



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:27 AM UTC

PDB ID : 8IRC / pdb\_00008irc  
Title : XFEL structure of cyanobacterial photosystem II following one flash (1F) with a 5-millisecond delay (Single conformation)  
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](mailto: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>.

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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)  
Xtrriage (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

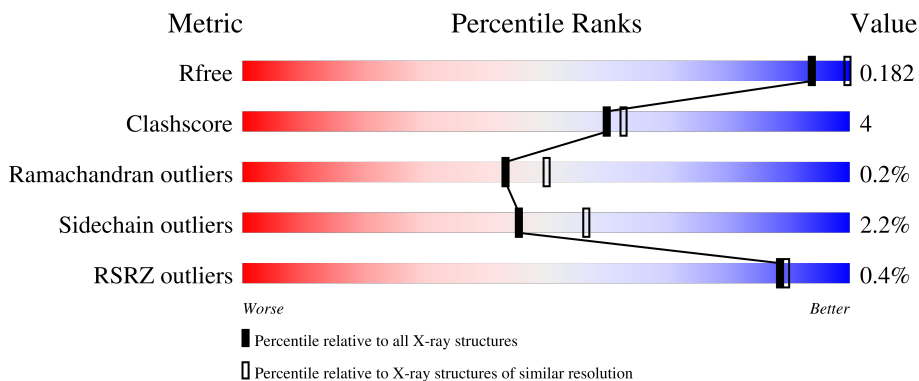
# 1 Overall quality at a glance

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.



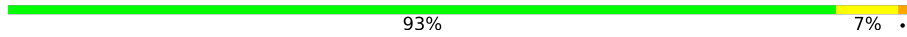

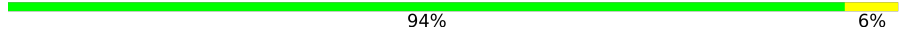




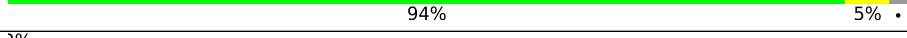
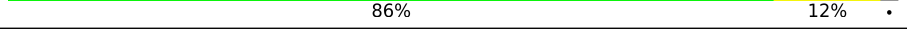

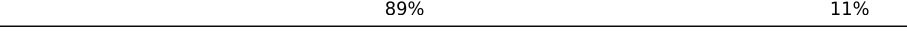
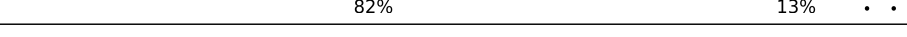
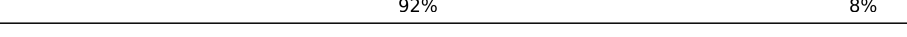
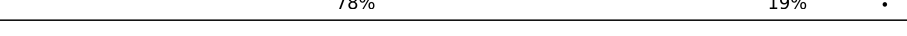

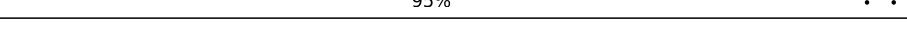
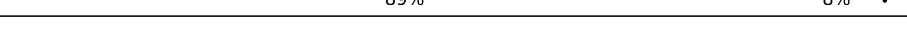

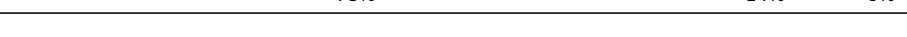






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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  $\geq 3$ , 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	92%
1	a	344	89% 8%
2	B	505	93% 7%
2	b	505	92% 7%
3	C	455	91% 9%

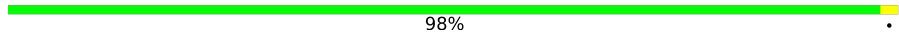
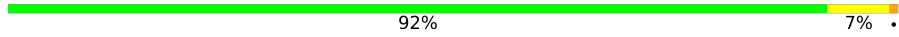







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Mol	Chain	Length	Quality of chain
3	c	455	 93% 7%
4	D	342	 91% 9%
4	d	342	 94% 6%
5	E	84	 80% 17%
5	e	84	 90% 6%
6	F	44	 64% 14% 23%
6	f	44	 57% 14% 30%
7	H	65	 94% 5%
7	h	65	 86% 12%
8	I	38	 76% 21%
8	i	38	 89% 11%
9	J	39	 82% 13%
9	j	39	 92% 8%
10	K	37	 78% 19%
10	k	37	 78% 16% 5%
11	L	37	 95%
11	l	37	 89% 8%
12	M	36	 81% 6% 6% 8%
12	m	36	 78% 14% 6%
13	O	244	 88% 12%
13	o	244	 91% 8%
14	T	32	 84% 9% 6%
14	t	32	 81% 12% 6%
15	U	104	 84% 9% 8%
15	u	104	 87% 6% 7%

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Mol	Chain	Length	Quality of chain
16	V	137	 98%
16	v	137	 92% 7%
17	X	40	 88% 8% 5%
17	x	40	 88% 8% 5%
18	Y	30	 87% 10% 3%
18	y	30	 70% 27%
19	Z	62	 89% 10%
19	z	62	 79% 19%
20	R	34	 71% 29% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	D	406	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
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23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
27	GOL	a	801	-	-	X	-

## 2 Entry composition i

There are 41 unique types of molecules in this entry. The entry contains 52977 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
			Total	C	N	O	S			
1	A	334	Total 2628	C 1722	N 432	O 459	S 15	0	1	0
1	a	334	Total 2629	C 1721	N 432	O 461	S 15	0	2	0

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
			Total	C	N	O	S			
2	B	504	Total 4029	C 2639	N 674	O 703	S 13	0	7	0
2	b	504	Total 4017	C 2636	N 669	O 699	S 13	0	6	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	Total 3497	C 2287	N 588	O 609	S 13	0	1	0
3	c	455	Total 3555	C 2327	N 595	O 620	S 13	0	5	0

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	1	0
			2732	1808	446	466	12			
4	d	341	Total	C	N	O	S	0	2	0
			2732	1808	447	465	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	S	0	0	0
			662	432	107	123				
5	e	79	Total	C	N	O	S	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	0	0
			296	197	47	52			
11	l	36	Total	C	N	O	0	0	0
			296	197	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			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	3	0
			1894	1181	321	388	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	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	1	0
			267	186	37	42	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	1	0
			774	491	129	154			
15	u	97	Total	C	N	O	0	1	0
			781	496	130	155			

- 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	2	0
			1082	685	179	214	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	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	0
			1	1		
21	a	1	Total	Fe	0	0
			1	1		

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

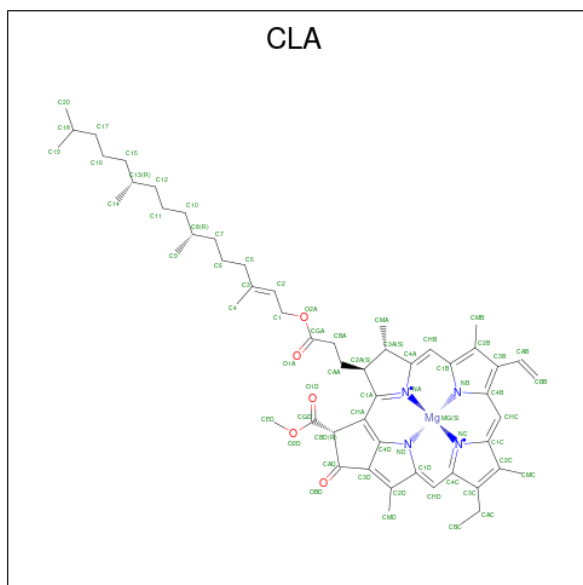
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



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

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

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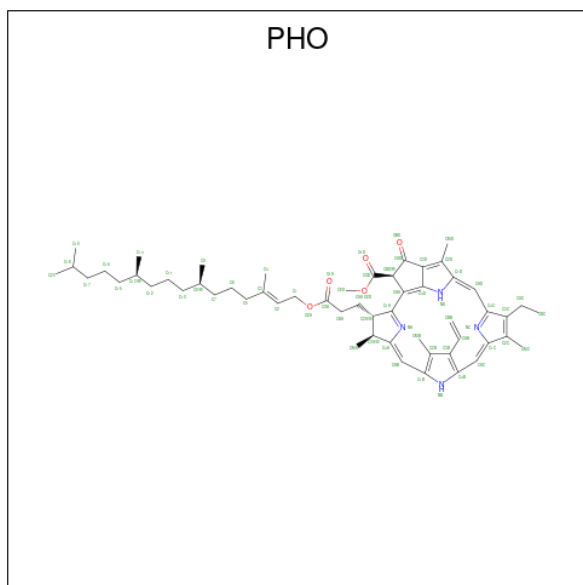
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
23	C	1	65	55	1	4	5	0	0
23	C	1	65	55	1	4	5	0	0
23	D	1	65	55	1	4	5	0	0
23	D	1	65	55	1	4	5	0	0
23	a	1	65	55	1	4	5	0	0
23	a	1	65	55	1	4	5	0	0
23	a	1	65	55	1	4	5	0	0
23	a	1	65	55	1	4	5	0	0
23	b	1	65	55	1	4	5	0	0
23	b	1	65	55	1	4	5	0	0
23	b	1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

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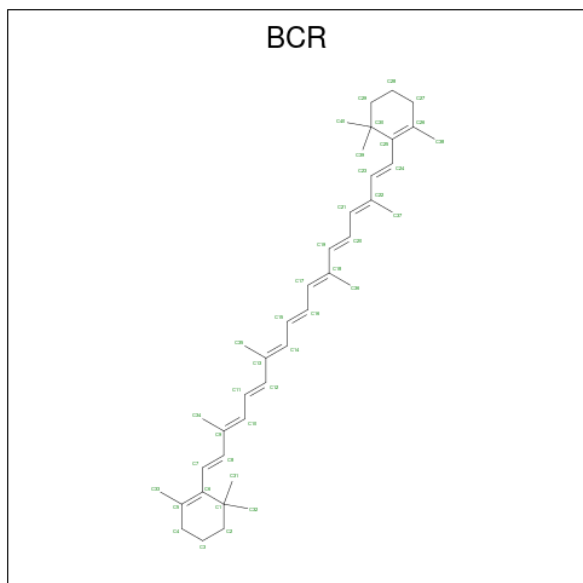
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



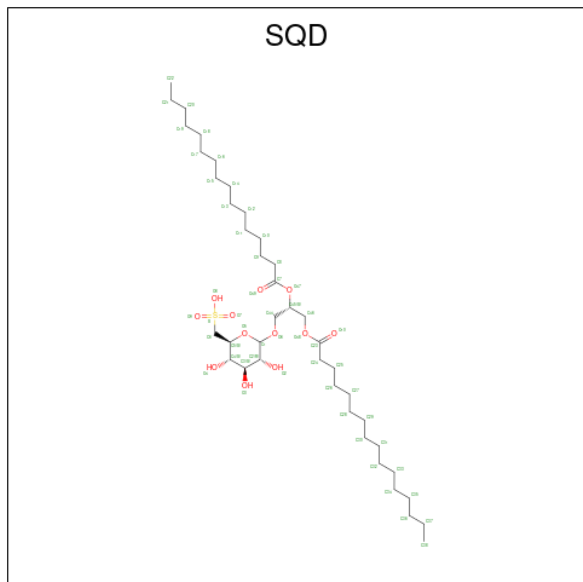
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
24	A	1	64	55	4	5	0	0
24	A	1	64	55	4	5	0	0
24	a	1	64	55	4	5	0	0
24	a	1	64	55	4	5	0	0

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



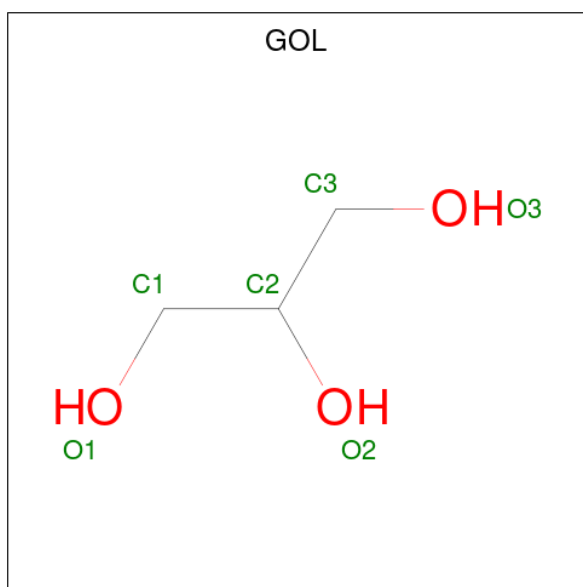
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



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

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



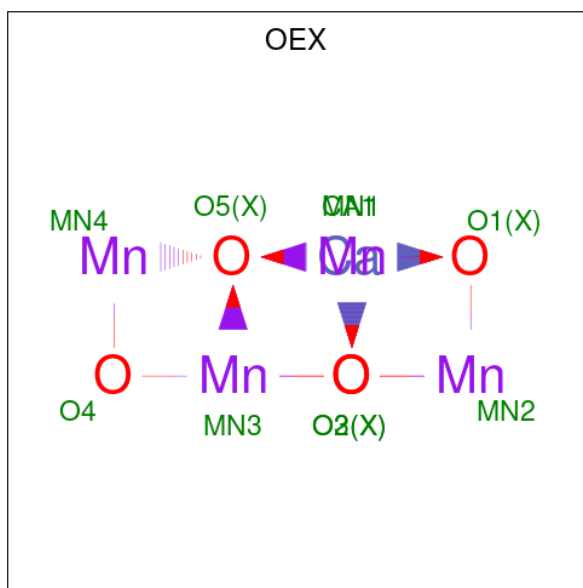
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 6 3 3	0	0
27	A	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	C	1	Total C O 6 3 3	0	0
27	D	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	V	1	Total C O 6 3 3	0	0
27	a	1	Total C O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

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

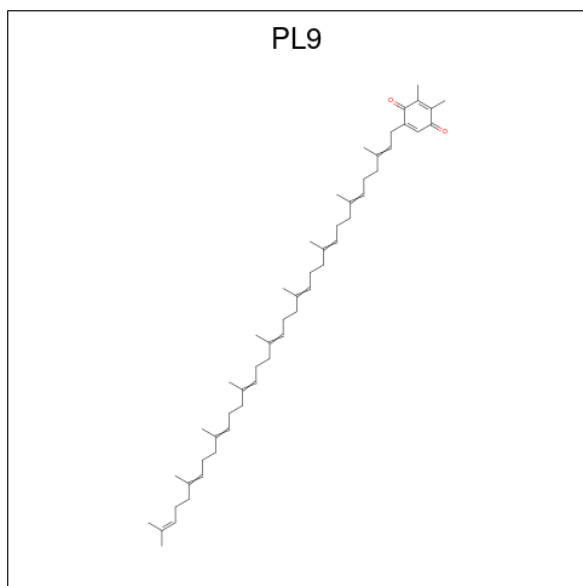
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



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

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

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



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

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

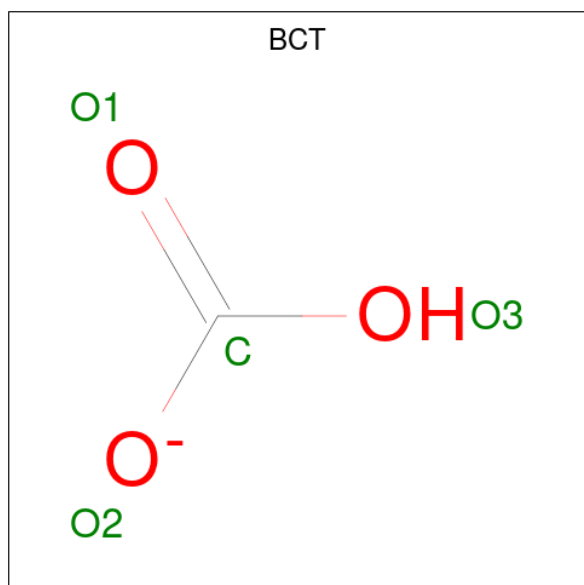
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	0
			34	29	5		
30	M	1	Total	C		0	0
			10	10			

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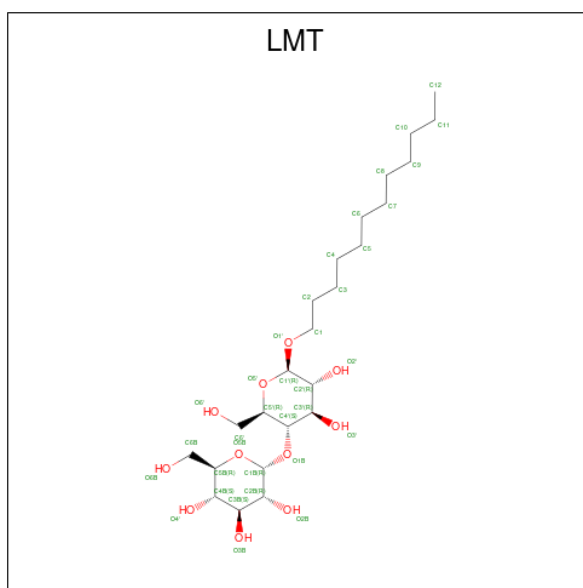
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	X	1	Total	C	O	0	0
			18	16	2		
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	1	Total	C	O	0	0
			33	28	5		
30	c	1	Total	C	O	0	0
			32	27	5		
30	d	2	Total	C	O	0	0
			53	47	6		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
	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

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 32 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



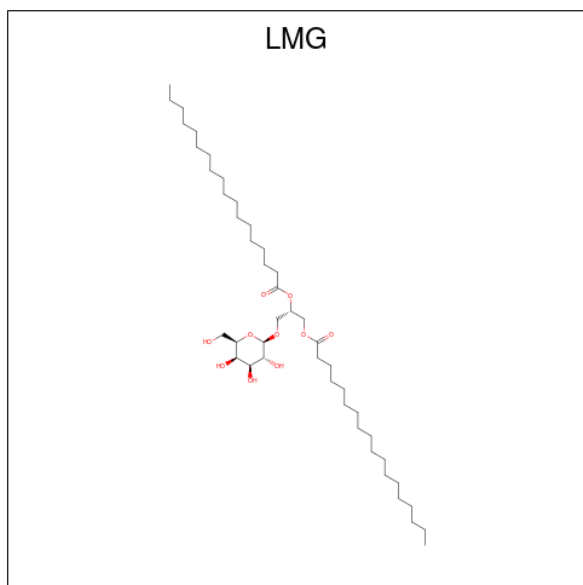
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			35	24	11		
32	D	1	Total	C	O	0	0
			35	24	11		
32	E	1	Total	C	O	0	0
			35	24	11		
32	I	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
32	t	1	26	19	7	0	0

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



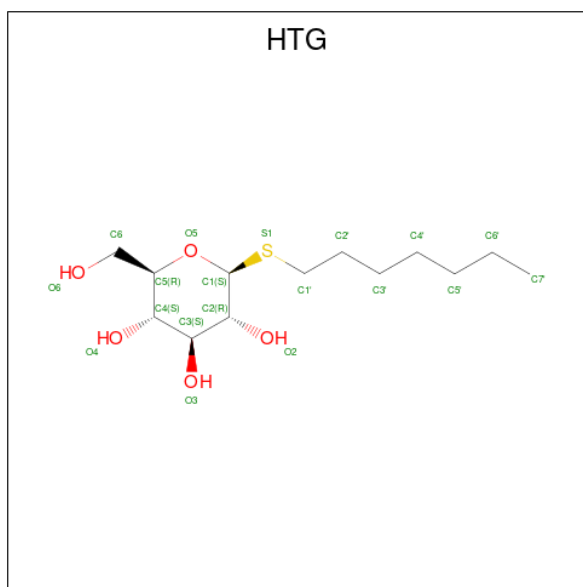
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
33	B	1	51	41	10	0	0
33	C	1	51	41	10	0	0
33	C	1	51	41	10	0	0
33	C	1	51	41	10	0	0
33	D	1	51	41	10	0	0
33	a	1	51	41	10	0	0
33	c	1	51	41	10	0	0
33	c	1	51	41	10	0	0
33	d	1	51	41	10	0	0
33	m	1	51	41	10	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).



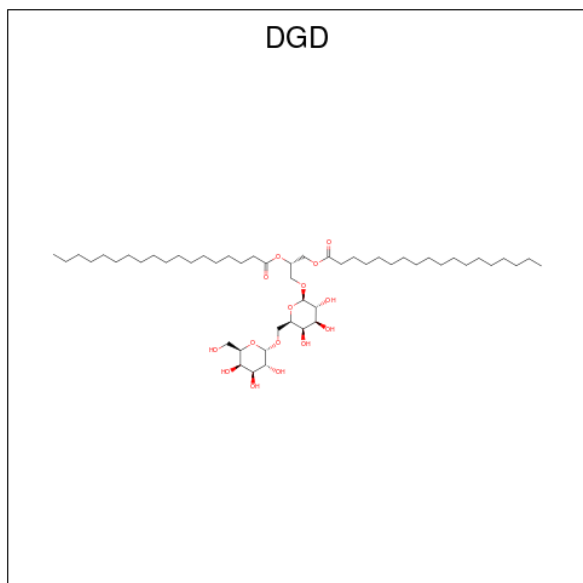
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	D	1	Total	C	O	S	0	0
			16	10	5	1		
34	V	1	Total	C	O		0	0
			11	6	5			
34	b	1	Total	C	O	S	0	0
			19	13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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
34	c	1	19	13	5	1	0	0
34	d	1	16	10	5	1	0	0

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

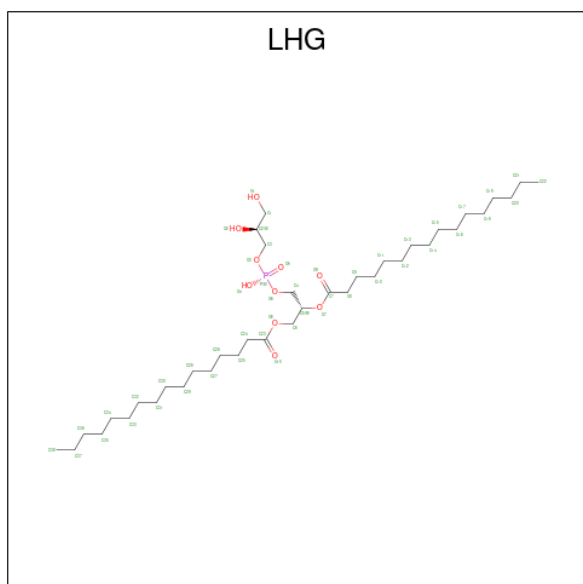


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
35	C	1	62	47	15	0	0
35	C	1	62	47	15	0	0
35	C	1	62	47	15	0	0
35	H	1	62	47	15	0	0
35	c	1	62	47	15	0	0
35	c	1	62	47	15	0	0
35	c	1	62	47	15	0	0
35	h	1	62	47	15	0	0

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



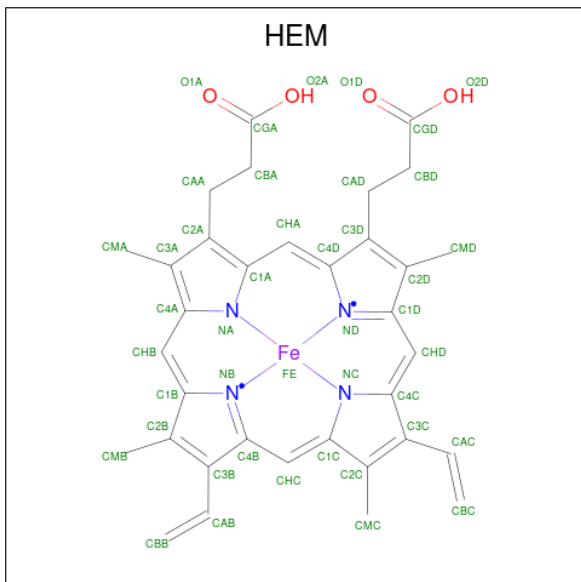
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	E	1	Total C O P 42 31 10 1	0	0
37	L	1	Total C O P 49 38 10 1	0	0

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

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

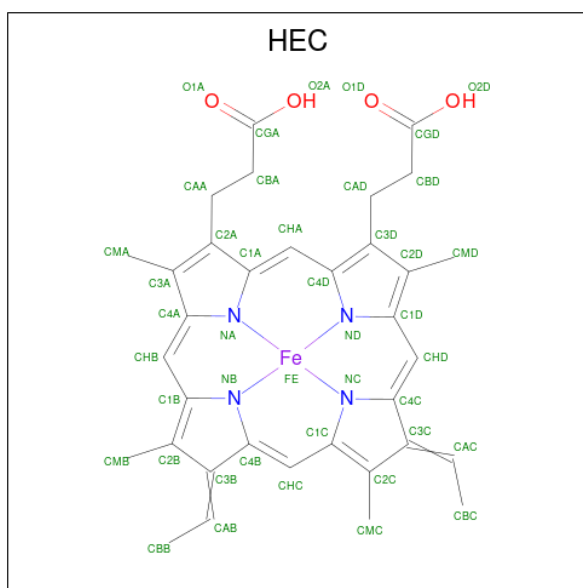


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
38	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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	126	Total	O	0	1
			127	127		
41	B	164	Total	O	0	0
			164	164		
41	C	141	Total	O	0	0
			141	141		
41	D	118	Total	O	0	0
			118	118		
41	E	14	Total	O	0	0
			14	14		
41	F	3	Total	O	0	0
			3	3		
41	H	17	Total	O	0	0
			17	17		
41	I	6	Total	O	0	0
			6	6		
41	J	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	K	5	Total O 5 5	0	0
41	L	3	Total O 3 3	0	0
41	M	5	Total O 5 5	0	0
41	O	70	Total O 70 70	0	0
41	T	8	Total O 8 8	0	0
41	U	32	Total O 32 32	0	0
41	V	65	Total O 65 65	0	0
41	X	1	Total O 1 1	0	0
41	a	128	Total O 128 128	0	0
41	b	182	Total O 182 182	0	0
41	c	133	Total O 133 133	0	0
41	d	109	Total O 109 109	0	0
41	e	8	Total O 8 8	0	0
41	f	3	Total O 3 3	0	0
41	h	15	Total O 15 15	0	0
41	i	3	Total O 3 3	0	0
41	j	2	Total O 2 2	0	0
41	k	3	Total O 3 3	0	0
41	l	4	Total O 4 4	0	0
41	m	14	Total O 14 14	0	0
41	o	76	Total O 76 76	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	t	6	Total O 6 6	0	0
41	u	47	Total O 47 47	0	0
41	v	41	Total O 41 41	0	0
41	x	2	Total O 2 2	0	0
41	y	1	Total O 1 1	0	0
41	G	264	Total O 264 264	0	1

### 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:  92%



- Molecule 1: Photosystem II protein D1

Chain a:  89%



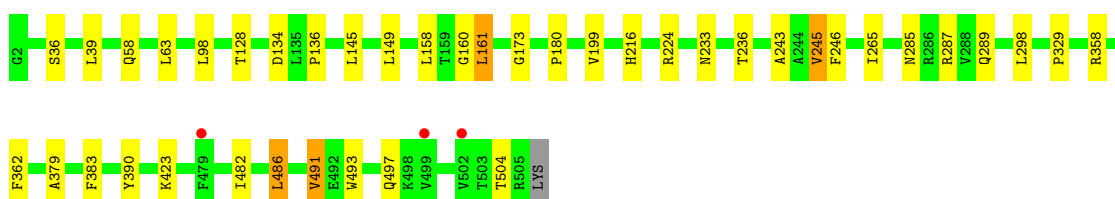
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  93%




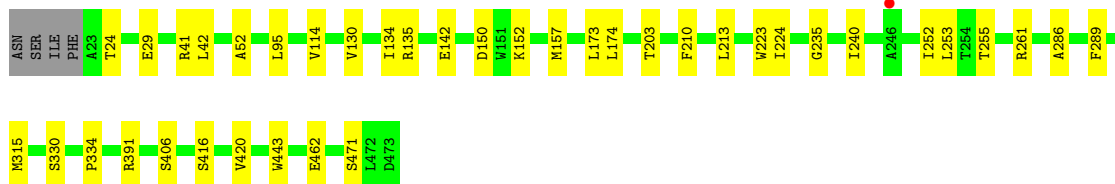
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  92%




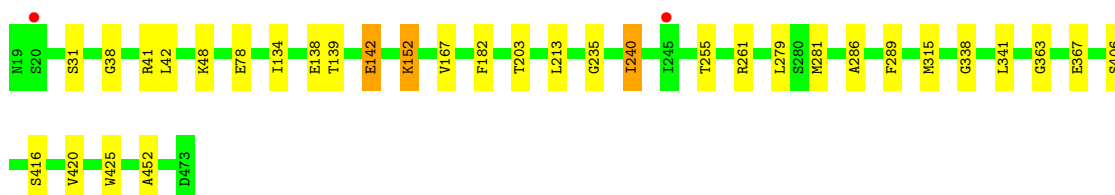
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  91% 9%




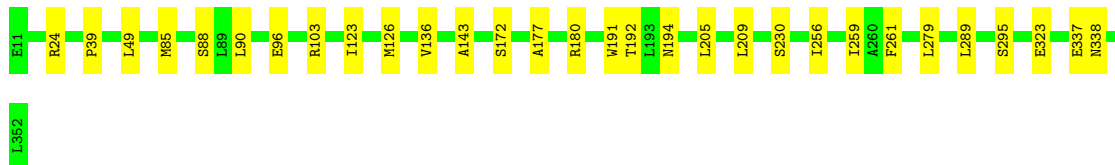
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  93% 7%



- Molecule 4: Photosystem II D2 protein

Chain D:  91% 9%




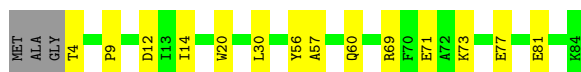
- Molecule 4: Photosystem II D2 protein

Chain d:  94% 6%




- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  80% 17%

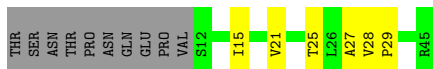


- Molecule 5: Cytochrome b559 subunit alpha

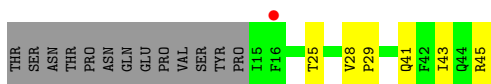
Chain e:  90% 6%



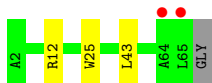
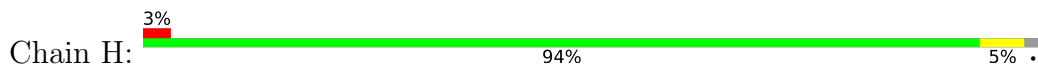
- Molecule 6: Cytochrome b559 subunit beta



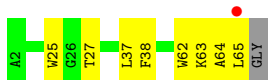
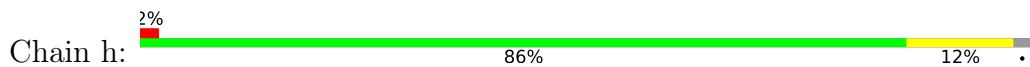
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



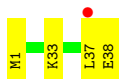
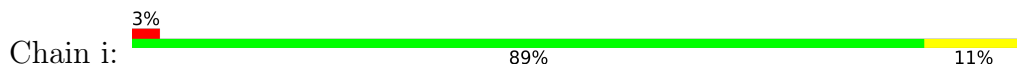
- Molecule 7: Photosystem II reaction center protein H




- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I




- Molecule 9: Photosystem II reaction center protein J

Chain J:  82% 13%




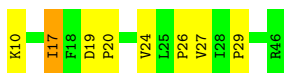
- Molecule 9: Photosystem II reaction center protein J

Chain j:  92% 8%




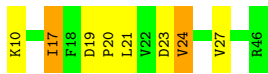
- Molecule 10: Photosystem II reaction center protein K

Chain K:  78% 19%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  78% 16% 5%




- Molecule 11: Photosystem II reaction center protein L

Chain L:  95%




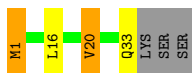
- Molecule 11: Photosystem II reaction center protein L

Chain l:  89% 8%




- Molecule 12: Photosystem II reaction center protein M

Chain M:  81% 6% 6% 8%




- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 14% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  88% 12%




- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  91% 8%




- Molecule 14: Photosystem II reaction center protein T

Chain T:  84% 9% 6%




- Molecule 14: Photosystem II reaction center protein T

Chain t:  81% 12% 6%




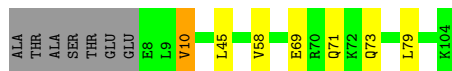
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  84% 9% 8%



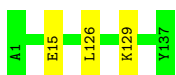
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  87% 6% 7%



- Molecule 16: Cytochrome c-550

Chain V:  98%




- Molecule 16: Cytochrome c-550

Chain v:  92% 7%




- Molecule 17: Photosystem II reaction center protein X

Chain X:  88% 8% 5%




- Molecule 17: Photosystem II reaction center protein X

Chain x:  88% 8% 5%



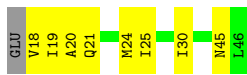
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  3% 87% 10%



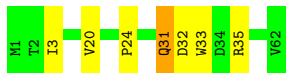
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  70% 27%




- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  89% 10%



- Molecule 19: Photosystem II reaction center protein Z

Chain z:  79% 19%



• Molecule 20: Photosystem II protein Y

Chain R:  9% 71% 29%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.26Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.145 , 0.180 0.146 , 0.182	Depositor DCC
$R_{free}$ test set	19914 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.9	Xtrriage
Anisotropy	0.487	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 69.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	52977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: HEC, HEM, BCT, LHG, MG, FE2, FME, DGD, LMT, BCR, CA, LMG, CL, HTG, UNL, CLA, PL9, PHO, GOL, OEX, SQD

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	0.36	0/2713	0.52	0/3700
1	a	0.33	0/2717	0.49	0/3705
2	B	0.33	0/4169	0.47	0/5679
2	b	0.30	0/4161	0.47	0/5669
3	C	0.29	0/3610	0.44	0/4914
3	c	0.29	0/3675	0.45	0/5002
4	D	0.37	0/2827	0.51	0/3852
4	d	0.34	0/2827	0.48	0/3852
5	E	0.28	0/681	0.47	0/928
5	e	0.25	0/690	0.44	0/939
6	F	0.28	0/284	0.44	0/387
6	f	0.25	0/269	0.38	0/365
7	H	0.29	0/519	0.46	0/708
7	h	0.26	0/530	0.44	0/722
8	I	0.27	0/311	0.45	0/419
8	i	0.30	0/311	0.43	0/419
9	J	0.27	0/278	0.36	0/376
9	j	0.27	0/283	0.40	0/383
10	K	0.29	0/303	0.46	0/416
10	k	0.33	0/303	0.44	0/416
11	L	0.33	0/303	0.46	0/412
11	l	0.35	0/303	0.44	0/412
12	M	0.34	0/261	0.47	0/357
12	m	0.31	0/279	0.44	0/380
13	O	0.30	0/1925	0.48	0/2609
13	o	0.29	0/1896	0.48	0/2571
14	T	0.34	0/266	0.43	0/362
14	t	0.31	0/257	0.42	0/349
15	U	0.32	0/785	0.52	0/1064
15	u	0.32	0/792	0.50	0/1074
16	V	0.32	0/1103	0.46	0/1497

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.27	0/1085	0.44	0/1473
17	X	0.21	0/292	0.33	0/395
17	x	0.20	0/284	0.32	0/384
18	Y	0.21	0/216	0.39	0/289
18	y	0.21	0/216	0.37	0/289
19	Z	0.19	0/490	0.34	0/669
19	z	0.19	0/490	0.36	0/669
20	R	0.21	0/279	0.32	0/383
All	All	0.31	0/42983	0.47	0/58489

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [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	2628	0	2527	10	0
1	a	2629	0	2526	21	0
2	B	4029	0	3880	24	0
2	b	4017	0	3872	33	0
3	C	3497	0	3419	23	0
3	c	3555	0	3480	23	0
4	D	2732	0	2631	24	0
4	d	2732	0	2632	14	0
5	E	662	0	648	11	0
5	e	670	0	655	2	0
6	F	275	0	282	4	0
6	f	261	0	269	5	0
7	H	506	0	529	3	0
7	h	517	0	541	5	0
8	I	314	0	328	5	0
8	i	314	0	328	2	0
9	J	272	0	279	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	2	0
10	K	293	0	305	4	0
10	k	293	0	305	7	0
11	L	296	0	304	1	0
11	l	296	0	304	3	0
12	M	268	0	285	4	0
12	m	286	0	305	8	0
13	O	1894	0	1860	15	0
13	o	1865	0	1838	8	0
14	T	267	0	267	0	0
14	t	258	0	261	3	0
15	U	774	0	772	4	0
15	u	781	0	781	4	0
16	V	1082	0	1083	1	0
16	v	1064	0	1073	5	0
17	X	289	0	322	2	0
17	x	281	0	312	3	0
18	Y	215	0	246	3	0
18	y	215	0	246	6	0
19	Z	479	0	516	3	0
19	z	479	0	516	3	0
20	R	273	0	305	5	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	260	0	288	7	0
23	B	1040	0	1152	24	0
23	C	845	0	936	27	0
23	D	130	0	144	3	0
23	a	260	0	288	10	0
23	b	1040	0	1152	28	0
23	c	845	0	936	25	0
23	d	130	0	144	4	0
24	A	128	0	148	3	0
24	a	128	0	148	1	0
25	A	40	0	56	2	0
25	B	120	0	168	6	0
25	C	80	0	112	2	0
25	D	40	0	56	2	0
25	H	40	0	56	2	0
25	K	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	40	0	56	6	0
25	Y	40	0	56	1	0
25	a	40	0	56	1	0
25	b	120	0	168	10	0
25	c	80	0	112	5	0
25	d	40	0	56	2	0
25	h	40	0	56	3	0
25	k	40	0	56	0	0
25	t	40	0	56	4	0
25	y	40	0	56	1	0
26	A	108	0	156	1	0
26	B	54	0	78	1	0
26	F	43	0	53	1	0
26	a	108	0	155	4	0
26	b	54	0	78	3	0
26	f	43	0	53	0	0
27	A	12	0	16	3	0
27	B	12	0	16	2	0
27	C	6	0	8	0	0
27	D	6	0	7	1	0
27	O	12	0	16	3	0
27	V	6	0	8	0	0
27	a	18	0	24	5	0
27	b	12	0	16	2	0
27	c	12	0	16	0	0
27	d	12	0	16	1	0
27	o	12	0	16	0	0
27	v	6	0	8	1	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	55	0	80	10	0
29	D	55	0	80	1	0
29	a	55	0	80	4	0
29	d	55	0	80	0	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	D	57	0	0	0	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	K	34	0	0	0	0
30	M	10	0	0	0	0
30	X	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	30	0	0	0	0
30	b	33	0	0	0	0
30	c	32	0	0	0	0
30	d	53	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	4	0	0	0	0
31	a	4	0	0	0	0
32	A	35	0	46	1	0
32	D	35	0	46	1	0
32	E	35	0	46	0	0
32	I	35	0	46	1	0
32	M	70	0	92	2	0
32	a	70	0	92	2	0
32	b	50	0	70	1	0
32	e	35	0	46	1	0
32	m	35	0	46	0	0
32	t	51	0	69	2	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	2	0
33	d	51	0	72	2	0
33	m	51	0	72	0	0
33	z	39	0	48	2	0
34	B	57	0	78	3	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	2	0
34	c	19	0	26	1	0
34	d	16	0	17	1	0
35	C	186	0	246	3	0
35	H	62	0	82	1	0
35	c	186	0	246	5	0
35	h	62	0	82	0	0
36	C	1	0	0	0	0
36	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	O	1	0	0	0	0
36	c	2	0	0	0	0
36	f	1	0	0	0	0
36	o	1	0	0	0	0
37	D	147	0	222	5	0
37	E	42	0	57	3	0
37	L	49	0	74	0	0
37	d	147	0	222	13	0
37	e	42	0	57	5	0
37	l	49	0	74	0	0
38	E	43	0	30	1	0
38	e	43	0	30	0	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	127	0	0	0	0
41	B	164	0	0	1	0
41	C	141	0	0	0	0
41	D	118	0	0	0	0
41	E	14	0	0	0	0
41	F	3	0	0	0	0
41	G	264	0	0	4	0
41	H	17	0	0	0	0
41	I	6	0	0	0	0
41	J	5	0	0	2	0
41	K	5	0	0	0	0
41	L	3	0	0	0	0
41	M	5	0	0	0	0
41	O	70	0	0	1	0
41	T	8	0	0	1	0
41	U	32	0	0	0	0
41	V	65	0	0	0	0
41	X	1	0	0	0	0
41	a	128	0	0	1	0
41	b	182	0	0	0	0
41	c	133	0	0	1	0
41	d	109	0	0	0	0
41	e	8	0	0	0	0
41	f	3	0	0	1	0
41	h	15	0	0	0	0
41	i	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	j	2	0	0	0	0
41	k	3	0	0	0	0
41	l	4	0	0	0	0
41	m	14	0	0	0	0
41	o	76	0	0	0	0
41	t	6	0	0	0	0
41	u	47	0	0	0	0
41	v	41	0	0	1	0
41	x	2	0	0	0	0
41	y	1	0	0	0	0
All	All	52977	0	52089	447	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 4.

All (447) 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:701:GOL:H11	12:M:1:FME:HG2	1.45	0.98
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.51	0.93
23:c:504:CLA:HBB1	23:c:513:CLA:H41	1.57	0.86
23:B:604:CLA:H42	23:B:605:CLA:H2	1.59	0.84
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.64	0.78
4:d:192:THR:HG23	23:d:402:CLA:HBC2	1.66	0.77
23:c:514:CLA:HBB1	25:c:515:BCR:H24C	1.65	0.77
23:A:406:CLA:H152	29:A:414:PL9:H252	1.67	0.76
23:B:601:CLA:H12	23:B:601:CLA:H71	1.66	0.75
23:c:506:CLA:HHC	23:c:506:CLA:HBB1	1.69	0.75
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.69	0.73
27:A:701:GOL:O2	41:T:202:HOH:O	2.08	0.72
23:C:514:CLA:H202	33:C:521:LMG:H402	1.72	0.70
1:a:253:GLY:HA3	2:b:491:VAL:HG12	1.75	0.69
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.74	0.69
23:C:502:CLA:H193	23:C:508:CLA:HBB1	1.76	0.68
37:D:411:LHG:H382	37:D:411:LHG:H112	1.76	0.68
23:c:512:CLA:H191	33:z:101:LMG:H241	1.76	0.68
23:a:409:CLA:H192	23:c:506:CLA:H142	1.76	0.67
23:C:504:CLA:HBB1	23:C:513:CLA:H41	1.78	0.66
23:C:506:CLA:CMD	23:C:508:CLA:HAB	2.25	0.66
23:C:507:CLA:H142	35:C:517:DGD:HAF2	1.77	0.66
23:C:506:CLA:HHC	23:C:506:CLA:HBB1	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:801:GOL:O2	41:G:68:HOH:O	2.12	0.66
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.78	0.65
23:a:409:CLA:H152	23:c:507:CLA:H142	1.77	0.65
23:c:506:CLA:CMD	23:c:508:CLA:HAB	2.26	0.65
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.78	0.65
23:B:615:CLA:H2	23:B:616:CLA:HBB2	1.78	0.64
3:c:261:ARG:NH1	8:i:38:GLU:OE2	2.30	0.64
23:a:406:CLA:HHC	23:a:406:CLA:HBB1	1.80	0.64
2:b:482:ILE:HD12	2:b:486:LEU:HD12	1.80	0.64
29:A:414:PL9:H262	37:E:101:LHG:H223	1.80	0.63
25:b:619:BCR:H331	25:b:619:BCR:HC8	1.79	0.63
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.80	0.63
33:z:101:LMG:H302	33:z:101:LMG:H141	1.80	0.62
26:a:411:SQD:H152	37:d:408:LHG:H172	1.82	0.62
3:c:213:LEU:HD13	23:c:507:CLA:H202	1.80	0.62
27:b:901:GOL:O3	27:b:901:GOL:O1	2.16	0.62
19:z:32:ASP:O	19:z:36:SER:OG	2.16	0.62
20:R:18:TRP:O	20:R:22:ASN:ND2	2.32	0.62
23:C:511:CLA:H192	23:C:511:CLA:HBC3	1.82	0.61
23:c:503:CLA:H61	23:c:513:CLA:H42	1.82	0.61
23:A:408:CLA:H193	23:C:507:CLA:H101	1.83	0.61
13:O:42:ARG:HH12	27:O:501:GOL:H12	1.65	0.61
10:k:17:ILE:HD13	10:k:17:ILE:H	1.66	0.61
27:a:701:GOL:H32	12:m:1:FME:HG3	1.82	0.60
23:b:606:CLA:H72	25:b:619:BCR:HC7	1.83	0.60
10:K:17:ILE:H	10:K:17:ILE:HD13	1.67	0.59
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.85	0.59
3:c:134[B]:ILE:HD13	23:c:512:CLA:H43	1.84	0.59
23:C:509:CLA:HBC3	23:C:511:CLA:H71	1.85	0.59
26:a:411:SQD:H141	37:d:408:LHG:H152	1.84	0.59
23:B:609:CLA:HHC	23:B:609:CLA:HBB1	1.83	0.58
4:D:123:ILE:HD11	35:H:102:DGD:HAH2	1.85	0.58
15:U:86[B]:GLU:H	15:U:86[B]:GLU:CD	2.12	0.58
23:B:606:CLA:H202	26:a:413:SQD:H302	1.86	0.58
12:M:33:GLN:HB2	12:m:33:GLN:HG3	1.85	0.58
2:B:357[B]:ARG:NH2	4:D:337:GLU:O	2.33	0.58
23:c:502:CLA:C4D	23:c:504:CLA:H2	2.34	0.58
13:O:169:ASP:OD1	27:O:601:GOL:H12	2.03	0.58
25:C:515:BCR:H352	33:C:521:LMG:H352	1.86	0.57
3:c:134[B]:ILE:HD11	23:c:512:CLA:H71	1.86	0.57
27:a:801:GOL:O3	14:t:2:GLU:OE1	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:601:CLA:H72	23:b:601:CLA:H2	1.86	0.57
4:D:192:THR:HG23	23:D:405:CLA:HBC2	1.87	0.57
25:y:101:BCR:H321	25:y:101:BCR:HC8	1.87	0.57
34:B:626:HTG:H61	1:a:102:LEU:HD12	1.87	0.57
23:a:407:CLA:H191	37:e:101:LHG:H111	1.85	0.57
2:b:285:ASN:O	2:b:289:GLN:HG2	2.04	0.57
3:c:78:GLU:OE2	16:v:106:ASN:ND2	2.38	0.56
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.40	0.56
3:C:261:ARG:NH1	8:I:38:GLU:OE2	2.38	0.56
25:t:103:BCR:H321	25:t:103:BCR:HC8	1.86	0.56
35:c:517:DGD:HG11	41:c:603:HOH:O	2.06	0.56
1:A:102:LEU:HD12	34:b:625:HTG:H61	1.88	0.55
2:b:216:HIS:HE1	23:b:609:CLA:C1A	2.19	0.55
24:a:353:PHO:HBC3	4:d:279:LEU:HD22	1.87	0.55
1:a:15:GLU:HB2	32:a:420:LMT:H6'2	1.88	0.55
25:b:619:BCR:H331	25:b:619:BCR:C8	2.37	0.55
4:D:323:GLU:O	27:D:701:GOL:O2	2.25	0.55
2:B:226:TYR:HA	2:B:231:MET:HG3	1.88	0.54
1:a:183:MET:HA	23:a:405:CLA:HMD1	1.89	0.54
16:v:134:LYS:HE2	27:v:401:GOL:H32	1.88	0.54
2:B:357[A]:ARG:HH12	27:B:624:GOL:H32	1.72	0.54
37:D:411:LHG:H382	37:D:411:LHG:H132	1.89	0.54
23:b:616:CLA:HHC	23:b:616:CLA:HBB1	1.89	0.54
23:a:407:CLA:H203	33:d:412:LMG:H412	1.89	0.54
32:e:102:LMT:H6'1	6:f:43:ILE:HG12	1.88	0.54
23:B:615:CLA:H2	23:B:616:CLA:CBB	2.38	0.54
26:F:101:SQD:H102	17:X:31:ILE:HD11	1.89	0.54
2:b:497:GLN:HB2	2:b:504:THR:HB	1.90	0.54
29:A:414:PL9:H253	23:D:405:CLA:H141	1.89	0.54
2:B:36[B]:SER:OG	25:B:618:BCR:H362	2.07	0.54
35:c:519:DGD:HBH2	37:d:408:LHG:H211	1.90	0.54
32:A:359:LMT:H71	2:b:39:LEU:HD13	1.90	0.53
1:a:334:ARG:NH2	41:a:627:HOH:O	2.42	0.53
10:k:21:LEU:HD13	18:y:24:MET:HE3	1.90	0.53
32:t:101:LMT:H6E	32:t:102:LMT:H6D	1.90	0.53
29:A:414:PL9:H472	4:D:39:PRO:HD3	1.91	0.53
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.90	0.53
23:C:502:CLA:C4D	23:C:504:CLA:H2	2.39	0.53
23:C:502:CLA:HHC	23:C:502:CLA:HBB1	1.89	0.53
5:E:20:TRP:CD1	9:J:7:ILE:HD12	2.44	0.52
33:c:521:LMG:H232	33:c:521:LMG:H391	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:233:ASN:O	2:b:236:THR:HG22	2.10	0.52
13:o:205:ASP:OD2	13:o:207:ARG:NH2	2.43	0.52
3:c:338:GLY:HA3	3:c:341:LEU:O	2.10	0.52
13:o:92:SER:HB3	13:o:131:PRO:HA	1.91	0.52
1:A:84:PRO:HA	1:A:112:TYR:CG	2.44	0.52
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.45	0.52
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.23	0.51
4:D:85:MET:CE	4:D:96:GLU:HG2	2.40	0.51
5:E:77:GLU:O	5:E:81:GLU:HG2	2.10	0.51
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.92	0.51
3:c:279:LEU:HD22	23:c:510:CLA:HED2	1.91	0.51
27:a:801:GOL:H31	12:m:1:FME:HG2	1.93	0.51
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.93	0.51
13:O:39[B]:ARG:NH1	13:O:244:GLU:OE2	2.35	0.51
26:B:620:SQD:H1	26:B:620:SQD:H462	1.92	0.51
18:y:20:ALA:O	18:y:24:MET:HG2	2.11	0.51
5:e:9:PRO:HA	37:e:101:LHG:HC31	1.92	0.50
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.36	0.50
6:F:21:VAL:O	6:F:25:THR:HG23	2.10	0.50
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.93	0.50
10:k:23:ASP:OD2	18:y:21:GLN:NE2	2.43	0.50
10:k:20:PRO:HB3	18:y:21:GLN:HG3	1.94	0.50
4:D:24:ARG:HD3	17:X:37:VAL:HG22	1.93	0.50
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.47	0.50
23:c:502:CLA:C3D	23:c:504:CLA:H2	2.42	0.50
2:b:149[B]:LEU:HD21	23:b:604:CLA:H171	1.94	0.50
13:O:66:VAL:HG21	13:O:110:MET:HE3	1.93	0.49
1:A:227:THR:HB	1:A:231:GLU:HG3	1.94	0.49
1:a:221[A]:SER:HB2	4:d:139:ARG:O	2.12	0.49
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.47	0.49
23:B:612:CLA:HBB1	23:B:612:CLA:HMB1	1.94	0.49
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.93	0.49
26:b:620:SQD:H462	26:b:620:SQD:H1	1.93	0.49
19:Z:32:ASP:OD2	19:Z:35:ARG:HB3	2.11	0.49
23:a:405:CLA:H201	37:d:407:LHG:H161	1.95	0.49
8:I:35:LYS:O	8:I:37:LEU:N	2.45	0.49
27:a:801:GOL:H11	12:m:1:FME:HE3	1.94	0.49
37:d:407:LHG:HC62	11:l:15:THR:HG23	1.95	0.49
19:Z:33:TRP:HZ2	33:Z:101:LMG:HC61	1.78	0.49
23:B:613:CLA:H162	23:B:613:CLA:H121	1.59	0.49
4:d:85:MET:CE	4:d:96:GLU:HG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:E:103:HEM:HAC	6:F:27:ALA:HB1	1.95	0.49
27:O:601:GOL:O1	41:O:414:HOH:O	2.20	0.49
2:B:149:LEU:HG	23:B:606:CLA:HBB2	1.96	0.48
23:b:602:CLA:HHC	23:b:602:CLA:HBB1	1.95	0.48
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.48	0.48
13:o:58:ASN:C	13:o:60:ARG:H	2.21	0.48
24:A:353:PHO:H3A	23:D:405:CLA:H142	1.94	0.48
4:D:230:SER:HB2	41:G:169:HOH:O	2.13	0.48
2:b:224:ARG:HH21	32:b:621:LMT:H1'	1.76	0.48
37:d:408:LHG:H122	37:d:408:LHG:C38	2.44	0.48
23:b:609:CLA:HMD1	7:h:27:THR:HB	1.95	0.48
35:c:518:DGD:HAT1	35:c:519:DGD:HBF2	1.96	0.48
25:T:101:BCR:H19C	25:b:618:BCR:H363	1.96	0.48
4:D:180:ARG:HD3	4:D:180:ARG:C	2.39	0.48
3:C:203:THR:O	3:C:235:GLY:HA3	2.12	0.48
3:c:42:LEU:HD21	23:c:512:CLA:H2A	1.95	0.48
3:C:406:SER:HA	3:C:420:VAL:HG23	1.96	0.48
37:D:410:LHG:HC62	11:L:15:THR:HG23	1.96	0.48
25:T:101:BCR:H311	25:T:101:BCR:HC8	1.95	0.48
2:b:36:SER:OG	25:b:618:BCR:H362	2.13	0.48
27:d:801:GOL:H32	14:t:25:GLU:HB2	1.95	0.48
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.49	0.47
13:O:42:ARG:O	13:O:241:ALA:HA	2.14	0.47
2:B:299:GLU:HG3	2:B:402:TYR:HD1	1.78	0.47
13:O:25:THR:O	13:O:27:ARG:N	2.46	0.47
12:m:5[B]:GLN:CD	12:m:5[B]:GLN:H	2.21	0.47
25:T:101:BCR:H331	25:T:101:BCR:HC7	1.59	0.47
15:u:45:LEU:HD21	15:u:71:GLN:HB3	1.97	0.47
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.94	0.47
24:A:353:PHO:HBC3	4:D:279:LEU:HD22	1.96	0.47
23:B:614:CLA:H112	23:B:614:CLA:H71	1.56	0.47
23:C:502:CLA:C3D	23:C:504:CLA:H2	2.44	0.47
1:a:84:PRO:HA	1:a:112:TYR:CG	2.49	0.47
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.50	0.47
23:b:604:CLA:H42	23:b:605:CLA:H2	1.96	0.47
3:c:31:SER:CB	3:c:41:ARG:HG2	2.44	0.47
3:c:406:SER:HA	3:c:420:VAL:HG23	1.97	0.47
37:d:408:LHG:H342	37:d:408:LHG:H151	1.97	0.47
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.97	0.47
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.49	0.47
32:M:101:LMT:H6'2	12:m:32:GLN:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:d:408:LHG:H302	37:d:408:LHG:H332	1.67	0.47
29:a:416:PL9:H351	6:f:25:THR:OG1	2.14	0.47
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.15	0.47
3:C:391[B]:ARG:HA	3:C:391[B]:ARG:HD3	1.73	0.47
29:a:416:PL9:H171	29:a:416:PL9:H151	1.58	0.47
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.49	0.47
2:B:363:PHE:HB3	2:B:365:SER:O	2.15	0.46
3:c:286:ALA:HB2	23:c:503:CLA:HMD1	1.95	0.46
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.97	0.46
13:O:205:ASP:OD1	13:O:207:ARG:HG3	2.16	0.46
23:c:509:CLA:HBC3	23:c:511:CLA:H71	1.96	0.46
7:h:38:PHE:HB2	25:h:101:BCR:C10	2.45	0.46
23:A:408:CLA:H18	23:C:506:CLA:H142	1.98	0.46
23:a:406:CLA:HBA1	23:a:406:CLA:C4A	2.45	0.46
23:b:614:CLA:H62	23:b:614:CLA:H41	1.64	0.46
23:c:513:CLA:HMB2	23:c:513:CLA:H192	1.97	0.46
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.96	0.46
26:a:411:SQD:H271	37:d:408:LHG:H141	1.97	0.46
3:c:240:ILE:HA	3:c:240:ILE:HD13	1.84	0.46
23:B:601:CLA:H72	23:B:601:CLA:C4D	2.45	0.46
5:E:14:ILE:HD12	9:J:12:VAL:HG11	1.98	0.46
25:h:101:BCR:C8	25:h:101:BCR:H331	2.46	0.46
13:o:216:GLU:CD	13:o:234:LYS:HD2	2.41	0.46
37:d:408:LHG:H331	37:d:408:LHG:H361	1.46	0.46
25:b:619:BCR:H15C	25:b:619:BCR:H351	1.84	0.46
26:b:620:SQD:H341	26:b:620:SQD:H311	1.69	0.45
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.98	0.45
25:A:409:BCR:H24C	25:A:409:BCR:H371	1.71	0.45
2:B:357[A]:ARG:HH12	27:B:624:GOL:C3	2.29	0.45
2:B:477:ASP:OD1	2:B:477:ASP:N	2.49	0.45
3:C:157:MET:HE2	3:C:157:MET:HA	1.98	0.45
25:T:101:BCR:H24C	25:T:101:BCR:H371	1.79	0.45
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	1.99	0.45
4:D:261:PHE:CZ	37:D:410:LHG:HC81	2.52	0.45
23:b:603:CLA:H62	23:b:603:CLA:H41	1.81	0.45
13:o:58:ASN:HB2	13:o:61:GLN:HG2	1.98	0.45
34:B:622:HTG:H6'2	34:B:622:HTG:H3'1	1.85	0.45
3:c:139:THR:OG1	3:c:142:GLU:OE2	2.26	0.45
37:d:408:LHG:H372	37:d:408:LHG:H142	1.97	0.45
23:C:507:CLA:H18	23:C:507:CLA:H152	1.52	0.45
9:J:2:SER:N	41:J:201:HOH:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:d:403:CLA:HHC	23:d:403:CLA:HBB1	1.99	0.45
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.47	0.45
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.99	0.45
32:t:102:LMT:H112	32:t:102:LMT:H81	1.64	0.45
3:C:42:LEU:HD21	23:C:512:CLA:H2A	1.99	0.45
4:D:194:ASN:HA	4:D:295[B]:SER:OG	2.17	0.45
37:E:101:LHG:H241	37:E:101:LHG:HC61	1.83	0.45
8:I:36:ASP:OD1	8:I:36:ASP:N	2.50	0.45
25:c:515:BCR:H15C	25:c:515:BCR:H351	1.80	0.45
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.98	0.45
2:B:144:PHE:CE2	2:B:148[A]:LEU:HD11	2.52	0.44
3:C:334:PRO:HA	13:O:153:THR:OG1	2.17	0.44
2:b:245:VAL:HG22	23:b:612:CLA:H202	1.99	0.44
23:b:605:CLA:H41	23:b:605:CLA:H62	1.62	0.44
1:a:105:TRP:CE2	1:a:110:GLY:HA3	2.52	0.44
25:d:404:BCR:C8	25:d:404:BCR:H331	2.48	0.44
29:A:414:PL9:H151	29:A:414:PL9:H171	1.55	0.44
29:A:414:PL9:H301	29:A:414:PL9:H322	1.76	0.44
25:T:101:BCR:HC8	25:T:101:BCR:H321	1.99	0.44
3:c:167:VAL:HG11	23:c:513:CLA:HBA2	2.00	0.44
25:t:103:BCR:HC7	25:t:103:BCR:H331	1.52	0.44
23:b:613:CLA:H203	23:b:613:CLA:H161	1.87	0.44
9:j:6:ARG:NH1	9:j:6:ARG:HA	2.32	0.44
15:u:10[A]:VAL:HG12	41:G:214:HOH:O	2.18	0.44
2:B:67:ALA:HA	2:B:71:VAL:O	2.17	0.44
23:B:601:CLA:HHC	23:B:601:CLA:HBB1	1.99	0.44
3:C:210:PHE:HA	3:C:213:LEU:HD13	2.00	0.44
10:K:24:VAL:HG13	18:Y:25:ILE:HD13	1.98	0.44
5:E:12:ASP:OD1	9:J:4:GLY:HA3	2.18	0.44
1:a:214:MET:HB3	29:a:416:PL9:H103	1.98	0.44
23:c:510:CLA:H142	23:c:510:CLA:H112	1.86	0.44
27:A:701:GOL:H31	12:M:1:FME:HE3	1.99	0.44
32:D:404:LMT:H62	32:D:404:LMT:H91	1.46	0.44
25:H:101:BCR:H371	25:H:101:BCR:H24C	1.69	0.44
32:M:101:LMT:H6D	11:l:9:PRO:HA	2.00	0.44
13:O:58:ASN:HD21	13:O:61:GLN:HG3	1.82	0.44
13:O:137:THR:C	13:O:139:SER:H	2.26	0.44
16:V:126:LEU:HB3	16:V:129:LYS:HB2	2.00	0.44
3:c:152:LYS:HD2	41:G:190:HOH:O	2.17	0.44
3:c:281:MET:HE3	3:c:281:MET:HB2	1.80	0.44
23:A:408:CLA:H41	23:A:408:CLA:H61	1.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:95:LEU:HD21	23:C:502:CLA:OBD	2.18	0.44
3:C:223:TRP:CG	3:C:224:ILE:H	2.36	0.44
4:D:103:ARG:HG3	5:E:73:LYS:HG3	2.00	0.44
12:M:20:VAL:HG22	12:m:20:VAL:HG11	2.00	0.44
25:T:101:BCR:H351	26:b:620:SQD:H211	2.00	0.44
2:b:145:LEU:HD22	23:b:604:CLA:H162	2.00	0.44
3:c:182:PHE:HA	34:c:522:HTG:H61	2.00	0.44
23:B:603:CLA:H61	23:B:603:CLA:H102	1.78	0.43
3:C:174:LEU:HB3	23:C:503:CLA:H152	2.00	0.43
3:C:330:SER:HB3	13:O:100:GLY:O	2.18	0.43
23:C:511:CLA:H152	23:C:511:CLA:H112	1.47	0.43
29:a:416:PL9:H28	37:e:101:LHG:H222	1.99	0.43
8:I:38:GLU:HG2	8:I:38:GLU:OXT	2.18	0.43
1:a:259:ILE:HG22	1:a:260:PHE:CD1	2.53	0.43
10:k:24:VAL:HG21	18:y:25:ILE:HB	2.00	0.43
3:C:41:ARG:NH1	23:C:512:CLA:HMD1	2.33	0.43
6:F:15:ILE:HD13	20:R:23:ILE:HD11	1.99	0.43
3:c:452:ALA:HB1	8:i:37:LEU:HD22	1.99	0.43
33:d:412:LMG:H221	33:d:412:LMG:H191	1.63	0.43
3:C:52:ALA:HB2	23:C:512:CLA:HMA2	2.00	0.43
4:D:126:MET:HE3	4:D:143:ALA:O	2.18	0.43
1:a:230:THR:HG21	11:l:8:GLN:NE2	2.34	0.43
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.81	0.43
6:f:45:ARG:HG2	41:f:201:HOH:O	2.18	0.43
29:A:414:PL9:HC2	29:A:414:PL9:HC8	1.71	0.43
29:A:414:PL9:H221	29:A:414:PL9:H201	1.88	0.43
29:D:408:PL9:H401	29:D:408:PL9:H422	1.75	0.43
15:U:53:ALA:HB1	15:U:54:PRO:HA	2.00	0.43
23:d:403:CLA:H61	23:d:403:CLA:H41	1.67	0.43
2:B:285:ASN:O	2:B:289:GLN:HG2	2.18	0.43
25:b:619:BCR:HC7	25:b:619:BCR:H311	1.69	0.43
23:B:601:CLA:H72	23:B:601:CLA:C3D	2.48	0.43
25:C:516:BCR:H11C	25:C:516:BCR:H341	1.91	0.43
26:A:410:SQD:H122	26:A:410:SQD:H152	1.52	0.43
3:C:286:ALA:HB2	23:C:503:CLA:HMD2	2.00	0.43
23:b:615:CLA:H61	23:b:615:CLA:H92	1.67	0.43
23:c:509:CLA:H18	35:c:518:DGD:HAT2	2.00	0.43
9:J:6:ARG:HG3	41:J:201:HOH:O	2.18	0.43
13:O:130:GLN:H	13:O:130:GLN:CD	2.26	0.43
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.54	0.43
25:c:516:BCR:H24C	25:c:516:BCR:H371	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:19:ASP:HB3	10:k:20:PRO:HD3	2.01	0.43
23:C:505:CLA:H62	23:C:505:CLA:H41	1.75	0.42
23:C:510:CLA:HMB1	23:C:510:CLA:HBB1	2.00	0.42
4:D:209:LEU:HD23	4:D:209:LEU:C	2.44	0.42
10:K:20:PRO:HB3	18:Y:21:GLN:HG3	2.00	0.42
1:a:261:GLN:HG3	2:b:493:TRP:CH2	2.54	0.42
2:b:98:LEU:HB2	34:b:622:HTG:H7'1	2.01	0.42
4:d:14:TRP:CD1	34:d:411:HTG:H61	2.54	0.42
4:d:90:LEU:HD23	4:d:90:LEU:HA	1.93	0.42
24:A:407:PHO:HAB	4:D:205:LEU:HD13	2.00	0.42
25:B:619:BCR:H331	25:B:619:BCR:C8	2.49	0.42
2:b:358:ARG:HB2	27:b:901:GOL:H31	2.01	0.42
2:b:379:ALA:HA	2:b:390:TYR:HB3	2.02	0.42
1:A:133:LEU:HD23	4:D:256:ILE:HG12	2.02	0.42
23:A:405:CLA:H203	23:A:405:CLA:H162	1.76	0.42
23:B:614:CLA:H8	25:B:617:BCR:H362	2.02	0.42
5:E:56:TYR:HA	5:E:60:GLN:HE21	1.84	0.42
5:E:57:ALA:H	5:E:60:GLN:HE21	1.66	0.42
2:b:58:GLN:C	2:b:329:PRO:HB3	2.44	0.42
23:b:609:CLA:NC	25:h:101:BCR:H332	2.35	0.42
13:o:40:ILE:HG12	13:o:243:ILE:HD13	2.01	0.42
1:A:82:VAL:HB	1:A:174:LEU:HB2	2.01	0.42
2:B:58:GLN:C	2:B:329:PRO:HB3	2.45	0.42
1:a:227:THR:HB	1:a:231:GLU:HG3	2.02	0.42
25:t:103:BCR:H24C	25:t:103:BCR:H371	1.86	0.42
25:B:617:BCR:H11C	25:B:617:BCR:H341	1.90	0.42
3:C:130:VAL:O	3:C:134:ILE:HG12	2.20	0.42
13:o:79:ASP:OD1	13:o:80:GLN:N	2.48	0.42
23:A:404:CLA:HBB1	23:A:404:CLA:HMB3	2.02	0.42
23:C:506:CLA:HAA1	23:C:506:CLA:HBD	2.01	0.42
5:E:57:ALA:HB3	5:E:60:GLN:HG2	2.01	0.42
25:b:618:BCR:H24C	25:b:618:BCR:H371	1.83	0.42
14:t:2:GLU:HG2	14:t:3:THR:N	2.35	0.42
1:A:183:MET:HA	23:A:404:CLA:HMD1	2.01	0.42
23:B:614:CLA:H61	23:B:614:CLA:H92	1.76	0.42
37:D:411:LHG:H302	37:D:411:LHG:H332	1.81	0.42
23:b:614:CLA:H112	23:b:614:CLA:H72	1.58	0.42
3:c:363:GLY:O	3:c:367:GLU:HG2	2.20	0.42
16:v:41:HIS:HA	16:v:45:ILE:O	2.20	0.42
20:R:8:VAL:O	20:R:11:PRO:HD2	2.20	0.42
23:b:605:CLA:HHC	23:b:605:CLA:CBB	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLU:CD	1:A:243:GLU:H	2.27	0.41
10:K:26:PRO:O	10:K:29:PRO:HD2	2.20	0.41
25:c:516:BCR:H20C	25:c:516:BCR:H361	1.96	0.41
6:f:28:VAL:HB	6:f:29:PRO:HD3	2.02	0.41
18:y:30:ILE:HD12	18:y:30:ILE:HA	1.96	0.41
23:C:509:CLA:H122	23:C:509:CLA:H162	1.86	0.41
23:b:604:CLA:H162	23:b:604:CLA:H192	1.91	0.41
4:d:293:LEU:HD12	4:d:293:LEU:HA	1.98	0.41
23:B:605:CLA:HBD	23:B:605:CLA:HAA1	2.03	0.41
13:O:142:PHE:HB2	13:O:199:LEU:HB2	2.02	0.41
23:c:506:CLA:HMD2	23:c:508:CLA:HAB	2.00	0.41
37:e:101:LHG:H241	37:e:101:LHG:HC61	1.90	0.41
1:A:231:GLU:HB3	41:B:827:HOH:O	2.20	0.41
2:B:138:MET:HE3	23:B:615:CLA:CHD	2.51	0.41
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.89	0.41
3:C:150:ASP:OD2	3:C:152:LYS:HB2	2.21	0.41
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.94	0.41
5:E:9:PRO:HA	37:E:101:LHG:HC31	2.02	0.41
23:b:605:CLA:HAA1	23:b:605:CLA:HBD	2.01	0.41
4:d:194:ASN:HA	4:d:295[B]:SER:OG	2.19	0.41
12:m:5[B]:GLN:H	12:m:5[B]:GLN:NE2	2.19	0.41
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.55	0.41
4:D:49:LEU:HD13	25:D:407:BCR:C15	2.49	0.41
23:a:406:CLA:HHC	23:a:406:CLA:CBB	2.48	0.41
23:a:409:CLA:H41	23:a:409:CLA:H61	1.84	0.41
23:b:613:CLA:H72	23:b:613:CLA:H111	1.88	0.41
25:c:516:BCR:H11C	25:c:516:BCR:H341	1.95	0.41
25:A:409:BCR:H11C	25:A:409:BCR:H341	1.85	0.41
29:A:414:PL9:H43	29:A:414:PL9:H471	1.69	0.41
33:B:621:LMG:H112	33:B:621:LMG:H141	1.85	0.41
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.03	0.41
3:c:203:THR:O	3:c:235:GLY:HA3	2.20	0.41
4:d:332[A]:GLN:NE2	41:v:320:HOH:O	2.53	0.41
25:d:404:BCR:H15C	25:d:404:BCR:H351	1.81	0.41
37:d:408:LHG:H131	37:d:408:LHG:H102	1.91	0.41
16:v:126:LEU:HB3	16:v:129:LYS:HB2	2.02	0.41
3:C:135:ARG:HA	3:C:135:ARG:HD2	1.94	0.41
23:C:513:CLA:H143	23:C:514:CLA:H142	2.01	0.41
25:a:410:BCR:H24C	25:a:410:BCR:H371	1.79	0.41
2:b:216:HIS:CE1	23:b:609:CLA:NA	2.87	0.41
3:c:38:GLY:HA3	23:c:512:CLA:HMD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:20:ASP:O	4:d:24:ARG:HG2	2.21	0.41
23:d:403:CLA:H162	7:h:37:LEU:HD21	2.02	0.41
7:h:62:TRP:C	7:h:64:ALA:H	2.28	0.41
23:B:602:CLA:H203	23:B:602:CLA:H162	1.72	0.41
25:B:618:BCR:H15C	25:B:618:BCR:H351	1.91	0.41
3:C:252:ILE:HG22	3:C:253:LEU:HD23	2.03	0.41
2:b:158:LEU:HB3	2:b:199:VAL:HG22	2.03	0.41
23:b:607:CLA:H112	23:b:607:CLA:H91	1.61	0.41
3:c:425:TRP:CD1	23:c:505:CLA:HMA2	2.56	0.41
2:B:491:VAL:HG12	4:D:136:VAL:HG13	2.03	0.41
25:B:619:BCR:H371	25:B:619:BCR:H24C	1.79	0.41
3:C:114:VAL:HG22	33:C:521:LMG:H182	2.03	0.41
3:C:173:LEU:HA	3:C:173:LEU:HD23	1.83	0.41
35:C:518:DGD:HAE2	35:C:518:DGD:HA81	1.91	0.41
35:C:519:DGD:HB81	35:C:519:DGD:HBE2	1.73	0.41
25:D:407:BCR:H20C	25:D:407:BCR:H361	1.90	0.41
34:D:414:HTG:H1'2	7:H:25:TRP:CZ3	2.56	0.41
5:E:30:LEU:HD23	20:R:12:VAL:HG22	2.03	0.41
8:I:2:GLU:O	8:I:6:ILE:HG12	2.21	0.41
1:a:14:TRP:HD1	32:a:420:LMT:H6'1	1.86	0.41
1:a:162:PRO:HB3	1:a:168:PHE:HA	2.03	0.41
23:b:615:CLA:H3A	23:b:615:CLA:HBA1	1.91	0.41
25:b:618:BCR:H15C	25:b:618:BCR:H351	1.84	0.41
3:c:48:LYS:HG3	3:c:138:GLU:HG3	2.03	0.41
25:t:103:BCR:H23C	25:t:103:BCR:H382	2.02	0.41
17:x:14:LEU:HD12	17:x:14:LEU:HA	1.83	0.41
17:x:23:LEU:HD23	17:x:23:LEU:HA	1.91	0.41
33:Z:101:LMG:H141	33:Z:101:LMG:H111	1.89	0.41
29:A:414:PL9:HC8	29:A:414:PL9:H121	1.79	0.41
3:C:443:TRP:CZ2	23:C:509:CLA:HMD1	2.55	0.41
32:I:101:LMT:H6'2	32:I:101:LMT:O3'	2.21	0.41
2:b:149[B]:LEU:HD11	23:b:604:CLA:H122	2.02	0.41
33:c:520:LMG:H181	10:k:27:VAL:HG11	2.02	0.41
15:u:69:GLU:O	15:u:73:GLN:HG3	2.21	0.41
2:b:298:LEU:HD12	2:b:298:LEU:HA	1.83	0.40
37:e:101:LHG:H142	37:e:101:LHG:H172	1.83	0.40
19:z:34:ASP:OD1	19:z:34:ASP:N	2.52	0.40
25:K:102:BCR:H24C	25:K:102:BCR:H371	1.71	0.40
2:b:134:ASP:OD1	2:b:136:PRO:HD2	2.21	0.40
37:d:408:LHG:H242	37:d:408:LHG:H272	1.92	0.40
1:A:132:GLU:O	1:A:136:ARG:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:161:LEU:HD12	2:b:161:LEU:HA	1.88	0.40
2:B:30:VAL:HG12	23:B:605:CLA:HHD	2.03	0.40
2:B:188:ASP:OD2	2:B:194:ASN:ND2	2.47	0.40
34:B:623:HTG:H4'2	34:B:623:HTG:H7'3	1.85	0.40
13:O:24:ASP:HA	13:O:203:LYS:HE2	2.04	0.40
1:a:261:GLN:HG3	2:b:493:TRP:CZ3	2.55	0.40
2:b:216:HIS:CE1	23:b:609:CLA:C1A	3.03	0.40
23:b:614:CLA:H8	25:b:617:BCR:H362	2.04	0.40
35:c:518:DGD:HBF2	35:c:518:DGD:HBE1	1.91	0.40
25:H:101:BCR:C8	25:H:101:BCR:H331	2.51	0.40
18:Y:35:ILE:HD13	19:Z:24:PRO:HG3	2.03	0.40
1:a:131:TRP:CH2	23:c:506:CLA:HAA2	2.57	0.40
4:d:24:ARG:NH1	17:x:37:VAL:HG22	2.37	0.40
20:R:2:ASP:HB3	20:R:5:VAL:HG23	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	328 (98%)	4 (1%)	1 (0%)	36	40
1	a	334/344 (97%)	327 (98%)	6 (2%)	1 (0%)	36	40
2	B	509/505 (101%)	501 (98%)	8 (2%)	0	100	100
2	b	508/505 (101%)	497 (98%)	11 (2%)	0	100	100
3	C	450/455 (99%)	441 (98%)	8 (2%)	1 (0%)	43	50
3	c	458/455 (101%)	450 (98%)	7 (2%)	1 (0%)	43	50
4	D	341/342 (100%)	328 (96%)	13 (4%)	0	100	100
4	d	341/342 (100%)	332 (97%)	9 (3%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	3 (5%)	1 (2%)	7	4
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%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	34/37 (92%)	34 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	244/244 (100%)	236 (97%)	7 (3%)	1 (0%)	30	31
13	o	241/244 (99%)	236 (98%)	5 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
16	V	137/137 (100%)	133 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	131 (97%)	4 (3%)	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%)	25 (93%)	2 (7%)	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	5252/5384 (98%)	5135 (98%)	108 (2%)	9 (0%)	43	50

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP
13	O	26	ALA
3	c	416	SER
19	Z	31	GLN
19	z	30	PRO
7	h	63	LYS
1	A	259	ILE
1	a	259	ILE

### 5.3.2 Protein sidechains [i](#)

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	270/279 (97%)	268 (99%)	2 (1%)	76	82
1	a	271/279 (97%)	270 (100%)	1 (0%)	84	89
2	B	409/403 (102%)	404 (99%)	5 (1%)	63	74
2	b	408/403 (101%)	400 (98%)	8 (2%)	48	59
3	C	353/356 (99%)	345 (98%)	8 (2%)	44	55
3	c	361/356 (101%)	355 (98%)	6 (2%)	53	65
4	D	278/277 (100%)	276 (99%)	2 (1%)	76	82
4	d	278/277 (100%)	275 (99%)	3 (1%)	65	75
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	48
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%)	54 (98%)	1 (2%)	51	63
8	I	34/34 (100%)	32 (94%)	2 (6%)	18	18
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (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	209/207 (101%)	203 (97%)	6 (3%)	37	47
13	o	206/207 (100%)	199 (97%)	7 (3%)	32	40
14	T	27/28 (96%)	24 (89%)	3 (11%)	6	4
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/89 (94%)	82 (98%)	2 (2%)	43	54
15	u	85/89 (96%)	83 (98%)	2 (2%)	43	54
16	V	119/117 (102%)	118 (99%)	1 (1%)	73	80
16	v	117/117 (100%)	113 (97%)	4 (3%)	32	40
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%)	19 (86%)	3 (14%)	3	2
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18	19
19	z	52/52 (100%)	44 (85%)	8 (15%)	2	1
20	R	29/29 (100%)	27 (93%)	2 (7%)	14	13
All	All	4358/4403 (99%)	4257 (98%)	101 (2%)	45	55

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	GLU
1	A	244	GLU
2	B	161	LEU
2	B	294	SER
2	B	299	GLU
2	B	362	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	389	LYS
3	C	24	THR
3	C	29	GLU
3	C	142	GLU
3	C	255	THR
3	C	289	PHE
3	C	315	MET
3	C	462	GLU
3	C	471	SER
4	D	259	ILE
4	D	338	ASN
5	E	4	THR
5	E	71	GLU
7	H	12	ARG
7	H	43	LEU
8	I	33	LYS
8	I	34	ARG
9	J	6	ARG
9	J	9	LEU
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
10	K	27	VAL
12	M	16[A]	LEU
12	M	16[B]	LEU
12	M	20	VAL
13	O	4	THR
13	O	55	GLU
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	THR
15	U	10	VAL
15	U	70	ARG
16	V	15	GLU
17	X	14	LEU
1	a	13	LEU
2	b	63	LEU
2	b	128	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	b	161	LEU
2	b	245	VAL
2	b	287	ARG
2	b	362	PHE
2	b	486	LEU
2	b	491	VAL
3	c	142	GLU
3	c	152	LYS
3	c	240	ILE
3	c	255	THR
3	c	289	PHE
3	c	315	MET
4	d	230	SER
4	d	259	ILE
4	d	272	LEU
5	e	71	GLU
7	h	65	LEU
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
16	v	106	ASN
18	y	18	VAL
18	y	19	ILE
18	y	45	ASN
19	Z	3	ILE
19	Z	20	VAL

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Mol	Chain	Res	Type
19	Z	31	GLN
20	R	4	ARG
20	R	29	LYS
19	z	2	THR
19	z	3	ILE
19	z	4	LEU
19	z	7	LEU
19	z	20	VAL
19	z	21	ILE
19	z	34	ASP
19	z	42	LEU

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

Mol	Chain	Res	Type
1	A	165	GLN
1	A	234	ASN
3	C	322	GLN
3	C	415	ASN
4	D	186	GLN
5	E	60	GLN
11	L	8	GLN
15	U	78	ASN
1	a	165	GLN
1	a	296	ASN
2	b	331	ASN
4	d	186	GLN
4	d	301	GLN
11	l	8	GLN
13	o	58	ASN
15	u	78	ASN
16	v	86	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	-	8,9,10	0.69	0	8,9,11	2.09	3 (37%)
8	FME	I	1	-	8,9,10	0.64	0	8,9,11	1.34	2 (25%)
12	FME	m	1	-	8,9,10	0.58	0	8,9,11	1.30	2 (25%)
8	FME	i	1	-	8,9,10	0.69	0	8,9,11	1.15	1 (12%)
14	FME	t	1	-	8,9,10	0.79	0	8,9,11	1.39	1 (12%)
12	FME	M	1	-	8,9,10	0.65	0	8,9,11	1.05	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	-	-	1/7/9/11	-
8	FME	I	1	-	-	0/7/9/11	-
12	FME	m	1	-	-	1/7/9/11	-
8	FME	i	1	-	-	0/7/9/11	-
14	FME	t	1	-	-	1/7/9/11	-
12	FME	M	1	-	-	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	CA-N-CN	3.40	128.05	122.82
14	T	1	FME	CB-CA-N	-2.91	105.22	110.52
14	T	1	FME	C-CA-N	2.74	114.79	109.50
14	t	1	FME	O-C-CA	-2.48	118.39	124.77
8	I	1	FME	O-C-CA	-2.33	118.78	124.77
12	m	1	FME	O1-CN-N	-2.20	119.63	125.32
12	m	1	FME	O-C-CA	-2.11	119.33	124.77
12	M	1	FME	O-C-CA	-2.03	119.55	124.77
8	I	1	FME	CA-N-CN	-2.01	119.74	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	O-C-CA	-2.00	119.62	124.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	3	0
12	M	1	FME	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 225 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 192 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	c	513	-	69,73,73	2.06	19 (27%)	82,113,113	2.65	34 (41%)
23	CLA	b	613	-	69,73,73	1.98	20 (28%)	82,113,113	2.68	31 (37%)
29	PL9	D	408	-	55,55,55	0.65	1 (1%)	68,69,69	1.61	17 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	C	502	-	69,73,73	1.98	19 (27%)	82,113,113	2.73	33 (40%)
23	CLA	A	406	-	69,73,73	2.01	19 (27%)	82,113,113	2.69	33 (40%)
23	CLA	b	612	-	69,73,73	1.97	19 (27%)	82,113,113	2.68	29 (35%)
27	GOL	b	624	-	5,5,5	1.21	1 (20%)	5,5,5	0.84	0
35	DGD	H	102	-	63,63,67	0.85	3 (4%)	77,77,81	1.03	5 (6%)
25	BCR	C	516	-	41,41,41	1.06	1 (2%)	56,56,56	1.33	7 (12%)
23	CLA	b	611	-	69,73,73	1.91	18 (26%)	82,113,113	2.82	31 (37%)
34	HTG	B	622	-	19,19,19	0.96	1 (5%)	23,24,24	1.60	5 (21%)
23	CLA	c	507	-	69,73,73	2.02	20 (28%)	82,113,113	2.65	30 (36%)
34	HTG	D	414	-	16,16,19	0.96	1 (6%)	20,21,24	1.20	1 (5%)
23	CLA	D	406	-	69,73,73	2.06	19 (27%)	82,113,113	2.65	31 (37%)
23	CLA	C	513	-	69,73,73	2.01	20 (28%)	82,113,113	2.74	35 (42%)
23	CLA	C	510	-	69,73,73	2.05	20 (28%)	82,113,113	2.70	29 (35%)
32	LMT	D	404	-	36,36,36	1.15	3 (8%)	47,47,47	1.32	6 (12%)
32	LMT	E	102	-	36,36,36	1.03	1 (2%)	47,47,47	1.04	3 (6%)
23	CLA	c	514	-	69,73,73	2.09	21 (30%)	82,113,113	2.73	32 (39%)
26	SQD	f	102	-	41,43,54	1.13	2 (4%)	51,54,65	1.55	10 (19%)
31	BCT	A	348	-	3,3,3	0.55	0	2,3,3	1.29	0
23	CLA	b	601	-	69,73,73	2.05	20 (28%)	82,113,113	2.70	31 (37%)
23	CLA	b	603	-	69,73,73	1.94	19 (27%)	82,113,113	2.76	32 (39%)
32	LMT	I	101	-	36,36,36	1.02	2 (5%)	47,47,47	1.17	4 (8%)
27	GOL	O	501	-	5,5,5	0.96	0	5,5,5	1.03	0
27	GOL	a	801	-	5,5,5	1.19	1 (20%)	5,5,5	1.06	1 (20%)
37	LHG	d	408	-	48,48,48	0.92	2 (4%)	51,54,54	1.02	3 (5%)
40	HEC	v	202	-	46,50,50	1.93	6 (13%)	58,82,82	1.86	6 (10%)
27	GOL	D	701	-	5,5,5	1.38	1 (20%)	5,5,5	0.97	0
25	BCR	B	617	-	41,41,41	1.09	1 (2%)	56,56,56	1.37	10 (17%)
25	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.40	10 (17%)
31	BCT	a	404	-	3,3,3	0.49	0	2,3,3	1.49	0
32	LMT	b	627	-	25,25,36	0.89	0	30,30,47	1.12	3 (10%)
23	CLA	B	604	-	69,73,73	2.02	19 (27%)	82,113,113	2.57	31 (37%)
27	GOL	A	701	-	5,5,5	1.47	2 (40%)	5,5,5	1.11	1 (20%)
23	CLA	C	514	-	69,73,73	2.01	19 (27%)	82,113,113	2.72	31 (37%)
33	LMG	C	501	-	51,51,55	0.93	2 (3%)	59,59,63	1.38	7 (11%)
25	BCR	k	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.44	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	B	619	-	41,41,41	1.08	1 (2%)	56,56,56	1.37	9 (16%)
23	CLA	A	408	-	69,73,73	1.95	19 (27%)	82,113,113	2.80	34 (41%)
23	CLA	c	511	-	69,73,73	1.95	20 (28%)	82,113,113	2.71	32 (39%)
33	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.10	4 (6%)
34	HTG	b	622	-	19,19,19	1.09	2 (10%)	23,24,24	1.86	7 (30%)
26	SQD	b	620	-	52,54,54	1.00	3 (5%)	62,65,65	1.58	11 (17%)
23	CLA	C	509	-	69,73,73	2.02	18 (26%)	82,113,113	2.65	30 (36%)
33	LMG	D	415	-	51,51,55	0.82	2 (3%)	59,59,63	1.05	3 (5%)
29	PL9	a	416	-	55,55,55	0.68	2 (3%)	68,69,69	2.03	23 (33%)
33	LMG	Z	101	-	37,37,55	1.01	3 (8%)	45,45,63	1.43	5 (11%)
23	CLA	B	614	-	69,73,73	1.99	19 (27%)	82,113,113	2.87	33 (40%)
23	CLA	B	602	-	69,73,73	2.00	19 (27%)	82,113,113	2.71	32 (39%)
23	CLA	B	610	-	69,73,73	2.01	19 (27%)	82,113,113	2.78	33 (40%)
25	BCR	D	407	-	41,41,41	1.12	1 (2%)	56,56,56	1.82	15 (26%)
23	CLA	B	609	-	69,73,73	2.00	18 (26%)	82,113,113	2.65	31 (37%)
23	CLA	c	504	-	69,73,73	2.04	19 (27%)	82,113,113	2.70	30 (36%)
27	GOL	B	624	-	5,5,5	0.88	0	5,5,5	1.28	1 (20%)
23	CLA	C	512	-	69,73,73	2.02	22 (31%)	82,113,113	2.60	28 (34%)
23	CLA	B	612	-	69,73,73	1.95	19 (27%)	82,113,113	2.67	31 (37%)
27	GOL	C	523	-	5,5,5	1.16	0	5,5,5	0.94	0
25	BCR	C	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	5 (8%)
35	DGD	C	519	-	63,63,67	0.88	3 (4%)	77,77,81	1.00	3 (3%)
25	BCR	b	618	-	41,41,41	1.02	1 (2%)	56,56,56	1.23	6 (10%)
27	GOL	d	801	-	5,5,5	0.98	0	5,5,5	1.05	1 (20%)
23	CLA	C	504	-	69,73,73	1.98	19 (27%)	82,113,113	2.67	30 (36%)
29	PL9	d	405	-	55,55,55	0.72	1 (1%)	68,69,69	1.61	17 (25%)
34	HTG	C	522	-	19,19,19	0.83	1 (5%)	23,24,24	1.32	2 (8%)
26	SQD	a	413	-	52,54,54	1.02	3 (5%)	62,65,65	1.15	6 (9%)
27	GOL	c	743	-	5,5,5	1.24	1 (20%)	5,5,5	0.97	0
27	GOL	o	501	-	5,5,5	1.04	0	5,5,5	1.04	0
24	PHO	A	407	-	58,69,69	2.66	12 (20%)	55,99,99	2.93	14 (25%)
26	SQD	A	412	-	52,54,54	0.97	2 (3%)	62,65,65	1.15	5 (8%)
33	LMG	a	419	-	51,51,55	0.93	2 (3%)	59,59,63	1.20	6 (10%)
34	HTG	B	626	-	19,19,19	0.95	2 (10%)	23,24,24	1.28	4 (17%)
26	SQD	F	101	-	41,43,54	1.15	3 (7%)	51,54,65	2.03	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	LHG	d	711	-	48,48,48	0.89	3 (6%)	51,54,54	1.13	4 (7%)
32	LMT	e	102	-	36,36,36	0.99	1 (2%)	47,47,47	1.01	1 (2%)
32	LMT	M	103	-	36,36,36	1.04	2 (5%)	47,47,47	1.07	2 (4%)
34	HTG	V	203	-	11,11,19	0.28	0	15,15,24	1.13	1 (6%)
25	BCR	d	404	-	41,41,41	1.14	2 (4%)	56,56,56	1.91	14 (25%)
23	CLA	B	615	-	69,73,73	2.00	20 (28%)	82,113,113	2.68	30 (36%)
34	HTG	b	623	-	19,19,19	0.96	1 (5%)	23,24,24	1.60	2 (8%)
29	PL9	A	414	-	55,55,55	0.71	3 (5%)	68,69,69	2.05	25 (36%)
23	CLA	d	402	-	69,73,73	1.94	19 (27%)	82,113,113	2.64	33 (40%)
33	LMG	m	101	-	51,51,55	0.88	2 (3%)	59,59,63	1.25	5 (8%)
23	CLA	b	610	-	69,73,73	1.98	20 (28%)	82,113,113	2.74	34 (41%)
27	GOL	v	401	-	5,5,5	1.26	0	5,5,5	0.88	0
32	LMT	t	102	-	26,26,36	0.90	1 (3%)	31,31,47	1.33	2 (6%)
35	DGD	c	518	-	63,63,67	0.85	3 (4%)	77,77,81	0.98	4 (5%)
33	LMG	d	412	-	51,51,55	0.89	2 (3%)	59,59,63	1.09	4 (6%)
23	CLA	b	602	-	69,73,73	2.05	19 (27%)	82,113,113	2.81	35 (42%)
23	CLA	C	511	-	69,73,73	2.03	20 (28%)	82,113,113	2.76	33 (40%)
24	PHO	a	353	-	58,69,69	2.79	14 (24%)	55,99,99	3.05	17 (30%)
23	CLA	b	609	-	69,73,73	1.97	18 (26%)	82,113,113	2.67	32 (39%)
27	GOL	V	401	-	5,5,5	1.41	1 (20%)	5,5,5	0.86	0
35	DGD	h	102	-	63,63,67	0.86	3 (4%)	77,77,81	1.10	5 (6%)
25	BCR	K	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.46	13 (23%)
23	CLA	a	405	-	69,73,73	1.97	19 (27%)	82,113,113	2.75	34 (41%)
35	DGD	c	517	-	63,63,67	0.86	2 (3%)	77,77,81	1.10	8 (10%)
23	CLA	C	507	-	69,73,73	2.00	20 (28%)	82,113,113	2.69	33 (40%)
23	CLA	B	611	-	69,73,73	2.46	21 (30%)	82,113,113	3.59	32 (39%)
23	CLA	a	407	-	69,73,73	1.96	19 (27%)	82,113,113	2.67	32 (39%)
27	GOL	B	901	-	5,5,5	1.11	0	5,5,5	1.03	0
27	GOL	a	701	-	5,5,5	1.09	0	5,5,5	1.09	1 (20%)
33	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.10	4 (8%)
37	LHG	D	410	-	48,48,48	0.88	3 (6%)	51,54,54	1.02	3 (5%)
23	CLA	b	615	-	69,73,73	1.97	20 (28%)	82,113,113	2.67	33 (40%)
23	CLA	A	405	-	69,73,73	2.00	18 (26%)	82,113,113	2.70	35 (42%)
35	DGD	C	518	-	63,63,67	0.91	3 (4%)	77,77,81	1.04	5 (6%)
38	HEM	E	103	-	50,50,50	1.55	8 (16%)	67,82,82	1.81	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LMG	B	621	-	51,51,55	0.93	2 (3%)	59,59,63	1.26	4 (6%)
40	HEC	V	202	-	46,50,50	1.91	5 (10%)	58,82,82	1.83	8 (13%)
23	CLA	B	603	-	69,73,73	1.98	20 (28%)	82,113,113	2.80	31 (37%)
23	CLA	A	404	-	69,73,73	1.98	19 (27%)	82,113,113	2.74	31 (37%)
34	HTG	b	625	-	19,19,19	0.92	2 (10%)	23,24,24	1.56	3 (13%)
37	LHG	l	101	-	48,48,48	0.84	3 (6%)	51,54,54	1.05	4 (7%)
25	BCR	b	619	-	41,41,41	1.10	1 (2%)	56,56,56	1.39	7 (12%)
34	HTG	B	623	-	19,19,19	0.72	1 (5%)	23,24,24	1.18	1 (4%)
23	CLA	a	406	-	69,73,73	2.01	17 (24%)	82,113,113	2.72	31 (37%)
23	CLA	c	503	-	69,73,73	2.00	18 (26%)	82,113,113	2.66	28 (34%)
25	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.59	13 (23%)
32	LMT	M	101	-	36,36,36	1.11	3 (8%)	47,47,47	1.20	4 (8%)
23	CLA	B	601	-	69,73,73	2.05	19 (27%)	82,113,113	2.74	31 (37%)
25	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.35	9 (16%)
23	CLA	B	606	-	69,73,73	2.00	18 (26%)	82,113,113	2.84	33 (40%)
24	PHO	A	353	-	58,69,69	2.81	14 (24%)	55,99,99	2.93	16 (29%)
32	LMT	A	359	-	36,36,36	0.91	1 (2%)	47,47,47	1.02	1 (2%)
27	GOL	A	411	-	5,5,5	1.10	0	5,5,5	0.78	0
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.35	6 (10%)
34	HTG	c	522	-	19,19,19	0.86	1 (5%)	23,24,24	1.44	1 (4%)
27	GOL	c	742	-	5,5,5	1.04	0	5,5,5	1.05	0
23	CLA	C	503	-	69,73,73	2.00	20 (28%)	82,113,113	2.58	29 (35%)
23	CLA	B	607	-	69,73,73	1.95	19 (27%)	82,113,113	2.66	32 (39%)
23	CLA	c	505	-	69,73,73	2.02	21 (30%)	82,113,113	2.67	33 (40%)
34	HTG	d	411	-	16,16,19	0.91	1 (6%)	20,21,24	1.33	1 (5%)
32	LMT	b	621	-	25,25,36	0.95	1 (4%)	30,30,47	1.18	3 (10%)
25	BCR	H	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.43	10 (17%)
25	BCR	y	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.64	9 (16%)
33	LMG	c	521	-	51,51,55	1.01	2 (3%)	59,59,63	1.37	7 (11%)
35	DGD	c	519	-	63,63,67	0.88	3 (4%)	77,77,81	0.99	4 (5%)
23	CLA	b	606	-	69,73,73	1.99	19 (27%)	82,113,113	2.71	31 (37%)
23	CLA	B	616	-	69,73,73	1.94	19 (27%)	82,113,113	2.74	27 (32%)
25	BCR	Y	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.75	13 (23%)
23	CLA	c	506	-	69,73,73	1.99	19 (27%)	82,113,113	2.68	29 (35%)
37	LHG	D	411	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	LHG	L	101	-	48,48,48	0.89	3 (6%)	51,54,54	1.16	4 (7%)
27	GOL	d	701	-	5,5,5	1.08	0	5,5,5	1.01	0
37	LHG	D	409	-	48,48,48	0.87	2 (4%)	51,54,54	1.29	6 (11%)
23	CLA	b	616	-	69,73,73	1.99	19 (27%)	82,113,113	2.80	30 (36%)
23	CLA	C	505	-	69,73,73	1.96	20 (28%)	82,113,113	2.66	31 (37%)
28	OEX	a	415	-	0,15,15	-	-	-	-	-
23	CLA	c	510	-	69,73,73	2.05	18 (26%)	82,113,113	2.74	32 (39%)
26	SQD	a	411	-	52,54,54	0.89	2 (3%)	62,65,65	1.80	11 (17%)
33	LMG	C	521	-	51,51,55	1.06	3 (5%)	59,59,63	1.33	6 (10%)
23	CLA	b	614	-	69,73,73	1.97	20 (28%)	82,113,113	2.77	29 (35%)
35	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.20	6 (7%)
23	CLA	C	506	-	69,73,73	2.01	18 (26%)	82,113,113	2.68	31 (37%)
23	CLA	d	403	-	69,73,73	2.02	19 (27%)	82,113,113	2.69	31 (37%)
32	LMT	t	101	-	25,25,36	0.88	2 (8%)	30,30,47	1.13	3 (10%)
25	BCR	a	410	-	41,41,41	1.05	1 (2%)	56,56,56	1.31	7 (12%)
32	LMT	m	103	-	36,36,36	1.03	3 (8%)	47,47,47	1.11	3 (6%)
27	GOL	a	412	-	5,5,5	0.93	0	5,5,5	1.18	1 (20%)
32	LMT	a	414	-	36,36,36	0.98	3 (8%)	47,47,47	1.13	3 (6%)
23	CLA	b	605	-	69,73,73	1.95	20 (28%)	82,113,113	2.77	31 (37%)
38	HEM	e	87	-	50,50,50	1.50	6 (12%)	67,82,82	1.64	12 (17%)
28	OEX	A	413	-	0,15,15	-	-	-	-	-
23	CLA	b	608	-	69,73,73	1.97	20 (28%)	82,113,113	2.68	34 (41%)
23	CLA	c	508	-	69,73,73	2.00	18 (26%)	82,113,113	2.74	31 (37%)
23	CLA	c	512	-	69,73,73	2.04	19 (27%)	82,113,113	2.62	31 (37%)
27	GOL	O	601	-	5,5,5	0.99	0	5,5,5	1.22	1 (20%)
25	BCR	A	409	-	41,41,41	1.01	1 (2%)	56,56,56	1.41	10 (17%)
25	BCR	t	103	-	41,41,41	1.02	1 (2%)	56,56,56	1.50	10 (17%)
37	LHG	E	101	-	41,41,48	1.08	2 (4%)	44,47,54	1.12	3 (6%)
32	LMT	a	420	-	36,36,36	0.99	1 (2%)	47,47,47	1.04	1 (2%)
27	GOL	o	601	-	5,5,5	1.16	1 (20%)	5,5,5	1.10	0
27	GOL	b	901	-	5,5,5	0.44	0	5,5,5	1.58	1 (20%)
33	LMG	c	520	-	51,51,55	0.91	2 (3%)	59,59,63	1.09	5 (8%)
23	CLA	B	613	-	69,73,73	2.03	18 (26%)	82,113,113	2.62	29 (35%)
23	CLA	c	509	-	69,73,73	2.11	20 (28%)	82,113,113	2.61	30 (36%)
23	CLA	C	508	-	69,73,73	1.98	20 (28%)	82,113,113	2.72	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	b	604	-	69,73,73	1.99	20 (28%)	82,113,113	2.67	30 (36%)
23	CLA	b	607	-	69,73,73	1.99	19 (27%)	82,113,113	2.73	31 (37%)
25	BCR	c	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.38	10 (17%)
25	BCR	c	515	-	41,41,41	1.00	1 (2%)	56,56,56	1.58	10 (17%)
23	CLA	c	502	-	69,73,73	1.98	21 (30%)	82,113,113	2.69	29 (35%)
37	LHG	d	407	-	48,48,48	0.87	2 (4%)	51,54,54	1.06	4 (7%)
23	CLA	B	605	-	69,73,73	2.01	19 (27%)	82,113,113	2.73	30 (36%)
37	LHG	e	101	-	41,41,48	1.06	2 (4%)	44,47,54	0.93	2 (4%)
23	CLA	B	608	-	69,73,73	1.89	20 (28%)	82,113,113	2.69	33 (40%)
26	SQD	B	620	-	52,54,54	1.02	3 (5%)	62,65,65	1.75	11 (17%)
26	SQD	A	410	-	52,54,54	0.86	2 (3%)	62,65,65	1.85	10 (16%)
23	CLA	D	405	-	69,73,73	1.98	19 (27%)	82,113,113	2.74	34 (41%)
23	CLA	a	409	-	69,73,73	1.98	18 (26%)	82,113,113	2.78	32 (39%)
24	PHO	a	408	-	58,69,69	2.77	13 (22%)	55,99,99	2.94	14 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	513	-	1/1/15/20	13/39/115/115	-
23	CLA	b	613	-	1/1/15/20	5/39/115/115	-
29	PL9	D	408	-	-	6/53/73/73	0/1/1/1
23	CLA	C	502	-	1/1/15/20	4/39/115/115	-
23	CLA	b	612	-	1/1/15/20	4/39/115/115	-
23	CLA	A	406	-	-	5/39/115/115	-
27	GOL	b	624	-	-	2/4/4/4	-
35	DGD	H	102	-	-	11/51/91/95	0/2/2/2
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
23	CLA	b	611	-	1/1/15/20	2/39/115/115	-
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
23	CLA	c	507	-	1/1/15/20	7/39/115/115	-
34	HTG	D	414	-	-	3/7/27/30	0/1/1/1
23	CLA	D	406	-	1/1/15/20	13/39/115/115	-
23	CLA	C	513	-	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	510	-	1/1/15/20	5/39/115/115	-
32	LMT	D	404	-	-	12/21/61/61	0/2/2/2
32	LMT	E	102	-	-	8/21/61/61	0/2/2/2
23	CLA	c	514	-	1/1/15/20	10/39/115/115	-
26	SQD	f	102	-	-	9/38/58/69	0/1/1/1
23	CLA	b	601	-	1/1/15/20	15/39/115/115	-
23	CLA	b	603	-	1/1/15/20	6/39/115/115	-
32	LMT	I	101	-	-	16/21/61/61	0/2/2/2
27	GOL	O	501	-	-	2/4/4/4	-
27	GOL	a	801	-	-	1/4/4/4	-
37	LHG	d	408	-	-	12/53/53/53	-
40	HEC	v	202	-	-	6/14/54/54	-
27	GOL	D	701	-	-	4/4/4/4	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
32	LMT	b	627	-	-	10/17/37/61	0/1/1/2
23	CLA	B	604	-	1/1/15/20	1/39/115/115	-
27	GOL	A	701	-	-	0/4/4/4	-
23	CLA	C	514	-	1/1/15/20	7/39/115/115	-
33	LMG	C	501	-	-	14/46/66/70	0/1/1/1
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	A	408	-	1/1/15/20	8/39/115/115	-
23	CLA	c	511	-	1/1/15/20	8/39/115/115	-
33	LMG	C	520	-	-	9/46/66/70	0/1/1/1
34	HTG	b	622	-	-	6/10/30/30	0/1/1/1
26	SQD	b	620	-	-	17/49/69/69	0/1/1/1
23	CLA	C	509	-	1/1/15/20	2/39/115/115	-
33	LMG	D	415	-	-	7/46/66/70	0/1/1/1
29	PL9	a	416	-	-	14/53/73/73	0/1/1/1
33	LMG	Z	101	-	-	9/31/51/70	0/1/1/1
23	CLA	B	614	-	1/1/15/20	11/39/115/115	-
23	CLA	B	602	-	1/1/15/20	9/39/115/115	-
23	CLA	B	610	-	1/1/15/20	7/39/115/115	-
25	BCR	D	407	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	609	-	1/1/15/20	1/39/115/115	-
23	CLA	c	504	-	1/1/15/20	2/39/115/115	-
27	GOL	B	624	-	-	4/4/4/4	-
23	CLA	C	512	-	1/1/15/20	4/39/115/115	-
23	CLA	B	612	-	1/1/15/20	5/39/115/115	-
27	GOL	C	523	-	-	0/4/4/4	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
35	DGD	C	519	-	-	15/51/91/95	0/2/2/2
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
27	GOL	d	801	-	-	2/4/4/4	-
23	CLA	C	504	-	1/1/15/20	2/39/115/115	-
29	PL9	d	405	-	-	6/53/73/73	0/1/1/1
34	HTG	C	522	-	-	0/10/30/30	0/1/1/1
26	SQD	a	413	-	-	11/49/69/69	0/1/1/1
27	GOL	c	743	-	-	3/4/4/4	-
27	GOL	o	501	-	-	2/4/4/4	-
24	PHO	A	407	-	-	0/37/103/103	0/5/6/6
26	SQD	A	412	-	-	14/49/69/69	0/1/1/1
33	LMG	a	419	-	-	13/46/66/70	0/1/1/1
34	HTG	B	626	-	-	5/10/30/30	0/1/1/1
26	SQD	F	101	-	-	15/38/58/69	0/1/1/1
37	LHG	d	711	-	-	15/53/53/53	-
32	LMT	e	102	-	-	15/21/61/61	0/2/2/2
32	LMT	M	103	-	-	7/21/61/61	0/2/2/2
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
25	BCR	d	404	-	-	6/29/63/63	0/2/2/2
23	CLA	B	615	-	1/1/15/20	5/39/115/115	-
34	HTG	b	623	-	-	4/10/30/30	0/1/1/1
29	PL9	A	414	-	-	14/53/73/73	0/1/1/1
23	CLA	d	402	-	1/1/15/20	4/39/115/115	-
33	LMG	m	101	-	-	12/46/66/70	0/1/1/1
23	CLA	b	610	-	1/1/15/20	6/39/115/115	-
27	GOL	v	401	-	-	2/4/4/4	-
32	LMT	t	102	-	-	9/17/38/61	0/1/1/2
35	DGD	c	518	-	-	16/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	d	412	-	-	10/46/66/70	0/1/1/1
23	CLA	b	602	-	1/1/15/20	4/39/115/115	-
23	CLA	C	511	-	1/1/15/20	13/39/115/115	-
24	PHO	a	353	-	-	1/37/103/103	0/5/6/6
23	CLA	b	609	-	1/1/15/20	2/39/115/115	-
27	GOL	V	401	-	-	2/4/4/4	-
35	DGD	h	102	-	-	13/51/91/95	0/2/2/2
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
23	CLA	a	405	-	1/1/15/20	4/39/115/115	-
35	DGD	c	517	-	-	17/51/91/95	0/2/2/2
23	CLA	C	507	-	1/1/15/20	12/39/115/115	-
23	CLA	B	611	-	1/1/15/20	2/39/115/115	-
23	CLA	a	407	-	-	6/39/115/115	-
27	GOL	B	901	-	-	2/4/4/4	-
27	GOL	a	701	-	-	2/4/4/4	-
33	LMG	z	101	-	-	9/34/54/70	0/1/1/1
37	LHG	D	410	-	-	17/53/53/53	-
23	CLA	b	615	-	1/1/15/20	7/39/115/115	-
23	CLA	A	405	-	1/1/15/20	1/39/115/115	-
35	DGD	C	518	-	-	12/51/91/95	0/2/2/2
38	HEM	E	103	-	-	6/14/54/54	-
33	LMG	B	621	-	-	20/46/66/70	0/1/1/1
40	HEC	V	202	-	-	6/14/54/54	-
23	CLA	B	603	-	1/1/15/20	6/39/115/115	-
23	CLA	A	404	-	1/1/15/20	3/39/115/115	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
37	LHG	l	101	-	-	15/53/53/53	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
34	HTG	B	623	-	-	2/10/30/30	0/1/1/1
23	CLA	a	406	-	1/1/15/20	4/39/115/115	-
23	CLA	c	503	-	1/1/15/20	5/39/115/115	-
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
32	LMT	M	101	-	-	5/21/61/61	0/2/2/2
23	CLA	B	601	-	1/1/15/20	12/39/115/115	-
25	BCR	h	101	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	606	-	1/1/15/20	8/39/115/115	-
24	PHO	A	353	-	-	1/37/103/103	0/5/6/6
32	LMT	A	359	-	-	7/21/61/61	0/2/2/2
27	GOL	A	411	-	-	2/4/4/4	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
34	HTG	c	522	-	-	1/10/30/30	0/1/1/1
27	GOL	c	742	-	-	0/4/4/4	-
23	CLA	C	503	-	1/1/15/20	11/39/115/115	-
23	CLA	B	607	-	1/1/15/20	3/39/115/115	-
23	CLA	c	505	-	1/1/15/20	5/39/115/115	-
34	HTG	d	411	-	-	1/7/27/30	0/1/1/1
32	LMT	b	621	-	-	8/17/37/61	0/1/1/2
25	BCR	H	101	-	-	1/29/63/63	0/2/2/2
25	BCR	y	101	-	-	3/29/63/63	0/2/2/2
33	LMG	c	521	-	-	10/46/66/70	0/1/1/1
35	DGD	c	519	-	-	11/51/91/95	0/2/2/2
23	CLA	b	606	-	1/1/15/20	11/39/115/115	-
23	CLA	B	616	-	1/1/15/20	6/39/115/115	-
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
23	CLA	c	506	-	1/1/15/20	6/39/115/115	-
37	LHG	D	411	-	-	13/53/53/53	-
37	LHG	L	101	-	-	20/53/53/53	-
27	GOL	d	701	-	-	2/4/4/4	-
37	LHG	D	409	-	-	14/53/53/53	-
23	CLA	b	616	-	1/1/15/20	9/39/115/115	-
23	CLA	C	505	-	1/1/15/20	8/39/115/115	-
23	CLA	c	510	-	1/1/15/20	14/39/115/115	-
26	SQD	a	411	-	-	9/49/69/69	0/1/1/1
33	LMG	C	521	-	-	13/46/66/70	0/1/1/1
23	CLA	b	614	-	1/1/15/20	11/39/115/115	-
35	DGD	C	517	-	-	15/51/91/95	0/2/2/2
23	CLA	C	506	-	1/1/15/20	6/39/115/115	-
23	CLA	d	403	-	1/1/15/20	8/39/115/115	-
32	LMT	t	101	-	-	11/17/37/61	0/1/1/2
25	BCR	a	410	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMT	m	103	-	-	7/21/61/61	0/2/2/2
27	GOL	a	412	-	-	4/4/4/4	-
32	LMT	a	414	-	-	10/21/61/61	0/2/2/2
23	CLA	b	605	-	1/1/15/20	5/39/115/115	-
38	HEM	e	87	-	-	6/14/54/54	-
23	CLA	c	508	-	1/1/15/20	7/39/115/115	-
23	CLA	c	512	-	1/1/15/20	5/39/115/115	-
23	CLA	b	608	-	-	5/39/115/115	-
27	GOL	O	601	-	-	2/4/4/4	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
25	BCR	t	103	-	-	0/29/63/63	0/2/2/2
37	LHG	E	101	-	-	21/46/46/53	-
32	LMT	a	420	-	-	11/21/61/61	0/2/2/2
27	GOL	o	601	-	-	4/4/4/4	-
27	GOL	b	901	-	-	0/4/4/4	-
33	LMG	c	520	-	-	11/46/66/70	0/1/1/1
23	CLA	B	613	-	1/1/15/20	8/39/115/115	-
23	CLA	c	509	-	1/1/15/20	4/39/115/115	-
23	CLA	C	508	-	1/1/15/20	10/39/115/115	-
23	CLA	b	604	-	1/1/15/20	12/39/115/115	-
23	CLA	b	607	-	1/1/15/20	2/39/115/115	-
25	BCR	c	516	-	-	1/29/63/63	0/2/2/2
25	BCR	c	515	-	-	2/29/63/63	0/2/2/2
23	CLA	c	502	-	1/1/15/20	3/39/115/115	-
37	LHG	d	407	-	-	12/53/53/53	-
23	CLA	B	605	-	1/1/15/20	3/39/115/115	-
37	LHG	e	101	-	-	16/46/46/53	-
23	CLA	B	608	-	-	4/39/115/115	-
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
26	SQD	A	410	-	-	12/49/69/69	0/1/1/1
23	CLA	D	405	-	1/1/15/20	2/39/115/115	-
23	CLA	a	409	-	1/1/15/20	10/39/115/115	-
24	PHO	a	408	-	-	6/37/103/103	0/5/6/6

