C3D-C4D-ND	4.65	117.55	109.99
23	b	601	CLA	C2B-C1B-NB	4.65	115.15	110.33
23	c	512	CLA	C1-C2-C3	-4.65	118.58	126.20
23	b	605	CLA	C2B-C1B-NB	4.65	115.15	110.33
23	B	613	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
23	b	611	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
23	c	511	CLA	C2C-C1C-NC	4.64	114.86	109.98
23	D	402[B]	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	b	608	CLA	C2C-C1C-NC	4.64	114.86	109.98
25	C	515	BCR	C33-C5-C6	-4.64	119.43	124.48
29	A	414[B]	PL9	C32-C33-C34	-4.63	117.02	127.62
23	B	603	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
23	b	609	CLA	C4A-NA-C1A	-4.63	104.57	106.68
23	a	406[B]	CLA	CHD-C1D-ND	-4.63	118.29	124.80
23	b	615	CLA	C3B-C2B-C1B	-4.63	101.72	107.17
23	C	509	CLA	CMD-C2D-C1D	4.62	132.87	124.73
23	a	404[B]	CLA	C2C-C1C-NC	4.62	114.84	109.98
23	d	402[A]	CLA	C3D-C4D-ND	4.62	117.50	109.99
23	c	507	CLA	CHD-C1D-ND	-4.62	118.30	124.80
23	b	606	CLA	C2C-C1C-NC	4.62	114.83	109.98
23	b	601	CLA	C3B-C2B-C1B	-4.61	101.73	107.17
23	B	604	CLA	C3C-C4C-NC	4.61	116.34	110.43
23	B	603	CLA	C2C-C1C-NC	4.61	114.83	109.98
33	a	416	LMG	O7-C10-C11	4.61	121.45	111.48
23	A	406[A]	CLA	O2D-CGD-CBD	4.61	119.28	111.23
25	d	404	BCR	C7-C8-C9	-4.61	119.42	126.23
23	b	615	CLA	C3D-C2D-C1D	-4.61	99.55	105.83
23	b	612	CLA	C3B-C2B-C1B	-4.61	101.74	107.17
23	B	608	CLA	C3B-C2B-C1B	-4.60	101.74	107.17
23	b	612	CLA	C1-C2-C3	-4.60	118.66	126.20
23	b	609	CLA	C3C-C4C-NC	4.60	116.32	110.43
23	c	510	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	C	514	CLA	O2D-CGD-CBD	4.59	119.26	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404[A]	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
23	A	405[A]	CLA	C1C-C2C-C3C	-4.59	102.15	106.98
23	B	610	CLA	C2B-C1B-NB	4.59	115.08	110.33
23	c	501	CLA	C3D-C4D-ND	4.59	117.44	109.99
23	b	606	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	C	509	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	c	507	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
23	C	511	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
23	B	613	CLA	C2C-C1C-NC	4.57	114.78	109.98
23	b	616	CLA	C1D-CHD-C4C	-4.57	116.32	126.02
23	b	611	CLA	C3D-C4D-ND	4.56	117.40	109.99
23	c	505	CLA	C3D-C4D-ND	4.56	117.40	109.99
23	b	605	CLA	C3D-C4D-ND	4.56	117.39	109.99
23	b	614	CLA	C4A-NA-C1A	-4.55	104.60	106.68
23	c	501	CLA	CHD-C1D-ND	-4.54	118.41	124.80
23	C	504	CLA	C3D-C4D-ND	4.54	117.37	109.99
23	C	507	CLA	C3D-C4D-ND	4.54	117.37	109.99
23	a	406[A]	CLA	O2D-CGD-CBD	4.54	119.17	111.23
33	C	501	LMG	O1-C1-C2	4.54	115.17	108.27
23	A	408	CLA	CHD-C1D-ND	-4.54	118.42	124.80
23	c	513	CLA	C3D-C4D-ND	4.54	117.36	109.99
23	A	405[A]	CLA	C2B-C1B-NB	4.53	115.03	110.33
23	C	505	CLA	CHD-C1D-ND	-4.53	118.42	124.80
23	B	609	CLA	C3D-C4D-ND	4.53	117.35	109.99
23	b	609	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	b	610	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	b	616	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
23	c	511	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
23	D	403	CLA	C3D-C4D-ND	4.52	117.34	109.99
23	C	503	CLA	O2D-CGD-CBD	4.52	119.13	111.23
23	C	510	CLA	C3B-C2B-C1B	-4.51	101.85	107.17
23	b	615	CLA	C2B-C1B-NB	4.51	115.00	110.33
34	d	410	HTG	C1'-S1-C1	4.51	110.18	100.45
23	B	611	CLA	CHD-C1D-ND	-4.51	118.46	124.80
29	A	414[A]	PL9	C32-C33-C34	-4.51	117.31	127.62
23	A	406[A]	CLA	CMB-C2B-C1B	4.50	132.27	125.42
23	b	616	CLA	C2B-C1B-NB	4.50	114.99	110.33
23	A	405[A]	CLA	C3D-C4D-ND	4.50	117.30	109.99
25	d	404	BCR	C29-C30-C25	4.50	116.97	110.44
23	b	609	CLA	C2C-C1C-NC	4.49	114.70	109.98
23	B	611	CLA	CHD-C4C-NC	4.49	131.20	124.23
23	c	502	CLA	C3D-C4D-ND	4.49	117.29	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	402[A]	CLA	C3C-C4C-NC	4.49	116.18	110.43
25	h	101	BCR	C7-C8-C9	-4.49	119.59	126.23
23	B	614	CLA	C4A-NA-C1A	-4.49	104.63	106.68
23	C	513	CLA	C1-C2-C3	-4.49	118.84	126.20
23	c	505	CLA	C2C-C1C-NC	4.48	114.69	109.98
23	C	510	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
23	b	608	CLA	C1C-C2C-C3C	-4.48	102.27	106.98
23	C	509	CLA	C1-C2-C3	-4.48	118.86	126.20
23	D	402[B]	CLA	O2D-CGD-CBD	4.48	119.06	111.23
23	C	507	CLA	C1-C2-C3	-4.48	118.86	126.20
23	C	507	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	b	610	CLA	C3D-C4D-ND	4.47	117.25	109.99
25	b	617	BCR	C33-C5-C6	-4.47	119.61	124.48
23	a	406[A]	CLA	C3B-C2B-C1B	-4.47	101.90	107.17
23	B	616	CLA	C3B-C4B-NB	4.47	114.52	110.53
23	b	612	CLA	C4A-NA-C1A	-4.46	104.64	106.68
23	A	405[B]	CLA	C2B-C1B-NB	4.46	114.95	110.33
23	C	502	CLA	C2B-C1B-NB	4.46	114.95	110.33
23	B	615	CLA	C2C-C1C-NC	4.45	114.65	109.98
23	b	610	CLA	O2A-CGA-CBA	4.44	125.38	111.83
23	B	610	CLA	C4A-NA-C1A	-4.44	104.65	106.68
23	b	603	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	C	511	CLA	C3B-C4B-NB	4.44	114.49	110.53
23	B	613	CLA	O2D-CGD-CBD	4.44	118.99	111.23
23	a	405[B]	CLA	C1D-CHD-C4C	-4.44	116.59	126.02
23	C	508	CLA	O2D-CGD-O1D	-4.43	115.22	123.85
23	c	507	CLA	CMB-C2B-C1B	4.43	132.17	125.42
23	b	611	CLA	C2B-C1B-NB	4.43	114.92	110.33
24	A	416[B]	PHO	C1-C2-C3	-4.43	118.94	126.20
23	C	514	CLA	C2B-C1B-NB	4.43	114.92	110.33
23	b	610	CLA	C2C-C1C-NC	4.43	114.63	109.98
23	d	403	CLA	C4A-NA-C1A	-4.42	104.66	106.68
23	c	512	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
23	a	406[A]	CLA	C3D-C4D-ND	4.42	117.17	109.99
23	b	609	CLA	C3D-C4D-ND	4.42	117.17	109.99
23	B	612	CLA	C3B-C2B-C1B	-4.42	101.96	107.17
23	B	602	CLA	C3D-C4D-ND	4.42	117.17	109.99
23	a	404[A]	CLA	C3D-C4D-ND	4.42	117.17	109.99
23	b	611	CLA	C3C-C4C-NC	4.42	116.09	110.43
23	a	404[A]	CLA	C1C-C2C-C3C	-4.41	102.34	106.98
23	C	513	CLA	C3D-C4D-ND	4.41	117.15	109.99
23	a	404[B]	CLA	C1D-CHD-C4C	-4.41	116.65	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405[A]	CLA	C1C-C2C-C3C	-4.41	102.34	106.98
23	b	613	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
23	a	405[B]	CLA	C4A-NA-C1A	-4.41	104.67	106.68
23	B	605	CLA	C2C-C1C-NC	4.40	114.61	109.98
23	C	512	CLA	C2B-C1B-NB	4.40	114.89	110.33
23	C	511	CLA	CHD-C1D-ND	-4.40	118.61	124.80
23	B	610	CLA	C3B-C2B-C1B	-4.40	101.98	107.17
23	A	404[B]	CLA	C3B-C4B-NB	4.40	114.46	110.53
23	a	406[A]	CLA	C2B-C1B-NB	4.40	114.89	110.33
23	C	514	CLA	C3D-C4D-ND	4.40	117.13	109.99
23	c	502	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
23	a	405[A]	CLA	C2B-C1B-NB	4.39	114.88	110.33
23	C	508	CLA	C2C-C1C-NC	4.39	114.60	109.98
24	A	416[A]	PHO	C1-C2-C3	-4.39	119.00	126.20
23	A	405[A]	CLA	C3B-C2B-C1B	-4.39	102.00	107.17
23	d	403	CLA	CHD-C1D-ND	-4.39	118.63	124.80
23	b	613	CLA	C3C-C4C-NC	4.39	116.05	110.43
23	c	511	CLA	O2D-CGD-CBD	4.39	118.90	111.23
23	D	402[B]	CLA	C3D-C4D-ND	4.38	117.11	109.99
23	B	614	CLA	C1C-C2C-C3C	-4.38	102.37	106.98
23	B	603	CLA	C3D-C4D-ND	4.38	117.11	109.99
23	B	610	CLA	C2C-C1C-NC	4.38	114.58	109.98
23	B	601	CLA	C4A-NA-C1A	-4.38	104.68	106.68
23	B	607	CLA	C1C-C2C-C3C	-4.38	102.37	106.98
23	C	502	CLA	C3D-C4D-ND	4.38	117.11	109.99
33	C	501	LMG	O7-C10-C11	4.38	120.95	111.48
23	B	602	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
23	C	507	CLA	CHD-C1D-ND	-4.38	118.64	124.80
23	A	405[B]	CLA	C3D-C4D-ND	4.38	117.10	109.99
23	B	609	CLA	C3D-C2D-C1D	-4.37	99.86	105.83
23	b	612	CLA	C3D-C4D-ND	4.37	117.10	109.99
23	c	506	CLA	C3D-C4D-ND	4.37	117.10	109.99
25	k	101	BCR	C29-C30-C25	4.37	116.79	110.44
23	A	406[A]	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
23	C	504	CLA	C2B-C1B-NB	4.37	114.86	110.33
23	c	504	CLA	C1-O2A-CGA	4.36	127.21	116.65
23	d	402[A]	CLA	C1C-C2C-C3C	-4.36	102.39	106.98
23	C	506	CLA	C3D-C4D-ND	4.36	117.08	109.99
23	B	607	CLA	C3D-C4D-ND	4.36	117.07	109.99
23	C	509	CLA	O2D-CGD-CBD	4.36	118.85	111.23
23	B	613	CLA	C3C-C4C-NC	4.35	116.01	110.43
32	E	101[A]	LHG	O7-C7-C8	4.35	120.90	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	C3B-C2B-C1B	-4.35	102.04	107.17
23	c	511	CLA	C3D-C4D-ND	4.35	117.06	109.99
23	c	503	CLA	C3B-C2B-C1B	-4.35	102.04	107.17
23	A	404[B]	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
23	B	612	CLA	O2D-CGD-O1D	-4.34	115.40	123.85
23	C	512	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
23	c	510	CLA	C2C-C1C-NC	4.34	114.54	109.98
23	C	511	CLA	C2B-C1B-NB	4.34	114.82	110.33
23	b	607	CLA	C1C-C2C-C3C	-4.33	102.42	106.98
23	A	404[B]	CLA	C4B-C3B-C2B	-4.33	101.91	107.30
23	B	614	CLA	C2B-C1B-NB	4.33	114.82	110.33
23	c	503	CLA	C2B-C1B-NB	4.33	114.82	110.33
23	c	513	CLA	CHD-C1D-ND	-4.33	118.70	124.80
23	c	505	CLA	C3B-C2B-C1B	-4.33	102.06	107.17
23	a	404[B]	CLA	C3B-C4B-NB	4.33	114.39	110.53
23	b	601	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
23	C	505	CLA	C3B-C4B-NB	4.33	114.39	110.53
29	a	413[B]	PL9	C7-C3-C4	4.32	120.47	116.91
23	D	403	CLA	C2B-C1B-NB	4.32	114.81	110.33
23	C	512	CLA	C1D-CHD-C4C	-4.32	116.84	126.02
23	d	403	CLA	C3D-C4D-ND	4.32	117.00	109.99
23	B	609	CLA	C2B-C1B-NB	4.32	114.80	110.33
23	A	404[A]	CLA	C3B-C4B-NB	4.31	114.38	110.53
23	C	506	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
23	C	502	CLA	C2C-C1C-NC	4.31	114.51	109.98
23	A	404[B]	CLA	C2B-C1B-NB	4.31	114.79	110.33
23	C	505	CLA	C3D-C4D-ND	4.30	116.98	109.99
23	D	402[B]	CLA	CHD-C1D-ND	-4.30	118.75	124.80
23	A	406[A]	CLA	C2C-C1C-NC	4.30	114.50	109.98
23	C	503	CLA	C4A-NA-C1A	-4.30	104.72	106.68
23	b	614	CLA	C3D-C4D-ND	4.30	116.97	109.99
23	B	606	CLA	C3D-C4D-ND	4.30	116.97	109.99
23	c	509	CLA	C3B-C4B-NB	4.29	114.36	110.53
23	c	511	CLA	C1D-CHD-C4C	-4.29	116.90	126.02
23	a	406[A]	CLA	C2C-C1C-NC	4.29	114.49	109.98
23	C	510	CLA	C1-C2-C3	-4.29	119.17	126.20
23	c	503	CLA	C2C-C1C-NC	4.29	114.48	109.98
23	A	406[B]	CLA	C3B-C2B-C1B	-4.28	102.12	107.17
23	a	408	CLA	C3C-C4C-NC	4.28	115.91	110.43
23	C	503	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
23	B	612	CLA	C2C-C1C-NC	4.28	114.48	109.98
23	B	605	CLA	CHD-C1D-ND	-4.28	118.78	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C3D-C4D-ND	4.28	116.94	109.99
23	b	612	CLA	C3C-C4C-NC	4.28	115.91	110.43
23	C	507	CLA	C2B-C1B-NB	4.27	114.76	110.33
23	B	605	CLA	C3D-C4D-ND	4.27	116.93	109.99
33	m	101	LMG	O7-C10-C11	4.27	120.72	111.48
23	b	606	CLA	C4-C3-C5	4.27	122.64	115.23
26	a	410[A]	SQD	C1-C2-C3	-4.27	101.02	110.01
23	B	615	CLA	CHD-C1D-ND	-4.27	118.79	124.80
23	B	615	CLA	CMB-C2B-C1B	4.27	131.92	125.42
23	c	504	CLA	C4A-NA-C1A	-4.27	104.73	106.68
23	a	404[A]	CLA	C2B-C1B-NB	4.27	114.75	110.33
23	a	404[A]	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	b	615	CLA	C3D-C4D-ND	4.26	116.91	109.99
23	B	610	CLA	CAA-C2A-C3A	-4.26	101.48	113.00
23	A	406[B]	CLA	CHD-C1D-ND	-4.26	118.81	124.80
23	A	406[A]	CLA	CHD-C1D-ND	-4.26	118.81	124.80
23	a	405[B]	CLA	C3D-C4D-ND	4.26	116.91	109.99
32	E	101[B]	LHG	O7-C7-C8	4.26	120.69	111.48
23	a	405[A]	CLA	C3D-C4D-ND	4.26	116.91	109.99
23	A	406[A]	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
23	B	603	CLA	C3C-C4C-NC	4.26	115.88	110.43
23	d	402[B]	CLA	C3C-C4C-NC	4.26	115.88	110.43
23	a	405[A]	CLA	C4A-NA-C1A	-4.25	104.74	106.68
23	a	406[A]	CLA	CHD-C1D-ND	-4.25	118.81	124.80
23	D	402[A]	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
23	B	603	CLA	CHD-C1D-ND	-4.25	118.82	124.80
23	C	503	CLA	C2B-C1B-NB	4.25	114.73	110.33
23	c	509	CLA	C3D-C4D-ND	4.25	116.89	109.99
23	b	606	CLA	C3C-C4C-NC	4.25	115.87	110.43
23	c	509	CLA	C3D-C2D-C1D	-4.25	100.04	105.83
23	B	604	CLA	C3B-C2B-C1B	-4.25	102.17	107.17
23	b	613	CLA	C1-C2-C3	-4.24	119.24	126.20
23	c	502	CLA	C2B-C1B-NB	4.24	114.73	110.33
23	C	508	CLA	C2B-C1B-NB	4.24	114.73	110.33
23	b	603	CLA	C3B-C2B-C1B	-4.24	102.17	107.17
23	c	512	CLA	C3D-C4D-ND	4.24	116.88	109.99
38	F	102	HEM	CHD-C4C-NC	4.24	129.07	124.45
23	B	608	CLA	C2B-C1B-NB	4.24	114.72	110.33
23	B	606	CLA	C2C-C1C-NC	4.24	114.44	109.98
23	b	602	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
23	C	503	CLA	C3D-C4D-ND	4.24	116.88	109.99
23	A	404[A]	CLA	CHD-C1D-ND	-4.24	118.83	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	C3D-C4D-ND	4.24	116.88	109.99
23	c	513	CLA	O2D-CGD-CBD	4.24	118.64	111.23
23	C	513	CLA	C3C-C4C-NC	4.24	115.86	110.43
23	b	603	CLA	C3C-C4C-NC	4.24	115.86	110.43
23	B	614	CLA	C1D-CHD-C4C	-4.24	117.02	126.02
32	A	419[A]	LHG	O8-C23-O10	-4.23	113.04	123.63
23	b	606	CLA	O2D-CGD-O1D	-4.23	115.61	123.85
23	a	408	CLA	CMC-C2C-C1C	4.23	131.65	125.03
23	b	604	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
23	A	408	CLA	C3C-C4C-NC	4.23	115.85	110.43
23	B	605	CLA	C1D-CHD-C4C	-4.23	117.03	126.02
23	C	513	CLA	C1D-CHD-C4C	-4.23	117.03	126.02
23	b	609	CLA	O2D-CGD-CBD	4.23	118.62	111.23
23	C	510	CLA	C3C-C4C-NC	4.23	115.84	110.43
23	C	509	CLA	C2B-C1B-NB	4.23	114.71	110.33
23	B	602	CLA	C2B-C1B-NB	4.23	114.71	110.33
23	a	405[B]	CLA	C2B-C1B-NB	4.23	114.71	110.33
33	Z	101	LMG	O7-C10-C11	4.23	120.62	111.48
23	a	405[A]	CLA	CAA-C2A-C3A	-4.22	101.59	113.00
23	C	503	CLA	C1C-C2C-C3C	-4.22	102.54	106.98
23	d	402[A]	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
23	B	609	CLA	C3C-C4C-NC	4.22	115.84	110.43
23	c	505	CLA	C2B-C1B-NB	4.22	114.70	110.33
29	a	413[A]	PL9	C32-C33-C34	-4.22	117.96	127.62
23	c	501	CLA	C3B-C2B-C1B	-4.22	102.19	107.17
23	b	607	CLA	O2D-CGD-CBD	4.22	118.60	111.23
23	c	506	CLA	CHD-C1D-ND	-4.22	118.87	124.80
23	A	408	CLA	C3D-C4D-ND	4.21	116.84	109.99
29	a	413[A]	PL9	C7-C3-C2	-4.21	118.42	123.39
29	a	413[B]	PL9	C7-C3-C2	-4.21	118.43	123.39
23	A	404[A]	CLA	C2B-C1B-NB	4.21	114.69	110.33
23	B	609	CLA	O2D-CGD-CBD	4.21	118.59	111.23
23	c	507	CLA	C1C-C2C-C3C	-4.21	102.56	106.98
23	c	508	CLA	C3B-C2B-C1B	-4.21	102.21	107.17
23	D	402[A]	CLA	C3D-C4D-ND	4.21	116.82	109.99
23	B	605	CLA	CMB-C2B-C1B	4.20	131.82	125.42
23	B	614	CLA	C3B-C4B-NB	4.20	114.28	110.53
23	A	405[B]	CLA	C1C-C2C-C3C	-4.20	102.56	106.98
23	a	404[A]	CLA	CAA-C2A-C3A	-4.20	101.65	113.00
23	c	508	CLA	C3C-C4C-NC	4.20	115.81	110.43
23	d	402[A]	CLA	C3B-C2B-C1B	-4.19	102.23	107.17
23	c	506	CLA	O2D-CGD-CBD	4.19	118.56	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	514	CLA	C1C-C2C-C3C	-4.19	102.57	106.98
23	C	510	CLA	C3D-C4D-ND	4.19	116.80	109.99
23	c	509	CLA	C2B-C1B-NB	4.19	114.67	110.33
23	c	503	CLA	C1D-CHD-C4C	-4.19	117.11	126.02
23	a	404[A]	CLA	C1D-CHD-C4C	-4.19	117.12	126.02
33	c	520	LMG	O7-C10-C11	4.19	120.54	111.48
23	b	605	CLA	O2D-CGD-O1D	-4.19	115.70	123.85
23	C	509	CLA	C3D-C4D-ND	4.19	116.79	109.99
23	C	504	CLA	O2D-CGD-CBD	4.18	118.55	111.23
23	b	607	CLA	C3B-C4B-NB	4.18	114.27	110.53
23	c	507	CLA	C3D-C4D-ND	4.18	116.79	109.99
23	b	607	CLA	C4A-NA-C1A	-4.18	104.77	106.68
23	b	616	CLA	O2D-CGD-O1D	-4.18	115.71	123.85
23	d	402[A]	CLA	O2D-CGD-CBD	4.18	118.53	111.23
23	B	612	CLA	C3D-C2D-C1D	-4.18	100.13	105.83
23	C	506	CLA	C3D-C2D-C1D	-4.18	100.13	105.83
23	b	607	CLA	C3D-C4D-ND	4.18	116.78	109.99
23	C	504	CLA	CHD-C1D-ND	-4.17	118.93	124.80
29	D	405[B]	PL9	C42-C43-C44	-4.17	118.07	127.62
23	b	606	CLA	C1D-CHD-C4C	-4.17	117.16	126.02
23	d	402[B]	CLA	C3D-C2D-C1D	-4.17	100.15	105.83
23	a	405[A]	CLA	C3B-C2B-C1B	-4.17	102.26	107.17
23	B	603	CLA	C2B-C1B-NB	4.16	114.64	110.33
23	A	404[A]	CLA	C3D-C4D-ND	4.16	116.75	109.99
23	D	403	CLA	O2D-CGD-O1D	-4.16	115.75	123.85
23	b	606	CLA	CHD-C1D-ND	-4.16	118.94	124.80
23	A	404[B]	CLA	O2D-CGD-CBD	4.16	118.50	111.23
29	a	413[B]	PL9	C32-C33-C34	-4.16	118.10	127.62
23	b	615	CLA	C1D-CHD-C4C	-4.16	117.18	126.02
23	b	609	CLA	C2B-C1B-NB	4.16	114.64	110.33
23	c	513	CLA	C1D-CHD-C4C	-4.16	117.19	126.02
23	b	611	CLA	O2D-CGD-O1D	-4.15	115.76	123.85
23	D	402[A]	CLA	O2D-CGD-CBD	4.15	118.49	111.23
23	c	501	CLA	C2B-C1B-NB	4.15	114.63	110.33
23	C	506	CLA	C3C-C4C-NC	4.15	115.75	110.43
23	C	514	CLA	CHD-C1D-ND	-4.15	118.96	124.80
23	a	404[B]	CLA	CHD-C1D-ND	-4.15	118.97	124.80
23	b	608	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
23	B	607	CLA	C3B-C2B-C1B	-4.14	102.28	107.17
23	c	501	CLA	C2C-C1C-NC	4.14	114.33	109.98
23	b	611	CLA	CHD-C1D-ND	-4.14	118.97	124.80
23	C	509	CLA	C1C-C2C-C3C	-4.14	102.62	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	C3D-C4D-ND	4.14	116.72	109.99
23	A	405[B]	CLA	C3B-C2B-C1B	-4.14	102.29	107.17
23	c	504	CLA	C3D-C4D-ND	4.13	116.71	109.99
23	c	502	CLA	O2D-CGD-O1D	-4.13	115.81	123.85
23	c	506	CLA	C3B-C2B-C1B	-4.13	102.30	107.17
23	c	504	CLA	C2B-C1B-NB	4.13	114.61	110.33
23	a	408	CLA	C2B-C1B-NB	4.13	114.61	110.33
23	A	406[B]	CLA	C2C-C1C-NC	4.12	114.31	109.98
23	C	504	CLA	C2C-C1C-NC	4.12	114.31	109.98
23	c	504	CLA	C3C-C4C-NC	4.12	115.71	110.43
23	C	511	CLA	C4A-NA-C1A	-4.12	104.80	106.68
23	b	616	CLA	C3D-C4D-ND	4.12	116.68	109.99
23	b	601	CLA	CHD-C1D-ND	-4.12	119.01	124.80
23	c	506	CLA	C1-C2-C3	-4.11	119.45	126.20
23	b	616	CLA	C2C-C1C-NC	4.11	114.30	109.98
23	B	604	CLA	C1D-CHD-C4C	-4.11	117.28	126.02
23	D	402[A]	CLA	CHD-C1D-ND	-4.11	119.02	124.80
23	B	610	CLA	C3C-C4C-NC	4.11	115.69	110.43
33	d	411	LMG	O7-C10-C11	4.11	120.37	111.48
23	c	509	CLA	C4A-NA-C1A	-4.11	104.81	106.68
23	C	510	CLA	C2B-C1B-NB	4.10	114.58	110.33
23	b	602	CLA	O2D-CGD-O1D	-4.10	115.86	123.85
23	B	601	CLA	CHD-C1D-ND	-4.10	119.03	124.80
23	a	405[A]	CLA	C1D-CHD-C4C	-4.10	117.30	126.02
23	b	606	CLA	C3D-C4D-ND	4.10	116.65	109.99
23	D	403	CLA	C2C-C1C-NC	4.10	114.29	109.98
23	C	508	CLA	CHD-C1D-ND	-4.10	119.03	124.80
23	a	408	CLA	C1C-C2C-C3C	-4.10	102.67	106.98
23	c	505	CLA	C3D-C2D-C1D	-4.10	100.24	105.83
23	b	610	CLA	C2B-C1B-NB	4.10	114.57	110.33
23	b	610	CLA	C3C-C4C-NC	4.10	115.68	110.43
23	c	510	CLA	C3C-C4C-NC	4.10	115.68	110.43
33	C	521	LMG	O6-C5-C4	4.09	117.07	109.70
23	a	405[B]	CLA	C3B-C2B-C1B	-4.09	102.35	107.17
23	b	603	CLA	C1D-CHD-C4C	-4.09	117.33	126.02
23	B	613	CLA	C3D-C4D-ND	4.09	116.63	109.99
23	a	406[B]	CLA	C2C-C1C-NC	4.09	114.27	109.98
23	b	616	CLA	O2A-CGA-CBA	4.08	124.29	111.83
23	c	508	CLA	C3D-C4D-ND	4.08	116.62	109.99
23	d	402[A]	CLA	C3C-C4C-NC	4.08	115.66	110.43
25	B	618	BCR	C29-C30-C25	4.08	116.37	110.44
38	F	102	HEM	CHC-C4B-NB	4.08	128.81	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	C3B-C2B-C1B	-4.08	102.36	107.17
23	C	510	CLA	CHD-C1D-ND	-4.08	119.06	124.80
24	A	407[A]	PHO	C1A-C2A-C3A	-4.08	98.96	102.84
23	B	602	CLA	O2D-CGD-O1D	-4.07	115.92	123.85
23	B	608	CLA	C3D-C4D-ND	4.07	116.61	109.99
23	B	609	CLA	CHD-C1D-ND	-4.07	119.08	124.80
23	A	404[B]	CLA	C3D-C4D-ND	4.06	116.59	109.99
23	D	402[A]	CLA	C1-C2-C3	-4.06	119.54	126.20
23	b	604	CLA	C3B-C2B-C1B	-4.06	102.38	107.17
23	B	605	CLA	C2B-C1B-NB	4.06	114.54	110.33
23	a	405[A]	CLA	CMB-C2B-C1B	4.06	131.60	125.42
25	d	404	BCR	C40-C30-C25	-4.06	103.88	110.24
23	c	512	CLA	C1D-CHD-C4C	-4.06	117.39	126.02
23	C	505	CLA	C3B-C2B-C1B	-4.06	102.39	107.17
23	C	505	CLA	C4A-NA-C1A	-4.06	104.83	106.68
23	b	603	CLA	CHD-C1D-ND	-4.05	119.10	124.80
23	b	608	CLA	CHD-C1D-ND	-4.05	119.11	124.80
23	C	506	CLA	C1D-CHD-C4C	-4.04	117.42	126.02
23	b	614	CLA	O2D-CGD-O1D	-4.04	115.98	123.85
23	c	513	CLA	C3B-C4B-NB	4.04	114.14	110.53
23	C	502	CLA	C1D-CHD-C4C	-4.04	117.43	126.02
29	a	413[A]	PL9	C7-C3-C4	4.04	120.24	116.91
25	K	102	BCR	C7-C8-C9	-4.04	120.26	126.23
29	A	414[A]	PL9	C7-C3-C2	-4.03	118.63	123.39
23	C	514	CLA	C3C-C4C-NC	4.03	115.60	110.43
23	c	503	CLA	CHD-C1D-ND	-4.03	119.13	124.80
23	A	404[A]	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
23	B	606	CLA	C1C-C2C-C3C	-4.03	102.75	106.98
23	b	613	CLA	C2B-C1B-NB	4.03	114.50	110.33
23	B	604	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
23	b	603	CLA	C2B-C1B-NB	4.02	114.50	110.33
23	b	610	CLA	O2D-CGD-O1D	-4.02	116.02	123.85
23	b	610	CLA	C1D-CHD-C4C	-4.02	117.47	126.02
23	D	402[B]	CLA	C3C-C4C-NC	4.02	115.58	110.43
23	c	506	CLA	C1C-C2C-C3C	-4.02	102.76	106.98
23	B	608	CLA	C3B-C4B-NB	4.02	114.11	110.53
23	c	508	CLA	C1-C2-C3	-4.01	119.62	126.20
23	A	408	CLA	C1C-C2C-C3C	-4.01	102.76	106.98
23	c	504	CLA	C3B-C4B-NB	4.01	114.11	110.53
23	c	511	CLA	CHD-C1D-ND	-4.01	119.16	124.80
23	B	602	CLA	C1C-C2C-C3C	-4.01	102.76	106.98
26	f	102	SQD	C1-O5-C5	4.01	121.55	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	CMC-C2C-C1C	4.01	131.30	125.03
23	b	612	CLA	O2D-CGD-CBD	4.01	118.24	111.23
23	B	611	CLA	C1D-CHD-C4C	-4.01	117.50	126.02
23	C	512	CLA	O2D-CGD-O1D	-4.01	116.05	123.85
23	b	601	CLA	C1D-CHD-C4C	-4.00	117.51	126.02
23	b	614	CLA	C3C-C4C-NC	4.00	115.56	110.43
23	C	503	CLA	C1-C2-C3	-4.00	119.64	126.20
23	c	503	CLA	C3C-C4C-NC	4.00	115.56	110.43
33	C	521	LMG	O7-C10-C11	4.00	120.14	111.48
23	a	404[B]	CLA	C3B-C2B-C1B	-4.00	102.45	107.17
23	c	512	CLA	C2C-C1C-NC	4.00	114.18	109.98
23	B	616	CLA	C4C-C3C-C2C	-4.00	101.07	106.89
23	d	403	CLA	C2C-C1C-NC	4.00	114.18	109.98
33	c	520	LMG	O6-C5-C4	4.00	116.90	109.70
23	c	511	CLA	C3B-C4B-NB	4.00	114.10	110.53
23	B	614	CLA	CHD-C1D-ND	-3.99	119.18	124.80
34	b	625	HTG	C1-O5-C5	3.99	119.73	112.56
35	C	518[A]	DGD	O2G-C1B-C2B	3.99	120.12	111.48
23	b	607	CLA	C3C-C4C-NC	3.99	115.55	110.43
23	b	604	CLA	C3C-C4C-NC	3.99	115.54	110.43
23	B	609	CLA	C3B-C2B-C1B	-3.98	102.47	107.17
23	b	601	CLA	C2C-C1C-NC	3.97	114.15	109.98
23	b	613	CLA	C1C-C2C-C3C	-3.97	102.80	106.98
23	D	402[B]	CLA	C2B-C1B-NB	3.97	114.44	110.33
23	C	509	CLA	C3B-C4B-NB	3.97	114.07	110.53
23	c	508	CLA	C1D-CHD-C4C	-3.97	117.59	126.02
23	a	404[A]	CLA	O2D-CGD-CBD	3.96	118.16	111.23
23	b	607	CLA	CHD-C1D-ND	-3.96	119.22	124.80
35	C	517[A]	DGD	O2G-C1B-C2B	3.96	120.05	111.48
40	V	201	HEC	CBD-CAD-C3D	-3.96	101.58	112.53
23	A	404[A]	CLA	CAA-C2A-C3A	-3.96	102.30	113.00
23	b	602	CLA	CHD-C1D-ND	-3.96	119.23	124.80
26	a	411	SQD	O47-C7-C8	3.96	120.04	111.48
23	C	512	CLA	C3C-C4C-NC	3.95	115.49	110.43
23	c	508	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
23	B	605	CLA	C4-C3-C5	3.95	122.08	115.23
23	C	502	CLA	C3B-C2B-C1B	-3.95	102.52	107.17
23	b	605	CLA	C3C-C4C-NC	3.95	115.49	110.43
23	c	506	CLA	C2B-C1B-NB	3.95	114.42	110.33
23	B	601	CLA	C3C-C4C-NC	3.95	115.48	110.43
23	B	610	CLA	C3D-C4D-ND	3.94	116.40	109.99
23	c	511	CLA	C3C-C4C-NC	3.94	115.48	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	CLA	O2D-CGD-CBD	3.94	118.12	111.23
23	b	608	CLA	O2D-CGD-O1D	-3.94	116.18	123.85
23	a	406[B]	CLA	C1-C2-C3	-3.94	119.75	126.20
34	C	522	HTG	C1'-S1-C1	3.93	108.95	100.45
23	A	404[B]	CLA	CAA-C2A-C3A	-3.93	102.37	113.00
23	c	506	CLA	C3B-C4B-NB	3.93	114.04	110.53
23	B	613	CLA	C2B-C1B-NB	3.93	114.40	110.33
23	b	613	CLA	CHD-C1D-ND	-3.93	119.27	124.80
23	D	403	CLA	C1D-CHD-C4C	-3.93	117.67	126.02
23	A	404[A]	CLA	O2A-CGA-CBA	3.93	123.81	111.83
23	a	404[B]	CLA	C4B-C3B-C2B	-3.92	102.42	107.30
23	a	406[A]	CLA	C3C-C4C-NC	3.92	115.45	110.43
23	a	405[B]	CLA	CAA-C2A-C3A	-3.92	102.41	113.00
23	a	404[B]	CLA	O2D-CGD-CBD	3.91	118.07	111.23
25	c	514	BCR	C11-C10-C9	-3.91	121.79	127.28
23	B	601	CLA	C1D-CHD-C4C	-3.91	117.70	126.02
23	A	406[A]	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
23	D	403	CLA	CHD-C1D-ND	-3.91	119.30	124.80
32	A	419[B]	LHG	O7-C7-C8	3.91	119.94	111.48
23	C	508	CLA	C3D-C4D-ND	3.91	116.34	109.99
23	b	614	CLA	C1D-CHD-C4C	-3.91	117.71	126.02
23	c	507	CLA	C2B-C1B-NB	3.91	114.38	110.33
23	b	614	CLA	C1-C2-C3	-3.91	119.80	126.20
23	c	504	CLA	CHD-C1D-ND	-3.90	119.31	124.80
23	b	615	CLA	C3C-C4C-NC	3.90	115.43	110.43
23	c	501	CLA	C3C-C4C-NC	3.90	115.43	110.43
23	C	510	CLA	C1C-C2C-C3C	-3.90	102.88	106.98
23	D	402[A]	CLA	C3B-C4B-NB	3.90	114.01	110.53
23	B	607	CLA	C3C-C4C-NC	3.90	115.42	110.43
23	c	510	CLA	C3D-C4D-ND	3.89	116.32	109.99
34	V	202	HTG	C1-O5-C5	3.89	117.40	112.19
23	B	608	CLA	O2D-CGD-O1D	-3.89	116.28	123.85
23	B	615	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
23	C	509	CLA	C4A-NA-C1A	-3.89	104.91	106.68
31	B	627	LMT	C1'-O5'-C5'	-3.89	106.13	113.72
35	C	518[B]	DGD	O2G-C1B-C2B	3.89	119.89	111.48
23	b	612	CLA	C3D-C2D-C1D	-3.88	100.53	105.83
23	B	602	CLA	C3C-C4C-NC	3.88	115.40	110.43
23	c	503	CLA	O2D-CGD-CBD	3.88	118.02	111.23
23	b	612	CLA	C3B-C4B-NB	3.88	113.99	110.53
23	B	611	CLA	O2D-CGD-O1D	-3.88	116.31	123.85
23	B	614	CLA	C3D-C4D-ND	3.88	116.29	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	416	LMG	C8-O7-C10	-3.87	108.53	117.80
23	A	408	CLA	C1-C2-C3	-3.87	119.85	126.20
23	B	615	CLA	C2B-C1B-NB	3.87	114.34	110.33
33	Z	101	LMG	C1-C2-C3	3.87	118.15	110.01
35	c	516[B]	DGD	O2G-C1B-C2B	3.87	119.85	111.48
23	c	501	CLA	CMB-C2B-C1B	3.86	131.30	125.42
23	c	509	CLA	C1D-CHD-C4C	-3.86	117.81	126.02
23	b	603	CLA	CAA-C2A-C3A	-3.86	102.56	113.00
23	d	402[B]	CLA	C1D-CHD-C4C	-3.86	117.81	126.02
23	b	603	CLA	C3B-C4B-NB	3.86	113.98	110.53
26	A	410[B]	SQD	O47-C7-C8	3.86	119.83	111.48
23	B	613	CLA	C3B-C4B-NB	3.86	113.97	110.53
23	c	507	CLA	CMC-C2C-C1C	3.86	131.06	125.03
23	b	610	CLA	CAA-C2A-C3A	-3.86	102.57	113.00
23	B	615	CLA	CMC-C2C-C1C	3.86	131.06	125.03
23	B	613	CLA	CAC-C3C-C4C	3.86	129.81	124.79
23	C	506	CLA	C2B-C1B-NB	3.86	114.32	110.33
23	B	615	CLA	C1C-C2C-C3C	-3.85	102.93	106.98
34	b	622	HTG	O2-C2-C1	3.85	117.14	110.30
23	b	601	CLA	O2D-CGD-O1D	-3.85	116.36	123.85
23	b	609	CLA	CAC-C3C-C4C	3.85	129.79	124.79
23	B	602	CLA	C1D-CHD-C4C	-3.85	117.85	126.02
23	A	405[A]	CLA	CMC-C2C-C1C	3.84	131.04	125.03
23	b	609	CLA	C3B-C2B-C1B	-3.84	102.64	107.17
29	D	405[A]	PL9	C42-C43-C44	-3.84	118.83	127.62
23	c	511	CLA	C4A-NA-C1A	-3.84	104.93	106.68
23	B	616	CLA	C1D-CHD-C4C	-3.84	117.85	126.02
23	B	606	CLA	O2D-CGD-O1D	-3.84	116.37	123.85
26	A	410[B]	SQD	C1-C2-C3	-3.84	101.93	110.01
23	B	604	CLA	C3D-C4D-ND	3.84	116.23	109.99
23	c	509	CLA	C1C-C2C-C3C	-3.84	102.94	106.98
23	b	602	CLA	C1D-CHD-C4C	-3.84	117.86	126.02
23	b	616	CLA	C3C-C4C-NC	3.84	115.34	110.43
23	a	405[A]	CLA	CHD-C1D-ND	-3.83	119.41	124.80
23	C	505	CLA	C1-O2A-CGA	3.83	125.92	116.65
33	c	520	LMG	C3-C4-C5	3.83	117.17	110.23
23	C	511	CLA	C1-C2-C3	-3.82	119.94	126.20
23	B	608	CLA	CHD-C1D-ND	-3.82	119.43	124.80
23	C	511	CLA	C1D-CHD-C4C	-3.82	117.90	126.02
23	C	503	CLA	C3C-C4C-NC	3.82	115.32	110.43
23	A	408	CLA	C3B-C4B-NB	3.82	113.94	110.53
23	C	502	CLA	CHD-C1D-ND	-3.82	119.43	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	413[B]	PL9	C27-C28-C29	-3.82	118.89	127.62
23	b	605	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
23	b	603	CLA	O2D-CGD-O1D	-3.81	116.43	123.85
23	A	404[A]	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
23	B	615	CLA	C3B-C2B-C1B	-3.81	102.68	107.17
23	A	405[A]	CLA	CBC-CAC-C3C	-3.81	102.10	112.42
23	A	405[B]	CLA	C1D-CHD-C4C	-3.81	117.93	126.02
23	D	403	CLA	C3B-C2B-C1B	-3.80	102.69	107.17
23	A	405[B]	CLA	C4A-NA-C1A	-3.80	104.94	106.68
23	C	506	CLA	C1-C2-C3	-3.80	119.97	126.20
23	b	612	CLA	C4-C3-C5	3.80	121.83	115.23
23	B	606	CLA	C1D-CHD-C4C	-3.80	117.94	126.02
23	A	404[A]	CLA	O2D-CGD-CBD	3.80	117.88	111.23
23	b	610	CLA	C4A-NA-C1A	-3.80	104.94	106.68
25	h	101	BCR	C38-C26-C25	-3.80	120.34	124.48
23	d	402[A]	CLA	C2B-C1B-NB	3.80	114.26	110.33
23	b	616	CLA	CBC-CAC-C3C	-3.80	102.13	112.42
23	B	603	CLA	C1D-CHD-C4C	-3.80	117.95	126.02
23	a	405[A]	CLA	C3C-C4C-NC	3.80	115.29	110.43
23	B	608	CLA	C3C-C4C-NC	3.79	115.29	110.43
23	c	510	CLA	CHD-C1D-ND	-3.79	119.47	124.80
23	b	606	CLA	C1-C2-C3	-3.79	119.99	126.20
23	B	605	CLA	CHD-C4C-NC	3.79	130.10	124.23
23	a	408	CLA	C1D-CHD-C4C	-3.79	117.97	126.02
23	C	508	CLA	C3C-C4C-NC	3.79	115.28	110.43
32	d	413[A]	LHG	O8-C23-O10	-3.78	114.17	123.63
23	C	507	CLA	C3B-C4B-NB	3.78	113.91	110.53
23	C	508	CLA	C1D-CHD-C4C	-3.78	117.98	126.02
23	A	405[A]	CLA	CHD-C1D-ND	-3.78	119.48	124.80
23	B	615	CLA	C3C-C4C-NC	3.78	115.27	110.43
23	B	603	CLA	O2D-CGD-O1D	-3.78	116.49	123.85
23	B	602	CLA	CAA-C2A-C3A	-3.78	102.79	113.00
23	A	408	CLA	CAA-C2A-C3A	-3.78	102.79	113.00
24	A	416[B]	PHO	C1A-C2A-C3A	-3.78	99.25	102.84
38	F	102	HEM	C1B-NB-C4B	3.78	109.68	105.21
23	C	505	CLA	C2B-C1B-NB	3.78	114.24	110.33
32	L	101[B]	LHG	O7-C7-C8	3.77	119.65	111.48
24	A	407[B]	PHO	C1A-C2A-C3A	-3.77	99.25	102.84
23	C	514	CLA	C3B-C4B-NB	3.77	113.89	110.53
23	B	604	CLA	C2B-C1B-NB	3.77	114.23	110.33
38	F	102	HEM	CHD-C1D-ND	3.77	128.48	124.42
23	C	511	CLA	O2D-CGD-O1D	-3.77	116.52	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	C1D-CHD-C4C	-3.77	118.01	126.02
23	b	612	CLA	C1C-C2C-C3C	-3.77	103.02	106.98
23	B	609	CLA	CMB-C2B-C1B	3.76	131.15	125.42
26	a	410[B]	SQD	C1-O5-C5	-3.76	106.37	113.72
23	b	604	CLA	C3D-C4D-ND	3.76	116.10	109.99
23	b	602	CLA	CMC-C2C-C1C	3.76	130.91	125.03
23	B	609	CLA	C1C-C2C-C3C	-3.76	103.03	106.98
23	b	603	CLA	C1C-C2C-C3C	-3.76	103.03	106.98
25	H	101	BCR	C16-C17-C18	-3.76	122.01	127.28
23	B	606	CLA	C3B-C2B-C1B	-3.76	102.74	107.17
29	d	405[A]	PL9	C42-C43-C44	-3.76	119.02	127.62
32	D	407[B]	LHG	O7-C7-C8	3.75	119.60	111.48
29	A	414[B]	PL9	C37-C38-C39	-3.75	119.03	127.62
23	C	504	CLA	C1D-CHD-C4C	-3.75	118.04	126.02
23	B	601	CLA	C2C-C1C-NC	3.75	113.92	109.98
23	A	405[B]	CLA	CHD-C1D-ND	-3.75	119.52	124.80
23	c	512	CLA	C3C-C4C-NC	3.75	115.23	110.43
25	D	404	BCR	C10-C11-C12	-3.75	112.34	123.20
23	B	606	CLA	C3C-C4C-NC	3.75	115.23	110.43
26	B	620	SQD	C3-C4-C5	3.75	117.03	110.23
29	A	414[A]	PL9	C22-C23-C24	-3.74	119.05	127.62
23	c	510	CLA	C1C-C2C-C3C	-3.74	103.04	106.98
23	c	505	CLA	CAC-C3C-C4C	3.74	129.66	124.79
23	c	505	CLA	O2D-CGD-O1D	-3.74	116.57	123.85
23	B	611	CLA	C2A-C1A-CHA	-3.74	117.38	123.87
25	C	515	BCR	C7-C8-C9	-3.74	120.71	126.23
29	A	414[A]	PL9	C7-C3-C4	3.74	119.99	116.91
23	C	504	CLA	C1-C2-C3	-3.73	120.08	126.20
23	a	404[A]	CLA	CHD-C1D-ND	-3.73	119.55	124.80
23	b	613	CLA	O2A-CGA-O1A	-3.73	114.30	123.63
23	B	602	CLA	CMC-C2C-C1C	3.73	130.86	125.03
32	d	413[A]	LHG	O8-C23-C24	3.73	123.21	111.83
24	a	407[A]	PHO	O1D-CGD-CBD	-3.73	119.07	124.72
23	B	612	CLA	CAC-C3C-C4C	3.73	129.64	124.79
25	C	516	BCR	C7-C8-C9	-3.73	120.72	126.23
23	D	403	CLA	C3C-C4C-NC	3.73	115.20	110.43
26	A	412	SQD	O47-C7-C8	3.73	119.54	111.48
23	C	505	CLA	C3C-C4C-NC	3.73	115.20	110.43
25	c	514	BCR	C15-C14-C13	-3.72	122.05	127.28
29	A	414[B]	PL9	C22-C23-C24	-3.72	119.10	127.62
25	B	617	BCR	C33-C5-C6	-3.72	120.42	124.48
38	f	101	HEM	CHA-C4D-ND	3.72	128.97	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	C3C-C4C-NC	3.72	115.19	110.43
23	C	503	CLA	CHD-C1D-ND	-3.72	119.57	124.80
23	B	605	CLA	O2A-CGA-O1A	-3.72	114.33	123.63
23	B	616	CLA	C2B-C1B-NB	3.72	114.18	110.33
23	B	604	CLA	C3D-C2D-C1D	-3.72	100.76	105.83
23	D	402[B]	CLA	C1C-C2C-C3C	-3.72	103.07	106.98
23	c	510	CLA	C1D-CHD-C4C	-3.72	118.12	126.02
23	b	609	CLA	C4C-C3C-C2C	-3.71	101.49	106.89
23	d	402[B]	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
23	B	612	CLA	C4C-C3C-C2C	-3.71	101.49	106.89
26	a	410[A]	SQD	C44-O6-C1	-3.71	105.84	113.80
23	C	506	CLA	CAC-C3C-C4C	3.71	129.62	124.79
32	L	101[A]	LHG	O7-C7-C8	3.71	119.50	111.48
23	c	513	CLA	C3C-C4C-NC	3.71	115.18	110.43
23	a	404[B]	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
23	A	404[B]	CLA	C3C-C4C-NC	3.70	115.17	110.43
33	B	621	LMG	O8-C28-C29	3.70	123.13	111.83
23	B	611	CLA	C3C-C4C-NC	3.70	115.17	110.43
23	c	511	CLA	C2B-C1B-NB	3.70	114.16	110.33
32	b	629[B]	LHG	O7-C7-C8	3.70	119.48	111.48
23	d	402[B]	CLA	C2B-C1B-NB	3.70	114.16	110.33
23	b	602	CLA	CAA-C2A-C3A	-3.70	103.00	113.00
25	T	101	BCR	C11-C10-C9	-3.70	122.09	127.28
29	a	413[B]	PL9	C7-C8-C9	-3.70	120.47	126.83
23	c	507	CLA	C3C-C4C-NC	3.69	115.16	110.43
23	b	610	CLA	O2A-CGA-O1A	-3.69	114.39	123.63
23	b	606	CLA	C1C-C2C-C3C	-3.69	103.10	106.98
23	D	402[A]	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
23	d	402[B]	CLA	C1-C2-C3	-3.68	120.17	126.20
23	b	612	CLA	C1D-CHD-C4C	-3.68	118.20	126.02
23	b	609	CLA	CHD-C1D-ND	-3.67	119.63	124.80
23	b	608	CLA	C3B-C4B-NB	3.67	113.81	110.53
29	a	413[A]	PL9	C15-C14-C16	3.67	121.60	115.23
25	D	404	BCR	C28-C27-C26	-3.67	107.51	114.06
23	c	512	CLA	CHD-C1D-ND	-3.67	119.64	124.80
33	c	519	LMG	O7-C10-C11	3.67	119.42	111.48
23	A	406[B]	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
23	b	607	CLA	C2B-C1B-NB	3.67	114.13	110.33
26	B	620	SQD	C1-O5-C5	-3.67	106.56	113.72
23	a	406[A]	CLA	C1D-CHD-C4C	-3.67	118.23	126.02
23	b	605	CLA	C1-C2-C3	-3.66	120.19	126.20
23	B	605	CLA	C1-C2-C3	-3.66	120.19	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404[A]	CLA	O2A-CGA-O1A	-3.66	114.47	123.63
23	a	406[A]	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
23	b	614	CLA	CHD-C1D-ND	-3.66	119.65	124.80
23	c	509	CLA	C3C-C4C-NC	3.66	115.12	110.43
23	b	604	CLA	C2B-C1B-NB	3.66	114.12	110.33
31	B	627	LMT	C4B-C3B-C2B	3.66	117.25	110.83
23	c	507	CLA	O2D-CGD-O1D	-3.65	116.73	123.85
26	F	103	SQD	O8-S-C6	3.65	113.03	105.97
23	b	605	CLA	C1D-CHD-C4C	-3.65	118.26	126.02
23	A	405[A]	CLA	CAA-C2A-C3A	-3.65	103.13	113.00
23	B	610	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
23	C	509	CLA	C1D-CHD-C4C	-3.64	118.27	126.02
23	b	602	CLA	C2C-C1C-NC	3.64	113.81	109.98
23	C	506	CLA	CHD-C1D-ND	-3.64	119.68	124.80
23	B	614	CLA	O2D-CGD-O1D	-3.64	116.77	123.85
29	A	414[B]	PL9	C15-C14-C16	3.64	121.54	115.23
23	a	404[A]	CLA	C3C-C4C-NC	3.64	115.09	110.43
23	B	613	CLA	O2D-CGD-O1D	-3.64	116.77	123.85
35	c	516[A]	DGD	O2G-C1B-C2B	3.64	119.34	111.48
25	y	101	BCR	C38-C26-C25	-3.63	120.52	124.48
23	B	609	CLA	CBC-CAC-C3C	-3.63	102.57	112.42
23	b	613	CLA	O2D-CGD-CBD	3.63	117.58	111.23
23	d	402[A]	CLA	CHD-C1D-ND	-3.63	119.69	124.80
23	b	604	CLA	CHD-C1D-ND	-3.63	119.69	124.80
40	V	201	HEC	CBC-CAC-C3C	-3.63	120.18	127.43
38	F	102	HEM	CBD-CAD-C3D	-3.63	102.50	112.53
23	C	514	CLA	C1D-CHD-C4C	-3.63	118.31	126.02
23	c	508	CLA	C2B-C1B-NB	3.63	114.09	110.33
23	B	605	CLA	C1C-C2C-C3C	-3.63	103.17	106.98
23	B	610	CLA	CMB-C2B-C1B	3.63	130.94	125.42
29	d	405[A]	PL9	C37-C38-C39	-3.63	119.33	127.62
23	c	510	CLA	CMC-C2C-C1C	3.62	130.70	125.03
23	B	612	CLA	CHD-C1D-ND	-3.62	119.70	124.80
23	b	613	CLA	C3B-C4B-NB	3.62	113.76	110.53
23	c	502	CLA	C1D-CHD-C4C	-3.62	118.33	126.02
23	C	513	CLA	CHD-C1D-ND	-3.62	119.71	124.80
23	C	504	CLA	C3C-C4C-NC	3.62	115.06	110.43
25	T	101	BCR	C15-C16-C17	-3.62	116.12	123.52
23	c	505	CLA	C4C-C3C-C2C	-3.61	101.63	106.89
23	c	502	CLA	C1-C2-C3	-3.61	120.28	126.20
23	a	404[A]	CLA	C1-C2-C3	-3.61	120.28	126.20
31	B	629	LMT	O1'-C1'-C2'	3.61	113.75	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	C3B-C4B-NB	3.61	113.75	110.53
23	C	503	CLA	C1D-CHD-C4C	-3.61	118.36	126.02
23	d	402[A]	CLA	O2A-CGA-CBA	3.61	122.83	111.83
23	B	607	CLA	CHD-C1D-ND	-3.60	119.73	124.80
25	C	515	BCR	C15-C14-C13	-3.60	122.22	127.28
23	c	502	CLA	CMC-C2C-C1C	3.60	130.66	125.03
29	a	413[B]	PL9	C15-C14-C16	3.60	121.48	115.23
23	c	506	CLA	CAC-C3C-C4C	3.60	129.48	124.79
23	B	607	CLA	O2D-CGD-O1D	-3.60	116.84	123.85
23	A	406[B]	CLA	C1C-C2C-C3C	-3.60	103.20	106.98
23	A	405[A]	CLA	C1D-CHD-C4C	-3.59	118.38	126.02
23	b	612	CLA	CAC-C3C-C4C	3.59	129.46	124.79
23	B	607	CLA	CBC-CAC-C3C	-3.59	102.68	112.42
23	a	405[B]	CLA	CHD-C1D-ND	-3.59	119.75	124.80
25	b	619	BCR	C24-C23-C22	-3.59	120.92	126.23
33	C	520	LMG	O7-C10-C11	3.59	119.25	111.48
23	d	402[A]	CLA	C3B-C4B-NB	3.59	113.73	110.53
23	d	403	CLA	C3C-C4C-NC	3.59	115.03	110.43
23	c	509	CLA	CHD-C1D-ND	-3.59	119.75	124.80
23	B	608	CLA	C1C-C2C-C3C	-3.59	103.21	106.98
23	c	504	CLA	C1D-CHD-C4C	-3.59	118.39	126.02
23	b	614	CLA	CMB-C2B-C1B	3.59	130.88	125.42
23	b	608	CLA	C1D-CHD-C4C	-3.59	118.40	126.02
23	B	603	CLA	C1C-C2C-C3C	-3.58	103.21	106.98
29	a	413[A]	PL9	C30-C29-C31	3.58	121.44	115.23
23	A	406[A]	CLA	C3C-C4C-NC	3.58	115.02	110.43
23	b	614	CLA	C1C-C2C-C3C	-3.58	103.22	106.98
23	C	512	CLA	C3D-C4D-ND	3.58	115.81	109.99
23	a	406[B]	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
23	A	406[A]	CLA	C1D-CHD-C4C	-3.57	118.42	126.02
23	B	611	CLA	CHB-C4A-NA	3.57	129.56	124.40
23	b	611	CLA	C3B-C4B-NB	3.57	113.72	110.53
23	B	610	CLA	CHD-C1D-ND	-3.57	119.78	124.80
23	d	403	CLA	C1C-C2C-C3C	-3.57	103.23	106.98
35	c	517[A]	DGD	O2G-C1B-C2B	3.56	119.19	111.48
29	A	414[A]	PL9	C15-C14-C16	3.56	121.41	115.23
25	d	404	BCR	C15-C14-C13	-3.56	122.28	127.28
29	D	405[B]	PL9	C10-C9-C11	3.56	121.41	115.23
23	b	615	CLA	C1C-C2C-C3C	-3.56	103.23	106.98
23	b	605	CLA	CHD-C4C-NC	3.56	129.75	124.23
23	b	610	CLA	C4C-C3C-C2C	-3.56	101.71	106.89
23	A	404[B]	CLA	CHD-C1D-ND	-3.56	119.80	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	v	201	HEC	C4D-ND-C1D	3.56	111.62	105.82
23	b	604	CLA	C3B-C4B-NB	3.56	113.70	110.53
33	c	520	LMG	C9-C8-C7	-3.56	103.50	111.78
31	A	417	LMT	O5B-C5B-C4B	3.55	116.10	109.70
35	c	517[B]	DGD	O2G-C1B-C2B	3.55	119.16	111.48
23	b	615	CLA	CHD-C1D-ND	-3.55	119.81	124.80
23	A	404[A]	CLA	C3C-C4C-NC	3.55	114.98	110.43
23	b	604	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
26	A	410[A]	SQD	O47-C7-C8	3.55	119.16	111.48
23	c	502	CLA	C3B-C4B-NB	3.55	113.70	110.53
23	A	406[B]	CLA	C3C-C4C-NC	3.55	114.97	110.43
23	C	508	CLA	CMB-C2B-C1B	3.55	130.82	125.42
23	c	506	CLA	C3C-C4C-NC	3.55	114.97	110.43
23	B	616	CLA	CAC-C3C-C4C	3.55	129.40	124.79
23	c	506	CLA	C1D-CHD-C4C	-3.54	118.49	126.02
23	B	610	CLA	O2A-CGA-O1A	-3.54	114.76	123.63
23	a	408	CLA	O2D-CGD-O1D	-3.54	116.95	123.85
23	c	502	CLA	C3C-C4C-NC	3.54	114.97	110.43
23	b	611	CLA	C1-C2-C3	-3.54	120.40	126.20
23	B	608	CLA	CAC-C3C-C4C	3.54	129.39	124.79
29	a	413[A]	PL9	C27-C28-C29	-3.54	119.53	127.62
25	Y	101	BCR	C16-C17-C18	-3.53	122.32	127.28
29	A	414[A]	PL9	C37-C38-C39	-3.53	119.54	127.62
23	D	403	CLA	CMB-C2B-C1B	3.53	130.80	125.42
23	B	610	CLA	C1D-CHD-C4C	-3.53	118.52	126.02
23	C	502	CLA	C1C-C2C-C3C	-3.53	103.27	106.98
23	c	502	CLA	CBC-CAC-C3C	-3.52	102.87	112.42
23	B	606	CLA	CHD-C4C-NC	3.52	129.69	124.23
29	A	414[A]	PL9	C27-C28-C29	-3.52	119.56	127.62
23	c	504	CLA	C4C-C3C-C2C	-3.52	101.77	106.89
26	a	410[A]	SQD	O9-S-C6	3.52	112.01	106.76
23	d	402[A]	CLA	C1-C2-C3	-3.52	120.43	126.20
23	B	609	CLA	C1D-CHD-C4C	-3.52	118.54	126.02
23	b	615	CLA	O2D-CGD-CBD	3.52	117.38	111.23
23	C	507	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
23	a	404[B]	CLA	C3C-C4C-NC	3.52	114.93	110.43
23	B	603	CLA	CAA-C2A-C3A	-3.51	103.50	113.00
23	B	613	CLA	C4A-NA-C1A	-3.51	105.08	106.68
29	d	405[B]	PL9	C42-C43-C44	-3.51	119.59	127.62
23	C	513	CLA	C2C-C1C-NC	3.51	113.67	109.98
23	c	511	CLA	C4-C3-C5	3.51	121.32	115.23
32	d	407[B]	LHG	O7-C7-C8	3.51	119.07	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	C1C-C2C-C3C	-3.51	103.29	106.98
23	d	402[B]	CLA	O2A-CGA-CBA	3.51	122.53	111.83
23	b	606	CLA	C3B-C4B-NB	3.51	113.66	110.53
23	B	612	CLA	O2A-CGA-O1A	-3.51	114.86	123.63
23	c	501	CLA	C1-C2-C3	-3.50	120.45	126.20
23	B	605	CLA	C4C-C3C-C2C	-3.50	101.79	106.89
29	d	405[B]	PL9	C7-C3-C4	3.50	119.79	116.91
33	C	521	LMG	C3-C4-C5	3.50	116.58	110.23
23	c	511	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
23	b	613	CLA	O2A-CGA-CBA	3.50	122.50	111.83
23	A	404[A]	CLA	O2A-CGA-O1A	-3.50	114.89	123.63
23	a	405[A]	CLA	C3B-C4B-NB	3.49	113.65	110.53
32	A	419[A]	LHG	O7-C7-C8	3.49	119.04	111.48
23	d	402[B]	CLA	C3B-C4B-NB	3.49	113.65	110.53
32	d	413[B]	LHG	O7-C7-C8	3.49	119.03	111.48
23	C	502	CLA	CBC-CAC-C3C	-3.49	102.96	112.42
23	b	612	CLA	CMC-C2C-C1C	3.49	130.48	125.03
23	b	616	CLA	CHD-C4C-NC	3.49	129.64	124.23
23	A	404[B]	CLA	O2A-CGA-CBA	3.49	122.46	111.83
29	d	405[A]	PL9	C40-C39-C41	3.49	121.28	115.23
25	T	101	BCR	C16-C17-C18	-3.48	122.39	127.28
23	C	505	CLA	C4B-C3B-C2B	-3.48	102.97	107.30
23	d	403	CLA	CMB-C2B-C1B	3.48	130.72	125.42
23	C	508	CLA	C1C-C2C-C3C	-3.48	103.32	106.98
23	a	405[B]	CLA	C3C-C4C-NC	3.48	114.89	110.43
23	a	404[A]	CLA	O2A-CGA-CBA	3.48	122.45	111.83
23	c	505	CLA	C1D-CHD-C4C	-3.48	118.62	126.02
23	A	404[B]	CLA	C3B-C2B-C1B	-3.48	103.07	107.17
23	b	613	CLA	C3D-C4D-ND	3.48	115.64	109.99
23	a	406[B]	CLA	C3C-C4C-NC	3.47	114.88	110.43
23	c	504	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
23	C	513	CLA	CHD-C4C-NC	3.47	129.62	124.23
23	B	614	CLA	C1-C2-C3	-3.47	120.52	126.20
23	C	507	CLA	C1D-CHD-C4C	-3.47	118.65	126.02
24	A	416[A]	PHO	C1A-C2A-C3A	-3.46	99.54	102.84
23	C	512	CLA	C1C-C2C-C3C	-3.46	103.34	106.98
23	B	614	CLA	CMC-C2C-C1C	3.46	130.44	125.03
23	A	405[A]	CLA	C3C-C4C-NC	3.46	114.86	110.43
29	a	413[A]	PL9	C37-C38-C39	-3.46	119.71	127.62
23	c	502	CLA	CMD-C2D-C1D	3.46	130.82	124.73
23	B	614	CLA	C3C-C4C-NC	3.46	114.86	110.43
25	c	515	BCR	C32-C1-C6	-3.46	104.82	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	CLA	C3C-C4C-NC	3.46	114.86	110.43
23	A	405[B]	CLA	C4B-C3B-C2B	-3.45	103.01	107.30
23	a	405[B]	CLA	CHD-C4C-NC	3.45	129.59	124.23
23	a	405[A]	CLA	CHD-C4C-NC	3.45	129.58	124.23
23	b	610	CLA	CHD-C1D-ND	-3.45	119.95	124.80
23	B	613	CLA	C4-C3-C5	3.45	121.21	115.23
23	B	606	CLA	CMC-C2C-C1C	3.45	130.42	125.03
23	A	405[B]	CLA	C3C-C4C-NC	3.45	114.84	110.43
31	M	101	LMT	C1'-O5'-C5'	-3.44	107.00	113.72
23	D	402[A]	CLA	C2B-C1B-NB	3.44	113.90	110.33
23	B	611	CLA	C1-C2-C3	-3.44	120.56	126.20
23	b	613	CLA	C1D-CHD-C4C	-3.44	118.70	126.02
23	A	408	CLA	C1D-CHD-C4C	-3.44	118.71	126.02
23	b	608	CLA	CBC-CAC-C3C	-3.44	103.09	112.42
23	C	513	CLA	C4-C3-C5	3.44	121.20	115.23
23	c	511	CLA	C1C-C2C-C3C	-3.44	103.36	106.98
23	c	513	CLA	C1C-C2C-C3C	-3.44	103.37	106.98
23	c	510	CLA	C3B-C4B-NB	3.43	113.59	110.53
23	c	511	CLA	C1-C2-C3	-3.43	120.58	126.20
23	a	404[B]	CLA	CAA-C2A-C3A	-3.43	103.73	113.00
23	D	402[B]	CLA	C3B-C4B-NB	3.43	113.59	110.53
24	a	407[A]	PHO	C1A-C2A-C3A	-3.43	99.58	102.84
32	A	419[A]	LHG	O8-C23-C24	3.42	122.28	111.83
23	A	405[B]	CLA	C3B-C4B-NB	3.42	113.59	110.53
23	C	512	CLA	CAC-C3C-C4C	3.42	129.24	124.79
23	c	508	CLA	C3B-C4B-NB	3.42	113.58	110.53
23	d	402[B]	CLA	CAC-C3C-C4C	3.42	129.24	124.79
23	c	503	CLA	CMB-C2B-C1B	3.42	130.62	125.42
23	c	505	CLA	CHD-C1D-ND	-3.42	120.00	124.80
23	a	408	CLA	CHD-C1D-ND	-3.42	120.00	124.80
23	c	511	CLA	CHD-C4C-NC	3.41	129.52	124.23
32	d	407[A]	LHG	O7-C7-C8	3.41	118.86	111.48
23	a	404[A]	CLA	C3B-C4B-NB	3.41	113.58	110.53
23	C	503	CLA	CMB-C2B-C1B	3.41	130.61	125.42
23	A	406[A]	CLA	CAA-C2A-C3A	-3.41	103.78	113.00
25	B	617	BCR	C31-C1-C6	-3.41	104.90	110.24
23	C	506	CLA	C4-C3-C5	3.41	121.15	115.23
23	B	612	CLA	O2A-CGA-CBA	3.40	122.22	111.83
25	D	404	BCR	C29-C30-C25	3.40	115.38	110.44
23	b	609	CLA	C4B-C3B-C2B	-3.40	103.07	107.30
25	b	619	BCR	C38-C26-C25	-3.40	120.77	124.48
23	D	403	CLA	C1C-C2C-C3C	-3.40	103.40	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	605	CLA	C4-C3-C5	3.40	121.13	115.23
23	B	606	CLA	C2B-C1B-NB	3.40	113.85	110.33
23	B	607	CLA	C1D-CHD-C4C	-3.40	118.80	126.02
23	C	502	CLA	C3C-C4C-NC	3.40	114.78	110.43
23	A	406[A]	CLA	C3B-C4B-NB	3.40	113.56	110.53
25	d	404	BCR	C38-C26-C25	-3.40	120.78	124.48
23	B	612	CLA	C1D-CHD-C4C	-3.40	118.80	126.02
23	A	404[A]	CLA	C1-C2-C3	-3.40	120.63	126.20
23	c	505	CLA	CMC-C2C-C1C	3.40	130.34	125.03
23	B	610	CLA	CAA-CBA-CGA	-3.39	103.57	113.21
23	a	406[B]	CLA	C1D-CHD-C4C	-3.39	118.81	126.02
23	A	404[B]	CLA	C1C-C2C-C3C	-3.39	103.41	106.98
23	B	601	CLA	C4C-C3C-C2C	-3.39	101.95	106.89
23	b	611	CLA	C1D-CHD-C4C	-3.39	118.82	126.02
23	d	402[B]	CLA	CHD-C1D-ND	-3.39	120.03	124.80
23	b	603	CLA	CMA-C3A-C2A	-3.39	100.89	113.98
29	D	405[B]	PL9	C27-C28-C29	-3.38	119.88	127.62
33	C	520	LMG	O8-C28-C29	3.38	122.15	111.83
23	C	507	CLA	C3C-C4C-NC	3.38	114.76	110.43
23	B	614	CLA	CHD-C4C-NC	3.38	129.47	124.23
23	c	506	CLA	C4B-C3B-C2B	-3.38	103.10	107.30
23	a	404[B]	CLA	C1-C2-C3	-3.38	120.66	126.20
23	c	501	CLA	C1C-C2C-C3C	-3.38	103.43	106.98
23	C	504	CLA	C4-C3-C5	3.37	121.09	115.23
26	A	410[A]	SQD	C44-O6-C1	-3.37	106.57	113.80
23	b	614	CLA	C3B-C4B-NB	3.37	113.54	110.53
23	B	613	CLA	O2A-CGA-O1A	-3.37	115.20	123.63
23	C	506	CLA	C4C-C3C-C2C	-3.37	101.99	106.89
23	d	402[B]	CLA	C4C-C3C-C2C	-3.37	101.99	106.89
23	b	616	CLA	C1C-C2C-C3C	-3.36	103.44	106.98
23	C	504	CLA	CMB-C2B-C1B	3.36	130.54	125.42
23	C	509	CLA	C4C-C3C-C2C	-3.36	102.00	106.89
23	b	609	CLA	C3B-C4B-NB	3.36	113.53	110.53
23	B	613	CLA	C1C-C2C-C3C	-3.36	103.45	106.98
29	a	413[A]	PL9	C17-C18-C19	-3.36	119.94	127.62
23	B	613	CLA	C1D-CHD-C4C	-3.36	118.89	126.02
23	B	607	CLA	C4-C3-C5	3.36	121.05	115.23
23	D	402[A]	CLA	C4C-C3C-C2C	-3.35	102.01	106.89
23	A	404[A]	CLA	CAC-C3C-C4C	3.35	129.15	124.79
38	f	101	HEM	CBD-CAD-C3D	-3.35	103.26	112.53
23	C	510	CLA	O2A-CGA-O1A	-3.35	115.24	123.63
40	V	201	HEC	C4D-ND-C1D	3.35	111.28	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	O2A-CGA-O1A	-3.35	115.25	123.63
23	B	611	CLA	C4A-NA-C1A	-3.35	105.15	106.68
29	D	405[A]	PL9	C17-C18-C19	-3.35	119.96	127.62
25	h	101	BCR	C33-C5-C6	-3.35	120.83	124.48
32	b	629[A]	LHG	O7-C7-C8	3.34	118.72	111.48
23	c	513	CLA	CAC-C3C-C4C	3.34	129.14	124.79
23	C	514	CLA	CMC-C2C-C1C	3.34	130.26	125.03
23	d	403	CLA	C1D-CHD-C4C	-3.34	118.92	126.02
25	D	404	BCR	C38-C26-C25	-3.34	120.84	124.48
23	b	608	CLA	C1-C2-C3	-3.34	120.73	126.20
26	B	620	SQD	O48-C23-C24	3.34	122.01	111.83
23	C	502	CLA	CAC-C3C-C4C	3.34	129.13	124.79
23	C	505	CLA	O2D-CGD-O1D	-3.34	117.36	123.85
32	d	406[B]	LHG	O7-C7-C8	3.34	118.70	111.48
25	b	617	BCR	C29-C30-C25	3.33	115.28	110.44
23	C	507	CLA	CAC-C3C-C4C	3.33	129.13	124.79
23	A	404[A]	CLA	CAA-C2A-C1A	-3.33	101.05	111.97
29	a	413[B]	PL9	C37-C38-C39	-3.33	120.00	127.62
23	C	510	CLA	C1D-CHD-C4C	-3.33	118.94	126.02
23	c	512	CLA	CMB-C2B-C1B	3.33	130.49	125.42
23	b	614	CLA	CAC-C3C-C4C	3.33	129.12	124.79
23	d	402[A]	CLA	C1D-CHD-C4C	-3.33	118.95	126.02
23	b	616	CLA	CMB-C2B-C1B	3.33	130.48	125.42
23	C	502	CLA	C4B-C3B-C2B	-3.33	103.17	107.30
23	a	404[A]	CLA	CAA-C2A-C1A	-3.32	101.10	111.97
23	b	607	CLA	C4B-C3B-C2B	-3.32	103.18	107.30
23	B	602	CLA	CHD-C1D-ND	-3.32	120.14	124.80
23	C	508	CLA	CBC-CAC-C3C	-3.31	103.44	112.42
29	a	413[B]	PL9	C30-C29-C31	3.31	120.98	115.23
31	b	627	LMT	C3'-C4'-C5'	-3.31	103.60	110.93
26	a	410[A]	SQD	C45-O47-C7	-3.31	109.88	117.80
23	B	613	CLA	CHD-C1D-ND	-3.31	120.15	124.80
23	A	406[B]	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
23	A	408	CLA	C4C-C3C-C2C	-3.30	102.08	106.89
23	B	603	CLA	C4C-C3C-C2C	-3.30	102.08	106.89
23	B	605	CLA	CED-O2D-CGD	3.30	123.40	115.92
23	B	601	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
23	a	404[A]	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
23	B	608	CLA	C1D-CHD-C4C	-3.30	119.02	126.02
23	b	603	CLA	C4B-C3B-C2B	-3.29	103.21	107.30
23	a	405[B]	CLA	C3B-C4B-NB	3.29	113.47	110.53
23	b	607	CLA	CAA-C2A-C3A	-3.29	104.11	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	b	622	HTG	O5-C5-C4	3.29	115.63	109.70
29	d	405[B]	PL9	C37-C38-C39	-3.29	120.10	127.62
23	b	601	CLA	C1-O2A-CGA	3.29	124.60	116.65
23	C	513	CLA	C4C-C3C-C2C	-3.29	102.11	106.89
26	A	410[B]	SQD	C44-O6-C1	-3.28	106.75	113.80
23	c	506	CLA	CHC-C1C-C2C	-3.28	117.62	126.95
23	A	406[B]	CLA	CMB-C2B-C1B	3.28	130.41	125.42
38	f	101	HEM	CHD-C4C-NC	3.28	128.02	124.45
23	b	602	CLA	C1-C2-C3	-3.28	120.82	126.20
23	C	504	CLA	C1C-C2C-C3C	-3.27	103.54	106.98
23	B	610	CLA	C4C-C3C-C2C	-3.27	102.13	106.89
23	b	612	CLA	C4C-C3C-C2C	-3.27	102.13	106.89
26	A	410[A]	SQD	O9-S-C6	3.27	111.64	106.76
23	A	406[A]	CLA	O2A-CGA-O1A	-3.27	115.45	123.63
23	D	402[B]	CLA	C1D-CHD-C4C	-3.27	119.07	126.02
32	A	419[B]	LHG	C5-O7-C7	-3.27	109.97	117.80
23	c	503	CLA	C4C-C3C-C2C	-3.27	102.13	106.89
24	a	415[A]	PHO	C4-C3-C5	3.27	120.90	115.23
24	a	415[B]	PHO	C4-C3-C5	3.27	120.90	115.23
26	F	103	SQD	C44-O6-C1	-3.27	106.79	113.80
23	B	615	CLA	CED-O2D-CGD	3.27	123.33	115.92
23	A	406[B]	CLA	O2A-CGA-O1A	-3.26	115.46	123.63
23	b	612	CLA	C2B-C1B-NB	3.26	113.71	110.33
23	d	402[A]	CLA	C4-C3-C5	3.26	120.89	115.23
23	b	612	CLA	CHD-C1D-ND	-3.26	120.21	124.80
23	b	606	CLA	CHD-C4C-NC	3.26	129.28	124.23
26	a	411	SQD	O48-C23-C24	3.26	121.77	111.83
23	C	512	CLA	CMC-C2C-C1C	3.26	130.12	125.03
23	B	610	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
23	b	601	CLA	CHD-C4C-NC	3.25	129.27	124.23
23	b	616	CLA	O2A-CGA-O1A	-3.25	115.51	123.63
33	c	519	LMG	O1-C7-C8	-3.25	102.92	110.82
23	B	615	CLA	O2D-CGD-CBD	3.25	116.91	111.23
24	a	407[A]	PHO	O2A-CGA-O1A	-3.25	115.51	123.63
29	A	414[B]	PL9	C27-C28-C29	-3.25	120.19	127.62
23	B	606	CLA	O2A-CGA-O1A	-3.24	115.51	123.63
29	a	413[B]	PL9	C17-C18-C19	-3.24	120.20	127.62
23	A	404[B]	CLA	CHC-C1C-C2C	-3.24	117.73	126.95
23	a	408	CLA	CAA-C2A-C3A	-3.24	104.23	113.00
23	C	506	CLA	C1C-C2C-C3C	-3.24	103.57	106.98
35	C	517[B]	DGD	O2G-C1B-C2B	3.24	118.49	111.48
23	c	512	CLA	O2A-CGA-CBA	3.24	121.72	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	102	BCR	C24-C23-C22	-3.24	121.44	126.23
23	c	512	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
23	b	616	CLA	CHD-C1D-ND	-3.24	120.25	124.80
23	A	404[B]	CLA	C4C-C3C-C2C	-3.23	102.18	106.89
23	B	613	CLA	C4C-C3C-C2C	-3.23	102.19	106.89
23	B	604	CLA	C3B-C4B-NB	3.23	113.41	110.53
23	C	510	CLA	C4C-C3C-C2C	-3.23	102.19	106.89
29	a	413[B]	PL9	C42-C43-C44	-3.23	120.23	127.62
23	b	611	CLA	C4C-C3C-C2C	-3.23	102.19	106.89
23	c	502	CLA	CHD-C1D-ND	-3.23	120.26	124.80
23	b	615	CLA	C11-C10-C8	-3.23	105.24	115.97
23	c	509	CLA	CAC-C3C-C4C	3.22	128.99	124.79
23	c	512	CLA	C1C-C2C-C3C	-3.22	103.59	106.98
23	A	406[A]	CLA	C4B-C3B-C2B	-3.22	103.29	107.30
23	A	404[B]	CLA	CAC-C3C-C4C	3.22	128.98	124.79
23	d	402[A]	CLA	O2A-CGA-O1A	-3.22	115.57	123.63
23	D	403	CLA	CMC-C2C-C1C	3.22	130.06	125.03
23	C	511	CLA	CHC-C1C-C2C	-3.22	117.81	126.95
29	D	405[A]	PL9	C25-C24-C26	3.22	120.81	115.23
23	a	406[A]	CLA	CAA-C2A-C3A	-3.22	104.31	113.00
24	a	407[A]	PHO	O2A-CGA-CBA	3.21	121.63	111.83
35	h	102	DGD	O1G-C1A-O1A	-3.21	115.59	123.63
38	f	101	HEM	CHD-C1D-ND	3.21	127.88	124.42
29	A	414[B]	PL9	C7-C3-C2	-3.21	119.61	123.39
23	C	510	CLA	O2A-CGA-CBA	3.21	121.62	111.83
23	c	501	CLA	C4C-C3C-C2C	-3.21	102.22	106.89
23	B	607	CLA	C3B-C4B-NB	3.20	113.39	110.53
23	b	604	CLA	C4B-C3B-C2B	-3.20	103.32	107.30
32	d	413[B]	LHG	O8-C23-C24	3.20	121.60	111.83
23	c	509	CLA	CHC-C1C-C2C	-3.20	117.85	126.95
34	o	301	HTG	O5-C1-C2	3.20	114.73	110.32
23	D	402[A]	CLA	C4B-C3B-C2B	-3.20	103.33	107.30
23	B	615	CLA	C4-C3-C5	3.20	120.78	115.23
23	b	607	CLA	CHC-C1C-C2C	-3.20	117.86	126.95
23	C	502	CLA	C3B-C4B-NB	3.20	113.38	110.53
23	b	605	CLA	CMB-C2B-C1B	3.19	130.28	125.42
33	Z	101	LMG	C4-C3-C2	3.19	116.44	110.83
23	A	405[B]	CLA	CHC-C1C-C2C	-3.19	117.87	126.95
23	c	512	CLA	C4-C3-C5	3.19	120.77	115.23
23	A	405[B]	CLA	CAA-C2A-C3A	-3.19	104.37	113.00
23	B	614	CLA	CAC-C3C-C4C	3.19	128.94	124.79
29	A	414[A]	PL9	O1-C4-C3	-3.19	117.37	120.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	CHD-C4C-NC	3.19	129.18	124.23
23	c	510	CLA	C4-C3-C5	3.19	120.76	115.23
23	B	613	CLA	CMC-C2C-C1C	3.19	130.02	125.03
25	D	404	BCR	C37-C22-C23	3.19	122.96	118.09
23	c	509	CLA	C4B-C3B-C2B	-3.19	103.34	107.30
38	f	101	HEM	CAD-CBD-CGD	3.19	122.11	113.67
23	a	408	CLA	O2A-CGA-CBA	3.18	121.55	111.83
29	D	405[B]	PL9	C25-C24-C26	3.18	120.76	115.23
23	b	615	CLA	C4-C3-C5	3.18	120.75	115.23
33	z	101	LMG	O7-C10-C11	3.18	118.36	111.48
25	b	618	BCR	C15-C14-C13	-3.18	122.82	127.28
23	b	614	CLA	CHC-C1C-C2C	-3.18	117.91	126.95
23	a	405[B]	CLA	C4B-C3B-C2B	-3.18	103.35	107.30
23	a	406[A]	CLA	C3B-C4B-NB	3.18	113.37	110.53
23	B	604	CLA	C4C-C3C-C2C	-3.18	102.27	106.89
23	b	612	CLA	C2A-C1A-CHA	-3.18	118.35	123.87
23	a	404[B]	CLA	CHC-C1C-C2C	-3.17	117.93	126.95
23	b	608	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
23	C	503	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
26	A	412	SQD	O48-C23-C24	3.17	121.50	111.83
23	b	603	CLA	C2A-C1A-CHA	-3.17	118.36	123.87
25	c	514	BCR	C16-C17-C18	-3.17	122.83	127.28
23	C	510	CLA	C3B-C4B-NB	3.17	113.36	110.53
25	a	409	BCR	C40-C30-C25	-3.17	105.27	110.24
25	D	404	BCR	C16-C17-C18	-3.17	122.83	127.28
23	a	405[A]	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
35	C	519	DGD	O1G-C1A-C2A	3.17	121.49	111.83
23	C	507	CLA	CHC-C1C-C2C	-3.17	117.95	126.95
23	B	616	CLA	C1C-C2C-C3C	-3.17	103.65	106.98
32	D	406[B]	LHG	O7-C7-C8	3.17	118.33	111.48
29	A	414[B]	PL9	C17-C18-C19	-3.16	120.38	127.62
23	B	615	CLA	CAC-C3C-C4C	3.16	128.90	124.79
23	b	605	CLA	CMC-C2C-C1C	3.16	129.97	125.03
26	a	410[B]	SQD	C44-O6-C1	-3.16	107.02	113.80
35	h	102	DGD	O1G-C1A-C2A	3.16	121.47	111.83
23	d	402[A]	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
32	D	407[A]	LHG	O8-C23-C24	3.16	121.46	111.83
23	A	404[A]	CLA	C4B-C3B-C2B	-3.16	103.38	107.30
23	b	612	CLA	O2A-CGA-CBA	3.16	121.46	111.83
23	c	508	CLA	CMB-C2B-C1B	3.15	130.22	125.42
23	A	406[B]	CLA	CAA-C2A-C3A	-3.15	104.48	113.00
23	a	406[A]	CLA	CHD-C4C-NC	3.15	129.12	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	CHD-C4C-NC	3.15	129.12	124.23
23	a	408	CLA	C4-C3-C5	3.15	120.70	115.23
23	c	505	CLA	C1C-C2C-C3C	-3.15	103.67	106.98
25	C	515	BCR	C16-C17-C18	-3.15	122.86	127.28
38	f	101	HEM	C1B-NB-C4B	3.15	108.93	105.21
33	Z	101	LMG	O6-C1-C2	3.15	116.83	110.37
23	c	508	CLA	C4C-C3C-C2C	-3.14	102.31	106.89
23	c	505	CLA	CMB-C2B-C1B	3.14	130.21	125.42
23	c	503	CLA	C1C-C2C-C3C	-3.14	103.67	106.98
23	A	404[B]	CLA	C1-C2-C3	-3.14	121.05	126.20
23	B	609	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
29	d	405[A]	PL9	C22-C23-C24	-3.14	120.44	127.62
23	C	506	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
23	D	402[A]	CLA	C1D-CHD-C4C	-3.13	119.36	126.02
23	d	403	CLA	CAA-C2A-C3A	-3.13	104.53	113.00
38	F	102	HEM	CHB-C1B-NB	3.13	128.24	124.37
29	A	414[A]	PL9	C17-C18-C19	-3.13	120.45	127.62
25	d	404	BCR	C10-C11-C12	-3.13	114.12	123.20
23	D	402[B]	CLA	C4C-C3C-C2C	-3.13	102.33	106.89
23	b	614	CLA	C4C-C3C-C2C	-3.13	102.33	106.89
23	b	606	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
23	b	612	CLA	O2A-CGA-O1A	-3.13	115.80	123.63
23	c	513	CLA	C4C-C3C-C2C	-3.13	102.33	106.89
23	C	502	CLA	C1-O2A-CGA	3.13	124.23	116.65
29	a	413[B]	PL9	C22-C23-C24	-3.13	120.46	127.62
23	A	405[A]	CLA	CMB-C2B-C1B	3.13	130.18	125.42
23	c	513	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
23	b	615	CLA	C4C-C3C-C2C	-3.13	102.34	106.89
23	D	403	CLA	C4-C3-C5	3.13	120.66	115.23
23	c	511	CLA	C4C-C3C-C2C	-3.13	102.34	106.89
23	C	510	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
23	B	607	CLA	CMB-C2B-C1B	3.13	130.18	125.42
23	A	405[A]	CLA	CAC-C3C-C4C	3.13	128.86	124.79
23	b	602	CLA	CAC-C3C-C4C	3.13	128.86	124.79
23	C	511	CLA	CHD-C4C-NC	3.13	129.08	124.23
26	b	620	SQD	C3-C4-C5	3.12	115.90	110.23
29	a	413[A]	PL9	C25-C24-C26	3.12	120.65	115.23
23	c	508	CLA	CHD-C1D-ND	-3.12	120.41	124.80
23	A	405[A]	CLA	C3B-C4B-NB	3.12	113.32	110.53
26	B	620	SQD	O7-S-C6	3.12	111.42	106.76
23	b	614	CLA	O2A-CGA-O1A	-3.12	115.82	123.63
32	D	406[A]	LHG	O8-C23-O10	-3.12	115.82	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	CHD-C4C-NC	3.12	129.07	124.23
23	a	408	CLA	CAC-C3C-C4C	3.12	128.85	124.79
23	B	612	CLA	C4B-C3B-C2B	-3.12	103.42	107.30
23	C	510	CLA	CMC-C2C-C1C	3.12	129.91	125.03
29	a	413[B]	PL9	C25-C24-C26	3.12	120.64	115.23
23	c	510	CLA	CHD-C4C-NC	3.12	129.07	124.23
23	C	514	CLA	CBC-CAC-C3C	-3.12	103.96	112.42
23	B	609	CLA	O2A-CGA-CBA	3.12	121.34	111.83
33	C	521	LMG	O8-C28-C29	3.12	121.34	111.83
24	A	416[A]	PHO	C4-C3-C5	3.12	120.64	115.23
23	B	614	CLA	O2A-CGA-O1A	-3.12	115.83	123.63
23	C	502	CLA	CMC-C2C-C1C	3.11	129.90	125.03
25	t	102	BCR	C21-C20-C19	-3.11	114.18	123.20
23	C	512	CLA	C4-C3-C5	3.11	120.63	115.23
23	c	509	CLA	C1-O2A-CGA	3.11	124.19	116.65
23	b	602	CLA	CMB-C2B-C1B	3.11	130.16	125.42
35	h	102	DGD	O2G-C1B-C2B	3.11	118.21	111.48
29	a	413[A]	PL9	C42-C43-C44	-3.11	120.50	127.62
23	b	604	CLA	CMC-C2C-C1C	3.11	129.89	125.03
23	B	607	CLA	CAA-C2A-C3A	-3.11	104.60	113.00
23	b	603	CLA	C4C-C3C-C2C	-3.10	102.37	106.89
23	C	513	CLA	C1C-C2C-C3C	-3.10	103.72	106.98
23	B	603	CLA	O2A-CGA-O1A	-3.10	115.87	123.63
23	b	604	CLA	C1D-CHD-C4C	-3.10	119.43	126.02
32	D	407[A]	LHG	O7-C7-C8	3.10	118.19	111.48
25	T	101	BCR	C2-C1-C6	3.10	114.94	110.44
23	b	610	CLA	CMB-C2B-C1B	3.10	130.14	125.42
23	B	605	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
23	C	506	CLA	C3B-C4B-NB	3.10	113.30	110.53
23	C	512	CLA	C3B-C4B-NB	3.10	113.30	110.53
23	C	511	CLA	C3C-C4C-NC	3.09	114.39	110.43
23	a	406[A]	CLA	CMB-C2B-C1B	3.09	130.12	125.42
23	a	405[A]	CLA	CMA-C3A-C2A	-3.09	102.03	113.98
23	c	508	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
23	C	511	CLA	CBC-CAC-C3C	-3.09	104.05	112.42
23	B	614	CLA	CHC-C1C-C2C	-3.09	118.17	126.95
25	T	101	BCR	C12-C13-C14	-3.09	114.15	119.01
23	A	408	CLA	O2A-CGA-CBA	3.09	121.25	111.83
23	b	608	CLA	CAC-C3C-C4C	3.09	128.81	124.79
23	b	601	CLA	C1C-C2C-C3C	-3.08	103.74	106.98
23	b	601	CLA	C4-C3-C5	3.08	120.58	115.23
23	c	503	CLA	C1-C2-C3	-3.08	121.15	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
23	b	602	CLA	C2A-C1A-CHA	-3.08	118.52	123.87
23	D	403	CLA	CAC-C3C-C4C	3.08	128.79	124.79
23	a	404[A]	CLA	C4-C3-C5	3.08	120.57	115.23
23	b	610	CLA	CMC-C2C-C1C	3.07	129.84	125.03
23	C	512	CLA	C4C-C3C-C2C	-3.07	102.42	106.89
26	A	412	SQD	O8-S-C6	3.07	111.90	105.97
23	B	607	CLA	C2B-C1B-NB	3.07	113.51	110.33
23	d	403	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
23	c	503	CLA	CAC-C3C-C4C	3.07	128.78	124.79
34	b	622	HTG	C1'-S1-C1	3.07	107.07	100.45
23	b	613	CLA	C4C-C3C-C2C	-3.06	102.43	106.89
23	B	615	CLA	C3B-C4B-NB	3.06	113.27	110.53
23	D	403	CLA	C4B-C3B-C2B	-3.06	103.49	107.30
23	B	607	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
35	C	517[A]	DGD	C2G-O2G-C1B	-3.06	110.47	117.80
23	B	612	CLA	C11-C12-C13	-3.06	105.80	115.97
23	C	507	CLA	CMC-C2C-C1C	3.06	129.81	125.03
23	b	602	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
23	A	405[B]	CLA	CHD-C4C-NC	3.05	128.97	124.23
29	d	405[B]	PL9	C10-C9-C11	3.05	120.53	115.23
32	D	407[A]	LHG	O8-C23-O10	-3.05	115.99	123.63
23	b	615	CLA	CMB-C2B-C1B	3.05	130.07	125.42
32	a	420[A]	LHG	O7-C7-C8	3.05	118.08	111.48
23	c	507	CLA	C1D-CHD-C4C	-3.05	119.53	126.02
23	b	601	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
23	a	406[B]	CLA	CHD-C4C-NC	3.05	128.96	124.23
23	c	512	CLA	CHD-C4C-NC	3.05	128.96	124.23
23	B	604	CLA	CAC-C3C-C4C	3.05	128.76	124.79
24	A	416[B]	PHO	C4D-CHA-CBD	3.05	109.92	108.45
24	A	407[B]	PHO	C1-C2-C3	-3.05	121.21	126.20
32	a	420[B]	LHG	O7-C7-C8	3.05	118.07	111.48
23	A	405[B]	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
23	C	509	CLA	CAC-C3C-C4C	3.05	128.75	124.79
23	B	616	CLA	O2A-CGA-CBA	3.05	121.12	111.83
25	k	101	BCR	C7-C8-C9	-3.05	121.73	126.23
23	b	611	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
23	B	611	CLA	C4B-C3B-C2B	3.04	111.09	107.30
23	b	616	CLA	C4C-C3C-C2C	-3.04	102.46	106.89
23	a	404[B]	CLA	O2A-CGA-CBA	3.04	121.11	111.83
23	a	404[B]	CLA	CHD-C4C-NC	3.04	128.94	124.23
26	F	103	SQD	O7-S-C6	3.04	111.29	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402[B]	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
23	b	605	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
23	c	509	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
29	d	405[B]	PL9	C40-C39-C41	3.04	120.50	115.23
23	A	406[B]	CLA	C4B-C3B-C2B	-3.04	103.53	107.30
29	a	413[A]	PL9	C35-C34-C36	3.03	120.49	115.23
23	B	612	CLA	C1C-C2C-C3C	-3.03	103.79	106.98
32	d	413[A]	LHG	O7-C7-C8	3.03	118.04	111.48
23	A	408	CLA	CHC-C1C-C2C	-3.03	118.33	126.95
23	A	406[A]	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
24	A	407[B]	PHO	O1D-CGD-CBD	-3.03	120.13	124.72
23	B	616	CLA	C4B-C3B-C2B	-3.03	103.53	107.30
23	b	612	CLA	C4B-C3B-C2B	-3.03	103.53	107.30
23	A	406[B]	CLA	CHD-C4C-NC	3.03	128.93	124.23
23	B	603	CLA	C4-C3-C5	3.03	120.48	115.23
32	E	101[A]	LHG	O8-C23-C24	3.03	121.06	111.83
23	A	405[B]	CLA	CBC-CAC-C3C	-3.02	104.23	112.42
23	C	509	CLA	CHC-C1C-C2C	-3.02	118.36	126.95
23	b	610	CLA	C1C-C2C-C3C	-3.02	103.80	106.98
23	b	602	CLA	C1C-C2C-C3C	-3.02	103.81	106.98
23	c	509	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
23	a	405[B]	CLA	CBC-CAC-C3C	-3.02	104.24	112.42
23	C	506	CLA	CHC-C1C-C2C	-3.02	118.38	126.95
23	B	606	CLA	CBC-CAC-C3C	-3.02	104.25	112.42
25	H	101	BCR	C10-C11-C12	-3.01	114.47	123.20
23	a	406[B]	CLA	CMB-C2B-C1B	3.01	130.01	125.42
23	b	602	CLA	CMA-C3A-C4A	-3.01	103.67	111.77
25	B	619	BCR	C29-C30-C25	3.01	114.81	110.44
23	a	408	CLA	CMA-C3A-C2A	-3.01	102.34	113.98
23	C	508	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
23	B	602	CLA	C2A-C1A-CHA	-3.01	118.64	123.87
23	D	403	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
23	D	402[A]	CLA	O2A-CGA-CBA	3.01	121.00	111.83
35	c	518	DGD	O1G-C1A-C2A	3.01	121.00	111.83
23	B	603	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
23	B	608	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
23	B	615	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
23	A	406[B]	CLA	O2A-CGA-CBA	3.00	121.00	111.83
23	B	610	CLA	C3B-C4B-NB	3.00	113.21	110.53
23	D	402[A]	CLA	CAA-C2A-C3A	-3.00	104.89	113.00
23	d	402[A]	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
23	c	506	CLA	O2D-CGD-O1D	-3.00	118.01	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	406[B]	CLA	CAA-C2A-C3A	-3.00	104.89	113.00
26	a	410[B]	SQD	C1-C2-C3	-3.00	103.70	110.01
23	A	406[B]	CLA	C1-C2-C3	-3.00	121.28	126.20
23	c	501	CLA	C1D-CHD-C4C	-3.00	119.65	126.02
23	a	404[A]	CLA	CHC-C1C-C2C	-3.00	118.43	126.95
23	a	406[A]	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
23	A	405[B]	CLA	CMB-C2B-C1B	3.00	129.98	125.42
23	B	601	CLA	C1C-C2C-C3C	-3.00	103.83	106.98
33	C	501	LMG	O6-C1-O1	-3.00	102.97	110.04
31	B	627	LMT	O1'-C1'-C2'	2.99	112.82	108.27
35	H	102	DGD	O6E-C5E-C6E	2.99	113.86	106.44
23	C	503	CLA	C3B-C4B-NB	2.99	113.20	110.53
23	C	511	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
23	B	603	CLA	C3B-C4B-NB	2.99	113.20	110.53
23	C	504	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
23	c	503	CLA	C3B-C4B-NB	2.99	113.20	110.53
23	c	508	CLA	C4-C3-C5	2.98	120.41	115.23
32	E	101[B]	LHG	O8-C23-C24	2.98	120.93	111.83
23	B	609	CLA	C4B-C3B-C2B	-2.98	103.59	107.30
23	B	610	CLA	C4B-C3B-C2B	-2.98	103.59	107.30
24	a	415[A]	PHO	O2D-CGD-O1D	-2.98	118.05	123.85
23	B	608	CLA	CHC-C1C-C2C	-2.98	118.48	126.95
33	c	519	LMG	O8-C28-C29	2.98	120.92	111.83
24	a	415[A]	PHO	CBA-CAA-C2A	-2.98	105.00	113.78
23	D	402[B]	CLA	O2A-CGA-CBA	2.98	120.92	111.83
26	A	410[B]	SQD	O48-C23-C24	2.98	120.92	111.83
23	a	404[A]	CLA	CMA-C3A-C4A	-2.98	103.77	111.77
23	b	601	CLA	C4B-C3B-C2B	-2.98	103.60	107.30
23	b	606	CLA	O2A-CGA-O1A	-2.98	116.18	123.63
25	B	618	BCR	C2-C1-C6	2.98	114.76	110.44
23	B	602	CLA	C4B-C3B-C2B	-2.98	103.60	107.30
23	d	403	CLA	CBC-CAC-C3C	-2.98	104.35	112.42
29	a	413[A]	PL9	C10-C9-C11	2.97	120.39	115.23
23	D	403	CLA	CHD-C4C-NC	2.97	128.84	124.23
23	C	512	CLA	C1-C2-C3	-2.97	121.33	126.20
23	B	610	CLA	CHC-C1C-C2C	-2.97	118.50	126.95
26	a	410[A]	SQD	O47-C7-O49	-2.97	116.75	123.70
23	b	606	CLA	C4C-C3C-C2C	-2.97	102.56	106.89
23	d	402[A]	CLA	C4C-C3C-C2C	-2.97	102.56	106.89
38	f	101	HEM	CHB-C1B-NB	2.97	128.04	124.37
23	A	404[A]	CLA	CMC-C2C-C1C	2.97	129.68	125.03
23	A	404[B]	CLA	O2A-CGA-O1A	-2.97	116.20	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	402[A]	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
29	A	414[A]	PL9	C20-C19-C21	2.97	120.38	115.23
23	b	607	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
26	F	103	SQD	O48-C23-C24	2.97	120.88	111.83
26	F	103	SQD	C1-C2-C3	-2.97	103.77	110.01
29	A	414[B]	PL9	C20-C19-C21	2.97	120.38	115.23
23	B	604	CLA	CHC-C1C-C2C	-2.97	118.52	126.95
23	b	615	CLA	O2A-CGA-CBA	2.97	120.88	111.83
23	D	403	CLA	CMA-C3A-C2A	-2.96	102.52	113.98
23	c	508	CLA	CHC-C1C-C2C	-2.96	118.53	126.95
23	c	501	CLA	CAC-C3C-C4C	2.96	128.65	124.79
23	B	603	CLA	O2A-CGA-CBA	2.96	120.87	111.83
23	a	404[B]	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
29	D	405[A]	PL9	C37-C38-C39	-2.96	120.85	127.62
23	b	613	CLA	CHD-C4C-NC	2.96	128.81	124.23
23	c	511	CLA	C4B-C3B-C2B	-2.96	103.63	107.30
26	a	410[B]	SQD	C45-O47-C7	-2.96	110.72	117.80
23	b	608	CLA	C3C-C4C-NC	2.96	114.22	110.43
32	A	419[A]	LHG	C5-O7-C7	-2.95	110.73	117.80
33	m	101	LMG	C8-O7-C10	-2.95	110.73	117.80
25	a	409	BCR	C38-C26-C25	-2.95	121.27	124.48
34	C	522	HTG	C1-O5-C5	2.95	117.85	112.56
23	B	615	CLA	CHD-C4C-NC	2.95	128.80	124.23
23	a	405[B]	CLA	CHC-C1C-C2C	-2.95	118.57	126.95
23	c	502	CLA	CMB-C2B-C1B	2.95	129.91	125.42
33	z	101	LMG	O8-C28-C29	2.95	120.83	111.83
29	A	414[B]	PL9	C30-C29-C31	2.95	120.35	115.23
25	y	101	BCR	C21-C20-C19	-2.95	114.66	123.20
26	A	410[A]	SQD	O48-C23-C24	2.95	120.82	111.83
33	m	101	LMG	O8-C28-C29	2.95	120.82	111.83
23	c	511	CLA	O2A-CGA-CBA	2.95	120.82	111.83
23	b	607	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
23	B	602	CLA	CMB-C2B-C1B	2.95	129.90	125.42
23	C	513	CLA	O2A-CGA-CBA	2.95	120.82	111.83
23	A	405[A]	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
23	a	406[B]	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
26	A	410[B]	SQD	O9-S-C6	2.94	111.15	106.76
23	A	406[B]	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
23	A	406[A]	CLA	O2A-CGA-CBA	2.94	120.80	111.83
25	d	404	BCR	C37-C22-C23	2.94	122.58	118.09
23	B	608	CLA	C11-C12-C13	-2.94	106.20	115.97
23	D	403	CLA	C3B-C4B-NB	2.94	113.15	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404[A]	CLA	C2A-C1A-CHA	-2.94	118.77	123.87
23	b	612	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
23	C	504	CLA	CHD-C4C-NC	2.93	128.78	124.23
23	A	405[A]	CLA	CHD-C4C-NC	2.93	128.78	124.23
29	a	413[A]	PL9	C22-C23-C24	-2.93	120.92	127.62
23	c	509	CLA	CMB-C2B-C1B	2.93	129.88	125.42
23	c	508	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
33	a	416	LMG	C7-O1-C1	-2.93	107.52	113.80
23	b	606	CLA	CHC-C1C-C2C	-2.93	118.62	126.95
23	A	405[A]	CLA	CMA-C3A-C4A	-2.93	103.90	111.77
23	b	602	CLA	C11-C12-C13	-2.93	106.23	115.97
23	C	502	CLA	CHD-C4C-NC	2.93	128.77	124.23
23	b	602	CLA	CHD-C4C-NC	2.92	128.77	124.23
23	c	513	CLA	O2A-CGA-CBA	2.92	120.75	111.83
23	A	404[A]	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
23	B	609	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
23	c	502	CLA	CHD-C4C-NC	2.92	128.76	124.23
32	L	101[A]	LHG	O8-C23-C24	2.92	120.75	111.83
38	F	102	HEM	CBA-CAA-C2A	-2.92	104.46	112.53
23	a	408	CLA	O2A-CGA-O1A	-2.92	116.33	123.63
23	B	604	CLA	C6-C5-C3	-2.92	106.36	113.47
23	b	611	CLA	CHC-C1C-C2C	-2.92	118.66	126.95
25	T	101	BCR	C21-C20-C19	-2.92	114.75	123.20
23	c	512	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
23	B	614	CLA	O2A-CGA-CBA	2.91	120.72	111.83
23	B	614	CLA	CBC-CAC-C3C	-2.91	104.53	112.42
23	B	613	CLA	O2A-CGA-CBA	2.91	120.71	111.83
23	b	609	CLA	CBC-CAC-C3C	-2.91	104.53	112.42
23	B	601	CLA	C1-O2A-CGA	2.91	123.69	116.65
23	D	402[B]	CLA	CHC-C1C-C2C	-2.91	118.69	126.95
33	D	411	LMG	O8-C28-C29	2.91	120.69	111.83
23	d	402[B]	CLA	CHC-C1C-C2C	-2.91	118.69	126.95
23	B	609	CLA	CMC-C2C-C1C	2.91	129.57	125.03
23	C	512	CLA	CHD-C1D-ND	-2.91	120.71	124.80
23	b	609	CLA	C1C-C2C-C3C	-2.90	103.92	106.98
23	A	406[A]	CLA	CHD-C4C-NC	2.90	128.73	124.23
23	A	406[A]	CLA	CMC-C2C-C1C	2.90	129.57	125.03
25	b	619	BCR	C7-C8-C9	-2.90	121.94	126.23
29	d	405[A]	PL9	C10-C9-C11	2.90	120.27	115.23
29	d	405[B]	PL9	C17-C18-C19	-2.90	120.98	127.62
23	c	503	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
23	b	615	CLA	C1-C2-C3	-2.90	121.45	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402[A]	CLA	CHC-C1C-C2C	-2.90	118.71	126.95
23	C	505	CLA	CHC-C1C-C2C	-2.90	118.71	126.95
23	a	404[A]	CLA	CMC-C2C-C1C	2.90	129.56	125.03
24	A	407[A]	PHO	C1-C2-C3	-2.90	121.45	126.20
34	b	625	HTG	O5-C5-C4	2.90	114.92	109.70
29	a	413[B]	PL9	C35-C34-C36	2.90	120.26	115.23
23	C	512	CLA	C1-O2A-CGA	2.90	123.66	116.65
23	c	504	CLA	C4B-C3B-C2B	-2.90	103.70	107.30
23	B	602	CLA	C1-C2-C3	-2.89	121.45	126.20
23	C	504	CLA	CBC-CAC-C3C	-2.89	104.57	112.42
23	b	615	CLA	CHD-C4C-NC	2.89	128.72	124.23
23	b	601	CLA	C3B-C4B-NB	2.89	113.11	110.53
23	C	507	CLA	C4B-C3B-C2B	-2.89	103.70	107.30
25	A	409	BCR	C15-C14-C13	-2.89	123.22	127.28
24	A	416[A]	PHO	O2D-CGD-O1D	-2.89	118.22	123.85
24	A	416[B]	PHO	C4-C3-C5	2.89	120.25	115.23
23	C	510	CLA	CAC-C3C-C4C	2.89	128.55	124.79
23	b	611	CLA	CHD-C4C-NC	2.89	128.71	124.23
23	B	614	CLA	C4B-C3B-C2B	-2.89	103.71	107.30
23	B	606	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
23	A	408	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
23	C	514	CLA	C1-C2-C3	-2.88	121.47	126.20
23	B	616	CLA	CHD-C1D-ND	-2.88	120.75	124.80
23	C	509	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
23	b	610	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
35	C	517[A]	DGD	O6D-C1D-O3G	-2.88	103.24	110.04
32	d	406[A]	LHG	O7-C7-C8	2.88	117.71	111.48
23	b	604	CLA	CHC-C1C-C2C	-2.88	118.76	126.95
23	C	514	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
23	B	606	CLA	C4-C3-C5	2.88	120.23	115.23
23	b	615	CLA	CHC-C1C-C2C	-2.88	118.77	126.95
23	d	403	CLA	O2A-CGA-CBA	2.88	120.61	111.83
32	b	629[B]	LHG	O8-C23-C24	2.88	120.61	111.83
23	b	607	CLA	C1D-CHD-C4C	-2.88	119.90	126.02
31	M	101	LMT	C3'-C4'-C5'	-2.88	104.55	110.93
24	a	415[A]	PHO	C4A-C3A-C2A	-2.88	100.10	102.84
23	c	507	CLA	C4-C3-C5	2.88	120.22	115.23
23	c	501	CLA	C3B-C4B-NB	2.88	113.10	110.53
23	a	404[A]	CLA	CAC-C3C-C4C	2.88	128.53	124.79
25	d	404	BCR	C39-C30-C25	-2.88	105.73	110.24
23	d	403	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
23	d	403	CLA	CHD-C4C-NC	2.87	128.69	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	101	BCR	C15-C14-C13	2.87	131.31	127.28
25	Y	101	BCR	C15-C14-C13	-2.87	123.25	127.28
25	y	101	BCR	C34-C9-C8	2.87	122.47	118.09
23	B	613	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
23	a	405[A]	CLA	O2A-CGA-CBA	2.87	120.58	111.83
29	D	405[A]	PL9	C10-C9-C11	2.87	120.20	115.23
23	c	509	CLA	C4-C3-C5	2.86	120.20	115.23
23	a	405[A]	CLA	CHC-C1C-C2C	-2.86	118.81	126.95
25	B	619	BCR	C7-C8-C9	-2.86	122.00	126.23
23	b	608	CLA	CHC-C1C-C2C	-2.86	118.81	126.95
32	D	407[B]	LHG	O8-C23-C24	2.86	120.57	111.83
23	B	608	CLA	C4C-C3C-C2C	-2.86	102.72	106.89
25	B	617	BCR	C16-C17-C18	-2.86	123.26	127.28
32	d	406[B]	LHG	O8-C23-O10	-2.86	116.47	123.63
23	A	408	CLA	CMB-C2B-C1B	2.86	129.77	125.42
23	a	405[B]	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
23	B	602	CLA	CAC-C3C-C4C	2.86	128.51	124.79
23	c	502	CLA	O2A-CGA-CBA	2.86	120.55	111.83
25	b	619	BCR	C15-C14-C13	-2.86	123.27	127.28
29	D	405[A]	PL9	C53-C6-C1	2.86	121.13	115.28
31	m	103	LMT	C3'-C4'-C5'	-2.85	104.61	110.93
23	c	507	CLA	O2A-CGA-CBA	2.85	120.53	111.83
23	a	406[A]	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
25	k	101	BCR	C39-C30-C25	-2.85	105.77	110.24
23	B	611	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
23	c	504	CLA	O2A-CGA-CBA	2.85	120.52	111.83
23	D	402[A]	CLA	C4-C3-C5	2.85	120.17	115.23
25	k	101	BCR	C2-C1-C6	2.85	114.58	110.44
23	C	502	CLA	C1-C2-C3	-2.85	121.53	126.20
25	B	618	BCR	C15-C14-C13	-2.85	123.29	127.28
29	d	405[A]	PL9	C27-C28-C29	-2.85	121.11	127.62
23	b	602	CLA	C1-O2A-CGA	2.85	123.54	116.65
23	c	503	CLA	C4B-C3B-C2B	-2.84	103.77	107.30
23	B	604	CLA	CMB-C2B-C1B	2.84	129.75	125.42
24	A	416[B]	PHO	O2D-CGD-O1D	-2.84	118.31	123.85
23	b	605	CLA	CHC-C1C-C2C	-2.84	118.87	126.95
34	o	301	HTG	C1-O5-C5	2.84	117.66	112.56
23	B	612	CLA	C4A-NA-C1A	-2.84	105.38	106.68
35	C	518[B]	DGD	C2G-O2G-C1B	-2.84	111.00	117.80
25	D	404	BCR	C15-C16-C17	-2.84	117.71	123.52
25	y	101	BCR	C24-C23-C22	-2.84	122.04	126.23
23	B	603	CLA	CHD-C4C-NC	2.84	128.63	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	CHC-C1C-C2C	-2.84	118.89	126.95
23	b	609	CLA	CHC-C1C-C2C	-2.84	118.89	126.95
23	C	504	CLA	O2A-CGA-O1A	-2.83	116.54	123.63
25	t	102	BCR	C11-C10-C9	-2.83	123.31	127.28
23	c	513	CLA	CAA-C2A-C3A	-2.83	105.35	113.00
23	a	406[A]	CLA	C4B-C3B-C2B	-2.83	103.78	107.30
23	A	404[A]	CLA	CMA-C3A-C2A	-2.83	103.05	113.98
23	C	505	CLA	C1D-CHD-C4C	-2.83	120.01	126.02
23	B	608	CLA	CMA-C3A-C4A	-2.83	104.18	111.77
25	c	514	BCR	C33-C5-C6	-2.83	121.40	124.48
23	B	616	CLA	C1-O2A-CGA	2.83	123.49	116.65
23	A	404[A]	CLA	CHC-C1C-C2C	-2.83	118.92	126.95
23	B	609	CLA	CHC-C1C-C2C	-2.82	118.93	126.95
33	D	411	LMG	O7-C10-C11	2.82	117.59	111.48
23	A	408	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
29	A	414[B]	PL9	C35-C34-C36	2.82	120.13	115.23
23	B	610	CLA	CMA-C3A-C4A	-2.82	104.19	111.77
23	c	503	CLA	C4-C3-C5	2.82	120.12	115.23
23	B	604	CLA	C6-C7-C8	-2.82	106.60	115.97
23	a	406[B]	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
29	A	414[B]	PL9	C12-C13-C14	-2.82	121.18	127.62
34	o	301	HTG	O2-C2-C3	-2.82	103.74	110.38
23	b	607	CLA	CBC-CAC-C3C	-2.82	104.79	112.42
23	C	505	CLA	CMC-C2C-C1C	2.81	129.43	125.03
23	A	404[B]	CLA	CHD-C4C-NC	2.81	128.59	124.23
24	a	415[A]	PHO	CMB-C2B-C3B	2.81	130.30	124.68
23	B	609	CLA	CHD-C4C-NC	2.81	128.59	124.23
29	D	405[B]	PL9	C53-C6-C1	2.81	121.04	115.28
24	A	407[A]	PHO	O1D-CGD-CBD	-2.81	120.46	124.72
23	b	603	CLA	O2A-CGA-CBA	2.81	120.41	111.83
23	b	605	CLA	O2A-CGA-O1A	-2.81	116.59	123.63
23	A	406[A]	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
23	d	402[B]	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
23	C	509	CLA	C4-C3-C5	2.81	120.11	115.23
23	C	509	CLA	CHD-C1D-ND	-2.81	120.85	124.80
23	c	513	CLA	CMB-C2B-C1B	2.81	129.70	125.42
26	A	412	SQD	C4-C3-C2	-2.81	105.90	110.83
23	C	511	CLA	C4-C3-C5	2.81	120.11	115.23
23	B	606	CLA	C1-C2-C3	-2.81	121.59	126.20
29	D	405[B]	PL9	C17-C18-C19	-2.81	121.19	127.62
23	c	502	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
23	A	405[A]	CLA	CHC-C1C-C2C	-2.81	118.97	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	CBC-CAC-C3C	-2.80	104.82	112.42
23	a	406[A]	CLA	CHC-C1C-C2C	-2.80	118.98	126.95
23	C	511	CLA	O2A-CGA-CBA	2.80	120.38	111.83
23	a	406[A]	CLA	O2A-CGA-O1A	-2.80	116.62	123.63
23	B	603	CLA	C2A-C1A-CHA	-2.80	119.01	123.87
23	D	403	CLA	CMA-C3A-C4A	-2.80	104.25	111.77
23	c	508	CLA	O2A-CGA-CBA	2.80	120.36	111.83
26	f	102	SQD	O48-C23-C24	2.80	120.36	111.83
31	A	420	LMT	O5B-C5B-C4B	2.80	114.74	109.70
31	F	101	LMT	C1'-O5'-C5'	-2.79	108.26	113.72
23	C	502	CLA	CHC-C1C-C2C	-2.79	119.01	126.95
23	c	508	CLA	O2A-CGA-O1A	-2.79	116.64	123.63
23	B	604	CLA	O2A-CGA-O1A	-2.79	116.65	123.63
23	A	405[A]	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
31	a	417	LMT	C3'-C4'-C5'	-2.79	104.75	110.93
32	d	413[B]	LHG	O8-C23-O10	-2.79	116.66	123.63
35	C	519	DGD	O2G-C1B-C2B	2.78	117.50	111.48
23	b	609	CLA	C16-C15-C13	-2.78	106.71	115.97
25	d	404	BCR	C11-C10-C9	-2.78	123.37	127.28
32	b	629[A]	LHG	O8-C23-C24	2.78	120.32	111.83
23	C	503	CLA	O2A-CGA-CBA	2.78	120.32	111.83
29	d	405[B]	PL9	C7-C8-C9	-2.78	122.04	126.83
25	H	101	BCR	C16-C15-C14	-2.78	117.83	123.52
34	o	301	HTG	C1'-S1-C1	2.78	106.45	100.45
23	B	609	CLA	O2A-CGA-O1A	-2.78	116.68	123.63
23	b	604	CLA	CMB-C2B-C1B	2.78	129.65	125.42
23	B	608	CLA	CMC-C2C-C1C	2.78	129.37	125.03
23	B	611	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
23	b	609	CLA	CHD-C4C-NC	2.77	128.53	124.23
26	f	102	SQD	C4-C3-C2	-2.77	105.96	110.83
33	c	520	LMG	O8-C28-C29	2.77	120.29	111.83
23	A	406[B]	CLA	C2A-C1A-CHA	-2.77	119.06	123.87
23	B	602	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
23	c	511	CLA	CHC-C1C-C2C	-2.77	119.07	126.95
23	c	504	CLA	CHC-C1C-C2C	-2.77	119.08	126.95
35	c	518	DGD	O2G-C1B-C2B	2.77	117.47	111.48
29	A	414[B]	PL9	C40-C39-C41	2.77	120.03	115.23
23	D	403	CLA	O2A-CGA-O1A	-2.77	116.70	123.63
25	K	102	BCR	C20-C21-C22	-2.77	123.40	127.28
23	C	503	CLA	O2A-CGA-O1A	-2.77	116.71	123.63
23	b	612	CLA	CMB-C2B-C1B	2.77	129.63	125.42
25	c	515	BCR	C21-C20-C19	-2.77	115.18	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	514	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
23	a	408	CLA	C4C-C3C-C2C	-2.76	102.87	106.89
23	C	503	CLA	CHC-C1C-C2C	-2.76	119.10	126.95
23	C	507	CLA	CAA-C2A-C3A	-2.76	105.54	113.00
32	a	420[A]	LHG	O8-C23-C24	2.76	120.25	111.83
23	c	504	CLA	CED-O2D-CGD	2.76	122.18	115.92
25	T	101	BCR	C33-C5-C6	-2.76	121.47	124.48
23	C	506	CLA	O2A-CGA-O1A	-2.76	116.73	123.63
23	b	605	CLA	C1-O2A-CGA	2.76	123.33	116.65
23	D	403	CLA	C2A-C1A-CHA	-2.76	119.08	123.87
23	B	604	CLA	O2A-CGA-CBA	2.76	120.24	111.83
29	A	414[A]	PL9	C35-C34-C36	2.76	120.01	115.23
23	a	404[B]	CLA	C2A-C1A-CHA	-2.76	119.08	123.87
29	D	405[B]	PL9	C22-C23-C24	-2.76	121.31	127.62
23	B	603	CLA	CHC-C1C-C2C	-2.76	119.12	126.95
23	B	608	CLA	O2A-CGA-O1A	-2.75	116.74	123.63
23	A	405[A]	CLA	CMA-C3A-C2A	-2.75	103.33	113.98
25	B	617	BCR	C7-C8-C9	-2.75	122.16	126.23
23	d	402[B]	CLA	C4-C3-C5	2.75	120.01	115.23
23	A	406[B]	CLA	C3B-C4B-NB	2.75	112.99	110.53
32	A	419[B]	LHG	O8-C23-O10	-2.75	116.74	123.63
32	D	406[A]	LHG	O7-C7-C8	2.75	117.44	111.48
23	D	402[B]	CLA	C4B-C3B-C2B	-2.75	103.88	107.30
23	c	507	CLA	CAC-C3C-C4C	2.75	128.37	124.79
29	D	405[A]	PL9	C51-C49-C50	2.75	120.92	114.59
35	H	102	DGD	O1G-C1A-C2A	2.75	120.21	111.83
23	B	615	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
29	A	414[B]	PL9	C53-C6-C1	2.75	120.91	115.28
23	b	603	CLA	C4-C3-C5	2.75	120.00	115.23
23	A	406[A]	CLA	C4-C3-C5	2.75	119.99	115.23
29	A	414[A]	PL9	C30-C29-C31	2.75	119.99	115.23
29	D	405[B]	PL9	C40-C39-C41	2.75	119.99	115.23
23	c	510	CLA	O2A-CGA-O1A	-2.74	116.76	123.63
23	B	616	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
32	D	406[A]	LHG	O8-C23-C24	2.74	120.20	111.83
23	C	506	CLA	O2A-CGA-CBA	2.74	120.20	111.83
23	c	513	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
33	m	101	LMG	C7-O1-C1	-2.74	107.92	113.80
26	b	620	SQD	O8-S-C6	2.74	111.27	105.97
23	a	406[B]	CLA	C4-C3-C5	2.74	119.99	115.23
26	B	620	SQD	O9-S-C6	2.74	110.85	106.76
25	d	404	BCR	C28-C27-C26	-2.74	109.17	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	C1-C2-C3	-2.74	121.71	126.20
23	c	505	CLA	C1-O2A-CGA	2.74	123.28	116.65
23	C	511	CLA	O2A-CGA-O1A	-2.74	116.78	123.63
23	C	514	CLA	CHD-C4C-NC	2.74	128.48	124.23
25	y	101	BCR	C10-C11-C12	-2.74	115.27	123.20
33	D	411	LMG	O8-C28-O10	-2.74	116.78	123.63
23	B	607	CLA	CED-O2D-CGD	2.74	122.12	115.92
23	B	604	CLA	C4A-NA-C1A	-2.74	105.43	106.68
23	b	614	CLA	CHD-C4C-NC	2.73	128.47	124.23
23	b	603	CLA	O2A-CGA-O1A	-2.73	116.79	123.63
23	c	501	CLA	O2A-CGA-CBA	2.73	120.16	111.83
32	L	101[A]	LHG	O8-C23-O10	-2.73	116.80	123.63
24	a	415[B]	PHO	O1D-CGD-CBD	-2.73	120.58	124.72
23	a	405[B]	CLA	CMB-C2B-C1B	2.73	129.57	125.42
23	c	511	CLA	CMB-C2B-C1B	2.73	129.57	125.42
23	c	506	CLA	CMC-C2C-C1C	2.73	129.30	125.03
23	c	506	CLA	C4C-C3C-C2C	-2.73	102.92	106.89
23	c	510	CLA	C4B-C3B-C2B	-2.73	103.91	107.30
23	B	605	CLA	CMC-C2C-C1C	2.72	129.29	125.03
23	c	507	CLA	O1D-CGD-CBD	-2.72	119.14	124.52
29	d	405[A]	PL9	C36-C34-C33	-2.72	115.05	121.17
23	C	503	CLA	CBC-CAC-C3C	-2.72	105.03	112.42
23	a	408	CLA	CBC-CAC-C3C	-2.72	105.04	112.42
23	a	406[B]	CLA	CHC-C1C-C2C	-2.72	119.21	126.95
23	C	503	CLA	CHD-C4C-NC	2.72	128.45	124.23
23	b	611	CLA	O2A-CGA-O1A	-2.72	116.82	123.63
23	a	405[B]	CLA	CMA-C3A-C2A	-2.72	103.46	113.98
23	b	603	CLA	CHC-C1C-C2C	-2.72	119.22	126.95
23	C	506	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
23	C	514	CLA	O2A-CGA-CBA	2.72	120.13	111.83
23	c	512	CLA	CHC-C1C-C2C	-2.72	119.22	126.95
23	a	404[A]	CLA	C2A-C1A-CHA	-2.72	119.15	123.87
26	B	620	SQD	O48-C23-O10	-2.72	116.83	123.63
26	f	102	SQD	O5-C1-C2	2.72	115.95	110.37
23	C	514	CLA	C2A-C1A-CHA	-2.72	119.15	123.87
23	c	513	CLA	C2A-C1A-CHA	-2.72	119.15	123.87
23	b	616	CLA	CMC-C2C-C1C	2.72	129.28	125.03
23	b	607	CLA	O2A-CGA-O1A	-2.72	116.83	123.63
23	B	601	CLA	O2A-CGA-CBA	2.72	120.12	111.83
23	B	602	CLA	CHD-C4C-NC	2.72	128.44	124.23
27	b	628	GOL	C3-C2-C1	-2.72	101.84	111.80
32	a	420[B]	LHG	O8-C23-C24	2.71	120.11	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	CMB-C2B-C1B	2.71	129.55	125.42
23	B	612	CLA	C3B-C4B-NB	2.71	112.95	110.53
25	b	618	BCR	C37-C22-C21	-2.71	118.42	122.82
23	a	406[A]	CLA	O2A-CGA-CBA	2.71	120.10	111.83
23	A	404[B]	CLA	C2A-C1A-CHA	-2.71	119.16	123.87
25	h	101	BCR	C20-C21-C22	-2.71	123.48	127.28
32	d	407[A]	LHG	O8-C23-C24	2.71	120.09	111.83
26	B	620	SQD	C4-C3-C2	2.71	115.58	110.83
29	D	405[A]	PL9	C2-C1-C6	2.71	122.22	119.00
23	a	406[B]	CLA	C3B-C4B-NB	2.71	112.95	110.53
24	a	407[B]	PHO	O1D-CGD-CBD	-2.71	120.62	124.72
26	F	103	SQD	O47-C7-O49	-2.71	117.38	123.70
23	D	403	CLA	CAA-C2A-C3A	-2.71	105.69	113.00
29	a	413[A]	PL9	C53-C6-C1	2.71	120.82	115.28
23	A	406[B]	CLA	CBC-CAC-C3C	-2.71	105.09	112.42
23	B	610	CLA	CAC-C3C-C4C	2.70	128.31	124.79
23	B	607	CLA	C2A-C1A-CHA	-2.70	119.17	123.87
23	B	616	CLA	C2A-C1A-CHA	-2.70	119.18	123.87
23	B	604	CLA	C4B-C3B-C2B	-2.70	103.94	107.30
23	C	512	CLA	CHD-C4C-NC	2.70	128.42	124.23
23	c	510	CLA	CAC-C3C-C4C	2.70	128.30	124.79
23	c	501	CLA	CHC-C1C-C2C	-2.70	119.28	126.95
23	D	402[A]	CLA	CAC-C3C-C4C	2.70	128.30	124.79
24	A	407[A]	PHO	O2A-CGA-CBA	2.69	120.05	111.83
24	a	407[B]	PHO	C1A-C2A-C3A	-2.69	100.28	102.84
25	c	514	BCR	C28-C27-C26	-2.69	109.25	114.06
23	B	606	CLA	O2A-CGA-CBA	2.69	120.05	111.83
23	d	402[B]	CLA	C2A-C1A-CHA	-2.69	119.19	123.87
23	C	508	CLA	O2A-CGA-CBA	2.69	120.05	111.83
29	A	414[A]	PL9	C2-C1-C6	2.69	122.20	119.00
23	d	403	CLA	CMC-C2C-C1C	2.69	129.24	125.03
23	C	509	CLA	O2A-CGA-O1A	-2.69	116.90	123.63
35	C	518[A]	DGD	O1G-C1A-O1A	-2.69	116.90	123.63
29	d	405[B]	PL9	C12-C13-C14	-2.69	121.47	127.62
29	D	405[B]	PL9	C51-C49-C50	2.69	120.78	114.59
23	b	615	CLA	C3B-C4B-NB	2.69	112.93	110.53
25	h	101	BCR	C16-C15-C14	-2.69	118.02	123.52
23	c	501	CLA	CHD-C4C-NC	2.69	128.40	124.23
23	B	611	CLA	C3B-C4B-NB	2.68	112.93	110.53
23	b	609	CLA	CMC-C2C-C1C	2.68	129.23	125.03
23	C	514	CLA	C4C-C3C-C2C	-2.68	102.98	106.89
23	c	504	CLA	O2A-CGA-O1A	-2.68	116.92	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	CHD-C4C-NC	2.68	128.39	124.23
23	b	608	CLA	O2A-CGA-O1A	-2.68	116.92	123.63
23	C	508	CLA	C4-C3-C5	2.68	119.88	115.23
23	B	608	CLA	CMA-C3A-C2A	-2.68	103.62	113.98
24	a	415[B]	PHO	CMB-C2B-C3B	2.68	130.04	124.68
23	a	404[B]	CLA	CAA-C2A-C1A	-2.68	103.20	111.97
23	c	509	CLA	O2A-CGA-CBA	2.68	120.00	111.83
32	A	419[B]	LHG	O8-C23-C24	2.68	120.00	111.83
31	b	621	LMT	C1'-O5'-C5'	-2.68	108.49	113.72
25	y	101	BCR	C11-C10-C9	-2.68	123.52	127.28
23	c	510	CLA	CHC-C1C-C2C	-2.68	119.34	126.95
23	C	514	CLA	CAA-C2A-C3A	-2.68	105.77	113.00
31	B	627	LMT	C2'-C3'-C4'	2.68	115.75	109.68
23	b	609	CLA	CMB-C2B-C1B	2.67	129.49	125.42
23	d	402[A]	CLA	C2A-C1A-CHA	-2.67	119.23	123.87
31	B	631	LMT	C3'-C4'-C5'	-2.67	105.00	110.93
23	C	508	CLA	CHC-C1C-C2C	-2.67	119.35	126.95
23	b	615	CLA	O2A-CGA-O1A	-2.67	116.94	123.63
23	d	403	CLA	C3B-C4B-NB	2.67	112.92	110.53
25	a	409	BCR	C29-C30-C25	2.67	114.32	110.44
23	b	609	CLA	O2A-CGA-CBA	2.67	119.98	111.83
23	D	402[A]	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
23	D	402[A]	CLA	C2A-C1A-CHA	-2.67	119.24	123.87
23	B	604	CLA	CMC-C2C-C1C	2.67	129.20	125.03
25	d	404	BCR	C21-C20-C19	-2.67	115.47	123.20
35	C	518[B]	DGD	O1G-C1A-O1A	-2.67	116.95	123.63
23	a	405[A]	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
23	c	501	CLA	CMC-C2C-C1C	2.67	129.20	125.03
23	c	504	CLA	CAC-C3C-C4C	2.67	128.26	124.79
23	a	405[A]	CLA	C4C-C3C-C2C	-2.67	103.01	106.89
31	M	103	LMT	C3'-C4'-C5'	-2.66	105.03	110.93
23	B	612	CLA	C4-C3-C5	2.66	119.85	115.23
32	A	419[B]	LHG	O7-C7-O9	-2.66	117.48	123.70
23	c	509	CLA	CHD-C4C-NC	2.66	128.36	124.23
23	C	510	CLA	CHD-C4C-NC	2.66	128.36	124.23
23	c	510	CLA	O2A-CGA-CBA	2.66	119.95	111.83
23	B	615	CLA	CHC-C1C-C2C	-2.66	119.39	126.95
23	d	402[A]	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
23	C	507	CLA	C2A-C1A-CHA	-2.66	119.25	123.87
23	b	611	CLA	C2A-C1A-CHA	-2.66	119.25	123.87
23	d	402[A]	CLA	CAC-C3C-C4C	2.66	128.25	124.79
31	e	101	LMT	O1'-C1'-C2'	2.66	112.31	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	CMC-C2C-C1C	2.66	129.18	125.03
29	d	405[B]	PL9	C27-C28-C29	-2.65	121.55	127.62
40	v	201	HEC	CMB-C2B-C1B	-2.65	121.38	125.42
23	a	408	CLA	C2A-C1A-CHA	-2.65	119.27	123.87
35	c	518	DGD	O3G-C1D-C2D	-2.65	104.25	108.27
25	d	404	BCR	C40-C30-C39	2.65	116.22	108.63
23	B	604	CLA	C11-C12-C13	-2.65	107.15	115.97
25	K	102	BCR	C2-C1-C6	2.65	114.29	110.44
23	b	614	CLA	CMC-C2C-C1C	2.65	129.17	125.03
35	C	518[B]	DGD	O1G-C1A-C2A	2.65	119.91	111.83
25	Y	101	BCR	C37-C22-C23	2.65	122.13	118.09
23	c	508	CLA	CAA-C2A-C3A	-2.65	105.84	113.00
23	A	406[A]	CLA	C1-C2-C3	-2.65	121.86	126.20
24	A	407[B]	PHO	O2A-CGA-CBA	2.65	119.91	111.83
23	b	603	CLA	CHD-C4C-NC	2.65	128.34	124.23
23	c	506	CLA	O2A-CGA-O1A	-2.65	117.01	123.63
23	B	608	CLA	CAA-C2A-C3A	-2.65	105.85	113.00
25	T	101	BCR	C35-C13-C12	2.64	122.13	118.09
29	a	413[A]	PL9	C47-C48-C49	-2.64	118.83	127.64
23	B	607	CLA	CMC-C2C-C1C	2.64	129.16	125.03
23	A	405[B]	CLA	C4C-C3C-C2C	-2.64	103.04	106.89
23	B	607	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
23	b	612	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
25	h	101	BCR	C10-C11-C12	-2.64	115.55	123.20
33	B	621	LMG	O8-C28-O10	-2.64	117.02	123.63
23	d	403	CLA	CHC-C1C-C2C	-2.64	119.45	126.95
23	D	402[B]	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
32	D	406[B]	LHG	O8-C23-O10	-2.64	117.03	123.63
23	B	612	CLA	C1-C2-C3	-2.64	121.88	126.20
24	a	407[B]	PHO	O2A-CGA-CBA	2.64	119.88	111.83
23	B	614	CLA	C4C-C3C-C2C	-2.64	103.05	106.89
23	C	502	CLA	CMB-C2B-C1B	2.64	129.44	125.42
38	F	102	HEM	O2A-CGA-CBA	2.64	122.33	114.00
23	C	507	CLA	C4-C3-C5	2.64	119.81	115.23
33	C	501	LMG	C8-O7-C10	-2.64	111.49	117.80
35	H	102	DGD	O3G-C3G-C2G	-2.64	104.41	110.82
23	b	608	CLA	O2A-CGA-CBA	2.63	119.87	111.83
23	B	612	CLA	C2B-C1B-NB	2.63	113.06	110.33
25	D	404	BCR	C40-C30-C25	-2.63	106.11	110.24
40	v	201	HEC	CBD-CAD-C3D	-2.63	105.26	112.53
23	B	614	CLA	C2A-C1A-CHA	-2.63	119.30	123.87
23	C	511	CLA	C2A-C1A-CHA	-2.63	119.30	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	101	BCR	C10-C11-C12	-2.63	115.58	123.20
25	K	102	BCR	C3-C4-C5	-2.63	109.36	114.06
23	C	510	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
40	v	201	HEC	CBA-CAA-C2A	-2.63	105.26	112.53
23	C	510	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
23	c	501	CLA	C4B-C3B-C2B	-2.63	104.03	107.30
23	b	616	CLA	C4B-C3B-C2B	-2.63	104.03	107.30
25	Y	101	BCR	C15-C16-C17	-2.63	118.14	123.52
23	B	612	CLA	CMC-C2C-C1C	2.63	129.14	125.03
23	c	504	CLA	CHD-C4C-NC	2.63	128.30	124.23
23	a	405[A]	CLA	O2A-CGA-O1A	-2.63	117.06	123.63
23	C	503	CLA	C2A-C1A-CHA	-2.62	119.31	123.87
23	C	506	CLA	CHD-C4C-NC	2.62	128.30	124.23
32	d	407[B]	LHG	O8-C23-C24	2.62	119.83	111.83
25	C	516	BCR	C29-C30-C25	2.62	114.25	110.44
23	b	613	CLA	CMA-C3A-C4A	-2.62	104.73	111.77
23	C	510	CLA	C16-C15-C13	-2.62	107.25	115.97
23	b	610	CLA	CAA-CBA-CGA	-2.62	105.77	113.21
23	C	513	CLA	CHB-C4A-NA	2.62	128.18	124.40
29	A	414[B]	PL9	C45-C44-C46	2.62	119.77	115.23
23	B	608	CLA	CHB-C4A-NA	2.62	128.18	124.40
23	b	601	CLA	CHC-C1C-C2C	-2.62	119.51	126.95
23	B	603	CLA	CAC-C3C-C4C	2.62	128.19	124.79
23	C	513	CLA	CBA-CAA-C2A	-2.62	106.01	113.79
25	k	101	BCR	C24-C23-C22	-2.61	122.37	126.23
23	b	603	CLA	CBC-CAC-C3C	-2.61	105.34	112.42
23	c	510	CLA	C4C-C3C-C2C	-2.61	103.09	106.89
31	M	103	LMT	C1'-O5'-C5'	-2.61	108.62	113.72
23	D	402[A]	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
25	t	102	BCR	C28-C27-C26	-2.61	109.40	114.06
23	C	512	CLA	CHC-C1C-C2C	-2.61	119.54	126.95
23	c	511	CLA	CBC-CAC-C3C	-2.61	105.35	112.42
23	a	404[A]	CLA	C4B-C3B-C2B	-2.61	104.06	107.30
26	A	410[A]	SQD	O48-C23-O10	-2.61	117.11	123.63
23	B	615	CLA	C4C-C3C-C2C	-2.60	103.10	106.89
23	b	611	CLA	CMC-C2C-C1C	2.60	129.10	125.03
24	A	407[A]	PHO	O2A-CGA-O1A	-2.60	117.12	123.63
23	b	610	CLA	CHC-C1C-C2C	-2.60	119.55	126.95
23	B	606	CLA	CHC-C1C-C2C	-2.60	119.55	126.95
23	C	502	CLA	C4-C3-C5	2.60	119.74	115.23
23	a	405[A]	CLA	CAA-CBA-CGA	2.60	120.59	113.21
25	H	101	BCR	C7-C8-C9	-2.60	122.39	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405[A]	CLA	C2A-C1A-CHA	-2.60	119.35	123.87
23	B	606	CLA	C2A-C1A-CHA	-2.60	119.35	123.87
23	b	606	CLA	CAA-C2A-C3A	-2.60	105.98	113.00
40	v	201	HEC	CHA-C1A-NA	2.60	127.28	124.45
23	A	406[A]	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
23	C	513	CLA	CMB-C2B-C1B	2.60	129.37	125.42
32	L	101[B]	LHG	O8-C23-C24	2.59	119.75	111.83
23	B	608	CLA	C1-C2-C3	-2.59	121.95	126.20
25	B	617	BCR	C15-C14-C13	-2.59	123.64	127.28
35	c	517[A]	DGD	O1G-C1A-C2A	2.59	119.74	111.83
29	d	405[B]	PL9	C7-C3-C2	-2.59	120.33	123.39
23	A	405[A]	CLA	C4-C3-C5	2.59	119.73	115.23
24	a	407[A]	PHO	CMB-C2B-C3B	2.59	129.86	124.68
23	b	602	CLA	CHB-C1B-C2B	-2.59	119.91	127.43
23	b	614	CLA	CBC-CAC-C3C	-2.59	105.40	112.42
23	C	509	CLA	CMB-C2B-C1B	2.59	129.36	125.42
29	a	413[A]	PL9	C40-C39-C41	2.59	119.72	115.23
25	c	514	BCR	C31-C1-C6	-2.59	106.18	110.24
23	c	501	CLA	O2A-CGA-O1A	-2.59	117.15	123.63
29	A	414[B]	PL9	C10-C9-C11	2.59	119.72	115.23
25	B	619	BCR	C21-C20-C19	-2.59	115.70	123.20
24	a	407[B]	PHO	CMA-C3A-C4A	-2.59	109.04	114.61
23	c	508	CLA	CAC-C3C-C4C	2.59	128.16	124.79
23	b	601	CLA	C2A-C1A-CHA	-2.59	119.38	123.87
23	C	502	CLA	C4C-C3C-C2C	-2.59	103.13	106.89
23	C	505	CLA	CBC-CAC-C3C	-2.59	105.41	112.42
23	A	408	CLA	CMA-C3A-C2A	-2.59	103.99	113.98
25	K	102	BCR	C38-C26-C25	-2.58	121.66	124.48
26	F	103	SQD	O9-S-C6	-2.58	102.90	106.76
35	c	516[B]	DGD	C2G-O2G-C1B	-2.58	111.62	117.80
23	A	405[A]	CLA	O2A-CGA-O1A	-2.58	117.17	123.63
23	D	402[B]	CLA	CAA-C2A-C3A	-2.58	106.03	113.00
23	a	408	CLA	CHD-C4C-NC	2.58	128.23	124.23
23	D	402[B]	CLA	CAC-C3C-C4C	2.58	128.14	124.79
29	a	413[A]	PL9	C10-C9-C8	-2.58	117.01	123.63
23	D	403	CLA	CHC-C1C-C2C	-2.58	119.63	126.95
29	A	414[A]	PL9	C40-C39-C41	2.58	119.70	115.23
23	D	402[B]	CLA	C2A-C1A-CHA	-2.58	119.40	123.87
23	a	406[A]	CLA	C1-C2-C3	-2.58	121.98	126.20
23	c	508	CLA	CHD-C4C-NC	2.58	128.22	124.23
29	A	414[A]	PL9	C47-C48-C49	-2.58	119.05	127.64
23	c	506	CLA	CAA-C2A-C3A	-2.58	106.04	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	629	LMT	O5'-C5'-C6'	2.57	112.82	106.44
23	B	609	CLA	C3B-C4B-NB	2.57	112.83	110.53
31	A	420	LMT	O1'-C1'-C2'	2.57	112.18	108.27
23	b	603	CLA	C7-C6-C5	-2.57	106.41	113.26
24	a	407[B]	PHO	C1-C2-C3	-2.57	121.98	126.20
23	b	613	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
24	A	407[B]	PHO	CMB-C2B-C3B	2.57	129.82	124.68
23	b	605	CLA	C3B-C4B-NB	2.57	112.82	110.53
23	a	406[B]	CLA	CBC-CAC-C3C	-2.57	105.46	112.42
23	A	406[B]	CLA	CMA-C3A-C2A	-2.57	104.05	113.98
23	c	511	CLA	CMC-C2C-C1C	2.57	129.05	125.03
23	b	610	CLA	C3B-C4B-NB	2.57	112.82	110.53
23	c	505	CLA	CHC-C1C-C2C	-2.57	119.66	126.95
31	b	621	LMT	C1-O1'-C1'	2.57	118.06	113.68
25	b	619	BCR	C29-C30-C25	2.57	114.17	110.44
23	B	607	CLA	C4C-C3C-C2C	-2.56	103.16	106.89
23	C	502	CLA	O2A-CGA-O1A	-2.56	117.21	123.63
23	A	405[B]	CLA	C4-C3-C5	2.56	119.68	115.23
33	m	101	LMG	C3-C4-C5	2.56	114.88	110.23
23	c	505	CLA	O2A-CGA-CBA	2.56	119.64	111.83
23	c	503	CLA	CHD-C4C-NC	2.56	128.20	124.23
23	c	513	CLA	C1-C2-C3	-2.56	122.00	126.20
35	H	102	DGD	C2G-O2G-C1B	-2.56	111.67	117.80
23	a	405[B]	CLA	O2A-CGA-CBA	2.56	119.64	111.83
23	B	607	CLA	CAA-CBA-CGA	2.56	120.47	113.21
29	A	414[B]	PL9	C42-C43-C44	-2.56	121.77	127.62
33	C	520	LMG	O8-C28-O10	-2.56	117.23	123.63
23	C	503	CLA	C4C-C3C-C2C	-2.56	103.17	106.89
31	A	420	LMT	O5'-C5'-C6'	2.56	112.78	106.44
23	b	604	CLA	C4-C3-C5	2.56	119.66	115.23
24	A	407[A]	PHO	CMA-C3A-C4A	-2.56	109.11	114.61
23	B	603	CLA	CMA-C3A-C2A	-2.55	104.11	113.98
38	f	101	HEM	C4D-ND-C1D	2.55	108.23	105.21
23	B	615	CLA	C2A-C1A-CHA	-2.55	119.44	123.87
23	c	504	CLA	CMB-C2B-C1B	2.55	129.30	125.42
23	A	405[B]	CLA	CED-O2D-CGD	2.55	121.70	115.92
23	C	509	CLA	O2A-CGA-CBA	2.55	119.61	111.83
23	C	504	CLA	CHC-C1C-C2C	-2.55	119.70	126.95
25	t	102	BCR	C36-C18-C19	2.55	121.98	118.09
25	H	101	BCR	C37-C22-C21	-2.55	118.69	122.82
26	a	410[B]	SQD	O47-C7-O49	-2.55	117.75	123.70
23	c	507	CLA	O2A-CGA-O1A	-2.55	117.25	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	CHC-C1C-C2C	-2.55	119.71	126.95
23	C	507	CLA	CBC-CAC-C3C	-2.55	105.52	112.42
23	c	513	CLA	O2A-CGA-O1A	-2.55	117.26	123.63
29	D	405[A]	PL9	C42-C41-C39	-2.55	104.75	113.19
35	H	102	DGD	O1G-C1A-O1A	-2.55	117.26	123.63
23	d	402[B]	CLA	O2A-CGA-O1A	-2.55	117.26	123.63
35	c	516[A]	DGD	C2G-O2G-C1B	-2.55	111.70	117.80
33	C	521	LMG	O1-C1-C2	2.54	112.14	108.27
25	c	515	BCR	C7-C8-C9	-2.54	122.47	126.23
35	C	519	DGD	O3G-C3G-C2G	-2.54	104.63	110.82
23	C	512	CLA	CMB-C2B-C1B	2.54	129.29	125.42
25	c	515	BCR	C11-C10-C9	-2.54	123.71	127.28
23	b	616	CLA	CHC-C1C-C2C	-2.54	119.72	126.95
23	B	613	CLA	CHC-C1C-C2C	-2.54	119.73	126.95
33	B	621	LMG	C3-C4-C5	2.54	114.84	110.23
25	D	404	BCR	C29-C28-C27	-2.54	105.69	111.28
29	A	414[A]	PL9	C10-C9-C8	-2.54	117.11	123.63
23	B	602	CLA	C11-C12-C13	-2.54	107.53	115.97
38	f	101	HEM	CMD-C2D-C1D	2.54	129.00	125.03
23	c	513	CLA	CMC-C2C-C1C	2.54	129.00	125.03
35	c	517[B]	DGD	O1G-C1A-C2A	2.54	119.56	111.83
23	C	509	CLA	O2D-CGD-O1D	-2.53	118.91	123.85
23	a	406[B]	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
23	B	601	CLA	CBC-CAC-C3C	-2.53	105.55	112.42
23	a	406[A]	CLA	CMC-C2C-C1C	2.53	128.99	125.03
35	c	516[B]	DGD	O3G-C3G-C2G	-2.53	104.66	110.82
23	A	406[A]	CLA	C2A-C1A-CHA	-2.53	119.47	123.87
23	C	507	CLA	O2A-CGA-CBA	2.53	119.55	111.83
25	t	102	BCR	C1-C6-C7	2.53	122.52	115.65
23	B	604	CLA	CHD-C1D-ND	-2.53	121.24	124.80
23	a	404[A]	CLA	CHD-C4C-NC	2.53	128.15	124.23
23	A	408	CLA	CHD-C4C-NC	2.53	128.15	124.23
23	B	605	CLA	O2A-CGA-CBA	2.53	119.54	111.83
33	d	411	LMG	O8-C28-O10	-2.53	117.31	123.63
23	A	406[B]	CLA	CMC-C2C-C1C	2.53	128.98	125.03
23	C	510	CLA	C2A-C1A-CHA	-2.53	119.48	123.87
23	b	607	CLA	CAC-C3C-C4C	2.53	128.08	124.79
33	d	411	LMG	O8-C28-C29	2.53	119.54	111.83
35	H	102	DGD	C3E-C4E-C5E	-2.53	105.65	110.23
23	a	404[A]	CLA	CMA-C3A-C2A	-2.53	104.22	113.98
23	A	406[B]	CLA	CHC-C1C-C2C	-2.52	119.78	126.95
23	b	607	CLA	C4-C3-C5	2.52	119.60	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405[A]	CLA	CBC-CAC-C3C	-2.52	105.59	112.42
23	c	503	CLA	C2A-C1A-CHA	-2.52	119.50	123.87
29	a	413[B]	PL9	C53-C6-C1	2.52	120.43	115.28
26	f	102	SQD	O47-C7-O49	-2.52	117.82	123.70
23	c	511	CLA	O2A-CGA-O1A	-2.52	117.34	123.63
31	B	627	LMT	C1B-C2B-C3B	2.51	115.30	110.01
29	D	405[B]	PL9	C37-C38-C39	-2.51	121.87	127.62
23	A	405[A]	CLA	CAA-CBA-CGA	2.51	120.34	113.21
23	c	509	CLA	O2A-C1-C2	2.51	117.77	108.11
23	B	603	CLA	C7-C6-C5	-2.51	106.57	113.26
23	b	604	CLA	CAC-C3C-C4C	2.51	128.05	124.79
23	C	508	CLA	CHD-C4C-NC	2.51	128.12	124.23
23	b	604	CLA	O2A-CGA-O1A	-2.51	117.36	123.63
29	d	405[A]	PL9	C17-C18-C19	-2.51	121.89	127.62
23	A	404[A]	CLA	CAA-CBA-CGA	-2.51	106.09	113.21
23	b	614	CLA	CAA-C2A-C3A	-2.51	106.23	113.00
23	C	511	CLA	CMB-C2B-C1B	2.50	129.23	125.42
23	c	506	CLA	CMB-C2B-C1B	2.50	129.23	125.42
23	b	615	CLA	C4B-C3B-C2B	-2.50	104.19	107.30
23	d	403	CLA	C4-C3-C5	2.50	119.57	115.23
25	c	515	BCR	C33-C5-C6	-2.50	121.75	124.48
25	C	516	BCR	C32-C1-C6	-2.50	106.32	110.24
23	b	605	CLA	C4B-C3B-C2B	-2.50	104.19	107.30
23	C	514	CLA	CHC-C1C-C2C	-2.50	119.84	126.95
23	A	408	CLA	C4-C3-C5	2.50	119.56	115.23
23	D	403	CLA	CBC-CAC-C3C	-2.50	105.65	112.42
23	a	406[B]	CLA	O2A-CGA-CBA	2.50	119.45	111.83
32	A	419[A]	LHG	O7-C7-O9	-2.50	117.87	123.70
23	B	602	CLA	CHC-C1C-C2C	-2.50	119.86	126.95
23	B	615	CLA	C6-C7-C8	-2.49	107.68	115.97
23	a	404[A]	CLA	C4C-C3C-C2C	-2.49	103.26	106.89
23	b	614	CLA	C4B-C3B-C2B	-2.49	104.20	107.30
23	a	405[B]	CLA	C4-C3-C5	2.49	119.55	115.23
25	c	514	BCR	C37-C22-C21	-2.49	118.78	122.82
23	c	507	CLA	C1-C2-C3	-2.49	122.12	126.20
23	b	614	CLA	C2A-C1A-CHA	-2.49	119.55	123.87
23	C	502	CLA	C11-C12-C13	-2.49	107.69	115.97
25	H	101	BCR	C24-C23-C22	-2.49	122.56	126.23
23	c	507	CLA	CHD-C4C-NC	2.49	128.09	124.23
23	c	502	CLA	C4B-C3B-C2B	-2.49	104.21	107.30
23	c	503	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
23	A	406[A]	CLA	CMA-C3A-C2A	-2.48	104.38	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	CMB-C2B-C1B	2.48	129.20	125.42
23	A	408	CLA	CAC-C3C-C4C	2.48	128.02	124.79
23	c	512	CLA	C3B-C4B-NB	2.48	112.74	110.53
23	A	408	CLA	CMC-C2C-C1C	2.48	128.91	125.03
29	a	413[B]	PL9	C20-C19-C21	2.48	119.53	115.23
23	b	613	CLA	CED-O2D-CGD	2.47	121.53	115.92
29	a	413[B]	PL9	C10-C9-C11	2.47	119.52	115.23
23	B	607	CLA	CHD-C4C-NC	2.47	128.07	124.23
29	a	413[B]	PL9	C47-C48-C49	-2.47	119.39	127.64
24	a	407[B]	PHO	O2A-CGA-O1A	-2.47	117.44	123.63
23	A	404[B]	CLA	CAA-C2A-C1A	-2.47	103.87	111.97
23	d	403	CLA	C1-O2A-CGA	2.47	122.64	116.65
38	F	102	HEM	C3B-C4B-NB	-2.47	107.69	109.47
25	h	101	BCR	C37-C22-C21	-2.47	118.81	122.82
24	a	407[B]	PHO	O2D-CGD-O1D	-2.47	119.04	123.85
25	T	101	BCR	C1-C6-C7	2.47	122.35	115.65
23	B	606	CLA	CMB-C2B-C1B	2.47	129.18	125.42
24	a	415[B]	PHO	O2D-CGD-O1D	-2.47	119.04	123.85
29	D	405[B]	PL9	C12-C13-C14	-2.47	121.97	127.62
25	k	101	BCR	C10-C11-C12	-2.47	116.04	123.20
25	c	514	BCR	C36-C18-C19	2.47	121.86	118.09
23	b	607	CLA	C1-O2A-CGA	2.47	122.62	116.65
23	c	507	CLA	C4C-C3C-C2C	-2.46	103.31	106.89
34	o	301	HTG	C2'-C1'-S1	-2.46	104.07	112.36
29	d	405[A]	PL9	C12-C13-C14	-2.46	121.99	127.62
25	c	515	BCR	C37-C22-C23	2.46	121.85	118.09
23	b	605	CLA	C2A-C1A-CHA	-2.46	119.60	123.87
23	C	514	CLA	CAC-C3C-C4C	2.46	127.99	124.79
24	a	415[B]	PHO	O2A-CGA-CBA	2.46	119.34	111.83
25	c	515	BCR	C38-C26-C25	-2.46	121.80	124.48
40	V	201	HEC	CHB-C4A-NA	2.46	127.13	124.45
23	a	405[B]	CLA	C4C-C3C-C2C	-2.46	103.31	106.89
24	A	407[B]	PHO	CMA-C3A-C4A	-2.46	109.31	114.61
32	d	406[B]	LHG	O8-C23-C24	2.46	119.33	111.83
23	B	606	CLA	C4C-C3C-C2C	-2.46	103.31	106.89
23	d	403	CLA	CAC-C3C-C4C	2.46	127.99	124.79
23	b	615	CLA	C6-C7-C8	-2.46	107.80	115.97
24	A	416[B]	PHO	C6-C5-C3	-2.46	107.49	113.47
23	C	505	CLA	C2A-C1A-CHA	-2.46	119.61	123.87
29	D	405[B]	PL9	C45-C44-C46	2.45	119.49	115.23
23	c	513	CLA	CHD-C4C-NC	2.45	128.04	124.23
23	B	601	CLA	CHC-C1C-C2C	-2.45	119.98	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	405[B]	PL9	C53-C6-C1	2.45	120.30	115.28
23	B	604	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
23	A	405[B]	CLA	C2A-C1A-CHA	-2.45	119.61	123.87
23	B	610	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
23	d	402[A]	CLA	CMC-C2C-C1C	2.45	128.86	125.03
23	B	606	CLA	C3B-C4B-NB	2.45	112.72	110.53
23	C	507	CLA	CHD-C4C-NC	2.45	128.03	124.23
33	C	501	LMG	C6-C5-C4	2.45	119.03	113.02
35	c	516[B]	DGD	C3G-C2G-C1G	-2.45	106.08	111.78
23	c	506	CLA	O2A-CGA-CBA	2.45	119.29	111.83
23	c	503	CLA	CMC-C2C-C1C	2.45	128.85	125.03
29	A	414[A]	PL9	C42-C43-C44	-2.44	122.03	127.62
23	b	612	CLA	CAA-C2A-C3A	-2.44	106.40	113.00
23	C	502	CLA	C2A-C1A-CHA	-2.44	119.63	123.87
23	B	613	CLA	CHB-C4A-NA	2.44	127.92	124.40
34	b	622	HTG	O2-C2-C3	-2.44	104.62	110.38
23	b	608	CLA	CMB-C2B-C3B	2.44	132.28	126.55
32	b	629[A]	LHG	O8-C23-O10	-2.44	117.53	123.63
23	c	504	CLA	C2A-C1A-CHA	-2.44	119.64	123.87
23	B	610	CLA	CHB-C4A-NA	2.44	127.92	124.40
25	c	515	BCR	C39-C30-C25	-2.44	106.42	110.24
32	d	407[A]	LHG	O8-C23-O10	-2.43	117.54	123.63
25	k	101	BCR	C15-C14-C13	-2.43	123.87	127.28
23	b	616	CLA	C3B-C4B-NB	2.43	112.70	110.53
26	A	412	SQD	O48-C23-O10	-2.43	117.55	123.63
23	B	605	CLA	CHC-C1C-C2C	-2.43	120.04	126.95
24	A	416[B]	PHO	O2A-CGA-CBA	2.43	119.25	111.83
24	a	415[A]	PHO	O1D-CGD-CBD	-2.43	121.04	124.72
32	D	406[B]	LHG	O8-C23-C24	2.43	119.24	111.83
23	b	609	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
26	a	410[B]	SQD	O48-C23-C24	2.43	119.24	111.83
23	C	512	CLA	C4B-C3B-C2B	-2.43	104.28	107.30
23	a	406[B]	CLA	CMC-C2C-C1C	2.43	128.83	125.03
23	b	610	CLA	CAC-C3C-C4C	2.43	127.95	124.79
23	b	614	CLA	O2A-CGA-CBA	2.42	119.23	111.83
23	b	601	CLA	O2A-CGA-CBA	2.42	119.23	111.83
23	b	604	CLA	O2A-CGA-CBA	2.42	119.23	111.83
23	C	511	CLA	CMC-C2C-C1C	2.42	128.82	125.03
23	C	507	CLA	CGD-CBD-CAD	-2.42	103.00	110.85
25	C	516	BCR	C11-C10-C9	-2.42	123.88	127.28
29	D	405[A]	PL9	C20-C19-C21	2.42	119.43	115.23
23	C	507	CLA	C4C-C3C-C2C	-2.42	103.37	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	C4-C3-C5	2.42	119.43	115.23
23	A	405[B]	CLA	OBD-CAD-C3D	-2.42	122.76	128.42
23	D	402[B]	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
23	b	606	CLA	CMC-C2C-C1C	2.42	128.82	125.03
23	B	616	CLA	CHD-C4C-NC	2.42	127.98	124.23
23	b	611	CLA	C7-C6-C5	-2.42	106.82	113.26
23	B	601	CLA	C4B-C3B-C2B	-2.42	104.30	107.30
25	B	619	BCR	C24-C23-C22	-2.42	122.66	126.23
25	Y	101	BCR	C38-C26-C25	-2.42	121.85	124.48
23	B	602	CLA	CMA-C3A-C4A	-2.42	105.28	111.77
32	D	407[B]	LHG	O8-C23-O10	-2.42	117.58	123.63
23	b	602	CLA	CMA-C3A-C2A	-2.42	104.64	113.98
23	b	602	CLA	C11-C10-C8	-2.41	107.94	115.97
23	a	406[B]	CLA	C2A-C1A-CHA	-2.41	119.68	123.87
25	Y	101	BCR	C40-C30-C25	-2.41	106.46	110.24
23	c	507	CLA	CHC-C1C-C2C	-2.41	120.08	126.95
23	A	408	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
25	c	514	BCR	C20-C21-C22	-2.41	123.89	127.28
25	B	619	BCR	C3-C4-C5	-2.41	109.75	114.06
40	V	201	HEC	C2A-C1A-NA	-2.41	108.00	110.32
25	b	619	BCR	C39-C30-C25	-2.41	106.46	110.24
23	B	616	CLA	CBC-CAC-C3C	-2.41	105.89	112.42
29	D	405[B]	PL9	C7-C8-C9	-2.41	122.68	126.83
23	c	502	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
23	c	512	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
23	B	610	CLA	CHD-C4C-NC	2.41	127.96	124.23
33	c	520	LMG	O8-C28-O10	-2.41	117.61	123.63
24	A	416[B]	PHO	CMB-C2B-C3B	2.40	129.49	124.68
23	c	505	CLA	C4B-C3B-C2B	-2.40	104.31	107.30
23	d	403	CLA	C4B-C3B-C2B	-2.40	104.31	107.30
26	b	620	SQD	O48-C23-C24	2.40	119.16	111.83
23	b	611	CLA	CAC-C3C-C4C	2.40	127.92	124.79
35	H	102	DGD	C3B-C2B-C1B	-2.40	104.89	113.69
35	C	517[B]	DGD	O3G-C3G-C2G	-2.40	104.98	110.82
25	b	618	BCR	C8-C7-C6	-2.40	120.58	127.00
23	b	608	CLA	C2A-C1A-CHA	-2.40	119.70	123.87
23	C	503	CLA	CMC-C2C-C1C	2.40	128.78	125.03
31	A	420	LMT	O5'-C5'-C4'	2.40	114.68	109.72
23	a	404[B]	CLA	C4-C3-C5	2.40	119.39	115.23
24	a	407[B]	PHO	CMB-C2B-C3B	2.40	129.47	124.68
24	a	407[A]	PHO	CMA-C3A-C4A	-2.40	109.45	114.61
29	D	405[A]	PL9	C40-C39-C41	2.40	119.39	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	CMA-C3A-C2A	-2.40	104.72	113.98
23	a	406[B]	CLA	C4B-C3B-C2B	-2.40	104.32	107.30
23	c	512	CLA	CHB-C4A-NA	2.40	127.86	124.40
23	B	613	CLA	CHD-C4C-NC	2.40	127.94	124.23
27	B	623	GOL	C3-C2-C1	-2.39	103.01	111.80
26	b	620	SQD	O47-C7-O49	-2.39	118.11	123.70
25	Y	101	BCR	C28-C27-C26	-2.39	109.79	114.06
32	L	101[B]	LHG	O8-C23-O10	-2.39	117.64	123.63
23	B	611	CLA	CMB-C2B-C3B	2.39	132.18	126.55
35	c	516[A]	DGD	C3G-C2G-C1G	-2.39	106.21	111.78
25	b	617	BCR	C16-C17-C18	-2.39	123.92	127.28
29	D	405[B]	PL9	C20-C19-C21	2.39	119.38	115.23
23	C	513	CLA	C2A-C1A-CHA	-2.39	119.72	123.87
23	c	507	CLA	CBC-CAC-C3C	-2.39	105.95	112.42
26	a	410[A]	SQD	O48-C23-C24	2.39	119.11	111.83
25	K	102	BCR	C29-C30-C25	2.39	113.90	110.44
38	F	102	HEM	C4C-NC-C1C	2.38	109.70	105.82
40	V	201	HEC	CBA-CAA-C2A	-2.38	105.95	112.53
23	C	502	CLA	O2A-CGA-CBA	2.38	119.10	111.83
23	A	406[A]	CLA	CAC-C3C-C4C	2.38	127.89	124.79
23	B	601	CLA	C3B-C4B-NB	2.38	112.66	110.53
31	b	621	LMT	C2'-C3'-C4'	2.38	115.08	109.68
23	C	503	CLA	C4-C3-C5	2.38	119.36	115.23
23	C	513	CLA	CHC-C1C-C2C	-2.38	120.19	126.95
23	B	608	CLA	CBC-CAC-C3C	-2.38	105.97	112.42
23	C	513	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
35	C	518[A]	DGD	C2G-O2G-C1B	-2.38	112.11	117.80
23	c	505	CLA	CHD-C4C-NC	2.38	127.91	124.23
23	A	405[B]	CLA	C1-C2-C3	-2.37	122.31	126.20
23	b	608	CLA	CMA-C3A-C4A	-2.37	105.39	111.77
23	B	610	CLA	C1-C2-C3	-2.37	122.31	126.20
24	a	415[B]	PHO	C4A-C3A-C2A	-2.37	100.58	102.84
25	b	618	BCR	C37-C22-C23	2.37	121.71	118.09
25	t	102	BCR	C29-C28-C27	-2.37	106.07	111.28
32	d	406[A]	LHG	C6-C5-C4	-2.37	106.27	111.78
24	a	415[A]	PHO	C1A-C2A-C3A	-2.36	100.59	102.84
25	Y	101	BCR	C36-C18-C19	2.36	121.69	118.09
23	B	602	CLA	C1-O2A-CGA	2.36	122.36	116.65
24	A	416[A]	PHO	C4D-CHA-CBD	2.36	109.59	108.45
38	F	102	HEM	O2D-CGD-CBD	2.36	121.46	114.00
33	m	101	LMG	O7-C10-O9	-2.36	118.19	123.70
23	C	510	CLA	C4-C3-C5	2.36	119.32	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	CAC-C3C-C4C	2.36	127.86	124.79
24	a	415[A]	PHO	O2A-CGA-CBA	2.36	119.03	111.83
23	B	608	CLA	CHD-C4C-NC	2.36	127.89	124.23
23	b	612	CLA	CHD-C4C-NC	2.36	127.89	124.23
23	D	403	CLA	O2A-CGA-CBA	2.36	119.03	111.83
25	y	101	BCR	C15-C14-C13	-2.36	123.97	127.28
23	a	408	CLA	C4B-C3B-C2B	-2.36	104.37	107.30
26	F	103	SQD	O5-C1-C2	-2.36	105.53	110.37
29	D	405[A]	PL9	C7-C8-C9	-2.36	122.77	126.83
38	F	102	HEM	CHA-C4D-ND	2.36	127.28	124.37
23	A	405[B]	CLA	O2A-CGA-O1A	-2.36	117.74	123.63
23	C	507	CLA	CMB-C2B-C1B	2.35	129.00	125.42
23	d	402[A]	CLA	CMB-C2B-C1B	2.35	129.00	125.42
23	A	404[B]	CLA	CHB-C1B-C2B	-2.35	120.60	127.43
23	A	406[B]	CLA	C4-C3-C5	2.35	119.31	115.23
23	C	508	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
33	C	521	LMG	C9-C8-C7	-2.35	106.31	111.78
23	B	615	CLA	C11-C10-C8	-2.35	108.16	115.97
23	c	512	CLA	CMC-C2C-C1C	2.35	128.70	125.03
29	d	405[B]	PL9	C45-C44-C46	2.35	119.30	115.23
26	F	103	SQD	O5-C1-O6	2.35	115.59	110.04
25	A	409	BCR	C8-C7-C6	-2.34	120.73	127.00
23	c	509	CLA	C4-C3-C2	-2.34	117.61	123.63
23	b	615	CLA	CHA-C1A-NA	-2.34	121.09	126.39
23	A	405[B]	CLA	CAC-C3C-C4C	2.34	127.83	124.79
25	D	404	BCR	C30-C25-C24	2.34	121.99	115.65
35	C	518[A]	DGD	O2G-C1B-O1B	-2.34	118.24	123.70
23	a	405[B]	CLA	C1-C2-C3	-2.34	122.37	126.20
25	y	101	BCR	C1-C6-C7	2.34	121.99	115.65
29	d	405[A]	PL9	C7-C8-C9	-2.34	122.81	126.83
31	B	631	LMT	O5'-C5'-C4'	2.34	114.55	109.72
23	c	503	CLA	OBD-CAD-C3D	-2.33	122.96	128.42
26	f	102	SQD	O48-C23-O10	-2.33	117.79	123.63
29	a	413[A]	PL9	C20-C19-C21	2.33	119.28	115.23
23	C	504	CLA	C2A-C1A-CHA	-2.33	119.82	123.87
25	C	516	BCR	C3-C4-C5	-2.33	109.90	114.06
23	B	605	CLA	C2A-C1A-CHA	-2.33	119.82	123.87
25	b	618	BCR	C33-C5-C6	-2.33	121.94	124.48
23	c	507	CLA	C3B-C4B-NB	2.33	112.61	110.53
25	d	404	BCR	C16-C15-C14	-2.33	118.75	123.52
23	a	404[B]	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
26	A	410[A]	SQD	O9-S-O7	-2.33	106.25	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	f	101	HEM	C4C-NC-C1C	2.33	109.62	105.82
25	c	514	BCR	C29-C30-C25	2.33	113.82	110.44
23	a	408	CLA	CMB-C2B-C1B	2.33	128.96	125.42
23	C	505	CLA	C4C-C3C-C2C	-2.33	103.50	106.89
26	A	410[A]	SQD	O8-S-C6	2.33	110.46	105.97
23	D	402[A]	CLA	CMC-C2C-C1C	2.33	128.67	125.03
35	C	517[B]	DGD	C3G-C2G-C1G	-2.33	106.36	111.78
29	A	414[A]	PL9	C12-C13-C14	-2.33	122.30	127.62
25	a	409	BCR	C7-C8-C9	-2.32	122.80	126.23
23	c	503	CLA	O2A-CGA-CBA	2.32	118.92	111.83
23	C	511	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
23	B	615	CLA	O2A-CGA-CBA	2.32	118.91	111.83
23	a	405[B]	CLA	C2A-C1A-CHA	-2.32	119.84	123.87
31	m	103	LMT	C1'-O5'-C5'	-2.32	109.19	113.72
23	c	509	CLA	CMC-C2C-C1C	2.32	128.66	125.03
35	C	517[A]	DGD	O6E-C5E-C4E	2.32	113.88	109.70
35	C	517[A]	DGD	C3G-C2G-C1G	-2.32	106.38	111.78
35	c	517[B]	DGD	O2G-C1B-O1B	-2.31	118.29	123.70
23	c	510	CLA	C4-C3-C2	-2.31	117.68	123.63
29	D	405[B]	PL9	C47-C48-C49	-2.31	119.93	127.64
23	B	614	CLA	CMA-C3A-C2A	-2.31	105.04	113.98
25	k	101	BCR	C36-C18-C19	2.31	121.62	118.09
23	B	605	CLA	OBD-CAD-C3D	-2.31	123.01	128.42
34	b	622	HTG	O5-C1-C2	2.31	113.50	110.32
32	d	406[B]	LHG	C5-O7-C7	-2.31	112.27	117.80
23	b	608	CLA	CAA-C2A-C3A	-2.31	106.76	113.00
25	b	619	BCR	C16-C15-C14	-2.31	118.80	123.52
26	f	102	SQD	O5-C5-C4	2.31	113.86	109.70
35	h	102	DGD	O3G-C1D-C2D	2.31	111.78	108.27
23	c	502	CLA	C2A-C1A-CHA	-2.31	119.86	123.87
29	a	413[B]	PL9	C40-C39-C41	2.31	119.23	115.23
23	d	403	CLA	C2A-C1A-CHA	-2.31	119.86	123.87
23	A	408	CLA	CHB-C4A-NA	2.31	127.73	124.40
23	B	608	CLA	O2A-CGA-CBA	2.30	118.86	111.83
23	A	405[B]	CLA	CAA-CBA-CGA	2.30	119.75	113.21
26	A	410[B]	SQD	O9-S-O7	-2.30	106.33	113.82
26	a	411	SQD	C1-O5-C5	2.30	118.22	113.72
24	A	407[A]	PHO	CMB-C2B-C3B	2.30	129.29	124.68
23	c	511	CLA	CAC-C3C-C4C	2.30	127.79	124.79
38	F	102	HEM	C4C-CHD-C1D	-2.30	121.12	126.02
23	a	408	CLA	CHC-C1C-C2C	-2.30	120.41	126.95
26	a	410[B]	SQD	O9-S-C6	2.30	110.19	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414[A]	PL9	C45-C44-C46	2.30	119.22	115.23
29	a	413[B]	PL9	C45-C44-C46	2.30	119.22	115.23
26	a	410[A]	SQD	O9-S-O7	-2.30	106.34	113.82
31	B	629	LMT	O5'-C5'-C4'	2.30	114.48	109.72
23	c	510	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
23	b	604	CLA	C4C-C3C-C2C	-2.30	103.54	106.89
23	b	606	CLA	CMB-C2B-C1B	2.30	128.92	125.42
23	D	402[A]	CLA	CMB-C2B-C1B	2.30	128.92	125.42
23	C	513	CLA	CMA-C3A-C4A	-2.30	105.60	111.77
23	b	616	CLA	C2A-C1A-CHA	-2.30	119.88	123.87
23	b	609	CLA	C7-C6-C5	-2.30	107.14	113.26
31	B	631	LMT	O1'-C1'-C2'	2.29	111.76	108.27
23	D	402[B]	CLA	CBC-CAC-C3C	-2.29	106.20	112.42
23	B	616	CLA	CMC-C2C-C1C	2.29	128.62	125.03
23	C	511	CLA	C4C-C3C-C2C	-2.29	103.56	106.89
23	A	404[B]	CLA	CMC-C2C-C1C	2.29	128.61	125.03
23	A	408	CLA	CBC-CAC-C3C	-2.29	106.22	112.42
23	b	608	CLA	CHB-C4A-NA	2.29	127.70	124.40
24	A	407[B]	PHO	CBC-CAC-C3C	-2.29	109.60	112.87
29	d	405[A]	PL9	C20-C19-C21	2.29	119.20	115.23
23	B	608	CLA	C11-C10-C8	-2.28	108.37	115.97
23	b	608	CLA	C11-C10-C8	-2.28	108.37	115.97
35	h	102	DGD	O4D-C4D-C3D	-2.28	104.99	110.38
25	B	618	BCR	C37-C22-C23	2.28	121.57	118.09
32	E	101[A]	LHG	O7-C7-O9	-2.28	118.37	123.70
23	b	609	CLA	CMA-C3A-C4A	-2.28	105.64	111.77
35	H	102	DGD	C1E-O6E-C5E	-2.28	109.27	113.72
23	A	408	CLA	C2A-C1A-CHA	-2.28	119.91	123.87
24	A	407[B]	PHO	O2A-CGA-O1A	-2.28	117.92	123.63
23	b	607	CLA	C2A-C1A-CHA	-2.28	119.91	123.87
23	A	404[B]	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
23	b	613	CLA	CMC-C2C-C1C	2.28	128.59	125.03
33	z	101	LMG	C8-O7-C10	-2.28	112.35	117.80
23	c	508	CLA	C2A-C1A-CHA	-2.28	119.92	123.87
23	C	513	CLA	CMC-C2C-C1C	2.27	128.59	125.03
23	a	404[B]	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
25	a	409	BCR	C33-C5-C6	-2.27	122.00	124.48
23	c	508	CLA	CMC-C2C-C1C	2.27	128.59	125.03
23	B	609	CLA	C16-C15-C13	-2.27	108.41	115.97
23	a	404[A]	CLA	C7-C6-C5	-2.27	107.20	113.26
23	a	405[A]	CLA	C2A-C1A-CHA	-2.27	119.92	123.87
23	A	404[B]	CLA	C4-C3-C5	2.27	119.17	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	C2A-C1A-CHA	-2.27	119.93	123.87
23	D	402[B]	CLA	CMB-C2B-C1B	2.27	128.88	125.42
23	d	403	CLA	CMA-C3A-C2A	-2.27	105.22	113.98
25	t	102	BCR	C7-C6-C5	-2.27	116.33	121.56
29	d	405[A]	PL9	C47-C48-C49	-2.27	120.08	127.64
23	B	602	CLA	CHB-C4A-NA	2.27	127.67	124.40
25	h	101	BCR	C39-C30-C25	-2.27	106.69	110.24
24	a	407[B]	PHO	C4A-C3A-C2A	-2.26	100.68	102.84
31	m	103	LMT	C3B-C4B-C5B	-2.26	106.13	110.23
25	C	516	BCR	C38-C26-C25	-2.26	122.01	124.48
23	b	611	CLA	O2A-CGA-CBA	2.26	118.74	111.83
23	c	513	CLA	C4-C3-C5	2.26	119.16	115.23
25	c	515	BCR	C29-C30-C25	2.26	113.73	110.44
26	f	102	SQD	O6-C1-C2	2.26	111.71	108.27
23	B	611	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
32	A	419[A]	LHG	O4-P-O5	2.26	122.96	112.44
25	C	515	BCR	C29-C30-C25	2.26	113.72	110.44
33	c	519	LMG	O8-C28-O10	-2.26	117.98	123.63
23	c	506	CLA	C4-C3-C5	2.26	119.15	115.23
33	d	411	LMG	O7-C10-O9	-2.26	118.42	123.70
23	c	504	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
23	b	611	CLA	CMB-C2B-C1B	2.26	128.85	125.42
23	a	405[A]	CLA	CMC-C2C-C1C	2.26	128.56	125.03
23	b	607	CLA	CAA-CBA-CGA	2.26	119.61	113.21
23	C	504	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
23	B	613	CLA	C2A-C1A-CHA	-2.25	119.95	123.87
23	D	402[A]	CLA	CED-O2D-CGD	2.25	121.03	115.92
34	b	623	HTG	O5-C1-C2	2.25	113.42	110.32
23	a	405[B]	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
32	d	406[A]	LHG	O8-C23-O10	-2.25	117.99	123.63
23	C	512	CLA	O2A-CGA-CBA	2.25	118.71	111.83
25	T	101	BCR	C7-C6-C5	-2.25	116.37	121.56
25	A	409	BCR	C33-C5-C6	-2.25	122.03	124.48
25	D	404	BCR	C3-C4-C5	-2.25	110.04	114.06
23	c	512	CLA	CBA-CAA-C2A	-2.25	107.10	113.79
23	B	603	CLA	CMC-C2C-C1C	2.25	128.55	125.03
23	B	612	CLA	C2A-C1A-CHA	-2.25	119.97	123.87
24	a	407[A]	PHO	C1-C2-C3	-2.25	122.51	126.20
23	c	511	CLA	C2A-C1A-CHA	-2.25	119.97	123.87
25	D	404	BCR	C39-C30-C25	-2.25	106.72	110.24
33	B	621	LMG	C8-O7-C10	-2.25	112.42	117.80
29	A	414[B]	PL9	C47-C48-C49	-2.25	120.15	127.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	405[A]	PL9	C12-C13-C14	-2.25	122.48	127.62
25	Y	101	BCR	C11-C10-C9	-2.25	124.13	127.28
23	b	615	CLA	CAC-C3C-C4C	2.25	127.71	124.79
23	A	405[A]	CLA	O2A-CGA-CBA	2.25	118.68	111.83
29	A	414[A]	PL9	C35-C34-C33	-2.25	117.86	123.63
29	A	414[B]	PL9	C7-C3-C4	2.24	118.76	116.91
23	A	406[B]	CLA	CAC-C3C-C4C	2.24	127.71	124.79
23	B	611	CLA	OBD-CAD-C3D	-2.24	123.17	128.42
23	b	601	CLA	CMC-C2C-C1C	2.24	128.54	125.03
23	C	508	CLA	CAC-C3C-C4C	2.24	127.71	124.79
33	B	621	LMG	C7-O1-C1	-2.24	108.99	113.80
23	a	404[B]	CLA	CHB-C1B-C2B	-2.24	120.92	127.43
23	A	404[A]	CLA	CHD-C4C-NC	2.24	127.71	124.23
23	d	402[A]	CLA	CMA-C3A-C2A	-2.24	105.31	113.98
23	B	609	CLA	CAC-C3C-C4C	2.24	127.71	124.79
24	A	416[A]	PHO	O1D-CGD-CBD	-2.24	121.33	124.72
23	b	602	CLA	CHC-C1C-C2C	-2.24	120.58	126.95
25	b	617	BCR	C20-C21-C22	-2.24	124.14	127.28
25	Y	101	BCR	C34-C9-C8	2.24	121.50	118.09
23	a	406[B]	CLA	CAC-C3C-C4C	2.24	127.70	124.79
29	d	405[B]	PL9	C15-C14-C16	2.24	119.11	115.23
23	b	610	CLA	CHB-C4A-NA	2.24	127.63	124.40
31	F	101	LMT	C3B-C4B-C5B	-2.24	106.18	110.23
23	C	503	CLA	CAC-C3C-C4C	2.24	127.70	124.79
35	C	517[B]	DGD	O1G-C1A-C2A	2.24	118.65	111.83
23	b	606	CLA	O2A-CGA-CBA	2.23	118.65	111.83
33	c	519	LMG	C8-O7-C10	-2.23	112.45	117.80
23	b	604	CLA	C6-C5-C3	-2.23	108.03	113.47
23	b	601	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
23	C	514	CLA	C4-C3-C5	2.23	119.11	115.23
38	F	102	HEM	CHD-C1D-C2D	-2.23	121.50	125.03
23	B	615	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
23	b	615	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
26	F	103	SQD	C46-C45-C44	-2.23	106.58	111.78
23	B	616	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
23	B	601	CLA	CAA-C2A-C3A	-2.23	106.97	113.00
23	B	614	CLA	CAA-C2A-C3A	-2.23	106.97	113.00
24	a	415[B]	PHO	CBA-CAA-C2A	-2.23	107.21	113.78
23	d	402[B]	CLA	CMB-C2B-C1B	2.23	128.81	125.42
23	a	408	CLA	C3B-C4B-NB	2.23	112.52	110.53
25	b	619	BCR	C7-C6-C5	2.23	126.69	121.56
23	C	511	CLA	CAC-C3C-C4C	2.23	127.69	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	CED-O2D-CGD	2.23	120.97	115.92
24	A	416[A]	PHO	CED-O2D-CGD	2.23	120.97	115.92
35	c	517[A]	DGD	O1G-C1A-O1A	-2.23	118.06	123.63
23	c	506	CLA	CAA-CBA-CGA	2.23	119.53	113.21
26	a	411	SQD	O7-S-C6	2.23	110.08	106.76
26	a	411	SQD	O47-C7-O49	-2.23	118.50	123.70
25	t	102	BCR	C35-C13-C12	2.22	121.49	118.09
23	B	614	CLA	OBD-CAD-C3D	-2.22	123.22	128.42
32	d	413[A]	LHG	O7-C7-O9	-2.22	118.51	123.70
25	d	404	BCR	C3-C4-C5	-2.22	110.09	114.06
23	c	502	CLA	C4C-C3C-C2C	-2.22	103.66	106.89
23	C	509	CLA	CMC-C2C-C1C	2.22	128.50	125.03
26	A	412	SQD	C1-C2-C3	-2.22	105.34	110.01
23	A	405[A]	CLA	C4C-C3C-C2C	-2.22	103.66	106.89
25	c	514	BCR	C36-C18-C17	-2.22	119.22	122.82
32	L	101[B]	LHG	C5-O7-C7	-2.22	112.49	117.80
29	a	413[B]	PL9	C12-C13-C14	-2.22	122.55	127.62
40	V	201	HEC	CAD-CBD-CGD	-2.22	107.78	113.67
23	c	504	CLA	CAA-C2A-C3A	-2.22	107.01	113.00
31	t	101	LMT	C1-O1'-C1'	2.22	117.47	113.68
23	B	601	CLA	CMC-C2C-C1C	2.22	128.50	125.03
32	d	406[A]	LHG	O8-C23-C24	2.21	118.59	111.83
23	D	402[A]	CLA	CMA-C3A-C4A	-2.21	105.82	111.77
23	b	606	CLA	C2A-C1A-CHA	-2.21	120.03	123.87
23	B	612	CLA	CHD-C4C-NC	2.21	127.66	124.23
23	a	404[B]	CLA	CMA-C3A-C2A	-2.21	105.44	113.98
26	B	620	SQD	O9-S-O7	-2.21	106.64	113.82
29	a	413[A]	PL9	C35-C34-C33	-2.21	117.95	123.63
23	C	504	CLA	O2A-CGA-CBA	2.21	118.57	111.83
31	B	627	LMT	O1B-C4'-C5'	-2.21	103.68	109.48
23	B	612	CLA	CMA-C3A-C2A	-2.21	105.44	113.98
26	F	103	SQD	O48-C23-O10	-2.21	118.11	123.63
23	c	504	CLA	CMC-C2C-C1C	2.21	128.48	125.03
24	A	407[A]	PHO	C4-C3-C5	2.21	119.06	115.23
25	k	101	BCR	C11-C10-C9	-2.21	124.18	127.28
23	B	601	CLA	C2A-C1A-CHA	-2.21	120.04	123.87
25	d	404	BCR	C30-C25-C24	2.21	121.64	115.65
23	b	606	CLA	CHB-C1B-C2B	-2.20	121.03	127.43
25	C	515	BCR	C40-C30-C25	-2.20	106.79	110.24
23	C	506	CLA	CHA-C1A-NA	-2.20	121.40	126.39
23	B	601	CLA	CHB-C4A-NA	2.20	127.58	124.40
23	D	402[B]	CLA	CHD-C4C-NC	2.20	127.64	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	101	BCR	C34-C9-C10	-2.20	119.25	122.82
23	C	509	CLA	CAA-C2A-C3A	-2.20	107.06	113.00
23	B	604	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
32	d	413[B]	LHG	O7-C7-O9	-2.20	118.57	123.70
26	a	411	SQD	O5-C5-C4	2.19	113.65	109.70
35	C	518[A]	DGD	O1G-C1A-C2A	2.19	118.53	111.83
32	E	101[B]	LHG	O7-C7-O9	-2.19	118.58	123.70
35	c	517[B]	DGD	C1D-O6D-C5D	2.19	118.00	113.72
35	c	516[A]	DGD	O3G-C3G-C2G	-2.19	105.48	110.82
29	d	405[A]	PL9	C51-C49-C50	2.19	119.63	114.59
25	B	617	BCR	C21-C20-C19	-2.19	116.85	123.20
26	F	103	SQD	O8-S-O7	-2.19	105.92	111.40
23	B	608	CLA	C2A-C1A-CHA	-2.19	120.07	123.87
23	b	614	CLA	CHB-C1B-NB	-2.19	120.77	124.05
29	A	414[A]	PL9	C25-C24-C26	2.18	119.02	115.23
29	d	405[B]	PL9	C20-C19-C21	2.18	119.02	115.23
23	B	605	CLA	CAA-C2A-C3A	-2.18	107.10	113.00
24	a	415[B]	PHO	C1A-C2A-C3A	-2.18	100.76	102.84
23	B	606	CLA	CHB-C1B-C2B	-2.18	121.09	127.43
23	D	403	CLA	C1-C2-C3	-2.18	122.62	126.20
23	C	509	CLA	CHD-C4C-NC	2.18	127.61	124.23
38	f	101	HEM	CHA-C4D-C3D	-2.18	121.21	125.23
23	b	613	CLA	CAC-C3C-C4C	2.18	127.63	124.79
40	V	201	HEC	CHA-C1A-NA	2.18	126.83	124.45
23	C	513	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
23	c	508	CLA	CMA-C3A-C2A	-2.18	105.56	113.98
23	C	505	CLA	C4-C3-C5	2.18	119.01	115.23
23	b	613	CLA	CMB-C2B-C1B	2.18	128.73	125.42
23	b	616	CLA	C4-C3-C5	2.18	119.01	115.23
23	C	513	CLA	C4B-C3B-C2B	-2.18	104.60	107.30
23	C	507	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
38	F	102	HEM	CHA-C1A-NA	2.17	127.80	123.86
24	A	416[B]	PHO	CMA-C3A-C4A	-2.17	109.92	114.61
23	b	606	CLA	CBC-CAC-C3C	-2.17	106.53	112.42
29	A	414[B]	PL9	C35-C34-C33	-2.17	118.05	123.63
24	a	407[A]	PHO	O2D-CGD-O1D	-2.17	119.62	123.85
23	b	602	CLA	O2A-CGA-CBA	2.17	118.46	111.83
32	d	413[B]	LHG	C5-O7-C7	-2.17	112.60	117.80
23	A	405[B]	CLA	CMC-C2C-C1C	2.17	128.43	125.03
23	b	601	CLA	CAC-C3C-C4C	2.17	127.61	124.79
23	A	405[B]	CLA	O2A-CGA-CBA	2.17	118.45	111.83
25	d	404	BCR	C29-C28-C27	-2.17	106.51	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	CHB-C1B-C2B	-2.17	121.13	127.43
23	d	402[B]	CLA	CAA-C2A-C3A	-2.17	107.14	113.00
23	B	613	CLA	CMA-C3A-C4A	-2.17	105.95	111.77
23	B	610	CLA	CMA-C3A-C2A	-2.17	105.60	113.98
23	B	612	CLA	C7-C6-C5	-2.17	107.49	113.26
23	A	404[B]	CLA	CMA-C3A-C2A	-2.17	105.61	113.98
23	C	513	CLA	O1D-CGD-CBD	-2.17	120.25	124.52
25	B	617	BCR	C29-C30-C25	2.17	113.58	110.44
35	c	516[A]	DGD	O6D-C1D-O3G	-2.16	104.93	110.04
24	a	415[A]	PHO	C4-C3-C2	-2.16	118.07	123.63
29	A	414[B]	PL9	C10-C9-C8	-2.16	118.07	123.63
29	d	405[A]	PL9	O2-C1-C6	-2.16	117.04	120.48
25	c	514	BCR	C37-C22-C23	2.16	121.39	118.09
24	A	416[A]	PHO	OBD-CAD-C3D	-2.16	124.52	127.89
25	k	101	BCR	C16-C17-C18	-2.16	124.25	127.28
24	a	407[B]	PHO	OBD-CAD-C3D	-2.16	124.52	127.89
23	D	402[A]	CLA	OBD-CAD-C3D	-2.16	123.37	128.42
35	C	517[B]	DGD	O1G-C1A-O1A	-2.16	118.22	123.63
23	A	406[B]	CLA	CHB-C4A-NA	2.16	127.52	124.40
26	A	412	SQD	O6-C1-C2	2.16	111.55	108.27
23	a	406[A]	CLA	CBC-CAC-C3C	-2.16	106.57	112.42
31	m	103	LMT	O5B-C5B-C6B	2.16	111.78	106.44
23	c	512	CLA	CHA-C1A-NA	-2.16	121.51	126.39
25	c	514	BCR	C38-C26-C25	-2.15	122.13	124.48
23	b	616	CLA	CHB-C1B-C2B	-2.15	121.18	127.43
25	K	102	BCR	C36-C18-C19	2.15	121.38	118.09
33	B	621	LMG	O7-C10-O9	-2.15	118.67	123.70
23	c	512	CLA	C4B-C3B-C2B	-2.15	104.63	107.30
35	C	517[A]	DGD	O3G-C3G-C2G	-2.15	105.59	110.82
24	A	407[B]	PHO	C4A-C3A-C2A	-2.15	100.79	102.84
23	b	613	CLA	C2A-C1A-CHA	-2.15	120.14	123.87
26	A	412	SQD	O6-C44-C45	-2.15	105.59	110.82
23	b	614	CLA	CED-O2D-CGD	2.15	120.79	115.92
25	C	516	BCR	C33-C5-C6	-2.15	122.14	124.48
29	D	405[A]	PL9	C27-C28-C29	-2.15	122.71	127.62
25	A	409	BCR	C28-C27-C26	-2.15	110.22	114.06
23	c	507	CLA	C7-C6-C5	-2.15	107.54	113.26
25	K	102	BCR	C39-C30-C25	-2.15	106.88	110.24
35	c	516[A]	DGD	O1G-C1A-O1A	-2.15	118.26	123.63
31	F	101	LMT	C2'-C3'-C4'	2.15	114.55	109.68
32	d	407[B]	LHG	O8-C23-O10	-2.14	118.27	123.63
25	B	619	BCR	C38-C26-C25	-2.14	122.14	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	CHA-C1A-NA	-2.14	121.54	126.39
25	a	409	BCR	C15-C16-C17	-2.14	119.13	123.52
25	D	404	BCR	C33-C5-C6	-2.14	122.15	124.48
23	B	613	CLA	C4-C3-C2	-2.14	118.12	123.63
25	k	101	BCR	C34-C9-C8	2.14	121.36	118.09
23	d	402[A]	CLA	CHD-C4C-NC	2.14	127.55	124.23
23	c	506	CLA	C2A-C1A-CHA	-2.14	120.15	123.87
35	C	518[B]	DGD	O2G-C1B-O1B	-2.14	118.70	123.70
25	D	404	BCR	C21-C20-C19	-2.14	117.00	123.20
23	B	615	CLA	CHA-C1A-NA	-2.14	121.55	126.39
31	F	101	LMT	O1'-C1'-C2'	2.14	111.52	108.27
23	B	609	CLA	C2A-C1A-CHA	-2.14	120.16	123.87
23	c	510	CLA	OBD-CAD-C3D	-2.14	123.42	128.42
23	c	504	CLA	CMA-C3A-C2A	-2.14	105.72	113.98
23	c	504	CLA	O1D-CGD-CBD	-2.14	120.31	124.52
33	a	416	LMG	O7-C10-O9	-2.14	118.71	123.70
23	B	611	CLA	CAA-C2A-C3A	-2.14	107.23	113.00
25	Y	101	BCR	C24-C23-C22	-2.14	123.08	126.23
23	b	607	CLA	CMB-C2B-C1B	2.14	128.67	125.42
23	c	509	CLA	C2A-C1A-CHA	-2.13	120.16	123.87
23	C	514	CLA	CMB-C2B-C1B	2.13	128.67	125.42
23	B	603	CLA	C5-C3-C2	-2.13	116.38	121.17
29	d	405[B]	PL9	C35-C34-C36	2.13	118.93	115.23
23	b	610	CLA	C4-C3-C2	-2.13	118.15	123.63
24	A	407[B]	PHO	C4-C3-C5	2.13	118.93	115.23
23	b	616	CLA	C1-C2-C3	-2.13	122.70	126.20
32	L	101[A]	LHG	O4-P-O5	2.13	122.36	112.44
24	A	416[A]	PHO	C6-C5-C3	-2.13	108.28	113.47
33	B	621	LMG	C12-C11-C10	-2.13	105.89	113.69
23	B	602	CLA	CMA-C3A-C2A	-2.13	105.74	113.98
23	c	505	CLA	CMA-C3A-C4A	-2.13	106.05	111.77
23	a	406[A]	CLA	C4-C3-C5	2.13	118.92	115.23
23	C	513	CLA	C4-C3-C2	-2.13	118.16	123.63
23	B	606	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
34	b	622	HTG	C6-C5-C4	-2.13	107.80	113.02
29	A	414[B]	PL9	C2-C3-C4	2.13	121.63	118.78
23	b	601	CLA	CAA-C2A-C3A	-2.12	107.26	113.00
23	b	609	CLA	O2D-CGD-O1D	-2.12	119.71	123.85
25	k	101	BCR	C3-C4-C5	-2.12	110.27	114.06
23	c	502	CLA	CAC-C3C-C4C	2.12	127.55	124.79
23	B	605	CLA	CAC-C3C-C2C	2.12	131.46	127.56
25	a	409	BCR	C8-C7-C6	-2.12	121.33	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	413[A]	PL9	C45-C44-C46	2.12	118.91	115.23
23	a	404[A]	CLA	CMB-C2B-C3B	2.12	131.54	126.55
23	b	615	CLA	C2A-C1A-CHA	-2.12	120.19	123.87
23	d	403	CLA	CGD-CBD-CAD	-2.12	103.98	110.85
23	c	505	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
23	A	406[A]	CLA	CHB-C4A-NA	2.12	127.46	124.40
25	Y	101	BCR	C3-C4-C5	-2.12	110.28	114.06
23	c	505	CLA	C3B-C4B-NB	2.12	112.42	110.53
35	c	517[B]	DGD	O1G-C1A-O1A	-2.12	118.33	123.63
23	C	513	CLA	CHB-C1B-C2B	-2.12	121.28	127.43
33	Z	101	LMG	C3-C4-C5	2.12	114.07	110.23
29	a	413[B]	PL9	C51-C49-C50	2.12	119.46	114.59
23	c	513	CLA	C1-O2A-CGA	2.12	121.77	116.65
23	b	608	CLA	C11-C12-C13	-2.12	108.93	115.97
23	B	616	CLA	OBD-CAD-C3D	-2.12	123.47	128.42
38	f	101	HEM	C3B-C4B-NB	-2.11	107.95	109.47
23	d	402[B]	CLA	CMA-C3A-C2A	-2.11	105.81	113.98
23	c	511	CLA	C4-C3-C2	-2.11	118.20	123.63
26	A	410[B]	SQD	O48-C23-O10	-2.11	118.34	123.63
23	b	616	CLA	OBD-CAD-C3D	-2.11	123.47	128.42
25	h	101	BCR	C16-C17-C18	-2.11	124.31	127.28
23	b	615	CLA	CMC-C2C-C1C	2.11	128.33	125.03
23	A	405[A]	CLA	CHB-C4A-NA	2.11	127.44	124.40
25	K	102	BCR	C32-C1-C6	-2.11	106.93	110.24
34	b	623	HTG	O5-C5-C6	2.11	111.67	106.44
32	b	629[A]	LHG	O7-C7-O9	-2.11	118.77	123.70
23	C	511	CLA	CHB-C4A-NA	2.11	127.44	124.40
23	c	501	CLA	C4-C3-C5	2.11	118.89	115.23
23	b	615	CLA	C6-C5-C3	-2.11	108.33	113.47
23	D	402[A]	CLA	CBC-CAC-C3C	-2.11	106.71	112.42
38	F	102	HEM	O2D-CGD-O1D	-2.11	117.92	123.33
24	A	416[B]	PHO	CED-O2D-CGD	2.11	120.69	115.92
23	A	404[A]	CLA	C7-C6-C5	-2.11	107.65	113.26
25	A	409	BCR	C16-C17-C18	-2.11	124.33	127.28
24	a	407[B]	PHO	CBA-CAA-C2A	-2.10	107.58	113.78
24	A	407[B]	PHO	O2D-CGD-O1D	-2.10	119.75	123.85
29	A	414[B]	PL9	C25-C24-C26	2.10	118.88	115.23
26	B	620	SQD	C44-O6-C1	-2.10	109.29	113.80
23	c	511	CLA	CMA-C3A-C4A	2.10	117.42	111.77
23	a	405[B]	CLA	CMC-C2C-C1C	2.10	128.32	125.03
23	a	405[A]	CLA	CHB-C4A-NA	2.10	127.43	124.40
29	d	405[A]	PL9	C45-C44-C46	2.10	118.87	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	416	LMG	O8-C28-C29	2.10	118.24	111.83
23	B	607	CLA	O2A-CGA-CBA	2.10	118.23	111.83
23	b	602	CLA	C4-C3-C5	2.10	118.87	115.23
25	k	101	BCR	C20-C21-C22	-2.10	124.34	127.28
35	c	516[A]	DGD	O1G-C1A-C2A	2.10	118.23	111.83
23	c	501	CLA	C2A-C1A-CHA	-2.10	120.23	123.87
23	a	406[A]	CLA	CAC-C3C-C4C	2.09	127.52	124.79
23	C	502	CLA	OBD-CAD-C3D	-2.09	123.52	128.42
31	B	627	LMT	O1B-C4'-C3'	2.09	112.55	107.23
23	C	514	CLA	C1-O2A-CGA	2.09	121.72	116.65
23	B	609	CLA	CHA-C1A-NA	-2.09	121.65	126.39
23	B	602	CLA	O2A-CGA-CBA	2.09	118.21	111.83
23	b	613	CLA	C16-C15-C13	-2.09	109.01	115.97
23	b	601	CLA	CHB-C1B-C2B	-2.09	121.36	127.43
23	b	608	CLA	C4-C3-C5	2.09	118.86	115.23
26	b	620	SQD	O5-C1-O6	2.09	114.98	110.04
23	d	402[A]	CLA	CBC-CAC-C3C	-2.09	106.75	112.42
23	b	613	CLA	C4-C3-C5	2.09	118.86	115.23
23	C	505	CLA	CAC-C3C-C4C	2.09	127.51	124.79
25	t	102	BCR	C39-C30-C25	-2.09	106.97	110.24
23	b	613	CLA	OBD-CAD-C3D	-2.09	123.54	128.42
25	a	409	BCR	C10-C11-C12	-2.09	117.15	123.20
23	c	504	CLA	CBC-CAC-C3C	-2.09	106.76	112.42
24	a	415[B]	PHO	CED-O2D-CGD	2.09	120.64	115.92
23	B	605	CLA	C3B-C4B-NB	2.08	112.39	110.53
29	d	405[A]	PL9	C2-C1-C6	2.08	121.48	119.00
23	B	607	CLA	C6-C7-C8	-2.08	109.04	115.97
23	a	404[B]	CLA	CMA-C3A-C4A	-2.08	106.17	111.77
23	b	616	CLA	CAC-C3C-C4C	2.08	127.50	124.79
23	B	608	CLA	CMB-C2B-C1B	2.08	128.59	125.42
23	A	404[B]	CLA	CBB-CAB-C3B	-2.08	117.12	127.53
31	a	417	LMT	O5B-C1B-C2B	2.08	114.65	110.37
23	A	406[B]	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
24	a	407[B]	PHO	C4-C3-C5	2.08	118.84	115.23
23	b	602	CLA	CHB-C4A-NA	2.08	127.40	124.40
29	A	414[A]	PL9	C53-C6-C1	2.08	119.54	115.28
23	B	611	CLA	C4-C3-C5	2.08	118.84	115.23
31	b	627	LMT	O1'-C1'-C2'	2.08	111.43	108.27
23	c	511	CLA	C1-O2A-CGA	2.08	121.68	116.65
24	a	407[B]	PHO	CAC-C3C-C4C	2.08	129.37	124.03
26	a	410[A]	SQD	C3-C4-C5	2.08	114.00	110.23
23	b	607	CLA	C11-C10-C8	-2.08	109.06	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	CAA-C2A-C3A	-2.08	107.39	113.00
23	C	512	CLA	OBD-CAD-C3D	-2.08	123.56	128.42
23	D	402[A]	CLA	CMA-C3A-C2A	-2.08	105.96	113.98
23	A	406[A]	CLA	CBC-CAC-C3C	-2.08	106.79	112.42
34	b	625	HTG	C1-C2-C3	-2.07	106.49	110.55
24	a	415[A]	PHO	O2A-CGA-O1A	-2.07	118.44	123.63
25	T	101	BCR	C39-C30-C25	-2.07	106.99	110.24
25	Y	101	BCR	C1-C6-C7	2.07	121.27	115.65
33	Z	101	LMG	C9-C8-C7	-2.07	106.96	111.78
23	c	507	CLA	C2A-C1A-CHA	-2.07	120.28	123.87
23	B	609	CLA	C1-O2A-CGA	2.07	121.66	116.65
26	b	620	SQD	C44-O6-C1	-2.07	109.36	113.80
23	B	605	CLA	CHA-C1A-NA	-2.07	121.71	126.39
26	a	411	SQD	O48-C23-O10	-2.07	118.46	123.63
23	b	602	CLA	CAA-CBA-CGA	-2.07	107.34	113.21
23	c	512	CLA	CMA-C3A-C4A	-2.06	106.22	111.77
31	M	101	LMT	O5B-C5B-C6B	2.06	111.56	106.44
23	B	616	CLA	C4-C3-C2	-2.06	118.33	123.63
25	h	101	BCR	C34-C9-C8	2.06	121.24	118.09
31	A	417	LMT	O1'-C1'-C2'	2.06	111.41	108.27
23	b	615	CLA	C11-C12-C13	-2.06	109.11	115.97
25	A	409	BCR	C11-C10-C9	-2.06	124.39	127.28
23	a	406[A]	CLA	CAA-CBA-CGA	2.06	119.06	113.21
23	a	406[B]	CLA	CHB-C4A-NA	2.06	127.38	124.40
23	B	607	CLA	C11-C10-C8	-2.06	109.11	115.97
23	C	503	CLA	C4B-C3B-C2B	-2.06	104.74	107.30
23	A	405[A]	CLA	C1-C2-C3	-2.06	122.82	126.20
23	c	501	CLA	C1-O2A-CGA	2.06	121.63	116.65
33	C	501	LMG	C12-C11-C10	-2.06	106.16	113.69
23	b	614	CLA	CMA-C3A-C2A	-2.06	106.03	113.98
25	b	617	BCR	C32-C1-C6	-2.06	107.02	110.24
29	A	414[B]	PL9	C2-C1-C6	2.06	121.44	119.00
35	c	516[B]	DGD	O6D-C1D-O3G	-2.06	105.19	110.04
23	b	610	CLA	CMA-C3A-C4A	-2.06	106.25	111.77
31	M	101	LMT	C3B-C4B-C5B	-2.05	106.51	110.23
24	A	416[A]	PHO	O2A-CGA-CBA	2.05	118.10	111.83
23	D	402[B]	CLA	CMC-C2C-C1C	2.05	128.24	125.03
23	B	601	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
25	b	619	BCR	C21-C20-C19	-2.05	117.25	123.20
23	b	607	CLA	C1-C2-C3	-2.05	122.83	126.20
23	B	604	CLA	CHB-C4A-NA	2.05	127.36	124.40
23	c	510	CLA	O1D-CGD-CBD	-2.05	120.47	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	405[A]	PL9	C47-C48-C49	-2.05	120.81	127.64
23	B	603	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
29	d	405[A]	PL9	C40-C39-C38	-2.05	118.37	123.63
23	B	602	CLA	C16-C15-C13	-2.05	109.16	115.97
23	c	512	CLA	CAC-C3C-C4C	2.05	127.45	124.79
33	B	621	LMG	O3-C3-C2	-2.05	105.55	110.38
23	B	609	CLA	CAA-C2A-C3A	-2.05	107.47	113.00
29	A	414[B]	PL9	C51-C49-C50	2.05	119.30	114.59
23	C	509	CLA	C2A-C1A-CHA	-2.05	120.32	123.87
25	b	617	BCR	C16-C15-C14	-2.04	119.34	123.52
23	C	513	CLA	CAC-C3C-C2C	2.04	131.31	127.56
23	b	604	CLA	CHA-C1A-NA	-2.04	121.76	126.39
23	d	402[A]	CLA	CBB-CAB-C3B	-2.04	117.32	127.53
25	D	404	BCR	C37-C22-C21	-2.04	119.51	122.82
23	B	611	CLA	C7-C6-C5	-2.04	107.82	113.26
35	c	517[B]	DGD	C2G-O2G-C1B	-2.04	112.91	117.80
23	c	502	CLA	C4D-C3D-CAD	-2.04	105.89	108.11
23	a	406[A]	CLA	CHA-C1A-NA	-2.04	121.77	126.39
25	b	618	BCR	C35-C13-C14	-2.04	119.51	122.82
23	b	604	CLA	C4-C3-C2	-2.04	118.39	123.63
27	o	304	GOL	C3-C2-C1	-2.04	104.32	111.80
29	A	414[A]	PL9	C10-C9-C11	2.04	118.77	115.23
33	D	411	LMG	C4-C3-C2	-2.04	107.25	110.83
29	a	413[A]	PL9	C47-C46-C44	-2.04	106.43	113.19
25	a	409	BCR	C11-C10-C9	-2.04	124.42	127.28
23	C	508	CLA	C6-C7-C8	-2.04	109.19	115.97
23	A	404[B]	CLA	OBD-CAD-C3D	-2.04	123.66	128.42
23	C	508	CLA	C3B-C4B-NB	2.04	112.35	110.53
23	A	408	CLA	CMA-C3A-C4A	-2.03	106.31	111.77
25	c	515	BCR	C37-C22-C21	-2.03	119.52	122.82
23	b	608	CLA	C4C-C3C-C2C	-2.03	103.93	106.89
23	B	605	CLA	C7-C6-C5	-2.03	107.84	113.26
25	B	618	BCR	C38-C26-C25	-2.03	122.27	124.48
26	a	410[B]	SQD	O8-S-C6	2.03	109.89	105.97
23	b	608	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
23	b	602	CLA	C4B-C3B-C2B	-2.03	104.78	107.30
23	C	509	CLA	C6-C7-C8	-2.03	109.22	115.97
34	b	623	HTG	C1-C2-C3	2.03	114.52	110.55
27	l	801[A]	GOL	C3-C2-C1	-2.03	104.36	111.80
25	K	102	BCR	C11-C10-C9	-2.03	124.43	127.28
35	h	102	DGD	C3B-C2B-C1B	-2.03	106.27	113.69
35	c	517[A]	DGD	O6E-C1E-O5D	-2.03	105.26	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	416[B]	PHO	OBD-CAD-C3D	-2.03	124.73	127.89
23	B	606	CLA	C1-O2A-CGA	2.02	121.55	116.65
23	c	512	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
29	a	413[A]	PL9	C51-C49-C50	2.02	119.25	114.59
23	C	504	CLA	C4B-C3B-C2B	-2.02	104.78	107.30
32	E	101[B]	LHG	C5-O7-C7	-2.02	112.95	117.80
26	a	411	SQD	C3-C4-C5	2.02	113.90	110.23
23	b	612	CLA	CMA-C3A-C2A	-2.02	106.16	113.98
33	C	501	LMG	O8-C28-C29	2.02	118.00	111.83
23	a	404[B]	CLA	CAC-C3C-C4C	2.02	127.42	124.79
23	a	404[B]	CLA	CMC-C2C-C1C	2.02	128.19	125.03
25	y	101	BCR	C40-C30-C25	-2.02	107.07	110.24
33	C	501	LMG	C9-C8-C7	-2.02	107.07	111.78
25	B	617	BCR	C37-C22-C23	2.02	121.17	118.09
25	h	101	BCR	C36-C18-C19	2.02	121.17	118.09
26	B	620	SQD	C9-C8-C7	-2.02	106.30	113.69
35	H	102	DGD	O2G-C1B-C2B	2.02	115.84	111.48
29	D	405[B]	PL9	C15-C14-C16	2.02	118.73	115.23
32	D	407[A]	LHG	O4-P-O5	2.01	121.82	112.44
29	A	414[A]	PL9	C51-C49-C50	2.01	119.22	114.59
23	b	615	CLA	CBC-CAC-C3C	-2.01	106.96	112.42
35	C	517[B]	DGD	C2G-O2G-C1B	-2.01	112.98	117.80
23	b	616	CLA	CHA-C1A-NA	-2.01	121.83	126.39
23	B	612	CLA	CMA-C3A-C4A	-2.01	106.36	111.77
23	A	405[B]	CLA	CMA-C3A-C2A	-2.01	106.20	113.98
29	a	413[B]	PL9	C35-C34-C33	-2.01	118.46	123.63
23	C	513	CLA	CBC-CAC-C3C	-2.01	106.97	112.42
29	D	405[A]	PL9	C45-C44-C46	2.01	118.72	115.23
23	d	403	CLA	CHB-C4A-NA	2.01	127.30	124.40
23	b	611	CLA	OBD-CAD-C3D	-2.01	123.72	128.42
23	D	402[B]	CLA	C4-C3-C5	2.01	118.72	115.23
33	z	101	LMG	O8-C28-O10	-2.01	118.60	123.63
40	v	201	HEC	CHA-C4D-ND	2.01	127.50	123.86
29	A	414[B]	PL9	C32-C31-C29	-2.01	106.53	113.19
35	c	516[A]	DGD	O2G-C1B-O1B	-2.01	119.01	123.70
25	c	514	BCR	C21-C20-C19	-2.01	117.39	123.20
25	d	404	BCR	C24-C23-C22	-2.00	123.27	126.23
31	M	101	LMT	O5'-C1'-O1'	-2.00	105.31	110.04
25	b	618	BCR	C29-C30-C25	2.00	113.35	110.44
29	D	405[A]	PL9	C22-C23-C24	-2.00	123.04	127.62
33	Z	101	LMG	C9-O8-C28	2.00	122.02	117.08

