



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 13, 2026 – 11:13 AM JST

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

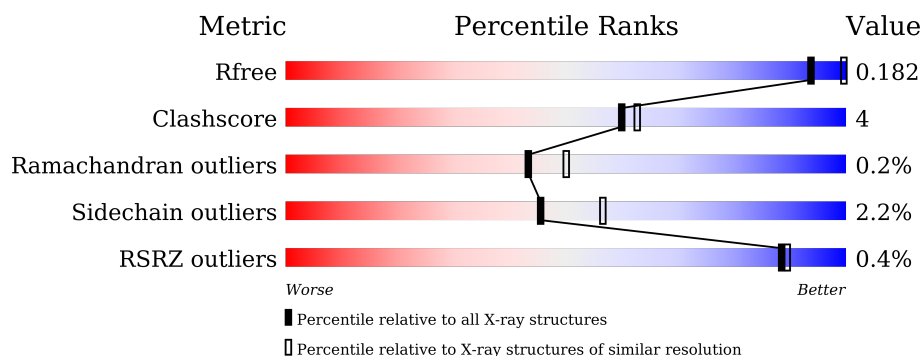
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



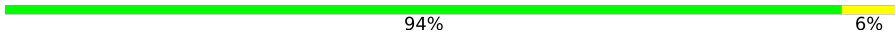
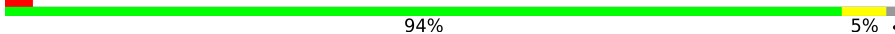
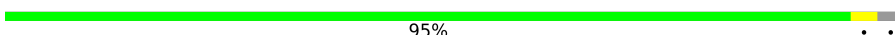
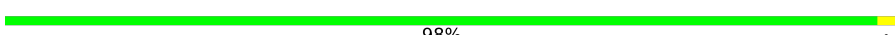
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	344	92%
1	a	344	% 89% 8%
2	B	505	93% 7%
2	b	505	% 92% 7%
3	C	455	91% 9%
3	c	455	93% 7%

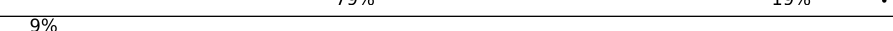
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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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

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
27	GOL	a	801	-	-	X	-
40	HEC	V	202	X	-	-	-
40	HEC	v	202	X	-	-	-

2 Entry composition

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
1	A	334	Total	C	N	O	S	0	1	0
			2628	1722	432	459	15			
1	a	334	Total	C	N	O	S	0	2	0
			2629	1721	432	461	15			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	7	0
			4029	2639	674	703	13			
2	b	504	Total	C	N	O	S	0	6	0
			4017	2636	669	699	13			

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

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

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	0	0	0
			662	432	107	123			
5	e	79	Total	C	N	O	0	2	0
			670	439	110	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	31	Total	C	N	O	S	0	1	0
			261	179	43	38	1			

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	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).

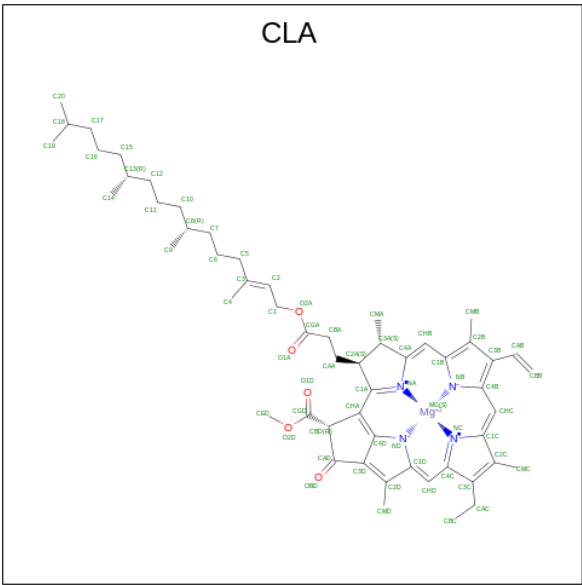
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		

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

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



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

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

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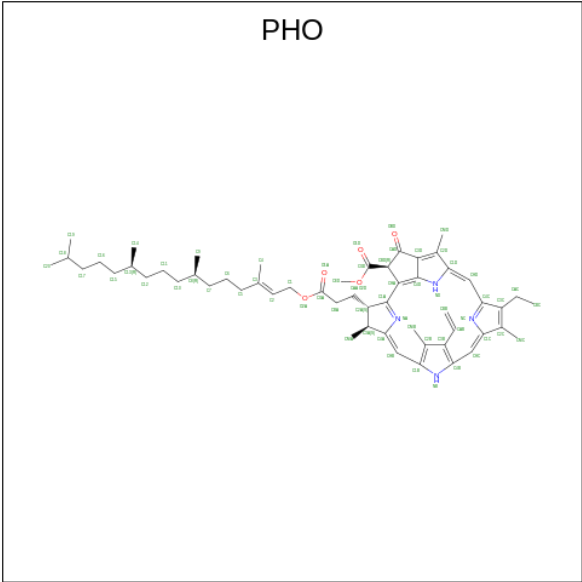
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23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55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

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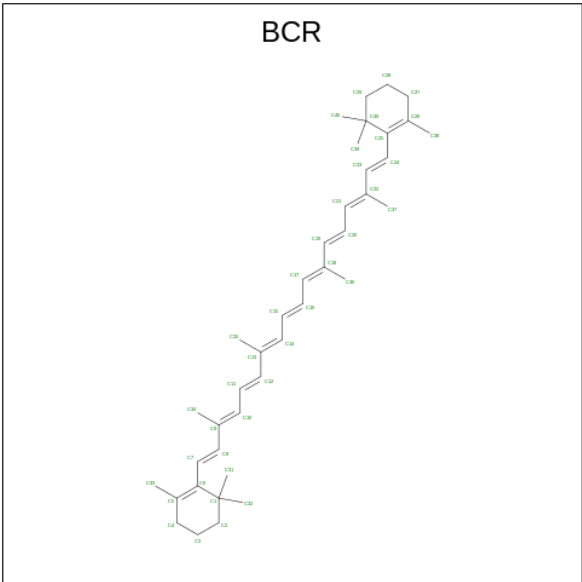
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



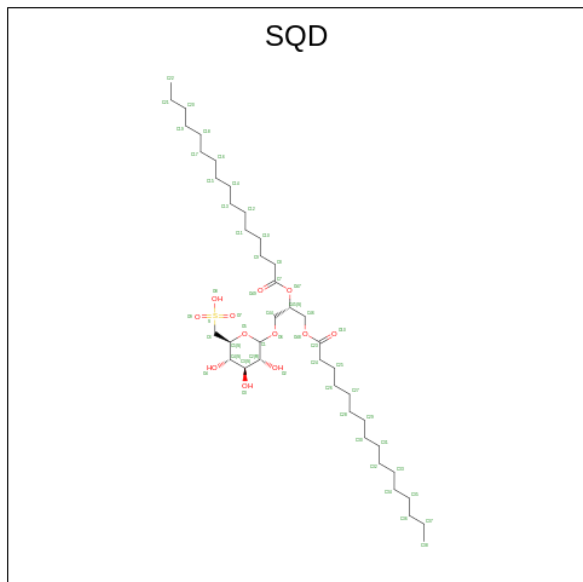
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



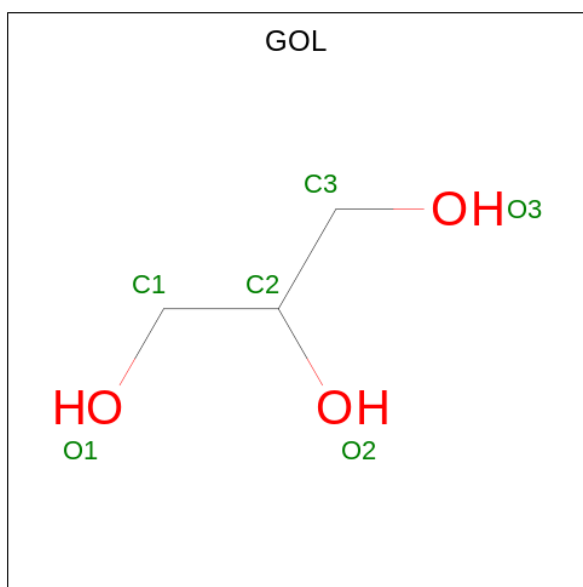
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

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



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

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



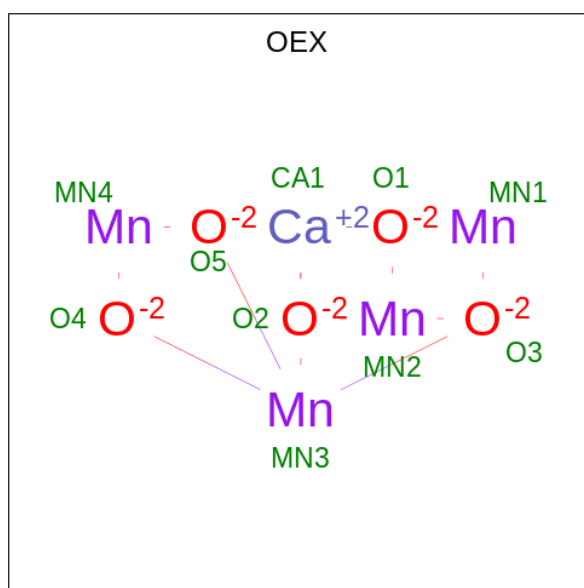
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	D	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27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

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

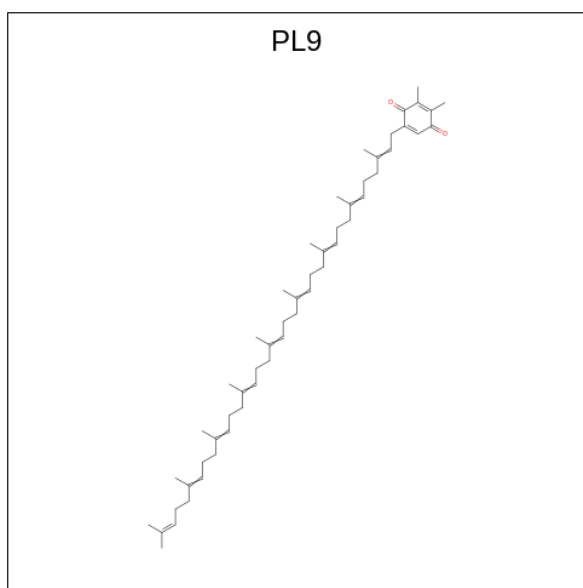
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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:).

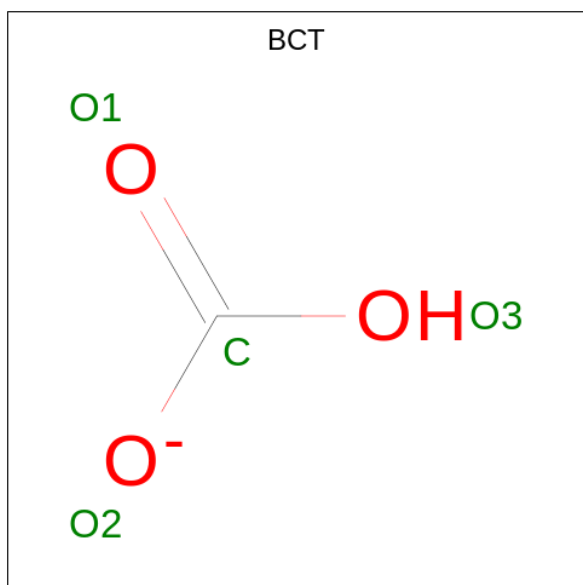
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	0
			34	29	5		
30	M	1	Total	C		0	0
			10	10			

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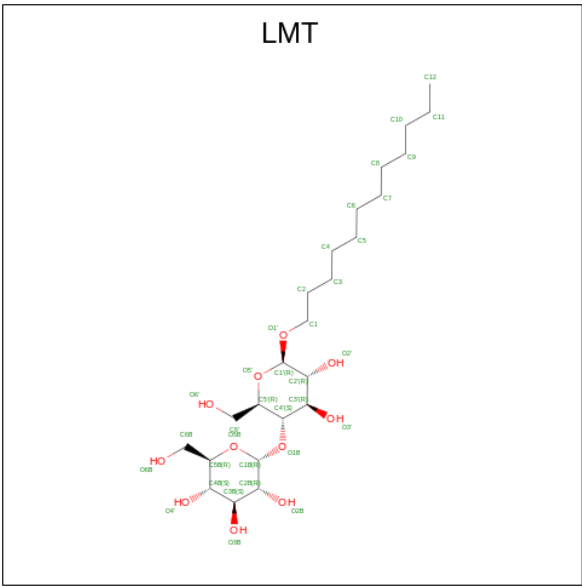
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	X	1	Total	C	O	0	0
			18	16	2		
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	1	Total	C	O	0	0
			33	28	5		
30	c	1	Total	C	O	0	0
			32	27	5		
30	d	2	Total	C	O	0	0
			53	47	6		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
	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

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: 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: C₂₄H₄₆O₁₁).



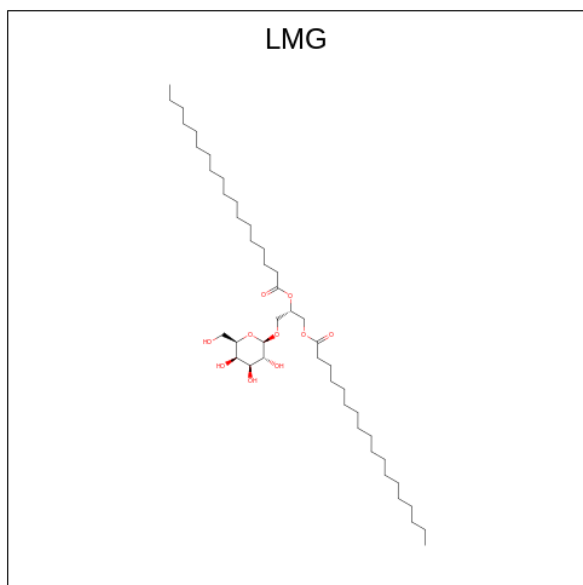
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 35 24 11	0	0
32	D	1	Total C O 35 24 11	0	0
32	E	1	Total C O 35 24 11	0	0
32	I	1	Total C O 35 24 11	0	0
32	M	1	Total C O 35 24 11	0	0
32	M	1	Total C O 35 24 11	0	0
32	a	1	Total C O 35 24 11	0	0
32	a	1	Total C O 35 24 11	0	0
32	b	1	Total C O 25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

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

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



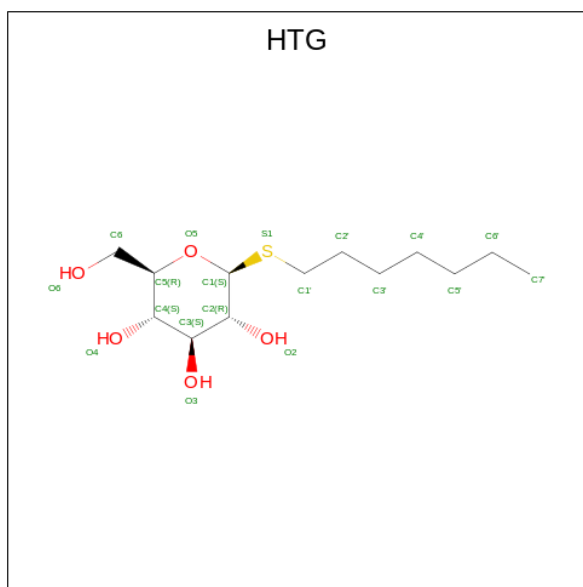
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	D	1	Total	C	O	0	0
			51	41	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total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

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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: C₁₃H₂₆O₅S).



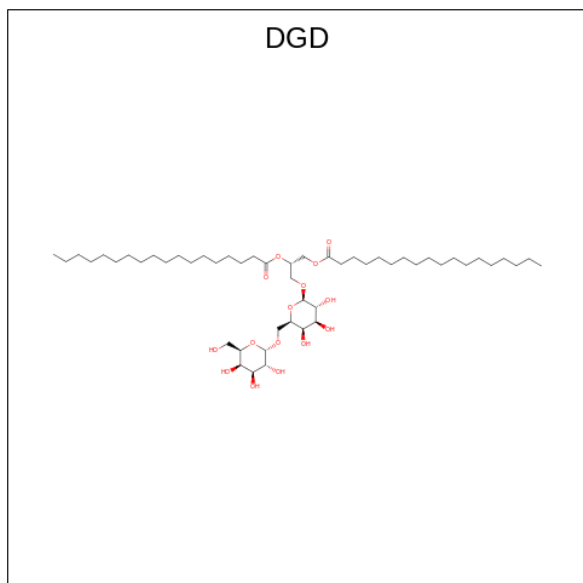
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	D	1	Total	C	O	S	0	0
			16	10	5	1		
34	V	1	Total	C	O		0	0
			11	6	5			
34	b	1	Total	C	O	S	0	0
			19	13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

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

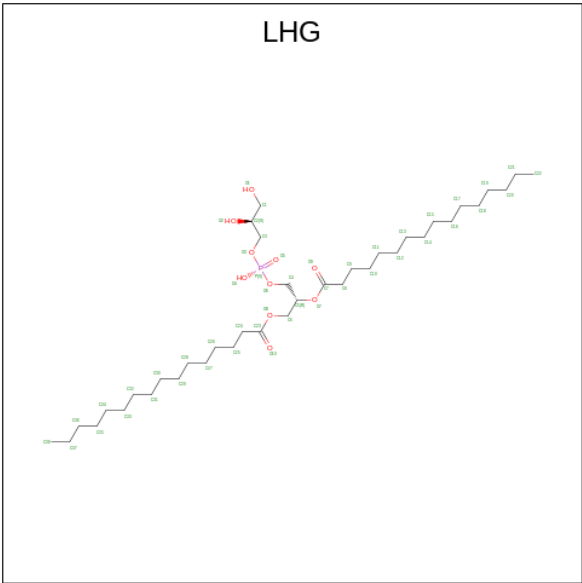


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	C	1	Total	C	O		0	0
			62	47	15			
35	C	1	Total	C	O		0	0
			62	47	15			
35	C	1	Total	C	O		0	0
			62	47	15			
35	H	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15	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

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

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

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



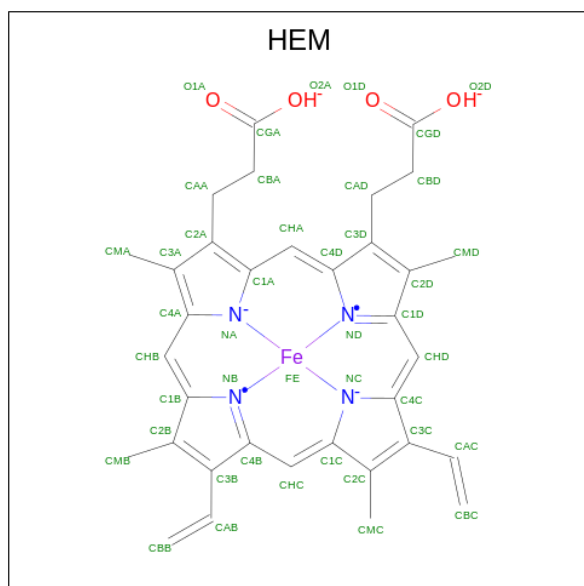
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	E	1	Total	C	O	P	0	0
			42	31	10	1		
37	L	1	Total	C	O	P	0	0
			49	38	10	1		

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

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

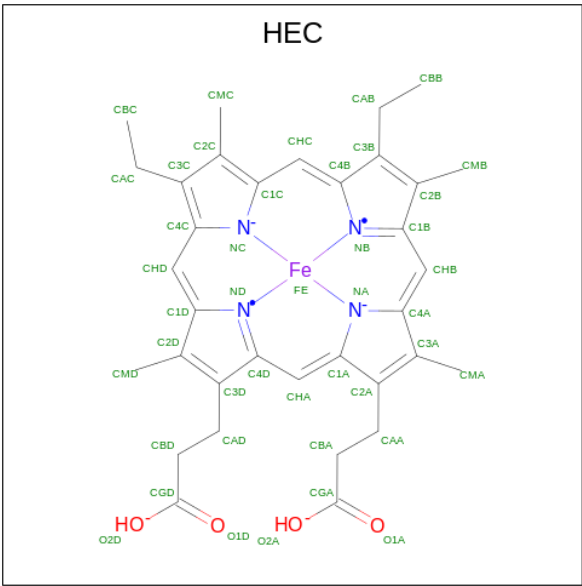


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
38	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

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

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

3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1

Chain A:  92%

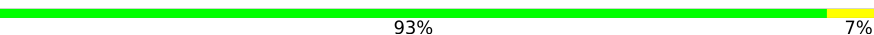


- Molecule 1: Photosystem II protein D1

Chain a:  89% 8%

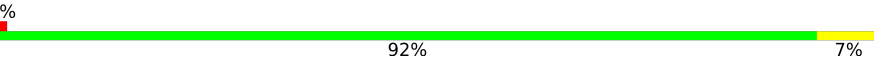


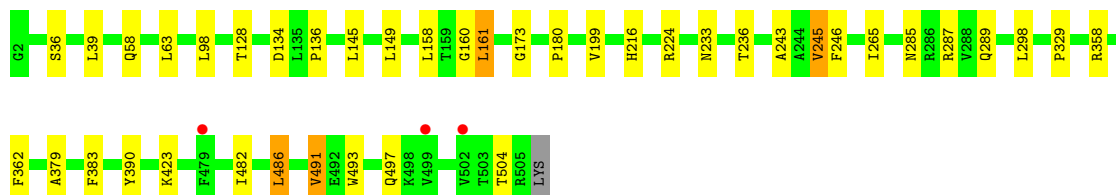
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  93% 7%



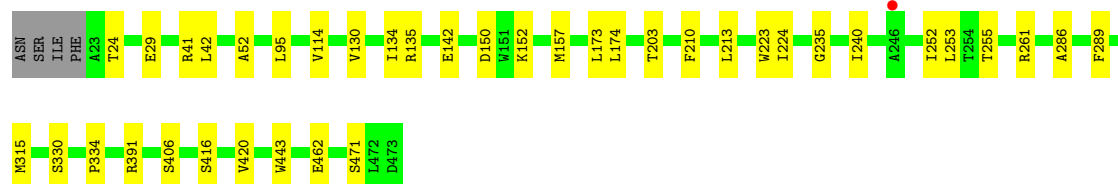
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  92% 7%



- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  91% 9%



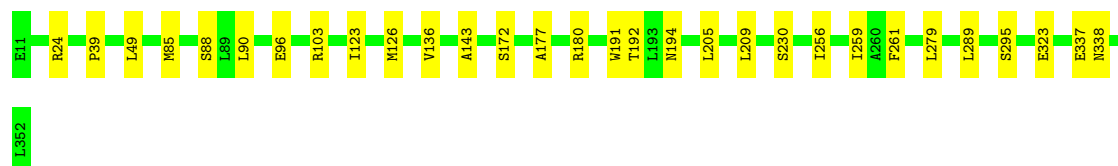
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  93% 7%



- Molecule 4: Photosystem II D2 protein

Chain D:  91% 9%



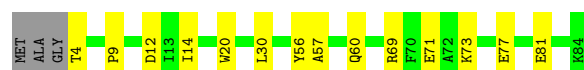
- Molecule 4: Photosystem II D2 protein

Chain d:  94% 6%

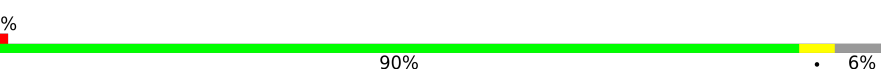


- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  80% 17%



- Molecule 5: Cytochrome b559 subunit alpha

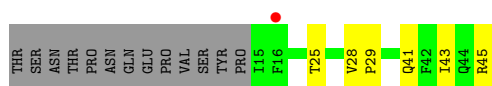
Chain e:  90% 6%



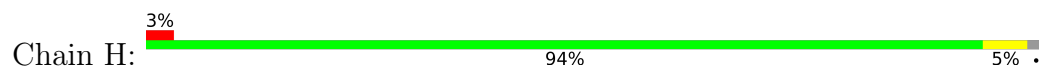
- Molecule 6: Cytochrome b559 subunit beta



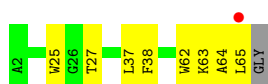
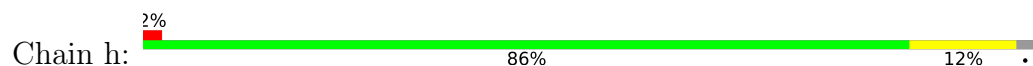
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



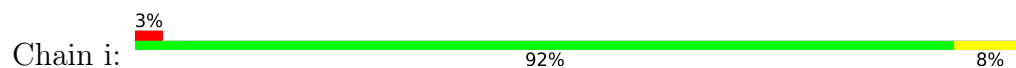
- Molecule 7: Photosystem II reaction center protein H



- 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% .

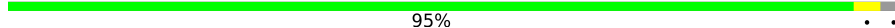


- Molecule 10: Photosystem II reaction center protein K

Chain k:  78% 16% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  95% . .



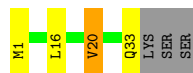
- Molecule 11: Photosystem II reaction center protein L

Chain l:  89% 8% .



- Molecule 12: Photosystem II reaction center protein M

Chain M:  81% 8% . 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%



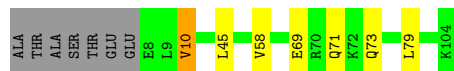
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  84% 9% 8%

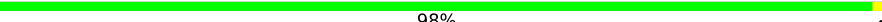


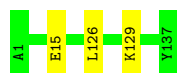
- Molecule 15: Photosystem II 12 kDa extrinsic protein

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:  87% 10% 3% .



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  70% 27% .

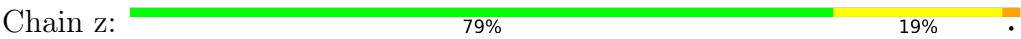


- Molecule 19: Photosystem II reaction center protein Z

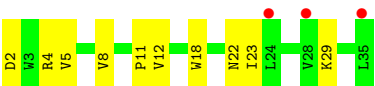
Chain Z:  89% 10% .



- Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.77Å 231.76Å 288.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.25 19.99 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.25) 99.8 (19.99-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.26Å)	Xtriage
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 ²)	50.9	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	52977	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HTG, LHG, PL9, BCT, HEC, GOL, PHO, BCR, FE2, CA, HEM, LMT, UNL, CL, SQD, CLA, OEX, MG, LMG, FME, DGD

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

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:HB2	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:I: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:H221	29:A:414:PL9:H201	1.88	0.43
29:A:414:PL9:HC2	29:A:414:PL9:HC8	1.71	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 ⓘ

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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Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
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 ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	FME	T	1	14	8,9,10	0.69	0	7,9,11	2.01	2 (28%)
14	FME	t	1	14	8,9,10	0.75	0	7,9,11	1.49	1 (14%)
12	FME	m	1	12	8,9,10	0.56	0	7,9,11	1.33	2 (28%)
12	FME	M	1	12	8,9,10	0.62	0	7,9,11	1.13	0
8	FME	I	1	8	8,9,10	0.60	0	7,9,11	1.40	2 (28%)
8	FME	i	1	8	8,9,10	0.65	0	7,9,11	1.19	0

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

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

There are no bond length outliers.

All (7) 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	C-CA-N	2.80	114.79	109.73
14	t	1	FME	O-C-CA	-2.44	118.39	124.78
8	I	1	FME	O-C-CA	-2.29	118.78	124.78
12	m	1	FME	O1-CN-N	-2.14	119.63	125.27
12	m	1	FME	O-C-CA	-2.08	119.33	124.78
8	I	1	FME	CA-N-CN	-2.01	119.74	122.82

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$
25	BCR	C	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.32	7 (12%)
33	LMG	C	521	-	51,51,55	1.06	3 (5%)	59,59,63	1.32	6 (10%)
33	LMG	Z	101	-	37,37,55	1.00	2 (5%)	45,45,63	1.43	5 (11%)
23	CLA	c	507	3	69,73,73	2.04	20 (28%)	83,113,113	2.77	29 (34%)
23	CLA	c	506	3	69,73,73	2.01	19 (27%)	83,113,113	2.82	28 (33%)
24	PHO	A	353	-	58,69,69	2.79	15 (25%)	56,99,99	2.85	15 (26%)
23	CLA	b	604	2	69,73,73	2.01	20 (28%)	83,113,113	2.77	29 (34%)
28	OEX	a	415	1,3,41	0,14,14	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HTG	C	522	-	19,19,19	0.89	1 (5%)	23,24,24	1.46	2 (8%)
23	CLA	b	610	41	69,73,73	2.00	20 (28%)	83,113,113	2.86	33 (39%)
32	LMT	D	404	-	36,36,36	1.17	4 (11%)	47,47,47	1.31	5 (10%)
25	BCR	b	619	-	41,41,41	1.09	1 (2%)	56,56,56	1.39	6 (10%)
23	CLA	c	512	3	69,73,73	2.06	19 (27%)	83,113,113	2.76	31 (37%)
33	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.39	7 (11%)
23	CLA	B	611	2	69,73,73	2.48	21 (30%)	83,113,113	3.98	31 (37%)
35	DGD	H	102	-	63,63,67	0.84	3 (4%)	77,77,81	1.02	5 (6%)
25	BCR	T	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.57	13 (23%)
33	LMG	c	521	-	51,51,55	1.00	2 (3%)	59,59,63	1.36	7 (11%)
35	DGD	c	518	-	63,63,67	0.85	3 (4%)	77,77,81	0.97	3 (3%)
34	HTG	B	623	-	19,19,19	0.78	1 (5%)	23,24,24	1.33	1 (4%)
27	GOL	V	401	-	5,5,5	1.34	0	5,5,5	0.80	0
37	LHG	D	411	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
23	CLA	A	405	41	69,73,73	2.02	18 (26%)	83,113,113	2.85	33 (39%)
23	CLA	b	612	2	69,73,73	1.99	19 (27%)	83,113,113	2.80	29 (34%)
27	GOL	B	624	-	5,5,5	0.86	0	5,5,5	1.18	1 (20%)
23	CLA	C	512	3	69,73,73	2.05	22 (31%)	83,113,113	2.74	28 (33%)
26	SQD	f	102	-	42,43,54	1.18	3 (7%)	51,54,65	1.57	11 (21%)
27	GOL	o	601	-	5,5,5	1.10	1 (20%)	5,5,5	1.02	0
23	CLA	C	510	3	69,73,73	2.07	20 (28%)	83,113,113	2.86	29 (34%)
34	HTG	b	625	-	19,19,19	1.00	2 (10%)	23,24,24	1.59	3 (13%)
37	LHG	d	408	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	3 (5%)
27	GOL	d	801	-	5,5,5	0.93	0	5,5,5	0.98	0
27	GOL	o	501	-	5,5,5	0.99	0	5,5,5	0.96	0
23	CLA	C	511	3	69,73,73	2.05	20 (28%)	83,113,113	2.89	32 (38%)
27	GOL	v	401	-	5,5,5	1.20	0	5,5,5	0.82	0
23	CLA	D	406	4	69,73,73	2.09	19 (27%)	83,113,113	2.79	31 (37%)
26	SQD	a	411	-	53,54,54	0.96	3 (5%)	62,65,65	1.83	13 (20%)
23	CLA	c	508	41	69,73,73	2.02	18 (26%)	83,113,113	2.88	29 (34%)
29	PL9	d	405	-	55,55,55	0.70	1 (1%)	68,69,69	1.63	18 (26%)
32	LMT	e	102	-	36,36,36	1.02	4 (11%)	47,47,47	0.99	1 (2%)
23	CLA	B	605	2	69,73,73	2.03	19 (27%)	83,113,113	2.85	29 (34%)
37	LHG	D	409	-	48,48,48	0.87	2 (4%)	51,54,54	1.27	6 (11%)
25	BCR	b	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.34	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	A	404	1	69,73,73	2.00	20 (28%)	83,113,113	2.87	30 (36%)
27	GOL	c	743	-	5,5,5	1.16	0	5,5,5	0.89	0
23	CLA	B	608	2	69,73,73	1.91	21 (30%)	83,113,113	2.84	34 (40%)
35	DGD	C	517	-	63,63,67	0.83	2 (3%)	77,77,81	1.20	8 (10%)
23	CLA	A	406	41	69,73,73	2.04	19 (27%)	83,113,113	2.85	32 (38%)
34	HTG	d	411	-	16,16,19	0.99	1 (6%)	20,21,24	1.50	1 (5%)
40	HEC	v	202	16	50,50,50	1.79	7 (14%)	68,82,82	1.39	8 (11%)
23	CLA	b	615	2	69,73,73	1.98	20 (28%)	83,113,113	2.81	31 (37%)
27	GOL	b	624	-	5,5,5	1.14	1 (20%)	5,5,5	0.78	0
26	SQD	F	101	-	42,43,54	1.20	4 (9%)	51,54,65	2.06	10 (19%)
32	LMT	A	359	-	36,36,36	0.94	3 (8%)	47,47,47	1.01	1 (2%)
25	BCR	H	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.43	10 (17%)
32	LMT	t	102	-	26,26,36	0.91	2 (7%)	31,31,47	1.30	2 (6%)
33	LMG	d	412	39	51,51,55	0.89	2 (3%)	59,59,63	1.09	4 (6%)
23	CLA	c	513	3	69,73,73	2.08	19 (27%)	83,113,113	2.81	32 (38%)
33	LMG	c	520	-	51,51,55	0.90	2 (3%)	59,59,63	1.09	5 (8%)
29	PL9	A	414	-	55,55,55	0.69	2 (3%)	68,69,69	2.01	24 (35%)
23	CLA	B	607	41	69,73,73	1.97	19 (27%)	83,113,113	2.80	31 (37%)
23	CLA	C	504	3	69,73,73	2.00	19 (27%)	83,113,113	2.82	29 (34%)
37	LHG	D	410	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	3 (5%)
25	BCR	A	409	-	41,41,41	0.99	1 (2%)	56,56,56	1.41	11 (19%)
23	CLA	a	409	1	69,73,73	2.00	18 (26%)	83,113,113	2.93	31 (37%)
23	CLA	B	615	2	69,73,73	2.02	20 (28%)	83,113,113	2.83	30 (36%)
32	LMT	M	101	-	36,36,36	1.14	3 (8%)	47,47,47	1.19	4 (8%)
28	OEX	A	413	1,3,41	0,14,14	-	-	-	-	-
32	LMT	E	102	-	36,36,36	1.05	1 (2%)	47,47,47	1.03	3 (6%)
27	GOL	C	523	-	5,5,5	1.11	0	5,5,5	0.88	0
37	LHG	e	101	-	41,41,48	1.06	2 (4%)	44,47,54	0.92	2 (4%)
33	LMG	B	621	-	51,51,55	0.93	2 (3%)	59,59,63	1.26	4 (6%)
23	CLA	B	616	2	69,73,73	1.96	20 (28%)	83,113,113	2.86	27 (32%)
23	CLA	C	506	3	69,73,73	2.03	18 (26%)	83,113,113	2.81	31 (37%)
23	CLA	b	601	41	69,73,73	2.08	20 (28%)	83,113,113	2.84	29 (34%)
23	CLA	d	403	4	69,73,73	2.04	19 (27%)	83,113,113	2.85	29 (34%)
23	CLA	b	613	2	69,73,73	2.00	20 (28%)	83,113,113	2.82	30 (36%)
23	CLA	d	402	4	69,73,73	1.95	20 (28%)	83,113,113	2.76	32 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	a	410	-	41,41,41	1.03	1 (2%)	56,56,56	1.30	8 (14%)
25	BCR	t	103	-	41,41,41	1.00	1 (2%)	56,56,56	1.48	9 (16%)
35	DGD	h	102	-	63,63,67	0.85	3 (4%)	77,77,81	1.09	5 (6%)
23	CLA	a	405	1	69,73,73	1.99	20 (28%)	83,113,113	2.87	33 (39%)
40	HEC	V	202	16	50,50,50	1.77	7 (14%)	68,82,82	1.51	12 (17%)
32	LMT	b	621	-	25,25,36	0.96	2 (8%)	30,30,47	1.16	2 (6%)
27	GOL	b	901	-	5,5,5	0.43	0	5,5,5	1.48	1 (20%)
37	LHG	E	101	-	41,41,48	1.08	2 (4%)	44,47,54	1.10	3 (6%)
23	CLA	b	608	2	69,73,73	1.99	19 (27%)	83,113,113	2.81	32 (38%)
23	CLA	B	606	2	69,73,73	2.02	18 (26%)	83,113,113	3.00	32 (38%)
25	BCR	k	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.42	9 (16%)
27	GOL	A	411	-	5,5,5	1.05	0	5,5,5	0.72	0
37	LHG	d	711	-	48,48,48	0.89	2 (4%)	51,54,54	1.11	4 (7%)
38	HEM	E	103	6,5	50,50,50	1.54	8 (16%)	66,82,82	1.92	14 (21%)
23	CLA	c	504	3	69,73,73	2.06	19 (27%)	83,113,113	2.84	29 (34%)
25	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.73	13 (23%)
23	CLA	b	611	2	69,73,73	1.92	19 (27%)	83,113,113	2.99	29 (34%)
23	CLA	b	603	2	69,73,73	1.96	19 (27%)	83,113,113	2.89	32 (38%)
23	CLA	B	612	2	69,73,73	1.97	21 (30%)	83,113,113	2.79	30 (36%)
25	BCR	D	407	-	41,41,41	1.11	1 (2%)	56,56,56	1.79	15 (26%)
23	CLA	C	502	3	69,73,73	2.00	19 (27%)	83,113,113	2.87	31 (37%)
23	CLA	a	407	41	69,73,73	1.98	19 (27%)	83,113,113	2.83	30 (36%)
23	CLA	b	602	2	69,73,73	2.08	19 (27%)	83,113,113	2.97	35 (42%)
24	PHO	a	353	-	58,69,69	2.77	13 (22%)	56,99,99	2.94	17 (30%)
26	SQD	A	410	-	53,54,54	0.93	3 (5%)	62,65,65	1.88	10 (16%)
23	CLA	B	613	2	69,73,73	2.04	19 (27%)	83,113,113	2.74	28 (33%)
27	GOL	c	742	-	5,5,5	1.00	0	5,5,5	0.98	0
33	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.09	4 (8%)
23	CLA	c	510	3	69,73,73	2.07	19 (27%)	83,113,113	2.87	31 (37%)
25	BCR	B	617	-	41,41,41	1.07	1 (2%)	56,56,56	1.36	9 (16%)
35	DGD	c	519	-	63,63,67	0.87	3 (4%)	77,77,81	0.98	4 (5%)
25	BCR	C	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.39	5 (8%)
23	CLA	B	604	2	69,73,73	2.03	20 (28%)	83,113,113	2.67	31 (37%)
34	HTG	b	622	-	19,19,19	1.15	2 (10%)	23,24,24	1.91	7 (30%)
27	GOL	D	701	-	5,5,5	1.33	1 (20%)	5,5,5	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	603	2	69,73,73	2.00	20 (28%)	83,113,113	2.93	30 (36%)
27	GOL	O	601	-	5,5,5	0.95	0	5,5,5	1.14	1 (20%)
23	CLA	c	509	3	69,73,73	2.13	20 (28%)	83,113,113	2.75	29 (34%)
37	LHG	l	101	-	48,48,48	0.83	2 (4%)	51,54,54	1.04	4 (7%)
27	GOL	B	901	-	5,5,5	1.05	0	5,5,5	0.96	0
23	CLA	b	616	2	69,73,73	2.01	19 (27%)	83,113,113	2.94	29 (34%)
35	DGD	c	517	-	63,63,67	0.85	2 (3%)	77,77,81	1.10	7 (9%)
23	CLA	B	614	2	69,73,73	2.01	20 (28%)	83,113,113	3.03	32 (38%)
27	GOL	O	501	-	5,5,5	0.92	0	5,5,5	0.95	0
37	LHG	d	407	-	48,48,48	0.87	2 (4%)	51,54,54	1.04	4 (7%)
33	LMG	D	415	39	51,51,55	0.81	2 (3%)	59,59,63	1.05	3 (5%)
34	HTG	B	622	-	19,19,19	1.02	2 (10%)	23,24,24	1.70	6 (26%)
25	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.35	9 (16%)
25	BCR	c	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.38	10 (17%)
29	PL9	D	408	-	55,55,55	0.63	1 (1%)	68,69,69	1.61	17 (25%)
23	CLA	B	609	2	69,73,73	2.02	19 (27%)	83,113,113	2.81	29 (34%)
33	LMG	m	101	-	51,51,55	0.88	2 (3%)	59,59,63	1.24	5 (8%)
23	CLA	c	505	41	69,73,73	2.05	21 (30%)	83,113,113	2.82	32 (38%)
27	GOL	A	701	-	5,5,5	1.40	2 (40%)	5,5,5	1.04	1 (20%)
34	HTG	b	623	-	19,19,19	1.04	1 (5%)	23,24,24	1.80	2 (8%)
23	CLA	B	610	41	69,73,73	2.03	19 (27%)	83,113,113	2.92	32 (38%)
25	BCR	h	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.35	11 (19%)
27	GOL	a	801	-	5,5,5	1.13	0	5,5,5	0.98	0
23	CLA	b	614	2	69,73,73	1.99	20 (28%)	83,113,113	2.93	30 (36%)
26	SQD	A	412	-	53,54,54	1.02	3 (5%)	62,65,65	1.19	6 (9%)
25	BCR	y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.62	11 (19%)
35	DGD	C	518	-	63,63,67	0.90	3 (4%)	77,77,81	1.03	5 (6%)
23	CLA	c	502	3	69,73,73	2.00	21 (30%)	83,113,113	2.84	28 (33%)
23	CLA	C	513	3	69,73,73	2.03	19 (27%)	83,113,113	2.90	34 (40%)
25	BCR	b	618	-	41,41,41	1.01	1 (2%)	56,56,56	1.24	6 (10%)
32	LMT	a	414	-	36,36,36	1.01	3 (8%)	47,47,47	1.12	3 (6%)
32	LMT	M	103	-	36,36,36	1.06	3 (8%)	47,47,47	1.06	2 (4%)
26	SQD	b	620	-	53,54,54	1.05	3 (5%)	62,65,65	1.61	10 (16%)
23	CLA	C	503	3	69,73,73	2.02	20 (28%)	83,113,113	2.73	28 (33%)
32	LMT	b	627	-	25,25,36	0.90	0	30,30,47	1.10	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMG	a	419	-	51,51,55	0.92	2 (3%)	59,59,63	1.20	6 (10%)
38	HEM	e	87	6,5	50,50,50	1.49	6 (12%)	66,82,82	1.76	14 (21%)
32	LMT	t	101	-	25,25,36	0.89	2 (8%)	30,30,47	1.12	3 (10%)
24	PHO	A	407	-	58,69,69	2.66	12 (20%)	56,99,99	2.81	14 (25%)
23	CLA	b	609	2	69,73,73	2.00	19 (27%)	83,113,113	2.80	31 (37%)
23	CLA	b	605	2	69,73,73	1.97	20 (28%)	83,113,113	2.92	30 (36%)
34	HTG	B	626	-	19,19,19	1.03	2 (10%)	23,24,24	1.35	4 (17%)
37	LHG	L	101	-	48,48,48	0.88	2 (4%)	51,54,54	1.15	4 (7%)
23	CLA	B	602	2	69,73,73	2.02	20 (28%)	83,113,113	2.83	31 (37%)
23	CLA	c	514	3	69,73,73	2.11	21 (30%)	83,113,113	2.89	32 (38%)
23	CLA	C	505	41	69,73,73	1.98	20 (28%)	83,113,113	2.82	30 (36%)
34	HTG	c	522	-	19,19,19	0.93	2 (10%)	23,24,24	1.63	2 (8%)
23	CLA	c	511	3	69,73,73	1.97	20 (28%)	83,113,113	2.85	31 (37%)
33	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.09	4 (6%)
26	SQD	a	413	-	53,54,54	1.07	4 (7%)	62,65,65	1.17	7 (11%)
25	BCR	c	515	-	41,41,41	0.99	1 (2%)	56,56,56	1.60	11 (19%)
23	CLA	C	508	41	69,73,73	1.99	21 (30%)	83,113,113	2.86	31 (37%)
23	CLA	D	405	4	69,73,73	2.00	20 (28%)	83,113,113	2.86	32 (38%)
27	GOL	d	701	-	5,5,5	1.05	0	5,5,5	0.93	0
35	DGD	C	519	-	63,63,67	0.87	3 (4%)	77,77,81	1.00	3 (3%)
32	LMT	I	101	-	36,36,36	1.05	3 (8%)	47,47,47	1.15	4 (8%)
27	GOL	a	701	-	5,5,5	1.03	0	5,5,5	1.02	0
29	PL9	a	416	-	55,55,55	0.65	2 (3%)	68,69,69	2.01	22 (32%)
34	HTG	V	203	-	11,11,19	0.28	0	15,15,24	1.13	1 (6%)
34	HTG	D	414	-	16,16,19	1.04	2 (12%)	20,21,24	1.40	1 (5%)
23	CLA	B	601	41	69,73,73	2.07	19 (27%)	83,113,113	2.91	29 (34%)
31	BCT	a	404	21	2,3,3	0.59	0	2,3,3	1.49	0
25	BCR	B	618	-	41,41,41	0.96	1 (2%)	56,56,56	1.39	9 (16%)
23	CLA	c	503	3	69,73,73	2.02	18 (26%)	83,113,113	2.81	27 (32%)
24	PHO	a	408	-	58,69,69	2.74	13 (22%)	56,99,99	2.81	14 (25%)
23	CLA	C	507	3	69,73,73	2.02	20 (28%)	83,113,113	2.84	33 (39%)
32	LMT	a	420	-	36,36,36	1.02	1 (2%)	47,47,47	1.03	1 (2%)
25	BCR	K	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.45	12 (21%)
23	CLA	C	514	3	69,73,73	2.03	19 (27%)	83,113,113	2.88	31 (37%)
31	BCT	A	348	21	2,3,3	0.64	0	2,3,3	1.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	406	41	69,73,73	2.04	17 (24%)	83,113,113	2.86	32 (38%)
23	CLA	b	606	2	69,73,73	2.01	19 (27%)	83,113,113	2.87	30 (36%)
23	CLA	b	607	41	69,73,73	2.00	20 (28%)	83,113,113	2.87	31 (37%)
23	CLA	A	408	1	69,73,73	1.96	21 (30%)	83,113,113	2.96	35 (42%)
26	SQD	B	620	-	53,54,54	1.07	4 (7%)	62,65,65	1.78	10 (16%)
25	BCR	d	404	-	41,41,41	1.11	2 (4%)	56,56,56	1.88	15 (26%)
32	LMT	m	103	-	36,36,36	1.05	3 (8%)	47,47,47	1.10	2 (4%)
23	CLA	C	509	3	69,73,73	2.04	19 (27%)	83,113,113	2.76	29 (34%)
27	GOL	a	412	-	5,5,5	0.88	0	5,5,5	1.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
33	LMG	C	521	-	-	12/46/66/70	0/1/1/1
33	LMG	Z	101	-	-	9/31/51/70	0/1/1/1
23	CLA	c	507	3	-	8/39/115/115	-
23	CLA	c	506	3	-	8/39/115/115	-
24	PHO	A	353	-	-	1/37/103/103	0/5/6/6
23	CLA	b	604	2	-	12/39/115/115	-
34	HTG	C	522	-	-	0/10/30/30	0/1/1/1
23	CLA	b	610	41	-	7/39/115/115	-
32	LMT	D	404	-	-	12/21/61/61	0/2/2/2
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	c	512	3	-	5/39/115/115	-
33	LMG	C	501	-	-	14/46/66/70	0/1/1/1
23	CLA	B	611	2	-	2/39/115/115	-
35	DGD	H	102	-	-	11/51/91/95	0/2/2/2
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
33	LMG	c	521	-	-	11/46/66/70	0/1/1/1
35	DGD	c	518	-	-	16/51/91/95	0/2/2/2
34	HTG	B	623	-	-	2/10/30/30	0/1/1/1
27	GOL	V	401	-	-	2/4/4/4	-
37	LHG	D	411	-	-	14/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	405	41	-	3/39/115/115	-
23	CLA	b	612	2	-	5/39/115/115	-
27	GOL	B	624	-	-	4/4/4/4	-
23	CLA	C	512	3	-	5/39/115/115	-
26	SQD	f	102	-	-	9/38/58/69	0/1/1/1
27	GOL	o	601	-	-	4/4/4/4	-
23	CLA	C	510	3	-	6/39/115/115	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
37	LHG	d	408	-	-	13/53/53/53	-
27	GOL	d	801	-	-	1/4/4/4	-
27	GOL	o	501	-	-	2/4/4/4	-
23	CLA	C	511	3	-	13/39/115/115	-
27	GOL	v	401	-	-	2/4/4/4	-
23	CLA	D	406	4	-	13/39/115/115	-
26	SQD	a	411	-	-	9/49/69/69	0/1/1/1
23	CLA	c	508	41	-	7/39/115/115	-
29	PL9	d	405	-	-	7/53/73/73	0/1/1/1
32	LMT	e	102	-	-	15/21/61/61	0/2/2/2
23	CLA	B	605	2	-	6/39/115/115	-
37	LHG	D	409	-	-	14/53/53/53	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	A	404	1	-	3/39/115/115	-
27	GOL	c	743	-	-	3/4/4/4	-
23	CLA	B	608	2	-	4/39/115/115	-
35	DGD	C	517	-	-	14/51/91/95	0/2/2/2
23	CLA	A	406	41	-	5/39/115/115	-
34	HTG	d	411	-	-	1/7/27/30	0/1/1/1
40	HEC	v	202	16	1/1/3/7	5/14/54/54	-
23	CLA	b	615	2	-	7/39/115/115	-
27	GOL	b	624	-	-	2/4/4/4	-
26	SQD	F	101	-	-	15/38/58/69	0/1/1/1
32	LMT	A	359	-	-	7/21/61/61	0/2/2/2
25	BCR	H	101	-	-	3/29/63/63	0/2/2/2
32	LMT	t	102	-	-	9/17/38/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	d	412	39	-	10/46/66/70	0/1/1/1
23	CLA	c	513	3	-	14/39/115/115	-
33	LMG	c	520	-	-	11/46/66/70	0/1/1/1
29	PL9	A	414	-	-	15/53/73/73	0/1/1/1
23	CLA	B	607	41	-	3/39/115/115	-
23	CLA	C	504	3	-	2/39/115/115	-
37	LHG	D	410	-	-	17/53/53/53	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
23	CLA	a	409	1	-	10/39/115/115	-
23	CLA	B	615	2	-	6/39/115/115	-
32	LMT	M	101	-	-	5/21/61/61	0/2/2/2
32	LMT	E	102	-	-	8/21/61/61	0/2/2/2
27	GOL	C	523	-	-	0/4/4/4	-
37	LHG	e	101	-	-	16/46/46/53	-
33	LMG	B	621	-	-	20/46/66/70	0/1/1/1
23	CLA	B	616	2	-	6/39/115/115	-
23	CLA	C	506	3	-	6/39/115/115	-
23	CLA	b	601	41	-	17/39/115/115	-
23	CLA	d	403	4	-	8/39/115/115	-
23	CLA	b	613	2	-	6/39/115/115	-
23	CLA	d	402	4	-	4/39/115/115	-
25	BCR	a	410	-	-	1/29/63/63	0/2/2/2
25	BCR	t	103	-	-	0/29/63/63	0/2/2/2
35	DGD	h	102	-	-	13/51/91/95	0/2/2/2
23	CLA	a	405	1	-	4/39/115/115	-
40	HEC	V	202	16	1/1/3/7	6/14/54/54	-
32	LMT	b	621	-	-	8/17/37/61	0/1/1/2
27	GOL	b	901	-	-	0/4/4/4	-
37	LHG	E	101	-	-	22/46/46/53	-
23	CLA	b	608	2	-	6/39/115/115	-
23	CLA	B	606	2	-	10/39/115/115	-
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
27	GOL	A	411	-	-	2/4/4/4	-
37	LHG	d	711	-	-	17/53/53/53	-
38	HEM	E	103	6,5	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	504	3	-	1/39/115/115	-
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
23	CLA	b	611	2	-	2/39/115/115	-
23	CLA	b	603	2	-	7/39/115/115	-
23	CLA	B	612	2	-	5/39/115/115	-
25	BCR	D	407	-	-	4/29/63/63	0/2/2/2
23	CLA	C	502	3	-	4/39/115/115	-
23	CLA	a	407	41	-	8/39/115/115	-
23	CLA	b	602	2	-	4/39/115/115	-
24	PHO	a	353	-	-	1/37/103/103	0/5/6/6
26	SQD	A	410	-	-	12/49/69/69	0/1/1/1
23	CLA	B	613	2	-	9/39/115/115	-
27	GOL	c	742	-	-	0/4/4/4	-
33	LMG	z	101	-	-	9/34/54/70	0/1/1/1
23	CLA	c	510	3	-	13/39/115/115	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
35	DGD	c	519	-	-	11/51/91/95	0/2/2/2
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
23	CLA	B	604	2	-	2/39/115/115	-
34	HTG	b	622	-	-	6/10/30/30	0/1/1/1
27	GOL	D	701	-	-	4/4/4/4	-
23	CLA	B	603	2	-	7/39/115/115	-
27	GOL	O	601	-	-	2/4/4/4	-
23	CLA	c	509	3	-	6/39/115/115	-
37	LHG	l	101	-	-	14/53/53/53	-
27	GOL	B	901	-	-	2/4/4/4	-
23	CLA	b	616	2	-	9/39/115/115	-
35	DGD	c	517	-	-	18/51/91/95	0/2/2/2
23	CLA	B	614	2	-	13/39/115/115	-
27	GOL	O	501	-	-	2/4/4/4	-
37	LHG	d	407	-	-	13/53/53/53	-
33	LMG	D	415	39	-	9/46/66/70	0/1/1/1
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	BCR	c	516	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PL9	D	408	-	-	6/53/73/73	0/1/1/1
23	CLA	B	609	2	-	2/39/115/115	-
33	LMG	m	101	-	-	12/46/66/70	0/1/1/1
23	CLA	c	505	41	-	5/39/115/115	-
27	GOL	A	701	-	-	1/4/4/4	-
34	HTG	b	623	-	-	4/10/30/30	0/1/1/1
23	CLA	B	610	41	-	8/39/115/115	-
25	BCR	h	101	-	-	2/29/63/63	0/2/2/2
27	GOL	a	801	-	-	1/4/4/4	-
23	CLA	b	614	2	-	15/39/115/115	-
26	SQD	A	412	-	-	14/49/69/69	0/1/1/1
25	BCR	y	101	-	-	4/29/63/63	0/2/2/2
35	DGD	C	518	-	-	13/51/91/95	0/2/2/2
23	CLA	c	502	3	-	4/39/115/115	-
23	CLA	C	513	3	-	10/39/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
32	LMT	a	414	-	-	10/21/61/61	0/2/2/2
32	LMT	M	103	-	-	7/21/61/61	0/2/2/2
26	SQD	b	620	-	-	16/49/69/69	0/1/1/1
23	CLA	C	503	3	-	12/39/115/115	-
32	LMT	b	627	-	-	11/17/37/61	0/1/1/2
33	LMG	a	419	-	-	13/46/66/70	0/1/1/1
38	HEM	e	87	6,5	-	5/14/54/54	-
32	LMT	t	101	-	-	11/17/37/61	0/1/1/2
24	PHO	A	407	-	-	3/37/103/103	0/5/6/6
23	CLA	b	609	2	-	3/39/115/115	-
23	CLA	b	605	2	-	6/39/115/115	-
34	HTG	B	626	-	-	5/10/30/30	0/1/1/1
37	LHG	L	101	-	-	20/53/53/53	-
23	CLA	B	602	2	-	10/39/115/115	-
23	CLA	c	514	3	-	10/39/115/115	-
23	CLA	C	505	41	-	8/39/115/115	-
34	HTG	c	522	-	-	1/10/30/30	0/1/1/1
23	CLA	c	511	3	-	10/39/115/115	-
33	LMG	C	520	-	-	9/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	a	413	-	-	12/49/69/69	0/1/1/1
25	BCR	c	515	-	-	2/29/63/63	0/2/2/2
23	CLA	C	508	41	-	11/39/115/115	-
23	CLA	D	405	4	-	2/39/115/115	-
27	GOL	d	701	-	-	2/4/4/4	-
35	DGD	C	519	-	-	16/51/91/95	0/2/2/2
32	LMT	I	101	-	-	16/21/61/61	0/2/2/2
27	GOL	a	701	-	-	2/4/4/4	-
29	PL9	a	416	-	-	14/53/73/73	0/1/1/1
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
34	HTG	D	414	-	-	3/7/27/30	0/1/1/1
23	CLA	B	601	41	-	13/39/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	c	503	3	-	8/39/115/115	-
24	PHO	a	408	-	-	6/37/103/103	0/5/6/6
23	CLA	C	507	3	-	14/39/115/115	-
32	LMT	a	420	-	-	11/21/61/61	0/2/2/2
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
23	CLA	C	514	3	-	7/39/115/115	-
23	CLA	a	406	41	-	8/39/115/115	-
23	CLA	b	606	2	-	14/39/115/115	-
23	CLA	b	607	41	-	2/39/115/115	-
23	CLA	A	408	1	-	9/39/115/115	-
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
25	BCR	d	404	-	-	6/29/63/63	0/2/2/2
32	LMT	m	103	-	-	7/21/61/61	0/2/2/2
23	CLA	C	509	3	-	4/39/115/115	-
27	GOL	a	412	-	-	4/4/4/4	-

All (1626) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408	PHO	C1B-C2B	9.21	1.49	1.39
24	A	407	PHO	C1D-C2D	8.89	1.49	1.39
24	a	353	PHO	C1B-C2B	8.69	1.49	1.39
24	A	353	PHO	C1B-C2B	8.65	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	353	PHO	C1D-C2D	8.62	1.49	1.39
24	A	353	PHO	C1D-C2D	8.53	1.49	1.39
24	A	407	PHO	C1B-C2B	8.45	1.48	1.39
24	a	408	PHO	C1D-C2D	8.40	1.48	1.39
40	v	202	HEC	C3D-C2D	8.07	1.53	1.36
40	V	202	HEC	C3D-C2D	7.54	1.52	1.36
24	a	353	PHO	C3B-C4B	7.31	1.49	1.41
24	A	353	PHO	C3B-C4B	7.11	1.49	1.41
23	B	611	CLA	CMB-C2B	6.71	1.65	1.50
24	a	408	PHO	C3B-C4B	6.66	1.49	1.41
23	B	611	CLA	C1D-ND	6.63	1.45	1.37
24	a	408	PHO	C4D-CHA	6.54	1.50	1.39
23	B	611	CLA	C1B-C2B	6.42	1.58	1.43
24	a	408	PHO	C3B-C2B	6.39	1.49	1.40
24	A	353	PHO	C4D-CHA	6.27	1.49	1.39
24	A	407	PHO	C3B-C4B	6.16	1.48	1.41
24	A	407	PHO	C4D-CHA	6.13	1.49	1.39
24	A	407	PHO	C3B-C2B	6.13	1.48	1.40
24	a	353	PHO	C4D-CHA	6.05	1.49	1.39
24	A	353	PHO	C3B-C2B	5.94	1.48	1.40
24	a	353	PHO	C3B-C2B	5.88	1.48	1.40
24	a	353	PHO	C3C-C2C	5.86	1.49	1.36
23	c	509	CLA	C1D-ND	5.82	1.44	1.37
24	A	353	PHO	C3C-C2C	5.72	1.48	1.36
24	A	407	PHO	C3C-C2C	5.71	1.48	1.36
23	C	511	CLA	C1D-ND	5.65	1.44	1.37
23	B	610	CLA	C3C-C2C	5.63	1.48	1.36
23	B	611	CLA	C3C-C2C	5.63	1.48	1.36
23	a	406	CLA	C3C-C2C	5.58	1.48	1.36
23	D	406	CLA	C3C-C2C	5.57	1.48	1.36
23	c	514	CLA	C1D-ND	5.56	1.44	1.37
23	c	513	CLA	C3C-C2C	5.51	1.48	1.36
23	C	510	CLA	C3C-C2C	5.51	1.48	1.36
23	c	509	CLA	C3C-C2C	5.50	1.48	1.36
23	c	510	CLA	C3C-C2C	5.49	1.48	1.36
23	D	406	CLA	C1D-ND	5.48	1.44	1.37
23	c	503	CLA	C1D-ND	5.48	1.44	1.37
23	d	403	CLA	C3C-C2C	5.47	1.48	1.36
24	a	353	PHO	C3D-C2D	5.46	1.49	1.39
24	a	408	PHO	C3D-C2D	5.46	1.49	1.39
23	c	504	CLA	C3C-C2C	5.45	1.48	1.36
23	B	611	CLA	CHC-C1C	5.45	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	C3C-C2C	5.45	1.48	1.36
23	c	503	CLA	C3C-C2C	5.44	1.48	1.36
23	C	504	CLA	C3C-C2C	5.44	1.48	1.36
23	A	404	CLA	C3C-C2C	5.43	1.48	1.36
23	a	406	CLA	C1D-ND	5.42	1.44	1.37
23	c	512	CLA	C1D-ND	5.41	1.44	1.37
23	B	605	CLA	C3C-C2C	5.40	1.48	1.36
23	b	601	CLA	C1D-ND	5.39	1.44	1.37
23	C	513	CLA	C3C-C2C	5.36	1.48	1.36
23	b	612	CLA	C3C-C2C	5.36	1.48	1.36
24	a	408	PHO	C3C-C2C	5.36	1.48	1.36
23	c	505	CLA	O2D-CGD	5.36	1.46	1.33
23	B	603	CLA	C3C-C2C	5.35	1.48	1.36
23	C	508	CLA	C3C-C2C	5.35	1.48	1.36
23	b	606	CLA	C3C-C2C	5.34	1.48	1.36
24	A	353	PHO	C3D-C2D	5.33	1.49	1.39
23	b	601	CLA	C3C-C2C	5.33	1.48	1.36
23	d	403	CLA	C1D-ND	5.33	1.44	1.37
23	B	601	CLA	C3C-C2C	5.32	1.48	1.36
23	b	614	CLA	C3C-C2C	5.31	1.48	1.36
23	b	604	CLA	C1D-ND	5.31	1.44	1.37
23	C	502	CLA	C3C-C2C	5.31	1.48	1.36
23	a	407	CLA	C3C-C2C	5.31	1.48	1.36
23	D	405	CLA	C3C-C2C	5.30	1.48	1.36
24	a	353	PHO	OBD-CAD	5.30	1.29	1.22
23	C	509	CLA	C3C-C2C	5.30	1.48	1.36
23	a	409	CLA	C3C-C2C	5.29	1.48	1.36
24	A	353	PHO	OBD-CAD	5.28	1.29	1.22
23	c	514	CLA	C3C-C2C	5.28	1.48	1.36
23	b	611	CLA	C3C-C2C	5.28	1.47	1.36
23	C	511	CLA	C3C-C2C	5.27	1.47	1.36
23	C	503	CLA	C1D-ND	5.27	1.44	1.37
23	B	614	CLA	C3C-C2C	5.27	1.47	1.36
23	c	510	CLA	O2D-CGD	5.26	1.46	1.33
23	c	506	CLA	C3C-C2C	5.26	1.47	1.36
23	B	601	CLA	C1D-ND	5.26	1.44	1.37
23	b	615	CLA	C3C-C2C	5.25	1.47	1.36
23	B	604	CLA	C3C-C2C	5.25	1.47	1.36
23	b	616	CLA	C3C-C2C	5.25	1.47	1.36
23	C	512	CLA	O2D-CGD	5.24	1.46	1.33
23	c	504	CLA	C1D-ND	5.24	1.44	1.37
23	B	606	CLA	C3C-C2C	5.24	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408	PHO	O2D-CGD	5.24	1.46	1.33
23	c	509	CLA	O2D-CGD	5.23	1.46	1.33
23	B	605	CLA	O2D-CGD	5.22	1.45	1.33
23	b	609	CLA	O2D-CGD	5.22	1.45	1.33
23	C	507	CLA	O2D-CGD	5.20	1.45	1.33
23	B	612	CLA	C3C-C2C	5.20	1.47	1.36
23	c	510	CLA	C1D-ND	5.18	1.44	1.37
23	b	602	CLA	C3C-C2C	5.16	1.47	1.36
23	c	505	CLA	C1D-ND	5.16	1.44	1.37
23	b	610	CLA	C3C-C2C	5.15	1.47	1.36
23	c	502	CLA	C1D-ND	5.14	1.44	1.37
38	e	87	HEM	FE-NB	5.14	2.10	1.94
23	b	607	CLA	C3C-C2C	5.14	1.47	1.36
23	A	405	CLA	O2D-CGD	5.14	1.45	1.33
23	a	409	CLA	CHC-C1C	5.13	1.48	1.38
23	B	602	CLA	C1D-ND	5.13	1.44	1.37
23	A	406	CLA	C3C-C2C	5.13	1.47	1.36
23	B	609	CLA	C3C-C2C	5.13	1.47	1.36
23	a	405	CLA	C1D-ND	5.13	1.44	1.37
23	A	404	CLA	C1D-ND	5.13	1.44	1.37
23	b	606	CLA	C1D-ND	5.12	1.44	1.37
23	c	512	CLA	C3C-C2C	5.11	1.47	1.36
23	B	606	CLA	CHC-C1C	5.11	1.48	1.38
23	C	514	CLA	C3C-C2C	5.11	1.47	1.36
23	c	513	CLA	C1D-ND	5.11	1.44	1.37
23	A	408	CLA	C3C-C2C	5.11	1.47	1.36
23	b	602	CLA	O2D-CGD	5.11	1.45	1.33
23	B	606	CLA	C1D-ND	5.09	1.44	1.37
23	C	513	CLA	CHC-C1C	5.09	1.48	1.38
23	d	402	CLA	C3C-C2C	5.09	1.47	1.36
23	B	613	CLA	C3C-C2C	5.09	1.47	1.36
23	c	509	CLA	CHC-C1C	5.08	1.48	1.38
23	B	604	CLA	CHC-C1C	5.08	1.48	1.38
23	c	511	CLA	C3C-C2C	5.08	1.47	1.36
23	B	615	CLA	C3C-C2C	5.08	1.47	1.36
23	C	503	CLA	C3C-C2C	5.07	1.47	1.36
23	B	605	CLA	C1D-ND	5.06	1.44	1.37
23	c	514	CLA	O2D-CGD	5.06	1.45	1.33
23	b	603	CLA	O2D-CGD	5.05	1.45	1.33
23	B	613	CLA	O2D-CGD	5.05	1.45	1.33
23	C	503	CLA	O2D-CGD	5.04	1.45	1.33
23	C	506	CLA	C3C-C2C	5.04	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	502	CLA	C3C-C2C	5.04	1.47	1.36
23	c	507	CLA	O2D-CGD	5.04	1.45	1.33
23	b	613	CLA	O2D-CGD	5.03	1.45	1.33
25	d	404	BCR	C23-C22	-5.03	1.35	1.45
23	C	508	CLA	CHC-C1C	5.03	1.48	1.38
23	b	603	CLA	C3C-C2C	5.03	1.47	1.36
23	c	507	CLA	C3C-C2C	5.02	1.47	1.36
23	a	405	CLA	C3C-C2C	5.02	1.47	1.36
25	C	515	BCR	C23-C22	-5.02	1.35	1.45
23	c	508	CLA	C1D-ND	5.02	1.44	1.37
23	c	505	CLA	C3C-C2C	5.02	1.47	1.36
23	d	403	CLA	CHC-C1C	5.01	1.48	1.38
23	B	601	CLA	O2D-CGD	5.01	1.45	1.33
23	b	605	CLA	C1D-ND	5.01	1.43	1.37
23	B	607	CLA	C3C-C2C	5.01	1.47	1.36
25	k	101	BCR	C23-C22	-5.00	1.35	1.45
23	C	514	CLA	C1D-ND	5.00	1.43	1.37
23	C	506	CLA	C1D-ND	5.00	1.43	1.37
23	C	509	CLA	C1D-ND	4.99	1.43	1.37
23	B	616	CLA	C3C-C2C	4.99	1.47	1.36
23	B	602	CLA	C3C-C2C	4.98	1.47	1.36
23	c	503	CLA	O2D-CGD	4.98	1.45	1.33
23	c	507	CLA	C1D-ND	4.97	1.43	1.37
23	b	613	CLA	C3C-C2C	4.97	1.47	1.36
23	C	509	CLA	O2D-CGD	4.97	1.45	1.33
23	b	613	CLA	C1D-ND	4.97	1.43	1.37
23	A	405	CLA	C3C-C2C	4.96	1.47	1.36
23	a	406	CLA	O2D-CGD	4.95	1.45	1.33
24	A	353	PHO	O2D-CGD	4.95	1.45	1.33
23	C	514	CLA	O2D-CGD	4.95	1.45	1.33
23	b	609	CLA	C3C-C2C	4.95	1.47	1.36
23	C	505	CLA	C3C-C2C	4.95	1.47	1.36
23	A	406	CLA	CHC-C1C	4.95	1.48	1.38
23	C	502	CLA	C1D-ND	4.94	1.43	1.37
23	b	613	CLA	CHC-C1C	4.94	1.48	1.38
23	B	601	CLA	O2A-CGA	4.94	1.47	1.33
23	c	513	CLA	O2D-CGD	4.94	1.45	1.33
23	b	610	CLA	O2D-CGD	4.93	1.45	1.33
23	c	506	CLA	CHC-C1C	4.93	1.48	1.38
23	B	613	CLA	CHC-C1C	4.93	1.48	1.38
23	B	609	CLA	O2D-CGD	4.93	1.45	1.33
23	C	506	CLA	CHC-C1C	4.92	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	O2D-CGD	4.92	1.45	1.33
25	D	407	BCR	C23-C22	-4.91	1.35	1.45
23	b	616	CLA	O2D-CGD	4.91	1.45	1.33
23	b	616	CLA	CHC-C1C	4.91	1.48	1.38
23	c	508	CLA	O2D-CGD	4.91	1.45	1.33
24	A	407	PHO	O2D-CGD	4.91	1.45	1.33
23	b	616	CLA	C1D-ND	4.90	1.43	1.37
23	B	601	CLA	CHC-C1C	4.89	1.48	1.38
23	C	505	CLA	O2D-CGD	4.88	1.45	1.33
23	D	405	CLA	O2D-CGD	4.88	1.45	1.33
23	b	602	CLA	CHC-C1C	4.88	1.48	1.38
23	B	615	CLA	C1D-ND	4.88	1.43	1.37
23	c	511	CLA	O2D-CGD	4.87	1.45	1.33
23	D	406	CLA	O2D-CGD	4.87	1.45	1.33
23	c	513	CLA	CHC-C1C	4.86	1.48	1.38
23	C	507	CLA	C3C-C2C	4.86	1.47	1.36
23	b	602	CLA	C1D-ND	4.86	1.43	1.37
23	c	508	CLA	C3C-C2C	4.86	1.47	1.36
23	C	506	CLA	O2D-CGD	4.86	1.45	1.33
23	B	606	CLA	O2D-CGD	4.85	1.45	1.33
23	B	615	CLA	O2D-CGD	4.85	1.45	1.33
23	B	603	CLA	O2D-CGD	4.85	1.45	1.33
24	a	353	PHO	O2D-CGD	4.84	1.45	1.33
23	B	611	CLA	O2D-CGD	4.84	1.45	1.33
23	B	616	CLA	O2D-CGD	4.83	1.45	1.33
25	C	516	BCR	C23-C22	-4.83	1.35	1.45
23	c	504	CLA	CHC-C1C	4.82	1.48	1.38
23	B	608	CLA	C3C-C2C	4.82	1.47	1.36
23	C	502	CLA	CHC-C1C	4.82	1.48	1.38
23	b	615	CLA	CHC-C1C	4.82	1.48	1.38
25	K	102	BCR	C23-C22	-4.81	1.35	1.45
23	b	601	CLA	O2D-CGD	4.81	1.44	1.33
23	B	610	CLA	O2D-CGD	4.80	1.44	1.33
23	B	603	CLA	C1D-ND	4.80	1.43	1.37
23	C	511	CLA	O2D-CGD	4.80	1.44	1.33
40	V	202	HEC	FE-ND	4.80	2.09	1.94
25	c	516	BCR	C23-C22	-4.80	1.35	1.45
23	b	614	CLA	CHC-C1C	4.79	1.48	1.38
23	b	608	CLA	C3C-C2C	4.79	1.46	1.36
23	B	614	CLA	C1D-ND	4.79	1.43	1.37
24	A	407	PHO	C3D-C2D	4.79	1.48	1.39
23	b	603	CLA	CHC-C1C	4.79	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	O2D-CGD	4.79	1.44	1.33
23	b	601	CLA	O2A-CGA	4.78	1.47	1.33
25	B	619	BCR	C23-C22	-4.78	1.35	1.45
23	A	404	CLA	O2D-CGD	4.77	1.44	1.33
23	B	609	CLA	CHC-C1C	4.77	1.48	1.38
23	B	604	CLA	O2D-CGD	4.76	1.44	1.33
23	b	615	CLA	O2D-CGD	4.75	1.44	1.33
25	y	101	BCR	C23-C22	-4.75	1.35	1.45
25	b	619	BCR	C23-C22	-4.74	1.35	1.45
23	C	512	CLA	C3C-C2C	4.74	1.46	1.36
23	B	602	CLA	O2D-CGD	4.74	1.44	1.33
23	B	612	CLA	CHC-C1C	4.73	1.48	1.38
23	A	406	CLA	O2D-CGD	4.73	1.44	1.33
23	c	514	CLA	CHC-C1C	4.72	1.48	1.38
25	T	101	BCR	C23-C22	-4.72	1.35	1.45
23	C	510	CLA	O2D-CGD	4.72	1.44	1.33
26	F	101	SQD	O47-C7	4.71	1.47	1.34
23	b	604	CLA	C3C-C2C	4.71	1.46	1.36
23	b	610	CLA	CHC-C1C	4.70	1.48	1.38
23	c	513	CLA	CHD-C1D	4.70	1.47	1.38
23	B	610	CLA	C1D-ND	4.70	1.43	1.37
38	E	103	HEM	FE-NB	4.69	2.09	1.94
23	C	510	CLA	C1D-ND	4.69	1.43	1.37
23	C	512	CLA	C1D-ND	4.69	1.43	1.37
23	b	614	CLA	O2D-CGD	4.69	1.44	1.33
23	a	409	CLA	O2D-CGD	4.68	1.44	1.33
23	b	608	CLA	O2D-CGD	4.67	1.44	1.33
23	b	602	CLA	CHD-C1D	4.67	1.47	1.38
25	b	617	BCR	C23-C22	-4.67	1.35	1.45
23	c	511	CLA	C1D-ND	4.67	1.43	1.37
23	A	408	CLA	O2D-CGD	4.66	1.44	1.33
23	b	606	CLA	CHC-C1C	4.66	1.48	1.38
23	b	605	CLA	O2D-CGD	4.66	1.44	1.33
33	c	521	LMG	O7-C10	4.65	1.47	1.34
23	a	407	CLA	O2D-CGD	4.65	1.44	1.33
23	a	405	CLA	CHC-C1C	4.64	1.47	1.38
23	C	514	CLA	CHC-C1C	4.64	1.47	1.38
23	b	609	CLA	CHC-C1C	4.64	1.47	1.38
25	B	617	BCR	C23-C22	-4.64	1.36	1.45
23	C	513	CLA	C1D-ND	4.63	1.43	1.37
23	C	508	CLA	C1D-ND	4.63	1.43	1.37
23	b	604	CLA	CHC-C1C	4.63	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	CHC-C1C	4.62	1.47	1.38
23	b	601	CLA	CHC-C1C	4.62	1.47	1.38
23	B	608	CLA	O2D-CGD	4.62	1.44	1.33
23	A	405	CLA	CHC-C1C	4.61	1.47	1.38
23	a	407	CLA	CHC-C1C	4.61	1.47	1.38
23	c	512	CLA	CHC-C1C	4.61	1.47	1.38
23	C	505	CLA	CHC-C1C	4.60	1.47	1.38
23	B	609	CLA	C1D-ND	4.59	1.43	1.37
23	c	502	CLA	CHC-C1C	4.59	1.47	1.38
23	c	504	CLA	O2D-CGD	4.59	1.44	1.33
33	C	521	LMG	O8-C28	4.59	1.46	1.33
26	a	413	SQD	O48-C23	4.59	1.46	1.33
23	d	402	CLA	O2D-CGD	4.59	1.44	1.33
23	b	614	CLA	C1D-ND	4.59	1.43	1.37
23	C	504	CLA	CHC-C1C	4.58	1.47	1.38
23	C	507	CLA	C1D-ND	4.58	1.43	1.37
23	b	607	CLA	O2D-CGD	4.57	1.44	1.33
26	f	102	SQD	O47-C7	4.57	1.47	1.34
33	C	521	LMG	O7-C10	4.57	1.47	1.34
23	B	607	CLA	CHC-C1C	4.57	1.47	1.38
37	E	101	LHG	O8-C23	4.57	1.46	1.33
23	B	614	CLA	C4B-NB	-4.57	1.32	1.37
23	B	605	CLA	CHC-C1C	4.57	1.47	1.38
23	c	504	CLA	CHD-C1D	4.56	1.47	1.38
23	b	611	CLA	CHC-C1C	4.56	1.47	1.38
23	c	506	CLA	O2D-CGD	4.55	1.44	1.33
25	t	103	BCR	C23-C22	-4.55	1.36	1.45
25	c	515	BCR	C23-C22	-4.55	1.36	1.45
23	A	405	CLA	C1D-ND	4.55	1.43	1.37
23	B	613	CLA	C1D-ND	4.54	1.43	1.37
23	D	405	CLA	CHC-C1C	4.54	1.47	1.38
23	C	504	CLA	C1D-ND	4.54	1.43	1.37
23	B	604	CLA	C1D-ND	4.53	1.43	1.37
25	A	409	BCR	C23-C22	-4.53	1.36	1.45
23	D	406	CLA	CHC-C1C	4.53	1.47	1.38
23	c	514	CLA	CHD-C1D	4.53	1.47	1.38
23	b	611	CLA	C1D-ND	4.53	1.43	1.37
23	B	616	CLA	CHC-C1C	4.52	1.47	1.38
23	b	606	CLA	O2D-CGD	4.51	1.44	1.33
23	C	510	CLA	CHD-C1D	4.50	1.47	1.38
37	e	101	LHG	O8-C23	4.50	1.46	1.33
23	B	604	CLA	CHD-C1D	4.49	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	CHC-C1C	4.49	1.47	1.38
23	B	602	CLA	CHC-C1C	4.49	1.47	1.38
23	B	610	CLA	CHC-C1C	4.49	1.47	1.38
23	c	506	CLA	C1D-ND	4.48	1.43	1.37
26	A	412	SQD	O48-C23	4.48	1.46	1.33
23	a	407	CLA	C1D-ND	4.48	1.43	1.37
23	A	404	CLA	CHC-C1C	4.48	1.47	1.38
23	C	505	CLA	C1D-ND	4.48	1.43	1.37
23	c	505	CLA	CHC-C1C	4.47	1.47	1.38
33	C	520	LMG	O8-C28	4.47	1.46	1.33
26	B	620	SQD	O47-C7	4.47	1.46	1.34
23	C	507	CLA	CHD-C1D	4.47	1.47	1.38
23	c	510	CLA	C1B-NB	-4.46	1.32	1.37
23	B	614	CLA	O2D-CGD	4.46	1.44	1.33
23	b	609	CLA	C1D-ND	4.46	1.43	1.37
23	b	615	CLA	C1D-ND	4.46	1.43	1.37
25	h	101	BCR	C23-C22	-4.46	1.36	1.45
23	C	502	CLA	CHD-C1D	4.46	1.47	1.38
23	B	615	CLA	CHC-C1C	4.46	1.47	1.38
23	C	504	CLA	O2D-CGD	4.45	1.44	1.33
23	B	611	CLA	CHC-C4B	4.45	1.49	1.39
23	c	508	CLA	CHC-C1C	4.45	1.47	1.38
23	D	406	CLA	CHD-C1D	4.44	1.47	1.38
23	C	511	CLA	CHC-C1C	4.44	1.47	1.38
23	B	603	CLA	CHC-C1C	4.44	1.47	1.38
23	a	406	CLA	CHC-C1C	4.44	1.47	1.38
23	b	607	CLA	CHC-C1C	4.44	1.47	1.38
23	B	611	CLA	C4B-NB	-4.43	1.32	1.37
23	c	514	CLA	O2A-CGA	4.42	1.46	1.33
25	b	618	BCR	C23-C22	-4.42	1.36	1.45
23	b	604	CLA	O2D-CGD	4.41	1.44	1.33
23	B	612	CLA	CHB-C1B	4.41	1.49	1.39
23	b	610	CLA	C1D-ND	4.41	1.43	1.37
23	c	509	CLA	O2A-CGA	4.40	1.46	1.33
23	b	612	CLA	O2D-CGD	4.40	1.43	1.33
25	H	101	BCR	C23-C22	-4.40	1.36	1.45
23	c	511	CLA	CHC-C1C	4.40	1.47	1.38
33	z	101	LMG	O8-C28	4.40	1.46	1.33
23	d	403	CLA	O2A-CGA	4.39	1.46	1.33
23	a	405	CLA	O2D-CGD	4.38	1.43	1.33
33	B	621	LMG	O8-C28	4.37	1.46	1.33
23	c	503	CLA	CHC-C1C	4.37	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	409	CLA	O2A-CGA	4.37	1.46	1.33
23	C	508	CLA	O2D-CGD	4.37	1.43	1.33
23	C	510	CLA	CHC-C1C	4.37	1.47	1.38
23	b	604	CLA	CHD-C1D	4.35	1.46	1.38
23	B	609	CLA	CHD-C1D	4.35	1.46	1.38
23	C	512	CLA	CHC-C1C	4.35	1.47	1.38
23	c	513	CLA	O2A-CGA	4.34	1.46	1.33
23	b	611	CLA	O2D-CGD	4.34	1.43	1.33
25	Y	101	BCR	C23-C22	-4.34	1.36	1.45
26	b	620	SQD	O47-C7	4.34	1.46	1.34
23	b	612	CLA	CHC-C1C	4.34	1.47	1.38
23	c	512	CLA	CHD-C1D	4.33	1.46	1.38
23	A	406	CLA	C1B-NB	-4.33	1.32	1.37
40	v	202	HEC	FE-NB	4.33	2.08	1.94
23	B	615	CLA	CHD-C1D	4.33	1.46	1.38
23	A	408	CLA	C1D-ND	4.33	1.43	1.37
23	d	403	CLA	CHD-C1D	4.31	1.46	1.38
26	B	620	SQD	O48-C23	4.31	1.45	1.33
23	c	509	CLA	C3D-C2D	4.31	1.50	1.39
23	c	510	CLA	CHD-C1D	4.31	1.46	1.38
23	a	406	CLA	C3D-C2D	4.30	1.50	1.39
23	C	506	CLA	CHD-C1D	4.30	1.46	1.38
26	b	620	SQD	O48-C23	4.30	1.45	1.33
23	b	606	CLA	CHD-C1D	4.30	1.46	1.38
23	c	507	CLA	CHD-C1D	4.30	1.46	1.38
23	b	608	CLA	C1D-ND	4.29	1.43	1.37
23	c	507	CLA	O2A-CGA	4.29	1.45	1.33
23	B	608	CLA	C1D-ND	4.29	1.43	1.37
37	e	101	LHG	O7-C7	4.28	1.46	1.34
23	c	510	CLA	CHC-C1C	4.28	1.47	1.38
23	b	602	CLA	CHD-C4C	4.27	1.49	1.39
23	b	601	CLA	CHD-C1D	4.26	1.46	1.38
23	C	502	CLA	O2D-CGD	4.26	1.43	1.33
23	A	408	CLA	O2A-CGA	4.26	1.45	1.33
23	b	605	CLA	CHC-C1C	4.26	1.47	1.38
23	B	616	CLA	C1D-ND	4.26	1.43	1.37
33	m	101	LMG	O8-C28	4.26	1.45	1.33
23	C	509	CLA	CHD-C1D	4.25	1.46	1.38
23	D	405	CLA	C1D-ND	4.25	1.43	1.37
38	E	103	HEM	FE-NC	4.25	2.09	1.95
23	C	514	CLA	O2A-CGA	4.24	1.45	1.33
23	a	409	CLA	C1D-ND	4.24	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	521	LMG	O8-C28	4.24	1.45	1.33
23	B	602	CLA	CHD-C1D	4.24	1.46	1.38
23	C	509	CLA	O2A-CGA	4.23	1.45	1.33
23	A	408	CLA	CHD-C1D	4.23	1.46	1.38
35	C	519	DGD	O1G-C1A	4.23	1.45	1.33
23	c	512	CLA	O2A-CGA	4.23	1.45	1.33
35	c	519	DGD	O1G-C1A	4.22	1.45	1.33
23	b	610	CLA	CHD-C1D	4.22	1.46	1.38
37	E	101	LHG	O7-C7	4.22	1.46	1.34
23	B	607	CLA	O2D-CGD	4.21	1.43	1.33
23	c	509	CLA	CHD-C1D	4.21	1.46	1.38
25	a	410	BCR	C23-C22	-4.21	1.36	1.45
23	B	605	CLA	CHB-C1B	4.21	1.48	1.39
23	d	402	CLA	CHC-C1C	4.21	1.47	1.38
23	C	512	CLA	O2A-CGA	4.21	1.45	1.33
23	b	607	CLA	C1D-ND	4.20	1.43	1.37
23	c	504	CLA	CHD-C4C	4.20	1.48	1.39
23	C	513	CLA	CHD-C1D	4.20	1.46	1.38
23	C	509	CLA	C3D-C2D	4.20	1.50	1.39
23	B	606	CLA	O2A-CGA	4.20	1.45	1.33
37	d	408	LHG	O8-C23	4.19	1.45	1.33
23	c	502	CLA	CHD-C1D	4.19	1.46	1.38
23	B	614	CLA	CHC-C1C	4.19	1.47	1.38
23	C	508	CLA	O2A-CGA	4.19	1.45	1.33
23	c	514	CLA	CHD-C4C	4.19	1.48	1.39
23	D	405	CLA	CHD-C1D	4.19	1.46	1.38
23	B	613	CLA	CHD-C1D	4.19	1.46	1.38
23	B	613	CLA	CHB-C1B	4.18	1.48	1.39
26	f	102	SQD	O48-C23	4.18	1.45	1.33
23	b	612	CLA	C1D-ND	4.18	1.42	1.37
23	D	405	CLA	O2A-CGA	4.18	1.45	1.33
23	D	406	CLA	C3D-C2D	4.17	1.50	1.39
23	C	512	CLA	CHD-C1D	4.17	1.46	1.38
23	c	508	CLA	CHD-C1D	4.16	1.46	1.38
33	a	419	LMG	O8-C28	4.15	1.45	1.33
23	b	602	CLA	CHC-C4B	4.15	1.48	1.39
23	B	611	CLA	O2A-CGA	4.15	1.45	1.33
23	b	609	CLA	CHB-C1B	4.15	1.48	1.39
23	C	514	CLA	CHD-C1D	4.14	1.46	1.38
23	b	607	CLA	CHD-C1D	4.14	1.46	1.38
26	F	101	SQD	O48-C23	4.14	1.45	1.33
23	B	614	CLA	CHB-C1B	4.14	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	CHD-C1D	4.13	1.46	1.38
33	Z	101	LMG	O7-C10	4.13	1.46	1.34
23	C	508	CLA	CHD-C1D	4.13	1.46	1.38
23	c	506	CLA	CHD-C1D	4.13	1.46	1.38
23	B	615	CLA	O2A-CGA	4.13	1.45	1.33
23	d	403	CLA	O2D-CGD	4.13	1.43	1.33
35	C	517	DGD	O2G-C1B	4.13	1.46	1.34
24	A	407	PHO	OBD-CAD	4.13	1.28	1.22
23	C	502	CLA	O2A-CGA	4.13	1.45	1.33
23	b	612	CLA	OBD-CAD	4.12	1.29	1.22
23	a	406	CLA	O2A-CGA	4.12	1.45	1.33
38	e	87	HEM	FE-NC	4.12	2.09	1.95
23	c	503	CLA	CHD-C1D	4.12	1.46	1.38
23	a	405	CLA	CHD-C1D	4.11	1.46	1.38
23	C	513	CLA	O2A-CGA	4.11	1.45	1.33
23	C	504	CLA	CHD-C1D	4.11	1.46	1.38
23	a	406	CLA	C1B-NB	-4.11	1.32	1.37
23	A	406	CLA	CHD-C1D	4.10	1.46	1.38
23	C	507	CLA	CHC-C1C	4.10	1.46	1.38
23	A	405	CLA	C3D-C2D	4.10	1.50	1.39
23	b	601	CLA	CHD-C4C	4.10	1.48	1.39
23	a	405	CLA	CHD-C4C	4.10	1.48	1.39
23	B	608	CLA	CHD-C1D	4.10	1.46	1.38
23	C	503	CLA	C3D-C2D	4.10	1.50	1.39
23	A	408	CLA	CHC-C1C	4.10	1.46	1.38
23	B	608	CLA	C3D-C2D	4.09	1.50	1.39
26	a	413	SQD	O47-C7	4.09	1.45	1.34
23	b	608	CLA	CHC-C1C	4.09	1.46	1.38
23	A	406	CLA	C1D-ND	4.09	1.42	1.37
23	c	502	CLA	O2D-CGD	4.08	1.43	1.33
23	b	611	CLA	O2A-CGA	4.08	1.45	1.33
23	c	504	CLA	CHB-C1B	4.08	1.48	1.39
23	C	509	CLA	CHC-C1C	4.08	1.46	1.38
23	B	609	CLA	O2A-CGA	4.08	1.45	1.33
23	b	608	CLA	O2A-CGA	4.07	1.45	1.33
23	A	405	CLA	O2A-CGA	4.07	1.45	1.33
23	c	513	CLA	CHD-C4C	4.07	1.48	1.39
23	c	503	CLA	O2A-CGA	4.07	1.45	1.33
23	b	603	CLA	CHD-C1D	4.07	1.46	1.38
33	C	501	LMG	O8-C28	4.07	1.45	1.33
23	B	606	CLA	CHD-C1D	4.06	1.46	1.38
23	B	609	CLA	C3D-C2D	4.06	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	CHB-C1B	4.06	1.48	1.39
33	c	520	LMG	O7-C10	4.06	1.45	1.34
23	C	506	CLA	CHD-C4C	4.05	1.48	1.39
23	C	507	CLA	O2A-CGA	4.05	1.45	1.33
26	a	411	SQD	O47-C7	4.05	1.45	1.34
23	b	613	CLA	C1B-NB	-4.05	1.32	1.37
33	c	520	LMG	O8-C28	4.04	1.45	1.33
23	C	513	CLA	CHC-C4B	4.04	1.48	1.39
23	B	602	CLA	CHD-C4C	4.04	1.48	1.39
23	B	601	CLA	CHC-C4B	4.04	1.48	1.39
23	b	601	CLA	C3D-C2D	4.04	1.50	1.39
23	B	604	CLA	CHD-C4C	4.04	1.48	1.39
23	c	512	CLA	CHB-C1B	4.03	1.48	1.39
23	c	506	CLA	CHC-C4B	4.03	1.48	1.39
23	b	616	CLA	O2A-CGA	4.03	1.45	1.33
23	C	512	CLA	CHD-C4C	4.03	1.48	1.39
33	a	419	LMG	O7-C10	4.03	1.45	1.34
23	b	609	CLA	CHD-C1D	4.03	1.46	1.38
23	b	616	CLA	CHD-C1D	4.03	1.46	1.38
23	c	504	CLA	O2A-CGA	4.03	1.45	1.33
33	z	101	LMG	O7-C10	4.03	1.45	1.34
23	b	615	CLA	CHD-C1D	4.02	1.46	1.38
23	B	616	CLA	O2A-CGA	4.02	1.45	1.33
23	D	405	CLA	CHB-C1B	4.02	1.48	1.39
23	B	612	CLA	O2D-CGD	4.02	1.43	1.33
23	B	601	CLA	CHD-C1D	4.02	1.46	1.38
24	A	353	PHO	O2A-CGA	4.02	1.45	1.33
33	C	501	LMG	O7-C10	4.02	1.45	1.34
23	b	612	CLA	CHB-C1B	4.02	1.48	1.39
23	B	615	CLA	CHB-C1B	4.01	1.48	1.39
23	a	405	CLA	CHB-C1B	4.01	1.48	1.39
23	C	510	CLA	C3D-C2D	4.01	1.50	1.39
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	b	608	CLA	CHD-C1D	4.01	1.46	1.38
33	B	621	LMG	O7-C10	4.01	1.45	1.34
23	c	511	CLA	CHB-C1B	4.01	1.48	1.39
23	B	611	CLA	C3B-C2B	4.01	1.54	1.41
35	c	518	DGD	O1G-C1A	4.00	1.45	1.33
23	C	505	CLA	CHB-C1B	4.00	1.48	1.39
23	c	505	CLA	C3D-C2D	4.00	1.50	1.39
23	C	513	CLA	C3D-C2D	4.00	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	OBD-CAD	4.00	1.29	1.22
23	c	509	CLA	OBD-CAD	3.99	1.29	1.22
23	c	508	CLA	O2A-CGA	3.99	1.45	1.33
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	506	CLA	CHB-C1B	3.99	1.48	1.39
23	C	503	CLA	O2A-CGA	3.99	1.45	1.33
23	d	402	CLA	CHB-C1B	3.99	1.48	1.39
33	C	520	LMG	O7-C10	3.98	1.45	1.34
23	c	503	CLA	CHD-C4C	3.98	1.48	1.39
23	C	511	CLA	CHD-C4C	3.98	1.48	1.39
23	B	613	CLA	C3D-C2D	3.98	1.50	1.39
23	A	405	CLA	CHD-C1D	3.97	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
26	a	411	SQD	O48-C23	3.97	1.44	1.33
23	b	604	CLA	CHC-C4B	3.97	1.48	1.39
23	B	602	CLA	O2A-CGA	3.97	1.44	1.33
23	b	613	CLA	C3D-C2D	3.97	1.50	1.39
23	b	606	CLA	CHD-C4C	3.97	1.48	1.39
23	B	610	CLA	OBD-CAD	3.97	1.29	1.22
23	B	606	CLA	CHC-C4B	3.97	1.48	1.39
23	B	616	CLA	C3D-C2D	3.97	1.49	1.39
23	C	511	CLA	CHB-C1B	3.96	1.48	1.39
23	C	504	CLA	CHD-C4C	3.96	1.48	1.39
23	B	603	CLA	CHB-C1B	3.96	1.48	1.39
23	a	407	CLA	O2A-CGA	3.96	1.44	1.33
23	a	407	CLA	C3D-C2D	3.96	1.49	1.39
23	B	611	CLA	CHB-C1B	3.96	1.48	1.39
23	d	402	CLA	O2A-CGA	3.96	1.44	1.33
23	C	504	CLA	O2A-CGA	3.95	1.44	1.33
23	C	507	CLA	CHD-C4C	3.95	1.48	1.39
23	C	511	CLA	CHD-C1D	3.95	1.46	1.38
23	c	508	CLA	OBD-CAD	3.95	1.29	1.22
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	B	612	CLA	C1D-ND	3.95	1.42	1.37
23	A	406	CLA	OBD-CAD	3.95	1.29	1.22
23	b	612	CLA	CHD-C1D	3.95	1.46	1.38
23	c	512	CLA	CHD-C4C	3.95	1.48	1.39
23	C	502	CLA	CHC-C4B	3.95	1.48	1.39
23	A	406	CLA	C3D-C2D	3.95	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	CHB-C1B	3.95	1.48	1.39
23	d	403	CLA	CHC-C4B	3.95	1.48	1.39
33	d	412	LMG	O8-C28	3.94	1.44	1.33
23	c	505	CLA	CHD-C1D	3.94	1.46	1.38
23	c	502	CLA	O2A-CGA	3.94	1.44	1.33
23	C	510	CLA	CHD-C4C	3.94	1.48	1.39
23	b	607	CLA	CHB-C1B	3.94	1.48	1.39
23	c	507	CLA	CHD-C4C	3.94	1.48	1.39
23	c	505	CLA	O2A-CGA	3.94	1.44	1.33
23	C	509	CLA	OBD-CAD	3.93	1.29	1.22
23	b	614	CLA	C3D-C2D	3.93	1.49	1.39
23	c	511	CLA	O2A-CGA	3.93	1.44	1.33
23	d	402	CLA	CHD-C1D	3.93	1.46	1.38
23	C	502	CLA	CHD-C4C	3.92	1.48	1.39
23	B	612	CLA	CHD-C1D	3.92	1.46	1.38
23	B	609	CLA	CHD-C4C	3.92	1.48	1.39
37	L	101	LHG	O8-C23	3.92	1.44	1.33
23	B	609	CLA	CHC-C4B	3.91	1.48	1.39
23	b	605	CLA	CHB-C1B	3.91	1.48	1.39
23	C	514	CLA	C3D-C2D	3.91	1.49	1.39
23	b	608	CLA	C1B-NB	-3.91	1.33	1.37
23	c	510	CLA	O2A-CGA	3.91	1.44	1.33
37	D	411	LHG	O8-C23	3.91	1.44	1.33
23	c	510	CLA	CHD-C4C	3.90	1.48	1.39
23	B	603	CLA	CHD-C1D	3.90	1.46	1.38
23	B	615	CLA	OBD-CAD	3.90	1.29	1.22
37	d	407	LHG	O7-C7	3.90	1.45	1.34
23	c	503	CLA	C3D-C2D	3.90	1.49	1.39
37	D	411	LHG	O7-C7	3.89	1.45	1.34
23	B	613	CLA	CHD-C4C	3.89	1.48	1.39
23	c	506	CLA	CHD-C4C	3.88	1.48	1.39
23	D	406	CLA	CHC-C4B	3.88	1.48	1.39
23	c	502	CLA	CHD-C4C	3.88	1.48	1.39
23	c	510	CLA	CHB-C1B	3.88	1.48	1.39
23	C	504	CLA	CHC-C4B	3.88	1.48	1.39
24	a	408	PHO	OBD-CAD	3.87	1.27	1.22
23	c	511	CLA	C3D-C2D	3.87	1.49	1.39
23	C	505	CLA	CHD-C1D	3.87	1.45	1.38
23	c	513	CLA	C3D-C2D	3.87	1.49	1.39
40	v	202	HEC	FE-ND	3.86	2.06	1.94
23	B	607	CLA	C1D-ND	3.86	1.42	1.37
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	B	604	CLA	CHB-C1B	3.86	1.48	1.39
23	C	506	CLA	CHB-C1B	3.86	1.48	1.39
23	b	608	CLA	OBD-CAD	3.86	1.29	1.22
23	b	616	CLA	CHC-C4B	3.86	1.48	1.39
23	c	509	CLA	CHD-C4C	3.86	1.48	1.39
23	B	611	CLA	CHD-C1D	3.86	1.45	1.38
23	b	614	CLA	O2A-CGA	3.85	1.44	1.33
23	C	505	CLA	O2A-CGA	3.85	1.44	1.33
23	B	614	CLA	CHD-C4C	3.85	1.48	1.39
23	D	406	CLA	CHB-C1B	3.85	1.48	1.39
23	C	511	CLA	O2A-CGA	3.85	1.44	1.33
24	a	353	PHO	O2A-CGA	3.84	1.44	1.33
35	C	518	DGD	O2G-C1B	3.84	1.45	1.34
23	a	406	CLA	OBD-CAD	3.84	1.29	1.22
23	c	513	CLA	CHC-C4B	3.84	1.48	1.39
23	b	609	CLA	C3D-C2D	3.84	1.49	1.39
23	D	406	CLA	CHD-C4C	3.84	1.48	1.39
23	c	508	CLA	CHD-C4C	3.84	1.48	1.39
23	c	507	CLA	CHB-C1B	3.84	1.48	1.39
23	b	610	CLA	CHB-C1B	3.83	1.48	1.39
23	b	602	CLA	C3D-C2D	3.83	1.49	1.39
23	B	613	CLA	C1B-NB	-3.83	1.33	1.37
23	b	614	CLA	CHD-C1D	3.83	1.45	1.38
23	c	502	CLA	C3D-C2D	3.83	1.49	1.39
23	c	513	CLA	OBD-CAD	3.83	1.29	1.22
23	B	608	CLA	CHC-C1C	3.82	1.46	1.38
23	c	502	CLA	CHB-C1B	3.82	1.48	1.39
23	C	508	CLA	CHB-C1B	3.82	1.48	1.39
23	c	507	CLA	C3D-C2D	3.81	1.49	1.39
23	C	513	CLA	CHD-C4C	3.81	1.47	1.39
23	B	615	CLA	C3D-C2D	3.81	1.49	1.39
35	c	517	DGD	O2G-C1B	3.81	1.45	1.34
23	B	610	CLA	CHB-C1B	3.81	1.48	1.39
23	C	510	CLA	C4B-NB	-3.81	1.33	1.37
23	C	505	CLA	C3D-C2D	3.81	1.49	1.39
23	A	404	CLA	C3D-C2D	3.81	1.49	1.39
23	b	609	CLA	O2A-CGA	3.80	1.44	1.33
23	B	603	CLA	O2A-CGA	3.80	1.44	1.33
23	c	508	CLA	CHB-C1B	3.80	1.47	1.39
23	B	610	CLA	C3D-C2D	3.80	1.49	1.39
23	C	514	CLA	CHB-C1B	3.80	1.47	1.39
23	b	606	CLA	O2A-CGA	3.80	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	CHB-C1B	3.80	1.47	1.39
25	B	618	BCR	C23-C22	-3.80	1.37	1.45
23	C	510	CLA	O2A-CGA	3.80	1.44	1.33
23	A	404	CLA	CHB-C1B	3.80	1.47	1.39
23	C	508	CLA	CHC-C4B	3.80	1.47	1.39
23	C	512	CLA	C3D-C2D	3.79	1.49	1.39
23	B	607	CLA	CHD-C4C	3.79	1.47	1.39
35	C	519	DGD	O2G-C1B	3.79	1.45	1.34
35	C	518	DGD	O1G-C1A	3.79	1.44	1.33
23	B	607	CLA	CHD-C1D	3.79	1.45	1.38
23	b	607	CLA	C3D-C2D	3.79	1.49	1.39
23	A	405	CLA	CHD-C4C	3.79	1.47	1.39
23	a	407	CLA	CHD-C4C	3.79	1.47	1.39
23	b	609	CLA	OBD-CAD	3.79	1.29	1.22
23	b	608	CLA	C3D-C2D	3.78	1.49	1.39
23	b	604	CLA	CHD-C4C	3.78	1.47	1.39
35	c	517	DGD	O1G-C1A	3.78	1.44	1.33
23	C	507	CLA	C3D-C2D	3.78	1.49	1.39
23	c	514	CLA	C3D-C2D	3.77	1.49	1.39
34	b	622	HTG	C1'-S1	-3.77	1.76	1.81
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	c	512	CLA	OBD-CAD	3.77	1.29	1.22
23	c	510	CLA	C3D-C2D	3.77	1.49	1.39
24	A	407	PHO	O2A-CGA	3.77	1.44	1.33
23	B	614	CLA	O2A-CGA	3.76	1.44	1.33
23	A	405	CLA	CHC-C4B	3.76	1.47	1.39
23	b	611	CLA	CHC-C4B	3.76	1.47	1.39
23	B	604	CLA	OBD-CAD	3.76	1.29	1.22
23	b	615	CLA	CHC-C4B	3.76	1.47	1.39
23	c	506	CLA	O2A-CGA	3.76	1.44	1.33
23	b	605	CLA	C3D-C2D	3.76	1.49	1.39
23	C	506	CLA	CHC-C4B	3.76	1.47	1.39
23	b	615	CLA	C3D-C2D	3.76	1.49	1.39
26	A	410	SQD	O48-C23	3.76	1.44	1.33
23	b	615	CLA	CHD-C4C	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	605	CLA	OBD-CAD	3.76	1.29	1.22
23	b	612	CLA	CHC-C4B	3.76	1.47	1.39
23	b	604	CLA	C3D-C2D	3.75	1.49	1.39
23	C	511	CLA	OBD-CAD	3.75	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	H	102	DGD	O1G-C1A	3.75	1.44	1.33
23	C	510	CLA	OBD-CAD	3.75	1.28	1.22
23	d	403	CLA	C3D-C2D	3.75	1.49	1.39
23	b	604	CLA	CHB-C1B	3.75	1.47	1.39
23	b	616	CLA	C3D-C2D	3.75	1.49	1.39
23	B	607	CLA	C1B-NB	-3.74	1.33	1.37
23	B	612	CLA	C1B-NB	-3.74	1.33	1.37
23	c	502	CLA	CHC-C4B	3.74	1.47	1.39
23	B	605	CLA	CHD-C1D	3.74	1.45	1.38
23	a	405	CLA	OBD-CAD	3.74	1.28	1.22
23	c	505	CLA	CHD-C4C	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	A	406	CLA	O2A-CGA	3.73	1.44	1.33
23	B	603	CLA	CHD-C4C	3.73	1.47	1.39
23	B	611	CLA	OBD-CAD	3.73	1.28	1.22
23	a	409	CLA	CHC-C4B	3.73	1.47	1.39
23	b	607	CLA	C1B-NB	-3.73	1.33	1.37
23	B	601	CLA	C3D-C2D	3.73	1.49	1.39
23	b	601	CLA	OBD-CAD	3.73	1.28	1.22
23	C	507	CLA	OBD-CAD	3.73	1.28	1.22
23	b	603	CLA	CHD-C4C	3.73	1.47	1.39
35	h	102	DGD	O1G-C1A	3.73	1.44	1.33
23	C	503	CLA	CHC-C4B	3.73	1.47	1.39
23	c	514	CLA	CHB-C1B	3.73	1.47	1.39
23	b	605	CLA	O2A-CGA	3.72	1.44	1.33
23	B	611	CLA	C1C-C2C	3.72	1.51	1.44
23	b	613	CLA	O2A-CGA	3.72	1.44	1.33
23	c	512	CLA	C3D-C2D	3.72	1.49	1.39
23	a	409	CLA	CHD-C1D	3.72	1.45	1.38
23	B	614	CLA	CHD-C1D	3.72	1.45	1.38
23	B	602	CLA	C3D-C2D	3.72	1.49	1.39
23	c	508	CLA	C3D-C2D	3.72	1.49	1.39
23	b	614	CLA	CHB-C1B	3.72	1.47	1.39
23	b	616	CLA	CHD-C4C	3.71	1.47	1.39
23	c	508	CLA	CHC-C4B	3.71	1.47	1.39
23	b	614	CLA	CHD-C4C	3.71	1.47	1.39
23	B	606	CLA	CHD-C4C	3.71	1.47	1.39
23	B	601	CLA	CHD-C4C	3.71	1.47	1.39
23	d	403	CLA	CHD-C4C	3.71	1.47	1.39
23	A	406	CLA	CHD-C4C	3.70	1.47	1.39
34	b	623	HTG	C1'-S1	-3.70	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	CHD-C1D	3.70	1.45	1.38
23	C	511	CLA	C3D-C2D	3.70	1.49	1.39
23	b	605	CLA	CHD-C4C	3.70	1.47	1.39
23	b	603	CLA	CHC-C4B	3.70	1.47	1.39
23	b	603	CLA	C1D-ND	3.70	1.42	1.37
23	b	612	CLA	C3D-C2D	3.70	1.49	1.39
23	D	406	CLA	O2A-CGA	3.70	1.44	1.33
23	c	511	CLA	CHC-C4B	3.70	1.47	1.39
23	A	404	CLA	CHD-C1D	3.70	1.45	1.38
23	B	613	CLA	O2A-CGA	3.69	1.44	1.33
23	b	615	CLA	O2A-CGA	3.69	1.44	1.33
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	CHC-C4B	3.69	1.47	1.39
23	b	610	CLA	CHD-C4C	3.69	1.47	1.39
23	c	511	CLA	CHD-C4C	3.69	1.47	1.39
23	b	613	CLA	CHD-C1D	3.68	1.45	1.38
23	c	509	CLA	CHC-C4B	3.68	1.47	1.39
37	L	101	LHG	O7-C7	3.68	1.44	1.34
23	B	616	CLA	CHB-C1B	3.68	1.47	1.39
26	A	410	SQD	O47-C7	3.68	1.44	1.34
23	B	603	CLA	C3D-C2D	3.68	1.49	1.39
23	C	510	CLA	C1B-NB	-3.68	1.33	1.37
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	505	CLA	CHD-C4C	3.68	1.47	1.39
23	b	613	CLA	CHB-C1B	3.68	1.47	1.39
23	C	503	CLA	CHB-C1B	3.67	1.47	1.39
23	B	605	CLA	C3D-C2D	3.67	1.49	1.39
23	b	611	CLA	CHD-C4C	3.67	1.47	1.39
23	C	503	CLA	OBD-CAD	3.67	1.28	1.22
23	B	605	CLA	O2A-CGA	3.67	1.44	1.33
23	a	405	CLA	C3D-C2D	3.67	1.49	1.39
23	c	509	CLA	CHB-C1B	3.67	1.47	1.39
23	c	511	CLA	CHD-C1D	3.67	1.45	1.38
23	A	404	CLA	CHD-C4C	3.67	1.47	1.39
23	B	612	CLA	CHD-C4C	3.66	1.47	1.39
23	b	609	CLA	CHD-C4C	3.66	1.47	1.39
23	b	614	CLA	CHC-C4B	3.66	1.47	1.39
37	D	410	LHG	O7-C7	3.66	1.44	1.34
23	B	603	CLA	CHC-C4B	3.66	1.47	1.39
23	C	510	CLA	CHC-C4B	3.66	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	C3D-C2D	3.66	1.49	1.39
23	B	601	CLA	OBD-CAD	3.66	1.28	1.22
23	c	513	CLA	CHB-C1B	3.66	1.47	1.39
23	b	602	CLA	O2A-CGA	3.66	1.44	1.33
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	607	CLA	O2A-CGA	3.65	1.44	1.33
35	C	517	DGD	O1G-C1A	3.65	1.44	1.33
23	A	405	CLA	CHB-C1B	3.65	1.47	1.39
23	a	406	CLA	CHD-C1D	3.65	1.45	1.38
37	d	711	LHG	O8-C23	3.64	1.44	1.33
23	D	405	CLA	CHD-C4C	3.64	1.47	1.39
23	A	406	CLA	CHC-C4B	3.64	1.47	1.39
23	b	608	CLA	C4B-NB	-3.64	1.33	1.37
23	b	615	CLA	CHB-C1B	3.64	1.47	1.39
23	b	605	CLA	CHD-C1D	3.64	1.45	1.38
23	d	403	CLA	CHB-C1B	3.64	1.47	1.39
23	b	606	CLA	CHB-C1B	3.64	1.47	1.39
23	C	510	CLA	CHB-C1B	3.63	1.47	1.39
24	A	353	PHO	CHA-CBD	-3.63	1.47	1.51
23	B	611	CLA	CHD-C4C	3.63	1.47	1.39
23	b	601	CLA	CHB-C1B	3.62	1.47	1.39
23	A	408	CLA	C3D-C2D	3.62	1.49	1.39
23	C	504	CLA	C3D-C2D	3.62	1.49	1.39
23	d	402	CLA	C1D-ND	3.61	1.42	1.37
23	B	615	CLA	CHD-C4C	3.61	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	B	610	CLA	CHC-C4B	3.61	1.47	1.39
23	a	407	CLA	CHD-C1D	3.61	1.45	1.38
23	d	402	CLA	OBD-CAD	3.61	1.28	1.22
23	C	502	CLA	CHB-C1B	3.61	1.47	1.39
37	l	101	LHG	O7-C7	3.60	1.44	1.34
23	A	406	CLA	CHB-C1B	3.60	1.47	1.39
23	b	611	CLA	C3D-C2D	3.60	1.49	1.39
37	D	410	LHG	O8-C23	3.60	1.43	1.33
23	A	408	CLA	CHD-C4C	3.60	1.47	1.39
23	b	603	CLA	C3D-C2D	3.60	1.49	1.39
23	B	614	CLA	C3D-C2D	3.60	1.49	1.39
23	d	402	CLA	CHD-C4C	3.60	1.47	1.39
23	b	615	CLA	OBD-CAD	3.60	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	CHD-C4C	3.60	1.47	1.39
23	b	601	CLA	CHC-C4B	3.60	1.47	1.39
37	D	409	LHG	O7-C7	3.60	1.44	1.34
23	b	606	CLA	OBD-CAD	3.59	1.28	1.22
23	D	406	CLA	OBD-CAD	3.59	1.28	1.22
23	B	602	CLA	C1B-NB	-3.59	1.33	1.37
23	B	610	CLA	CHD-C1D	3.59	1.45	1.38
23	C	514	CLA	CHD-C4C	3.59	1.47	1.39
23	B	604	CLA	O2A-CGA	3.58	1.43	1.33
23	b	606	CLA	C3D-C2D	3.58	1.48	1.39
23	C	514	CLA	OBD-CAD	3.58	1.28	1.22
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	c	505	CLA	CHB-C1B	3.57	1.47	1.39
23	b	615	CLA	C1B-NB	-3.56	1.33	1.37
23	b	603	CLA	CHB-C1B	3.56	1.47	1.39
23	A	404	CLA	C4B-NB	-3.56	1.33	1.37
23	b	613	CLA	CHD-C4C	3.56	1.47	1.39
23	B	610	CLA	CHD-C4C	3.56	1.47	1.39
23	C	508	CLA	CHD-C4C	3.56	1.47	1.39
33	D	415	LMG	O7-C10	3.55	1.44	1.34
23	C	513	CLA	OBD-CAD	3.55	1.28	1.22
23	a	405	CLA	CHC-C4B	3.55	1.47	1.39
23	C	508	CLA	C3D-C2D	3.55	1.48	1.39
23	a	407	CLA	CHB-C1B	3.55	1.47	1.39
23	B	607	CLA	C3D-C2D	3.55	1.48	1.39
23	D	405	CLA	C3D-C2D	3.55	1.48	1.39
23	b	610	CLA	C3D-C2D	3.54	1.48	1.39
23	b	607	CLA	CHD-C4C	3.54	1.47	1.39
23	b	608	CLA	CHD-C4C	3.54	1.47	1.39
35	c	518	DGD	O2G-C1B	3.54	1.44	1.34
23	b	606	CLA	CHC-C4B	3.54	1.47	1.39
23	B	601	CLA	CHB-C1B	3.53	1.47	1.39
23	c	507	CLA	CHC-C4B	3.53	1.47	1.39
23	c	506	CLA	OBD-CAD	3.53	1.28	1.22
23	B	610	CLA	C1B-NB	-3.53	1.33	1.37
23	d	402	CLA	C3D-C2D	3.53	1.48	1.39
23	B	609	CLA	C3B-C4B	3.53	1.51	1.42
23	b	616	CLA	OBD-CAD	3.53	1.28	1.22
23	c	507	CLA	OBD-CAD	3.53	1.28	1.22
40	V	202	HEC	FE-NB	3.52	2.05	1.94
23	a	406	CLA	CHD-C4C	3.52	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	O2A-CGA	3.52	1.43	1.33
23	B	606	CLA	C3D-C2D	3.51	1.48	1.39
23	b	607	CLA	CHC-C4B	3.51	1.47	1.39
23	B	608	CLA	O2A-CGA	3.51	1.43	1.33
23	a	409	CLA	CHD-C4C	3.51	1.47	1.39
23	b	611	CLA	CHD-C1D	3.51	1.45	1.38
37	d	711	LHG	O7-C7	3.50	1.44	1.34
23	B	611	CLA	C3B-C4B	3.50	1.50	1.42
23	a	409	CLA	C1B-NB	-3.50	1.33	1.37
23	D	405	CLA	CHC-C4B	3.50	1.47	1.39
23	a	407	CLA	OBD-CAD	3.50	1.28	1.22
23	B	605	CLA	CHD-C4C	3.50	1.47	1.39
37	D	409	LHG	O8-C23	3.49	1.43	1.33
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	c	514	CLA	OBD-CAD	3.49	1.28	1.22
23	B	616	CLA	CHC-C4B	3.48	1.47	1.39
23	A	405	CLA	C1B-NB	-3.48	1.33	1.37
23	b	602	CLA	C3B-C4B	3.48	1.50	1.42
23	c	506	CLA	C3D-C2D	3.48	1.48	1.39
23	c	512	CLA	CHC-C4B	3.48	1.47	1.39
23	a	406	CLA	CHB-C1B	3.48	1.47	1.39
23	C	509	CLA	CHC-C4B	3.48	1.47	1.39
23	C	507	CLA	C4B-NB	-3.47	1.33	1.37
23	B	612	CLA	C4B-NB	-3.47	1.33	1.37
23	C	512	CLA	C4B-NB	-3.47	1.33	1.37
23	d	403	CLA	OBD-CAD	3.47	1.28	1.22
23	C	506	CLA	OBD-CAD	3.46	1.28	1.22
23	b	612	CLA	C4B-NB	-3.46	1.33	1.37
34	B	622	HTG	C1'-S1	-3.46	1.77	1.81
23	C	507	CLA	CHB-C1B	3.46	1.47	1.39
23	C	504	CLA	OBD-CAD	3.46	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	603	CLA	OBD-CAD	3.45	1.28	1.22
23	b	609	CLA	CHC-C4B	3.45	1.47	1.39
38	E	103	HEM	C4D-ND	-3.45	1.34	1.40
23	B	609	CLA	CHB-C1B	3.44	1.47	1.39
23	c	514	CLA	CHC-C4B	3.44	1.47	1.39
23	A	408	CLA	CHB-C1B	3.44	1.47	1.39
33	D	415	LMG	O8-C28	3.44	1.43	1.33
23	b	614	CLA	OBD-CAD	3.44	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	C1B-NB	-3.43	1.33	1.37
23	b	607	CLA	O2A-CGA	3.43	1.43	1.33
23	b	610	CLA	OBD-CAD	3.42	1.28	1.22
23	c	503	CLA	CHC-C4B	3.42	1.47	1.39
23	B	612	CLA	C3D-C2D	3.42	1.48	1.39
23	B	613	CLA	CHC-C4B	3.42	1.47	1.39
23	b	611	CLA	CHB-C1B	3.42	1.47	1.39
34	B	626	HTG	C1'-S1	-3.42	1.77	1.81
23	B	608	CLA	CHD-C4C	3.42	1.47	1.39
23	b	614	CLA	C1B-NB	-3.41	1.33	1.37
23	b	616	CLA	C1B-NB	-3.41	1.33	1.37
23	d	402	CLA	C1B-NB	-3.41	1.33	1.37
23	b	605	CLA	C1B-NB	-3.41	1.33	1.37
23	c	505	CLA	OBD-CAD	3.41	1.28	1.22
23	b	610	CLA	C1B-NB	-3.40	1.33	1.37
38	e	87	HEM	C4D-ND	-3.40	1.34	1.40
23	c	510	CLA	OBD-CAD	3.40	1.28	1.22
23	A	408	CLA	C4B-NB	-3.39	1.33	1.37
37	l	101	LHG	O8-C23	3.39	1.43	1.33
23	C	505	CLA	CHC-C4B	3.39	1.47	1.39
23	C	509	CLA	CHD-C4C	3.39	1.47	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	B	606	CLA	OBD-CAD	3.38	1.28	1.22
23	C	506	CLA	C3D-C2D	3.38	1.48	1.39
23	C	502	CLA	C1B-NB	-3.38	1.33	1.37
23	b	604	CLA	O2A-CGA	3.38	1.43	1.33
23	d	402	CLA	CHC-C4B	3.38	1.47	1.39
23	B	603	CLA	OBD-CAD	3.37	1.28	1.22
23	C	511	CLA	C1B-NB	-3.37	1.33	1.37
23	C	507	CLA	C1B-NB	-3.37	1.33	1.37
23	b	612	CLA	CHD-C4C	3.37	1.46	1.39
35	H	102	DGD	O2G-C1B	3.37	1.43	1.34
23	C	512	CLA	OBD-CAD	3.37	1.28	1.22
23	A	406	CLA	C3B-C4B	3.36	1.50	1.42
23	C	511	CLA	CHC-C4B	3.36	1.46	1.39
23	A	405	CLA	OBD-CAD	3.36	1.28	1.22
23	c	514	CLA	C4B-NB	-3.36	1.33	1.37
23	B	608	CLA	C4B-NB	-3.36	1.33	1.37
24	a	408	PHO	O2A-CGA	3.35	1.43	1.33
23	B	601	CLA	C3B-C4B	3.35	1.50	1.42
23	b	602	CLA	C1B-NB	-3.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	OBD-CAD	3.34	1.28	1.22
23	c	505	CLA	CHC-C4B	3.34	1.46	1.39
23	B	604	CLA	C3D-C2D	3.33	1.48	1.39
23	B	615	CLA	CHC-C4B	3.33	1.46	1.39
23	A	404	CLA	OBD-CAD	3.33	1.28	1.22
23	b	607	CLA	C1B-C2B	3.32	1.51	1.43
23	c	508	CLA	C1B-NB	-3.32	1.33	1.37
23	c	514	CLA	C1B-NB	-3.31	1.33	1.37
23	D	406	CLA	C3B-C4B	3.31	1.50	1.42
23	A	408	CLA	C1B-NB	-3.31	1.33	1.37
40	V	202	HEC	FE-NC	3.30	2.06	1.95
23	C	511	CLA	C4B-NB	-3.30	1.33	1.37
23	c	504	CLA	C3D-C2D	3.30	1.48	1.39
23	B	611	CLA	C3D-C2D	3.30	1.48	1.39
23	C	513	CLA	CHB-C1B	3.29	1.46	1.39
23	C	505	CLA	C1B-NB	-3.28	1.33	1.37
23	B	609	CLA	OBD-CAD	3.28	1.28	1.22
23	A	404	CLA	O2A-CGA	3.28	1.42	1.33
23	a	409	CLA	C3D-C2D	3.28	1.48	1.39
23	c	510	CLA	C4B-NB	-3.27	1.33	1.37
23	b	604	CLA	OBD-CAD	3.27	1.28	1.22
34	d	411	HTG	C1'-S1	-3.27	1.77	1.81
23	a	407	CLA	CHC-C4B	3.27	1.46	1.39
38	E	103	HEM	C1B-NB	-3.26	1.34	1.40
23	c	508	CLA	C4B-NB	-3.26	1.33	1.37
23	A	408	CLA	CHC-C4B	3.26	1.46	1.39
23	D	405	CLA	OBD-CAD	3.24	1.28	1.22
23	a	406	CLA	CHC-C4B	3.23	1.46	1.39
23	b	602	CLA	CHB-C1B	3.23	1.46	1.39
38	e	87	HEM	C1B-NB	-3.23	1.34	1.40
23	c	507	CLA	C1B-NB	-3.22	1.33	1.37
23	B	612	CLA	CHC-C4B	3.22	1.46	1.39
23	C	505	CLA	OBD-CAD	3.22	1.28	1.22
23	B	616	CLA	C1B-NB	-3.22	1.33	1.37
23	a	409	CLA	OBD-CAD	3.21	1.28	1.22
23	b	604	CLA	C1B-NB	-3.21	1.33	1.37
34	D	414	HTG	C1'-S1	-3.21	1.77	1.81
23	B	603	CLA	C4B-NB	-3.21	1.33	1.37
23	b	608	CLA	CHC-C4B	3.20	1.46	1.39
23	c	511	CLA	OBD-CAD	3.20	1.28	1.22
23	c	505	CLA	C1B-NB	-3.20	1.33	1.37
23	B	602	CLA	OBD-CAD	3.20	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	514	CLA	C4B-NB	-3.20	1.33	1.37
23	C	507	CLA	CHC-C4B	3.20	1.46	1.39
23	D	405	CLA	C1B-NB	-3.20	1.33	1.37
23	B	603	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	CHB-C1B	3.18	1.46	1.39
23	c	504	CLA	C3B-C4B	3.18	1.50	1.42
40	v	202	HEC	FE-NC	3.17	2.05	1.95
23	C	513	CLA	C3B-C4B	3.17	1.50	1.42
23	A	405	CLA	C3B-C4B	3.17	1.50	1.42
23	B	616	CLA	CHD-C4C	3.17	1.46	1.39
23	B	604	CLA	C1B-NB	-3.17	1.33	1.37
23	c	506	CLA	C3B-C4B	3.16	1.50	1.42
34	b	625	HTG	C1'-S1	-3.16	1.77	1.81
23	b	616	CLA	C3B-C4B	3.14	1.50	1.42
23	B	610	CLA	C4B-NB	-3.13	1.33	1.37
23	c	509	CLA	C3B-C4B	3.12	1.50	1.42
23	C	506	CLA	C1B-NB	-3.12	1.34	1.37
23	B	604	CLA	C1B-C2B	3.11	1.50	1.43
23	C	506	CLA	C1B-C2B	3.11	1.50	1.43
23	b	609	CLA	C1B-NB	-3.11	1.34	1.37
23	B	607	CLA	C4B-NB	-3.10	1.34	1.37
23	b	611	CLA	OBD-CAD	3.10	1.27	1.22
23	A	404	CLA	C1B-NB	-3.09	1.34	1.37
23	d	402	CLA	C4B-NB	-3.09	1.34	1.37
23	C	502	CLA	C3B-C4B	3.09	1.50	1.42
23	b	610	CLA	O2A-CGA	3.09	1.42	1.33
23	B	612	CLA	C1B-C2B	3.09	1.50	1.43
23	C	506	CLA	C3B-C4B	3.09	1.50	1.42
23	a	409	CLA	C3B-C4B	3.08	1.50	1.42
23	B	605	CLA	C3B-C4B	3.08	1.50	1.42
23	B	605	CLA	OBD-CAD	3.08	1.27	1.22
23	b	611	CLA	C1B-NB	-3.08	1.34	1.37
23	D	406	CLA	C1C-C2C	3.08	1.50	1.44
23	C	513	CLA	C1C-C2C	3.07	1.50	1.44
23	B	615	CLA	C1B-C2B	3.07	1.50	1.43
34	C	522	HTG	C1'-S1	-3.07	1.77	1.81
23	C	513	CLA	C1B-NB	-3.07	1.34	1.37
23	b	606	CLA	C1B-NB	-3.07	1.34	1.37
23	B	616	CLA	OBD-CAD	3.07	1.27	1.22
23	B	614	CLA	OBD-CAD	3.06	1.27	1.22
23	a	405	CLA	C1B-NB	-3.06	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	405	CLA	C4B-NB	-3.05	1.34	1.37
23	b	612	CLA	C1C-C2C	3.05	1.50	1.44
23	b	601	CLA	C1B-NB	-3.05	1.34	1.37
23	c	510	CLA	C1B-C2B	3.04	1.50	1.43
23	a	407	CLA	C1B-NB	-3.04	1.34	1.37
23	C	509	CLA	C1B-C2B	3.04	1.50	1.43
23	C	508	CLA	OBD-CAD	3.03	1.27	1.22
23	c	512	CLA	C1B-NB	-3.03	1.34	1.37
23	c	512	CLA	C1B-C2B	3.03	1.50	1.43
23	c	505	CLA	C4B-NB	-3.02	1.34	1.37
23	c	510	CLA	CHC-C4B	3.02	1.46	1.39
23	B	615	CLA	C1C-C2C	3.01	1.50	1.44
23	B	606	CLA	C1C-C2C	3.01	1.50	1.44
23	a	409	CLA	C1C-C2C	3.01	1.50	1.44
23	A	404	CLA	CHC-C4B	3.01	1.46	1.39
23	B	606	CLA	C3B-C4B	3.00	1.49	1.42
23	B	610	CLA	C1C-C2C	3.00	1.50	1.44
23	d	403	CLA	C3B-C4B	2.99	1.49	1.42
23	B	612	CLA	OBD-CAD	2.99	1.27	1.22
23	A	408	CLA	OBD-CAD	2.99	1.27	1.22
23	b	603	CLA	C1B-NB	-2.99	1.34	1.37
23	a	407	CLA	C3B-C4B	2.98	1.49	1.42
23	b	613	CLA	C4B-NB	-2.98	1.34	1.37
34	c	522	HTG	C1'-S1	-2.98	1.77	1.81
23	c	513	CLA	C3B-C4B	2.98	1.49	1.42
23	A	406	CLA	C1B-C2B	2.96	1.50	1.43
23	B	605	CLA	C4B-NB	-2.96	1.34	1.37
23	b	603	CLA	C1B-C2B	2.96	1.50	1.43
23	b	601	CLA	C3B-C4B	2.96	1.49	1.42
23	a	409	CLA	C1B-C2B	2.95	1.50	1.43
23	C	504	CLA	C3B-C4B	2.95	1.49	1.42
23	C	514	CLA	C1B-C2B	2.95	1.50	1.43
23	b	614	CLA	C1B-C2B	2.95	1.50	1.43
23	c	504	CLA	C1B-NB	-2.95	1.34	1.37
23	b	610	CLA	C1C-C2C	2.95	1.50	1.44
23	B	616	CLA	C1B-C2B	2.94	1.50	1.43
23	c	505	CLA	C1B-C2B	2.94	1.50	1.43
23	B	605	CLA	C1B-C2B	2.93	1.50	1.43
23	b	603	CLA	C3B-C4B	2.93	1.49	1.42
23	C	505	CLA	C4B-NB	-2.93	1.34	1.37
23	b	612	CLA	C1B-NB	-2.93	1.34	1.37
23	C	514	CLA	C1B-NB	-2.93	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	OBD-CAD	2.92	1.27	1.22
23	B	608	CLA	CHC-C4B	2.92	1.46	1.39
23	C	512	CLA	C4D-CHA	2.92	1.48	1.38
23	C	508	CLA	C1B-NB	-2.92	1.34	1.37
23	b	602	CLA	C1C-C2C	2.92	1.50	1.44
23	C	503	CLA	C1B-NB	-2.91	1.34	1.37
23	C	508	CLA	C1C-C2C	2.91	1.50	1.44
23	a	407	CLA	C1C-C2C	2.91	1.50	1.44
23	B	612	CLA	C1C-C2C	2.91	1.50	1.44
23	C	502	CLA	OBD-CAD	2.90	1.27	1.22
23	b	607	CLA	C4B-NB	-2.90	1.34	1.37
23	c	511	CLA	C1C-C2C	2.90	1.50	1.44
23	c	503	CLA	C1B-C2B	2.90	1.50	1.43
23	B	614	CLA	C1B-NB	-2.89	1.34	1.37
23	b	604	CLA	C1B-C2B	2.89	1.50	1.43
23	c	502	CLA	C1B-NB	-2.89	1.34	1.37
23	D	406	CLA	C1B-C2B	2.89	1.50	1.43
23	C	509	CLA	C4B-NB	-2.89	1.34	1.37
23	D	406	CLA	C1B-NB	-2.88	1.34	1.37
23	b	601	CLA	C4B-NB	-2.88	1.34	1.37
23	b	609	CLA	C3B-C4B	2.88	1.49	1.42
23	c	507	CLA	C4B-NB	-2.88	1.34	1.37
23	B	607	CLA	C4D-CHA	2.88	1.48	1.38
23	C	503	CLA	C4B-NB	-2.88	1.34	1.37
23	B	610	CLA	C3B-C4B	2.88	1.49	1.42
23	B	605	CLA	C1C-C2C	2.88	1.50	1.44
23	B	608	CLA	OBD-CAD	2.87	1.27	1.22
23	c	514	CLA	C3B-C4B	2.87	1.49	1.42
23	D	405	CLA	C4B-NB	-2.86	1.34	1.37
23	b	606	CLA	C3B-C4B	2.86	1.49	1.42
23	B	614	CLA	C4D-CHA	2.86	1.48	1.38
23	d	403	CLA	C1B-NB	-2.86	1.34	1.37
23	b	607	CLA	C1C-C2C	2.86	1.50	1.44
23	B	615	CLA	C3B-C4B	2.85	1.49	1.42
23	C	504	CLA	C1B-NB	-2.85	1.34	1.37
23	A	404	CLA	C4C-C3C	2.84	1.49	1.45
23	c	506	CLA	C4C-C3C	2.84	1.49	1.45
23	a	406	CLA	C3B-C4B	2.84	1.49	1.42
23	b	607	CLA	C4C-C3C	2.83	1.49	1.45
23	C	511	CLA	C1C-C2C	2.83	1.50	1.44
23	a	409	CLA	C4B-NB	-2.83	1.34	1.37
23	b	604	CLA	C4D-CHA	2.83	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C1B-C2B	2.83	1.49	1.43
23	c	508	CLA	C1C-C2C	2.83	1.50	1.44
23	b	610	CLA	C3B-C4B	2.81	1.49	1.42
29	A	414	PL9	C6-C5	2.81	1.49	1.35
23	B	607	CLA	C1B-C2B	2.80	1.49	1.43
23	c	506	CLA	C1B-NB	-2.80	1.34	1.37
23	b	612	CLA	C1B-C2B	2.80	1.49	1.43
23	A	408	CLA	C1B-C2B	2.80	1.49	1.43
23	B	616	CLA	C1C-C2C	2.80	1.50	1.44
23	b	613	CLA	C4D-CHA	2.80	1.48	1.38
23	b	611	CLA	C1B-C2B	2.80	1.49	1.43
23	c	514	CLA	C1C-C2C	2.80	1.50	1.44
23	b	604	CLA	C1C-C2C	2.80	1.50	1.44
23	D	405	CLA	C1B-C2B	2.79	1.49	1.43
23	d	402	CLA	C4C-C3C	2.79	1.49	1.45
23	c	511	CLA	C3B-C4B	2.79	1.49	1.42
23	B	601	CLA	C1C-C2C	2.79	1.50	1.44
23	C	502	CLA	C1B-C2B	2.79	1.49	1.43
23	c	511	CLA	C4B-NB	-2.78	1.34	1.37
23	c	512	CLA	C4B-NB	-2.78	1.34	1.37
23	c	504	CLA	C4B-NB	-2.78	1.34	1.37
23	c	511	CLA	C1B-C2B	2.78	1.49	1.43
23	B	613	CLA	C4B-NB	-2.78	1.34	1.37
23	B	616	CLA	C4B-NB	-2.77	1.34	1.37
23	B	615	CLA	C1B-NB	-2.77	1.34	1.37
23	A	404	CLA	C1B-C2B	2.76	1.49	1.43
24	A	407	PHO	CBD-CGD	-2.76	1.48	1.52
23	C	502	CLA	C1C-C2C	2.76	1.49	1.44
23	C	505	CLA	C1C-C2C	2.76	1.49	1.44
26	A	410	SQD	C6-S	-2.76	1.67	1.77
23	B	613	CLA	C1B-C2B	2.75	1.49	1.43
23	b	612	CLA	C3B-C4B	2.75	1.49	1.42
23	A	408	CLA	C4D-CHA	2.75	1.48	1.38
23	C	505	CLA	C4D-CHA	2.75	1.48	1.38
23	B	602	CLA	C1C-C2C	2.75	1.49	1.44
23	B	611	CLA	MG-NB	2.75	2.11	2.05
23	c	513	CLA	C1B-NB	-2.75	1.34	1.37
23	c	506	CLA	C1C-C2C	2.75	1.49	1.44
23	B	607	CLA	C3B-C4B	2.74	1.49	1.42
23	c	502	CLA	C3B-C4B	2.74	1.49	1.42
34	b	625	HTG	C1-S1	-2.74	1.76	1.80
23	a	407	CLA	C4B-NB	-2.74	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	416	PL9	C6-C5	2.74	1.49	1.35
23	B	616	CLA	C4D-CHA	2.74	1.48	1.38
23	c	503	CLA	C3B-C4B	2.74	1.49	1.42
23	C	514	CLA	C1C-C2C	2.74	1.49	1.44
23	b	614	CLA	C4B-NB	-2.74	1.34	1.37
23	c	507	CLA	C1B-C2B	2.74	1.49	1.43
23	c	509	CLA	C4D-CHA	2.74	1.48	1.38
23	c	504	CLA	C1B-C2B	2.74	1.49	1.43
23	B	601	CLA	C4B-NB	-2.73	1.34	1.37
26	a	411	SQD	C6-S	-2.73	1.67	1.77
23	C	508	CLA	C4D-CHA	2.73	1.48	1.38
23	B	606	CLA	C1B-NB	-2.73	1.34	1.37
23	a	406	CLA	C4B-NB	-2.73	1.34	1.37
23	A	405	CLA	C1C-C2C	2.73	1.49	1.44
23	C	512	CLA	C1B-NB	-2.73	1.34	1.37
23	b	616	CLA	C1C-C2C	2.72	1.49	1.44
23	C	506	CLA	C4C-C3C	2.72	1.49	1.45
23	b	614	CLA	C3B-C4B	2.72	1.49	1.42
23	b	613	CLA	C1B-C2B	2.72	1.49	1.43
23	A	405	CLA	C4B-NB	-2.72	1.34	1.37
23	B	612	CLA	C4D-CHA	2.72	1.48	1.38
23	b	613	CLA	OBD-CAD	2.72	1.27	1.22
23	D	406	CLA	C4C-C3C	2.71	1.49	1.45
23	c	508	CLA	C1B-C2B	2.71	1.49	1.43
23	C	502	CLA	C4D-CHA	2.71	1.48	1.38
23	B	605	CLA	C1B-NB	-2.71	1.34	1.37
23	B	609	CLA	C1C-C2C	2.71	1.49	1.44
23	c	506	CLA	C1B-C2B	2.70	1.49	1.43
23	B	608	CLA	C4D-CHA	2.70	1.48	1.38
23	B	613	CLA	C4D-CHA	2.70	1.48	1.38
23	B	615	CLA	C4D-CHA	2.70	1.48	1.38
23	c	514	CLA	C1B-C2B	2.70	1.49	1.43
23	C	514	CLA	C3B-C4B	2.69	1.49	1.42
23	A	405	CLA	C1B-C2B	2.69	1.49	1.43
23	B	604	CLA	C4C-C3C	2.69	1.49	1.45
23	C	511	CLA	C1B-C2B	2.69	1.49	1.43
23	c	502	CLA	C4D-CHA	2.69	1.48	1.38
23	c	513	CLA	C4D-CHA	2.69	1.48	1.38
23	A	405	CLA	C4D-CHA	2.69	1.48	1.38
23	b	609	CLA	C4B-NB	-2.69	1.34	1.37
33	Z	101	LMG	O8-C28	2.69	1.46	1.33
23	b	605	CLA	C3B-C4B	2.68	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C3B-C4B	2.68	1.49	1.42
23	B	608	CLA	C3B-C4B	2.68	1.49	1.42
23	C	503	CLA	C1B-C2B	2.68	1.49	1.43
23	C	508	CLA	C4B-NB	-2.68	1.34	1.37
23	C	507	CLA	C1B-C2B	2.68	1.49	1.43
23	B	601	CLA	C1B-NB	-2.68	1.34	1.37
23	C	503	CLA	C3B-C4B	2.68	1.49	1.42
23	a	407	CLA	C4D-CHA	2.67	1.47	1.38
23	b	603	CLA	C4B-NB	-2.67	1.34	1.37
23	c	509	CLA	C1C-C2C	2.67	1.49	1.44
23	B	604	CLA	C4D-CHA	2.67	1.47	1.38
23	C	510	CLA	C3B-C4B	2.67	1.49	1.42
23	a	407	CLA	C1B-C2B	2.67	1.49	1.43
26	A	412	SQD	C6-S	-2.67	1.67	1.77
23	c	509	CLA	C1B-C2B	2.67	1.49	1.43
34	b	622	HTG	O5-C1	2.67	1.46	1.42
23	B	610	CLA	C1B-C2B	2.67	1.49	1.43
32	t	102	LMT	O3'-C3'	-2.67	1.36	1.43
23	a	406	CLA	C1B-C2B	2.66	1.49	1.43
23	C	509	CLA	C4D-CHA	2.66	1.47	1.38
26	a	413	SQD	C6-S	-2.66	1.67	1.77
23	c	513	CLA	C4B-NB	-2.66	1.34	1.37
23	b	609	CLA	C4D-CHA	2.66	1.47	1.38
26	f	102	SQD	C6-S	-2.66	1.67	1.77
23	C	505	CLA	C1B-C2B	2.66	1.49	1.43
23	b	604	CLA	C3B-C4B	2.65	1.49	1.42
23	C	507	CLA	C4D-CHA	2.65	1.47	1.38
23	c	512	CLA	C4D-CHA	2.65	1.47	1.38
23	C	507	CLA	C4C-C3C	2.65	1.49	1.45
23	B	608	CLA	C1B-NB	-2.64	1.34	1.37
23	c	505	CLA	C4D-CHA	2.64	1.47	1.38
23	c	510	CLA	C4D-CHA	2.64	1.47	1.38
23	b	605	CLA	C4B-NB	-2.64	1.34	1.37
23	C	505	CLA	C3B-C4B	2.64	1.48	1.42
23	C	508	CLA	C1B-C2B	2.64	1.49	1.43
23	B	608	CLA	C1B-C2B	2.63	1.49	1.43
23	A	408	CLA	C3D-C4D	-2.63	1.38	1.44
40	V	202	HEC	CAC-C3C	2.63	1.57	1.51
23	B	610	CLA	C4C-C3C	2.63	1.49	1.45
23	B	610	CLA	C4D-CHA	2.63	1.47	1.38
23	c	504	CLA	C4D-CHA	2.63	1.47	1.38
23	b	602	CLA	C3D-C4D	-2.63	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	C3B-C4B	2.62	1.48	1.42
23	b	607	CLA	C4D-CHA	2.62	1.47	1.38
23	d	403	CLA	C1C-C2C	2.62	1.49	1.44
23	c	511	CLA	C1B-NB	-2.62	1.34	1.37
23	c	507	CLA	C4C-C3C	2.62	1.49	1.45
23	c	508	CLA	C4D-CHA	2.62	1.47	1.38
23	c	505	CLA	C3B-C4B	2.62	1.48	1.42
23	c	504	CLA	C1C-C2C	2.61	1.49	1.44
23	D	405	CLA	C4D-CHA	2.61	1.47	1.38
23	b	615	CLA	C1B-C2B	2.61	1.49	1.43
23	c	503	CLA	C1B-NB	-2.61	1.34	1.37
23	C	513	CLA	C4D-CHA	2.61	1.47	1.38
23	c	507	CLA	C3B-C4B	2.61	1.48	1.42
26	b	620	SQD	C6-S	-2.60	1.67	1.77
23	B	602	CLA	C1B-C2B	2.60	1.49	1.43
23	d	402	CLA	C4D-CHA	2.60	1.47	1.38
23	C	510	CLA	C4C-C3C	2.60	1.49	1.45
23	c	503	CLA	C4D-CHA	2.60	1.47	1.38
23	B	606	CLA	C1B-C2B	2.60	1.49	1.43
23	c	511	CLA	C4D-CHA	2.60	1.47	1.38
23	C	511	CLA	C4C-C3C	2.60	1.49	1.45
23	c	504	CLA	C3D-C4D	-2.60	1.38	1.44
23	B	614	CLA	C1B-C2B	2.60	1.49	1.43
23	A	406	CLA	C4D-CHA	2.58	1.47	1.38
24	a	408	PHO	CBD-CGD	-2.58	1.49	1.52
23	B	605	CLA	C4D-CHA	2.58	1.47	1.38
23	C	504	CLA	C4B-NB	-2.58	1.34	1.37
23	C	514	CLA	C4D-CHA	2.58	1.47	1.38
23	b	615	CLA	C4D-CHA	2.57	1.47	1.38
23	C	510	CLA	C4D-CHA	2.57	1.47	1.38
23	b	605	CLA	C4D-CHA	2.57	1.47	1.38
23	B	602	CLA	C4D-CHA	2.57	1.47	1.38
32	M	101	LMT	O2'-C2'	-2.56	1.36	1.43
23	c	502	CLA	C1B-C2B	2.56	1.49	1.43
23	C	509	CLA	C3B-C2B	2.56	1.49	1.41
23	b	606	CLA	C4D-CHA	2.56	1.47	1.38
23	b	601	CLA	C4D-CHA	2.56	1.47	1.38
35	H	102	DGD	O5D-C1E	2.56	1.44	1.40
23	C	506	CLA	C1C-C2C	2.56	1.49	1.44
23	a	405	CLA	C4D-CHA	2.55	1.47	1.38
23	B	613	CLA	C4C-C3C	2.55	1.49	1.45
23	B	602	CLA	C4B-NB	-2.55	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	C1C-C2C	2.55	1.49	1.44
23	d	402	CLA	C1C-C2C	2.55	1.49	1.44
23	B	603	CLA	C3B-C4B	2.55	1.48	1.42
23	B	607	CLA	C4C-C3C	2.55	1.49	1.45
23	A	406	CLA	C4B-NB	-2.55	1.34	1.37
23	B	603	CLA	C4D-CHA	2.54	1.47	1.38
23	A	404	CLA	C4D-CHA	2.54	1.47	1.38
34	B	623	HTG	C1'-S1	-2.54	1.78	1.81
23	C	512	CLA	C3B-C4B	2.54	1.48	1.42
23	b	610	CLA	C4B-NB	-2.54	1.34	1.37
32	D	404	LMT	C3'-C2'	2.53	1.58	1.52
23	C	512	CLA	C4C-C3C	2.53	1.49	1.45
23	C	506	CLA	C4D-CHA	2.53	1.47	1.38
23	c	502	CLA	C4C-C3C	2.53	1.49	1.45
23	c	506	CLA	C4D-CHA	2.53	1.47	1.38
23	b	613	CLA	C3B-C4B	2.53	1.48	1.42
23	b	610	CLA	C1B-C2B	2.53	1.49	1.43
23	C	509	CLA	C4C-C3C	2.52	1.49	1.45
23	b	606	CLA	C1B-C2B	2.52	1.49	1.43
34	B	626	HTG	C1-S1	-2.52	1.76	1.80
23	a	406	CLA	C4D-CHA	2.52	1.47	1.38
23	b	615	CLA	C3B-C4B	2.52	1.48	1.42
23	c	503	CLA	C4B-NB	-2.52	1.34	1.37
24	a	353	PHO	C3A-C2A	-2.52	1.52	1.54
23	b	614	CLA	C4D-CHA	2.52	1.47	1.38
23	b	608	CLA	C3B-C4B	2.52	1.48	1.42
32	M	101	LMT	O2B-C2B	-2.52	1.37	1.43
32	I	101	LMT	O3'-C3'	-2.51	1.37	1.43
23	c	502	CLA	C1C-C2C	2.51	1.49	1.44
23	c	502	CLA	C4B-NB	-2.51	1.34	1.37
23	b	616	CLA	C1B-C2B	2.51	1.49	1.43
23	C	504	CLA	C4C-C3C	2.51	1.49	1.45
23	b	602	CLA	C4D-CHA	2.51	1.47	1.38
23	c	507	CLA	C4D-CHA	2.51	1.47	1.38
23	d	402	CLA	C1B-C2B	2.51	1.49	1.43
23	C	512	CLA	C1C-C2C	2.51	1.49	1.44
23	b	610	CLA	C4C-C3C	2.51	1.49	1.45
23	C	511	CLA	C3B-C4B	2.51	1.48	1.42
23	B	616	CLA	C3B-C2B	2.51	1.49	1.41
23	D	406	CLA	C4D-CHA	2.50	1.47	1.38
23	b	606	CLA	C4B-NB	-2.50	1.34	1.37
23	c	509	CLA	C4C-C3C	2.50	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	C4D-CHA	2.50	1.47	1.38
23	C	503	CLA	C1C-C2C	2.50	1.49	1.44
26	F	101	SQD	C6-S	-2.50	1.68	1.77
29	D	408	PL9	C6-C5	2.50	1.48	1.35
23	C	504	CLA	C4D-CHA	2.50	1.47	1.38
23	c	513	CLA	C1B-C2B	2.50	1.49	1.43
23	c	502	CLA	C3D-C4D	-2.49	1.38	1.44
23	B	607	CLA	C1C-C2C	2.49	1.49	1.44
23	b	611	CLA	C1C-C2C	2.49	1.49	1.44
38	e	87	HEM	C1C-C2C	-2.49	1.40	1.45
23	c	514	CLA	C4C-C3C	2.49	1.49	1.45
23	B	602	CLA	C3D-C4D	-2.49	1.38	1.44
23	B	614	CLA	C1C-C2C	2.49	1.49	1.44
23	b	610	CLA	C4D-CHA	2.49	1.47	1.38
23	c	509	CLA	C4B-NB	-2.49	1.34	1.37
23	B	609	CLA	C4D-CHA	2.49	1.47	1.38
23	c	512	CLA	C3B-C4B	2.48	1.48	1.42
23	b	604	CLA	C4B-NB	-2.48	1.34	1.37
23	C	510	CLA	C1B-C2B	2.48	1.49	1.43
23	B	607	CLA	C3D-C4D	-2.48	1.38	1.44
26	B	620	SQD	C6-S	-2.48	1.68	1.77
23	b	608	CLA	C4D-CHA	2.48	1.47	1.38
23	C	512	CLA	C3B-C2B	2.48	1.49	1.41
23	B	614	CLA	C3B-C4B	2.48	1.48	1.42
24	A	353	PHO	C3D-C4D	-2.48	1.37	1.41
23	B	609	CLA	C1B-C2B	2.48	1.49	1.43
23	b	611	CLA	C4D-CHA	2.47	1.47	1.38
23	a	405	CLA	C1C-C2C	2.47	1.49	1.44
23	b	611	CLA	C3B-C4B	2.47	1.48	1.42
23	C	509	CLA	C1C-C2C	2.47	1.49	1.44
23	a	405	CLA	C1B-C2B	2.47	1.49	1.43
23	b	601	CLA	C1C-C2C	2.46	1.49	1.44
23	d	403	CLA	C4D-CHA	2.46	1.47	1.38
23	D	405	CLA	C1C-C2C	2.46	1.49	1.44
23	c	514	CLA	C4D-CHA	2.46	1.47	1.38
23	C	514	CLA	C3B-C2B	2.45	1.49	1.41
32	e	102	LMT	O3'-C3'	-2.45	1.37	1.43
33	C	521	LMG	O1-C1	2.45	1.44	1.40
23	b	605	CLA	C1B-C2B	2.45	1.49	1.43
23	b	602	CLA	C4B-NB	-2.45	1.34	1.37
23	b	612	CLA	C4D-CHA	2.45	1.47	1.38
23	b	606	CLA	C1C-C2C	2.45	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	C3D-C4D	-2.45	1.38	1.44
23	B	602	CLA	C3B-C4B	2.45	1.48	1.42
23	d	402	CLA	C3D-C4D	-2.45	1.38	1.44
23	b	612	CLA	C3B-C2B	2.45	1.49	1.41
23	d	403	CLA	C1B-C2B	2.44	1.49	1.43
32	t	101	LMT	O3'-C3'	-2.44	1.37	1.43
23	B	603	CLA	C3B-C2B	2.44	1.49	1.41
23	B	608	CLA	C4C-C3C	2.44	1.49	1.45
23	b	613	CLA	C1C-C2C	2.43	1.49	1.44
23	C	503	CLA	C4D-CHA	2.43	1.47	1.38
23	B	612	CLA	C3B-C4B	2.43	1.48	1.42
23	c	504	CLA	C4C-C3C	2.43	1.49	1.45
23	c	510	CLA	C4C-C3C	2.43	1.49	1.45
23	C	504	CLA	C1B-C2B	2.43	1.49	1.43
23	B	616	CLA	C3B-C4B	2.43	1.48	1.42
23	A	404	CLA	C3B-C4B	2.43	1.48	1.42
23	D	405	CLA	C3D-C4D	-2.43	1.38	1.44
23	d	403	CLA	C3D-C4D	-2.43	1.38	1.44
23	B	608	CLA	C3D-C4D	-2.43	1.38	1.44
23	C	510	CLA	C3B-C2B	2.43	1.49	1.41
40	V	202	HEC	CMB-C2B	2.43	1.55	1.50
23	B	605	CLA	C3D-C4D	-2.43	1.38	1.44
32	M	103	LMT	O3'-C3'	-2.42	1.37	1.43
23	b	608	CLA	C1B-C2B	2.42	1.49	1.43
23	B	608	CLA	C3B-C2B	2.42	1.49	1.41
23	A	404	CLA	C1C-C2C	2.42	1.49	1.44
23	b	601	CLA	C1B-C2B	2.42	1.48	1.43
32	M	101	LMT	O3'-C3'	-2.42	1.37	1.43
23	b	608	CLA	C3D-C4D	-2.42	1.38	1.44
32	b	621	LMT	C3'-C2'	2.42	1.58	1.52
23	c	510	CLA	C3B-C4B	2.41	1.48	1.42
23	d	402	CLA	C3B-C4B	2.41	1.48	1.42
23	B	602	CLA	C4C-C3C	2.41	1.49	1.45
23	b	615	CLA	C4C-C3C	2.41	1.49	1.45
23	B	601	CLA	C4D-CHA	2.41	1.47	1.38
23	C	509	CLA	C3B-C4B	2.41	1.48	1.42
23	B	612	CLA	C3B-C2B	2.41	1.49	1.41
23	b	610	CLA	C3D-C4D	-2.40	1.38	1.44
24	a	353	PHO	C4B-NB	-2.40	1.34	1.38
23	C	512	CLA	C3D-C4D	-2.40	1.38	1.44
23	B	614	CLA	C3D-C4D	-2.39	1.38	1.44
24	a	408	PHO	C4B-NB	-2.39	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406	CLA	C1C-C2C	2.39	1.49	1.44
23	C	507	CLA	C3D-C4D	-2.39	1.38	1.44
32	a	420	LMT	O3'-C3'	-2.38	1.37	1.43
23	b	611	CLA	C3B-C2B	2.38	1.49	1.41
23	D	405	CLA	C3B-C2B	2.38	1.49	1.41
23	b	609	CLA	C1C-C2C	2.38	1.49	1.44
23	c	512	CLA	C3B-C2B	2.38	1.49	1.41
23	b	615	CLA	C3D-C4D	-2.38	1.38	1.44
24	A	353	PHO	C4B-NB	-2.38	1.34	1.38
23	C	507	CLA	C1C-C2C	2.37	1.49	1.44
23	b	603	CLA	C4D-CHA	2.37	1.46	1.38
23	b	616	CLA	C4D-CHA	2.37	1.46	1.38
23	B	608	CLA	C1C-NC	-2.37	1.34	1.37
23	a	407	CLA	C3D-C4D	-2.36	1.38	1.44
23	b	603	CLA	C3B-C2B	2.36	1.49	1.41
24	A	353	PHO	C3A-C2A	-2.36	1.52	1.54
23	b	603	CLA	C1C-C2C	2.36	1.49	1.44
23	C	503	CLA	C4C-C3C	2.36	1.49	1.45
23	c	511	CLA	C3B-C2B	2.36	1.49	1.41
23	C	504	CLA	C1C-C2C	2.36	1.49	1.44
23	c	512	CLA	C1C-C2C	2.36	1.49	1.44
23	a	405	CLA	C4C-C3C	2.36	1.49	1.45
23	C	508	CLA	C3B-C4B	2.35	1.48	1.42
40	v	202	HEC	CAC-C3C	2.35	1.57	1.51
23	a	409	CLA	C4D-CHA	2.35	1.46	1.38
23	c	514	CLA	C3D-C4D	-2.35	1.38	1.44
23	c	513	CLA	C4C-C3C	2.35	1.49	1.45
23	b	613	CLA	C4C-C3C	2.34	1.49	1.45
23	b	614	CLA	C1C-C2C	2.34	1.49	1.44
23	b	609	CLA	C1B-C2B	2.34	1.48	1.43
23	B	604	CLA	C3D-C4D	-2.34	1.38	1.44
23	B	615	CLA	C4B-NB	-2.33	1.34	1.37
23	B	601	CLA	C1B-C2B	2.33	1.48	1.43
23	A	408	CLA	C3B-C4B	2.33	1.48	1.42
23	c	507	CLA	C3D-C4D	-2.33	1.38	1.44
29	d	405	PL9	C6-C5	2.33	1.47	1.35
32	a	414	LMT	O2'-C2'	-2.32	1.37	1.43
23	c	505	CLA	C4C-C3C	2.32	1.49	1.45
23	B	616	CLA	C3D-C4D	-2.32	1.38	1.44
23	C	511	CLA	C4D-CHA	2.32	1.46	1.38
23	C	510	CLA	C1C-C2C	2.32	1.49	1.44
23	B	603	CLA	C1B-C2B	2.31	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	C1C-C2C	2.31	1.49	1.44
32	A	359	LMT	O3'-C3'	-2.31	1.37	1.43
23	C	513	CLA	C1B-C2B	2.31	1.48	1.43
23	c	503	CLA	C3B-C2B	2.31	1.49	1.41
23	d	403	CLA	C4B-NB	-2.31	1.34	1.37
23	b	607	CLA	C1D-C2D	2.31	1.49	1.45
23	b	616	CLA	C3D-C4D	-2.30	1.39	1.44
23	B	603	CLA	C1C-C2C	2.30	1.49	1.44
23	C	513	CLA	C3D-C4D	-2.30	1.39	1.44
23	d	403	CLA	C4C-C3C	2.30	1.49	1.45
23	b	602	CLA	C4C-C3C	2.30	1.49	1.45
23	b	608	CLA	C3B-C2B	2.30	1.49	1.41
35	c	519	DGD	O2G-C2G	-2.30	1.40	1.46
32	E	102	LMT	O3'-C3'	-2.30	1.37	1.43
23	c	513	CLA	C1C-C2C	2.29	1.49	1.44
23	B	614	CLA	C4C-C3C	2.29	1.49	1.45
23	b	605	CLA	C1C-C2C	2.29	1.49	1.44
23	C	502	CLA	C3D-C4D	-2.28	1.39	1.44
32	D	404	LMT	O3'-C3'	-2.28	1.37	1.43
38	e	87	HEM	C1D-ND	-2.28	1.34	1.38
23	C	513	CLA	C4B-NB	-2.28	1.35	1.37
23	c	505	CLA	C1C-NC	-2.28	1.34	1.37
23	b	608	CLA	C1C-C2C	2.27	1.49	1.44
23	b	611	CLA	C3D-C4D	-2.27	1.39	1.44
38	E	103	HEM	C3C-C4C	-2.27	1.42	1.46
26	F	101	SQD	O6-C1	2.27	1.44	1.40
23	B	602	CLA	C3B-C2B	2.27	1.48	1.41
23	c	509	CLA	C1B-NB	-2.26	1.35	1.37
23	B	609	CLA	C3D-C4D	-2.26	1.39	1.44
23	C	508	CLA	C3D-C4D	-2.25	1.39	1.44
23	A	405	CLA	C3D-C4D	-2.25	1.39	1.44
23	c	505	CLA	C3B-C2B	2.25	1.48	1.41
24	a	408	PHO	C1D-ND	-2.25	1.34	1.38
23	C	505	CLA	C3B-C2B	2.25	1.48	1.41
23	b	606	CLA	C3D-C4D	-2.25	1.39	1.44
35	C	519	DGD	O2G-C2G	-2.25	1.41	1.46
23	c	508	CLA	C4C-C3C	2.25	1.48	1.45
23	b	612	CLA	C4C-C3C	2.24	1.48	1.45
32	a	414	LMT	O2B-C2B	-2.24	1.37	1.43
23	B	613	CLA	C1C-C2C	2.24	1.48	1.44
27	A	701	GOL	C3-C2	2.24	1.60	1.51
23	b	601	CLA	C3B-C2B	2.24	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	E	103	HEM	C3B-C4B	2.23	1.49	1.44
23	A	408	CLA	C1C-NC	-2.23	1.34	1.37
23	c	513	CLA	C3D-C4D	-2.23	1.39	1.44
23	c	507	CLA	C3B-C2B	2.23	1.48	1.41
35	C	518	DGD	O5D-C1E	2.22	1.44	1.40
23	B	611	CLA	C4D-CHA	2.22	1.46	1.38
23	B	601	CLA	C3B-C2B	2.22	1.48	1.41
23	B	605	CLA	C4C-C3C	2.22	1.48	1.45
23	B	613	CLA	C3B-C2B	2.22	1.48	1.41
32	m	103	LMT	C3'-C2'	2.22	1.58	1.52
23	D	406	CLA	C4B-NB	-2.21	1.35	1.37
23	C	512	CLA	C1C-NC	-2.21	1.34	1.37
23	c	512	CLA	C4C-C3C	2.21	1.48	1.45
23	B	606	CLA	C3D-C4D	-2.21	1.39	1.44
35	h	102	DGD	O5D-C1E	2.21	1.44	1.40
23	A	408	CLA	C3B-C2B	2.21	1.48	1.41
23	c	505	CLA	C3D-C4D	-2.21	1.39	1.44
23	b	602	CLA	C1B-C2B	2.21	1.48	1.43
23	b	615	CLA	C1C-C2C	2.21	1.48	1.44
23	A	404	CLA	C3B-C2B	2.20	1.48	1.41
23	c	509	CLA	C3B-C2B	2.20	1.48	1.41
23	b	614	CLA	C3B-C2B	2.20	1.48	1.41
23	B	616	CLA	C1C-NC	-2.20	1.34	1.37
27	D	701	GOL	O2-C2	-2.20	1.36	1.43
23	B	613	CLA	C3B-C4B	2.20	1.47	1.42
23	B	612	CLA	C4C-C3C	2.19	1.48	1.45
40	V	202	HEC	CMA-C3A	2.19	1.55	1.50
23	a	405	CLA	C3B-C4B	2.19	1.47	1.42
23	c	507	CLA	C1C-C2C	2.19	1.48	1.44
23	b	604	CLA	C3B-C2B	2.19	1.48	1.41
23	C	514	CLA	C3D-C4D	-2.19	1.39	1.44
23	b	605	CLA	C4C-C3C	2.19	1.48	1.45
23	B	615	CLA	C3D-C4D	-2.18	1.39	1.44
23	c	511	CLA	C4C-C3C	2.18	1.48	1.45
23	b	611	CLA	C4B-NB	-2.18	1.35	1.37
23	C	510	CLA	C1D-C2D	2.18	1.49	1.45
23	C	503	CLA	C3B-C2B	2.18	1.48	1.41
32	M	103	LMT	O3B-C3B	-2.18	1.37	1.43
24	A	353	PHO	C1D-ND	-2.18	1.34	1.38
23	D	405	CLA	C4C-C3C	2.18	1.48	1.45
23	b	605	CLA	C3D-C4D	-2.18	1.39	1.44
23	B	612	CLA	C3D-C4D	-2.17	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	C3D-C4D	-2.17	1.39	1.44
23	B	604	CLA	C3B-C2B	2.17	1.48	1.41
23	c	514	CLA	C1D-C2D	2.17	1.49	1.45
23	c	511	CLA	C3D-C4D	-2.17	1.39	1.44
23	C	511	CLA	C3D-C4D	-2.17	1.39	1.44
23	a	409	CLA	C4C-C3C	2.17	1.48	1.45
23	A	408	CLA	C4C-C3C	2.17	1.48	1.45
23	b	607	CLA	C3B-C4B	2.17	1.47	1.42
32	a	414	LMT	O3'-C3'	-2.16	1.37	1.43
23	a	405	CLA	C3B-C2B	2.16	1.48	1.41
23	B	609	CLA	C4C-C3C	2.16	1.48	1.45
23	C	506	CLA	C3D-C4D	-2.16	1.39	1.44
23	b	610	CLA	C3B-C2B	2.16	1.48	1.41
23	D	405	CLA	C3B-C4B	2.15	1.47	1.42
23	b	613	CLA	C3B-C2B	2.15	1.48	1.41
32	D	404	LMT	O5'-C5'	-2.15	1.39	1.44
32	m	103	LMT	O2B-C2B	-2.15	1.37	1.43
23	b	616	CLA	C4B-NB	-2.15	1.35	1.37
23	b	605	CLA	C3B-C2B	2.15	1.48	1.41
23	C	507	CLA	C3B-C2B	2.15	1.48	1.41
32	m	103	LMT	O3'-C3'	-2.14	1.37	1.43
23	b	607	CLA	C1A-CHA	2.14	1.52	1.43
23	B	601	CLA	C3D-C4D	-2.14	1.39	1.44
23	b	616	CLA	C3B-C2B	2.14	1.48	1.41
23	b	603	CLA	C4C-C3C	2.13	1.48	1.45
27	o	601	GOL	C1-C2	2.13	1.60	1.51
23	B	603	CLA	C3D-C4D	-2.13	1.39	1.44
23	B	615	CLA	C4C-C3C	2.13	1.48	1.45
32	t	101	LMT	O2'-C2'	-2.13	1.38	1.43
27	A	701	GOL	O2-C2	-2.13	1.37	1.43
23	C	505	CLA	C3D-C4D	-2.13	1.39	1.44
38	E	103	HEM	C1C-C2C	-2.13	1.41	1.45
23	C	513	CLA	C3B-C2B	2.13	1.48	1.41
40	v	202	HEC	CMD-C2D	2.12	1.55	1.50
29	a	416	PL9	C2-C3	2.12	1.40	1.34
27	b	624	GOL	C3-C2	2.12	1.60	1.51
32	I	101	LMT	O2'-C2'	-2.12	1.38	1.43
23	a	406	CLA	C1C-C2C	2.12	1.48	1.44
23	A	406	CLA	C1C-NC	-2.12	1.34	1.37
23	c	510	CLA	C3B-C2B	2.11	1.48	1.41
23	C	508	CLA	C4C-C3C	2.11	1.48	1.45
23	A	406	CLA	C3D-C4D	-2.11	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	404	BCR	C30-C25	-2.11	1.50	1.53
23	C	502	CLA	C3B-C2B	2.11	1.48	1.41
23	c	510	CLA	C3D-C4D	-2.11	1.39	1.44
23	b	615	CLA	C4B-NB	-2.10	1.35	1.37
23	C	505	CLA	C4C-C3C	2.10	1.48	1.45
32	D	404	LMT	O4'-C4B	-2.10	1.38	1.43
23	b	604	CLA	C4C-C3C	2.10	1.48	1.45
23	c	502	CLA	C3B-C2B	2.10	1.48	1.41
34	D	414	HTG	C1-S1	-2.10	1.77	1.80
23	a	405	CLA	C3D-C4D	-2.10	1.39	1.44
23	a	407	CLA	C4C-C3C	2.10	1.48	1.45
23	C	502	CLA	C4C-C3C	2.10	1.48	1.45
23	b	601	CLA	C4C-C3C	2.10	1.48	1.45
23	b	606	CLA	C3B-C2B	2.09	1.48	1.41
32	e	102	LMT	O2B-C2B	-2.09	1.38	1.43
23	b	604	CLA	C1A-CHA	2.09	1.51	1.43
23	d	402	CLA	C3B-C2B	2.09	1.48	1.41
23	b	614	CLA	C3D-C4D	-2.09	1.39	1.44
24	a	353	PHO	C1B-NB	-2.08	1.34	1.38
23	B	604	CLA	C1C-C2C	2.08	1.48	1.44
32	A	359	LMT	O2B-C2B	-2.08	1.38	1.43
32	t	102	LMT	O2'-C2'	-2.08	1.38	1.43
23	C	511	CLA	C3B-C2B	2.08	1.48	1.41
23	b	615	CLA	C3B-C2B	2.08	1.48	1.41
23	b	613	CLA	C3D-C4D	-2.08	1.39	1.44
23	B	606	CLA	C3B-C2B	2.07	1.48	1.41
35	c	518	DGD	O2G-C2G	-2.07	1.41	1.46
23	B	603	CLA	C4C-C3C	2.07	1.48	1.45
40	v	202	HEC	CMC-C2C	2.07	1.55	1.50
38	E	103	HEM	C1D-ND	-2.07	1.34	1.38
23	c	514	CLA	C3B-C2B	2.06	1.48	1.41
23	B	609	CLA	C4B-NB	-2.06	1.35	1.37
23	c	502	CLA	C1C-NC	-2.06	1.34	1.37
32	e	102	LMT	O2'-C2'	-2.06	1.38	1.43
26	a	413	SQD	O6-C1	2.06	1.43	1.40
23	B	611	CLA	C1D-C2D	2.06	1.49	1.45
23	c	508	CLA	C3D-C4D	-2.06	1.39	1.44
23	C	508	CLA	C3B-C2B	2.06	1.48	1.41
23	B	608	CLA	C1C-C2C	2.05	1.48	1.44
23	B	615	CLA	MG-NA	2.05	2.11	2.06
23	c	509	CLA	C3D-C4D	-2.05	1.39	1.44
32	e	102	LMT	O3B-C3B	-2.05	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	622	HTG	O5-C1	2.05	1.45	1.42
32	M	103	LMT	O2'-C2'	-2.05	1.38	1.43
24	A	407	PHO	C1B-NB	-2.05	1.34	1.38
23	B	611	CLA	C3D-C4D	-2.04	1.39	1.44
32	A	359	LMT	O2'-C2'	-2.04	1.38	1.43
23	b	614	CLA	C4C-C3C	2.04	1.48	1.45
23	c	506	CLA	C3B-C2B	2.04	1.48	1.41
29	A	414	PL9	C2-C1	-2.04	1.39	1.44
23	D	406	CLA	C3D-C4D	-2.03	1.39	1.44
23	A	404	CLA	C3D-C4D	-2.03	1.39	1.44
32	I	101	LMT	O2B-C2B	-2.03	1.38	1.43
26	B	620	SQD	O6-C1	2.02	1.43	1.40
23	C	503	CLA	C3D-C4D	-2.02	1.39	1.44
23	C	508	CLA	C1D-C2D	2.02	1.49	1.45
23	b	601	CLA	C3D-C4D	-2.02	1.39	1.44
23	C	509	CLA	C3D-C4D	-2.02	1.39	1.44
32	b	621	LMT	O3'-C3'	-2.02	1.38	1.43
34	c	522	HTG	C1-S1	-2.01	1.77	1.80
23	B	612	CLA	C1C-NC	-2.01	1.34	1.37
23	B	614	CLA	C3B-C2B	2.01	1.48	1.41
23	B	610	CLA	C3D-C4D	-2.01	1.39	1.44
23	B	604	CLA	C4B-NB	-2.01	1.35	1.37
23	A	408	CLA	C1C-C2C	2.01	1.48	1.44
23	C	512	CLA	C1A-CHA	2.01	1.51	1.43
23	c	506	CLA	C3D-C4D	-2.01	1.39	1.44
23	b	609	CLA	C1C-NC	-2.00	1.34	1.37