All (1593) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408	PHO	C1B-C2B	9.37	1.49	1.39
24	A	407	PHO	C1D-C2D	9.05	1.49	1.39
24	a	353	PHO	C1B-C2B	8.84	1.49	1.39
24	A	353	PHO	C1B-C2B	8.80	1.49	1.39
24	a	353	PHO	C1D-C2D	8.76	1.49	1.39
24	A	353	PHO	C1D-C2D	8.67	1.49	1.39
24	A	407	PHO	C1B-C2B	8.59	1.48	1.39
24	a	408	PHO	C1D-C2D	8.55	1.48	1.39
24	a	353	PHO	C3B-C4B	8.28	1.49	1.41
24	A	353	PHO	C3B-C4B	8.05	1.49	1.41
24	a	408	PHO	C3B-C4B	7.53	1.49	1.41
40	V	202	HEC	CAC-C3C	7.04	1.57	1.35
24	a	408	PHO	C4D-CHA	7.01	1.50	1.39
24	A	407	PHO	C3B-C4B	6.95	1.48	1.41
23	B	611	CLA	CMB-C2B	6.94	1.65	1.50
40	v	202	HEC	CAC-C3C	6.81	1.57	1.35
24	A	353	PHO	C4D-CHA	6.72	1.49	1.39
24	A	407	PHO	C4D-CHA	6.57	1.49	1.39
24	a	408	PHO	C3B-C2B	6.55	1.49	1.40
23	B	611	CLA	C1B-C2B	6.49	1.58	1.43
24	a	353	PHO	C4D-CHA	6.48	1.49	1.39
40	v	202	HEC	CAB-C3B	6.47	1.56	1.35
40	V	202	HEC	CAB-C3B	6.32	1.55	1.35
24	A	407	PHO	C3B-C2B	6.28	1.48	1.40
23	B	611	CLA	C1D-ND	6.15	1.45	1.37
24	A	353	PHO	C3B-C2B	6.09	1.48	1.40
24	a	353	PHO	C3B-C2B	6.02	1.48	1.40
40	v	202	HEC	C3D-C2D	5.75	1.53	1.38
24	a	353	PHO	OBD-CAD	5.65	1.29	1.22
24	A	353	PHO	OBD-CAD	5.63	1.29	1.22
24	a	353	PHO	C3D-C2D	5.62	1.49	1.39
24	a	408	PHO	C3D-C2D	5.61	1.49	1.39
23	B	611	CLA	CHC-C1C	5.54	1.49	1.38
23	B	610	CLA	C3C-C2C	5.54	1.48	1.36
23	B	611	CLA	C3C-C2C	5.53	1.48	1.36
23	a	406	CLA	C3C-C2C	5.48	1.48	1.36
24	A	353	PHO	C3D-C2D	5.48	1.49	1.39
23	D	406	CLA	C3C-C2C	5.47	1.48	1.36
23	c	513	CLA	C3C-C2C	5.41	1.48	1.36
23	C	510	CLA	C3C-C2C	5.41	1.48	1.36
23	c	509	CLA	C3C-C2C	5.40	1.48	1.36
23	c	510	CLA	C3C-C2C	5.39	1.48	1.36
23	c	509	CLA	C1D-ND	5.39	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	403	CLA	C3C-C2C	5.38	1.48	1.36
23	c	504	CLA	C3C-C2C	5.36	1.48	1.36
23	b	605	CLA	C3C-C2C	5.35	1.48	1.36
23	c	503	CLA	C3C-C2C	5.35	1.48	1.36
23	C	504	CLA	C3C-C2C	5.35	1.48	1.36
23	A	404	CLA	C3C-C2C	5.33	1.48	1.36
40	V	202	HEC	C3D-C2D	5.32	1.52	1.38
23	B	605	CLA	C3C-C2C	5.30	1.48	1.36
23	c	505	CLA	O2D-CGD	5.30	1.46	1.33
23	C	513	CLA	C3C-C2C	5.27	1.48	1.36
23	b	612	CLA	C3C-C2C	5.27	1.48	1.36
23	B	603	CLA	C3C-C2C	5.26	1.48	1.36
23	C	508	CLA	C3C-C2C	5.25	1.48	1.36
23	b	606	CLA	C3C-C2C	5.25	1.48	1.36
23	b	601	CLA	C3C-C2C	5.23	1.48	1.36
23	C	511	CLA	C1D-ND	5.23	1.44	1.37
23	a	409	CLA	CHC-C1C	5.22	1.48	1.38
23	B	601	CLA	C3C-C2C	5.22	1.48	1.36
23	b	614	CLA	C3C-C2C	5.22	1.48	1.36
23	c	510	CLA	O2D-CGD	5.21	1.46	1.33
23	C	502	CLA	C3C-C2C	5.21	1.48	1.36
23	a	407	CLA	C3C-C2C	5.21	1.48	1.36
23	D	405	CLA	C3C-C2C	5.21	1.48	1.36
23	C	509	CLA	C3C-C2C	5.20	1.48	1.36
23	B	606	CLA	CHC-C1C	5.20	1.48	1.38
23	a	409	CLA	C3C-C2C	5.20	1.48	1.36
23	C	512	CLA	O2D-CGD	5.19	1.46	1.33
23	c	514	CLA	C3C-C2C	5.19	1.48	1.36
24	a	408	PHO	O2D-CGD	5.19	1.46	1.33
23	C	513	CLA	CHC-C1C	5.18	1.48	1.38
23	b	611	CLA	C3C-C2C	5.18	1.47	1.36
23	C	511	CLA	C3C-C2C	5.18	1.47	1.36
23	c	509	CLA	O2D-CGD	5.18	1.46	1.33
23	B	614	CLA	C3C-C2C	5.18	1.47	1.36
23	c	509	CLA	CHC-C1C	5.17	1.48	1.38
23	B	605	CLA	O2D-CGD	5.17	1.45	1.33
23	B	604	CLA	CHC-C1C	5.17	1.48	1.38
23	b	609	CLA	O2D-CGD	5.17	1.45	1.33
23	c	506	CLA	C3C-C2C	5.17	1.47	1.36
38	e	87	HEM	FE-NB	5.16	2.10	1.94
23	b	615	CLA	C3C-C2C	5.15	1.47	1.36
23	B	604	CLA	C3C-C2C	5.15	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	C3C-C2C	5.15	1.47	1.36
23	C	507	CLA	O2D-CGD	5.15	1.45	1.33
23	B	606	CLA	C3C-C2C	5.15	1.47	1.36
23	c	514	CLA	C1D-ND	5.14	1.44	1.37
23	C	508	CLA	CHC-C1C	5.12	1.48	1.38
23	d	403	CLA	CHC-C1C	5.10	1.48	1.38
23	B	612	CLA	C3C-C2C	5.10	1.47	1.36
23	A	405	CLA	O2D-CGD	5.09	1.45	1.33
23	D	406	CLA	C1D-ND	5.07	1.44	1.37
23	c	503	CLA	C1D-ND	5.07	1.44	1.37
23	b	602	CLA	C3C-C2C	5.07	1.47	1.36
23	b	610	CLA	C3C-C2C	5.06	1.47	1.36
23	b	602	CLA	O2D-CGD	5.05	1.45	1.33
25	d	404	BCR	C23-C22	-5.05	1.35	1.46
23	b	607	CLA	C3C-C2C	5.05	1.47	1.36
25	C	515	BCR	C23-C22	-5.04	1.35	1.46
23	A	406	CLA	C3C-C2C	5.04	1.47	1.36
23	B	609	CLA	C3C-C2C	5.04	1.47	1.36
23	A	406	CLA	CHC-C1C	5.03	1.48	1.38
23	b	613	CLA	CHC-C1C	5.03	1.48	1.38
25	k	101	BCR	C23-C22	-5.03	1.35	1.46
23	c	512	CLA	C3C-C2C	5.02	1.47	1.36
23	c	506	CLA	CHC-C1C	5.02	1.48	1.38
23	C	514	CLA	C3C-C2C	5.02	1.47	1.36
23	B	613	CLA	CHC-C1C	5.02	1.48	1.38
23	A	408	CLA	C3C-C2C	5.01	1.47	1.36
23	a	406	CLA	C1D-ND	5.01	1.44	1.37
23	C	506	CLA	CHC-C1C	5.01	1.48	1.38
23	c	512	CLA	C1D-ND	5.01	1.44	1.37
23	c	514	CLA	O2D-CGD	5.01	1.45	1.33
23	b	603	CLA	O2D-CGD	5.00	1.45	1.33
23	B	613	CLA	O2D-CGD	5.00	1.45	1.33
23	b	616	CLA	CHC-C1C	5.00	1.48	1.38
23	d	402	CLA	C3C-C2C	5.00	1.47	1.36
23	B	613	CLA	C3C-C2C	4.99	1.47	1.36
23	C	503	CLA	O2D-CGD	4.99	1.45	1.33
23	b	601	CLA	C1D-ND	4.99	1.44	1.37
23	c	507	CLA	O2D-CGD	4.99	1.45	1.33
23	c	511	CLA	C3C-C2C	4.99	1.47	1.36
23	b	613	CLA	O2D-CGD	4.98	1.45	1.33
23	B	615	CLA	C3C-C2C	4.98	1.47	1.36
23	B	601	CLA	CHC-C1C	4.98	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	C3C-C2C	4.98	1.47	1.36
23	b	602	CLA	CHC-C1C	4.97	1.48	1.38
23	B	601	CLA	O2D-CGD	4.96	1.45	1.33
23	B	601	CLA	O2A-CGA	4.95	1.47	1.33
23	c	513	CLA	CHC-C1C	4.95	1.48	1.38
23	C	506	CLA	C3C-C2C	4.95	1.47	1.36
23	c	502	CLA	C3C-C2C	4.94	1.47	1.36
25	D	407	BCR	C23-C22	-4.94	1.35	1.46
23	b	603	CLA	C3C-C2C	4.94	1.47	1.36
23	c	507	CLA	C3C-C2C	4.93	1.47	1.36
23	c	503	CLA	O2D-CGD	4.93	1.45	1.33
23	a	405	CLA	C3C-C2C	4.93	1.47	1.36
23	c	505	CLA	C3C-C2C	4.93	1.47	1.36
23	d	403	CLA	C1D-ND	4.93	1.44	1.37
23	C	509	CLA	O2D-CGD	4.92	1.45	1.33
23	B	607	CLA	C3C-C2C	4.91	1.47	1.36
24	A	407	PHO	C3D-C2D	4.91	1.48	1.39
23	b	604	CLA	C1D-ND	4.91	1.44	1.37
23	c	504	CLA	CHC-C1C	4.91	1.48	1.38
23	C	502	CLA	CHC-C1C	4.91	1.48	1.38
23	b	615	CLA	CHC-C1C	4.91	1.48	1.38
23	a	406	CLA	O2D-CGD	4.90	1.45	1.33
24	A	353	PHO	O2D-CGD	4.90	1.45	1.33
23	C	514	CLA	O2D-CGD	4.90	1.45	1.33
23	B	616	CLA	C3C-C2C	4.90	1.47	1.36
23	B	602	CLA	C3C-C2C	4.89	1.47	1.36
23	c	513	CLA	O2D-CGD	4.89	1.45	1.33
23	b	610	CLA	O2D-CGD	4.88	1.45	1.33
23	b	613	CLA	C3C-C2C	4.88	1.47	1.36
23	b	614	CLA	CHC-C1C	4.88	1.48	1.38
23	b	603	CLA	CHC-C1C	4.88	1.48	1.38
23	B	609	CLA	O2D-CGD	4.88	1.45	1.33
23	C	503	CLA	C1D-ND	4.88	1.44	1.37
23	c	512	CLA	O2D-CGD	4.87	1.45	1.33
23	A	405	CLA	C3C-C2C	4.87	1.47	1.36
23	b	616	CLA	O2D-CGD	4.86	1.45	1.33
23	c	508	CLA	O2D-CGD	4.86	1.45	1.33
23	B	601	CLA	C1D-ND	4.86	1.44	1.37
24	A	407	PHO	O2D-CGD	4.86	1.45	1.33
23	B	609	CLA	CHC-C1C	4.86	1.48	1.38
23	b	609	CLA	C3C-C2C	4.86	1.47	1.36
23	C	505	CLA	C3C-C2C	4.85	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	C1D-ND	4.85	1.44	1.37
25	C	516	BCR	C23-C22	-4.85	1.35	1.46
25	K	102	BCR	C23-C22	-4.84	1.35	1.46
23	C	505	CLA	O2D-CGD	4.83	1.45	1.33
23	D	405	CLA	O2D-CGD	4.83	1.45	1.33
23	c	511	CLA	O2D-CGD	4.82	1.45	1.33
23	D	406	CLA	O2D-CGD	4.82	1.45	1.33
25	c	516	BCR	C23-C22	-4.82	1.35	1.46
23	B	612	CLA	CHC-C1C	4.82	1.48	1.38
23	C	506	CLA	O2D-CGD	4.81	1.45	1.33
23	c	514	CLA	CHC-C1C	4.81	1.48	1.38
25	B	619	BCR	C23-C22	-4.80	1.35	1.46
23	B	606	CLA	O2D-CGD	4.80	1.45	1.33
23	B	615	CLA	O2D-CGD	4.80	1.45	1.33
23	B	603	CLA	O2D-CGD	4.80	1.45	1.33
23	b	601	CLA	O2A-CGA	4.79	1.47	1.33
24	a	353	PHO	O2D-CGD	4.79	1.45	1.33
23	B	611	CLA	O2D-CGD	4.79	1.45	1.33
23	b	610	CLA	CHC-C1C	4.79	1.48	1.38
23	c	510	CLA	C1D-ND	4.79	1.44	1.37
23	B	616	CLA	O2D-CGD	4.78	1.45	1.33
25	y	101	BCR	C23-C22	-4.77	1.35	1.46
23	C	507	CLA	C3C-C2C	4.77	1.47	1.36
23	c	508	CLA	C3C-C2C	4.77	1.47	1.36
23	c	505	CLA	C1D-ND	4.77	1.44	1.37
25	b	619	BCR	C23-C22	-4.77	1.35	1.46
23	b	601	CLA	O2D-CGD	4.76	1.44	1.33
23	c	502	CLA	C1D-ND	4.76	1.44	1.37
23	B	610	CLA	O2D-CGD	4.76	1.44	1.33
23	C	511	CLA	O2D-CGD	4.75	1.44	1.33
23	B	602	CLA	C1D-ND	4.75	1.44	1.37
25	T	101	BCR	C23-C22	-4.74	1.35	1.46
23	b	606	CLA	CHC-C1C	4.74	1.48	1.38
23	a	405	CLA	C1D-ND	4.74	1.44	1.37
23	C	513	CLA	O2D-CGD	4.74	1.44	1.33
23	A	404	CLA	C1D-ND	4.74	1.44	1.37
23	b	606	CLA	C1D-ND	4.73	1.44	1.37
23	B	608	CLA	C3C-C2C	4.73	1.47	1.36
23	a	405	CLA	CHC-C1C	4.72	1.47	1.38
23	A	404	CLA	O2D-CGD	4.72	1.44	1.33
23	c	513	CLA	C1D-ND	4.72	1.44	1.37
23	C	514	CLA	CHC-C1C	4.72	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	CHC-C1C	4.72	1.47	1.38
23	B	604	CLA	O2D-CGD	4.71	1.44	1.33
23	b	604	CLA	CHC-C1C	4.71	1.47	1.38
23	C	503	CLA	CHC-C1C	4.71	1.47	1.38
38	E	103	HEM	FE-NB	4.71	2.09	1.94
26	F	101	SQD	O47-C7	4.71	1.47	1.34
23	B	606	CLA	C1D-ND	4.71	1.44	1.37
23	b	601	CLA	CHC-C1C	4.71	1.47	1.38
23	b	615	CLA	O2D-CGD	4.71	1.44	1.33
23	b	608	CLA	C3C-C2C	4.70	1.46	1.36
23	A	405	CLA	CHC-C1C	4.69	1.47	1.38
23	a	407	CLA	CHC-C1C	4.69	1.47	1.38
23	c	512	CLA	CHC-C1C	4.69	1.47	1.38
23	B	602	CLA	O2D-CGD	4.69	1.44	1.33
25	b	617	BCR	C23-C22	-4.69	1.35	1.46
23	C	505	CLA	CHC-C1C	4.68	1.47	1.38
23	B	605	CLA	C1D-ND	4.68	1.44	1.37
23	A	406	CLA	O2D-CGD	4.68	1.44	1.33
23	c	502	CLA	CHC-C1C	4.68	1.47	1.38
23	C	510	CLA	O2D-CGD	4.67	1.44	1.33
23	C	504	CLA	CHC-C1C	4.67	1.47	1.38
23	c	513	CLA	CHD-C1D	4.66	1.47	1.38
25	B	617	BCR	C23-C22	-4.66	1.36	1.46
33	c	521	LMG	O7-C10	4.65	1.47	1.34
23	B	607	CLA	CHC-C1C	4.65	1.47	1.38
23	B	605	CLA	CHC-C1C	4.65	1.47	1.38
23	C	512	CLA	C3C-C2C	4.65	1.46	1.36
23	b	611	CLA	CHC-C1C	4.64	1.47	1.38
23	b	614	CLA	O2D-CGD	4.64	1.44	1.33
23	c	508	CLA	C1D-ND	4.64	1.44	1.37
23	a	409	CLA	O2D-CGD	4.63	1.44	1.33
23	b	602	CLA	CHD-C1D	4.63	1.47	1.38
23	b	605	CLA	C1D-ND	4.63	1.43	1.37
23	b	608	CLA	O2D-CGD	4.63	1.44	1.33
23	C	514	CLA	C1D-ND	4.62	1.43	1.37
23	C	506	CLA	C1D-ND	4.62	1.43	1.37
23	D	405	CLA	CHC-C1C	4.62	1.47	1.38
23	b	604	CLA	C3C-C2C	4.62	1.46	1.36
23	A	408	CLA	O2D-CGD	4.61	1.44	1.33
23	D	406	CLA	CHC-C1C	4.61	1.47	1.38
23	C	509	CLA	C1D-ND	4.61	1.43	1.37
23	b	605	CLA	O2D-CGD	4.61	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	407	CLA	O2D-CGD	4.60	1.44	1.33
23	B	616	CLA	CHC-C1C	4.60	1.47	1.38
33	C	521	LMG	O8-C28	4.60	1.46	1.33
23	c	507	CLA	C1D-ND	4.60	1.43	1.37
26	a	413	SQD	O48-C23	4.60	1.46	1.33
23	b	613	CLA	C1D-ND	4.60	1.43	1.37
37	E	101	LHG	O8-C23	4.58	1.46	1.33
23	c	507	CLA	CHC-C1C	4.57	1.47	1.38
23	B	602	CLA	CHC-C1C	4.57	1.47	1.38
23	B	608	CLA	O2D-CGD	4.57	1.44	1.33
26	f	102	SQD	O47-C7	4.57	1.47	1.34
25	t	103	BCR	C23-C22	-4.57	1.36	1.46
33	C	521	LMG	O7-C10	4.57	1.47	1.34
23	B	610	CLA	CHC-C1C	4.57	1.47	1.38
25	c	515	BCR	C23-C22	-4.57	1.36	1.46
23	C	502	CLA	C1D-ND	4.57	1.43	1.37
23	A	404	CLA	CHC-C1C	4.56	1.47	1.38
23	c	505	CLA	CHC-C1C	4.55	1.47	1.38
25	A	409	BCR	C23-C22	-4.55	1.36	1.46
23	c	504	CLA	O2D-CGD	4.55	1.44	1.33
23	d	402	CLA	O2D-CGD	4.54	1.44	1.33
23	B	615	CLA	CHC-C1C	4.54	1.47	1.38
23	b	616	CLA	C1D-ND	4.53	1.43	1.37
23	c	508	CLA	CHC-C1C	4.53	1.47	1.38
23	b	607	CLA	O2D-CGD	4.53	1.44	1.33
23	C	511	CLA	CHC-C1C	4.52	1.47	1.38
23	B	603	CLA	CHC-C1C	4.52	1.47	1.38
23	a	406	CLA	CHC-C1C	4.52	1.47	1.38
23	c	504	CLA	CHD-C1D	4.52	1.47	1.38
23	b	607	CLA	CHC-C1C	4.52	1.47	1.38
37	e	101	LHG	O8-C23	4.51	1.46	1.33
23	c	506	CLA	O2D-CGD	4.51	1.44	1.33
23	B	615	CLA	C1D-ND	4.51	1.43	1.37
23	b	602	CLA	C1D-ND	4.49	1.43	1.37
23	c	514	CLA	CHD-C1D	4.49	1.47	1.38
26	A	412	SQD	O48-C23	4.49	1.46	1.33
33	C	520	LMG	O8-C28	4.48	1.46	1.33
25	h	101	BCR	C23-C22	-4.48	1.36	1.46
23	c	511	CLA	CHC-C1C	4.48	1.47	1.38
26	B	620	SQD	O47-C7	4.47	1.46	1.34
23	C	510	CLA	CHD-C1D	4.47	1.47	1.38
23	b	606	CLA	O2D-CGD	4.46	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	CHD-C1D	4.46	1.47	1.38
23	c	503	CLA	CHC-C1C	4.45	1.47	1.38
23	B	611	CLA	CHC-C4B	4.45	1.49	1.39
23	C	510	CLA	CHC-C1C	4.45	1.47	1.38
25	b	618	BCR	C23-C22	-4.44	1.36	1.46
23	B	603	CLA	C1D-ND	4.44	1.43	1.37
23	C	512	CLA	CHC-C1C	4.43	1.47	1.38
23	c	514	CLA	O2A-CGA	4.43	1.46	1.33
23	C	507	CLA	CHD-C1D	4.43	1.47	1.38
23	B	614	CLA	C1D-ND	4.43	1.43	1.37
23	C	502	CLA	CHD-C1D	4.42	1.47	1.38
23	B	614	CLA	O2D-CGD	4.42	1.44	1.33
25	H	101	BCR	C23-C22	-4.42	1.36	1.46
23	b	612	CLA	CHC-C1C	4.41	1.47	1.38
23	c	509	CLA	O2A-CGA	4.41	1.46	1.33
23	C	504	CLA	O2D-CGD	4.41	1.44	1.33
23	B	612	CLA	CHB-C1B	4.41	1.49	1.39
23	D	406	CLA	CHD-C1D	4.41	1.47	1.38
24	A	407	PHO	OBD-CAD	4.41	1.28	1.22
33	z	101	LMG	O8-C28	4.40	1.46	1.33
23	d	403	CLA	O2A-CGA	4.40	1.46	1.33
33	B	621	LMG	O8-C28	4.38	1.46	1.33
23	a	409	CLA	O2A-CGA	4.38	1.46	1.33
23	b	604	CLA	O2D-CGD	4.37	1.44	1.33
23	c	509	CLA	C3D-C2D	4.36	1.50	1.39
25	Y	101	BCR	C23-C22	-4.36	1.36	1.46
23	a	406	CLA	C3D-C2D	4.36	1.50	1.39
38	E	103	HEM	FE-NC	4.35	2.09	1.95
23	b	612	CLA	O2D-CGD	4.35	1.43	1.33
23	c	510	CLA	CHC-C1C	4.35	1.47	1.38
23	c	513	CLA	O2A-CGA	4.35	1.46	1.33
23	B	610	CLA	C1D-ND	4.34	1.43	1.37
26	b	620	SQD	O47-C7	4.34	1.46	1.34
23	a	405	CLA	O2D-CGD	4.34	1.43	1.33
23	b	605	CLA	CHC-C1C	4.34	1.47	1.38
23	B	614	CLA	C4B-NB	-4.34	1.32	1.37
23	C	510	CLA	C1D-ND	4.33	1.43	1.37
23	C	512	CLA	C1D-ND	4.33	1.43	1.37
23	C	508	CLA	O2D-CGD	4.33	1.43	1.33
23	b	604	CLA	CHD-C1D	4.32	1.46	1.38
26	B	620	SQD	O48-C23	4.32	1.45	1.33
23	B	609	CLA	CHD-C1D	4.31	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	620	SQD	O48-C23	4.31	1.45	1.33
23	c	511	CLA	C1D-ND	4.31	1.43	1.37
23	c	512	CLA	CHD-C1D	4.30	1.46	1.38
23	c	507	CLA	O2A-CGA	4.30	1.45	1.33
23	b	602	CLA	CHD-C4C	4.30	1.49	1.39
23	B	615	CLA	CHD-C1D	4.30	1.46	1.38
23	b	611	CLA	O2D-CGD	4.30	1.43	1.33
37	e	101	LHG	O7-C7	4.28	1.46	1.34
23	d	402	CLA	CHC-C1C	4.28	1.47	1.38
23	C	513	CLA	C1D-ND	4.28	1.43	1.37
23	d	403	CLA	CHD-C1D	4.28	1.46	1.38
23	C	508	CLA	C1D-ND	4.27	1.43	1.37
23	c	510	CLA	CHD-C1D	4.27	1.46	1.38
23	A	408	CLA	O2A-CGA	4.27	1.45	1.33
23	B	614	CLA	CHC-C1C	4.27	1.47	1.38
23	C	506	CLA	CHD-C1D	4.27	1.46	1.38
33	m	101	LMG	O8-C28	4.27	1.45	1.33
23	b	606	CLA	CHD-C1D	4.27	1.46	1.38
23	c	507	CLA	CHD-C1D	4.26	1.46	1.38
23	C	514	CLA	O2A-CGA	4.25	1.45	1.33
23	C	509	CLA	C3D-C2D	4.25	1.50	1.39
33	c	521	LMG	O8-C28	4.24	1.45	1.33
23	B	609	CLA	C1D-ND	4.24	1.43	1.37
23	C	509	CLA	O2A-CGA	4.24	1.45	1.33
23	c	510	CLA	C1B-NB	-4.24	1.32	1.37
35	C	519	DGD	O1G-C1A	4.24	1.45	1.33
23	c	512	CLA	O2A-CGA	4.23	1.45	1.33
23	b	614	CLA	C1D-ND	4.23	1.43	1.37
23	C	507	CLA	C1D-ND	4.23	1.43	1.37
35	c	519	DGD	O1G-C1A	4.23	1.45	1.33
23	c	504	CLA	CHD-C4C	4.23	1.48	1.39
23	b	601	CLA	CHD-C1D	4.23	1.46	1.38
25	a	410	BCR	C23-C22	-4.23	1.36	1.46
23	D	406	CLA	C3D-C2D	4.22	1.50	1.39
38	e	87	HEM	FE-NC	4.22	2.09	1.95
23	C	509	CLA	CHD-C1D	4.22	1.46	1.38
23	C	502	CLA	O2D-CGD	4.22	1.43	1.33
37	E	101	LHG	O7-C7	4.22	1.46	1.34
23	c	514	CLA	CHD-C4C	4.22	1.48	1.39
23	C	512	CLA	O2A-CGA	4.21	1.45	1.33
23	B	606	CLA	O2A-CGA	4.21	1.45	1.33
23	B	611	CLA	C4B-NB	-4.20	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	CHB-C1B	4.20	1.48	1.39
37	d	408	LHG	O8-C23	4.20	1.45	1.33
23	B	602	CLA	CHD-C1D	4.20	1.46	1.38
23	C	508	CLA	O2A-CGA	4.20	1.45	1.33
23	A	405	CLA	C1D-ND	4.20	1.43	1.37
23	A	408	CLA	CHD-C1D	4.20	1.46	1.38
23	B	613	CLA	C1D-ND	4.19	1.43	1.37
26	f	102	SQD	O48-C23	4.19	1.45	1.33
23	C	504	CLA	C1D-ND	4.19	1.43	1.37
23	D	405	CLA	O2A-CGA	4.19	1.45	1.33
23	B	604	CLA	C1D-ND	4.18	1.43	1.37
23	b	610	CLA	CHD-C1D	4.18	1.46	1.38
23	B	613	CLA	CHB-C1B	4.18	1.48	1.39
23	b	611	CLA	C1D-ND	4.18	1.43	1.37
23	C	507	CLA	CHC-C1C	4.18	1.46	1.38
23	c	509	CLA	CHD-C1D	4.17	1.46	1.38
23	A	408	CLA	CHC-C1C	4.17	1.46	1.38
23	C	513	CLA	CHD-C1D	4.17	1.46	1.38
23	B	607	CLA	O2D-CGD	4.17	1.43	1.33
23	b	608	CLA	CHC-C1C	4.17	1.46	1.38
33	a	419	LMG	O8-C28	4.16	1.45	1.33
23	c	502	CLA	CHD-C1D	4.16	1.46	1.38
23	B	611	CLA	O2A-CGA	4.16	1.45	1.33
23	D	405	CLA	CHD-C1D	4.16	1.46	1.38
23	A	405	CLA	C3D-C2D	4.15	1.50	1.39
23	B	613	CLA	CHD-C1D	4.15	1.46	1.38
23	C	509	CLA	CHC-C1C	4.15	1.46	1.38
26	F	101	SQD	O48-C23	4.15	1.45	1.33
23	C	503	CLA	C3D-C2D	4.15	1.50	1.39
23	b	602	CLA	CHC-C4B	4.15	1.48	1.39
23	B	608	CLA	C3D-C2D	4.15	1.50	1.39
23	b	609	CLA	CHB-C1B	4.14	1.48	1.39
23	B	615	CLA	O2A-CGA	4.14	1.45	1.33
23	c	506	CLA	C1D-ND	4.14	1.43	1.37
23	C	512	CLA	CHD-C1D	4.14	1.46	1.38
23	C	502	CLA	O2A-CGA	4.14	1.45	1.33
23	B	614	CLA	CHB-C1B	4.14	1.48	1.39
33	Z	101	LMG	O7-C10	4.14	1.46	1.34
23	a	407	CLA	C1D-ND	4.13	1.43	1.37
35	C	517	DGD	O2G-C1B	4.13	1.46	1.34
23	C	505	CLA	C1D-ND	4.13	1.43	1.37
24	a	408	PHO	OBD-CAD	4.13	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	CHD-C1D	4.13	1.46	1.38
23	a	406	CLA	O2A-CGA	4.13	1.45	1.33
23	b	601	CLA	CHD-C4C	4.13	1.48	1.39
23	a	405	CLA	CHD-C4C	4.12	1.48	1.39
23	b	612	CLA	OBD-CAD	4.12	1.29	1.22
23	C	513	CLA	O2A-CGA	4.12	1.45	1.33
23	b	609	CLA	C1D-ND	4.12	1.43	1.37
23	b	615	CLA	C1D-ND	4.12	1.43	1.37
23	A	406	CLA	C1B-NB	-4.11	1.32	1.37
23	B	609	CLA	C3D-C2D	4.11	1.50	1.39
23	C	514	CLA	CHD-C1D	4.11	1.46	1.38
23	b	607	CLA	CHD-C1D	4.11	1.46	1.38
23	C	503	CLA	CHD-C1D	4.10	1.46	1.38
23	C	508	CLA	CHD-C1D	4.10	1.46	1.38
23	c	506	CLA	CHD-C1D	4.10	1.46	1.38
23	c	513	CLA	CHD-C4C	4.10	1.48	1.39
26	a	413	SQD	O47-C7	4.09	1.45	1.34
23	b	601	CLA	C3D-C2D	4.09	1.50	1.39
23	d	403	CLA	O2D-CGD	4.09	1.43	1.33
23	b	611	CLA	O2A-CGA	4.09	1.45	1.33
23	c	503	CLA	CHD-C1D	4.09	1.46	1.38
23	B	609	CLA	O2A-CGA	4.08	1.45	1.33
23	b	608	CLA	O2A-CGA	4.08	1.45	1.33
23	a	405	CLA	CHD-C1D	4.08	1.46	1.38
23	A	405	CLA	O2A-CGA	4.08	1.45	1.33
23	C	506	CLA	CHD-C4C	4.08	1.48	1.39
23	C	504	CLA	CHD-C1D	4.08	1.46	1.38
23	c	503	CLA	O2A-CGA	4.07	1.45	1.33
23	c	504	CLA	CHB-C1B	4.07	1.48	1.39
33	C	501	LMG	O8-C28	4.07	1.45	1.33
23	A	406	CLA	CHD-C1D	4.07	1.46	1.38
23	B	602	CLA	CHD-C4C	4.07	1.48	1.39
23	B	608	CLA	CHD-C1D	4.07	1.46	1.38
23	b	610	CLA	C1D-ND	4.06	1.43	1.37
23	C	510	CLA	C3D-C2D	4.06	1.50	1.39
23	B	604	CLA	CHD-C4C	4.06	1.48	1.39
23	C	507	CLA	O2A-CGA	4.06	1.45	1.33
33	c	520	LMG	O7-C10	4.06	1.45	1.34
23	C	512	CLA	CHD-C4C	4.06	1.48	1.39
23	C	509	CLA	CHB-C1B	4.05	1.48	1.39
23	c	505	CLA	C3D-C2D	4.05	1.50	1.39
26	a	411	SQD	O47-C7	4.05	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	520	LMG	O8-C28	4.05	1.45	1.33
23	C	513	CLA	C3D-C2D	4.05	1.50	1.39
23	B	611	CLA	C3B-C2B	4.04	1.54	1.41
23	b	616	CLA	O2A-CGA	4.04	1.45	1.33
23	c	502	CLA	O2D-CGD	4.04	1.43	1.33
23	C	513	CLA	CHC-C4B	4.04	1.48	1.39
23	c	504	CLA	O2A-CGA	4.04	1.45	1.33
23	B	601	CLA	CHC-C4B	4.04	1.48	1.39
33	a	419	LMG	O7-C10	4.03	1.45	1.34
23	b	603	CLA	CHD-C1D	4.03	1.46	1.38
23	c	512	CLA	CHB-C1B	4.03	1.48	1.39
23	B	616	CLA	O2A-CGA	4.03	1.45	1.33
23	c	506	CLA	CHC-C4B	4.03	1.48	1.39
23	B	606	CLA	CHD-C1D	4.03	1.46	1.38
33	z	101	LMG	O7-C10	4.03	1.45	1.34
23	B	613	CLA	C3D-C2D	4.03	1.50	1.39
24	A	353	PHO	O2A-CGA	4.03	1.45	1.33
23	b	613	CLA	C3D-C2D	4.02	1.50	1.39
23	D	405	CLA	CHB-C1B	4.02	1.48	1.39
33	C	501	LMG	O7-C10	4.02	1.45	1.34
23	B	616	CLA	C3D-C2D	4.02	1.49	1.39
23	b	612	CLA	CHB-C1B	4.01	1.48	1.39
23	a	407	CLA	C3D-C2D	4.01	1.49	1.39
23	B	615	CLA	CHB-C1B	4.01	1.48	1.39
33	B	621	LMG	O7-C10	4.01	1.45	1.34
23	a	405	CLA	CHB-C1B	4.01	1.48	1.39
35	c	518	DGD	O1G-C1A	4.01	1.45	1.33
23	b	610	CLA	CHC-C4B	4.01	1.48	1.39
23	B	605	CLA	CHC-C4B	4.01	1.48	1.39
23	c	503	CLA	CHD-C4C	4.01	1.48	1.39
23	c	511	CLA	CHB-C1B	4.00	1.48	1.39
23	C	511	CLA	CHD-C4C	4.00	1.48	1.39
23	c	508	CLA	O2A-CGA	4.00	1.45	1.33
23	b	609	CLA	CHD-C1D	4.00	1.46	1.38
23	A	406	CLA	C3D-C2D	4.00	1.49	1.39
23	C	503	CLA	O2A-CGA	4.00	1.45	1.33
23	b	616	CLA	CHD-C1D	4.00	1.46	1.38
23	B	613	CLA	OBD-CAD	4.00	1.29	1.22
23	c	509	CLA	OBD-CAD	4.00	1.29	1.22
23	C	505	CLA	CHB-C1B	4.00	1.48	1.39
23	b	606	CLA	CHD-C4C	3.99	1.48	1.39
23	b	615	CLA	CHD-C1D	3.99	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	408	CLA	C1D-ND	3.99	1.43	1.37
23	B	602	CLA	CHB-C1B	3.99	1.48	1.39
23	c	504	CLA	CHC-C4B	3.99	1.48	1.39
23	C	504	CLA	CHD-C4C	3.99	1.48	1.39
23	c	506	CLA	CHB-C1B	3.99	1.48	1.39
23	d	402	CLA	CHB-C1B	3.99	1.48	1.39
23	B	601	CLA	CHD-C1D	3.99	1.46	1.38
33	C	520	LMG	O7-C10	3.99	1.45	1.34
23	b	614	CLA	C3D-C2D	3.99	1.49	1.39
23	C	507	CLA	CHD-C4C	3.98	1.48	1.39
23	B	612	CLA	O2D-CGD	3.98	1.43	1.33
26	a	411	SQD	O48-C23	3.98	1.44	1.33
23	B	602	CLA	O2A-CGA	3.98	1.44	1.33
23	b	608	CLA	CHD-C1D	3.98	1.46	1.38
35	h	102	DGD	O2G-C1B	3.97	1.45	1.34
26	A	412	SQD	O47-C7	3.97	1.45	1.34
23	c	512	CLA	CHD-C4C	3.97	1.48	1.39
23	B	610	CLA	OBD-CAD	3.97	1.29	1.22
23	b	604	CLA	CHC-C4B	3.97	1.48	1.39
23	C	510	CLA	CHD-C4C	3.97	1.48	1.39
23	a	407	CLA	O2A-CGA	3.97	1.44	1.33
23	c	507	CLA	CHD-C4C	3.97	1.48	1.39
23	C	514	CLA	C3D-C2D	3.96	1.49	1.39
23	d	402	CLA	O2A-CGA	3.96	1.44	1.33
23	B	606	CLA	CHC-C4B	3.96	1.48	1.39
23	C	504	CLA	O2A-CGA	3.96	1.44	1.33
23	C	511	CLA	CHB-C1B	3.96	1.48	1.39
23	b	608	CLA	C1D-ND	3.96	1.43	1.37
23	B	603	CLA	CHB-C1B	3.96	1.48	1.39
23	B	611	CLA	CHB-C1B	3.96	1.48	1.39
23	B	608	CLA	C1D-ND	3.95	1.43	1.37
23	c	508	CLA	OBD-CAD	3.95	1.29	1.22
23	A	406	CLA	OBD-CAD	3.95	1.29	1.22
33	d	412	LMG	O8-C28	3.95	1.44	1.33
23	C	502	CLA	CHD-C4C	3.95	1.48	1.39
23	c	503	CLA	C3D-C2D	3.95	1.49	1.39
23	c	502	CLA	O2A-CGA	3.95	1.44	1.33
23	B	607	CLA	CHB-C1B	3.95	1.48	1.39
23	a	409	CLA	CHB-C1B	3.95	1.48	1.39
23	C	502	CLA	CHC-C4B	3.94	1.48	1.39
23	B	609	CLA	CHD-C4C	3.94	1.48	1.39
23	c	505	CLA	O2A-CGA	3.94	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	CHB-C1B	3.94	1.48	1.39
23	d	403	CLA	CHC-C4B	3.94	1.48	1.39
23	A	405	CLA	CHD-C1D	3.94	1.46	1.38
23	c	511	CLA	O2A-CGA	3.94	1.44	1.33
23	C	509	CLA	OBD-CAD	3.94	1.29	1.22
23	b	607	CLA	CHB-C1B	3.94	1.48	1.39
23	c	510	CLA	CHD-C4C	3.93	1.48	1.39
23	B	616	CLA	C1D-ND	3.93	1.43	1.37
23	c	511	CLA	C3D-C2D	3.92	1.49	1.39
37	L	101	LHG	O8-C23	3.92	1.44	1.33
23	C	511	CLA	CHD-C1D	3.92	1.46	1.38
23	D	405	CLA	C1D-ND	3.92	1.43	1.37
23	c	513	CLA	C3D-C2D	3.92	1.49	1.39
23	b	612	CLA	CHD-C1D	3.92	1.46	1.38
23	c	510	CLA	O2A-CGA	3.92	1.44	1.33
37	D	411	LHG	O8-C23	3.91	1.44	1.33
23	B	613	CLA	CHD-C4C	3.91	1.48	1.39
23	B	609	CLA	CHC-C4B	3.91	1.48	1.39
23	c	505	CLA	CHD-C1D	3.91	1.46	1.38
23	b	605	CLA	CHB-C1B	3.91	1.48	1.39
23	c	506	CLA	CHD-C4C	3.91	1.48	1.39
23	a	409	CLA	C1D-ND	3.91	1.43	1.37
23	c	502	CLA	CHD-C4C	3.91	1.48	1.39
23	B	615	CLA	OBD-CAD	3.90	1.29	1.22
23	a	406	CLA	C1B-NB	-3.90	1.32	1.37
37	d	407	LHG	O7-C7	3.90	1.45	1.34
23	d	402	CLA	CHD-C1D	3.89	1.46	1.38
37	D	411	LHG	O7-C7	3.89	1.45	1.34
23	B	608	CLA	CHC-C1C	3.89	1.46	1.38
23	b	609	CLA	C3D-C2D	3.89	1.49	1.39
23	B	612	CLA	CHD-C1D	3.89	1.46	1.38
23	b	602	CLA	C3D-C2D	3.89	1.49	1.39
23	c	502	CLA	C3D-C2D	3.88	1.49	1.39
23	c	509	CLA	CHD-C4C	3.88	1.48	1.39
23	D	406	CLA	CHC-C4B	3.88	1.48	1.39
23	b	607	CLA	C1D-ND	3.88	1.43	1.37
23	c	510	CLA	CHB-C1B	3.87	1.48	1.39
23	B	614	CLA	CHD-C4C	3.87	1.48	1.39
23	C	504	CLA	CHC-C4B	3.87	1.48	1.39
23	B	603	CLA	CHD-C1D	3.87	1.46	1.38
23	c	507	CLA	C3D-C2D	3.87	1.49	1.39
33	d	412	LMG	O7-C10	3.86	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	406	CLA	CHD-C4C	3.86	1.48	1.39
23	c	508	CLA	CHD-C4C	3.86	1.48	1.39
23	B	615	CLA	C3D-C2D	3.86	1.49	1.39
23	b	608	CLA	OBD-CAD	3.86	1.29	1.22
23	b	614	CLA	O2A-CGA	3.86	1.44	1.33
23	B	604	CLA	CHB-C1B	3.86	1.48	1.39
23	C	506	CLA	CHB-C1B	3.86	1.48	1.39
23	C	505	CLA	C3D-C2D	3.86	1.49	1.39
23	C	505	CLA	O2A-CGA	3.86	1.44	1.33
23	A	404	CLA	C3D-C2D	3.86	1.49	1.39
23	B	610	CLA	C3D-C2D	3.85	1.49	1.39
23	b	612	CLA	C1D-ND	3.85	1.42	1.37
23	b	616	CLA	CHC-C4B	3.85	1.48	1.39
23	C	511	CLA	O2A-CGA	3.85	1.44	1.33
24	a	353	PHO	O2A-CGA	3.85	1.44	1.33
23	b	613	CLA	C1B-NB	-3.85	1.32	1.37
35	C	518	DGD	O2G-C1B	3.85	1.45	1.34
23	C	512	CLA	C3D-C2D	3.85	1.49	1.39
23	D	406	CLA	CHB-C1B	3.84	1.48	1.39
23	a	406	CLA	OBD-CAD	3.84	1.29	1.22
23	b	607	CLA	C3D-C2D	3.84	1.49	1.39
23	C	505	CLA	CHD-C1D	3.84	1.45	1.38
23	c	513	CLA	CHC-C4B	3.84	1.48	1.39
23	b	608	CLA	C3D-C2D	3.84	1.49	1.39
23	C	513	CLA	CHD-C4C	3.84	1.47	1.39
23	c	507	CLA	CHB-C1B	3.83	1.48	1.39
23	b	610	CLA	CHB-C1B	3.83	1.48	1.39
23	c	513	CLA	OBD-CAD	3.83	1.29	1.22
23	C	507	CLA	C3D-C2D	3.83	1.49	1.39
23	c	514	CLA	C3D-C2D	3.83	1.49	1.39
23	B	611	CLA	CHD-C1D	3.83	1.45	1.38
23	c	510	CLA	C3D-C2D	3.82	1.49	1.39
23	B	607	CLA	CHD-C4C	3.82	1.47	1.39
25	B	618	BCR	C23-C22	-3.82	1.37	1.46
23	c	502	CLA	CHB-C1B	3.82	1.48	1.39
23	C	508	CLA	CHB-C1B	3.81	1.48	1.39
23	A	405	CLA	CHD-C4C	3.81	1.47	1.39
23	b	605	CLA	C3D-C2D	3.81	1.49	1.39
35	c	517	DGD	O2G-C1B	3.81	1.45	1.34
23	a	407	CLA	CHD-C4C	3.81	1.47	1.39
23	b	609	CLA	O2A-CGA	3.81	1.44	1.33
23	B	603	CLA	O2A-CGA	3.81	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	C3D-C2D	3.81	1.49	1.39
23	b	604	CLA	CHD-C4C	3.81	1.47	1.39
23	b	604	CLA	C3D-C2D	3.81	1.49	1.39
23	B	610	CLA	CHB-C1B	3.80	1.48	1.39
23	b	606	CLA	O2A-CGA	3.80	1.44	1.33
23	d	403	CLA	C3D-C2D	3.80	1.49	1.39
23	C	510	CLA	O2A-CGA	3.80	1.44	1.33
23	c	508	CLA	CHB-C1B	3.80	1.47	1.39
23	b	614	CLA	CHD-C1D	3.80	1.45	1.38
23	b	616	CLA	C3D-C2D	3.80	1.49	1.39
23	C	514	CLA	CHB-C1B	3.80	1.47	1.39
35	C	518	DGD	O1G-C1A	3.80	1.44	1.33
23	B	606	CLA	CHB-C1B	3.79	1.47	1.39
35	C	519	DGD	O2G-C1B	3.79	1.45	1.34
23	A	404	CLA	CHB-C1B	3.79	1.47	1.39
23	C	508	CLA	CHC-C4B	3.79	1.47	1.39
23	b	609	CLA	OBD-CAD	3.79	1.29	1.22
35	c	517	DGD	O1G-C1A	3.79	1.44	1.33
23	b	615	CLA	CHD-C4C	3.78	1.47	1.39
23	B	601	CLA	C3D-C2D	3.78	1.49	1.39
24	A	407	PHO	O2A-CGA	3.77	1.44	1.33
23	c	512	CLA	OBD-CAD	3.77	1.29	1.22
23	c	512	CLA	C3D-C2D	3.77	1.49	1.39
23	B	614	CLA	O2A-CGA	3.77	1.44	1.33
23	c	506	CLA	O2A-CGA	3.77	1.44	1.33
23	A	406	CLA	C1D-ND	3.77	1.42	1.37
23	b	608	CLA	CHB-C1B	3.77	1.47	1.39
23	b	613	CLA	CHC-C4B	3.77	1.47	1.39
23	B	602	CLA	C3D-C2D	3.77	1.49	1.39
23	c	508	CLA	C3D-C2D	3.77	1.49	1.39
23	B	604	CLA	OBD-CAD	3.77	1.29	1.22
26	A	410	SQD	O48-C23	3.76	1.44	1.33
23	c	505	CLA	CHD-C4C	3.76	1.47	1.39
23	B	607	CLA	CHD-C1D	3.76	1.45	1.38
23	A	405	CLA	CHC-C4B	3.76	1.47	1.39
23	b	611	CLA	CHC-C4B	3.76	1.47	1.39
33	m	101	LMG	O7-C10	3.76	1.44	1.34
35	c	519	DGD	O2G-C1B	3.76	1.44	1.34
23	b	615	CLA	CHC-C4B	3.76	1.47	1.39
35	H	102	DGD	O1G-C1A	3.76	1.44	1.33
24	A	353	PHO	CHA-CBD	-3.76	1.47	1.51
23	b	605	CLA	OBD-CAD	3.76	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	CHC-C4B	3.76	1.47	1.39
23	B	603	CLA	CHD-C4C	3.76	1.47	1.39
23	C	511	CLA	OBD-CAD	3.75	1.28	1.22
23	C	510	CLA	OBD-CAD	3.75	1.28	1.22
23	C	511	CLA	C3D-C2D	3.75	1.49	1.39
23	b	603	CLA	CHD-C4C	3.75	1.47	1.39
23	b	612	CLA	CHC-C4B	3.75	1.47	1.39
23	b	612	CLA	C3D-C2D	3.75	1.49	1.39
23	b	604	CLA	CHB-C1B	3.74	1.47	1.39
23	C	506	CLA	O2A-CGA	3.74	1.44	1.33
23	b	612	CLA	O2A-CGA	3.74	1.44	1.33
23	b	616	CLA	CHD-C4C	3.74	1.47	1.39
23	a	405	CLA	OBD-CAD	3.74	1.28	1.22
23	b	614	CLA	CHD-C4C	3.74	1.47	1.39
23	A	406	CLA	O2A-CGA	3.74	1.44	1.33
23	B	606	CLA	CHD-C4C	3.74	1.47	1.39
23	B	601	CLA	CHD-C4C	3.74	1.47	1.39
23	d	403	CLA	CHD-C4C	3.74	1.47	1.39
23	c	502	CLA	CHC-C4B	3.73	1.47	1.39
35	h	102	DGD	O1G-C1A	3.73	1.44	1.33
23	B	611	CLA	OBD-CAD	3.73	1.28	1.22
23	B	603	CLA	C3D-C2D	3.73	1.49	1.39
23	b	601	CLA	OBD-CAD	3.73	1.28	1.22
23	A	406	CLA	CHD-C4C	3.73	1.47	1.39
23	C	507	CLA	OBD-CAD	3.73	1.28	1.22
23	a	409	CLA	CHC-C4B	3.73	1.47	1.39
23	b	605	CLA	O2A-CGA	3.73	1.44	1.33
23	b	613	CLA	O2A-CGA	3.73	1.44	1.33
23	B	605	CLA	C3D-C2D	3.73	1.49	1.39
23	b	605	CLA	CHD-C4C	3.73	1.47	1.39
23	C	503	CLA	CHC-C4B	3.72	1.47	1.39
23	c	514	CLA	CHB-C1B	3.72	1.47	1.39
23	a	405	CLA	C3D-C2D	3.72	1.49	1.39
23	b	608	CLA	C1B-NB	-3.72	1.33	1.37
23	C	502	CLA	C3D-C2D	3.71	1.49	1.39
23	b	614	CLA	CHB-C1B	3.71	1.47	1.39
23	b	610	CLA	CHD-C4C	3.71	1.47	1.39
23	c	508	CLA	CHC-C4B	3.71	1.47	1.39
23	c	511	CLA	CHD-C4C	3.71	1.47	1.39
23	B	605	CLA	CHD-C1D	3.71	1.45	1.38
23	D	406	CLA	O2A-CGA	3.70	1.44	1.33
23	C	505	CLA	CHD-C4C	3.70	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	O2A-CGA	3.70	1.44	1.33
23	b	615	CLA	O2A-CGA	3.70	1.44	1.33
23	b	611	CLA	CHD-C4C	3.70	1.47	1.39
23	b	603	CLA	CHC-C4B	3.70	1.47	1.39
23	c	511	CLA	CHC-C4B	3.69	1.47	1.39
23	A	404	CLA	CHD-C4C	3.69	1.47	1.39
23	a	409	CLA	CHD-C1D	3.69	1.45	1.38
23	B	607	CLA	CHC-C4B	3.69	1.47	1.39
23	C	504	CLA	CHB-C1B	3.69	1.47	1.39
23	B	614	CLA	CHD-C1D	3.69	1.45	1.38
23	B	614	CLA	CHC-C4B	3.69	1.47	1.39
23	B	612	CLA	CHD-C4C	3.69	1.47	1.39
23	b	609	CLA	CHD-C4C	3.69	1.47	1.39
37	L	101	LHG	O7-C7	3.69	1.44	1.34
26	A	410	SQD	O47-C7	3.68	1.44	1.34
23	B	610	CLA	O2A-CGA	3.68	1.44	1.33
37	d	408	LHG	O7-C7	3.68	1.44	1.34
23	c	509	CLA	CHC-C4B	3.68	1.47	1.39
23	B	616	CLA	CHB-C1B	3.68	1.47	1.39
23	B	605	CLA	O2A-CGA	3.68	1.44	1.33
23	B	616	CLA	CHD-C1D	3.67	1.45	1.38
23	C	503	CLA	OBD-CAD	3.67	1.28	1.22
23	A	408	CLA	C3D-C2D	3.67	1.49	1.39
23	b	613	CLA	CHB-C1B	3.67	1.47	1.39
23	C	503	CLA	CHB-C1B	3.67	1.47	1.39
23	D	405	CLA	CHD-C4C	3.67	1.47	1.39
23	C	504	CLA	C3D-C2D	3.67	1.49	1.39
23	A	404	CLA	CHD-C1D	3.67	1.45	1.38
37	D	410	LHG	O7-C7	3.67	1.44	1.34
23	c	509	CLA	CHB-C1B	3.67	1.47	1.39
23	b	602	CLA	O2A-CGA	3.66	1.44	1.33
23	B	601	CLA	OBD-CAD	3.66	1.28	1.22
23	b	614	CLA	CHC-C4B	3.66	1.47	1.39
23	B	603	CLA	CHC-C4B	3.66	1.47	1.39
23	C	510	CLA	CHC-C4B	3.66	1.47	1.39
23	c	513	CLA	CHB-C1B	3.66	1.47	1.39
23	b	613	CLA	CHD-C1D	3.66	1.45	1.38
23	B	607	CLA	O2A-CGA	3.66	1.44	1.33
35	C	517	DGD	O1G-C1A	3.66	1.44	1.33
23	b	611	CLA	C3D-C2D	3.65	1.49	1.39
23	b	603	CLA	C3D-C2D	3.65	1.49	1.39
23	B	614	CLA	C3D-C2D	3.65	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	d	711	LHG	O8-C23	3.65	1.44	1.33
23	B	611	CLA	CHD-C4C	3.65	1.47	1.39
23	c	503	CLA	CHB-C1B	3.65	1.47	1.39
23	B	602	CLA	CHC-C4B	3.65	1.47	1.39
23	B	608	CLA	CHB-C1B	3.65	1.47	1.39
23	B	613	CLA	C1B-NB	-3.65	1.33	1.37
23	A	405	CLA	CHB-C1B	3.65	1.47	1.39
23	c	511	CLA	CHD-C1D	3.64	1.45	1.38
23	B	615	CLA	CHD-C4C	3.64	1.47	1.39
23	B	612	CLA	C1D-ND	3.64	1.42	1.37
23	A	406	CLA	CHC-C4B	3.64	1.47	1.39
23	b	615	CLA	CHB-C1B	3.64	1.47	1.39
23	b	606	CLA	C3D-C2D	3.63	1.48	1.39
23	d	403	CLA	CHB-C1B	3.63	1.47	1.39
23	b	606	CLA	CHB-C1B	3.63	1.47	1.39
23	C	510	CLA	CHB-C1B	3.63	1.47	1.39
23	A	408	CLA	CHD-C4C	3.63	1.47	1.39
23	d	402	CLA	CHD-C4C	3.62	1.47	1.39
23	C	503	CLA	CHD-C4C	3.62	1.47	1.39
23	C	510	CLA	C4B-NB	-3.62	1.33	1.37
23	a	406	CLA	CHD-C1D	3.62	1.45	1.38
23	b	601	CLA	CHB-C1B	3.62	1.47	1.39
23	b	602	CLA	OBD-CAD	3.61	1.28	1.22
23	c	503	CLA	OBD-CAD	3.61	1.28	1.22
23	C	514	CLA	CHD-C4C	3.61	1.47	1.39
23	b	605	CLA	CHD-C1D	3.61	1.45	1.38
23	d	402	CLA	OBD-CAD	3.61	1.28	1.22
37	l	101	LHG	O7-C7	3.61	1.44	1.34
37	D	410	LHG	O8-C23	3.61	1.43	1.33
23	B	610	CLA	CHC-C4B	3.61	1.47	1.39
23	C	502	CLA	CHB-C1B	3.60	1.47	1.39
23	C	508	CLA	C3D-C2D	3.60	1.48	1.39
23	A	406	CLA	CHB-C1B	3.60	1.47	1.39
23	B	607	CLA	C3D-C2D	3.60	1.48	1.39
23	b	615	CLA	OBD-CAD	3.60	1.28	1.22
37	D	409	LHG	O7-C7	3.60	1.44	1.34
23	D	405	CLA	C3D-C2D	3.60	1.48	1.39
23	b	610	CLA	C3D-C2D	3.60	1.48	1.39
23	b	606	CLA	OBD-CAD	3.59	1.28	1.22
23	b	601	CLA	CHC-C4B	3.59	1.47	1.39
23	D	406	CLA	OBD-CAD	3.59	1.28	1.22
23	B	604	CLA	O2A-CGA	3.59	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	O2A-CGA	3.58	1.43	1.33
37	d	407	LHG	O8-C23	3.58	1.43	1.33
23	a	407	CLA	CHD-C1D	3.58	1.45	1.38
23	d	402	CLA	C3D-C2D	3.58	1.48	1.39
23	b	613	CLA	CHD-C4C	3.58	1.47	1.39
23	C	514	CLA	OBD-CAD	3.58	1.28	1.22
23	B	610	CLA	CHD-C4C	3.58	1.47	1.39
23	C	508	CLA	CHD-C4C	3.58	1.47	1.39
23	B	611	CLA	C1C-C2C	3.57	1.51	1.44
23	c	505	CLA	CHB-C1B	3.57	1.47	1.39
23	b	607	CLA	CHD-C4C	3.57	1.47	1.39
23	B	606	CLA	C3D-C2D	3.57	1.48	1.39
23	B	610	CLA	CHD-C1D	3.56	1.45	1.38
23	B	607	CLA	C1B-NB	-3.56	1.33	1.37
23	b	608	CLA	CHD-C4C	3.56	1.47	1.39
33	D	415	LMG	O7-C10	3.56	1.44	1.34
23	B	612	CLA	C1B-NB	-3.56	1.33	1.37
23	b	603	CLA	CHB-C1B	3.56	1.47	1.39
23	B	607	CLA	C1D-ND	3.56	1.42	1.37
23	C	513	CLA	OBD-CAD	3.55	1.28	1.22
23	b	607	CLA	C1B-NB	-3.55	1.33	1.37
23	a	405	CLA	CHC-C4B	3.55	1.47	1.39
23	a	407	CLA	CHB-C1B	3.55	1.47	1.39
23	a	406	CLA	CHD-C4C	3.55	1.47	1.39
35	c	518	DGD	O2G-C1B	3.54	1.44	1.34
23	a	409	CLA	CHD-C4C	3.53	1.47	1.39
23	c	506	CLA	OBD-CAD	3.53	1.28	1.22
23	c	506	CLA	C3D-C2D	3.53	1.48	1.39
23	b	606	CLA	CHC-C4B	3.53	1.47	1.39
23	b	616	CLA	OBD-CAD	3.53	1.28	1.22
23	B	601	CLA	CHB-C1B	3.53	1.47	1.39
23	c	507	CLA	OBD-CAD	3.53	1.28	1.22
23	c	507	CLA	CHC-C4B	3.53	1.47	1.39
23	B	612	CLA	O2A-CGA	3.52	1.43	1.33
23	B	605	CLA	CHD-C4C	3.52	1.47	1.39
23	B	608	CLA	O2A-CGA	3.52	1.43	1.33
23	b	607	CLA	CHC-C4B	3.51	1.47	1.39
37	d	711	LHG	O7-C7	3.51	1.44	1.34
23	C	510	CLA	C1B-NB	-3.50	1.33	1.37
37	D	409	LHG	O8-C23	3.50	1.43	1.33
23	a	407	CLA	OBD-CAD	3.50	1.28	1.22
23	D	405	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	514	CLA	OBD-CAD	3.49	1.28	1.22
23	B	604	CLA	CHC-C4B	3.49	1.47	1.39
23	C	512	CLA	CHC-C4B	3.49	1.47	1.39
23	B	616	CLA	CHC-C4B	3.48	1.47	1.39
23	b	611	CLA	CHD-C1D	3.48	1.45	1.38
23	c	512	CLA	CHC-C4B	3.48	1.47	1.39
23	a	406	CLA	CHB-C1B	3.47	1.47	1.39
23	B	612	CLA	C3D-C2D	3.47	1.48	1.39
23	C	509	CLA	CHC-C4B	3.47	1.47	1.39
23	d	403	CLA	OBD-CAD	3.47	1.28	1.22
23	b	608	CLA	C4B-NB	-3.47	1.33	1.37
23	C	506	CLA	OBD-CAD	3.46	1.28	1.22
23	C	504	CLA	OBD-CAD	3.46	1.28	1.22
23	C	507	CLA	CHB-C1B	3.45	1.47	1.39
23	b	603	CLA	OBD-CAD	3.45	1.28	1.22
23	b	605	CLA	CHC-C4B	3.45	1.47	1.39
23	C	514	CLA	CHC-C4B	3.45	1.47	1.39
23	b	609	CLA	CHC-C4B	3.45	1.47	1.39
33	D	415	LMG	O8-C28	3.44	1.43	1.33
23	B	609	CLA	CHB-C1B	3.44	1.47	1.39
23	B	608	CLA	CHD-C4C	3.44	1.47	1.39
23	c	514	CLA	CHC-C4B	3.44	1.47	1.39
23	b	614	CLA	OBD-CAD	3.44	1.28	1.22
23	A	408	CLA	CHB-C1B	3.44	1.47	1.39
23	b	607	CLA	O2A-CGA	3.44	1.43	1.33
23	C	506	CLA	C3D-C2D	3.43	1.48	1.39
34	b	622	HTG	C1'-S1	-3.43	1.76	1.81
23	b	610	CLA	OBD-CAD	3.42	1.28	1.22
23	B	602	CLA	C1B-NB	-3.42	1.33	1.37
23	c	503	CLA	CHC-C4B	3.42	1.47	1.39
23	B	613	CLA	CHC-C4B	3.42	1.47	1.39
23	b	611	CLA	CHB-C1B	3.41	1.47	1.39
23	C	509	CLA	CHD-C4C	3.41	1.47	1.39
23	c	505	CLA	OBD-CAD	3.41	1.28	1.22
23	b	603	CLA	C1D-ND	3.40	1.42	1.37
23	c	510	CLA	OBD-CAD	3.40	1.28	1.22
37	l	101	LHG	O8-C23	3.40	1.43	1.33
38	E	103	HEM	C4D-ND	-3.40	1.34	1.40
23	b	615	CLA	C1B-NB	-3.39	1.33	1.37
23	b	612	CLA	CHD-C4C	3.39	1.46	1.39
23	A	404	CLA	C4B-NB	-3.39	1.33	1.37
23	b	607	CLA	C1B-C2B	3.39	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	C3D-C2D	3.39	1.48	1.39
23	c	502	CLA	OBD-CAD	3.39	1.28	1.22
23	B	607	CLA	OBD-CAD	3.38	1.28	1.22
23	C	505	CLA	CHC-C4B	3.38	1.47	1.39
23	B	606	CLA	OBD-CAD	3.38	1.28	1.22
23	b	604	CLA	O2A-CGA	3.38	1.43	1.33
23	B	603	CLA	OBD-CAD	3.37	1.28	1.22
23	d	402	CLA	CHC-C4B	3.37	1.47	1.39
35	H	102	DGD	O2G-C1B	3.37	1.43	1.34
23	C	512	CLA	OBD-CAD	3.36	1.28	1.22
23	B	610	CLA	C1B-NB	-3.36	1.33	1.37
34	b	623	HTG	C1'-S1	-3.36	1.76	1.81
23	A	405	CLA	OBD-CAD	3.36	1.28	1.22
23	C	511	CLA	CHC-C4B	3.36	1.46	1.39
24	a	408	PHO	O2A-CGA	3.36	1.43	1.33
38	e	87	HEM	C4D-ND	-3.35	1.34	1.40
23	c	504	CLA	C3D-C2D	3.35	1.48	1.39
23	B	611	CLA	C3D-C2D	3.35	1.48	1.39
23	b	607	CLA	OBD-CAD	3.34	1.28	1.22
23	a	409	CLA	C1B-NB	-3.33	1.33	1.37
23	c	505	CLA	CHC-C4B	3.33	1.46	1.39
23	A	404	CLA	OBD-CAD	3.33	1.28	1.22
23	a	409	CLA	C3D-C2D	3.33	1.48	1.39
23	B	615	CLA	CHC-C4B	3.33	1.46	1.39
23	d	402	CLA	C1D-ND	3.32	1.42	1.37
23	A	405	CLA	C1B-NB	-3.32	1.33	1.37
23	C	507	CLA	C4B-NB	-3.31	1.33	1.37
23	B	612	CLA	C4B-NB	-3.31	1.33	1.37
23	C	512	CLA	C4B-NB	-3.30	1.33	1.37
23	b	612	CLA	C4B-NB	-3.29	1.33	1.37
23	C	513	CLA	CHB-C1B	3.29	1.46	1.39
23	A	404	CLA	O2A-CGA	3.28	1.42	1.33
23	B	609	CLA	OBD-CAD	3.28	1.28	1.22
23	B	609	CLA	C1B-NB	-3.27	1.33	1.37
23	b	604	CLA	OBD-CAD	3.27	1.28	1.22
23	a	407	CLA	CHC-C4B	3.26	1.46	1.39
23	b	614	CLA	C1B-NB	-3.25	1.33	1.37
23	b	616	CLA	C1B-NB	-3.25	1.33	1.37
23	A	408	CLA	CHC-C4B	3.25	1.46	1.39
23	d	402	CLA	C1B-NB	-3.25	1.33	1.37
23	b	605	CLA	C1B-NB	-3.25	1.33	1.37
23	b	610	CLA	C1B-NB	-3.25	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	405	CLA	OBD-CAD	3.24	1.28	1.22
23	A	408	CLA	C4B-NB	-3.23	1.33	1.37
23	a	406	CLA	CHC-C4B	3.23	1.46	1.39
23	C	502	CLA	C1B-NB	-3.22	1.33	1.37
23	b	602	CLA	CHB-C1B	3.22	1.46	1.39
23	C	505	CLA	OBD-CAD	3.22	1.28	1.22
23	B	612	CLA	CHC-C4B	3.22	1.46	1.39
23	C	511	CLA	C1B-NB	-3.21	1.33	1.37
23	a	409	CLA	OBD-CAD	3.21	1.28	1.22
23	C	507	CLA	C1B-NB	-3.21	1.33	1.37
38	E	103	HEM	C1B-NB	-3.21	1.34	1.40
23	c	514	CLA	C4B-NB	-3.20	1.33	1.37
23	c	511	CLA	OBD-CAD	3.20	1.28	1.22
23	B	608	CLA	C4B-NB	-3.20	1.33	1.37
23	b	608	CLA	CHC-C4B	3.20	1.46	1.39
23	B	602	CLA	OBD-CAD	3.20	1.28	1.22
23	b	602	CLA	C1B-NB	-3.19	1.33	1.37
23	a	405	CLA	O2A-CGA	3.19	1.42	1.33
23	B	616	CLA	CHD-C4C	3.19	1.46	1.39
23	C	507	CLA	CHC-C4B	3.19	1.46	1.39
23	b	616	CLA	CHB-C1B	3.18	1.46	1.39
38	e	87	HEM	C1B-NB	-3.18	1.34	1.40
23	B	604	CLA	C1B-C2B	3.18	1.50	1.43
23	C	506	CLA	C1B-C2B	3.18	1.50	1.43
23	c	508	CLA	C1B-NB	-3.17	1.33	1.37
23	c	514	CLA	C1B-NB	-3.16	1.33	1.37
23	A	408	CLA	C1B-NB	-3.16	1.33	1.37
23	B	612	CLA	C1B-C2B	3.15	1.50	1.43
23	C	511	CLA	C4B-NB	-3.15	1.33	1.37
23	B	615	CLA	C1B-C2B	3.14	1.50	1.43
34	B	622	HTG	C1'-S1	-3.14	1.77	1.81
23	C	505	CLA	C1B-NB	-3.13	1.33	1.37
23	c	510	CLA	C4B-NB	-3.12	1.33	1.37
23	c	508	CLA	C4B-NB	-3.11	1.33	1.37
23	c	510	CLA	C1B-C2B	3.11	1.50	1.43
23	C	509	CLA	C1B-C2B	3.11	1.50	1.43
34	B	626	HTG	C1'-S1	-3.10	1.77	1.81
23	b	611	CLA	OBD-CAD	3.10	1.27	1.22
23	c	512	CLA	C1B-C2B	3.09	1.50	1.43
23	b	610	CLA	O2A-CGA	3.09	1.42	1.33
23	B	605	CLA	OBD-CAD	3.08	1.27	1.22
23	c	507	CLA	C1B-NB	-3.07	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C1B-NB	-3.07	1.33	1.37
23	b	604	CLA	C1B-NB	-3.07	1.33	1.37
23	B	616	CLA	OBD-CAD	3.06	1.27	1.22
23	B	603	CLA	C4B-NB	-3.06	1.33	1.37
23	B	614	CLA	OBD-CAD	3.06	1.27	1.22
23	c	505	CLA	C1B-NB	-3.05	1.33	1.37
23	C	514	CLA	C4B-NB	-3.05	1.33	1.37
23	D	405	CLA	C1B-NB	-3.05	1.33	1.37
23	B	603	CLA	C1B-NB	-3.05	1.33	1.37
23	C	508	CLA	OBD-CAD	3.03	1.27	1.22
23	C	512	CLA	C4D-CHA	3.03	1.48	1.38
23	A	406	CLA	C1B-C2B	3.03	1.50	1.43
23	B	604	CLA	C1B-NB	-3.02	1.33	1.37
23	b	603	CLA	C1B-C2B	3.02	1.50	1.43
23	a	409	CLA	C1B-C2B	3.02	1.50	1.43
23	C	514	CLA	C1B-C2B	3.02	1.50	1.43
23	b	614	CLA	C1B-C2B	3.01	1.50	1.43
23	c	510	CLA	CHC-C4B	3.01	1.46	1.39
23	B	616	CLA	C1B-C2B	3.01	1.50	1.43
23	A	404	CLA	CHC-C4B	3.01	1.46	1.39
23	c	505	CLA	C1B-C2B	3.00	1.50	1.43
23	B	605	CLA	C1B-C2B	3.00	1.50	1.43
29	A	414	PL9	C6-C5	2.99	1.49	1.35
23	B	612	CLA	OBD-CAD	2.99	1.27	1.22
24	A	407	PHO	CBD-CGD	-2.99	1.48	1.52
23	A	408	CLA	OBD-CAD	2.99	1.27	1.22
23	B	610	CLA	C4B-NB	-2.99	1.33	1.37
23	B	607	CLA	C4D-CHA	2.98	1.48	1.38
23	C	506	CLA	C1B-NB	-2.98	1.34	1.37
23	B	614	CLA	C4D-CHA	2.97	1.48	1.38
23	b	609	CLA	C1B-NB	-2.97	1.34	1.37
34	d	411	HTG	C1'-S1	-2.97	1.77	1.81
23	c	503	CLA	C1B-C2B	2.96	1.50	1.43
23	B	607	CLA	C4B-NB	-2.96	1.34	1.37
23	b	604	CLA	C1B-C2B	2.96	1.50	1.43
23	D	406	CLA	C1C-C2C	2.96	1.50	1.44
23	A	404	CLA	C1B-NB	-2.95	1.34	1.37
23	C	513	CLA	C1C-C2C	2.95	1.50	1.44
23	d	402	CLA	C4B-NB	-2.95	1.34	1.37
23	D	406	CLA	C1B-C2B	2.95	1.50	1.43
23	b	611	CLA	C1B-NB	-2.94	1.34	1.37
23	b	604	CLA	C4D-CHA	2.94	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	C1B-NB	-2.93	1.34	1.37
23	b	612	CLA	C1C-C2C	2.93	1.50	1.44
23	b	606	CLA	C1B-NB	-2.93	1.34	1.37
23	c	504	CLA	OBD-CAD	2.92	1.27	1.22
29	a	416	PL9	C6-C5	2.92	1.49	1.35
23	B	608	CLA	CHC-C4B	2.92	1.46	1.39
23	a	405	CLA	C1B-NB	-2.92	1.34	1.37
34	D	414	HTG	C1'-S1	-2.91	1.77	1.81
23	a	405	CLA	C4B-NB	-2.91	1.34	1.37
23	b	601	CLA	C1B-NB	-2.91	1.34	1.37
23	a	407	CLA	C1B-NB	-2.91	1.34	1.37
23	b	613	CLA	C4D-CHA	2.91	1.48	1.38
23	C	502	CLA	OBD-CAD	2.90	1.27	1.22
23	c	512	CLA	C1B-NB	-2.90	1.34	1.37
23	B	615	CLA	C1C-C2C	2.90	1.50	1.44
23	B	606	CLA	C1C-C2C	2.89	1.50	1.44
23	a	409	CLA	C1C-C2C	2.89	1.50	1.44
23	C	512	CLA	C1B-C2B	2.89	1.49	1.43
23	A	404	CLA	C4C-C3C	2.88	1.49	1.45
23	c	505	CLA	C4B-NB	-2.88	1.34	1.37
23	B	610	CLA	C1C-C2C	2.88	1.50	1.44
23	c	506	CLA	C4C-C3C	2.88	1.49	1.45
23	b	607	CLA	C4C-C3C	2.88	1.49	1.45
23	B	608	CLA	OBD-CAD	2.87	1.27	1.22
23	B	607	CLA	C1B-C2B	2.87	1.49	1.43
23	b	612	CLA	C1B-C2B	2.87	1.49	1.43
34	b	625	HTG	C1'-S1	-2.87	1.77	1.81
23	A	408	CLA	C1B-C2B	2.87	1.49	1.43
23	b	611	CLA	C1B-C2B	2.86	1.49	1.43
23	D	405	CLA	C1B-C2B	2.86	1.49	1.43
23	A	408	CLA	C4D-CHA	2.86	1.48	1.38
23	b	603	CLA	C1B-NB	-2.85	1.34	1.37
23	C	505	CLA	C4D-CHA	2.85	1.48	1.38
23	b	613	CLA	C4B-NB	-2.85	1.34	1.37
23	C	502	CLA	C1B-C2B	2.85	1.49	1.43
23	B	609	CLA	C3B-C4B	2.85	1.51	1.42
23	B	616	CLA	C4D-CHA	2.84	1.48	1.38
23	c	511	CLA	C1B-C2B	2.84	1.49	1.43
23	c	509	CLA	C4D-CHA	2.84	1.48	1.38
23	d	402	CLA	C4C-C3C	2.84	1.49	1.45
23	B	605	CLA	C4B-NB	-2.83	1.34	1.37
23	b	610	CLA	C1C-C2C	2.83	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	C4D-CHA	2.83	1.48	1.38
23	A	404	CLA	C1B-C2B	2.83	1.49	1.43
23	B	611	CLA	C3B-C4B	2.82	1.50	1.42
23	B	613	CLA	C1B-C2B	2.82	1.49	1.43
23	B	612	CLA	C4D-CHA	2.82	1.48	1.38
23	c	504	CLA	C1B-NB	-2.82	1.34	1.37
23	C	502	CLA	C4D-CHA	2.81	1.48	1.38
23	b	602	CLA	C3B-C4B	2.81	1.50	1.42
23	B	608	CLA	C4D-CHA	2.80	1.48	1.38
23	b	602	CLA	C1C-C2C	2.80	1.50	1.44
23	c	507	CLA	C1B-C2B	2.80	1.49	1.43
23	C	505	CLA	C4B-NB	-2.80	1.34	1.37
23	b	612	CLA	C1B-NB	-2.80	1.34	1.37
23	c	504	CLA	C1B-C2B	2.80	1.49	1.43
23	B	613	CLA	C4D-CHA	2.80	1.48	1.38
23	B	615	CLA	C4D-CHA	2.80	1.48	1.38
23	C	514	CLA	C1B-NB	-2.80	1.34	1.37
23	C	508	CLA	C1C-C2C	2.80	1.50	1.44
23	a	407	CLA	C1C-C2C	2.79	1.50	1.44
23	B	612	CLA	C1C-C2C	2.79	1.50	1.44
23	c	511	CLA	C1C-C2C	2.79	1.50	1.44
23	c	502	CLA	C4D-CHA	2.79	1.48	1.38
23	C	508	CLA	C1B-NB	-2.79	1.34	1.37
23	c	513	CLA	C4D-CHA	2.79	1.48	1.38
23	A	405	CLA	C4D-CHA	2.79	1.48	1.38
24	a	408	PHO	CBD-CGD	-2.79	1.49	1.52
34	C	522	HTG	C1'-S1	-2.79	1.77	1.81
23	C	503	CLA	C1B-NB	-2.78	1.34	1.37
23	b	613	CLA	C1B-C2B	2.78	1.49	1.43
23	c	508	CLA	C1B-C2B	2.78	1.49	1.43
23	b	607	CLA	C4B-NB	-2.78	1.34	1.37
23	a	407	CLA	C4D-CHA	2.77	1.47	1.38
23	B	604	CLA	C4D-CHA	2.77	1.47	1.38
23	B	614	CLA	C1B-NB	-2.77	1.34	1.37
23	c	506	CLA	C1B-C2B	2.77	1.49	1.43
23	C	506	CLA	C4C-C3C	2.76	1.49	1.45
23	B	605	CLA	C1C-C2C	2.76	1.50	1.44
23	c	502	CLA	C1B-NB	-2.76	1.34	1.37
23	C	509	CLA	C4D-CHA	2.76	1.47	1.38
23	C	509	CLA	C4B-NB	-2.76	1.34	1.37
23	c	514	CLA	C1B-C2B	2.76	1.49	1.43
23	D	406	CLA	C1B-NB	-2.76	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	C4B-NB	-2.76	1.34	1.37
23	b	609	CLA	C4D-CHA	2.76	1.47	1.38
23	A	405	CLA	C1B-C2B	2.76	1.49	1.43
23	D	406	CLA	C4C-C3C	2.76	1.49	1.45
33	Z	101	LMG	O8-C28	2.76	1.46	1.33
23	C	511	CLA	C1B-C2B	2.75	1.49	1.43
23	c	507	CLA	C4B-NB	-2.75	1.34	1.37
23	C	503	CLA	C4B-NB	-2.75	1.34	1.37
23	C	507	CLA	C4D-CHA	2.75	1.47	1.38
23	B	611	CLA	MG-NB	2.75	2.11	2.05
23	b	607	CLA	C1C-C2C	2.75	1.50	1.44
23	c	512	CLA	C4D-CHA	2.75	1.47	1.38
23	C	503	CLA	C1B-C2B	2.74	1.49	1.43
23	c	505	CLA	C4D-CHA	2.74	1.47	1.38
23	c	510	CLA	C4D-CHA	2.74	1.47	1.38
23	C	507	CLA	C1B-C2B	2.74	1.49	1.43
23	D	405	CLA	C4B-NB	-2.74	1.34	1.37
23	d	403	CLA	C1B-NB	-2.73	1.34	1.37
23	a	407	CLA	C1B-C2B	2.73	1.49	1.43
23	B	604	CLA	C4C-C3C	2.73	1.49	1.45
23	c	509	CLA	C1B-C2B	2.73	1.49	1.43
23	B	610	CLA	C1B-C2B	2.73	1.49	1.43
23	a	406	CLA	C1B-C2B	2.73	1.49	1.43
23	B	610	CLA	C4D-CHA	2.73	1.47	1.38
23	c	504	CLA	C4D-CHA	2.73	1.47	1.38
23	C	511	CLA	C1C-C2C	2.72	1.50	1.44
23	C	504	CLA	C1B-NB	-2.72	1.34	1.37
23	b	607	CLA	C4D-CHA	2.72	1.47	1.38
23	C	505	CLA	C1B-C2B	2.72	1.49	1.43
23	c	508	CLA	C1C-C2C	2.72	1.50	1.44
23	c	508	CLA	C4D-CHA	2.71	1.47	1.38
23	A	406	CLA	C3B-C4B	2.71	1.50	1.42
23	b	613	CLA	OBD-CAD	2.71	1.27	1.22
23	D	405	CLA	C4D-CHA	2.71	1.47	1.38
23	a	409	CLA	C4B-NB	-2.71	1.34	1.37
23	C	513	CLA	C4D-CHA	2.71	1.47	1.38
34	c	522	HTG	C1'-S1	-2.70	1.77	1.81
23	B	601	CLA	C3B-C4B	2.70	1.50	1.42
23	C	508	CLA	C1B-C2B	2.70	1.49	1.43
23	B	608	CLA	C1B-C2B	2.70	1.49	1.43
23	d	402	CLA	C4D-CHA	2.70	1.47	1.38
23	c	503	CLA	C4D-CHA	2.69	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C1C-C2C	2.69	1.50	1.44
23	c	511	CLA	C4D-CHA	2.69	1.47	1.38
23	c	514	CLA	C1C-C2C	2.69	1.50	1.44
23	b	604	CLA	C1C-C2C	2.69	1.50	1.44
23	C	507	CLA	C4C-C3C	2.69	1.49	1.45
23	c	506	CLA	C1B-NB	-2.68	1.34	1.37
23	B	601	CLA	C1C-C2C	2.68	1.50	1.44
23	b	615	CLA	C1B-C2B	2.67	1.49	1.43
23	A	406	CLA	C4D-CHA	2.67	1.47	1.38
23	B	610	CLA	C4C-C3C	2.67	1.49	1.45
24	a	353	PHO	C3A-C2A	-2.67	1.52	1.54
23	B	605	CLA	C4D-CHA	2.67	1.47	1.38
23	D	406	CLA	C3B-C4B	2.67	1.50	1.42
23	C	514	CLA	C4D-CHA	2.67	1.47	1.38
23	b	615	CLA	C4D-CHA	2.67	1.47	1.38
23	C	510	CLA	C4D-CHA	2.67	1.47	1.38
23	b	605	CLA	C4D-CHA	2.67	1.47	1.38
23	c	511	CLA	C4B-NB	-2.66	1.34	1.37
23	c	512	CLA	C4B-NB	-2.66	1.34	1.37
23	B	602	CLA	C1B-C2B	2.66	1.49	1.43
23	B	602	CLA	C4D-CHA	2.66	1.47	1.38
23	B	606	CLA	C1B-C2B	2.66	1.49	1.43
23	c	504	CLA	C4B-NB	-2.66	1.34	1.37
23	B	614	CLA	C1B-C2B	2.66	1.49	1.43
29	D	408	PL9	C6-C5	2.66	1.48	1.35
23	c	507	CLA	C4C-C3C	2.66	1.49	1.45
23	B	613	CLA	C4B-NB	-2.66	1.34	1.37
23	B	616	CLA	C4B-NB	-2.66	1.34	1.37
23	b	606	CLA	C4D-CHA	2.65	1.47	1.38
23	C	502	CLA	C1C-C2C	2.65	1.49	1.44
23	C	505	CLA	C1C-C2C	2.65	1.49	1.44
23	B	615	CLA	C1B-NB	-2.65	1.34	1.37
23	b	601	CLA	C4D-CHA	2.65	1.47	1.38
23	a	405	CLA	C4D-CHA	2.65	1.47	1.38
23	A	408	CLA	C3D-C4D	-2.65	1.38	1.44
23	B	602	CLA	C1C-C2C	2.64	1.49	1.44
23	b	602	CLA	C3D-C4D	-2.64	1.38	1.44
23	c	506	CLA	C1C-C2C	2.64	1.49	1.44
23	C	510	CLA	C4C-C3C	2.64	1.49	1.45
23	B	603	CLA	C4D-CHA	2.64	1.47	1.38
23	C	511	CLA	C4C-C3C	2.64	1.49	1.45
23	C	514	CLA	C1C-C2C	2.64	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404	CLA	C4D-CHA	2.64	1.47	1.38
23	c	513	CLA	C1B-NB	-2.63	1.34	1.37
23	a	407	CLA	C4B-NB	-2.63	1.34	1.37
23	C	506	CLA	C4D-CHA	2.62	1.47	1.38
23	b	614	CLA	C4B-NB	-2.62	1.34	1.37
23	A	405	CLA	C1C-C2C	2.62	1.49	1.44
23	c	502	CLA	C1B-C2B	2.62	1.49	1.43
23	c	506	CLA	C4D-CHA	2.62	1.47	1.38
23	b	616	CLA	C1C-C2C	2.62	1.49	1.44
23	B	601	CLA	C4B-NB	-2.62	1.34	1.37
23	a	406	CLA	C4D-CHA	2.61	1.47	1.38
35	H	102	DGD	O5D-C1E	2.61	1.44	1.40
23	B	606	CLA	C1B-NB	-2.61	1.34	1.37
23	a	406	CLA	C4B-NB	-2.61	1.34	1.37
23	c	504	CLA	C3D-C4D	-2.61	1.38	1.44
23	C	512	CLA	C1B-NB	-2.61	1.34	1.37
23	b	614	CLA	C4D-CHA	2.61	1.47	1.38
23	b	602	CLA	C4D-CHA	2.60	1.47	1.38
23	c	507	CLA	C4D-CHA	2.60	1.47	1.38
24	A	353	PHO	C3D-C4D	-2.60	1.37	1.41
23	B	609	CLA	C1C-C2C	2.60	1.49	1.44
23	A	405	CLA	C4B-NB	-2.60	1.34	1.37
34	b	622	HTG	O5-C1	2.60	1.46	1.42
23	D	406	CLA	C4D-CHA	2.60	1.47	1.38
23	B	606	CLA	C4D-CHA	2.59	1.47	1.38
23	B	605	CLA	C1B-NB	-2.59	1.34	1.37
23	B	613	CLA	C4C-C3C	2.59	1.49	1.45
23	b	610	CLA	C1B-C2B	2.59	1.49	1.43
23	B	607	CLA	C4C-C3C	2.59	1.49	1.45
23	C	504	CLA	C4D-CHA	2.59	1.47	1.38
23	b	606	CLA	C1B-C2B	2.59	1.49	1.43
23	b	610	CLA	C4D-CHA	2.58	1.47	1.38
23	C	509	CLA	C3B-C2B	2.58	1.49	1.41
23	B	609	CLA	C4D-CHA	2.58	1.47	1.38
23	b	616	CLA	C1B-C2B	2.58	1.49	1.43
23	b	609	CLA	C4B-NB	-2.57	1.34	1.37
23	d	402	CLA	C1B-C2B	2.57	1.49	1.43
23	C	512	CLA	C4C-C3C	2.57	1.49	1.45
23	b	608	CLA	C4D-CHA	2.57	1.47	1.38
23	c	509	CLA	C1C-C2C	2.57	1.49	1.44
23	c	502	CLA	C4C-C3C	2.57	1.49	1.45
23	c	504	CLA	C3B-C4B	2.56	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	C4B-NB	-2.56	1.34	1.37
23	b	611	CLA	C4D-CHA	2.56	1.47	1.38
23	B	601	CLA	C1B-NB	-2.56	1.34	1.37
23	C	509	CLA	C4C-C3C	2.56	1.49	1.45
23	b	603	CLA	C4B-NB	-2.56	1.34	1.37
23	c	513	CLA	C1B-C2B	2.56	1.49	1.43
23	C	513	CLA	C3B-C4B	2.56	1.50	1.42
23	A	405	CLA	C3B-C4B	2.56	1.50	1.42
23	d	403	CLA	C4D-CHA	2.55	1.47	1.38
23	c	514	CLA	C4D-CHA	2.55	1.47	1.38
23	C	504	CLA	C4C-C3C	2.55	1.49	1.45
23	c	506	CLA	C3B-C4B	2.55	1.50	1.42
23	c	513	CLA	C4B-NB	-2.55	1.34	1.37
23	b	610	CLA	C4C-C3C	2.55	1.49	1.45
23	C	510	CLA	C1B-C2B	2.54	1.49	1.43
23	c	509	CLA	C4C-C3C	2.54	1.49	1.45
23	b	612	CLA	C4D-CHA	2.54	1.47	1.38
23	B	609	CLA	C1B-C2B	2.54	1.49	1.43
23	B	608	CLA	C1B-NB	-2.53	1.34	1.37
23	b	616	CLA	C3B-C4B	2.53	1.50	1.42
23	a	405	CLA	C1B-C2B	2.53	1.49	1.43
23	b	605	CLA	C4B-NB	-2.53	1.34	1.37
23	c	514	CLA	C4C-C3C	2.53	1.49	1.45
32	t	102	LMT	O3'-C3'	-2.53	1.36	1.43
23	C	503	CLA	C4D-CHA	2.52	1.47	1.38
23	B	616	CLA	C3B-C2B	2.52	1.49	1.41
23	d	403	CLA	C1C-C2C	2.52	1.49	1.44
23	c	509	CLA	C3B-C4B	2.52	1.50	1.42
40	V	202	HEC	CMB-C2B	2.52	1.55	1.50
23	c	504	CLA	C1C-C2C	2.51	1.49	1.44
34	b	625	HTG	C1-S1	-2.51	1.76	1.80
23	b	605	CLA	C1B-C2B	2.51	1.49	1.43
23	c	511	CLA	C1B-NB	-2.51	1.34	1.37
24	A	353	PHO	C3A-C2A	-2.51	1.52	1.54
23	c	502	CLA	C3D-C4D	-2.51	1.38	1.44
23	d	403	CLA	C1B-C2B	2.51	1.49	1.43
33	C	521	LMG	O1-C1	2.51	1.44	1.40
23	c	503	CLA	C1B-NB	-2.50	1.34	1.37
23	B	602	CLA	C3D-C4D	-2.50	1.38	1.44
23	B	601	CLA	C4D-CHA	2.50	1.47	1.38
24	a	353	PHO	C4B-NB	-2.50	1.34	1.38
23	C	512	CLA	C3B-C2B	2.49	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	C3D-C4D	-2.49	1.38	1.44
23	C	504	CLA	C1B-C2B	2.49	1.49	1.43
23	C	502	CLA	C3B-C4B	2.49	1.50	1.42
38	e	87	HEM	C1C-C2C	-2.49	1.40	1.45
23	C	506	CLA	C3B-C4B	2.49	1.50	1.42
23	b	608	CLA	C1B-C2B	2.49	1.49	1.43
23	a	409	CLA	C3B-C4B	2.49	1.50	1.42
24	a	408	PHO	C4B-NB	-2.48	1.34	1.38
23	B	605	CLA	C3B-C4B	2.48	1.50	1.42
32	D	404	LMT	C3'-C2'	2.48	1.58	1.52
23	b	601	CLA	C1B-C2B	2.48	1.48	1.43
29	d	405	PL9	C6-C5	2.48	1.47	1.35
23	B	608	CLA	C4C-C3C	2.47	1.49	1.45
24	A	353	PHO	C4B-NB	-2.47	1.34	1.38
23	C	514	CLA	C3B-C2B	2.47	1.49	1.41
23	c	504	CLA	C4C-C3C	2.47	1.49	1.45
23	c	510	CLA	C4C-C3C	2.47	1.49	1.45
23	C	504	CLA	C4B-NB	-2.47	1.34	1.37
23	b	612	CLA	C3B-C2B	2.46	1.49	1.41
23	C	504	CLA	C3D-C4D	-2.46	1.38	1.44
23	d	402	CLA	C3D-C4D	-2.46	1.38	1.44
23	C	506	CLA	C1C-C2C	2.46	1.49	1.44
23	b	603	CLA	C4D-CHA	2.46	1.46	1.38
23	b	616	CLA	C4D-CHA	2.46	1.46	1.38
23	B	603	CLA	C3B-C2B	2.46	1.49	1.41
23	c	505	CLA	C1C-C2C	2.45	1.49	1.44
23	d	402	CLA	C1C-C2C	2.45	1.49	1.44
23	B	602	CLA	C4C-C3C	2.45	1.49	1.45
23	b	615	CLA	C4C-C3C	2.45	1.49	1.45
23	B	602	CLA	C4B-NB	-2.45	1.34	1.37
35	c	519	DGD	O2G-C2G	-2.44	1.40	1.46
23	A	406	CLA	C4B-NB	-2.44	1.34	1.37
23	C	510	CLA	C3B-C2B	2.44	1.49	1.41
23	D	405	CLA	C3D-C4D	-2.44	1.38	1.44
23	d	403	CLA	C3D-C4D	-2.44	1.38	1.44
23	B	608	CLA	C3D-C4D	-2.44	1.38	1.44
23	B	605	CLA	C3D-C4D	-2.44	1.38	1.44
23	B	608	CLA	C3B-C2B	2.44	1.49	1.41
23	b	610	CLA	C4B-NB	-2.43	1.34	1.37
23	a	409	CLA	C4D-CHA	2.43	1.46	1.38
23	b	608	CLA	C3D-C4D	-2.43	1.38	1.44
32	M	101	LMT	O2'-C2'	-2.43	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C3B-C2B	2.42	1.49	1.41
23	B	606	CLA	C3B-C4B	2.42	1.49	1.42
38	e	87	HEM	C1D-ND	-2.42	1.34	1.38
23	c	502	CLA	C1C-C2C	2.42	1.49	1.44
23	b	610	CLA	C3D-C4D	-2.42	1.38	1.44
23	c	503	CLA	C4B-NB	-2.42	1.34	1.37
23	C	512	CLA	C1C-C2C	2.41	1.49	1.44
23	d	403	CLA	C3B-C4B	2.41	1.49	1.42
23	c	502	CLA	C4B-NB	-2.41	1.34	1.37
23	C	512	CLA	C3D-C4D	-2.41	1.38	1.44
23	a	407	CLA	C3B-C4B	2.41	1.49	1.42
23	B	614	CLA	C3D-C4D	-2.41	1.38	1.44
23	C	511	CLA	C4D-CHA	2.40	1.46	1.38
23	b	609	CLA	C1B-C2B	2.40	1.48	1.43
23	C	503	CLA	C1C-C2C	2.40	1.49	1.44
23	b	606	CLA	C4B-NB	-2.40	1.34	1.37
27	A	701	GOL	C3-C2	2.40	1.60	1.51
23	b	611	CLA	C3B-C2B	2.40	1.49	1.41
23	C	507	CLA	C3D-C4D	-2.40	1.38	1.44
23	c	513	CLA	C3B-C4B	2.40	1.49	1.42
23	C	503	CLA	C4C-C3C	2.40	1.49	1.45
23	B	607	CLA	C1C-C2C	2.40	1.49	1.44
23	D	405	CLA	C3B-C2B	2.40	1.49	1.41
23	b	611	CLA	C1C-C2C	2.40	1.49	1.44
23	B	601	CLA	C1B-C2B	2.40	1.48	1.43
23	a	405	CLA	C4C-C3C	2.39	1.49	1.45
23	B	614	CLA	C1C-C2C	2.39	1.49	1.44
23	c	512	CLA	C3B-C2B	2.39	1.49	1.41
23	b	615	CLA	C3D-C4D	-2.39	1.38	1.44
35	C	519	DGD	O2G-C2G	-2.39	1.41	1.46
23	c	509	CLA	C4B-NB	-2.39	1.34	1.37
32	M	101	LMT	O2B-C2B	-2.38	1.37	1.43
23	b	601	CLA	C3B-C4B	2.38	1.49	1.42
32	I	101	LMT	O3'-C3'	-2.38	1.37	1.43
23	b	604	CLA	C4B-NB	-2.38	1.34	1.37
23	C	504	CLA	C3B-C4B	2.38	1.49	1.42
23	c	513	CLA	C4C-C3C	2.38	1.49	1.45
23	b	603	CLA	C3B-C2B	2.38	1.49	1.41
23	a	407	CLA	C3D-C4D	-2.38	1.38	1.44
23	b	613	CLA	C4C-C3C	2.38	1.49	1.45
23	a	405	CLA	C1C-C2C	2.38	1.49	1.44
23	C	509	CLA	C1C-C2C	2.38	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	C3B-C2B	2.38	1.49	1.41
23	B	603	CLA	C1B-C2B	2.37	1.48	1.43
23	b	601	CLA	C1C-C2C	2.37	1.49	1.44
23	D	405	CLA	C1C-C2C	2.37	1.49	1.44
23	C	513	CLA	C1B-C2B	2.37	1.48	1.43
32	b	621	LMT	C3'-C2'	2.37	1.58	1.52
23	b	603	CLA	C3B-C4B	2.36	1.49	1.42
23	c	514	CLA	C3D-C4D	-2.36	1.38	1.44
23	b	606	CLA	C1C-C2C	2.36	1.49	1.44
23	c	505	CLA	C4C-C3C	2.36	1.49	1.45
23	B	604	CLA	C3D-C4D	-2.35	1.38	1.44
23	b	602	CLA	C4B-NB	-2.35	1.34	1.37
23	b	613	CLA	C1C-C2C	2.34	1.49	1.44
23	c	507	CLA	C3D-C4D	-2.34	1.38	1.44
24	a	408	PHO	C1D-ND	-2.34	1.34	1.38
23	d	403	CLA	C4C-C3C	2.34	1.49	1.45
23	b	602	CLA	C4C-C3C	2.34	1.49	1.45
23	B	616	CLA	C3D-C4D	-2.33	1.38	1.44
23	A	404	CLA	C1C-C2C	2.33	1.49	1.44
23	b	609	CLA	C3B-C4B	2.32	1.49	1.42
23	B	614	CLA	C4C-C3C	2.32	1.49	1.45
32	e	102	LMT	O3'-C3'	-2.32	1.37	1.43
23	c	503	CLA	C3B-C2B	2.32	1.49	1.41
23	B	610	CLA	C3B-C4B	2.32	1.49	1.42
23	b	616	CLA	C3D-C4D	-2.32	1.39	1.44
23	C	513	CLA	C3D-C4D	-2.32	1.39	1.44
26	F	101	SQD	O6-C1	2.32	1.44	1.40
23	b	608	CLA	C3B-C2B	2.31	1.49	1.41
23	c	514	CLA	C3B-C4B	2.31	1.49	1.42
32	t	101	LMT	O3'-C3'	-2.31	1.37	1.43
34	B	626	HTG	C1-S1	-2.31	1.76	1.80
23	b	606	CLA	C3B-C4B	2.31	1.49	1.42
34	B	623	HTG	C1'-S1	-2.31	1.78	1.81
23	B	608	CLA	C1C-NC	-2.30	1.34	1.37
23	B	611	CLA	C4D-CHA	2.30	1.46	1.38
23	A	406	CLA	C1C-C2C	2.30	1.49	1.44
23	B	615	CLA	C3B-C4B	2.30	1.49	1.42
23	C	502	CLA	C3D-C4D	-2.30	1.39	1.44
32	M	103	LMT	O3'-C3'	-2.30	1.37	1.43
23	b	607	CLA	C1D-C2D	2.29	1.49	1.45
23	b	609	CLA	C1C-C2C	2.29	1.49	1.44
32	M	101	LMT	O3'-C3'	-2.29	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	o	601	GOL	C1-C2	2.29	1.60	1.51
23	a	406	CLA	C3B-C4B	2.29	1.49	1.42
23	b	611	CLA	C3D-C4D	-2.29	1.39	1.44
23	C	507	CLA	C1C-C2C	2.29	1.49	1.44
23	B	602	CLA	C3B-C2B	2.28	1.48	1.41
38	E	103	HEM	C3C-C4C	-2.28	1.42	1.46
23	c	508	CLA	C4C-C3C	2.28	1.48	1.45
23	b	612	CLA	C4C-C3C	2.28	1.48	1.45
25	d	404	BCR	C30-C25	-2.28	1.50	1.53
23	b	603	CLA	C1C-C2C	2.28	1.49	1.44
40	V	202	HEC	CMA-C3A	2.28	1.55	1.50
23	C	504	CLA	C1C-C2C	2.27	1.49	1.44
38	E	103	HEM	C3B-C4B	2.27	1.49	1.44
23	c	512	CLA	C1C-C2C	2.27	1.49	1.44
23	B	609	CLA	C3D-C4D	-2.27	1.39	1.44
35	C	518	DGD	O5D-C1E	2.27	1.44	1.40
27	b	624	GOL	C3-C2	2.27	1.60	1.51
23	b	610	CLA	C3B-C4B	2.27	1.49	1.42
23	b	602	CLA	C1B-C2B	2.27	1.48	1.43
23	C	508	CLA	C3D-C4D	-2.27	1.39	1.44
23	c	505	CLA	C3B-C2B	2.27	1.48	1.41
23	A	405	CLA	C3D-C4D	-2.26	1.39	1.44
24	A	353	PHO	C1D-ND	-2.26	1.34	1.38
23	C	505	CLA	C3B-C2B	2.26	1.48	1.41
23	b	606	CLA	C3D-C4D	-2.26	1.39	1.44
32	a	420	LMT	O3'-C3'	-2.26	1.37	1.43
23	b	614	CLA	C1C-C2C	2.25	1.49	1.44
35	h	102	DGD	O5D-C1E	2.25	1.44	1.40
23	b	601	CLA	C3B-C2B	2.25	1.48	1.41
23	c	511	CLA	C3B-C4B	2.25	1.49	1.42
27	D	701	GOL	O2-C2	-2.25	1.36	1.43
23	B	605	CLA	C4C-C3C	2.25	1.48	1.45
23	B	615	CLA	C4B-NB	-2.24	1.34	1.37
23	c	512	CLA	C4C-C3C	2.24	1.48	1.45
23	c	507	CLA	C3B-C2B	2.24	1.48	1.41
23	c	513	CLA	C3D-C4D	-2.24	1.39	1.44
23	B	601	CLA	C3B-C2B	2.24	1.48	1.41
23	C	510	CLA	C1C-C2C	2.23	1.49	1.44
23	B	613	CLA	C3B-C2B	2.23	1.48	1.41
23	B	612	CLA	C4C-C3C	2.23	1.48	1.45
23	c	503	CLA	C1C-C2C	2.23	1.49	1.44
29	a	416	PL9	C2-C3	2.22	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	C4C-C3C	2.22	1.48	1.45
23	B	606	CLA	C3D-C4D	-2.22	1.39	1.44
23	A	408	CLA	C3B-C2B	2.22	1.48	1.41
23	b	612	CLA	C3B-C4B	2.22	1.49	1.42
23	c	505	CLA	C3D-C4D	-2.22	1.39	1.44
23	B	603	CLA	C1C-C2C	2.22	1.49	1.44
23	c	505	CLA	C1C-NC	-2.22	1.34	1.37
23	d	403	CLA	C4B-NB	-2.22	1.34	1.37
23	A	404	CLA	C3B-C2B	2.22	1.48	1.41
23	c	509	CLA	C3B-C2B	2.22	1.48	1.41
23	c	511	CLA	C4C-C3C	2.22	1.48	1.45
23	b	614	CLA	C3B-C2B	2.22	1.48	1.41
23	B	607	CLA	C3B-C4B	2.21	1.49	1.42
23	c	502	CLA	C3B-C4B	2.21	1.49	1.42
23	D	405	CLA	C4C-C3C	2.21	1.48	1.45
23	c	503	CLA	C3B-C4B	2.21	1.49	1.42
23	c	513	CLA	C1C-C2C	2.21	1.49	1.44
35	c	518	DGD	O2G-C2G	-2.21	1.41	1.46
40	v	202	HEC	CMD-C2D	2.20	1.55	1.50
23	b	604	CLA	C3B-C2B	2.20	1.48	1.41
23	b	605	CLA	C1C-C2C	2.20	1.49	1.44
23	C	514	CLA	C3D-C4D	-2.20	1.39	1.44
32	a	414	LMT	O2'-C2'	-2.20	1.37	1.43
23	a	409	CLA	C4C-C3C	2.20	1.48	1.45
23	A	408	CLA	C4C-C3C	2.20	1.48	1.45
23	B	615	CLA	C3D-C4D	-2.20	1.39	1.44
23	b	614	CLA	C3B-C4B	2.20	1.49	1.42
38	E	103	HEM	C1D-ND	-2.19	1.34	1.38
23	C	503	CLA	C3B-C2B	2.19	1.48	1.41
23	C	513	CLA	C4B-NB	-2.19	1.35	1.37
23	B	609	CLA	C4C-C3C	2.19	1.48	1.45
23	b	605	CLA	C3D-C4D	-2.19	1.39	1.44
32	A	359	LMT	O3'-C3'	-2.19	1.37	1.43
23	b	608	CLA	C1C-C2C	2.19	1.49	1.44
23	B	612	CLA	C3D-C4D	-2.19	1.39	1.44
23	b	609	CLA	C3D-C4D	-2.18	1.39	1.44
23	B	604	CLA	C3B-C2B	2.18	1.48	1.41
23	c	511	CLA	C3D-C4D	-2.18	1.39	1.44
27	A	701	GOL	O2-C2	-2.18	1.37	1.43
23	C	511	CLA	C3D-C4D	-2.18	1.39	1.44
23	A	408	CLA	C1C-NC	-2.18	1.34	1.37
32	E	102	LMT	O3'-C3'	-2.18	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	405	CLA	C3B-C2B	2.18	1.48	1.41
23	C	514	CLA	C3B-C4B	2.17	1.49	1.42
23	c	509	CLA	C1B-NB	-2.17	1.35	1.37
23	C	506	CLA	C3D-C4D	-2.17	1.39	1.44
23	b	610	CLA	C3B-C2B	2.17	1.48	1.41
32	m	103	LMT	C3'-C2'	2.17	1.58	1.52
23	C	510	CLA	C1D-C2D	2.17	1.49	1.45
23	b	603	CLA	C4C-C3C	2.17	1.48	1.45
23	b	613	CLA	C3B-C2B	2.17	1.48	1.41
23	B	615	CLA	C4C-C3C	2.16	1.48	1.45
24	a	353	PHO	C1B-NB	-2.16	1.34	1.38
32	D	404	LMT	O3'-C3'	-2.16	1.37	1.43
23	b	605	CLA	C3B-C4B	2.16	1.49	1.42
23	b	605	CLA	C3B-C2B	2.16	1.48	1.41
23	C	507	CLA	C3B-C4B	2.16	1.49	1.42
23	B	608	CLA	C3B-C4B	2.16	1.49	1.42
23	B	613	CLA	C1C-C2C	2.16	1.48	1.44
23	C	512	CLA	C1C-NC	-2.16	1.34	1.37
23	C	507	CLA	C3B-C2B	2.16	1.48	1.41
23	b	607	CLA	C1A-CHA	2.16	1.52	1.43
23	C	503	CLA	C3B-C4B	2.16	1.49	1.42
23	c	514	CLA	C1D-C2D	2.16	1.49	1.45
23	B	601	CLA	C3D-C4D	-2.15	1.39	1.44
23	C	510	CLA	C3B-C4B	2.15	1.49	1.42
32	D	404	LMT	O5'-C5'	-2.15	1.39	1.44
40	v	202	HEC	CMC-C2C	2.15	1.55	1.50
23	b	616	CLA	C3B-C2B	2.15	1.48	1.41
23	B	616	CLA	C1C-NC	-2.15	1.34	1.37
23	B	603	CLA	C3D-C4D	-2.15	1.39	1.44
23	C	508	CLA	C4C-C3C	2.14	1.48	1.45
23	C	505	CLA	C3D-C4D	-2.14	1.39	1.44
23	C	513	CLA	C3B-C2B	2.14	1.48	1.41
23	b	604	CLA	C3B-C4B	2.14	1.49	1.42
23	C	505	CLA	C4C-C3C	2.13	1.48	1.45
23	b	604	CLA	C4C-C3C	2.13	1.48	1.45
23	a	407	CLA	C4C-C3C	2.13	1.48	1.45
23	C	502	CLA	C4C-C3C	2.13	1.48	1.45
23	D	406	CLA	C4B-NB	-2.13	1.35	1.37
23	C	505	CLA	C3B-C4B	2.13	1.48	1.42
23	b	601	CLA	C4C-C3C	2.13	1.48	1.45
23	c	510	CLA	C3B-C2B	2.13	1.48	1.41
38	E	103	HEM	C1C-C2C	-2.13	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	C1C-C2C	2.13	1.48	1.44
23	A	406	CLA	C3D-C4D	-2.12	1.39	1.44
32	a	414	LMT	O2B-C2B	-2.12	1.37	1.43
24	A	407	PHO	C1B-NB	-2.12	1.34	1.38
23	C	502	CLA	C3B-C2B	2.12	1.48	1.41
23	c	510	CLA	C3D-C4D	-2.12	1.39	1.44
37	d	711	LHG	O7-C5	-2.12	1.41	1.46
23	B	604	CLA	C3B-C4B	2.12	1.48	1.42
29	A	414	PL9	C2-C1	-2.12	1.39	1.44
27	c	743	GOL	C3-C2	2.11	1.59	1.51
23	c	502	CLA	C3B-C2B	2.11	1.48	1.41
23	c	507	CLA	C1C-C2C	2.11	1.48	1.44
23	a	405	CLA	C3D-C4D	-2.11	1.39	1.44
23	c	505	CLA	C3B-C4B	2.11	1.48	1.42
23	b	604	CLA	C1A-CHA	2.11	1.51	1.43
27	a	801	GOL	C1-C2	2.11	1.59	1.51
23	b	606	CLA	C3B-C2B	2.10	1.48	1.41
23	c	507	CLA	C3B-C4B	2.10	1.48	1.42
23	B	603	CLA	C4C-C3C	2.10	1.48	1.45
23	b	611	CLA	C4B-NB	-2.10	1.35	1.37
26	a	413	SQD	O6-C1	2.10	1.43	1.40
23	d	402	CLA	C3B-C2B	2.10	1.48	1.41
23	b	614	CLA	C3D-C4D	-2.10	1.39	1.44
23	C	511	CLA	C3B-C2B	2.09	1.48	1.41
23	b	615	CLA	C3B-C2B	2.09	1.48	1.41
23	b	613	CLA	C3D-C4D	-2.09	1.39	1.44
23	B	606	CLA	C3B-C2B	2.09	1.48	1.41
37	D	410	LHG	O7-C5	-2.08	1.41	1.46
23	c	514	CLA	C3B-C2B	2.08	1.48	1.41
24	A	407	PHO	C4B-NB	-2.08	1.34	1.38
23	b	614	CLA	C4C-C3C	2.07	1.48	1.45
23	b	616	CLA	C4B-NB	-2.07	1.35	1.37
23	c	508	CLA	C3D-C4D	-2.07	1.39	1.44
23	C	508	CLA	C3B-C2B	2.07	1.48	1.41
23	A	406	CLA	C1C-NC	-2.07	1.34	1.37
26	B	620	SQD	O6-C1	2.06	1.43	1.40
32	M	103	LMT	O3B-C3B	-2.06	1.37	1.43
23	c	509	CLA	C3D-C4D	-2.06	1.39	1.44
23	B	611	CLA	C3D-C4D	-2.06	1.39	1.44
23	B	603	CLA	C3B-C4B	2.06	1.48	1.42
23	c	506	CLA	C3B-C2B	2.05	1.48	1.41
23	B	615	CLA	MG-NA	2.05	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	414	LMT	O3'-C3'	-2.05	1.37	1.43
23	C	512	CLA	C3B-C4B	2.05	1.48	1.42
40	v	202	HEC	C3B-C2B	-2.05	1.34	1.41
23	D	406	CLA	C3D-C4D	-2.05	1.39	1.44
29	A	414	PL9	C2-C3	2.05	1.39	1.34
23	B	611	CLA	C1D-C2D	2.05	1.49	1.45
23	A	404	CLA	C3D-C4D	-2.04	1.39	1.44
37	l	101	LHG	O7-C5	-2.04	1.41	1.46
27	V	401	GOL	C1-C2	2.04	1.59	1.51
23	a	406	CLA	C1C-C2C	2.04	1.48	1.44
23	b	613	CLA	C3B-C4B	2.04	1.48	1.42
32	m	103	LMT	O2B-C2B	-2.04	1.37	1.43
23	C	503	CLA	C3D-C4D	-2.04	1.39	1.44
24	a	408	PHO	CHA-CBD	-2.03	1.49	1.51
23	b	601	CLA	C3D-C4D	-2.03	1.39	1.44
23	C	509	CLA	C3D-C4D	-2.03	1.39	1.44
23	b	615	CLA	C3B-C4B	2.03	1.48	1.42
32	m	103	LMT	O3'-C3'	-2.03	1.37	1.43
23	b	608	CLA	C3B-C4B	2.03	1.48	1.42
23	b	615	CLA	C4B-NB	-2.03	1.35	1.37
24	a	353	PHO	C1D-ND	-2.03	1.35	1.38
37	L	101	LHG	O7-C5	-2.02	1.41	1.46
23	B	610	CLA	C3D-C4D	-2.02	1.39	1.44
23	C	512	CLA	C1A-CHA	2.02	1.51	1.43
23	B	614	CLA	C3B-C2B	2.02	1.48	1.41
23	C	511	CLA	C3B-C4B	2.02	1.48	1.42
32	t	101	LMT	O2'-C2'	-2.02	1.38	1.43
23	c	506	CLA	C3D-C4D	-2.02	1.39	1.44
26	b	620	SQD	O6-C1	2.02	1.43	1.40
23	c	502	CLA	C1C-NC	-2.02	1.34	1.37
23	C	513	CLA	C4C-C3C	2.01	1.48	1.45
23	C	508	CLA	C1D-C2D	2.01	1.49	1.45
23	B	604	CLA	C1C-C2C	2.01	1.48	1.44
32	I	101	LMT	O2'-C2'	-2.01	1.38	1.43
23	c	512	CLA	C3B-C4B	2.00	1.48	1.42
33	Z	101	LMG	O1-C1	2.00	1.43	1.40
24	a	353	PHO	CHA-CBD	-2.00	1.49	1.51
23	b	608	CLA	C4C-C3C	2.00	1.48	1.45