All (72) 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[A]	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	503	CLA	ND
23	C	504	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	C	514	CLA	ND
23	D	402[A]	CLA	ND
23	D	402[B]	CLA	ND
23	D	403	CLA	ND
23	a	404[A]	CLA	ND
23	a	404[B]	CLA	ND
23	a	405[A]	CLA	ND
23	a	405[B]	CLA	ND
23	a	408	CLA	ND
23	b	601	CLA	ND
23	b	602	CLA	ND

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Mol	Chain	Res	Type	Atom
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	CLA	ND

All (1597) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	404[B]	CLA	C2B-C3B-CAB-CBB
23	A	404[B]	CLA	C4B-C3B-CAB-CBB
23	B	601	CLA	CAD-CBD-CGD-O2D
23	B	603	CLA	C4-C3-C5-C6
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	508	CLA	C2B-C3B-CAB-CBB
23	C	508	CLA	C4B-C3B-CAB-CBB
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	a	404[B]	CLA	C2B-C3B-CAB-CBB
23	a	404[B]	CLA	C4B-C3B-CAB-CBB
23	a	408	CLA	C2-C3-C5-C6
23	a	408	CLA	C4-C3-C5-C6
23	b	606	CLA	C12-C13-C15-C16
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	C11-C12-C13-C14
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	D	404	BCR	C21-C22-C23-C24
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
26	A	410[B]	SQD	C8-C7-O47-C45
26	A	412	SQD	O6-C44-C45-O47
26	B	620	SQD	O49-C7-O47-C45
26	F	103	SQD	C2-C1-O6-C44
26	F	103	SQD	O49-C7-O47-C45
26	F	103	SQD	C8-C7-O47-C45
26	a	411	SQD	O6-C44-C45-O47
26	a	411	SQD	C5-C6-S-O7
26	a	411	SQD	C5-C6-S-O8
26	a	411	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-C3
27	B	623	GOL	O1-C1-C2-C3
27	B	628	GOL	O1-C1-C2-C3
27	D	412	GOL	C1-C2-C3-O3
27	O	302	GOL	O1-C1-C2-C3
27	V	203[A]	GOL	C1-C2-C3-O3
27	V	203[B]	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
27	V	203[B]	GOL	O2-C2-C3-O3
27	b	624	GOL	C1-C2-C3-O3
27	c	526	GOL	C1-C2-C3-O3
27	o	303	GOL	C1-C2-C3-O3
27	o	304	GOL	C1-C2-C3-O3
27	v	202[B]	GOL	O1-C1-C2-O2
29	A	414[A]	PL9	C9-C11-C12-C13
29	A	414[B]	PL9	C9-C11-C12-C13
29	a	413[A]	PL9	C23-C24-C26-C27
29	a	413[A]	PL9	C25-C24-C26-C27
31	A	417	LMT	O5'-C1'-O1'-C1
31	A	420	LMT	C2'-C1'-O1'-C1
31	A	420	LMT	O5'-C1'-O1'-C1
31	B	629	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-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

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Mol	Chain	Res	Type	Atoms
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
32	a	420[A]	LHG	C3-O3-P-O4
32	a	420[A]	LHG	C3-O3-P-O6
32	a	420[A]	LHG	C4-O6-P-O3
32	a	420[A]	LHG	C4-O6-P-O5
32	a	420[A]	LHG	O10-C23-O8-C6
32	a	420[A]	LHG	C24-C23-O8-C6
32	a	420[B]	LHG	C3-O3-P-O4
32	a	420[B]	LHG	C3-O3-P-O6
32	a	420[B]	LHG	C4-O6-P-O3
32	a	420[B]	LHG	C4-O6-P-O5
32	a	420[B]	LHG	O10-C23-O8-C6
32	a	420[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	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	O2-C2-C3-O3
32	d	406[B]	LHG	C3-O3-P-O4
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	d	413[A]	LHG	C3-O3-P-O5
33	C	521	LMG	C11-C10-O7-C8
33	c	520	LMG	O9-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
38	F	102	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
38	F	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
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	629	LMT	C4'-C5'-C6'-O6'
26	A	410[A]	SQD	O49-C7-O47-C45
26	A	410[B]	SQD	O49-C7-O47-C45
26	b	620	SQD	O49-C7-O47-C45
33	C	521	LMG	O9-C10-O7-C8
33	z	101	LMG	O9-C10-O7-C8
23	B	614	CLA	C3-C5-C6-C7
23	D	403	CLA	C3-C5-C6-C7
23	b	616	CLA	C3-C5-C6-C7
23	d	403	CLA	C3-C5-C6-C7
31	a	417	LMT	O5B-C5B-C6B-O6B
26	B	620	SQD	C8-C7-O47-C45
33	c	520	LMG	C11-C10-O7-C8
23	A	408	CLA	C4-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
23	D	403	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
23	d	403	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C15-C14-C16-C17
29	a	413[B]	PL9	C25-C24-C26-C27
23	B	603	CLA	C2-C3-C5-C6
23	C	505	CLA	C2-C3-C5-C6
23	D	403	CLA	C2-C3-C5-C6
23	d	403	CLA	C2-C3-C5-C6
23	D	403	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	C3-C5-C6-C7
34	D	410	HTG	O5-C5-C6-O6
31	M	103	LMT	C4B-C5B-C6B-O6B
31	F	101	LMT	O5'-C5'-C6'-O6'
31	b	621	LMT	O5'-C5'-C6'-O6'
31	m	103	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C3-C5-C6-C7
32	d	406[A]	LHG	O2-C2-C3-O3
31	B	629	LMT	O5B-C5B-C6B-O6B
31	M	103	LMT	O5'-C5'-C6'-O6'
31	B	627	LMT	C4'-C5'-C6'-O6'
26	A	410[A]	SQD	C8-C7-O47-C45
33	z	101	LMG	C11-C10-O7-C8
31	b	627	LMT	O5'-C5'-C6'-O6'
33	C	521	LMG	O6-C5-C6-O5
31	a	417	LMT	C4B-C5B-C6B-O6B
34	D	410	HTG	S1-C1'-C2'-C3'
23	b	614	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C20-C19-C21-C22
29	A	414[B]	PL9	C30-C29-C31-C32
29	a	413[A]	PL9	C15-C14-C16-C17
29	a	413[A]	PL9	C30-C29-C31-C32
29	a	413[B]	PL9	C15-C14-C16-C17
29	a	413[B]	PL9	C30-C29-C31-C32
23	A	408	CLA	C2-C3-C5-C6
23	C	508	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
23	c	507	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	414[B]	PL9	C18-C19-C21-C22
29	a	413[A]	PL9	C13-C14-C16-C17
29	a	413[A]	PL9	C28-C29-C31-C32
29	a	413[B]	PL9	C13-C14-C16-C17
29	a	413[B]	PL9	C28-C29-C31-C32
31	B	627	LMT	O5B-C5B-C6B-O6B
31	m	103	LMT	O5B-C5B-C6B-O6B
29	A	414[A]	PL9	C14-C16-C17-C18
29	A	414[A]	PL9	C44-C46-C47-C48
29	A	414[B]	PL9	C14-C16-C17-C18
29	A	414[B]	PL9	C44-C46-C47-C48
29	D	405[A]	PL9	C39-C41-C42-C43
29	D	405[B]	PL9	C39-C41-C42-C43
29	a	413[A]	PL9	C9-C11-C12-C13
29	a	413[A]	PL9	C14-C16-C17-C18
29	a	413[B]	PL9	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	a	413[B]	PL9	C14-C16-C17-C18
29	d	405[B]	PL9	C39-C41-C42-C43
33	c	520	LMG	C4-C5-C6-O5
31	M	103	LMT	C4'-C5'-C6'-O6'
34	D	410	HTG	C4-C5-C6-O6
31	A	420	LMT	O5B-C5B-C6B-O6B
31	B	627	LMT	O5'-C5'-C6'-O6'
31	B	629	LMT	C4B-C5B-C6B-O6B
23	C	514	CLA	CBD-CGD-O2D-CED
23	c	513	CLA	CBD-CGD-O2D-CED
31	M	103	LMT	O5B-C5B-C6B-O6B
31	A	420	LMT	O5'-C5'-C6'-O6'
31	B	629	LMT	O5'-C5'-C6'-O6'
31	B	631	LMT	O5'-C5'-C6'-O6'
23	c	510	CLA	CBD-CGD-O2D-CED
34	b	625	HTG	S1-C1'-C2'-C3'
32	d	406[A]	LHG	C1-C2-C3-O3
23	a	408	CLA	CBA-CGA-O2A-C1
34	b	625	HTG	O5-C5-C6-O6
31	B	631	LMT	C4'-C5'-C6'-O6'
31	B	627	LMT	C6-C7-C8-C9
31	A	420	LMT	C4B-C5B-C6B-O6B
31	e	101	LMT	C4'-C5'-C6'-O6'
23	B	605	CLA	C4-C3-C5-C6
23	C	508	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
29	A	414[B]	PL9	C15-C14-C16-C17
29	A	414[B]	PL9	C20-C19-C21-C22
23	B	605	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
29	a	413[B]	PL9	C23-C24-C26-C27
23	C	504	CLA	CBD-CGD-O2D-CED
23	B	602	CLA	C6-C7-C8-C9
23	C	503	CLA	C14-C13-C15-C16
23	C	507	CLA	C14-C13-C15-C16
23	b	601	CLA	C11-C10-C8-C9
23	b	604	CLA	C6-C7-C8-C9
23	b	616	CLA	C6-C7-C8-C9
31	F	101	LMT	C4'-C5'-C6'-O6'
31	b	627	LMT	C4'-C5'-C6'-O6'
31	A	417	LMT	C2'-C1'-O1'-C1
32	D	406[B]	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
25	D	404	BCR	C37-C22-C23-C24
31	B	627	LMT	C5'-C4'-O1B-C1B
26	F	103	SQD	C23-C24-C25-C26
35	c	517[B]	DGD	C1B-C2B-C3B-C4B
23	B	601	CLA	C10-C11-C12-C13
23	b	601	CLA	C10-C11-C12-C13
23	A	408	CLA	C5-C6-C7-C8
23	c	509	CLA	C3-C5-C6-C7
31	b	621	LMT	C4'-C5'-C6'-O6'
23	A	408	CLA	C12-C13-C15-C16
23	B	614	CLA	C11-C10-C8-C7
29	A	414[A]	PL9	C30-C29-C31-C32
25	T	101	BCR	C13-C14-C15-C16
31	A	420	LMT	O1'-C1-C2-C3
29	d	405[A]	PL9	C39-C41-C42-C43
23	B	601	CLA	C5-C6-C7-C8
23	b	604	CLA	C8-C10-C11-C12
23	b	611	CLA	C15-C16-C17-C18
35	c	517[A]	DGD	C1B-C2B-C3B-C4B
23	B	602	CLA	C13-C15-C16-C17
31	B	627	LMT	C4B-C5B-C6B-O6B
23	b	606	CLA	C2A-CAA-CBA-CGA
23	C	508	CLA	C5-C6-C7-C8
32	E	101[A]	LHG	C23-C24-C25-C26
33	Z	101	LMG	C10-C11-C12-C13
23	B	616	CLA	C3-C5-C6-C7
26	B	620	SQD	O5-C1-O6-C44
26	F	103	SQD	O5-C1-O6-C44
31	B	629	LMT	O5'-C1'-O1'-C1
31	b	621	LMT	O5'-C1'-O1'-C1
31	e	101	LMT	O5'-C1'-O1'-C1
35	c	518	DGD	C2B-C3B-C4B-C5B
23	B	603	CLA	C13-C15-C16-C17
23	c	512	CLA	C15-C16-C17-C18
33	B	621	LMG	C39-C40-C41-C42
23	a	408	CLA	O1A-CGA-O2A-C1
31	A	420	LMT	C4'-C5'-C6'-O6'
31	a	417	LMT	O1'-C1-C2-C3
23	B	606	CLA	C10-C11-C12-C13
23	c	513	CLA	C10-C11-C12-C13
26	B	620	SQD	C7-C8-C9-C10
31	A	420	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
31	e	101	LMT	O5B-C5B-C6B-O6B
23	B	614	CLA	C8-C10-C11-C12
23	B	615	CLA	C10-C11-C12-C13
23	D	403	CLA	C10-C11-C12-C13
23	b	606	CLA	C13-C15-C16-C17
23	b	614	CLA	C8-C10-C11-C12
35	C	519	DGD	C6B-C7B-C8B-C9B
35	h	102	DGD	C6B-C7B-C8B-C9B
23	a	404[A]	CLA	C15-C16-C17-C18
32	D	407[B]	LHG	C33-C34-C35-C36
33	d	411	LMG	C10-C11-C12-C13
32	D	406[A]	LHG	C1-C2-C3-O3
32	d	406[B]	LHG	C1-C2-C3-O3
23	B	606	CLA	C2A-CAA-CBA-CGA
23	c	507	CLA	C2A-CAA-CBA-CGA
26	b	620	SQD	C18-C19-C20-C21
32	D	407[A]	LHG	C33-C34-C35-C36
23	C	503	CLA	C13-C15-C16-C17
23	C	509	CLA	C10-C11-C12-C13
23	a	404[B]	CLA	C15-C16-C17-C18
23	b	611	CLA	C8-C10-C11-C12
23	c	506	CLA	C15-C16-C17-C18
23	C	502	CLA	CBD-CGD-O2D-CED
35	C	517[B]	DGD	O6D-C5D-C6D-O5D
35	c	516[B]	DGD	O6D-C5D-C6D-O5D
23	B	614	CLA	C10-C11-C12-C13
23	b	606	CLA	C10-C11-C12-C13
31	t	101	LMT	O5'-C5'-C6'-O6'
34	b	622	HTG	S1-C1'-C2'-C3'
23	C	511	CLA	C10-C11-C12-C13
23	b	604	CLA	C5-C6-C7-C8
33	c	520	LMG	O6-C5-C6-O5
34	B	624	HTG	O5-C5-C6-O6
33	B	621	LMG	C11-C10-O7-C8
33	B	621	LMG	O9-C10-O7-C8
26	A	412	SQD	C2-C1-O6-C44
31	B	631	LMT	C2'-C1'-O1'-C1
31	M	101	LMT	C2'-C1'-O1'-C1
31	b	621	LMT	C2'-C1'-O1'-C1
31	e	101	LMT	C2'-C1'-O1'-C1
31	t	101	LMT	C2'-C1'-O1'-C1
35	C	518[A]	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
35	C	518[B]	DGD	C2E-C1E-O5D-C6D
26	A	410[A]	SQD	C7-C8-C9-C10
26	A	410[B]	SQD	C7-C8-C9-C10
34	b	623	HTG	C1'-C2'-C3'-C4'
23	B	615	CLA	C16-C17-C18-C19
23	a	408	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C20
31	A	417	LMT	O1'-C1-C2-C3
25	b	619	BCR	C7-C8-C9-C34
31	e	101	LMT	O5'-C5'-C6'-O6'
25	b	619	BCR	C7-C8-C9-C10
23	D	403	CLA	O1D-CGD-O2D-CED
31	a	417	LMT	C1-C2-C3-C4
27	B	623	GOL	C1-C2-C3-O3
27	B	628	GOL	C1-C2-C3-O3
27	D	412	GOL	O1-C1-C2-C3
27	O	303	GOL	O1-C1-C2-C3
27	a	418	GOL	O1-C1-C2-C3
27	d	412	GOL	O1-C1-C2-C3
27	l	801[B]	GOL	O1-C1-C2-C3
27	v	202[A]	GOL	O1-C1-C2-C3
27	v	202[B]	GOL	O1-C1-C2-C3
32	A	419[B]	LHG	O1-C1-C2-C3
33	a	416	LMG	C4-C5-C6-O5
26	B	620	SQD	C30-C31-C32-C33
23	B	603	CLA	C16-C17-C18-C20
23	a	408	CLA	C16-C17-C18-C20
31	M	101	LMT	O5'-C1'-O1'-C1
35	c	516[B]	DGD	C4D-C5D-C6D-O5D
26	A	410[A]	SQD	C12-C13-C14-C15
23	B	616	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C1-O2A-CGA
23	B	603	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C20
23	c	508	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
26	f	102	SQD	C32-C33-C34-C35
32	L	101[A]	LHG	C15-C16-C17-C18
32	L	101[A]	LHG	C17-C18-C19-C20
33	a	416	LMG	C30-C31-C32-C33
35	C	518[B]	DGD	CCB-CDB-CEB-CFB
35	c	516[B]	DGD	C5A-C6A-C7A-C8A
35	c	517[A]	DGD	C9A-CAA-CBA-CCA
26	F	103	SQD	C30-C31-C32-C33
31	B	627	LMT	C5-C6-C7-C8
31	t	101	LMT	C4-C5-C6-C7
32	d	413[B]	LHG	C16-C17-C18-C19
33	D	411	LMG	C19-C20-C21-C22
35	C	517[B]	DGD	C5B-C6B-C7B-C8B
23	A	405[B]	CLA	C15-C16-C17-C18
23	b	606	CLA	C15-C16-C17-C18
23	b	614	CLA	C10-C11-C12-C13
35	c	516[A]	DGD	O6D-C5D-C6D-O5D
35	c	516[A]	DGD	C9A-CAA-CBA-CCA
35	c	517[B]	DGD	CBA-CCA-CDA-CEA
35	h	102	DGD	C7B-C8B-C9B-CAB
27	A	411	GOL	O1-C1-C2-O2
27	B	623	GOL	O2-C2-C3-O3
27	B	628	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	O	303	GOL	O1-C1-C2-O2
27	V	203[A]	GOL	O2-C2-C3-O3
27	a	418	GOL	O1-C1-C2-O2
27	b	624	GOL	O2-C2-C3-O3
27	c	526	GOL	O2-C2-C3-O3
31	M	103	LMT	C2-C1-O1'-C1'
31	t	101	LMT	C2-C1-O1'-C1'
31	b	627	LMT	C7-C8-C9-C10
23	D	402[B]	CLA	C4B-C3B-CAB-CBB
23	b	606	CLA	C4B-C3B-CAB-CBB
23	c	507	CLA	C4B-C3B-CAB-CBB
32	d	413[A]	LHG	C16-C17-C18-C19
35	c	516[B]	DGD	C9A-CAA-CBA-CCA
23	B	615	CLA	C16-C17-C18-C20
31	B	631	LMT	C11-C10-C9-C8
34	B	622	HTG	C3'-C4'-C5'-C6'

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Mol	Chain	Res	Type	Atoms
35	c	517[B]	DGD	C9A-CAA-CBA-CCA
23	A	405[A]	CLA	C15-C16-C17-C18
31	A	420	LMT	C1-C2-C3-C4
26	b	620	SQD	C27-C28-C29-C30
32	L	101[B]	LHG	C25-C26-C27-C28
35	h	102	DGD	C9A-CAA-CBA-CCA
23	C	511	CLA	C11-C12-C13-C15
33	C	501	LMG	C17-C18-C19-C20
35	c	516[A]	DGD	C5A-C6A-C7A-C8A
23	B	615	CLA	C5-C6-C7-C8
26	A	410[B]	SQD	C15-C16-C17-C18
31	M	103	LMT	C7-C8-C9-C10
32	d	413[A]	LHG	C32-C33-C34-C35
35	C	517[B]	DGD	C4D-C5D-C6D-O5D
31	B	627	LMT	C3'-C4'-O1B-C1B
32	a	420[A]	LHG	C26-C27-C28-C29
32	d	413[B]	LHG	C32-C33-C34-C35
35	C	517[A]	DGD	C5B-C6B-C7B-C8B
26	b	620	SQD	C31-C32-C33-C34
32	D	406[A]	LHG	C16-C17-C18-C19
32	D	407[B]	LHG	C32-C33-C34-C35
23	b	605	CLA	C8-C10-C11-C12
32	E	101[B]	LHG	C23-C24-C25-C26
23	d	402[A]	CLA	C16-C17-C18-C20
23	d	402[B]	CLA	C16-C17-C18-C20
35	C	517[A]	DGD	O6D-C5D-C6D-O5D
31	B	631	LMT	C4-C5-C6-C7
35	c	517[A]	DGD	CBA-CCA-CDA-CEA
31	B	631	LMT	C3-C4-C5-C6
32	D	407[A]	LHG	C32-C33-C34-C35
33	C	501	LMG	C36-C37-C38-C39
33	D	411	LMG	C12-C13-C14-C15
33	m	101	LMG	C35-C36-C37-C38
23	d	403	CLA	CBA-CGA-O2A-C1
35	c	516[B]	DGD	C2A-C1A-O1G-C1G
33	D	411	LMG	C35-C36-C37-C38
35	c	516[A]	DGD	C2B-C3B-C4B-C5B
35	c	516[B]	DGD	C2B-C3B-C4B-C5B
35	c	517[A]	DGD	CAA-CBA-CCA-CDA
34	o	301	HTG	C1'-C2'-C3'-C4'
32	E	101[B]	LHG	C24-C25-C26-C27
32	L	101[A]	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
32	L	101[A]	LHG	C13-C14-C15-C16
32	a	420[B]	LHG	C26-C27-C28-C29
32	b	629[A]	LHG	C16-C17-C18-C19
35	C	517[A]	DGD	C4B-C5B-C6B-C7B
35	C	518[A]	DGD	CCB-CDB-CEB-CFB
26	A	410[A]	SQD	C15-C16-C17-C18
31	e	101	LMT	C5-C6-C7-C8
32	E	101[A]	LHG	C24-C25-C26-C27
32	d	413[A]	LHG	C29-C30-C31-C32
33	B	621	LMG	C34-C35-C36-C37
31	B	629	LMT	C2-C3-C4-C5
32	b	629[B]	LHG	C27-C28-C29-C30
35	H	102	DGD	C5B-C6B-C7B-C8B
23	A	406[B]	CLA	C13-C15-C16-C17
31	b	627	LMT	C3-C4-C5-C6
23	B	610	CLA	C16-C17-C18-C19
33	a	416	LMG	C10-C11-C12-C13
23	b	606	CLA	C2B-C3B-CAB-CBB
23	c	507	CLA	C2B-C3B-CAB-CBB
32	D	407[B]	LHG	C29-C30-C31-C32
32	d	406[B]	LHG	C34-C35-C36-C37
31	e	101	LMT	C4-C5-C6-C7
32	D	406[B]	LHG	C16-C17-C18-C19
33	C	501	LMG	C12-C13-C14-C15
33	a	416	LMG	C34-C35-C36-C37
23	b	610	CLA	C2A-CAA-CBA-CGA
26	a	411	SQD	C25-C26-C27-C28
31	A	420	LMT	C3-C4-C5-C6
32	L	101[A]	LHG	C25-C26-C27-C28
33	C	521	LMG	C19-C20-C21-C22
23	d	403	CLA	O1A-CGA-O2A-C1
33	B	621	LMG	C17-C18-C19-C20
32	L	101[B]	LHG	C12-C13-C14-C15
35	c	517[B]	DGD	CAA-CBA-CCA-CDA
23	C	513	CLA	CBA-CGA-O2A-C1
23	c	512	CLA	CBA-CGA-O2A-C1
33	m	101	LMG	C39-C40-C41-C42
35	c	518	DGD	CBB-CCB-CDB-CEB
23	B	608	CLA	C13-C15-C16-C17
32	b	629[B]	LHG	C14-C15-C16-C17
34	b	622	HTG	C2'-C3'-C4'-C5'
26	A	412	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
33	B	621	LMG	O6-C1-O1-C7
35	C	518[A]	DGD	O6E-C1E-O5D-C6D
35	C	518[B]	DGD	O6E-C1E-O5D-C6D
35	c	516[B]	DGD	O6E-C1E-O5D-C6D
33	Z	101	LMG	O6-C5-C6-O5
33	B	621	LMG	C2-C1-O1-C7
23	b	604	CLA	C15-C16-C17-C18
32	b	629[A]	LHG	C14-C15-C16-C17
33	C	521	LMG	C18-C19-C20-C21
33	c	519	LMG	C31-C32-C33-C34
31	b	621	LMT	C3'-C4'-O1B-C1B
32	L	101[B]	LHG	C13-C14-C15-C16
32	E	101[A]	LHG	O2-C2-C3-O3
32	d	407[B]	LHG	C27-C28-C29-C30
23	c	502	CLA	C16-C17-C18-C19
33	m	101	LMG	C11-C10-O7-C8
32	b	629[B]	LHG	C12-C13-C14-C15
23	C	503	CLA	C15-C16-C17-C18
23	b	610	CLA	C15-C16-C17-C18
33	m	101	LMG	O9-C10-O7-C8
35	c	516[B]	DGD	C7A-C8A-C9A-CAA
31	m	103	LMT	C7-C8-C9-C10
33	C	520	LMG	C16-C17-C18-C19
34	B	624	HTG	S1-C1'-C2'-C3'
26	A	412	SQD	C26-C27-C28-C29
35	c	516[A]	DGD	C7A-C8A-C9A-CAA
33	C	501	LMG	C19-C20-C21-C22
23	B	610	CLA	C16-C17-C18-C20
23	c	508	CLA	C16-C17-C18-C20
23	d	403	CLA	C16-C17-C18-C19
31	b	621	LMT	C11-C10-C9-C8
29	D	405[B]	PL9	C15-C14-C16-C17
32	L	101[B]	LHG	C27-C28-C29-C30
35	H	102	DGD	C9B-CAB-CBB-CCB
32	d	407[A]	LHG	C29-C30-C31-C32
35	C	517[B]	DGD	C4B-C5B-C6B-C7B
33	C	501	LMG	C39-C40-C41-C42
33	m	101	LMG	C38-C39-C40-C41
33	m	101	LMG	C14-C15-C16-C17
32	A	419[A]	LHG	C12-C13-C14-C15
34	b	622	HTG	C3'-C4'-C5'-C6'
35	C	517[A]	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
32	d	407[A]	LHG	C27-C28-C29-C30
33	C	521	LMG	C17-C18-C19-C20
35	c	516[B]	DGD	O1A-C1A-O1G-C1G
26	B	620	SQD	C11-C10-C9-C8
26	F	103	SQD	C24-C25-C26-C27
32	L	101[B]	LHG	C15-C16-C17-C18
33	B	621	LMG	C32-C33-C34-C35
33	C	501	LMG	C10-C11-C12-C13
31	A	420	LMT	C3'-C4'-O1B-C1B
23	c	513	CLA	O1D-CGD-O2D-CED
32	d	407[A]	LHG	C25-C26-C27-C28
23	C	512	CLA	C3-C5-C6-C7
26	A	410[A]	SQD	O6-C44-C45-O47
26	A	410[B]	SQD	O6-C44-C45-O47
32	A	419[B]	LHG	C34-C35-C36-C37
35	c	518	DGD	CBA-CCA-CDA-CEA
32	d	413[A]	LHG	C24-C25-C26-C27
32	b	629[A]	LHG	C27-C28-C29-C30
35	c	516[A]	DGD	C4D-C5D-C6D-O5D
31	B	629	LMT	C5-C6-C7-C8
32	D	406[A]	LHG	C12-C13-C14-C15
23	d	402[A]	CLA	C16-C17-C18-C19
23	d	402[B]	CLA	C16-C17-C18-C19
31	B	631	LMT	O1'-C1-C2-C3
26	F	103	SQD	C29-C30-C31-C32
31	A	417	LMT	O5B-C5B-C6B-O6B
33	C	521	LMG	C13-C14-C15-C16
26	a	411	SQD	C31-C32-C33-C34
31	A	420	LMT	C5-C6-C7-C8
32	D	407[A]	LHG	C15-C16-C17-C18
32	d	406[B]	LHG	C16-C17-C18-C19
23	C	514	CLA	O1D-CGD-O2D-CED
34	b	623	HTG	O5-C5-C6-O6
31	e	101	LMT	C1-C2-C3-C4
26	A	412	SQD	C27-C28-C29-C30
32	A	419[A]	LHG	C34-C35-C36-C37
23	C	507	CLA	C15-C16-C17-C18
27	B	628	GOL	O2-C2-C3-O3
27	o	303	GOL	O2-C2-C3-O3
27	o	304	GOL	O2-C2-C3-O3
23	C	513	CLA	O1A-CGA-O2A-C1
32	d	407[A]	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
35	C	517[B]	DGD	C9A-CAA-CBA-CCA
23	B	604	CLA	C1A-C2A-CAA-CBA
23	B	611	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	C1A-C2A-CAA-CBA
23	B	601	CLA	C15-C16-C17-C18
23	C	513	CLA	C10-C11-C12-C13
23	a	404[B]	CLA	C2C-C3C-CAC-CBC
32	D	407[B]	LHG	C13-C14-C15-C16
33	d	411	LMG	C29-C30-C31-C32
24	A	416[B]	PHO	C2C-C3C-CAC-CBC
35	c	517[A]	DGD	C6A-C7A-C8A-C9A
35	c	516[B]	DGD	O6E-C5E-C6E-O5E
32	b	629[B]	LHG	C16-C17-C18-C19
32	d	406[A]	LHG	C34-C35-C36-C37
23	B	613	CLA	C11-C10-C8-C7
23	C	505	CLA	C12-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
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	505	CLA	C11-C12-C13-C15
23	c	510	CLA	C12-C13-C15-C16
23	c	512	CLA	C12-C13-C15-C16
31	B	629	LMT	C6-C7-C8-C9
23	b	606	CLA	C16-C17-C18-C20
23	A	406[A]	CLA	C13-C15-C16-C17
35	c	517[A]	DGD	C4A-C5A-C6A-C7A
23	b	601	CLA	C8-C10-C11-C12
23	b	601	CLA	C13-C15-C16-C17
23	b	605	CLA	C5-C6-C7-C8
33	c	519	LMG	C10-C11-C12-C13
33	D	411	LMG	C30-C31-C32-C33
23	C	511	CLA	C4-C3-C5-C6
23	c	505	CLA	C4-C3-C5-C6
29	a	413[A]	PL9	C12-C11-C9-C10
29	D	405[B]	PL9	C13-C14-C16-C17
33	c	519	LMG	C34-C35-C36-C37
31	b	627	LMT	C5-C6-C7-C8
33	D	411	LMG	C36-C37-C38-C39
23	B	610	CLA	C2A-CAA-CBA-CGA
23	C	506	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	D	403	CLA	C14-C13-C15-C16
26	b	620	SQD	C26-C27-C28-C29
33	B	621	LMG	C29-C30-C31-C32
31	M	101	LMT	O5'-C5'-C6'-O6'
23	c	509	CLA	CBA-CGA-O2A-C1
32	d	407[B]	LHG	C25-C26-C27-C28
35	h	102	DGD	CCB-CDB-CEB-CFB
23	A	404[B]	CLA	C13-C15-C16-C17
33	a	416	LMG	C29-C30-C31-C32
26	A	410[B]	SQD	O6-C44-C45-C46
26	A	412	SQD	O6-C44-C45-C46
26	a	410[A]	SQD	O6-C44-C45-C46
26	f	102	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
29	a	413[B]	PL9	C24-C26-C27-C28
32	E	101[A]	LHG	C4-C5-C6-O8
32	E	101[B]	LHG	C4-C5-C6-O8
32	D	407[A]	LHG	C13-C14-C15-C16
35	c	516[A]	DGD	CAA-CBA-CCA-CDA
33	C	520	LMG	C17-C18-C19-C20
23	c	511	CLA	C8-C10-C11-C12
32	A	419[A]	LHG	O2-C2-C3-O3
35	c	516[A]	DGD	C2A-C1A-O1G-C1G
35	c	518	DGD	C2A-C1A-O1G-C1G
31	m	103	LMT	O5'-C5'-C6'-O6'
33	D	411	LMG	O6-C5-C6-O5
33	d	411	LMG	O6-C5-C6-O5
35	C	517[A]	DGD	O6E-C5E-C6E-O5E
35	c	516[A]	DGD	O6E-C5E-C6E-O5E
23	c	509	CLA	O1A-CGA-O2A-C1
31	a	417	LMT	O5'-C5'-C6'-O6'
31	M	101	LMT	C3-C4-C5-C6
32	D	406[B]	LHG	C13-C14-C15-C16
23	c	510	CLA	O1D-CGD-O2D-CED
33	C	521	LMG	C35-C36-C37-C38
35	h	102	DGD	C9B-CAB-CBB-CCB
26	b	620	SQD	C13-C14-C15-C16
23	C	511	CLA	C2-C3-C5-C6
23	c	505	CLA	C2-C3-C5-C6
29	d	405[B]	PL9	C13-C14-C16-C17
26	A	412	SQD	C17-C18-C19-C20
32	d	413[A]	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
35	c	516[B]	DGD	CAA-CBA-CCA-CDA
35	C	517[B]	DGD	O6E-C5E-C6E-O5E
23	c	512	CLA	O1A-CGA-O2A-C1
23	C	507	CLA	C5-C6-C7-C8
32	D	407[A]	LHG	C29-C30-C31-C32
32	D	407[B]	LHG	C15-C16-C17-C18
35	C	517[A]	DGD	C8A-C9A-CAA-CBA
23	B	614	CLA	C5-C6-C7-C8
35	c	517[A]	DGD	C2B-C3B-C4B-C5B
27	l	801[A]	GOL	O1-C1-C2-C3
23	B	601	CLA	CBA-CGA-O2A-C1
23	b	601	CLA	CBA-CGA-O2A-C1
23	c	511	CLA	CBA-CGA-O2A-C1
26	b	620	SQD	C24-C23-O48-C46
26	B	620	SQD	C46-C45-O47-C7
23	a	405[A]	CLA	C2C-C3C-CAC-CBC
26	f	102	SQD	C25-C26-C27-C28
35	H	102	DGD	CCB-CDB-CEB-CFB
31	b	627	LMT	C1-C2-C3-C4
26	a	410[A]	SQD	C9-C10-C11-C12
32	A	419[A]	LHG	C26-C27-C28-C29
32	A	419[B]	LHG	C12-C13-C14-C15
23	c	502	CLA	C16-C17-C18-C20
33	C	520	LMG	C37-C38-C39-C40
23	B	607	CLA	C3-C5-C6-C7
35	C	517[B]	DGD	C8A-C9A-CAA-CBA
26	a	410[B]	SQD	C12-C13-C14-C15
32	d	407[A]	LHG	C28-C29-C30-C31
23	b	616	CLA	CBA-CGA-O2A-C1
33	c	520	LMG	C29-C28-O8-C9
26	b	620	SQD	C14-C15-C16-C17
33	B	621	LMG	C15-C16-C17-C18
23	C	506	CLA	C2-C3-C5-C6
32	L	101[B]	LHG	C17-C18-C19-C20
35	H	102	DGD	CCA-CDA-CEA-CFA
31	B	627	LMT	C1-C2-C3-C4
31	b	621	LMT	C3-C4-C5-C6
35	C	519	DGD	C2B-C3B-C4B-C5B
35	C	518[A]	DGD	CDA-CEA-CFA-CGA
26	a	410[A]	SQD	C12-C13-C14-C15
32	D	406[A]	LHG	C10-C11-C12-C13
26	B	620	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
32	b	629[A]	LHG	C9-C10-C11-C12
33	Z	101	LMG	C11-C12-C13-C14
35	h	102	DGD	CBA-CCA-CDA-CEA
23	C	513	CLA	C3-C5-C6-C7
26	a	410[B]	SQD	C9-C10-C11-C12
34	B	622	HTG	C4'-C5'-C6'-C7'
31	t	101	LMT	C7-C8-C9-C10
23	c	512	CLA	CBD-CGD-O2D-CED
32	E	101[A]	LHG	C25-C26-C27-C28
31	b	621	LMT	C7-C8-C9-C10
33	z	101	LMG	C14-C15-C16-C17
32	d	413[A]	LHG	C33-C34-C35-C36
35	C	518[B]	DGD	CDA-CEA-CFA-CGA
31	a	417	LMT	C2-C3-C4-C5
33	a	416	LMG	C35-C36-C37-C38
23	c	511	CLA	C3-C5-C6-C7
35	c	517[B]	DGD	C4A-C5A-C6A-C7A
23	C	504	CLA	O1D-CGD-O2D-CED
29	D	405[A]	PL9	C45-C44-C46-C47
29	d	405[A]	PL9	C13-C14-C16-C17
32	D	407[B]	LHG	C24-C23-O8-C6
26	A	410[A]	SQD	C11-C10-C9-C8
33	c	519	LMG	C33-C34-C35-C36
27	B	626	GOL	O1-C1-C2-O2
27	v	202[A]	GOL	O1-C1-C2-O2
31	A	420	LMT	C2-C1-O1'-C1'
31	b	627	LMT	C2-C1-O1'-C1'
23	B	614	CLA	C14-C13-C15-C16
23	C	505	CLA	C14-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C9
23	C	514	CLA	C11-C10-C8-C9
23	b	601	CLA	C6-C7-C8-C9
23	b	606	CLA	C11-C10-C8-C9
23	b	610	CLA	C11-C12-C13-C14
23	c	512	CLA	C6-C7-C8-C9
32	d	406[B]	LHG	C13-C14-C15-C16
23	B	605	CLA	C5-C6-C7-C8
23	B	602	CLA	C4B-C3B-CAB-CBB
23	a	406[A]	CLA	C4B-C3B-CAB-CBB
31	F	101	LMT	C4-C5-C6-C7
32	d	407[A]	LHG	C33-C34-C35-C36
32	d	413[B]	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
33	z	101	LMG	C20-C21-C22-C23
34	b	622	HTG	C1'-C2'-C3'-C4'
32	E	101[B]	LHG	C25-C26-C27-C28
23	A	404[A]	CLA	C13-C15-C16-C17
33	C	520	LMG	C11-C12-C13-C14
32	D	407[A]	LHG	C17-C18-C19-C20
35	H	102	DGD	C7A-C8A-C9A-CAA
33	m	101	LMG	C2-C1-O1-C7
23	B	602	CLA	C15-C16-C17-C18
31	a	417	LMT	C3-C4-C5-C6
32	D	407[B]	LHG	C17-C18-C19-C20
32	d	406[B]	LHG	C11-C10-C9-C8
35	c	517[B]	DGD	C2B-C3B-C4B-C5B
33	c	519	LMG	C4-C5-C6-O5
32	L	101[B]	LHG	O6-C4-C5-C6
35	C	517[A]	DGD	C4D-C5D-C6D-O5D
35	C	519	DGD	CDB-CEB-CFB-CGB
23	B	610	CLA	C12-C13-C15-C16
23	B	614	CLA	C12-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C10
23	b	601	CLA	C6-C7-C8-C10
23	b	604	CLA	C6-C7-C8-C10
23	b	606	CLA	C11-C10-C8-C7
23	b	616	CLA	C6-C7-C8-C10
23	c	504	CLA	C11-C12-C13-C15
23	c	506	CLA	C11-C10-C8-C7
23	c	509	CLA	C6-C7-C8-C10
23	d	402[B]	CLA	C11-C12-C13-C15
23	c	512	CLA	C10-C11-C12-C13
35	c	516[A]	DGD	O1A-C1A-O1G-C1G
32	E	101[A]	LHG	C13-C14-C15-C16
31	B	629	LMT	C1-C2-C3-C4
23	c	511	CLA	O1A-CGA-O2A-C1
35	c	518	DGD	O1A-C1A-O1G-C1G
29	a	413[B]	PL9	C12-C11-C9-C10
23	C	509	CLA	C5-C6-C7-C8
29	A	414[A]	PL9	C12-C11-C9-C8
29	D	405[A]	PL9	C13-C14-C16-C17
23	B	601	CLA	O1A-CGA-O2A-C1
23	b	601	CLA	O1A-CGA-O2A-C1
31	e	101	LMT	C9-C10-C11-C12
23	C	511	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	B	604	CLA	C3-C5-C6-C7
32	D	406[B]	LHG	C26-C27-C28-C29
33	d	411	LMG	C28-C29-C30-C31
32	D	406[B]	LHG	C11-C10-C9-C8
32	d	407[B]	LHG	C9-C10-C11-C12
33	m	101	LMG	C37-C38-C39-C40
33	z	101	LMG	C19-C20-C21-C22
26	A	410[A]	SQD	O6-C44-C45-C46
26	a	410[B]	SQD	O6-C44-C45-C46
32	a	420[A]	LHG	C4-C5-C6-O8
32	a	420[B]	LHG	C4-C5-C6-O8
33	a	416	LMG	C7-C8-C9-O8
35	c	517[B]	DGD	C9B-CAB-CBB-CCB
35	h	102	DGD	CDB-CEB-CFB-CGB
26	A	410[B]	SQD	C12-C13-C14-C15
31	B	629	LMT	C3-C4-C5-C6
32	b	629[B]	LHG	C13-C14-C15-C16
35	c	517[A]	DGD	CBB-CCB-CDB-CEB
26	b	620	SQD	C11-C10-C9-C8
23	C	506	CLA	C4-C3-C5-C6
24	a	407[B]	PHO	C4-C3-C5-C6
29	A	414[A]	PL9	C45-C44-C46-C47
29	d	405[B]	PL9	C15-C14-C16-C17
32	a	420[A]	LHG	C23-C24-C25-C26
35	c	518	DGD	C1A-C2A-C3A-C4A
33	C	520	LMG	C30-C31-C32-C33
29	D	405[A]	PL9	C43-C44-C46-C47
32	d	407[B]	LHG	C28-C29-C30-C31
32	d	407[B]	LHG	C34-C35-C36-C37
23	a	406[A]	CLA	C2B-C3B-CAB-CBB
25	D	404	BCR	C23-C24-C25-C30
25	b	617	BCR	C1-C6-C7-C8
25	b	619	BCR	C5-C6-C7-C8
35	C	517[A]	DGD	CCA-CDA-CEA-CFA
32	a	420[A]	LHG	C10-C11-C12-C13
33	c	519	LMG	C30-C31-C32-C33
35	c	517[B]	DGD	C6A-C7A-C8A-C9A
23	b	602	CLA	C10-C11-C12-C13
26	F	103	SQD	C34-C35-C36-C37
32	d	407[B]	LHG	C29-C30-C31-C32
32	d	413[B]	LHG	C25-C26-C27-C28
32	d	413[B]	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
23	b	606	CLA	C16-C17-C18-C19
26	a	410[A]	SQD	O6-C44-C45-O47
26	a	410[B]	SQD	O6-C44-C45-O47
26	b	620	SQD	O47-C45-C46-O48
29	D	405[B]	PL9	C4-C3-C7-C8
34	b	623	HTG	O5-C1-S1-C1'
35	h	102	DGD	CAA-CBA-CCA-CDA
23	b	616	CLA	O1A-CGA-O2A-C1
32	L	101[A]	LHG	C27-C28-C29-C30
35	C	517[B]	DGD	CCA-CDA-CEA-CFA
24	a	407[B]	PHO	C2-C3-C5-C6
32	A	419[B]	LHG	C26-C27-C28-C29
35	C	517[B]	DGD	C7A-C8A-C9A-CAA
23	B	608	CLA	C16-C17-C18-C19
23	B	608	CLA	C16-C17-C18-C20
26	B	620	SQD	C29-C30-C31-C32
35	C	517[A]	DGD	C7A-C8A-C9A-CAA
35	C	517[A]	DGD	C3B-C4B-C5B-C6B
35	C	519	DGD	CAA-CBA-CCA-CDA
26	F	103	SQD	C7-C8-C9-C10
23	C	502	CLA	O1D-CGD-O2D-CED
33	C	520	LMG	C34-C35-C36-C37
23	B	613	CLA	C11-C12-C13-C14
23	C	513	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C12-C13-C14
23	c	509	CLA	C6-C7-C8-C9
23	c	510	CLA	C11-C10-C8-C9
31	a	417	LMT	C9-C10-C11-C12
35	c	516[A]	DGD	O6E-C1E-O5D-C6D
32	d	413[B]	LHG	C33-C34-C35-C36
26	F	103	SQD	C32-C33-C34-C35
32	D	407[B]	LHG	O10-C23-O8-C6
29	A	414[A]	PL9	C39-C41-C42-C43
29	a	413[A]	PL9	C24-C26-C27-C28
33	C	520	LMG	C31-C32-C33-C34
33	d	411	LMG	C35-C36-C37-C38
24	a	415[B]	PHO	C2C-C3C-CAC-CBC
31	t	101	LMT	O1'-C1-C2-C3
23	b	603	CLA	C5-C6-C7-C8
35	C	517[A]	DGD	C1B-C2B-C3B-C4B
23	C	511	CLA	C13-C15-C16-C17
27	B	623	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
27	c	526	GOL	O1-C1-C2-O2
32	A	419[B]	LHG	O1-C1-C2-O2
23	A	406[A]	CLA	C16-C17-C18-C20
26	b	620	SQD	O10-C23-O48-C46
32	d	406[B]	LHG	C25-C26-C27-C28
32	A	419[A]	LHG	C1-C2-C3-O3
32	L	101[B]	LHG	C26-C27-C28-C29
31	A	420	LMT	C4-C5-C6-C7
25	Y	101	BCR	C37-C22-C23-C24
26	a	410[B]	SQD	C34-C35-C36-C37
35	C	517[B]	DGD	C3B-C4B-C5B-C6B
23	C	511	CLA	C12-C13-C15-C16
23	a	408	CLA	C11-C10-C8-C7
23	c	509	CLA	C11-C10-C8-C7
23	c	510	CLA	C11-C10-C8-C7
32	D	407[A]	LHG	C27-C28-C29-C30
32	b	629[A]	LHG	C34-C35-C36-C37
34	o	301	HTG	C2'-C3'-C4'-C5'
35	h	102	DGD	CAB-CBB-CCB-CDB
23	c	503	CLA	C8-C10-C11-C12
25	Y	101	BCR	C21-C22-C23-C24
25	b	619	BCR	C21-C22-C23-C24
23	C	511	CLA	O1A-CGA-O2A-C1
33	c	520	LMG	O10-C28-O8-C9
35	C	518[A]	DGD	C2G-C3G-O3G-C1D
35	C	518[B]	DGD	C5D-C6D-O5D-C1E
35	c	517[A]	DGD	C5D-C6D-O5D-C1E
35	c	517[B]	DGD	C5D-C6D-O5D-C1E
32	A	419[B]	LHG	C18-C19-C20-C21
23	B	615	CLA	C13-C15-C16-C17
23	B	601	CLA	C2A-CAA-CBA-CGA
32	L	101[A]	LHG	C11-C10-C9-C8
29	d	405[A]	PL9	C45-C44-C46-C47
29	a	413[A]	PL9	C12-C11-C9-C8
38	f	101	HEM	C2B-C3B-CAB-CBB
38	f	101	HEM	C2C-C3C-CAC-CBC
23	C	511	CLA	C8-C10-C11-C12
27	B	626	GOL	C1-C2-C3-O3
35	C	518[B]	DGD	C5B-C6B-C7B-C8B
35	c	517[B]	DGD	C5A-C6A-C7A-C8A
26	b	620	SQD	C46-C45-O47-C7
26	A	410[A]	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
35	C	518[A]	DGD	C5B-C6B-C7B-C8B
32	a	420[B]	LHG	C10-C11-C12-C13
33	C	520	LMG	C29-C30-C31-C32
24	a	407[B]	PHO	C2C-C3C-CAC-CBC
32	b	629[A]	LHG	C13-C14-C15-C16
35	C	518[A]	DGD	C8B-C9B-CAB-CBB
32	D	406[A]	LHG	C11-C10-C9-C8
32	b	629[B]	LHG	C34-C35-C36-C37
35	c	516[A]	DGD	CCB-CDB-CEB-CFB
33	C	521	LMG	C4-C5-C6-O5
32	D	406[B]	LHG	C28-C29-C30-C31
32	E	101[A]	LHG	O6-C4-C5-O7
32	L	101[A]	LHG	O6-C4-C5-O7
32	L	101[B]	LHG	O6-C4-C5-O7
26	a	410[A]	SQD	C27-C28-C29-C30
35	c	517[A]	DGD	O6E-C1E-O5D-C6D
35	c	517[B]	DGD	O6E-C1E-O5D-C6D
31	t	101	LMT	C11-C10-C9-C8
26	a	411	SQD	O6-C44-C45-C46
26	b	620	SQD	C44-C45-C46-O48
29	A	414[B]	PL9	C39-C41-C42-C43
32	a	420[B]	LHG	C23-C24-C25-C26
38	f	101	HEM	C4C-C3C-CAC-CBC
32	L	101[A]	LHG	C24-C25-C26-C27
31	A	417	LMT	C9-C10-C11-C12
33	B	621	LMG	C14-C15-C16-C17
33	B	621	LMG	C36-C37-C38-C39
35	C	519	DGD	C6A-C7A-C8A-C9A
23	B	606	CLA	C8-C10-C11-C12
32	d	406[A]	LHG	C13-C14-C15-C16
29	A	414[B]	PL9	C28-C29-C31-C32
32	D	407[A]	LHG	C10-C11-C12-C13
35	C	518[A]	DGD	C7A-C8A-C9A-CAA
26	a	410[A]	SQD	C34-C35-C36-C37
33	d	411	LMG	C11-C12-C13-C14
35	C	519	DGD	CAB-CBB-CCB-CDB
23	B	602	CLA	C3-C5-C6-C7
26	B	620	SQD	O47-C45-C46-O48
26	f	102	SQD	O47-C45-C46-O48
32	a	420[A]	LHG	O7-C5-C6-O8
33	B	621	LMG	O1-C7-C8-O7
23	b	616	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	c	506	CLA	C6-C7-C8-C9
35	C	518[B]	DGD	C8B-C9B-CAB-CBB
33	m	101	LMG	C32-C33-C34-C35
31	b	627	LMT	C6-C7-C8-C9
23	B	610	CLA	C13-C15-C16-C17
31	F	101	LMT	C6-C7-C8-C9
32	a	420[A]	LHG	C7-C8-C9-C10
35	C	518[B]	DGD	C3B-C4B-C5B-C6B
33	a	416	LMG	C21-C22-C23-C24
23	C	510	CLA	C2-C1-O2A-CGA
33	Z	101	LMG	C2-C1-O1-C7
35	c	516[A]	DGD	C2E-C1E-O5D-C6D
35	c	516[B]	DGD	C2E-C1E-O5D-C6D
35	c	517[A]	DGD	C2E-C1E-O5D-C6D
35	c	517[B]	DGD	C2E-C1E-O5D-C6D
23	c	512	CLA	C13-C15-C16-C17
32	D	407[B]	LHG	C2-C3-O3-P
32	b	629[B]	LHG	C17-C18-C19-C20
35	C	519	DGD	C9A-CAA-CBA-CCA
29	d	405[B]	PL9	C45-C44-C46-C47
29	a	413[B]	PL9	C12-C11-C9-C8
32	A	419[A]	LHG	C32-C33-C34-C35
23	a	405[B]	CLA	C15-C16-C17-C18
32	E	101[B]	LHG	O2-C2-C3-O3
23	C	507	CLA	C16-C17-C18-C20
32	d	407[A]	LHG	C9-C10-C11-C12
23	C	510	CLA	CBD-CGD-O2D-CED
26	A	410[A]	SQD	C34-C35-C36-C37
33	C	520	LMG	C36-C37-C38-C39
33	C	501	LMG	C18-C19-C20-C21
32	d	413[B]	LHG	C13-C14-C15-C16
23	a	404[B]	CLA	C4C-C3C-CAC-CBC
32	d	406[A]	LHG	C11-C10-C9-C8
23	b	607	CLA	C3-C5-C6-C7
25	b	619	BCR	C37-C22-C23-C24
26	A	412	SQD	C30-C31-C32-C33
35	H	102	DGD	CAB-CBB-CCB-CDB
23	C	513	CLA	C4B-C3B-CAB-CBB
23	C	514	CLA	C1A-C2A-CAA-CBA
23	a	405[A]	CLA	C1A-C2A-CAA-CBA
31	B	631	LMT	C2-C3-C4-C5
34	b	625	HTG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
26	a	410[A]	SQD	C35-C36-C37-C38
25	d	404	BCR	C21-C22-C23-C24
26	a	411	SQD	C14-C15-C16-C17
31	A	417	LMT	C7-C8-C9-C10
31	B	627	LMT	C7-C8-C9-C10
32	L	101[A]	LHG	O6-C4-C5-C6
32	d	413[A]	LHG	C18-C19-C20-C21
33	C	501	LMG	C11-C12-C13-C14
31	a	417	LMT	C4'-C5'-C6'-O6'
23	A	406[A]	CLA	C12-C13-C15-C16
23	A	406[B]	CLA	C12-C13-C15-C16
23	B	602	CLA	C6-C7-C8-C10
23	B	602	CLA	C11-C12-C13-C15
23	B	616	CLA	C12-C13-C15-C16
23	C	503	CLA	C12-C13-C15-C16
23	C	507	CLA	C12-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C7
23	b	615	CLA	C12-C13-C15-C16
23	c	505	CLA	C12-C13-C15-C16
23	d	402[A]	CLA	C11-C12-C13-C15
23	b	612	CLA	C8-C10-C11-C12
33	z	101	LMG	C13-C14-C15-C16
31	e	101	LMT	O1'-C1-C2-C3
32	d	406[A]	LHG	C16-C17-C18-C19
35	c	516[B]	DGD	C7B-C8B-C9B-CAB
26	A	412	SQD	C24-C23-O48-C46
33	C	501	LMG	C29-C30-C31-C32
23	A	406[B]	CLA	C16-C17-C18-C20
32	E	101[B]	LHG	C13-C14-C15-C16
23	C	508	CLA	C13-C15-C16-C17
26	A	410[B]	SQD	C34-C35-C36-C37
23	C	511	CLA	C14-C13-C15-C16
23	a	408	CLA	C11-C10-C8-C9
23	c	506	CLA	C11-C10-C8-C9
23	d	402[B]	CLA	C11-C12-C13-C14
26	f	102	SQD	C28-C29-C30-C31
35	C	517[A]	DGD	C6A-C7A-C8A-C9A
23	B	613	CLA	C15-C16-C17-C18
23	c	506	CLA	C13-C15-C16-C17
32	b	629[B]	LHG	C28-C29-C30-C31
34	B	624	HTG	C2'-C3'-C4'-C5'
31	A	420	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
32	A	419[B]	LHG	C32-C33-C34-C35
32	L	101[A]	LHG	C26-C27-C28-C29
33	B	621	LMG	C18-C19-C20-C21
33	c	519	LMG	C29-C30-C31-C32
35	c	517[A]	DGD	C7B-C8B-C9B-CAB
31	M	101	LMT	C2-C3-C4-C5
31	B	627	LMT	C9-C10-C11-C12
26	F	103	SQD	O47-C45-C46-O48
32	E	101[A]	LHG	O7-C5-C6-O8
32	a	420[B]	LHG	O7-C5-C6-O8
33	a	416	LMG	O7-C8-C9-O8
23	c	509	CLA	C15-C16-C17-C18
34	d	410	HTG	S1-C1'-C2'-C3'
32	d	406[B]	LHG	C9-C10-C11-C12
26	B	620	SQD	C44-C45-C46-O48
33	C	501	LMG	C7-C8-C9-O8
33	C	501	LMG	C20-C21-C22-C23
29	a	413[A]	PL9	C43-C44-C46-C47
29	a	413[B]	PL9	C43-C44-C46-C47
32	a	420[B]	LHG	C7-C8-C9-C10
33	a	416	LMG	C33-C34-C35-C36
23	C	503	CLA	CAD-CBD-CGD-O2D
23	C	505	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
26	A	410[A]	SQD	C13-C14-C15-C16
35	C	518[B]	DGD	C7A-C8A-C9A-CAA
32	D	406[A]	LHG	C34-C35-C36-C37
23	C	508	CLA	C2A-CAA-CBA-CGA
23	b	615	CLA	C13-C15-C16-C17
35	C	519	DGD	C8B-C9B-CAB-CBB
32	d	413[B]	LHG	C17-C18-C19-C20
35	C	518[A]	DGD	C8A-C9A-CAA-CBA
34	c	521	HTG	C4'-C5'-C6'-C7'
26	b	620	SQD	C28-C29-C30-C31
32	E	101[B]	LHG	C17-C18-C19-C20
33	C	521	LMG	C12-C13-C14-C15
23	B	601	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	508	CLA	CHA-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
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	420[A]	LHG	C4-O6-P-O4
32	a	420[B]	LHG	C4-O6-P-O4
32	d	413[B]	LHG	C3-O3-P-O5
23	b	613	CLA	CBD-CGD-O2D-CED
35	c	517[A]	DGD	C5A-C6A-C7A-C8A
23	b	604	CLA	C13-C15-C16-C17
23	D	402[B]	CLA	C2B-C3B-CAB-CBB
25	b	619	BCR	C1-C6-C7-C8
29	A	414[A]	PL9	C28-C29-C31-C32
32	D	407[A]	LHG	C2-C3-O3-P
32	d	407[A]	LHG	C2-C3-O3-P
32	d	407[B]	LHG	C2-C3-O3-P
35	C	519	DGD	C7B-C8B-C9B-CAB
32	d	407[A]	LHG	C32-C33-C34-C35
33	d	411	LMG	C18-C19-C20-C21
26	A	412	SQD	O10-C23-O48-C46
32	D	406[A]	LHG	C26-C27-C28-C29
35	C	518[B]	DGD	C1A-C2A-C3A-C4A
29	A	414[B]	PL9	C4-C3-C7-C8
29	a	413[A]	PL9	C4-C3-C7-C8
29	a	413[B]	PL9	C4-C3-C7-C8
32	A	419[A]	LHG	O1-C1-C2-C3
26	f	102	SQD	C34-C35-C36-C37
23	B	613	CLA	C13-C15-C16-C17
32	d	413[A]	LHG	C34-C35-C36-C37
33	D	411	LMG	C18-C19-C20-C21
26	B	620	SQD	C24-C25-C26-C27
35	C	519	DGD	CDA-CEA-CFA-CGA
23	c	506	CLA	C10-C11-C12-C13
26	a	411	SQD	C24-C25-C26-C27
32	d	413[A]	LHG	C11-C12-C13-C14
32	D	406[B]	LHG	O6-C4-C5-C6
32	E	101[A]	LHG	O6-C4-C5-C6
32	b	629[B]	LHG	O6-C4-C5-C6
34	B	624	HTG	C4'-C5'-C6'-C7'
35	C	518[A]	DGD	C7B-C8B-C9B-CAB
23	A	406[B]	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C11-C12-C13-C14
23	B	610	CLA	C14-C13-C15-C16
23	B	614	CLA	C11-C10-C8-C9
23	D	403	CLA	C11-C10-C8-C9
23	b	603	CLA	C11-C10-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	c	513	CLA	C6-C7-C8-C9
23	d	402[A]	CLA	C11-C12-C13-C14
23	d	403	CLA	C11-C12-C13-C14
32	b	629[B]	LHG	O6-C4-C5-O7
31	t	101	LMT	C2-C3-C4-C5
32	D	407[B]	LHG	C10-C11-C12-C13
23	D	403	CLA	O1A-CGA-O2A-C1
23	b	612	CLA	C10-C11-C12-C13
33	Z	101	LMG	C21-C22-C23-C24
23	c	504	CLA	C4-C3-C5-C6
29	D	405[A]	PL9	C15-C14-C16-C17
26	a	410[B]	SQD	C27-C28-C29-C30
31	a	417	LMT	C7-C8-C9-C10
32	D	406[A]	LHG	C13-C14-C15-C16
26	a	411	SQD	C26-C27-C28-C29
33	B	621	LMG	C20-C21-C22-C23
32	E	101[B]	LHG	O7-C5-C6-O8
23	b	601	CLA	CAA-CBA-CGA-O2A
35	H	102	DGD	O2G-C1B-C2B-C3B
32	b	629[A]	LHG	C28-C29-C30-C31
32	d	407[A]	LHG	C10-C11-C12-C13
23	a	408	CLA	C15-C16-C17-C18
26	A	410[B]	SQD	C11-C10-C9-C8
31	B	631	LMT	C1-C2-C3-C4
23	C	507	CLA	C4-C3-C5-C6
23	b	601	CLA	C4-C3-C5-C6
29	D	405[B]	PL9	C45-C44-C46-C47
23	B	601	CLA	CAA-CBA-CGA-O2A
35	c	517[B]	DGD	C5B-C6B-C7B-C8B
23	a	405[A]	CLA	C15-C16-C17-C18
33	B	621	LMG	O1-C7-C8-C9
23	b	601	CLA	C3-C5-C6-C7
26	a	410[B]	SQD	C35-C36-C37-C38
23	c	507	CLA	C5-C6-C7-C8
25	d	404	BCR	C7-C8-C9-C34
26	A	412	SQD	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	m	101	LMG	C11-C12-C13-C14
35	c	516[B]	DGD	C5D-C6D-O5D-C1E
35	c	517[A]	DGD	C2G-C3G-O3G-C1D
23	B	612	CLA	C10-C11-C12-C13
23	a	404[B]	CLA	C2A-CAA-CBA-CGA
26	a	411	SQD	C15-C16-C17-C18
29	a	413[A]	PL9	C45-C44-C46-C47
29	a	413[B]	PL9	C45-C44-C46-C47
29	A	414[B]	PL9	C12-C11-C9-C8
26	A	410[A]	SQD	C16-C17-C18-C19
26	B	620	SQD	C9-C10-C11-C12
23	c	512	CLA	O1D-CGD-O2D-CED
35	H	102	DGD	C6A-C7A-C8A-C9A
31	e	101	LMT	C2-C1-O1'-C1'
23	A	406[A]	CLA	C14-C13-C15-C16
23	B	602	CLA	C11-C12-C13-C14
23	C	511	CLA	C11-C12-C13-C14
32	D	406[A]	LHG	C28-C29-C30-C31
24	a	407[A]	PHO	C2C-C3C-CAC-CBC
23	D	402[A]	CLA	C4B-C3B-CAB-CBB
23	a	406[B]	CLA	C4B-C3B-CAB-CBB
23	b	610	CLA	C13-C15-C16-C17
32	b	629[B]	LHG	C9-C10-C11-C12
31	M	103	LMT	C9-C10-C11-C12
35	h	102	DGD	C6A-C7A-C8A-C9A
26	F	103	SQD	C24-C23-O48-C46
32	L	101[A]	LHG	C23-C24-C25-C26
35	c	516[B]	DGD	CBA-CCA-CDA-CEA
23	b	616	CLA	C4-C3-C5-C6
23	b	601	CLA	C2-C3-C5-C6
29	d	405[A]	PL9	C43-C44-C46-C47
23	C	510	CLA	C3-C5-C6-C7
32	D	407[A]	LHG	O10-C23-O8-C6
33	C	521	LMG	C38-C39-C40-C41
26	b	620	SQD	C33-C34-C35-C36
23	a	405[A]	CLA	C4C-C3C-CAC-CBC
32	D	406[B]	LHG	C12-C13-C14-C15
32	L	101[B]	LHG	C11-C10-C9-C8
23	b	615	CLA	C11-C12-C13-C15
23	b	605	CLA	C13-C15-C16-C17
23	b	615	CLA	C10-C11-C12-C13
33	c	519	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
33	c	520	LMG	C31-C32-C33-C34
32	D	407[A]	LHG	C24-C23-O8-C6
23	A	404[B]	CLA	C2C-C3C-CAC-CBC
35	h	102	DGD	O2G-C1B-C2B-C3B
33	a	416	LMG	C31-C32-C33-C34
23	B	616	CLA	C16-C17-C18-C19
32	L	101[B]	LHG	C24-C25-C26-C27
33	C	521	LMG	C10-C11-C12-C13
32	D	406[B]	LHG	C9-C10-C11-C12
23	A	405[B]	CLA	C13-C15-C16-C17
33	c	520	LMG	O1-C7-C8-O7
33	B	621	LMG	O8-C28-C29-C30
23	B	604	CLA	C2C-C3C-CAC-CBC
32	a	420[B]	LHG	C24-C25-C26-C27
26	a	410[A]	SQD	C11-C12-C13-C14
23	b	613	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
23	B	601	CLA	C13-C15-C16-C17
23	a	405[B]	CLA	C2C-C3C-CAC-CBC
25	K	102	BCR	C7-C8-C9-C10
25	d	404	BCR	C7-C8-C9-C10
23	c	510	CLA	C4-C3-C5-C6
32	D	406[B]	LHG	C1-C2-C3-O3
32	d	413[A]	LHG	C1-C2-C3-O3
33	Z	101	LMG	C29-C28-O8-C9
26	A	410[B]	SQD	C18-C19-C20-C21
23	C	502	CLA	C2A-CAA-CBA-CGA
23	B	604	CLA	C4C-C3C-CAC-CBC
35	C	518[B]	DGD	C8A-C9A-CAA-CBA
26	a	411	SQD	C33-C34-C35-C36
23	B	610	CLA	C11-C12-C13-C14
23	B	614	CLA	C6-C7-C8-C9
23	C	510	CLA	C6-C7-C8-C9
23	a	406[A]	CLA	C14-C13-C15-C16
23	a	406[B]	CLA	C11-C12-C13-C14
23	c	504	CLA	C14-C13-C15-C16
23	c	505	CLA	C14-C13-C15-C16
33	z	101	LMG	C10-C11-C12-C13
23	B	616	CLA	C16-C17-C18-C20
26	a	410[B]	SQD	C11-C12-C13-C14
35	c	516[A]	DGD	C4B-C5B-C6B-C7B
23	c	513	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	b	608	CLA	C16-C17-C18-C20
33	z	101	LMG	O7-C10-C11-C12
23	c	510	CLA	C2-C3-C5-C6
27	A	418	GOL	O1-C1-C2-O2
23	b	605	CLA	C3-C5-C6-C7
40	V	201	HEC	CAD-CBD-CGD-O1D
32	E	101[A]	LHG	C12-C13-C14-C15
26	a	410[A]	SQD	C10-C11-C12-C13
26	a	411	SQD	C16-C17-C18-C19
32	d	406[A]	LHG	C9-C10-C11-C12
23	a	406[A]	CLA	C1A-C2A-CAA-CBA
23	c	511	CLA	C1A-C2A-CAA-CBA
23	A	405[B]	CLA	C2C-C3C-CAC-CBC
23	D	403	CLA	CBA-CGA-O2A-C1
23	A	408	CLA	C16-C17-C18-C19
31	b	627	LMT	O1'-C1-C2-C3
24	A	416[A]	PHO	C2C-C3C-CAC-CBC
23	C	513	CLA	C2B-C3B-CAB-CBB
23	D	402[A]	CLA	C2B-C3B-CAB-CBB
23	a	406[B]	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
23	c	502	CLA	C2B-C3B-CAB-CBB
25	D	404	BCR	C23-C24-C25-C26
25	b	617	BCR	C5-C6-C7-C8
25	t	102	BCR	C5-C6-C7-C8
23	B	615	CLA	C8-C10-C11-C12
23	c	507	CLA	C8-C10-C11-C12
32	D	406[A]	LHG	C17-C18-C19-C20
23	A	406[A]	CLA	C16-C17-C18-C19
29	D	405[B]	PL9	C35-C34-C36-C37
32	d	406[B]	LHG	O6-C4-C5-C6
23	b	616	CLA	C2-C3-C5-C6
29	D	405[B]	PL9	C43-C44-C46-C47
32	D	406[B]	LHG	C34-C35-C36-C37
32	A	419[A]	LHG	C29-C30-C31-C32
23	C	506	CLA	C12-C13-C15-C16
23	D	403	CLA	C11-C10-C8-C7
23	b	601	CLA	C11-C12-C13-C15
23	b	608	CLA	C12-C13-C15-C16
23	b	614	CLA	C12-C13-C15-C16
32	b	629[A]	LHG	C10-C11-C12-C13
23	A	404[B]	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
35	C	519	DGD	C7A-C8A-C9A-CAA
33	C	501	LMG	O7-C8-C9-O8
40	V	201	HEC	CAD-CBD-CGD-O2D
29	A	414[A]	PL9	C4-C3-C7-C8
35	c	516[A]	DGD	CBA-CCA-CDA-CEA
38	F	102	HEM	CAD-CBD-CGD-O1D
33	C	521	LMG	C20-C21-C22-C23
23	b	615	CLA	C5-C6-C7-C8
25	K	102	BCR	C7-C8-C9-C34
29	D	405[A]	PL9	C35-C34-C36-C37
29	d	405[B]	PL9	C43-C44-C46-C47
23	A	404[B]	CLA	C2-C1-O2A-CGA
23	C	504	CLA	C8-C10-C11-C12
31	e	101	LMT	C3-C4-C5-C6
23	b	613	CLA	O1D-CGD-O2D-CED
32	L	101[A]	LHG	C10-C11-C12-C13
35	C	519	DGD	CBA-CCA-CDA-CEA
23	B	606	CLA	C11-C10-C8-C9
31	F	101	LMT	C2-C3-C4-C5
32	a	420[A]	LHG	C24-C25-C26-C27
29	A	414[A]	PL9	C25-C24-C26-C27
29	D	405[B]	PL9	C18-C19-C21-C22
26	F	103	SQD	O10-C23-O48-C46
33	c	519	LMG	C28-C29-C30-C31
35	c	516[B]	DGD	C4B-C5B-C6B-C7B
35	H	102	DGD	O1G-C1G-C2G-C3G
26	f	102	SQD	C11-C10-C9-C8
38	F	102	HEM	CAD-CBD-CGD-O2D
23	c	510	CLA	O1A-CGA-O2A-C1
32	L	101[B]	LHG	O9-C7-O7-C5
27	d	412	GOL	O1-C1-C2-O2
27	l	801[B]	GOL	O1-C1-C2-O2
32	A	419[A]	LHG	O1-C1-C2-O2
32	d	413[A]	LHG	C27-C28-C29-C30
32	D	406[B]	LHG	O6-C4-C5-O7
32	d	406[B]	LHG	O6-C4-C5-O7
23	B	614	CLA	C4-C3-C5-C6
32	d	413[A]	LHG	C17-C18-C19-C20
33	a	416	LMG	O8-C28-C29-C30
23	b	604	CLA	C4B-C3B-CAB-CBB
23	c	502	CLA	C4B-C3B-CAB-CBB
23	B	612	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	d	406[A]	LHG	C25-C26-C27-C28
35	C	519	DGD	CCB-CDB-CEB-CFB
35	c	517[B]	DGD	CBB-CCB-CDB-CEB
23	C	512	CLA	O1A-CGA-O2A-C1
23	C	507	CLA	C16-C17-C18-C19
34	b	623	HTG	S1-C1'-C2'-C3'
24	a	407[A]	PHO	CHA-CBD-CGD-O1D
23	B	602	CLA	C8-C10-C11-C12
23	C	509	CLA	C13-C15-C16-C17
23	b	612	CLA	C13-C15-C16-C17
33	B	621	LMG	C37-C38-C39-C40
35	C	519	DGD	O1A-C1A-O1G-C1G
23	C	502	CLA	C16-C17-C18-C20
38	f	101	HEM	CAA-CBA-CGA-O2A
40	v	201	HEC	CAD-CBD-CGD-O2D
38	f	101	HEM	CAD-CBD-CGD-O1D
32	d	413[A]	LHG	C9-C10-C11-C12
35	c	518	DGD	CDB-CEB-CFB-CGB
32	A	419[A]	LHG	C17-C18-C19-C20
23	a	406[A]	CLA	C11-C12-C13-C14
23	b	606	CLA	C14-C13-C15-C16
35	C	519	DGD	O6D-C5D-C6D-O5D
33	d	411	LMG	C19-C20-C21-C22
35	C	518[B]	DGD	C2G-C3G-O3G-C1D
35	c	516[A]	DGD	CDB-CEB-CFB-CGB
23	C	507	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	d	402[B]	CLA	C2-C1-O2A-CGA
35	c	518	DGD	O6D-C5D-C6D-O5D
33	a	416	LMG	O6-C5-C6-O5
23	b	608	CLA	C13-C15-C16-C17
32	d	413[B]	LHG	C27-C28-C29-C30
38	F	102	HEM	C2B-C3B-CAB-CBB
26	A	412	SQD	C7-C8-C9-C10
23	c	504	CLA	C5-C6-C7-C8
24	a	407[A]	PHO	O2A-C1-C2-C3
26	b	620	SQD	C30-C31-C32-C33
35	C	519	DGD	C4A-C5A-C6A-C7A
31	e	101	LMT	C4B-C5B-C6B-O6B
32	b	629[A]	LHG	C25-C26-C27-C28
26	A	412	SQD	C25-C26-C27-C28
38	f	101	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
32	E	101[B]	LHG	O6-C4-C5-O7
33	m	101	LMG	O6-C1-O1-C7
40	v	201	HEC	CAD-CBD-CGD-O1D
33	C	520	LMG	O1-C7-C8-C9
23	B	611	CLA	C8-C10-C11-C12
38	F	102	HEM	C4B-C3B-CAB-CBB
38	f	101	HEM	C4B-C3B-CAB-CBB
32	d	407[B]	LHG	C33-C34-C35-C36
33	d	411	LMG	C36-C37-C38-C39
23	B	612	CLA	CBA-CGA-O2A-C1
23	A	404[B]	CLA	C4C-C3C-CAC-CBC
32	L	101[A]	LHG	C11-C12-C13-C14
32	b	629[B]	LHG	C32-C33-C34-C35
33	d	411	LMG	C16-C17-C18-C19
23	B	601	CLA	C3-C5-C6-C7
23	B	616	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	C	514	CLA	C6-C7-C8-C9
23	a	404[A]	CLA	C2C-C3C-CAC-CBC
33	C	521	LMG	C11-C12-C13-C14
23	C	513	CLA	CAA-CBA-CGA-O2A
32	A	419[A]	LHG	O8-C23-C24-C25
32	A	419[B]	LHG	O8-C23-C24-C25
32	a	420[B]	LHG	O8-C23-C24-C25
32	b	629[B]	LHG	O7-C7-C8-C9
23	A	404[A]	CLA	C2C-C3C-CAC-CBC
33	m	101	LMG	C29-C30-C31-C32
23	C	511	CLA	CAA-CBA-CGA-O2A
35	c	517[A]	DGD	C1A-C2A-C3A-C4A
23	B	601	CLA	C11-C12-C13-C15
23	B	606	CLA	C11-C10-C8-C7
23	a	406[A]	CLA	C11-C12-C13-C15
23	a	406[B]	CLA	C11-C12-C13-C15
23	b	614	CLA	C11-C10-C8-C7
23	c	508	CLA	C12-C13-C15-C16
24	A	407[B]	PHO	C6-C7-C8-C10
23	B	602	CLA	C2B-C3B-CAB-CBB
23	b	612	CLA	C2B-C3B-CAB-CBB
25	B	617	BCR	C1-C6-C7-C8
25	H	101	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C30
31	M	103	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
32	a	420[A]	LHG	O8-C23-C24-C25
23	A	408	CLA	C2-C1-O2A-CGA
33	D	411	LMG	C34-C35-C36-C37
23	D	403	CLA	C8-C10-C11-C12
31	A	417	LMT	C2B-C1B-O1B-C4'
35	C	517[B]	DGD	C6A-C7A-C8A-C9A
32	L	101[B]	LHG	O7-C7-C8-C9
24	a	407[A]	PHO	C2-C3-C5-C6
29	d	405[B]	PL9	C28-C29-C31-C32
32	E	101[B]	LHG	C11-C10-C9-C8
34	o	301	HTG	C2'-C1'-S1-C1
33	C	501	LMG	C13-C14-C15-C16
33	c	520	LMG	C28-C29-C30-C31
32	d	407[B]	LHG	C32-C33-C34-C35
33	Z	101	LMG	C19-C20-C21-C22
32	L	101[A]	LHG	O7-C7-C8-C9
32	b	629[A]	LHG	O7-C7-C8-C9
34	b	623	HTG	C4'-C5'-C6'-C7'
24	a	407[A]	PHO	C4-C3-C5-C6
33	Z	101	LMG	O7-C10-C11-C12
23	C	507	CLA	C2-C3-C5-C6
23	c	504	CLA	C2-C3-C5-C6
26	A	410[B]	SQD	C23-C24-C25-C26
26	f	102	SQD	C23-C24-C25-C26
31	e	101	LMT	C2B-C1B-O1B-C4'
23	B	614	CLA	C2A-CAA-CBA-CGA
35	C	517[B]	DGD	C2A-C1A-O1G-C1G
31	B	627	LMT	C2-C1-O1'-C1'
31	F	101	LMT	C2-C1-O1'-C1'
35	C	517[B]	DGD	O1A-C1A-O1G-C1G
32	d	413[A]	LHG	C30-C31-C32-C33
33	C	520	LMG	C35-C36-C37-C38
23	b	608	CLA	C14-C13-C15-C16
26	b	620	SQD	C16-C17-C18-C19
23	b	604	CLA	C2C-C3C-CAC-CBC
26	F	103	SQD	C44-C45-C46-O48
24	a	415[A]	PHO	C2C-C3C-CAC-CBC
32	d	407[B]	LHG	C11-C10-C9-C8
23	B	610	CLA	C4B-C3B-CAB-CBB
23	C	506	CLA	C4B-C3B-CAB-CBB
23	a	406[B]	CLA	C1A-C2A-CAA-CBA
23	c	501	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	L	101[B]	LHG	C11-C12-C13-C14
35	C	517[B]	DGD	O6E-C1E-O5D-C6D
32	E	101[B]	LHG	O7-C7-C8-C9
33	c	519	LMG	O7-C10-C11-C12
38	f	101	HEM	CAD-CBD-CGD-O2D
35	C	519	DGD	C8A-C9A-CAA-CBA
23	C	503	CLA	C3-C5-C6-C7
23	c	510	CLA	CAA-CBA-CGA-O2A
32	D	407[B]	LHG	C26-C27-C28-C29
23	b	611	CLA	C13-C15-C16-C17
33	C	520	LMG	C12-C13-C14-C15
23	b	613	CLA	CAA-CBA-CGA-O2A
23	B	605	CLA	C8-C10-C11-C12
23	B	608	CLA	C2-C1-O2A-CGA
23	B	613	CLA	C2-C1-O2A-CGA
23	a	404[A]	CLA	C2-C1-O2A-CGA
23	c	513	CLA	C2-C1-O2A-CGA
23	C	502	CLA	C11-C12-C13-C15
23	C	508	CLA	C11-C12-C13-C15
23	c	504	CLA	C12-C13-C15-C16
23	c	513	CLA	C12-C13-C15-C16
23	a	404[A]	CLA	C4C-C3C-CAC-CBC
23	b	608	CLA	C16-C17-C18-C19
32	d	406[B]	LHG	C30-C31-C32-C33
35	C	517[A]	DGD	C3A-C4A-C5A-C6A
23	B	613	CLA	CAA-CBA-CGA-O2A
33	a	416	LMG	C13-C14-C15-C16
33	c	520	LMG	C39-C40-C41-C42
32	A	419[A]	LHG	C18-C19-C20-C21
32	d	407[A]	LHG	C30-C31-C32-C33
29	A	414[B]	PL9	C46-C47-C48-C49
29	d	405[B]	PL9	C11-C12-C13-C14
29	d	405[A]	PL9	C34-C36-C37-C38
23	b	602	CLA	C8-C10-C11-C12
32	E	101[A]	LHG	O7-C7-C8-C9
23	c	513	CLA	C2-C3-C5-C6
31	e	101	LMT	C2-C3-C4-C5
23	C	513	CLA	CAA-CBA-CGA-O1A
32	b	629[A]	LHG	O9-C7-C8-C9
23	A	404[A]	CLA	C4C-C3C-CAC-CBC
23	C	512	CLA	C8-C10-C11-C12
23	c	512	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
32	d	407[A]	LHG	O10-C23-O8-C6
23	c	510	CLA	CBA-CGA-O2A-C1
35	C	519	DGD	C2A-C1A-O1G-C1G
23	B	601	CLA	C11-C12-C13-C14
23	C	505	CLA	C11-C12-C13-C14
23	b	601	CLA	C11-C12-C13-C14
23	c	513	CLA	C14-C13-C15-C16
32	E	101[B]	LHG	O9-C7-C8-C9
26	A	410[B]	SQD	C13-C14-C15-C16
32	A	419[B]	LHG	O10-C23-C24-C25
32	L	101[A]	LHG	O9-C7-C8-C9
32	b	629[B]	LHG	O9-C7-C8-C9
33	c	519	LMG	C35-C36-C37-C38
26	f	102	SQD	O5-C5-C6-S
38	F	102	HEM	CAA-CBA-CGA-O1A
27	l	801[A]	GOL	O1-C1-C2-O2
33	C	520	LMG	C15-C16-C17-C18
32	A	419[A]	LHG	C30-C31-C32-C33
25	y	101	BCR	C21-C22-C23-C24
32	A	419[A]	LHG	O10-C23-C24-C25
32	a	420[A]	LHG	O10-C23-C24-C25
33	c	519	LMG	O9-C10-C11-C12
26	B	620	SQD	C11-C12-C13-C14
26	a	410[B]	SQD	C10-C11-C12-C13
23	b	603	CLA	C13-C15-C16-C17
32	D	407[A]	LHG	C28-C29-C30-C31
33	C	521	LMG	C8-C7-O1-C1
35	C	517[A]	DGD	C5D-C6D-O5D-C1E
35	C	517[B]	DGD	C5D-C6D-O5D-C1E
35	C	518[A]	DGD	C5D-C6D-O5D-C1E
35	c	516[A]	DGD	C5D-C6D-O5D-C1E
35	H	102	DGD	O1G-C1G-C2G-O2G
23	b	604	CLA	C4C-C3C-CAC-CBC
32	E	101[A]	LHG	C11-C10-C9-C8
23	C	511	CLA	CAA-CBA-CGA-O1A
32	a	420[B]	LHG	O10-C23-C24-C25
33	C	520	LMG	O7-C10-C11-C12
35	C	518[A]	DGD	O2G-C1B-C2B-C3B
23	b	602	CLA	C2A-CAA-CBA-CGA
35	C	517[A]	DGD	CBA-CCA-CDA-CEA
23	c	512	CLA	CAA-CBA-CGA-O1A
33	Z	101	LMG	O9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	d	405[A]	PL9	C11-C12-C13-C14
23	c	509	CLA	C8-C10-C11-C12
35	c	517[A]	DGD	CDA-CEA-CFA-CGA
24	a	407[B]	PHO	C8-C10-C11-C12
32	L	101[B]	LHG	O9-C7-C8-C9
23	b	612	CLA	O1A-CGA-O2A-C1
23	B	609	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O2D
23	c	512	CLA	CAD-CBD-CGD-O2D
24	a	407[A]	PHO	CAD-CBD-CGD-O2D
32	L	101[A]	LHG	C32-C33-C34-C35
26	a	410[B]	SQD	O47-C7-C8-C9
33	D	411	LMG	O7-C10-C11-C12
26	a	411	SQD	C18-C19-C20-C21
33	d	411	LMG	C40-C41-C42-C43
35	c	516[B]	DGD	C2A-C3A-C4A-C5A
23	B	613	CLA	CAA-CBA-CGA-O1A
32	E	101[A]	LHG	O8-C23-C24-C25
33	B	621	LMG	C30-C31-C32-C33
32	b	629[A]	LHG	C17-C18-C19-C20
23	b	613	CLA	CAA-CBA-CGA-O1A
26	A	412	SQD	O48-C23-C24-C25
26	a	411	SQD	O48-C23-C24-C25
32	D	407[A]	LHG	O8-C23-C24-C25
32	E	101[B]	LHG	O8-C23-C24-C25
33	c	520	LMG	O7-C10-C11-C12
32	E	101[A]	LHG	O9-C7-C8-C9
23	c	501	CLA	CAA-CBA-CGA-O2A
32	D	407[B]	LHG	O8-C23-C24-C25
38	F	102	HEM	CAA-CBA-CGA-O2A
33	C	520	LMG	O9-C10-C11-C12
33	D	411	LMG	O9-C10-C11-C12

There are no ring outliers.