All (2827) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C2B-C1B-NB	16.36	121.20	110.23
23	B	611	CLA	C3B-C2B-C1B	-12.98	91.49	107.16
24	A	407	PHO	C2D-C1D-ND	11.89	117.73	109.53
23	B	611	CLA	C1D-ND-C4D	-11.74	97.99	106.33
24	a	353	PHO	C2D-C1D-ND	11.37	117.38	109.53
24	a	408	PHO	C2D-C1D-ND	11.17	117.24	109.53
24	A	353	PHO	C2D-C1D-ND	10.94	117.08	109.53
23	B	612	CLA	C1D-ND-C4D	-10.65	98.77	106.33
23	a	409	CLA	C1D-ND-C4D	-10.54	98.85	106.33
23	B	601	CLA	C1D-ND-C4D	-10.12	99.15	106.33
23	B	611	CLA	CHB-C1B-NB	-10.12	113.55	124.26
23	C	514	CLA	C1D-ND-C4D	-9.95	99.27	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	C1D-ND-C4D	-9.91	99.30	106.33
23	b	611	CLA	C1D-ND-C4D	-9.90	99.31	106.33
23	b	607	CLA	C1D-ND-C4D	-9.87	99.33	106.33
23	c	506	CLA	C1D-ND-C4D	-9.81	99.37	106.33
23	b	603	CLA	C1D-ND-C4D	-9.77	99.40	106.33
23	B	611	CLA	C2D-C1D-ND	9.75	117.29	110.10
23	d	403	CLA	C1D-ND-C4D	-9.67	99.46	106.33
23	A	408	CLA	C1D-ND-C4D	-9.62	99.50	106.33
23	c	514	CLA	C1D-ND-C4D	-9.59	99.52	106.33
23	b	605	CLA	C1D-ND-C4D	-9.58	99.53	106.33
23	B	614	CLA	C1D-ND-C4D	-9.57	99.53	106.33
23	C	504	CLA	C1D-ND-C4D	-9.54	99.56	106.33
23	C	502	CLA	C1D-ND-C4D	-9.48	99.60	106.33
23	c	504	CLA	C1D-ND-C4D	-9.40	99.65	106.33
23	b	614	CLA	C1D-ND-C4D	-9.40	99.66	106.33
23	C	511	CLA	C1D-ND-C4D	-9.36	99.68	106.33
23	B	615	CLA	C1D-ND-C4D	-9.36	99.69	106.33
23	a	409	CLA	C2D-C1D-ND	9.35	117.00	110.10
23	B	605	CLA	C1D-ND-C4D	-9.34	99.70	106.33
23	b	610	CLA	C1D-ND-C4D	-9.32	99.71	106.33
23	C	506	CLA	C1D-ND-C4D	-9.31	99.72	106.33
23	b	601	CLA	C1D-ND-C4D	-9.31	99.72	106.33
23	B	610	CLA	C1D-ND-C4D	-9.30	99.73	106.33
23	b	611	CLA	C2D-C1D-ND	9.29	116.95	110.10
23	C	510	CLA	C1D-ND-C4D	-9.28	99.74	106.33
23	c	512	CLA	C1D-ND-C4D	-9.26	99.75	106.33
23	B	603	CLA	C1D-ND-C4D	-9.26	99.76	106.33
23	B	614	CLA	C2D-C1D-ND	9.22	116.90	110.10
23	b	616	CLA	C1D-ND-C4D	-9.19	99.81	106.33
23	C	505	CLA	C1D-ND-C4D	-9.19	99.81	106.33
23	b	612	CLA	C1D-ND-C4D	-9.18	99.81	106.33
23	a	407	CLA	C1D-ND-C4D	-9.17	99.82	106.33
23	D	405	CLA	C1D-ND-C4D	-9.16	99.83	106.33
23	b	614	CLA	C2D-C1D-ND	9.16	116.86	110.10
23	c	503	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	b	615	CLA	C1D-ND-C4D	-9.12	99.86	106.33
23	c	502	CLA	C1D-ND-C4D	-9.12	99.86	106.33
23	C	505	CLA	C2D-C1D-ND	9.12	116.82	110.10
23	c	507	CLA	C1D-ND-C4D	-9.10	99.87	106.33
23	d	402	CLA	C1D-ND-C4D	-9.09	99.88	106.33
23	B	612	CLA	C2D-C1D-ND	9.09	116.80	110.10
23	A	406	CLA	C1D-ND-C4D	-9.08	99.89	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	C1D-ND-C4D	-9.04	99.91	106.33
23	C	503	CLA	C1D-ND-C4D	-9.04	99.91	106.33
23	a	406	CLA	C1D-ND-C4D	-9.04	99.91	106.33
23	C	513	CLA	C1D-ND-C4D	-9.03	99.92	106.33
23	c	510	CLA	C1D-ND-C4D	-9.01	99.94	106.33
23	B	616	CLA	C1D-ND-C4D	-9.01	99.94	106.33
23	B	610	CLA	C2D-C1D-ND	8.99	116.73	110.10
23	B	607	CLA	C1D-ND-C4D	-8.98	99.96	106.33
23	C	507	CLA	C1D-ND-C4D	-8.97	99.96	106.33
23	c	508	CLA	C1D-ND-C4D	-8.97	99.96	106.33
23	b	606	CLA	C1D-ND-C4D	-8.97	99.97	106.33
23	b	613	CLA	C2D-C1D-ND	8.96	116.71	110.10
23	B	609	CLA	C1D-ND-C4D	-8.95	99.98	106.33
23	b	609	CLA	C1D-ND-C4D	-8.91	100.00	106.33
23	A	405	CLA	C1D-ND-C4D	-8.91	100.01	106.33
23	B	602	CLA	C1D-ND-C4D	-8.90	100.02	106.33
23	B	615	CLA	C2D-C1D-ND	8.89	116.66	110.10
23	B	616	CLA	C2D-C1D-ND	8.88	116.65	110.10
23	b	607	CLA	C2D-C1D-ND	8.88	116.65	110.10
23	B	606	CLA	C2D-C1D-ND	8.87	116.64	110.10
23	C	514	CLA	C2D-C1D-ND	8.84	116.62	110.10
23	a	405	CLA	C1D-ND-C4D	-8.83	100.06	106.33
23	B	601	CLA	C2D-C1D-ND	8.82	116.60	110.10
23	B	613	CLA	C1D-ND-C4D	-8.81	100.08	106.33
23	C	508	CLA	C1D-ND-C4D	-8.79	100.09	106.33
23	a	406	CLA	C2D-C1D-ND	8.75	116.56	110.10
23	b	613	CLA	C1D-ND-C4D	-8.75	100.12	106.33
23	D	406	CLA	C1D-ND-C4D	-8.74	100.12	106.33
23	A	408	CLA	C2D-C1D-ND	8.74	116.54	110.10
23	a	407	CLA	C2D-C1D-ND	8.65	116.48	110.10
23	c	511	CLA	C1D-ND-C4D	-8.64	100.19	106.33
23	B	608	CLA	C1D-ND-C4D	-8.63	100.20	106.33
23	c	505	CLA	C1D-ND-C4D	-8.63	100.21	106.33
23	B	608	CLA	C2D-C1D-ND	8.60	116.44	110.10
23	C	512	CLA	C1D-ND-C4D	-8.58	100.24	106.33
23	c	509	CLA	C1D-ND-C4D	-8.52	100.28	106.33
23	C	509	CLA	C1D-ND-C4D	-8.51	100.29	106.33
23	b	603	CLA	C2D-C1D-ND	8.51	116.38	110.10
23	D	405	CLA	C2D-C1D-ND	8.50	116.37	110.10
23	A	404	CLA	C1D-ND-C4D	-8.50	100.30	106.33
23	B	613	CLA	C2D-C1D-ND	8.50	116.36	110.10
23	b	602	CLA	C2B-C1B-NB	8.49	115.93	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	C4A-NA-C1A	-8.49	102.89	106.71
23	b	608	CLA	C1D-ND-C4D	-8.43	100.35	106.33
23	c	513	CLA	C2B-C1B-NB	8.42	115.88	110.23
23	b	615	CLA	C2D-C1D-ND	8.41	116.30	110.10
23	b	605	CLA	C2D-C1D-ND	8.38	116.28	110.10
23	c	513	CLA	C1D-ND-C4D	-8.38	100.39	106.33
23	C	513	CLA	C2D-C1D-ND	8.34	116.25	110.10
23	B	605	CLA	C2D-C1D-ND	8.33	116.24	110.10
23	C	504	CLA	C2D-C1D-ND	8.29	116.21	110.10
23	A	405	CLA	C2D-C1D-ND	8.25	116.18	110.10
23	C	513	CLA	C2B-C1B-NB	8.24	115.76	110.23
23	c	503	CLA	C2D-C1D-ND	8.23	116.17	110.10
23	B	607	CLA	C2D-C1D-ND	8.22	116.16	110.10
23	c	509	CLA	C2D-C1D-ND	8.20	116.14	110.10
23	b	604	CLA	C1D-ND-C4D	-8.18	100.52	106.33
23	c	511	CLA	C2D-C1D-ND	8.18	116.13	110.10
23	C	509	CLA	C2D-C1D-ND	8.18	116.13	110.10
23	B	603	CLA	C2D-C1D-ND	8.16	116.11	110.10
23	A	406	CLA	C2D-C1D-ND	8.15	116.11	110.10
23	B	609	CLA	C2D-C1D-ND	8.15	116.11	110.10
23	b	609	CLA	C2D-C1D-ND	8.14	116.11	110.10
23	c	505	CLA	C2D-C1D-ND	8.14	116.11	110.10
24	a	408	PHO	O2D-CGD-CBD	8.14	121.31	111.00
23	C	503	CLA	C2D-C1D-ND	8.13	116.10	110.10
23	c	508	CLA	C2D-C1D-ND	8.09	116.07	110.10
23	c	502	CLA	C2D-C1D-ND	8.09	116.07	110.10
23	b	610	CLA	C2D-C1D-ND	8.08	116.06	110.10
23	c	512	CLA	C2D-C1D-ND	8.06	116.05	110.10
23	b	612	CLA	C2D-C1D-ND	8.05	116.04	110.10
23	b	601	CLA	C2D-C1D-ND	8.01	116.00	110.10
23	b	616	CLA	C2D-C1D-ND	7.98	115.98	110.10
23	C	508	CLA	C2D-C1D-ND	7.97	115.98	110.10
23	C	502	CLA	C2D-C1D-ND	7.96	115.97	110.10
23	d	403	CLA	C2D-C1D-ND	7.96	115.97	110.10
23	D	406	CLA	C2D-C1D-ND	7.95	115.97	110.10
23	c	504	CLA	C2D-C1D-ND	7.90	115.93	110.10
23	c	506	CLA	C2D-C1D-ND	7.86	115.90	110.10
23	B	602	CLA	C2D-C1D-ND	7.84	115.88	110.10
23	c	510	CLA	C2D-C1D-ND	7.84	115.88	110.10
24	a	353	PHO	O2D-CGD-CBD	7.83	120.91	111.00
23	d	402	CLA	C2D-C1D-ND	7.82	115.87	110.10
23	c	514	CLA	C2D-C1D-ND	7.77	115.83	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	C2D-C1D-ND	7.75	115.82	110.10
23	C	510	CLA	C2B-C1B-NB	7.72	115.41	110.23
23	c	507	CLA	C2D-C1D-ND	7.71	115.79	110.10
23	C	507	CLA	C2D-C1D-ND	7.69	115.77	110.10
23	b	606	CLA	C2B-C1B-NB	7.68	115.38	110.23
23	c	514	CLA	C2B-C1B-NB	7.68	115.38	110.23
23	C	512	CLA	C2D-C1D-ND	7.66	115.75	110.10
23	B	601	CLA	C2B-C1B-NB	7.66	115.36	110.23
23	C	511	CLA	C2D-C1D-ND	7.64	115.74	110.10
23	A	404	CLA	C2D-C1D-ND	7.64	115.73	110.10
23	B	611	CLA	CHD-C4C-C3C	-7.63	113.63	124.84
23	b	614	CLA	C2B-C1B-NB	7.60	115.32	110.23
23	B	604	CLA	C1D-ND-C4D	-7.54	100.98	106.33
23	b	606	CLA	C2D-C1D-ND	7.54	115.66	110.10
23	A	406	CLA	C2B-C1B-NB	7.52	115.27	110.23
23	b	608	CLA	C2D-C1D-ND	7.51	115.64	110.10
23	d	403	CLA	C2B-C1B-NB	7.49	115.25	110.23
24	A	353	PHO	C2B-C1B-NB	7.46	114.68	109.53
24	A	353	PHO	O2D-CGD-CBD	7.46	120.44	111.00
23	b	616	CLA	C2B-C1B-NB	7.46	115.23	110.23
23	c	505	CLA	C2B-C1B-NB	7.45	115.23	110.23
23	b	604	CLA	C2D-C1D-ND	7.45	115.59	110.10
23	C	506	CLA	C2D-C1D-ND	7.42	115.58	110.10
23	C	507	CLA	C2B-C1B-NB	7.41	115.20	110.23
23	B	611	CLA	CMD-C2D-C1D	7.36	137.69	124.71
24	A	407	PHO	C4D-ND-C1D	-7.35	101.35	108.83
23	B	609	CLA	C2B-C1B-NB	7.35	115.16	110.23
23	a	405	CLA	C2D-C1D-ND	7.32	115.50	110.10
23	B	606	CLA	CMD-C2D-C1D	7.28	137.55	124.71
23	B	606	CLA	C4A-NA-C1A	-7.27	103.44	106.71
23	b	608	CLA	C2B-C1B-NB	7.26	115.10	110.23
23	c	509	CLA	C2B-C1B-NB	7.25	115.09	110.23
23	A	408	CLA	C2B-C1B-NB	7.24	115.09	110.23
23	B	608	CLA	C2B-C1B-NB	7.23	115.08	110.23
23	c	502	CLA	CMD-C2D-C1D	7.23	137.45	124.71
23	C	514	CLA	C2B-C1B-NB	7.22	115.07	110.23
23	D	405	CLA	C4A-NA-C1A	-7.21	103.46	106.71
23	B	614	CLA	C2B-C1B-NB	7.17	115.04	110.23
23	b	601	CLA	C2B-C1B-NB	7.17	115.04	110.23
26	F	101	SQD	O6-C1-C2	7.17	119.50	108.30
23	A	405	CLA	C2B-C1B-NB	7.15	115.03	110.23
23	B	605	CLA	CHD-C4C-C3C	-7.15	114.33	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	C2B-C1B-NB	7.15	115.02	110.23
23	C	512	CLA	C2B-C1B-NB	7.14	115.02	110.23
23	C	511	CLA	CMD-C2D-C1D	7.14	137.29	124.71
23	b	616	CLA	C4A-NA-C1A	-7.13	103.50	106.71
23	B	611	CLA	CMB-C2B-C1B	7.13	136.22	125.37
34	b	623	HTG	C1'-S1-C1	7.11	113.38	100.09
23	c	511	CLA	C2B-C1B-NB	7.09	114.99	110.23
23	C	508	CLA	CMD-C2D-C1D	7.09	137.22	124.71
23	B	609	CLA	C4A-NA-C1A	-7.07	103.53	106.71
23	c	513	CLA	C2D-C1D-ND	7.06	115.31	110.10
23	c	514	CLA	CMD-C2D-C1D	7.06	137.15	124.71
23	c	503	CLA	C2B-C1B-NB	7.04	114.95	110.23
23	b	602	CLA	C2D-C1D-ND	7.04	115.29	110.10
23	b	611	CLA	C2B-C1B-NB	7.02	114.94	110.23
23	B	606	CLA	CHD-C1D-ND	-7.01	118.01	124.45
23	c	510	CLA	C2B-C1B-NB	7.01	114.93	110.23
23	b	611	CLA	CHD-C1D-ND	-7.00	118.02	124.45
23	C	502	CLA	C2B-C1B-NB	6.99	114.92	110.23
23	c	504	CLA	CMD-C2D-C1D	6.99	137.03	124.71
23	d	403	CLA	CMD-C2D-C1D	6.99	137.02	124.71
23	b	611	CLA	CMD-C2D-C1D	6.97	137.00	124.71
23	C	511	CLA	C2B-C1B-NB	6.97	114.90	110.23
23	b	615	CLA	C4A-NA-C1A	-6.95	103.58	106.71
23	a	407	CLA	C2B-C1B-NB	6.94	114.89	110.23
23	a	406	CLA	C2B-C1B-NB	6.94	114.88	110.23
24	a	353	PHO	C2B-C1B-NB	6.92	114.30	109.53
23	B	616	CLA	CHD-C4C-C3C	-6.91	114.68	124.84
23	c	508	CLA	CMD-C2D-C1D	6.91	136.89	124.71
23	c	504	CLA	C2B-C1B-NB	6.90	114.86	110.23
23	b	603	CLA	C2B-C1B-NB	6.89	114.85	110.23
23	D	406	CLA	C2B-C1B-NB	6.88	114.85	110.23
23	b	606	CLA	CMD-C2D-C1D	6.88	136.84	124.71
23	c	502	CLA	CHD-C1D-ND	-6.88	118.13	124.45
23	b	606	CLA	C4A-NA-C1A	-6.87	103.62	106.71
23	c	508	CLA	O2D-CGD-CBD	6.86	123.46	111.27
23	a	409	CLA	C2B-C1B-NB	6.86	114.83	110.23
23	a	409	CLA	CHD-C4C-C3C	-6.85	114.77	124.84
23	C	509	CLA	C2C-C1C-NC	6.85	116.39	109.97
23	b	605	CLA	C2B-C1B-NB	6.83	114.81	110.23
23	B	616	CLA	O2D-CGD-CBD	6.83	123.40	111.27
23	b	601	CLA	O2D-CGD-CBD	6.83	123.40	111.27
23	b	607	CLA	C2C-C1C-NC	6.81	116.35	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	O2D-CGD-CBD	6.78	123.32	111.27
23	B	601	CLA	CHD-C4C-C3C	-6.74	114.93	124.84
23	a	405	CLA	C2B-C1B-NB	6.74	114.75	110.23
23	C	513	CLA	C4A-NA-C1A	-6.74	103.68	106.71
23	C	503	CLA	C2B-C1B-NB	6.74	114.75	110.23
24	a	353	PHO	C4D-ND-C1D	-6.72	101.99	108.83
23	b	611	CLA	CHD-C4C-C3C	-6.71	114.98	124.84
23	A	404	CLA	CMD-C2D-C1D	6.70	136.53	124.71
34	c	522	HTG	C1'-S1-C1	6.69	112.60	100.09
23	B	614	CLA	CMD-C2D-C1D	6.69	136.50	124.71
23	b	616	CLA	O2D-CGD-CBD	6.68	123.14	111.27
23	b	610	CLA	C2B-C1B-NB	6.66	114.69	110.23
23	A	404	CLA	C2B-C1B-NB	6.65	114.69	110.23
23	b	616	CLA	CHD-C4C-C3C	-6.65	115.07	124.84
23	c	504	CLA	C4A-NA-C1A	-6.65	103.72	106.71
23	C	513	CLA	CHD-C4C-C3C	-6.62	115.11	124.84
23	b	605	CLA	CHD-C4C-C3C	-6.62	115.11	124.84
23	a	406	CLA	CHD-C4C-C3C	-6.61	115.12	124.84
23	C	504	CLA	CMD-C2D-C1D	6.61	136.35	124.71
23	C	505	CLA	C2B-C1B-NB	6.59	114.65	110.23
23	b	615	CLA	C2B-C1B-NB	6.59	114.65	110.23
23	B	607	CLA	C2B-C1B-NB	6.58	114.65	110.23
23	C	508	CLA	O2D-CGD-CBD	6.58	122.97	111.27
23	B	606	CLA	CHD-C4C-C3C	-6.58	115.17	124.84
23	B	610	CLA	C2B-C1B-NB	6.57	114.63	110.23
23	B	606	CLA	C2B-C1B-NB	6.55	114.62	110.23
23	b	613	CLA	C2B-C1B-NB	6.54	114.62	110.23
23	c	502	CLA	C2B-C1B-NB	6.54	114.61	110.23
23	B	601	CLA	CMD-C2D-C1D	6.52	136.21	124.71
23	C	504	CLA	C4A-NA-C1A	-6.52	103.77	106.71
23	B	615	CLA	CHD-C4C-C3C	-6.52	115.25	124.84
23	C	514	CLA	CHD-C4C-C3C	-6.51	115.27	124.84
23	c	514	CLA	CHD-C1D-ND	-6.51	118.47	124.45
23	B	603	CLA	C2B-C1B-NB	6.51	114.60	110.23
23	b	605	CLA	CMD-C2D-C1D	6.49	136.16	124.71
23	d	402	CLA	C2C-C1C-NC	6.49	116.05	109.97
24	a	408	PHO	C2B-C1B-NB	6.49	114.01	109.53
23	b	616	CLA	CMD-C2D-C1D	6.49	136.15	124.71
23	B	602	CLA	C2B-C1B-NB	6.48	114.58	110.23
24	a	408	PHO	C1C-C2C-C3C	-6.48	103.22	108.61
23	b	612	CLA	CHD-C4C-C3C	-6.47	115.33	124.84
23	b	609	CLA	C2B-C1B-NB	6.47	114.57	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	C2C-C1C-NC	6.47	116.03	109.97
23	C	506	CLA	CMD-C2D-C1D	6.46	136.10	124.71
23	b	610	CLA	CHD-C4C-C3C	-6.46	115.35	124.84
23	C	510	CLA	CHD-C1D-ND	-6.45	118.53	124.45
23	A	404	CLA	C4A-NA-C1A	-6.44	103.81	106.71
26	A	410	SQD	O6-C1-C2	6.44	118.36	108.30
24	A	353	PHO	C1C-C2C-C3C	-6.44	103.26	108.61
23	c	503	CLA	CHD-C4C-C3C	-6.43	115.39	124.84
24	A	353	PHO	C4D-ND-C1D	-6.43	102.29	108.83
23	c	508	CLA	CHD-C1D-ND	-6.42	118.55	124.45
23	B	614	CLA	CHD-C1D-ND	-6.42	118.55	124.45
23	c	506	CLA	C2B-C1B-NB	6.41	114.53	110.23
23	a	407	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
23	B	613	CLA	C2B-C1B-NB	6.39	114.52	110.23
23	b	613	CLA	CHD-C4C-C3C	-6.38	115.46	124.84
23	b	609	CLA	CHD-C4C-C3C	-6.38	115.46	124.84
23	c	512	CLA	C2B-C1B-NB	6.38	114.51	110.23
23	B	604	CLA	C2D-C1D-ND	6.37	114.80	110.10
23	b	606	CLA	CHD-C1D-ND	-6.37	118.60	124.45
23	B	602	CLA	C4A-NA-C1A	-6.37	103.84	106.71
23	B	611	CLA	CHD-C1D-ND	-6.36	118.61	124.45
23	C	508	CLA	CHD-C4C-C3C	-6.35	115.50	124.84
23	C	507	CLA	CHD-C1D-ND	-6.34	118.63	124.45
23	B	616	CLA	C2B-C1B-NB	6.33	114.47	110.23
23	b	604	CLA	C2C-C1C-NC	6.32	115.90	109.97
23	C	506	CLA	C2B-C1B-NB	6.32	114.47	110.23
24	a	353	PHO	C1C-C2C-C3C	-6.32	103.36	108.61
23	C	508	CLA	CHD-C1D-ND	-6.31	118.66	124.45
23	A	408	CLA	CMD-C2D-C1D	6.30	135.82	124.71
23	c	507	CLA	C2B-C1B-NB	6.29	114.45	110.23
23	A	408	CLA	C2C-C1C-NC	6.29	115.87	109.97
23	b	605	CLA	CHD-C1D-ND	-6.29	118.67	124.45
23	b	609	CLA	C4A-NA-C1A	-6.29	103.88	106.71
23	c	506	CLA	C4A-NA-C1A	-6.29	103.88	106.71
23	c	507	CLA	CMD-C2D-C1D	6.27	135.76	124.71
23	B	603	CLA	CHD-C4C-C3C	-6.27	115.62	124.84
23	b	614	CLA	O2D-CGD-CBD	6.26	122.39	111.27
23	B	610	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
23	B	604	CLA	C2B-C1B-NB	6.25	114.42	110.23
23	C	502	CLA	C4A-NA-C1A	-6.25	103.90	106.71
23	C	510	CLA	C4A-NA-C1A	-6.25	103.90	106.71
23	c	511	CLA	CHD-C4C-C3C	-6.24	115.66	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	CHD-C4C-C3C	-6.24	115.67	124.84
24	A	407	PHO	O2D-CGD-CBD	6.23	118.89	111.00
23	A	408	CLA	CHD-C1D-ND	-6.23	118.73	124.45
23	B	601	CLA	CHD-C1D-ND	-6.23	118.73	124.45
23	b	603	CLA	C4A-NA-C1A	-6.23	103.91	106.71
23	d	403	CLA	CHD-C1D-ND	-6.22	118.73	124.45
23	c	512	CLA	CMD-C2D-C1D	6.22	135.67	124.71
23	c	506	CLA	CMD-C2D-C1D	6.21	135.66	124.71
23	B	605	CLA	CMD-C2D-C1D	6.21	135.66	124.71
23	c	510	CLA	CMD-C2D-C1D	6.21	135.66	124.71
24	A	407	PHO	C1C-C2C-C3C	-6.21	103.45	108.61
23	a	405	CLA	C2C-C1C-NC	6.21	115.79	109.97
26	F	101	SQD	O47-C7-C8	6.19	124.85	111.50
23	a	405	CLA	C4A-NA-C1A	-6.18	103.93	106.71
23	B	604	CLA	C2C-C1C-NC	6.17	115.76	109.97
23	b	605	CLA	C4A-NA-C1A	-6.17	103.93	106.71
40	V	202	HEC	C1D-ND-C4D	6.17	111.45	105.07
23	a	407	CLA	C4A-NA-C1A	-6.17	103.93	106.71
23	D	406	CLA	C4A-NA-C1A	-6.16	103.94	106.71
23	A	406	CLA	CHD-C1D-ND	-6.14	118.81	124.45
24	A	407	PHO	C2B-C1B-NB	6.14	113.77	109.53
23	b	602	CLA	CHD-C1D-ND	-6.14	118.81	124.45
23	B	610	CLA	O2D-CGD-CBD	6.14	122.17	111.27
23	a	407	CLA	CHD-C1D-ND	-6.14	118.81	124.45
23	b	601	CLA	CMD-C2D-C1D	6.13	135.52	124.71
23	b	601	CLA	CHD-C4C-C3C	-6.13	115.84	124.84
23	b	603	CLA	CHD-C4C-C3C	-6.12	115.85	124.84
23	B	601	CLA	O2D-CGD-CBD	6.12	122.14	111.27
23	A	404	CLA	CHD-C1D-ND	-6.11	118.83	124.45
23	c	505	CLA	CMD-C2D-C1D	6.11	135.49	124.71
23	C	507	CLA	CMD-C2D-C1D	6.11	135.48	124.71
23	C	511	CLA	CHD-C1D-ND	-6.11	118.84	124.45
23	D	405	CLA	CMD-C2D-C1D	6.10	135.47	124.71
23	B	609	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
23	c	513	CLA	C4A-NA-C1A	-6.10	103.96	106.71
23	C	508	CLA	C4A-NA-C1A	-6.10	103.96	106.71
23	B	604	CLA	CMD-C2D-C1D	6.10	135.46	124.71
23	c	507	CLA	C2C-C1C-NC	6.10	115.68	109.97
23	C	509	CLA	CHD-C4C-C3C	-6.10	115.88	124.84
23	B	602	CLA	CMD-C2D-C1D	6.09	135.45	124.71
23	C	502	CLA	CHD-C4C-C3C	-6.08	115.91	124.84
23	C	505	CLA	C2C-C1C-NC	6.08	115.66	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	v	202	HEC	C1D-ND-C4D	6.07	111.35	105.07
23	c	504	CLA	CHD-C4C-C3C	-6.07	115.91	124.84
23	a	405	CLA	CMD-C2D-C1D	6.07	135.41	124.71
23	b	608	CLA	C2C-C1C-NC	6.07	115.66	109.97
23	b	612	CLA	C2B-C1B-NB	6.06	114.29	110.23
23	C	502	CLA	O2D-CGD-CBD	6.06	122.03	111.27
23	c	506	CLA	CHD-C1D-ND	-6.06	118.89	124.45
23	B	612	CLA	CHD-C4C-C3C	-6.06	115.94	124.84
24	a	408	PHO	C4D-ND-C1D	-6.05	102.68	108.83
23	B	606	CLA	O2D-CGD-CBD	6.05	122.01	111.27
23	B	614	CLA	C4A-NA-C1A	-6.04	103.99	106.71
23	c	505	CLA	CHD-C1D-ND	-6.04	118.91	124.45
23	c	513	CLA	CMD-C2D-C1D	6.03	135.35	124.71
23	B	614	CLA	C2C-C1C-NC	6.03	115.62	109.97
23	c	508	CLA	CHD-C4C-C3C	-6.03	115.97	124.84
23	B	610	CLA	CMD-C2D-C1D	6.03	135.34	124.71
23	C	502	CLA	CMD-C2D-C1D	6.02	135.33	124.71
23	b	604	CLA	CHD-C4C-C3C	-6.02	115.98	124.84
23	B	605	CLA	C4A-NA-C1A	-6.02	104.00	106.71
23	c	507	CLA	CHD-C1D-ND	-6.02	118.92	124.45
23	d	402	CLA	C2B-C1B-NB	6.01	114.26	110.23
23	B	614	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
23	b	616	CLA	CHD-C1D-ND	-6.01	118.93	124.45
23	C	505	CLA	CHD-C1D-ND	-6.01	118.93	124.45
23	C	504	CLA	CHD-C1D-ND	-6.00	118.94	124.45
23	B	603	CLA	C4A-NA-C1A	-6.00	104.01	106.71
23	b	604	CLA	O2D-CGD-CBD	6.00	121.92	111.27
23	B	615	CLA	C2B-C1B-NB	5.98	114.24	110.23
23	C	506	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
23	C	508	CLA	C2B-C1B-NB	5.97	114.24	110.23
23	b	615	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
23	b	601	CLA	CHD-C1D-ND	-5.97	118.97	124.45
23	B	608	CLA	C2C-C1C-NC	5.96	115.56	109.97
23	c	512	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
23	b	602	CLA	CMD-C2D-C1D	5.95	135.20	124.71
23	B	615	CLA	CMD-C2D-C1D	5.95	135.20	124.71
23	b	606	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
23	a	406	CLA	CMD-C2D-C1D	5.93	135.16	124.71
23	c	503	CLA	C2C-C1C-NC	5.92	115.52	109.97
23	A	406	CLA	C4A-NA-C1A	-5.91	104.05	106.71
23	D	405	CLA	CHD-C1D-ND	-5.91	119.02	124.45
23	C	503	CLA	CHD-C4C-C3C	-5.91	116.16	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	CMD-C2D-C1D	5.91	135.12	124.71
23	B	602	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
23	b	613	CLA	C2C-C1C-NC	5.90	115.50	109.97
23	c	508	CLA	C2C-C1C-NC	5.90	115.50	109.97
23	C	511	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
23	A	406	CLA	CMD-C2D-C1D	5.89	135.10	124.71
23	c	509	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
23	c	508	CLA	C2B-C1B-NB	5.89	114.18	110.23
23	C	504	CLA	CHD-C4C-C3C	-5.89	116.19	124.84
23	B	608	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
23	D	405	CLA	C2C-C1C-NC	5.88	115.48	109.97
23	b	615	CLA	CMD-C2D-C1D	5.87	135.06	124.71
23	B	609	CLA	CMD-C2D-C1D	5.86	135.04	124.71
23	B	613	CLA	C2C-C1C-NC	5.86	115.46	109.97
23	B	607	CLA	C2C-C1C-NC	5.86	115.46	109.97
23	A	406	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
23	C	502	CLA	CHD-C1D-ND	-5.84	119.08	124.45
23	b	607	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
23	A	404	CLA	C2C-C1C-NC	5.84	115.44	109.97
23	b	602	CLA	O2D-CGD-CBD	5.84	121.64	111.27
23	b	612	CLA	C2C-C1C-NC	5.83	115.43	109.97
23	B	615	CLA	C2C-C1C-NC	5.82	115.43	109.97
34	D	414	HTG	C1'-S1-C1	5.82	110.98	100.09
23	B	612	CLA	CHD-C1D-ND	-5.82	119.10	124.45
26	B	620	SQD	O6-C1-C2	5.82	117.39	108.30
23	C	512	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
23	B	609	CLA	CHD-C1D-ND	-5.81	119.12	124.45
23	C	514	CLA	CHD-C1D-ND	-5.81	119.12	124.45
23	b	607	CLA	CMD-C2D-C1D	5.81	134.94	124.71
23	C	509	CLA	C2B-C1B-NB	5.80	114.12	110.23
23	C	510	CLA	CMD-C2D-C1D	5.77	134.89	124.71
23	C	505	CLA	CHD-C4C-C3C	-5.77	116.35	124.84
23	B	607	CLA	CHD-C1D-ND	-5.77	119.15	124.45
23	A	405	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
23	b	607	CLA	CHD-C1D-ND	-5.77	119.15	124.45
23	B	603	CLA	CMD-C2D-C1D	5.77	134.88	124.71
23	C	512	CLA	C2C-C1C-NC	5.76	115.37	109.97
23	c	511	CLA	CMD-C2D-C1D	5.76	134.86	124.71
23	C	511	CLA	C2C-C1C-NC	5.75	115.36	109.97
23	c	506	CLA	O2D-CGD-CBD	5.75	121.48	111.27
23	B	607	CLA	CMD-C2D-C1D	5.74	134.84	124.71
23	b	613	CLA	C4A-NA-C1A	-5.74	104.12	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	C2C-C1C-NC	5.72	115.33	109.97
38	E	103	HEM	CAD-CBD-CGD	5.71	125.90	113.60
23	c	510	CLA	C1-C2-C3	-5.70	116.18	126.04
26	a	411	SQD	O6-C1-C2	5.69	117.19	108.30
23	d	403	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
23	D	406	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
23	b	611	CLA	C4A-NA-C1A	-5.69	104.15	106.71
23	A	408	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
23	b	608	CLA	CMD-C2D-C1D	5.68	134.73	124.71
23	b	608	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
23	c	506	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
23	B	611	CLA	O2D-CGD-CBD	5.66	121.33	111.27
23	C	505	CLA	CMD-C2D-C1D	5.65	134.66	124.71
23	B	615	CLA	CHD-C1D-ND	-5.65	119.27	124.45
23	b	609	CLA	CHD-C1D-ND	-5.65	119.27	124.45
23	c	504	CLA	CHD-C1D-ND	-5.65	119.27	124.45
26	A	410	SQD	C1-O5-C5	-5.64	102.61	113.69
23	b	615	CLA	C2C-C1C-NC	5.64	115.25	109.97
23	c	502	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
23	B	614	CLA	O2D-CGD-CBD	5.63	121.28	111.27
23	B	610	CLA	CHD-C1D-ND	-5.63	119.28	124.45
23	c	513	CLA	CHD-C1D-ND	-5.62	119.29	124.45
23	c	514	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
23	C	510	CLA	C2C-C1C-NC	5.62	115.23	109.97
23	c	505	CLA	CHD-C4C-C3C	-5.62	116.59	124.84
23	c	512	CLA	CHD-C1D-ND	-5.61	119.30	124.45
23	c	511	CLA	C4A-NA-C1A	-5.61	104.19	106.71
23	C	513	CLA	O2D-CGD-CBD	5.60	121.22	111.27
23	b	604	CLA	C1-C2-C3	-5.60	116.36	126.04
23	b	604	CLA	CMD-C2D-C1D	5.59	134.57	124.71
23	C	503	CLA	C2C-C1C-NC	5.59	115.21	109.97
23	b	602	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
23	C	514	CLA	CMD-C2D-C1D	5.59	134.56	124.71
23	b	607	CLA	C2B-C1B-NB	5.58	113.98	110.23
23	b	613	CLA	CMD-C2D-C1D	5.58	134.55	124.71
23	b	604	CLA	C2B-C1B-NB	5.57	113.97	110.23
23	c	509	CLA	C2C-C1C-NC	5.57	115.19	109.97
34	d	411	HTG	C1'-S1-C1	5.57	110.51	100.09
23	b	614	CLA	CMD-C2D-C1D	5.56	134.52	124.71
23	a	409	CLA	CHD-C1D-ND	-5.56	119.34	124.45
23	B	611	CLA	C3D-C2D-C1D	-5.56	98.24	105.83
23	B	603	CLA	C2C-C1C-NC	5.56	115.18	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	522	HTG	C1'-S1-C1	5.55	110.48	100.09
23	A	405	CLA	C2C-C1C-NC	5.54	115.17	109.97
23	D	405	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
23	C	506	CLA	CHD-C1D-ND	-5.53	119.38	124.45
23	B	602	CLA	C2C-C1C-NC	5.52	115.14	109.97
23	d	403	CLA	C4A-NA-C1A	-5.52	104.22	106.71
23	b	608	CLA	CHD-C1D-ND	-5.52	119.39	124.45
23	B	605	CLA	C2B-C1B-NB	5.51	113.93	110.23
23	b	601	CLA	C4A-NA-C1A	-5.51	104.23	106.71
23	b	603	CLA	O2D-CGD-CBD	5.51	121.06	111.27
23	b	605	CLA	C2C-C1C-NC	5.51	115.14	109.97
23	c	510	CLA	C2C-C1C-NC	5.51	115.13	109.97
23	a	405	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
23	a	406	CLA	C2C-C1C-NC	5.50	115.13	109.97
23	d	402	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
23	b	611	CLA	C3D-C2D-C1D	-5.50	98.33	105.83
23	c	510	CLA	CHD-C1D-ND	-5.50	119.40	124.45
23	b	610	CLA	O2D-CGD-CBD	5.49	121.03	111.27
23	a	406	CLA	CHD-C1D-ND	-5.49	119.41	124.45
25	D	407	BCR	C7-C8-C9	-5.49	117.94	126.23
23	B	607	CLA	CHD-C4C-C3C	-5.49	116.78	124.84
23	a	407	CLA	CMD-C2D-C1D	5.49	134.38	124.71
23	B	616	CLA	C4A-NA-C1A	-5.49	104.24	106.71
23	c	514	CLA	C2C-C1C-NC	5.48	115.11	109.97
23	B	614	CLA	C3D-C2D-C1D	-5.48	98.35	105.83
23	C	503	CLA	CHD-C1D-ND	-5.48	119.42	124.45
23	B	612	CLA	O2D-CGD-CBD	5.47	120.99	111.27
23	B	613	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
23	c	510	CLA	O2D-CGD-CBD	5.47	120.98	111.27
23	D	405	CLA	C2B-C1B-NB	5.47	113.90	110.23
23	C	512	CLA	CMD-C2D-C1D	5.46	134.33	124.71
23	c	511	CLA	CHD-C1D-ND	-5.45	119.44	124.45
23	d	402	CLA	CMD-C2D-C1D	5.44	134.30	124.71
23	c	513	CLA	CHD-C4C-C3C	-5.43	116.86	124.84
23	D	406	CLA	CMD-C2D-C1D	5.43	134.28	124.71
23	B	602	CLA	O2D-CGD-CBD	5.42	120.91	111.27
23	c	510	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
23	C	511	CLA	O2D-CGD-CBD	5.41	120.88	111.27
23	A	405	CLA	CHD-C1D-ND	-5.41	119.48	124.45
23	c	503	CLA	O2D-CGD-CBD	5.41	120.88	111.27
26	B	620	SQD	O47-C7-C8	5.41	123.15	111.50
23	b	609	CLA	CMD-C2D-C1D	5.41	134.24	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	CHD-C1D-ND	-5.39	119.50	124.45
24	a	353	PHO	C1-C2-C3	-5.39	116.72	126.04
23	B	608	CLA	O2D-CGD-CBD	5.39	120.84	111.27
23	A	405	CLA	C4A-NA-C1A	-5.38	104.29	106.71
23	B	616	CLA	C3C-C4C-NC	5.38	116.60	110.57
23	B	602	CLA	CHD-C1D-ND	-5.37	119.52	124.45
23	c	509	CLA	C4A-NA-C1A	-5.37	104.29	106.71
23	c	512	CLA	C2C-C1C-NC	5.36	115.00	109.97
23	C	506	CLA	O2D-CGD-CBD	5.36	120.80	111.27
23	C	513	CLA	CHD-C1D-ND	-5.35	119.54	124.45
23	b	603	CLA	CHD-C1D-ND	-5.35	119.54	124.45
26	A	410	SQD	C1-C2-C3	-5.35	98.86	110.00
23	b	612	CLA	C3C-C4C-NC	5.35	116.57	110.57
23	b	603	CLA	C2C-C1C-NC	5.34	114.98	109.97
23	a	405	CLA	CHD-C1D-ND	-5.34	119.55	124.45
24	A	407	PHO	C3D-C4D-ND	5.34	115.00	107.72
23	C	505	CLA	C3D-C2D-C1D	-5.33	98.55	105.83
23	B	609	CLA	C2C-C1C-NC	5.31	114.95	109.97
23	B	608	CLA	CHD-C1D-ND	-5.31	119.57	124.45
23	c	507	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
23	B	607	CLA	O2D-CGD-CBD	5.31	120.70	111.27
23	a	409	CLA	CMD-C2D-C1D	5.29	134.03	124.71
23	B	613	CLA	C1-C2-C3	-5.29	116.90	126.04
23	B	615	CLA	C4A-NA-C1A	-5.28	104.33	106.71
23	C	513	CLA	CMD-C2D-C1D	5.27	134.01	124.71
23	D	406	CLA	CHD-C1D-ND	-5.27	119.61	124.45
23	B	608	CLA	CMD-C2D-C1D	5.27	134.00	124.71
23	C	503	CLA	CMD-C2D-C1D	5.27	134.00	124.71
23	a	409	CLA	O2D-CGD-CBD	5.27	120.62	111.27
23	C	510	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
23	C	503	CLA	C4A-NA-C1A	-5.25	104.34	106.71
23	c	502	CLA	O2D-CGD-CBD	5.25	120.60	111.27
23	c	502	CLA	C2C-C1C-NC	5.25	114.89	109.97
23	b	614	CLA	CHD-C1D-ND	-5.24	119.63	124.45
23	c	513	CLA	O2D-CGD-CBD	5.24	120.59	111.27
23	C	514	CLA	C2C-C1C-NC	5.24	114.88	109.97
23	B	604	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
23	B	605	CLA	CHD-C1D-ND	-5.23	119.65	124.45
23	c	511	CLA	C2C-C1C-NC	5.22	114.86	109.97
23	c	514	CLA	C4A-NA-C1A	-5.20	104.37	106.71
23	B	612	CLA	CMD-C2D-C1D	5.20	133.88	124.71
23	b	606	CLA	C2C-C1C-NC	5.20	114.84	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
23	c	506	CLA	C2C-C1C-NC	5.20	114.84	109.97
23	b	608	CLA	C4A-NA-C1A	-5.19	104.37	106.71
23	b	613	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
24	a	353	PHO	C3D-C4D-ND	5.19	114.79	107.72
23	c	509	CLA	CMD-C2D-C1D	5.18	133.85	124.71
23	d	402	CLA	CHD-C1D-ND	-5.18	119.69	124.45
23	C	512	CLA	O2D-CGD-CBD	5.18	120.48	111.27
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	B	610	CLA	C2C-C1C-NC	5.17	114.82	109.97
23	B	605	CLA	C2C-C1C-NC	5.16	114.81	109.97
26	b	620	SQD	O6-C1-C2	5.16	116.36	108.30
23	c	504	CLA	C2C-C1C-NC	5.16	114.80	109.97
23	B	615	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
23	B	611	CLA	CMC-C2C-C1C	5.15	132.88	125.04
23	b	610	CLA	CHD-C1D-ND	-5.15	119.72	124.45
23	C	512	CLA	C3B-C2B-C1B	-5.14	100.95	107.16
23	b	612	CLA	O2D-CGD-CBD	5.14	120.40	111.27
34	B	623	HTG	C1'-S1-C1	5.14	109.70	100.09
23	b	606	CLA	O2D-CGD-CBD	5.13	120.39	111.27
23	A	404	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
23	B	616	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
23	c	503	CLA	CMD-C2D-C1D	5.13	133.75	124.71
23	B	614	CLA	C3B-C2B-C1B	-5.13	100.97	107.16
23	B	616	CLA	C2C-C1C-NC	5.12	114.77	109.97
23	C	509	CLA	O2D-CGD-CBD	5.12	120.36	111.27
23	B	610	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
23	b	615	CLA	CHD-C1D-ND	-5.11	119.76	124.45
23	c	505	CLA	O2D-CGD-CBD	5.11	120.34	111.27
23	b	614	CLA	C2C-C1C-NC	5.10	114.75	109.97
23	b	614	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
23	D	406	CLA	C2C-C1C-NC	5.10	114.75	109.97
23	C	504	CLA	C2C-C1C-NC	5.09	114.74	109.97
23	c	502	CLA	C4A-NA-C1A	-5.09	104.42	106.71
23	c	505	CLA	C2C-C1C-NC	5.09	114.74	109.97
23	b	605	CLA	O2D-CGD-CBD	5.09	120.31	111.27
23	c	509	CLA	O2D-CGD-CBD	5.08	120.30	111.27
23	c	513	CLA	C3B-C2B-C1B	-5.08	101.03	107.16
26	a	411	SQD	O47-C7-C8	5.08	122.45	111.50
23	a	406	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
23	C	509	CLA	C3C-C4C-NC	5.08	116.26	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	101	BCR	C33-C5-C6	-5.07	118.83	124.53
23	B	604	CLA	C1-C2-C3	-5.07	117.28	126.04
23	C	514	CLA	C3B-C2B-C1B	-5.06	101.05	107.16
23	D	405	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
23	c	505	CLA	C3B-C2B-C1B	-5.06	101.06	107.16
23	B	608	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
23	c	505	CLA	C4A-NA-C1A	-5.06	104.43	106.71
23	C	506	CLA	C4A-NA-C1A	-5.05	104.43	106.71
23	D	406	CLA	O2D-CGD-CBD	5.05	120.24	111.27
23	B	605	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	c	507	CLA	C4A-NA-C1A	-5.04	104.44	106.71
23	b	611	CLA	O2D-CGD-CBD	5.04	120.23	111.27
23	C	505	CLA	O2D-CGD-CBD	5.03	120.20	111.27
23	a	409	CLA	C2C-C1C-NC	5.03	114.68	109.97
26	b	620	SQD	O47-C7-C8	5.02	122.31	111.50
23	c	503	CLA	CHD-C1D-ND	-5.01	119.85	124.45
23	B	615	CLA	C3C-C4C-NC	5.01	116.19	110.57
23	A	405	CLA	O2D-CGD-CBD	5.01	120.17	111.27
23	B	616	CLA	CMD-C2D-C1D	5.01	133.54	124.71
23	B	605	CLA	C3C-C4C-NC	5.00	116.18	110.57
23	D	405	CLA	C3C-C4C-NC	5.00	116.18	110.57
23	B	613	CLA	CMD-C2D-C1D	5.00	133.52	124.71
23	C	510	CLA	C3B-C2B-C1B	-4.98	101.15	107.16
29	a	416	PL9	C7-C8-C9	-4.98	118.50	126.79
23	b	610	CLA	C2C-C1C-NC	4.98	114.63	109.97
23	a	407	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
24	A	353	PHO	C3D-C4D-ND	4.96	114.48	107.72
23	c	511	CLA	O2D-CGD-CBD	4.95	120.07	111.27
23	C	513	CLA	C3B-C2B-C1B	-4.95	101.18	107.16
23	b	607	CLA	C3C-C4C-NC	4.95	116.12	110.57
23	b	609	CLA	C2C-C1C-NC	4.95	114.61	109.97
29	A	414	PL9	C7-C8-C9	-4.94	118.56	126.79
23	c	502	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
23	c	505	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
38	e	87	HEM	CHC-C4B-NB	4.93	129.77	124.42
23	c	509	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
25	y	101	BCR	C33-C5-C6	-4.92	119.01	124.53
26	f	102	SQD	O47-C7-C8	4.91	122.09	111.50
23	b	614	CLA	C3B-C2B-C1B	-4.91	101.23	107.16
23	c	504	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
23	b	604	CLA	C3C-C4C-NC	4.91	116.08	110.57
23	b	601	CLA	C2C-C1C-NC	4.91	114.57	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	411	SQD	C1-O5-C5	-4.91	104.05	113.69
23	B	605	CLA	O2D-CGD-CBD	4.90	119.98	111.27
23	b	605	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
23	C	508	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
23	B	601	CLA	C3D-C2D-C1D	-4.89	99.15	105.83
23	d	402	CLA	C4A-NA-C1A	-4.89	104.51	106.71
23	a	409	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
25	t	103	BCR	C33-C5-C6	-4.87	119.06	124.53
23	c	508	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
23	C	507	CLA	C1C-C2C-C3C	-4.86	101.84	106.96
23	C	508	CLA	C2C-C1C-NC	4.86	114.52	109.97
23	B	606	CLA	C2C-C1C-NC	4.85	114.52	109.97
23	b	611	CLA	C2C-C1C-NC	4.85	114.52	109.97
23	b	613	CLA	CHD-C1D-ND	-4.85	120.00	124.45
23	b	613	CLA	C3C-C4C-NC	4.84	116.00	110.57
25	d	404	BCR	C7-C8-C9	-4.84	118.92	126.23
23	b	615	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
23	A	406	CLA	C2C-C1C-NC	4.83	114.50	109.97
23	b	612	CLA	CMD-C2D-C1D	4.83	133.22	124.71
23	a	407	CLA	C2C-C1C-NC	4.82	114.49	109.97
23	b	604	CLA	CHD-C1D-ND	-4.82	120.02	124.45
23	c	511	CLA	C3B-C2B-C1B	-4.82	101.35	107.16
23	b	608	CLA	O2D-CGD-CBD	4.81	119.82	111.27
23	B	612	CLA	C2B-C1B-NB	4.81	113.45	110.23
23	a	409	CLA	C3C-C4C-NC	4.80	115.96	110.57
23	A	408	CLA	C3B-C2B-C1B	-4.80	101.37	107.16
23	B	604	CLA	C3C-C4C-NC	4.80	115.95	110.57
23	B	602	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	C	514	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
23	b	602	CLA	C3B-C2B-C1B	-4.79	101.38	107.16
38	E	103	HEM	C1B-NB-C4B	4.78	110.01	105.07
23	c	503	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
23	B	612	CLA	C2C-C1C-NC	4.78	114.45	109.97
23	A	405	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	c	513	CLA	C2C-C1C-NC	4.78	114.45	109.97
23	d	403	CLA	O2D-CGD-CBD	4.78	119.75	111.27
23	C	508	CLA	C3B-C2B-C1B	-4.77	101.40	107.16
23	B	616	CLA	CHD-C1D-ND	-4.77	120.07	124.45
23	B	611	CLA	C3C-C4C-NC	4.77	115.92	110.57
23	A	405	CLA	CMD-C2D-C1D	4.77	133.12	124.71
23	c	508	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
23	c	506	CLA	C3C-C4C-NC	4.76	115.91	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	b	622	HTG	C1-O5-C5	4.76	121.36	112.58
23	b	607	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
23	b	610	CLA	C3C-C4C-NC	4.76	115.91	110.57
23	B	613	CLA	O2D-CGD-CBD	4.76	119.72	111.27
23	b	609	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	B	603	CLA	C3C-C4C-NC	4.73	115.88	110.57
23	C	507	CLA	C3B-C2B-C1B	-4.73	101.46	107.16
23	c	514	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
23	C	506	CLA	C3C-C4C-NC	4.72	115.87	110.57
23	b	614	CLA	O2D-CGD-O1D	-4.72	114.61	123.84
23	b	603	CLA	CMD-C2D-C1D	4.72	133.03	124.71
23	C	514	CLA	O2D-CGD-CBD	4.72	119.65	111.27
23	b	603	CLA	C3D-C4D-ND	4.72	117.87	110.24
23	b	610	CLA	C4A-NA-C1A	-4.72	104.59	106.71
23	b	607	CLA	C3D-C4D-ND	4.71	117.86	110.24
23	C	514	CLA	C3C-C4C-NC	4.71	115.86	110.57
23	d	403	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
23	a	405	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
23	D	406	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	c	502	CLA	O2D-CGD-O1D	-4.71	114.64	123.84
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	b	607	CLA	O2D-CGD-CBD	4.69	119.61	111.27
23	c	514	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	B	612	CLA	C3D-C4D-ND	4.69	117.82	110.24
23	C	505	CLA	C3C-C4C-NC	4.69	115.83	110.57
23	B	613	CLA	CHD-C1D-ND	-4.68	120.15	124.45
23	b	602	CLA	C3D-C4D-ND	4.68	117.82	110.24
23	c	506	CLA	C3D-C4D-ND	4.68	117.81	110.24
23	B	615	CLA	CMB-C2B-C1B	4.68	132.50	125.37
33	C	501	LMG	C7-O1-C1	-4.68	104.60	113.74
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	503	CLA	C1C-C2C-C3C	-4.67	102.04	106.96
23	B	601	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
23	B	608	CLA	C3B-C2B-C1B	-4.67	101.53	107.16
23	B	604	CLA	C4A-NA-C1A	-4.67	104.61	106.71
23	C	504	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
33	B	621	LMG	O7-C10-C11	4.66	121.54	111.50
23	c	511	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
23	B	609	CLA	C3C-C4C-NC	4.64	115.78	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	408	PHO	C3D-C4D-ND	4.64	114.04	107.72
23	B	603	CLA	C3B-C2B-C1B	-4.64	101.56	107.16
23	C	510	CLA	C3D-C4D-ND	4.64	117.74	110.24
23	B	604	CLA	O2D-CGD-CBD	4.63	119.49	111.27
23	a	406	CLA	O2D-CGD-CBD	4.63	119.49	111.27
23	C	509	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
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	610	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
23	c	509	CLA	C3B-C2B-C1B	-4.61	101.59	107.16
23	C	503	CLA	C3B-C2B-C1B	-4.61	101.59	107.16
23	b	606	CLA	C3B-C2B-C1B	-4.61	101.60	107.16
23	c	510	CLA	C3B-C2B-C1B	-4.61	101.60	107.16
23	C	502	CLA	C2C-C1C-NC	4.61	114.29	109.97
23	b	609	CLA	C3C-C4C-NC	4.60	115.73	110.57
23	b	608	CLA	C1C-C2C-C3C	-4.60	102.12	106.96
23	B	606	CLA	C3C-C4C-NC	4.60	115.73	110.57
23	c	503	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	b	607	CLA	C1C-C2C-C3C	-4.60	102.12	106.96
23	b	611	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
23	C	511	CLA	C4A-NA-C1A	-4.60	104.64	106.71
23	A	404	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
23	B	607	CLA	C4A-NA-C1A	-4.59	104.64	106.71
23	C	505	CLA	C1C-C2C-C3C	-4.59	102.13	106.96
23	C	511	CLA	C1-C2-C3	-4.59	118.11	126.04
23	B	611	CLA	C3D-C4D-ND	4.58	117.65	110.24
23	B	612	CLA	C3C-C4C-NC	4.58	115.70	110.57
23	c	507	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	A	404	CLA	C3B-C2B-C1B	-4.57	101.64	107.16
23	d	403	CLA	C3B-C2B-C1B	-4.57	101.64	107.16
23	A	405	CLA	C1C-C2C-C3C	-4.57	102.15	106.96
23	C	508	CLA	C3C-C4C-NC	4.57	115.69	110.57
23	B	610	CLA	C3C-C4C-NC	4.56	115.69	110.57
23	C	510	CLA	O2D-CGD-CBD	4.56	119.38	111.27
23	c	503	CLA	C4A-NA-C1A	-4.56	104.66	106.71
23	A	408	CLA	O2D-CGD-CBD	4.56	119.37	111.27
23	C	506	CLA	CMB-C2B-C1B	4.55	132.30	125.37
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
23	c	512	CLA	C3B-C2B-C1B	-4.55	101.67	107.16
23	b	603	CLA	C3C-C4C-NC	4.55	115.67	110.57
23	d	403	CLA	C3D-C4D-ND	4.55	117.59	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	C3B-C2B-C1B	-4.55	101.67	107.16
26	f	102	SQD	C1-O5-C5	4.54	122.61	113.69
23	C	512	CLA	CHD-C1D-ND	-4.54	120.28	124.45
23	b	601	CLA	C3B-C2B-C1B	-4.54	101.68	107.16
23	b	615	CLA	C3C-C4C-NC	4.54	115.66	110.57
23	d	402	CLA	C3C-C4C-NC	4.54	115.66	110.57
23	A	406	CLA	CMB-C2B-C1B	4.53	132.27	125.37
23	c	509	CLA	C3C-C4C-NC	4.53	115.65	110.57
23	c	507	CLA	O2D-CGD-CBD	4.53	119.32	111.27
23	A	406	CLA	C3D-C4D-ND	4.53	117.56	110.24
23	a	409	CLA	C3D-C4D-ND	4.53	117.56	110.24
23	c	510	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
23	b	603	CLA	C3B-C2B-C1B	-4.52	101.70	107.16
23	c	508	CLA	CMB-C2B-C1B	4.52	132.25	125.37
23	C	502	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
23	c	514	CLA	C3D-C4D-ND	4.51	117.54	110.24
23	c	512	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
23	A	406	CLA	O2D-CGD-CBD	4.51	119.28	111.27
23	C	514	CLA	C3D-C4D-ND	4.51	117.53	110.24
33	a	419	LMG	O7-C10-C11	4.50	121.20	111.50
23	d	403	CLA	C2C-C1C-NC	4.50	114.19	109.97
23	b	602	CLA	C2C-C1C-NC	4.49	114.18	109.97
23	C	511	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
23	d	402	CLA	C3D-C4D-ND	4.49	117.50	110.24
23	a	409	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
23	b	605	CLA	C3D-C4D-ND	4.49	117.50	110.24
23	b	610	CLA	C1-C2-C3	-4.48	118.29	126.04
23	C	511	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	B	608	CLA	C3C-C4C-NC	4.48	115.59	110.57
23	b	608	CLA	C3B-C2B-C1B	-4.47	101.76	107.16
23	C	503	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
23	c	504	CLA	O2D-CGD-CBD	4.47	119.22	111.27
23	b	605	CLA	C3C-C4C-NC	4.47	115.58	110.57
23	b	607	CLA	C3B-C4B-NB	4.47	114.66	110.52
23	B	613	CLA	C4A-NA-C1A	-4.46	104.70	106.71
23	c	508	CLA	C3C-C4C-NC	4.45	115.57	110.57
23	C	507	CLA	C3D-C4D-ND	4.45	117.43	110.24
23	a	407	CLA	O2D-CGD-CBD	4.44	119.17	111.27
23	B	610	CLA	O2A-CGA-CBA	4.44	125.85	111.91
23	C	509	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
23	c	507	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	C	513	CLA	C3C-C4C-NC	4.44	115.55	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	c	504	CLA	C1D-CHD-C4C	-4.44	116.49	126.06
23	B	604	CLA	CHD-C1D-ND	-4.44	120.38	124.45
23	C	503	CLA	C3C-C4C-NC	4.43	115.54	110.57
23	b	608	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
23	C	502	CLA	C3D-C4D-ND	4.43	117.40	110.24
23	C	512	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
23	c	504	CLA	C3C-C4C-NC	4.42	115.53	110.57
23	B	601	CLA	C3D-C4D-ND	4.42	117.39	110.24
23	c	511	CLA	C3C-C4C-NC	4.42	115.53	110.57
23	b	612	CLA	CHD-C1D-ND	-4.42	120.40	124.45
23	b	605	CLA	C3B-C2B-C1B	-4.41	101.83	107.16
23	C	511	CLA	C3D-C4D-ND	4.41	117.38	110.24
23	D	406	CLA	C3C-C4C-NC	4.41	115.52	110.57
23	B	612	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
23	B	612	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
23	B	601	CLA	C3C-C4C-NC	4.41	115.52	110.57
23	C	503	CLA	C3D-C4D-ND	4.41	117.37	110.24
23	c	512	CLA	O2D-CGD-CBD	4.41	119.10	111.27
23	b	611	CLA	C3C-C4C-NC	4.41	115.51	110.57
23	B	602	CLA	C3B-C2B-C1B	-4.40	101.84	107.16
23	C	509	CLA	CMD-C2D-C1D	4.40	132.47	124.71
23	b	610	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
23	c	509	CLA	CHD-C1D-ND	-4.40	120.41	124.45
23	C	512	CLA	C3C-C4C-NC	4.40	115.51	110.57
23	B	607	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
32	t	102	LMT	C3'-C4'-C5'	-4.40	100.84	110.93
26	F	101	SQD	C1-O5-C5	-4.40	105.06	113.69
23	a	405	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
23	a	406	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
23	c	514	CLA	O2D-CGD-CBD	4.38	119.05	111.27
23	C	503	CLA	O2D-CGD-CBD	4.38	119.05	111.27
23	a	406	CLA	C4A-NA-C1A	-4.38	104.74	106.71
23	B	607	CLA	C3B-C2B-C1B	-4.38	101.88	107.16
23	C	509	CLA	C1-C2-C3	-4.37	118.48	126.04
23	A	406	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
23	B	610	CLA	C4A-NA-C1A	-4.37	104.74	106.71
23	A	405	CLA	C3D-C4D-ND	4.36	117.30	110.24
37	E	101	LHG	O7-C7-C8	4.36	120.90	111.50
38	E	103	HEM	CHC-C4B-NB	4.36	129.15	124.42
23	b	604	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
23	a	407	CLA	C3B-C2B-C1B	-4.36	101.90	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	c	511	CLA	C1-C2-C3	-4.35	118.52	126.04
23	c	510	CLA	C4A-NA-C1A	-4.35	104.75	106.71
23	b	614	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	b	612	CLA	C3B-C2B-C1B	-4.35	101.92	107.16
33	c	521	LMG	O6-C5-C4	4.35	117.59	109.69
23	B	616	CLA	C3B-C4B-NB	4.35	114.55	110.52
23	b	610	CLA	C3D-C4D-ND	4.34	117.27	110.24
23	d	402	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
23	b	615	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
23	B	613	CLA	C3C-C4C-NC	4.34	115.44	110.57
23	B	609	CLA	C3D-C4D-ND	4.34	117.25	110.24
23	B	612	CLA	O2D-CGD-O1D	-4.33	115.36	123.84
23	B	603	CLA	O2D-CGD-O1D	-4.33	115.37	123.84
25	H	101	BCR	C38-C26-C25	-4.33	119.67	124.53
23	C	504	CLA	C3D-C4D-ND	4.33	117.24	110.24
23	C	506	CLA	C3D-C4D-ND	4.32	117.23	110.24
23	b	604	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
33	C	501	LMG	O7-C10-C11	4.31	120.80	111.50
23	c	502	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
23	b	613	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
23	C	505	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
23	b	609	CLA	O2D-CGD-CBD	4.31	118.92	111.27
26	a	411	SQD	C1-C2-C3	-4.31	101.02	110.00
23	A	408	CLA	C3B-C4B-NB	4.30	114.51	110.52
23	b	611	CLA	C3D-C4D-ND	4.30	117.20	110.24
23	c	504	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
26	B	620	SQD	O7-S-C6	4.30	112.05	106.94
29	A	414	PL9	C32-C33-C34	-4.30	117.31	127.66
23	A	408	CLA	C3D-C4D-ND	4.29	117.19	110.24
25	d	404	BCR	C15-C14-C13	-4.29	121.18	127.31
23	b	616	CLA	C3D-C4D-ND	4.29	117.18	110.24
23	b	612	CLA	C3D-C4D-ND	4.29	117.18	110.24
23	A	408	CLA	C3C-C4C-NC	4.29	115.39	110.57
34	b	625	HTG	C1-O5-C5	4.29	120.50	112.58
23	c	510	CLA	C3B-C4B-NB	4.29	114.50	110.52
23	a	407	CLA	C3D-C4D-ND	4.29	117.17	110.24
23	a	405	CLA	C3D-C4D-ND	4.28	117.17	110.24
38	E	103	HEM	C4C-NC-C1C	4.28	109.54	105.35
23	A	405	CLA	C3B-C2B-C1B	-4.28	102.00	107.16
23	B	605	CLA	C3D-C4D-ND	4.28	117.16	110.24
23	B	616	CLA	C3B-C2B-C1B	-4.28	102.00	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C1C-C2C-C3C	-4.27	102.46	106.96
23	B	602	CLA	C3C-C4C-NC	4.27	115.36	110.57
23	b	614	CLA	C3D-C4D-ND	4.27	117.14	110.24
26	a	411	SQD	O9-S-C6	4.27	112.01	106.94
23	b	608	CLA	CMC-C2C-C1C	4.27	131.54	125.04
23	B	610	CLA	C3B-C2B-C1B	-4.27	102.01	107.16
23	C	502	CLA	O2D-CGD-O1D	-4.26	115.50	123.84
23	c	513	CLA	C3D-C2D-C1D	-4.26	100.01	105.83
25	Y	101	BCR	C16-C17-C18	-4.26	121.22	127.31
23	a	405	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	A	408	CLA	C4A-NA-C1A	-4.26	104.79	106.71
23	b	602	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	c	508	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
23	b	603	CLA	C1D-CHD-C4C	-4.25	116.89	126.06
23	B	603	CLA	C3D-C4D-ND	4.25	117.11	110.24
23	B	607	CLA	C3C-C4C-NC	4.24	115.33	110.57
23	c	512	CLA	C4A-NA-C1A	-4.24	104.80	106.71
23	D	406	CLA	C3D-C4D-ND	4.24	117.09	110.24
26	F	101	SQD	O8-S-C6	4.23	112.48	105.74
23	d	402	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
23	c	503	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	C	509	CLA	C1C-C2C-C3C	-4.21	102.53	106.96
23	B	605	CLA	C1D-CHD-C4C	-4.21	116.97	126.06
23	a	406	CLA	C3C-C4C-NC	4.21	115.29	110.57
23	b	612	CLA	C4A-NA-C1A	-4.21	104.81	106.71
23	b	609	CLA	C3D-C4D-ND	4.21	117.04	110.24
23	B	613	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
23	b	616	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
23	B	606	CLA	C3D-C4D-ND	4.20	117.03	110.24
23	B	614	CLA	C3C-C4C-NC	4.20	115.28	110.57
23	B	614	CLA	C1C-C2C-C3C	-4.20	102.55	106.96
33	d	412	LMG	O7-C10-C11	4.19	120.53	111.50
26	B	620	SQD	C3-C4-C5	4.19	117.70	110.24
23	C	506	CLA	C3D-C2D-C1D	-4.18	100.12	105.83
37	D	409	LHG	O8-C23-O10	-4.18	113.04	123.59
23	B	613	CLA	C3B-C4B-NB	4.17	114.39	110.52
23	c	510	CLA	C3D-C4D-ND	4.17	116.99	110.24
25	C	515	BCR	C7-C8-C9	-4.17	119.93	126.23
33	c	521	LMG	O7-C10-C11	4.17	120.50	111.50
23	C	512	CLA	C1D-CHD-C4C	-4.17	117.06	126.06
23	C	513	CLA	C3D-C4D-ND	4.17	116.98	110.24
23	A	404	CLA	C3B-C4B-NB	4.17	114.38	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	C3B-C4B-NB	4.17	114.38	110.52
23	b	605	CLA	O2D-CGD-O1D	-4.16	115.69	123.84
23	b	607	CLA	C3B-C2B-C1B	-4.16	102.13	107.16
23	b	615	CLA	C3D-C4D-ND	4.16	116.97	110.24
23	B	605	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
23	c	514	CLA	C1D-CHD-C4C	-4.16	117.08	126.06
23	B	607	CLA	C3D-C4D-ND	4.15	116.96	110.24
23	c	512	CLA	C3D-C4D-ND	4.15	116.95	110.24
23	A	406	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
23	b	610	CLA	O2A-CGA-CBA	4.15	124.92	111.91
23	D	405	CLA	C3B-C2B-C1B	-4.15	102.16	107.16
23	a	405	CLA	C1D-CHD-C4C	-4.14	117.12	126.06
23	b	603	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
23	B	604	CLA	C3B-C2B-C1B	-4.14	102.16	107.16
23	b	606	CLA	C3D-C4D-ND	4.14	116.94	110.24
23	b	612	CLA	C1-C2-C3	-4.14	118.89	126.04
23	b	616	CLA	C3C-C4C-NC	4.14	115.21	110.57
29	a	416	PL9	C7-C3-C4	4.13	120.24	116.88
23	D	406	CLA	C3B-C2B-C1B	-4.13	102.18	107.16
25	b	617	BCR	C33-C5-C6	-4.13	119.89	124.53
23	B	603	CLA	C1D-CHD-C4C	-4.13	117.15	126.06
23	B	610	CLA	C3D-C4D-ND	4.13	116.92	110.24
23	a	406	CLA	C3D-C4D-ND	4.12	116.91	110.24
23	c	505	CLA	C3C-C4C-NC	4.12	115.19	110.57
23	c	502	CLA	C3D-C4D-ND	4.12	116.90	110.24
23	C	510	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
38	E	103	HEM	CHD-C4C-NC	4.12	128.89	124.44
38	e	87	HEM	CAD-CBD-CGD	4.11	122.45	113.60
23	C	502	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
23	c	513	CLA	C3D-C4D-ND	4.11	116.88	110.24
23	C	504	CLA	C3C-C4C-NC	4.11	115.17	110.57
23	c	504	CLA	C3D-C4D-ND	4.10	116.88	110.24
23	C	509	CLA	C3D-C4D-ND	4.10	116.87	110.24
23	c	512	CLA	C1D-CHD-C4C	-4.10	117.21	126.06
23	c	508	CLA	CMC-C2C-C1C	4.10	131.28	125.04
23	C	509	CLA	C3B-C4B-NB	4.09	114.31	110.52
23	b	612	CLA	O2D-CGD-O1D	-4.09	115.84	123.84
23	a	406	CLA	CMB-C2B-C1B	4.09	131.60	125.37
23	a	409	CLA	C4A-NA-C1A	-4.09	104.87	106.71
23	C	513	CLA	C2C-C1C-NC	4.09	113.80	109.97
23	d	402	CLA	O2D-CGD-CBD	4.09	118.53	111.27
23	d	402	CLA	C3B-C2B-C1B	-4.09	102.23	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	C3D-C4D-ND	4.09	116.85	110.24
23	a	406	CLA	CAA-C2A-C3A	-4.09	101.59	112.78
23	B	615	CLA	C3B-C2B-C1B	-4.09	102.23	107.16
23	B	615	CLA	C3D-C4D-ND	4.08	116.84	110.24
23	B	601	CLA	C4A-NA-C1A	-4.08	104.87	106.71
23	B	615	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
23	c	506	CLA	C3B-C2B-C1B	-4.08	102.24	107.16
23	C	507	CLA	C4A-NA-C1A	-4.08	104.87	106.71
23	b	604	CLA	CMC-C2C-C1C	4.08	131.25	125.04
24	A	407	PHO	C1A-C2A-C3A	-4.08	98.96	102.84
23	B	616	CLA	O2D-CGD-O1D	-4.08	115.87	123.84
23	B	608	CLA	C3B-C4B-NB	4.07	114.30	110.52
23	B	616	CLA	C3D-C4D-ND	4.07	116.83	110.24
23	c	507	CLA	C3B-C2B-C1B	-4.07	102.25	107.16
23	b	616	CLA	C1D-CHD-C4C	-4.07	117.28	126.06
23	D	405	CLA	C3D-C4D-ND	4.07	116.82	110.24
24	A	353	PHO	C1-C2-C3	-4.07	119.00	126.04
23	c	514	CLA	C3C-C4C-NC	4.07	115.13	110.57
23	b	616	CLA	C2C-C1C-NC	4.06	113.78	109.97
23	D	405	CLA	O2D-CGD-CBD	4.06	118.49	111.27
23	a	405	CLA	CAA-C2A-C3A	-4.06	101.65	112.78
23	a	406	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
23	c	503	CLA	C3C-C4C-NC	4.06	115.12	110.57
23	a	406	CLA	C1D-CHD-C4C	-4.06	117.30	126.06
38	e	87	HEM	C4C-NC-C1C	4.06	109.32	105.35
23	C	506	CLA	C3B-C2B-C1B	-4.06	102.27	107.16
33	Z	101	LMG	O7-C10-C11	4.05	120.23	111.50
23	B	606	CLA	C3B-C2B-C1B	-4.05	102.27	107.16
26	a	411	SQD	C44-O6-C1	-4.04	105.84	113.74
23	C	511	CLA	C3B-C4B-NB	4.04	114.26	110.52
23	C	502	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
26	b	620	SQD	C1-O5-C5	-4.04	105.76	113.69
23	c	506	CLA	C3D-C2D-C1D	-4.04	100.32	105.83
23	C	504	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
23	A	408	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
23	c	507	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
23	A	404	CLA	C3D-C4D-ND	4.03	116.75	110.24
23	a	405	CLA	C3C-C4C-NC	4.03	115.09	110.57
23	c	505	CLA	C1-O2A-CGA	4.03	127.01	116.44
23	B	613	CLA	C3D-C4D-ND	4.03	116.75	110.24
29	a	416	PL9	C32-C33-C34	-4.03	117.96	127.66
23	B	608	CLA	C3D-C4D-ND	4.02	116.75	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	C1D-CHD-C4C	-4.02	117.38	126.06
23	b	613	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
23	c	509	CLA	C3D-C4D-ND	4.02	116.74	110.24
23	b	608	CLA	C3D-C4D-ND	4.01	116.73	110.24
23	c	508	CLA	C4A-NA-C1A	-4.01	104.90	106.71
23	b	606	CLA	C3C-C4C-NC	4.01	115.07	110.57
23	C	505	CLA	C3D-C4D-ND	4.01	116.72	110.24
23	A	404	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
23	B	611	CLA	C1D-CHD-C4C	-4.01	117.42	126.06
23	C	505	CLA	C4A-NA-C1A	-4.00	104.91	106.71
35	C	518	DGD	O2G-C1B-C2B	4.00	120.12	111.50
23	c	506	CLA	CAC-C3C-C4C	4.00	130.00	124.81
23	c	507	CLA	C3B-C4B-NB	4.00	114.22	110.52
23	B	609	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
23	B	601	CLA	C2C-C1C-NC	3.99	113.71	109.97
23	c	508	CLA	C3D-C4D-ND	3.99	116.69	110.24
23	C	514	CLA	C4A-NA-C1A	-3.98	104.92	106.71
23	b	601	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
23	b	612	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
23	C	513	CLA	C1D-CHD-C4C	-3.98	117.48	126.06
23	b	606	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
35	C	517	DGD	O2G-C1B-C2B	3.97	120.05	111.50
23	A	406	CLA	C3C-C4C-NC	3.96	115.02	110.57
23	b	616	CLA	O2D-CGD-O1D	-3.96	116.09	123.84
23	b	603	CLA	CAA-C2A-C3A	-3.96	101.93	112.78
23	C	512	CLA	C4A-NA-C1A	-3.96	104.92	106.71
23	b	614	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
23	C	504	CLA	O2D-CGD-CBD	3.96	118.30	111.27
23	B	611	CLA	CHD-C4C-NC	3.96	130.44	124.20
23	C	509	CLA	CHD-C1D-ND	-3.96	120.82	124.45
26	A	410	SQD	O9-S-C6	3.96	111.64	106.94
23	b	614	CLA	C4A-NA-C1A	-3.95	104.93	106.71
23	c	505	CLA	C3D-C4D-ND	3.95	116.63	110.24
23	b	613	CLA	O2D-CGD-CBD	3.95	118.29	111.27
23	C	514	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
23	D	406	CLA	CMB-C2B-C1B	3.95	131.38	125.37
23	a	409	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
23	A	405	CLA	CMC-C2C-C1C	3.94	131.04	125.04
23	c	503	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
23	c	512	CLA	C3C-C4C-NC	3.94	114.99	110.57
23	c	502	CLA	C3C-C4C-NC	3.94	114.99	110.57
23	B	610	CLA	CAA-C2A-C3A	-3.93	102.01	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	CLA	O2D-CGD-O1D	-3.93	116.15	123.84
23	A	404	CLA	C3C-C4C-NC	3.93	114.98	110.57
23	B	609	CLA	O2D-CGD-CBD	3.92	118.24	111.27
23	c	504	CLA	C1-C2-C3	-3.92	119.27	126.04
23	C	508	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
23	b	606	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
23	b	610	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
23	c	514	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
23	D	406	CLA	O2D-CGD-O1D	-3.91	116.19	123.84
23	c	511	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
33	C	521	LMG	O6-C5-C4	3.91	116.79	109.69
23	B	615	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
23	C	508	CLA	C3D-C4D-ND	3.91	116.56	110.24
23	C	512	CLA	C3D-C4D-ND	3.91	116.56	110.24
23	a	409	CLA	C1D-CHD-C4C	-3.90	117.63	126.06
33	C	520	LMG	O7-C10-C11	3.90	119.92	111.50
23	c	511	CLA	C3D-C4D-ND	3.90	116.55	110.24
23	B	613	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
23	B	605	CLA	CMB-C2B-C1B	3.90	131.30	125.37
23	A	406	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
23	b	615	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
33	m	101	LMG	O7-C10-C11	3.88	119.87	111.50
33	c	521	LMG	C3-C4-C5	3.88	117.16	110.24
23	a	405	CLA	O2D-CGD-CBD	3.88	118.16	111.27
23	B	604	CLA	C3D-C2D-C1D	-3.88	100.54	105.83
23	C	507	CLA	C3B-C4B-NB	3.88	114.11	110.52
23	B	608	CLA	C4A-NA-C1A	-3.88	104.96	106.71
25	T	101	BCR	C15-C16-C17	-3.87	115.54	123.47
23	C	510	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
23	B	614	CLA	C3D-C4D-ND	3.87	116.49	110.24
23	b	609	CLA	C3B-C2B-C1B	-3.87	102.49	107.16
23	C	502	CLA	C3C-C4C-NC	3.87	114.91	110.57
26	F	101	SQD	C44-O6-C1	-3.86	106.20	113.74
23	b	608	CLA	C3C-C4C-NC	3.86	114.90	110.57
23	b	610	CLA	O2A-CGA-O1A	-3.86	113.86	123.59
23	c	510	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
23	C	506	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
23	c	513	CLA	C1D-CHD-C4C	-3.85	117.76	126.06
23	b	604	CLA	C3B-C2B-C1B	-3.85	102.52	107.16
23	d	403	CLA	C3C-C4C-NC	3.84	114.88	110.57
33	C	521	LMG	O7-C10-C11	3.84	119.78	111.50
23	a	409	CLA	CMC-C2C-C1C	3.84	130.89	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	B	614	CLA	O2D-CGD-O1D	-3.84	116.33	123.84
29	A	414	PL9	C7-C3-C4	3.83	119.99	116.88
23	A	404	CLA	CAA-C2A-C3A	-3.83	102.30	112.78
23	c	503	CLA	O2D-CGD-O1D	-3.83	116.36	123.84
23	A	405	CLA	C3C-C4C-NC	3.83	114.86	110.57
25	D	407	BCR	C38-C26-C25	-3.82	120.23	124.53
23	C	510	CLA	C3C-C4C-NC	3.82	114.86	110.57
23	C	509	CLA	C1D-CHD-C4C	-3.82	117.81	126.06
23	C	510	CLA	C1-C2-C3	-3.82	119.44	126.04
23	C	512	CLA	CAC-C3C-C4C	3.82	129.76	124.81
23	b	612	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
23	b	605	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
23	c	509	CLA	C1C-C2C-C3C	-3.81	102.96	106.96
23	B	602	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
33	Z	101	LMG	C1-C2-C3	3.80	117.91	110.00
23	B	608	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
34	B	622	HTG	C1'-S1-C1	3.80	107.19	100.09
25	B	618	BCR	C29-C30-C25	3.80	116.32	110.48
23	A	404	CLA	O2A-CGA-CBA	3.79	123.81	111.91
23	b	601	CLA	C3C-C4C-NC	3.79	114.82	110.57
32	D	404	LMT	C1'-O5'-C5'	-3.78	106.26	113.69
23	b	604	CLA	C4A-NA-C1A	-3.78	105.00	106.71
23	B	610	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
23	B	611	CLA	O2D-CGD-O1D	-3.78	116.45	123.84
23	c	504	CLA	CMB-C2B-C1B	3.78	131.12	125.37
23	c	513	CLA	C1-C2-C3	-3.77	119.52	126.04
23	A	404	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
23	C	509	CLA	C4A-NA-C1A	-3.77	105.01	106.71
23	c	512	CLA	C3B-C4B-NB	3.77	114.01	110.52
23	B	616	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
23	D	405	CLA	C3B-C4B-NB	3.77	114.01	110.52
23	b	609	CLA	C1-C2-C3	-3.77	119.53	126.04
23	B	606	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
23	c	514	CLA	C3B-C4B-NB	3.77	114.01	110.52
29	a	416	PL9	C15-C14-C16	3.76	121.60	115.27
23	C	507	CLA	C1-C2-C3	-3.76	119.54	126.04
23	b	603	CLA	O2D-CGD-O1D	-3.76	116.48	123.84
23	D	405	CLA	C1-C2-C3	-3.76	119.54	126.04
23	B	614	CLA	C3B-C4B-NB	3.76	114.00	110.52
23	B	609	CLA	C1C-C2C-C3C	-3.76	103.01	106.96
23	B	604	CLA	C1C-C2C-C3C	-3.76	103.01	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	CMC-C2C-C1C	3.76	130.76	125.04
23	C	507	CLA	O2D-CGD-CBD	3.75	117.94	111.27
23	C	503	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
23	c	509	CLA	C1D-CHD-C4C	-3.75	117.96	126.06
26	A	412	SQD	O8-S-C6	3.75	111.72	105.74
23	b	612	CLA	C4-C3-C5	3.75	121.58	115.27
23	A	405	CLA	CBC-CAC-C3C	-3.75	102.10	112.43
23	b	604	CLA	O2D-CGD-O1D	-3.75	116.52	123.84
23	c	507	CLA	C3C-C4C-NC	3.74	114.76	110.57
23	C	513	CLA	C1-C2-C3	-3.74	119.58	126.04
23	C	514	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
23	C	511	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
23	b	612	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
37	d	711	LHG	O8-C23-O10	-3.73	114.17	123.59
23	d	403	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
23	b	604	CLA	C3D-C4D-ND	3.73	116.27	110.24
23	B	603	CLA	C4-C3-C5	3.73	121.54	115.27
23	c	510	CLA	C3C-C4C-NC	3.72	114.75	110.57
23	A	404	CLA	O2D-CGD-CBD	3.72	117.88	111.27
23	B	604	CLA	C3B-C4B-NB	3.71	113.96	110.52
23	B	602	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
37	L	101	LHG	O7-C7-C8	3.71	119.50	111.50
29	a	416	PL9	C7-C3-C2	-3.71	118.42	123.30
23	b	611	CLA	C1-C2-C3	-3.71	119.63	126.04
23	C	511	CLA	C3C-C4C-NC	3.70	114.73	110.57
23	c	502	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
23	B	611	CLA	C4A-NA-C1A	-3.70	105.04	106.71
23	b	604	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
23	b	613	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
23	c	507	CLA	CAC-C3C-C4C	3.69	129.59	124.81
23	B	615	CLA	O2D-CGD-CBD	3.68	117.81	111.27
23	b	613	CLA	C3D-C4D-ND	3.68	116.19	110.24
23	B	614	CLA	O2A-CGA-O1A	-3.68	114.30	123.59
26	A	412	SQD	O47-C7-C8	3.68	119.43	111.50
23	b	606	CLA	C4-C3-C5	3.68	121.46	115.27
26	A	410	SQD	C44-O6-C1	-3.67	106.57	113.74
33	c	520	LMG	O7-C10-C11	3.67	119.41	111.50
34	B	622	HTG	O5-C1-C2	3.67	114.93	110.31
29	a	416	PL9	C30-C29-C31	3.67	121.44	115.27
25	D	407	BCR	C28-C27-C26	-3.67	107.53	114.08
29	D	408	PL9	C42-C43-C44	-3.67	118.83	127.66
23	A	408	CLA	C1-C2-C3	-3.67	119.70	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	C3B-C4B-NB	3.67	113.92	110.52
25	d	404	BCR	C38-C26-C25	-3.67	120.41	124.53
23	B	603	CLA	C1C-C2C-C3C	-3.66	103.10	106.96
23	b	612	CLA	C3B-C4B-NB	3.66	113.91	110.52
23	D	405	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
23	c	505	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
23	B	602	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
23	B	614	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
23	B	616	CLA	C4C-C3C-C2C	-3.65	101.57	106.90
29	A	414	PL9	C15-C14-C16	3.65	121.41	115.27
23	b	608	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
23	D	406	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
25	h	101	BCR	C38-C26-C25	-3.65	120.43	124.53
25	b	617	BCR	C7-C8-C9	-3.65	120.72	126.23
23	a	407	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
35	c	517	DGD	O2G-C1B-C2B	3.64	119.34	111.50
23	C	506	CLA	C1-C2-C3	-3.64	119.75	126.04
23	c	512	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
25	d	404	BCR	C29-C30-C25	3.63	116.07	110.48
23	a	407	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
23	A	408	CLA	CAC-C3C-C4C	3.62	129.51	124.81
25	y	101	BCR	C15-C14-C13	-3.62	122.14	127.31
23	b	613	CLA	C1-C2-C3	-3.62	119.79	126.04
38	e	87	HEM	C1B-NB-C4B	3.62	108.81	105.07
23	a	405	CLA	O2A-CGA-O1A	-3.62	114.47	123.59
33	C	521	LMG	C3-C4-C5	3.61	116.69	110.24
23	D	406	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
23	b	611	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
23	b	609	CLA	C1D-CHD-C4C	-3.61	118.28	126.06
23	c	510	CLA	C1C-C2C-C3C	-3.61	103.17	106.96
23	c	511	CLA	C1D-CHD-C4C	-3.60	118.28	126.06
23	C	505	CLA	C3B-C4B-NB	3.60	113.86	110.52
23	b	602	CLA	C3C-C4C-NC	3.60	114.61	110.57
37	d	711	LHG	O8-C23-C24	3.60	123.21	111.91
25	d	404	BCR	C40-C30-C25	-3.60	104.46	110.30
23	B	604	CLA	C3D-C4D-ND	3.60	116.06	110.24
23	c	511	CLA	CMC-C2C-C1C	3.60	130.52	125.04
23	b	601	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
25	Y	101	BCR	C15-C14-C13	-3.59	122.19	127.31
23	B	602	CLA	CAA-C2A-C3A	-3.59	102.96	112.78
29	d	405	PL9	C42-C43-C44	-3.59	119.02	127.66
26	a	413	SQD	O47-C7-C8	3.59	119.23	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	626	HTG	C1'-S1-C1	3.58	106.79	100.09
33	C	501	LMG	O1-C1-C2	3.58	113.89	108.30
29	A	414	PL9	C22-C23-C24	-3.57	119.05	127.66
29	d	405	PL9	C40-C39-C41	3.57	121.28	115.27
23	d	403	CLA	CMB-C2B-C1B	3.57	130.81	125.37
35	c	518	DGD	O2G-C1B-C2B	3.57	119.19	111.50
23	b	602	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
23	b	613	CLA	C3B-C4B-NB	3.56	113.82	110.52
23	b	603	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
23	A	405	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
23	b	616	CLA	O2A-CGA-CBA	3.56	123.07	111.91
25	c	515	BCR	C11-C10-C9	-3.56	122.23	127.31
23	C	504	CLA	C1-C2-C3	-3.55	119.89	126.04
23	C	507	CLA	C3C-C4C-NC	3.55	114.56	110.57
23	b	615	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
26	A	410	SQD	O47-C7-C8	3.55	119.16	111.50
23	b	602	CLA	CAA-C2A-C3A	-3.55	103.05	112.78
23	B	610	CLA	C1D-CHD-C4C	-3.55	118.40	126.06
29	A	414	PL9	C7-C3-C2	-3.55	118.63	123.30
23	C	512	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
23	A	408	CLA	C1D-CHD-C4C	-3.55	118.40	126.06
23	b	603	CLA	C3B-C4B-NB	3.55	113.81	110.52
23	c	513	CLA	C3C-C4C-NC	3.54	114.55	110.57
23	b	605	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
23	A	406	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
23	b	604	CLA	C3B-C4B-NB	3.54	113.80	110.52
23	b	602	CLA	C1D-CHD-C4C	-3.54	118.43	126.06
23	C	508	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
23	C	509	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
23	c	507	CLA	C1-C2-C3	-3.53	119.93	126.04
23	b	611	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
38	E	103	HEM	CHB-C1B-NB	3.53	128.73	124.37
25	d	404	BCR	C16-C17-C18	-3.53	122.27	127.31
23	b	614	CLA	C3B-C4B-NB	3.53	113.79	110.52
23	c	505	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
23	B	608	CLA	C1D-CHD-C4C	-3.53	118.45	126.06
23	b	611	CLA	C3B-C4B-NB	3.52	113.78	110.52
23	C	512	CLA	C3B-C4B-NB	3.52	113.78	110.52
23	A	405	CLA	CAA-C2A-C3A	-3.52	103.13	112.78
23	b	607	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
23	B	613	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
23	d	403	CLA	C1D-CHD-C4C	-3.52	118.47	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	C3B-C4B-NB	3.52	113.78	110.52
23	C	506	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
25	c	515	BCR	C15-C14-C13	-3.51	122.30	127.31
23	B	603	CLA	CAA-C2A-C3A	-3.51	103.18	112.78
23	B	614	CLA	CMC-C2C-C1C	3.51	130.38	125.04
23	C	513	CLA	C4-C3-C5	3.50	121.16	115.27
23	b	616	CLA	CHD-C4C-NC	3.50	129.72	124.20
37	D	409	LHG	O7-C7-C8	3.50	119.04	111.50
23	B	608	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
23	B	607	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
34	V	203	HTG	C1-O5-C5	3.48	116.91	112.19
23	B	605	CLA	O2A-CGA-O1A	-3.48	114.81	123.59
23	d	402	CLA	O2A-CGA-CBA	3.48	122.83	111.91
23	C	514	CLA	C3B-C4B-NB	3.48	113.74	110.52
23	C	505	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
23	b	615	CLA	O2D-CGD-CBD	3.48	117.45	111.27
23	C	504	CLA	C4-C3-C5	3.48	121.12	115.27
23	b	612	CLA	C4C-C3C-C2C	-3.47	101.84	106.90
23	d	402	CLA	C3B-C4B-NB	3.47	113.73	110.52
23	B	610	CLA	CAA-CBA-CGA	-3.47	103.11	113.25
24	A	353	PHO	C1A-C2A-C3A	-3.46	99.54	102.84
29	d	405	PL9	C37-C38-C39	-3.46	119.33	127.66
23	b	614	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
23	b	610	CLA	O2D-CGD-O1D	-3.46	117.07	123.84
23	B	608	CLA	CAC-C3C-C4C	3.46	129.30	124.81
23	c	506	CLA	C4C-C3C-C2C	-3.45	101.87	106.90
23	A	404	CLA	O2A-CGA-O1A	-3.45	114.89	123.59
23	B	610	CLA	CMB-C2B-C1B	3.45	130.62	125.37
23	c	507	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
25	C	515	BCR	C33-C5-C6	-3.44	120.66	124.53
23	b	615	CLA	C4-C3-C5	3.44	121.06	115.27
23	B	609	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
23	B	604	CLA	CAC-C3C-C4C	3.43	129.27	124.81
25	D	407	BCR	C10-C11-C12	-3.43	112.50	123.22
23	C	511	CLA	C4-C3-C5	3.43	121.05	115.27
23	B	605	CLA	C4C-C3C-C2C	-3.43	101.89	106.90
23	c	513	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
33	B	621	LMG	O8-C28-C29	3.43	122.67	111.91
23	C	508	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
23	C	512	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
24	a	408	PHO	C1A-C2A-C3A	-3.43	99.58	102.84
23	B	606	CLA	O2D-CGD-O1D	-3.43	117.14	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	617	BCR	C33-C5-C6	-3.42	120.68	124.53
23	b	608	CLA	CAC-C3C-C4C	3.42	129.25	124.81
23	B	601	CLA	O2D-CGD-O1D	-3.42	117.14	123.84
25	A	409	BCR	C24-C23-C22	-3.42	121.06	126.23
34	b	622	HTG	C1'-S1-C1	3.42	106.48	100.09
23	C	507	CLA	CBC-CAC-C3C	-3.42	103.01	112.43
37	d	408	LHG	O7-C7-C8	3.42	118.86	111.50
23	a	406	CLA	CHD-C4C-NC	3.41	129.58	124.20
23	B	604	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
23	C	502	CLA	C1C-C2C-C3C	-3.41	103.38	106.96
38	e	87	HEM	CHA-C4D-ND	3.41	128.57	124.37
23	B	616	CLA	CAC-C3C-C4C	3.41	129.23	124.81
24	a	408	PHO	O1D-CGD-CBD	-3.41	119.07	124.74
23	c	513	CLA	CMB-C2B-C1B	3.40	130.55	125.37
23	B	611	CLA	CHB-C4A-NA	3.40	129.21	124.51
23	B	601	CLA	CHD-C4C-NC	3.40	129.55	124.20
23	b	604	CLA	CAC-C3C-C4C	3.39	129.21	124.81
23	C	503	CLA	CMB-C2B-C1B	3.39	130.53	125.37
23	b	607	CLA	C4-C3-C5	3.38	120.96	115.27
23	B	611	CLA	C4C-C3C-C2C	-3.38	101.97	106.90
23	B	613	CLA	C4-C3-C5	3.38	120.96	115.27
23	C	514	CLA	CMC-C2C-C1C	3.38	130.19	125.04
23	B	607	CLA	C3B-C4B-NB	3.38	113.65	110.52
23	a	406	CLA	C3B-C4B-NB	3.38	113.65	110.52
29	a	416	PL9	C27-C28-C29	-3.38	119.53	127.66
23	b	601	CLA	C4-C3-C5	3.38	120.95	115.27
23	b	607	CLA	C1D-CHD-C4C	-3.38	118.78	126.06
29	A	414	PL9	C37-C38-C39	-3.37	119.54	127.66
23	B	609	CLA	CMB-C2B-C1B	3.37	130.51	125.37
23	B	601	CLA	C4C-C3C-C2C	-3.37	101.98	106.90
23	d	403	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
23	B	608	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
23	B	611	CLA	C2A-C1A-CHA	-3.37	117.97	123.86
23	a	409	CLA	O2D-CGD-O1D	-3.37	117.26	123.84
25	a	410	BCR	C38-C26-C25	-3.37	120.75	124.53
29	A	414	PL9	C27-C28-C29	-3.36	119.56	127.66
23	c	506	CLA	CMB-C2B-C1B	3.36	130.49	125.37
23	b	611	CLA	CHD-C4C-NC	3.36	129.50	124.20
23	a	405	CLA	O2A-CGA-CBA	3.36	122.45	111.91
40	V	202	HEC	CBD-CAD-C3D	-3.36	103.30	112.63
23	D	405	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
23	B	605	CLA	CHD-C4C-NC	3.35	129.49	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	CMC-C2C-C1C	3.35	130.15	125.04
26	B	620	SQD	C1-O5-C5	-3.35	107.11	113.69
23	C	507	CLA	CMC-C2C-C1C	3.35	130.15	125.04
23	c	503	CLA	CHD-C4C-NC	3.35	129.48	124.20
23	A	404	CLA	CAC-C3C-C4C	3.35	129.15	124.81
37	l	101	LHG	O7-C7-C8	3.35	118.72	111.50
25	B	619	BCR	C7-C8-C9	-3.35	121.18	126.23
24	a	353	PHO	C4-C3-C5	3.35	120.90	115.27
23	b	610	CLA	C4C-C3C-C2C	-3.34	102.02	106.90
23	B	604	CLA	C4C-C3C-C2C	-3.34	102.02	106.90
23	A	408	CLA	CAA-C2A-C3A	-3.34	103.63	112.78
23	b	602	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
23	d	402	CLA	C4-C3-C5	3.34	120.89	115.27
23	B	615	CLA	CMC-C2C-C1C	3.34	130.12	125.04
23	B	612	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
23	b	612	CLA	CAC-C3C-C4C	3.33	129.14	124.81
23	a	405	CLA	C1-C2-C3	-3.33	120.28	126.04
23	A	404	CLA	CAA-C2A-C1A	-3.33	101.05	111.97
23	B	610	CLA	C4C-C3C-C2C	-3.33	102.04	106.90
23	C	513	CLA	CMC-C2C-C1C	3.33	130.11	125.04
23	C	508	CLA	CMB-C2B-C1B	3.32	130.43	125.37
23	B	602	CLA	CMC-C2C-C1C	3.32	130.10	125.04
23	b	609	CLA	CBC-CAC-C3C	-3.32	103.28	112.43
23	a	405	CLA	CAA-C2A-C1A	-3.32	101.10	111.97
23	B	605	CLA	C4-C3-C5	3.32	120.85	115.27
23	B	612	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
23	b	611	CLA	CMC-C2C-C1C	3.32	130.09	125.04
23	C	504	CLA	C1C-C2C-C3C	-3.31	103.47	106.96
25	k	101	BCR	C29-C30-C25	3.31	115.57	110.48
23	b	610	CLA	C1C-C2C-C3C	-3.31	103.48	106.96
23	C	506	CLA	CAC-C3C-C4C	3.31	129.10	124.81
23	C	503	CLA	O2D-CGD-O1D	-3.31	117.38	123.84
37	D	409	LHG	O8-C23-C24	3.30	122.28	111.91
23	b	615	CLA	CMB-C2B-C1B	3.30	130.40	125.37
29	a	416	PL9	C37-C38-C39	-3.30	119.71	127.66
23	a	405	CLA	C3B-C4B-NB	3.30	113.58	110.52
33	a	419	LMG	C8-O7-C10	-3.30	109.67	117.79
23	d	402	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
25	Y	101	BCR	C28-C27-C26	-3.29	108.20	114.08
23	c	508	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
29	D	408	PL9	C25-C24-C26	3.29	120.81	115.27
34	b	625	HTG	O5-C5-C4	3.29	115.67	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	C3B-C4B-NB	3.29	113.56	110.52
23	c	511	CLA	C4-C3-C5	3.28	120.80	115.27
23	A	406	CLA	CAA-C2A-C3A	-3.28	103.78	112.78
23	B	605	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
33	z	101	LMG	O7-C10-C11	3.28	118.57	111.50
23	a	405	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
23	B	606	CLA	CMC-C2C-C1C	3.27	130.03	125.04
33	C	520	LMG	O8-C28-C29	3.27	122.17	111.91
23	A	408	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
23	C	507	CLA	CHC-C1C-C2C	-3.27	117.65	126.73
25	K	102	BCR	C7-C8-C9	-3.27	121.30	126.23
23	c	504	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
23	C	513	CLA	CHD-C4C-NC	3.26	129.34	124.20
23	C	506	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
23	b	601	CLA	CHD-C4C-NC	3.26	129.34	124.20
23	b	611	CLA	C1D-CHD-C4C	-3.26	119.03	126.06
23	c	510	CLA	CHC-C1C-C2C	-3.25	117.70	126.73
23	b	612	CLA	CMC-C2C-C1C	3.25	129.99	125.04
23	b	616	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
23	c	509	CLA	C1-C2-C3	-3.25	120.43	126.04
25	C	516	BCR	C7-C8-C9	-3.25	121.33	126.23
38	E	103	HEM	CBD-CAD-C3D	-3.25	103.61	112.63
23	C	509	CLA	C4C-C3C-C2C	-3.25	102.17	106.90
23	d	402	CLA	C1-C2-C3	-3.24	120.43	126.04
23	B	612	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
23	b	605	CLA	CHD-C4C-NC	3.24	129.31	124.20
23	b	609	CLA	C4C-C3C-C2C	-3.24	102.18	106.90
23	B	614	CLA	C1-C2-C3	-3.23	120.45	126.04
23	c	508	CLA	C1D-CHD-C4C	-3.23	119.08	126.06
23	c	507	CLA	CHC-C1C-C2C	-3.23	117.75	126.73
23	B	603	CLA	O2A-CGA-O1A	-3.23	115.43	123.59
23	C	507	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
25	K	102	BCR	C20-C21-C22	-3.23	122.70	127.31
35	h	102	DGD	O2G-C1B-C2B	3.23	118.46	111.50
23	C	503	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
23	A	406	CLA	O2A-CGA-O1A	-3.23	115.45	123.59
26	a	413	SQD	O48-C23-C24	3.23	122.03	111.91
23	b	614	CLA	O2A-CGA-O1A	-3.22	115.45	123.59
23	B	603	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
23	c	503	CLA	C3B-C4B-NB	3.22	113.51	110.52
23	C	512	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
23	b	608	CLA	C1-C2-C3	-3.22	120.47	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	502	CLA	CMB-C2B-C1B	3.22	130.28	125.37
23	a	409	CLA	CMB-C2B-C1B	3.22	130.28	125.37
23	B	604	CLA	O2A-CGA-O1A	-3.22	115.47	123.59
23	a	409	CLA	CHD-C4C-NC	3.22	129.27	124.20
23	B	607	CLA	CMC-C2C-C1C	3.21	129.94	125.04
26	a	411	SQD	C45-O47-C7	-3.21	109.88	117.79
33	Z	101	LMG	O6-C1-C2	3.21	117.15	110.35
23	b	605	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
23	c	505	CLA	CMB-C2B-C1B	3.21	130.25	125.37
29	a	416	PL9	C17-C18-C19	-3.21	119.94	127.66
24	a	408	PHO	O2A-CGA-O1A	-3.20	115.51	123.59
33	c	521	LMG	C9-C8-C7	-3.20	104.22	111.79
23	B	615	CLA	C3B-C4B-NB	3.20	113.48	110.52
29	a	416	PL9	C25-C24-C26	3.20	120.65	115.27
23	b	609	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
23	c	506	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
25	T	101	BCR	C16-C17-C18	-3.20	122.75	127.31
23	b	615	CLA	C11-C10-C8	-3.20	105.59	115.92
29	D	408	PL9	C17-C18-C19	-3.20	119.96	127.66
33	m	101	LMG	O8-C28-C29	3.19	121.93	111.91
24	A	353	PHO	C4-C3-C5	3.19	120.64	115.27
23	b	615	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
38	e	87	HEM	CBD-CAD-C3D	-3.19	103.77	112.63
23	c	510	CLA	CAC-C3C-C4C	3.18	128.94	124.81
23	B	612	CLA	CMC-C2C-C1C	3.18	129.89	125.04
23	c	512	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
23	c	513	CLA	O2A-CGA-CBA	3.18	121.89	111.91
23	c	502	CLA	C1D-CHD-C4C	-3.18	119.20	126.06
23	d	402	CLA	O2A-CGA-O1A	-3.18	115.57	123.59
23	C	508	CLA	C4C-C3C-C2C	-3.17	102.27	106.90
33	a	419	LMG	C7-O1-C1	-3.17	107.54	113.74
33	Z	101	LMG	C4-C3-C2	3.17	116.36	110.82
33	D	415	LMG	O8-C28-O10	-3.17	115.59	123.59
23	b	606	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
34	b	622	HTG	O5-C1-C2	3.17	114.30	110.31
23	C	504	CLA	CMB-C2B-C1B	3.17	130.19	125.37
23	b	614	CLA	C1-C2-C3	-3.17	120.57	126.04
23	b	606	CLA	C3B-C4B-NB	3.16	113.45	110.52
23	A	405	CLA	CMB-C2B-C1B	3.16	130.18	125.37
23	C	502	CLA	CHD-C4C-NC	3.16	129.18	124.20
23	c	508	CLA	C4-C3-C5	3.16	120.59	115.27
23	B	612	CLA	CAC-C3C-C4C	3.16	128.91	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
23	C	507	CLA	CAC-C3C-C4C	3.16	128.91	124.81
25	C	516	BCR	C33-C5-C6	-3.16	120.98	124.53
23	C	502	CLA	CMC-C2C-C1C	3.15	129.84	125.04
23	a	405	CLA	C4-C3-C5	3.15	120.57	115.27
23	c	511	CLA	C3B-C4B-NB	3.15	113.44	110.52
23	b	616	CLA	CBC-CAC-C3C	-3.15	103.76	112.43
23	b	602	CLA	C1-C2-C3	-3.14	120.61	126.04
25	H	101	BCR	C24-C23-C22	-3.14	121.49	126.23
32	b	627	LMT	C3'-C4'-C5'	-3.14	103.73	110.93
23	C	502	CLA	CMB-C2B-C1B	3.14	130.15	125.37
23	C	505	CLA	C1-O2A-CGA	3.14	124.68	116.44
23	B	614	CLA	O2A-CGA-CBA	3.14	121.75	111.91
23	b	614	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
23	b	603	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
23	c	505	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
23	c	506	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
25	A	409	BCR	C11-C10-C9	-3.13	122.84	127.31
23	A	404	CLA	C1-C2-C3	-3.13	120.63	126.04
23	A	408	CLA	CHC-C1C-C2C	-3.13	118.04	126.73
23	C	513	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
23	c	507	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
23	c	513	CLA	C4-C3-C5	3.13	120.53	115.27
23	b	608	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
23	B	608	CLA	CMA-C3A-C4A	-3.12	103.37	111.77
23	a	407	CLA	CMB-C2B-C1B	3.12	130.12	125.37
23	c	509	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
23	B	608	CLA	CHC-C1C-C2C	-3.12	118.06	126.73
23	C	508	CLA	CBC-CAC-C3C	-3.12	103.83	112.43
23	A	405	CLA	CAC-C3C-C4C	3.12	128.86	124.81
23	B	616	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
23	C	509	CLA	CAC-C3C-C4C	3.12	128.86	124.81
23	c	510	CLA	CHB-C1B-NB	-3.12	120.95	124.26
26	b	620	SQD	C3-C4-C5	3.12	115.80	110.24
23	a	407	CLA	CHD-C4C-NC	3.12	129.12	124.20
23	B	604	CLA	CMB-C2B-C1B	3.12	130.11	125.37
23	B	607	CLA	C4-C3-C5	3.11	120.51	115.27
23	b	609	CLA	C3B-C4B-NB	3.11	113.40	110.52
25	B	617	BCR	C7-C8-C9	-3.11	121.54	126.23
23	b	602	CLA	CMB-C2B-C1B	3.11	130.10	125.37
23	b	612	CLA	O2A-CGA-CBA	3.11	121.66	111.91
23	c	504	CLA	C1C-C2C-C3C	-3.11	103.69	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	CAC-C3C-C4C	3.11	128.84	124.81
23	c	502	CLA	C1-C2-C3	-3.11	120.67	126.04
38	e	87	HEM	CHD-C4C-NC	3.11	127.80	124.44
23	D	405	CLA	C1D-CHD-C4C	-3.11	119.36	126.06
23	C	511	CLA	CHD-C4C-NC	3.11	129.10	124.20
23	C	504	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
29	a	416	PL9	C35-C34-C36	3.10	120.49	115.27
26	A	412	SQD	O48-C23-C24	3.10	121.65	111.91
23	B	606	CLA	CHD-C4C-NC	3.10	129.09	124.20
37	D	411	LHG	O7-C7-C8	3.10	118.19	111.50
23	c	510	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
24	a	408	PHO	O2A-CGA-CBA	3.10	121.63	111.91
23	c	509	CLA	CMB-C2B-C1B	3.10	130.09	125.37
26	B	620	SQD	O9-S-C6	3.09	110.61	106.94
23	a	407	CLA	CAA-C2A-C3A	-3.09	104.31	112.78
23	C	505	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
25	k	101	BCR	C7-C8-C9	-3.09	121.57	126.23
23	B	610	CLA	C3B-C4B-NB	3.09	113.38	110.52
25	y	101	BCR	C38-C26-C25	-3.09	121.06	124.53
23	D	406	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
32	A	359	LMT	O5B-C5B-C4B	3.08	115.29	109.69
37	D	410	LHG	O8-C23-O10	-3.08	115.82	123.59
25	y	101	BCR	C24-C23-C22	-3.08	121.58	126.23
23	B	609	CLA	CMC-C2C-C1C	3.08	129.73	125.04
23	B	615	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
25	D	407	BCR	C29-C30-C25	3.08	115.22	110.48
25	T	101	BCR	C15-C14-C13	3.08	131.70	127.31
23	c	512	CLA	C4-C3-C5	3.08	120.44	115.27
38	E	103	HEM	CHD-C1D-ND	3.07	127.76	124.42
23	a	407	CLA	C3B-C4B-NB	3.07	113.37	110.52
38	e	87	HEM	CHD-C1D-ND	3.07	127.75	124.42
23	C	512	CLA	CMC-C2C-C1C	3.07	129.71	125.04
25	b	618	BCR	C37-C22-C21	-3.07	118.62	122.92
23	B	604	CLA	CHC-C1C-C2C	-3.07	118.21	126.73
23	C	510	CLA	C1D-CHD-C4C	-3.07	119.44	126.06
23	c	504	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
26	f	102	SQD	O5-C1-C2	3.06	116.83	110.35
23	c	510	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
25	b	619	BCR	C15-C14-C13	-3.06	122.94	127.31
25	T	101	BCR	C11-C10-C9	-3.06	122.95	127.31
37	e	101	LHG	O7-C7-C8	3.05	118.08	111.50
35	C	519	DGD	O1G-C1A-C2A	3.05	121.48	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	CHC-C1C-C2C	-3.05	118.26	126.73
23	b	613	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	B	607	CLA	C1D-CHD-C4C	-3.05	119.49	126.06
23	C	514	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
23	A	404	CLA	CMC-C2C-C1C	3.05	129.68	125.04
23	B	602	CLA	C3B-C4B-NB	3.05	113.34	110.52
37	D	411	LHG	O8-C23-C24	3.05	121.46	111.91
29	A	414	PL9	O1-C4-C3	-3.05	117.37	120.72
23	B	614	CLA	CBC-CAC-C3C	-3.04	104.04	112.43
29	a	416	PL9	C10-C9-C11	3.04	120.39	115.27
23	A	408	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
23	C	503	CLA	C3B-C4B-NB	3.04	113.33	110.52
29	A	414	PL9	C20-C19-C21	3.04	120.38	115.27
23	B	614	CLA	CAC-C3C-C4C	3.04	128.75	124.81
23	C	510	CLA	O2A-CGA-CBA	3.04	121.44	111.91
23	b	603	CLA	C4-C3-C5	3.04	120.38	115.27
37	d	711	LHG	O7-C7-C8	3.03	118.04	111.50
23	b	616	CLA	C3B-C4B-NB	3.03	113.32	110.52
23	C	506	CLA	C4-C3-C5	3.03	120.36	115.27
23	B	611	CLA	C1-C2-C3	-3.03	120.81	126.04
26	F	101	SQD	C1-C2-C3	-3.03	103.69	110.00
25	c	516	BCR	C7-C8-C9	-3.03	121.66	126.23
23	C	513	CLA	C1C-C2C-C3C	-3.03	103.78	106.96
23	C	509	CLA	CHC-C1C-C2C	-3.02	118.33	126.73
23	A	405	CLA	C3B-C4B-NB	3.02	113.32	110.52
23	C	510	CLA	CHC-C1C-C2C	-3.02	118.34	126.73
33	D	415	LMG	O8-C28-C29	3.02	121.38	111.91
23	c	503	CLA	CBC-CAC-C3C	-3.02	104.11	112.43
23	a	409	CLA	O2A-CGA-CBA	3.02	121.38	111.91
24	a	353	PHO	CBA-CAA-C2A	-3.02	105.00	113.81
23	b	616	CLA	CMB-C2B-C1B	3.02	129.96	125.37
23	b	603	CLA	C2A-C1A-CHA	-3.02	118.59	123.86
23	B	607	CLA	CBC-CAC-C3C	-3.01	104.12	112.43
23	A	406	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
37	D	411	LHG	O8-C23-O10	-3.01	115.99	123.59
24	a	353	PHO	CMB-C2B-C3B	3.01	130.30	124.68
23	b	609	CLA	CAC-C3C-C4C	3.01	128.71	124.81
23	B	610	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
23	B	602	CLA	CAC-C3C-C4C	3.00	128.71	124.81
23	D	406	CLA	CAC-C3C-C4C	3.00	128.71	124.81
29	D	408	PL9	C53-C6-C1	3.00	121.13	114.99
25	c	515	BCR	C16-C17-C18	-3.00	123.03	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	CMB-C2B-C1B	3.00	129.94	125.37
29	d	405	PL9	C22-C23-C24	-3.00	120.44	127.66
23	c	512	CLA	CHD-C4C-NC	3.00	128.93	124.20
29	d	405	PL9	C36-C34-C33	-3.00	115.05	121.12
23	a	407	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
23	b	613	CLA	CHC-C1C-C2C	-3.00	118.41	126.73
23	C	503	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
26	B	620	SQD	C4-C3-C2	3.00	116.05	110.82
23	C	502	CLA	CAC-C3C-C4C	3.00	128.70	124.81
29	A	414	PL9	C17-C18-C19	-2.99	120.45	127.66
23	D	406	CLA	C3B-C4B-NB	2.99	113.29	110.52
38	e	87	HEM	C4D-ND-C1D	2.99	108.16	105.07
23	C	512	CLA	C1-C2-C3	-2.99	120.87	126.04
23	C	512	CLA	CMB-C2B-C1B	2.99	129.92	125.37
23	c	506	CLA	CMC-C2C-C1C	2.99	129.59	125.04
23	a	405	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
25	T	101	BCR	C33-C5-C6	-2.99	121.17	124.53
23	b	607	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
23	c	502	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
23	d	402	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	b	616	CLA	O2A-CGA-O1A	-2.98	116.07	123.59
25	B	618	BCR	C2-C1-C6	2.98	115.07	110.48
23	a	405	CLA	CMA-C3A-C4A	-2.98	103.77	111.77
25	h	101	BCR	C7-C8-C9	-2.98	121.74	126.23
23	A	406	CLA	CMC-C2C-C1C	2.98	129.57	125.04
23	C	509	CLA	CMC-C2C-C1C	2.97	129.57	125.04
35	C	517	DGD	C2G-O2G-C1B	-2.97	110.47	117.79
23	d	402	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
23	B	613	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
29	a	416	PL9	C42-C43-C44	-2.97	120.50	127.66
23	a	405	CLA	CMC-C2C-C1C	2.97	129.56	125.04
23	B	607	CLA	CAA-C2A-C3A	-2.97	104.64	112.78
23	B	603	CLA	O2A-CGA-CBA	2.97	121.23	111.91
29	d	405	PL9	C10-C9-C11	2.97	120.27	115.27
23	B	605	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
26	f	102	SQD	C4-C3-C2	-2.97	105.64	110.82
23	C	502	CLA	C3B-C4B-NB	2.97	113.27	110.52
33	C	521	LMG	O8-C28-C29	2.97	121.22	111.91
23	C	511	CLA	CHC-C1C-C2C	-2.97	118.49	126.73
23	b	614	CLA	CHD-C4C-NC	2.97	128.88	124.20
23	C	514	CLA	CHD-C4C-NC	2.97	128.88	124.20
23	b	610	CLA	CAA-C2A-C3A	-2.96	104.66	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	410	SQD	O8-S-C6	2.96	110.46	105.74
24	a	353	PHO	O2D-CGD-O1D	-2.96	118.05	123.84
34	b	622	HTG	O5-C5-C4	2.96	115.07	109.69
23	B	609	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
25	C	515	BCR	C15-C14-C13	-2.96	123.09	127.31
23	B	610	CLA	O2A-CGA-O1A	-2.96	116.13	123.59
23	c	505	CLA	CBC-CAC-C3C	-2.95	104.29	112.43
23	D	405	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
23	d	403	CLA	C4-C3-C5	2.95	120.23	115.27
23	C	503	CLA	CAC-C3C-C4C	2.95	128.64	124.81
23	a	409	CLA	C3B-C4B-NB	2.95	113.25	110.52
23	d	403	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
23	b	606	CLA	CHC-C1C-C2C	-2.95	118.54	126.73
23	c	513	CLA	CHC-C1C-C2C	-2.95	118.55	126.73
23	b	608	CLA	CHC-C1C-C2C	-2.94	118.55	126.73
23	C	511	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
23	d	403	CLA	C2A-C1A-CHA	-2.94	118.71	123.86
23	B	613	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
23	C	514	CLA	C1-C2-C3	-2.94	120.96	126.04
23	B	606	CLA	CMB-C2B-C1B	2.94	129.85	125.37
23	C	506	CLA	C3B-C4B-NB	2.94	113.24	110.52
23	c	510	CLA	O2A-CGA-CBA	2.94	121.13	111.91
23	b	614	CLA	CHC-C1C-C2C	-2.94	118.57	126.73
33	c	520	LMG	O1-C7-C8	-2.94	103.81	110.90
23	c	502	CLA	CAC-C3C-C4C	2.93	128.62	124.81
23	C	510	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
23	b	606	CLA	O2A-CGA-O1A	-2.93	116.19	123.59
23	b	605	CLA	O2A-CGA-O1A	-2.93	116.19	123.59
23	C	507	CLA	C4-C3-C5	2.93	120.20	115.27
25	t	103	BCR	C21-C20-C19	-2.93	114.07	123.22
29	D	408	PL9	C10-C9-C11	2.93	120.20	115.27
23	B	613	CLA	O2A-CGA-O1A	-2.93	116.20	123.59
23	b	616	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
23	C	513	CLA	O2A-CGA-CBA	2.93	121.10	111.91
23	b	606	CLA	CHD-C4C-NC	2.93	128.82	124.20
23	A	405	CLA	CMA-C3A-C4A	-2.93	103.90	111.77
23	c	506	CLA	C1D-CHD-C4C	-2.93	119.74	126.06
23	c	510	CLA	O2A-C1-C2	2.92	116.32	108.64
23	A	404	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
23	a	406	CLA	CMA-C3A-C2A	-2.92	102.03	113.83
25	b	619	BCR	C38-C26-C25	-2.92	121.25	124.53
23	b	612	CLA	O2A-CGA-O1A	-2.92	116.22	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	CHD-C4C-NC	2.92	128.81	124.20
23	b	605	CLA	C2A-C1A-CHA	-2.92	118.75	123.86
23	C	508	CLA	CHD-C4C-NC	2.92	128.81	124.20
23	B	604	CLA	C6-C5-C3	-2.92	105.80	113.45
26	B	620	SQD	O48-C23-C24	2.92	121.07	111.91
23	b	605	CLA	C4-C3-C5	2.92	120.18	115.27
23	B	601	CLA	C1C-C2C-C3C	-2.92	103.89	106.96
23	b	611	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
23	b	609	CLA	CHD-C4C-NC	2.92	128.80	124.20
37	E	101	LHG	O8-C23-C24	2.92	121.06	111.91
23	a	409	CLA	C4-C3-C5	2.92	120.18	115.27
23	c	504	CLA	C3B-C4B-NB	2.91	113.22	110.52
23	b	603	CLA	O2A-CGA-O1A	-2.91	116.24	123.59
23	B	613	CLA	O2A-CGA-CBA	2.91	121.05	111.91
23	D	405	CLA	C4-C3-C5	2.91	120.17	115.27
23	c	514	CLA	CAC-C3C-C4C	2.91	128.59	124.81
23	C	512	CLA	C4-C3-C5	2.91	120.17	115.27
23	A	404	CLA	C2A-C1A-CHA	-2.91	118.77	123.86
25	H	101	BCR	C7-C8-C9	-2.91	121.84	126.23
23	B	609	CLA	O2A-CGA-CBA	2.91	121.03	111.91
23	b	609	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	a	409	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
23	C	506	CLA	CMC-C2C-C1C	2.90	129.46	125.04
23	A	405	CLA	CHD-C4C-NC	2.90	128.78	124.20
23	c	512	CLA	CHC-C1C-C2C	-2.90	118.67	126.73
23	D	405	CLA	O2A-CGA-CBA	2.90	121.00	111.91
23	b	609	CLA	CMC-C2C-C1C	2.90	129.45	125.04
23	A	408	CLA	CMC-C2C-C1C	2.90	129.45	125.04
23	b	607	CLA	CBC-CAC-C3C	-2.90	104.45	112.43
23	c	502	CLA	CHC-C1C-C2C	-2.90	118.69	126.73
23	b	602	CLA	CHD-C4C-NC	2.90	128.77	124.20
25	b	619	BCR	C24-C23-C22	-2.89	121.86	126.23
35	h	102	DGD	O3G-C1D-C2D	2.89	112.82	108.30
23	B	603	CLA	CHC-C1C-C2C	-2.89	118.69	126.73
33	z	101	LMG	O8-C28-C29	2.89	120.98	111.91
23	C	510	CLA	O2A-CGA-O1A	-2.89	116.30	123.59
23	B	615	CLA	C4-C3-C5	2.89	120.13	115.27
23	b	605	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
25	c	515	BCR	C38-C26-C25	-2.89	121.28	124.53
23	C	507	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
23	d	402	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
23	B	611	CLA	C3B-C4B-NB	2.89	113.19	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
23	b	606	CLA	CAA-C2A-C3A	-2.88	104.88	112.78
23	b	610	CLA	CHD-C4C-NC	2.88	128.75	124.20
25	d	404	BCR	C21-C20-C19	-2.88	114.22	123.22
23	C	504	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
37	d	407	LHG	O7-C7-C8	2.88	117.71	111.50
23	D	405	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
23	C	510	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
24	a	353	PHO	C4A-C3A-C2A	-2.88	100.10	102.84
23	b	615	CLA	CHC-C1C-C2C	-2.88	118.74	126.73
32	I	101	LMT	O5B-C5B-C4B	2.88	114.92	109.69
26	b	620	SQD	O8-S-C6	2.88	110.32	105.74
23	A	406	CLA	CHD-C4C-NC	2.88	128.73	124.20
26	a	411	SQD	O47-C7-O49	-2.87	116.75	123.70
23	C	504	CLA	CAC-C3C-C4C	2.87	128.54	124.81
23	C	503	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
24	A	353	PHO	O2D-CGD-O1D	-2.87	118.22	123.84
23	B	616	CLA	CMC-C2C-C1C	2.87	129.41	125.04
23	c	514	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
23	a	405	CLA	CAC-C3C-C4C	2.87	128.53	124.81
23	B	616	CLA	CHD-C4C-NC	2.87	128.72	124.20
23	b	604	CLA	CMB-C2B-C1B	2.87	129.74	125.37
37	D	409	LHG	C5-O7-C7	-2.87	110.73	117.79
34	b	622	HTG	O2-C2-C1	2.86	115.53	110.27
23	B	606	CLA	O2A-CGA-CBA	2.86	120.89	111.91
23	C	509	CLA	CMB-C2B-C1B	2.86	129.73	125.37
23	c	503	CLA	CMB-C2B-C1B	2.86	129.72	125.37
23	B	602	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
23	c	512	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
29	D	408	PL9	C51-C49-C50	2.86	120.92	114.60
32	M	101	LMT	C1'-O5'-C5'	-2.86	108.08	113.69
23	B	603	CLA	C2A-C1A-CHA	-2.85	118.87	123.86
26	b	620	SQD	O7-S-C6	2.85	110.33	106.94
23	c	510	CLA	C4-C3-C5	2.85	120.07	115.27
23	a	406	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
29	a	416	PL9	C53-C6-C1	2.85	120.82	114.99
23	c	505	CLA	CAC-C3C-C4C	2.85	128.51	124.81
23	C	506	CLA	CHC-C1C-C2C	-2.85	118.82	126.73
23	c	509	CLA	CHC-C1C-C2C	-2.85	118.82	126.73
23	B	613	CLA	CAC-C3C-C4C	2.85	128.50	124.81
35	h	102	DGD	O1G-C1A-O1A	-2.85	116.41	123.59
35	C	517	DGD	O6D-C1D-O3G	-2.85	103.24	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	C3B-C4B-NB	2.84	113.15	110.52
25	k	101	BCR	C15-C14-C13	-2.84	123.25	127.31
23	B	614	CLA	CHD-C4C-NC	2.84	128.68	124.20
38	E	103	HEM	CBA-CAA-C2A	-2.84	104.73	112.63
25	H	101	BCR	C10-C11-C12	-2.84	114.35	123.22
26	A	410	SQD	O48-C23-C24	2.84	120.82	111.91
25	K	102	BCR	C38-C26-C25	-2.84	121.34	124.53
23	B	614	CLA	CHC-C1C-C2C	-2.84	118.84	126.73
23	c	502	CLA	C3B-C4B-NB	2.84	113.15	110.52
23	a	407	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
23	A	406	CLA	O2A-CGA-CBA	2.83	120.80	111.91
23	B	610	CLA	CHD-C4C-NC	2.83	128.66	124.20
25	d	404	BCR	C28-C27-C26	-2.83	109.02	114.08
23	c	507	CLA	O2A-CGA-O1A	-2.83	116.45	123.59
23	B	607	CLA	CMB-C2B-C1B	2.83	129.68	125.37
25	D	407	BCR	C37-C22-C23	2.83	122.53	118.08
23	c	514	CLA	O2A-CGA-CBA	2.83	120.78	111.91
29	D	408	PL9	C37-C38-C39	-2.83	120.85	127.66
23	b	613	CLA	C4-C3-C5	2.83	120.02	115.27
23	b	608	CLA	CBC-CAC-C3C	-2.82	104.65	112.43
25	K	102	BCR	C36-C18-C19	2.82	122.52	118.08
23	B	608	CLA	CHB-C4A-NA	2.82	128.41	124.51
23	C	511	CLA	CBC-CAC-C3C	-2.82	104.66	112.43
25	d	404	BCR	C10-C11-C12	-2.82	114.42	123.22
23	B	613	CLA	CHC-C1C-C2C	-2.82	118.90	126.73
29	A	414	PL9	C35-C34-C36	2.82	120.01	115.27
23	c	505	CLA	CED-O2D-CGD	2.82	122.31	115.94
23	c	510	CLA	C1-O2A-CGA	2.82	123.84	116.44
23	B	616	CLA	O2A-CGA-CBA	2.82	120.75	111.91
23	d	403	CLA	CHD-C4C-NC	2.82	128.64	124.20
23	A	408	CLA	C4-C3-C5	2.82	120.01	115.27
37	L	101	LHG	O8-C23-C24	2.82	120.75	111.91
23	C	504	CLA	CHD-C4C-NC	2.81	128.64	124.20
23	A	404	CLA	CHC-C1C-C2C	-2.81	118.92	126.73
23	A	406	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
23	b	605	CLA	C3B-C4B-NB	2.81	113.12	110.52
23	A	406	CLA	C4-C3-C5	2.81	119.99	115.27
29	A	414	PL9	C30-C29-C31	2.81	119.99	115.27
23	b	601	CLA	C3B-C4B-NB	2.80	113.12	110.52
23	C	503	CLA	C2A-C1A-CHA	-2.80	118.95	123.86
23	C	512	CLA	CHC-C1C-C2C	-2.80	118.94	126.73
23	B	606	CLA	C4C-C3C-C2C	-2.80	102.81	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	CAC-C3C-C4C	2.80	128.45	124.81
29	a	416	PL9	C22-C23-C24	-2.80	120.92	127.66
23	b	610	CLA	CMC-C2C-C1C	2.80	129.30	125.04
23	C	511	CLA	CMC-C2C-C1C	2.80	129.30	125.04
23	b	602	CLA	CMA-C3A-C4A	-2.80	104.26	111.77
23	b	610	CLA	CMB-C2B-C1B	2.79	129.62	125.37
23	b	604	CLA	CHC-C1C-C2C	-2.79	118.97	126.73
23	A	405	CLA	CHC-C1C-C2C	-2.79	118.97	126.73
23	C	505	CLA	CHC-C1C-C2C	-2.79	118.97	126.73
23	B	612	CLA	C3B-C4B-NB	2.79	113.10	110.52
23	B	608	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
23	a	407	CLA	CHC-C1C-C2C	-2.79	118.98	126.73
26	f	102	SQD	O48-C23-C24	2.79	120.65	111.91
23	c	513	CLA	CHD-C4C-NC	2.79	128.59	124.20
23	c	513	CLA	CAC-C3C-C4C	2.79	128.42	124.81
38	e	87	HEM	CHB-C1B-NB	2.78	127.81	124.37
23	c	511	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
23	b	615	CLA	O2A-CGA-O1A	-2.78	116.58	123.59
23	b	608	CLA	CHD-C4C-NC	2.78	128.58	124.20
23	c	513	CLA	C3B-C4B-NB	2.78	113.09	110.52
32	m	103	LMT	C3'-C4'-C5'	-2.78	104.56	110.93
23	b	603	CLA	CMB-C2B-C1B	2.78	129.60	125.37
23	B	614	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
23	C	514	CLA	CBC-CAC-C3C	-2.78	104.77	112.43
25	a	410	BCR	C33-C5-C6	-2.78	121.41	124.53
23	b	602	CLA	CAC-C3C-C4C	2.78	128.41	124.81
23	B	615	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
23	b	603	CLA	O2A-CGA-CBA	2.77	120.61	111.91
25	b	618	BCR	C15-C14-C13	-2.77	123.35	127.31
26	F	101	SQD	O48-C23-C24	2.77	120.61	111.91
23	A	405	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
23	b	601	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
24	a	408	PHO	CMB-C2B-C3B	2.77	129.86	124.68
23	C	502	CLA	C4-C3-C5	2.77	119.93	115.27
32	a	414	LMT	O1'-C1'-C2'	2.77	112.62	108.30
23	c	505	CLA	CHC-C1C-C2C	-2.76	119.05	126.73
23	a	406	CLA	O2A-CGA-CBA	2.76	120.58	111.91
32	a	420	LMT	C3'-C4'-C5'	-2.76	104.59	110.93
23	C	502	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
23	a	407	CLA	O2A-CGA-O1A	-2.76	116.62	123.59
23	b	612	CLA	C2A-C1A-CHA	-2.76	119.03	123.86
23	B	615	CLA	CHD-C4C-NC	2.76	128.55	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	514	CLA	C2A-C1A-CHA	-2.76	119.04	123.86
23	B	605	CLA	C2A-C1A-CHA	-2.76	119.04	123.86
23	c	509	CLA	O2A-CGA-CBA	2.76	120.55	111.91
37	D	410	LHG	O7-C7-C8	2.75	117.44	111.50
23	c	504	CLA	CHD-C4C-NC	2.75	128.54	124.20
23	C	514	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
23	c	511	CLA	CAC-C3C-C4C	2.75	128.38	124.81
23	b	613	CLA	CHD-C4C-NC	2.75	128.54	124.20
23	B	608	CLA	CMC-C2C-C1C	2.75	129.22	125.04
23	c	507	CLA	CMC-C2C-C1C	2.75	129.22	125.04
23	b	604	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
23	c	504	CLA	CAC-C3C-C4C	2.75	128.38	124.81
23	D	406	CLA	C4-C3-C5	2.75	119.89	115.27
23	C	502	CLA	CHC-C1C-C2C	-2.74	119.11	126.73
25	a	410	BCR	C40-C30-C25	-2.74	105.85	110.30
29	d	405	PL9	C36-C37-C38	-2.74	102.86	111.88
23	b	614	CLA	O2A-CGA-CBA	2.74	120.52	111.91
23	c	514	CLA	CHC-C1C-C2C	-2.74	119.11	126.73
23	b	615	CLA	C3B-C4B-NB	2.74	113.06	110.52
23	b	603	CLA	CMA-C3A-C2A	-2.74	102.77	113.83
23	c	513	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
23	b	609	CLA	CHC-C1C-C2C	-2.74	119.13	126.73
23	c	511	CLA	O2A-CGA-CBA	2.74	120.50	111.91
23	b	607	CLA	CMC-C2C-C1C	2.74	129.21	125.04
23	b	610	CLA	C4-C3-C5	2.74	119.87	115.27
23	B	611	CLA	C2C-C1C-NC	2.73	112.53	109.97
23	b	601	CLA	CHC-C1C-C2C	-2.73	119.14	126.73
23	B	601	CLA	O2A-CGA-CBA	2.73	120.47	111.91
23	D	406	CLA	CMC-C2C-C1C	2.73	129.19	125.04
23	b	602	CLA	C11-C12-C13	-2.73	107.10	115.92
23	A	408	CLA	O2A-CGA-CBA	2.73	120.47	111.91
27	b	901	GOL	C3-C2-C1	-2.73	101.10	111.70
35	H	102	DGD	O1G-C1A-C2A	2.73	120.46	111.91
23	c	514	CLA	CMB-C2B-C1B	2.73	129.52	125.37
34	B	626	HTG	O5-C5-C4	2.73	114.64	109.69
23	b	604	CLA	C4-C3-C5	2.72	119.86	115.27
32	D	404	LMT	C4B-C3B-C2B	2.72	115.58	110.82
23	b	602	CLA	C4-C3-C5	2.72	119.85	115.27
23	C	504	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
23	B	601	CLA	CMB-C2B-C1B	2.72	129.52	125.37
23	b	601	CLA	CMC-C2C-C1C	2.72	129.19	125.04
23	B	603	CLA	CHD-C4C-NC	2.72	128.49	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	405	PL9	C27-C28-C29	-2.72	121.11	127.66
23	b	613	CLA	O2A-CGA-CBA	2.72	120.44	111.91
23	B	609	CLA	CHC-C1C-C2C	-2.72	119.18	126.73
25	b	617	BCR	C20-C21-C22	-2.72	123.43	127.31
25	B	617	BCR	C31-C1-C6	-2.72	105.89	110.30
23	B	606	CLA	O2A-CGA-O1A	-2.72	116.74	123.59
25	c	516	BCR	C32-C1-C6	-2.72	105.89	110.30
33	c	520	LMG	O8-C28-C29	2.72	120.43	111.91
23	b	603	CLA	CHD-C4C-NC	2.71	128.48	124.20
23	c	503	CLA	O2A-CGA-CBA	2.71	120.42	111.91
23	C	504	CLA	CBC-CAC-C3C	-2.71	104.95	112.43
23	B	614	CLA	C2A-C1A-CHA	-2.71	119.12	123.86
23	b	614	CLA	CBC-CAC-C3C	-2.71	104.96	112.43
23	b	611	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
23	D	406	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
25	D	407	BCR	C40-C30-C25	-2.71	105.91	110.30
23	C	503	CLA	C1-C2-C3	-2.71	121.36	126.04
23	C	505	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
23	B	602	CLA	CHD-C4C-NC	2.71	128.47	124.20
26	f	102	SQD	O8-S-C6	2.70	110.05	105.74
23	B	612	CLA	C2A-C1A-CHA	-2.70	119.13	123.86
23	c	506	CLA	C1-C2-C3	-2.70	121.37	126.04
25	D	407	BCR	C3-C4-C5	-2.70	109.26	114.08
23	B	615	CLA	CED-O2D-CGD	2.70	122.04	115.94
23	C	514	CLA	CMB-C2B-C1B	2.70	129.48	125.37
23	c	508	CLA	CHD-C4C-NC	2.70	128.46	124.20
23	c	502	CLA	CHD-C4C-NC	2.70	128.45	124.20
32	D	404	LMT	C2'-C3'-C4'	2.70	115.84	109.68
23	a	405	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
23	b	603	CLA	CHC-C1C-C2C	-2.69	119.25	126.73
37	L	101	LHG	O8-C23-O10	-2.69	116.80	123.59
23	b	613	CLA	CMC-C2C-C1C	2.69	129.13	125.04
23	D	405	CLA	CAC-C3C-C4C	2.69	128.30	124.81
35	H	102	DGD	O1G-C1A-O1A	-2.69	116.81	123.59
25	T	101	BCR	C12-C13-C14	-2.69	114.82	118.94
23	C	508	CLA	C4-C3-C5	2.69	119.79	115.27
23	b	609	CLA	O2A-CGA-O1A	-2.68	116.82	123.59
23	C	507	CLA	O2A-CGA-O1A	-2.68	116.82	123.59
37	l	101	LHG	O8-C23-C24	2.68	120.32	111.91
23	c	512	CLA	O2A-CGA-CBA	2.68	120.32	111.91
23	c	508	CLA	CAC-C3C-C4C	2.68	128.29	124.81
23	B	603	CLA	CAC-C3C-C4C	2.68	128.28	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	C2A-C1A-CHA	-2.68	119.18	123.86
25	B	619	BCR	C24-C23-C22	-2.68	122.19	126.23
23	A	404	CLA	CMA-C3A-C2A	-2.67	103.05	113.83
33	c	521	LMG	O8-C28-C29	2.67	120.30	111.91
35	H	102	DGD	O2G-C1B-C2B	2.67	117.26	111.50
23	b	613	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
23	D	406	CLA	CHC-C1C-C2C	-2.67	119.31	126.73
23	B	615	CLA	CHC-C1C-C2C	-2.67	119.32	126.73
25	C	516	BCR	C11-C10-C9	-2.67	123.50	127.31
23	B	607	CLA	CHC-C1C-C2C	-2.67	119.33	126.73
23	a	406	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
23	c	508	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
23	c	506	CLA	CHC-C1C-C2C	-2.66	119.33	126.73
25	A	409	BCR	C15-C14-C13	-2.66	123.51	127.31
23	b	609	CLA	CMB-C2B-C1B	2.66	129.43	125.37
23	b	603	CLA	CMC-C2C-C1C	2.66	129.09	125.04
23	B	610	CLA	CMC-C2C-C1C	2.66	129.09	125.04
37	e	101	LHG	O8-C23-C24	2.66	120.25	111.91
40	V	202	HEC	C4B-NB-C1B	2.66	107.82	105.07
25	K	102	BCR	C24-C23-C22	-2.66	122.22	126.23
23	c	507	CLA	C4C-C3C-C2C	-2.66	103.03	106.90
24	A	407	PHO	C1-C2-C3	-2.66	121.45	126.04
23	c	508	CLA	C3B-C4B-NB	2.66	112.98	110.52
23	b	614	CLA	CHB-C1B-NB	-2.66	121.45	124.26
23	C	514	CLA	CHB-C1B-NB	-2.65	121.45	124.26
23	D	405	CLA	CHC-C1C-C2C	-2.65	119.36	126.73
23	C	503	CLA	CMC-C2C-C1C	2.65	129.08	125.04
34	B	626	HTG	C3-C4-C5	2.65	114.97	110.24
23	b	608	CLA	CMA-C3A-C4A	-2.65	104.65	111.77
35	h	102	DGD	O1G-C1A-C2A	2.65	120.23	111.91
23	a	406	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
23	d	402	CLA	CAC-C3C-C4C	2.65	128.25	124.81
35	C	518	DGD	O1G-C1A-O1A	-2.65	116.90	123.59
23	d	402	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
23	A	405	CLA	C4-C3-C5	2.65	119.73	115.27
23	B	602	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
25	y	101	BCR	C10-C11-C12	-2.65	114.96	123.22
29	a	416	PL9	C40-C39-C41	2.65	119.72	115.27
23	b	601	CLA	C1-O2A-CGA	2.65	123.39	116.44
23	c	510	CLA	CHD-C4C-NC	2.65	128.37	124.20
23	b	607	CLA	CMB-C2B-C1B	2.64	129.40	125.37
23	D	405	CLA	C2A-C1A-CHA	-2.64	119.24	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D	410	LHG	O8-C23-C24	2.64	120.20	111.91
23	c	514	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
23	B	607	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
32	D	404	LMT	O1'-C1'-C2'	2.64	112.43	108.30
23	C	510	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
23	a	409	CLA	CAA-C2A-C3A	-2.64	105.55	112.78
23	b	601	CLA	CBC-CAC-C3C	-2.63	105.17	112.43
23	b	606	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
23	c	513	CLA	CHB-C4A-NA	2.63	128.15	124.51
23	B	609	CLA	CHD-C4C-NC	2.63	128.35	124.20
33	m	101	LMG	C7-O1-C1	-2.63	108.60	113.74
23	B	603	CLA	C3B-C4B-NB	2.63	112.96	110.52
29	A	414	PL9	C40-C39-C41	2.63	119.70	115.27
23	C	512	CLA	C1-O2A-CGA	2.63	123.35	116.44
25	t	103	BCR	C36-C18-C19	2.63	122.22	118.08
23	C	513	CLA	CMB-C2B-C1B	2.63	129.38	125.37
23	B	612	CLA	CHD-C4C-NC	2.63	128.35	124.20
23	C	510	CLA	C16-C15-C13	-2.63	107.42	115.92
23	c	508	CLA	O1D-CGD-CBD	-2.63	119.11	124.48
23	B	602	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
23	D	406	CLA	C2A-C1A-CHA	-2.62	119.27	123.86
23	c	514	CLA	CMC-C2C-C1C	2.62	129.03	125.04
23	b	611	CLA	CHC-C1C-C2C	-2.62	119.44	126.73
23	c	512	CLA	CMB-C2B-C1B	2.62	129.36	125.37
23	C	507	CLA	CMB-C2B-C1B	2.62	129.36	125.37
23	b	613	CLA	CAC-C3C-C4C	2.62	128.21	124.81
23	c	503	CLA	C1-C2-C3	-2.62	121.51	126.04
23	C	507	CLA	O2A-CGA-CBA	2.62	120.13	111.91
23	c	511	CLA	CHC-C1C-C2C	-2.62	119.46	126.73
23	b	607	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
23	D	406	CLA	CMA-C3A-C2A	-2.62	103.28	113.83
35	C	519	DGD	O2G-C1B-C2B	2.61	117.13	111.50
26	a	413	SQD	C1-O5-C5	2.61	118.82	113.69
23	D	406	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
23	B	612	CLA	O2A-CGA-CBA	2.61	120.10	111.91
29	a	416	PL9	C47-C48-C49	-2.61	118.83	127.75
23	b	614	CLA	CMC-C2C-C1C	2.61	129.01	125.04
23	a	407	CLA	O2A-CGA-CBA	2.61	120.10	111.91
23	b	616	CLA	C4-C3-C5	2.61	119.66	115.27
34	b	623	HTG	O5-C1-C2	2.61	113.59	110.31
23	C	505	CLA	CMC-C2C-C1C	2.61	129.01	125.04
37	d	408	LHG	O8-C23-C24	2.61	120.09	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	v	202	HEC	CHA-C4D-ND	2.61	127.25	124.42
35	c	519	DGD	O1G-C1A-C2A	2.61	120.09	111.91
23	C	502	CLA	CBC-CAC-C3C	-2.61	105.25	112.43
23	c	508	CLA	O2A-CGA-CBA	2.61	120.08	111.91
32	M	103	LMT	C3'-C4'-C5'	-2.60	104.96	110.93
23	A	405	CLA	CMA-C3A-C2A	-2.60	103.33	113.83
29	a	416	PL9	C10-C9-C8	-2.60	117.01	123.68
25	B	618	BCR	C37-C22-C21	-2.60	119.28	122.92
26	a	413	SQD	O7-S-C6	2.60	110.03	106.94
23	C	511	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
25	k	101	BCR	C2-C1-C6	2.60	114.48	110.48
23	b	602	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
23	b	601	CLA	CMB-C2B-C1B	2.60	129.32	125.37
23	a	407	CLA	CMC-C2C-C1C	2.60	128.99	125.04
23	B	601	CLA	C1-O2A-CGA	2.60	123.26	116.44
23	C	503	CLA	CHD-C4C-NC	2.60	128.29	124.20
24	A	407	PHO	O2A-CGA-CBA	2.59	120.05	111.91
23	c	504	CLA	C4-C3-C5	2.59	119.63	115.27
25	h	101	BCR	C16-C17-C18	-2.59	123.61	127.31
23	b	613	CLA	CED-O2D-CGD	2.59	121.80	115.94
25	K	102	BCR	C37-C22-C21	-2.59	119.29	122.92
23	C	514	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
23	c	514	CLA	CHD-C4C-NC	2.59	128.29	124.20
23	C	502	CLA	C1-C2-C3	-2.59	121.57	126.04
23	a	406	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
23	c	510	CLA	CMB-C2B-C1B	2.59	129.31	125.37
38	E	103	HEM	O2D-CGD-CBD	2.59	122.34	114.03
23	B	616	CLA	CHC-C1C-C2C	-2.58	119.55	126.73
25	c	515	BCR	C36-C18-C17	-2.58	119.30	122.92
23	b	602	CLA	C1-O2A-CGA	2.58	123.22	116.44
34	C	522	HTG	C1-O5-C5	2.58	117.34	112.58
23	b	612	CLA	CHC-C1C-C2C	-2.58	119.56	126.73
32	b	621	LMT	C1'-O5'-C5'	-2.58	108.62	113.69
34	B	622	HTG	O2-C2-C3	-2.58	104.38	110.35
23	b	615	CLA	CHD-C4C-NC	2.58	128.27	124.20
35	c	519	DGD	O2G-C1B-C2B	2.58	117.06	111.50
25	Y	101	BCR	C36-C18-C17	-2.58	119.31	122.92
25	B	617	BCR	C16-C17-C18	-2.58	123.63	127.31
23	a	409	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
23	c	502	CLA	O2A-CGA-O1A	-2.58	117.08	123.59
23	C	510	CLA	C11-C12-C13	-2.58	107.58	115.92
23	b	609	CLA	O2A-CGA-CBA	2.58	120.00	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	CHC-C1C-C2C	-2.58	119.57	126.73
25	c	515	BCR	C37-C22-C21	-2.58	119.31	122.92
34	B	622	HTG	C1-O5-C5	2.58	117.33	112.58
23	C	514	CLA	O2A-CGA-CBA	2.58	119.99	111.91
23	A	405	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
23	c	503	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
23	b	611	CLA	CBC-CAC-C3C	-2.58	105.33	112.43
23	D	405	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
23	c	512	CLA	CMC-C2C-C1C	2.57	128.96	125.04
23	C	513	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
23	d	403	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
24	A	407	PHO	O1D-CGD-CBD	-2.57	120.46	124.74
23	A	408	CLA	CMA-C3A-C2A	-2.57	103.46	113.83
26	A	410	SQD	O48-C23-O10	-2.57	117.11	123.59
33	D	415	LMG	O7-C10-C11	2.57	117.03	111.50
23	b	608	CLA	O2A-CGA-CBA	2.57	119.96	111.91
23	B	603	CLA	CMA-C3A-C2A	-2.57	103.47	113.83
23	B	611	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
24	A	407	PHO	O2A-CGA-O1A	-2.57	117.12	123.59
25	c	515	BCR	C20-C21-C22	-2.57	123.65	127.31
23	c	502	CLA	C4-C3-C5	2.57	119.59	115.27
23	C	507	CLA	CHD-C4C-NC	2.56	128.25	124.20
23	b	607	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
32	M	101	LMT	C3'-C4'-C5'	-2.56	105.05	110.93
23	B	604	CLA	C6-C7-C8	-2.56	107.64	115.92
23	b	614	CLA	CAC-C3C-C4C	2.56	128.13	124.81
32	I	101	LMT	O5'-C5'-C6'	2.56	112.81	106.44
26	F	101	SQD	O47-C7-O49	-2.56	117.51	123.70
23	b	611	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
23	C	511	CLA	O2A-CGA-CBA	2.56	119.94	111.91
29	A	414	PL9	C10-C9-C8	-2.56	117.11	123.68
23	d	403	CLA	CHC-C1C-C2C	-2.56	119.62	126.73
23	c	507	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
23	b	603	CLA	CBC-CAC-C3C	-2.56	105.38	112.43
23	c	504	CLA	CHC-C1C-C2C	-2.56	119.62	126.73
23	A	408	CLA	CHB-C1B-NB	-2.56	121.55	124.26
23	c	508	CLA	C1-C2-C3	-2.56	121.62	126.04
25	t	103	BCR	C1-C6-C7	2.56	123.01	115.78
25	Y	101	BCR	C10-C11-C12	-2.56	115.24	123.22
25	B	617	BCR	C15-C14-C13	-2.55	123.66	127.31
23	b	607	CLA	CAC-C3C-C4C	2.55	128.12	124.81
23	C	511	CLA	C4C-C3C-C2C	-2.55	103.18	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
23	B	609	CLA	CBC-CAC-C3C	-2.55	105.40	112.43
23	b	605	CLA	CMC-C2C-C1C	2.55	128.92	125.04
23	c	505	CLA	CHD-C4C-NC	2.55	128.22	124.20
23	c	511	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
25	h	101	BCR	C33-C5-C6	-2.55	121.67	124.53
23	A	405	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
23	d	402	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
29	A	414	PL9	C47-C48-C49	-2.54	119.05	127.75
25	H	101	BCR	C11-C10-C9	-2.54	123.68	127.31
23	c	508	CLA	CHC-C1C-C2C	-2.54	119.67	126.73
23	C	512	CLA	CHD-C4C-NC	2.54	128.21	124.20
32	e	102	LMT	O1'-C1'-C2'	2.54	112.27	108.30
23	d	403	CLA	O2A-CGA-CBA	2.54	119.88	111.91
23	B	610	CLA	CHC-C1C-C2C	-2.54	119.68	126.73
23	B	608	CLA	CHD-C4C-NC	2.54	128.20	124.20
23	b	615	CLA	C1-C2-C3	-2.54	121.65	126.04
23	c	507	CLA	CHD-C4C-NC	2.54	128.20	124.20
33	C	501	LMG	C8-O7-C10	-2.54	111.55	117.79
40	V	202	HEC	CAD-CBD-CGD	-2.53	108.15	113.60
23	C	506	CLA	O2A-CGA-CBA	2.53	119.85	111.91
25	C	516	BCR	C32-C1-C6	-2.53	106.19	110.30
23	C	508	CLA	C1-C2-C3	-2.53	121.67	126.04
23	B	612	CLA	C1-C2-C3	-2.53	121.67	126.04
23	B	605	CLA	O2A-CGA-CBA	2.53	119.84	111.91
23	b	606	CLA	CMC-C2C-C1C	2.53	128.89	125.04
23	B	613	CLA	CMC-C2C-C1C	2.52	128.88	125.04
23	c	511	CLA	O2A-CGA-O1A	-2.52	117.22	123.59
23	b	606	CLA	CMB-C2B-C1B	2.52	129.21	125.37
32	M	103	LMT	C1'-O5'-C5'	-2.52	108.74	113.69
26	A	412	SQD	C4-C3-C2	-2.52	106.42	110.82
23	C	506	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
23	c	505	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
23	B	615	CLA	C11-C10-C8	-2.52	107.78	115.92
25	C	515	BCR	C38-C26-C25	-2.52	121.70	124.53
23	B	604	CLA	CMC-C2C-C1C	2.51	128.87	125.04
23	b	602	CLA	CHB-C1B-C2B	-2.51	120.13	127.24
25	D	407	BCR	C16-C17-C18	-2.51	123.72	127.31
23	b	616	CLA	CHC-C1C-C2C	-2.51	119.75	126.73
23	c	509	CLA	CHD-C4C-NC	2.51	128.16	124.20
23	a	406	CLA	CAA-CBA-CGA	2.51	120.59	113.25
23	B	606	CLA	C4-C3-C5	2.51	119.50	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	CMC-C2C-C1C	2.51	128.86	125.04
23	d	402	CLA	CMC-C2C-C1C	2.51	128.86	125.04
25	d	404	BCR	C33-C5-C6	-2.51	121.71	124.53
23	A	406	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
23	B	608	CLA	O2A-CGA-CBA	2.51	119.78	111.91
23	a	405	CLA	CHD-C4C-NC	2.51	128.15	124.20
29	D	408	PL9	C42-C41-C39	-2.50	104.75	112.98
25	c	516	BCR	C2-C1-C6	2.50	114.33	110.48
23	c	504	CLA	CMC-C2C-C1C	2.50	128.84	125.04
35	c	518	DGD	O1G-C1A-C2A	2.50	119.74	111.91
23	A	408	CLA	CHD-C4C-NC	2.50	128.14	124.20
23	B	606	CLA	CHC-C1C-C2C	-2.50	119.80	126.73
25	T	101	BCR	C21-C20-C19	-2.50	115.43	123.22
23	c	502	CLA	CMC-C2C-C1C	2.50	128.84	125.04
23	a	405	CLA	C4C-C3C-C2C	-2.49	103.26	106.90
40	V	202	HEC	C2A-C1A-NA	-2.49	107.90	110.32
25	B	618	BCR	C15-C14-C13	-2.49	123.75	127.31
23	B	611	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
23	b	604	CLA	O2A-CGA-CBA	2.49	119.72	111.91
23	b	610	CLA	C3B-C4B-NB	2.49	112.82	110.52
38	E	103	HEM	CHA-C4D-ND	2.49	127.44	124.37
40	V	202	HEC	CMD-C2D-C1D	2.49	128.83	125.04
23	b	605	CLA	CAC-C3C-C4C	2.49	128.04	124.81
23	B	601	CLA	CMC-C2C-C1C	2.49	128.82	125.04
23	d	403	CLA	C3B-C4B-NB	2.49	112.82	110.52
23	b	608	CLA	O2A-CGA-O1A	-2.49	117.32	123.59
26	a	411	SQD	O8-S-C6	2.49	109.70	105.74
23	b	614	CLA	C2A-C1A-CHA	-2.48	119.51	123.86
23	c	511	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
23	C	508	CLA	O2A-CGA-CBA	2.48	119.70	111.91
23	a	406	CLA	CBC-CAC-C3C	-2.48	105.59	112.43
23	C	505	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
23	C	503	CLA	C4-C3-C5	2.48	119.44	115.27
23	C	508	CLA	CMC-C2C-C1C	2.48	128.81	125.04
23	b	612	CLA	CHD-C4C-NC	2.48	128.11	124.20
23	c	512	CLA	C1-O2A-CGA	2.48	122.94	116.44
29	D	408	PL9	C20-C19-C21	2.47	119.43	115.27
25	H	101	BCR	C37-C22-C21	-2.47	119.46	122.92
35	c	517	DGD	C2G-O2G-C1B	-2.47	111.70	117.79
23	B	607	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
25	d	404	BCR	C37-C22-C23	2.47	121.97	118.08
23	b	615	CLA	C6-C7-C8	-2.47	107.94	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	C1-C2-C3	-2.47	121.78	126.04
25	K	102	BCR	C29-C30-C25	2.47	114.28	110.48
23	C	511	CLA	C2A-C1A-CHA	-2.47	119.55	123.86
23	C	508	CLA	CHC-C1C-C2C	-2.47	119.88	126.73
23	B	612	CLA	C11-C12-C13	-2.46	107.95	115.92
23	A	408	CLA	CBC-CAC-C3C	-2.46	105.64	112.43
26	f	102	SQD	O5-C5-C4	2.46	114.17	109.69
24	A	407	PHO	CMB-C2B-C3B	2.46	129.29	124.68
23	b	604	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
23	C	509	CLA	C4-C3-C5	2.46	119.41	115.27
23	b	610	CLA	CHC-C1C-C2C	-2.46	119.89	126.73
23	B	603	CLA	CMC-C2C-C1C	2.46	128.78	125.04
23	C	506	CLA	CHD-C4C-NC	2.46	128.08	124.20
23	c	512	CLA	CBC-CAC-C3C	-2.46	105.66	112.43
23	c	513	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
25	k	101	BCR	C24-C23-C22	-2.45	122.53	126.23
34	b	625	HTG	O5-C1-S1	-2.45	103.96	109.82
23	b	605	CLA	CMB-C2B-C1B	2.45	129.10	125.37
35	C	519	DGD	O3G-C3G-C2G	-2.45	104.98	110.90
23	C	514	CLA	CAA-C2A-C3A	-2.45	106.07	112.78
23	b	610	CLA	CAA-CBA-CGA	-2.45	106.09	113.25
23	B	606	CLA	C3B-C4B-NB	2.45	112.79	110.52
23	A	404	CLA	CAA-CBA-CGA	-2.45	106.09	113.25
23	B	609	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
29	D	408	PL9	C40-C39-C41	2.45	119.39	115.27
23	B	610	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	C	505	CLA	CMB-C2B-C1B	2.45	129.10	125.37
23	B	605	CLA	CHC-C1C-C2C	-2.45	119.93	126.73
23	B	612	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
23	b	615	CLA	CAC-C3C-C4C	2.45	127.98	124.81
32	E	102	LMT	C1'-O5'-C5'	-2.44	108.89	113.69
23	B	601	CLA	CHC-C1C-C2C	-2.44	119.95	126.73
23	B	612	CLA	CHC-C1C-C2C	-2.44	119.95	126.73
25	c	516	BCR	C33-C5-C6	-2.44	121.79	124.53
23	b	605	CLA	C1-C2-C3	-2.44	121.83	126.04
23	B	611	CLA	OBD-CAD-C3D	-2.44	122.66	128.52
23	B	605	CLA	C1-C2-C3	-2.44	121.83	126.04
23	b	605	CLA	CED-O2D-CGD	2.44	121.45	115.94
25	T	101	BCR	C3-C4-C5	-2.43	109.73	114.08
23	c	511	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
25	c	516	BCR	C21-C20-C19	-2.43	115.63	123.22
23	C	504	CLA	O2A-CGA-CBA	2.43	119.54	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	516	BCR	C37-C22-C23	2.43	121.90	118.08
23	D	406	CLA	O2A-CGA-CBA	2.43	119.53	111.91
25	A	409	BCR	C38-C26-C25	-2.43	121.80	124.53
23	c	509	CLA	CAC-C3C-C4C	2.43	127.96	124.81
23	d	403	CLA	CBC-CAC-C3C	-2.43	105.74	112.43
40	v	202	HEC	C1D-C2D-C3D	-2.43	104.41	106.96
25	y	101	BCR	C16-C17-C18	-2.43	123.85	127.31
23	C	510	CLA	CHD-C4C-NC	2.42	128.02	124.20
23	A	405	CLA	CAA-CBA-CGA	2.42	120.34	113.25
23	c	510	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
23	C	514	CLA	CHC-C1C-C2C	-2.42	120.00	126.73
38	E	103	HEM	O2A-CGA-CBA	2.42	121.81	114.03
23	c	508	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
23	B	606	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
23	A	406	CLA	C1-C2-C3	-2.42	121.86	126.04
23	c	506	CLA	O2A-CGA-CBA	2.42	119.50	111.91
23	B	616	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
23	B	602	CLA	C11-C12-C13	-2.42	108.11	115.92
25	D	407	BCR	C15-C14-C13	-2.42	123.86	127.31
33	m	101	LMG	C8-O7-C10	-2.42	111.84	117.79
23	B	609	CLA	CAC-C3C-C4C	2.42	127.94	124.81
25	H	101	BCR	C16-C17-C18	-2.42	123.86	127.31
25	B	618	BCR	C38-C26-C25	-2.42	121.82	124.53
23	D	406	CLA	CHD-C4C-NC	2.41	128.01	124.20
29	D	408	PL9	C7-C8-C9	-2.41	122.77	126.79
23	B	610	CLA	C1-C2-C3	-2.41	121.87	126.04
25	B	619	BCR	C2-C1-C6	2.41	114.20	110.48
37	D	409	LHG	O7-C7-O9	-2.41	117.87	123.70
25	B	618	BCR	C11-C10-C9	-2.41	123.87	127.31
25	d	404	BCR	C39-C30-C25	-2.41	106.39	110.30
35	H	102	DGD	O6E-C5E-C6E	2.41	112.43	106.44
23	B	612	CLA	CHB-C1B-NB	-2.41	121.70	124.26
25	c	516	BCR	C37-C22-C21	-2.41	119.55	122.92
23	B	604	CLA	C11-C12-C13	-2.41	108.13	115.92
23	b	612	CLA	CHB-C1B-NB	-2.41	121.71	124.26
25	Y	101	BCR	C37-C22-C23	2.41	121.87	118.08
23	C	507	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
24	A	407	PHO	CMA-C3A-C4A	-2.41	109.11	114.38
23	B	604	CLA	O2A-CGA-CBA	2.41	119.46	111.91
25	c	515	BCR	C33-C5-C6	-2.41	121.83	124.53
23	c	505	CLA	CHB-C1B-NB	-2.40	121.71	124.26
23	c	502	CLA	O2A-CGA-CBA	2.40	119.45	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	C1-C2-C3	-2.40	121.89	126.04
25	y	101	BCR	C34-C9-C8	2.40	121.86	118.08
37	l	101	LHG	O8-C23-O10	-2.40	117.53	123.59
37	d	408	LHG	O8-C23-O10	-2.40	117.54	123.59
29	d	405	PL9	C17-C18-C19	-2.40	121.89	127.66
23	C	511	CLA	CMB-C2B-C1B	2.40	129.02	125.37
23	b	615	CLA	CMC-C2C-C1C	2.40	128.69	125.04
25	b	619	BCR	C11-C10-C9	-2.40	123.89	127.31
23	c	507	CLA	O2A-CGA-CBA	2.40	119.43	111.91
26	b	620	SQD	O48-C23-C24	2.40	119.43	111.91
23	A	408	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
29	d	405	PL9	C7-C8-C9	-2.39	122.81	126.79
25	d	404	BCR	C24-C23-C22	-2.39	122.62	126.23
23	B	609	CLA	C3B-C4B-NB	2.39	112.73	110.52
23	c	514	CLA	C4-C3-C5	2.39	119.29	115.27
32	E	102	LMT	C3B-C4B-C5B	-2.39	105.97	110.24
23	B	608	CLA	C1-C2-C3	-2.39	121.91	126.04
33	d	412	LMG	O8-C28-C29	2.39	119.41	111.91
23	c	504	CLA	OBD-CAD-C3D	-2.39	122.77	128.52
25	b	617	BCR	C11-C10-C9	-2.39	123.90	127.31
23	b	603	CLA	CAC-C3C-C4C	2.39	127.91	124.81
32	I	101	LMT	O1'-C1'-C2'	2.39	112.03	108.30
32	a	414	LMT	O5'-C5'-C6'	2.39	112.37	106.44
23	C	513	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	D	405	CLA	CMC-C2C-C1C	2.38	128.67	125.04
23	c	505	CLA	CMC-C2C-C1C	2.38	128.67	125.04
23	d	402	CLA	CMB-C2B-C1B	2.38	129.00	125.37
23	a	405	CLA	CMA-C3A-C2A	-2.38	104.22	113.83
23	B	612	CLA	C4-C3-C5	2.38	119.28	115.27
29	a	416	PL9	C20-C19-C21	2.38	119.28	115.27
26	B	620	SQD	O48-C23-O10	-2.38	117.58	123.59
23	d	403	CLA	CAC-C3C-C4C	2.38	127.90	124.81
23	C	502	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
25	h	101	BCR	C36-C18-C17	-2.38	119.59	122.92
23	B	603	CLA	C5-C3-C2	-2.38	116.31	121.12
29	D	408	PL9	C36-C37-C38	-2.38	104.07	111.88
33	B	621	LMG	O8-C28-O10	-2.38	117.59	123.59
34	b	622	HTG	C6-C5-C4	-2.38	107.44	113.00
26	B	620	SQD	C44-O6-C1	-2.38	109.10	113.74
25	C	515	BCR	C16-C17-C18	-2.37	123.92	127.31
23	c	514	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
23	A	406	CLA	CAC-C3C-C4C	2.37	127.89	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
32	I	101	LMT	O5'-C5'-C4'	2.37	114.75	109.75
23	b	604	CLA	CHD-C4C-NC	2.37	127.94	124.20
23	b	601	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
23	C	504	CLA	C3B-C4B-NB	2.37	112.71	110.52
23	c	509	CLA	C4-C3-C5	2.37	119.25	115.27
23	a	409	CLA	CHC-C1C-C2C	-2.37	120.15	126.73
23	B	601	CLA	CAC-C3C-C4C	2.37	127.88	124.81
24	A	353	PHO	C4D-CHA-CBD	2.37	109.59	108.52
23	c	506	CLA	C4-C3-C5	2.36	119.25	115.27
32	t	101	LMT	C3'-C4'-C5'	-2.36	105.51	110.93
23	B	601	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	C	512	CLA	O2A-CGA-CBA	2.36	119.33	111.91
23	c	510	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
23	b	615	CLA	O2A-CGA-CBA	2.36	119.32	111.91
24	a	353	PHO	C1A-C2A-C3A	-2.36	100.59	102.84
23	C	502	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
23	B	614	CLA	CAA-C2A-C3A	-2.36	106.31	112.78
23	C	510	CLA	CMC-C2C-C1C	2.36	128.63	125.04
25	b	619	BCR	C16-C17-C18	-2.36	123.94	127.31
23	C	503	CLA	O2A-CGA-CBA	2.36	119.31	111.91
35	c	517	DGD	C3G-C2G-C1G	-2.36	106.21	111.79
23	c	509	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
34	b	622	HTG	O2-C2-C3	-2.36	104.90	110.35
23	B	606	CLA	C2A-C1A-CHA	-2.36	119.74	123.86
26	f	102	SQD	O47-C7-O49	-2.36	118.00	123.70
23	c	514	CLA	CHB-C1B-NB	-2.36	121.76	124.26
29	d	405	PL9	C12-C13-C14	-2.36	121.99	127.66
25	h	101	BCR	C37-C22-C21	-2.36	119.62	122.92
23	c	503	CLA	C4C-C3C-C2C	-2.35	103.47	106.90
23	B	615	CLA	C6-C7-C8	-2.35	108.31	115.92
23	C	502	CLA	C11-C12-C13	-2.35	108.32	115.92
23	a	407	CLA	C1-C2-C3	-2.35	121.98	126.04
25	C	516	BCR	C3-C4-C5	-2.35	109.88	114.08
23	C	513	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
23	C	502	CLA	O2A-CGA-CBA	2.35	119.28	111.91
29	A	414	PL9	C45-C44-C46	2.35	119.22	115.27
23	b	602	CLA	CHC-C1C-C2C	-2.35	120.21	126.73
26	f	102	SQD	O48-C23-O10	-2.35	117.67	123.59
23	B	608	CLA	C11-C12-C13	-2.35	108.33	115.92
25	T	101	BCR	C2-C1-C6	2.34	114.09	110.48
23	c	504	CLA	C2A-C1A-CHA	-2.34	119.76	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	CAC-C3C-C2C	2.34	131.54	127.53
23	b	609	CLA	C16-C15-C13	-2.34	108.34	115.92
23	A	406	CLA	CMA-C3A-C2A	-2.34	104.38	113.83
23	C	502	CLA	C1-O2A-CGA	2.34	122.59	116.44
23	B	605	CLA	CMC-C2C-C1C	2.34	128.60	125.04
23	B	611	CLA	C4-C3-C5	2.34	119.21	115.27
23	B	607	CLA	CHD-C4C-NC	2.34	127.89	124.20
23	c	505	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
25	y	101	BCR	C34-C9-C10	-2.34	119.65	122.92
23	B	611	CLA	CMB-C2B-C3B	2.34	132.25	126.59
29	A	414	PL9	C42-C43-C44	-2.34	122.03	127.66
40	V	202	HEC	CBC-CAC-C3C	2.34	118.87	112.43
23	B	613	CLA	C2A-C1A-CHA	-2.34	119.78	123.86
25	a	410	BCR	C29-C30-C25	2.34	114.08	110.48
25	c	516	BCR	C11-C10-C9	-2.33	123.98	127.31
26	b	620	SQD	O47-C7-O49	-2.33	118.06	123.70
37	d	407	LHG	C6-C5-C4	-2.33	106.27	111.79
29	d	405	PL9	C20-C19-C21	2.33	119.20	115.27
25	c	515	BCR	C36-C18-C19	2.33	121.75	118.08
32	a	414	LMT	O5'-C5'-C4'	2.33	114.67	109.75
23	D	405	CLA	CMB-C2B-C1B	2.33	128.92	125.37
25	b	619	BCR	C7-C8-C9	-2.33	122.72	126.23
25	b	618	BCR	C29-C30-C25	2.33	114.07	110.48
32	M	101	LMT	C3B-C4B-C5B	-2.33	106.08	110.24
23	c	513	CLA	CMC-C2C-C1C	2.33	128.59	125.04
25	B	617	BCR	C11-C10-C9	-2.33	123.99	127.31
23	c	502	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
40	V	202	HEC	CHB-C4A-NA	2.32	126.95	124.44
23	d	403	CLA	CMC-C2C-C1C	2.32	128.58	125.04
23	C	514	CLA	CAC-C3C-C4C	2.32	127.82	124.81
23	b	613	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
23	C	509	CLA	CHD-C4C-NC	2.32	127.86	124.20
23	C	506	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
23	C	505	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
25	B	619	BCR	C38-C26-C25	-2.32	121.93	124.53
23	b	606	CLA	C1-C2-C3	-2.31	122.04	126.04
23	b	608	CLA	C4C-C3C-C2C	-2.31	103.53	106.90
23	b	609	CLA	C7-C6-C5	-2.31	107.08	113.36
23	a	409	CLA	CMA-C3A-C2A	-2.31	104.50	113.83
32	t	101	LMT	O5'-C5'-C4'	2.31	114.63	109.75
23	B	614	CLA	C4-C3-C5	2.31	119.16	115.27
23	a	406	CLA	CMC-C2C-C1C	2.31	128.56	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	514	CLA	C1-C2-C3	-2.31	122.05	126.04
32	m	103	LMT	C3B-C4B-C5B	-2.31	106.12	110.24
25	b	617	BCR	C29-C30-C25	2.31	114.04	110.48
40	v	202	HEC	C4A-NA-C1A	2.31	107.61	105.35
25	y	101	BCR	C21-C20-C19	-2.31	116.02	123.22
35	C	518	DGD	C2G-O2G-C1B	-2.31	112.11	117.79
32	t	101	LMT	O1'-C1'-C2'	2.31	111.90	108.30
25	c	515	BCR	C7-C8-C9	-2.31	122.75	126.23
23	B	605	CLA	C3B-C4B-NB	2.30	112.65	110.52
35	C	517	DGD	O6E-C5E-C4E	2.30	113.88	109.69
23	B	604	CLA	C4-C3-C5	2.30	119.14	115.27
38	E	103	HEM	C4A-NA-C1A	2.30	107.60	105.35
25	A	409	BCR	C16-C17-C18	-2.30	124.03	127.31
26	a	413	SQD	O8-S-C6	2.30	109.41	105.74
23	C	506	CLA	CHA-C1A-NA	-2.30	121.13	126.40
23	b	604	CLA	C6-C5-C3	-2.30	107.43	113.45
23	c	504	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
23	b	607	CLA	C4A-NA-C1A	-2.30	105.67	106.71
26	a	411	SQD	O48-C23-C24	2.30	119.11	111.91
23	c	509	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
23	C	513	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
33	B	621	LMG	C12-C11-C10	-2.29	105.29	113.62
25	t	103	BCR	C7-C6-C5	-2.29	115.91	121.46
23	b	616	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
26	a	413	SQD	C3-C4-C5	2.29	114.32	110.24
23	C	505	CLA	CHD-C4C-NC	2.29	127.81	124.20
33	C	520	LMG	C8-O7-C10	-2.29	112.16	117.79
23	c	513	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
35	C	517	DGD	C3G-C2G-C1G	-2.29	106.38	111.79
25	K	102	BCR	C2-C1-C6	2.29	114.00	110.48
40	v	202	HEC	C4B-NB-C1B	2.28	107.43	105.07
23	B	613	CLA	C4-C3-C2	-2.28	117.82	123.68
23	D	406	CLA	CMA-C3A-C4A	-2.28	105.64	111.77
23	C	507	CLA	CHB-C4A-NA	2.28	127.67	124.51
23	C	513	CLA	CHC-C1C-C2C	-2.28	120.40	126.73
23	c	505	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
29	d	405	PL9	C51-C49-C50	2.28	119.63	114.60
23	B	614	CLA	OBD-CAD-C3D	-2.27	123.05	128.52
25	Y	101	BCR	C38-C26-C25	-2.27	121.97	124.53
25	D	407	BCR	C24-C23-C22	-2.27	122.80	126.23
25	b	618	BCR	C20-C21-C22	-2.27	124.07	127.31
23	B	601	CLA	C3B-C4B-NB	2.27	112.62	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	O2A-CGA-CBA	2.27	119.03	111.91
24	a	353	PHO	O2A-CGA-CBA	2.27	119.03	111.91
29	A	414	PL9	C35-C34-C33	-2.27	117.86	123.68
25	Y	101	BCR	C15-C16-C17	-2.27	118.83	123.47
23	B	611	CLA	O2A-CGA-CBA	2.27	119.02	111.91
23	C	510	CLA	O2A-C1-C2	2.27	114.59	108.64
23	a	405	CLA	C7-C6-C5	-2.27	107.20	113.36
33	d	412	LMG	O7-C10-O9	-2.27	118.23	123.70
23	b	601	CLA	O2A-CGA-CBA	2.26	119.01	111.91
23	C	504	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
23	B	609	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
34	B	622	HTG	C6-C5-C4	-2.26	107.71	113.00
35	C	518	DGD	O2G-C1B-O1B	-2.26	118.24	123.70
23	b	607	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
23	B	613	CLA	CHD-C4C-NC	2.26	127.77	124.20
25	y	101	BCR	C1-C6-C7	2.26	122.17	115.78
23	c	505	CLA	O2A-CGA-CBA	2.26	119.00	111.91
23	b	607	CLA	CHB-C1B-NB	-2.26	121.87	124.26
23	C	508	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
23	B	610	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
40	V	202	HEC	C4A-NA-C1A	2.26	107.56	105.35
23	b	610	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
33	C	521	LMG	C9-C8-C7	-2.26	106.45	111.79
23	B	606	CLA	C1-O2A-CGA	2.25	122.36	116.44
40	V	202	HEC	C1D-C2D-C3D	-2.25	104.59	106.96
25	K	102	BCR	C33-C5-C6	-2.25	122.00	124.53
25	B	619	BCR	C31-C1-C6	-2.25	106.64	110.30
23	C	509	CLA	CHB-C1B-NB	-2.25	121.87	124.26
24	A	407	PHO	C4-C3-C5	2.25	119.06	115.27
25	T	101	BCR	C1-C6-C7	2.25	122.15	115.78
23	D	405	CLA	CED-O2D-CGD	2.25	121.03	115.94
24	a	408	PHO	CMA-C3A-C4A	-2.25	109.45	114.38
23	a	406	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
33	c	521	LMG	O8-C28-O10	-2.25	117.92	123.59
23	B	614	CLA	CMB-C2B-C1B	2.25	128.79	125.37
33	c	520	LMG	C8-O7-C10	-2.25	112.26	117.79
25	B	618	BCR	C37-C22-C23	2.25	121.62	118.08
23	C	506	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
23	b	610	CLA	CAC-C3C-C4C	2.25	127.72	124.81
23	B	602	CLA	CMB-C2B-C1B	2.24	128.79	125.37
35	c	517	DGD	O3G-C3G-C2G	-2.24	105.48	110.90
29	d	405	PL9	C47-C48-C49	-2.24	120.08	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	516	BCR	C29-C30-C25	2.24	113.93	110.48
23	C	504	CLA	CMC-C2C-C1C	2.24	128.45	125.04
23	b	608	CLA	CMB-C2B-C3B	2.24	132.01	126.59
23	c	504	CLA	O2A-CGA-CBA	2.24	118.93	111.91
23	C	505	CLA	CBC-CAC-C3C	-2.24	106.27	112.43
25	b	617	BCR	C15-C16-C17	-2.23	118.90	123.47
23	B	604	CLA	CHB-C1B-NB	-2.23	121.89	124.26
23	B	602	CLA	CAA-CBA-CGA	-2.23	106.73	113.25
25	k	101	BCR	C10-C11-C12	-2.23	116.25	123.22
29	a	416	PL9	C35-C34-C33	-2.23	117.95	123.68
23	C	505	CLA	C4-C3-C5	2.23	119.02	115.27
23	a	409	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
29	A	414	PL9	C25-C24-C26	2.23	119.02	115.27
23	c	505	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
25	B	619	BCR	C3-C4-C5	-2.23	110.10	114.08
23	a	409	CLA	CAC-C3C-C4C	2.23	127.70	124.81
23	c	506	CLA	C3B-C4B-NB	2.23	112.58	110.52
29	A	414	PL9	C12-C13-C14	-2.23	122.30	127.66
23	c	507	CLA	CMB-C2B-C1B	2.23	128.76	125.37
23	c	509	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
24	A	353	PHO	CED-O2D-CGD	2.22	120.97	115.94
29	A	414	PL9	C53-C6-C1	2.22	119.54	114.99
26	A	410	SQD	O9-S-O7	-2.22	106.25	113.95
23	A	404	CLA	CHD-C4C-NC	2.22	127.71	124.20
35	H	102	DGD	C2G-O2G-C1B	-2.22	112.32	117.79
24	a	353	PHO	O1D-CGD-CBD	-2.22	121.04	124.74
23	A	405	CLA	C4C-C3C-C2C	-2.22	103.66	106.90
23	B	606	CLA	C11-C12-C13	-2.22	108.74	115.92
23	c	506	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
23	c	514	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
26	f	102	SQD	C44-O6-C1	-2.22	109.40	113.74
37	d	407	LHG	O8-C23-O10	-2.22	117.99	123.59
33	Z	101	LMG	C1-O6-C5	2.22	118.04	113.69
23	C	507	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
23	C	505	CLA	CHB-C1B-NB	-2.22	121.91	124.26
23	C	509	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
26	A	412	SQD	O48-C23-O10	-2.22	118.00	123.59
33	C	520	LMG	O8-C28-O10	-2.22	118.00	123.59
33	C	521	LMG	O1-C1-C2	2.22	111.76	108.30
23	C	507	CLA	C4C-C3C-C2C	-2.22	103.67	106.90
25	D	407	BCR	C15-C16-C17	-2.21	118.94	123.47
23	D	405	CLA	CMA-C3A-C4A	-2.21	105.82	111.77