All (2881) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C3B-C2B-C1B	-13.30	91.49	107.17
23	B	611	CLA	C1D-ND-C4D	-11.86	97.99	106.31
24	A	407	PHO	C2D-C1D-ND	11.49	117.73	109.43
24	a	353	PHO	C2D-C1D-ND	10.99	117.38	109.43
24	a	408	PHO	C2D-C1D-ND	10.81	117.24	109.43
23	B	612	CLA	C1D-ND-C4D	-10.75	98.77	106.31
23	a	409	CLA	C1D-ND-C4D	-10.64	98.85	106.31
24	A	353	PHO	C2D-C1D-ND	10.58	117.08	109.43
23	B	611	CLA	C2B-C1B-NB	10.48	121.20	110.33
23	B	601	CLA	C1D-ND-C4D	-10.21	99.15	106.31
23	C	514	CLA	C1D-ND-C4D	-10.04	99.27	106.31
23	B	606	CLA	C1D-ND-C4D	-10.00	99.30	106.31
23	b	611	CLA	C1D-ND-C4D	-9.99	99.31	106.31
23	b	607	CLA	C1D-ND-C4D	-9.96	99.33	106.31
40	v	202	HEC	CBB-CAB-C3B	-9.90	107.64	127.43
23	c	506	CLA	C1D-ND-C4D	-9.90	99.37	106.31
23	b	603	CLA	C1D-ND-C4D	-9.86	99.40	106.31
23	d	403	CLA	C1D-ND-C4D	-9.76	99.46	106.31
23	A	408	CLA	C1D-ND-C4D	-9.71	99.50	106.31
23	c	514	CLA	C1D-ND-C4D	-9.68	99.52	106.31
23	b	605	CLA	C1D-ND-C4D	-9.67	99.53	106.31
23	B	614	CLA	C1D-ND-C4D	-9.66	99.53	106.31
23	C	504	CLA	C1D-ND-C4D	-9.63	99.56	106.31
23	C	502	CLA	C1D-ND-C4D	-9.57	99.60	106.31
23	c	504	CLA	C1D-ND-C4D	-9.49	99.65	106.31
23	b	614	CLA	C1D-ND-C4D	-9.48	99.66	106.31
23	C	511	CLA	C1D-ND-C4D	-9.45	99.68	106.31
23	B	615	CLA	C1D-ND-C4D	-9.44	99.69	106.31
24	a	408	PHO	O2D-CGD-CBD	9.43	121.31	110.95
23	B	605	CLA	C1D-ND-C4D	-9.43	99.70	106.31
23	b	610	CLA	C1D-ND-C4D	-9.41	99.71	106.31
23	C	506	CLA	C1D-ND-C4D	-9.40	99.72	106.31
23	b	601	CLA	C1D-ND-C4D	-9.39	99.72	106.31
23	B	610	CLA	C1D-ND-C4D	-9.38	99.73	106.31
23	C	510	CLA	C1D-ND-C4D	-9.36	99.74	106.31
23	c	512	CLA	C1D-ND-C4D	-9.35	99.75	106.31
23	B	603	CLA	C1D-ND-C4D	-9.34	99.76	106.31
23	b	616	CLA	C1D-ND-C4D	-9.27	99.81	106.31
23	C	505	CLA	C1D-ND-C4D	-9.27	99.81	106.31
23	b	612	CLA	C1D-ND-C4D	-9.27	99.81	106.31
23	a	407	CLA	C1D-ND-C4D	-9.26	99.82	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	405	CLA	C1D-ND-C4D	-9.24	99.83	106.31
23	c	503	CLA	C1D-ND-C4D	-9.22	99.84	106.31
40	V	202	HEC	CBB-CAB-C3B	-9.22	109.01	127.43
23	b	615	CLA	C1D-ND-C4D	-9.20	99.86	106.31
23	c	502	CLA	C1D-ND-C4D	-9.20	99.86	106.31
23	c	507	CLA	C1D-ND-C4D	-9.18	99.87	106.31
23	d	402	CLA	C1D-ND-C4D	-9.17	99.88	106.31
23	A	406	CLA	C1D-ND-C4D	-9.16	99.89	106.31
23	b	602	CLA	C1D-ND-C4D	-9.12	99.91	106.31
23	C	503	CLA	C1D-ND-C4D	-9.12	99.91	106.31
23	a	406	CLA	C1D-ND-C4D	-9.12	99.91	106.31
23	C	513	CLA	C1D-ND-C4D	-9.10	99.92	106.31
23	c	510	CLA	C1D-ND-C4D	-9.09	99.94	106.31
23	B	616	CLA	C1D-ND-C4D	-9.09	99.94	106.31
24	a	353	PHO	O2D-CGD-CBD	9.07	120.91	110.95
23	B	607	CLA	C1D-ND-C4D	-9.05	99.96	106.31
23	C	507	CLA	C1D-ND-C4D	-9.05	99.96	106.31
23	c	508	CLA	C1D-ND-C4D	-9.05	99.96	106.31
23	b	606	CLA	C1D-ND-C4D	-9.04	99.97	106.31
23	B	609	CLA	C1D-ND-C4D	-9.03	99.98	106.31
23	b	609	CLA	C1D-ND-C4D	-8.99	100.00	106.31
23	A	405	CLA	C1D-ND-C4D	-8.99	100.01	106.31
23	B	602	CLA	C1D-ND-C4D	-8.97	100.02	106.31
23	a	405	CLA	C1D-ND-C4D	-8.91	100.06	106.31
23	B	613	CLA	C1D-ND-C4D	-8.89	100.08	106.31
23	C	508	CLA	C1D-ND-C4D	-8.87	100.09	106.31
23	b	613	CLA	C1D-ND-C4D	-8.82	100.12	106.31
23	D	406	CLA	C1D-ND-C4D	-8.82	100.12	106.31
24	A	407	PHO	C3B-C4B-NB	8.75	113.17	107.46
23	c	511	CLA	C1D-ND-C4D	-8.72	100.19	106.31
23	B	608	CLA	C1D-ND-C4D	-8.71	100.20	106.31
23	c	505	CLA	C1D-ND-C4D	-8.70	100.21	106.31
23	C	512	CLA	C1D-ND-C4D	-8.66	100.24	106.31
24	A	353	PHO	O2D-CGD-CBD	8.64	120.44	110.95
23	c	509	CLA	C1D-ND-C4D	-8.59	100.28	106.31
23	C	509	CLA	C1D-ND-C4D	-8.59	100.29	106.31
23	A	404	CLA	C1D-ND-C4D	-8.57	100.30	106.31
23	b	608	CLA	C1D-ND-C4D	-8.50	100.35	106.31
23	c	513	CLA	C1D-ND-C4D	-8.45	100.39	106.31
23	b	602	CLA	C4A-NA-C1A	-8.31	102.89	106.68
23	b	604	CLA	C1D-ND-C4D	-8.25	100.52	106.31
24	a	408	PHO	C3B-C4B-NB	8.10	112.75	107.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	353	PHO	C3B-C4B-NB	7.89	112.61	107.46
23	B	611	CLA	CHD-C4C-C3C	-7.64	113.63	124.77
24	A	353	PHO	C3B-C4B-NB	7.61	112.43	107.46
23	B	604	CLA	C1D-ND-C4D	-7.60	100.98	106.31
26	F	101	SQD	O6-C1-C2	7.39	119.50	108.27
23	B	611	CLA	CMD-C2D-C1D	7.36	137.69	124.73
23	B	606	CLA	CMD-C2D-C1D	7.28	137.55	124.73
24	A	353	PHO	C2B-C1B-NB	7.26	114.68	109.43
23	B	611	CLA	C2D-C1D-ND	7.24	117.29	110.13
24	A	407	PHO	O2D-CGD-CBD	7.23	118.89	110.95
23	c	502	CLA	CMD-C2D-C1D	7.22	137.45	124.73
23	B	605	CLA	CHD-C4C-C3C	-7.16	114.33	124.77
23	C	511	CLA	CMD-C2D-C1D	7.14	137.29	124.73
23	B	606	CLA	C4A-NA-C1A	-7.11	103.44	106.68
23	B	611	CLA	CMB-C2B-C1B	7.10	136.22	125.42
23	C	508	CLA	CMD-C2D-C1D	7.09	137.22	124.73
23	c	514	CLA	CMD-C2D-C1D	7.05	137.15	124.73
23	D	405	CLA	C4A-NA-C1A	-7.05	103.46	106.68
23	B	611	CLA	CHB-C1B-NB	-7.00	113.55	124.05
23	c	508	CLA	O2D-CGD-CBD	7.00	123.46	111.23
23	c	504	CLA	CMD-C2D-C1D	6.99	137.03	124.73
23	d	403	CLA	CMD-C2D-C1D	6.98	137.02	124.73
23	b	616	CLA	C4A-NA-C1A	-6.97	103.50	106.68
23	b	611	CLA	CMD-C2D-C1D	6.97	137.00	124.73
23	B	616	CLA	O2D-CGD-CBD	6.96	123.40	111.23
23	b	601	CLA	O2D-CGD-CBD	6.96	123.40	111.23
23	a	409	CLA	C2D-C1D-ND	6.94	117.00	110.13
23	B	616	CLA	CHD-C4C-C3C	-6.92	114.68	124.77
23	B	603	CLA	O2D-CGD-CBD	6.92	123.32	111.23
23	c	508	CLA	CMD-C2D-C1D	6.91	136.89	124.73
23	B	609	CLA	C4A-NA-C1A	-6.90	103.53	106.68
23	b	611	CLA	C2D-C1D-ND	6.90	116.95	110.13
23	b	606	CLA	CMD-C2D-C1D	6.88	136.84	124.73
23	a	409	CLA	CHD-C4C-C3C	-6.86	114.77	124.77
23	B	614	CLA	C2D-C1D-ND	6.85	116.90	110.13
23	b	616	CLA	O2D-CGD-CBD	6.81	123.14	111.23
23	b	614	CLA	C2D-C1D-ND	6.80	116.86	110.13
23	b	615	CLA	C4A-NA-C1A	-6.79	103.58	106.68
23	C	505	CLA	C2D-C1D-ND	6.77	116.82	110.13
23	B	601	CLA	CHD-C4C-C3C	-6.75	114.93	124.77
23	B	612	CLA	C2D-C1D-ND	6.74	116.80	110.13
24	a	353	PHO	C2B-C1B-NB	6.74	114.30	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	CHD-C4C-C3C	-6.72	114.98	124.77
23	C	508	CLA	O2D-CGD-CBD	6.71	122.97	111.23
23	b	606	CLA	C4A-NA-C1A	-6.71	103.62	106.68
23	A	404	CLA	CMD-C2D-C1D	6.70	136.53	124.73
23	B	614	CLA	CMD-C2D-C1D	6.68	136.50	124.73
23	B	610	CLA	C2D-C1D-ND	6.67	116.73	110.13
23	b	616	CLA	CHD-C4C-C3C	-6.66	115.07	124.77
23	b	613	CLA	C2D-C1D-ND	6.65	116.71	110.13
26	A	410	SQD	O6-C1-C2	6.64	118.36	108.27
23	C	513	CLA	CHD-C4C-C3C	-6.63	115.11	124.77
23	b	605	CLA	CHD-C4C-C3C	-6.63	115.11	124.77
23	a	406	CLA	CHD-C4C-C3C	-6.62	115.12	124.77
23	C	504	CLA	CMD-C2D-C1D	6.60	136.35	124.73
23	B	615	CLA	C2D-C1D-ND	6.60	116.66	110.13
23	B	616	CLA	C2D-C1D-ND	6.59	116.65	110.13
23	b	607	CLA	C2D-C1D-ND	6.59	116.65	110.13
23	B	606	CLA	CHD-C4C-C3C	-6.59	115.17	124.77
23	B	606	CLA	C2D-C1D-ND	6.58	116.64	110.13
23	C	513	CLA	C4A-NA-C1A	-6.58	103.68	106.68
23	C	514	CLA	C2D-C1D-ND	6.56	116.62	110.13
23	B	601	CLA	C2D-C1D-ND	6.54	116.60	110.13
23	B	615	CLA	CHD-C4C-C3C	-6.53	115.25	124.77
23	B	601	CLA	CMD-C2D-C1D	6.52	136.21	124.73
23	C	514	CLA	CHD-C4C-C3C	-6.52	115.27	124.77
23	a	406	CLA	C2D-C1D-ND	6.50	116.56	110.13
23	c	504	CLA	C4A-NA-C1A	-6.49	103.72	106.68
23	b	605	CLA	CMD-C2D-C1D	6.49	136.16	124.73
23	A	408	CLA	C2D-C1D-ND	6.48	116.54	110.13
23	b	616	CLA	CMD-C2D-C1D	6.48	136.15	124.73
23	b	612	CLA	CHD-C4C-C3C	-6.48	115.33	124.77
23	b	610	CLA	CHD-C4C-C3C	-6.47	115.35	124.77
23	C	506	CLA	CMD-C2D-C1D	6.46	136.10	124.73
23	c	503	CLA	CHD-C4C-C3C	-6.43	115.39	124.77
23	a	407	CLA	C2D-C1D-ND	6.42	116.48	110.13
23	a	407	CLA	CHD-C4C-C3C	-6.41	115.43	124.77
23	b	613	CLA	CHD-C4C-C3C	-6.39	115.46	124.77
23	b	609	CLA	CHD-C4C-C3C	-6.39	115.46	124.77
23	b	614	CLA	O2D-CGD-CBD	6.38	122.39	111.23
23	B	608	CLA	C2D-C1D-ND	6.38	116.44	110.13
23	C	504	CLA	C4A-NA-C1A	-6.37	103.77	106.68
23	C	508	CLA	CHD-C4C-C3C	-6.36	115.50	124.77
24	a	408	PHO	C2B-C1B-NB	6.33	114.01	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	C2D-C1D-ND	6.31	116.38	110.13
23	D	405	CLA	C2D-C1D-ND	6.30	116.37	110.13
23	B	613	CLA	C2D-C1D-ND	6.30	116.36	110.13
23	A	408	CLA	CMD-C2D-C1D	6.30	135.82	124.73
23	A	404	CLA	C4A-NA-C1A	-6.29	103.81	106.68
24	A	407	PHO	C4D-ND-C1D	-6.28	101.35	108.87
23	B	603	CLA	CHD-C4C-C3C	-6.27	115.62	124.77
23	c	507	CLA	CMD-C2D-C1D	6.27	135.76	124.73
23	B	610	CLA	CHD-C4C-C3C	-6.26	115.64	124.77
23	B	610	CLA	O2D-CGD-CBD	6.26	122.17	111.23
23	c	511	CLA	CHD-C4C-C3C	-6.25	115.66	124.77
23	b	614	CLA	CHD-C4C-C3C	-6.24	115.67	124.77
23	b	615	CLA	C2D-C1D-ND	6.24	116.30	110.13
23	B	601	CLA	O2D-CGD-CBD	6.24	122.14	111.23
23	b	605	CLA	C2D-C1D-ND	6.22	116.28	110.13
23	c	512	CLA	CMD-C2D-C1D	6.21	135.67	124.73
23	B	602	CLA	C4A-NA-C1A	-6.21	103.84	106.68
23	c	506	CLA	CMD-C2D-C1D	6.21	135.66	124.73
23	B	605	CLA	CMD-C2D-C1D	6.21	135.66	124.73
23	c	510	CLA	CMD-C2D-C1D	6.21	135.66	124.73
23	C	513	CLA	C2D-C1D-ND	6.19	116.25	110.13
23	C	502	CLA	O2D-CGD-CBD	6.18	122.03	111.23
26	F	101	SQD	O47-C7-C8	6.18	124.85	111.48
23	B	605	CLA	C2D-C1D-ND	6.18	116.24	110.13
23	B	606	CLA	O2D-CGD-CBD	6.17	122.01	111.23
23	C	504	CLA	C2D-C1D-ND	6.15	116.21	110.13
23	b	609	CLA	C4A-NA-C1A	-6.14	103.88	106.68
23	c	506	CLA	C4A-NA-C1A	-6.14	103.88	106.68
23	b	601	CLA	CHD-C4C-C3C	-6.13	115.84	124.77
23	b	601	CLA	CMD-C2D-C1D	6.13	135.52	124.73
23	b	603	CLA	CHD-C4C-C3C	-6.12	115.85	124.77
23	A	405	CLA	C2D-C1D-ND	6.12	116.18	110.13
23	b	604	CLA	O2D-CGD-CBD	6.12	121.92	111.23
23	c	510	CLA	C1-C2-C3	-6.12	116.18	126.20
23	c	505	CLA	CMD-C2D-C1D	6.11	135.49	124.73
23	c	503	CLA	C2D-C1D-ND	6.11	116.17	110.13
23	B	609	CLA	CHD-C4C-C3C	-6.11	115.87	124.77
23	C	507	CLA	CMD-C2D-C1D	6.10	135.48	124.73
23	C	502	CLA	C4A-NA-C1A	-6.10	103.90	106.68
23	C	510	CLA	C4A-NA-C1A	-6.10	103.90	106.68
23	C	509	CLA	C2C-C1C-NC	6.10	116.39	109.98
23	B	607	CLA	C2D-C1D-ND	6.10	116.16	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	405	CLA	CMD-C2D-C1D	6.10	135.47	124.73
23	C	509	CLA	CHD-C4C-C3C	-6.10	115.88	124.77
23	B	604	CLA	CMD-C2D-C1D	6.09	135.46	124.73
23	B	602	CLA	CMD-C2D-C1D	6.09	135.45	124.73
23	c	509	CLA	C2D-C1D-ND	6.08	116.14	110.13
23	C	502	CLA	CHD-C4C-C3C	-6.08	115.91	124.77
23	b	603	CLA	C4A-NA-C1A	-6.08	103.91	106.68
23	c	504	CLA	CHD-C4C-C3C	-6.08	115.91	124.77
23	c	511	CLA	C2D-C1D-ND	6.07	116.13	110.13
23	a	405	CLA	CMD-C2D-C1D	6.07	135.41	124.73
23	C	509	CLA	C2D-C1D-ND	6.07	116.13	110.13
23	b	607	CLA	C2C-C1C-NC	6.06	116.35	109.98
23	B	612	CLA	CHD-C4C-C3C	-6.06	115.94	124.77
23	B	603	CLA	C2D-C1D-ND	6.05	116.11	110.13
23	A	406	CLA	C2D-C1D-ND	6.05	116.11	110.13
23	B	609	CLA	C2D-C1D-ND	6.04	116.11	110.13
23	b	609	CLA	C2D-C1D-ND	6.04	116.11	110.13
23	c	505	CLA	C2D-C1D-ND	6.04	116.11	110.13
23	c	508	CLA	CHD-C4C-C3C	-6.03	115.97	124.77
23	C	503	CLA	C2D-C1D-ND	6.03	116.10	110.13
23	a	405	CLA	C4A-NA-C1A	-6.03	103.93	106.68
23	c	513	CLA	CMD-C2D-C1D	6.03	135.35	124.73
23	b	604	CLA	CHD-C4C-C3C	-6.03	115.98	124.77
23	b	605	CLA	C4A-NA-C1A	-6.02	103.93	106.68
23	B	610	CLA	CMD-C2D-C1D	6.02	135.34	124.73
23	a	407	CLA	C4A-NA-C1A	-6.02	103.93	106.68
23	C	502	CLA	CMD-C2D-C1D	6.02	135.33	124.73
23	B	614	CLA	CHD-C4C-C3C	-6.02	116.00	124.77
23	D	406	CLA	C4A-NA-C1A	-6.01	103.94	106.68
26	B	620	SQD	O6-C1-C2	6.01	117.39	108.27
23	c	508	CLA	C2D-C1D-ND	6.00	116.07	110.13
23	c	502	CLA	C2D-C1D-ND	6.00	116.07	110.13
23	b	604	CLA	C1-C2-C3	-6.00	116.36	126.20
24	A	407	PHO	C2B-C1B-NB	6.00	113.77	109.43
23	b	610	CLA	C2D-C1D-ND	6.00	116.06	110.13
34	b	623	HTG	C1'-S1-C1	5.99	113.38	100.45
23	C	506	CLA	CHD-C4C-C3C	-5.98	116.05	124.77
23	c	512	CLA	C2D-C1D-ND	5.98	116.05	110.13
23	b	612	CLA	C2D-C1D-ND	5.98	116.04	110.13
23	b	615	CLA	CHD-C4C-C3C	-5.97	116.06	124.77
23	c	512	CLA	CHD-C4C-C3C	-5.96	116.08	124.77
23	b	602	CLA	O2D-CGD-CBD	5.95	121.64	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	C4A-NA-C1A	-5.95	103.96	106.68
23	C	508	CLA	C4A-NA-C1A	-5.95	103.96	106.68
23	b	602	CLA	CMD-C2D-C1D	5.95	135.20	124.73
23	B	615	CLA	CMD-C2D-C1D	5.95	135.20	124.73
23	b	606	CLA	CHD-C4C-C3C	-5.94	116.11	124.77
23	b	601	CLA	C2D-C1D-ND	5.94	116.00	110.13
23	a	406	CLA	CMD-C2D-C1D	5.93	135.16	124.73
23	b	616	CLA	C2D-C1D-ND	5.92	115.98	110.13
23	C	508	CLA	C2D-C1D-ND	5.91	115.98	110.13
23	C	503	CLA	CHD-C4C-C3C	-5.91	116.16	124.77
23	C	502	CLA	C2D-C1D-ND	5.91	115.97	110.13
23	d	403	CLA	C2D-C1D-ND	5.90	115.97	110.13
23	b	610	CLA	CMD-C2D-C1D	5.90	135.12	124.73
23	B	602	CLA	CHD-C4C-C3C	-5.90	116.17	124.77
23	D	406	CLA	C2D-C1D-ND	5.90	115.97	110.13
23	C	511	CLA	CHD-C4C-C3C	-5.90	116.18	124.77
23	c	509	CLA	CHD-C4C-C3C	-5.89	116.18	124.77
23	B	614	CLA	C4A-NA-C1A	-5.89	103.99	106.68
23	C	504	CLA	CHD-C4C-C3C	-5.89	116.19	124.77
23	A	406	CLA	CMD-C2D-C1D	5.89	135.10	124.73
23	B	608	CLA	CHD-C4C-C3C	-5.88	116.20	124.77
23	B	605	CLA	C4A-NA-C1A	-5.88	104.00	106.68
26	a	411	SQD	O6-C1-C2	5.87	117.19	108.27
23	b	615	CLA	CMD-C2D-C1D	5.87	135.06	124.73
23	c	506	CLA	O2D-CGD-CBD	5.86	121.48	111.23
23	c	504	CLA	C2D-C1D-ND	5.86	115.93	110.13
23	B	609	CLA	CMD-C2D-C1D	5.86	135.04	124.73
23	B	603	CLA	C4A-NA-C1A	-5.85	104.01	106.68
23	A	406	CLA	CHD-C4C-C3C	-5.85	116.25	124.77
23	b	607	CLA	CHD-C4C-C3C	-5.84	116.25	124.77
23	c	506	CLA	C2D-C1D-ND	5.83	115.90	110.13
23	C	512	CLA	CHD-C4C-C3C	-5.82	116.28	124.77
23	B	602	CLA	C2D-C1D-ND	5.81	115.88	110.13
23	c	510	CLA	C2D-C1D-ND	5.81	115.88	110.13
23	b	607	CLA	CMD-C2D-C1D	5.80	134.94	124.73
23	d	402	CLA	C2D-C1D-ND	5.80	115.87	110.13
24	a	353	PHO	C1-C2-C3	-5.78	116.72	126.20
23	d	402	CLA	C2C-C1C-NC	5.78	116.05	109.98
23	B	611	CLA	O2D-CGD-CBD	5.78	121.33	111.23
23	C	505	CLA	CHD-C4C-C3C	-5.77	116.35	124.77
23	A	405	CLA	CHD-C4C-C3C	-5.77	116.36	124.77
23	C	510	CLA	CMD-C2D-C1D	5.77	134.89	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	C4A-NA-C1A	-5.77	104.05	106.68
23	c	514	CLA	C2D-C1D-ND	5.77	115.83	110.13
23	B	603	CLA	CMD-C2D-C1D	5.76	134.88	124.73
23	C	507	CLA	C2C-C1C-NC	5.76	116.03	109.98
23	c	511	CLA	CMD-C2D-C1D	5.75	134.86	124.73
23	C	510	CLA	C2D-C1D-ND	5.75	115.82	110.13
23	B	614	CLA	O2D-CGD-CBD	5.75	121.28	111.23
24	a	353	PHO	C4D-ND-C1D	-5.74	101.99	108.87
23	B	607	CLA	CMD-C2D-C1D	5.74	134.84	124.73
23	c	507	CLA	C2D-C1D-ND	5.72	115.79	110.13
23	C	513	CLA	O2D-CGD-CBD	5.72	121.22	111.23
23	C	507	CLA	C2D-C1D-ND	5.71	115.77	110.13
23	d	403	CLA	CHD-C4C-C3C	-5.69	116.47	124.77
23	D	406	CLA	CHD-C4C-C3C	-5.69	116.47	124.77
23	A	408	CLA	CHD-C4C-C3C	-5.69	116.48	124.77
26	A	410	SQD	C1-O5-C5	-5.69	102.61	113.72
24	A	407	PHO	C3D-C4D-ND	5.69	115.00	107.71
23	C	512	CLA	C2D-C1D-ND	5.68	115.75	110.13
23	b	608	CLA	CMD-C2D-C1D	5.68	134.73	124.73
23	B	613	CLA	C1-C2-C3	-5.67	116.90	126.20
23	C	511	CLA	C2D-C1D-ND	5.67	115.74	110.13
23	A	404	CLA	C2D-C1D-ND	5.67	115.73	110.13
23	b	608	CLA	CHD-C4C-C3C	-5.66	116.52	124.77
23	c	506	CLA	CHD-C4C-C3C	-5.66	116.52	124.77
23	C	505	CLA	CMD-C2D-C1D	5.64	134.66	124.73
23	c	502	CLA	CHD-C4C-C3C	-5.63	116.56	124.77
23	b	604	CLA	C2C-C1C-NC	5.63	115.90	109.98
34	c	522	HTG	C1'-S1-C1	5.62	112.60	100.45
23	b	603	CLA	O2D-CGD-CBD	5.62	121.06	111.23
23	c	514	CLA	CHD-C4C-C3C	-5.62	116.58	124.77
23	c	505	CLA	CHD-C4C-C3C	-5.62	116.59	124.77
23	b	610	CLA	O2D-CGD-CBD	5.61	121.03	111.23
23	A	408	CLA	C2C-C1C-NC	5.60	115.87	109.98
25	D	407	BCR	C7-C8-C9	-5.60	117.94	126.23
23	b	613	CLA	C4A-NA-C1A	-5.60	104.12	106.68
23	b	606	CLA	C2D-C1D-ND	5.59	115.66	110.13
23	b	604	CLA	CMD-C2D-C1D	5.59	134.57	124.73
23	b	602	CLA	CHD-C4C-C3C	-5.59	116.62	124.77
23	B	612	CLA	O2D-CGD-CBD	5.58	120.99	111.23
23	C	514	CLA	CMD-C2D-C1D	5.58	134.56	124.73
23	c	510	CLA	O2D-CGD-CBD	5.58	120.98	111.23
23	b	613	CLA	CMD-C2D-C1D	5.58	134.55	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	C2D-C1D-ND	5.57	115.64	110.13
23	B	611	CLA	C3D-C2D-C1D	-5.56	98.24	105.83
23	b	614	CLA	CMD-C2D-C1D	5.56	134.52	124.73
23	b	611	CLA	C4A-NA-C1A	-5.55	104.15	106.68
23	D	405	CLA	CHD-C4C-C3C	-5.54	116.70	124.77
23	B	602	CLA	O2D-CGD-CBD	5.53	120.91	111.23
23	a	405	CLA	C2C-C1C-NC	5.53	115.79	109.98
24	a	353	PHO	C3D-C4D-ND	5.52	114.79	107.71
23	b	604	CLA	C2D-C1D-ND	5.52	115.59	110.13
23	C	511	CLA	O2D-CGD-CBD	5.52	120.88	111.23
23	c	503	CLA	O2D-CGD-CBD	5.52	120.88	111.23
23	a	405	CLA	CHD-C4C-C3C	-5.51	116.74	124.77
23	C	506	CLA	C2D-C1D-ND	5.51	115.58	110.13
23	B	608	CLA	O2D-CGD-CBD	5.50	120.84	111.23
23	B	604	CLA	C2C-C1C-NC	5.50	115.76	109.98
23	b	611	CLA	C3D-C2D-C1D	-5.50	98.33	105.83
23	d	402	CLA	CHD-C4C-C3C	-5.49	116.76	124.77
24	A	353	PHO	C4D-ND-C1D	-5.49	102.29	108.87
23	B	607	CLA	CHD-C4C-C3C	-5.48	116.78	124.77
23	a	407	CLA	CMD-C2D-C1D	5.48	134.38	124.73
23	B	614	CLA	C3D-C2D-C1D	-5.48	98.35	105.83
23	C	506	CLA	O2D-CGD-CBD	5.47	120.80	111.23
23	B	613	CLA	CHD-C4C-C3C	-5.47	116.80	124.77
23	c	511	CLA	C4A-NA-C1A	-5.46	104.19	106.68
23	C	512	CLA	CMD-C2D-C1D	5.45	134.33	124.73
23	B	604	CLA	C1-C2-C3	-5.45	117.28	126.20
23	d	402	CLA	CMD-C2D-C1D	5.43	134.30	124.73
23	c	507	CLA	C2C-C1C-NC	5.43	115.68	109.98
23	c	513	CLA	CHD-C4C-C3C	-5.43	116.86	124.77
23	a	405	CLA	C2D-C1D-ND	5.43	115.50	110.13
23	D	406	CLA	CMD-C2D-C1D	5.42	134.28	124.73
23	B	607	CLA	O2D-CGD-CBD	5.42	120.70	111.23
23	c	510	CLA	CHD-C4C-C3C	-5.41	116.88	124.77
23	C	505	CLA	C2C-C1C-NC	5.41	115.66	109.98
23	b	608	CLA	C2C-C1C-NC	5.40	115.66	109.98
23	b	609	CLA	CMD-C2D-C1D	5.40	134.24	124.73
23	b	602	CLA	C2B-C1B-NB	5.40	115.93	110.33
26	B	620	SQD	O47-C7-C8	5.40	123.15	111.48
23	d	403	CLA	C4A-NA-C1A	-5.38	104.22	106.68
23	b	601	CLA	C4A-NA-C1A	-5.37	104.23	106.68
23	a	409	CLA	O2D-CGD-CBD	5.37	120.62	111.23
23	B	614	CLA	C2C-C1C-NC	5.37	115.62	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	502	CLA	O2D-CGD-CBD	5.36	120.60	111.23
23	c	513	CLA	C2B-C1B-NB	5.35	115.88	110.33
23	c	513	CLA	O2D-CGD-CBD	5.35	120.59	111.23
23	B	616	CLA	C4A-NA-C1A	-5.35	104.24	106.68
23	C	505	CLA	C3D-C2D-C1D	-5.33	98.55	105.83
26	b	620	SQD	O6-C1-C2	5.32	116.36	108.27
23	B	608	CLA	C2C-C1C-NC	5.31	115.56	109.98
23	c	507	CLA	CHD-C4C-C3C	-5.31	117.03	124.77
26	A	410	SQD	C1-C2-C3	-5.30	98.86	110.01
23	C	512	CLA	O2D-CGD-CBD	5.29	120.48	111.23
24	A	353	PHO	C3D-C4D-ND	5.28	114.48	107.71
23	a	409	CLA	CMD-C2D-C1D	5.28	134.03	124.73
23	c	503	CLA	C2C-C1C-NC	5.27	115.52	109.98
23	C	512	CLA	C3B-C2B-C1B	-5.27	100.95	107.17
23	C	513	CLA	CMD-C2D-C1D	5.27	134.01	124.73
23	B	608	CLA	CMD-C2D-C1D	5.26	134.00	124.73
23	C	503	CLA	CMD-C2D-C1D	5.26	134.00	124.73
23	B	614	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
23	C	510	CLA	CHD-C4C-C3C	-5.25	117.12	124.77
23	b	613	CLA	C2C-C1C-NC	5.25	115.50	109.98
23	c	508	CLA	C2C-C1C-NC	5.25	115.50	109.98
23	b	612	CLA	O2D-CGD-CBD	5.25	120.40	111.23
23	b	606	CLA	O2D-CGD-CBD	5.24	120.39	111.23
23	A	405	CLA	C4A-NA-C1A	-5.24	104.29	106.68
23	C	513	CLA	C2B-C1B-NB	5.24	115.76	110.33
23	c	509	CLA	C4A-NA-C1A	-5.23	104.29	106.68
23	c	513	CLA	C2D-C1D-ND	5.23	115.31	110.13
23	D	405	CLA	C2C-C1C-NC	5.23	115.48	109.98
23	B	604	CLA	CHD-C4C-C3C	-5.23	117.15	124.77
23	C	509	CLA	O2D-CGD-CBD	5.22	120.36	111.23
23	b	602	CLA	C2D-C1D-ND	5.22	115.29	110.13
23	B	613	CLA	C2C-C1C-NC	5.21	115.46	109.98
23	B	607	CLA	C2C-C1C-NC	5.21	115.46	109.98
23	c	505	CLA	O2D-CGD-CBD	5.21	120.34	111.23
23	c	513	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
23	A	404	CLA	C2C-C1C-NC	5.20	115.44	109.98
23	B	612	CLA	CMD-C2D-C1D	5.20	133.88	124.73
23	C	507	CLA	CHD-C4C-C3C	-5.20	117.20	124.77
23	b	605	CLA	O2D-CGD-CBD	5.19	120.31	111.23
23	C	514	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
23	b	613	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	b	612	CLA	C2C-C1C-NC	5.19	115.43	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	O2D-CGD-CBD	5.19	120.30	111.23
23	c	505	CLA	C3B-C2B-C1B	-5.19	101.06	107.17
23	B	615	CLA	C2C-C1C-NC	5.19	115.43	109.98
23	B	606	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
23	A	408	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
23	c	509	CLA	CMD-C2D-C1D	5.18	133.85	124.73
25	Y	101	BCR	C33-C5-C6	-5.18	118.83	124.48
24	a	408	PHO	C4D-ND-C1D	-5.17	102.68	108.87
23	D	406	CLA	O2D-CGD-CBD	5.15	120.24	111.23
23	B	615	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
23	B	615	CLA	C4A-NA-C1A	-5.15	104.33	106.68
23	b	611	CLA	O2D-CGD-CBD	5.15	120.23	111.23
23	C	505	CLA	O2D-CGD-CBD	5.13	120.20	111.23
23	C	512	CLA	C2C-C1C-NC	5.13	115.37	109.98
23	B	616	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
23	A	404	CLA	CHD-C4C-C3C	-5.13	117.30	124.77
23	c	503	CLA	CMD-C2D-C1D	5.12	133.75	124.73
23	C	511	CLA	C2C-C1C-NC	5.12	115.36	109.98
23	C	503	CLA	C4A-NA-C1A	-5.12	104.34	106.68
23	B	610	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
23	A	405	CLA	O2D-CGD-CBD	5.11	120.17	111.23
23	C	510	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
23	b	614	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
23	C	506	CLA	C2C-C1C-NC	5.09	115.33	109.98
40	v	202	HEC	CBC-CAC-C3C	-5.09	117.27	127.43
23	C	513	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
23	a	406	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
26	a	411	SQD	O47-C7-C8	5.07	122.45	111.48
23	c	514	CLA	C4A-NA-C1A	-5.07	104.37	106.68
23	D	405	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
23	b	608	CLA	C4A-NA-C1A	-5.06	104.37	106.68
23	c	511	CLA	O2D-CGD-CBD	5.06	120.07	111.23
23	B	608	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
23	B	605	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	b	614	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
23	B	611	CLA	CMC-C2C-C1C	5.02	132.88	125.03
25	y	101	BCR	C33-C5-C6	-5.02	119.01	124.48
23	b	615	CLA	C2C-C1C-NC	5.02	115.25	109.98
26	b	620	SQD	O47-C7-C8	5.01	122.31	111.48
23	B	605	CLA	O2D-CGD-CBD	5.01	119.98	111.23
23	B	616	CLA	CMD-C2D-C1D	5.00	133.54	124.73
23	C	510	CLA	C2C-C1C-NC	5.00	115.23	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	CMD-C2D-C1D	4.99	133.52	124.73
23	c	508	CLA	C3B-C2B-C1B	-4.99	101.28	107.17
23	C	503	CLA	C2C-C1C-NC	4.98	115.21	109.98
25	t	103	BCR	C33-C5-C6	-4.97	119.06	124.48
38	e	87	HEM	CHC-C4B-NB	4.97	129.77	124.42
23	a	407	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
23	c	509	CLA	C2C-C1C-NC	4.96	115.19	109.98
23	c	502	CLA	C4A-NA-C1A	-4.96	104.42	106.68
26	a	411	SQD	C1-O5-C5	-4.95	104.05	113.72
25	d	404	BCR	C7-C8-C9	-4.95	118.92	126.23
23	B	603	CLA	C2C-C1C-NC	4.95	115.18	109.98
24	a	408	PHO	C3D-C4D-ND	4.94	114.04	107.71
23	c	511	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
23	c	502	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
23	C	511	CLA	C1-C2-C3	-4.94	118.11	126.20
23	A	405	CLA	C2C-C1C-NC	4.93	115.17	109.98
23	c	505	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
23	c	505	CLA	C4A-NA-C1A	-4.92	104.43	106.68
23	c	509	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
23	C	506	CLA	C4A-NA-C1A	-4.92	104.43	106.68
23	A	408	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
23	B	602	CLA	C2C-C1C-NC	4.91	115.14	109.98
23	b	608	CLA	O2D-CGD-CBD	4.91	119.82	111.23
23	c	504	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
23	c	507	CLA	C4A-NA-C1A	-4.91	104.44	106.68
23	b	602	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
23	b	605	CLA	C2C-C1C-NC	4.91	115.14	109.98
26	f	102	SQD	O47-C7-C8	4.91	122.09	111.48
34	b	622	HTG	C1-O5-C5	4.91	121.36	112.56
23	c	503	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
23	c	510	CLA	C2C-C1C-NC	4.90	115.13	109.98
23	b	605	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
23	a	406	CLA	C2C-C1C-NC	4.90	115.13	109.98
23	C	510	CLA	C2B-C1B-NB	4.90	115.41	110.33
23	C	508	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
23	C	508	CLA	C3B-C2B-C1B	-4.90	101.40	107.17
23	B	601	CLA	C3D-C2D-C1D	-4.89	99.15	105.83
23	C	507	CLA	C1C-C2C-C3C	-4.89	101.84	106.98
23	c	514	CLA	C2C-C1C-NC	4.88	115.11	109.98
23	a	409	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
34	D	414	HTG	C1'-S1-C1	4.88	110.98	100.45
23	d	403	CLA	O2D-CGD-CBD	4.88	119.75	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	C2B-C1B-NB	4.87	115.38	110.33
23	c	514	CLA	C2B-C1B-NB	4.87	115.38	110.33
23	B	601	CLA	C2B-C1B-NB	4.86	115.36	110.33
23	B	613	CLA	O2D-CGD-CBD	4.86	119.72	111.23
23	b	603	CLA	C3D-C4D-ND	4.85	117.87	109.99
23	C	507	CLA	C3B-C2B-C1B	-4.85	101.46	107.17
23	b	607	CLA	C3D-C4D-ND	4.85	117.86	109.99
23	c	514	CLA	C3B-C2B-C1B	-4.85	101.46	107.17
23	b	615	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
29	a	416	PL9	C7-C8-C9	-4.84	118.50	126.83
23	a	405	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
23	b	610	CLA	C1-C2-C3	-4.83	118.29	126.20
23	B	606	CLA	CHD-C1D-ND	-4.82	118.01	124.80
23	b	612	CLA	CMD-C2D-C1D	4.82	133.22	124.73
23	b	611	CLA	CHD-C1D-ND	-4.82	118.02	124.80
23	B	612	CLA	C3D-C4D-ND	4.82	117.82	109.99
23	b	614	CLA	C2B-C1B-NB	4.82	115.32	110.33
23	B	616	CLA	C3C-C4C-NC	4.82	116.60	110.43
23	b	602	CLA	C3D-C4D-ND	4.82	117.82	109.99
23	C	514	CLA	O2D-CGD-CBD	4.82	119.65	111.23
23	c	506	CLA	C3D-C4D-ND	4.82	117.81	109.99
29	A	414	PL9	C7-C8-C9	-4.80	118.56	126.83
23	B	602	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	b	607	CLA	O2D-CGD-CBD	4.79	119.61	111.23
23	B	601	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
23	b	612	CLA	C3C-C4C-NC	4.79	116.57	110.43
23	C	514	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
23	B	608	CLA	C3B-C2B-C1B	-4.79	101.53	107.17
23	A	405	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	c	512	CLA	C2C-C1C-NC	4.78	115.00	109.98
23	c	508	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
23	C	510	CLA	C3D-C4D-ND	4.77	117.74	109.99
23	A	406	CLA	C2B-C1B-NB	4.77	115.27	110.33
23	A	405	CLA	CMD-C2D-C1D	4.77	133.12	124.73
23	d	402	CLA	C4A-NA-C1A	-4.76	104.51	106.68
23	B	603	CLA	C3B-C2B-C1B	-4.76	101.56	107.17
23	b	607	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
23	b	603	CLA	C2C-C1C-NC	4.76	114.98	109.98
23	d	403	CLA	C2B-C1B-NB	4.75	115.25	110.33
23	b	614	CLA	O2D-CGD-O1D	-4.75	114.61	123.85
23	b	609	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	c	502	CLA	CHD-C1D-ND	-4.74	118.13	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	502	CLA	O2D-CGD-O1D	-4.73	114.64	123.85
23	c	509	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
23	B	609	CLA	C2C-C1C-NC	4.73	114.95	109.98
23	C	503	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
23	b	616	CLA	C2B-C1B-NB	4.73	115.23	110.33
23	c	505	CLA	C2B-C1B-NB	4.73	115.23	110.33
23	b	606	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
23	B	604	CLA	O2D-CGD-CBD	4.73	119.49	111.23
23	a	406	CLA	O2D-CGD-CBD	4.73	119.49	111.23
23	c	510	CLA	C3B-C2B-C1B	-4.72	101.60	107.17
23	B	604	CLA	C2D-C1D-ND	4.72	114.80	110.13
23	b	603	CLA	CMD-C2D-C1D	4.71	133.03	124.73
23	b	611	CLA	C3B-C2B-C1B	-4.71	101.61	107.17
23	B	611	CLA	C3D-C4D-ND	4.71	117.65	109.99
23	d	403	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
23	C	509	CLA	C1-C2-C3	-4.71	118.48	126.20
23	D	406	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	B	609	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	C	513	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	C	507	CLA	C2B-C1B-NB	4.70	115.20	110.33
23	c	503	CLA	C1C-C2C-C3C	-4.69	102.04	106.98
23	A	404	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
23	c	514	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	d	403	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
23	c	511	CLA	C1-C2-C3	-4.69	118.52	126.20
23	d	403	CLA	C3D-C4D-ND	4.68	117.59	109.99
23	b	616	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
23	B	607	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
23	B	613	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
23	c	502	CLA	C2C-C1C-NC	4.67	114.89	109.98
23	c	512	CLA	C3B-C2B-C1B	-4.67	101.67	107.17
23	C	504	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
23	C	514	CLA	C2C-C1C-NC	4.66	114.88	109.98
23	C	504	CLA	C3B-C2B-C1B	-4.66	101.67	107.17
23	A	406	CLA	C3D-C4D-ND	4.66	117.56	109.99
23	a	409	CLA	C3D-C4D-ND	4.66	117.56	109.99
23	B	609	CLA	C2B-C1B-NB	4.66	115.16	110.33
23	C	510	CLA	O2D-CGD-CBD	4.66	119.38	111.23
34	d	411	HTG	C1'-S1-C1	4.66	110.51	100.45
23	b	601	CLA	C3B-C2B-C1B	-4.66	101.68	107.17
23	c	511	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
23	A	408	CLA	O2D-CGD-CBD	4.65	119.37	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	B	621	LMG	O7-C10-C11	4.65	121.54	111.48
23	B	615	CLA	CMB-C2B-C1B	4.65	132.50	125.42
23	c	514	CLA	C3D-C4D-ND	4.65	117.54	109.99
23	c	511	CLA	C2C-C1C-NC	4.65	114.86	109.98
34	C	522	HTG	C1'-S1-C1	4.64	110.48	100.45
23	C	514	CLA	C3D-C4D-ND	4.64	117.53	109.99
23	b	603	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
23	b	606	CLA	C2C-C1C-NC	4.63	114.84	109.98
23	c	507	CLA	O2D-CGD-CBD	4.63	119.32	111.23
23	c	506	CLA	C2C-C1C-NC	4.63	114.84	109.98
23	C	509	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
23	b	608	CLA	C1C-C2C-C3C	-4.62	102.12	106.98
23	b	607	CLA	C3B-C4B-NB	4.62	114.66	110.53
23	d	402	CLA	C3D-C4D-ND	4.62	117.50	109.99
23	C	507	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
23	B	603	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
23	b	605	CLA	C3D-C4D-ND	4.62	117.50	109.99
23	b	610	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
23	b	607	CLA	C1C-C2C-C3C	-4.62	102.12	106.98
38	E	103	HEM	CAD-CBD-CGD	4.61	125.90	113.67
23	C	505	CLA	C1C-C2C-C3C	-4.61	102.13	106.98
23	A	406	CLA	O2D-CGD-CBD	4.61	119.28	111.23
23	C	511	CLA	C3B-C2B-C1B	-4.61	101.74	107.17
23	a	409	CLA	C3B-C2B-C1B	-4.60	101.74	107.17
23	B	610	CLA	C2C-C1C-NC	4.60	114.82	109.98
23	b	608	CLA	C2B-C1B-NB	4.60	115.10	110.33
23	c	509	CLA	C2B-C1B-NB	4.60	115.09	110.33
23	c	503	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	B	610	CLA	O2A-CGA-CBA	4.60	125.85	111.83
23	B	605	CLA	C2C-C1C-NC	4.59	114.81	109.98
23	A	408	CLA	C2B-C1B-NB	4.59	115.09	110.33
23	A	404	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
23	A	405	CLA	C1C-C2C-C3C	-4.59	102.15	106.98
23	c	504	CLA	C2C-C1C-NC	4.59	114.80	109.98
23	b	608	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
23	b	610	CLA	C4A-NA-C1A	-4.59	104.59	106.68
23	B	608	CLA	C2B-C1B-NB	4.58	115.08	110.33
23	C	507	CLA	C3D-C4D-ND	4.58	117.43	109.99
23	c	507	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	C	514	CLA	C2B-C1B-NB	4.57	115.07	110.33
23	c	507	CLA	C3D-C4D-ND	4.57	117.42	109.99
23	b	601	CLA	C3D-C4D-ND	4.57	117.42	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	O2D-CGD-CBD	4.57	119.22	111.23
23	B	616	CLA	C2C-C1C-NC	4.56	114.77	109.98
23	C	502	CLA	C3D-C4D-ND	4.56	117.40	109.99
23	C	509	CLA	C3B-C2B-C1B	-4.55	101.80	107.17
23	C	509	CLA	C3C-C4C-NC	4.55	116.26	110.43
26	f	102	SQD	C1-O5-C5	4.55	122.61	113.72
23	B	601	CLA	C3D-C4D-ND	4.55	117.39	109.99
23	b	606	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
23	b	601	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
32	t	102	LMT	C3'-C4'-C5'	-4.55	100.84	110.93
23	B	614	CLA	C2B-C1B-NB	4.55	115.04	110.33
23	C	511	CLA	C3D-C4D-ND	4.55	117.38	109.99
23	b	601	CLA	C2B-C1B-NB	4.54	115.04	110.33
23	b	614	CLA	C2C-C1C-NC	4.54	114.75	109.98
23	C	503	CLA	C3D-C4D-ND	4.54	117.37	109.99
23	a	407	CLA	O2D-CGD-CBD	4.54	119.17	111.23
23	B	604	CLA	C4A-NA-C1A	-4.54	104.61	106.68
23	D	406	CLA	C2C-C1C-NC	4.54	114.75	109.98
23	A	405	CLA	C2B-C1B-NB	4.53	115.03	110.33
23	C	504	CLA	C2C-C1C-NC	4.53	114.74	109.98
23	C	504	CLA	C2B-C1B-NB	4.53	115.02	110.33
23	c	505	CLA	C2C-C1C-NC	4.53	114.74	109.98
23	b	605	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
23	C	512	CLA	C2B-C1B-NB	4.53	115.02	110.33
23	B	612	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
23	c	510	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
23	C	506	CLA	CMB-C2B-C1B	4.52	132.30	125.42
23	B	602	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
23	b	610	CLA	C3B-C2B-C1B	-4.52	101.85	107.17
23	C	502	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
23	c	512	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
29	A	414	PL9	C32-C33-C34	-4.51	117.31	127.62
23	A	406	CLA	CMB-C2B-C1B	4.50	132.27	125.42
23	c	512	CLA	O2D-CGD-CBD	4.50	119.10	111.23
23	B	616	CLA	C3B-C4B-NB	4.50	114.55	110.53
23	c	514	CLA	CHD-C1D-ND	-4.50	118.47	124.80
23	A	405	CLA	C3D-C4D-ND	4.50	117.30	109.99
23	B	615	CLA	C3C-C4C-NC	4.50	116.19	110.43
23	c	511	CLA	C2B-C1B-NB	4.50	114.99	110.33
33	a	419	LMG	O7-C10-C11	4.49	121.20	111.48
23	B	605	CLA	C3C-C4C-NC	4.49	116.18	110.43
23	D	405	CLA	C3C-C4C-NC	4.49	116.18	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	CMB-C2B-C1B	4.49	132.25	125.42
23	B	607	CLA	C3B-C2B-C1B	-4.49	101.88	107.17
23	c	504	CLA	C1D-CHD-C4C	-4.48	116.49	126.02
23	C	511	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	b	610	CLA	C3D-C4D-ND	4.48	117.27	109.99
23	c	514	CLA	O2D-CGD-CBD	4.47	119.05	111.23
23	a	409	CLA	C2C-C1C-NC	4.47	114.68	109.98
23	C	503	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
23	C	503	CLA	O2D-CGD-CBD	4.47	119.05	111.23
23	B	609	CLA	C3D-C4D-ND	4.47	117.25	109.99
23	C	511	CLA	C4A-NA-C1A	-4.47	104.64	106.68
23	a	407	CLA	C3B-C2B-C1B	-4.47	101.90	107.17
23	B	607	CLA	C4A-NA-C1A	-4.46	104.64	106.68
23	b	612	CLA	C1-C2-C3	-4.46	118.89	126.20
23	c	503	CLA	C2B-C1B-NB	4.46	114.95	110.33
23	C	504	CLA	C3D-C4D-ND	4.46	117.24	109.99
23	C	510	CLA	CHD-C1D-ND	-4.46	118.53	124.80
23	b	612	CLA	C3B-C2B-C1B	-4.46	101.92	107.17
23	C	506	CLA	C3D-C4D-ND	4.46	117.23	109.99
23	A	408	CLA	C3B-C4B-NB	4.46	114.51	110.53
23	b	615	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
23	b	611	CLA	C2B-C1B-NB	4.45	114.94	110.33
23	b	607	CLA	C3C-C4C-NC	4.45	116.12	110.43
23	c	510	CLA	C3B-C4B-NB	4.44	114.50	110.53
23	c	508	CLA	CHD-C1D-ND	-4.44	118.55	124.80
23	c	510	CLA	C2B-C1B-NB	4.44	114.93	110.33
23	B	614	CLA	CHD-C1D-ND	-4.44	118.55	124.80
23	b	611	CLA	C3D-C4D-ND	4.44	117.20	109.99
26	F	101	SQD	C1-O5-C5	-4.43	105.06	113.72
23	b	608	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
23	c	503	CLA	C4A-NA-C1A	-4.43	104.66	106.68
23	C	502	CLA	C2B-C1B-NB	4.43	114.92	110.33
23	b	610	CLA	C2C-C1C-NC	4.43	114.63	109.98
23	A	408	CLA	C3D-C4D-ND	4.43	117.19	109.99
23	b	616	CLA	C3D-C4D-ND	4.43	117.18	109.99
23	b	612	CLA	C3D-C4D-ND	4.43	117.18	109.99
23	C	512	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
34	b	625	HTG	C1-O5-C5	4.42	120.50	112.56
23	a	407	CLA	C3D-C4D-ND	4.42	117.17	109.99
23	c	502	CLA	C3B-C2B-C1B	-4.42	101.96	107.17
23	B	607	CLA	C1C-C2C-C3C	-4.42	102.33	106.98
23	b	613	CLA	C3B-C2B-C1B	-4.42	101.96	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	C3B-C2B-C1B	-4.42	101.96	107.17
23	a	405	CLA	C3D-C4D-ND	4.42	117.17	109.99
25	H	101	BCR	C38-C26-C25	-4.41	119.67	124.48
23	a	405	CLA	C1C-C2C-C3C	-4.41	102.34	106.98
23	c	504	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
23	C	511	CLA	C2B-C1B-NB	4.41	114.90	110.33
23	B	605	CLA	C3D-C4D-ND	4.41	117.16	109.99
23	B	612	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
23	b	604	CLA	C3C-C4C-NC	4.41	116.08	110.43
23	a	406	CLA	C1C-C2C-C3C	-4.41	102.34	106.98
23	b	609	CLA	C2C-C1C-NC	4.41	114.61	109.98
23	b	606	CLA	CHD-C1D-ND	-4.40	118.60	124.80
23	b	614	CLA	C3D-C4D-ND	4.40	117.14	109.99
23	B	611	CLA	CHD-C1D-ND	-4.40	118.61	124.80
23	b	609	CLA	O2D-CGD-CBD	4.40	118.92	111.23
23	C	509	CLA	CMD-C2D-C1D	4.40	132.47	124.73
23	a	407	CLA	C2B-C1B-NB	4.40	114.89	110.33
38	E	103	HEM	CHC-C4B-NB	4.40	129.15	124.42
23	a	406	CLA	C2B-C1B-NB	4.39	114.88	110.33
24	A	353	PHO	C1-C2-C3	-4.39	119.00	126.20
23	A	405	CLA	C3B-C2B-C1B	-4.39	102.00	107.17
23	B	616	CLA	C3B-C2B-C1B	-4.39	102.00	107.17
23	C	507	CLA	CHD-C1D-ND	-4.39	118.63	124.80
23	B	603	CLA	C3D-C4D-ND	4.38	117.11	109.99
33	c	521	LMG	O6-C5-C4	4.38	117.59	109.70
23	B	610	CLA	C3B-C2B-C1B	-4.38	102.01	107.17
23	c	504	CLA	C2B-C1B-NB	4.37	114.86	110.33
23	D	406	CLA	C3D-C4D-ND	4.37	117.09	109.99
23	b	601	CLA	C2C-C1C-NC	4.37	114.57	109.98
23	A	406	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
23	C	508	CLA	CHD-C1D-ND	-4.37	118.66	124.80
23	d	402	CLA	C1C-C2C-C3C	-4.36	102.39	106.98
23	b	603	CLA	C2B-C1B-NB	4.36	114.85	110.33
23	D	406	CLA	C2B-C1B-NB	4.36	114.85	110.33
23	B	612	CLA	O2D-CGD-O1D	-4.36	115.36	123.85
23	b	605	CLA	CHD-C1D-ND	-4.36	118.67	124.80
23	b	604	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
23	B	603	CLA	O2D-CGD-O1D	-4.36	115.37	123.85
37	E	101	LHG	O7-C7-C8	4.35	120.90	111.48
23	c	503	CLA	C3D-C4D-ND	4.35	117.06	109.99
23	b	613	CLA	C3C-C4C-NC	4.35	116.00	110.43
25	d	404	BCR	C15-C14-C13	-4.35	121.18	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	409	CLA	C2B-C1B-NB	4.34	114.83	110.33
23	b	604	CLA	C1C-C2C-C3C	-4.34	102.41	106.98
23	B	613	CLA	C4A-NA-C1A	-4.34	104.70	106.68
23	b	609	CLA	C3D-C4D-ND	4.34	117.04	109.99
23	B	606	CLA	C3D-C4D-ND	4.34	117.03	109.99
23	b	605	CLA	C2B-C1B-NB	4.32	114.81	110.33
23	C	508	CLA	C2C-C1C-NC	4.32	114.52	109.98
23	B	613	CLA	C3B-C4B-NB	4.32	114.39	110.53
23	B	606	CLA	C2C-C1C-NC	4.32	114.52	109.98
25	Y	101	BCR	C16-C17-C18	-4.32	121.22	127.28
23	b	611	CLA	C2C-C1C-NC	4.32	114.52	109.98
23	A	408	CLA	CHD-C1D-ND	-4.32	118.73	124.80
23	a	409	CLA	C3C-C4C-NC	4.31	115.96	110.43
23	B	601	CLA	CHD-C1D-ND	-4.31	118.73	124.80
23	A	404	CLA	C3B-C4B-NB	4.31	114.38	110.53
23	B	613	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
23	b	616	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
23	b	608	CLA	C3B-C4B-NB	4.31	114.38	110.53
23	d	403	CLA	CHD-C1D-ND	-4.31	118.73	124.80
23	B	604	CLA	C3C-C4C-NC	4.31	115.95	110.43
23	c	510	CLA	C3D-C4D-ND	4.31	116.99	109.99
33	C	501	LMG	O7-C10-C11	4.31	120.80	111.48
23	C	513	CLA	C3D-C4D-ND	4.30	116.98	109.99
23	A	406	CLA	C2C-C1C-NC	4.30	114.50	109.98
23	b	615	CLA	C3D-C4D-ND	4.30	116.97	109.99
23	C	511	CLA	C1C-C2C-C3C	-4.30	102.46	106.98
23	b	603	CLA	C1D-CHD-C4C	-4.29	116.89	126.02
23	b	610	CLA	O2A-CGA-CBA	4.29	124.92	111.83
23	a	407	CLA	C2C-C1C-NC	4.29	114.49	109.98
33	C	501	LMG	C7-O1-C1	-4.29	104.60	113.80
23	B	607	CLA	C3D-C4D-ND	4.29	116.96	109.99
23	C	502	CLA	O2D-CGD-O1D	-4.29	115.50	123.85
23	B	611	CLA	C3C-C4C-NC	4.29	115.92	110.43
23	c	512	CLA	C3D-C4D-ND	4.29	116.95	109.99
34	B	623	HTG	C1'-S1-C1	4.28	109.70	100.45
40	V	202	HEC	CBC-CAC-C3C	-4.28	118.87	127.43
23	c	506	CLA	C3C-C4C-NC	4.28	115.91	110.43
23	c	505	CLA	C1-O2A-CGA	4.28	127.01	116.65
23	b	606	CLA	C3D-C4D-ND	4.27	116.94	109.99
23	b	610	CLA	C3C-C4C-NC	4.27	115.91	110.43
23	c	508	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
23	b	607	CLA	C3B-C2B-C1B	-4.27	102.13	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	411	SQD	C1-C2-C3	-4.27	101.02	110.01
23	B	605	CLA	C3B-C2B-C1B	-4.27	102.14	107.17
23	a	405	CLA	C2B-C1B-NB	4.27	114.75	110.33
23	C	503	CLA	C2B-C1B-NB	4.26	114.75	110.33
23	c	513	CLA	C3D-C2D-C1D	-4.26	100.01	105.83
25	C	515	BCR	C7-C8-C9	-4.26	119.93	126.23
23	B	610	CLA	C3D-C4D-ND	4.26	116.92	109.99
23	a	405	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	b	602	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	A	406	CLA	CHD-C1D-ND	-4.26	118.81	124.80
23	B	605	CLA	C1D-CHD-C4C	-4.26	116.97	126.02
23	a	406	CLA	C3D-C4D-ND	4.26	116.91	109.99
23	A	406	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
23	b	602	CLA	CHD-C1D-ND	-4.26	118.81	124.80
23	B	612	CLA	C2C-C1C-NC	4.25	114.45	109.98
23	a	406	CLA	C4A-NA-C1A	-4.25	104.74	106.68
23	a	407	CLA	CHD-C1D-ND	-4.25	118.81	124.80
23	c	502	CLA	C3D-C4D-ND	4.25	116.90	109.99
23	D	405	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
23	B	603	CLA	C3C-C4C-NC	4.25	115.88	110.43
23	c	513	CLA	C2C-C1C-NC	4.25	114.45	109.98
23	B	604	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
23	C	506	CLA	C3C-C4C-NC	4.24	115.87	110.43
23	B	610	CLA	C4A-NA-C1A	-4.24	104.74	106.68
23	c	513	CLA	C3D-C4D-ND	4.24	116.88	109.99
23	A	404	CLA	CHD-C1D-ND	-4.24	118.83	124.80
23	c	504	CLA	C3D-C4D-ND	4.24	116.88	109.99
23	C	509	CLA	C3D-C4D-ND	4.24	116.87	109.99
23	D	406	CLA	C3B-C2B-C1B	-4.24	102.18	107.17
23	C	514	CLA	C3C-C4C-NC	4.24	115.86	110.43
23	C	509	CLA	C3B-C4B-NB	4.24	114.31	110.53
23	C	511	CLA	CHD-C1D-ND	-4.24	118.84	124.80
23	C	509	CLA	C1C-C2C-C3C	-4.23	102.53	106.98
37	D	409	LHG	O8-C23-O10	-4.23	113.04	123.63
23	c	504	CLA	C1-C2-C3	-4.23	119.27	126.20
23	c	510	CLA	C4A-NA-C1A	-4.23	104.75	106.68
23	a	406	CLA	CAA-C2A-C3A	-4.22	101.59	113.00
23	B	602	CLA	C3D-C4D-ND	4.22	116.85	109.99
23	d	402	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
29	a	416	PL9	C32-C33-C34	-4.22	117.96	127.62
23	B	615	CLA	C3D-C4D-ND	4.22	116.84	109.99
23	B	608	CLA	C3B-C4B-NB	4.22	114.30	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	C3B-C2B-C1B	-4.22	102.20	107.17
23	B	614	CLA	C1C-C2C-C3C	-4.22	102.55	106.98
23	C	512	CLA	C1D-CHD-C4C	-4.21	117.06	126.02
23	C	505	CLA	C3C-C4C-NC	4.21	115.83	110.43
29	a	416	PL9	C7-C3-C2	-4.21	118.42	123.39
23	b	610	CLA	C2B-C1B-NB	4.21	114.69	110.33
23	A	404	CLA	C2B-C1B-NB	4.21	114.69	110.33
25	b	617	BCR	C33-C5-C6	-4.21	119.89	124.48
23	B	616	CLA	C3D-C4D-ND	4.21	116.83	109.99
23	c	514	CLA	C1D-CHD-C4C	-4.21	117.08	126.02
23	D	405	CLA	C3D-C4D-ND	4.21	116.82	109.99
23	c	506	CLA	CHD-C1D-ND	-4.20	118.89	124.80
23	a	405	CLA	CAA-C2A-C3A	-4.20	101.65	113.00
23	d	402	CLA	C3B-C2B-C1B	-4.19	102.23	107.17
23	B	615	CLA	C3B-C2B-C1B	-4.19	102.23	107.17
23	c	505	CLA	CHD-C1D-ND	-4.19	118.91	124.80
23	b	605	CLA	O2D-CGD-O1D	-4.19	115.69	123.85
23	a	405	CLA	C1D-CHD-C4C	-4.19	117.12	126.02
23	c	506	CLA	C3B-C2B-C1B	-4.19	102.24	107.17
23	C	506	CLA	C3D-C2D-C1D	-4.18	100.12	105.83
23	C	511	CLA	C3B-C4B-NB	4.18	114.26	110.53
33	d	412	LMG	O7-C10-C11	4.18	120.53	111.48
23	d	402	CLA	O2D-CGD-CBD	4.18	118.53	111.23
23	c	507	CLA	CHD-C1D-ND	-4.18	118.92	124.80
23	c	507	CLA	C3B-C2B-C1B	-4.18	102.25	107.17
23	b	616	CLA	CHD-C1D-ND	-4.17	118.93	124.80
23	B	603	CLA	C1D-CHD-C4C	-4.17	117.15	126.02
23	B	609	CLA	C3C-C4C-NC	4.17	115.78	110.43
23	C	505	CLA	CHD-C1D-ND	-4.17	118.93	124.80
23	C	505	CLA	C2B-C1B-NB	4.17	114.65	110.33
23	b	615	CLA	C2B-C1B-NB	4.17	114.65	110.33
33	c	521	LMG	O7-C10-C11	4.17	120.50	111.48
23	B	607	CLA	C2B-C1B-NB	4.17	114.65	110.33
23	a	406	CLA	C3B-C2B-C1B	-4.17	102.26	107.17
23	C	504	CLA	CHD-C1D-ND	-4.17	118.94	124.80
23	A	404	CLA	C3D-C4D-ND	4.16	116.75	109.99
23	B	613	CLA	C3D-C4D-ND	4.16	116.75	109.99
23	b	608	CLA	CMC-C2C-C1C	4.16	131.54	125.03
23	C	506	CLA	C3B-C2B-C1B	-4.16	102.27	107.17
23	B	608	CLA	C3D-C4D-ND	4.16	116.75	109.99
23	B	610	CLA	C2B-C1B-NB	4.15	114.63	110.33
23	B	606	CLA	C3B-C2B-C1B	-4.15	102.27	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	405	CLA	O2D-CGD-CBD	4.15	118.49	111.23
23	c	509	CLA	C3D-C4D-ND	4.15	116.74	109.99
23	b	608	CLA	C3D-C4D-ND	4.15	116.73	109.99
23	c	512	CLA	C1D-CHD-C4C	-4.14	117.21	126.02
23	B	606	CLA	C2B-C1B-NB	4.14	114.62	110.33
23	b	601	CLA	CHD-C1D-ND	-4.14	118.97	124.80
23	C	505	CLA	C3D-C4D-ND	4.14	116.72	109.99
23	b	603	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
23	b	609	CLA	C3C-C4C-NC	4.14	115.73	110.43
23	A	408	CLA	C4A-NA-C1A	-4.14	104.79	106.68
23	b	613	CLA	C2B-C1B-NB	4.14	114.62	110.33
23	B	606	CLA	C3C-C4C-NC	4.14	115.73	110.43
23	c	507	CLA	C3B-C4B-NB	4.14	114.22	110.53
23	c	502	CLA	C2B-C1B-NB	4.14	114.61	110.33
23	C	510	CLA	C1-C2-C3	-4.13	119.44	126.20
23	c	508	CLA	C3D-C4D-ND	4.12	116.69	109.99
26	B	620	SQD	C3-C4-C5	4.12	117.70	110.23
23	C	510	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
23	B	612	CLA	C3C-C4C-NC	4.12	115.70	110.43
23	B	603	CLA	C2B-C1B-NB	4.12	114.60	110.33
23	c	512	CLA	C4A-NA-C1A	-4.12	104.80	106.68
23	b	612	CLA	O2D-CGD-O1D	-4.12	115.84	123.85
23	b	616	CLA	C1D-CHD-C4C	-4.11	117.28	126.02
23	D	405	CLA	CHD-C1D-ND	-4.11	119.02	124.80
23	C	508	CLA	C3C-C4C-NC	4.11	115.69	110.43
23	B	610	CLA	C3C-C4C-NC	4.11	115.69	110.43
23	B	615	CLA	C1C-C2C-C3C	-4.10	102.67	106.98
23	a	406	CLA	C1D-CHD-C4C	-4.10	117.30	126.02
23	B	616	CLA	O2D-CGD-O1D	-4.10	115.87	123.85
23	B	602	CLA	C2B-C1B-NB	4.10	114.58	110.33
23	C	502	CLA	C2C-C1C-NC	4.10	114.29	109.98
23	b	603	CLA	CAA-C2A-C3A	-4.10	101.93	113.00
23	B	609	CLA	C3B-C2B-C1B	-4.10	102.34	107.17
23	b	603	CLA	C3C-C4C-NC	4.09	115.67	110.43
23	b	609	CLA	C2B-C1B-NB	4.09	114.57	110.33
23	b	612	CLA	C4A-NA-C1A	-4.09	104.81	106.68
23	c	505	CLA	C3D-C4D-ND	4.09	116.63	109.99
23	b	615	CLA	C3C-C4C-NC	4.08	115.66	110.43
23	d	402	CLA	C3C-C4C-NC	4.08	115.66	110.43
23	C	502	CLA	C1D-CHD-C4C	-4.08	117.34	126.02
23	c	513	CLA	C1-C2-C3	-4.08	119.52	126.20
23	c	509	CLA	C3C-C4C-NC	4.08	115.65	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	C1D-CHD-C4C	-4.08	117.35	126.02
24	A	407	PHO	C1A-C2A-C3A	-4.08	98.96	102.84
26	b	620	SQD	C1-O5-C5	-4.08	105.76	113.72
38	E	103	HEM	CHD-C4C-NC	4.08	128.89	124.45
23	b	609	CLA	C1-C2-C3	-4.07	119.53	126.20
23	B	610	CLA	CAA-C2A-C3A	-4.07	102.01	113.00
23	B	601	CLA	C1D-CHD-C4C	-4.07	117.38	126.02
23	C	507	CLA	C1-C2-C3	-4.07	119.54	126.20
23	D	405	CLA	C1-C2-C3	-4.06	119.54	126.20
23	C	502	CLA	CHD-C1D-ND	-4.06	119.08	124.80
23	a	406	CLA	CMB-C2B-C1B	4.06	131.60	125.42
38	E	103	HEM	C1B-NB-C4B	4.06	110.01	105.21
25	B	618	BCR	C29-C30-C25	4.05	116.32	110.44
23	A	408	CLA	C1C-C2C-C3C	-4.05	102.72	106.98
23	c	507	CLA	C1C-C2C-C3C	-4.05	102.72	106.98
23	c	506	CLA	C2B-C1B-NB	4.05	114.53	110.33
23	B	612	CLA	CHD-C1D-ND	-4.05	119.10	124.80
23	B	611	CLA	C1D-CHD-C4C	-4.05	117.42	126.02
23	C	504	CLA	O2D-CGD-CBD	4.05	118.30	111.23
23	b	613	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
33	Z	101	LMG	O7-C10-C11	4.04	120.23	111.48
23	B	613	CLA	C2B-C1B-NB	4.04	114.52	110.33
23	C	508	CLA	C3D-C4D-ND	4.04	116.56	109.99
23	C	512	CLA	C3D-C4D-ND	4.04	116.56	109.99
23	B	609	CLA	CHD-C1D-ND	-4.04	119.12	124.80
23	C	514	CLA	CHD-C1D-ND	-4.04	119.12	124.80
23	C	513	CLA	C1-C2-C3	-4.04	119.58	126.20
29	a	416	PL9	C7-C3-C4	4.04	120.24	116.91
23	c	506	CLA	C3D-C2D-C1D	-4.04	100.32	105.83
23	c	511	CLA	C3D-C4D-ND	4.04	116.55	109.99
23	b	613	CLA	O2D-CGD-CBD	4.04	118.29	111.23
29	A	414	PL9	C7-C3-C2	-4.03	118.63	123.39
23	c	512	CLA	C2B-C1B-NB	4.03	114.51	110.33
23	B	608	CLA	C3C-C4C-NC	4.03	115.59	110.43
23	A	404	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
23	b	601	CLA	C1D-CHD-C4C	-4.02	117.47	126.02
23	b	605	CLA	C3C-C4C-NC	4.02	115.58	110.43
23	C	513	CLA	C1D-CHD-C4C	-4.02	117.48	126.02
23	B	607	CLA	CHD-C1D-ND	-4.02	119.15	124.80
23	b	607	CLA	CHD-C1D-ND	-4.02	119.15	124.80
23	C	507	CLA	C3B-C4B-NB	4.01	114.11	110.53
23	b	606	CLA	C1D-CHD-C4C	-4.01	117.50	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	C3C-C4C-NC	4.01	115.57	110.43
23	B	609	CLA	O2D-CGD-CBD	4.01	118.24	111.23
23	b	611	CLA	C1-C2-C3	-4.01	119.63	126.20
23	B	611	CLA	CHD-C4C-NC	4.00	130.44	124.23
23	c	506	CLA	CAC-C3C-C4C	4.00	130.00	124.79
23	B	614	CLA	C3D-C4D-ND	4.00	116.49	109.99
23	d	403	CLA	C2C-C1C-NC	4.00	114.19	109.98
23	B	616	CLA	C2B-C1B-NB	4.00	114.47	110.33
23	b	614	CLA	C1D-CHD-C4C	-4.00	117.52	126.02
23	c	508	CLA	CMC-C2C-C1C	4.00	131.28	125.03
23	b	602	CLA	C2C-C1C-NC	4.00	114.18	109.98
23	C	513	CLA	C3C-C4C-NC	4.00	115.55	110.43
35	C	518	DGD	O2G-C1B-C2B	3.99	120.12	111.48
23	C	506	CLA	C2B-C1B-NB	3.99	114.47	110.33
23	C	503	CLA	C3C-C4C-NC	3.99	115.54	110.43
23	C	514	CLA	C1D-CHD-C4C	-3.99	117.54	126.02
23	b	616	CLA	O2D-CGD-O1D	-3.99	116.09	123.85
23	c	503	CLA	C1D-CHD-C4C	-3.98	117.56	126.02
23	b	612	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
23	c	504	CLA	C3C-C4C-NC	3.98	115.53	110.43
23	c	507	CLA	C2B-C1B-NB	3.98	114.45	110.33
23	c	511	CLA	C3C-C4C-NC	3.98	115.53	110.43
23	b	604	CLA	CMC-C2C-C1C	3.98	131.25	125.03
23	D	406	CLA	C3C-C4C-NC	3.97	115.52	110.43
23	a	409	CLA	C4A-NA-C1A	-3.97	104.87	106.68
23	B	601	CLA	C3C-C4C-NC	3.97	115.52	110.43
23	a	409	CLA	C1C-C2C-C3C	-3.97	102.81	106.98
23	b	611	CLA	C3C-C4C-NC	3.97	115.51	110.43
23	A	408	CLA	C1-C2-C3	-3.97	119.70	126.20
23	b	609	CLA	C3B-C2B-C1B	-3.97	102.49	107.17
23	a	405	CLA	O2D-CGD-CBD	3.96	118.16	111.23
23	B	601	CLA	C4A-NA-C1A	-3.96	104.87	106.68
23	C	512	CLA	C3C-C4C-NC	3.96	115.51	110.43
23	C	507	CLA	C4A-NA-C1A	-3.96	104.87	106.68
35	C	517	DGD	O2G-C1B-C2B	3.96	120.05	111.48
23	A	404	CLA	CAA-C2A-C3A	-3.96	102.30	113.00
23	C	508	CLA	C1D-CHD-C4C	-3.96	117.61	126.02
23	b	601	CLA	O2D-CGD-O1D	-3.95	116.15	123.85
23	b	610	CLA	C1D-CHD-C4C	-3.95	117.62	126.02
23	B	604	CLA	C2B-C1B-NB	3.95	114.42	110.33
23	B	615	CLA	C1D-CHD-C4C	-3.95	117.63	126.02
23	a	409	CLA	C1D-CHD-C4C	-3.95	117.63	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	C3B-C2B-C1B	-3.95	102.52	107.17
23	b	606	CLA	C1C-C2C-C3C	-3.94	102.84	106.98
33	C	521	LMG	O6-C5-C4	3.94	116.79	109.70
23	B	615	CLA	CHD-C1D-ND	-3.93	119.27	124.80
23	b	609	CLA	CHD-C1D-ND	-3.93	119.27	124.80
23	c	504	CLA	CHD-C1D-ND	-3.93	119.27	124.80
23	C	506	CLA	C1-C2-C3	-3.93	119.75	126.20
23	c	514	CLA	C1C-C2C-C3C	-3.93	102.84	106.98
23	D	406	CLA	O2D-CGD-O1D	-3.93	116.19	123.85
23	c	511	CLA	C1C-C2C-C3C	-3.93	102.85	106.98
23	b	615	CLA	C1D-CHD-C4C	-3.93	117.67	126.02
23	A	404	CLA	O2A-CGA-CBA	3.93	123.81	111.83
23	B	610	CLA	CHD-C1D-ND	-3.92	119.28	124.80
23	a	407	CLA	C3C-C4C-NC	3.92	115.45	110.43
23	c	513	CLA	CHD-C1D-ND	-3.92	119.29	124.80
23	b	614	CLA	C3C-C4C-NC	3.92	115.45	110.43
23	B	613	CLA	C1C-C2C-C3C	-3.92	102.86	106.98
23	D	406	CLA	CMB-C2B-C1B	3.92	131.38	125.42
23	b	613	CLA	C1-C2-C3	-3.91	119.79	126.20
23	A	406	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
23	c	512	CLA	CHD-C1D-ND	-3.91	119.30	124.80
23	B	613	CLA	C3C-C4C-NC	3.91	115.44	110.43
23	b	610	CLA	O2A-CGA-O1A	-3.90	113.86	123.63
23	c	512	CLA	C3B-C4B-NB	3.90	114.01	110.53
33	C	520	LMG	O7-C10-C11	3.90	119.92	111.48
23	D	405	CLA	C3B-C4B-NB	3.90	114.01	110.53
25	T	101	BCR	C15-C16-C17	-3.90	115.54	123.52
23	c	514	CLA	C3B-C4B-NB	3.90	114.01	110.53
25	D	407	BCR	C38-C26-C25	-3.89	120.23	124.48
23	c	508	CLA	C4A-NA-C1A	-3.89	104.90	106.68
23	c	510	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
23	C	510	CLA	C1C-C2C-C3C	-3.89	102.89	106.98
23	C	506	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
23	B	614	CLA	C3B-C4B-NB	3.89	114.00	110.53
23	C	505	CLA	C4A-NA-C1A	-3.89	104.91	106.68
23	c	513	CLA	C1D-CHD-C4C	-3.89	117.76	126.02
23	a	409	CLA	CHD-C1D-ND	-3.88	119.34	124.80
33	m	101	LMG	O7-C10-C11	3.88	119.87	111.48
23	B	604	CLA	C3D-C2D-C1D	-3.88	100.54	105.83
25	d	404	BCR	C29-C30-C25	3.88	116.07	110.44
23	A	408	CLA	C3C-C4C-NC	3.87	115.39	110.43
23	C	514	CLA	C4A-NA-C1A	-3.87	104.92	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	C3D-C4D-ND	3.87	116.27	109.99
23	B	605	CLA	CMB-C2B-C1B	3.86	131.30	125.42
23	B	606	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
23	B	614	CLA	O2D-CGD-O1D	-3.86	116.33	123.85
23	C	509	CLA	C1D-CHD-C4C	-3.86	117.81	126.02
23	C	506	CLA	CHD-C1D-ND	-3.86	119.38	124.80
23	b	612	CLA	C1D-CHD-C4C	-3.85	117.83	126.02
23	B	602	CLA	C3C-C4C-NC	3.85	115.36	110.43
23	b	608	CLA	CHD-C1D-ND	-3.85	119.39	124.80
23	c	503	CLA	O2D-CGD-O1D	-3.85	116.36	123.85
23	b	605	CLA	C1D-CHD-C4C	-3.85	117.84	126.02
23	C	504	CLA	C1-C2-C3	-3.85	119.89	126.20
23	A	405	CLA	CMC-C2C-C1C	3.84	131.04	125.03
23	C	512	CLA	C4A-NA-C1A	-3.84	104.92	106.68
29	D	408	PL9	C42-C43-C44	-3.84	118.83	127.62
23	B	604	CLA	C3B-C4B-NB	3.84	113.96	110.53
23	B	602	CLA	C1D-CHD-C4C	-3.84	117.86	126.02
23	b	614	CLA	C4A-NA-C1A	-3.84	104.93	106.68
33	C	521	LMG	O7-C10-C11	3.84	119.78	111.48
23	C	507	CLA	O2D-CGD-CBD	3.84	117.94	111.23
23	c	510	CLA	CHD-C1D-ND	-3.84	119.40	124.80
23	a	406	CLA	CHD-C1D-ND	-3.83	119.41	124.80
23	b	612	CLA	C2B-C1B-NB	3.83	114.29	110.33
23	c	509	CLA	C1C-C2C-C3C	-3.83	102.96	106.98
23	B	607	CLA	C3C-C4C-NC	3.82	115.33	110.43
23	C	503	CLA	CHD-C1D-ND	-3.82	119.42	124.80
23	c	507	CLA	C1-C2-C3	-3.82	119.93	126.20
23	C	512	CLA	CAC-C3C-C4C	3.82	129.76	124.79
32	D	404	LMT	C1'-O5'-C5'	-3.82	106.26	113.72
23	B	608	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
33	c	521	LMG	C3-C4-C5	3.82	117.16	110.23
23	b	613	CLA	C3D-C4D-ND	3.82	116.19	109.99
23	A	404	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
23	B	616	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
23	c	511	CLA	CHD-C1D-ND	-3.81	119.44	124.80
23	A	405	CLA	CBC-CAC-C3C	-3.81	102.10	112.42
23	B	606	CLA	C1D-CHD-C4C	-3.80	117.93	126.02
23	B	610	CLA	C1C-C2C-C3C	-3.80	102.98	106.98
23	A	404	CLA	O2D-CGD-CBD	3.80	117.88	111.23
23	B	611	CLA	O2D-CGD-O1D	-3.80	116.45	123.85
23	d	402	CLA	C2B-C1B-NB	3.80	114.26	110.33
23	a	406	CLA	C3C-C4C-NC	3.80	115.29	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	C3B-C4B-NB	3.79	113.92	110.53
23	c	509	CLA	C1D-CHD-C4C	-3.79	117.96	126.02
23	b	612	CLA	C3B-C4B-NB	3.79	113.91	110.53
23	B	614	CLA	C3C-C4C-NC	3.79	115.28	110.43
23	b	603	CLA	O2D-CGD-O1D	-3.78	116.48	123.85
37	d	711	LHG	O8-C23-O10	-3.78	114.17	123.63
23	A	405	CLA	CHD-C1D-ND	-3.78	119.48	124.80
23	B	609	CLA	C1C-C2C-C3C	-3.78	103.01	106.98
23	B	615	CLA	C2B-C1B-NB	3.78	114.24	110.33
23	B	604	CLA	C1C-C2C-C3C	-3.78	103.01	106.98
23	C	503	CLA	C1C-C2C-C3C	-3.77	103.01	106.98
23	C	511	CLA	C1D-CHD-C4C	-3.77	118.00	126.02
23	C	508	CLA	C2B-C1B-NB	3.77	114.24	110.33
23	B	603	CLA	CHD-C1D-ND	-3.77	119.50	124.80
23	b	604	CLA	O2D-CGD-O1D	-3.77	116.52	123.85
23	B	615	CLA	O2D-CGD-CBD	3.76	117.81	111.23
23	B	608	CLA	C4A-NA-C1A	-3.76	104.96	106.68
23	C	514	CLA	C1C-C2C-C3C	-3.76	103.03	106.98
29	d	405	PL9	C42-C43-C44	-3.76	119.02	127.62
33	Z	101	LMG	C1-C2-C3	3.76	117.91	110.01
23	b	612	CLA	C1C-C2C-C3C	-3.76	103.03	106.98
23	B	602	CLA	CHD-C1D-ND	-3.76	119.52	124.80
23	d	403	CLA	O2D-CGD-O1D	-3.75	116.55	123.85
23	a	409	CLA	CMC-C2C-C1C	3.75	130.89	125.03
29	A	414	PL9	C22-C23-C24	-3.74	119.05	127.62
23	c	504	CLA	CMB-C2B-C1B	3.74	131.12	125.42
23	C	513	CLA	CHD-C1D-ND	-3.74	119.54	124.80
23	b	603	CLA	CHD-C1D-ND	-3.74	119.54	124.80
23	b	604	CLA	C1D-CHD-C4C	-3.74	118.07	126.02
23	B	604	CLA	C3D-C4D-ND	3.74	116.06	109.99
29	A	414	PL9	C7-C3-C4	3.74	119.99	116.91
23	a	405	CLA	CHD-C1D-ND	-3.73	119.55	124.80
23	B	602	CLA	C1C-C2C-C3C	-3.73	103.05	106.98
25	d	404	BCR	C38-C26-C25	-3.73	120.41	124.48
23	b	616	CLA	C3C-C4C-NC	3.73	115.21	110.43
37	d	711	LHG	O8-C23-C24	3.73	123.21	111.83
24	a	408	PHO	O1D-CGD-CBD	-3.73	119.07	124.72
23	B	614	CLA	O2A-CGA-O1A	-3.73	114.30	123.63
23	b	613	CLA	C1D-CHD-C4C	-3.73	118.10	126.02
23	C	505	CLA	C3B-C4B-NB	3.73	113.86	110.53
23	c	502	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
25	b	617	BCR	C7-C8-C9	-3.72	120.72	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	C3C-C4C-NC	3.72	115.19	110.43
23	B	602	CLA	CAA-C2A-C3A	-3.72	102.96	113.00
23	c	508	CLA	C2B-C1B-NB	3.72	114.18	110.33
23	B	608	CLA	CHD-C1D-ND	-3.72	119.57	124.80
25	h	101	BCR	C38-C26-C25	-3.71	120.43	124.48
26	a	411	SQD	C44-O6-C1	-3.71	105.84	113.80
37	L	101	LHG	O7-C7-C8	3.71	119.50	111.48
23	C	504	CLA	C3C-C4C-NC	3.70	115.17	110.43
33	C	501	LMG	O1-C1-C2	3.70	113.89	108.27
23	c	505	CLA	C1D-CHD-C4C	-3.69	118.17	126.02
23	B	614	CLA	C1D-CHD-C4C	-3.69	118.17	126.02
25	D	407	BCR	C10-C11-C12	-3.69	112.50	123.20
23	c	507	CLA	CAC-C3C-C4C	3.69	129.59	124.79
23	D	406	CLA	CHD-C1D-ND	-3.69	119.61	124.80
25	d	404	BCR	C40-C30-C25	-3.69	104.46	110.24
23	b	613	CLA	C3B-C4B-NB	3.69	113.82	110.53
23	b	616	CLA	O2A-CGA-CBA	3.69	123.07	111.83
23	b	608	CLA	C1D-CHD-C4C	-3.69	118.19	126.02
23	B	603	CLA	C1C-C2C-C3C	-3.69	103.10	106.98
23	b	602	CLA	CAA-C2A-C3A	-3.68	103.05	113.00
23	D	405	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
23	B	602	CLA	O2D-CGD-O1D	-3.68	116.69	123.85
26	A	412	SQD	O47-C7-C8	3.67	119.43	111.48
23	b	614	CLA	CHD-C1D-ND	-3.67	119.63	124.80
29	a	416	PL9	C15-C14-C16	3.67	121.60	115.23
23	c	514	CLA	C3C-C4C-NC	3.67	115.13	110.43
23	b	603	CLA	C3B-C4B-NB	3.67	113.81	110.53
23	b	604	CLA	C4A-NA-C1A	-3.67	105.00	106.68
23	D	406	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
33	c	520	LMG	O7-C10-C11	3.67	119.41	111.48
23	a	407	CLA	C1D-CHD-C4C	-3.67	118.23	126.02
23	c	503	CLA	C3C-C4C-NC	3.66	115.12	110.43
23	b	602	CLA	CMC-C2C-C1C	3.66	130.76	125.03
25	D	407	BCR	C28-C27-C26	-3.66	107.53	114.06
23	a	405	CLA	O2A-CGA-O1A	-3.66	114.47	123.63
23	B	605	CLA	CHD-C1D-ND	-3.66	119.65	124.80
25	y	101	BCR	C15-C14-C13	-3.66	122.14	127.28
23	a	407	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
23	b	612	CLA	C4-C3-C5	3.66	121.58	115.23
23	b	604	CLA	C3B-C4B-NB	3.66	113.80	110.53
23	C	509	CLA	C4A-NA-C1A	-3.66	105.01	106.68
23	C	509	CLA	C2B-C1B-NB	3.66	114.12	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	C1C-C2C-C3C	-3.66	103.14	106.98
23	B	616	CLA	C4C-C3C-C2C	-3.65	101.57	106.89
23	A	405	CLA	CAA-C2A-C3A	-3.65	103.13	113.00
23	b	614	CLA	C3B-C4B-NB	3.65	113.79	110.53
23	b	611	CLA	C3B-C4B-NB	3.65	113.78	110.53
23	D	406	CLA	C1D-CHD-C4C	-3.64	118.27	126.02
23	C	512	CLA	C3B-C4B-NB	3.64	113.78	110.53
23	b	609	CLA	C1D-CHD-C4C	-3.64	118.28	126.02
23	c	511	CLA	C1D-CHD-C4C	-3.64	118.28	126.02
23	C	513	CLA	C2C-C1C-NC	3.64	113.80	109.98
23	c	505	CLA	C3B-C4B-NB	3.64	113.78	110.53
23	a	405	CLA	C3C-C4C-NC	3.64	115.09	110.43
23	B	603	CLA	C4-C3-C5	3.64	121.54	115.23
35	c	517	DGD	O2G-C1B-C2B	3.64	119.34	111.48
23	B	603	CLA	CAA-C2A-C3A	-3.63	103.18	113.00
23	d	402	CLA	CHD-C1D-ND	-3.63	119.69	124.80
23	b	611	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
23	A	408	CLA	CAC-C3C-C4C	3.63	129.51	124.79
25	Y	101	BCR	C15-C14-C13	-3.63	122.19	127.28
23	c	510	CLA	C1C-C2C-C3C	-3.63	103.17	106.98
29	d	405	PL9	C37-C38-C39	-3.63	119.33	127.62
23	b	606	CLA	C3C-C4C-NC	3.62	115.07	110.43
23	b	616	CLA	C2C-C1C-NC	3.62	113.78	109.98
23	a	405	CLA	C1-C2-C3	-3.61	120.28	126.20
23	b	601	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
23	b	610	CLA	CHD-C1D-ND	-3.61	119.72	124.80
23	d	402	CLA	O2A-CGA-CBA	3.61	122.83	111.83
23	C	514	CLA	C3B-C4B-NB	3.60	113.74	110.53
25	c	515	BCR	C11-C10-C9	-3.60	122.23	127.28
23	A	405	CLA	C1D-CHD-C4C	-3.59	118.38	126.02
23	d	402	CLA	C3B-C4B-NB	3.59	113.73	110.53
23	b	606	CLA	C4-C3-C5	3.59	121.46	115.23
23	B	611	CLA	C4A-NA-C1A	-3.59	105.04	106.68
23	B	610	CLA	C1D-CHD-C4C	-3.59	118.40	126.02
23	b	602	CLA	C1C-C2C-C3C	-3.59	103.21	106.98
23	b	615	CLA	CHD-C1D-ND	-3.58	119.76	124.80
23	A	408	CLA	C1D-CHD-C4C	-3.58	118.40	126.02
26	a	413	SQD	O47-C7-C8	3.58	119.23	111.48
23	b	603	CLA	C1C-C2C-C3C	-3.58	103.21	106.98
29	a	416	PL9	C30-C29-C31	3.58	121.44	115.23
23	A	406	CLA	C3C-C4C-NC	3.58	115.02	110.43
23	b	615	CLA	C1C-C2C-C3C	-3.57	103.22	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	C1D-CHD-C4C	-3.57	118.42	126.02
23	b	602	CLA	C1D-CHD-C4C	-3.57	118.43	126.02
23	C	512	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
23	b	608	CLA	C4B-C3B-C2B	-3.57	102.86	107.30
25	d	404	BCR	C16-C17-C18	-3.57	122.27	127.28
35	c	518	DGD	O2G-C1B-C2B	3.56	119.19	111.48
29	A	414	PL9	C15-C14-C16	3.56	121.41	115.23
23	b	605	CLA	C1C-C2C-C3C	-3.56	103.23	106.98
23	B	608	CLA	C1D-CHD-C4C	-3.56	118.45	126.02
33	C	521	LMG	C3-C4-C5	3.56	116.69	110.23
23	c	512	CLA	C3C-C4C-NC	3.56	114.99	110.43
23	b	615	CLA	O2D-CGD-CBD	3.56	117.45	111.23
23	c	502	CLA	C3C-C4C-NC	3.56	114.99	110.43
23	C	508	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
23	B	610	CLA	CAA-CBA-CGA	-3.56	103.11	113.21
23	B	613	CLA	C1D-CHD-C4C	-3.56	118.46	126.02
23	C	509	CLA	O2D-CGD-O1D	-3.55	116.93	123.85
33	B	621	LMG	O8-C28-C29	3.55	122.67	111.83
23	b	611	CLA	C1C-C2C-C3C	-3.55	103.24	106.98
23	d	403	CLA	C1D-CHD-C4C	-3.55	118.47	126.02
23	B	601	CLA	C2C-C1C-NC	3.55	113.71	109.98
23	A	404	CLA	C3C-C4C-NC	3.55	114.98	110.43
26	A	410	SQD	O47-C7-C8	3.55	119.16	111.48
23	c	505	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
25	c	515	BCR	C15-C14-C13	-3.55	122.30	127.28
26	B	620	SQD	O7-S-C6	3.55	112.05	106.76
26	F	101	SQD	C44-O6-C1	-3.54	106.20	113.80
23	b	607	CLA	O2D-CGD-O1D	-3.54	116.95	123.85
23	b	616	CLA	CHD-C4C-NC	3.54	129.72	124.23
23	d	403	CLA	CMB-C2B-C1B	3.54	130.81	125.42
29	a	416	PL9	C27-C28-C29	-3.54	119.53	127.62
25	k	101	BCR	C29-C30-C25	3.53	115.57	110.44
23	C	506	CLA	C1C-C2C-C3C	-3.53	103.26	106.98
29	A	414	PL9	C37-C38-C39	-3.53	119.54	127.62
23	B	605	CLA	O2A-CGA-O1A	-3.53	114.81	123.63
38	E	103	HEM	CHB-C1B-NB	3.53	128.73	124.37
34	V	203	HTG	C1-O5-C5	3.52	116.91	112.19
23	c	509	CLA	C1-C2-C3	-3.52	120.43	126.20
23	c	503	CLA	CHD-C1D-ND	-3.52	119.85	124.80
29	A	414	PL9	C27-C28-C29	-3.52	119.56	127.62
23	b	607	CLA	C2B-C1B-NB	3.52	113.98	110.33
26	a	411	SQD	O9-S-C6	3.52	112.01	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	C1-C2-C3	-3.52	120.43	126.20
23	B	608	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
23	b	604	CLA	C2B-C1B-NB	3.51	113.97	110.33
23	C	505	CLA	C1D-CHD-C4C	-3.51	118.55	126.02
23	c	511	CLA	CMC-C2C-C1C	3.51	130.52	125.03
23	B	614	CLA	C1-C2-C3	-3.51	120.45	126.20
23	B	607	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
23	B	616	CLA	C4B-C3B-C2B	-3.50	102.94	107.30
25	C	515	BCR	C33-C5-C6	-3.50	120.66	124.48
23	b	608	CLA	C1-C2-C3	-3.50	120.47	126.20
25	A	409	BCR	C24-C23-C22	-3.50	121.06	126.23
23	A	404	CLA	O2A-CGA-O1A	-3.50	114.89	123.63
23	B	607	CLA	C3B-C4B-NB	3.50	113.65	110.53
23	C	502	CLA	C3C-C4C-NC	3.49	114.91	110.43
23	a	406	CLA	C3B-C4B-NB	3.49	113.65	110.53
37	D	409	LHG	O7-C7-C8	3.49	119.04	111.48
23	b	608	CLA	C3C-C4C-NC	3.49	114.90	110.43
29	d	405	PL9	C40-C39-C41	3.49	121.28	115.23
25	B	617	BCR	C33-C5-C6	-3.48	120.68	124.48
23	b	614	CLA	C1C-C2C-C3C	-3.48	103.32	106.98
23	b	610	CLA	O2D-CGD-O1D	-3.48	117.07	123.85
23	a	405	CLA	O2A-CGA-CBA	3.48	122.45	111.83
23	c	507	CLA	C1D-CHD-C4C	-3.48	118.63	126.02
23	d	403	CLA	C3C-C4C-NC	3.47	114.88	110.43
23	B	605	CLA	C2B-C1B-NB	3.47	113.93	110.33
23	b	612	CLA	C4C-C3C-C2C	-3.47	101.84	106.89
23	C	507	CLA	CBC-CAC-C3C	-3.47	103.01	112.42
23	B	609	CLA	C1D-CHD-C4C	-3.47	118.64	126.02
23	A	408	CLA	CAA-C2A-C3A	-3.47	103.63	113.00
23	B	608	CLA	CAC-C3C-C4C	3.46	129.30	124.79
24	A	353	PHO	C1A-C2A-C3A	-3.46	99.54	102.84
23	A	405	CLA	C3C-C4C-NC	3.46	114.86	110.43
29	a	416	PL9	C37-C38-C39	-3.46	119.71	127.62
23	C	510	CLA	C3C-C4C-NC	3.46	114.86	110.43
23	c	506	CLA	C4C-C3C-C2C	-3.45	101.87	106.89
40	V	202	HEC	C4D-ND-C1D	3.45	111.45	105.82
23	c	513	CLA	C1C-C2C-C3C	-3.45	103.35	106.98
23	a	406	CLA	CHD-C4C-NC	3.45	129.58	124.23
23	C	508	CLA	C1C-C2C-C3C	-3.45	103.35	106.98
23	C	512	CLA	C1C-C2C-C3C	-3.45	103.35	106.98
23	B	606	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
23	B	604	CLA	C1D-CHD-C4C	-3.45	118.70	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	O2D-CGD-O1D	-3.44	117.14	123.85
23	D	405	CLA	C2B-C1B-NB	3.44	113.90	110.33
23	c	507	CLA	C4B-C3B-C2B	-3.44	103.02	107.30
23	B	604	CLA	CAC-C3C-C4C	3.44	129.27	124.79
23	b	614	CLA	C1-C2-C3	-3.44	120.57	126.20
23	B	605	CLA	C4C-C3C-C2C	-3.43	101.89	106.89
23	B	601	CLA	CHD-C4C-NC	3.43	129.55	124.23
23	b	608	CLA	CAC-C3C-C4C	3.43	129.25	124.79
23	b	601	CLA	C3C-C4C-NC	3.43	114.82	110.43
23	C	502	CLA	C1C-C2C-C3C	-3.43	103.38	106.98
24	a	408	PHO	C1A-C2A-C3A	-3.43	99.58	102.84
37	D	409	LHG	O8-C23-C24	3.42	122.28	111.83
25	a	410	BCR	C38-C26-C25	-3.42	120.75	124.48
23	B	613	CLA	C4B-C3B-C2B	-3.42	103.05	107.30
23	B	614	CLA	CMC-C2C-C1C	3.42	130.38	125.03
23	C	513	CLA	C4-C3-C5	3.42	121.16	115.23
25	B	619	BCR	C7-C8-C9	-3.42	121.18	126.23
23	B	610	CLA	CMB-C2B-C1B	3.42	130.62	125.42
23	b	613	CLA	CHD-C1D-ND	-3.41	120.00	124.80
37	d	408	LHG	O7-C7-C8	3.41	118.86	111.48
23	a	405	CLA	C3B-C4B-NB	3.41	113.58	110.53
23	B	616	CLA	CAC-C3C-C4C	3.41	129.23	124.79
23	A	406	CLA	CAA-C2A-C3A	-3.41	103.78	113.00
23	b	602	CLA	C1-C2-C3	-3.41	120.61	126.20
23	b	607	CLA	C1D-CHD-C4C	-3.41	118.78	126.02
23	c	510	CLA	C4B-C3B-C2B	-3.40	103.07	107.30
38	e	87	HEM	CHA-C4D-ND	3.40	128.57	124.37
23	b	611	CLA	CHD-C4C-NC	3.40	129.50	124.23
23	b	604	CLA	CAC-C3C-C4C	3.40	129.21	124.79
23	A	406	CLA	C3B-C4B-NB	3.40	113.56	110.53
23	B	611	CLA	C2A-C1A-CHA	-3.40	117.97	123.87
23	b	604	CLA	CHD-C1D-ND	-3.40	120.02	124.80
23	A	404	CLA	C1-C2-C3	-3.40	120.63	126.20
33	a	419	LMG	C8-O7-C10	-3.40	109.67	117.80
23	C	504	CLA	C4-C3-C5	3.39	121.12	115.23
23	d	403	CLA	C1C-C2C-C3C	-3.39	103.41	106.98
23	B	605	CLA	CHD-C4C-NC	3.39	129.49	124.23
33	C	520	LMG	O8-C28-C29	3.39	122.17	111.83
40	v	202	HEC	C4D-ND-C1D	3.39	111.35	105.82
26	B	620	SQD	C1-O5-C5	-3.39	107.11	113.72
23	a	409	CLA	O2D-CGD-O1D	-3.39	117.26	123.85
23	c	503	CLA	CHD-C4C-NC	3.39	129.48	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C4C-C3C-C2C	-3.38	101.97	106.89
23	c	507	CLA	C3C-C4C-NC	3.38	114.76	110.43
23	c	502	CLA	C1-C2-C3	-3.37	120.67	126.20
23	B	601	CLA	C4C-C3C-C2C	-3.37	101.98	106.89
23	b	609	CLA	CBC-CAC-C3C	-3.37	103.28	112.42
26	F	101	SQD	O8-S-C6	3.37	112.48	105.97
23	c	513	CLA	CMB-C2B-C1B	3.37	130.55	125.42
26	A	410	SQD	C44-O6-C1	-3.37	106.57	113.80
23	c	510	CLA	C3C-C4C-NC	3.37	114.75	110.43
23	B	608	CLA	C4C-C3C-C2C	-3.37	101.99	106.89
23	B	616	CLA	CHD-C1D-ND	-3.36	120.07	124.80
23	b	602	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
23	b	615	CLA	C4-C3-C5	3.36	121.06	115.23
29	a	416	PL9	C17-C18-C19	-3.36	119.94	127.62
23	C	503	CLA	CMB-C2B-C1B	3.36	130.53	125.42
23	D	405	CLA	C4C-C3C-C2C	-3.35	102.01	106.89
23	A	404	CLA	CAC-C3C-C4C	3.35	129.15	124.79
23	C	511	CLA	C3C-C4C-NC	3.35	114.73	110.43
23	C	511	CLA	C4-C3-C5	3.35	121.05	115.23
38	E	103	HEM	C3B-C4B-NB	-3.35	107.06	109.47
23	B	612	CLA	C1D-CHD-C4C	-3.35	118.90	126.02
29	D	408	PL9	C17-C18-C19	-3.35	119.96	127.62
34	B	622	HTG	O5-C1-C2	3.35	114.93	110.32
26	a	413	SQD	O48-C23-C24	3.35	122.03	111.83
23	b	610	CLA	C4C-C3C-C2C	-3.34	102.02	106.89
37	l	101	LHG	O7-C7-C8	3.34	118.72	111.48
23	B	604	CLA	C4C-C3C-C2C	-3.34	102.02	106.89
23	B	609	CLA	CMB-C2B-C1B	3.34	130.51	125.42
23	b	612	CLA	CAC-C3C-C4C	3.34	129.14	124.79
40	V	202	HEC	CBD-CAD-C3D	-3.34	103.30	112.53
25	K	102	BCR	C7-C8-C9	-3.34	121.30	126.23
23	B	612	CLA	C4C-C3C-C2C	-3.34	102.03	106.89
23	c	503	CLA	C3B-C4B-NB	3.33	113.51	110.53
23	A	404	CLA	CAA-C2A-C1A	-3.33	101.05	111.97
23	B	611	CLA	CHB-C4A-NA	3.33	129.21	124.40
23	C	504	CLA	C1C-C2C-C3C	-3.33	103.47	106.98
23	B	610	CLA	C4C-C3C-C2C	-3.33	102.04	106.89
23	c	506	CLA	CMB-C2B-C1B	3.33	130.49	125.42
23	b	610	CLA	C1C-C2C-C3C	-3.33	103.48	106.98
23	d	402	CLA	C1D-CHD-C4C	-3.33	118.95	126.02
23	C	503	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
23	a	405	CLA	CAA-C2A-C1A	-3.32	101.10	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	C4B-C3B-C2B	-3.32	103.17	107.30
25	C	516	BCR	C7-C8-C9	-3.32	121.33	126.23
23	C	505	CLA	C1-O2A-CGA	3.32	124.68	116.65
38	e	87	HEM	CAD-CBD-CGD	3.31	122.45	113.67
23	c	508	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
34	b	625	HTG	O5-C5-C4	3.31	115.67	109.70
23	C	506	CLA	CAC-C3C-C4C	3.31	129.10	124.79
33	m	101	LMG	O8-C28-C29	3.31	121.93	111.83
23	B	615	CLA	C3B-C4B-NB	3.31	113.48	110.53
23	b	604	CLA	C4B-C3B-C2B	-3.31	103.19	107.30
26	a	411	SQD	C45-O47-C7	-3.31	109.88	117.80
23	B	613	CLA	CHD-C1D-ND	-3.31	120.15	124.80
23	b	607	CLA	C4-C3-C5	3.30	120.96	115.23
23	B	613	CLA	C4-C3-C5	3.30	120.96	115.23
23	B	605	CLA	C1C-C2C-C3C	-3.30	103.51	106.98
33	Z	101	LMG	O6-C1-C2	3.30	117.15	110.37
23	C	514	CLA	CMC-C2C-C1C	3.30	130.19	125.03
23	C	513	CLA	CHD-C4C-NC	3.30	129.34	124.23
23	c	513	CLA	O2A-CGA-CBA	3.30	121.89	111.83
23	a	405	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
23	b	601	CLA	C4-C3-C5	3.30	120.95	115.23
23	b	601	CLA	CHD-C4C-NC	3.29	129.34	124.23
23	C	508	CLA	CMB-C2B-C1B	3.29	130.43	125.42
23	b	611	CLA	C1D-CHD-C4C	-3.29	119.03	126.02
23	A	408	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
25	D	407	BCR	C29-C30-C25	3.29	115.22	110.44
23	B	611	CLA	C1-C2-C3	-3.29	120.81	126.20
25	Y	101	BCR	C28-C27-C26	-3.29	108.20	114.06
23	b	605	CLA	CHD-C4C-NC	3.28	129.31	124.23
33	z	101	LMG	O7-C10-C11	3.28	118.57	111.48
23	B	603	CLA	O2A-CGA-O1A	-3.28	115.43	123.63
23	c	503	CLA	CMC-C2C-C1C	3.27	130.15	125.03
23	C	507	CLA	CMC-C2C-C1C	3.27	130.15	125.03
23	b	615	CLA	CMB-C2B-C1B	3.27	130.40	125.42
26	A	410	SQD	O9-S-C6	3.27	111.64	106.76
23	A	406	CLA	O2A-CGA-O1A	-3.27	115.45	123.63
23	C	507	CLA	CHC-C1C-C2C	-3.27	117.65	126.95
23	b	606	CLA	C3B-C4B-NB	3.27	113.45	110.53
24	a	353	PHO	C4-C3-C5	3.27	120.90	115.23
23	b	614	CLA	O2A-CGA-O1A	-3.27	115.45	123.63
23	b	612	CLA	C4B-C3B-C2B	-3.27	103.24	107.30
23	B	612	CLA	C1C-C2C-C3C	-3.26	103.55	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	C4C-C3C-C2C	-3.26	102.14	106.89
23	c	508	CLA	C1D-CHD-C4C	-3.26	119.08	126.02
23	b	613	CLA	C4B-C3B-C2B	-3.26	103.24	107.30
23	b	602	CLA	C3C-C4C-NC	3.26	114.61	110.43
25	K	102	BCR	C20-C21-C22	-3.26	122.70	127.28
23	C	507	CLA	C1D-CHD-C4C	-3.26	119.09	126.02
23	C	506	CLA	C4C-C3C-C2C	-3.26	102.14	106.89
23	B	604	CLA	O2A-CGA-O1A	-3.26	115.47	123.63
23	d	402	CLA	C4-C3-C5	3.26	120.89	115.23
23	C	503	CLA	C1D-CHD-C4C	-3.26	119.09	126.02
23	B	615	CLA	CMC-C2C-C1C	3.26	130.12	125.03
23	c	511	CLA	C3B-C4B-NB	3.26	113.44	110.53
23	c	510	CLA	CHC-C1C-C2C	-3.26	117.70	126.95
23	a	409	CLA	CHD-C4C-NC	3.25	129.27	124.23
23	B	614	CLA	O2A-CGA-CBA	3.25	121.75	111.83
23	C	512	CLA	C1-C2-C3	-3.25	120.87	126.20
32	b	627	LMT	C3'-C4'-C5'	-3.25	103.73	110.93
23	b	616	CLA	C4C-C3C-C2C	-3.25	102.16	106.89
23	C	513	CLA	CMC-C2C-C1C	3.25	130.11	125.03
33	c	521	LMG	C9-C8-C7	-3.25	104.22	111.78
24	a	408	PHO	O2A-CGA-O1A	-3.25	115.51	123.63
23	C	509	CLA	C4C-C3C-C2C	-3.25	102.17	106.89
23	B	605	CLA	C4-C3-C5	3.24	120.85	115.23
23	B	602	CLA	CMC-C2C-C1C	3.24	130.10	125.03
23	c	507	CLA	CHC-C1C-C2C	-3.24	117.75	126.95
23	b	609	CLA	C4C-C3C-C2C	-3.24	102.18	106.89
23	b	611	CLA	CMC-C2C-C1C	3.23	130.09	125.03
25	T	101	BCR	C16-C17-C18	-3.23	122.75	127.28
38	E	103	HEM	CBD-CAD-C3D	-3.23	103.61	112.53
35	h	102	DGD	O2G-C1B-C2B	3.23	118.46	111.48
23	B	603	CLA	C4C-C3C-C2C	-3.22	102.20	106.89
23	A	406	CLA	C4B-C3B-C2B	-3.22	103.29	107.30
23	b	612	CLA	O2A-CGA-CBA	3.22	121.66	111.83
23	C	512	CLA	C4C-C3C-C2C	-3.22	102.20	106.89
23	C	507	CLA	C3C-C4C-NC	3.22	114.56	110.43
23	d	402	CLA	O2A-CGA-O1A	-3.22	115.57	123.63
26	A	412	SQD	O48-C23-C24	3.22	121.65	111.83
23	b	609	CLA	C1C-C2C-C3C	-3.22	103.59	106.98
23	c	506	CLA	C1C-C2C-C3C	-3.22	103.59	106.98
29	D	408	PL9	C25-C24-C26	3.22	120.81	115.23
23	a	407	CLA	CAA-C2A-C3A	-3.22	104.31	113.00
23	b	609	CLA	C3B-C4B-NB	3.21	113.40	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	CHD-C1D-ND	-3.21	120.28	124.80
24	a	408	PHO	O2A-CGA-CBA	3.21	121.63	111.83
23	c	513	CLA	C3C-C4C-NC	3.21	114.55	110.43
33	D	415	LMG	O8-C28-O10	-3.21	115.59	123.63
23	b	605	CLA	C4C-C3C-C2C	-3.21	102.22	106.89
23	c	511	CLA	C4-C3-C5	3.21	120.80	115.23
25	H	101	BCR	C24-C23-C22	-3.21	121.49	126.23
25	C	516	BCR	C33-C5-C6	-3.21	120.98	124.48
23	c	502	CLA	C1D-CHD-C4C	-3.21	119.20	126.02
23	c	512	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
23	D	405	CLA	C4B-C3B-C2B	-3.20	103.33	107.30
23	C	514	CLA	C1-C2-C3	-3.20	120.96	126.20
23	b	616	CLA	CBC-CAC-C3C	-3.20	103.76	112.42
23	C	502	CLA	CHD-C4C-NC	3.19	129.18	124.23
23	B	606	CLA	CMC-C2C-C1C	3.19	130.03	125.03
23	B	610	CLA	C3B-C4B-NB	3.19	113.38	110.53
23	b	615	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
23	c	510	CLA	CAC-C3C-C4C	3.19	128.94	124.79
23	c	502	CLA	CMB-C2B-C1B	3.19	130.28	125.42
29	A	414	PL9	O1-C4-C3	-3.19	117.37	120.73
23	a	409	CLA	CMB-C2B-C1B	3.19	130.28	125.42
23	b	606	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
23	C	505	CLA	C4B-C3B-C2B	-3.19	103.34	107.30
25	B	618	BCR	C2-C1-C6	3.19	115.07	110.44
23	a	407	CLA	C3B-C4B-NB	3.18	113.37	110.53
25	B	617	BCR	C7-C8-C9	-3.18	121.54	126.23
23	c	505	CLA	CMB-C2B-C1B	3.18	130.25	125.42
23	C	508	CLA	C4C-C3C-C2C	-3.17	102.27	106.89
23	C	511	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
23	b	612	CLA	CMC-C2C-C1C	3.17	129.99	125.03
38	e	87	HEM	CBD-CAD-C3D	-3.17	103.77	112.53
23	C	508	CLA	CBC-CAC-C3C	-3.17	103.83	112.42
23	a	406	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
23	B	612	CLA	CAC-C3C-C4C	3.17	128.91	124.79
23	C	507	CLA	CAC-C3C-C4C	3.16	128.91	124.79
35	C	519	DGD	O1G-C1A-C2A	3.16	121.48	111.83
25	A	409	BCR	C11-C10-C9	-3.16	122.84	127.28
23	B	608	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
23	d	402	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
37	D	411	LHG	O8-C23-C24	3.16	121.46	111.83
23	A	404	CLA	C4B-C3B-C2B	-3.16	103.38	107.30
23	c	509	CLA	C4C-C3C-C2C	-3.16	102.30	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	k	101	BCR	C7-C8-C9	-3.16	121.57	126.23
25	T	101	BCR	C15-C14-C13	3.15	131.70	127.28
25	t	103	BCR	C21-C20-C19	-3.15	114.07	123.20
23	a	407	CLA	CHD-C4C-NC	3.15	129.12	124.23
23	c	506	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
33	Z	101	LMG	C4-C3-C2	3.15	116.36	110.83
23	C	510	CLA	O2A-CGA-CBA	3.15	121.44	111.83
23	B	604	CLA	C6-C5-C3	-3.15	105.80	113.47
23	B	602	CLA	C3B-C4B-NB	3.15	113.34	110.53
23	c	507	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
23	b	609	CLA	C4B-C3B-C2B	-3.15	103.39	107.30
25	y	101	BCR	C24-C23-C22	-3.15	121.58	126.23
23	b	608	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
23	B	604	CLA	CHD-C1D-ND	-3.14	120.38	124.80
26	f	102	SQD	O5-C1-C2	3.14	116.83	110.37
23	c	509	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
23	C	503	CLA	C3B-C4B-NB	3.14	113.33	110.53
23	B	616	CLA	C1C-C2C-C3C	-3.14	103.68	106.98
23	C	511	CLA	CHD-C4C-NC	3.14	129.10	124.23
29	d	405	PL9	C22-C23-C24	-3.14	120.44	127.62
23	B	606	CLA	CHD-C4C-NC	3.14	129.09	124.23
23	B	607	CLA	CMC-C2C-C1C	3.14	129.94	125.03
23	C	504	CLA	CMB-C2B-C1B	3.14	130.19	125.42
25	y	101	BCR	C38-C26-C25	-3.14	121.06	124.48
23	D	405	CLA	C1D-CHD-C4C	-3.13	119.36	126.02
23	b	614	CLA	C4C-C3C-C2C	-3.13	102.33	106.89
23	A	408	CLA	CHC-C1C-C2C	-3.13	118.04	126.95
23	b	603	CLA	C4C-C3C-C2C	-3.13	102.33	106.89
23	c	505	CLA	C4C-C3C-C2C	-3.13	102.33	106.89
29	A	414	PL9	C17-C18-C19	-3.13	120.45	127.62
23	C	510	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
23	b	612	CLA	CHD-C1D-ND	-3.13	120.40	124.80
33	D	415	LMG	O8-C28-C29	3.13	121.38	111.83
23	b	616	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
23	A	405	CLA	CMB-C2B-C1B	3.13	130.18	125.42
23	a	409	CLA	O2A-CGA-CBA	3.13	121.38	111.83
23	c	504	CLA	C1C-C2C-C3C	-3.13	103.69	106.98
23	b	616	CLA	C3B-C4B-NB	3.13	113.32	110.53
23	B	608	CLA	CHC-C1C-C2C	-3.13	118.06	126.95
23	C	513	CLA	C4C-C3C-C2C	-3.13	102.34	106.89
23	A	405	CLA	CAC-C3C-C4C	3.13	128.86	124.79
23	C	509	CLA	CAC-C3C-C4C	3.13	128.86	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	CMA-C3A-C4A	-3.12	103.37	111.77
29	a	416	PL9	C25-C24-C26	3.12	120.65	115.23
23	A	405	CLA	C3B-C4B-NB	3.12	113.32	110.53
23	b	615	CLA	C11-C10-C8	-3.12	105.59	115.97
34	B	622	HTG	C1'-S1-C1	3.12	107.19	100.45
37	D	410	LHG	O8-C23-O10	-3.12	115.82	123.63
23	c	509	CLA	CHD-C1D-ND	-3.12	120.41	124.80
23	c	510	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
24	A	353	PHO	C4-C3-C5	3.12	120.64	115.23
23	C	510	CLA	CAC-C3C-C4C	3.11	128.84	124.79
23	C	505	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
29	a	416	PL9	C42-C43-C44	-3.11	120.50	127.62
23	C	502	CLA	CMB-C2B-C1B	3.11	130.15	125.42
23	B	612	CLA	CMC-C2C-C1C	3.11	129.89	125.03
23	C	504	CLA	C4C-C3C-C2C	-3.11	102.37	106.89
23	B	604	CLA	C4B-C3B-C2B	-3.10	103.44	107.30
32	A	359	LMT	O5B-C5B-C4B	3.10	115.29	109.70
37	D	411	LHG	O7-C7-C8	3.10	118.19	111.48
38	E	103	HEM	CHD-C1D-ND	3.10	127.76	124.42
25	d	404	BCR	C21-C20-C19	-3.10	114.22	123.20
38	e	87	HEM	CHD-C1D-ND	3.10	127.75	124.42
23	C	510	CLA	C1D-CHD-C4C	-3.09	119.44	126.02
23	D	406	CLA	C3B-C4B-NB	3.09	113.29	110.53
23	B	607	CLA	CAA-C2A-C3A	-3.09	104.64	113.00
23	B	614	CLA	CBC-CAC-C3C	-3.09	104.04	112.42
23	a	407	CLA	CMB-C2B-C1B	3.09	130.12	125.42
23	a	406	CLA	CMA-C3A-C2A	-3.09	102.03	113.98
25	c	516	BCR	C7-C8-C9	-3.09	121.66	126.23
25	b	619	BCR	C15-C14-C13	-3.09	122.94	127.28
25	T	101	BCR	C11-C10-C9	-3.09	122.95	127.28
23	c	508	CLA	C4-C3-C5	3.09	120.59	115.23
23	b	610	CLA	CAA-C2A-C3A	-3.09	104.66	113.00
23	D	406	CLA	C4C-C3C-C2C	-3.08	102.40	106.89
23	B	604	CLA	CMB-C2B-C1B	3.08	130.11	125.42
23	c	504	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
23	B	603	CLA	O2A-CGA-CBA	3.08	121.23	111.83
23	a	405	CLA	C4-C3-C5	3.08	120.57	115.23
23	b	602	CLA	CMB-C2B-C1B	3.08	130.10	125.42
33	C	521	LMG	O8-C28-C29	3.08	121.22	111.83
23	B	615	CLA	C4C-C3C-C2C	-3.08	102.41	106.89
23	C	507	CLA	C4B-C3B-C2B	-3.08	103.48	107.30
23	B	604	CLA	CHC-C1C-C2C	-3.07	118.21	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	CMC-C2C-C1C	3.07	129.84	125.03
23	B	607	CLA	C1D-CHD-C4C	-3.07	119.49	126.02
38	e	87	HEM	CHD-C4C-NC	3.07	127.80	124.45
23	A	408	CLA	C4B-C3B-C2B	-3.07	103.48	107.30
26	b	620	SQD	C3-C4-C5	3.07	115.80	110.23
23	c	509	CLA	CMB-C2B-C1B	3.07	130.09	125.42
23	C	502	CLA	C3B-C4B-NB	3.07	113.27	110.53
23	c	503	CLA	CBC-CAC-C3C	-3.07	104.11	112.42
23	B	607	CLA	CBC-CAC-C3C	-3.06	104.12	112.42
23	c	510	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
23	b	603	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
35	C	517	DGD	C2G-O2G-C1B	-3.06	110.47	117.80
23	B	607	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
23	b	607	CLA	CHC-C1C-C2C	-3.06	118.26	126.95
23	c	513	CLA	C4-C3-C5	3.05	120.53	115.23
25	H	101	BCR	C10-C11-C12	-3.05	114.35	123.20
37	D	411	LHG	O8-C23-O10	-3.05	115.99	123.63
37	e	101	LHG	O7-C7-C8	3.05	118.08	111.48
23	c	510	CLA	O2A-CGA-CBA	3.05	121.13	111.83
23	b	613	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
23	a	409	CLA	C3B-C4B-NB	3.05	113.25	110.53
23	C	513	CLA	C1C-C2C-C3C	-3.05	103.78	106.98
23	C	514	CLA	C4C-C3C-C2C	-3.05	102.46	106.89
23	B	614	CLA	CAC-C3C-C4C	3.04	128.75	124.79
23	b	603	CLA	C2A-C1A-CHA	-3.04	118.59	123.87
23	B	607	CLA	C4-C3-C5	3.04	120.51	115.23
38	e	87	HEM	C1B-NB-C4B	3.04	108.81	105.21
25	h	101	BCR	C7-C8-C9	-3.04	121.74	126.23
23	A	408	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
23	C	513	CLA	O2A-CGA-CBA	3.04	121.10	111.83
23	C	506	CLA	C3B-C4B-NB	3.04	113.24	110.53
25	T	101	BCR	C33-C5-C6	-3.04	121.17	124.48
29	a	416	PL9	C35-C34-C36	3.03	120.49	115.23
23	C	509	CLA	CHC-C1C-C2C	-3.03	118.33	126.95
25	d	404	BCR	C10-C11-C12	-3.03	114.42	123.20
37	d	711	LHG	O7-C7-C8	3.03	118.04	111.48
25	c	515	BCR	C16-C17-C18	-3.03	123.03	127.28
23	C	502	CLA	C4B-C3B-C2B	-3.03	103.53	107.30
23	A	406	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
23	c	514	CLA	C4B-C3B-C2B	-3.03	103.54	107.30
23	c	512	CLA	CHD-C4C-NC	3.03	128.93	124.23
23	C	510	CLA	CHC-C1C-C2C	-3.03	118.34	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	620	SQD	O48-C23-C24	3.03	121.07	111.83
37	E	101	LHG	O8-C23-C24	3.03	121.06	111.83
23	B	610	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
23	B	613	CLA	O2A-CGA-CBA	3.02	121.05	111.83
23	b	616	CLA	O2A-CGA-O1A	-3.02	116.07	123.63
23	B	609	CLA	O2A-CGA-CBA	3.02	121.03	111.83
23	B	612	CLA	C2B-C1B-NB	3.02	113.45	110.33
23	b	609	CLA	CAC-C3C-C4C	3.01	128.71	124.79
23	c	504	CLA	C3B-C4B-NB	3.01	113.22	110.53
23	B	602	CLA	CAC-C3C-C4C	3.01	128.71	124.79
23	D	406	CLA	CAC-C3C-C4C	3.01	128.71	124.79
23	D	405	CLA	O2A-CGA-CBA	3.01	121.00	111.83
23	b	613	CLA	CHC-C1C-C2C	-3.01	118.41	126.95
23	b	606	CLA	CAA-C2A-C3A	-3.01	104.88	113.00
23	c	512	CLA	C4-C3-C5	3.00	120.44	115.23
23	B	609	CLA	CMC-C2C-C1C	3.00	129.73	125.03
26	F	101	SQD	C1-C2-C3	-3.00	103.69	110.01
23	C	502	CLA	CAC-C3C-C4C	3.00	128.70	124.79
23	D	405	CLA	CAA-C2A-C3A	-3.00	104.89	113.00
23	d	402	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
33	z	101	LMG	O8-C28-C29	3.00	120.98	111.83
23	c	505	CLA	CBC-CAC-C3C	-3.00	104.29	112.42
23	a	405	CLA	CHC-C1C-C2C	-3.00	118.43	126.95
23	a	407	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
23	B	610	CLA	O2A-CGA-O1A	-3.00	116.13	123.63
23	b	614	CLA	CHD-C4C-NC	3.00	128.88	124.23
23	C	503	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
23	C	514	CLA	CHD-C4C-NC	3.00	128.88	124.23
35	h	102	DGD	O3G-C1D-C2D	2.99	112.82	108.27
23	C	512	CLA	CMC-C2C-C1C	2.99	129.71	125.03
23	B	613	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
23	b	607	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
23	B	605	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
25	C	515	BCR	C15-C14-C13	-2.99	123.09	127.28
23	B	611	CLA	C3B-C4B-NB	2.98	113.19	110.53
23	b	616	CLA	CMB-C2B-C1B	2.98	129.96	125.42
23	c	502	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
23	c	512	CLA	C4B-C3B-C2B	-2.98	103.59	107.30
24	a	353	PHO	O2D-CGD-O1D	-2.98	118.05	123.85
24	a	353	PHO	CBA-CAA-C2A	-2.98	105.00	113.78
34	b	622	HTG	O5-C5-C4	2.98	115.07	109.70
23	a	405	CLA	CMA-C3A-C4A	-2.98	103.77	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	412	SQD	O8-S-C6	2.98	111.72	105.97
23	C	511	CLA	CHC-C1C-C2C	-2.98	118.49	126.95
23	b	606	CLA	O2A-CGA-O1A	-2.97	116.19	123.63
26	B	620	SQD	C4-C3-C2	2.97	116.05	110.83
23	b	605	CLA	O2A-CGA-O1A	-2.97	116.19	123.63
29	a	416	PL9	C10-C9-C11	2.97	120.39	115.23
26	a	411	SQD	O47-C7-O49	-2.97	116.75	123.70
23	d	402	CLA	C4C-C3C-C2C	-2.97	102.56	106.89
23	A	404	CLA	CMC-C2C-C1C	2.97	129.68	125.03
23	B	613	CLA	O2A-CGA-O1A	-2.97	116.20	123.63
25	H	101	BCR	C7-C8-C9	-2.97	121.84	126.23
23	B	606	CLA	O2A-CGA-CBA	2.97	120.89	111.83
23	D	405	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
23	d	403	CLA	C2A-C1A-CHA	-2.97	118.71	123.87
29	A	414	PL9	C20-C19-C21	2.97	120.38	115.23
23	c	510	CLA	C1-O2A-CGA	2.97	123.84	116.65
23	b	614	CLA	CMB-C2B-C1B	2.97	129.94	125.42
25	b	619	BCR	C38-C26-C25	-2.97	121.25	124.48
23	C	509	CLA	C4B-C3B-C2B	-2.97	103.61	107.30
23	b	603	CLA	C4-C3-C5	2.97	120.38	115.23
23	b	612	CLA	O2A-CGA-O1A	-2.96	116.22	123.63
23	C	511	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
23	B	609	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
23	b	606	CLA	CHD-C4C-NC	2.96	128.82	124.23
23	b	606	CLA	CHC-C1C-C2C	-2.96	118.54	126.95
23	C	512	CLA	CMB-C2B-C1B	2.96	129.92	125.42
23	B	609	CLA	C4C-C3C-C2C	-2.96	102.59	106.89
23	C	506	CLA	C4-C3-C5	2.96	120.36	115.23
29	D	408	PL9	C37-C38-C39	-2.96	120.85	127.62
23	C	503	CLA	CAC-C3C-C4C	2.96	128.64	124.79
23	c	513	CLA	CHC-C1C-C2C	-2.96	118.55	126.95
25	b	619	BCR	C24-C23-C22	-2.96	121.86	126.23
23	b	603	CLA	O2A-CGA-O1A	-2.96	116.24	123.63
26	f	102	SQD	C4-C3-C2	-2.95	105.64	110.83
23	B	610	CLA	C4B-C3B-C2B	-2.95	103.63	107.30
23	b	608	CLA	CHC-C1C-C2C	-2.95	118.55	126.95
23	c	506	CLA	C1D-CHD-C4C	-2.95	119.74	126.02
23	C	503	CLA	C1-C2-C3	-2.95	121.36	126.20
23	b	616	CLA	C1C-C2C-C3C	-2.95	103.88	106.98
23	c	511	CLA	CHD-C4C-NC	2.95	128.81	124.23
37	D	409	LHG	C5-O7-C7	-2.95	110.73	117.80
23	C	508	CLA	CHD-C4C-NC	2.95	128.81	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	403	CLA	C4C-C3C-C2C	-2.95	102.60	106.89
23	b	605	CLA	C2A-C1A-CHA	-2.95	118.75	123.87
26	A	410	SQD	O48-C23-C24	2.95	120.82	111.83
23	b	614	CLA	CHC-C1C-C2C	-2.95	118.57	126.95
23	b	609	CLA	CHD-C4C-NC	2.95	128.80	124.23
23	c	506	CLA	C1-C2-C3	-2.95	121.37	126.20
23	A	405	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
34	b	622	HTG	O2-C2-C1	2.94	115.53	110.30
23	c	502	CLA	CAC-C3C-C4C	2.94	128.62	124.79
23	A	406	CLA	O2A-CGA-CBA	2.94	120.80	111.83
23	b	607	CLA	CBC-CAC-C3C	-2.94	104.45	112.42
23	B	613	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
23	c	509	CLA	C3B-C4B-NB	2.94	113.15	110.53
23	B	601	CLA	C1C-C2C-C3C	-2.94	103.89	106.98
23	A	404	CLA	C2A-C1A-CHA	-2.94	118.77	123.87
23	C	510	CLA	C4C-C3C-C2C	-2.93	102.62	106.89
34	B	626	HTG	C1'-S1-C1	2.93	106.79	100.45
23	c	514	CLA	O2A-CGA-CBA	2.93	120.78	111.83
23	c	502	CLA	C3B-C4B-NB	2.93	113.15	110.53
25	c	515	BCR	C38-C26-C25	-2.93	121.28	124.48
23	A	405	CLA	CHD-C4C-NC	2.93	128.78	124.23
29	a	416	PL9	C22-C23-C24	-2.93	120.92	127.62
23	C	510	CLA	O2A-CGA-O1A	-2.93	116.30	123.63
23	A	405	CLA	CMA-C3A-C4A	-2.93	103.90	111.77
23	b	609	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
23	b	602	CLA	CHD-C4C-NC	2.92	128.77	124.23
23	A	404	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
23	B	616	CLA	O2A-CGA-CBA	2.92	120.75	111.83
37	L	101	LHG	O8-C23-C24	2.92	120.75	111.83
23	c	514	CLA	CAC-C3C-C4C	2.92	128.59	124.79
33	a	419	LMG	C7-O1-C1	-2.92	107.54	113.80
23	b	611	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
23	c	506	CLA	CMC-C2C-C1C	2.92	129.59	125.03
27	b	901	GOL	C3-C2-C1	-2.92	101.10	111.80
23	b	610	CLA	CHD-C4C-NC	2.91	128.75	124.23
23	c	512	CLA	CHC-C1C-C2C	-2.91	118.67	126.95
25	D	407	BCR	C37-C22-C23	2.91	122.53	118.09
23	B	606	CLA	CMB-C2B-C1B	2.91	129.85	125.42
23	a	409	CLA	C4C-C3C-C2C	-2.91	102.66	106.89
23	c	502	CLA	CHC-C1C-C2C	-2.91	118.69	126.95
23	C	507	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
23	b	605	CLA	C3B-C4B-NB	2.90	113.12	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	CHC-C1C-C2C	-2.90	118.69	126.95
23	A	406	CLA	CHD-C4C-NC	2.90	128.73	124.23
23	A	406	CLA	CMC-C2C-C1C	2.90	129.57	125.03
25	K	102	BCR	C36-C18-C19	2.90	122.52	118.09
29	d	405	PL9	C10-C9-C11	2.90	120.27	115.23
23	C	509	CLA	CMC-C2C-C1C	2.90	129.57	125.03
23	b	605	CLA	CHC-C1C-C2C	-2.90	118.70	126.95
23	d	402	CLA	CHC-C1C-C2C	-2.90	118.71	126.95
23	b	603	CLA	CMA-C3A-C2A	-2.90	102.77	113.98
23	a	405	CLA	CMC-C2C-C1C	2.90	129.56	125.03
23	b	601	CLA	C3B-C4B-NB	2.90	113.12	110.53
24	A	407	PHO	C1-C2-C3	-2.90	121.45	126.20
23	c	503	CLA	CHC-C1C-C2C	-2.90	118.71	126.95
32	I	101	LMT	O5B-C5B-C4B	2.90	114.92	109.70
23	B	602	CLA	C4B-C3B-C2B	-2.90	103.70	107.30
23	B	616	CLA	CHD-C4C-NC	2.90	128.72	124.23
23	C	510	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
23	C	504	CLA	CHC-C1C-C2C	-2.89	118.72	126.95
26	f	102	SQD	O48-C23-C24	2.89	120.65	111.83
24	A	353	PHO	O2D-CGD-O1D	-2.89	118.22	123.85
23	b	615	CLA	CHC-C1C-C2C	-2.89	118.74	126.95
34	b	622	HTG	O5-C1-C2	2.89	114.30	110.32
32	M	101	LMT	C1'-O5'-C5'	-2.89	108.08	113.72
35	h	102	DGD	O1G-C1A-O1A	-2.89	116.41	123.63
23	C	503	CLA	CHC-C1C-C2C	-2.89	118.75	126.95
23	d	403	CLA	C4-C3-C5	2.88	120.23	115.23
23	B	612	CLA	C3B-C4B-NB	2.88	113.10	110.53
25	K	102	BCR	C38-C26-C25	-2.88	121.34	124.48
23	C	504	CLA	CAC-C3C-C4C	2.88	128.54	124.79
23	D	406	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
35	C	517	DGD	O6D-C1D-O3G	-2.88	103.24	110.04
37	d	407	LHG	O7-C7-C8	2.88	117.71	111.48
23	B	603	CLA	C2A-C1A-CHA	-2.88	118.87	123.87
33	c	520	LMG	O1-C7-C8	-2.88	103.81	110.82
23	b	603	CLA	O2A-CGA-CBA	2.88	120.61	111.83
24	a	353	PHO	C4A-C3A-C2A	-2.88	100.10	102.84
26	F	101	SQD	O48-C23-C24	2.88	120.61	111.83
32	m	103	LMT	C3'-C4'-C5'	-2.88	104.56	110.93
23	a	405	CLA	CAC-C3C-C4C	2.88	128.53	124.79
25	k	101	BCR	C15-C14-C13	-2.87	123.25	127.28
23	B	614	CLA	CHD-C4C-NC	2.87	128.68	124.23
23	c	513	CLA	C3B-C4B-NB	2.87	113.09	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	514	CLA	C4C-C3C-C2C	-2.87	102.72	106.89
23	c	507	CLA	O2A-CGA-O1A	-2.87	116.45	123.63
23	a	406	CLA	O2A-CGA-CBA	2.87	120.58	111.83
23	b	608	CLA	CBC-CAC-C3C	-2.87	104.65	112.42
23	C	507	CLA	C4-C3-C5	2.87	120.20	115.23
29	D	408	PL9	C10-C9-C11	2.87	120.20	115.23
23	B	612	CLA	C4B-C3B-C2B	-2.87	103.74	107.30
23	b	611	CLA	C4B-C3B-C2B	-2.86	103.74	107.30
23	C	511	CLA	CBC-CAC-C3C	-2.86	104.66	112.42
23	a	406	CLA	CHC-C1C-C2C	-2.86	118.81	126.95
32	a	414	LMT	O1'-C1'-C2'	2.86	112.62	108.27
23	C	506	CLA	CHC-C1C-C2C	-2.86	118.82	126.95
23	c	509	CLA	CHC-C1C-C2C	-2.86	118.82	126.95
23	c	509	CLA	O2A-CGA-CBA	2.86	120.55	111.83
23	B	602	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
23	c	512	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
23	c	503	CLA	C1-C2-C3	-2.86	121.51	126.20
32	a	420	LMT	C3'-C4'-C5'	-2.86	104.59	110.93
23	B	610	CLA	CHD-C4C-NC	2.86	128.66	124.23
23	c	505	CLA	CAC-C3C-C4C	2.86	128.51	124.79
29	D	408	PL9	C53-C6-C1	2.86	121.13	115.28
23	B	613	CLA	CAC-C3C-C4C	2.85	128.50	124.79
23	b	605	CLA	C4-C3-C5	2.85	120.18	115.23
23	a	407	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
23	B	614	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
23	a	409	CLA	C4-C3-C5	2.85	120.18	115.23
23	D	405	CLA	C4-C3-C5	2.85	120.17	115.23
23	b	614	CLA	O2A-CGA-CBA	2.85	120.52	111.83
29	d	405	PL9	C27-C28-C29	-2.85	121.11	127.62
23	C	512	CLA	C4-C3-C5	2.85	120.17	115.23
23	d	403	CLA	CHD-C4C-NC	2.85	128.64	124.23
25	y	101	BCR	C10-C11-C12	-2.84	114.96	123.20
23	C	504	CLA	CHD-C4C-NC	2.84	128.64	124.23
23	c	511	CLA	O2A-CGA-CBA	2.84	120.50	111.83
23	b	604	CLA	CMB-C2B-C1B	2.84	129.74	125.42
23	b	615	CLA	C3B-C4B-NB	2.83	113.06	110.53
23	B	613	CLA	CHC-C1C-C2C	-2.83	118.90	126.95
23	B	601	CLA	O2A-CGA-CBA	2.83	120.47	111.83
23	C	506	CLA	CMC-C2C-C1C	2.83	129.46	125.03
23	A	408	CLA	O2A-CGA-CBA	2.83	120.47	111.83
23	C	509	CLA	CHD-C1D-ND	-2.83	120.82	124.80
23	C	503	CLA	C2A-C1A-CHA	-2.83	118.95	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	CMB-C2B-C1B	2.83	129.73	125.42
23	a	407	CLA	C4B-C3B-C2B	-2.83	103.78	107.30
35	H	102	DGD	O1G-C1A-C2A	2.83	120.46	111.83
23	B	608	CLA	O2A-CGA-O1A	-2.83	116.55	123.63
23	A	404	CLA	CMA-C3A-C2A	-2.83	103.05	113.98
23	b	609	CLA	CMC-C2C-C1C	2.83	129.45	125.03
23	c	503	CLA	CMB-C2B-C1B	2.83	129.72	125.42
23	A	408	CLA	CMC-C2C-C1C	2.83	129.45	125.03
23	C	502	CLA	C1-C2-C3	-2.83	121.57	126.20
23	B	615	CLA	C4-C3-C5	2.83	120.13	115.23
23	A	404	CLA	CHC-C1C-C2C	-2.83	118.92	126.95
23	b	613	CLA	O2A-CGA-CBA	2.82	120.44	111.83
25	d	404	BCR	C28-C27-C26	-2.82	109.02	114.06
38	E	103	HEM	CBA-CAA-C2A	-2.82	104.73	112.53
23	C	514	CLA	CBC-CAC-C3C	-2.82	104.77	112.42
23	c	505	CLA	CED-O2D-CGD	2.82	122.31	115.92
23	b	615	CLA	O2A-CGA-O1A	-2.82	116.58	123.63
33	c	520	LMG	O8-C28-C29	2.82	120.43	111.83
25	a	410	BCR	C33-C5-C6	-2.82	121.41	124.48
23	C	512	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
23	c	503	CLA	O2A-CGA-CBA	2.82	120.42	111.83
23	c	513	CLA	CHD-C4C-NC	2.81	128.59	124.23
24	a	353	PHO	CMB-C2B-C3B	2.81	130.30	124.68
24	A	407	PHO	O1D-CGD-CBD	-2.81	120.46	124.72
23	A	406	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
23	c	512	CLA	CAC-C3C-C4C	2.81	128.45	124.79
23	b	608	CLA	CHD-C4C-NC	2.81	128.58	124.23
23	b	604	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
23	A	405	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
23	C	505	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
23	b	601	CLA	C4B-C3B-C2B	-2.80	103.81	107.30
23	B	606	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
23	a	407	CLA	CHC-C1C-C2C	-2.80	118.98	126.95
25	a	410	BCR	C40-C30-C25	-2.80	105.85	110.24
23	B	616	CLA	CMC-C2C-C1C	2.80	129.41	125.03
23	a	407	CLA	O2A-CGA-O1A	-2.80	116.62	123.63
25	b	618	BCR	C15-C14-C13	-2.80	123.35	127.28
23	B	607	CLA	CMB-C2B-C1B	2.80	129.68	125.42
23	b	602	CLA	CMA-C3A-C4A	-2.80	104.26	111.77
23	b	605	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
34	b	622	HTG	C1'-S1-C1	2.79	106.48	100.45
23	c	508	CLA	C1-C2-C3	-2.79	121.62	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	CAC-C3C-C4C	2.79	128.42	124.79
23	B	615	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
23	c	510	CLA	C4-C3-C5	2.79	120.07	115.23
23	A	405	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	B	615	CLA	CHD-C4C-NC	2.79	128.55	124.23
23	b	612	CLA	C2A-C1A-CHA	-2.78	119.03	123.87
23	a	409	CLA	C4B-C3B-C2B	-2.78	103.84	107.30
23	c	514	CLA	C2A-C1A-CHA	-2.78	119.04	123.87
37	l	101	LHG	O8-C23-C24	2.78	120.32	111.83
23	b	602	CLA	CAC-C3C-C4C	2.78	128.41	124.79
23	c	511	CLA	C4C-C3C-C2C	-2.78	102.84	106.89
23	b	601	CLA	C1-O2A-CGA	2.78	123.39	116.65
23	c	512	CLA	O2A-CGA-CBA	2.78	120.32	111.83
25	k	101	BCR	C2-C1-C6	2.78	114.48	110.44
23	B	605	CLA	C2A-C1A-CHA	-2.78	119.04	123.87
23	B	608	CLA	CHB-C4A-NA	2.78	128.41	124.40
38	e	87	HEM	CHB-C1B-NB	2.78	127.81	124.37
23	c	504	CLA	CHD-C4C-NC	2.78	128.54	124.23
23	c	505	CLA	CHC-C1C-C2C	-2.78	119.05	126.95
23	B	614	CLA	C4C-C3C-C2C	-2.78	102.85	106.89
23	b	613	CLA	CHD-C4C-NC	2.78	128.54	124.23
23	C	514	CLA	C2A-C1A-CHA	-2.78	119.05	123.87
33	c	521	LMG	O8-C28-C29	2.77	120.30	111.83
25	B	617	BCR	C31-C1-C6	-2.77	105.89	110.24
25	c	516	BCR	C32-C1-C6	-2.77	105.89	110.24
23	b	615	CLA	C1-C2-C3	-2.77	121.65	126.20
23	b	601	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
23	D	406	CLA	CMA-C3A-C2A	-2.77	103.28	113.98
23	C	512	CLA	C1-O2A-CGA	2.77	123.35	116.65
23	b	614	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
25	D	407	BCR	C40-C30-C25	-2.77	105.91	110.24
23	C	508	CLA	C1-C2-C3	-2.76	121.67	126.20
23	B	612	CLA	C1-C2-C3	-2.76	121.67	126.20
23	b	613	CLA	C4-C3-C5	2.76	120.02	115.23
23	C	504	CLA	O2A-CGA-O1A	-2.76	116.72	123.63
23	b	610	CLA	CMB-C2B-C1B	2.76	129.62	125.42
23	b	606	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
23	C	502	CLA	C4C-C3C-C2C	-2.76	102.87	106.89
37	e	101	LHG	O8-C23-C24	2.76	120.25	111.83
23	C	506	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
23	c	514	CLA	CAA-C2A-C3A	-2.76	105.54	113.00
23	C	502	CLA	CHC-C1C-C2C	-2.76	119.11	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	CAC-C3C-C4C	2.76	128.38	124.79
29	A	414	PL9	C35-C34-C36	2.76	120.01	115.23
23	c	514	CLA	CHC-C1C-C2C	-2.76	119.11	126.95
23	c	504	CLA	CAC-C3C-C4C	2.76	128.38	124.79
23	a	409	CLA	CAA-C2A-C3A	-2.76	105.55	113.00
23	B	606	CLA	O2A-CGA-O1A	-2.76	116.74	123.63
23	C	504	CLA	CBC-CAC-C3C	-2.75	104.95	112.42
23	A	408	CLA	C4-C3-C5	2.75	120.01	115.23
23	c	504	CLA	C4B-C3B-C2B	-2.75	103.88	107.30
23	A	405	CLA	CMA-C3A-C2A	-2.75	103.33	113.98
37	D	410	LHG	O7-C7-C8	2.75	117.44	111.48
35	h	102	DGD	O1G-C1A-C2A	2.75	120.23	111.83
23	b	614	CLA	CBC-CAC-C3C	-2.75	104.96	112.42
23	b	609	CLA	CHC-C1C-C2C	-2.75	119.13	126.95
29	D	408	PL9	C51-C49-C50	2.75	120.92	114.59
23	b	611	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
23	D	406	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
23	B	603	CLA	CHD-C4C-NC	2.75	128.49	124.23
23	b	604	CLA	C4C-C3C-C2C	-2.75	102.89	106.89
25	Y	101	BCR	C10-C11-C12	-2.75	115.24	123.20
23	b	601	CLA	CHC-C1C-C2C	-2.75	119.14	126.95
23	b	603	CLA	CMB-C2B-C1B	2.75	129.60	125.42
23	A	406	CLA	C4-C3-C5	2.75	119.99	115.23
29	A	414	PL9	C30-C29-C31	2.75	119.99	115.23
23	c	508	CLA	O1D-CGD-CBD	-2.74	119.11	124.52
34	B	626	HTG	O5-C5-C4	2.74	114.64	109.70
37	D	410	LHG	O8-C23-C24	2.74	120.20	111.83
23	c	508	CLA	C3B-C4B-NB	2.74	112.98	110.53
25	b	617	BCR	C20-C21-C22	-2.74	123.43	127.28
23	b	603	CLA	CHD-C4C-NC	2.74	128.48	124.23
23	c	513	CLA	C4C-C3C-C2C	-2.74	102.90	106.89
23	B	614	CLA	C2A-C1A-CHA	-2.74	119.12	123.87
32	D	404	LMT	O1'-C1'-C2'	2.73	112.43	108.27
23	B	609	CLA	CHC-C1C-C2C	-2.73	119.18	126.95
25	B	619	BCR	C24-C23-C22	-2.73	122.19	126.23
23	b	610	CLA	CMC-C2C-C1C	2.73	129.30	125.03
23	B	602	CLA	CHD-C4C-NC	2.73	128.47	124.23
23	C	511	CLA	CMC-C2C-C1C	2.73	129.30	125.03
37	L	101	LHG	O8-C23-O10	-2.73	116.80	123.63
23	B	601	CLA	C1-O2A-CGA	2.73	123.26	116.65
23	B	612	CLA	C2A-C1A-CHA	-2.73	119.13	123.87
23	D	406	CLA	CAA-C2A-C3A	-2.73	105.63	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	C4B-C3B-C2B	-2.73	103.91	107.30
35	H	102	DGD	O1G-C1A-O1A	-2.73	116.81	123.63
29	d	405	PL9	C36-C34-C33	-2.72	115.05	121.17
23	c	508	CLA	CHD-C4C-NC	2.72	128.46	124.23
23	B	603	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
23	c	502	CLA	CHD-C4C-NC	2.72	128.45	124.23
23	b	609	CLA	O2A-CGA-O1A	-2.72	116.82	123.63
23	A	408	CLA	CMA-C3A-C2A	-2.72	103.46	113.98
23	C	507	CLA	O2A-CGA-O1A	-2.72	116.82	123.63
23	C	507	CLA	O2A-CGA-CBA	2.72	120.13	111.83
23	B	603	CLA	C3B-C4B-NB	2.72	112.96	110.53
23	a	405	CLA	C2A-C1A-CHA	-2.72	119.15	123.87
23	B	603	CLA	CMA-C3A-C2A	-2.72	103.47	113.98
23	b	602	CLA	C1-O2A-CGA	2.72	123.22	116.65
32	D	404	LMT	C2'-C3'-C4'	2.71	115.84	109.68
25	K	102	BCR	C24-C23-C22	-2.71	122.22	126.23
25	t	103	BCR	C1-C6-C7	2.71	123.01	115.65
23	B	612	CLA	O2A-CGA-CBA	2.71	120.10	111.83
23	a	407	CLA	O2A-CGA-CBA	2.71	120.10	111.83
23	b	613	CLA	O2A-CGA-O1A	-2.71	116.85	123.63
37	d	408	LHG	O8-C23-C24	2.71	120.09	111.83
29	D	408	PL9	C2-C1-C6	2.71	122.22	119.00
23	C	502	CLA	C4-C3-C5	2.71	119.93	115.23
23	b	603	CLA	CHC-C1C-C2C	-2.71	119.25	126.95
23	C	505	CLA	C4C-C3C-C2C	-2.71	102.95	106.89
35	c	519	DGD	O1G-C1A-C2A	2.71	120.09	111.83
25	t	103	BCR	C36-C18-C19	2.71	122.22	118.09
23	c	508	CLA	O2A-CGA-CBA	2.71	120.08	111.83
29	a	416	PL9	C53-C6-C1	2.71	120.82	115.28
32	D	404	LMT	C4B-C3B-C2B	2.71	115.58	110.83
23	c	502	CLA	C4B-C3B-C2B	-2.70	103.94	107.30
23	b	602	CLA	C2A-C1A-CHA	-2.70	119.18	123.87
23	B	615	CLA	CED-O2D-CGD	2.70	122.04	115.92
23	b	607	CLA	C1-C2-C3	-2.70	121.78	126.20
23	D	405	CLA	CAC-C3C-C4C	2.70	128.30	124.79
24	A	407	PHO	O2A-CGA-CBA	2.69	120.05	111.83
23	b	610	CLA	C4B-C3B-C2B	-2.69	103.95	107.30
23	c	514	CLA	CMB-C2B-C1B	2.69	129.52	125.42
32	M	103	LMT	C3'-C4'-C5'	-2.69	104.96	110.93
25	C	516	BCR	C11-C10-C9	-2.69	123.50	127.28
23	C	514	CLA	C4B-C3B-C2B	-2.69	103.95	107.30
29	A	414	PL9	C2-C1-C6	2.69	122.20	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	CMB-C2B-C1B	2.69	129.52	125.42
25	D	407	BCR	C3-C4-C5	-2.69	109.26	114.06
25	A	409	BCR	C15-C14-C13	-2.69	123.51	127.28
35	C	518	DGD	O1G-C1A-O1A	-2.69	116.90	123.63
23	c	508	CLA	CAC-C3C-C4C	2.69	128.29	124.79
23	D	406	CLA	CHC-C1C-C2C	-2.69	119.31	126.95
23	d	403	CLA	CAA-C2A-C3A	-2.69	105.74	113.00
23	D	406	CLA	C4-C3-C5	2.69	119.89	115.23
23	B	603	CLA	CAC-C3C-C4C	2.69	128.28	124.79
23	B	615	CLA	CHC-C1C-C2C	-2.68	119.32	126.95
23	b	615	CLA	C4B-C3B-C2B	-2.68	103.97	107.30
23	B	607	CLA	CHC-C1C-C2C	-2.68	119.33	126.95
23	B	608	CLA	CMC-C2C-C1C	2.68	129.22	125.03
23	c	507	CLA	CMC-C2C-C1C	2.68	129.22	125.03
25	T	101	BCR	C21-C20-C19	-2.68	115.43	123.20
23	c	506	CLA	CHC-C1C-C2C	-2.68	119.33	126.95
23	b	607	CLA	CAA-C2A-C3A	-2.68	105.76	113.00
25	c	516	BCR	C2-C1-C6	2.68	114.33	110.44
23	b	609	CLA	O2A-CGA-CBA	2.68	120.00	111.83
23	b	610	CLA	C4-C3-C5	2.68	119.87	115.23
23	C	514	CLA	O2A-CGA-CBA	2.68	119.99	111.83
23	b	601	CLA	CBC-CAC-C3C	-2.67	105.17	112.42
23	d	402	CLA	C2A-C1A-CHA	-2.67	119.23	123.87
23	B	602	CLA	C2A-C1A-CHA	-2.67	119.23	123.87
35	H	102	DGD	O2G-C1B-C2B	2.67	117.26	111.48
23	c	510	CLA	CHD-C4C-NC	2.67	128.37	124.23
23	b	607	CLA	CMC-C2C-C1C	2.67	129.21	125.03
23	D	405	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
23	D	405	CLA	C2A-C1A-CHA	-2.67	119.24	123.87
23	a	406	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
23	b	605	CLA	C1-C2-C3	-2.67	121.83	126.20
23	B	605	CLA	C1-C2-C3	-2.67	121.83	126.20
34	C	522	HTG	C1-O5-C5	2.67	117.34	112.56
23	b	602	CLA	C11-C12-C13	-2.67	107.10	115.97
23	C	514	CLA	CMB-C2B-C1B	2.67	129.48	125.42
23	b	608	CLA	O2A-CGA-CBA	2.67	119.96	111.83
25	T	101	BCR	C12-C13-C14	-2.67	114.82	119.01
23	b	604	CLA	C4-C3-C5	2.67	119.86	115.23
23	a	406	CLA	C4C-C3C-C2C	-2.67	103.01	106.89
23	c	508	CLA	C4C-C3C-C2C	-2.67	103.01	106.89
23	C	510	CLA	C2A-C1A-CHA	-2.67	119.24	123.87
23	b	602	CLA	C4-C3-C5	2.66	119.85	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	406	CLA	CMC-C2C-C1C	2.66	129.19	125.03
34	B	622	HTG	C1-O5-C5	2.66	117.33	112.56
23	d	402	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
23	B	606	CLA	C4B-C3B-C2B	-2.66	103.99	107.30
23	C	511	CLA	O2A-CGA-CBA	2.66	119.94	111.83
23	d	402	CLA	CAC-C3C-C4C	2.66	128.25	124.79
23	B	609	CLA	CHD-C4C-NC	2.66	128.35	124.23
23	b	601	CLA	CMC-C2C-C1C	2.66	129.19	125.03
23	c	507	CLA	C4C-C3C-C2C	-2.66	103.03	106.89
23	B	612	CLA	CHD-C4C-NC	2.65	128.35	124.23
32	M	101	LMT	C3'-C4'-C5'	-2.65	105.05	110.93
23	b	608	CLA	CMA-C3A-C4A	-2.65	104.65	111.77
23	D	406	CLA	C2A-C1A-CHA	-2.65	119.27	123.87
26	F	101	SQD	O47-C7-O49	-2.65	117.51	123.70
23	A	406	CLA	C1-C2-C3	-2.65	121.86	126.20
23	C	502	CLA	CBC-CAC-C3C	-2.65	105.25	112.42
23	B	602	CLA	CHC-C1C-C2C	-2.65	119.43	126.95
29	a	416	PL9	C47-C48-C49	-2.64	118.83	127.64
25	K	102	BCR	C29-C30-C25	2.64	114.28	110.44
23	B	610	CLA	C1-C2-C3	-2.64	121.87	126.20
23	b	611	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
23	B	607	CLA	C4C-C3C-C2C	-2.64	103.05	106.89
23	b	607	CLA	C2A-C1A-CHA	-2.64	119.28	123.87
38	E	103	HEM	O2D-CGD-CBD	2.64	122.34	114.00
23	d	403	CLA	O2A-CGA-CBA	2.64	119.88	111.83
23	C	511	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
23	c	511	CLA	CHC-C1C-C2C	-2.64	119.46	126.95
23	C	503	CLA	C4B-C3B-C2B	-2.64	104.03	107.30
23	c	505	CLA	C4B-C3B-C2B	-2.64	104.03	107.30
23	b	606	CLA	C4C-C3C-C2C	-2.63	103.06	106.89
23	b	609	CLA	CMB-C2B-C1B	2.63	129.43	125.42
32	e	102	LMT	O1'-C1'-C2'	2.63	112.27	108.27
23	B	602	CLA	C1-C2-C3	-2.63	121.89	126.20
23	C	506	CLA	O2A-CGA-CBA	2.63	119.85	111.83
23	C	508	CLA	C4-C3-C5	2.63	119.79	115.23
23	b	613	CLA	CAC-C3C-C4C	2.63	128.21	124.79
23	B	605	CLA	O2A-CGA-CBA	2.63	119.84	111.83
23	a	406	CLA	O2A-CGA-O1A	-2.63	117.06	123.63
23	b	613	CLA	CMC-C2C-C1C	2.62	129.13	125.03
23	C	503	CLA	CHD-C4C-NC	2.62	128.29	124.23
23	c	502	CLA	O2A-CGA-O1A	-2.62	117.08	123.63
23	B	608	CLA	C1-C2-C3	-2.62	121.91	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	h	101	BCR	C16-C17-C18	-2.62	123.61	127.28
23	c	514	CLA	CHD-C4C-NC	2.62	128.29	124.23
23	C	512	CLA	C4B-C3B-C2B	-2.62	104.05	107.30
23	b	611	CLA	CBC-CAC-C3C	-2.61	105.33	112.42
23	c	503	CLA	O2A-CGA-O1A	-2.61	117.09	123.63
34	B	626	HTG	C3-C4-C5	2.61	114.97	110.23
25	c	516	BCR	C21-C20-C19	-2.61	115.63	123.20
23	c	511	CLA	C4B-C3B-C2B	-2.61	104.05	107.30
32	b	621	LMT	C1'-O5'-C5'	-2.61	108.62	113.72
23	b	607	CLA	CMB-C2B-C1B	2.61	129.40	125.42
35	C	519	DGD	O2G-C1B-C2B	2.61	117.13	111.48
33	C	501	LMG	C8-O7-C10	-2.61	111.55	117.80
23	B	614	CLA	C4B-C3B-C2B	-2.61	104.06	107.30
23	D	405	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
26	a	413	SQD	C1-O5-C5	2.61	118.82	113.72
23	C	514	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
23	a	405	CLA	C4B-C3B-C2B	-2.61	104.06	107.30
23	b	615	CLA	CHD-C4C-NC	2.61	128.27	124.23
26	A	410	SQD	O48-C23-O10	-2.61	117.11	123.63
23	a	409	CLA	C2A-C1A-CHA	-2.61	119.35	123.87
23	B	608	CLA	O2A-CGA-CBA	2.60	119.78	111.83
25	B	617	BCR	C16-C17-C18	-2.60	123.63	127.28
24	A	407	PHO	O2A-CGA-O1A	-2.60	117.12	123.63
23	B	616	CLA	CHC-C1C-C2C	-2.60	119.55	126.95
23	a	406	CLA	CAA-CBA-CGA	2.60	120.59	113.21
23	b	612	CLA	CHC-C1C-C2C	-2.60	119.56	126.95
23	c	513	CLA	CHB-C4A-NA	2.60	128.15	124.40
23	A	405	CLA	C2A-C1A-CHA	-2.60	119.35	123.87
23	b	603	CLA	CBC-CAC-C3C	-2.60	105.38	112.42
23	c	512	CLA	C1-O2A-CGA	2.60	122.94	116.65
23	b	603	CLA	CMC-C2C-C1C	2.60	129.09	125.03
23	C	513	CLA	CMB-C2B-C1B	2.60	129.38	125.42
23	b	602	CLA	C4C-C3C-C2C	-2.60	103.11	106.89
23	A	406	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
23	C	505	CLA	CAA-C2A-C3A	-2.60	105.98	113.00
23	b	613	CLA	CED-O2D-CGD	2.60	121.80	115.92
23	B	610	CLA	CMC-C2C-C1C	2.59	129.09	125.03
35	c	518	DGD	O1G-C1A-C2A	2.59	119.74	111.83
23	A	405	CLA	C4-C3-C5	2.59	119.73	115.23
24	a	408	PHO	CMB-C2B-C3B	2.59	129.86	124.68
23	B	609	CLA	CBC-CAC-C3C	-2.59	105.40	112.42
23	c	512	CLA	CMB-C2B-C1B	2.59	129.36	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	CMB-C2B-C1B	2.59	129.36	125.42
29	a	416	PL9	C40-C39-C41	2.59	119.72	115.23
23	B	607	CLA	O2A-CGA-O1A	-2.59	117.15	123.63
23	C	507	CLA	CHD-C4C-NC	2.59	128.25	124.23
25	c	515	BCR	C20-C21-C22	-2.59	123.65	127.28
23	B	611	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
23	C	503	CLA	CMC-C2C-C1C	2.59	129.08	125.03
23	c	506	CLA	C4B-C3B-C2B	-2.59	104.08	107.30
25	B	619	BCR	C2-C1-C6	2.59	114.20	110.44
23	C	513	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
25	b	618	BCR	C37-C22-C21	-2.59	118.62	122.82
23	b	604	CLA	O2A-CGA-CBA	2.59	119.72	111.83
23	b	611	CLA	C2A-C1A-CHA	-2.58	119.38	123.87
26	B	620	SQD	O9-S-C6	2.58	110.61	106.76
23	c	507	CLA	C2A-C1A-CHA	-2.58	119.38	123.87
25	C	516	BCR	C32-C1-C6	-2.58	106.19	110.24
23	A	405	CLA	O2A-CGA-O1A	-2.58	117.17	123.63
25	h	101	BCR	C33-C5-C6	-2.58	121.67	124.48
35	c	519	DGD	O2G-C1B-C2B	2.58	117.06	111.48
23	C	508	CLA	O2A-CGA-CBA	2.58	119.70	111.83
23	d	403	CLA	CHC-C1C-C2C	-2.58	119.62	126.95
23	c	504	CLA	CHC-C1C-C2C	-2.58	119.62	126.95
29	a	416	PL9	C10-C9-C8	-2.58	117.01	123.63
25	B	617	BCR	C15-C14-C13	-2.58	123.66	127.28
29	A	414	PL9	C40-C39-C41	2.58	119.70	115.23
23	a	407	CLA	C1-C2-C3	-2.58	121.98	126.20
29	A	414	PL9	C47-C48-C49	-2.58	119.05	127.64
23	c	505	CLA	CHD-C4C-NC	2.57	128.22	124.23
23	C	510	CLA	C16-C15-C13	-2.57	107.42	115.97
23	b	614	CLA	CAC-C3C-C4C	2.57	128.13	124.79
23	b	610	CLA	C3B-C4B-NB	2.57	112.82	110.53
32	I	101	LMT	O5 <sup>1</sup> -C5 <sup>3</sup> -C6 <sup>7</sup>	2.57	112.81	106.44
23	c	503	CLA	C4B-C3B-C2B	-2.57	104.11	107.30
33	D	415	LMG	O7-C10-C11	2.57	117.03	111.48
23	d	403	CLA	C3B-C4B-NB	2.57	112.82	110.53
23	C	512	CLA	CHD-C4C-NC	2.57	128.21	124.23
23	c	511	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
25	H	101	BCR	C11-C10-C9	-2.57	123.68	127.28
23	b	601	CLA	CMB-C2B-C1B	2.57	129.32	125.42
23	C	514	CLA	CAA-C2A-C3A	-2.57	106.07	113.00
23	c	508	CLA	CHC-C1C-C2C	-2.56	119.67	126.95
23	B	608	CLA	CHD-C4C-NC	2.56	128.20	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	CAC-C3C-C4C	2.56	128.12	124.79
23	c	507	CLA	CHD-C4C-NC	2.56	128.20	124.23
23	c	514	CLA	CMC-C2C-C1C	2.56	129.03	125.03
23	c	511	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
23	B	610	CLA	CHC-C1C-C2C	-2.56	119.68	126.95
23	C	506	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
23	c	505	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
24	A	407	PHO	CMA-C3A-C4A	-2.56	109.11	114.61
23	b	616	CLA	C4-C3-C5	2.55	119.66	115.23
23	c	510	CLA	CMB-C2B-C1B	2.55	129.31	125.42
23	C	511	CLA	C4C-C3C-C2C	-2.55	103.18	106.89
32	M	103	LMT	C1'-O5'-C5'	-2.55	108.74	113.72
25	C	515	BCR	C38-C26-C25	-2.55	121.70	124.48
23	b	614	CLA	CMC-C2C-C1C	2.55	129.01	125.03
29	D	408	PL9	C42-C41-C39	-2.55	104.75	113.19
23	C	505	CLA	CMC-C2C-C1C	2.55	129.01	125.03
23	B	601	CLA	C4B-C3B-C2B	-2.55	104.14	107.30
35	c	517	DGD	C2G-O2G-C1B	-2.55	111.70	117.80
34	B	622	HTG	O2-C2-C3	-2.54	104.38	110.38
23	c	509	CLA	C4B-C3B-C2B	-2.54	104.14	107.30
25	d	404	BCR	C33-C5-C6	-2.54	121.71	124.48
25	d	404	BCR	C37-C22-C23	2.54	121.97	118.09
23	c	504	CLA	C4-C3-C5	2.54	119.63	115.23
29	A	414	PL9	C10-C9-C8	-2.54	117.11	123.63
23	b	606	CLA	C1-C2-C3	-2.54	122.04	126.20
23	c	509	CLA	CHD-C4C-NC	2.54	128.16	124.23
25	D	407	BCR	C16-C17-C18	-2.54	123.72	127.28
23	b	616	CLA	CHC-C1C-C2C	-2.53	119.75	126.95
23	a	407	CLA	CMC-C2C-C1C	2.53	128.99	125.03
23	c	514	CLA	C1-C2-C3	-2.53	122.05	126.20
23	B	611	CLA	C4B-C3B-C2B	2.53	110.45	107.30
23	A	406	CLA	C2A-C1A-CHA	-2.53	119.47	123.87
23	a	405	CLA	CHD-C4C-NC	2.53	128.15	124.23
23	B	606	CLA	C3B-C4B-NB	2.53	112.79	110.53
23	B	611	CLA	O2A-CGA-O1A	-2.53	117.31	123.63
23	C	504	CLA	O2A-CGA-CBA	2.53	119.54	111.83
23	a	405	CLA	CMA-C3A-C2A	-2.53	104.22	113.98
23	D	406	CLA	O2A-CGA-CBA	2.52	119.53	111.83
23	b	608	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
23	C	510	CLA	C11-C12-C13	-2.52	107.58	115.97
23	a	406	CLA	CBC-CAC-C3C	-2.52	105.59	112.42
23	A	408	CLA	CHD-C4C-NC	2.52	128.14	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	CHC-C1C-C2C	-2.52	119.80	126.95
40	V	202	HEC	C2A-C1A-NA	-2.51	107.90	110.32
25	T	101	BCR	C2-C1-C6	2.51	114.09	110.44
25	B	618	BCR	C15-C14-C13	-2.51	123.75	127.28
23	c	506	CLA	O2A-CGA-CBA	2.51	119.50	111.83
23	b	602	CLA	CHB-C1B-C2B	-2.51	120.13	127.43
23	A	405	CLA	CAA-CBA-CGA	2.51	120.34	113.21
23	c	502	CLA	C4-C3-C5	2.51	119.59	115.23
26	A	412	SQD	C4-C3-C2	-2.51	106.42	110.83
23	c	512	CLA	CMC-C2C-C1C	2.51	128.96	125.03
23	b	614	CLA	C2A-C1A-CHA	-2.51	119.51	123.87
23	c	511	CLA	C2A-C1A-CHA	-2.51	119.52	123.87
29	d	405	PL9	C17-C18-C19	-2.51	121.89	127.62
25	k	101	BCR	C24-C23-C22	-2.51	122.53	126.23
23	b	610	CLA	CAA-CBA-CGA	-2.51	106.09	113.21
23	B	604	CLA	C6-C7-C8	-2.51	107.64	115.97
23	A	404	CLA	CAA-CBA-CGA	-2.51	106.09	113.21
25	a	410	BCR	C29-C30-C25	2.50	114.08	110.44
23	A	408	CLA	CBC-CAC-C3C	-2.50	105.64	112.42
23	B	604	CLA	O2A-CGA-CBA	2.50	119.46	111.83
23	b	612	CLA	CHD-C4C-NC	2.50	128.11	124.23
23	c	502	CLA	O2A-CGA-CBA	2.50	119.45	111.83
23	b	604	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
25	b	618	BCR	C29-C30-C25	2.50	114.07	110.44
25	c	516	BCR	C37-C22-C23	2.50	121.90	118.09
38	e	87	HEM	C4D-ND-C1D	2.50	108.16	105.21
37	D	409	LHG	O7-C7-O9	-2.50	117.87	123.70
23	b	605	CLA	CAC-C3C-C4C	2.49	128.04	124.79
23	c	512	CLA	CBC-CAC-C3C	-2.49	105.66	112.42
23	a	405	CLA	C4C-C3C-C2C	-2.49	103.26	106.89
23	B	607	CLA	C2A-C1A-CHA	-2.49	119.54	123.87
23	c	507	CLA	O2A-CGA-CBA	2.49	119.43	111.83
26	b	620	SQD	O48-C23-C24	2.49	119.43	111.83
23	C	511	CLA	C2A-C1A-CHA	-2.49	119.55	123.87
23	b	606	CLA	CMB-C2B-C1B	2.49	129.21	125.42
33	m	101	LMG	C8-O7-C10	-2.49	111.84	117.80
23	b	605	CLA	CMC-C2C-C1C	2.49	128.92	125.03
23	C	508	CLA	CHC-C1C-C2C	-2.49	119.88	126.95
38	E	103	HEM	CHA-C4D-ND	2.49	127.44	124.37
23	A	406	CLA	CMA-C3A-C2A	-2.48	104.38	113.98
33	d	412	LMG	O8-C28-C29	2.48	119.41	111.83
23	B	612	CLA	O2A-CGA-O1A	-2.48	117.42	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
23	C	506	CLA	CHD-C4C-NC	2.48	128.08	124.23
23	b	604	CLA	C6-C5-C3	-2.48	107.43	113.47
26	f	102	SQD	O5-C5-C4	2.48	114.17	109.70
25	y	101	BCR	C21-C20-C19	-2.48	116.02	123.20
25	Y	101	BCR	C37-C22-C23	2.48	121.87	118.09
25	b	617	BCR	C29-C30-C25	2.48	114.04	110.44
23	B	614	CLA	CAA-C2A-C3A	-2.48	106.31	113.00
32	I	101	LMT	O1'-C1'-C2'	2.47	112.03	108.27
32	E	102	LMT	C1'-O5'-C5'	-2.47	108.89	113.72
25	c	516	BCR	C33-C5-C6	-2.47	121.79	124.48
38	E	103	HEM	O2A-CGA-CBA	2.47	121.81	114.00
25	y	101	BCR	C34-C9-C8	2.47	121.86	118.09
23	c	513	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
23	B	609	CLA	C3B-C4B-NB	2.47	112.73	110.53
23	c	511	CLA	CBC-CAC-C3C	-2.47	105.73	112.42
23	B	605	CLA	CHC-C1C-C2C	-2.47	119.93	126.95
23	b	606	CLA	CMC-C2C-C1C	2.47	128.89	125.03
23	B	611	CLA	OBD-CAD-C3D	-2.46	122.66	128.42
23	B	609	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
23	B	615	CLA	C11-C10-C8	-2.46	107.78	115.97
23	B	613	CLA	CMC-C2C-C1C	2.46	128.88	125.03
23	d	403	CLA	CBC-CAC-C3C	-2.46	105.74	112.42
23	B	601	CLA	CHC-C1C-C2C	-2.46	119.95	126.95
23	B	612	CLA	CHC-C1C-C2C	-2.46	119.95	126.95
29	d	405	PL9	C12-C13-C14	-2.46	121.99	127.62
25	d	404	BCR	C39-C30-C25	-2.46	106.39	110.24
23	B	606	CLA	C4-C3-C5	2.46	119.50	115.23
25	A	409	BCR	C38-C26-C25	-2.46	121.80	124.48
23	c	508	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
23	C	512	CLA	O2A-CGA-CBA	2.46	119.33	111.83
23	B	606	CLA	CBC-CAC-C3C	-2.46	105.76	112.42
23	b	615	CLA	O2A-CGA-CBA	2.46	119.32	111.83
23	B	616	CLA	CBC-CAC-C3C	-2.45	105.77	112.42
23	b	615	CLA	CAC-C3C-C4C	2.45	127.98	124.79
23	B	604	CLA	CMC-C2C-C1C	2.45	128.87	125.03
23	C	502	CLA	C1-O2A-CGA	2.45	122.59	116.65
23	C	503	CLA	O2A-CGA-CBA	2.45	119.31	111.83
23	a	409	CLA	CMA-C3A-C2A	-2.45	104.50	113.98
25	K	102	BCR	C2-C1-C6	2.45	114.00	110.44
23	b	616	CLA	CMC-C2C-C1C	2.45	128.86	125.03
25	t	103	BCR	C7-C6-C5	-2.45	115.91	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	CMC-C2C-C1C	2.45	128.86	125.03
32	t	101	LMT	C3'-C4'-C5'	-2.45	105.51	110.93
23	C	510	CLA	CHD-C4C-NC	2.45	128.02	124.23
25	B	618	BCR	C38-C26-C25	-2.45	121.82	124.48
25	y	101	BCR	C16-C17-C18	-2.45	123.85	127.28
23	c	510	CLA	C2A-C1A-CHA	-2.44	119.62	123.87
23	C	504	CLA	C3B-C4B-NB	2.44	112.71	110.53
25	d	404	BCR	C24-C23-C22	-2.44	122.62	126.23
29	A	414	PL9	C42-C43-C44	-2.44	122.03	127.62
23	C	514	CLA	CHC-C1C-C2C	-2.44	120.00	126.95
23	C	502	CLA	O2A-CGA-CBA	2.44	119.28	111.83
23	b	605	CLA	CED-O2D-CGD	2.44	121.45	115.92
26	f	102	SQD	O47-C7-O49	-2.44	118.00	123.70
25	D	407	BCR	C15-C14-C13	-2.44	123.86	127.28
37	l	101	LHG	O8-C23-O10	-2.44	117.53	123.63
23	c	504	CLA	CMC-C2C-C1C	2.44	128.84	125.03
23	D	406	CLA	CHD-C4C-NC	2.44	128.01	124.23
25	c	515	BCR	C33-C5-C6	-2.44	121.83	124.48
23	c	509	CLA	CAC-C3C-C4C	2.44	127.96	124.79
25	H	101	BCR	C16-C17-C18	-2.44	123.86	127.28
23	c	502	CLA	CMC-C2C-C1C	2.43	128.84	125.03
37	d	408	LHG	O8-C23-O10	-2.43	117.54	123.63
25	B	618	BCR	C11-C10-C9	-2.43	123.87	127.28
23	C	507	CLA	C2A-C1A-CHA	-2.43	119.65	123.87
32	I	101	LMT	O5'-C5'-C4'	2.43	114.75	109.72
24	a	353	PHO	O1D-CGD-CBD	-2.43	121.04	124.72
23	B	611	CLA	C2C-C1C-NC	2.43	112.53	109.98
23	C	503	CLA	C4-C3-C5	2.43	119.44	115.23
23	B	601	CLA	CMC-C2C-C1C	2.43	128.82	125.03
25	T	101	BCR	C3-C4-C5	-2.43	109.73	114.06
33	m	101	LMG	C7-O1-C1	-2.43	108.60	113.80
23	B	601	CLA	C1-C2-C3	-2.42	122.22	126.20
23	B	609	CLA	CAC-C3C-C4C	2.42	127.94	124.79
23	B	611	CLA	CMB-C2B-C3B	2.42	132.25	126.55
23	B	610	CLA	CHB-C4A-NA	2.42	127.90	124.40
29	D	408	PL9	C20-C19-C21	2.42	119.43	115.23
23	C	506	CLA	O1D-CGD-CBD	-2.42	119.74	124.52
23	b	605	CLA	CMB-C2B-C1B	2.42	129.10	125.42
23	d	403	CLA	C4B-C3B-C2B	-2.42	104.29	107.30
23	A	408	CLA	C2A-C1A-CHA	-2.42	119.67	123.87
23	C	508	CLA	CMC-C2C-C1C	2.42	128.81	125.03
35	H	102	DGD	O6E-C5E-C6E	2.42	112.43	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	619	BCR	C11-C10-C9	-2.42	123.89	127.28
26	B	620	SQD	O48-C23-O10	-2.42	117.58	123.63
23	c	504	CLA	OBD-CAD-C3D	-2.42	122.77	128.42
23	C	505	CLA	CMB-C2B-C1B	2.41	129.10	125.42
26	b	620	SQD	O47-C7-O49	-2.41	118.06	123.70
23	b	615	CLA	C6-C7-C8	-2.41	107.94	115.97
33	B	621	LMG	O8-C28-O10	-2.41	117.59	123.63
23	B	612	CLA	C11-C12-C13	-2.41	107.95	115.97
23	C	509	CLA	C4-C3-C5	2.41	119.41	115.23
25	b	617	BCR	C11-C10-C9	-2.41	123.90	127.28
25	C	516	BCR	C29-C30-C25	2.41	113.93	110.44
23	c	509	CLA	CAA-C2A-C3A	-2.40	106.50	113.00
25	y	101	BCR	C1-C6-C7	2.40	122.17	115.65
23	C	502	CLA	C2A-C1A-CHA	-2.40	119.70	123.87
35	C	519	DGD	O3G-C3G-C2G	-2.40	104.98	110.82
23	B	603	CLA	CMC-C2C-C1C	2.40	128.78	125.03
25	c	515	BCR	C36-C18-C19	2.40	121.75	118.09
23	c	510	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
25	k	101	BCR	C10-C11-C12	-2.40	116.25	123.20
23	C	502	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
23	b	603	CLA	CAC-C3C-C4C	2.40	127.91	124.79
24	a	408	PHO	CMA-C3A-C4A	-2.40	109.45	114.61
29	D	408	PL9	C40-C39-C41	2.40	119.39	115.23
23	B	605	CLA	C4B-C3B-C2B	-2.40	104.32	107.30
25	T	101	BCR	C1-C6-C7	2.40	122.15	115.65
23	c	509	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
26	b	620	SQD	O7-S-C6	2.39	110.33	106.76
25	C	515	BCR	C16-C17-C18	-2.39	123.92	127.28
35	c	517	DGD	C3G-C2G-C1G	-2.39	106.21	111.78
32	a	414	LMT	O5 <sup>1</sup> -C5 <sup>1</sup> -C4 <sup>1</sup>	2.39	114.67	109.72
32	a	414	LMT	O5 <sup>1</sup> -C5 <sup>1</sup> -C6 <sup>1</sup>	2.39	112.37	106.44
23	b	601	CLA	C2A-C1A-CHA	-2.39	119.72	123.87
23	a	409	CLA	CHC-C1C-C2C	-2.39	120.15	126.95
32	t	101	LMT	O1 <sup>1</sup> -C1 <sup>1</sup> -C2 <sup>1</sup>	2.39	111.90	108.27
23	b	604	CLA	CHD-C4C-NC	2.39	127.94	124.23
23	c	514	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
23	d	403	CLA	CAC-C3C-C4C	2.39	127.90	124.79
26	a	411	SQD	O48-C23-C24	2.39	119.11	111.83
23	C	504	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
23	C	513	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
26	f	102	SQD	O48-C23-O10	-2.38	117.67	123.63
23	A	406	CLA	CAC-C3C-C4C	2.38	127.89	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	C2A-C1A-CHA	-2.38	119.74	123.87
25	b	619	BCR	C7-C8-C9	-2.38	122.72	126.23
25	b	619	BCR	C16-C17-C18	-2.38	123.94	127.28
23	B	605	CLA	C3B-C4B-NB	2.38	112.65	110.53
34	b	623	HTG	O5-C1-C2	2.38	113.59	110.32
23	B	601	CLA	CAC-C3C-C4C	2.38	127.88	124.79
35	C	518	DGD	C2G-O2G-C1B	-2.38	112.11	117.80
32	t	101	LMT	O5'-C5'-C4'	2.37	114.63	109.72
23	b	602	CLA	CHC-C1C-C2C	-2.37	120.21	126.95
23	C	504	CLA	C4B-C3B-C2B	-2.37	104.36	107.30
23	c	504	CLA	C2A-C1A-CHA	-2.37	119.76	123.87
37	d	407	LHG	C6-C5-C4	-2.37	106.27	111.78
23	C	511	CLA	CMB-C2B-C1B	2.37	129.02	125.42
23	B	602	CLA	C11-C12-C13	-2.36	108.11	115.97
23	C	513	CLA	CHB-C4A-NA	2.36	127.81	124.40
24	a	353	PHO	C1A-C2A-C3A	-2.36	100.59	102.84
23	B	607	CLA	CHD-C4C-NC	2.36	127.89	124.23
23	c	502	CLA	CBC-CAC-C3C	-2.36	106.02	112.42
25	B	619	BCR	C21-C20-C19	-2.36	116.36	123.20
23	b	606	CLA	O2A-CGA-CBA	2.36	119.03	111.83
24	A	353	PHO	C4D-CHA-CBD	2.36	109.59	108.45
23	B	610	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
24	a	353	PHO	O2A-CGA-CBA	2.36	119.03	111.83
23	B	606	CLA	C1-O2A-CGA	2.36	122.36	116.65
23	B	613	CLA	C2A-C1A-CHA	-2.36	119.78	123.87
23	B	604	CLA	C11-C12-C13	-2.36	108.13	115.97
23	B	611	CLA	O2A-CGA-CBA	2.36	119.02	111.83
29	D	408	PL9	C7-C8-C9	-2.36	122.77	126.83
23	c	505	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
33	C	520	LMG	C8-O7-C10	-2.36	112.16	117.80
25	c	515	BCR	C7-C8-C9	-2.36	122.75	126.23
23	b	601	CLA	O2A-CGA-CBA	2.35	119.01	111.83
23	c	503	CLA	C4C-C3C-C2C	-2.35	103.47	106.89
25	c	516	BCR	C11-C10-C9	-2.35	123.98	127.28
27	O	601	GOL	C3-C2-C1	-2.35	103.17	111.80
23	C	505	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
23	d	402	CLA	CMB-C2B-C1B	2.35	129.00	125.42
23	c	505	CLA	O2A-CGA-CBA	2.35	119.00	111.83
32	E	102	LMT	C3B-C4B-C5B	-2.35	105.97	110.23
27	B	624	GOL	C3-C2-C1	-2.35	103.19	111.80
25	B	617	BCR	C11-C10-C9	-2.35	123.99	127.28
33	d	412	LMG	O7-C10-O9	-2.34	118.23	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	CHB-C4A-NA	2.34	127.78	124.40
25	B	619	BCR	C38-C26-C25	-2.34	121.93	124.48
23	B	601	CLA	C3B-C4B-NB	2.34	112.62	110.53
23	c	514	CLA	C4-C3-C5	2.34	119.29	115.23
25	C	516	BCR	C3-C4-C5	-2.34	109.88	114.06
23	b	615	CLA	CMC-C2C-C1C	2.34	128.69	125.03
23	c	505	CLA	CAA-C2A-C3A	-2.34	106.68	113.00
35	C	518	DGD	O2G-C1B-O1B	-2.34	118.24	123.70
23	C	509	CLA	CHD-C4C-NC	2.34	127.86	124.23
29	d	405	PL9	C7-C8-C9	-2.34	122.81	126.83
23	b	613	CLA	O2D-CGD-O1D	-2.33	119.30	123.85
23	c	504	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
23	B	612	CLA	C4-C3-C5	2.33	119.28	115.23
29	a	416	PL9	C20-C19-C21	2.33	119.28	115.23
23	C	514	CLA	CAC-C3C-C4C	2.33	127.82	124.79
23	B	608	CLA	CMA-C3A-C2A	-2.33	104.97	113.98
23	C	507	CLA	CAA-C2A-C3A	-2.33	106.70	113.00
26	A	410	SQD	O9-S-O7	-2.33	106.25	113.82
23	C	513	CLA	CBC-CAC-C3C	-2.33	106.11	112.42
26	A	410	SQD	O8-S-C6	2.33	110.46	105.97
23	c	504	CLA	O2A-CGA-CBA	2.33	118.93	111.83
23	D	405	CLA	CMC-C2C-C1C	2.33	128.67	125.03
23	c	505	CLA	CMC-C2C-C1C	2.33	128.67	125.03
29	A	414	PL9	C12-C13-C14	-2.33	122.30	127.62
34	b	622	HTG	O2-C2-C3	-2.32	104.90	110.38
25	T	101	BCR	C7-C6-C5	-2.32	116.20	121.56
25	B	617	BCR	C29-C30-C25	2.32	113.81	110.44
23	C	506	CLA	CHA-C1A-NA	-2.32	121.13	126.39
23	c	513	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
23	b	608	CLA	CMB-C2B-C3B	2.32	132.01	126.55
25	D	407	BCR	C24-C23-C22	-2.32	122.80	126.23
23	b	609	CLA	C7-C6-C5	-2.32	107.08	113.26
23	c	509	CLA	C4-C3-C5	2.32	119.25	115.23
35	C	517	DGD	O6E-C5E-C4E	2.32	113.88	109.70
25	A	409	BCR	C16-C17-C18	-2.32	124.03	127.28
35	C	517	DGD	C3G-C2G-C1G	-2.32	106.38	111.78
23	c	506	CLA	C4-C3-C5	2.32	119.25	115.23
33	c	520	LMG	C8-O7-C10	-2.31	112.26	117.80
23	b	608	CLA	C4C-C3C-C2C	-2.31	103.53	106.89
23	b	616	CLA	C2A-C1A-CHA	-2.31	119.86	123.87
25	B	618	BCR	C37-C22-C23	2.31	121.62	118.09
23	C	513	CLA	O1D-CGD-CBD	-2.31	119.96	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	CHD-C4C-NC	2.31	127.81	124.23
23	C	510	CLA	CMC-C2C-C1C	2.30	128.63	125.03
24	A	407	PHO	CMB-C2B-C3B	2.30	129.29	124.68
23	B	615	CLA	C6-C7-C8	-2.30	108.31	115.97
23	C	513	CLA	CHC-C1C-C2C	-2.30	120.40	126.95
25	h	101	BCR	C10-C11-C12	-2.30	116.53	123.20
23	C	502	CLA	C11-C12-C13	-2.30	108.32	115.97
29	A	414	PL9	C45-C44-C46	2.30	119.22	115.23
26	a	411	SQD	O9-S-O7	-2.30	106.34	113.82
25	Y	101	BCR	C38-C26-C25	-2.30	121.97	124.48
23	c	505	CLA	C2A-C1A-CHA	-2.30	119.88	123.87
23	B	609	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
23	B	614	CLA	OBD-CAD-C3D	-2.30	123.05	128.42
33	C	521	LMG	O1-C1-C2	2.30	111.76	108.27
23	D	405	CLA	CMB-C2B-C1B	2.30	128.92	125.42
40	V	202	HEC	CHB-C4A-NA	2.30	126.95	124.45
25	D	407	BCR	C30-C25-C24	2.30	121.88	115.65
23	c	506	CLA	C3B-C4B-NB	2.30	112.58	110.53
23	B	608	CLA	C11-C12-C13	-2.30	108.33	115.97
25	B	619	BCR	C31-C1-C6	-2.30	106.64	110.24
23	b	616	CLA	C1-C2-C3	-2.29	122.44	126.20
23	b	607	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
33	B	621	LMG	C12-C11-C10	-2.29	105.29	113.69
23	B	611	CLA	C4-C3-C5	2.29	119.21	115.23
23	b	609	CLA	C16-C15-C13	-2.29	108.34	115.97
23	C	508	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
23	B	607	CLA	C1-O2A-CGA	2.29	122.20	116.65
25	Y	101	BCR	C15-C16-C17	-2.29	118.83	123.52
23	b	602	CLA	C4B-C3B-C2B	-2.29	104.45	107.30
35	H	102	DGD	C2G-O2G-C1B	-2.29	112.32	117.80
32	M	101	LMT	C3B-C4B-C5B	-2.29	106.08	110.23
25	b	618	BCR	C20-C21-C22	-2.29	124.07	127.28
33	C	521	LMG	C9-C8-C7	-2.29	106.45	111.78
23	B	602	CLA	CMA-C3A-C2A	-2.29	105.14	113.98
29	d	405	PL9	C20-C19-C21	2.29	119.20	115.23
23	C	504	CLA	C2A-C1A-CHA	-2.29	119.90	123.87
23	B	605	CLA	CMC-C2C-C1C	2.29	128.60	125.03
33	c	521	LMG	O8-C28-O10	-2.28	117.92	123.63
37	E	101	LHG	O7-C7-O9	-2.28	118.37	123.70
38	E	103	HEM	C4C-NC-C1C	2.28	109.54	105.82
23	D	406	CLA	CMA-C3A-C4A	-2.28	105.64	111.77
23	B	602	CLA	CAA-CBA-CGA	-2.28	106.73	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	102	BCR	C33-C5-C6	-2.28	122.00	124.48
23	B	613	CLA	CHD-C4C-NC	2.28	127.77	124.23
23	b	610	CLA	C2A-C1A-CHA	-2.28	119.91	123.87
34	b	622	HTG	C6-C5-C4	-2.27	107.44	113.02
23	c	513	CLA	CMC-C2C-C1C	2.27	128.59	125.03
27	A	701	GOL	C3-C2-C1	-2.27	103.46	111.80
23	a	405	CLA	C7-C6-C5	-2.27	107.20	113.26
23	a	406	CLA	C2A-C1A-CHA	-2.27	119.92	123.87
23	C	505	CLA	CBC-CAC-C3C	-2.27	106.27	112.42
32	m	103	LMT	C3B-C4B-C5B	-2.27	106.12	110.23
23	d	403	CLA	CMC-C2C-C1C	2.27	128.58	125.03
29	d	405	PL9	C47-C48-C49	-2.27	120.08	127.64
23	B	614	CLA	C4-C3-C5	2.26	119.16	115.23
23	a	409	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
23	C	507	CLA	CHB-C4A-NA	2.26	127.67	124.40
23	b	602	CLA	O2A-CGA-CBA	2.26	118.73	111.83
37	D	409	LHG	O4-P-O5	2.26	122.96	112.44
23	c	507	CLA	CAA-C2A-C3A	-2.26	106.89	113.00
23	C	506	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
23	B	613	CLA	C4-C3-C2	-2.26	117.82	123.63
23	C	509	CLA	O2A-CGA-CBA	2.26	118.73	111.83
25	Y	101	BCR	C34-C9-C8	2.26	121.54	118.09
25	B	619	BCR	C29-C30-C25	2.26	113.72	110.44
25	b	617	BCR	C15-C16-C17	-2.26	118.90	123.52
23	B	604	CLA	C4-C3-C5	2.26	119.14	115.23
26	a	413	SQD	C3-C4-C5	2.26	114.32	110.23
23	a	406	CLA	CMC-C2C-C1C	2.26	128.56	125.03
23	b	610	CLA	CAC-C3C-C4C	2.25	127.72	124.79
23	B	608	CLA	CAA-C2A-C3A	-2.25	106.91	113.00
23	c	514	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
23	D	405	CLA	CED-O2D-CGD	2.25	121.03	115.92
37	d	407	LHG	O8-C23-O10	-2.25	117.99	123.63
26	b	620	SQD	O8-S-C6	2.25	110.32	105.97
33	z	101	LMG	C8-O7-C10	-2.25	112.40	117.80
26	A	412	SQD	O48-C23-O10	-2.25	118.00	123.63
33	C	520	LMG	O8-C28-O10	-2.25	118.00	123.63
24	a	408	PHO	C1-C2-C3	-2.25	122.51	126.20
25	B	619	BCR	C10-C11-C12	-2.25	116.69	123.20
29	D	408	PL9	C12-C13-C14	-2.25	122.48	127.62
23	c	509	CLA	C2A-C1A-CHA	-2.25	119.97	123.87
23	C	503	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
23	A	405	CLA	O2A-CGA-CBA	2.25	118.68	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414	PL9	C35-C34-C33	-2.25	117.86	123.63
23	B	606	CLA	CAA-C2A-C3A	-2.24	106.93	113.00
25	T	101	BCR	C35-C13-C12	2.24	121.52	118.09
23	B	609	CLA	CAA-C2A-C3A	-2.24	106.94	113.00
33	m	101	LMG	O8-C28-O10	-2.24	118.02	123.63
23	A	404	CLA	CHD-C4C-NC	2.24	127.71	124.23
23	c	506	CLA	C2A-C1A-CHA	-2.24	119.98	123.87
23	d	402	CLA	CMA-C3A-C2A	-2.24	105.31	113.98
24	A	353	PHO	O1D-CGD-CBD	-2.24	121.33	124.72
25	D	407	BCR	C15-C16-C17	-2.24	118.94	123.52
23	C	509	CLA	C2A-C1A-CHA	-2.24	119.98	123.87
25	A	409	BCR	C40-C30-C25	-2.24	106.73	110.24
40	V	202	HEC	CMD-C2D-C1D	2.24	128.83	125.42
23	C	508	CLA	O1D-CGD-CBD	-2.24	120.11	124.52
23	a	409	CLA	CBC-CAC-C3C	-2.24	106.36	112.42
25	D	407	BCR	C21-C20-C19	-2.24	116.72	123.20
23	a	409	CLA	CAC-C3C-C4C	2.24	127.70	124.79
25	H	101	BCR	C29-C30-C25	2.24	113.69	110.44
23	b	615	CLA	C2A-C1A-CHA	-2.23	119.99	123.87
23	b	606	CLA	C2A-C1A-CHA	-2.23	119.99	123.87
33	d	412	LMG	O8-C28-O10	-2.23	118.05	123.63
25	a	410	BCR	C7-C8-C9	-2.23	122.94	126.23
25	c	516	BCR	C29-C30-C25	2.23	113.68	110.44
24	A	353	PHO	CED-O2D-CGD	2.23	120.97	115.92
25	b	618	BCR	C8-C7-C6	-2.23	121.05	127.00
35	c	518	DGD	O1G-C1A-O1A	-2.23	118.06	123.63
23	B	607	CLA	C1-C2-C3	-2.23	122.55	126.20
23	c	512	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
23	B	614	CLA	CMA-C3A-C2A	-2.22	105.39	113.98
37	d	711	LHG	O7-C7-O9	-2.22	118.51	123.70
23	b	611	CLA	CAC-C3C-C4C	2.22	127.68	124.79
23	A	405	CLA	C4C-C3C-C2C	-2.22	103.66	106.89
25	t	103	BCR	C11-C10-C9	-2.22	124.17	127.28
25	B	619	BCR	C3-C4-C5	-2.22	110.10	114.06
23	B	612	CLA	CMA-C3A-C2A	-2.22	105.41	113.98
35	h	102	DGD	C3B-C2B-C1B	-2.22	105.58	113.69
23	C	513	CLA	CHB-C1B-C2B	-2.21	121.00	127.43
23	C	513	CLA	C4B-C3B-C2B	-2.21	104.55	107.30
23	C	507	CLA	C4C-C3C-C2C	-2.21	103.67	106.89
37	d	407	LHG	O8-C23-C24	2.21	118.59	111.83
23	D	405	CLA	CMA-C3A-C4A	-2.21	105.82	111.77
23	B	614	CLA	CMB-C2B-C1B	2.21	128.79	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	CMA-C3A-C4A	-2.21	105.82	111.77
33	Z	101	LMG	C1-O6-C5	2.21	118.04	113.72
23	B	602	CLA	CMB-C2B-C1B	2.21	128.79	125.42
23	b	601	CLA	CAA-C2A-C3A	-2.21	107.02	113.00
33	C	501	LMG	O8-C28-C29	2.21	118.58	111.83
23	B	605	CLA	CED-O2D-CGD	2.21	120.93	115.92
23	A	408	CLA	CMA-C3A-C4A	-2.21	105.83	111.77
29	a	416	PL9	C35-C34-C33	-2.21	117.95	123.63
25	Y	101	BCR	C1-C6-C7	2.21	121.64	115.65
23	B	608	CLA	C2A-C1A-CHA	-2.21	120.03	123.87
24	A	407	PHO	C4-C3-C5	2.21	119.06	115.23
23	C	513	CLA	CAC-C3C-C4C	2.21	127.66	124.79
23	c	514	CLA	C1-O2A-CGA	2.21	121.99	116.65
23	B	615	CLA	O2A-CGA-CBA	2.21	118.56	111.83
23	b	607	CLA	C4A-NA-C1A	-2.21	105.67	106.68
25	k	101	BCR	C36-C18-C19	2.20	121.46	118.09
23	d	403	CLA	C1-O2A-CGA	2.20	121.99	116.65
23	c	513	CLA	C4B-C3B-C2B	-2.20	104.56	107.30
33	C	501	LMG	O7-C10-O9	-2.20	118.56	123.70
23	C	505	CLA	C1-C2-C3	-2.20	122.59	126.20
25	C	516	BCR	C21-C20-C19	-2.20	116.83	123.20
23	B	615	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
25	c	516	BCR	C15-C14-C13	-2.20	124.20	127.28
25	b	618	BCR	C37-C22-C23	2.19	121.44	118.09
35	C	518	DGD	O1G-C1A-C2A	2.19	118.53	111.83
35	c	517	DGD	O3G-C3G-C2G	-2.19	105.48	110.82
23	b	615	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
23	C	511	CLA	CAC-C3C-C4C	2.19	127.64	124.79
23	c	507	CLA	CMB-C2B-C1B	2.19	128.76	125.42
26	a	413	SQD	O7-S-C6	2.19	110.03	106.76
29	d	405	PL9	C51-C49-C50	2.19	119.63	114.59
23	C	505	CLA	O2A-CGA-CBA	2.19	118.52	111.83
23	B	601	CLA	C2A-C1A-CHA	-2.19	120.06	123.87
26	B	620	SQD	C44-O6-C1	-2.19	109.10	113.80
23	A	408	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
32	b	621	LMT	C2'-C3'-C4'	2.19	114.65	109.68
23	C	504	CLA	CMC-C2C-C1C	2.19	128.45	125.03
25	B	617	BCR	C37-C22-C23	2.19	121.43	118.09
23	C	505	CLA	C4-C3-C5	2.19	119.02	115.23
23	c	511	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
29	A	414	PL9	C25-C24-C26	2.18	119.02	115.23
23	A	408	CLA	CHB-C4A-NA	2.18	127.55	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	e	87	HEM	CHA-C1A-NA	2.18	127.82	123.86
25	B	618	BCR	C37-C22-C21	-2.18	119.28	122.82
23	A	408	CLA	CMB-C2B-C1B	2.18	128.74	125.42
23	b	613	CLA	C2A-C1A-CHA	-2.18	120.08	123.87
33	a	419	LMG	O7-C10-O9	-2.18	118.61	123.70
25	t	103	BCR	C2-C1-C6	2.18	113.61	110.44
23	C	507	CLA	CGD-CBD-CAD	-2.18	103.79	110.85
25	d	404	BCR	C40-C30-C39	2.18	114.88	108.63
25	h	101	BCR	C24-C23-C22	-2.18	123.01	126.23
23	b	607	CLA	CHD-C4C-NC	2.18	127.61	124.23
23	B	607	CLA	CMA-C3A-C2A	-2.18	105.56	113.98
34	b	625	HTG	O5-C1-S1	-2.18	103.96	109.94
25	Y	101	BCR	C36-C18-C19	2.18	121.41	118.09
23	c	505	CLA	C1-C2-C3	-2.18	122.63	126.20
25	K	102	BCR	C37-C22-C21	-2.18	119.29	122.82
33	a	419	LMG	O8-C28-C29	2.17	118.47	111.83
23	b	606	CLA	CHB-C1B-C2B	-2.17	121.12	127.43
23	B	606	CLA	C11-C12-C13	-2.17	108.74	115.97
23	b	602	CLA	CHB-C4A-NA	2.17	127.54	124.40
24	a	408	PHO	O2D-CGD-O1D	-2.17	119.62	123.85
23	B	607	CLA	CAC-C3C-C4C	2.17	127.62	124.79
23	C	513	CLA	CBA-CAA-C2A	-2.17	107.33	113.79
23	c	508	CLA	C2A-C1A-CHA	-2.17	120.10	123.87
25	A	409	BCR	C2-C1-C6	2.17	113.59	110.44
26	a	413	SQD	O48-C23-O10	-2.17	118.20	123.63
23	C	511	CLA	C4-C3-C2	-2.17	118.05	123.63
25	c	515	BCR	C36-C18-C17	-2.17	119.30	122.82
25	t	103	BCR	C19-C18-C17	-2.17	115.60	119.01
38	E	103	HEM	CHA-C1A-NA	2.17	127.79	123.86
23	B	616	CLA	C1-O2A-CGA	2.17	121.90	116.65
25	Y	101	BCR	C11-C10-C9	-2.17	124.24	127.28
23	B	605	CLA	CAC-C3C-C2C	2.17	131.54	127.56
23	B	609	CLA	C1-C2-C3	-2.17	122.65	126.20
33	a	419	LMG	O6-C5-C4	2.17	113.60	109.70
25	Y	101	BCR	C36-C18-C17	-2.17	119.31	122.82
23	B	603	CLA	C5-C3-C2	-2.17	116.31	121.17
23	b	608	CLA	C11-C12-C13	-2.16	108.77	115.97
35	c	517	DGD	O6D-C1D-O3G	-2.16	104.93	110.04
24	a	353	PHO	C4-C3-C2	-2.16	118.07	123.63
29	d	405	PL9	O2-C1-C6	-2.16	117.04	120.48
25	a	410	BCR	C11-C10-C9	-2.16	124.24	127.28
23	c	510	CLA	C4-C3-C2	-2.16	118.07	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	353	PHO	OBD-CAD-C3D	-2.16	124.52	127.89
25	c	515	BCR	C37-C22-C21	-2.16	119.31	122.82
34	B	622	HTG	C6-C5-C4	-2.16	107.71	113.02
23	b	605	CLA	C1-O2A-CGA	2.16	121.89	116.65
25	k	101	BCR	C3-C4-C5	-2.16	110.20	114.06
40	v	202	HEC	CMC-C2C-C1C	-2.16	122.13	125.42
23	B	611	CLA	C4D-CHA-C1A	-2.16	118.67	121.24
23	D	405	CLA	OBD-CAD-C3D	-2.16	123.37	128.42
23	B	610	CLA	CMA-C3A-C2A	-2.16	105.63	113.98
23	b	602	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
26	F	101	SQD	O5-C1-O6	2.16	115.15	110.04
23	a	407	CLA	CBC-CAC-C3C	-2.16	106.57	112.42
23	b	612	CLA	C11-C12-C13	-2.16	108.80	115.97
23	b	611	CLA	C7-C6-C5	-2.15	107.53	113.26
25	h	101	BCR	C34-C9-C8	2.15	121.37	118.09
23	c	506	CLA	CHD-C4C-NC	2.15	127.57	124.23
35	C	517	DGD	O3G-C3G-C2G	-2.15	105.59	110.82
23	C	514	CLA	C4-C3-C5	2.15	118.96	115.23
25	B	618	BCR	C15-C16-C17	-2.15	119.12	123.52
29	D	408	PL9	C27-C28-C29	-2.15	122.71	127.62
35	c	519	DGD	O3G-C1D-C2D	-2.15	105.01	108.27
38	e	87	HEM	C4C-NC-C1C	2.15	109.32	105.82
35	c	517	DGD	O1G-C1A-O1A	-2.15	118.26	123.63
23	b	615	CLA	CHA-C1A-NA	-2.14	121.54	126.39
23	b	609	CLA	CHA-C1A-NA	-2.14	121.54	126.39
25	H	101	BCR	C33-C5-C6	-2.14	122.15	124.48
23	d	402	CLA	CHD-C4C-NC	2.14	127.55	124.23
25	k	101	BCR	C38-C26-C25	-2.14	122.15	124.48
35	c	519	DGD	O3G-C3G-C2G	-2.14	105.62	110.82
23	b	609	CLA	CMA-C3A-C4A	-2.14	106.03	111.77
23	b	605	CLA	O2A-CGA-CBA	2.14	118.35	111.83
23	a	409	CLA	C1-O2A-CGA	2.14	121.82	116.65
23	c	510	CLA	O2A-C1-C2	2.13	116.32	108.11
32	b	627	LMT	O1'-C1'-C2'	2.13	111.51	108.27
38	e	87	HEM	CMD-C2D-C1D	2.13	128.37	125.03
37	L	101	LHG	O4-P-O5	2.13	122.36	112.44
24	A	353	PHO	C6-C5-C3	-2.13	108.28	113.47
23	C	506	CLA	CBC-CAC-C3C	-2.13	106.65	112.42
23	a	407	CLA	C4-C3-C5	2.13	118.92	115.23
33	c	520	LMG	O8-C28-O10	-2.13	118.30	123.63
25	B	618	BCR	C40-C30-C25	-2.13	106.91	110.24
23	b	607	CLA	CAA-CBA-CGA	2.13	119.25	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	514	CLA	CBC-CAC-C3C	-2.13	106.65	112.42
23	c	506	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
33	C	501	LMG	O6-C1-O1	-2.13	105.02	110.04
23	C	513	CLA	CMA-C3A-C4A	-2.12	106.06	111.77
23	B	616	CLA	C2A-C1A-CHA	-2.12	120.18	123.87
29	a	416	PL9	C45-C44-C46	2.12	118.91	115.23
23	a	405	CLA	CMB-C2B-C3B	2.12	131.54	126.55
23	c	507	CLA	C4-C3-C5	2.12	118.91	115.23
23	A	406	CLA	CHB-C4A-NA	2.12	127.46	124.40
23	B	606	CLA	CHB-C1B-C2B	-2.12	121.28	127.43
25	K	102	BCR	C11-C10-C9	-2.12	124.31	127.28
23	b	606	CLA	CAC-C3C-C4C	2.12	127.54	124.79
23	B	609	CLA	C2A-C1A-CHA	-2.12	120.20	123.87
25	B	618	BCR	C10-C11-C12	-2.11	117.08	123.20
23	b	613	CLA	C16-C15-C13	-2.11	108.95	115.97
25	A	409	BCR	C8-C7-C6	-2.11	121.36	127.00
26	f	102	SQD	O8-S-C6	2.11	110.05	105.97
23	C	509	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
23	A	405	CLA	CHB-C4A-NA	2.11	127.44	124.40
23	B	615	CLA	C2A-C1A-CHA	-2.11	120.21	123.87
37	l	101	LHG	O7-C7-O9	-2.11	118.77	123.70
23	b	604	CLA	C4-C3-C2	-2.11	118.21	123.63
23	C	508	CLA	C6-C7-C8	-2.11	108.96	115.97
25	t	103	BCR	C35-C13-C12	2.11	121.31	118.09
23	c	511	CLA	C4-C3-C2	-2.11	118.22	123.63
23	D	405	CLA	CBC-CAC-C3C	-2.11	106.71	112.42
23	A	404	CLA	C7-C6-C5	-2.11	107.65	113.26
40	v	202	HEC	C1D-C2D-C3D	-2.11	104.41	106.82
23	b	608	CLA	C4-C3-C5	2.10	118.88	115.23
23	c	513	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
23	a	406	CLA	CHB-C4A-NA	2.10	127.43	124.40
29	d	405	PL9	C45-C44-C46	2.10	118.87	115.23
23	b	611	CLA	O2A-CGA-CBA	2.10	118.24	111.83
35	c	517	DGD	O1G-C1A-C2A	2.10	118.23	111.83
23	a	407	CLA	CAC-C3C-C4C	2.09	127.52	124.79
23	c	505	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
23	b	615	CLA	C6-C5-C3	-2.09	108.37	113.47
27	a	801	GOL	C3-C2-C1	-2.09	104.12	111.80
25	h	101	BCR	C16-C15-C14	-2.09	119.24	123.52
23	d	402	CLA	CBC-CAC-C3C	-2.09	106.75	112.42
23	c	513	CLA	CBC-CAC-C3C	-2.09	106.76	112.42
25	A	409	BCR	C28-C27-C26	-2.09	110.33	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C6-C5-C3	-2.09	108.38	113.47
25	K	102	BCR	C28-C27-C26	-2.09	110.34	114.06
23	b	611	CLA	OBD-CAD-C3D	-2.08	123.54	128.42
29	d	405	PL9	C2-C1-C6	2.08	121.48	119.00
23	B	609	CLA	CHA-C1A-NA	-2.08	121.67	126.39
23	b	611	CLA	CAA-C2A-C3A	-2.08	107.37	113.00
25	a	410	BCR	C8-C7-C6	-2.08	121.44	127.00
23	b	610	CLA	CHB-C4A-NA	2.08	127.40	124.40
40	V	202	HEC	CAD-CBD-CGD	-2.08	108.15	113.67
29	A	414	PL9	C53-C6-C1	2.08	119.54	115.28
26	a	411	SQD	C3-C4-C5	2.08	114.00	110.23
23	b	601	CLA	CAC-C3C-C4C	2.08	127.49	124.79
23	c	512	CLA	C11-C10-C8	-2.08	109.06	115.97
23	c	513	CLA	CHA-C1A-NA	-2.08	121.69	126.39
23	B	602	CLA	OBD-CAD-C3D	-2.08	123.56	128.42
23	B	602	CLA	C4-C3-C5	2.08	118.83	115.23
23	D	405	CLA	CMA-C3A-C2A	-2.08	105.96	113.98
23	A	406	CLA	CBC-CAC-C3C	-2.08	106.79	112.42
24	a	353	PHO	O2A-CGA-O1A	-2.07	118.44	123.63
23	c	512	CLA	CMA-C3A-C4A	2.07	117.34	111.77
25	H	101	BCR	C37-C22-C21	-2.07	119.46	122.82
23	B	612	CLA	C4A-NA-C1A	-2.07	105.73	106.68
23	c	513	CLA	CMA-C3A-C4A	-2.07	106.21	111.77
25	T	101	BCR	C7-C8-C9	-2.07	123.17	126.23
34	B	626	HTG	C1-O5-C5	2.07	116.27	112.56
32	b	627	LMT	C1'-O5'-C5'	-2.07	109.68	113.72
23	B	603	CLA	CHB-C1B-C2B	-2.07	121.43	127.43
23	c	503	CLA	C2A-C1A-CHA	-2.07	120.28	123.87
23	C	508	CLA	C3B-C4B-NB	2.07	112.38	110.53
23	C	508	CLA	CHA-C1A-NA	-2.07	121.71	126.39
23	c	511	CLA	C11-C10-C8	-2.07	109.10	115.97
23	b	601	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
23	b	610	CLA	CMA-C3A-C4A	-2.06	106.22	111.77
33	z	101	LMG	O8-C28-O10	-2.06	118.47	123.63
23	c	510	CLA	CHB-C1B-NB	-2.06	120.95	124.05
23	a	407	CLA	CAA-CBA-CGA	2.06	119.06	113.21
23	A	405	CLA	C1-C2-C3	-2.06	122.82	126.20
25	b	619	BCR	C21-C20-C19	-2.06	117.23	123.20
23	B	601	CLA	C4-C3-C5	2.06	118.80	115.23
25	A	409	BCR	C31-C1-C6	-2.06	107.02	110.24
23	C	505	CLA	OBD-CAD-C3D	-2.06	123.61	128.42
23	b	608	CLA	C2A-C1A-CHA	-2.06	120.30	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	H	101	BCR	C16-C15-C14	-2.06	119.31	123.52
25	K	102	BCR	C3-C4-C5	-2.05	110.39	114.06
25	K	102	BCR	C10-C11-C12	-2.05	117.25	123.20
24	A	353	PHO	O2A-CGA-CBA	2.05	118.10	111.83
23	C	514	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
23	C	511	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
32	M	101	LMT	O5B-C5B-C6B	2.05	111.52	106.44
29	D	408	PL9	C47-C48-C49	-2.05	120.81	127.64
26	f	102	SQD	C44-O6-C1	-2.05	109.40	113.80
23	B	610	CLA	C4-C3-C5	2.05	118.78	115.23
23	B	601	CLA	CAA-C2A-C3A	-2.05	107.46	113.00
26	b	620	SQD	O5-C1-C2	-2.05	106.16	110.37
29	d	405	PL9	C40-C39-C38	-2.05	118.37	123.63
33	c	521	LMG	C1-C2-C3	-2.04	105.71	110.01
23	d	402	CLA	CBB-CAB-C3B	-2.04	117.32	127.53
26	b	620	SQD	C44-O6-C1	-2.04	109.42	113.80
23	b	603	CLA	C7-C6-C5	-2.04	107.82	113.26
23	a	407	CLA	CHA-C1A-NA	-2.04	121.77	126.39
26	b	620	SQD	C1-C2-C3	-2.04	105.72	110.01
27	a	412	GOL	C3-C2-C1	-2.04	104.31	111.80
23	C	502	CLA	CAA-C2A-C3A	-2.04	107.49	113.00
29	A	414	PL9	C10-C9-C11	2.04	118.77	115.23
23	C	513	CLA	C2A-C1A-CHA	-2.04	120.33	123.87
23	B	604	CLA	CHA-C1A-NA	-2.04	121.78	126.39
29	a	416	PL9	C47-C46-C44	-2.04	106.43	113.19
32	t	102	LMT	O5'-C1'-O1'	-2.04	105.23	110.04
26	F	101	SQD	O5-C1-C2	-2.04	106.19	110.37
23	C	513	CLA	C3B-C4B-NB	2.03	112.35	110.53
25	B	617	BCR	C21-C20-C19	-2.03	117.31	123.20
23	B	604	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
23	C	508	CLA	CAC-C3C-C4C	2.03	127.44	124.79
23	b	613	CLA	CHA-C1A-NA	-2.03	121.79	126.39
25	D	407	BCR	C39-C30-C25	-2.03	107.06	110.24
23	B	606	CLA	CAC-C3C-C4C	2.03	127.43	124.79
23	b	616	CLA	CHB-C1B-C2B	-2.03	121.54	127.43
27	d	801	GOL	C3-C2-C1	-2.03	104.36	111.80
23	C	509	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
35	c	518	DGD	O6E-C1E-O5D	-2.03	105.26	110.04
32	E	102	LMT	C2'-C3'-C4'	2.02	114.28	109.68
29	a	416	PL9	C51-C49-C50	2.02	119.25	114.59
25	B	617	BCR	C3-C4-C5	-2.02	110.45	114.06
32	m	103	LMT	C1'-O5'-C5'	-2.02	109.77	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	CED-O2D-CGD	2.02	120.50	115.92
23	c	513	CLA	CAA-C2A-C3A	-2.02	107.54	113.00
23	b	608	CLA	C11-C10-C8	-2.02	109.25	115.97
25	c	516	BCR	C37-C22-C21	-2.02	119.55	122.82
40	v	202	HEC	CBD-CAD-C3D	-2.02	106.95	112.53
32	D	404	LMT	C1B-C2B-C3B	2.02	114.25	110.01
25	h	101	BCR	C20-C21-C22	-2.02	124.45	127.28
27	a	701	GOL	C3-C2-C1	-2.01	104.41	111.80
37	D	411	LHG	O4-P-O5	2.01	121.82	112.44
29	A	414	PL9	C51-C49-C50	2.01	119.22	114.59
23	c	509	CLA	CMC-C2C-C1C	2.01	128.18	125.03
29	D	408	PL9	C45-C44-C46	2.01	118.72	115.23
23	B	608	CLA	CMB-C2B-C1B	2.01	128.48	125.42
26	B	620	SQD	O5-C1-C2	-2.01	106.24	110.37
23	C	511	CLA	CHB-C4A-NA	2.01	127.30	124.40
23	c	508	CLA	C4B-C3B-C2B	-2.01	104.81	107.30
35	c	517	DGD	O2G-C1B-O1B	-2.01	119.01	123.70
23	c	508	CLA	CBC-CAC-C3C	-2.01	106.98	112.42
25	t	103	BCR	C20-C21-C22	-2.01	124.47	127.28
23	d	403	CLA	CMA-C3A-C2A	-2.00	106.23	113.98
32	D	404	LMT	O1B-C4'-C5'	-2.00	104.22	109.48
23	b	610	CLA	C4-C3-C2	-2.00	118.48	123.63
23	C	508	CLA	C2A-C1A-CHA	-2.00	120.39	123.87
29	D	408	PL9	C22-C23-C24	-2.00	123.04	127.62
23	b	608	CLA	CAA-C2A-C3A	-2.00	107.59	113.00
32	b	621	LMT	C1-O1'-C1'	2.00	117.10	113.68