177 monomers are involved in 358 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	a	408	CLA	3	0
23	A	408	CLA	3	0
23	B	601	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	H	101	BCR	2	0
23	c	506	CLA	4	0
23	C	503	CLA	2	0
23	A	406[A]	CLA	1	0
35	C	519	DGD	2	0
31	B	631	LMT	1	0
34	o	301	HTG	3	0
23	C	509	CLA	3	0
26	a	410[A]	SQD	4	0
32	d	406[A]	LHG	2	0
23	d	403	CLA	1	0
23	b	612	CLA	1	0
23	D	402[B]	CLA	4	0
26	B	620	SQD	1	0
23	b	601	CLA	2	0
32	D	407[A]	LHG	4	0
32	E	101[A]	LHG	4	0
27	B	623	GOL	2	0
31	B	629	LMT	2	0
24	a	407[B]	PHO	2	0
23	c	507	CLA	2	0
34	c	521	HTG	1	0
24	a	415[B]	PHO	1	0
29	a	413[B]	PL9	4	0
38	f	101	HEM	1	0
33	d	411	LMG	3	0
23	A	405[B]	CLA	5	0
23	b	610	CLA	1	0
25	a	409	BCR	1	0
27	l	801[A]	GOL	1	0
23	c	513	CLA	1	0
32	d	407[B]	LHG	8	0
23	C	507	CLA	4	0
24	A	407[B]	PHO	2	0
25	B	619	BCR	2	0
35	c	517[A]	DGD	4	0
23	a	404[A]	CLA	2	0
32	A	419[B]	LHG	1	0
27	v	202[A]	GOL	1	0
33	c	519	LMG	1	0
23	a	406[A]	CLA	2	0
23	b	606	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	d	402[B]	CLA	4	0
33	Z	101	LMG	2	0
35	C	518[A]	DGD	1	0
23	b	614	CLA	1	0
23	c	503	CLA	3	0
31	A	420	LMT	2	0
32	a	420[B]	LHG	4	0
35	H	102	DGD	1	0
23	c	505	CLA	4	0
27	D	412	GOL	3	0
31	M	103	LMT	1	0
33	C	521	LMG	3	0
32	d	413[B]	LHG	1	0
23	b	603	CLA	2	0
29	A	414[B]	PL9	9	0
27	a	419	GOL	5	0
35	C	517[B]	DGD	1	0
23	B	604	CLA	2	0
23	C	505	CLA	1	0
27	a	418	GOL	1	0
25	B	617	BCR	1	0
23	B	615	CLA	4	0
26	A	410[B]	SQD	2	0
23	b	605	CLA	2	0
25	B	618	BCR	2	0
25	h	101	BCR	5	0
23	A	406[B]	CLA	3	0
27	B	628	GOL	1	0
23	C	504	CLA	5	0
33	B	621	LMG	1	0
25	c	514	BCR	3	0
29	D	405[A]	PL9	1	0
26	a	410[B]	SQD	3	0
32	d	406[B]	LHG	3	0
23	B	613	CLA	4	0
23	A	404[A]	CLA	2	0
32	D	407[B]	LHG	2	0
23	B	609	CLA	3	0
32	E	101[B]	LHG	2	0
25	T	101	BCR	6	0
25	b	618	BCR	4	0
23	a	405[A]	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	616	CLA	3	0
24	A	416[B]	PHO	2	0
35	c	516[A]	DGD	1	0
23	B	614	CLA	3	0
25	Y	101	BCR	2	0
32	d	407[A]	LHG	11	0
23	B	612	CLA	2	0
27	A	418	GOL	4	0
32	D	406[B]	LHG	1	0
34	b	622	HTG	2	0
31	m	103	LMT	2	0
26	A	412	SQD	1	0
32	L	101[B]	LHG	1	0
25	d	404	BCR	2	0
23	a	404[B]	CLA	5	0
27	b	628	GOL	2	0
31	a	417	LMT	1	0
23	d	402[A]	CLA	1	0
23	c	509	CLA	3	0
26	F	103	SQD	1	0
27	v	202[B]	GOL	3	0
33	c	520	LMG	2	0
34	D	410	HTG	1	0
38	F	102	HEM	1	0
23	a	406[B]	CLA	3	0
23	C	513	CLA	2	0
23	C	512	CLA	2	0
31	t	101	LMT	2	0
23	c	502	CLA	1	0
23	c	501	CLA	3	0
25	b	619	BCR	5	0
23	c	508	CLA	6	0
34	b	625	HTG	1	0
25	D	404	BCR	1	0
23	C	514	CLA	1	0
35	C	518[B]	DGD	1	0
35	c	518	DGD	5	0
23	D	402[A]	CLA	3	0
29	A	414[A]	PL9	10	0
23	b	604	CLA	2	0
25	t	102	BCR	6	0
23	C	510	CLA	2	0

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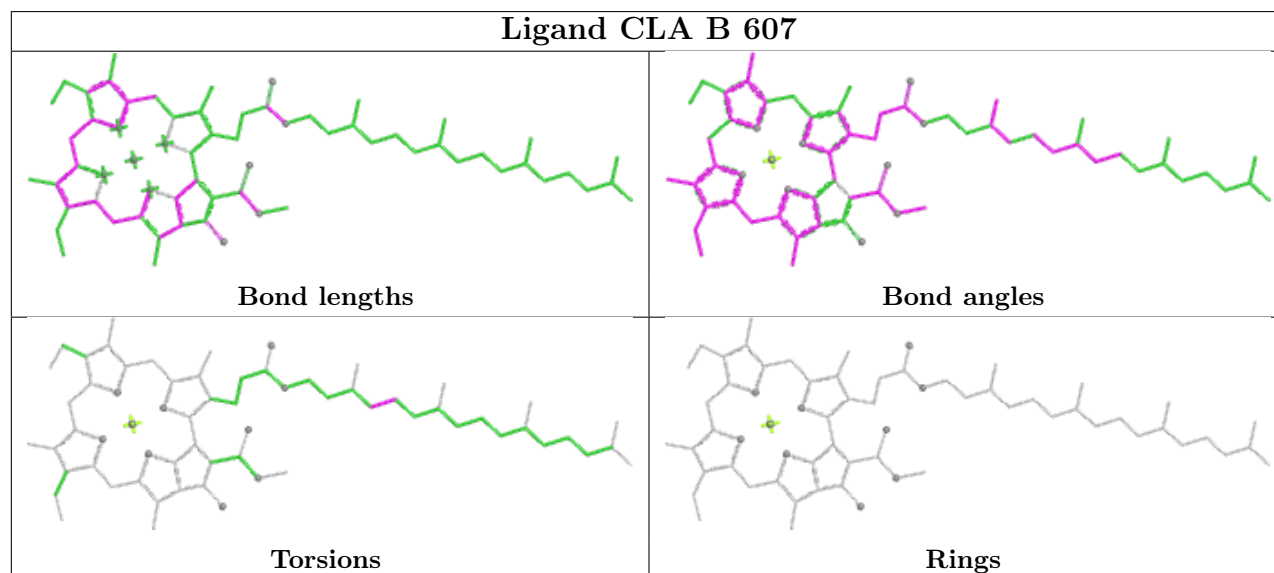
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	626	GOL	1	0
23	C	502	CLA	4	0
25	b	617	BCR	1	0
25	A	409	BCR	2	0
35	c	517[B]	DGD	3	0
23	b	615	CLA	2	0
24	a	415[A]	PHO	1	0
23	C	506	CLA	5	0
26	A	410[A]	SQD	1	0
29	a	413[A]	PL9	5	0
31	e	101	LMT	1	0
23	A	405[A]	CLA	1	0
23	B	602	CLA	3	0
23	c	504	CLA	3	0
23	B	603	CLA	1	0
23	c	511	CLA	5	0
27	O	302	GOL	1	0
27	O	303	GOL	1	0
24	A	407[A]	PHO	1	0
25	y	101	BCR	3	0
23	b	609	CLA	5	0
32	A	419[A]	LHG	1	0
27	l	801[B]	GOL	1	0
34	B	624	HTG	1	0
23	B	616	CLA	3	0
24	A	416[A]	PHO	1	0
23	B	605	CLA	3	0
23	A	404[B]	CLA	4	0
23	b	607	CLA	1	0
25	C	515	BCR	1	0
32	D	406[A]	LHG	2	0
23	C	508	CLA	2	0
23	a	405[B]	CLA	5	0
32	a	420[A]	LHG	5	0
35	c	516[B]	DGD	1	0
31	B	627	LMT	1	0
31	M	101	LMT	1	0
26	b	620	SQD	2	0
31	b	621	LMT	2	0
35	C	517[A]	DGD	1	0
23	B	606	CLA	3	0
33	z	101	LMG	2	0

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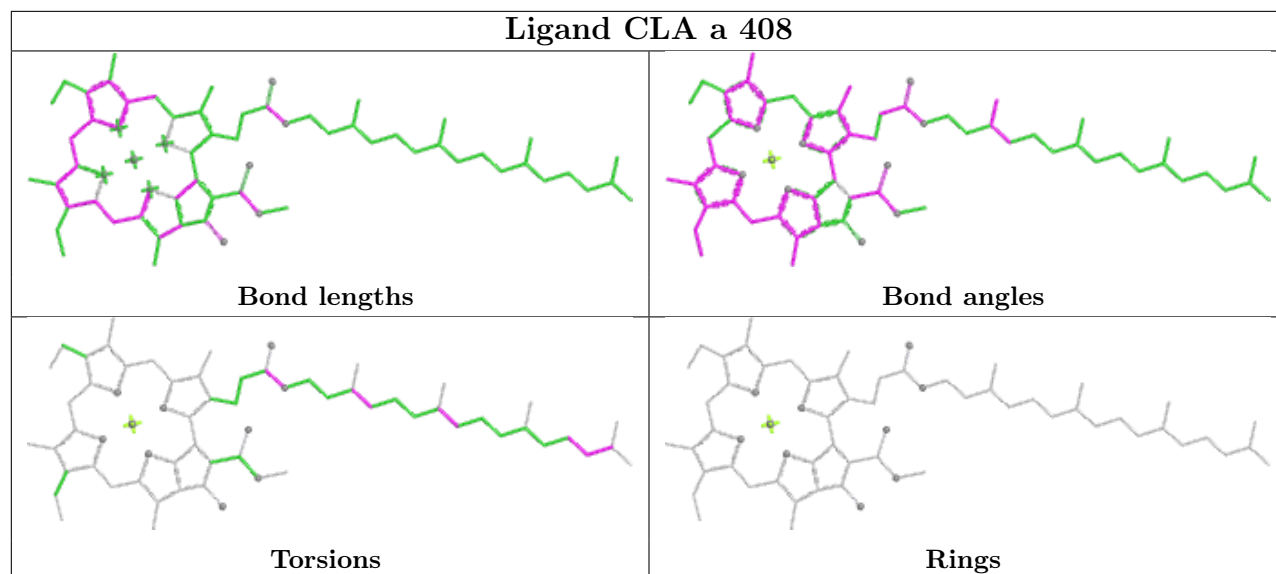
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	512	CLA	6	0
26	a	411	SQD	1	0
23	C	511	CLA	3	0
23	b	611	CLA	2	0
34	B	622	HTG	1	0
25	k	101	BCR	2	0

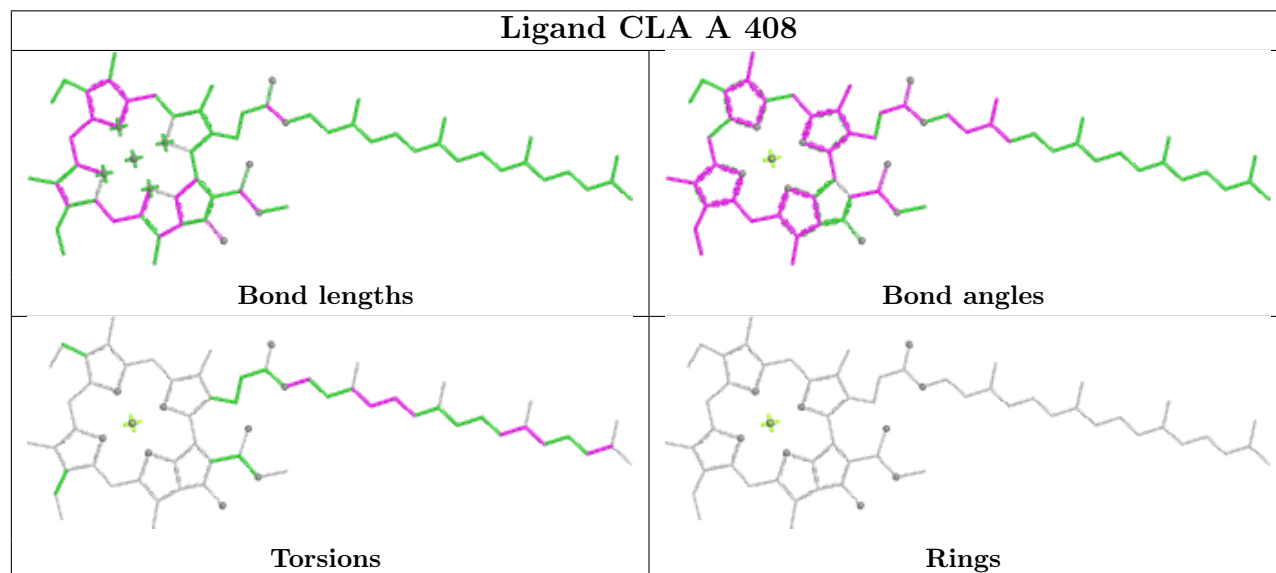
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



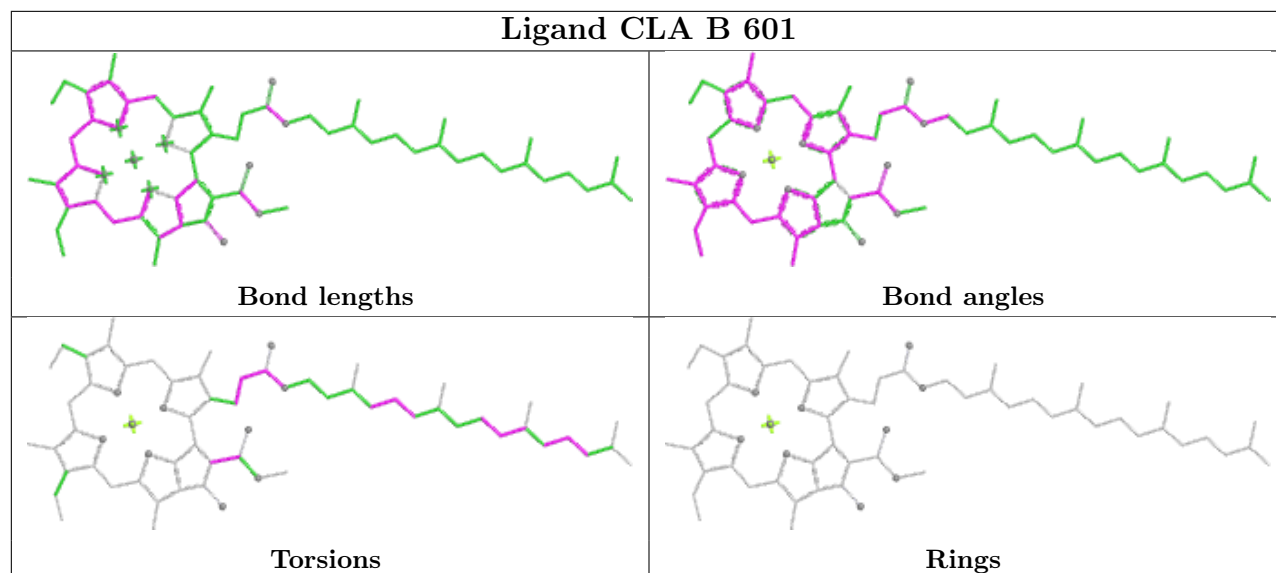
Ligand CLA a 408

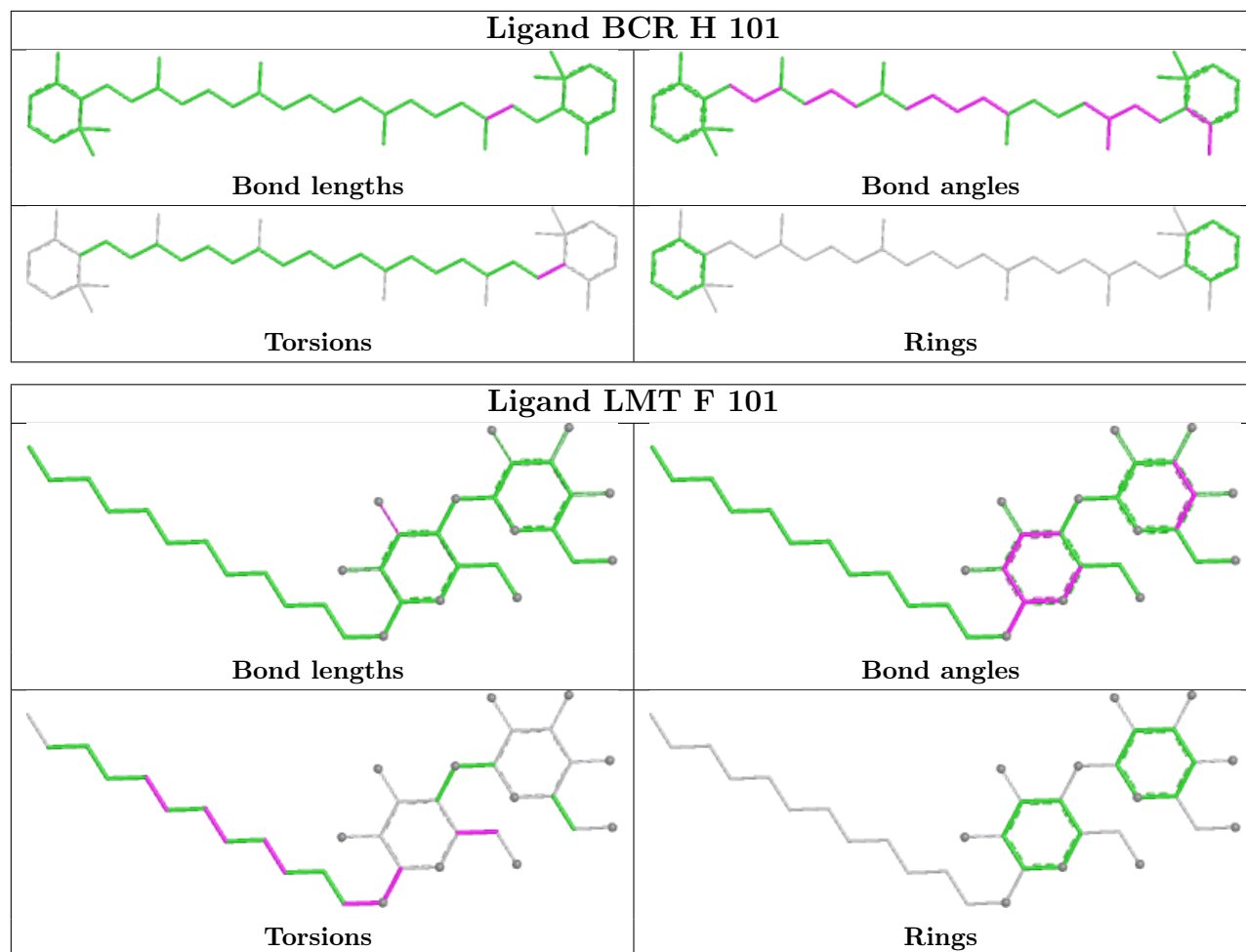


Ligand CLA A 408

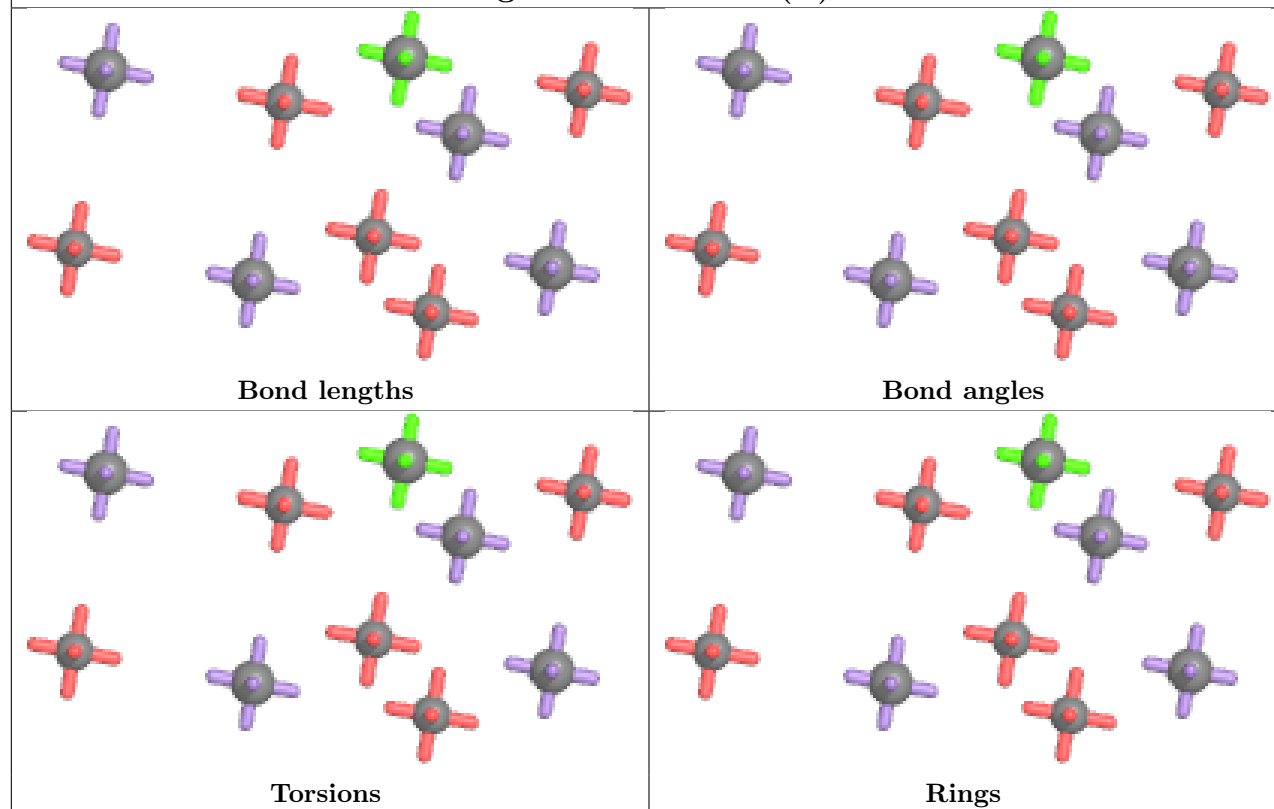


Ligand CLA B 601

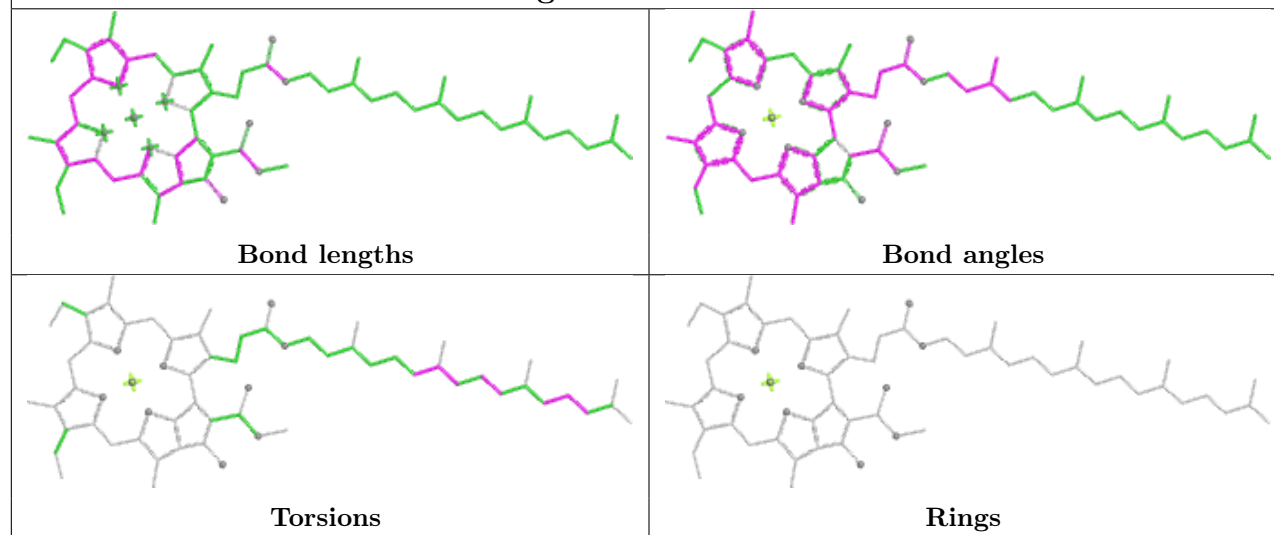




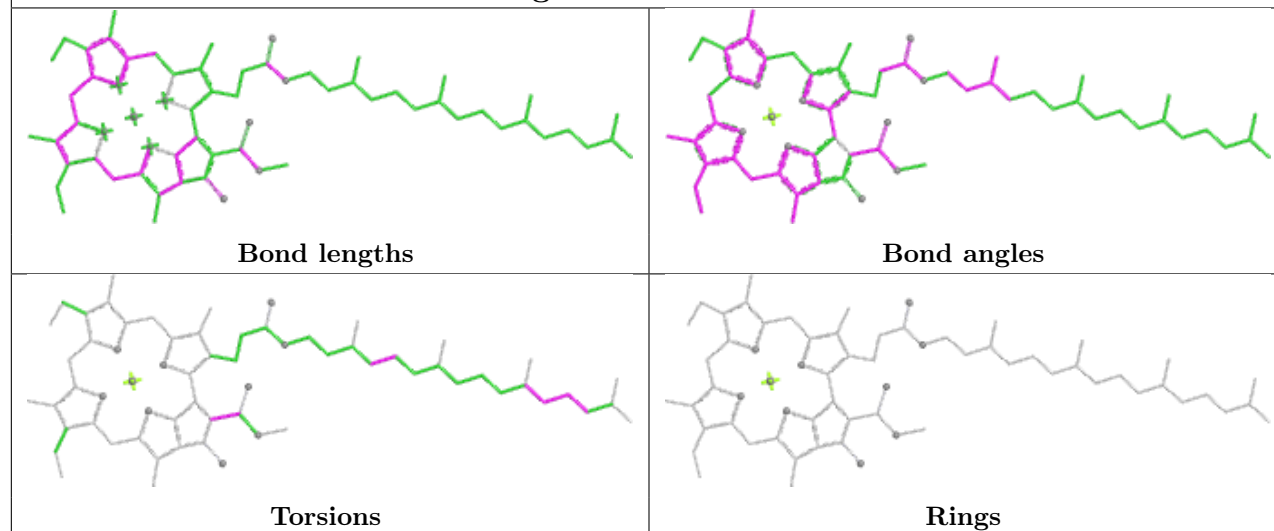
Ligand OEX A 413 (B)



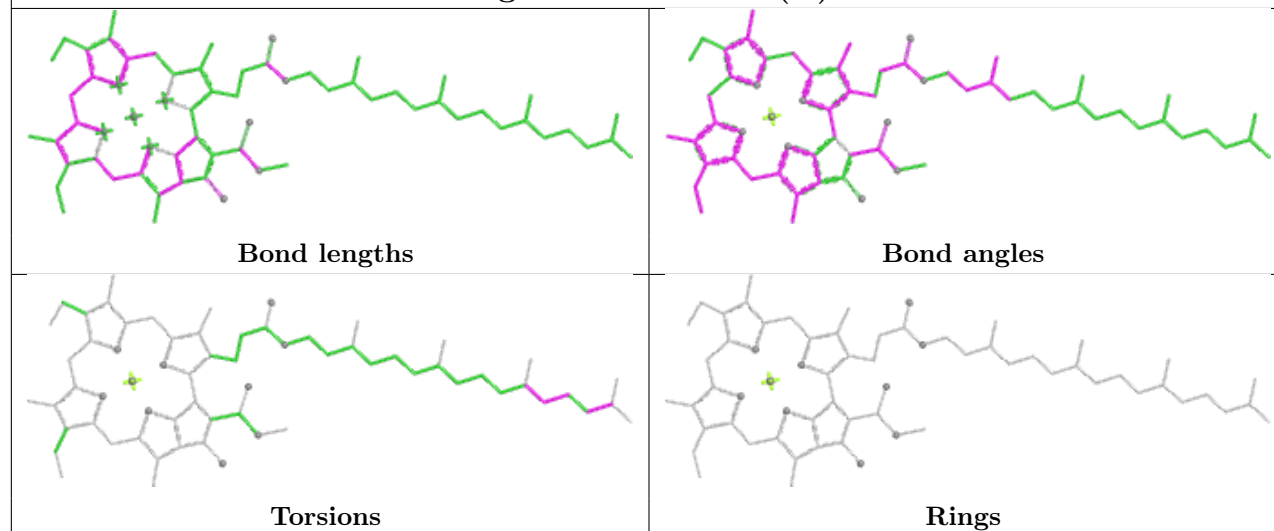
Ligand CLA c 506



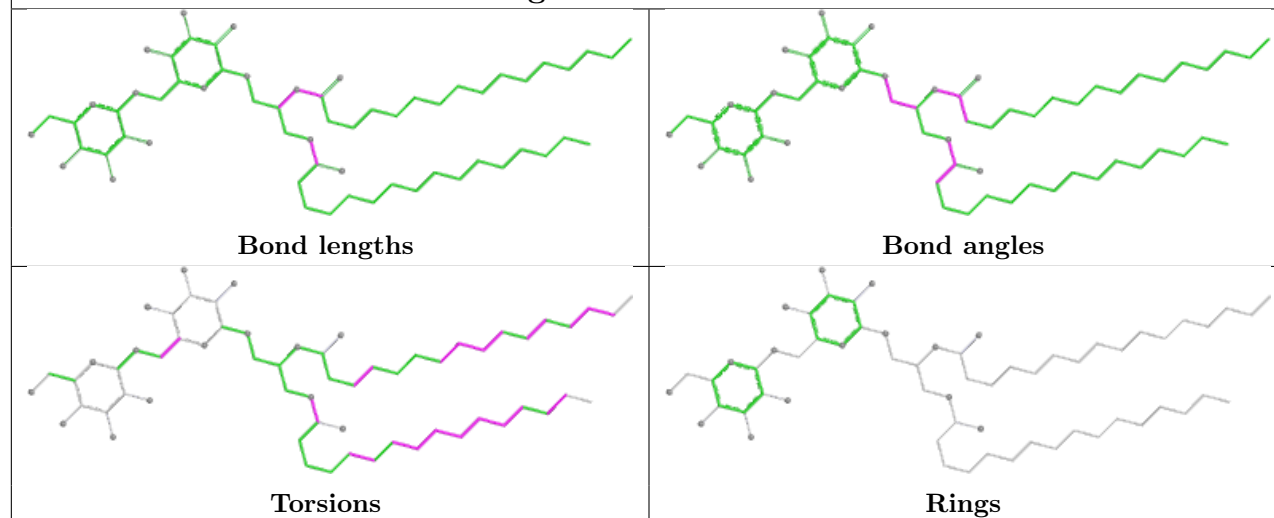
Ligand CLA C 503

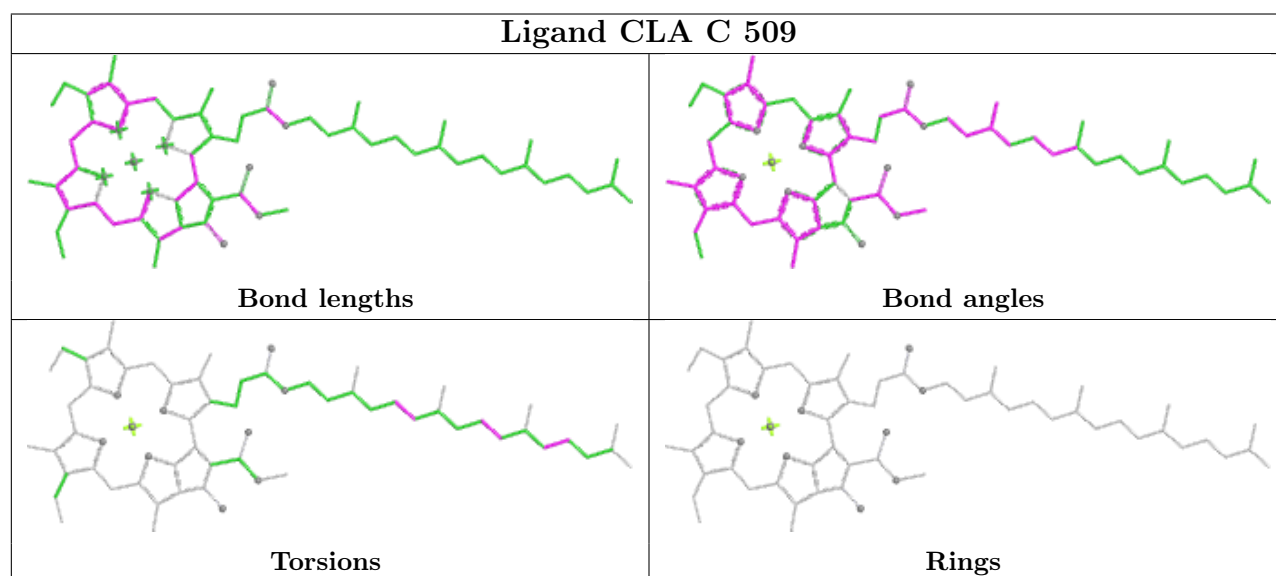
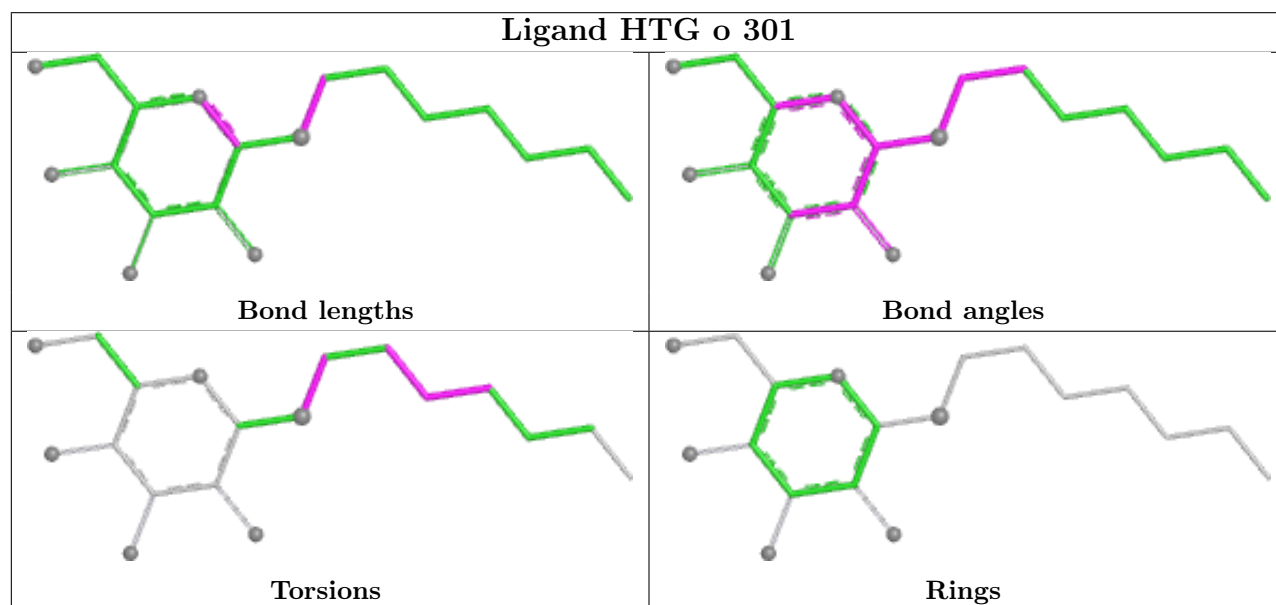
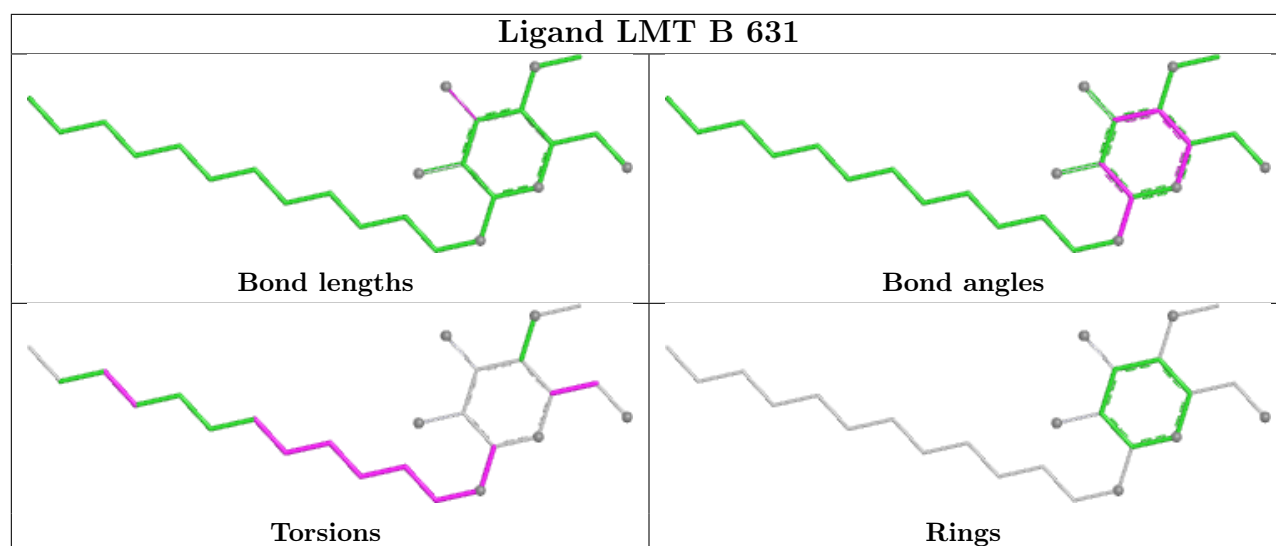


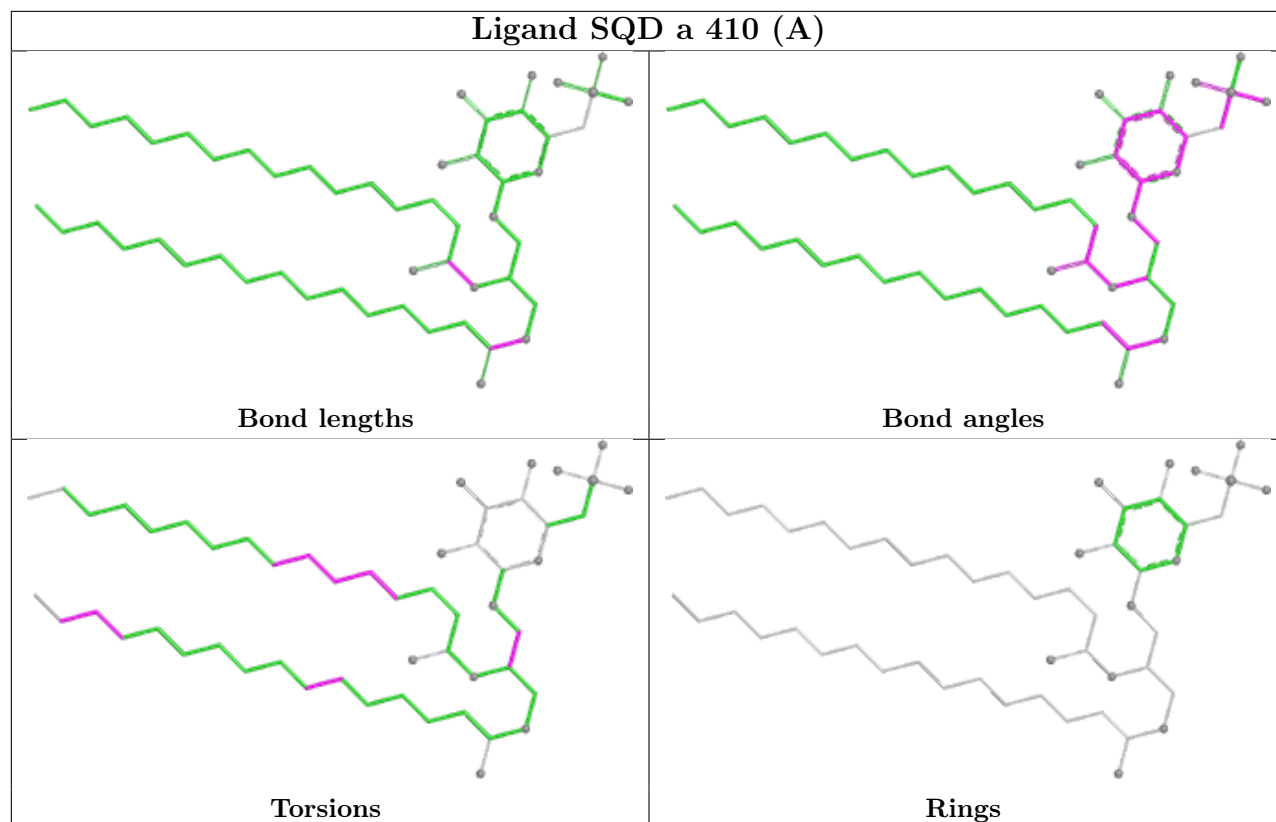
Ligand CLA A 406 (A)



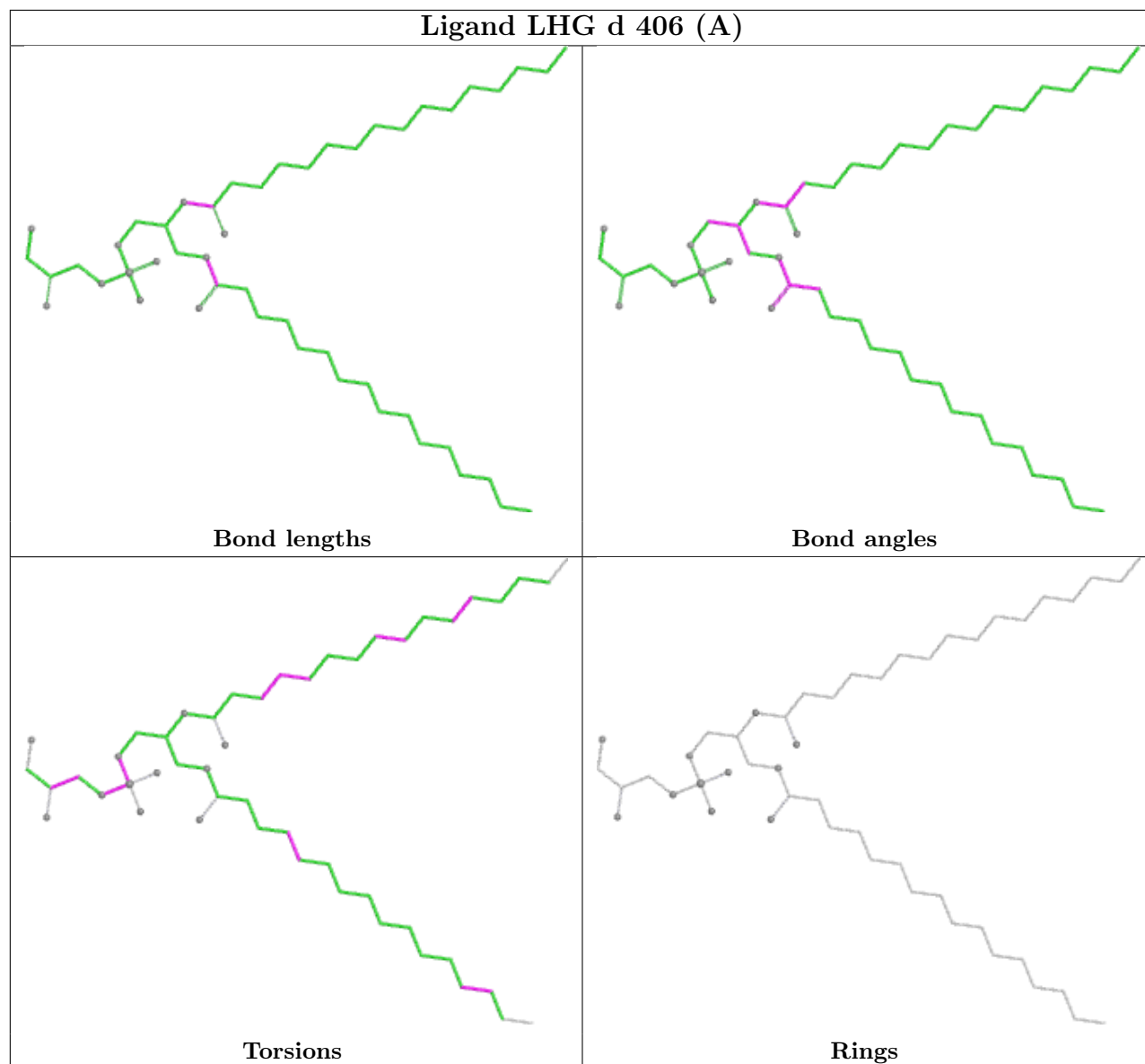
Ligand DGD C 519



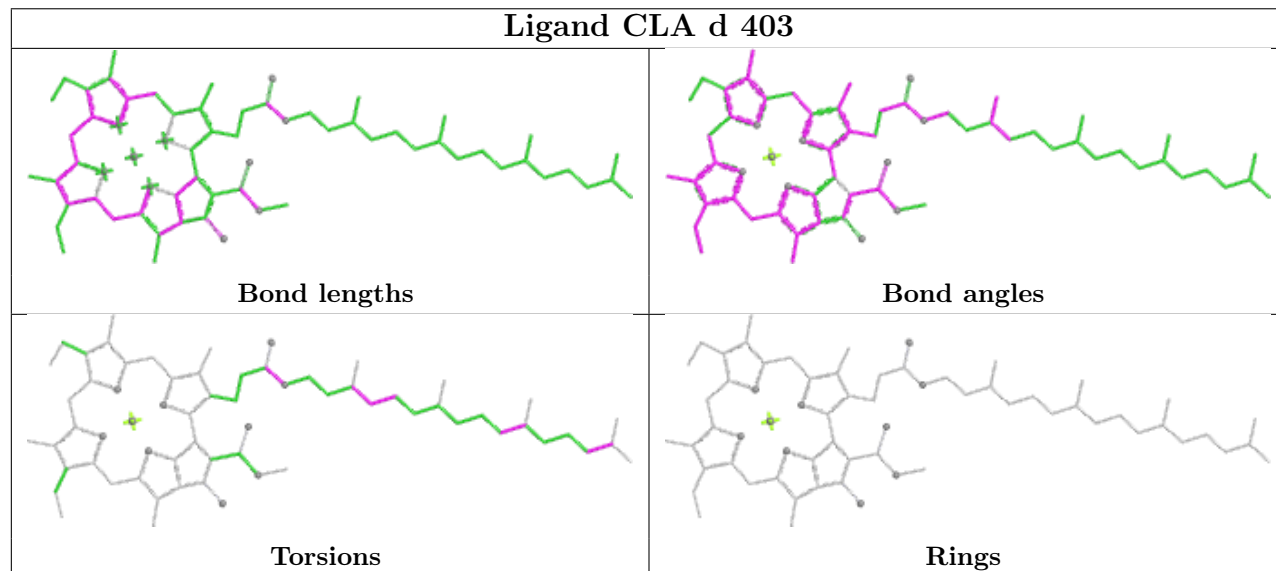




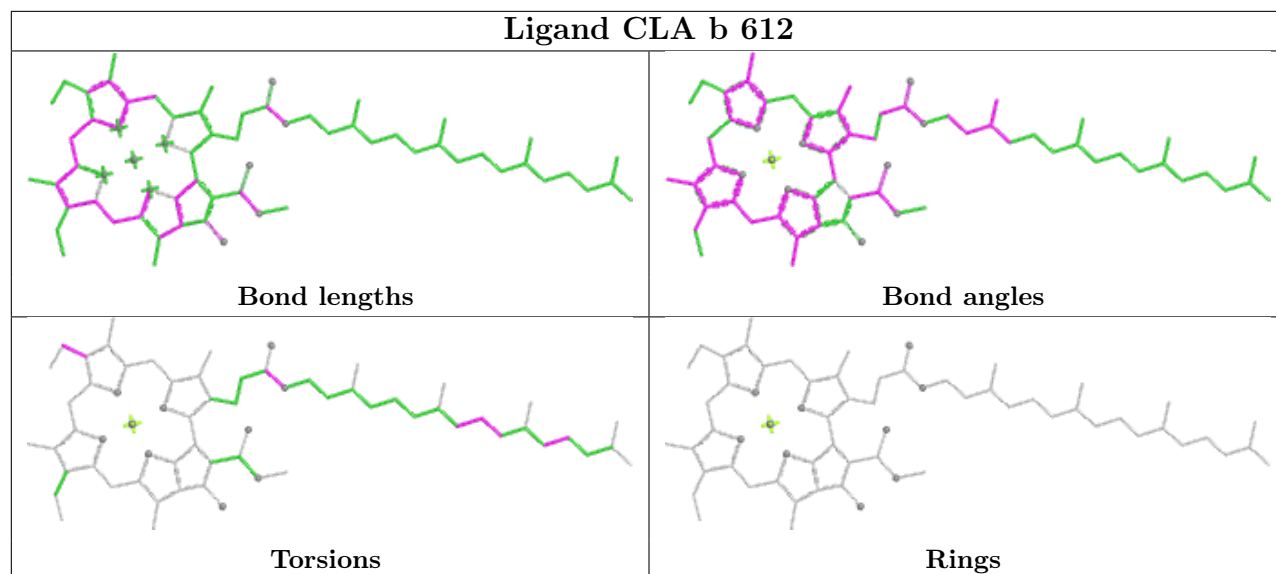
Ligand LHG d 406 (A)



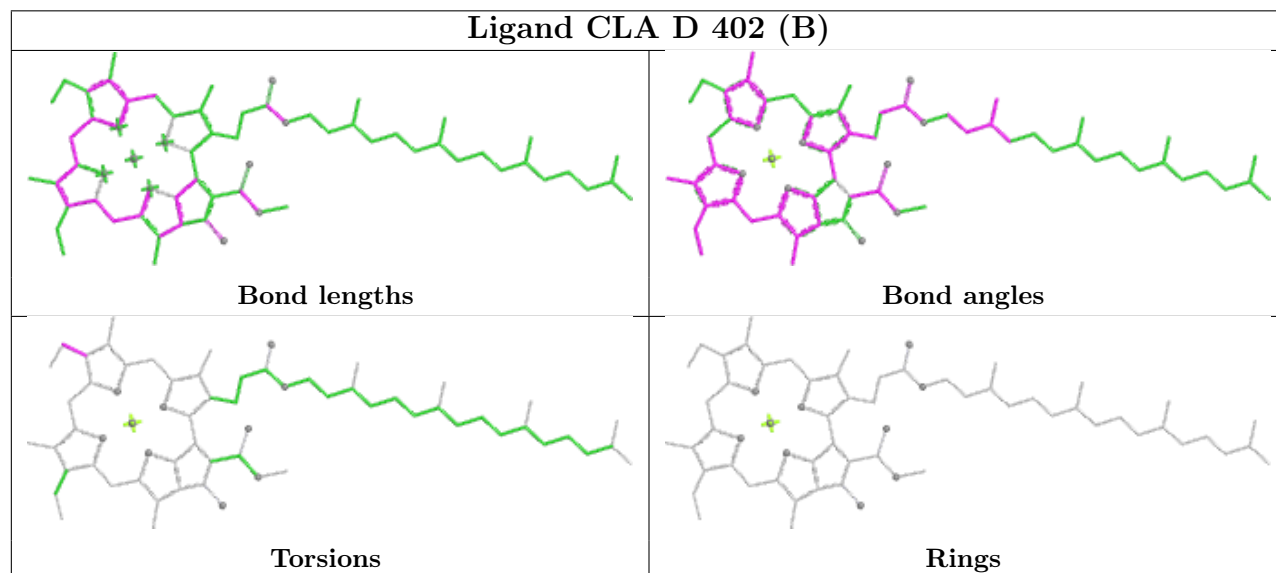
Ligand CLA d 403

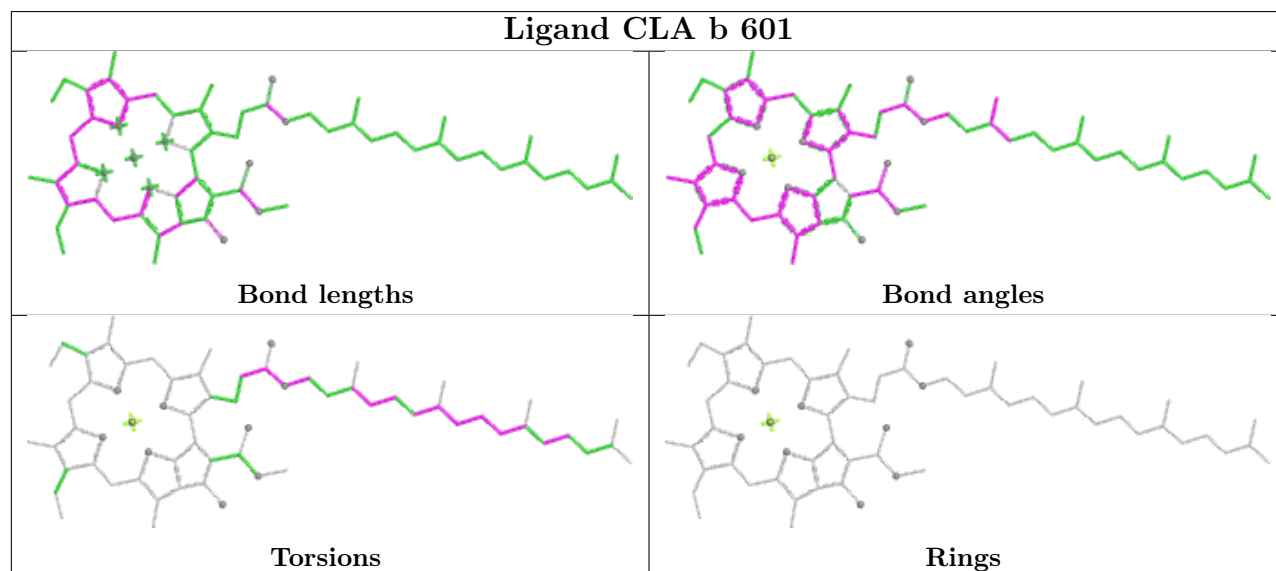
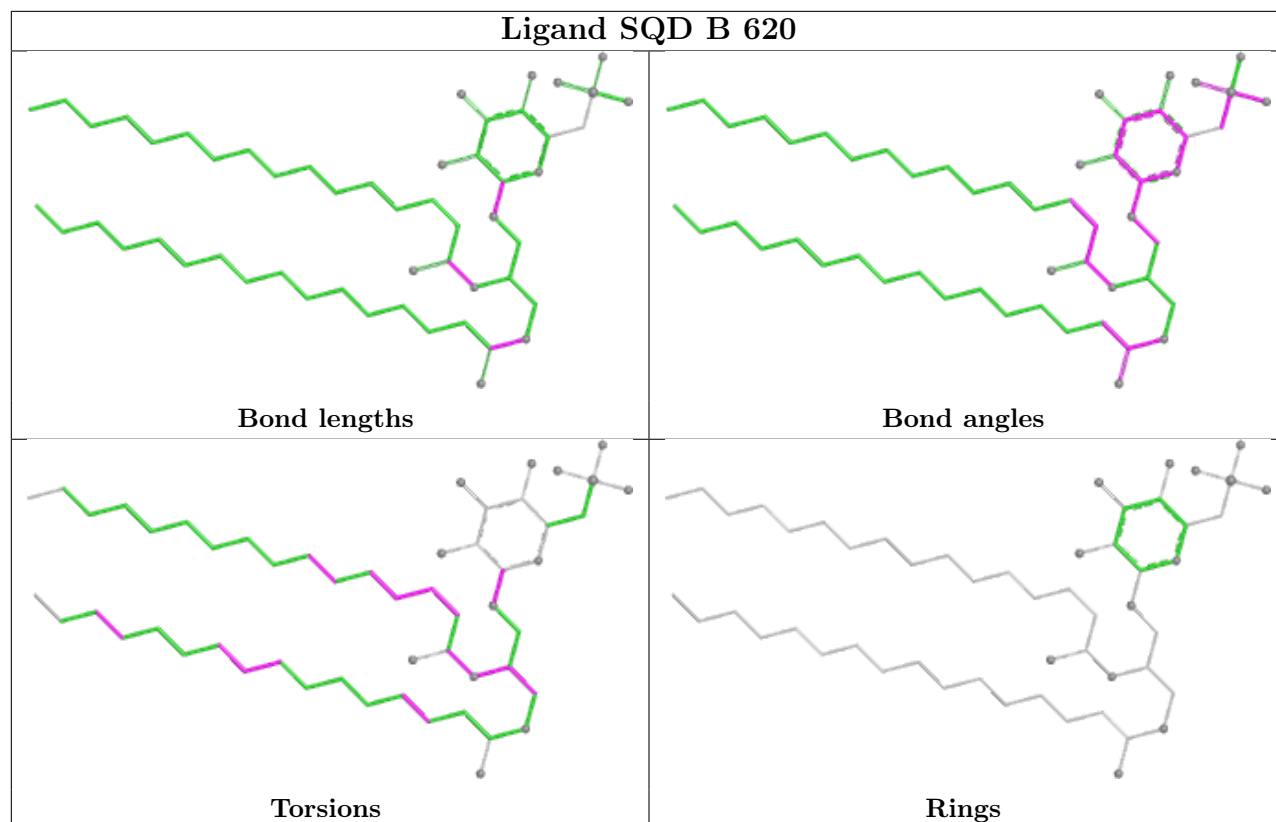


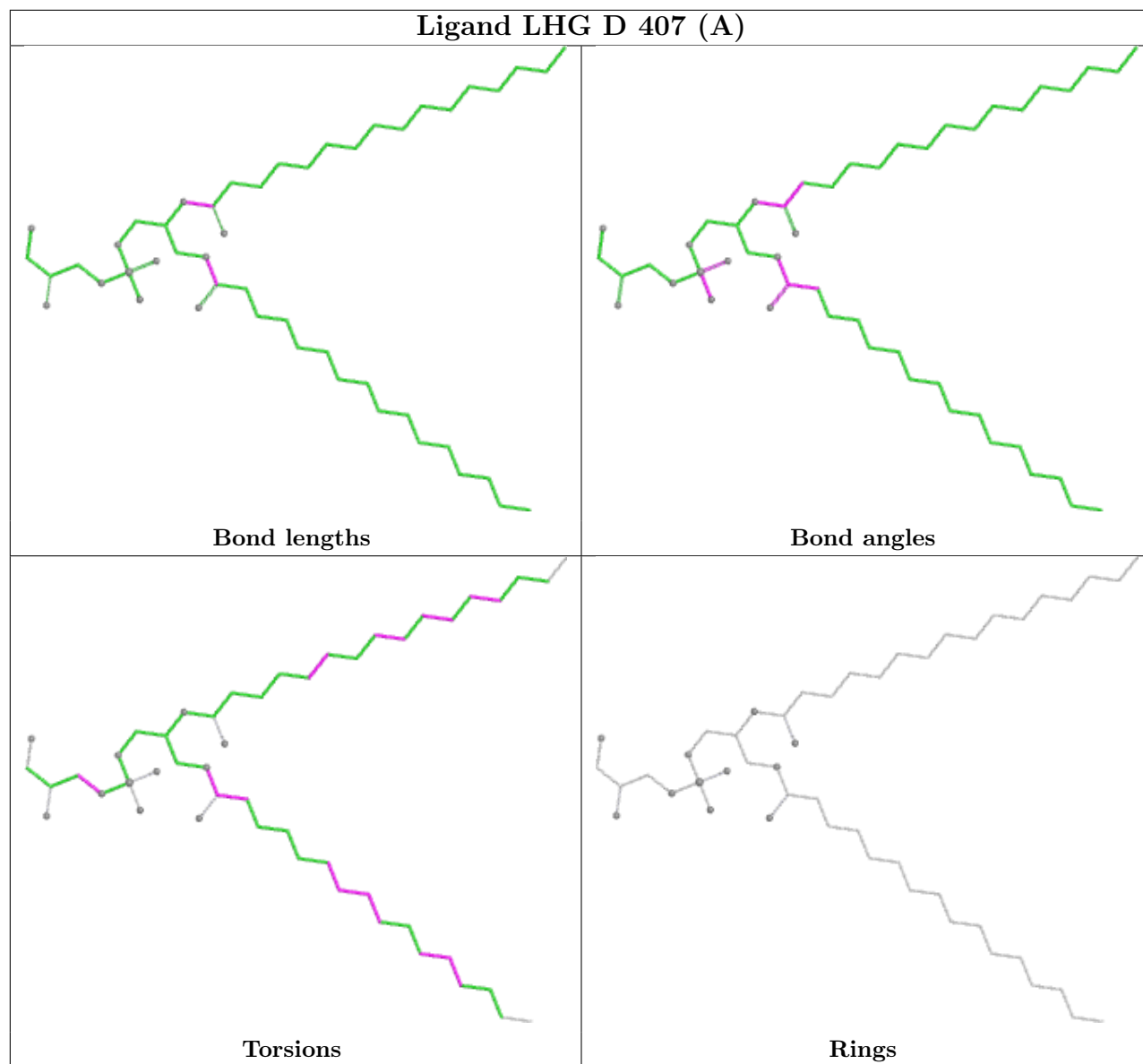
Ligand CLA b 612

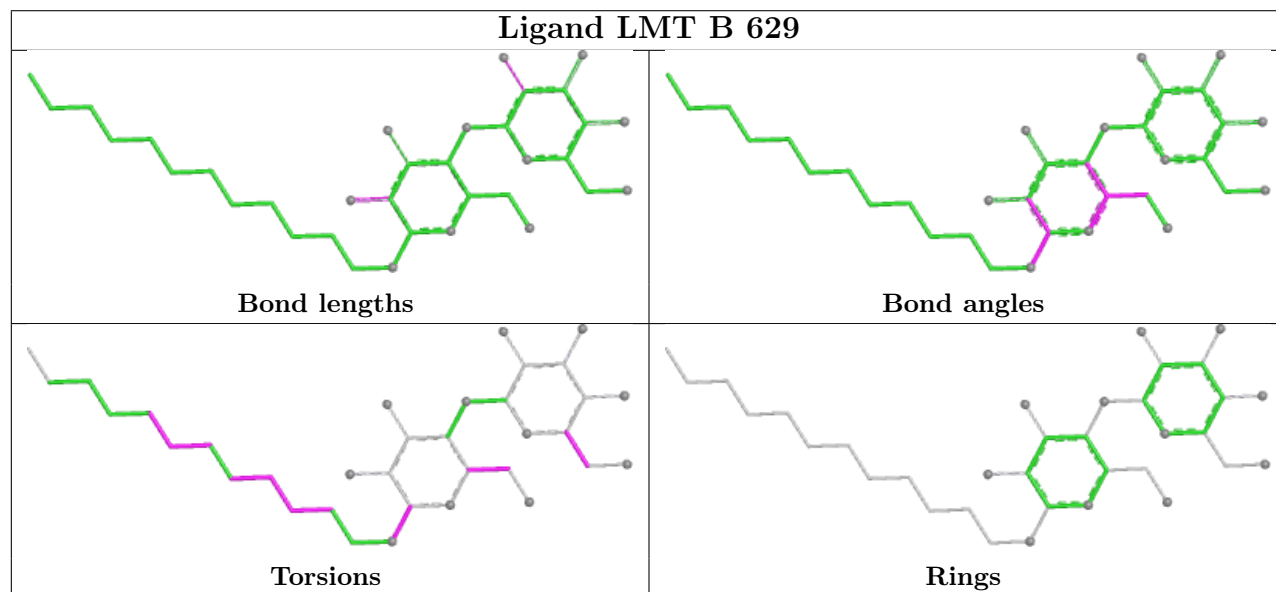
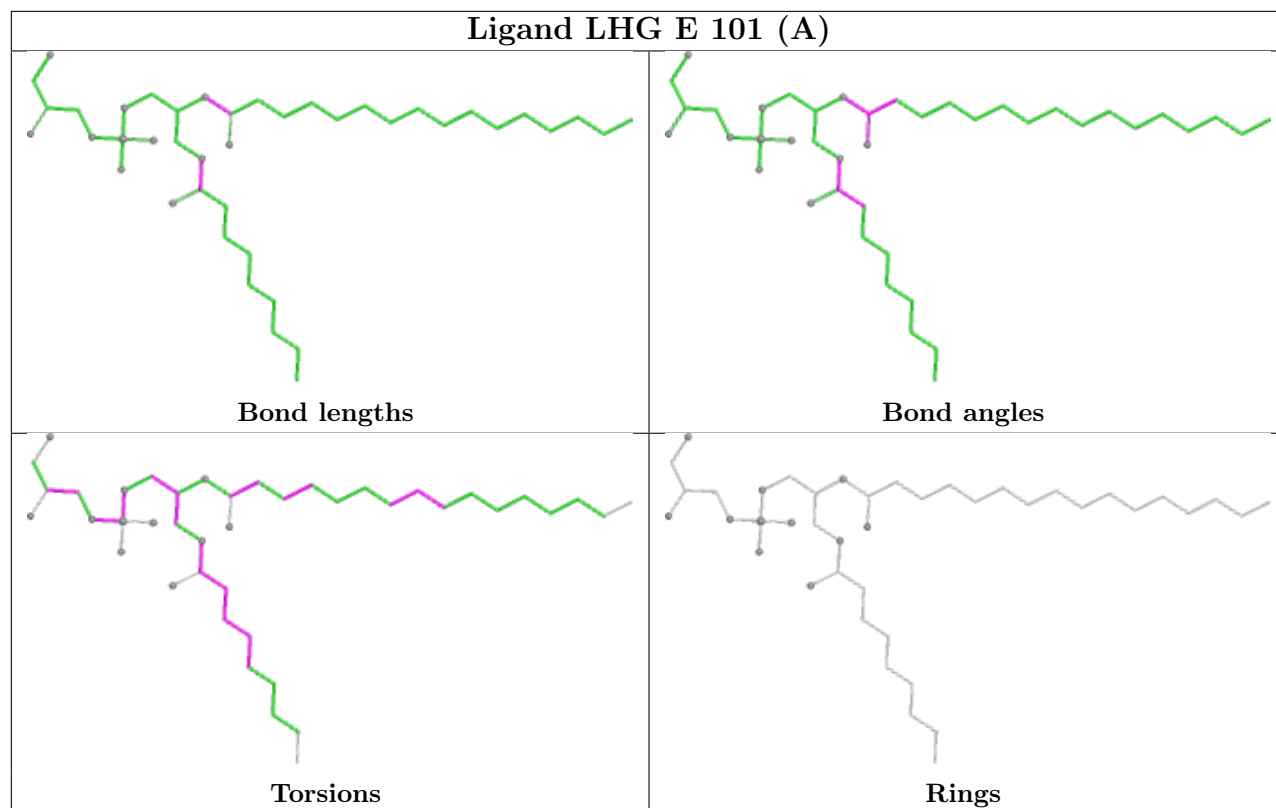


Ligand CLA D 402 (B)

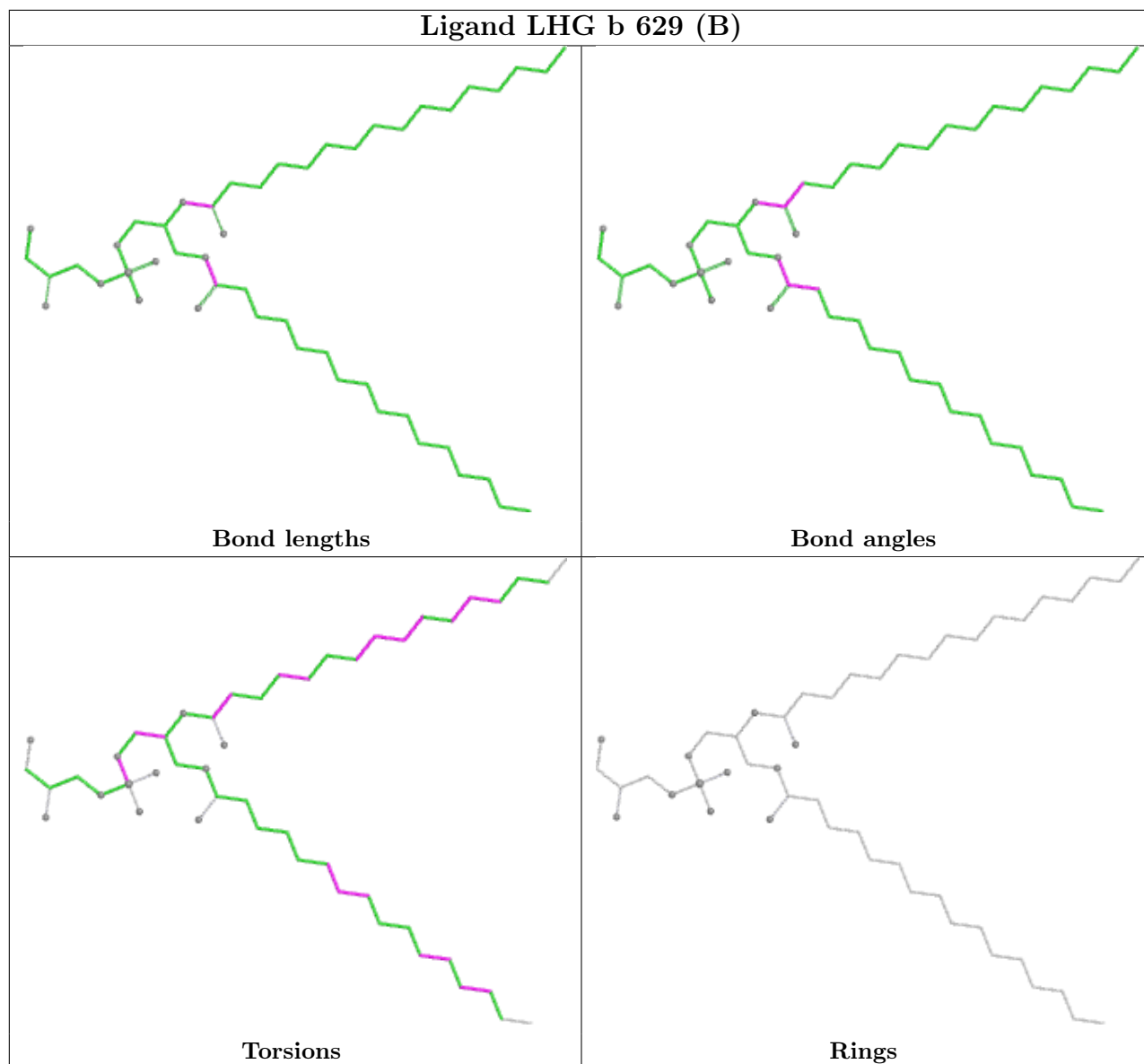




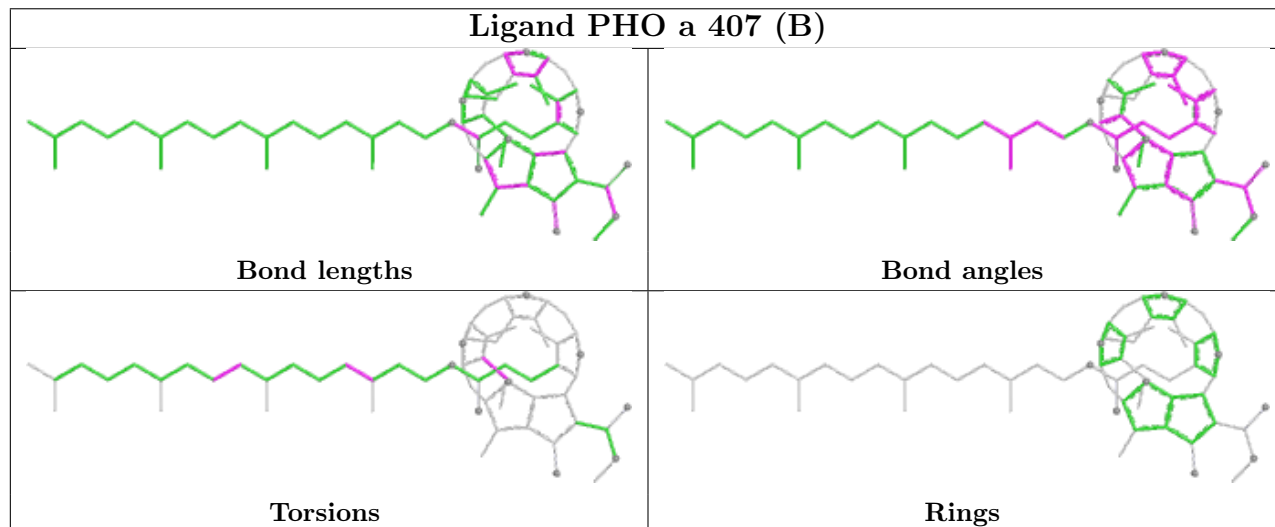


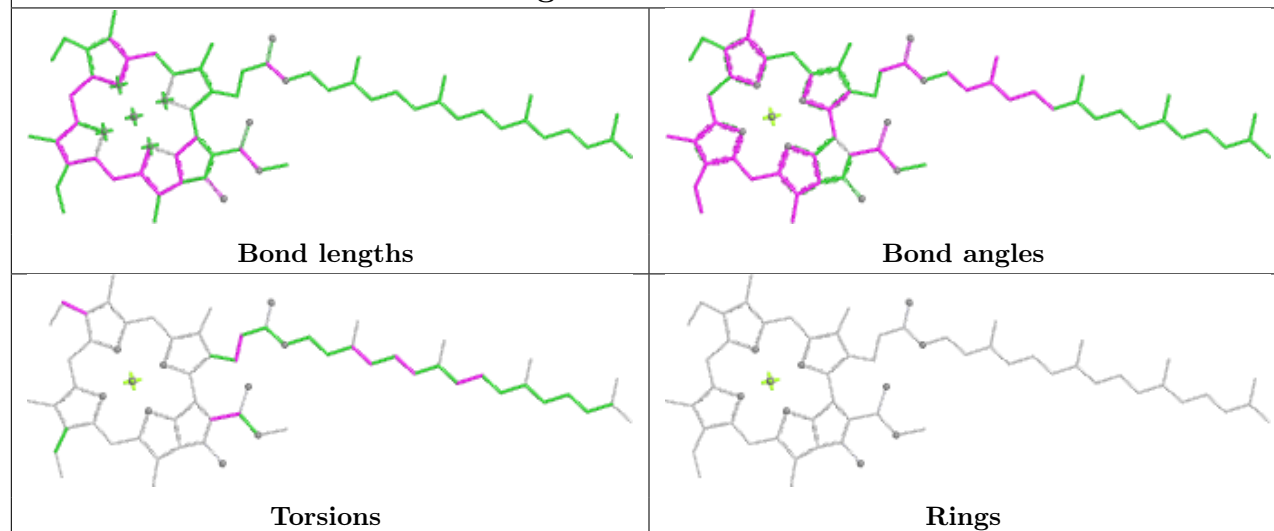
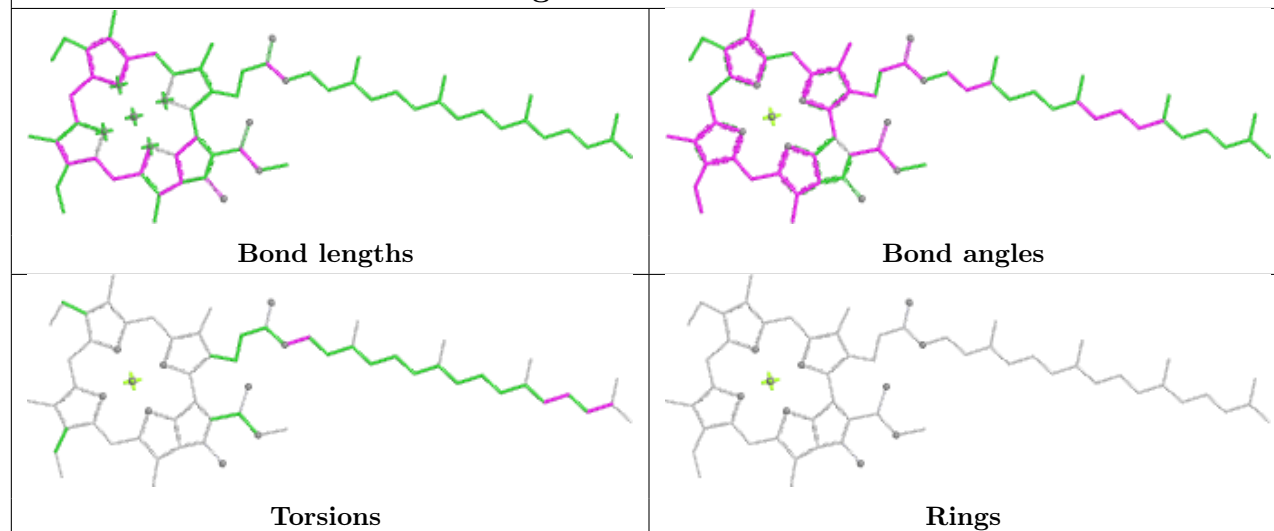


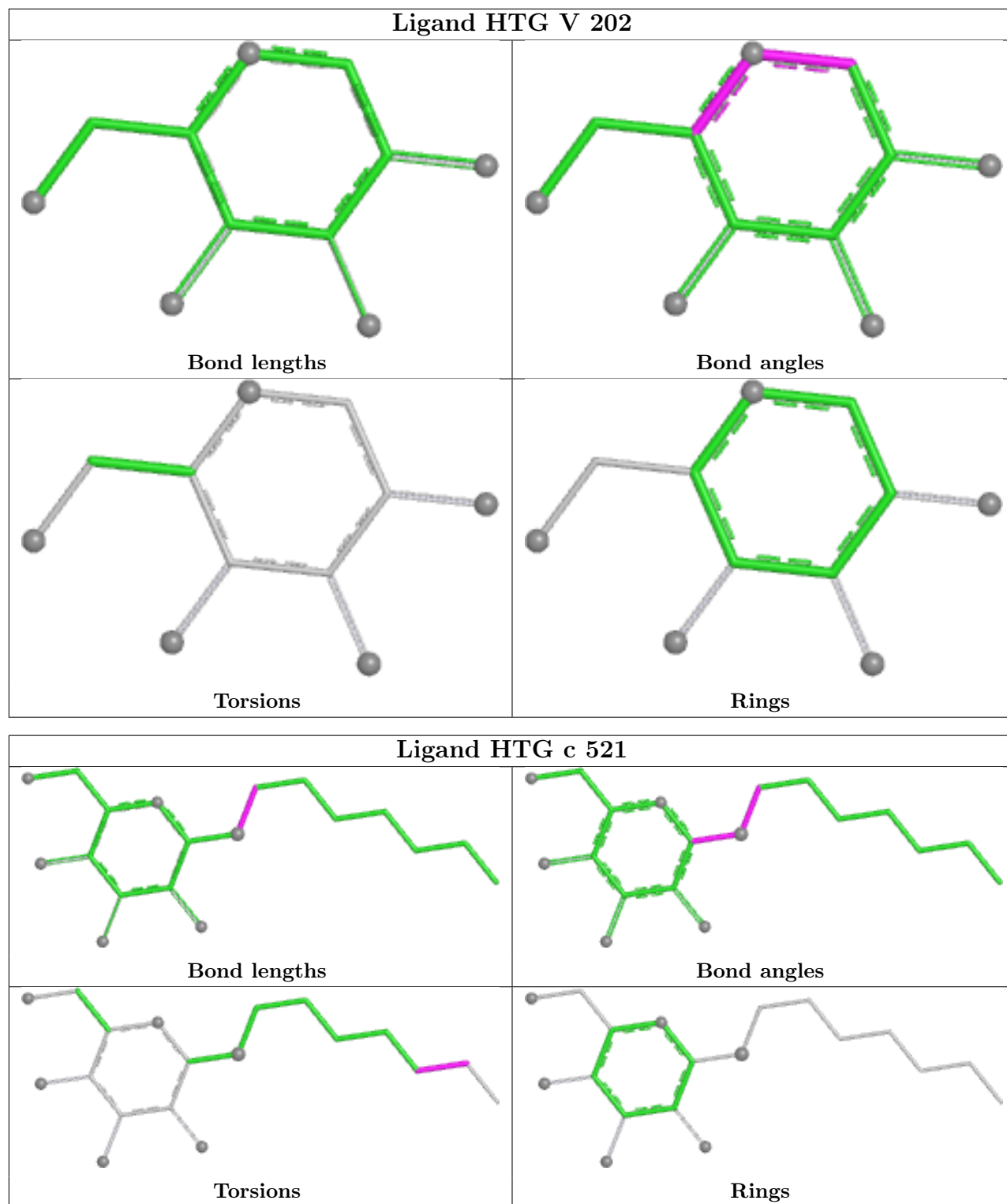
Ligand LHG b 629 (B)

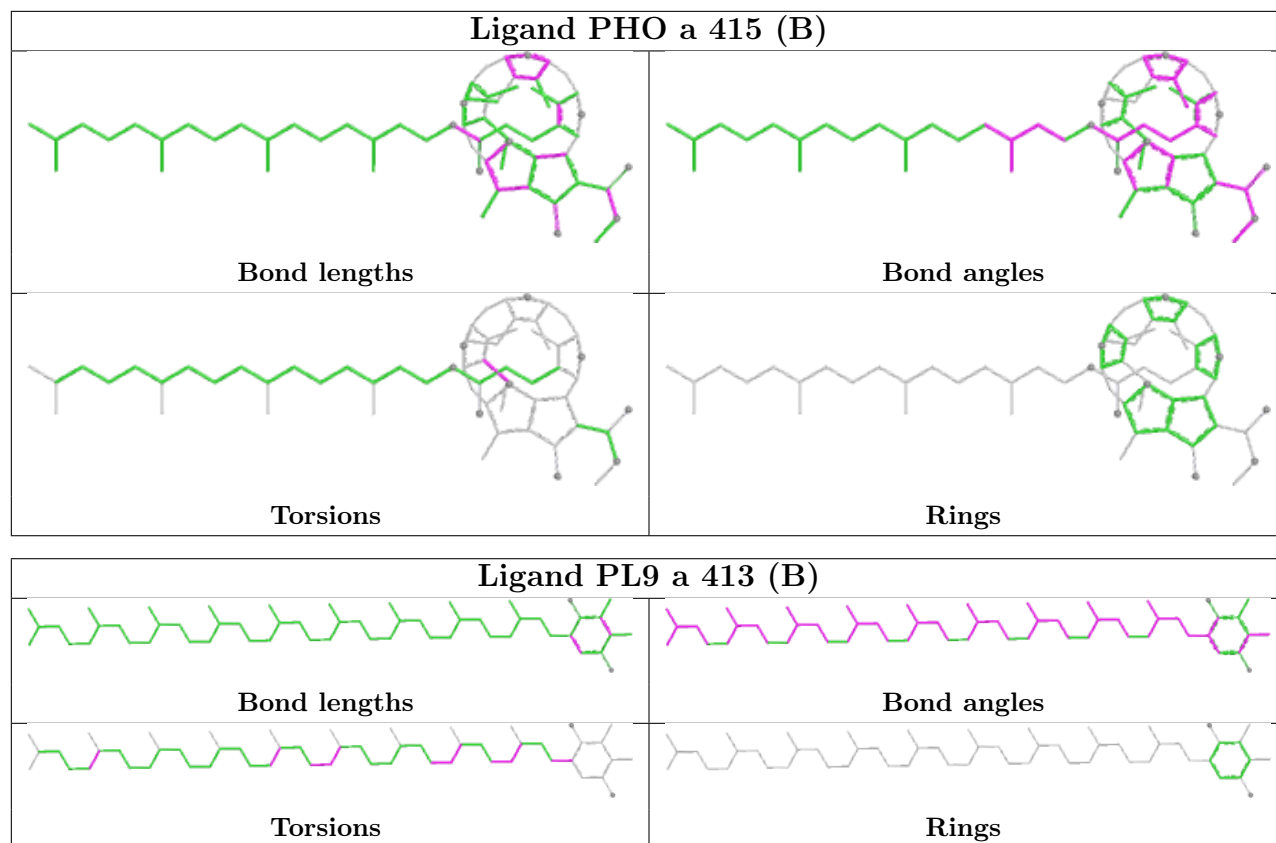


Ligand PHO a 407 (B)

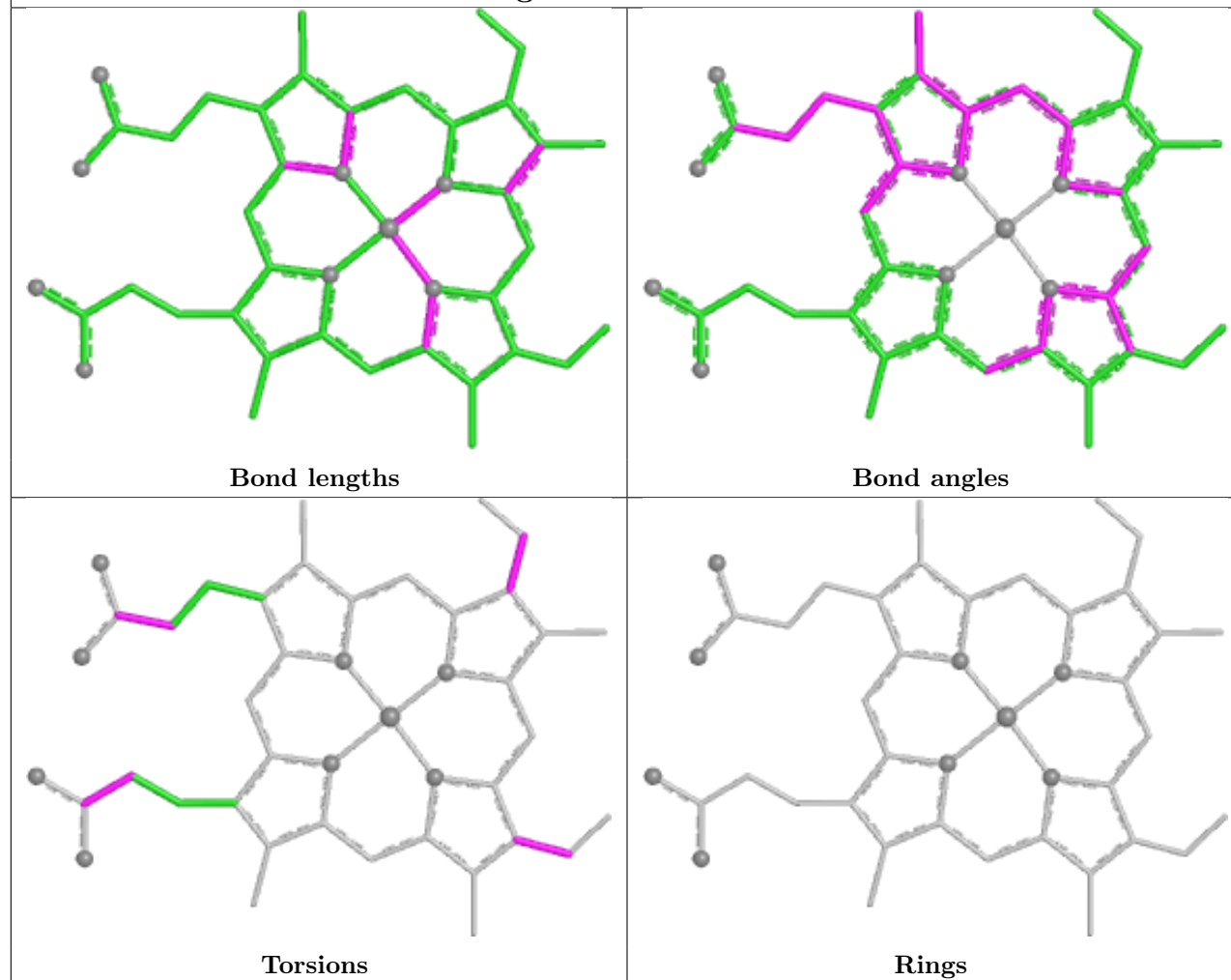


Ligand CLA c 507**Ligand CLA B 608**

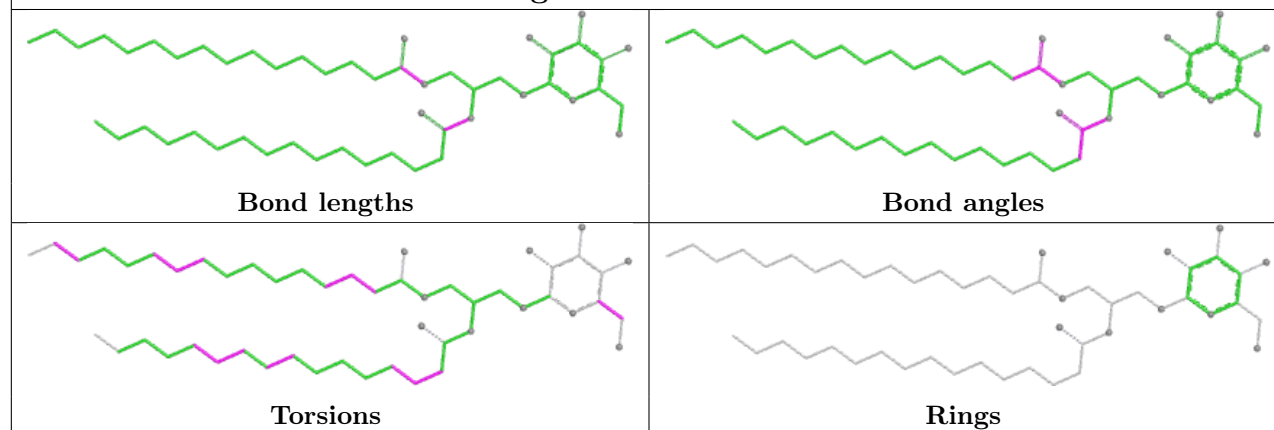




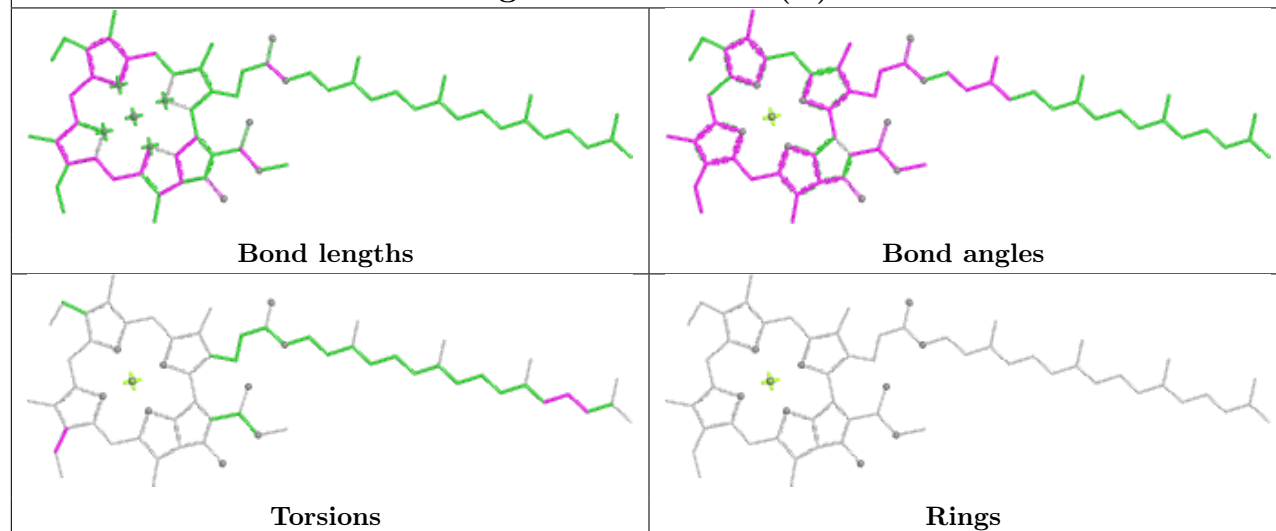
Ligand HEM f 101



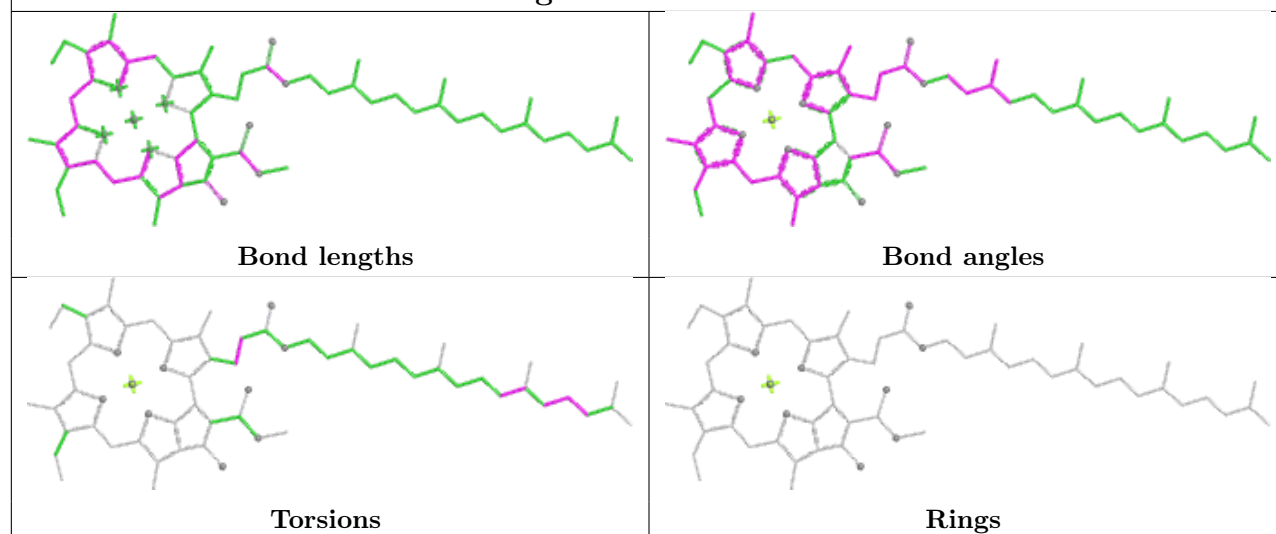
Ligand LMG d 411



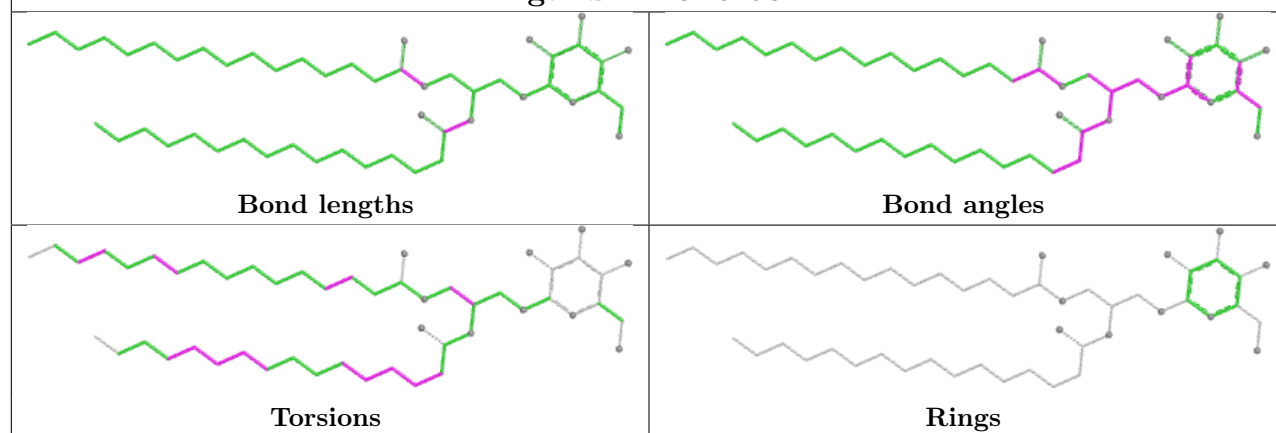
Ligand CLA A 405 (B)

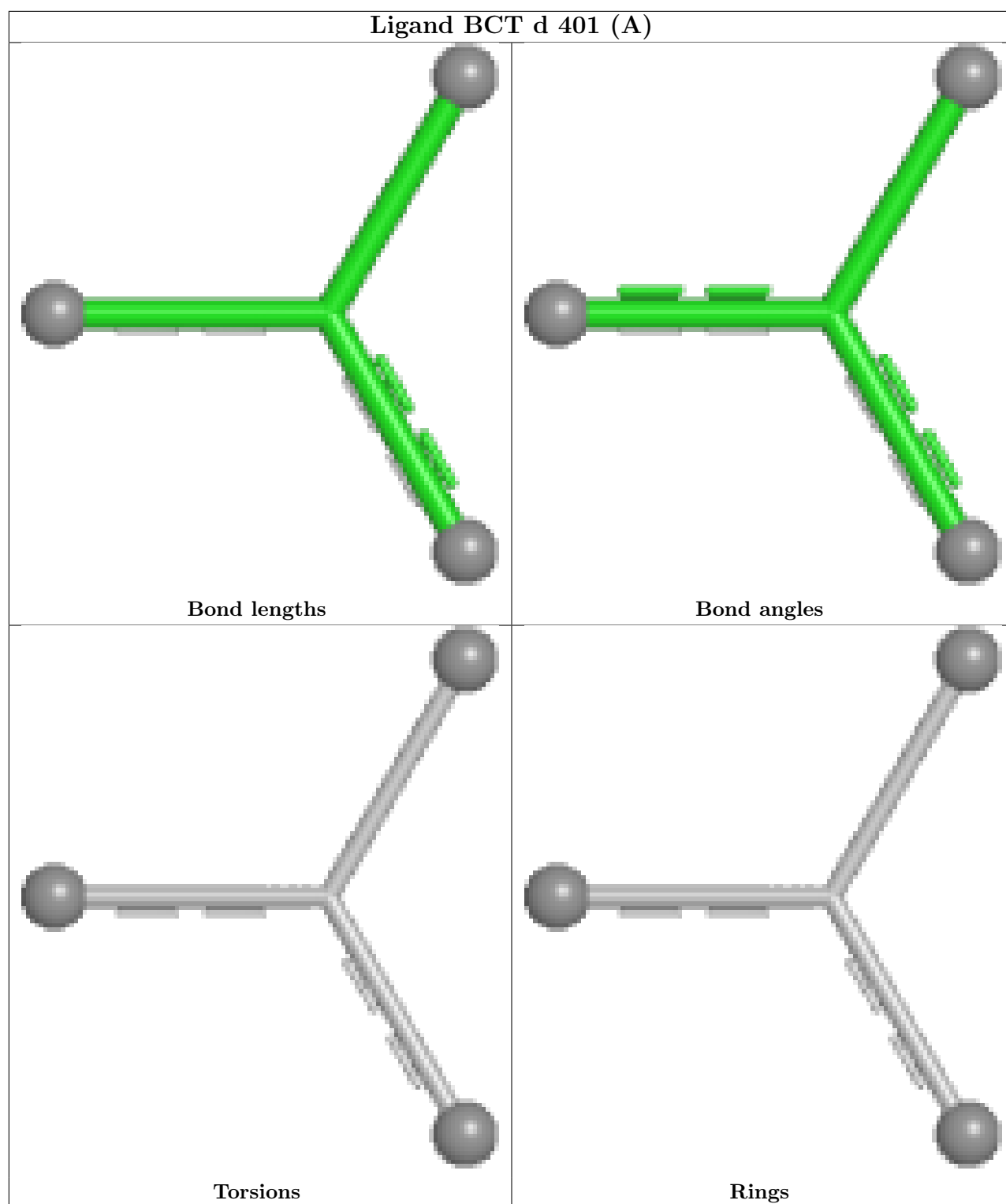


Ligand CLA b 610

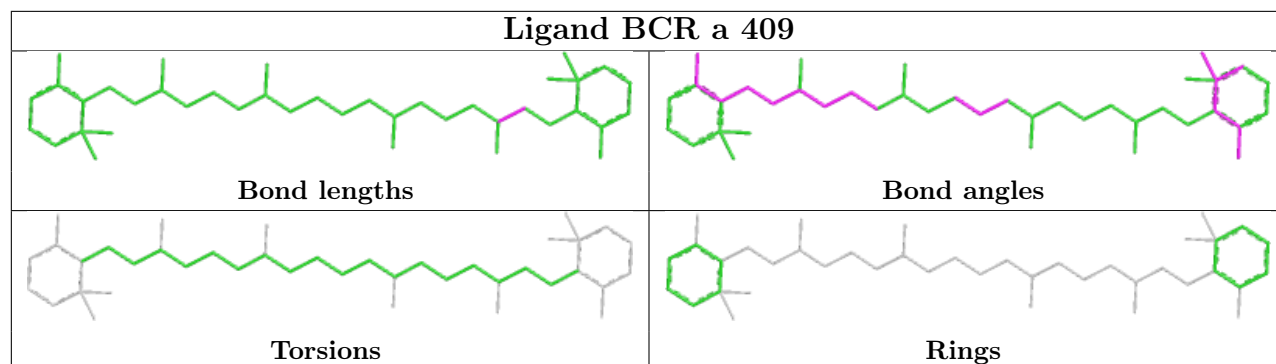


Ligand LMG C 501

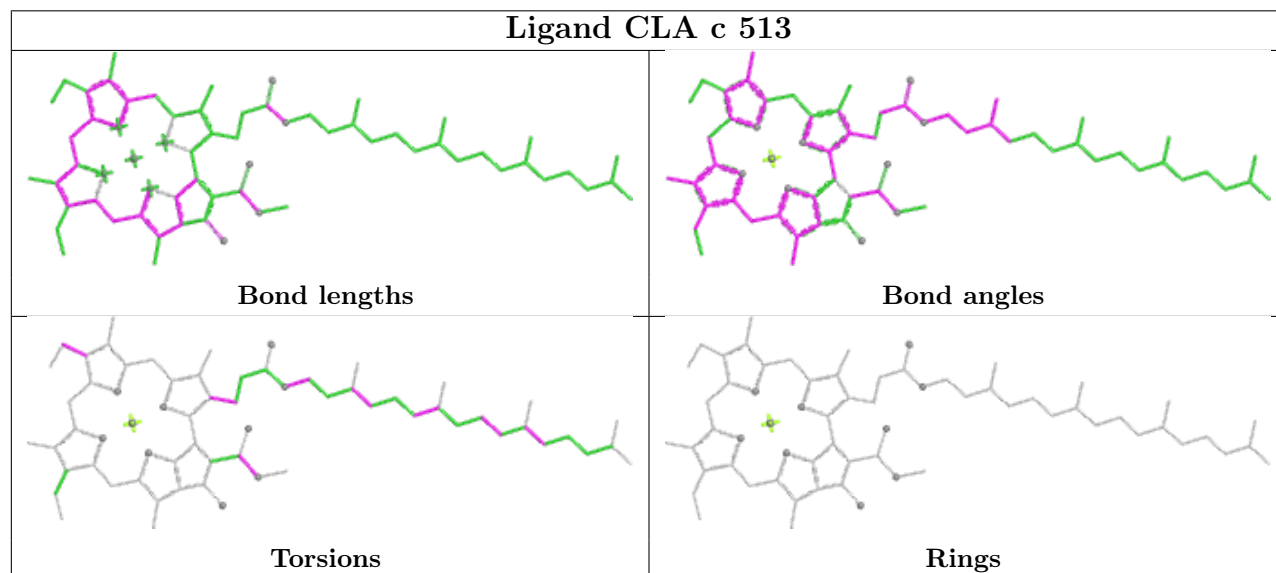




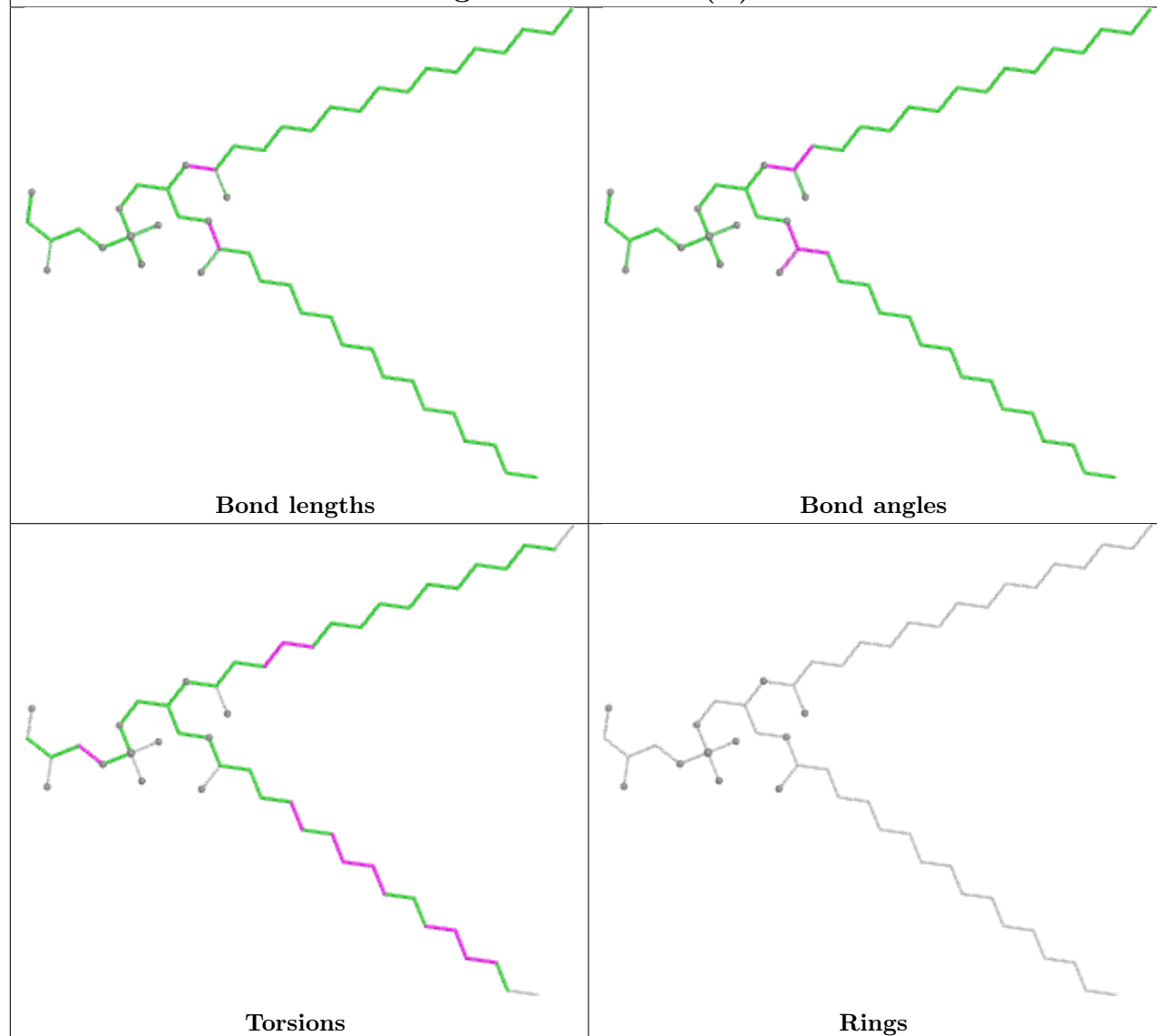
Ligand BCR a 409



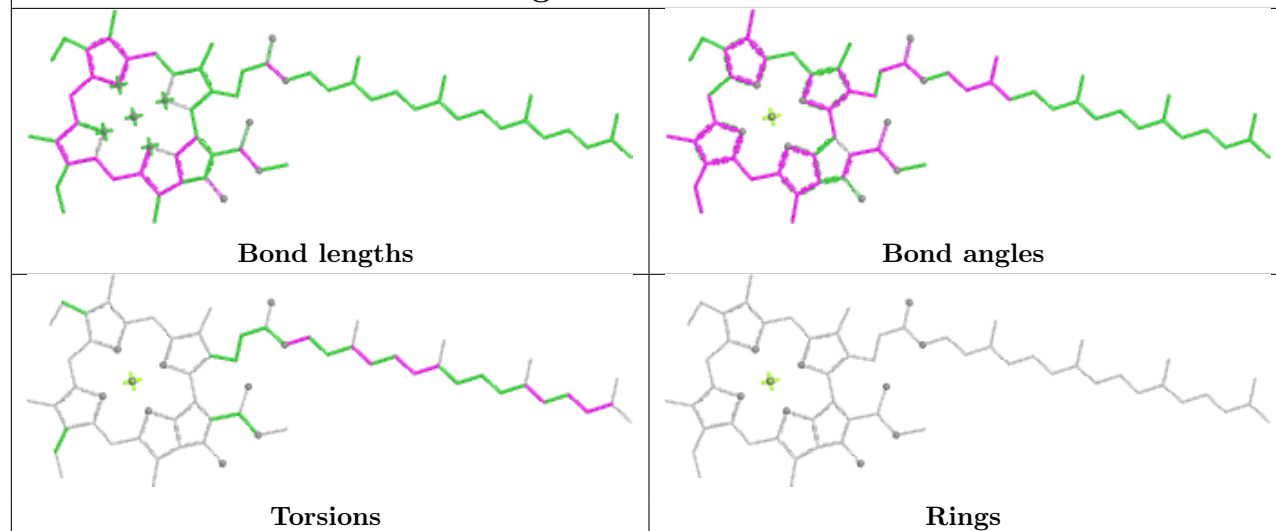
Ligand CLA c 513



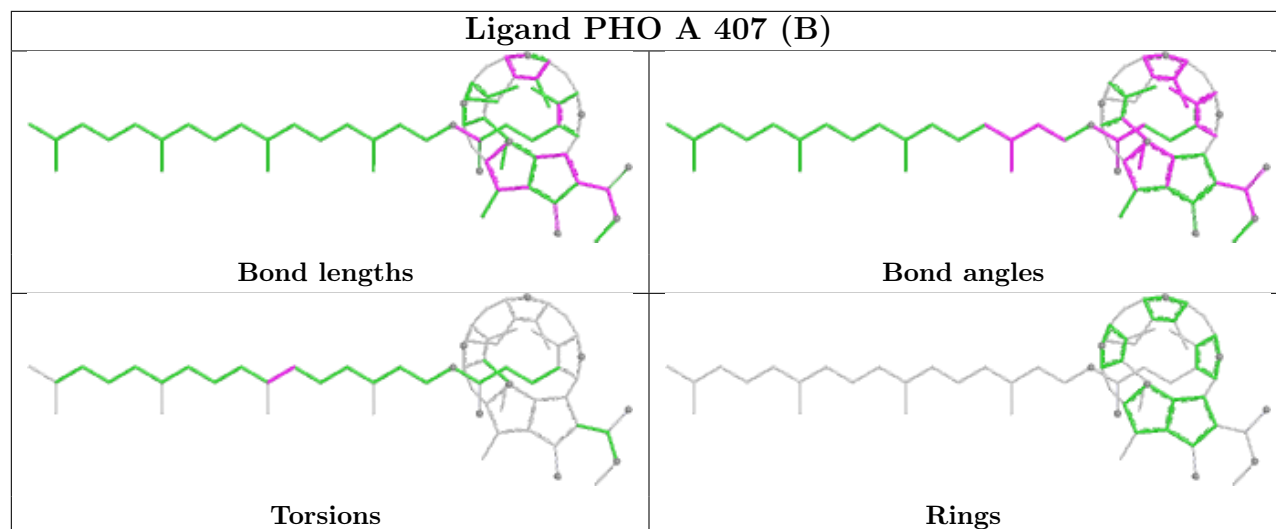
Ligand LHG d 407 (B)



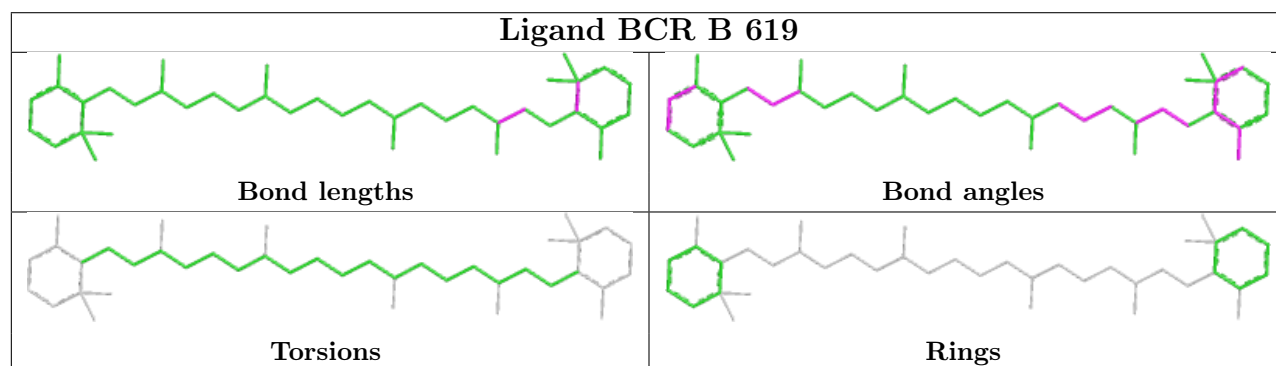
Ligand CLA C 507



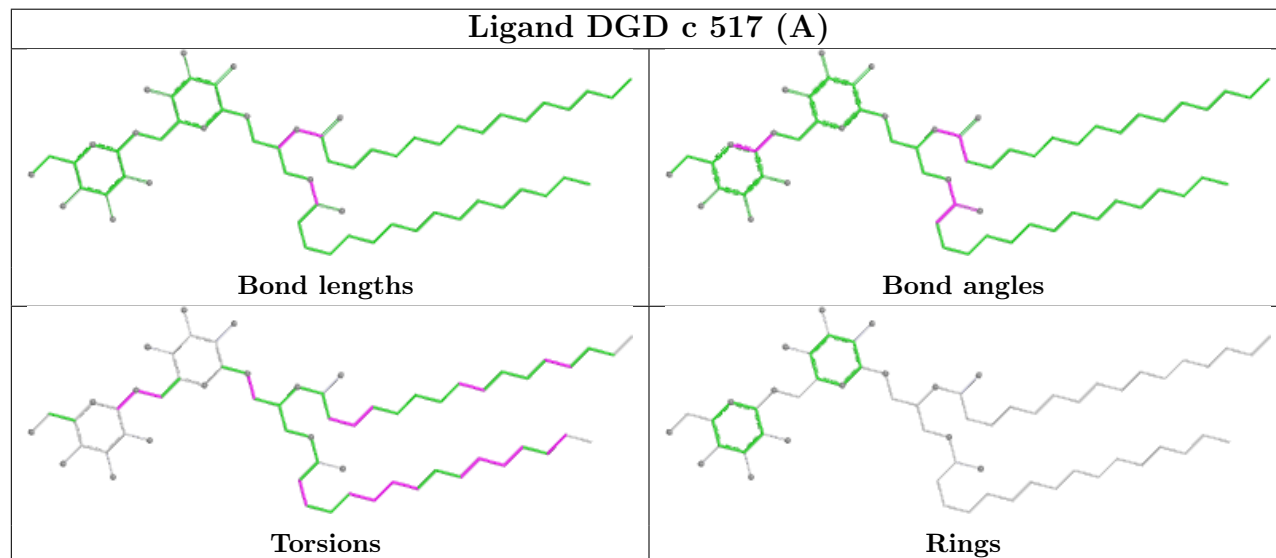
Ligand PHO A 407 (B)



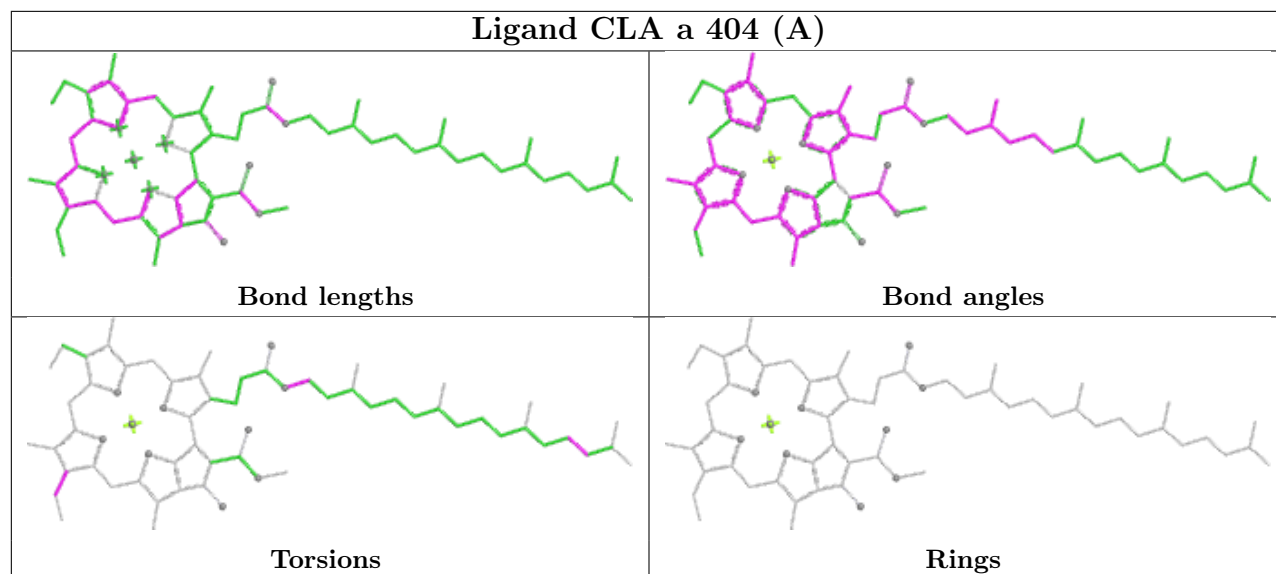
Ligand BCR B 619



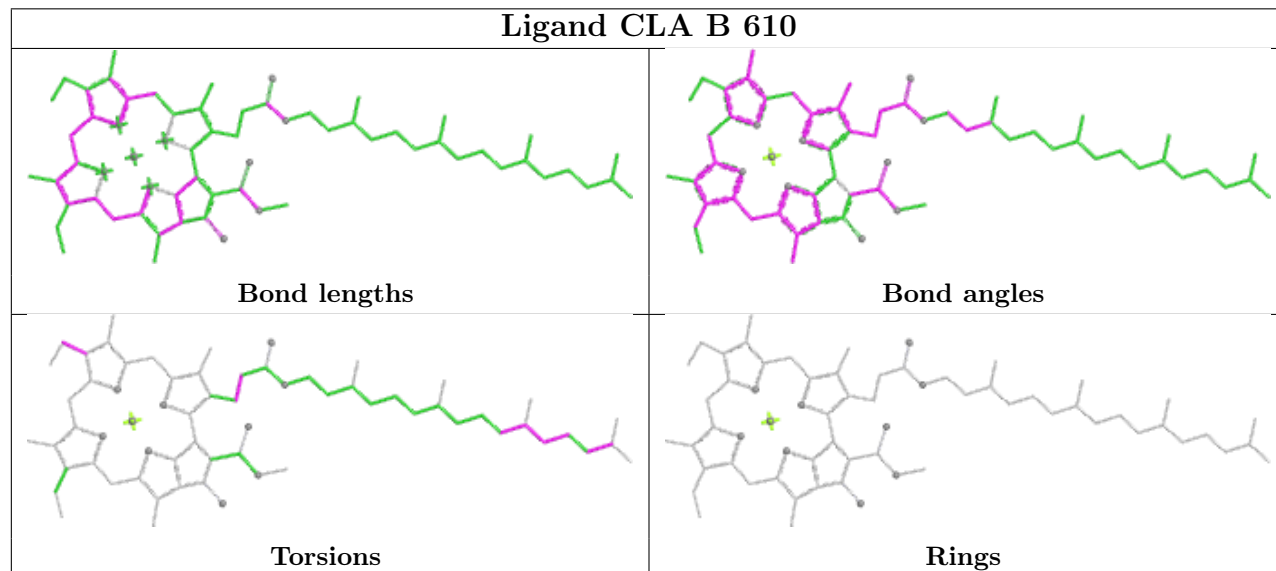
Ligand DGD c 517 (A)



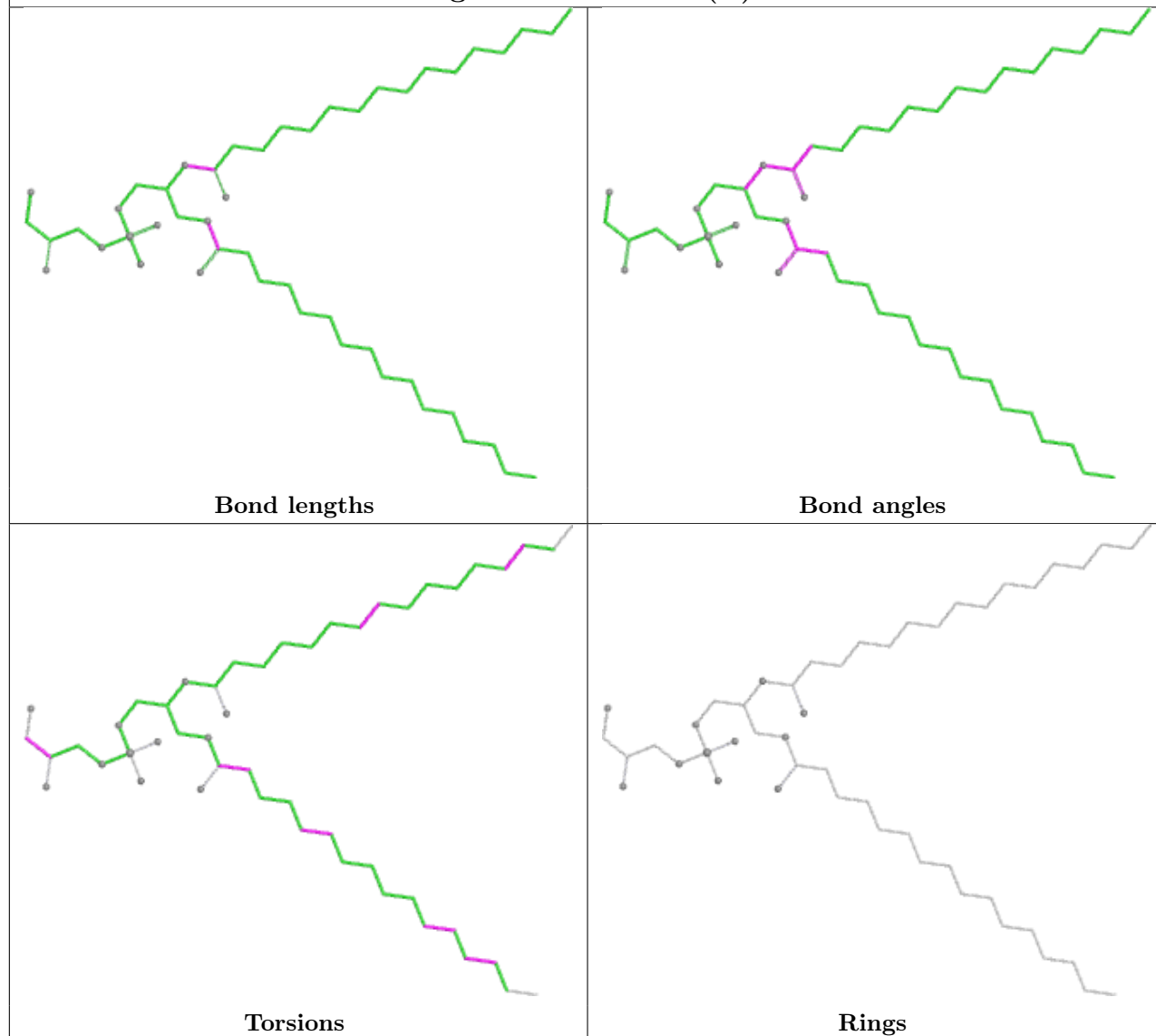
Ligand CLA a 404 (A)



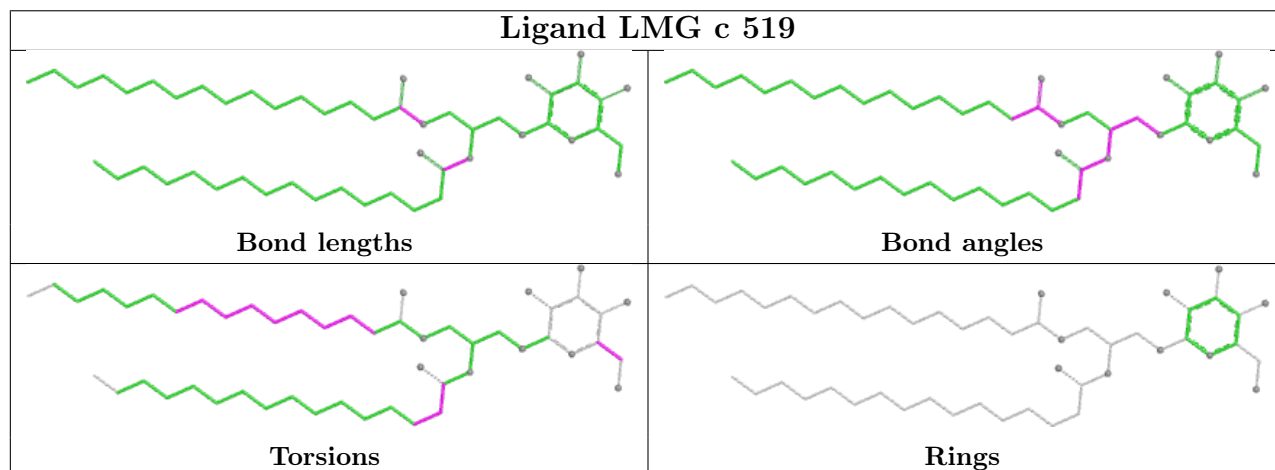
Ligand CLA B 610

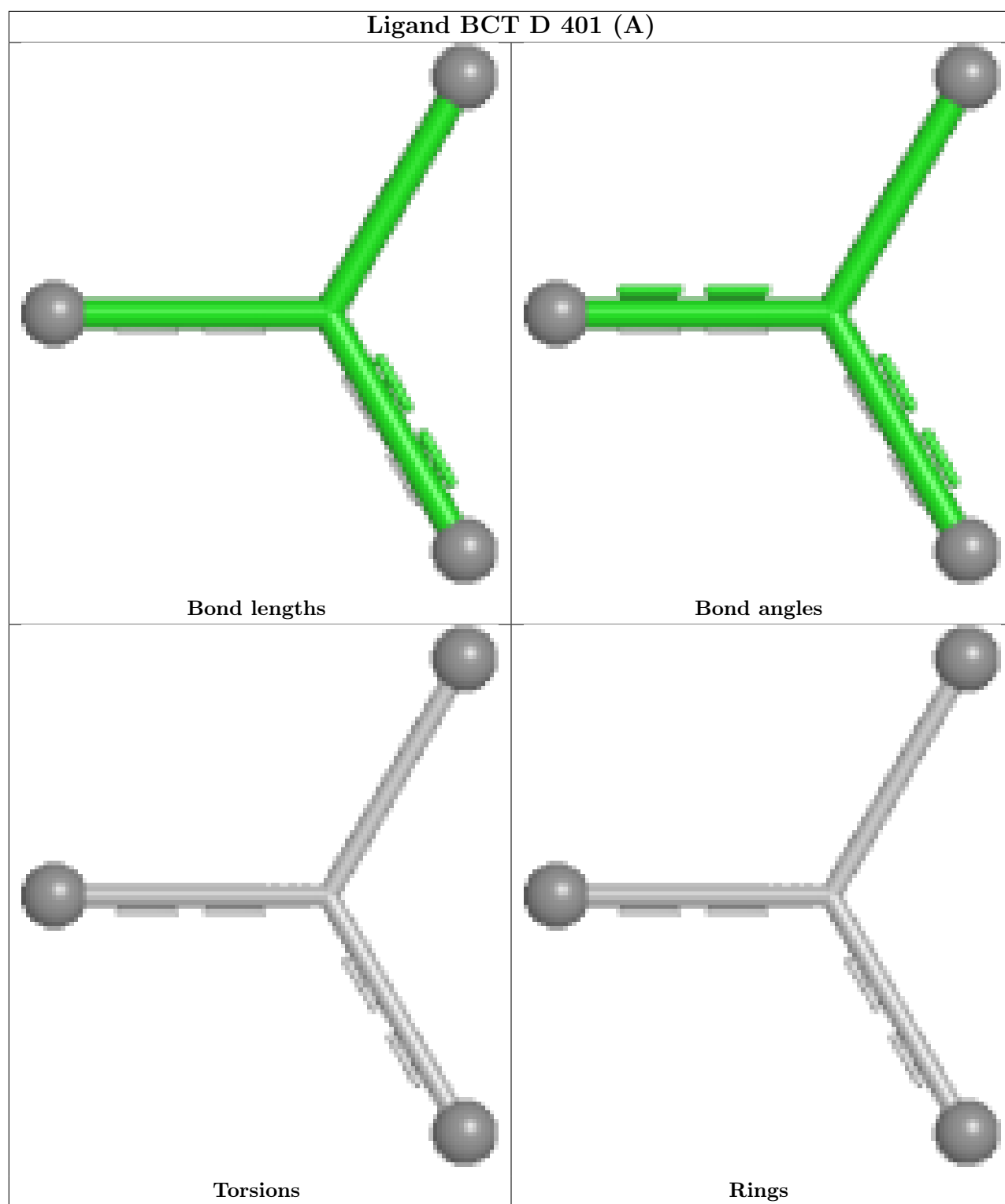


Ligand LHG A 419 (B)

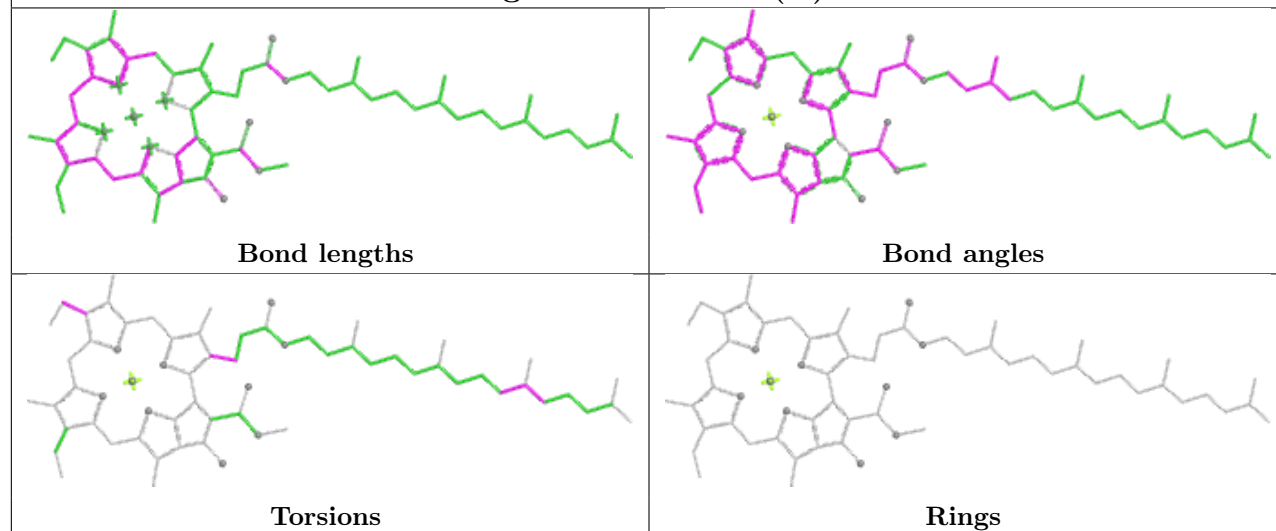


Ligand LMG c 519

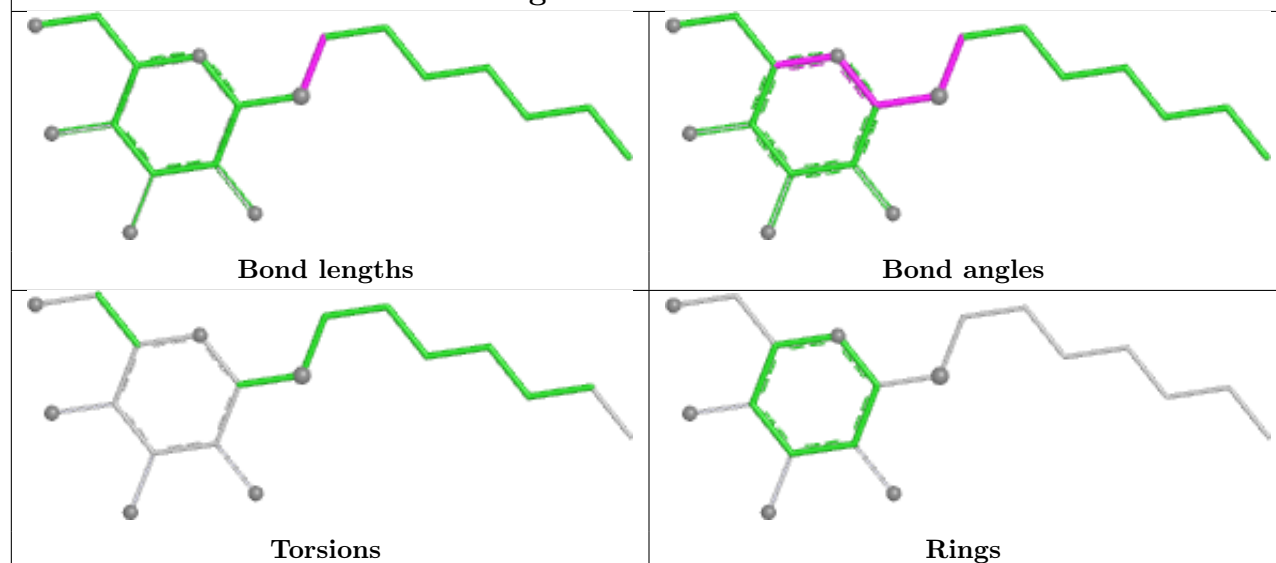




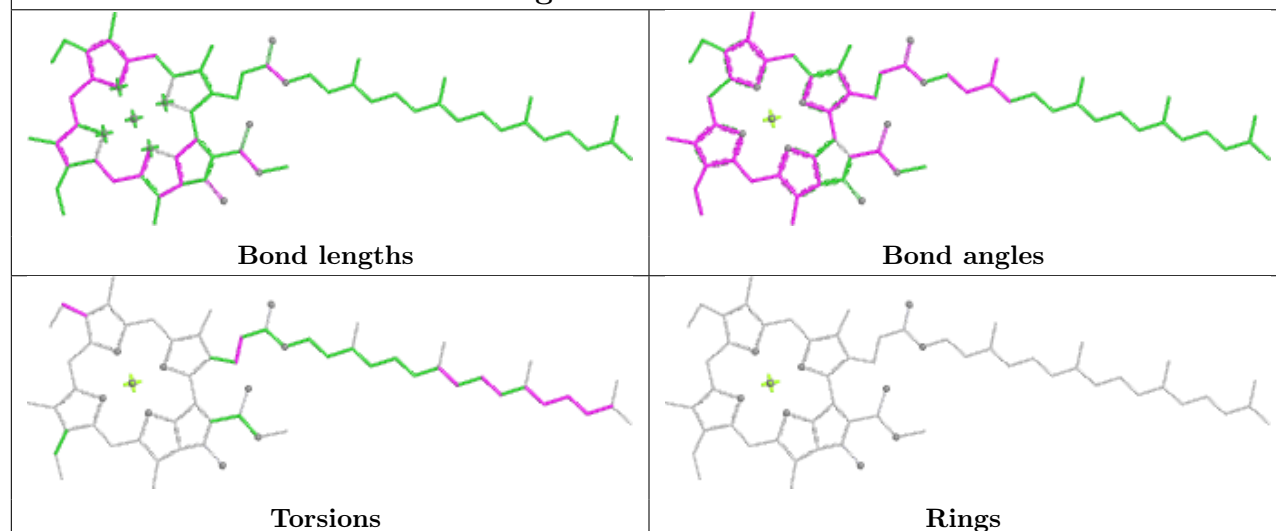
Ligand CLA a 406 (A)



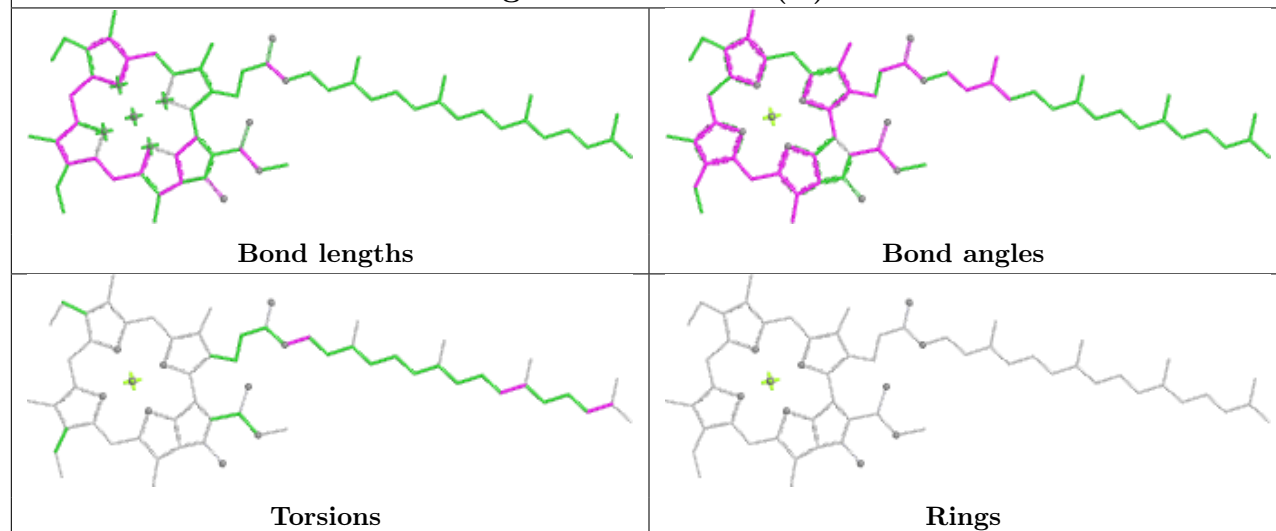
Ligand HTG C 522



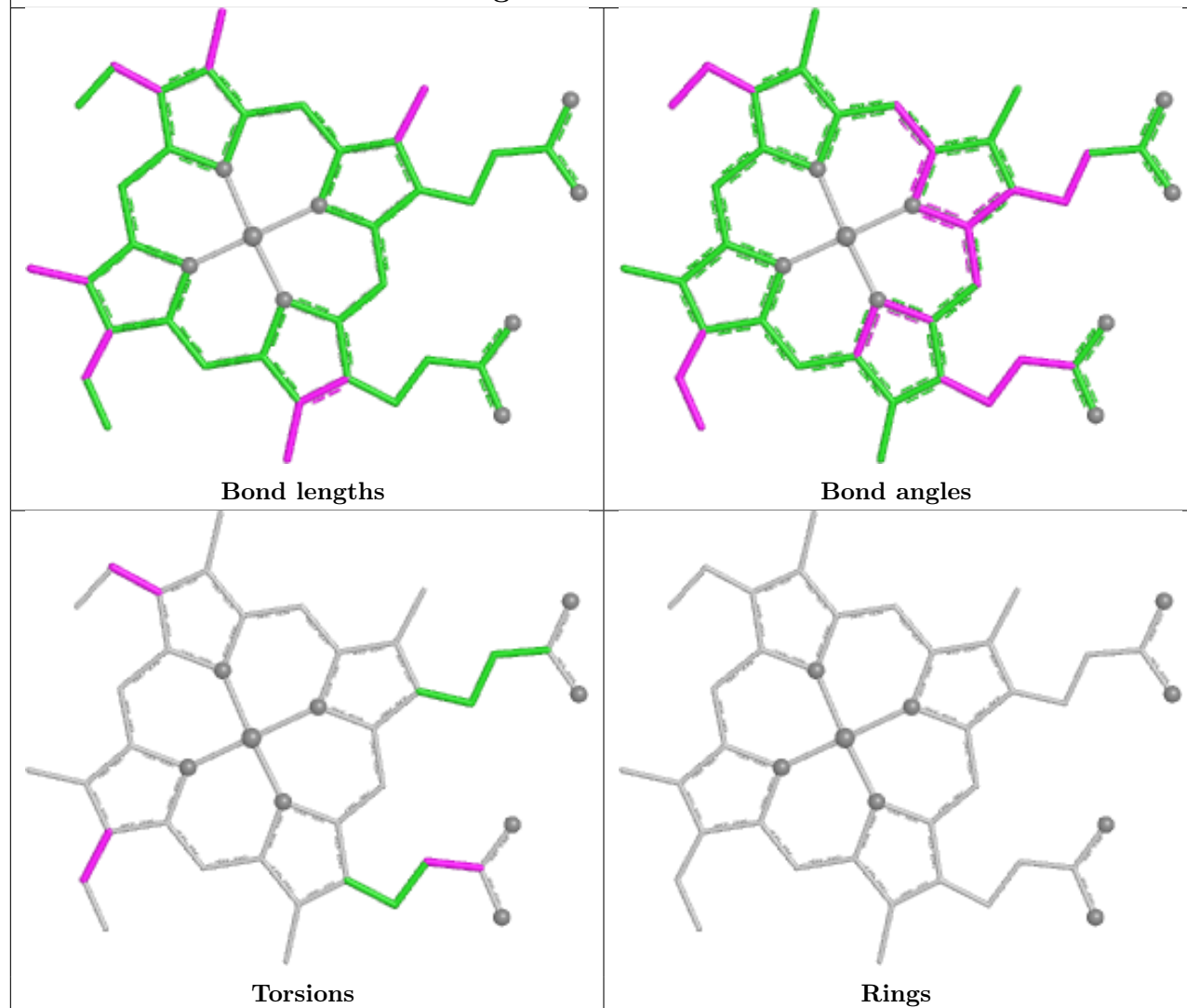
Ligand CLA b 606

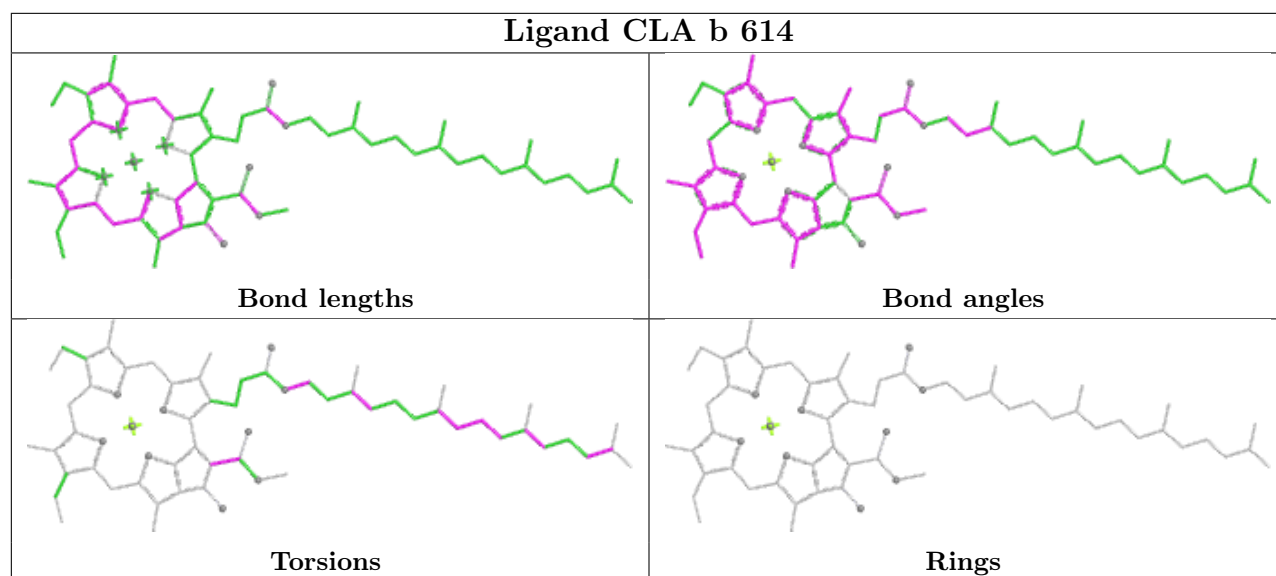
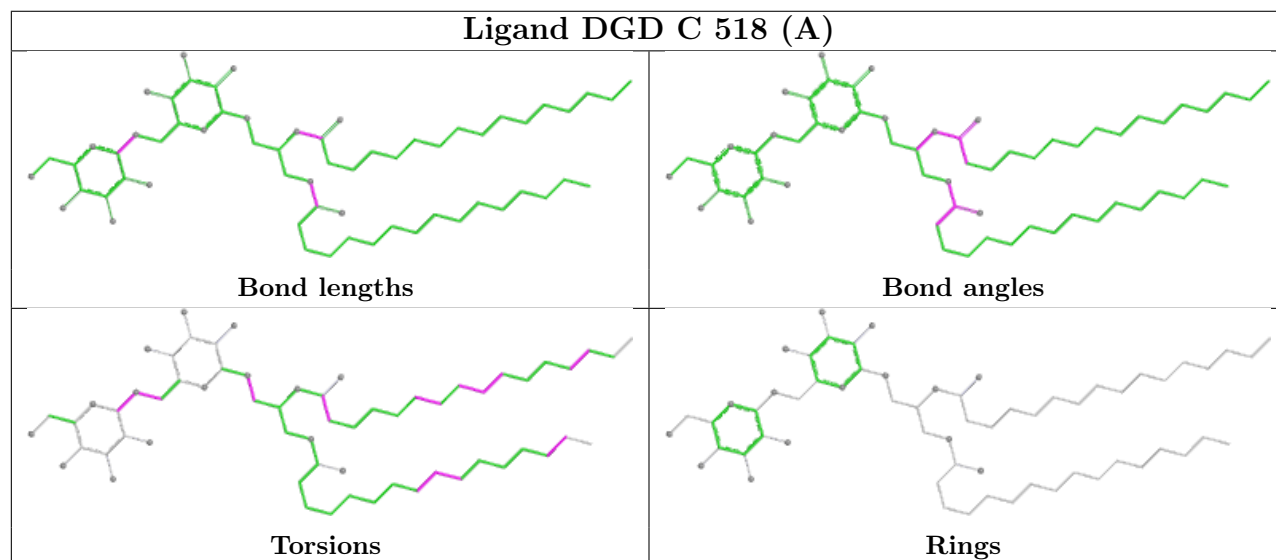
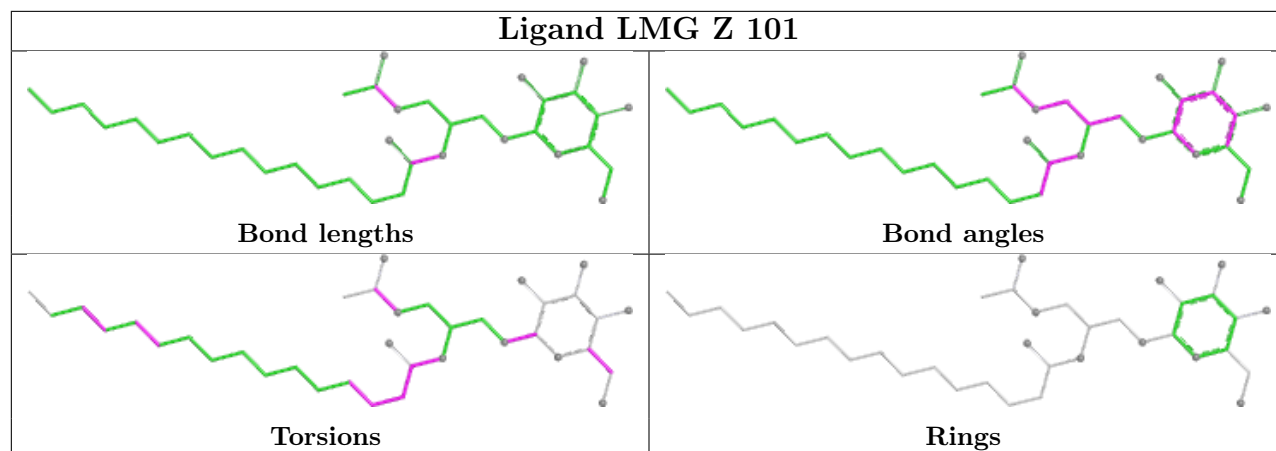