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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
23	C	513	CLA	CBA-CAA-C2A	-2.21	107.33	113.86
23	A	408	CLA	CMB-C2B-C1B	2.21	128.74	125.37
26	f	102	SQD	O7-S-C6	2.21	109.57	106.94
23	b	611	CLA	CAC-C3C-C4C	2.21	127.68	124.81
23	C	503	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
23	b	608	CLA	C11-C12-C13	-2.21	108.77	115.92
35	h	102	DGD	C3B-C2B-C1B	-2.21	105.58	113.62
23	b	615	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
23	A	408	CLA	CMA-C3A-C4A	-2.21	105.83	111.77
26	b	620	SQD	C44-O6-C1	-2.21	109.42	113.74
23	b	606	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
23	C	513	CLA	CHB-C1B-C2B	-2.21	121.00	127.24
23	C	513	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
23	B	605	CLA	CED-O2D-CGD	2.21	120.93	115.94
33	m	101	LMG	O8-C28-O10	-2.21	118.02	123.59
23	B	601	CLA	C1-C2-C3	-2.21	122.22	126.04
37	E	101	LHG	O7-C7-O9	-2.21	118.37	123.70
25	t	103	BCR	C11-C10-C9	-2.20	124.17	127.31
23	a	409	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
23	b	612	CLA	C11-C12-C13	-2.20	108.80	115.92
35	C	517	DGD	O3G-C3G-C2G	-2.20	105.59	110.90
23	C	512	CLA	CHB-C1B-NB	-2.20	121.93	124.26
26	a	411	SQD	O9-S-O7	-2.20	106.34	113.95
25	A	409	BCR	C40-C30-C25	-2.20	106.73	110.30
23	A	408	CLA	CHB-C4A-NA	2.20	127.55	124.51
23	C	513	CLA	CAC-C3C-C4C	2.20	127.66	124.81
25	B	619	BCR	C21-C20-C19	-2.20	116.36	123.22
33	d	412	LMG	O8-C28-O10	-2.20	118.05	123.59
25	Y	101	BCR	C34-C9-C8	2.20	121.54	118.08
23	B	608	CLA	CMA-C3A-C2A	-2.20	104.97	113.83
27	O	601	GOL	C3-C2-C1	-2.20	103.17	111.70
23	B	607	CLA	C1-O2A-CGA	2.19	122.20	116.44
35	c	518	DGD	O1G-C1A-O1A	-2.19	118.06	123.59
23	C	514	CLA	C4-C3-C5	2.19	118.96	115.27
23	C	511	CLA	C4-C3-C2	-2.19	118.05	123.68
25	b	618	BCR	C8-C7-C6	-2.19	121.05	127.20
23	c	512	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
27	B	624	GOL	C3-C2-C1	-2.19	103.19	111.70
23	C	506	CLA	CHB-C1B-NB	-2.19	121.94	124.26
35	c	519	DGD	O3G-C3G-C2G	-2.19	105.62	110.90
33	z	101	LMG	C8-O7-C10	-2.19	112.40	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
24	a	353	PHO	C4-C3-C2	-2.19	118.07	123.68
23	b	602	CLA	CHB-C4A-NA	2.19	127.54	124.51
23	c	510	CLA	C4-C3-C2	-2.19	118.07	123.68
26	F	101	SQD	O5-C1-O6	2.18	115.15	109.97
38	e	87	HEM	CMD-C2D-C1D	2.18	128.37	125.04
23	C	511	CLA	CAC-C3C-C4C	2.18	127.64	124.81
25	a	410	BCR	C7-C8-C9	-2.18	122.94	126.23
25	T	101	BCR	C35-C13-C12	2.18	121.52	118.08
25	c	516	BCR	C15-C14-C13	-2.18	124.20	127.31
23	b	615	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
25	t	103	BCR	C19-C18-C17	-2.18	115.60	118.94
32	b	621	LMT	C2'-C3'-C4'	2.18	114.65	109.68
23	b	602	CLA	O2A-CGA-CBA	2.18	118.73	111.91
26	F	101	SQD	O7-S-C6	2.17	109.52	106.94
23	C	509	CLA	O2A-CGA-CBA	2.17	118.73	111.91
23	a	407	CLA	C4-C3-C5	2.17	118.92	115.27
25	T	101	BCR	C7-C6-C5	-2.17	116.20	121.46
25	k	101	BCR	C3-C4-C5	-2.17	110.20	114.08
23	B	601	CLA	C2A-C1A-CHA	-2.17	120.06	123.86
37	D	409	LHG	O4-P-O5	2.17	122.96	112.24
23	b	606	CLA	CHB-C1B-C2B	-2.17	121.12	127.24
38	e	87	HEM	C4A-NA-C1A	2.17	107.47	105.35
25	B	617	BCR	C29-C30-C25	2.17	113.81	110.48
29	a	416	PL9	C45-C44-C46	2.16	118.91	115.27
23	B	607	CLA	CAC-C3C-C4C	2.16	127.62	124.81
23	c	507	CLA	C4-C3-C5	2.16	118.91	115.27
23	B	615	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
23	b	607	CLA	CHD-C4C-NC	2.16	127.61	124.20
23	B	612	CLA	C4A-NA-C1A	-2.16	105.73	106.71
23	b	613	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
23	A	405	CLA	O2A-CGA-CBA	2.16	118.68	111.91
38	e	87	HEM	CHA-C1A-NA	2.16	127.82	123.85
24	a	408	PHO	O2D-CGD-O1D	-2.16	119.62	123.84
25	A	409	BCR	C37-C22-C21	-2.16	119.90	122.92
23	b	613	CLA	C16-C15-C13	-2.16	108.95	115.92
25	D	407	BCR	C30-C25-C24	2.16	121.88	115.78
23	A	408	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
23	C	508	CLA	C6-C7-C8	-2.15	108.96	115.92
23	B	602	CLA	CMA-C3A-C2A	-2.15	105.14	113.83
33	a	419	LMG	O6-C5-C4	2.15	113.60	109.69
25	Y	101	BCR	C11-C10-C9	-2.15	124.24	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
23	c	507	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
29	D	408	PL9	C12-C13-C14	-2.15	122.48	127.66
37	d	711	LHG	O7-C7-O9	-2.15	118.51	123.70
25	a	410	BCR	C11-C10-C9	-2.15	124.24	127.31
23	b	611	CLA	C7-C6-C5	-2.15	107.53	113.36
23	b	608	CLA	C4-C3-C5	2.15	118.88	115.27
23	C	507	CLA	CGD-CBD-CAD	-2.14	103.79	110.73
25	k	101	BCR	C36-C18-C19	2.14	121.46	118.08
23	B	608	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
38	E	103	HEM	CHA-C1A-NA	2.14	127.79	123.85
25	h	101	BCR	C10-C11-C12	-2.14	116.53	123.22
29	d	405	PL9	C45-C44-C46	2.14	118.87	115.27
23	D	405	CLA	OBD-CAD-C3D	-2.14	123.37	128.52
23	C	508	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
23	b	609	CLA	CMA-C3A-C4A	-2.14	106.03	111.77
26	a	413	SQD	O48-C23-O10	-2.14	118.20	123.59
25	b	618	BCR	C37-C22-C23	2.14	121.44	118.08
23	B	606	CLA	CAA-C2A-C3A	-2.13	106.93	112.78
25	h	101	BCR	C24-C23-C22	-2.13	123.01	126.23
23	c	506	CLA	CHD-C4C-NC	2.13	127.57	124.20
23	B	609	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
34	c	522	HTG	O5-C1-C2	2.13	113.00	110.31
40	V	202	HEC	CAA-CBA-CGA	-2.13	109.02	113.60
23	b	604	CLA	C4-C3-C2	-2.13	118.21	123.68
35	c	517	DGD	O6D-C1D-O3G	-2.13	104.93	109.97
23	A	406	CLA	CHB-C4A-NA	2.13	127.46	124.51
33	C	501	LMG	O7-C10-O9	-2.13	118.56	123.70
35	C	517	DGD	O5D-C6D-C5D	-2.13	105.11	109.05
23	c	511	CLA	C4-C3-C2	-2.13	118.22	123.68
37	d	407	LHG	O8-C23-C24	2.13	118.59	111.91
40	v	202	HEC	CMC-C2C-C1C	-2.13	122.13	125.37
33	C	501	LMG	O8-C28-C29	2.13	118.58	111.91
25	D	407	BCR	C38-C26-C27	2.13	117.70	113.62
25	B	617	BCR	C37-C22-C23	2.13	121.43	118.08
23	b	602	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
40	V	202	HEC	C3D-C4D-ND	-2.13	108.30	110.36
23	a	407	CLA	CBC-CAC-C3C	-2.12	106.57	112.43
25	B	618	BCR	C15-C16-C17	-2.12	119.12	123.47
23	C	513	CLA	CMA-C3A-C4A	-2.12	106.06	111.77
23	d	402	CLA	CHD-C4C-NC	2.12	127.55	124.20
23	B	611	CLA	C4D-CHA-C1A	-2.12	118.67	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	CHA-C1A-NA	-2.12	121.54	126.40
23	c	512	CLA	C11-C10-C8	-2.12	109.06	115.92
23	A	405	CLA	CHB-C4A-NA	2.12	127.44	124.51
27	A	701	GOL	C3-C2-C1	-2.12	103.46	111.70
23	b	609	CLA	CHA-C1A-NA	-2.12	121.54	126.40
23	B	615	CLA	O2A-CGA-CBA	2.12	118.56	111.91
25	H	101	BCR	C33-C5-C6	-2.12	122.15	124.53
25	a	410	BCR	C37-C22-C21	-2.12	119.95	122.92
25	k	101	BCR	C38-C26-C25	-2.12	122.15	124.53
25	Y	101	BCR	C36-C18-C19	2.12	121.41	118.08
23	B	602	CLA	C4-C3-C5	2.12	118.83	115.27
23	c	514	CLA	C1-O2A-CGA	2.11	121.99	116.44
35	c	517	DGD	O1G-C1A-O1A	-2.11	118.26	123.59
23	a	406	CLA	CHB-C4A-NA	2.11	127.43	124.51
23	d	403	CLA	C1-O2A-CGA	2.11	121.99	116.44
23	d	402	CLA	CMA-C3A-C2A	-2.11	105.31	113.83
23	c	511	CLA	C11-C10-C8	-2.11	109.10	115.92
23	B	606	CLA	CHB-C1B-C2B	-2.11	121.28	127.24
35	C	518	DGD	O1G-C1A-C2A	2.11	118.53	111.91
33	a	419	LMG	O7-C10-O9	-2.11	118.61	123.70
23	b	603	CLA	C5-C3-C2	-2.11	116.85	121.12
35	c	519	DGD	O3G-C1D-C2D	-2.11	105.01	108.30
26	a	411	SQD	C3-C4-C5	2.11	114.00	110.24
23	C	507	CLA	CHB-C1B-NB	-2.11	122.03	124.26
23	b	606	CLA	CAC-C3C-C4C	2.11	127.54	124.81
23	C	505	CLA	O2A-CGA-CBA	2.11	118.52	111.91
29	d	405	PL9	C31-C32-C33	-2.10	104.97	111.88
23	a	406	CLA	CAC-C3C-C2C	2.10	131.13	127.53
25	B	619	BCR	C29-C30-C25	2.10	113.72	110.48
23	B	616	CLA	C2A-C1A-CHA	-2.10	120.18	123.86
23	b	601	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
29	a	416	PL9	C51-C49-C50	2.10	119.25	114.60
25	K	102	BCR	C11-C10-C9	-2.10	124.31	127.31
23	A	404	CLA	C7-C6-C5	-2.10	107.65	113.36
25	A	409	BCR	C28-C27-C26	-2.10	110.33	114.08
23	B	601	CLA	C4-C3-C5	2.10	118.80	115.27
23	C	506	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
23	c	514	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
33	c	520	LMG	O8-C28-O10	-2.10	118.30	123.59
25	K	102	BCR	C28-C27-C26	-2.10	110.34	114.08
23	B	609	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
23	c	506	CLA	O2A-CGA-O1A	-2.09	118.31	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	h	101	BCR	C34-C9-C8	2.09	121.37	118.08
29	A	414	PL9	C51-C49-C50	2.09	119.22	114.60
23	B	614	CLA	CMA-C3A-C2A	-2.09	105.39	113.83
25	B	618	BCR	C40-C30-C25	-2.09	106.91	110.30
25	B	619	BCR	C10-C11-C12	-2.09	116.69	123.22
33	C	501	LMG	O6-C1-O1	-2.09	105.02	109.97
23	b	610	CLA	CHB-C4A-NA	2.09	127.40	124.51
33	a	419	LMG	O8-C28-C29	2.09	118.47	111.91
23	B	615	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
23	B	610	CLA	C4-C3-C5	2.09	118.78	115.27
40	v	202	HEC	CAD-CBD-CGD	-2.09	109.11	113.60
23	B	612	CLA	CMA-C3A-C2A	-2.09	105.41	113.83
24	A	353	PHO	OBD-CAD-C3D	-2.09	124.52	127.98
23	b	616	CLA	C1-C2-C3	-2.08	122.44	126.04
23	a	407	CLA	CAC-C3C-C4C	2.08	127.52	124.81
23	a	406	CLA	CHB-C1B-NB	-2.08	122.05	124.26
25	H	101	BCR	C29-C30-C25	2.08	113.69	110.48
25	D	407	BCR	C21-C20-C19	-2.08	116.72	123.22
25	A	409	BCR	C8-C7-C6	-2.08	121.36	127.20
29	A	414	PL9	C10-C9-C11	2.08	118.77	115.27
23	B	615	CLA	CHB-C1B-NB	-2.08	122.06	124.26
23	B	616	CLA	C1-O2A-CGA	2.08	121.90	116.44
23	C	509	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
25	c	516	BCR	C29-C30-C25	2.08	113.68	110.48
23	c	511	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
23	D	405	CLA	CBC-CAC-C3C	-2.07	106.71	112.43
23	b	605	CLA	C1-O2A-CGA	2.07	121.89	116.44
25	Y	101	BCR	C1-C6-C7	2.07	121.64	115.78
23	c	512	CLA	CMA-C3A-C4A	2.07	117.34	111.77
29	d	405	PL9	C40-C39-C38	-2.07	118.37	123.68
23	c	513	CLA	CMA-C3A-C4A	-2.07	106.21	111.77
23	d	402	CLA	CBB-CAB-C3B	-2.07	117.32	127.62
25	d	404	BCR	C38-C26-C27	2.07	117.59	113.62
23	b	611	CLA	OBD-CAD-C3D	-2.07	123.54	128.52
25	d	404	BCR	C40-C30-C39	2.07	114.88	108.53
23	b	601	CLA	CAC-C3C-C4C	2.07	127.49	124.81
25	h	101	BCR	C16-C15-C14	-2.07	119.24	123.47
25	K	102	BCR	C3-C4-C5	-2.06	110.39	114.08
23	b	610	CLA	CMA-C3A-C4A	-2.06	106.22	111.77
23	B	609	CLA	CHA-C1A-NA	-2.06	121.67	126.40
23	b	608	CLA	C11-C10-C8	-2.06	109.25	115.92
23	c	509	CLA	CMC-C2C-C1C	2.06	128.18	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	515	BCR	C35-C13-C14	-2.06	120.04	122.92
23	B	602	CLA	OBD-CAD-C3D	-2.06	123.56	128.52
23	d	402	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
33	c	521	LMG	C1-C2-C3	-2.06	105.71	110.00
23	c	513	CLA	CBC-CAC-C3C	-2.06	106.76	112.43
23	B	603	CLA	CHB-C1B-C2B	-2.06	121.43	127.24
29	D	408	PL9	C27-C28-C29	-2.06	122.71	127.66
23	c	513	CLA	CHA-C1A-NA	-2.06	121.69	126.40
32	b	627	LMT	O1'-C1'-C2'	2.06	111.51	108.30
26	b	620	SQD	C1-C2-C3	-2.05	105.72	110.00
23	b	605	CLA	O2A-CGA-CBA	2.05	118.35	111.91
25	a	410	BCR	C8-C7-C6	-2.05	121.44	127.20
29	d	405	PL9	O2-C1-C6	-2.05	117.04	120.59
23	b	607	CLA	CAA-CBA-CGA	2.05	119.25	113.25
23	B	607	CLA	CMA-C3A-C2A	-2.05	105.56	113.83
24	A	353	PHO	O1D-CGD-CBD	-2.05	121.33	124.74
34	B	622	HTG	C2'-C1'-S1	-2.05	105.78	112.40
25	t	103	BCR	C35-C13-C12	2.05	121.31	118.08
29	D	408	PL9	C45-C44-C46	2.05	118.72	115.27
25	y	101	BCR	C35-C13-C14	-2.05	120.05	122.92
23	a	409	CLA	C1-O2A-CGA	2.05	121.82	116.44
25	C	516	BCR	C21-C20-C19	-2.05	116.83	123.22
23	c	503	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
37	L	101	LHG	O4-P-O5	2.05	122.36	112.24
23	C	508	CLA	CHA-C1A-NA	-2.05	121.71	126.40
32	M	101	LMT	O5B-C5B-C6B	2.05	111.52	106.44
23	a	405	CLA	CMB-C2B-C3B	2.05	131.54	126.59
23	A	406	CLA	CBC-CAC-C3C	-2.04	106.79	112.43
32	D	404	LMT	C1B-C2B-C3B	2.04	114.25	110.00
23	B	608	CLA	CMB-C2B-C1B	2.04	128.48	125.37
40	v	202	HEC	CBD-CAD-C3D	-2.04	106.95	112.63
24	a	353	PHO	O2A-CGA-O1A	-2.04	118.44	123.59
32	b	627	LMT	C1'-O5'-C5'	-2.04	109.68	113.69
24	a	408	PHO	C1-C2-C3	-2.04	122.51	126.04
23	D	406	CLA	CHB-C1B-NB	-2.04	122.10	124.26
23	C	505	CLA	OBD-CAD-C3D	-2.04	123.61	128.52
37	l	101	LHG	O7-C7-O9	-2.04	118.77	123.70
23	B	616	CLA	CHB-C1B-NB	-2.04	122.10	124.26
23	b	603	CLA	C7-C6-C5	-2.04	107.82	113.36
23	B	608	CLA	C4-C3-C5	2.04	118.70	115.27
23	b	608	CLA	C2A-C1A-CHA	-2.04	120.30	123.86
25	B	617	BCR	C3-C4-C5	-2.03	110.45	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	C11-C10-C8	-2.03	109.35	115.92
23	B	610	CLA	CMA-C3A-C2A	-2.03	105.63	113.83
29	D	408	PL9	C47-C48-C49	-2.03	120.81	127.75
25	H	101	BCR	C16-C15-C14	-2.03	119.31	123.47
29	D	408	PL9	C21-C22-C23	-2.03	105.21	111.88
33	z	101	LMG	O8-C28-O10	-2.03	118.47	123.59
25	t	103	BCR	C2-C1-C6	2.03	113.61	110.48
26	A	412	SQD	O6-C44-C45	-2.03	106.01	110.90
23	A	408	CLA	C11-C12-C13	-2.03	109.37	115.92
25	T	101	BCR	C7-C8-C9	-2.03	123.17	126.23
23	b	610	CLA	C4-C3-C2	-2.02	118.48	123.68
25	A	409	BCR	C31-C1-C6	-2.02	107.02	110.30
23	C	508	CLA	CAC-C3C-C4C	2.02	127.44	124.81
25	A	409	BCR	C2-C1-C6	2.02	113.59	110.48
23	B	606	CLA	CAC-C3C-C4C	2.02	127.43	124.81
23	a	407	CLA	CHA-C1A-NA	-2.02	121.77	126.40
23	B	604	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
23	B	607	CLA	C1-C2-C3	-2.02	122.55	126.04
23	C	514	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	C	513	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
23	c	512	CLA	CHB-C1B-NB	-2.02	122.12	124.26
23	b	616	CLA	CHB-C1B-C2B	-2.02	121.54	127.24
26	a	411	SQD	O4-C4-C3	-2.02	105.68	110.35
23	B	604	CLA	CHA-C1A-NA	-2.02	121.78	126.40
23	b	611	CLA	O2A-CGA-CBA	2.02	118.24	111.91
23	b	602	CLA	CED-O2D-CGD	2.02	120.50	115.94
23	b	614	CLA	C11-C10-C8	-2.02	109.40	115.92
23	C	511	CLA	CHB-C4A-NA	2.02	127.30	124.51
35	c	517	DGD	O1G-C1A-C2A	2.01	118.23	111.91
23	C	511	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
23	b	613	CLA	CHA-C1A-NA	-2.01	121.79	126.40
32	E	102	LMT	C2'-C3'-C4'	2.01	114.28	109.68
23	c	513	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
38	e	87	HEM	CHA-C4D-C3D	-2.01	121.56	125.33
23	B	608	CLA	C11-C10-C8	-2.01	109.43	115.92
23	C	508	CLA	C3B-C4B-NB	2.00	112.38	110.52
25	h	101	BCR	C20-C21-C22	-2.00	124.45	127.31
24	A	353	PHO	CMB-C2B-C3B	2.00	128.43	124.68
32	t	102	LMT	O5'-C1'-O1'	-2.00	105.23	109.97
35	C	517	DGD	C4E-C3E-C2E	-2.00	107.33	110.82
23	c	505	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
23	C	513	CLA	C4-C3-C2	-2.00	118.54	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	626	HTG	C1-O5-C5	2.00	116.27	112.58