All (66) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	405	CLA	ND
23	A	408	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	609	CLA	ND
23	B	610	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	502	CLA	ND
23	C	503	CLA	ND
23	C	504	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	C	514	CLA	ND
23	D	405	CLA	ND
23	D	406	CLA	ND
23	a	405	CLA	ND
23	a	406	CLA	ND
23	a	409	CLA	ND
23	b	601	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	c	502	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND

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

All (1263) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	603	CLA	C2-C3-C5-C6
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	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	510	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O2D
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	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C2-C1-O2A-CGA
23	c	510	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C11-C10-C8-C9
23	c	514	CLA	C2B-C3B-CAB-CBB
23	c	514	CLA	C4B-C3B-CAB-CBB
25	D	407	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

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Mol	Chain	Res	Type	Atoms
26	A	412	SQD	O6-C44-C45-O47
26	B	620	SQD	O49-C7-O47-C45
26	F	101	SQD	C2-C1-O6-C44
26	F	101	SQD	O49-C7-O47-C45
26	F	101	SQD	C8-C7-O47-C45
26	a	413	SQD	O6-C44-C45-O47
26	a	413	SQD	C5-C6-S-O7
26	a	413	SQD	C5-C6-S-O8
26	a	413	SQD	C5-C6-S-O9
26	b	620	SQD	C8-C7-O47-C45
26	f	102	SQD	O6-C44-C45-O47
26	f	102	SQD	O49-C7-O47-C45
26	f	102	SQD	C8-C7-O47-C45
27	A	411	GOL	O1-C1-C2-C3
27	B	624	GOL	C1-C2-C3-O3
27	D	701	GOL	C1-C2-C3-O3
27	V	401	GOL	C1-C2-C3-O3
27	a	412	GOL	O1-C1-C2-C3
27	b	624	GOL	C1-C2-C3-O3
27	c	743	GOL	C1-C2-C3-O3
27	o	601	GOL	O1-C1-C2-C3
27	o	601	GOL	C1-C2-C3-O3
29	A	414	PL9	C9-C11-C12-C13
29	a	416	PL9	C23-C24-C26-C27
29	a	416	PL9	C25-C24-C26-C27
32	A	359	LMT	C2'-C1'-O1'-C1
32	A	359	LMT	O5'-C1'-O1'-C1
32	E	102	LMT	C2'-C1'-O1'-C1
32	E	102	LMT	O5'-C1'-O1'-C1
32	I	101	LMT	O5'-C1'-O1'-C1
32	a	414	LMT	C2'-C1'-O1'-C1
32	b	627	LMT	C2'-C1'-O1'-C1
32	b	627	LMT	O5'-C1'-O1'-C1
32	t	101	LMT	O5'-C1'-O1'-C1
32	t	101	LMT	C2-C1-O1'-C1'
32	t	102	LMT	O5'-C1'-O1'-C1
33	C	521	LMG	C11-C10-O7-C8
33	c	521	LMG	O9-C10-O7-C8
33	c	521	LMG	C11-C10-O7-C8
33	Z	101	LMG	O9-C10-O7-C8
33	Z	101	LMG	C11-C10-O7-C8
33	z	101	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
37	D	410	LHG	O2-C2-C3-O3
37	D	410	LHG	C3-O3-P-O4
37	D	410	LHG	C3-O3-P-O5
37	D	410	LHG	C3-O3-P-O6
37	D	410	LHG	C4-O6-P-O4
37	E	101	LHG	C3-O3-P-O4
37	E	101	LHG	C3-O3-P-O5
37	E	101	LHG	C3-O3-P-O6
37	E	101	LHG	C4-O6-P-O3
37	E	101	LHG	O10-C23-O8-C6
37	E	101	LHG	C24-C23-O8-C6
37	L	101	LHG	C4-O6-P-O3
37	L	101	LHG	C4-O6-P-O4
37	L	101	LHG	C4-O6-P-O5
37	d	407	LHG	C3-O3-P-O4
37	d	407	LHG	C3-O3-P-O5
37	d	407	LHG	C3-O3-P-O6
37	d	407	LHG	C4-O6-P-O4
37	d	711	LHG	C3-O3-P-O5
37	e	101	LHG	C3-O3-P-O4
37	e	101	LHG	C3-O3-P-O6
37	e	101	LHG	C4-O6-P-O3
37	e	101	LHG	C4-O6-P-O5
37	e	101	LHG	O10-C23-O8-C6
37	e	101	LHG	C24-C23-O8-C6
37	l	101	LHG	C4-O6-P-O3
37	l	101	LHG	C4-O6-P-O4
37	l	101	LHG	C4-O6-P-O5
38	E	103	HEM	C2C-C3C-CAC-CBC
38	E	103	HEM	C4C-C3C-CAC-CBC
40	V	202	HEC	C2B-C3B-CAB-CBB
40	V	202	HEC	C4B-C3B-CAB-CBB
40	V	202	HEC	C2C-C3C-CAC-CBC
40	V	202	HEC	C4C-C3C-CAC-CBC
40	v	202	HEC	C2B-C3B-CAB-CBB
40	v	202	HEC	C4B-C3B-CAB-CBB
40	v	202	HEC	C2C-C3C-CAC-CBC
40	v	202	HEC	C4C-C3C-CAC-CBC
32	I	101	LMT	O5B-C1B-O1B-C4'
32	a	414	LMT	C4'-C5'-C6'-O6'
26	A	410	SQD	O49-C7-O47-C45
26	b	620	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
23	B	614	CLA	C3-C5-C6-C7
23	D	406	CLA	C3-C5-C6-C7
23	c	513	CLA	C3-C5-C6-C7
23	d	403	CLA	C3-C5-C6-C7
32	M	103	LMT	C4B-C5B-C6B-O6B
26	B	620	SQD	C8-C7-O47-C45
23	A	408	CLA	C4-C3-C5-C6
23	a	409	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	c	508	CLA	C4-C3-C5-C6
23	d	403	CLA	C4-C3-C5-C6
29	A	414	PL9	C15-C14-C16-C17
23	A	408	CLA	C2-C3-C5-C6
23	d	403	CLA	C2-C3-C5-C6
32	M	103	LMT	O5'-C5'-C6'-O6'
32	a	420	LMT	O5B-C5B-C6B-O6B
23	b	616	CLA	C3-C5-C6-C7
32	E	102	LMT	O5'-C5'-C6'-O6'
32	m	103	LMT	O5B-C5B-C6B-O6B
32	m	103	LMT	C4B-C5B-C6B-O6B
25	T	101	BCR	C13-C14-C15-C16
33	C	521	LMG	O9-C10-O7-C8
32	b	621	LMT	O5'-C5'-C6'-O6'
34	D	414	HTG	O5-C5-C6-O6
32	D	404	LMT	C4'-C5'-C6'-O6'
23	A	408	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
32	D	404	LMT	C6-C7-C8-C9
37	d	407	LHG	O2-C2-C3-O3
32	a	414	LMT	O5B-C5B-C6B-O6B
26	A	410	SQD	C8-C7-O47-C45
33	z	101	LMG	C11-C10-O7-C8
32	b	627	LMT	O5'-C5'-C6'-O6'
33	C	521	LMG	O6-C5-C6-O5
34	b	625	HTG	O5-C5-C6-O6
33	c	521	LMG	C4-C5-C6-O5
32	M	103	LMT	C4'-C5'-C6'-O6'
34	b	625	HTG	S1-C1'-C2'-C3'
23	B	605	CLA	C4-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
23	C	508	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C4-C3-C5-C6
29	A	414	PL9	C20-C19-C21-C22
29	a	416	PL9	C15-C14-C16-C17
29	a	416	PL9	C30-C29-C31-C32
23	B	605	CLA	C2-C3-C5-C6
23	C	508	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
23	c	508	CLA	C2-C3-C5-C6
29	A	414	PL9	C13-C14-C16-C17
29	A	414	PL9	C18-C19-C21-C22
29	a	416	PL9	C13-C14-C16-C17
29	a	416	PL9	C28-C29-C31-C32
33	z	101	LMG	O9-C10-O7-C8
29	A	414	PL9	C14-C16-C17-C18
29	A	414	PL9	C44-C46-C47-C48
29	D	408	PL9	C39-C41-C42-C43
29	a	416	PL9	C9-C11-C12-C13
29	a	416	PL9	C14-C16-C17-C18
34	D	414	HTG	C4-C5-C6-O6
32	I	101	LMT	O5B-C5B-C6B-O6B
32	e	102	LMT	O5'-C1'-O1'-C1
32	D	404	LMT	O5'-C5'-C6'-O6'
32	I	101	LMT	O5'-C5'-C6'-O6'
32	M	103	LMT	O5B-C5B-C6B-O6B
32	t	101	LMT	O5'-C5'-C6'-O6'
32	a	420	LMT	C4B-C5B-C6B-O6B
23	D	406	CLA	CBD-CGD-O2D-CED
23	c	514	CLA	CBD-CGD-O2D-CED
32	a	414	LMT	O5'-C5'-C6'-O6'
33	c	521	LMG	O6-C5-C6-O5
32	D	404	LMT	O5B-C5B-C6B-O6B
32	a	414	LMT	C4B-C5B-C6B-O6B
32	e	102	LMT	C4'-C5'-C6'-O6'
23	c	511	CLA	CBD-CGD-O2D-CED
32	E	102	LMT	C4'-C5'-C6'-O6'
37	d	407	LHG	C1-C2-C3-O3
23	a	409	CLA	CBA-CGA-O2A-C1
23	C	505	CLA	C2-C3-C5-C6
23	a	409	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	B	602	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	B	613	CLA	C11-C12-C13-C14
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
23	c	505	CLA	C11-C12-C13-C14
32	I	101	LMT	C2'-C1'-O1'-C1
26	F	101	SQD	C23-C24-C25-C26
32	I	101	LMT	C5'-C4'-O1B-C1B
34	B	626	HTG	O5-C5-C6-O6
25	D	407	BCR	C37-C22-C23-C24
32	e	102	LMT	O5B-C5B-C6B-O6B
32	b	627	LMT	C4'-C5'-C6'-O6'
32	I	101	LMT	C4B-C5B-C6B-O6B
32	t	102	LMT	O5'-C5'-C6'-O6'
32	D	404	LMT	C4B-C5B-C6B-O6B
32	t	101	LMT	C4'-C5'-C6'-O6'
23	c	510	CLA	CBA-CGA-O2A-C1
23	a	409	CLA	O1A-CGA-O2A-C1
34	b	622	HTG	O5-C5-C6-O6
27	a	412	GOL	O1-C1-C2-O2
23	c	510	CLA	C3-C5-C6-C7
23	B	601	CLA	C5-C6-C7-C8
32	b	621	LMT	C4'-C5'-C6'-O6'
23	C	511	CLA	C11-C12-C13-C15
23	b	606	CLA	C12-C13-C15-C16
23	D	406	CLA	C4-C3-C5-C6
29	A	414	PL9	C30-C29-C31-C32
32	m	103	LMT	O5'-C5'-C6'-O6'
29	d	405	PL9	C39-C41-C42-C43
32	I	101	LMT	C4'-C5'-C6'-O6'
32	I	101	LMT	O1'-C1-C2-C3
35	c	518	DGD	C1B-C2B-C3B-C4B
23	C	514	CLA	CBD-CGD-O2D-CED
23	c	513	CLA	CBD-CGD-O2D-CED
23	A	408	CLA	C5-C6-C7-C8
23	b	601	CLA	C10-C11-C12-C13
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
32	D	404	LMT	C5'-C4'-O1B-C1B
23	C	508	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	Z	101	LMG	C10-C11-C12-C13
37	E	101	LHG	C23-C24-C25-C26
23	c	510	CLA	O1A-CGA-O2A-C1
34	D	414	HTG	S1-C1'-C2'-C3'
34	b	622	HTG	S1-C1'-C2'-C3'
26	B	620	SQD	O5-C1-O6-C44
32	a	414	LMT	O5'-C1'-O1'-C1
32	b	621	LMT	O5'-C1'-O1'-C1
32	a	420	LMT	O1'-C1-C2-C3
23	B	601	CLA	C10-C11-C12-C13
23	B	602	CLA	C13-C15-C16-C17
23	b	604	CLA	C8-C10-C11-C12
23	b	606	CLA	C10-C11-C12-C13
23	b	606	CLA	C13-C15-C16-C17
23	b	614	CLA	C8-C10-C11-C12
33	B	621	LMG	C39-C40-C41-C42
32	e	102	LMT	O5'-C5'-C6'-O6'
23	B	606	CLA	C10-C11-C12-C13
23	c	513	CLA	C15-C16-C17-C18
26	B	620	SQD	C7-C8-C9-C10
23	c	514	CLA	C10-C11-C12-C13
23	b	605	CLA	C8-C10-C11-C12
23	a	405	CLA	C15-C16-C17-C18
23	b	611	CLA	C15-C16-C17-C18
37	D	410	LHG	C1-C2-C3-O3
35	h	102	DGD	C6B-C7B-C8B-C9B
37	D	411	LHG	C33-C34-C35-C36
23	B	608	CLA	C13-C15-C16-C17
23	B	614	CLA	C5-C6-C7-C8
23	B	614	CLA	C10-C11-C12-C13
23	b	604	CLA	C5-C6-C7-C8
23	D	406	CLA	C10-C11-C12-C13
23	b	611	CLA	C8-C10-C11-C12
26	b	620	SQD	C31-C32-C33-C34
34	d	411	HTG	S1-C1'-C2'-C3'
23	B	614	CLA	C8-C10-C11-C12
23	B	615	CLA	C10-C11-C12-C13
23	C	509	CLA	C10-C11-C12-C13
33	B	621	LMG	C11-C10-O7-C8
33	B	621	LMG	O9-C10-O7-C8
32	b	621	LMT	C2'-C1'-O1'-C1
32	e	102	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
32	t	101	LMT	C2'-C1'-O1'-C1
32	t	102	LMT	C2'-C1'-O1'-C1
35	C	518	DGD	C2E-C1E-O5D-C6D
35	C	519	DGD	C6B-C7B-C8B-C9B
26	A	410	SQD	C7-C8-C9-C10
34	B	622	HTG	C1'-C2'-C3'-C4'
34	b	623	HTG	C1'-C2'-C3'-C4'
25	b	619	BCR	C7-C8-C9-C34
25	b	619	BCR	C7-C8-C9-C10
23	B	610	CLA	C2A-CAA-CBA-CGA
27	B	624	GOL	O1-C1-C2-C3
27	D	701	GOL	O1-C1-C2-C3
27	O	501	GOL	O1-C1-C2-C3
27	O	601	GOL	O1-C1-C2-C3
27	a	412	GOL	C1-C2-C3-O3
27	a	701	GOL	O1-C1-C2-C3
27	d	701	GOL	O1-C1-C2-C3
27	v	401	GOL	O1-C1-C2-C3
23	b	602	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C20
26	F	101	SQD	O5-C1-O6-C44
23	D	406	CLA	C2-C3-C5-C6
26	A	410	SQD	C12-C13-C14-C15
23	b	614	CLA	C10-C11-C12-C13
23	c	507	CLA	C15-C16-C17-C18
33	Z	101	LMG	O6-C5-C6-O5
23	C	510	CLA	C2-C1-O2A-CGA
23	a	409	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C20
32	I	101	LMT	C1-C2-C3-C4
32	t	101	LMT	C3-C4-C5-C6
35	c	518	DGD	C9A-CAA-CBA-CCA
37	L	101	LHG	C15-C16-C17-C18
37	L	101	LHG	C17-C18-C19-C20
33	m	101	LMG	C35-C36-C37-C38
33	D	415	LMG	C35-C36-C37-C38
34	B	623	HTG	C3'-C4'-C5'-C6'
35	c	517	DGD	O6D-C5D-C6D-O5D
32	a	420	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
26	F	101	SQD	C30-C31-C32-C33
32	t	102	LMT	C4-C5-C6-C7
35	c	517	DGD	C9A-CAA-CBA-CCA
35	h	102	DGD	C9A-CAA-CBA-CCA
27	A	411	GOL	O1-C1-C2-O2
27	B	624	GOL	O2-C2-C3-O3
27	D	701	GOL	O1-C1-C2-O2
27	D	701	GOL	O2-C2-C3-O3
27	O	501	GOL	O1-C1-C2-O2
27	O	601	GOL	O1-C1-C2-O2
27	V	401	GOL	O2-C2-C3-O3
27	b	624	GOL	O2-C2-C3-O3
27	c	743	GOL	O2-C2-C3-O3
27	o	601	GOL	O2-C2-C3-O3
32	M	103	LMT	C2-C1-O1'-C1'
32	t	102	LMT	C2-C1-O1'-C1'
23	C	505	CLA	C4B-C3B-CAB-CBB
37	d	711	LHG	C16-C17-C18-C19
32	A	359	LMT	O5B-C5B-C6B-O6B
23	b	615	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C19
23	b	610	CLA	C2A-CAA-CBA-CGA
33	C	501	LMG	C17-C18-C19-C20
23	A	405	CLA	C15-C16-C17-C18
33	m	101	LMG	C11-C10-O7-C8
26	A	412	SQD	C17-C18-C19-C20
23	A	408	CLA	C12-C13-C15-C16
23	b	614	CLA	C12-C13-C15-C16
26	f	102	SQD	C32-C33-C34-C35
33	C	501	LMG	C36-C37-C38-C39
33	a	419	LMG	C30-C31-C32-C33
35	c	517	DGD	C5A-C6A-C7A-C8A
32	I	101	LMT	C3'-C4'-O1B-C1B
23	C	511	CLA	C10-C11-C12-C13
23	b	606	CLA	C15-C16-C17-C18
32	I	101	LMT	C3-C4-C5-C6
33	D	415	LMG	C19-C20-C21-C22
37	d	711	LHG	C32-C33-C34-C35
32	b	621	LMT	C3'-C4'-O1B-C1B
23	c	507	CLA	C3A-C2A-CAA-CBA
35	C	517	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
37	e	101	LHG	C26-C27-C28-C29
37	D	410	LHG	C16-C17-C18-C19
23	C	503	CLA	C13-C15-C16-C17
23	C	513	CLA	C10-C11-C12-C13
23	c	514	CLA	O1D-CGD-O2D-CED
32	A	359	LMT	O1'-C1-C2-C3
23	B	603	CLA	C16-C17-C18-C19
23	B	603	CLA	C16-C17-C18-C20
23	d	402	CLA	C16-C17-C18-C20
35	C	517	DGD	O6D-C5D-C6D-O5D
35	c	518	DGD	CBA-CCA-CDA-CEA
33	C	501	LMG	C12-C13-C14-C15
37	D	411	LHG	C32-C33-C34-C35
32	t	102	LMT	O1'-C1-C2-C3
32	b	627	LMT	C7-C8-C9-C10
32	e	102	LMT	C4-C5-C6-C7
33	B	621	LMG	C17-C18-C19-C20
35	c	517	DGD	C2B-C3B-C4B-C5B
35	c	518	DGD	CAA-CBA-CCA-CDA
33	a	419	LMG	C10-C11-C12-C13
33	c	520	LMG	C10-C11-C12-C13
32	M	103	LMT	C7-C8-C9-C10
33	B	621	LMG	C34-C35-C36-C37
34	b	622	HTG	C2'-C3'-C4'-C5'
34	b	622	HTG	C3'-C4'-C5'-C6'
35	C	517	DGD	C4B-C5B-C6B-C7B
35	C	518	DGD	CCB-CDB-CEB-CFB
37	L	101	LHG	C12-C13-C14-C15
37	L	101	LHG	C13-C14-C15-C16
37	l	101	LHG	C16-C17-C18-C19
26	A	410	SQD	C15-C16-C17-C18
26	F	101	SQD	C24-C25-C26-C27
33	D	415	LMG	C12-C13-C14-C15
37	E	101	LHG	C24-C25-C26-C27
37	d	711	LHG	C29-C30-C31-C32
34	b	625	HTG	C4-C5-C6-O6
33	C	521	LMG	C18-C19-C20-C21
33	a	419	LMG	C34-C35-C36-C37
23	B	610	CLA	C16-C17-C18-C19
23	B	615	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C20
32	b	627	LMT	C3-C4-C5-C6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
33	C	521	LMG	C17-C18-C19-C20
35	c	519	DGD	CBB-CCB-CDB-CEB
23	C	504	CLA	CBD-CGD-O2D-CED
23	c	513	CLA	CBA-CGA-O2A-C1
23	C	512	CLA	C3-C5-C6-C7
32	a	414	LMT	C2-C3-C4-C5
35	h	102	DGD	C7B-C8B-C9B-CAB
33	C	520	LMG	C16-C17-C18-C19
23	B	615	CLA	C5-C6-C7-C8
37	L	101	LHG	C25-C26-C27-C28
33	m	101	LMG	O9-C10-O7-C8
23	C	511	CLA	C4-C3-C5-C6
35	h	102	DGD	CAA-CBA-CCA-CDA
26	a	413	SQD	C25-C26-C27-C28
32	e	102	LMT	C5-C6-C7-C8
32	t	101	LMT	C4-C5-C6-C7
35	H	102	DGD	C5B-C6B-C7B-C8B
32	e	102	LMT	C1-C2-C3-C4
23	b	610	CLA	C11-C12-C13-C14
33	C	501	LMG	C19-C20-C21-C22
35	C	518	DGD	O6E-C1E-O5D-C6D
33	C	521	LMG	C13-C14-C15-C16
23	b	601	CLA	C8-C10-C11-C12
33	m	101	LMG	C39-C40-C41-C42
37	l	101	LHG	C14-C15-C16-C17
37	E	101	LHG	O2-C2-C3-O3
26	B	620	SQD	C11-C10-C9-C8
32	D	404	LMT	C5-C6-C7-C8
23	B	615	CLA	C16-C17-C18-C20
23	a	409	CLA	C16-C17-C18-C20
23	b	606	CLA	C16-C17-C18-C20
32	D	404	LMT	C3'-C4'-O1B-C1B
23	B	603	CLA	C13-C15-C16-C17
23	C	503	CLA	C15-C16-C17-C18
33	c	520	LMG	C33-C34-C35-C36
25	d	404	BCR	C37-C22-C23-C24
33	D	415	LMG	C36-C37-C38-C39
35	c	517	DGD	C7A-C8A-C9A-CAA
25	d	404	BCR	C21-C22-C23-C24
33	d	412	LMG	C29-C30-C31-C32
23	B	610	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	c	509	CLA	C16-C17-C18-C20
33	B	621	LMG	C15-C16-C17-C18
37	d	408	LHG	C29-C30-C31-C32
32	D	404	LMT	C1-C2-C3-C4
26	F	101	SQD	C29-C30-C31-C32
26	a	413	SQD	C31-C32-C33-C34
35	h	102	DGD	C2B-C3B-C4B-C5B
33	D	415	LMG	O6-C5-C6-O5
35	C	517	DGD	C9A-CAA-CBA-CCA
37	D	409	LHG	C12-C13-C14-C15
37	d	408	LHG	C27-C28-C29-C30
33	C	501	LMG	C39-C40-C41-C42
35	H	102	DGD	CCB-CDB-CEB-CFB
37	d	408	LHG	C25-C26-C27-C28
34	b	623	HTG	O5-C5-C6-O6
26	A	410	SQD	O6-C44-C45-O47
26	b	620	SQD	C27-C28-C29-C30
37	d	711	LHG	C24-C25-C26-C27
26	b	620	SQD	C14-C15-C16-C17
26	f	102	SQD	C25-C26-C27-C28
37	l	101	LHG	C27-C28-C29-C30
35	c	517	DGD	C4D-C5D-C6D-O5D
32	t	101	LMT	C11-C10-C9-C8
33	C	501	LMG	C13-C14-C15-C16
33	C	520	LMG	C17-C18-C19-C20
33	c	520	LMG	C31-C32-C33-C34
37	D	410	LHG	C12-C13-C14-C15
23	b	601	CLA	C2-C1-O2A-CGA
23	d	402	CLA	C16-C17-C18-C19
35	c	519	DGD	CBA-CCA-CDA-CEA
26	b	620	SQD	C13-C14-C15-C16
32	b	621	LMT	C11-C10-C9-C8
37	D	411	LHG	C15-C16-C17-C18
37	D	409	LHG	C34-C35-C36-C37
27	a	412	GOL	O2-C2-C3-O3
27	a	701	GOL	O1-C1-C2-O2
23	c	513	CLA	O1A-CGA-O2A-C1
37	d	408	LHG	C34-C35-C36-C37
23	C	512	CLA	C1A-C2A-CAA-CBA
23	c	507	CLA	C1A-C2A-CAA-CBA
23	B	610	CLA	C13-C15-C16-C17
33	C	521	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
35	H	102	DGD	C7A-C8A-C9A-CAA
33	c	520	LMG	C34-C35-C36-C37
35	c	518	DGD	C6A-C7A-C8A-C9A
37	d	407	LHG	C34-C35-C36-C37
23	B	602	CLA	C11-C12-C13-C15
23	B	613	CLA	C11-C10-C8-C7
23	B	614	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	D	406	CLA	C12-C13-C15-C16
23	b	601	CLA	C11-C10-C8-C7
23	b	606	CLA	C11-C10-C8-C7
23	c	505	CLA	C11-C12-C13-C15
23	c	506	CLA	C11-C12-C13-C15
23	c	510	CLA	C11-C10-C8-C7
23	c	513	CLA	C12-C13-C15-C16
23	A	406	CLA	C13-C15-C16-C17
35	c	518	DGD	C4A-C5A-C6A-C7A
33	C	501	LMG	C10-C11-C12-C13
29	a	416	PL9	C12-C11-C9-C10
32	M	101	LMT	O1'-C1-C2-C3
26	b	620	SQD	C18-C19-C20-C21
23	b	606	CLA	C11-C10-C8-C9
23	c	511	CLA	C11-C10-C8-C9
26	A	412	SQD	C26-C27-C28-C29
33	D	415	LMG	C30-C31-C32-C33
26	b	620	SQD	C24-C23-O48-C46
33	d	412	LMG	O6-C5-C6-O5
33	z	101	LMG	C19-C20-C21-C22
26	A	412	SQD	O6-C44-C45-C46
26	a	411	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
33	a	419	LMG	C7-C8-C9-O8
37	E	101	LHG	C4-C5-C6-O8
35	c	517	DGD	CAA-CBA-CCA-CDA
37	D	411	LHG	C13-C14-C15-C16
23	c	512	CLA	C8-C10-C11-C12
37	D	409	LHG	O2-C2-C3-O3
35	c	517	DGD	C2A-C1A-O1G-C1G
35	c	519	DGD	C2A-C1A-O1G-C1G
35	C	517	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
35	c	517	DGD	O6E-C5E-C6E-O5E
35	h	102	DGD	CAB-CBB-CCB-CDB
23	C	511	CLA	C2-C3-C5-C6
33	m	101	LMG	C38-C39-C40-C41
37	d	711	LHG	C25-C26-C27-C28
32	m	103	LMT	C7-C8-C9-C10
35	C	517	DGD	C8A-C9A-CAA-CBA
37	D	411	LHG	C29-C30-C31-C32
35	c	518	DGD	C2B-C3B-C4B-C5B
27	d	801	GOL	O1-C1-C2-C3
32	M	101	LMT	C3-C4-C5-C6
23	C	513	CLA	CBA-CGA-O2A-C1
26	B	620	SQD	C46-C45-O47-C7
26	b	620	SQD	C46-C45-O47-C7
23	a	406	CLA	C2C-C3C-CAC-CBC
26	a	411	SQD	C9-C10-C11-C12
37	D	409	LHG	C26-C27-C28-C29
32	b	627	LMT	C5-C6-C7-C8
23	D	406	CLA	O1D-CGD-O2D-CED
23	c	513	CLA	O1D-CGD-O2D-CED
26	b	620	SQD	C26-C27-C28-C29
37	d	408	LHG	C28-C29-C30-C31
23	d	403	CLA	CBA-CGA-O2A-C1
33	C	501	LMG	C11-C12-C13-C14
35	H	102	DGD	C9B-CAB-CBB-CCB
35	C	518	DGD	CDA-CEA-CFA-CGA
26	A	412	SQD	C27-C28-C29-C30
26	a	411	SQD	C12-C13-C14-C15
33	m	101	LMG	C37-C38-C39-C40
37	D	410	LHG	C10-C11-C12-C13
32	M	101	LMT	O5'-C5'-C6'-O6'
35	H	102	DGD	CAB-CBB-CCB-CDB
35	h	102	DGD	CDB-CEB-CFB-CGB
34	B	622	HTG	C2'-C3'-C4'-C5'
37	l	101	LHG	C9-C10-C11-C12
23	B	601	CLA	C2A-CAA-CBA-CGA
23	B	616	CLA	C2-C1-O2A-CGA
32	t	101	LMT	O1'-C1-C2-C3
35	h	102	DGD	CBA-CCA-CDA-CEA
37	E	101	LHG	C25-C26-C27-C28
32	t	102	LMT	C4'-C5'-C6'-O6'
32	a	414	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	d	412	LMG	C11-C12-C13-C14
23	B	601	CLA	CBA-CGA-O2A-C1
33	c	521	LMG	C29-C28-O8-C9
32	I	101	LMT	C5-C6-C7-C8
32	t	102	LMT	C7-C8-C9-C10
37	d	711	LHG	C33-C34-C35-C36
32	a	414	LMT	C3-C4-C5-C6
32	a	414	LMT	C6-C7-C8-C9
23	b	607	CLA	C3-C5-C6-C7
33	C	501	LMG	C18-C19-C20-C21
33	a	419	LMG	C29-C30-C31-C32
23	c	511	CLA	O1D-CGD-O2D-CED
35	C	519	DGD	C2B-C3B-C4B-C5B
29	D	408	PL9	C45-C44-C46-C47
23	C	506	CLA	C2-C3-C5-C6
29	d	405	PL9	C13-C14-C16-C17
23	B	613	CLA	C13-C15-C16-C17
23	C	507	CLA	C5-C6-C7-C8
26	A	410	SQD	C11-C10-C9-C8
33	C	520	LMG	C37-C38-C39-C40
27	B	624	GOL	O1-C1-C2-O2
27	o	501	GOL	O2-C2-C3-O3
27	v	401	GOL	O1-C1-C2-O2
32	D	404	LMT	C2-C1-O1'-C1'
32	E	102	LMT	C2-C1-O1'-C1'
32	I	101	LMT	C2-C1-O1'-C1'
32	e	102	LMT	C2-C1-O1'-C1'
32	m	103	LMT	C2-C1-O1'-C1'
23	C	505	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	C	507	CLA	C6-C7-C8-C9
23	C	514	CLA	C11-C10-C8-C9
23	D	406	CLA	C14-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C9
23	c	506	CLA	C11-C12-C13-C14
23	c	507	CLA	C10-C11-C12-C13
23	C	503	CLA	C4B-C3B-CAB-CBB
23	a	407	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C4B-C3B-CAB-CBB
23	b	606	CLA	C4B-C3B-CAB-CBB
23	c	503	CLA	C4B-C3B-CAB-CBB
33	a	419	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
37	d	408	LHG	C33-C34-C35-C36
23	A	404	CLA	C13-C15-C16-C17
32	a	420	LMT	C9-C10-C11-C12
32	a	420	LMT	C2-C3-C4-C5
37	D	411	LHG	C17-C18-C19-C20
26	A	412	SQD	C2-C1-O6-C44
23	c	508	CLA	C5-C6-C7-C8
33	C	520	LMG	C34-C35-C36-C37
34	c	522	HTG	C4'-C5'-C6'-C7'
35	C	517	DGD	C4D-C5D-C6D-O5D
23	B	614	CLA	C12-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C10
23	C	511	CLA	C12-C13-C15-C16
23	a	409	CLA	C11-C10-C8-C7
23	b	601	CLA	C6-C7-C8-C10
23	b	604	CLA	C6-C7-C8-C10
23	c	507	CLA	C11-C10-C8-C7
23	c	510	CLA	C6-C7-C8-C10
23	c	511	CLA	C11-C10-C8-C7
23	c	513	CLA	C10-C11-C12-C13
26	b	620	SQD	O10-C23-O48-C46
35	c	517	DGD	O1A-C1A-O1G-C1G
32	a	420	LMT	O5'-C5'-C6'-O6'
37	E	101	LHG	C13-C14-C15-C16
35	C	519	DGD	CDB-CEB-CFB-CGB
23	C	507	CLA	C3A-C2A-CAA-CBA
23	b	603	CLA	C5-C6-C7-C8
29	A	414	PL9	C12-C11-C9-C8
29	D	408	PL9	C13-C14-C16-C17
33	a	419	LMG	C4-C5-C6-O5
26	b	620	SQD	C28-C29-C30-C31
23	d	403	CLA	O1A-CGA-O2A-C1
35	c	519	DGD	O1A-C1A-O1G-C1G
23	b	601	CLA	CBA-CGA-O2A-C1
23	b	610	CLA	C15-C16-C17-C18
33	z	101	LMG	C14-C15-C16-C17
32	e	102	LMT	C4B-C5B-C6B-O6B
26	B	620	SQD	C34-C35-C36-C37
35	H	102	DGD	CCA-CDA-CEA-CFA
26	A	410	SQD	O6-C44-C45-C46
26	a	413	SQD	O6-C44-C45-C46
26	b	620	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
26	f	102	SQD	O6-C44-C45-C46
37	e	101	LHG	C4-C5-C6-O8
23	B	607	CLA	C3-C5-C6-C7
23	C	503	CLA	C16-C17-C18-C19
23	B	606	CLA	C8-C10-C11-C12
33	C	521	LMG	C12-C13-C14-C15
35	c	518	DGD	CBB-CCB-CDB-CEB
23	C	512	CLA	C8-C10-C11-C12
23	C	506	CLA	C4-C3-C5-C6
29	A	414	PL9	C45-C44-C46-C47
37	e	101	LHG	C23-C24-C25-C26
29	D	408	PL9	C43-C44-C46-C47
23	C	513	CLA	O1A-CGA-O2A-C1
23	C	514	CLA	O1D-CGD-O2D-CED
23	a	407	CLA	C2B-C3B-CAB-CBB
23	b	606	CLA	C2B-C3B-CAB-CBB
25	D	407	BCR	C23-C24-C25-C30
25	b	617	BCR	C1-C6-C7-C8
25	b	619	BCR	C5-C6-C7-C8
23	b	615	CLA	C10-C11-C12-C13
35	C	517	DGD	CCA-CDA-CEA-CFA
33	d	412	LMG	C18-C19-C20-C21
37	e	101	LHG	C10-C11-C12-C13
23	b	605	CLA	C5-C6-C7-C8
33	C	520	LMG	C31-C32-C33-C34
34	B	626	HTG	S1-C1'-C2'-C3'
26	B	620	SQD	O47-C45-C46-O48
26	a	411	SQD	O6-C44-C45-O47
26	b	620	SQD	O47-C45-C46-O48
26	f	102	SQD	O47-C45-C46-O48
32	a	420	LMT	C3-C4-C5-C6
34	b	623	HTG	O5-C1-S1-C1'
33	d	412	LMG	C10-C11-C12-C13
23	c	506	CLA	C4-C3-C5-C6
33	c	520	LMG	C29-C30-C31-C32
37	L	101	LHG	C27-C28-C29-C30
23	c	506	CLA	C2-C3-C5-C6
33	B	621	LMG	C32-C33-C34-C35
33	C	520	LMG	C30-C31-C32-C33
23	b	606	CLA	C16-C17-C18-C19
26	F	101	SQD	C34-C35-C36-C37
35	C	517	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
35	C	517	DGD	C3B-C4B-C5B-C6B
35	h	102	DGD	C3B-C4B-C5B-C6B
33	a	419	LMG	C21-C22-C23-C24
23	B	610	CLA	C14-C13-C15-C16
23	B	614	CLA	C14-C13-C15-C16
23	C	511	CLA	C14-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C9
23	c	514	CLA	C6-C7-C8-C9
23	c	513	CLA	C13-C15-C16-C17
26	A	412	SQD	O5-C1-O6-C44
35	c	517	DGD	O6E-C1E-O5D-C6D
32	I	101	LMT	C4-C5-C6-C7
33	a	419	LMG	C33-C34-C35-C36
29	A	414	PL9	C39-C41-C42-C43
29	a	416	PL9	C24-C26-C27-C28
33	c	520	LMG	C4-C5-C6-O5
32	e	102	LMT	C9-C10-C11-C12
33	Z	101	LMG	C19-C20-C21-C22
32	a	420	LMT	C4'-C5'-C6'-O6'
35	C	517	DGD	C1B-C2B-C3B-C4B
35	c	519	DGD	C1A-C2A-C3A-C4A
27	B	901	GOL	O1-C1-C2-O2
27	c	743	GOL	O1-C1-C2-O2
27	o	601	GOL	O1-C1-C2-O2
32	b	627	LMT	C1-C2-C3-C4
23	A	406	CLA	C16-C17-C18-C20
23	C	503	CLA	C16-C17-C18-C20
26	F	101	SQD	C32-C33-C34-C35
37	D	409	LHG	C1-C2-C3-O3
23	B	601	CLA	O1A-CGA-O2A-C1
23	B	601	CLA	C15-C16-C17-C18
25	Y	101	BCR	C37-C22-C23-C24
34	B	626	HTG	C4'-C5'-C6'-C7'
23	B	610	CLA	C12-C13-C15-C16
23	C	503	CLA	C12-C13-C15-C16
33	c	520	LMG	C28-C29-C30-C31
37	D	411	LHG	C27-C28-C29-C30
37	l	101	LHG	C34-C35-C36-C37
23	b	605	CLA	C13-C15-C16-C17
25	Y	101	BCR	C21-C22-C23-C24
23	C	511	CLA	CBA-CGA-O2A-C1
23	c	512	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	C	501	LMG	C20-C21-C22-C23
35	C	518	DGD	C2G-C3G-O3G-C1D
35	c	518	DGD	C5D-C6D-O5D-C1E
37	L	101	LHG	C11-C10-C9-C8
33	m	101	LMG	C14-C15-C16-C17
35	h	102	DGD	C6A-C7A-C8A-C9A
29	d	405	PL9	C45-C44-C46-C47
29	a	416	PL9	C12-C11-C9-C8
27	o	501	GOL	C1-C2-C3-O3
26	b	620	SQD	C11-C10-C9-C8
32	E	102	LMT	C2-C3-C4-C5
32	b	627	LMT	C6-C7-C8-C9
35	h	102	DGD	C9B-CAB-CBB-CCB
33	c	521	LMG	O10-C28-O8-C9
26	A	410	SQD	C18-C19-C20-C21
35	C	518	DGD	C5B-C6B-C7B-C8B
23	B	612	CLA	C10-C11-C12-C13
33	z	101	LMG	C20-C21-C22-C23
35	C	518	DGD	C8B-C9B-CAB-CBB
37	l	101	LHG	C13-C14-C15-C16
23	C	511	CLA	O1A-CGA-O2A-C1
23	b	601	CLA	O1A-CGA-O2A-C1
23	c	512	CLA	O1A-CGA-O2A-C1
35	c	517	DGD	CCB-CDB-CEB-CFB
37	D	410	LHG	C11-C10-C9-C8
37	E	101	LHG	O6-C4-C5-O7
37	L	101	LHG	O6-C4-C5-O7
26	a	411	SQD	C27-C28-C29-C30
33	B	621	LMG	O6-C1-O1-C7
35	c	518	DGD	O6E-C1E-O5D-C6D
33	B	621	LMG	C18-C19-C20-C21
26	B	620	SQD	C44-C45-C46-O48
37	L	101	LHG	C24-C25-C26-C27
37	d	407	LHG	C13-C14-C15-C16
35	C	518	DGD	C7A-C8A-C9A-CAA
37	D	411	LHG	C10-C11-C12-C13
26	a	411	SQD	C34-C35-C36-C37
32	E	102	LMT	C4-C5-C6-C7
33	a	419	LMG	O7-C8-C9-O8
37	e	101	LHG	O7-C5-C6-O8
23	B	602	CLA	C11-C12-C13-C14
23	C	514	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	c	513	CLA	C6-C7-C8-C9
23	d	403	CLA	C11-C12-C13-C14
33	d	412	LMG	C16-C17-C18-C19
33	a	419	LMG	C31-C32-C33-C34
33	C	520	LMG	C36-C37-C38-C39
23	B	605	CLA	C5-C6-C7-C8
23	b	601	CLA	C13-C15-C16-C17
37	e	101	LHG	C7-C8-C9-C10
33	C	521	LMG	C35-C36-C37-C38
33	B	621	LMG	C2-C1-O1-C7
35	c	517	DGD	C2E-C1E-O5D-C6D
35	c	518	DGD	C2E-C1E-O5D-C6D
23	C	507	CLA	C4-C3-C5-C6
37	D	409	LHG	C32-C33-C34-C35
23	B	601	CLA	C13-C15-C16-C17
37	d	408	LHG	C9-C10-C11-C12
23	b	613	CLA	CBD-CGD-O2D-CED
26	A	410	SQD	C34-C35-C36-C37
26	A	412	SQD	C30-C31-C32-C33
35	C	519	DGD	C2A-C3A-C4A-C5A
37	d	407	LHG	C11-C10-C9-C8
32	b	627	LMT	O1'-C1-C2-C3
23	C	513	CLA	C3-C5-C6-C7
32	D	404	LMT	C9-C10-C11-C12
23	B	611	CLA	C1A-C2A-CAA-CBA
23	C	513	CLA	C4B-C3B-CAB-CBB
23	a	406	CLA	C1A-C2A-CAA-CBA
23	c	502	CLA	C4B-C3B-CAB-CBB
23	c	512	CLA	C1A-C2A-CAA-CBA
23	C	504	CLA	O1D-CGD-O2D-CED
26	A	412	SQD	C24-C23-O48-C46
35	C	519	DGD	CBA-CCA-CDA-CEA
26	a	411	SQD	C35-C36-C37-C38
25	d	404	BCR	C7-C8-C9-C10
26	a	413	SQD	C24-C25-C26-C27
23	B	608	CLA	C16-C17-C18-C20
26	a	413	SQD	C16-C17-C18-C19
23	b	604	CLA	O1A-CGA-O2A-C1
37	L	101	LHG	O6-C4-C5-C6
37	d	711	LHG	C18-C19-C20-C21
32	b	621	LMT	C3-C4-C5-C6
23	A	406	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	B	602	CLA	C6-C7-C8-C10
23	B	616	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C10
23	d	402	CLA	C11-C12-C13-C15
23	C	502	CLA	C16-C17-C18-C20
37	d	407	LHG	C16-C17-C18-C19
23	b	604	CLA	CBA-CGA-O2A-C1
33	m	101	LMG	C32-C33-C34-C35
23	B	602	CLA	C15-C16-C17-C18
26	F	101	SQD	C7-C8-C9-C10
32	e	102	LMT	O1'-C1-C2-C3
35	c	519	DGD	C2B-C3B-C4B-C5B
23	C	511	CLA	C11-C12-C13-C14
23	a	409	CLA	C11-C10-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	B	606	CLA	C15-C16-C17-C18
23	C	507	CLA	C15-C16-C17-C18
35	C	517	DGD	C6A-C7A-C8A-C9A
23	c	507	CLA	C13-C15-C16-C17
33	c	520	LMG	C30-C31-C32-C33
35	C	519	DGD	CAB-CBB-CCB-CDB
35	c	518	DGD	C7B-C8B-C9B-CAB
37	L	101	LHG	C26-C27-C28-C29
26	B	620	SQD	C30-C31-C32-C33
26	F	101	SQD	O47-C45-C46-O48
37	E	101	LHG	O7-C5-C6-O8
34	b	623	HTG	S1-C1'-C2'-C3'
33	C	501	LMG	C7-C8-C9-O8
23	c	511	CLA	C4-C3-C5-C6
29	a	416	PL9	C43-C44-C46-C47
34	b	622	HTG	C1'-C2'-C3'-C4'
23	B	601	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CAD-CBD-CGD-O2D
23	B	613	CLA	C15-C16-C17-C18
26	A	412	SQD	O10-C23-O48-C46
26	A	410	SQD	C13-C14-C15-C16
23	b	604	CLA	C13-C15-C16-C17
23	B	606	CLA	C16-C17-C18-C19
33	Z	101	LMG	C11-C12-C13-C14
37	D	410	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
23	a	409	CLA	C15-C16-C17-C18
35	C	518	DGD	C8A-C9A-CAA-CBA
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
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	510	CLA	CHA-CBD-CGD-O1D
37	D	410	LHG	C4-O6-P-O3
37	D	410	LHG	C4-O6-P-O5
37	E	101	LHG	C4-O6-P-O5
37	e	101	LHG	C4-O6-P-O4
35	c	518	DGD	C5A-C6A-C7A-C8A
23	C	505	CLA	C2B-C3B-CAB-CBB
23	C	513	CLA	C2B-C3B-CAB-CBB
33	B	621	LMG	C29-C30-C31-C32
29	A	414	PL9	C28-C29-C31-C32
33	d	412	LMG	C35-C36-C37-C38
25	c	516	BCR	C7-C8-C9-C34
25	d	404	BCR	C7-C8-C9-C34
37	D	411	LHG	C2-C3-O3-P
37	d	408	LHG	C2-C3-O3-P
37	d	408	LHG	C32-C33-C34-C35
33	z	101	LMG	C10-C11-C12-C13
32	e	102	LMT	C3-C4-C5-C6
37	D	410	LHG	C26-C27-C28-C29
27	d	701	GOL	O1-C1-C2-O2
35	C	519	DGD	C6A-C7A-C8A-C9A
29	a	416	PL9	C4-C3-C7-C8
37	D	409	LHG	O1-C1-C2-C3
37	d	711	LHG	C34-C35-C36-C37
34	B	626	HTG	C4-C5-C6-O6
23	c	514	CLA	C4-C3-C5-C6
32	I	101	LMT	C7-C8-C9-C10
23	b	604	CLA	C15-C16-C17-C18
23	b	610	CLA	C13-C15-C16-C17
23	b	615	CLA	C5-C6-C7-C8
37	d	711	LHG	C11-C12-C13-C14
37	E	101	LHG	O6-C4-C5-C6
35	C	518	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C11-C12-C13-C14
23	D	406	CLA	C11-C10-C8-C9
23	c	507	CLA	C11-C10-C8-C9
23	d	402	CLA	C11-C12-C13-C14
23	D	406	CLA	C11-C10-C8-C7
23	c	506	CLA	C12-C13-C15-C16
33	B	621	LMG	O8-C28-C29-C30
35	C	519	DGD	C7B-C8B-C9B-CAB
35	C	519	DGD	C7A-C8A-C9A-CAA
33	m	101	LMG	C2-C1-O1-C7
33	Z	101	LMG	C2-C1-O1-C7
29	D	408	PL9	C15-C14-C16-C17
23	B	601	CLA	CAA-CBA-CGA-O2A
34	b	622	HTG	C4-C5-C6-O6
23	C	507	CLA	C16-C17-C18-C20
37	D	410	LHG	C13-C14-C15-C16
32	M	103	LMT	C3-C4-C5-C6
35	H	102	DGD	O2G-C1B-C2B-C3B
25	H	101	BCR	C9-C10-C11-C12
37	d	408	LHG	C10-C11-C12-C13
37	l	101	LHG	C28-C29-C30-C31
23	b	601	CLA	CAA-CBA-CGA-O2A
32	m	103	LMT	C4'-C5'-C6'-O6'
23	b	616	CLA	C4-C3-C5-C6
26	B	620	SQD	C29-C30-C31-C32
23	a	406	CLA	C15-C16-C17-C18
33	D	415	LMG	C18-C19-C20-C21
33	C	520	LMG	C11-C12-C13-C14
33	m	101	LMG	C11-C12-C13-C14
35	c	518	DGD	C2G-C3G-O3G-C1D
35	C	519	DGD	CAA-CBA-CCA-CDA
23	c	510	CLA	C15-C16-C17-C18
26	a	413	SQD	C26-C27-C28-C29
29	a	416	PL9	C45-C44-C46-C47
26	A	410	SQD	C16-C17-C18-C19
23	A	406	CLA	C14-C13-C15-C16
37	D	410	LHG	C28-C29-C30-C31
24	a	408	PHO	C2C-C3C-CAC-CBC
23	B	602	CLA	C4B-C3B-CAB-CBB
23	D	405	CLA	C4B-C3B-CAB-CBB
23	c	513	CLA	C4B-C3B-CAB-CBB
26	A	412	SQD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C16-C17-C18-C19
26	F	101	SQD	C24-C23-O48-C46
37	L	101	LHG	C23-C24-C25-C26
23	b	601	CLA	C4-C3-C5-C6
33	B	621	LMG	C14-C15-C16-C17
29	d	405	PL9	C43-C44-C46-C47
35	c	519	DGD	O6D-C5D-C6D-O5D
34	B	626	HTG	C2'-C3'-C4'-C5'
37	D	411	LHG	O10-C23-O8-C6
23	B	608	CLA	C16-C17-C18-C19
33	B	621	LMG	O6-C5-C6-O5
23	a	406	CLA	C4C-C3C-CAC-CBC
23	C	514	CLA	C11-C12-C13-C15
37	D	411	LHG	C24-C23-O8-C6
32	E	102	LMT	C6-C7-C8-C9
23	B	606	CLA	C16-C17-C18-C20
32	A	359	LMT	C7-C8-C9-C10
23	C	509	CLA	C5-C6-C7-C8
33	d	412	LMG	C38-C39-C40-C41
23	b	616	CLA	C2-C3-C5-C6
23	c	511	CLA	C2-C3-C5-C6
33	B	621	LMG	C37-C38-C39-C40
26	a	411	SQD	C11-C12-C13-C14
23	b	613	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
33	a	419	LMG	O8-C28-C29-C30
23	b	612	CLA	C10-C11-C12-C13
23	C	511	CLA	C13-C15-C16-C17
37	d	711	LHG	C1-C2-C3-O3
32	b	621	LMT	C7-C8-C9-C10
35	C	519	DGD	C8B-C9B-CAB-CBB
23	c	512	CLA	C3-C5-C6-C7
23	C	510	CLA	C6-C7-C8-C9
23	C	513	CLA	C6-C7-C8-C9
23	a	407	CLA	C14-C13-C15-C16
23	c	505	CLA	C14-C13-C15-C16
33	B	621	LMG	C20-C21-C22-C23
27	B	901	GOL	C1-C2-C3-O3
23	C	511	CLA	C8-C10-C11-C12
33	C	521	LMG	C4-C5-C6-O5
33	z	101	LMG	O7-C10-C11-C12
35	c	517	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
26	B	620	SQD	C33-C34-C35-C36
37	E	101	LHG	C12-C13-C14-C15
26	a	411	SQD	C10-C11-C12-C13
23	b	608	CLA	C13-C15-C16-C17
37	d	407	LHG	C9-C10-C11-C12
23	C	502	CLA	C1A-C2A-CAA-CBA
23	a	407	CLA	C1A-C2A-CAA-CBA
23	c	514	CLA	C1A-C2A-CAA-CBA
23	b	608	CLA	C16-C17-C18-C20
35	C	519	DGD	C8A-C9A-CAA-CBA
26	F	101	SQD	O10-C23-O48-C46
24	A	353	PHO	C2C-C3C-CAC-CBC
23	B	602	CLA	C2B-C3B-CAB-CBB
23	D	405	CLA	C2B-C3B-CAB-CBB
23	c	502	CLA	C2B-C3B-CAB-CBB
23	c	503	CLA	C2B-C3B-CAB-CBB
23	c	513	CLA	C2B-C3B-CAB-CBB
25	B	617	BCR	C1-C6-C7-C8
25	D	407	BCR	C23-C24-C25-C26
25	b	617	BCR	C5-C6-C7-C8
33	d	412	LMG	C19-C20-C21-C22
37	D	410	LHG	C17-C18-C19-C20
23	A	406	CLA	C16-C17-C18-C19
23	C	510	CLA	C3-C5-C6-C7
23	b	601	CLA	C3-C5-C6-C7
32	t	101	LMT	C2-C3-C4-C5
23	b	601	CLA	C2-C3-C5-C6
23	b	613	CLA	O1D-CGD-O2D-CED
38	e	87	HEM	CAD-CBD-CGD-O1D
33	c	521	LMG	C31-C32-C33-C34
37	D	409	LHG	C29-C30-C31-C32
23	B	601	CLA	C11-C12-C13-C15
23	B	613	CLA	C11-C12-C13-C15
23	B	613	CLA	C12-C13-C15-C16
23	C	507	CLA	C12-C13-C15-C16
23	b	615	CLA	C11-C12-C13-C15
37	l	101	LHG	C10-C11-C12-C13
23	C	502	CLA	C2A-CAA-CBA-CGA
33	C	501	LMG	O7-C8-C9-O8
33	c	521	LMG	O1-C7-C8-O7
35	H	102	DGD	O1G-C1G-C2G-O2G
38	E	103	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
35	H	102	DGD	C4E-C5E-C6E-O5E
29	A	414	PL9	C4-C3-C7-C8
35	c	517	DGD	CBA-CCA-CDA-CEA
33	B	621	LMG	C36-C37-C38-C39
25	K	102	BCR	C7-C8-C9-C34
35	C	519	DGD	CDA-CEA-CFA-CGA
29	D	408	PL9	C35-C34-C36-C37
23	b	609	CLA	C2-C3-C5-C6
23	C	502	CLA	CBD-CGD-O2D-CED
23	b	612	CLA	C8-C10-C11-C12
40	V	202	HEC	CAD-CBD-CGD-O2D
37	L	101	LHG	C10-C11-C12-C13
32	A	359	LMT	C9-C10-C11-C12
23	B	606	CLA	C11-C10-C8-C9
33	z	101	LMG	C13-C14-C15-C16
26	b	620	SQD	C30-C31-C32-C33
40	V	202	HEC	CAD-CBD-CGD-O1D
26	a	413	SQD	C15-C16-C17-C18
35	c	519	DGD	C9B-CAB-CBB-CCB
23	b	616	CLA	C5-C6-C7-C8
37	e	101	LHG	C24-C25-C26-C27
29	A	414	PL9	C25-C24-C26-C27
35	c	519	DGD	CDB-CEB-CFB-CGB
35	h	102	DGD	CCA-CDA-CEA-CFA
40	v	202	HEC	CAD-CBD-CGD-O2D
32	e	102	LMT	C2B-C1B-O1B-C4'
35	H	102	DGD	O1G-C1G-C2G-C3G
38	E	103	HEM	CAD-CBD-CGD-O2D
38	e	87	HEM	CAA-CBA-CGA-O2A
23	C	508	CLA	C2A-CAA-CBA-CGA
37	D	409	LHG	O1-C1-C2-O2
37	d	711	LHG	C27-C28-C29-C30
37	d	711	LHG	C17-C18-C19-C20
23	B	611	CLA	C8-C10-C11-C12
23	a	409	CLA	C4B-C3B-CAB-CBB
23	c	509	CLA	C4B-C3B-CAB-CBB
37	d	407	LHG	C25-C26-C27-C28
24	a	408	PHO	CHA-CBD-CGD-O1D
33	B	621	LMG	O1-C7-C8-O7
35	H	102	DGD	C8A-C9A-CAA-CBA
26	A	412	SQD	C15-C16-C17-C18
37	d	711	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
37	D	409	LHG	C17-C18-C19-C20
38	e	87	HEM	CAD-CBD-CGD-O2D
25	K	102	BCR	C7-C8-C9-C10
23	a	407	CLA	C11-C12-C13-C14
35	c	517	DGD	CDB-CEB-CFB-CGB
23	b	603	CLA	C2A-CAA-CBA-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	C	512	CLA	O1A-CGA-O2A-C1
33	C	520	LMG	C29-C30-C31-C32
40	v	202	HEC	CAD-CBD-CGD-O1D
23	C	507	CLA	C2-C3-C5-C6
38	E	103	HEM	C2B-C3B-CAB-CBB
38	e	87	HEM	C2C-C3C-CAC-CBC
23	b	607	CLA	C8-C10-C11-C12
35	h	102	DGD	O2G-C1B-C2B-C3B
24	a	408	PHO	O2A-C1-C2-C3
37	l	101	LHG	C25-C26-C27-C28
38	e	87	HEM	CAA-CBA-CGA-O1A
32	M	101	LMT	C2-C3-C4-C5
32	M	101	LMT	O5'-C1'-O1'-C1
33	B	621	LMG	O1-C7-C8-C9
23	b	612	CLA	C13-C15-C16-C17
38	E	103	HEM	C4B-C3B-CAB-CBB
33	C	521	LMG	C10-C11-C12-C13
23	c	503	CLA	C16-C17-C18-C19
26	B	620	SQD	C24-C25-C26-C27
37	L	101	LHG	C11-C12-C13-C14
23	b	614	CLA	C14-C13-C15-C16
23	b	610	CLA	C16-C17-C18-C20
23	a	405	CLA	C2C-C3C-CAC-CBC
37	D	409	LHG	O8-C23-C24-C25
23	A	404	CLA	C2C-C3C-CAC-CBC
33	C	501	LMG	C29-C30-C31-C32
35	c	519	DGD	CDA-CEA-CFA-CGA
23	b	609	CLA	C4-C3-C5-C6
33	Z	101	LMG	O7-C10-C11-C12
35	c	518	DGD	C1A-C2A-C3A-C4A
23	c	504	CLA	C2A-CAA-CBA-CGA
23	B	606	CLA	C11-C10-C8-C7
23	B	616	CLA	C11-C12-C13-C15
23	a	407	CLA	C11-C12-C13-C15
23	b	608	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	c	505	CLA	C12-C13-C15-C16
23	c	509	CLA	C12-C13-C15-C16
23	C	503	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
25	B	617	BCR	C5-C6-C7-C8
25	b	619	BCR	C1-C6-C7-C8
25	c	515	BCR	C23-C24-C25-C26
25	c	515	BCR	C23-C24-C25-C30
25	d	404	BCR	C23-C24-C25-C26
25	d	404	BCR	C23-C24-C25-C30
25	h	101	BCR	C23-C24-C25-C30
23	b	613	CLA	CAA-CBA-CGA-O2A
37	e	101	LHG	O8-C23-C24-C25
23	C	507	CLA	C2-C1-O2A-CGA
23	C	514	CLA	C2-C1-O2A-CGA
23	b	610	CLA	C16-C17-C18-C19
33	m	101	LMG	O6-C1-O1-C7
33	c	520	LMG	O7-C10-C11-C12
24	a	408	PHO	C2-C3-C5-C6
23	c	511	CLA	O1A-CGA-O2A-C1
33	B	621	LMG	C30-C31-C32-C33
34	B	622	HTG	C2'-C1'-S1-C1
23	B	612	CLA	CBA-CGA-O2A-C1
37	L	101	LHG	O7-C7-C8-C9
37	l	101	LHG	O7-C7-C8-C9
23	C	503	CLA	C3-C5-C6-C7
23	b	602	CLA	C10-C11-C12-C13
23	B	613	CLA	CAA-CBA-CGA-O2A
23	D	406	CLA	O1A-CGA-O2A-C1
23	b	608	CLA	C16-C17-C18-C19
24	a	408	PHO	C4-C3-C5-C6
23	c	514	CLA	C2-C3-C5-C6
35	C	519	DGD	C9A-CAA-CBA-CCA
32	e	102	LMT	C2-C3-C4-C5
33	a	419	LMG	C14-C15-C16-C17
32	D	404	LMT	C7-C8-C9-C10
37	d	711	LHG	C30-C31-C32-C33
23	B	601	CLA	C11-C12-C13-C14
23	B	614	CLA	C6-C7-C8-C9
23	B	614	CLA	C11-C10-C8-C9
23	D	406	CLA	C6-C7-C8-C9
26	A	412	SQD	O48-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
26	F	101	SQD	C44-C45-C46-O48
24	a	353	PHO	C2C-C3C-CAC-CBC
23	D	406	CLA	C8-C10-C11-C12
23	B	610	CLA	C4B-C3B-CAB-CBB
33	C	501	LMG	C31-C32-C33-C34
23	b	604	CLA	C10-C11-C12-C13
32	a	420	LMT	O5'-C1'-O1'-C1
23	C	513	CLA	CAA-CBA-CGA-O2A
25	y	101	BCR	C21-C22-C23-C24
25	a	410	BCR	C19-C20-C21-C22
23	c	510	CLA	C13-C15-C16-C17
23	b	616	CLA	O1A-CGA-O2A-C1
23	C	507	CLA	C16-C17-C18-C19
23	C	511	CLA	CAA-CBA-CGA-O2A
32	t	102	LMT	C11-C10-C9-C8
33	c	520	LMG	C32-C33-C34-C35
23	B	612	CLA	O1A-CGA-O2A-C1
23	c	511	CLA	CAA-CBA-CGA-O2A
23	B	615	CLA	C8-C10-C11-C12
32	a	420	LMT	C7-C8-C9-C10
34	B	623	HTG	C4'-C5'-C6'-C7'
23	a	405	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2-C1-O2A-CGA
33	C	521	LMG	C11-C12-C13-C14
23	C	506	CLA	C12-C13-C15-C16
23	C	508	CLA	C11-C12-C13-C15
23	b	603	CLA	C11-C10-C8-C7
23	c	504	CLA	C6-C7-C8-C10
23	C	508	CLA	C10-C11-C12-C13
23	a	405	CLA	C4C-C3C-CAC-CBC
33	m	101	LMG	C30-C31-C32-C33
35	C	517	DGD	C3A-C4A-C5A-C6A
32	m	103	LMT	C4-C5-C6-C7
23	B	612	CLA	CAA-CBA-CGA-O2A
33	c	521	LMG	C34-C35-C36-C37
23	B	602	CLA	C2A-CAA-CBA-CGA
23	B	603	CLA	C2A-CAA-CBA-CGA
37	D	409	LHG	C18-C19-C20-C21
37	d	408	LHG	C30-C31-C32-C33
29	d	405	PL9	C34-C36-C37-C38
23	B	604	CLA	C5-C6-C7-C8
23	b	604	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	b	602	CLA	O1A-CGA-O2A-C1
37	E	101	LHG	O7-C7-C8-C9
37	l	101	LHG	O9-C7-C8-C9
23	A	404	CLA	C4C-C3C-CAC-CBC
37	d	408	LHG	O10-C23-O8-C6
34	B	622	HTG	C3'-C4'-C5'-C6'
23	b	616	CLA	CBA-CGA-O2A-C1
23	B	616	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C9
23	c	506	CLA	C14-C13-C15-C16
33	Z	101	LMG	O9-C10-C11-C12
25	h	101	BCR	C9-C10-C11-C12
37	L	101	LHG	O9-C7-C8-C9
35	c	519	DGD	C2A-C3A-C4A-C5A
26	f	102	SQD	O5-C5-C6-S
23	B	612	CLA	CAA-CBA-CGA-O1A
27	a	801	GOL	O2-C2-C3-O3
27	d	801	GOL	O1-C1-C2-O2
37	D	409	LHG	C30-C31-C32-C33
23	b	612	CLA	CAA-CBA-CGA-O2A
35	C	519	DGD	O1G-C1A-C2A-C3A
23	B	613	CLA	CAA-CBA-CGA-O1A
23	C	513	CLA	CAA-CBA-CGA-O1A
26	A	412	SQD	O10-C23-C24-C25
33	c	520	LMG	O9-C10-C11-C12
37	D	409	LHG	O10-C23-C24-C25
37	e	101	LHG	O10-C23-C24-C25
37	D	411	LHG	C28-C29-C30-C31
33	C	521	LMG	C8-C7-O1-C1
35	C	517	DGD	C5D-C6D-O5D-C1E
35	C	518	DGD	C5D-C6D-O5D-C1E
35	c	517	DGD	C5D-C6D-O5D-C1E
32	A	359	LMT	C2B-C1B-O1B-C4'
37	E	101	LHG	C11-C10-C9-C8
32	t	101	LMT	C6-C7-C8-C9
23	b	613	CLA	CAA-CBA-CGA-O1A
35	C	518	DGD	O2G-C1B-C2B-C3B
23	c	502	CLA	C2A-CAA-CBA-CGA
35	C	517	DGD	CBA-CCA-CDA-CEA
29	d	405	PL9	C11-C12-C13-C14
35	c	518	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
38	e	87	HEM	C2B-C3B-CAB-CBB
33	d	412	LMG	C28-C29-C30-C31
23	B	607	CLA	CAD-CBD-CGD-O2D
23	B	609	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	C	505	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
24	a	408	PHO	CAD-CBD-CGD-O2D
37	L	101	LHG	C32-C33-C34-C35
26	b	620	SQD	C10-C11-C12-C13
23	A	408	CLA	C2-C1-O2A-CGA
23	B	608	CLA	C2-C1-O2A-CGA
23	C	511	CLA	CAA-CBA-CGA-O1A
37	E	101	LHG	O8-C23-C24-C25
37	l	101	LHG	C17-C18-C19-C20
33	c	521	LMG	C28-C29-C30-C31
37	D	411	LHG	O8-C23-C24-C25
37	E	101	LHG	O9-C7-C8-C9
23	c	513	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

143 monomers are involved in 261 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	513	CLA	4	0
23	b	613	CLA	2	0
29	D	408	PL9	1	0
23	C	502	CLA	5	0
23	A	406	CLA	1	0
23	b	612	CLA	1	0
35	H	102	DGD	1	0
25	C	516	BCR	1	0
34	B	622	HTG	1	0
23	c	507	CLA	2	0
34	D	414	HTG	1	0
23	C	513	CLA	2	0
23	C	510	CLA	1	0
32	D	404	LMT	1	0
23	c	514	CLA	1	0
23	b	601	CLA	1	0
23	b	603	CLA	1	0
32	I	101	LMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	O	501	GOL	1	0
27	a	801	GOL	4	0
37	d	408	LHG	11	0
27	D	701	GOL	1	0
25	B	617	BCR	2	0
25	B	618	BCR	2	0
23	B	604	CLA	1	0
27	A	701	GOL	3	0
23	C	514	CLA	2	0
25	B	619	BCR	2	0
23	A	408	CLA	3	0
23	c	511	CLA	1	0
34	b	622	HTG	1	0
26	b	620	SQD	3	0
23	C	509	CLA	3	0
29	a	416	PL9	4	0
33	Z	101	LMG	2	0
23	B	614	CLA	3	0
23	B	602	CLA	1	0
25	D	407	BCR	2	0
23	B	609	CLA	2	0
23	c	504	CLA	3	0
27	B	624	GOL	2	0
23	C	512	CLA	3	0
23	B	612	CLA	1	0
25	C	515	BCR	1	0
35	C	519	DGD	1	0
25	b	618	BCR	4	0
27	d	801	GOL	1	0
23	C	504	CLA	3	0
26	a	413	SQD	1	0
24	A	407	PHO	1	0
34	B	626	HTG	1	0
26	F	101	SQD	1	0
32	e	102	LMT	1	0
25	d	404	BCR	2	0
23	B	615	CLA	3	0
29	A	414	PL9	10	0
23	d	402	CLA	1	0
27	v	401	GOL	1	0
32	t	102	LMT	2	0
35	c	518	DGD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	d	412	LMG	2	0
23	b	602	CLA	1	0
23	C	511	CLA	3	0
24	a	353	PHO	1	0
23	b	609	CLA	5	0
25	K	102	BCR	1	0
23	a	405	CLA	2	0
35	c	517	DGD	1	0
23	C	507	CLA	3	0
23	a	407	CLA	2	0
27	a	701	GOL	1	0
33	z	101	LMG	2	0
37	D	410	LHG	2	0
23	b	615	CLA	2	0
23	A	405	CLA	1	0
35	C	518	DGD	1	0
38	E	103	HEM	1	0
33	B	621	LMG	1	0
23	B	603	CLA	1	0
23	A	404	CLA	2	0
34	b	625	HTG	1	0
25	b	619	BCR	5	0
34	B	623	HTG	1	0
23	a	406	CLA	3	0
23	c	503	CLA	2	0
25	T	101	BCR	6	0
32	M	101	LMT	2	0
23	B	601	CLA	4	0
25	h	101	BCR	3	0
23	B	606	CLA	2	0
24	A	353	PHO	2	0
32	A	359	LMT	1	0
25	b	617	BCR	1	0
34	c	522	HTG	1	0
23	C	503	CLA	2	0
23	c	505	CLA	1	0
34	d	411	HTG	1	0
32	b	621	LMT	1	0
25	H	101	BCR	2	0
25	y	101	BCR	1	0
33	c	521	LMG	1	0
35	c	519	DGD	2	0

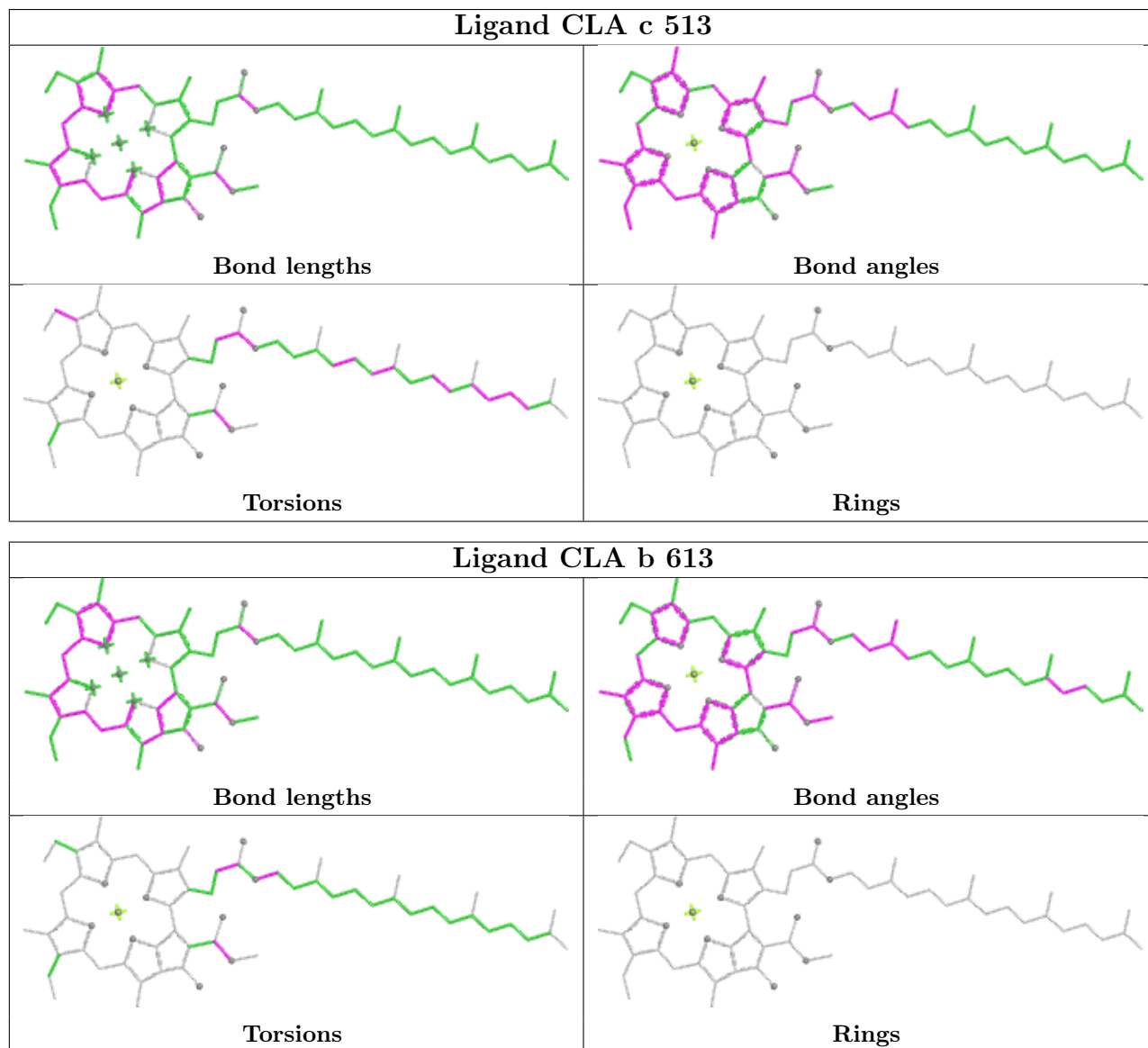
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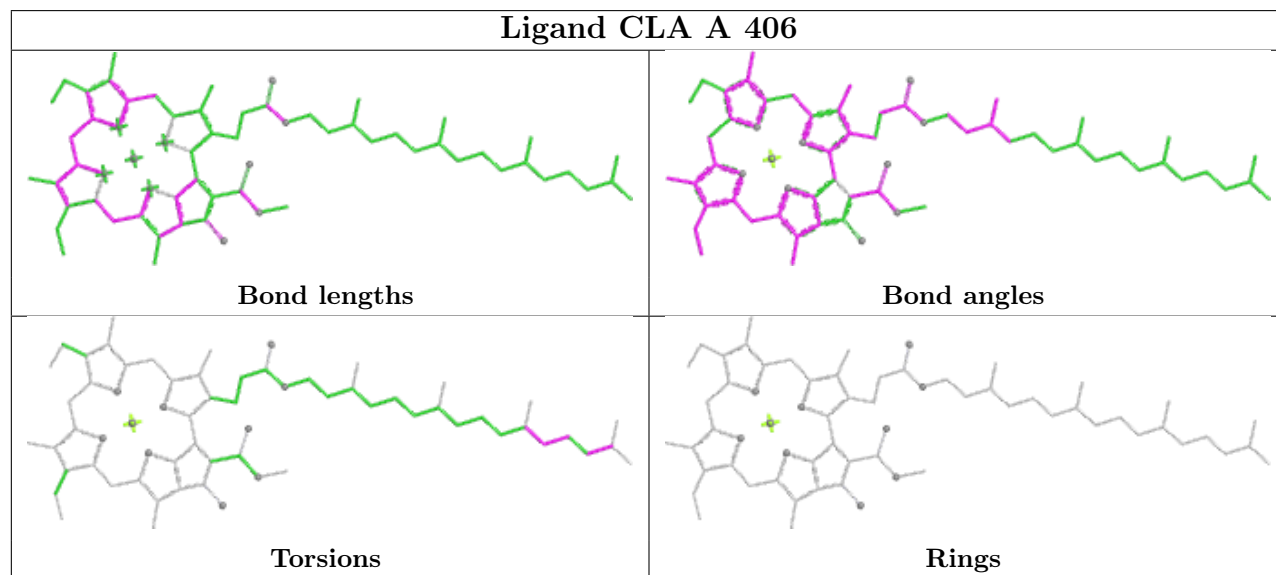
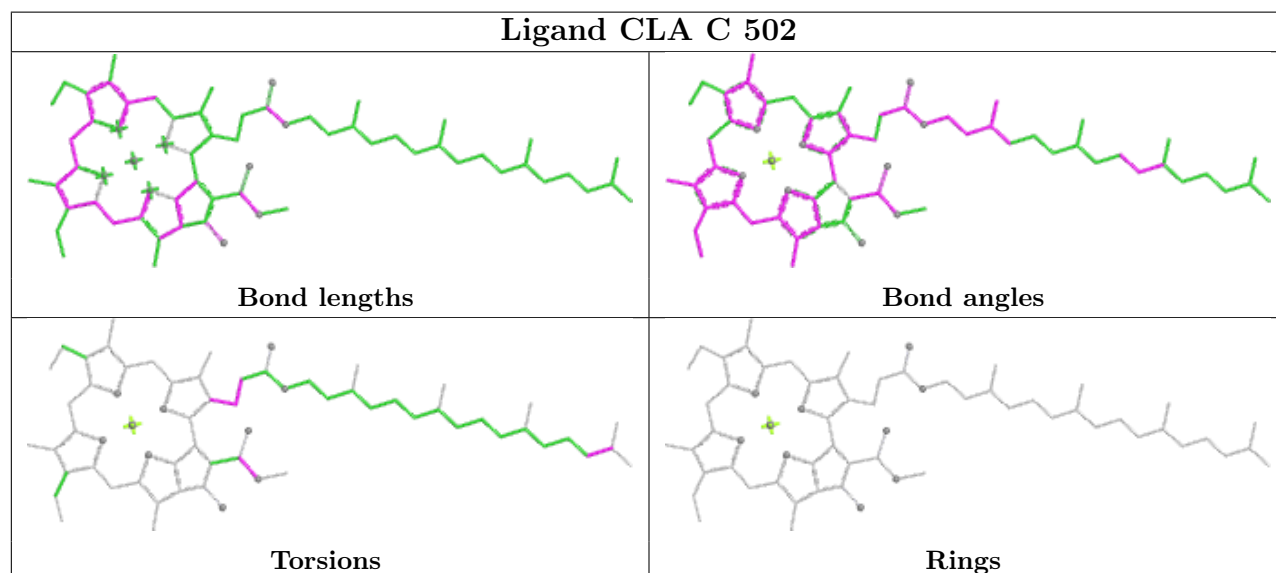
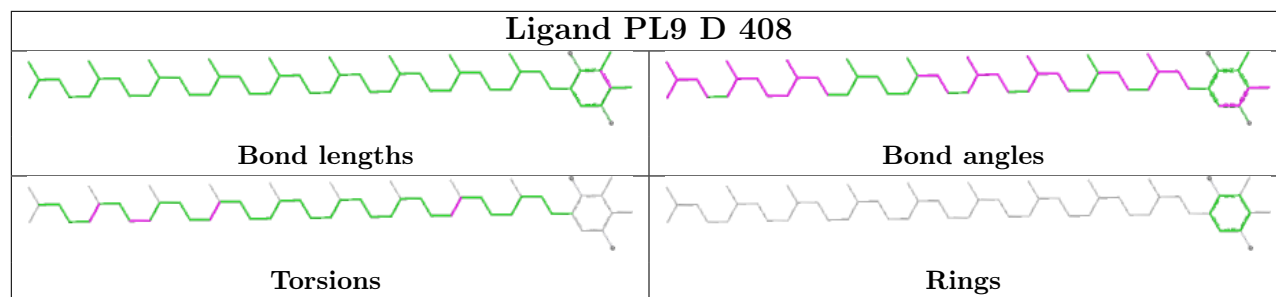
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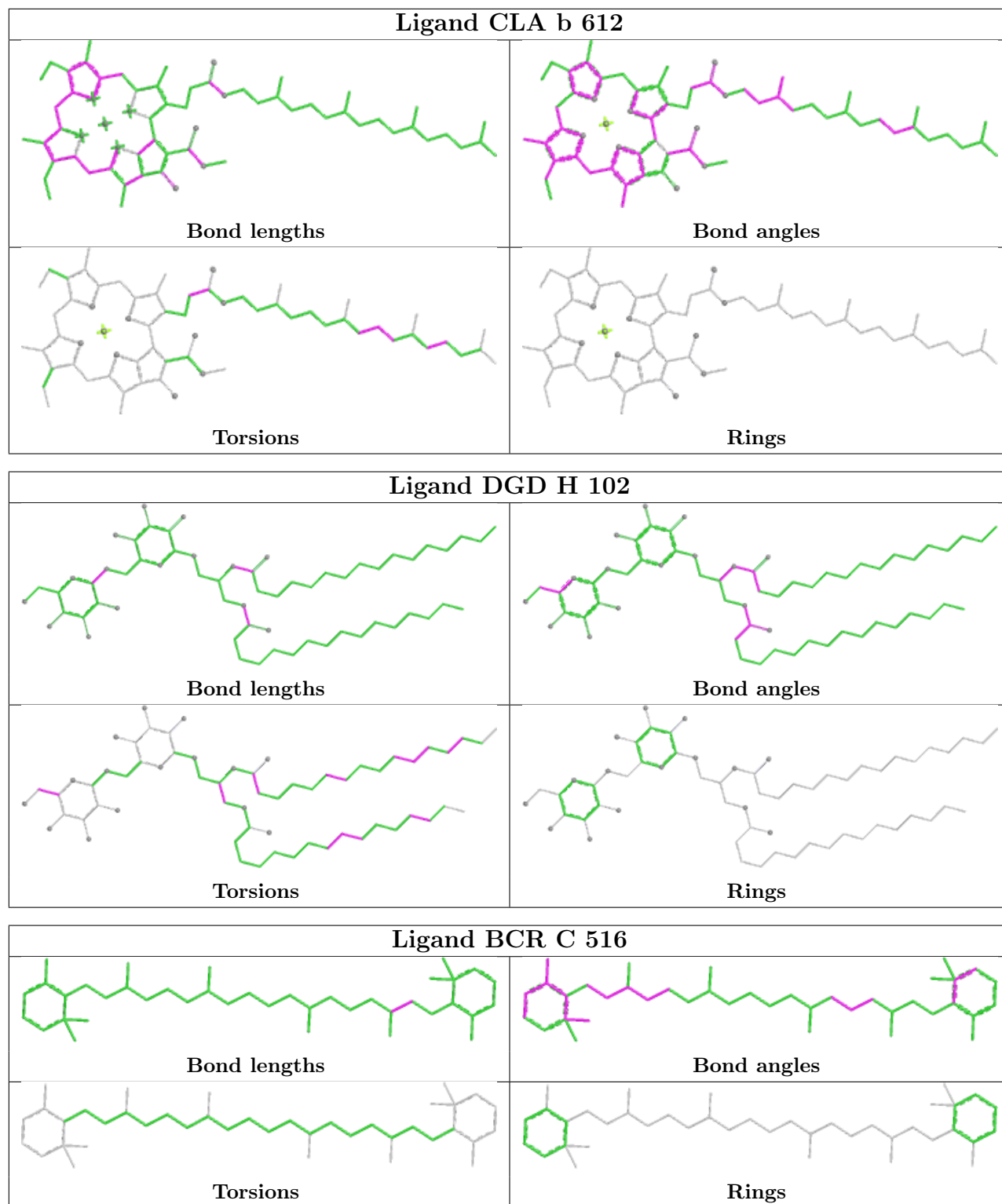
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	606	CLA	1	0
23	B	616	CLA	3	0
25	Y	101	BCR	1	0
23	c	506	CLA	5	0
37	D	411	LHG	3	0
23	b	616	CLA	1	0
23	C	505	CLA	1	0
23	c	510	CLA	2	0
26	a	411	SQD	3	0
33	C	521	LMG	3	0
23	b	614	CLA	3	0
35	C	517	DGD	1	0
23	C	506	CLA	4	0
23	d	403	CLA	3	0
32	t	101	LMT	1	0
25	a	410	BCR	1	0
23	b	605	CLA	5	0
23	c	508	CLA	2	0
23	c	512	CLA	5	0
27	O	601	GOL	2	0
25	A	409	BCR	2	0
25	t	103	BCR	4	0
37	E	101	LHG	3	0
32	a	420	LMT	2	0
27	b	901	GOL	2	0
33	c	520	LMG	1	0
23	B	613	CLA	2	0
23	c	509	CLA	2	0
23	C	508	CLA	2	0
23	b	604	CLA	5	0
23	b	607	CLA	1	0
25	c	516	BCR	3	0
25	c	515	BCR	2	0
23	c	502	CLA	2	0
37	d	407	LHG	2	0
23	B	605	CLA	4	0
37	e	101	LHG	5	0
26	B	620	SQD	1	0
26	A	410	SQD	1	0
23	D	405	CLA	3	0
23	a	409	CLA	3	0

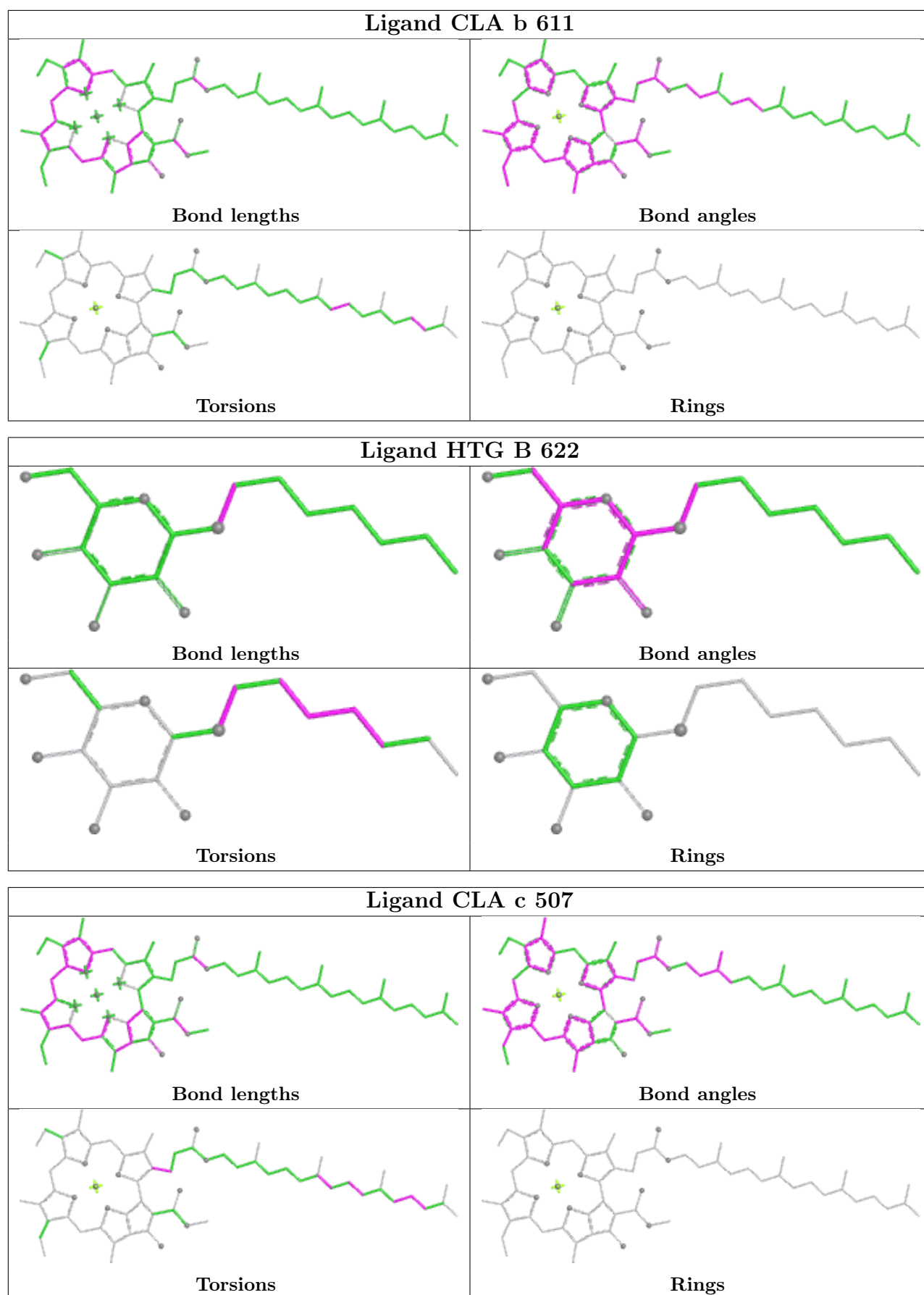
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

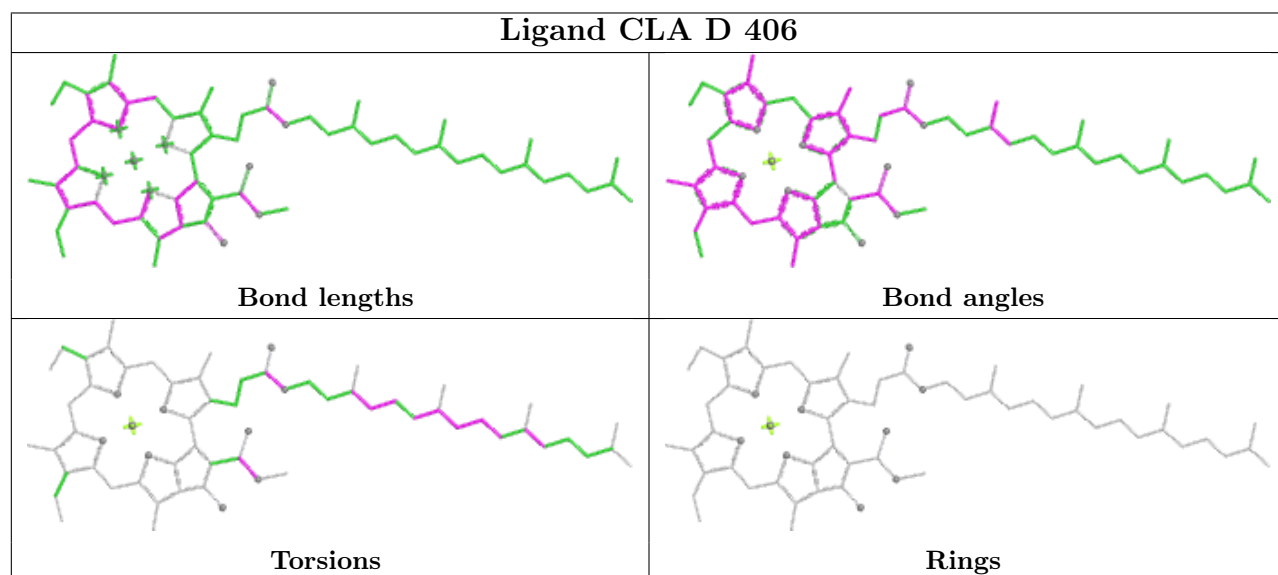
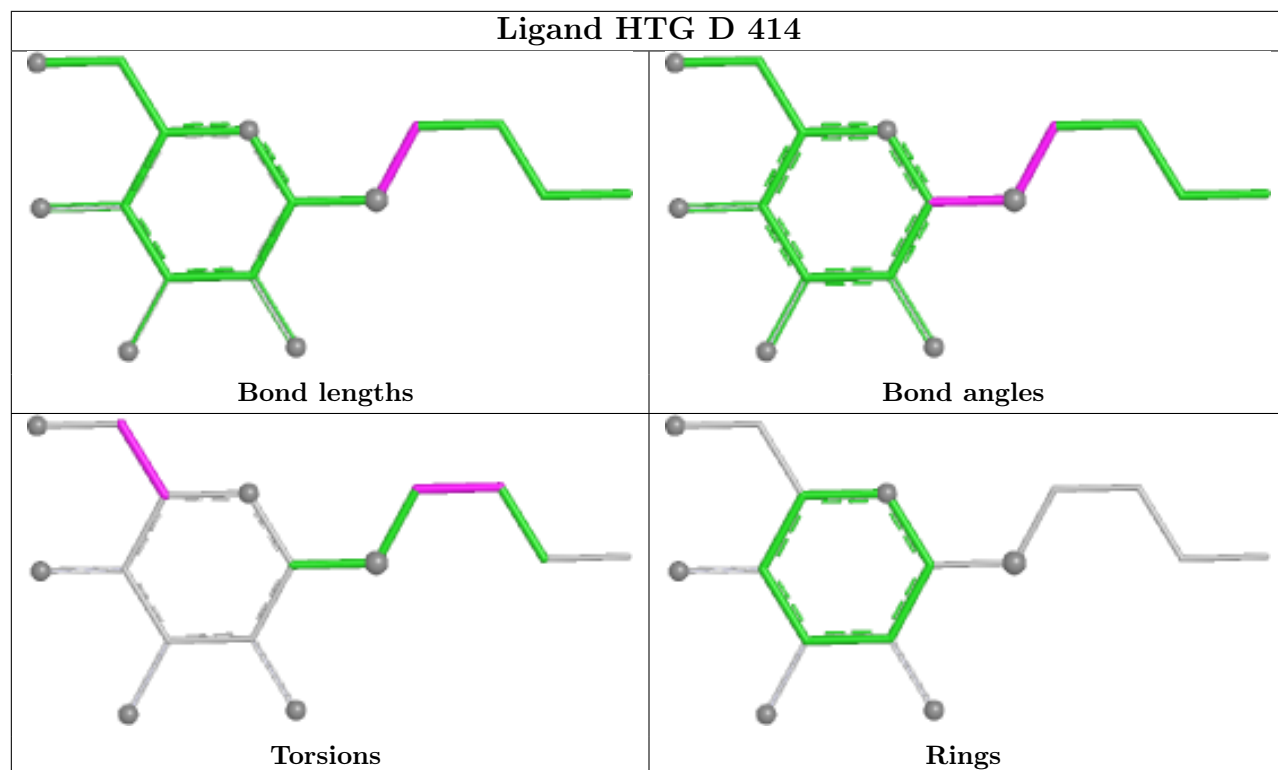
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

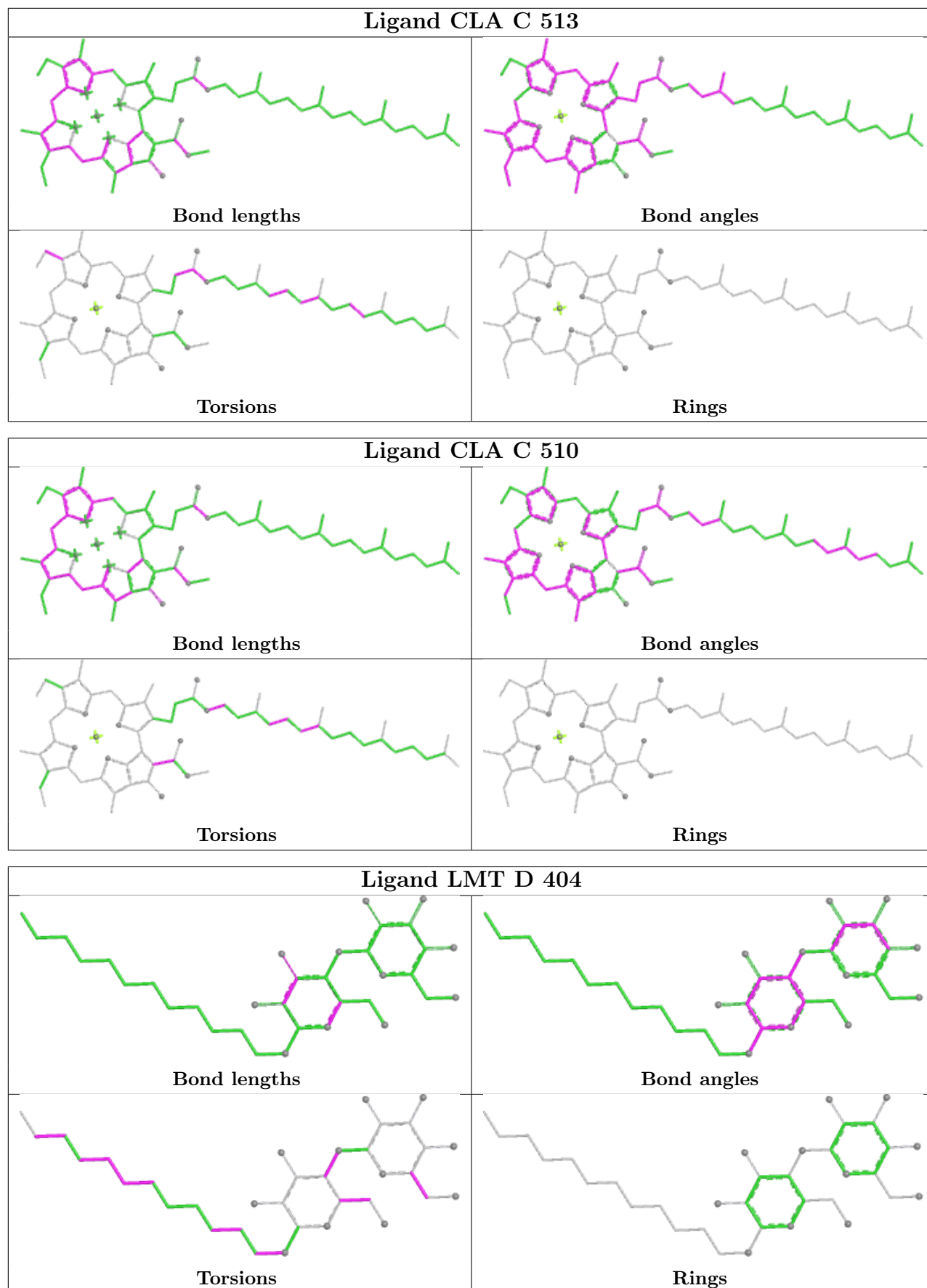


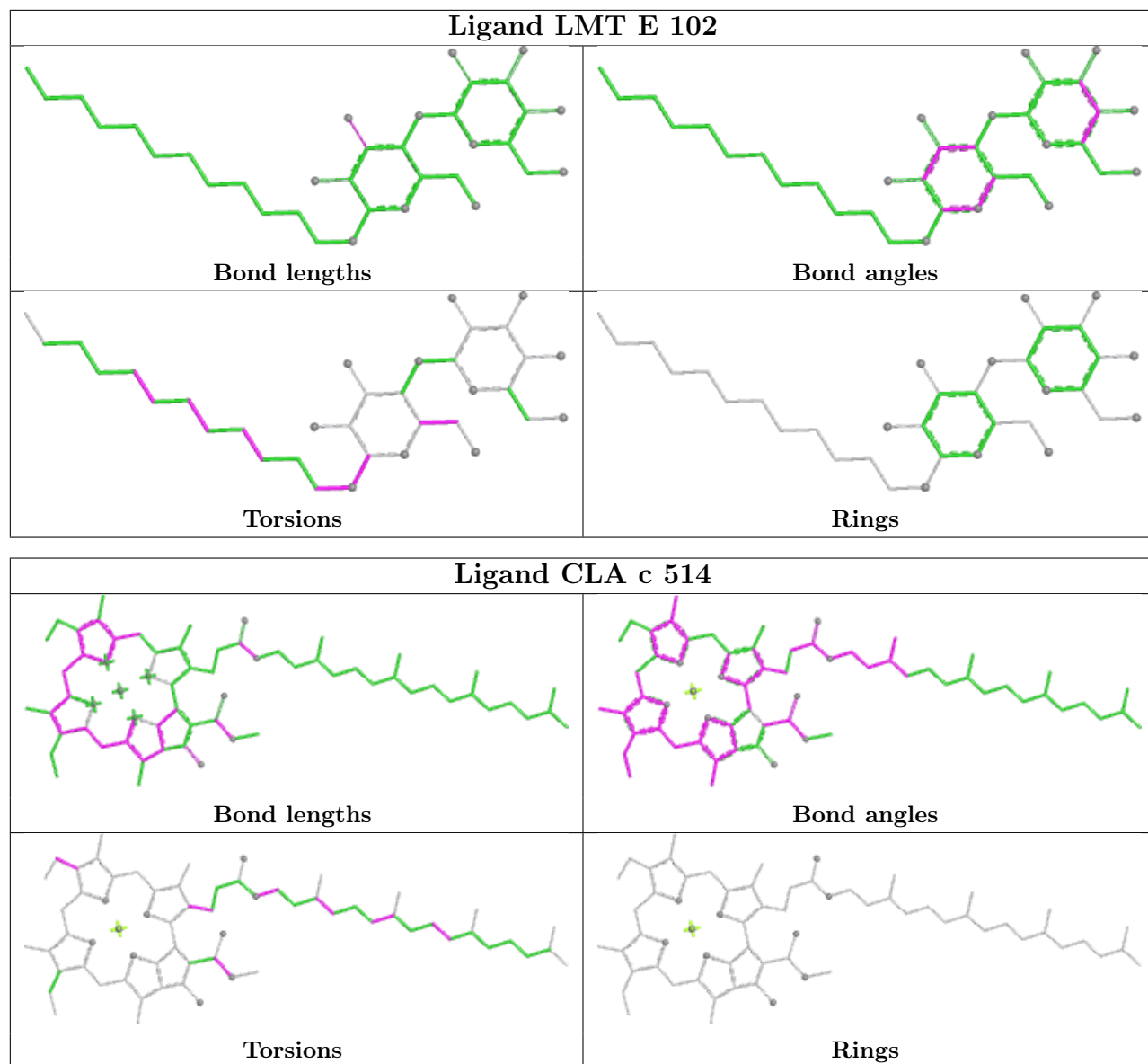


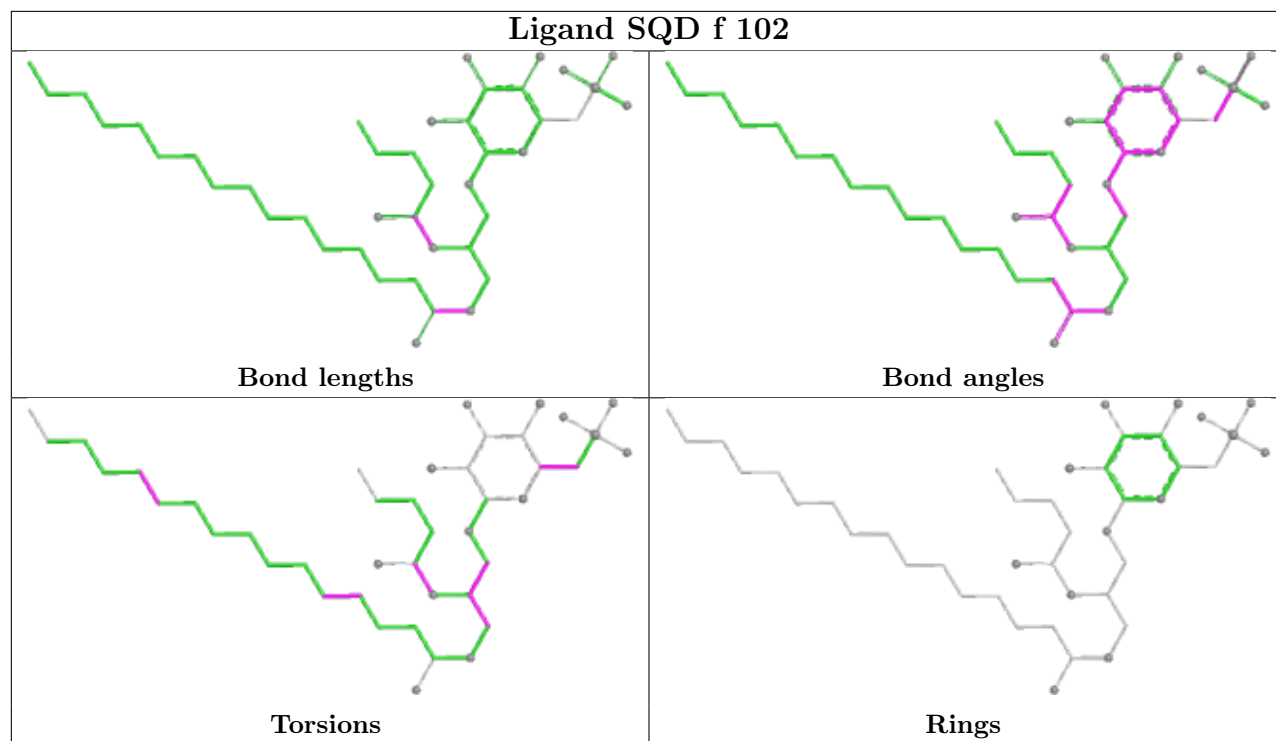


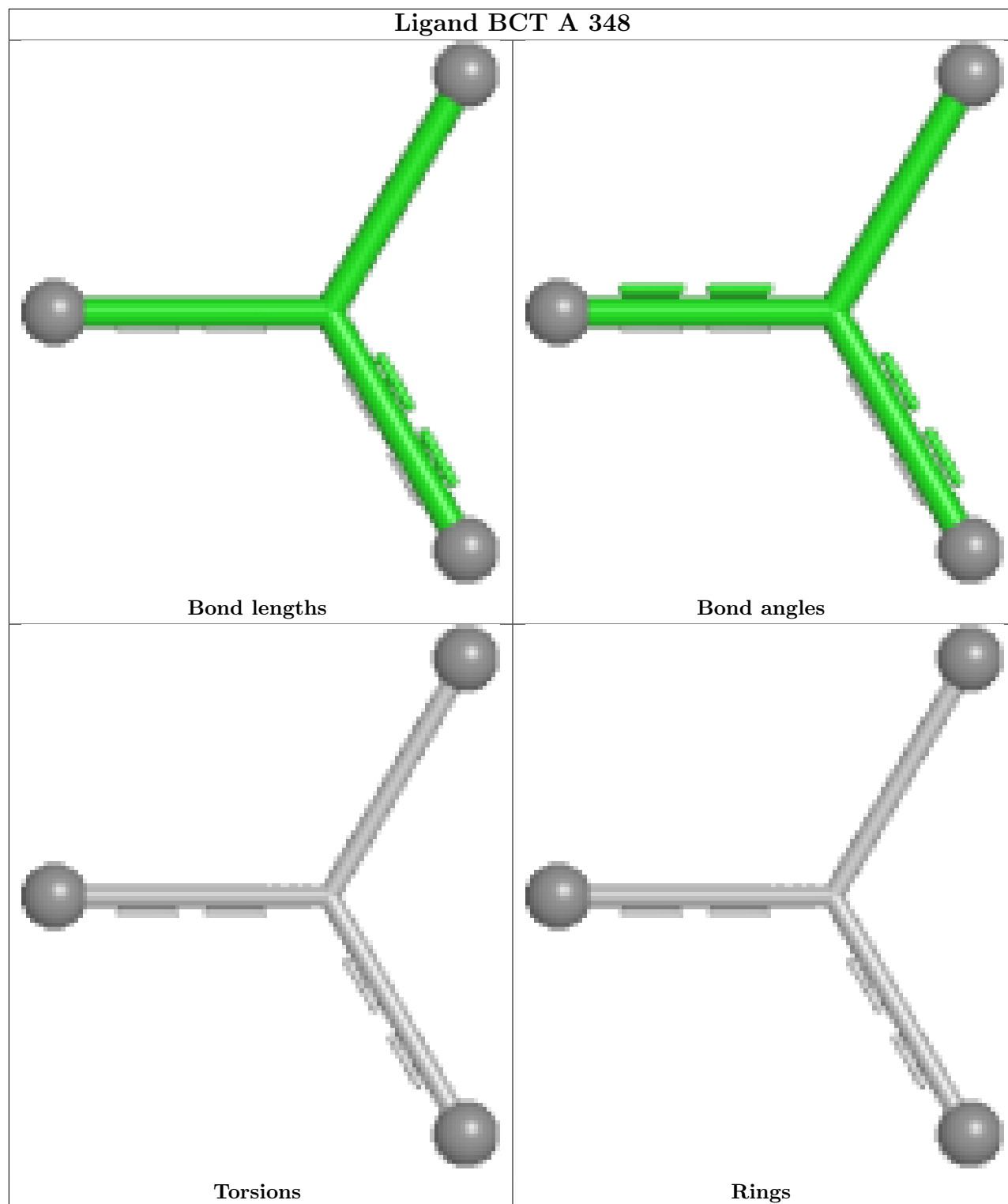


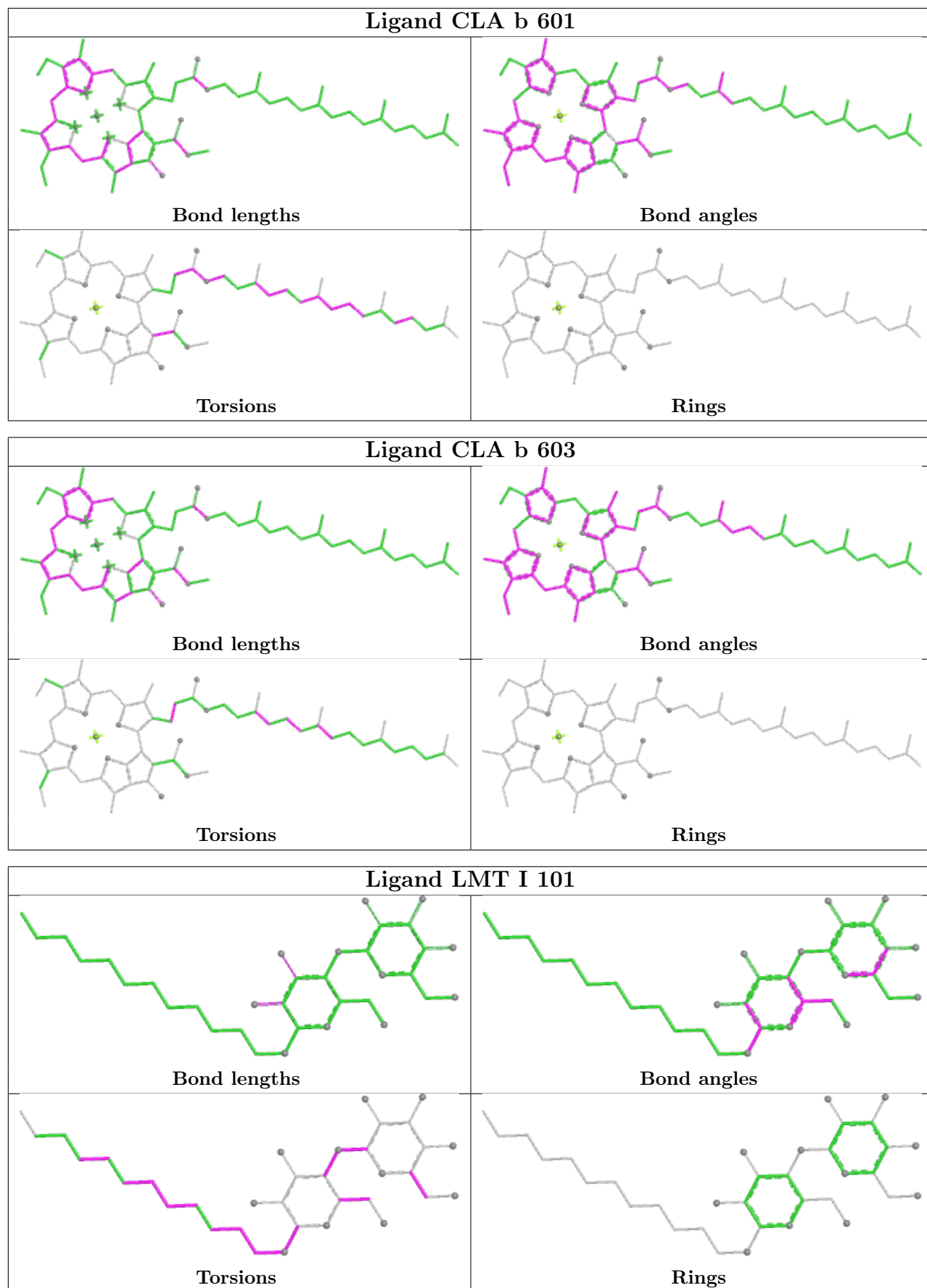


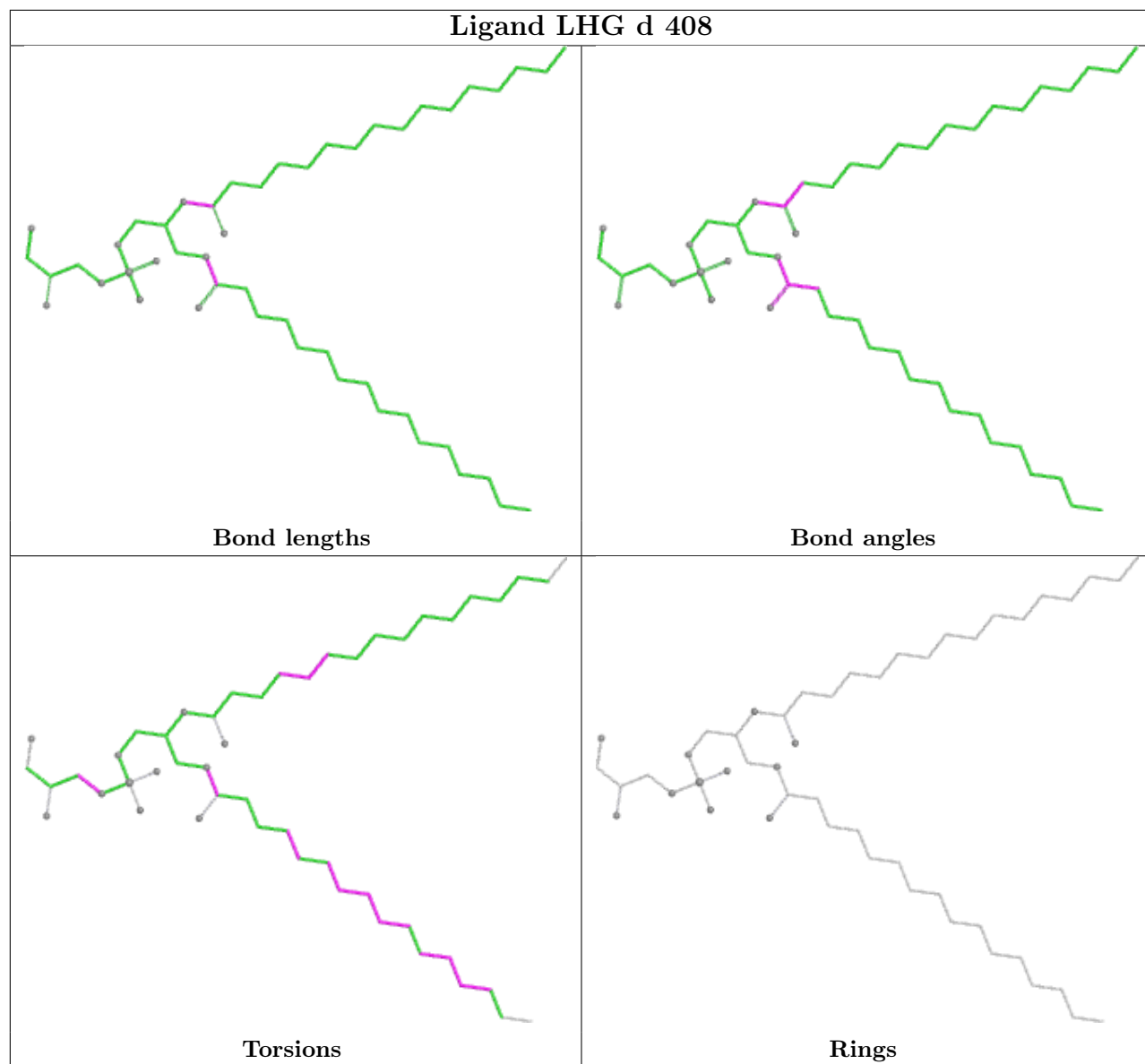


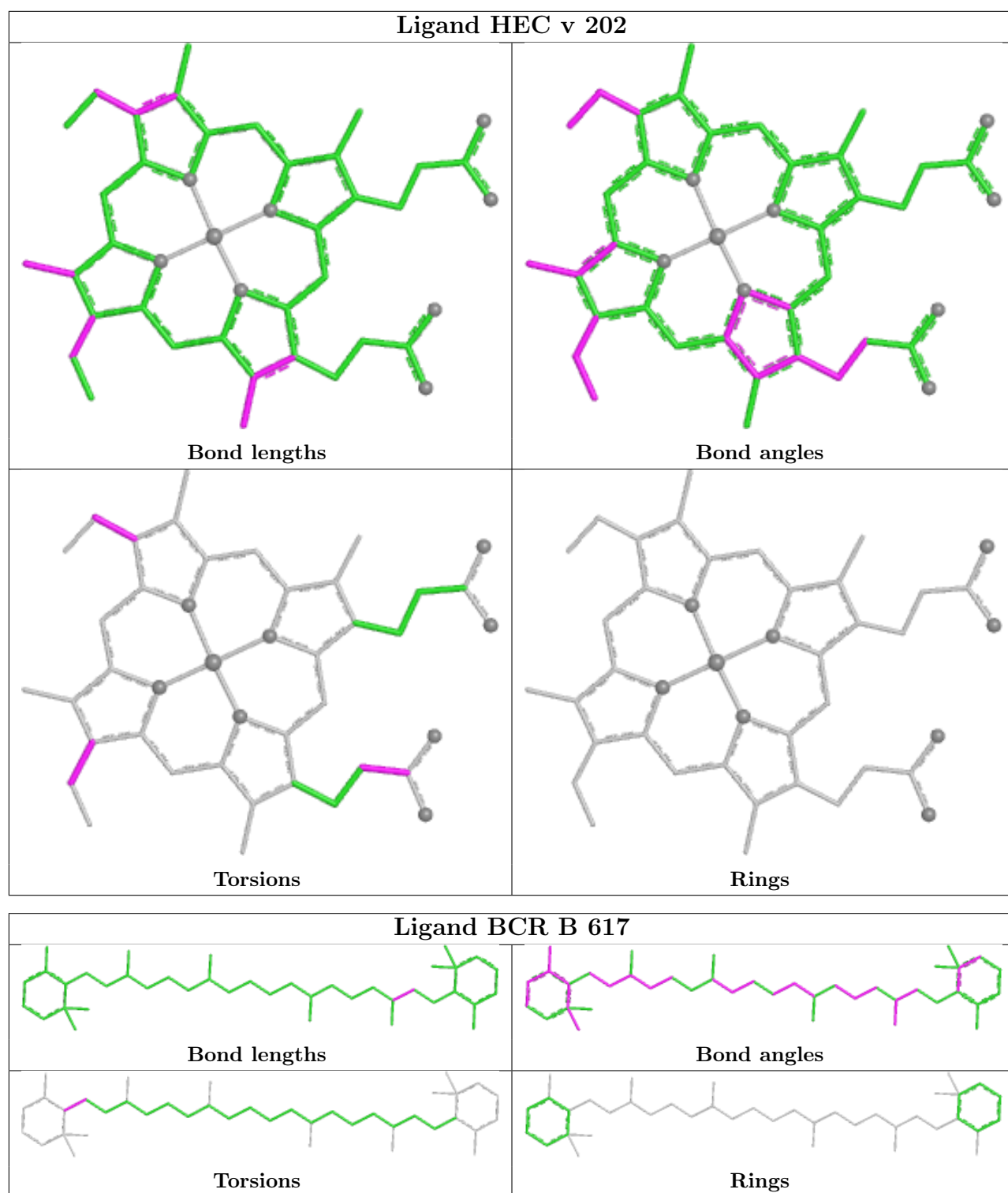


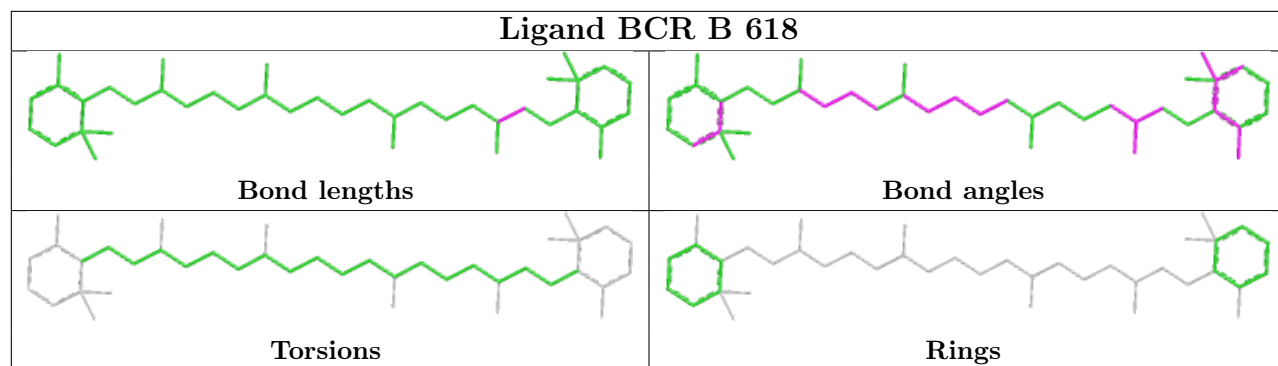


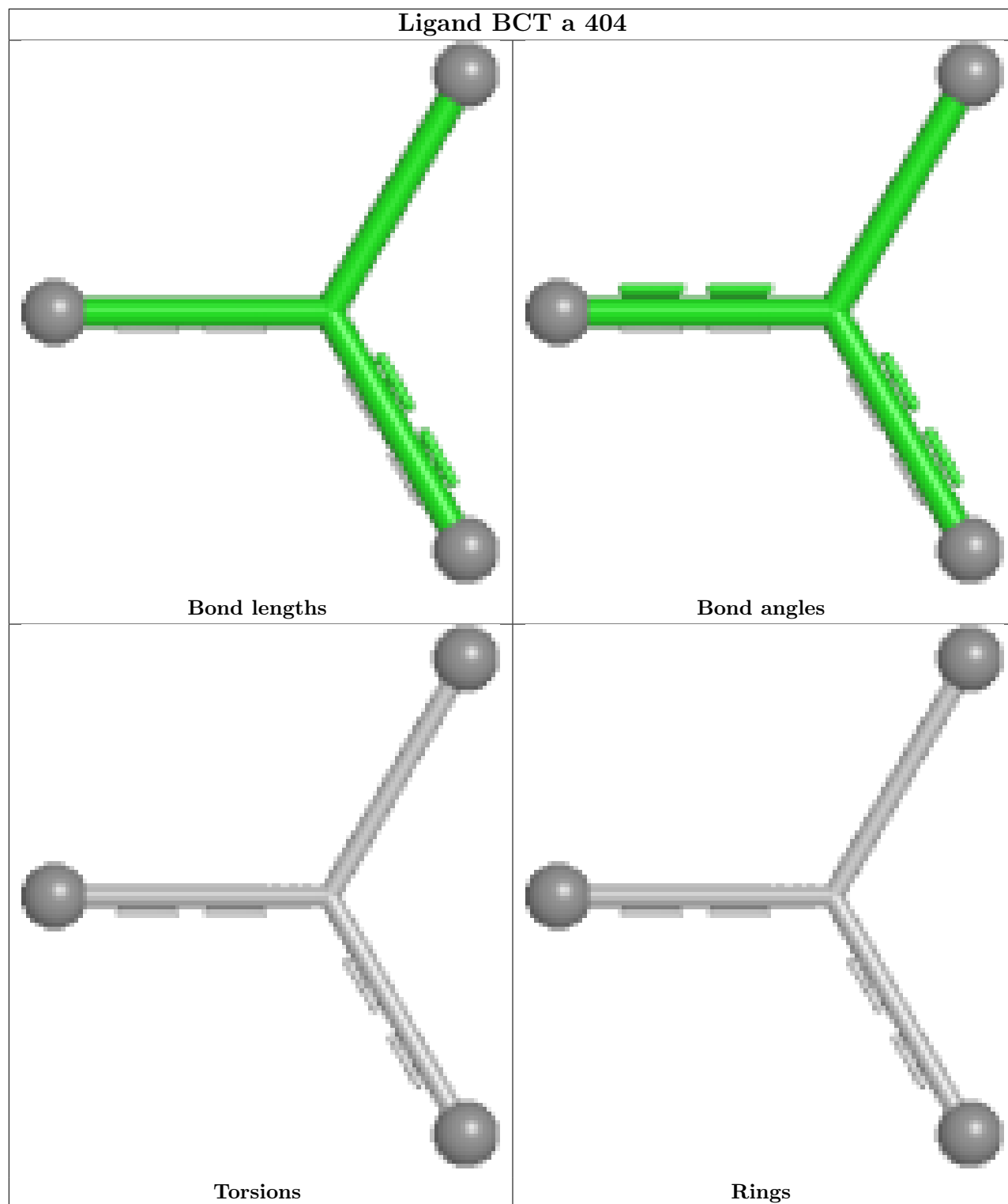


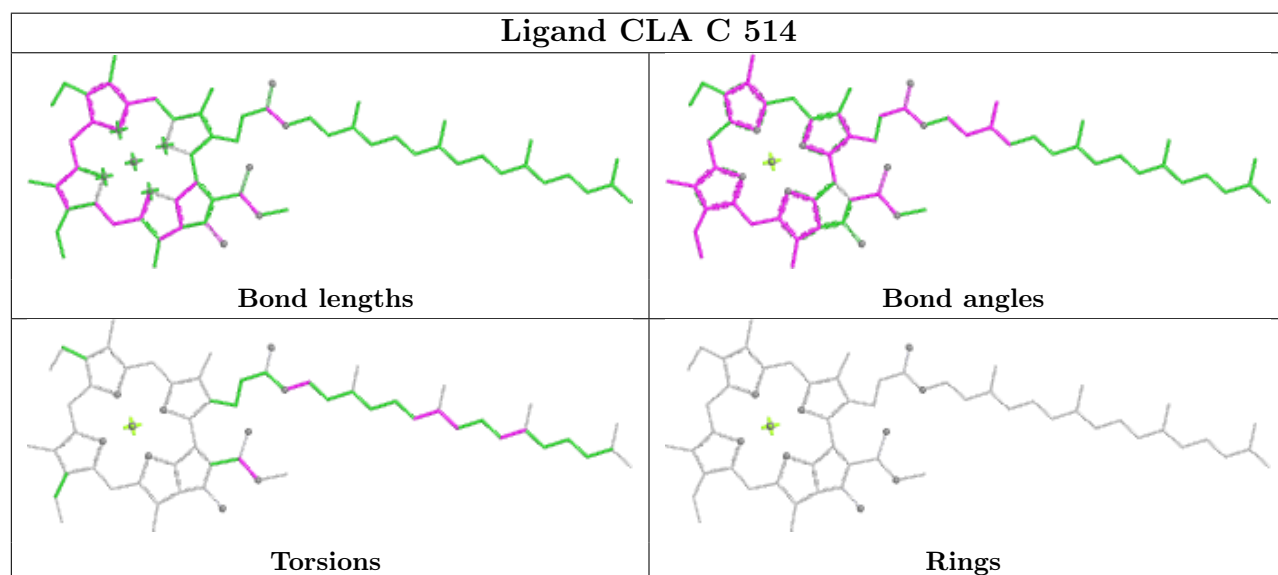
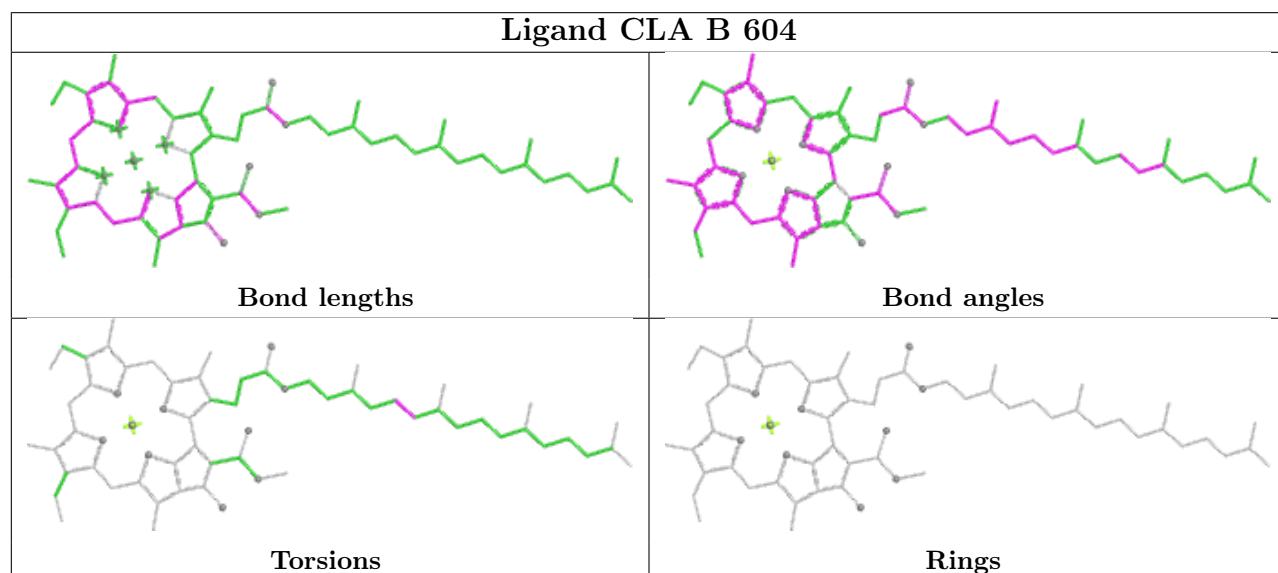
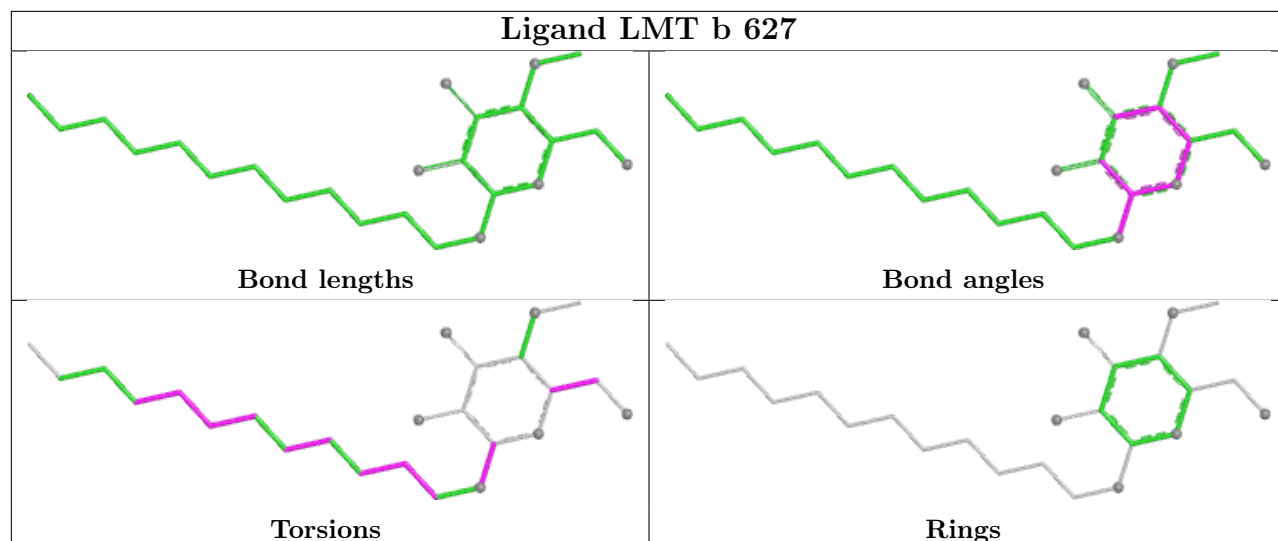