Ligand CLA d 402 (B)

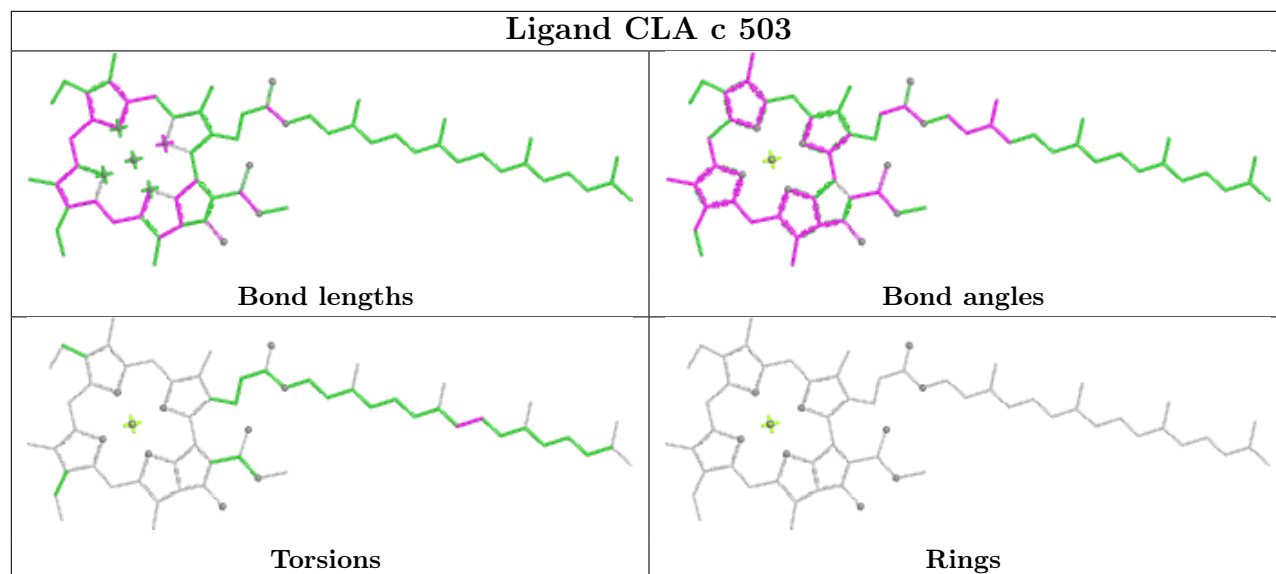


Ligand HEC V 201

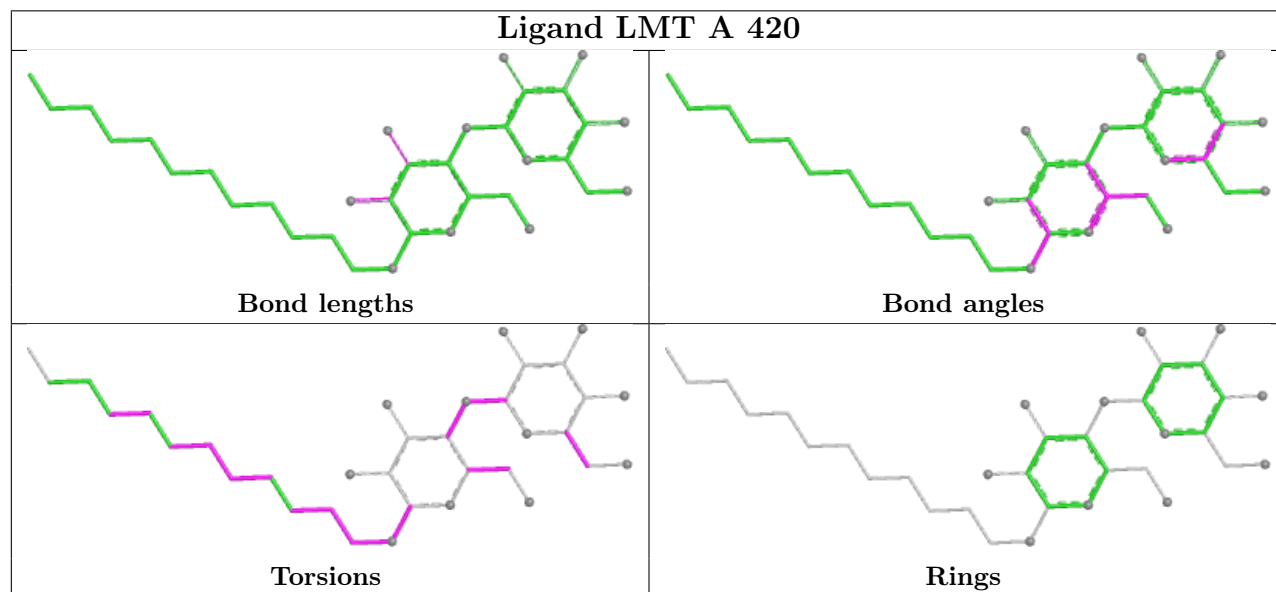




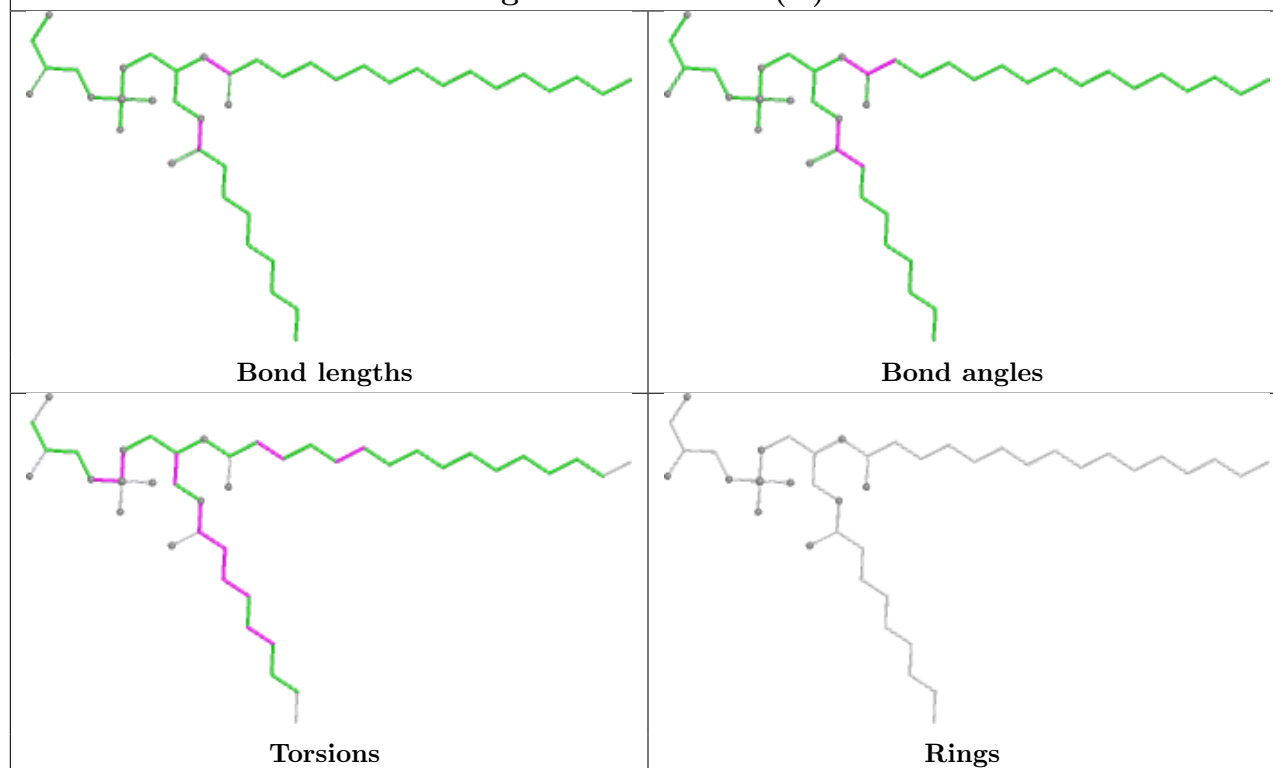
Ligand CLA c 503



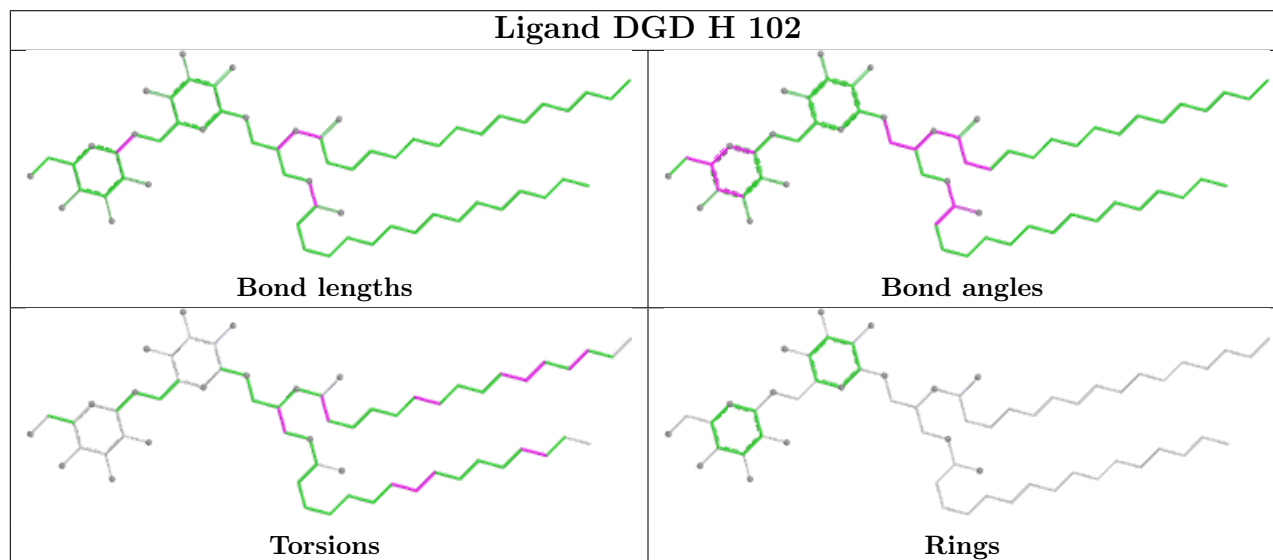
Ligand LMT A 420



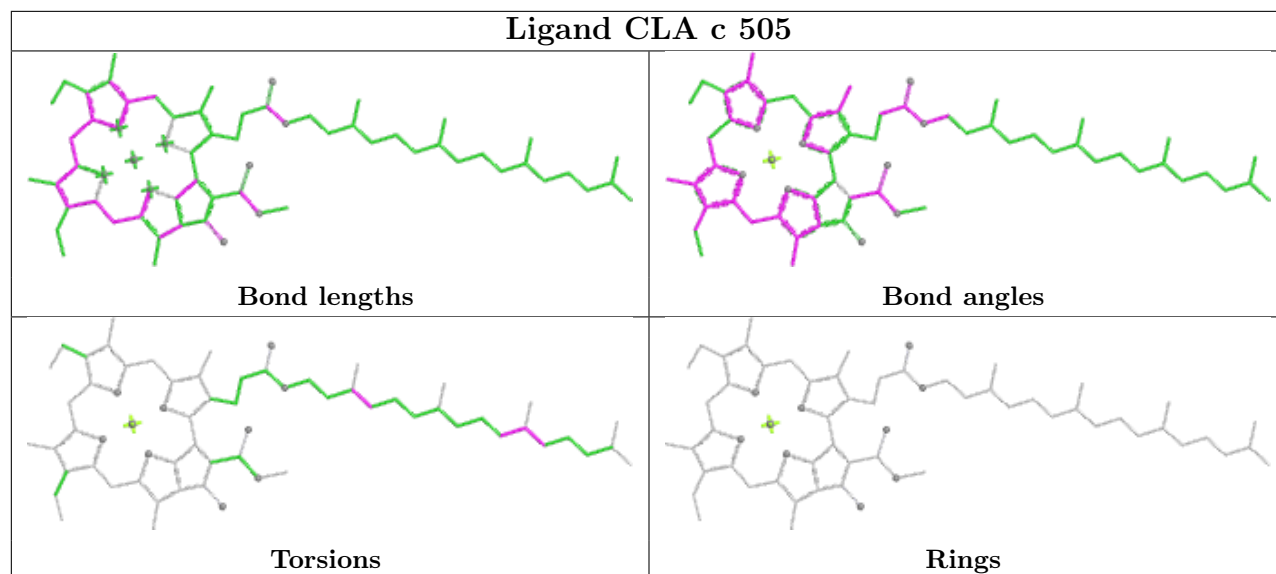
Ligand LHG a 420 (B)



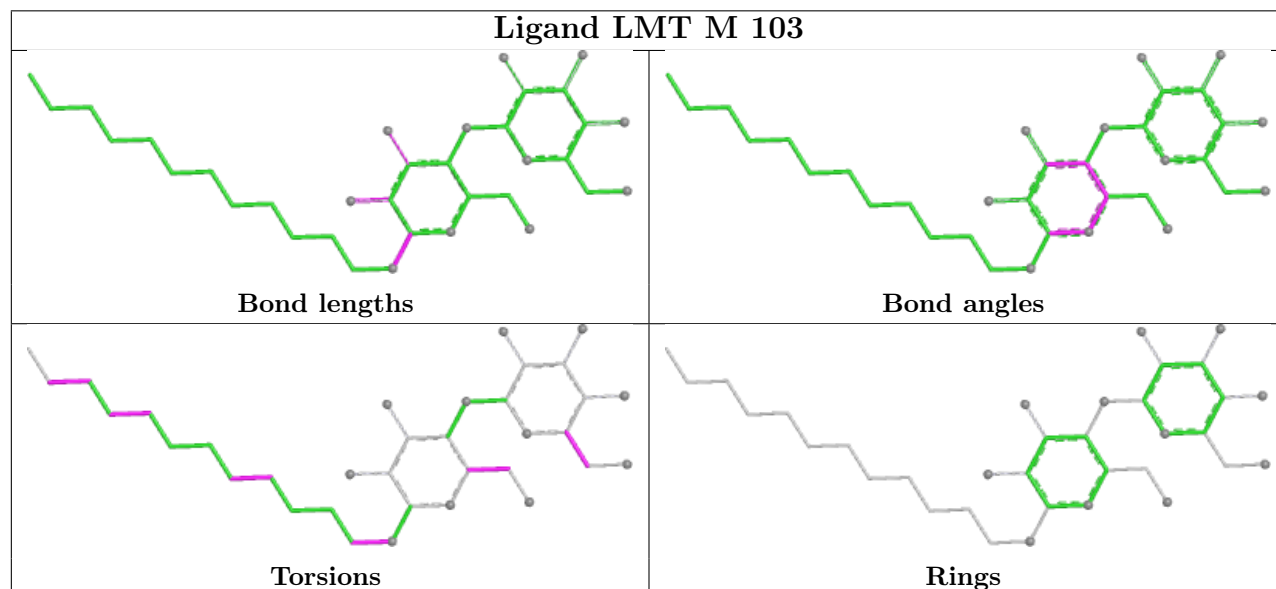
Ligand DGD H 102



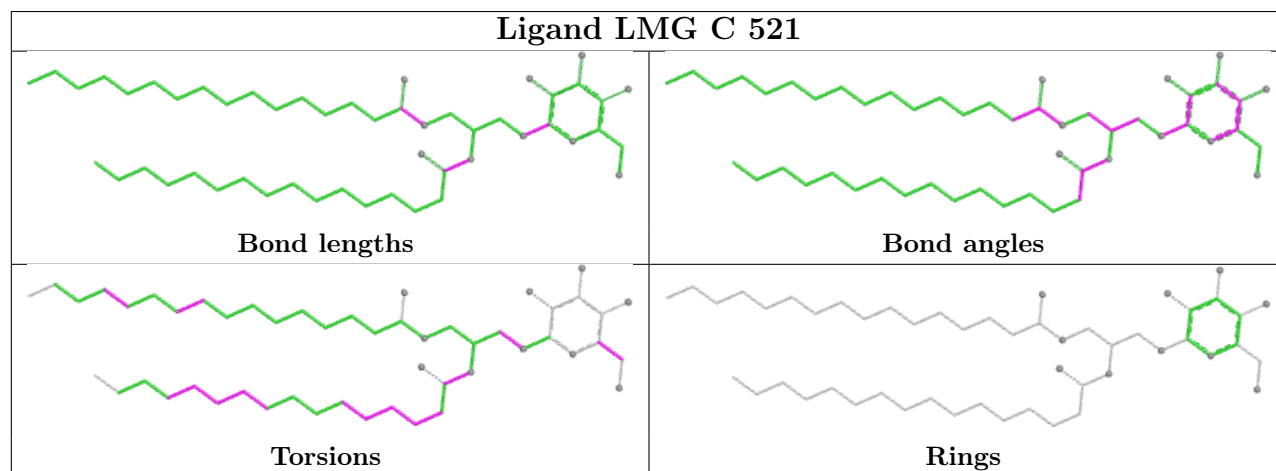
Ligand CLA c 505

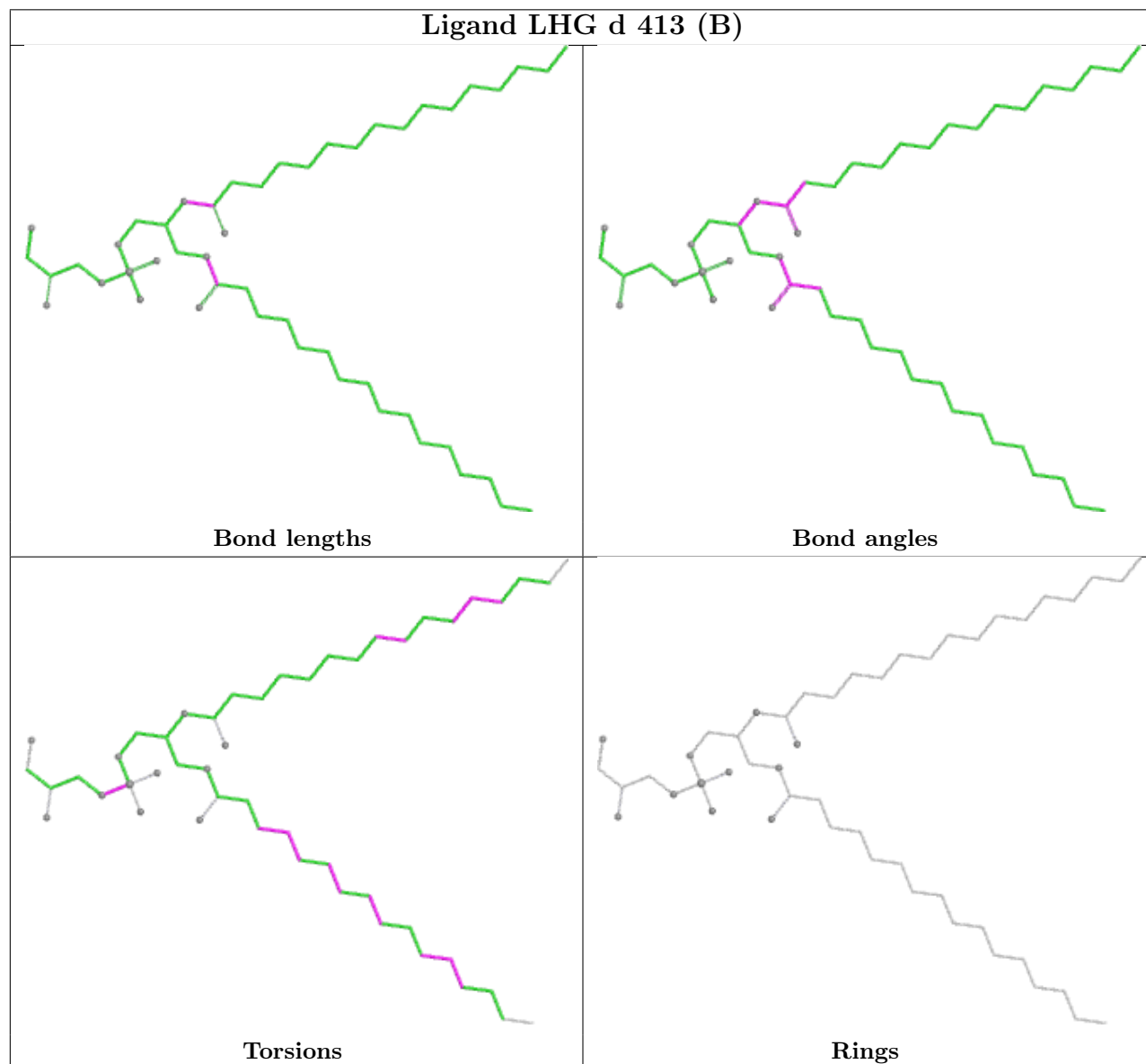
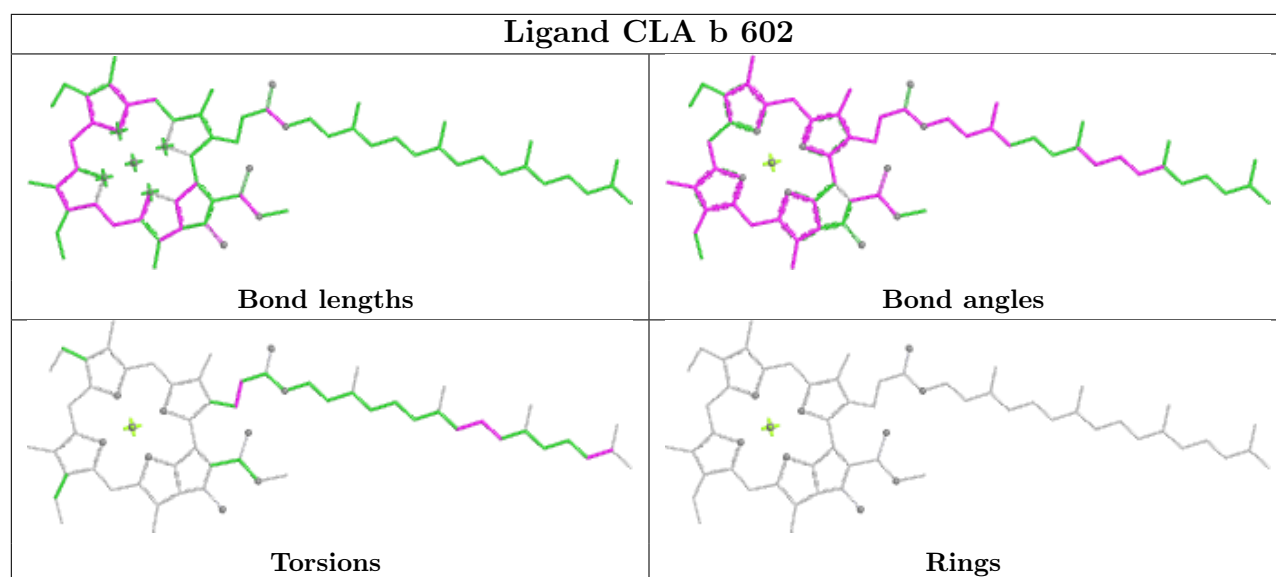


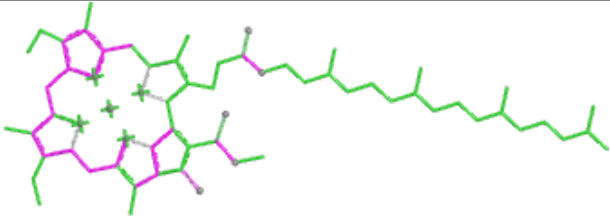
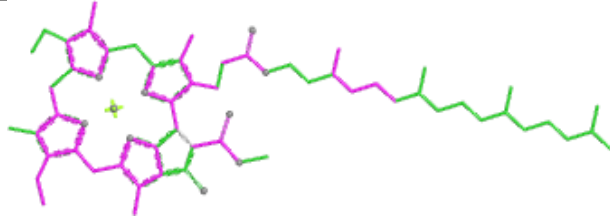
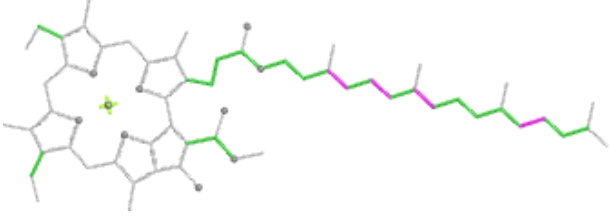
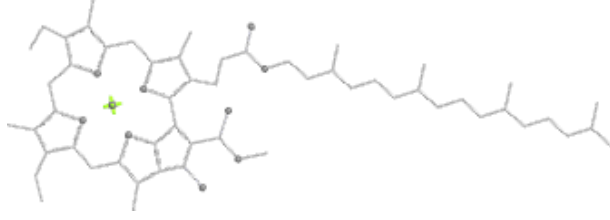
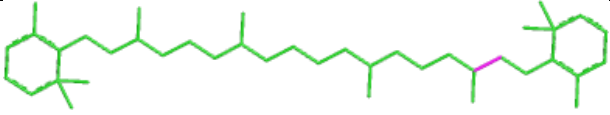
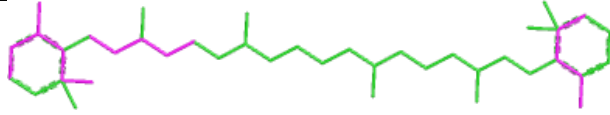
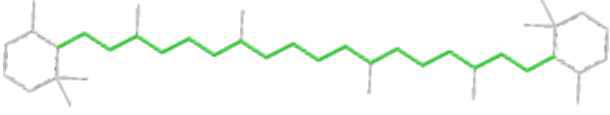
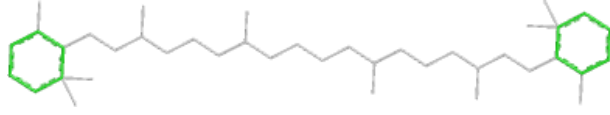
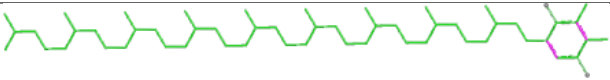
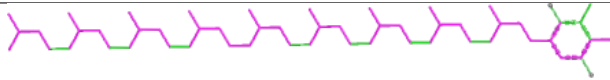
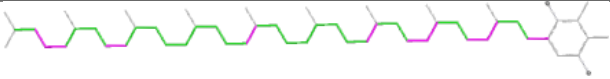
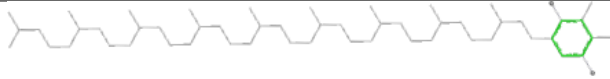
Ligand LMT M 103



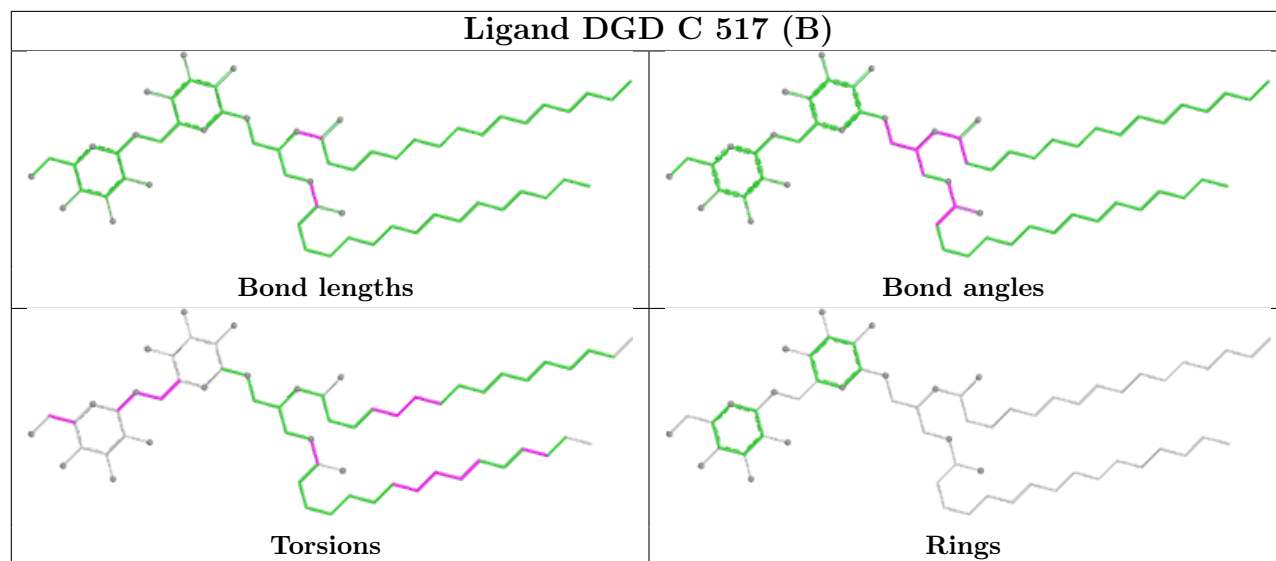
Ligand LMG C 521



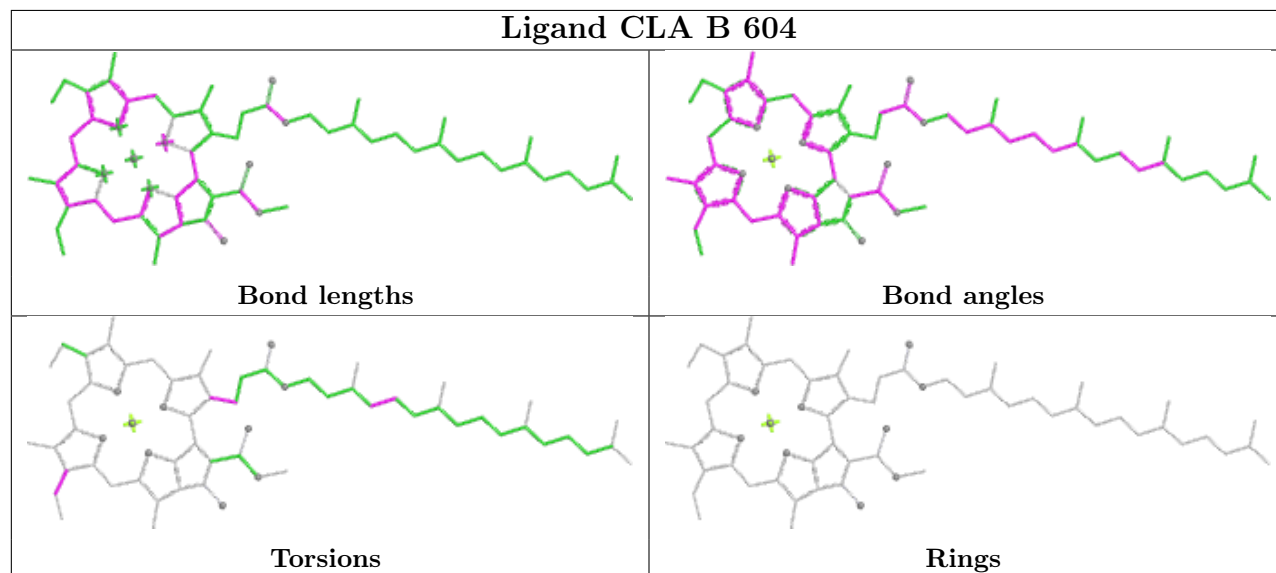


Ligand CLA b 603	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 516	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 A 414 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

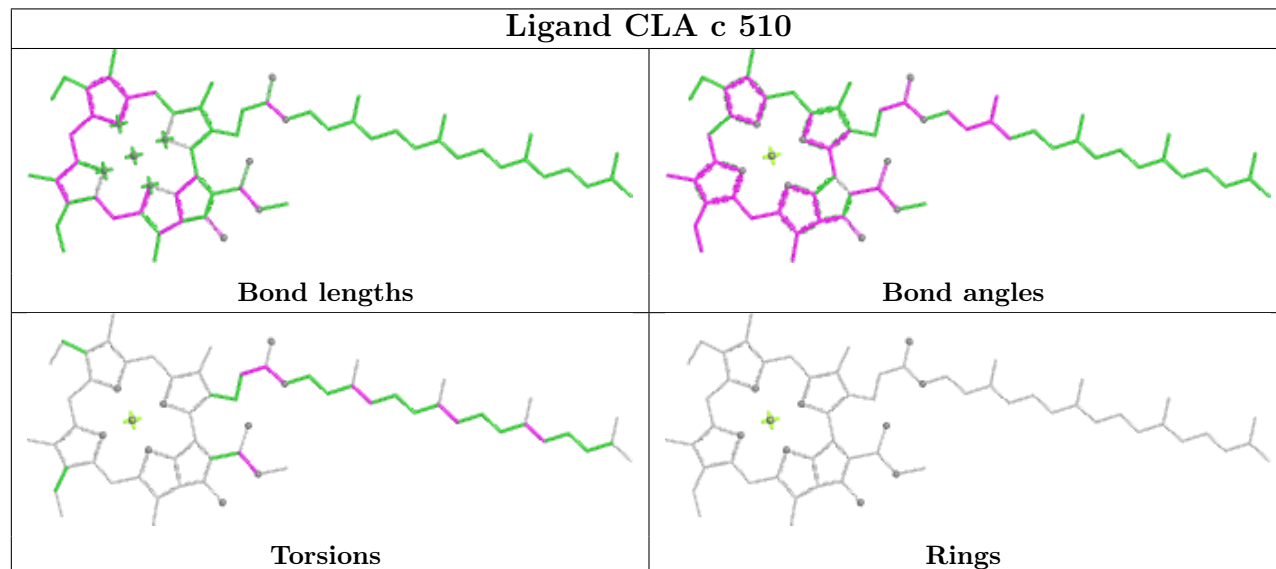
Ligand DGD C 517 (B)

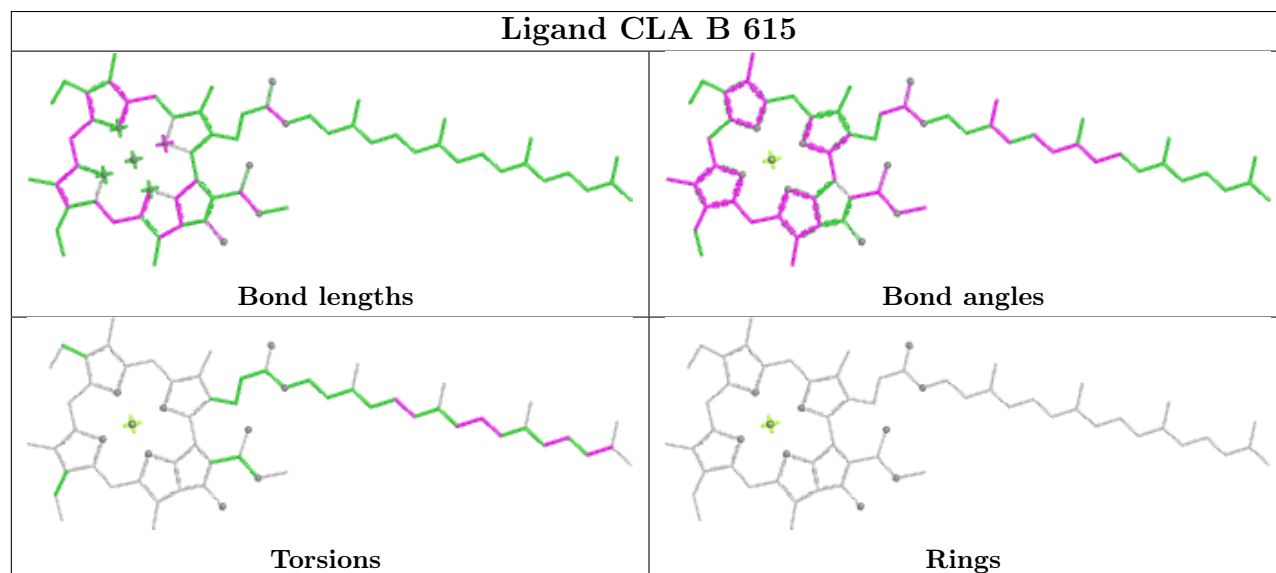
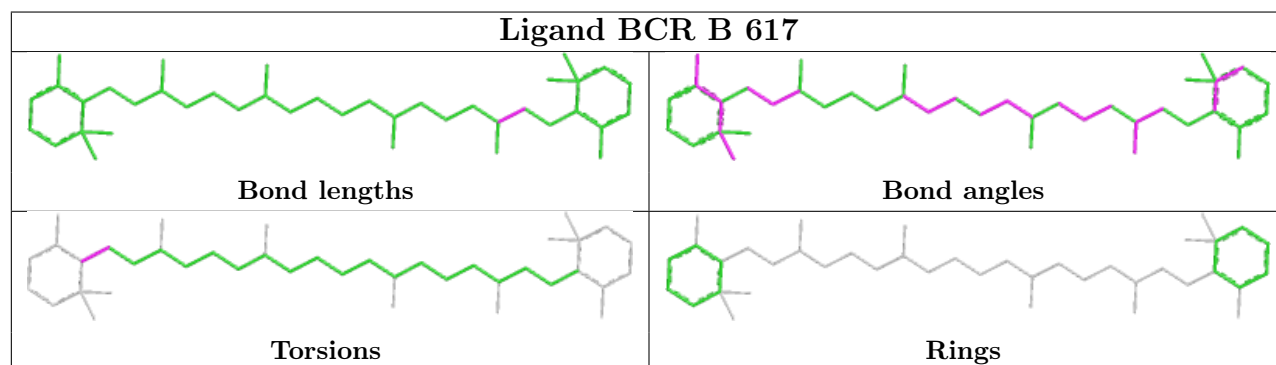
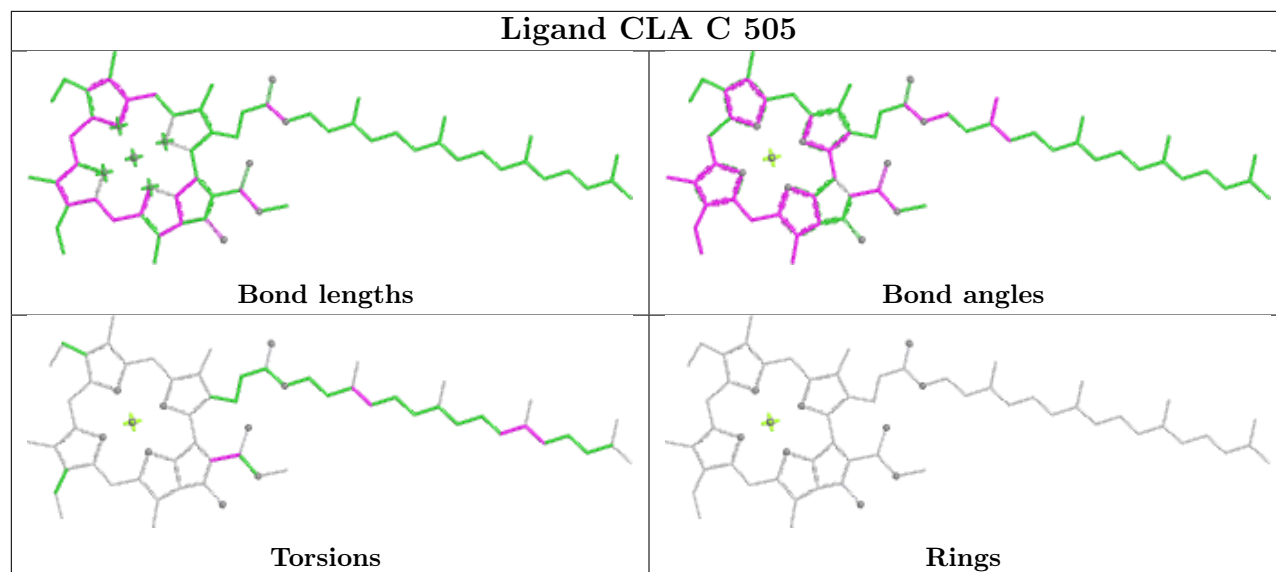


Ligand CLA B 604

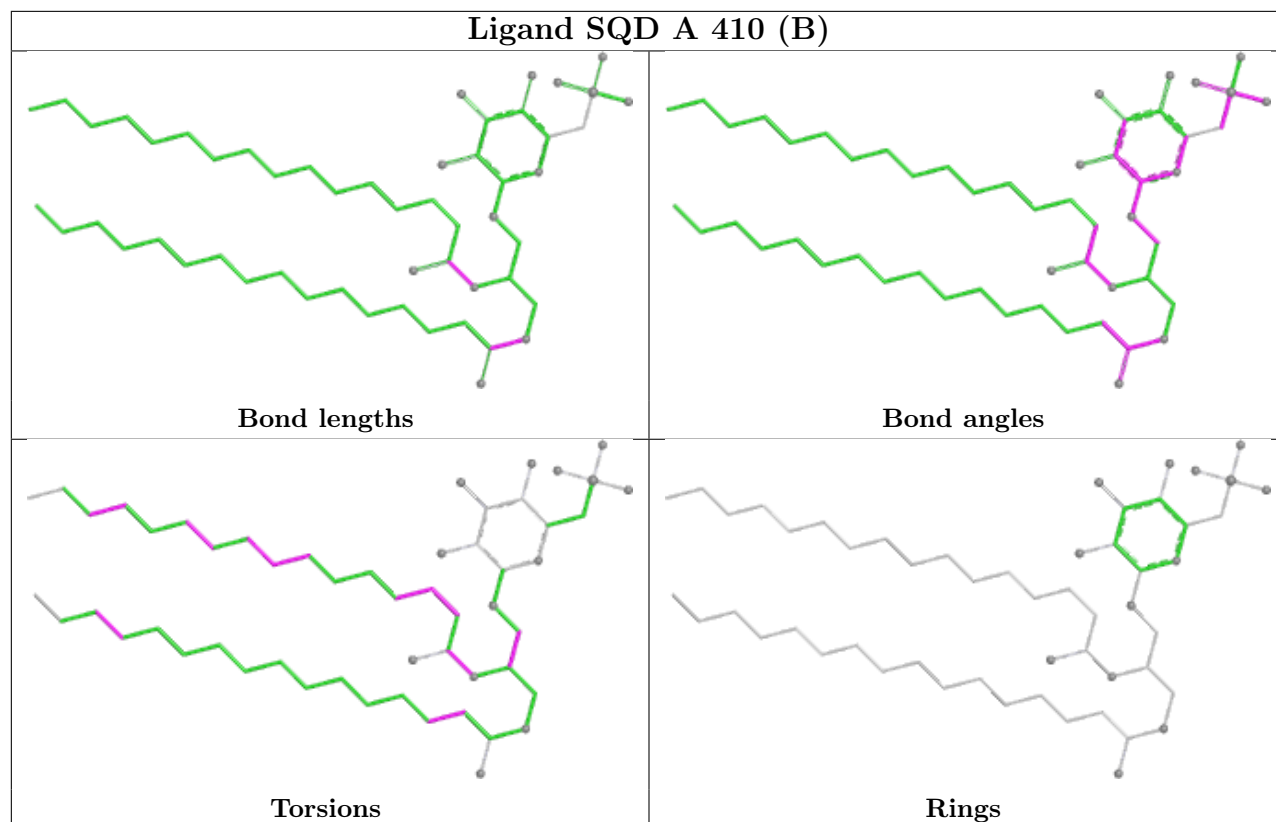


Ligand CLA c 510

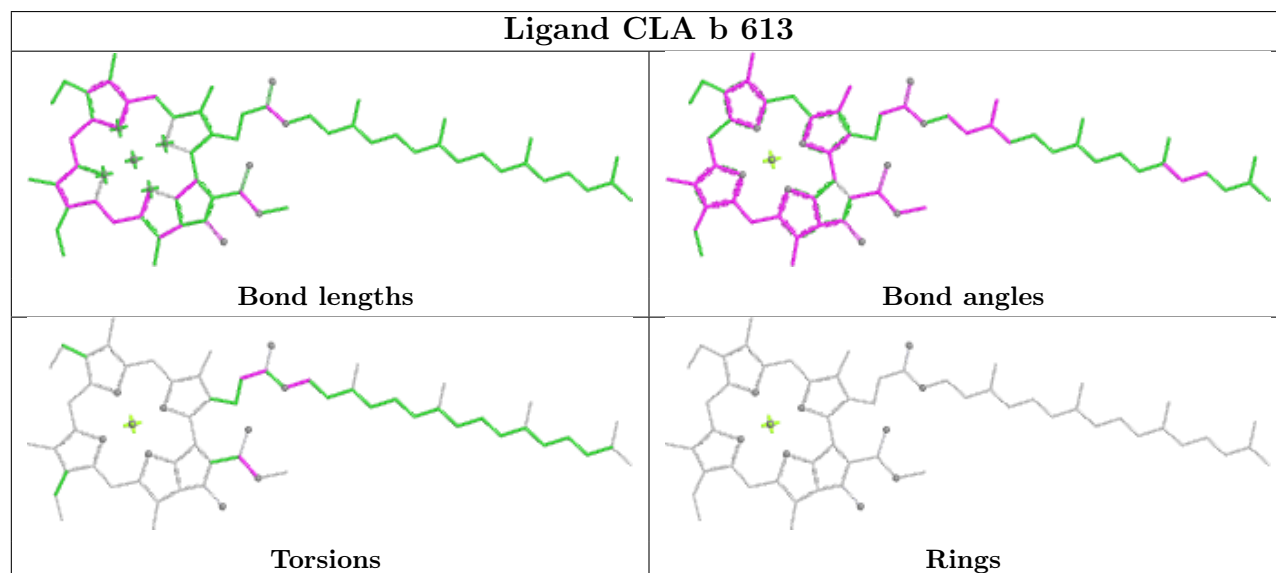


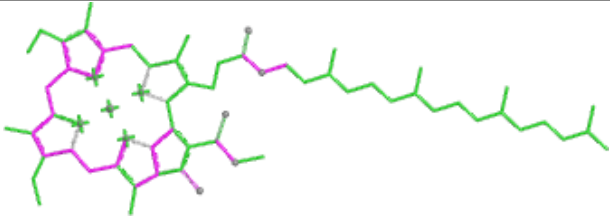
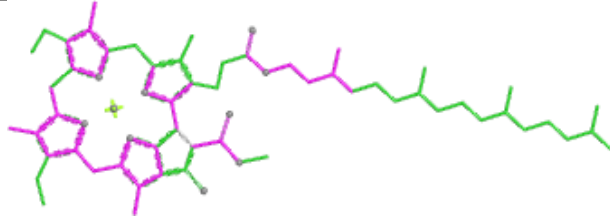
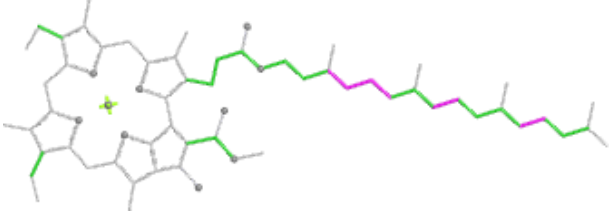
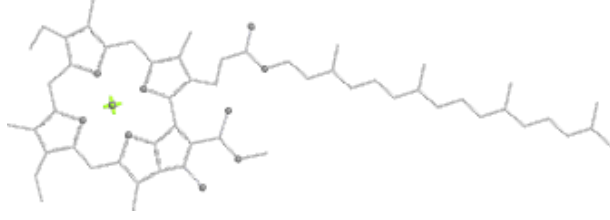
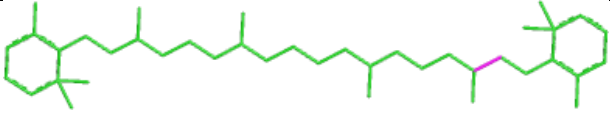
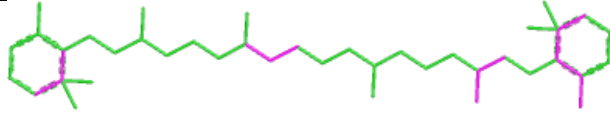
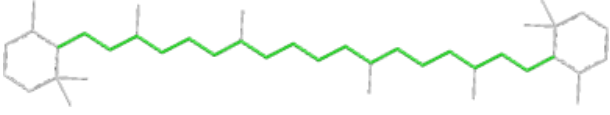
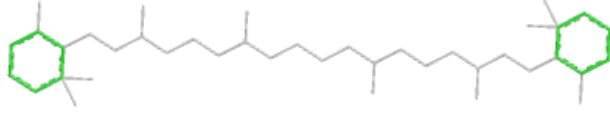
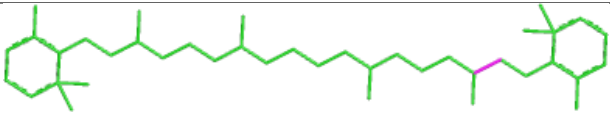
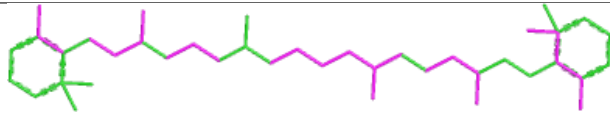
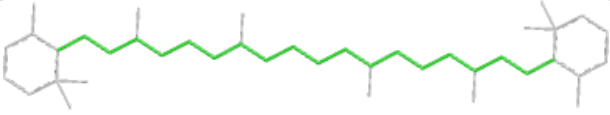
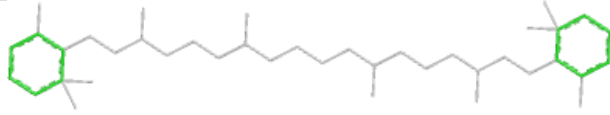


Ligand SQD A 410 (B)

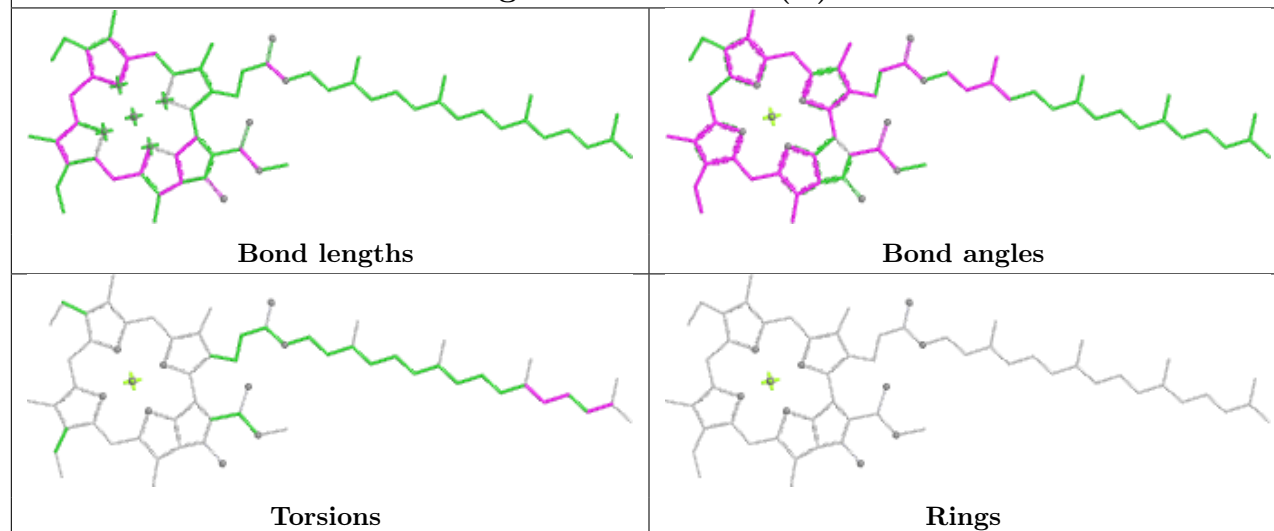


Ligand CLA b 613

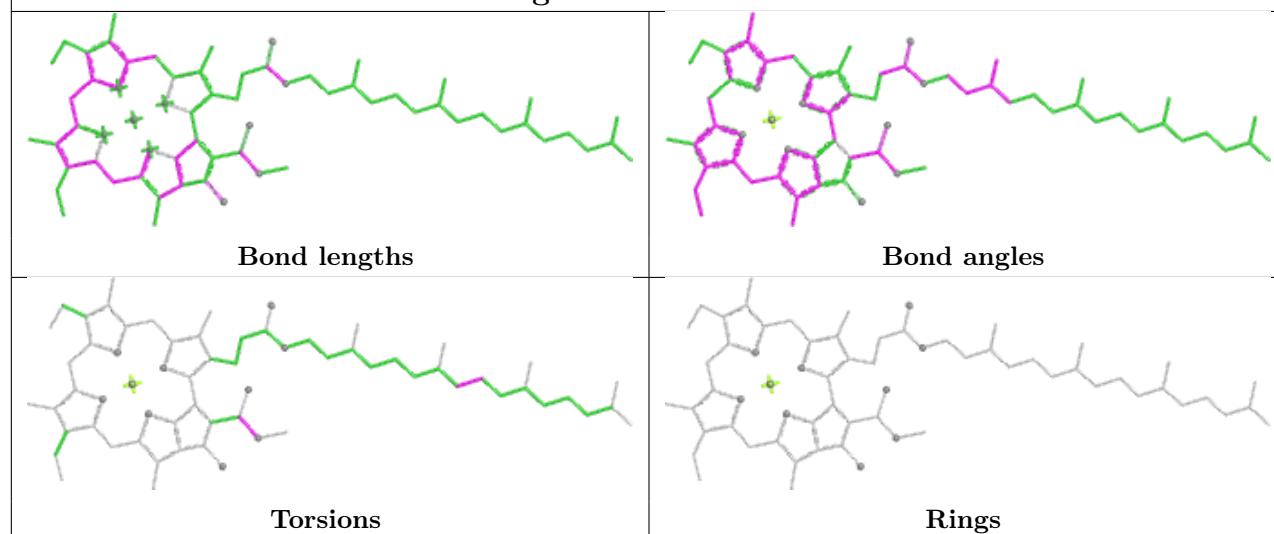


Ligand CLA b 605	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR h 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

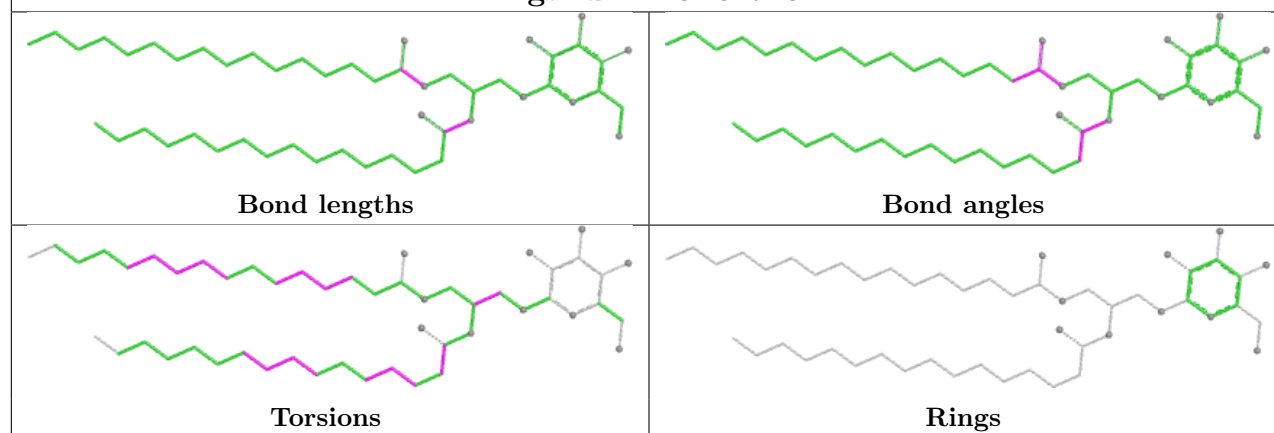
Ligand CLA A 406 (B)

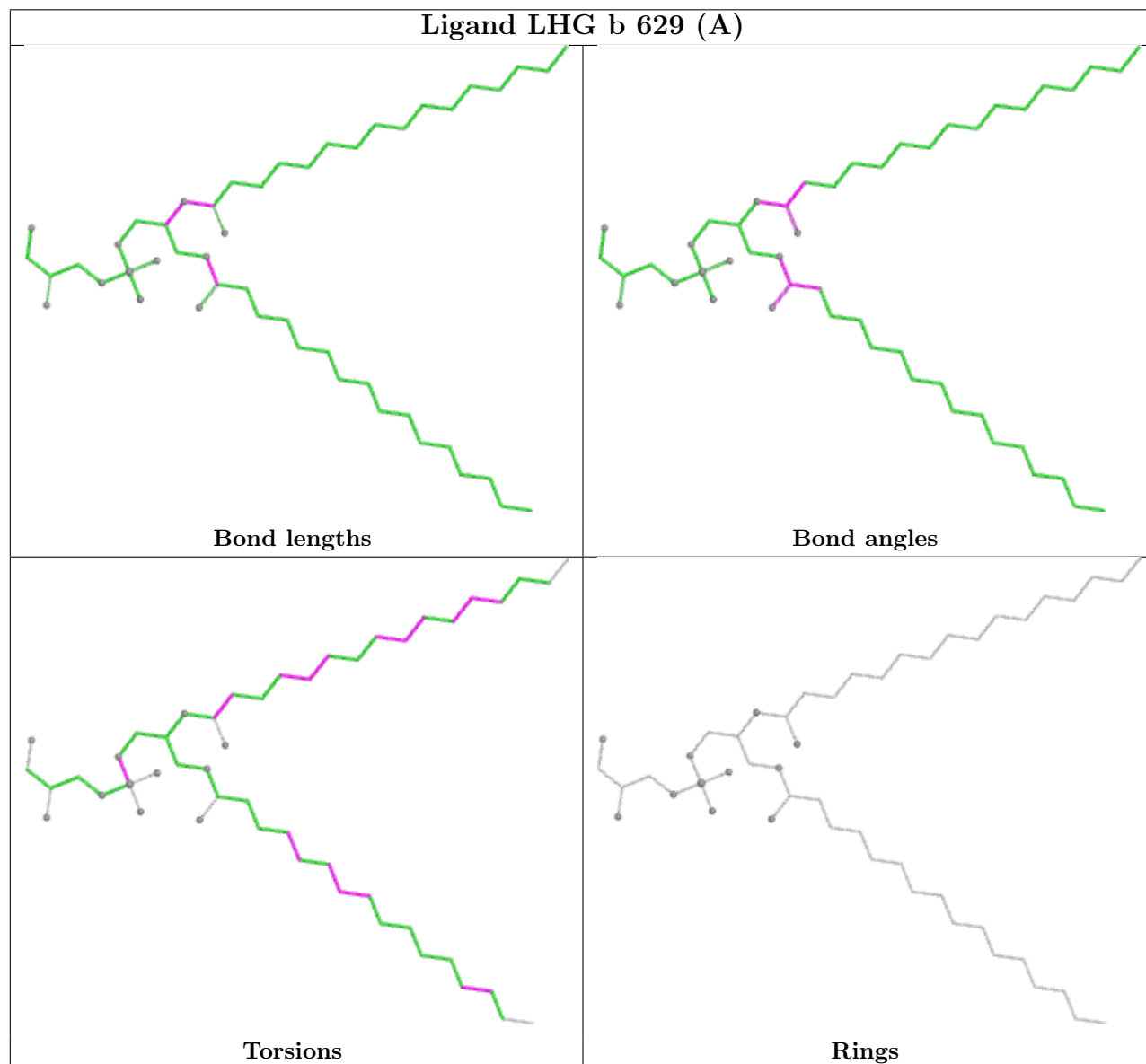
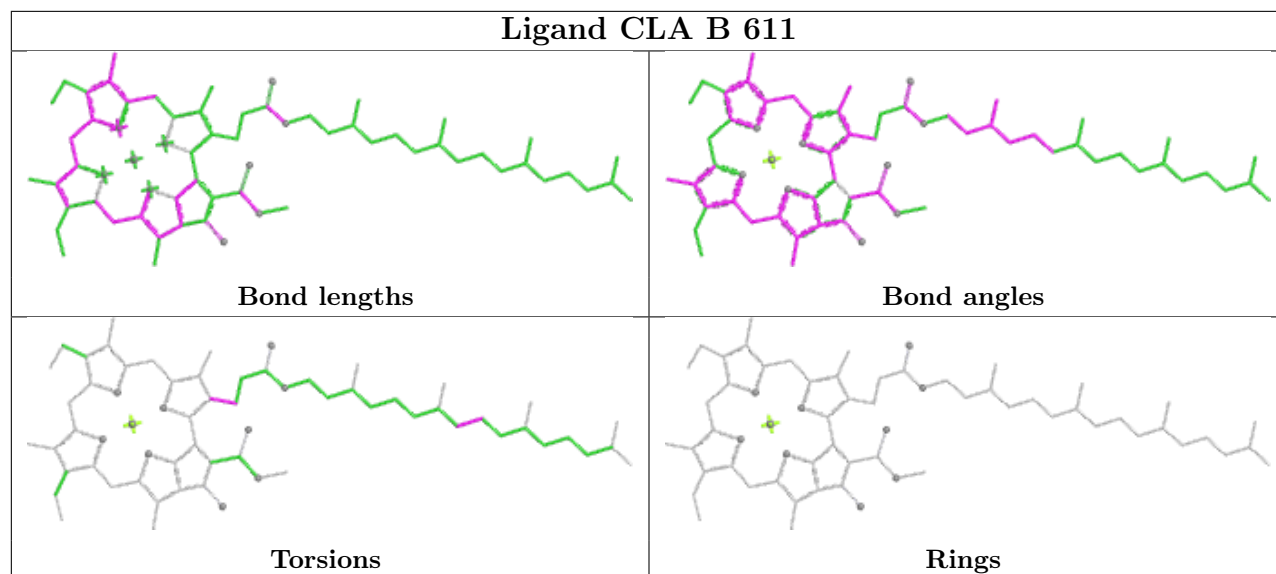


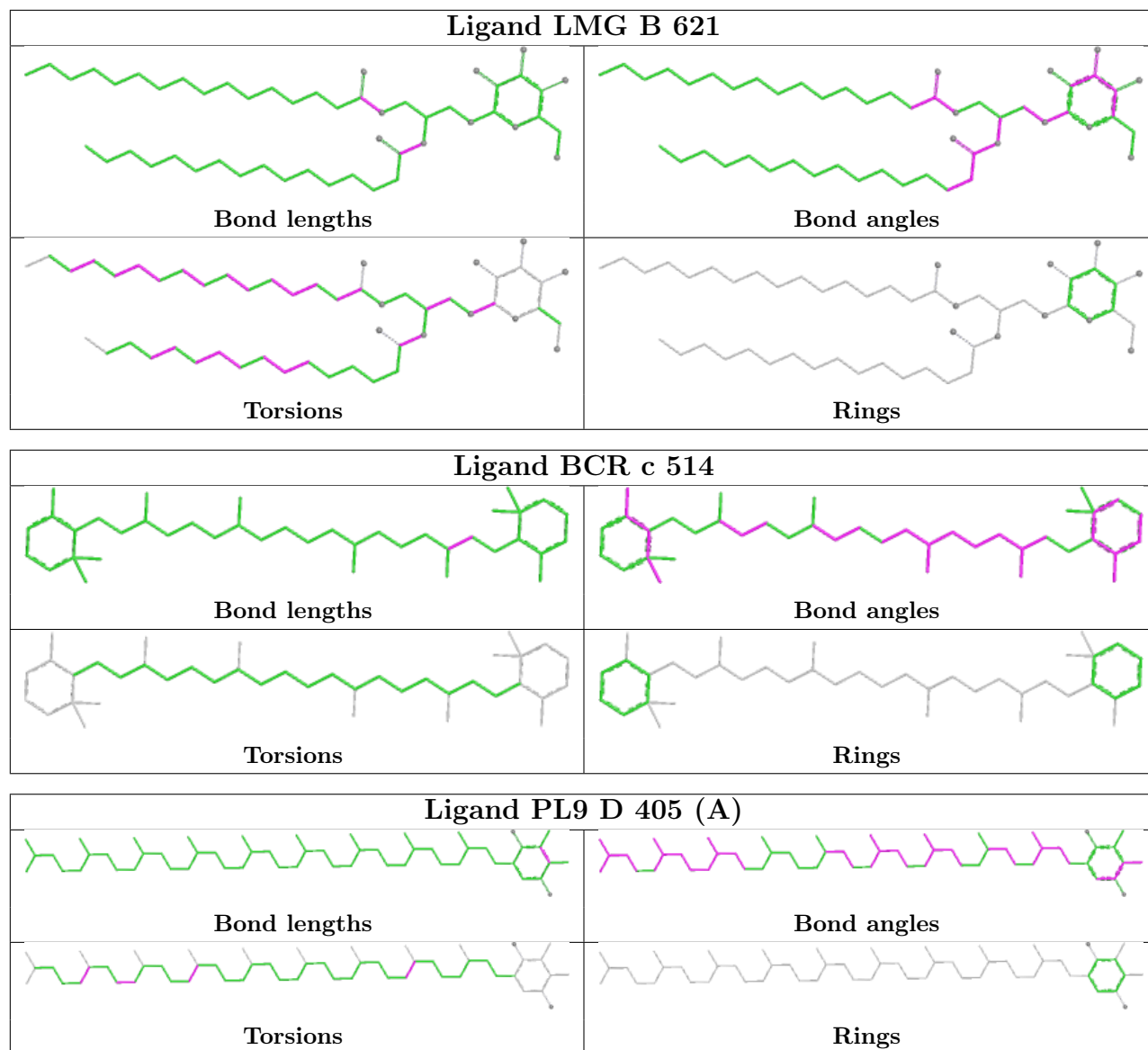
Ligand CLA C 504

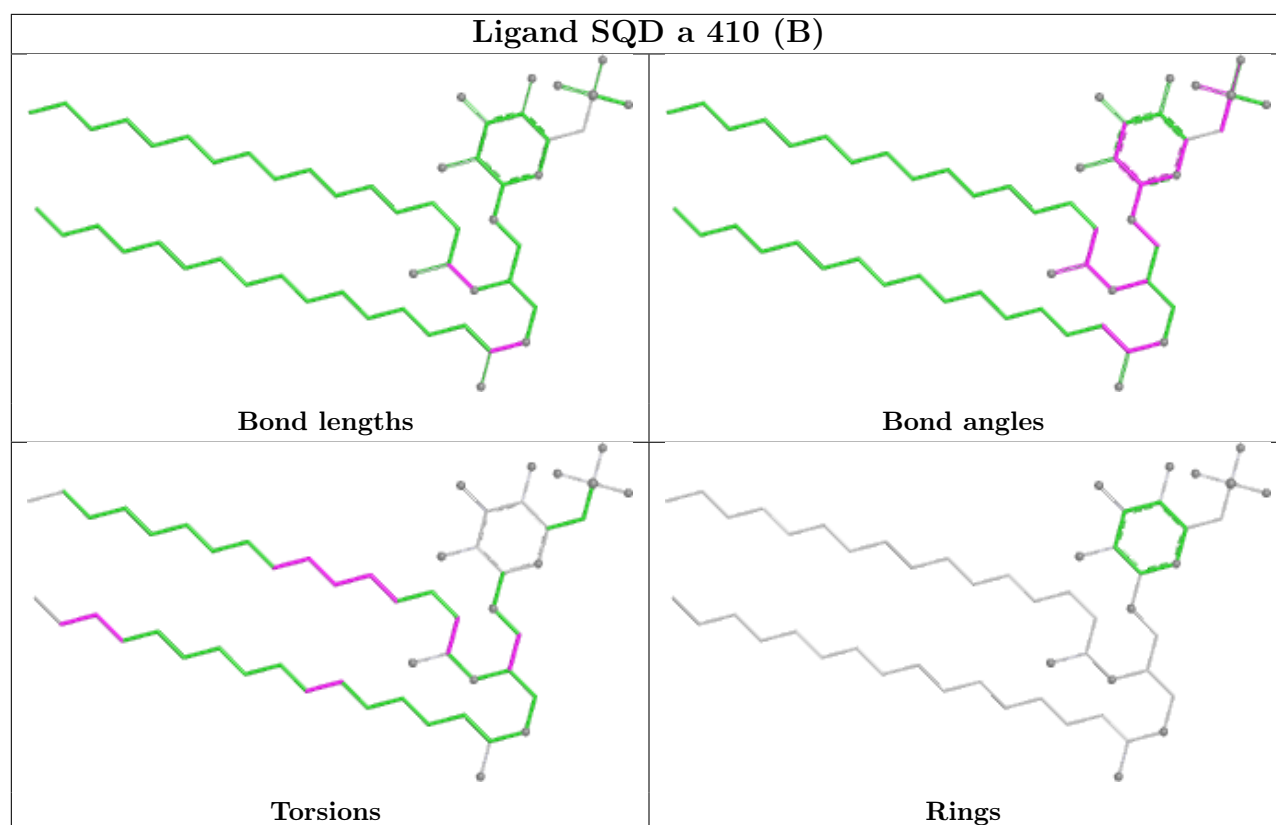


Ligand LMG C 520

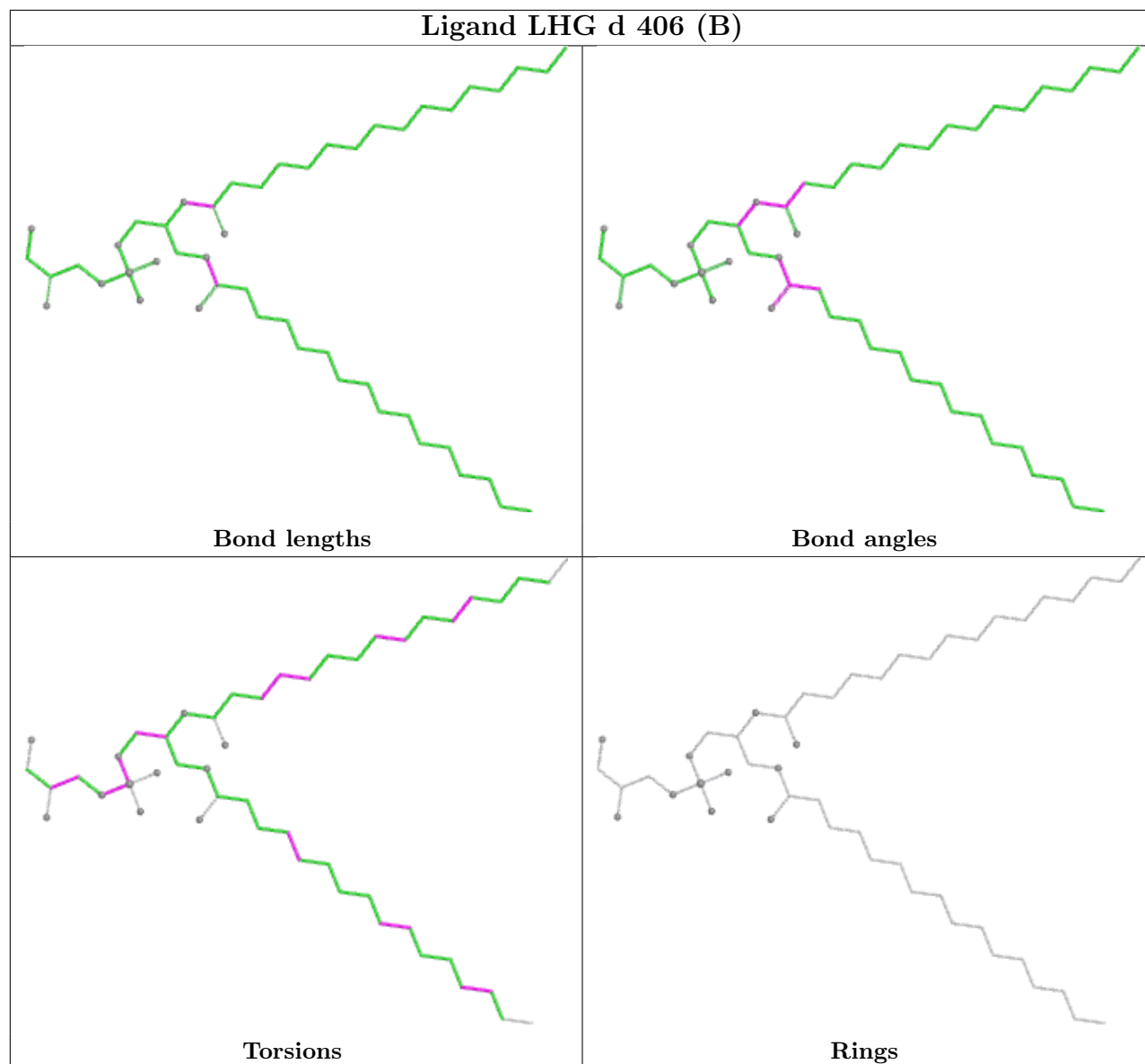




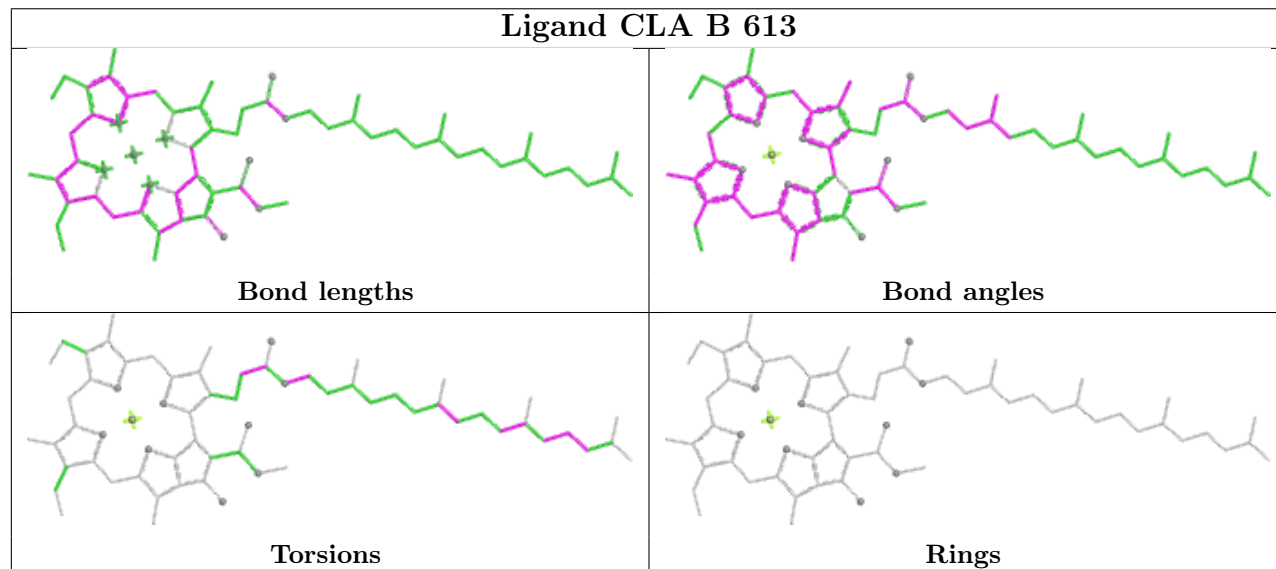




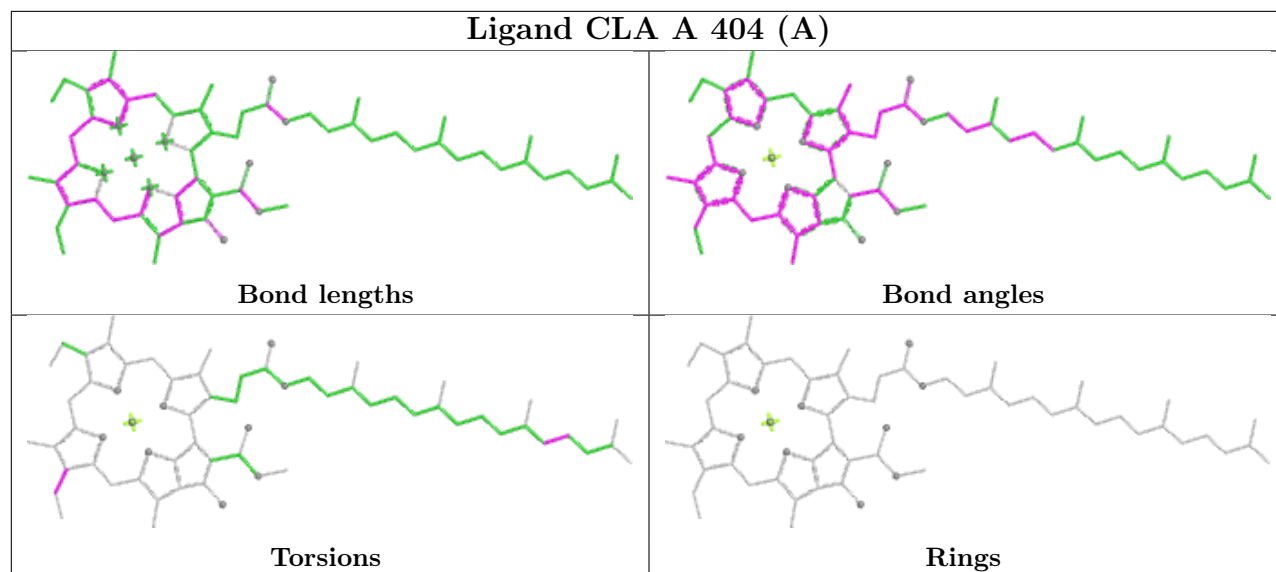
Ligand LHG d 406 (B)



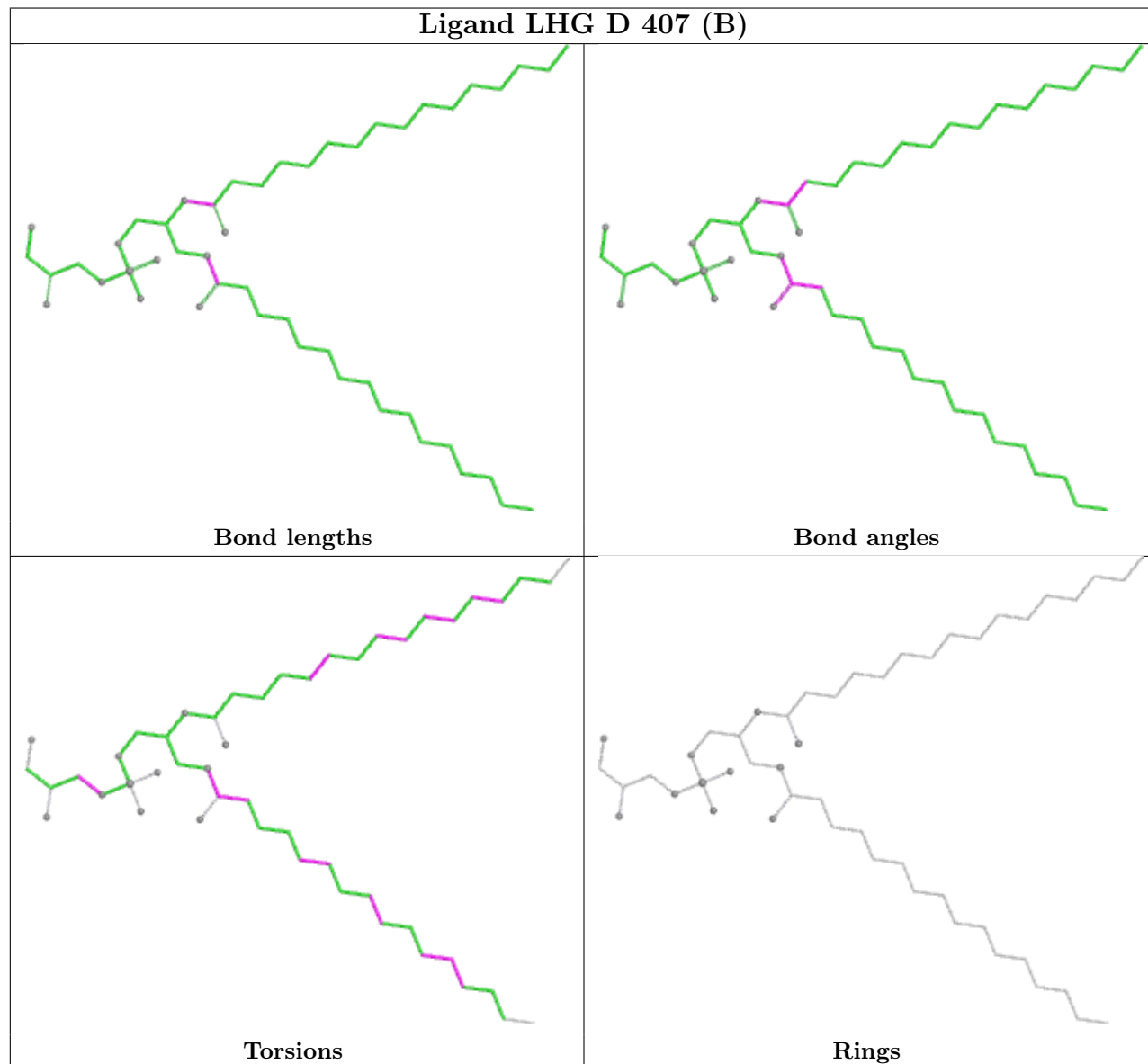
Ligand CLA B 613

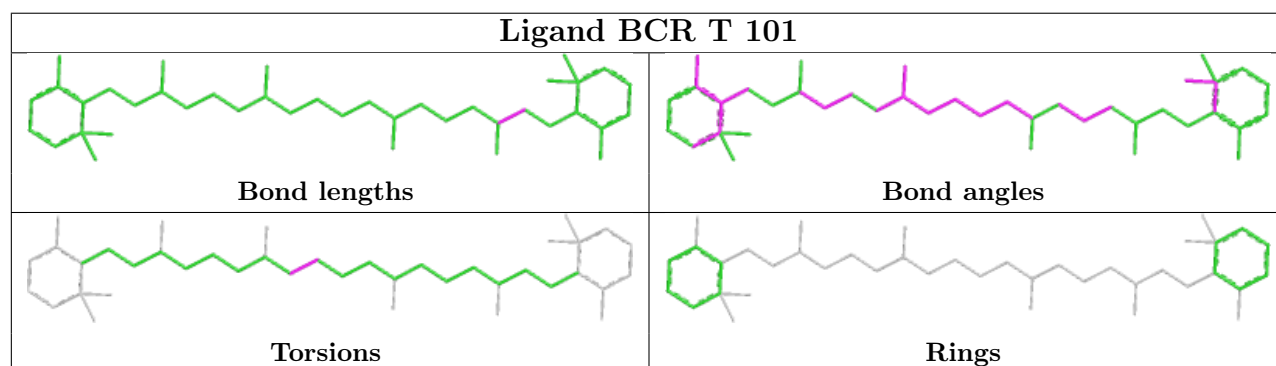
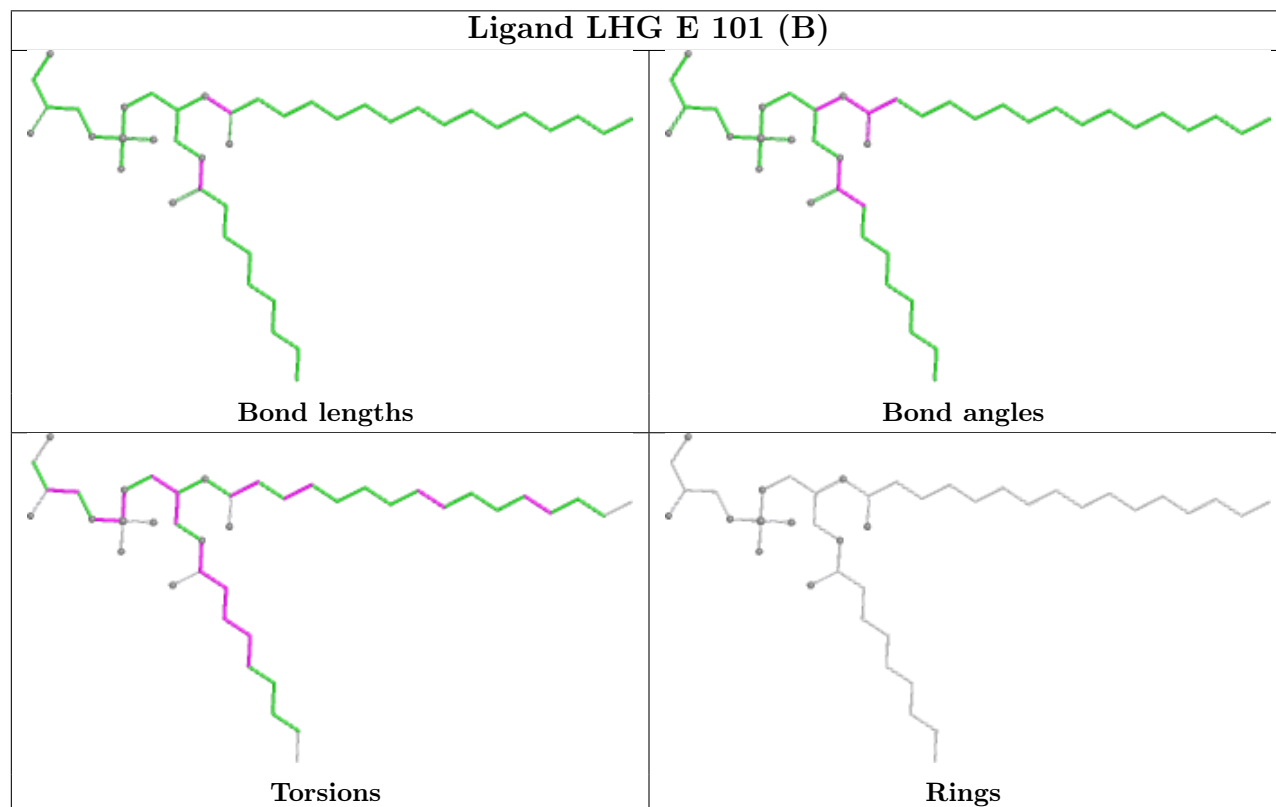
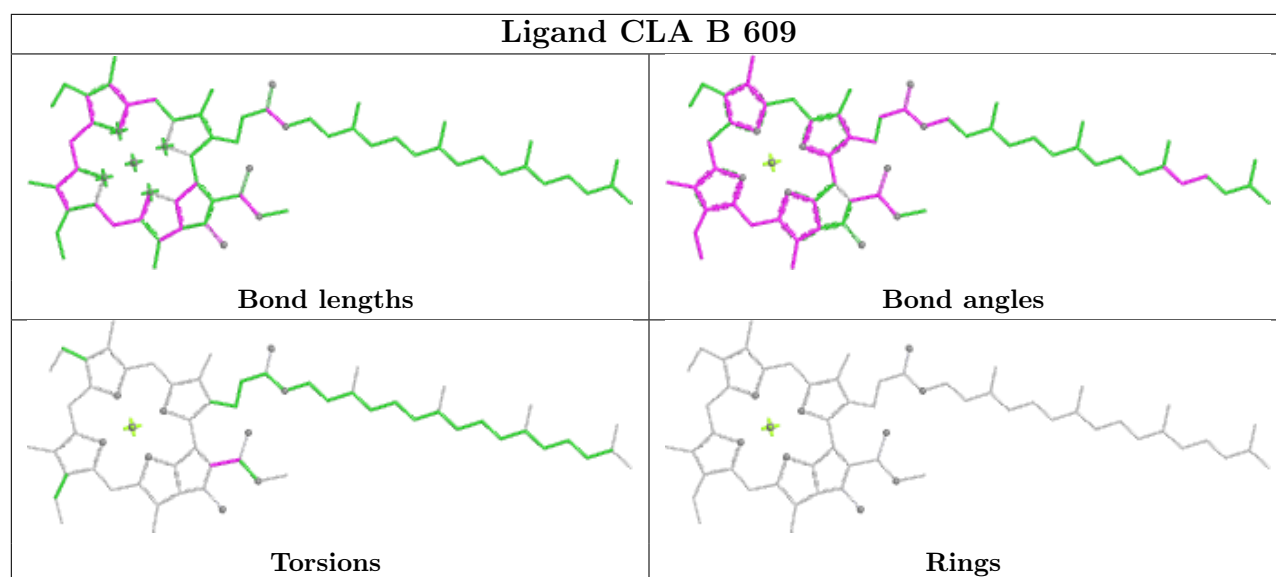


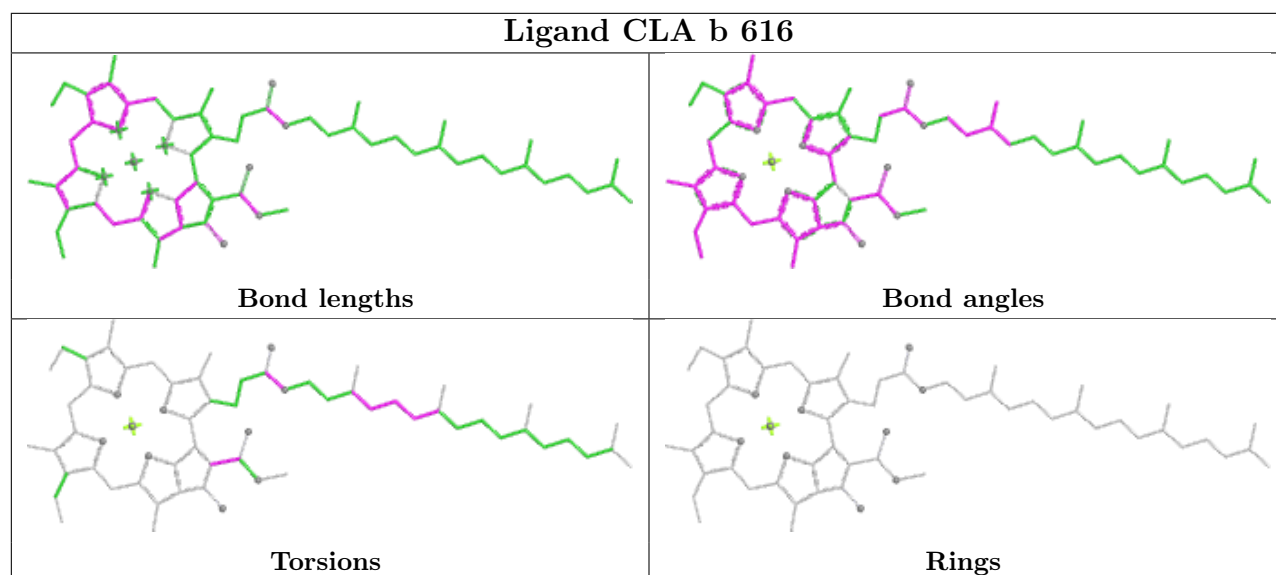
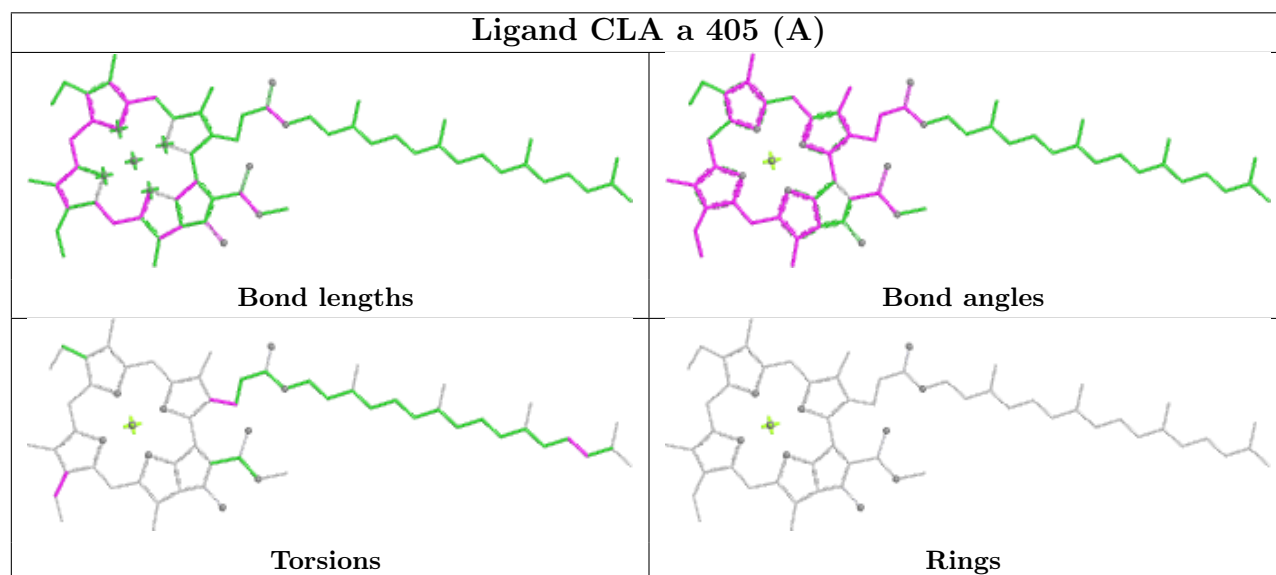
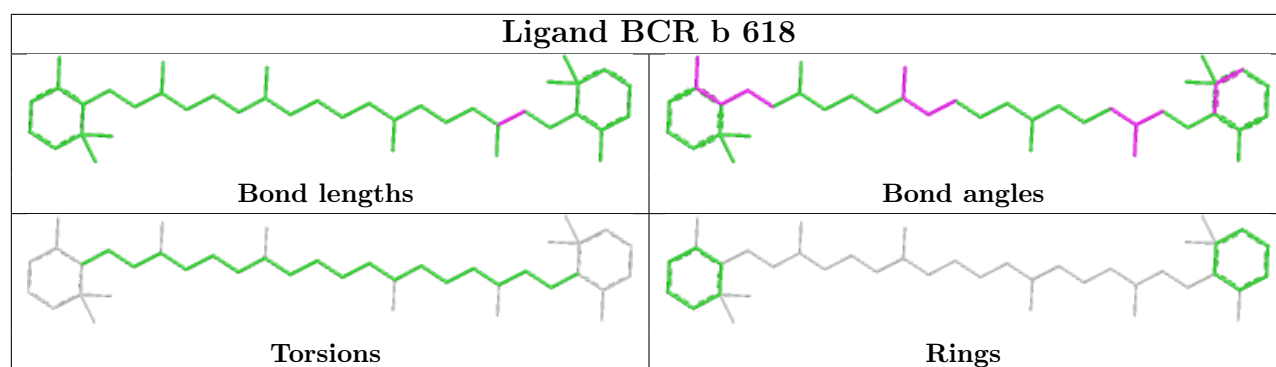
Ligand CLA A 404 (A)



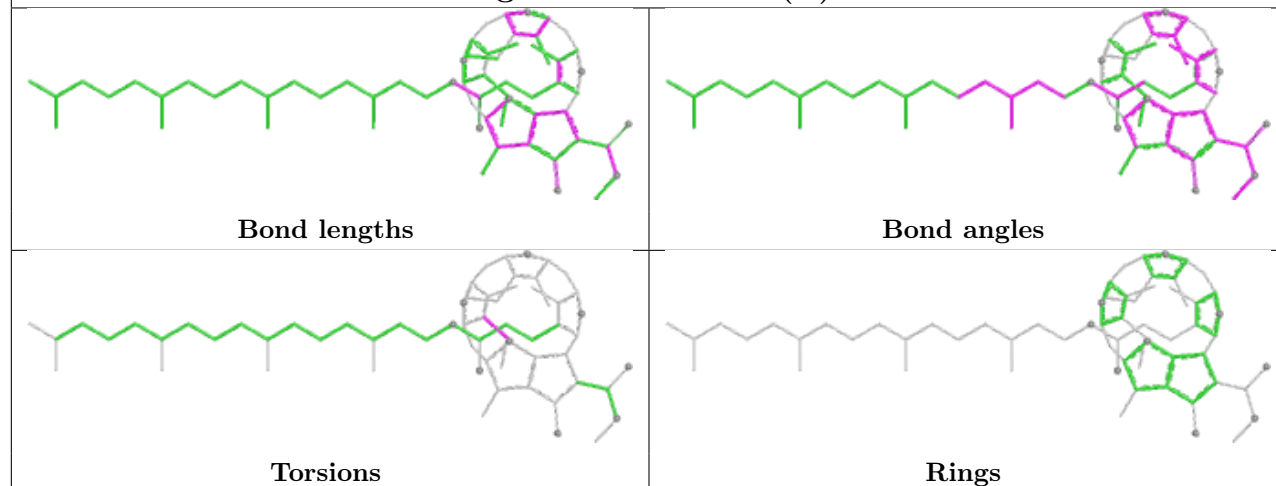
Ligand LHG D 407 (B)



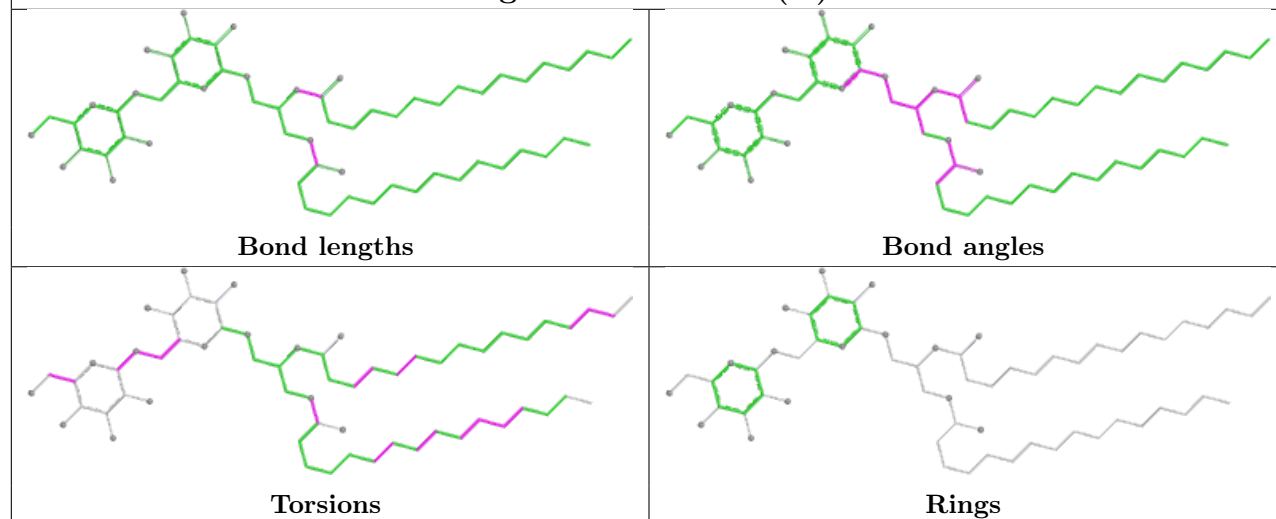




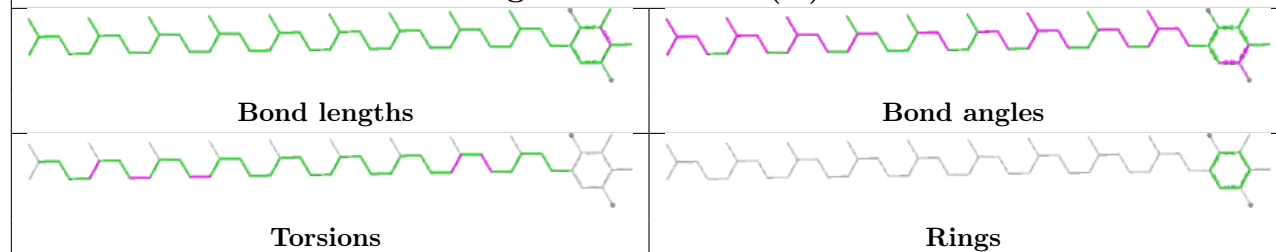
Ligand PHO A 416 (B)

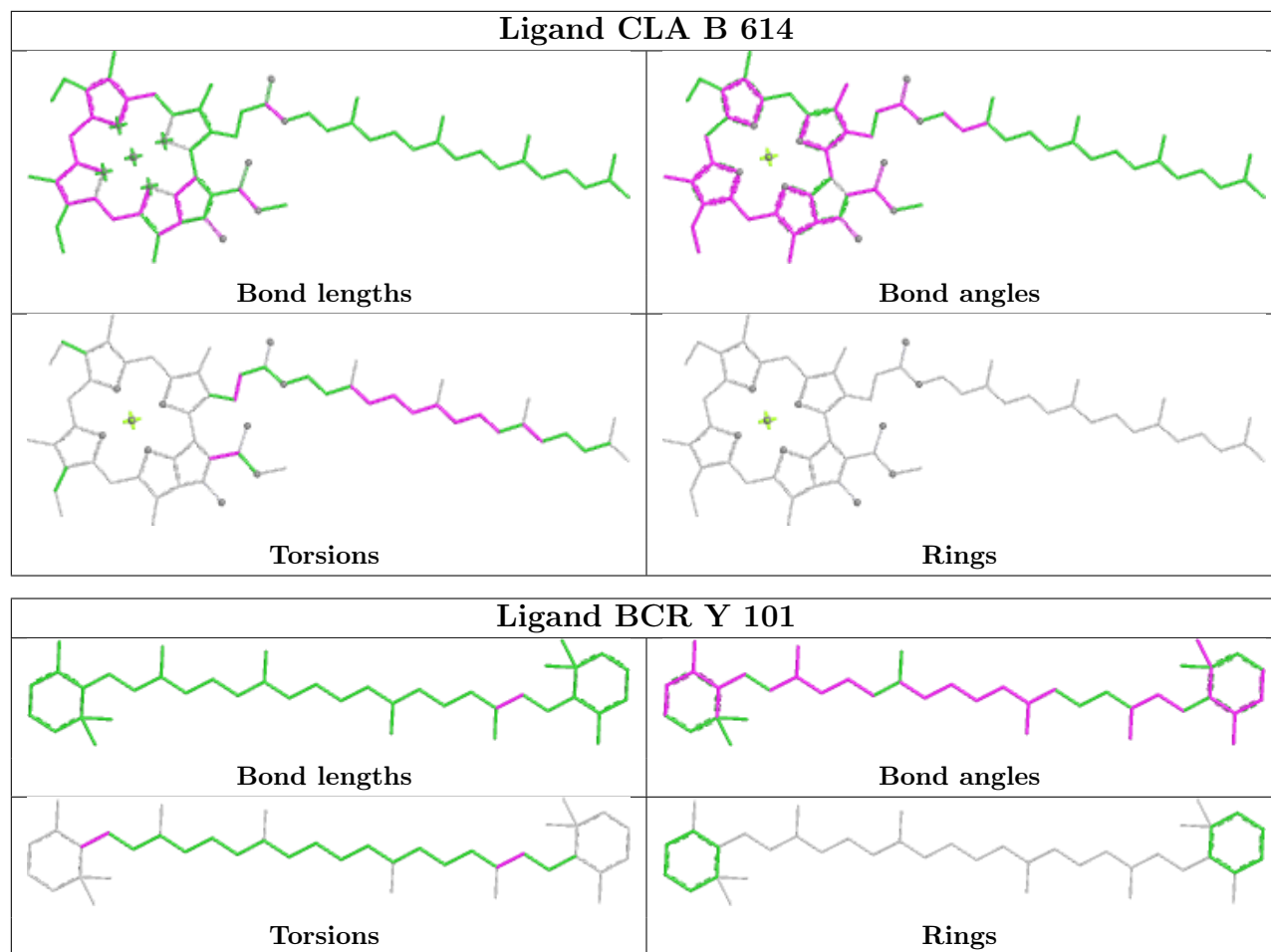


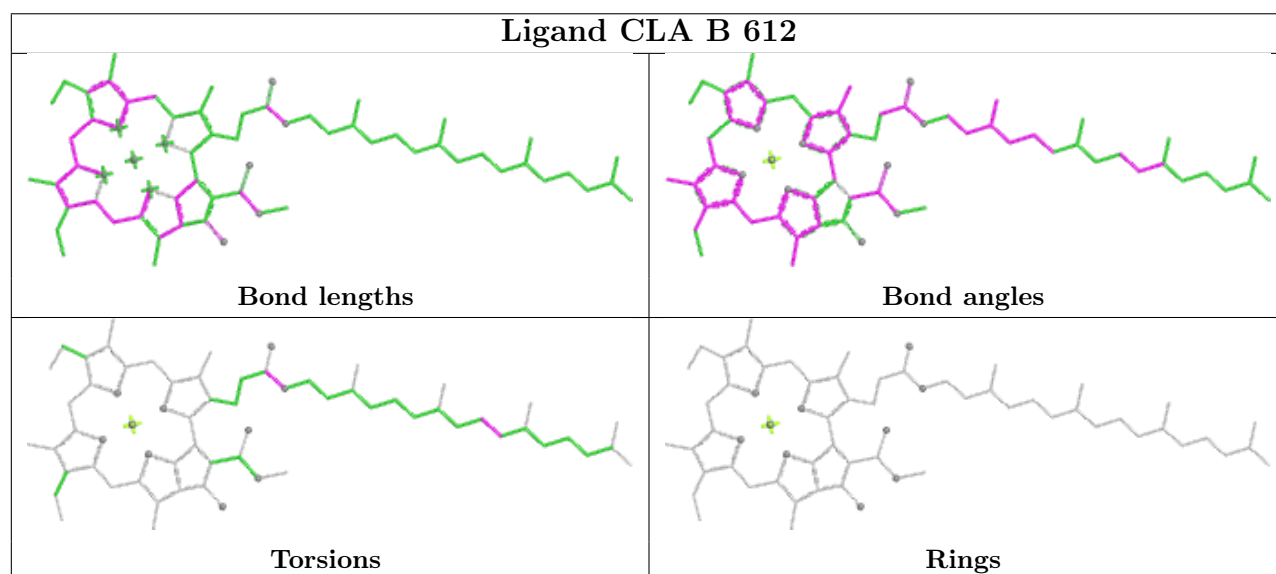
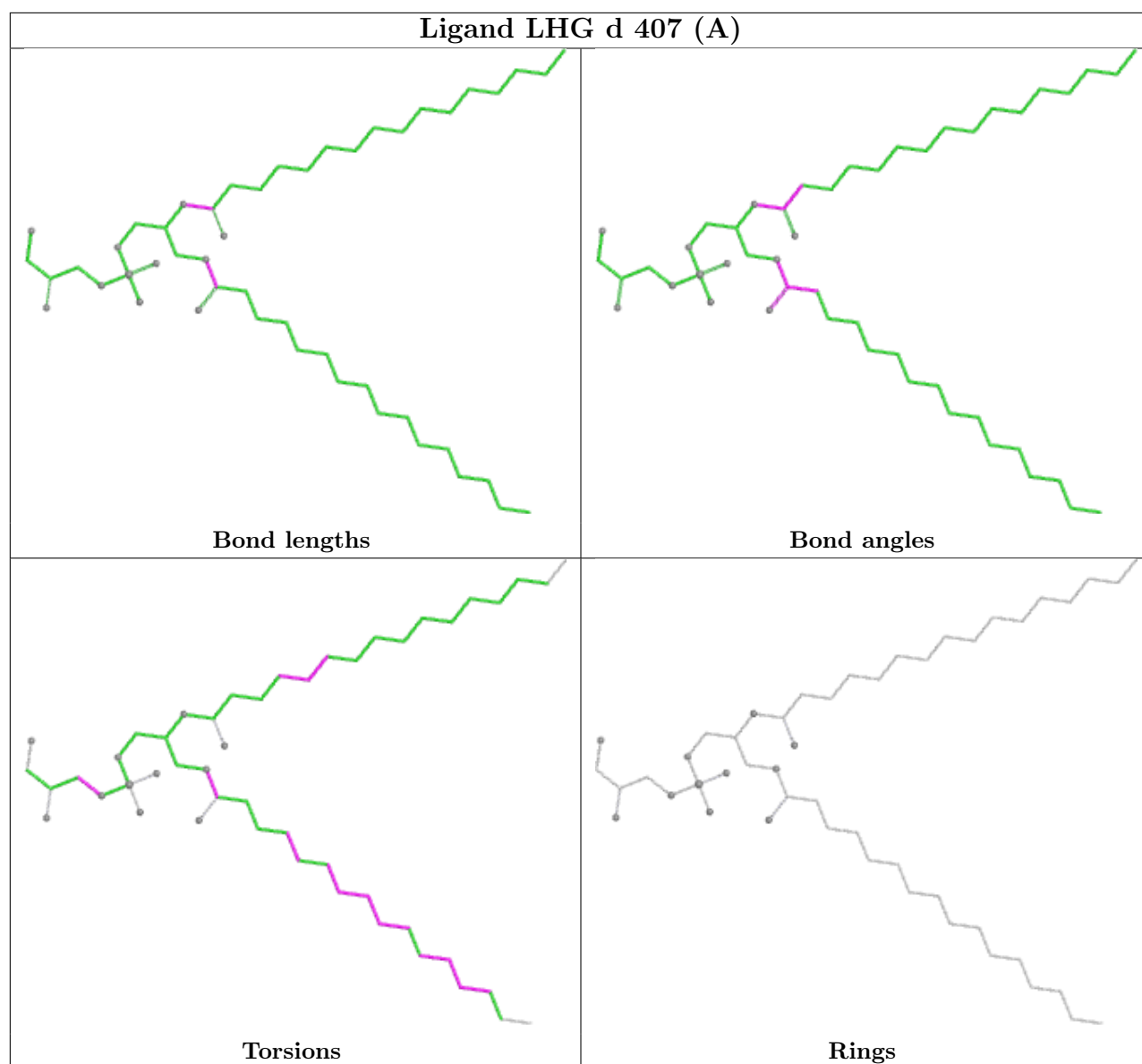
Ligand DGD c 516 (A)

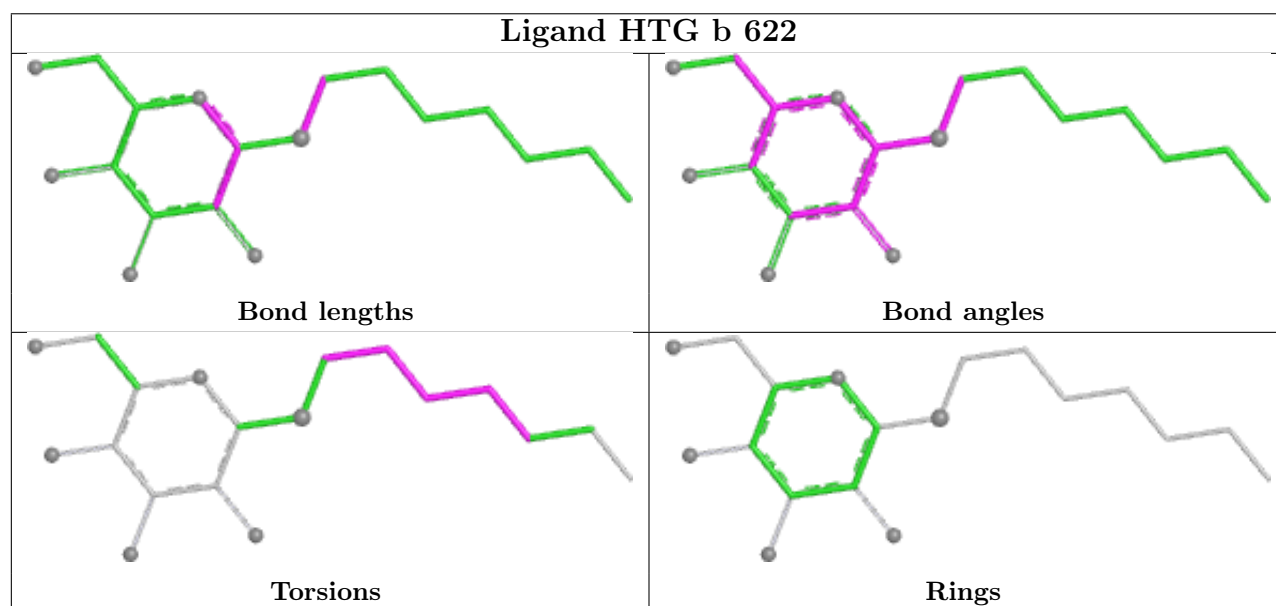
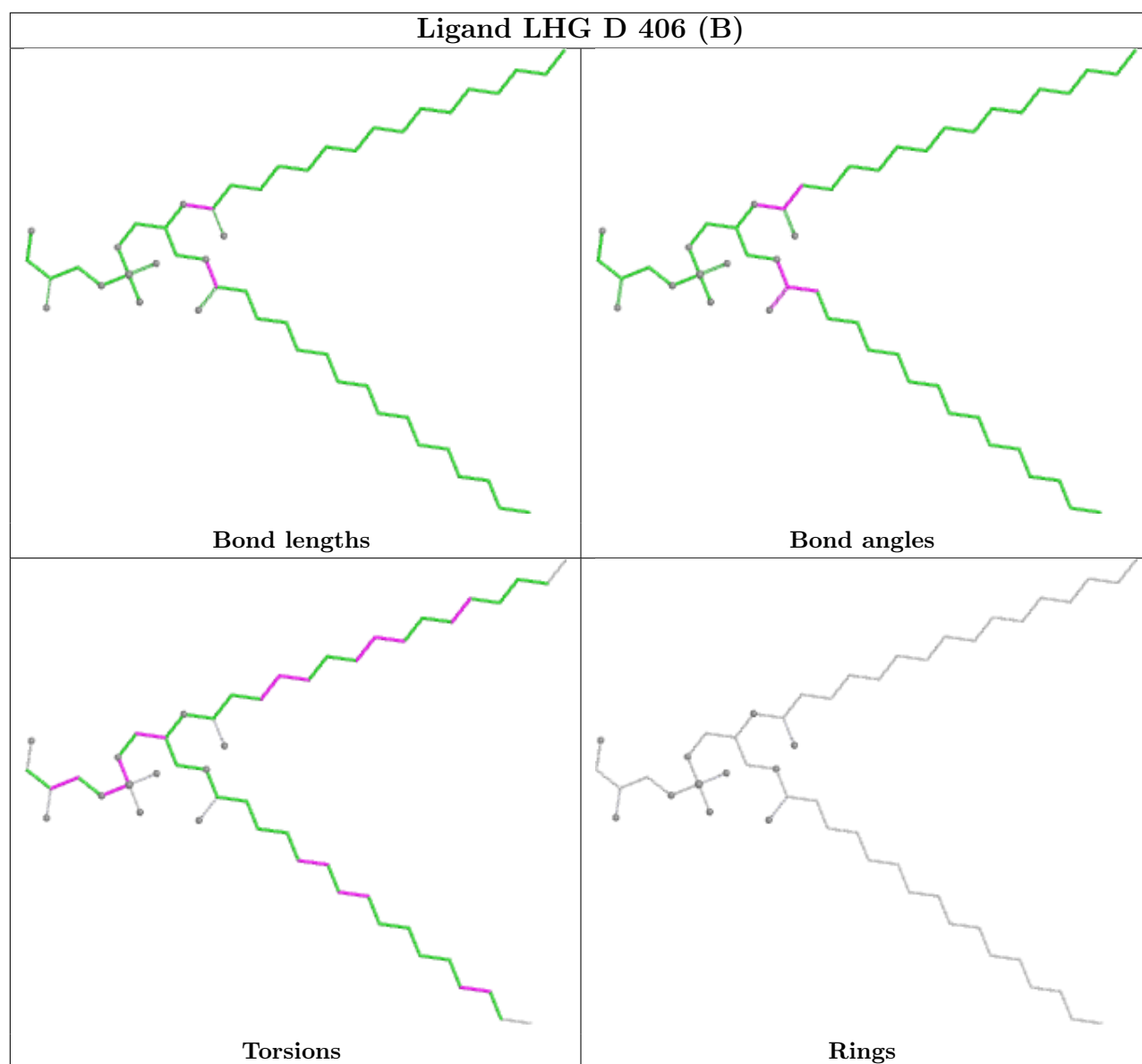


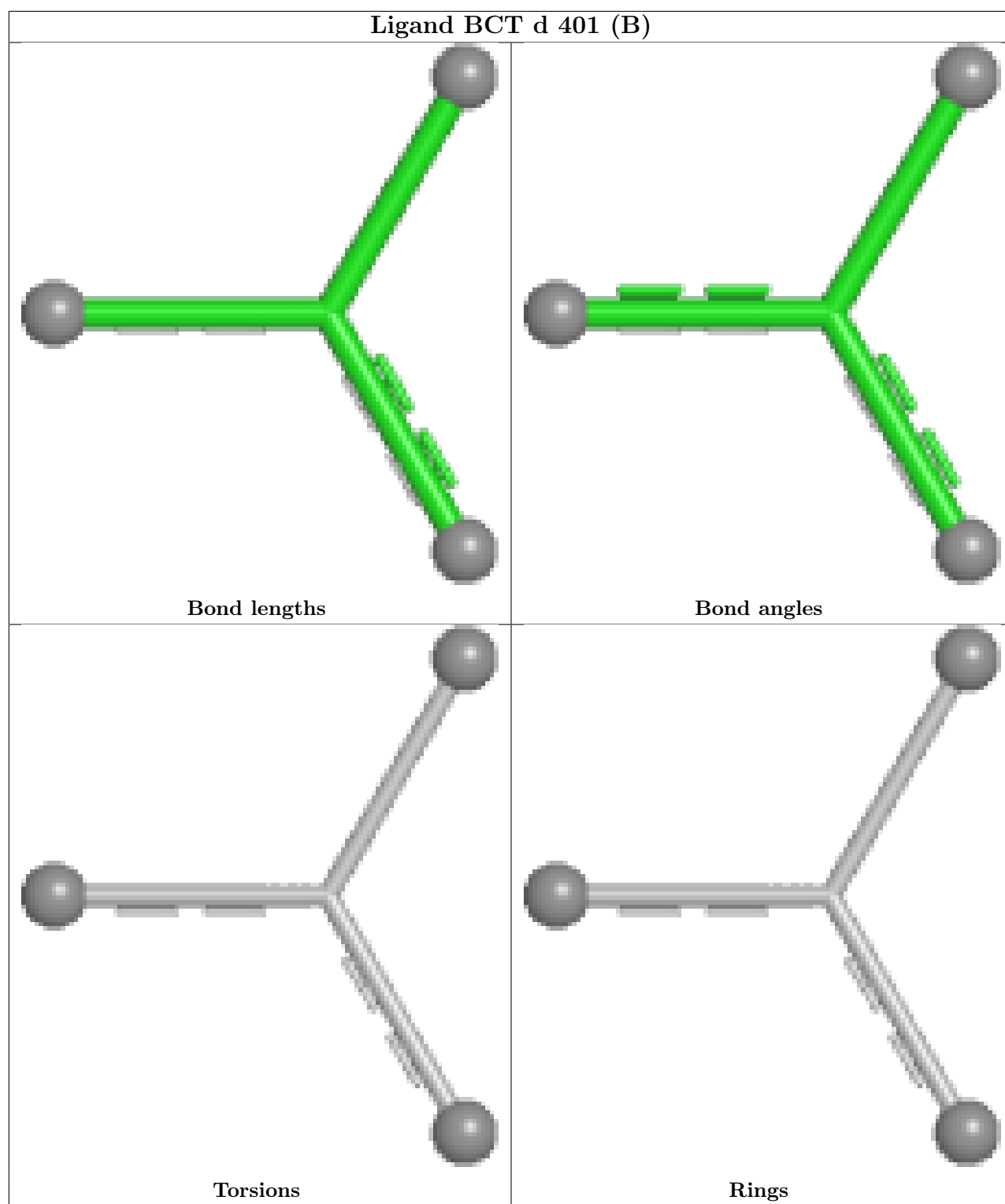
Ligand PL9 d 405 (A)

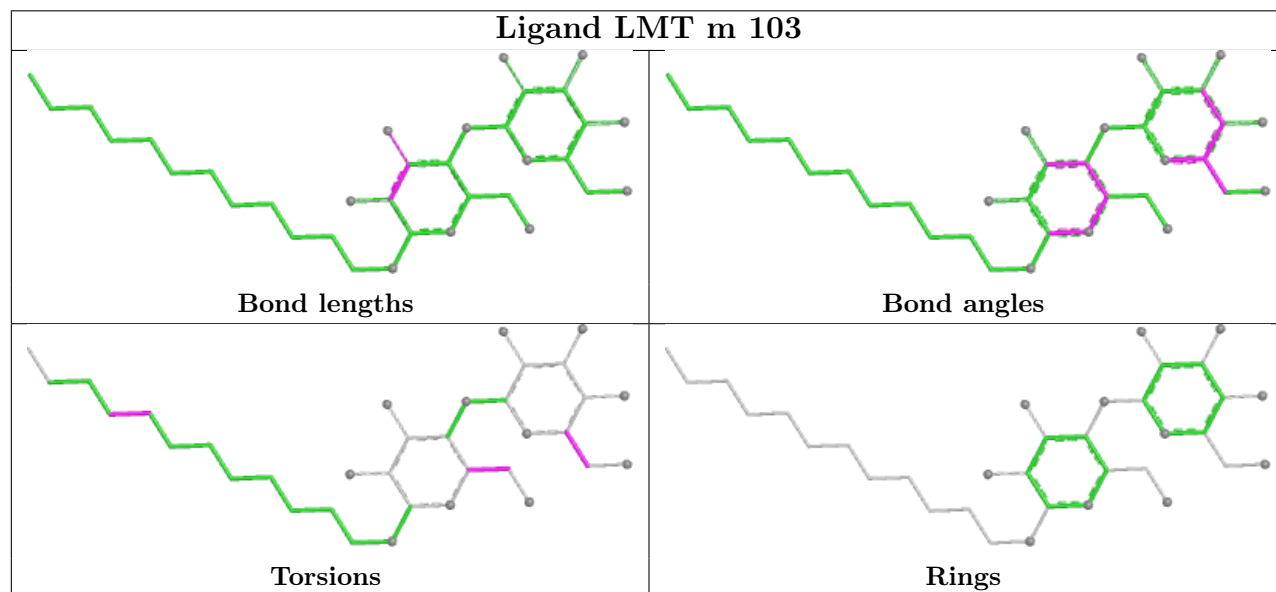
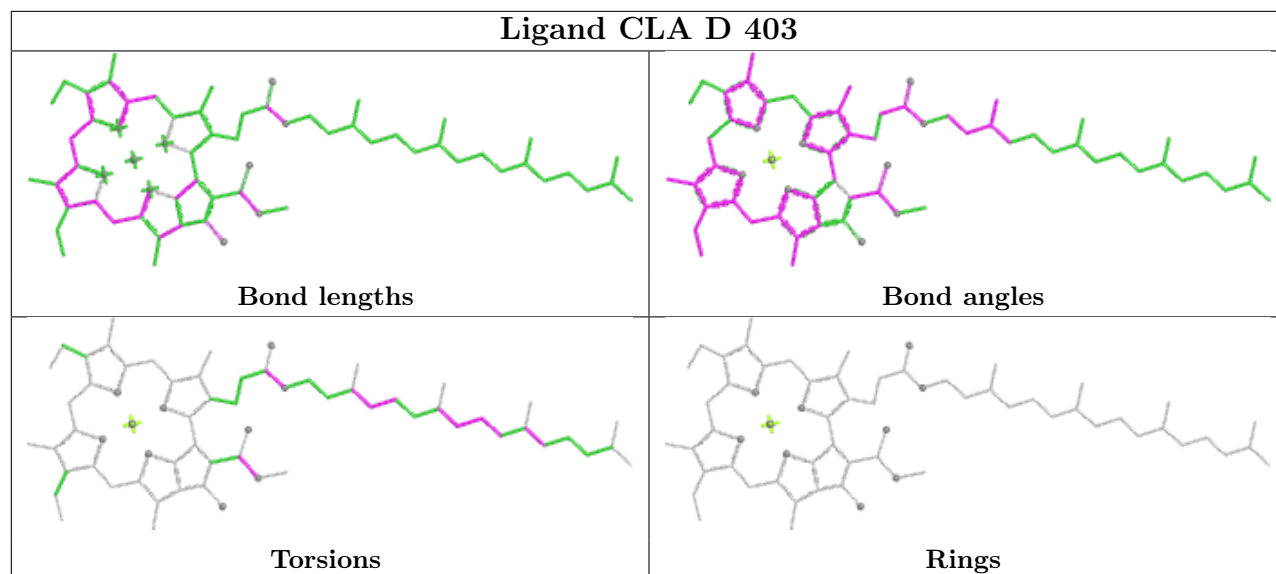


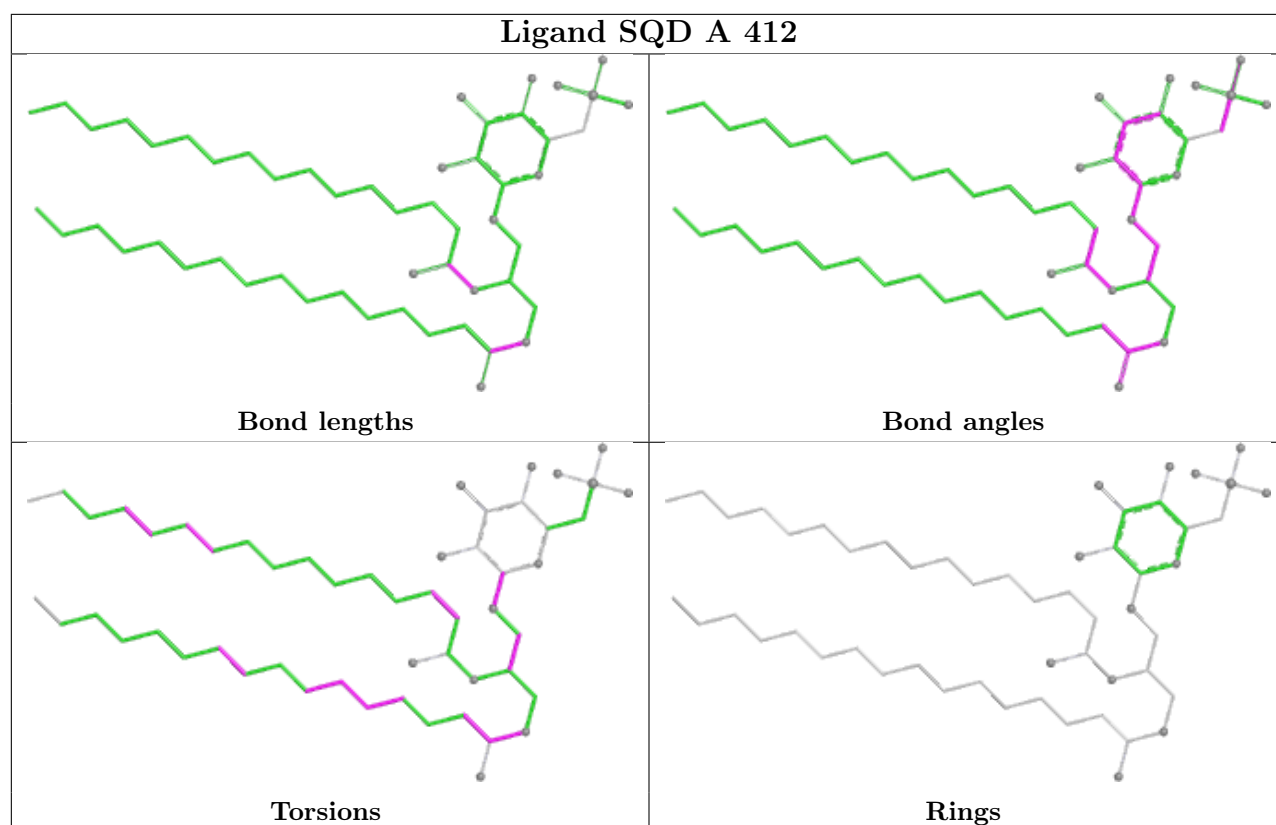




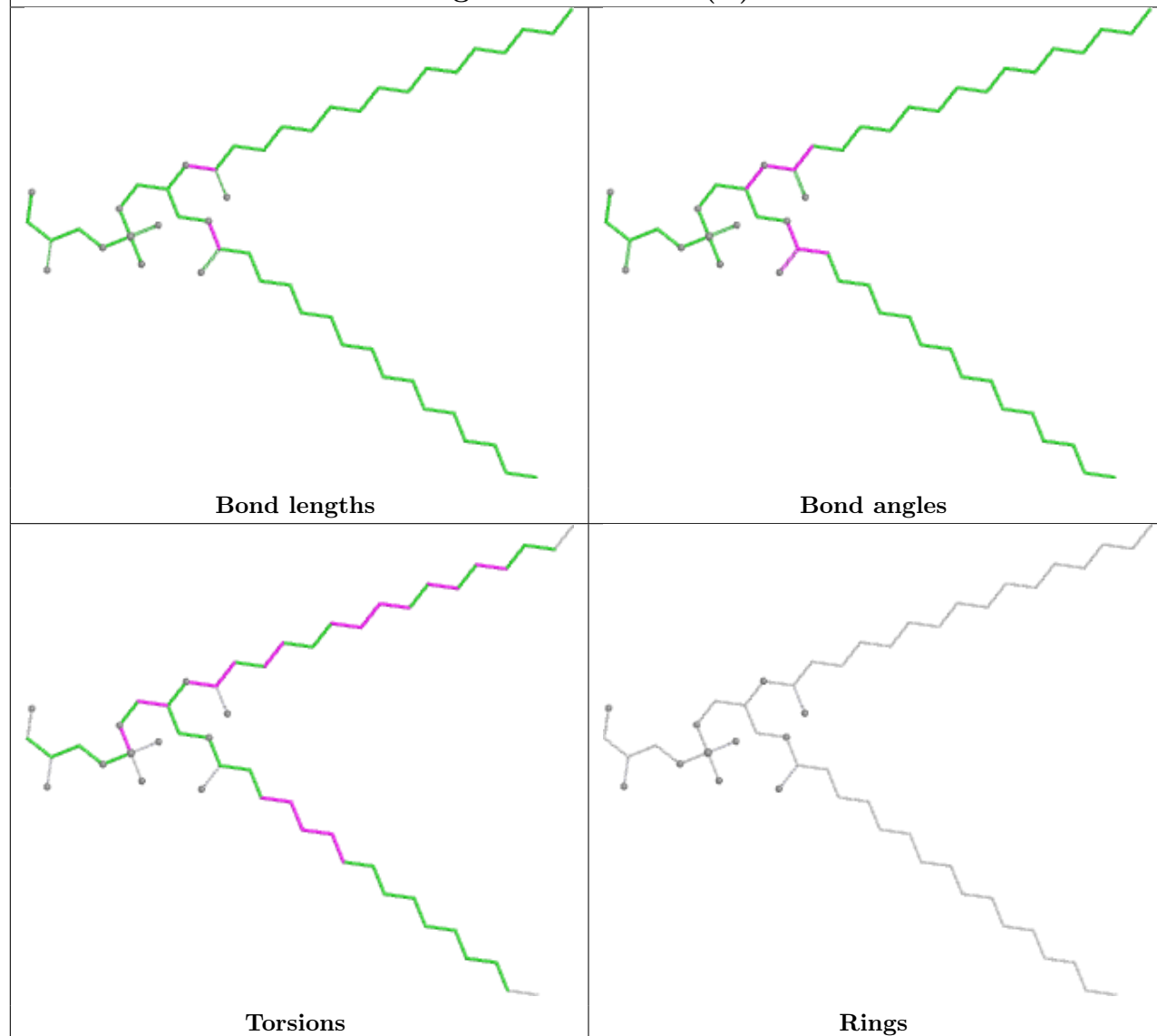




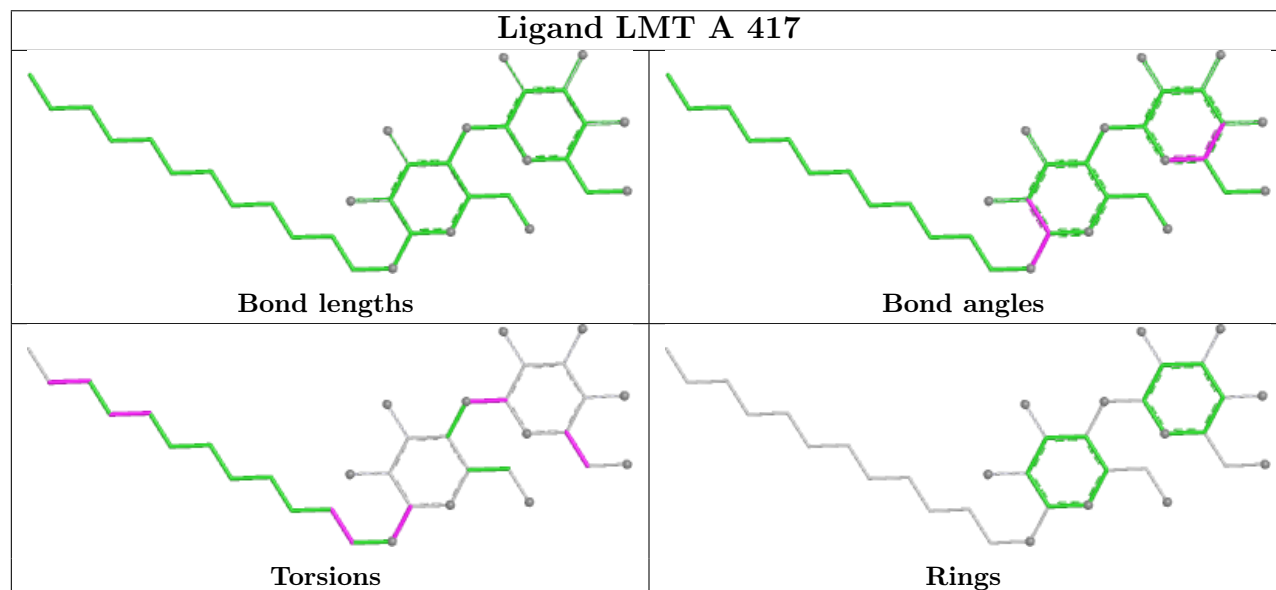


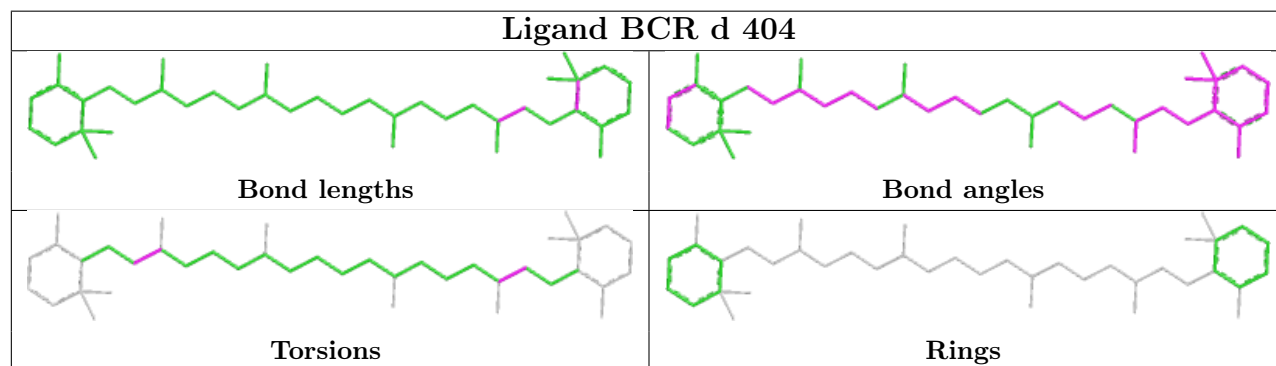
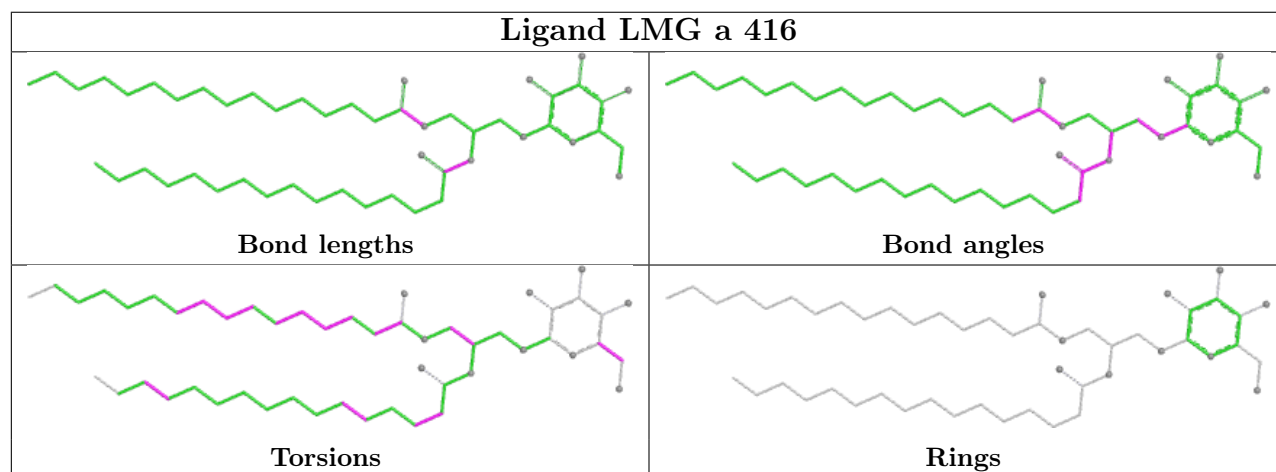
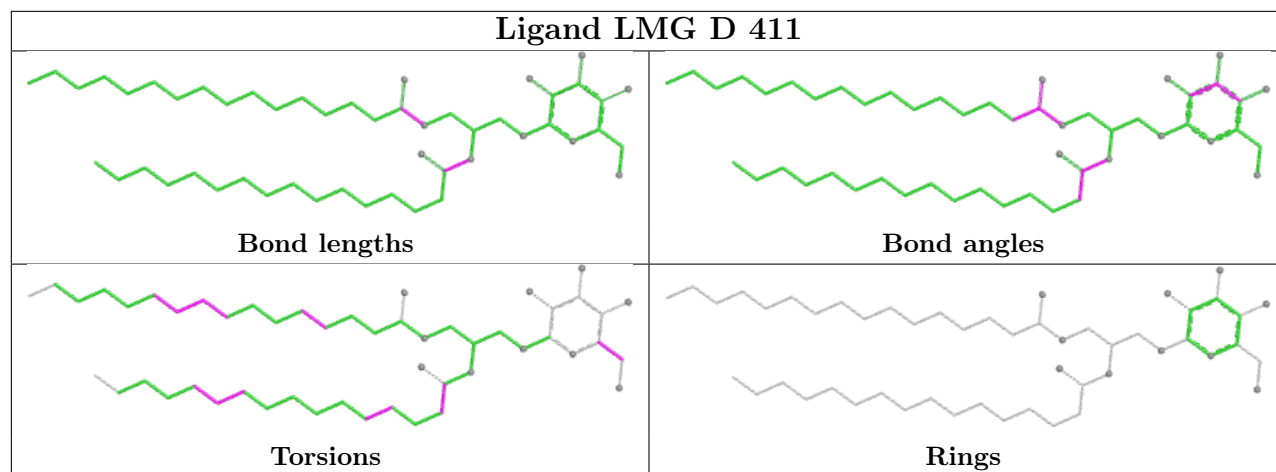


Ligand LHG L 101 (B)