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	202	HEC	NA
40	v	202	HEC	NA

All (1339) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C2-C3-C5-C6
23	A	408	CLA	C4-C3-C5-C6
23	B	603	CLA	C2-C3-C5-C6
23	B	603	CLA	C4-C3-C5-C6
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	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	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	b	603	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	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	C4-C3-C5-C6
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C2-C1-O2A-CGA
23	c	510	CLA	C11-C10-C8-C9
23	c	514	CLA	C2B-C3B-CAB-CBB
23	c	514	CLA	C4B-C3B-CAB-CBB
23	d	403	CLA	C2-C3-C5-C6
23	d	403	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	D	407	BCR	C21-C22-C23-C24
25	D	407	BCR	C37-C22-C23-C24
25	D	407	BCR	C23-C24-C25-C30
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	b	617	BCR	C1-C6-C7-C8
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
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	414	PL9	C15-C14-C16-C17
29	A	414	PL9	C14-C16-C17-C18
29	a	416	PL9	C9-C11-C12-C13
29	a	416	PL9	C14-C16-C17-C18
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

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Mol	Chain	Res	Type	Atoms
32	I	101	LMT	C2-C1-O1'-C1'
32	M	103	LMT	C2-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
32	t	102	LMT	C2-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
34	B	622	HTG	C2'-C1'-S1-C1
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	O10-C23-O8-C6
37	E	101	LHG	C24-C23-O8-C6
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	C4-O6-P-O4
37	d	711	LHG	C3-O3-P-O5
37	e	101	LHG	C3-O3-P-O4
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-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
32	I	101	LMT	O5B-C1B-O1B-C4'
32	a	414	LMT	C4'-C5'-C6'-O6'
26	A	410	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
26	b	620	SQD	O49-C7-O47-C45
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
32	M	103	LMT	O5'-C5'-C6'-O6'
32	a	420	LMT	O5B-C5B-C6B-O6B
32	E	102	LMT	O5'-C5'-C6'-O6'
23	C	505	CLA	C4-C3-C5-C6
23	a	409	CLA	C4-C3-C5-C6
29	A	414	PL9	C20-C19-C21-C22
23	c	508	CLA	C2-C3-C5-C6
29	A	414	PL9	C18-C19-C21-C22
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
23	b	616	CLA	C3-C5-C6-C7
32	m	103	LMT	O5B-C5B-C6B-O6B
32	m	103	LMT	C4B-C5B-C6B-O6B
32	D	404	LMT	C6-C7-C8-C9
34	b	625	HTG	S1-C1'-C2'-C3'
34	D	414	HTG	O5-C5-C6-O6
33	C	521	LMG	O9-C10-O7-C8
32	D	404	LMT	C4'-C5'-C6'-O6'
25	T	101	BCR	C13-C14-C15-C16
32	a	414	LMT	O5B-C5B-C6B-O6B
32	b	621	LMT	O5'-C5'-C6'-O6'
23	D	406	CLA	CBD-CGD-O2D-CED
23	c	514	CLA	CBD-CGD-O2D-CED
37	d	407	LHG	O2-C2-C3-O3
23	A	408	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
26	A	410	SQD	C8-C7-O47-C45
33	z	101	LMG	C11-C10-O7-C8
23	c	511	CLA	CBD-CGD-O2D-CED
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	I	101	LMT	O5B-C5B-C6B-O6B
32	M	103	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
32	I	101	LMT	O5'-C5'-C6'-O6'
32	M	103	LMT	O5B-C5B-C6B-O6B
32	t	101	LMT	O5'-C5'-C6'-O6'
33	z	101	LMG	O9-C10-O7-C8
34	D	414	HTG	C4-C5-C6-O6
32	D	404	LMT	O5'-C5'-C6'-O6'
32	a	414	LMT	O5'-C5'-C6'-O6'
23	B	605	CLA	C4-C3-C5-C6
23	C	508	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
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	603	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
29	A	414	PL9	C13-C14-C16-C17
29	a	416	PL9	C13-C14-C16-C17
29	a	416	PL9	C28-C29-C31-C32
32	D	404	LMT	O5B-C5B-C6B-O6B
33	c	521	LMG	O6-C5-C6-O5
32	a	414	LMT	C4B-C5B-C6B-O6B
32	a	420	LMT	C4B-C5B-C6B-O6B
32	e	102	LMT	C4'-C5'-C6'-O6'
26	B	620	SQD	O5-C1-O6-C44
32	e	102	LMT	O5'-C1'-O1'-C1
29	A	414	PL9	C44-C46-C47-C48
29	D	408	PL9	C39-C41-C42-C43
40	V	202	HEC	C2C-C3C-CAC-CBC
34	B	626	HTG	O5-C5-C6-O6
37	d	407	LHG	C1-C2-C3-O3
32	E	102	LMT	C4'-C5'-C6'-O6'
23	a	409	CLA	CBA-CGA-O2A-C1
26	F	101	SQD	C23-C24-C25-C26
32	I	101	LMT	C2'-C1'-O1'-C1
32	t	101	LMT	C2'-C1'-O1'-C1
32	t	102	LMT	C2'-C1'-O1'-C1
32	I	101	LMT	C5'-C4'-O1B-C1B
33	B	621	LMG	C39-C40-C41-C42
32	e	102	LMT	O5B-C5B-C6B-O6B
23	D	406	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	A	414	PL9	C30-C29-C31-C32
23	C	505	CLA	C2-C3-C5-C6
23	a	409	CLA	C2-C3-C5-C6
23	B	602	CLA	C6-C7-C8-C9
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
23	C	514	CLA	CBD-CGD-O2D-CED
23	c	513	CLA	CBD-CGD-O2D-CED
23	B	601	CLA	C5-C6-C7-C8
25	d	404	BCR	C37-C22-C23-C24
32	b	621	LMT	C4'-C5'-C6'-O6'
32	b	627	LMT	C4'-C5'-C6'-O6'
37	E	101	LHG	C23-C24-C25-C26
23	A	408	CLA	C5-C6-C7-C8
32	t	102	LMT	O5'-C5'-C6'-O6'
34	b	622	HTG	O5-C5-C6-O6
32	I	101	LMT	C4B-C5B-C6B-O6B
23	c	510	CLA	CBA-CGA-O2A-C1
23	b	601	CLA	C10-C11-C12-C13
32	D	404	LMT	C4B-C5B-C6B-O6B
32	t	101	LMT	C4'-C5'-C6'-O6'
23	a	409	CLA	O1A-CGA-O2A-C1
34	b	623	HTG	C1'-C2'-C3'-C4'
32	m	103	LMT	O5'-C5'-C6'-O6'
23	B	601	CLA	C10-C11-C12-C13
23	B	602	CLA	C13-C15-C16-C17
23	b	606	CLA	C10-C11-C12-C13
23	b	606	CLA	C13-C15-C16-C17
23	b	614	CLA	C8-C10-C11-C12
27	a	412	GOL	O1-C1-C2-O2
26	B	620	SQD	C7-C8-C9-C10
33	Z	101	LMG	C10-C11-C12-C13
35	c	518	DGD	C1B-C2B-C3B-C4B
23	C	508	CLA	C5-C6-C7-C8
23	b	604	CLA	C8-C10-C11-C12
23	c	510	CLA	C3-C5-C6-C7
35	h	102	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
34	D	414	HTG	S1-C1'-C2'-C3'
34	b	622	HTG	S1-C1'-C2'-C3'
32	I	101	LMT	O1'-C1-C2-C3
37	D	411	LHG	C33-C34-C35-C36
40	V	202	HEC	C4C-C3C-CAC-CBC
32	I	101	LMT	C4'-C5'-C6'-O6'
26	b	620	SQD	C31-C32-C33-C34
23	c	513	CLA	C15-C16-C17-C18
23	B	613	CLA	C11-C12-C13-C15
23	C	511	CLA	C11-C12-C13-C15
23	b	606	CLA	C12-C13-C15-C16
23	B	610	CLA	C2A-CAA-CBA-CGA
23	B	606	CLA	C10-C11-C12-C13
23	c	514	CLA	C10-C11-C12-C13
35	C	519	DGD	C6B-C7B-C8B-C9B
23	c	510	CLA	O1A-CGA-O2A-C1
32	a	414	LMT	O5'-C1'-O1'-C1
32	b	621	LMT	O5'-C1'-O1'-C1
23	a	405	CLA	C15-C16-C17-C18
23	b	605	CLA	C8-C10-C11-C12
23	b	611	CLA	C15-C16-C17-C18
29	d	405	PL9	C39-C41-C42-C43
32	D	404	LMT	C5'-C4'-O1B-C1B
32	a	420	LMT	O1'-C1-C2-C3
32	e	102	LMT	O5'-C5'-C6'-O6'
23	B	608	CLA	C13-C15-C16-C17
23	b	604	CLA	C5-C6-C7-C8
23	B	614	CLA	C5-C6-C7-C8
23	B	614	CLA	C10-C11-C12-C13
23	D	406	CLA	C10-C11-C12-C13
23	b	611	CLA	C8-C10-C11-C12
23	B	614	CLA	C8-C10-C11-C12
23	B	615	CLA	C10-C11-C12-C13
23	C	509	CLA	C10-C11-C12-C13
37	E	101	LHG	C3-O3-P-O6
37	E	101	LHG	C4-O6-P-O3
37	L	101	LHG	C4-O6-P-O3
37	d	407	LHG	C3-O3-P-O6
37	e	101	LHG	C3-O3-P-O6
37	e	101	LHG	C4-O6-P-O3
37	l	101	LHG	C4-O6-P-O3
26	A	410	SQD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
34	B	622	HTG	C1'-C2'-C3'-C4'
34	d	411	HTG	S1-C1'-C2'-C3'
37	D	410	LHG	C1-C2-C3-O3
23	C	511	CLA	C4-C3-C5-C6
26	A	410	SQD	C12-C13-C14-C15
23	b	610	CLA	C2A-CAA-CBA-CGA
32	t	101	LMT	C3-C4-C5-C6
33	B	621	LMG	C11-C10-O7-C8
23	b	614	CLA	C10-C11-C12-C13
26	F	101	SQD	C30-C31-C32-C33
33	m	101	LMG	C35-C36-C37-C38
34	B	623	HTG	C3'-C4'-C5'-C6'
35	c	517	DGD	C9A-CAA-CBA-CCA
35	c	518	DGD	C9A-CAA-CBA-CCA
37	L	101	LHG	C15-C16-C17-C18
37	L	101	LHG	C17-C18-C19-C20
23	b	602	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C20
33	C	501	LMG	C17-C18-C19-C20
33	D	415	LMG	C35-C36-C37-C38
37	d	711	LHG	C16-C17-C18-C19
33	B	621	LMG	O9-C10-O7-C8
26	A	412	SQD	C17-C18-C19-C20
32	t	102	LMT	C4-C5-C6-C7
35	h	102	DGD	C9A-CAA-CBA-CCA
32	I	101	LMT	C3-C4-C5-C6
33	D	415	LMG	C19-C20-C21-C22
35	C	517	DGD	C5B-C6B-C7B-C8B
37	D	410	LHG	C16-C17-C18-C19
37	d	711	LHG	C32-C33-C34-C35
32	b	627	LMT	C7-C8-C9-C10
32	e	102	LMT	C4-C5-C6-C7
34	b	622	HTG	C2'-C3'-C4'-C5'
35	c	517	DGD	C5A-C6A-C7A-C8A
35	c	518	DGD	CBA-CCA-CDA-CEA
37	e	101	LHG	C26-C27-C28-C29
32	b	621	LMT	C2'-C1'-O1'-C1
32	e	102	LMT	C2'-C1'-O1'-C1
35	C	518	DGD	C2E-C1E-O5D-C6D
26	f	102	SQD	C32-C33-C34-C35
33	B	621	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
33	C	501	LMG	C36-C37-C38-C39
33	a	419	LMG	C30-C31-C32-C33
35	C	517	DGD	C4B-C5B-C6B-C7B
35	c	517	DGD	C2B-C3B-C4B-C5B
35	c	518	DGD	CAA-CBA-CCA-CDA
23	c	507	CLA	C15-C16-C17-C18
23	a	409	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C20
33	C	501	LMG	C12-C13-C14-C15
37	L	101	LHG	C13-C14-C15-C16
23	a	407	CLA	C11-C12-C13-C14
23	b	610	CLA	C11-C12-C13-C14
23	c	505	CLA	C14-C13-C15-C16
26	A	410	SQD	C15-C16-C17-C18
33	C	521	LMG	C17-C18-C19-C20
33	C	521	LMG	C18-C19-C20-C21
35	C	518	DGD	CCB-CDB-CEB-CFB
35	H	102	DGD	C5B-C6B-C7B-C8B
35	c	519	DGD	CBB-CCB-CDB-CEB
33	Z	101	LMG	O6-C5-C6-O5
25	b	619	BCR	C7-C8-C9-C34
32	a	414	LMT	C2-C3-C4-C5
32	e	102	LMT	C5-C6-C7-C8
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	o	501	GOL	C1-C2-C3-O3
27	v	401	GOL	O1-C1-C2-C3
25	b	619	BCR	C7-C8-C9-C10
23	C	511	CLA	C10-C11-C12-C13
37	D	411	LHG	C32-C33-C34-C35
37	l	101	LHG	C14-C15-C16-C17
33	a	419	LMG	C10-C11-C12-C13
33	c	520	LMG	C10-C11-C12-C13
32	D	404	LMT	C5-C6-C7-C8
33	C	501	LMG	C19-C20-C21-C22
33	C	521	LMG	C13-C14-C15-C16
33	m	101	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
37	L	101	LHG	C12-C13-C14-C15
37	d	711	LHG	C29-C30-C31-C32
32	b	621	LMT	C3'-C4'-O1B-C1B
32	A	359	LMT	O5B-C5B-C6B-O6B
23	C	505	CLA	C4B-C3B-CAB-CBB
23	b	602	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C19
23	d	402	CLA	C16-C17-C18-C20
26	F	101	SQD	O5-C1-O6-C44
23	A	405	CLA	C15-C16-C17-C18
26	B	620	SQD	C11-C10-C9-C8
32	M	103	LMT	C7-C8-C9-C10
33	B	621	LMG	C34-C35-C36-C37
34	b	622	HTG	C3'-C4'-C5'-C6'
37	l	101	LHG	C16-C17-C18-C19
23	c	514	CLA	O1D-CGD-O2D-CED
26	F	101	SQD	C24-C25-C26-C27
33	D	415	LMG	C12-C13-C14-C15
33	d	412	LMG	C29-C30-C31-C32
23	b	606	CLA	C15-C16-C17-C18
26	F	101	SQD	C29-C30-C31-C32
33	a	419	LMG	C34-C35-C36-C37
35	C	517	DGD	C9A-CAA-CBA-CCA
37	d	408	LHG	C27-C28-C29-C30
23	c	507	CLA	C3A-C2A-CAA-CBA
23	C	503	CLA	C13-C15-C16-C17
23	C	513	CLA	C10-C11-C12-C13
32	I	101	LMT	C1-C2-C3-C4
32	D	404	LMT	C2-C1-O1'-C1'
32	E	102	LMT	C2-C1-O1'-C1'
32	e	102	LMT	C2-C1-O1'-C1'
32	m	103	LMT	C2-C1-O1'-C1'
37	E	101	LHG	C24-C25-C26-C27
23	B	603	CLA	C16-C17-C18-C19
23	B	603	CLA	C16-C17-C18-C20
23	B	615	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C19
32	b	627	LMT	C3-C4-C5-C6
33	C	520	LMG	C16-C17-C18-C19
35	H	102	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
37	L	101	LHG	C25-C26-C27-C28
40	v	202	HEC	C2C-C3C-CAC-CBC
23	C	504	CLA	CBD-CGD-O2D-CED
35	h	102	DGD	CAA-CBA-CCA-CDA
35	h	102	DGD	C7B-C8B-C9B-CAB
37	l	101	LHG	C27-C28-C29-C30
35	c	517	DGD	O6D-C5D-C6D-O5D
32	a	420	LMT	C1-C2-C3-C4
32	A	359	LMT	O1'-C1-C2-C3
23	c	506	CLA	C4-C3-C5-C6
23	D	406	CLA	C2-C3-C5-C6
23	c	506	CLA	C2-C3-C5-C6
29	A	414	PL9	C12-C11-C9-C8
29	D	408	PL9	C13-C14-C16-C17
33	m	101	LMG	C11-C10-O7-C8
26	a	413	SQD	C25-C26-C27-C28
32	t	101	LMT	C4-C5-C6-C7
33	c	520	LMG	C31-C32-C33-C34
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
26	f	102	SQD	C25-C26-C27-C28
32	t	101	LMT	C11-C10-C9-C8
32	t	102	LMT	O1'-C1-C2-C3
33	C	520	LMG	C17-C18-C19-C20
37	d	711	LHG	C24-C25-C26-C27
23	B	610	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C19
23	C	505	CLA	C2B-C3B-CAB-CBB
37	E	101	LHG	O2-C2-C3-O3
37	D	410	LHG	C12-C13-C14-C15
35	c	519	DGD	CBA-CCA-CDA-CEA
23	B	615	CLA	C5-C6-C7-C8
26	b	620	SQD	C13-C14-C15-C16
32	b	621	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
33	m	101	LMG	O9-C10-O7-C8
23	B	616	CLA	C2-C1-O2A-CGA
23	C	510	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C1-O2A-CGA
35	C	517	DGD	O6D-C5D-C6D-O5D
34	b	625	HTG	C4-C5-C6-O6
32	I	101	LMT	C3'-C4'-O1B-C1B
33	c	520	LMG	C33-C34-C35-C36
37	D	409	LHG	C34-C35-C36-C37
23	C	512	CLA	C3-C5-C6-C7
25	D	407	BCR	C23-C24-C25-C26
25	b	617	BCR	C5-C6-C7-C8
25	b	619	BCR	C5-C6-C7-C8
33	D	415	LMG	C36-C37-C38-C39
35	H	102	DGD	C7A-C8A-C9A-CAA
35	c	517	DGD	C7A-C8A-C9A-CAA
23	B	603	CLA	C13-C15-C16-C17
23	C	503	CLA	C15-C16-C17-C18
23	b	601	CLA	C8-C10-C11-C12
33	B	621	LMG	C15-C16-C17-C18
33	C	521	LMG	C19-C20-C21-C22
37	d	408	LHG	C29-C30-C31-C32
33	c	520	LMG	C34-C35-C36-C37
35	c	518	DGD	C6A-C7A-C8A-C9A
37	d	407	LHG	C34-C35-C36-C37
26	a	413	SQD	C31-C32-C33-C34
23	C	506	CLA	C4-C3-C5-C6
29	A	414	PL9	C45-C44-C46-C47
29	a	416	PL9	C12-C11-C9-C10
23	A	408	CLA	C12-C13-C15-C16
23	B	606	CLA	C11-C10-C8-C7
23	C	506	CLA	C2-C3-C5-C6
23	C	511	CLA	C2-C3-C5-C6
23	D	406	CLA	C11-C10-C8-C7
23	a	407	CLA	C11-C12-C13-C15
23	b	614	CLA	C12-C13-C15-C16
23	c	505	CLA	C12-C13-C15-C16
29	d	405	PL9	C13-C14-C16-C17
35	c	518	DGD	C4A-C5A-C6A-C7A
35	h	102	DGD	C2B-C3B-C4B-C5B
37	D	409	LHG	C12-C13-C14-C15
23	b	606	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	c	513	CLA	CBA-CGA-O2A-C1
32	e	102	LMT	C1-C2-C3-C4
33	D	415	LMG	C30-C31-C32-C33
33	C	501	LMG	C39-C40-C41-C42
37	d	408	LHG	C25-C26-C27-C28
26	b	620	SQD	C14-C15-C16-C17
26	b	620	SQD	C27-C28-C29-C30
33	C	501	LMG	C13-C14-C15-C16
35	c	517	DGD	CAA-CBA-CCA-CDA
37	D	411	LHG	C13-C14-C15-C16
33	z	101	LMG	C19-C20-C21-C22
33	D	415	LMG	O6-C5-C6-O5
35	C	518	DGD	O6E-C1E-O5D-C6D
35	h	102	DGD	CAB-CBB-CCB-CDB
37	D	411	LHG	C15-C16-C17-C18
33	C	501	LMG	C10-C11-C12-C13
26	A	410	SQD	O6-C44-C45-O47
26	b	620	SQD	C18-C19-C20-C21
37	d	408	LHG	C34-C35-C36-C37
37	d	711	LHG	C25-C26-C27-C28
23	B	615	CLA	C16-C17-C18-C20
23	a	409	CLA	C16-C17-C18-C20
32	m	103	LMT	C7-C8-C9-C10
23	B	610	CLA	C13-C15-C16-C17
32	M	101	LMT	C3-C4-C5-C6
23	B	602	CLA	C11-C12-C13-C14
23	B	606	CLA	C11-C10-C8-C9
23	D	406	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C10-C8-C9
32	D	404	LMT	C3'-C4'-O1B-C1B
35	c	518	DGD	C2B-C3B-C4B-C5B
32	D	404	LMT	C1-C2-C3-C4
34	b	623	HTG	O5-C5-C6-O6
23	A	406	CLA	C13-C15-C16-C17
25	d	404	BCR	C21-C22-C23-C24
23	C	512	CLA	C1A-C2A-CAA-CBA
23	c	507	CLA	C1A-C2A-CAA-CBA
23	B	610	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C20
26	a	411	SQD	C9-C10-C11-C12
37	D	409	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
37	D	410	LHG	C4-O6-P-O3
32	b	627	LMT	C5-C6-C7-C8
26	A	412	SQD	C26-C27-C28-C29
26	b	620	SQD	C26-C27-C28-C29
37	d	408	LHG	C28-C29-C30-C31
26	A	412	SQD	C27-C28-C29-C30
33	m	101	LMG	C37-C38-C39-C40
35	C	517	DGD	C8A-C9A-CAA-CBA
35	c	517	DGD	C4D-C5D-C6D-O5D
32	M	101	LMT	O1'-C1-C2-C3
23	c	512	CLA	C8-C10-C11-C12
35	H	102	DGD	C9B-CAB-CBB-CCB
23	c	513	CLA	O1A-CGA-O2A-C1
37	D	410	LHG	C10-C11-C12-C13
23	d	402	CLA	C16-C17-C18-C19
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
35	C	518	DGD	CDA-CEA-CFA-CGA
37	E	101	LHG	C4-C5-C6-O8
35	H	102	DGD	CAB-CBB-CCB-CDB
35	C	518	DGD	C2G-C3G-O3G-C1D
35	c	518	DGD	C2G-C3G-O3G-C1D
35	c	518	DGD	C5D-C6D-O5D-C1E
23	D	406	CLA	O1D-CGD-O2D-CED
23	c	513	CLA	O1D-CGD-O2D-CED
34	B	622	HTG	C2'-C3'-C4'-C5'
33	m	101	LMG	C38-C39-C40-C41
35	h	102	DGD	CBA-CCA-CDA-CEA
37	l	101	LHG	C9-C10-C11-C12
37	D	411	LHG	C29-C30-C31-C32
32	a	414	LMT	C5-C6-C7-C8
37	d	711	LHG	C33-C34-C35-C36
33	d	412	LMG	O6-C5-C6-O5
27	a	412	GOL	O2-C2-C3-O3
27	a	701	GOL	O1-C1-C2-O2
32	I	101	LMT	C5-C6-C7-C8
32	t	102	LMT	C7-C8-C9-C10
32	a	414	LMT	C3-C4-C5-C6
33	a	419	LMG	C29-C30-C31-C32
33	d	412	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
35	C	517	DGD	O6E-C5E-C6E-O5E
35	c	517	DGD	O6E-C5E-C6E-O5E
33	C	501	LMG	C11-C12-C13-C14
26	b	620	SQD	C24-C23-O48-C46
40	V	202	HEC	C2B-C3B-CAB-CBB
23	a	406	CLA	C2C-C3C-CAC-CBC
33	C	520	LMG	C37-C38-C39-C40
26	B	620	SQD	C46-C45-O47-C7
26	b	620	SQD	C46-C45-O47-C7
26	a	411	SQD	C12-C13-C14-C15
35	C	519	DGD	C2B-C3B-C4B-C5B
35	h	102	DGD	CDB-CEB-CFB-CGB
33	a	419	LMG	C35-C36-C37-C38
23	c	511	CLA	O1D-CGD-O2D-CED
32	a	420	LMT	C2-C3-C4-C5
32	a	420	LMT	C9-C10-C11-C12
35	c	517	DGD	C2A-C1A-O1G-C1G
35	c	519	DGD	C2A-C1A-O1G-C1G
37	D	411	LHG	C17-C18-C19-C20
32	t	102	LMT	C4'-C5'-C6'-O6'
26	A	410	SQD	C11-C10-C9-C8
33	C	520	LMG	C34-C35-C36-C37
37	D	409	LHG	O2-C2-C3-O3
23	c	507	CLA	C10-C11-C12-C13
26	A	412	SQD	C2-C1-O6-C44
37	E	101	LHG	C25-C26-C27-C28
37	d	408	LHG	C33-C34-C35-C36
33	C	501	LMG	C18-C19-C20-C21
37	E	101	LHG	C13-C14-C15-C16
23	A	404	CLA	C13-C15-C16-C17
32	a	414	LMT	C6-C7-C8-C9
32	t	101	LMT	O1'-C1-C2-C3
23	c	508	CLA	C5-C6-C7-C8
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	a	409	CLA	C11-C10-C8-C7
23	b	601	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	b	604	CLA	C6-C7-C8-C10
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	507	CLA	C11-C10-C8-C7
23	c	510	CLA	C11-C10-C8-C7
23	c	513	CLA	C12-C13-C15-C16
23	b	607	CLA	C3-C5-C6-C7
23	C	505	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	C	514	CLA	C11-C10-C8-C9
23	D	406	CLA	C14-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C14
23	c	511	CLA	C11-C10-C8-C9
23	C	513	CLA	CBA-CGA-O2A-C1
32	M	101	LMT	O5'-C5'-C6'-O6'
23	B	601	CLA	C2A-CAA-CBA-CGA
25	Y	101	BCR	C37-C22-C23-C24
33	z	101	LMG	C14-C15-C16-C17
34	c	522	HTG	C4'-C5'-C6'-C7'
35	C	519	DGD	CDB-CEB-CFB-CGB
27	d	801	GOL	O1-C1-C2-C3
23	b	603	CLA	C5-C6-C7-C8
26	B	620	SQD	C34-C35-C36-C37
23	d	403	CLA	CBA-CGA-O2A-C1
35	H	102	DGD	CCA-CDA-CEA-CFA
37	e	101	LHG	C23-C24-C25-C26
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
23	B	613	CLA	C13-C15-C16-C17
23	C	507	CLA	C5-C6-C7-C8
29	A	414	PL9	C39-C41-C42-C43
33	a	419	LMG	C4-C5-C6-O5
26	b	620	SQD	C28-C29-C30-C31
23	B	606	CLA	C8-C10-C11-C12
23	C	514	CLA	O1D-CGD-O2D-CED
29	D	408	PL9	C45-C44-C46-C47
23	C	512	CLA	C8-C10-C11-C12
35	c	518	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
32	a	420	LMT	O5'-C5'-C6'-O6'
23	c	513	CLA	C10-C11-C12-C13
23	B	601	CLA	CBA-CGA-O2A-C1
33	c	521	LMG	C29-C28-O8-C9
35	C	517	DGD	CCA-CDA-CEA-CFA
23	C	507	CLA	C3A-C2A-CAA-CBA
33	C	521	LMG	C12-C13-C14-C15
33	d	412	LMG	C18-C19-C20-C21
37	e	101	LHG	C10-C11-C12-C13
32	e	102	LMT	C4B-C5B-C6B-O6B
33	C	520	LMG	C31-C32-C33-C34
23	b	615	CLA	C10-C11-C12-C13
32	a	420	LMT	C3-C4-C5-C6
23	b	605	CLA	C5-C6-C7-C8
26	A	410	SQD	O6-C44-C45-C46
26	a	413	SQD	O6-C44-C45-C46
26	b	620	SQD	C44-C45-C46-O48
26	f	102	SQD	O6-C44-C45-C46
37	e	101	LHG	C4-C5-C6-O8
37	L	101	LHG	C27-C28-C29-C30
35	C	517	DGD	C1B-C2B-C3B-C4B
35	c	519	DGD	C1A-C2A-C3A-C4A
33	C	520	LMG	C30-C31-C32-C33
23	b	610	CLA	C15-C16-C17-C18
33	c	520	LMG	C29-C30-C31-C32
23	B	607	CLA	C3-C5-C6-C7
26	b	620	SQD	O10-C23-O48-C46
35	c	517	DGD	O1A-C1A-O1G-C1G
29	D	408	PL9	C15-C14-C16-C17
29	D	408	PL9	C43-C44-C46-C47
35	C	517	DGD	C4D-C5D-C6D-O5D
35	C	517	DGD	C7A-C8A-C9A-CAA
33	B	621	LMG	C32-C33-C34-C35
35	h	102	DGD	C3B-C4B-C5B-C6B
37	d	711	LHG	C3-O3-P-O6
33	c	520	LMG	C28-C29-C30-C31
26	F	101	SQD	C34-C35-C36-C37
27	B	624	GOL	O1-C1-C2-O2
27	o	501	GOL	O2-C2-C3-O3
27	v	401	GOL	O1-C1-C2-O2
35	C	517	DGD	C3B-C4B-C5B-C6B
23	b	601	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	a	419	LMG	C21-C22-C23-C24
23	d	403	CLA	O1A-CGA-O2A-C1
35	c	519	DGD	O1A-C1A-O1G-C1G
33	d	412	LMG	C10-C11-C12-C13
23	A	406	CLA	C16-C17-C18-C20
23	c	513	CLA	C13-C15-C16-C17
23	a	407	CLA	C2B-C3B-CAB-CBB
23	b	606	CLA	C2B-C3B-CAB-CBB
32	I	101	LMT	C4-C5-C6-C7
33	a	419	LMG	C33-C34-C35-C36
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
34	B	626	HTG	S1-C1'-C2'-C3'
23	C	503	CLA	C16-C17-C18-C19
23	b	606	CLA	C16-C17-C18-C19
33	Z	101	LMG	C19-C20-C21-C22
26	A	412	SQD	O5-C1-O6-C44
35	c	517	DGD	O6E-C1E-O5D-C6D
29	a	416	PL9	C24-C26-C27-C28
37	D	409	LHG	C1-C2-C3-O3
34	B	626	HTG	C4'-C5'-C6'-C7'
23	b	608	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
26	F	101	SQD	C32-C33-C34-C35
23	C	507	CLA	C6-C7-C8-C9
23	C	514	CLA	C6-C7-C8-C9
23	b	601	CLA	C6-C7-C8-C9
23	c	513	CLA	C6-C7-C8-C9
23	c	514	CLA	C6-C7-C8-C9
23	d	403	CLA	C11-C12-C13-C14
23	C	513	CLA	O1A-CGA-O2A-C1
32	a	420	LMT	C4'-C5'-C6'-O6'
37	D	411	LHG	C27-C28-C29-C30
37	l	101	LHG	C34-C35-C36-C37
25	B	617	BCR	C1-C6-C7-C8
25	B	617	BCR	C5-C6-C7-C8
25	c	515	BCR	C23-C24-C25-C26
25	d	404	BCR	C23-C24-C25-C26
23	B	601	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	C	501	LMG	C20-C21-C22-C23
32	b	627	LMT	C1-C2-C3-C4
33	c	520	LMG	C4-C5-C6-O5
25	Y	101	BCR	C21-C22-C23-C24
37	L	101	LHG	C11-C10-C9-C8
33	m	101	LMG	C14-C15-C16-C17
35	h	102	DGD	C6A-C7A-C8A-C9A
26	A	410	SQD	C18-C19-C20-C21
26	b	620	SQD	C11-C10-C9-C8
37	e	101	LHG	C7-C8-C9-C10
32	e	102	LMT	C9-C10-C11-C12
32	E	102	LMT	C2-C3-C4-C5
32	b	627	LMT	C6-C7-C8-C9
35	C	518	DGD	C5B-C6B-C7B-C8B
35	h	102	DGD	C9B-CAB-CBB-CCB
37	l	101	LHG	C13-C14-C15-C16
23	B	612	CLA	C10-C11-C12-C13
37	L	101	LHG	O6-C4-C5-C6
33	z	101	LMG	C20-C21-C22-C23
35	C	518	DGD	C8B-C9B-CAB-CBB
23	B	610	CLA	C12-C13-C15-C16
23	B	614	CLA	C12-C13-C15-C16
23	C	503	CLA	C12-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C10
23	C	511	CLA	C12-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C10
23	c	510	CLA	C6-C7-C8-C10
23	c	511	CLA	C11-C10-C8-C7
29	a	416	PL9	C12-C11-C9-C8
33	B	621	LMG	C18-C19-C20-C21
35	c	517	DGD	CCB-CDB-CEB-CFB
37	D	410	LHG	C11-C10-C9-C8
26	a	411	SQD	C27-C28-C29-C30
37	L	101	LHG	C24-C25-C26-C27
37	D	411	LHG	C10-C11-C12-C13
37	d	407	LHG	C13-C14-C15-C16
32	E	102	LMT	C4-C5-C6-C7
35	C	518	DGD	C7A-C8A-C9A-CAA
34	b	623	HTG	O5-C1-S1-C1'
33	a	419	LMG	C31-C32-C33-C34
33	C	520	LMG	C36-C37-C38-C39
23	B	605	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	b	601	CLA	C13-C15-C16-C17
23	b	613	CLA	CBD-CGD-O2D-CED
33	d	412	LMG	C16-C17-C18-C19
23	B	616	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O2D
24	a	408	PHO	CAD-CBD-CGD-O2D
38	e	87	HEM	C2C-C3C-CAC-CBC
23	b	605	CLA	C13-C15-C16-C17
23	C	511	CLA	CBA-CGA-O2A-C1
23	c	512	CLA	CBA-CGA-O2A-C1
29	d	405	PL9	C45-C44-C46-C47
26	a	411	SQD	C34-C35-C36-C37
33	B	621	LMG	O6-C1-O1-C7
35	c	518	DGD	O6E-C1E-O5D-C6D
26	B	620	SQD	C44-C45-C46-O48
33	C	501	LMG	C7-C8-C9-O8
23	B	601	CLA	O1A-CGA-O2A-C1
37	E	101	LHG	O6-C4-C5-O7
37	L	101	LHG	O6-C4-C5-O7
33	C	521	LMG	C35-C36-C37-C38
23	B	601	CLA	C13-C15-C16-C17
23	C	503	CLA	C16-C17-C18-C20
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O1D
32	D	404	LMT	C9-C10-C11-C12
33	B	621	LMG	C2-C1-O1-C7
35	c	517	DGD	C2E-C1E-O5D-C6D
35	c	518	DGD	C2E-C1E-O5D-C6D
37	D	409	LHG	C32-C33-C34-C35
33	a	419	LMG	O7-C8-C9-O8
37	e	101	LHG	O7-C5-C6-O8
26	A	410	SQD	C34-C35-C36-C37
33	c	521	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
27	B	901	GOL	O1-C1-C2-O2
27	c	743	GOL	O1-C1-C2-O2
27	o	601	GOL	O1-C1-C2-O2
23	C	504	CLA	O1D-CGD-O2D-CED
37	d	407	LHG	C11-C10-C9-C8
37	d	408	LHG	C9-C10-C11-C12
26	A	412	SQD	C30-C31-C32-C33
35	C	519	DGD	C2A-C3A-C4A-C5A
23	C	511	CLA	O1A-CGA-O2A-C1
23	b	601	CLA	O1A-CGA-O2A-C1
23	c	512	CLA	O1A-CGA-O2A-C1
26	F	101	SQD	C7-C8-C9-C10
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
35	C	519	DGD	CBA-CCA-CDA-CEA
26	a	413	SQD	C16-C17-C18-C19
26	a	413	SQD	C24-C25-C26-C27
25	c	516	BCR	C7-C8-C9-C34
25	d	404	BCR	C7-C8-C9-C34
25	d	404	BCR	C7-C8-C9-C10
37	d	711	LHG	C18-C19-C20-C21
23	B	611	CLA	C1A-C2A-CAA-CBA
23	a	406	CLA	C1A-C2A-CAA-CBA
23	c	512	CLA	C1A-C2A-CAA-CBA
23	C	502	CLA	C16-C17-C18-C20
37	d	407	LHG	C16-C17-C18-C19
32	b	621	LMT	C3-C4-C5-C6
26	a	411	SQD	C35-C36-C37-C38
23	C	507	CLA	C4-C3-C5-C6
37	D	411	LHG	C2-C3-O3-P
33	m	101	LMG	C32-C33-C34-C35
23	C	513	CLA	C4B-C3B-CAB-CBB
23	c	502	CLA	C4B-C3B-CAB-CBB
37	D	410	LHG	C4-O6-P-O5
37	E	101	LHG	C4-O6-P-O5
37	e	101	LHG	C4-O6-P-O4
33	z	101	LMG	C10-C11-C12-C13
35	c	519	DGD	C2B-C3B-C4B-C5B
23	B	606	CLA	C15-C16-C17-C18
26	A	412	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
37	E	101	LHG	O6-C4-C5-C6
32	b	627	LMT	O1'-C1-C2-C3
37	L	101	LHG	C26-C27-C28-C29
35	c	518	DGD	C7B-C8B-C9B-CAB
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
26	B	620	SQD	C30-C31-C32-C33
35	C	517	DGD	C6A-C7A-C8A-C9A
35	C	519	DGD	CAB-CBB-CCB-CDB
23	b	604	CLA	O1A-CGA-O2A-C1
33	c	520	LMG	C30-C31-C32-C33
34	b	623	HTG	S1-C1'-C2'-C3'
23	b	604	CLA	CBA-CGA-O2A-C1
23	C	507	CLA	C15-C16-C17-C18
23	B	608	CLA	C16-C17-C18-C20
23	A	406	CLA	C12-C13-C15-C16
23	B	602	CLA	C6-C7-C8-C10
23	B	616	CLA	C12-C13-C15-C16
23	b	609	CLA	C2-C3-C5-C6
23	b	615	CLA	C12-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C10
23	d	402	CLA	C11-C12-C13-C15
26	A	410	SQD	C13-C14-C15-C16
23	C	513	CLA	C3-C5-C6-C7
37	D	410	LHG	C34-C35-C36-C37
32	e	102	LMT	O1'-C1-C2-C3
33	Z	101	LMG	C11-C12-C13-C14
35	c	518	DGD	C5A-C6A-C7A-C8A
40	v	202	HEC	C4C-C3C-CAC-CBC
26	F	101	SQD	O47-C45-C46-O48
37	E	101	LHG	O7-C5-C6-O8
35	C	518	DGD	C8A-C9A-CAA-CBA
37	d	408	LHG	C32-C33-C34-C35
23	B	602	CLA	C15-C16-C17-C18
32	e	102	LMT	C3-C4-C5-C6
33	d	412	LMG	C35-C36-C37-C38
35	C	518	DGD	C5D-C6D-O5D-C1E

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Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CAA-CBA-CGA-O2A
33	B	621	LMG	O8-C28-C29-C30
23	b	604	CLA	C13-C15-C16-C17
23	b	604	CLA	C15-C16-C17-C18
23	b	610	CLA	C13-C15-C16-C17
33	B	621	LMG	C29-C30-C31-C32
37	d	408	LHG	C2-C3-O3-P
35	C	519	DGD	C6A-C7A-C8A-C9A
35	H	102	DGD	O2G-C1B-C2B-C3B
37	d	711	LHG	C34-C35-C36-C37
23	c	507	CLA	C13-C15-C16-C17
23	A	408	CLA	C11-C12-C13-C14
23	C	511	CLA	C11-C12-C13-C14
23	a	409	CLA	C11-C10-C8-C9
23	b	606	CLA	C14-C13-C15-C16
23	b	614	CLA	C11-C12-C13-C14
23	b	615	CLA	C14-C13-C15-C16
26	A	412	SQD	O10-C23-O48-C46
32	I	101	LMT	C7-C8-C9-C10
37	D	410	LHG	C26-C27-C28-C29
23	b	601	CLA	CAA-CBA-CGA-O2A
35	C	518	DGD	C7B-C8B-C9B-CAB
37	d	711	LHG	C11-C12-C13-C14
23	B	606	CLA	C16-C17-C18-C19
23	B	613	CLA	C15-C16-C17-C18
35	C	519	DGD	C7B-C8B-C9B-CAB
23	B	602	CLA	C2B-C3B-CAB-CBB
23	C	503	CLA	C2B-C3B-CAB-CBB
23	C	513	CLA	C2B-C3B-CAB-CBB
23	D	405	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
23	c	503	CLA	C2B-C3B-CAB-CBB
35	C	519	DGD	C7A-C8A-C9A-CAA
34	b	622	HTG	C1'-C2'-C3'-C4'
29	a	416	PL9	C43-C44-C46-C47
23	a	409	CLA	C15-C16-C17-C18
37	L	101	LHG	C23-C24-C25-C26
32	M	103	LMT	C3-C4-C5-C6
37	D	410	LHG	C13-C14-C15-C16
37	l	101	LHG	C28-C29-C30-C31
23	A	408	CLA	C2-C1-O2A-CGA
26	B	620	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
33	D	415	LMG	C18-C19-C20-C21
33	C	520	LMG	C11-C12-C13-C14
35	C	519	DGD	CAA-CBA-CCA-CDA
23	c	511	CLA	C4-C3-C5-C6
34	B	626	HTG	C4-C5-C6-O6
25	c	515	BCR	C23-C24-C25-C30
25	d	404	BCR	C23-C24-C25-C30
25	h	101	BCR	C23-C24-C25-C26
25	h	101	BCR	C23-C24-C25-C30
29	A	414	PL9	C28-C29-C31-C32
26	a	413	SQD	C26-C27-C28-C29
37	d	408	LHG	C10-C11-C12-C13
23	b	615	CLA	C5-C6-C7-C8
33	m	101	LMG	C2-C1-O1-C7
33	Z	101	LMG	C2-C1-O1-C7
34	b	622	HTG	C4-C5-C6-O6
33	m	101	LMG	C11-C12-C13-C14
26	A	410	SQD	C16-C17-C18-C19
33	B	621	LMG	C14-C15-C16-C17
23	c	514	CLA	C4-C3-C5-C6
34	B	626	HTG	C2'-C3'-C4'-C5'
23	c	506	CLA	C12-C13-C15-C16
23	a	406	CLA	C4C-C3C-CAC-CBC
32	m	103	LMT	C4'-C5'-C6'-O6'
23	A	406	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C9
23	d	402	CLA	C11-C12-C13-C14
23	A	408	CLA	C16-C17-C18-C19
23	C	507	CLA	C16-C17-C18-C20
37	D	410	LHG	C28-C29-C30-C31
24	a	408	PHO	C2C-C3C-CAC-CBC
32	E	102	LMT	C6-C7-C8-C9
26	A	412	SQD	C7-C8-C9-C10
32	A	359	LMT	C7-C8-C9-C10
27	B	901	GOL	C1-C2-C3-O3
37	D	409	LHG	O1-C1-C2-C3
23	a	406	CLA	C15-C16-C17-C18
23	b	609	CLA	C4-C3-C5-C6
27	d	701	GOL	O1-C1-C2-O2
26	F	101	SQD	C24-C23-O48-C46
33	B	621	LMG	O6-C5-C6-O5
38	e	87	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
26	a	411	SQD	C11-C12-C13-C14
23	C	509	CLA	C5-C6-C7-C8
23	c	510	CLA	C15-C16-C17-C18
37	D	411	LHG	O10-C23-O8-C6
37	D	411	LHG	C24-C23-O8-C6
23	B	602	CLA	C4B-C3B-CAB-CBB
23	D	405	CLA	C4B-C3B-CAB-CBB
23	a	409	CLA	C4B-C3B-CAB-CBB
23	c	509	CLA	C4B-C3B-CAB-CBB
23	c	513	CLA	C4B-C3B-CAB-CBB
32	M	101	LMT	O5'-C1'-O1'-C1
33	m	101	LMG	O6-C1-O1-C7
33	d	412	LMG	C38-C39-C40-C41
33	B	621	LMG	C37-C38-C39-C40
35	c	519	DGD	O6D-C5D-C6D-O5D
32	b	621	LMT	C7-C8-C9-C10
23	b	616	CLA	C4-C3-C5-C6
24	a	408	PHO	C4-C3-C5-C6
40	v	202	HEC	C2B-C3B-CAB-CBB
24	a	408	PHO	C2-C3-C5-C6
23	C	511	CLA	C13-C15-C16-C17
23	b	612	CLA	C10-C11-C12-C13
33	B	621	LMG	C20-C21-C22-C23
33	a	419	LMG	O8-C28-C29-C30
23	B	608	CLA	C2-C1-O2A-CGA
23	C	507	CLA	C2-C1-O2A-CGA
23	C	514	CLA	C2-C1-O2A-CGA
23	C	502	CLA	C2A-CAA-CBA-CGA
35	C	519	DGD	C8B-C9B-CAB-CBB
35	c	517	DGD	C4B-C5B-C6B-C7B
23	b	613	CLA	O1D-CGD-O2D-CED
26	B	620	SQD	C33-C34-C35-C36
33	z	101	LMG	O7-C10-C11-C12
37	d	407	LHG	C9-C10-C11-C12
23	b	608	CLA	C13-C15-C16-C17
32	e	102	LMT	C2B-C1B-O1B-C4'
37	D	410	LHG	C17-C18-C19-C20
38	E	103	HEM	CAD-CBD-CGD-O1D
23	C	502	CLA	CBD-CGD-O2D-CED
29	a	416	PL9	C4-C3-C7-C8
23	C	510	CLA	C6-C7-C8-C9
23	C	513	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	a	407	CLA	C14-C13-C15-C16
23	B	608	CLA	C16-C17-C18-C19
32	t	101	LMT	C2-C3-C4-C5
33	c	521	LMG	C31-C32-C33-C34
37	l	101	LHG	C10-C11-C12-C13
35	H	102	DGD	O1G-C1G-C2G-C3G
37	d	711	LHG	C1-C2-C3-O3
26	a	411	SQD	C10-C11-C12-C13
37	E	101	LHG	C12-C13-C14-C15
23	B	606	CLA	C16-C17-C18-C20
24	A	407	PHO	O2A-C1-C2-C3
24	a	408	PHO	O2A-C1-C2-C3
24	A	353	PHO	C2C-C3C-CAC-CBC
32	a	420	LMT	O5'-C1'-O1'-C1
35	c	517	DGD	CBA-CCA-CDA-CEA
25	K	102	BCR	C7-C8-C9-C34
33	B	621	LMG	C36-C37-C38-C39
35	C	519	DGD	C8A-C9A-CAA-CBA
29	a	416	PL9	C45-C44-C46-C47
23	C	502	CLA	C1A-C2A-CAA-CBA
23	a	407	CLA	C1A-C2A-CAA-CBA
23	c	514	CLA	C1A-C2A-CAA-CBA
35	C	519	DGD	CDA-CEA-CFA-CGA
33	C	521	LMG	C4-C5-C6-O5
23	B	601	CLA	C11-C12-C13-C15
23	C	507	CLA	C12-C13-C15-C16
23	C	514	CLA	C11-C12-C13-C15
33	d	412	LMG	C19-C20-C21-C22
25	H	101	BCR	C9-C10-C11-C12
37	D	409	LHG	C29-C30-C31-C32
37	L	101	LHG	C10-C11-C12-C13
26	F	101	SQD	O10-C23-O48-C46
32	A	359	LMT	C9-C10-C11-C12
23	C	508	CLA	C2A-CAA-CBA-CGA
23	C	511	CLA	C8-C10-C11-C12
26	a	413	SQD	C15-C16-C17-C18
35	c	519	DGD	C9B-CAB-CBB-CCB
23	b	601	CLA	C4-C3-C5-C6
23	b	616	CLA	C5-C6-C7-C8
23	c	502	CLA	C2B-C3B-CAB-CBB
23	c	513	CLA	C2B-C3B-CAB-CBB
35	h	102	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
38	E	103	HEM	CAD-CBD-CGD-O2D
23	b	608	CLA	C16-C17-C18-C20
33	z	101	LMG	C13-C14-C15-C16
26	b	620	SQD	C30-C31-C32-C33
35	H	102	DGD	C4E-C5E-C6E-O5E
33	C	501	LMG	O7-C8-C9-O8
33	c	521	LMG	O1-C7-C8-O7
35	H	102	DGD	O1G-C1G-C2G-O2G
40	V	202	HEC	C4B-C3B-CAB-CBB
23	c	512	CLA	C3-C5-C6-C7
37	d	711	LHG	C27-C28-C29-C30
37	e	101	LHG	C24-C25-C26-C27
23	A	406	CLA	C16-C17-C18-C19
37	d	711	LHG	C17-C18-C19-C20
38	e	87	HEM	CAD-CBD-CGD-O2D
40	V	202	HEC	CAD-CBD-CGD-O2D
37	d	407	LHG	C25-C26-C27-C28
23	B	613	CLA	C2-C1-O2A-CGA
23	a	405	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2-C1-O2A-CGA
23	c	511	CLA	C2-C3-C5-C6
29	d	405	PL9	C43-C44-C46-C47
35	c	519	DGD	CDB-CEB-CFB-CGB
23	c	503	CLA	C11-C12-C13-C14
40	V	202	HEC	CAD-CBD-CGD-O1D
23	b	612	CLA	C8-C10-C11-C12
23	b	603	CLA	C2A-CAA-CBA-CGA
25	H	101	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C30
25	b	619	BCR	C1-C6-C7-C8
25	y	101	BCR	C23-C24-C25-C30
35	H	102	DGD	C8A-C9A-CAA-CBA
25	K	102	BCR	C7-C8-C9-C10
26	A	412	SQD	C15-C16-C17-C18
37	d	711	LHG	C9-C10-C11-C12
23	b	616	CLA	C2-C3-C5-C6
29	A	414	PL9	C43-C44-C46-C47
23	C	510	CLA	C3-C5-C6-C7
23	b	601	CLA	C3-C5-C6-C7
38	e	87	HEM	CAA-CBA-CGA-O2A
40	v	202	HEC	CAD-CBD-CGD-O2D
37	D	409	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
35	c	517	DGD	CDB-CEB-CFB-CGB
33	C	521	LMG	C10-C11-C12-C13
33	C	520	LMG	C29-C30-C31-C32
23	c	504	CLA	C2A-CAA-CBA-CGA
23	b	607	CLA	C8-C10-C11-C12
35	c	518	DGD	C1A-C2A-C3A-C4A
29	D	408	PL9	C35-C34-C36-C37
23	B	613	CLA	C12-C13-C15-C16
23	b	615	CLA	C11-C12-C13-C15
23	c	503	CLA	C11-C12-C13-C15
23	B	611	CLA	C8-C10-C11-C12
23	C	512	CLA	O1A-CGA-O2A-C1
37	l	101	LHG	C25-C26-C27-C28
33	B	621	LMG	O1-C7-C8-O7
32	M	101	LMT	C2-C3-C4-C5
35	h	102	DGD	O2G-C1B-C2B-C3B
37	D	409	LHG	O8-C23-C24-C25
29	A	414	PL9	C25-C24-C26-C27
23	B	609	CLA	C2-C3-C5-C6
23	b	601	CLA	C2-C3-C5-C6
33	Z	101	LMG	O7-C10-C11-C12
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
23	a	407	CLA	C6-C7-C8-C9
23	b	614	CLA	C14-C13-C15-C16
23	b	613	CLA	CAA-CBA-CGA-O2A
33	c	520	LMG	O7-C10-C11-C12
37	e	101	LHG	O8-C23-C24-C25
23	B	603	CLA	CAD-CBD-CGD-O2D
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	609	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
24	A	407	PHO	CAD-CBD-CGD-O2D
38	E	103	HEM	C2B-C3B-CAB-CBB
40	v	202	HEC	CAD-CBD-CGD-O1D
26	B	620	SQD	C24-C25-C26-C27
37	L	101	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	B	613	CLA	CAA-CBA-CGA-O2A
37	L	101	LHG	O7-C7-C8-C9
38	e	87	HEM	CAA-CBA-CGA-O1A
37	l	101	LHG	O7-C7-C8-C9
25	y	101	BCR	C21-C22-C23-C24
33	B	621	LMG	O1-C7-C8-C9
35	c	519	DGD	CDA-CEA-CFA-CGA
33	C	501	LMG	C29-C30-C31-C32
23	B	602	CLA	O2A-C1-C2-C3
23	b	613	CLA	O2A-C1-C2-C3
38	E	103	HEM	C4B-C3B-CAB-CBB
23	B	612	CLA	CBA-CGA-O2A-C1
23	b	612	CLA	C13-C15-C16-C17
23	a	405	CLA	C2C-C3C-CAC-CBC
23	A	404	CLA	C2C-C3C-CAC-CBC
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	C	505	CLA	CHA-CBD-CGD-O1D
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	a	406	CLA	CHA-CBD-CGD-O1D
23	a	406	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	CHA-CBD-CGD-O2D
33	B	621	LMG	C30-C31-C32-C33
26	A	412	SQD	O48-C23-C24-C25
23	c	511	CLA	O1A-CGA-O2A-C1
23	C	513	CLA	CAA-CBA-CGA-O2A
23	c	503	CLA	C16-C17-C18-C19
24	A	407	PHO	CHA-CBD-CGD-O2D
24	a	408	PHO	CHA-CBD-CGD-O1D
37	D	409	LHG	O1-C1-C2-O2
23	b	602	CLA	C10-C11-C12-C13
23	C	511	CLA	CAA-CBA-CGA-O2A
32	A	359	LMT	C2B-C1B-O1B-C4'
35	C	519	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
23	D	406	CLA	O1A-CGA-O2A-C1
32	e	102	LMT	C2-C3-C4-C5
23	B	605	CLA	C11-C12-C13-C15
23	C	507	CLA	C2-C3-C5-C6
23	a	406	CLA	C11-C12-C13-C15
23	b	608	CLA	C12-C13-C15-C16
29	A	414	PL9	C4-C3-C7-C8
24	a	353	PHO	C2C-C3C-CAC-CBC
23	c	511	CLA	CAA-CBA-CGA-O2A
32	D	404	LMT	C7-C8-C9-C10
37	d	711	LHG	C30-C31-C32-C33
23	B	605	CLA	C11-C12-C13-C14
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
29	d	405	PL9	C34-C36-C37-C38
34	B	623	HTG	C4'-C5'-C6'-C7'
23	b	610	CLA	C16-C17-C18-C19
23	b	610	CLA	C16-C17-C18-C20
23	a	405	CLA	C4C-C3C-CAC-CBC
33	C	501	LMG	C31-C32-C33-C34
33	a	419	LMG	C14-C15-C16-C17
23	B	612	CLA	CAA-CBA-CGA-O2A
23	b	608	CLA	C16-C17-C18-C19
27	A	701	GOL	O1-C1-C2-C3
27	a	801	GOL	C1-C2-C3-O3
23	b	616	CLA	O1A-CGA-O2A-C1
23	b	604	CLA	C10-C11-C12-C13
33	Z	101	LMG	O9-C10-C11-C12
23	b	616	CLA	CBA-CGA-O2A-C1
23	c	510	CLA	C13-C15-C16-C17
23	C	507	CLA	C1A-C2A-CAA-CBA
37	l	101	LHG	O9-C7-C8-C9
32	a	420	LMT	C7-C8-C9-C10
33	C	521	LMG	C11-C12-C13-C14
23	B	612	CLA	O1A-CGA-O2A-C1
23	A	404	CLA	C4C-C3C-CAC-CBC
37	D	409	LHG	O10-C23-C24-C25
37	L	101	LHG	O9-C7-C8-C9
37	e	101	LHG	O10-C23-C24-C25
35	C	517	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
26	F	101	SQD	C44-C45-C46-O48
37	E	101	LHG	O7-C7-C8-C9
23	B	602	CLA	C2A-CAA-CBA-CGA
23	B	603	CLA	C2A-CAA-CBA-CGA
32	m	103	LMT	C4-C5-C6-C7
32	t	102	LMT	C11-C10-C9-C8
33	c	521	LMG	C34-C35-C36-C37
23	B	612	CLA	CAA-CBA-CGA-O1A
33	c	520	LMG	C32-C33-C34-C35
23	B	615	CLA	C8-C10-C11-C12
23	D	406	CLA	C8-C10-C11-C12
23	B	613	CLA	CAA-CBA-CGA-O1A
23	C	513	CLA	CAA-CBA-CGA-O1A
23	b	613	CLA	CAA-CBA-CGA-O1A
33	c	520	LMG	O9-C10-C11-C12
23	C	508	CLA	C10-C11-C12-C13
23	B	610	CLA	C4B-C3B-CAB-CBB
23	b	603	CLA	C4B-C3B-CAB-CBB
37	d	407	LHG	C4-O6-P-O5
23	C	507	CLA	C16-C17-C18-C19
33	d	412	LMG	C28-C29-C30-C31
26	A	412	SQD	O10-C23-C24-C25
23	b	602	CLA	O1A-CGA-O2A-C1
35	C	519	DGD	O1G-C1A-C2A-C3A
33	m	101	LMG	C30-C31-C32-C33
37	d	408	LHG	O10-C23-O8-C6
23	B	604	CLA	C5-C6-C7-C8
23	b	612	CLA	CAA-CBA-CGA-O2A
37	D	409	LHG	C18-C19-C20-C21
33	c	521	LMG	C28-C29-C30-C31
29	d	405	PL9	C15-C14-C16-C17
37	d	408	LHG	C30-C31-C32-C33
29	d	405	PL9	C11-C12-C13-C14
35	c	518	DGD	CDA-CEA-CFA-CGA
35	c	519	DGD	C2A-C3A-C4A-C5A
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	C3-C5-C6-C7
23	C	507	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
26	f	102	SQD	O5-C5-C6-S
23	C	511	CLA	CAA-CBA-CGA-O1A
35	C	518	DGD	O2G-C1B-C2B-C3B
37	E	101	LHG	O8-C23-C24-C25
23	A	408	CLA	C14-C13-C15-C16
23	B	615	CLA	C14-C13-C15-C16
23	C	508	CLA	C11-C12-C13-C14
23	C	512	CLA	C11-C12-C13-C14
23	a	406	CLA	C11-C12-C13-C14
23	b	608	CLA	C14-C13-C15-C16
37	D	409	LHG	C30-C31-C32-C33
37	D	411	LHG	C28-C29-C30-C31
32	t	101	LMT	C6-C7-C8-C9
35	C	517	DGD	CBA-CCA-CDA-CEA
37	L	101	LHG	C32-C33-C34-C35
23	c	502	CLA	C2A-CAA-CBA-CGA
37	D	411	LHG	O8-C23-C24-C25
34	B	622	HTG	C3'-C4'-C5'-C6'
23	B	616	CLA	C11-C12-C13-C15
23	C	506	CLA	C12-C13-C15-C16
23	C	508	CLA	C11-C12-C13-C15
23	C	510	CLA	C6-C7-C8-C10
23	a	407	CLA	C6-C7-C8-C10
23	b	603	CLA	C11-C10-C8-C7
23	b	614	CLA	C11-C12-C13-C15
23	c	509	CLA	C12-C13-C15-C16
23	c	514	CLA	C2-C3-C5-C6
37	E	101	LHG	O9-C7-C8-C9
37	E	101	LHG	O10-C23-C24-C25
23	c	513	CLA	CAA-CBA-CGA-O2A
26	a	413	SQD	O48-C23-C24-C25
35	c	517	DGD	O2G-C1B-C2B-C3B
25	c	516	BCR	C7-C8-C9-C10
23	c	513	CLA	CAA-CBA-CGA-O1A
35	c	517	DGD	O1B-C1B-C2B-C3B
37	D	411	LHG	O10-C23-C24-C25
25	a	410	BCR	C19-C20-C21-C22
32	b	627	LMT	C2-C1-O1'-C1'
23	c	506	CLA	CAA-CBA-CGA-O2A
23	c	511	CLA	CAA-CBA-CGA-O1A
33	D	415	LMG	O9-C10-C11-C12
35	C	518	DGD	O1B-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
37	d	711	LHG	C31-C32-C33-C34
33	D	415	LMG	O7-C10-C11-C12
33	c	521	LMG	O7-C10-C11-C12
35	C	519	DGD	O1A-C1A-C2A-C3A
37	E	101	LHG	C11-C10-C9-C8
37	d	408	LHG	O8-C23-C24-C25

There are no ring outliers.

143 monomers are involved in 261 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	516	BCR	1	0
33	C	521	LMG	3	0
33	Z	101	LMG	2	0
23	c	507	CLA	2	0
23	c	506	CLA	5	0
24	A	353	PHO	2	0
23	b	604	CLA	5	0
32	D	404	LMT	1	0
25	b	619	BCR	5	0
23	c	512	CLA	5	0
35	H	102	DGD	1	0
25	T	101	BCR	6	0
33	c	521	LMG	1	0
35	c	518	DGD	3	0
34	B	623	HTG	1	0
37	D	411	LHG	3	0
23	A	405	CLA	1	0
23	b	612	CLA	1	0
27	B	624	GOL	2	0
23	C	512	CLA	3	0
23	C	510	CLA	1	0
34	b	625	HTG	1	0
37	d	408	LHG	11	0
27	d	801	GOL	1	0
23	C	511	CLA	3	0
27	v	401	GOL	1	0
26	a	411	SQD	3	0
23	c	508	CLA	2	0
32	e	102	LMT	1	0
23	B	605	CLA	4	0
25	b	617	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	404	CLA	2	0
35	C	517	DGD	1	0
23	A	406	CLA	1	0
34	d	411	HTG	1	0
23	b	615	CLA	2	0
26	F	101	SQD	1	0
32	A	359	LMT	1	0
25	H	101	BCR	2	0
32	t	102	LMT	2	0
33	d	412	LMG	2	0
23	c	513	CLA	4	0
33	c	520	LMG	1	0
29	A	414	PL9	10	0
23	C	504	CLA	3	0
37	D	410	LHG	2	0
25	A	409	BCR	2	0
23	a	409	CLA	3	0
23	B	615	CLA	3	0
32	M	101	LMT	2	0
37	e	101	LHG	5	0
33	B	621	LMG	1	0
23	B	616	CLA	3	0
23	C	506	CLA	4	0
23	b	601	CLA	1	0
23	d	403	CLA	3	0
23	b	613	CLA	2	0
23	d	402	CLA	1	0
25	a	410	BCR	1	0
25	t	103	BCR	4	0
23	a	405	CLA	2	0
32	b	621	LMT	1	0
27	b	901	GOL	2	0
37	E	101	LHG	3	0
23	B	606	CLA	2	0
38	E	103	HEM	1	0
23	c	504	CLA	3	0
25	Y	101	BCR	1	0
23	b	603	CLA	1	0
23	B	612	CLA	1	0
25	D	407	BCR	2	0
23	C	502	CLA	5	0
23	a	407	CLA	2	0

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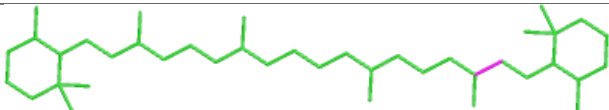
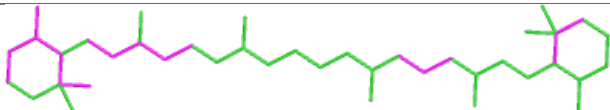
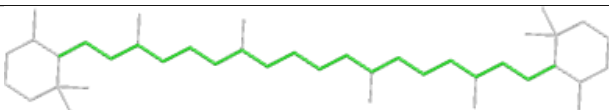
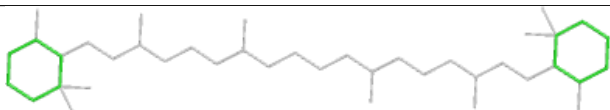
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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24	a	353	PHO	1	0
26	A	410	SQD	1	0
23	B	613	CLA	2	0
33	z	101	LMG	2	0
23	c	510	CLA	2	0
25	B	617	BCR	2	0
35	c	519	DGD	2	0
25	C	515	BCR	1	0
23	B	604	CLA	1	0
34	b	622	HTG	1	0
27	D	701	GOL	1	0
23	B	603	CLA	1	0
27	O	601	GOL	2	0
23	c	509	CLA	2	0
23	b	616	CLA	1	0
35	c	517	DGD	1	0
23	B	614	CLA	3	0
27	O	501	GOL	1	0
37	d	407	LHG	2	0
34	B	622	HTG	1	0
25	B	619	BCR	2	0
25	c	516	BCR	3	0
29	D	408	PL9	1	0
23	B	609	CLA	2	0
23	c	505	CLA	1	0
27	A	701	GOL	3	0
25	h	101	BCR	3	0
27	a	801	GOL	4	0
23	b	614	CLA	3	0
25	y	101	BCR	1	0
35	C	518	DGD	1	0
23	c	502	CLA	2	0
23	C	513	CLA	2	0
25	b	618	BCR	4	0
26	b	620	SQD	3	0
23	C	503	CLA	2	0
32	t	101	LMT	1	0
24	A	407	PHO	1	0
23	b	609	CLA	5	0
23	b	605	CLA	5	0
34	B	626	HTG	1	0

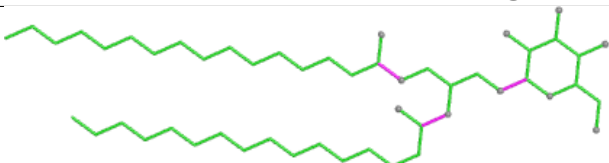
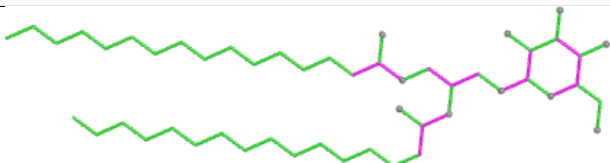
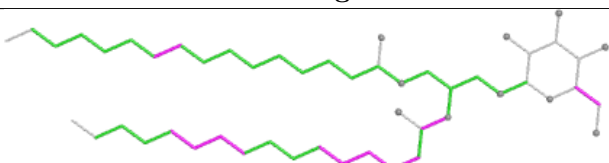
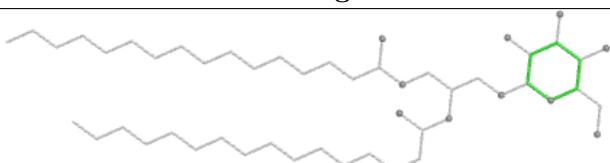
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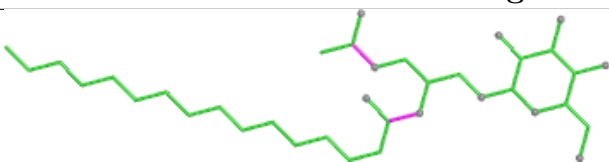
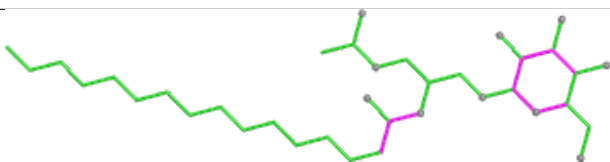
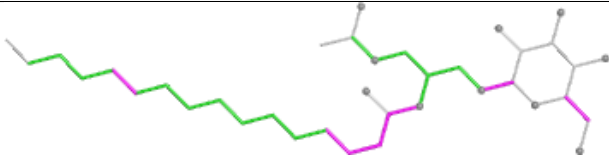
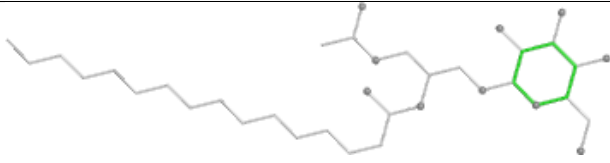
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	602	CLA	1	0
23	c	514	CLA	1	0
23	C	505	CLA	1	0
34	c	522	HTG	1	0
23	c	511	CLA	1	0
26	a	413	SQD	1	0
25	c	515	BCR	2	0
23	C	508	CLA	2	0
23	D	405	CLA	3	0
35	C	519	DGD	1	0
32	I	101	LMT	1	0
27	a	701	GOL	1	0
29	a	416	PL9	4	0
34	D	414	HTG	1	0
23	B	601	CLA	4	0
25	B	618	BCR	2	0
23	c	503	CLA	2	0
23	C	507	CLA	3	0
32	a	420	LMT	2	0
25	K	102	BCR	1	0
23	C	514	CLA	2	0
23	a	406	CLA	3	0
23	b	606	CLA	1	0
23	b	607	CLA	1	0
23	A	408	CLA	3	0
26	B	620	SQD	1	0
25	d	404	BCR	2	0
23	C	509	CLA	3	0

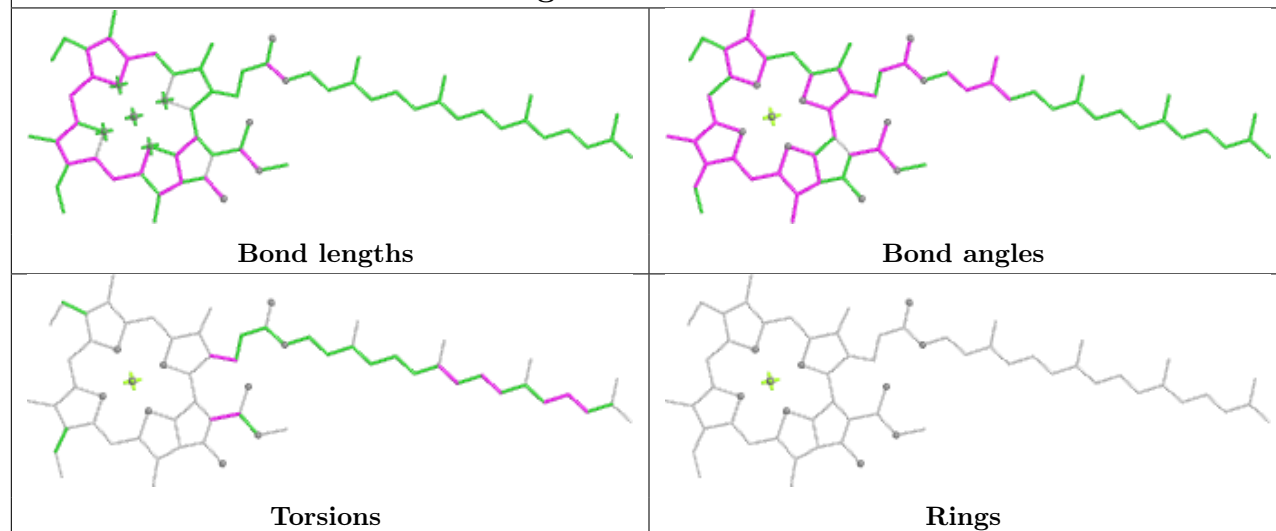
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand BCR C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

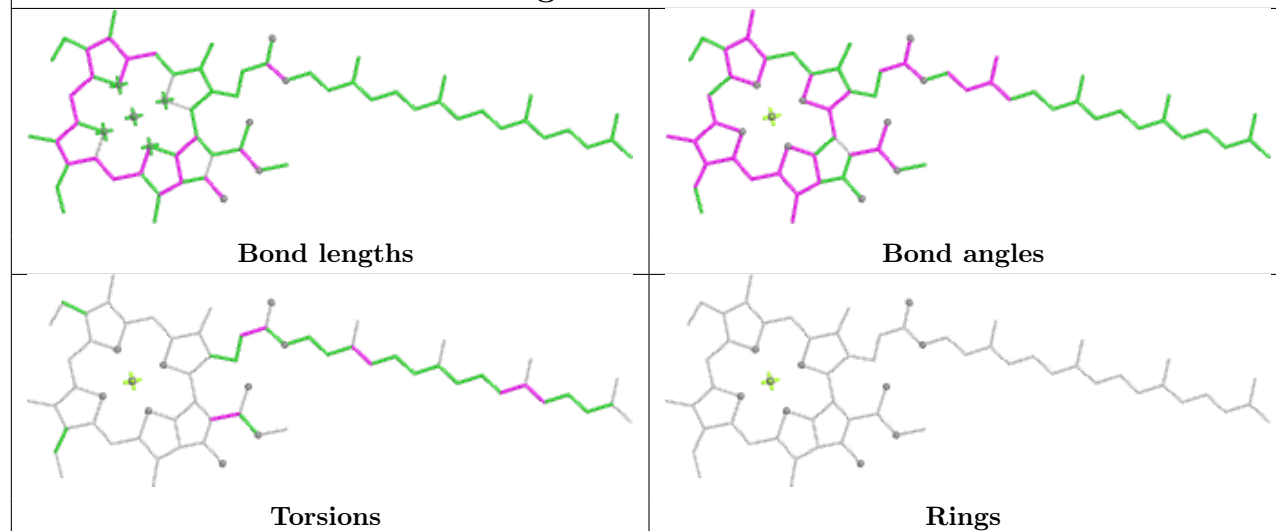
Ligand LMG C 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG Z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

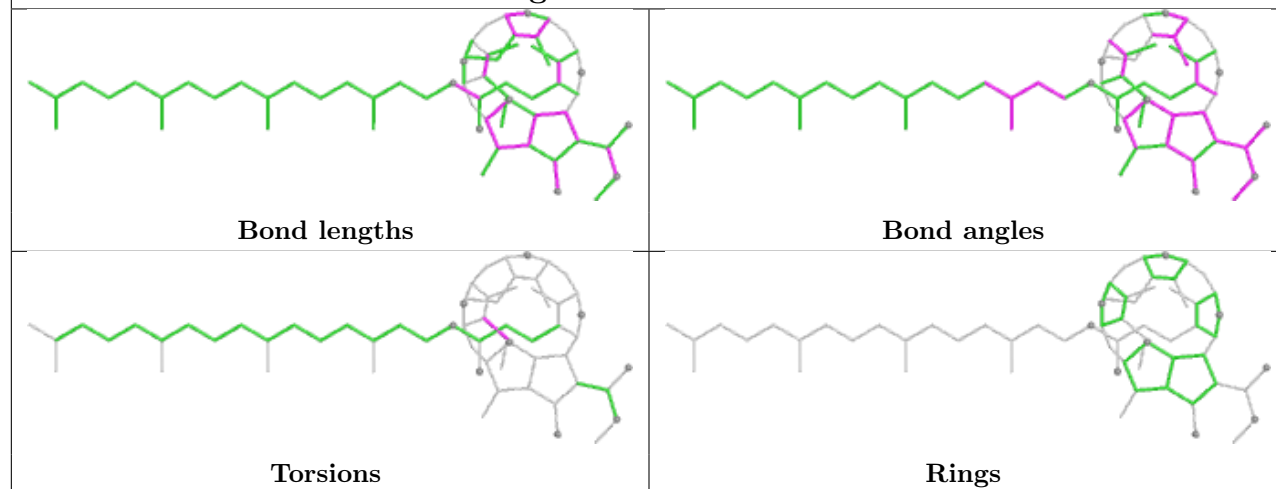
Ligand CLA c 507



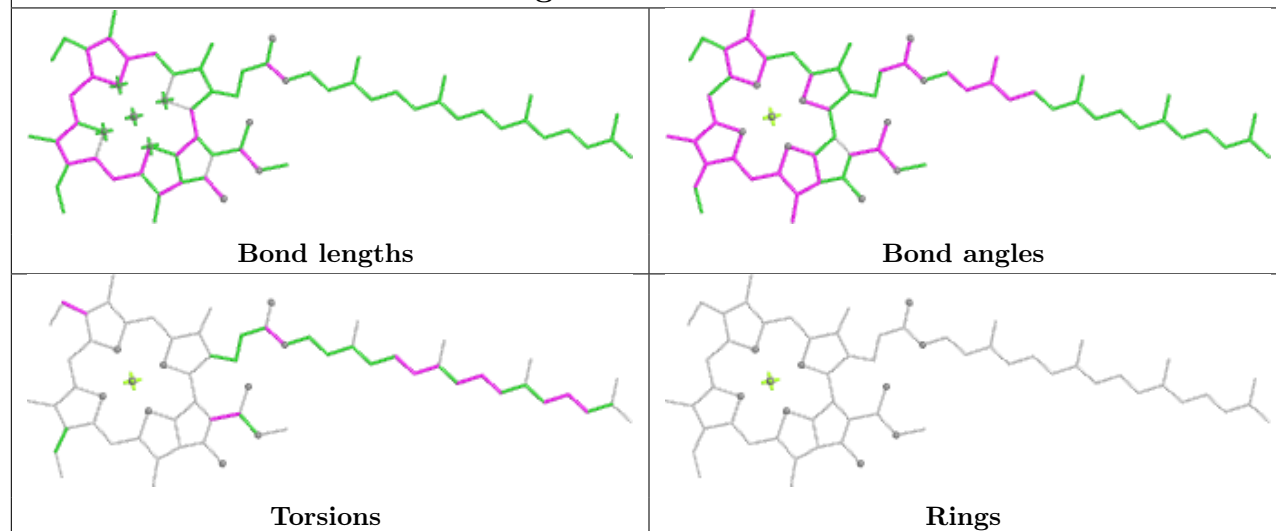
Ligand CLA c 506



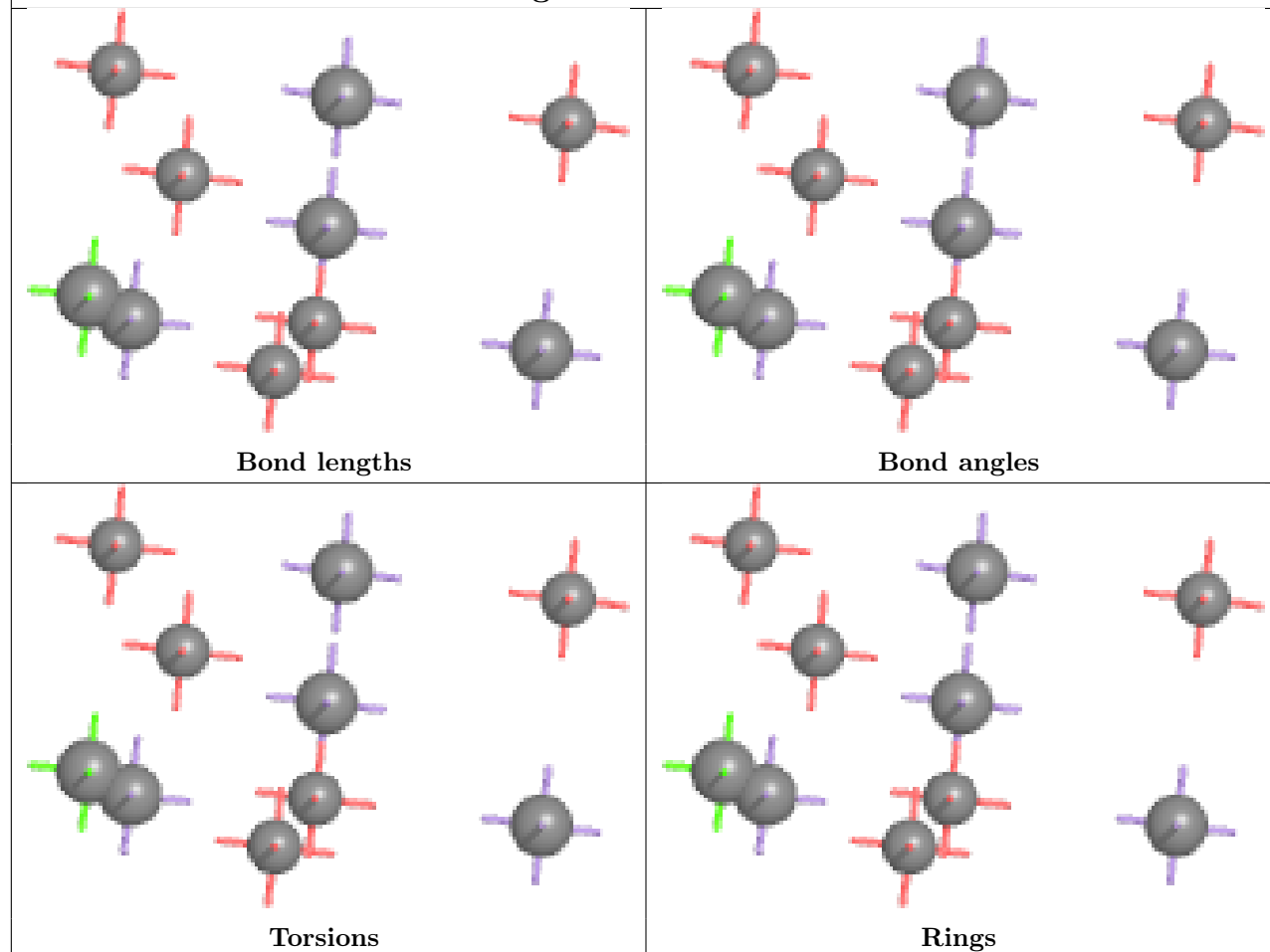
Ligand PHO A 353

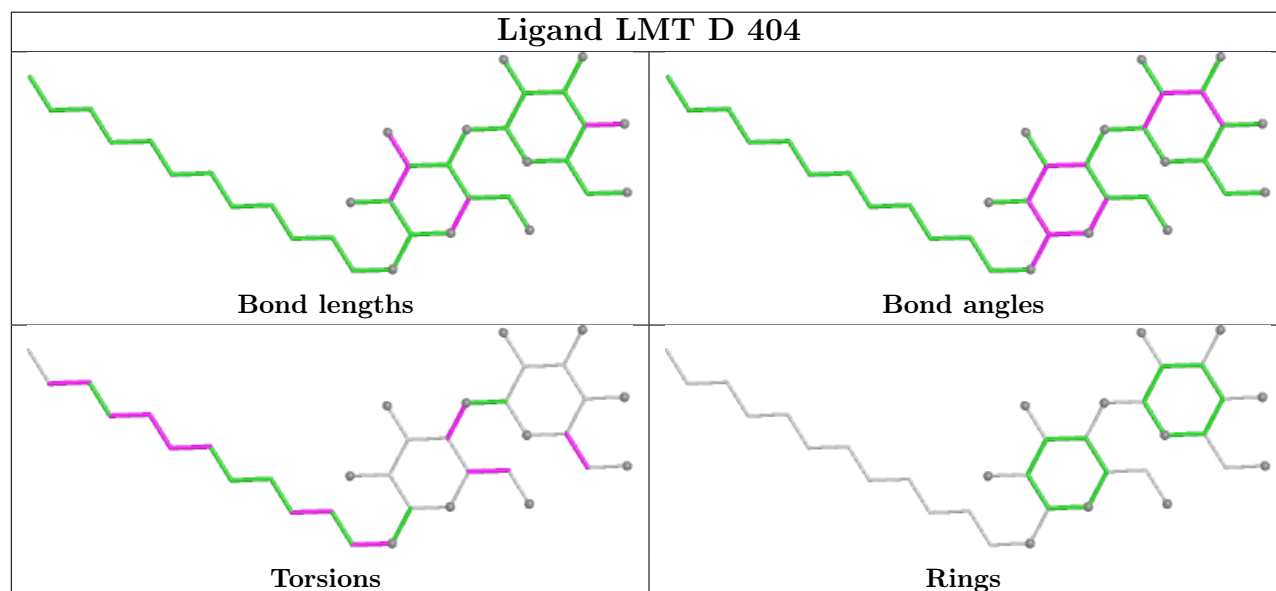
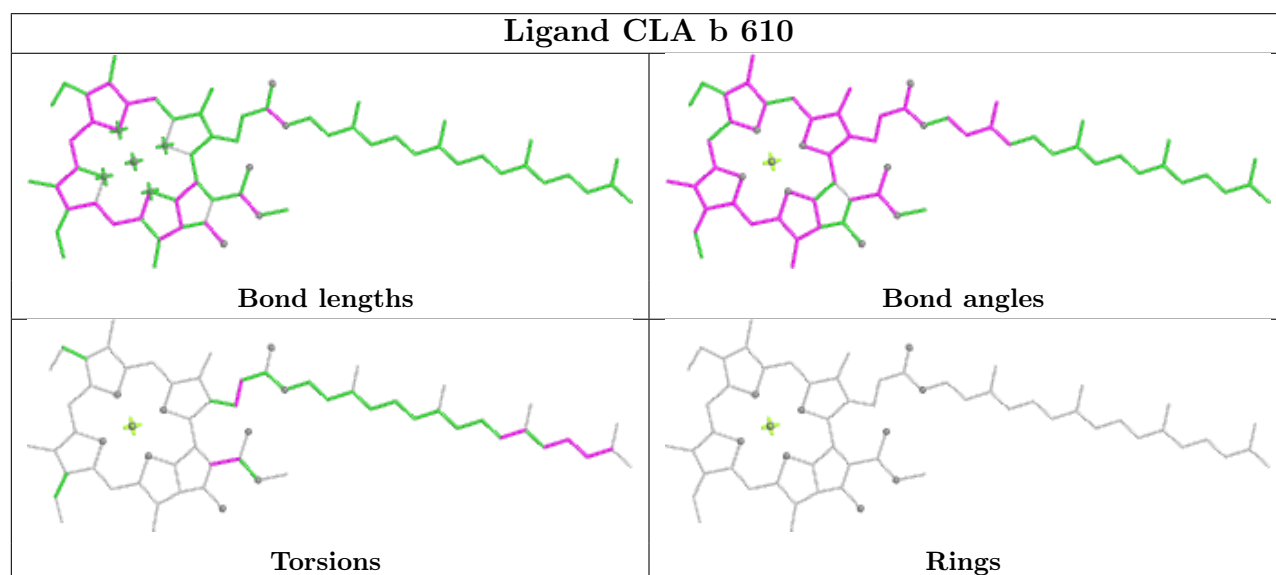
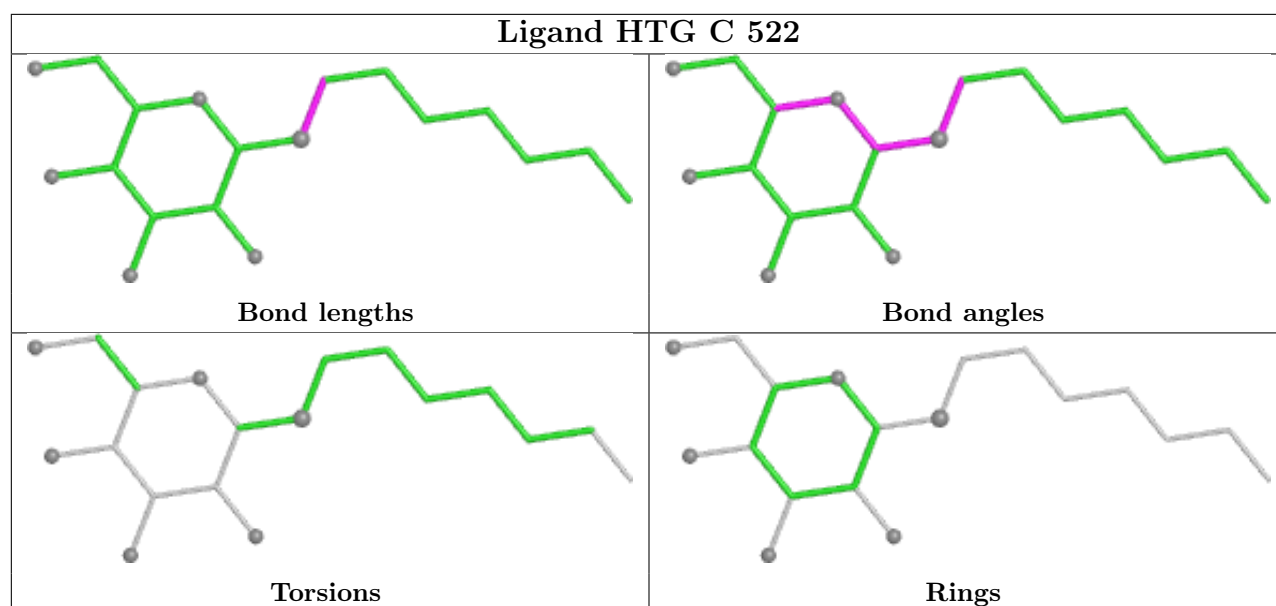


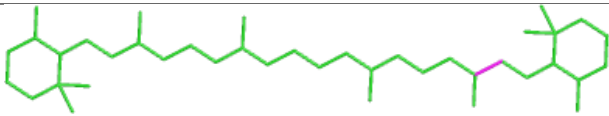
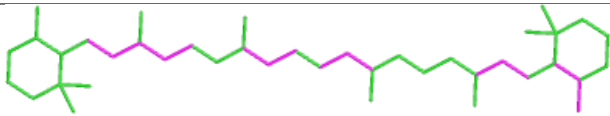
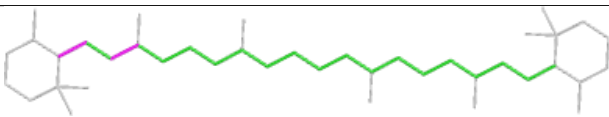
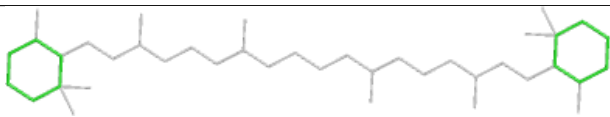
Ligand CLA b 604

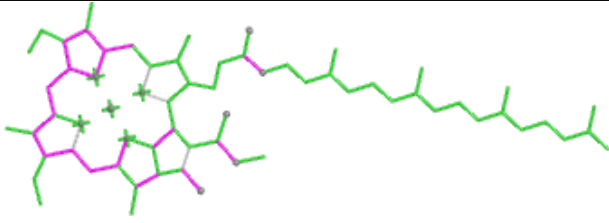
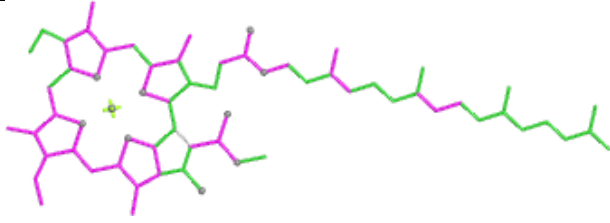
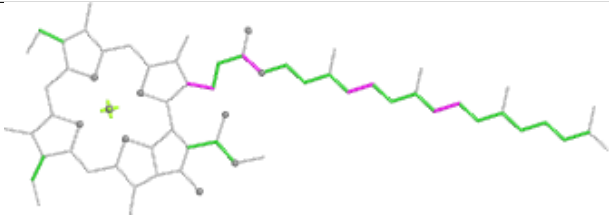
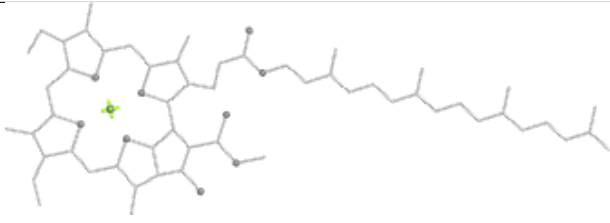


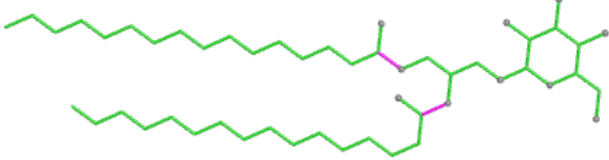
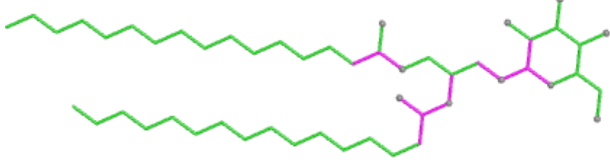
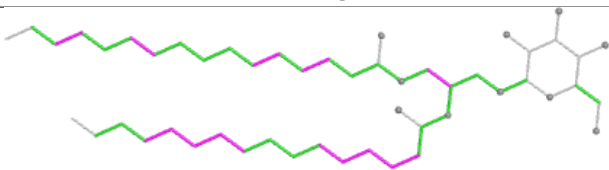
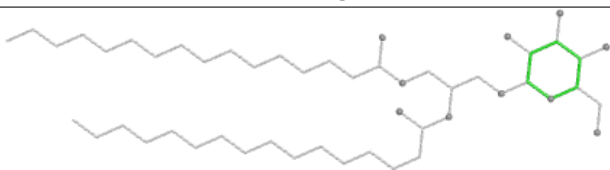
Ligand OEX a 415

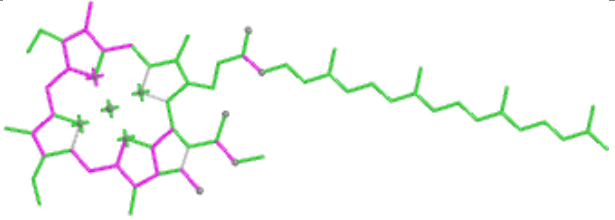
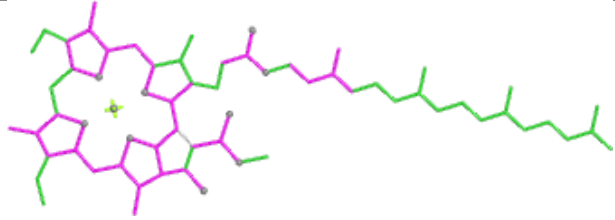
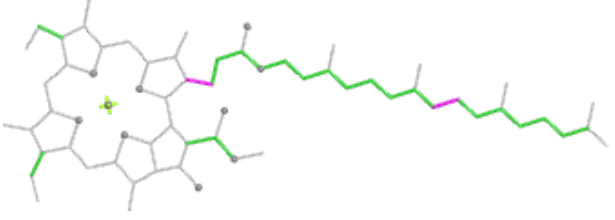
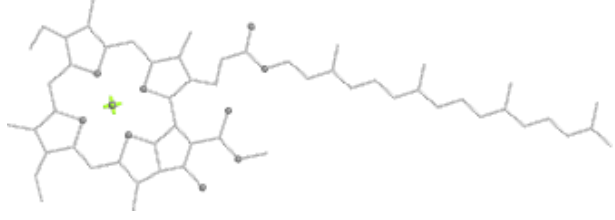
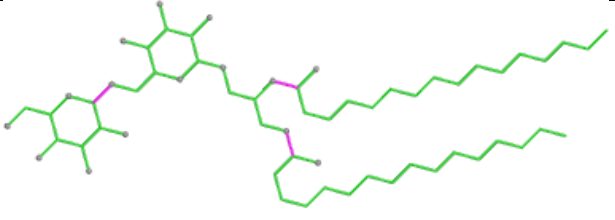
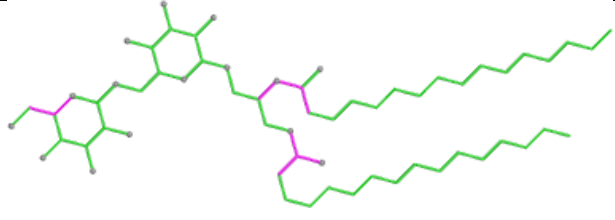
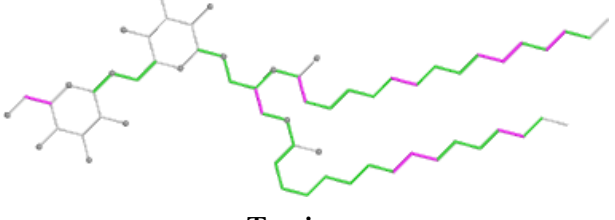
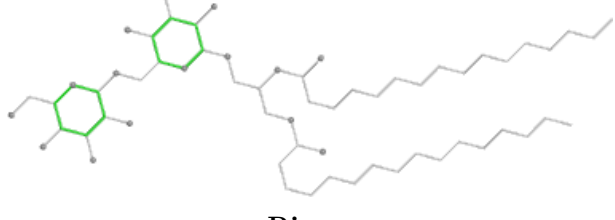
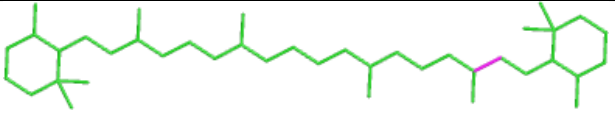
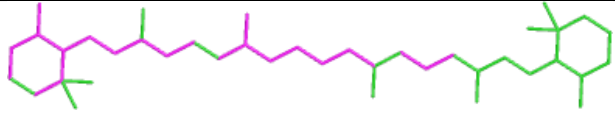
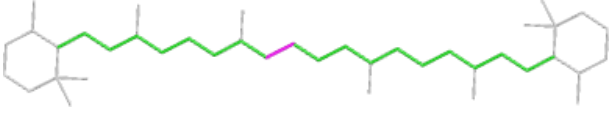
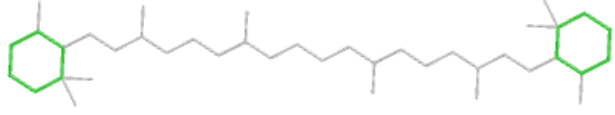


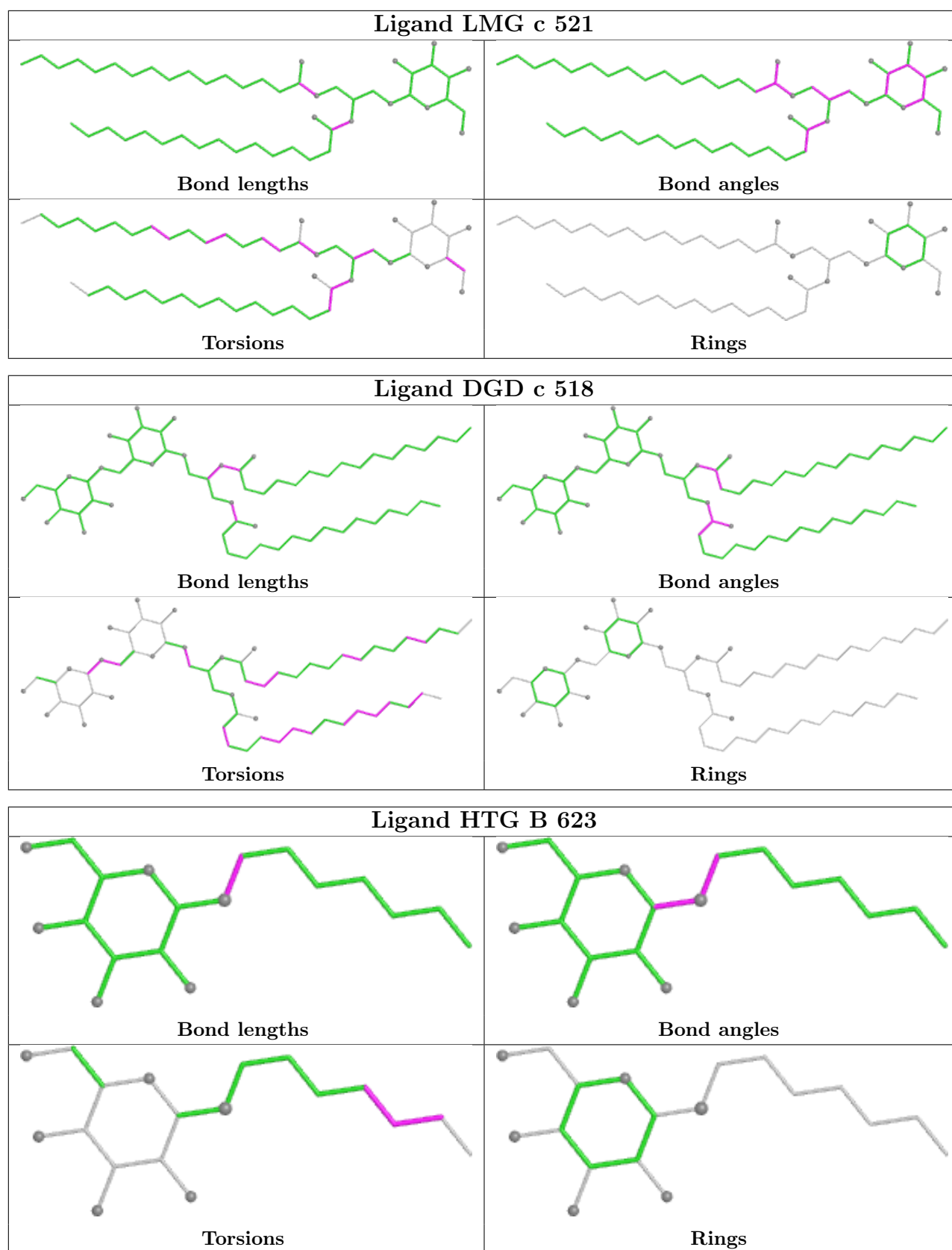


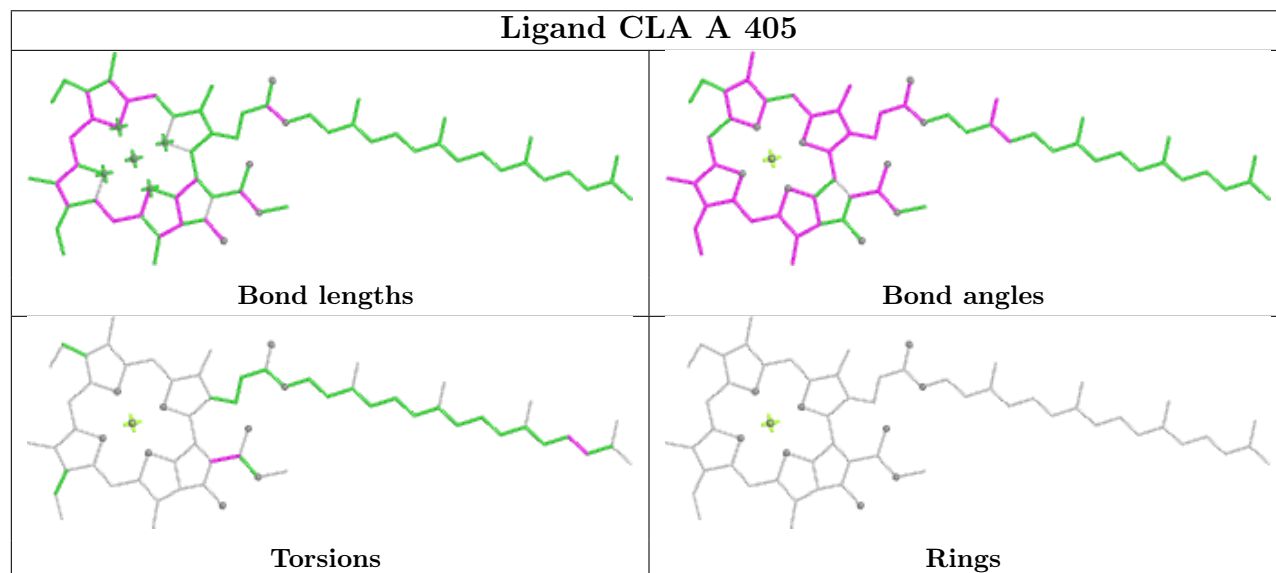
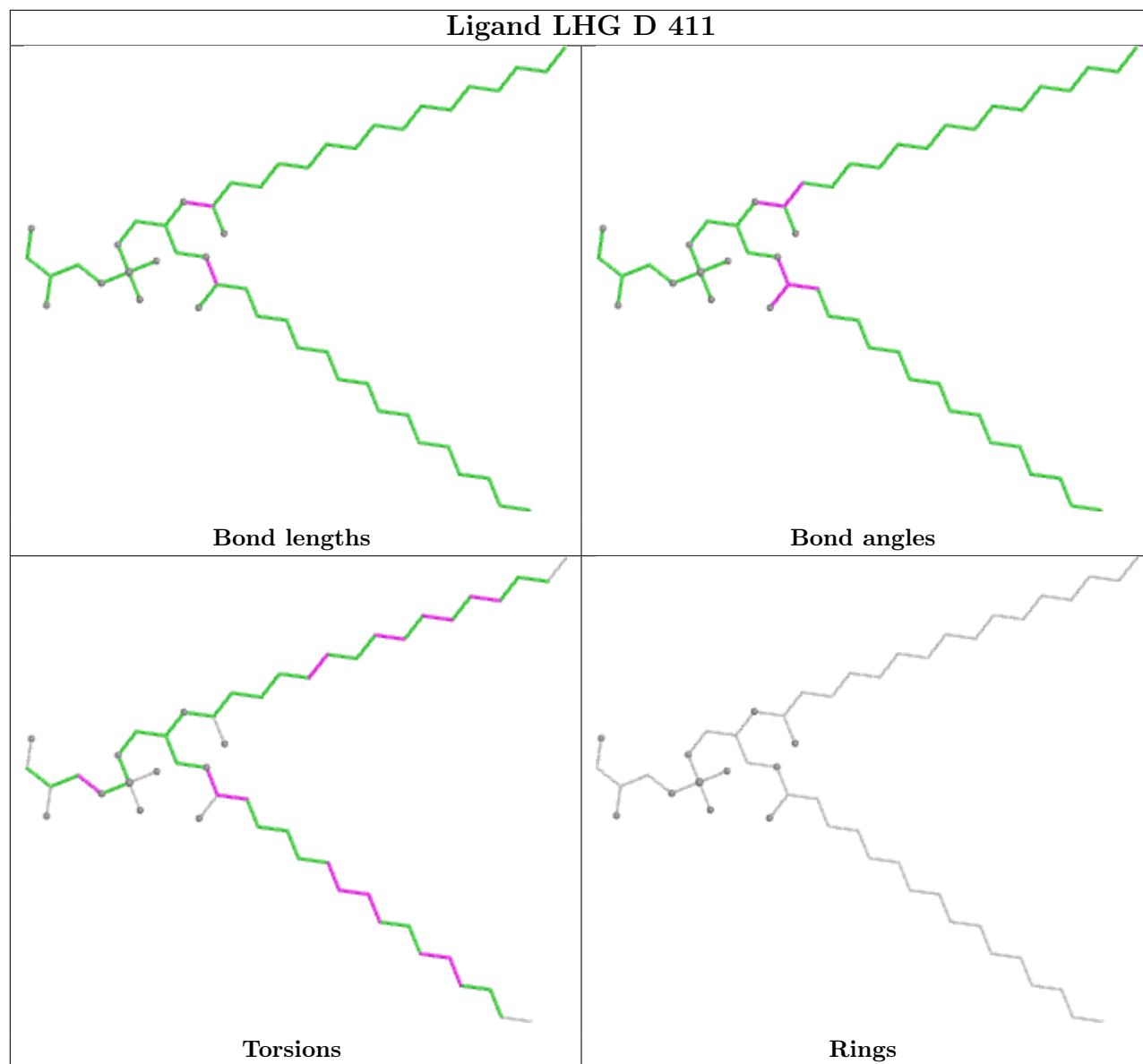
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

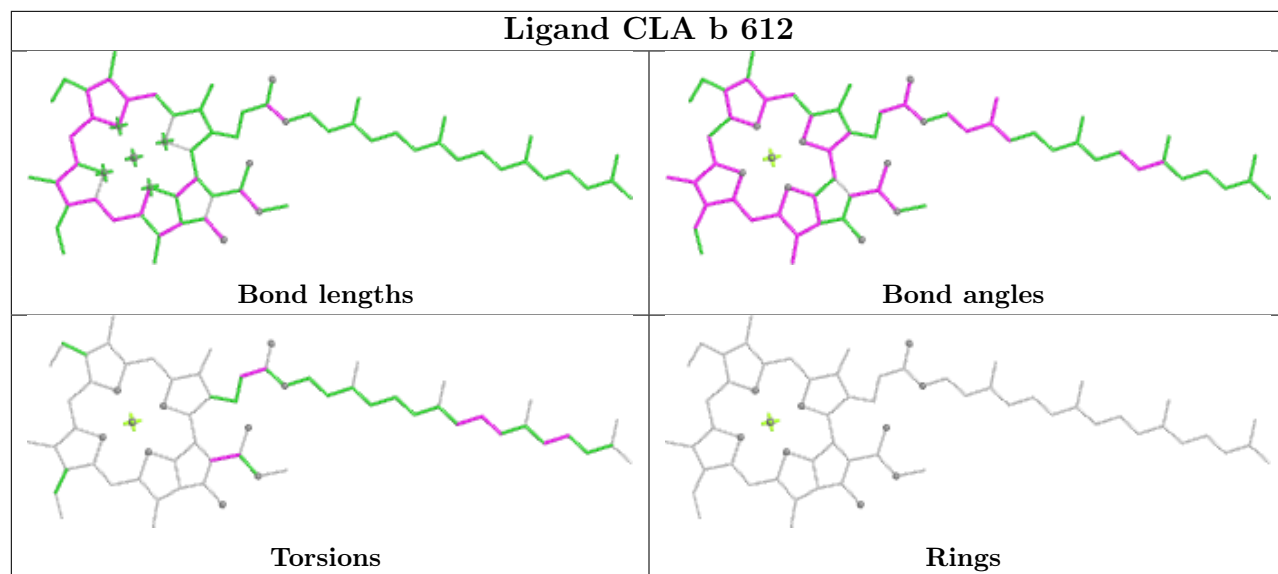
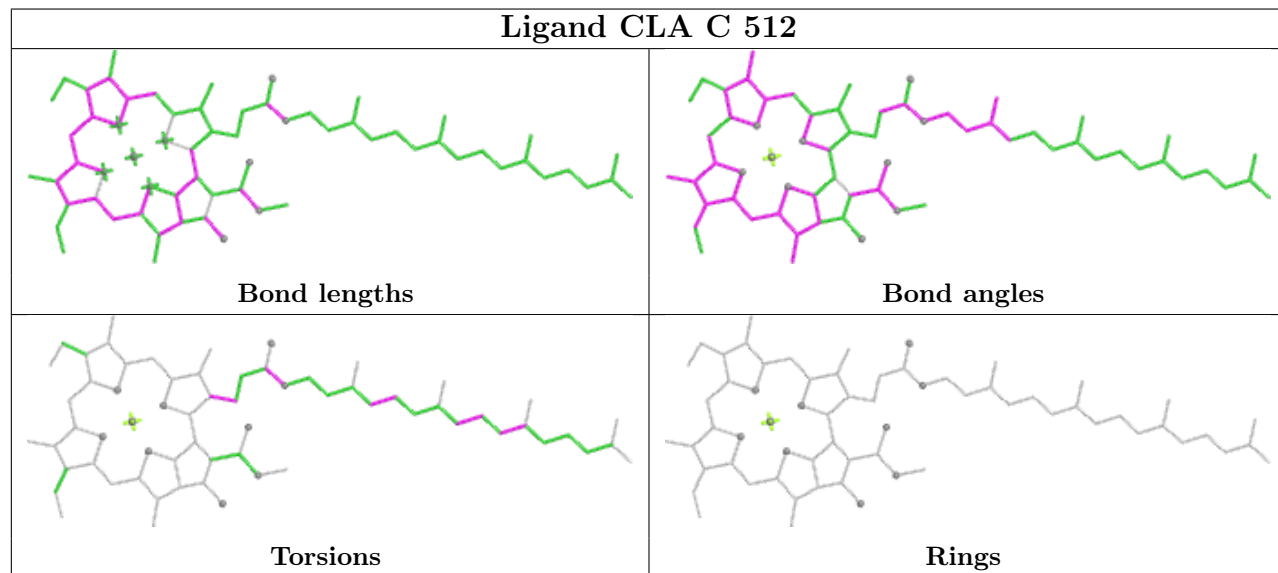
Ligand CLA c 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

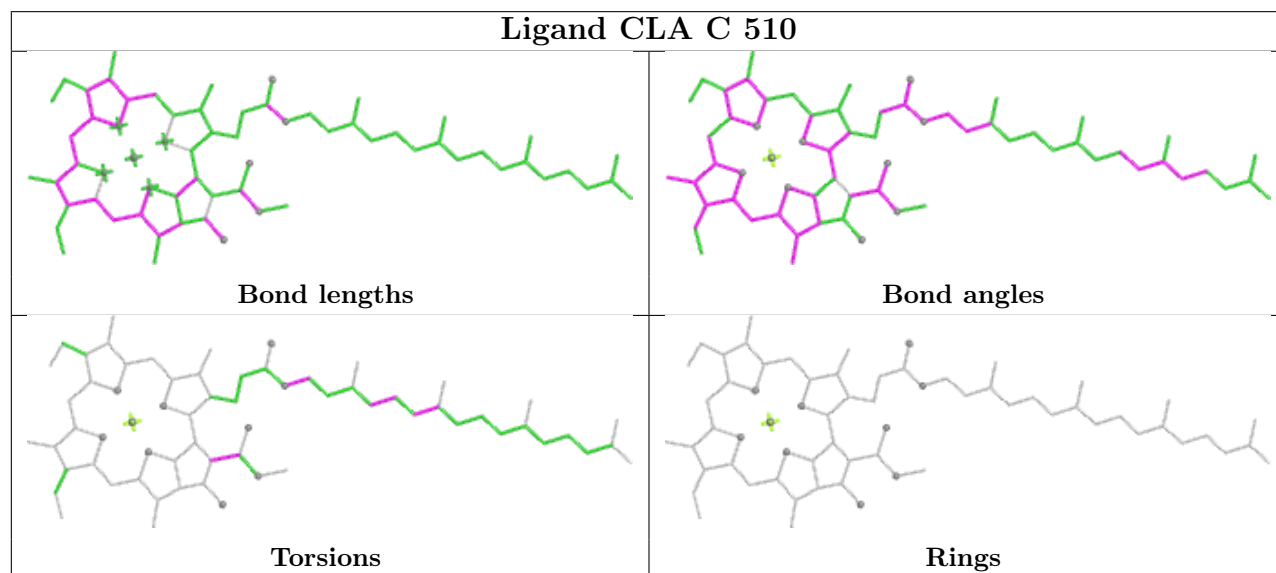
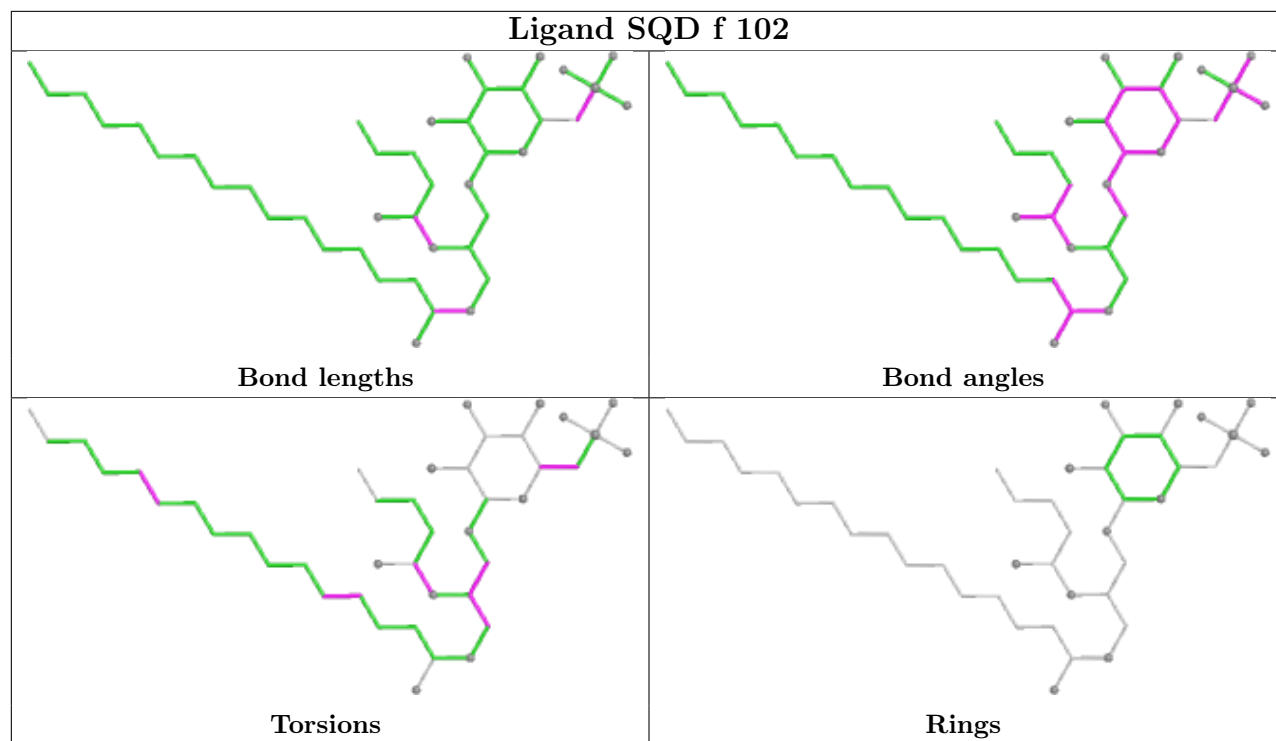
Ligand LMG C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