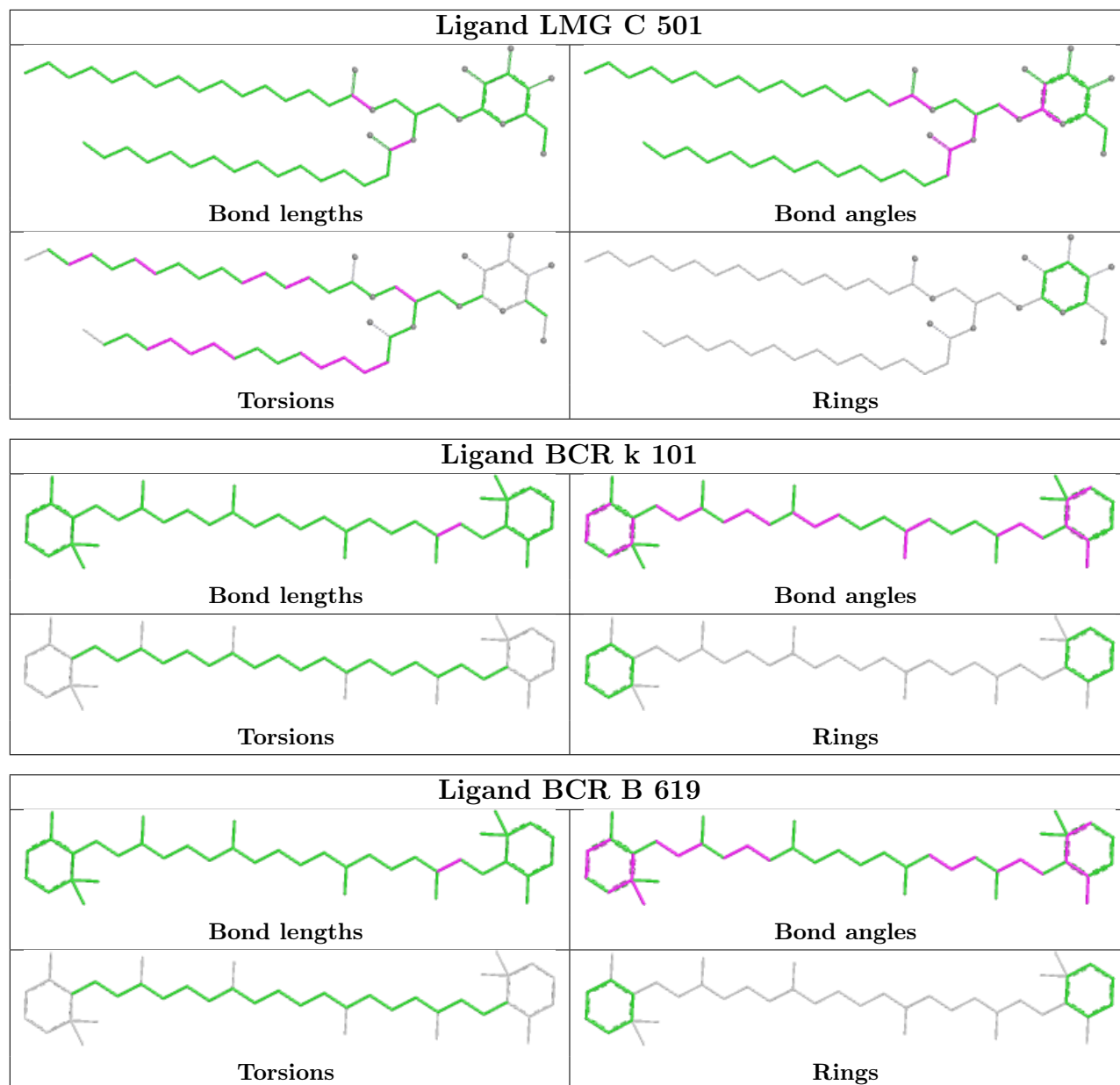


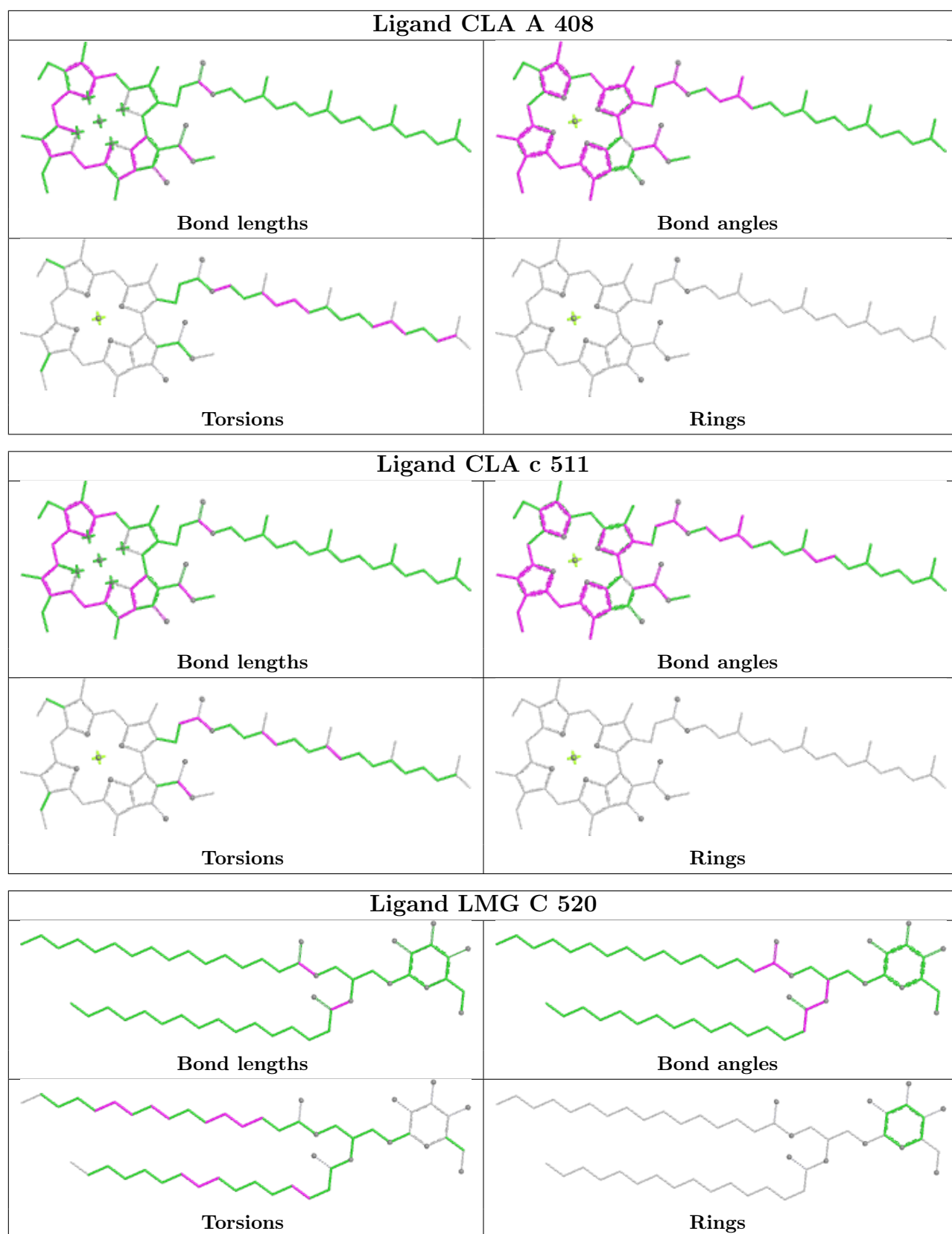


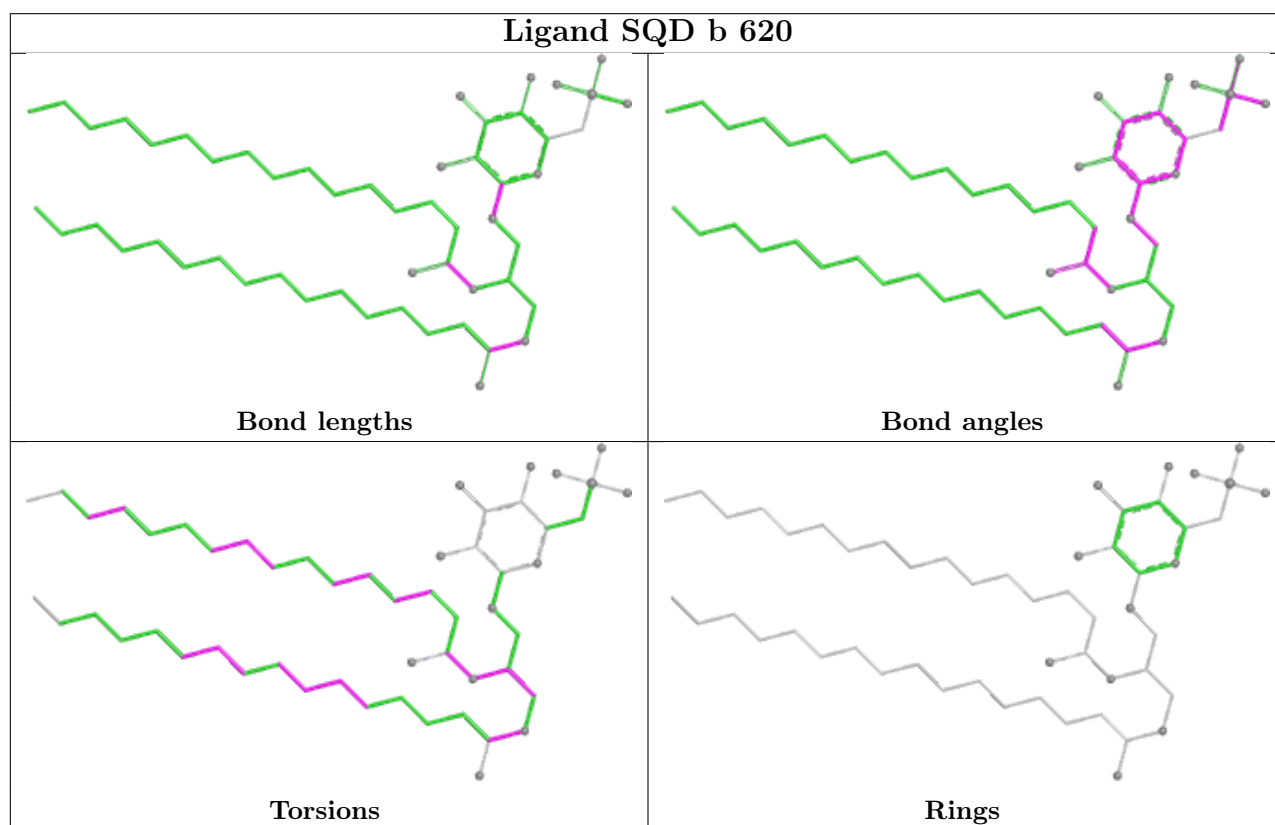
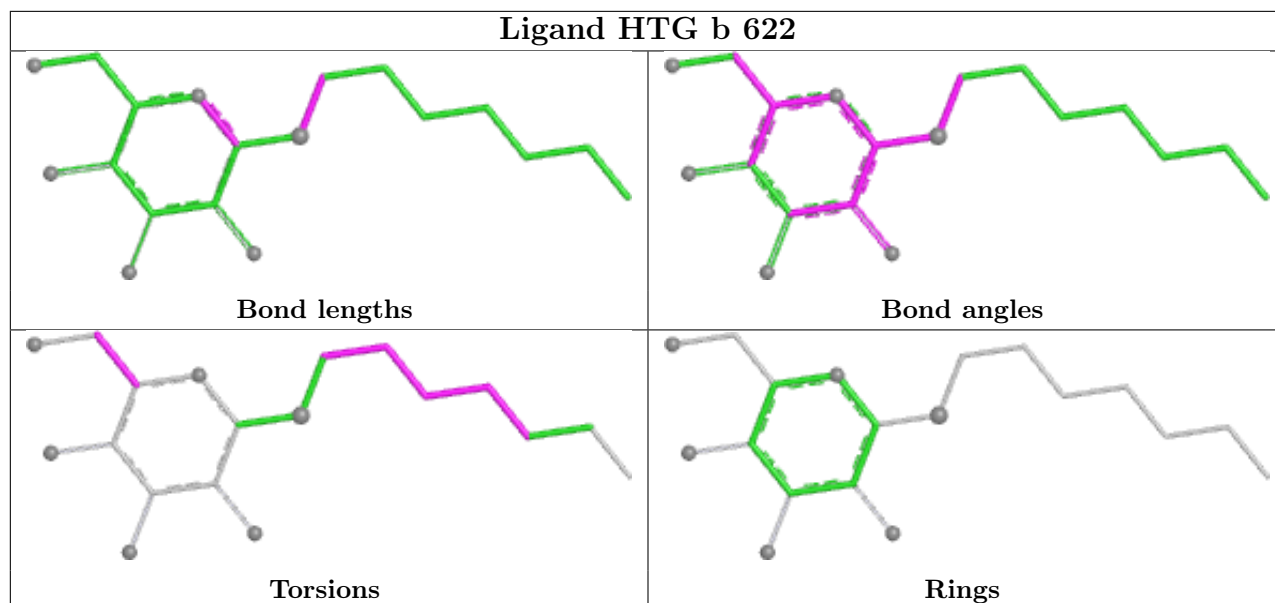


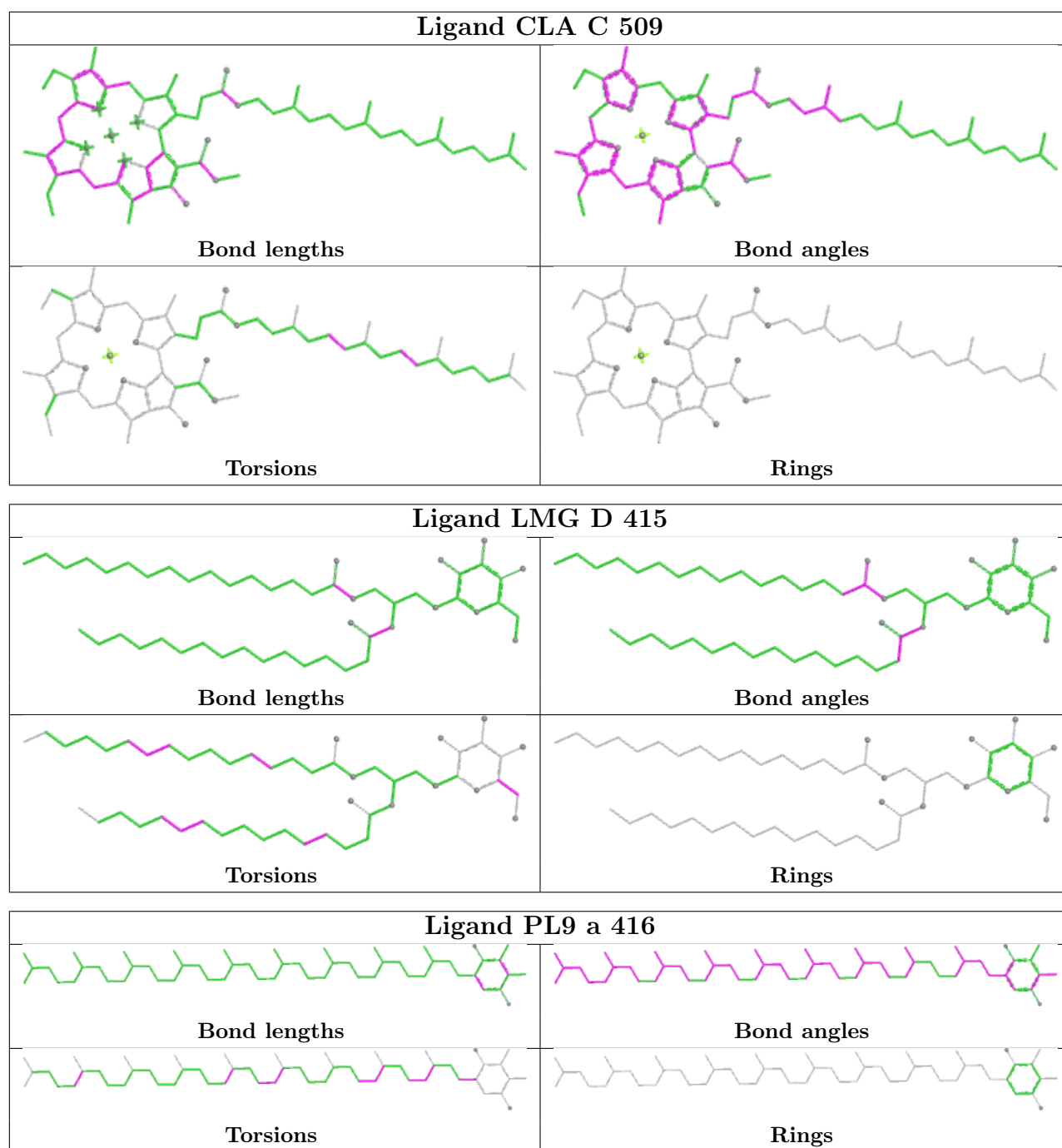


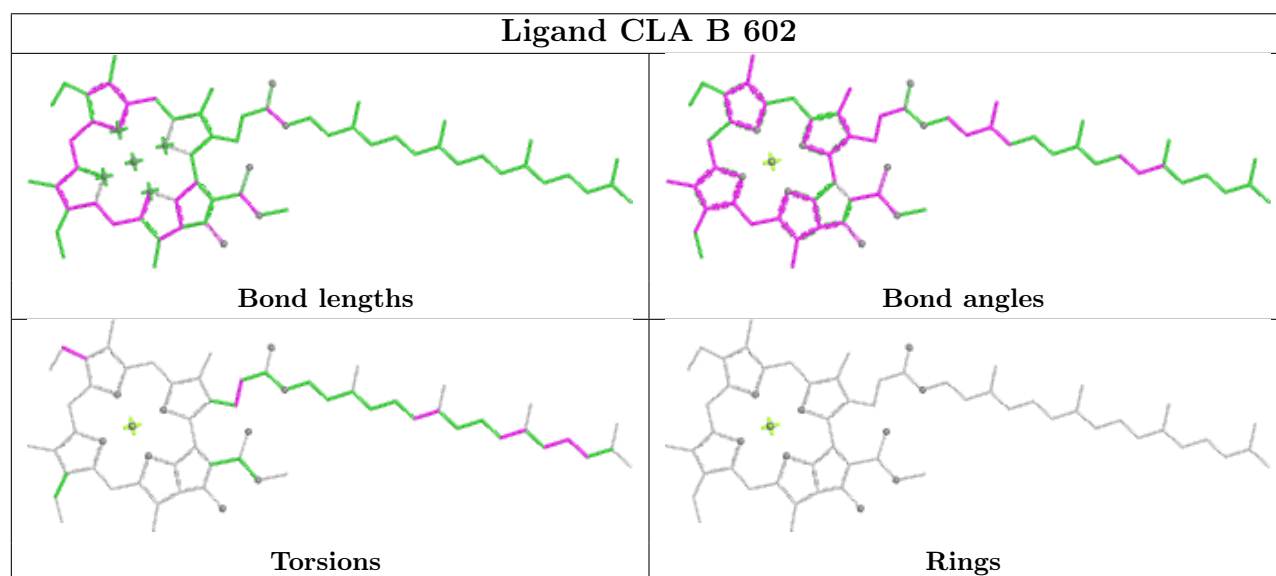
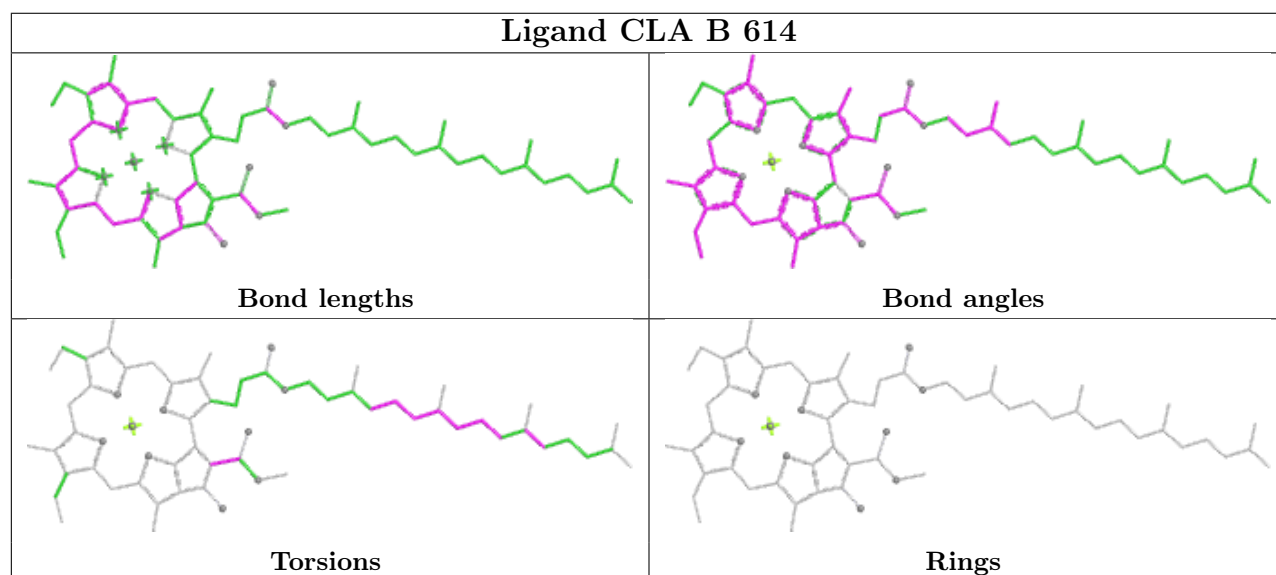
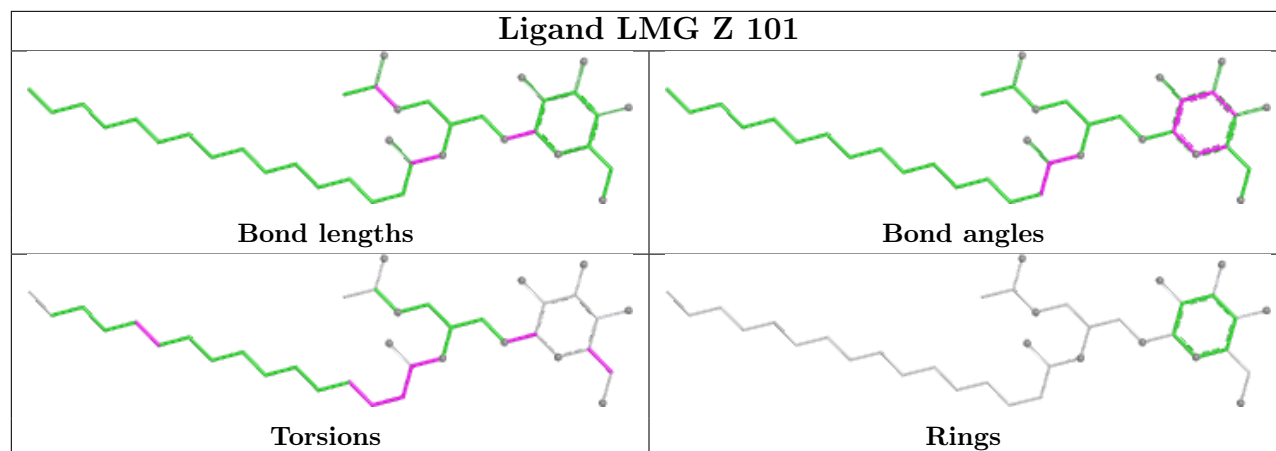


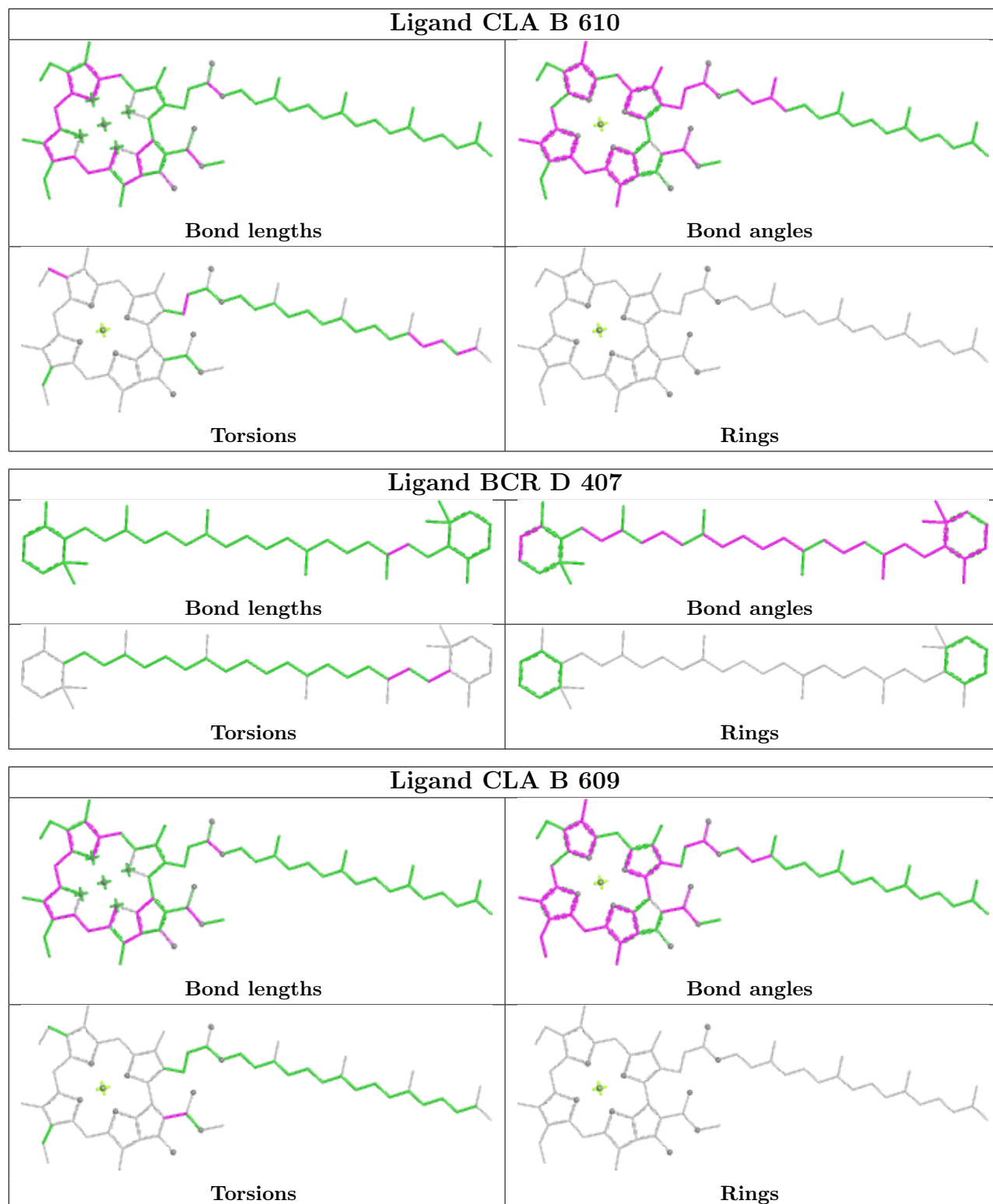


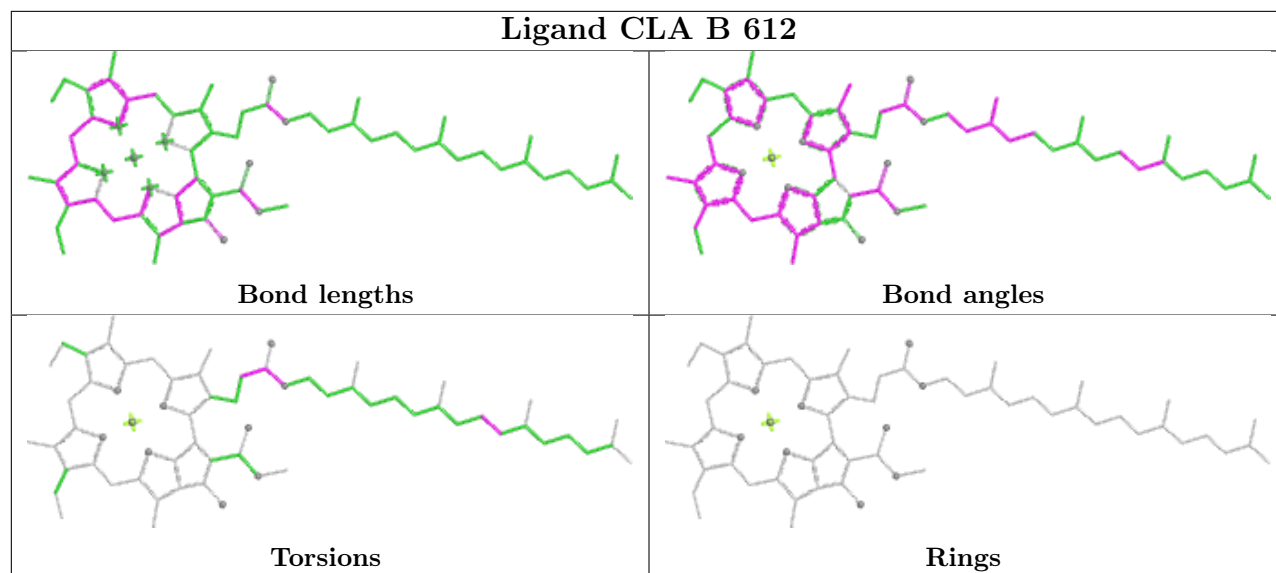
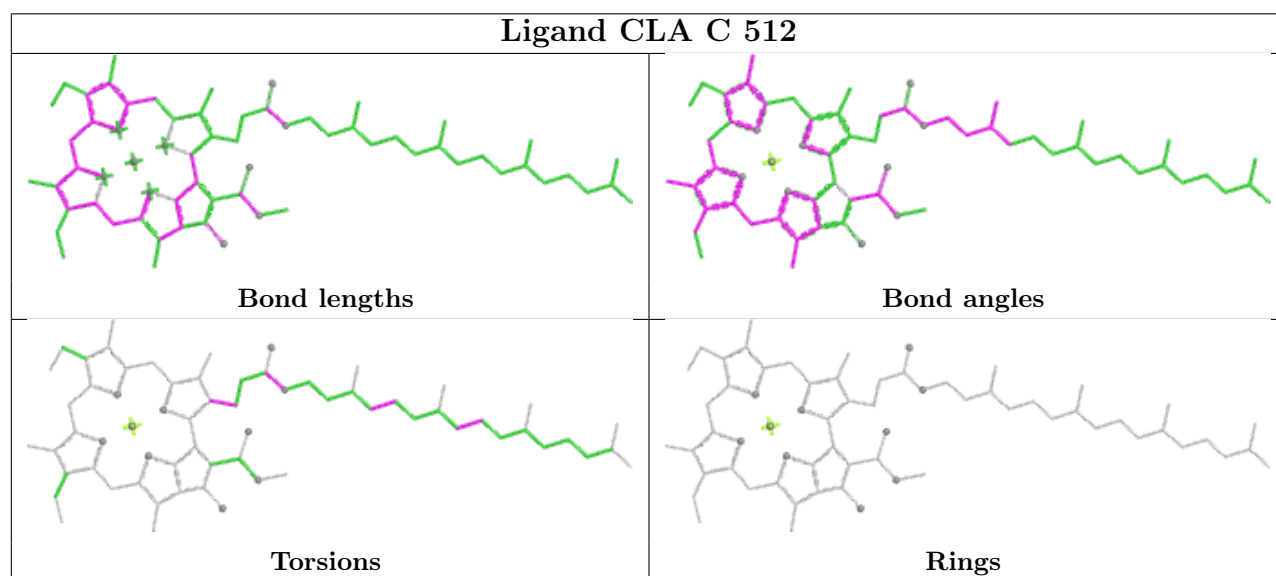
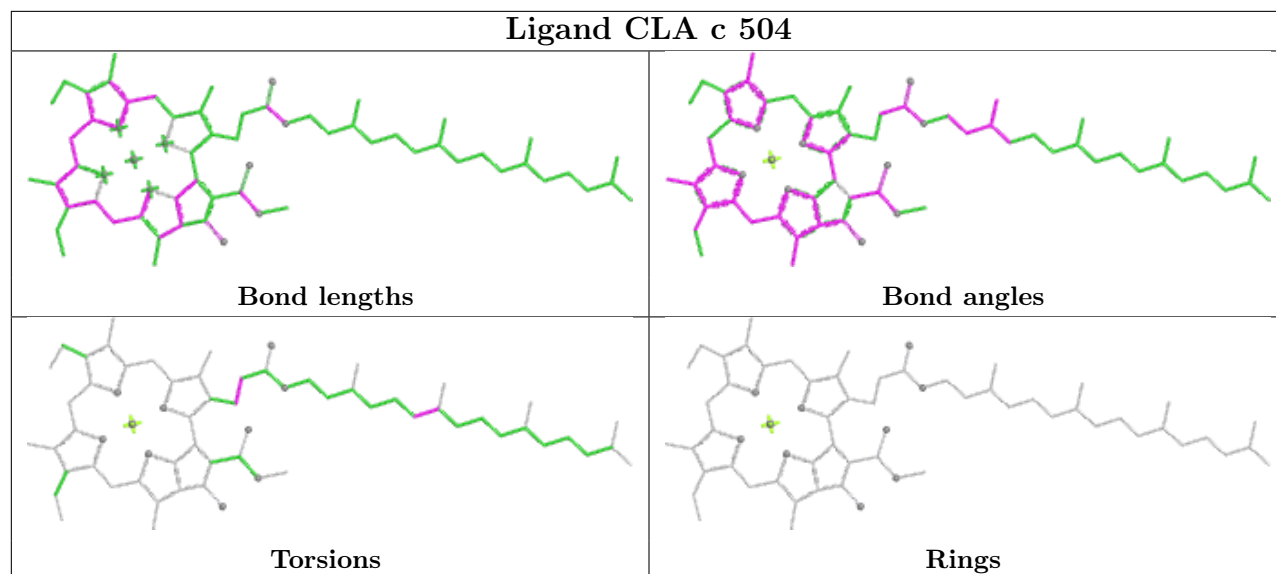


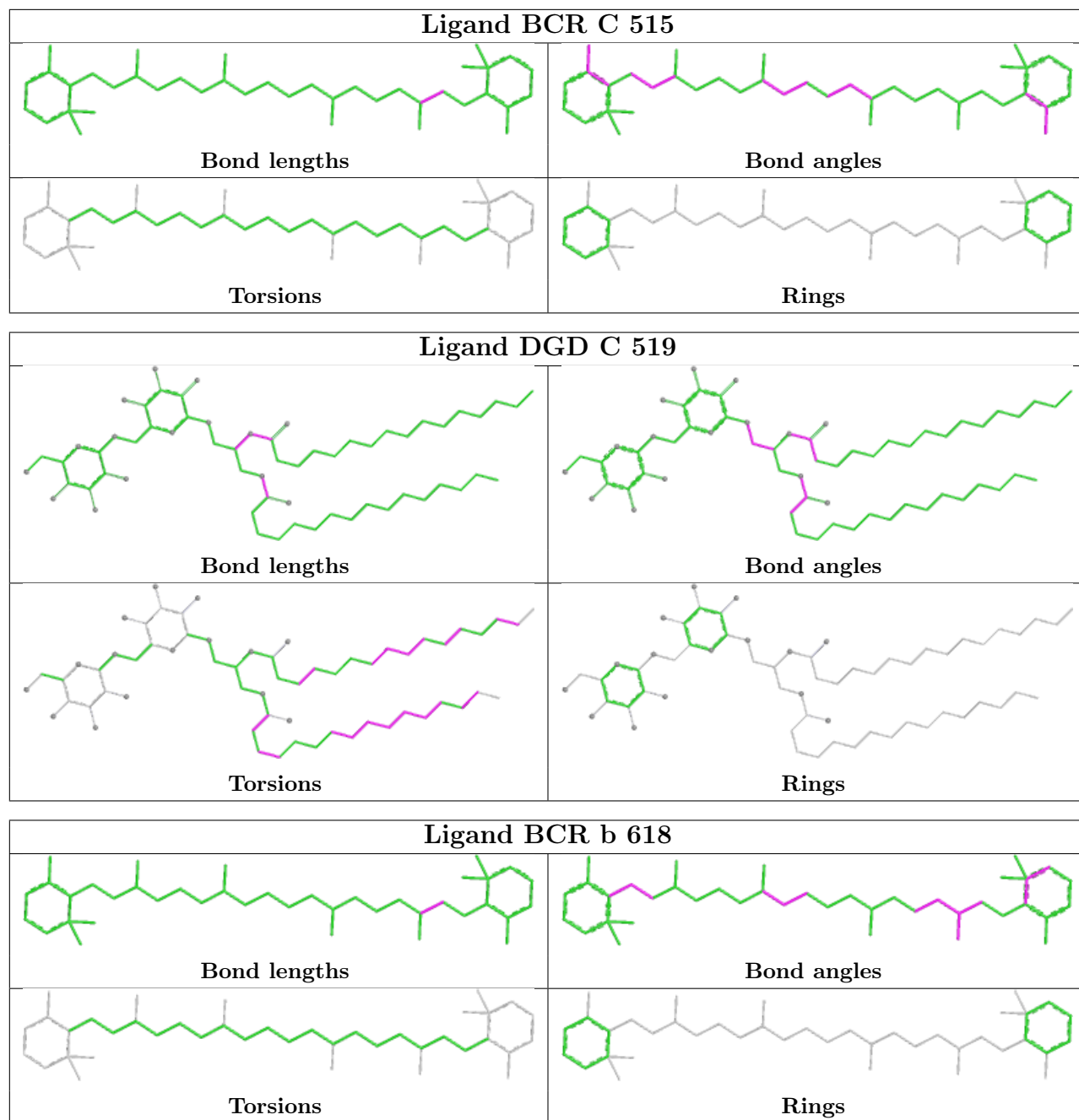


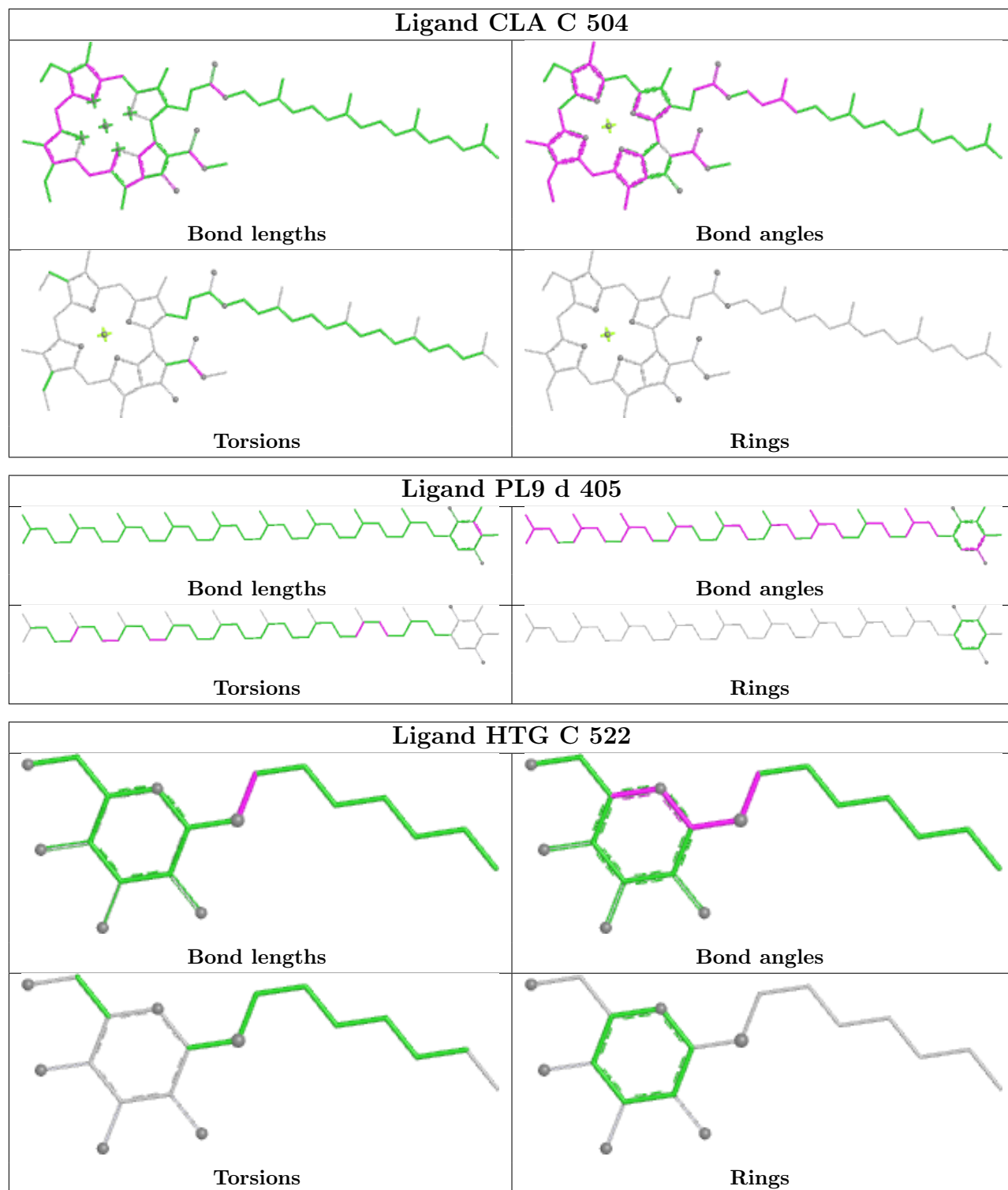


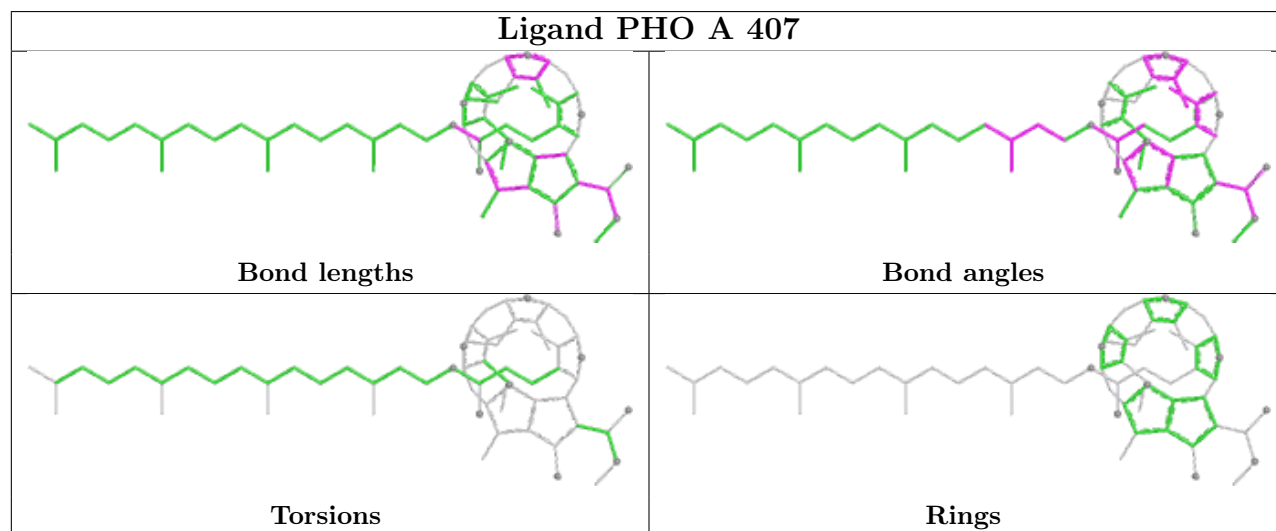
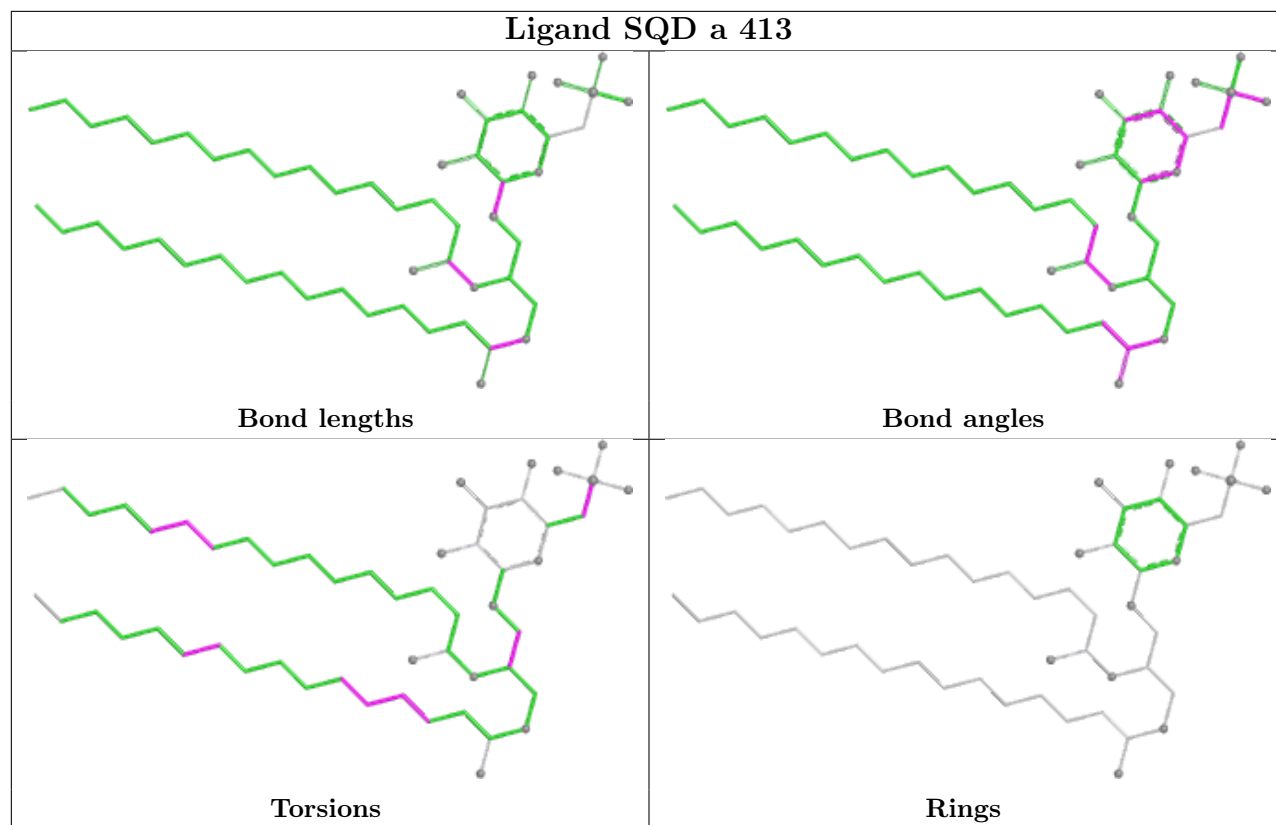


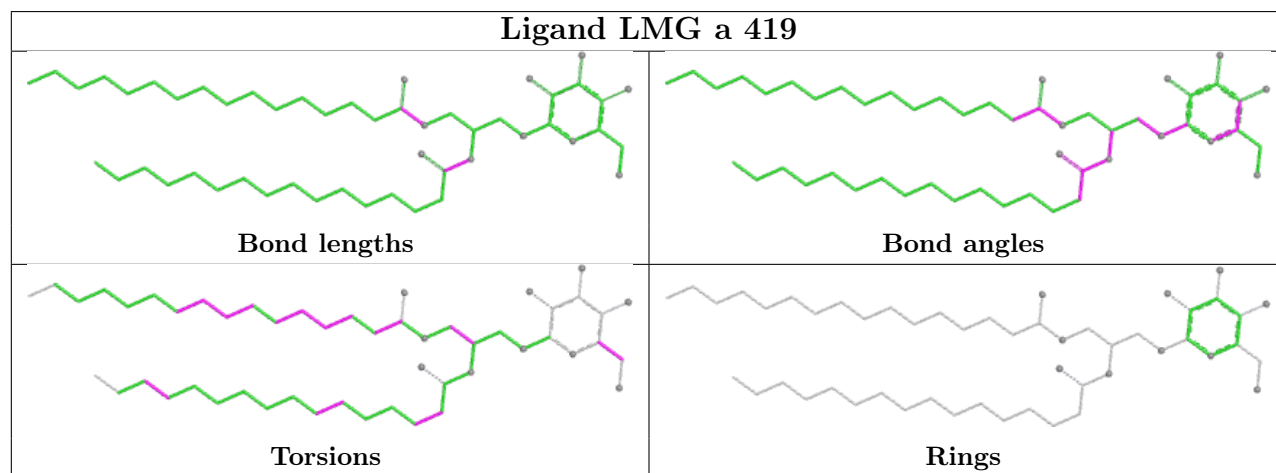
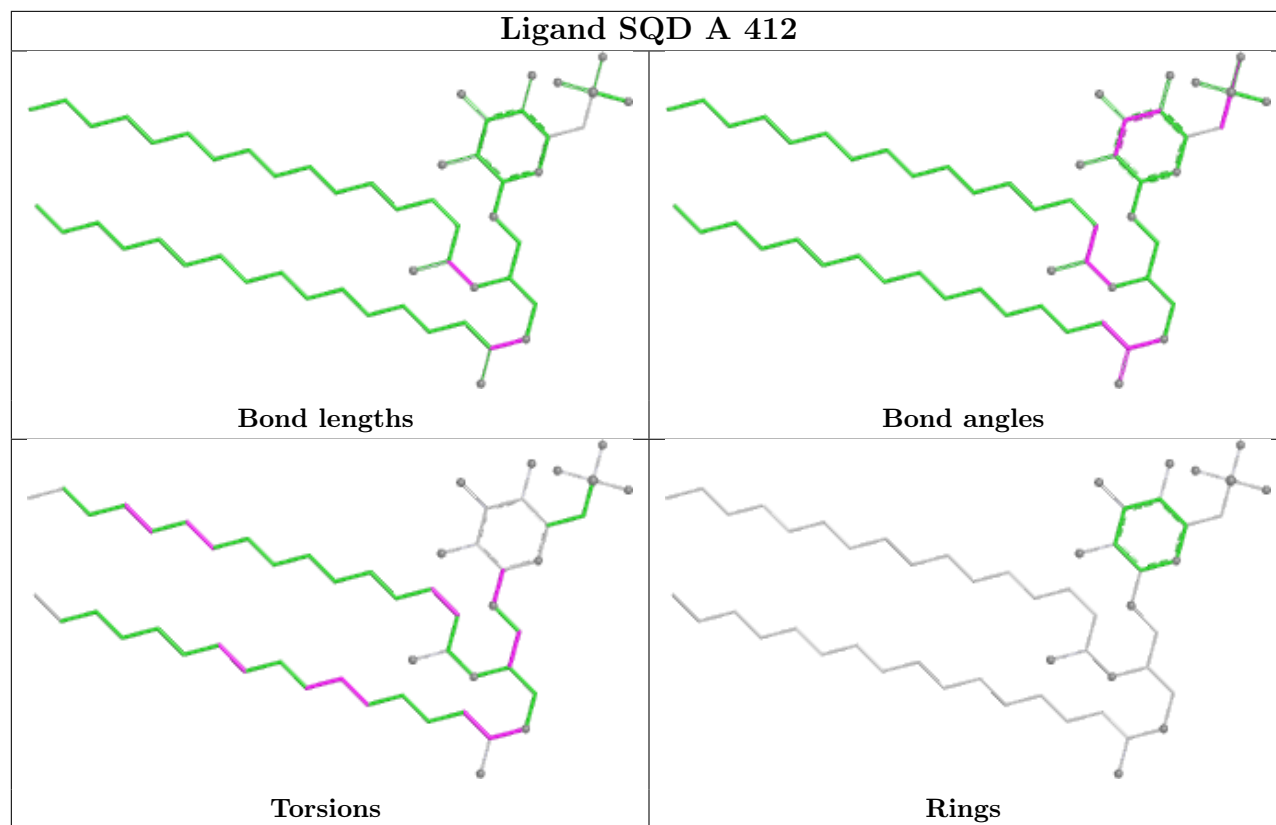


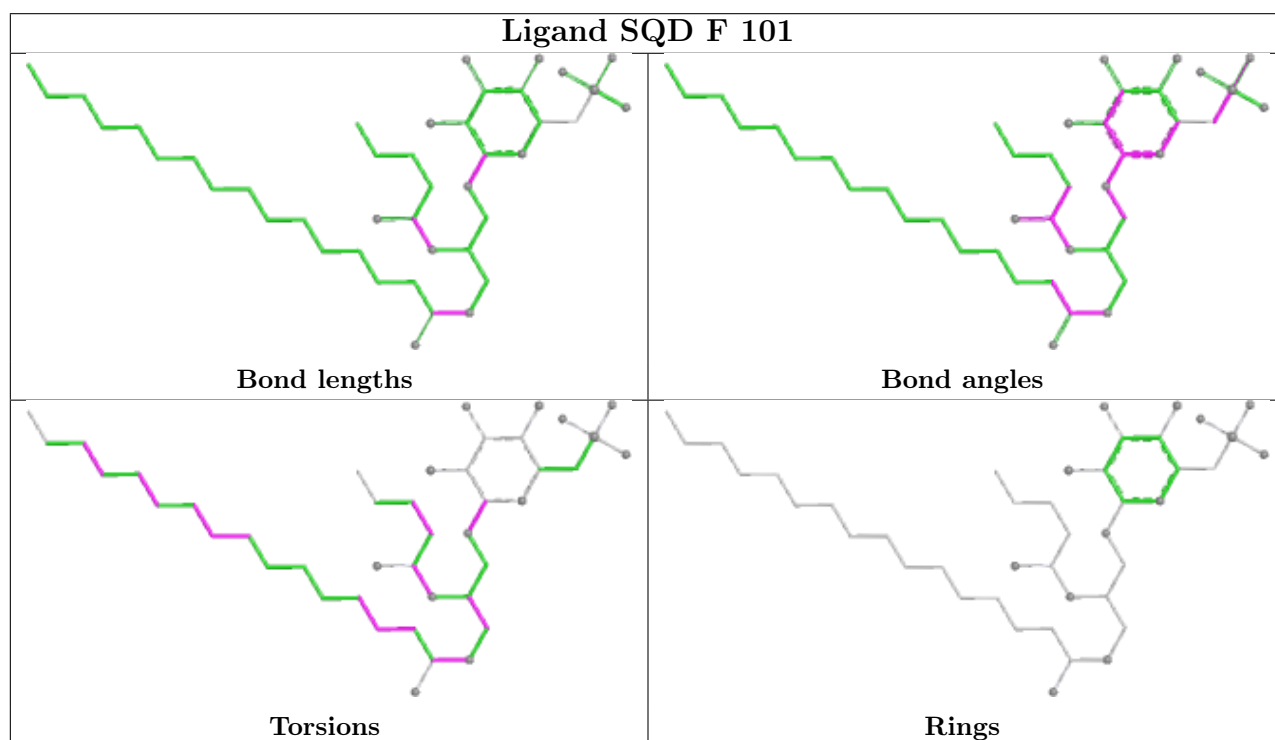
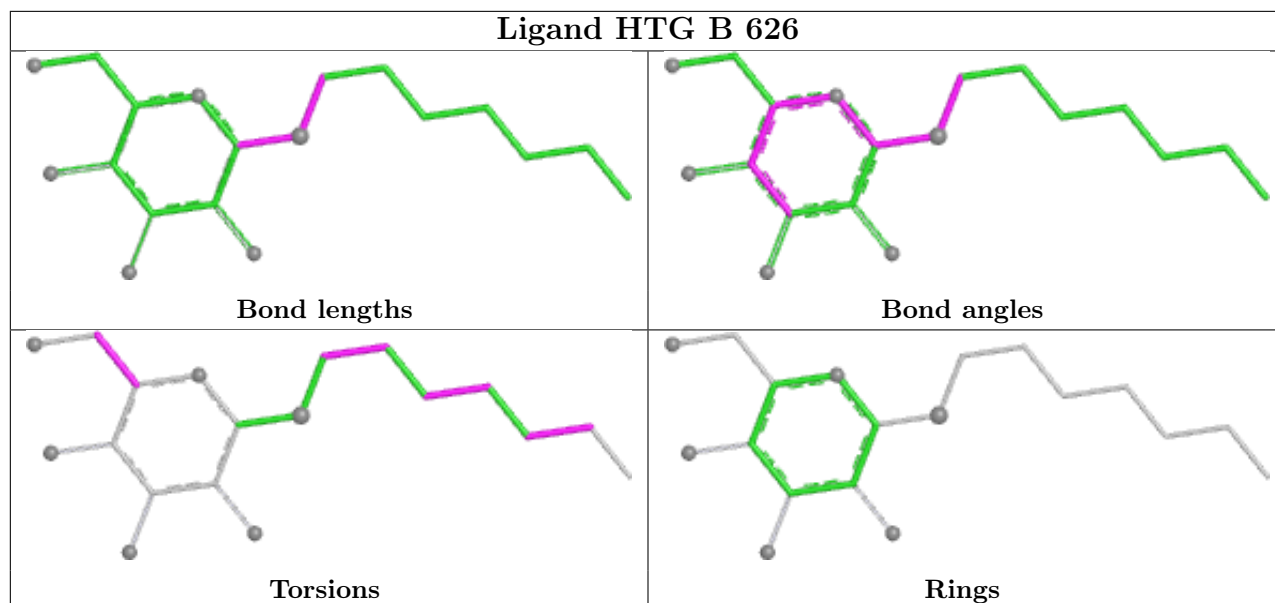


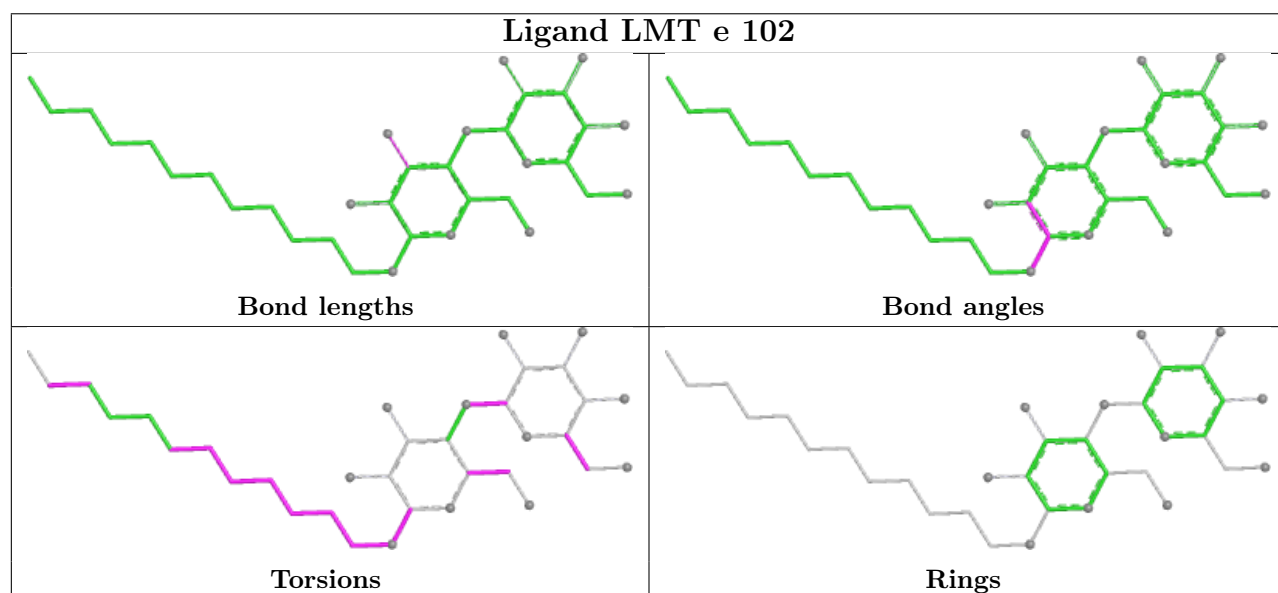
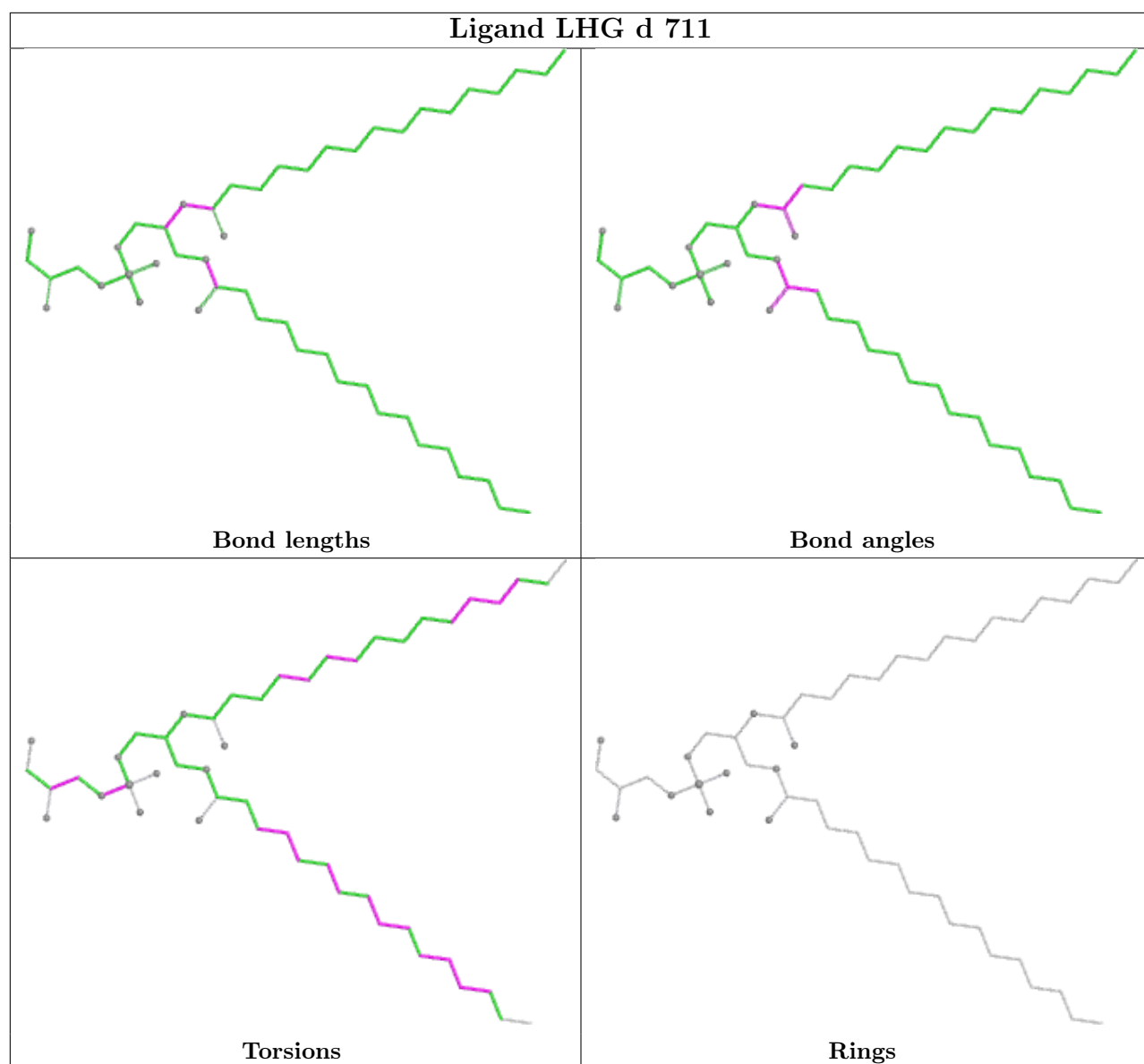


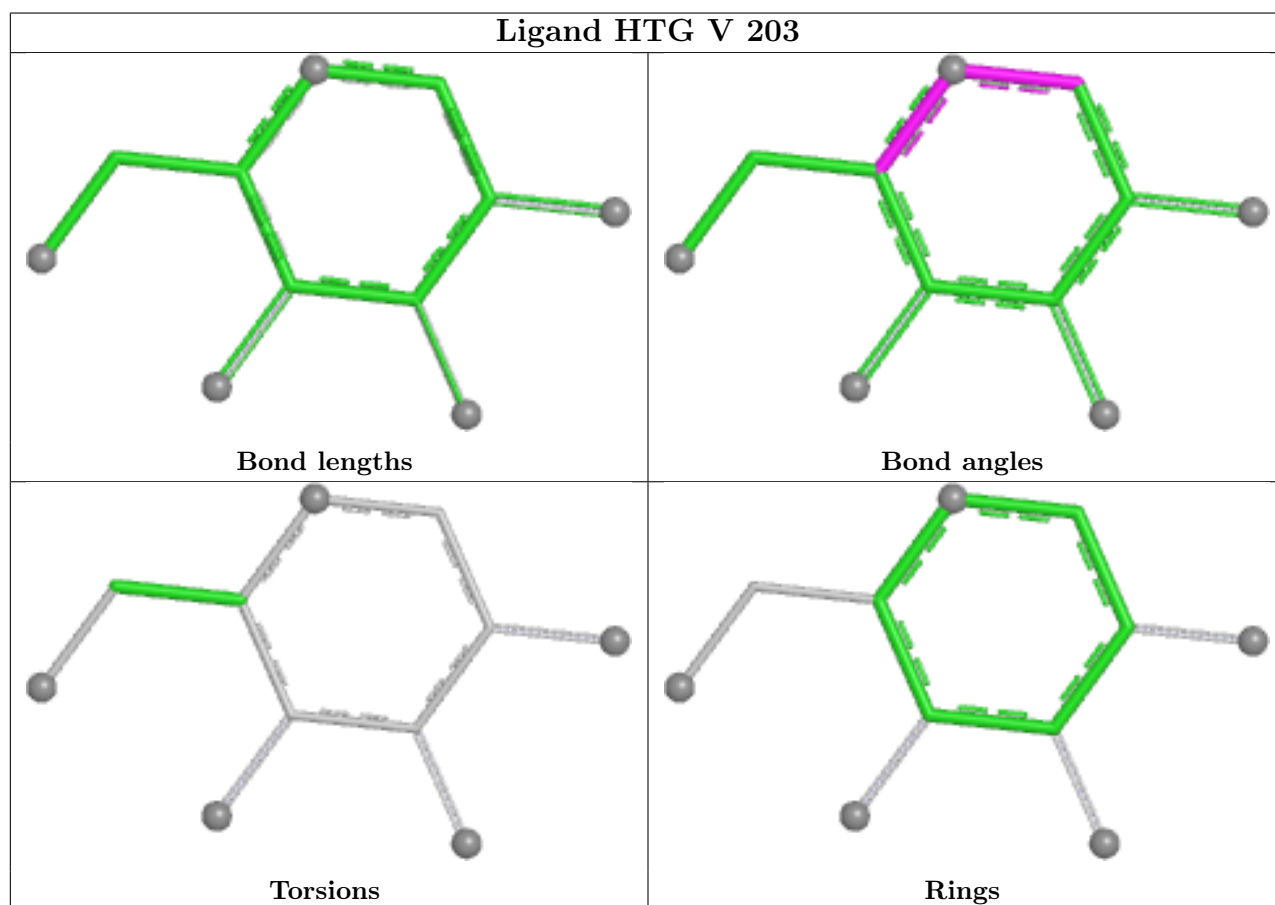
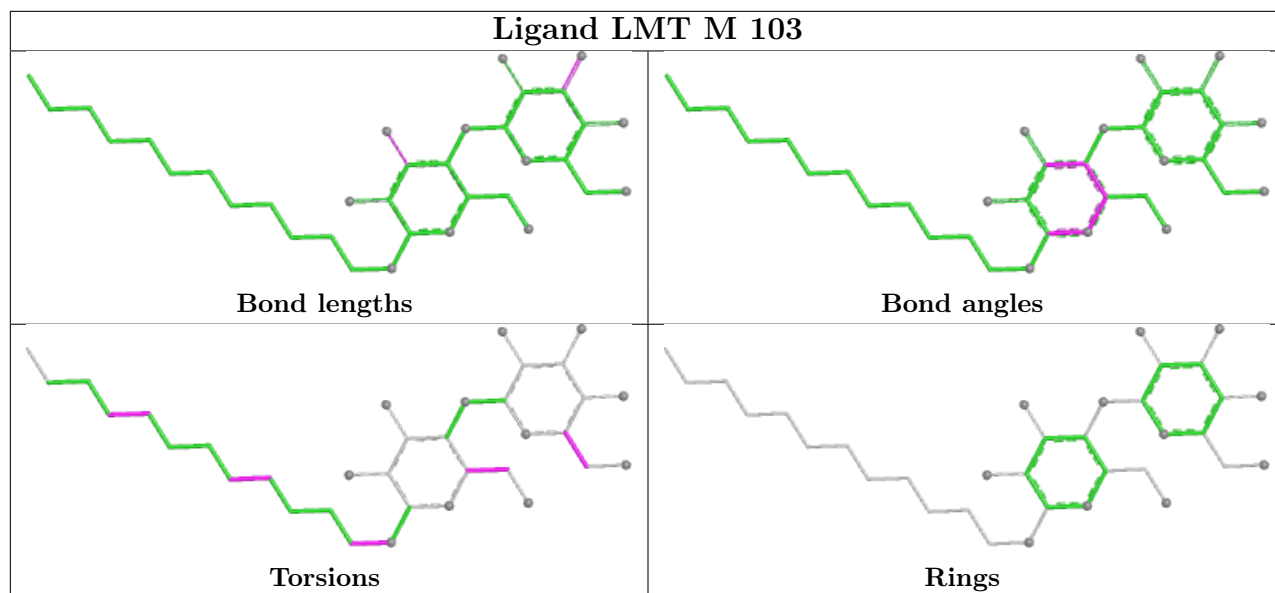


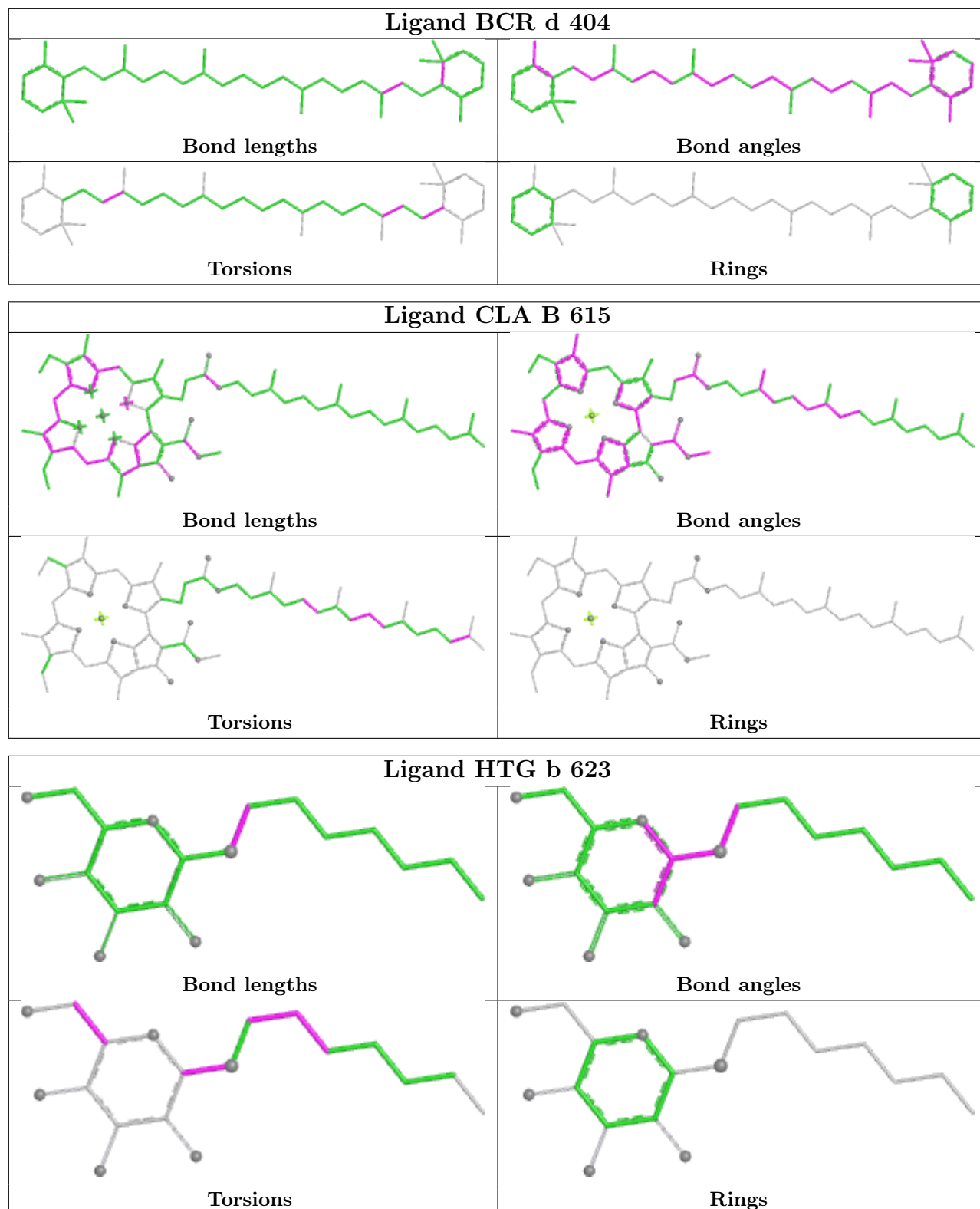


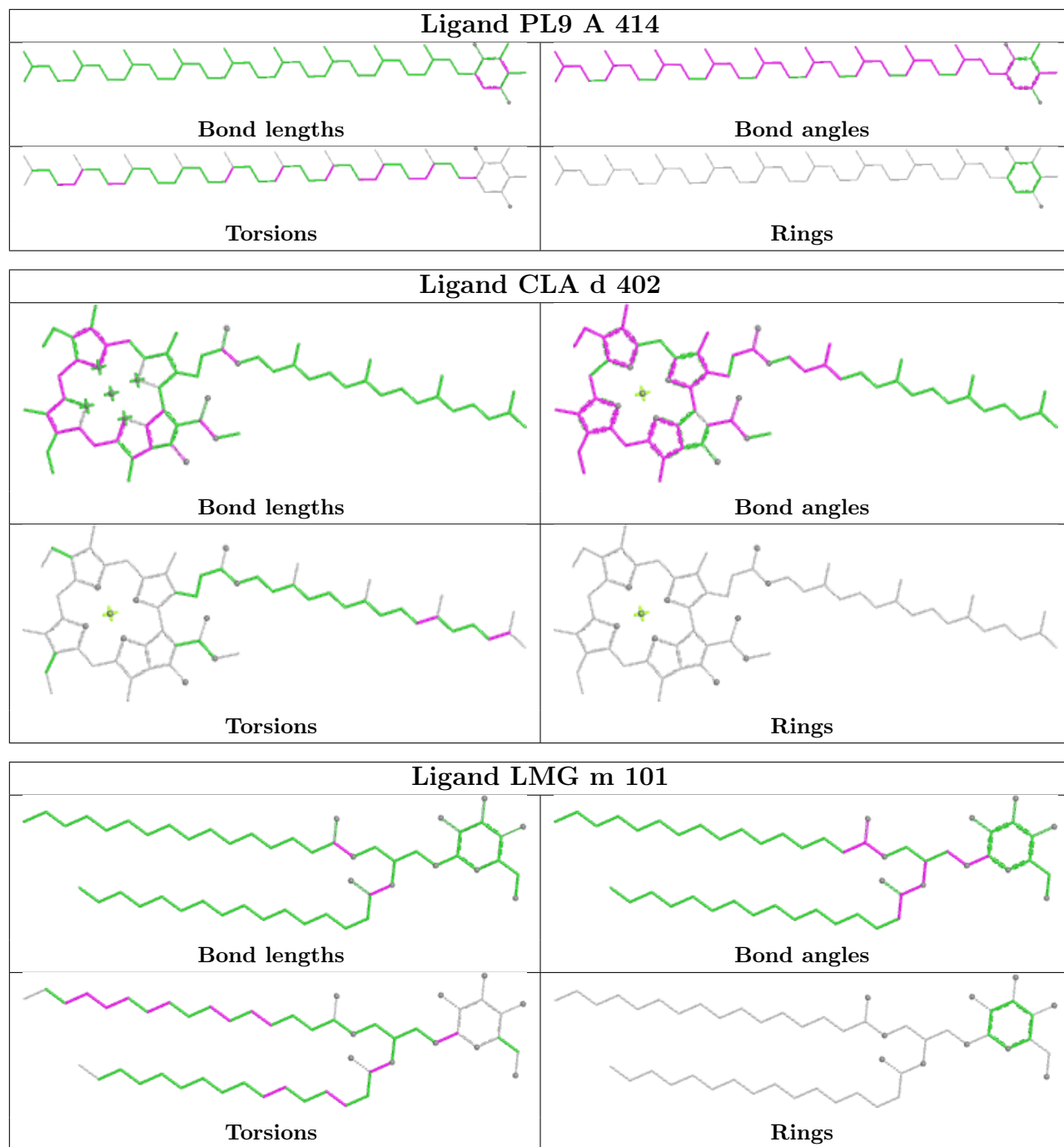


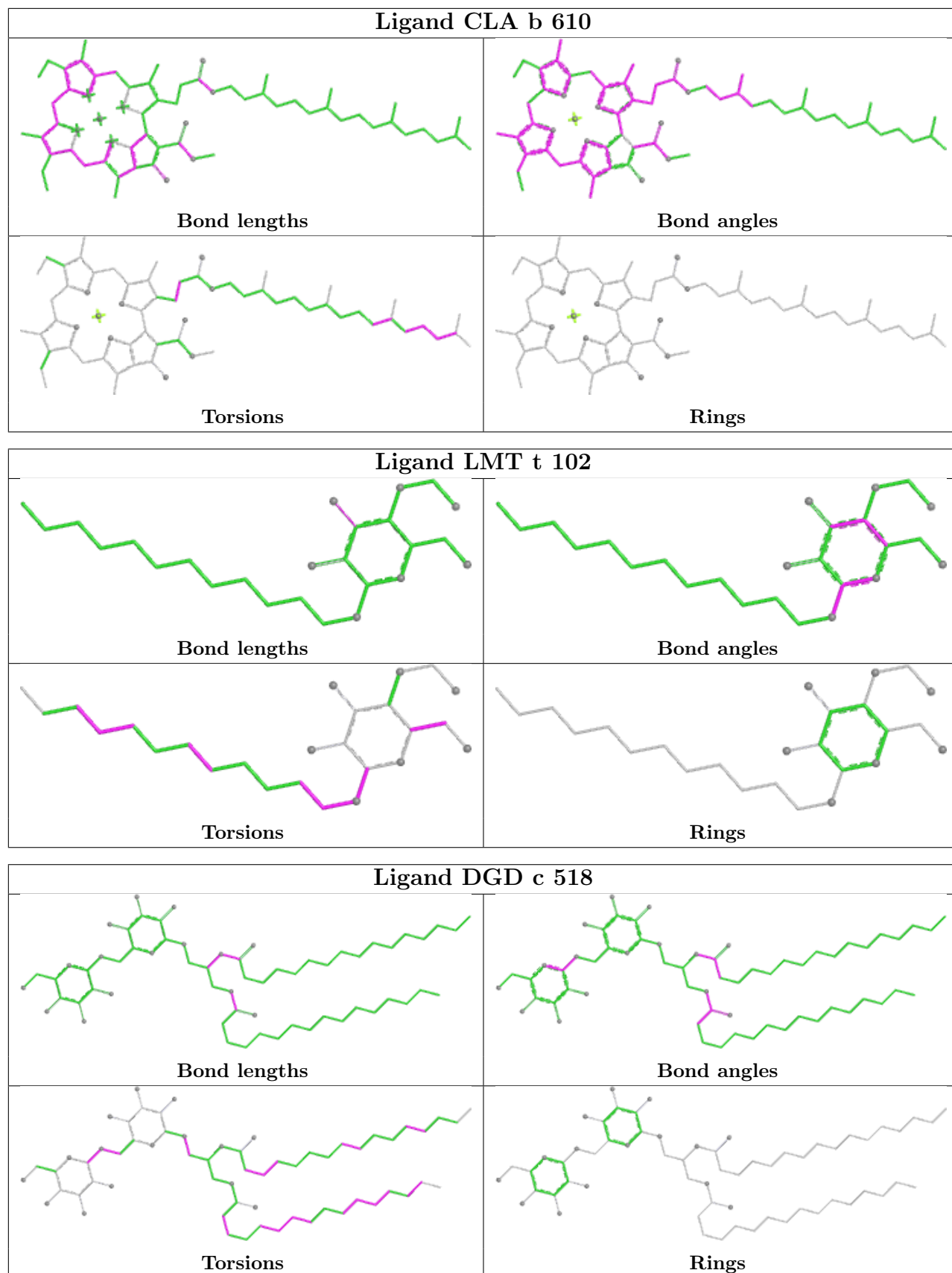


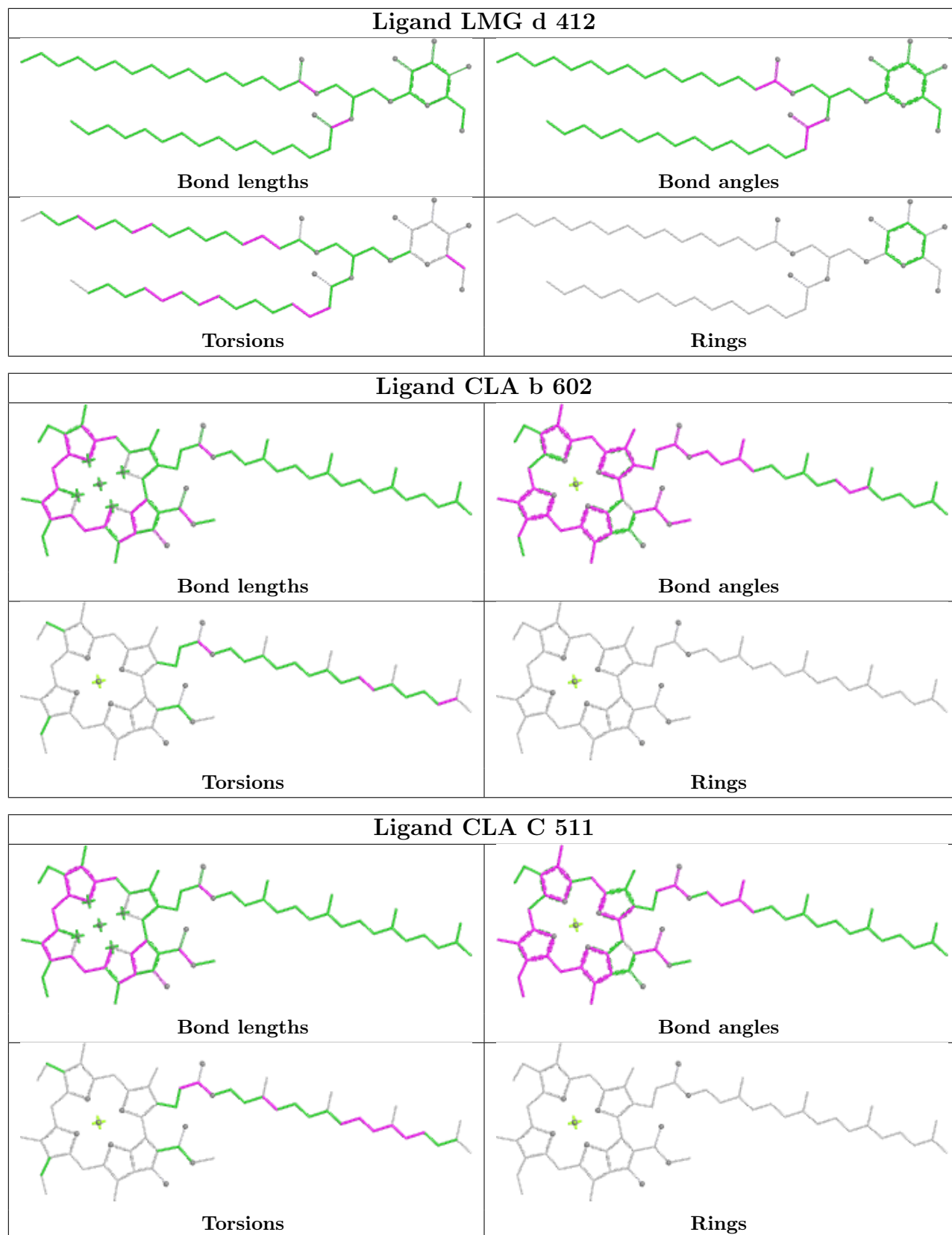


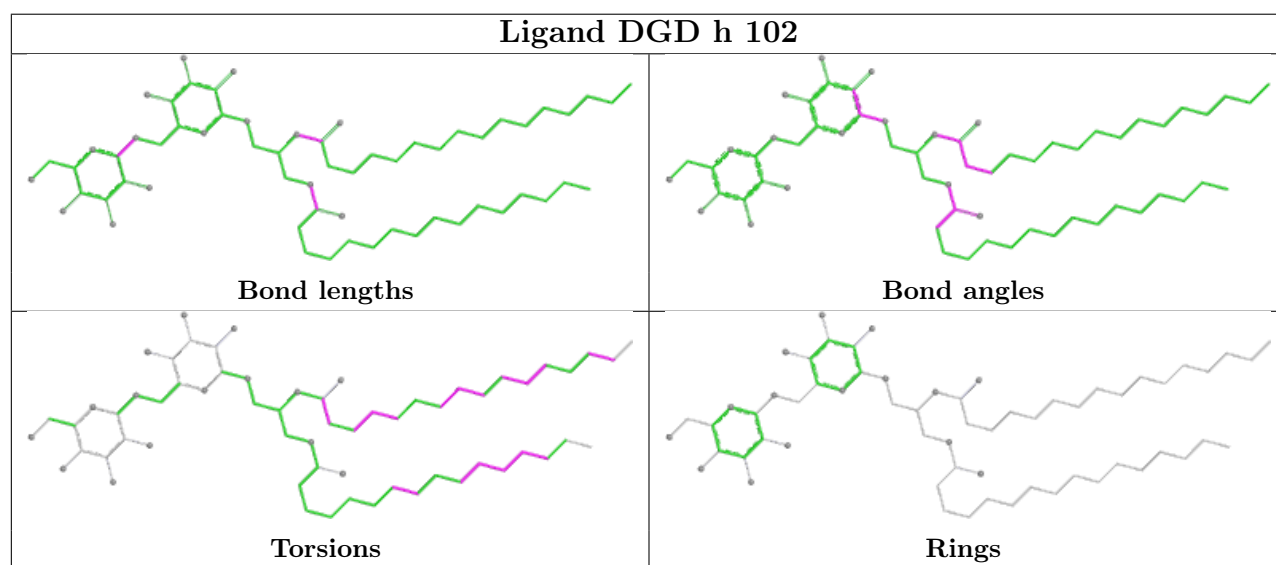
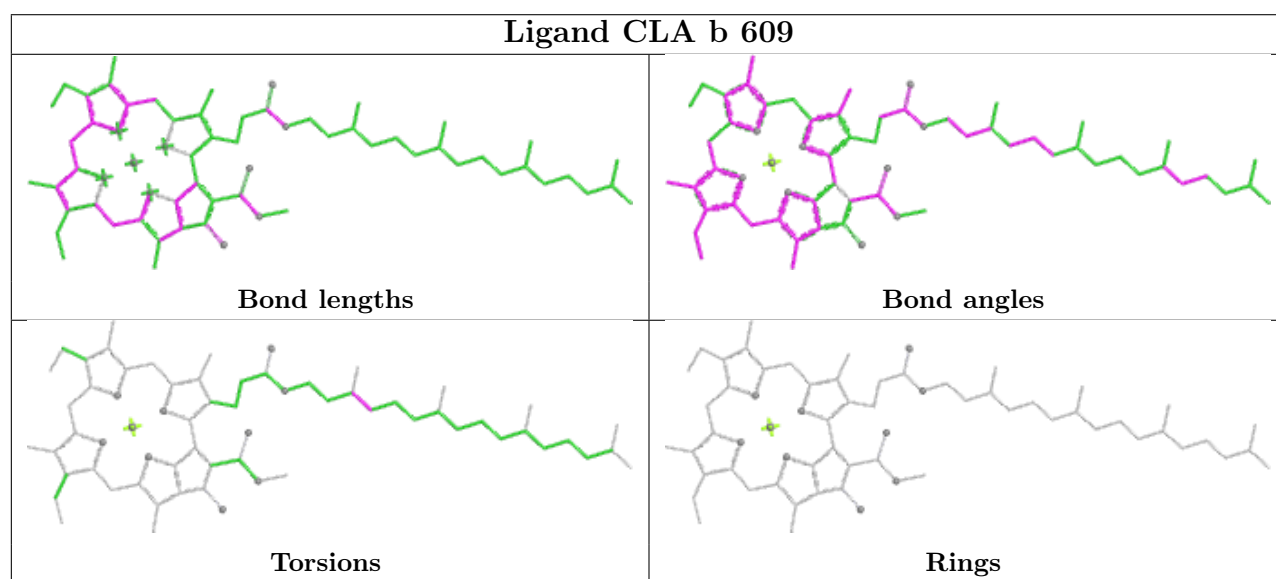
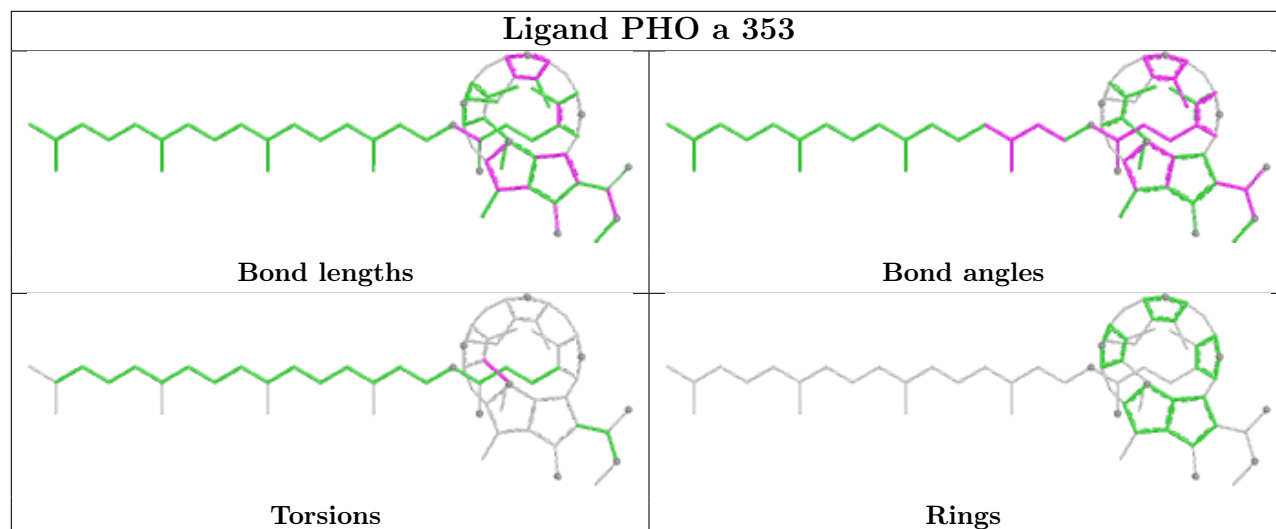


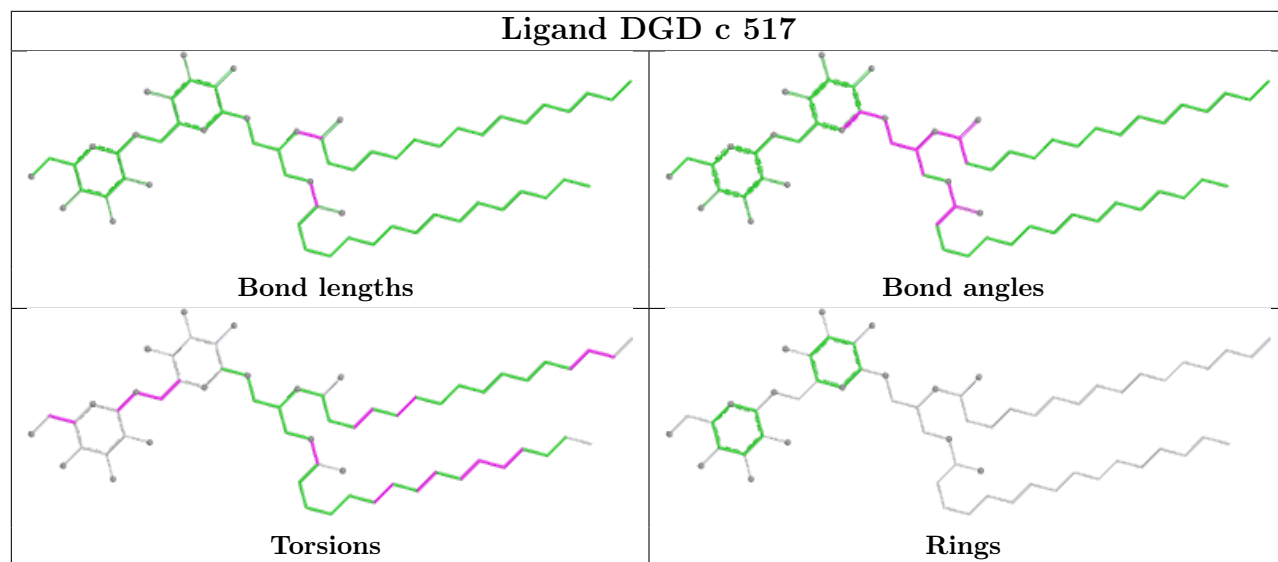
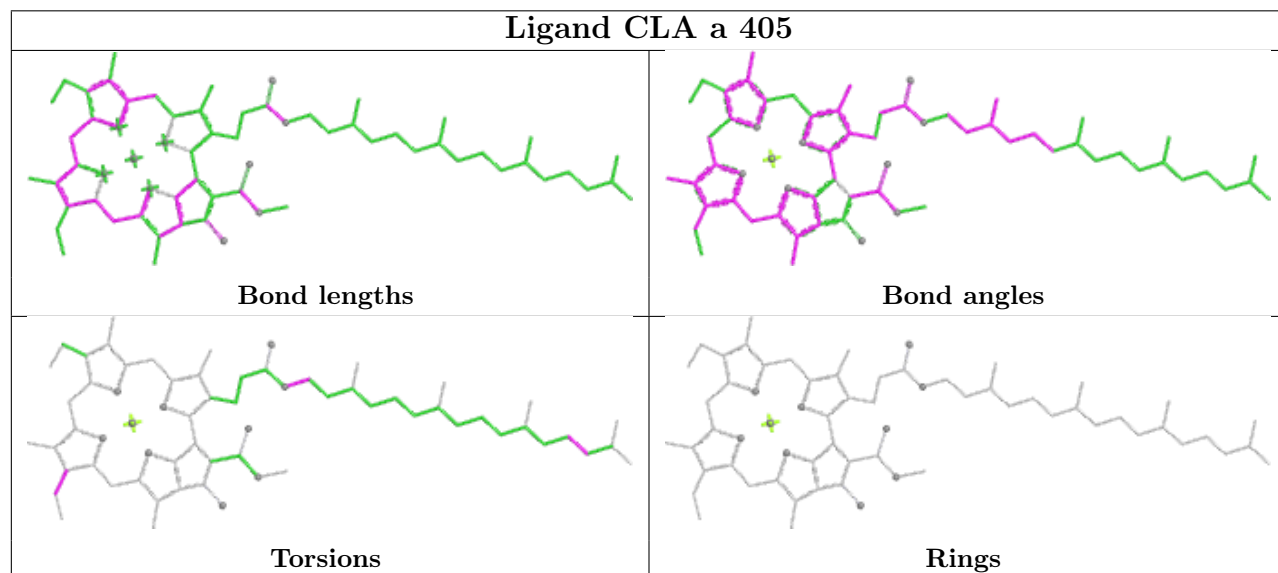
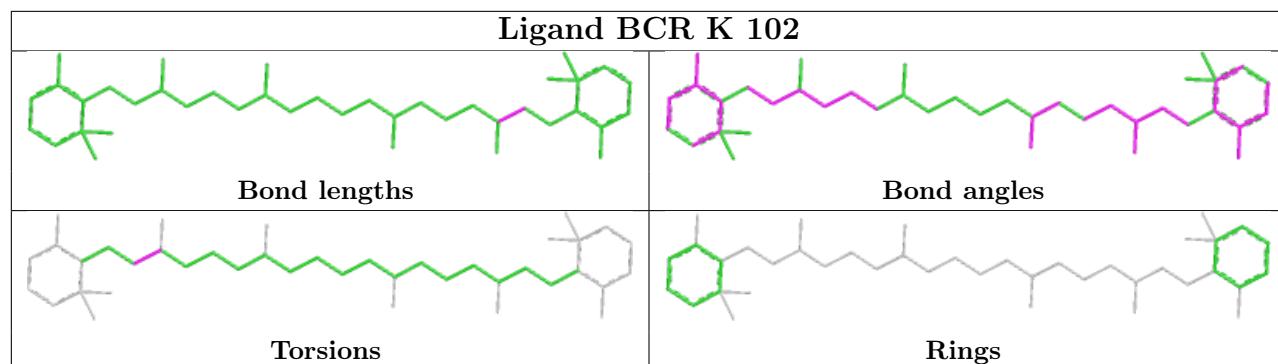


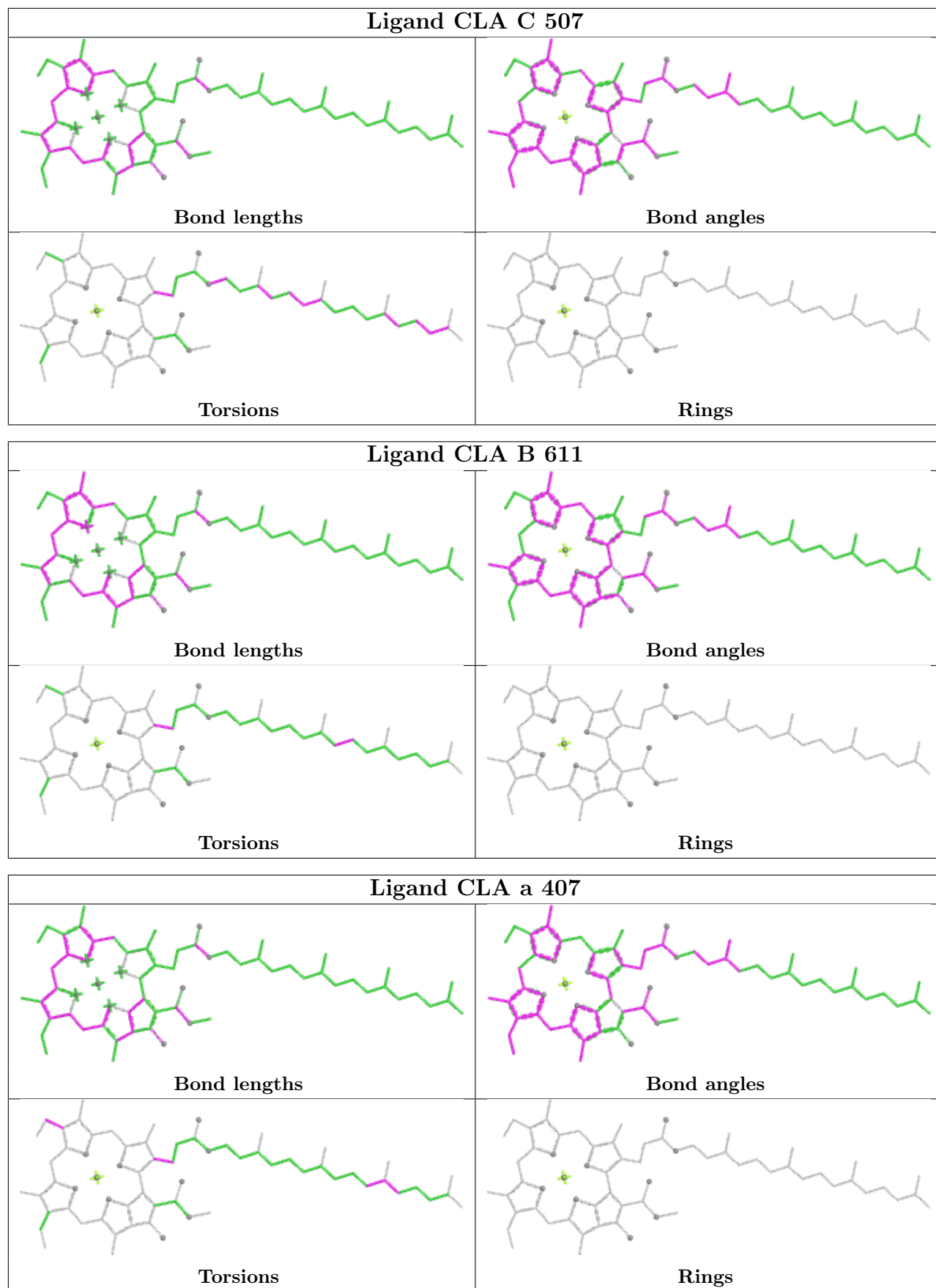


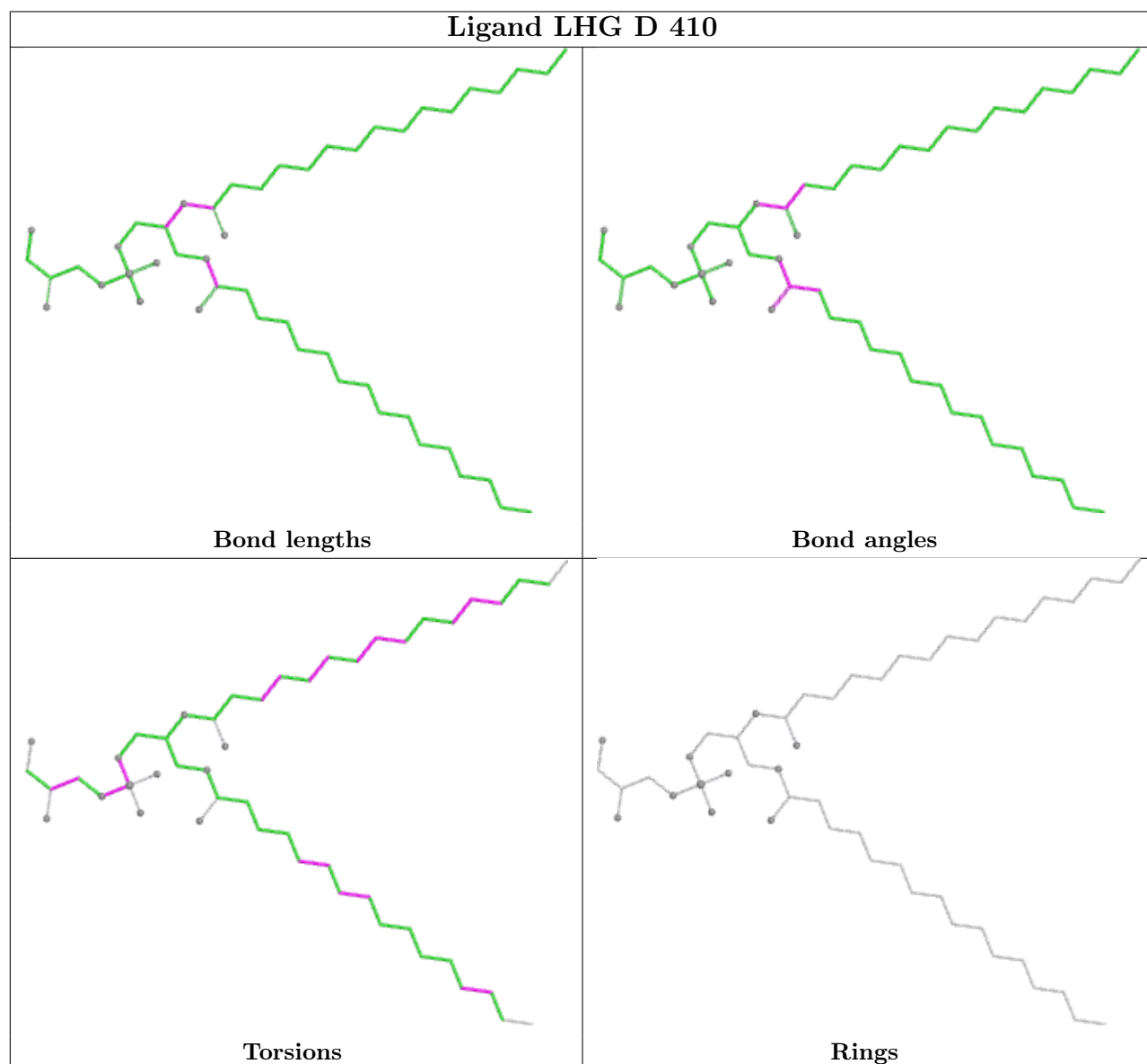
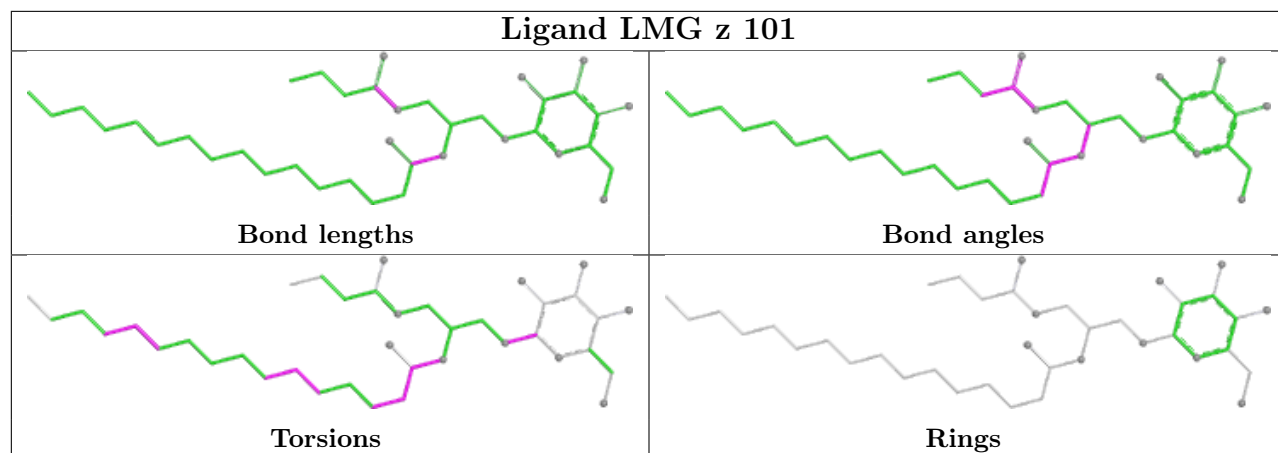


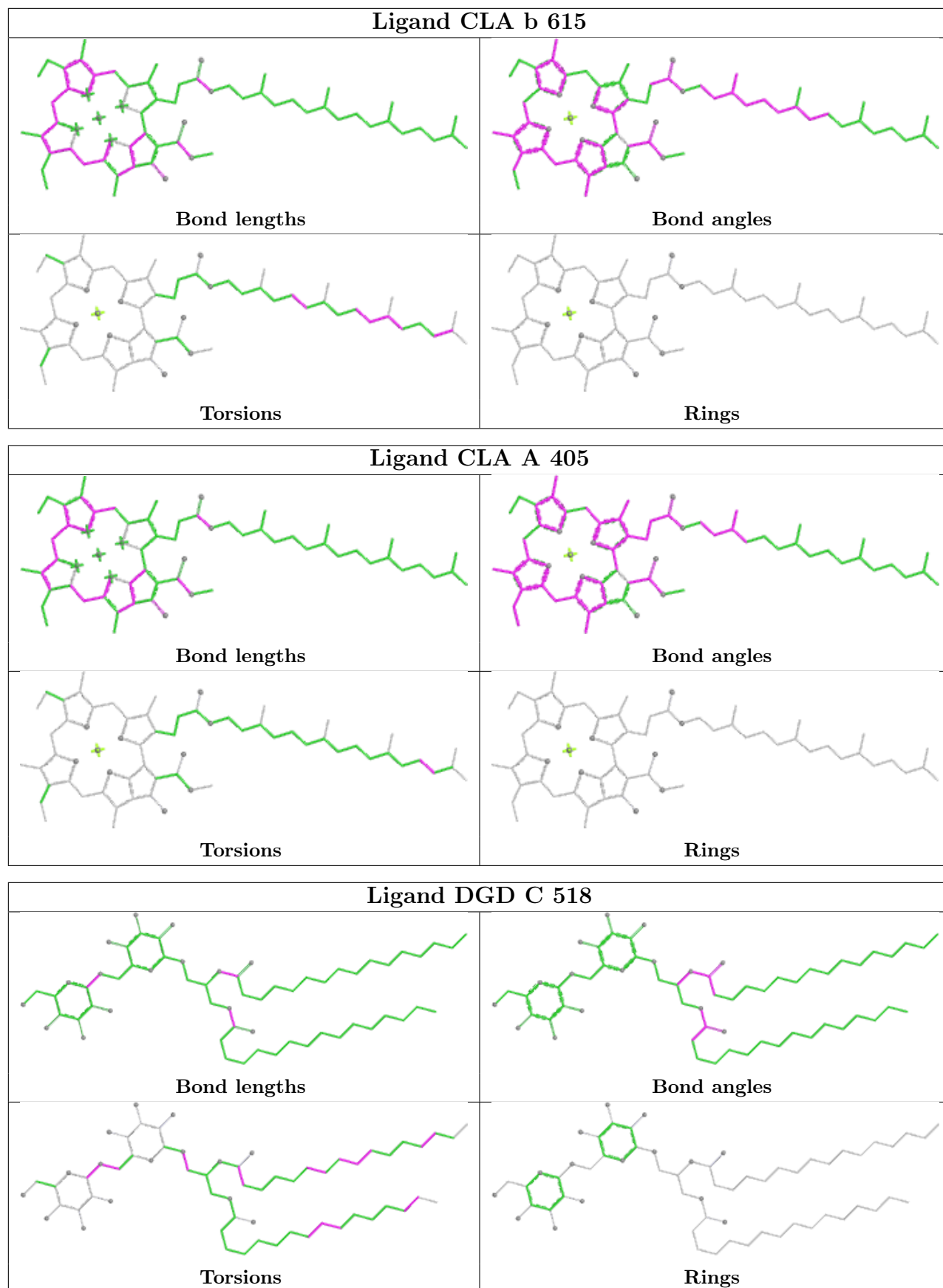


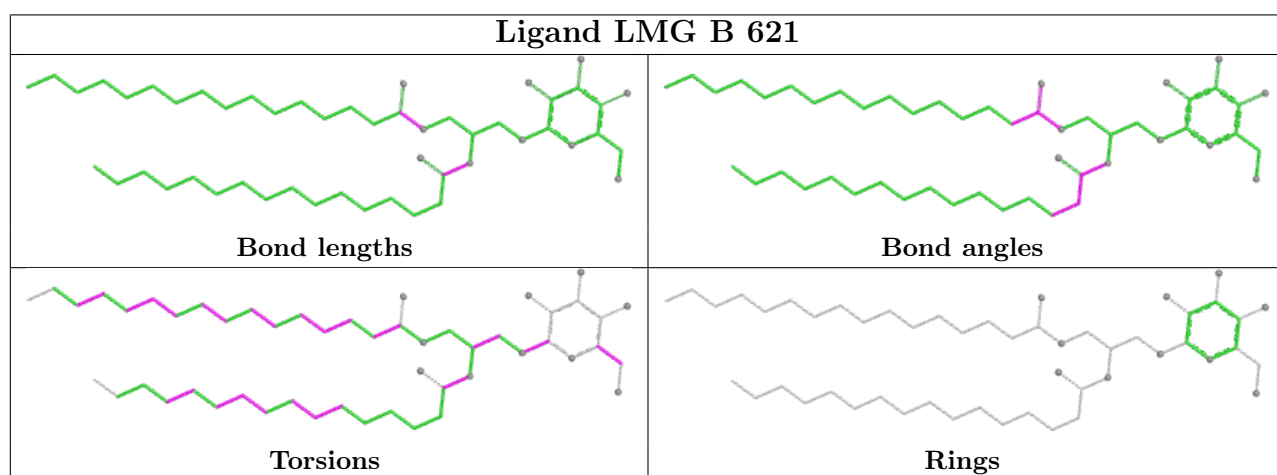
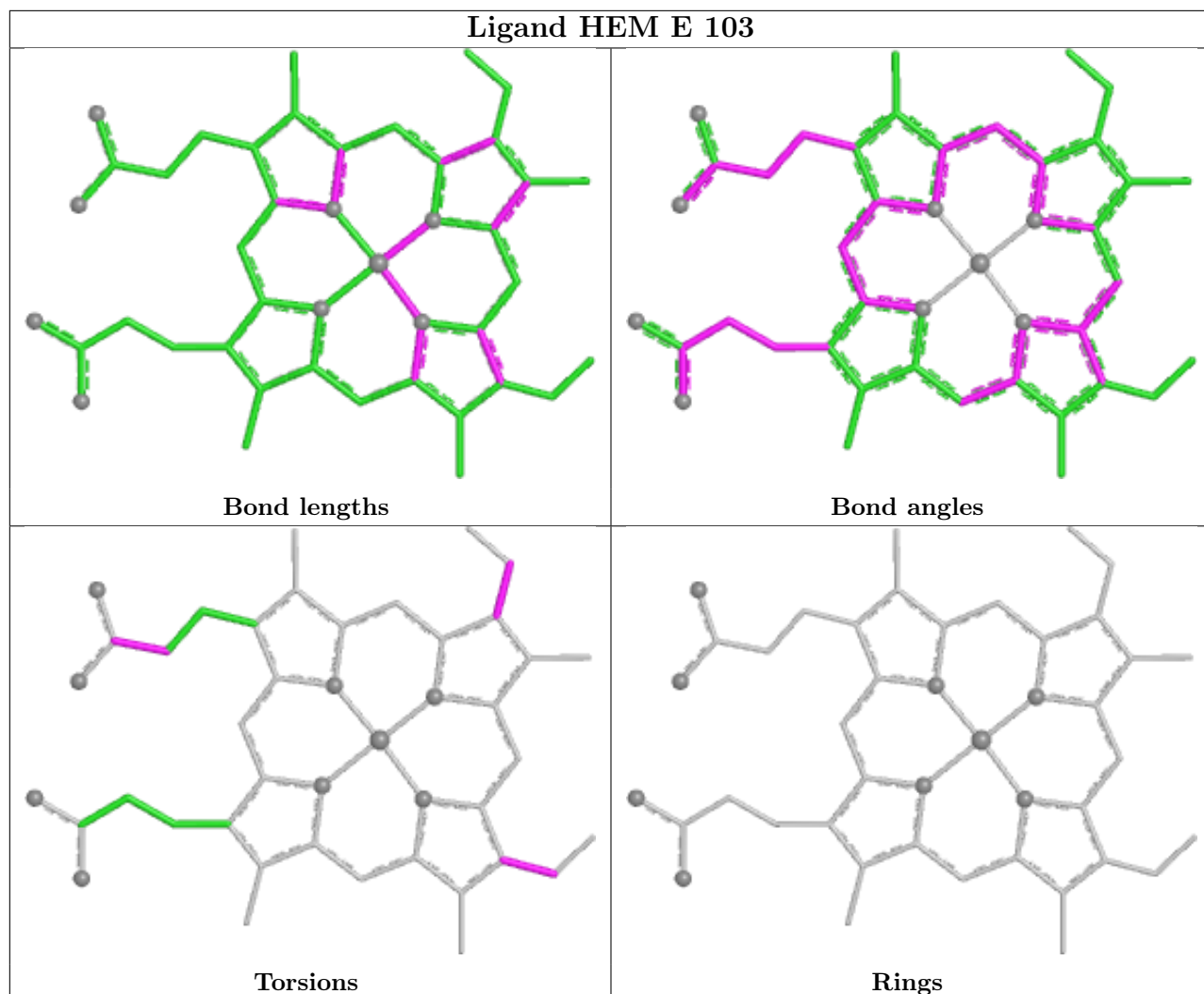


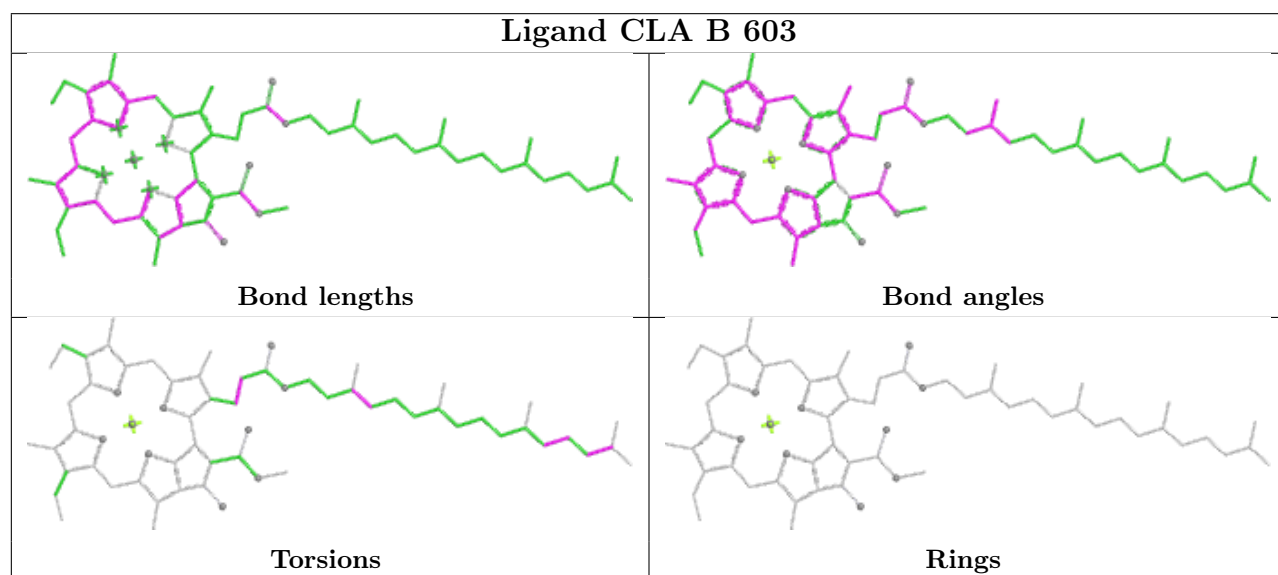
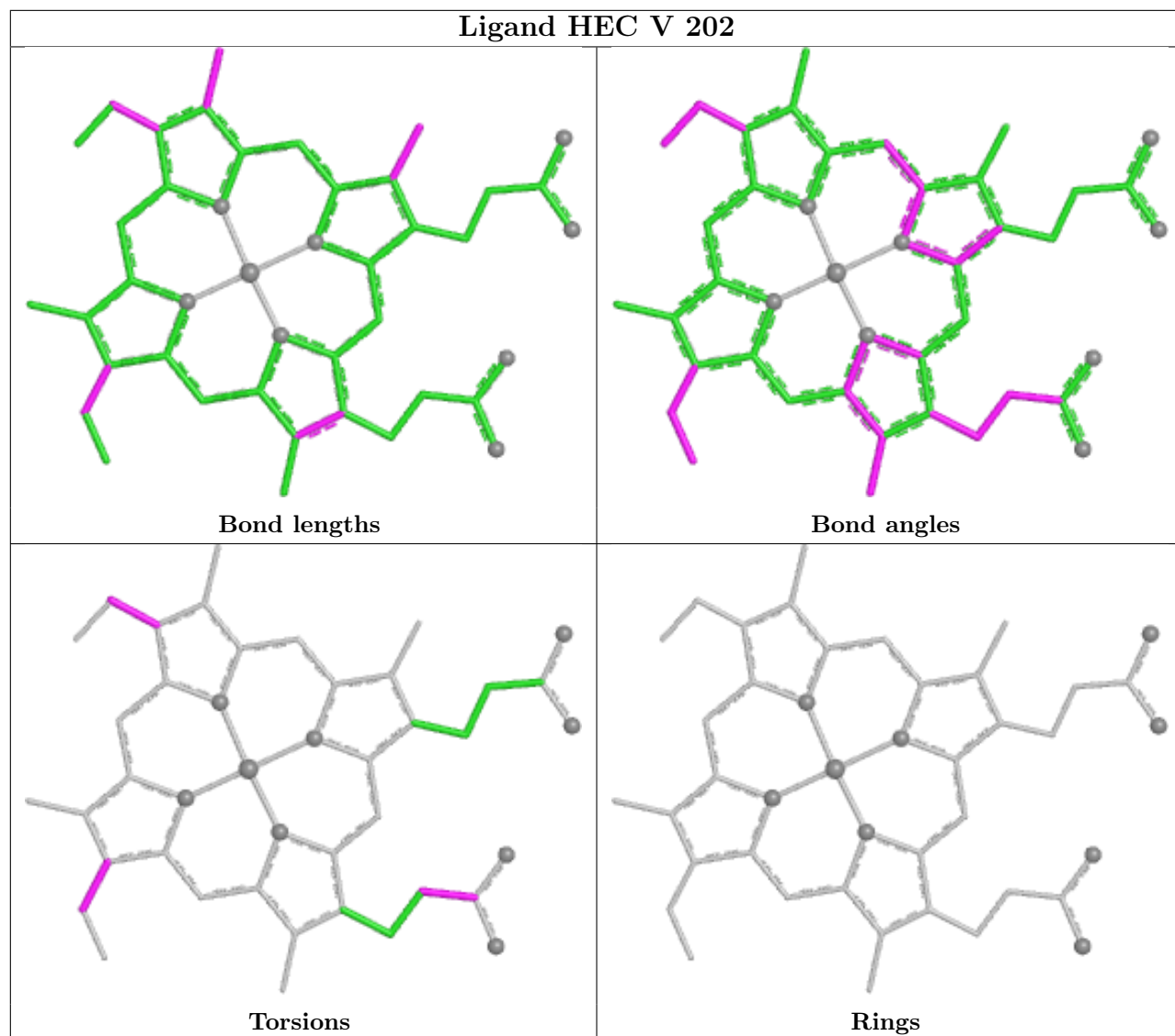


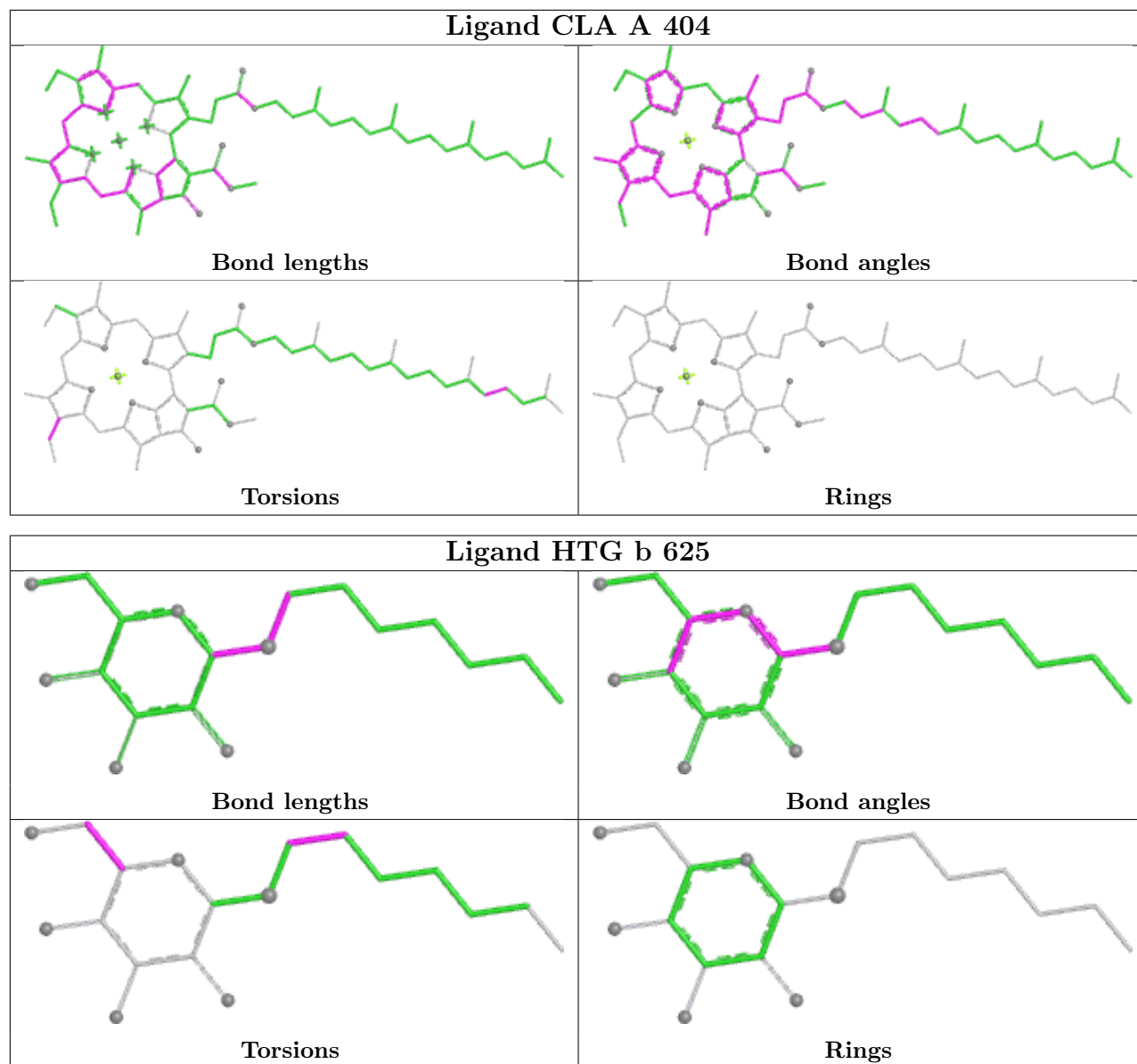


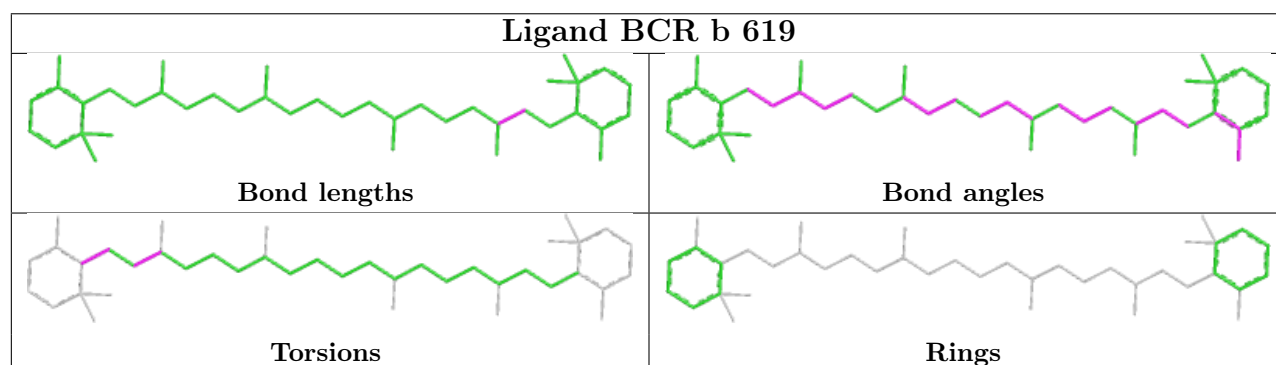
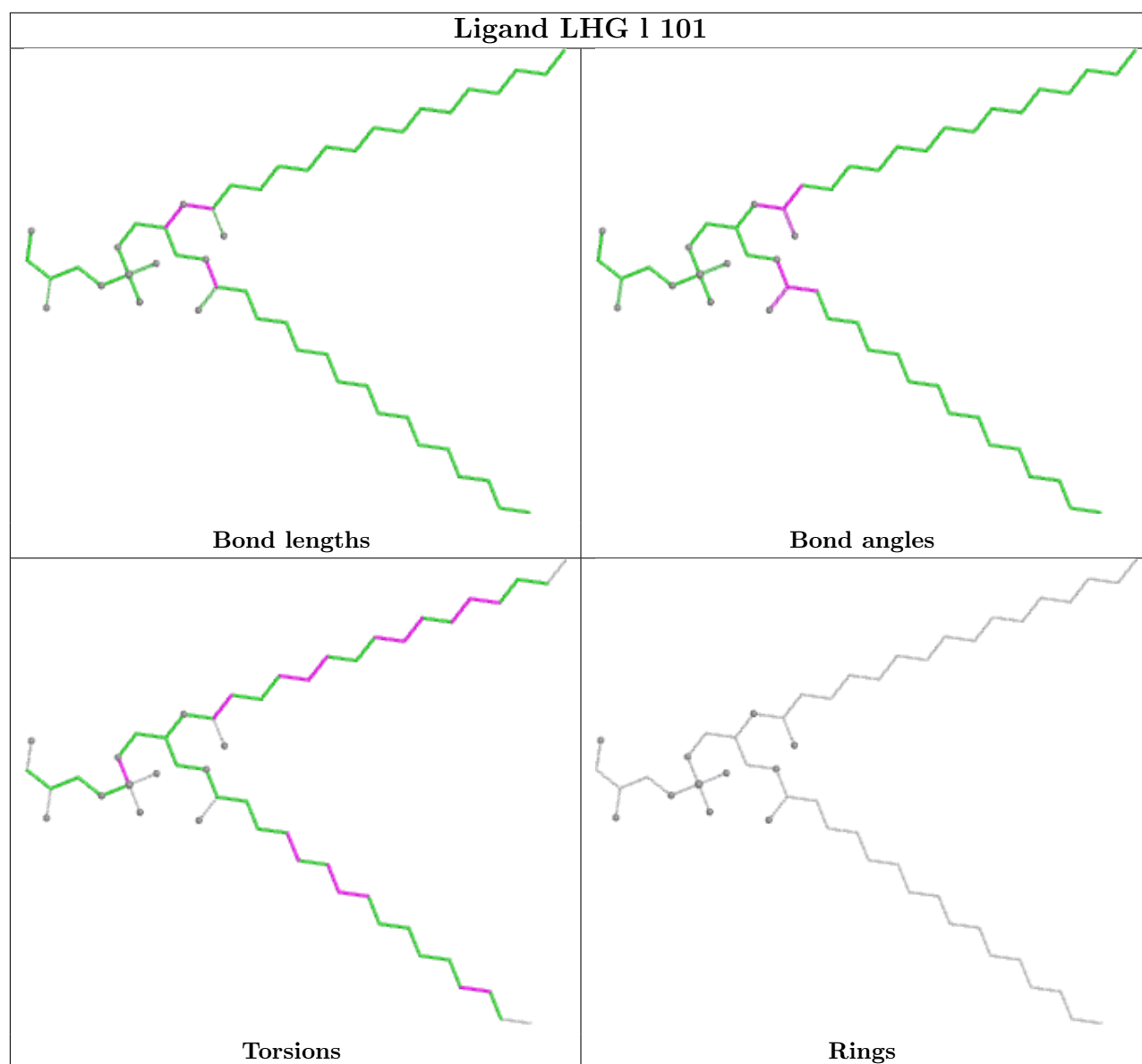


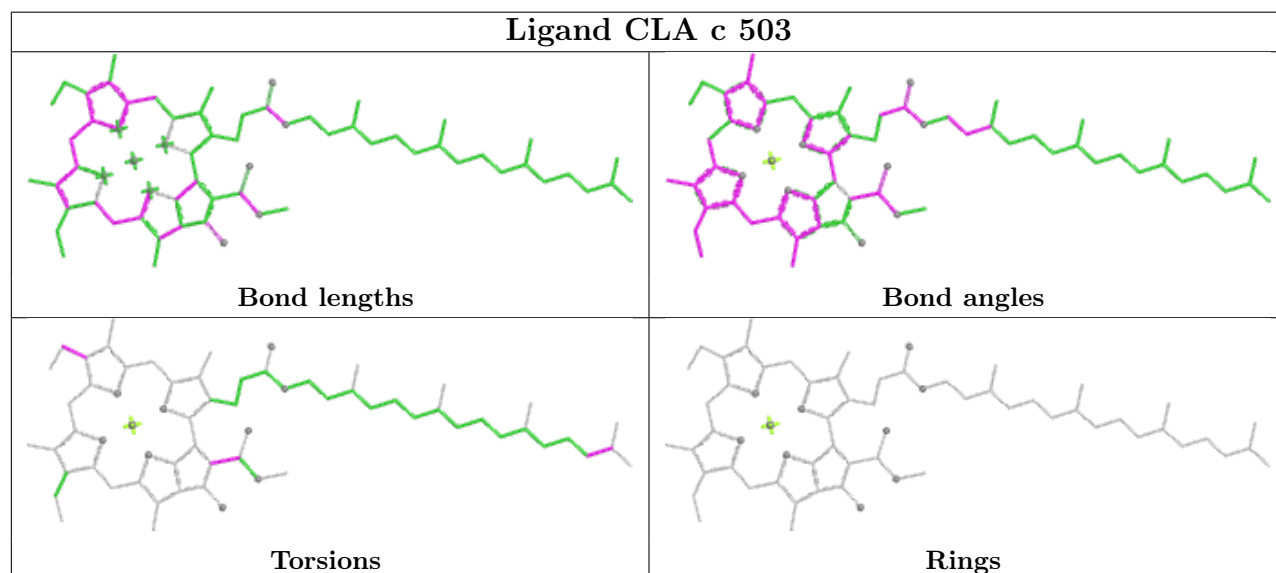
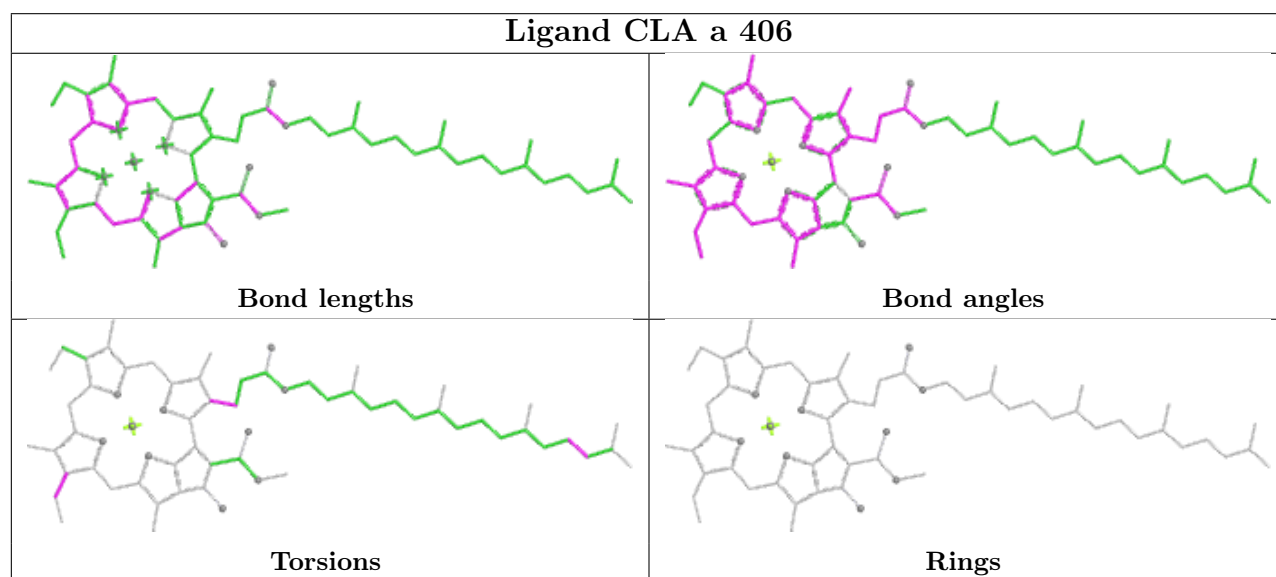
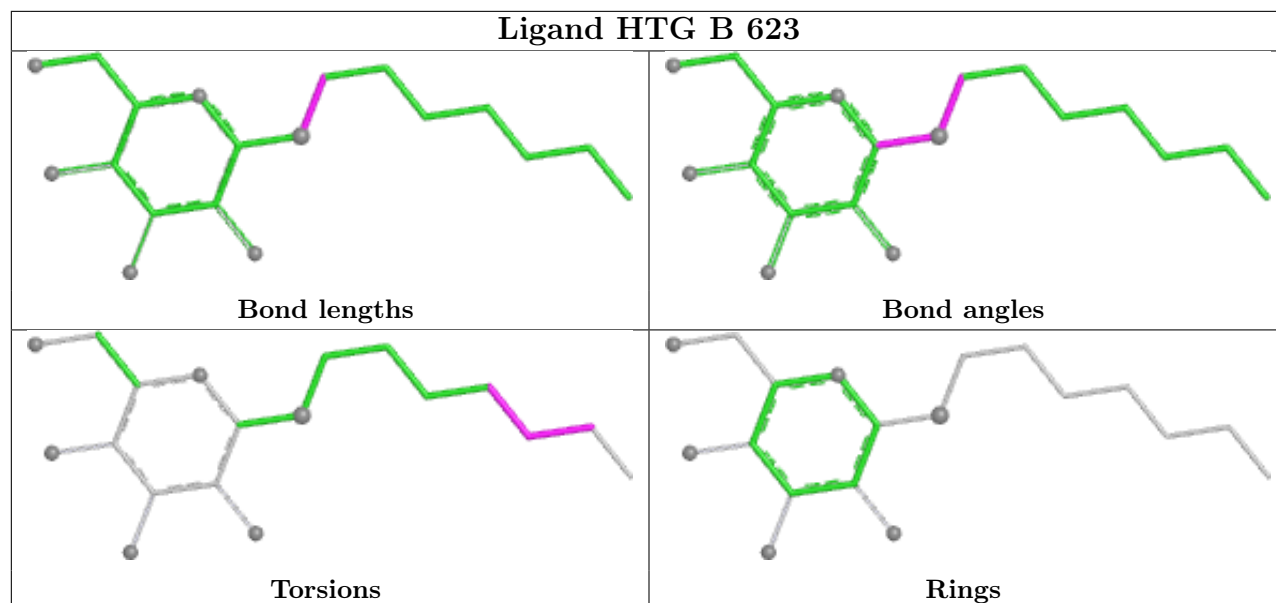