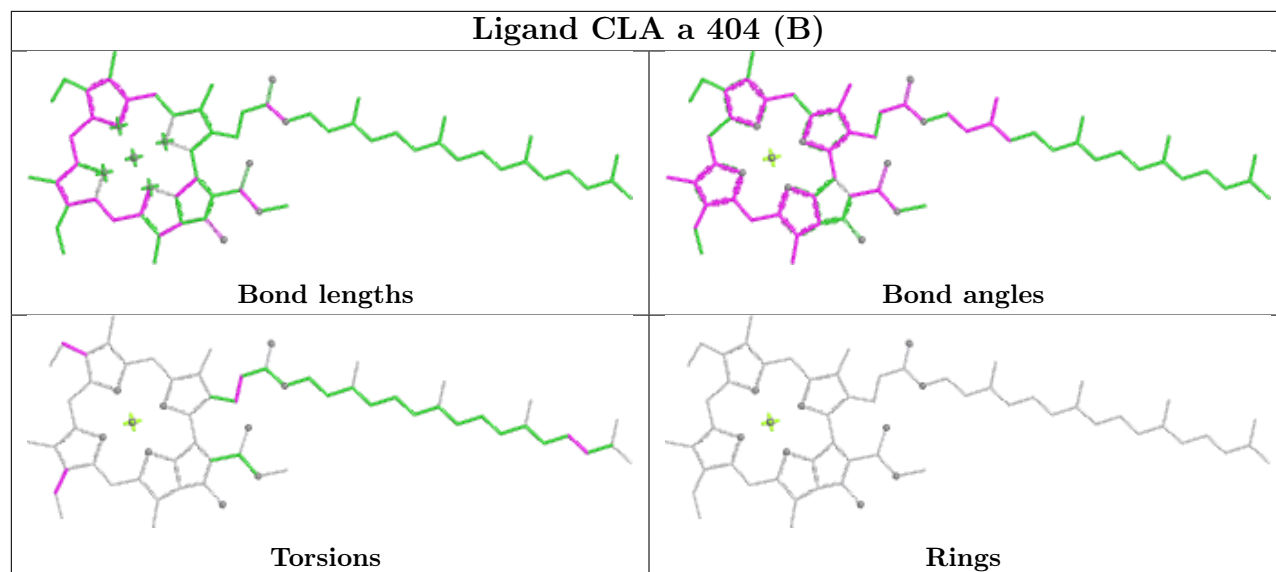


Ligand LMT A 417

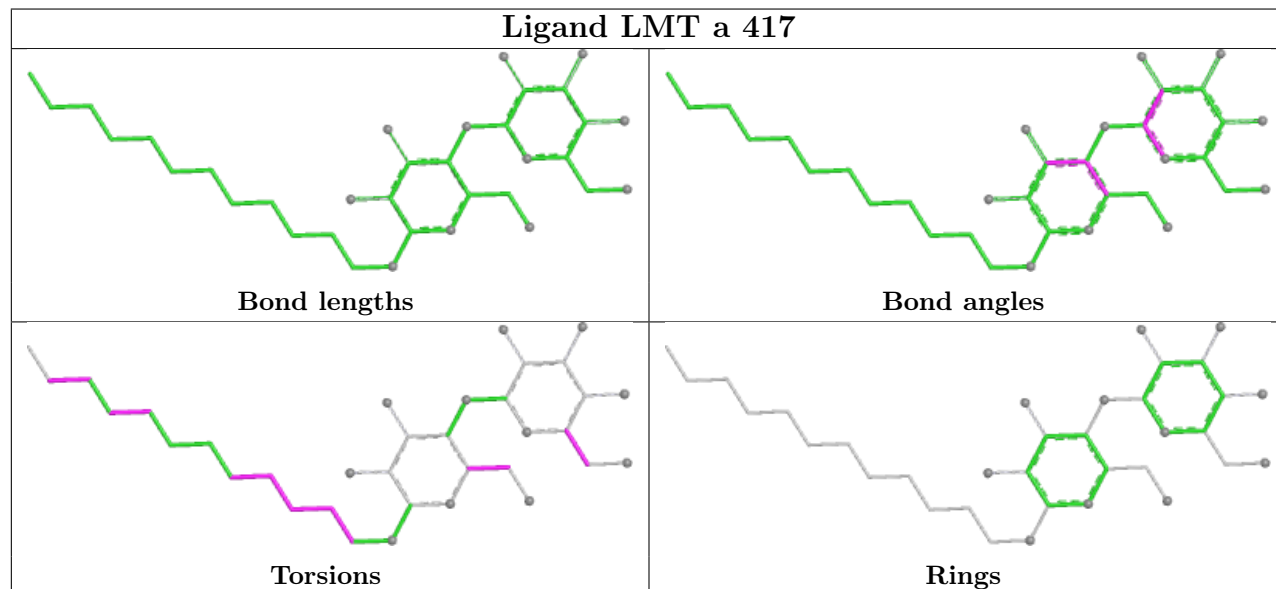




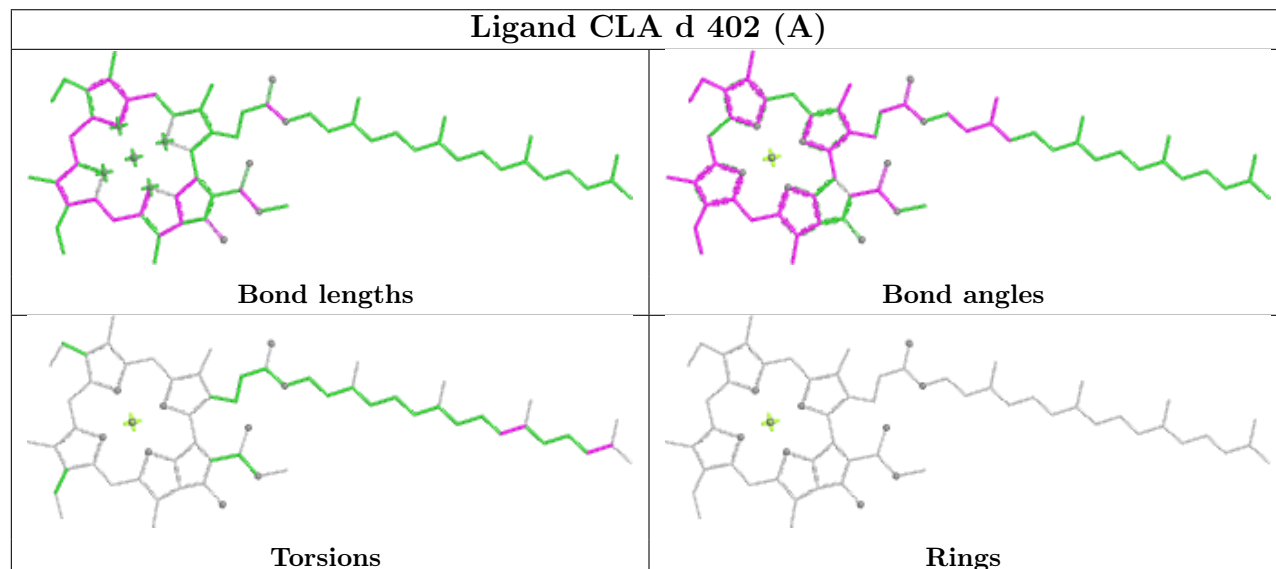
Ligand CLA a 404 (B)

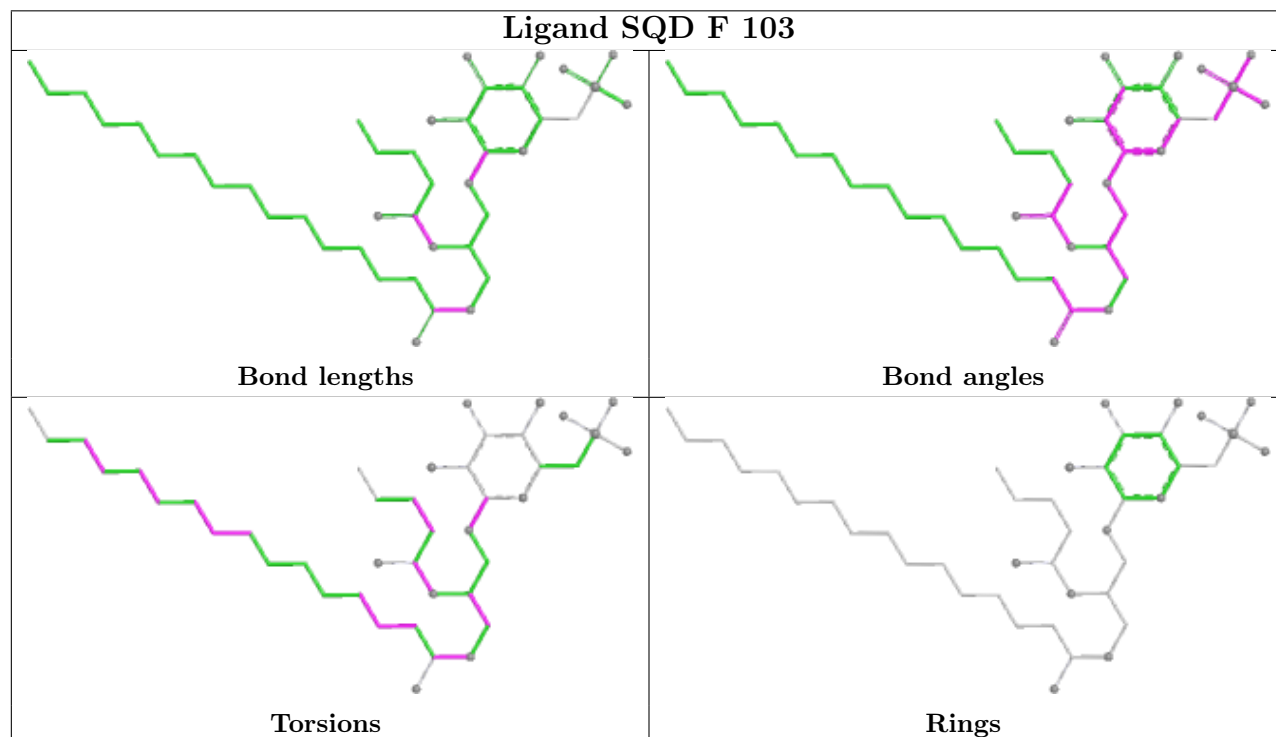
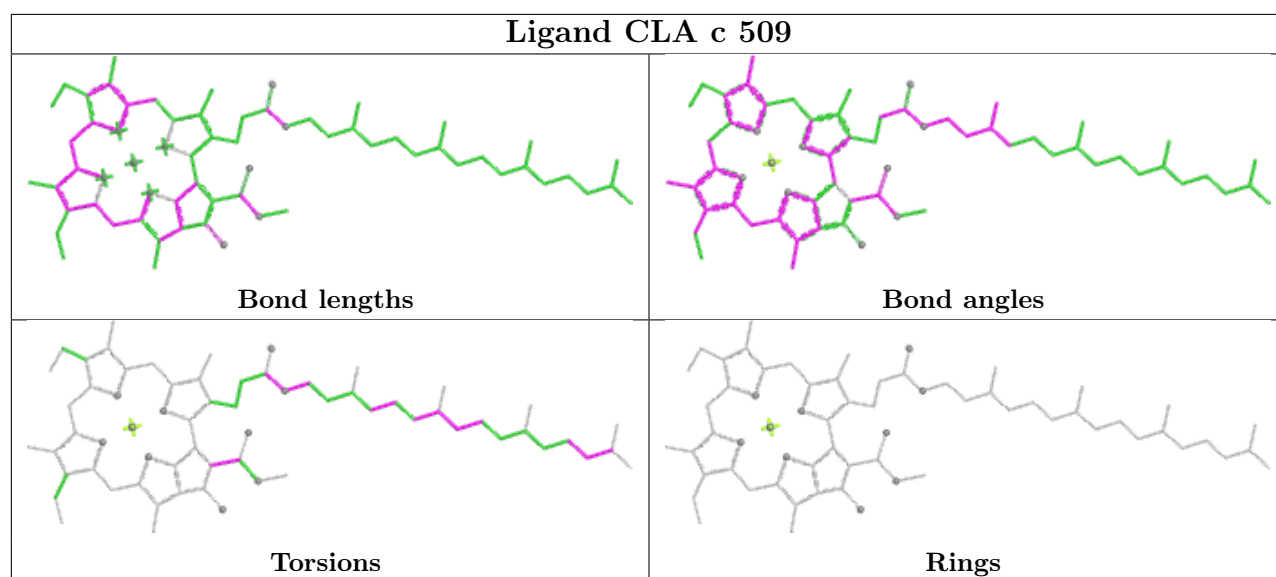


Ligand LMT a 417

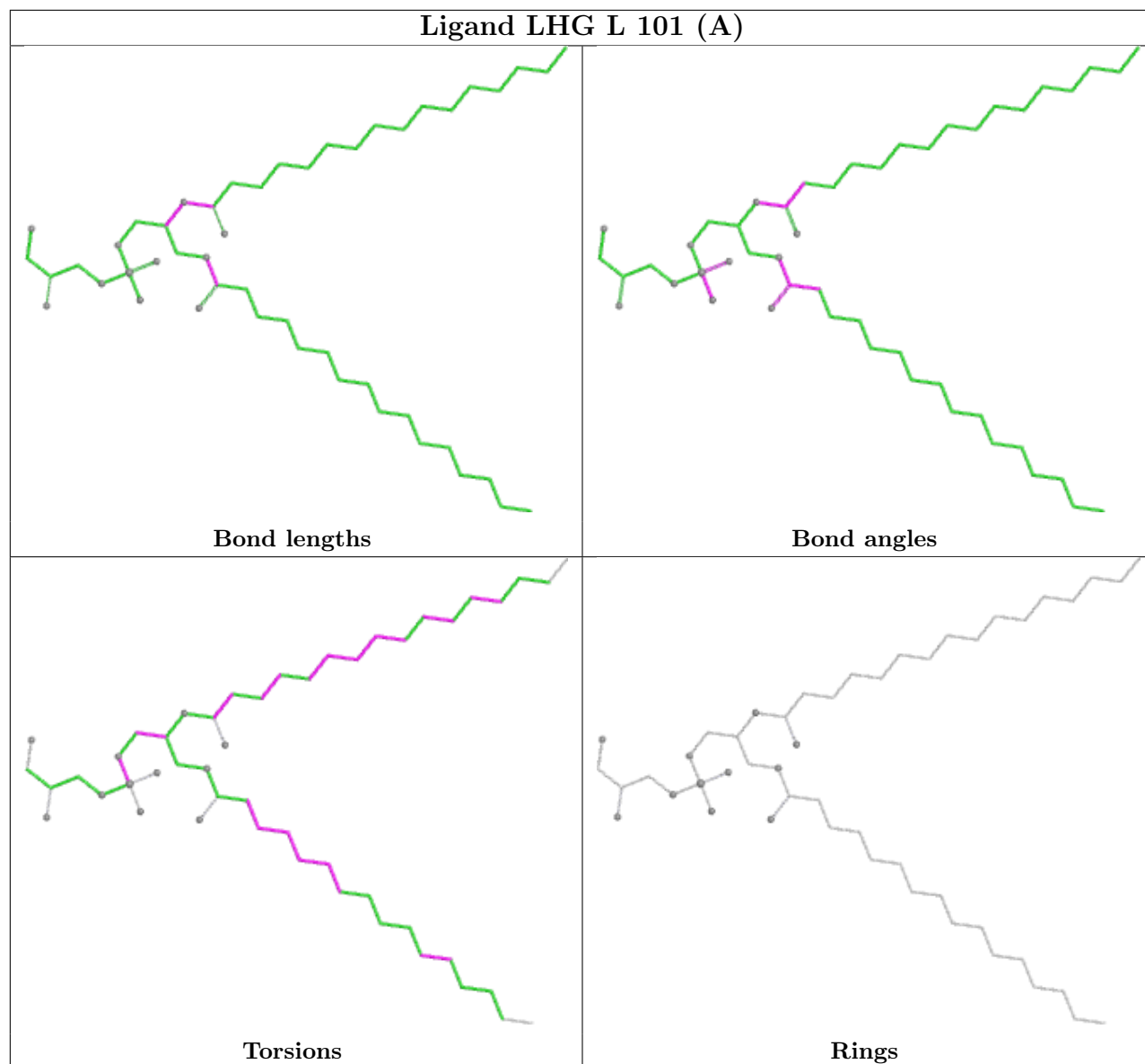


Ligand CLA d 402 (A)

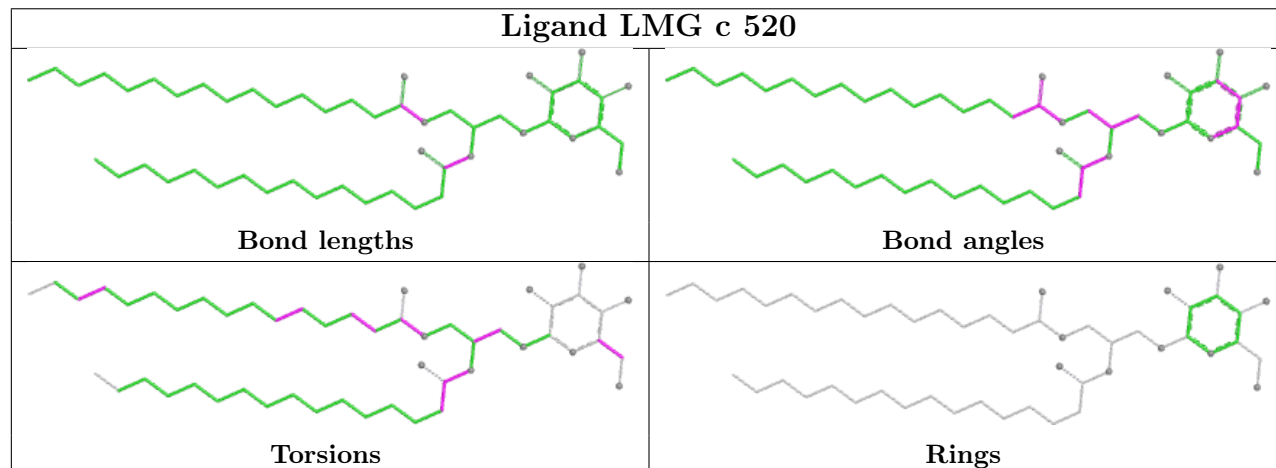


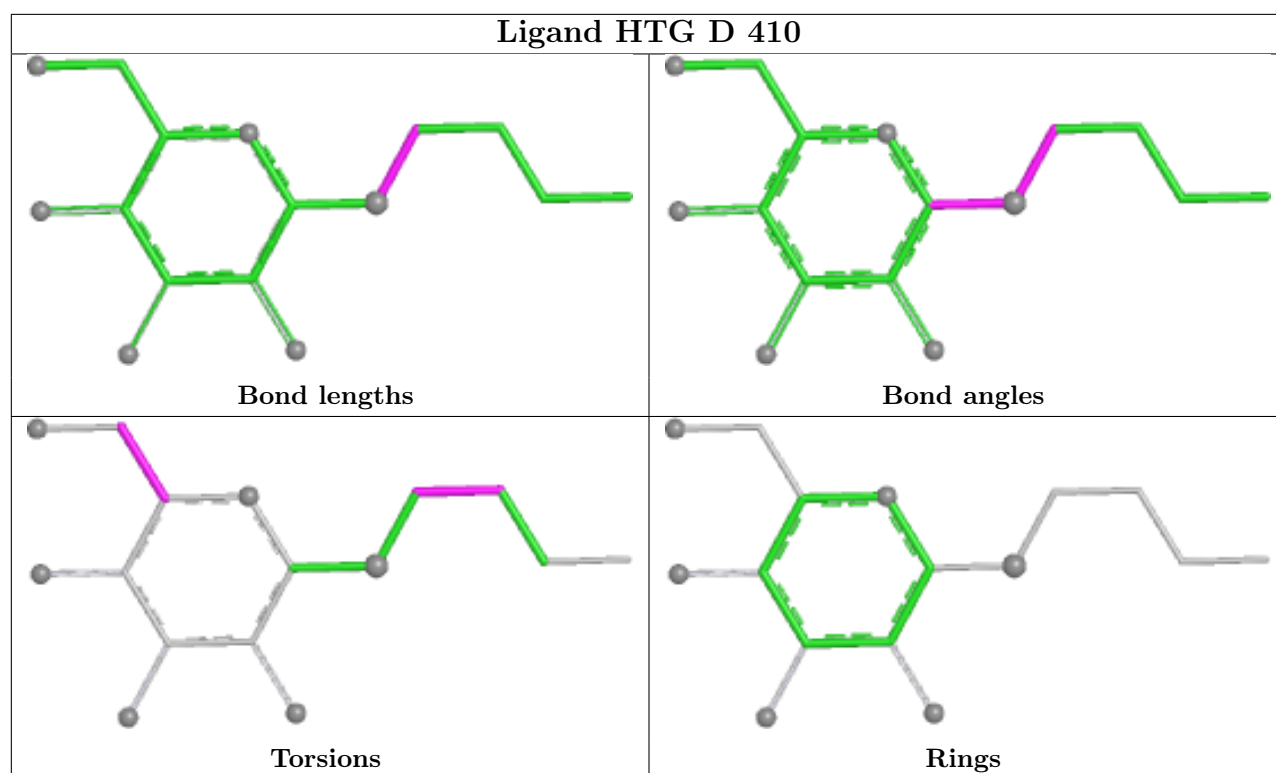


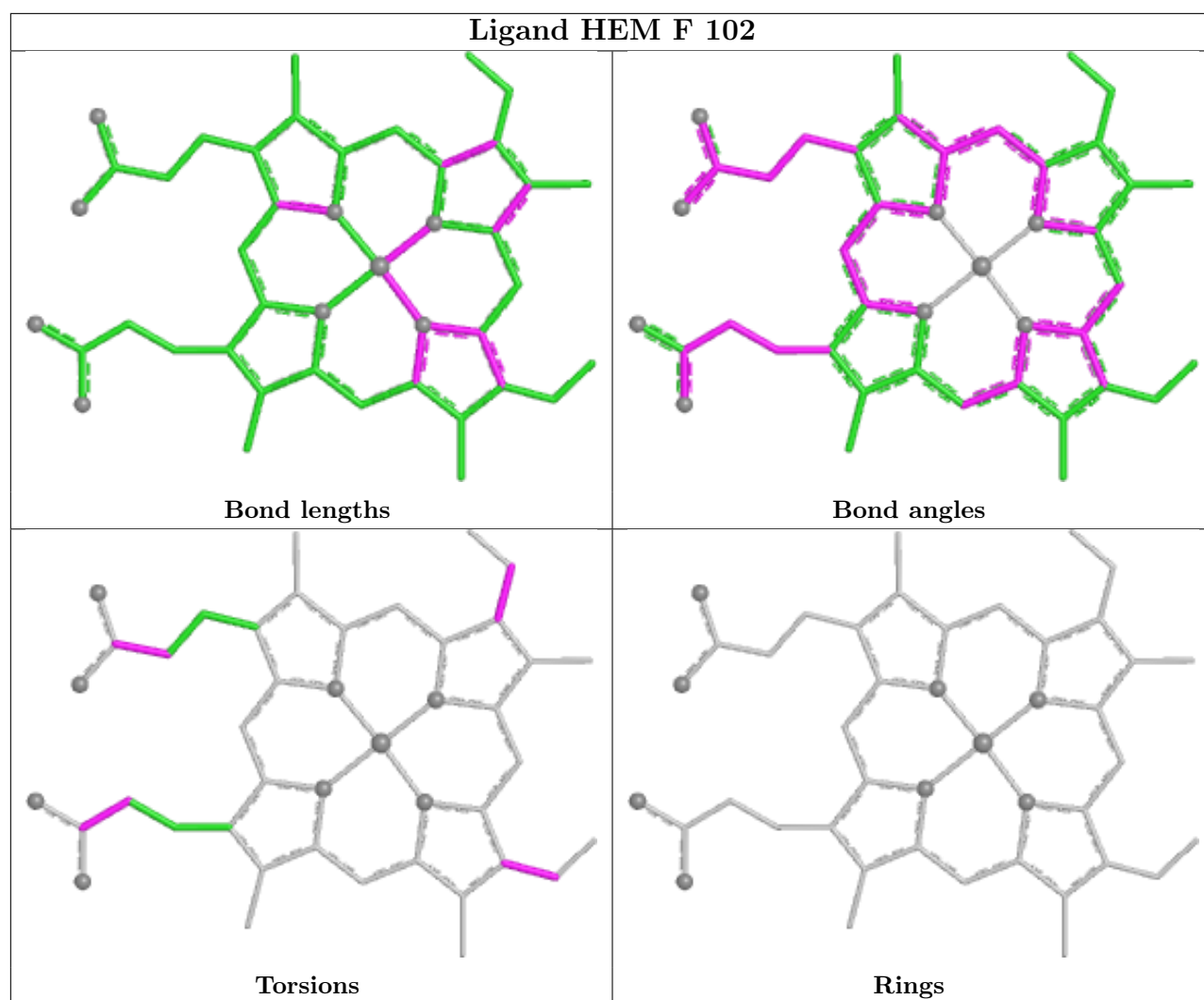
Ligand LHG L 101 (A)

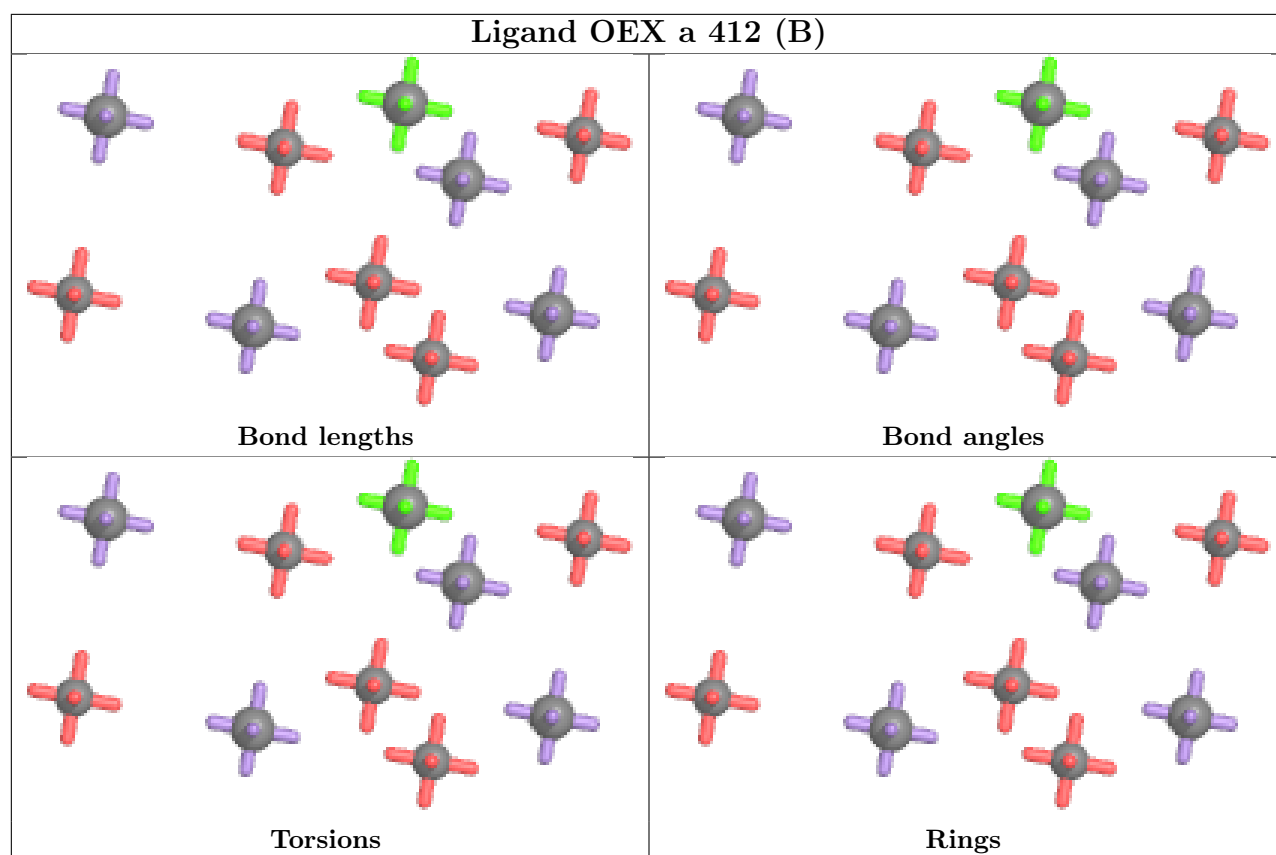


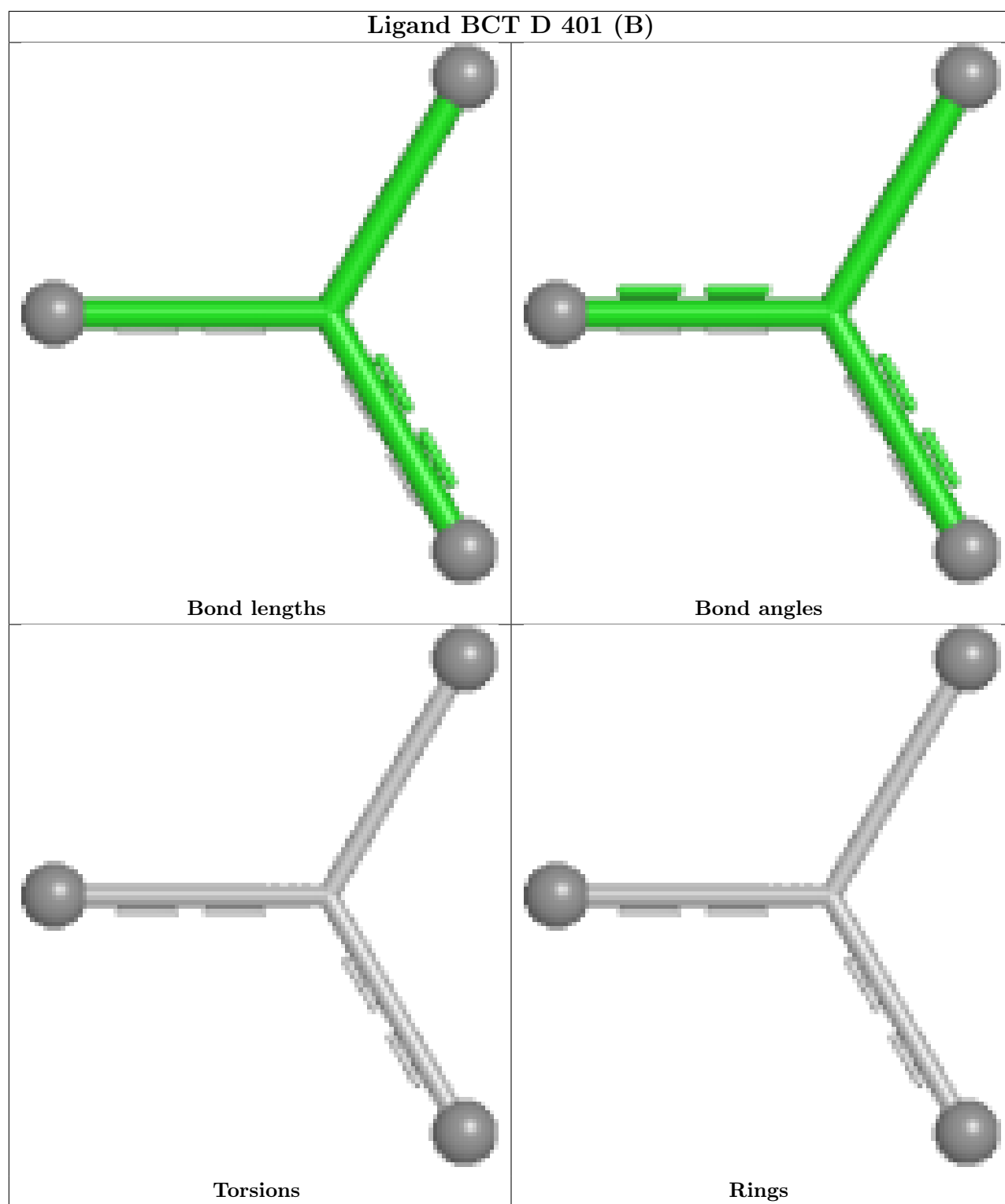
Ligand LMG c 520

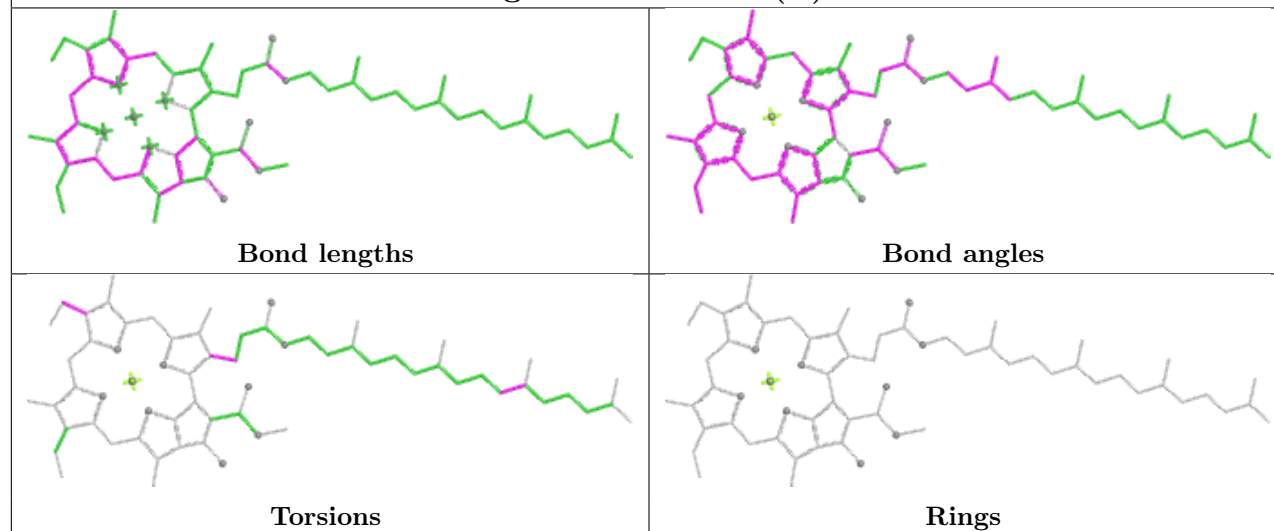
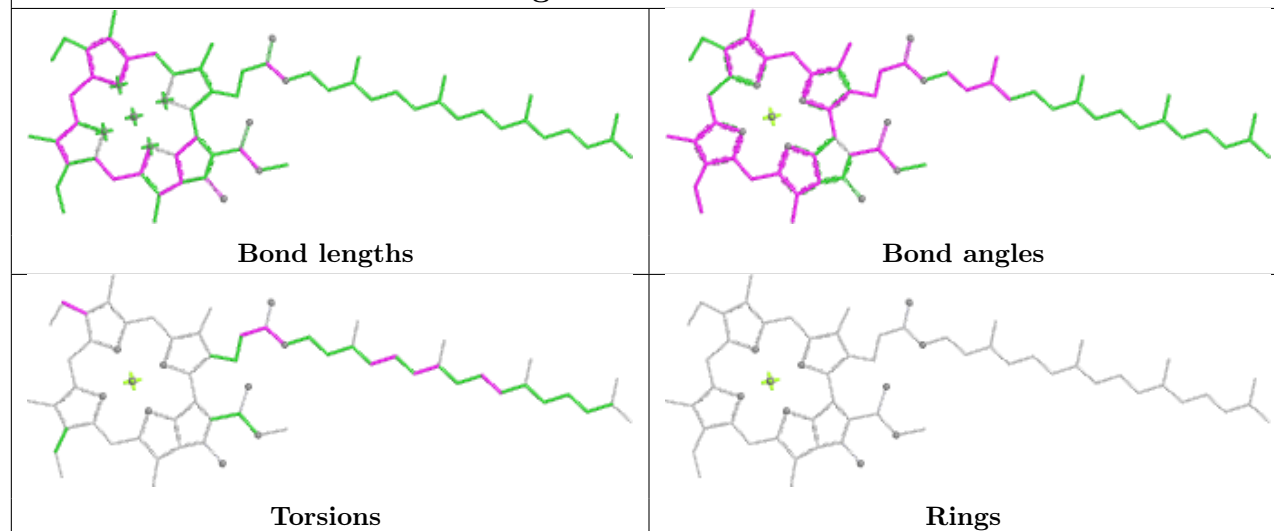




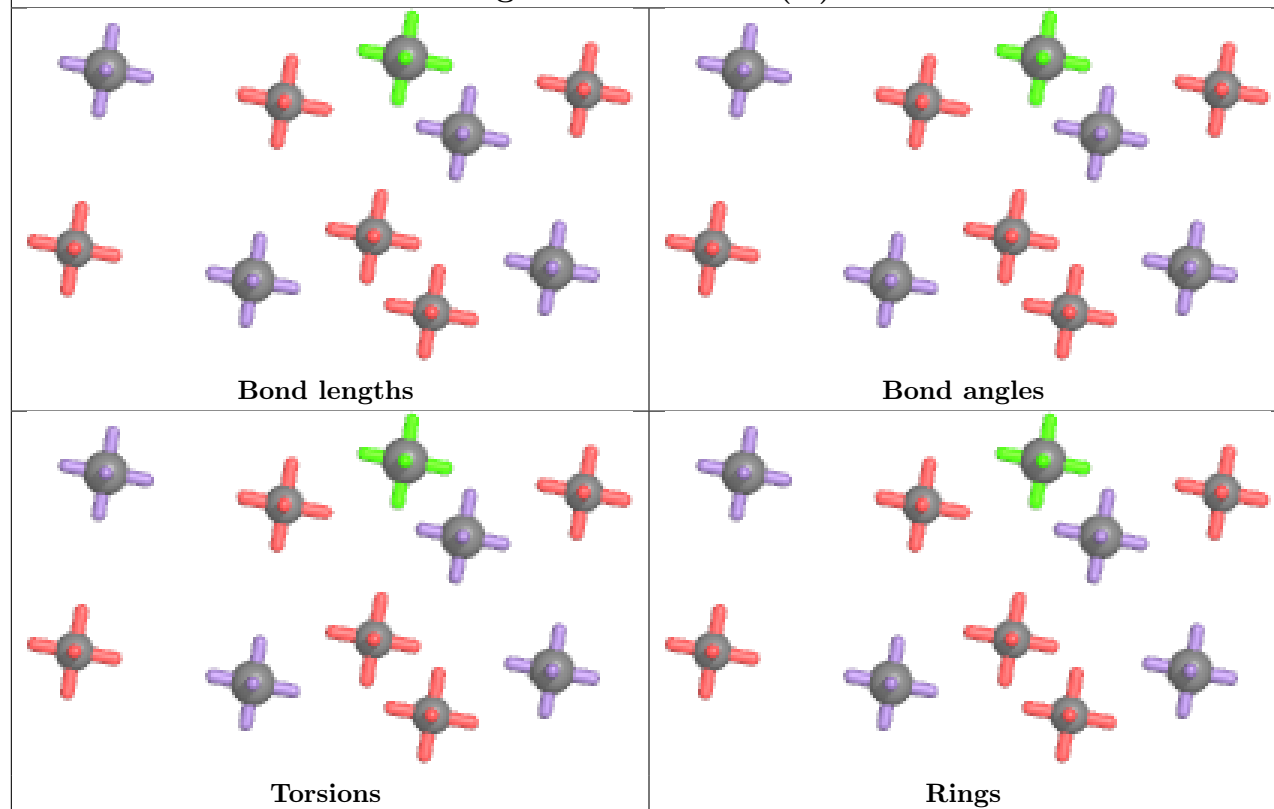




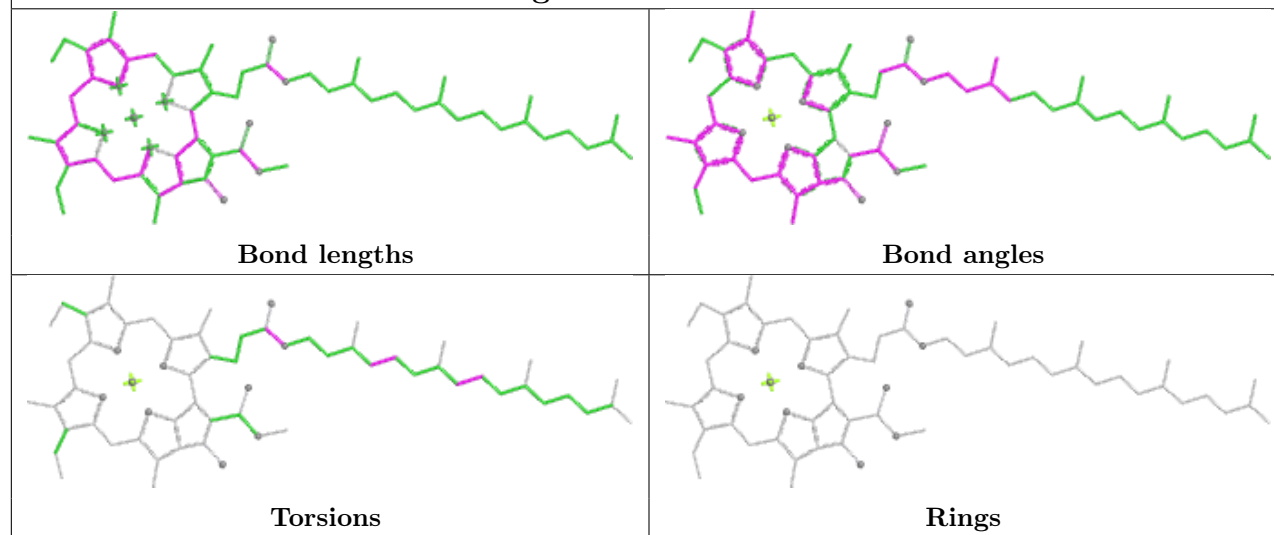


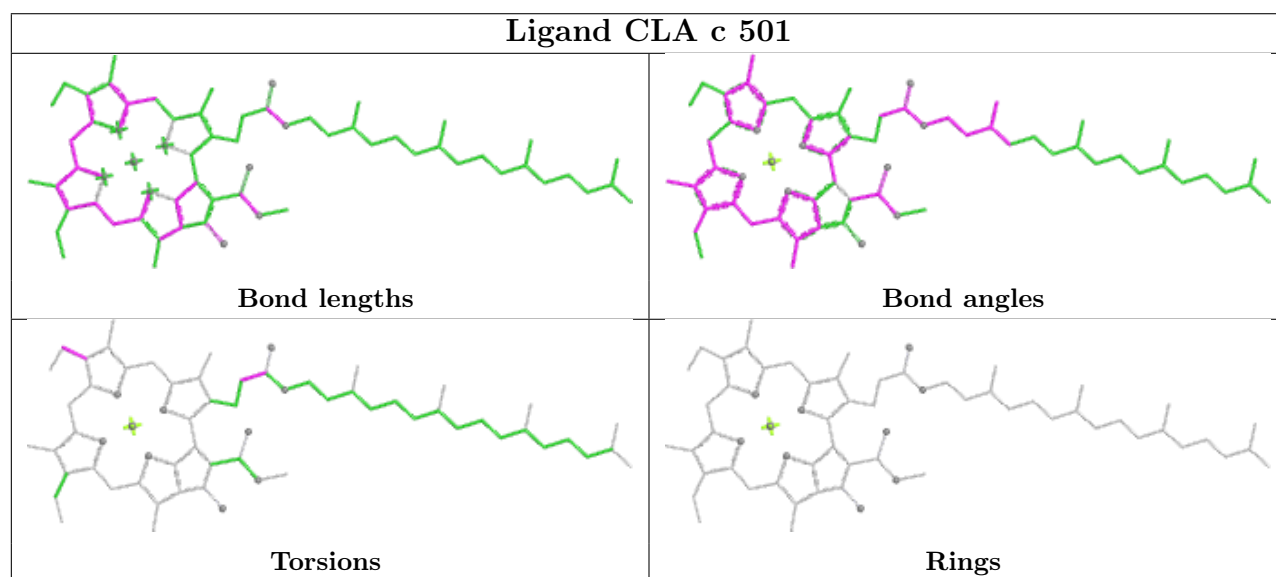
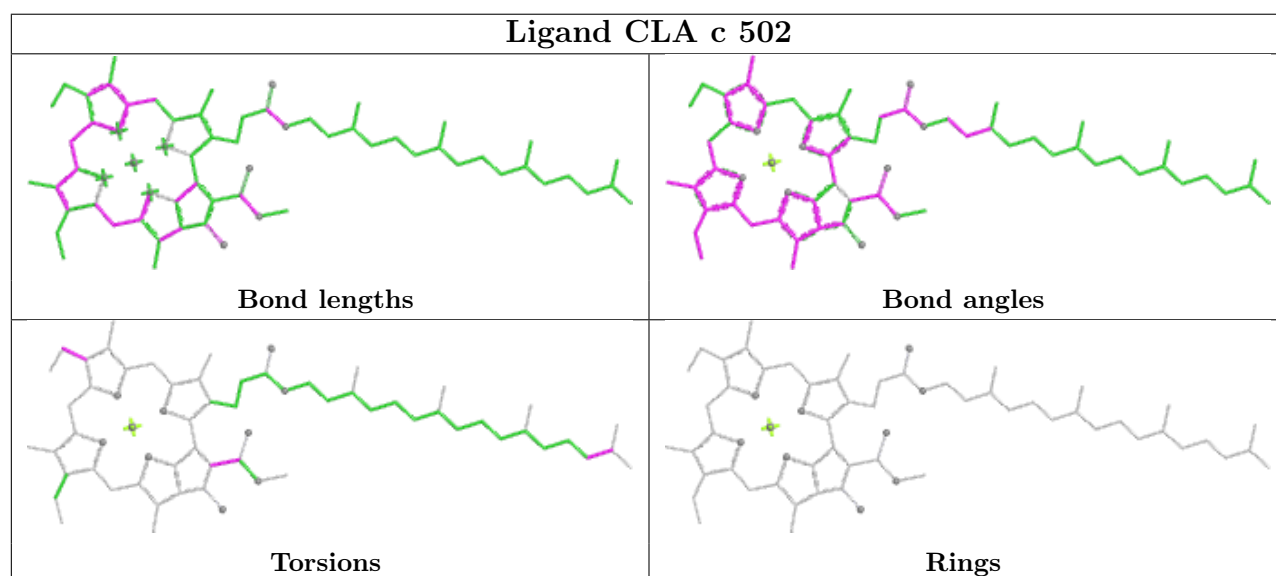
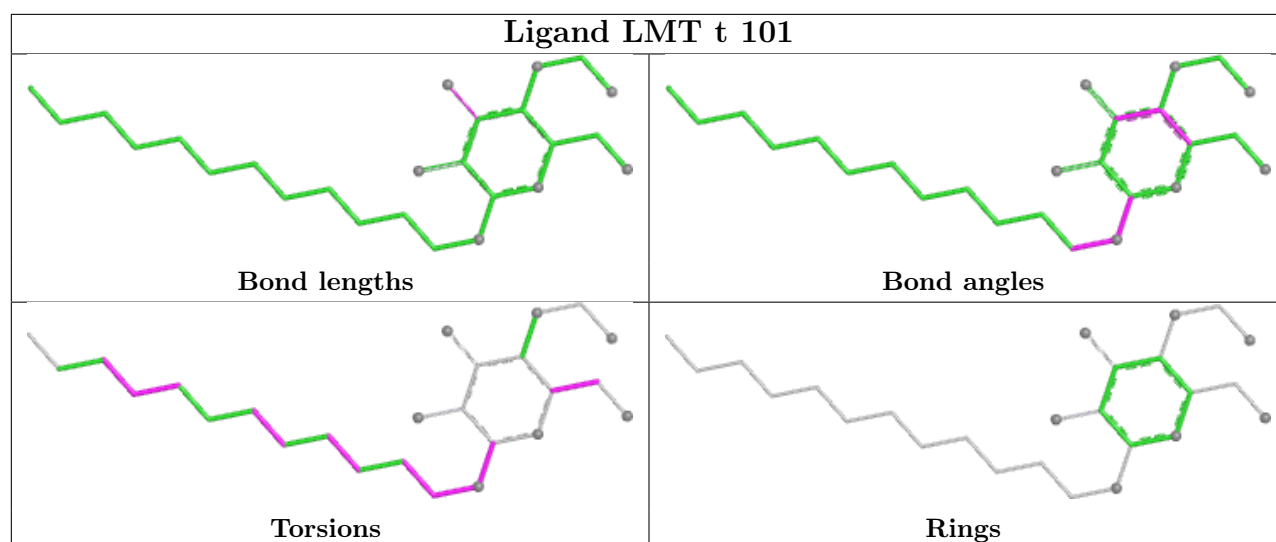
Ligand CLA a 406 (B)**Ligand CLA C 513**

Ligand OEX A 413 (A)

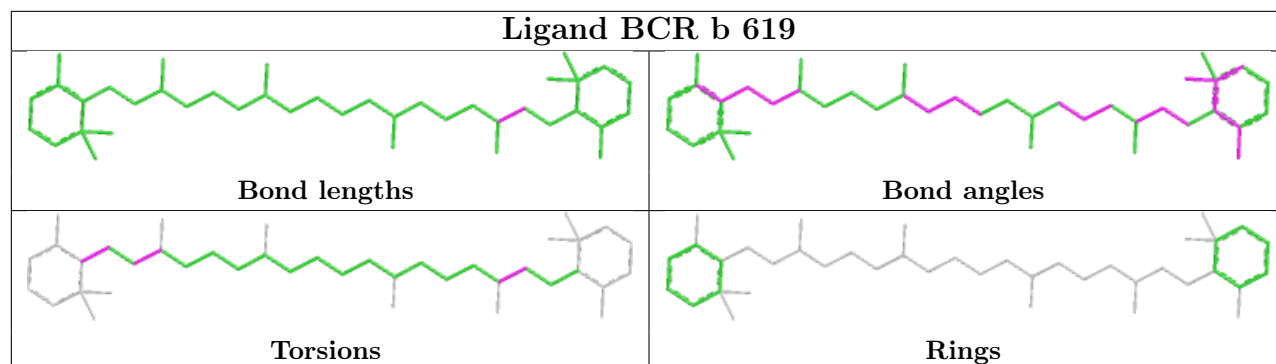


Ligand CLA C 512

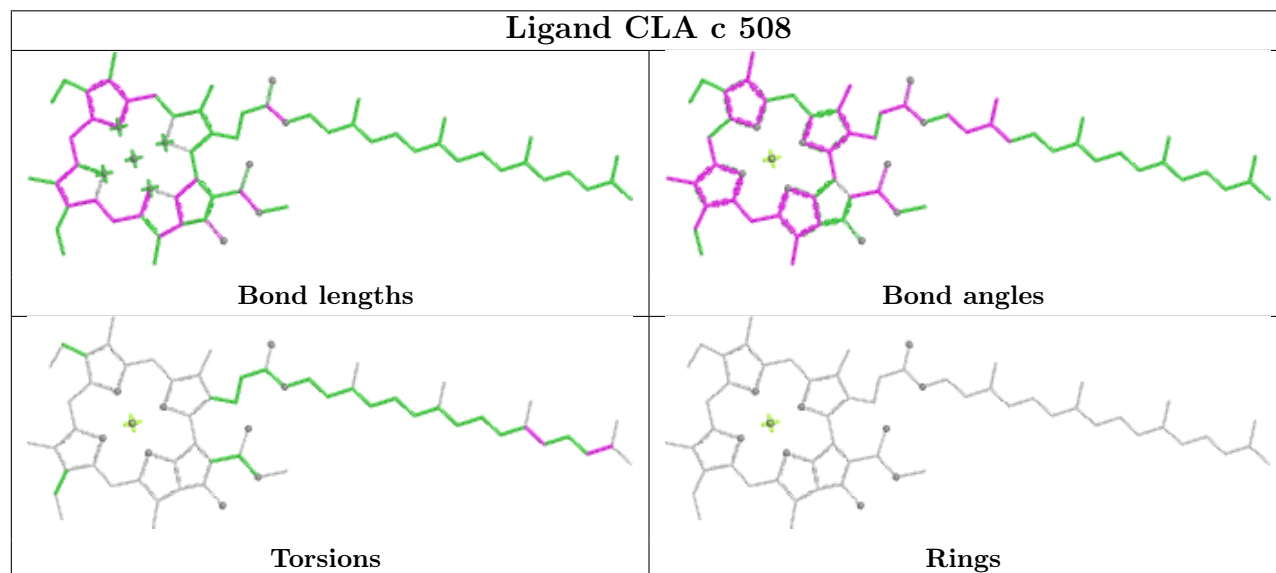




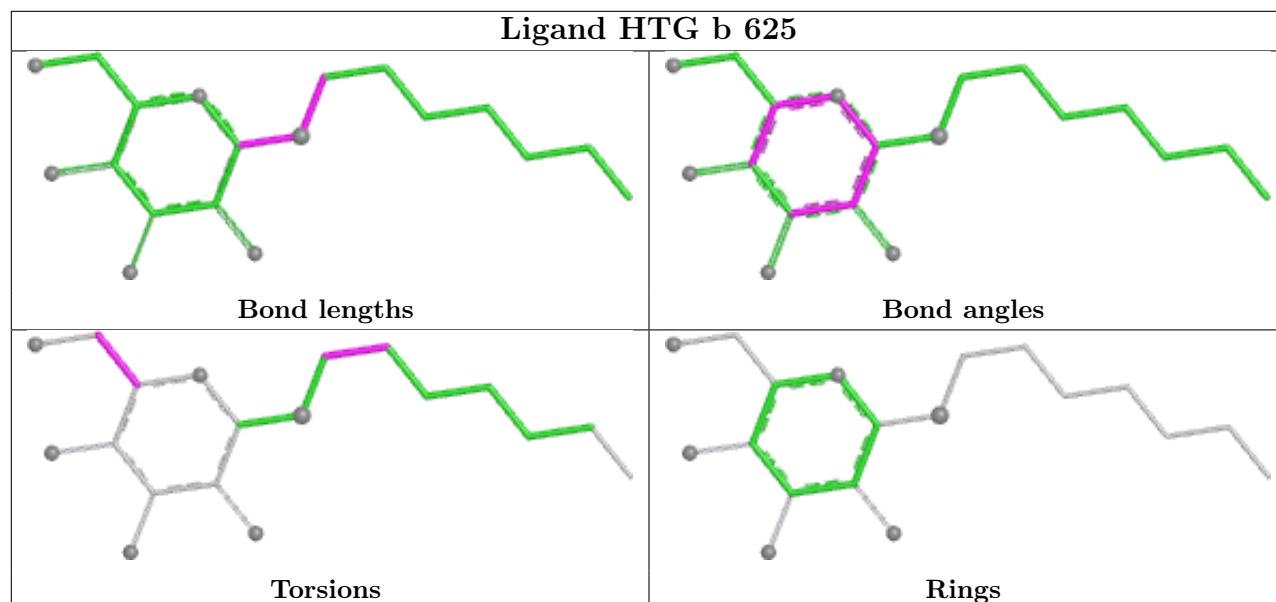
Ligand BCR b 619

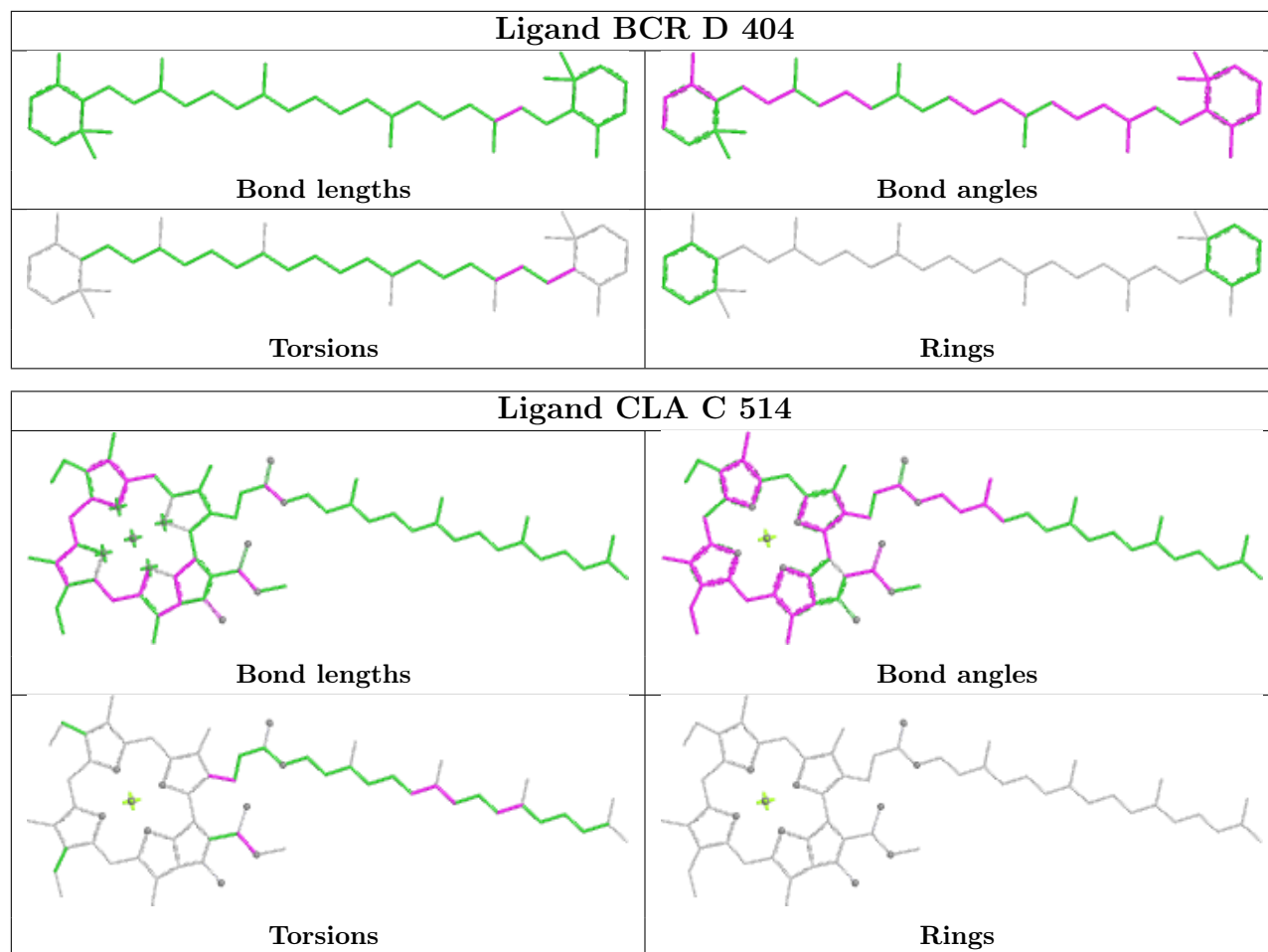


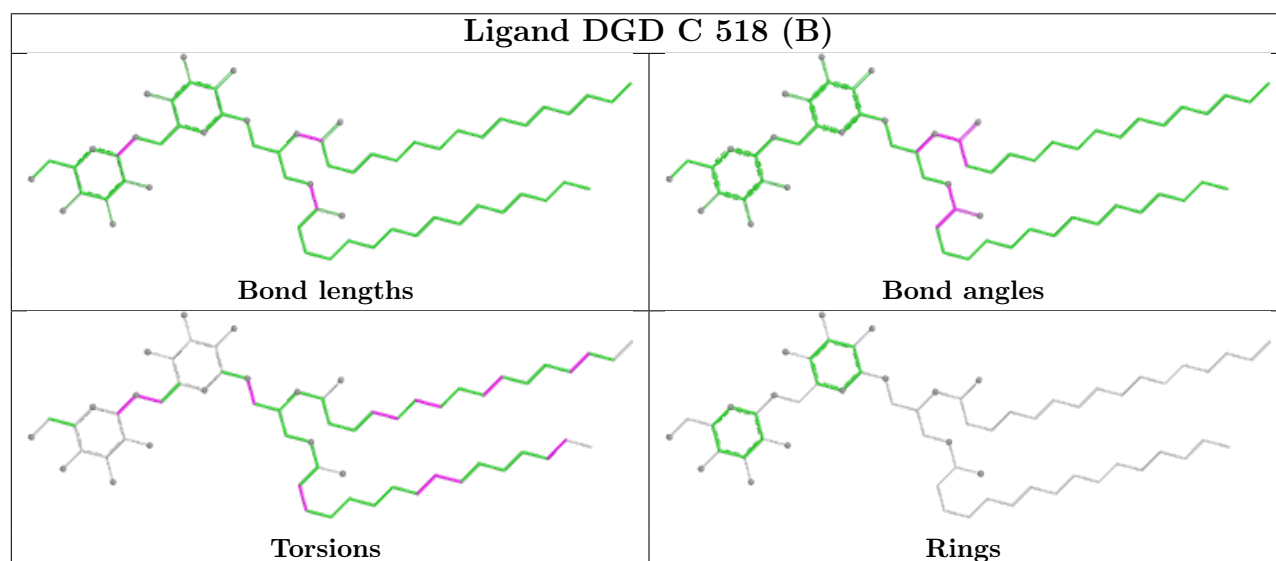
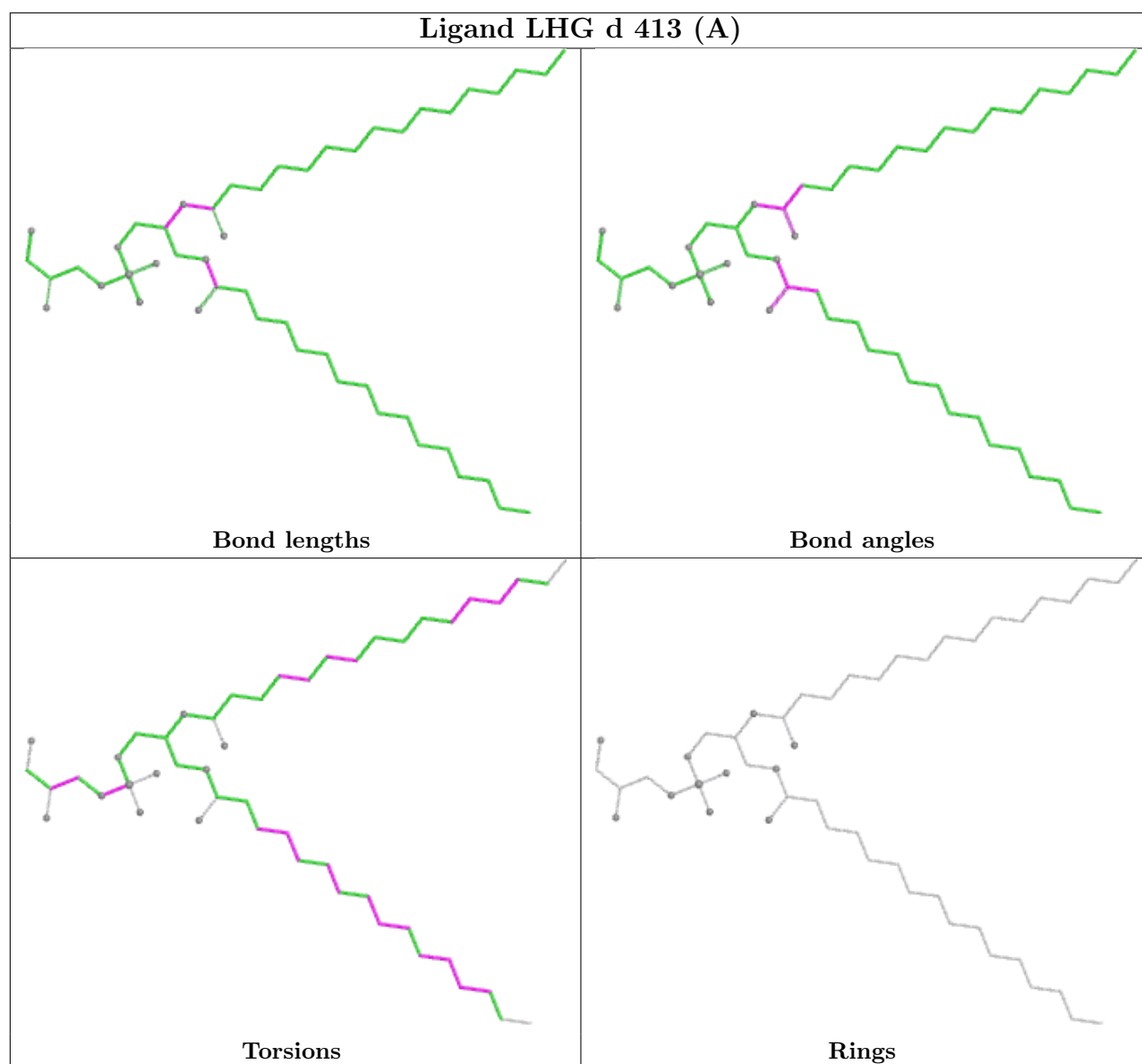
Ligand CLA c 508



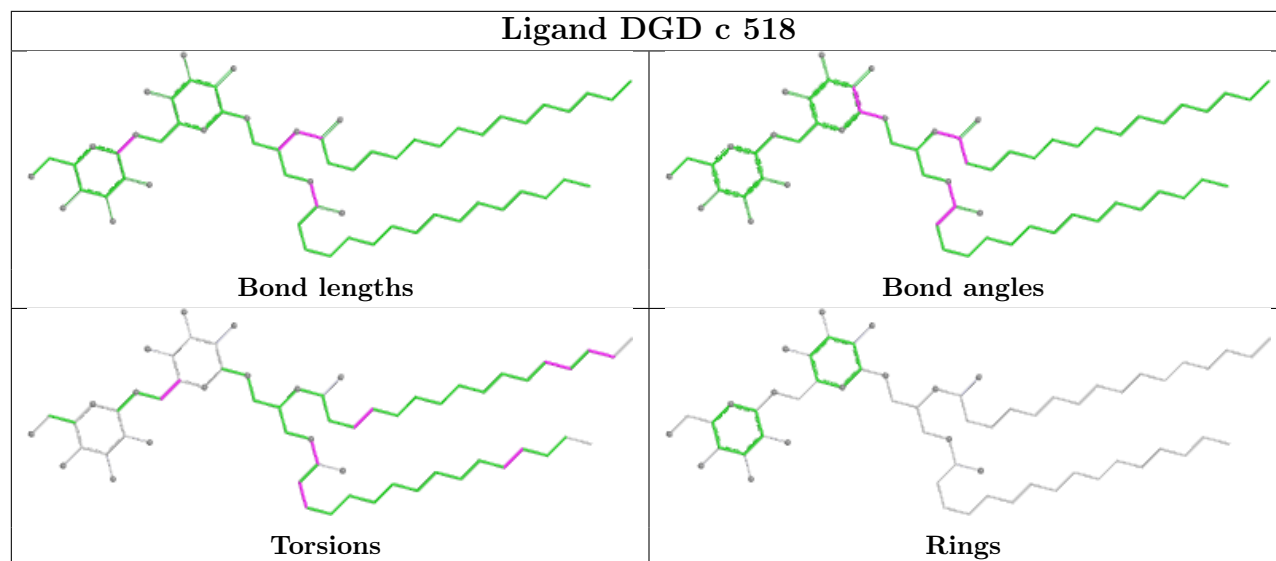
Ligand HTG b 625



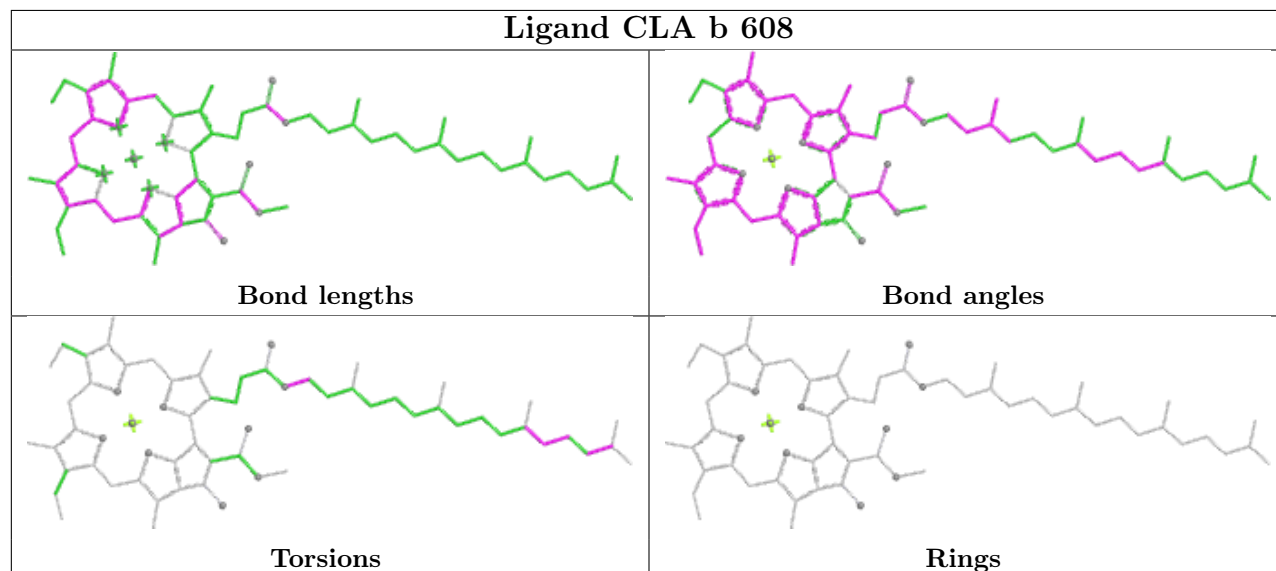




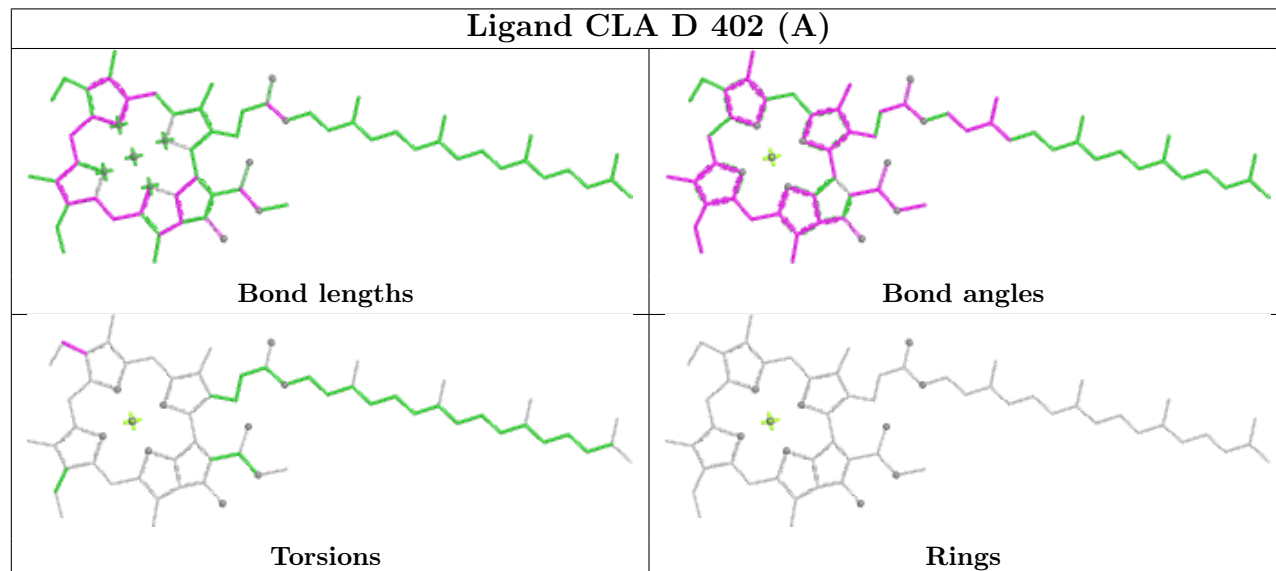
Ligand DGD c 518

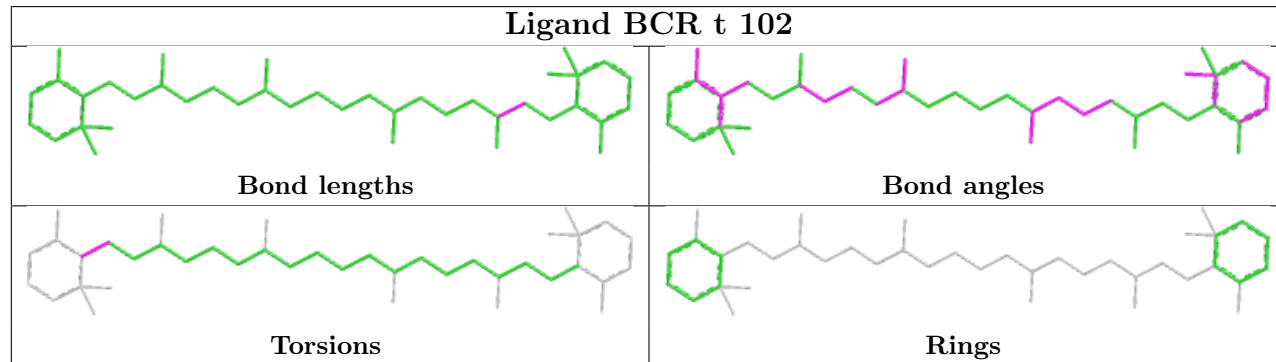
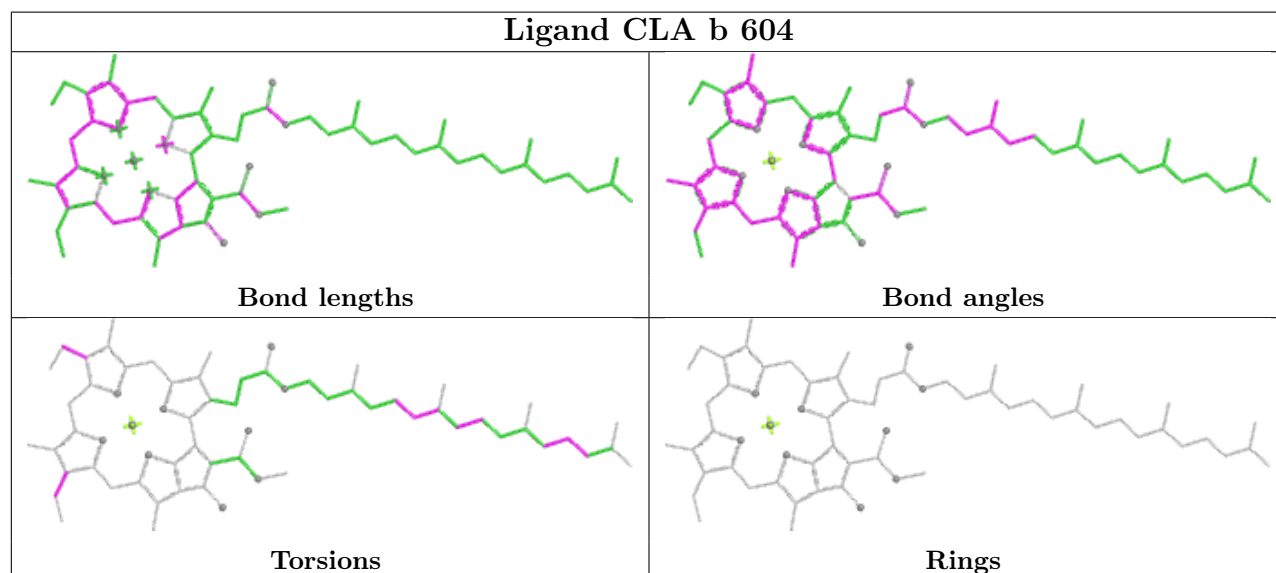
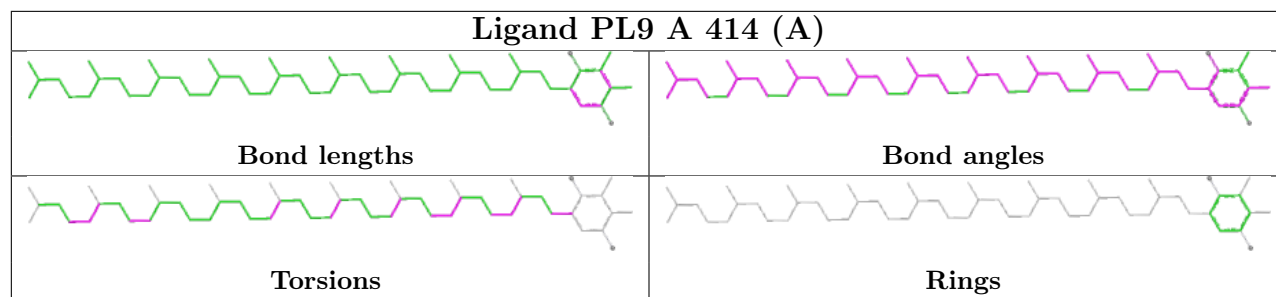


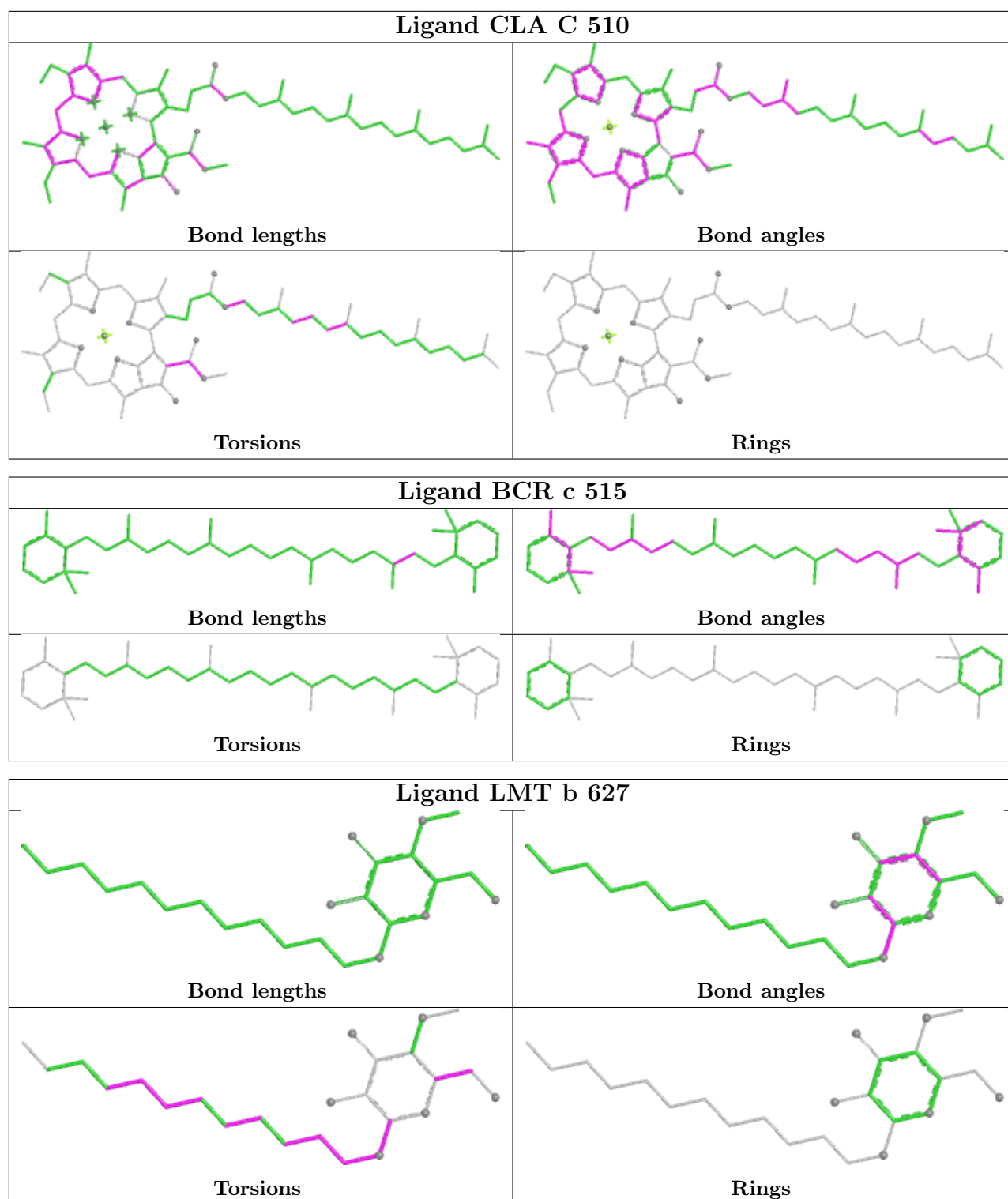
Ligand CLA b 608

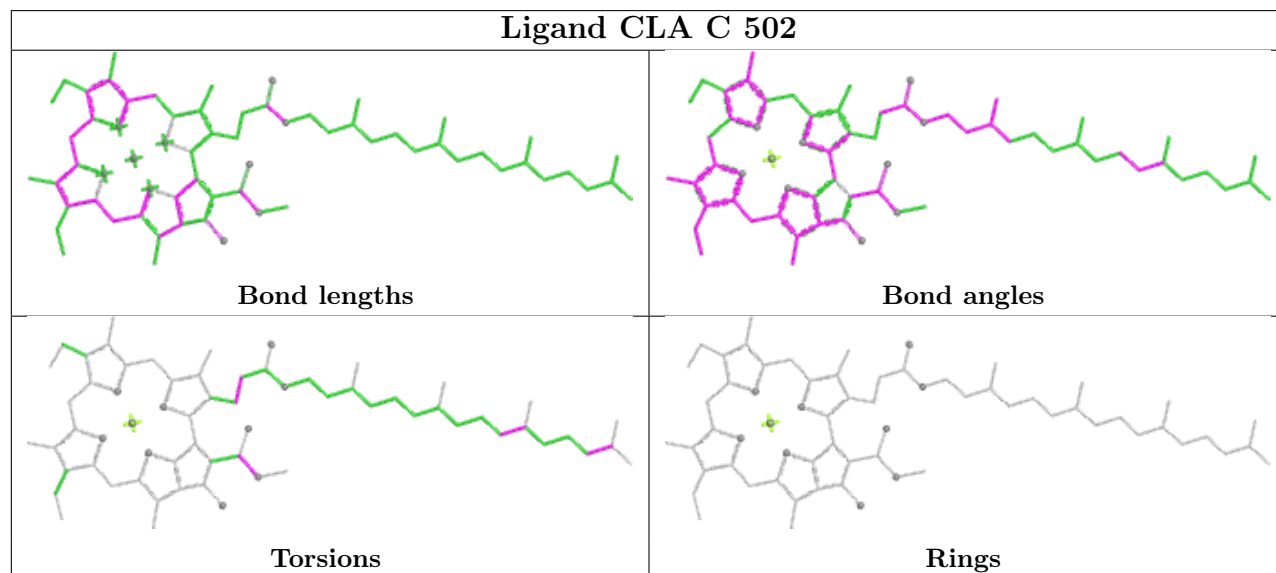
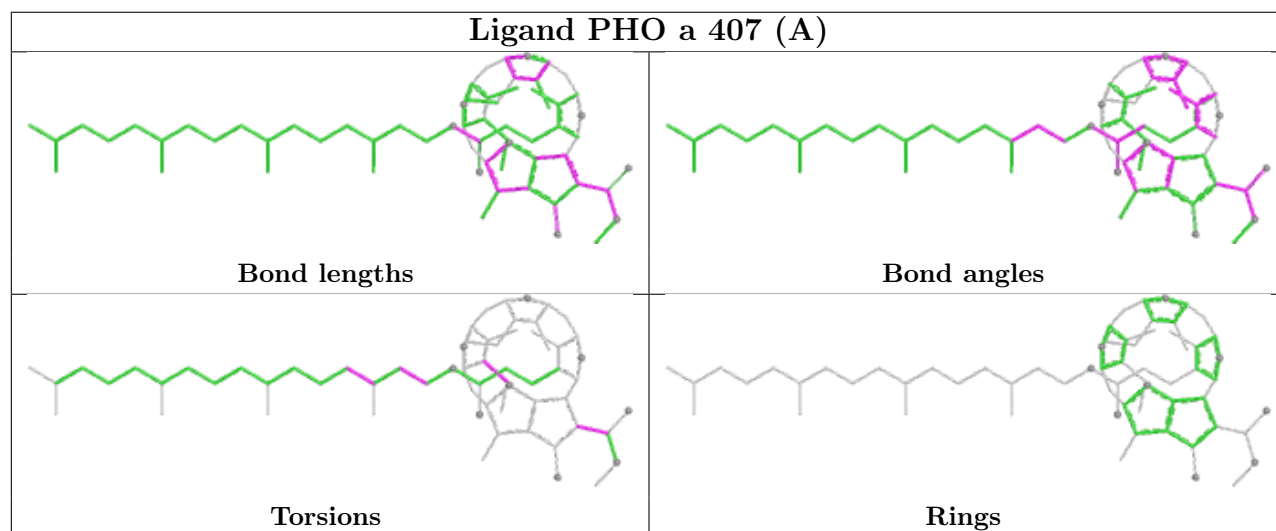
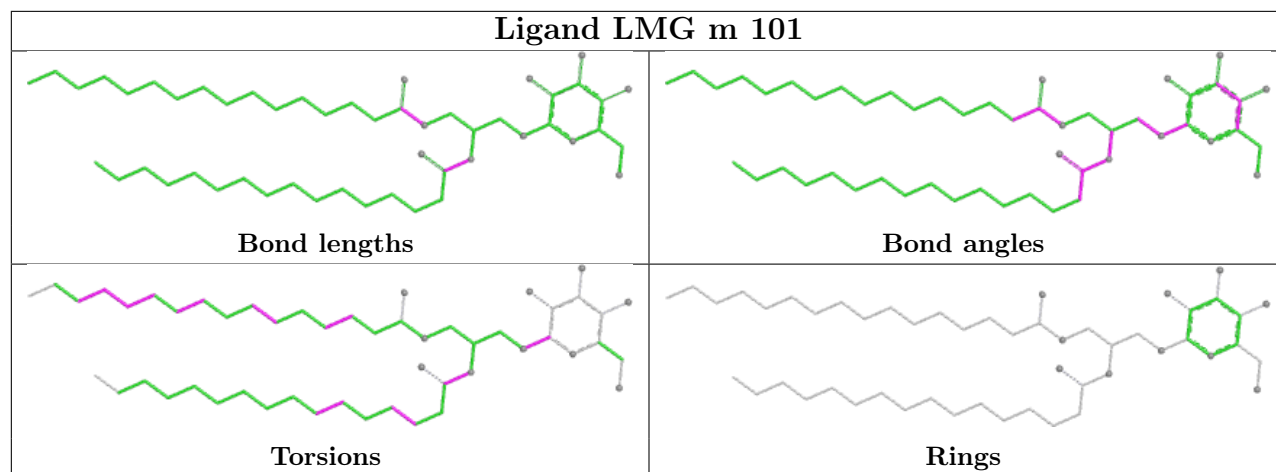


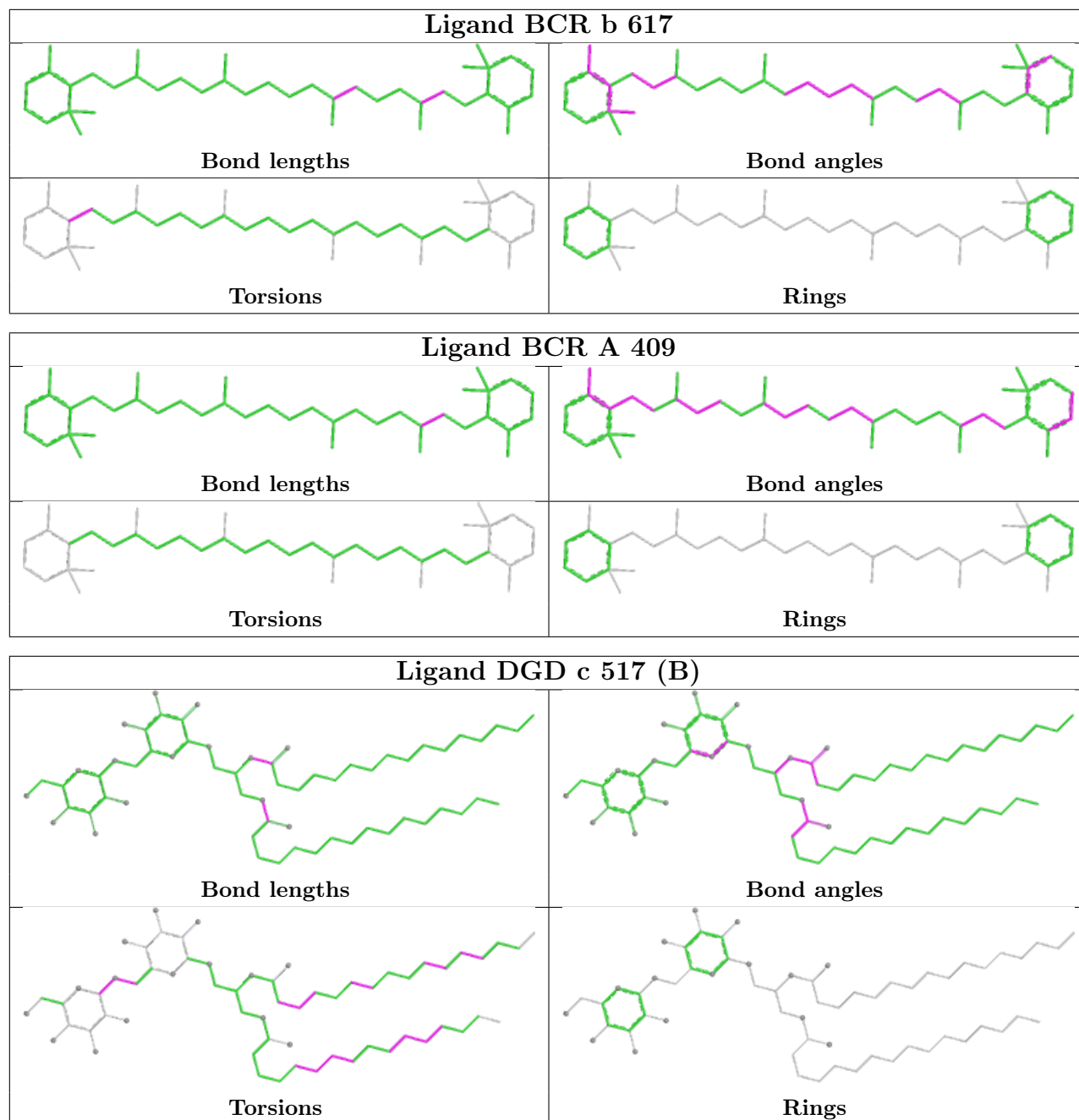
Ligand CLA D 402 (A)



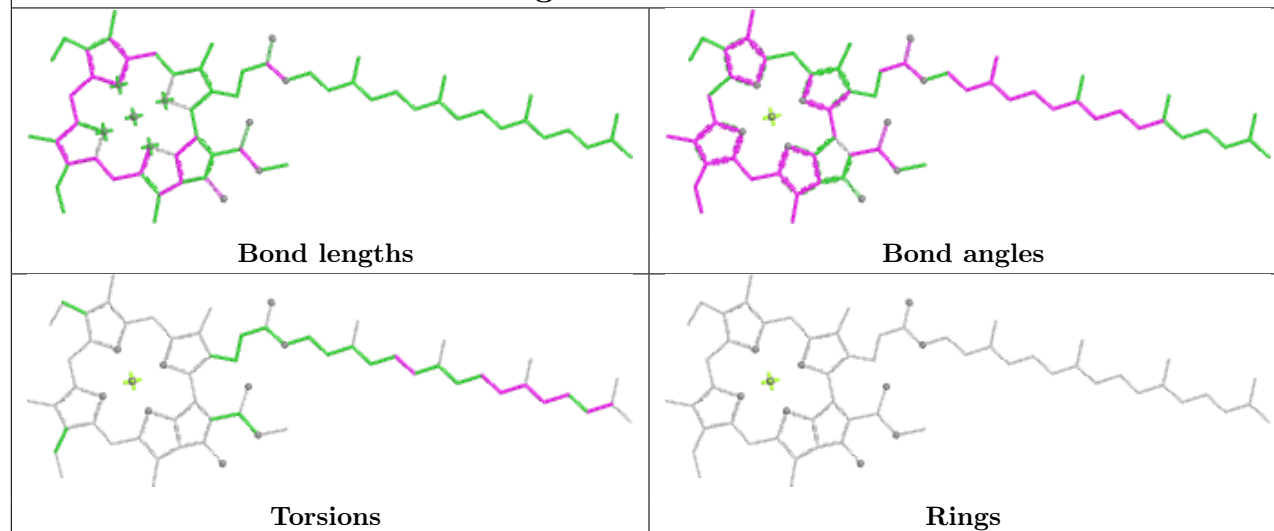




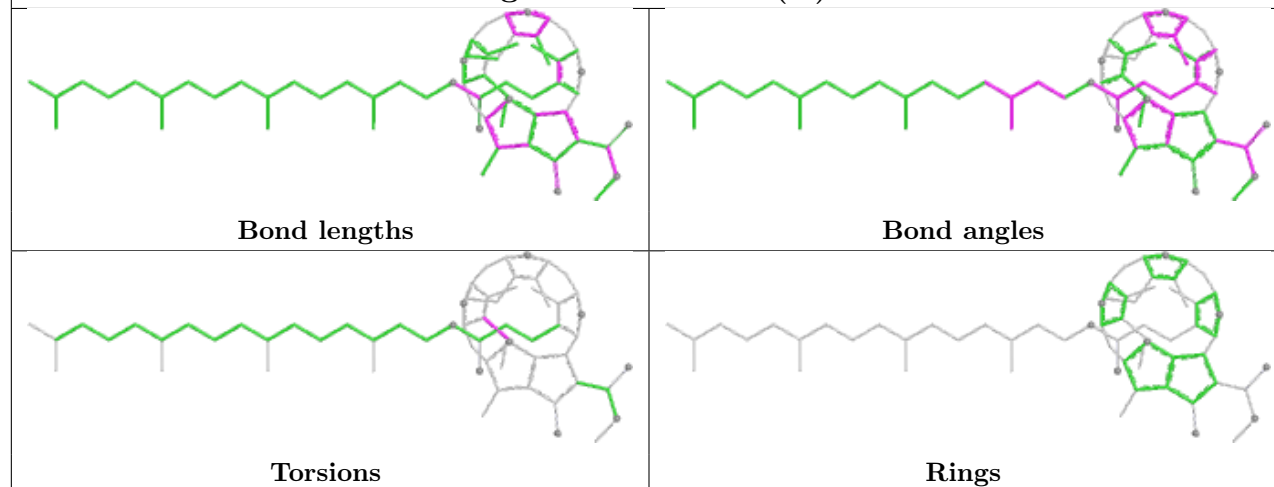




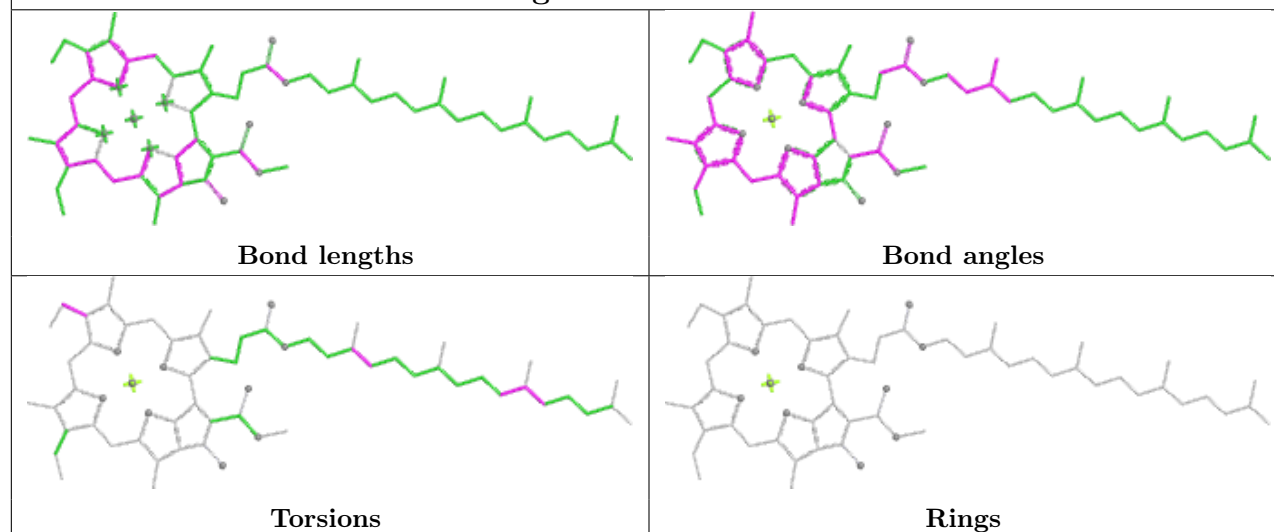
Ligand CLA b 615

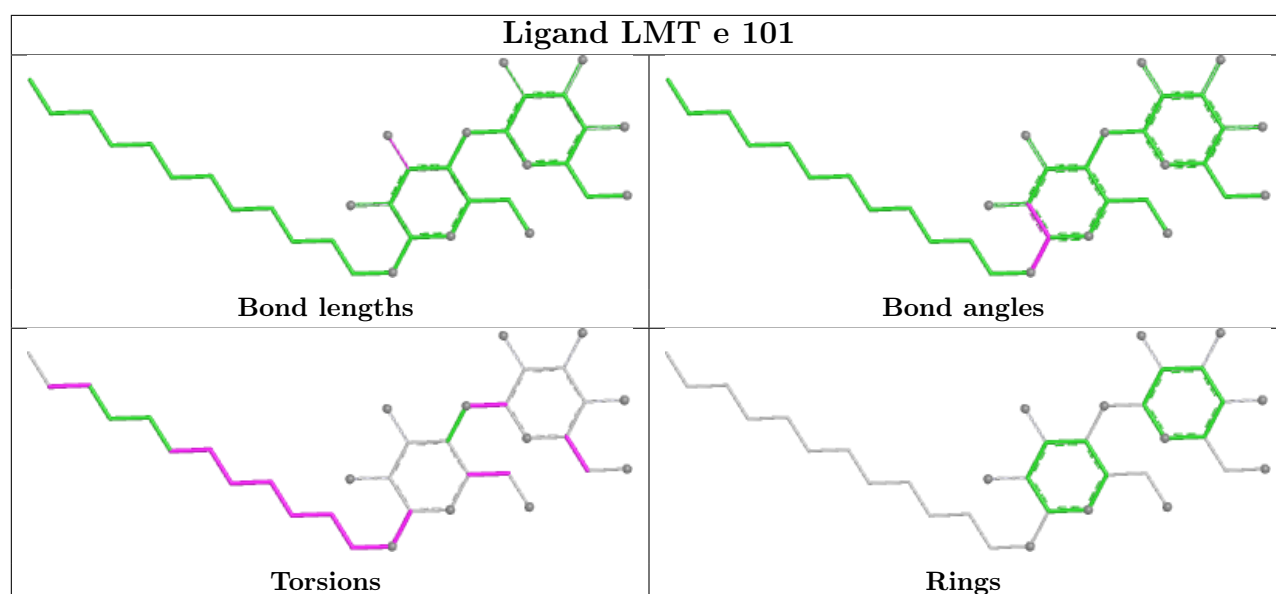
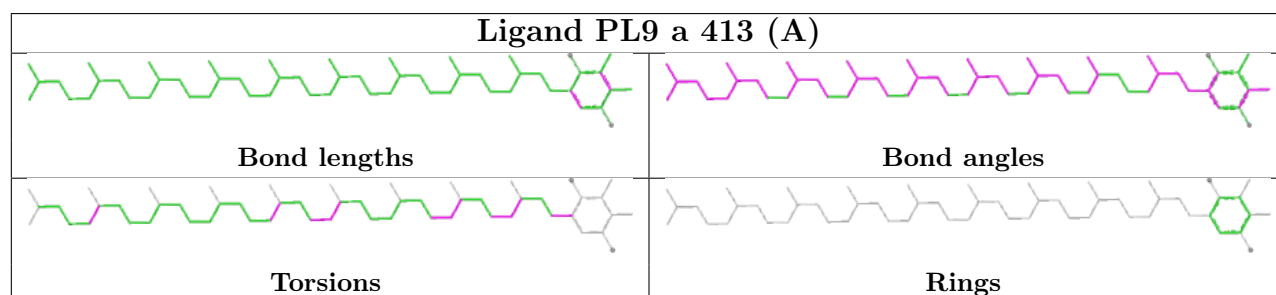
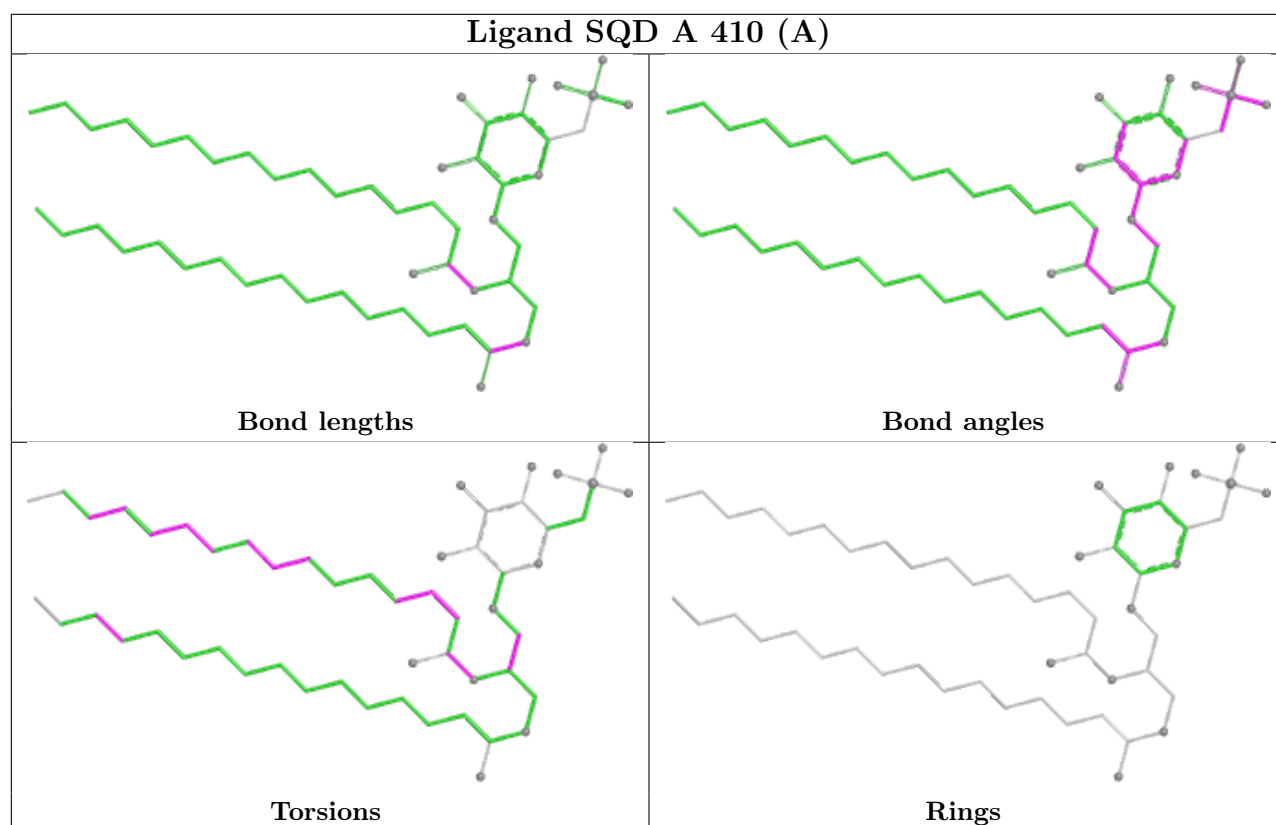


Ligand PHO a 415 (A)

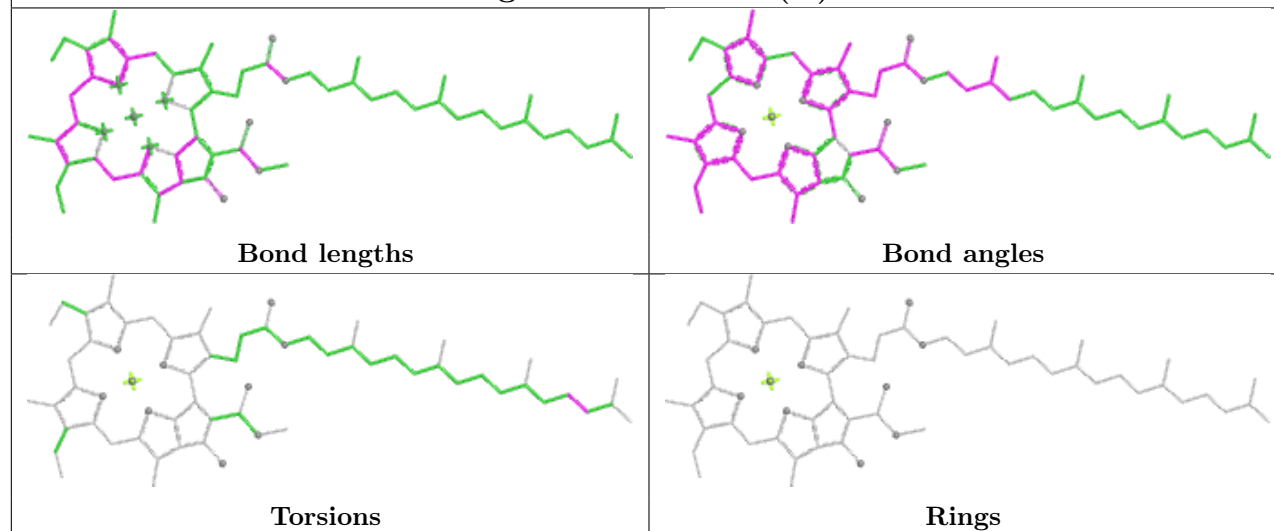


Ligand CLA C 506

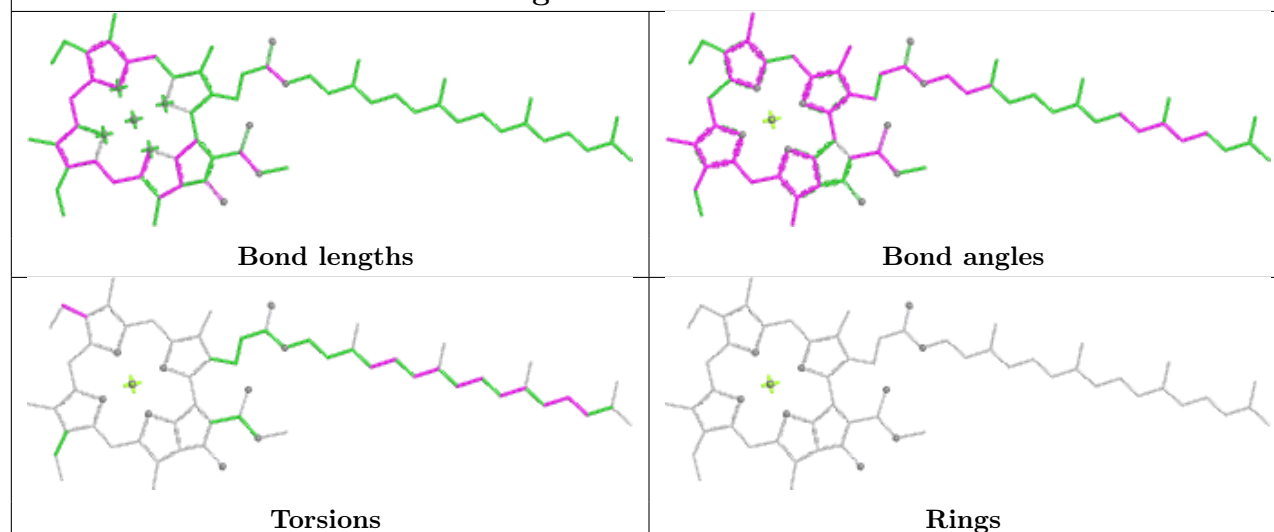




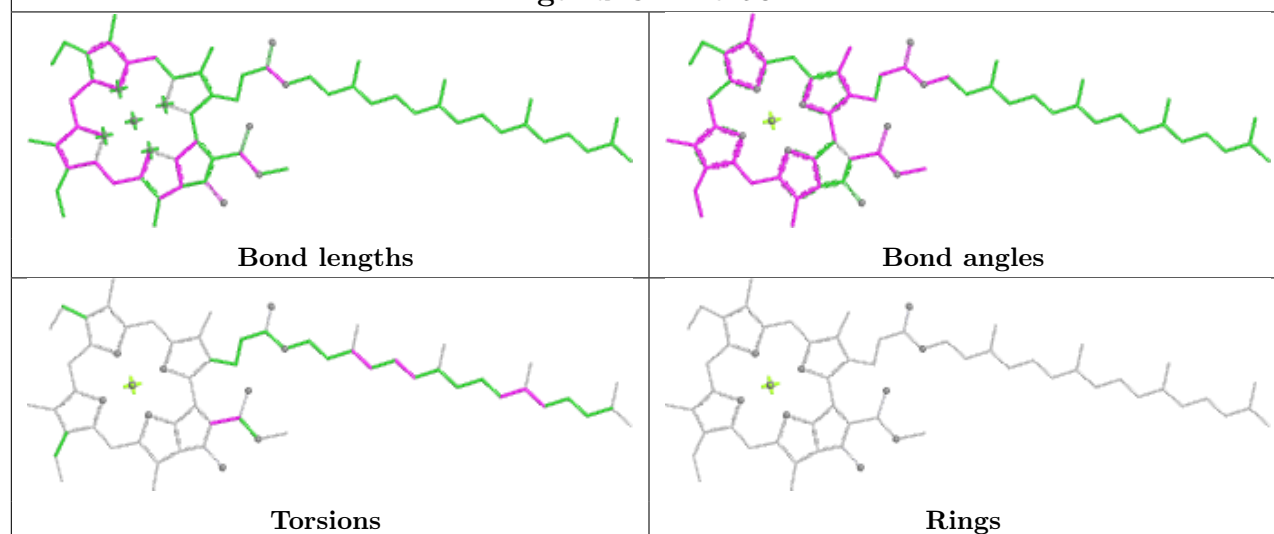
Ligand CLA A 405 (A)

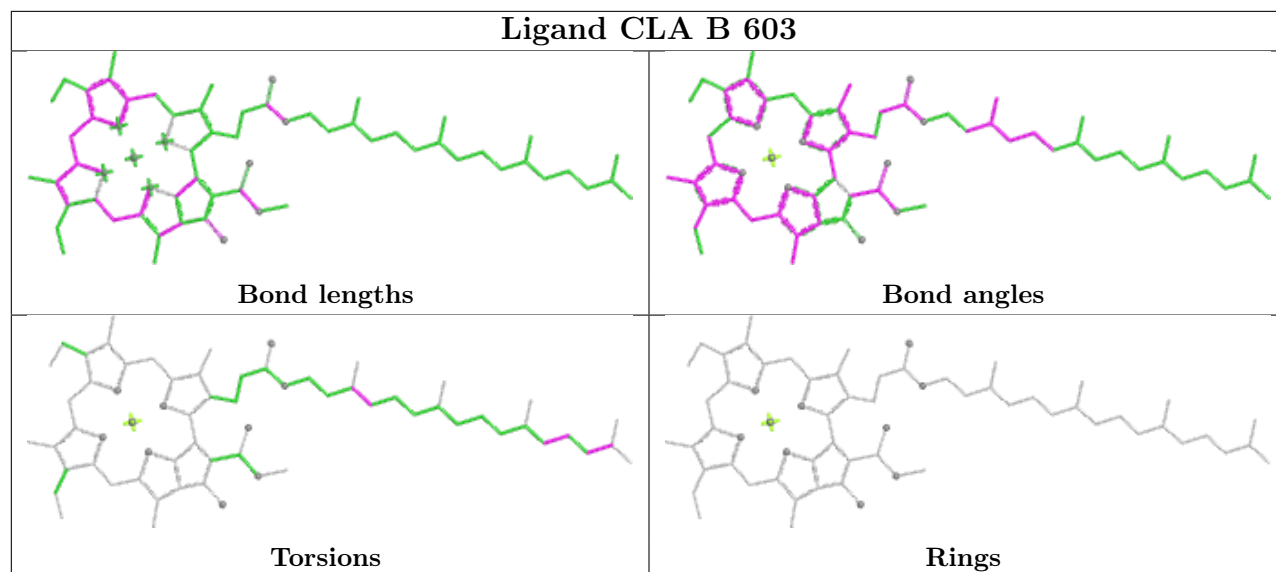
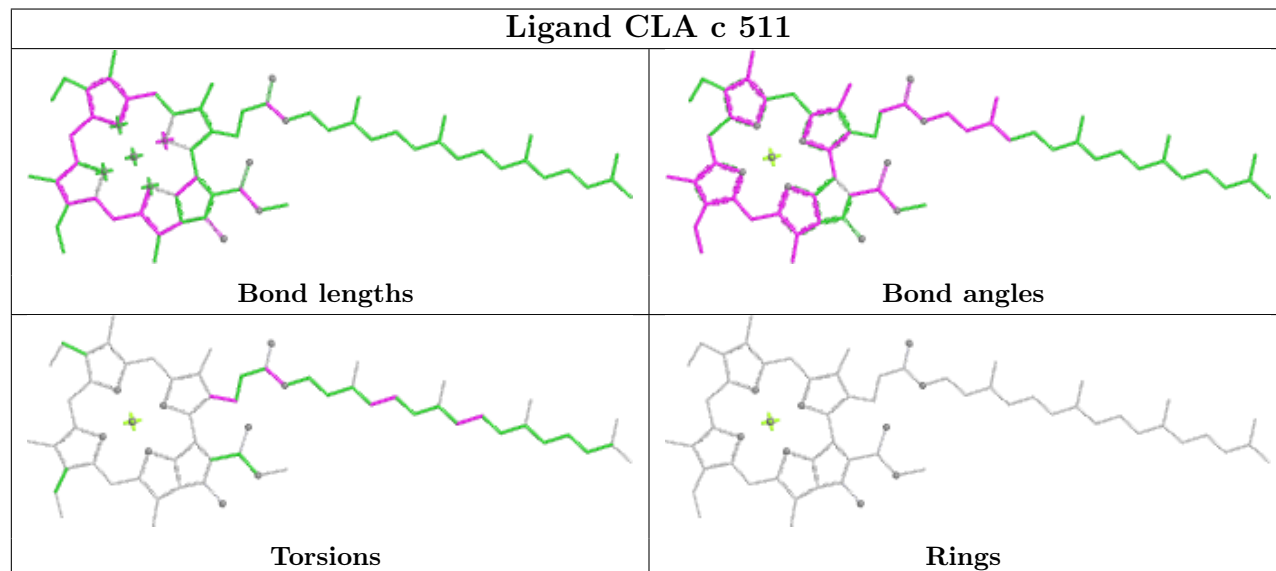
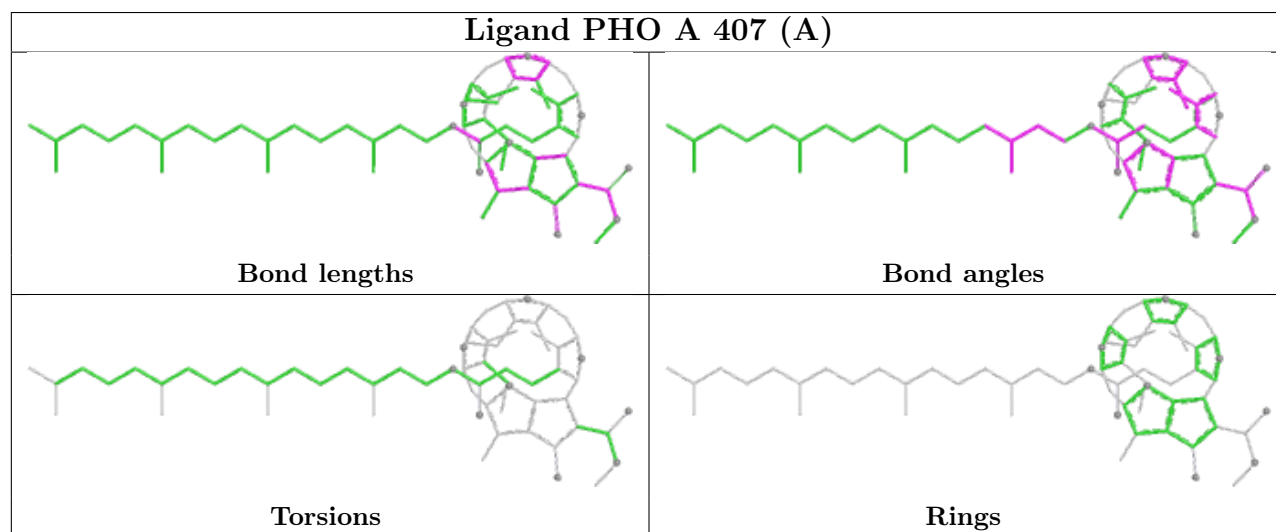


Ligand CLA B 602

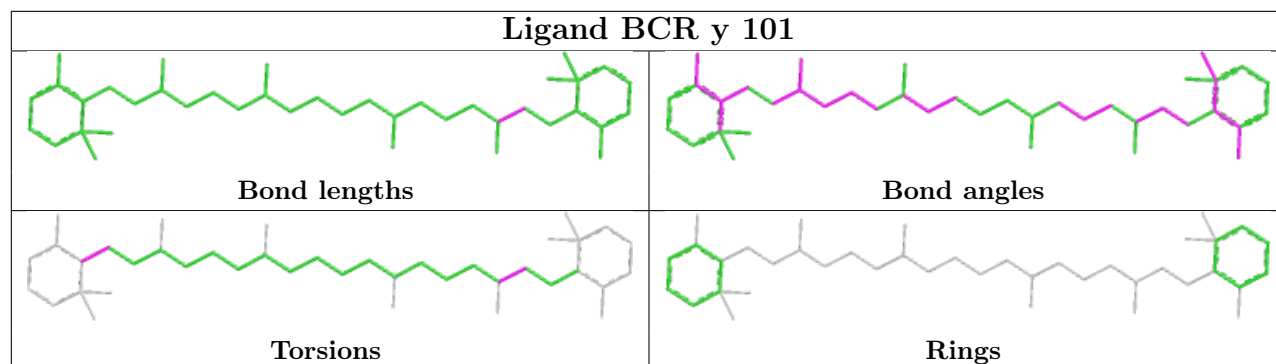


Ligand CLA c 504

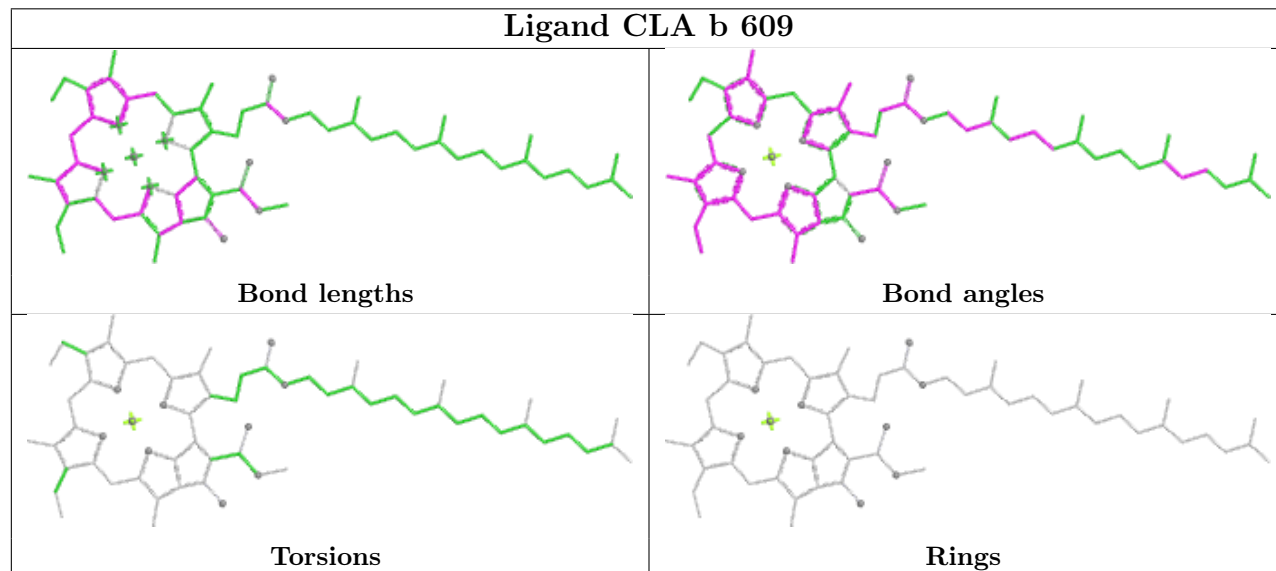


Ligand CLA B 603**Ligand CLA c 511****Ligand PHO A 407 (A)**

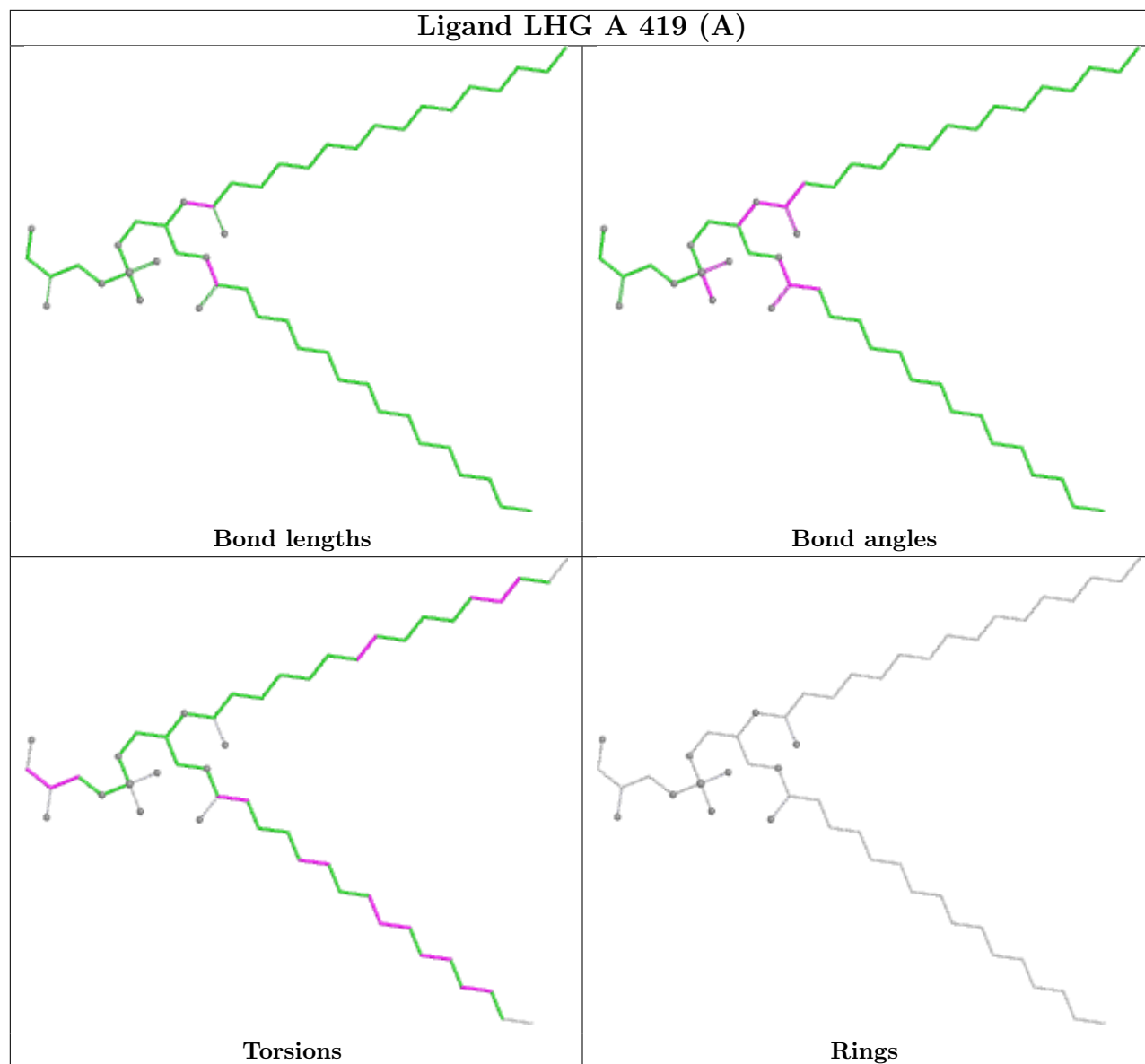
Ligand BCR y 101



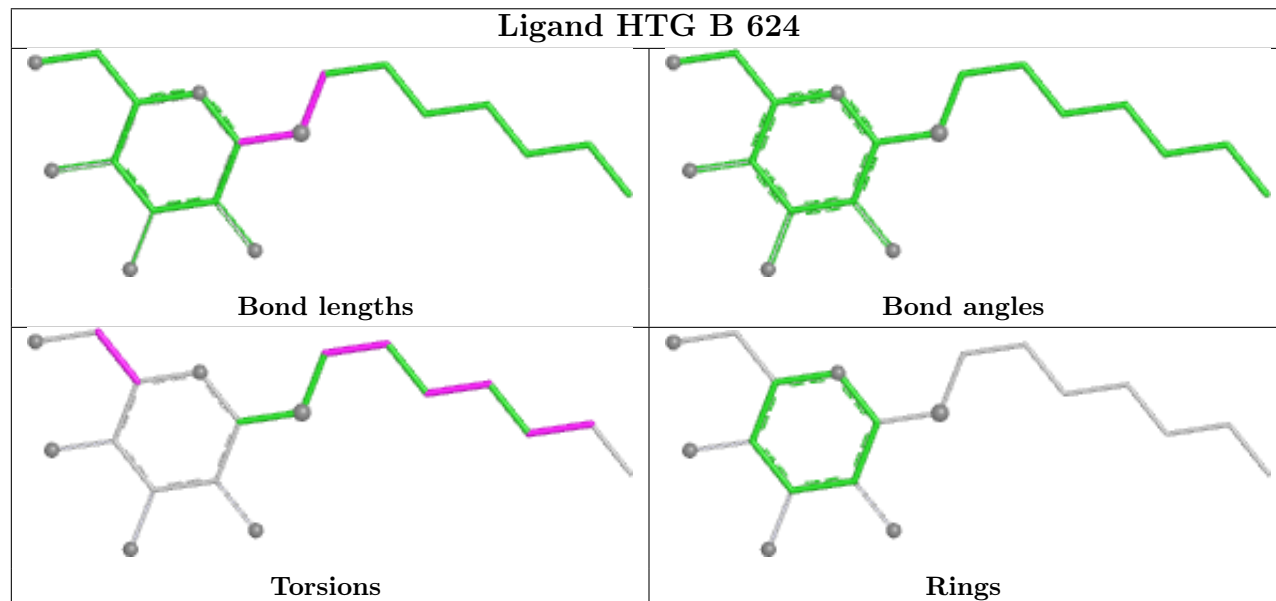
Ligand CLA b 609

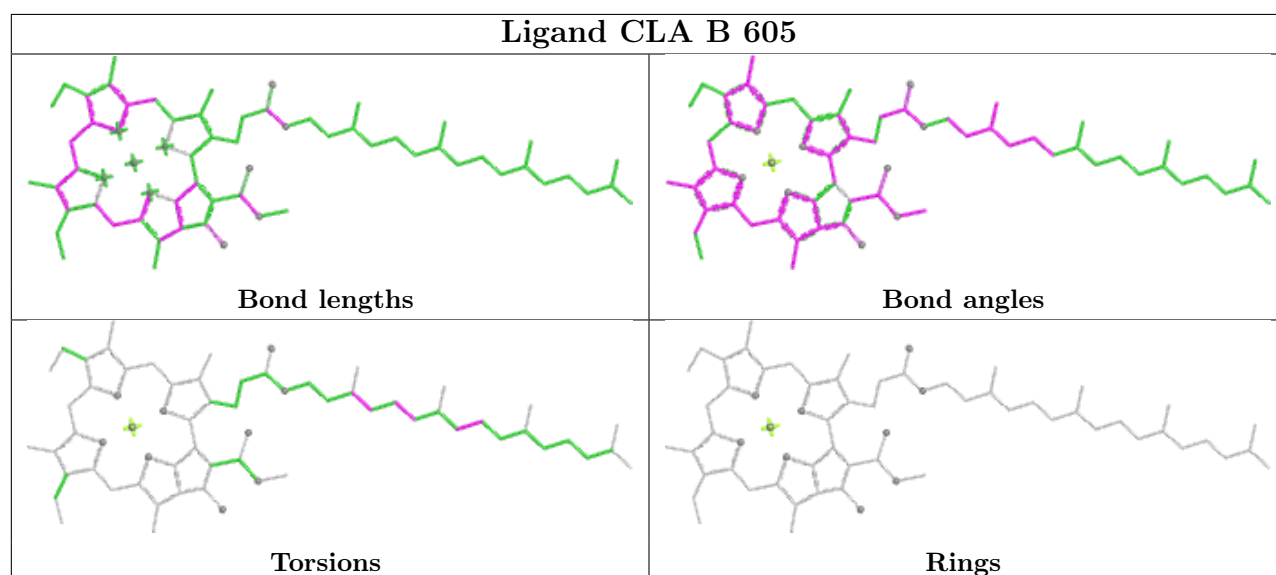
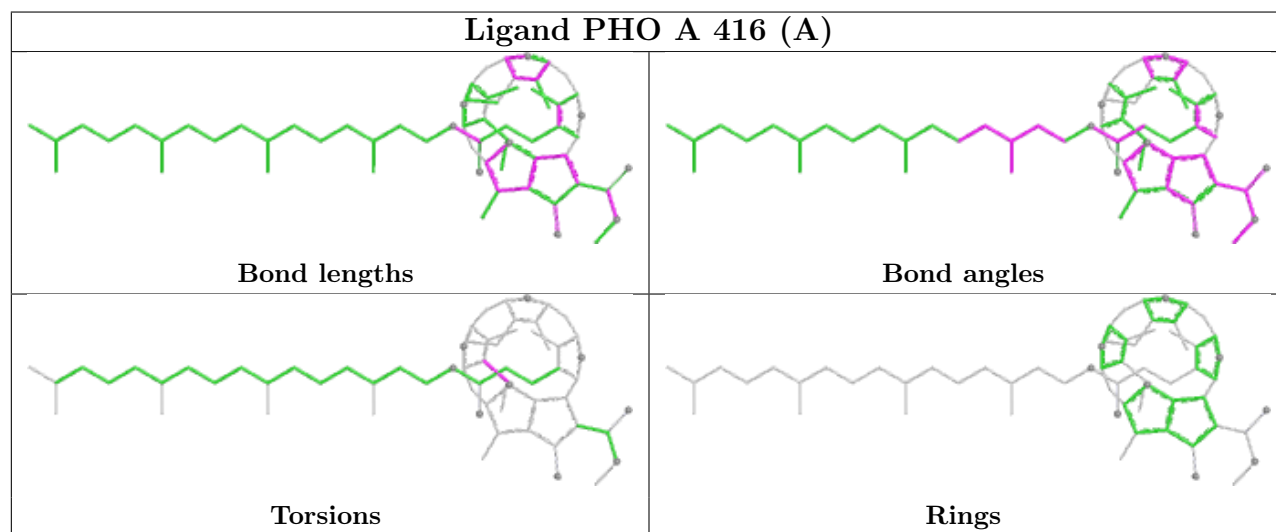
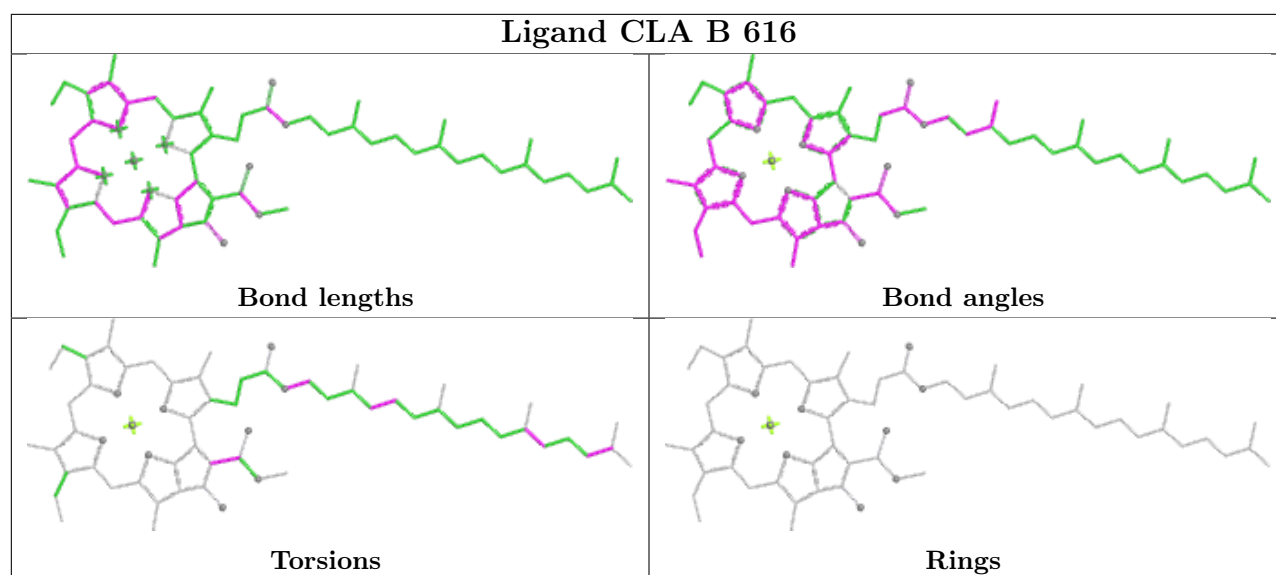


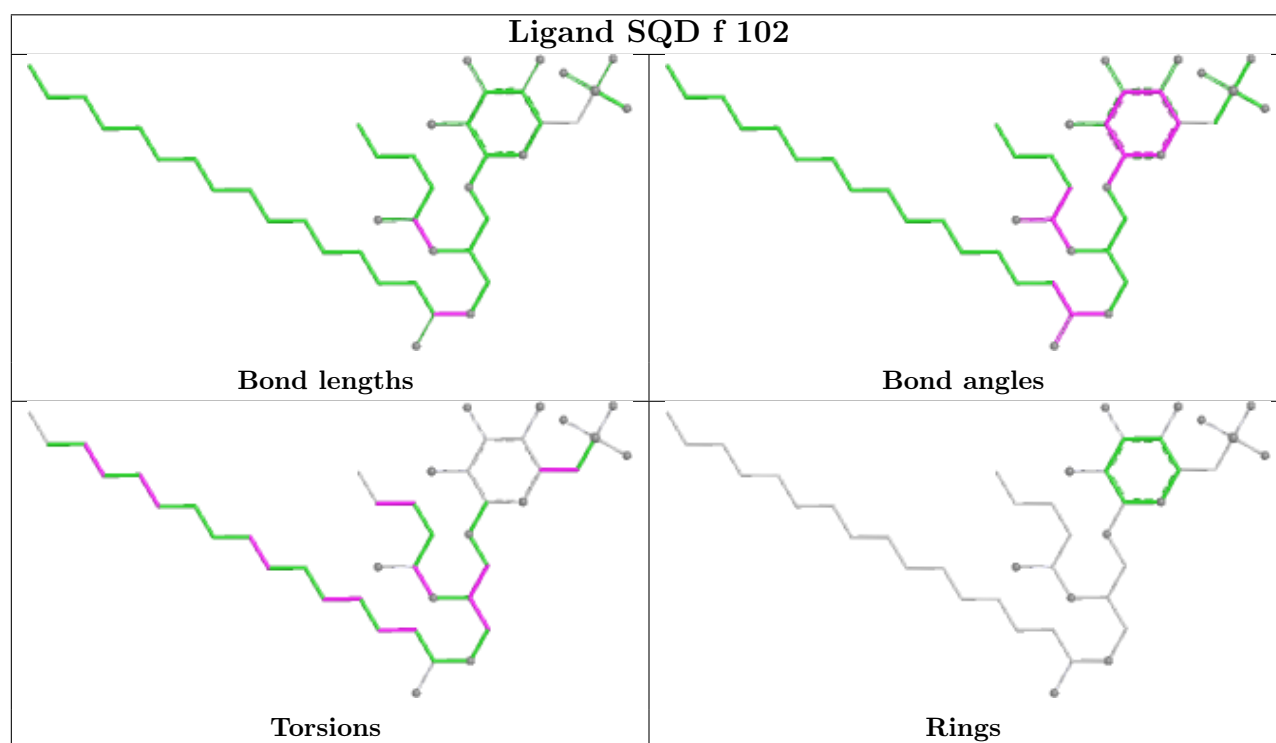
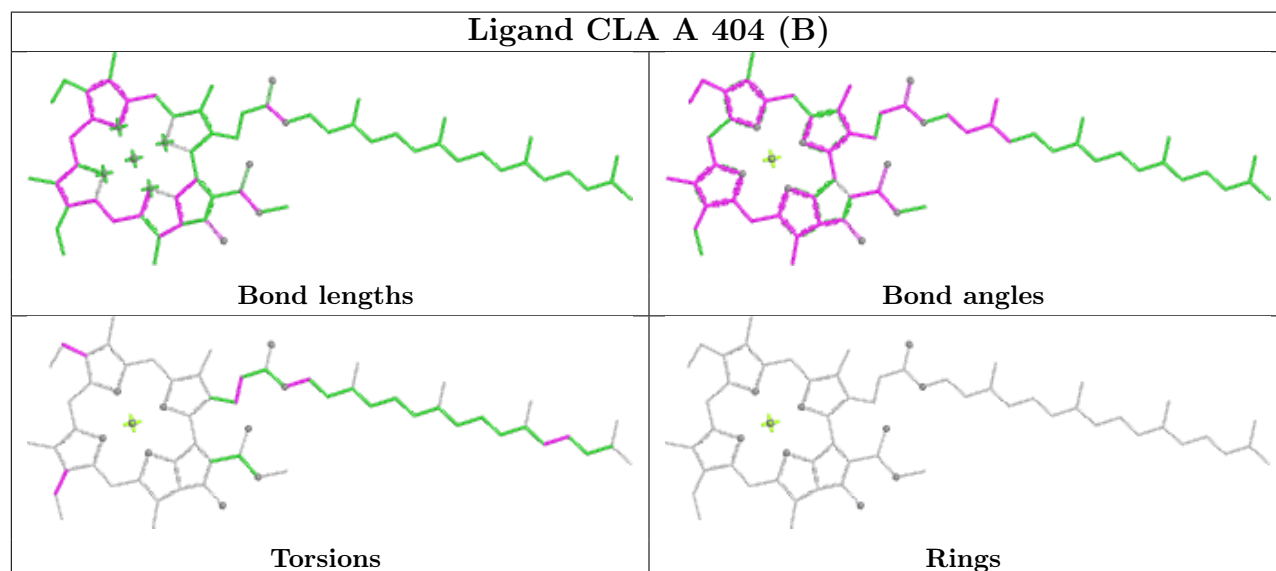
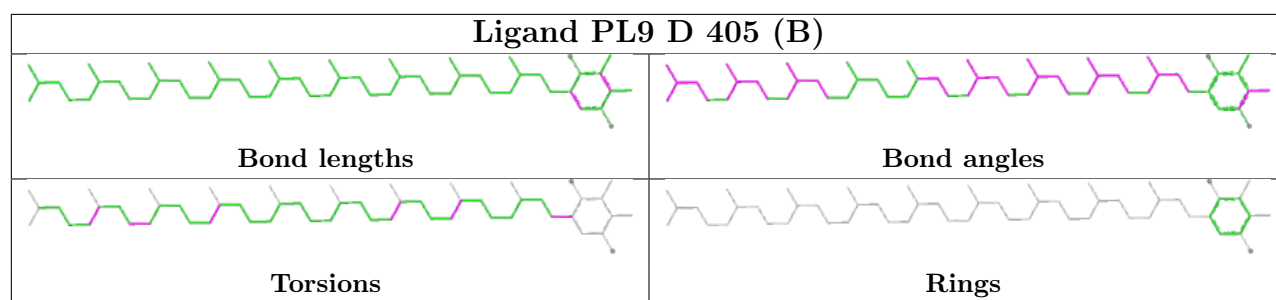
Ligand LHG A 419 (A)



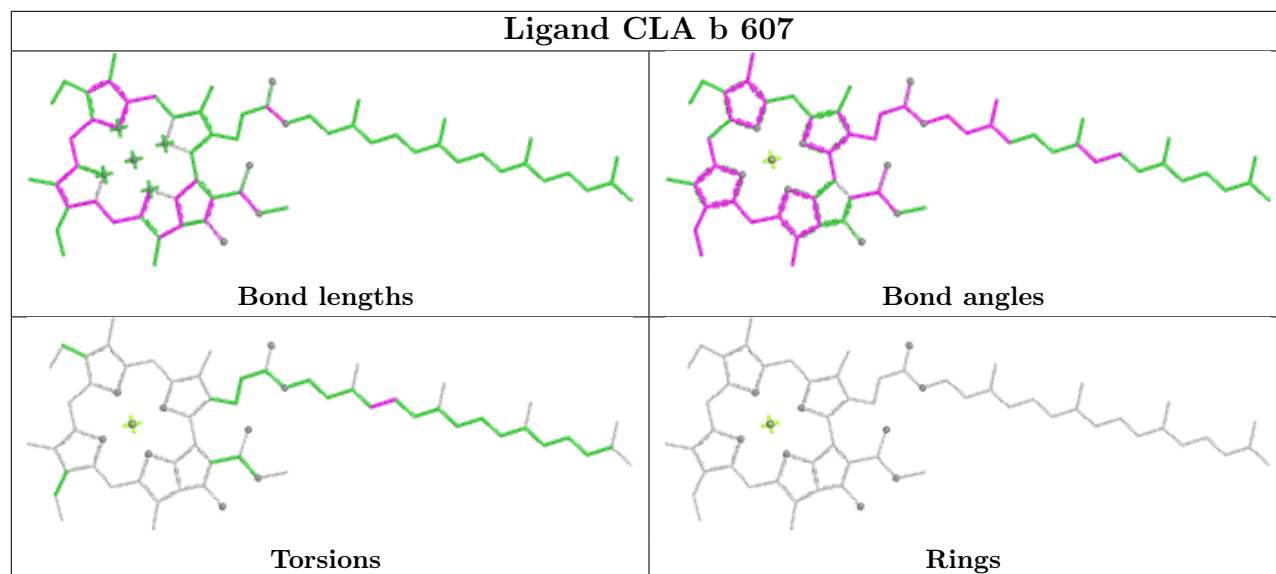
Ligand HTG B 624



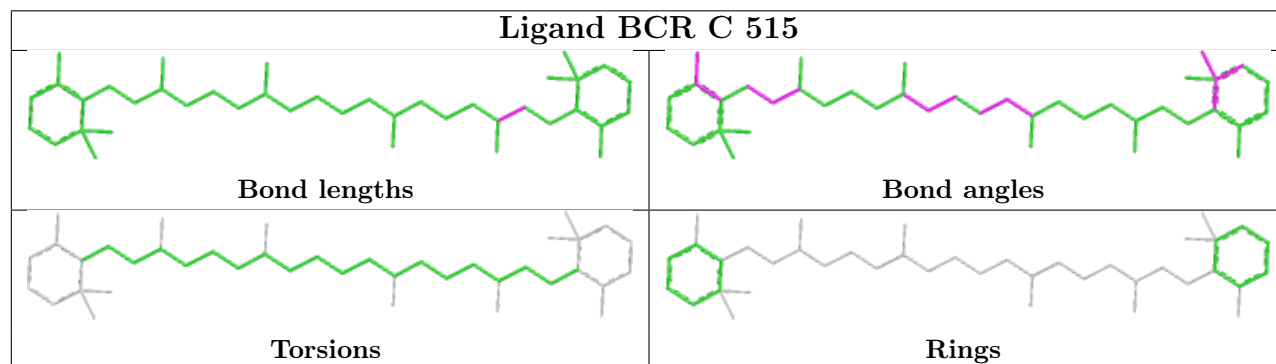




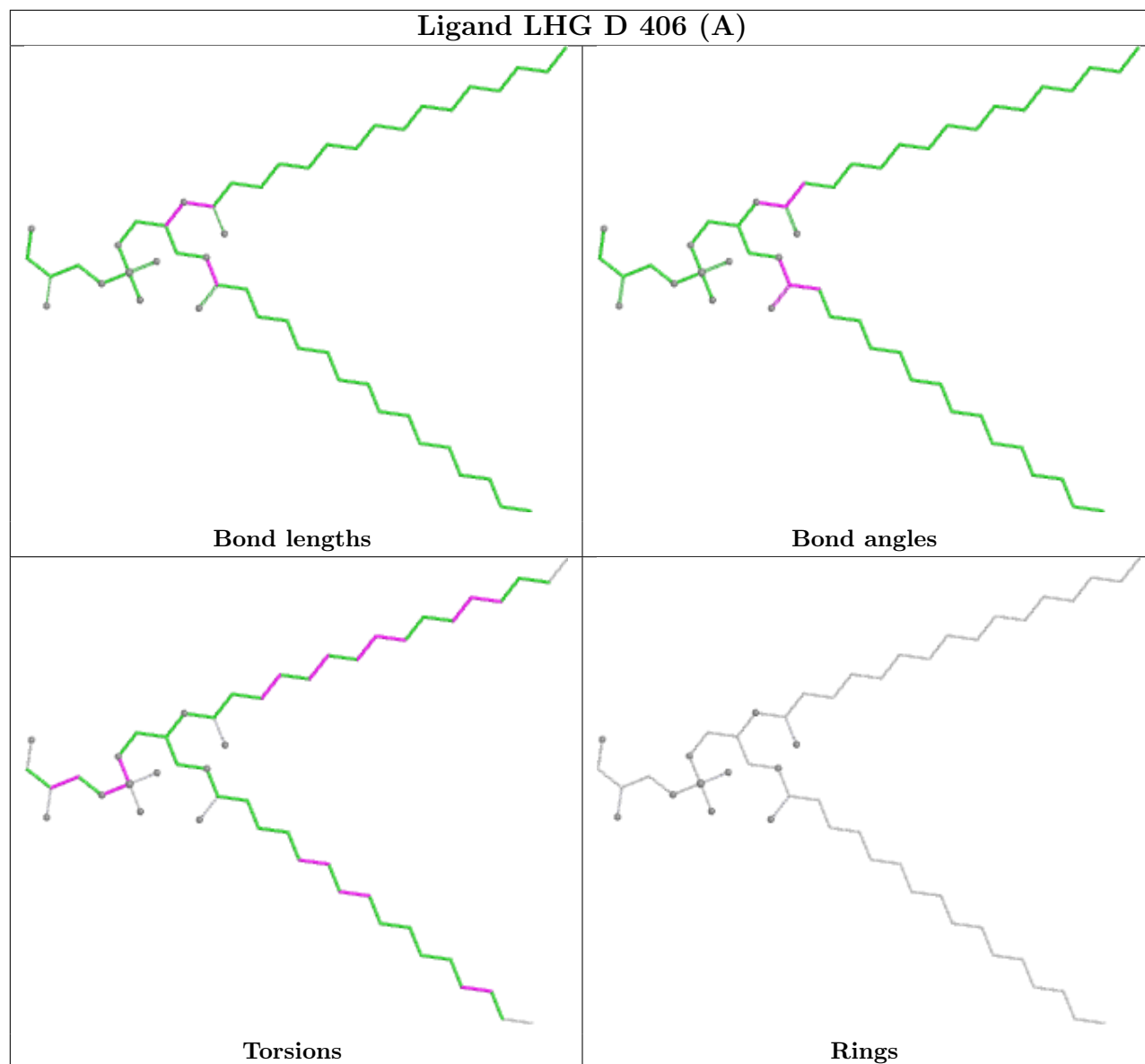
Ligand CLA b 607



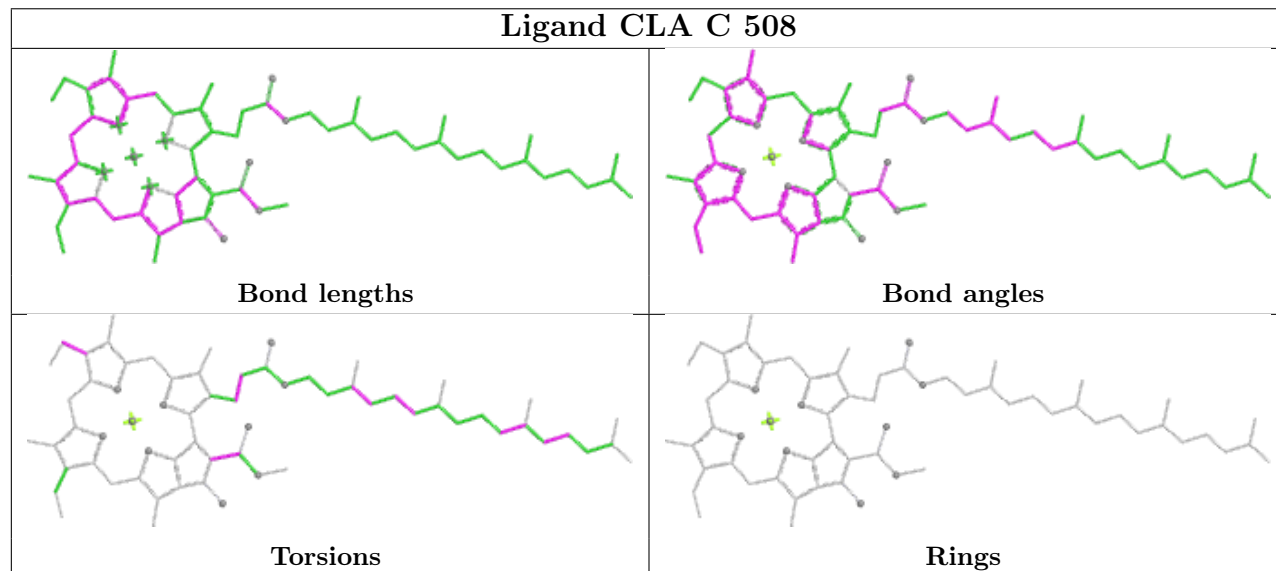
Ligand BCR C 515



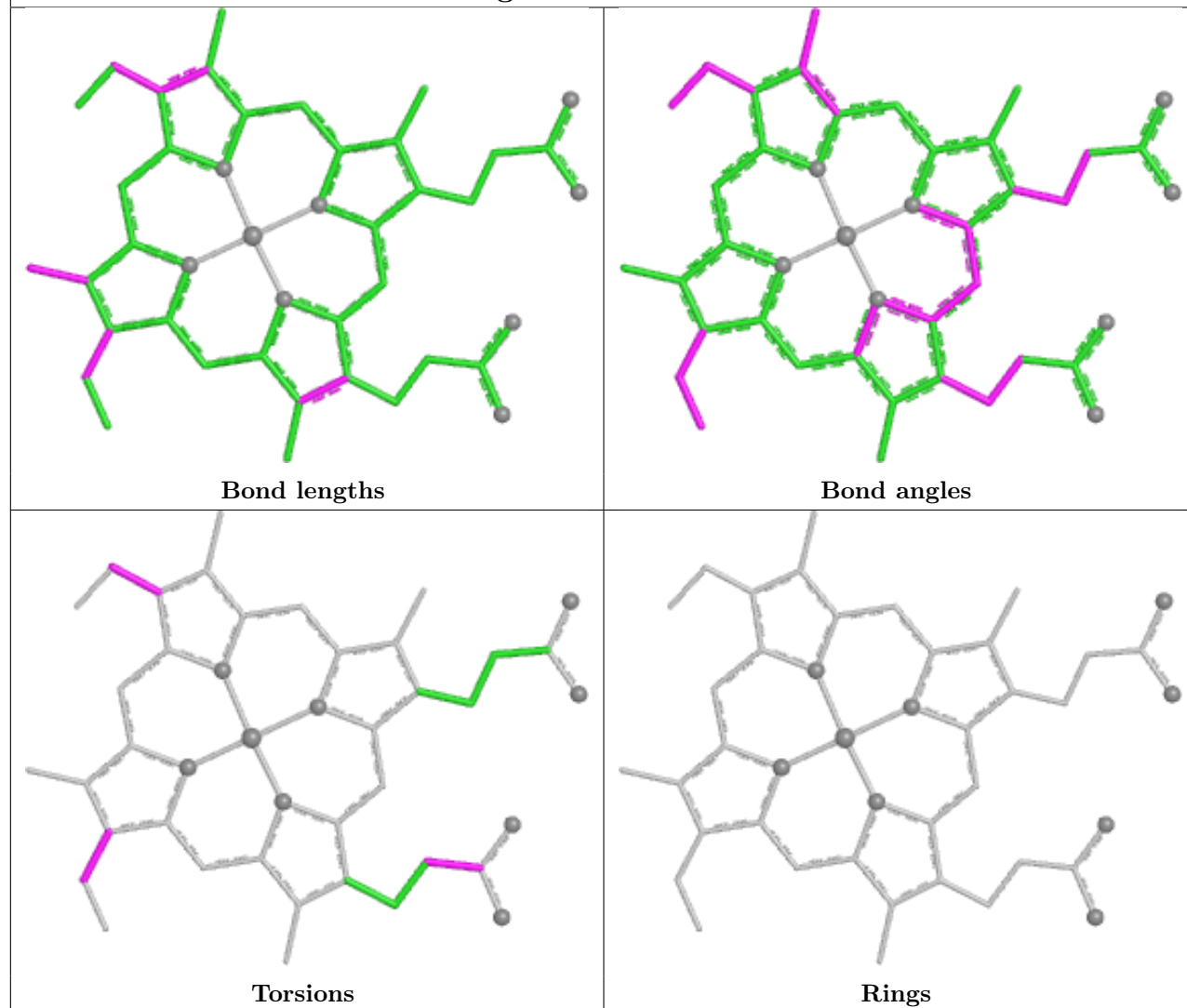
Ligand LHG D 406 (A)