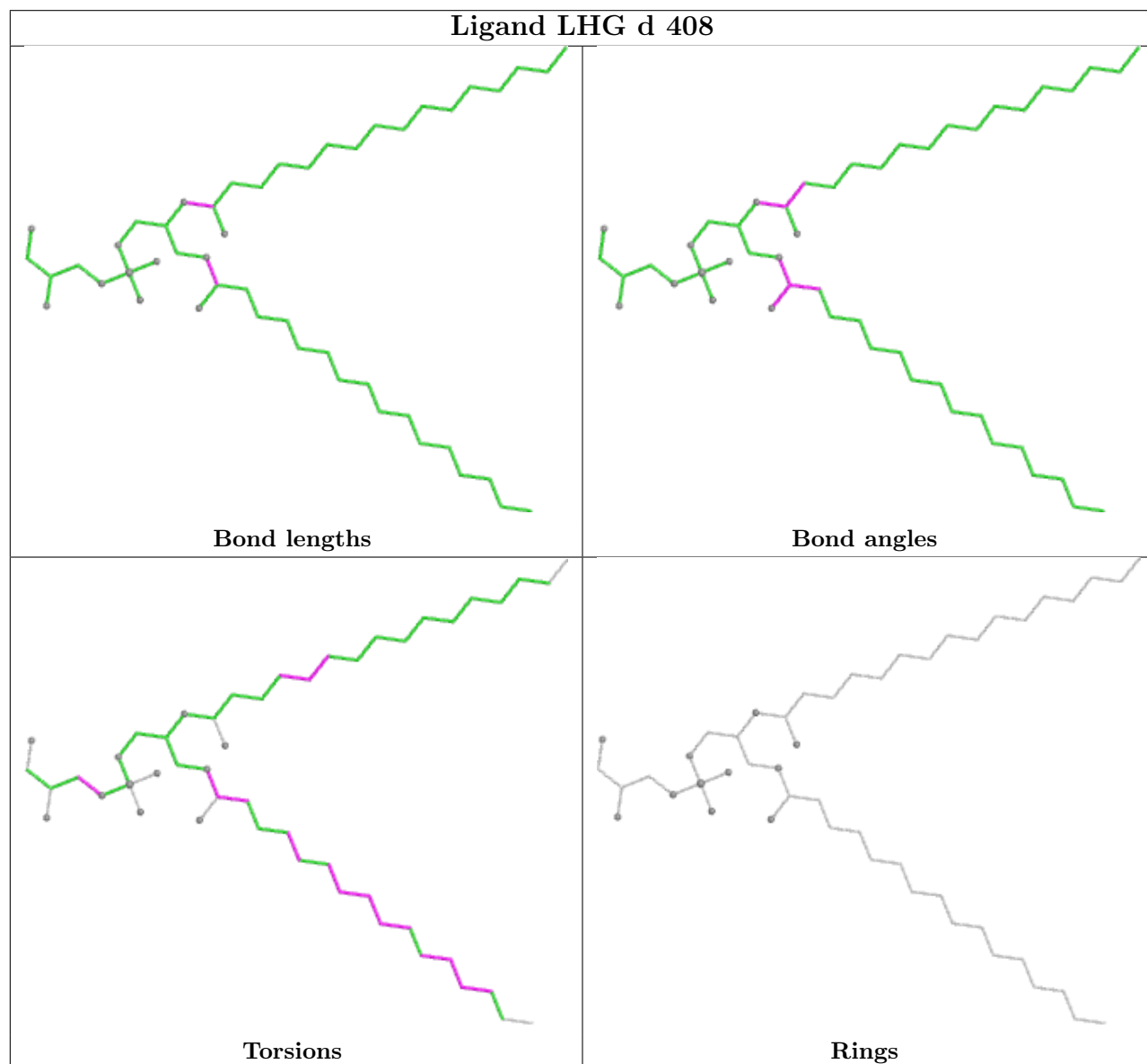
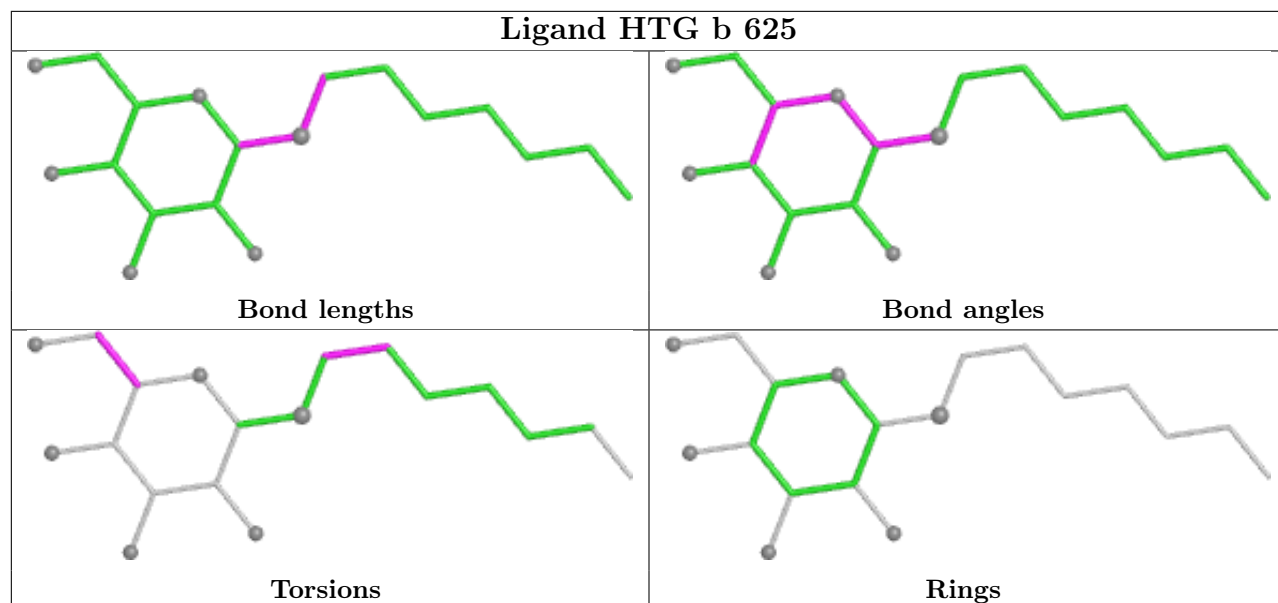
Ligand CLA B 611	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD H 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR T 101	
 Bond lengths	 Bond angles
 Torsions	 Rings



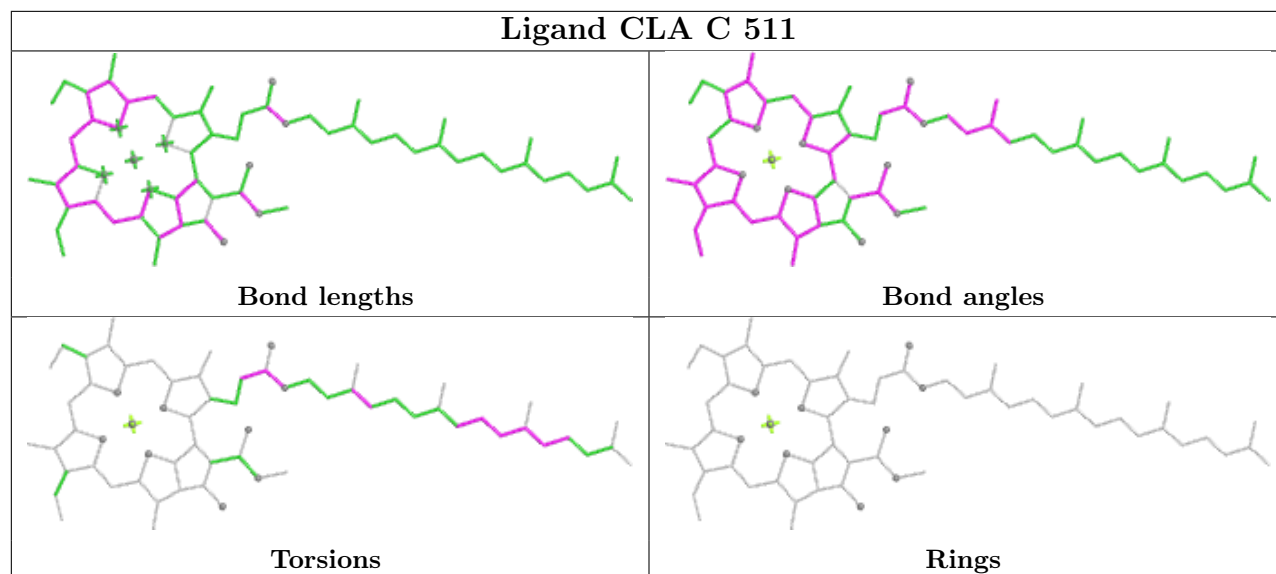


Ligand CLA b 612**Ligand CLA C 512**

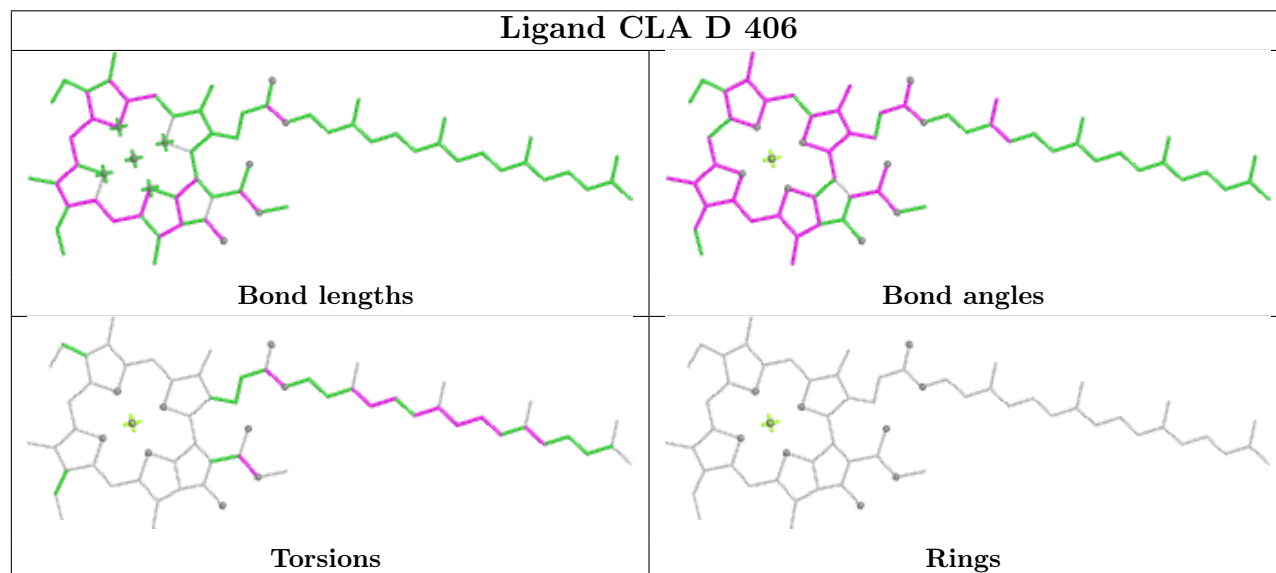


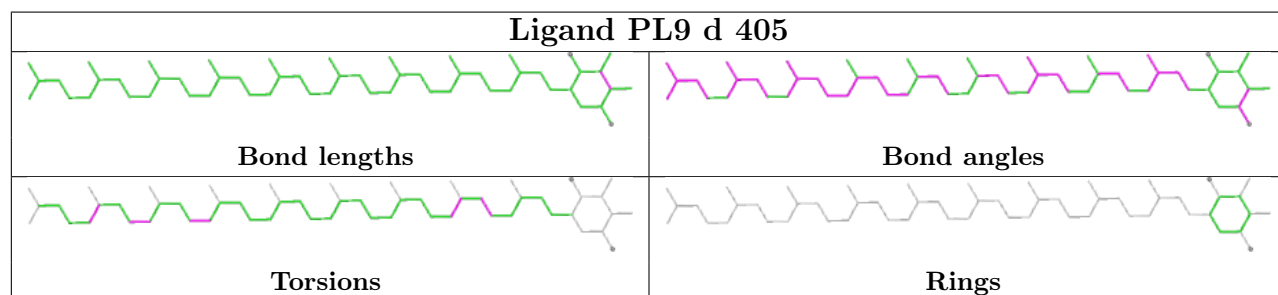
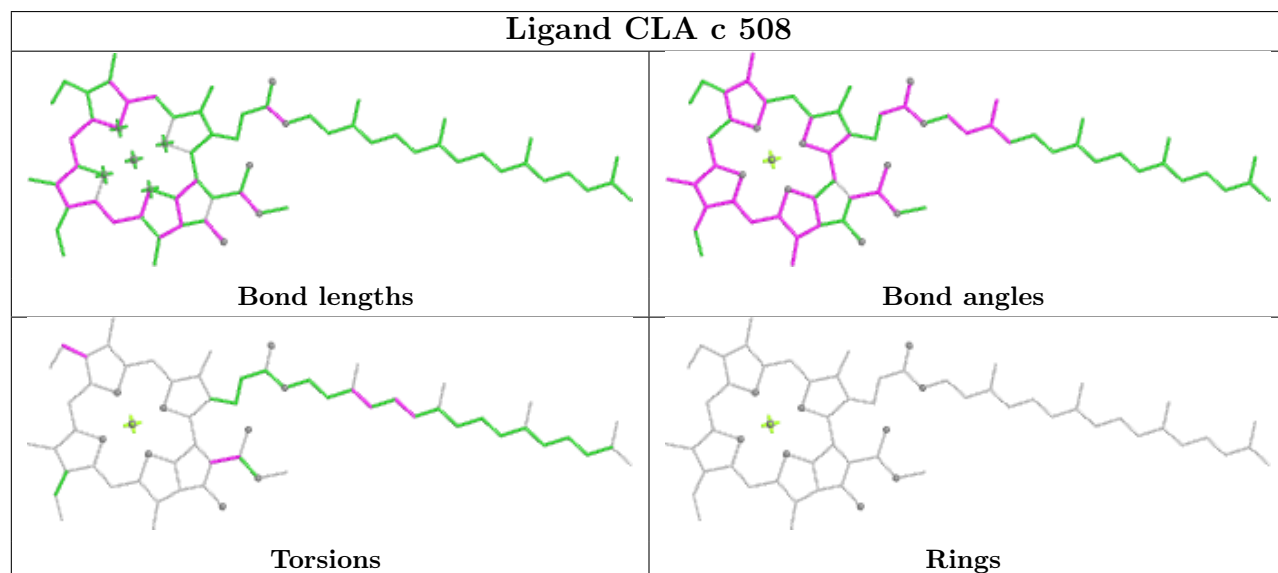
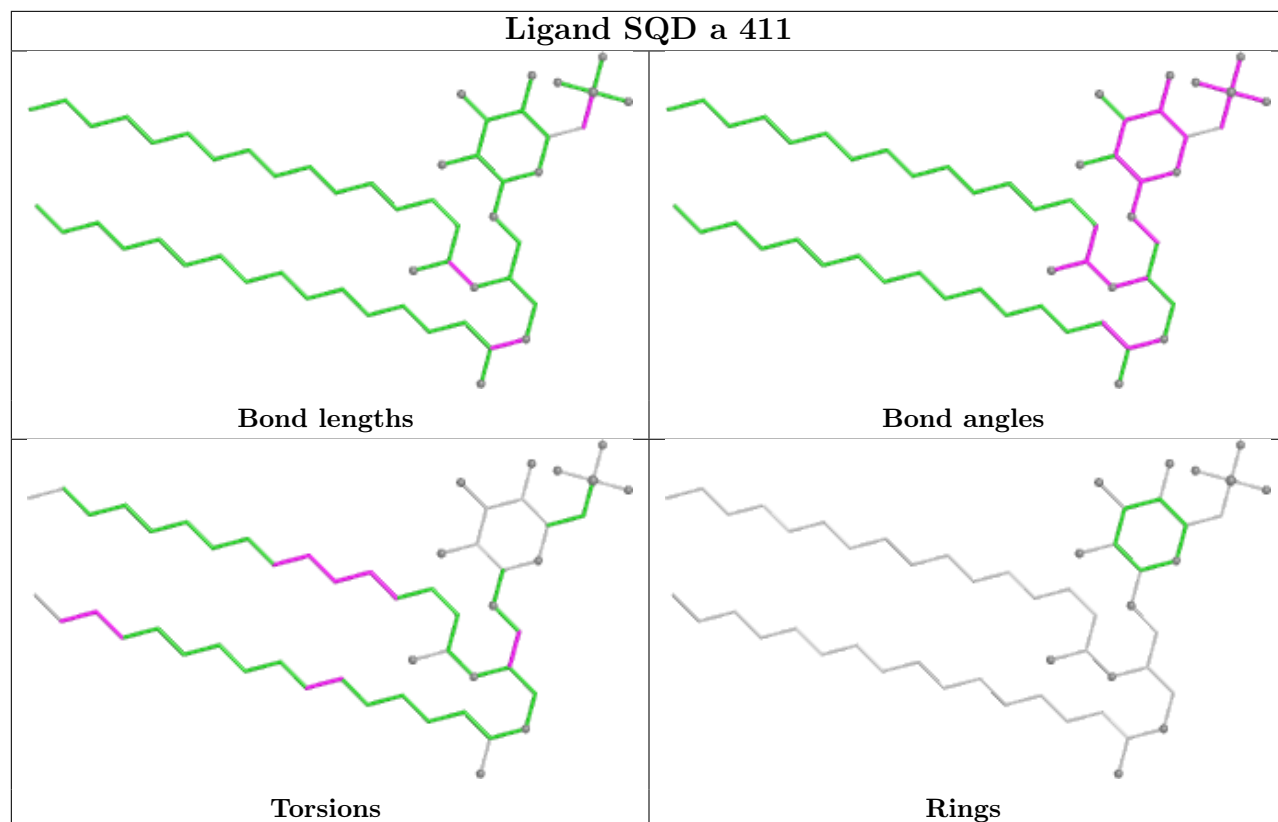


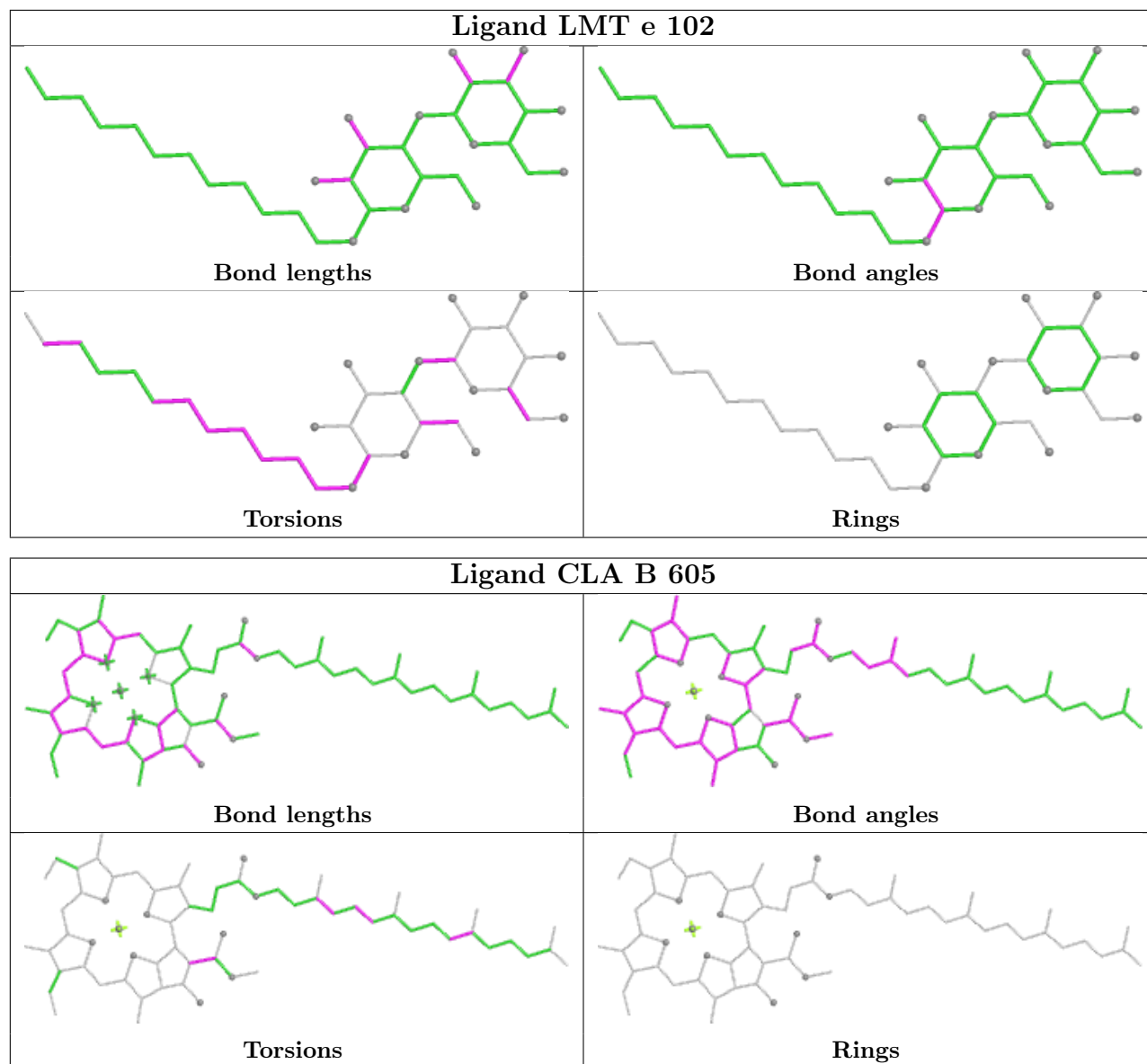
Ligand CLA C 511

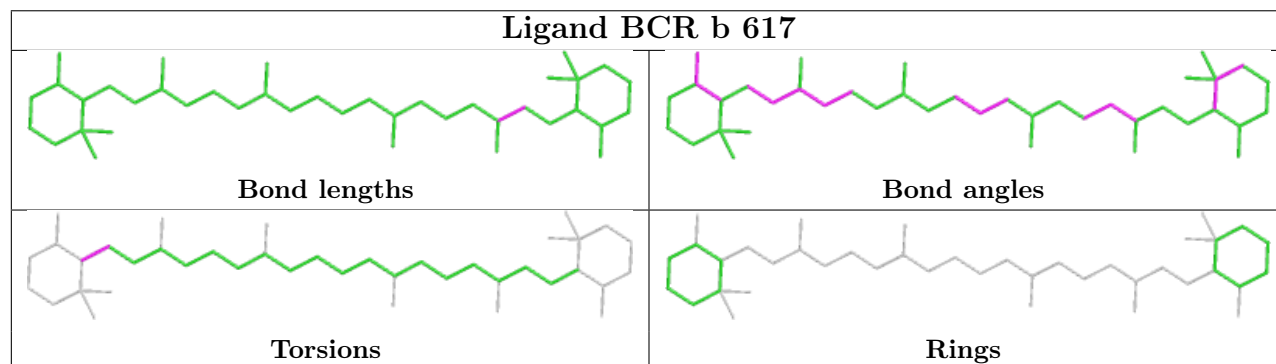
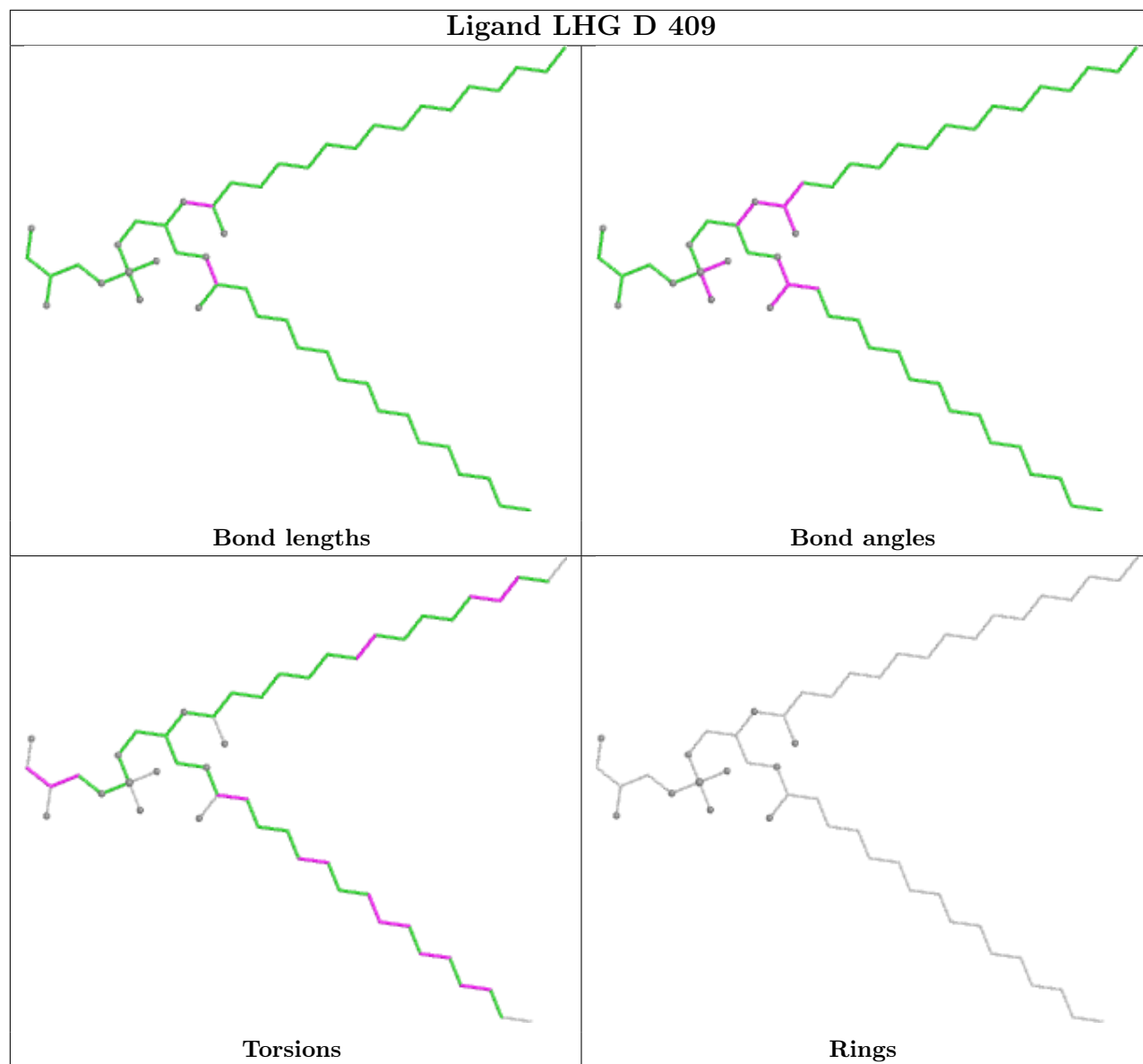


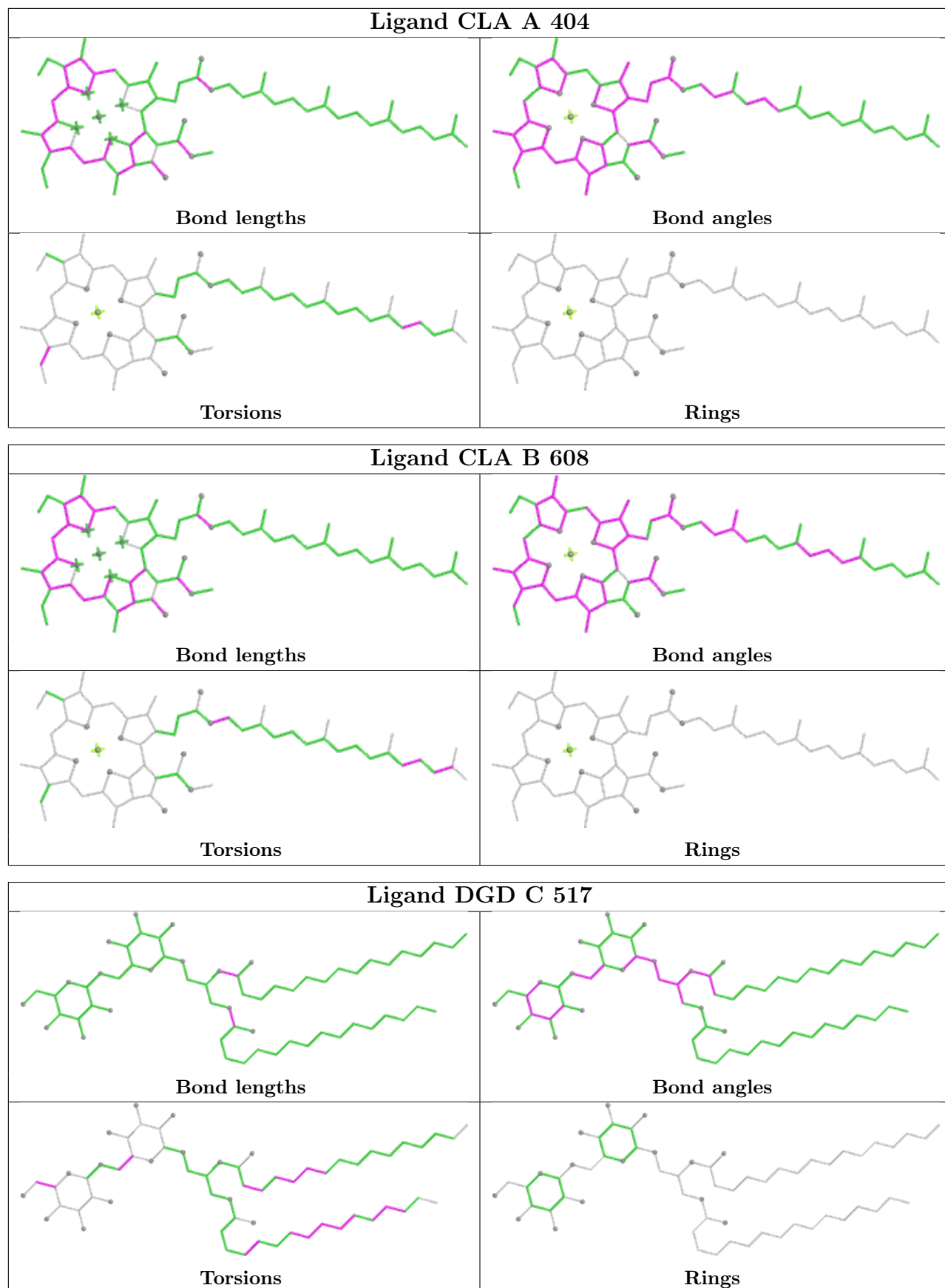
Ligand CLA D 406

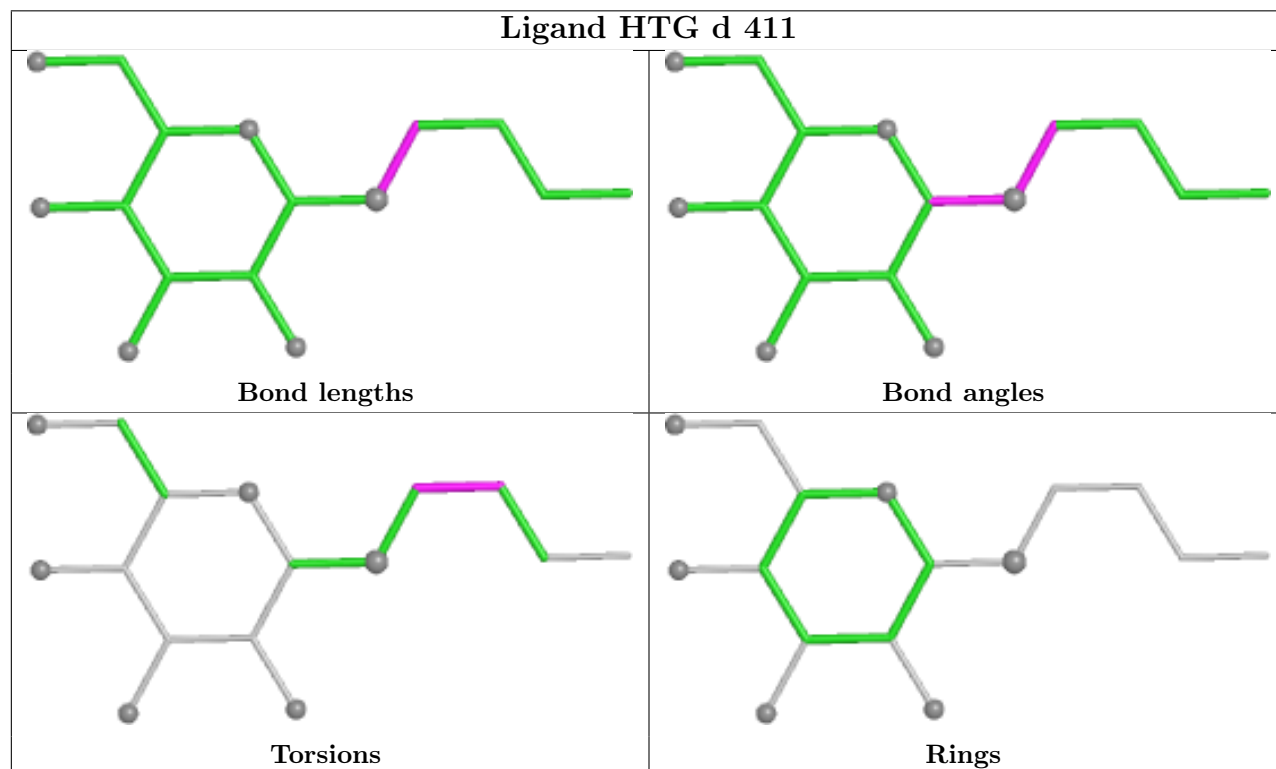
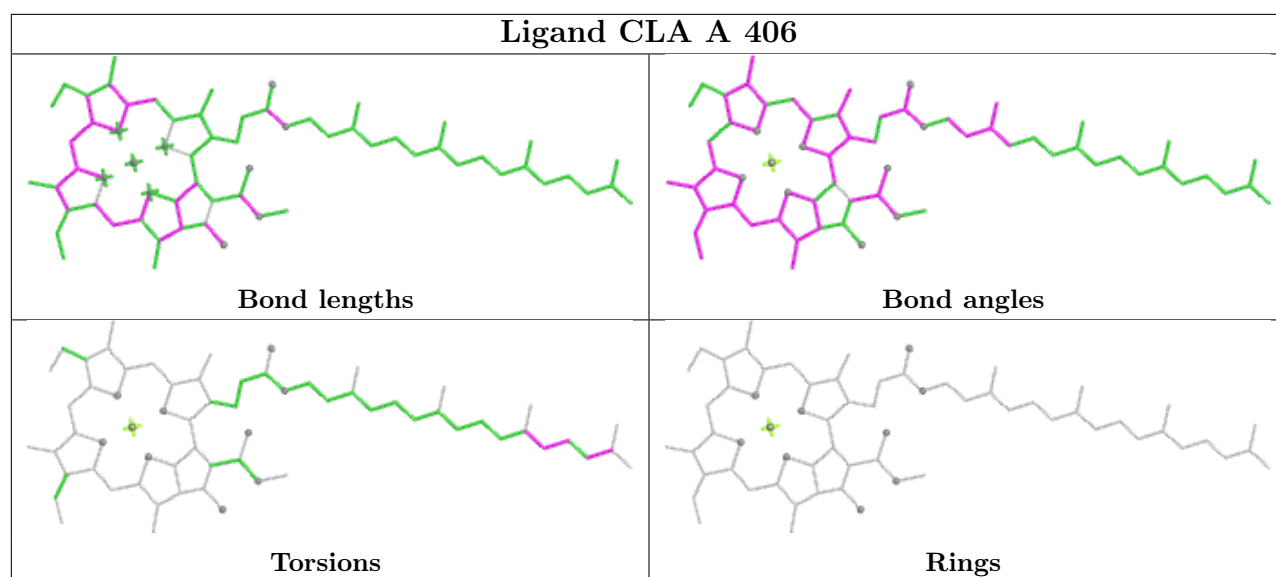




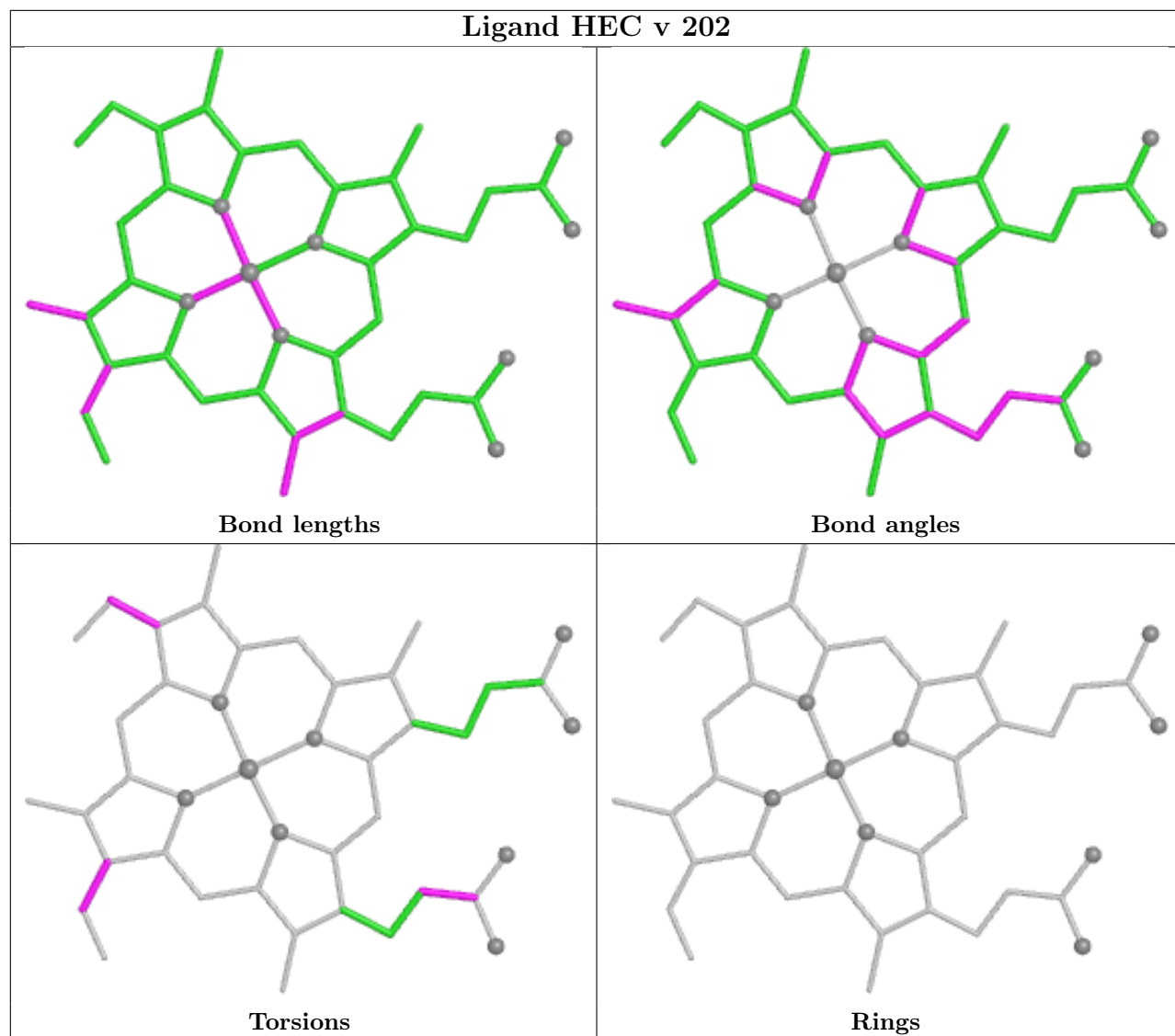




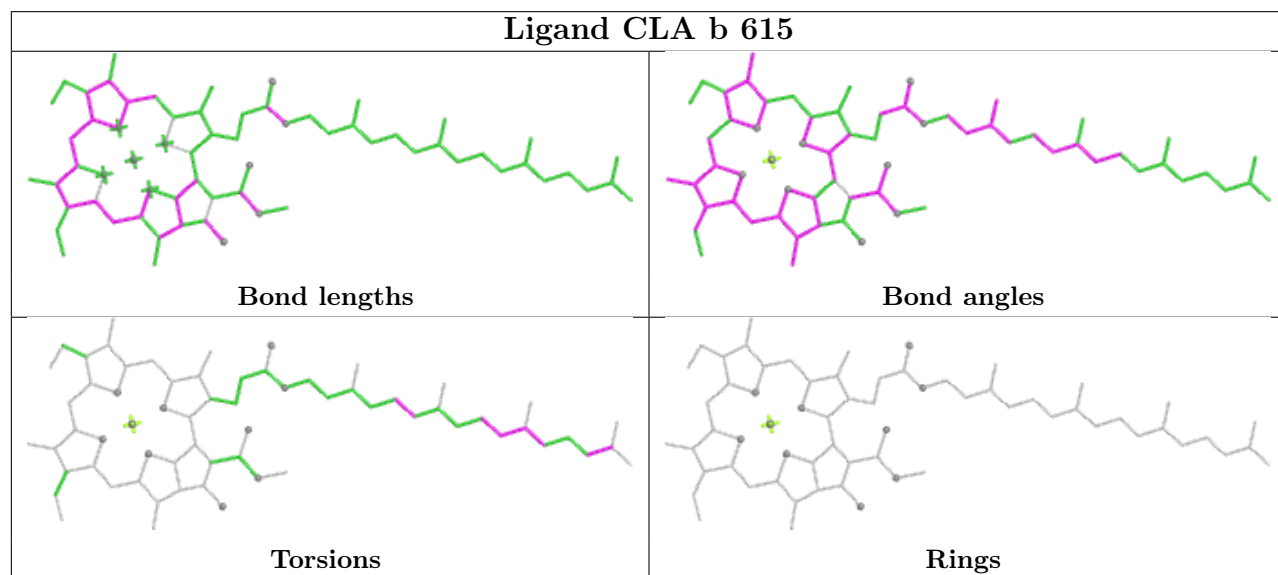


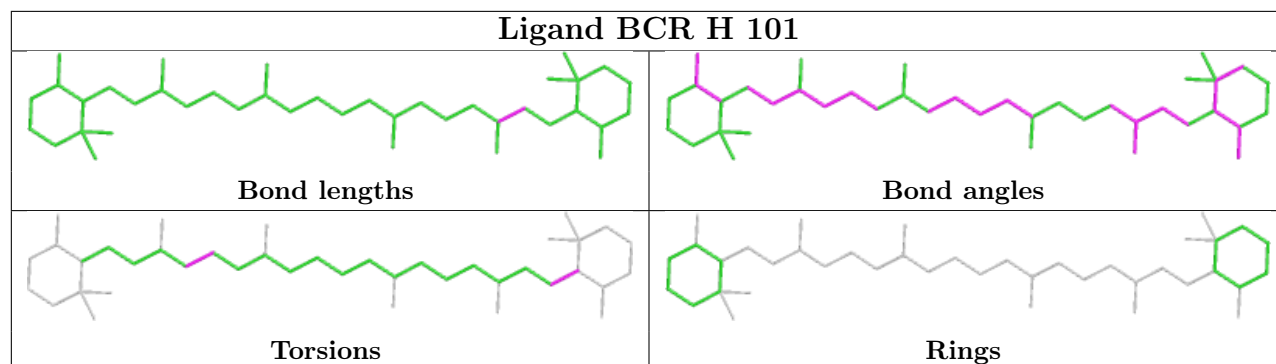
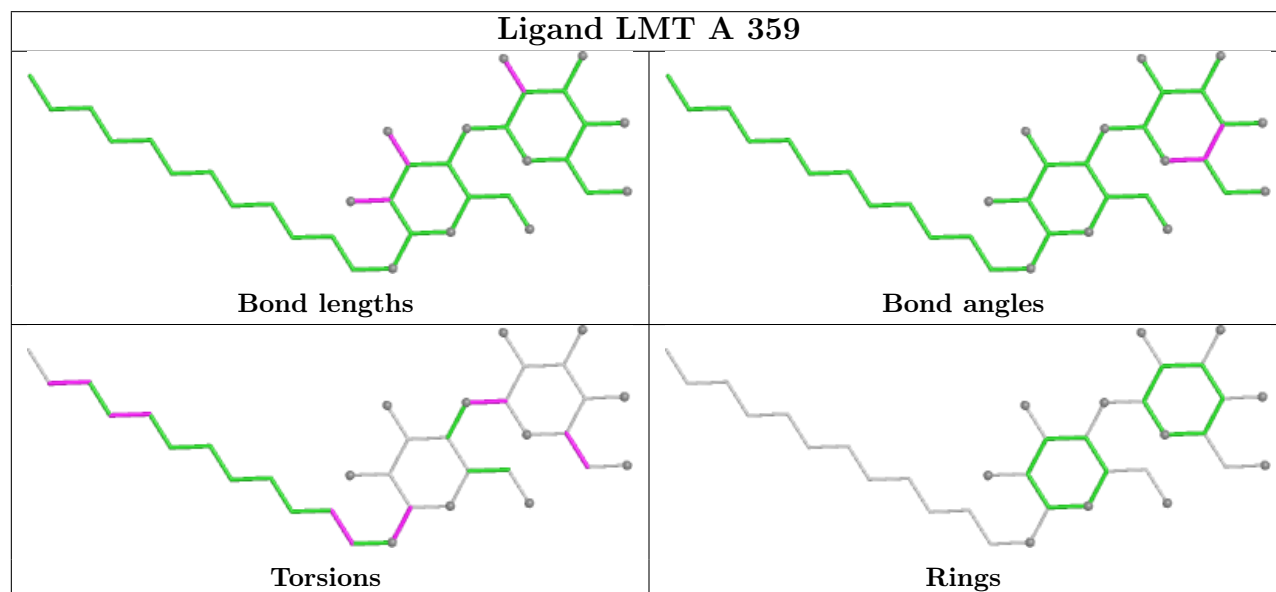
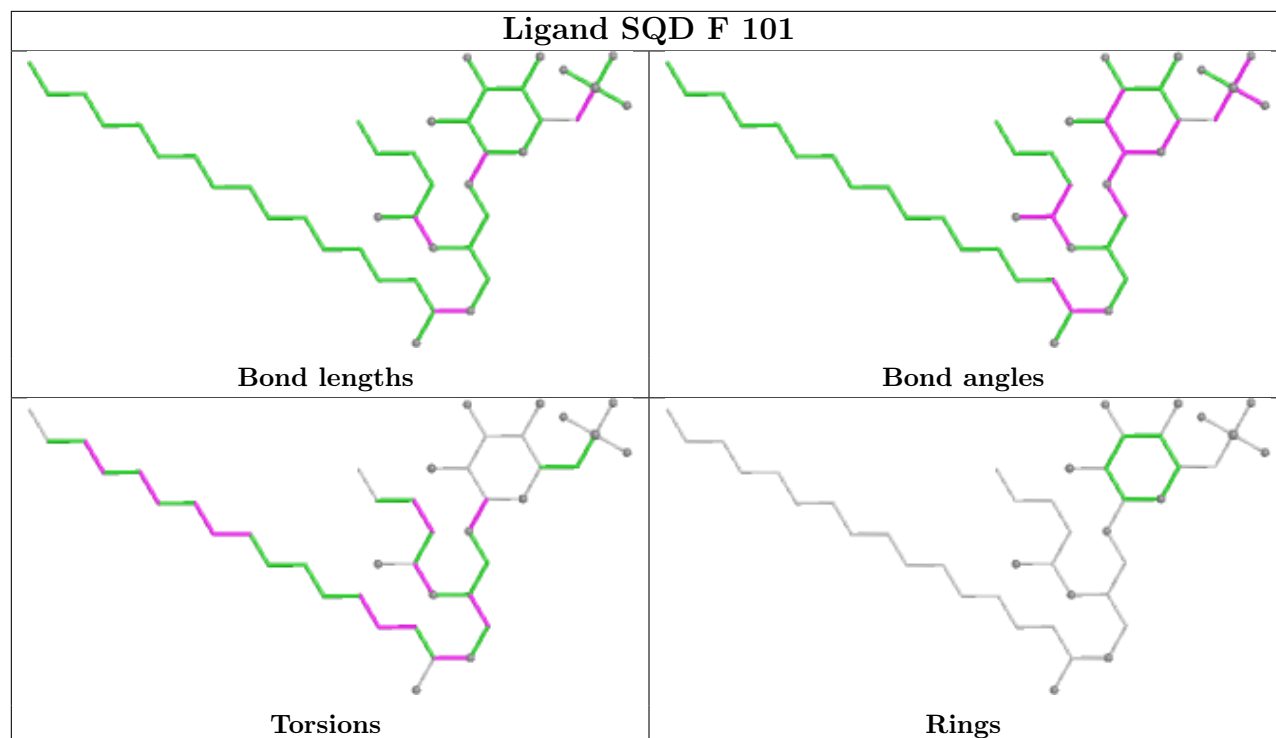


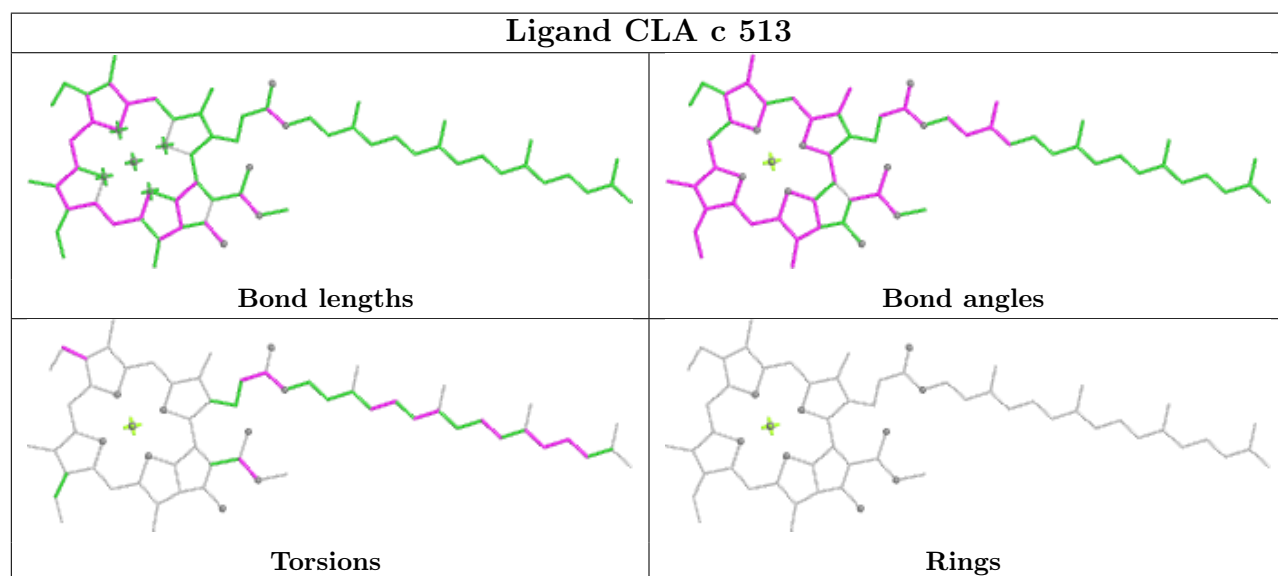
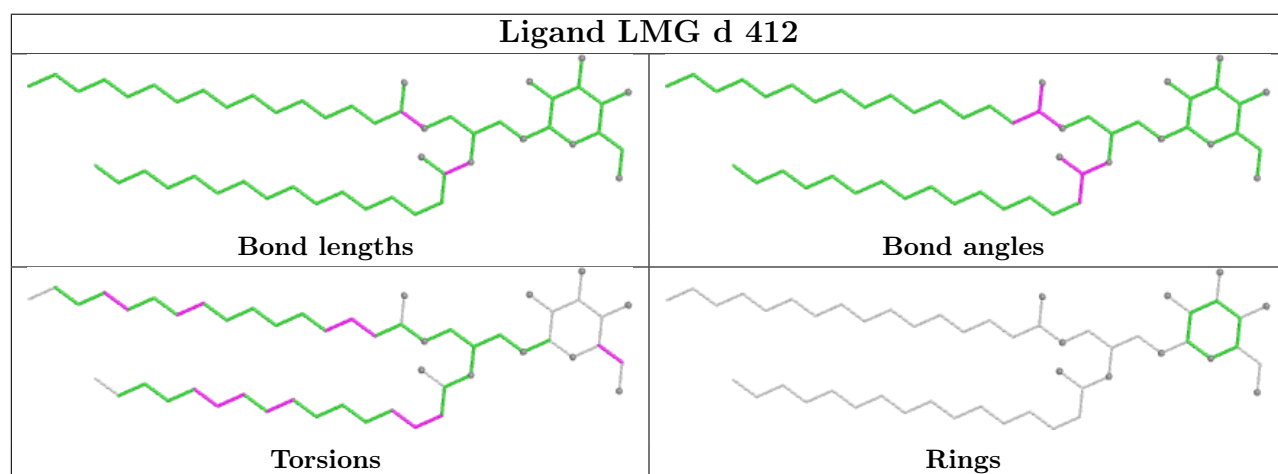
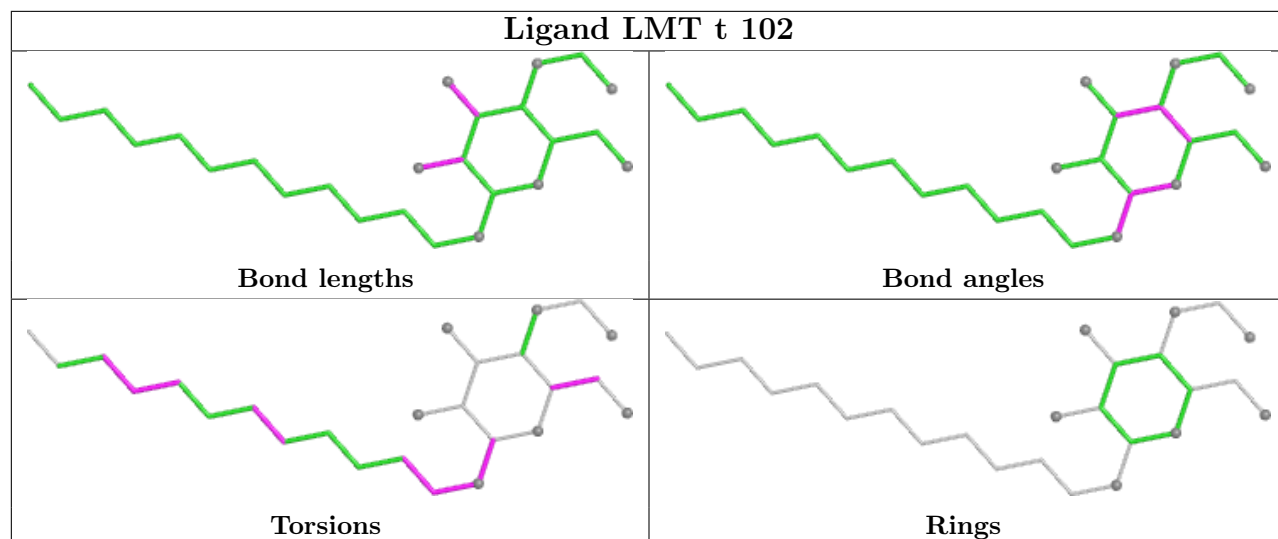
Ligand HEC v 202

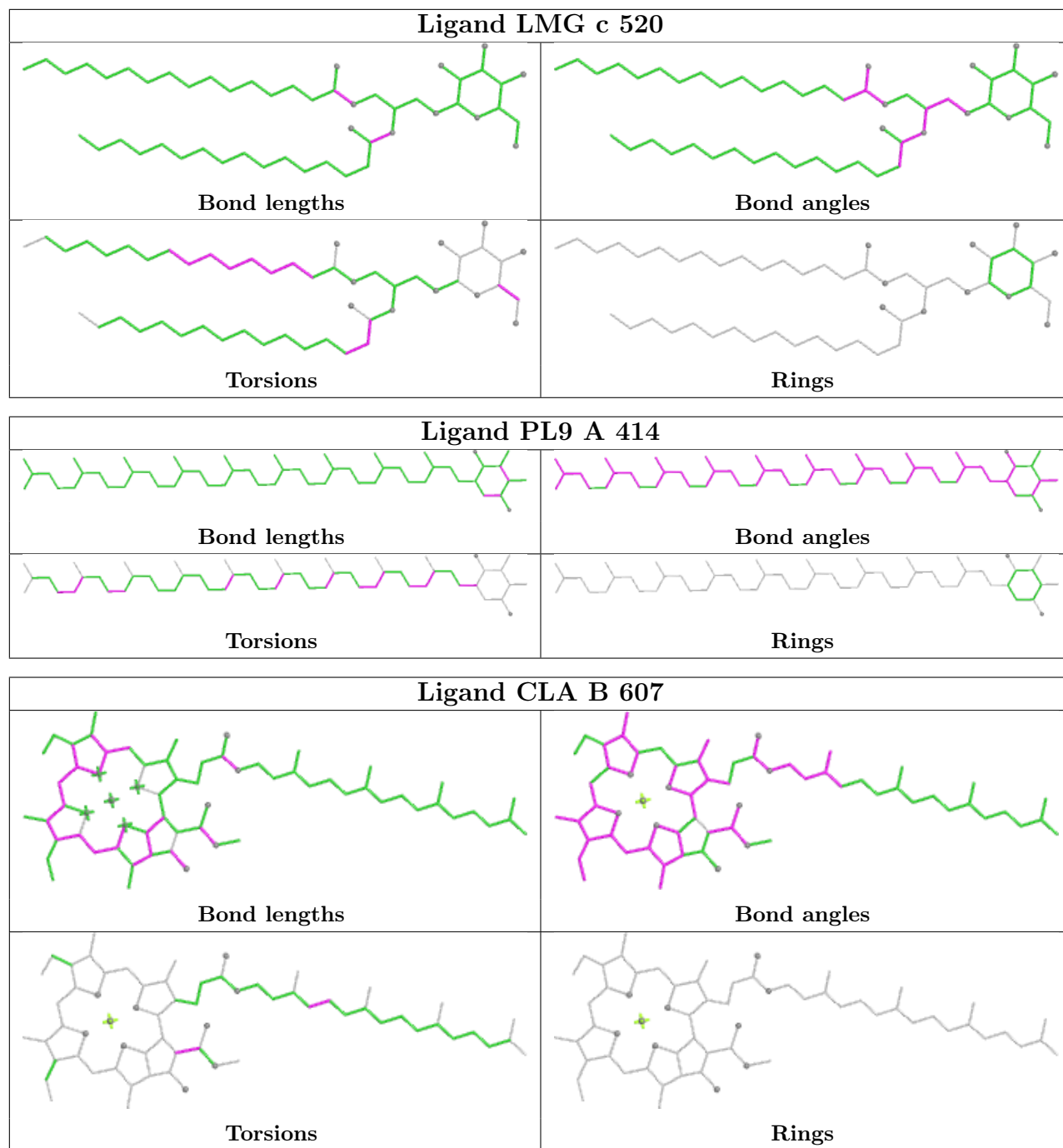


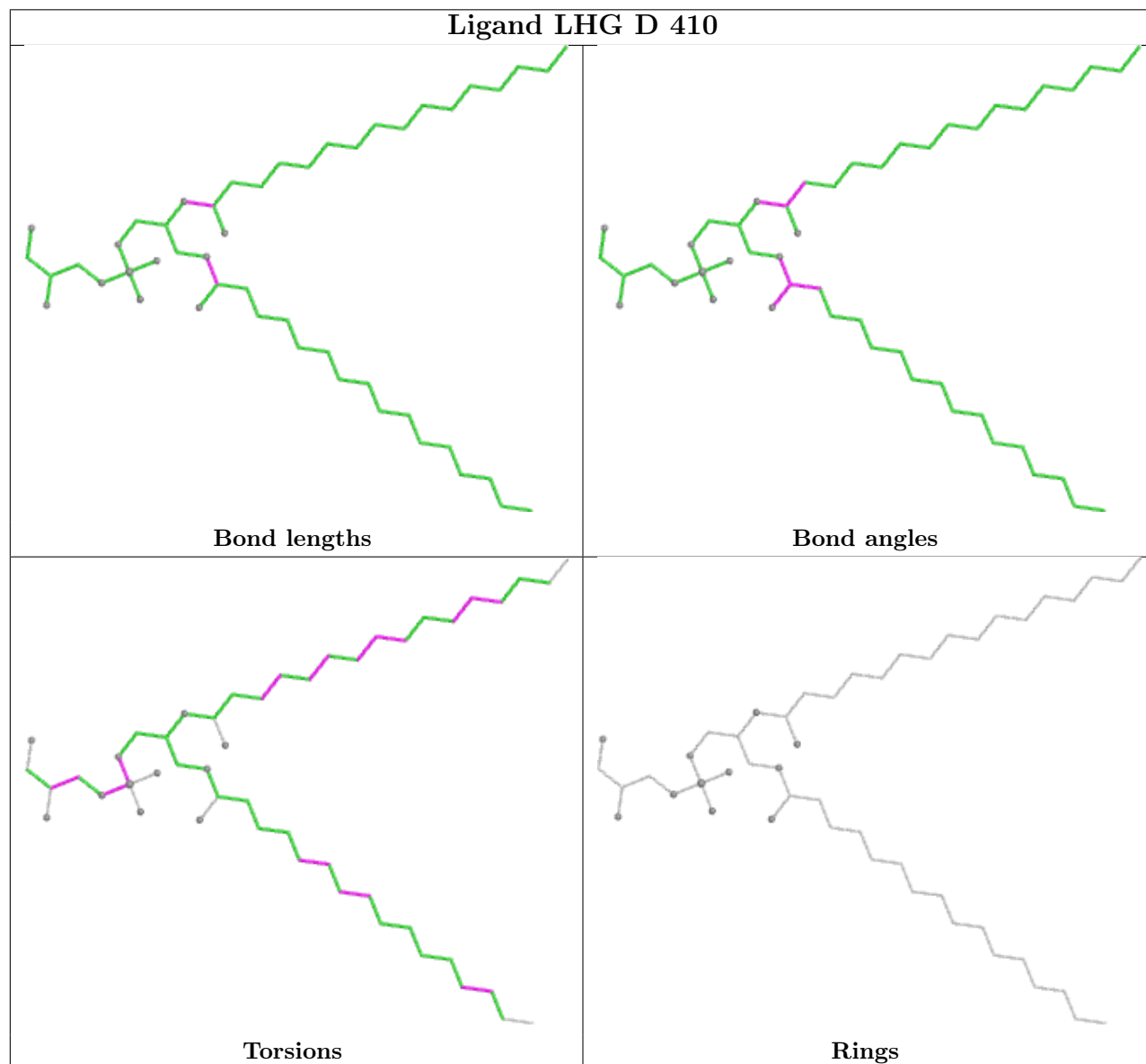
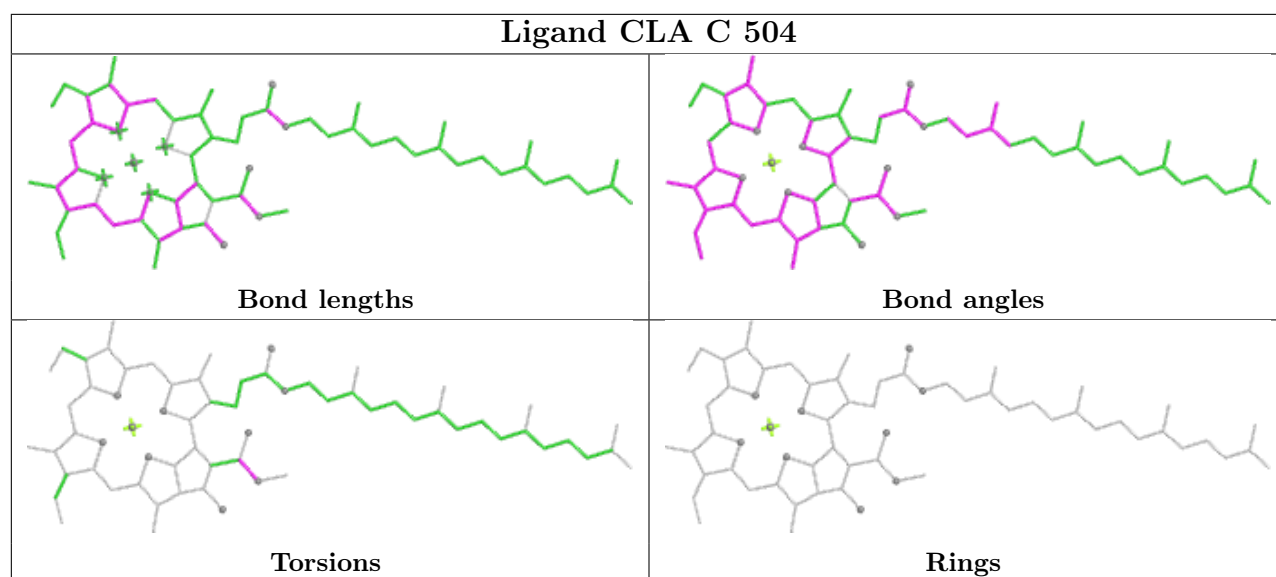
Ligand CLA b 615

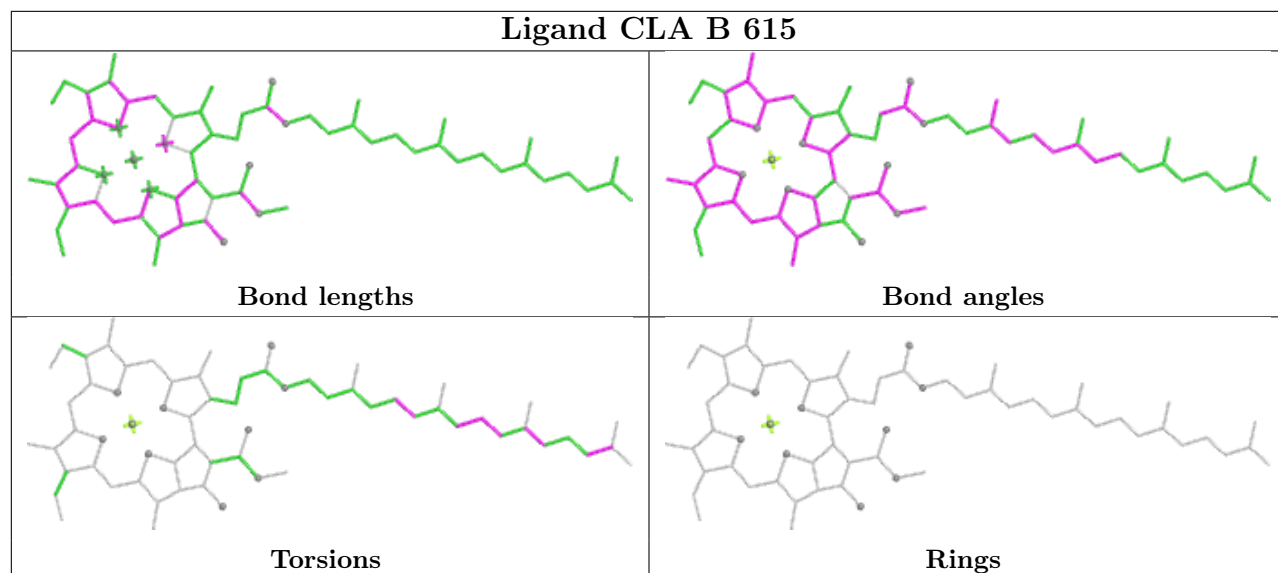
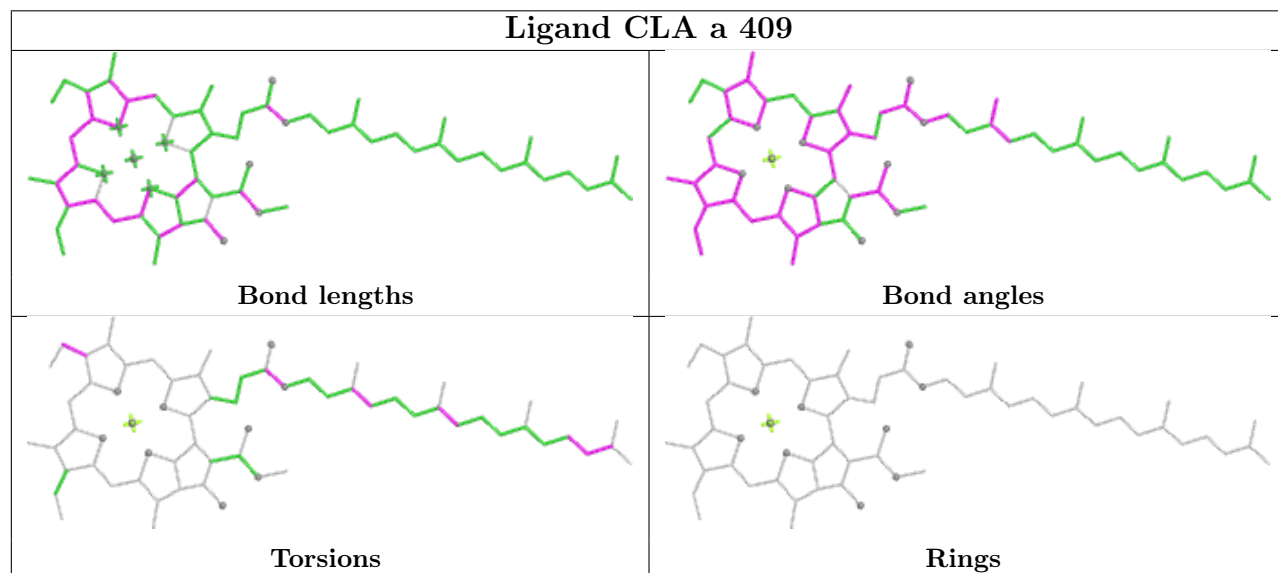
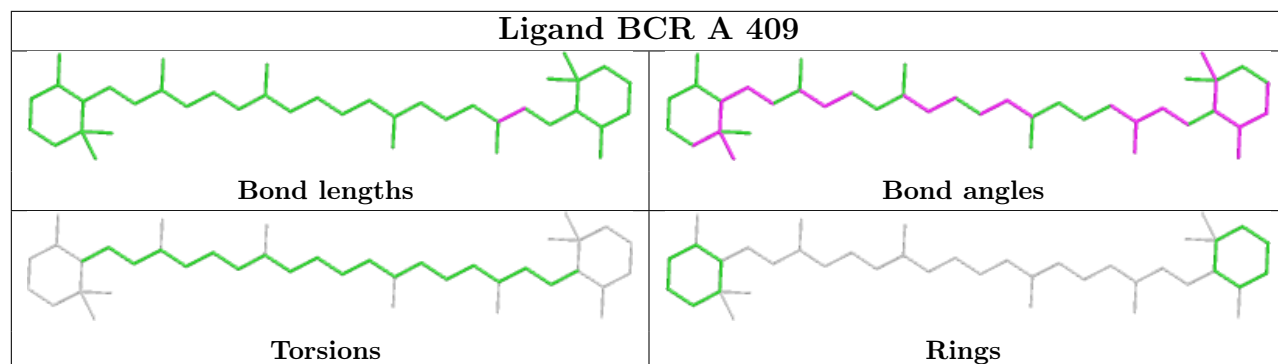


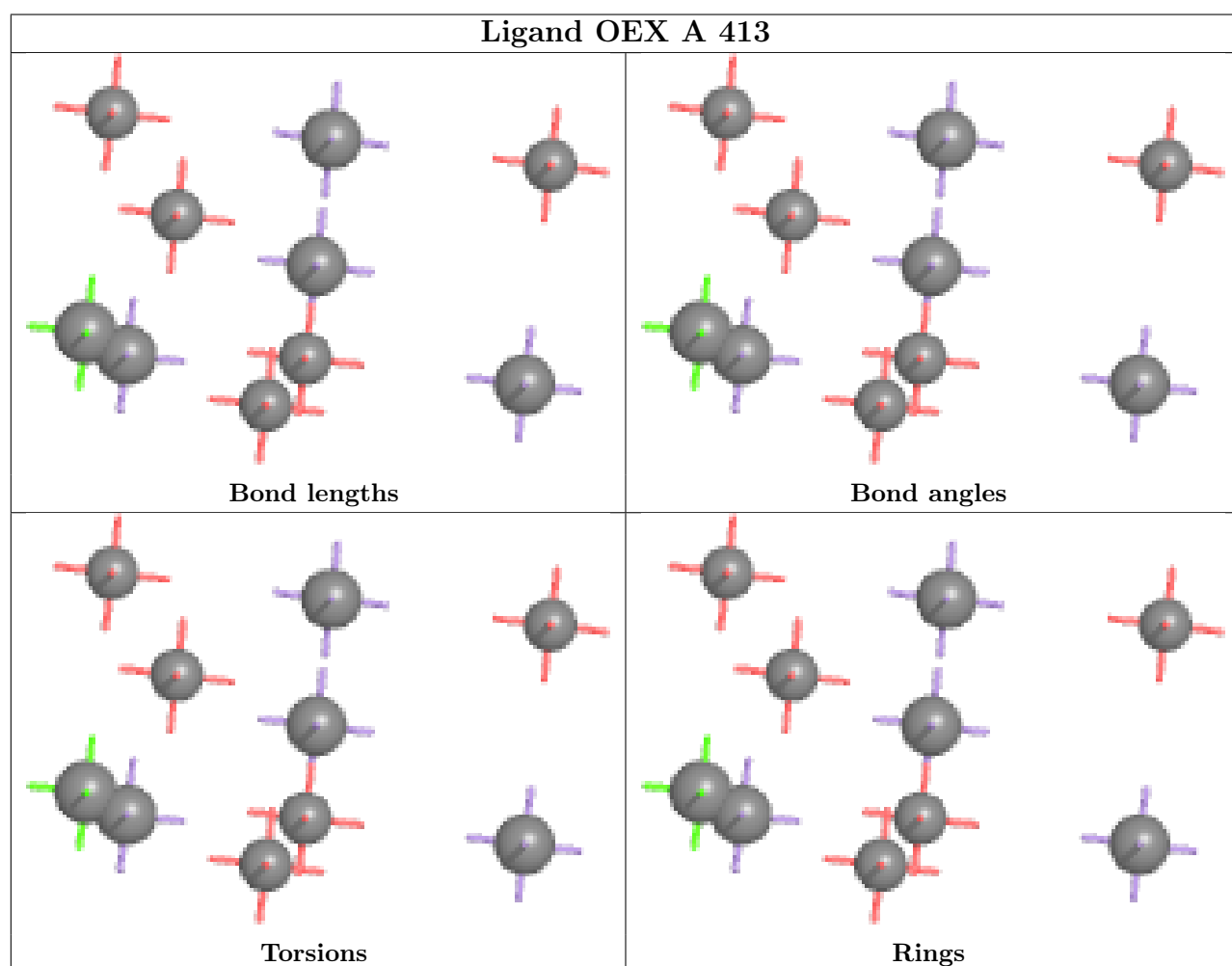
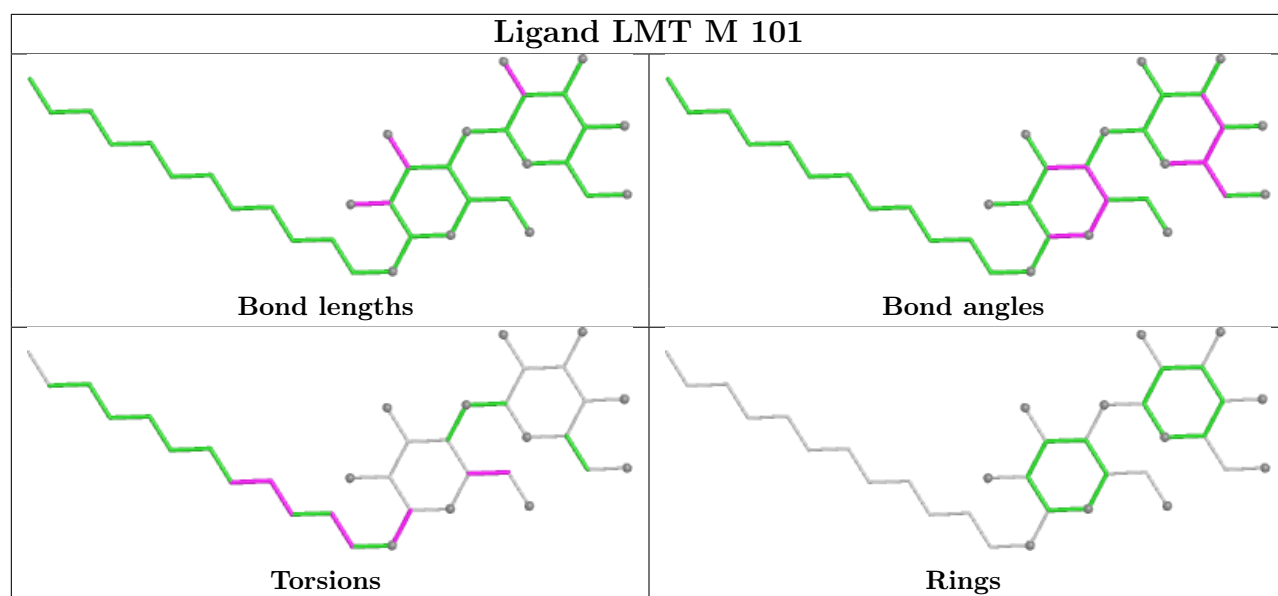


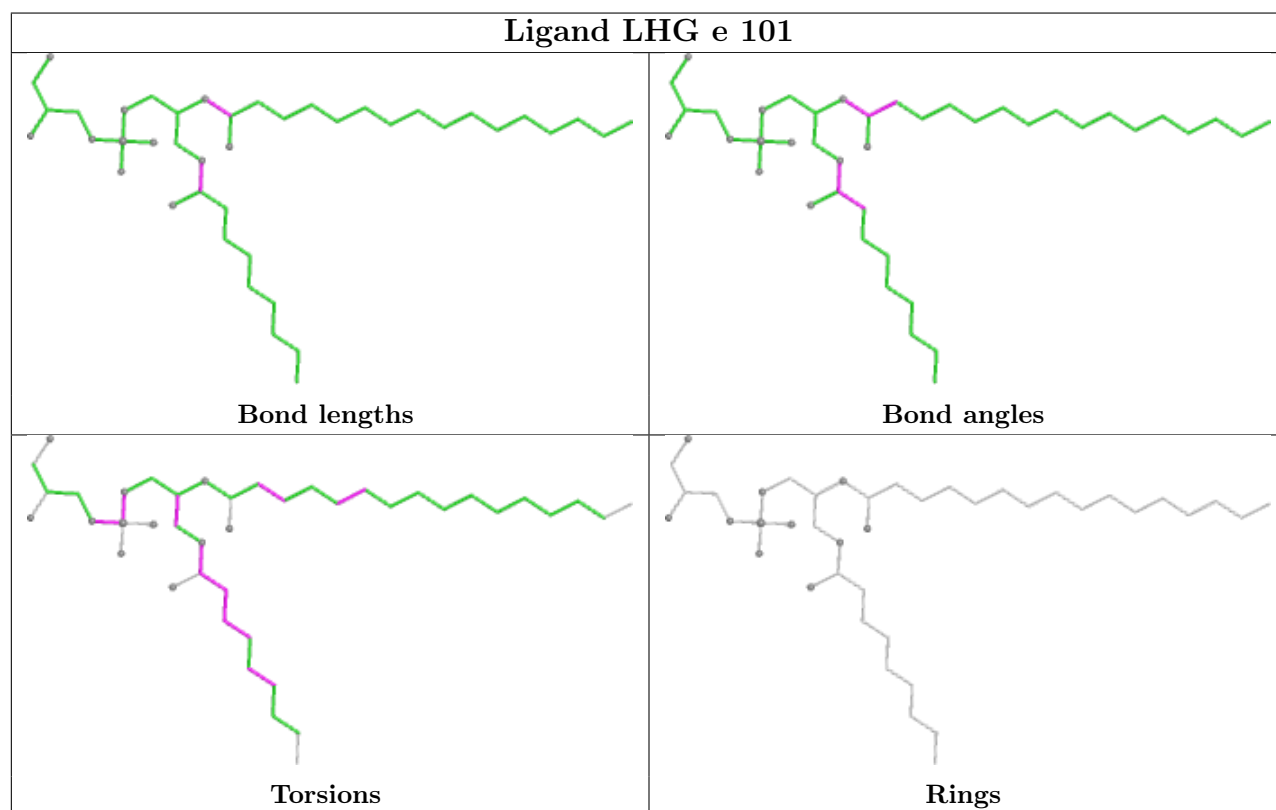
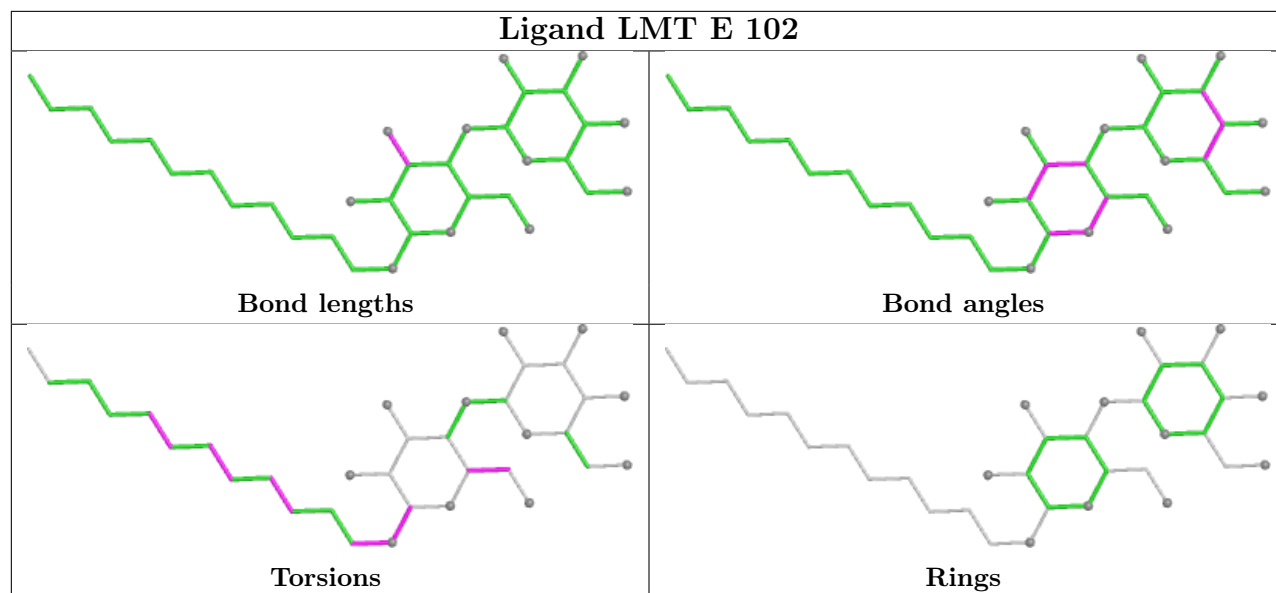


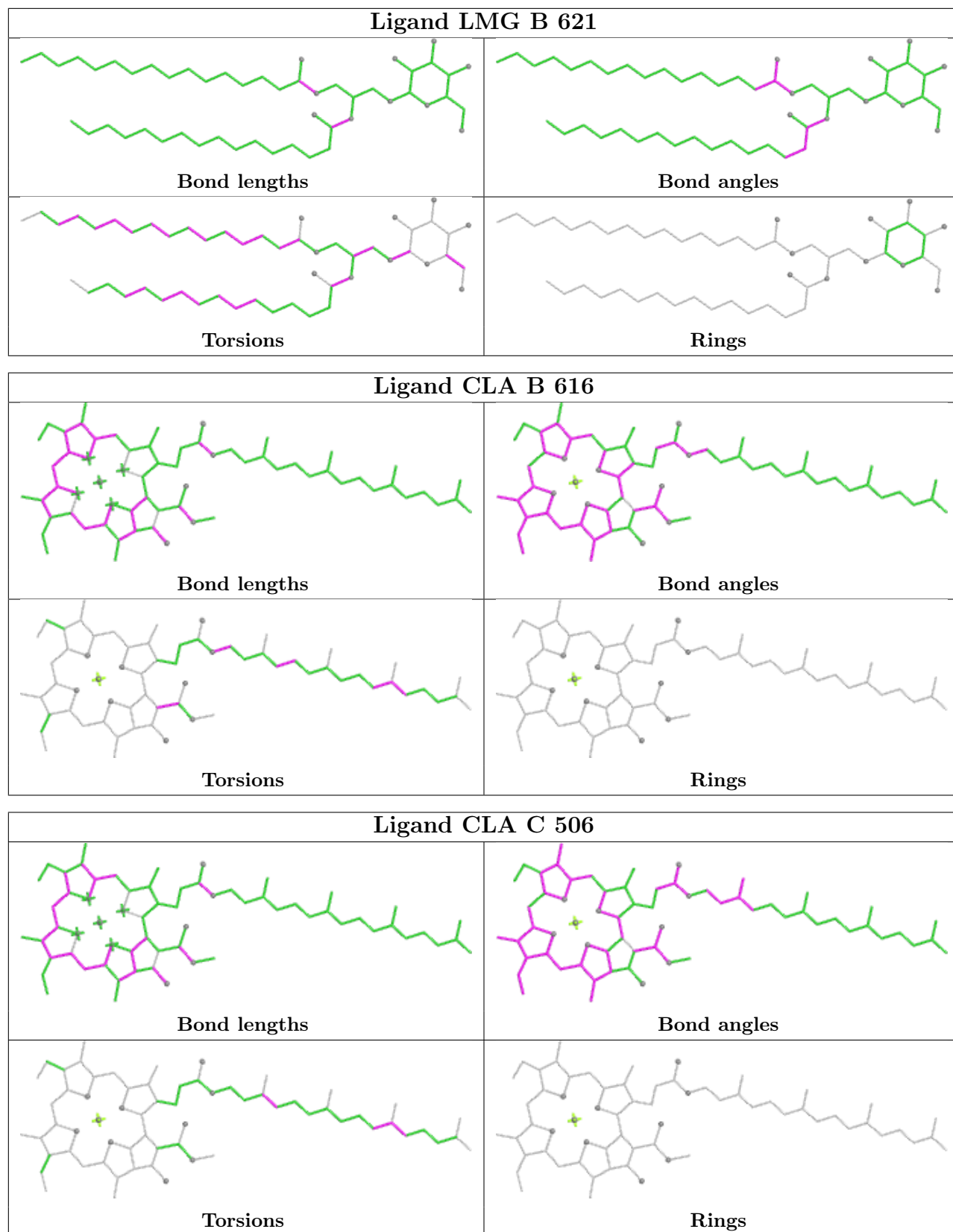




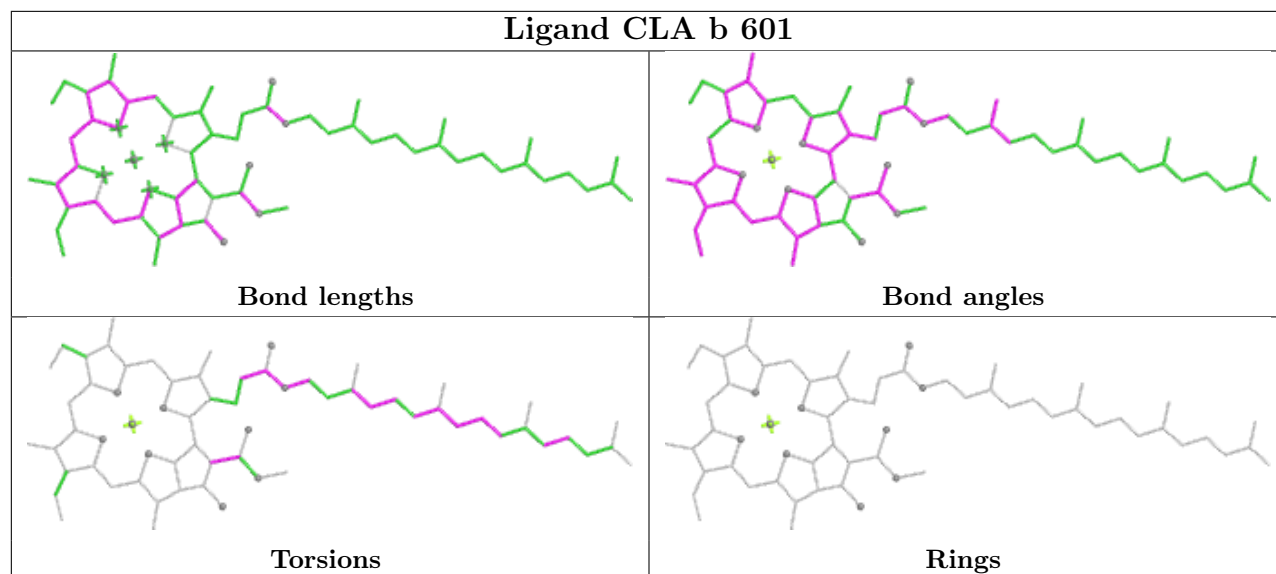




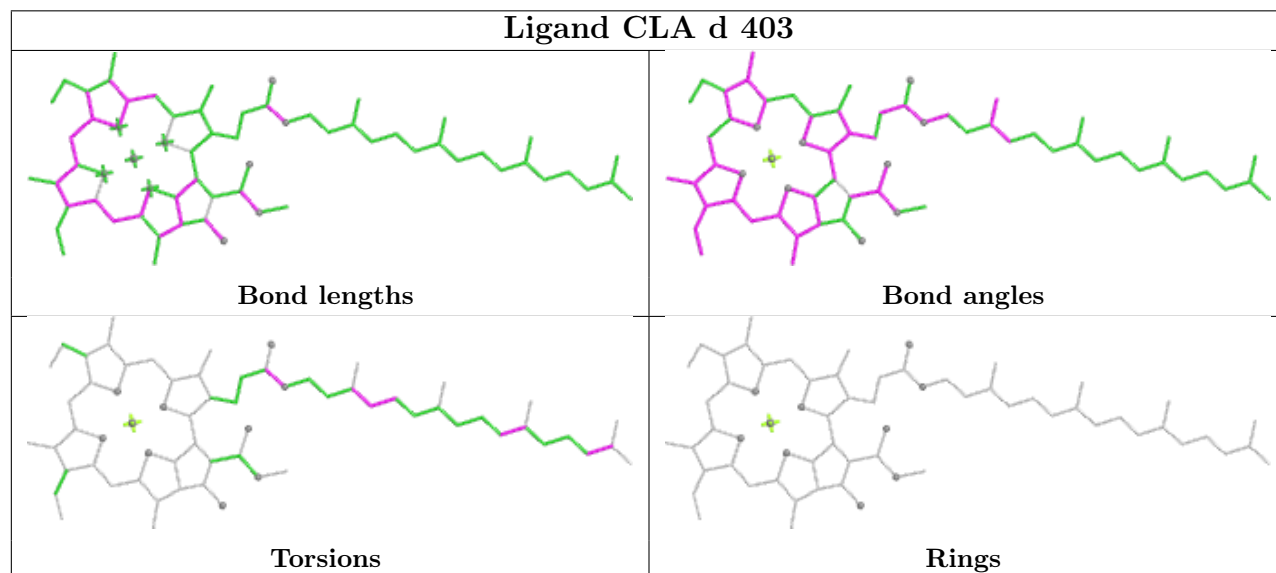




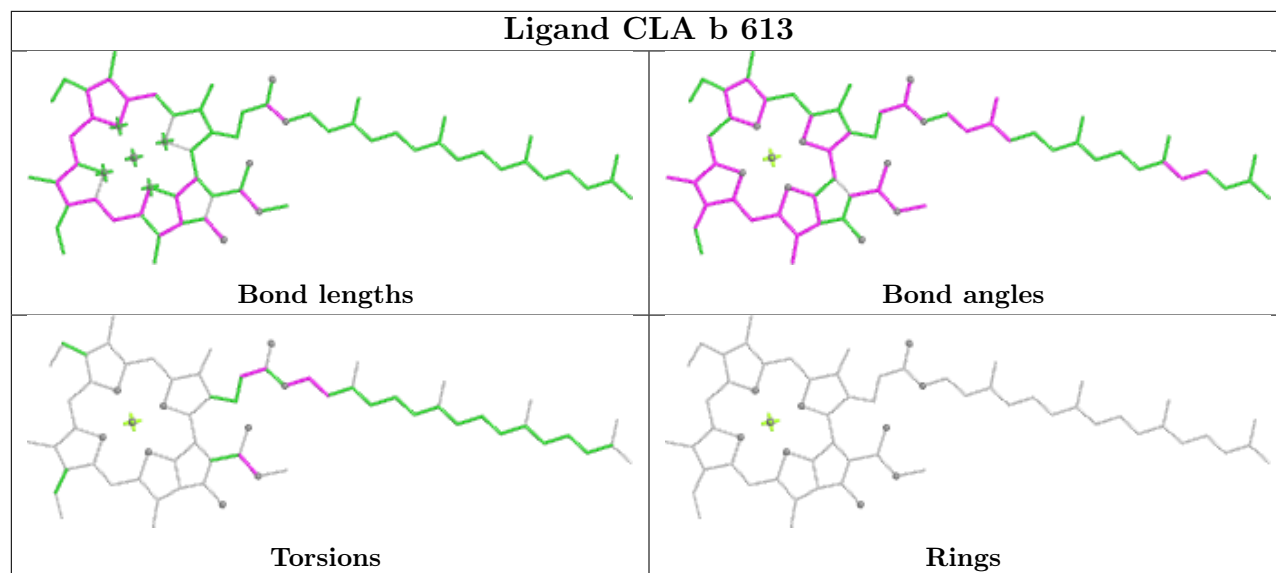
Ligand CLA b 601

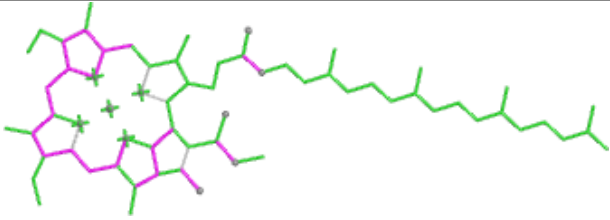
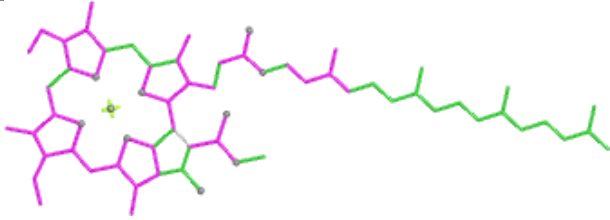
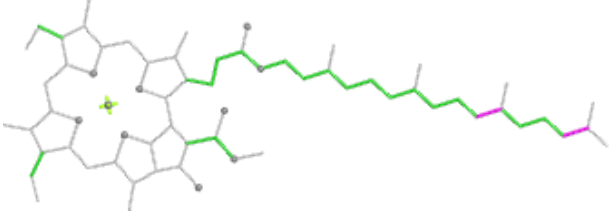
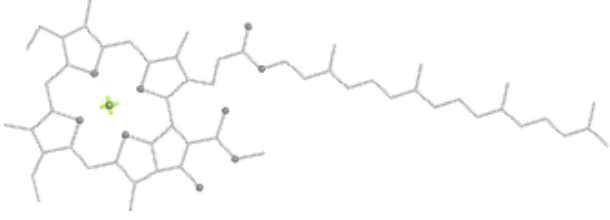
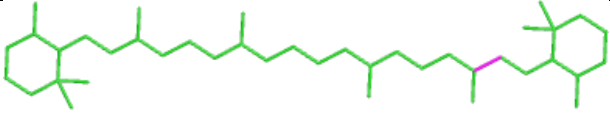
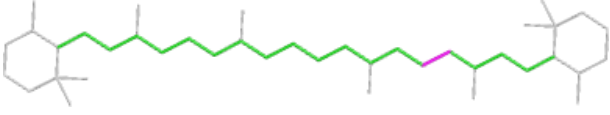
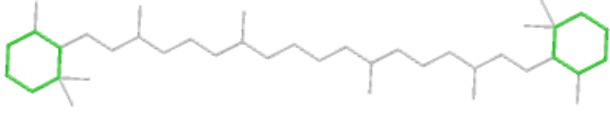
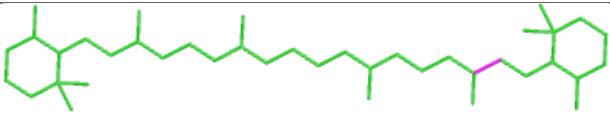
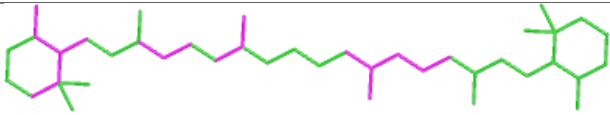
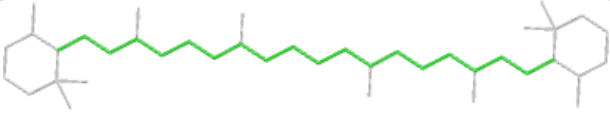
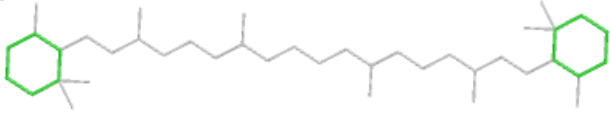


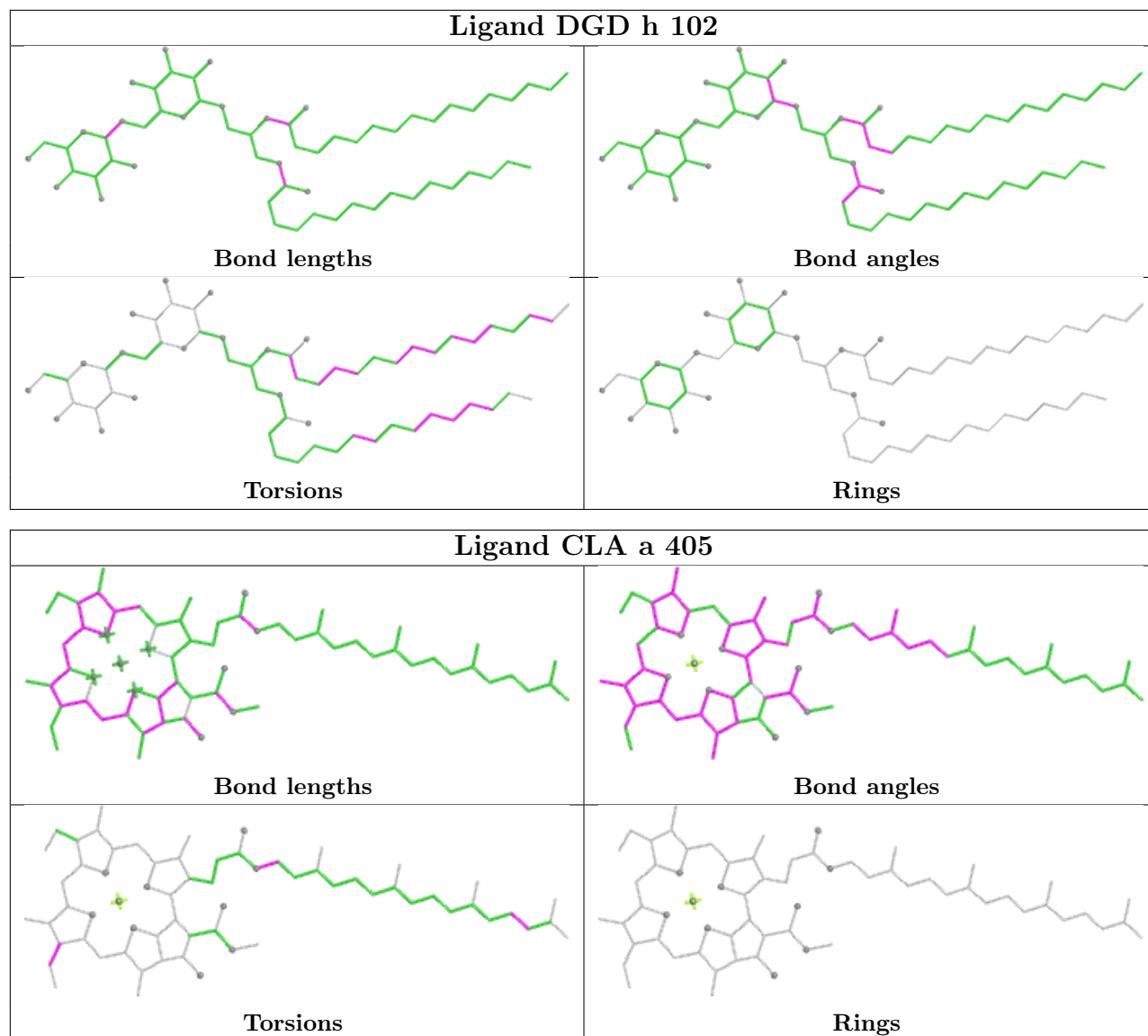
Ligand CLA d 403



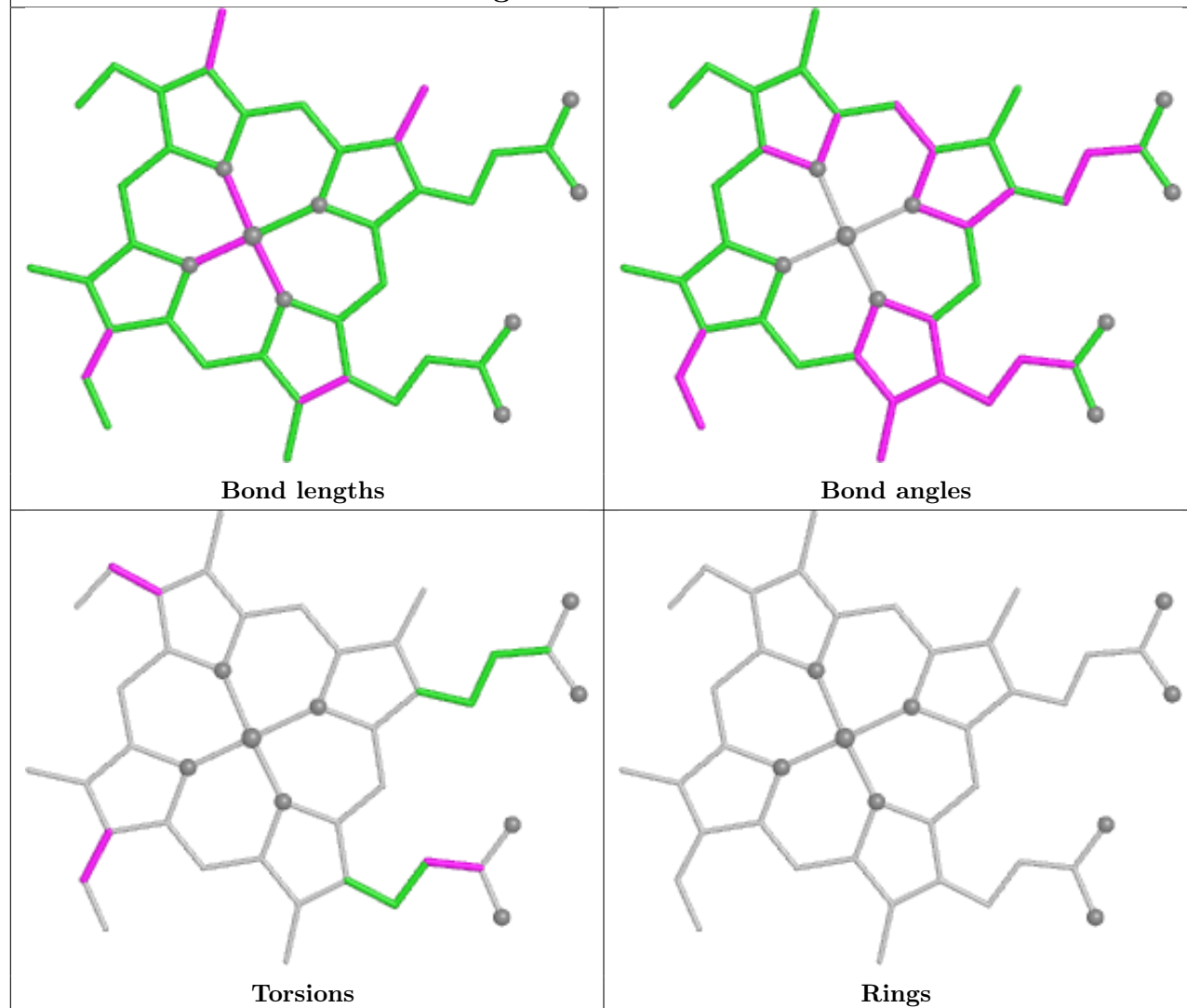
Ligand CLA b 613



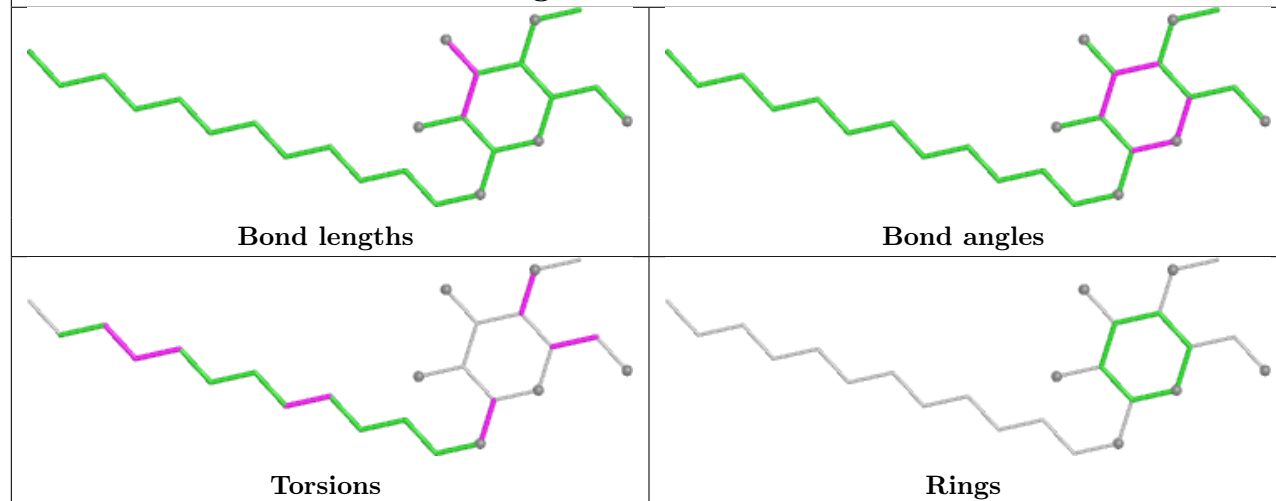
Ligand CLA d 402	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR a 410	
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 Torsions	 Rings

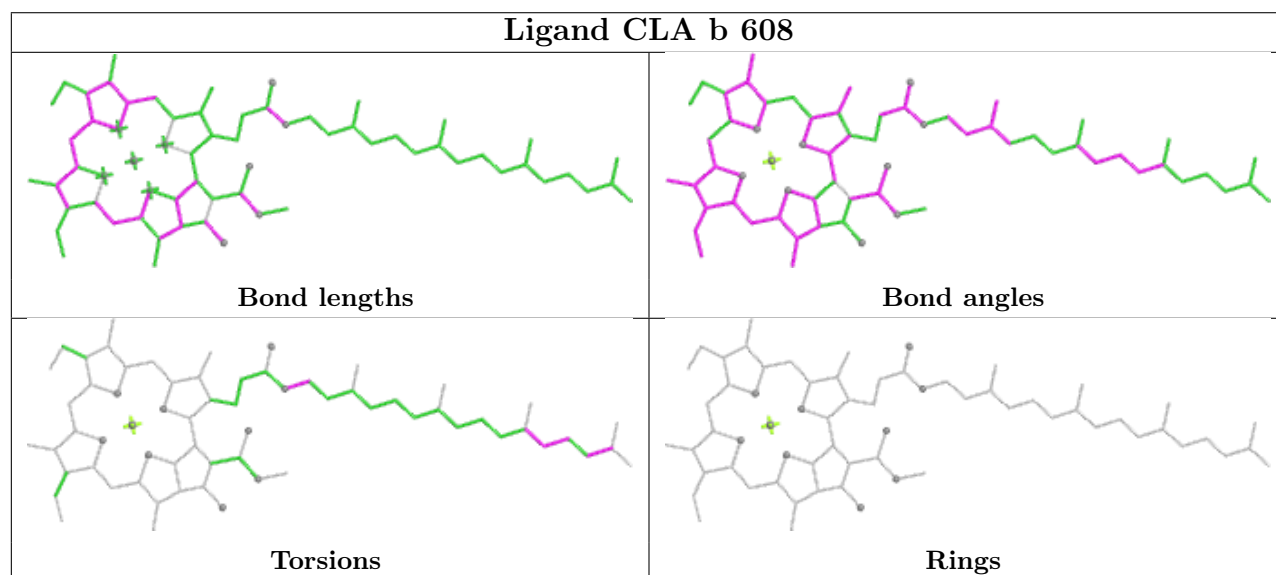
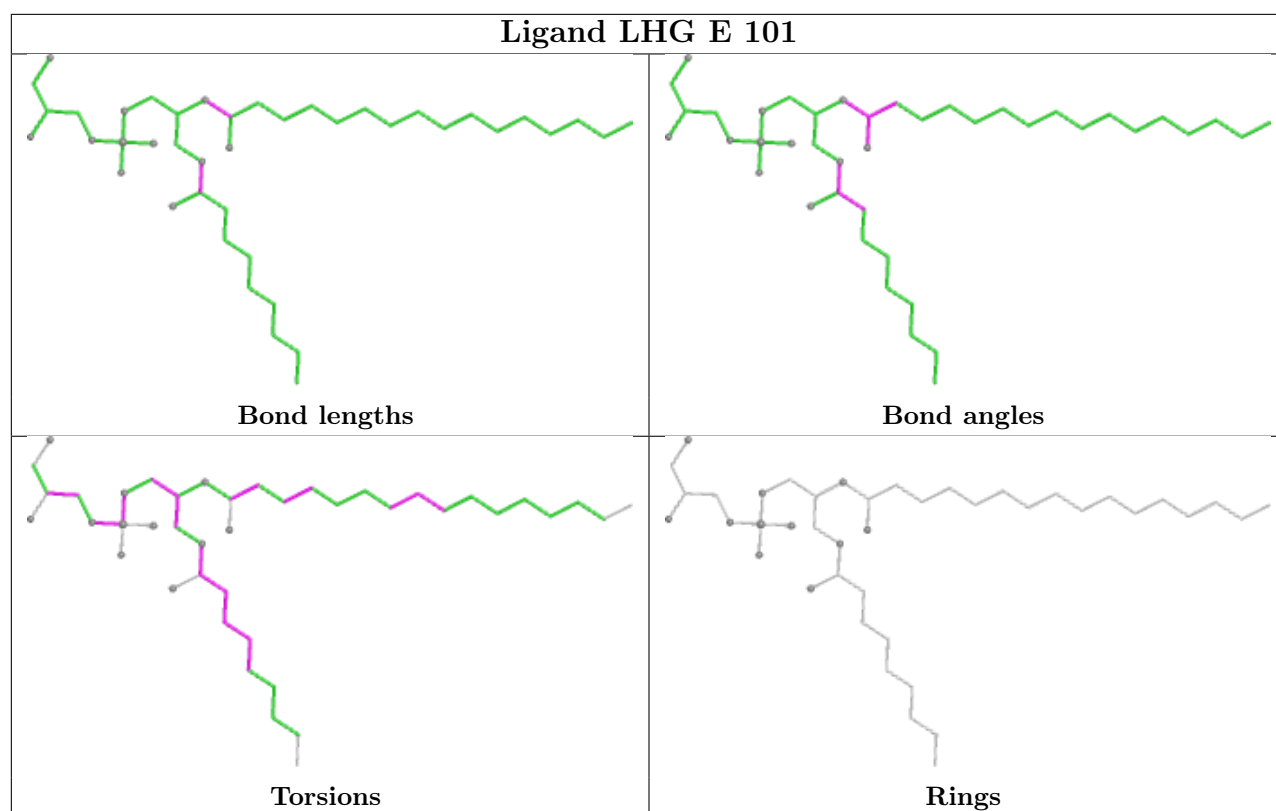