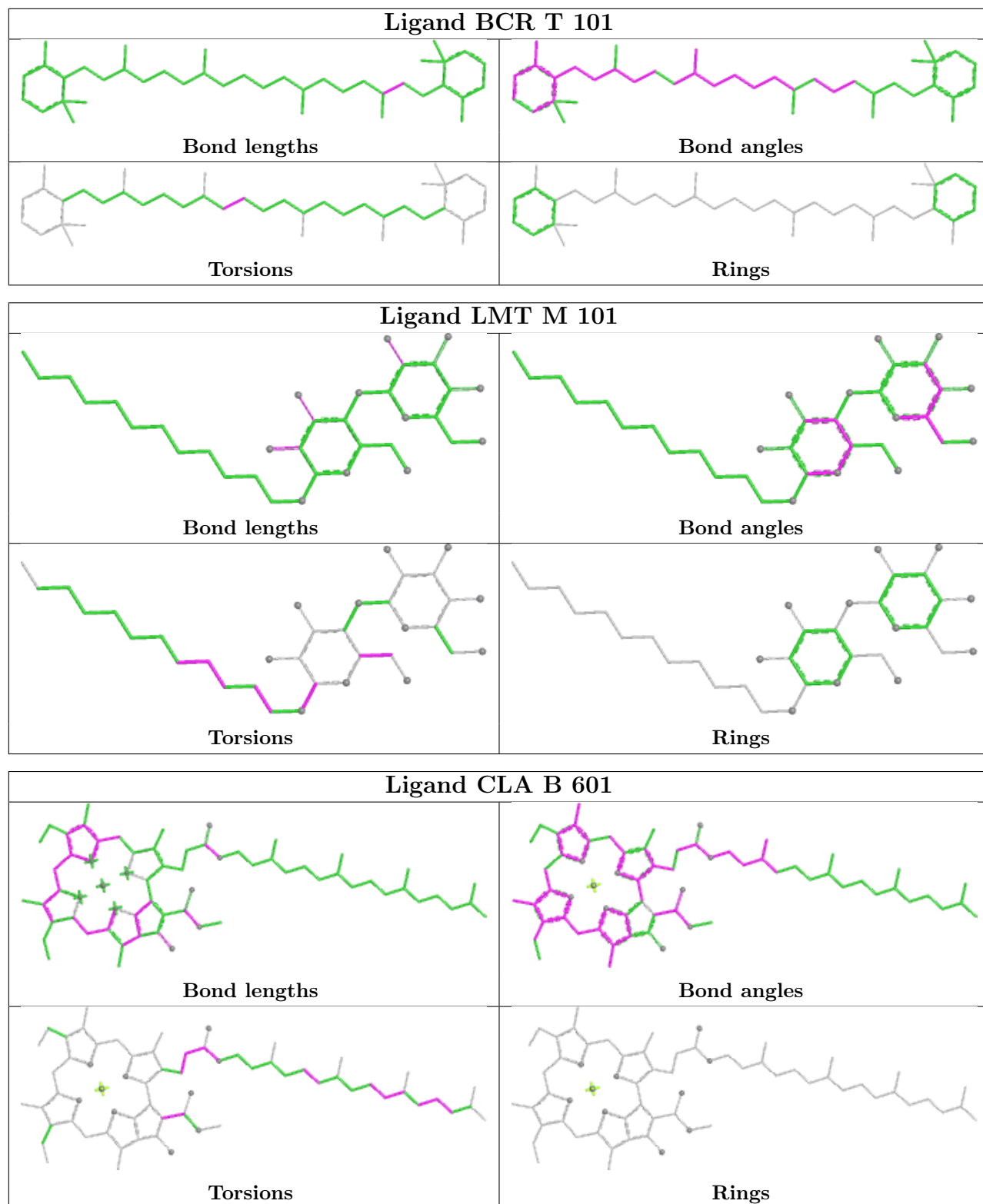


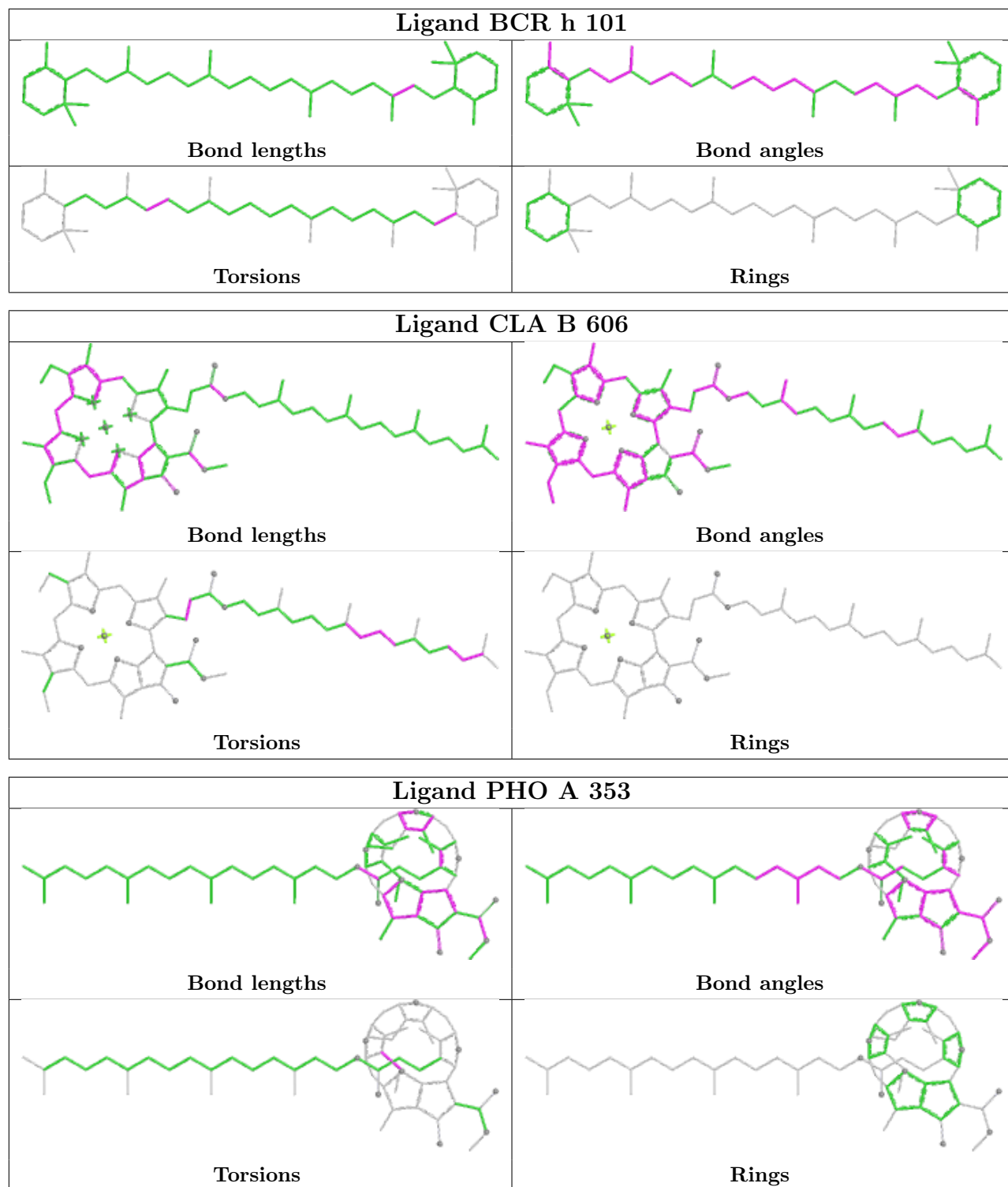


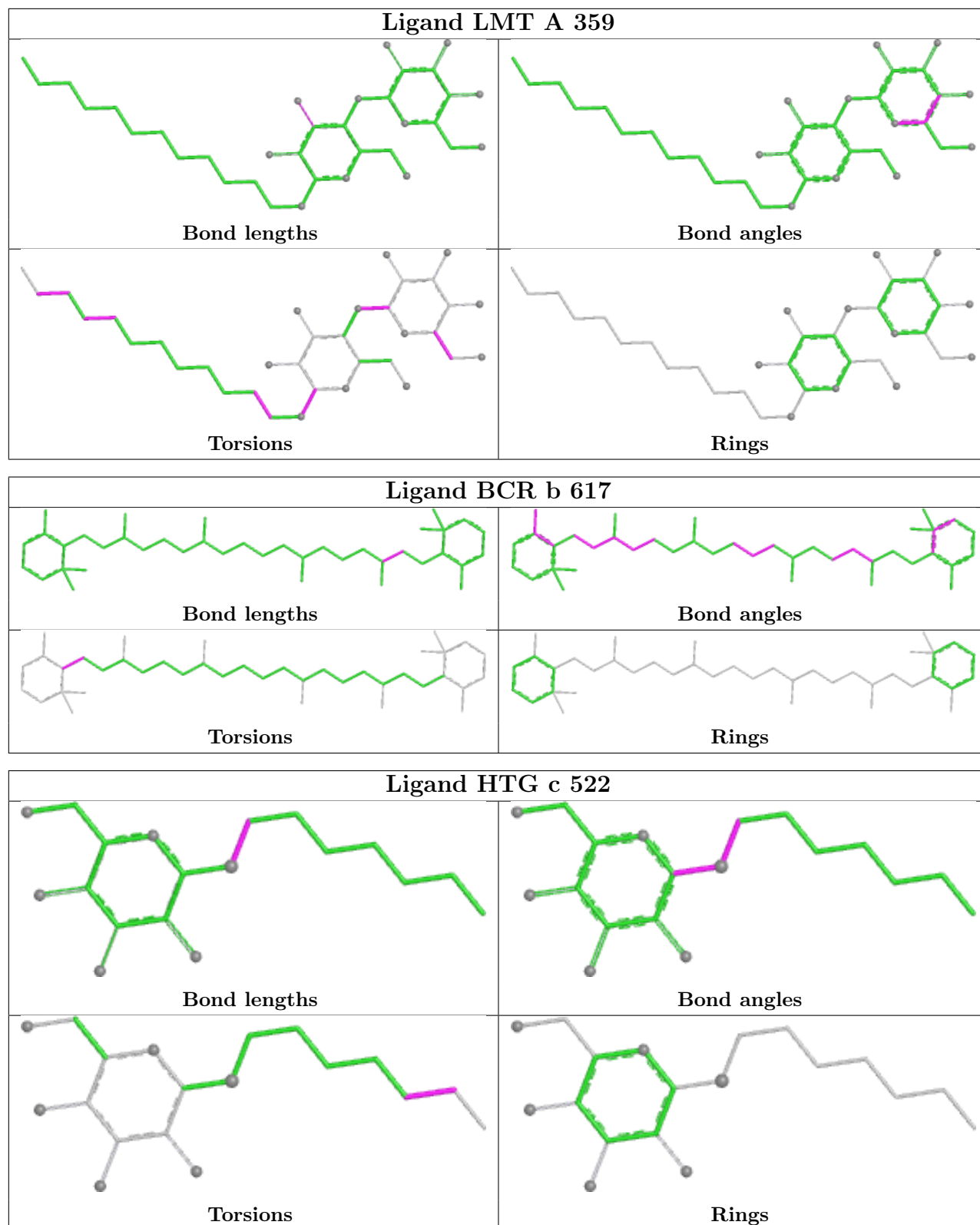


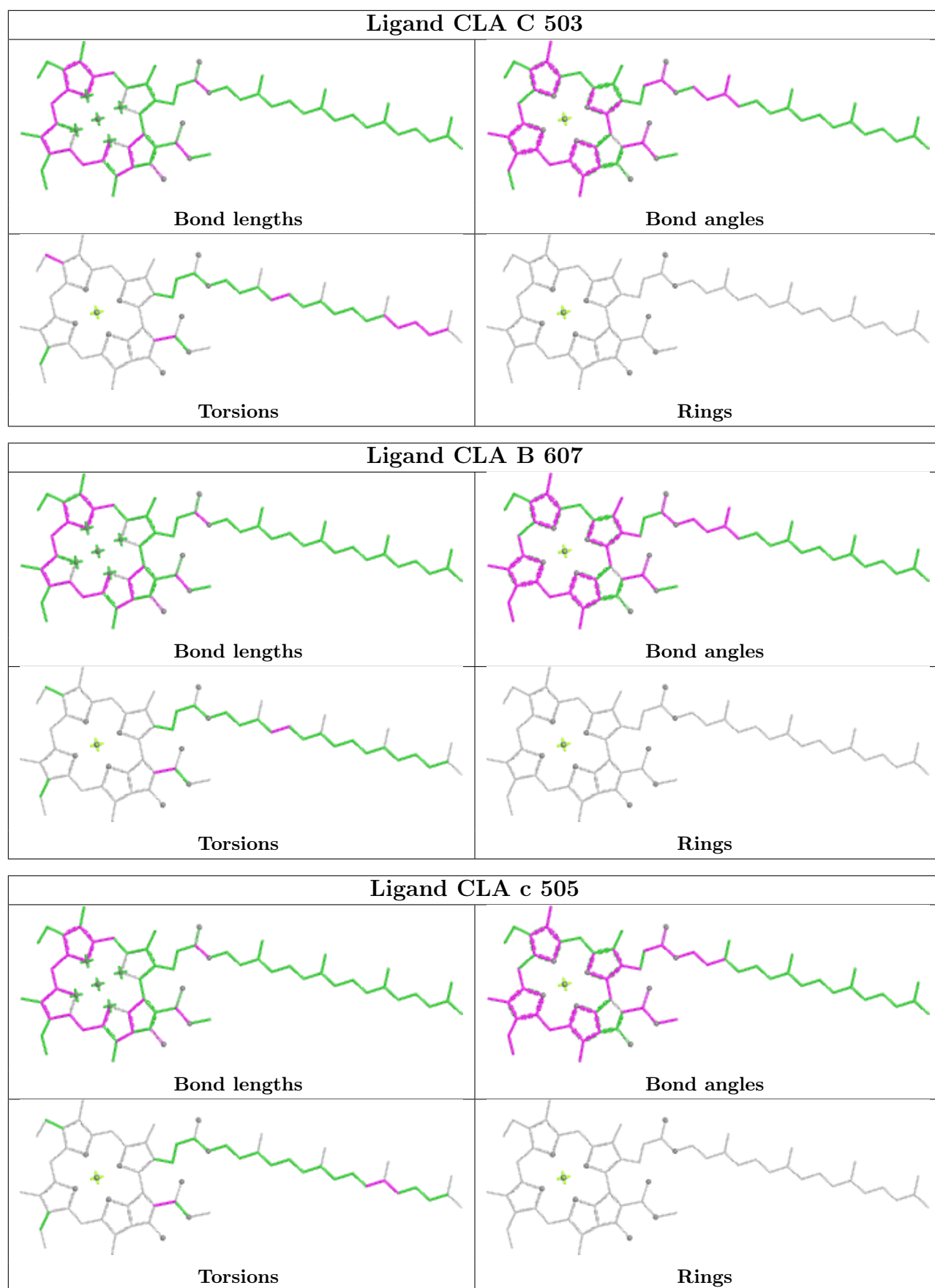


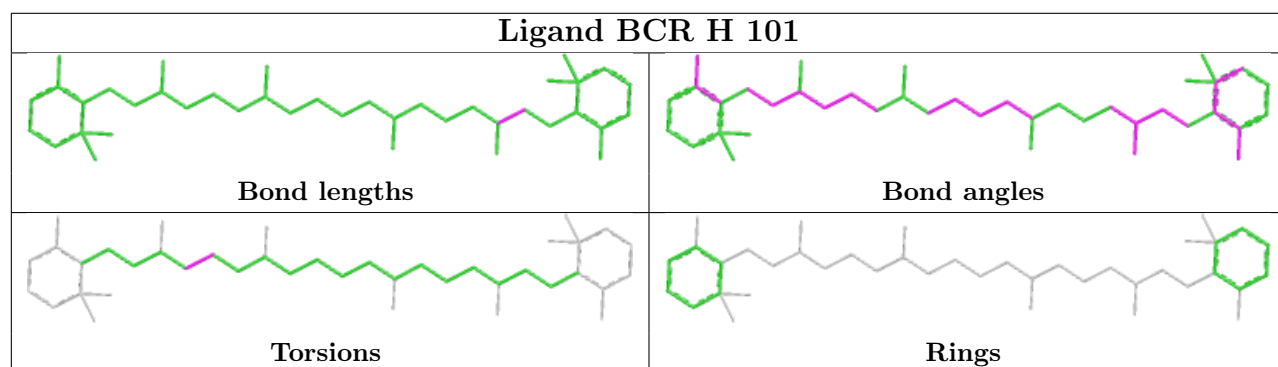
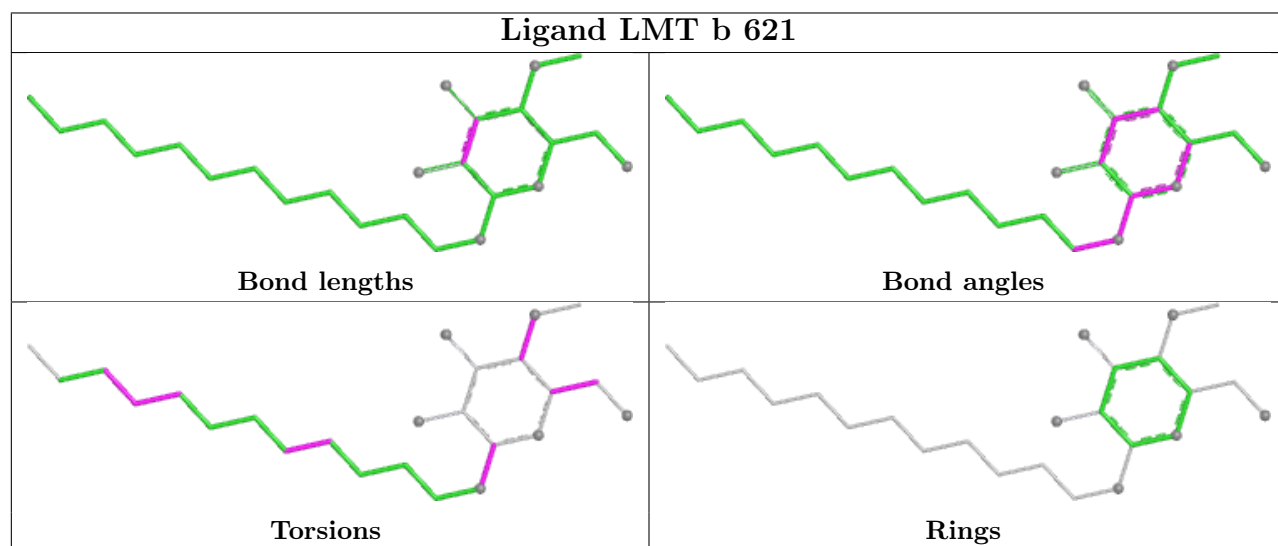
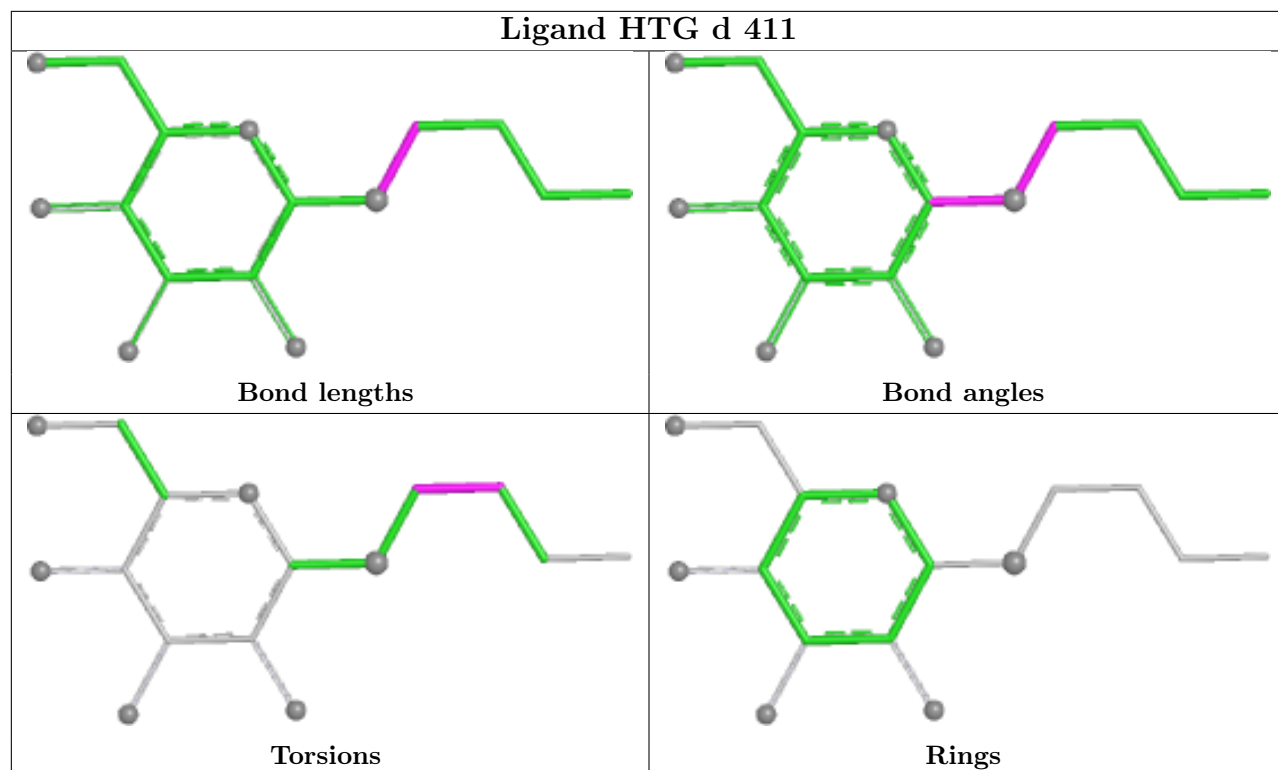


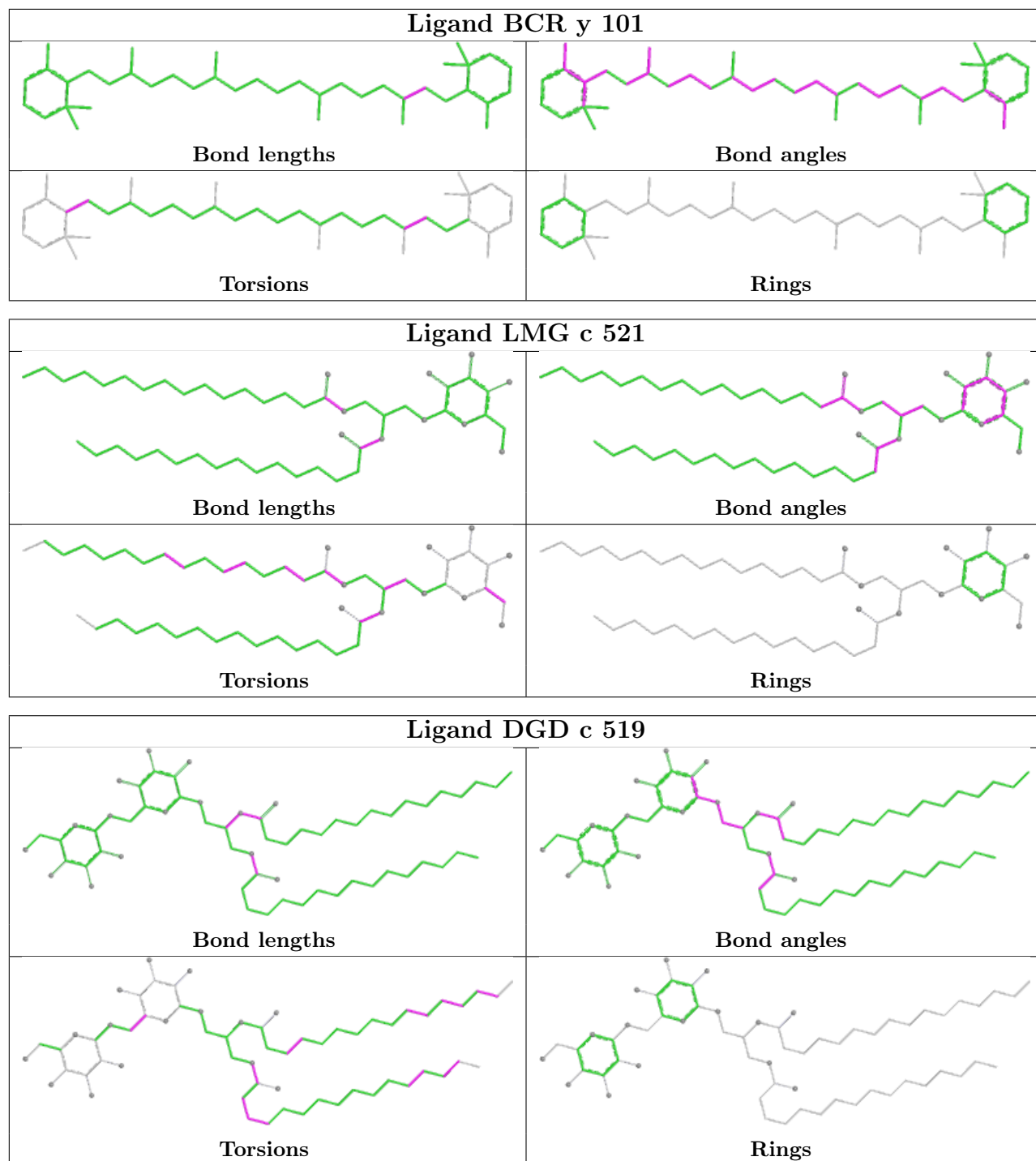


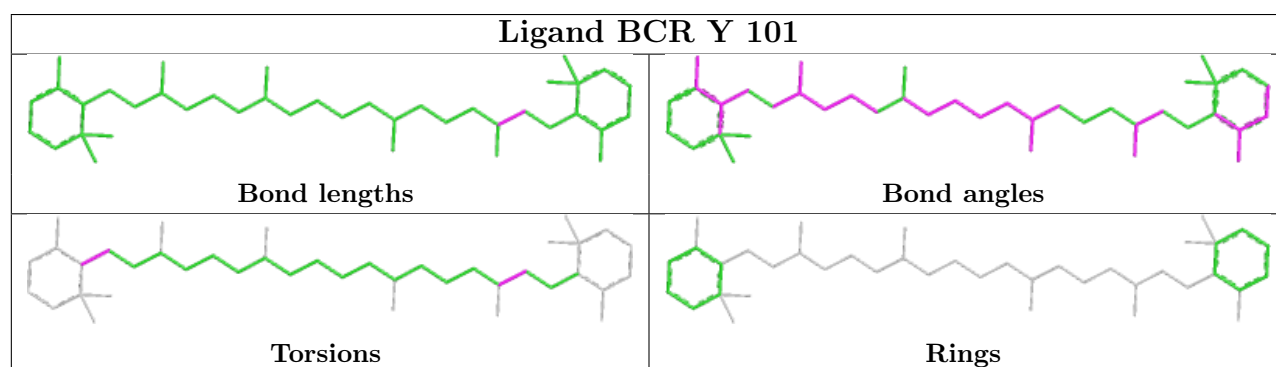
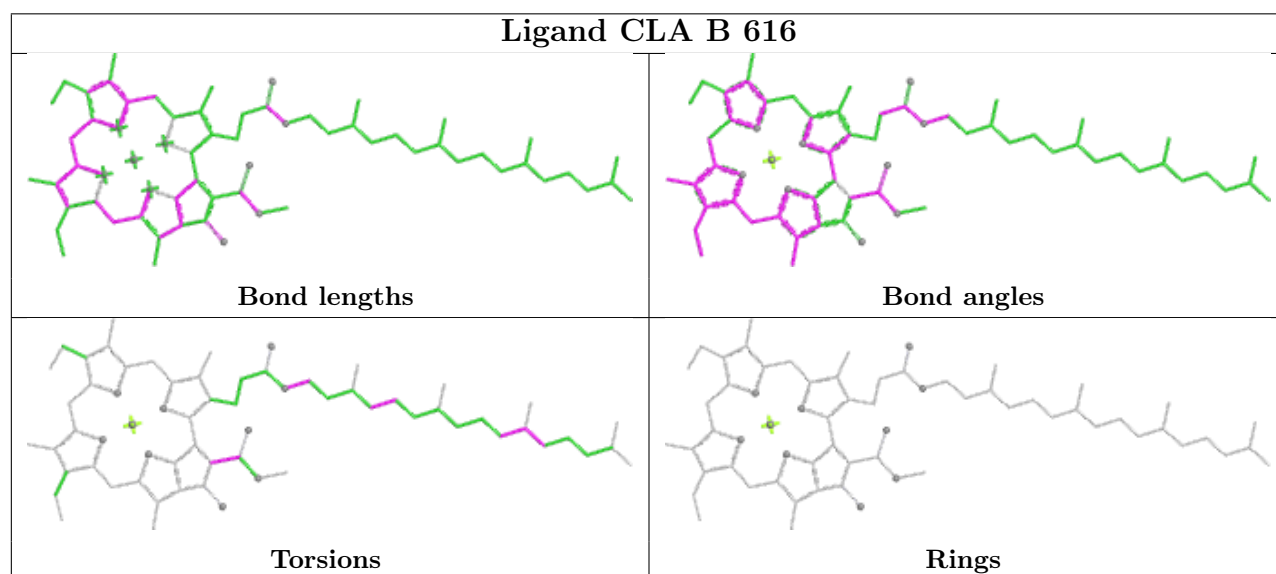
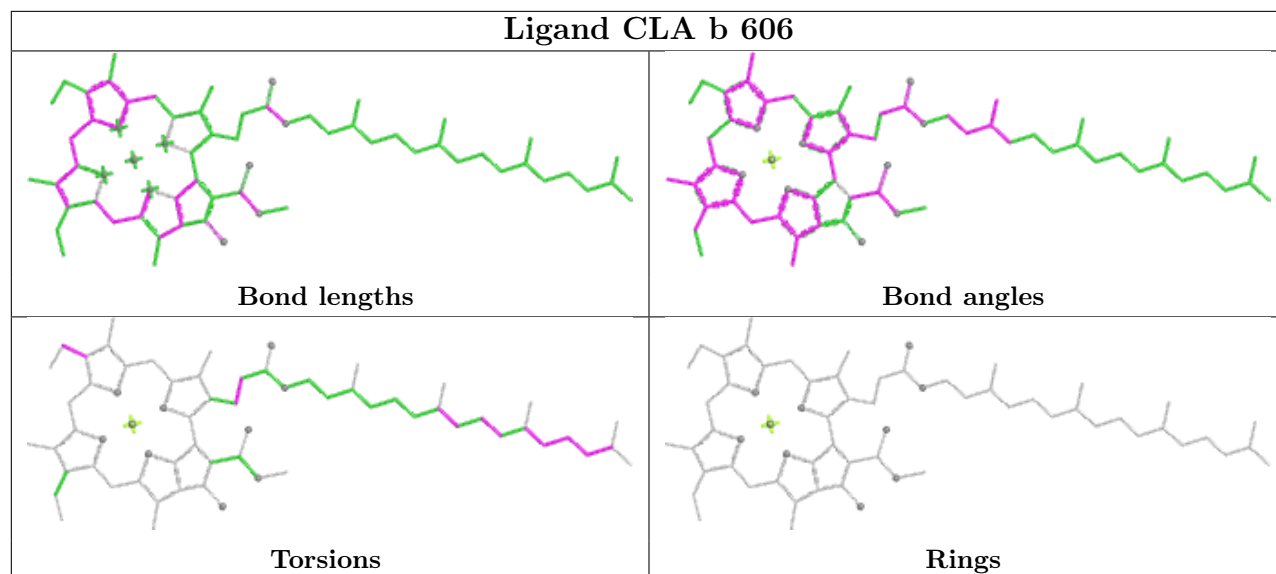


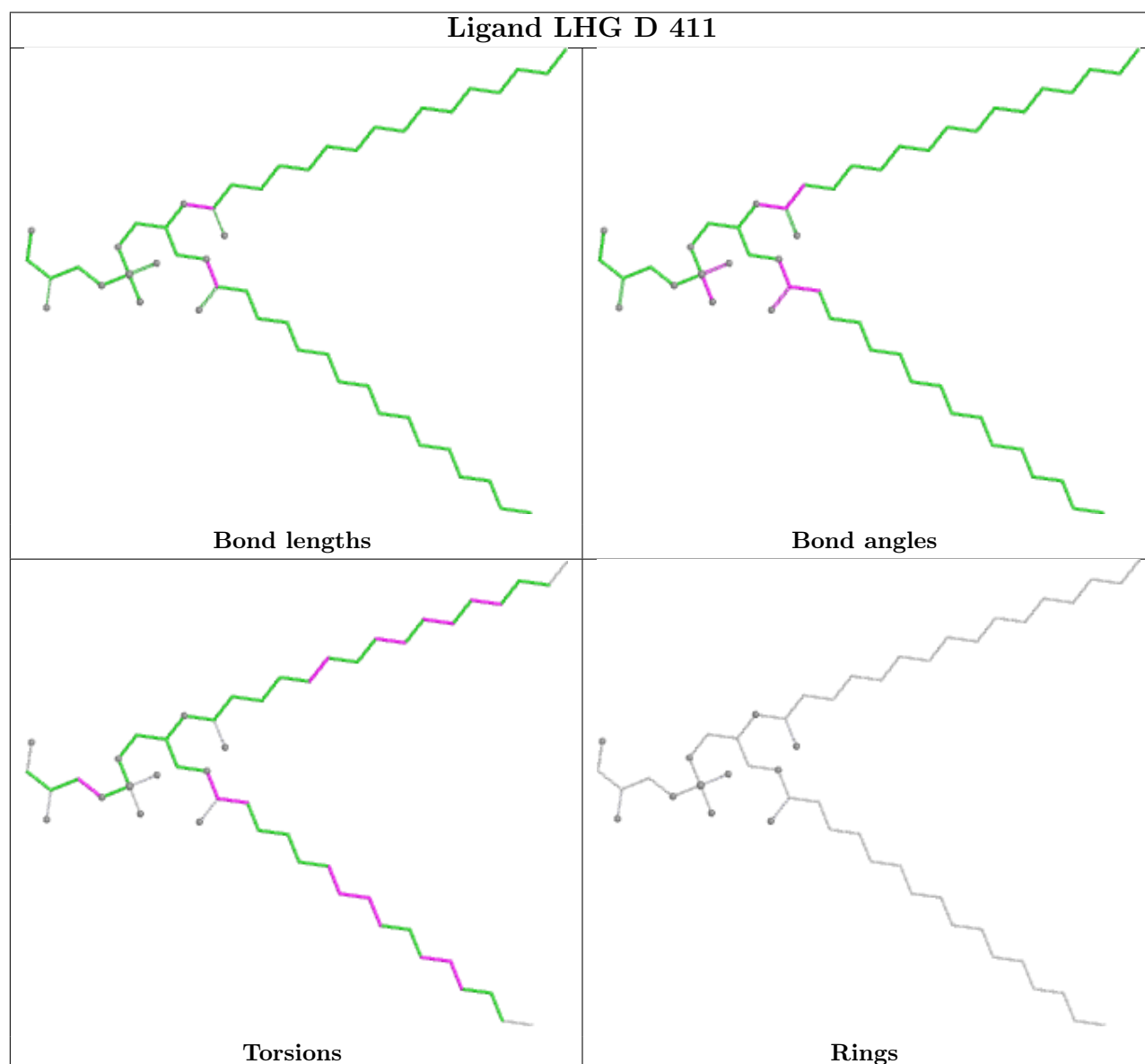
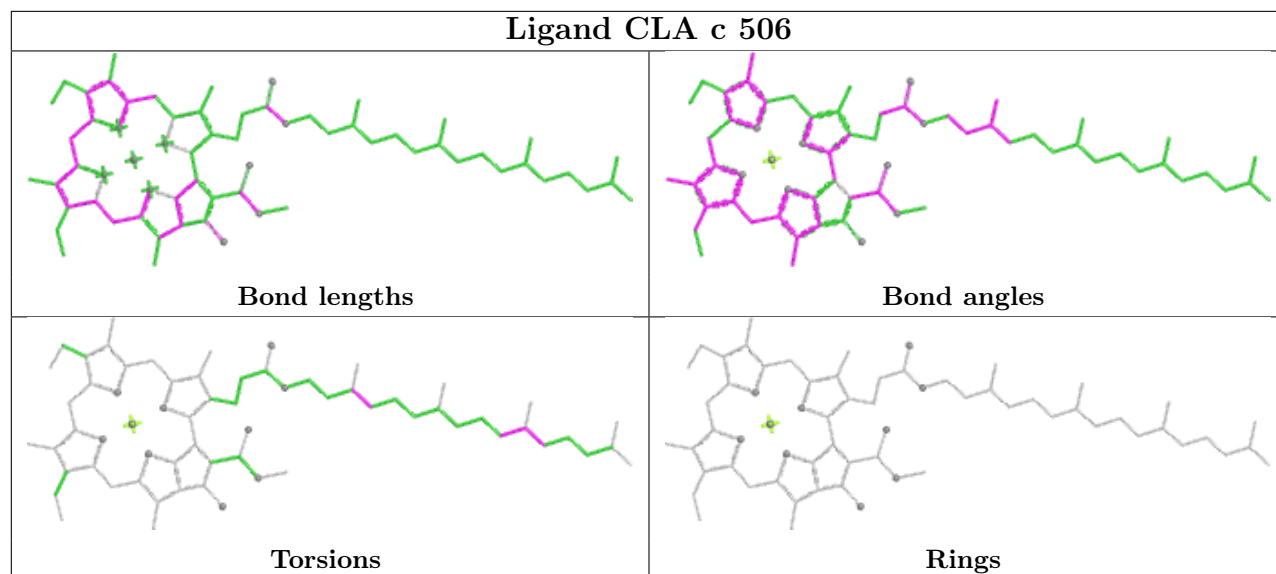


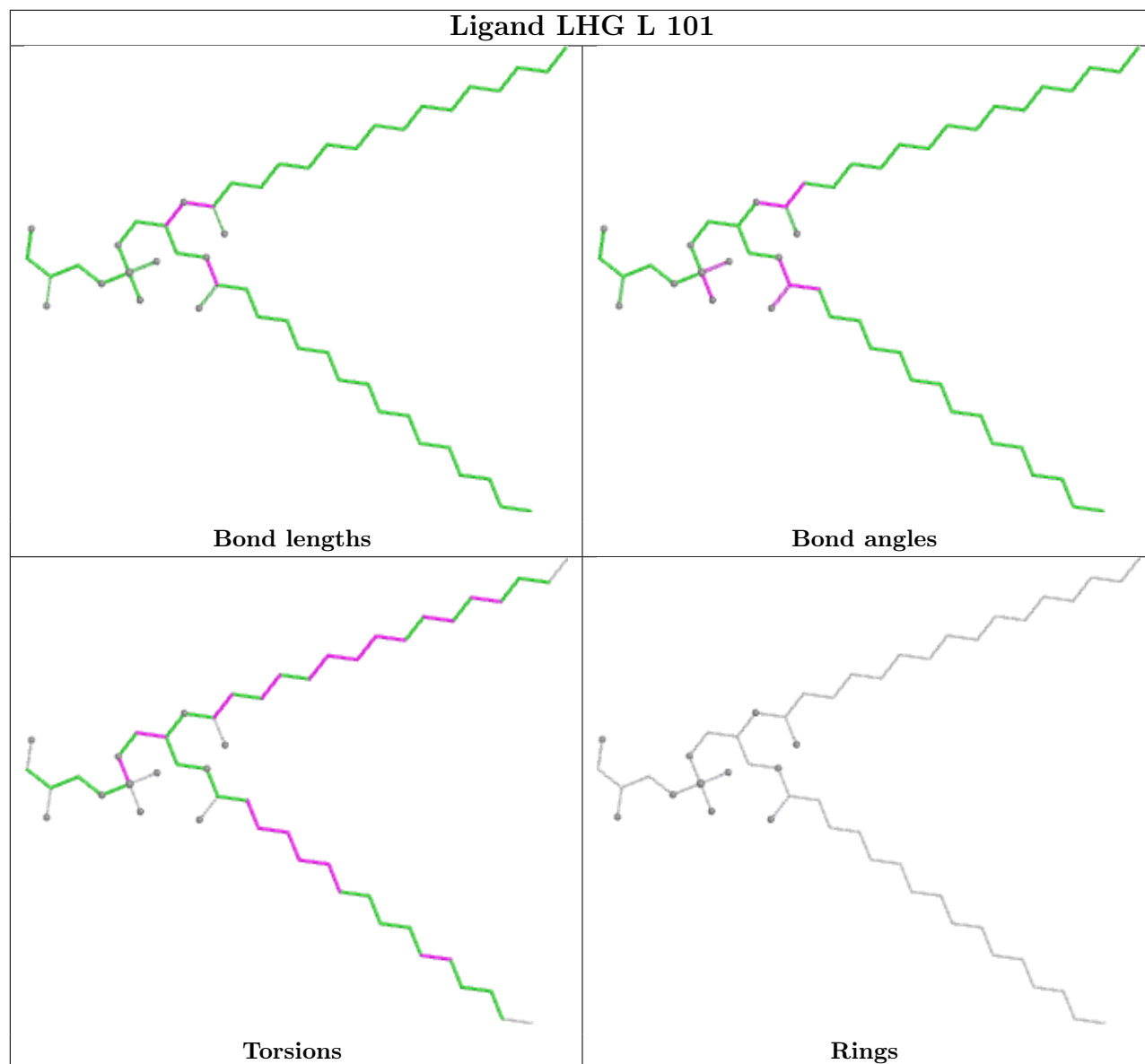


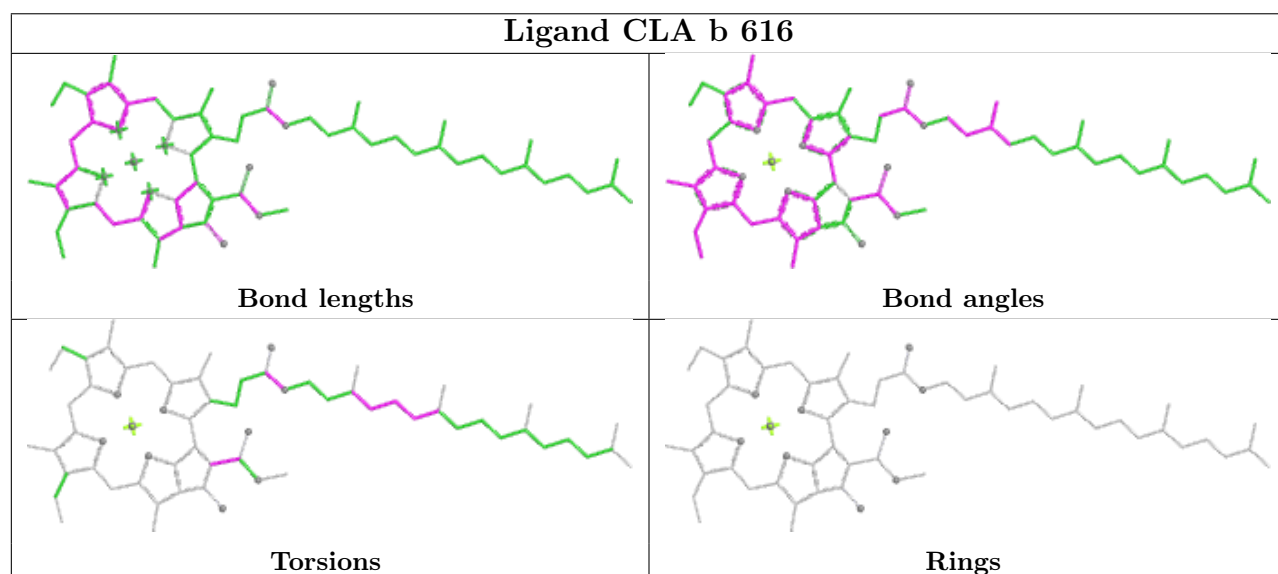
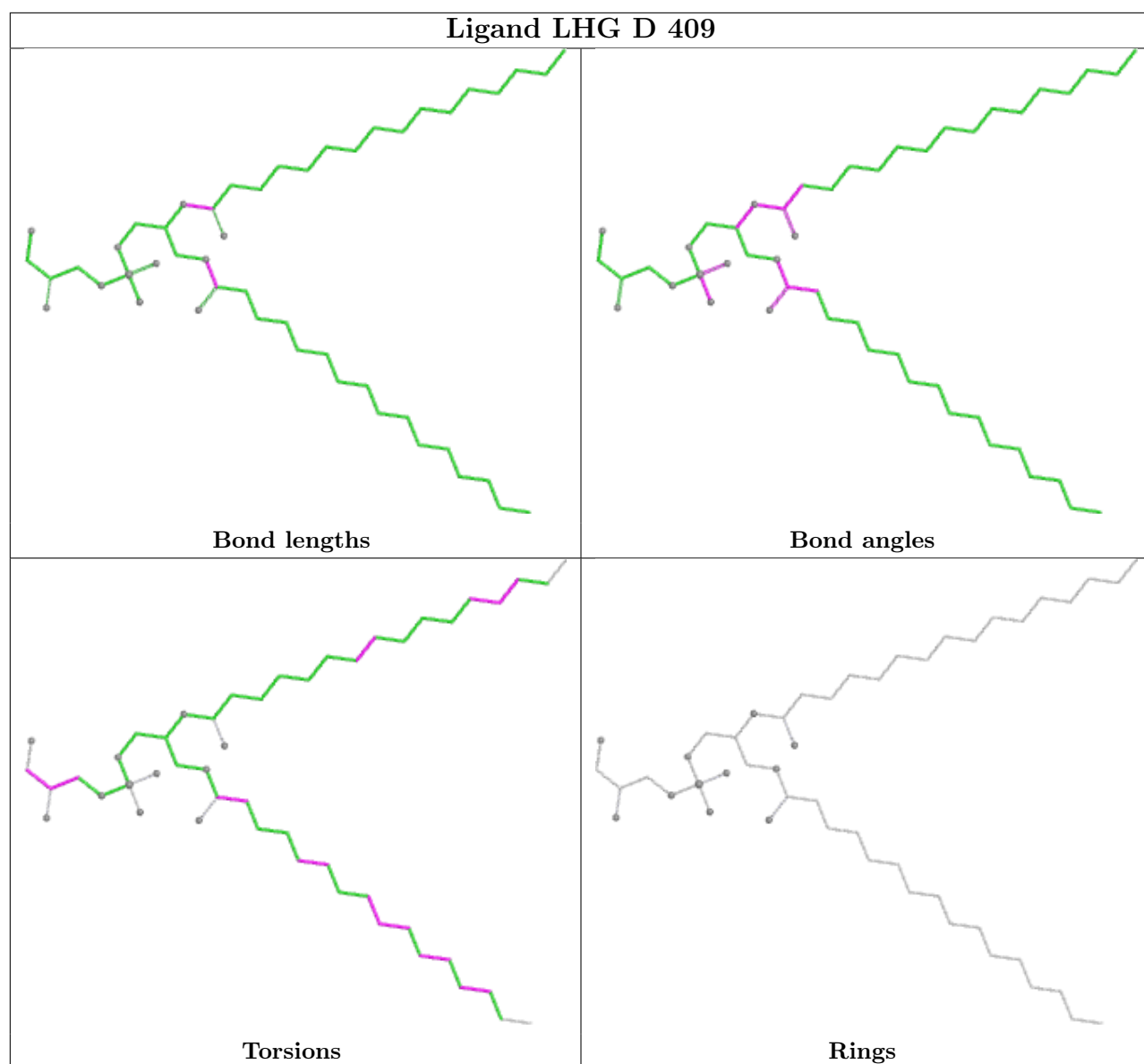


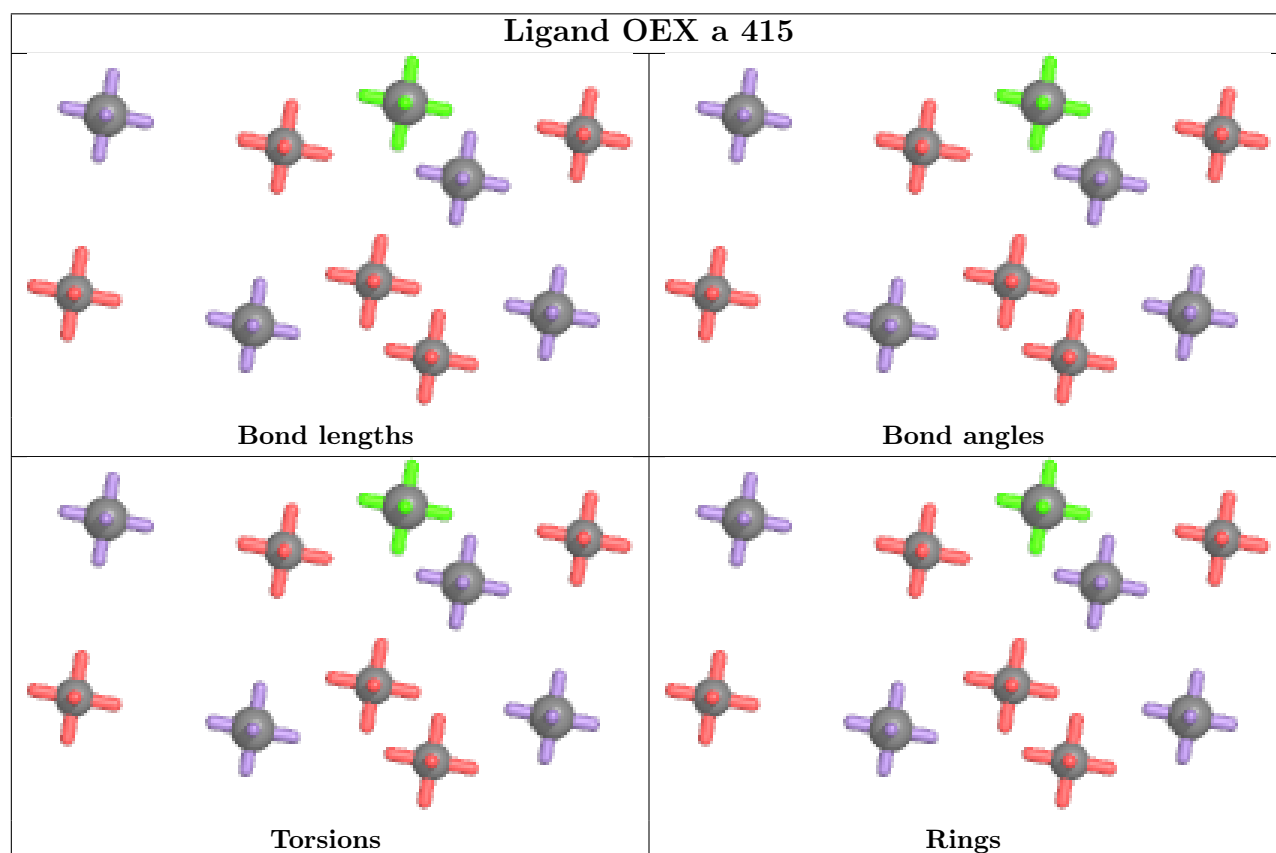
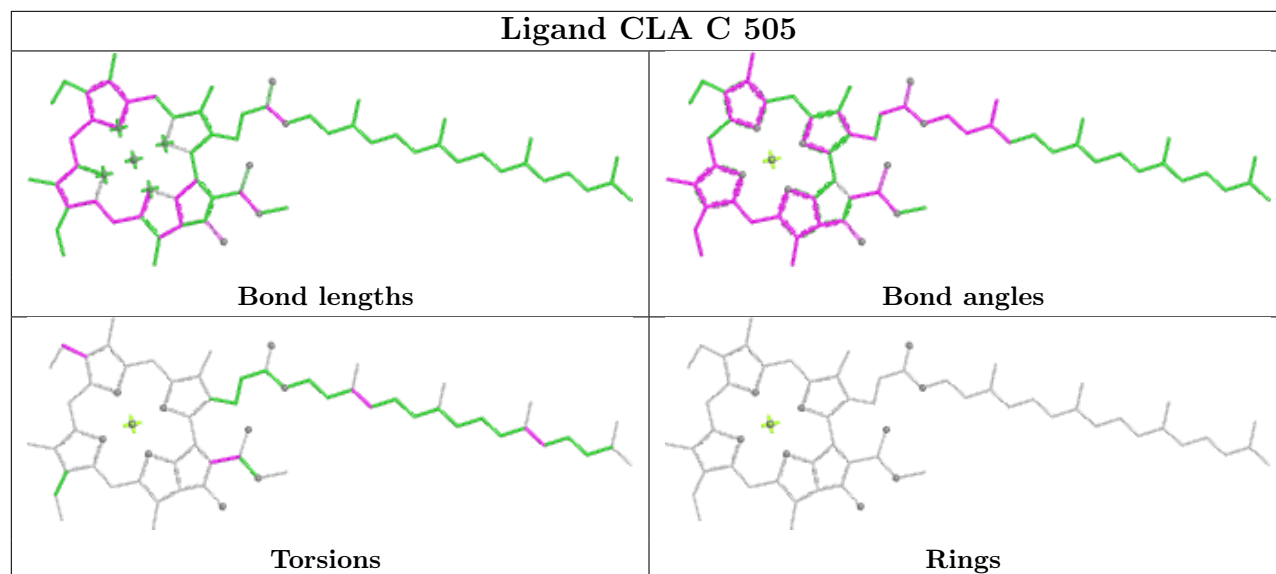


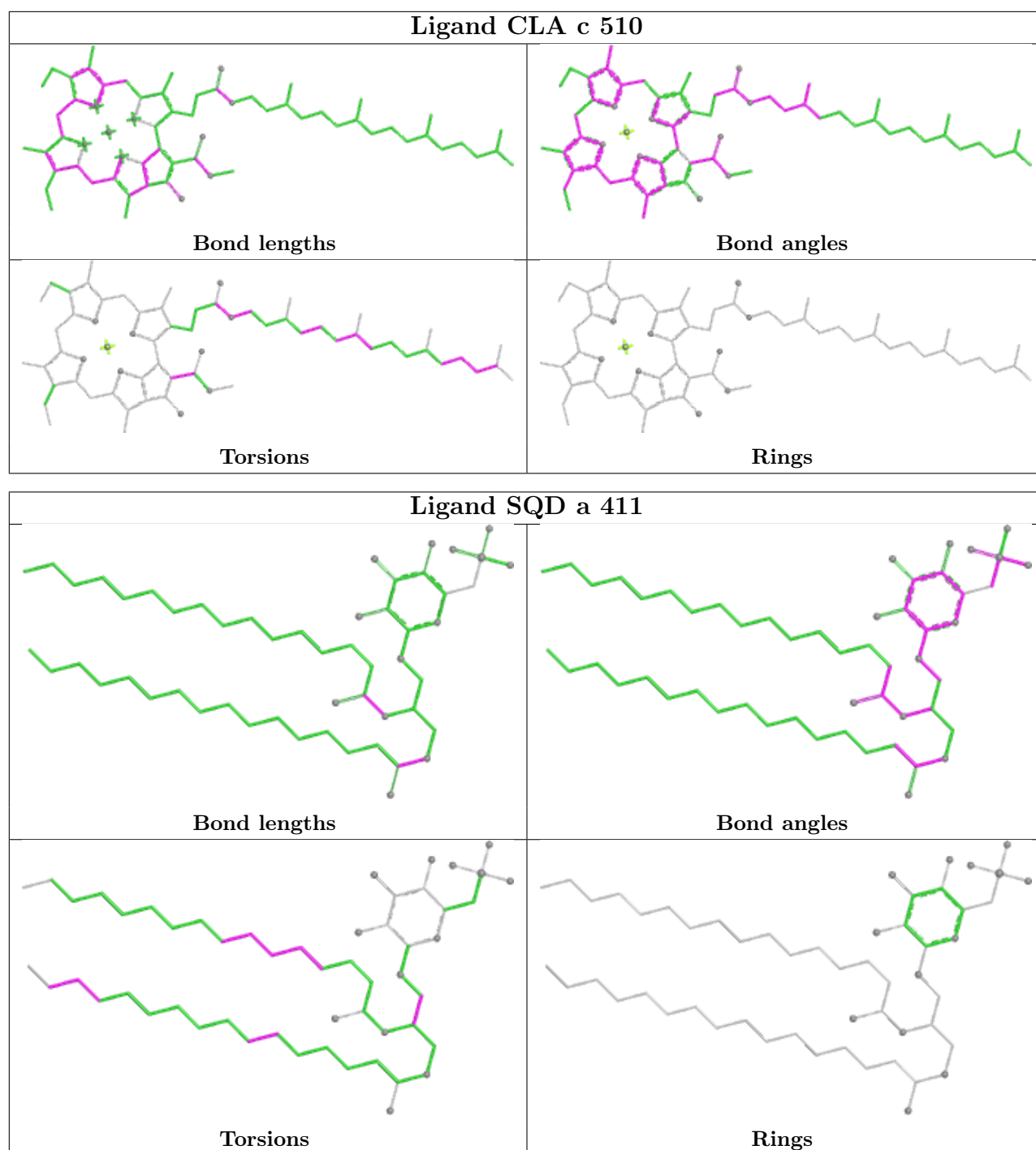


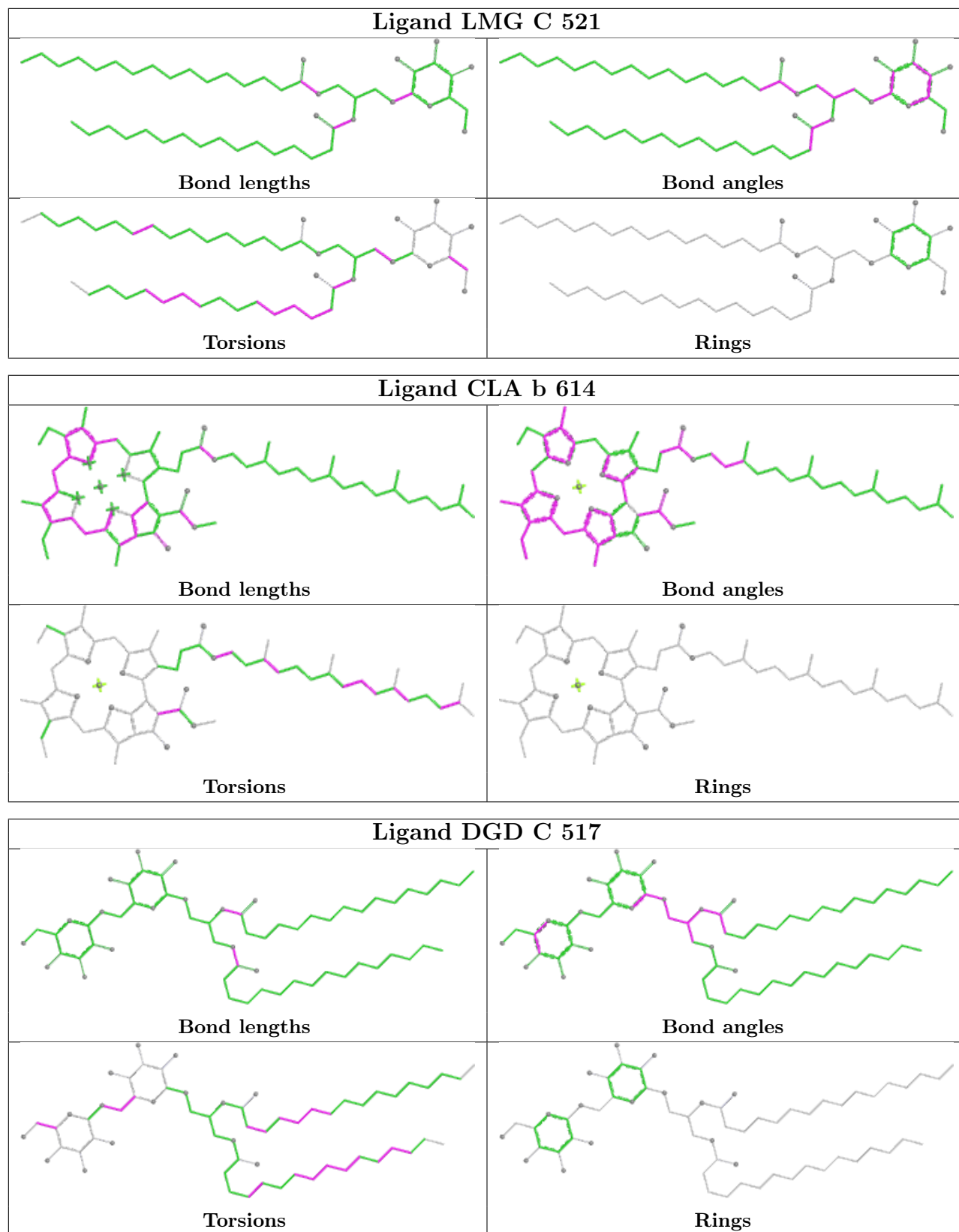


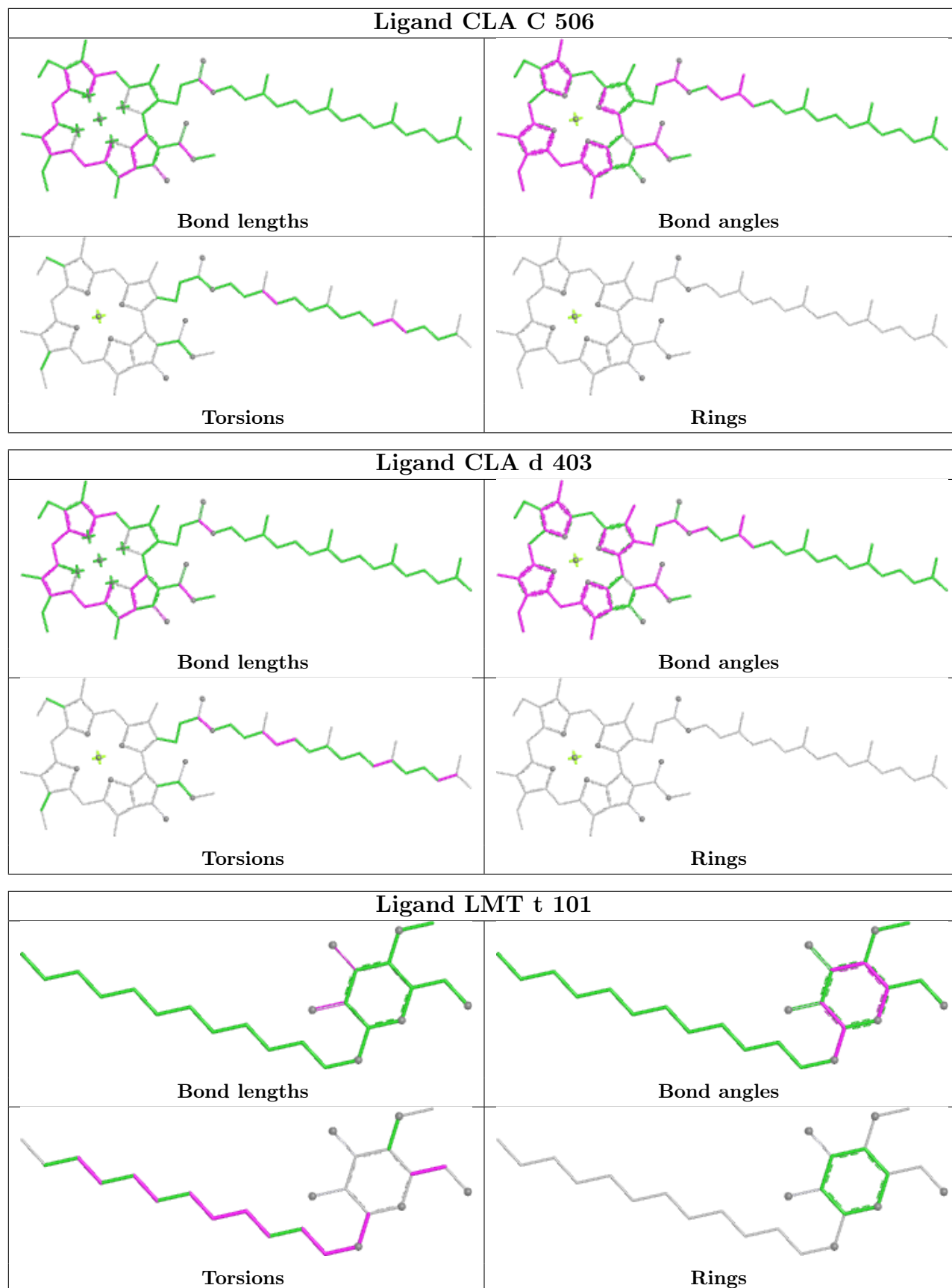


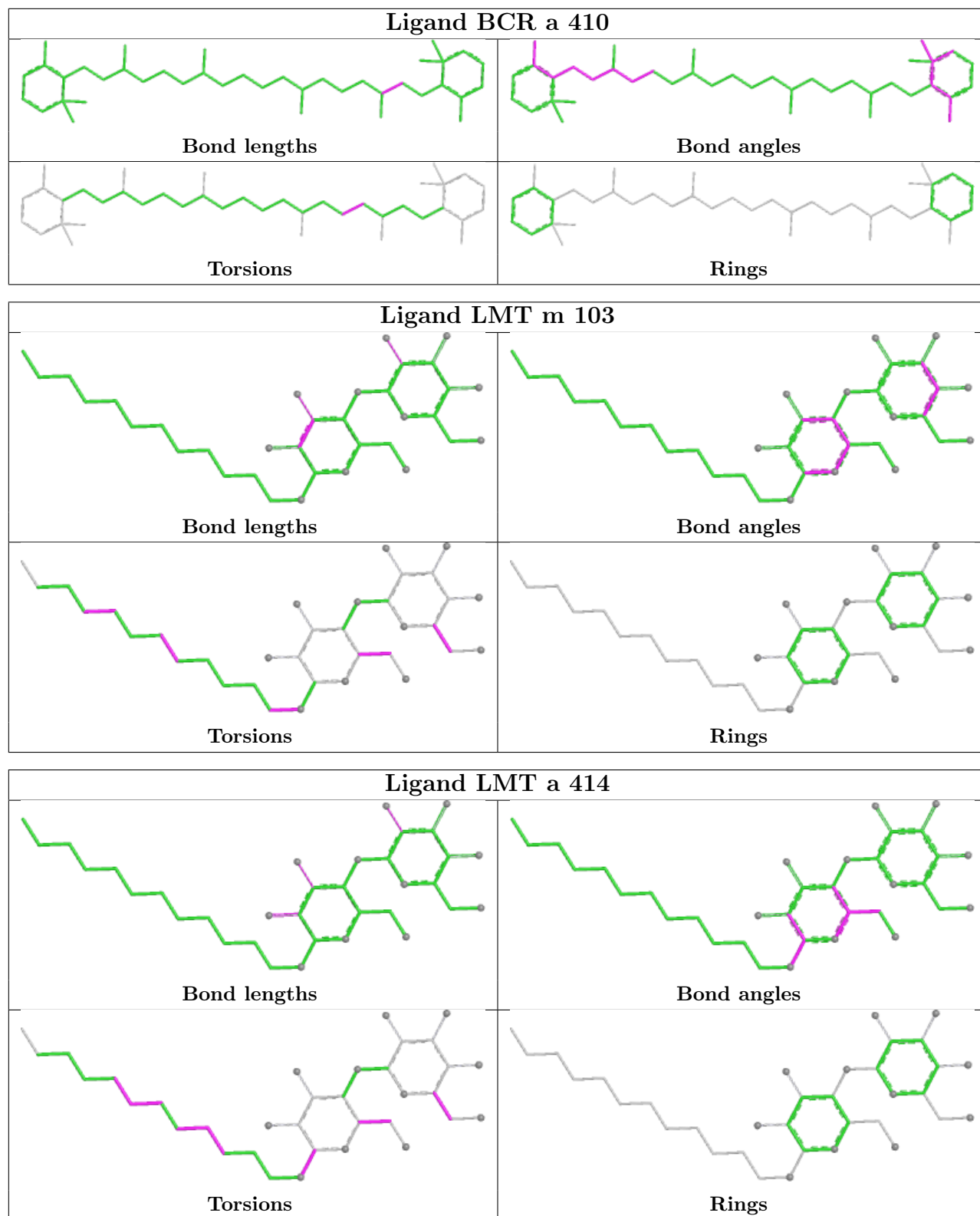


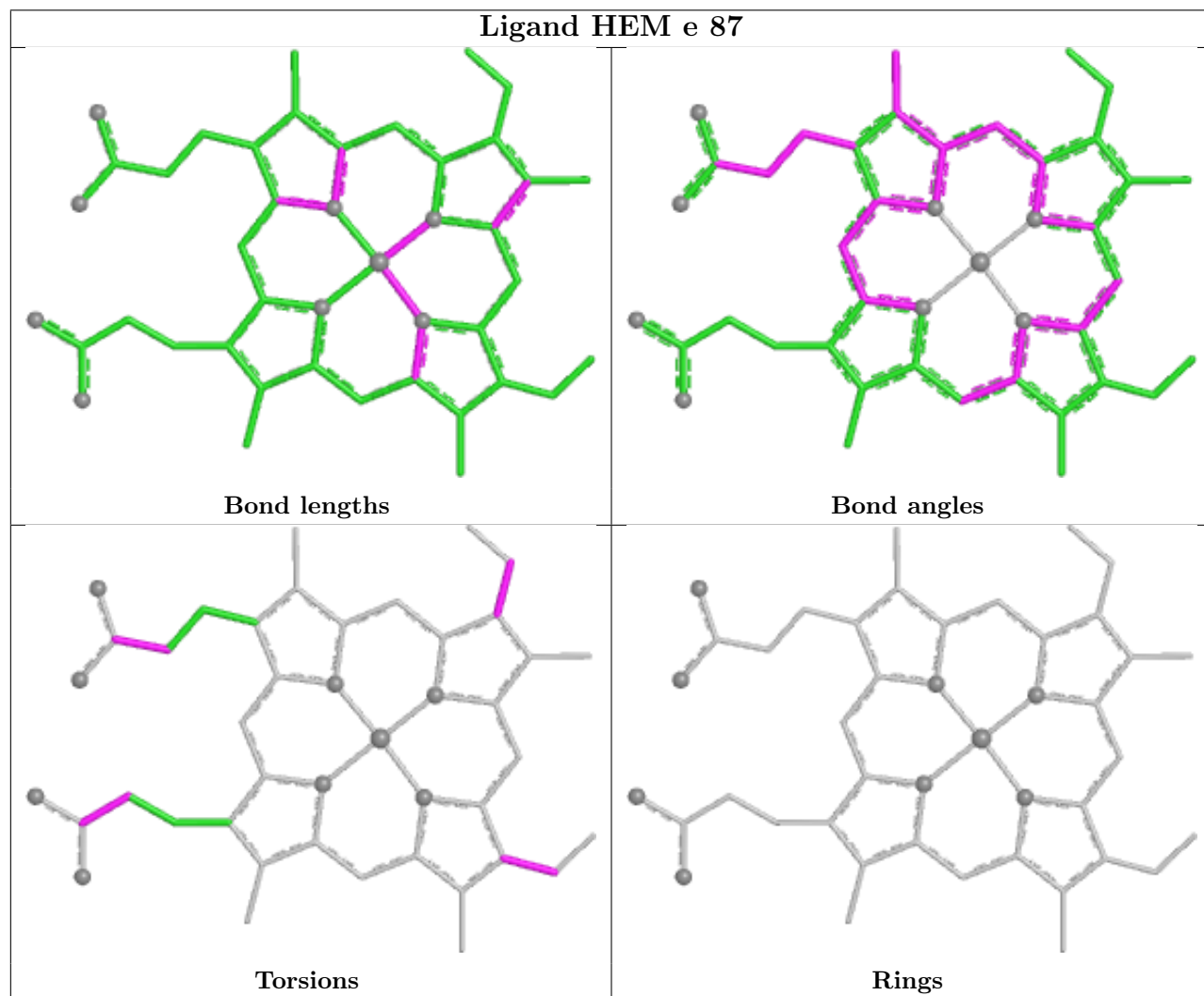
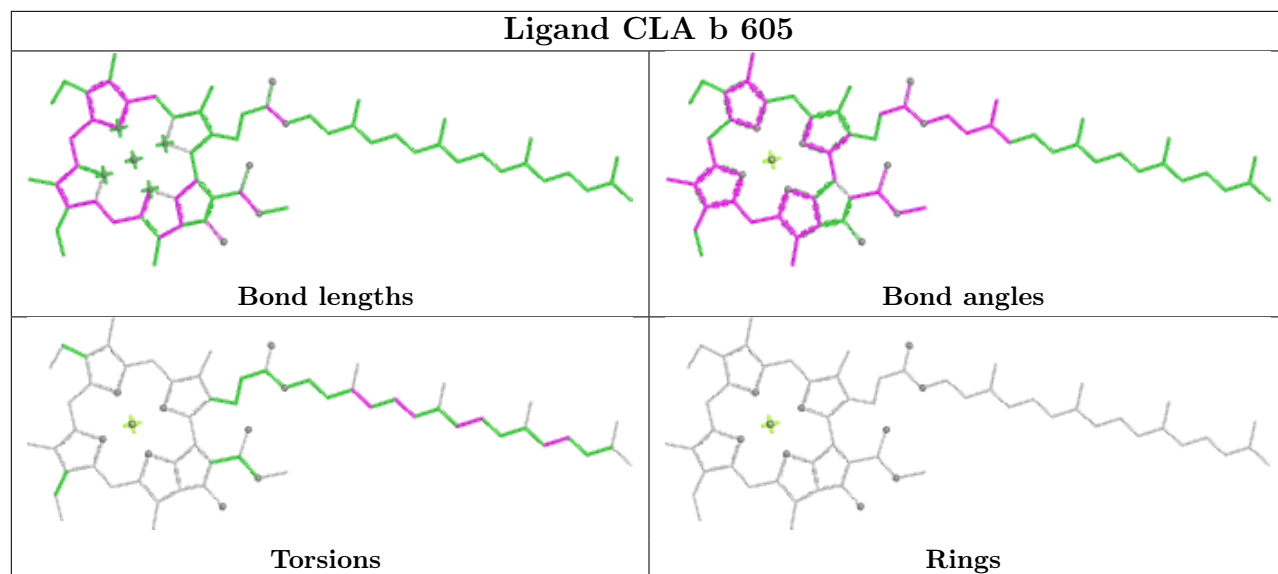


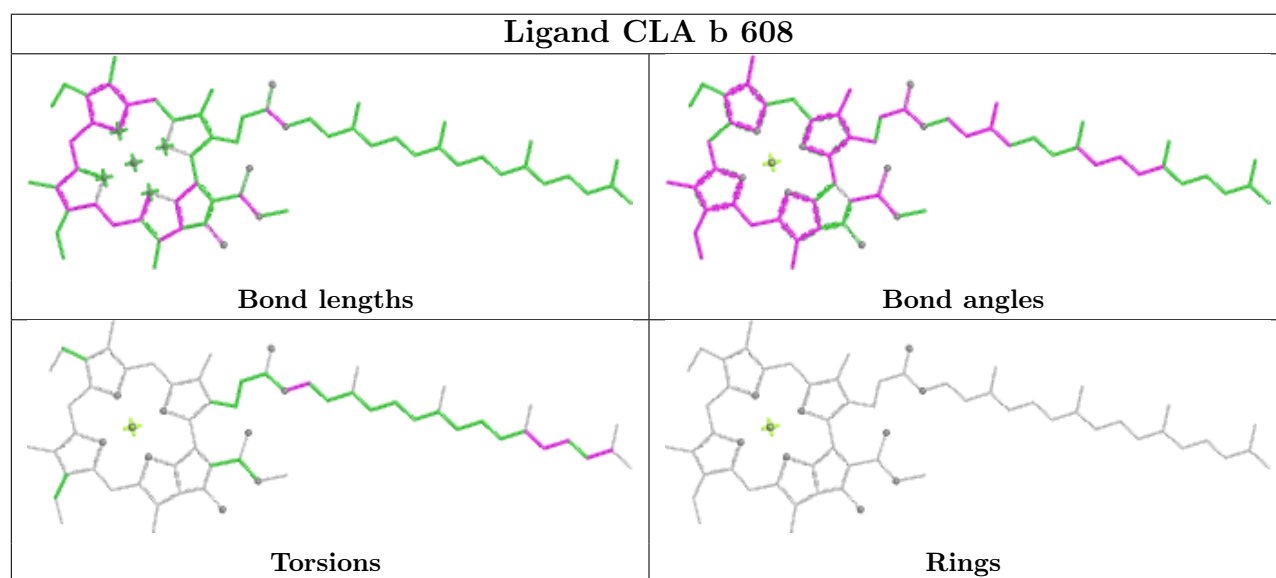
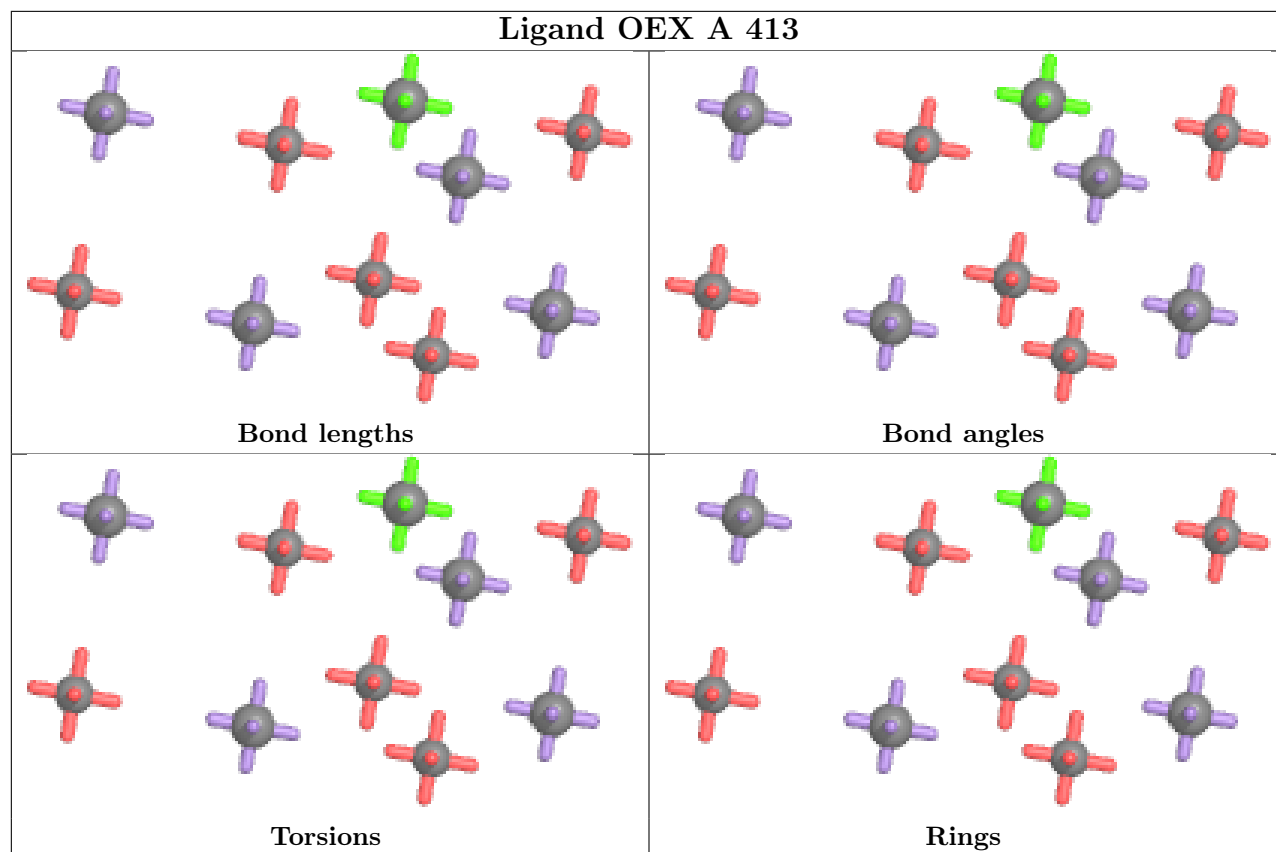


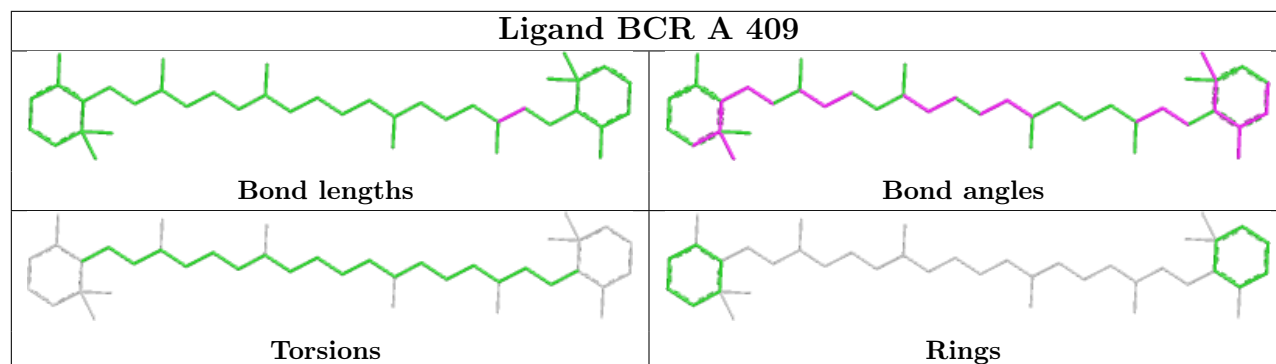
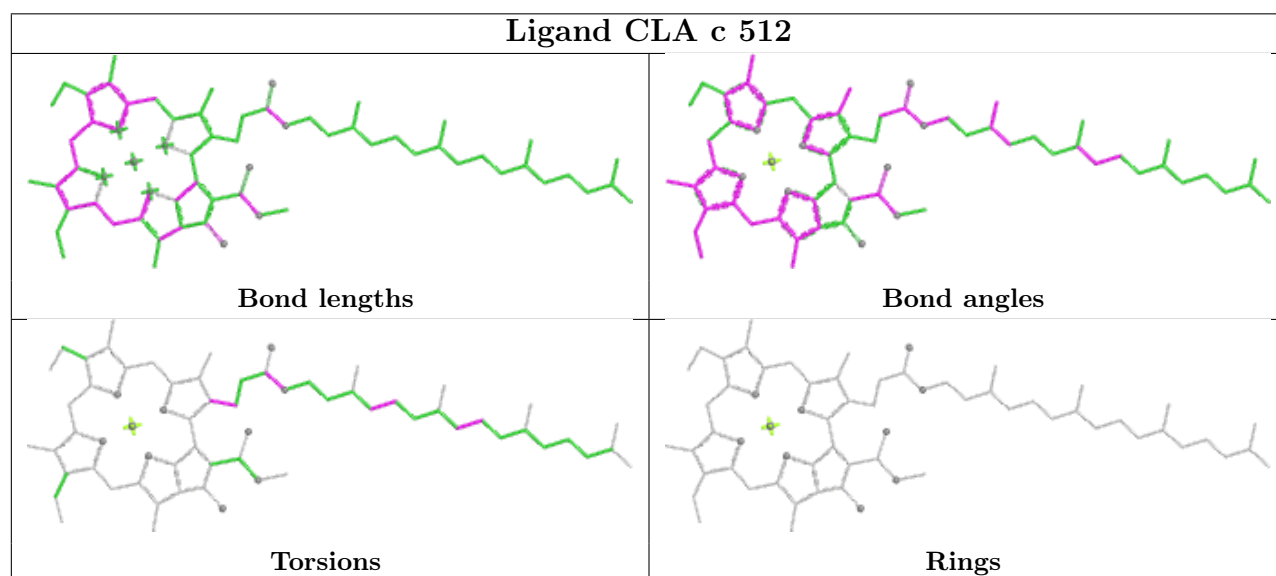
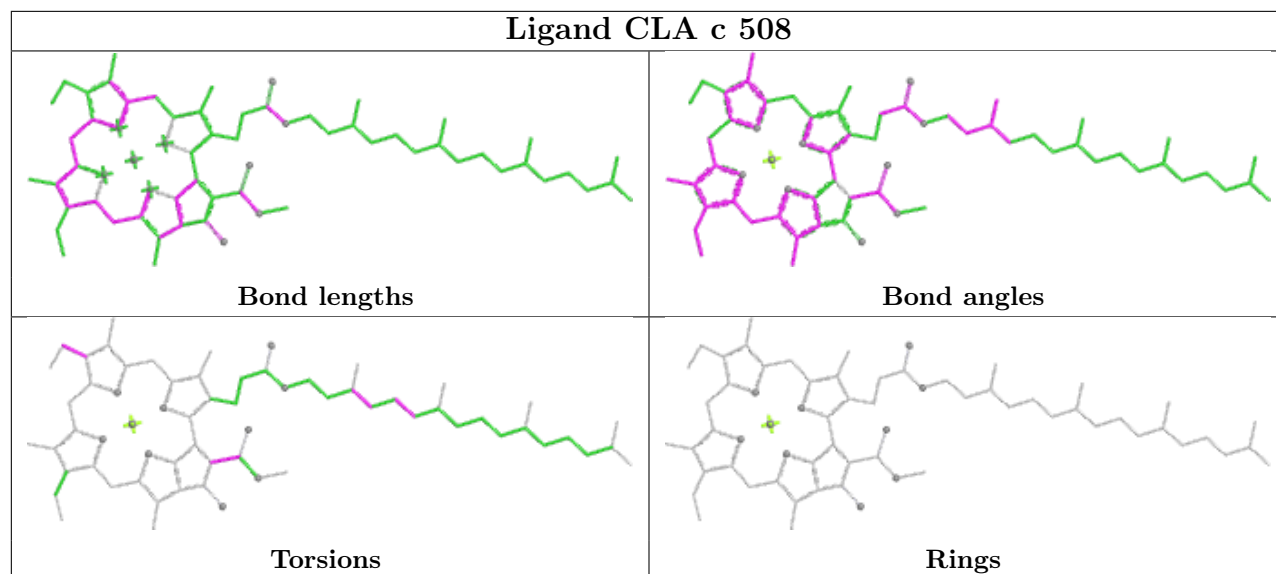


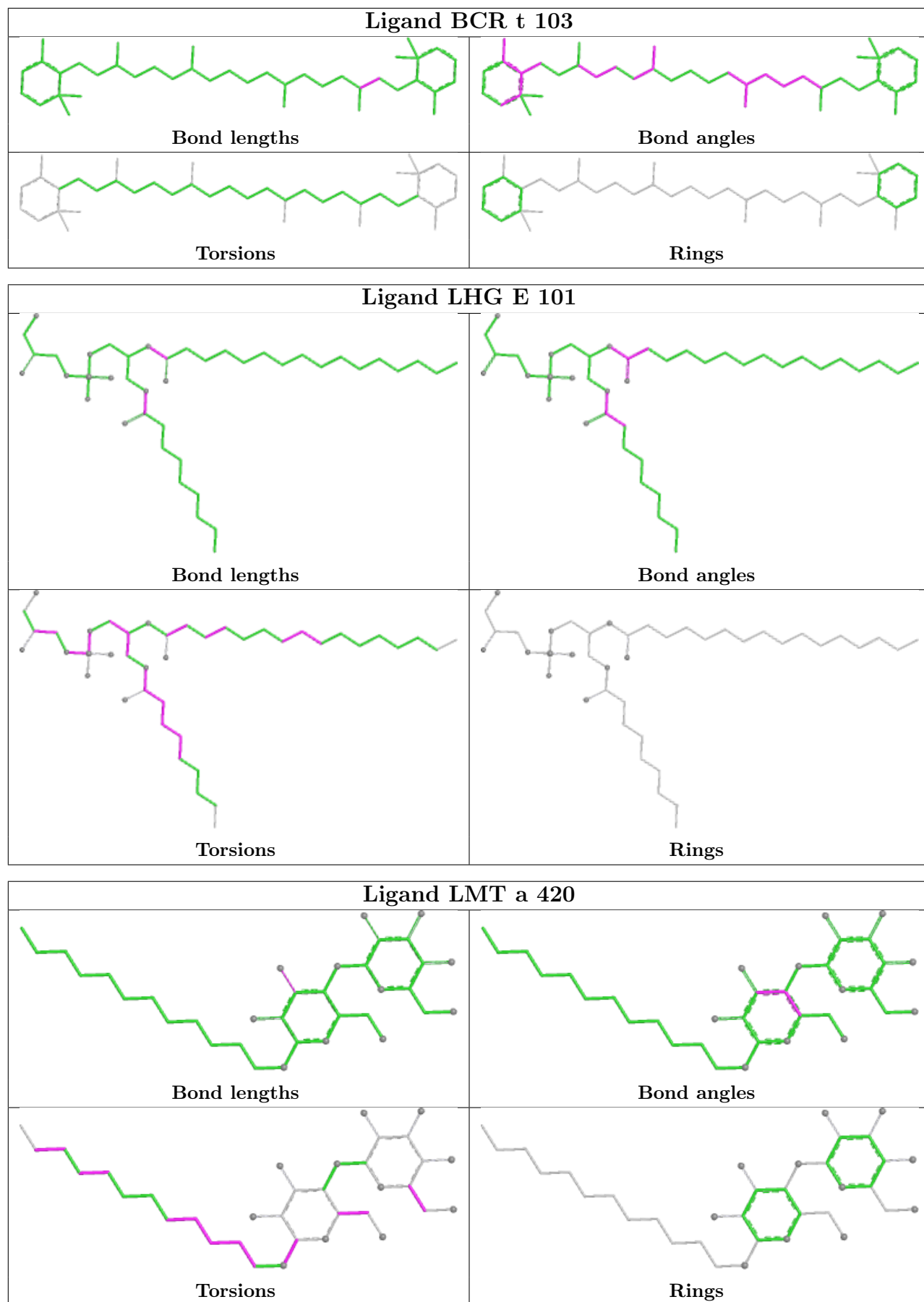


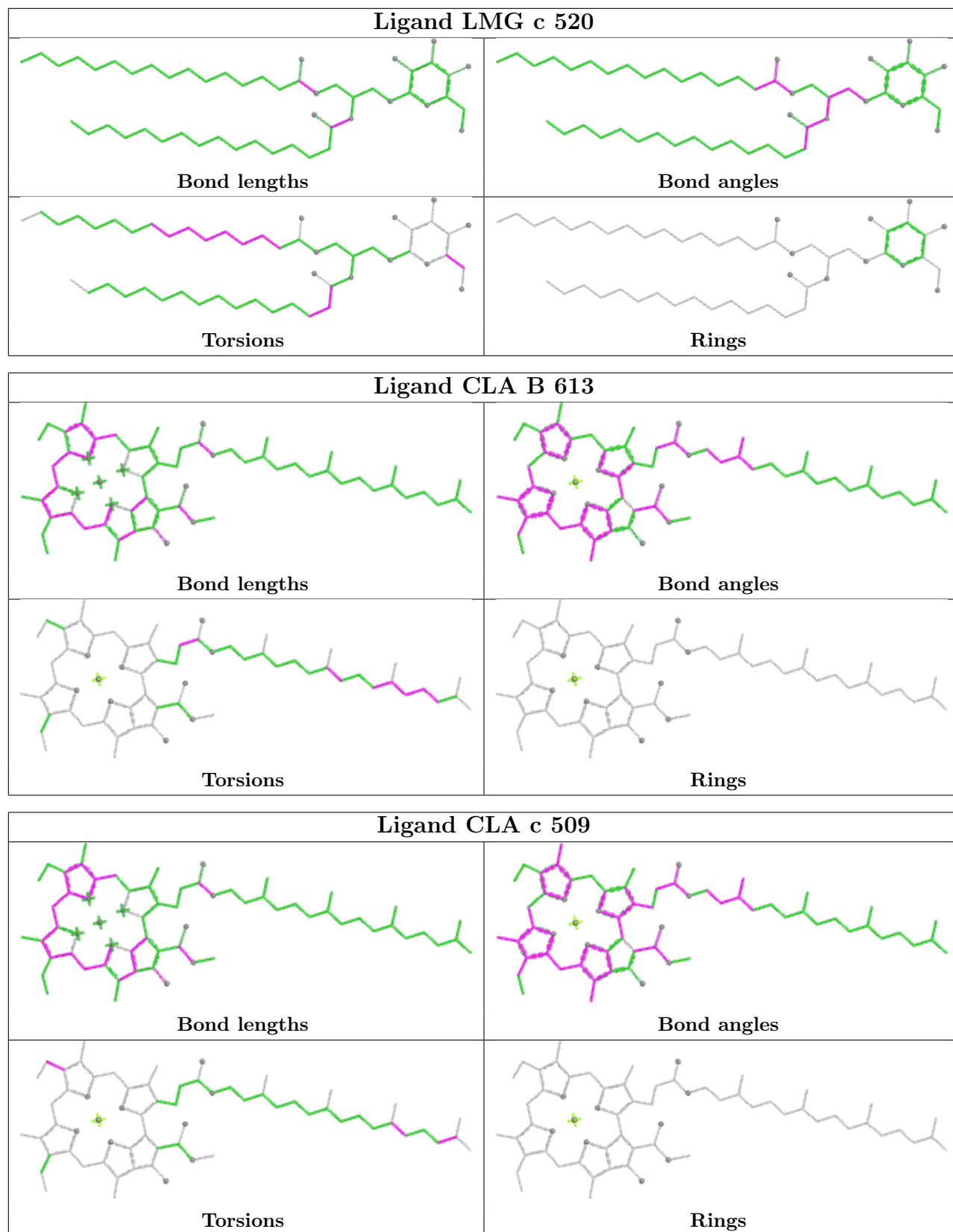


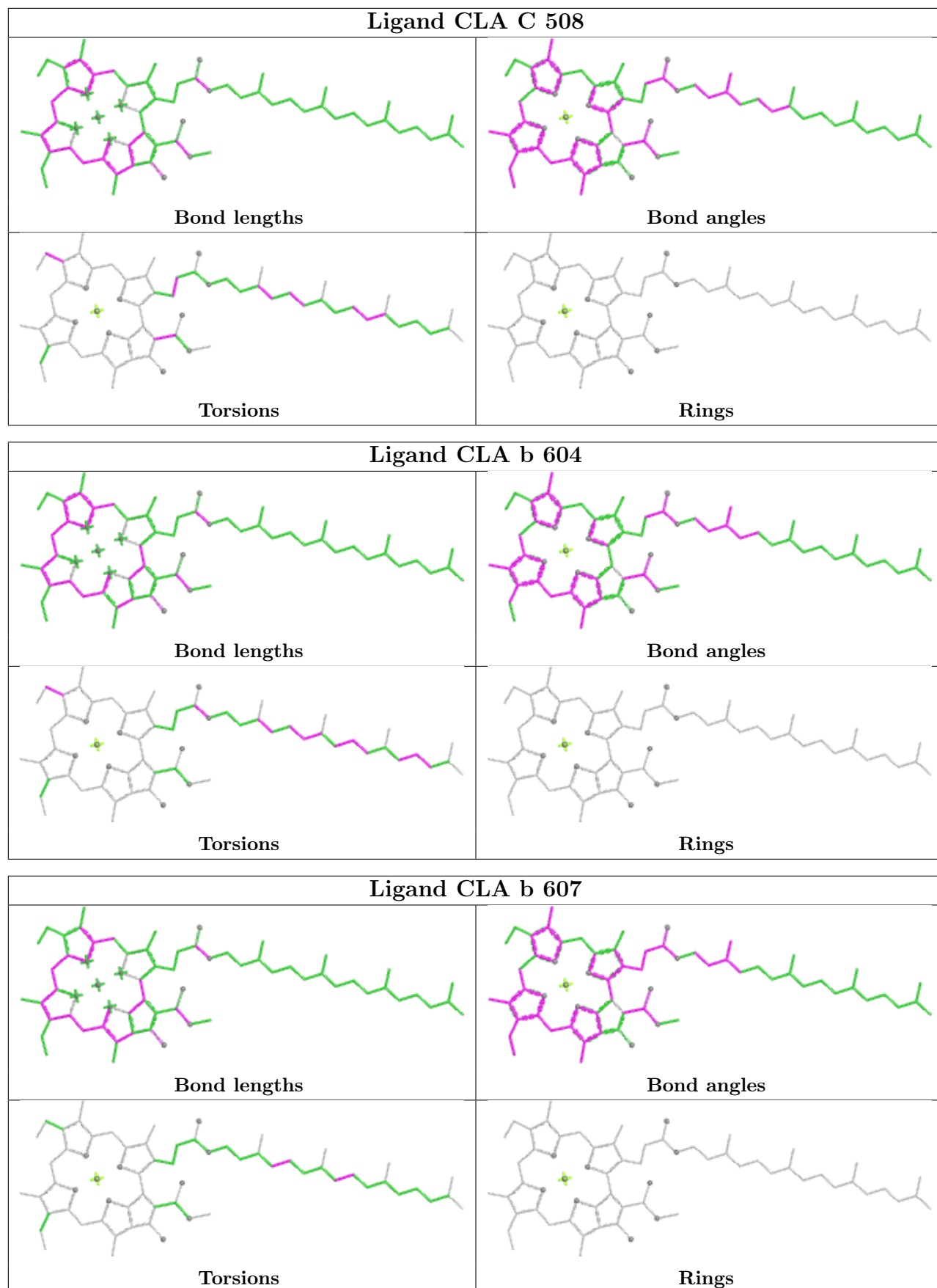


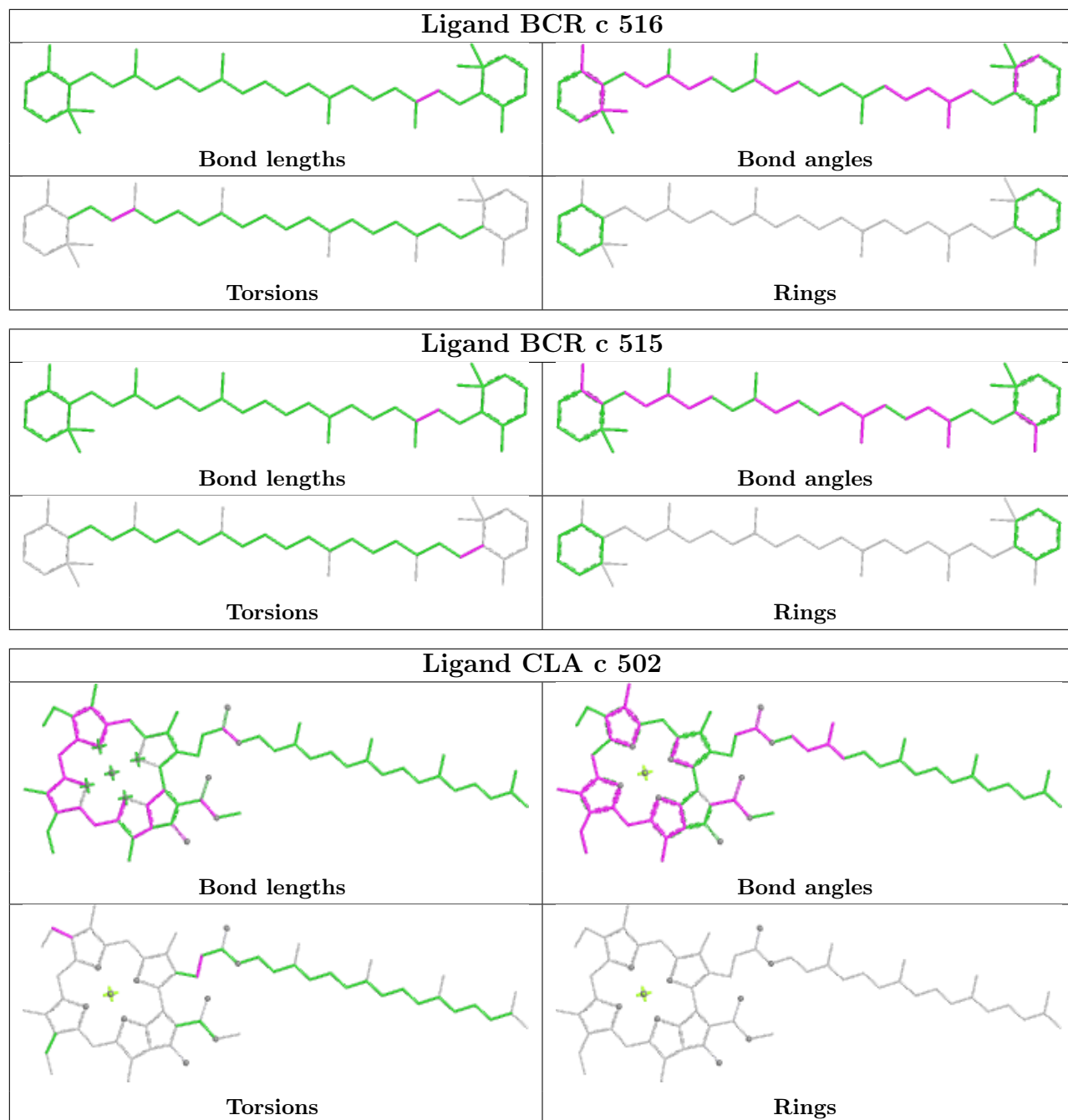


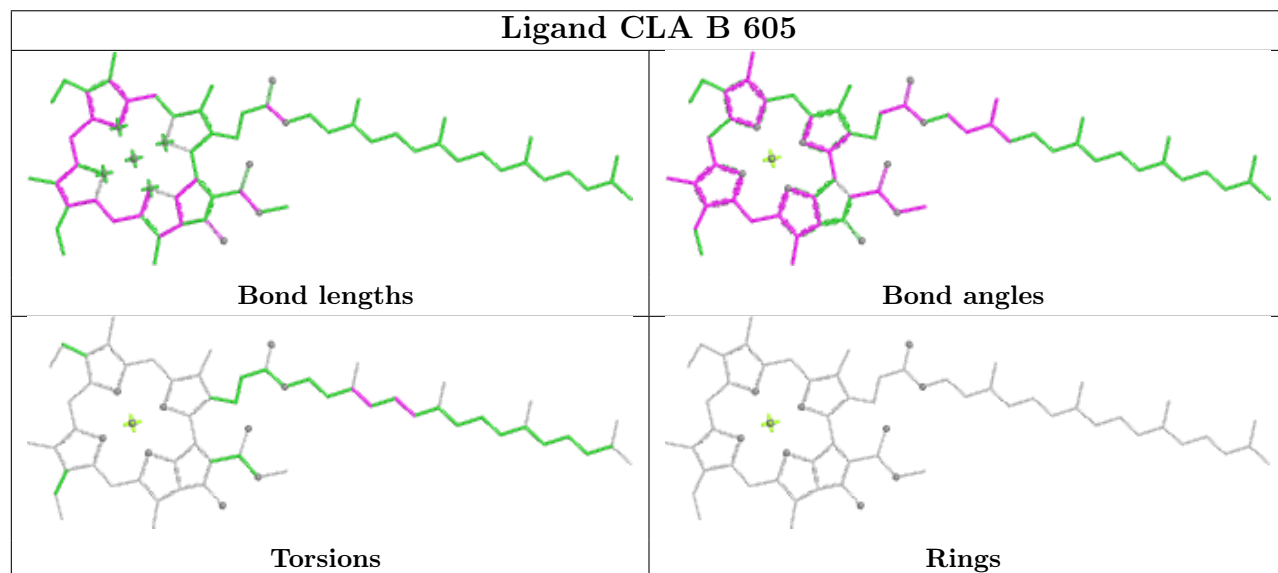
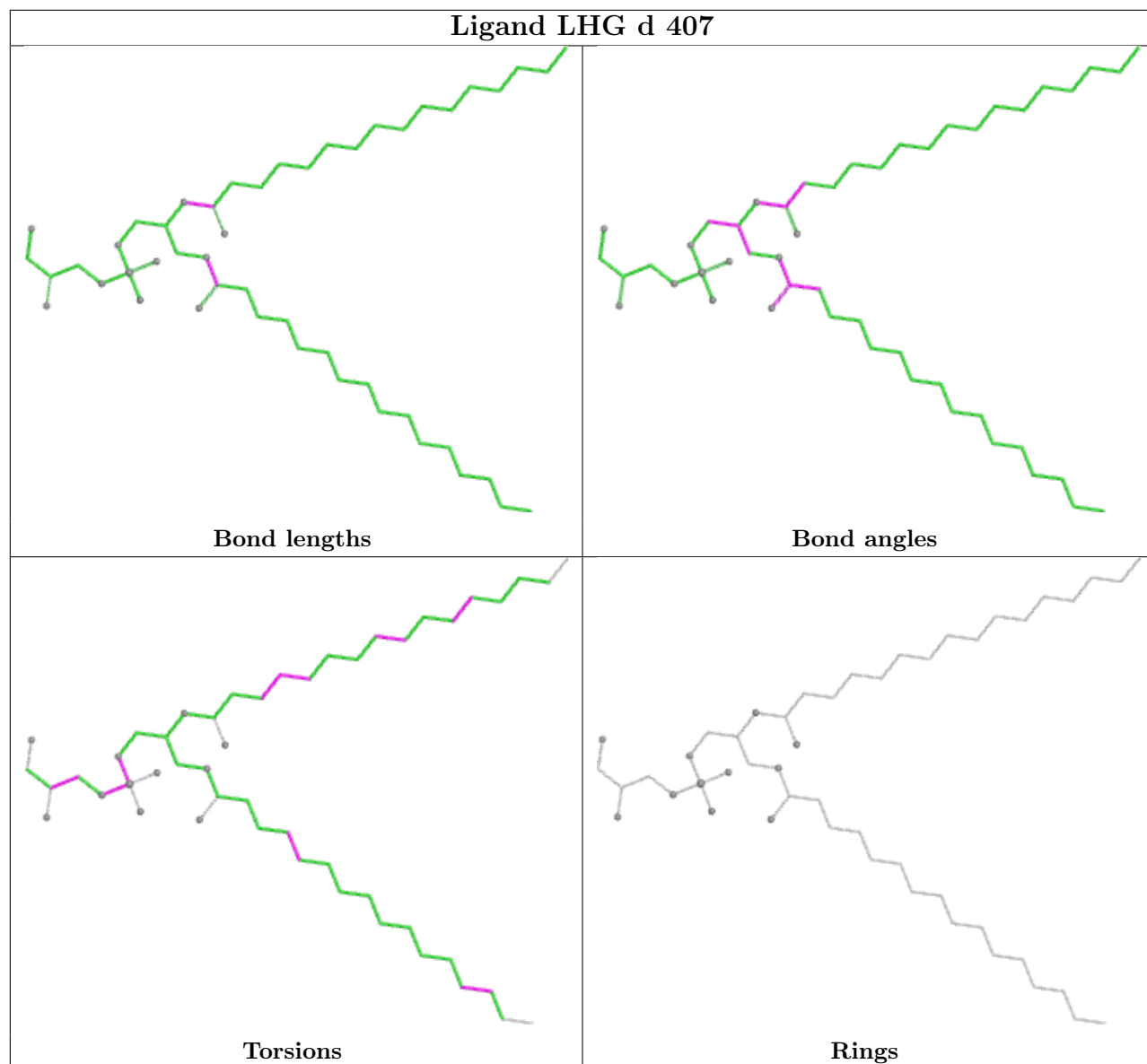


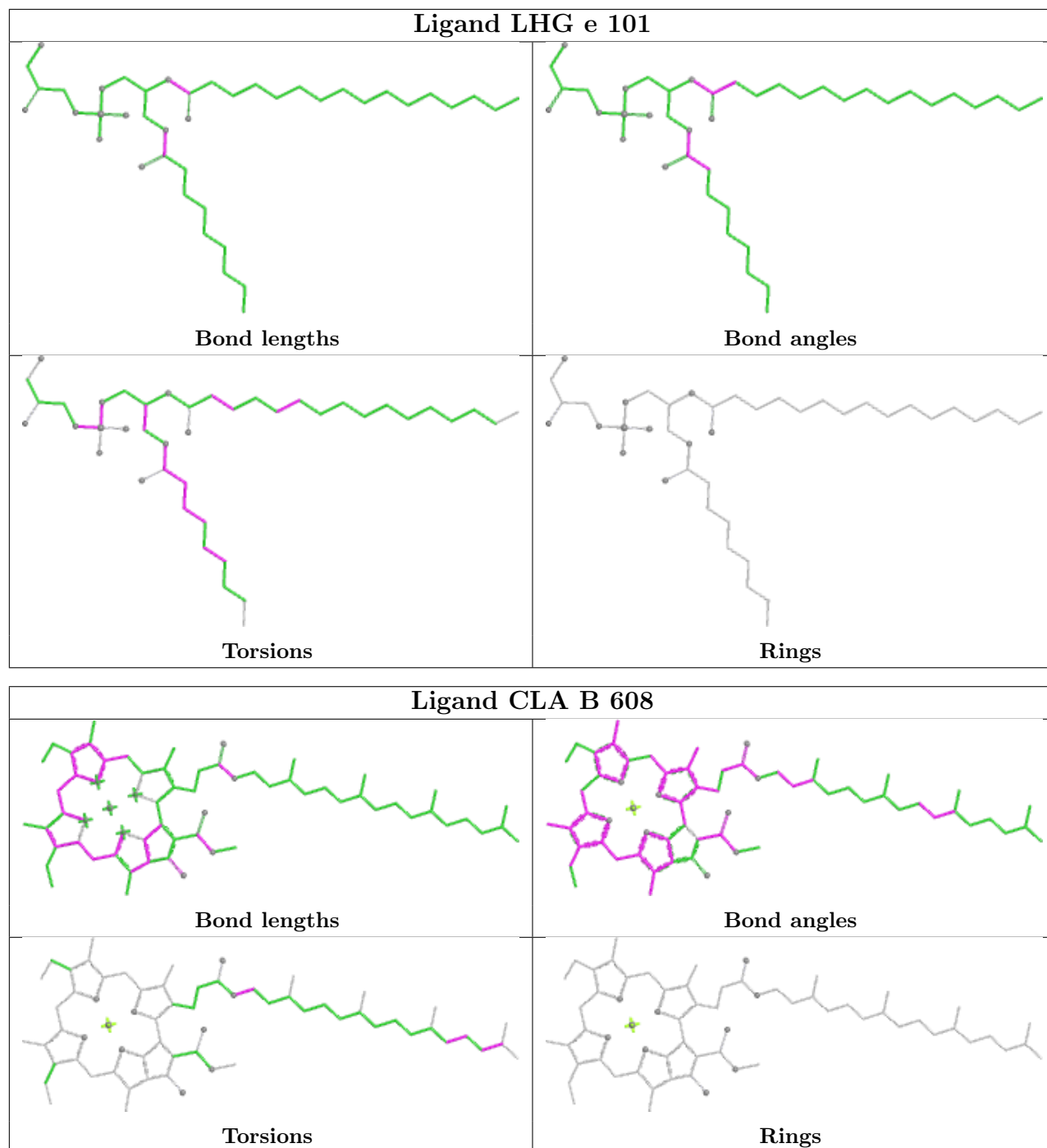


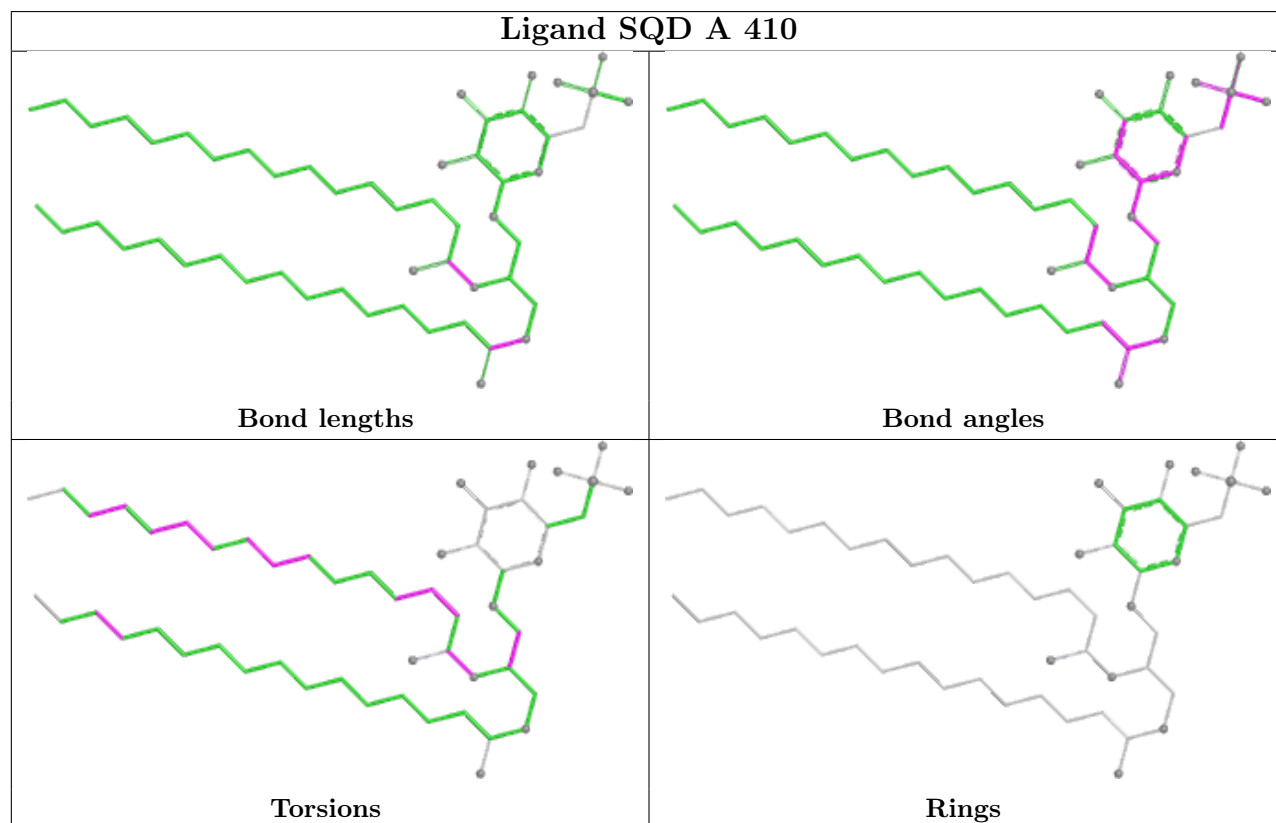
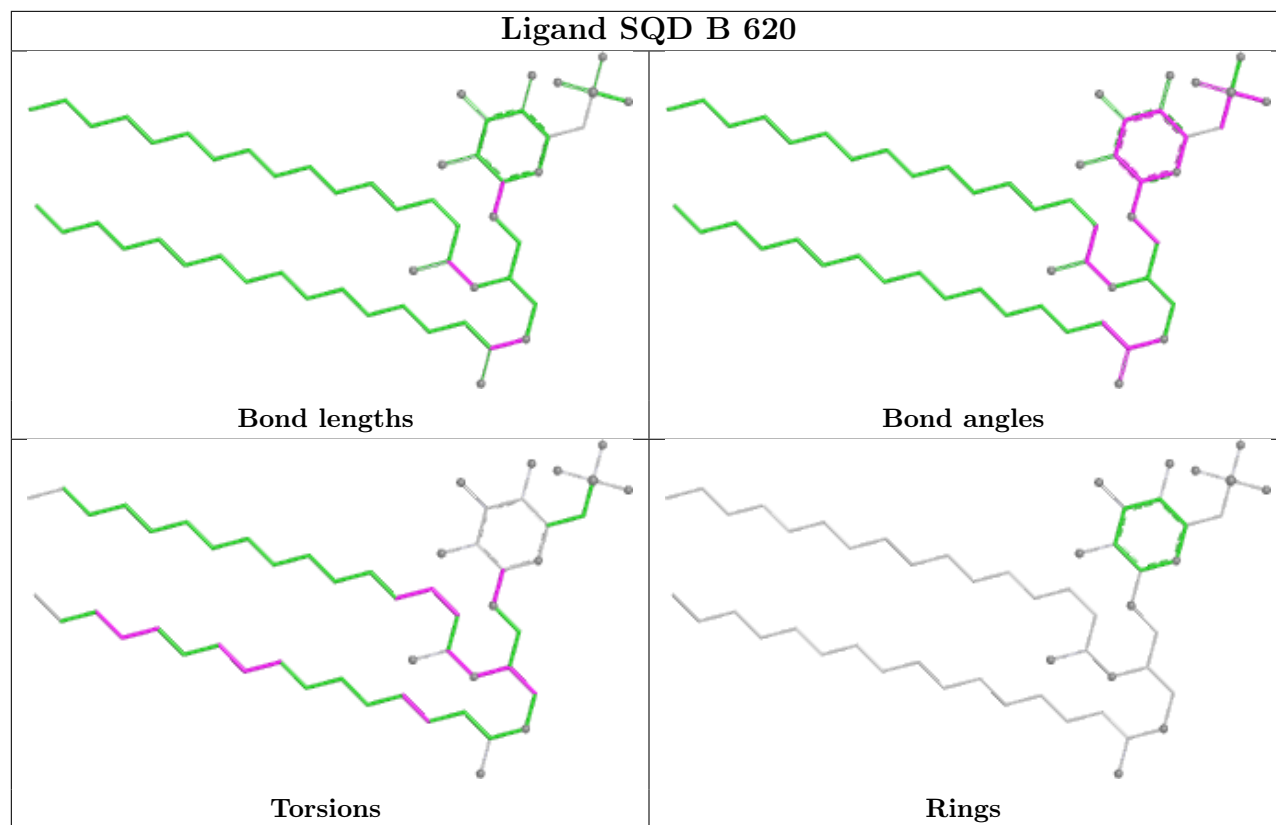


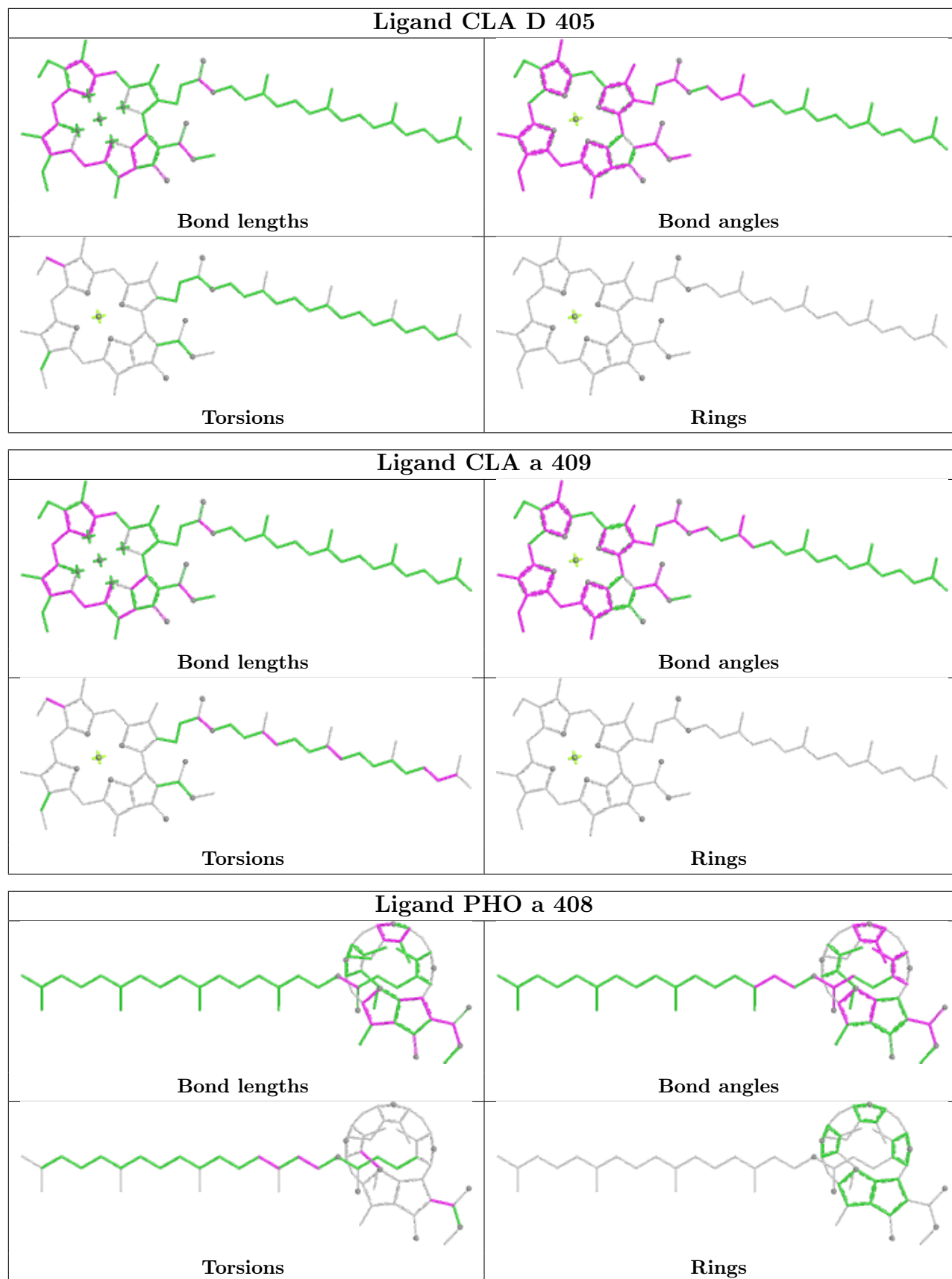












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	334/344 (97%)	-0.66	0 100 100	23, 46, 67, 111	1 (0%)
1	a	334/344 (97%)	-0.64	2 (0%) 85 86	27, 50, 77, 114	2 (0%)
2	B	504/505 (99%)	-0.53	1 (0%) 91 92	23, 53, 79, 105	7 (1%)
2	b	504/505 (99%)	-0.41	3 (0%) 85 86	26, 58, 95, 136	6 (1%)
3	C	451/455 (99%)	-0.53	1 (0%) 91 92	28, 59, 80, 116	1 (0%)
3	c	455/455 (100%)	-0.46	2 (0%) 88 89	30, 64, 86, 118	5 (1%)
4	D	342/342 (100%)	-0.68	0 100 100	20, 48, 66, 117	1 (0%)
4	d	341/342 (99%)	-0.67	0 100 100	22, 53, 78, 114	2 (0%)
5	E	81/84 (96%)	-0.25	0 100 100	53, 68, 89, 140	0
5	e	79/84 (94%)	-0.24	1 (1%) 75 76	32, 74, 107, 128	2 (2%)
6	F	34/44 (77%)	-0.54	0 100 100	52, 61, 86, 106	0
6	f	31/44 (70%)	-0.23	1 (3%) 50 50	53, 69, 89, 125	1 (3%)
7	H	64/65 (98%)	-0.27	2 (3%) 51 51	52, 63, 80, 92	0
7	h	64/65 (98%)	-0.22	1 (1%) 70 71	38, 73, 87, 91	1 (1%)
8	I	37/38 (97%)	-0.05	0 100 100	56, 64, 104, 127	0
8	i	37/38 (97%)	-0.18	1 (2%) 56 57	56, 65, 103, 117	0
9	J	38/39 (97%)	-0.37	0 100 100	50, 68, 108, 135	0
9	j	39/39 (100%)	-0.20	0 100 100	58, 77, 115, 133	0
10	K	37/37 (100%)	-0.63	0 100 100	56, 66, 82, 95	0
10	k	37/37 (100%)	-0.45	0 100 100	65, 73, 91, 101	0
11	L	36/37 (97%)	-0.63	0 100 100	38, 44, 87, 107	0
11	l	36/37 (97%)	-0.62	0 100 100	40, 46, 90, 95	0
12	M	32/36 (88%)	-0.57	0 100 100	24, 46, 68, 107	1 (3%)
12	m	33/36 (91%)	-0.57	0 100 100	23, 47, 68, 123	2 (6%)

*Continued on next page...*

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	-0.47	0 100 100	33, 63, 108, 147	3 (1%)
13	o	243/244 (99%)	-0.37	0 100 100	43, 67, 114, 143	0
14	T	29/32 (90%)	-0.70	0 100 100	28, 47, 72, 93	1 (3%)
14	t	29/32 (90%)	-0.64	0 100 100	43, 49, 75, 100	0
15	U	96/104 (92%)	-0.57	0 100 100	33, 56, 82, 90	1 (1%)
15	u	97/104 (93%)	-0.62	0 100 100	30, 61, 77, 106	1 (1%)
16	V	137/137 (100%)	-0.68	0 100 100	32, 55, 75, 96	2 (1%)
16	v	137/137 (100%)	-0.52	0 100 100	51, 70, 93, 116	0
17	X	38/40 (95%)	-0.13	0 100 100	35, 72, 92, 102	1 (2%)
17	x	38/40 (95%)	0.09	0 100 100	69, 80, 120, 138	0
18	Y	29/30 (96%)	0.03	1 (3%) 48 48	66, 82, 111, 113	0
18	y	29/30 (96%)	-0.10	0 100 100	77, 89, 105, 106	0
19	Z	62/62 (100%)	-0.18	0 100 100	69, 79, 123, 135	0
19	z	62/62 (100%)	0.21	0 100 100	81, 93, 129, 151	0
20	R	34/34 (100%)	0.90	3 (8%) 15 14	89, 106, 127, 134	0
All	All	5283/5384 (98%)	-0.49	19 (0%) 88 89	20, 58, 95, 151	41 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	479[A]	PHE	4.8
5	e	79[A]	PHE	4.2
7	H	65	LEU	3.6
6	f	16[A]	PHE	3.5
2	B	494	GLY	3.1
20	R	35	LEU	2.8
20	R	28	VAL	2.8
2	b	499	VAL	2.8
1	a	221[A]	SER	2.7
8	i	37	LEU	2.7
1	a	11	ALA	2.7
7	h	65	LEU	2.5
20	R	24	LEU	2.5
3	c	245[A]	ILE	2.3
18	Y	18	VAL	2.3
2	b	502	VAL	2.2
7	H	64	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
3	c	20	SER	2.0
3	C	246	ALA	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
14	FME	T	1	10/11	0.94	0.08	42,50,60,69	0
8	FME	I	1	10/11	0.95	0.07	62,71,80,84	0
14	FME	t	1	10/11	0.96	0.07	43,48,58,71	0
12	FME	m	1	10/11	0.97	0.07	47,59,81,89	0
8	FME	i	1	10/11	0.97	0.07	60,69,80,82	0
12	FME	M	1	10/11	0.98	0.06	45,57,82,83	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
27	GOL	a	701	6/6	0.58	0.17	67,76,80,87	0
32	LMT	a	414	35/35	0.58	0.16	63,88,104,110	0
30	UNL	a	417	30/-	0.60	0.14	83,97,111,115	0
32	LMT	E	102	35/35	0.60	0.16	91,110,128,136	0
30	UNL	A	415	28/-	0.60	0.15	85,97,103,113	0
32	LMT	e	102	35/35	0.60	0.16	100,117,141,148	0
32	LMT	A	359	35/35	0.62	0.14	62,87,99,103	0
32	LMT	a	420	35/35	0.66	0.14	98,106,117,123	0
32	LMT	I	101	35/35	0.67	0.13	95,106,125,127	0
30	UNL	I	102	40/-	0.67	0.16	73,93,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	UNL	K	101	34/-	0.69	0.14	70,94,106,109	0
30	UNL	J	101	10/-	0.70	0.21	62,76,78,81	0
26	SQD	f	102	43/54	0.71	0.13	95,111,133,137	0
34	HTG	C	522	19/19	0.71	0.13	101,105,118,120	0
27	GOL	o	601	6/6	0.72	0.16	69,76,81,81	0
37	LHG	e	101	42/49	0.72	0.13	77,123,136,141	0
30	UNL	i	101	40/-	0.73	0.13	73,92,119,122	0
30	UNL	m	102	10/-	0.73	0.18	66,69,81,84	0
34	HTG	b	623	19/19	0.74	0.13	82,117,123,124	0
30	UNL	j	101	10/-	0.74	0.17	73,86,89,91	0
30	UNL	M	102	10/-	0.75	0.15	61,69,82,85	0
32	LMT	b	621	25/35	0.75	0.14	78,101,125,128	0
32	LMT	t	102	26/35	0.76	0.13	65,87,107,111	0
30	UNL	c	525	32/-	0.76	0.13	84,98,109,116	0
30	UNL	d	410	36/-	0.76	0.12	68,87,107,111	0
30	UNL	D	413	40/-	0.76	0.13	66,84,105,112	0
33	LMG	C	521	51/55	0.77	0.12	62,105,124,128	0
32	LMT	M	103	35/35	0.77	0.12	63,100,125,128	0
32	LMT	t	101	25/35	0.77	0.14	57,76,105,116	0
27	GOL	o	501	6/6	0.77	0.15	78,88,93,93	0
34	HTG	D	414	16/19	0.78	0.12	85,93,108,117	0
34	HTG	B	623	19/19	0.78	0.15	62,74,92,96	0
30	UNL	b	626	33/-	0.78	0.13	68,91,132,133	0
32	LMT	D	404	35/35	0.79	0.12	67,94,113,116	0
27	GOL	O	501	6/6	0.79	0.10	80,89,94,96	0
30	UNL	B	627	33/-	0.79	0.14	56,95,117,120	0
27	GOL	A	411	6/6	0.79	0.13	61,70,75,76	0
32	LMT	b	627	25/35	0.80	0.13	56,78,111,117	0
34	HTG	c	522	19/19	0.80	0.10	106,114,122,125	0
34	HTG	d	411	16/19	0.80	0.12	92,107,116,125	0
34	HTG	V	203	11/19	0.80	0.10	79,95,104,104	0
27	GOL	c	743	6/6	0.81	0.17	84,89,90,93	0
27	GOL	d	701	6/6	0.82	0.21	51,59,69,72	0
34	HTG	b	622	19/19	0.82	0.12	57,74,82,89	0
27	GOL	B	901	6/6	0.82	0.15	62,69,78,92	0
26	SQD	a	413	54/54	0.82	0.10	65,85,111,118	0
29	PL9	A	414	55/55	0.82	0.12	58,81,99,103	0
29	PL9	a	416	55/55	0.82	0.14	71,90,100,107	0
33	LMG	c	521	51/55	0.83	0.11	74,112,132,135	0
27	GOL	b	624	6/6	0.83	0.14	78,85,87,93	0
26	SQD	A	412	54/54	0.84	0.10	63,79,104,118	0
27	GOL	d	801	6/6	0.84	0.16	56,86,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	CA	F	102	1/1	0.84	0.23	114,114,114,114	0
33	LMG	Z	101	37/55	0.84	0.14	71,110,125,133	0
32	LMT	m	103	35/35	0.85	0.11	60,77,86,90	0
27	GOL	O	601	6/6	0.85	0.18	67,71,76,78	0
32	LMT	M	101	35/35	0.85	0.11	58,81,89,94	0
33	LMG	z	101	39/55	0.85	0.12	78,116,128,136	0
34	HTG	B	622	19/19	0.85	0.12	63,76,85,85	0
30	UNL	D	412	17/-	0.86	0.11	57,70,92,98	0
26	SQD	B	620	54/54	0.86	0.10	61,81,106,110	0
23	CLA	b	601	65/65	0.87	0.10	68,87,110,121	0
26	SQD	b	620	54/54	0.87	0.10	58,83,99,104	0
36	CA	f	103	1/1	0.87	0.12	116,116,116,116	0
26	SQD	F	101	43/54	0.87	0.11	71,94,114,123	0
27	GOL	a	412	6/6	0.88	0.12	69,72,83,84	0
33	LMG	C	501	51/55	0.88	0.09	66,82,94,99	0
37	LHG	E	101	42/49	0.88	0.10	70,93,106,111	0
27	GOL	D	701	6/6	0.88	0.17	46,57,60,63	0
27	GOL	V	401	6/6	0.89	0.14	54,62,68,69	0
27	GOL	a	801	6/6	0.89	0.24	54,61,68,69	0
33	LMG	a	419	51/55	0.89	0.08	68,85,93,101	0
27	GOL	A	701	6/6	0.89	0.24	48,61,63,69	0
33	LMG	m	101	51/55	0.89	0.09	52,68,81,90	0
30	UNL	d	409	17/-	0.90	0.10	64,75,90,92	0
27	GOL	v	401	6/6	0.90	0.13	62,73,75,76	0
23	CLA	B	601	65/65	0.90	0.09	59,77,99,112	0
33	LMG	c	520	51/55	0.91	0.09	61,86,110,121	0
33	LMG	B	621	51/55	0.91	0.08	53,66,78,88	0
23	CLA	c	514	65/65	0.91	0.10	75,91,113,123	0
33	LMG	d	412	51/55	0.92	0.09	54,69,102,107	0
25	BCR	d	404	40/40	0.92	0.08	50,65,89,95	0
33	LMG	C	520	51/55	0.92	0.09	55,80,98,108	0
34	HTG	b	625	19/19	0.92	0.07	62,72,85,90	0
23	CLA	C	514	65/65	0.92	0.09	68,84,105,108	0
33	LMG	D	415	51/55	0.92	0.09	48,63,100,106	0
27	GOL	C	523	6/6	0.92	0.13	56,58,59,62	0
34	HTG	B	626	19/19	0.92	0.07	64,77,86,89	0
25	BCR	D	407	40/40	0.92	0.09	44,58,89,91	0
25	BCR	T	101	40/40	0.92	0.07	44,57,65,66	0
30	UNL	X	101	18/-	0.93	0.10	59,73,95,100	0
23	CLA	c	513	65/65	0.93	0.09	65,80,111,115	0
27	GOL	c	742	6/6	0.93	0.21	63,64,69,69	0
23	CLA	B	614	65/65	0.93	0.07	37,47,82,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	BCR	C	515	40/40	0.93	0.09	61,76,85,88	0
23	CLA	C	507	65/65	0.93	0.08	59,69,104,107	0
35	DGD	C	518	62/66	0.93	0.08	48,61,103,107	0
23	CLA	b	616	65/65	0.93	0.09	55,63,116,123	0
23	CLA	c	505	65/65	0.93	0.07	52,61,95,101	0
36	CA	o	301	1/1	0.93	0.06	107,107,107,107	0
37	LHG	D	409	49/49	0.93	0.08	47,59,75,81	0
25	BCR	t	103	40/40	0.93	0.07	46,55,69,73	0
23	CLA	c	507	65/65	0.93	0.09	56,68,100,106	0
23	CLA	B	606	65/65	0.94	0.08	46,56,97,106	0
23	CLA	C	509	65/65	0.94	0.07	50,55,107,116	0
23	CLA	C	513	65/65	0.94	0.09	60,74,100,108	0
26	SQD	a	411	54/54	0.94	0.08	58,77,107,109	0
23	CLA	A	408	65/65	0.94	0.09	42,51,108,112	0
23	CLA	d	403	65/65	0.94	0.09	56,65,110,122	0
23	CLA	a	409	65/65	0.94	0.10	46,55,108,116	0
23	CLA	B	616	65/65	0.94	0.09	46,57,106,111	0
25	BCR	K	102	40/40	0.94	0.09	59,65,71,72	0
27	GOL	B	624	6/6	0.94	0.12	62,64,69,71	0
23	CLA	b	606	65/65	0.94	0.08	47,61,100,110	0
25	BCR	Y	101	40/40	0.94	0.08	55,63,76,77	0
35	DGD	c	517	62/66	0.94	0.07	48,62,95,101	0
35	DGD	c	518	62/66	0.94	0.07	55,65,110,121	0
35	DGD	c	519	62/66	0.94	0.07	50,64,98,115	0
25	BCR	c	515	40/40	0.94	0.08	77,84,90,91	0
23	CLA	b	614	65/65	0.94	0.07	41,51,84,86	0
25	BCR	h	101	40/40	0.94	0.09	60,70,88,89	0
25	BCR	k	101	40/40	0.94	0.10	63,74,82,85	0
37	LHG	D	411	49/49	0.94	0.09	47,59,99,106	0
23	CLA	C	505	65/65	0.94	0.08	44,55,89,101	0
37	LHG	d	711	49/49	0.94	0.08	49,63,75,77	0
26	SQD	A	410	54/54	0.94	0.08	55,77,101,104	0
25	BCR	B	618	40/40	0.95	0.06	41,51,62,66	0
25	BCR	B	619	40/40	0.95	0.07	49,59,83,89	0
25	BCR	y	101	40/40	0.95	0.07	62,71,80,85	0
29	PL9	d	405	55/55	0.95	0.06	39,49,57,67	0
31	BCT	a	404	4/4	0.95	0.07	53,58,65,74	0
23	CLA	b	604	65/65	0.95	0.07	41,52,88,93	0
23	CLA	a	407	65/65	0.95	0.07	41,52,112,121	0
35	DGD	C	519	62/66	0.95	0.07	43,58,88,95	0
35	DGD	H	102	62/66	0.95	0.08	47,58,67,70	0
25	BCR	H	101	40/40	0.95	0.08	53,66,84,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	c	508	65/65	0.95	0.08	58,67,78,80	0
23	CLA	c	509	65/65	0.95	0.07	50,61,118,124	0
35	DGD	h	102	62/66	0.95	0.07	53,63,72,76	0
23	CLA	B	611	65/65	0.95	0.07	37,43,61,67	0
36	CA	O	301	1/1	0.95	0.04	98,98,98,98	0
36	CA	c	523	1/1	0.95	0.06	79,79,79,79	0
27	GOL	b	901	6/6	0.95	0.11	67,70,76,77	0
25	BCR	a	410	40/40	0.95	0.07	44,54,62,63	0
25	BCR	b	618	40/40	0.95	0.06	42,55,72,76	0
25	BCR	b	619	40/40	0.95	0.08	53,62,80,85	0
23	CLA	D	406	65/65	0.95	0.08	49,58,102,105	0
37	LHG	d	408	49/49	0.95	0.08	50,61,105,116	0
23	CLA	c	502	65/65	0.95	0.07	58,68,75,81	0
25	BCR	A	409	40/40	0.95	0.07	40,52,62,66	0
37	LHG	l	101	49/49	0.95	0.07	48,56,68,82	0
23	CLA	B	603	65/65	0.96	0.07	45,52,68,73	0
23	CLA	c	512	65/65	0.96	0.07	60,67,81,87	0
23	CLA	A	406	65/65	0.96	0.06	36,45,103,112	0
23	CLA	C	502	65/65	0.96	0.06	52,60,68,77	0
23	CLA	b	602	65/65	0.96	0.07	49,61,74,81	0
24	PHO	a	353	64/64	0.96	0.06	45,55,61,66	0
29	PL9	D	408	55/55	0.96	0.06	37,46,55,66	0
23	CLA	b	603	65/65	0.96	0.07	49,56,77,82	0
25	BCR	B	617	40/40	0.96	0.05	42,51,59,61	0
35	DGD	C	517	62/66	0.96	0.06	47,56,94,100	0
23	CLA	B	607	65/65	0.96	0.06	37,45,67,73	0
23	CLA	C	506	65/65	0.96	0.07	52,59,85,91	0
23	CLA	b	607	65/65	0.96	0.06	40,47,70,76	0
25	BCR	C	516	40/40	0.96	0.07	55,65,73,76	0
23	CLA	b	609	65/65	0.96	0.07	55,65,76,82	0
23	CLA	b	611	65/65	0.96	0.06	40,48,66,77	0
23	CLA	b	612	65/65	0.96	0.07	44,53,63,68	0
23	CLA	b	613	65/65	0.96	0.06	41,49,79,86	0
23	CLA	B	609	65/65	0.96	0.07	46,59,67,73	0
23	CLA	b	615	65/65	0.96	0.07	49,60,75,78	0
25	BCR	b	617	40/40	0.96	0.06	46,54,61,64	0
23	CLA	C	508	65/65	0.96	0.07	54,63,76,83	0
23	CLA	B	610	65/65	0.96	0.07	42,53,60,72	0
23	CLA	B	602	65/65	0.96	0.07	49,57,70,80	0
25	BCR	c	516	40/40	0.96	0.06	58,66,76,78	0
37	LHG	d	407	49/49	0.96	0.07	44,54,66,72	0
23	CLA	c	506	65/65	0.96	0.07	52,63,84,87	0

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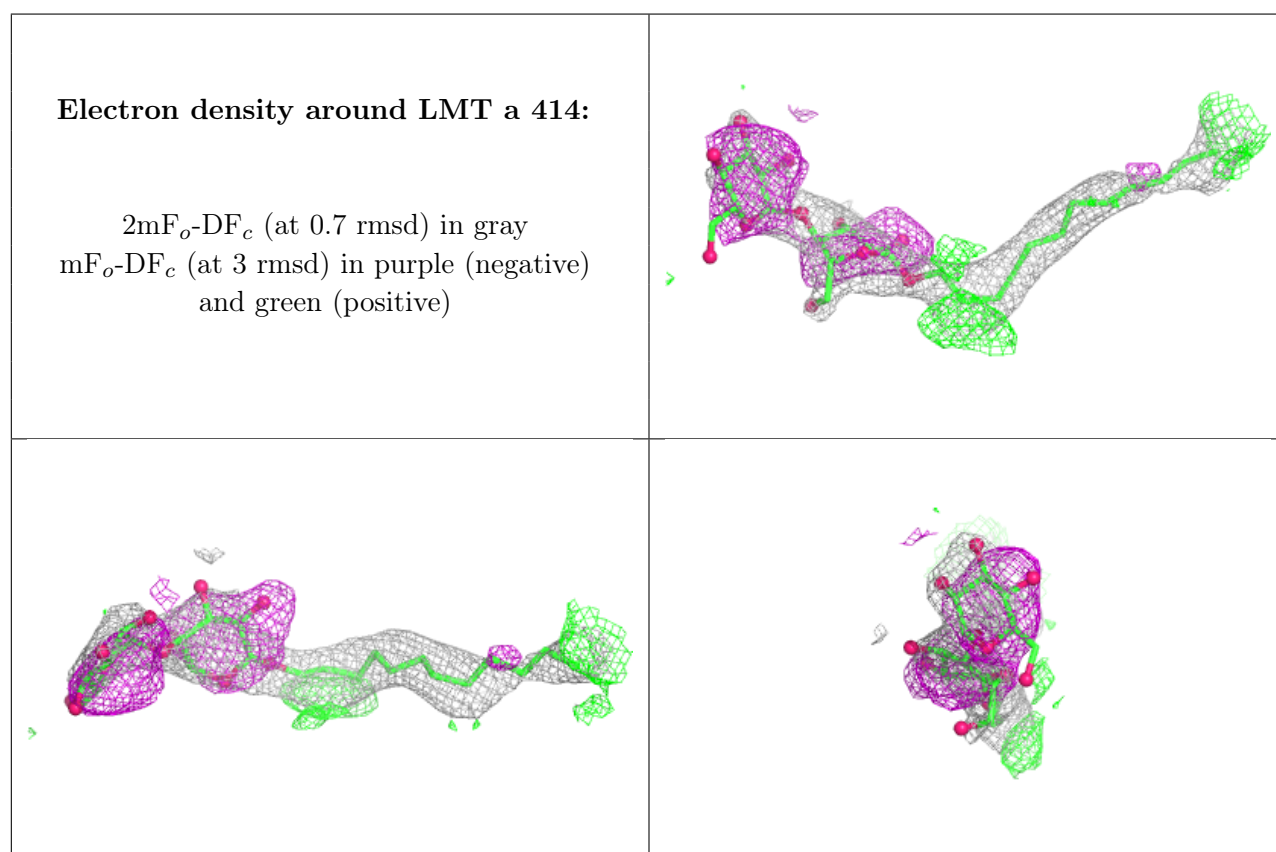
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	B	612	65/65	0.96	0.06	36,47,56,61	0
30	UNL	x	101	18/-	0.96	0.09	66,77,110,116	0
23	CLA	B	613	65/65	0.96	0.06	37,44,82,88	0
23	CLA	A	405	65/65	0.97	0.05	35,41,52,64	0
23	CLA	b	608	65/65	0.97	0.06	44,56,76,86	0
23	CLA	C	504	65/65	0.97	0.06	51,61,67,75	0
23	CLA	b	610	65/65	0.97	0.07	50,59,66,68	0
24	PHO	A	407	64/64	0.97	0.05	36,44,50,56	0
24	PHO	A	353	64/64	0.97	0.05	38,47,53,57	0
24	PHO	a	408	64/64	0.97	0.05	40,47,51,54	0
23	CLA	D	405	65/65	0.97	0.06	33,42,67,73	0
23	CLA	A	404	65/65	0.97	0.06	36,41,59,64	0
23	CLA	a	405	65/65	0.97	0.06	38,45,61,69	0
23	CLA	a	406	65/65	0.97	0.04	37,43,61,69	0
23	CLA	B	608	65/65	0.97	0.05	38,48,64,71	0
31	BCT	A	348	4/4	0.97	0.06	53,54,58,67	0
23	CLA	B	604	65/65	0.97	0.06	37,44,95,101	0
23	CLA	B	615	65/65	0.97	0.06	42,52,74,78	0
23	CLA	c	503	65/65	0.97	0.06	46,58,84,98	0
23	CLA	c	504	65/65	0.97	0.06	51,69,78,83	0
37	LHG	D	410	49/49	0.97	0.06	45,52,63,70	0
23	CLA	B	605	65/65	0.97	0.06	40,48,63,69	0
23	CLA	C	510	65/65	0.97	0.07	50,58,76,79	0
37	LHG	L	101	49/49	0.97	0.06	46,52,67,81	0
23	CLA	C	511	65/65	0.97	0.06	49,57,71,75	0
23	CLA	b	605	65/65	0.97	0.07	41,50,68,74	0
23	CLA	C	512	65/65	0.97	0.07	54,63,76,79	0
23	CLA	c	510	65/65	0.97	0.07	50,61,80,82	0
23	CLA	c	511	65/65	0.97	0.06	53,61,72,82	0
38	HEM	e	87	43/43	0.97	0.09	72,84,98,110	0
23	CLA	C	503	65/65	0.98	0.06	48,53,77,83	0
36	CA	C	524	1/1	0.98	0.04	77,77,77,77	0
38	HEM	E	103	43/43	0.98	0.06	57,69,77,88	0
23	CLA	d	402	65/65	0.98	0.05	39,46,72,86	0
40	HEC	V	202	43/43	0.98	0.06	42,50,54,56	0
40	HEC	v	202	43/43	0.98	0.07	54,61,68,70	0
22	CL	a	403	1/1	0.99	0.07	54,54,54,54	0
36	CA	c	524	1/1	0.99	0.05	76,76,76,76	0
22	CL	A	402	1/1	0.99	0.06	40,40,40,40	0
28	OEX	A	413	10/10	0.99	0.03	38,44,47,47	0
39	MG	J	102	1/1	0.99	0.03	57,57,57,57	0
39	MG	j	102	1/1	0.99	0.05	61,61,61,61	0

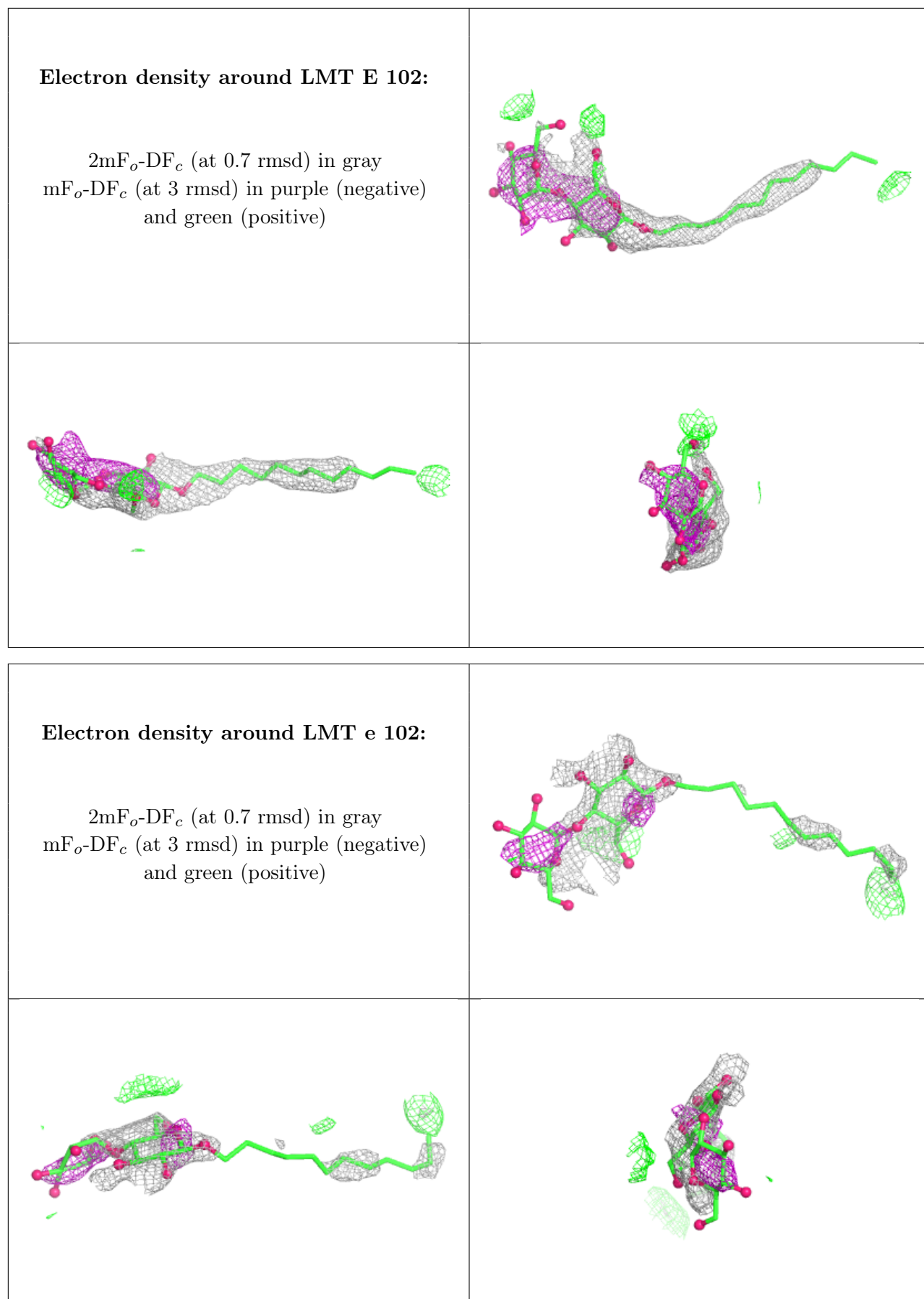
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CL	A	403	1/1	0.99	0.03	44,44,44,44	0
22	CL	a	402	1/1	0.99	0.07	47,47,47,47	0
28	OEX	a	415	10/10	1.00	0.02	45,48,51,54	0
21	FE2	A	401	1/1	1.00	0.01	49,49,49,49	0
21	FE2	a	401	1/1	1.00	0.01	52,52,52,52	0