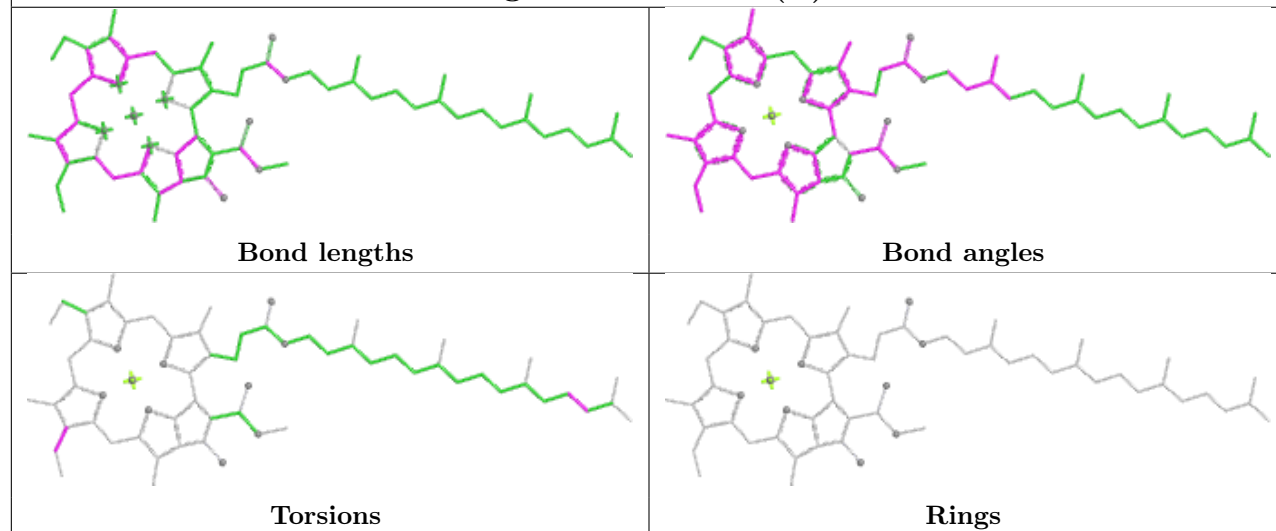
Ligand CLA C 508



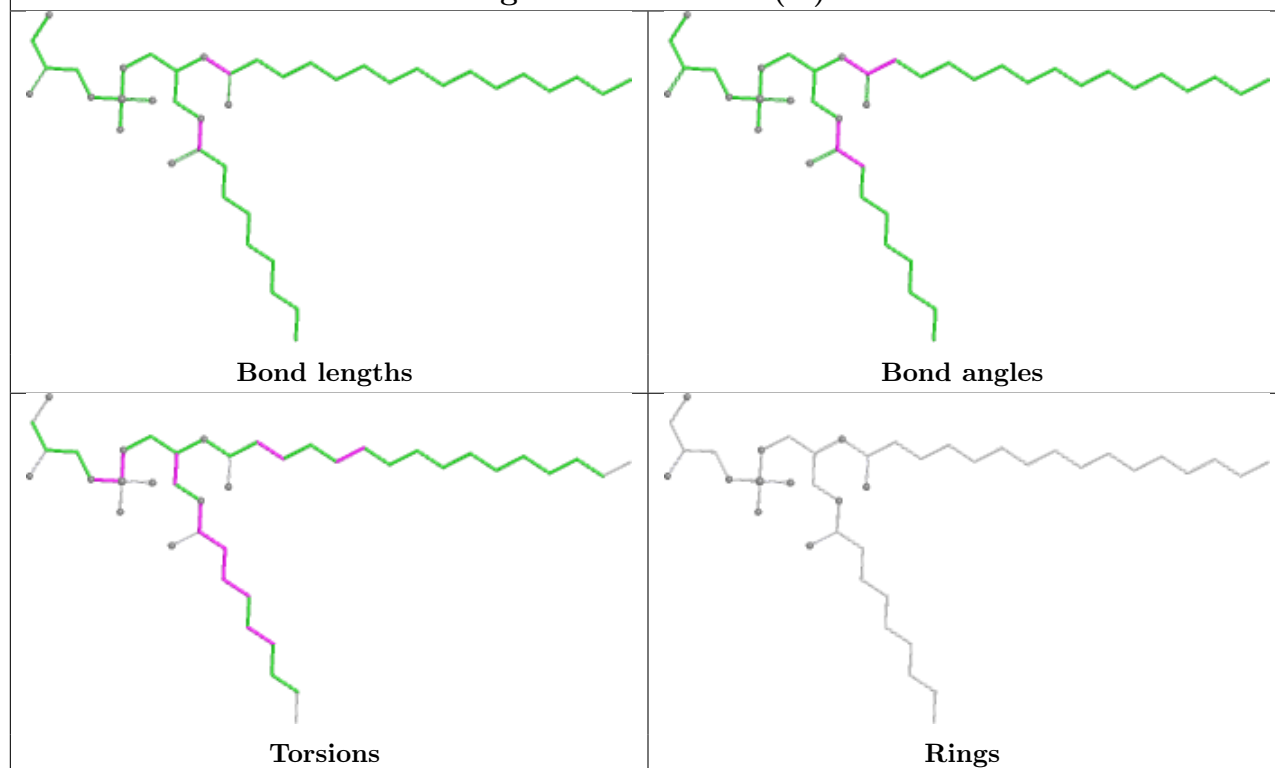
Ligand HEC v 201



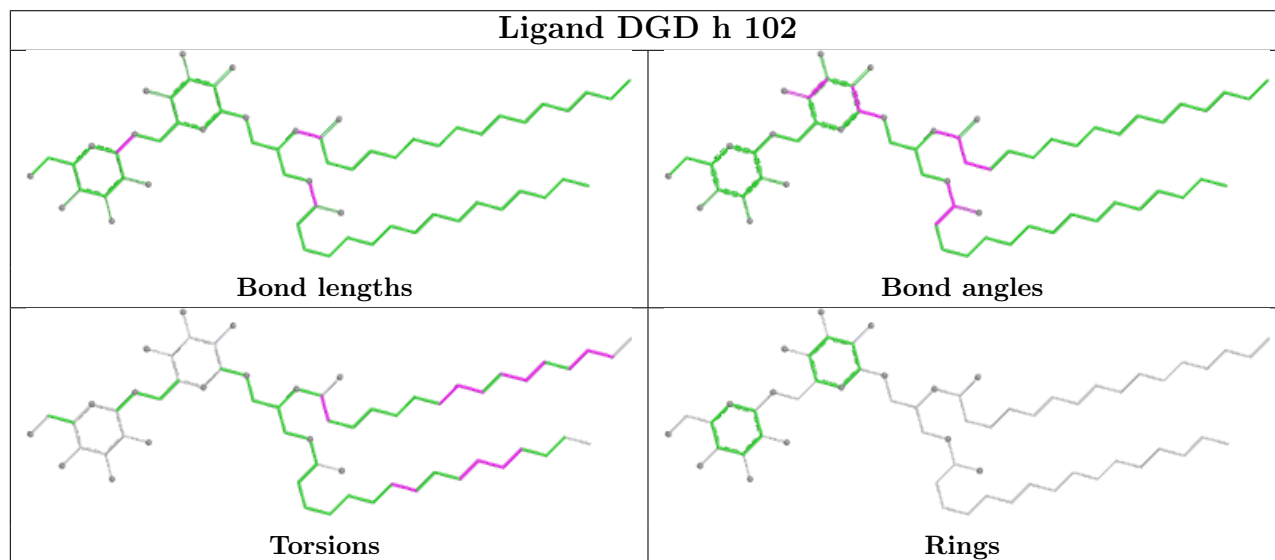
Ligand CLA a 405 (B)

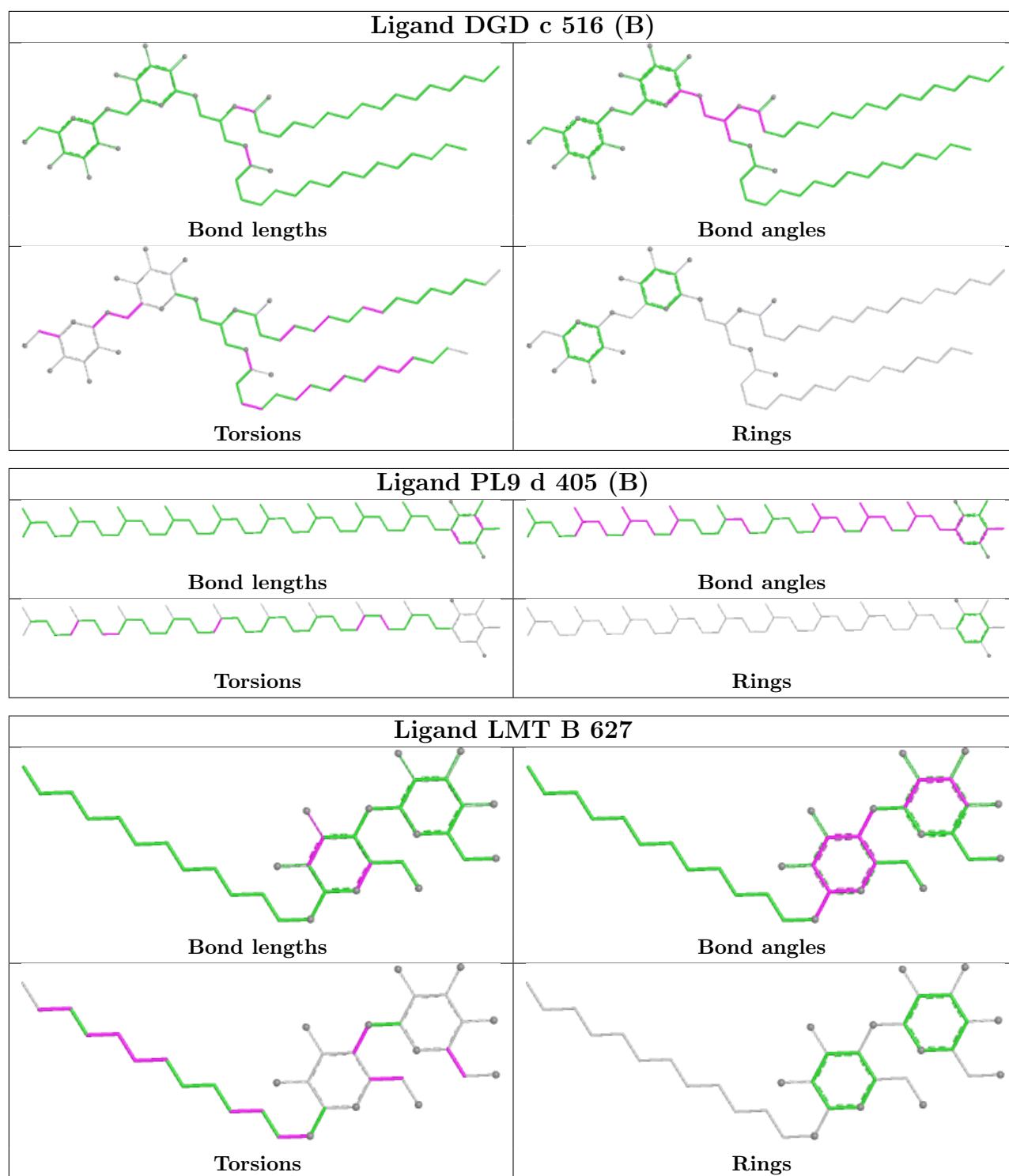


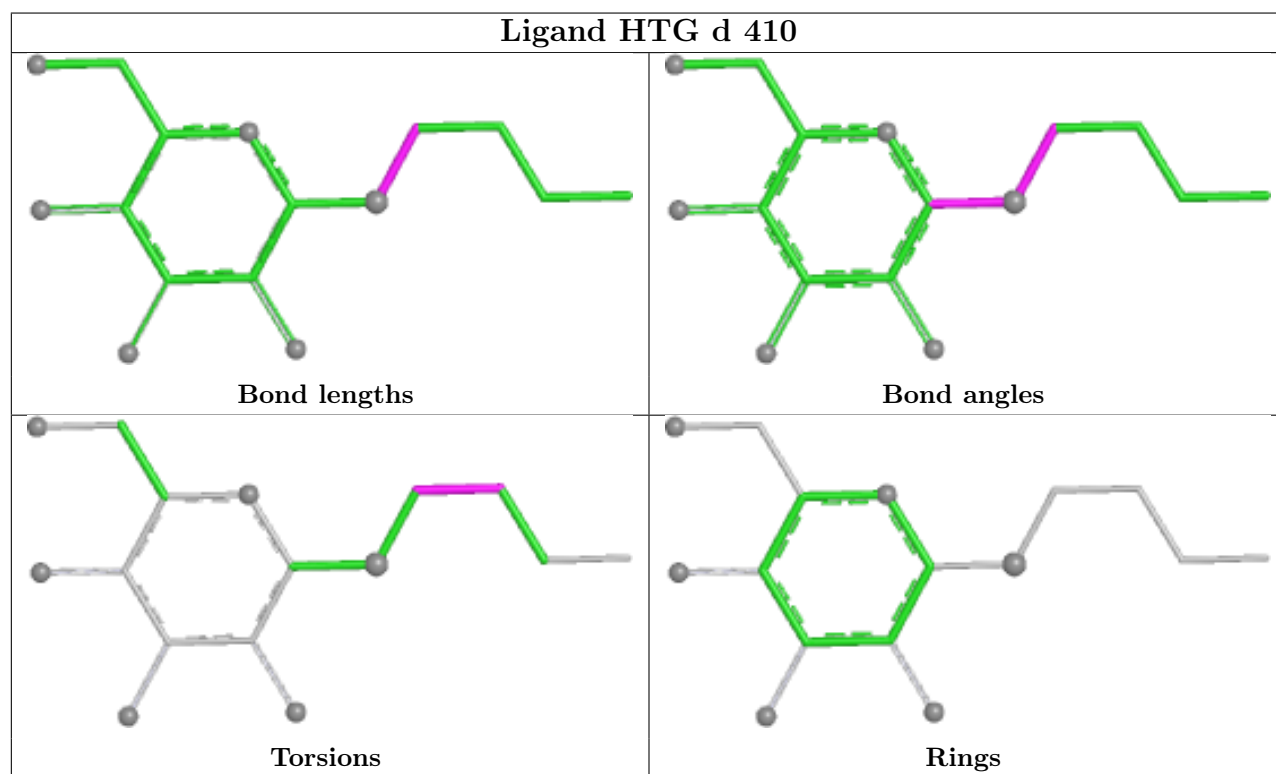
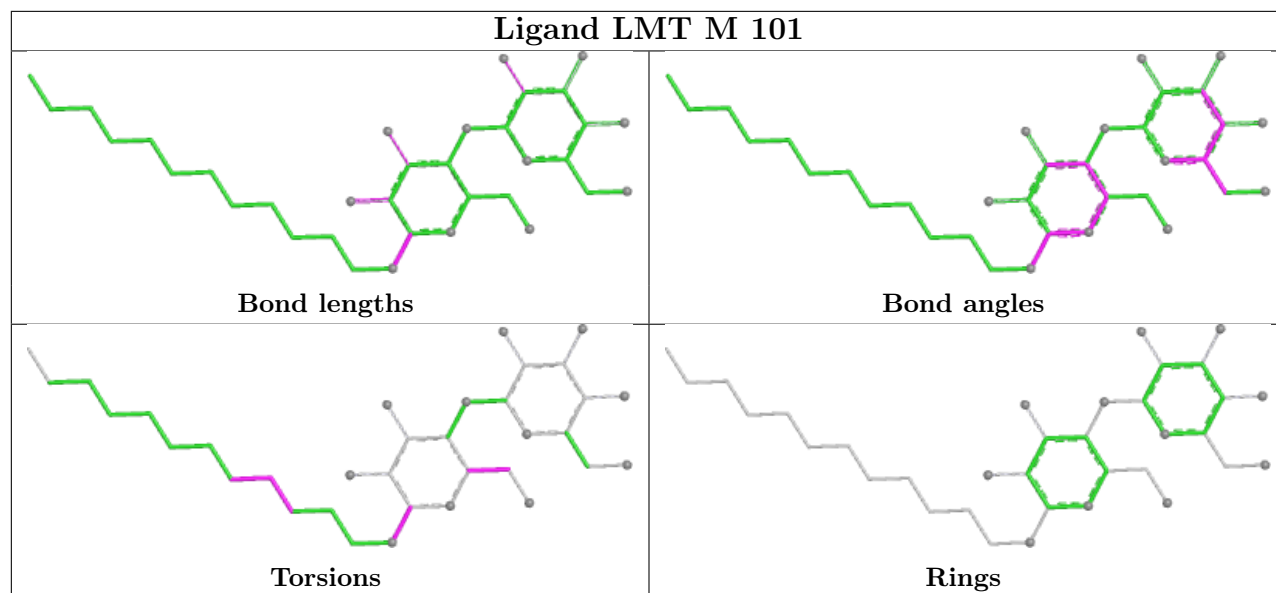
Ligand LHG a 420 (A)

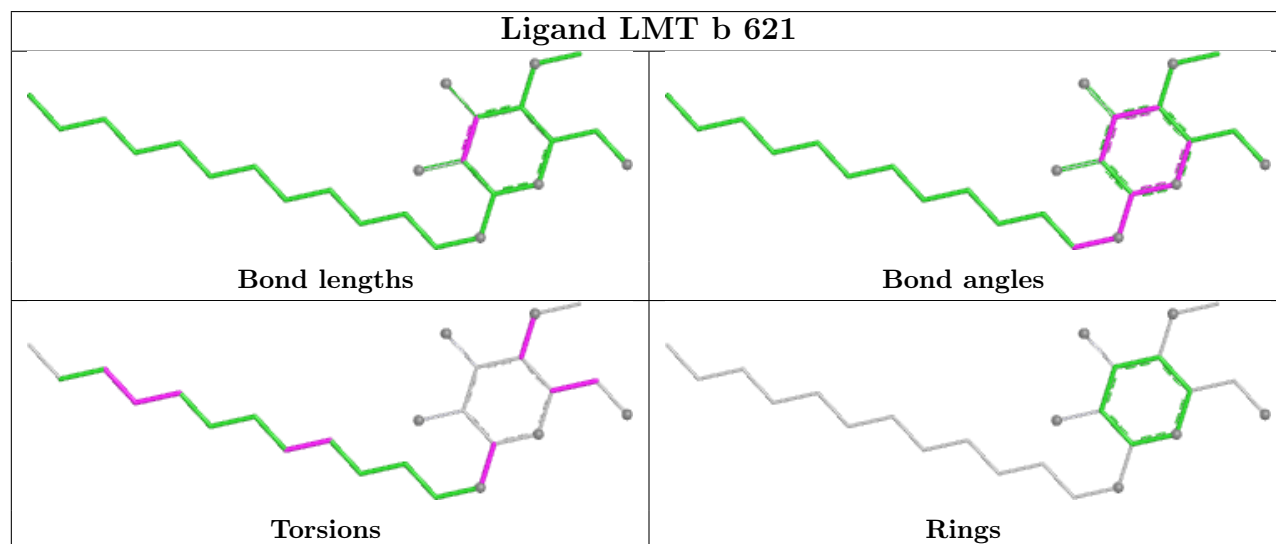
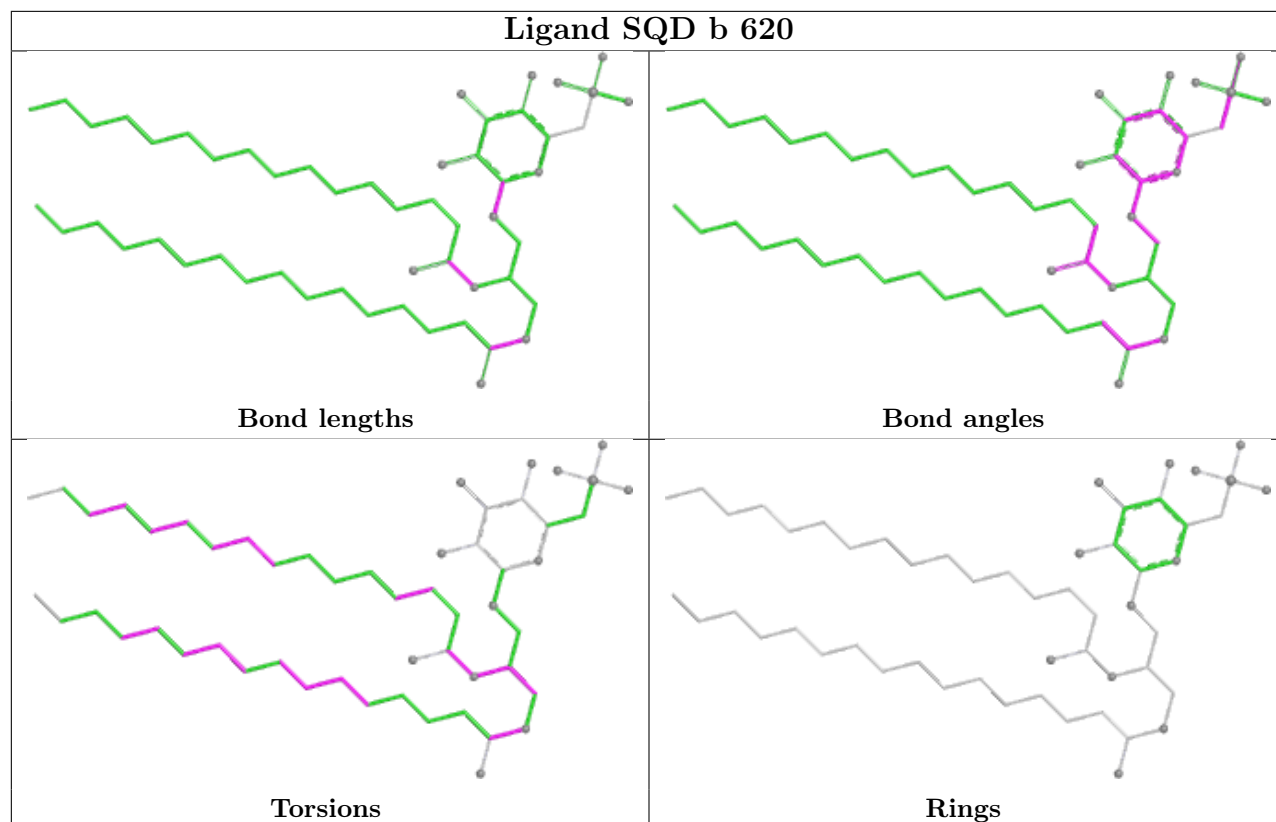


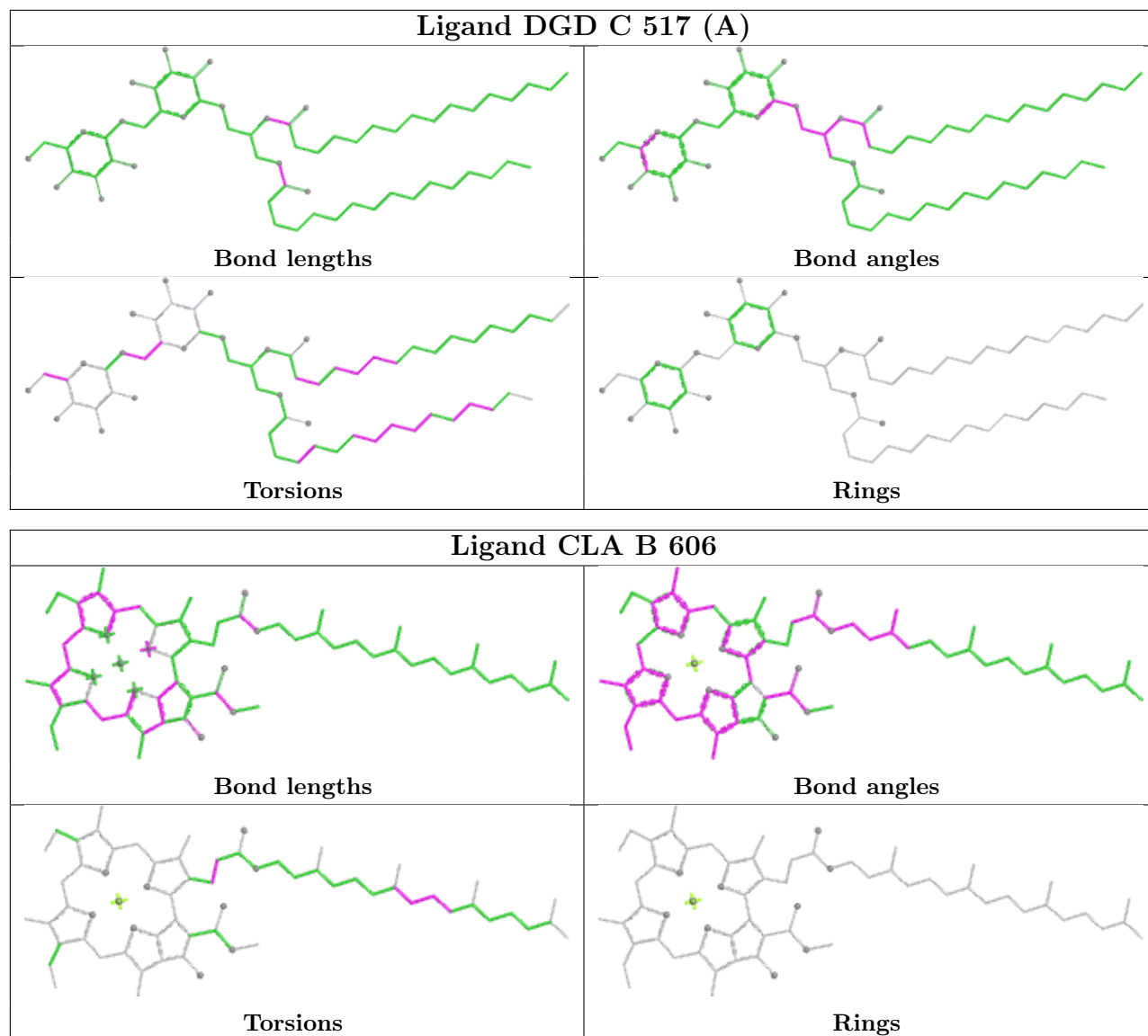
Ligand DGD h 102

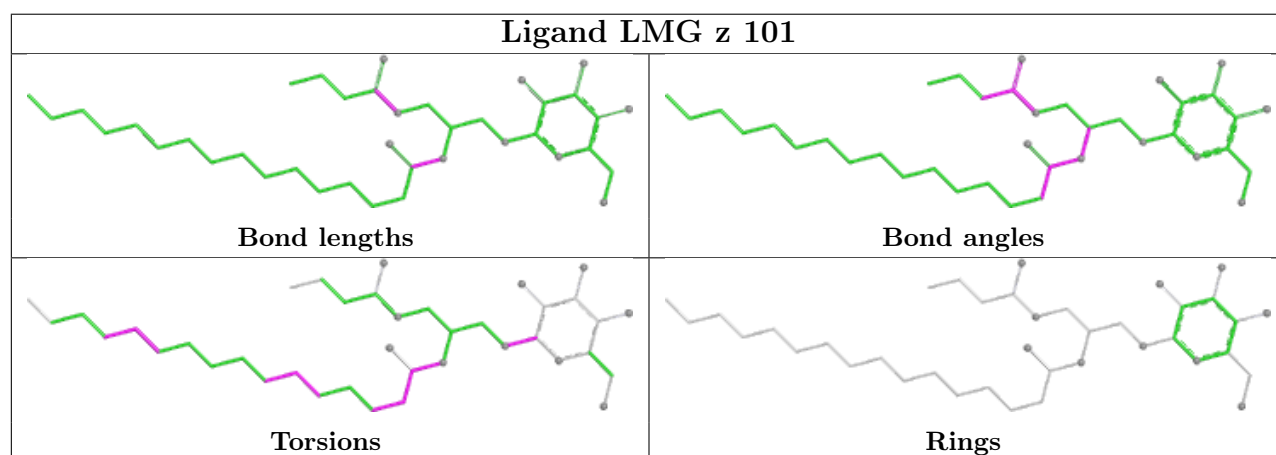
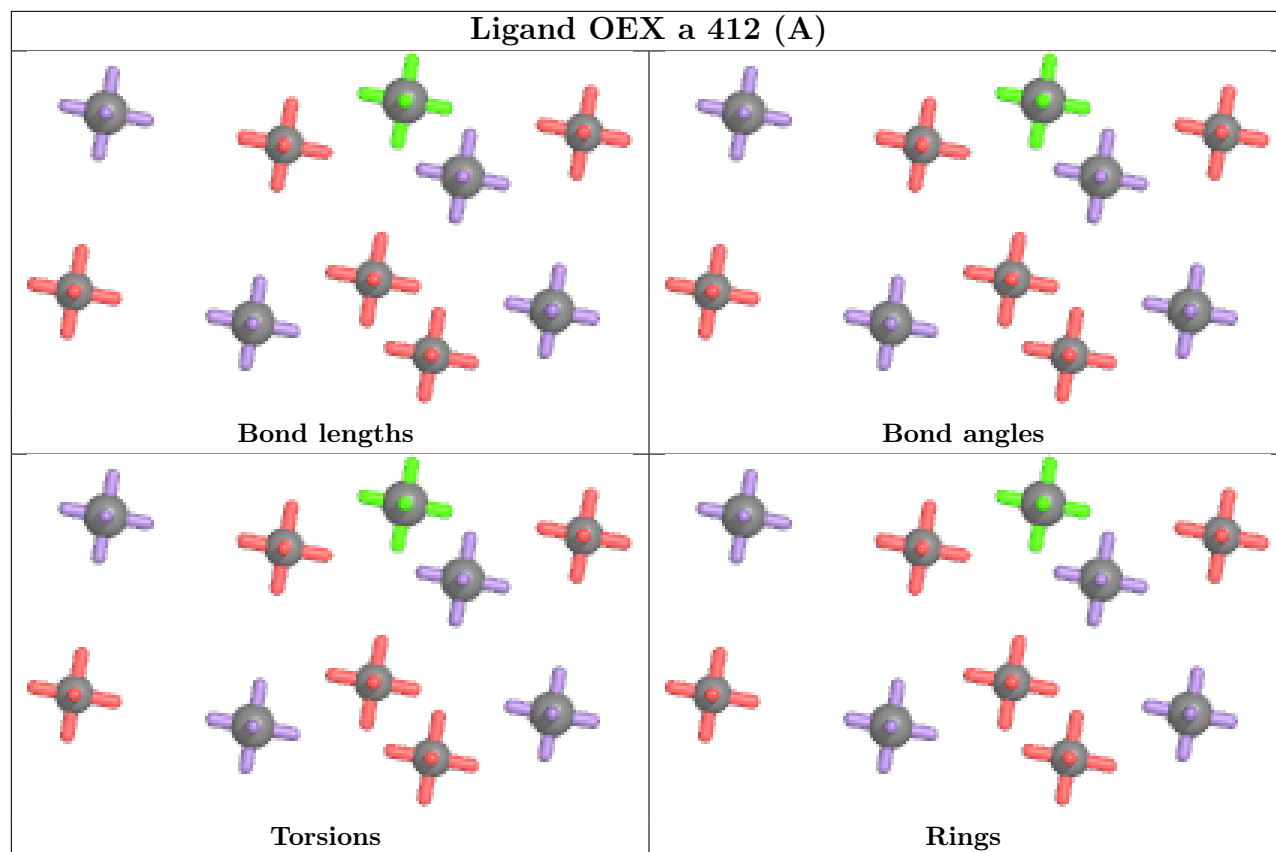




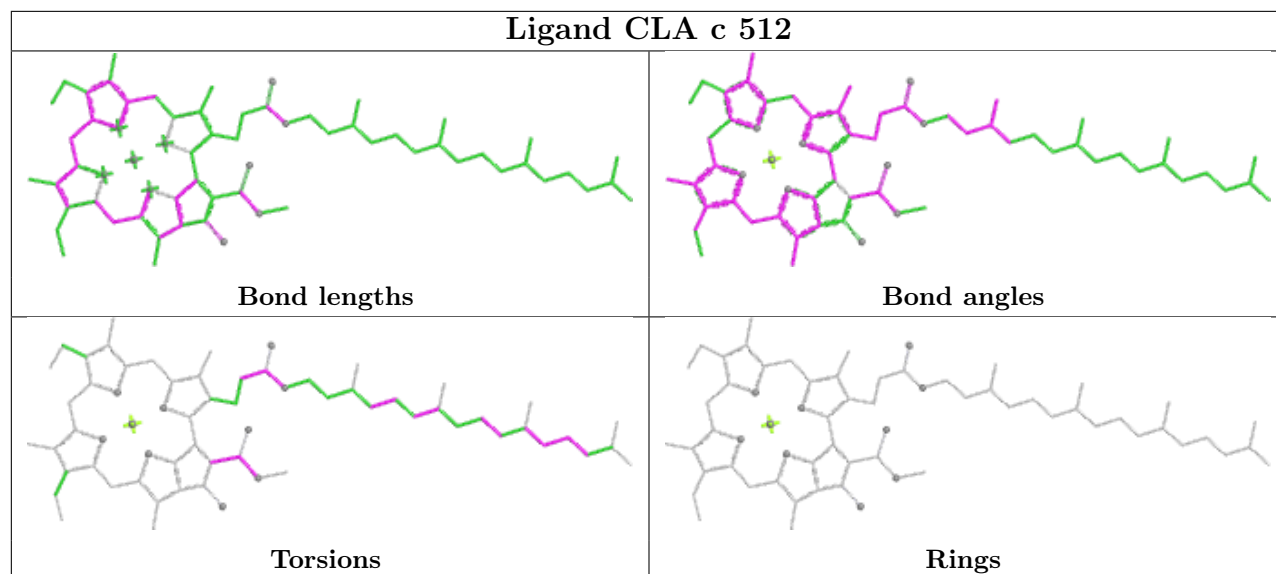




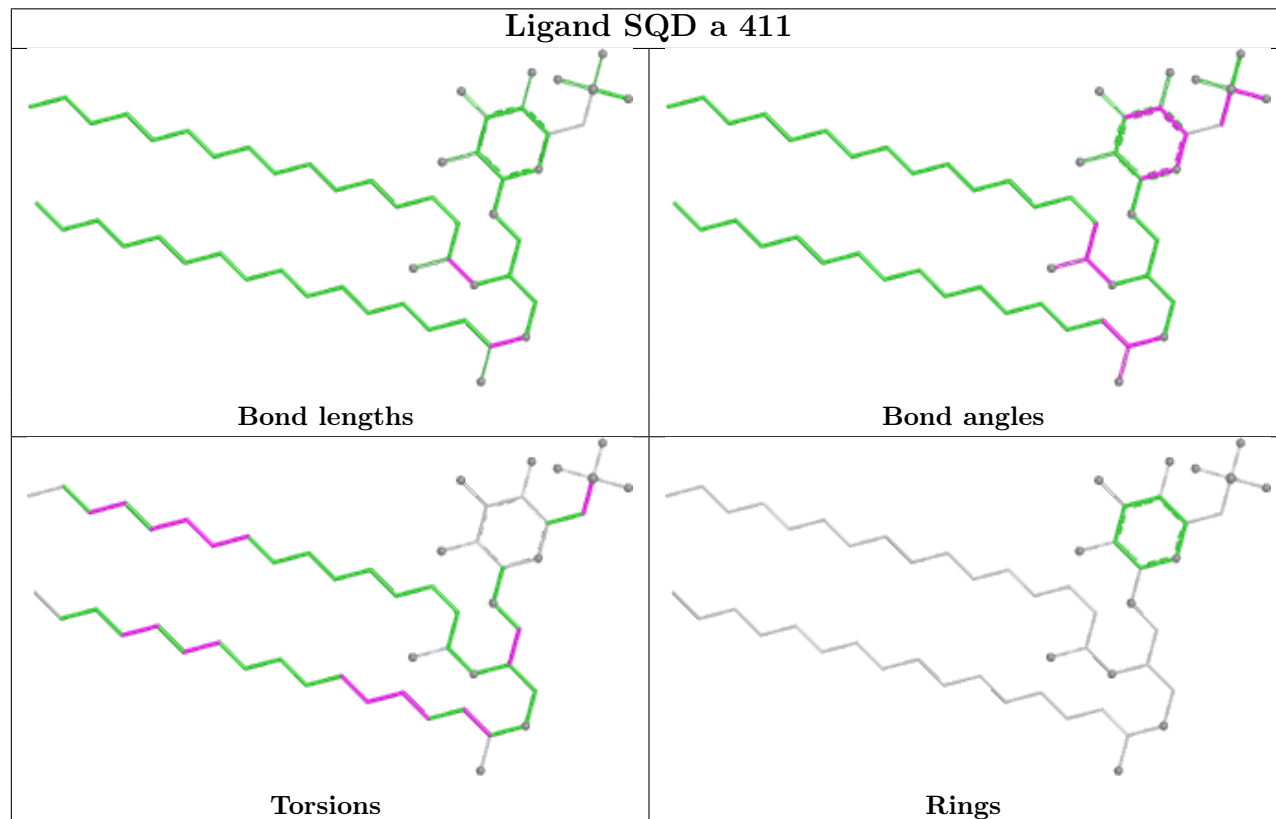




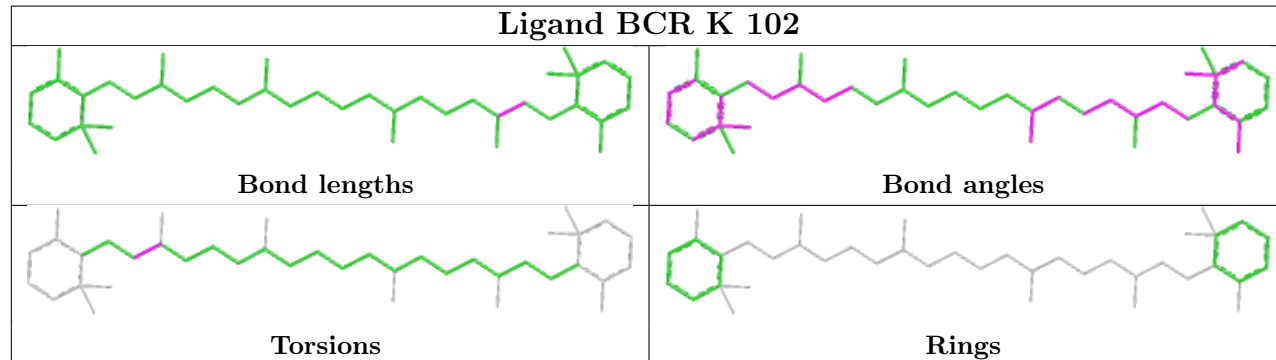
Ligand CLA c 512



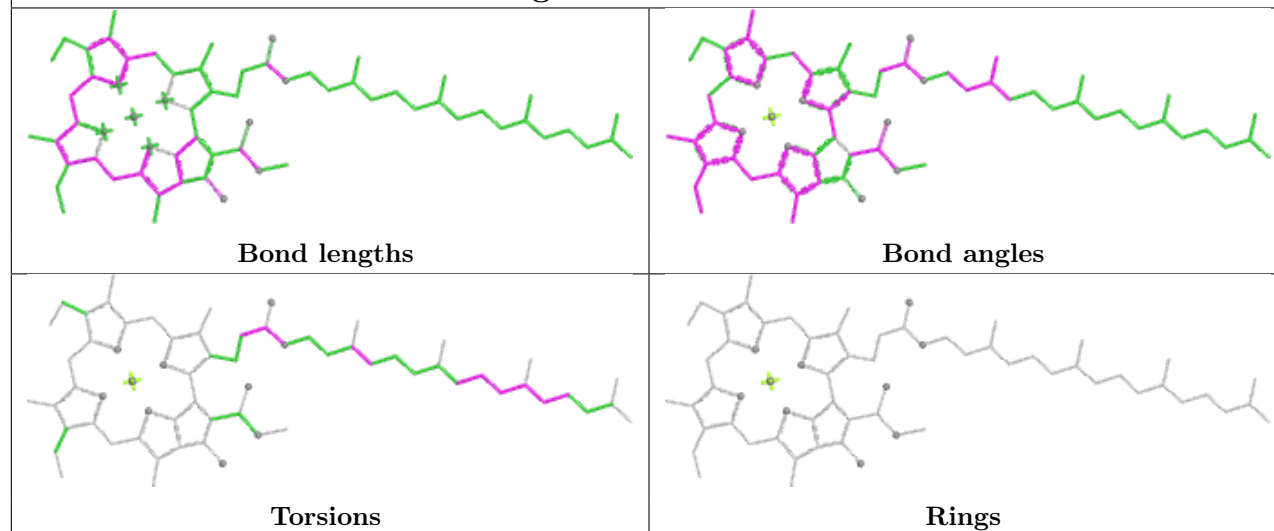
Ligand SQD a 411



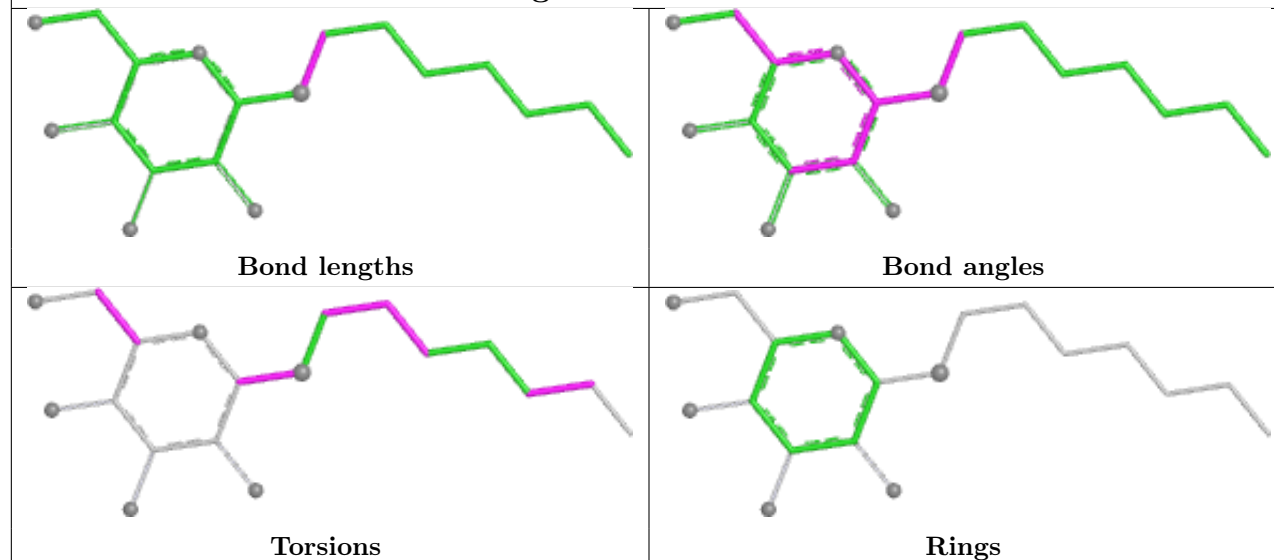
Ligand BCR K 102



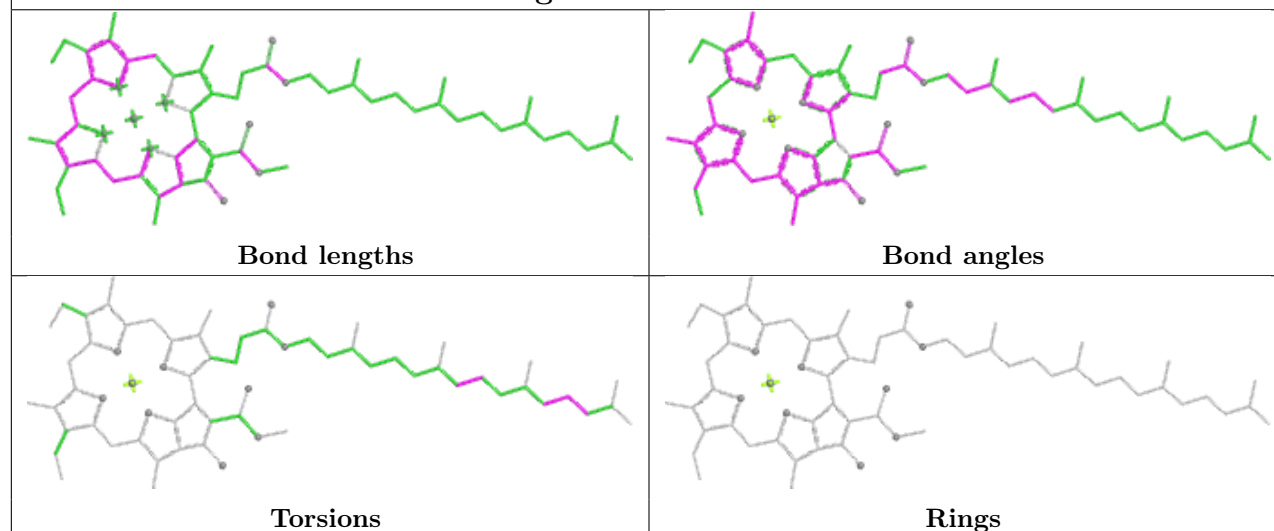
Ligand CLA C 511

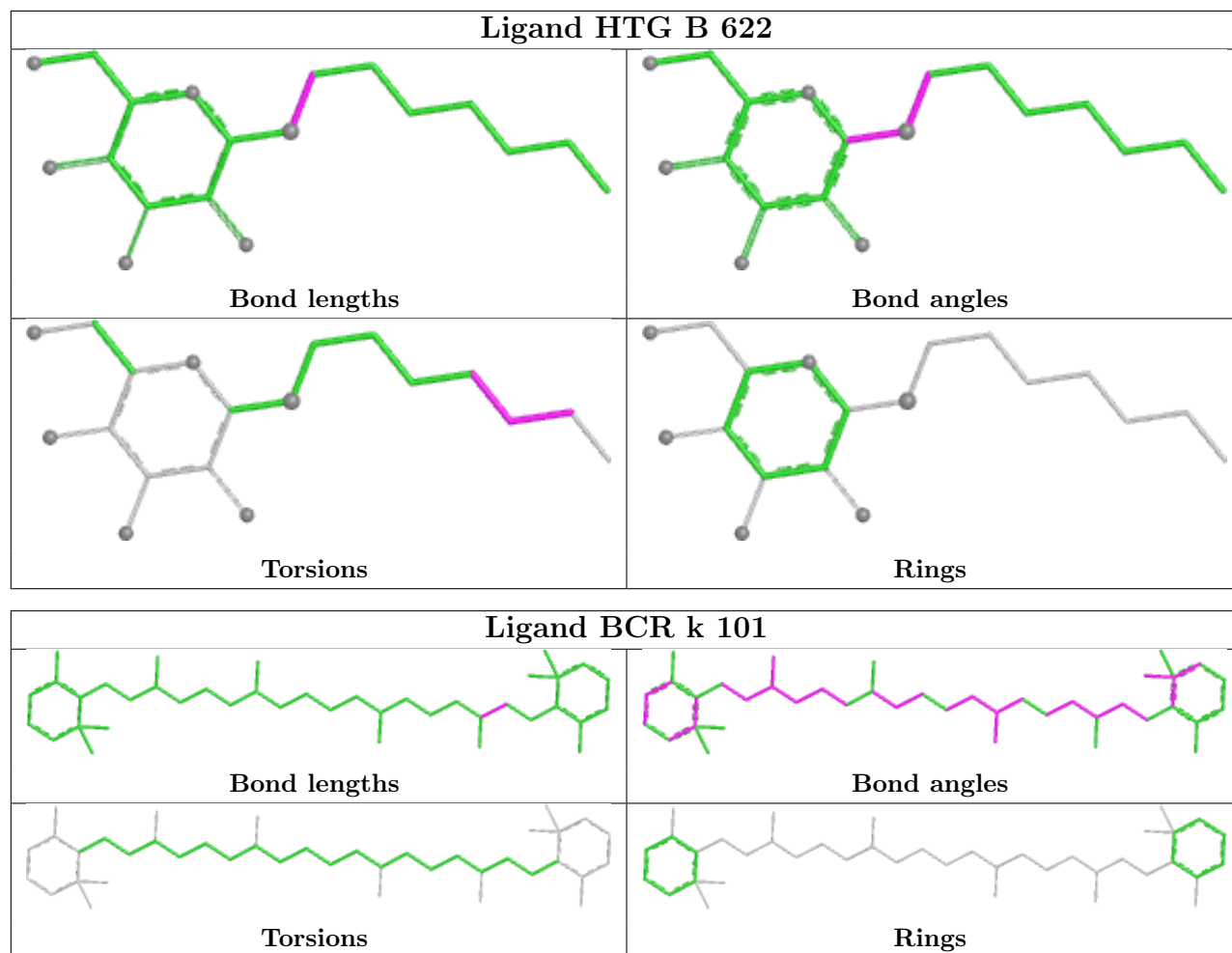


Ligand HTG b 623



Ligand CLA b 611





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%)	-0.65	0 100 100	19, 26, 61, 119	222 (66%)
1	a	334/344 (97%)	-0.63	1 (0%) 90 90	20, 28, 64, 128	221 (66%)
2	B	504/505 (99%)	-0.57	1 (0%) 91 92	22, 53, 82, 116	20 (3%)
2	b	504/505 (99%)	-0.46	2 (0%) 88 89	24, 58, 94, 150	19 (3%)
3	C	451/455 (99%)	-0.55	1 (0%) 91 92	22, 59, 83, 136	97 (21%)
3	c	455/455 (100%)	-0.50	2 (0%) 88 89	24, 65, 88, 128	100 (21%)
4	D	342/342 (100%)	-0.70	0 100 100	20, 45, 64, 135	114 (33%)
4	d	341/342 (99%)	-0.68	0 100 100	21, 50, 75, 133	116 (34%)
5	E	81/84 (96%)	-0.36	0 100 100	51, 69, 100, 158	0
5	e	79/84 (94%)	-0.35	1 (1%) 75 76	33, 76, 118, 147	2 (2%)
6	F	34/44 (77%)	-0.59	0 100 100	52, 62, 89, 115	0
6	f	31/44 (70%)	-0.35	1 (3%) 50 50	54, 68, 94, 138	1 (3%)
7	H	64/65 (98%)	-0.29	1 (1%) 70 71	53, 64, 88, 108	0
7	h	64/65 (98%)	-0.34	0 100 100	39, 73, 95, 104	1 (1%)
8	I	37/38 (97%)	-0.19	0 100 100	55, 66, 123, 149	0
8	i	37/38 (97%)	-0.34	1 (2%) 56 57	55, 64, 116, 132	0
9	J	38/39 (97%)	-0.41	0 100 100	48, 68, 117, 151	0
9	j	39/39 (100%)	-0.30	0 100 100	57, 77, 119, 150	0
10	K	37/37 (100%)	-0.65	0 100 100	56, 67, 88, 106	0
10	k	37/37 (100%)	-0.51	0 100 100	66, 75, 97, 113	0
11	L	36/37 (97%)	-0.68	0 100 100	22, 45, 103, 126	2 (5%)
11	l	36/37 (97%)	-0.65	0 100 100	23, 45, 101, 112	2 (5%)
12	M	32/36 (88%)	-0.64	0 100 100	26, 47, 72, 132	1 (3%)
12	m	33/36 (91%)	-0.58	0 100 100	23, 47, 69, 145	2 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.51	0 100 100	21, 65, 120, 162	10 (4%)
13	o	243/244 (99%)	-0.49	0 100 100	22, 68, 125, 158	8 (3%)
14	T	29/32 (90%)	-0.62	0 100 100	27, 46, 55, 65	6 (20%)
14	t	29/32 (90%)	-0.66	1 (3%) 48 48	27, 46, 59, 71	5 (17%)
15	U	96/104 (92%)	-0.63	0 100 100	25, 57, 91, 97	4 (4%)
15	u	97/104 (93%)	-0.67	0 100 100	28, 61, 80, 126	4 (4%)
16	V	137/137 (100%)	-0.72	0 100 100	23, 56, 81, 105	6 (4%)
16	v	137/137 (100%)	-0.58	0 100 100	26, 71, 102, 133	6 (4%)
17	X	38/40 (95%)	-0.22	0 100 100	34, 73, 93, 111	1 (2%)
17	x	38/40 (95%)	-0.04	0 100 100	68, 82, 125, 156	0
18	Y	29/30 (96%)	-0.05	1 (3%) 48 48	69, 84, 119, 128	0
18	y	29/30 (96%)	-0.21	0 100 100	76, 91, 110, 114	0
19	Z	62/62 (100%)	-0.32	0 100 100	67, 81, 131, 151	0
19	z	62/62 (100%)	0.09	0 100 100	82, 95, 140, 172	0
20	R	34/34 (100%)	0.54	2 (5%) 28 26	85, 109, 135, 146	0
All	All	5283/5384 (98%)	-0.53	15 (0%) 90 90	19, 58, 101, 172	970 (18%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	e	79[A]	PHE	4.0
7	H	65	LEU	3.5
6	f	16[A]	PHE	2.8
1	a	11	ALA	2.7
18	Y	18	VAL	2.6
2	b	499	VAL	2.5
3	c	245[A]	ILE	2.5
2	B	494	GLY	2.4
20	R	35	LEU	2.2
3	C	246	ALA	2.2
3	c	20	SER	2.2
14	t	30[A]	THR	2.1
2	b	502	VAL	2.1
20	R	28	VAL	2.0
8	i	37	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.94	0.08	42,51,66,69	0
8	FME	I	1	10/11	0.95	0.08	63,75,82,85	0
12	FME	M	1	10/11	0.97	0.07	45,59,93,93	0
8	FME	i	1	10/11	0.97	0.07	58,72,80,83	0
12	FME	m	1	10/11	0.97	0.07	49,61,90,112	0
14	FME	t	1	10/11	0.97	0.06	41,48,61,76	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
27	GOL	a	418	6/6	0.58	0.17	70,91,103,104	0
31	LMT	B	629	35/35	0.66	0.15	65,109,141,142	0
31	LMT	A	417	35/35	0.67	0.13	59,105,131,135	0
31	LMT	F	101	35/35	0.68	0.15	99,131,171,175	0
30	UNL	A	415	28/-	0.69	0.14	84,112,129,139	0
30	UNL	a	414	30/-	0.70	0.12	82,114,134,151	0
31	LMT	A	420	35/35	0.70	0.12	90,128,153,167	0
31	LMT	a	417	35/35	0.70	0.14	108,129,146,150	0
31	LMT	e	101	35/35	0.71	0.14	101,137,181,192	0
30	UNL	K	101[B]	34/-	0.72	0.14	82,103,115,118	34
30	UNL	K	101[A]	34/-	0.72	0.14	82,103,115,118	34
30	UNL	j	101	10/-	0.72	0.17	77,90,103,106	0
30	UNL	J	101	10/-	0.73	0.24	62,80,84,96	0
26	SQD	f	102	43/54	0.74	0.12	95,128,175,186	0
30	UNL	m	102	10/-	0.74	0.19	67,75,93,104	0
30	UNL	I	101	40/-	0.75	0.15	75,99,155,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	HTG	C	522	19/19	0.75	0.12	105,121,140,144	0
27	GOL	o	303	6/6	0.76	0.17	81,104,116,122	0
27	GOL	B	626	6/6	0.77	0.15	64,79,95,110	0
32	LHG	a	420[A]	42/49	0.77	0.11	88,132,149,155	42
32	LHG	a	420[B]	42/49	0.77	0.11	88,132,149,155	42
34	HTG	B	622	19/19	0.77	0.16	63,89,107,116	0
30	UNL	M	102	10/-	0.77	0.16	66,76,92,93	0
27	GOL	o	304	6/6	0.78	0.15	78,87,97,108	0
30	UNL	c	524[A]	32/-	0.78	0.14	87,105,121,128	32
30	UNL	c	524[B]	32/-	0.78	0.14	87,105,121,128	32
27	GOL	A	411	6/6	0.79	0.14	59,77,81,86	0
30	UNL	B	630	40/-	0.79	0.13	71,106,157,158	0
31	LMT	b	621	25/35	0.80	0.12	80,109,160,169	0
30	UNL	D	409	40/-	0.80	0.13	63,87,144,147	0
34	HTG	D	410	16/19	0.80	0.12	92,106,134,148	0
30	UNL	d	409	36/-	0.81	0.11	67,92,132,138	0
27	GOL	d	412	6/6	0.81	0.22	51,63,76,86	0
33	LMG	C	521	51/55	0.81	0.11	62,120,157,171	0
30	UNL	b	626	33/-	0.82	0.12	67,95,159,168	0
27	GOL	b	624	6/6	0.82	0.16	91,95,101,114	0
31	LMT	M	103	35/35	0.82	0.10	68,117,169,174	0
34	HTG	V	202	11/19	0.82	0.09	82,110,121,124	0
34	HTG	c	521	19/19	0.82	0.10	104,124,145,146	0
36	CA	F	104	1/1	0.82	0.21	120,120,120,120	0
31	LMT	t	101	26/35	0.83	0.11	69,96,138,154	0
29	PL9	a	413[B]	55/55	0.83	0.14	76,98,111,115	55
31	LMT	B	627	35/35	0.83	0.11	66,101,138,146	0
29	PL9	a	413[A]	55/55	0.83	0.14	76,98,111,115	55
30	UNL	B	625	33/-	0.83	0.14	51,115,144,151	0
27	GOL	l	801[B]	6/6	0.84	0.16	60,93,96,97	6
27	GOL	O	303	6/6	0.84	0.12	71,89,93,94	0
26	SQD	a	411	54/54	0.84	0.10	66,92,136,148	0
29	PL9	A	414[A]	55/55	0.84	0.13	58,89,104,114	55
34	HTG	b	622	19/19	0.84	0.13	58,85,108,115	0
34	HTG	b	623	19/19	0.84	0.11	83,131,156,160	0
29	PL9	A	414[B]	55/55	0.84	0.13	58,89,104,114	55
34	HTG	d	410	16/19	0.84	0.11	92,118,137,152	0
27	GOL	l	801[A]	6/6	0.84	0.16	60,93,96,97	6
33	LMG	Z	101	37/55	0.85	0.13	71,123,149,170	0
31	LMT	B	631	25/35	0.85	0.12	58,82,138,164	0
31	LMT	b	627	25/35	0.85	0.12	55,95,148,160	0
26	SQD	A	412	54/54	0.85	0.10	66,87,123,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LMT	m	103	35/35	0.85	0.11	57,89,102,112	0
27	GOL	c	526	6/6	0.86	0.16	91,101,113,116	0
36	CA	f	103	1/1	0.86	0.13	122,122,122,122	0
33	LMG	c	520	51/55	0.87	0.10	72,136,163,185	0
27	GOL	O	302	6/6	0.87	0.08	79,88,104,105	0
31	LMT	M	101	35/35	0.87	0.10	62,90,110,117	0
26	SQD	b	620	54/54	0.88	0.09	61,95,117,129	0
32	LHG	E	101[A]	42/49	0.88	0.11	73,98,112,119	42
32	LHG	E	101[B]	42/49	0.88	0.11	73,98,112,119	42
34	HTG	o	301	19/19	0.88	0.12	57,85,108,117	0
27	GOL	A	418	6/6	0.88	0.28	50,70,78,80	0
33	LMG	z	101	39/55	0.88	0.11	76,127,152,171	0
27	GOL	c	525[B]	6/6	0.89	0.09	65,69,73,75	6
26	SQD	B	620	54/54	0.89	0.10	60,90,130,146	0
26	SQD	F	103	43/54	0.89	0.11	74,103,133,140	0
23	CLA	b	601	65/65	0.89	0.09	60,87,126,155	0
27	GOL	c	525[A]	6/6	0.89	0.09	65,69,73,75	6
27	GOL	V	203[B]	6/6	0.90	0.12	60,69,72,78	6
30	UNL	D	408	17/-	0.90	0.10	59,74,104,122	0
27	GOL	D	412	6/6	0.90	0.16	47,61,66,84	0
27	GOL	v	202[A]	6/6	0.90	0.10	64,79,81,82	6
27	GOL	v	202[B]	6/6	0.90	0.10	64,79,81,82	6
27	GOL	V	203[A]	6/6	0.90	0.12	60,68,74,77	6
36	CA	o	302	1/1	0.90	0.07	112,112,112,112	0
27	GOL	a	419	6/6	0.91	0.23	53,77,78,81	0
33	LMG	a	416	51/55	0.91	0.08	66,94,109,119	0
23	CLA	B	601	65/65	0.91	0.09	59,78,116,151	0
33	LMG	m	101	51/55	0.91	0.08	50,74,96,116	0
27	GOL	B	628	6/6	0.91	0.10	72,76,91,94	0
33	LMG	C	501	51/55	0.91	0.09	68,86,115,124	0
33	LMG	B	621	51/55	0.92	0.08	49,69,93,112	0
33	LMG	c	519	51/55	0.92	0.09	58,93,138,159	0
30	UNL	d	408	17/-	0.92	0.09	64,80,107,110	0
34	HTG	B	624	19/19	0.92	0.08	63,74,94,99	0
23	CLA	c	513	65/65	0.92	0.10	71,96,136,156	0
26	SQD	A	410[A]	54/54	0.93	0.09	57,79,113,119	54
26	SQD	A	410[B]	54/54	0.93	0.09	57,79,113,119	54
23	CLA	b	616	65/65	0.93	0.08	50,63,129,139	0
23	CLA	c	512	65/65	0.93	0.10	65,83,131,143	0
27	GOL	C	523[A]	6/6	0.93	0.10	56,60,66,68	6
27	GOL	C	523[B]	6/6	0.93	0.10	56,60,66,68	6
33	LMG	C	520	51/55	0.93	0.09	54,83,114,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	C	514	65/65	0.93	0.09	63,88,116,127	0
34	HTG	b	625	19/19	0.93	0.07	65,82,94,105	0
33	LMG	D	411	51/55	0.93	0.09	49,67,124,138	0
25	BCR	D	404	40/40	0.93	0.08	43,60,102,103	0
25	BCR	T	101	40/40	0.93	0.06	45,59,73,74	0
35	DGD	C	518[A]	62/66	0.93	0.09	48,64,116,123	62
35	DGD	C	518[B]	62/66	0.93	0.09	48,64,116,123	62
35	DGD	c	517[A]	62/66	0.93	0.08	55,69,121,134	62
35	DGD	c	517[B]	62/66	0.93	0.08	55,68,121,135	62
25	BCR	d	404	40/40	0.93	0.08	48,66,101,113	0
32	LHG	A	419[A]	49/49	0.93	0.09	48,62,84,89	49
32	LHG	A	419[B]	49/49	0.93	0.09	48,63,84,89	49
27	GOL	B	623	6/6	0.94	0.07	67,74,84,86	0
30	UNL	X	101	18/-	0.94	0.10	58,72,105,116	0
25	BCR	C	515	40/40	0.94	0.08	57,76,91,93	0
23	CLA	C	505	65/65	0.94	0.07	40,56,105,126	0
32	LHG	d	413[A]	49/49	0.94	0.08	49,66,77,87	49
32	LHG	d	413[B]	49/49	0.94	0.08	49,66,77,87	49
25	BCR	K	102	40/40	0.94	0.09	56,65,75,81	0
23	CLA	C	507	65/65	0.94	0.08	55,72,130,146	0
26	SQD	a	410[A]	54/54	0.94	0.09	56,82,117,123	54
26	SQD	a	410[B]	54/54	0.94	0.09	56,81,117,123	54
25	BCR	Y	101	40/40	0.94	0.07	53,66,78,89	0
25	BCR	c	514	40/40	0.94	0.08	72,84,95,101	0
23	CLA	b	614	65/65	0.94	0.07	39,52,99,113	0
25	BCR	t	102	40/40	0.94	0.06	39,58,76,84	0
33	LMG	d	411	51/55	0.94	0.08	53,70,118,146	0
23	CLA	d	403	65/65	0.94	0.09	53,66,133,154	0
32	LHG	D	407[A]	49/49	0.94	0.09	48,59,109,112	49
32	LHG	D	407[B]	49/49	0.94	0.09	48,59,109,112	49
23	CLA	B	616	65/65	0.95	0.08	46,59,130,139	0
23	CLA	b	606	65/65	0.95	0.07	44,62,113,138	0
23	CLA	A	408	65/65	0.95	0.09	40,53,130,150	0
29	PL9	D	405[A]	55/55	0.95	0.07	37,47,58,65	55
29	PL9	D	405[B]	55/55	0.95	0.07	37,47,57,66	55
23	CLA	B	606	65/65	0.95	0.08	46,57,115,138	0
25	BCR	h	101	40/40	0.95	0.09	58,69,93,97	0
29	PL9	d	405[A]	55/55	0.95	0.07	38,50,60,73	55
29	PL9	d	405[B]	55/55	0.95	0.07	37,50,60,73	55
25	BCR	k	101	40/40	0.95	0.09	59,75,84,90	0
23	CLA	c	504	65/65	0.95	0.07	50,64,109,136	0
25	BCR	y	101	40/40	0.95	0.07	59,71,90,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	c	506	65/65	0.95	0.07	53,68,128,140	0
23	CLA	c	507	65/65	0.95	0.08	54,69,86,91	0
23	CLA	c	508	65/65	0.95	0.07	46,63,127,152	0
23	CLA	C	509	65/65	0.95	0.07	47,56,124,144	0
27	GOL	b	628	6/6	0.95	0.07	75,83,88,89	0
23	CLA	C	513	65/65	0.95	0.08	60,76,113,131	0
23	CLA	B	614	65/65	0.95	0.08	38,50,108,122	0
25	BCR	A	409	40/40	0.95	0.07	40,52,64,67	0
25	BCR	B	618	40/40	0.95	0.06	40,53,68,77	0
25	BCR	B	619	40/40	0.95	0.07	49,60,93,99	0
23	CLA	a	406[A]	65/65	0.95	0.07	41,53,126,135	65
23	CLA	a	406[B]	65/65	0.95	0.07	41,53,126,135	65
32	LHG	b	629[A]	49/49	0.95	0.08	47,57,73,92	49
35	DGD	C	519	62/66	0.95	0.07	44,57,96,110	0
35	DGD	H	102	62/66	0.95	0.08	46,62,73,86	0
35	DGD	c	516[A]	62/66	0.95	0.07	50,65,104,113	62
35	DGD	c	516[B]	62/66	0.95	0.07	49,65,104,113	62
32	LHG	b	629[B]	49/49	0.95	0.08	47,57,73,92	49
32	LHG	d	407[A]	49/49	0.95	0.08	51,62,114,129	49
35	DGD	c	518	62/66	0.95	0.07	49,68,101,134	0
35	DGD	h	102	62/66	0.95	0.08	54,66,77,83	0
32	LHG	d	407[B]	49/49	0.95	0.08	51,62,114,129	49
25	BCR	H	101	40/40	0.95	0.08	50,68,80,90	0
23	CLA	a	408	65/65	0.95	0.10	44,57,138,151	0
23	CLA	B	609	65/65	0.96	0.07	45,60,74,84	0
30	UNL	x	101	18/-	0.96	0.09	67,80,133,135	0
23	CLA	D	402[A]	65/65	0.96	0.06	33,43,65,73	65
23	CLA	D	402[B]	65/65	0.96	0.06	33,43,65,73	65
23	CLA	D	403	65/65	0.96	0.08	49,59,124,135	0
24	PHO	a	415[A]	64/64	0.96	0.06	45,55,62,70	64
24	PHO	a	415[B]	64/64	0.96	0.06	45,55,62,70	64
23	CLA	B	611	65/65	0.96	0.07	34,45,67,74	0
25	BCR	B	617	40/40	0.96	0.05	39,52,62,68	0
23	CLA	A	406[B]	65/65	0.96	0.06	38,47,111,122	65
23	CLA	A	404[A]	65/65	0.96	0.06	37,41,59,68	65
23	CLA	C	502	65/65	0.96	0.06	50,62,71,80	0
25	BCR	C	516	40/40	0.96	0.06	50,65,76,88	0
23	CLA	b	604	65/65	0.96	0.07	40,53,99,121	0
23	CLA	A	404[B]	65/65	0.96	0.06	36,42,60,68	65
23	CLA	b	607	65/65	0.96	0.06	37,46,83,89	0
23	CLA	b	611	65/65	0.96	0.06	39,48,72,79	0
23	CLA	b	612	65/65	0.96	0.07	42,54,65,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	LHG	D	406[A]	49/49	0.96	0.07	45,53,66,77	49
32	LHG	D	406[B]	49/49	0.96	0.07	45,53,66,78	49
25	BCR	a	409	40/40	0.96	0.06	45,55,65,68	0
25	BCR	b	617	40/40	0.96	0.06	44,54,64,74	0
35	DGD	C	517[A]	62/66	0.96	0.06	47,58,100,109	62
35	DGD	C	517[B]	62/66	0.96	0.06	46,58,100,109	62
25	BCR	b	618	40/40	0.96	0.05	44,55,79,87	0
25	BCR	b	619	40/40	0.96	0.07	50,62,88,95	0
23	CLA	C	506	65/65	0.96	0.07	50,61,96,107	0
25	BCR	c	515	40/40	0.96	0.07	54,66,82,89	0
23	CLA	B	602	65/65	0.96	0.07	47,58,75,88	0
23	CLA	c	501	65/65	0.96	0.07	52,69,82,95	0
32	LHG	d	406[A]	49/49	0.96	0.07	47,54,65,77	49
32	LHG	d	406[B]	49/49	0.96	0.07	48,54,65,77	49
23	CLA	c	503	65/65	0.96	0.07	50,71,86,89	0
23	CLA	C	508	65/65	0.96	0.08	53,65,84,98	0
23	CLA	c	505	65/65	0.96	0.07	51,65,93,96	0
36	CA	O	301	1/1	0.96	0.05	109,109,109,109	0
36	CA	c	522	1/1	0.96	0.07	77,77,77,77	0
23	CLA	B	603	65/65	0.96	0.07	42,53,72,83	0
23	CLA	A	406[A]	65/65	0.96	0.06	38,47,111,122	65
37	BCT	d	401[A]	4/4	0.96	0.06	56,59,66,78	4
37	BCT	d	401[B]	4/4	0.96	0.06	56,59,66,78	4
23	CLA	b	609	65/65	0.97	0.06	49,67,83,94	0
23	CLA	b	610	65/65	0.97	0.07	48,59,71,73	0
23	CLA	C	511	65/65	0.97	0.06	46,59,78,92	0
23	CLA	C	512	65/65	0.97	0.07	52,65,81,86	0
23	CLA	b	613	65/65	0.97	0.05	41,49,90,102	0
23	CLA	B	605	65/65	0.97	0.06	42,49,65,83	0
23	CLA	b	615	65/65	0.97	0.06	50,63,83,91	0
23	CLA	B	615	65/65	0.97	0.06	45,55,79,92	0
23	CLA	A	405[A]	65/65	0.97	0.05	34,42,57,74	65
23	CLA	c	502	65/65	0.97	0.06	43,59,88,103	0
23	CLA	B	607	65/65	0.97	0.06	35,46,73,83	0
23	CLA	C	503	65/65	0.97	0.06	44,54,82,93	0
23	CLA	a	404[A]	65/65	0.97	0.06	34,45,61,72	65
23	CLA	a	404[B]	65/65	0.97	0.06	38,46,61,72	65
23	CLA	a	405[A]	65/65	0.97	0.05	38,44,63,71	65
23	CLA	a	405[B]	65/65	0.97	0.05	38,44,64,71	65
23	CLA	c	509	65/65	0.97	0.07	45,61,87,94	0
23	CLA	c	510	65/65	0.97	0.06	49,62,79,95	0
23	CLA	c	511	65/65	0.97	0.07	57,69,86,101	0

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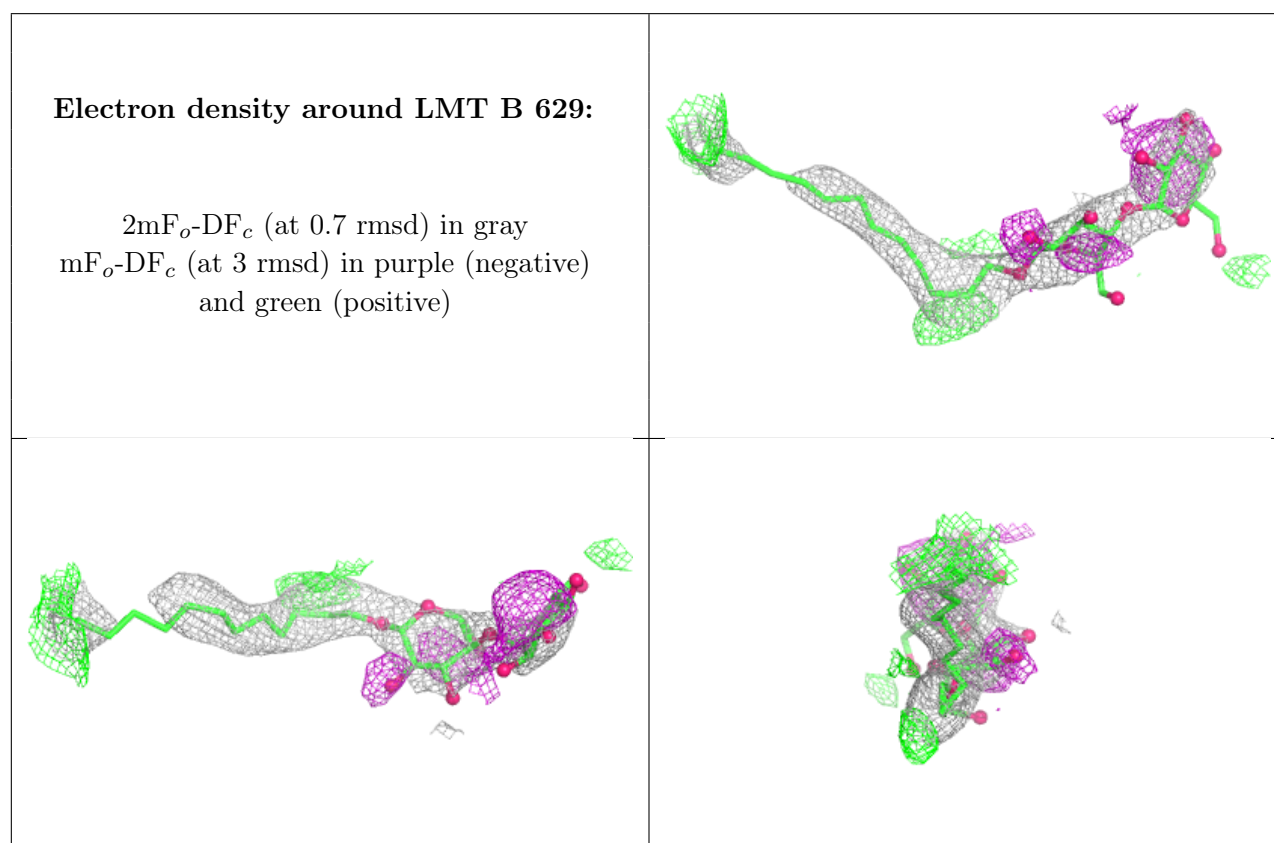
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	C	504	65/65	0.97	0.06	48,62,74,82	0
23	CLA	A	405[B]	65/65	0.97	0.05	34,42,57,74	65
23	CLA	d	402[A]	65/65	0.97	0.06	36,45,72,93	65
23	CLA	d	402[B]	65/65	0.97	0.06	36,45,72,93	65
23	CLA	B	610	65/65	0.97	0.08	40,54,67,83	0
24	PHO	A	407[A]	64/64	0.97	0.04	38,44,52,57	64
24	PHO	A	407[B]	64/64	0.97	0.04	38,44,51,57	64
32	LHG	L	101[A]	49/49	0.97	0.06	47,55,69,88	49
32	LHG	L	101[B]	49/49	0.97	0.06	47,55,69,88	49
24	PHO	A	416[A]	64/64	0.97	0.06	37,49,54,61	64
24	PHO	A	416[B]	64/64	0.97	0.06	37,49,54,61	64
24	PHO	a	407[A]	64/64	0.97	0.05	41,47,53,58	64
24	PHO	a	407[B]	64/64	0.97	0.05	41,47,53,58	64
23	CLA	B	604	65/65	0.97	0.06	38,47,106,132	0
36	CA	C	524	1/1	0.97	0.06	79,79,79,79	0
23	CLA	b	602	65/65	0.97	0.07	49,62,83,93	0
23	CLA	b	603	65/65	0.97	0.06	46,58,82,98	0
23	CLA	B	612	65/65	0.97	0.06	36,48,63,70	0
23	CLA	b	605	65/65	0.97	0.07	38,52,75,82	0
23	CLA	B	613	65/65	0.97	0.06	38,45,97,109	0
37	BCT	D	401[A]	4/4	0.97	0.07	51,52,58,69	4
37	BCT	D	401[B]	4/4	0.97	0.07	51,52,58,70	4
23	CLA	C	510	65/65	0.97	0.08	48,58,84,92	0
23	CLA	b	608	65/65	0.97	0.05	45,55,83,89	0
22	CL	a	403[B]	1/1	0.98	0.08	52,52,52,52	1
22	CL	A	403[A]	1/1	0.98	0.05	46,46,46,46	1
22	CL	A	403[B]	1/1	0.98	0.05	45,45,45,45	1
23	CLA	B	608	65/65	0.98	0.04	35,49,68,78	0
22	CL	a	403[A]	1/1	0.98	0.08	52,52,52,52	1
38	HEM	F	102	43/43	0.98	0.06	55,70,84,94	0
38	HEM	f	101	43/43	0.98	0.08	59,85,115,142	0
40	HEC	V	201	43/43	0.98	0.06	39,50,57,61	0
40	HEC	v	201	43/43	0.98	0.07	51,62,70,75	0
22	CL	A	402[A]	1/1	0.99	0.06	41,41,41,41	1
22	CL	A	402[B]	1/1	0.99	0.06	41,41,41,41	1
28	OEX	A	413[A]	10/10	0.99	0.03	37,44,49,50	10
36	CA	c	523	1/1	0.99	0.05	77,77,77,77	0
28	OEX	A	413[B]	10/10	0.99	0.03	37,45,48,50	10
39	MG	J	102	1/1	0.99	0.03	58,58,58,58	0
22	CL	a	402[A]	1/1	0.99	0.06	47,47,47,47	1
22	CL	a	402[B]	1/1	0.99	0.06	47,47,47,47	1
28	OEX	a	412[B]	10/10	1.00	0.02	46,49,54,55	10

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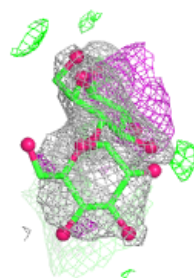
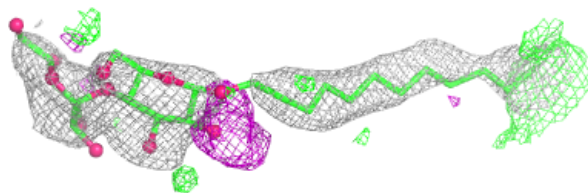
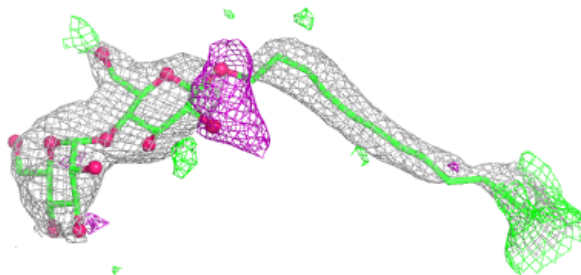
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	FE2	a	401[A]	1/1	1.00	0.01	53,53,53,53	1
21	FE2	a	401[B]	1/1	1.00	0.01	53,53,53,53	1
21	FE2	A	401[A]	1/1	1.00	0.01	49,49,49,49	1
39	MG	j	102	1/1	1.00	0.03	63,63,63,63	0
21	FE2	A	401[B]	1/1	1.00	0.01	49,49,49,49	1
28	OEX	a	412[A]	10/10	1.00	0.02	46,49,53,55	10

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.

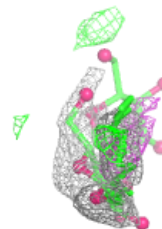
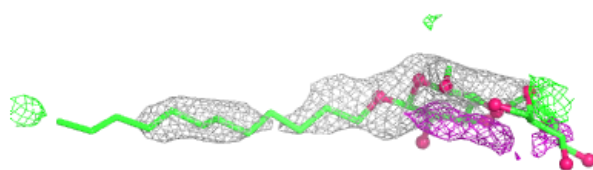
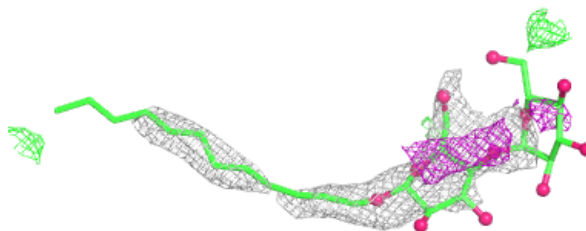


Electron density around LMT A 417:

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

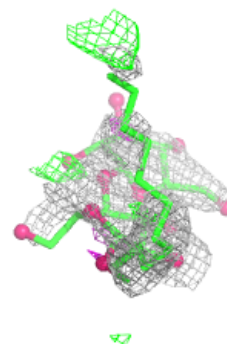
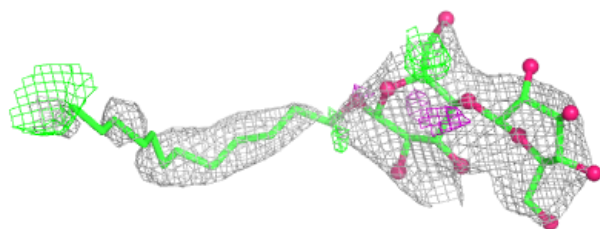
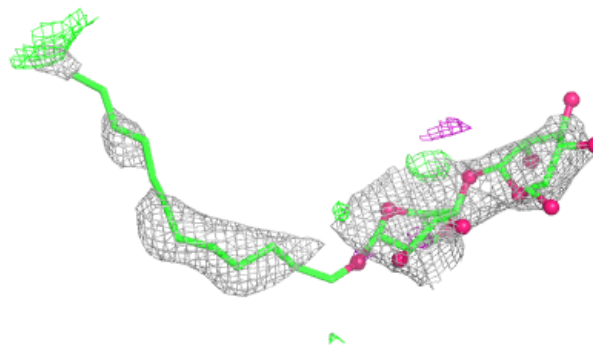
**Electron density around LMT F 101:**

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

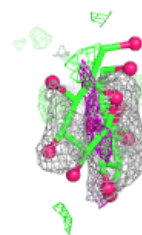
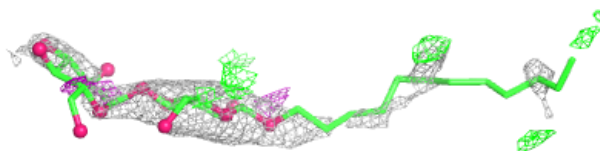
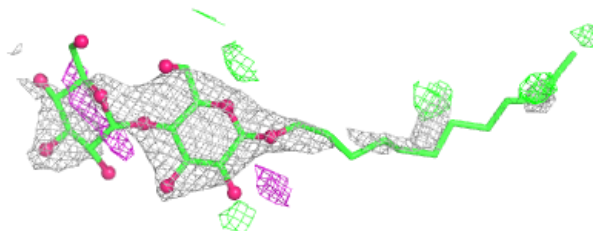


Electron density around LMT A 420:

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

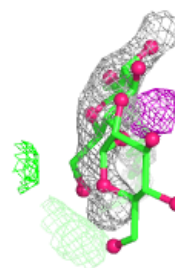
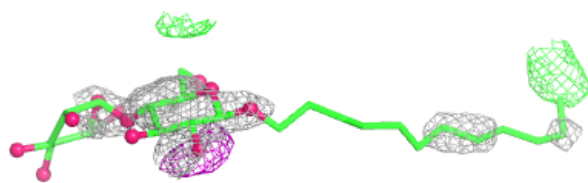
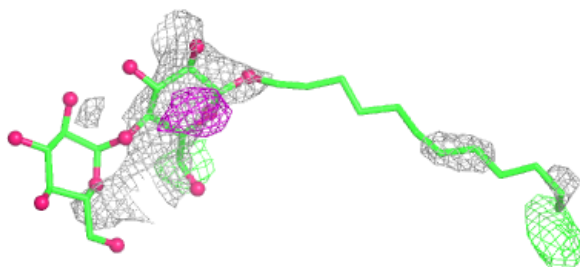
**Electron density around LMT a 417:**

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

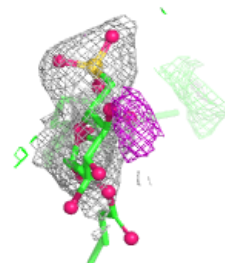
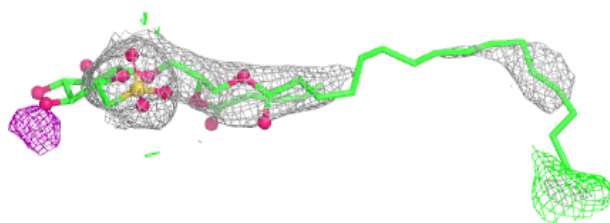
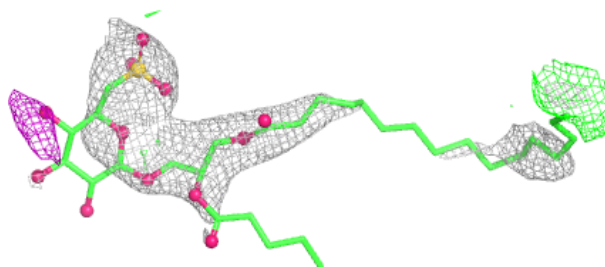


Electron density around LMT e 101:

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

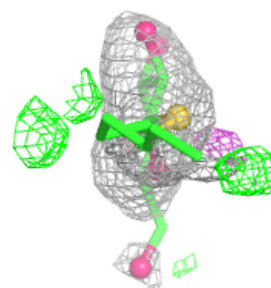
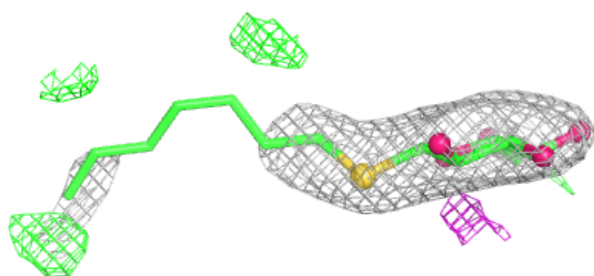
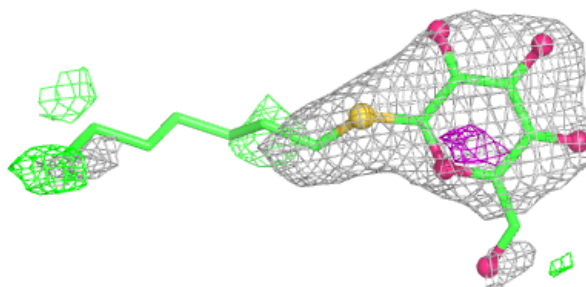
**Electron density around SQD f 102:**

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

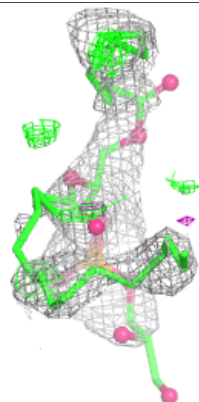
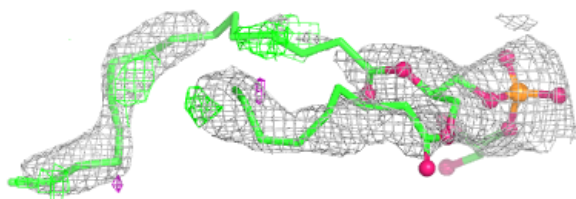
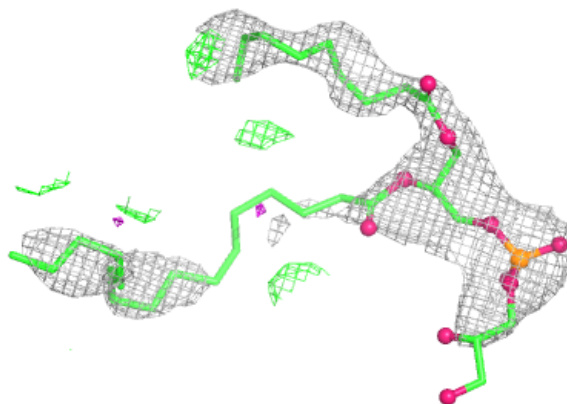


Electron density around HTG C 522:

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

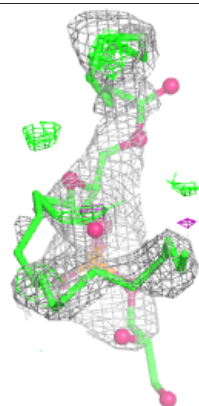
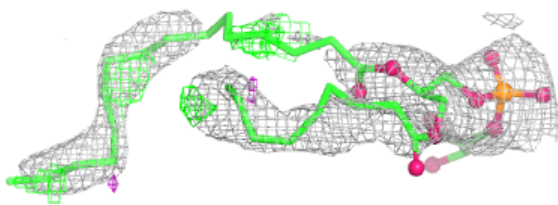
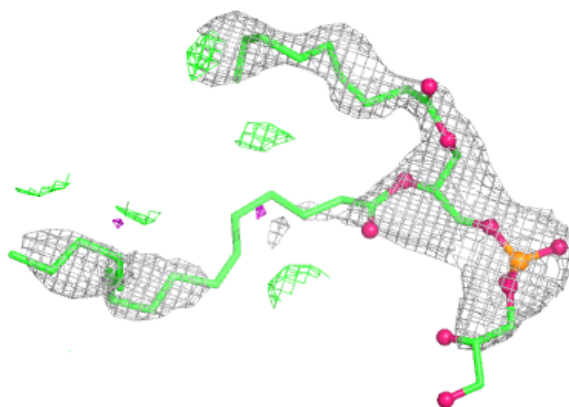
**Electron density around LHG a 420 (A):**

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

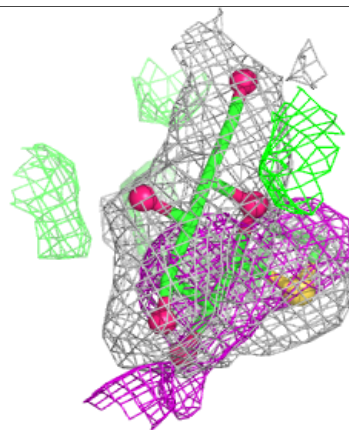
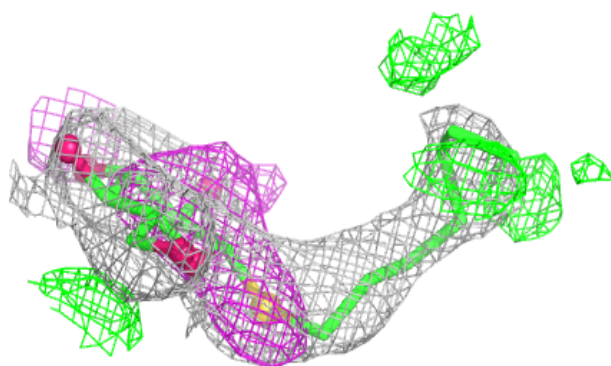
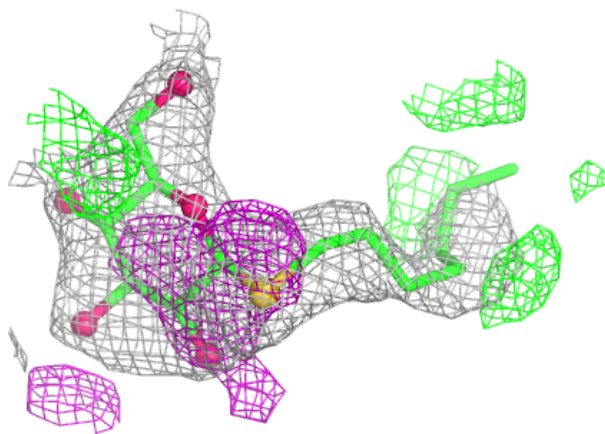


Electron density around LHG a 420 (B):

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

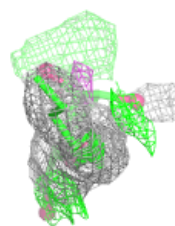
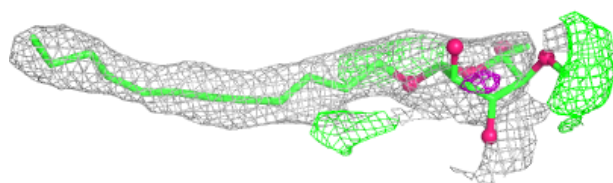
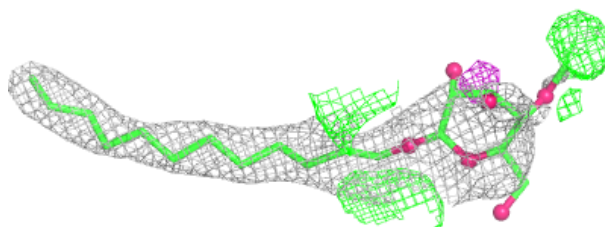
**Electron density around HTG B 622:**

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

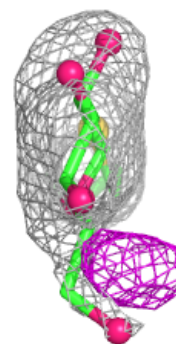
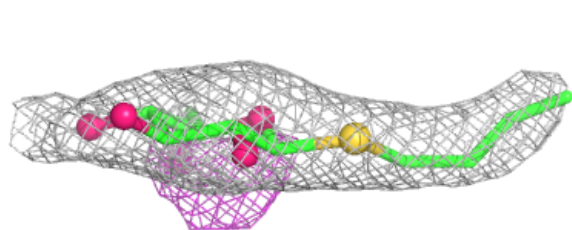
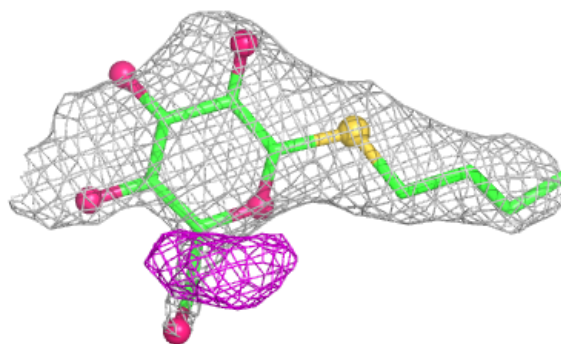


Electron density around LMT b 621:

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

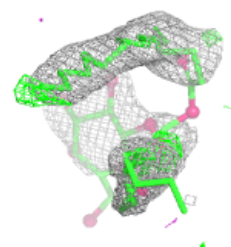
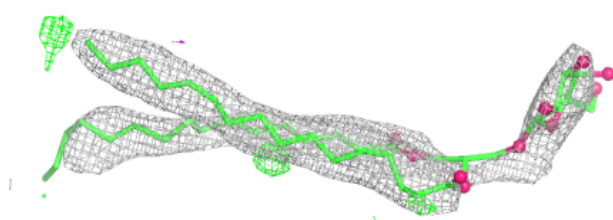
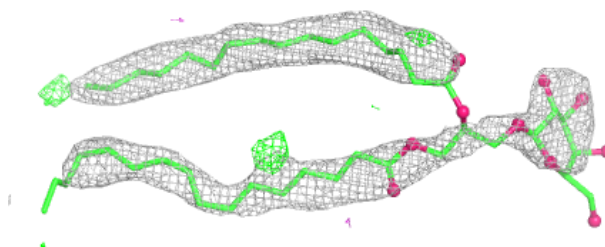
**Electron density around HTG D 410:**

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

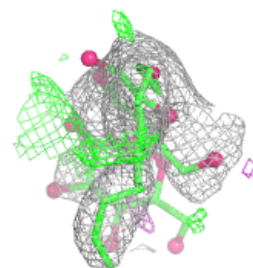
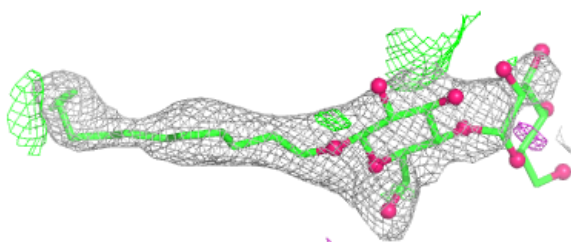
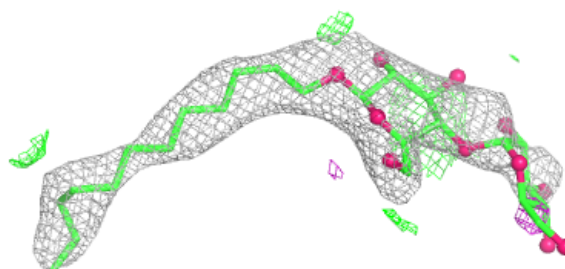


Electron density around LMG C 521:

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

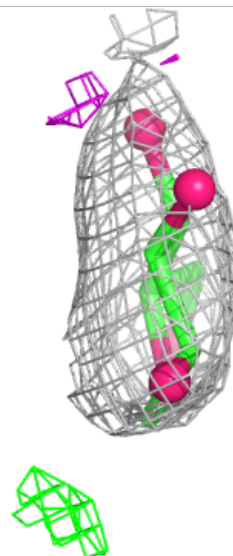
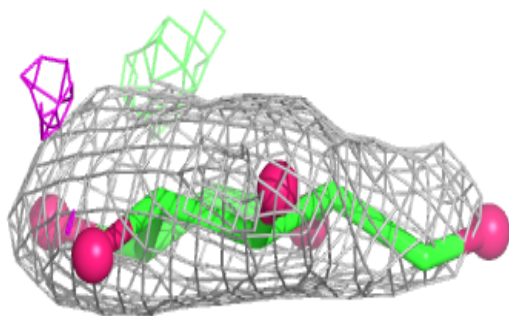
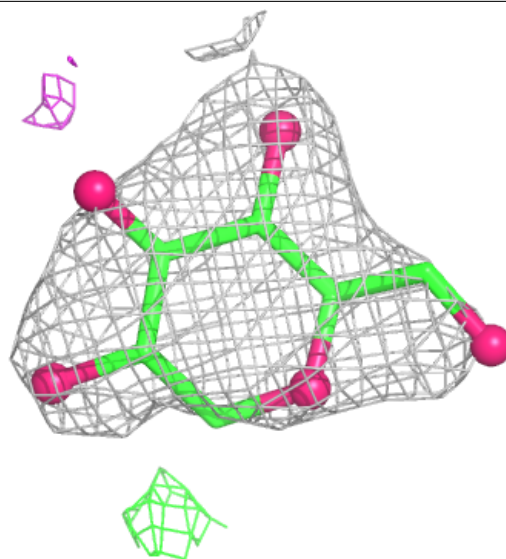
**Electron density around LMT M 103:**

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



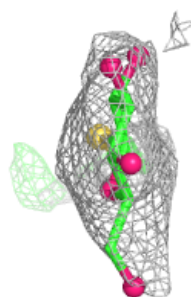
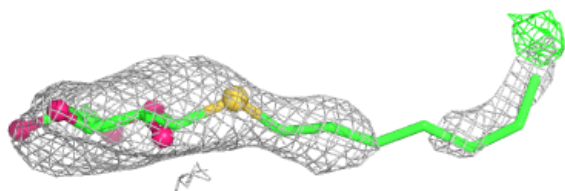
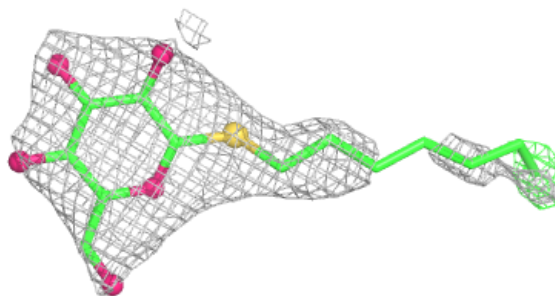
Electron density around HTG V 202:

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

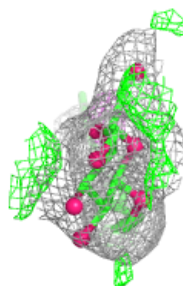
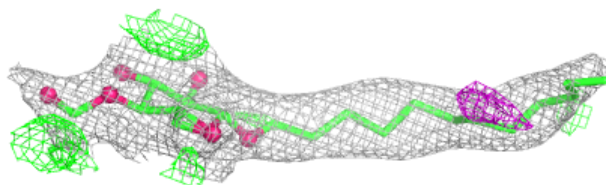
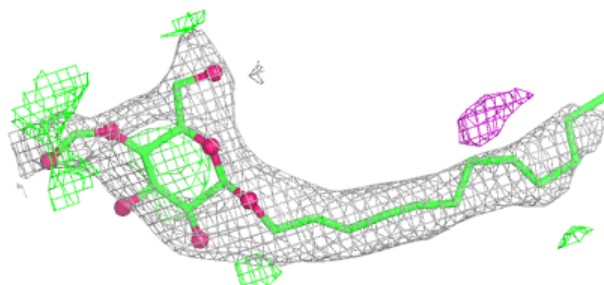


Electron density around HTG c 521:

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and green (positive)

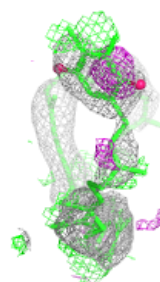
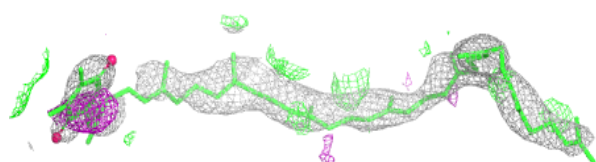
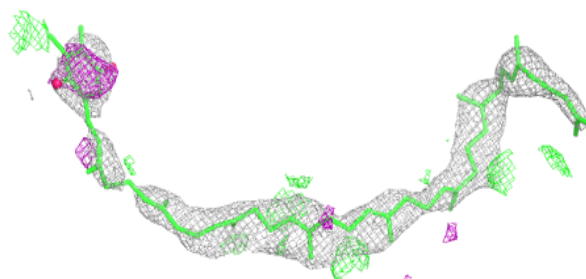
**Electron density around LMT t 101:**

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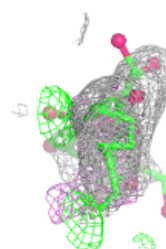
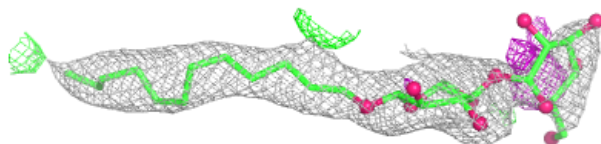
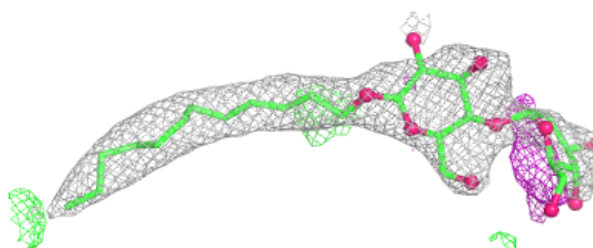


Electron density around PL9 a 413 (B):

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

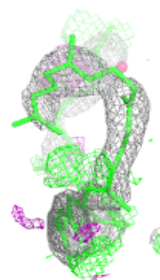
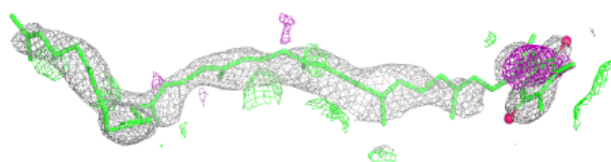
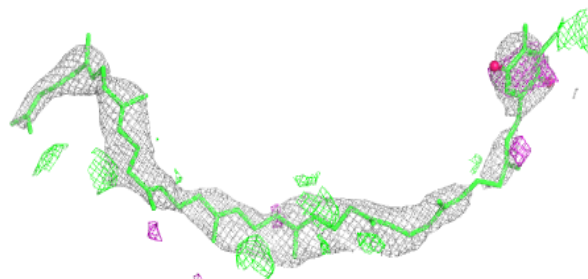
**Electron density around LMT B 627:**

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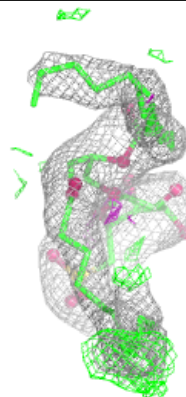
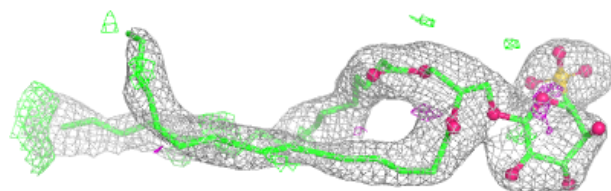
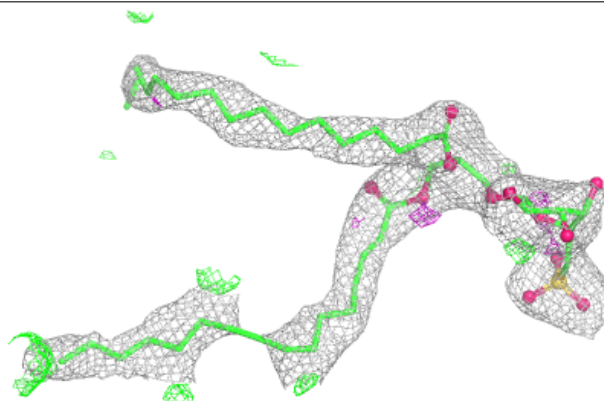


Electron density around PL9 a 413 (A):

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

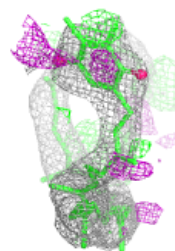
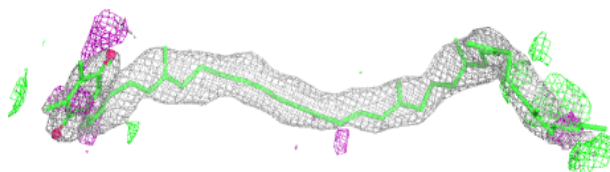
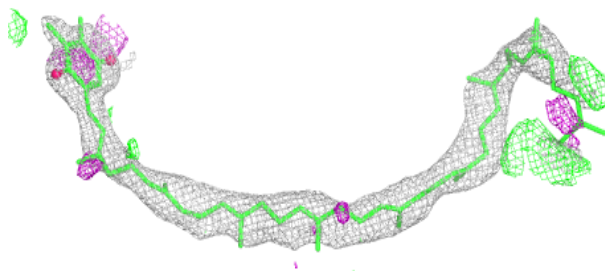
**Electron density around SQD a 411:**

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

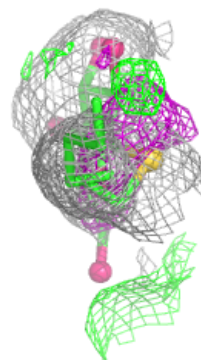
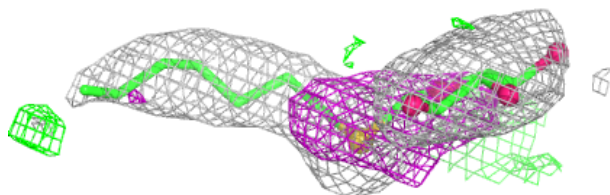
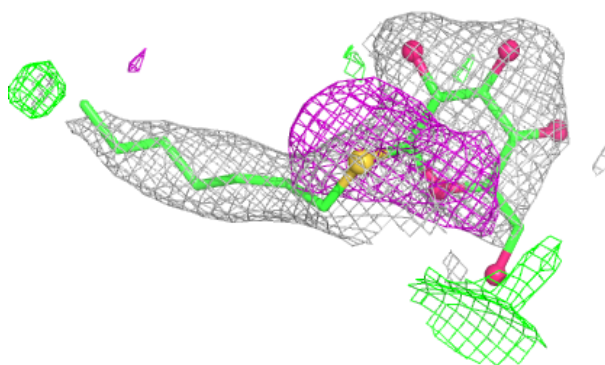


Electron density around PL9 A 414 (A):

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

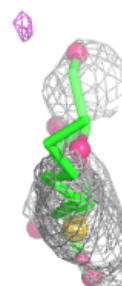
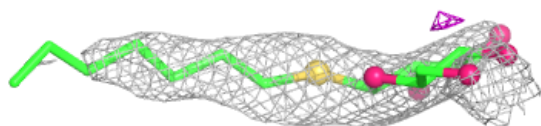
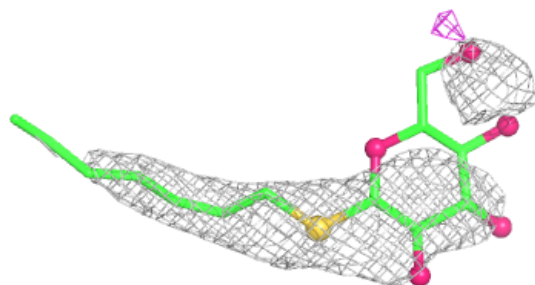
**Electron density around HTG b 622:**

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

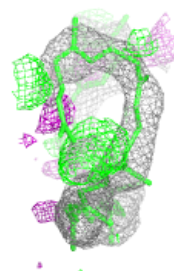
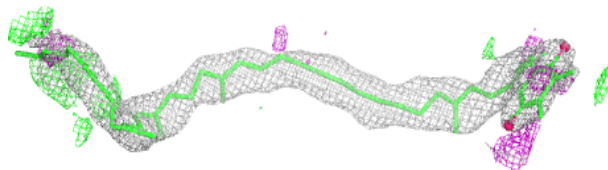
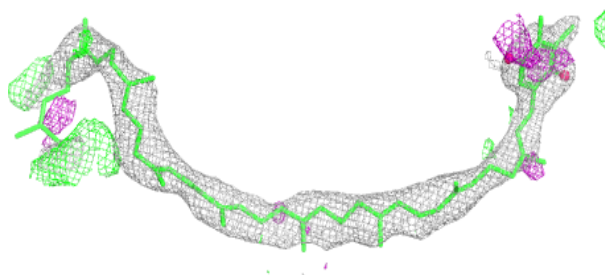


Electron density around HTG b 623:

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

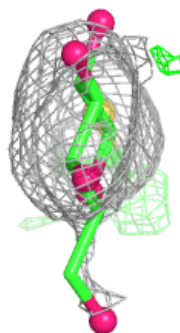
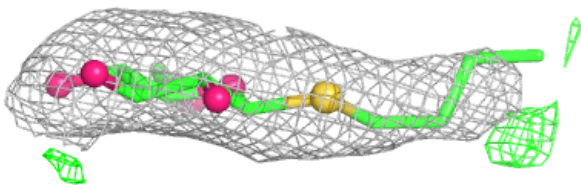
**Electron density around PL9 A 414 (B):**

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

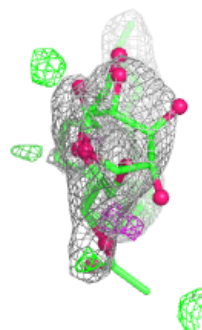
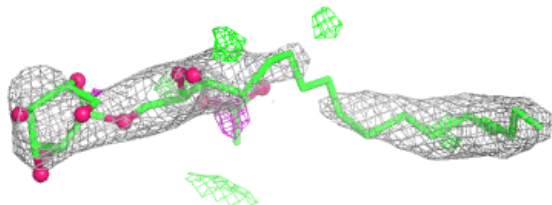
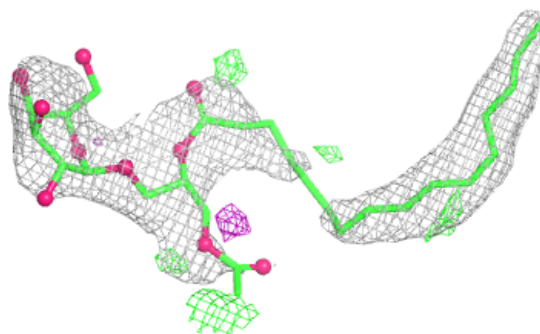


Electron density around HTG d 410:

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

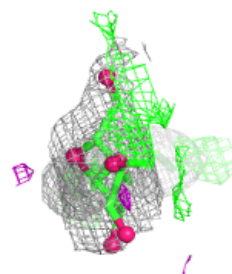
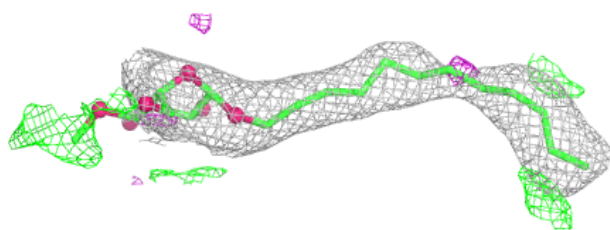
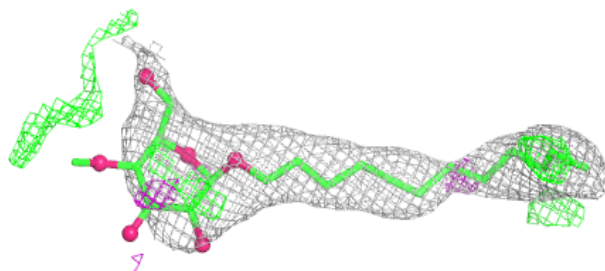
**Electron density around LMG Z 101:**

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

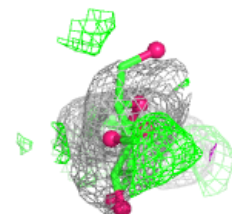
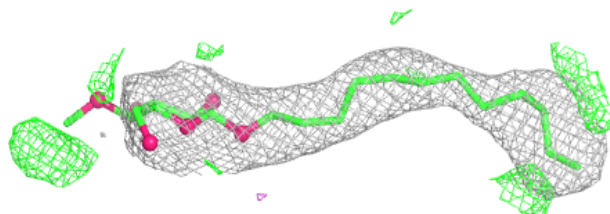
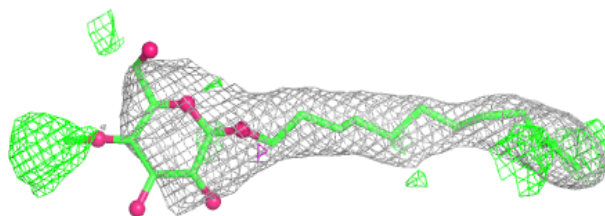


Electron density around LMT B 631:

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

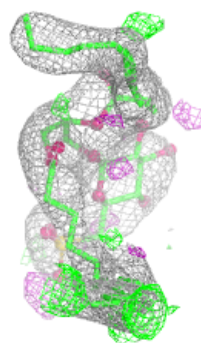
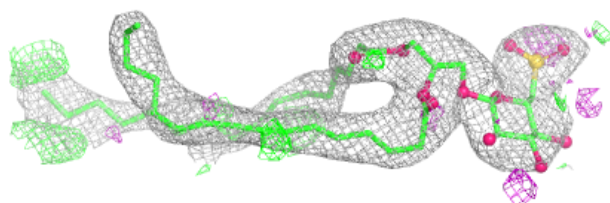
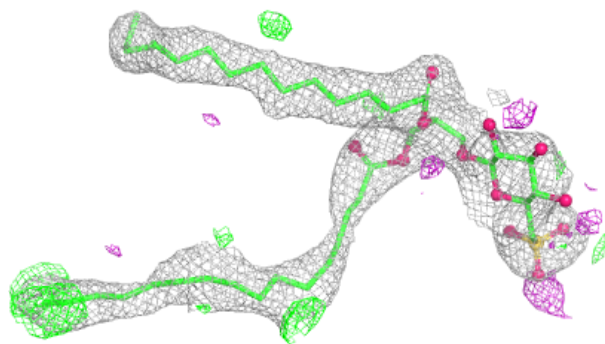
**Electron density around LMT b 627:**

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

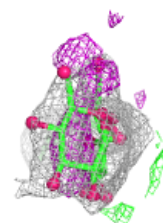
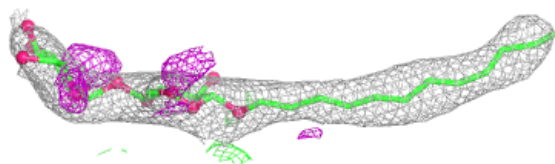
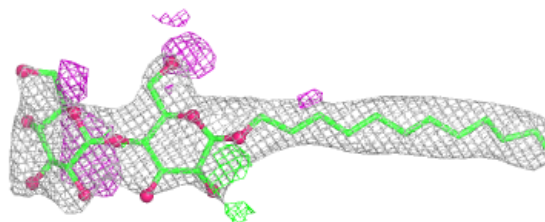


Electron density around SQD A 412:

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

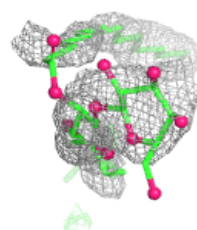
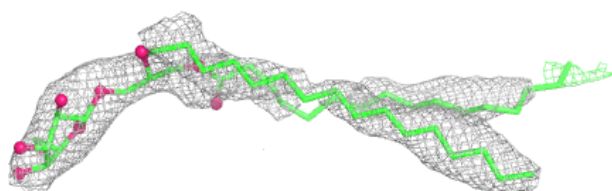
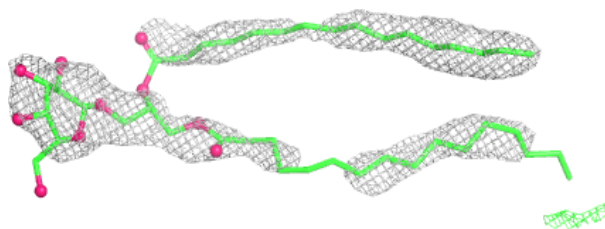
**Electron density around LMT m 103:**

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

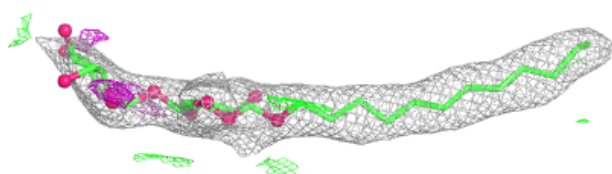
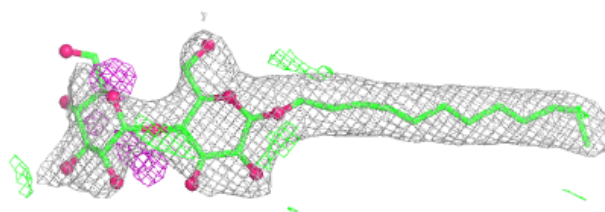


Electron density around LMG c 520:

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

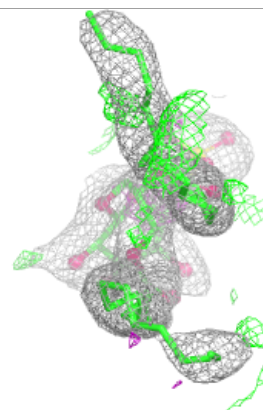
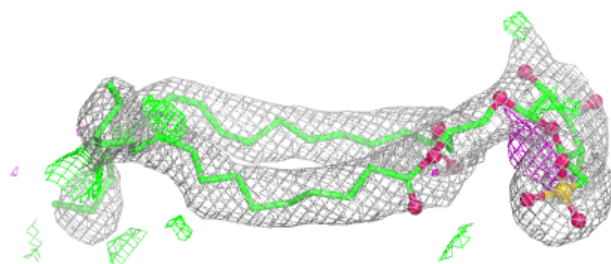
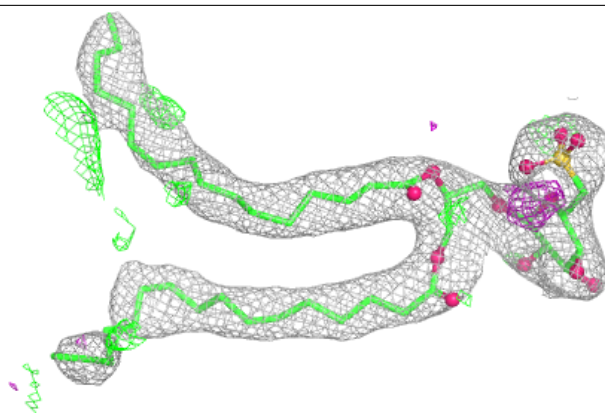
**Electron density around LMT M 101:**

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

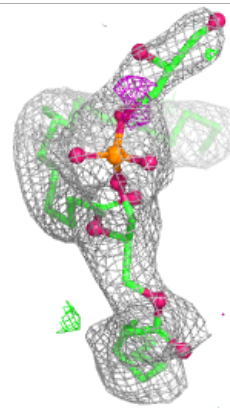
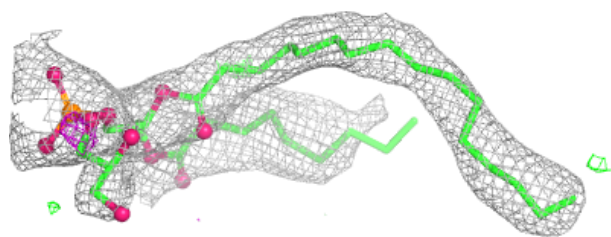
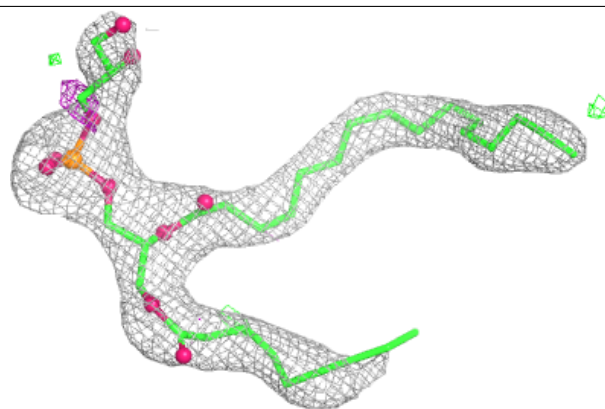


Electron density around SQD b 620:

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

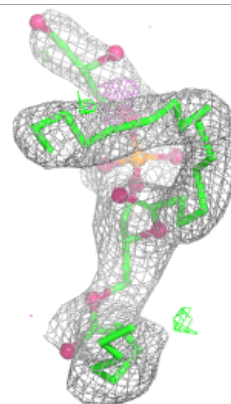
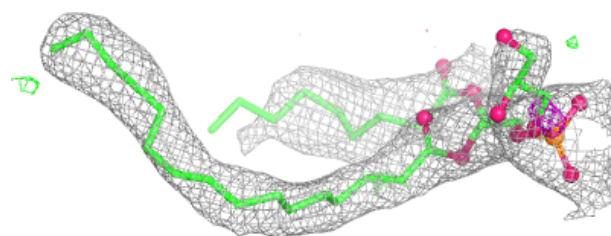
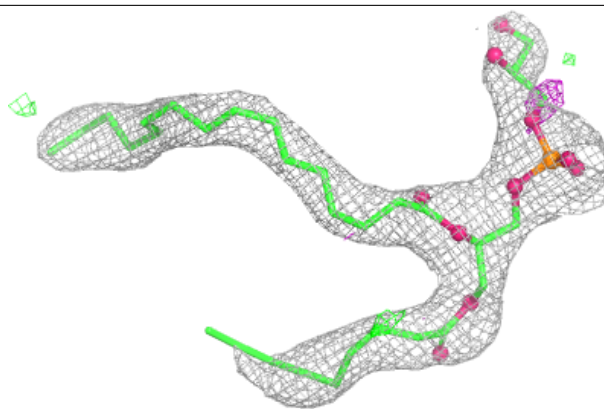
**Electron density around LHG E 101 (A):**

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

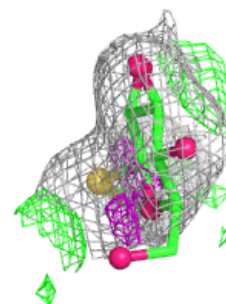
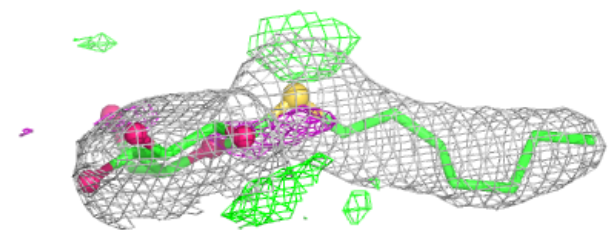
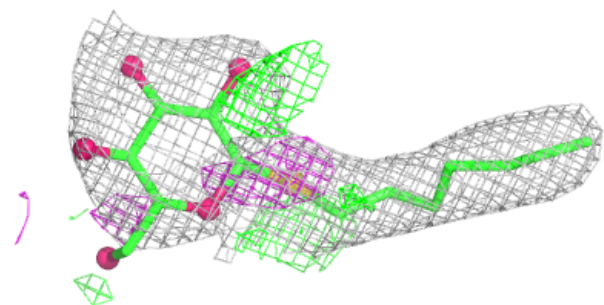


Electron density around LHG E 101 (B):

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

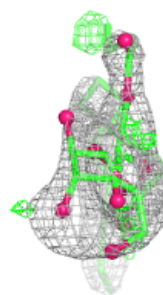
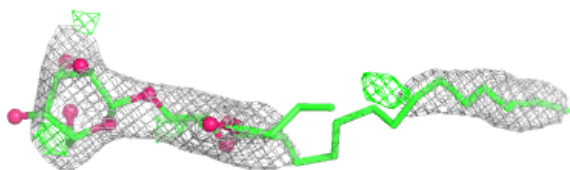
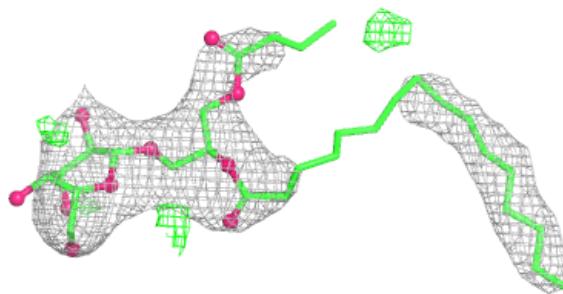
**Electron density around HTG o 301:**

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

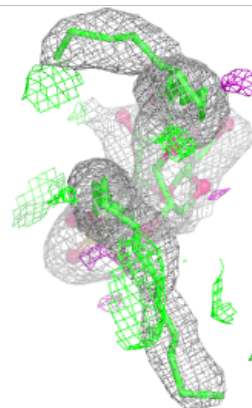
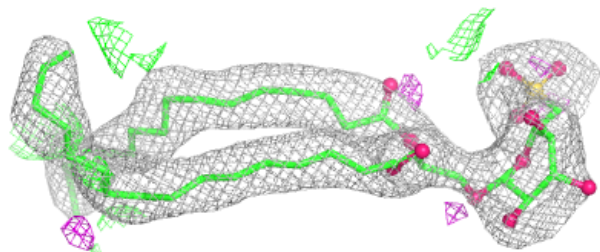
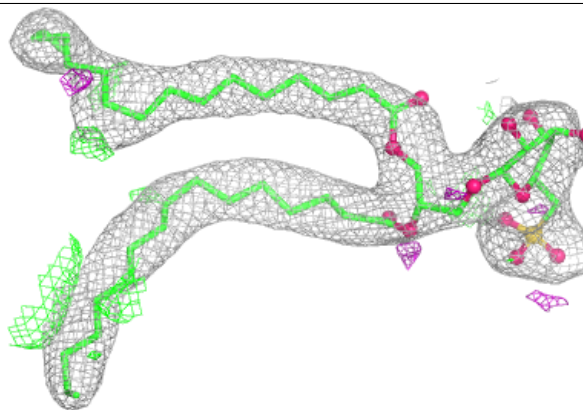


Electron density around LMG z 101:

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

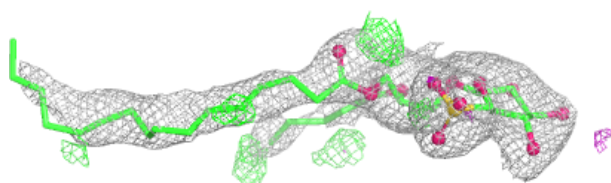
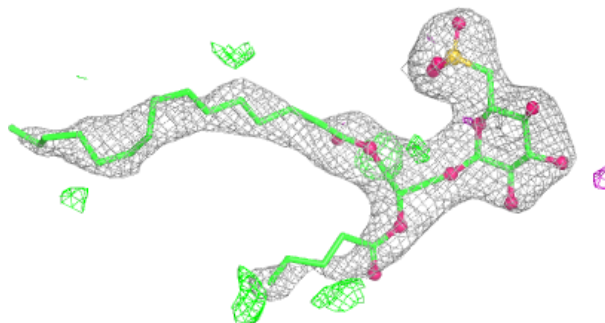
**Electron density around SQD B 620:**

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

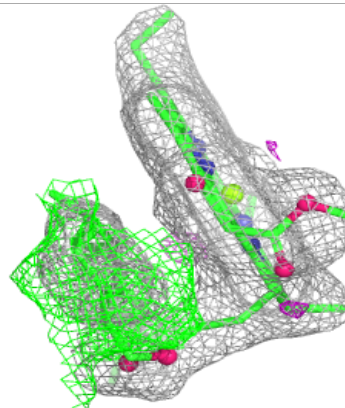
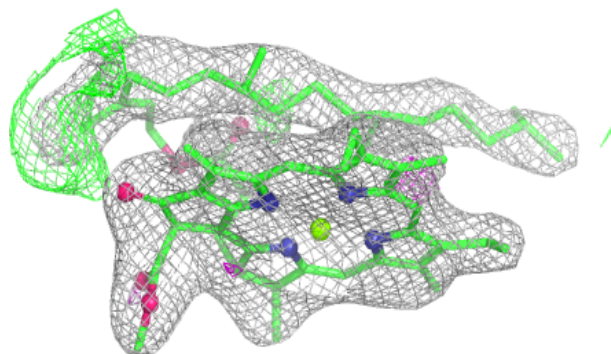
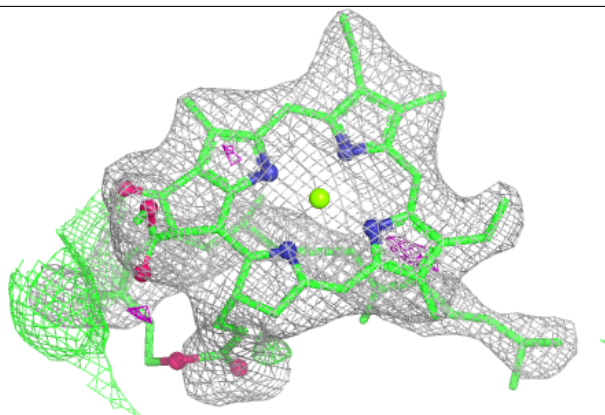


Electron density around SQD F 103:

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

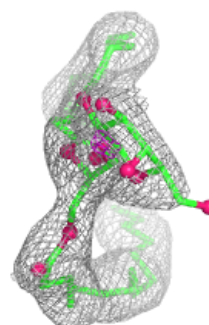
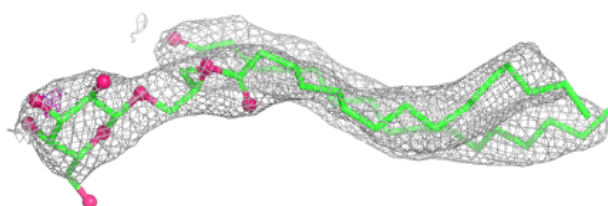
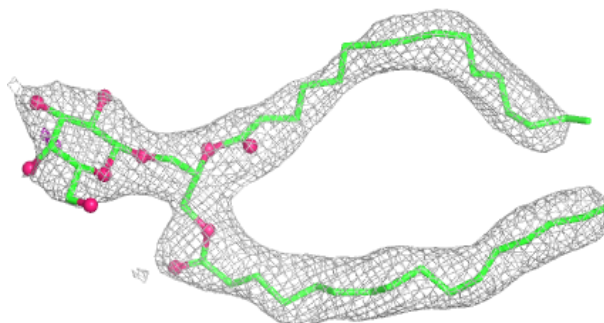
**Electron density around CLA b 601:**

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

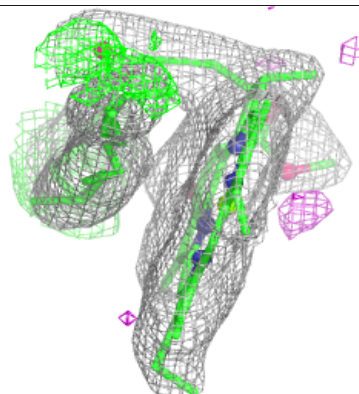
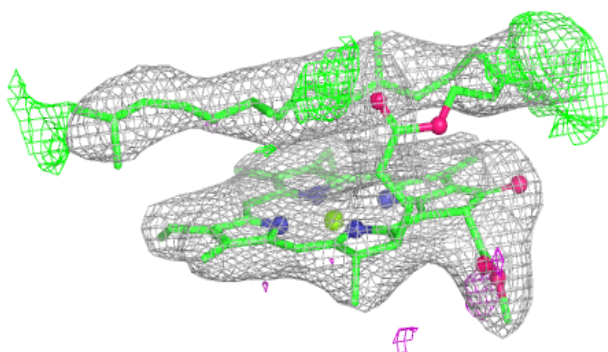
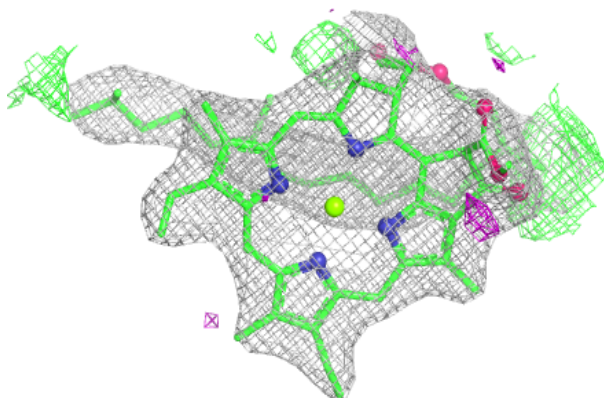


Electron density around LMG a 416:

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

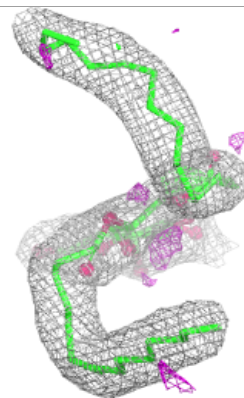
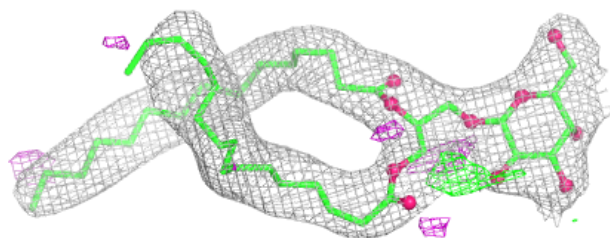
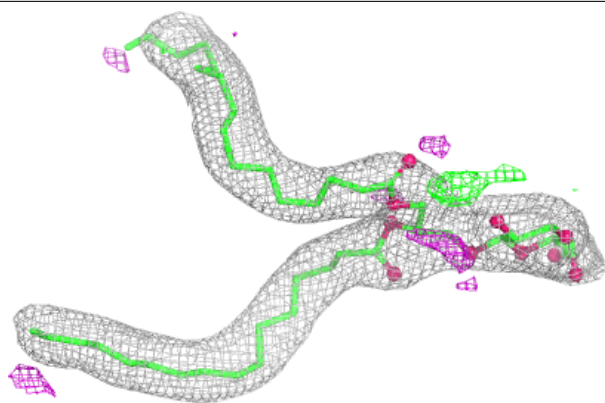
**Electron density around CLA B 601:**

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

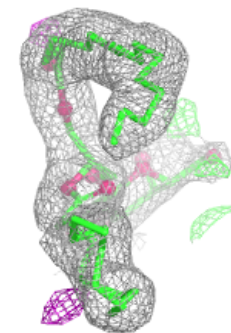
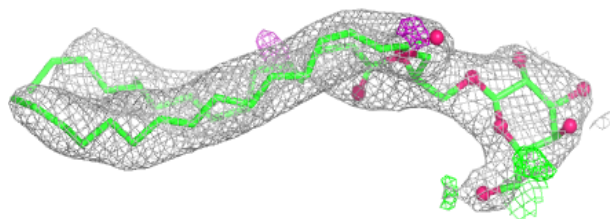
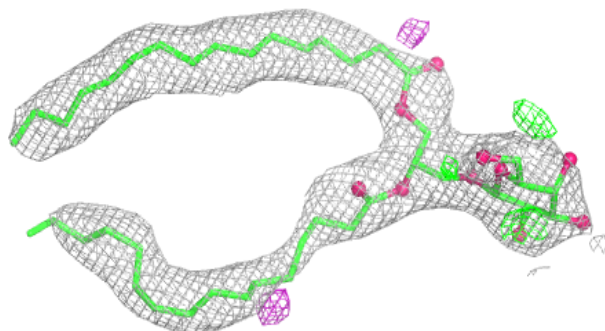


Electron density around LMG m 101:

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

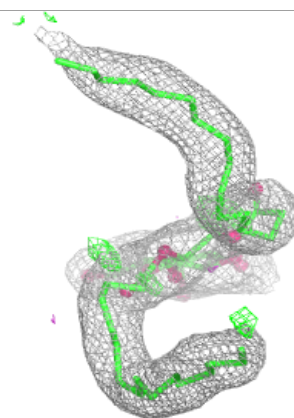
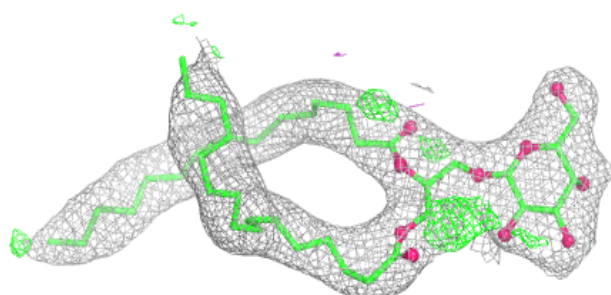
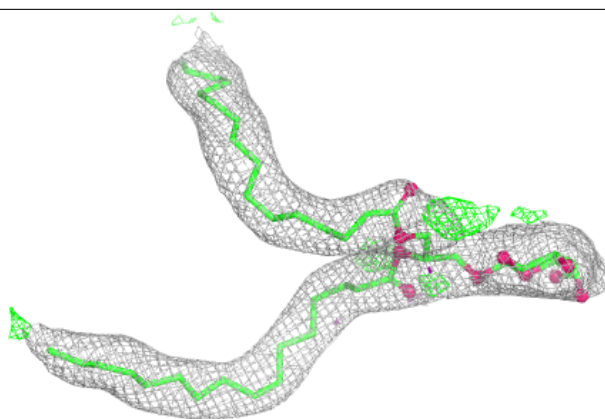
**Electron density around LMG C 501:**

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

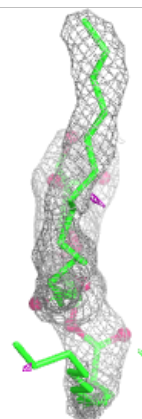
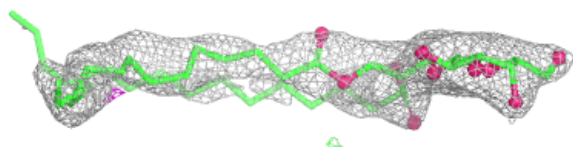
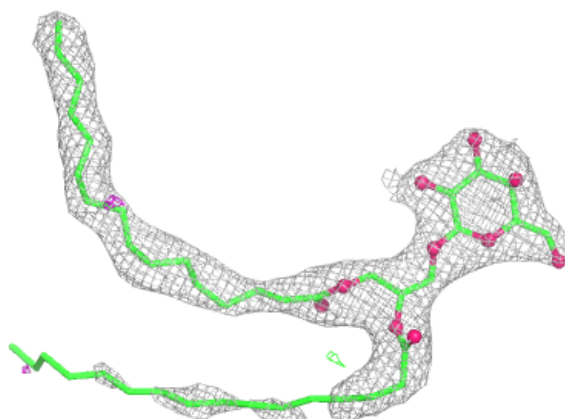