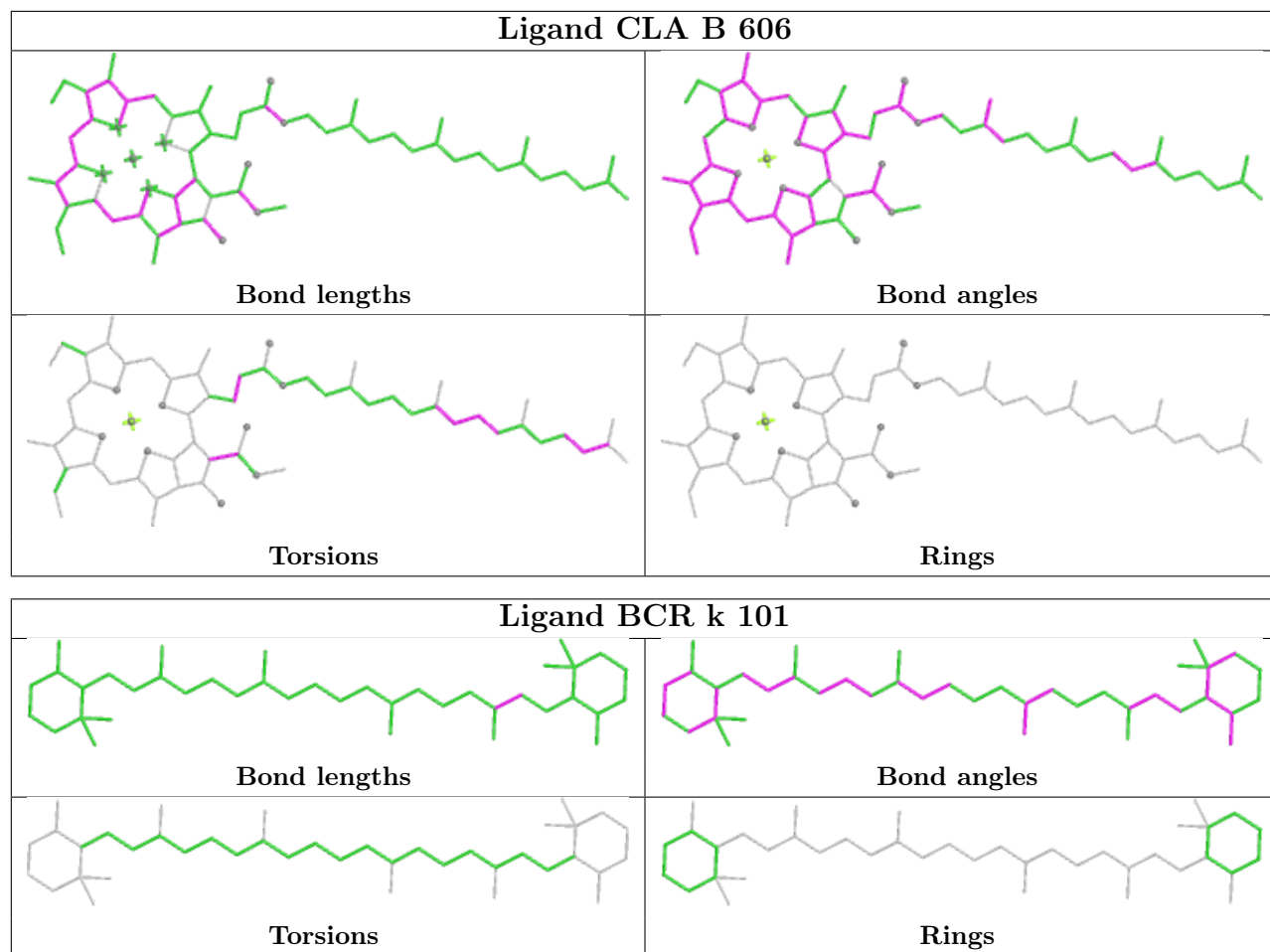
Ligand HEC V 202

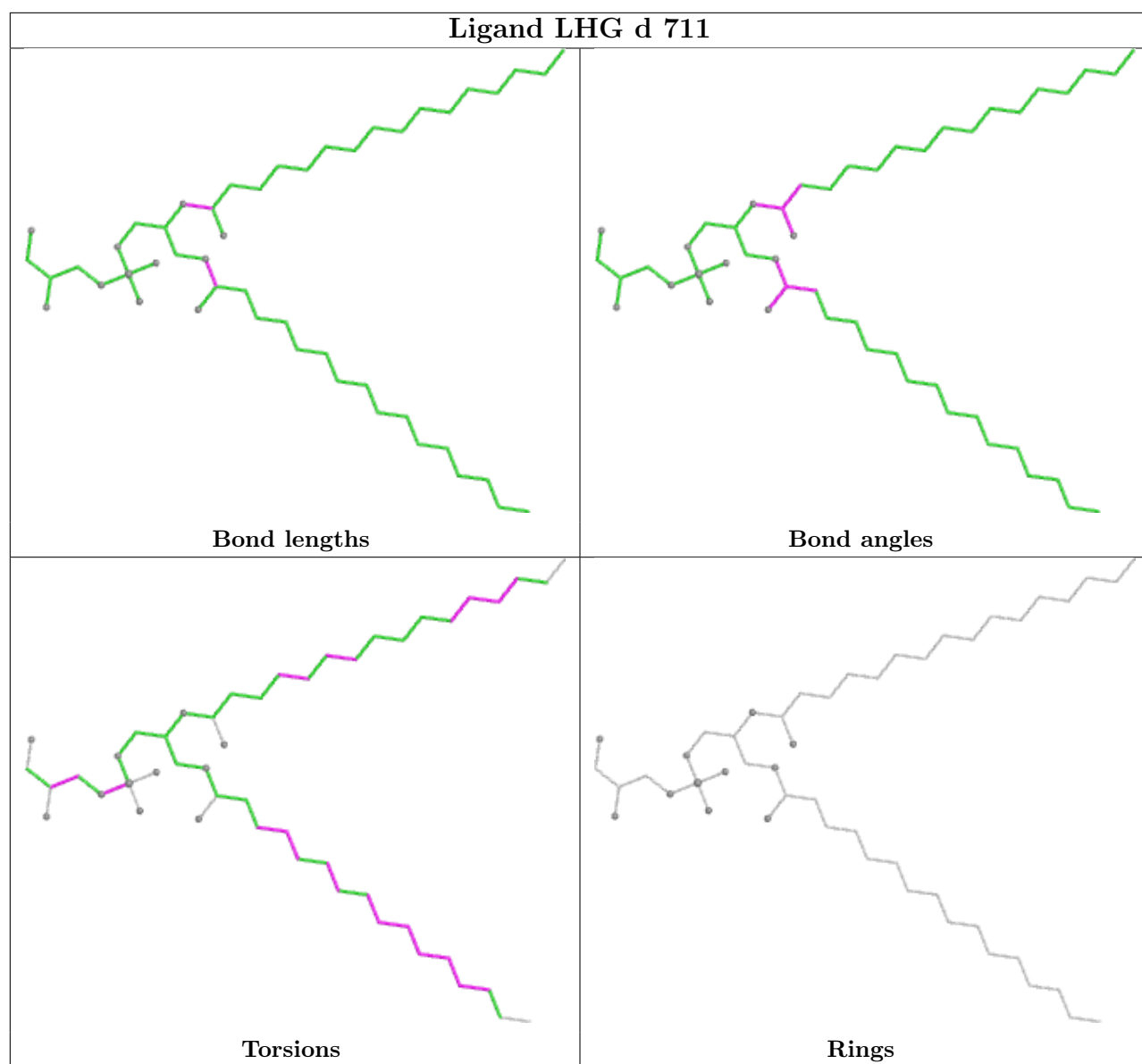


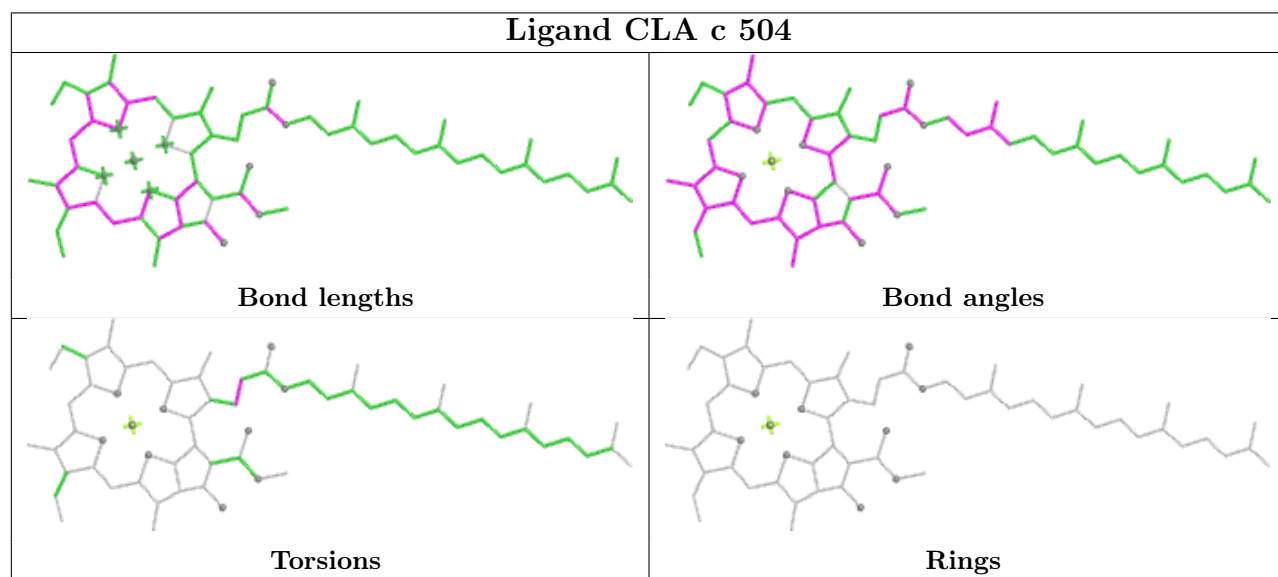
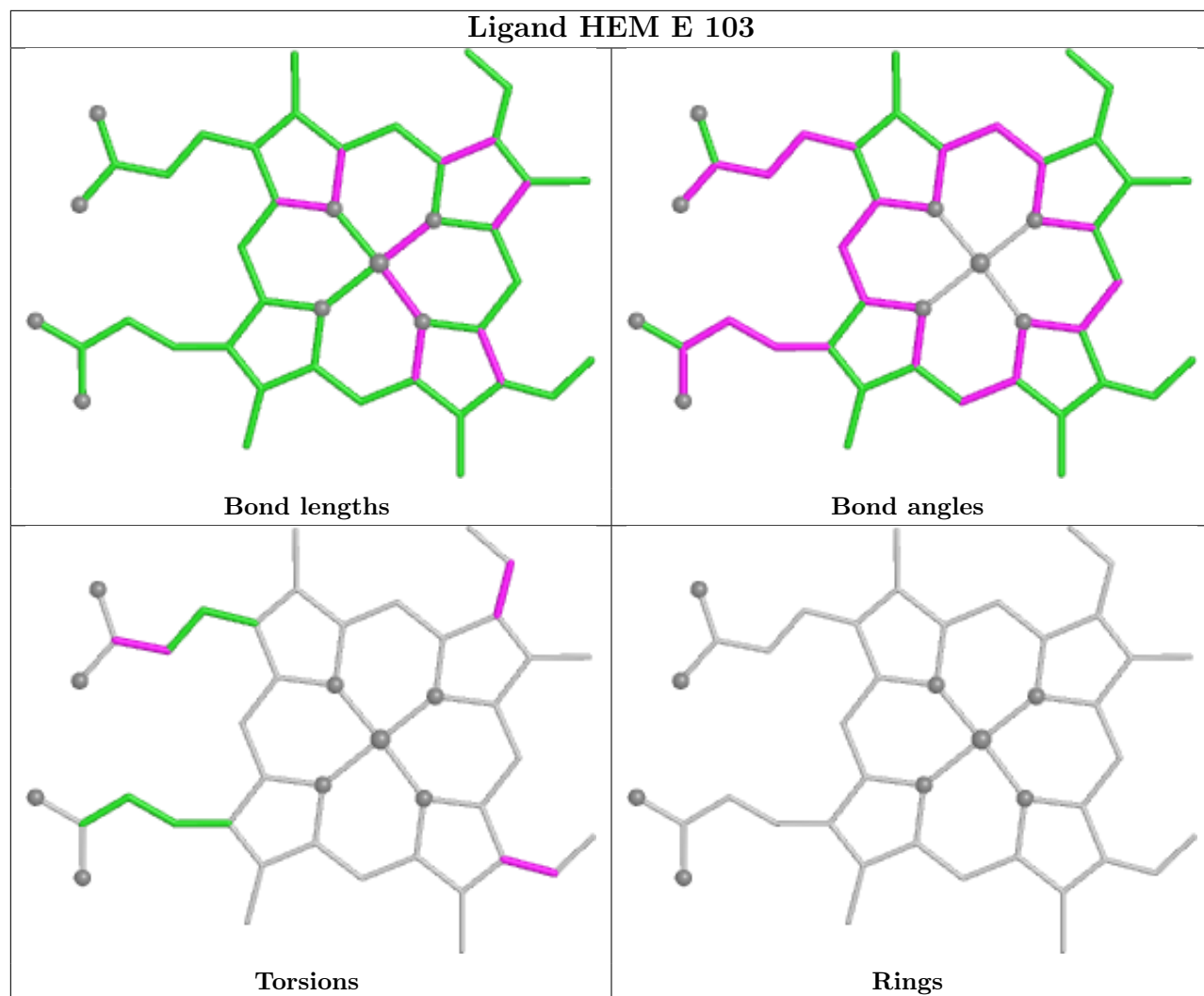
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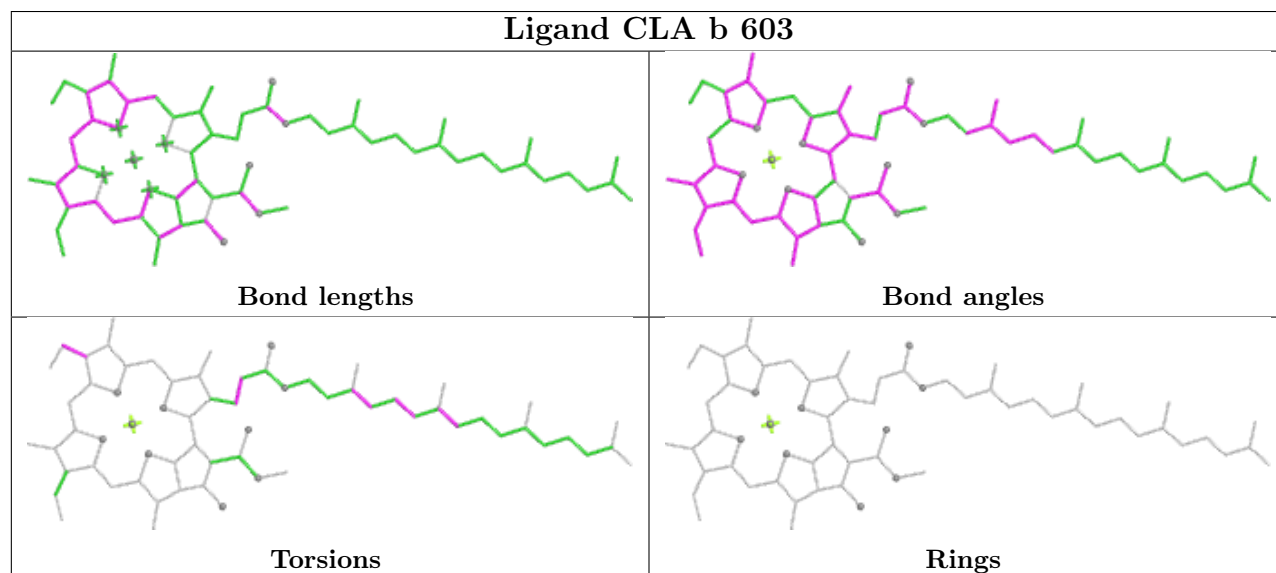
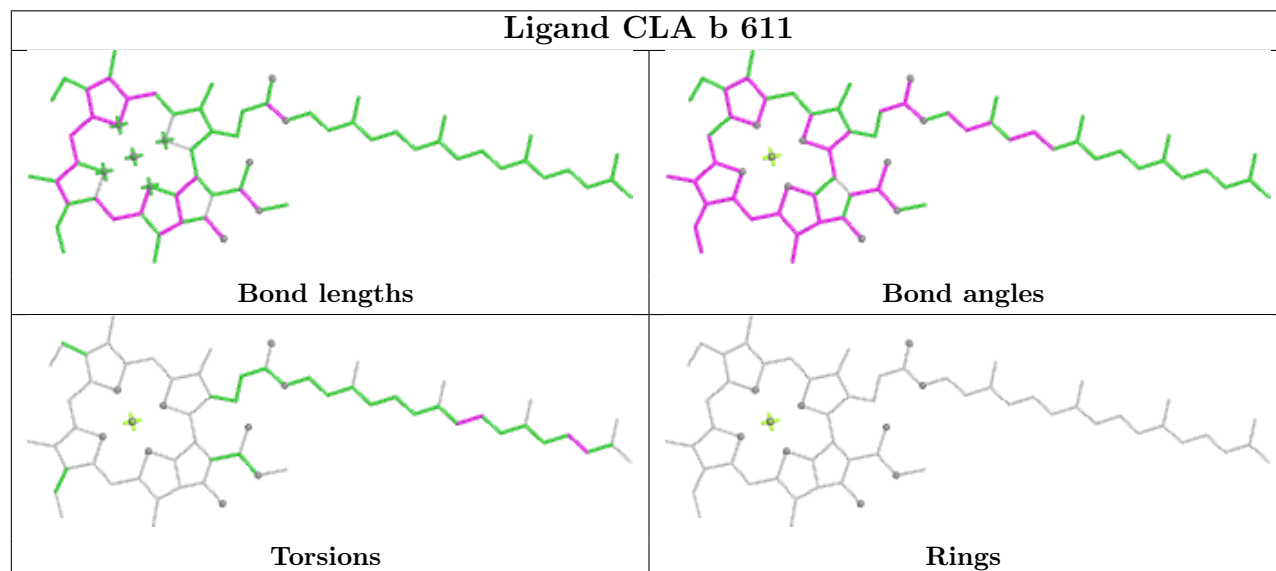
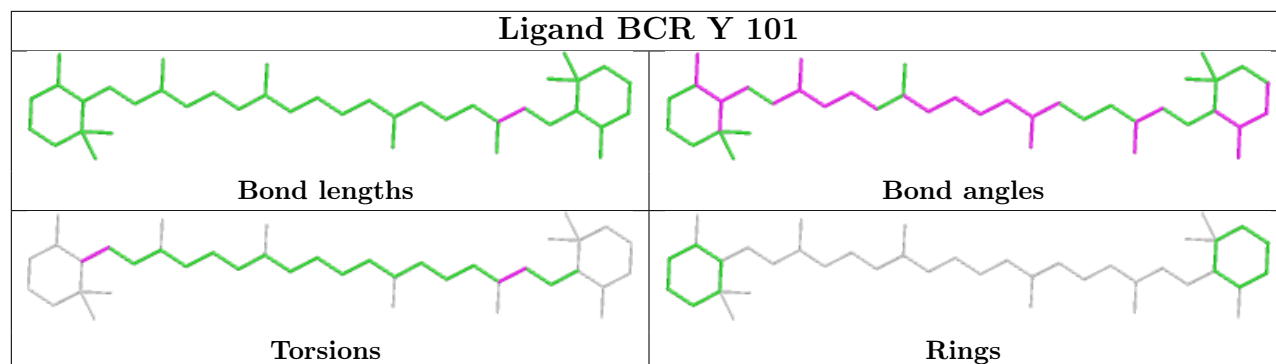


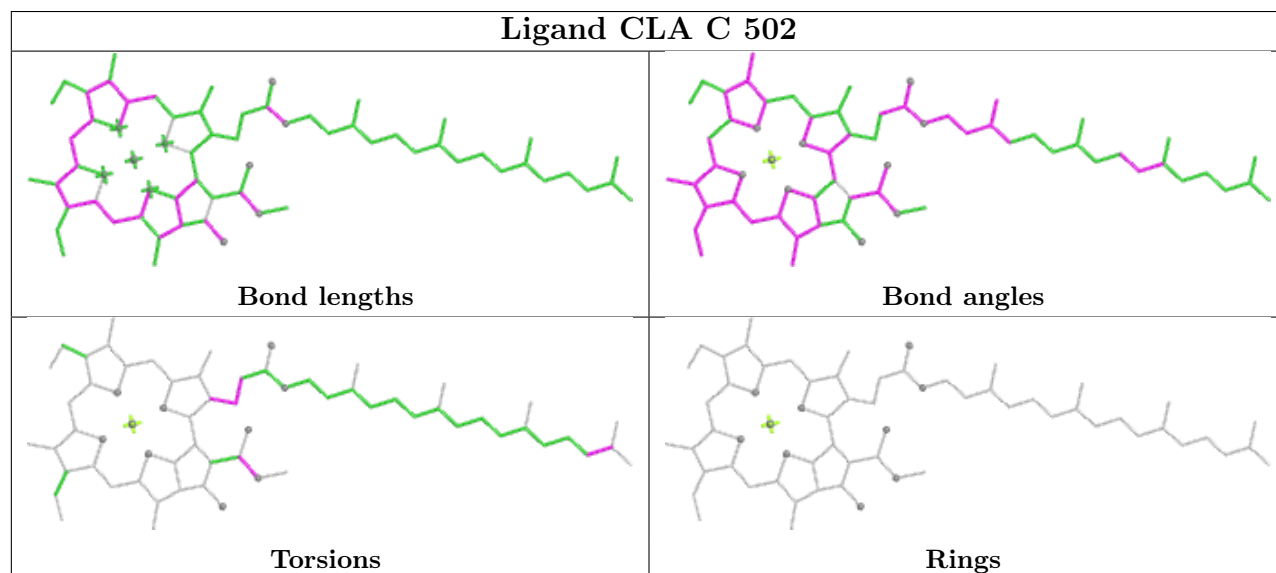
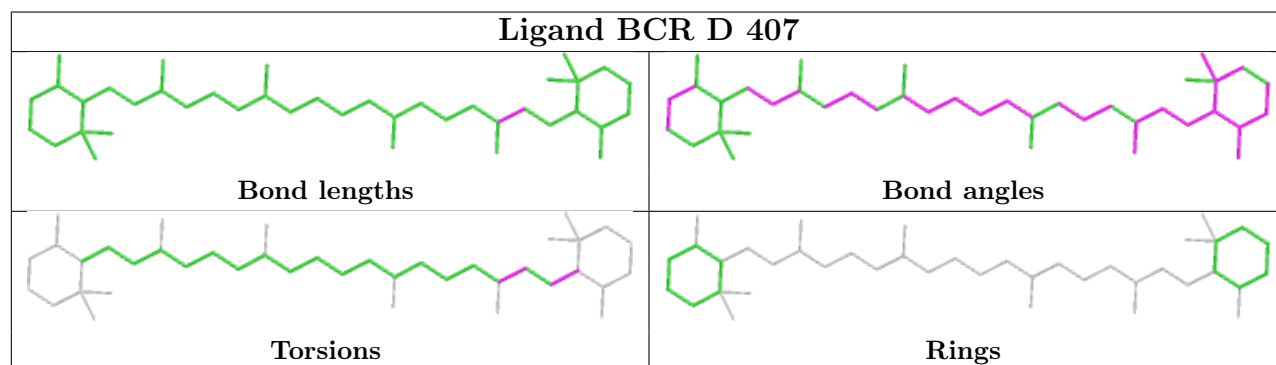
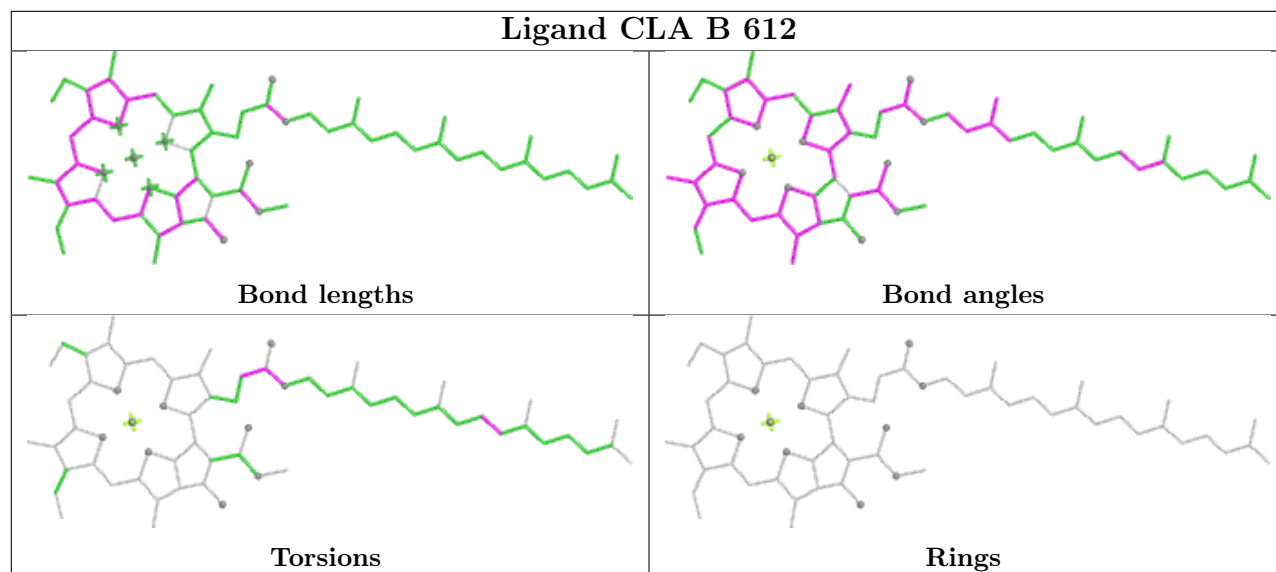




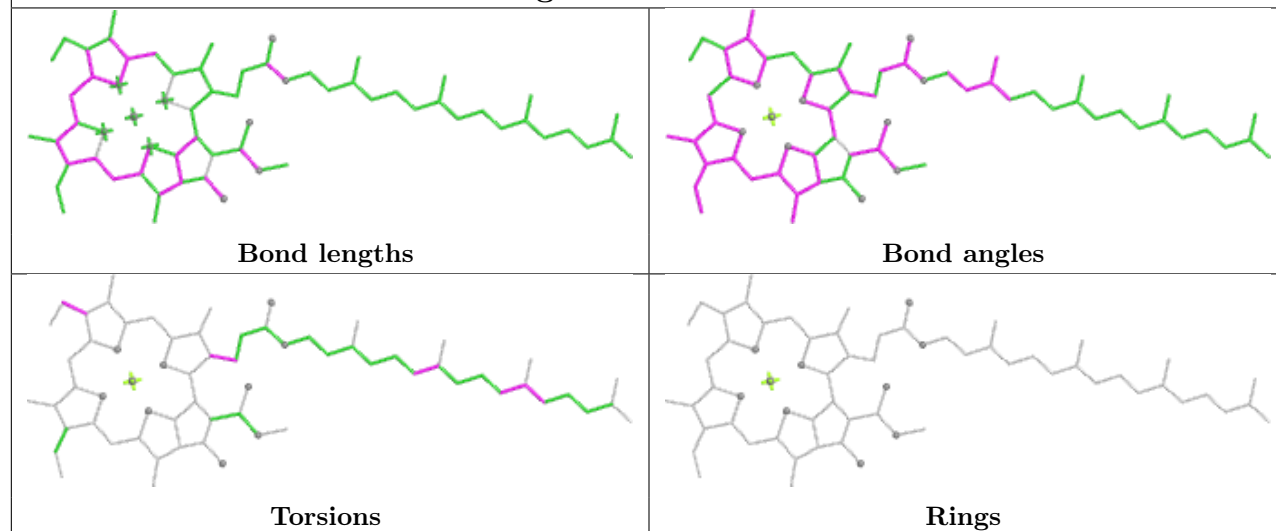




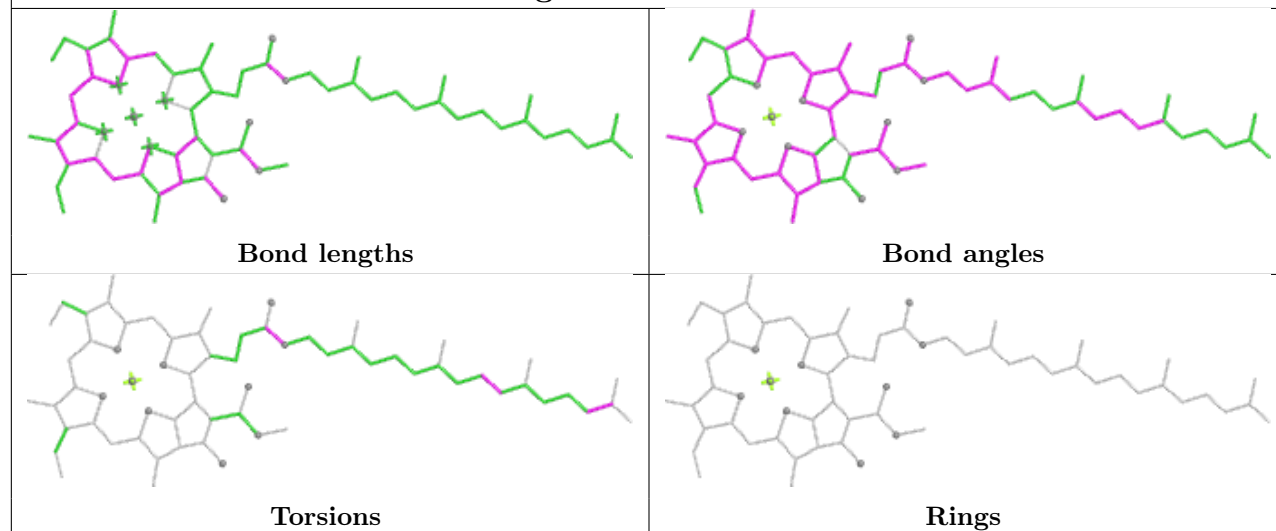




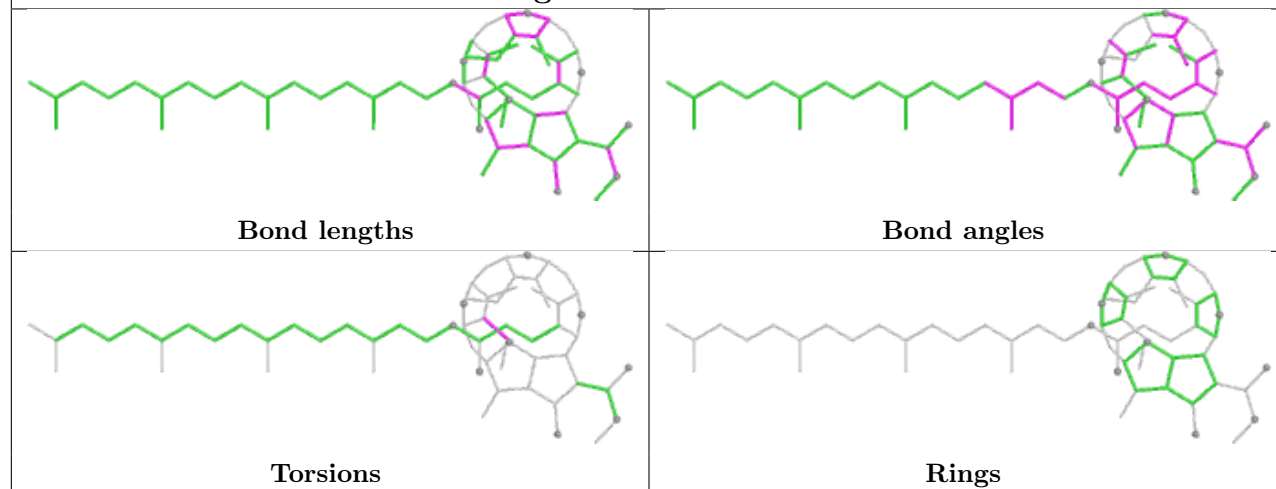
Ligand CLA a 407

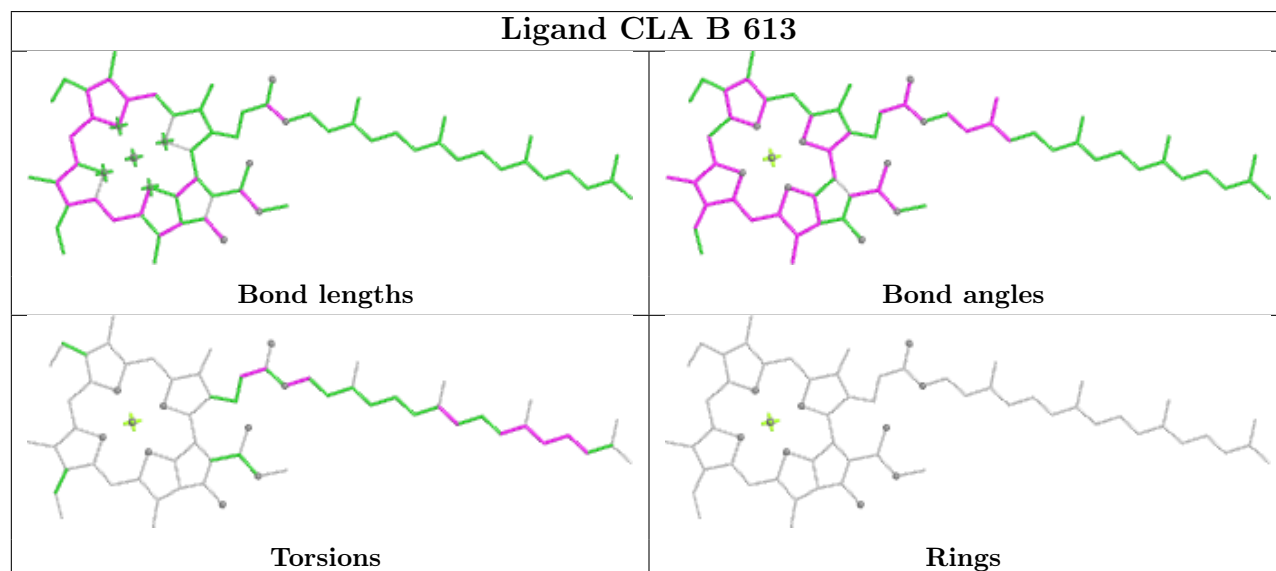
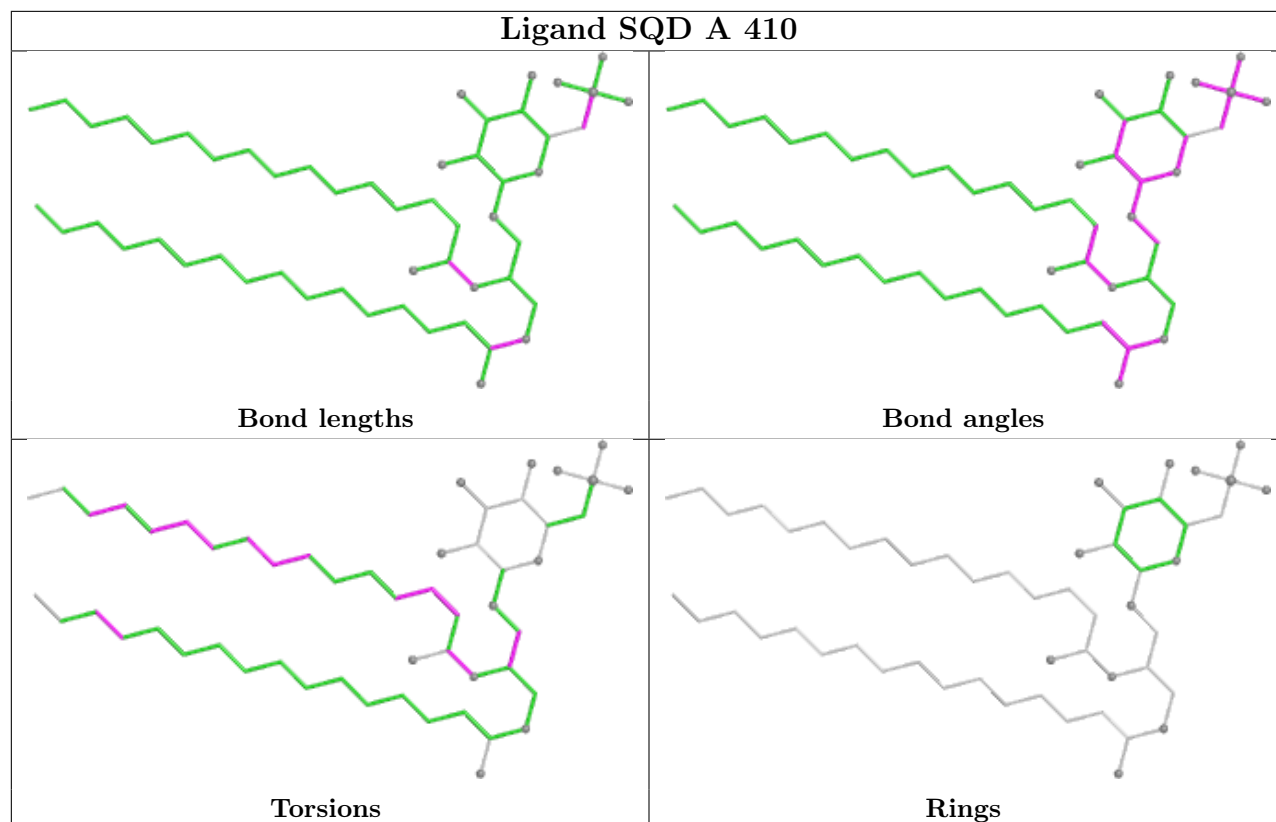


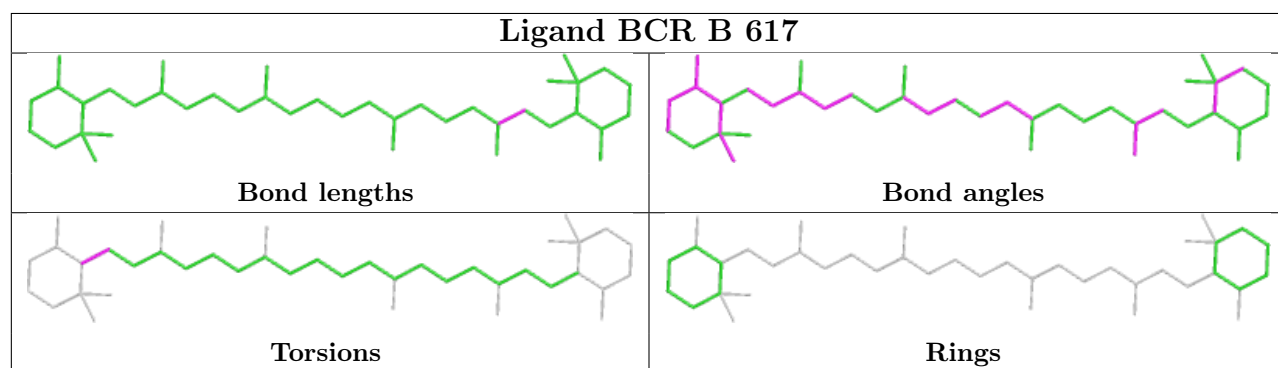
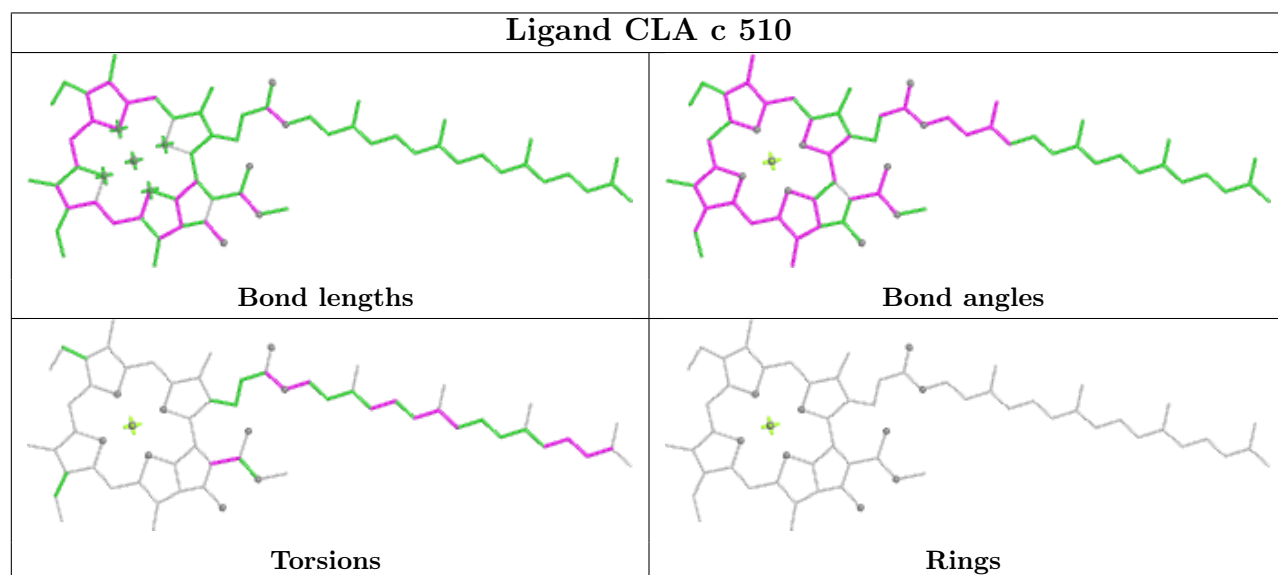
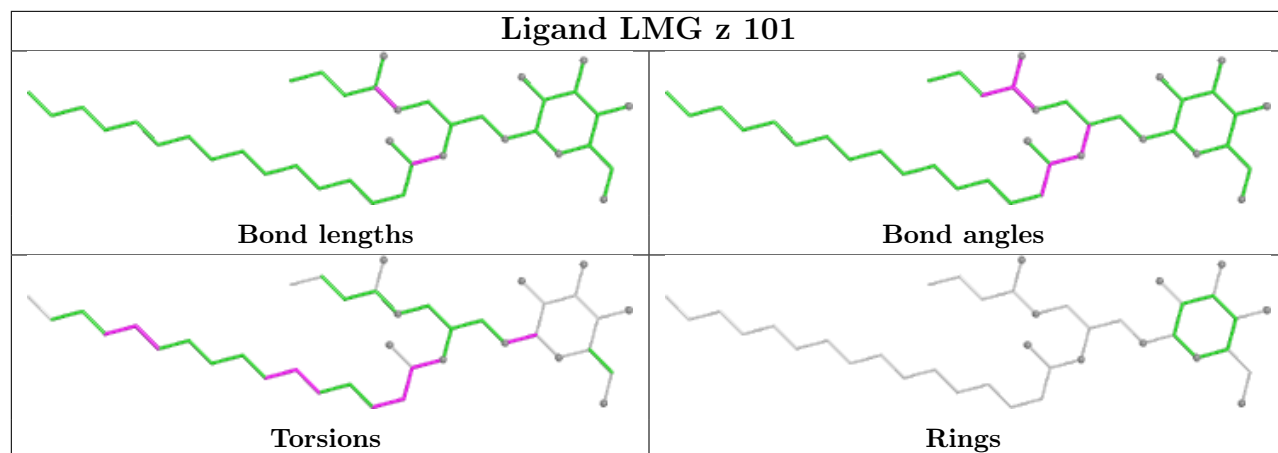
Ligand CLA b 602

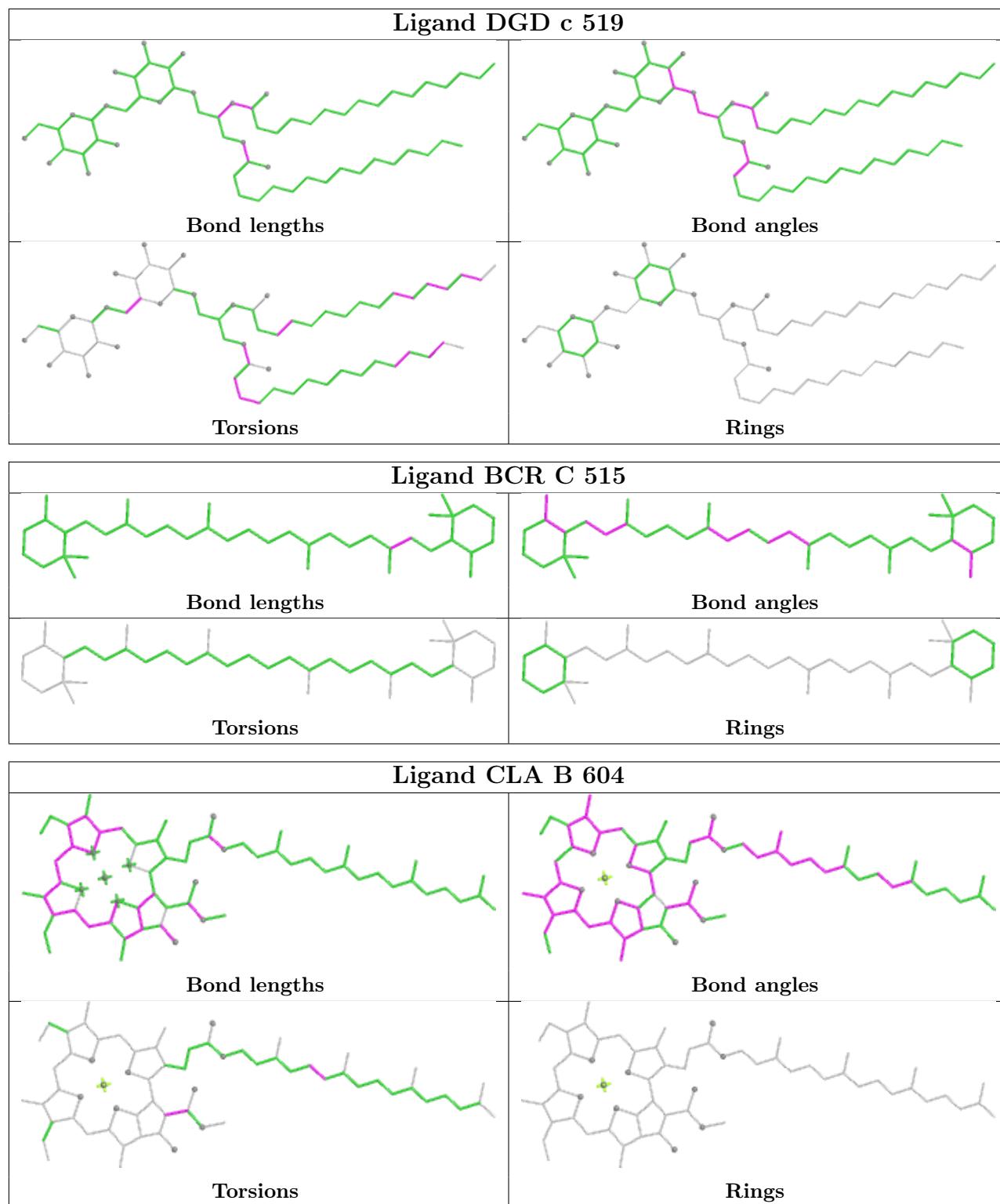


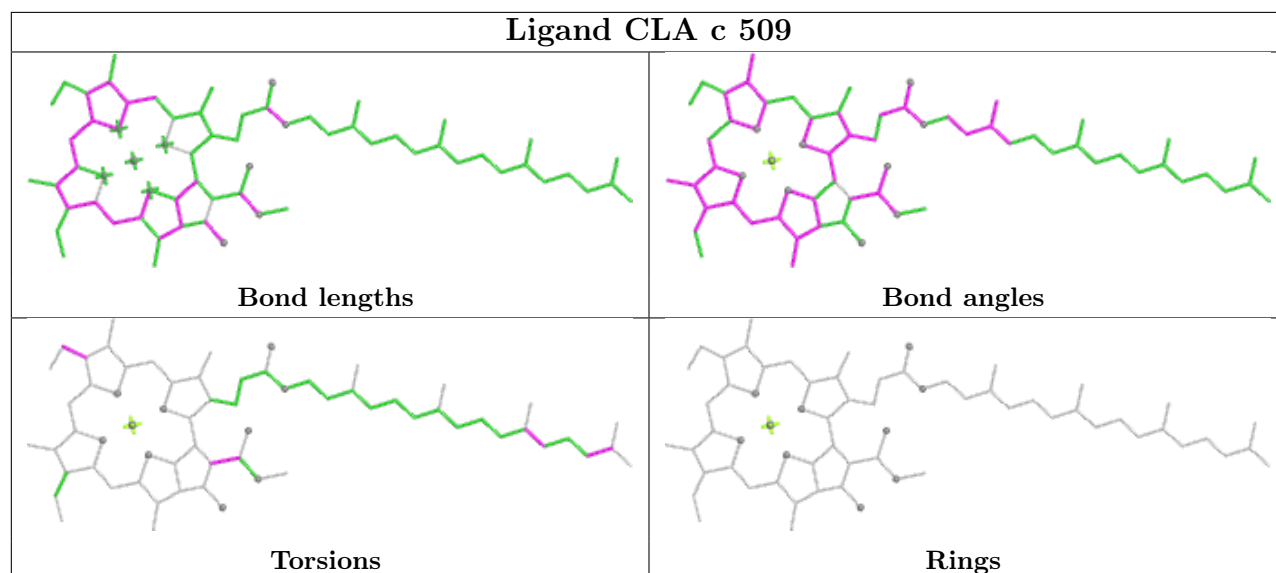
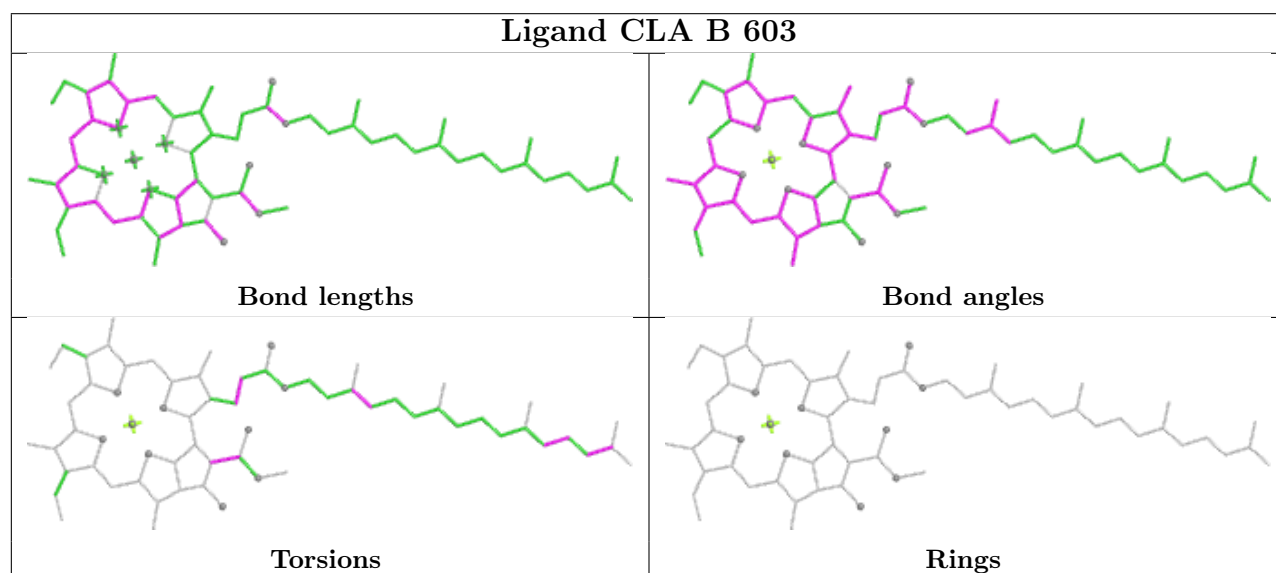
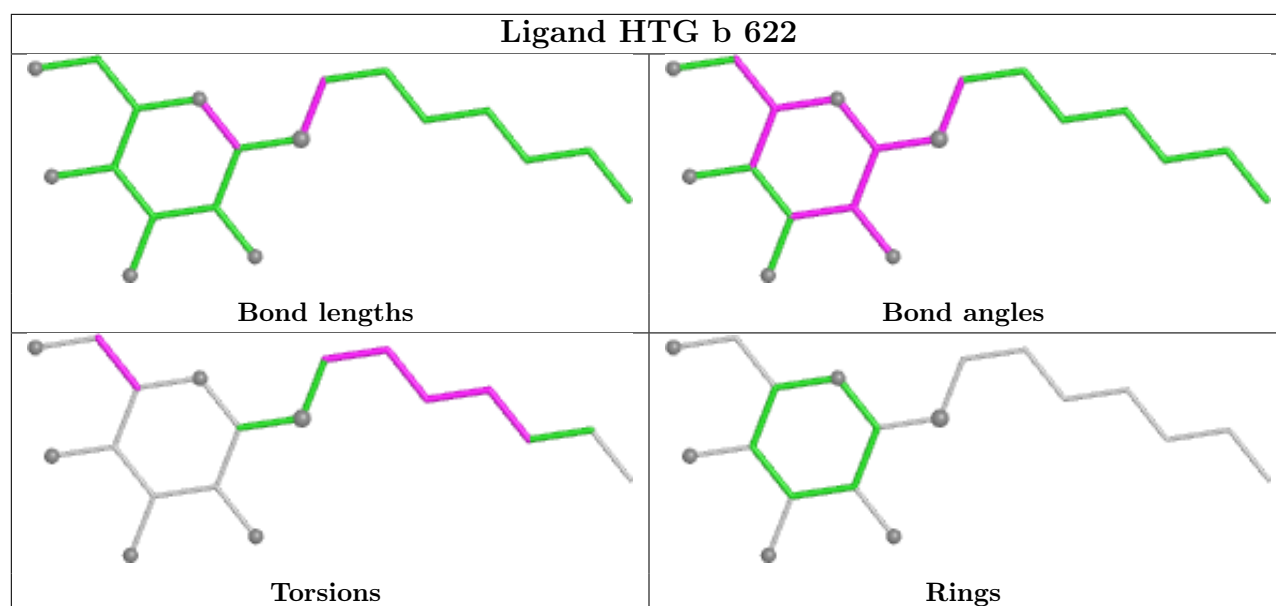
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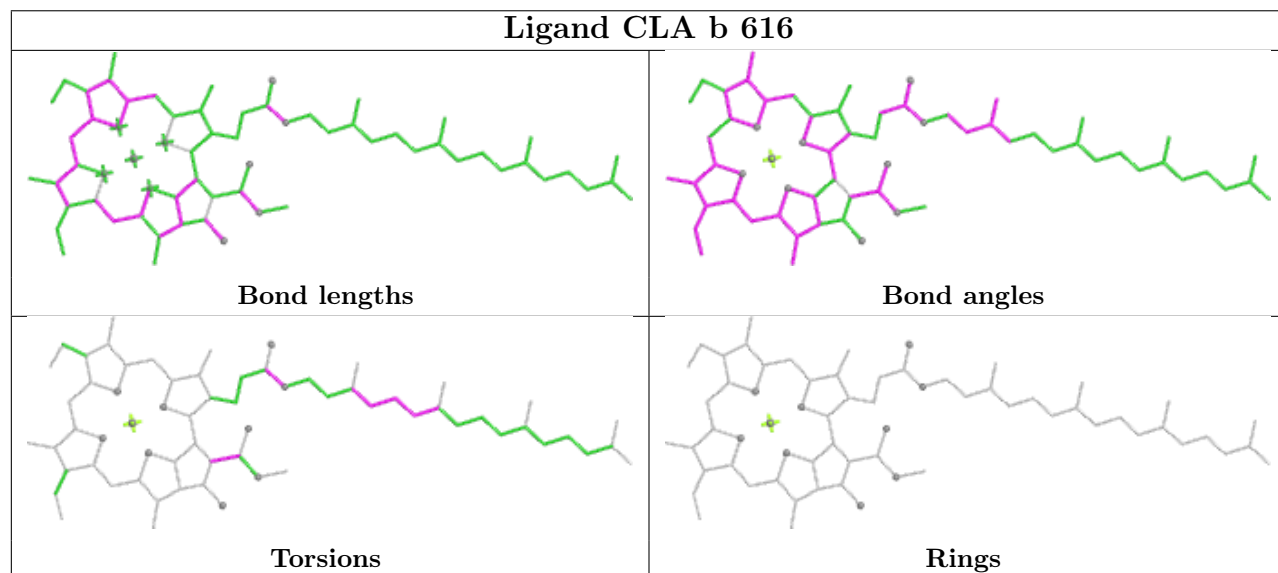
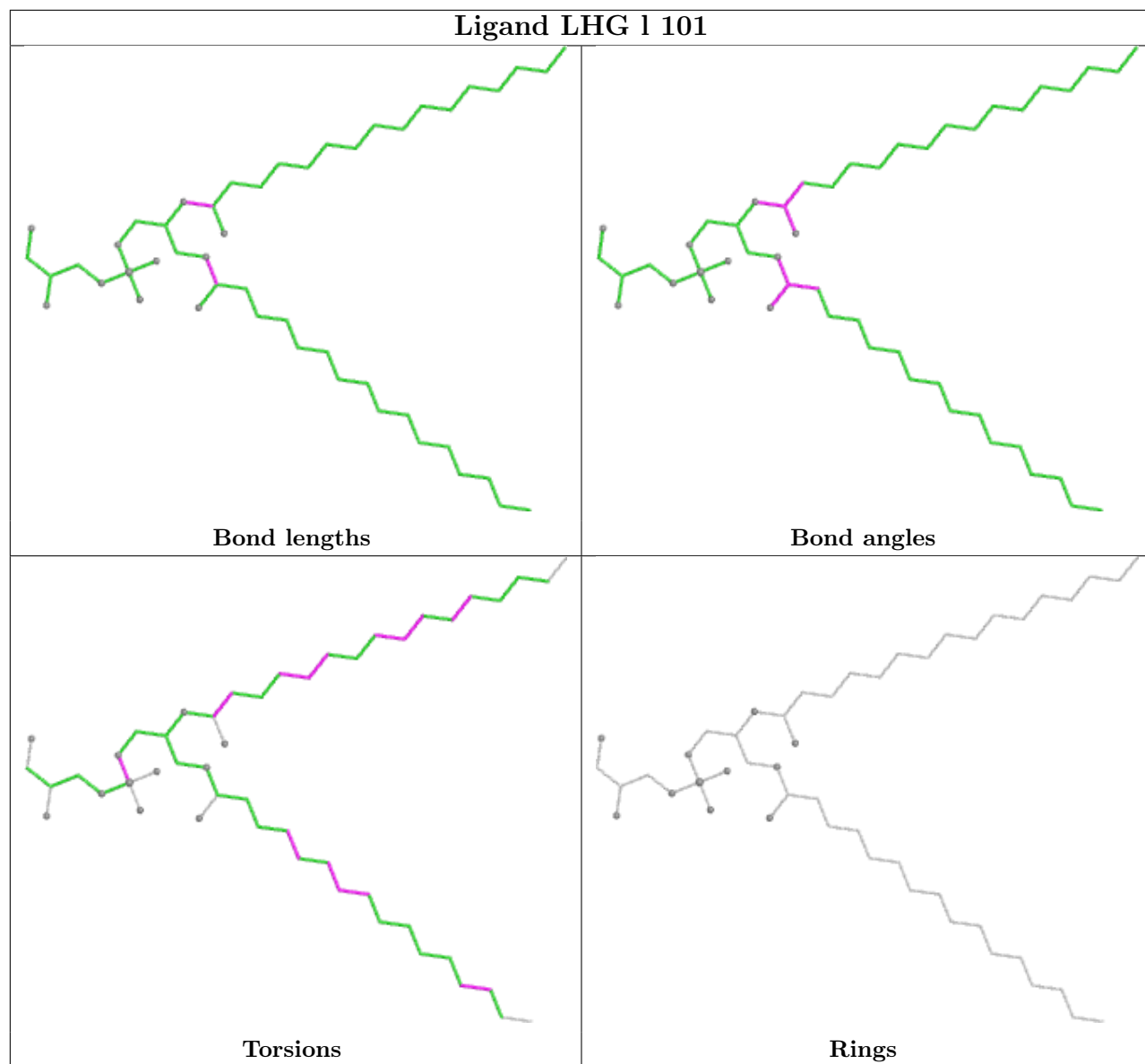


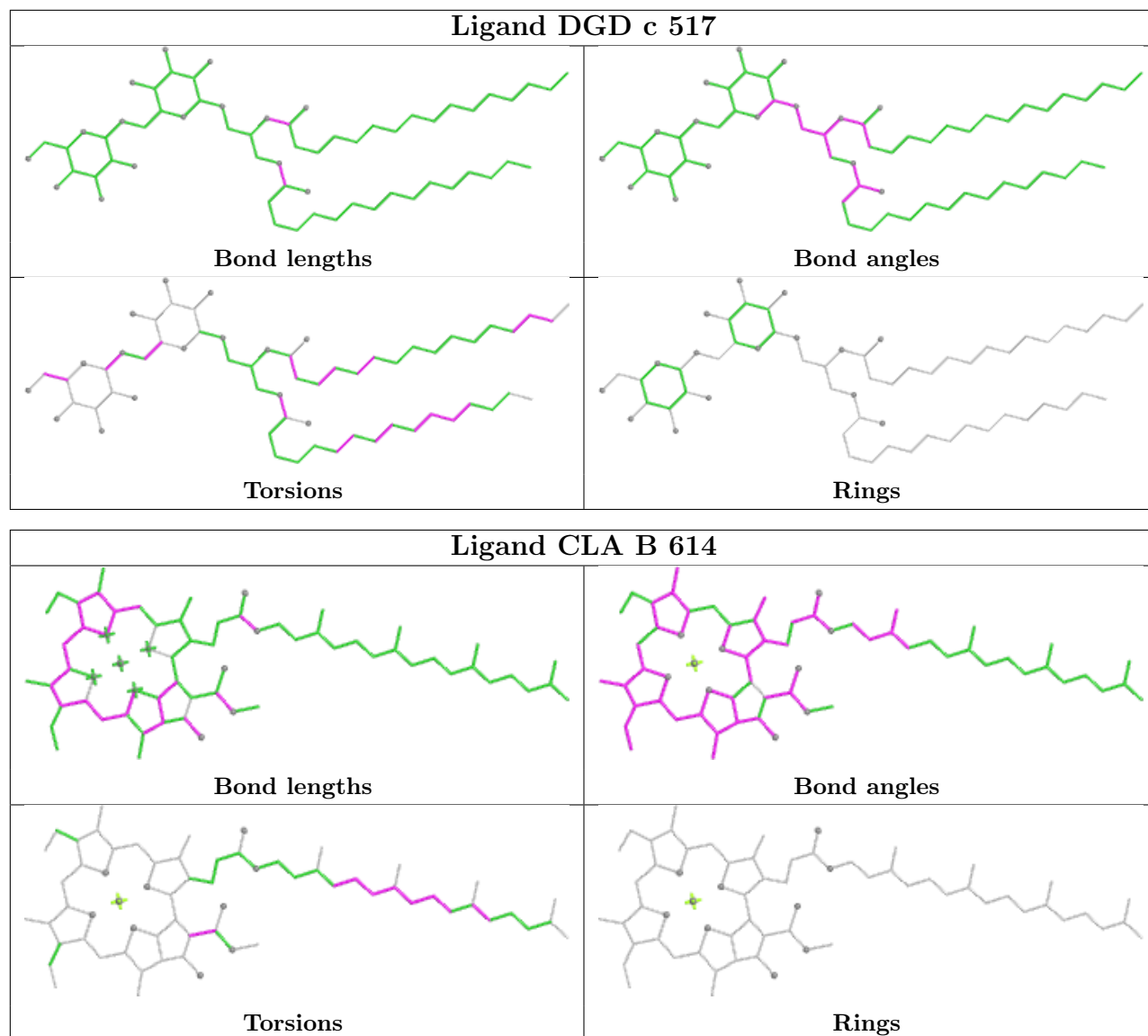


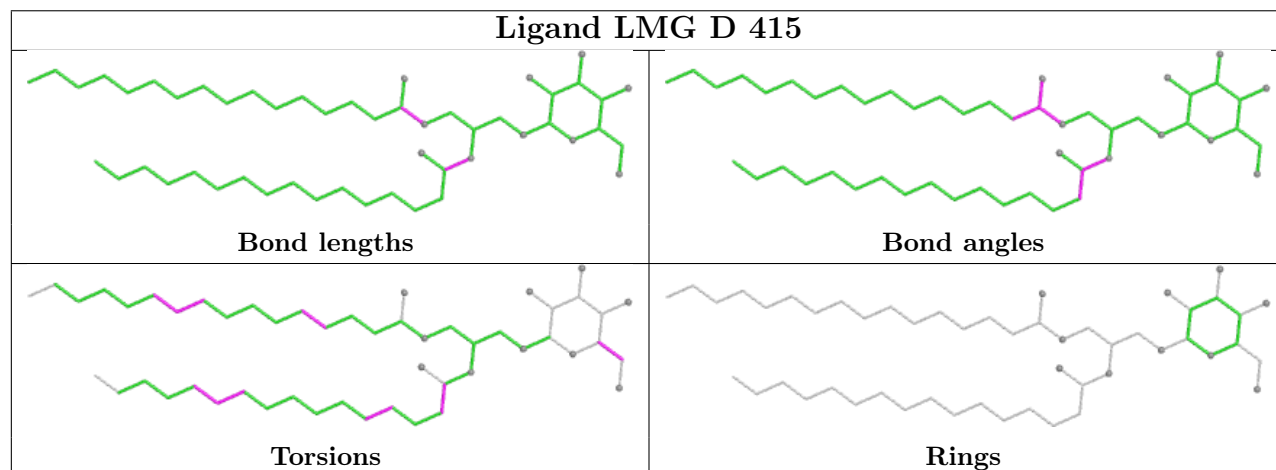
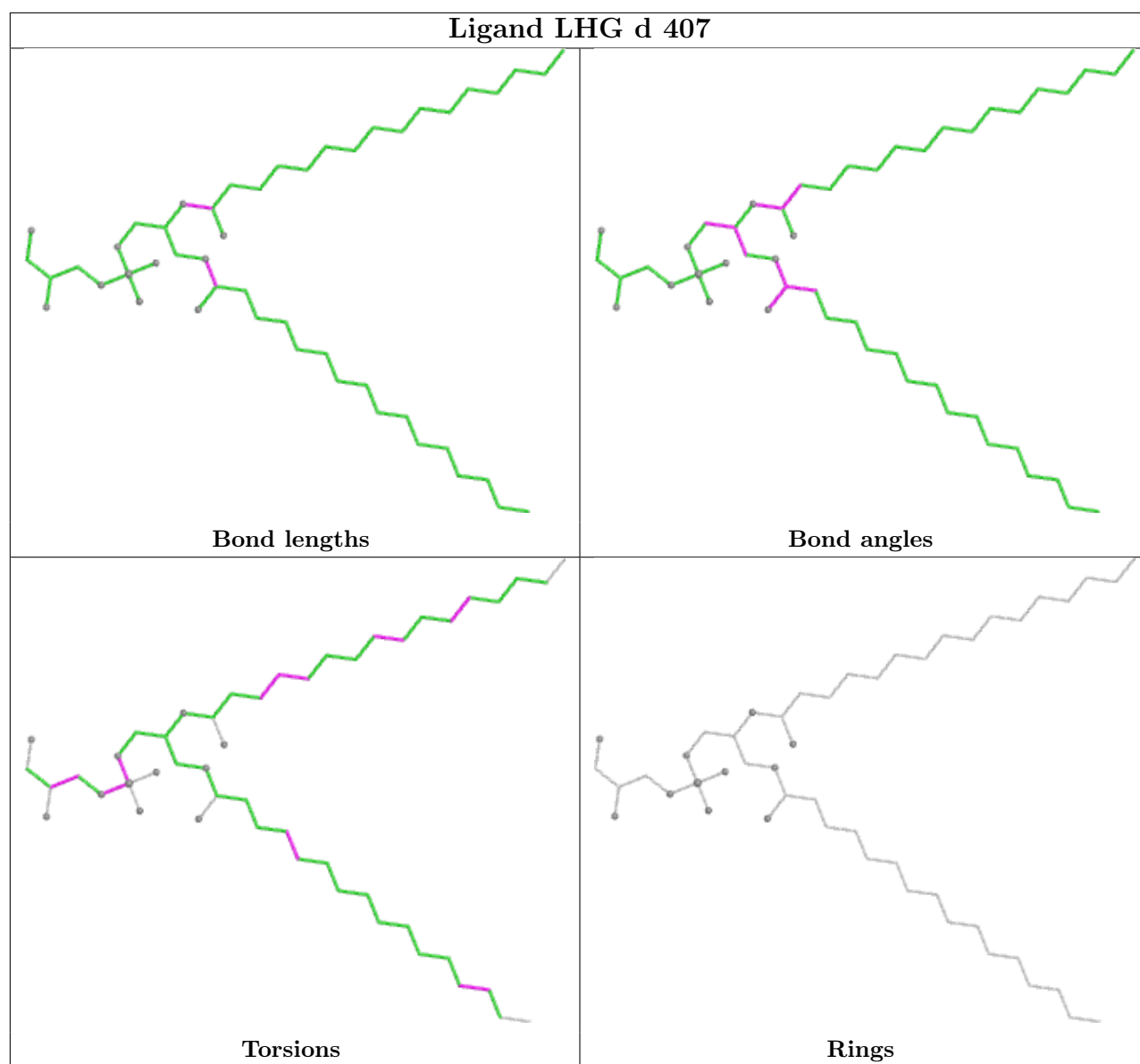


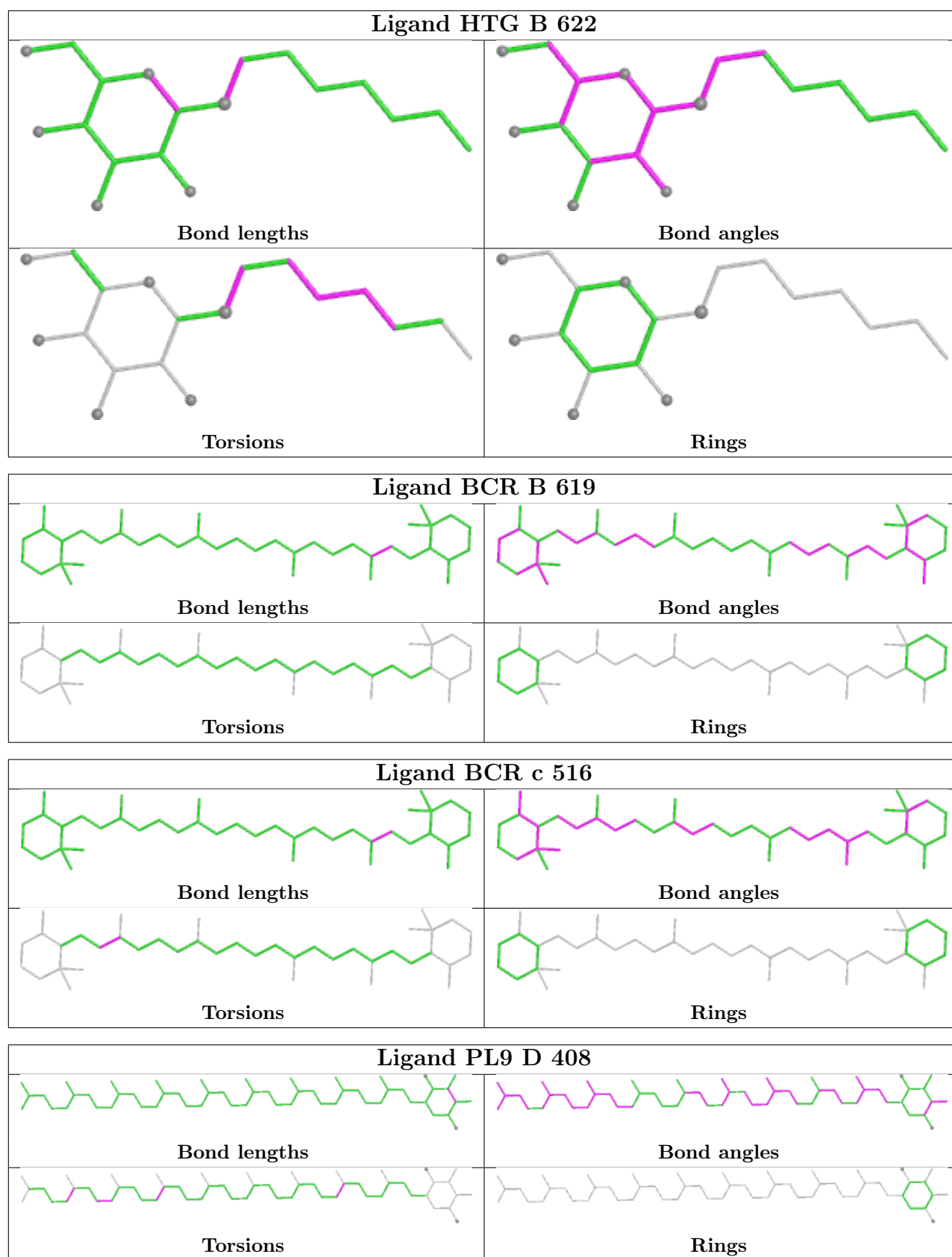


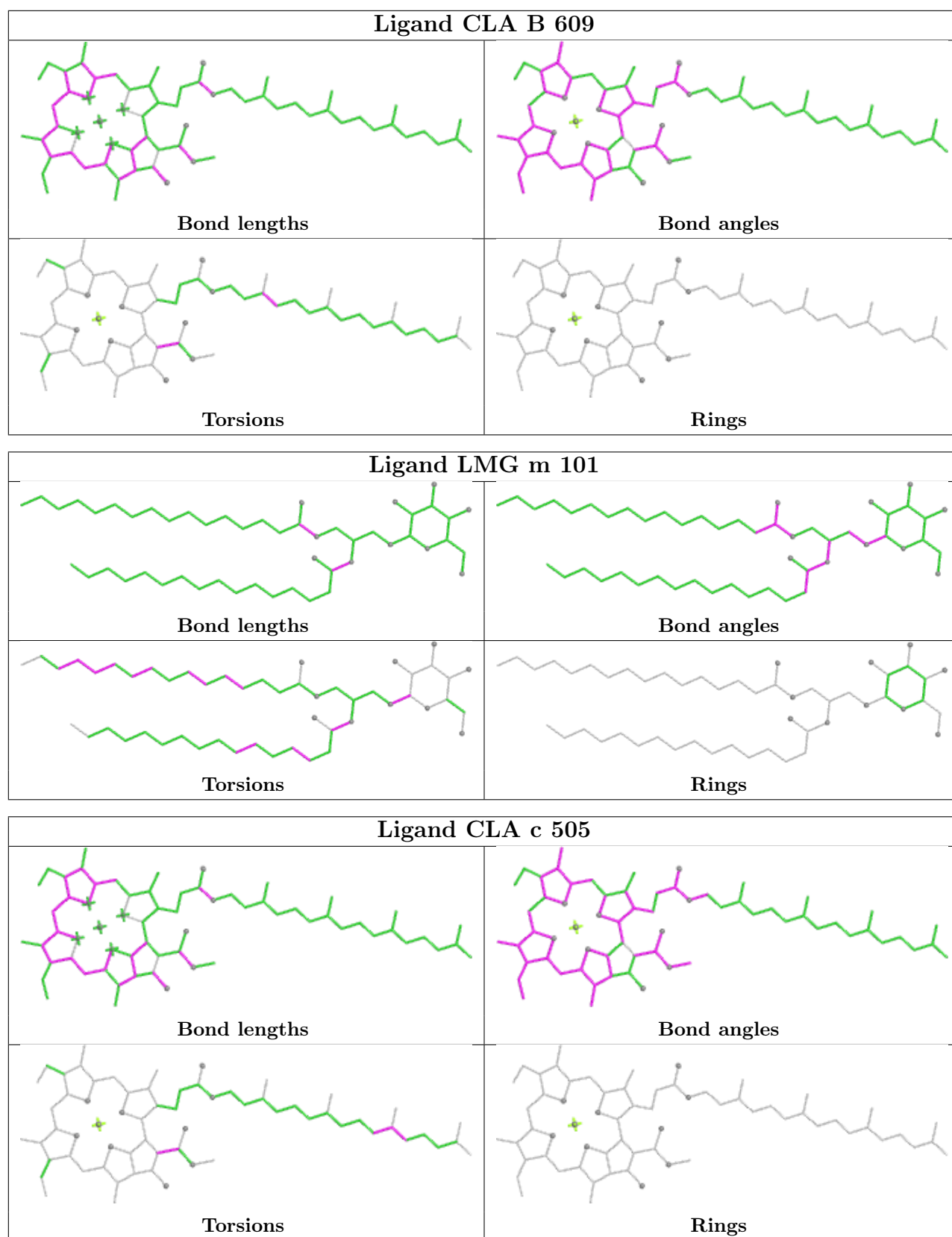


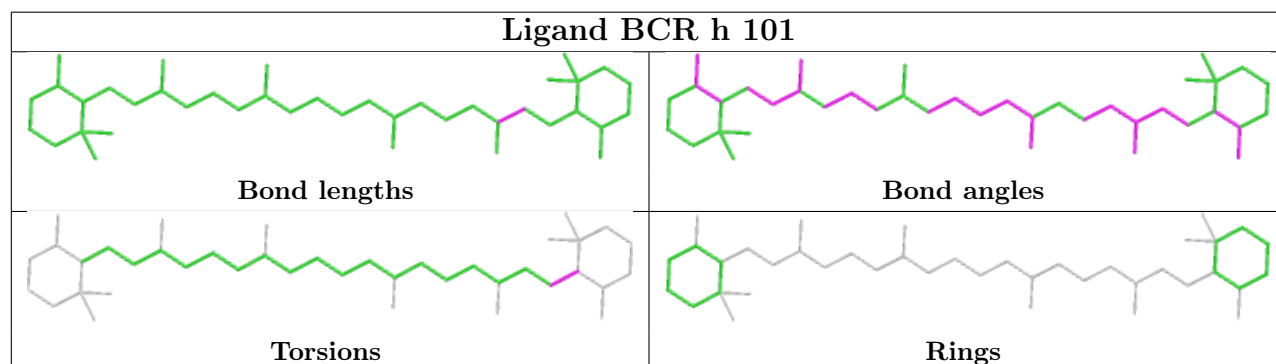
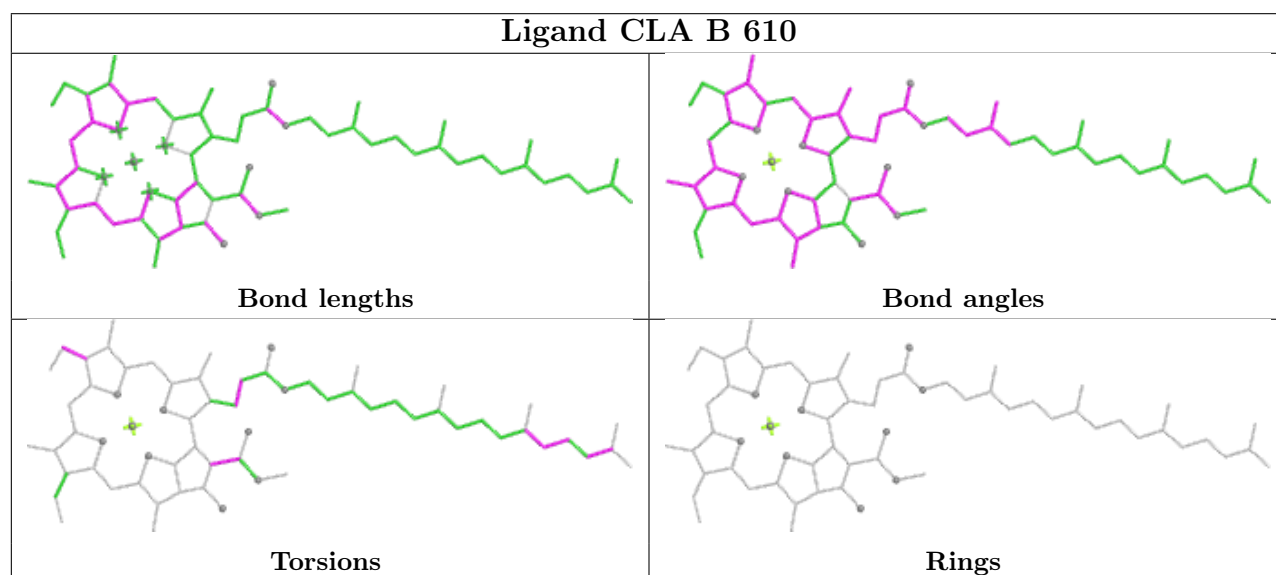
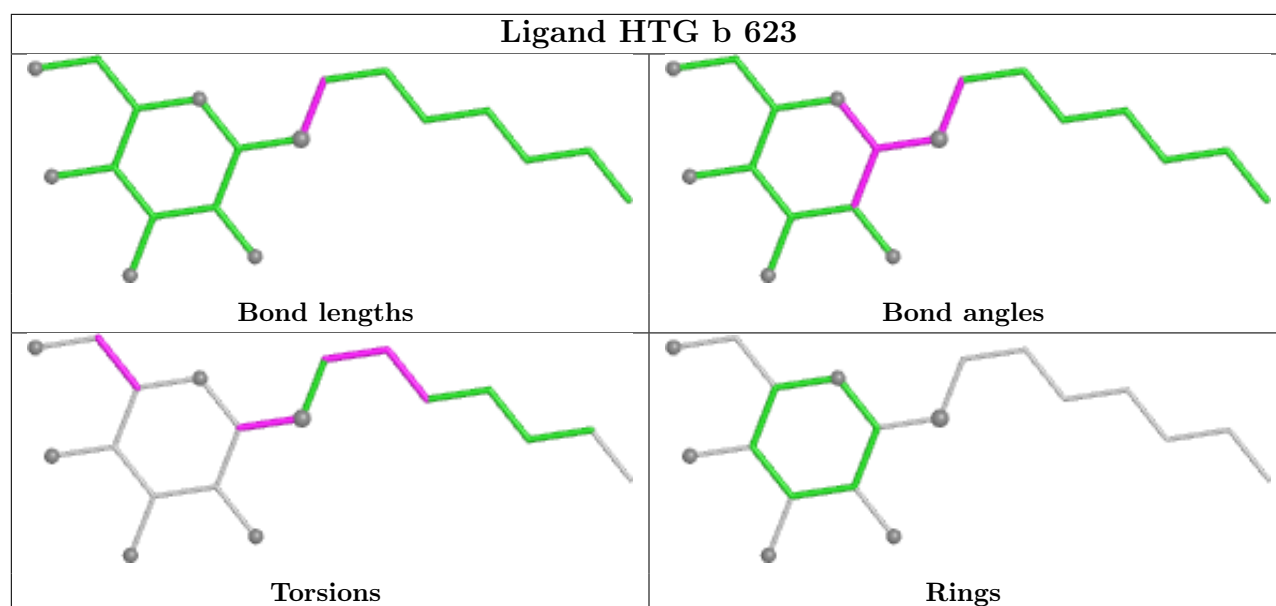


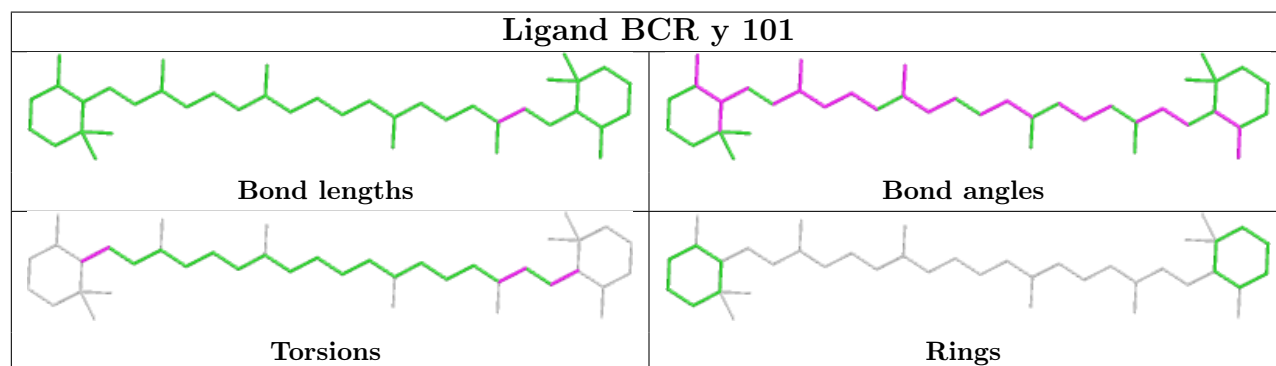
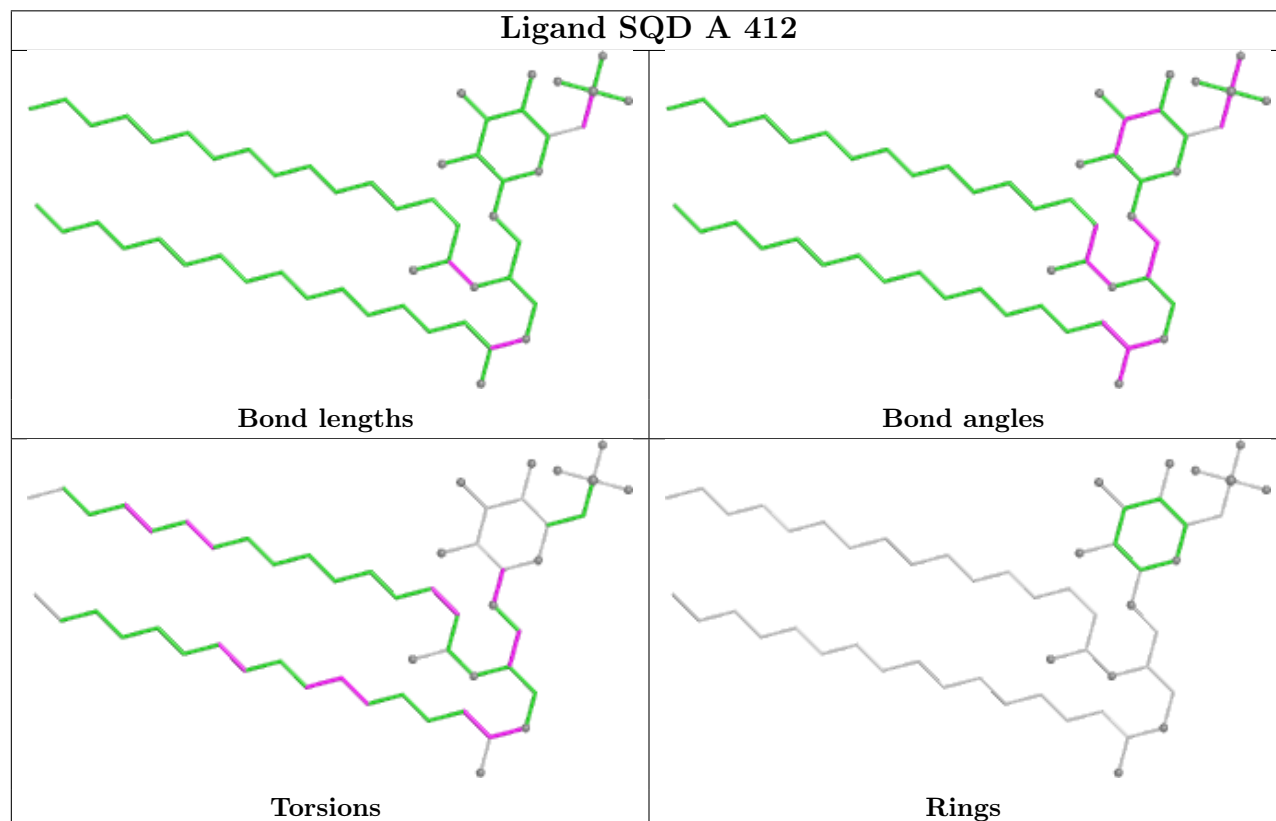
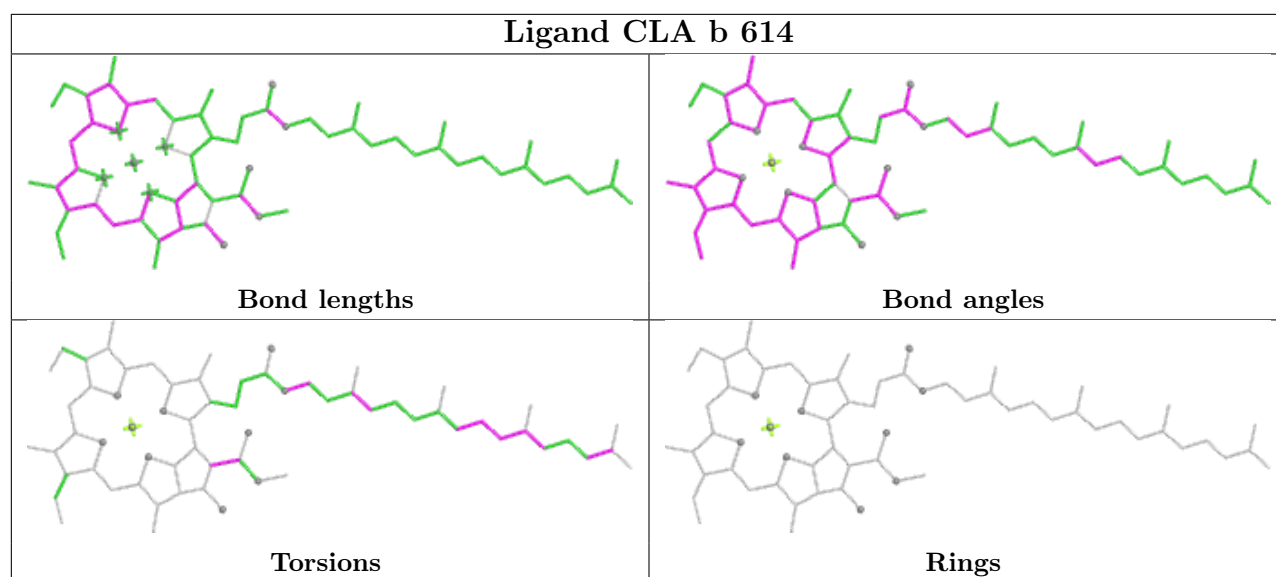


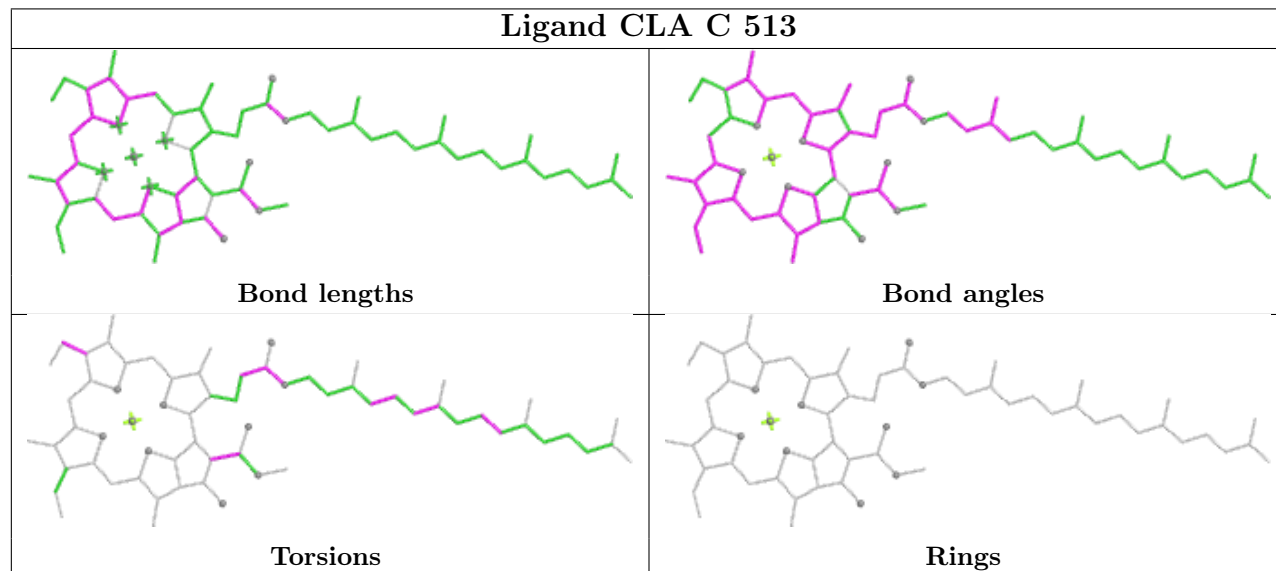
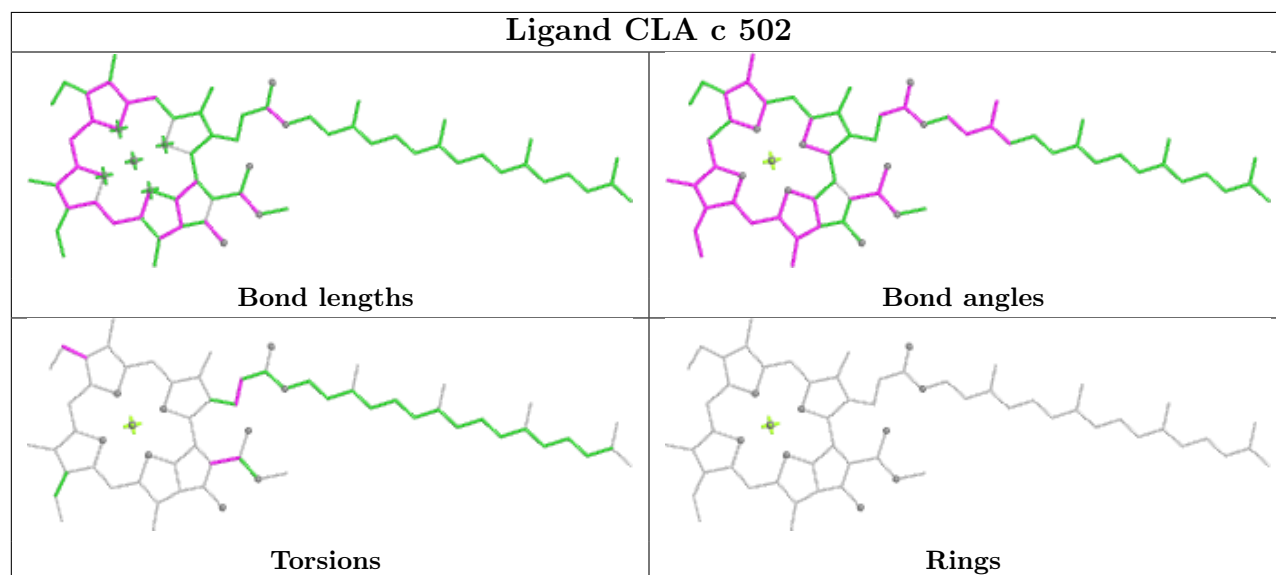
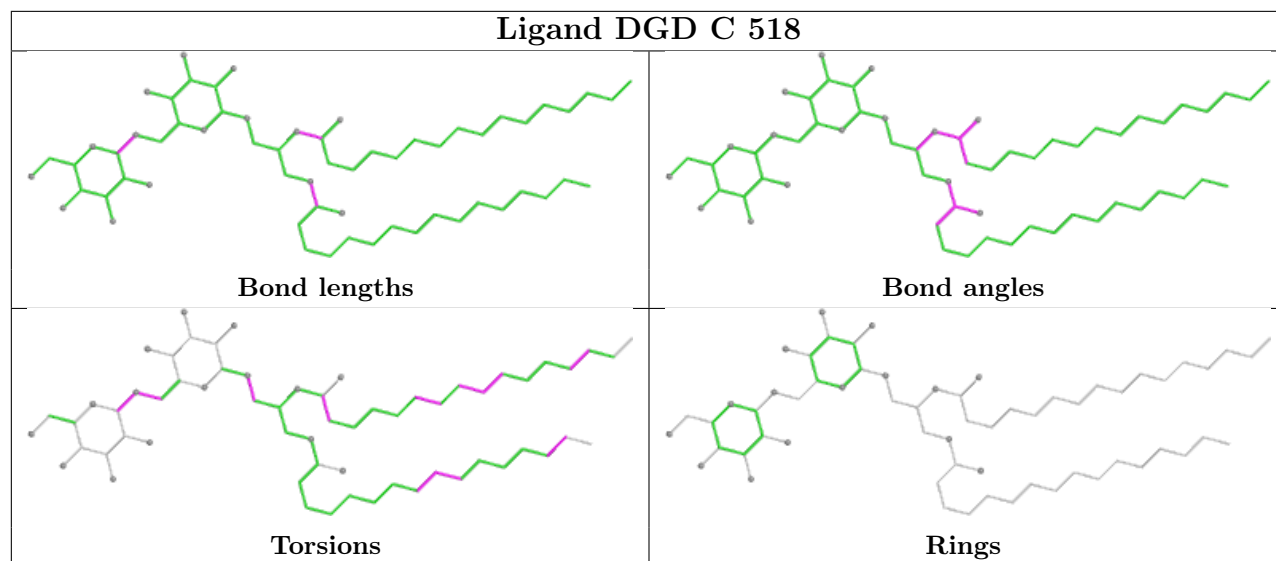


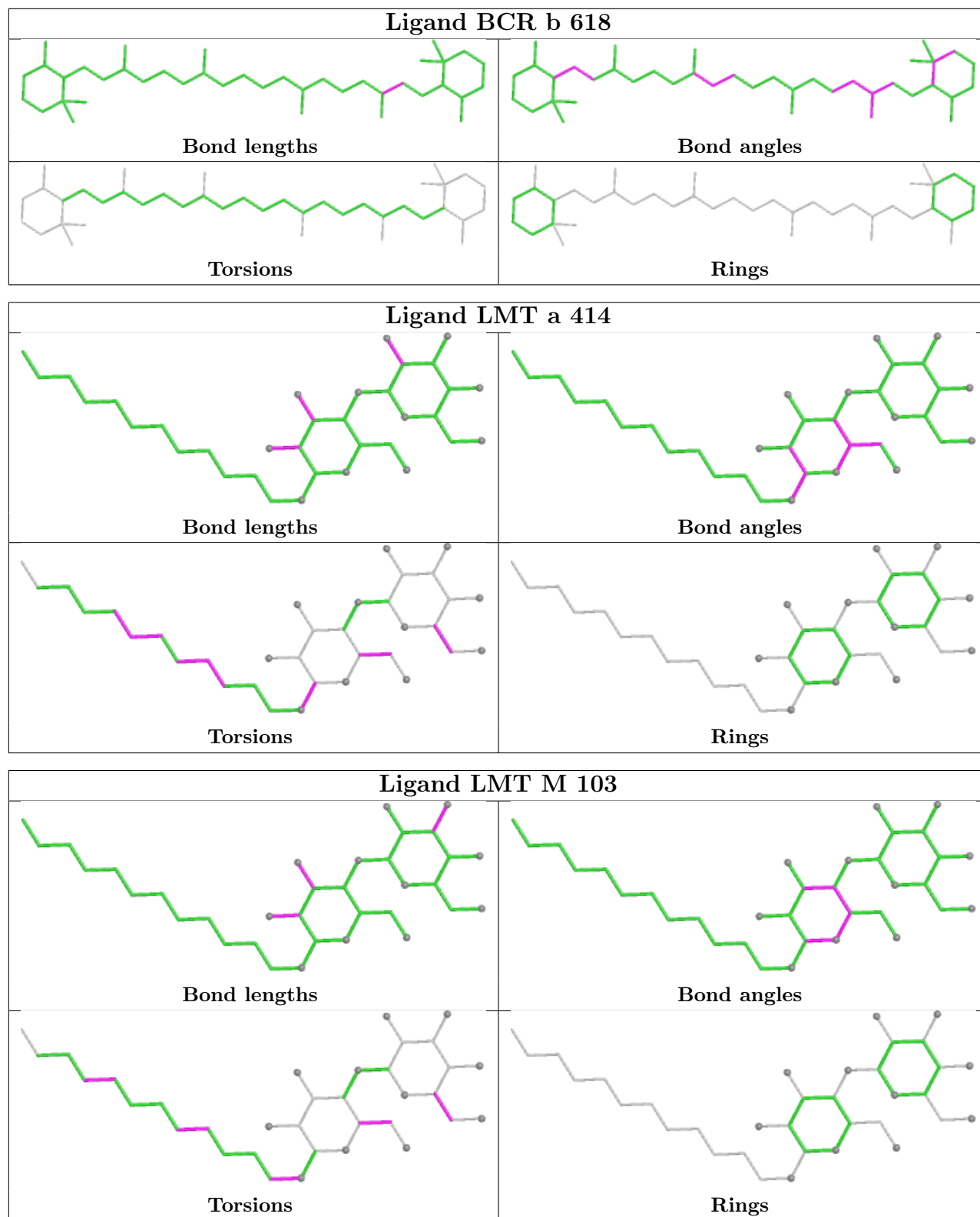


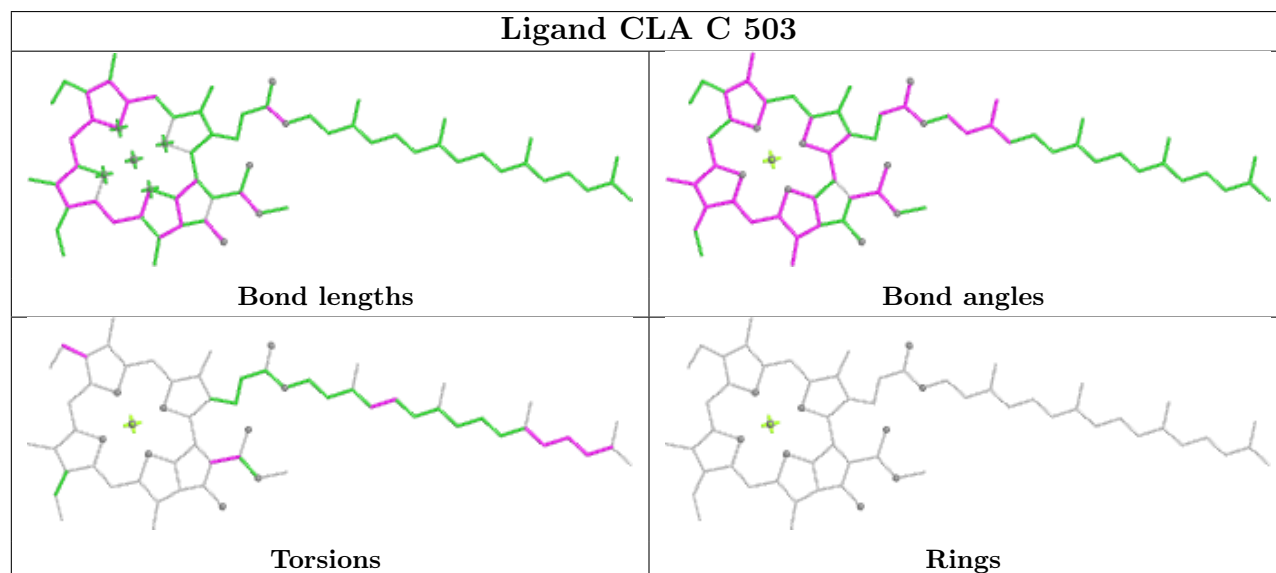
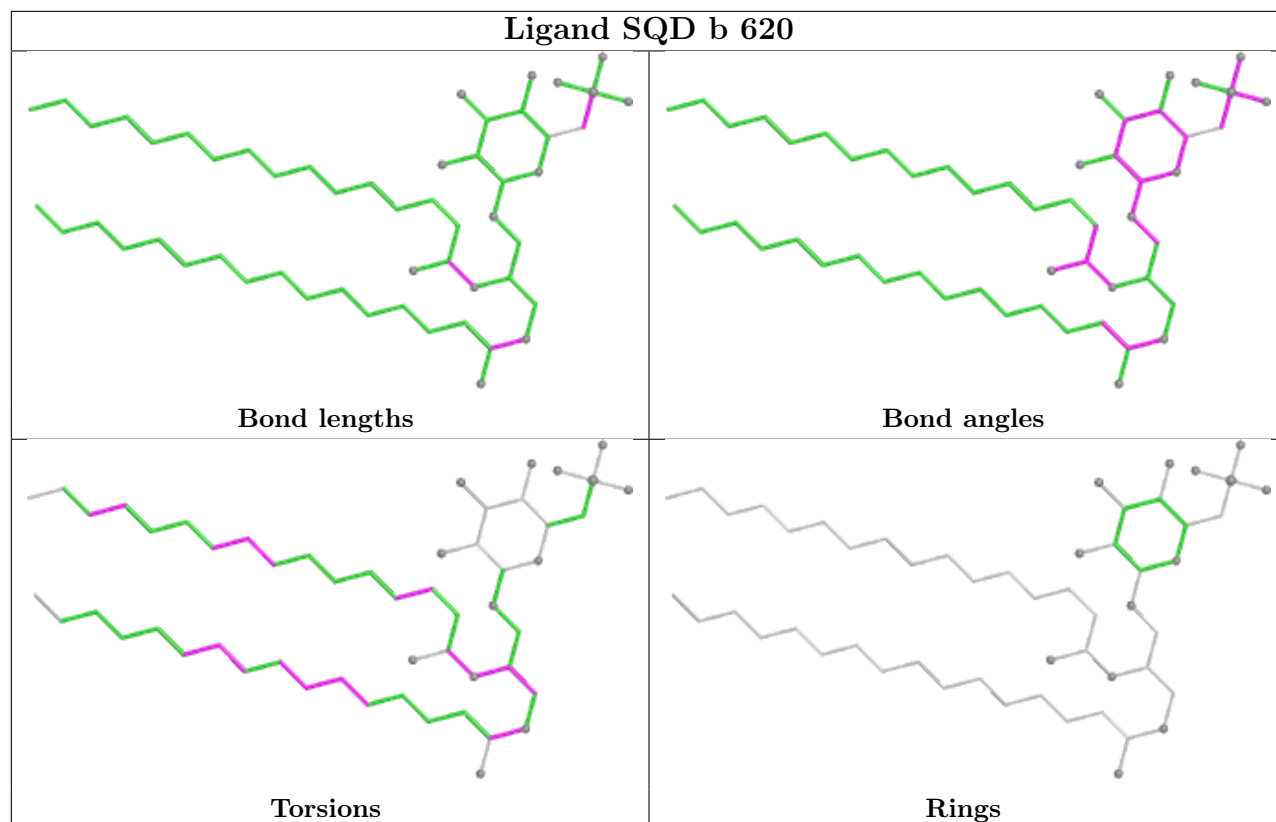


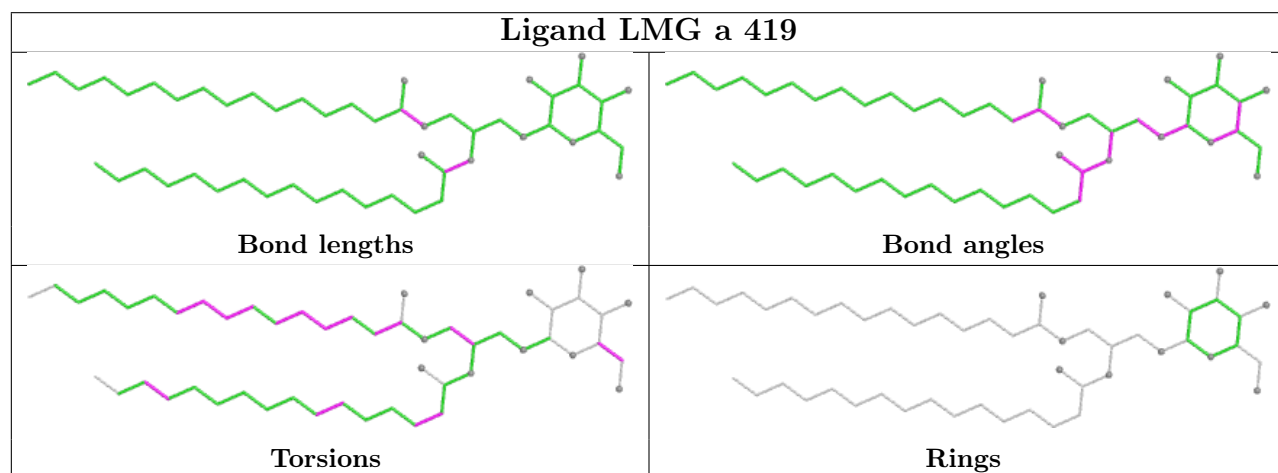
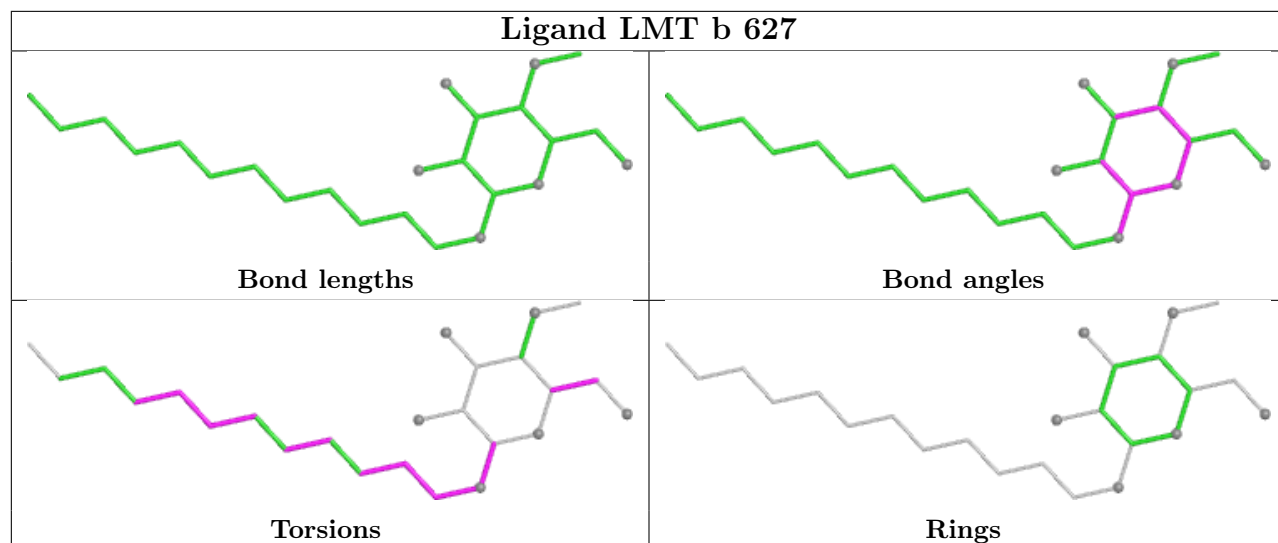




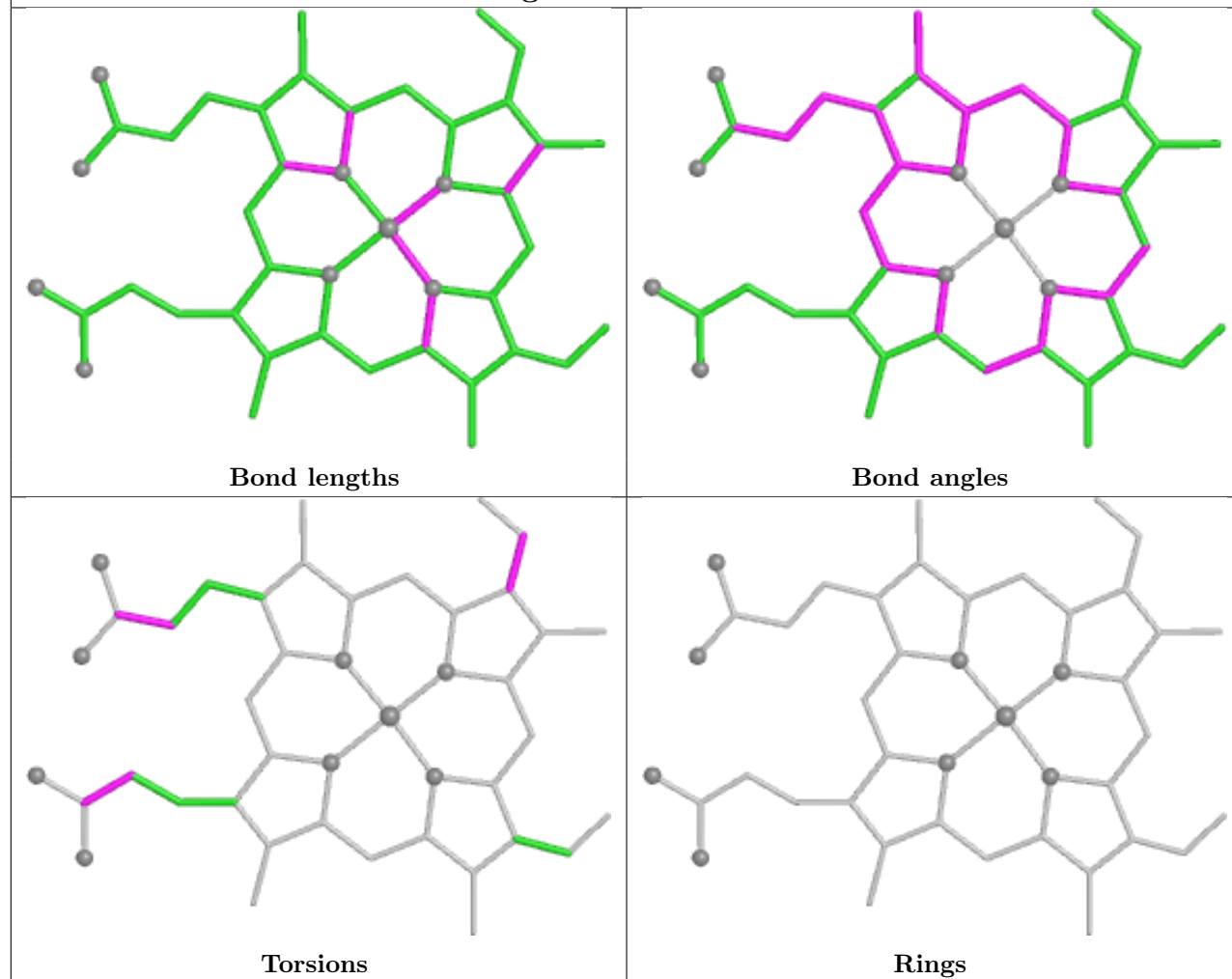




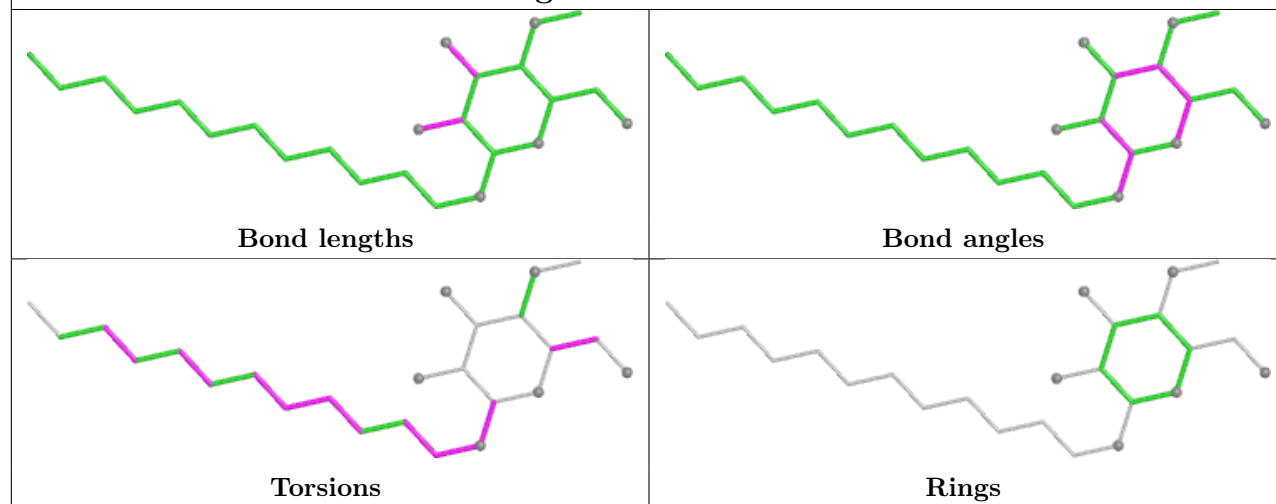


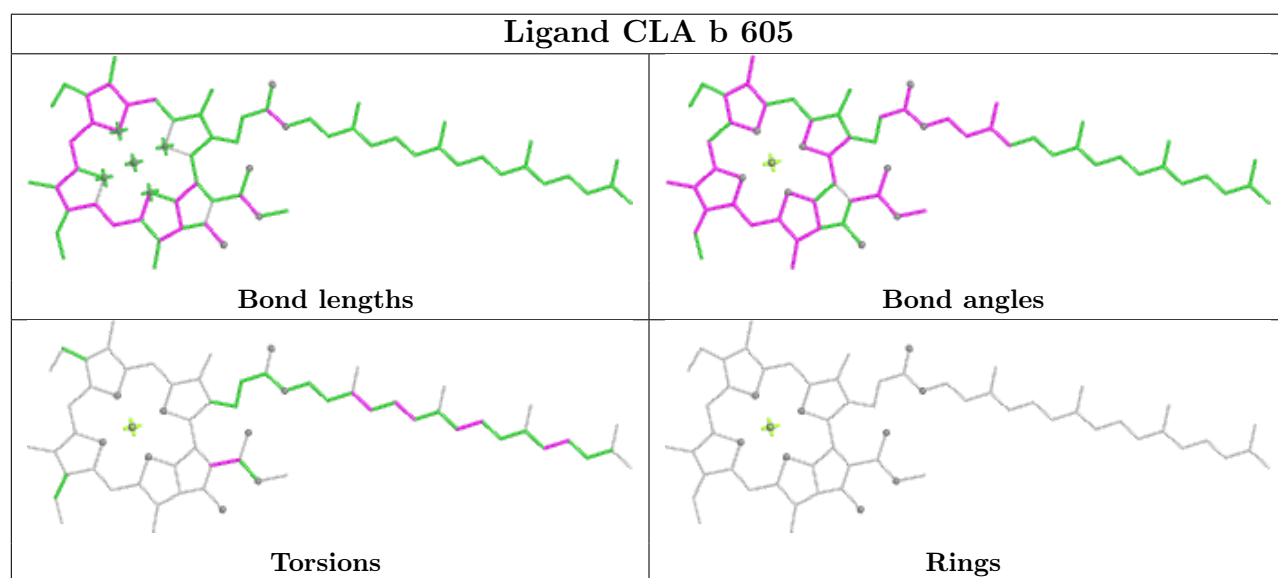
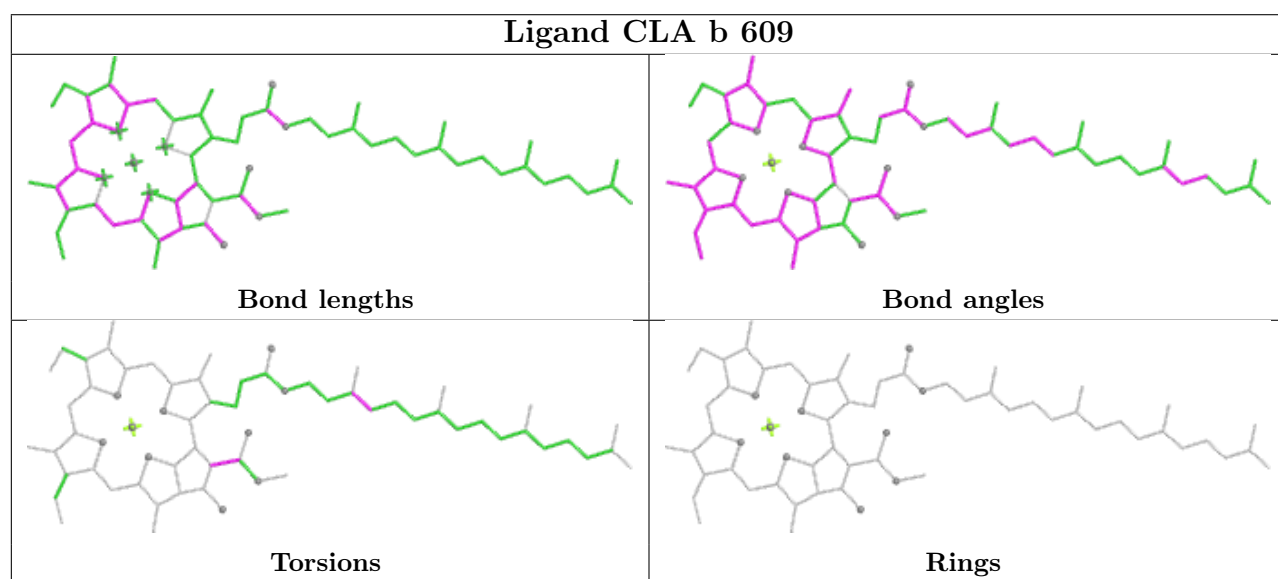
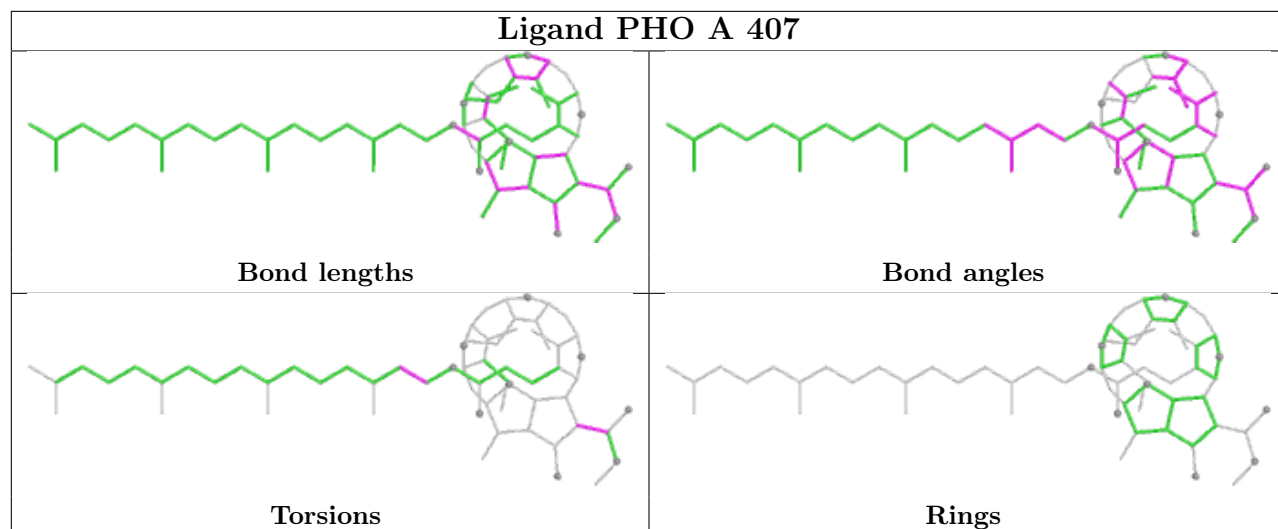


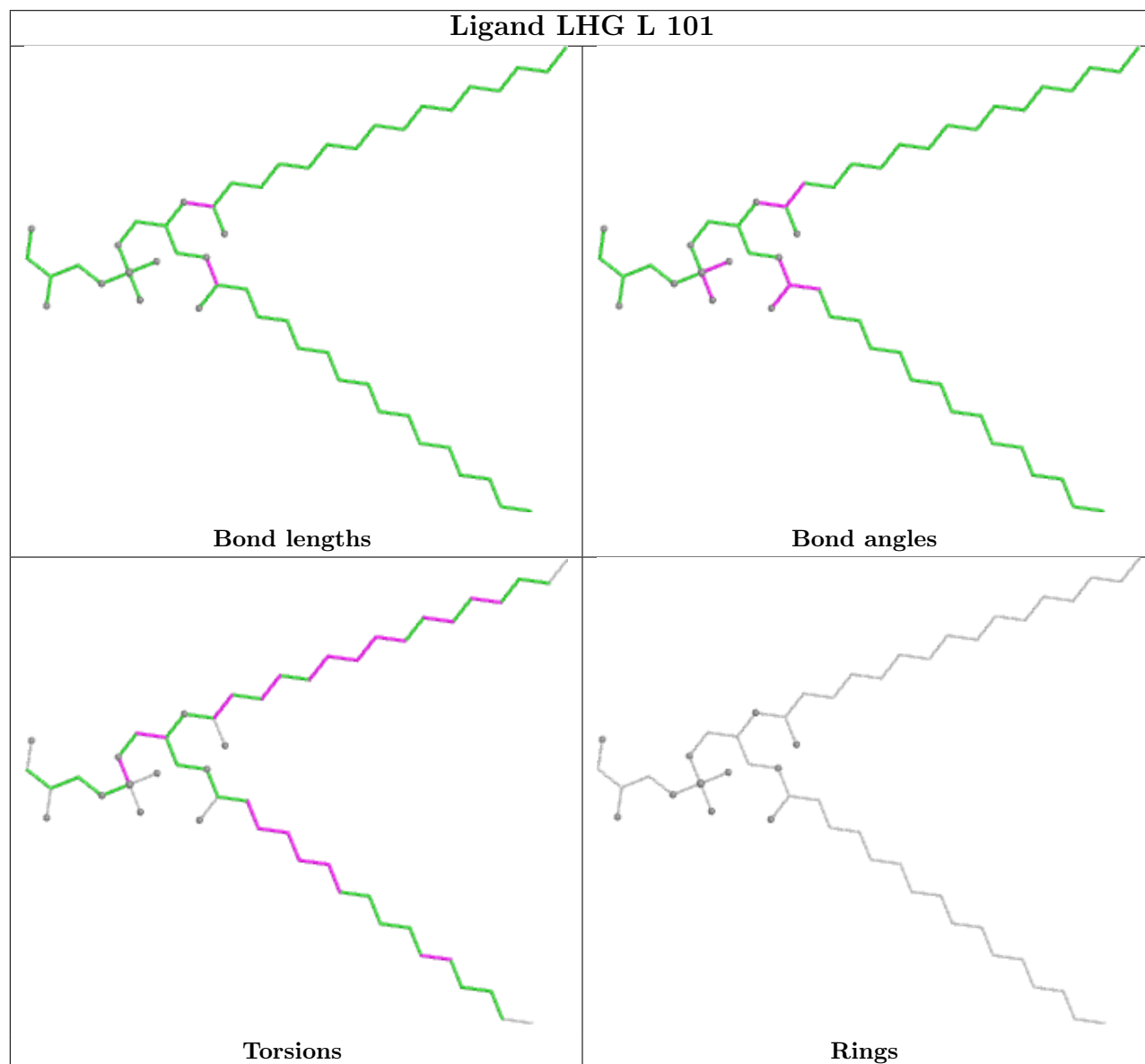
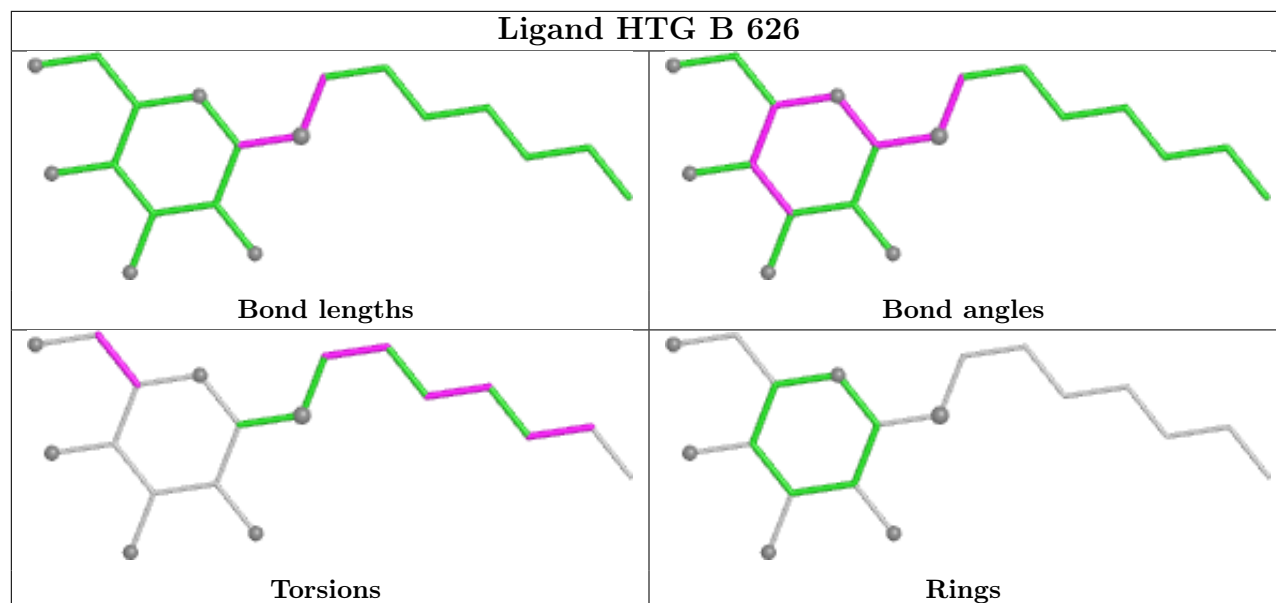
Ligand HEM e 87