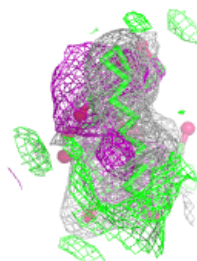
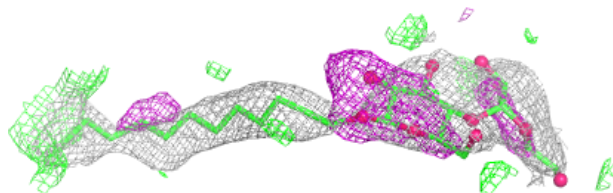
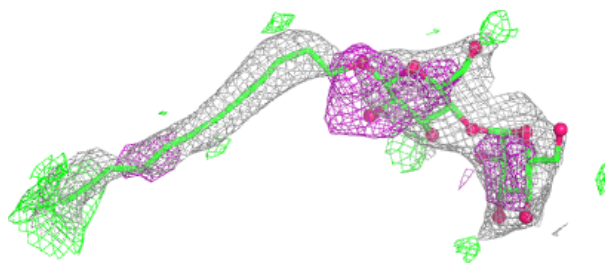
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



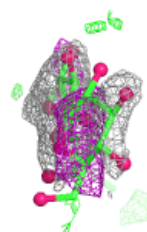
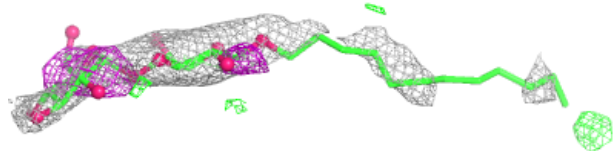
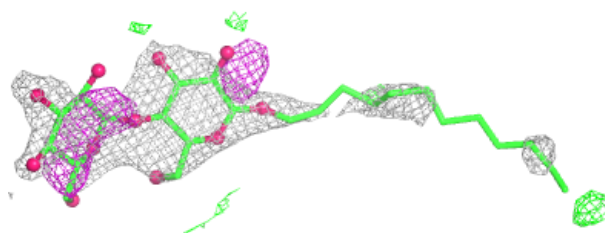


**Electron density around LMT A 359:**

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

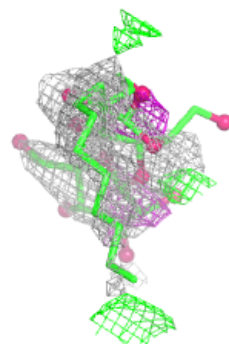
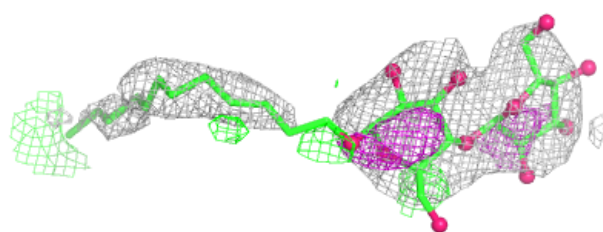
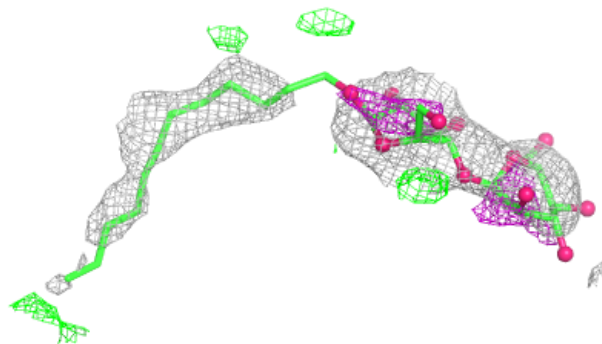
**Electron density around LMT a 420:**

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

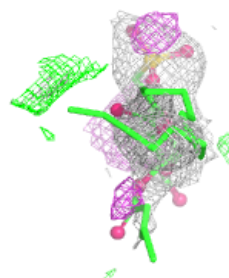
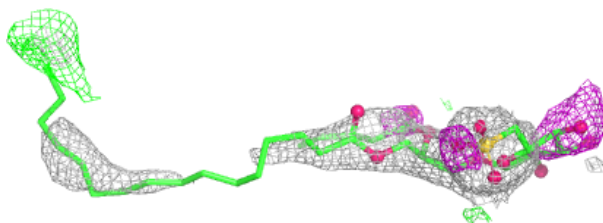
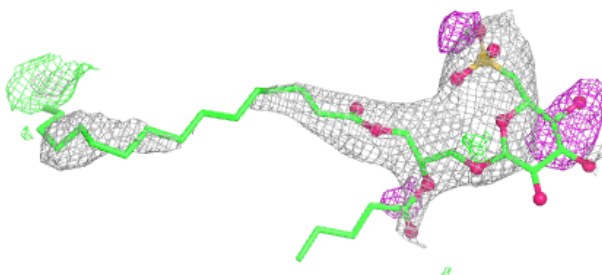


**Electron density around LMT I 101:**

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

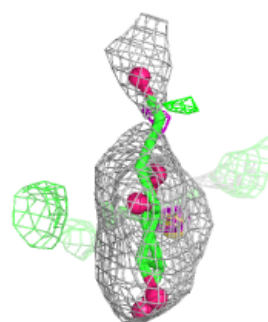
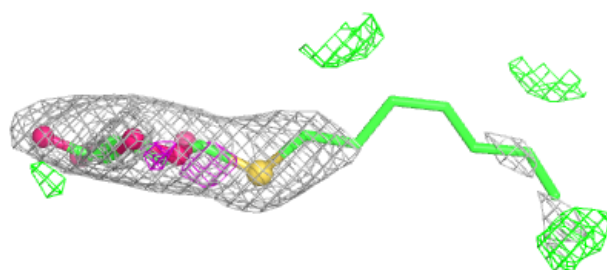
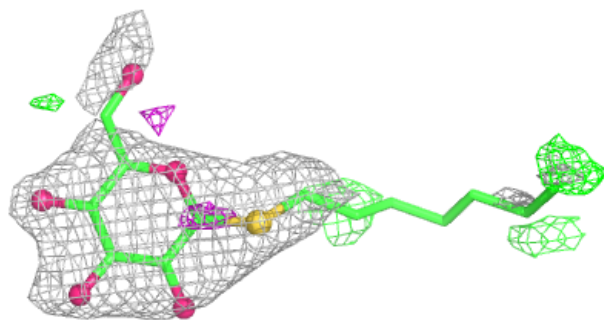
**Electron density around SQD f 102:**

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

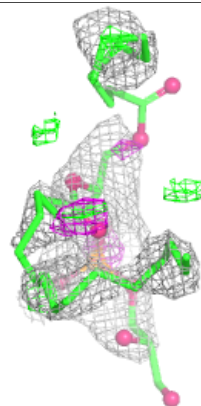
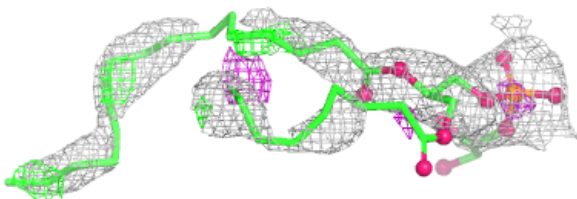
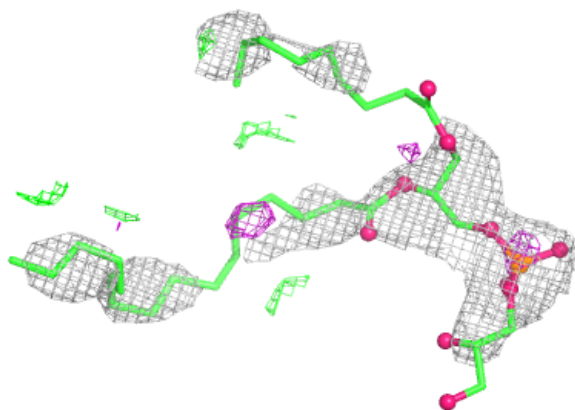


**Electron density around HTG C 522:**

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

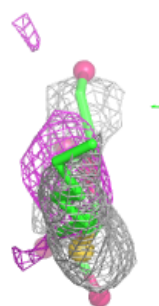
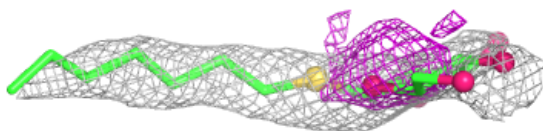
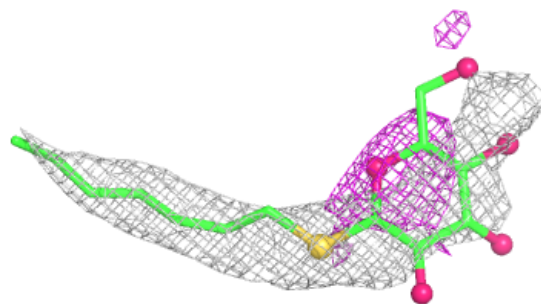
**Electron density around LHG e 101:**

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

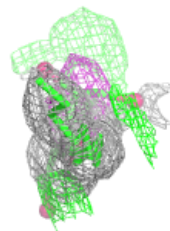
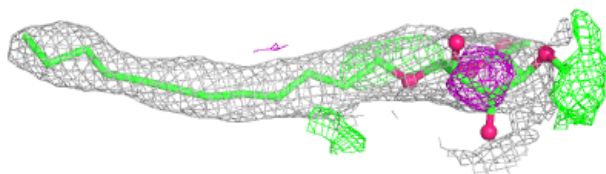
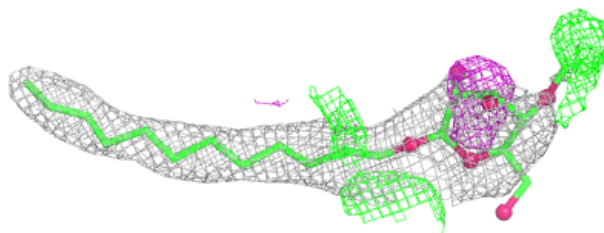


**Electron density around HTG b 623:**

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

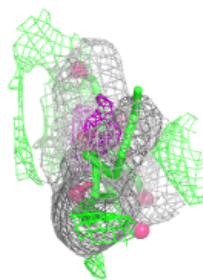
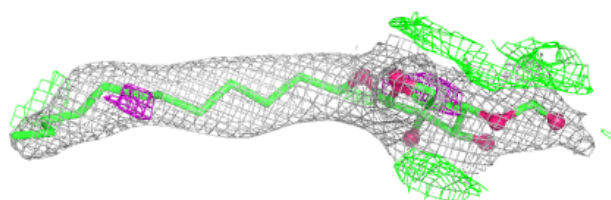
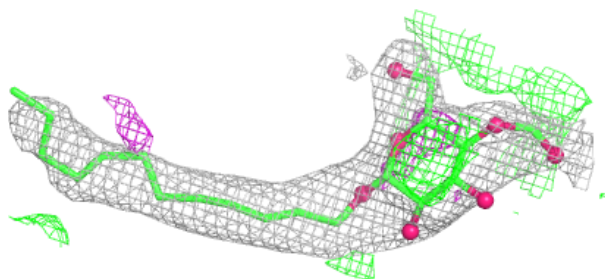
**Electron density around LMT b 621:**

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

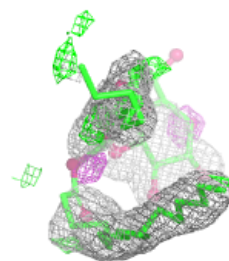
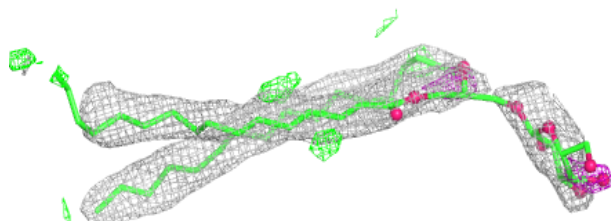
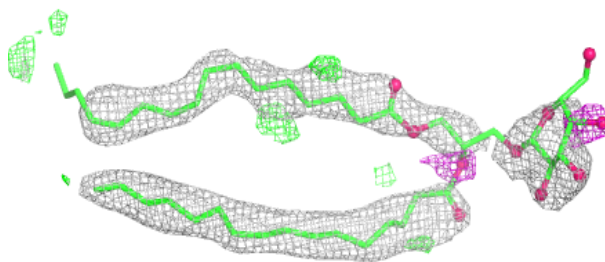


**Electron density around LMT t 102:**

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

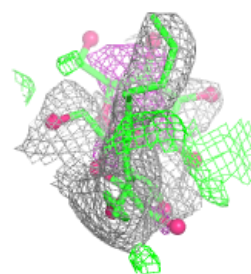
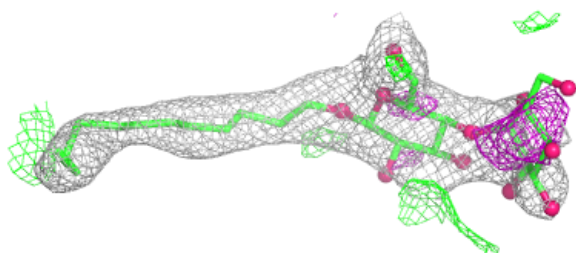
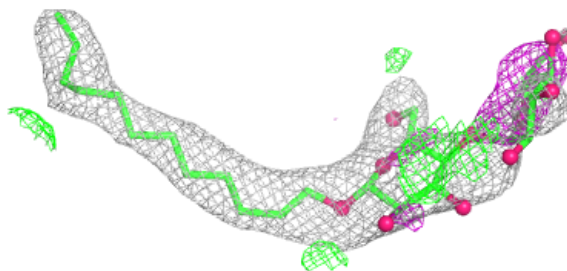
**Electron density around LMG C 521:**

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

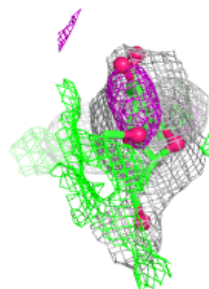
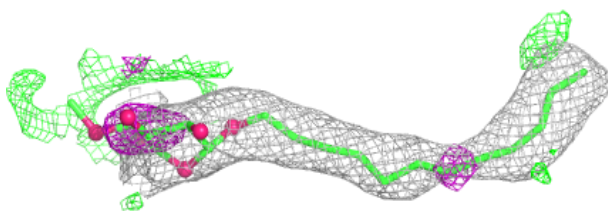
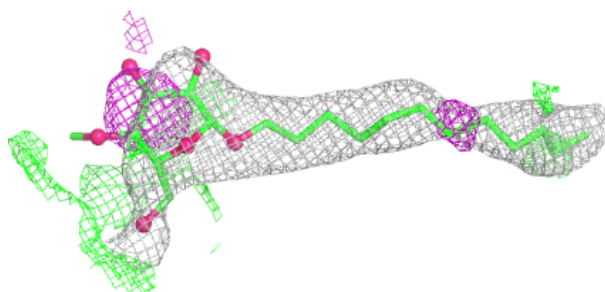


**Electron density around LMT M 103:**

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

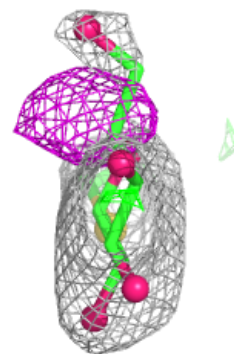
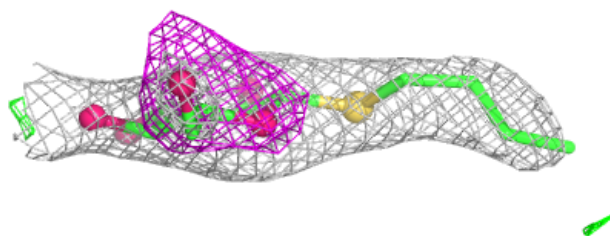
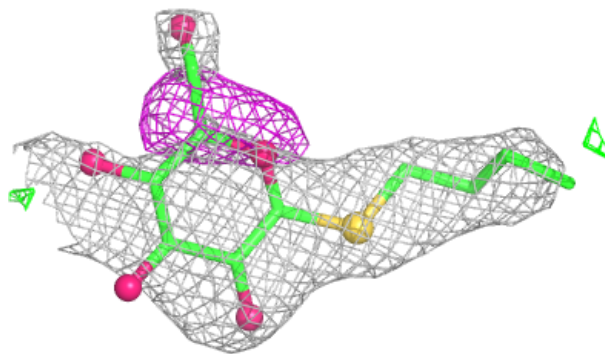
**Electron density around LMT t 101:**

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

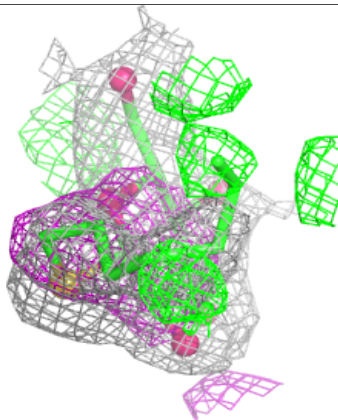
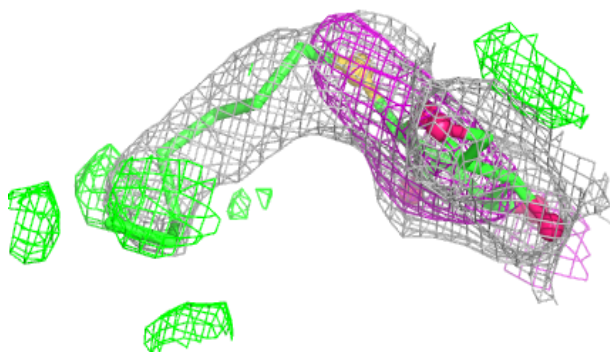
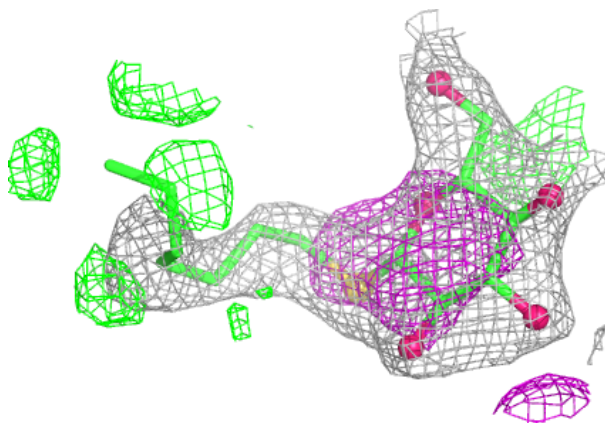


**Electron density around HTG D 414:**

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

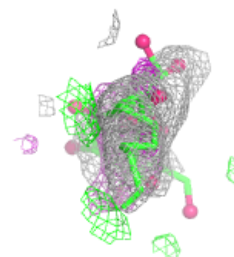
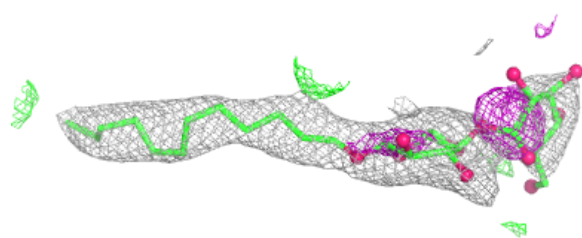
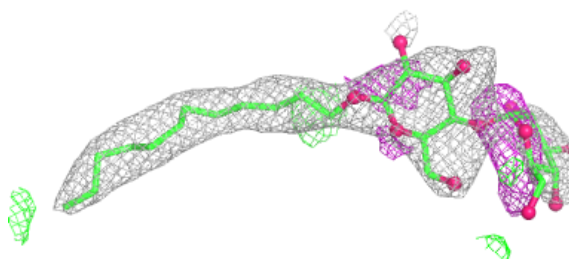
**Electron density around HTG B 623:**

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

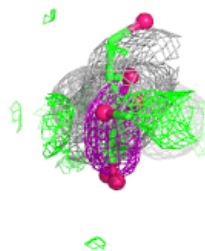
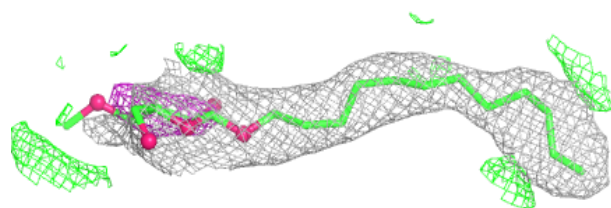
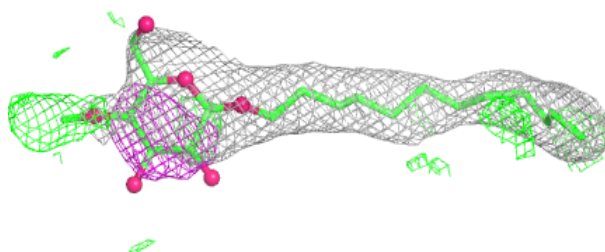


**Electron density around LMT D 404:**

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

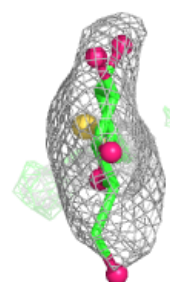
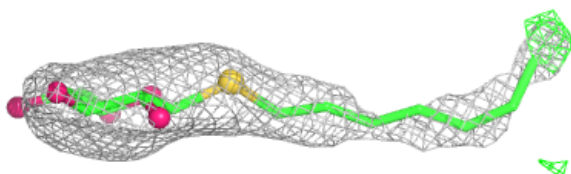
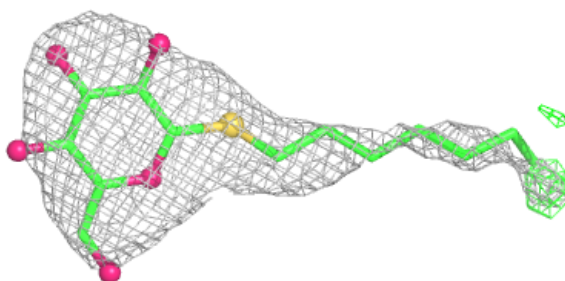
**Electron density around LMT b 627:**

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

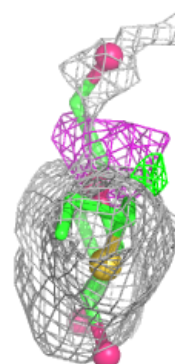
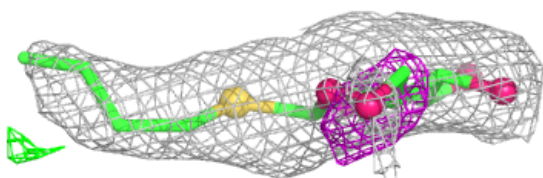
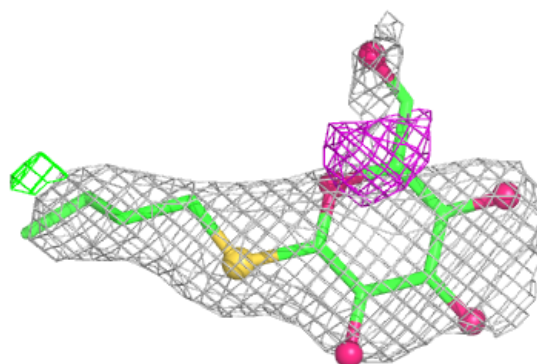


**Electron density around HTG c 522:**

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

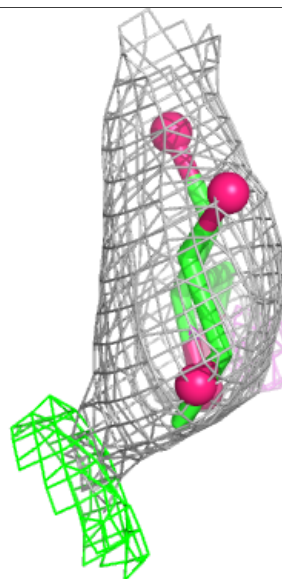
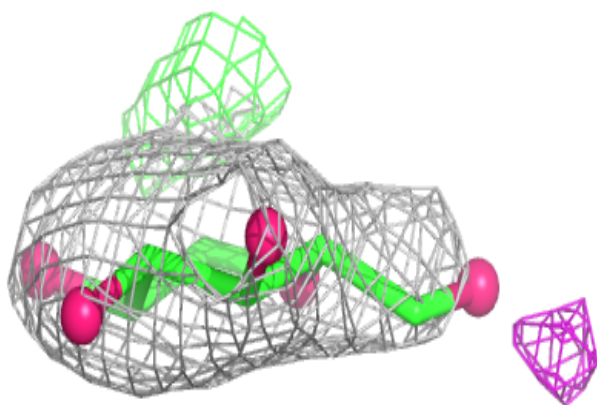
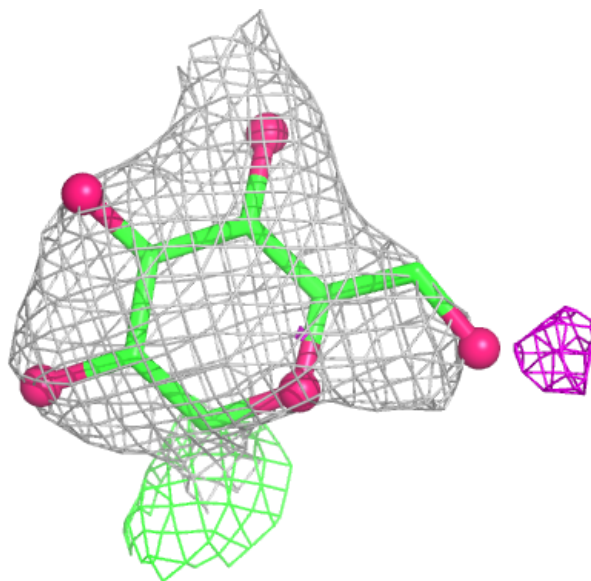
**Electron density around HTG d 411:**

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



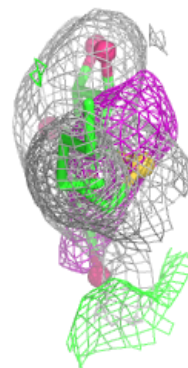
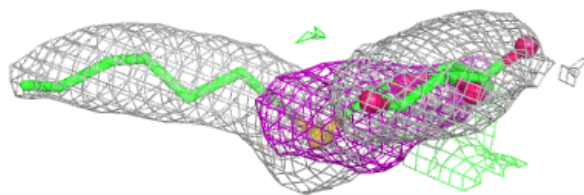
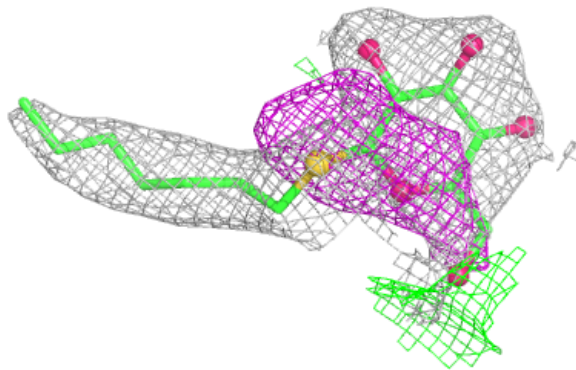
**Electron density around HTG V 203:**

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

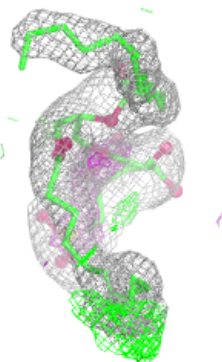
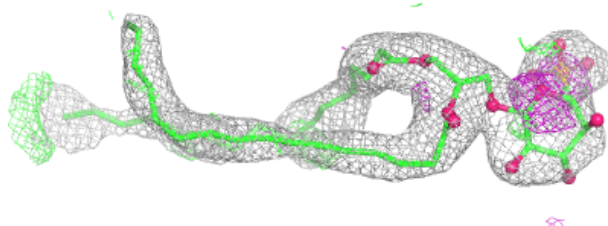
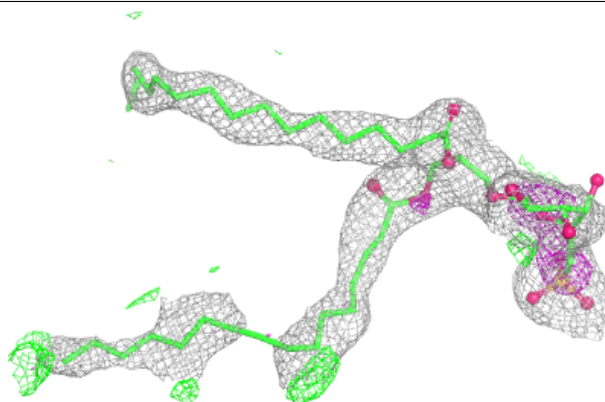


**Electron density around HTG b 622:**

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

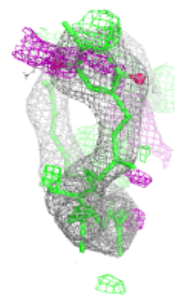
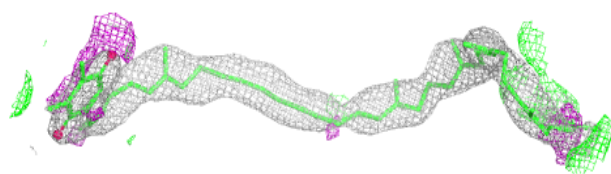
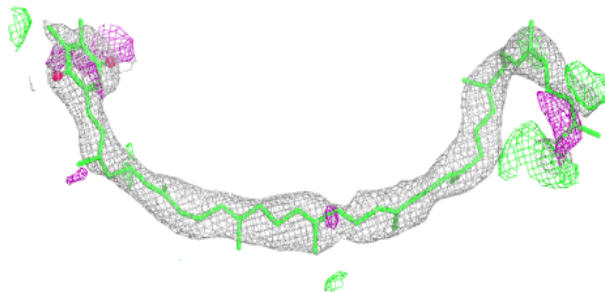
**Electron density around SQD a 413:**

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

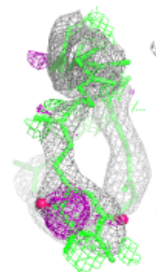
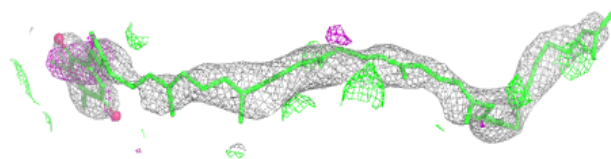
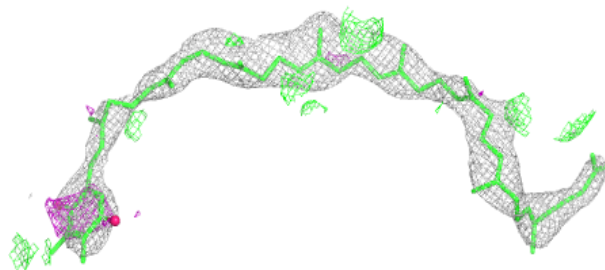


**Electron density around PL9 A 414:**

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

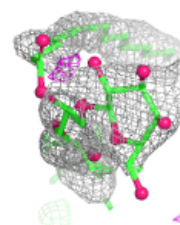
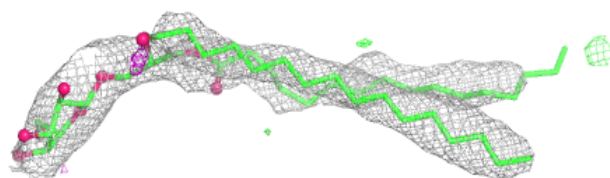
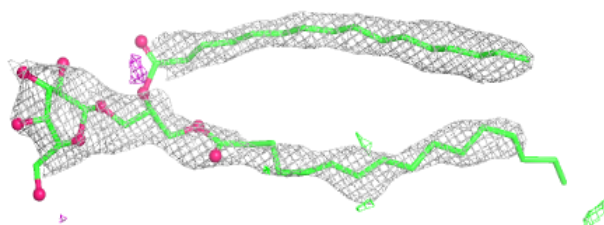
**Electron density around PL9 a 416:**

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

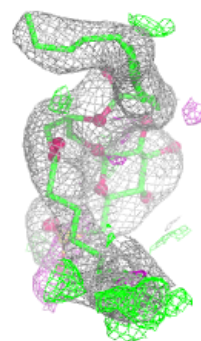
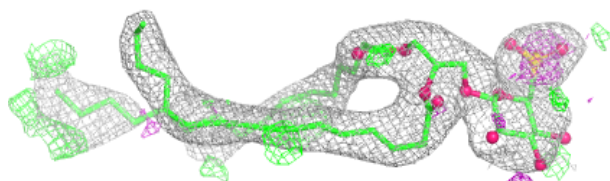
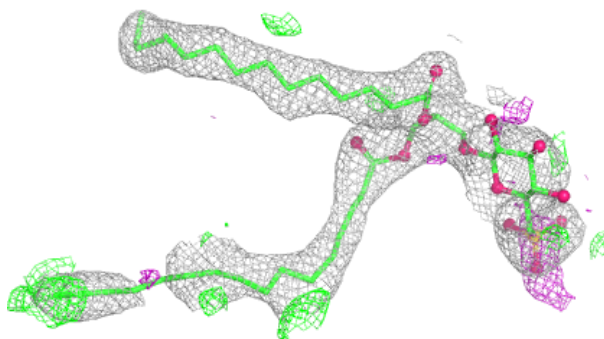


**Electron density around LMG c 521:**

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

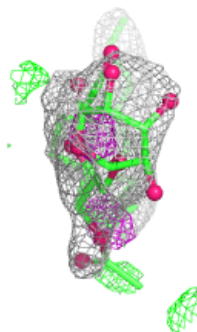
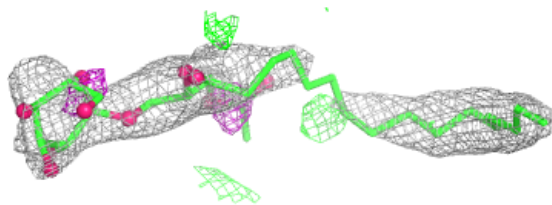
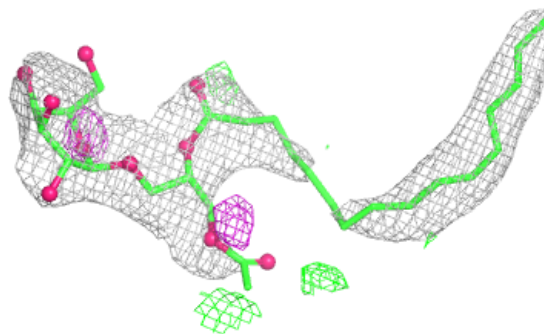
**Electron density around SQD A 412:**

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

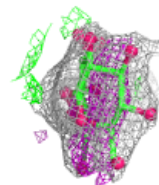
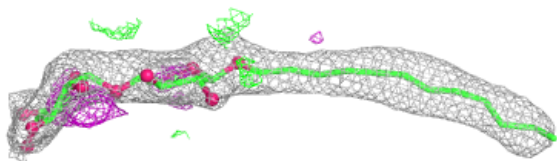
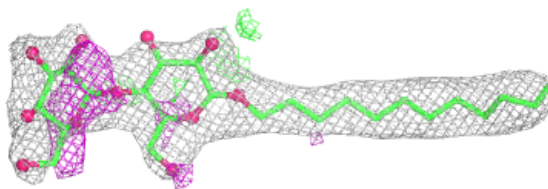


**Electron density around LMG Z 101:**

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

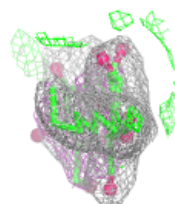
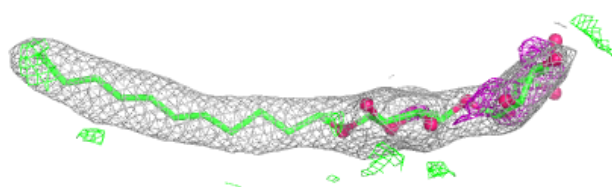
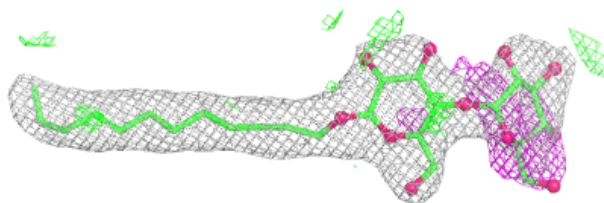
**Electron density around LMT m 103:**

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

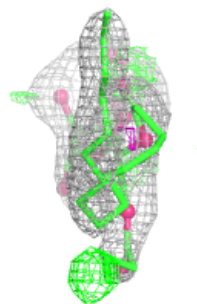
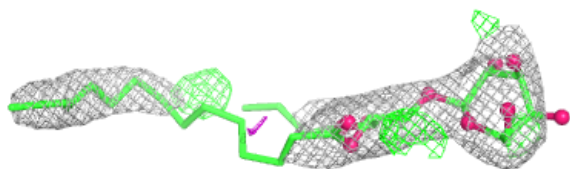
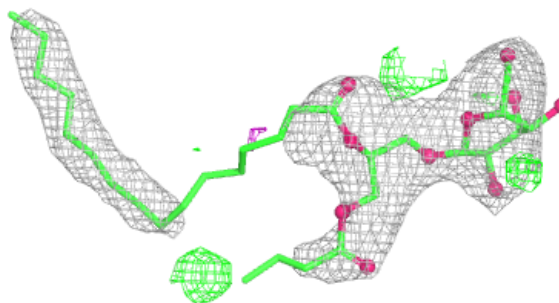


**Electron density around LMT M 101:**

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

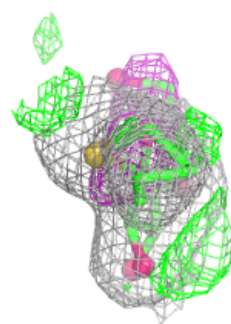
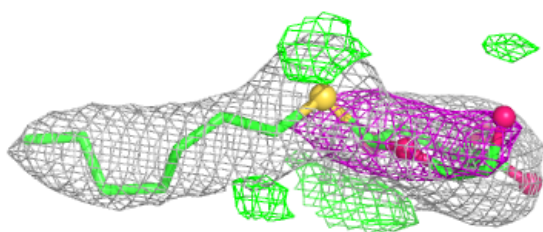
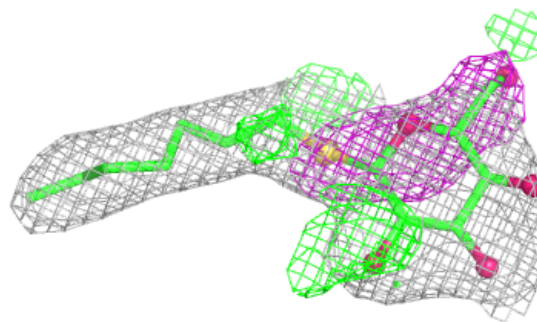
**Electron density around LMG z 101:**

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

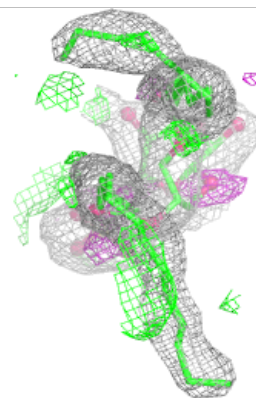
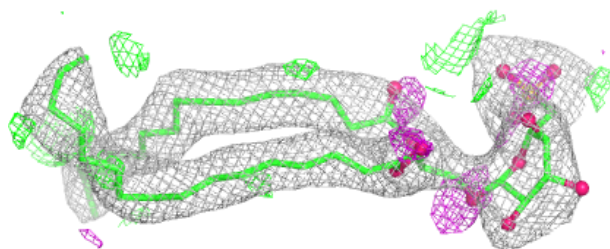
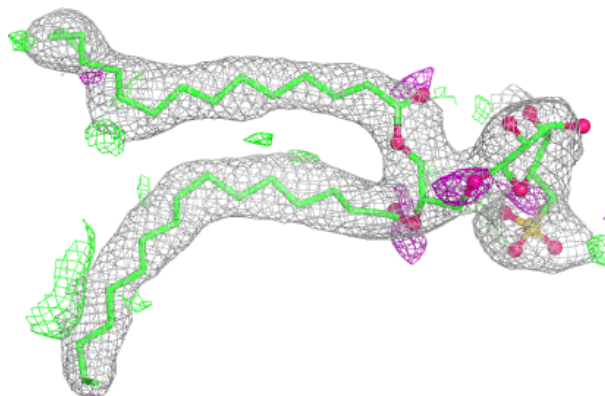


**Electron density around HTG B 622:**

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

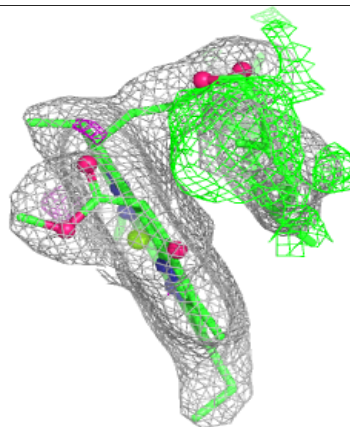
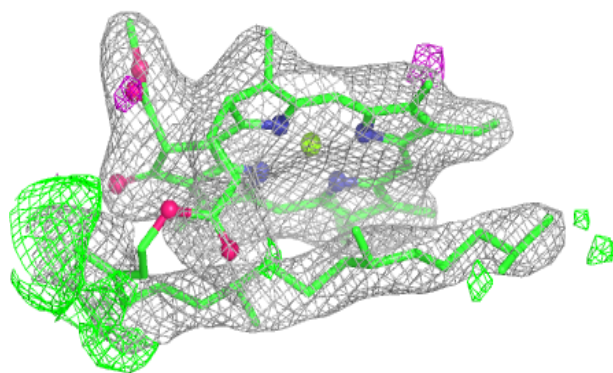
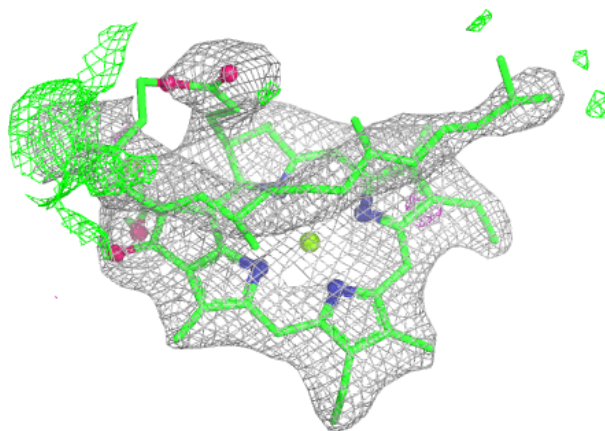
**Electron density around SQD B 620:**

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

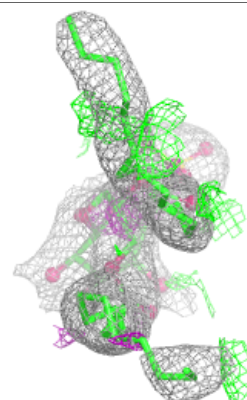
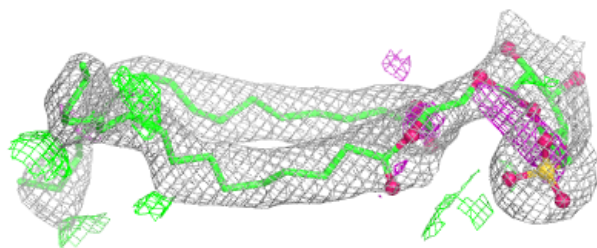
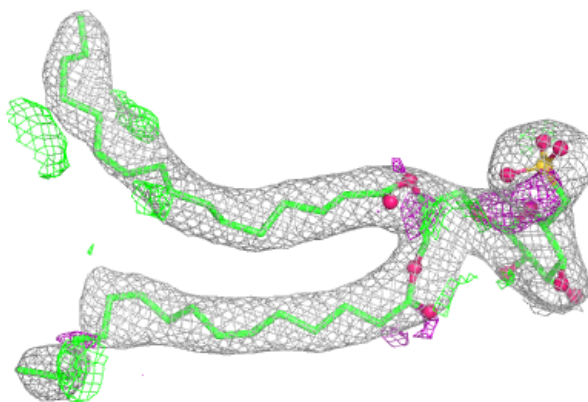


**Electron density around CLA b 601:**

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

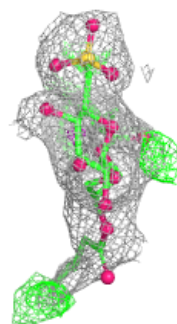
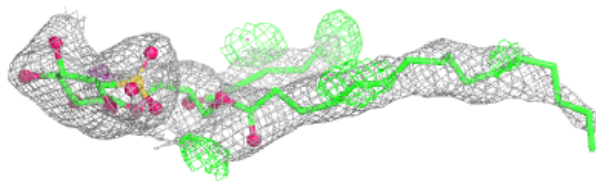
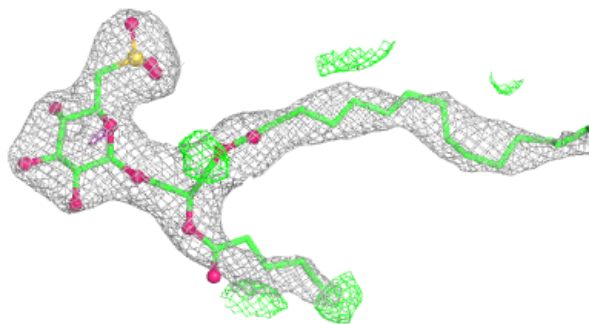
**Electron density around SQD b 620:**

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

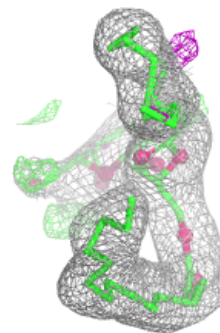
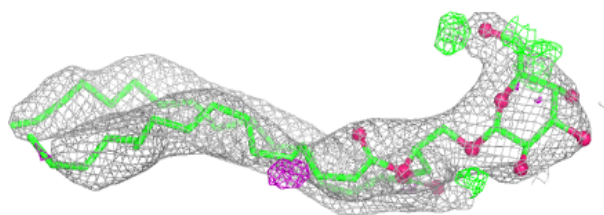
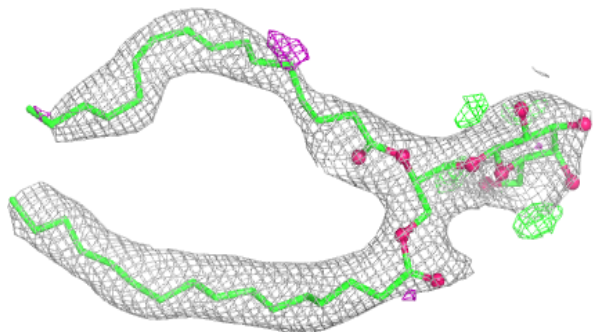


**Electron density around SQD F 101:**

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

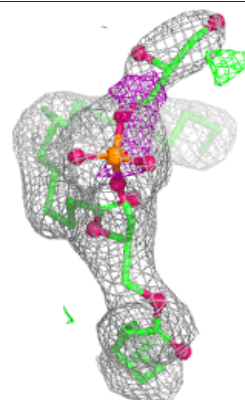
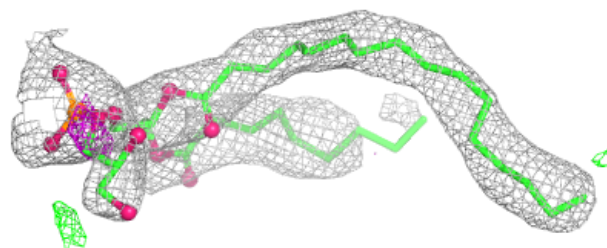
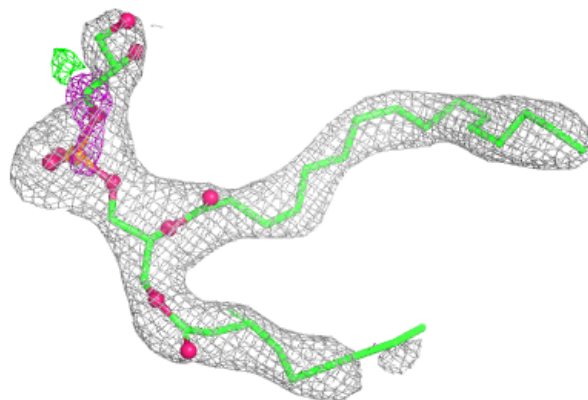
**Electron density around LMG C 501:**

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

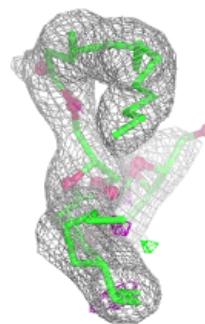
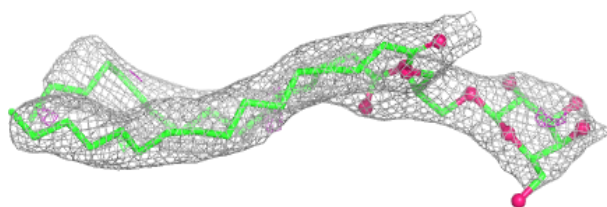
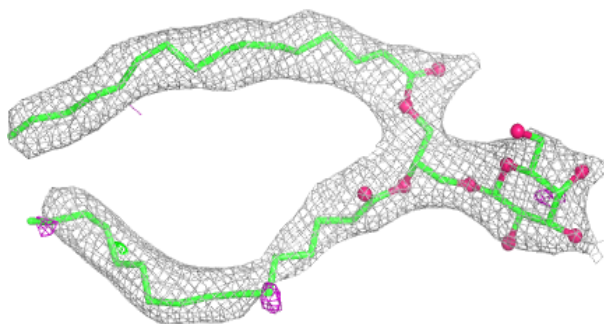


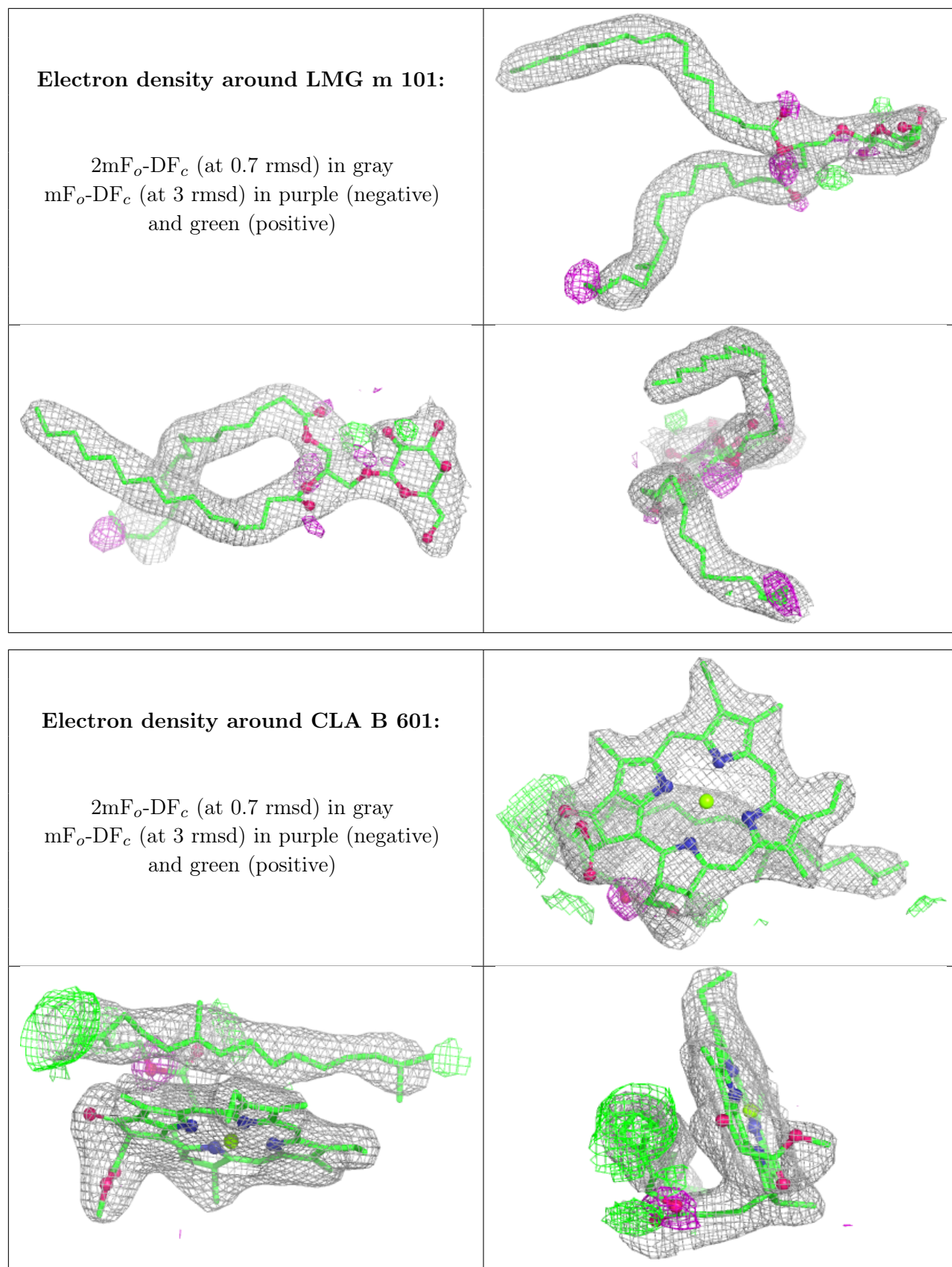
**Electron density around LHG E 101:**

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

**Electron density around LMG a 419:**

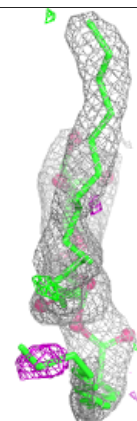
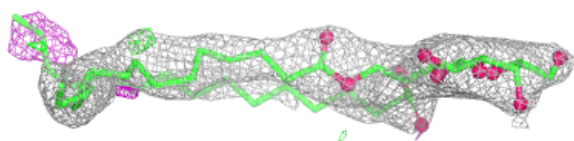
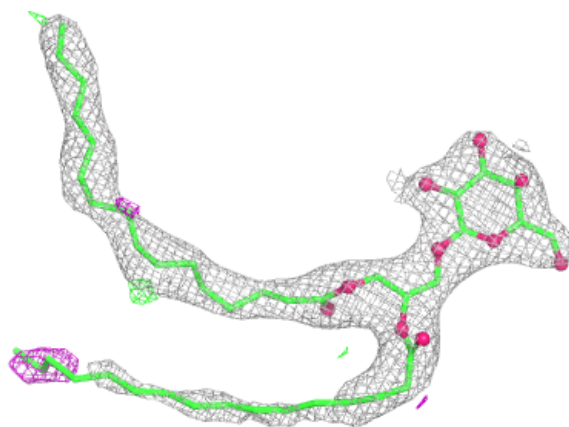
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



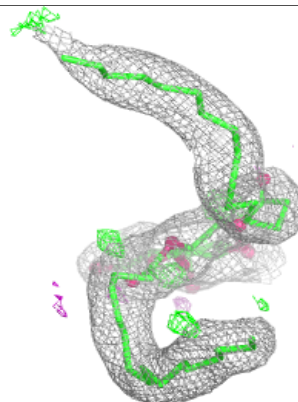
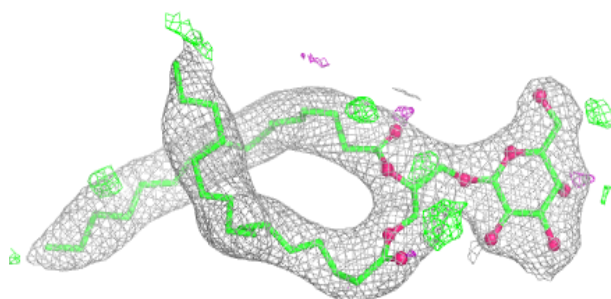
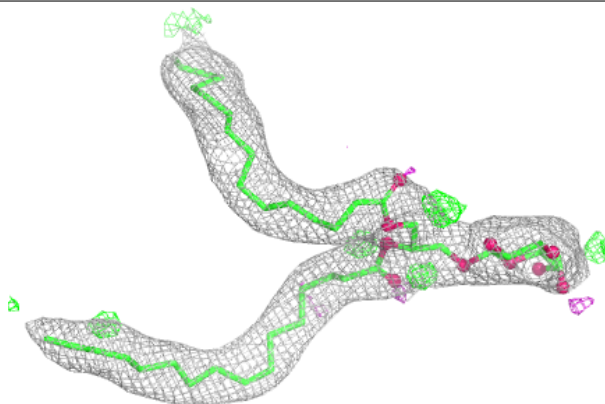


**Electron density around LMG c 520:**

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

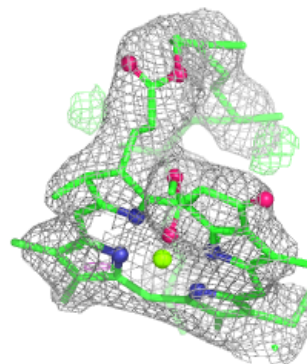
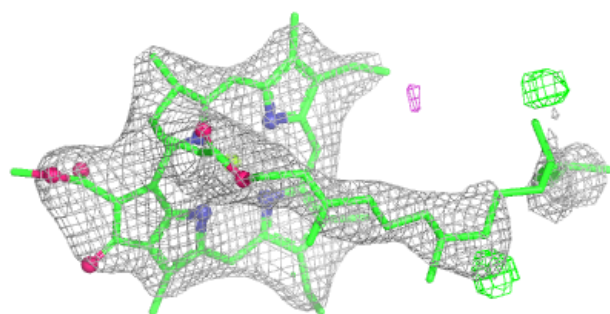
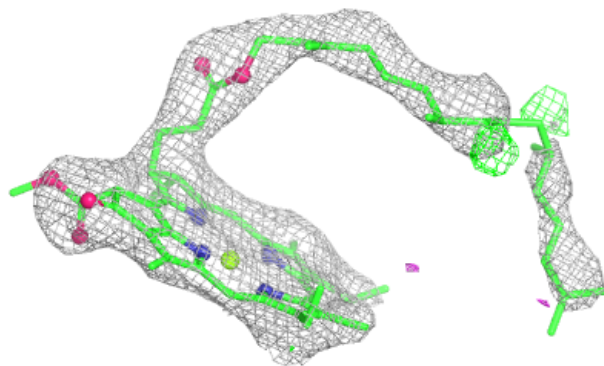
**Electron density around LMG B 621:**

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

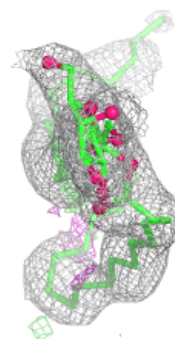
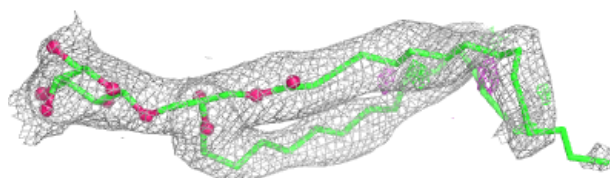
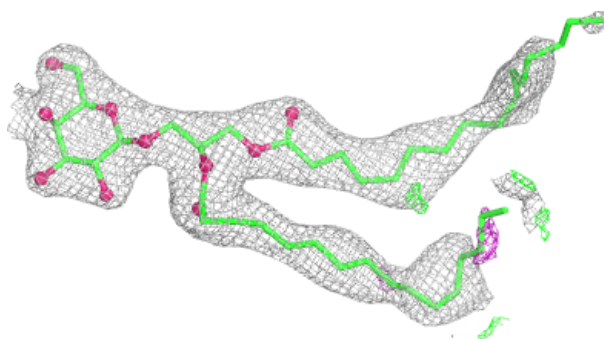


**Electron density around CLA c 514:**

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

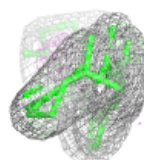
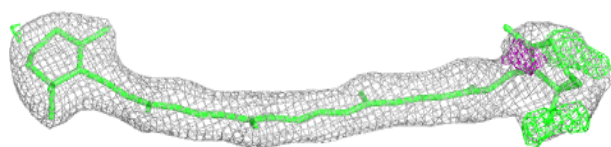
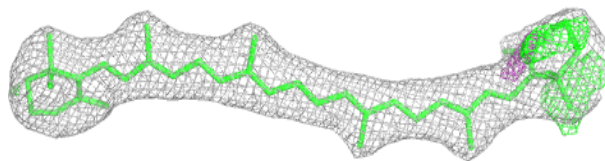
**Electron density around LMG d 412:**

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

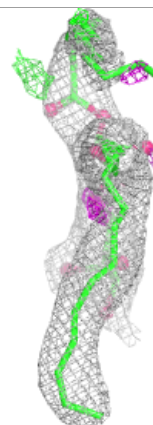
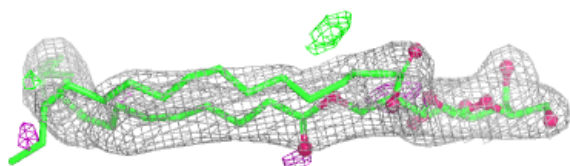
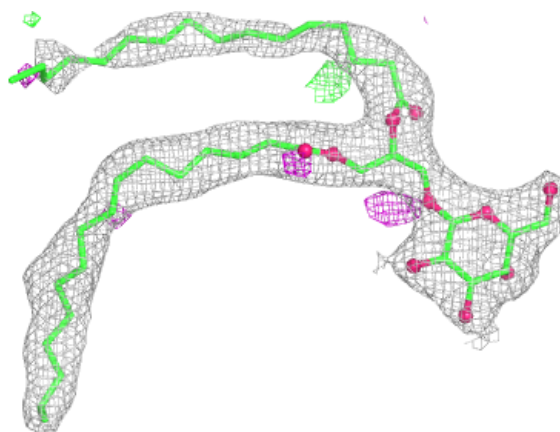


**Electron density around BCR d 404:**

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

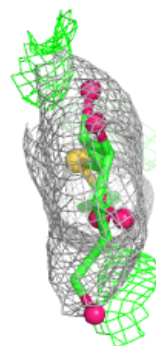
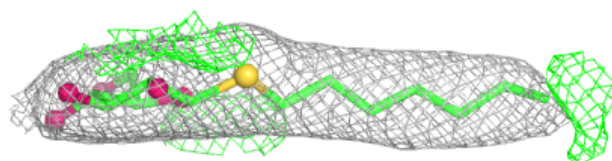
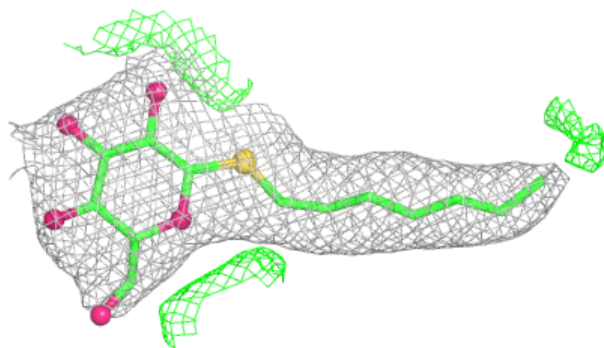
**Electron density around LMG C 520:**

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

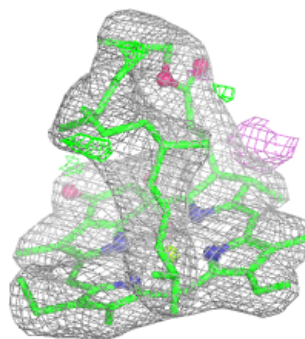
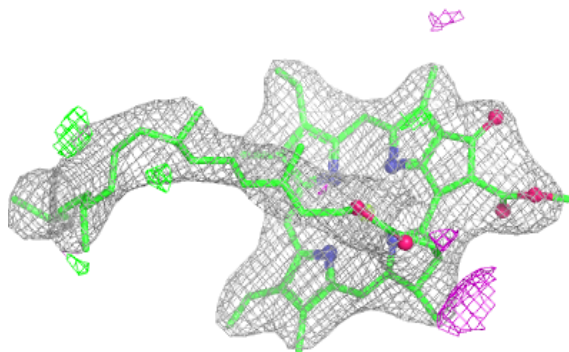
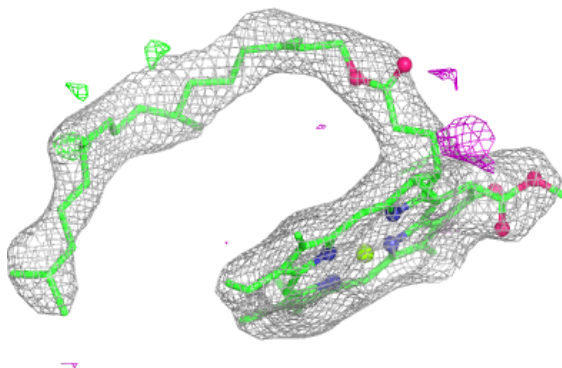


**Electron density around HTG b 625:**

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

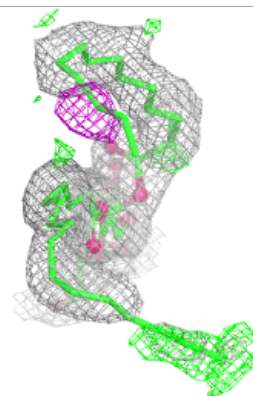
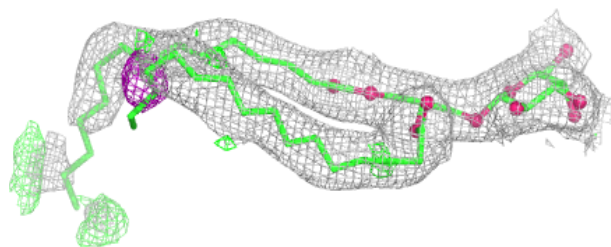
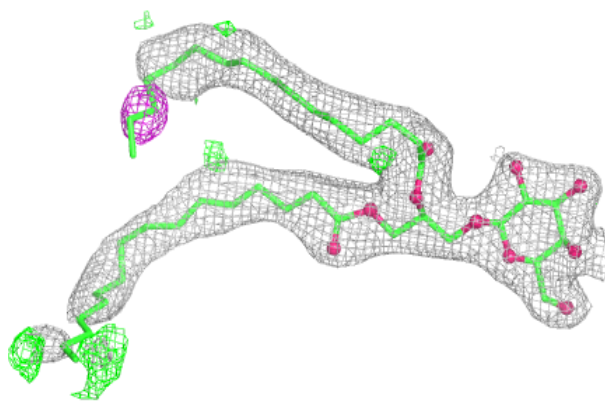
**Electron density around CLA C 514:**

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

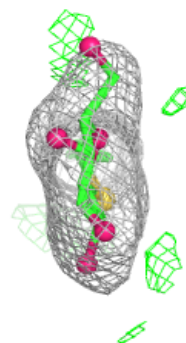
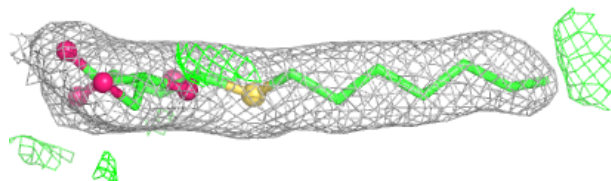
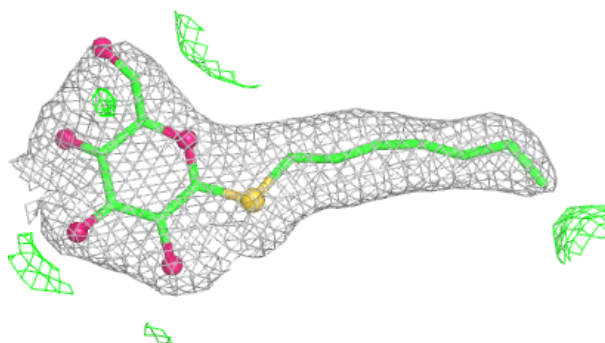


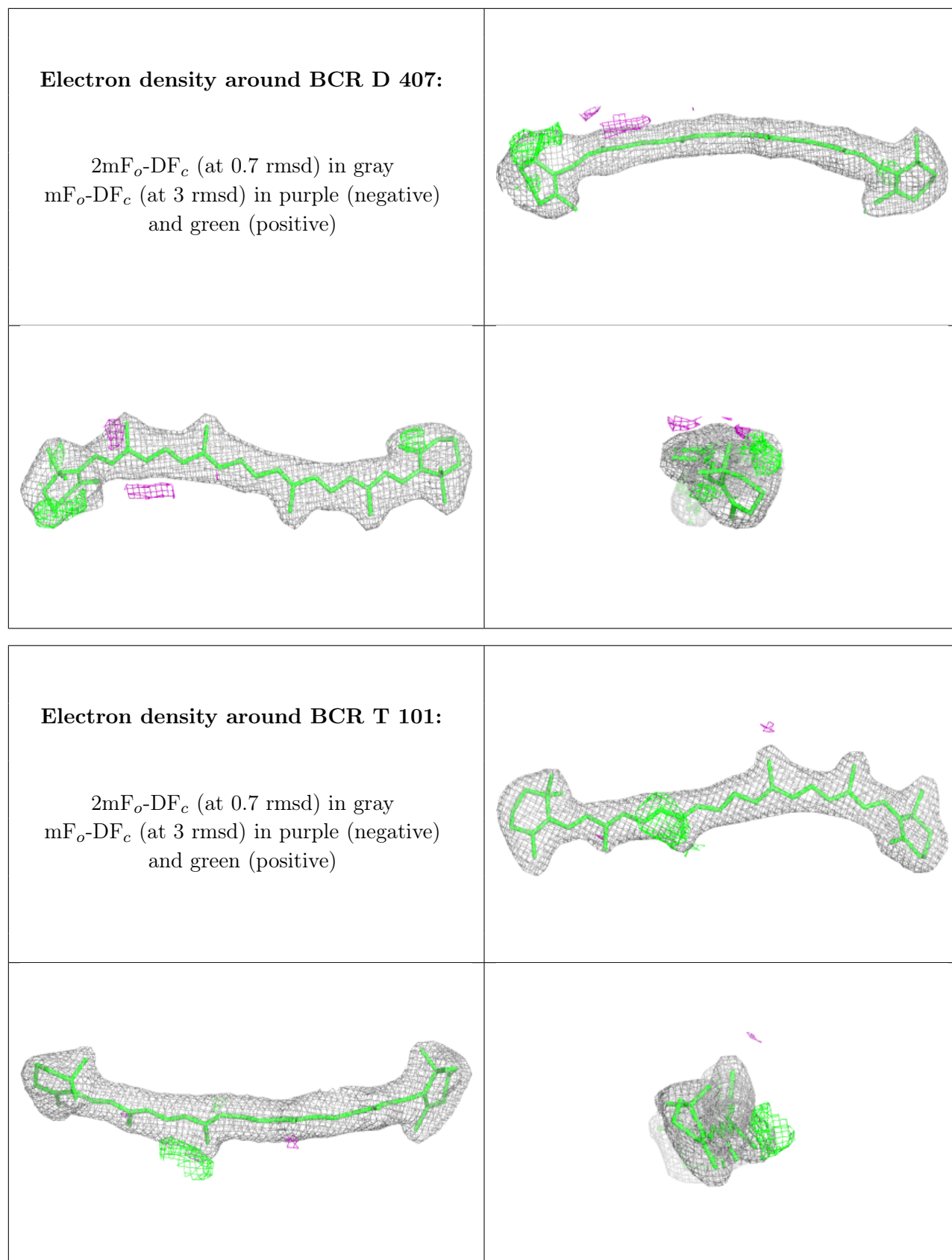
**Electron density around LMG D 415:**

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

**Electron density around HTG B 626:**

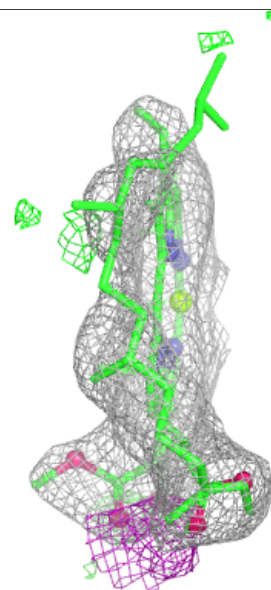
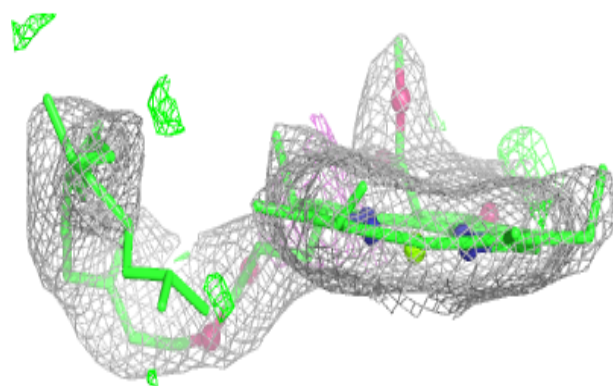
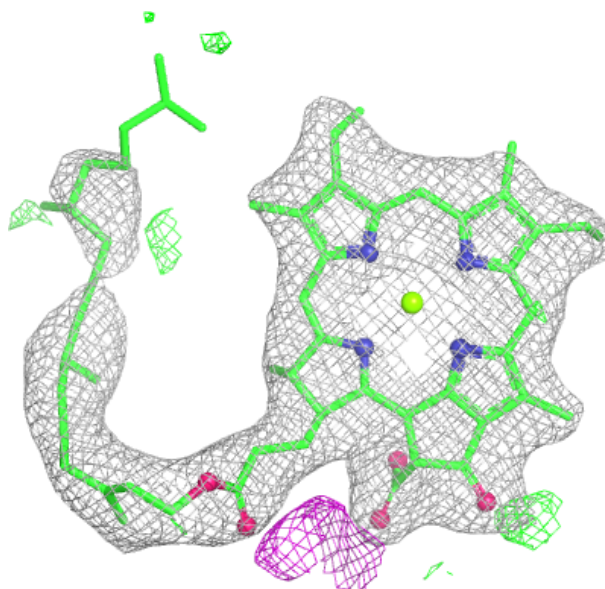
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





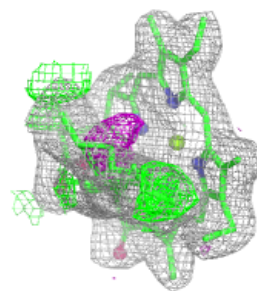
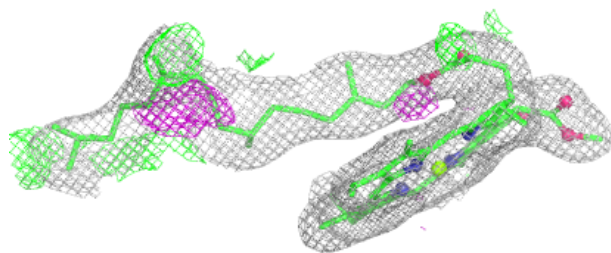
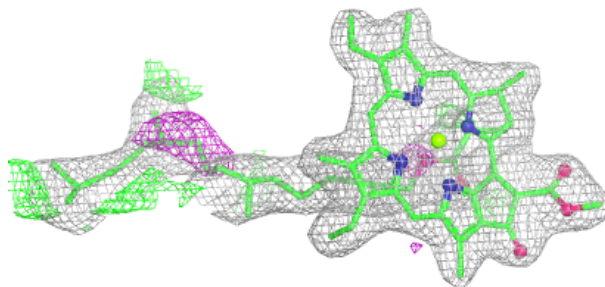
**Electron density around CLA c 513:**

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

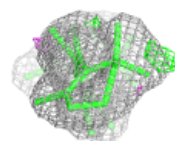
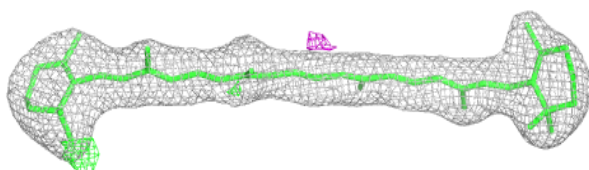
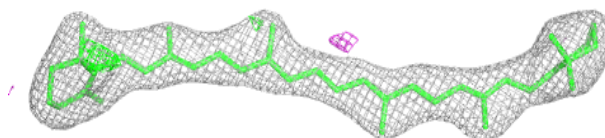


**Electron density around CLA B 614:**

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

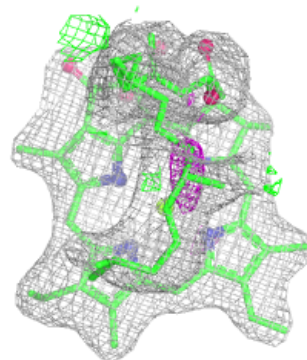
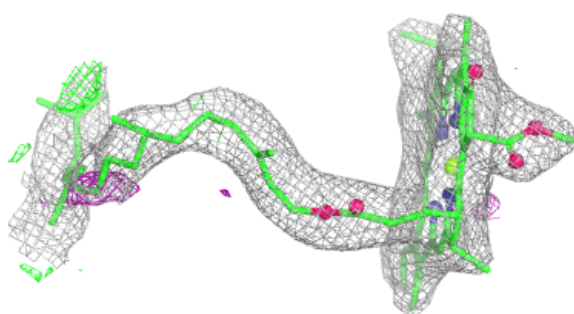
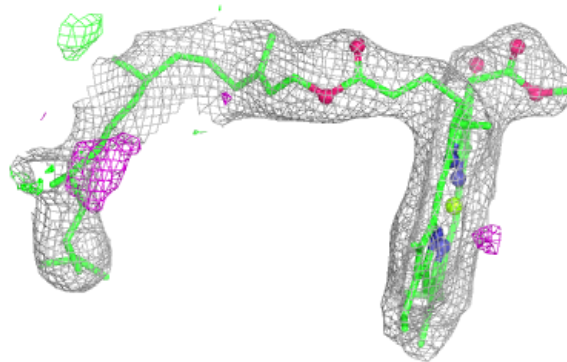
**Electron density around BCR C 515:**

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



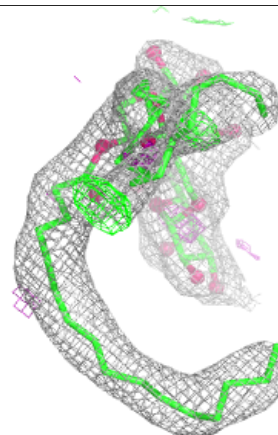
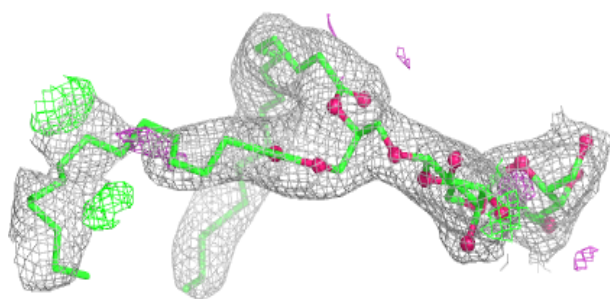
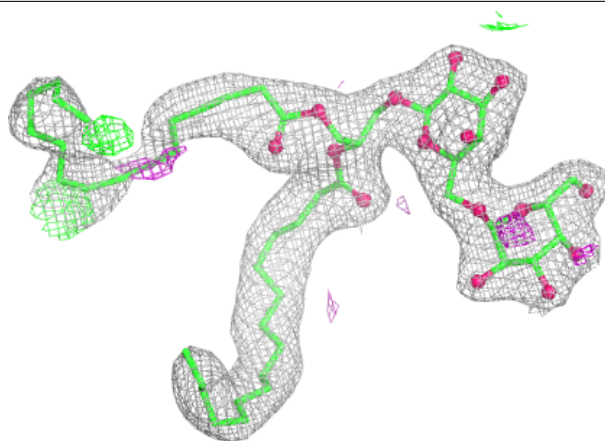
**Electron density around CLA C 507:**

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



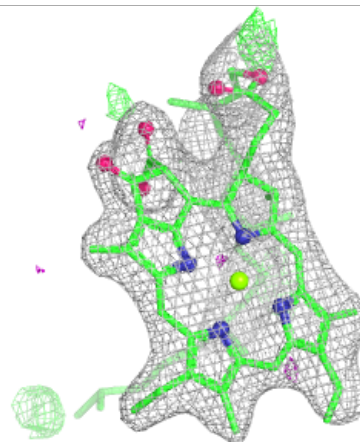
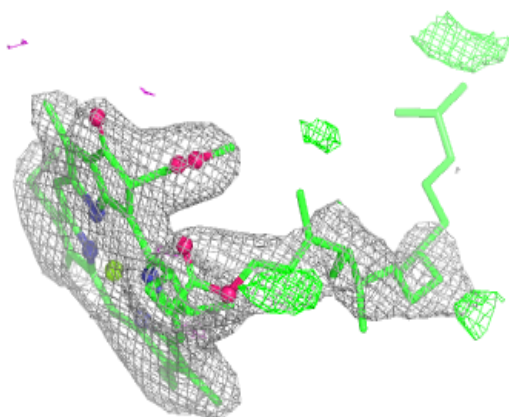
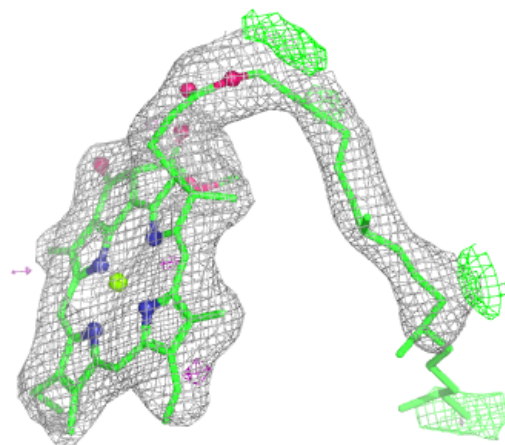
**Electron density around DGD C 518:**

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



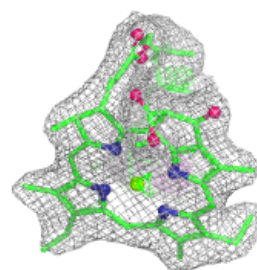
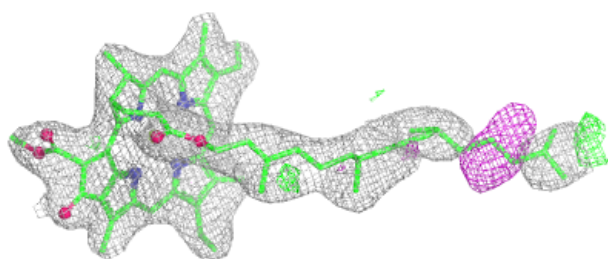
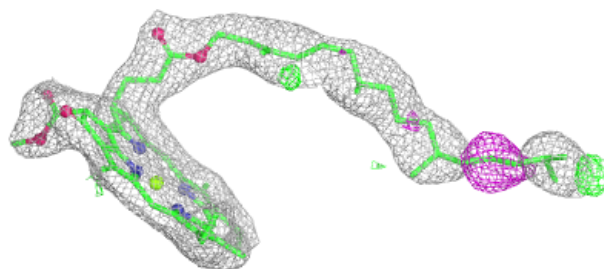
**Electron density around CLA b 616:**

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

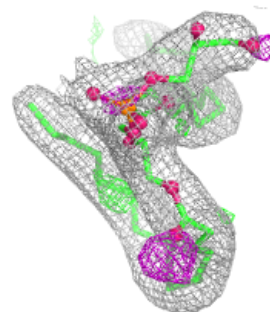
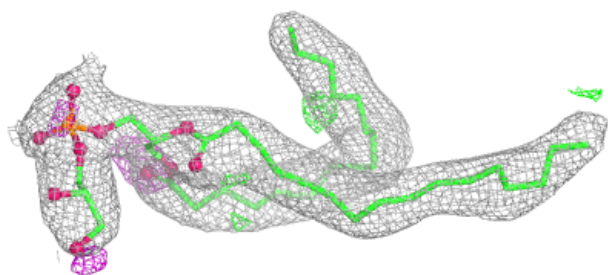
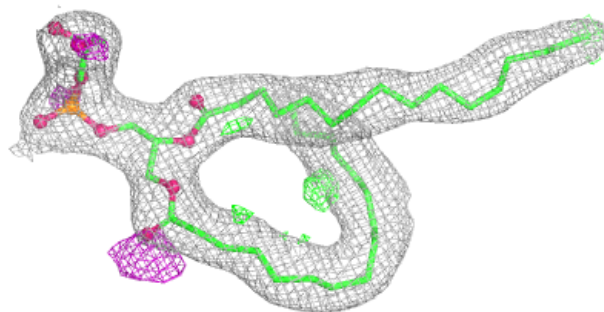


**Electron density around CLA c 505:**

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

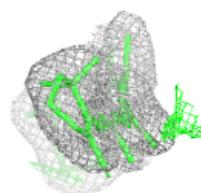
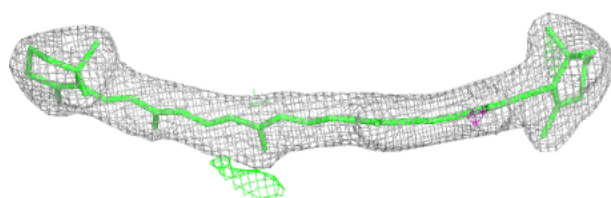
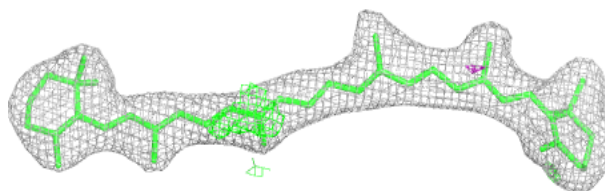
**Electron density around LHG D 409:**

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

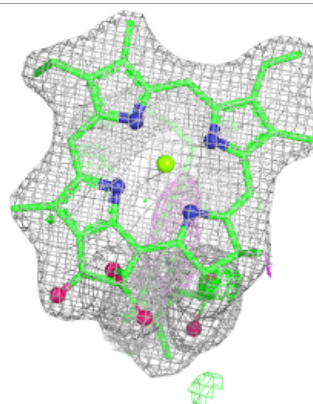
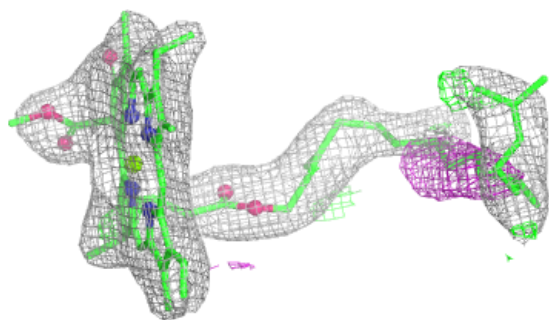
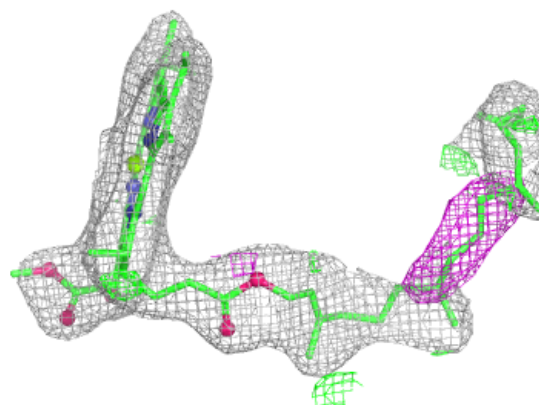


**Electron density around BCR t 103:**

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

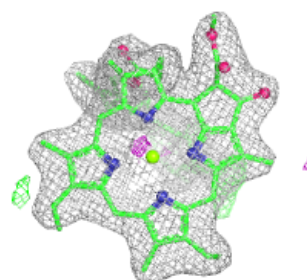
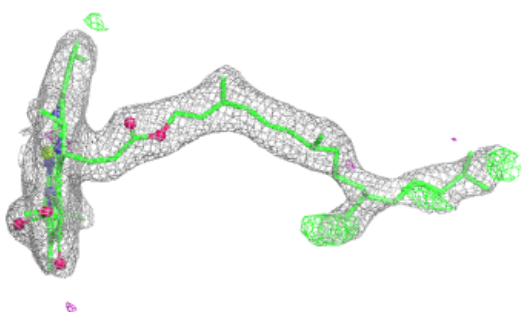
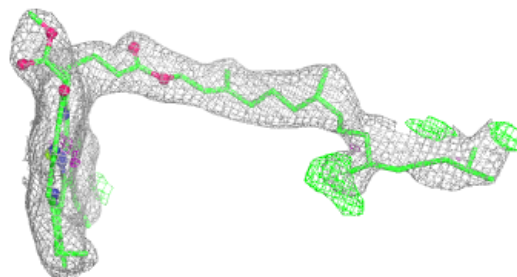
**Electron density around CLA c 507:**

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

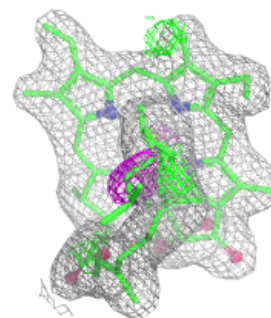
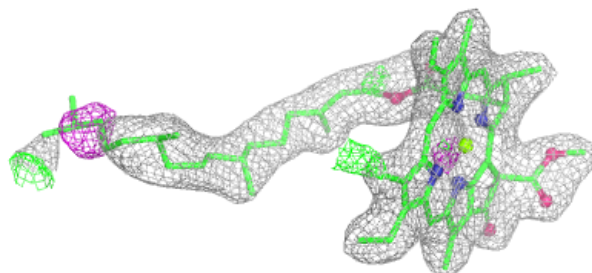
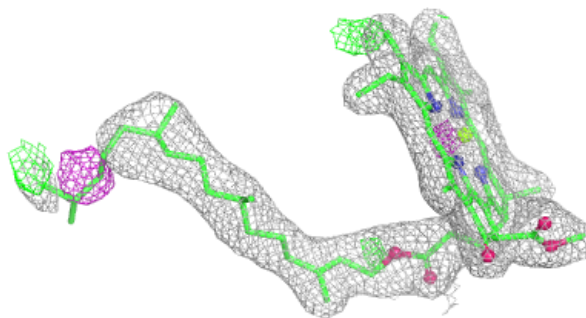


**Electron density around CLA B 606:**

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

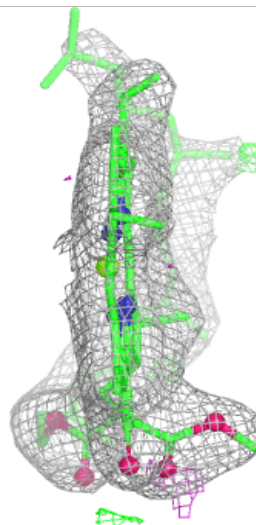
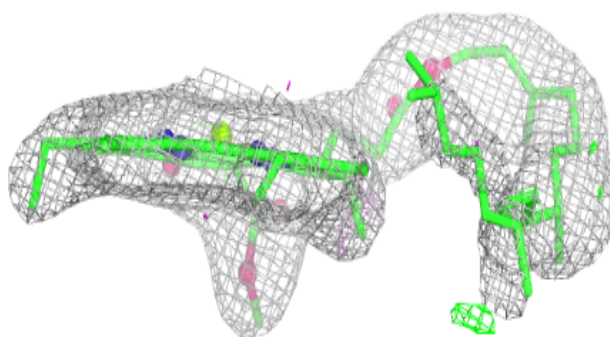
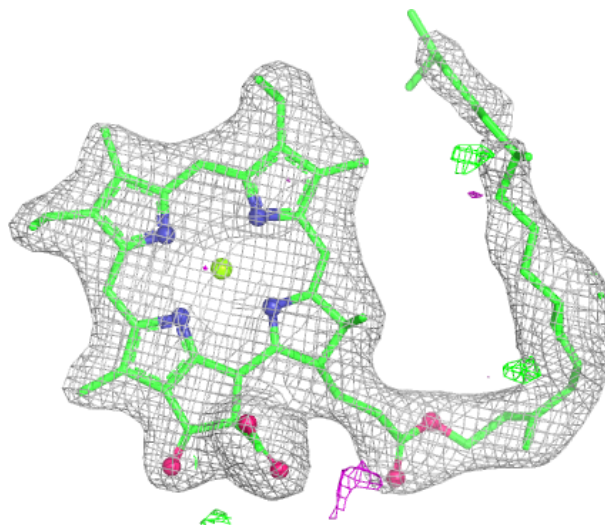
**Electron density around CLA C 509:**

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



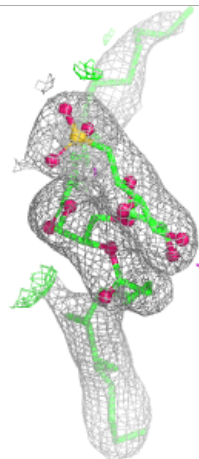
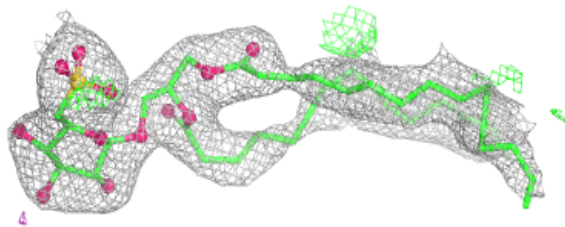
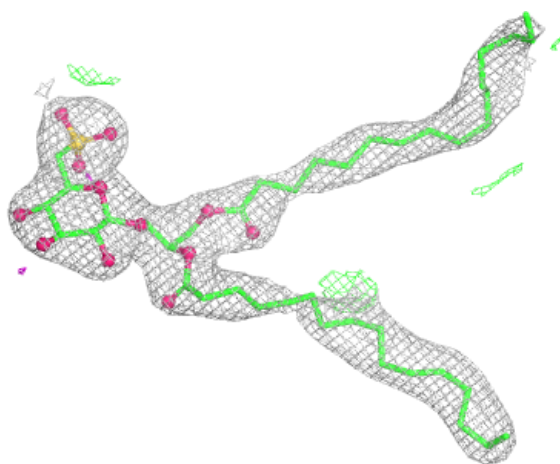
**Electron density around CLA C 513:**

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



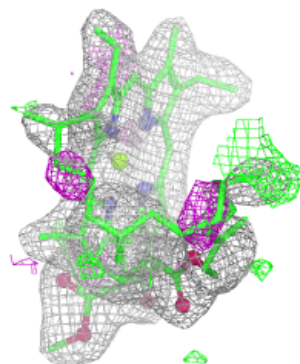
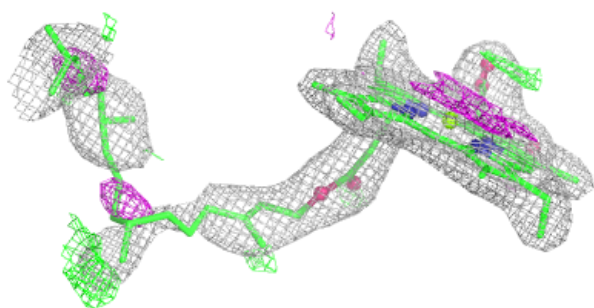
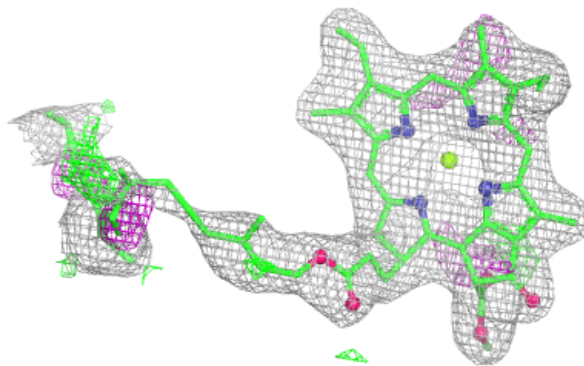
**Electron density around SQD a 411:**

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

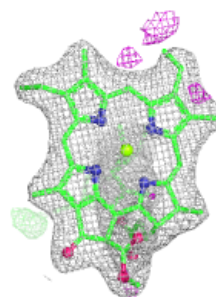
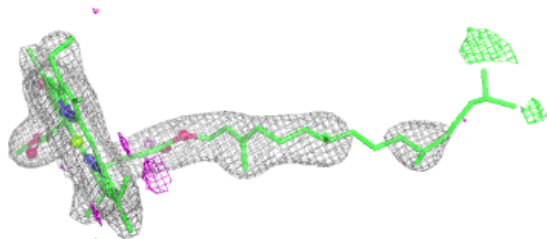
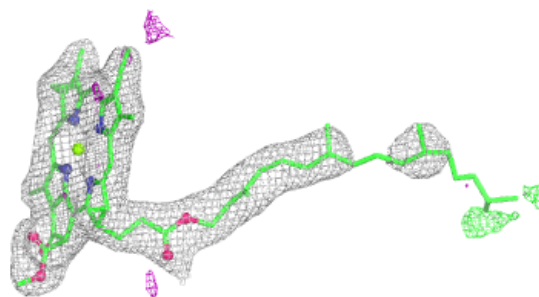


**Electron density around CLA A 408:**

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

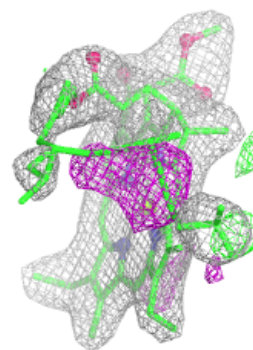
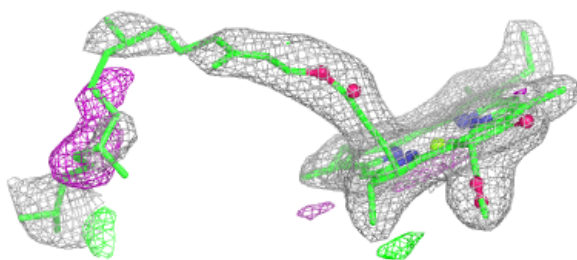
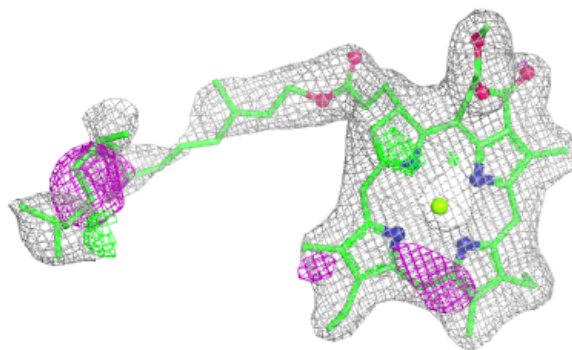
**Electron density around CLA d 403:**

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



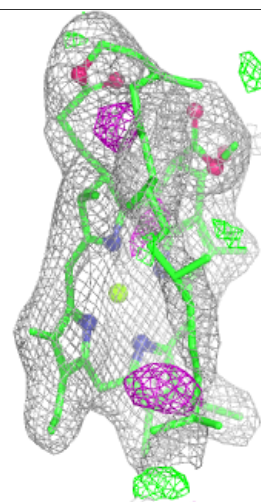
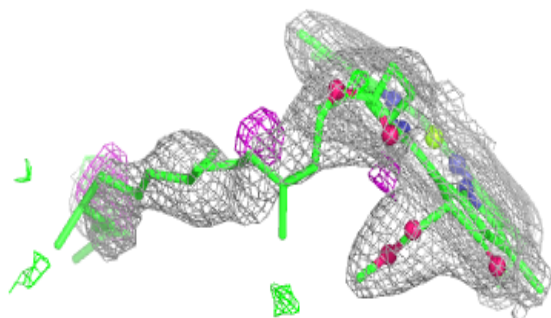
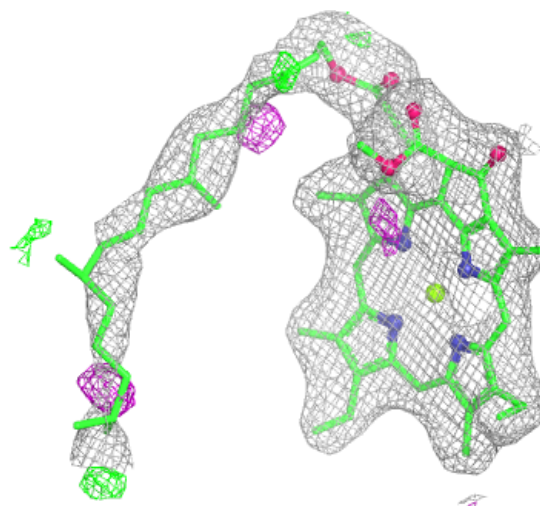
**Electron density around CLA a 409:**

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



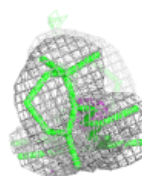
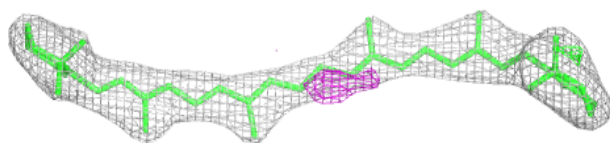
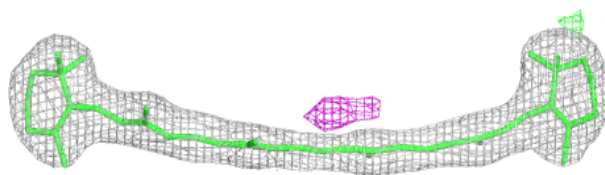
**Electron density around CLA B 616:**

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

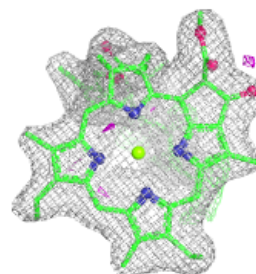
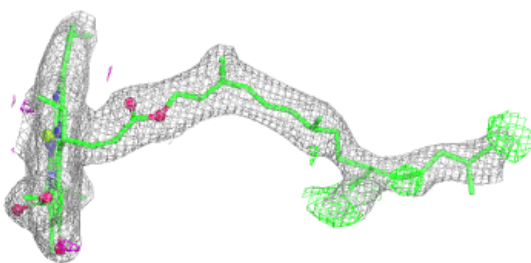
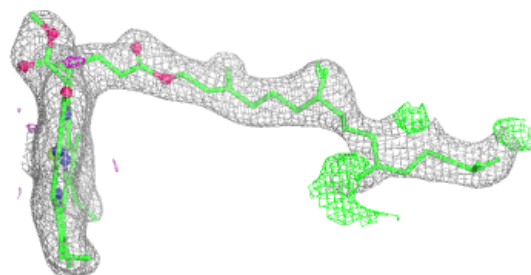


**Electron density around BCR K 102:**

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

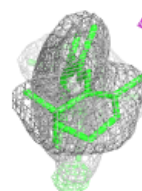
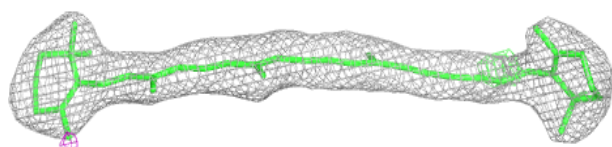
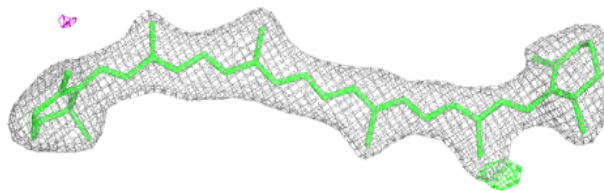
**Electron density around CLA b 606:**

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

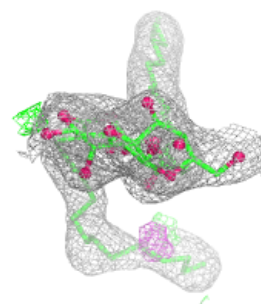
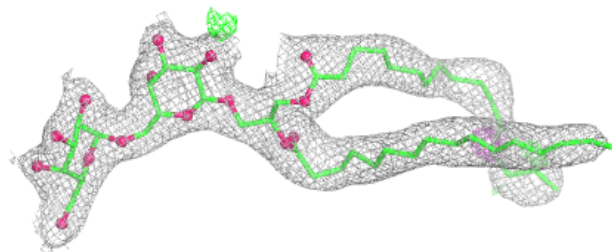
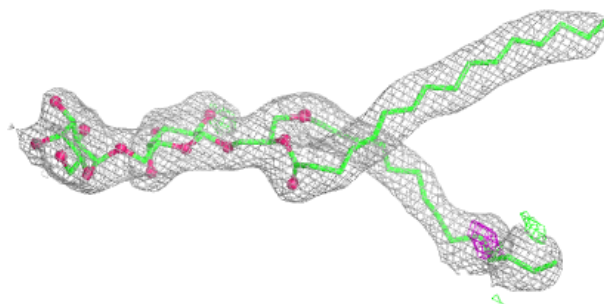


**Electron density around BCR Y 101:**

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

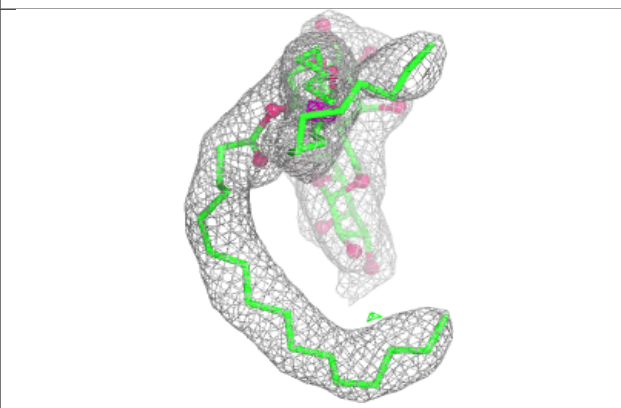
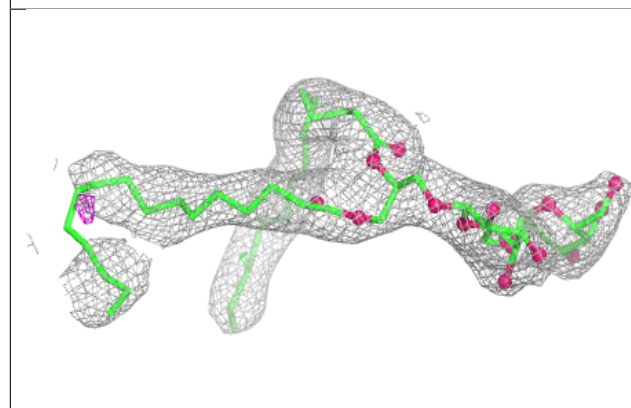
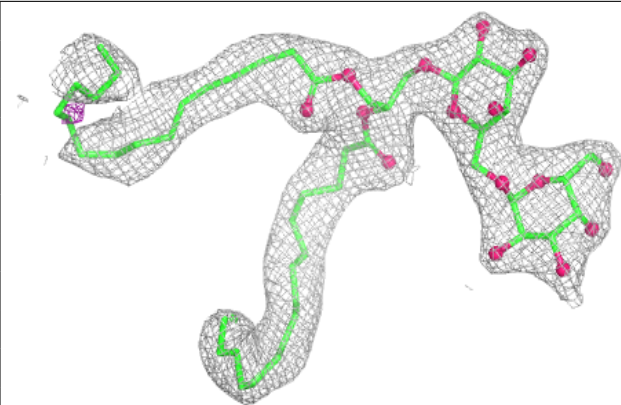
**Electron density around DGD c 517:**

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

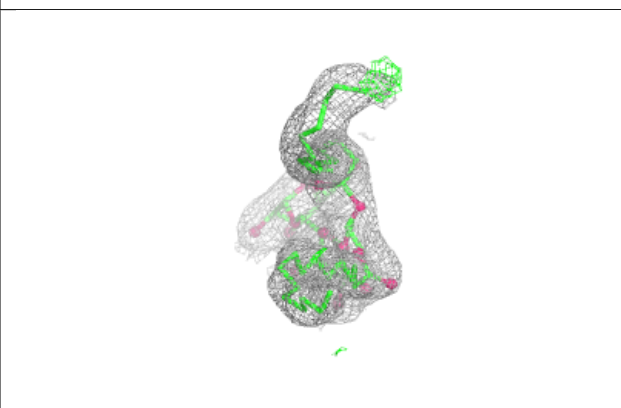
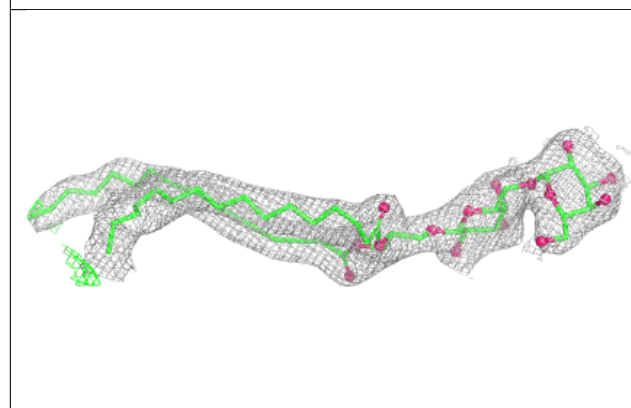
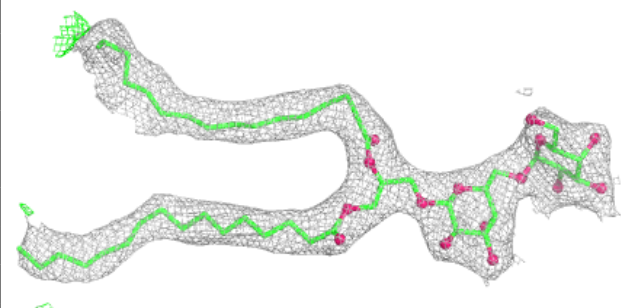


**Electron density around DGD c 518:**

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

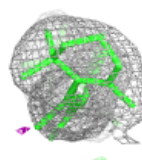
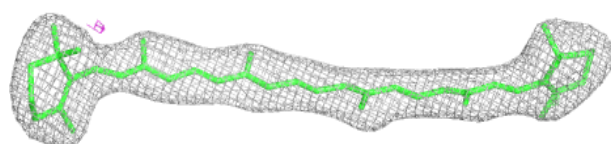
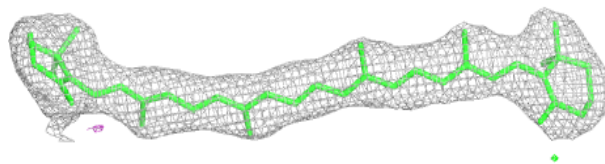
**Electron density around DGD c 519:**

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

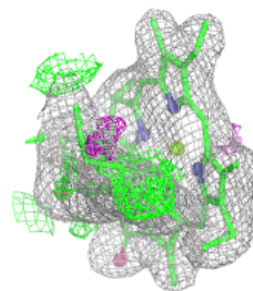
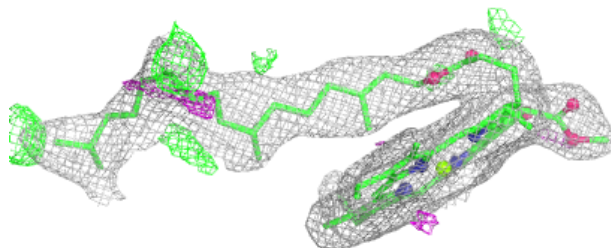
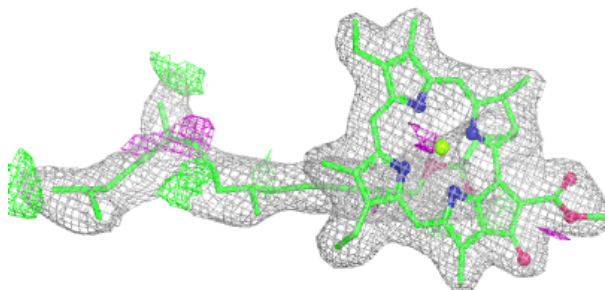


**Electron density around BCR c 515:**

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

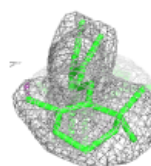
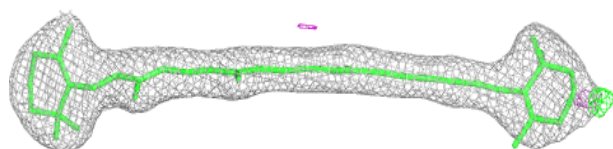
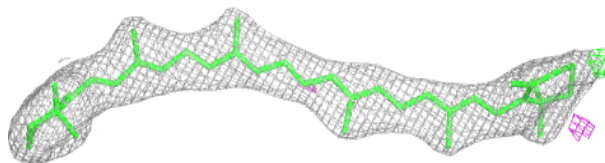
**Electron density around CLA b 614:**

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

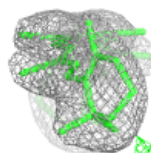
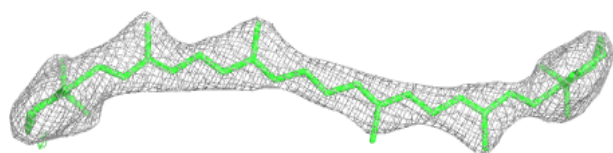
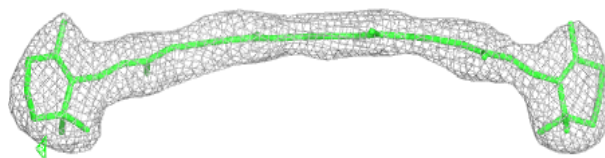


**Electron density around BCR h 101:**

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

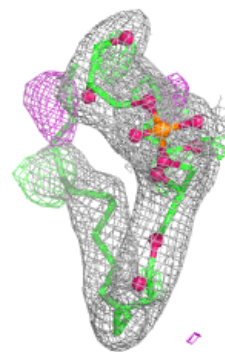
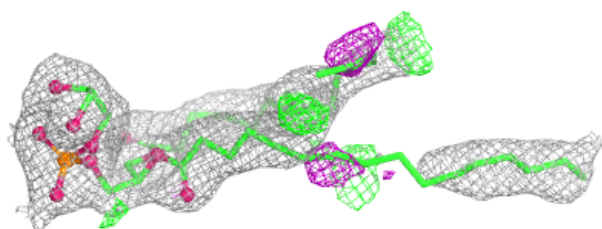
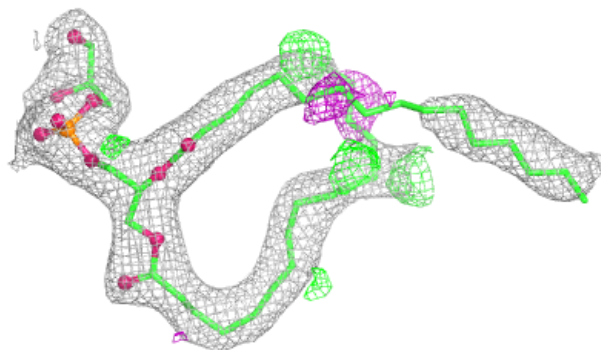
**Electron density around BCR k 101:**

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

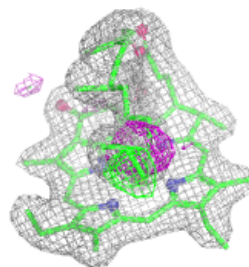
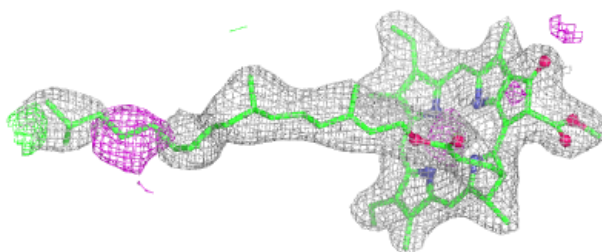
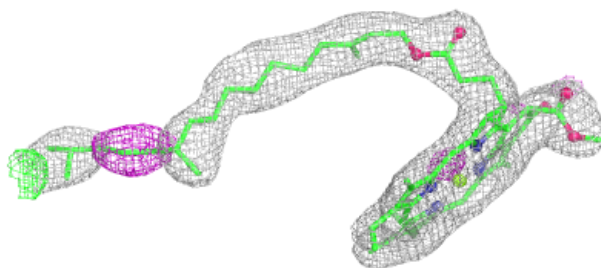


**Electron density around LHG D 411:**

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

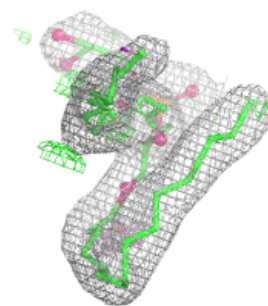
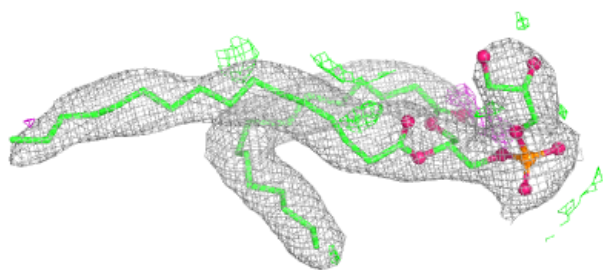
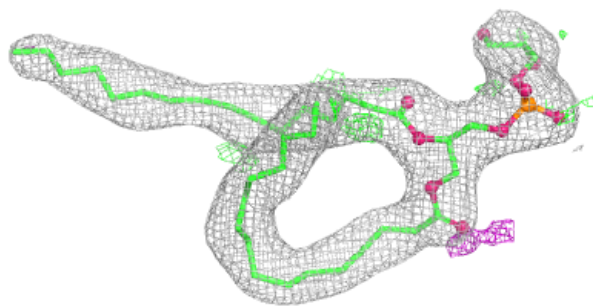
**Electron density around CLA C 505:**

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



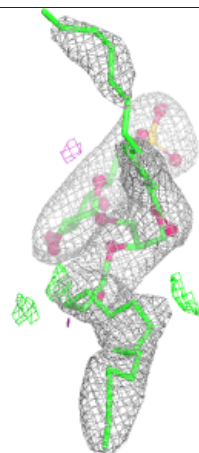
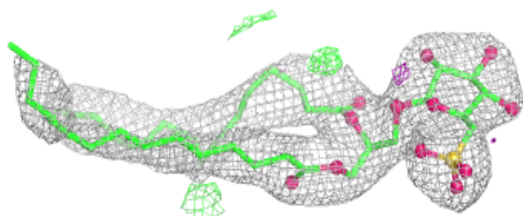
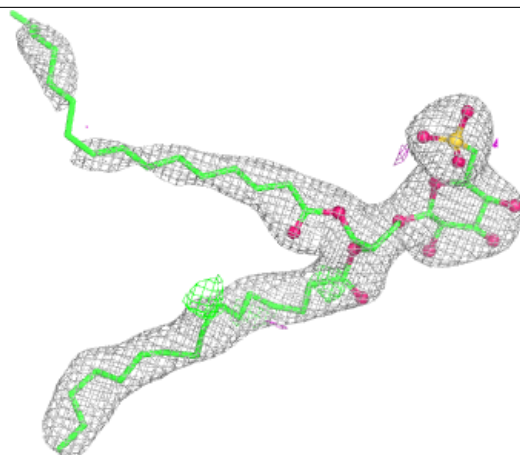
**Electron density around LHG d 711:**

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

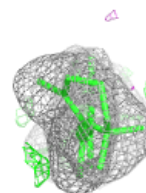
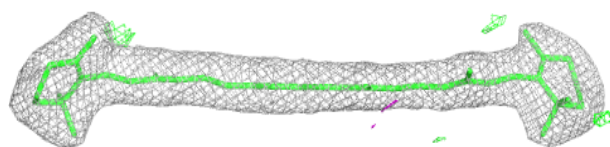
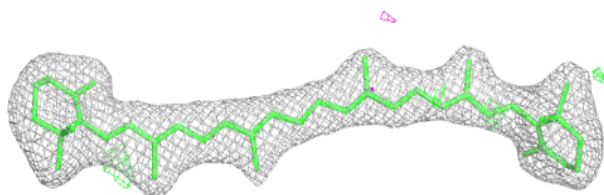


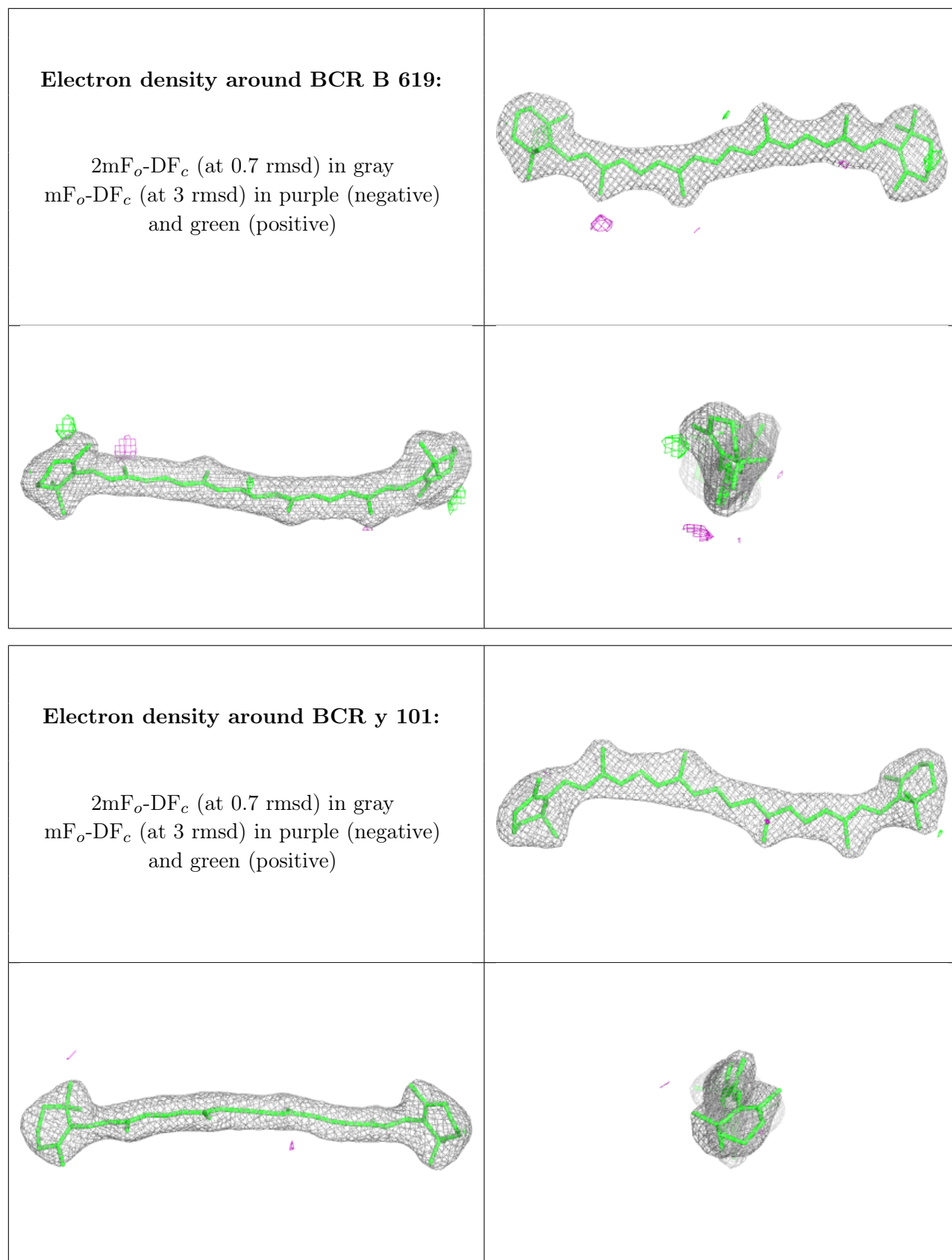
**Electron density around SQD A 410:**

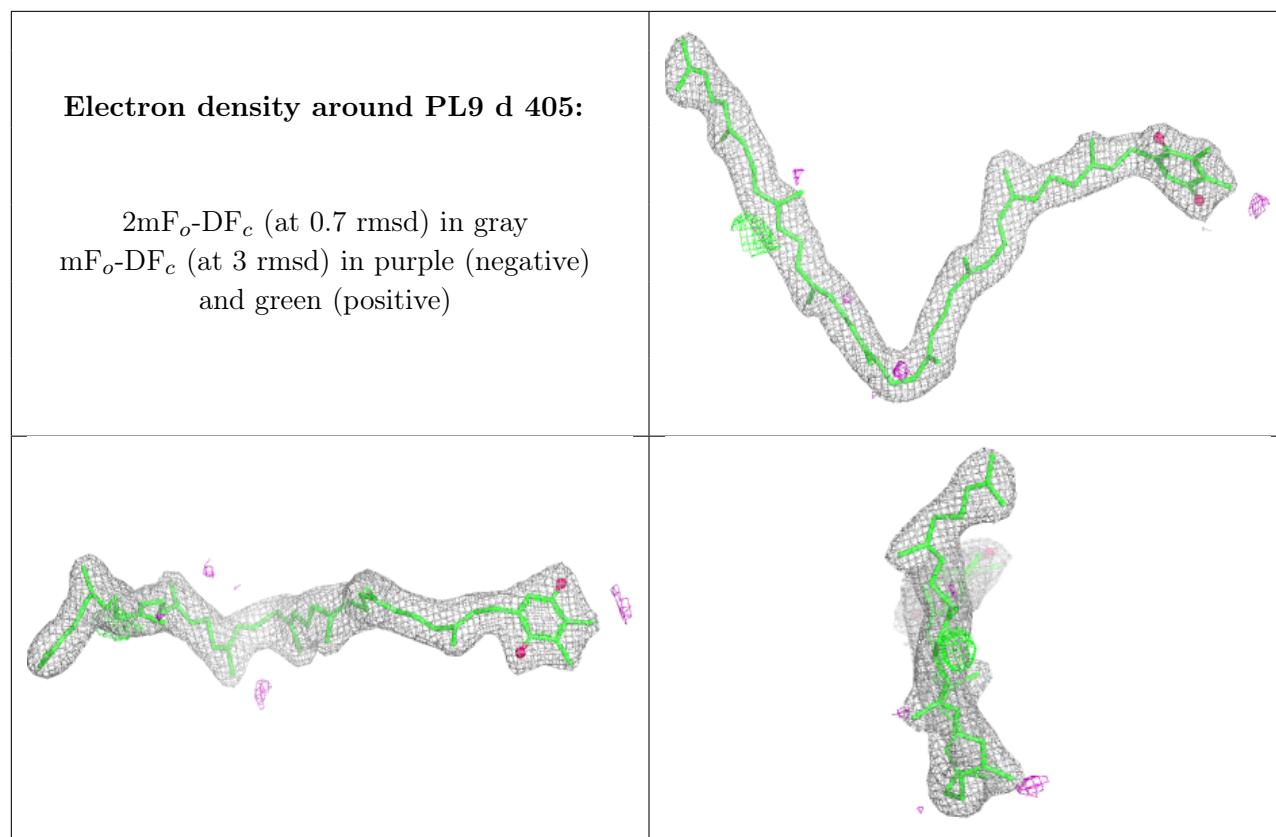
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 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)

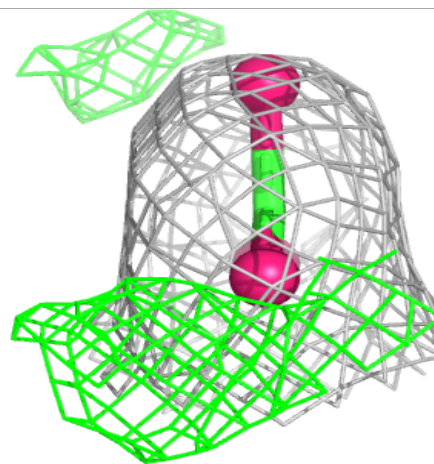
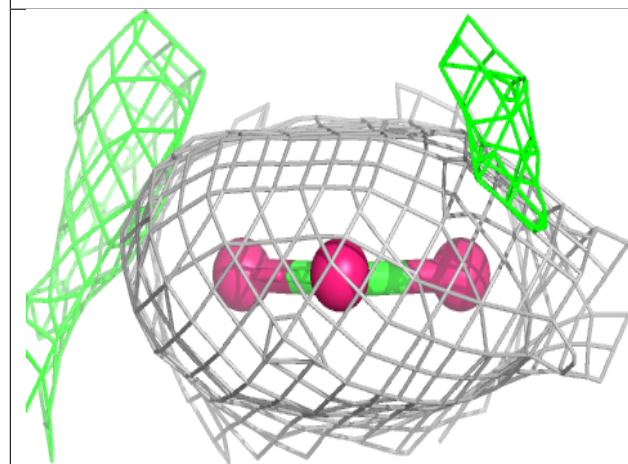
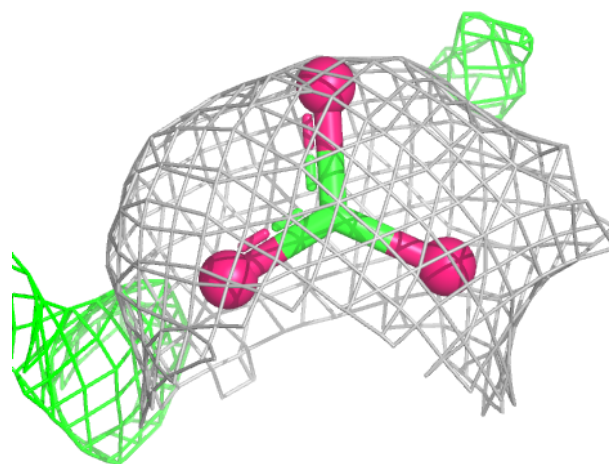






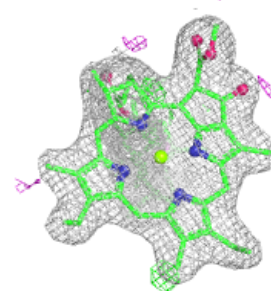
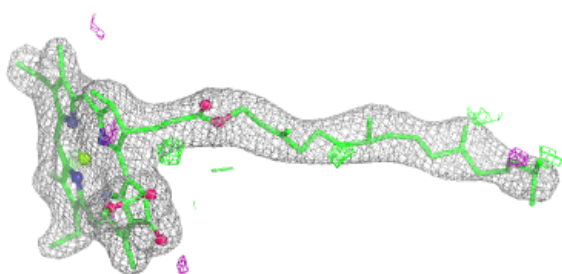
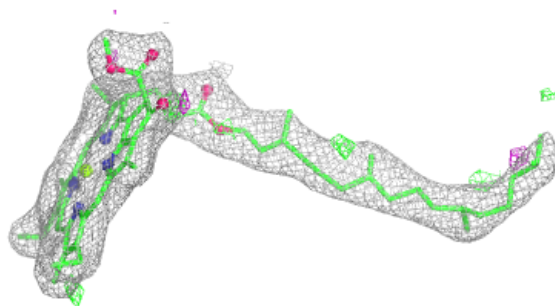
**Electron density around BCT a 404:**

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

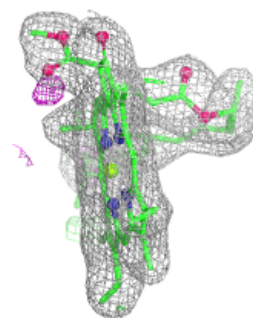
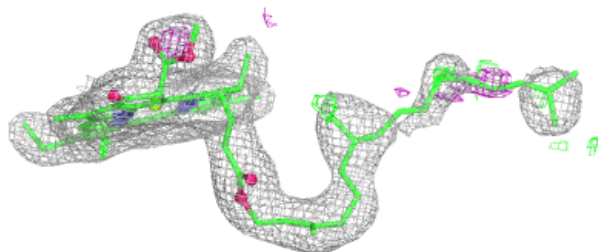
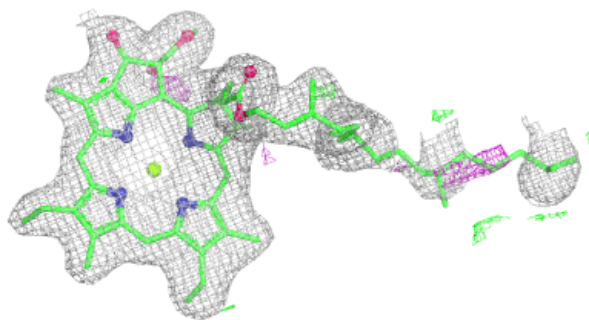


**Electron density around CLA b 604:**

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

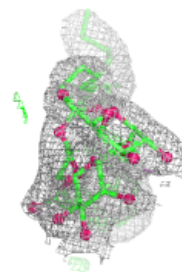
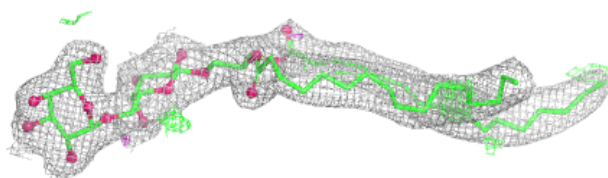
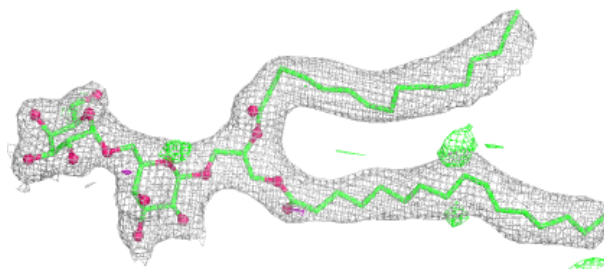
**Electron density around CLA a 407:**

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

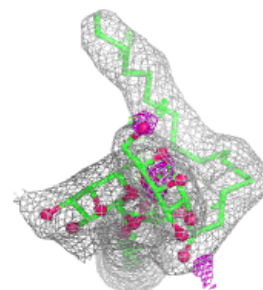
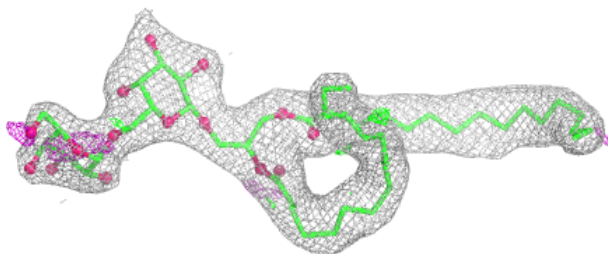
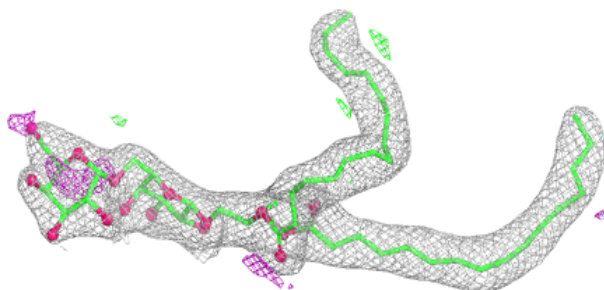


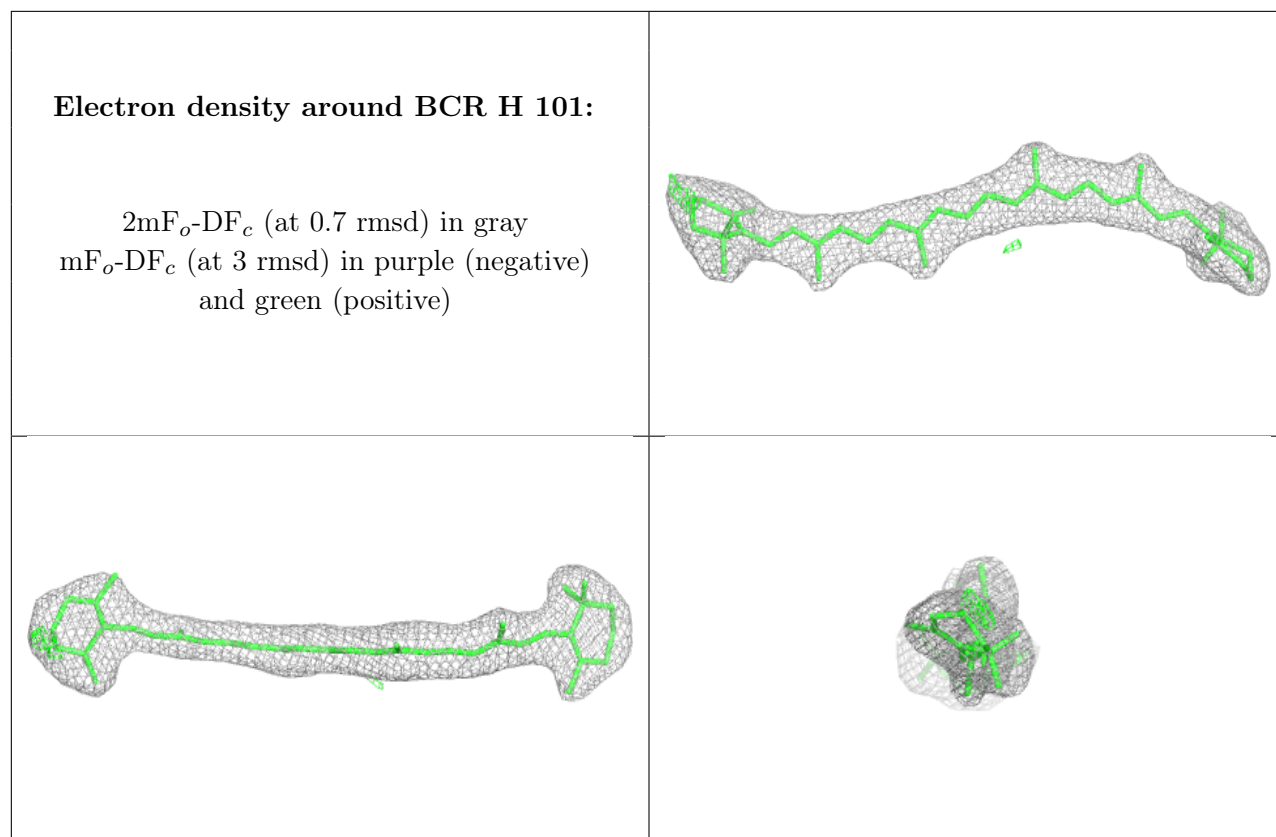
**Electron density around DGD C 519:**

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

**Electron density around DGD H 102:**

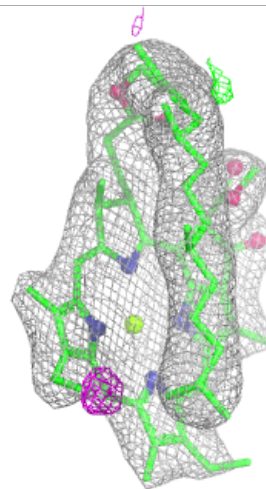
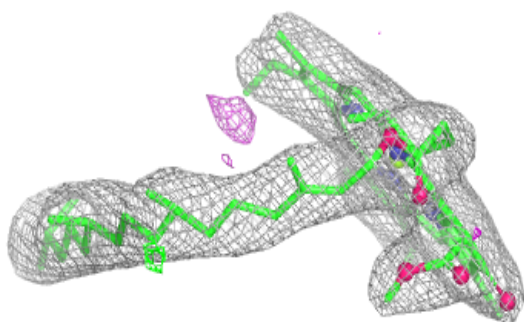
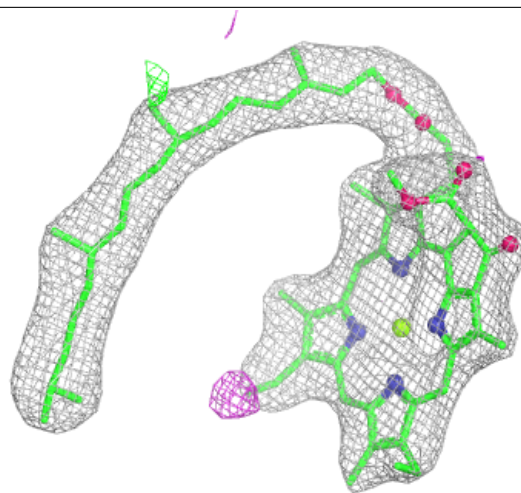
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





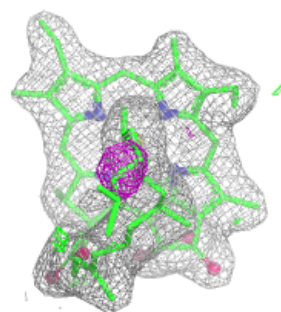
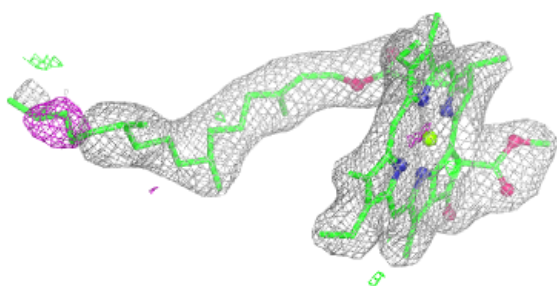
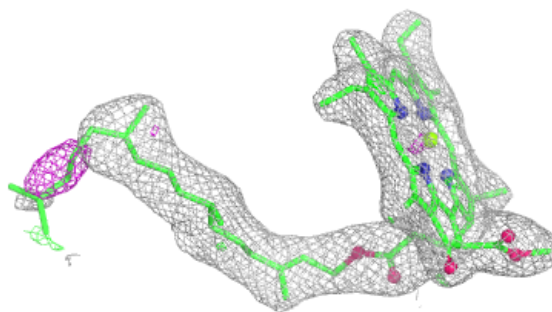
**Electron density around CLA c 508:**