Electron density around LMG B 621:

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

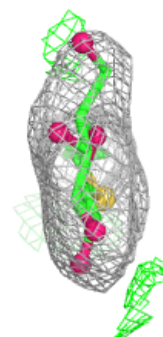
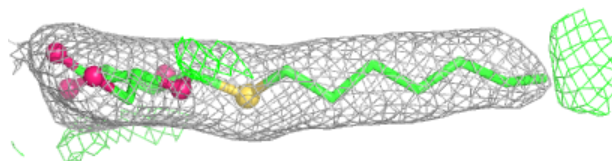
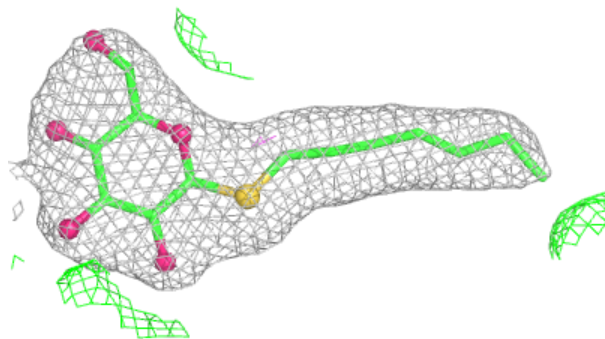
**Electron density around LMG c 519:**

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

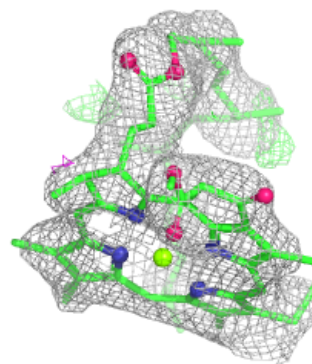
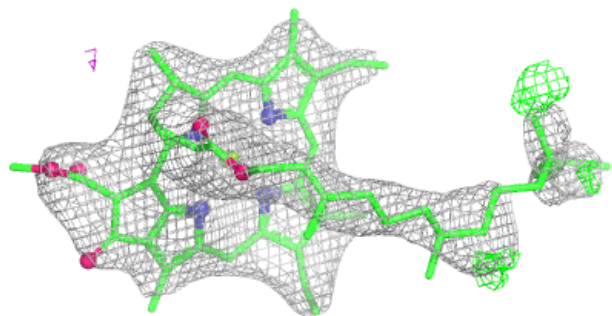
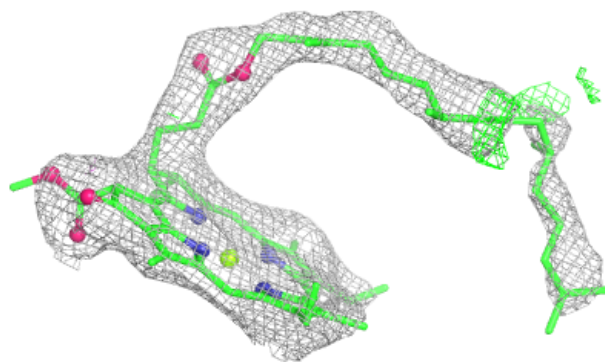


Electron density around HTG B 624:

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

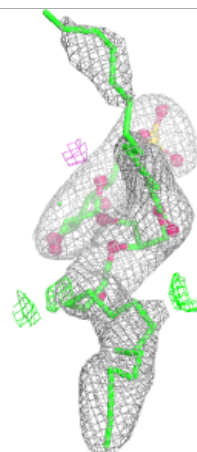
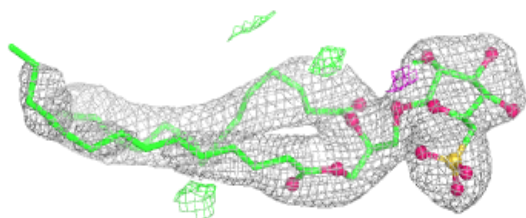
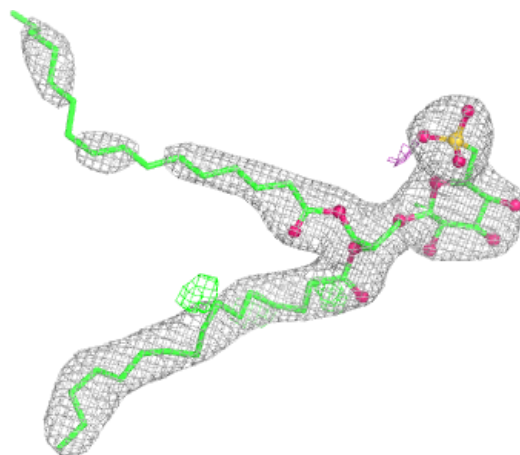
**Electron density around CLA c 513:**

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



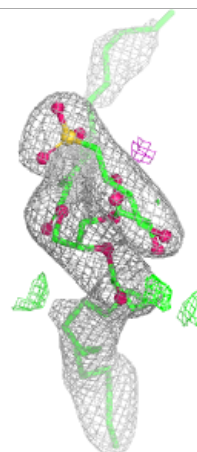
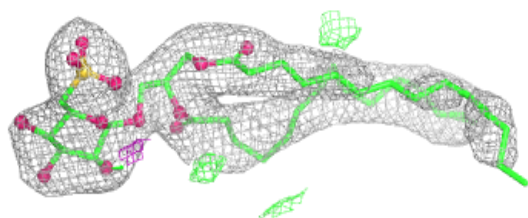
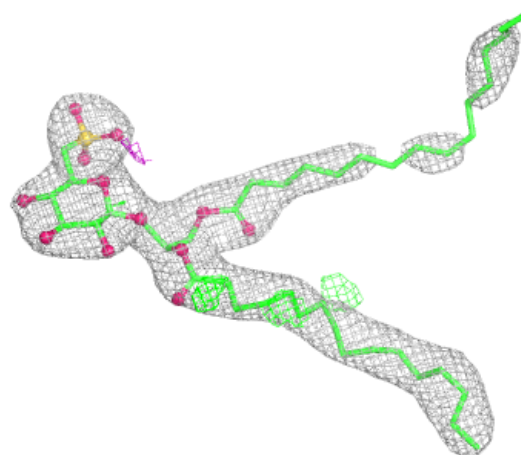
Electron density around SQD A 410 (A):

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



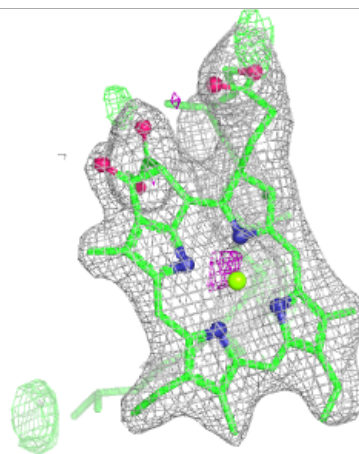
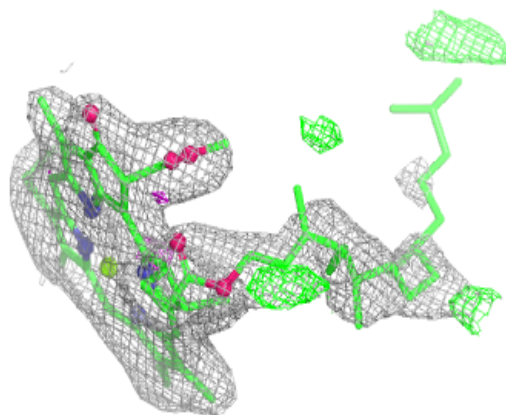
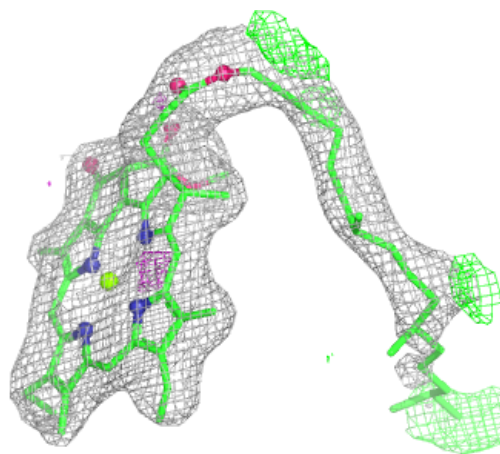
Electron density around SQD A 410 (B):

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



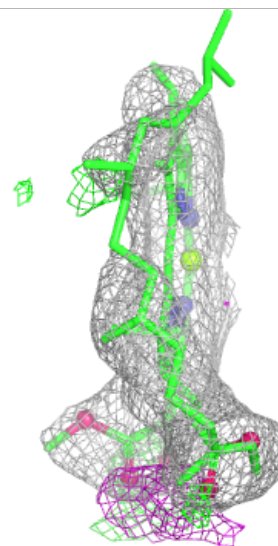
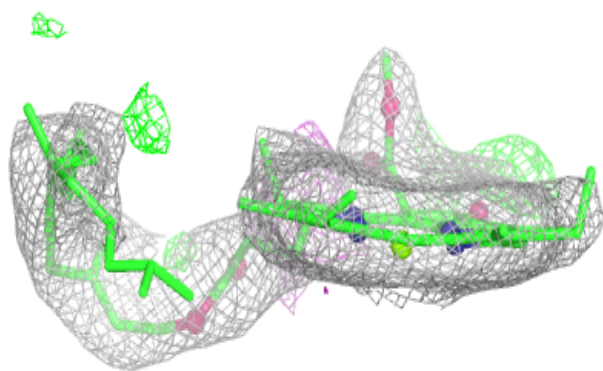
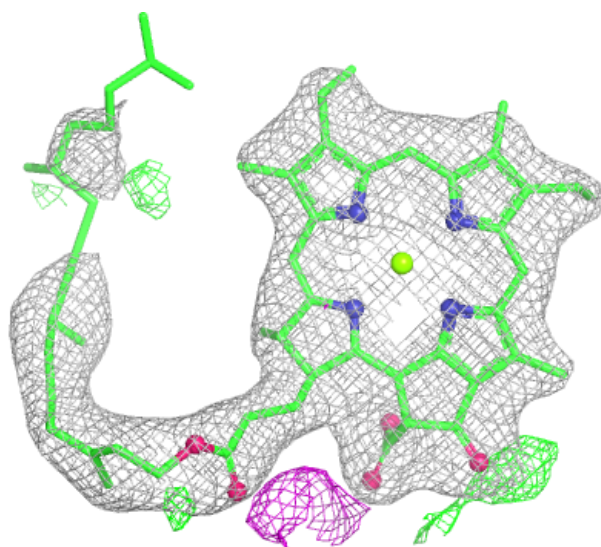
Electron density around CLA b 616:

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



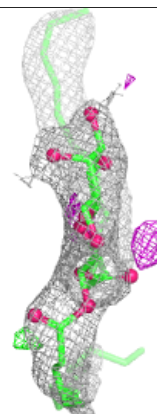
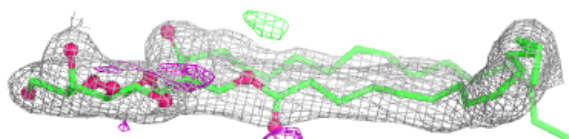
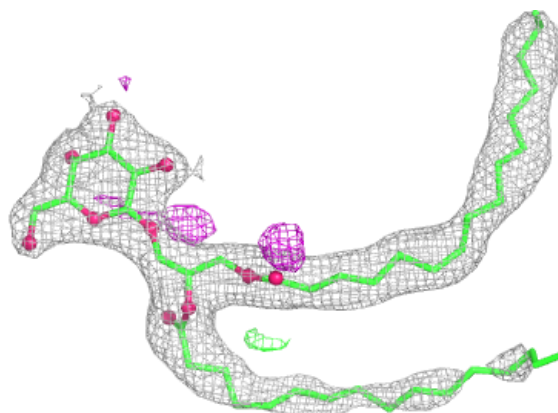
Electron density around CLA c 512:

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

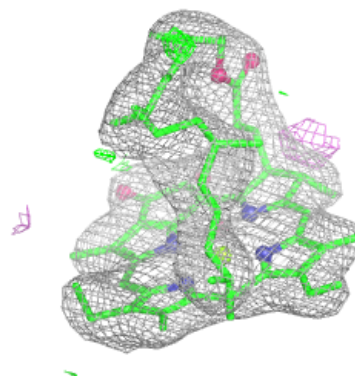
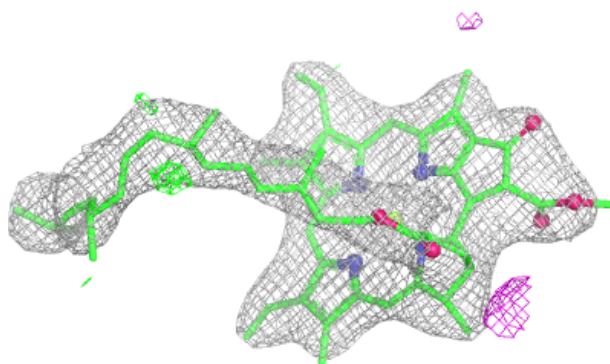
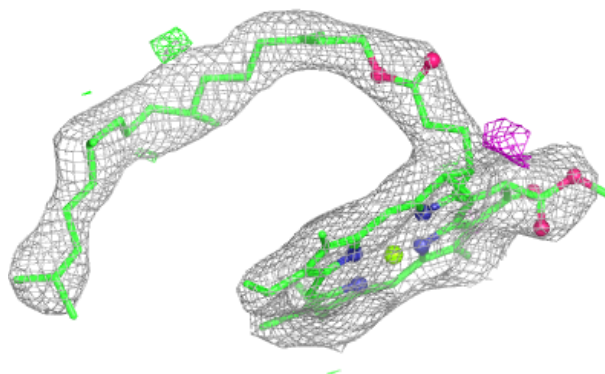


Electron density around LMG C 520:

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

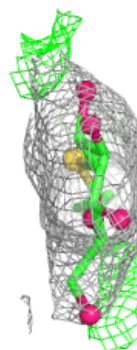
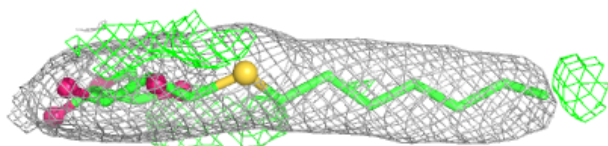
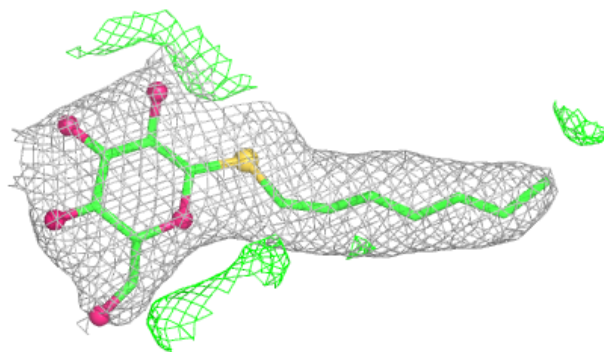
**Electron density around CLA C 514:**

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

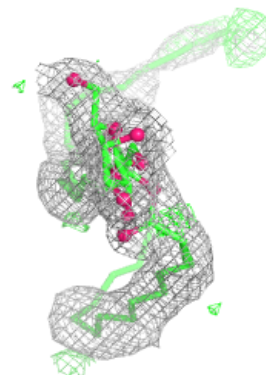
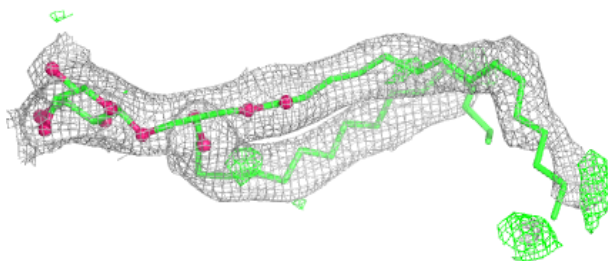
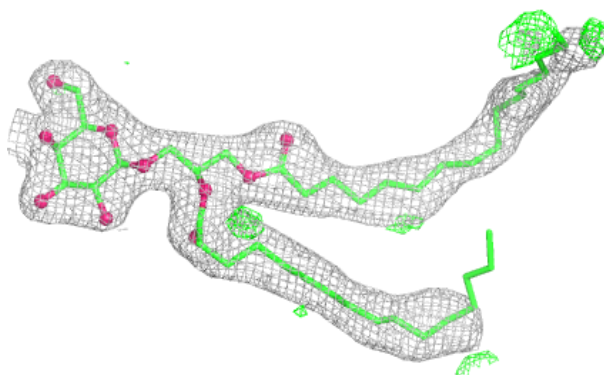


Electron density around HTG b 625:

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

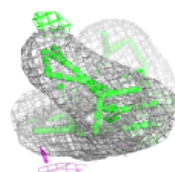
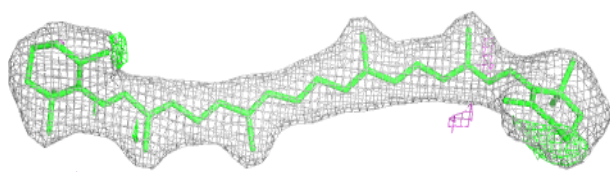
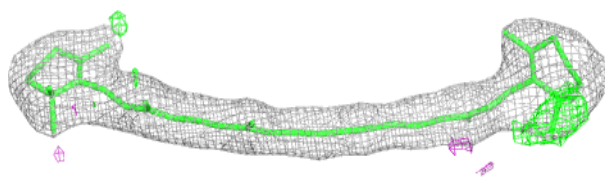
**Electron density around LMG D 411:**

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

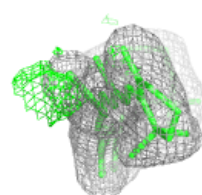
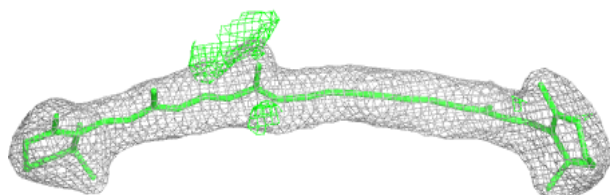
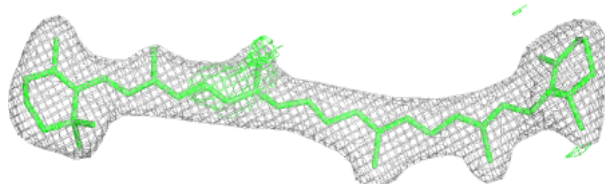


Electron density around BCR D 404:

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

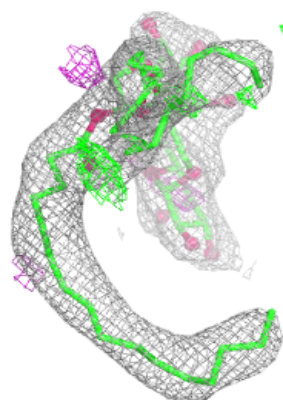
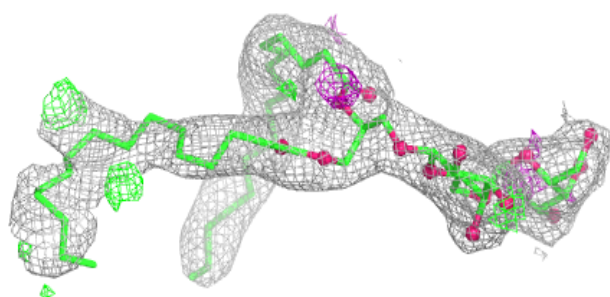
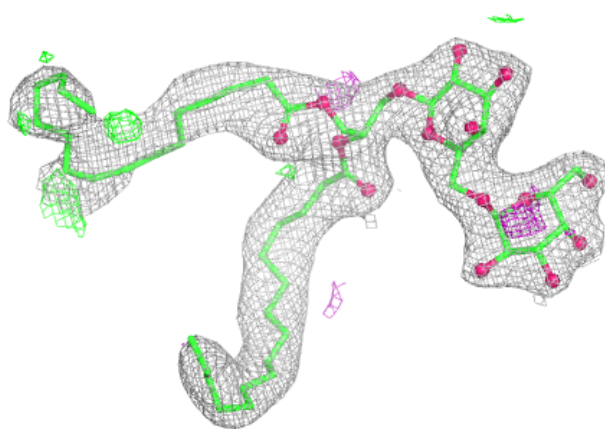
**Electron density around BCR T 101:**

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

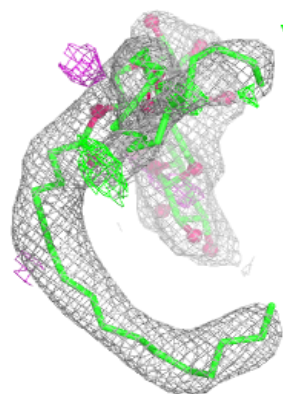
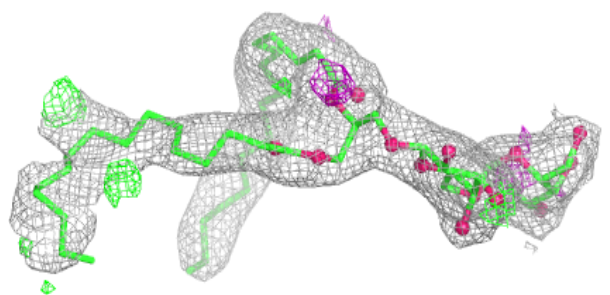
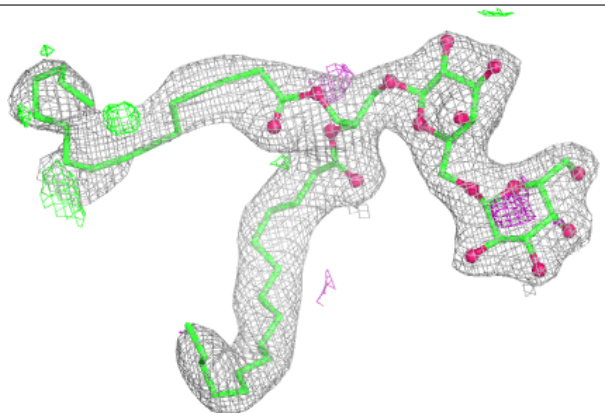


Electron density around DGD C 518 (A):

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

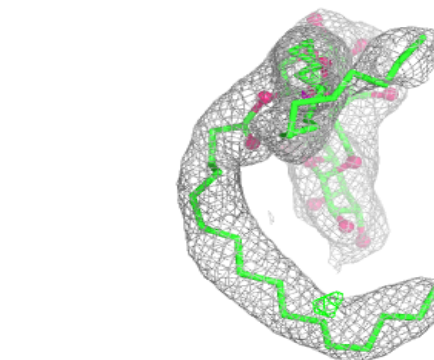
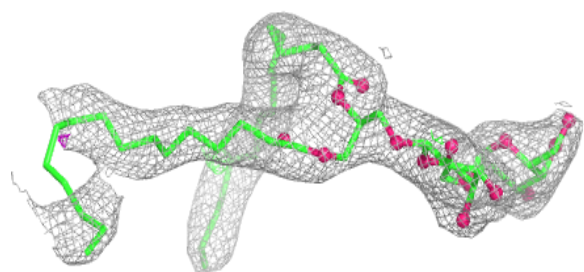
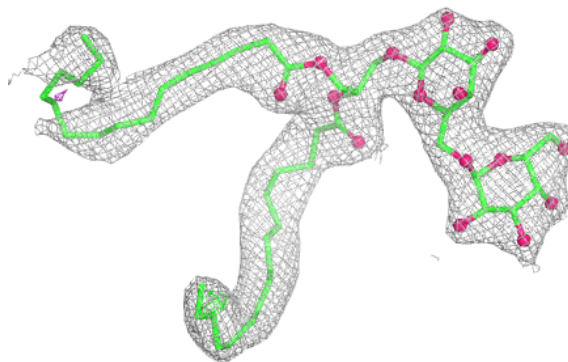
**Electron density around DGD C 518 (B):**

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

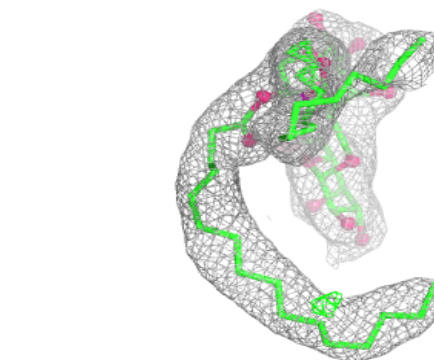
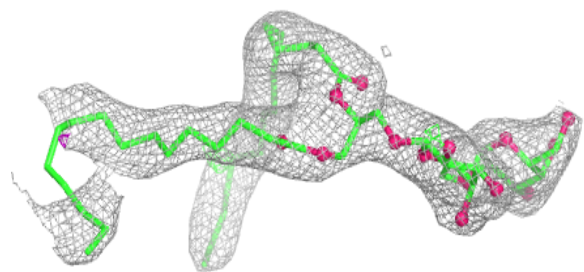
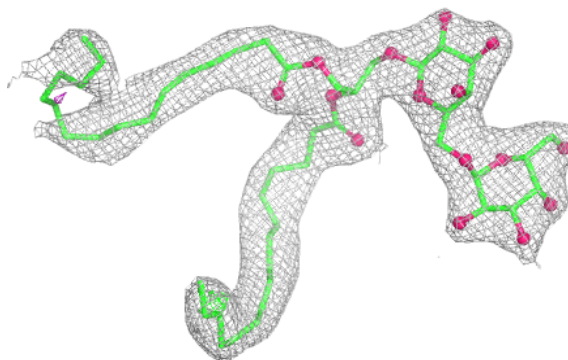


Electron density around DGD c 517 (A):

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

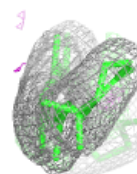
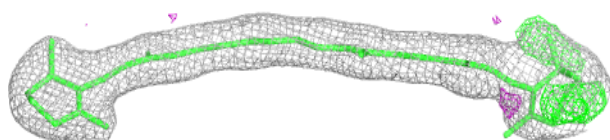
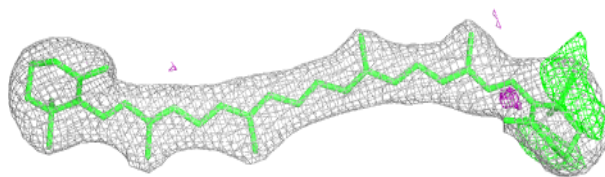
**Electron density around DGD c 517 (B):**

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

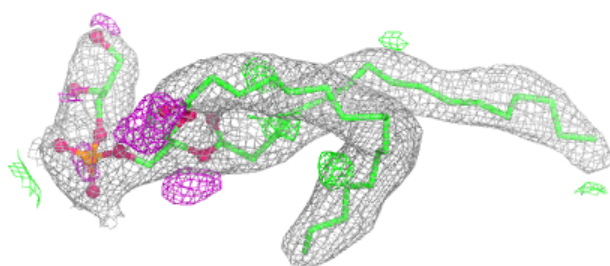
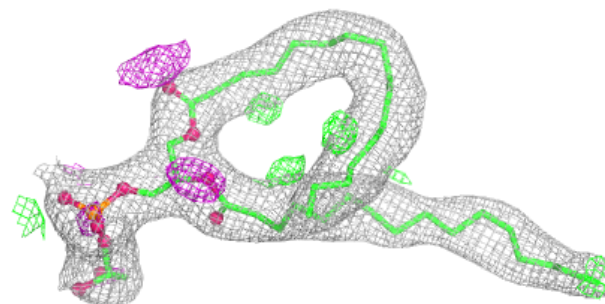


Electron density around BCR d 404:

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

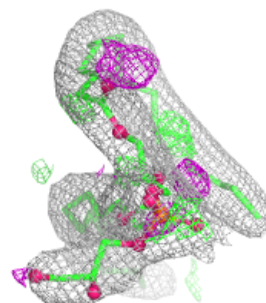
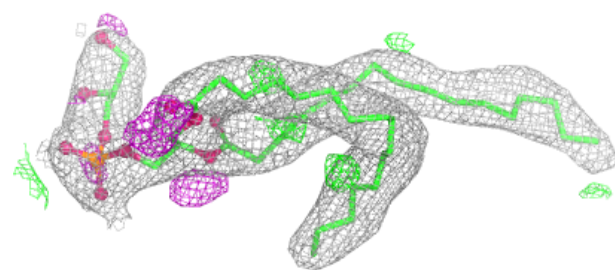
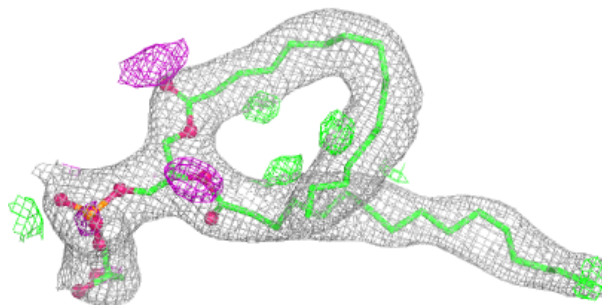
**Electron density around LHG A 419 (A):**

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

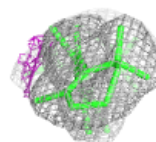
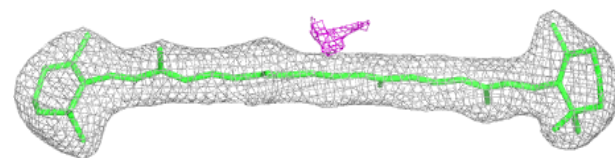
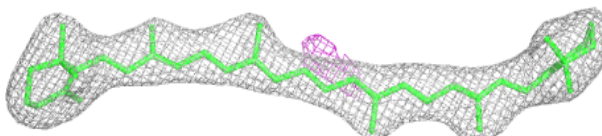


Electron density around LHG A 419 (B):

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

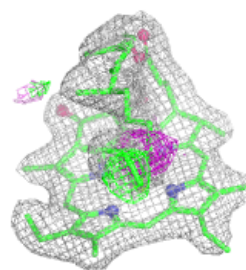
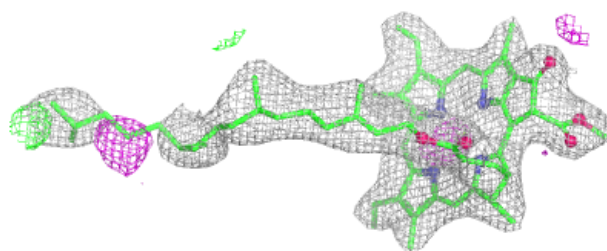
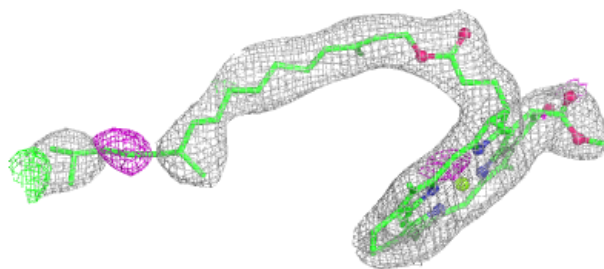
**Electron density around BCR C 515:**

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

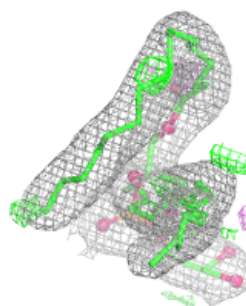
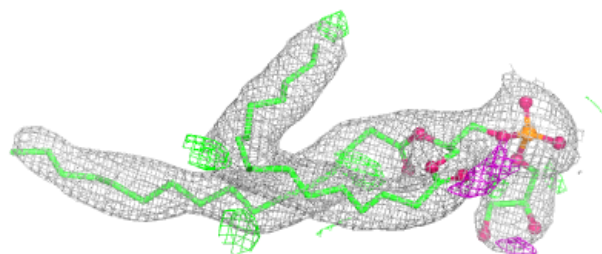
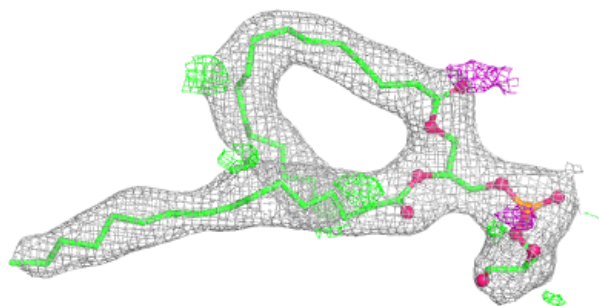


Electron density around CLA C 505:

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

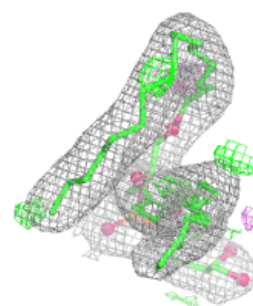
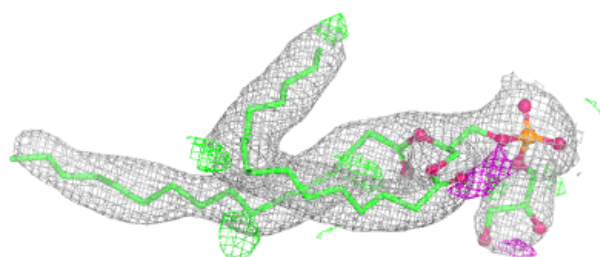
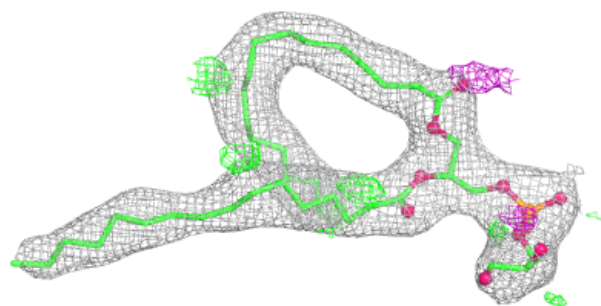
**Electron density around LHG d 413 (A):**

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

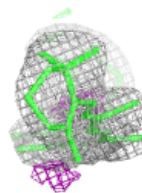
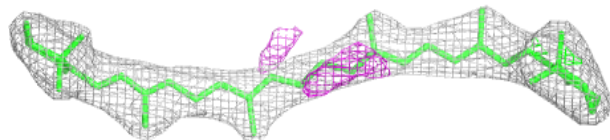
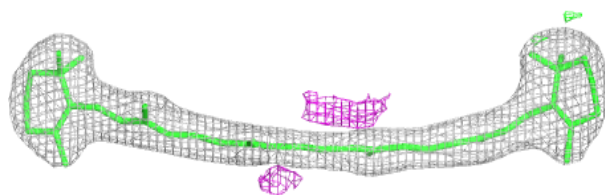


Electron density around LHG d 413 (B):

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

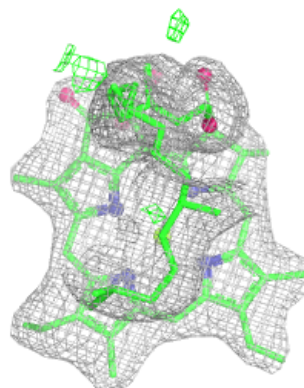
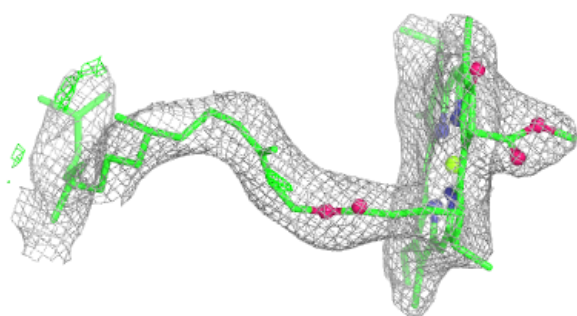
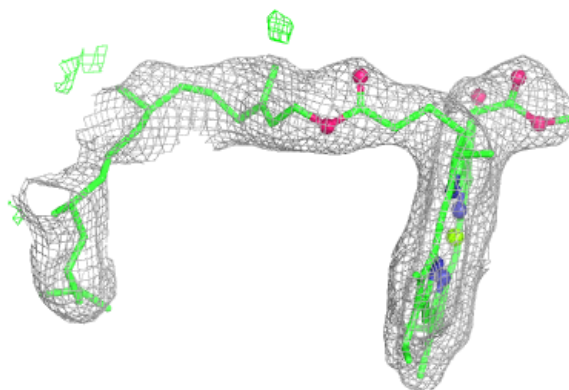
**Electron density around BCR K 102:**

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



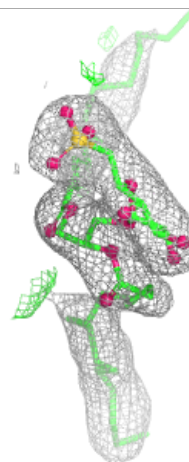
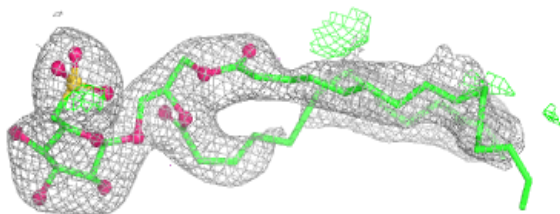
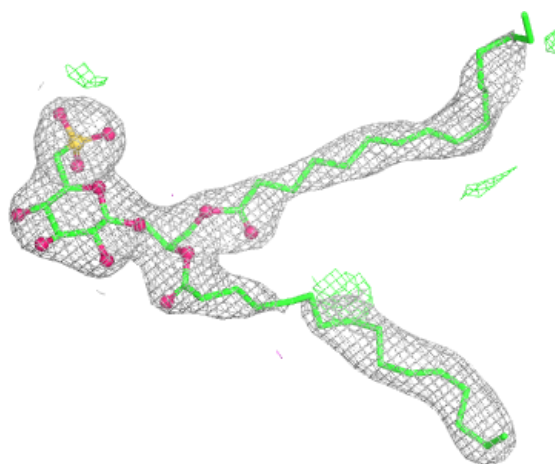
Electron density around CLA C 507:

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



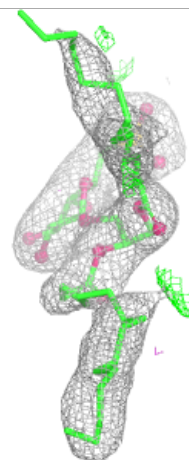
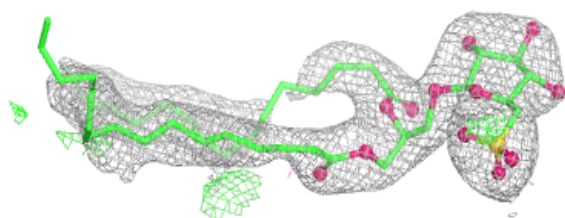
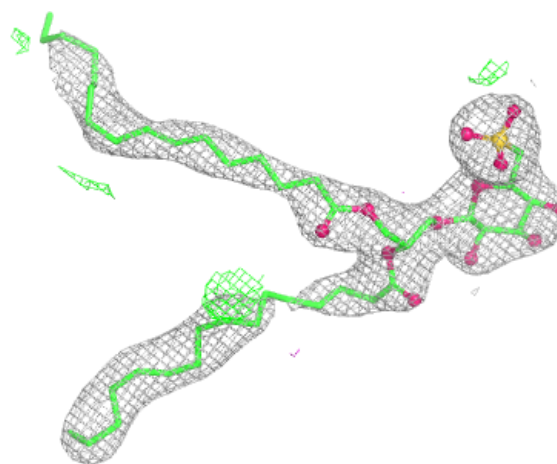
Electron density around SQD a 410 (A):

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



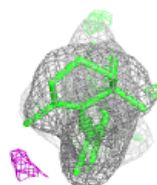
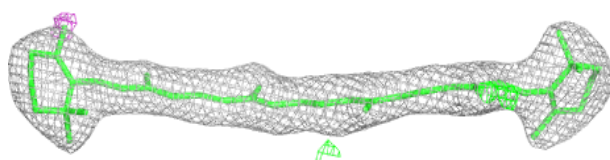
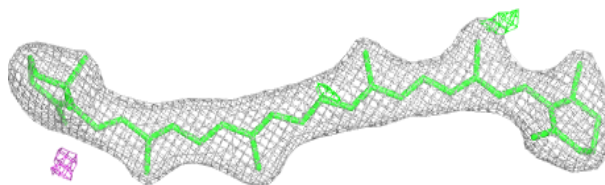
Electron density around SQD a 410 (B):

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

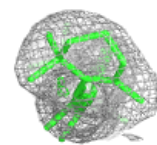
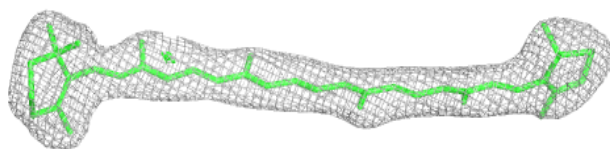
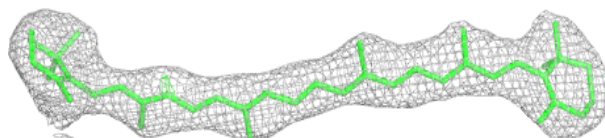


Electron density around BCR Y 101:

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

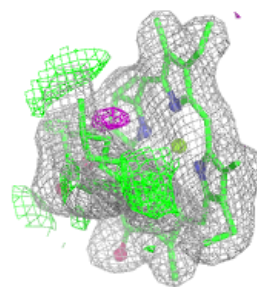
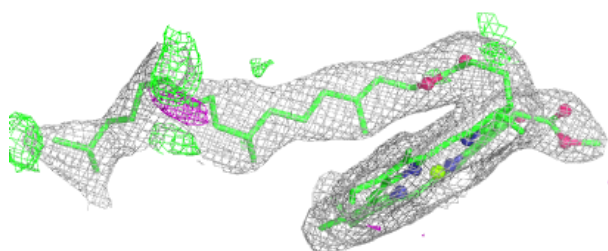
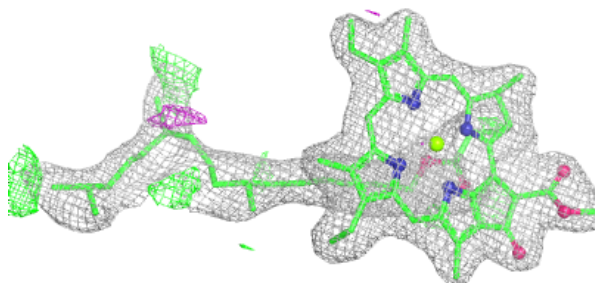
**Electron density around BCR c 514:**

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

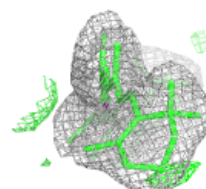
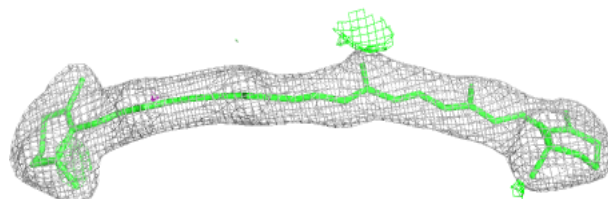
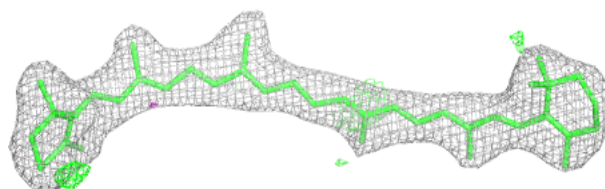


Electron density around CLA b 614:

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

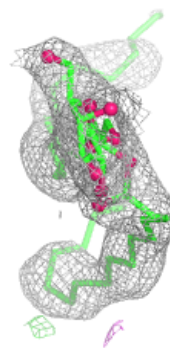
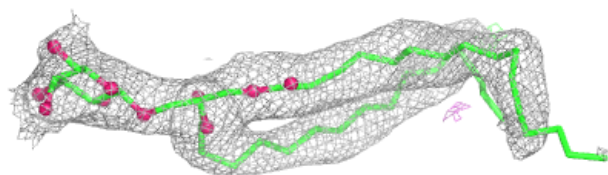
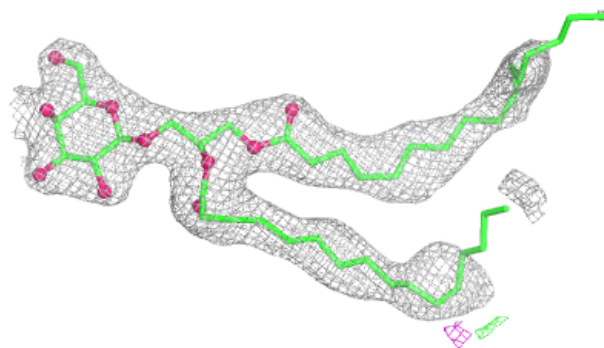
**Electron density around BCR t 102:**

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

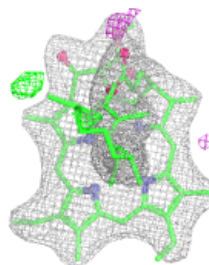
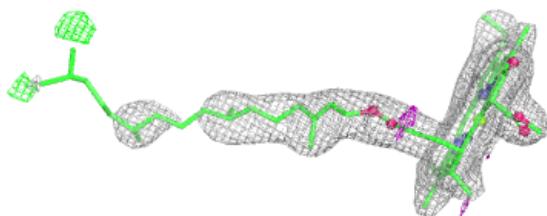
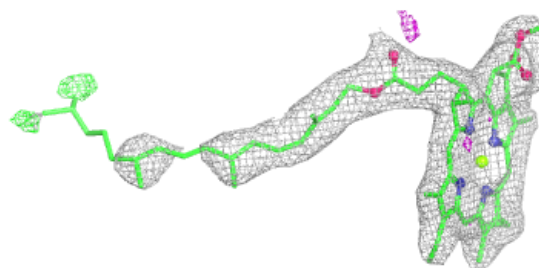


Electron density around LMG d 411:

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

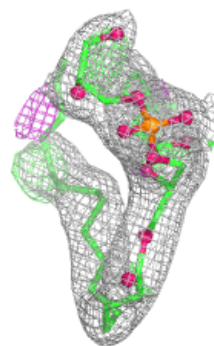
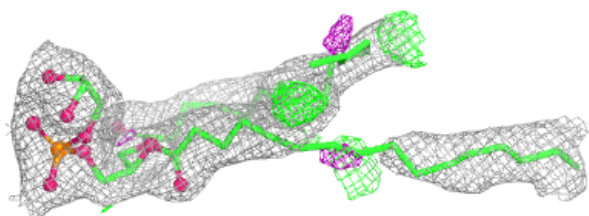
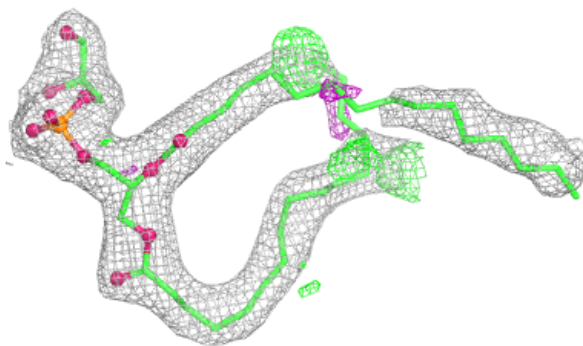
**Electron density around CLA d 403:**

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

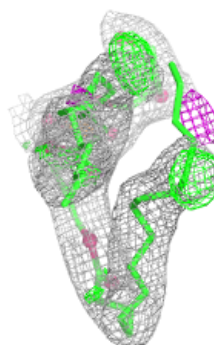
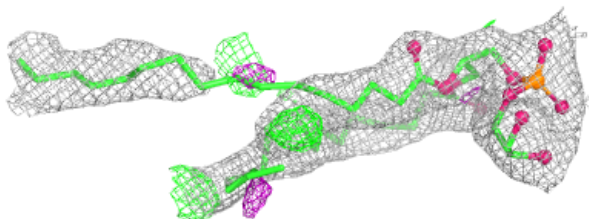
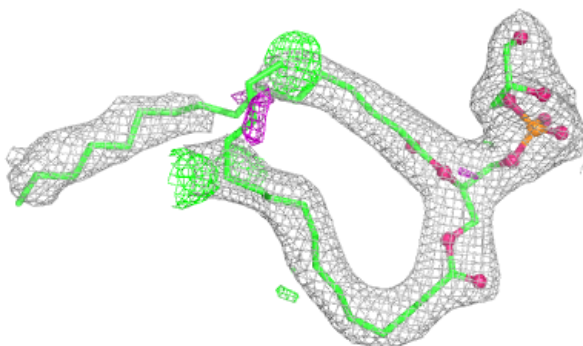


Electron density around LHG D 407 (A):

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

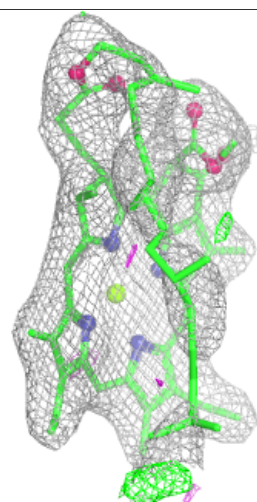
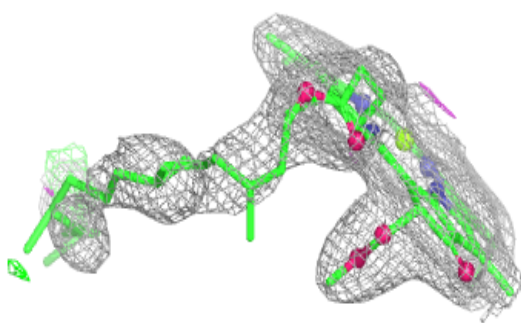
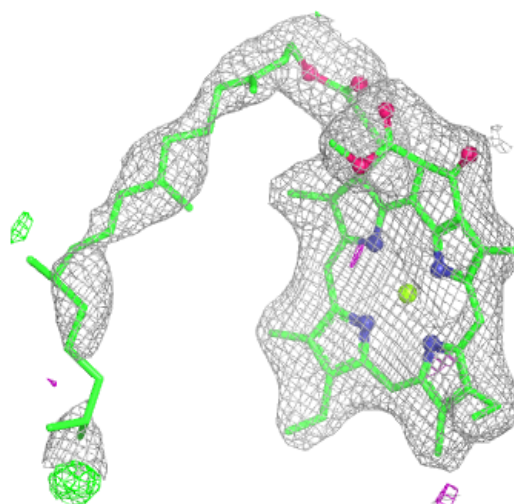
**Electron density around LHG D 407 (B):**

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



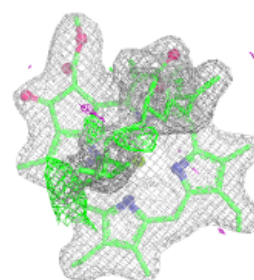
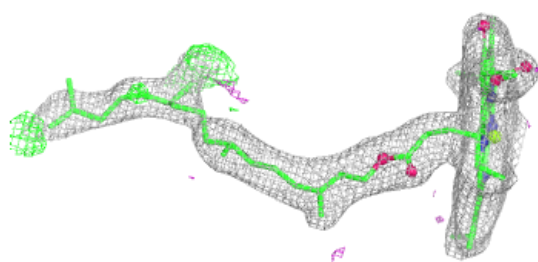
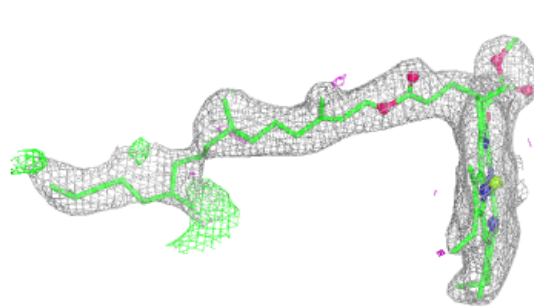
Electron density around CLA B 616:

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

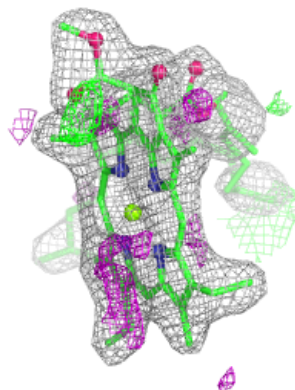
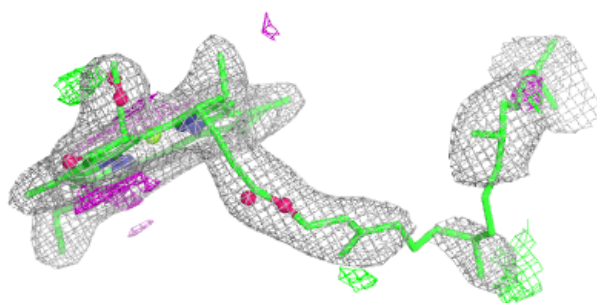
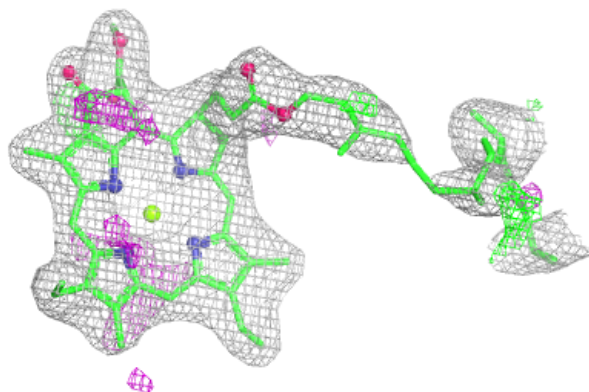


Electron density around CLA b 606:

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

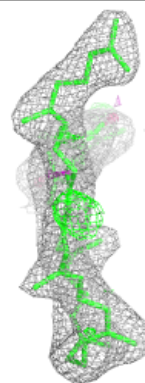
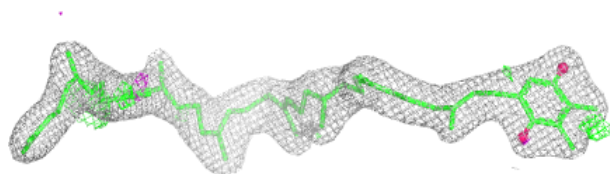
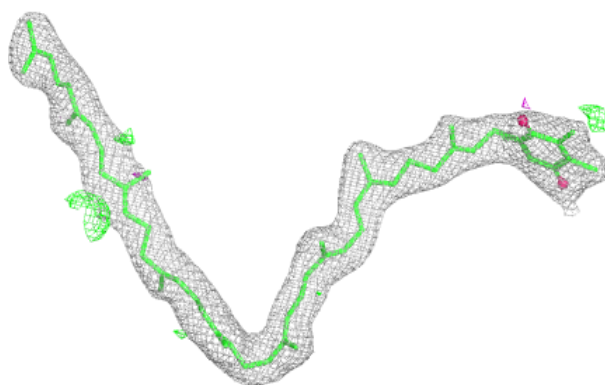
**Electron density around CLA A 408:**

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

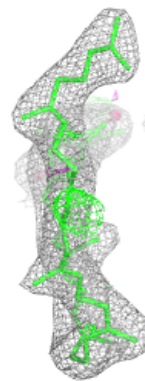
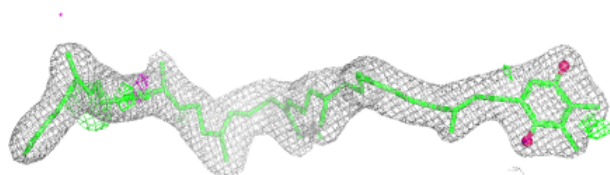
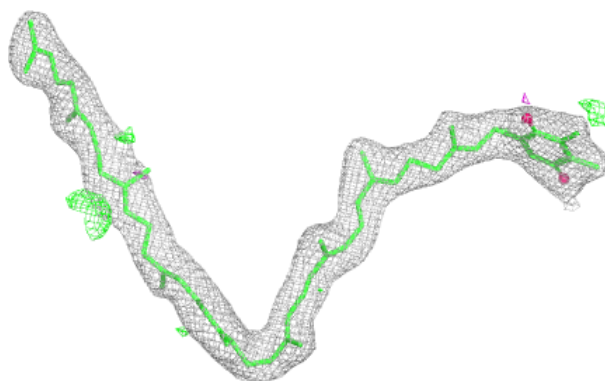


Electron density around PL9 D 405 (A):

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

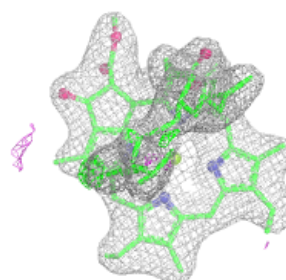
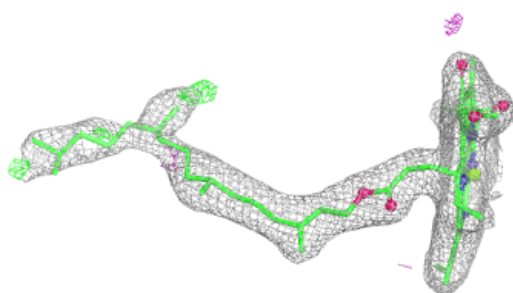
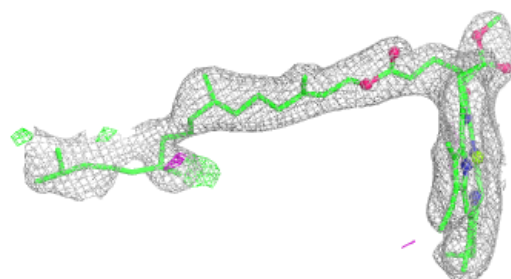
**Electron density around PL9 D 405 (B):**

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

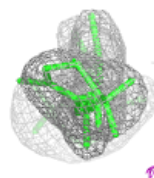
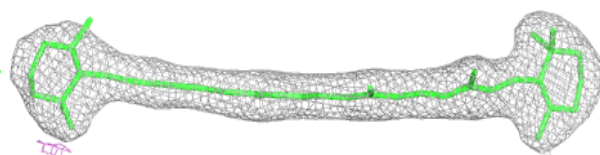
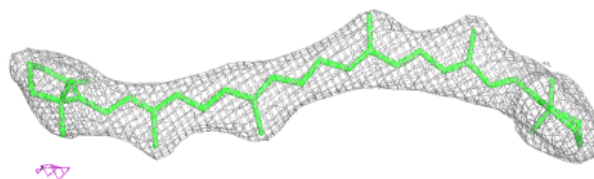


Electron density around CLA B 606:

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

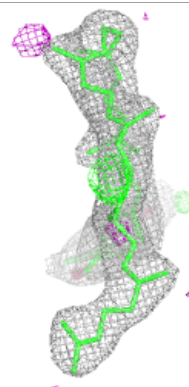
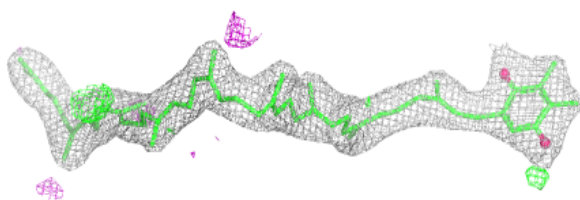
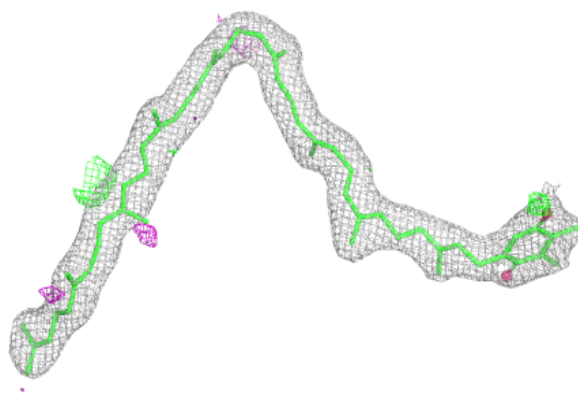
**Electron density around BCR h 101:**

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

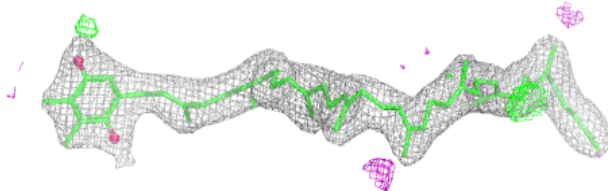
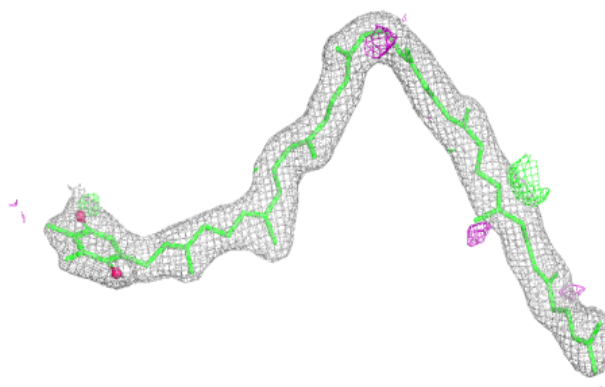


Electron density around PL9 d 405 (A):

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

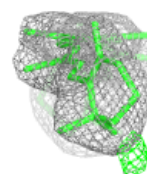
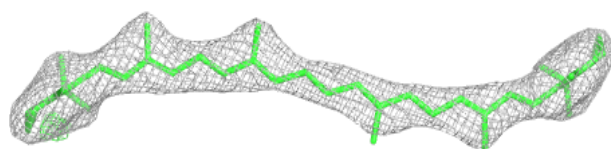
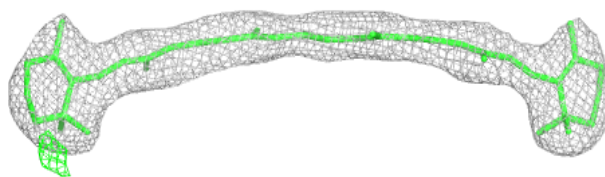
**Electron density around PL9 d 405 (B):**

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

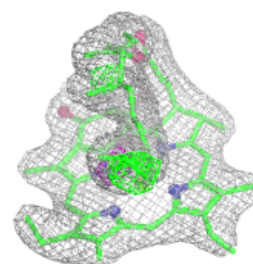
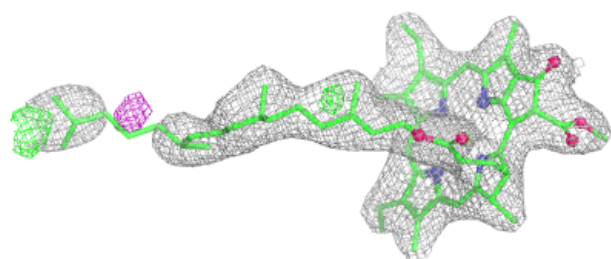
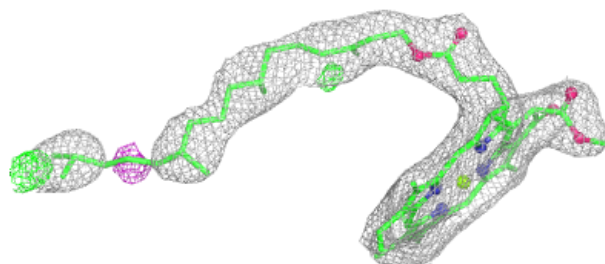


Electron density around BCR k 101:

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

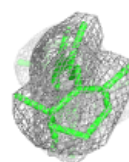
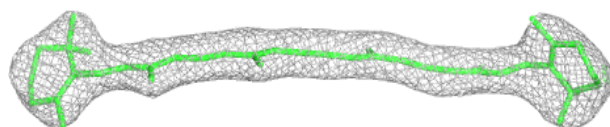
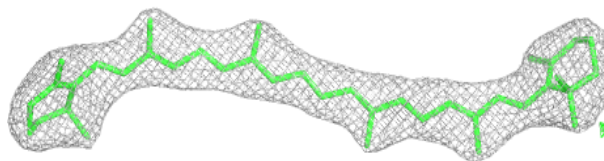
**Electron density around CLA c 504:**

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

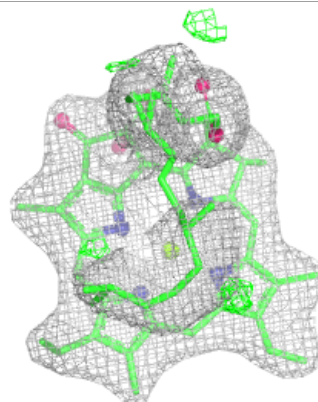
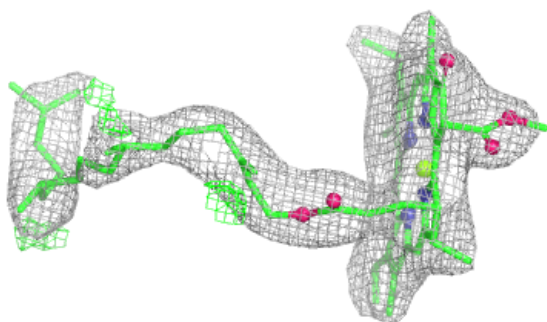
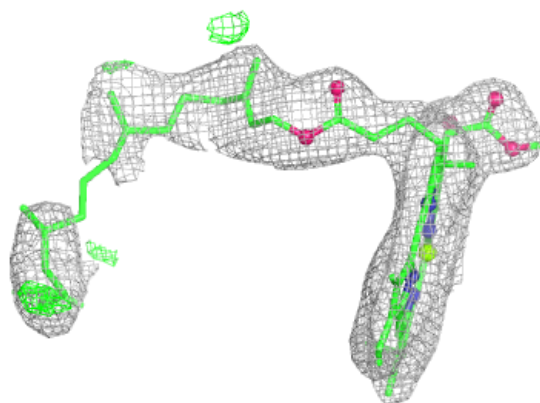


Electron density around BCR y 101:

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

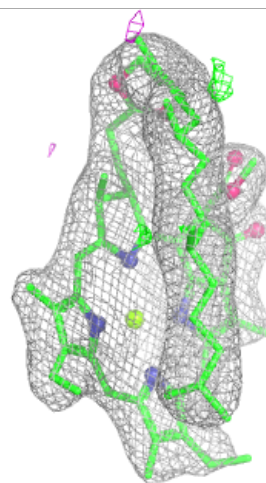
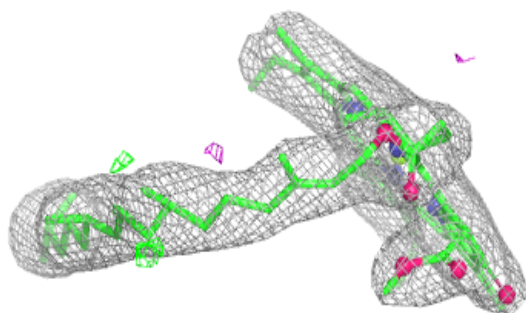
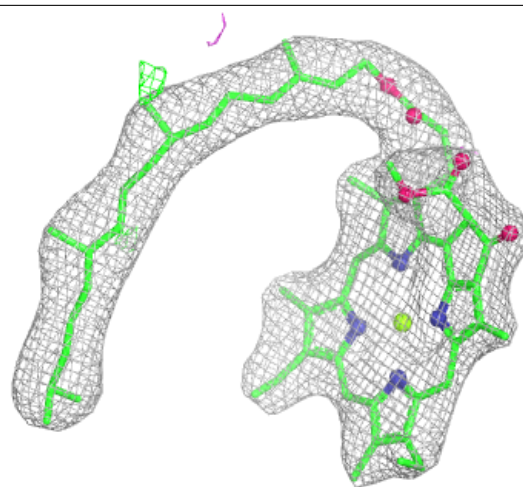
**Electron density around CLA c 506:**

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



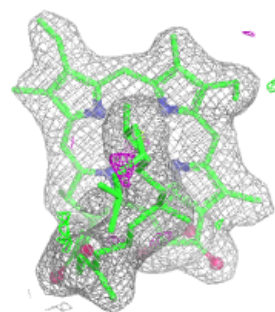
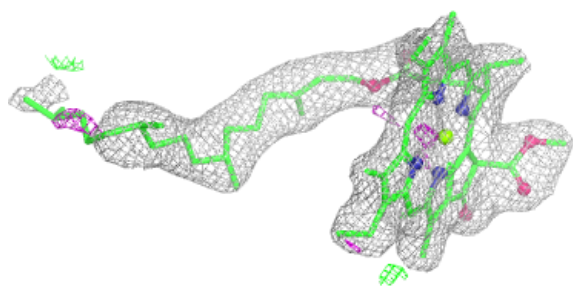
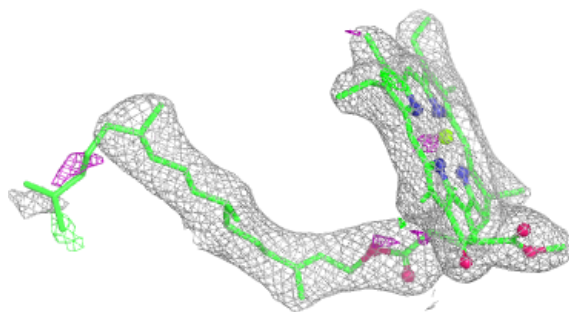
Electron density around CLA c 507:

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

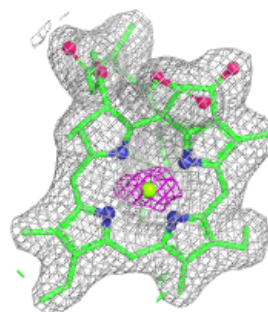
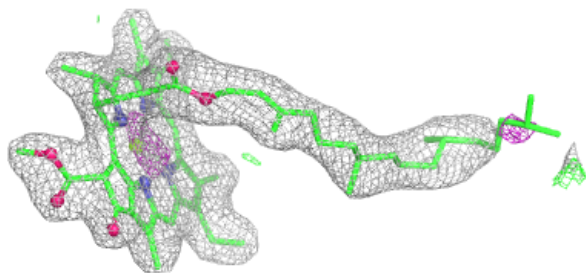
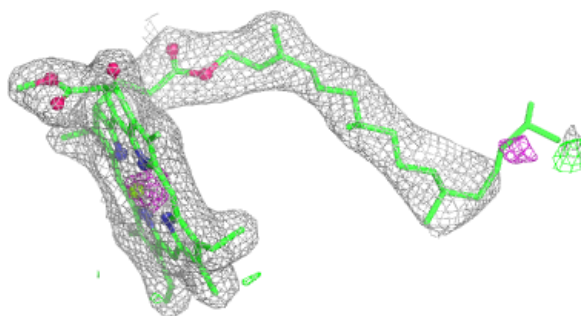


Electron density around CLA c 508:

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

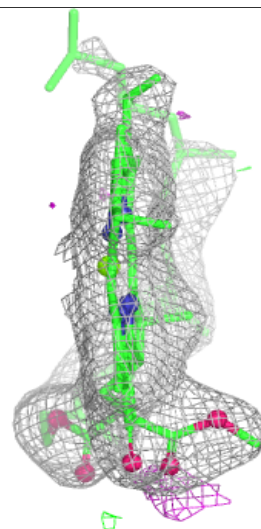
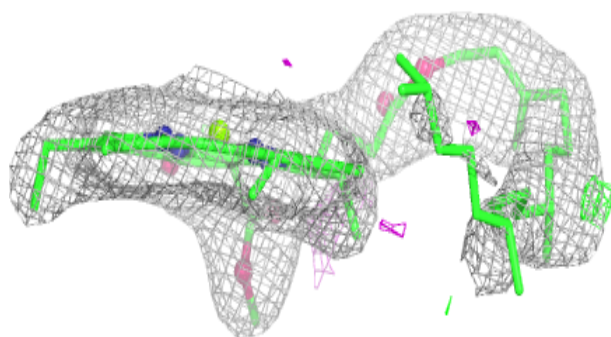
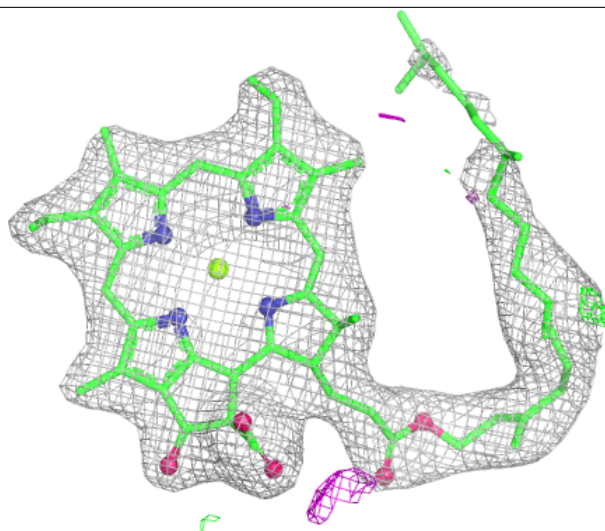
**Electron density around CLA C 509:**

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



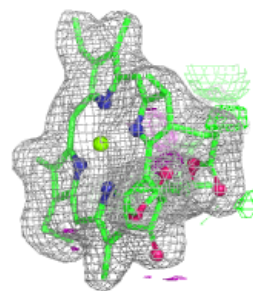
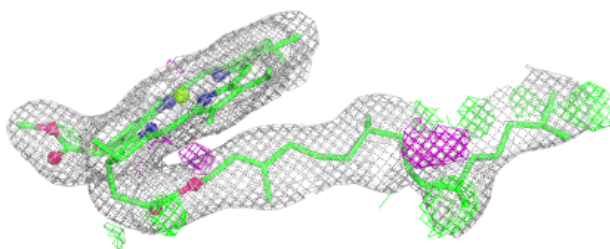
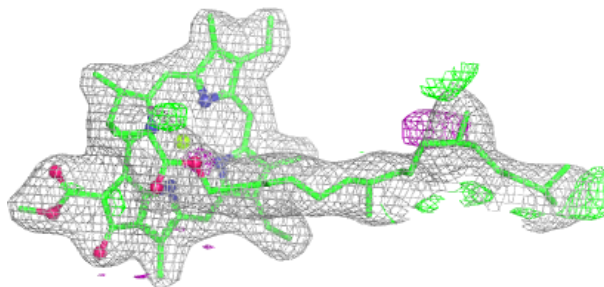
Electron density around CLA C 513:

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

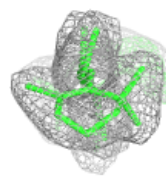
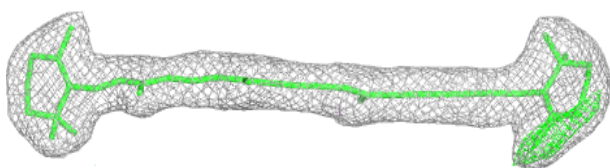
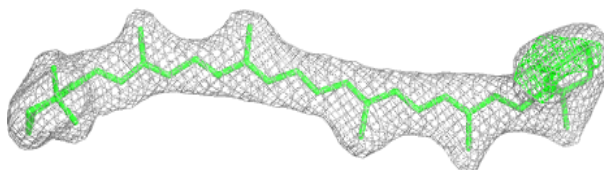


Electron density around CLA B 614:

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

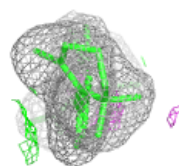
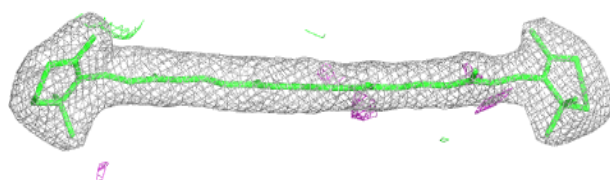
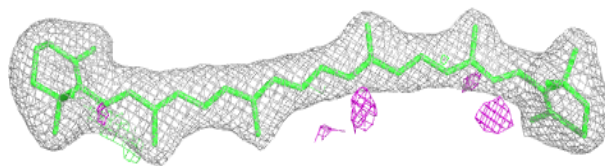
**Electron density around BCR A 409:**

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

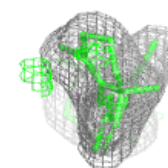
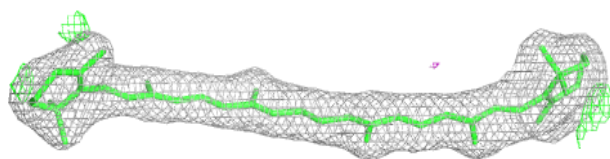
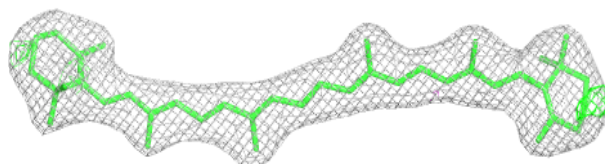


Electron density around BCR B 618:

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

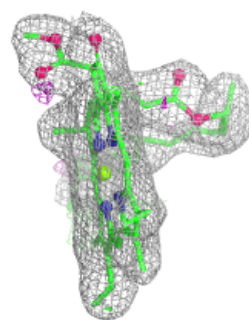
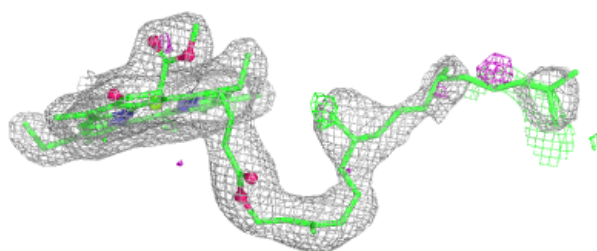
**Electron density around BCR B 619:**

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

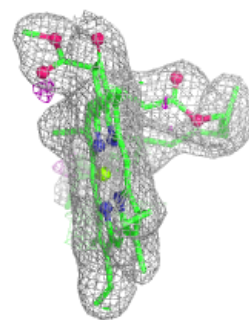
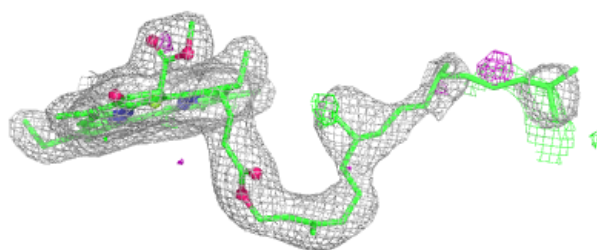
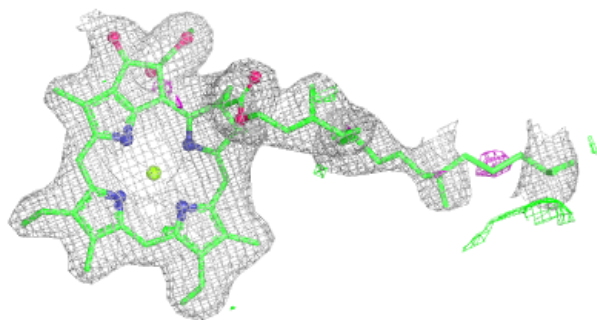


Electron density around CLA a 406 (A):

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

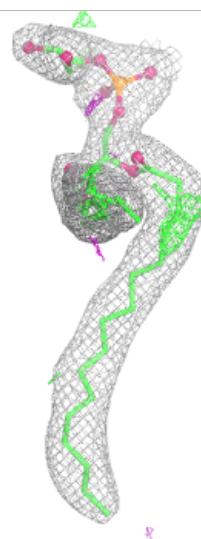
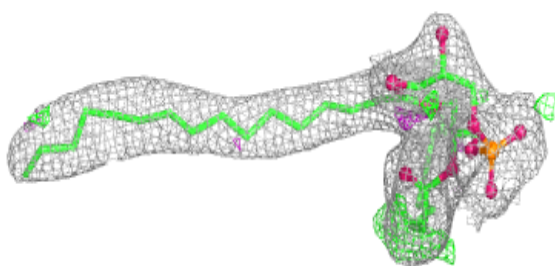
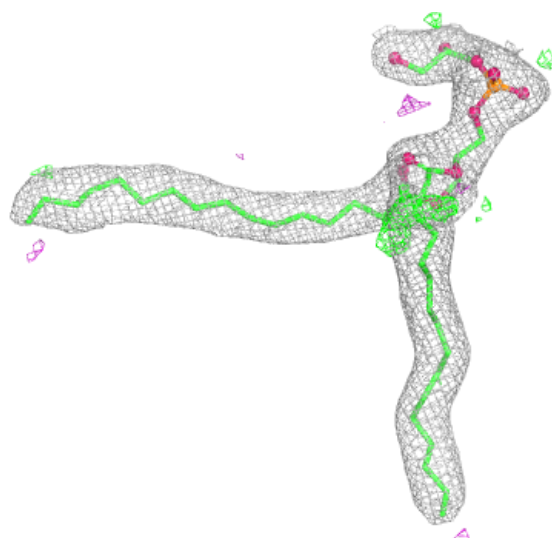
**Electron density around CLA a 406 (B):**

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



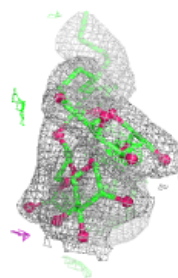
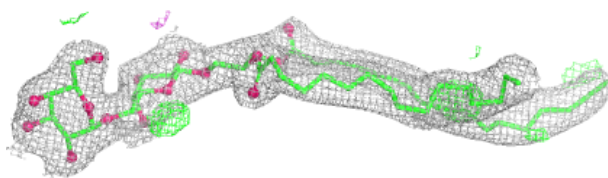
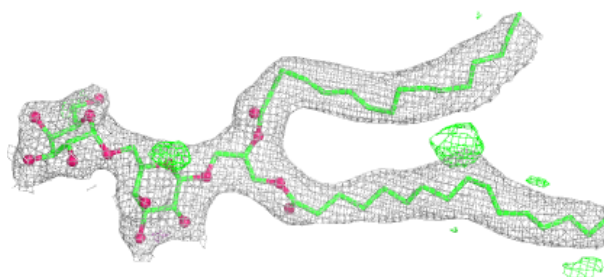
Electron density around LHG b 629 (A):

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

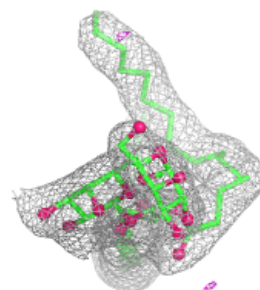
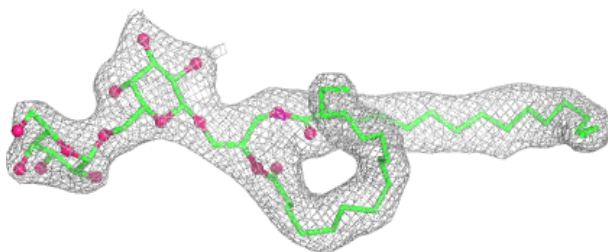
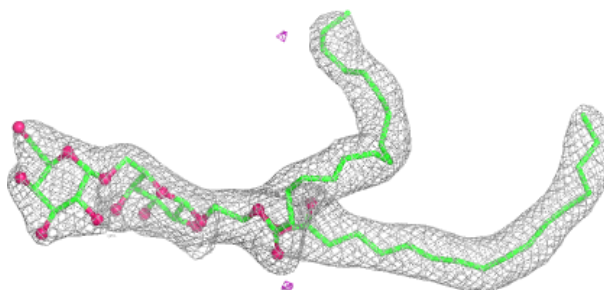


Electron density around DGD C 519:

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

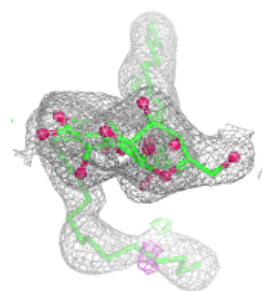
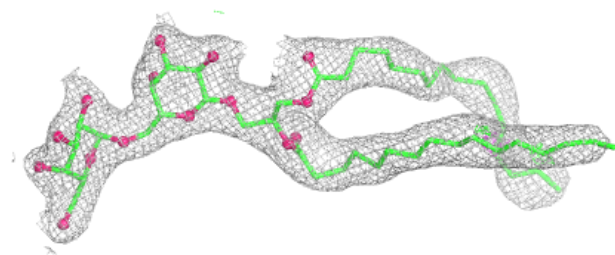
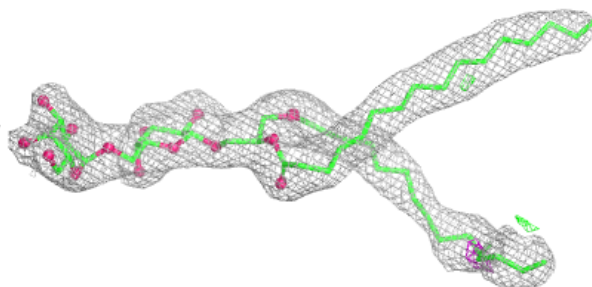
**Electron density around DGD H 102:**

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

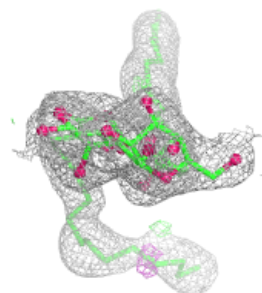
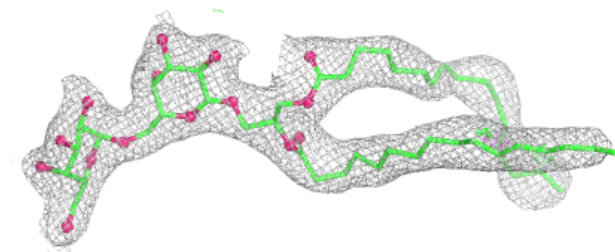
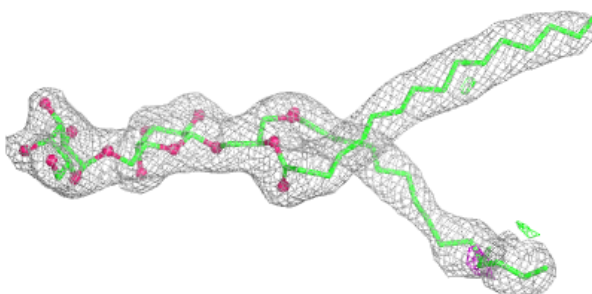


Electron density around DGD c 516 (A):

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

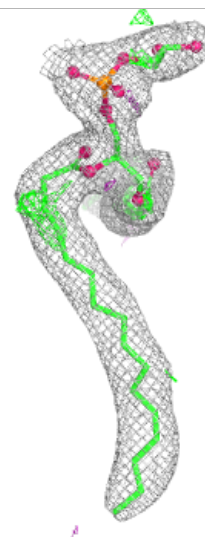
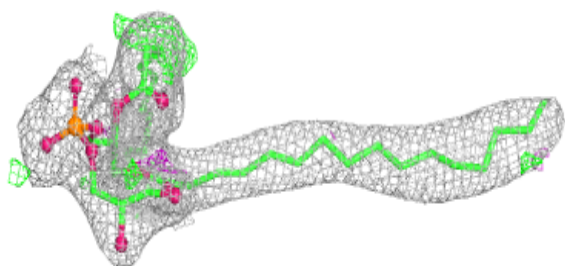
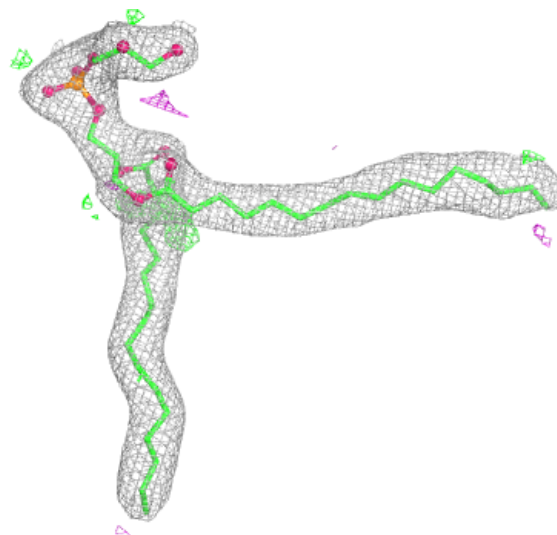
**Electron density around DGD c 516 (B):**

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



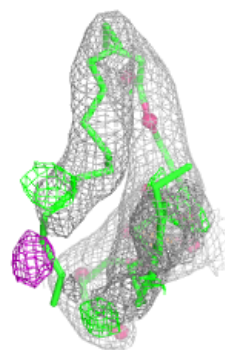
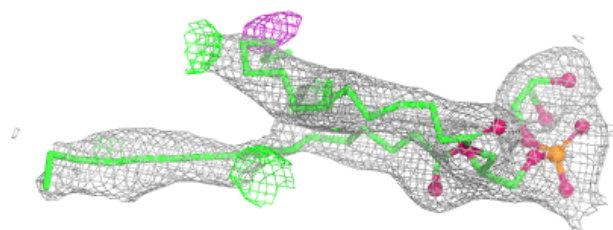
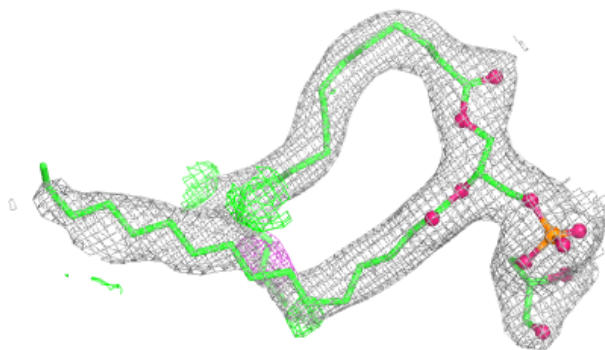
Electron density around LHG b 629 (B):

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

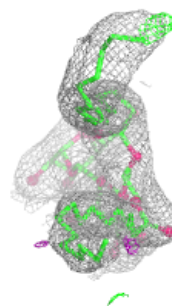
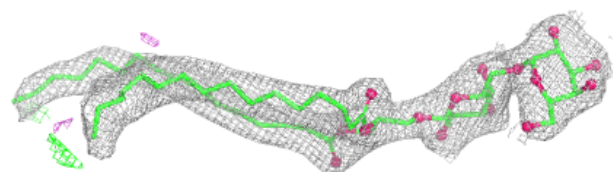
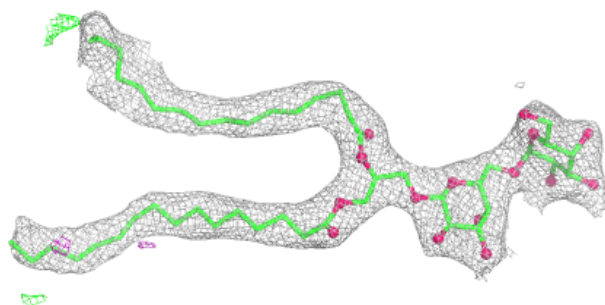


Electron density around LHG d 407 (A):

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

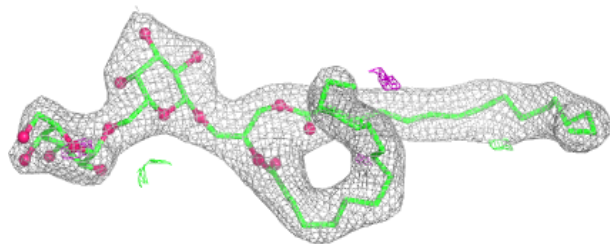
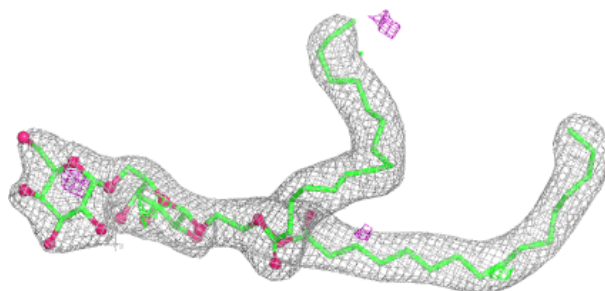
**Electron density around DGD c 518:**

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

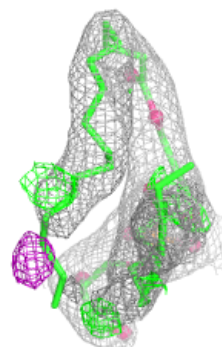
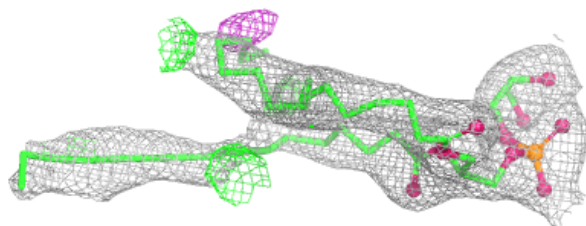
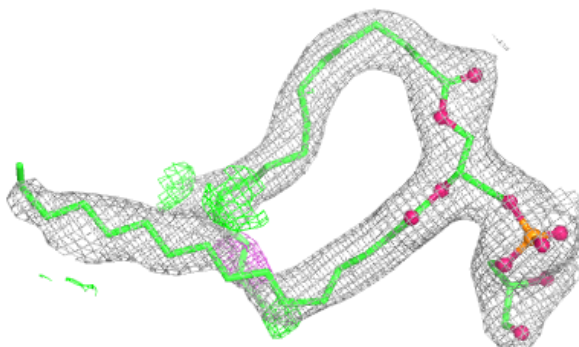


Electron density around DGD h 102:

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

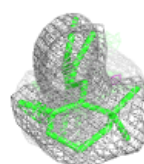
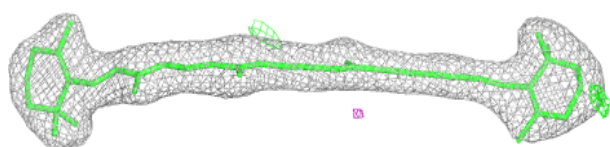
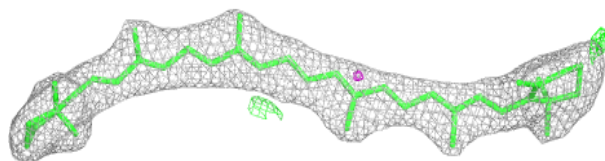
**Electron density around LHG d 407 (B):**

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

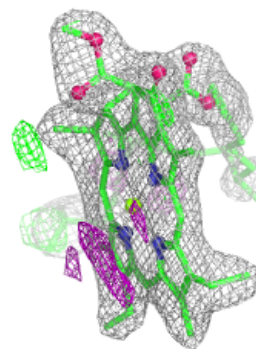
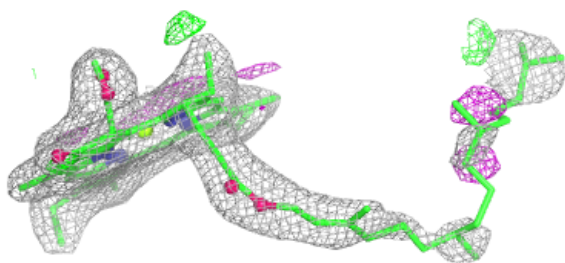
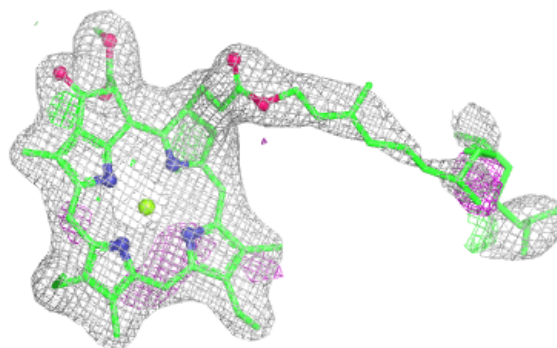


Electron density around BCR H 101:

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

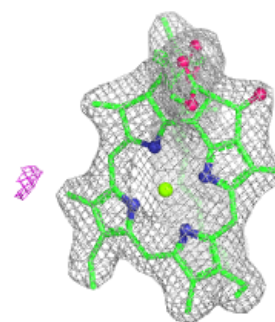
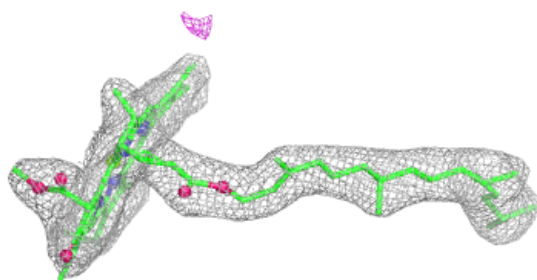
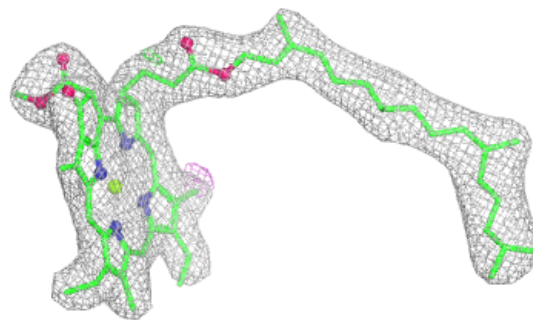
**Electron density around CLA a 408:**

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

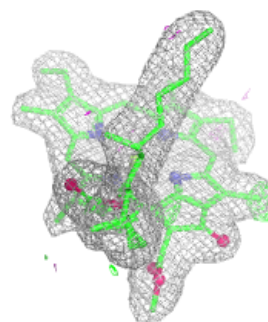
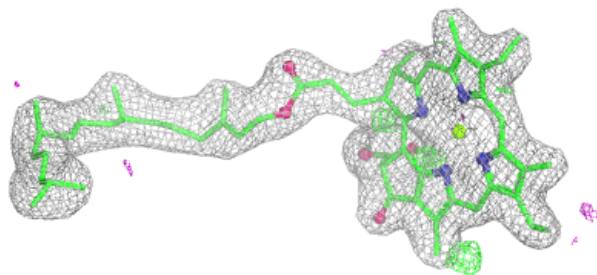
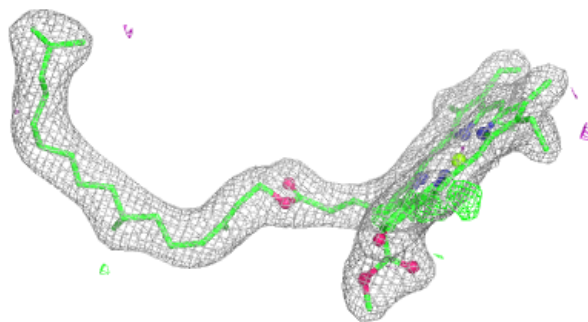


Electron density around CLA B 609:

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

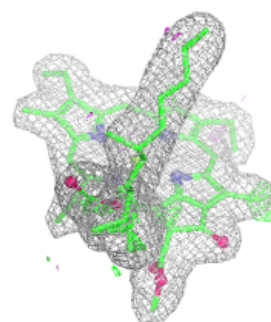
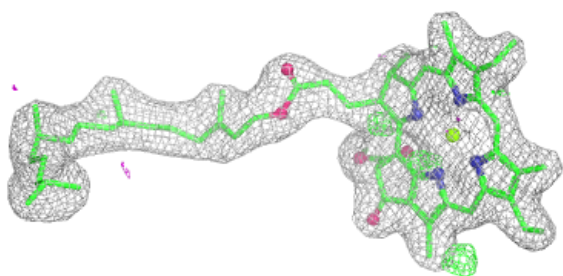
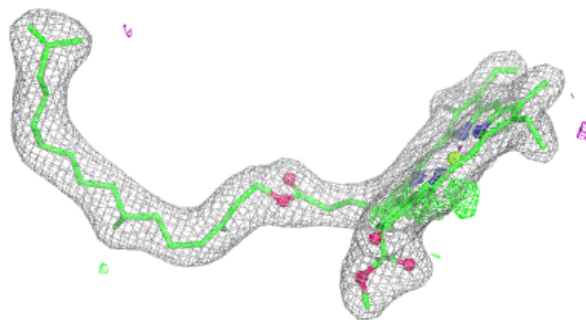
**Electron density around CLA D 402 (A):**

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

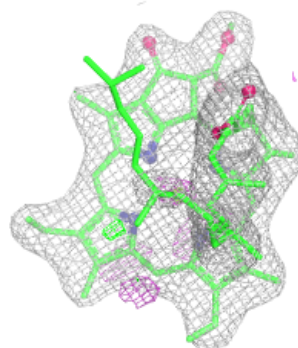
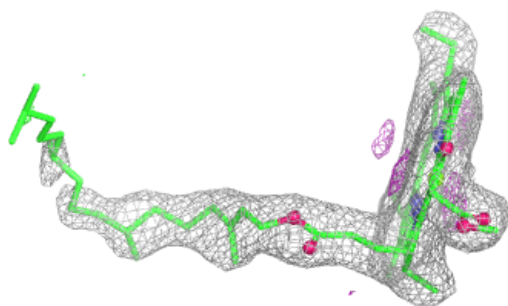
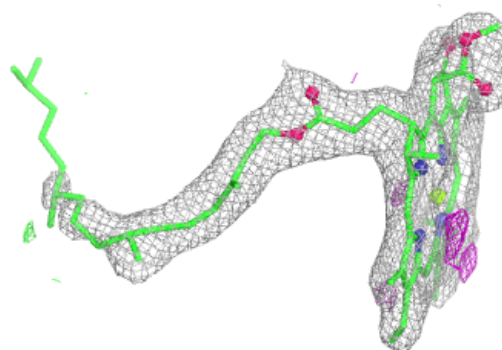


Electron density around CLA D 402 (B):

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

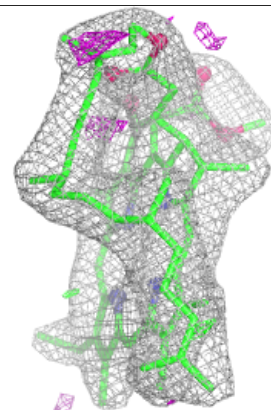
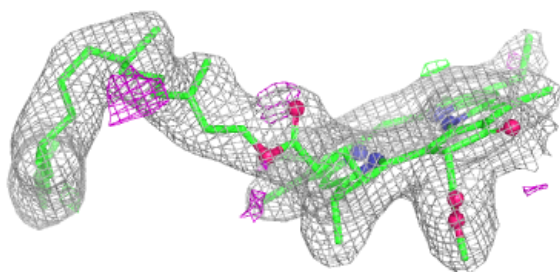
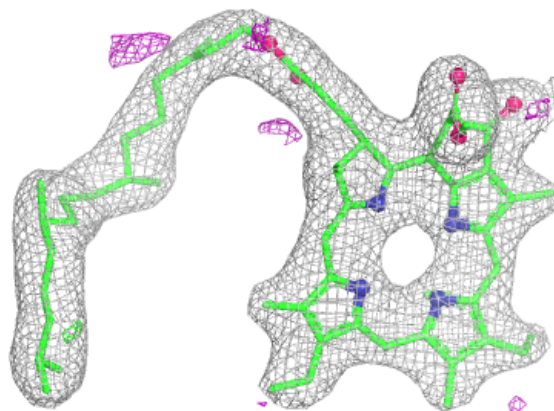
**Electron density around CLA D 403:**

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

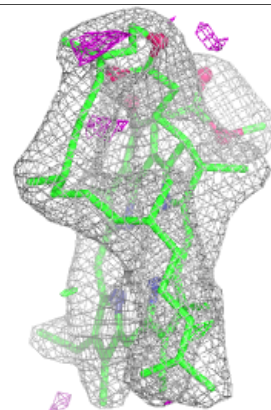
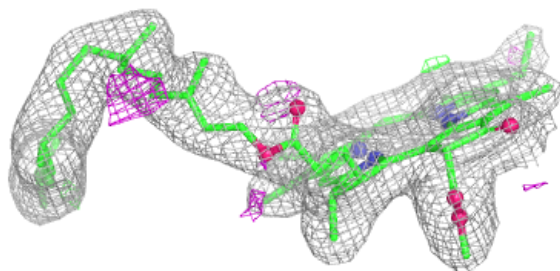
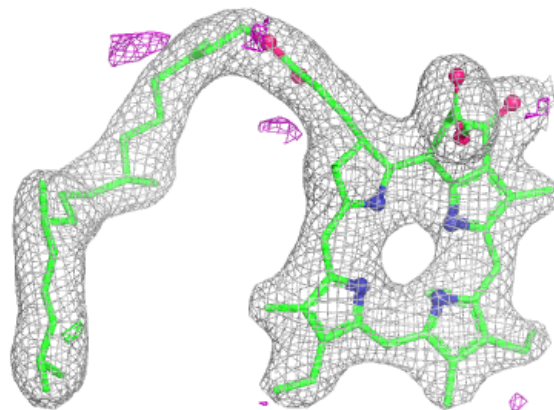


Electron density around PHO a 415 (A):

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

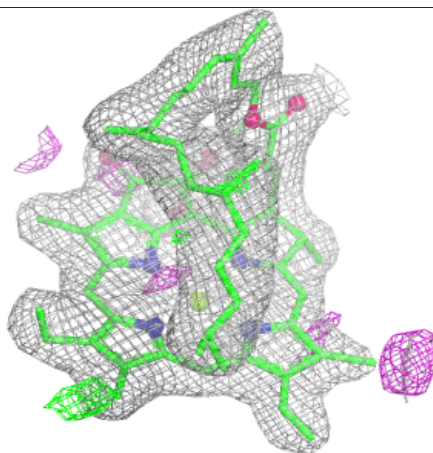
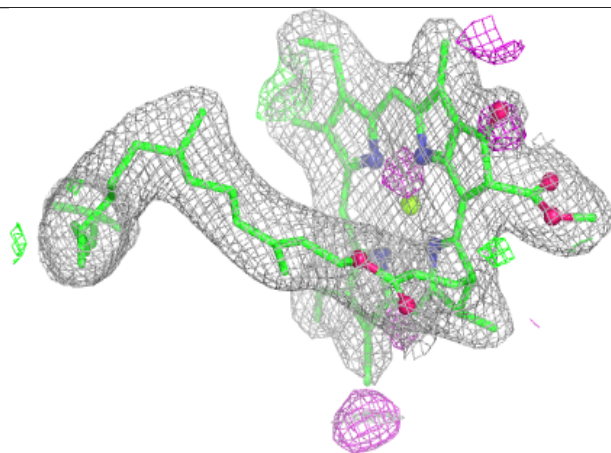
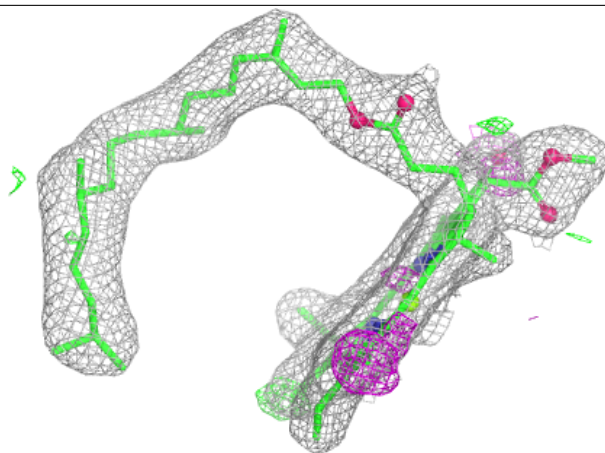
**Electron density around PHO a 415 (B):**

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

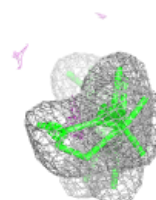
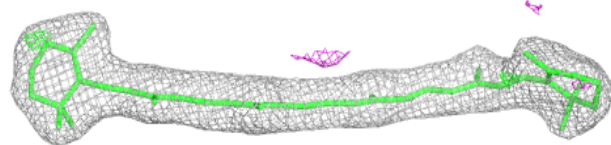
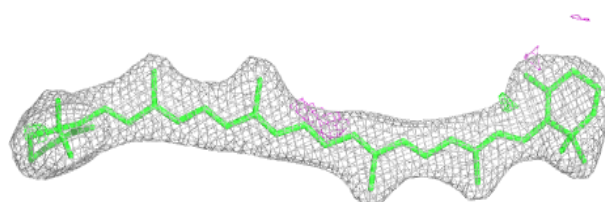


Electron density around CLA B 611:

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

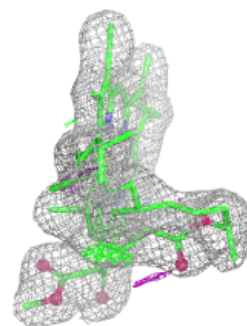
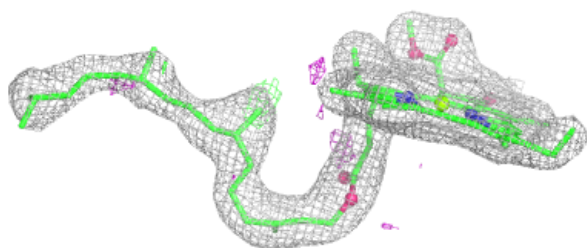
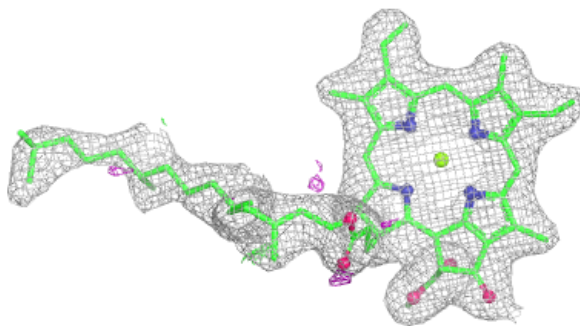
**Electron density around BCR B 617:**

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

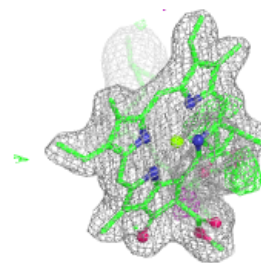
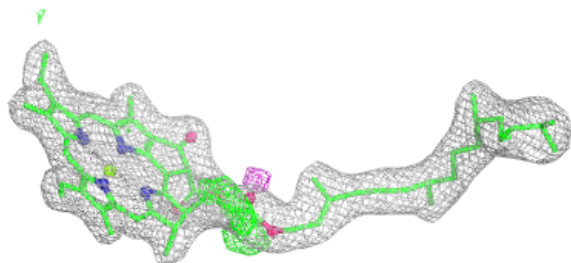
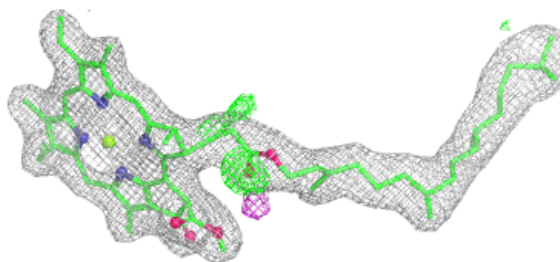


Electron density around CLA A 406 (B):

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

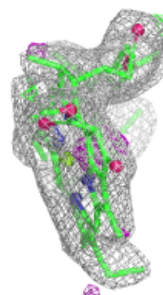
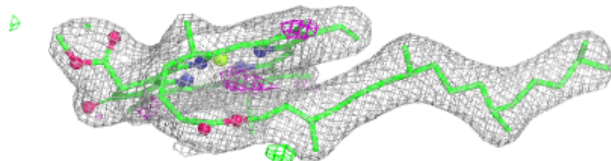
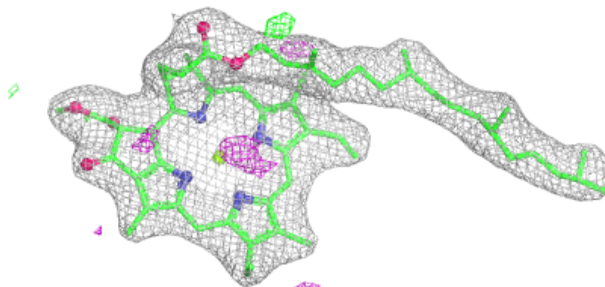
**Electron density around CLA A 404 (A):**

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

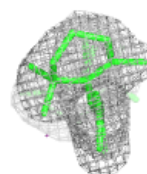
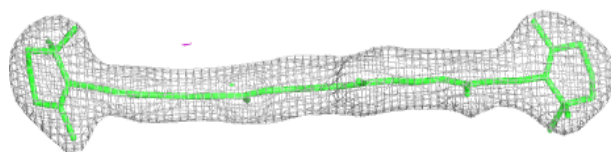
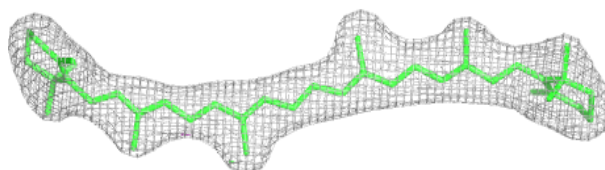


Electron density around CLA C 502:

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

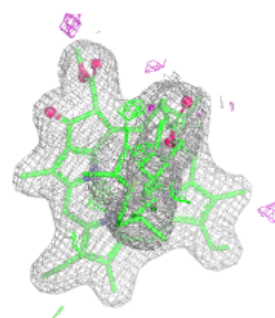
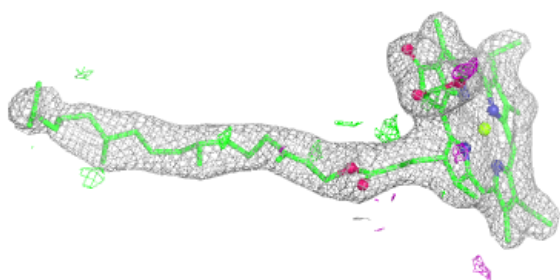
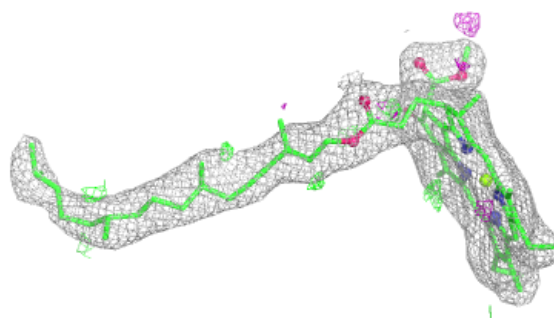
**Electron density around BCR C 516:**

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

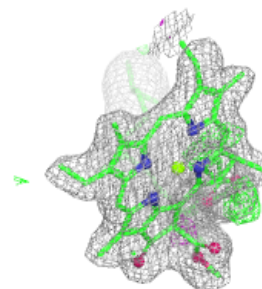
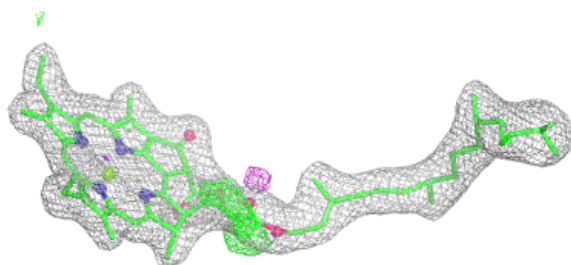
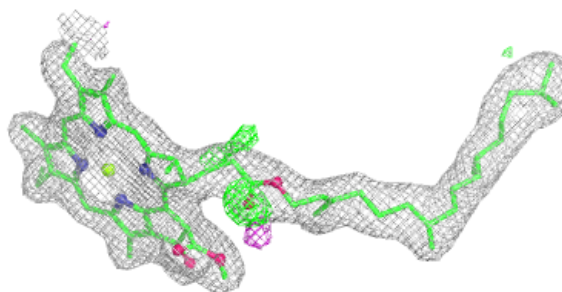


Electron density around CLA b 604:

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

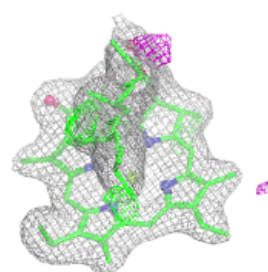
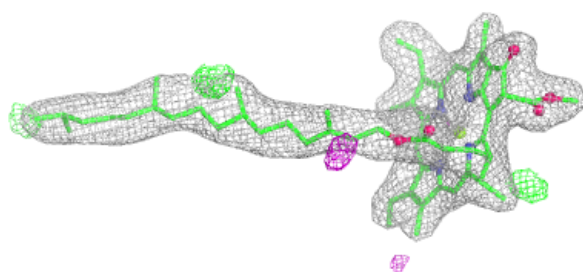
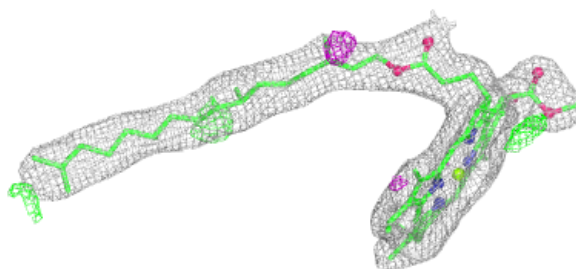
**Electron density around CLA A 404 (B):**

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



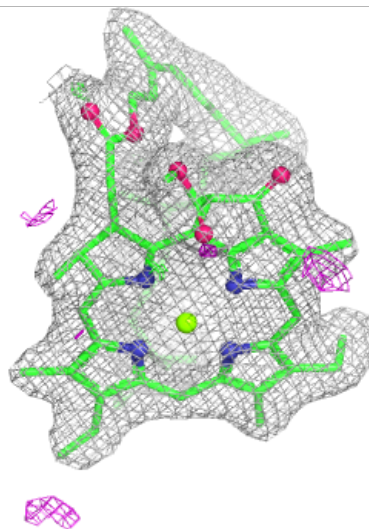
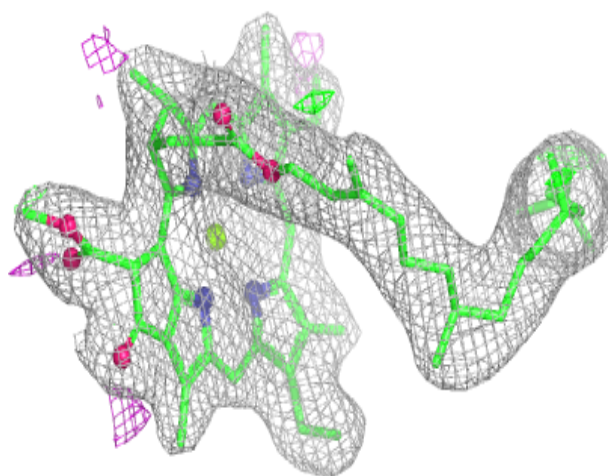
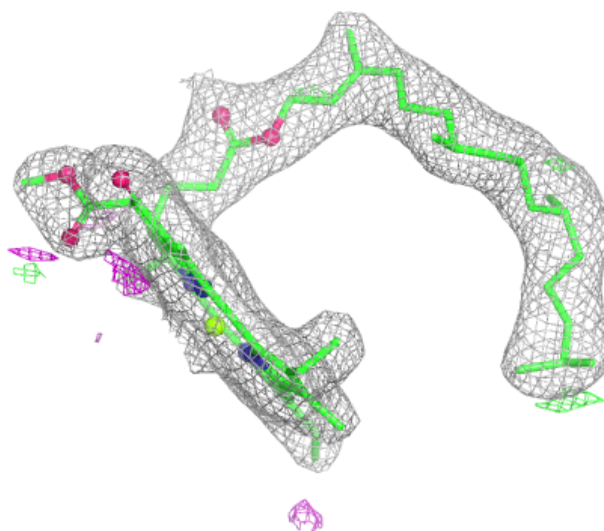
Electron density around CLA b 607:

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



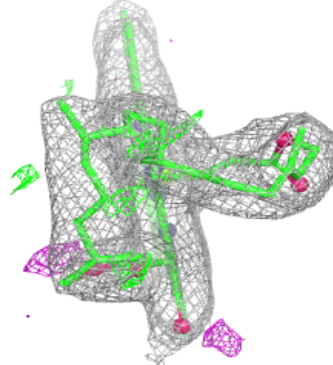
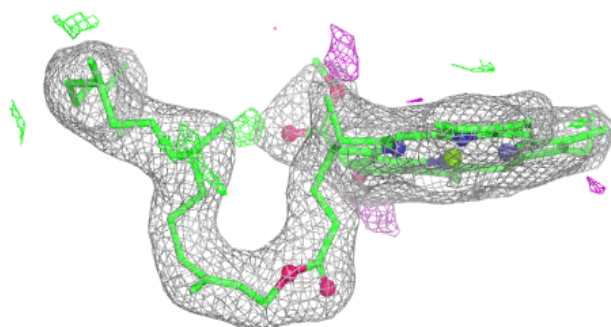
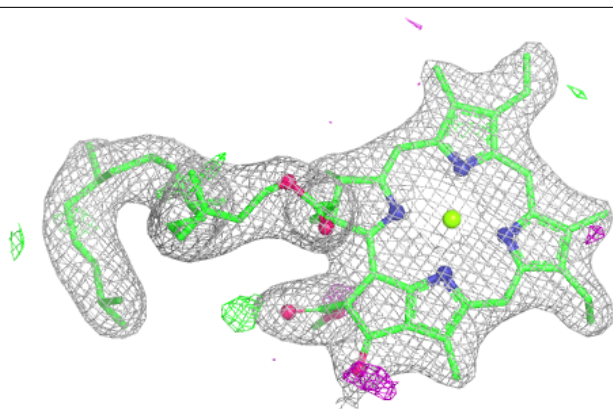
Electron density around CLA b 611:

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

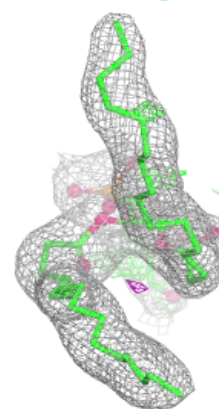
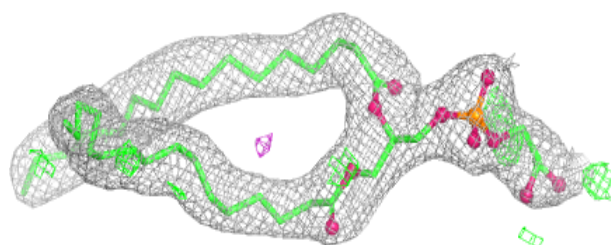
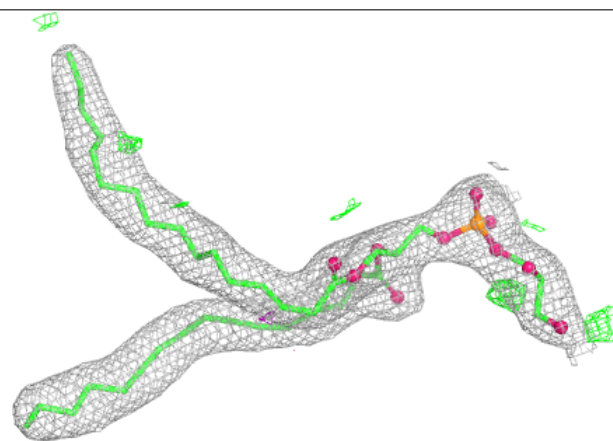


Electron density around CLA b 612:

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

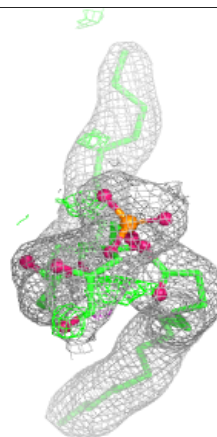
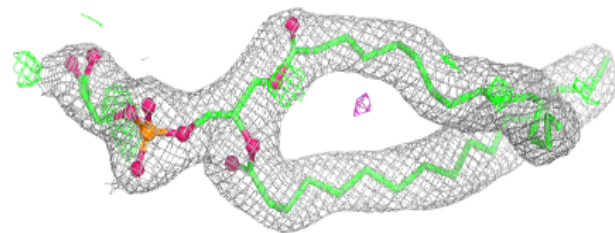
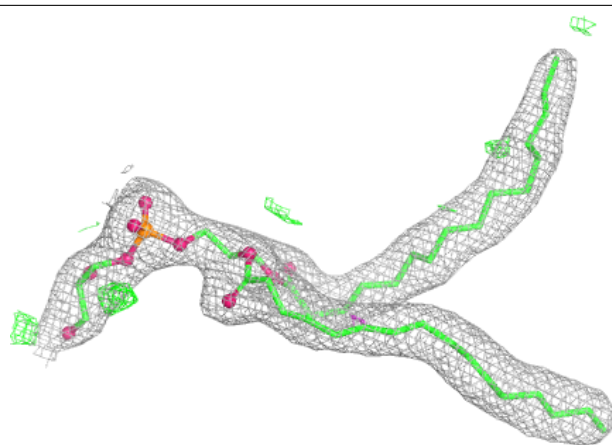
**Electron density around LHG D 406 (A):**

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

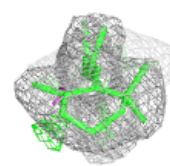
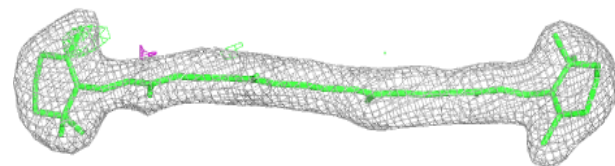
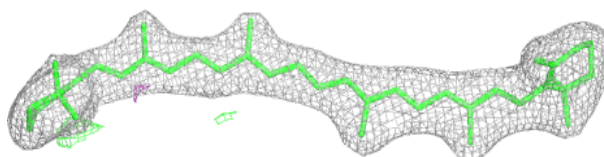


Electron density around LHG D 406 (B):

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

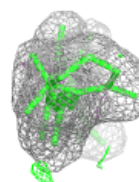
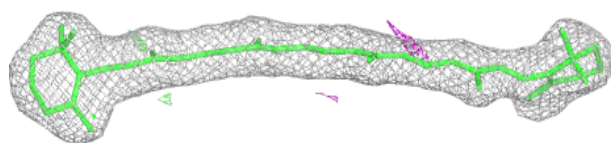
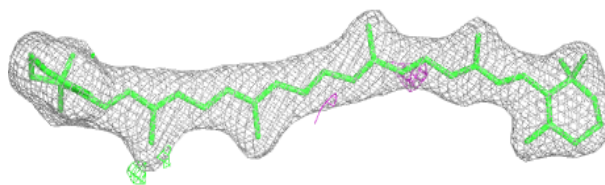
**Electron density around BCR a 409:**

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

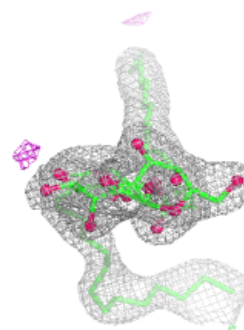
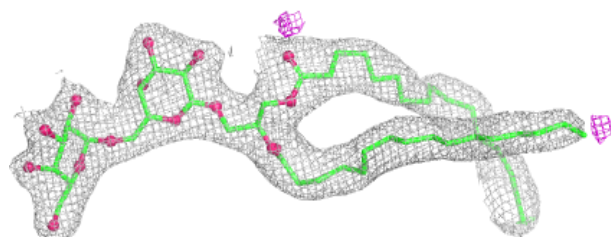
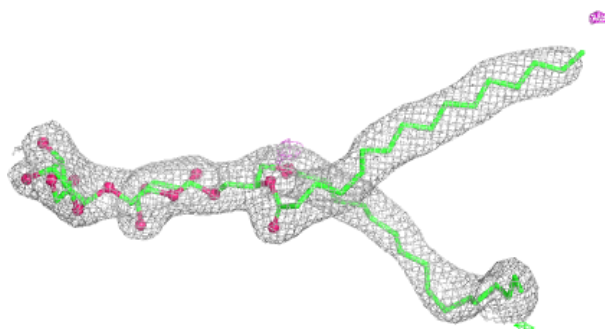


Electron density around BCR b 617:

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

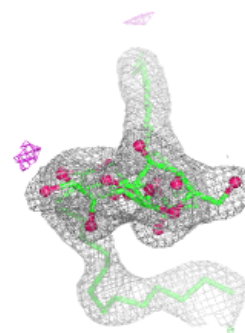
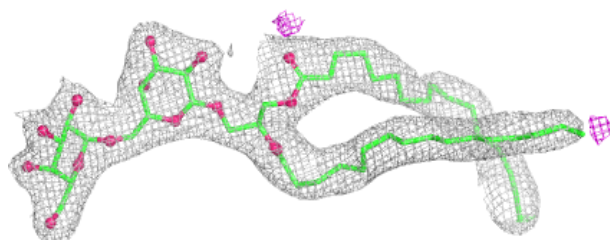
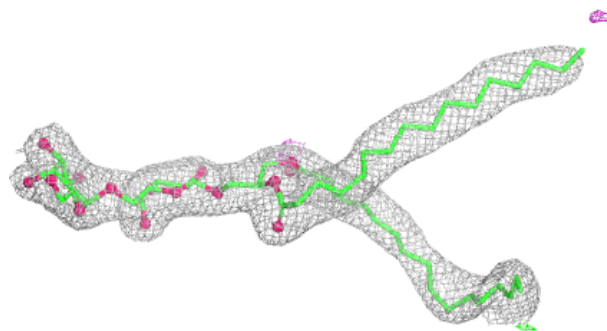
**Electron density around DGD C 517 (A):**

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

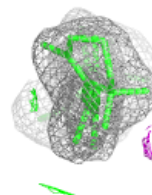
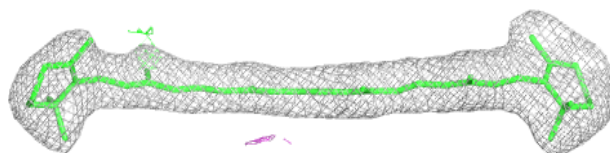
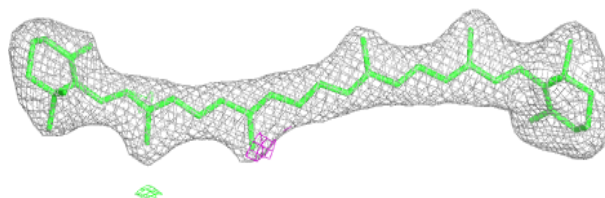


Electron density around DGD C 517 (B):

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

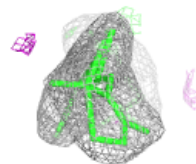
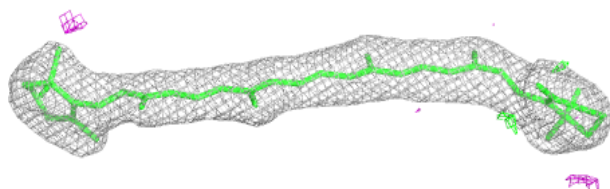
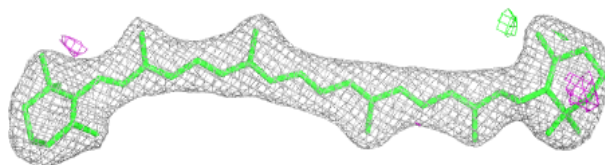
**Electron density around BCR b 618:**

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

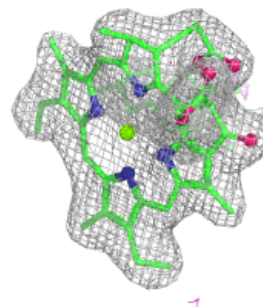
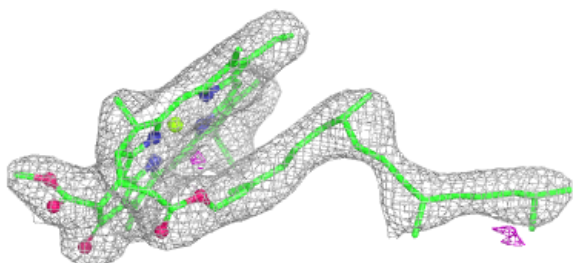
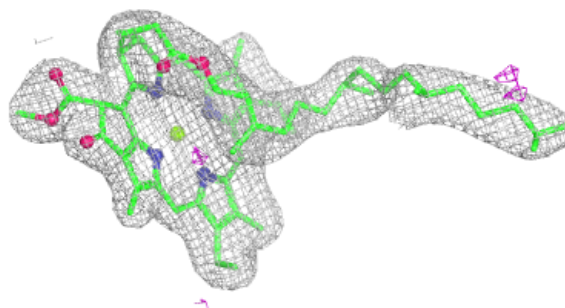


Electron density around BCR b 619:

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

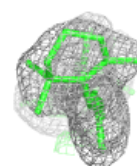
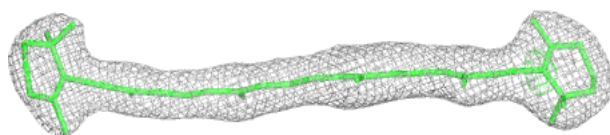
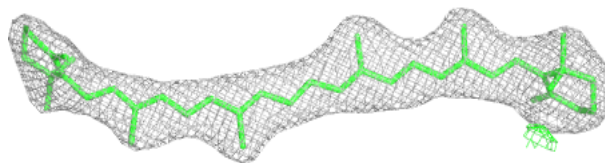
**Electron density around CLA C 506:**

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

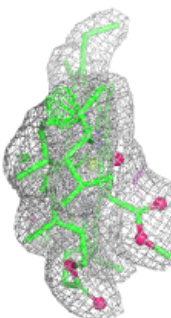
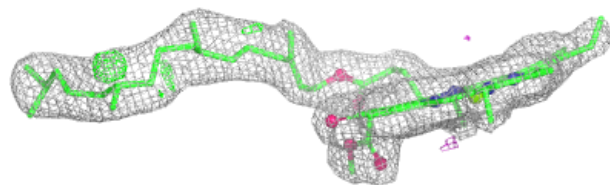
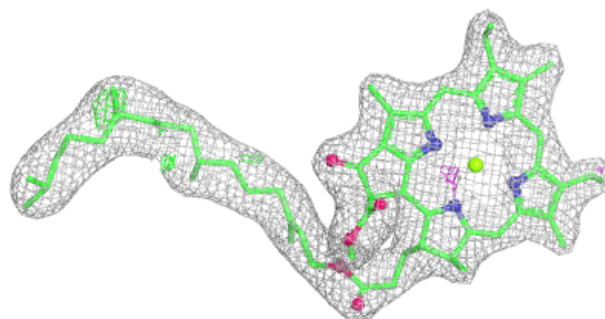


Electron density around BCR c 515:

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

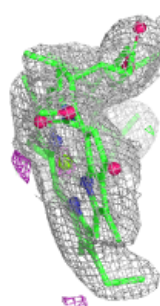
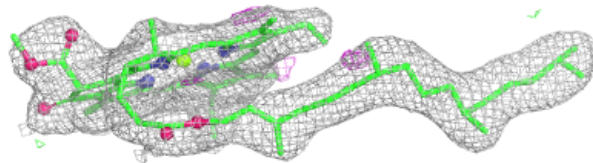
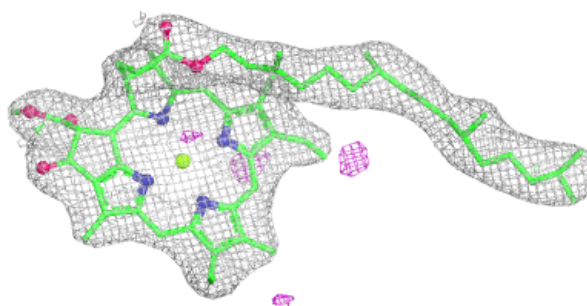
**Electron density around CLA B 602:**

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

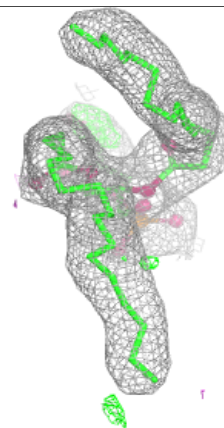
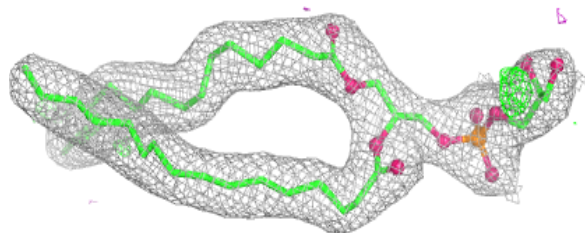
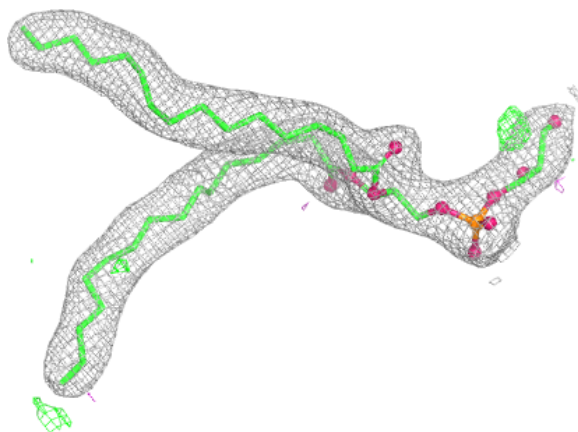


Electron density around CLA c 501:

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

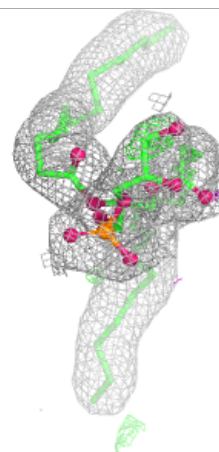
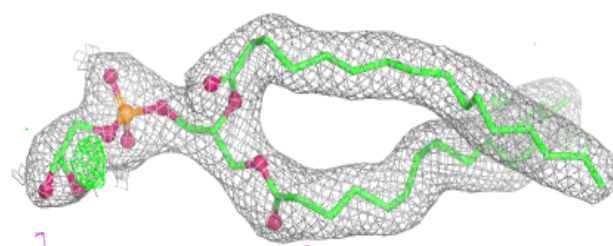
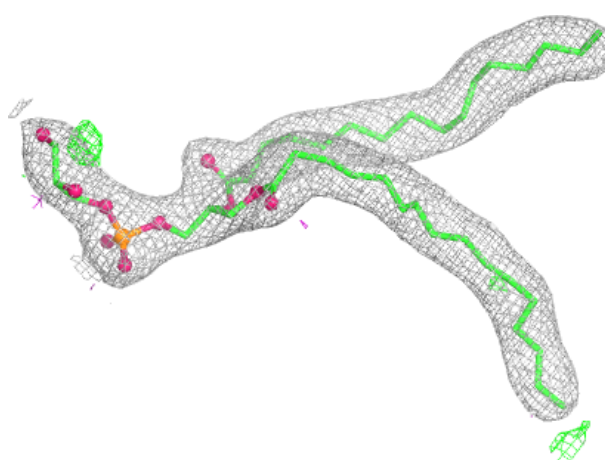
**Electron density around LHG d 406 (A):**

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



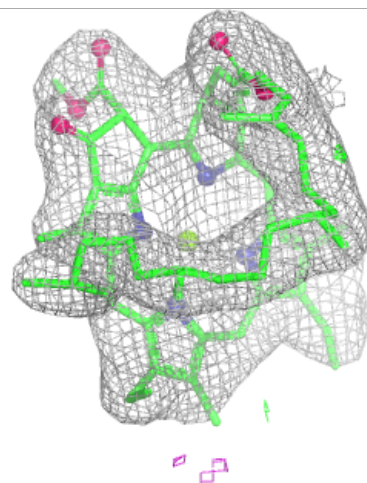
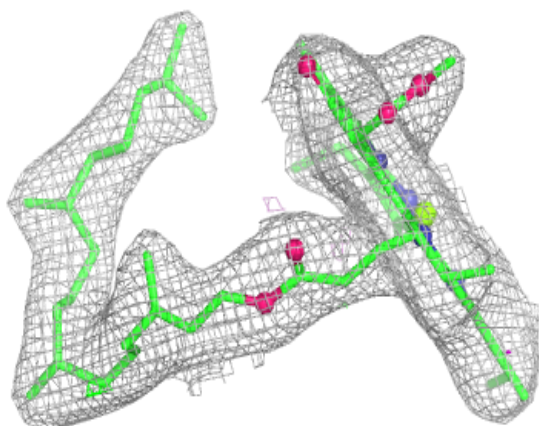
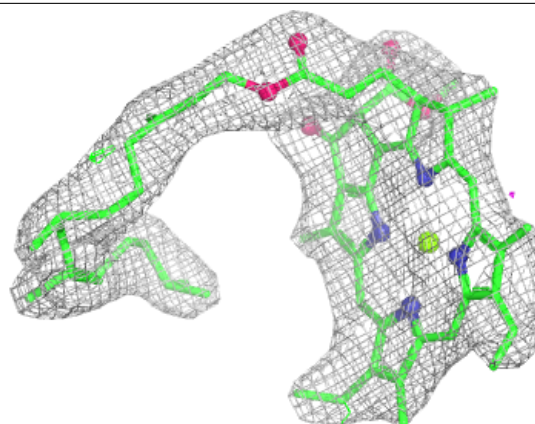
Electron density around LHG d 406 (B):

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



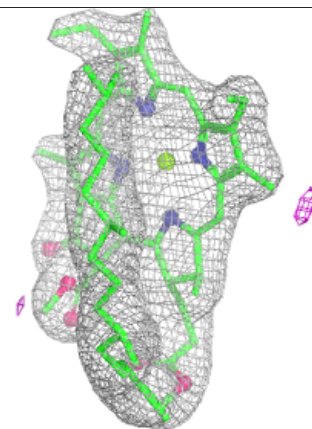
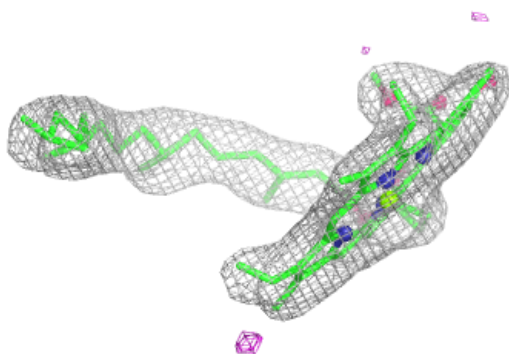
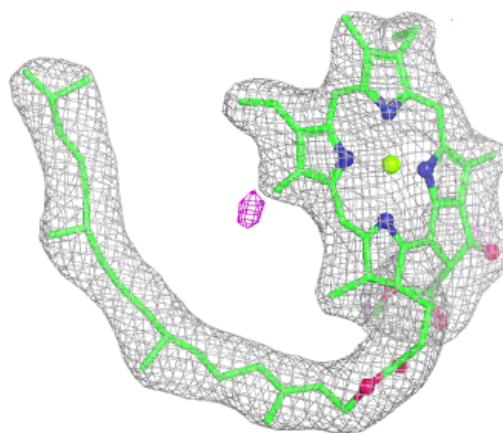
Electron density around CLA c 503:

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

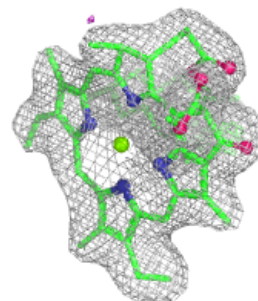
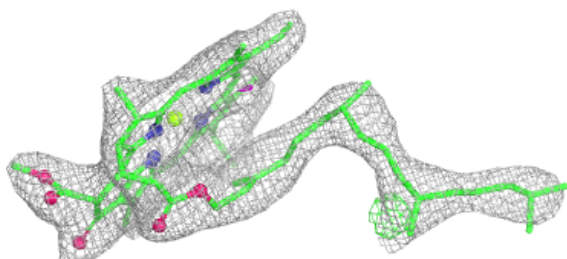
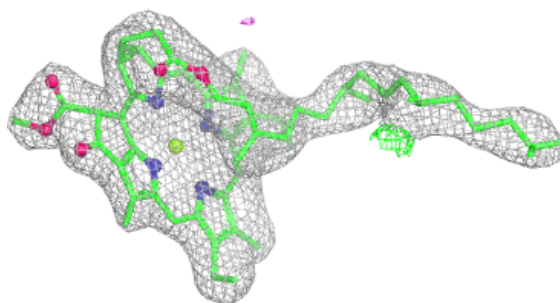


Electron density around CLA C 508:

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

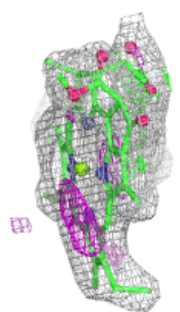
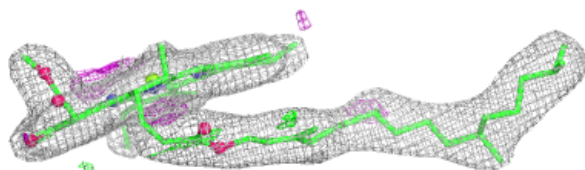
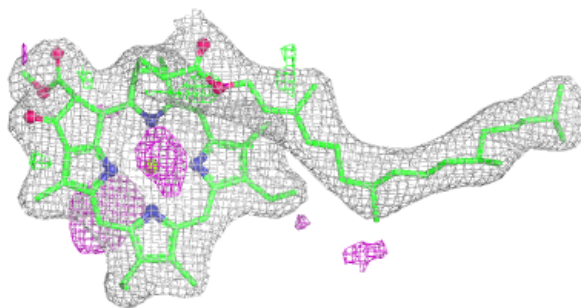
**Electron density around CLA c 505:**

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

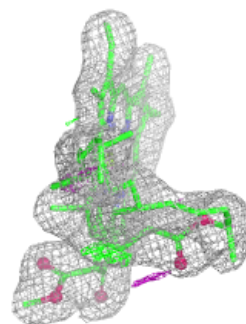
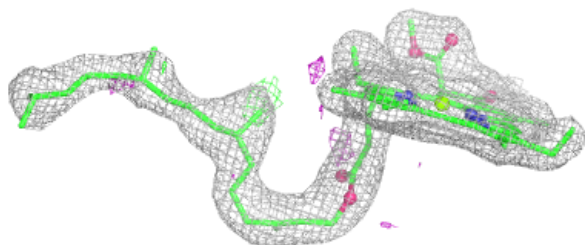
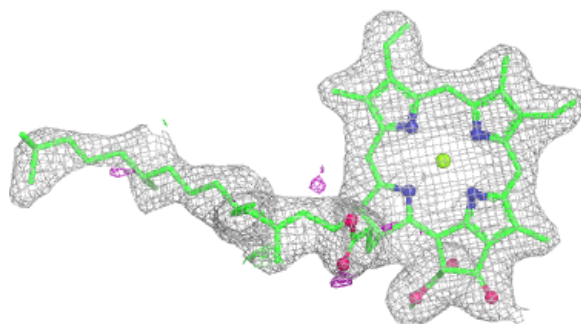