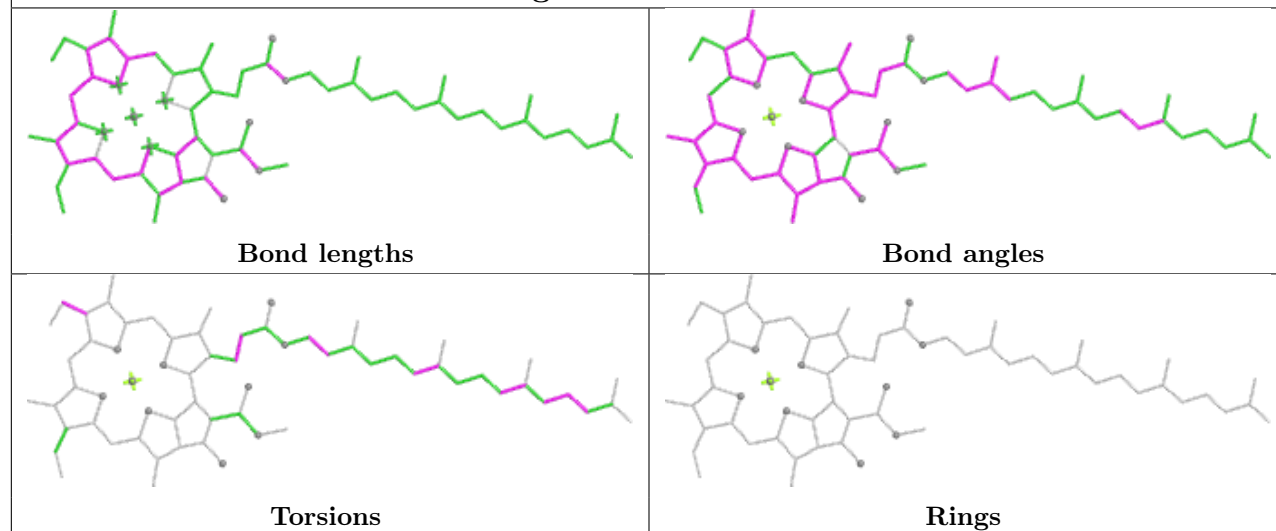
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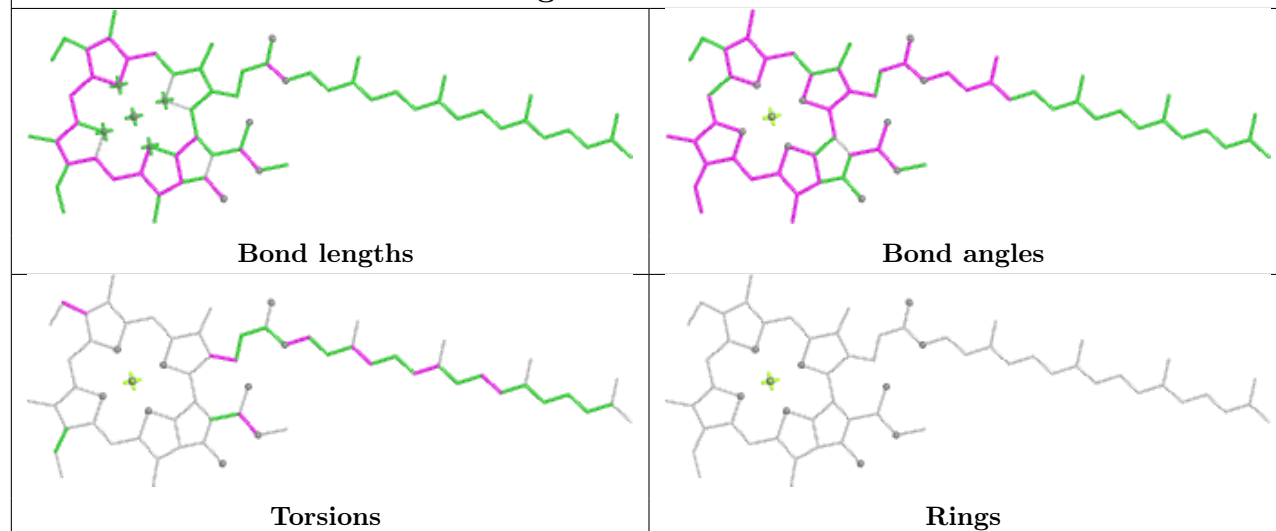




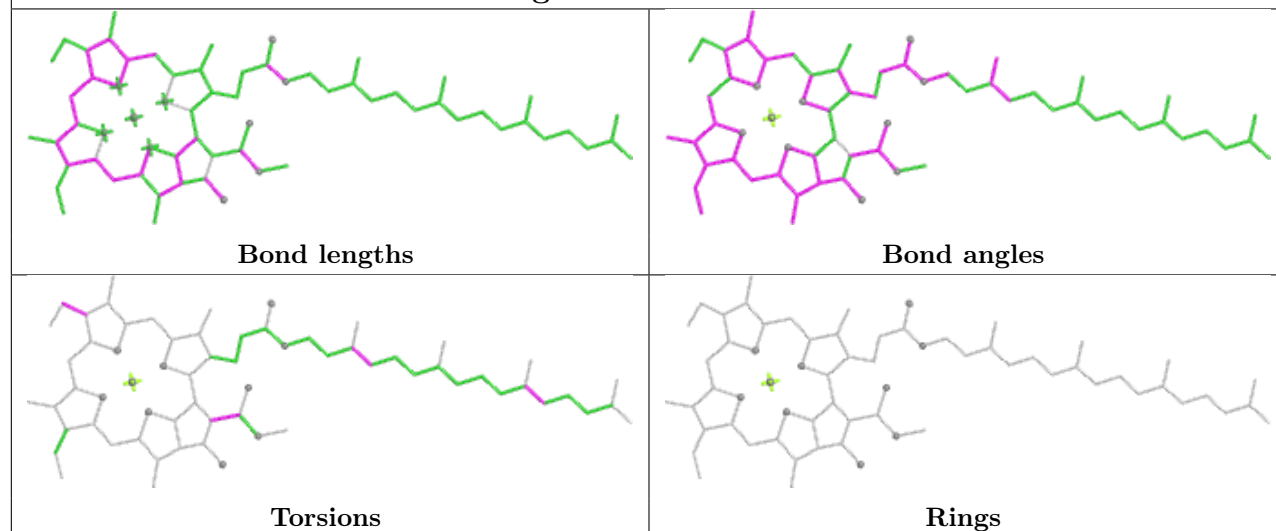
Ligand CLA B 602

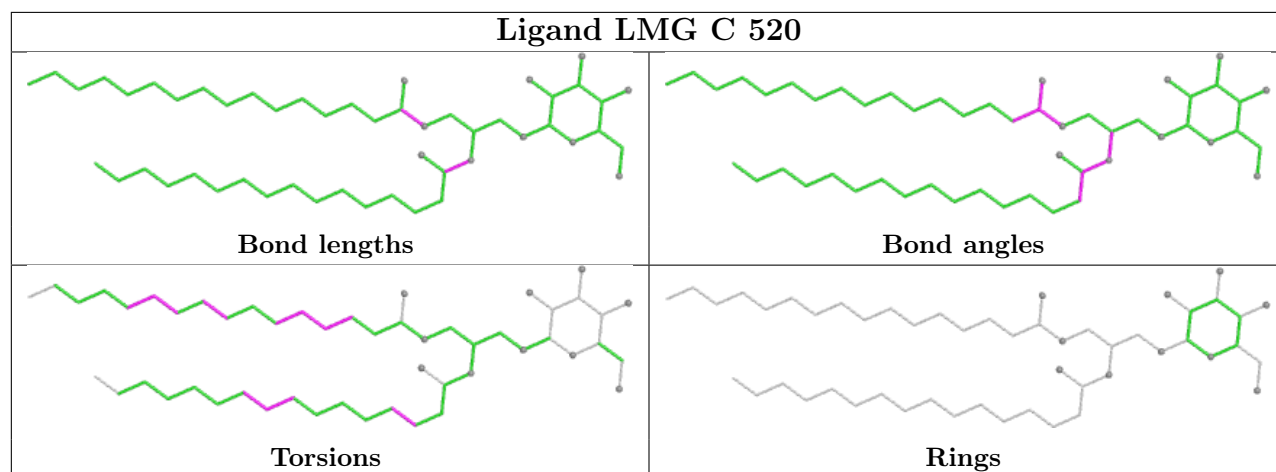
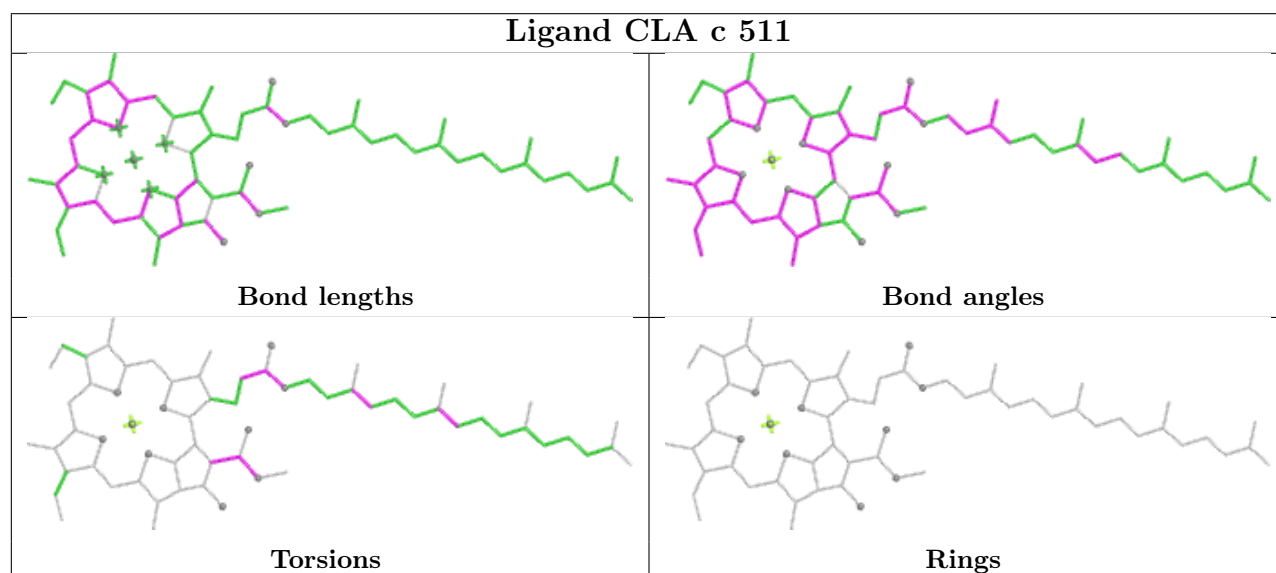
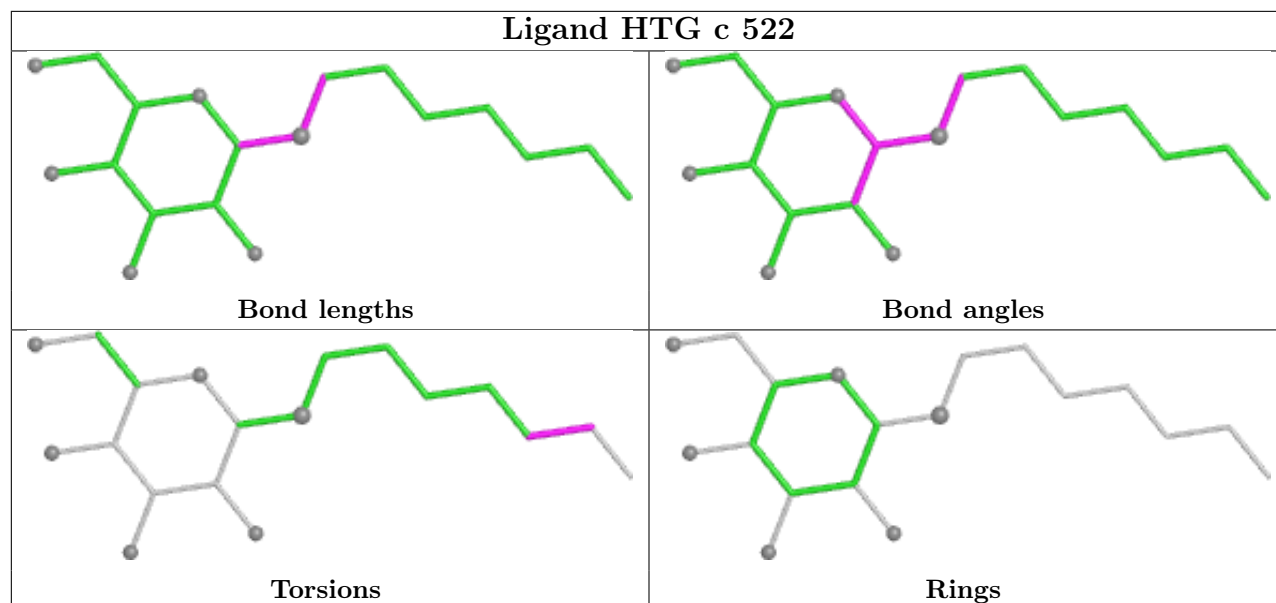


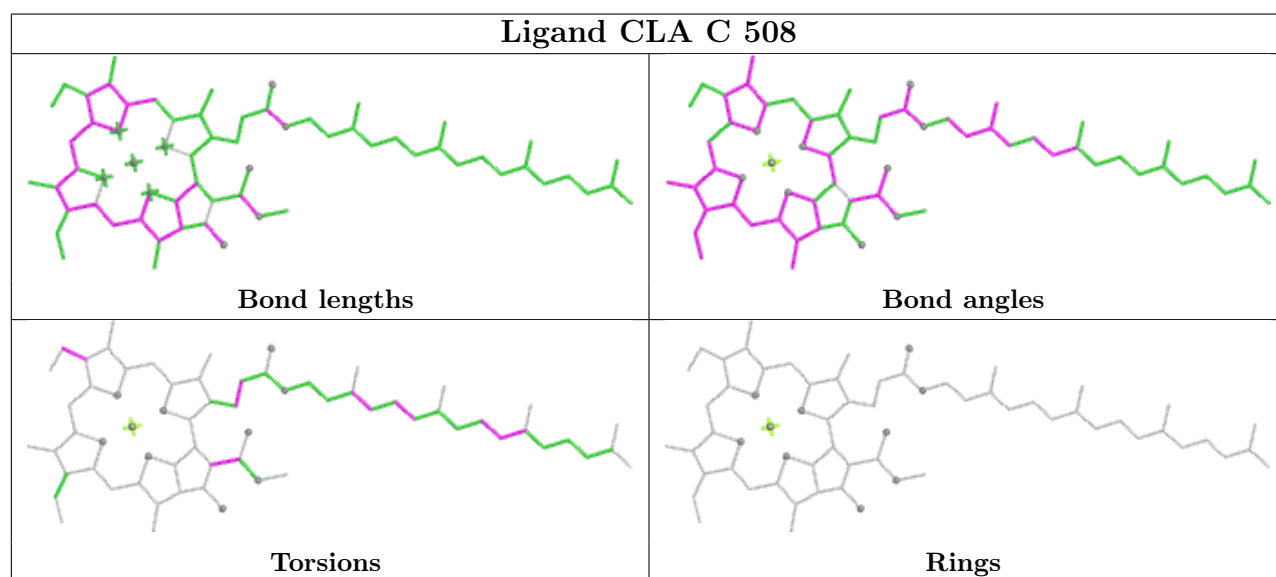
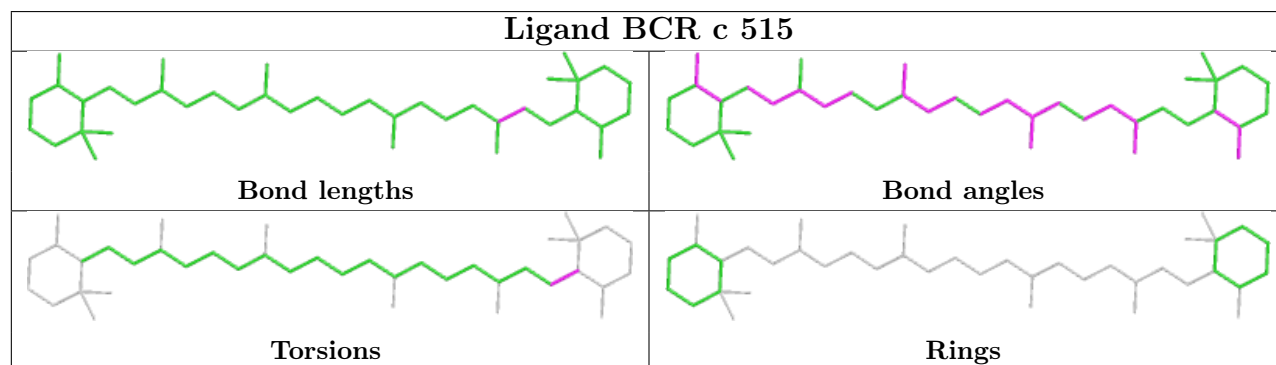
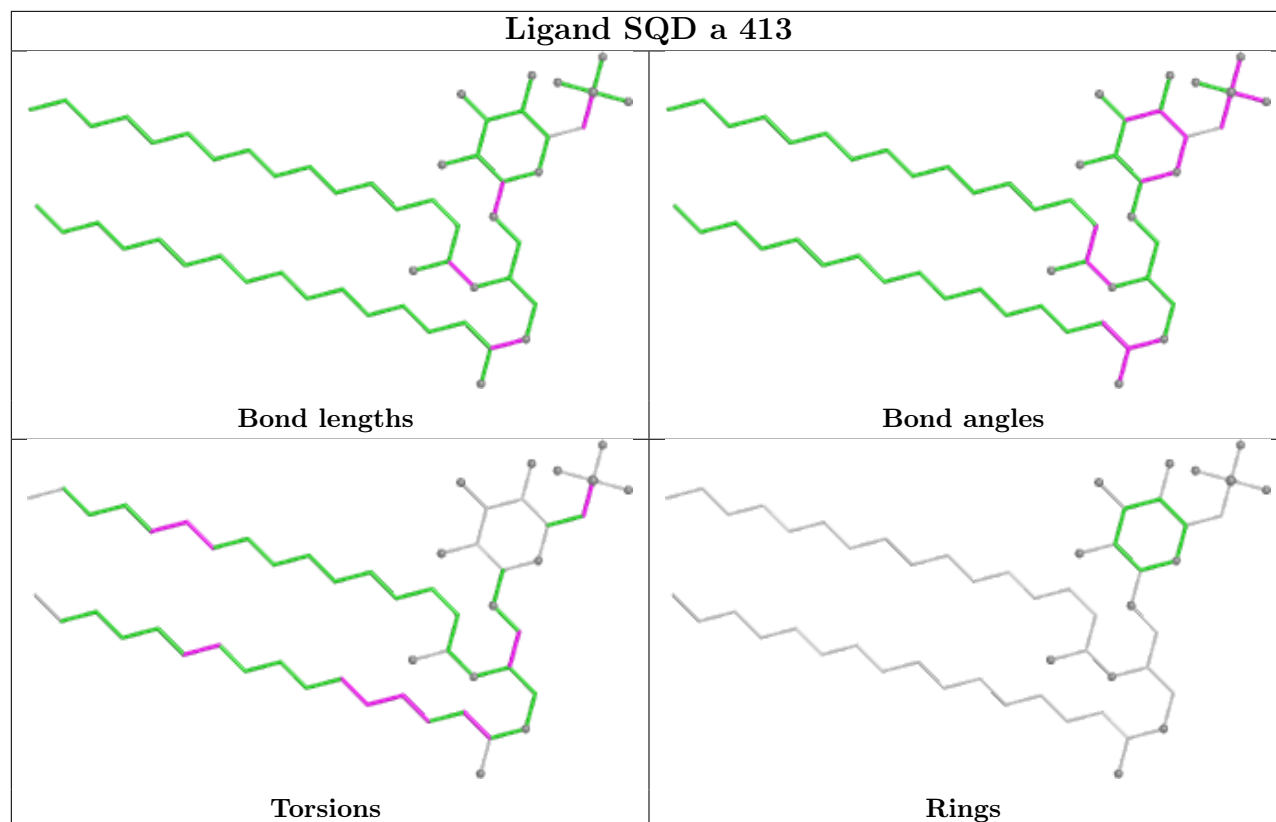
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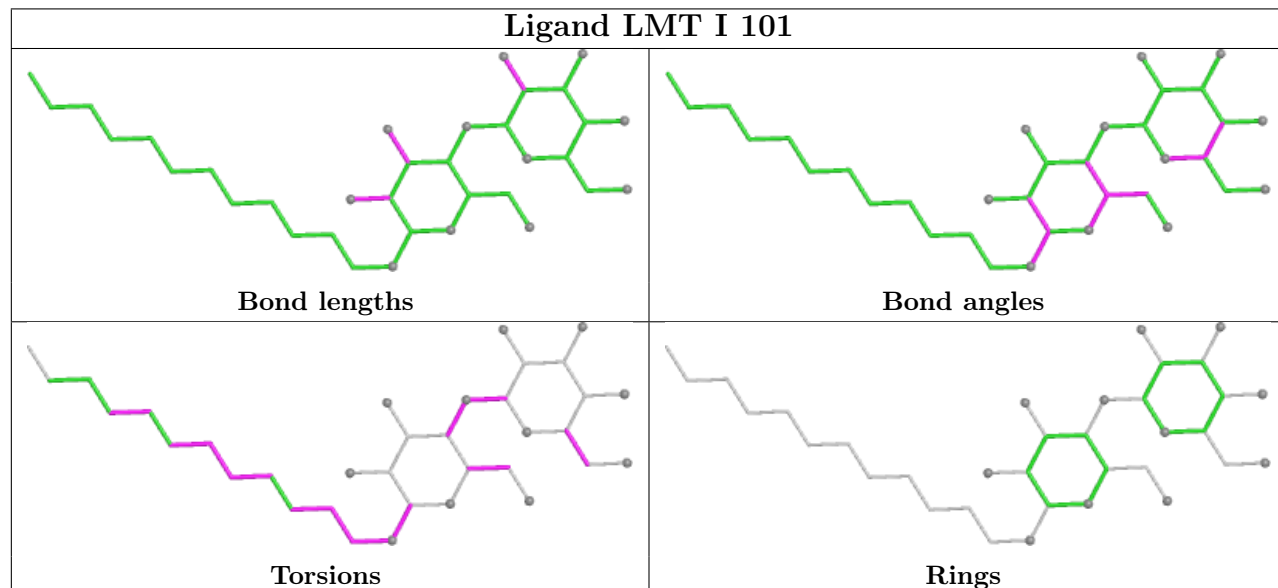
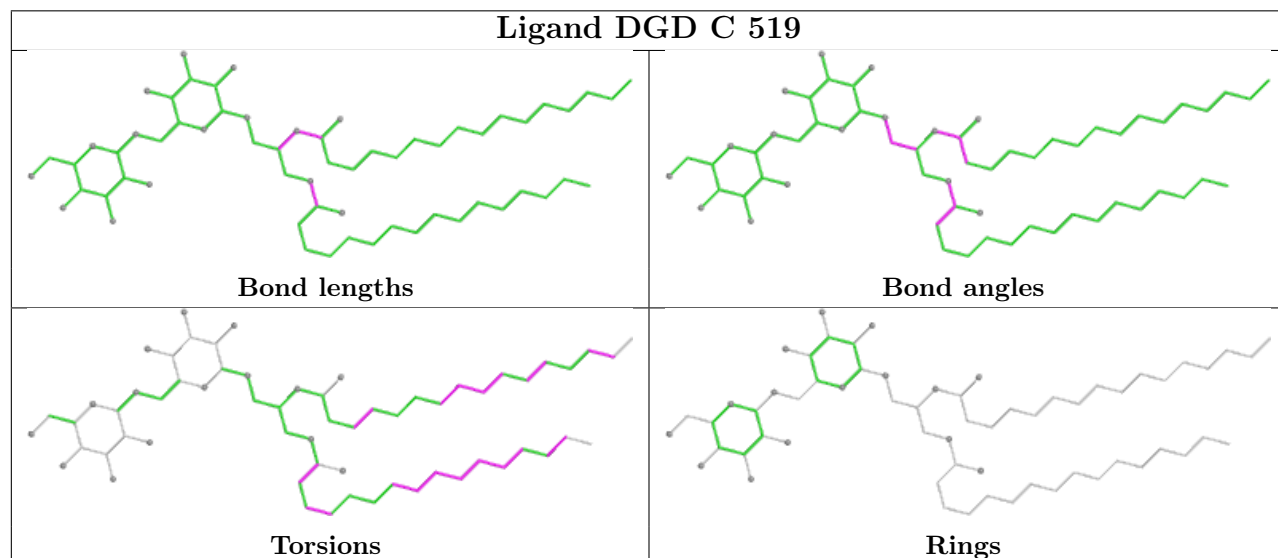
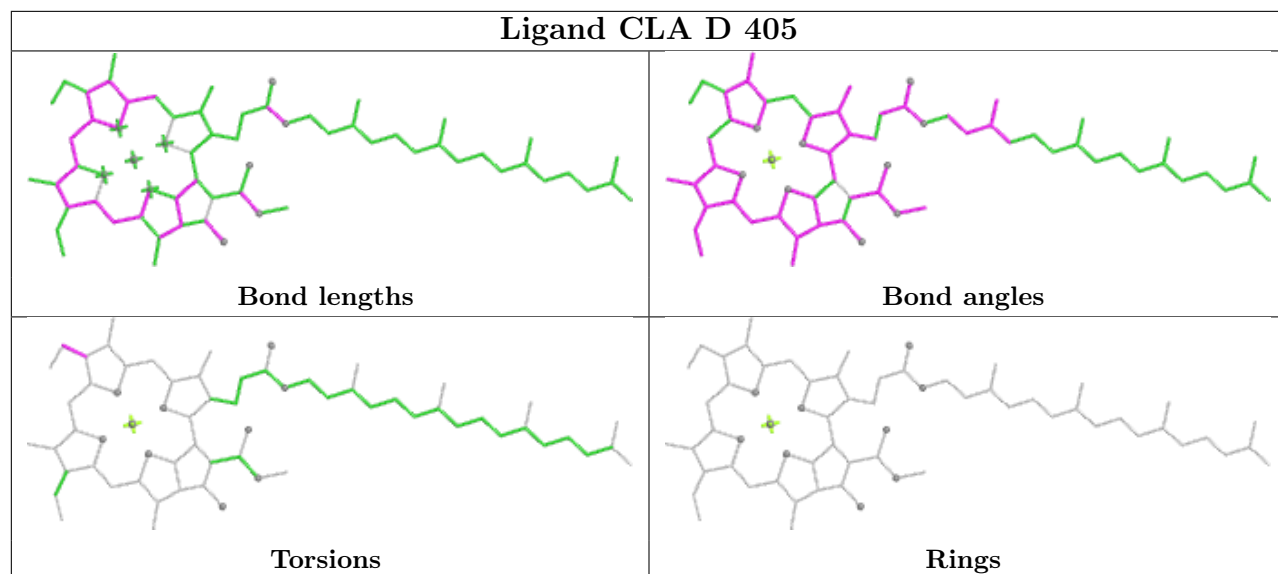


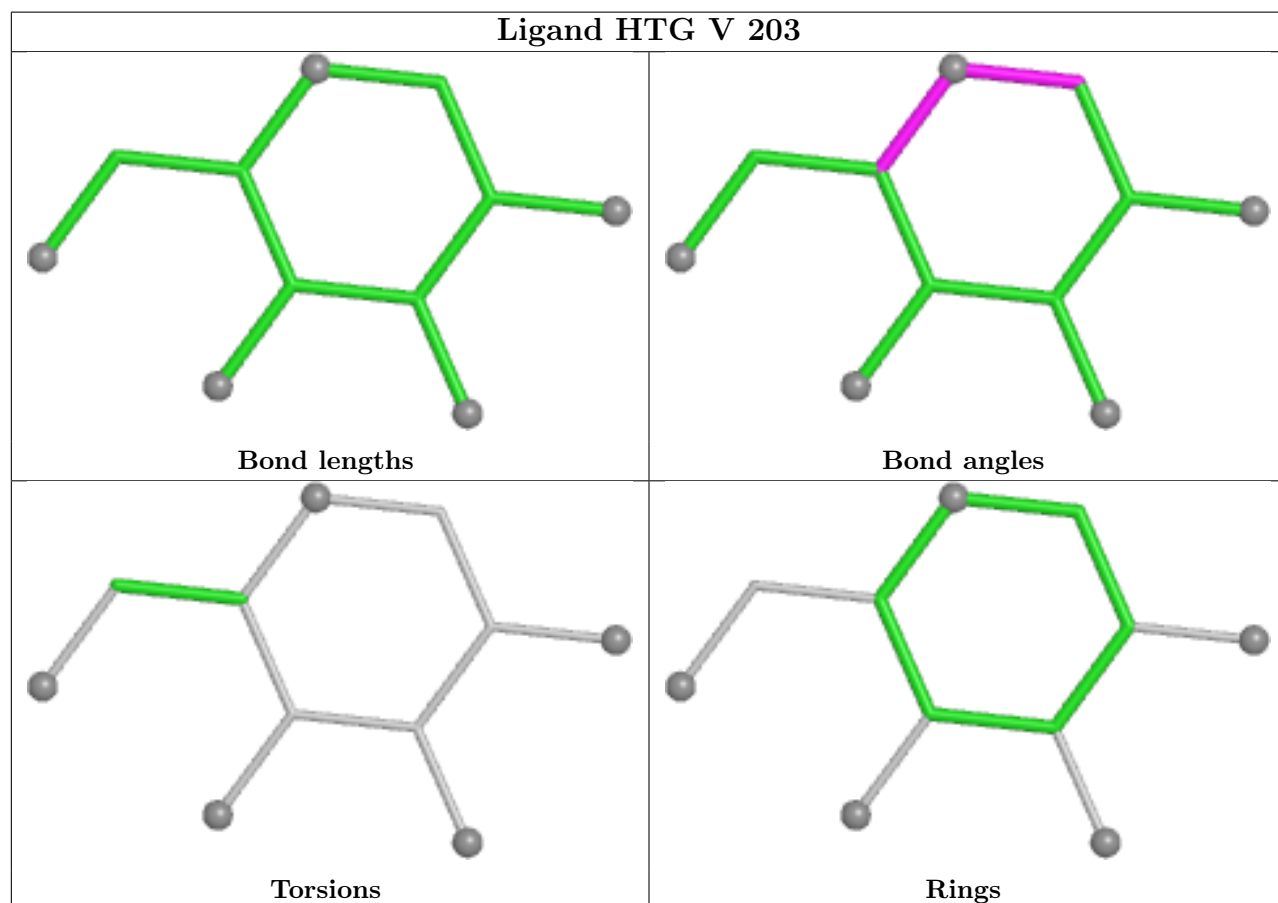
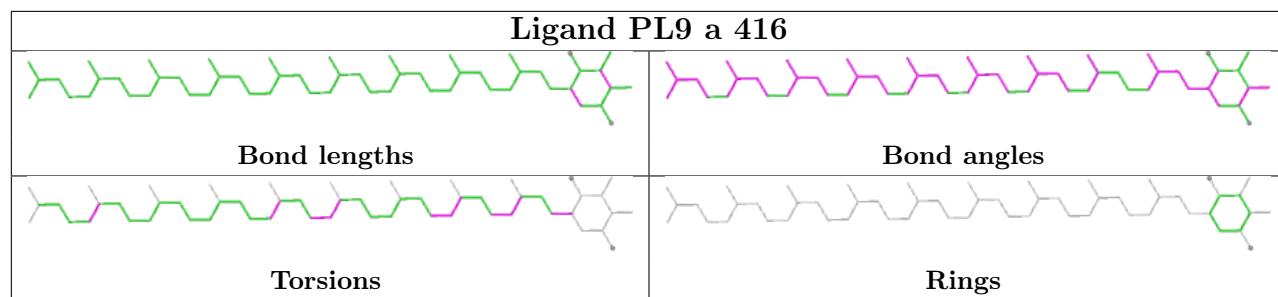
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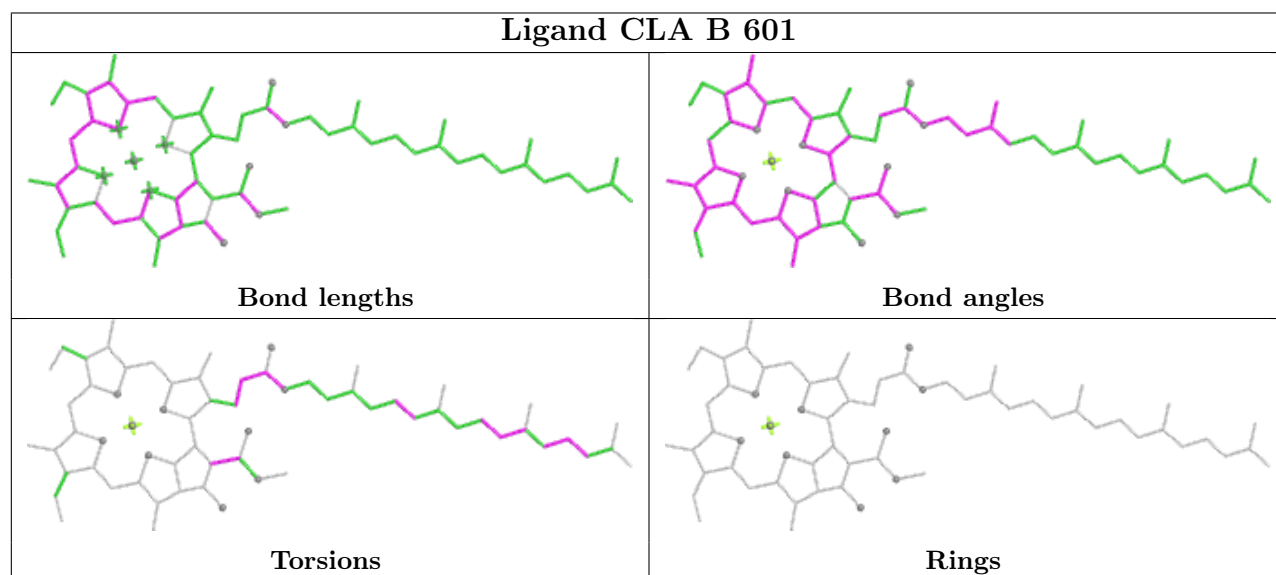
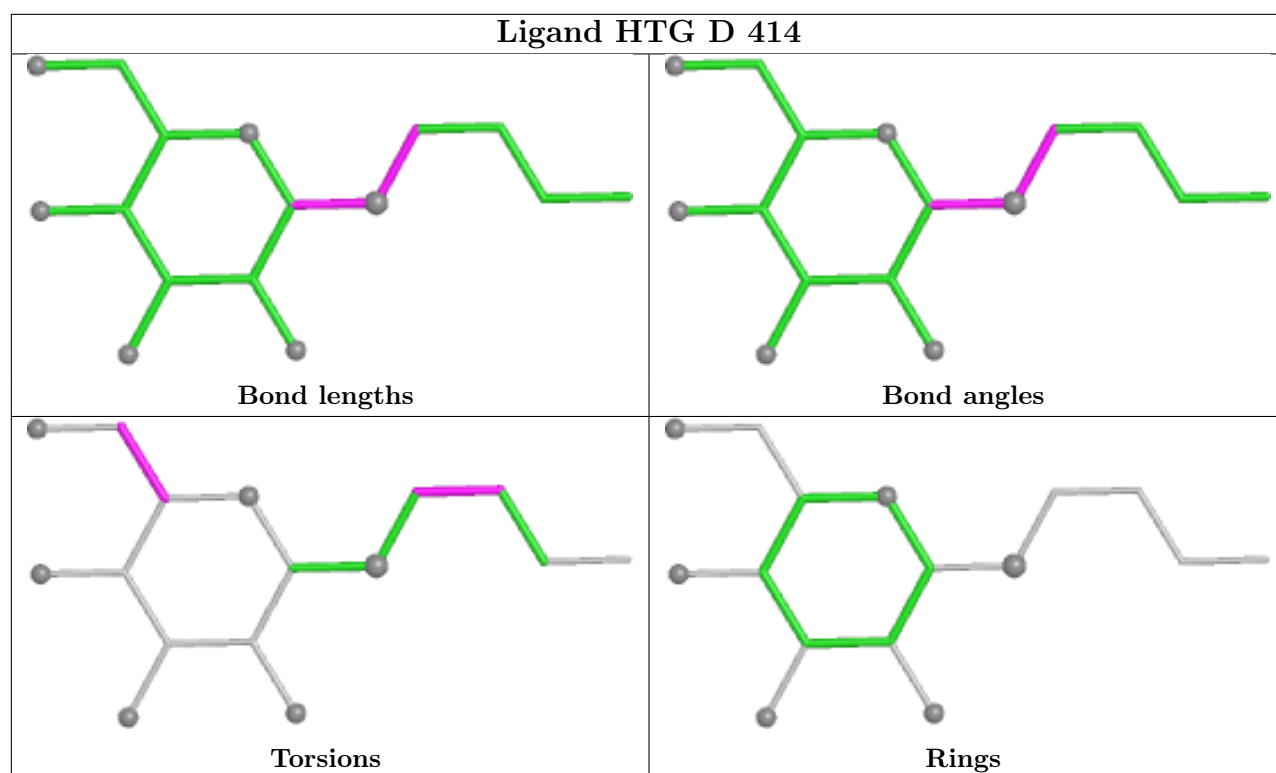


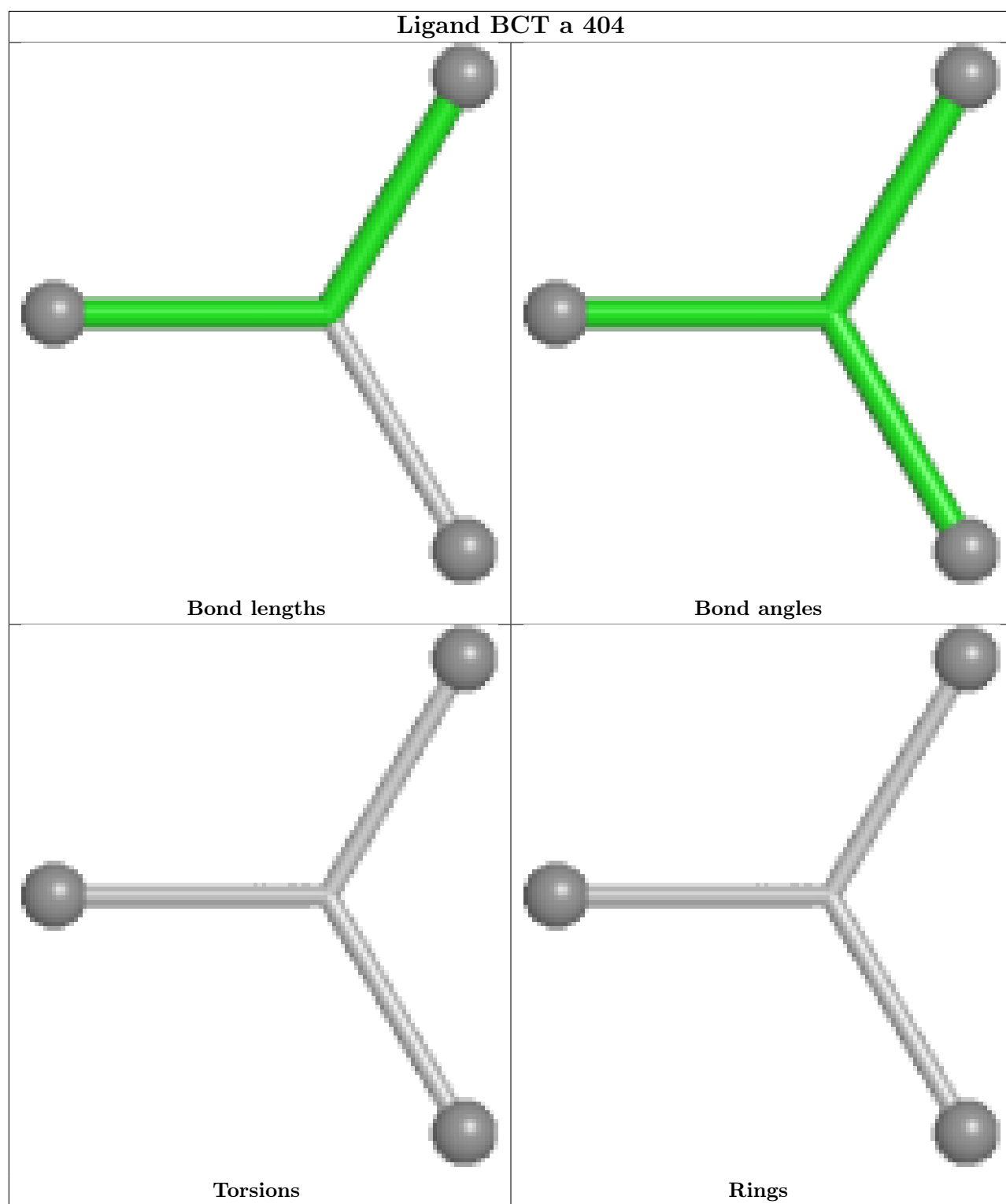


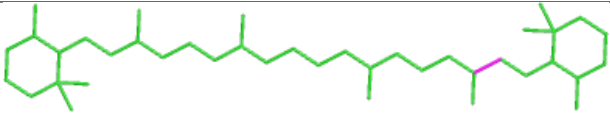
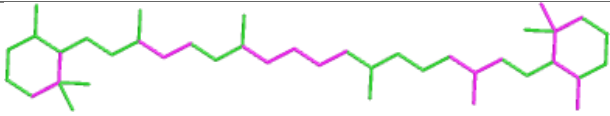
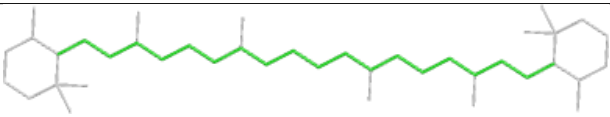
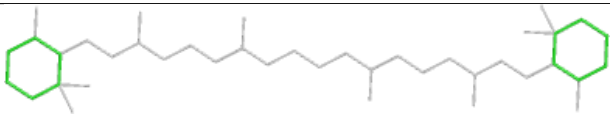
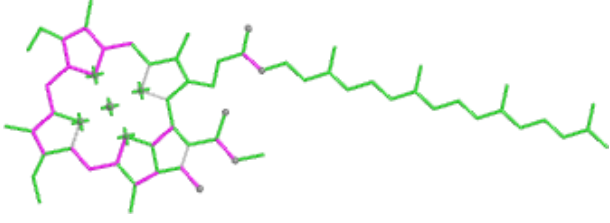
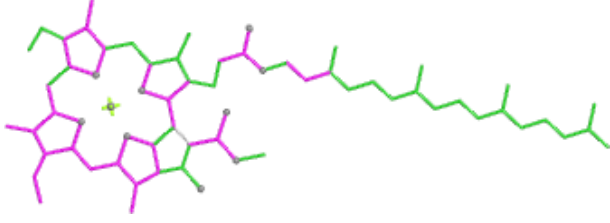
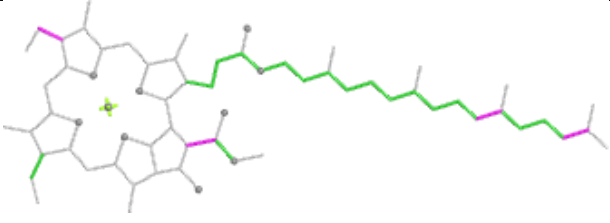
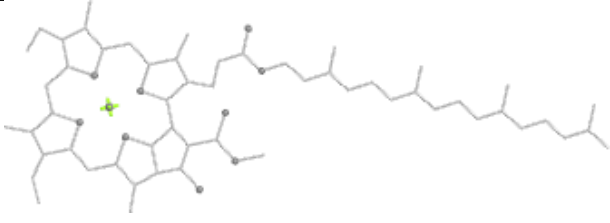
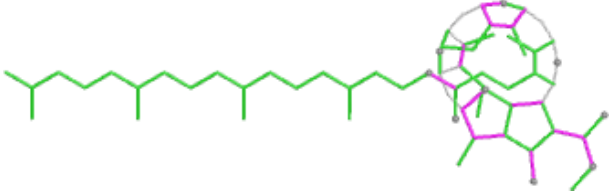
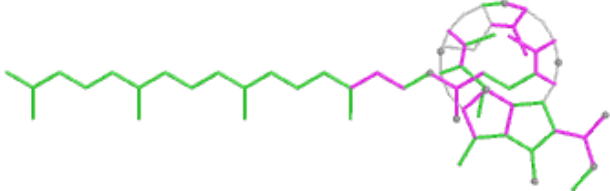
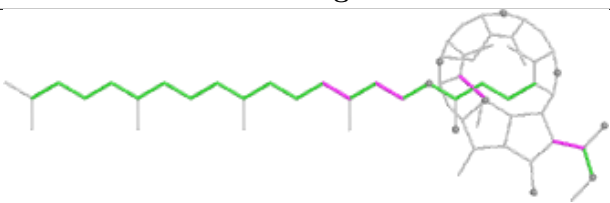
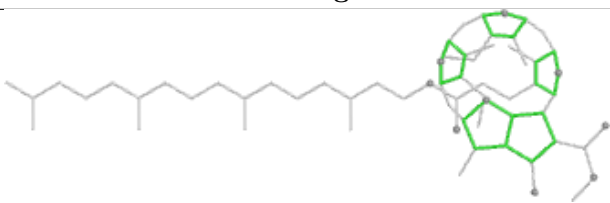


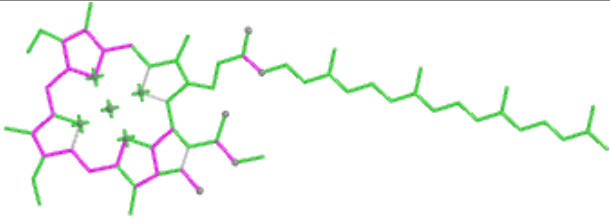
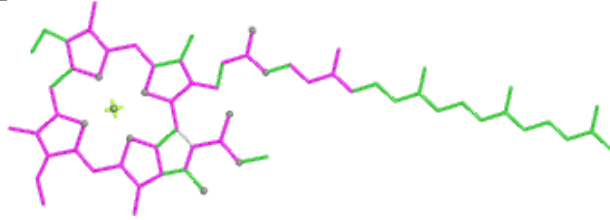
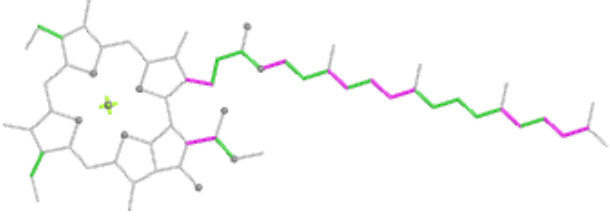
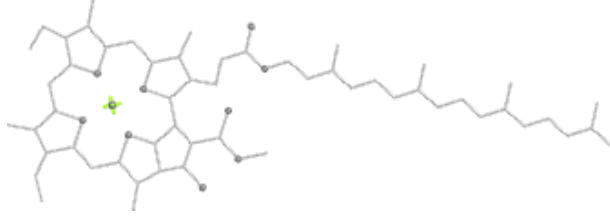
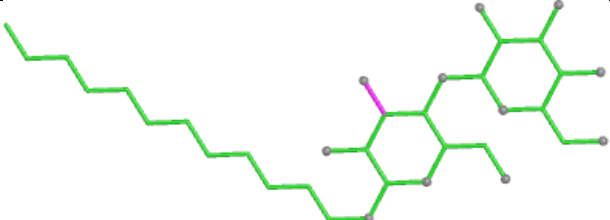
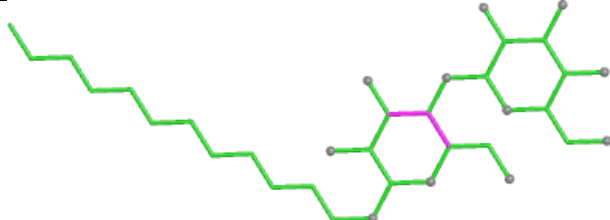
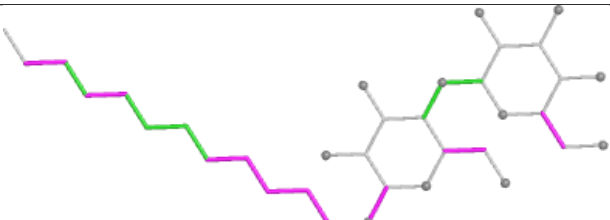
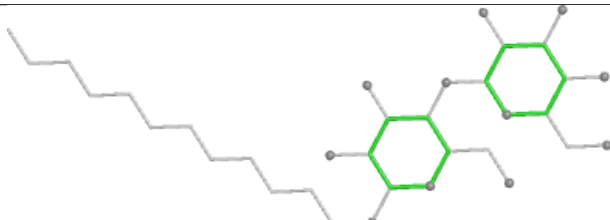
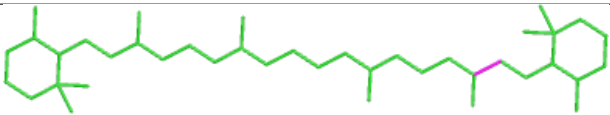
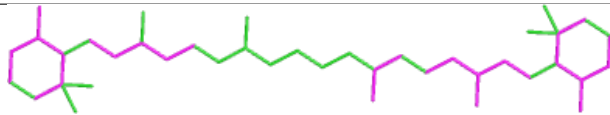
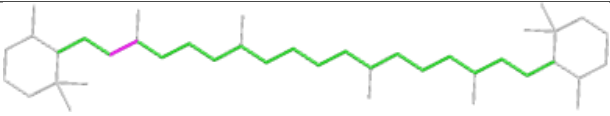
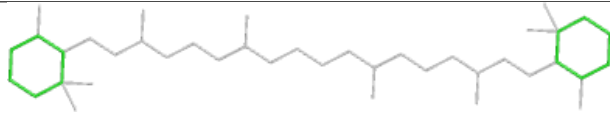


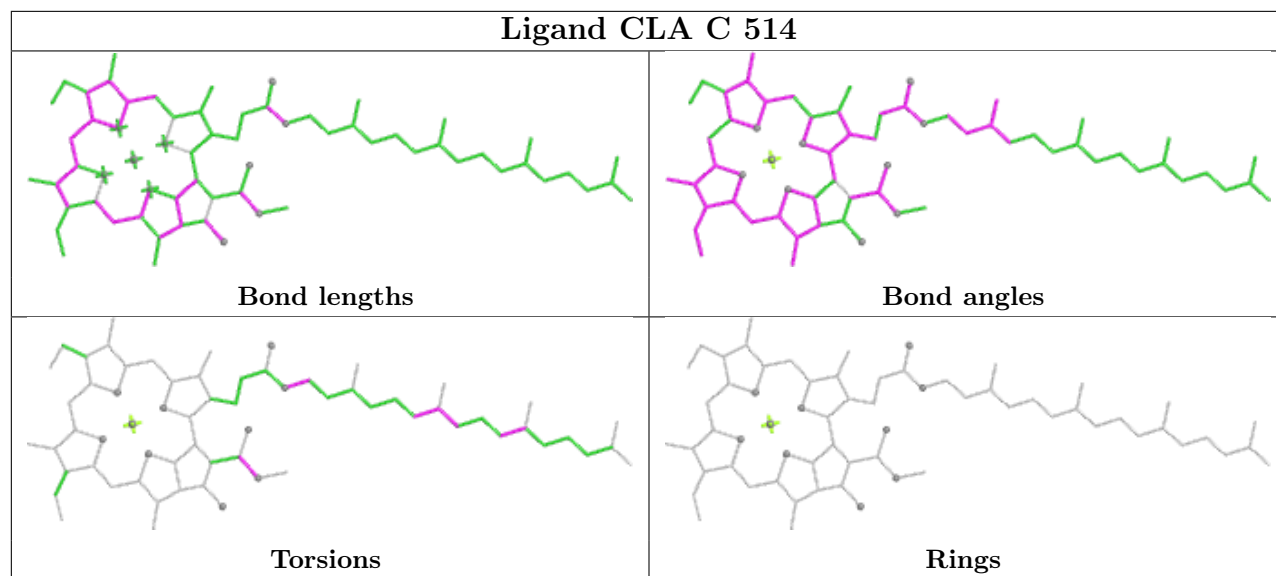


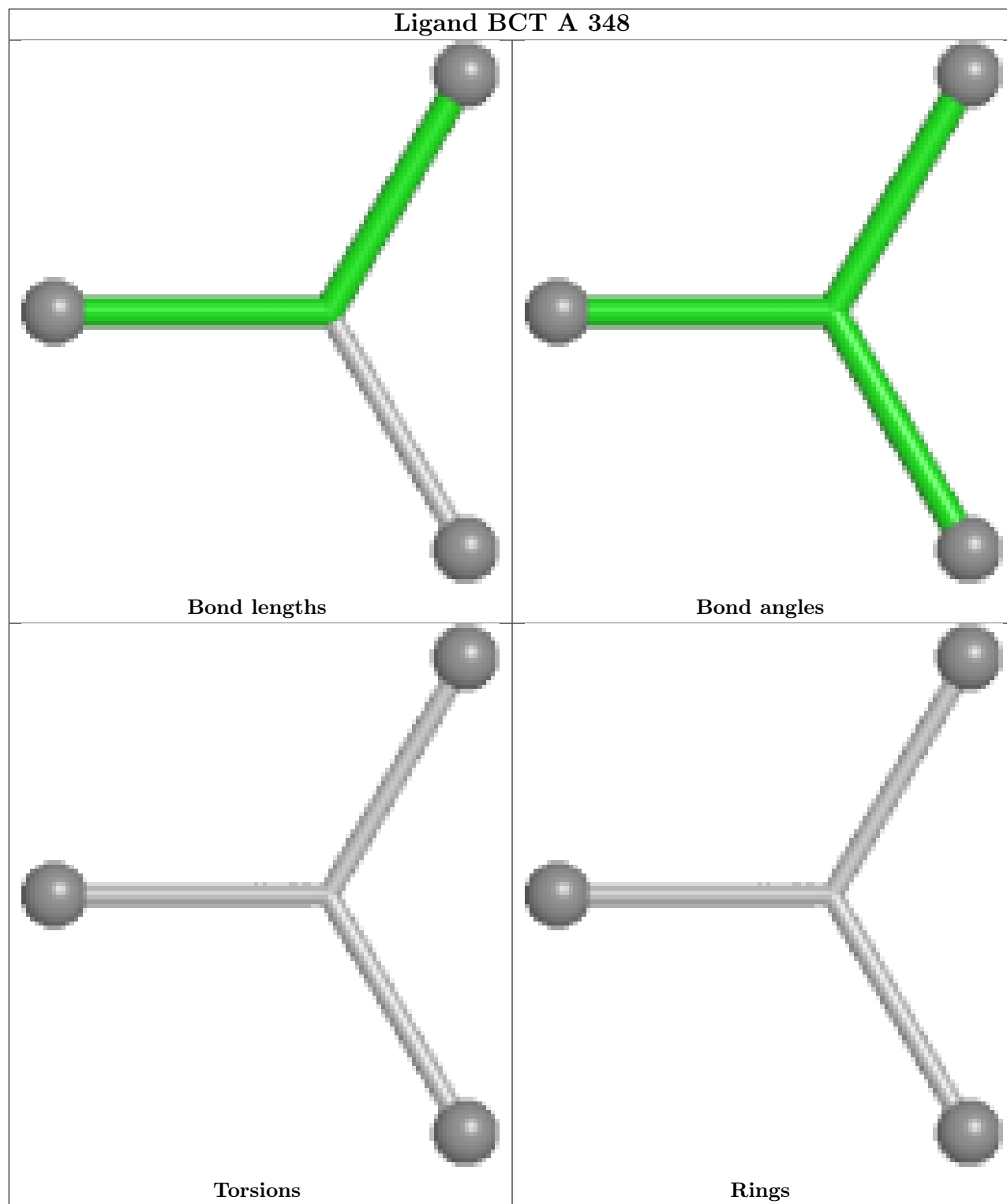




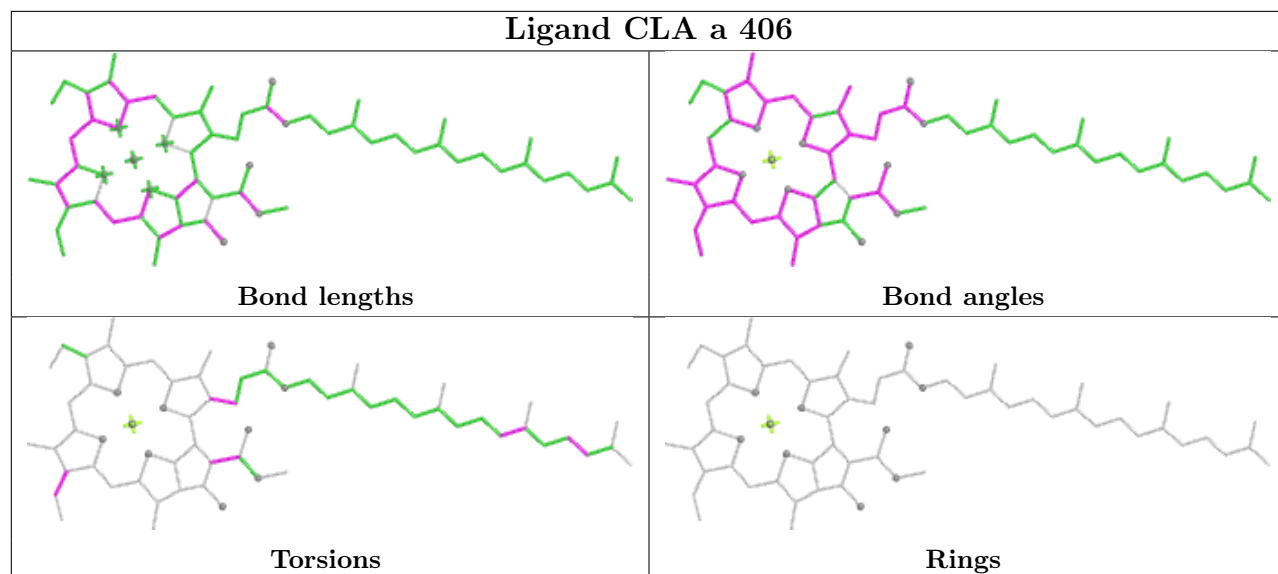
Ligand BCR B 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA c 503	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PHO a 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 507	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT a 420	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

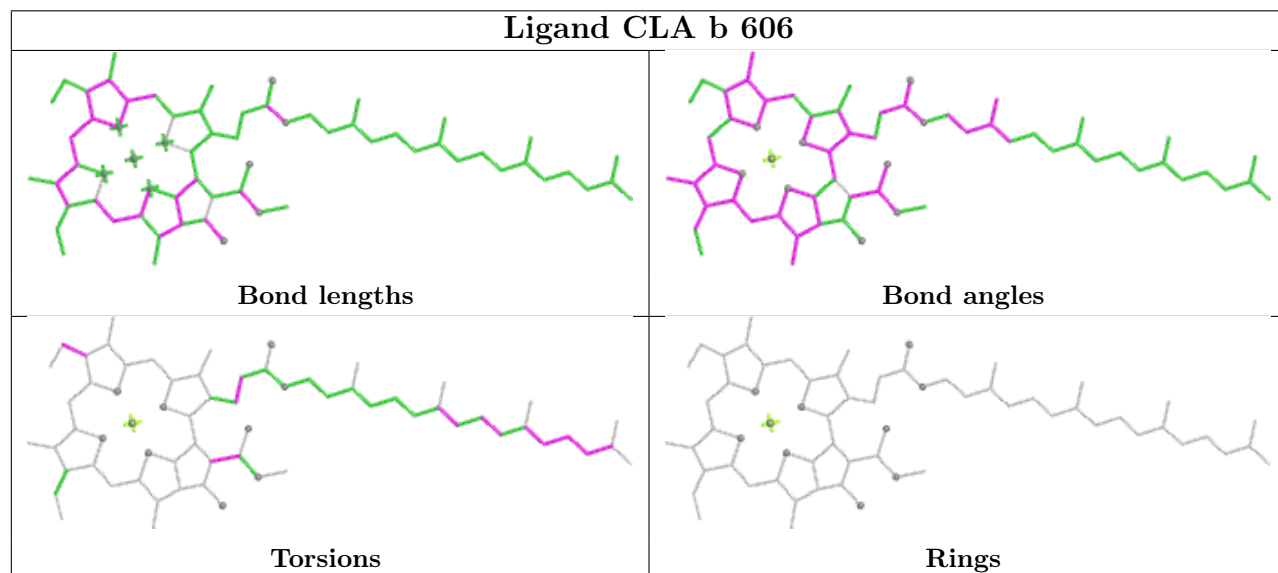




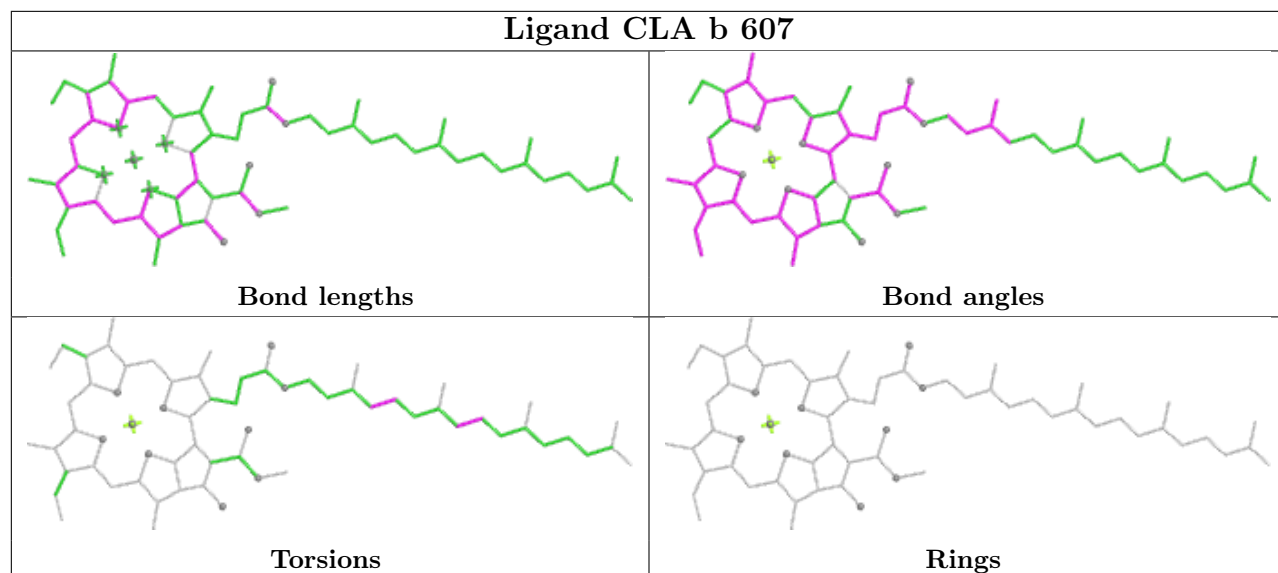
Ligand CLA a 406

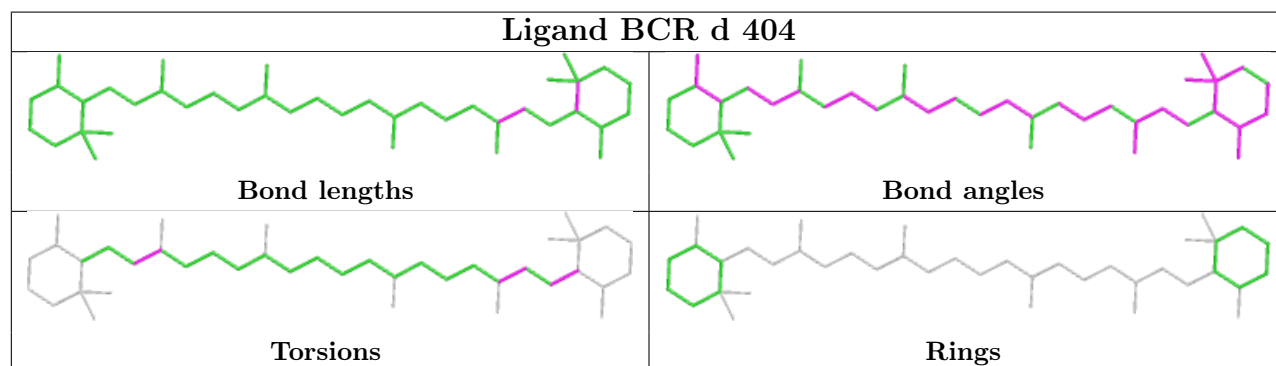
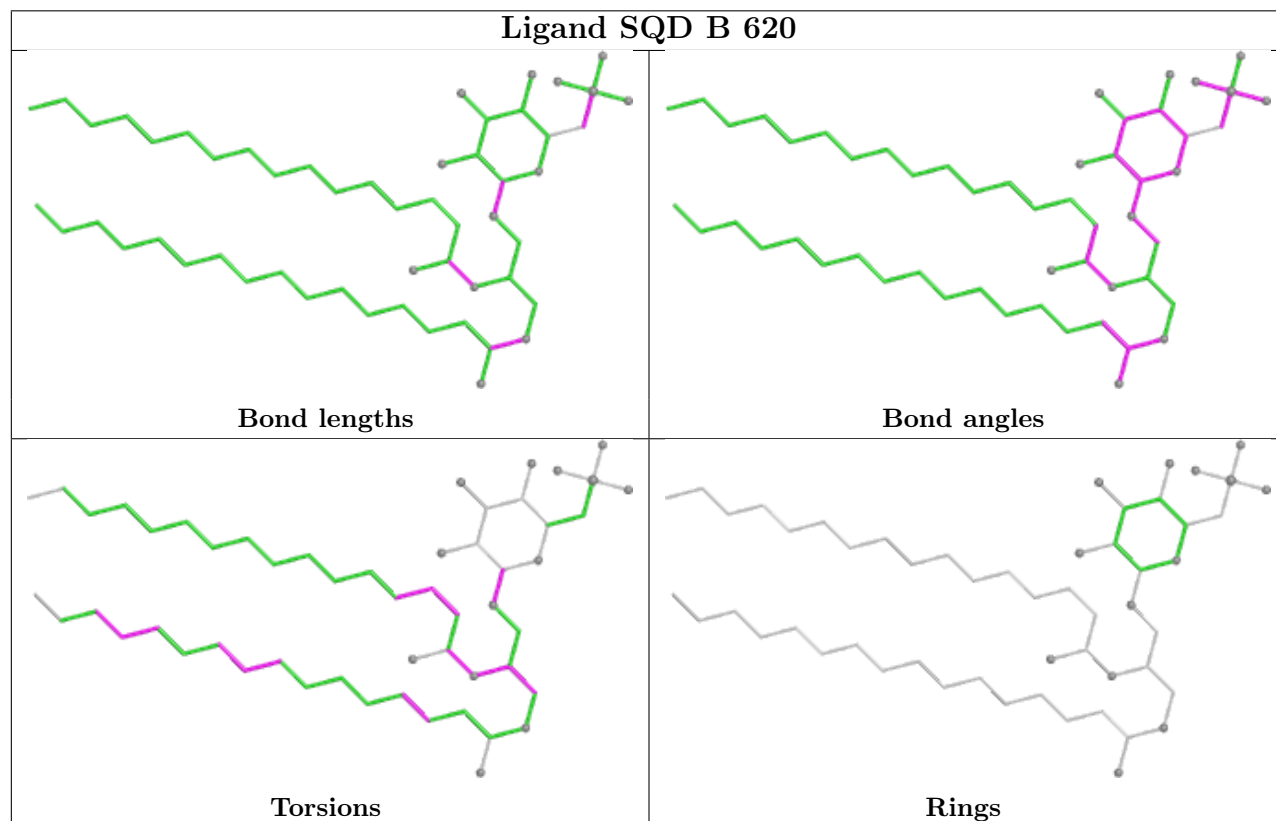
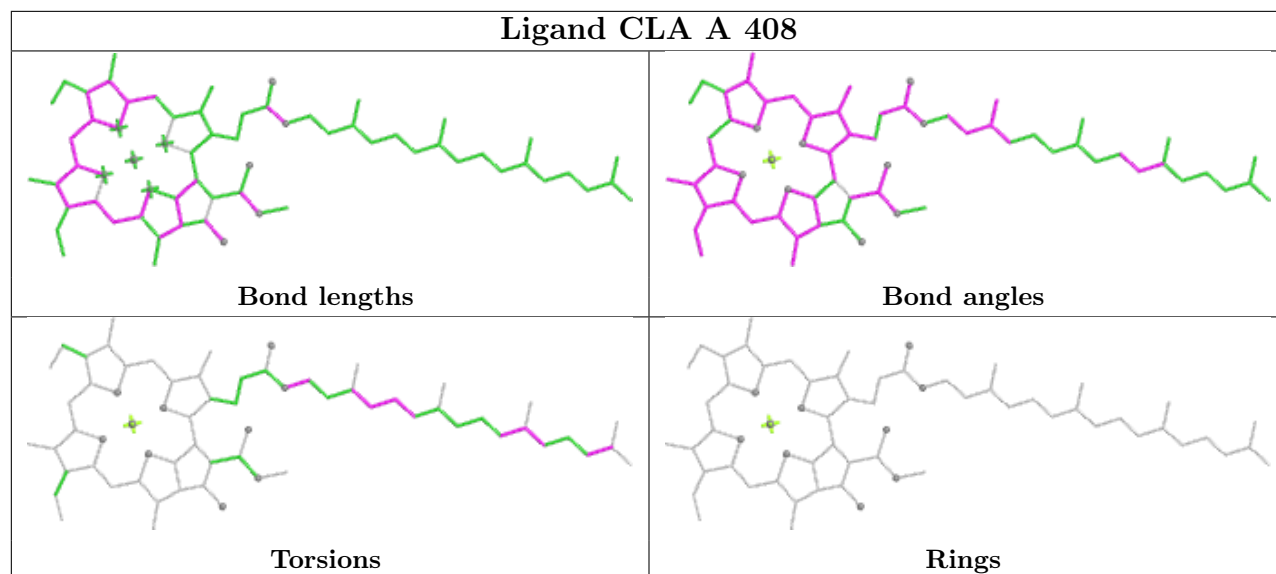


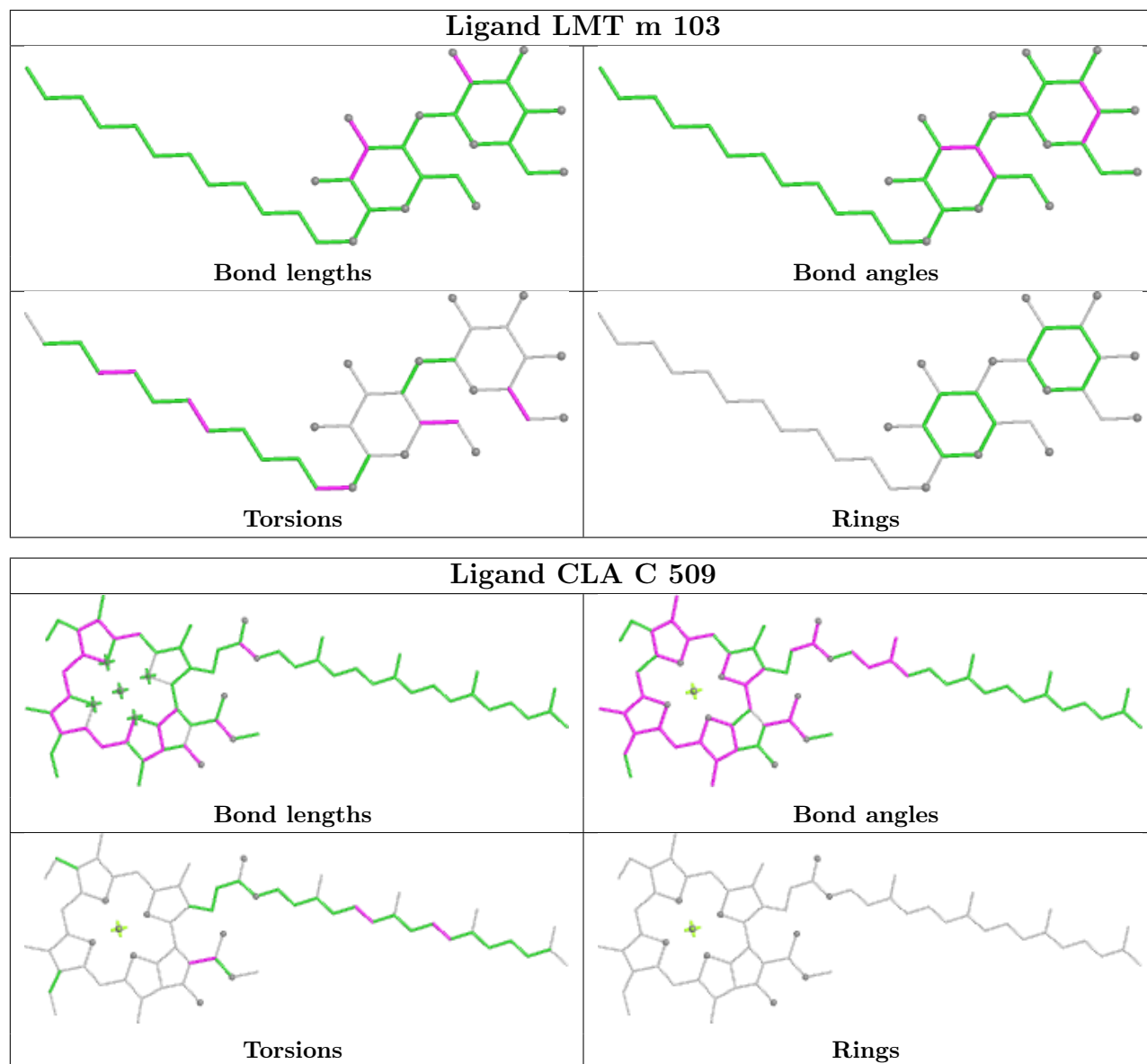
Ligand CLA b 606



Ligand CLA b 607







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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.66	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%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.47	0 100 100	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.94	0.08	42,50,60,69	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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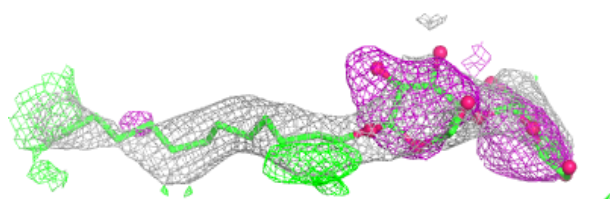
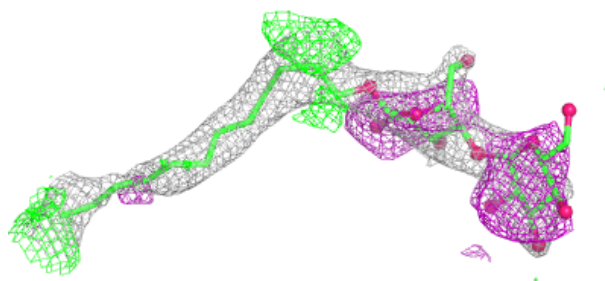
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CL	A	403	1/1	0.99	0.03	44,44,44,44	0
22	CL	a	402	1/1	0.99	0.07	47,47,47,47	0
28	OEX	a	415	10/10	1.00	0.02	45,48,51,54	0
21	FE2	A	401	1/1	1.00	0.01	49,49,49,49	0
21	FE2	a	401	1/1	1.00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

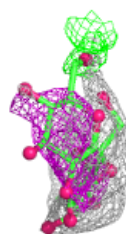
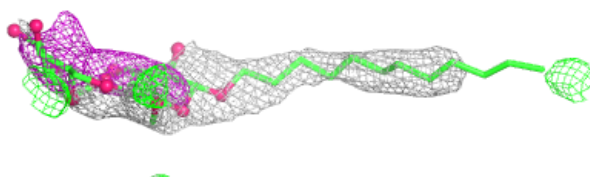
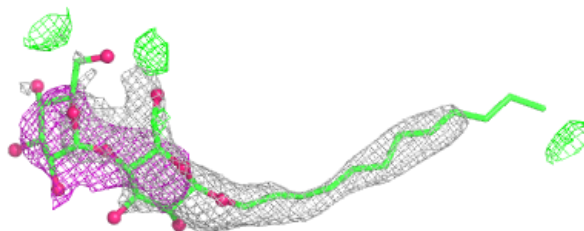
Electron density around LMT a 414:

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

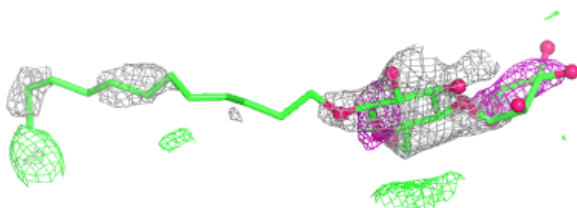
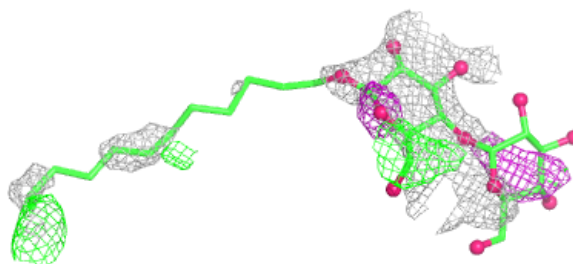


Electron density around LMT E 102:

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

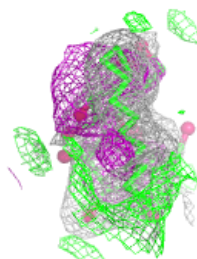
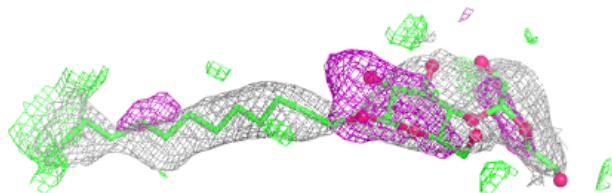
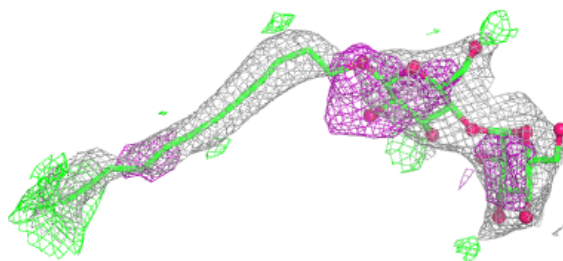
**Electron density around LMT e 102:**

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

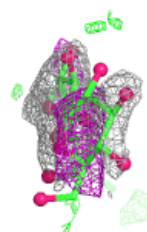
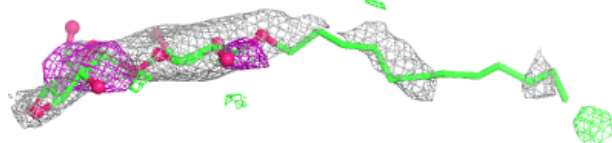
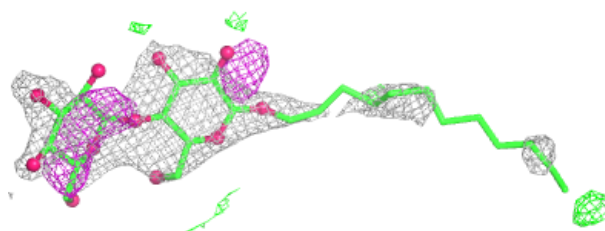


Electron density around LMT A 359:

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

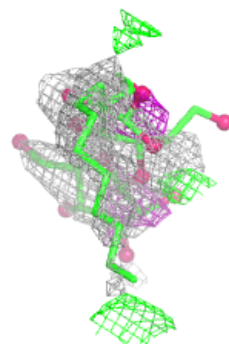
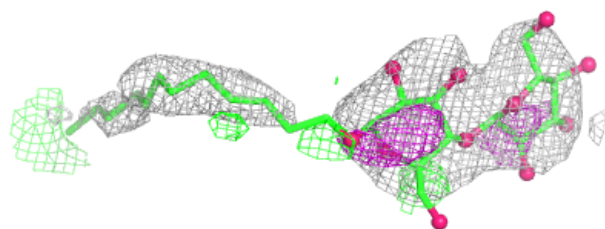
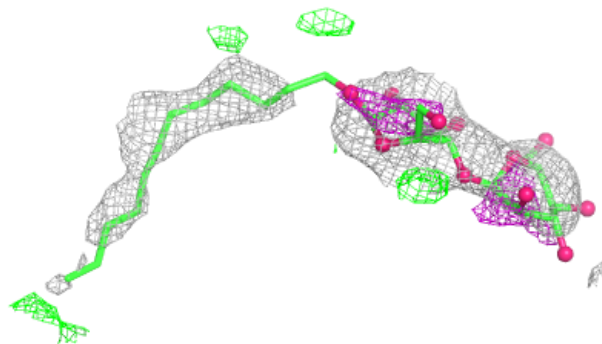
**Electron density around LMT a 420:**

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

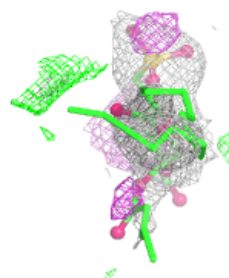
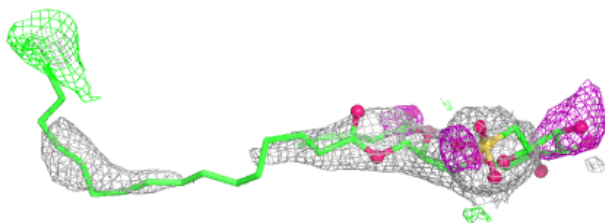
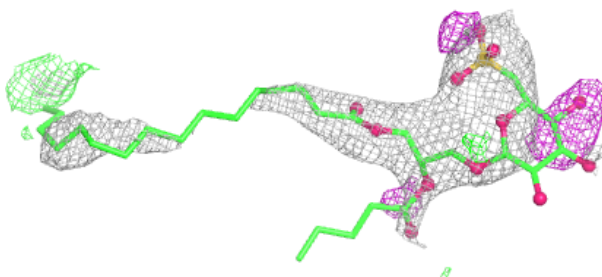


Electron density around LMT I 101:

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

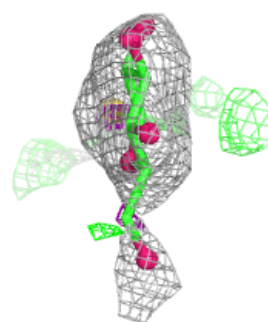
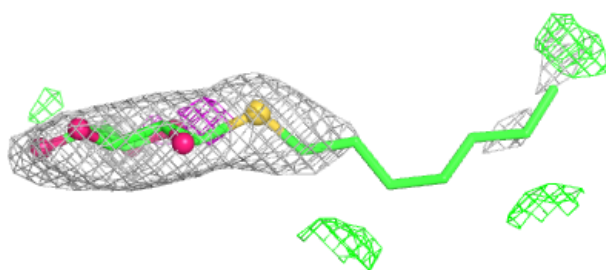
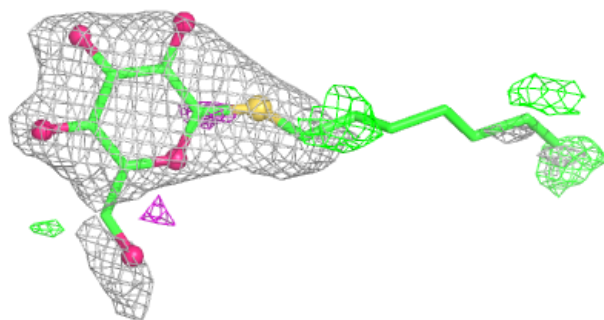
**Electron density around SQD f 102:**

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

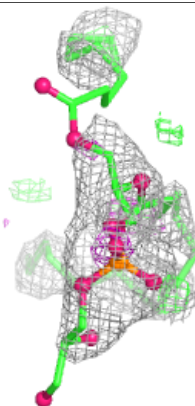
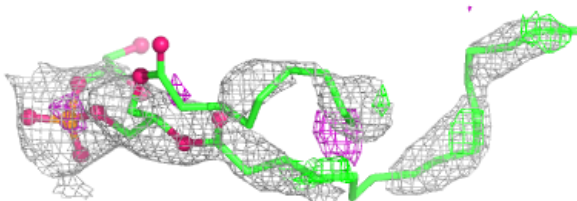
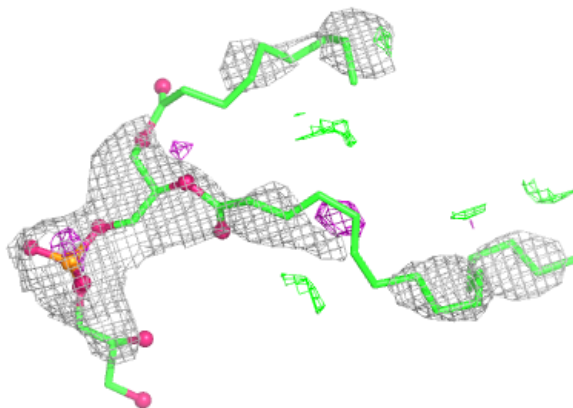


Electron density around HTG C 522:

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

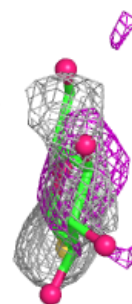
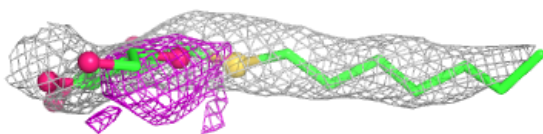
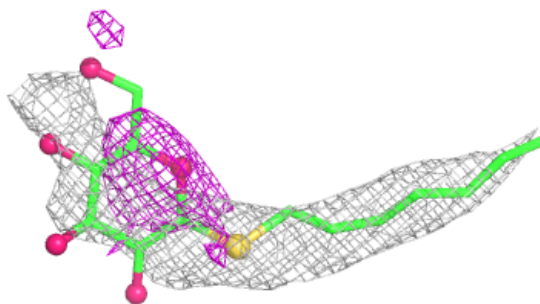
**Electron density around LHG e 101:**

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

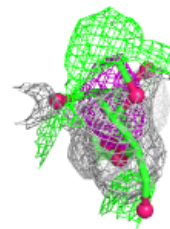
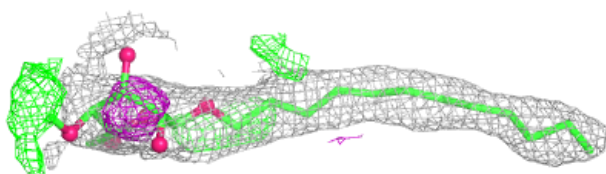
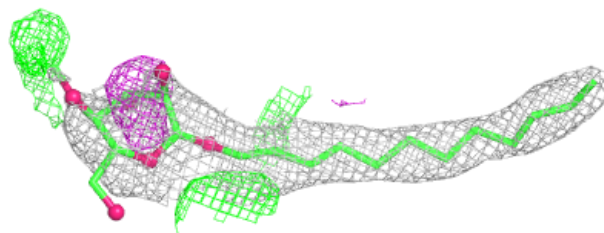


Electron density around HTG b 623:

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

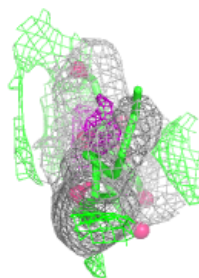
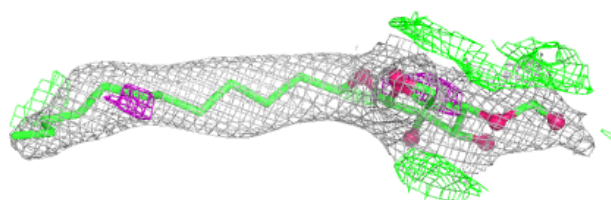
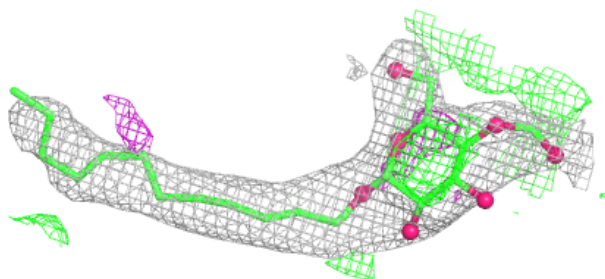
**Electron density around LMT b 621:**

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

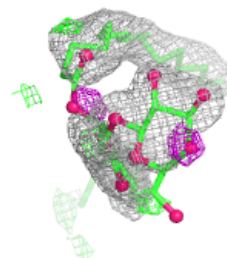
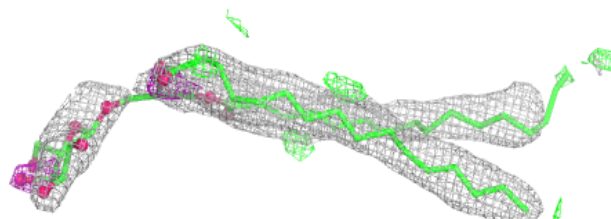
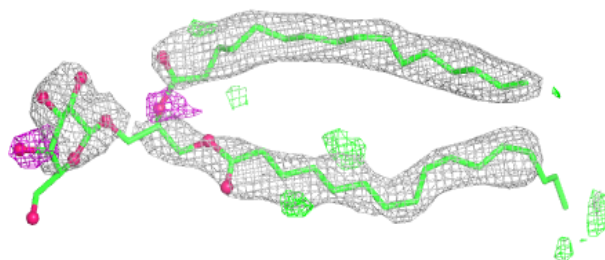


Electron density around LMT t 102:

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

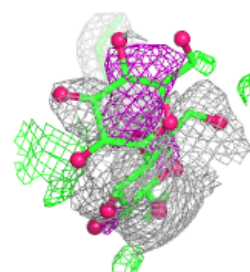
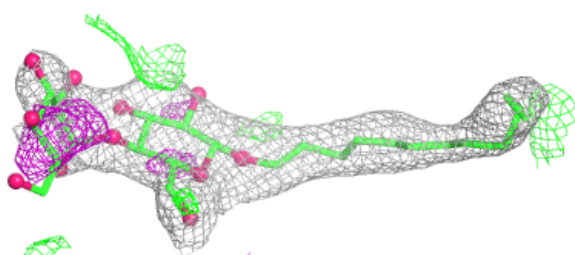
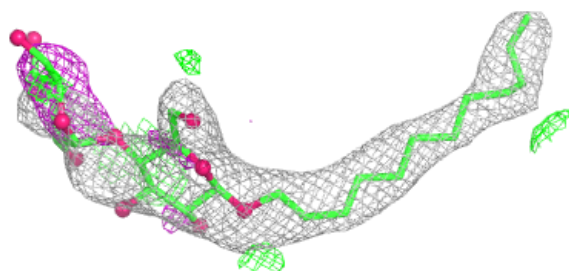
**Electron density around LMG C 521:**

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

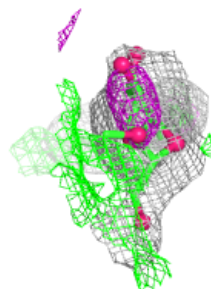
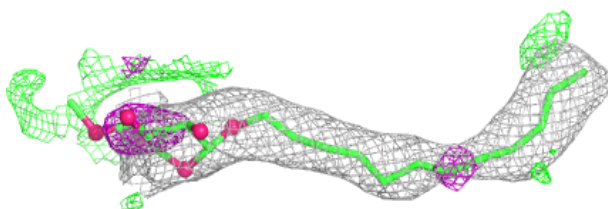
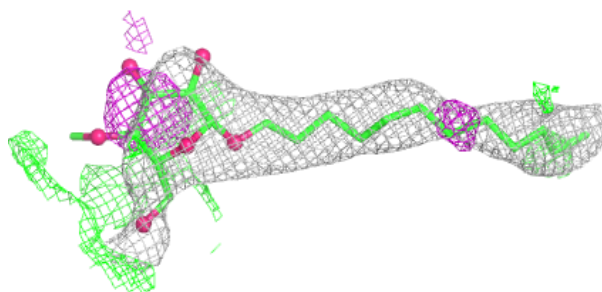


Electron density around LMT M 103:

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

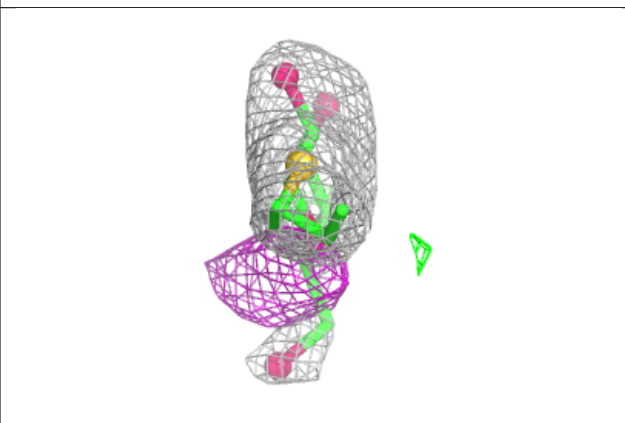
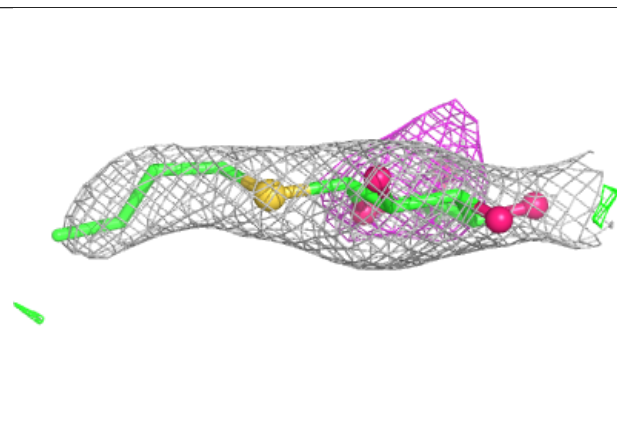
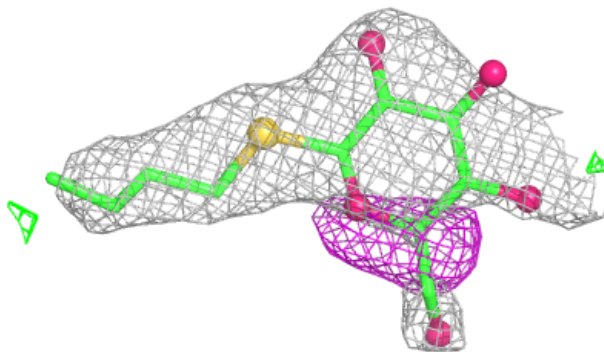
**Electron density around LMT t 101:**

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

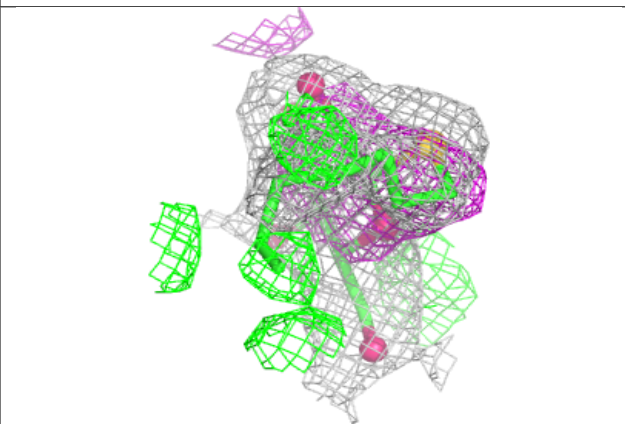
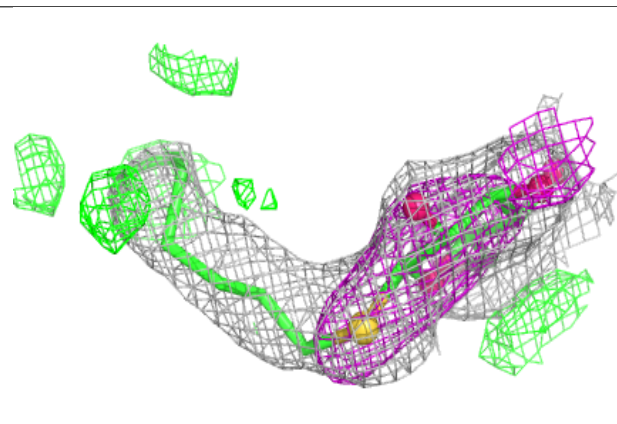
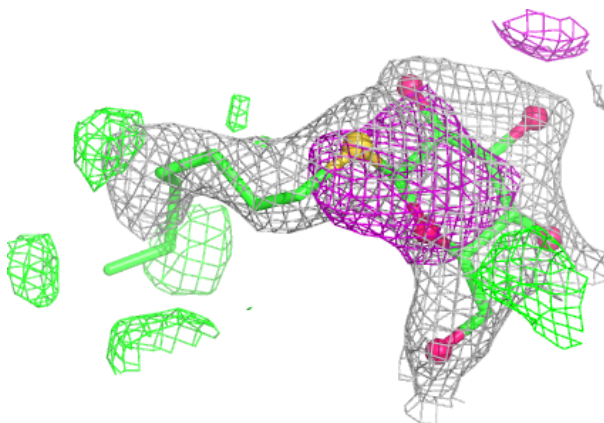


Electron density around HTG D 414:

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

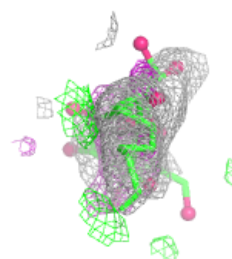
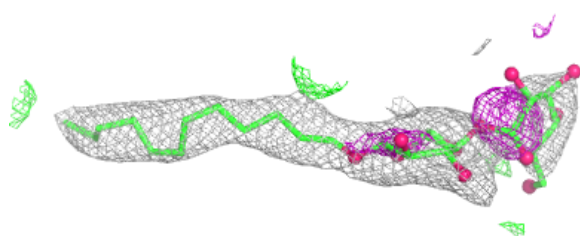
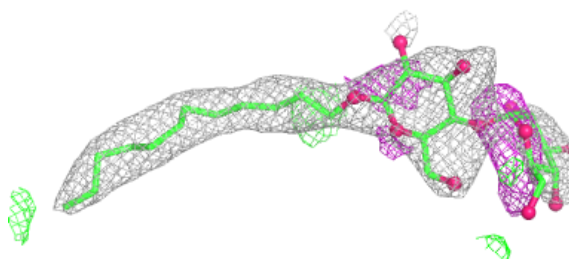
**Electron density around HTG B 623:**

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

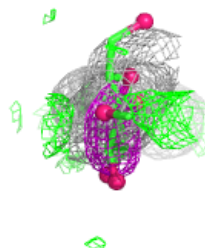
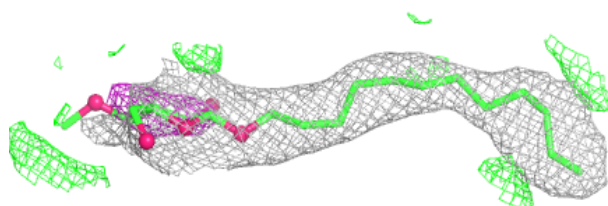
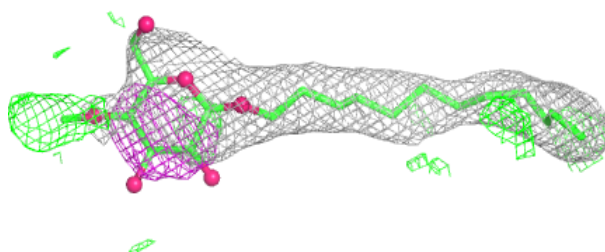


Electron density around LMT D 404:

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

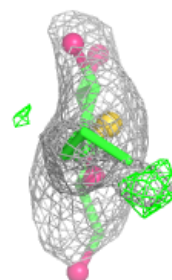
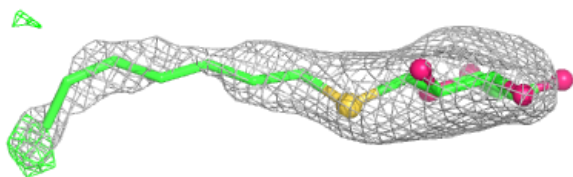
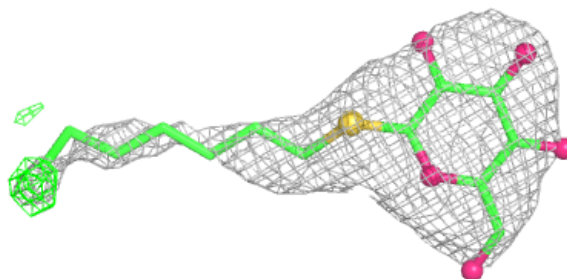
**Electron density around LMT b 627:**

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

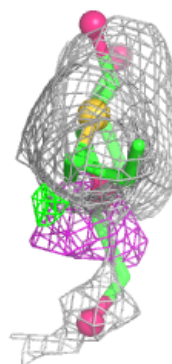
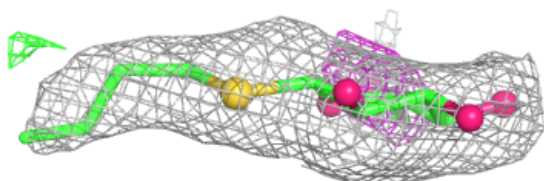
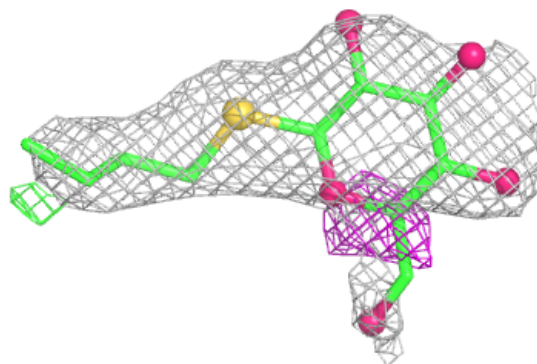


Electron density around HTG c 522:

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

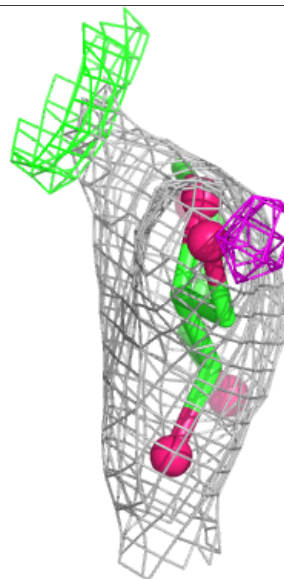
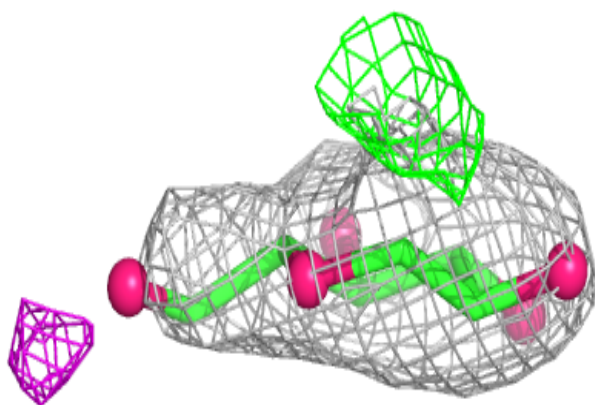
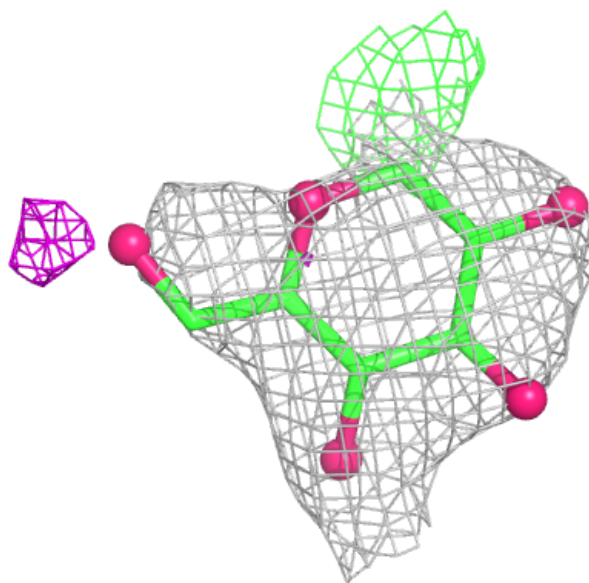
**Electron density around HTG d 411:**

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



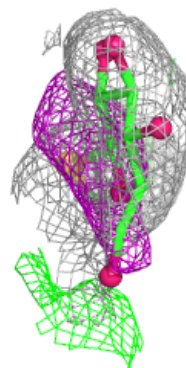
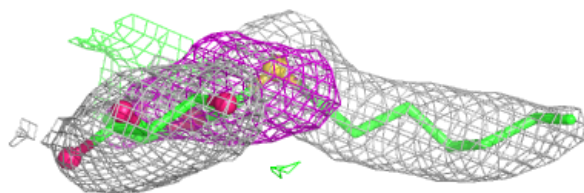
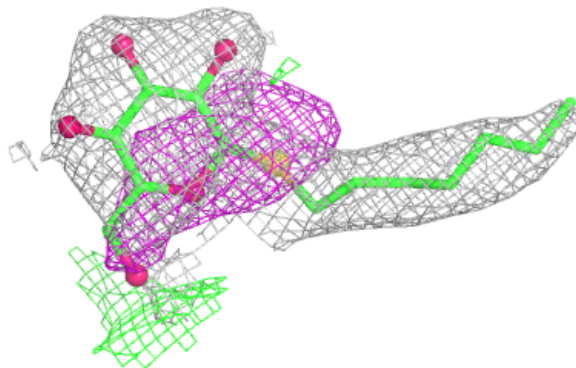
Electron density around HTG V 203:

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

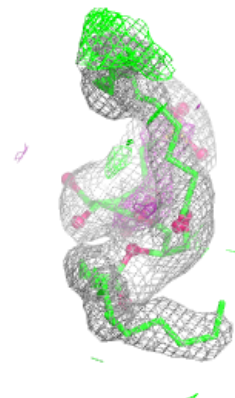
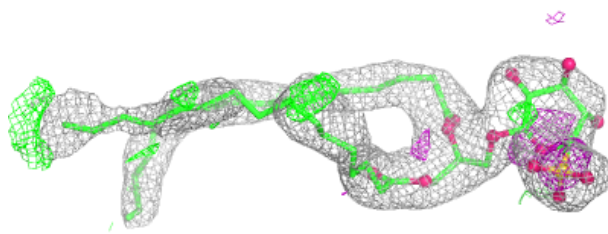
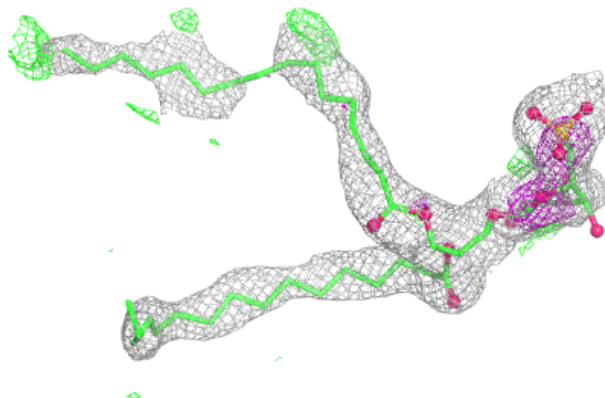


Electron density around HTG b 622:

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

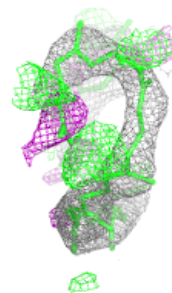
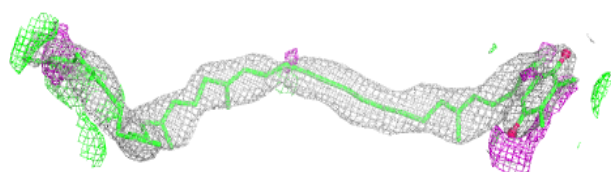
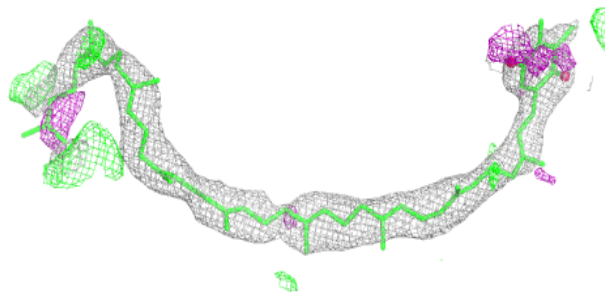
**Electron density around SQD a 413:**

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

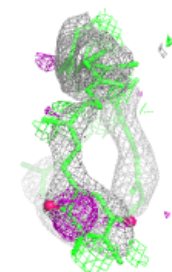
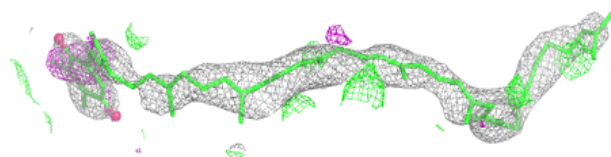
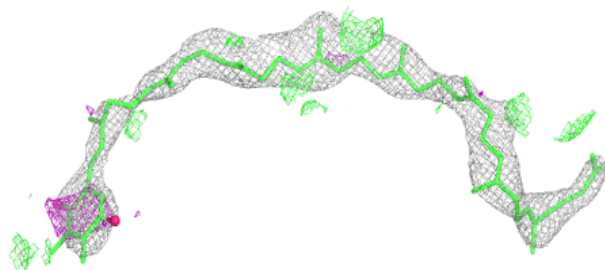


Electron density around PL9 A 414:

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

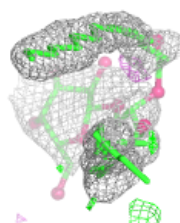
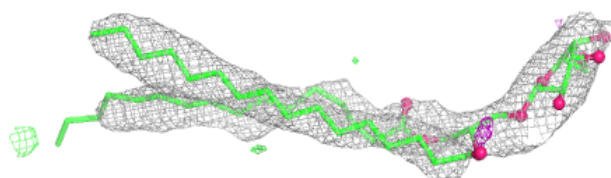
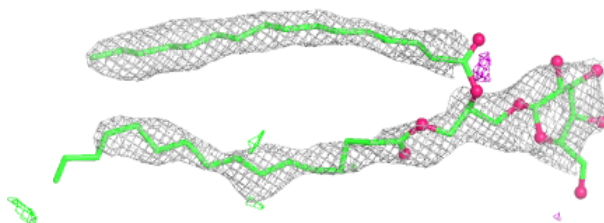
**Electron density around PL9 a 416:**

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

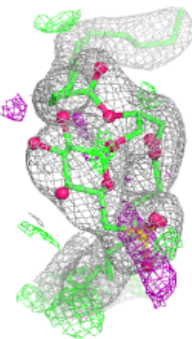
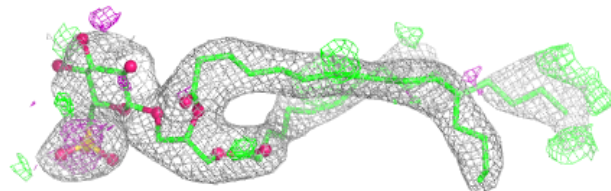
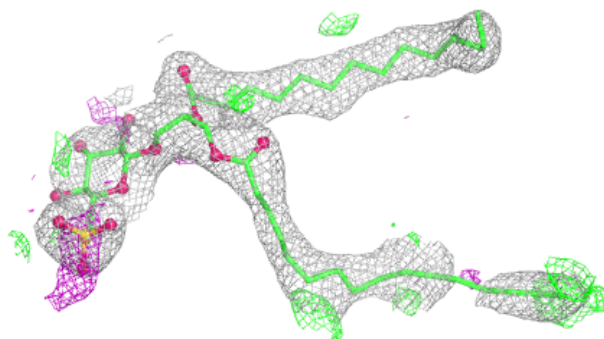


Electron density around LMG c 521:

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

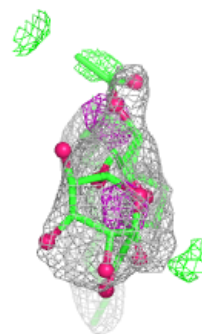
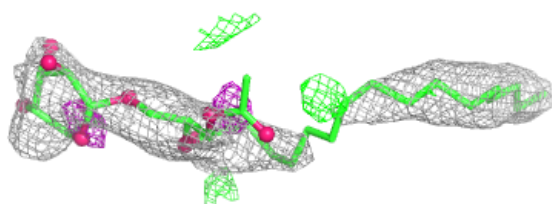
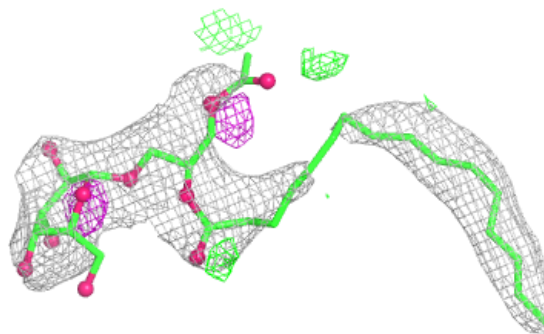
**Electron density around SQD A 412:**

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

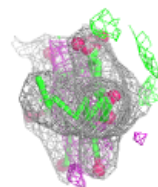
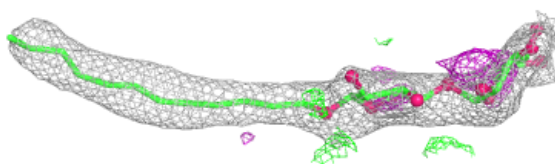
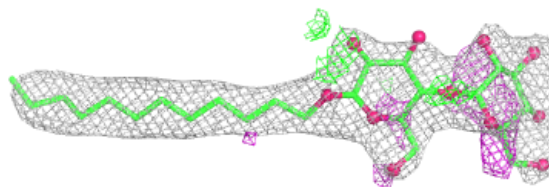


Electron density around LMG Z 101:

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

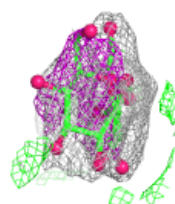
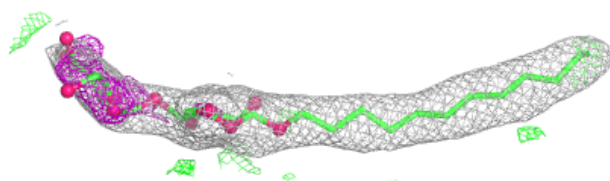
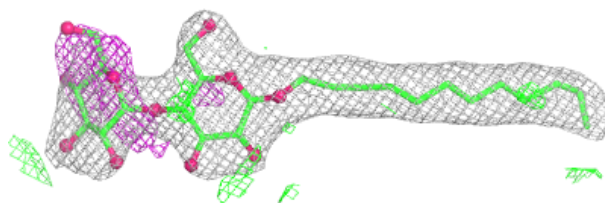
**Electron density around LMT m 103:**

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

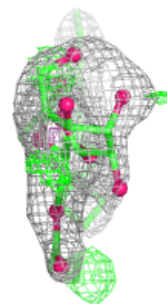
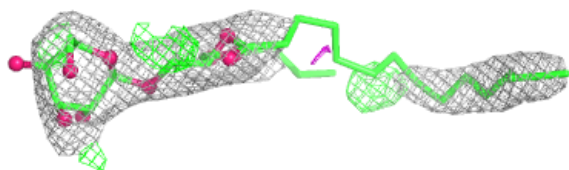
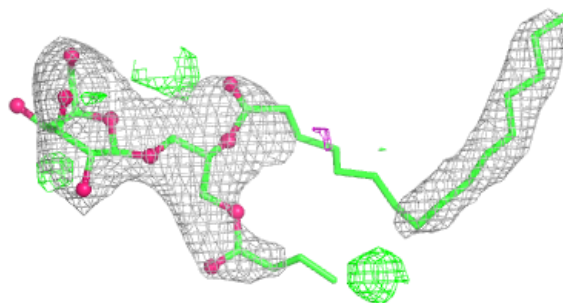


Electron density around LMT M 101:

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

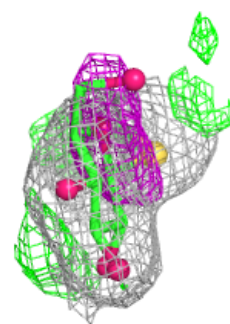
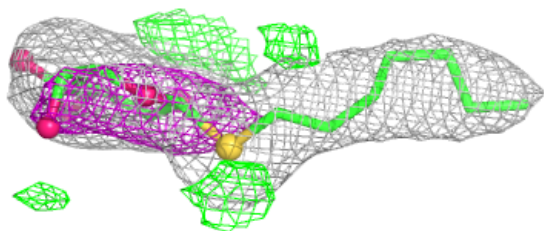
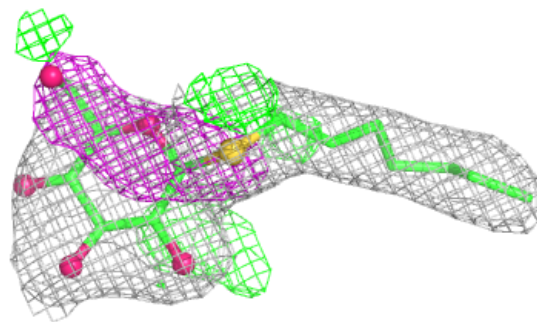
**Electron density around LMG z 101:**

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

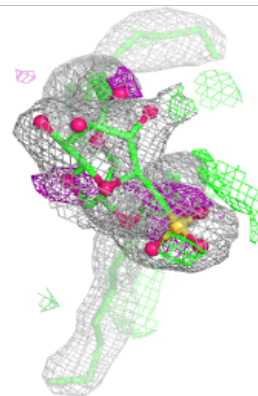
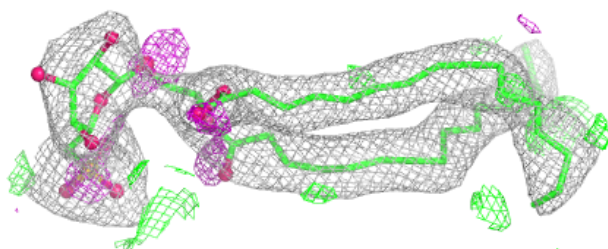
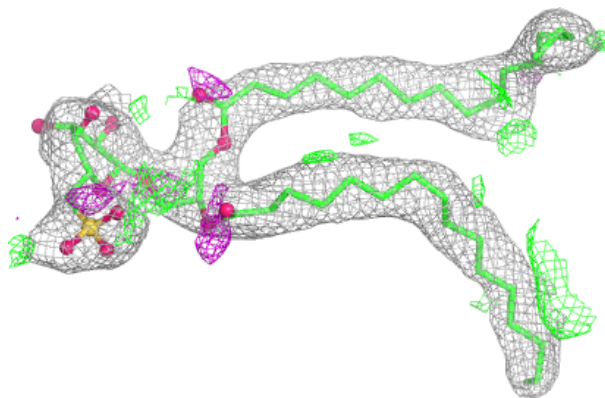


Electron density around HTG B 622:

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

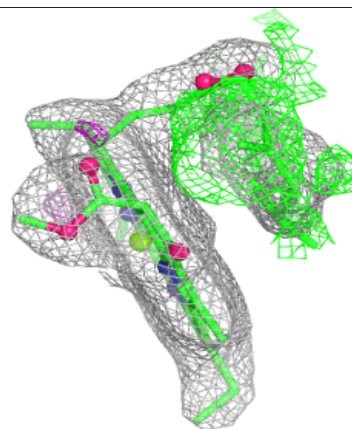
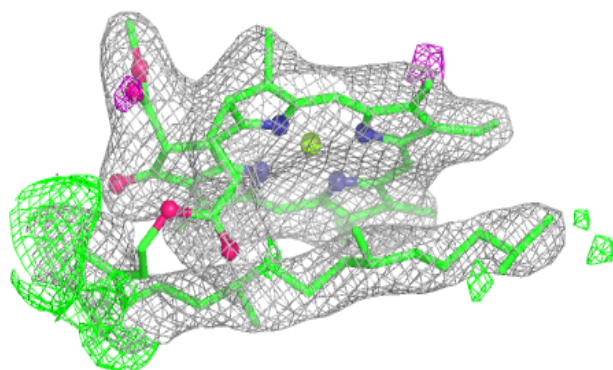
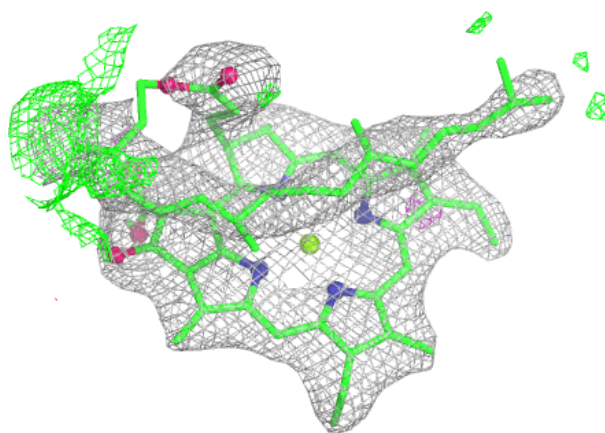
**Electron density around SQD B 620:**