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

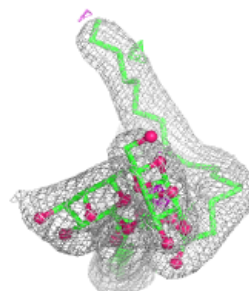
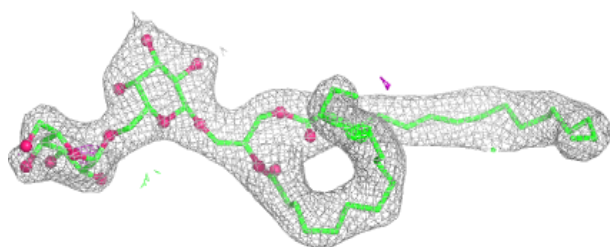
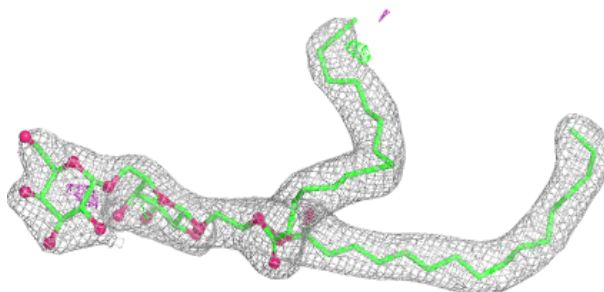


**Electron density around CLA c 509:**

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

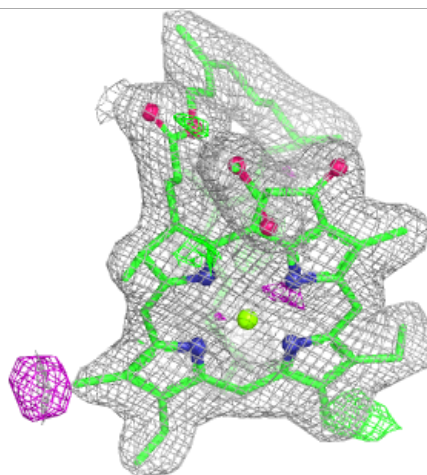
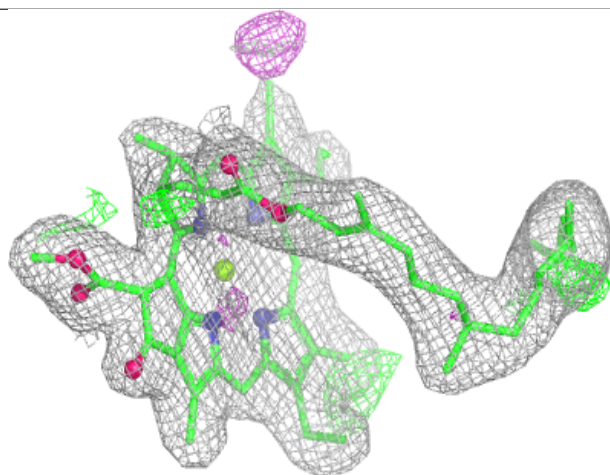
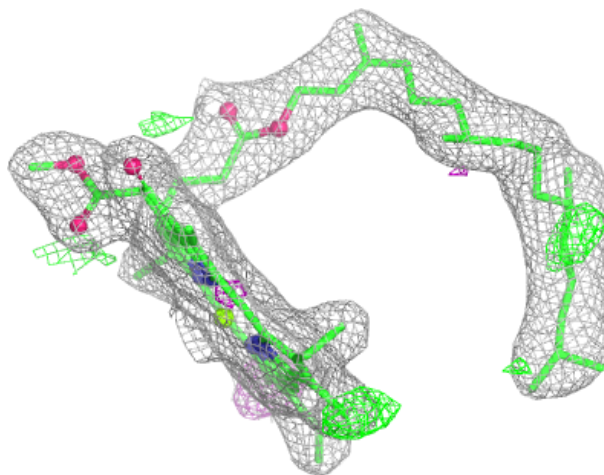
**Electron density around DGD h 102:**

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



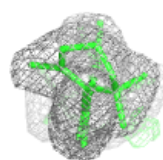
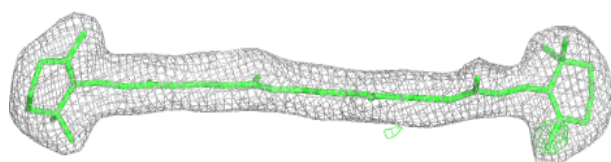
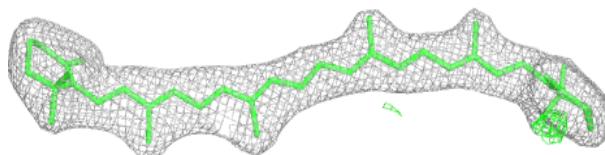
**Electron density around CLA B 611:**

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

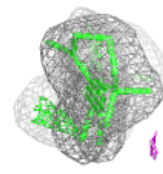
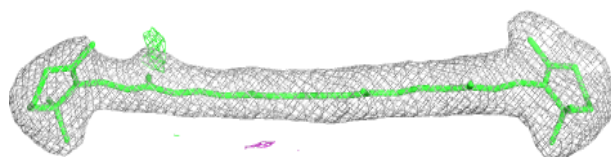
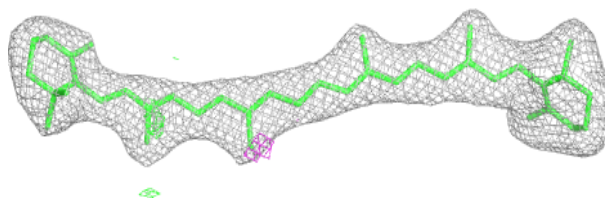


**Electron density around BCR a 410:**

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

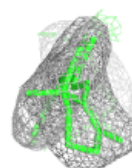
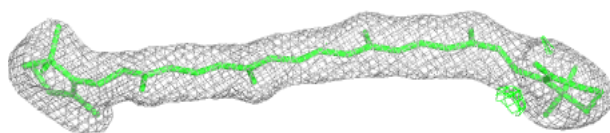
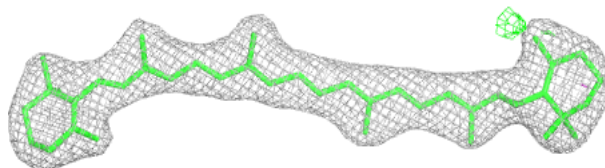
**Electron density around BCR b 618:**

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

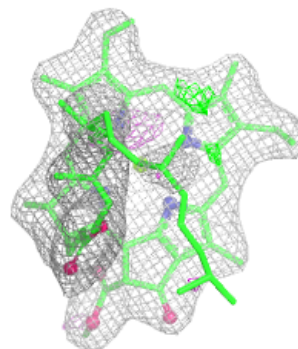
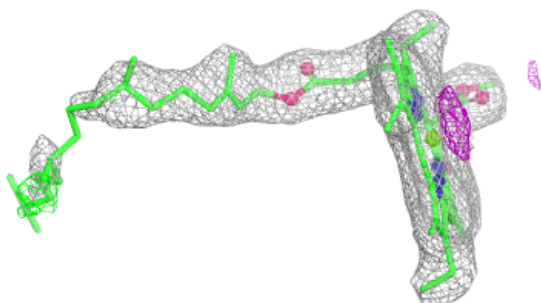
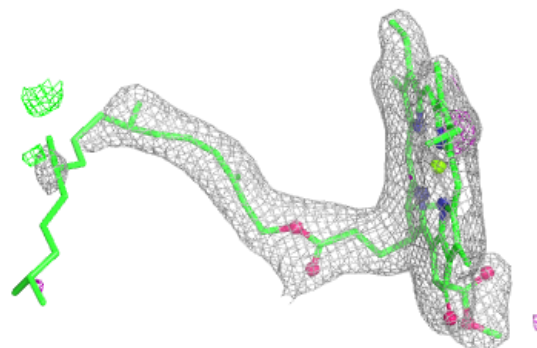


**Electron density around BCR b 619:**

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

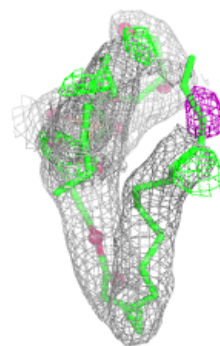
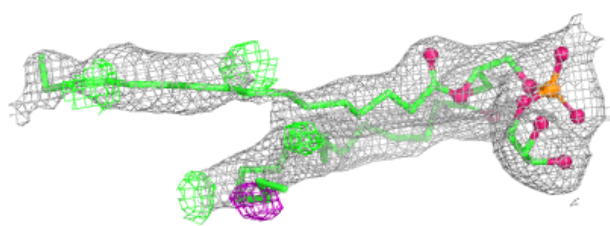
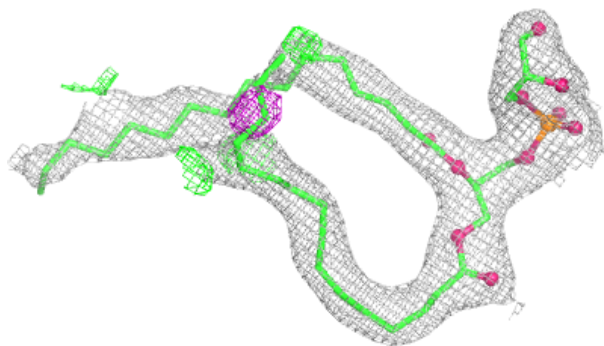
**Electron density around CLA D 406:**

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

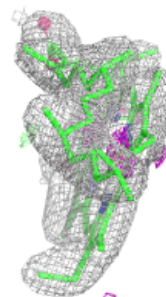
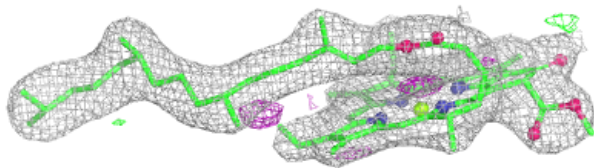
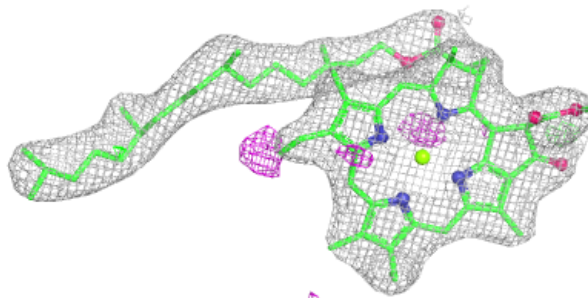


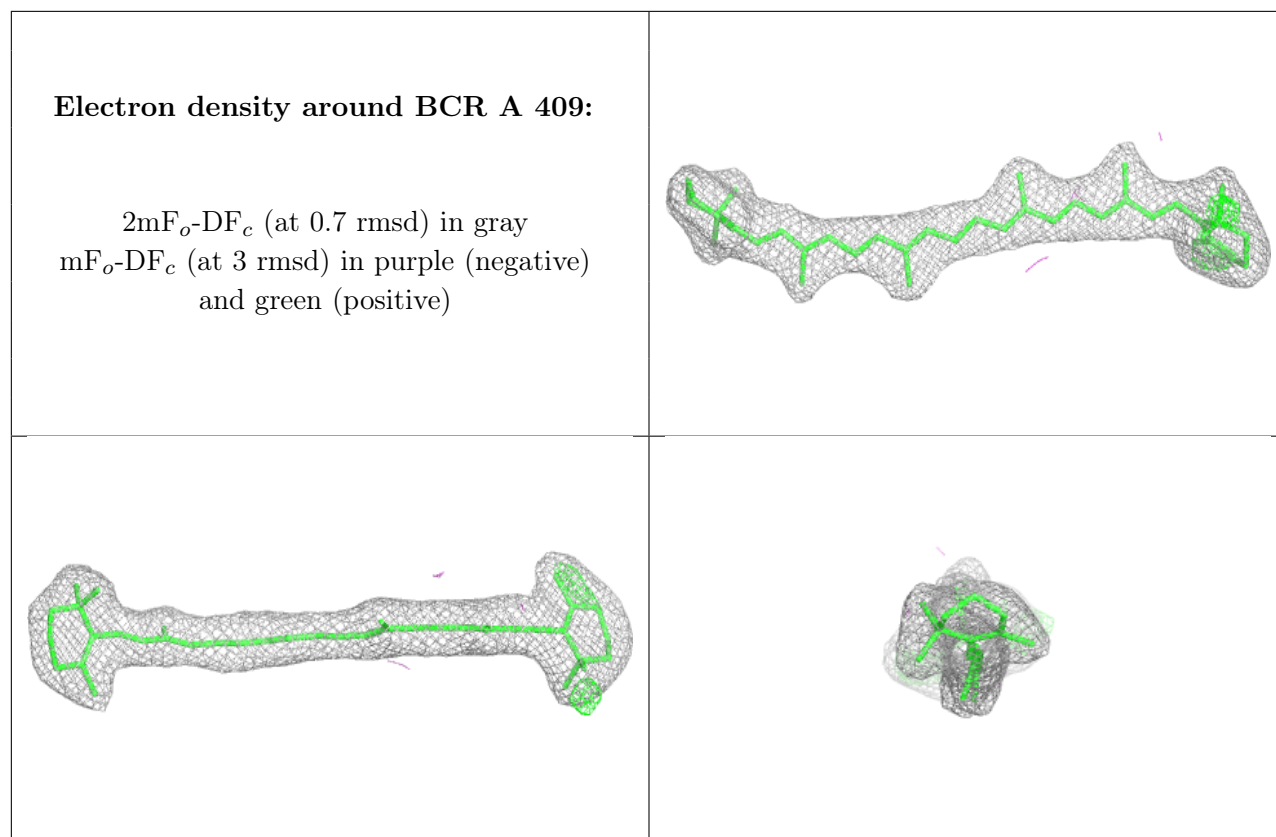
**Electron density around LHG d 408:**

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

**Electron density around CLA c 502:**

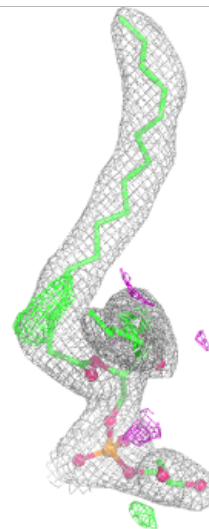
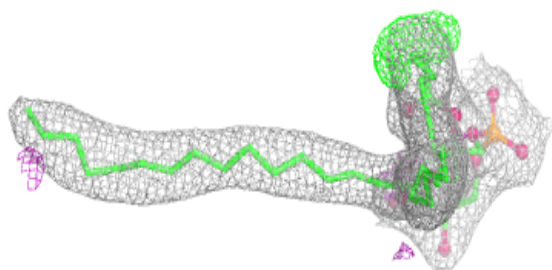
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





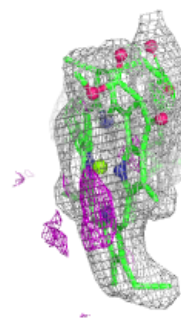
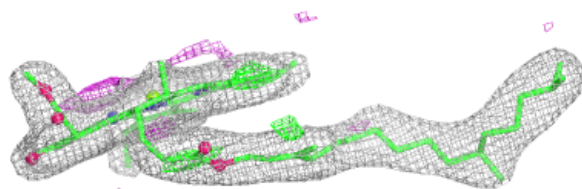
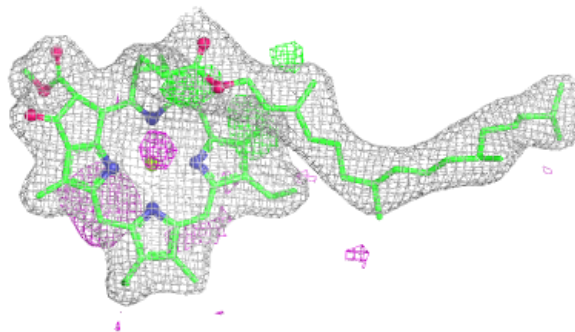
**Electron density around LHG 1 101:**

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

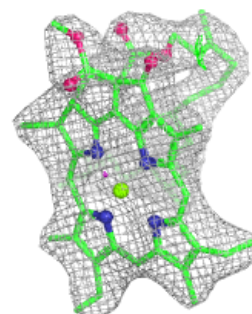
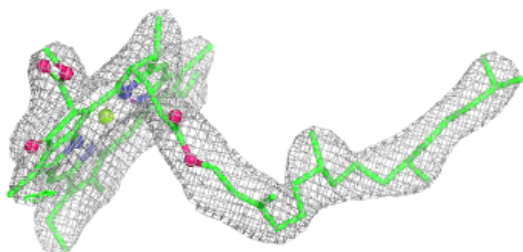
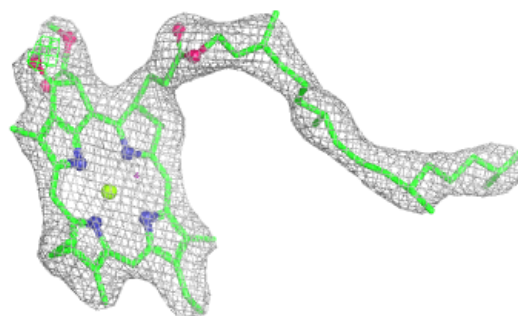


**Electron density around CLA B 603:**

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

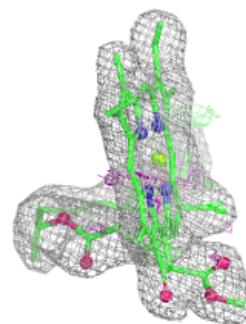
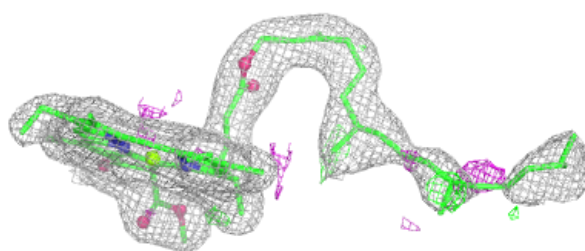
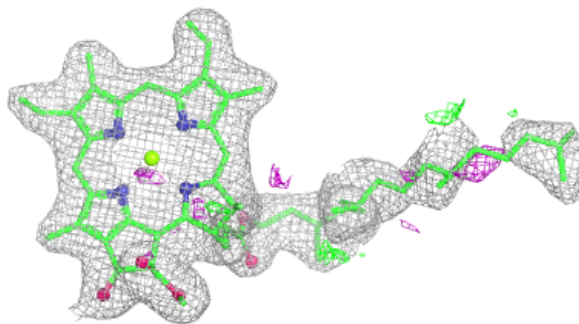
**Electron density around CLA c 512:**

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

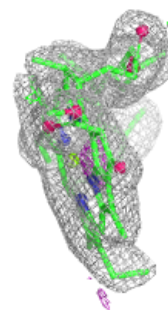
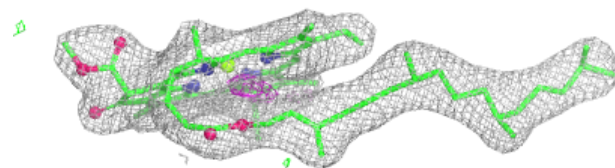
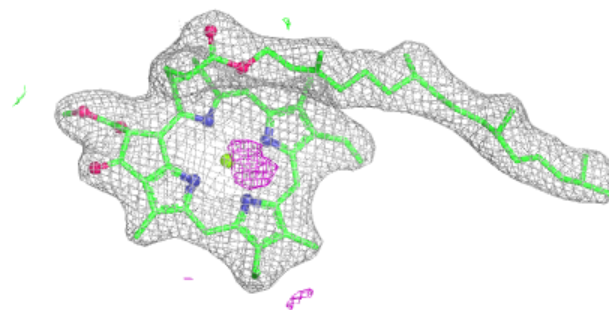


**Electron density around CLA A 406:**

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

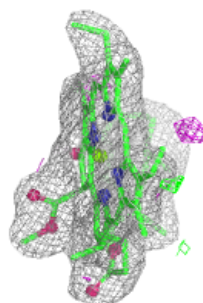
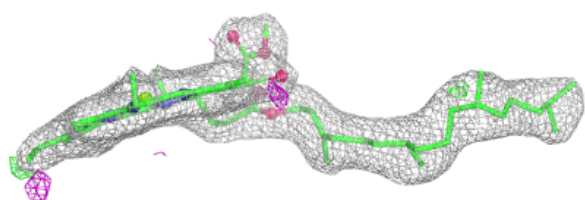
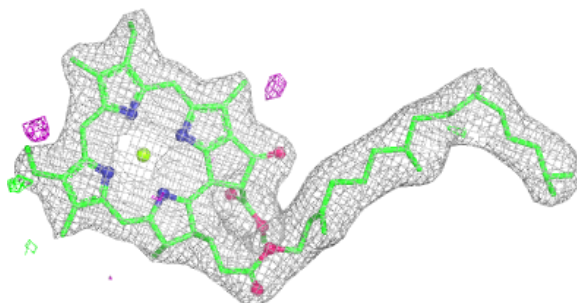
**Electron density around CLA C 502:**

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

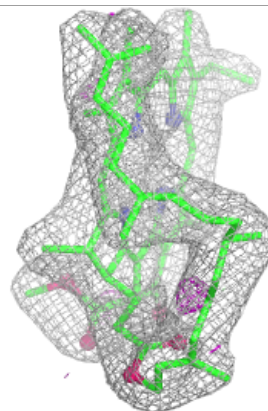
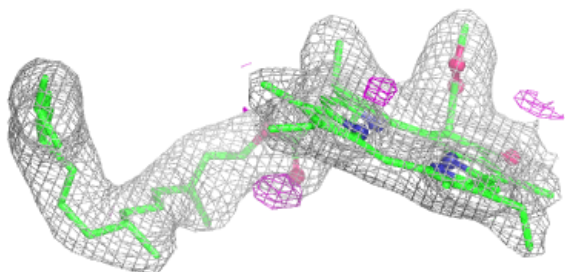
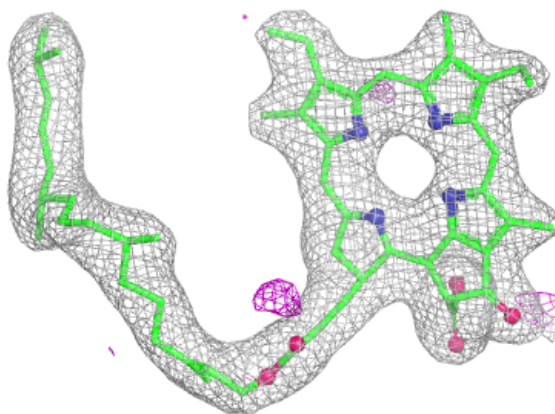


**Electron density around CLA b 602:**

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

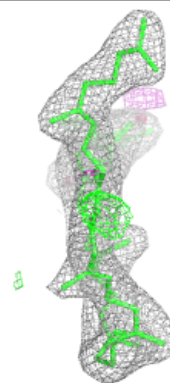
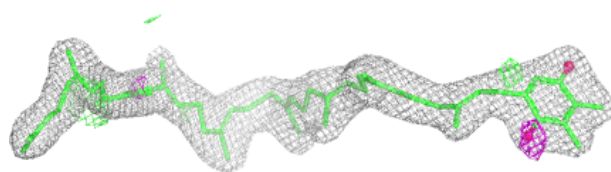
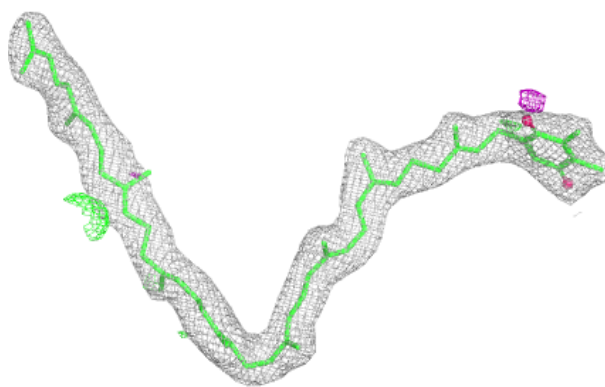
**Electron density around PHO a 353:**

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

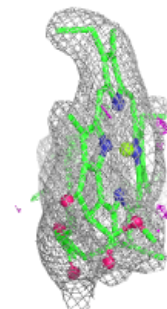
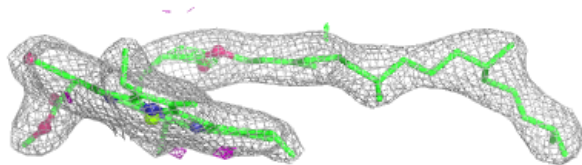
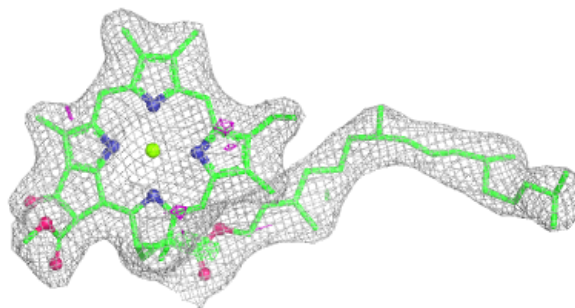


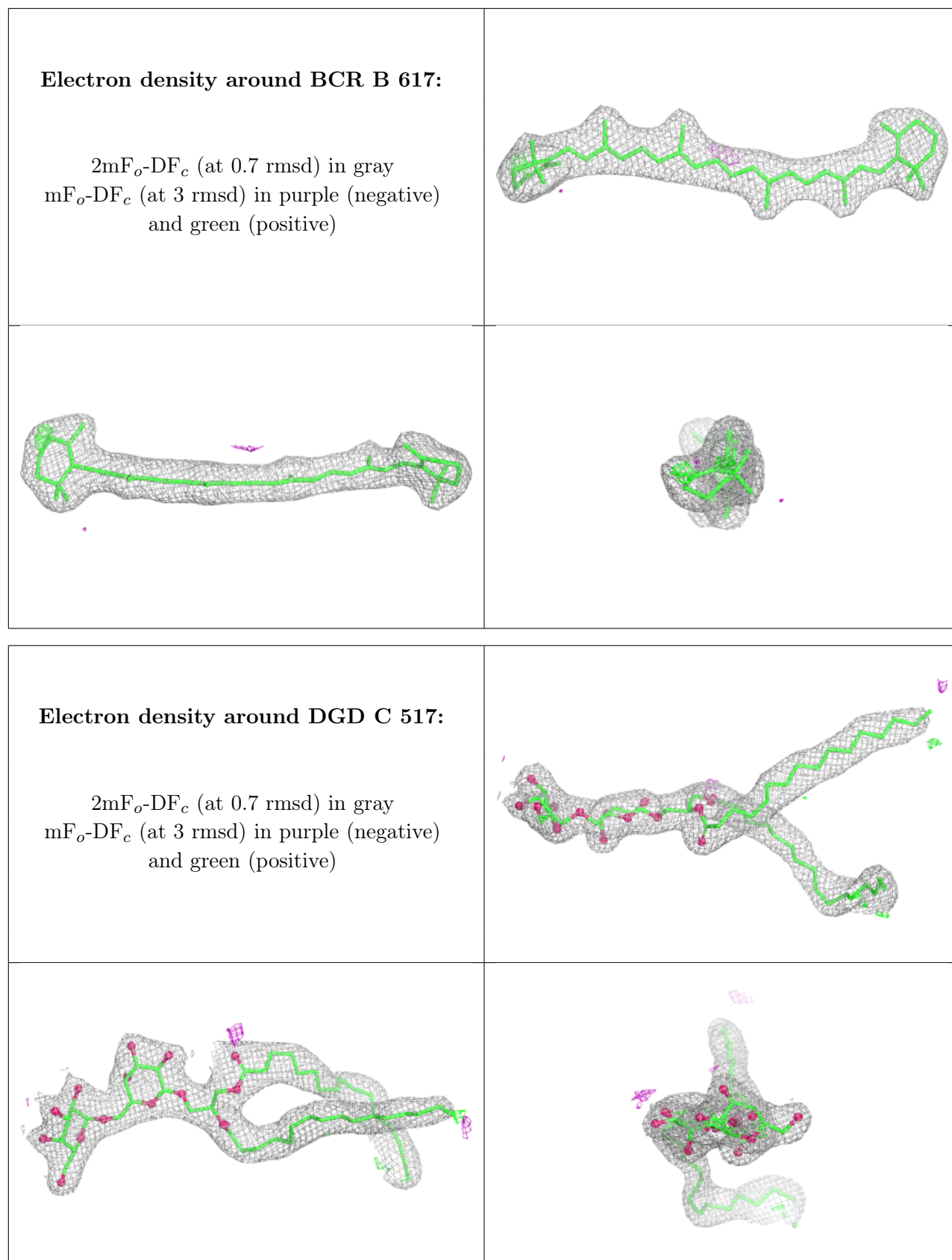
**Electron density around PL9 D 408:**

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

**Electron density around CLA b 603:**

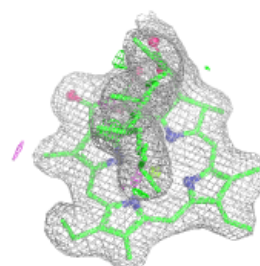
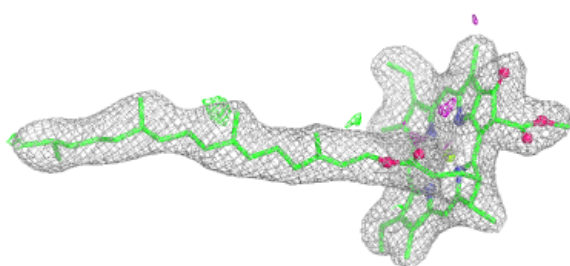
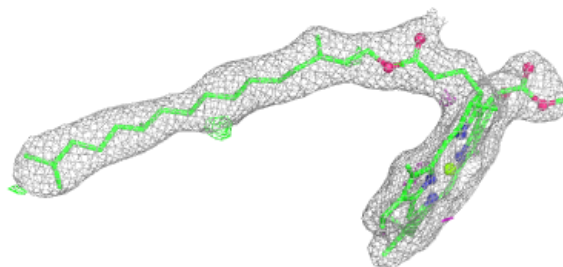
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



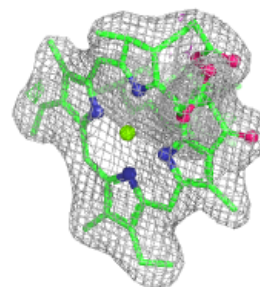
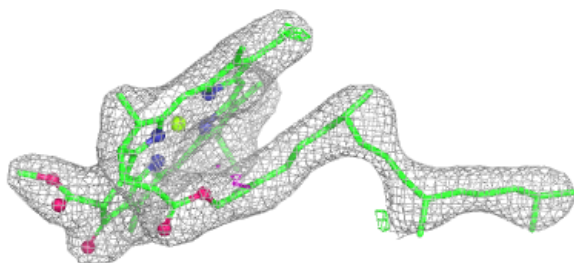
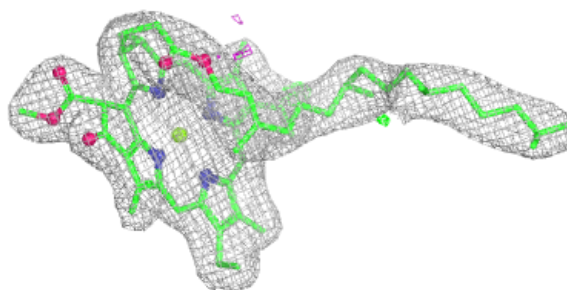


**Electron density around CLA B 607:**

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

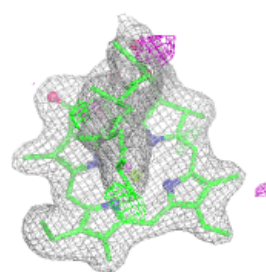
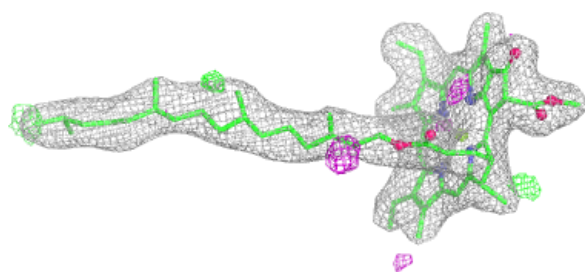
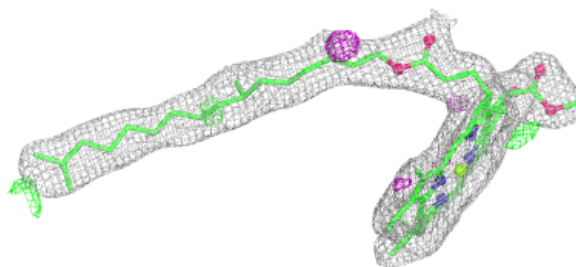
**Electron density around CLA C 506:**

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

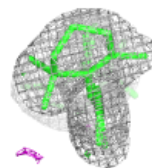
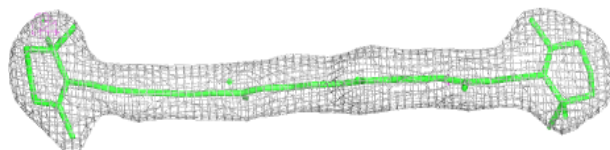
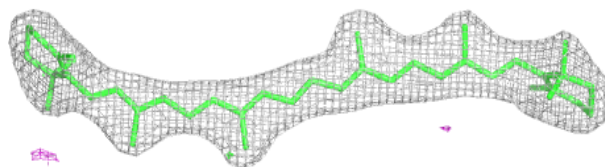


**Electron density around CLA b 607:**

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

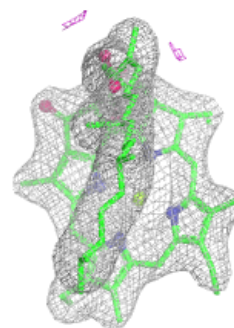
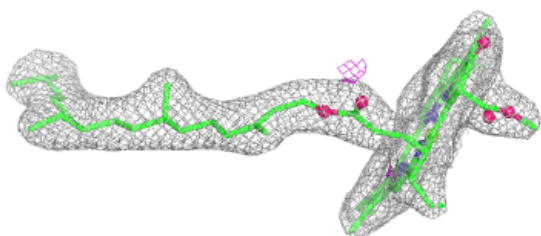
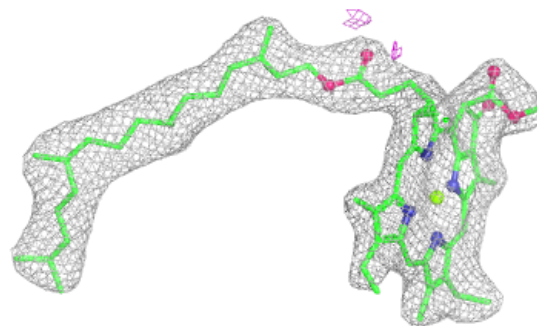
**Electron density around BCR C 516:**

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



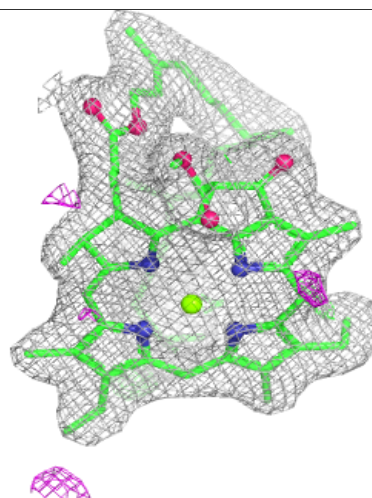
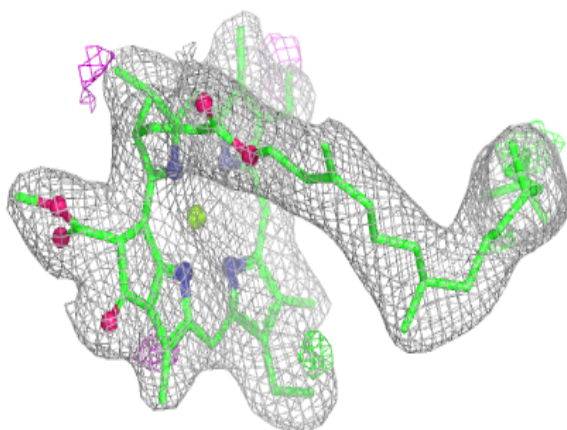
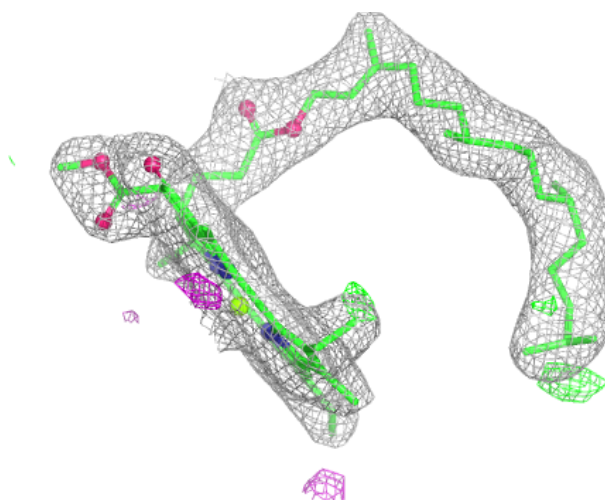
**Electron density around CLA b 609:**

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



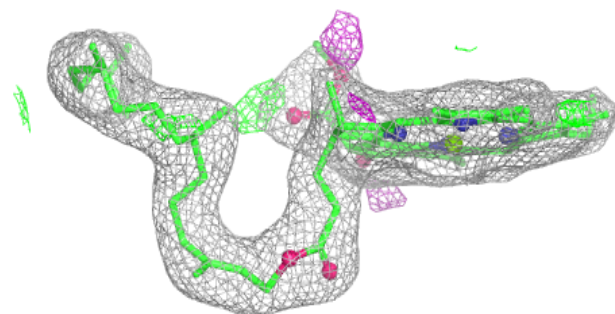
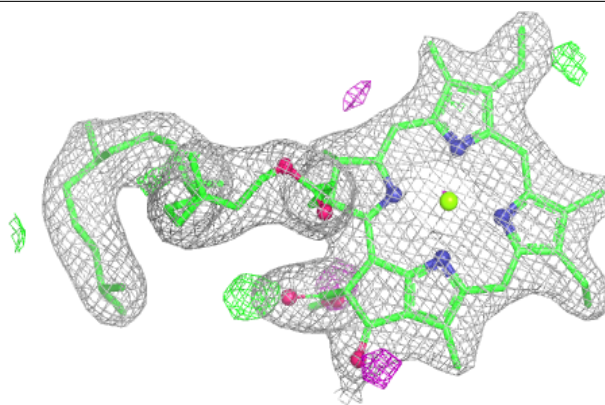
**Electron density around CLA b 611:**

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



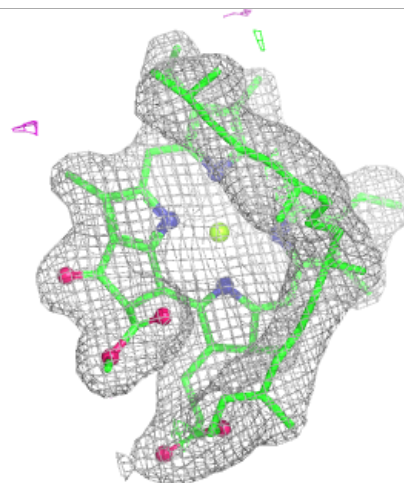
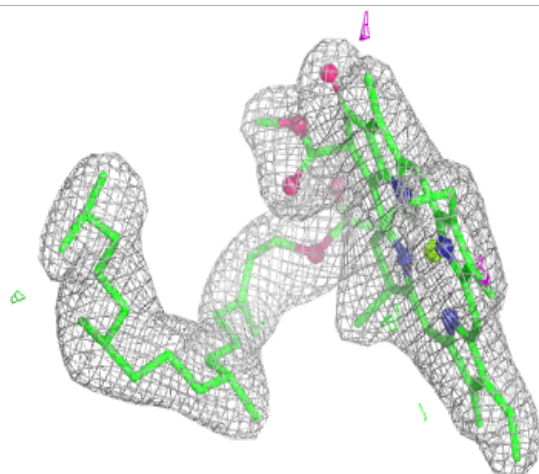
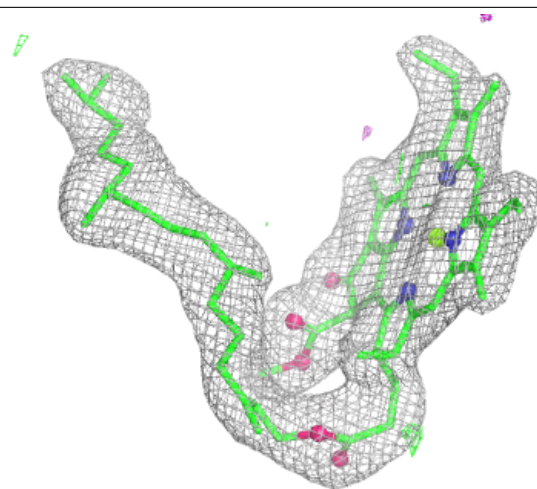
**Electron density around CLA b 612:**

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



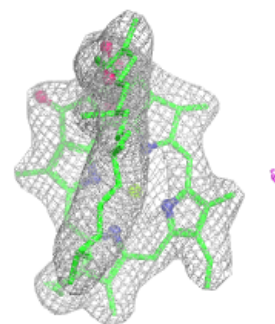
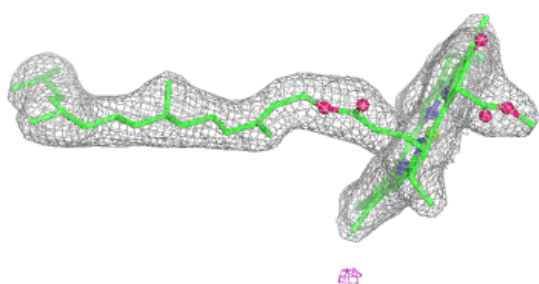
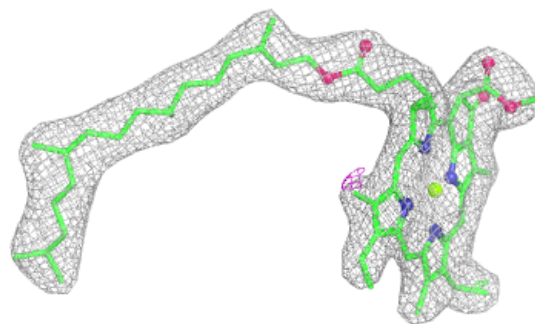
**Electron density around CLA b 613:**

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



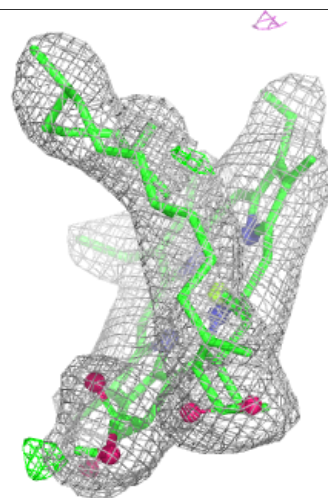
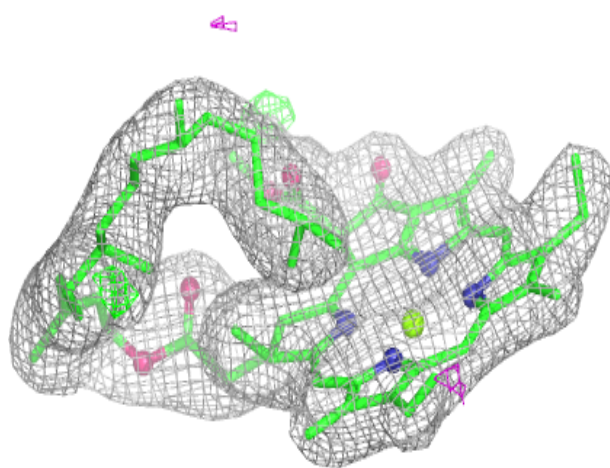
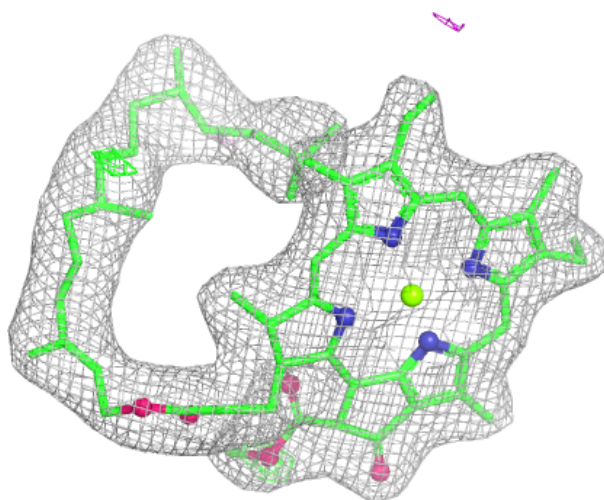
**Electron density around CLA B 609:**

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



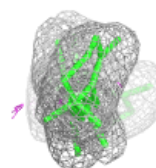
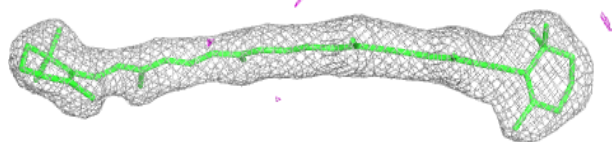
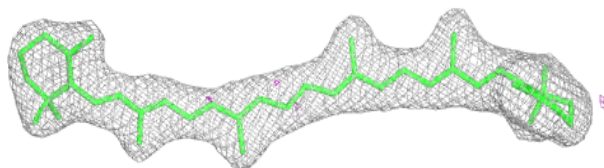
**Electron density around CLA b 615:**

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

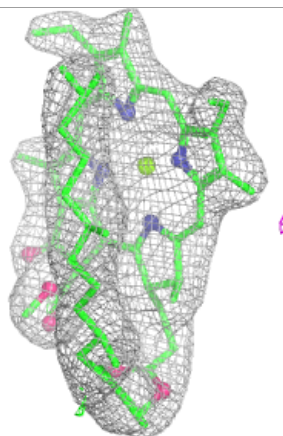
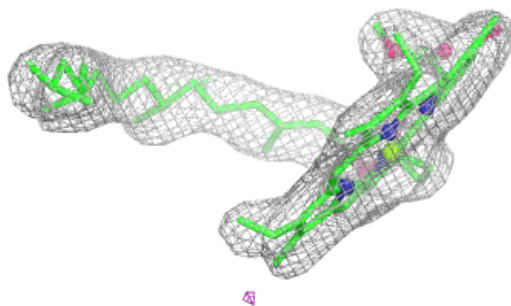
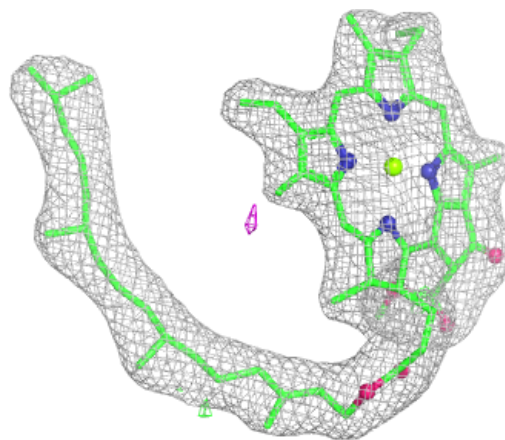


**Electron density around BCR b 617:**

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

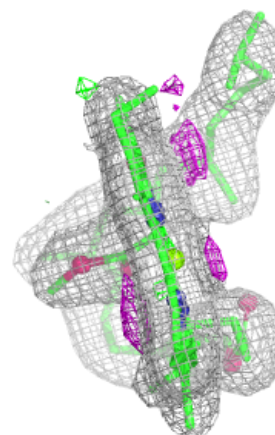
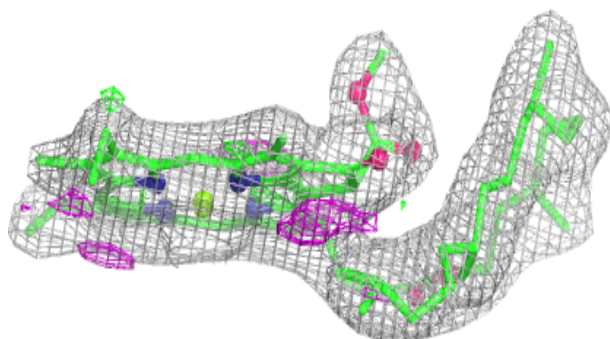
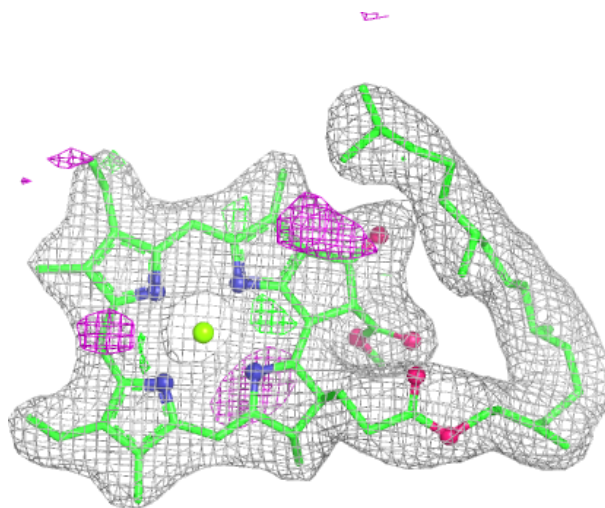
**Electron density around CLA C 508:**

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



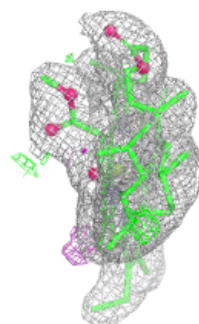
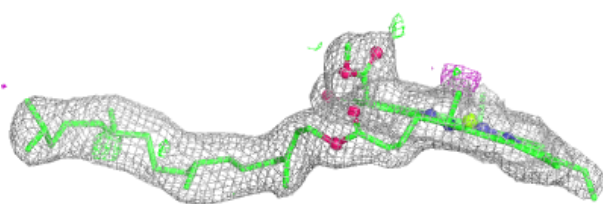
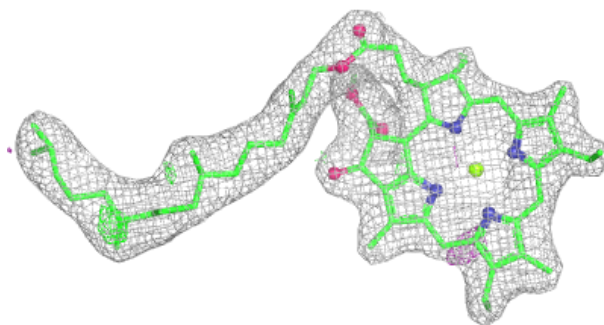
**Electron density around CLA B 610:**

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

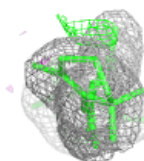
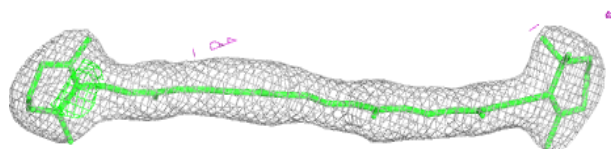
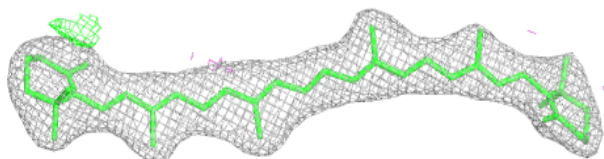


**Electron density around CLA B 602:**

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

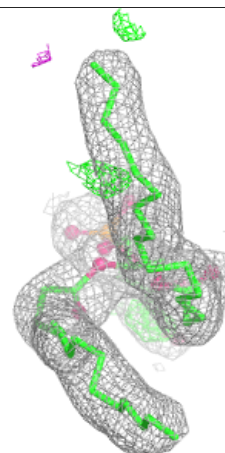
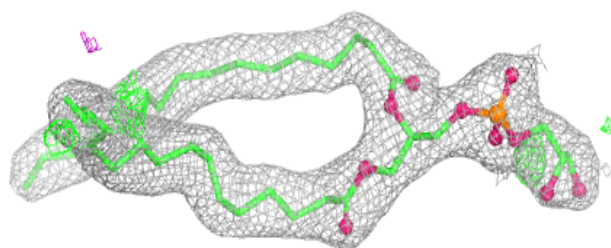
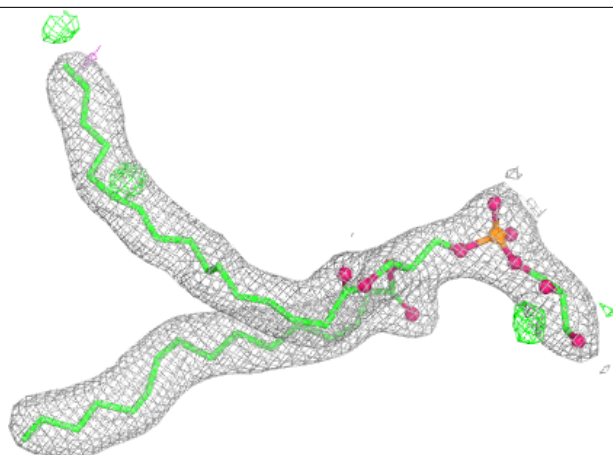
**Electron density around BCR c 516:**

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



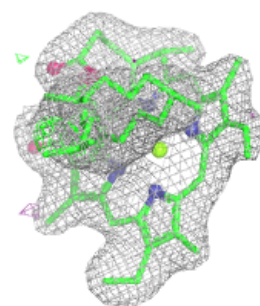
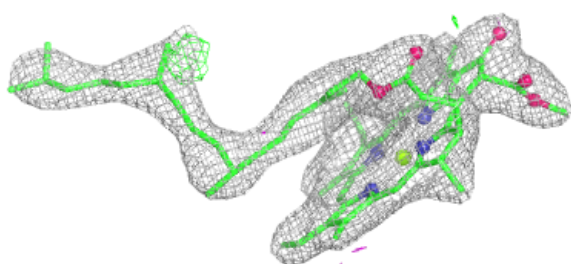
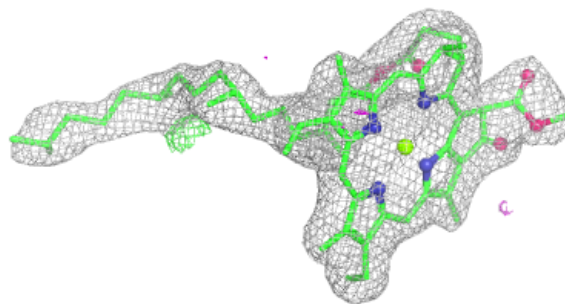
**Electron density around LHG d 407:**

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

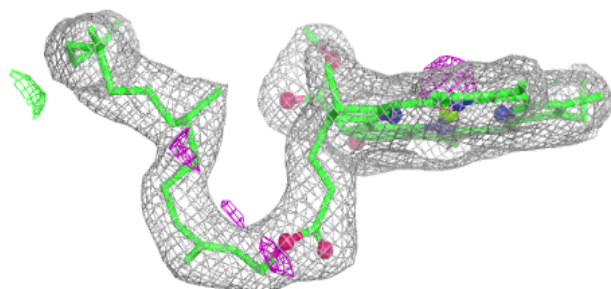
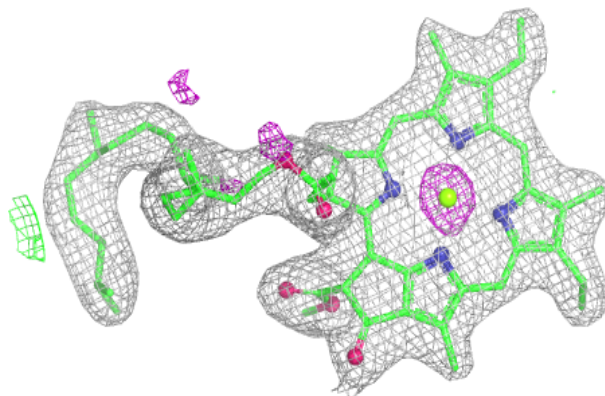


**Electron density around CLA c 506:**

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

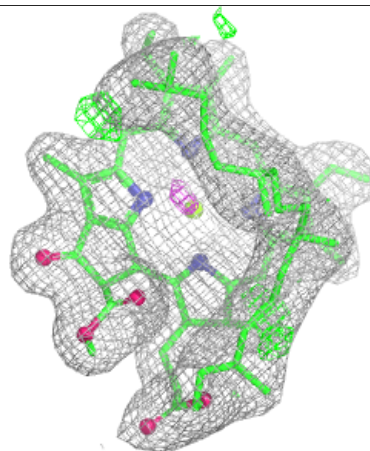
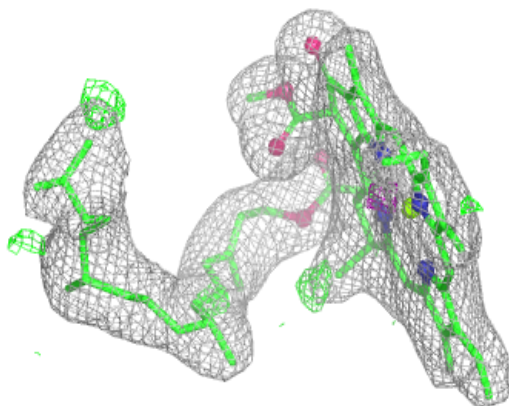
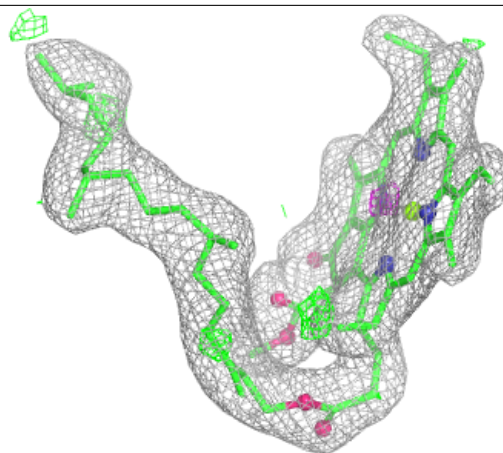
**Electron density around CLA B 612:**

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

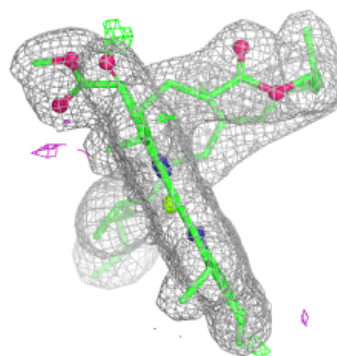
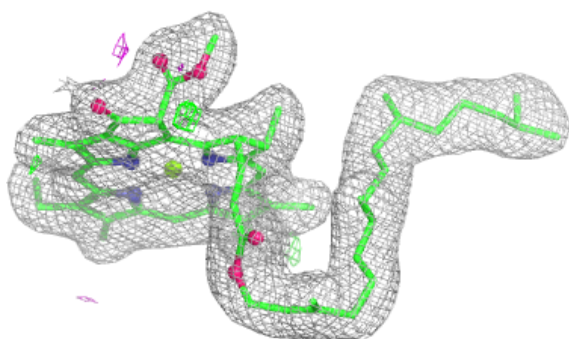
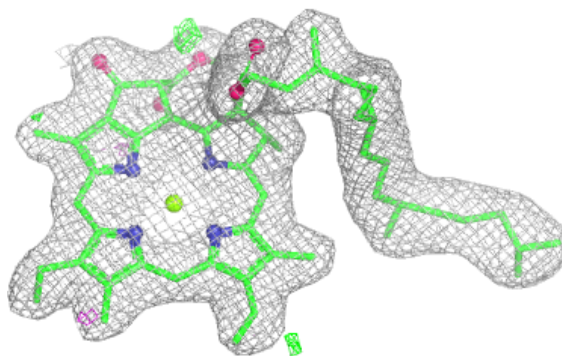


**Electron density around CLA B 613:**

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

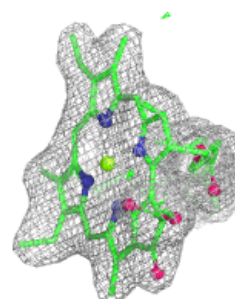
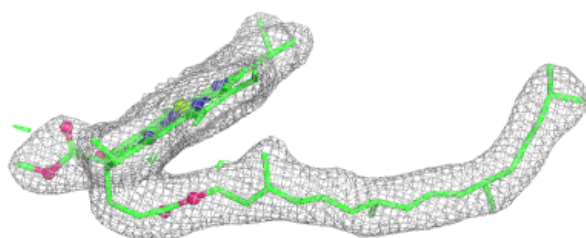
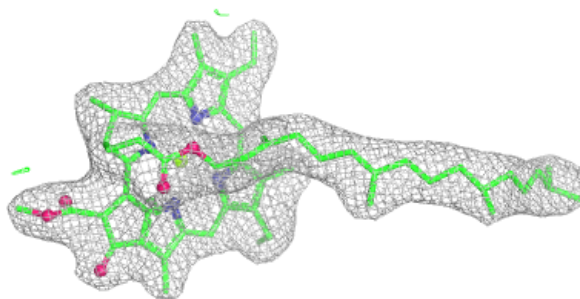
**Electron density around CLA A 405:**

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



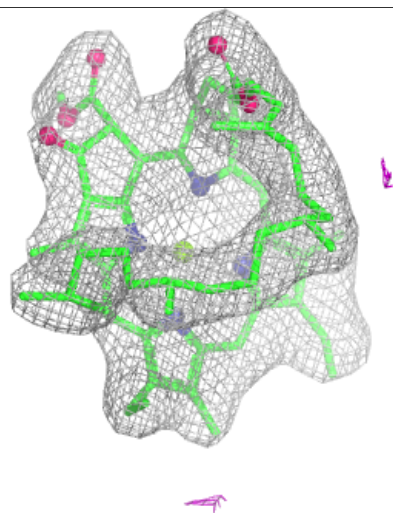
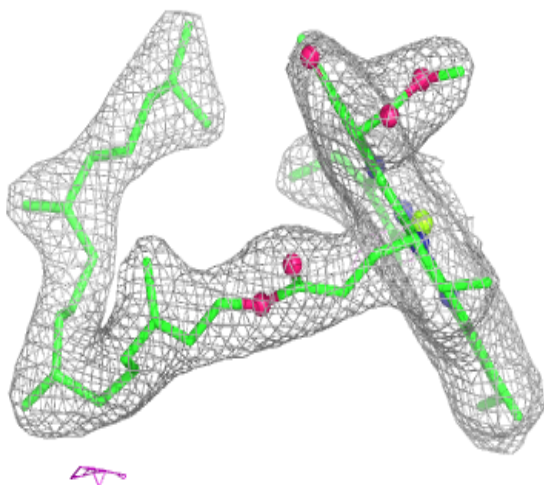
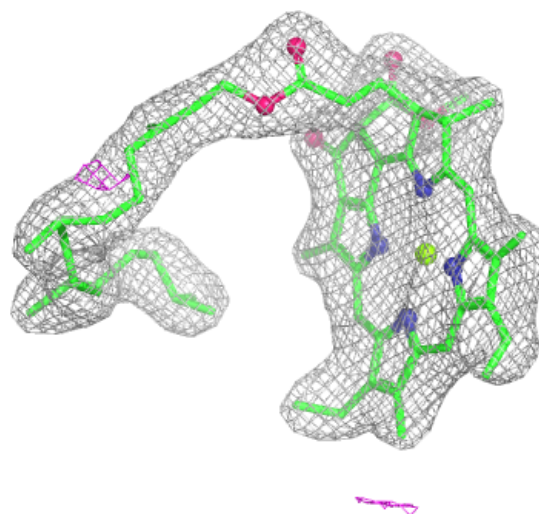
**Electron density around CLA b 608:**

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



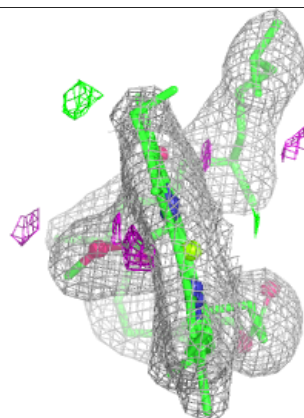
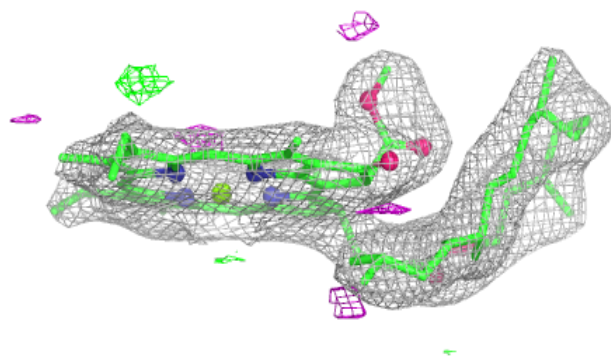
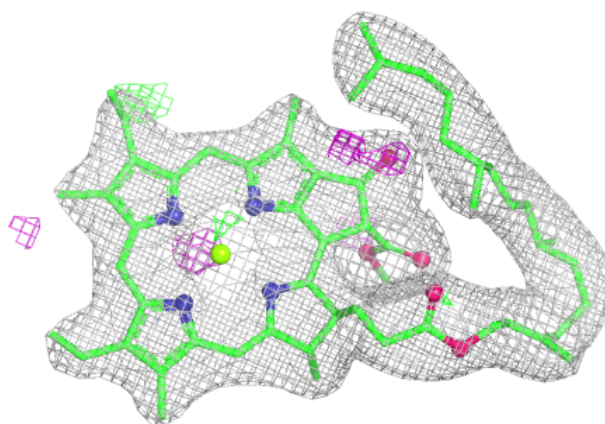
**Electron density around CLA C 504:**

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



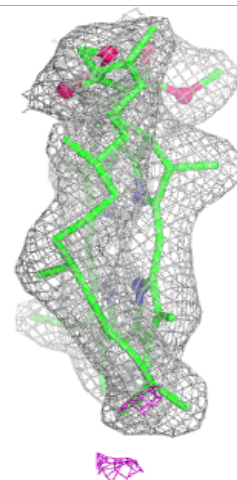
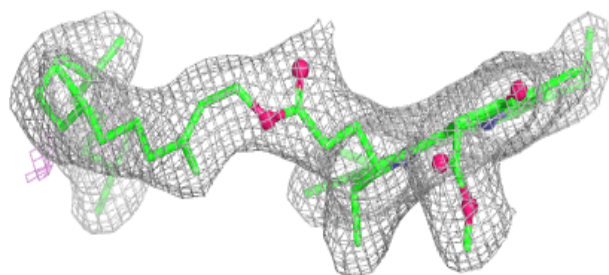
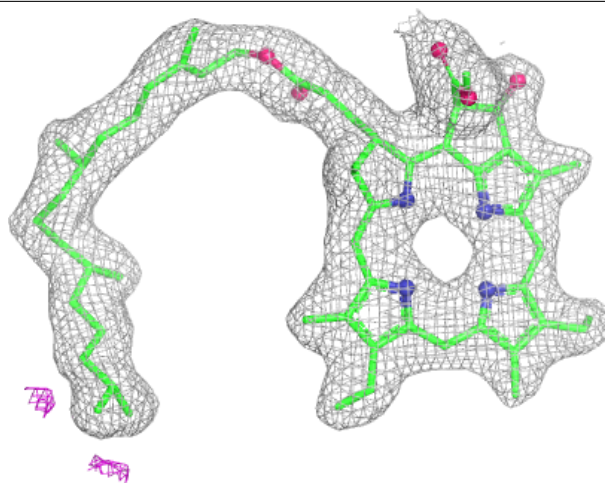
**Electron density around CLA b 610:**

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



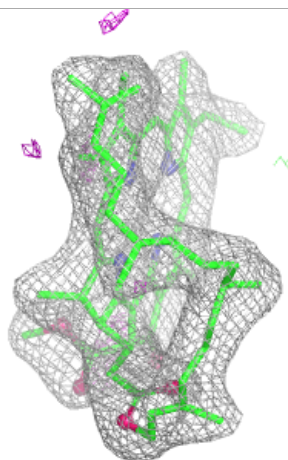
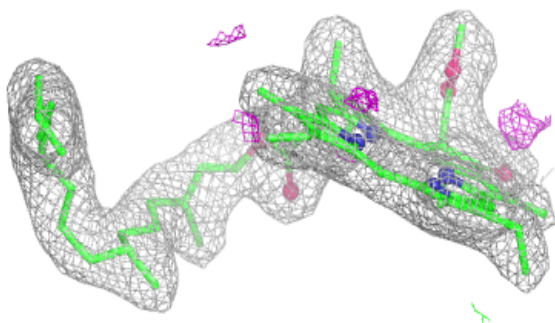
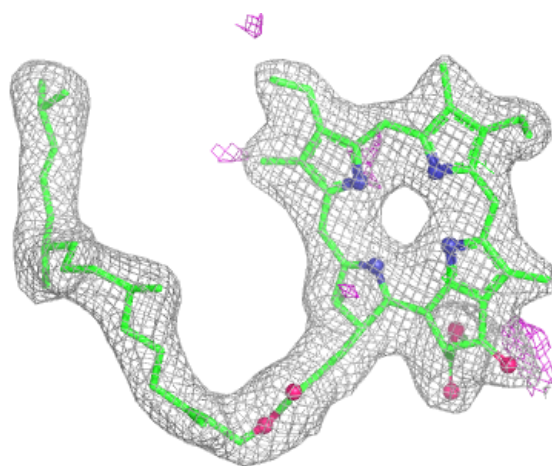
**Electron density around PHO A 407:**

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



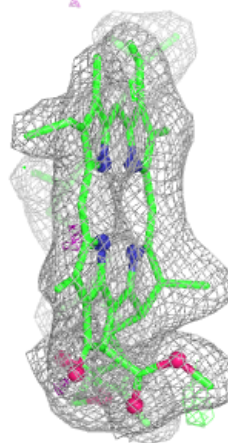
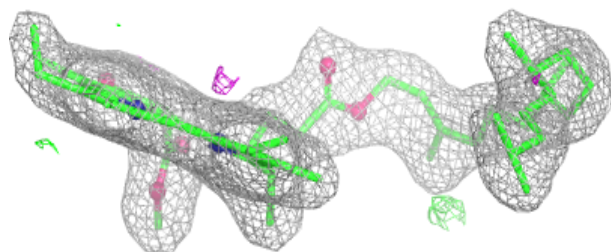
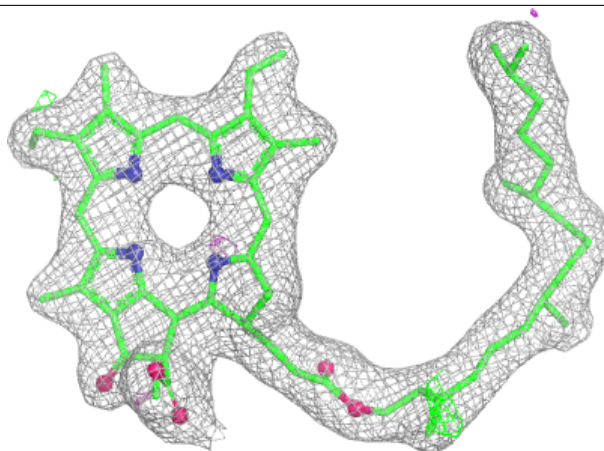
**Electron density around PHO A 353:**

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



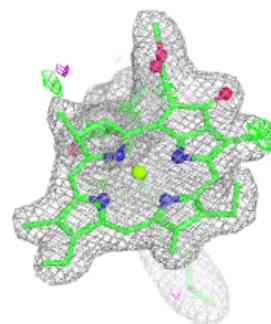
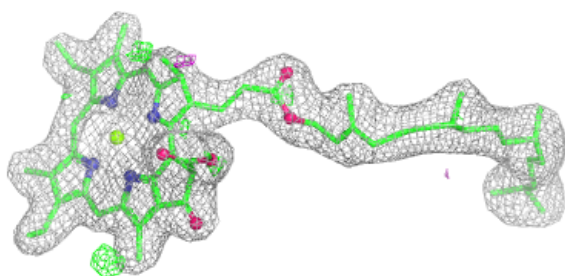
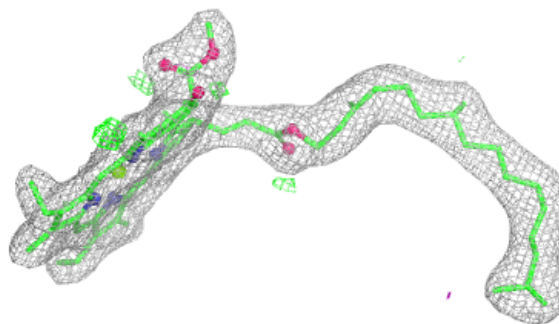
**Electron density around PHO a 408:**

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

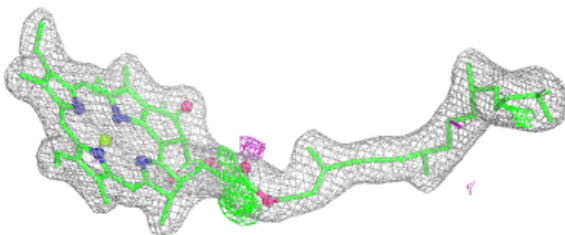
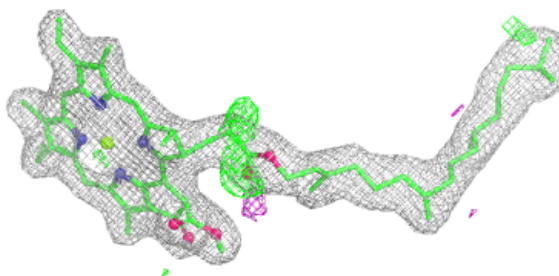


**Electron density around CLA D 405:**

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

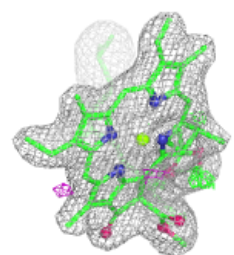
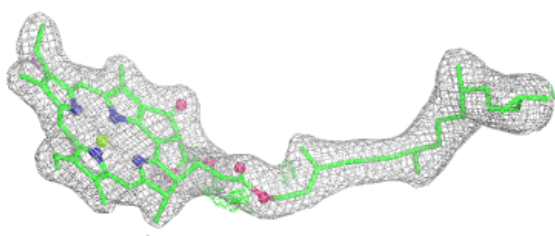
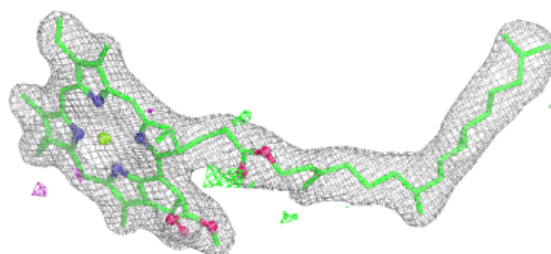
**Electron density around CLA A 404:**

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

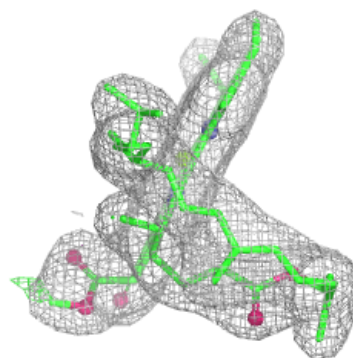
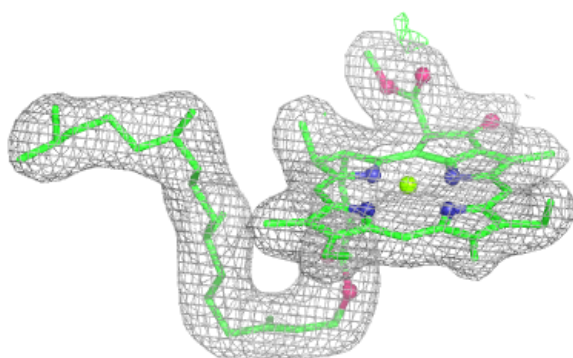
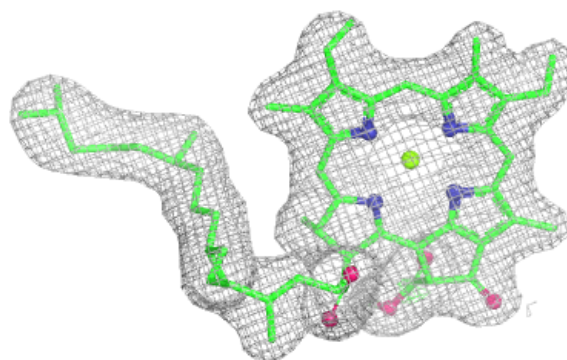


**Electron density around CLA a 405:**

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

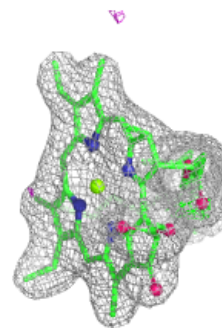
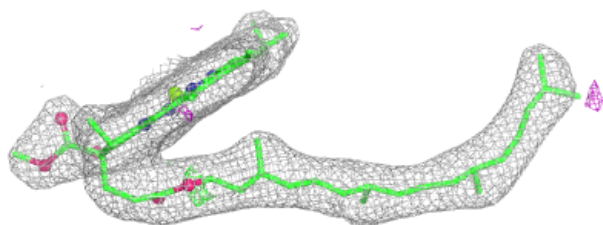
**Electron density around CLA a 406:**

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

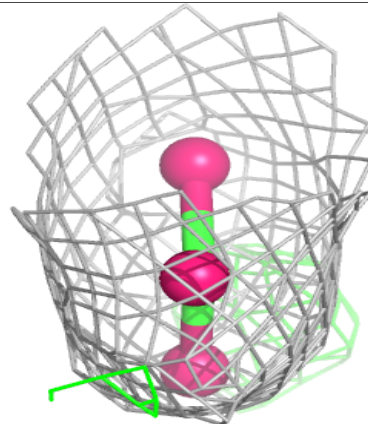
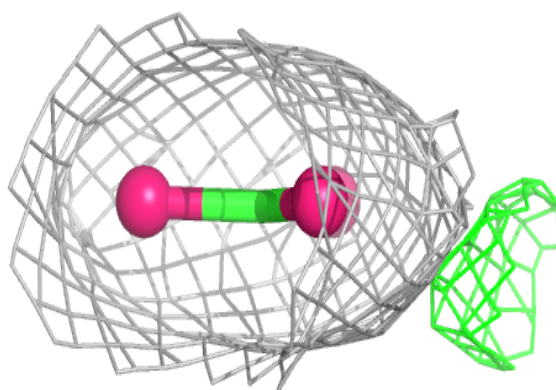
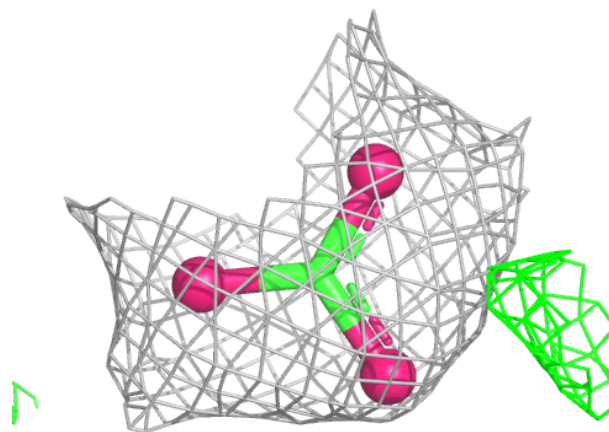


**Electron density around CLA B 608:**

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

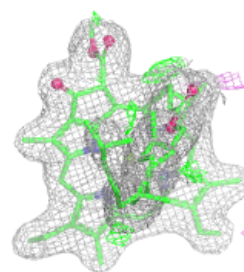
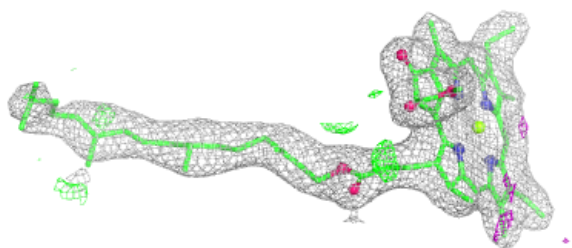
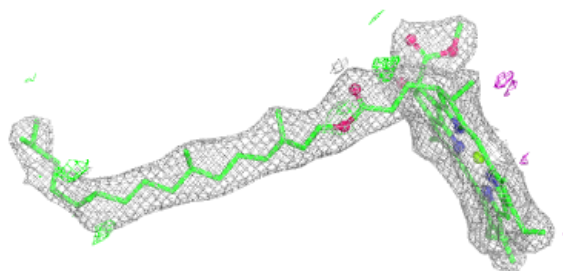
**Electron density around BCT A 348:**

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



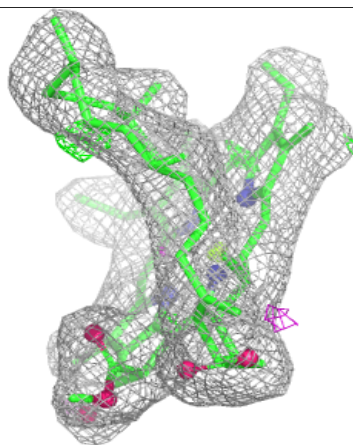
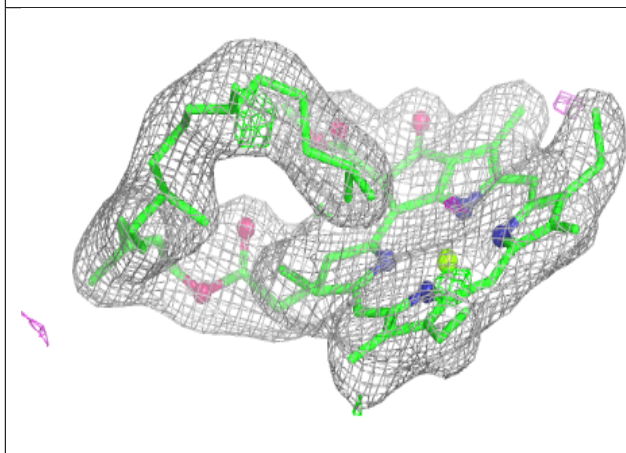
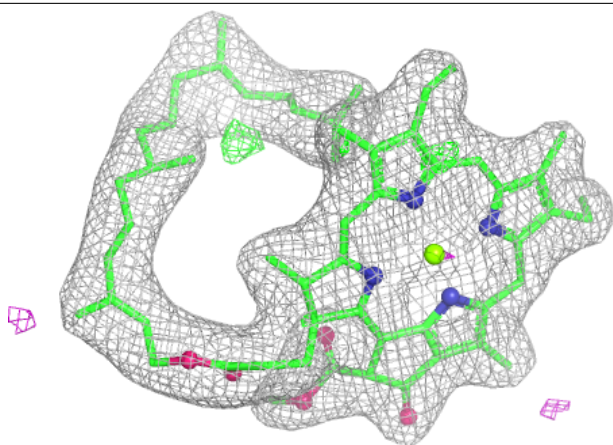
**Electron density around CLA B 604:**

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



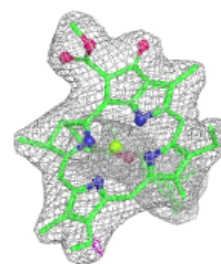
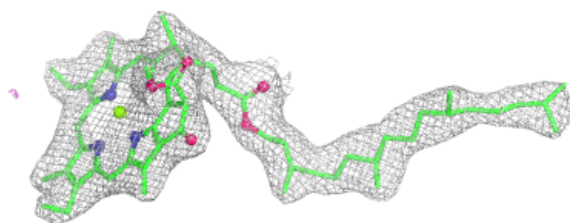
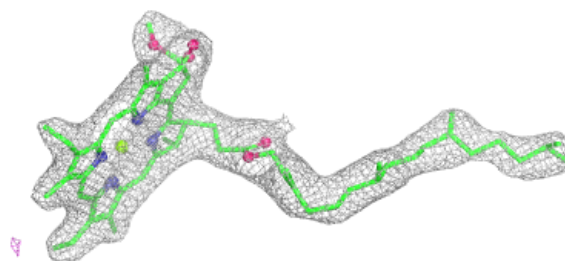
**Electron density around CLA B 615:**

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



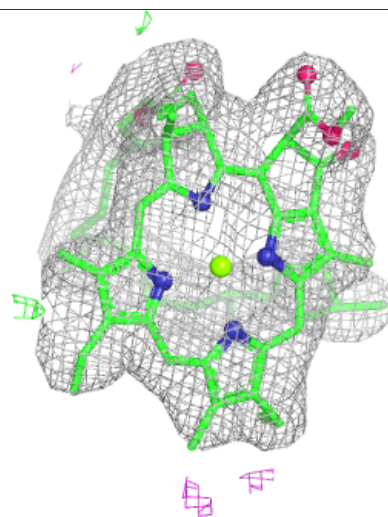
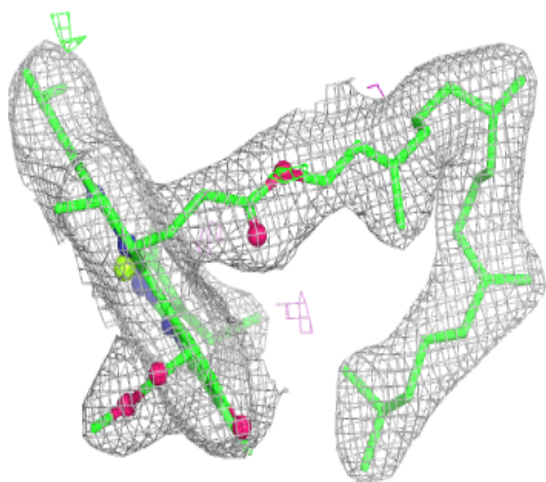
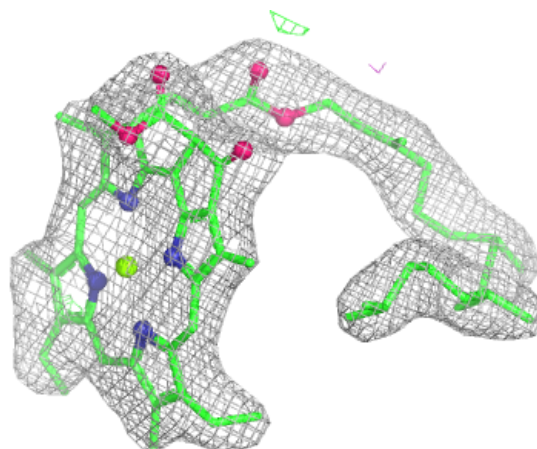
**Electron density around CLA c 503:**

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



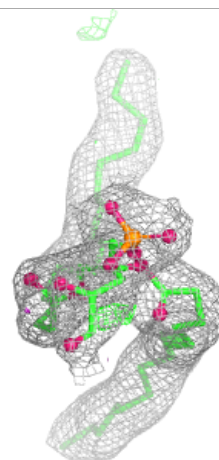
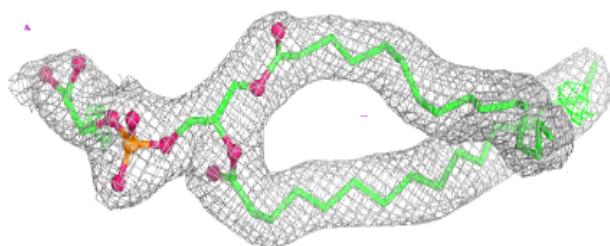
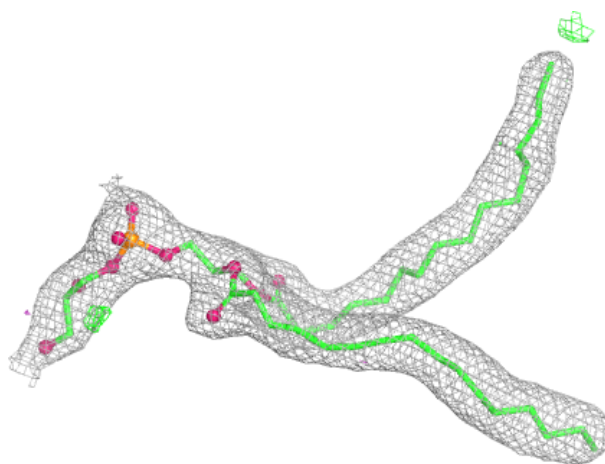
**Electron density around CLA c 504:**

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



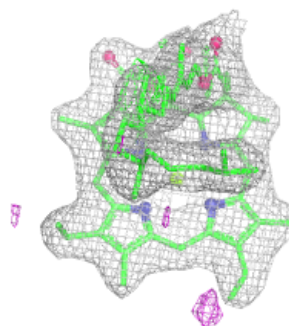
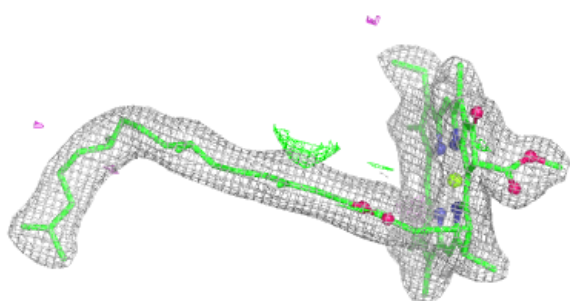
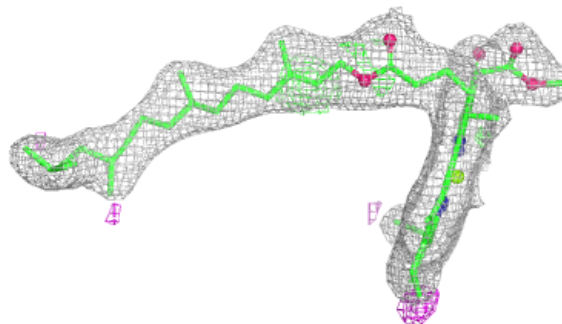
**Electron density around LHG D 410:**

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



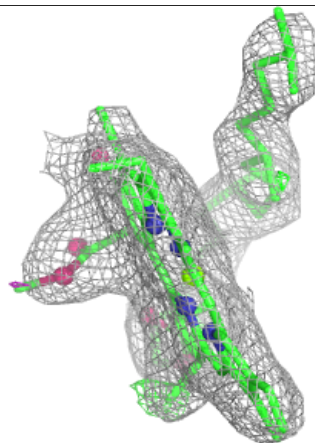
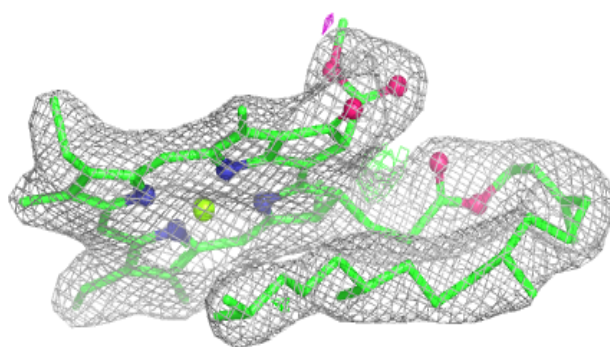
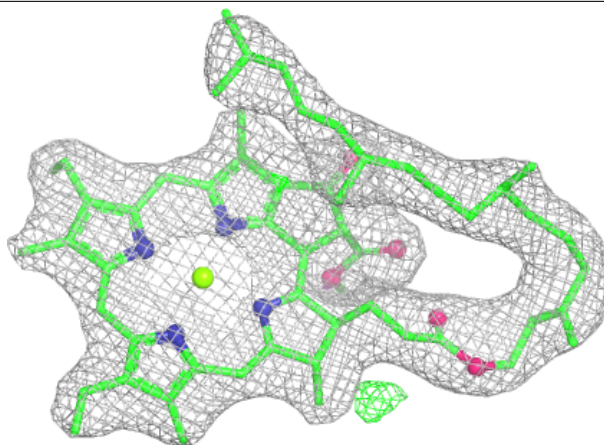
**Electron density around CLA B 605:**

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



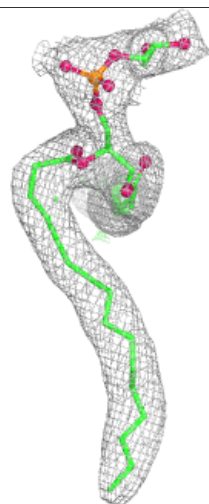
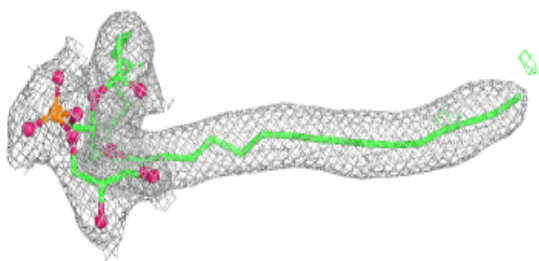
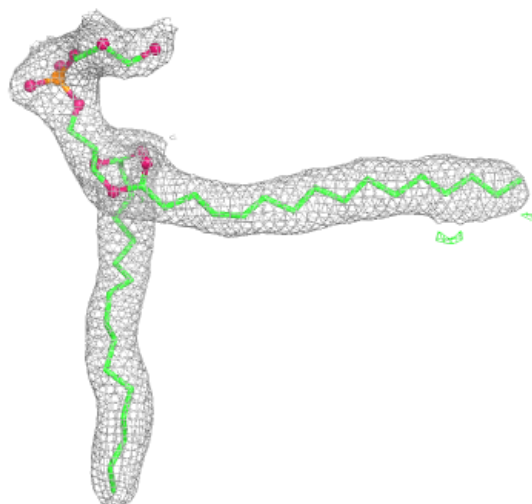
**Electron density around CLA C 510:**

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



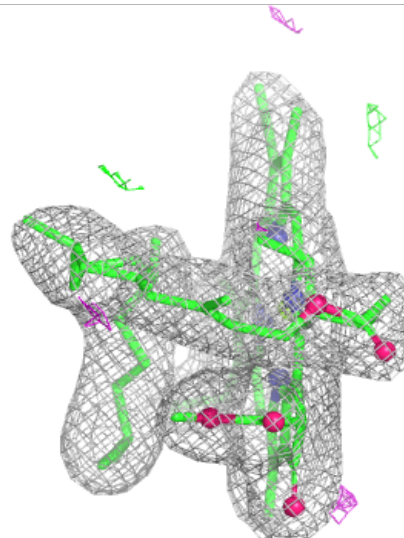
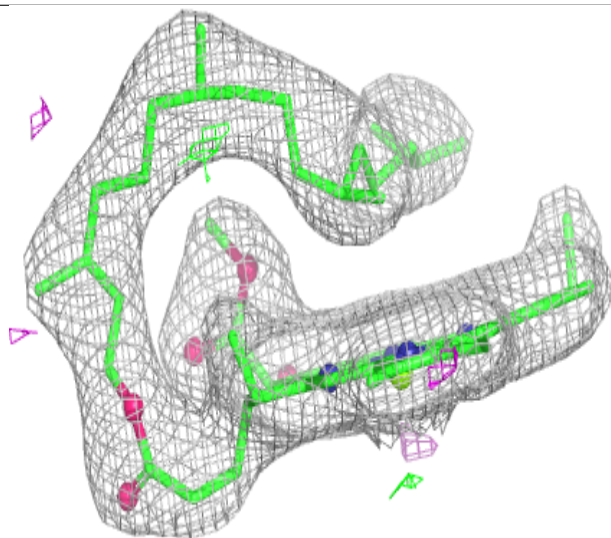
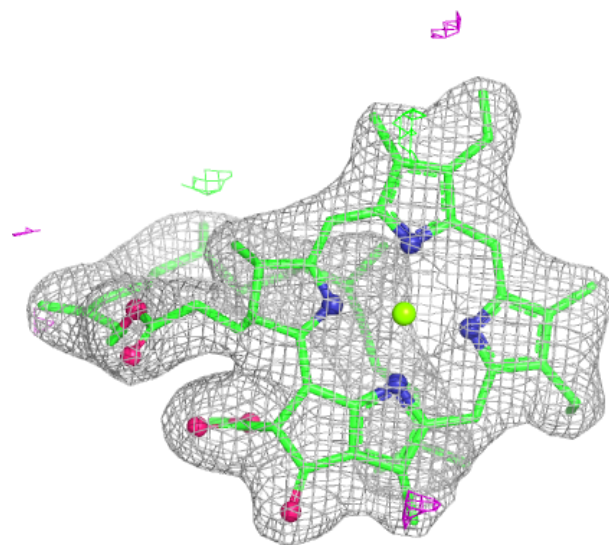
**Electron density around LHG L 101:**

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



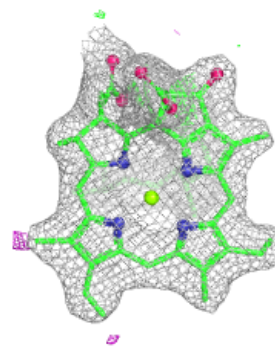
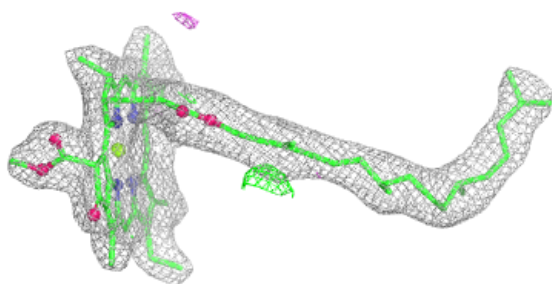
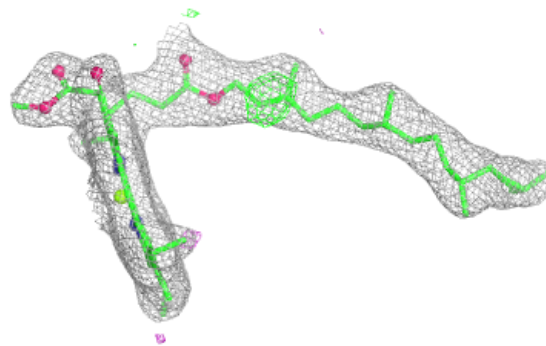
**Electron density around CLA C 511:**

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

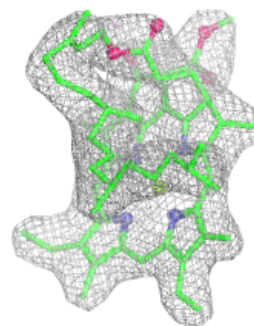
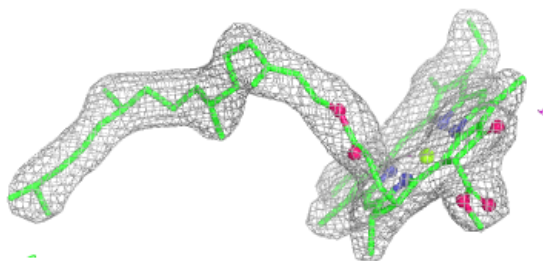
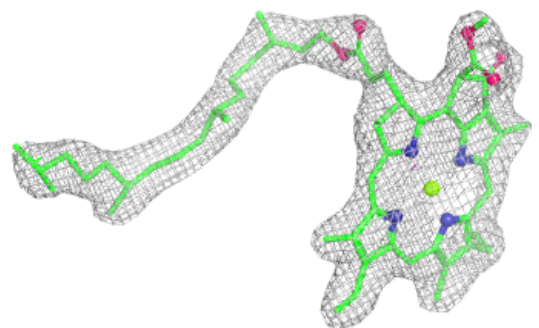


**Electron density around CLA b 605:**

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

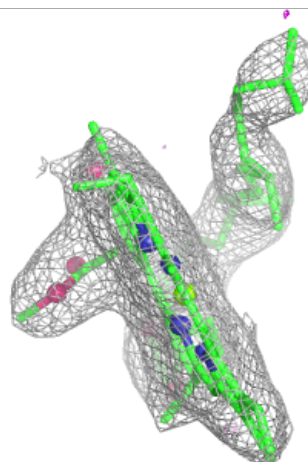
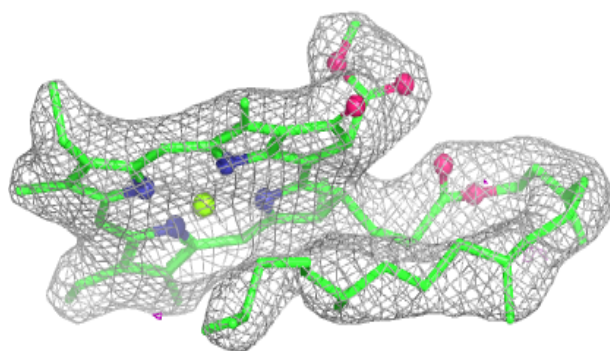
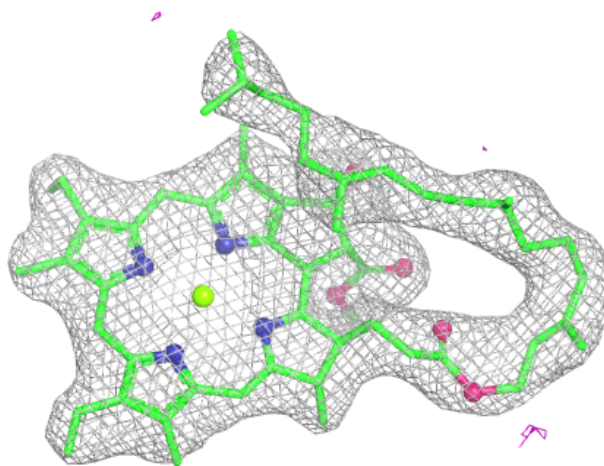
**Electron density around CLA C 512:**

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



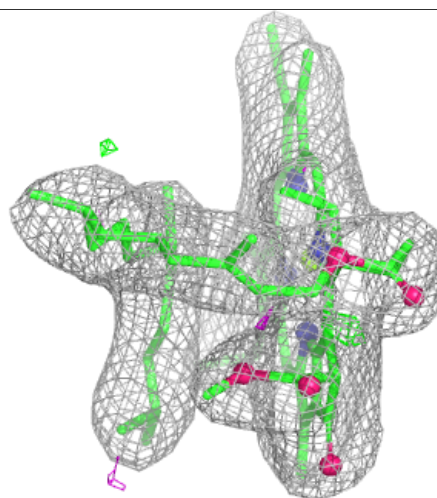
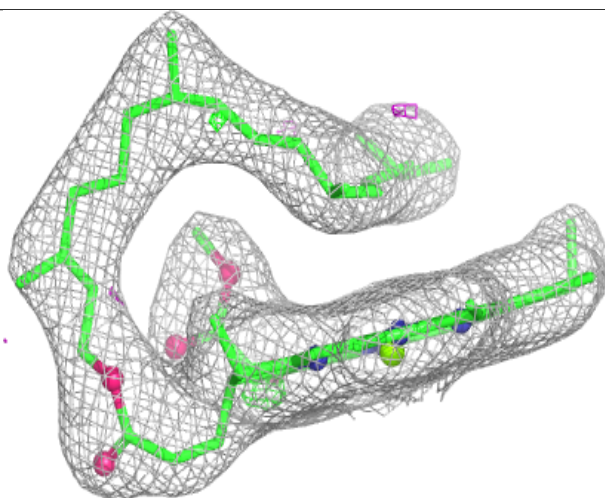
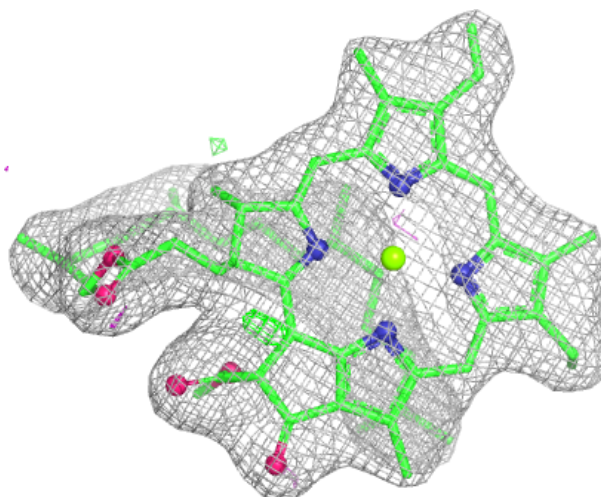
**Electron density around CLA c 510:**

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



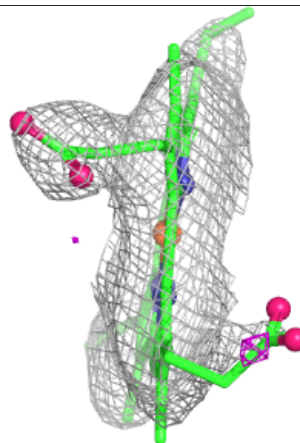
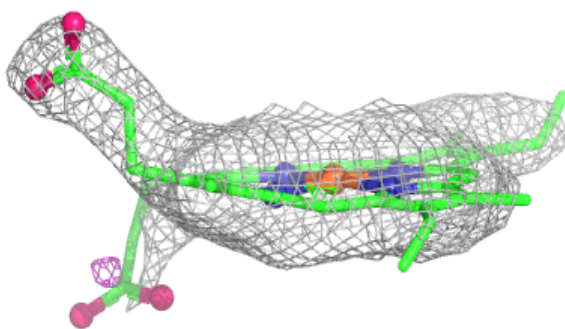
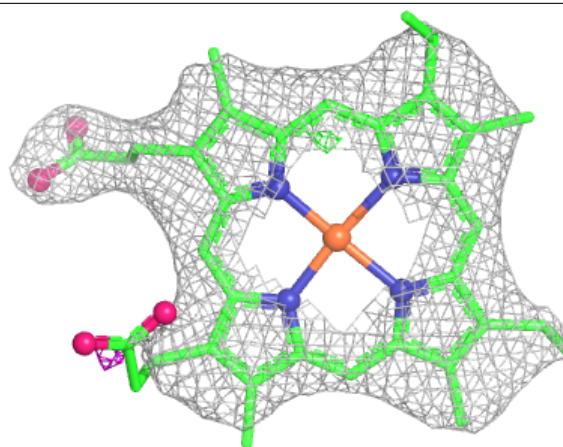
**Electron density around CLA c 511:**

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



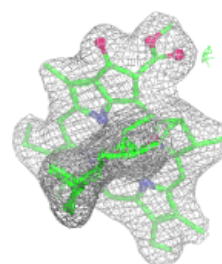
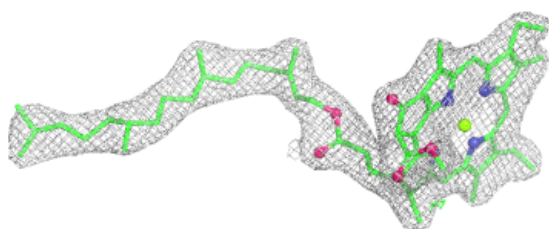
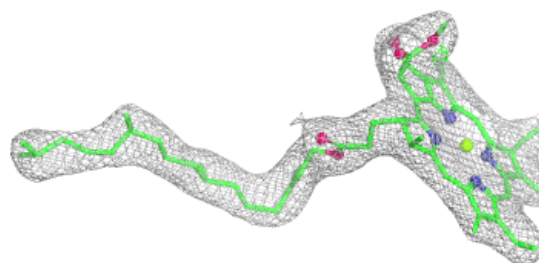
**Electron density around HEM e 87:**

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



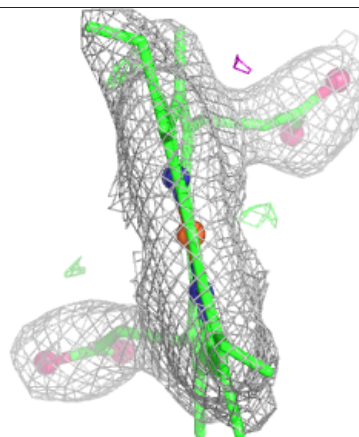
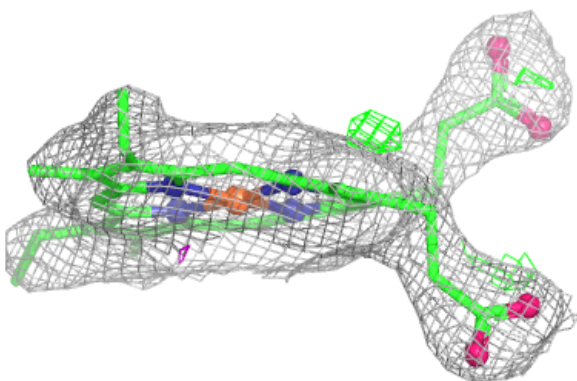
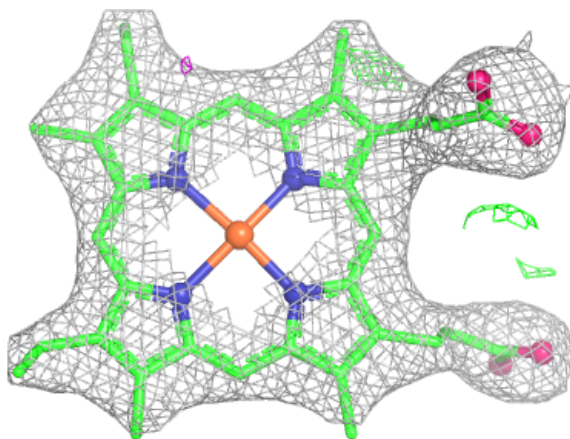
**Electron density around CLA C 503:**

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



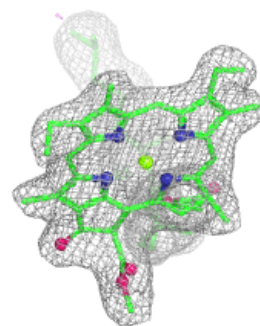
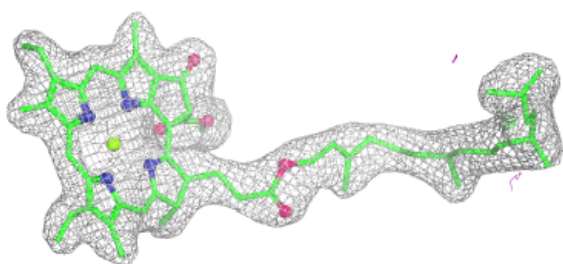
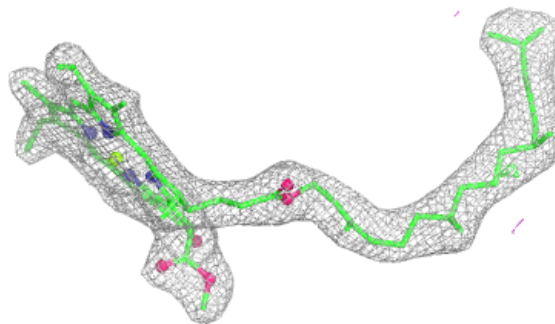
**Electron density around HEM E 103:**

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



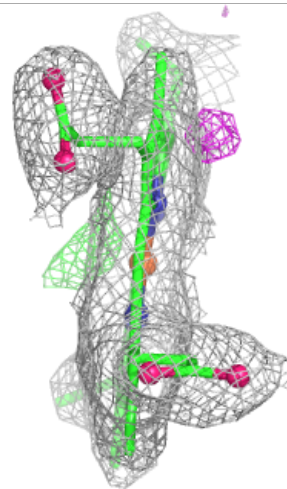
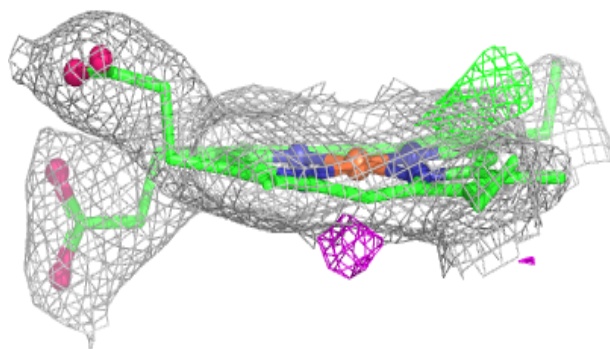
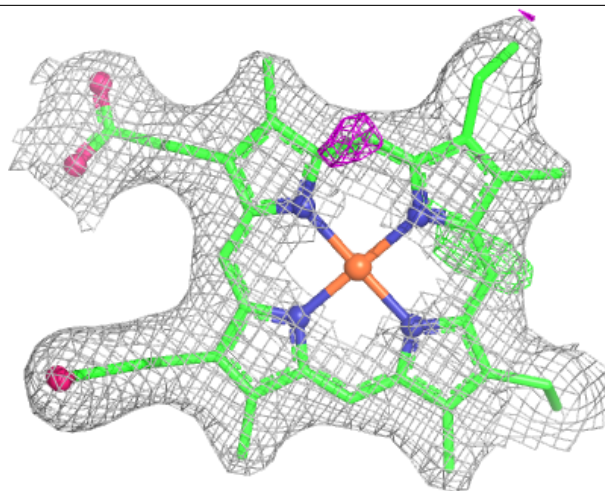
**Electron density around CLA d 402:**

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



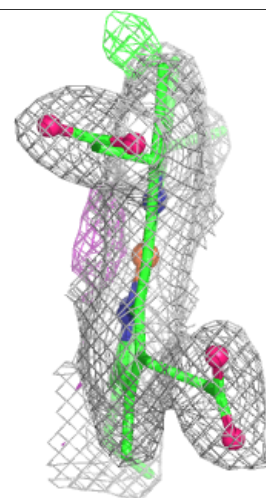
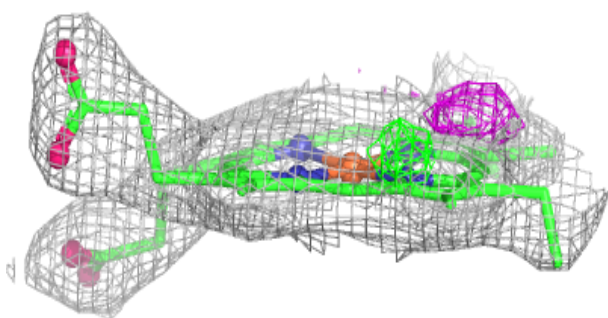
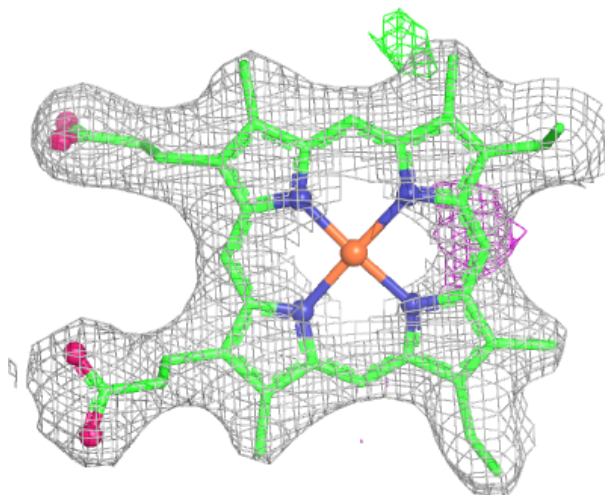
**Electron density around HEC V 202:**

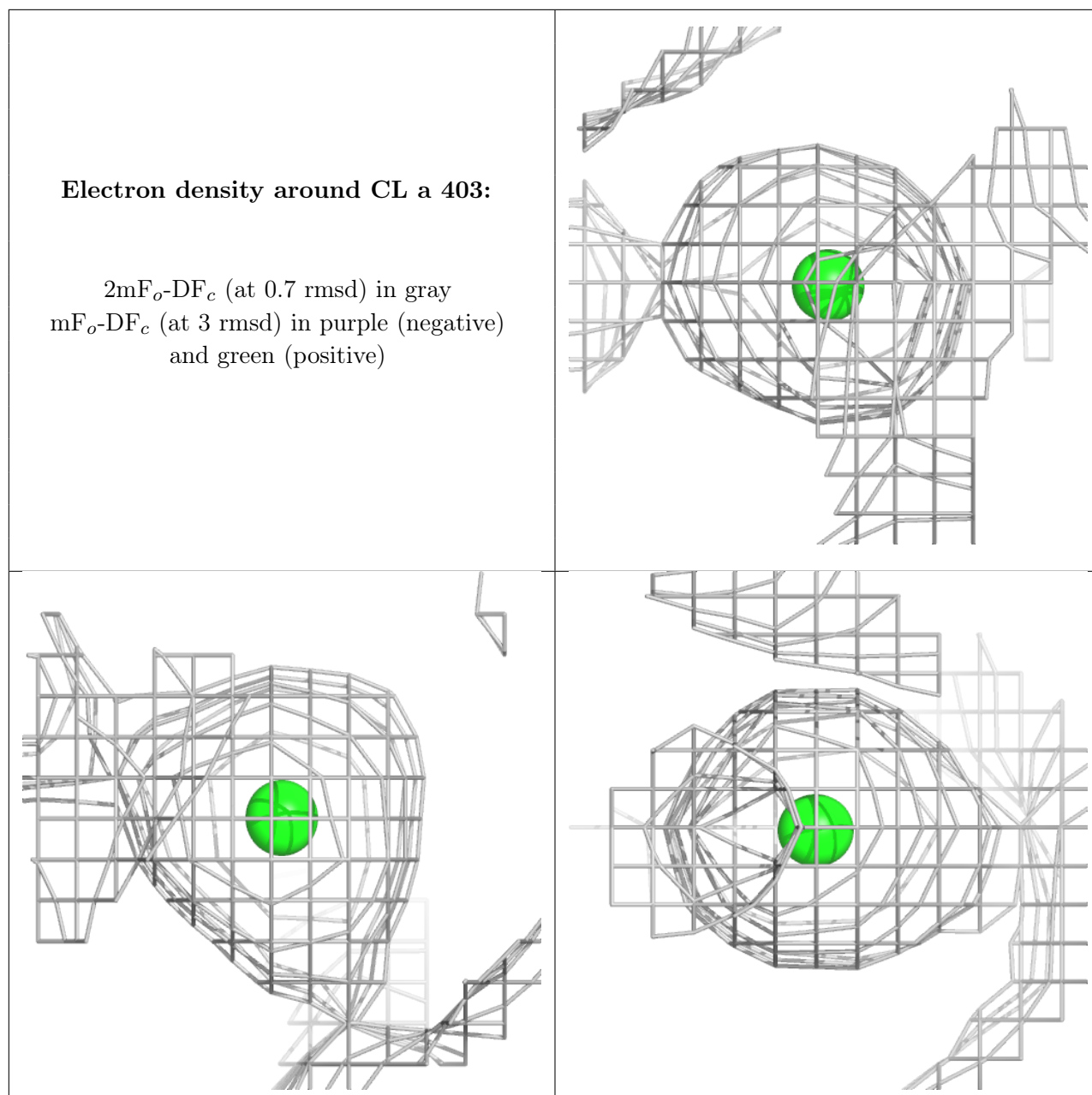
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC v 202:**

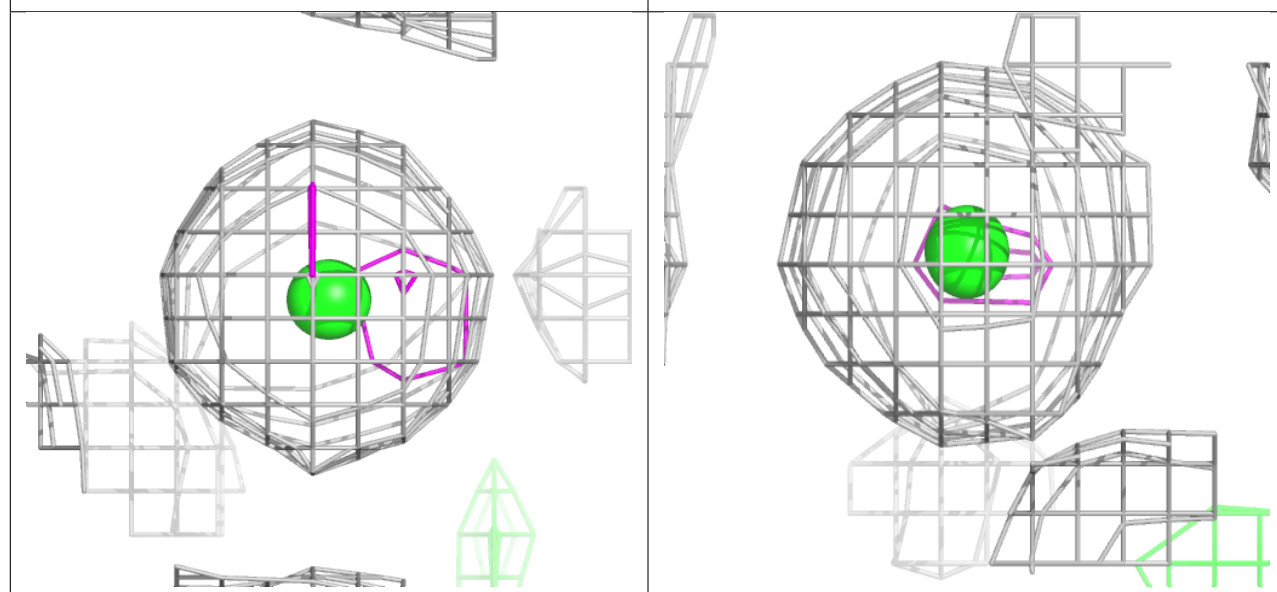
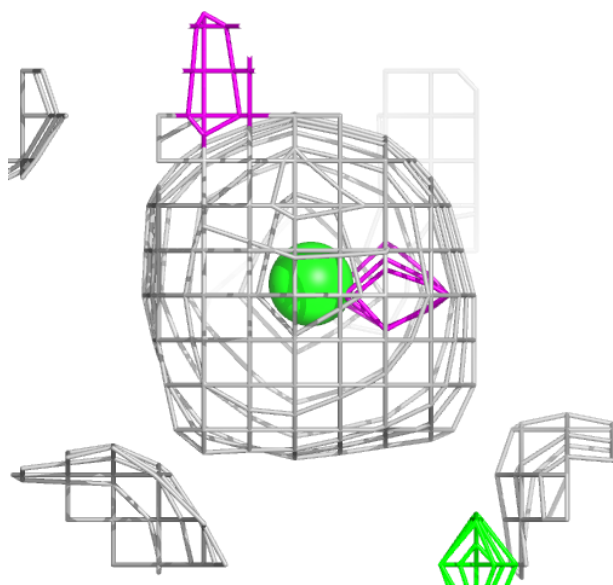
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





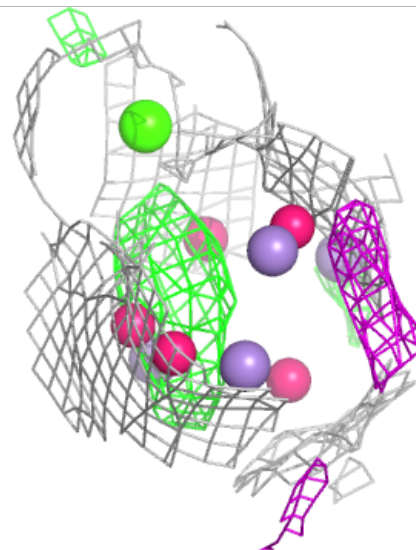
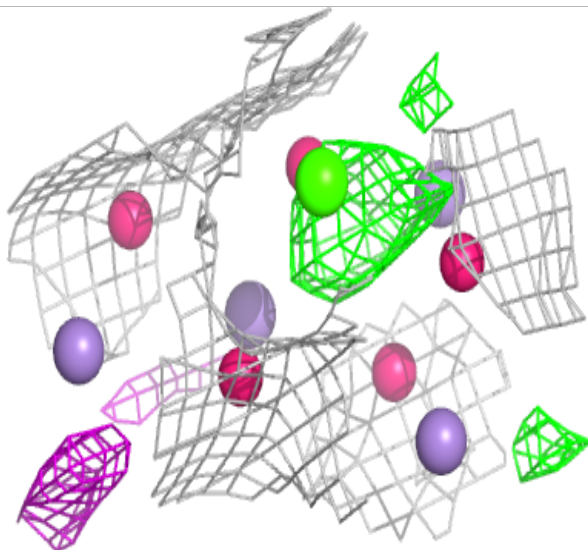
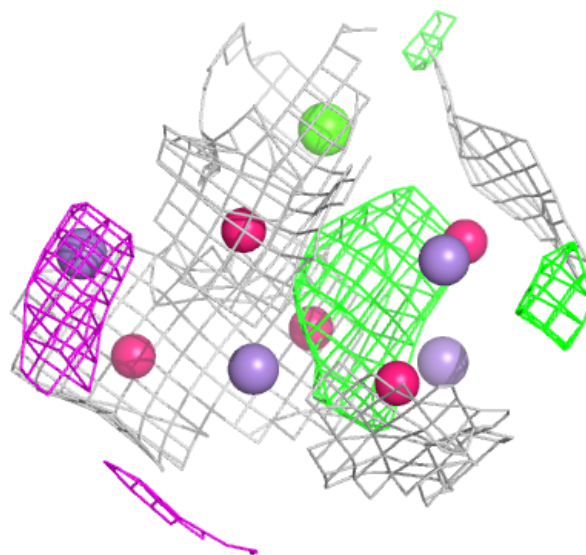
**Electron density around CL A 402:**

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



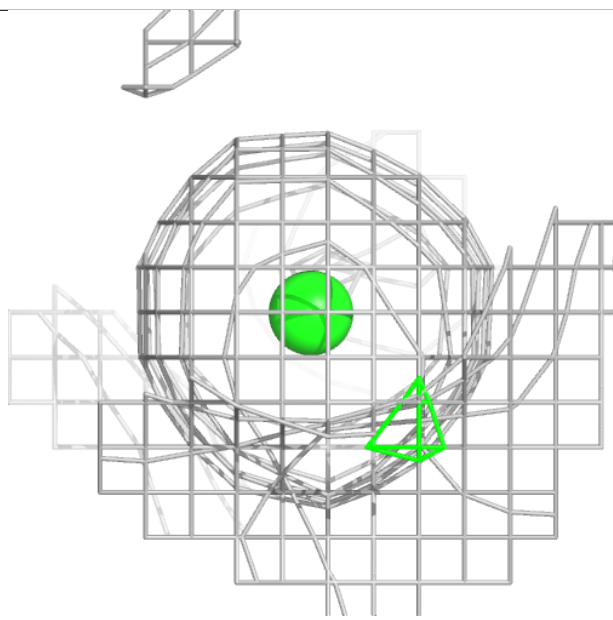
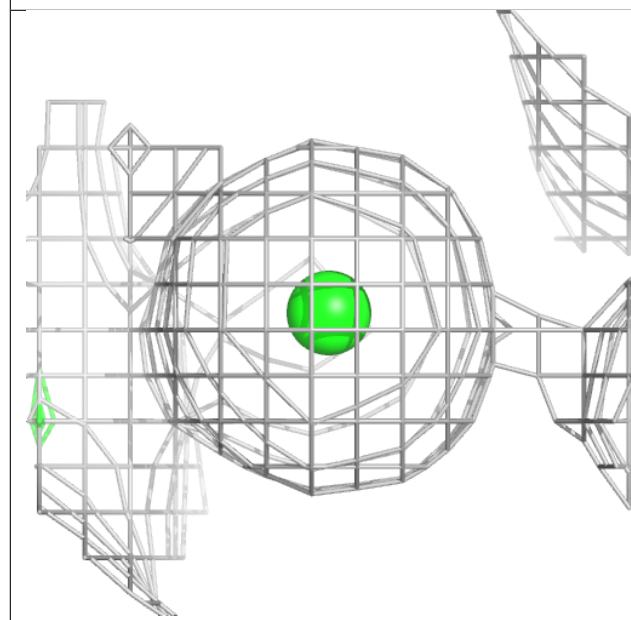
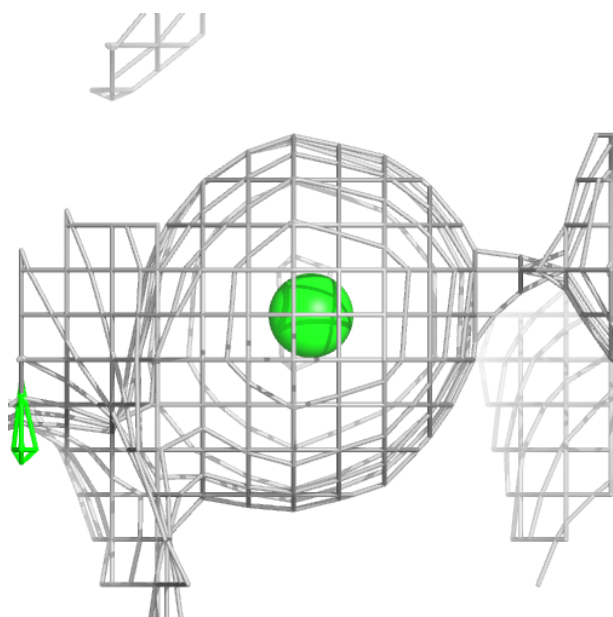
**Electron density around OEX A 413:**

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



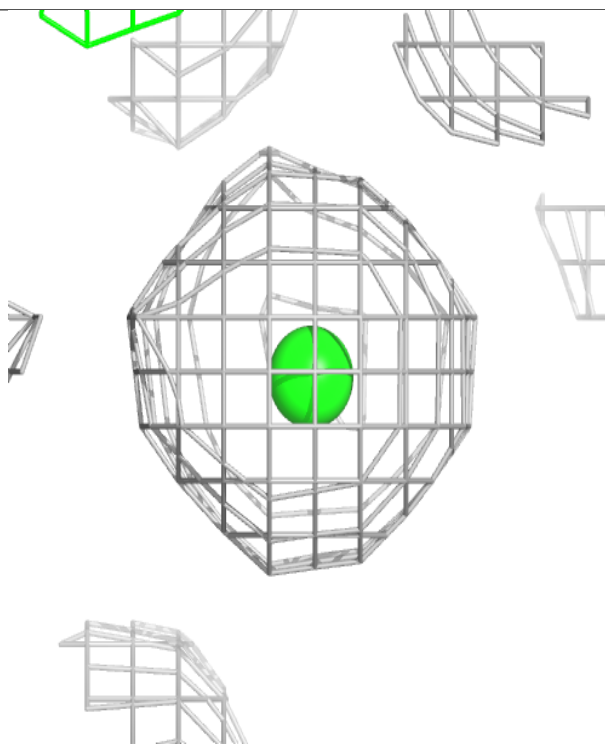
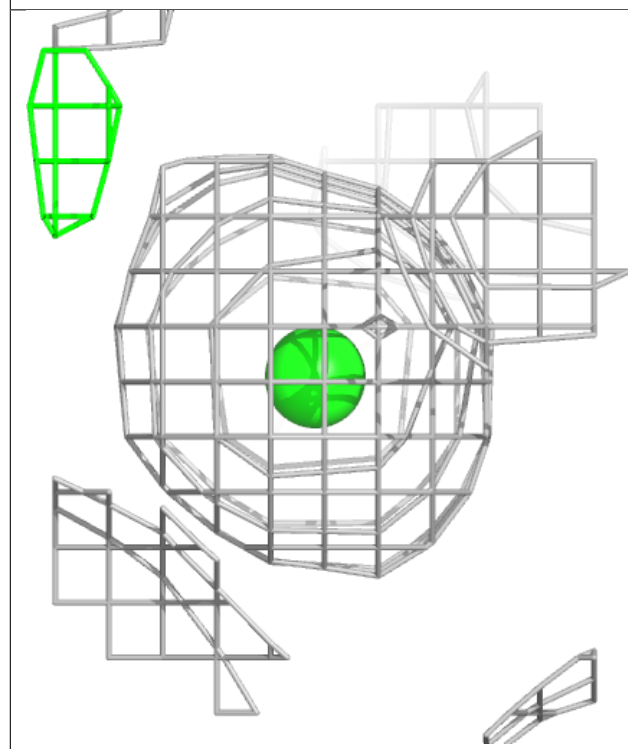
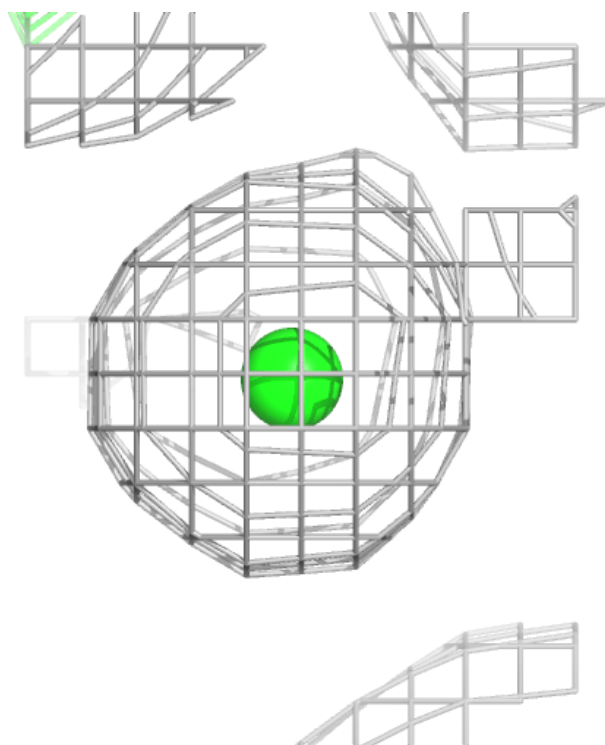
**Electron density around CL A 403:**

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



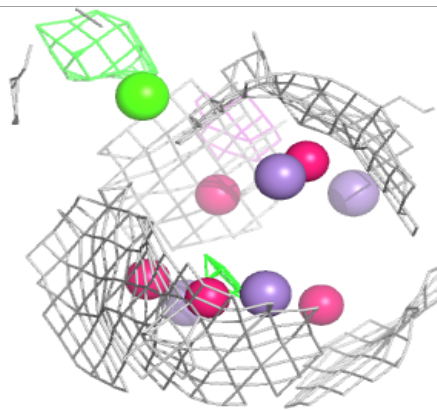
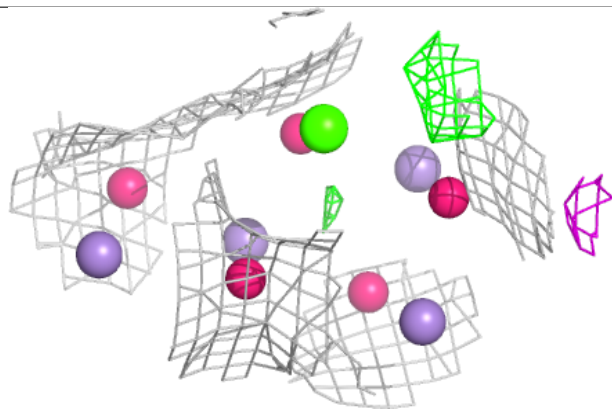
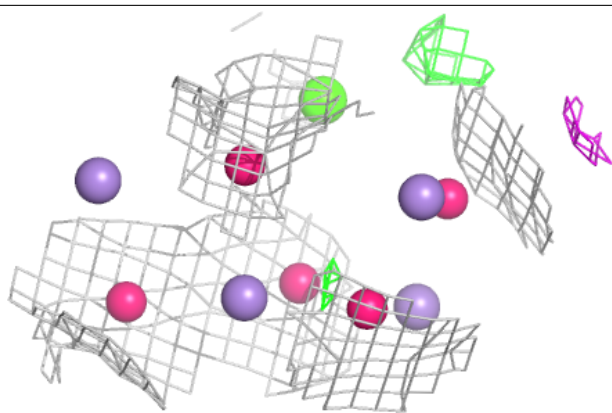
**Electron density around CL a 402:**

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



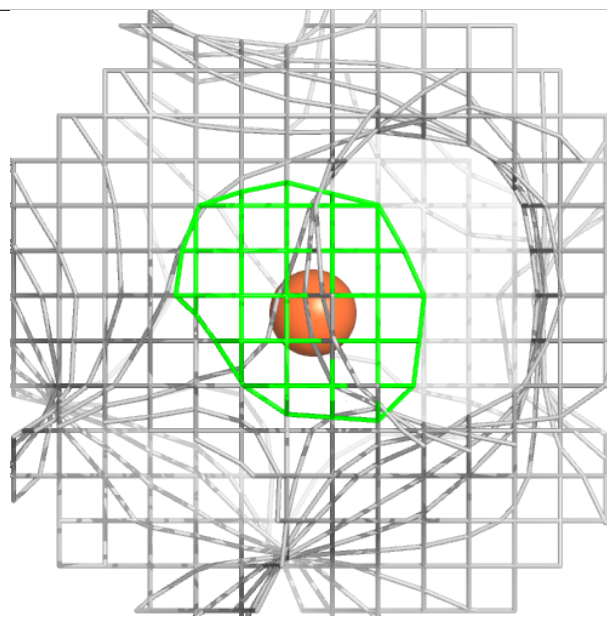
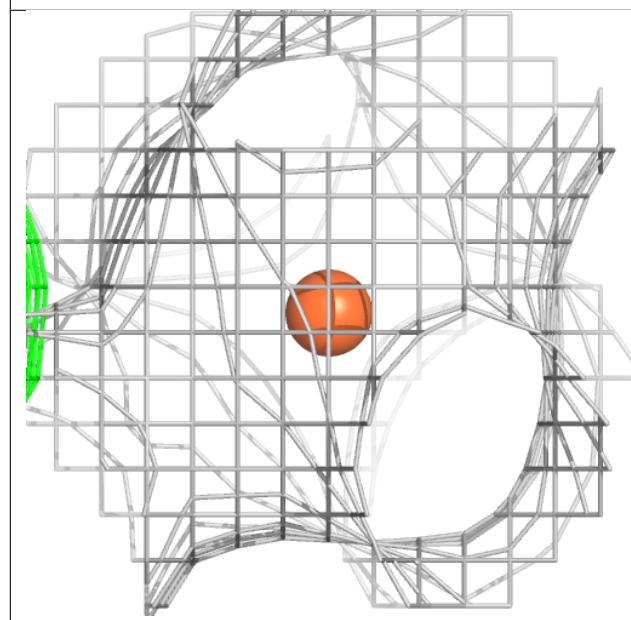
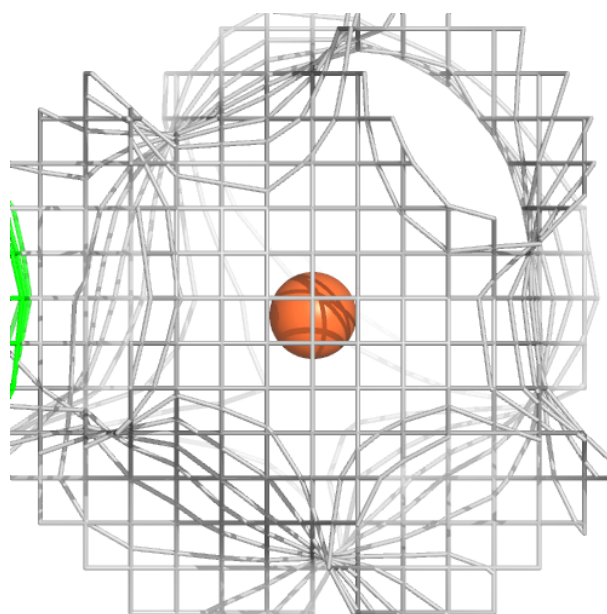
**Electron density around OEX a 415:**

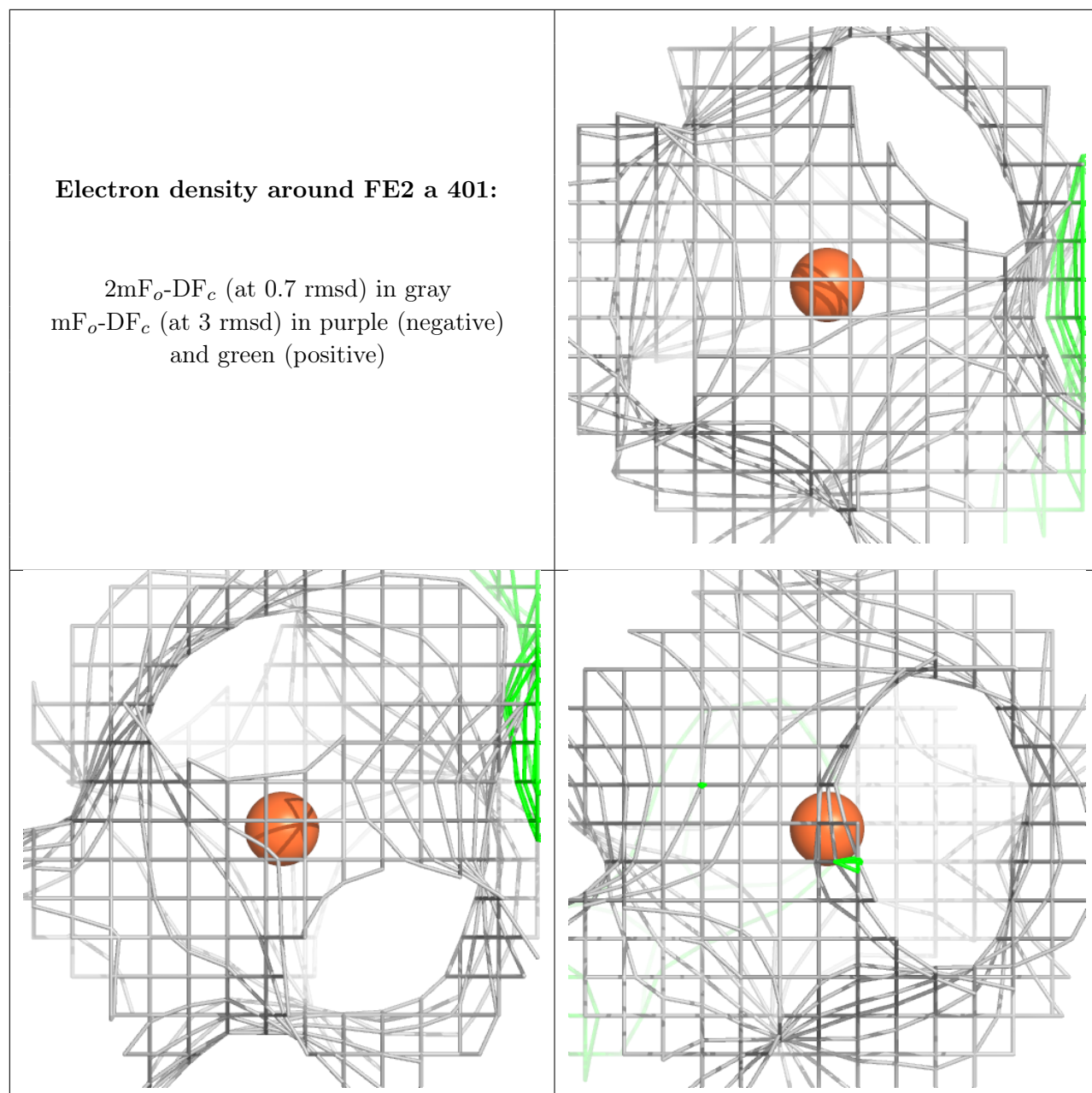
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)



**Electron density around FE2 A 401:**

$2mF_o-DF_c$  (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.