Electron density around CLA B 603:

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

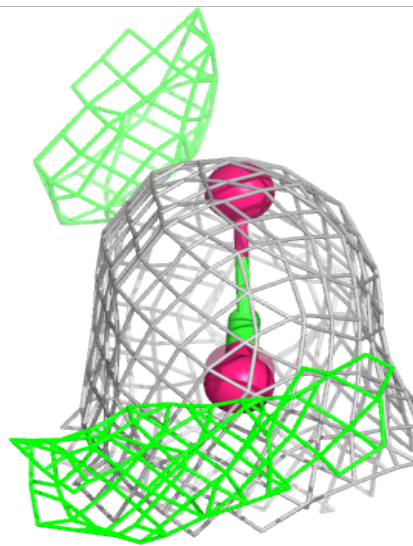
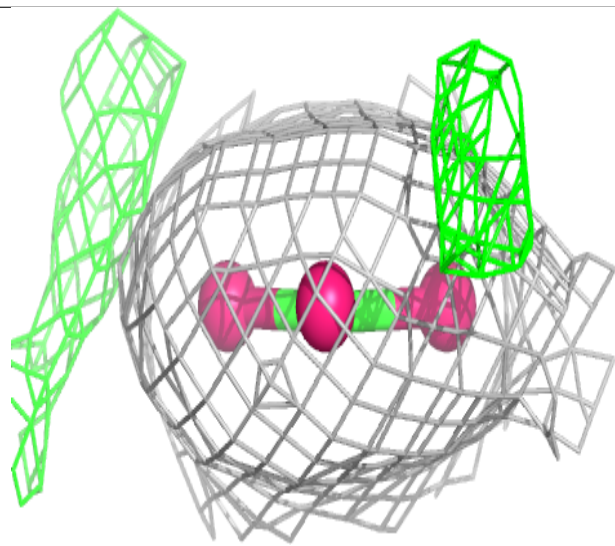
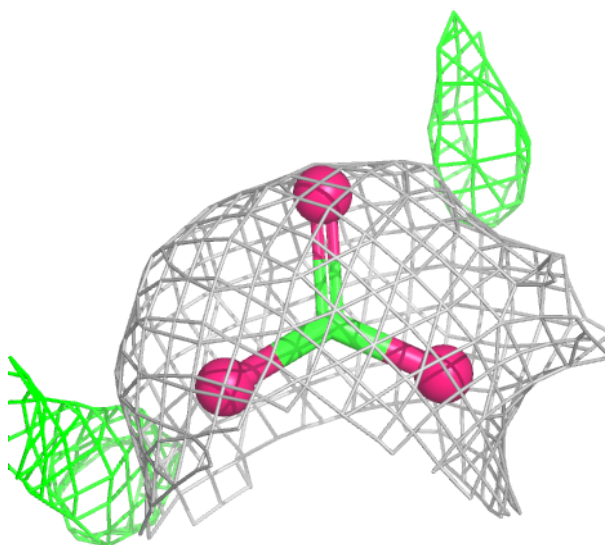
**Electron density around CLA A 406 (A):**

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



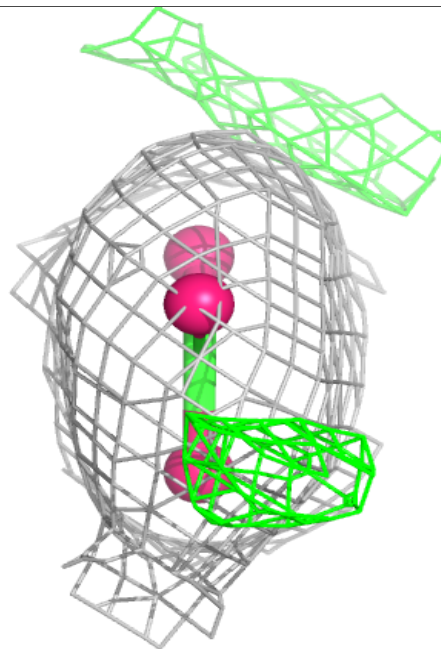
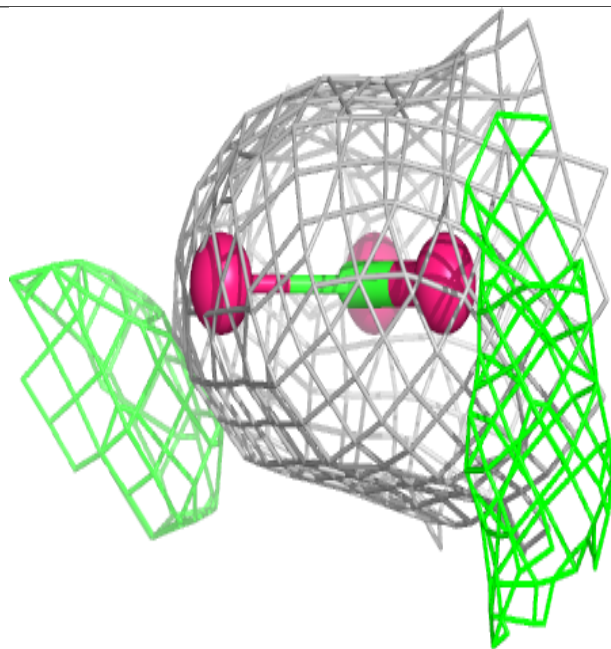
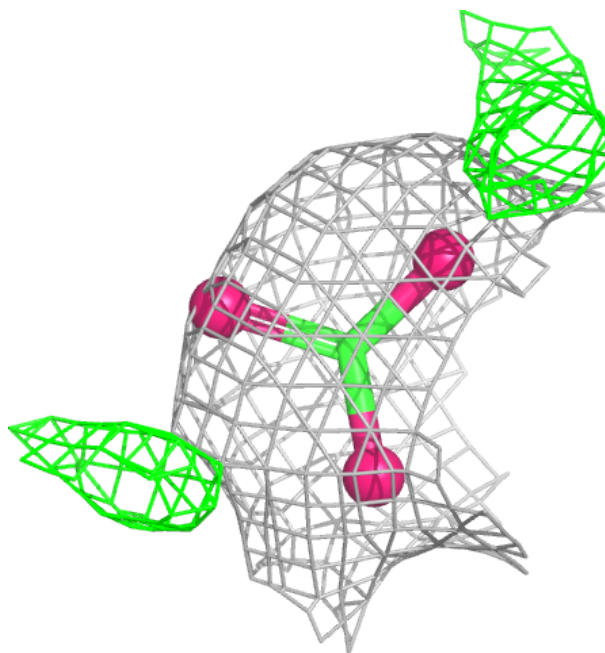
Electron density around BCT d 401 (A):

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



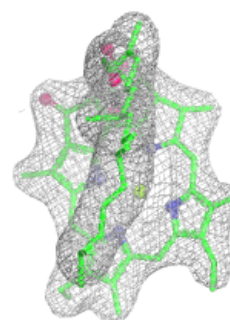
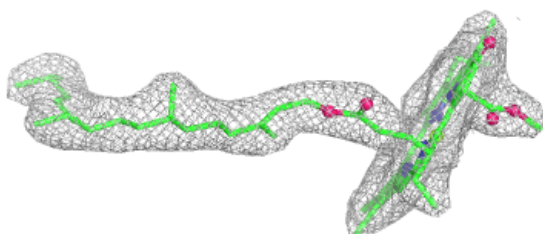
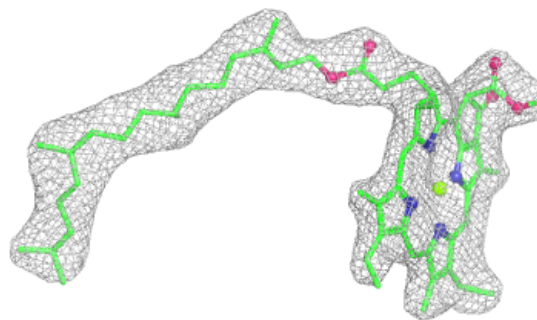
Electron density around BCT d 401 (B):

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

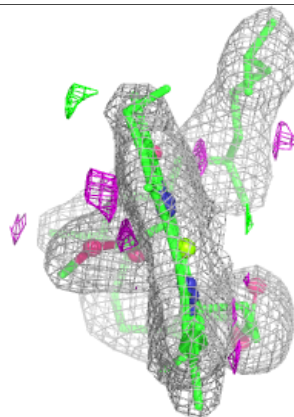
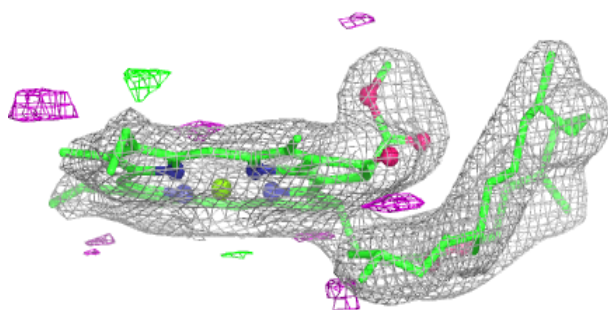
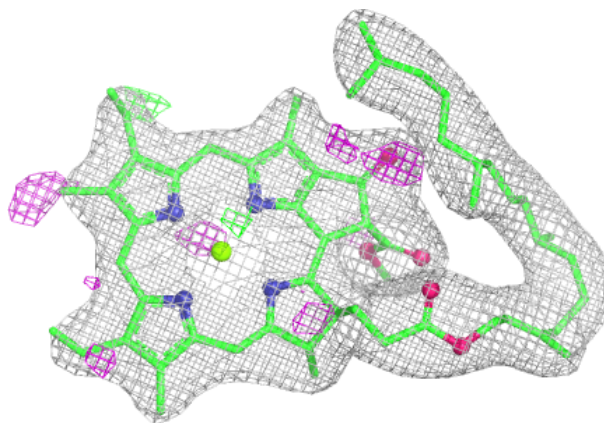


Electron density around CLA b 609:

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

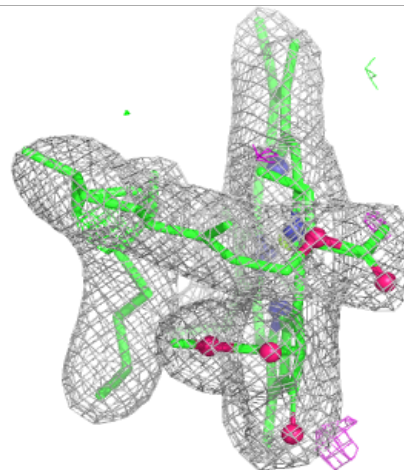
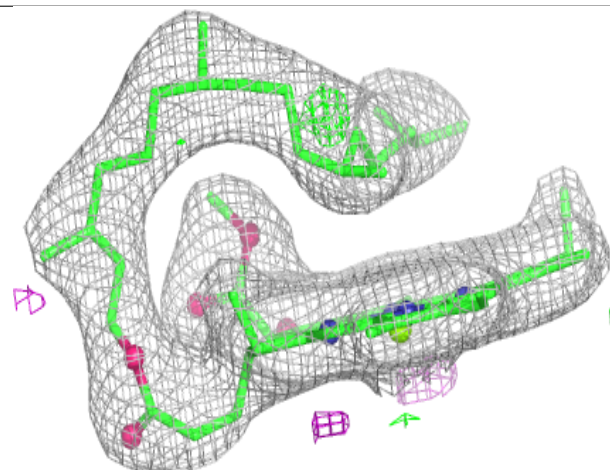
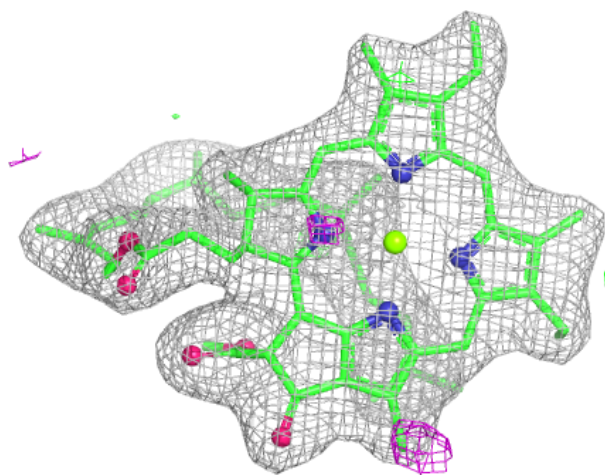
**Electron density around CLA b 610:**

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



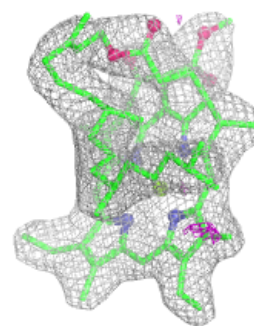
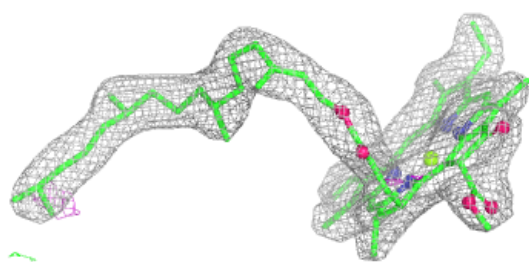
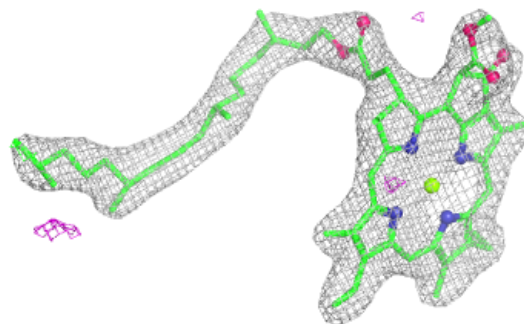
Electron density around CLA C 511:

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



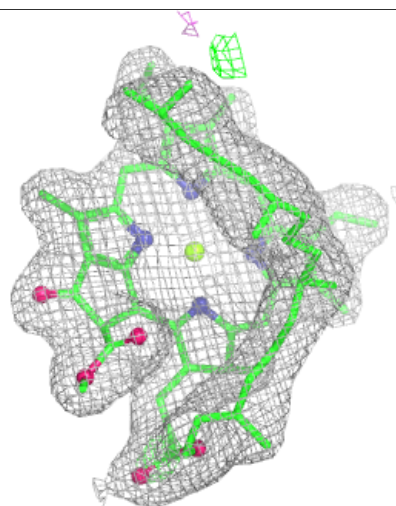
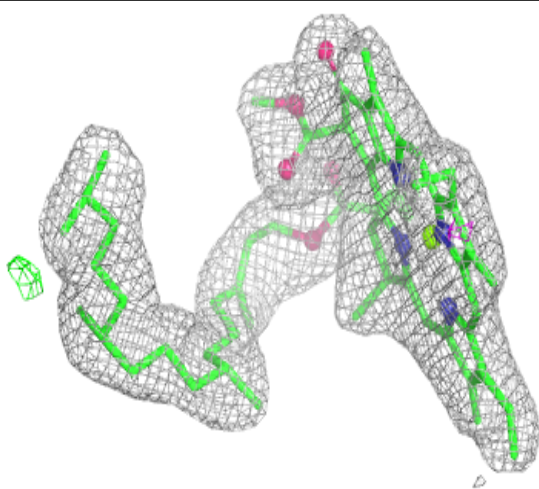
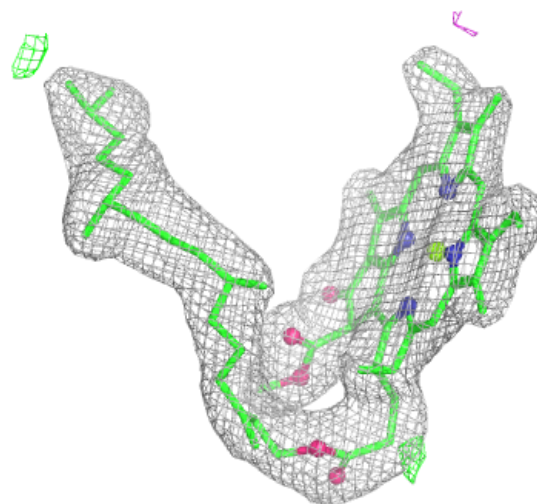
Electron density around CLA C 512:

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



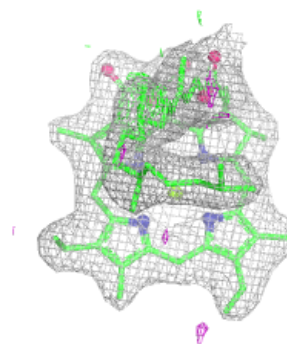
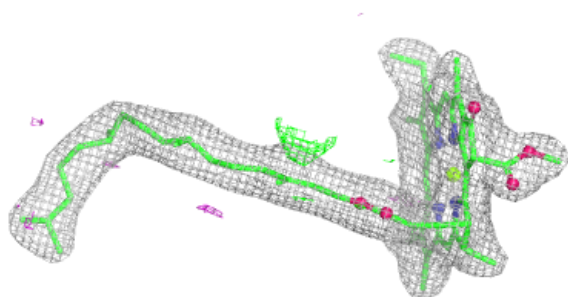
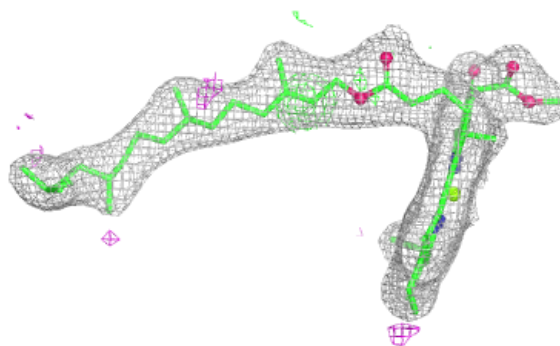
Electron density around CLA b 613:

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



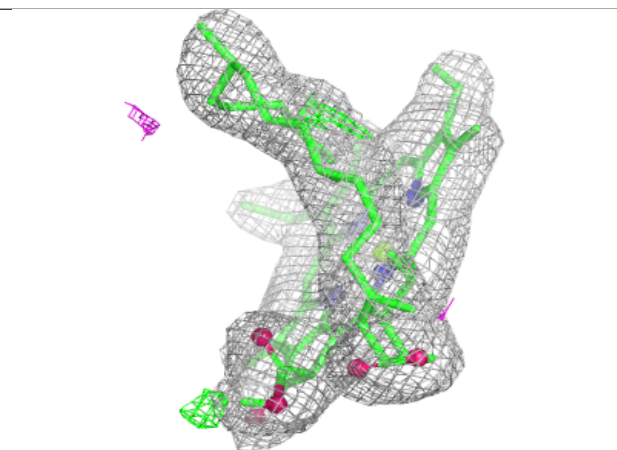
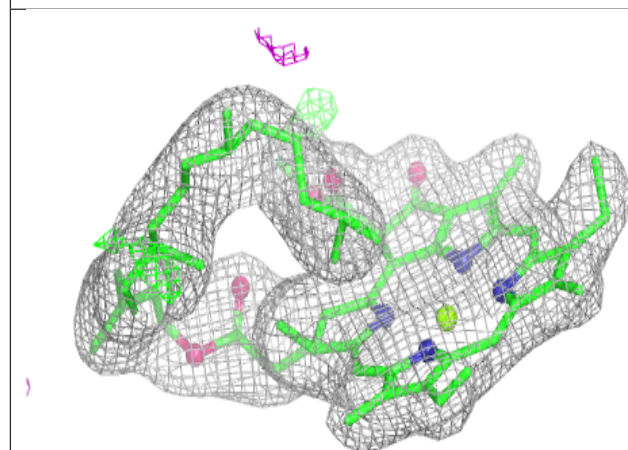
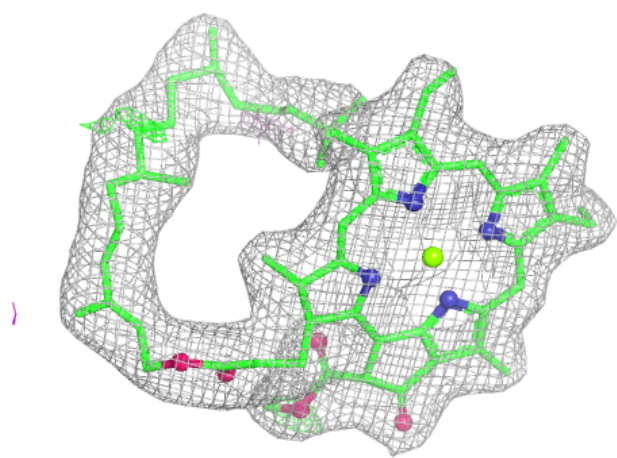
Electron density around CLA B 605:

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



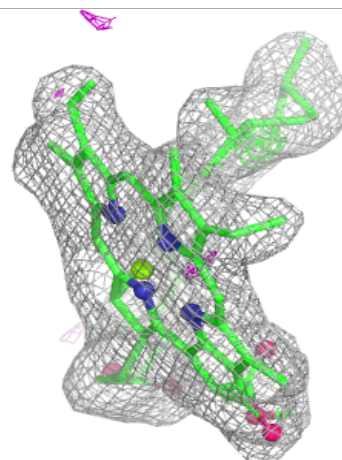
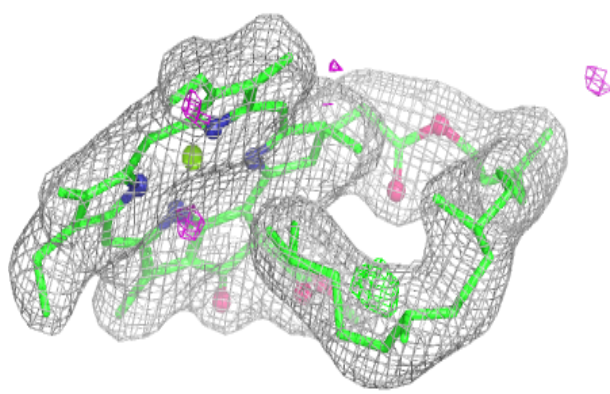
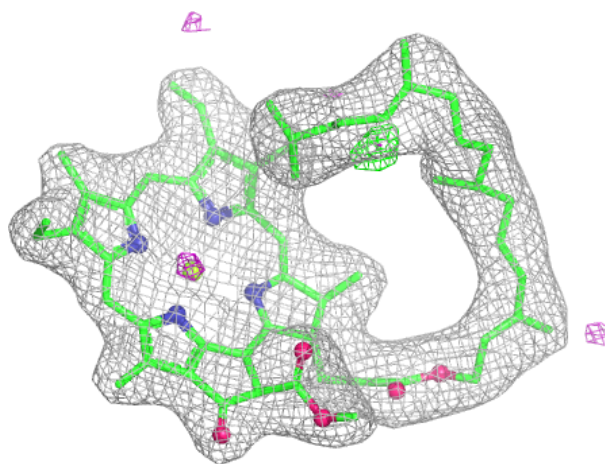
Electron density around CLA b 615:

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



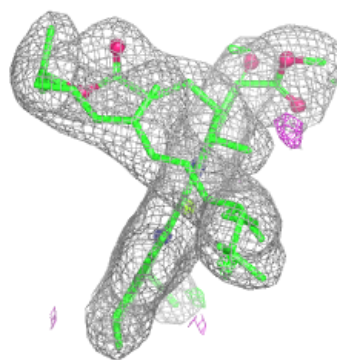
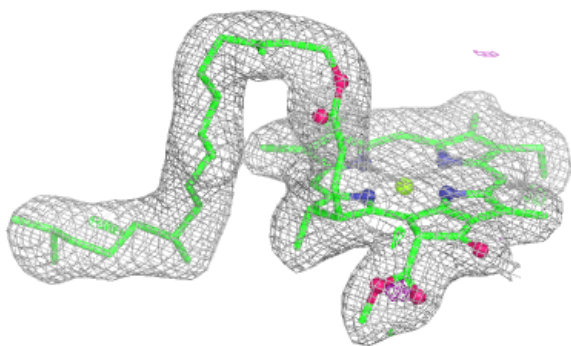
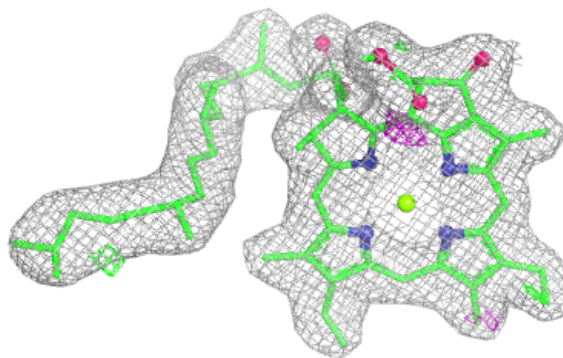
Electron density around CLA B 615:

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

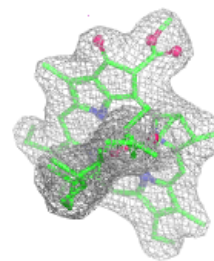
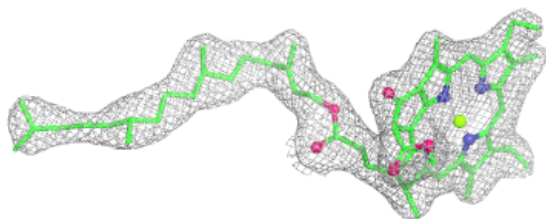
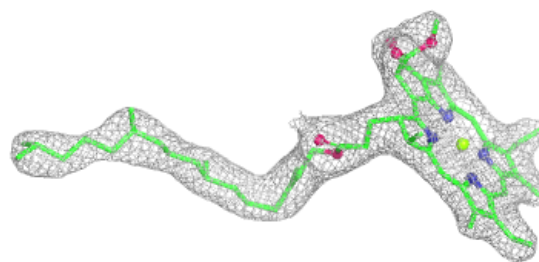


Electron density around CLA A 405 (A):

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

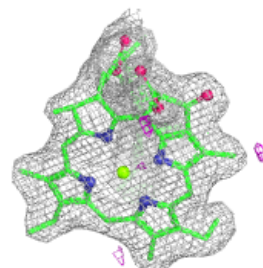
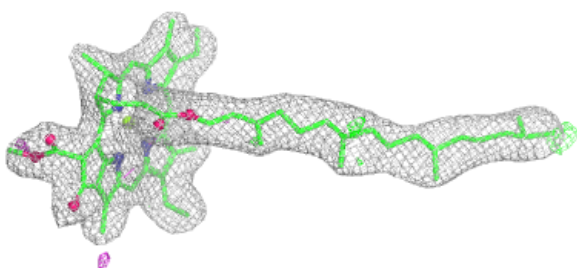
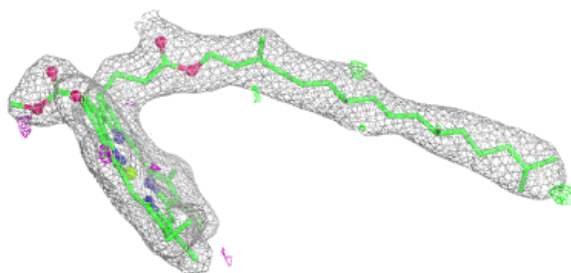
**Electron density around CLA c 502:**

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

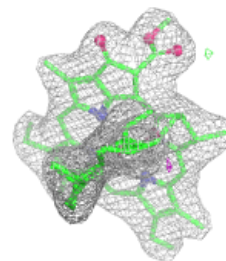
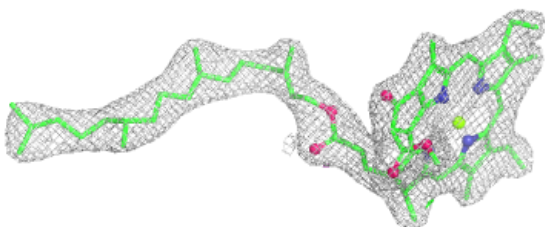
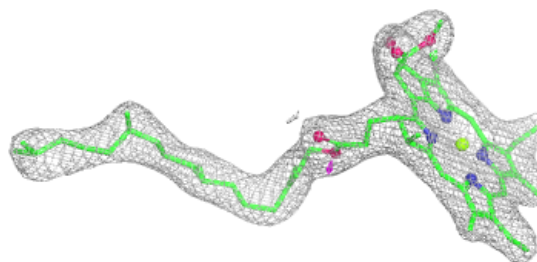


Electron density around CLA B 607:

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

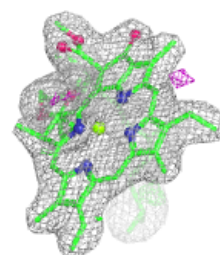
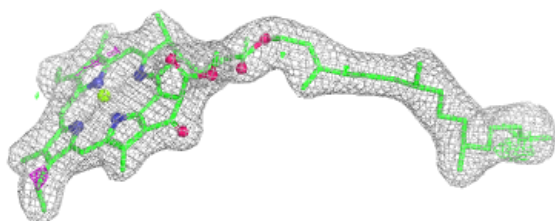
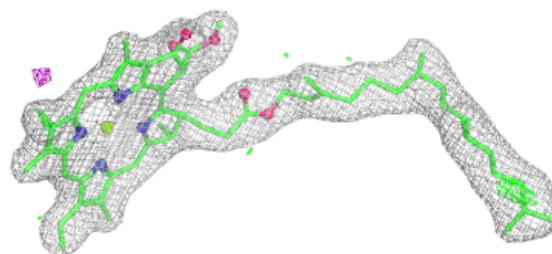
**Electron density around CLA C 503:**

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

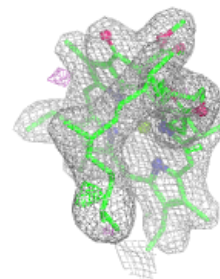
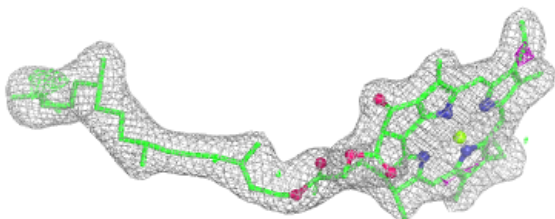
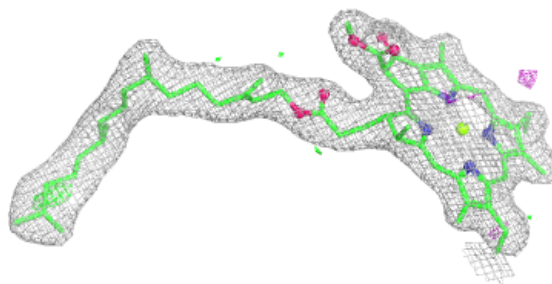


Electron density around CLA a 404 (A):

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

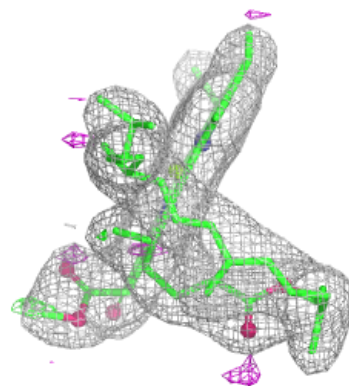
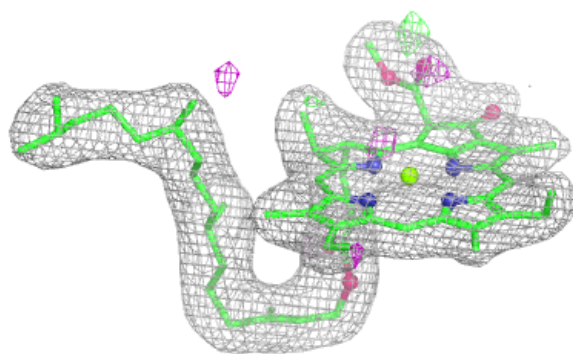
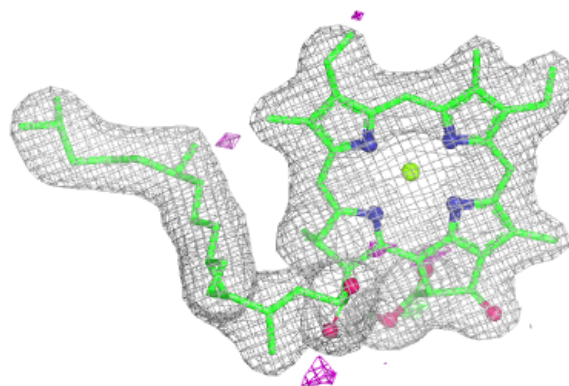
**Electron density around CLA a 404 (B):**

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

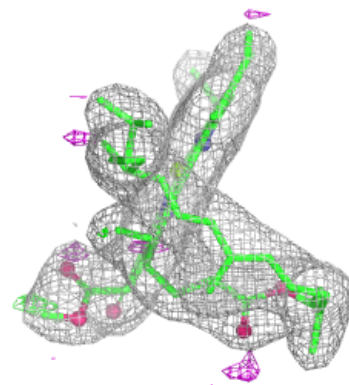
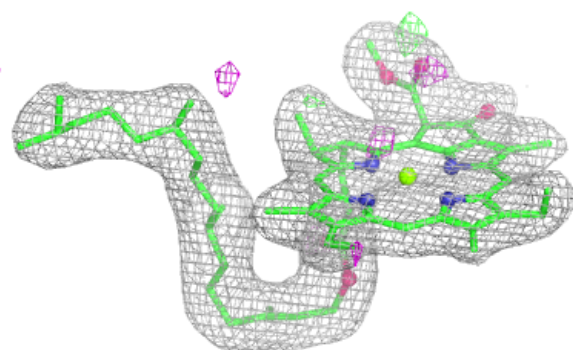
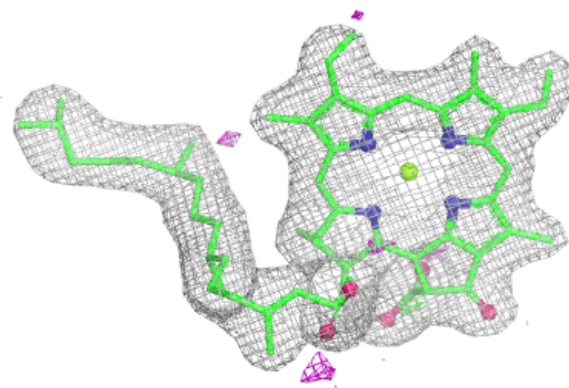


Electron density around CLA a 405 (A):

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

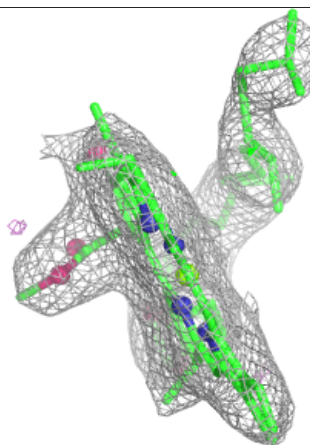
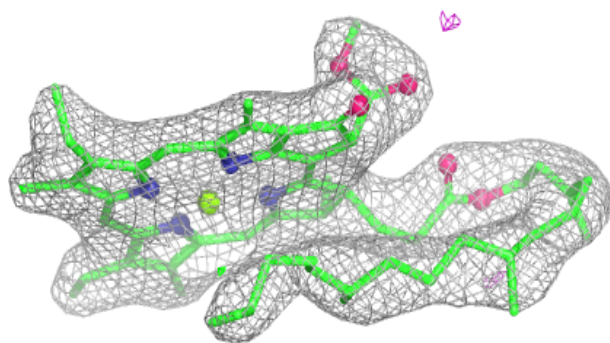
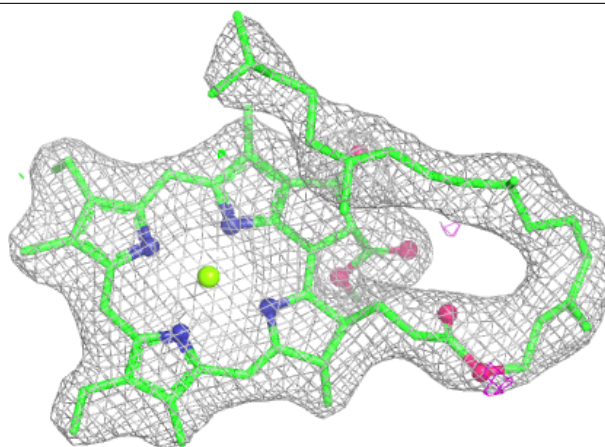
**Electron density around CLA a 405 (B):**

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



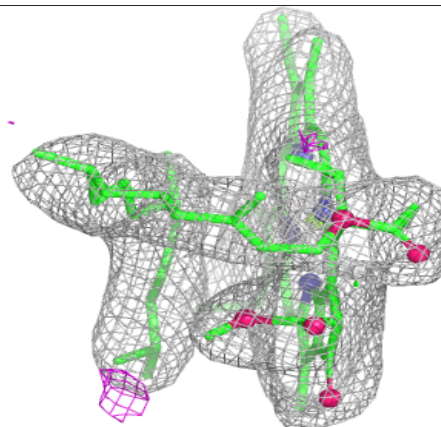
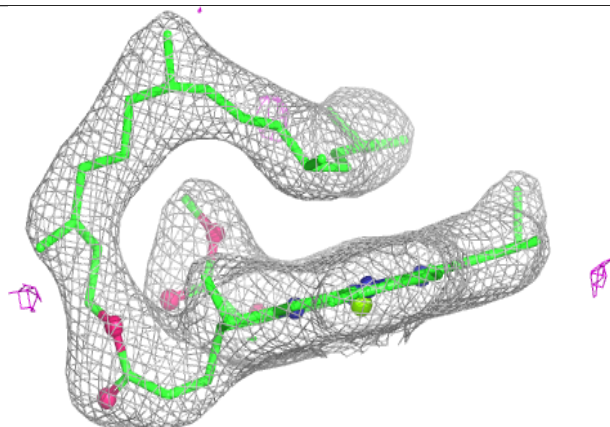
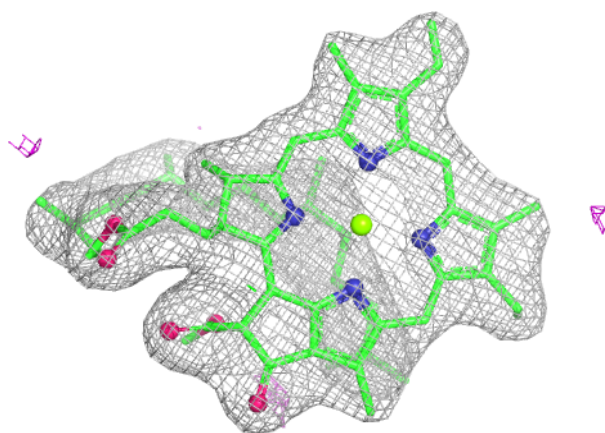
Electron density around CLA c 509:

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

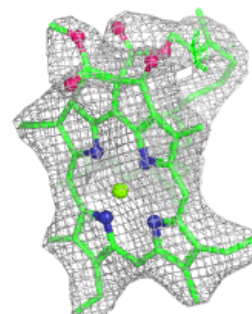
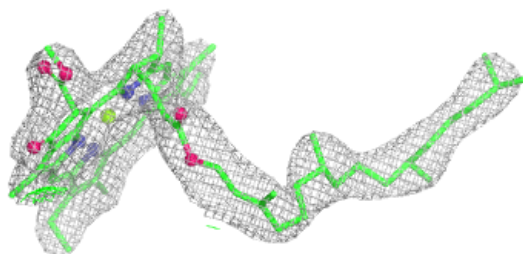
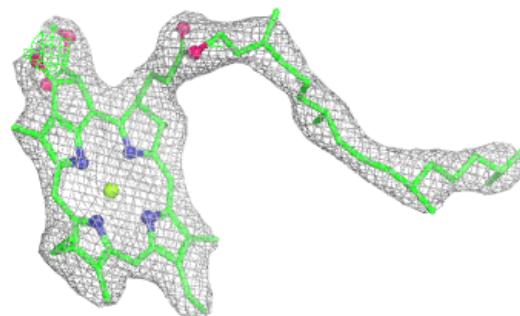


Electron density around CLA c 510:

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

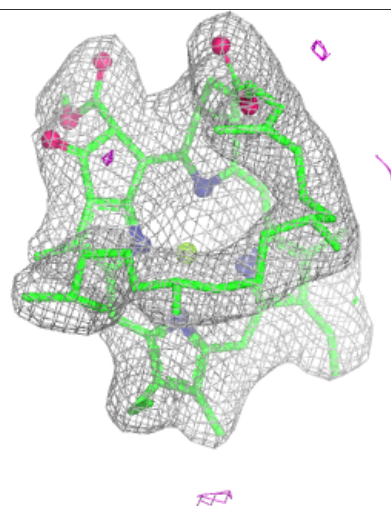
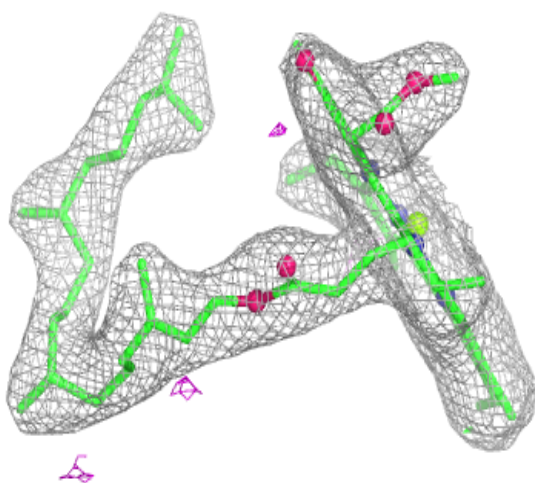
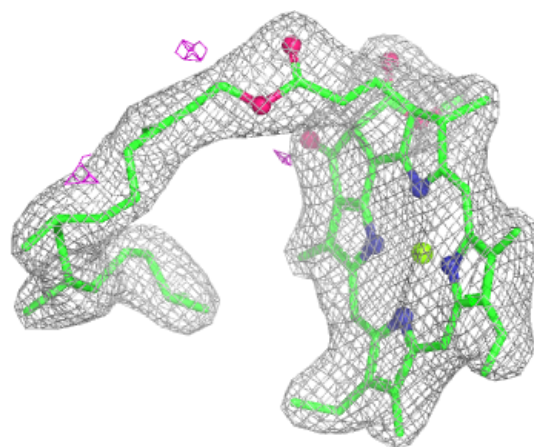
**Electron density around CLA c 511:**

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



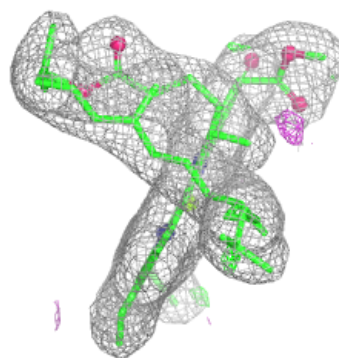
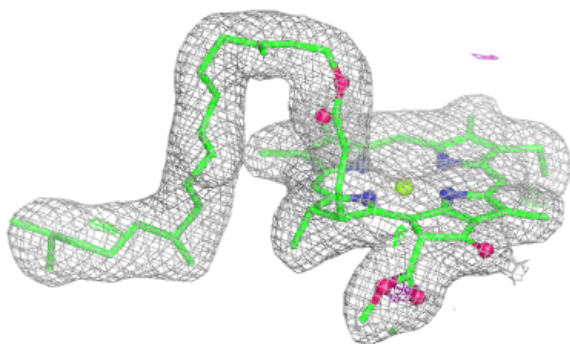
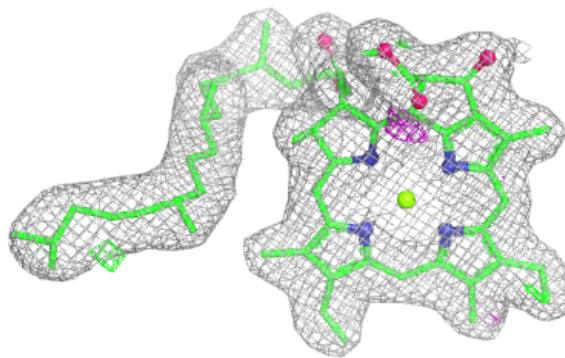
Electron density around CLA C 504:

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

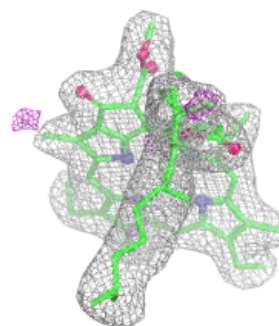
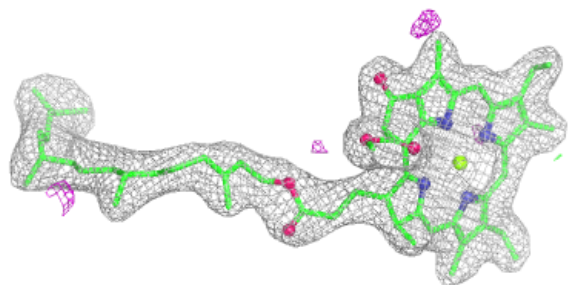
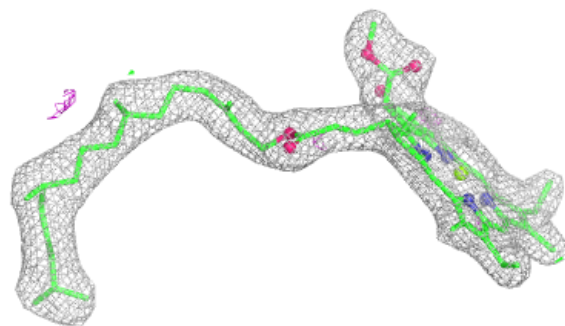


Electron density around CLA A 405 (B):

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

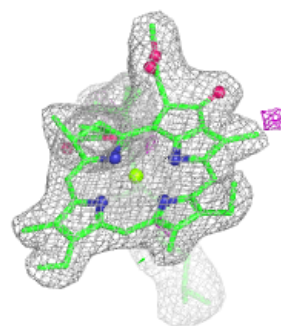
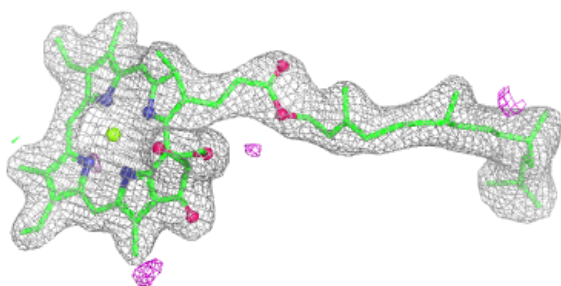
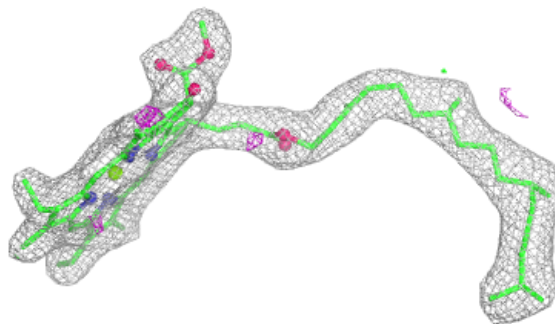
**Electron density around CLA d 402 (A):**

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



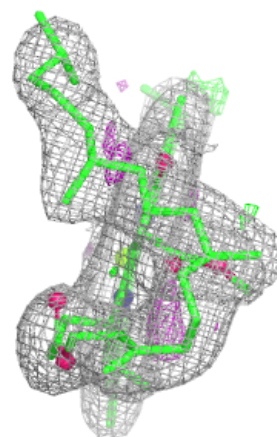
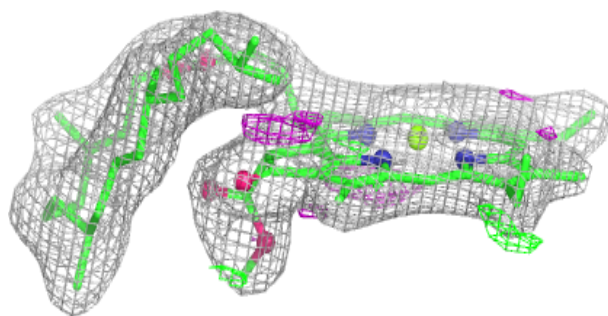
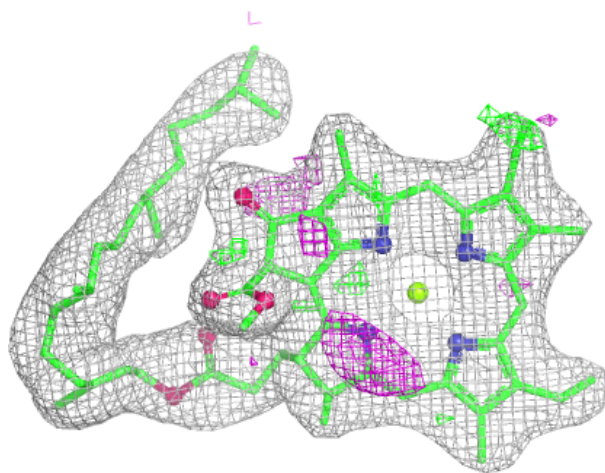
Electron density around CLA d 402 (B):

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



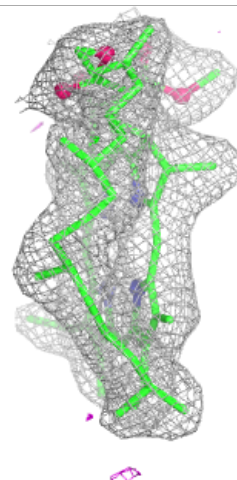
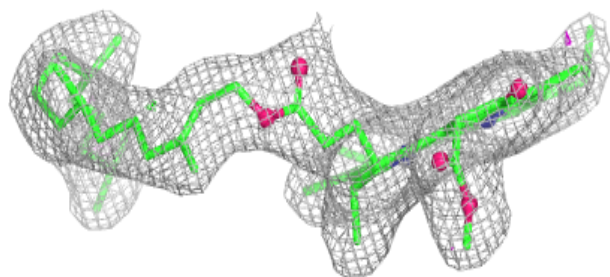
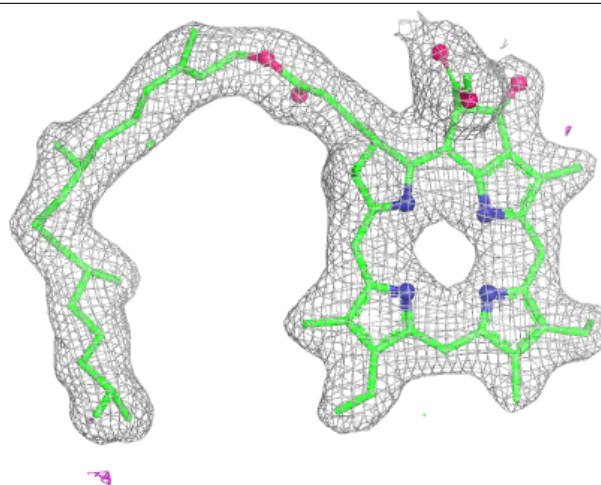
Electron density around CLA B 610:

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



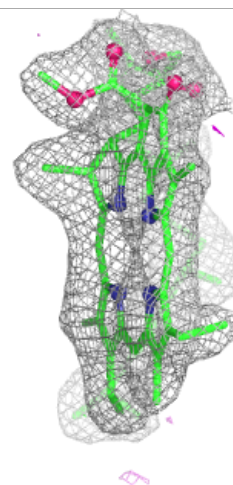
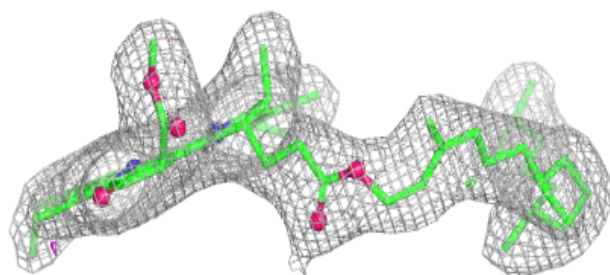
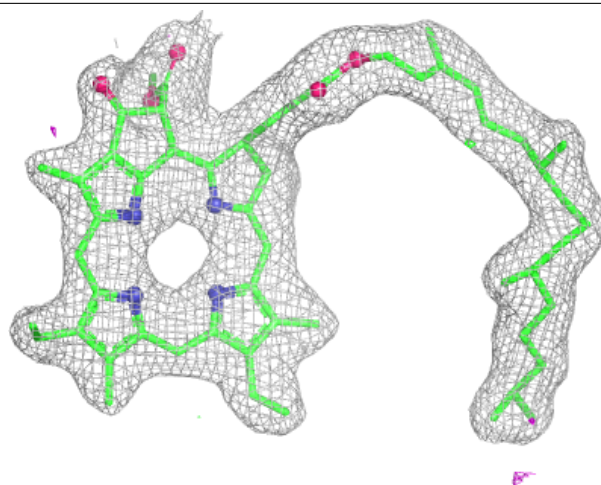
Electron density around PHO A 407 (A):

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



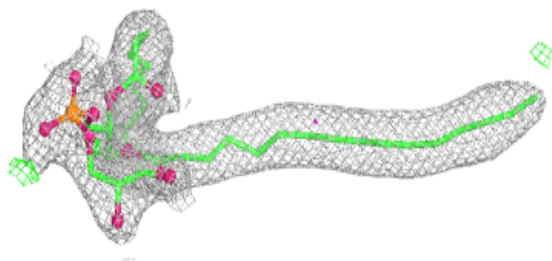
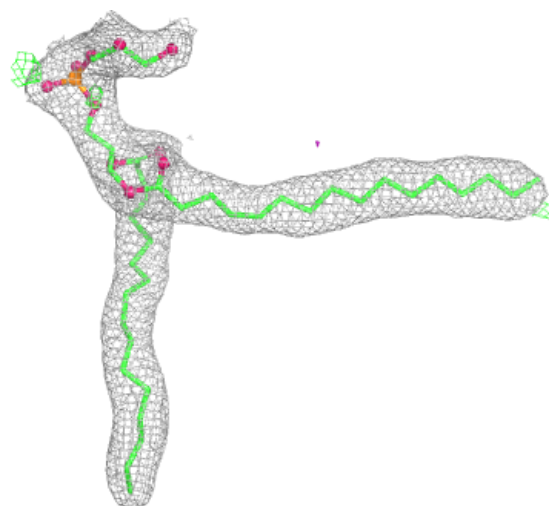
Electron density around PHO A 407 (B):

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



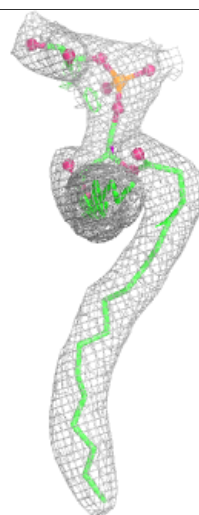
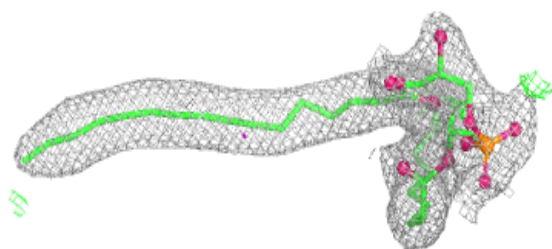
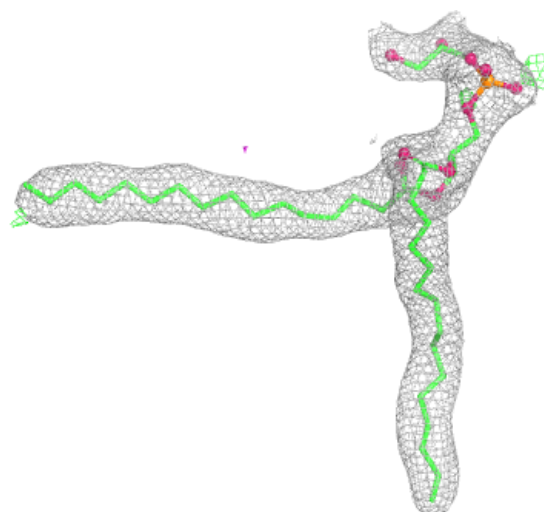
Electron density around LHG L 101 (A):

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



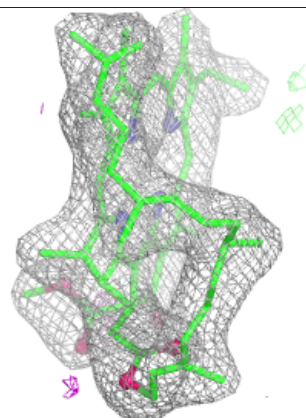
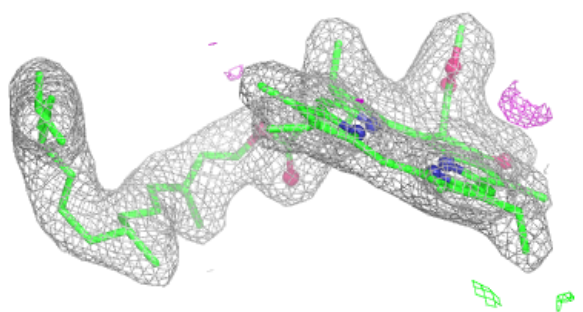
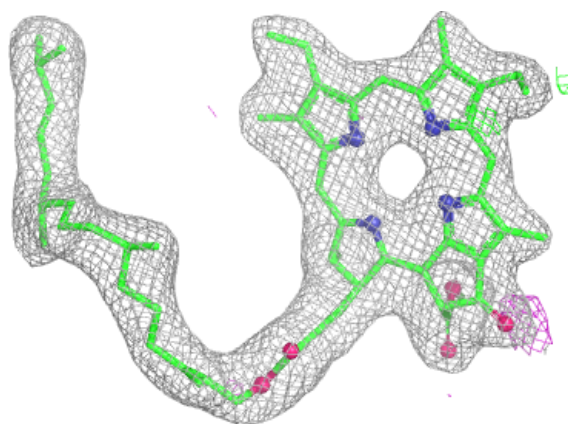
Electron density around LHG L 101 (B):

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

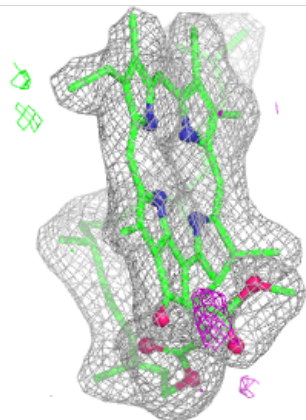
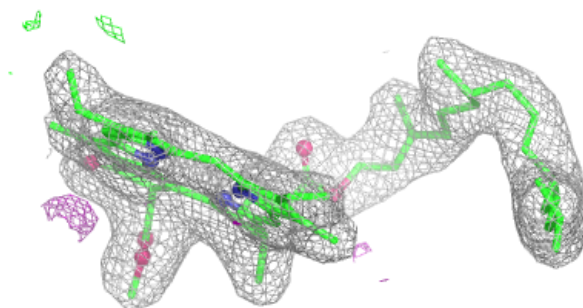
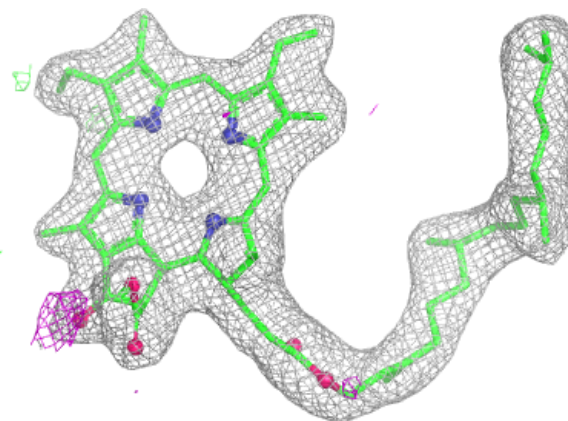


Electron density around PHO A 416 (A):

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

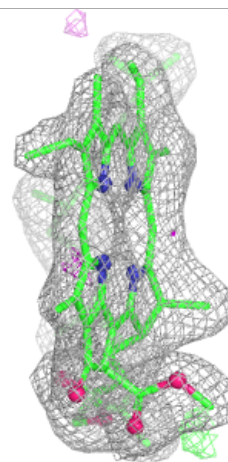
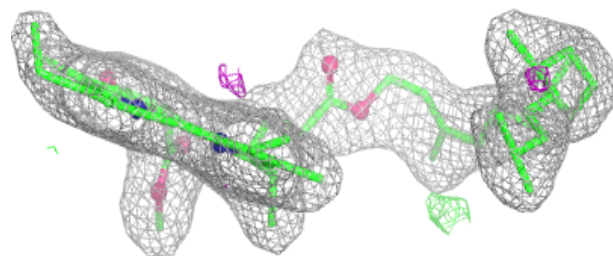
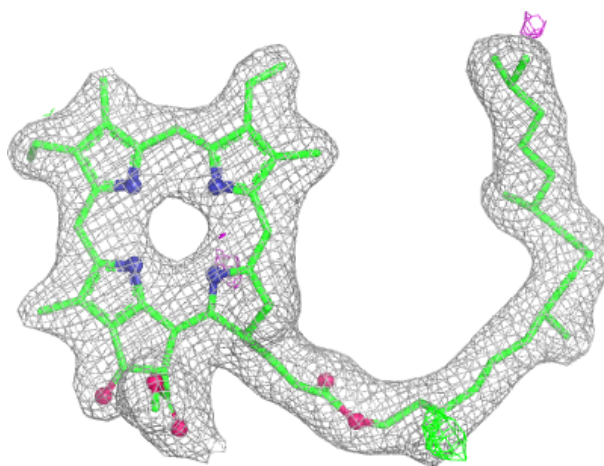
**Electron density around PHO A 416 (B):**

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



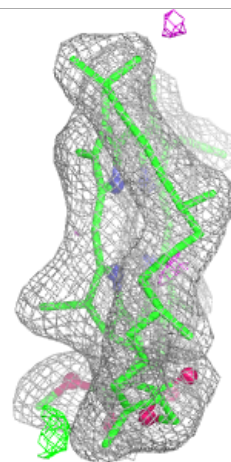
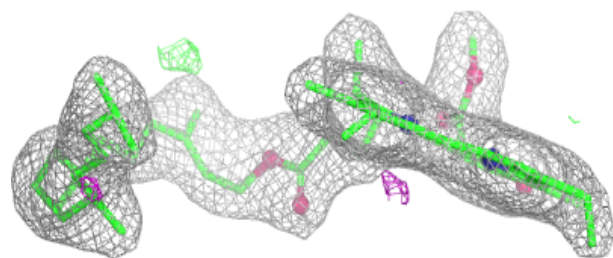
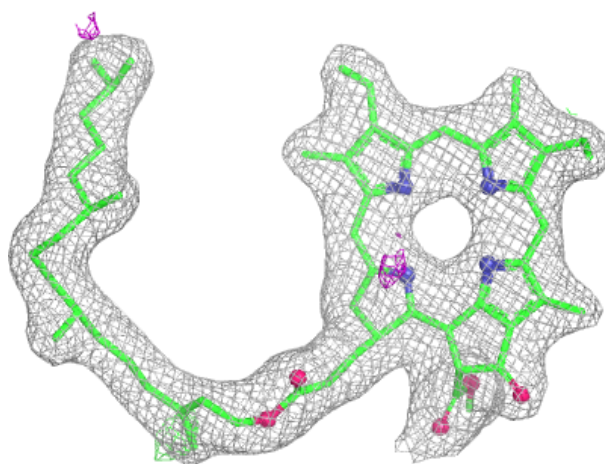
Electron density around PHO a 407 (A):

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



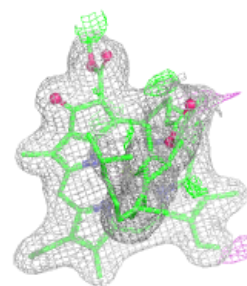
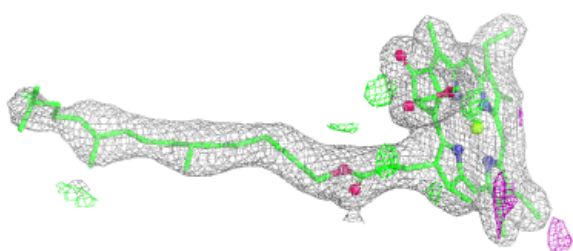
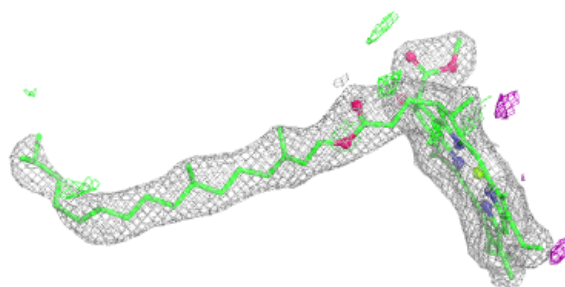
Electron density around PHO a 407 (B):

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

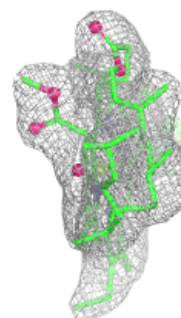
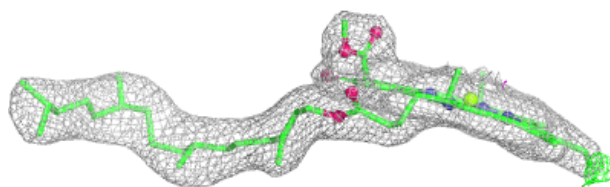
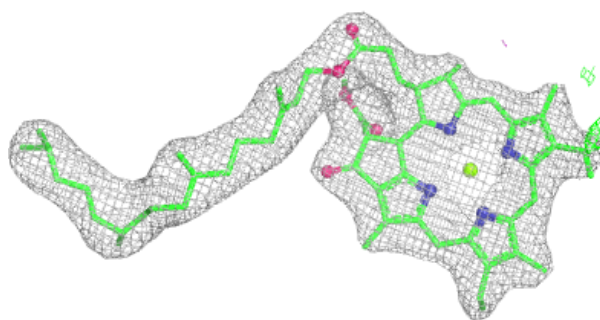


Electron density around CLA B 604:

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

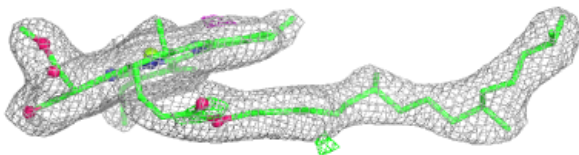
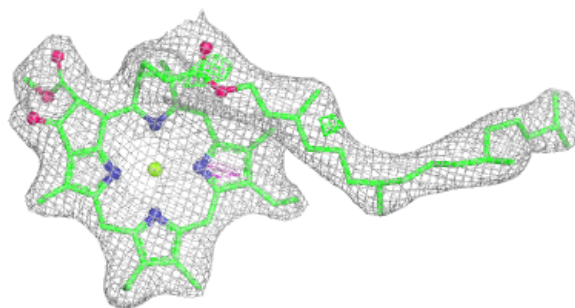
**Electron density around CLA b 602:**

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

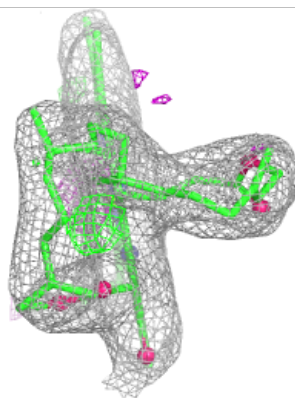
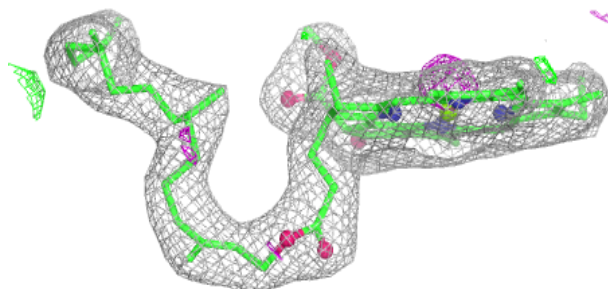
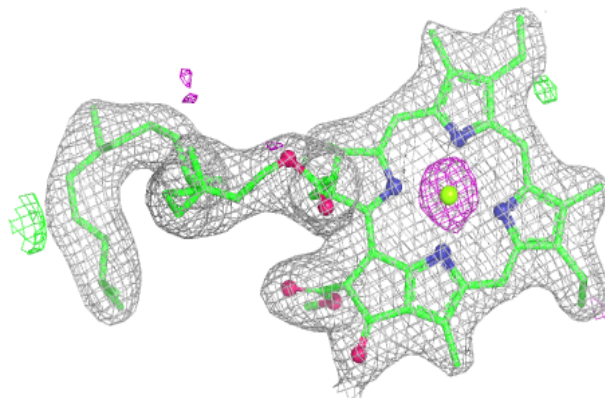


Electron density around CLA b 603:

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

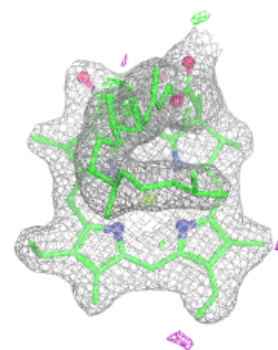
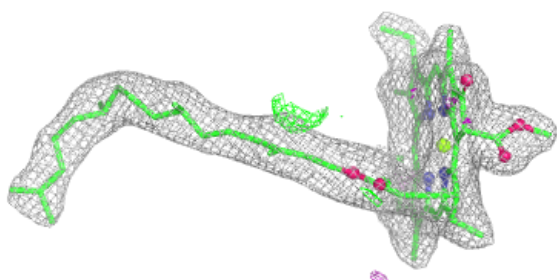
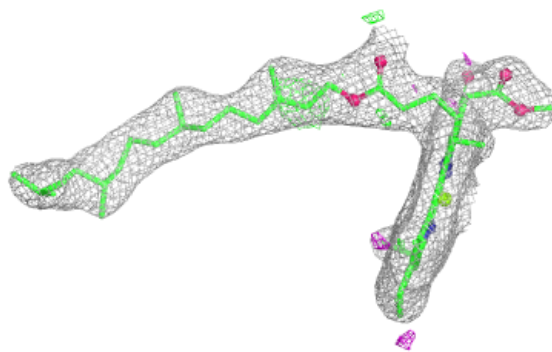
**Electron density around CLA B 612:**

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



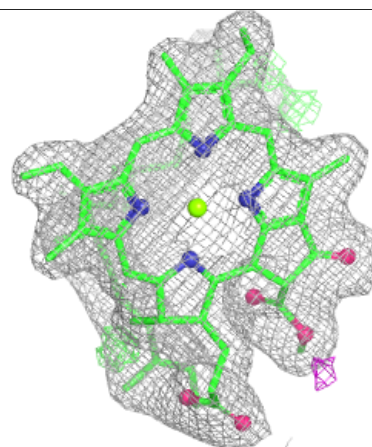
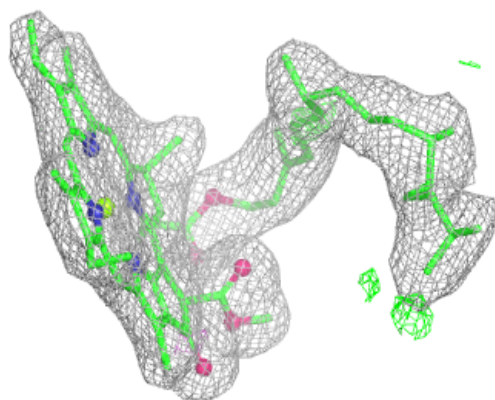
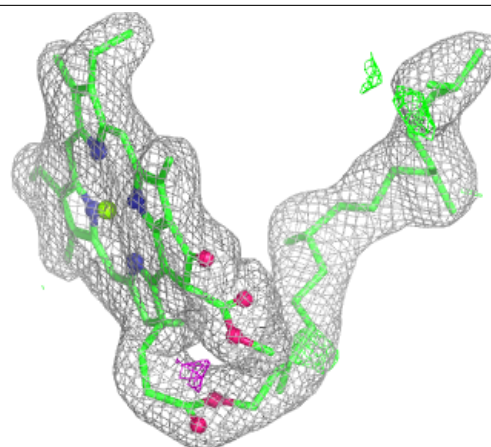
Electron density around CLA b 605:

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



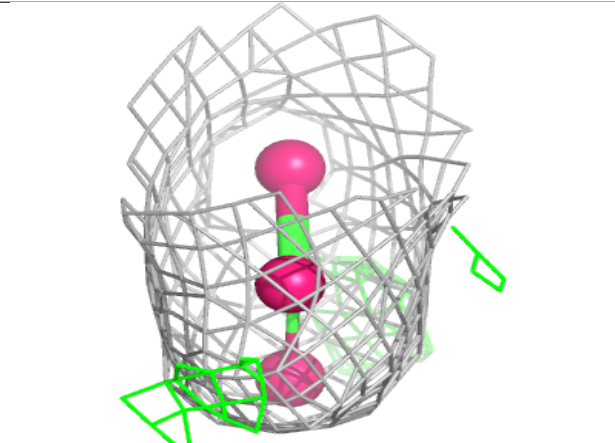
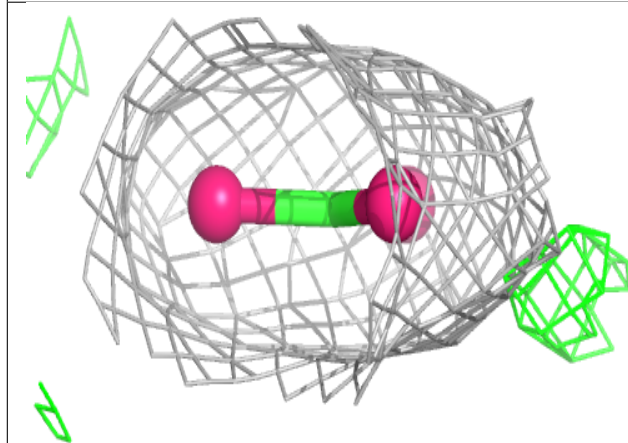
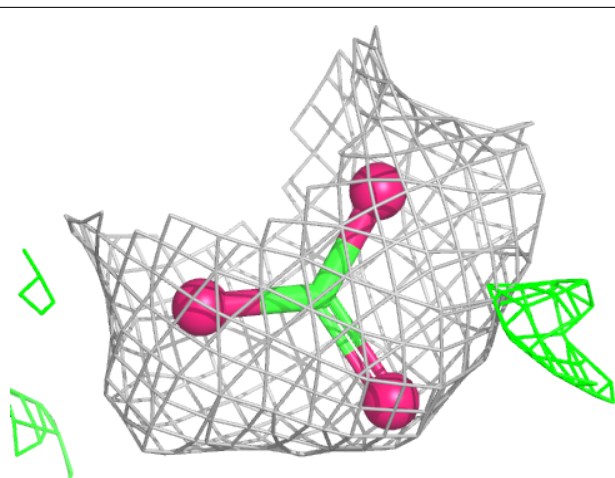
Electron density around CLA B 613:

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



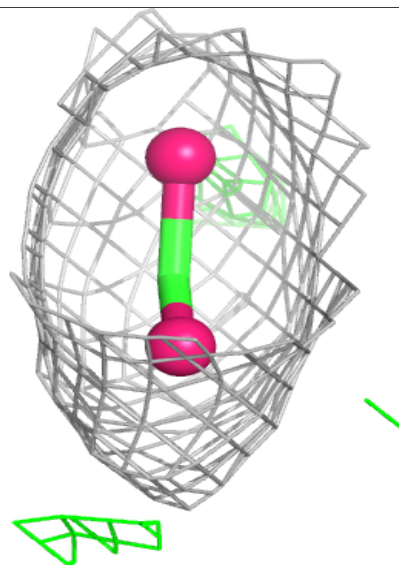
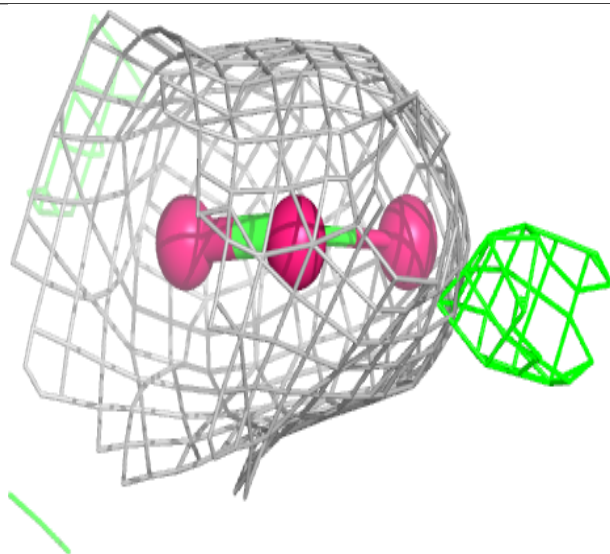
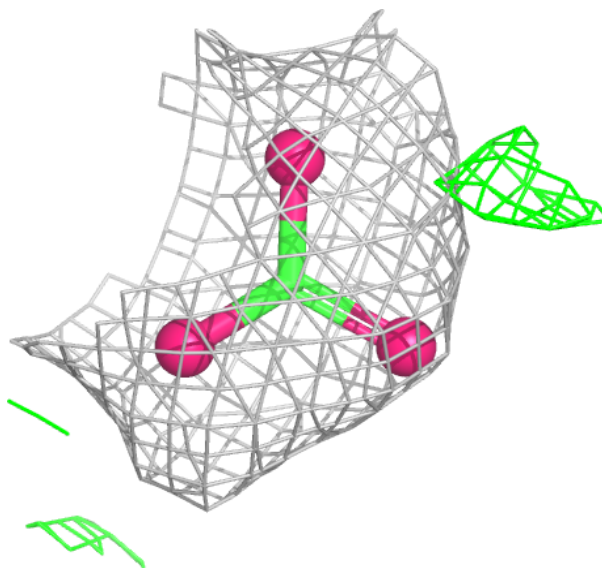
Electron density around BCT D 401 (A):

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



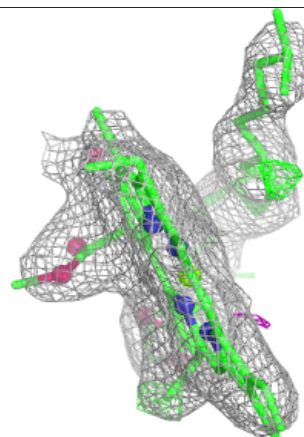
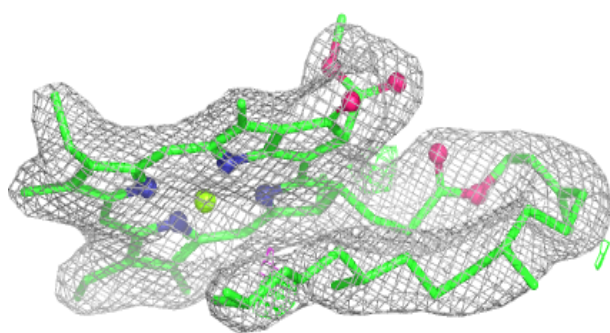
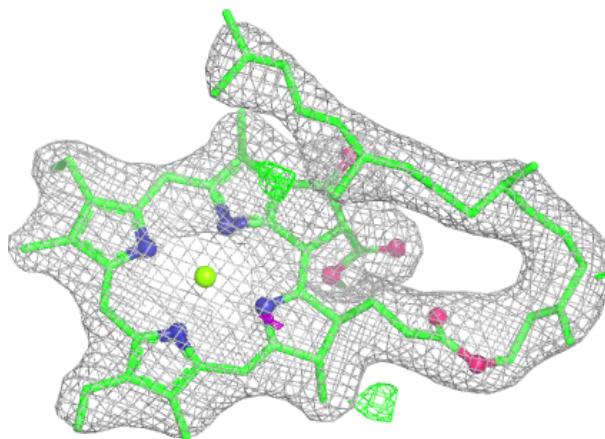
Electron density around BCT D 401 (B):

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



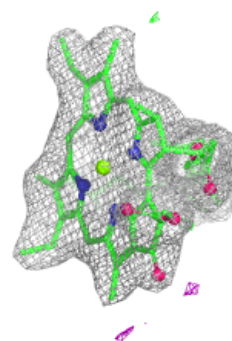
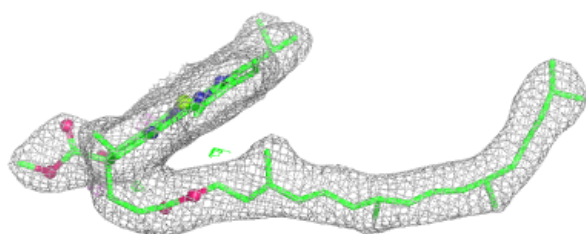
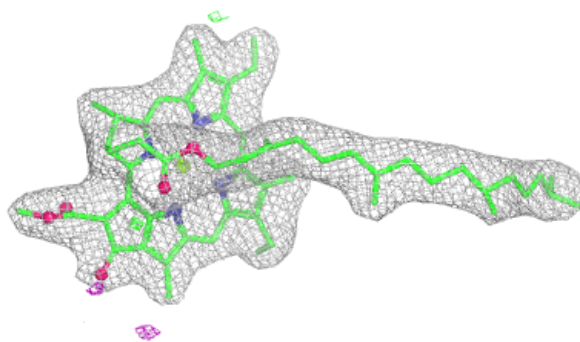
Electron density around CLA C 510:

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



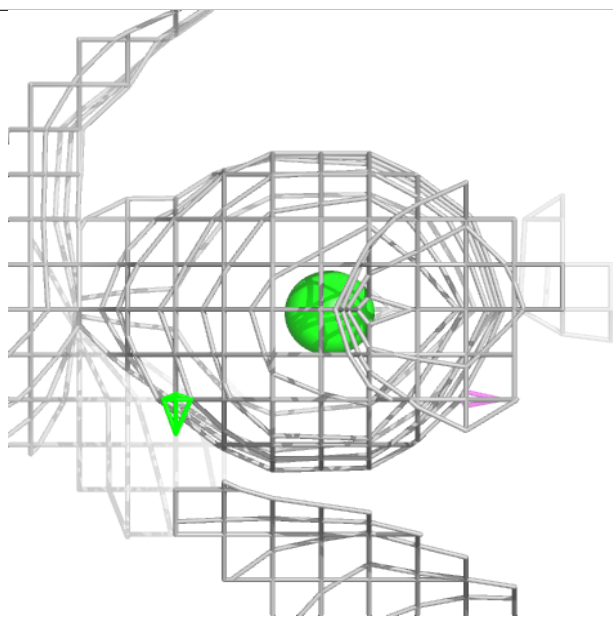
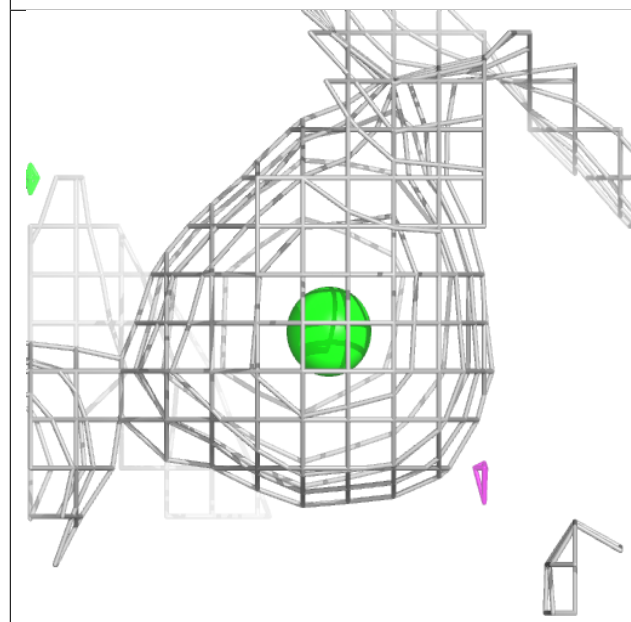
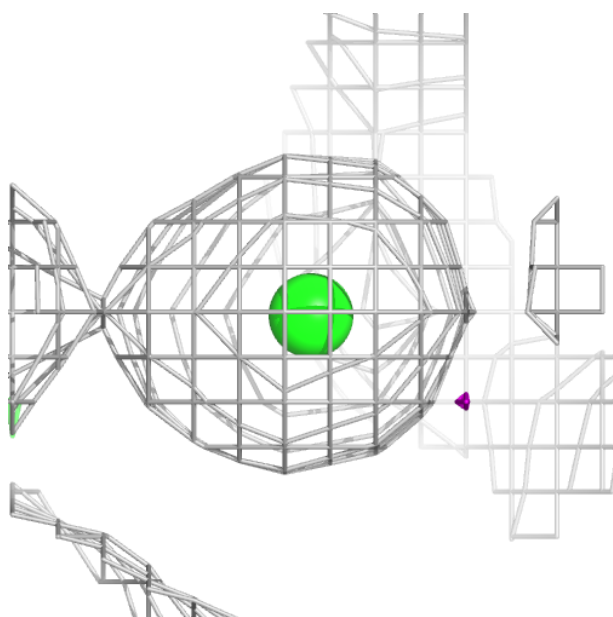
Electron density around CLA b 608:

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



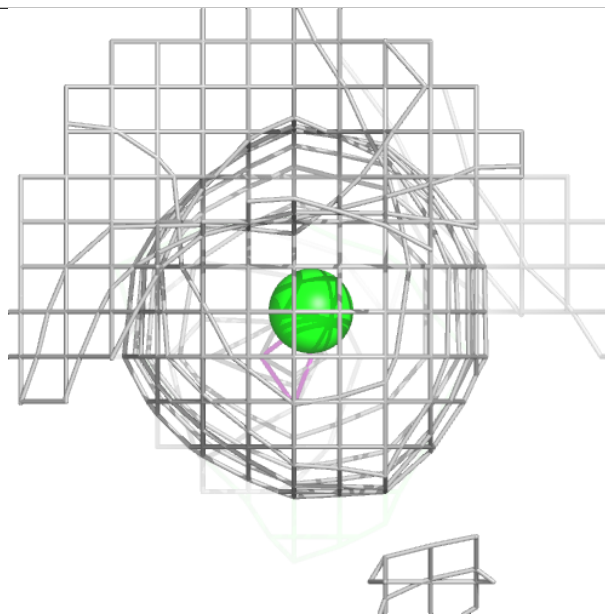
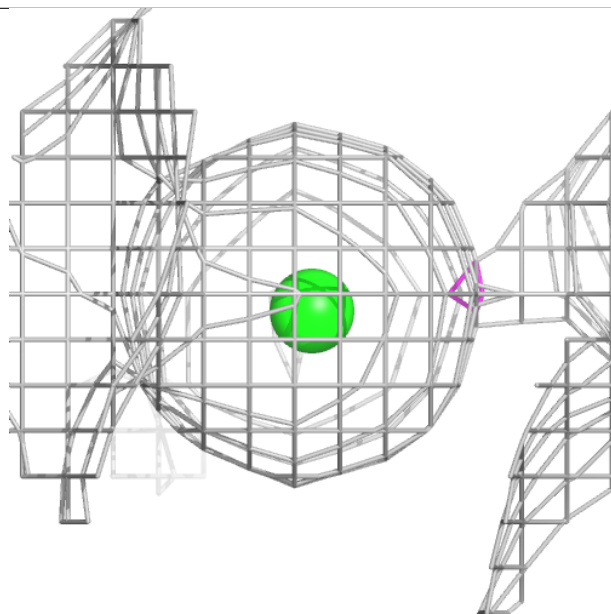
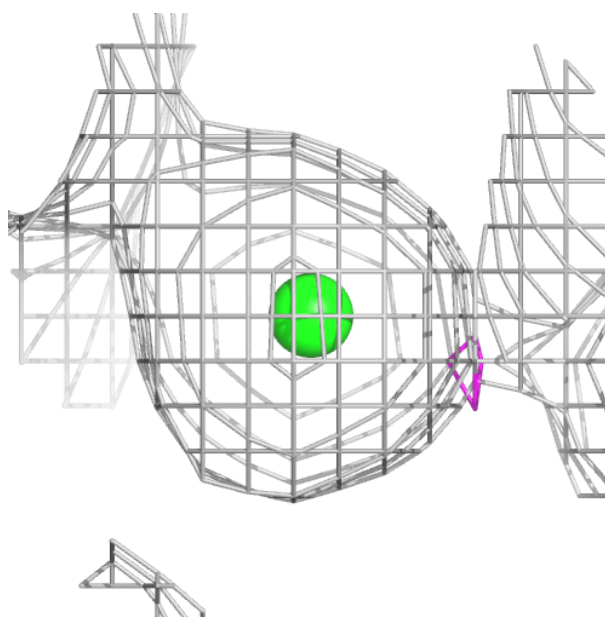
Electron density around CL a 403 (B):

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



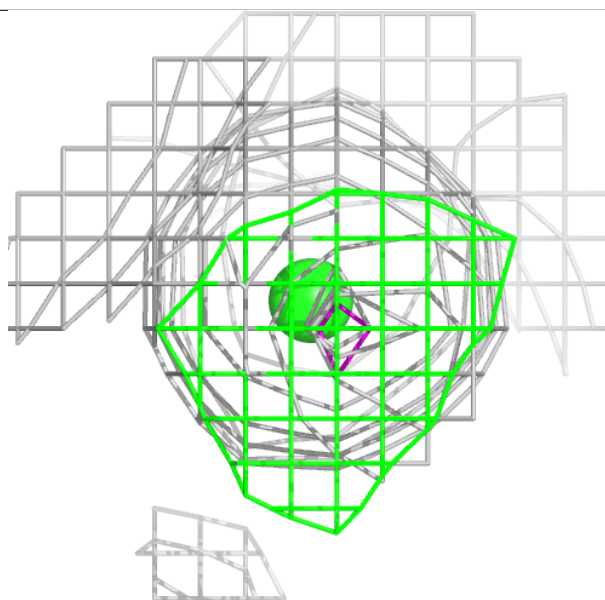
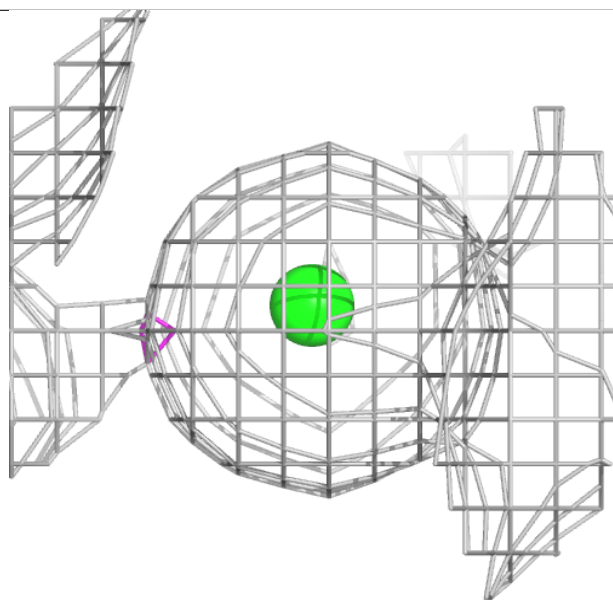
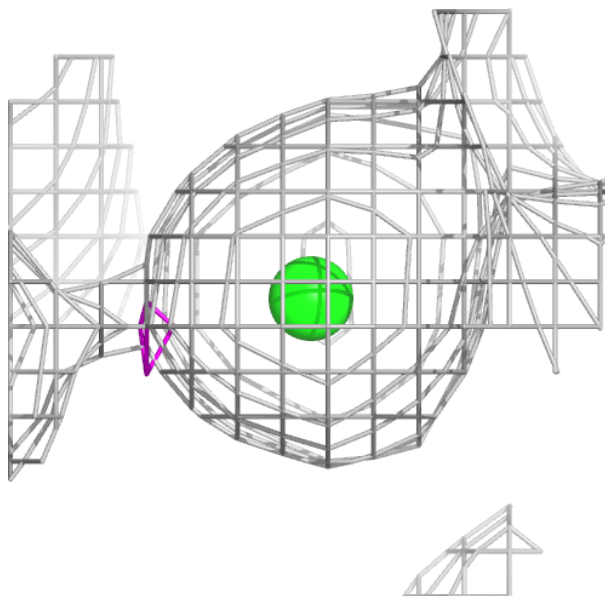
Electron density around CL A 403 (A):

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



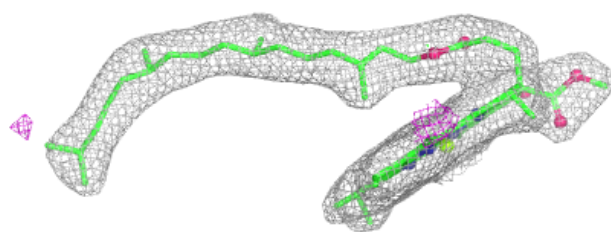
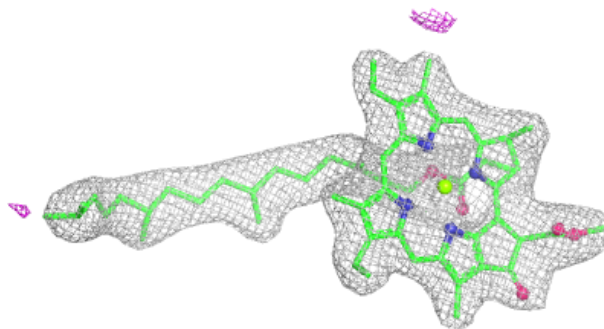
Electron density around CL A 403 (B):

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



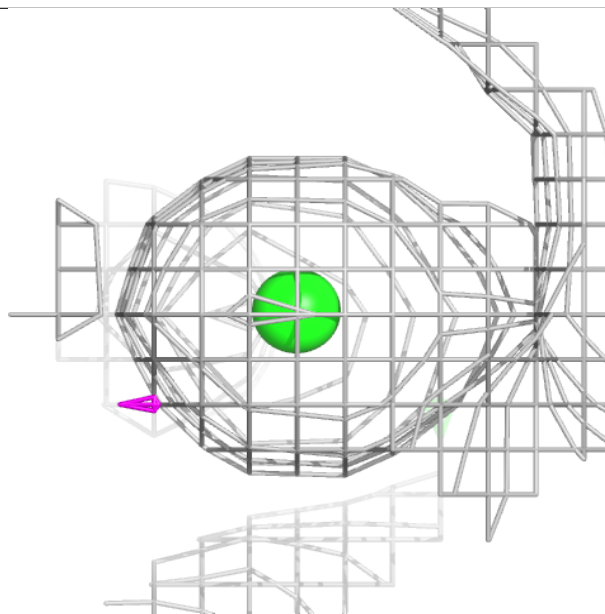
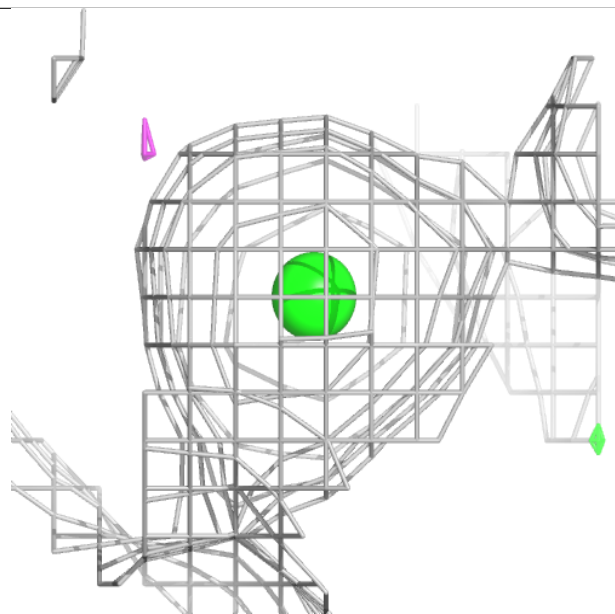
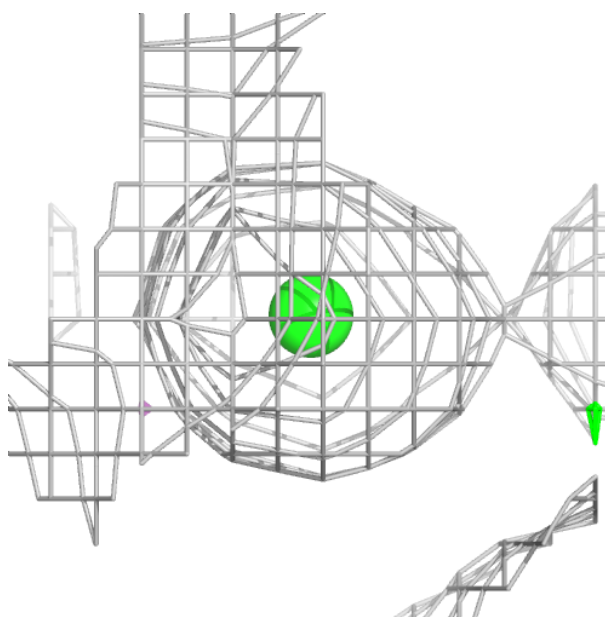
Electron density around CLA B 608:

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



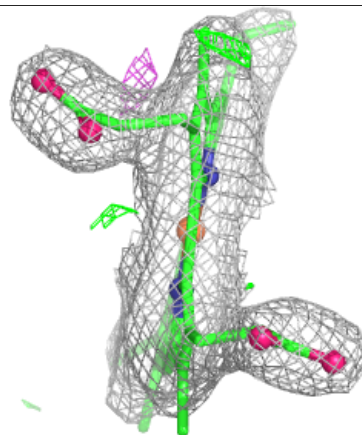
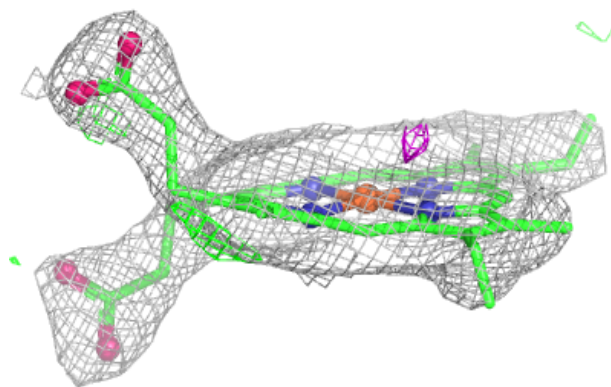
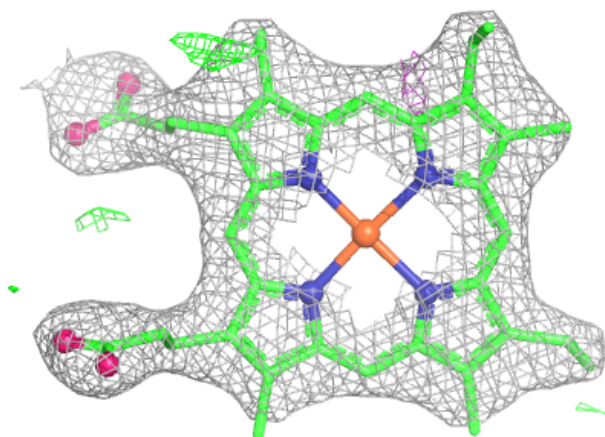
Electron density around CL a 403 (A):

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



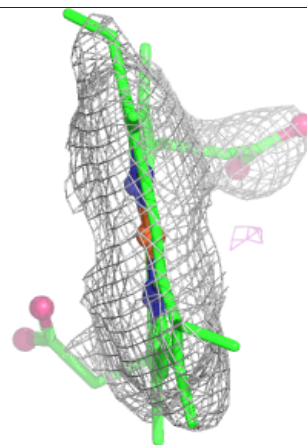
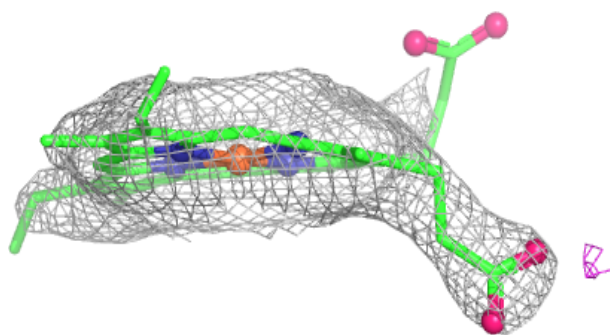
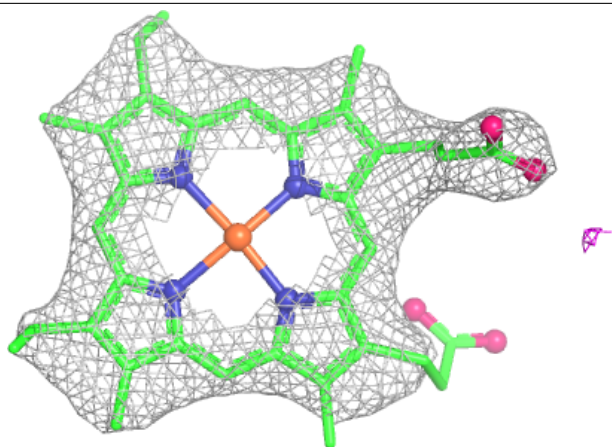
Electron density around HEM F 102:

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



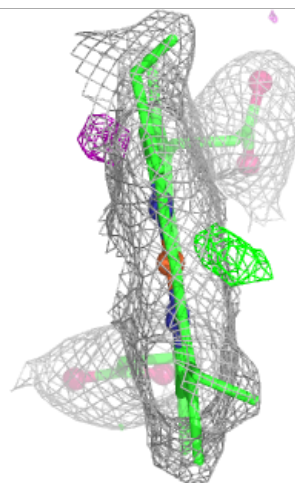
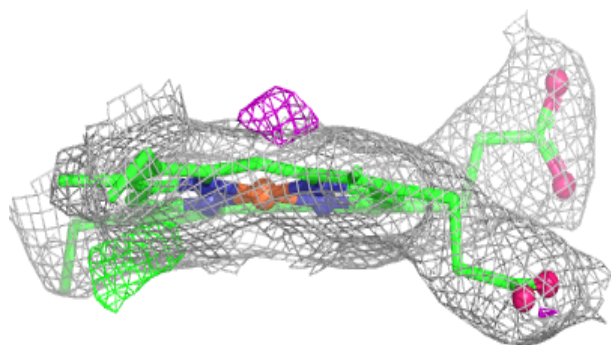
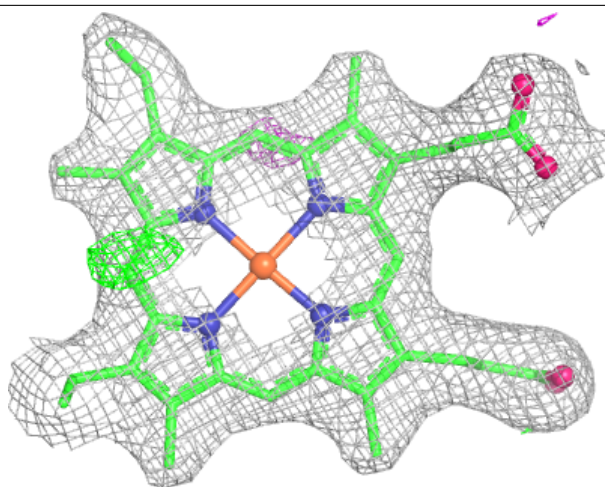
Electron density around HEM f 101:

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



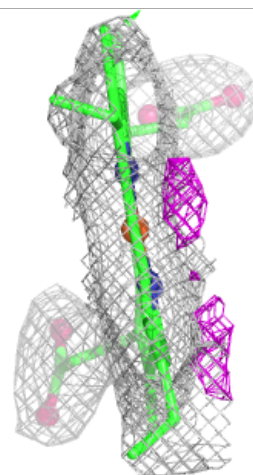
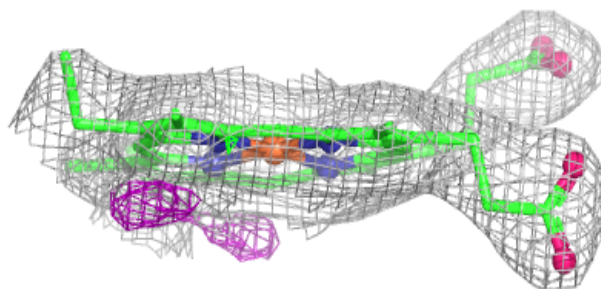
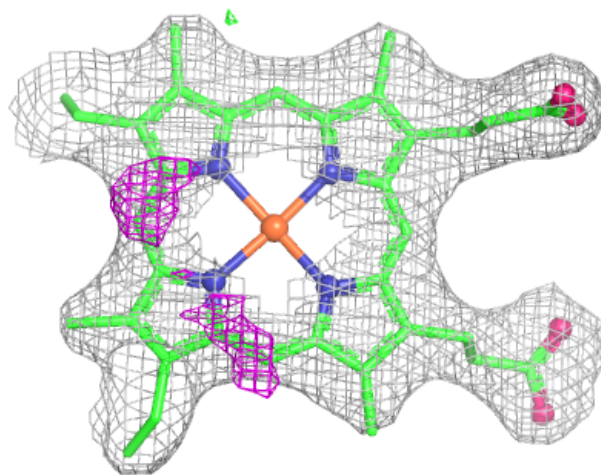
Electron density around HEC V 201:

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



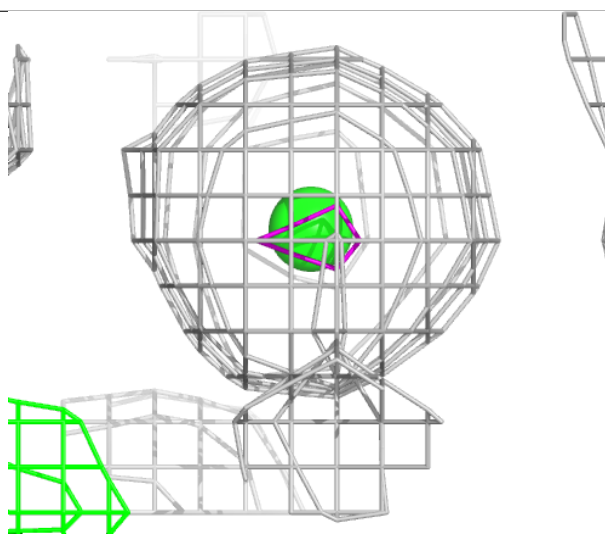
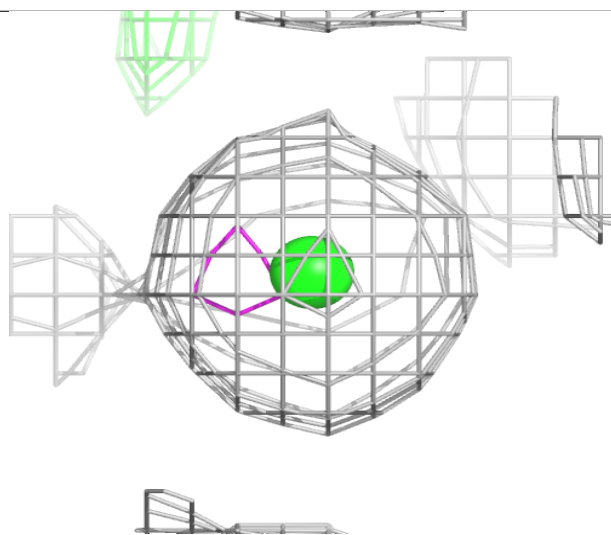
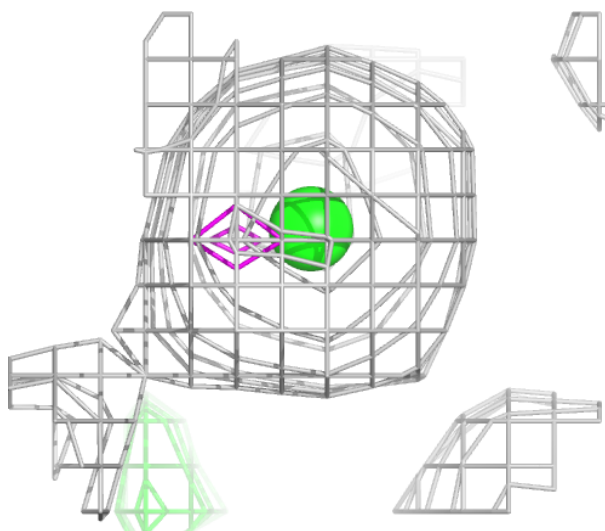
Electron density around HEC v 201:

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



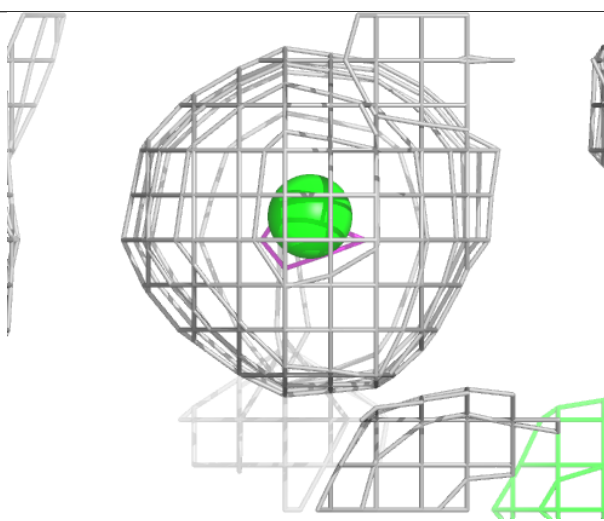
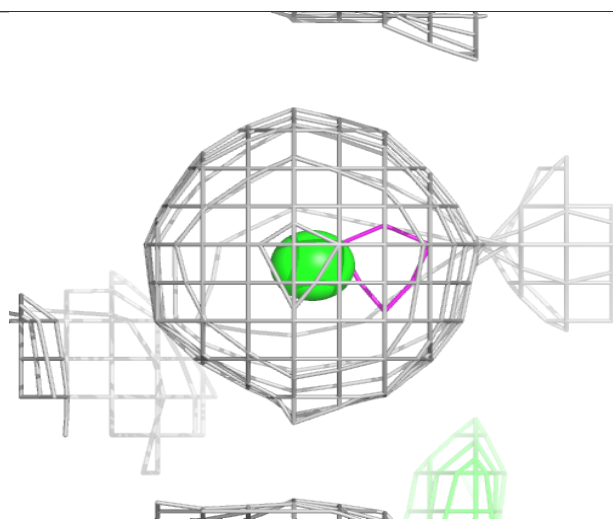
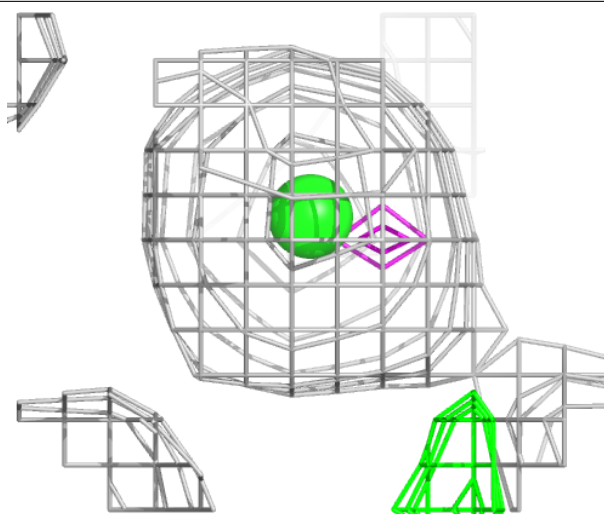
Electron density around CL A 402 (A):

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



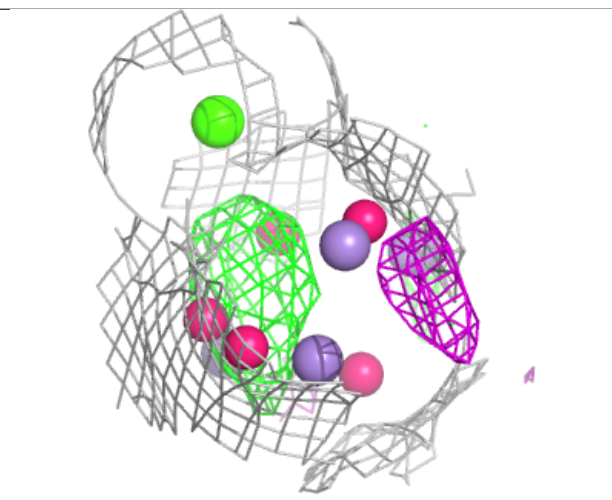
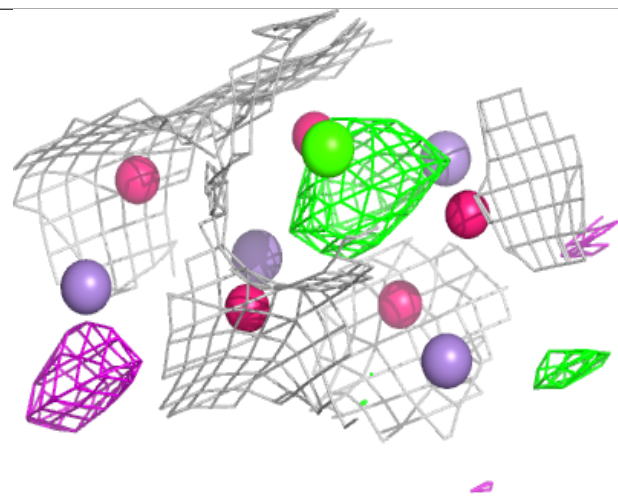
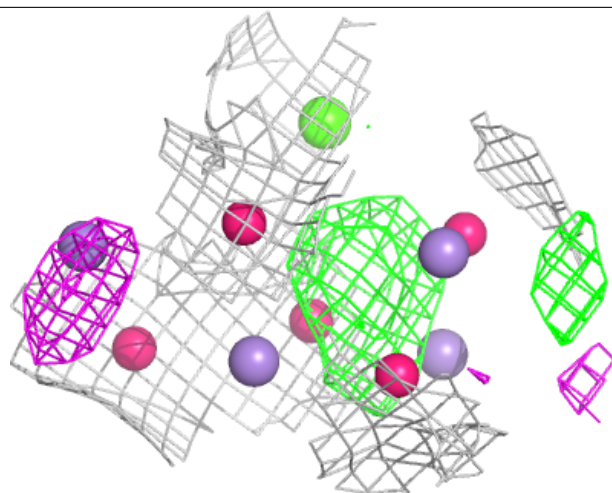
Electron density around CL A 402 (B):

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



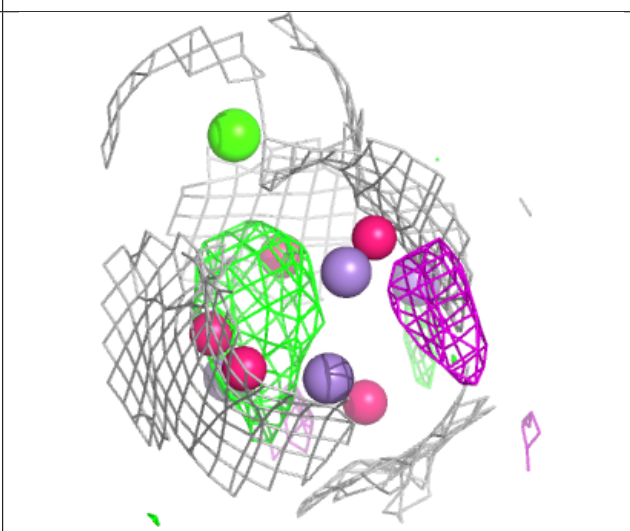
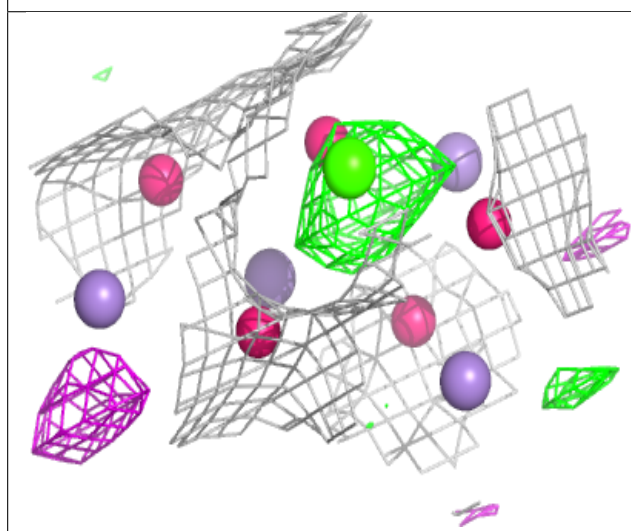
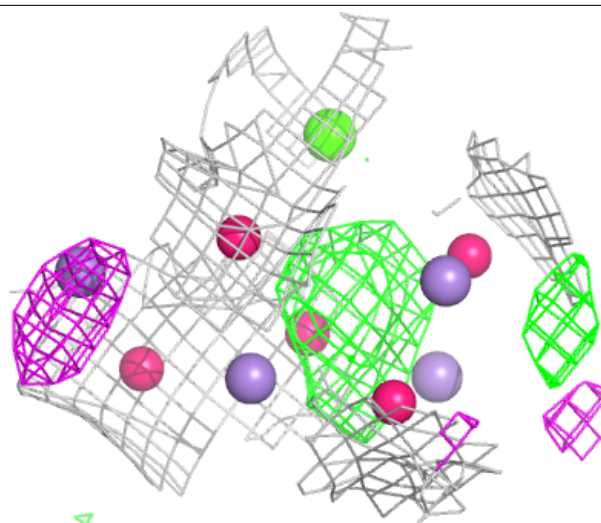
Electron density around OEX A 413 (A):

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



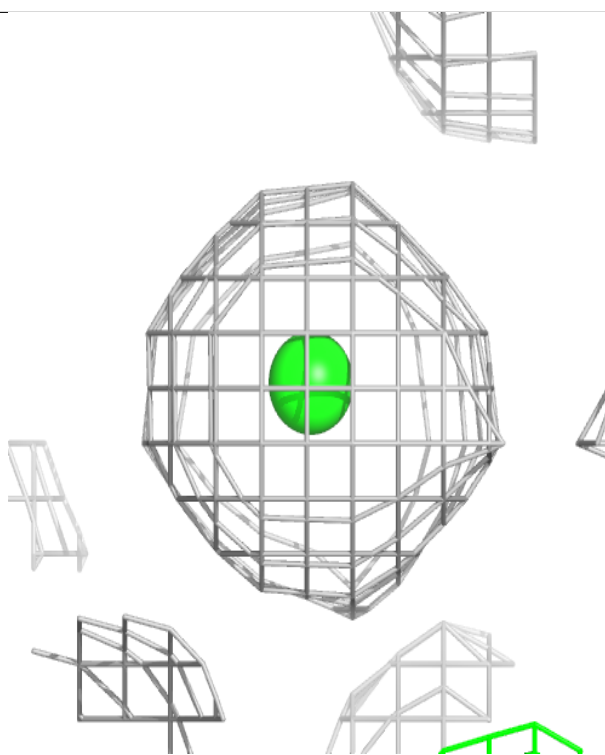
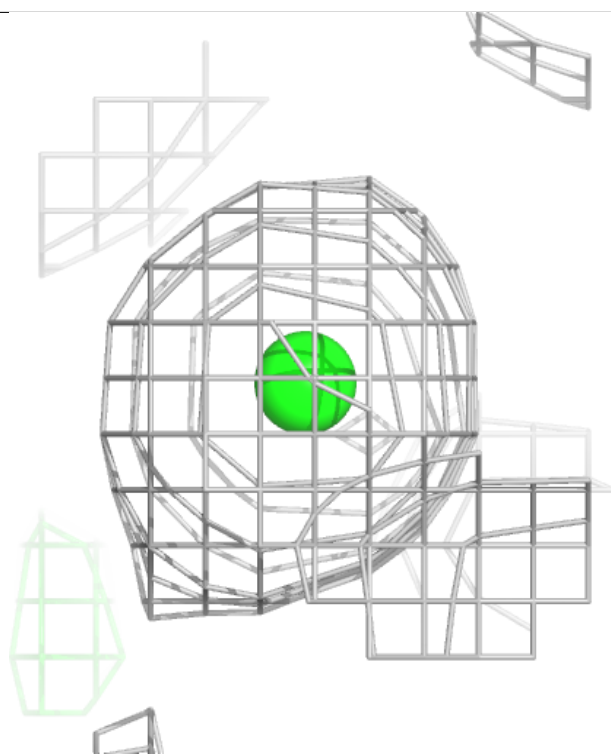
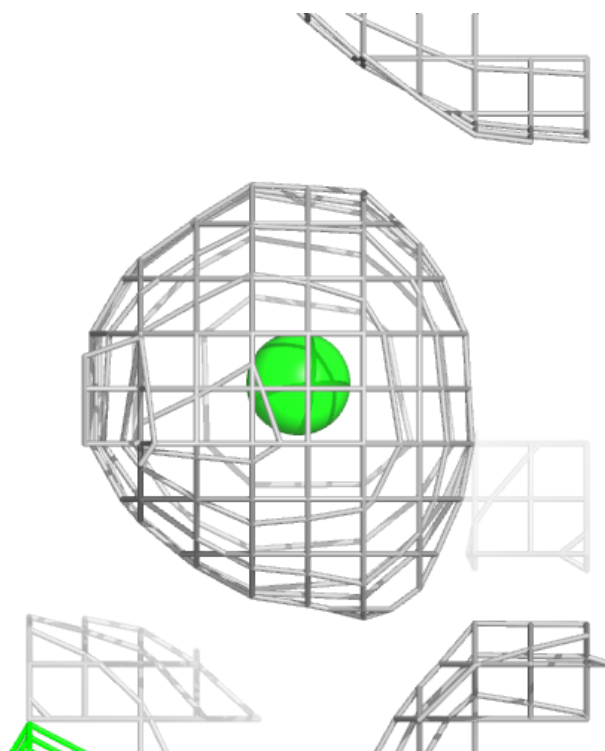
Electron density around OEX A 413 (B):

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



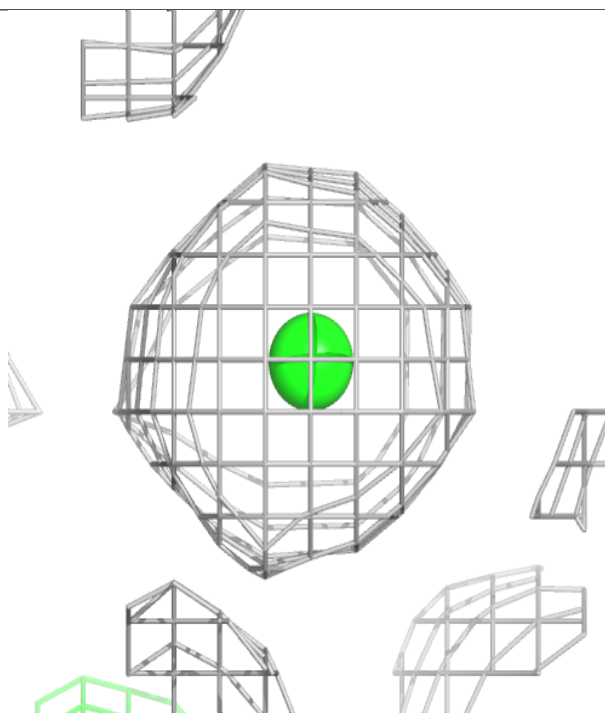
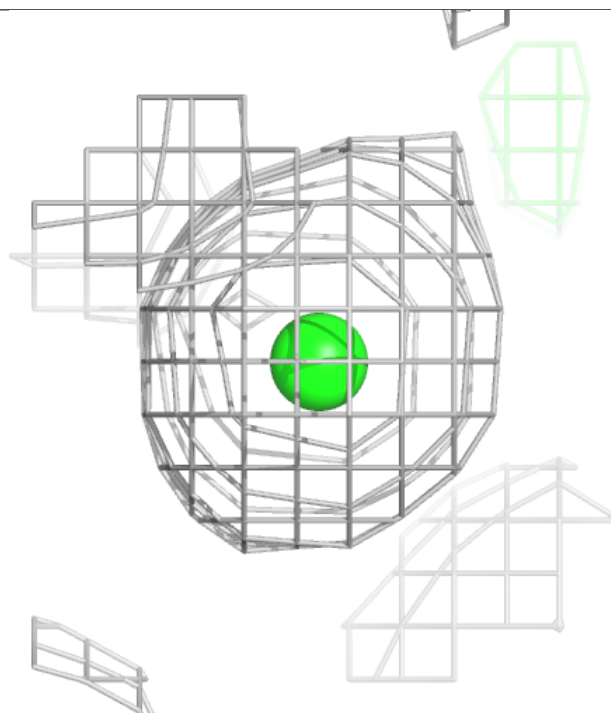
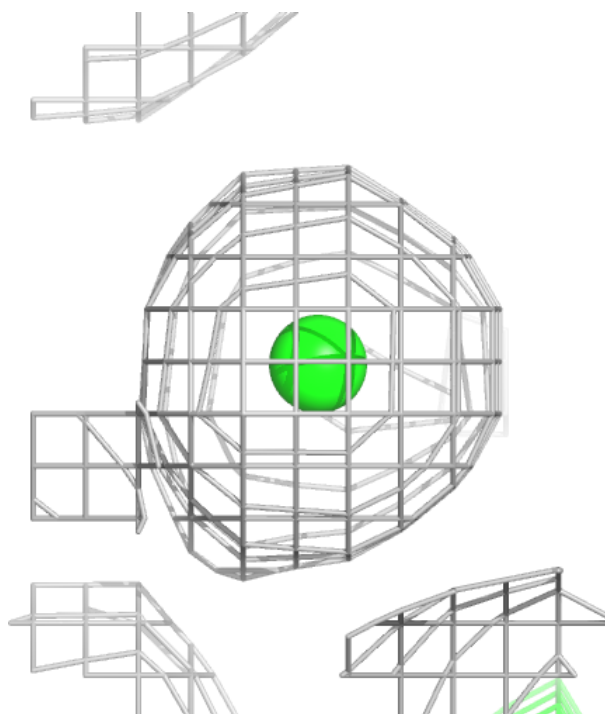
Electron density around CL a 402 (A):

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



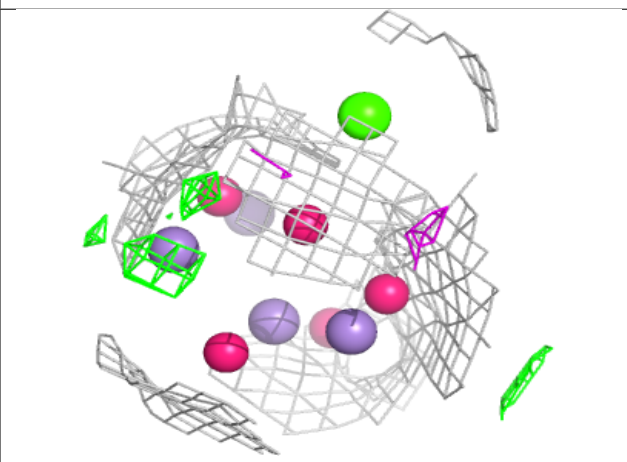
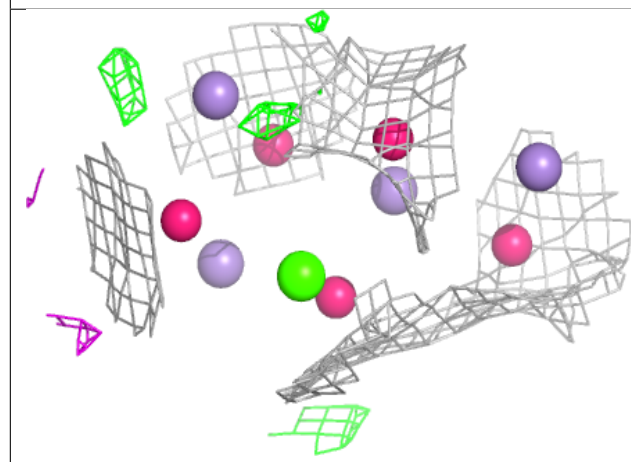
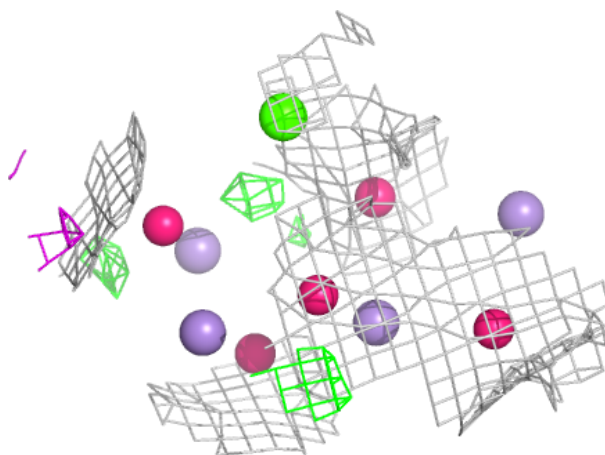
Electron density around CL a 402 (B):

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



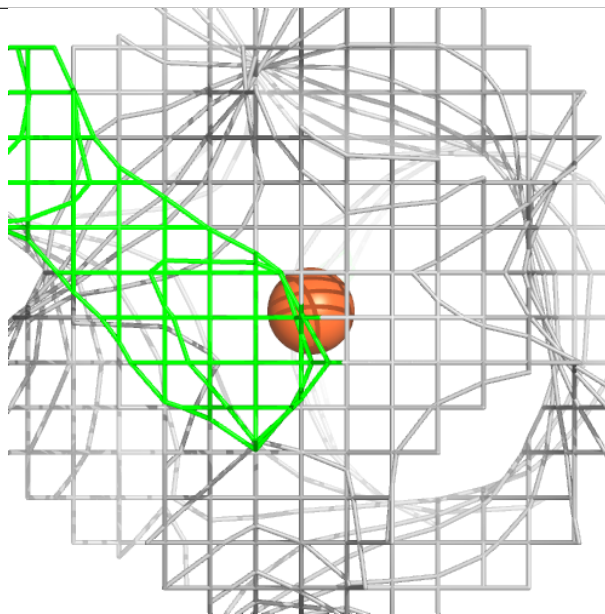
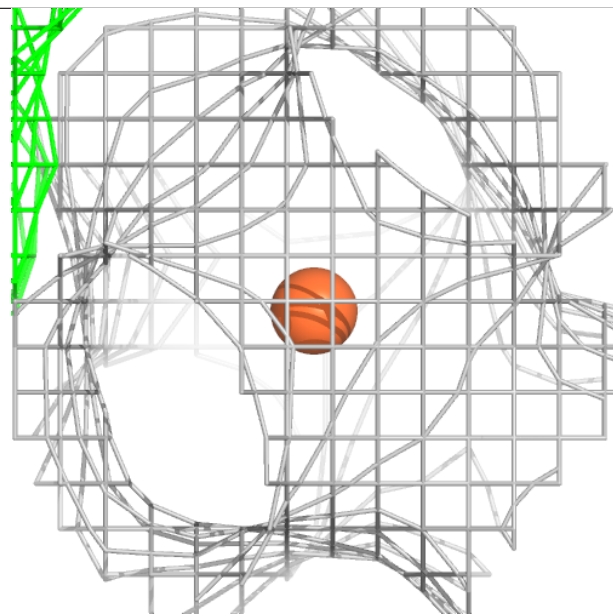
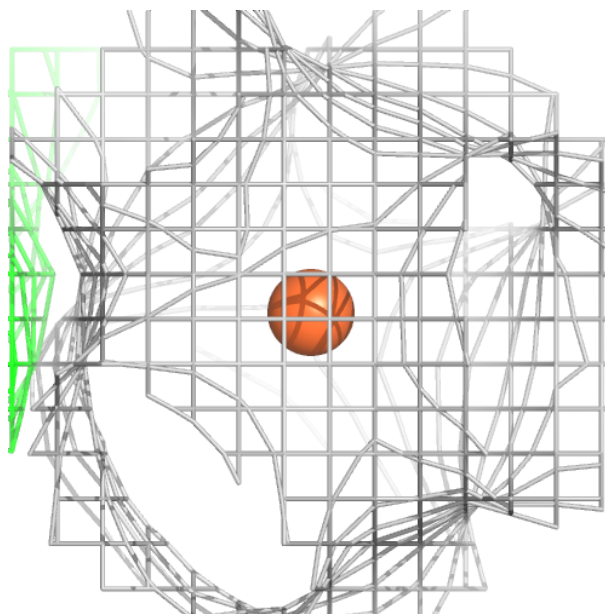
Electron density around OEX a 412 (B):

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



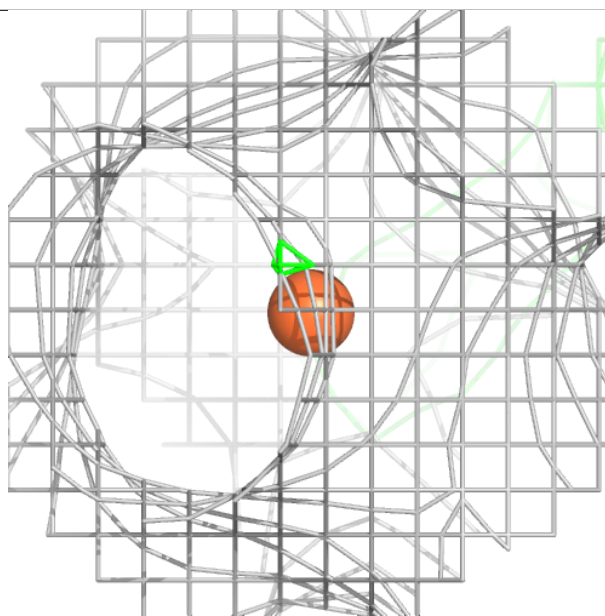
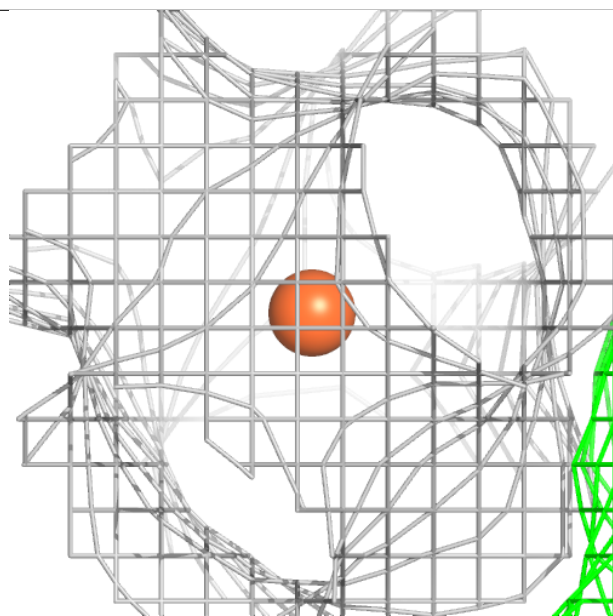
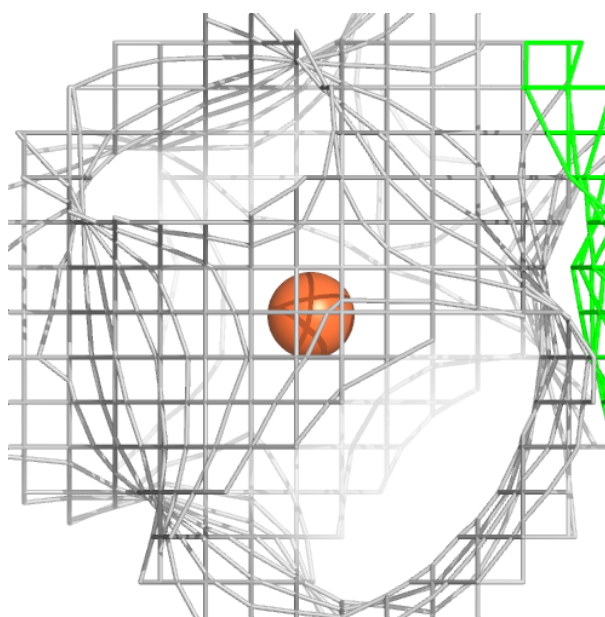
Electron density around FE2 a 401 (A):

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



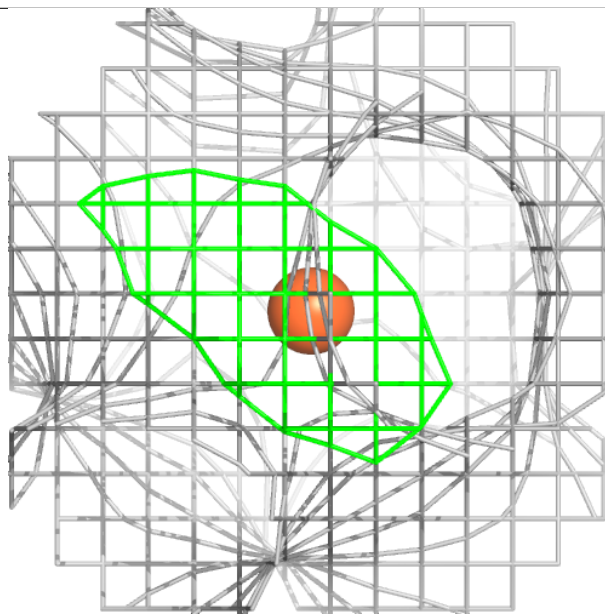
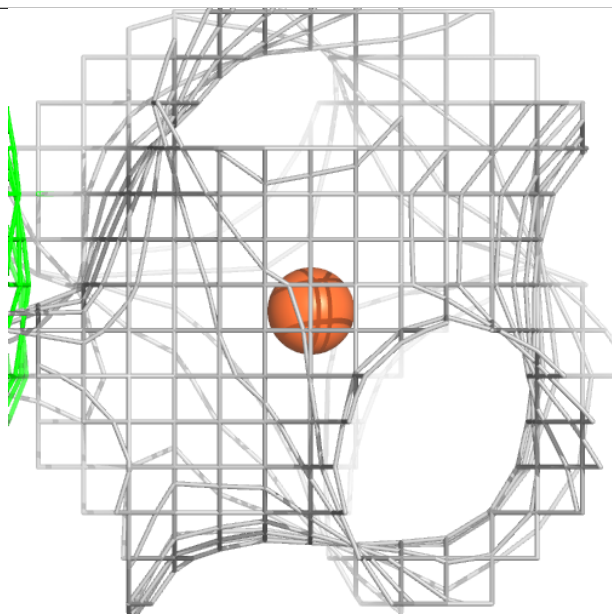
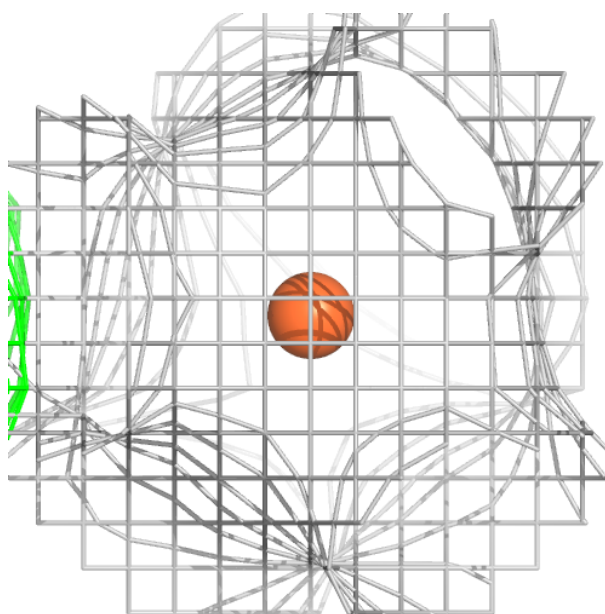
Electron density around FE2 a 401 (B):

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



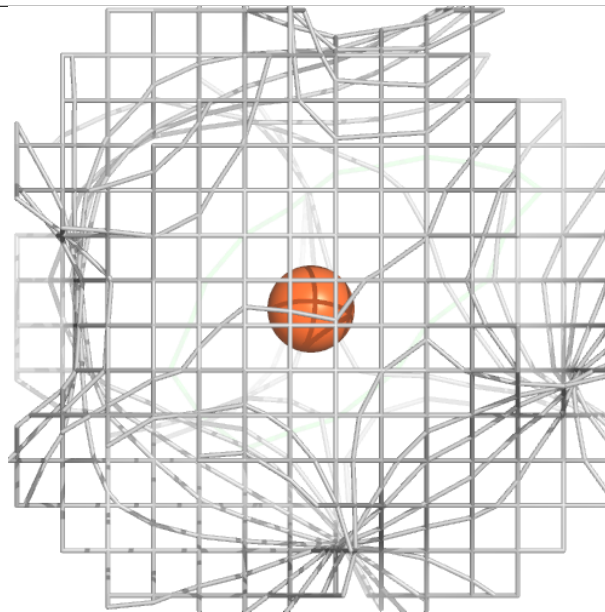
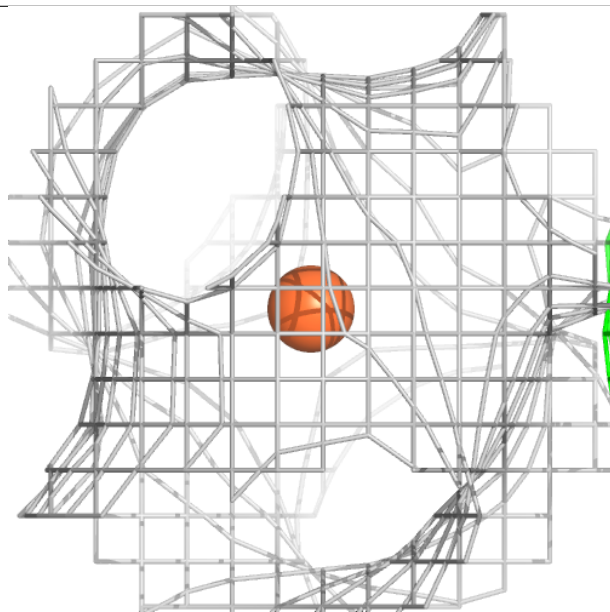
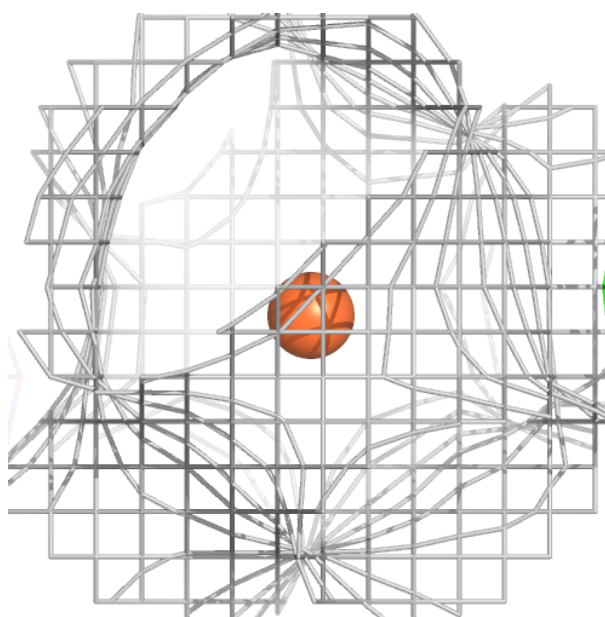
Electron density around FE2 A 401 (A):

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



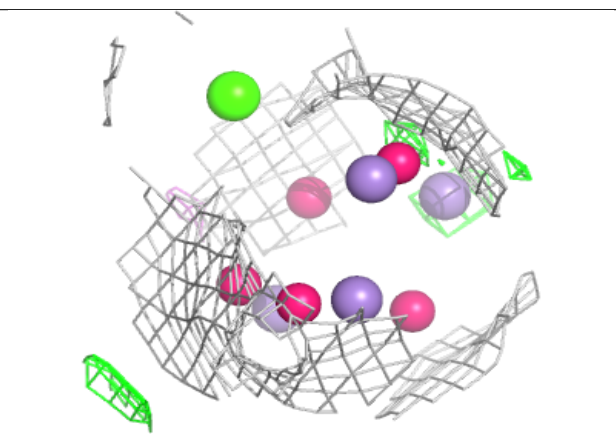
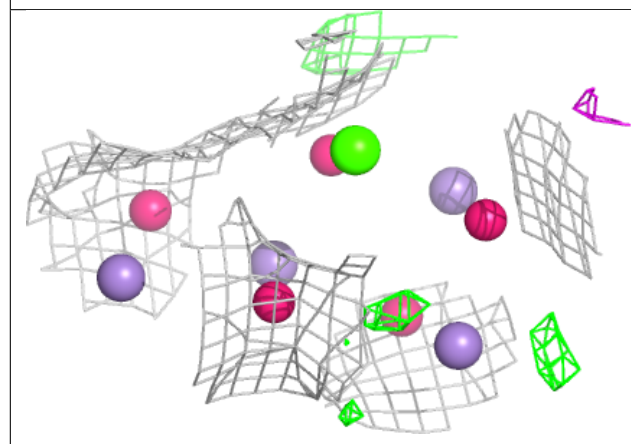
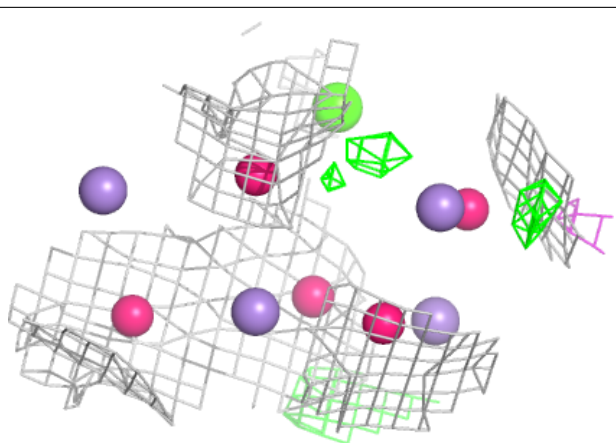
Electron density around FE2 A 401 (B):

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



Electron density around OEX 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.