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

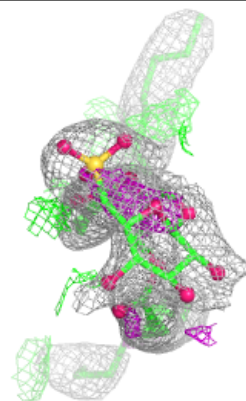
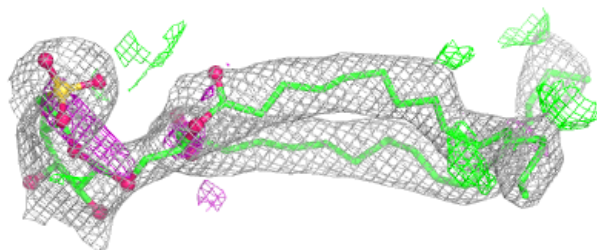
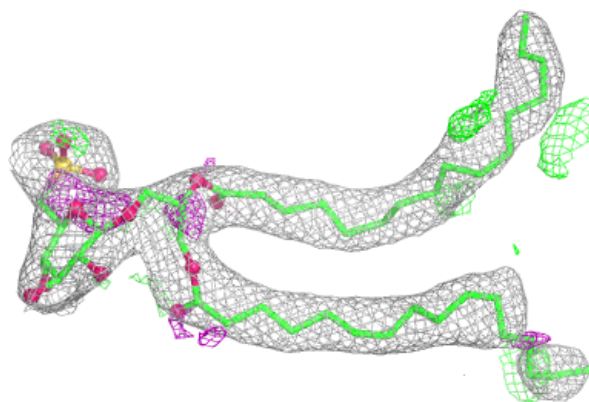


Electron density around CLA b 601:

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

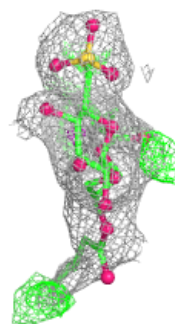
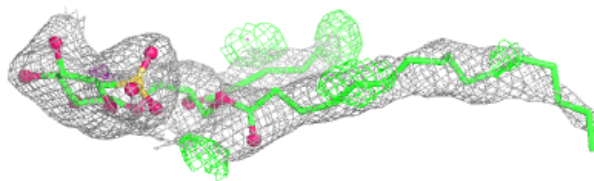
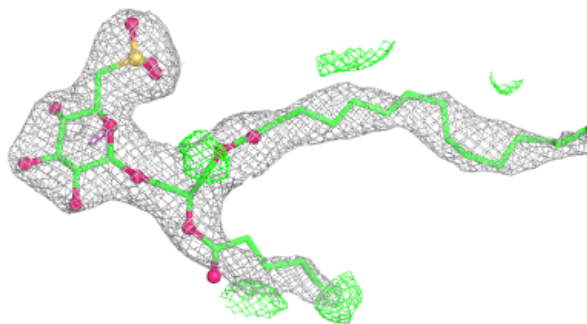
**Electron density around SQD b 620:**

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

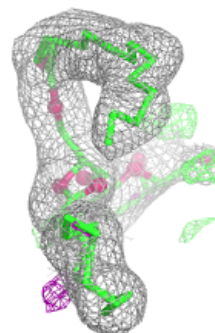
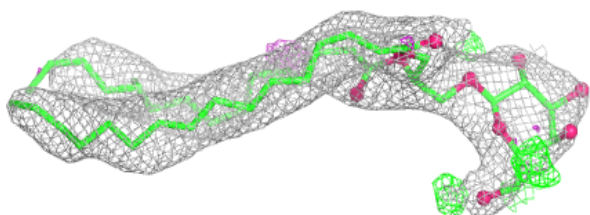
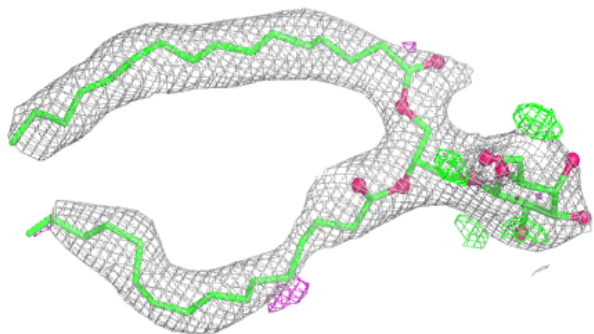


Electron density around SQD F 101:

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

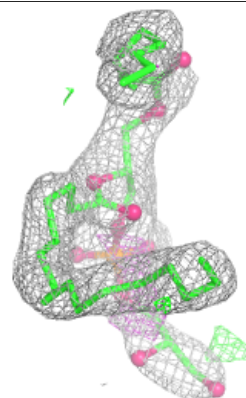
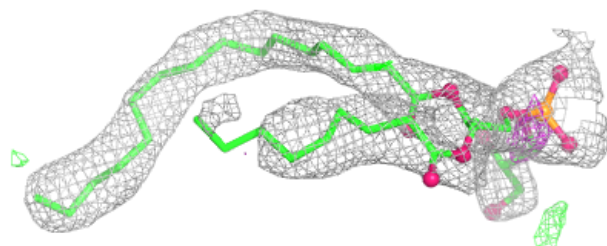
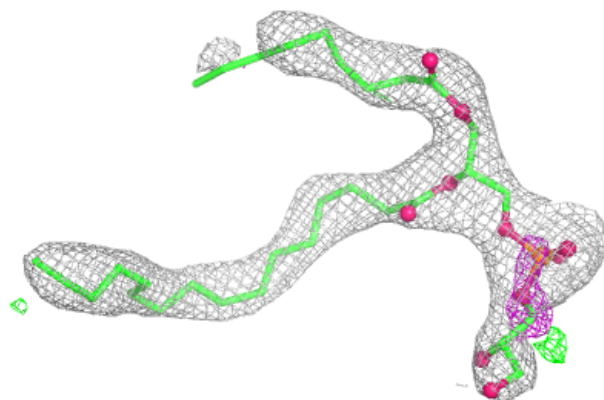
**Electron density around LMG C 501:**

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

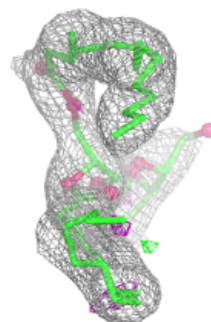
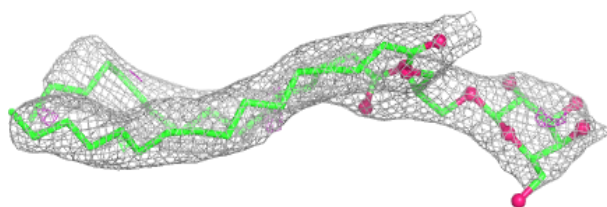
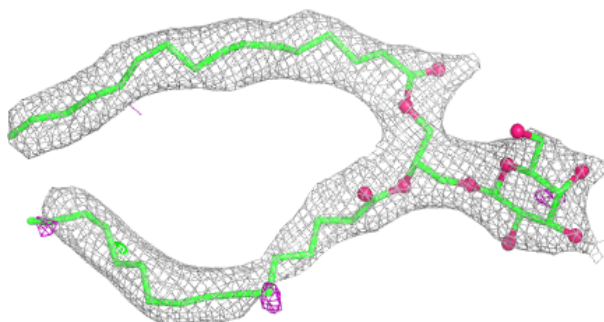


Electron density around LHG E 101:

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

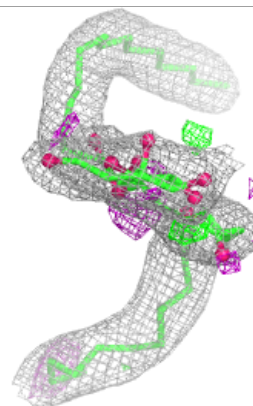
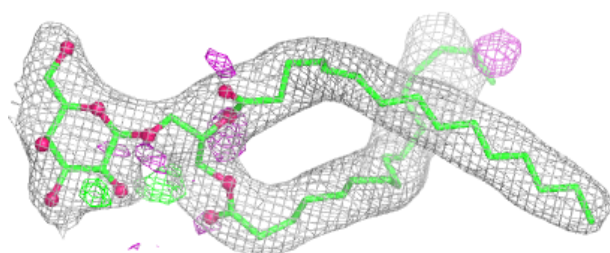
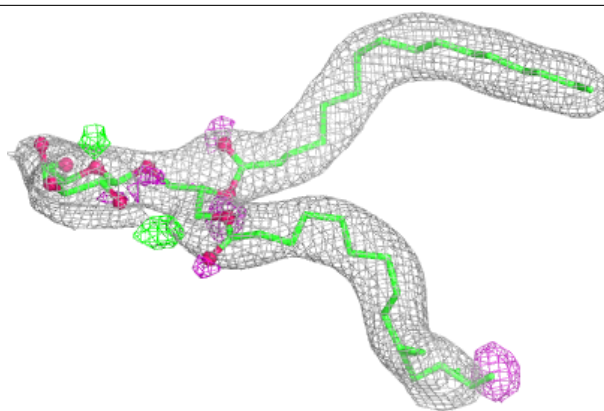
**Electron density around LMG a 419:**

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

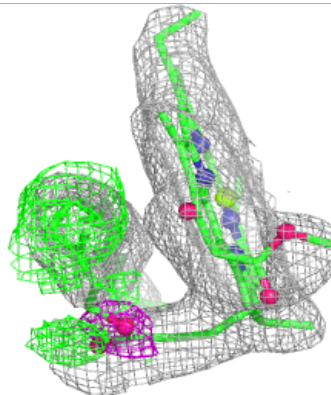
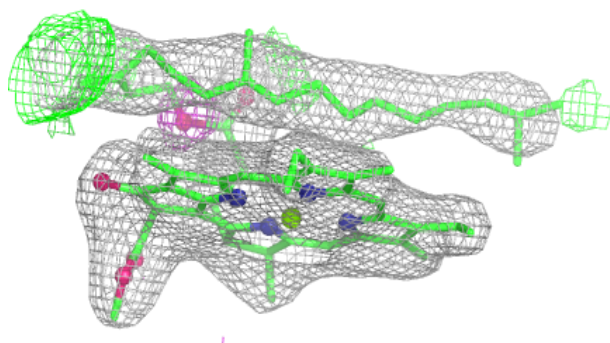
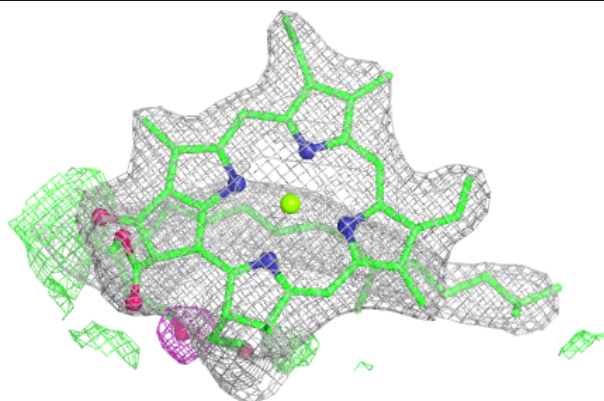


Electron density around LMG m 101:

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

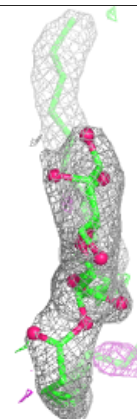
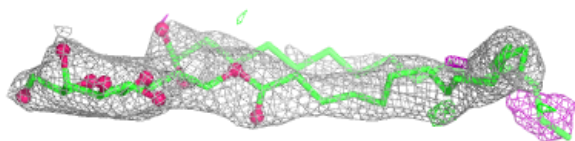
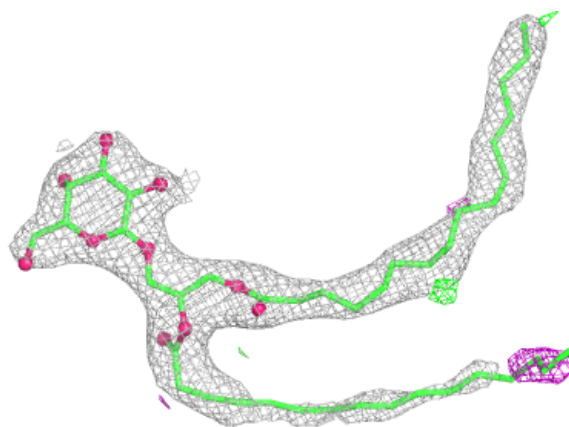
**Electron density around CLA B 601:**

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

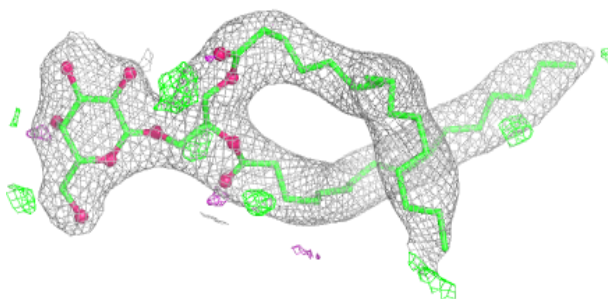
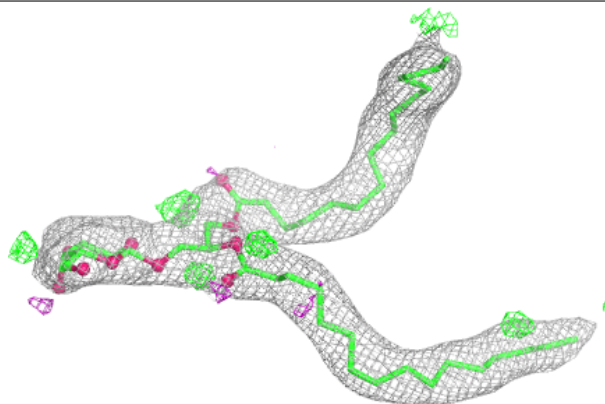


Electron density around LMG c 520:

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

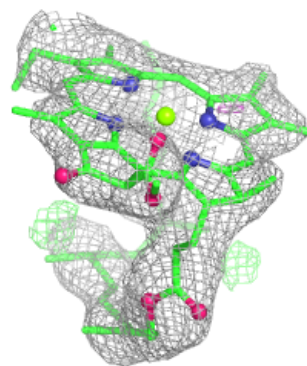
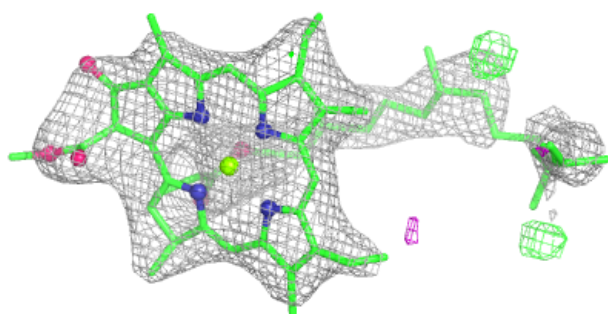
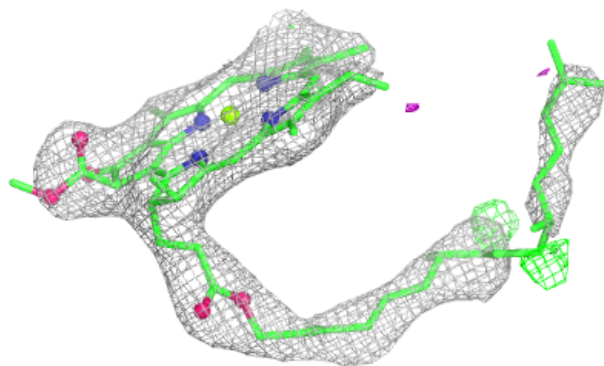
**Electron density around LMG B 621:**

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

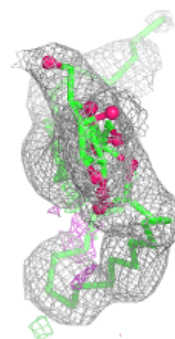
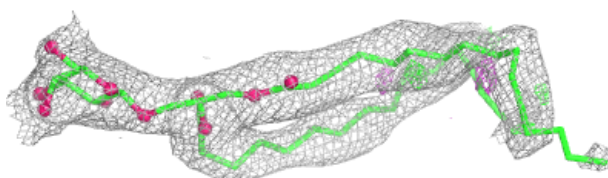
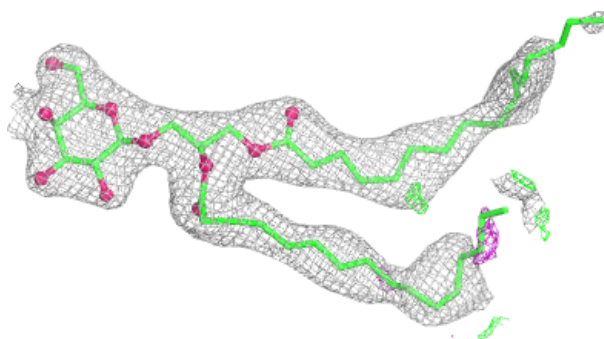


Electron density around CLA c 514:

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

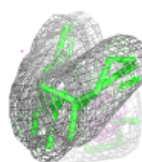
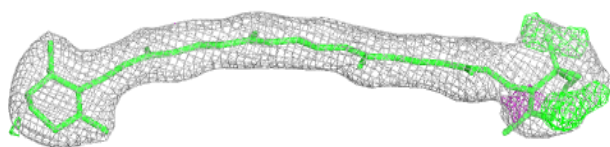
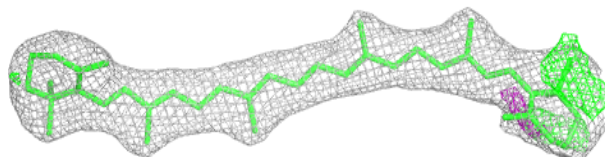
**Electron density around LMG d 412:**

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

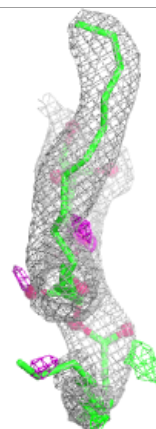
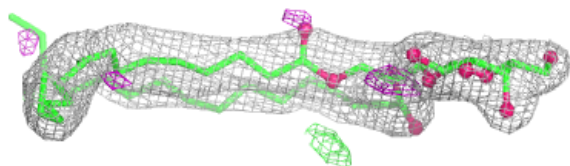
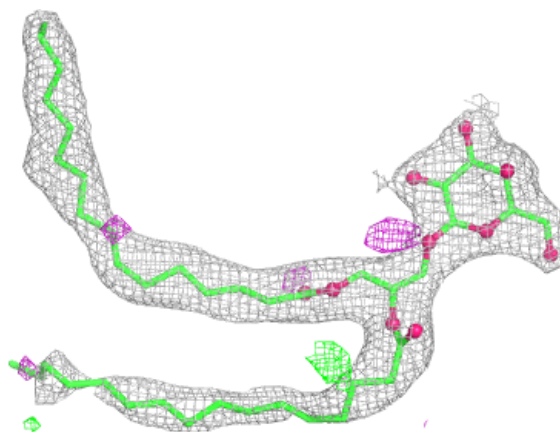


Electron density around BCR d 404:

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

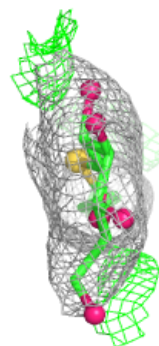
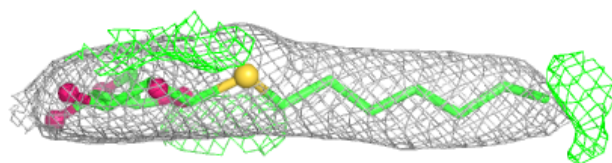
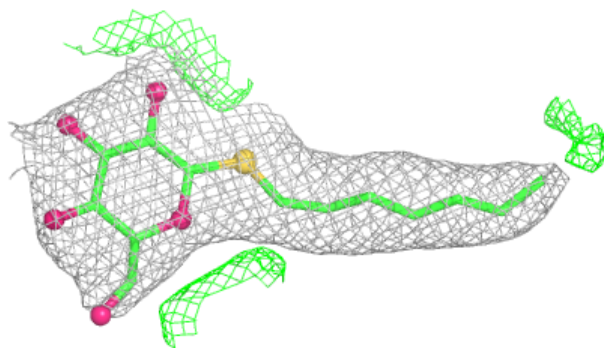
**Electron density around LMG C 520:**

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

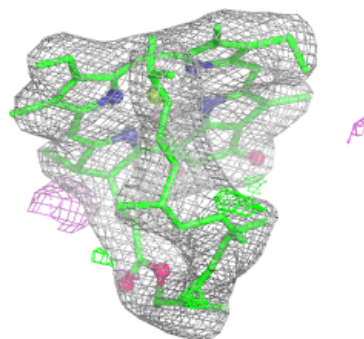
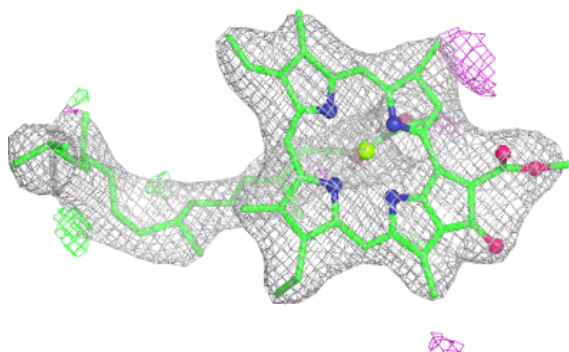
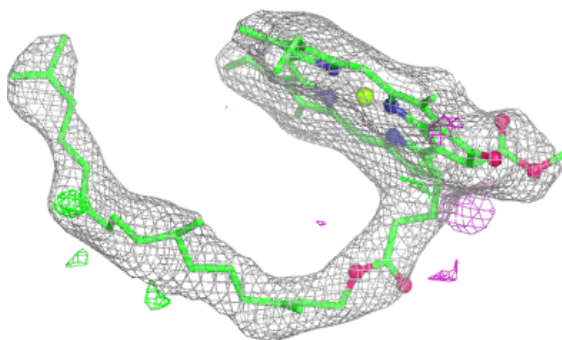


Electron density around HTG b 625:

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

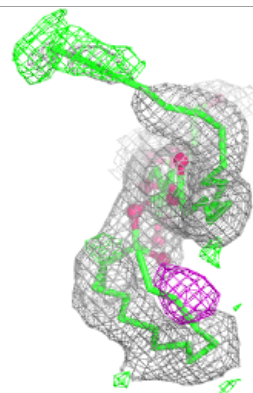
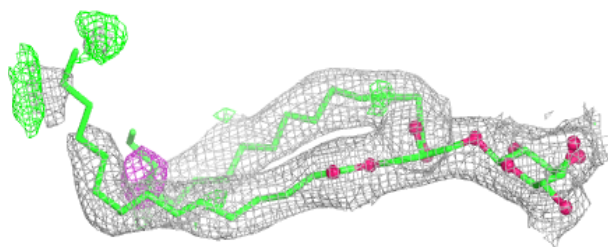
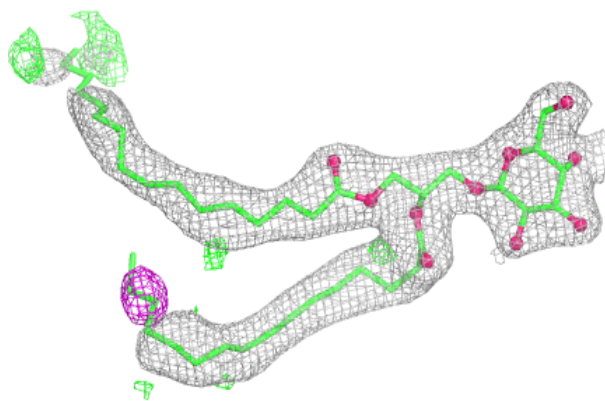
**Electron density around CLA C 514:**

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

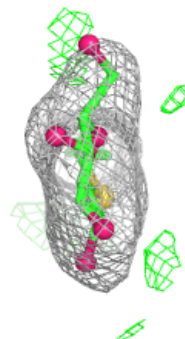
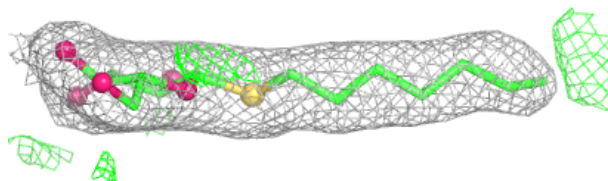
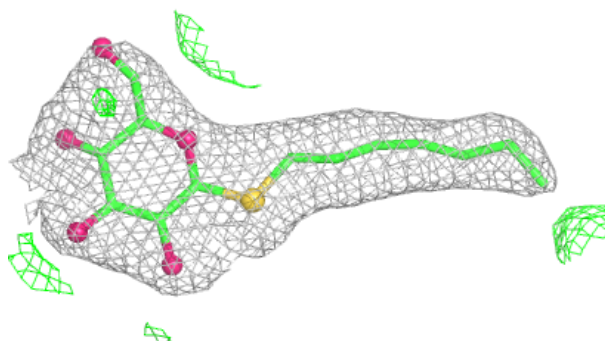


Electron density around LMG D 415:

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

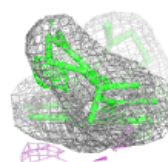
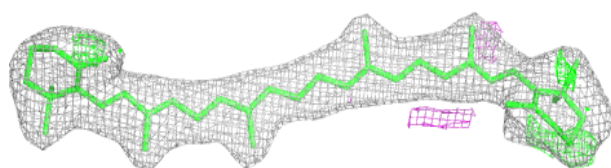
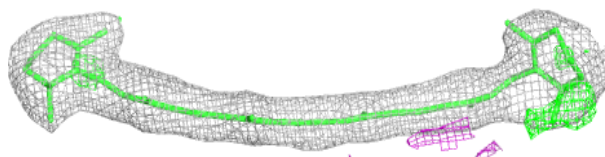
**Electron density around HTG B 626:**

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

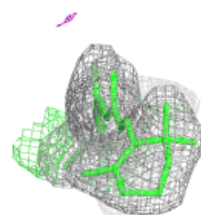
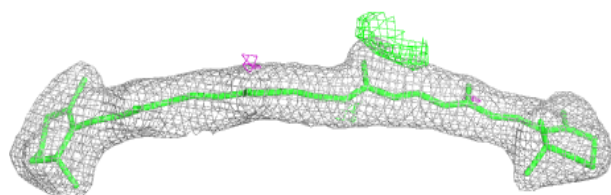
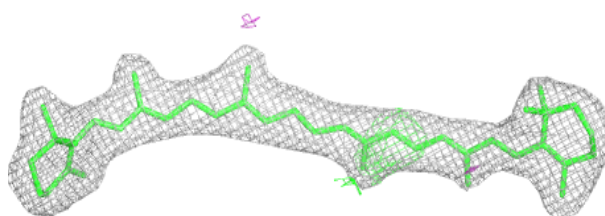


Electron density around BCR D 407:

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

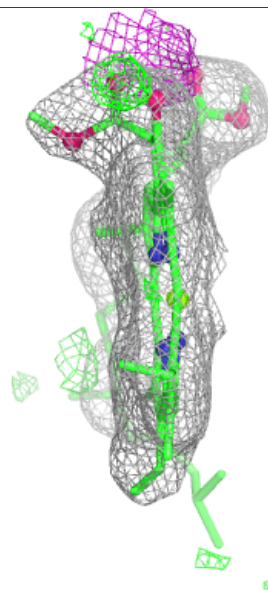
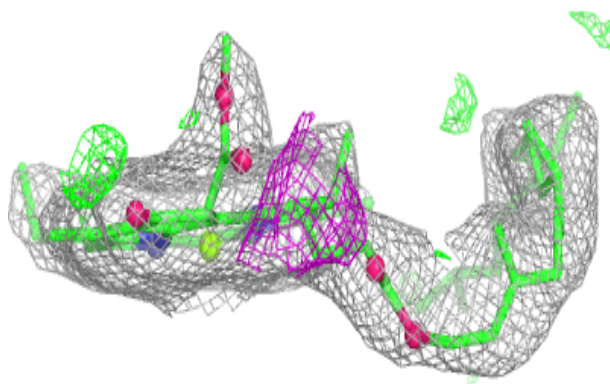
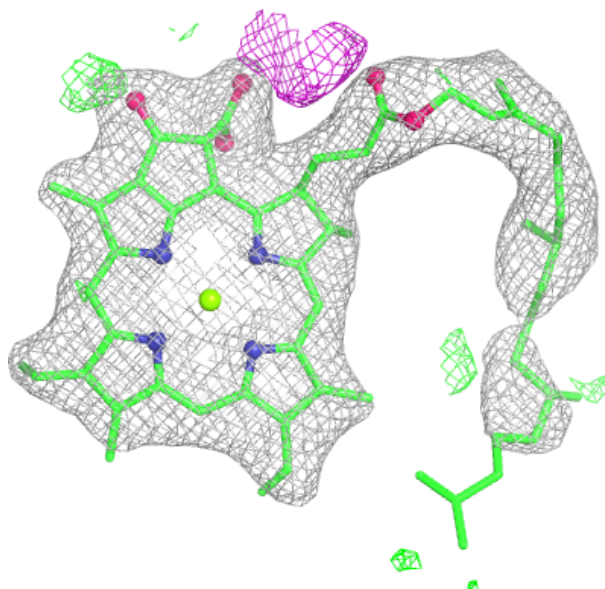
**Electron density around BCR T 101:**

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



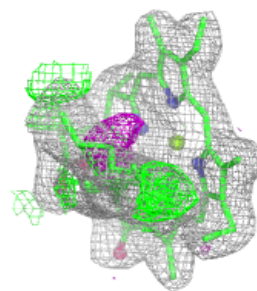
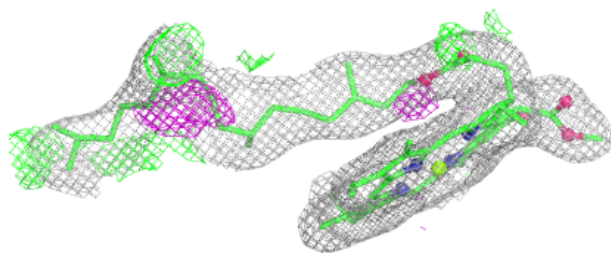
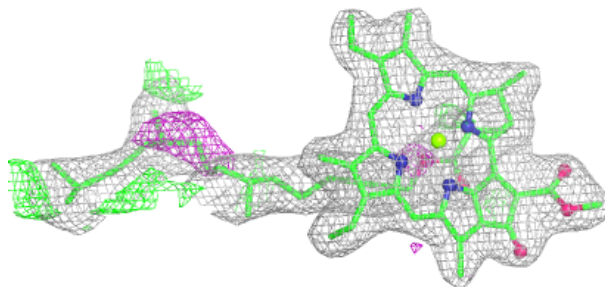
Electron density around CLA c 513:

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

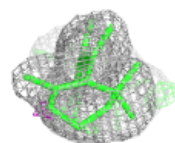
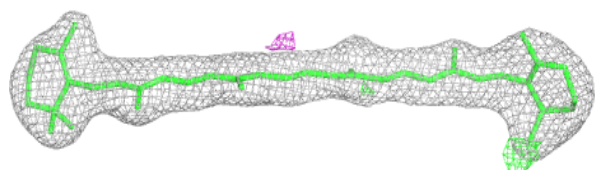
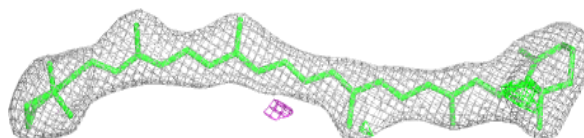


Electron density around CLA B 614:

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

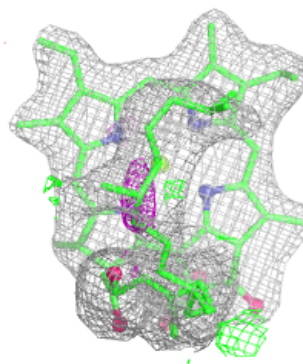
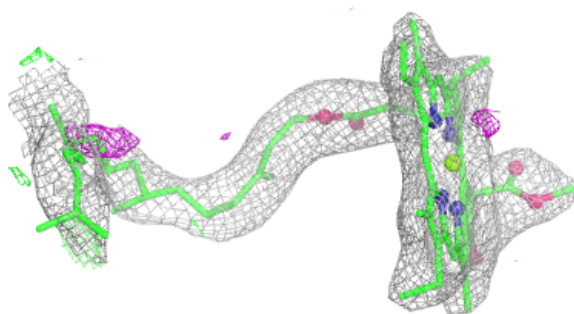
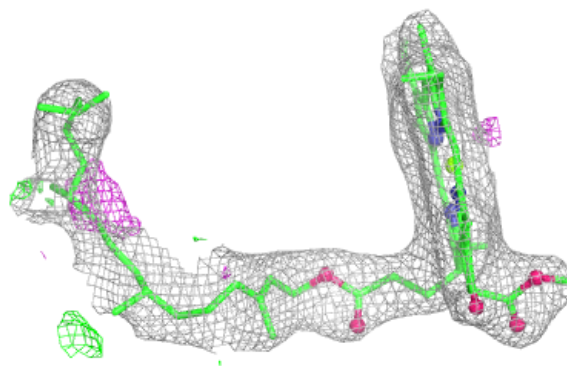
**Electron density around BCR C 515:**

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



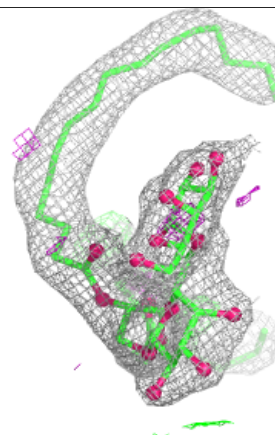
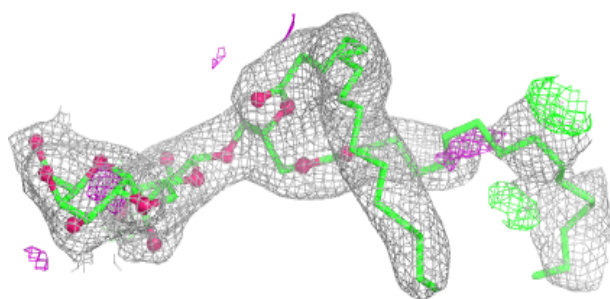
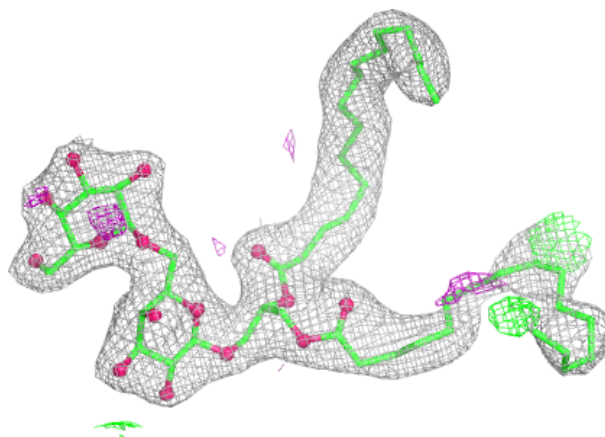
Electron density around CLA C 507:

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



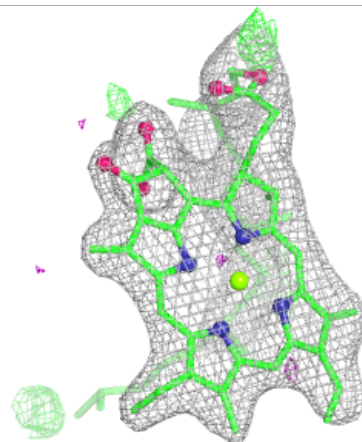
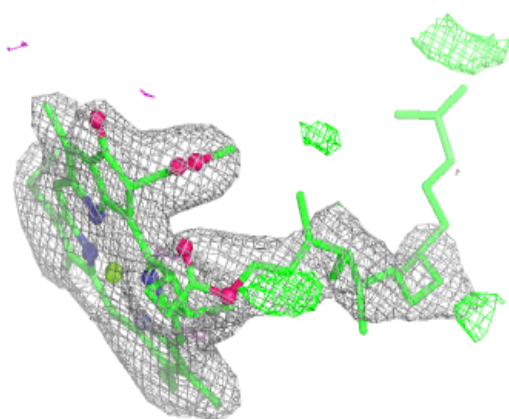
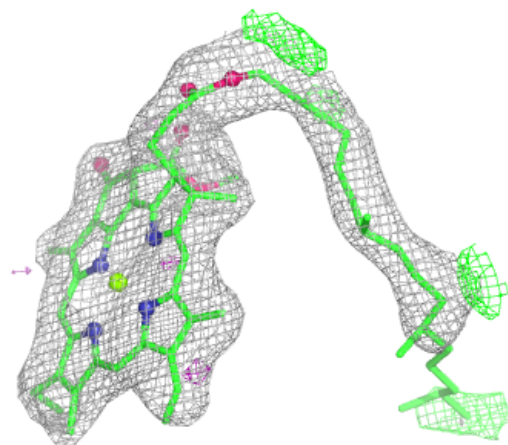
Electron density around DGD C 518:

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



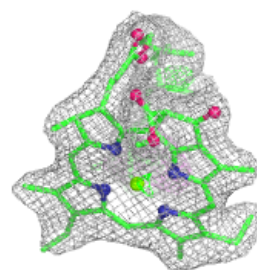
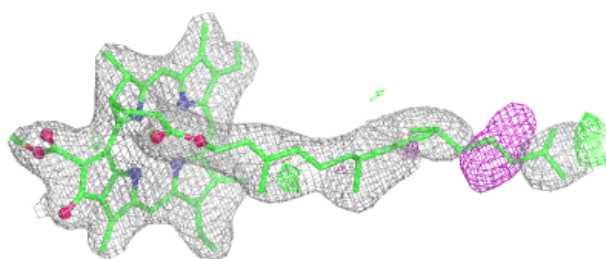
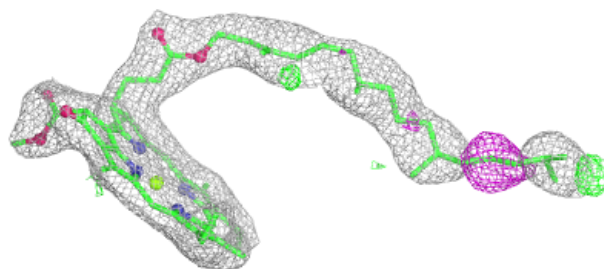
Electron density around CLA b 616:

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

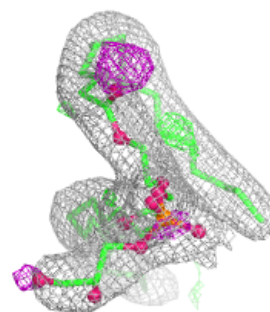
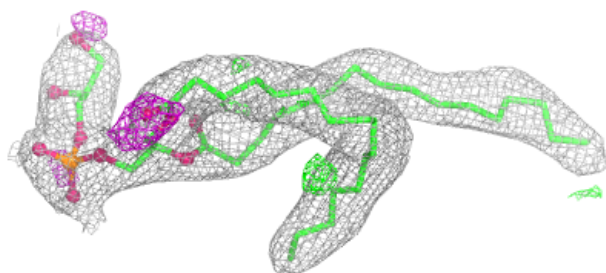
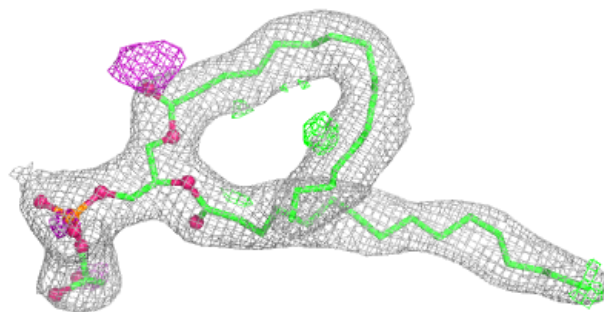


Electron density around CLA c 505:

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

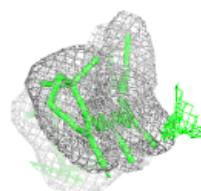
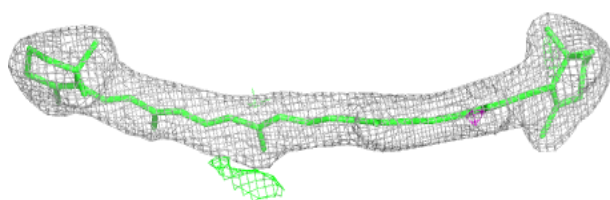
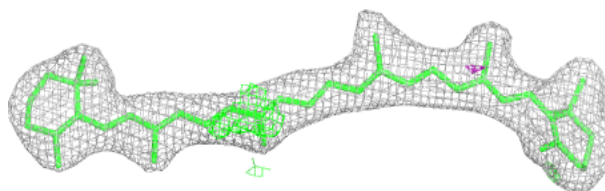
**Electron density around LHG D 409:**

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

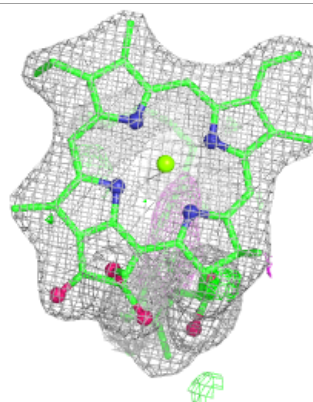
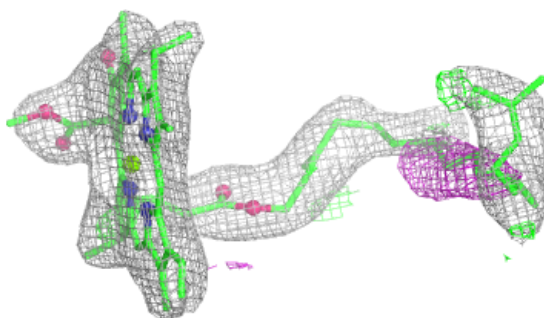
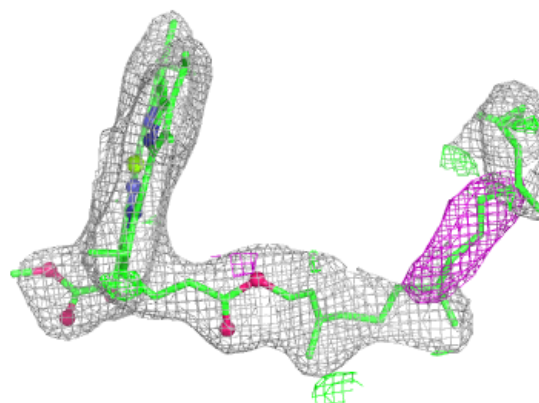


Electron density around BCR t 103:

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

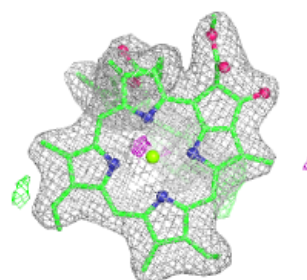
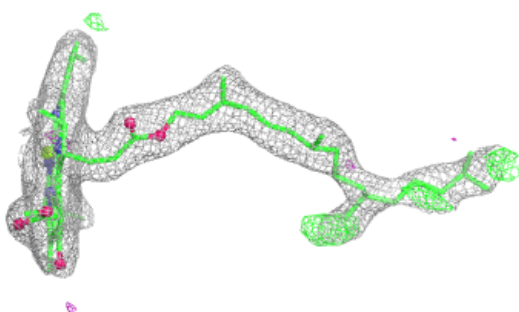
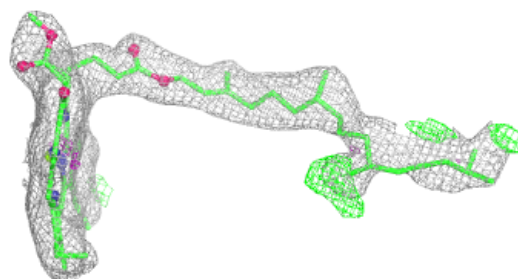
**Electron density around CLA c 507:**

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

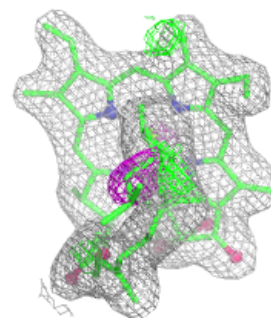
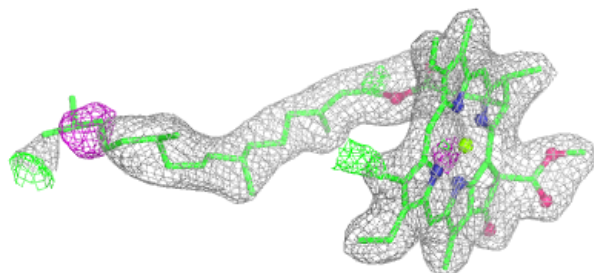
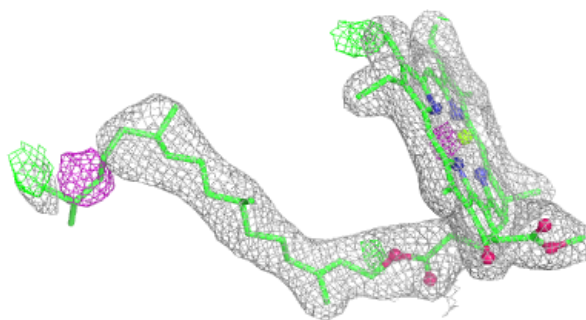


Electron density around CLA B 606:

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

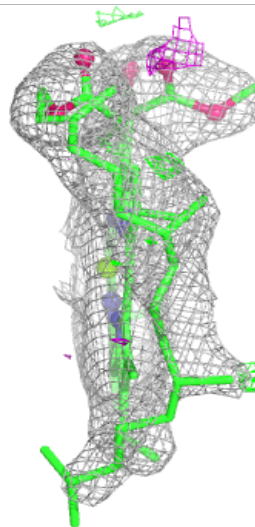
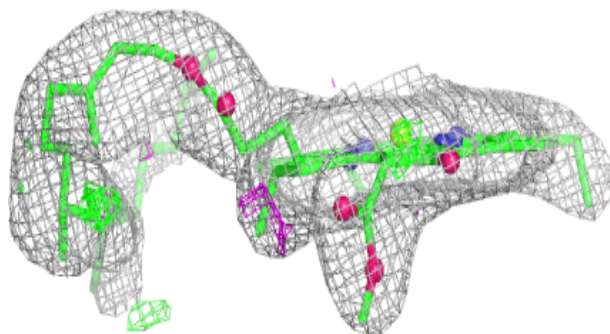
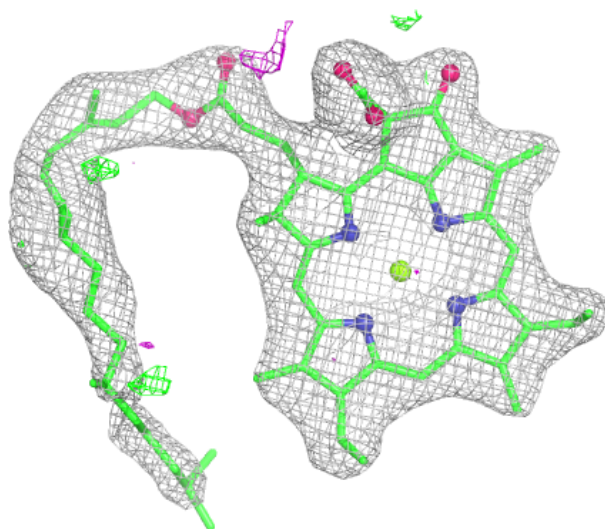
**Electron density around CLA C 509:**

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



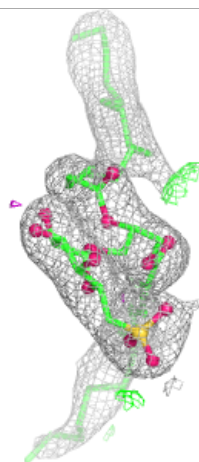
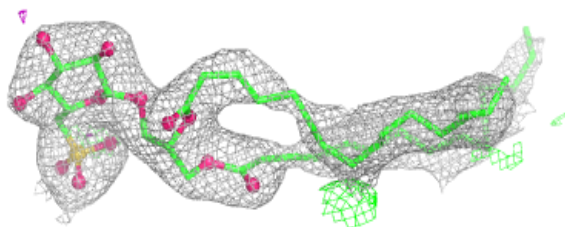
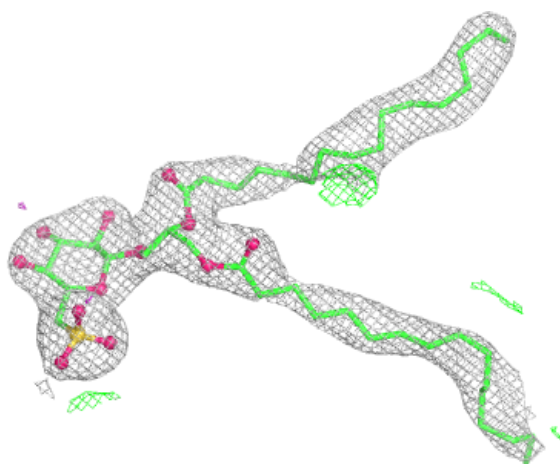
Electron density around CLA C 513:

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



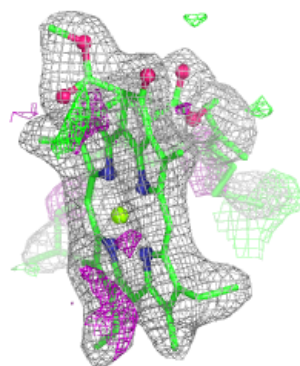
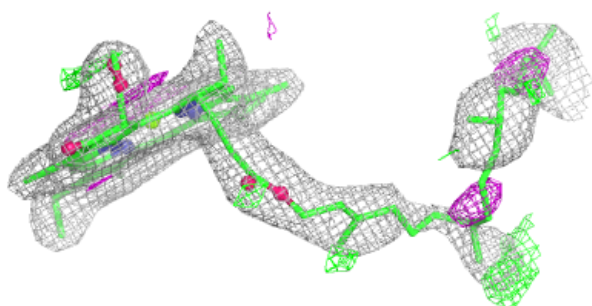
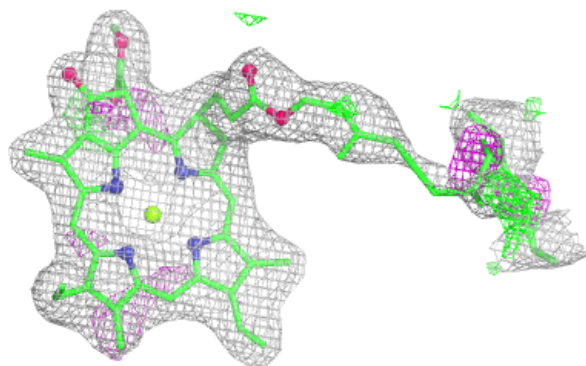
Electron density around SQD a 411:

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

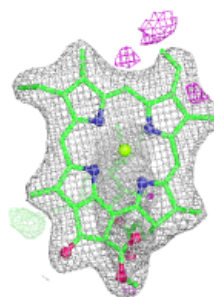
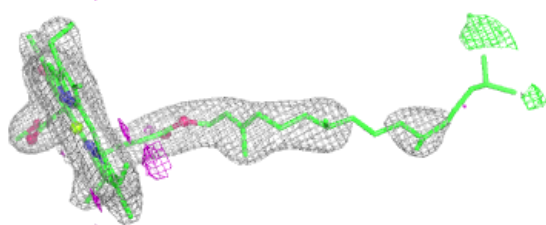
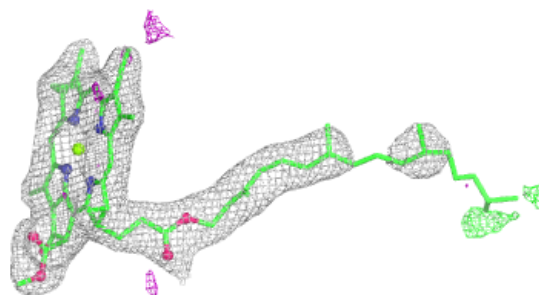


Electron density around CLA A 408:

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

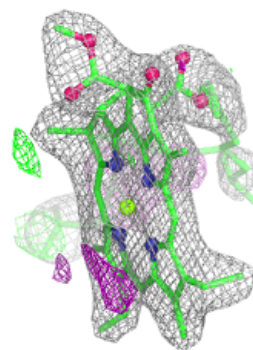
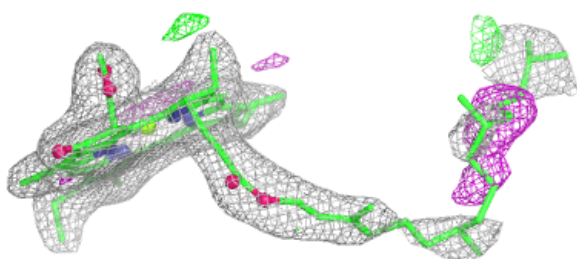
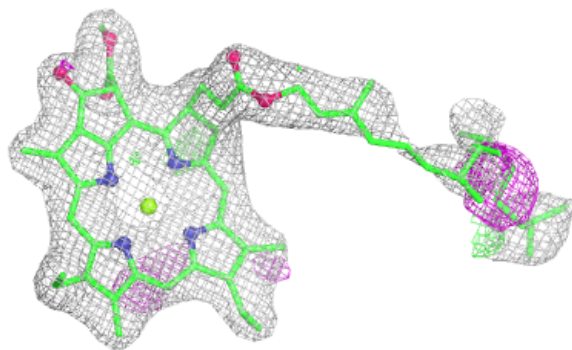
**Electron density around CLA d 403:**

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



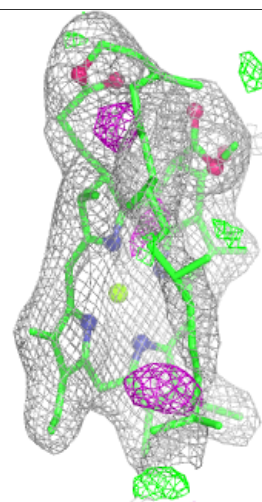
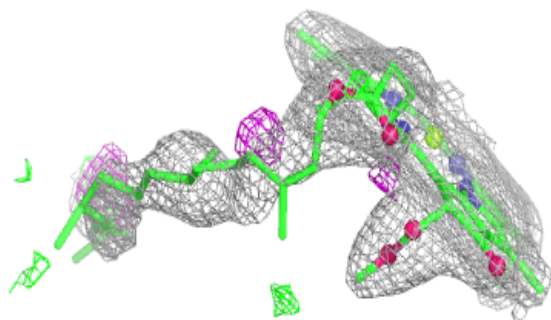
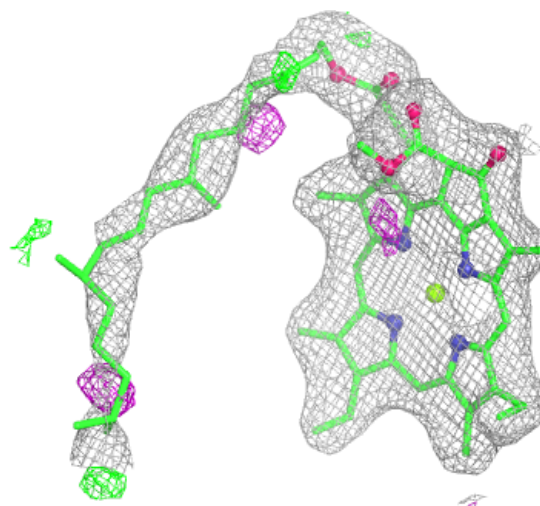
Electron density around CLA a 409:

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



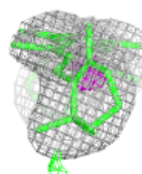
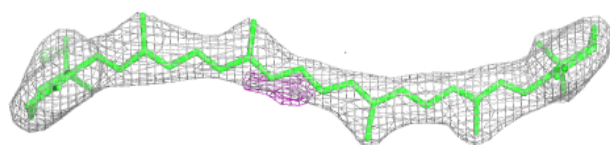
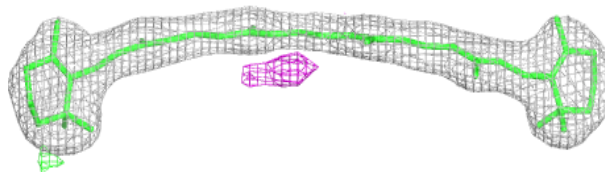
Electron density around CLA B 616:

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

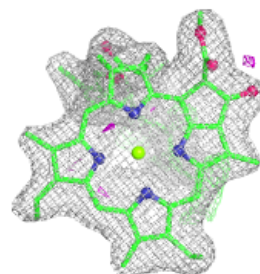
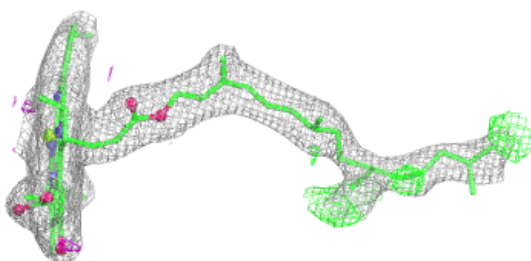
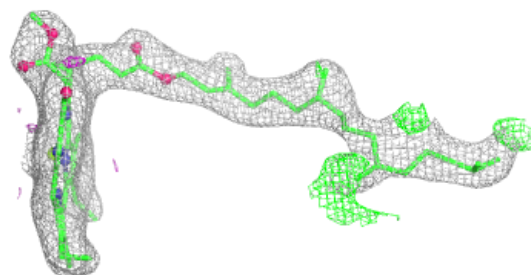


Electron density around BCR K 102:

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

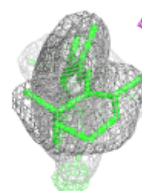
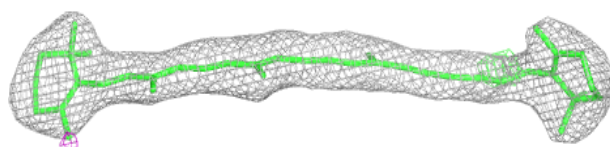
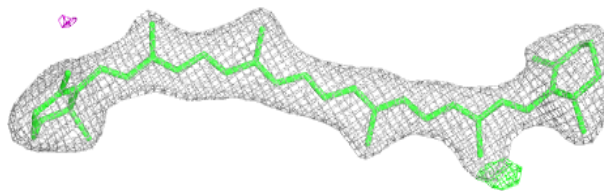
**Electron density around CLA b 606:**

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

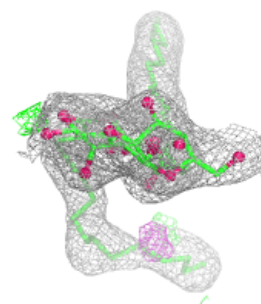
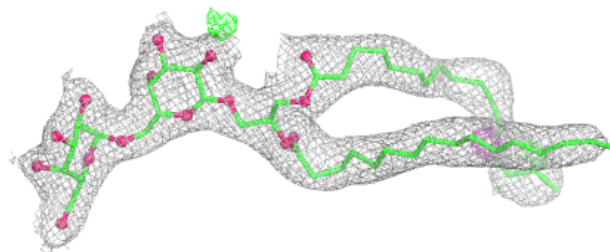
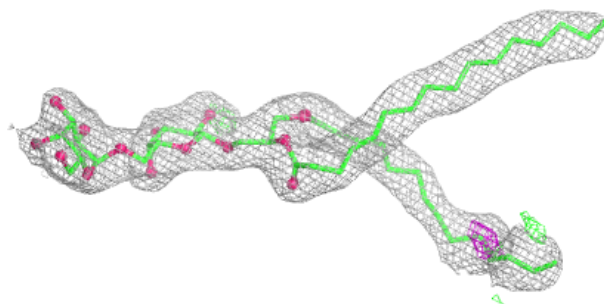


Electron density around BCR Y 101:

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

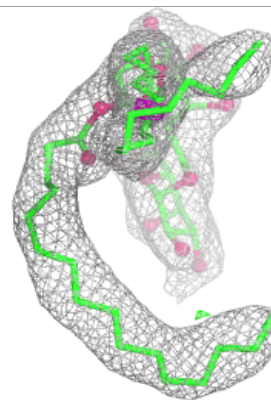
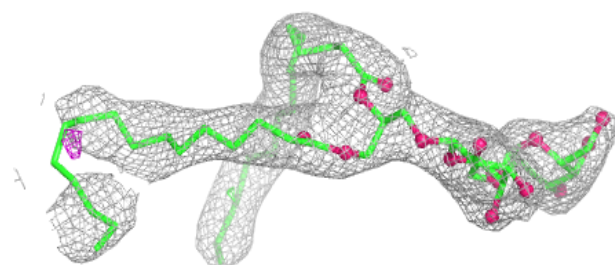
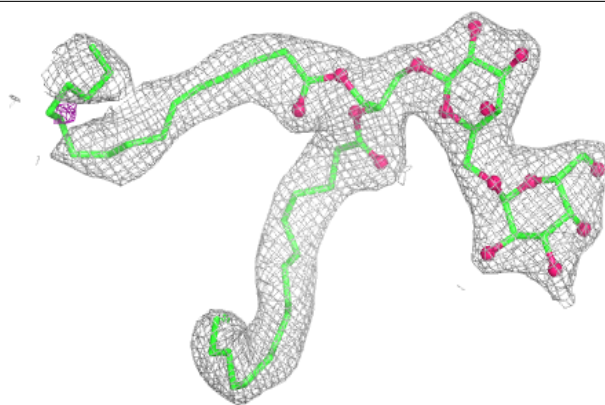
**Electron density around DGD c 517:**

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

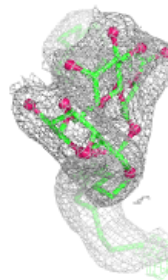
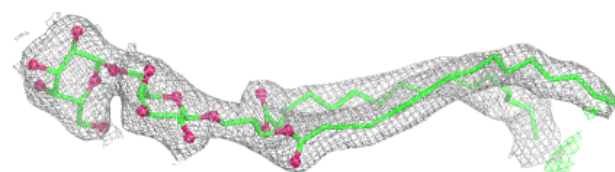
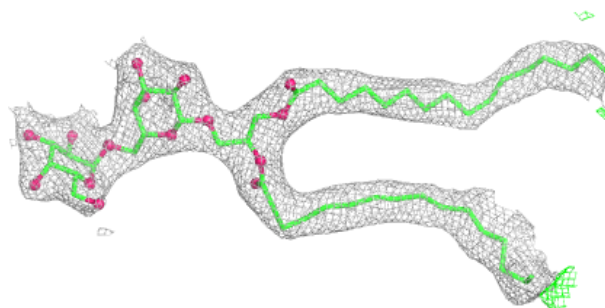


Electron density around DGD c 518:

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

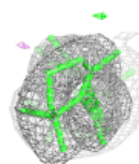
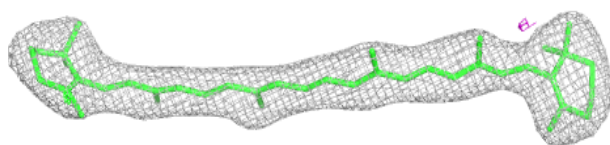
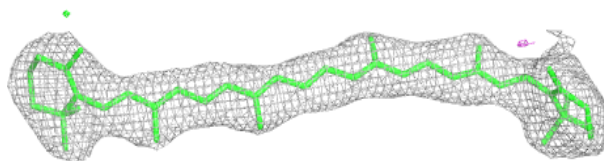
**Electron density around DGD c 519:**

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

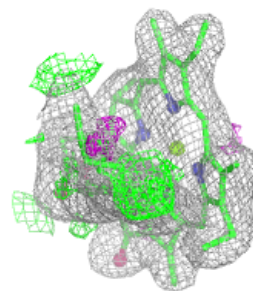
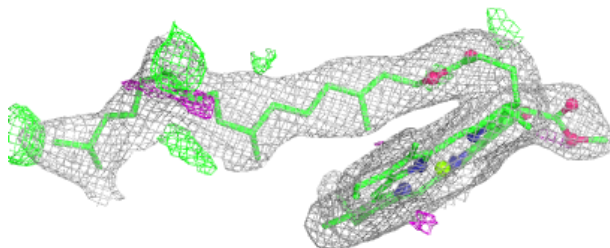
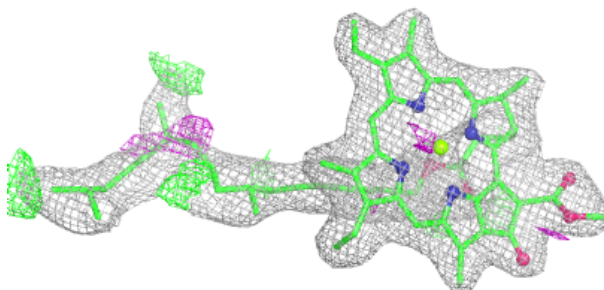


Electron density around BCR c 515:

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

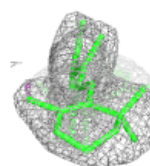
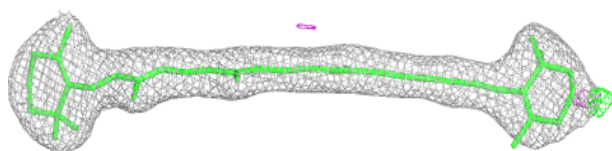
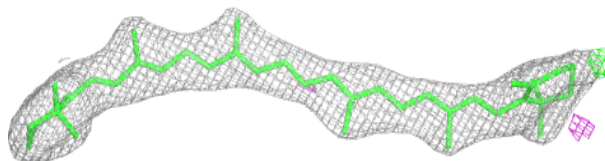
**Electron density around CLA b 614:**

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

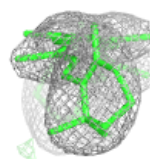
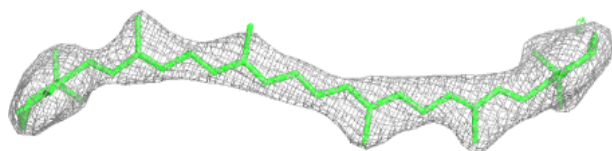
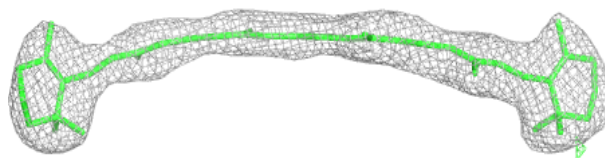


Electron density around BCR h 101:

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

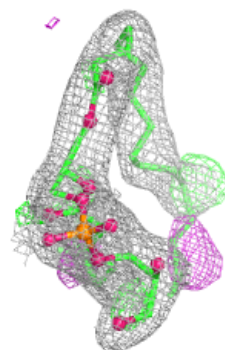
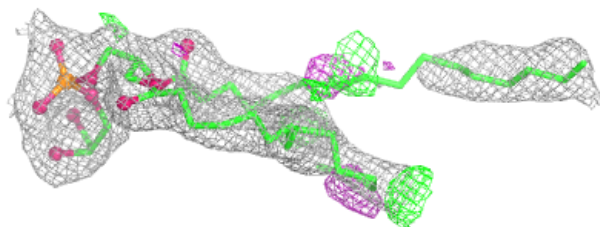
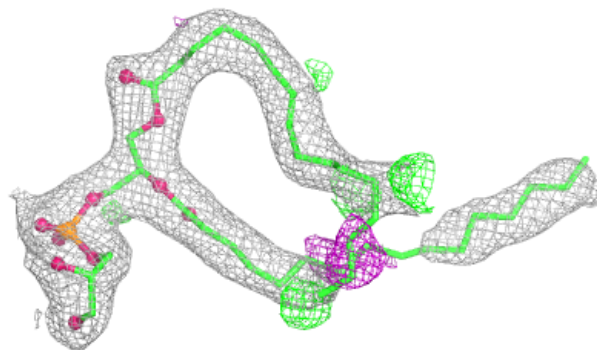
**Electron density around BCR k 101:**

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

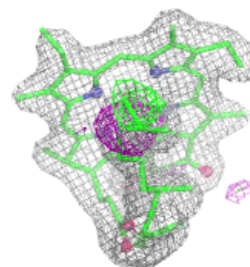
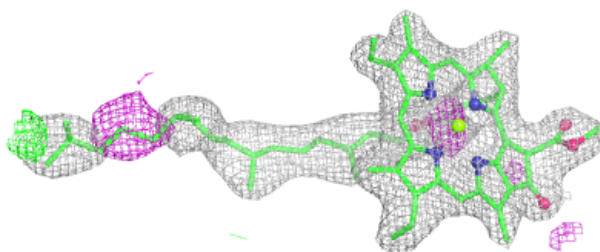
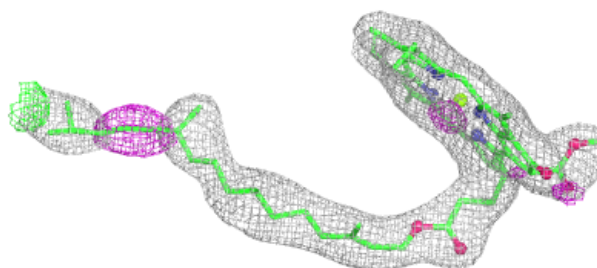


Electron density around LHG D 411:

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

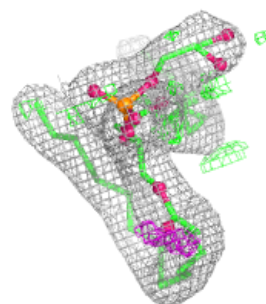
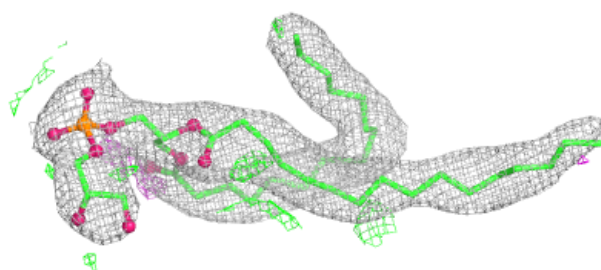
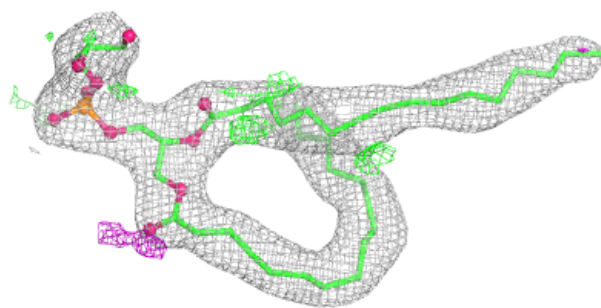
**Electron density around CLA C 505:**

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



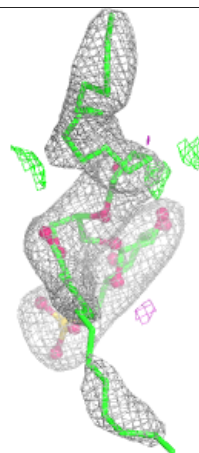
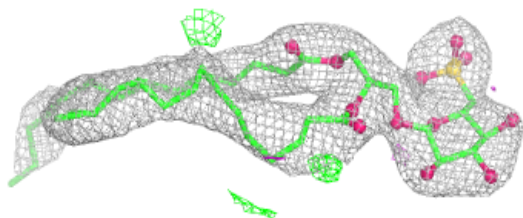
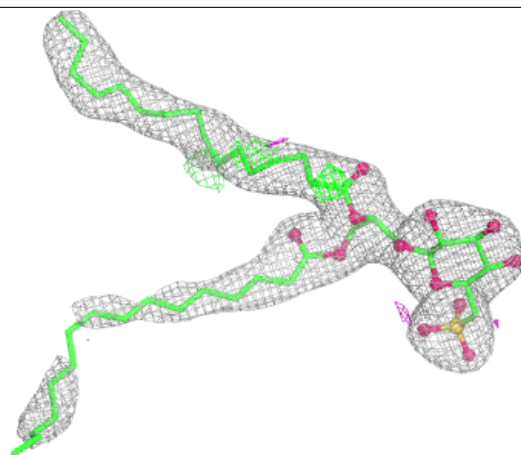
Electron density around LHG d 711:

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

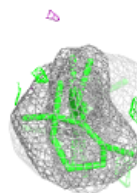
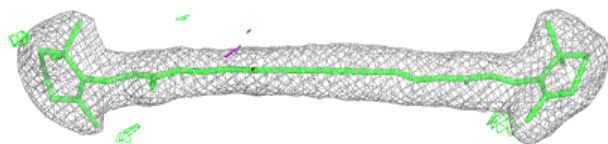
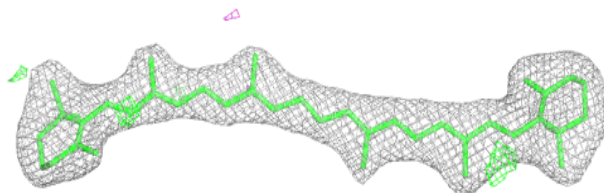


Electron density around SQD A 410:

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

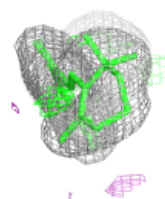
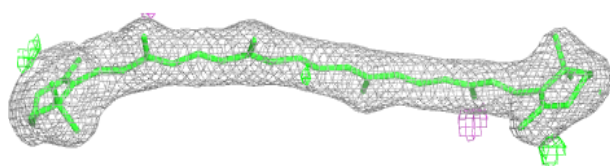
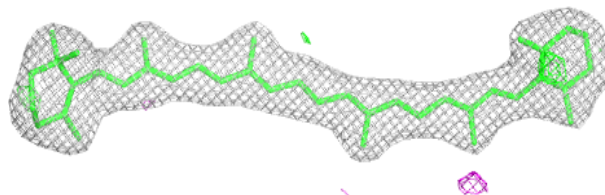
**Electron density around BCR B 618:**

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

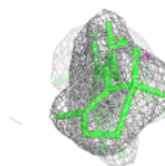
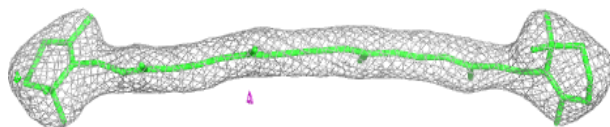
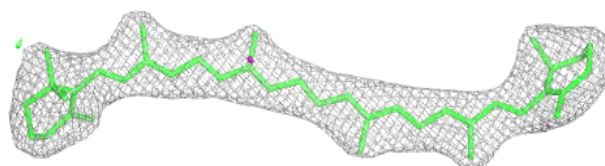


Electron density around BCR B 619:

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

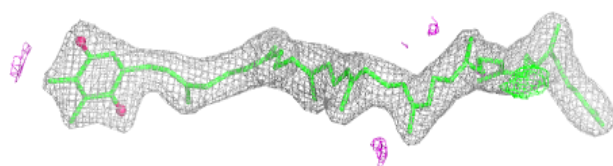
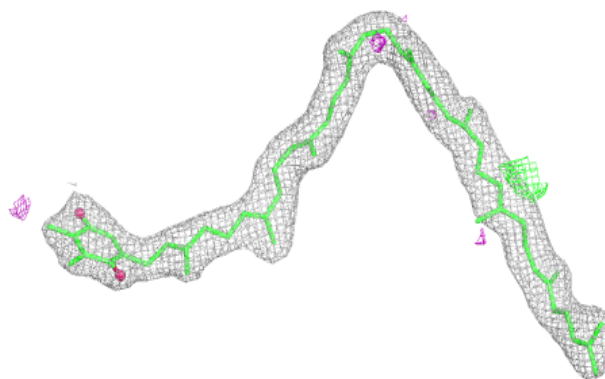
**Electron density around BCR y 101:**

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



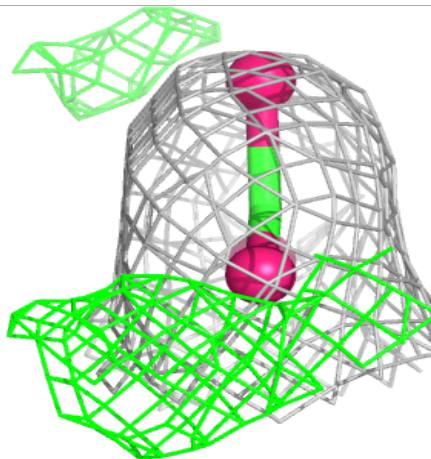
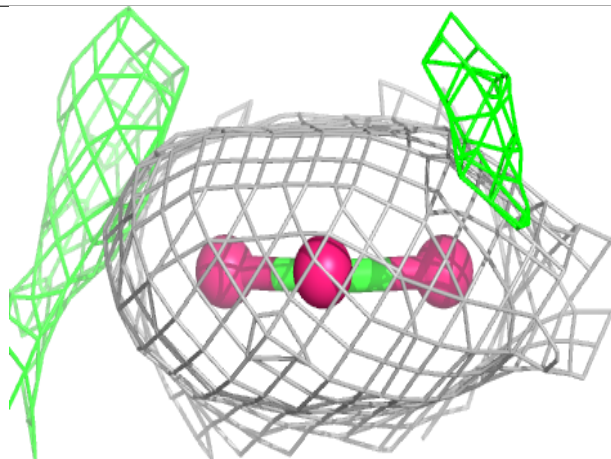
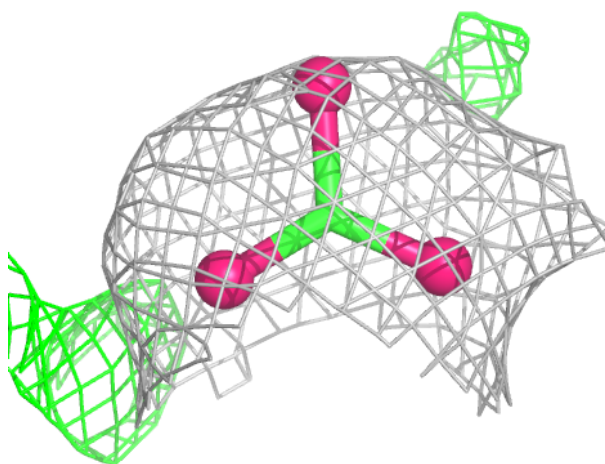
Electron density around PL9 d 405:

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



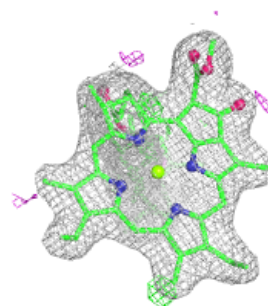
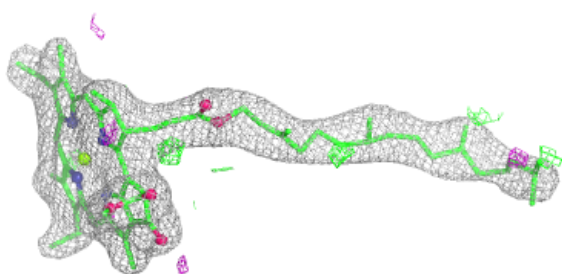
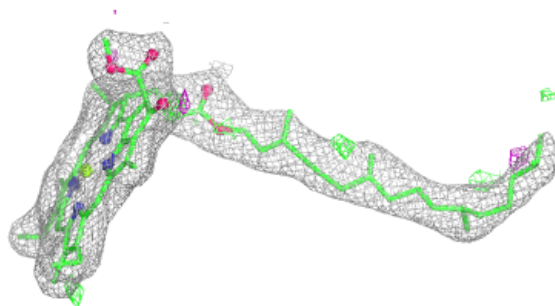
Electron density around BCT a 404:

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

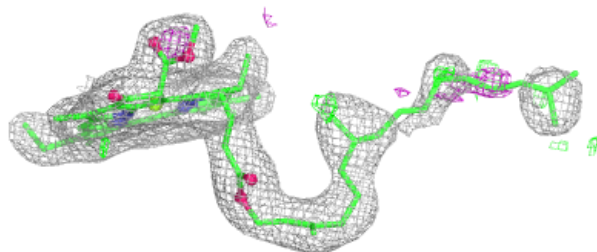
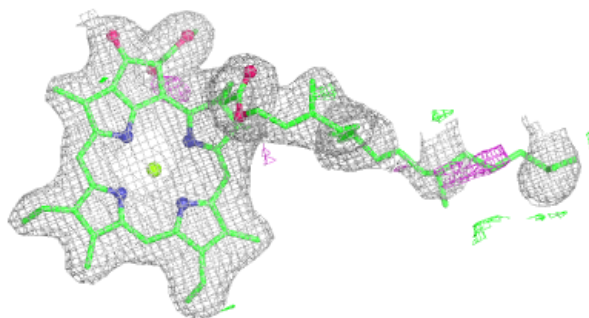


Electron density around CLA b 604:

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

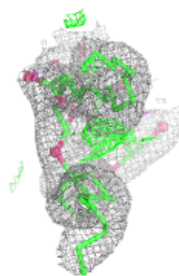
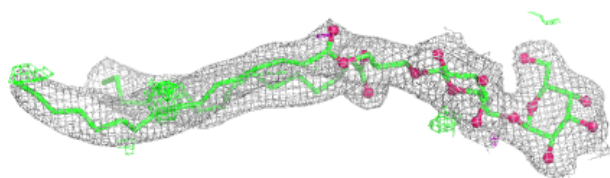
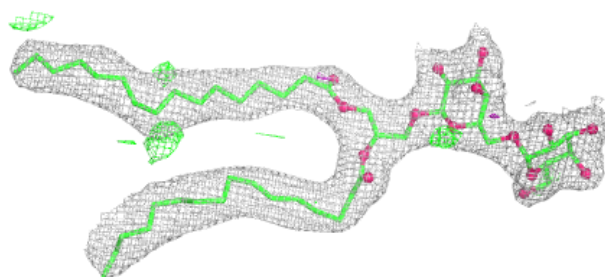
**Electron density around CLA a 407:**

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

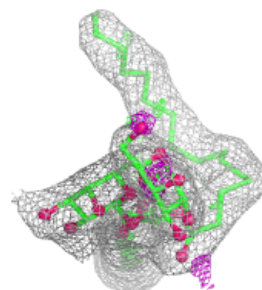
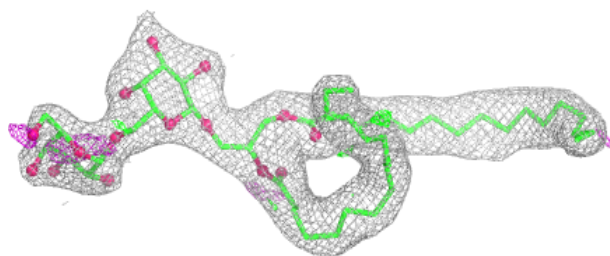
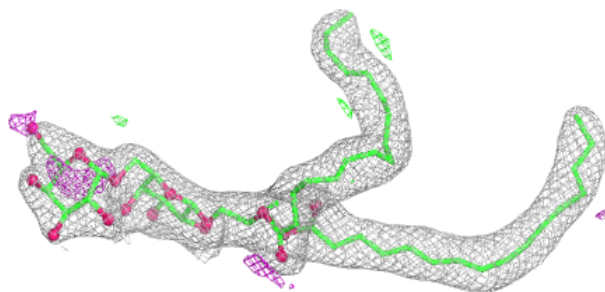


Electron density around DGD C 519:

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

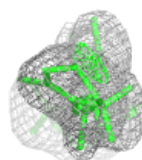
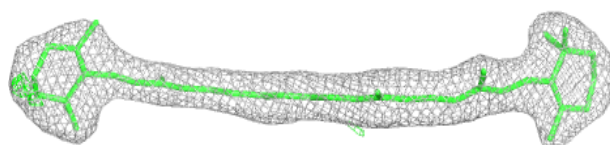
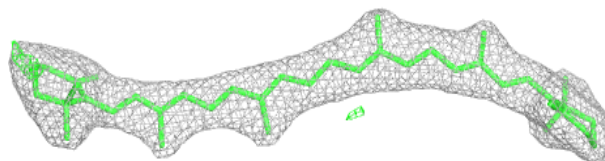
**Electron density around DGD H 102:**

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



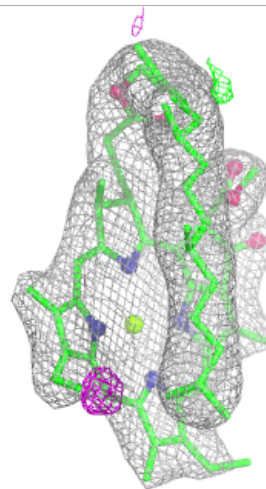
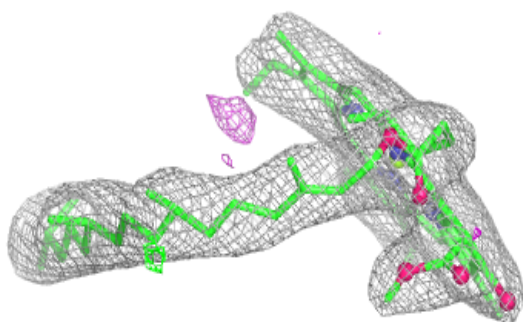
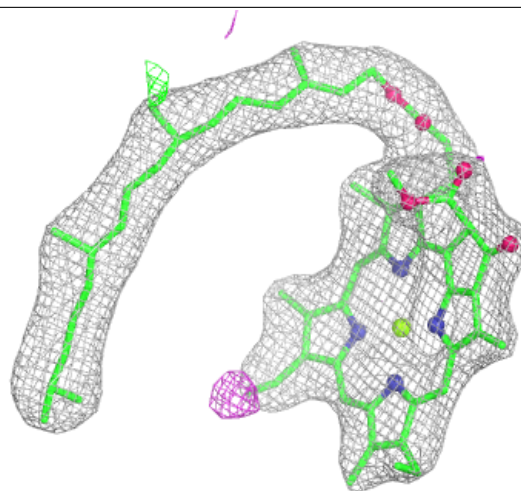
Electron density around BCR H 101:

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



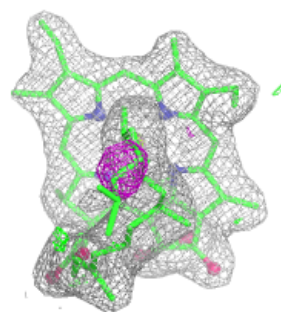
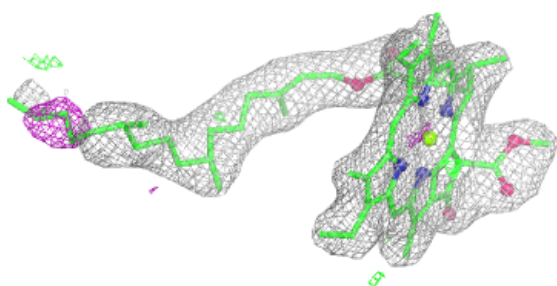
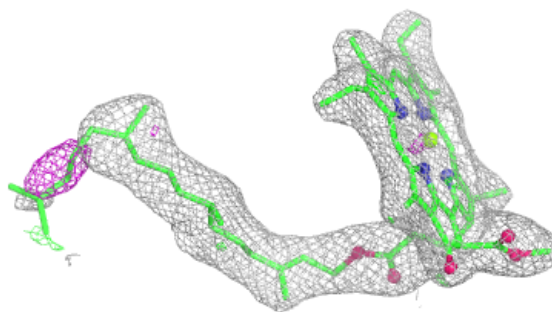
Electron density around CLA c 508:

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

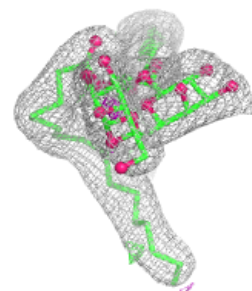
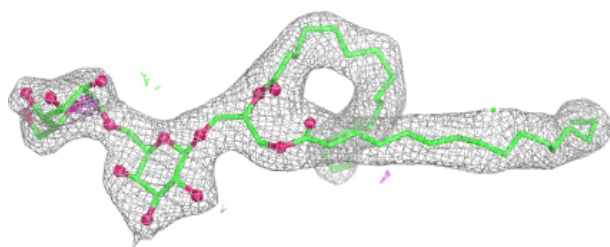
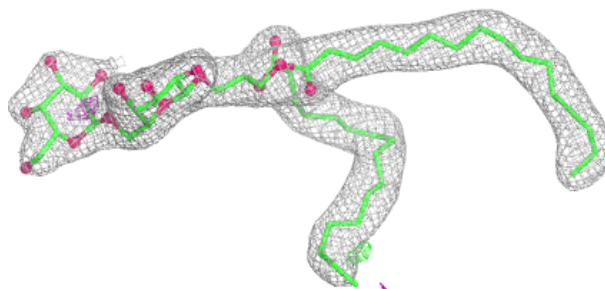


Electron density around CLA c 509:

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

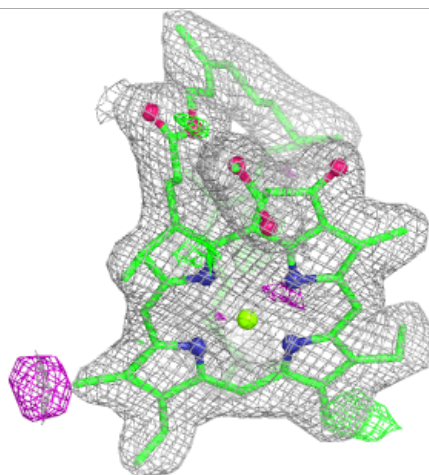
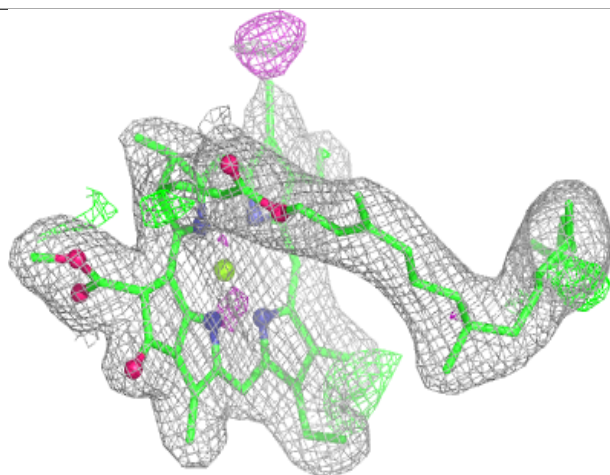
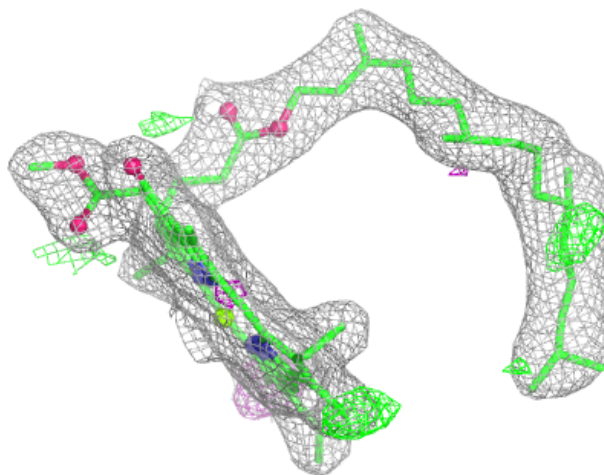
**Electron density around DGD h 102:**

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



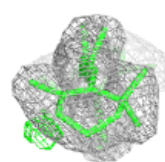
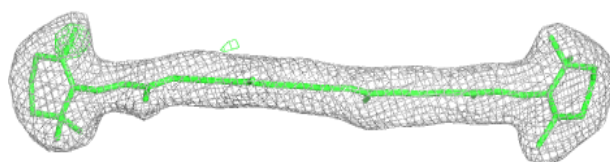
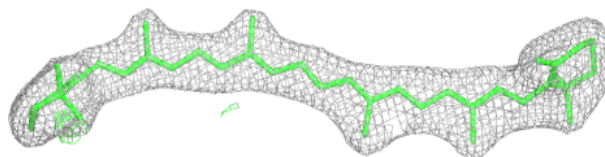
Electron density around CLA B 611:

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

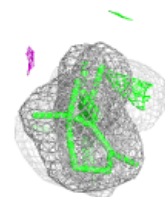
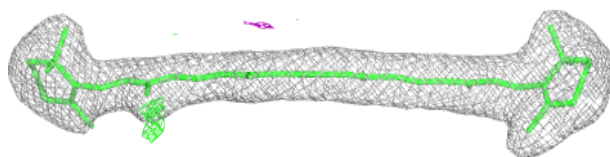
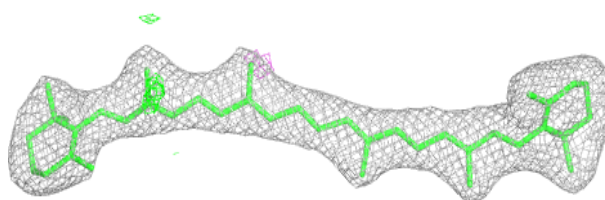


Electron density around BCR a 410:

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

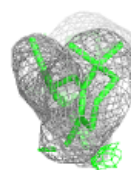
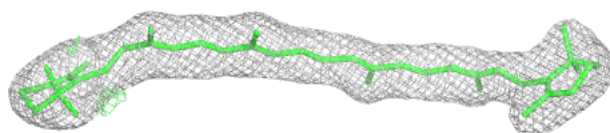
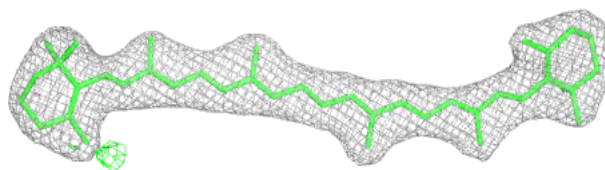
**Electron density around BCR b 618:**

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

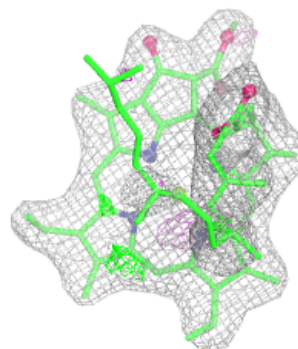
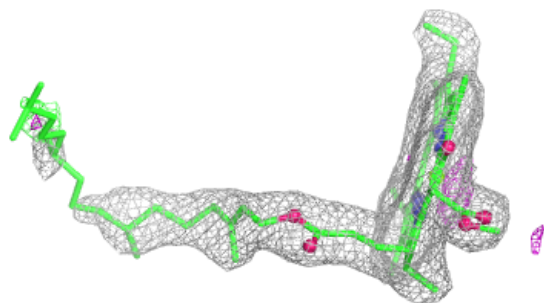
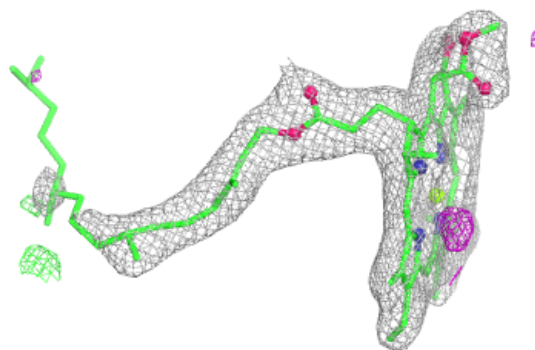


Electron density around BCR b 619:

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

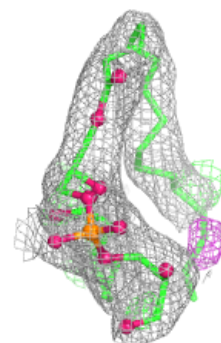
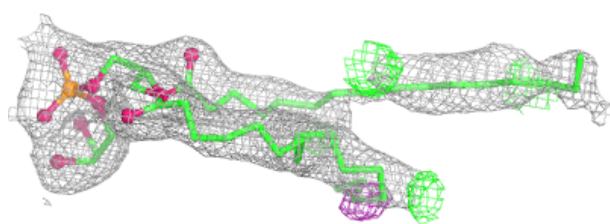
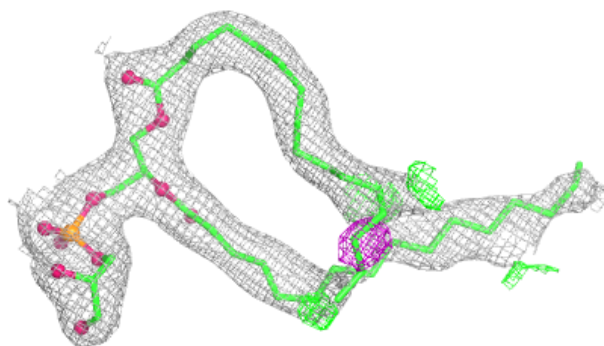
**Electron density around CLA D 406:**

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

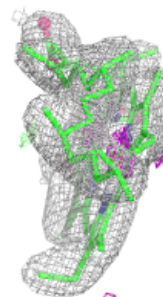
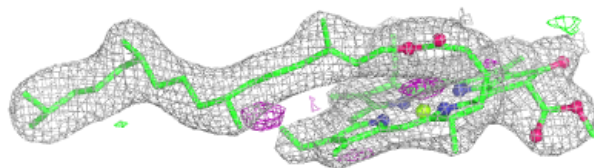
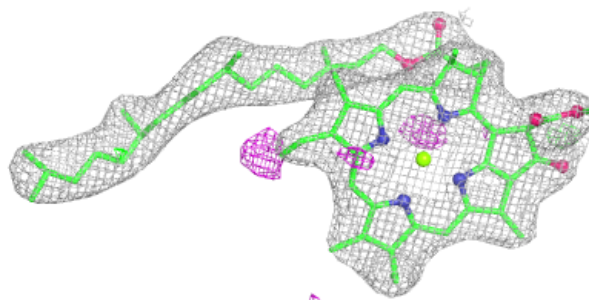


Electron density around LHG d 408:

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

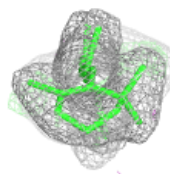
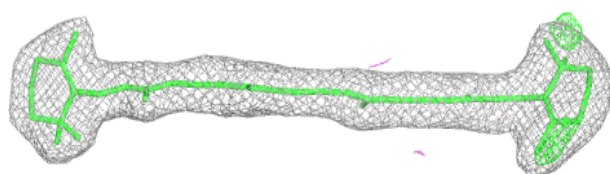
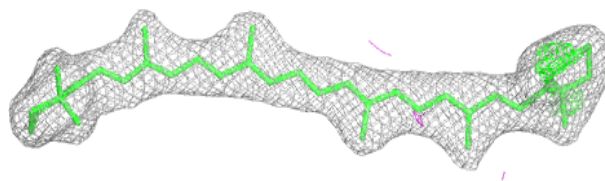
**Electron density around CLA c 502:**

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



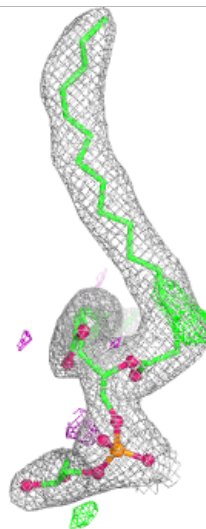
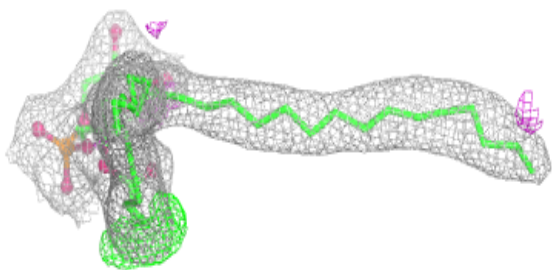
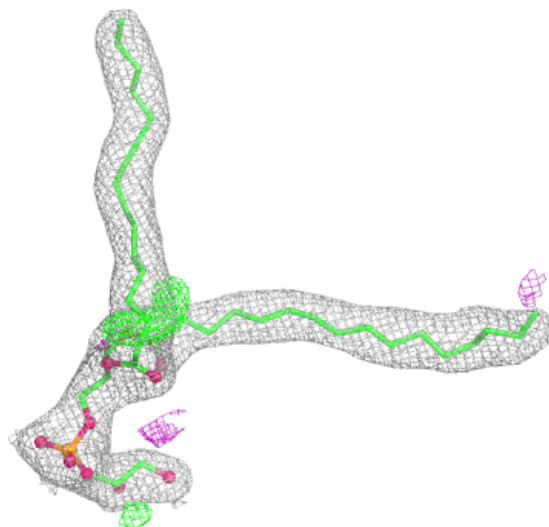
Electron density around BCR A 409:

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



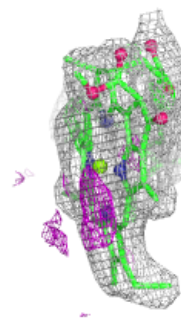
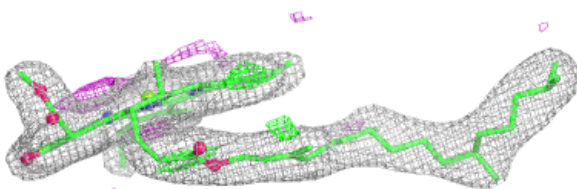
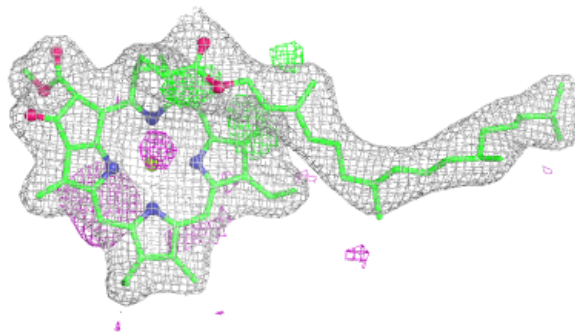
Electron density around LHG 1 101:

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

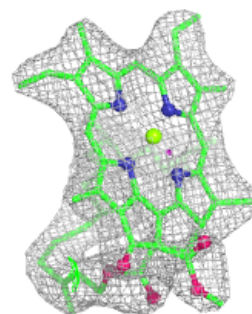
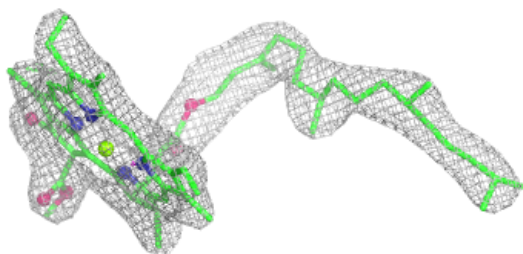
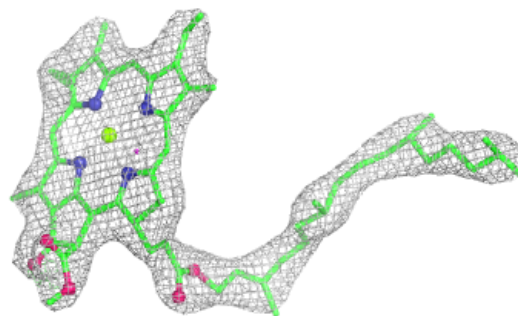


Electron density around CLA B 603:

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

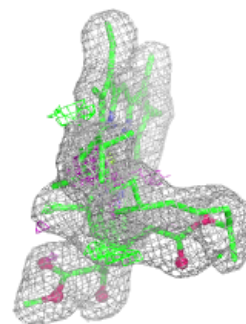
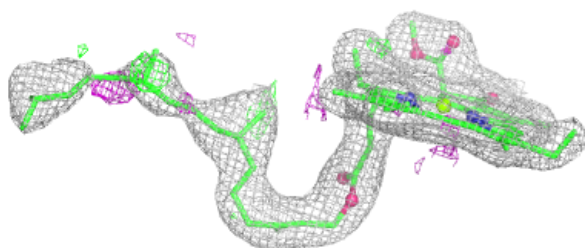
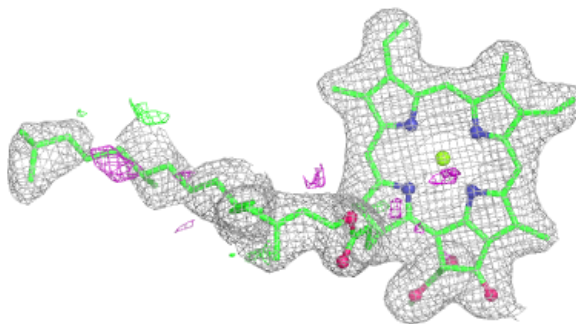
**Electron density around CLA c 512:**

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

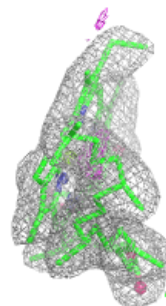
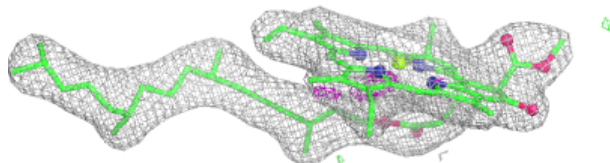
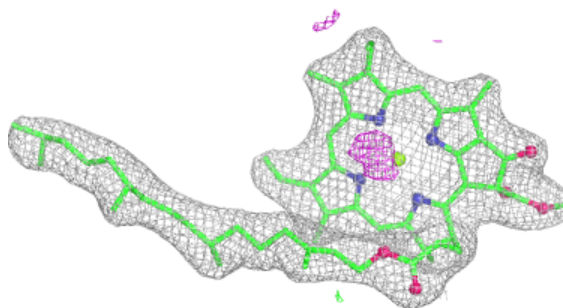


Electron density around CLA A 406:

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

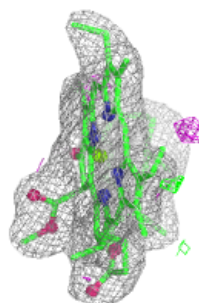
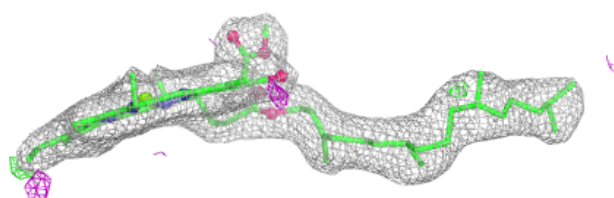
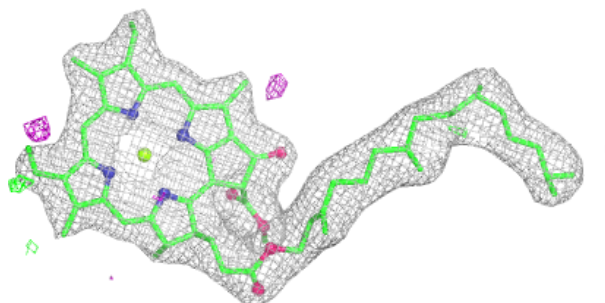
**Electron density around CLA C 502:**

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

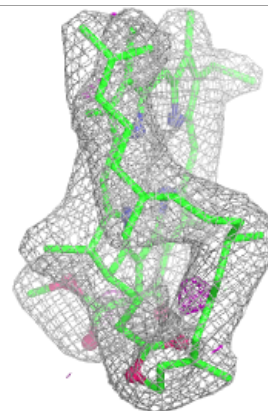
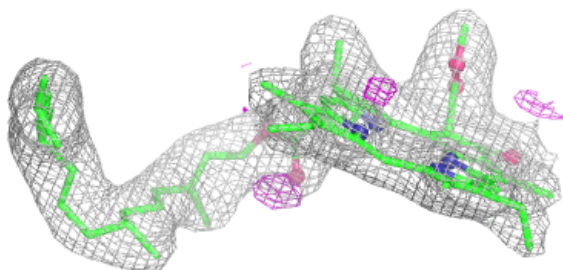
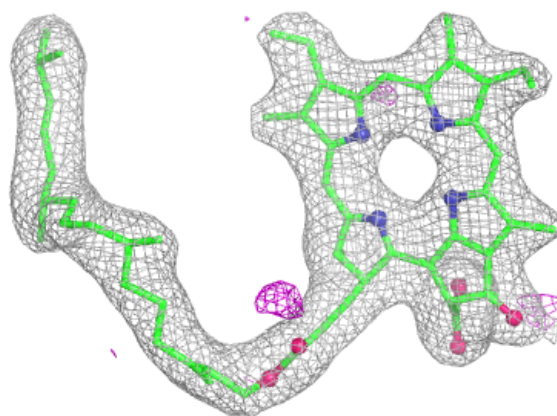


Electron density around CLA b 602:

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

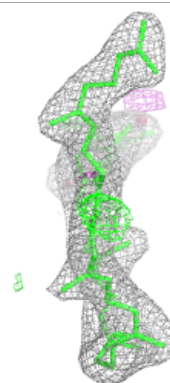
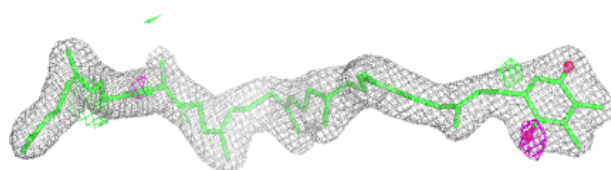
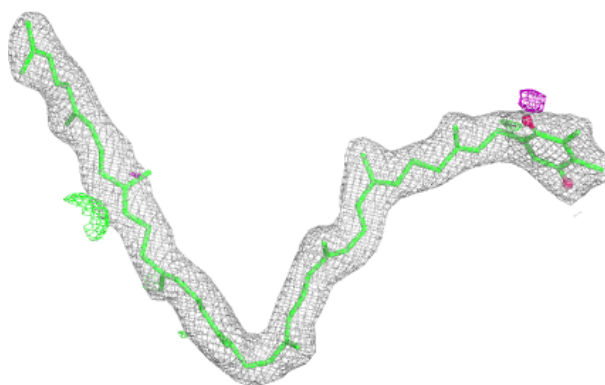
**Electron density around PHO a 353:**

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

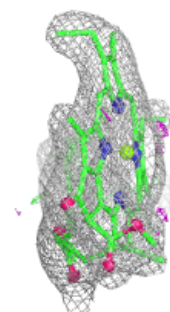
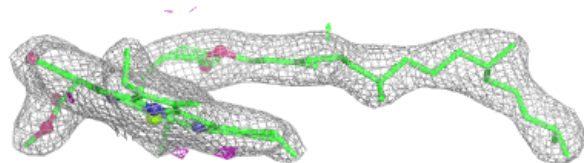
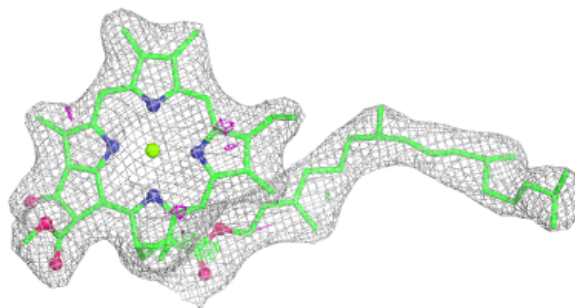


Electron density around PL9 D 408:

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

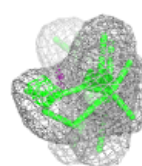
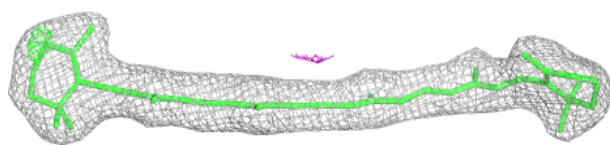
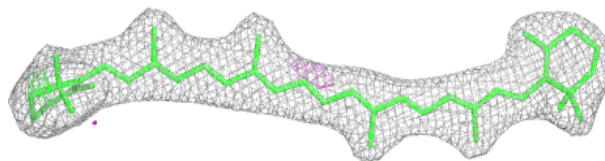
**Electron density around CLA b 603:**

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

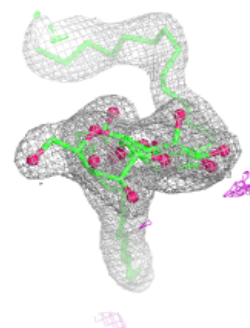
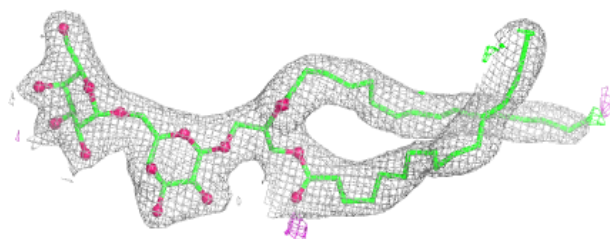
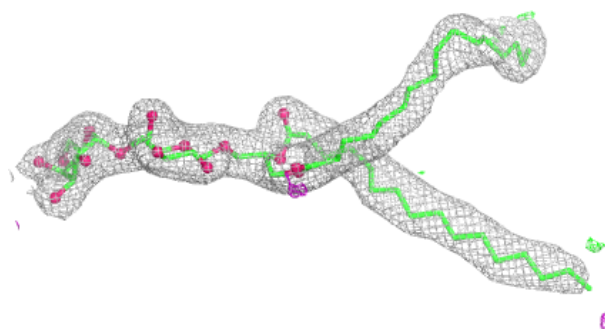


Electron density around BCR B 617:

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

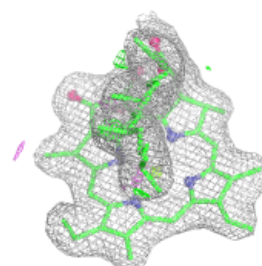
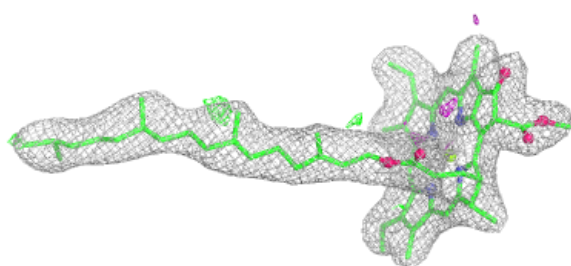
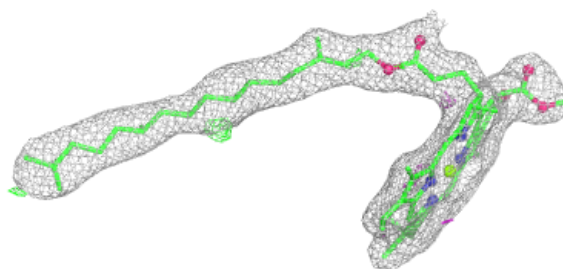
**Electron density around DGD C 517:**

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

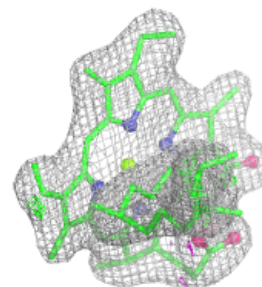
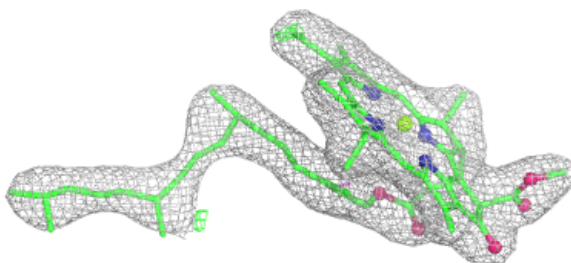
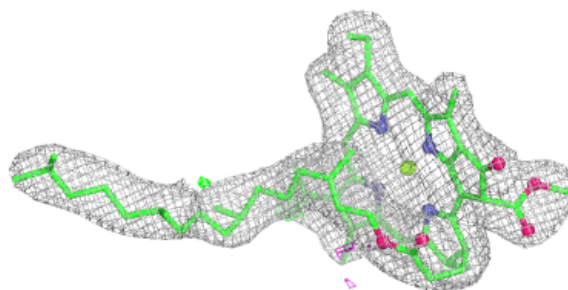


Electron density around CLA B 607:

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

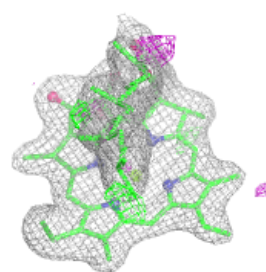
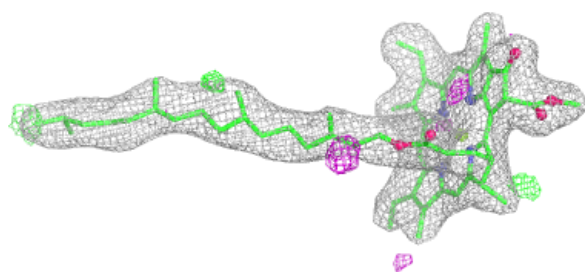
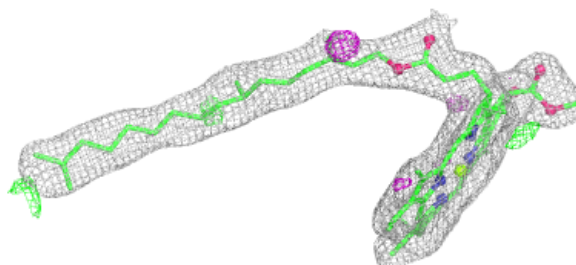
**Electron density around CLA C 506:**

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

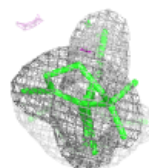
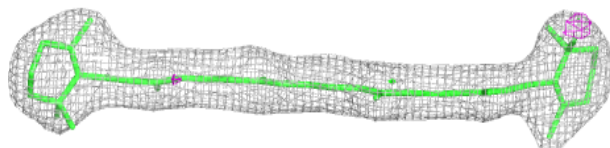
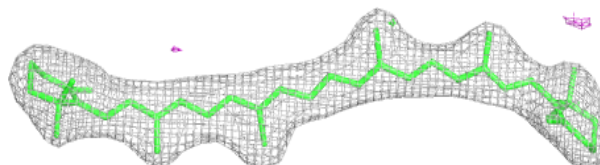


Electron density around CLA b 607:

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

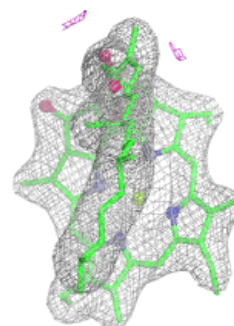
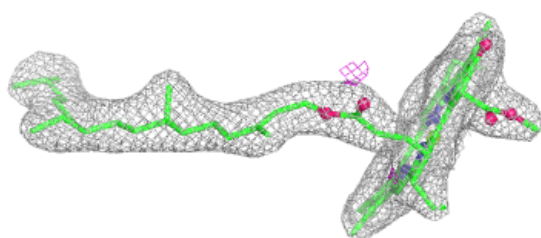
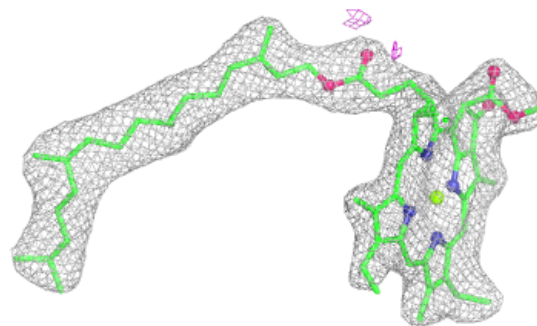
**Electron density around BCR C 516:**

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



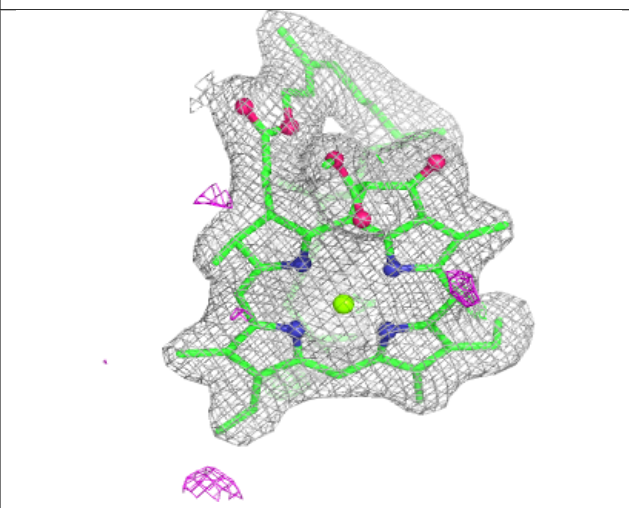
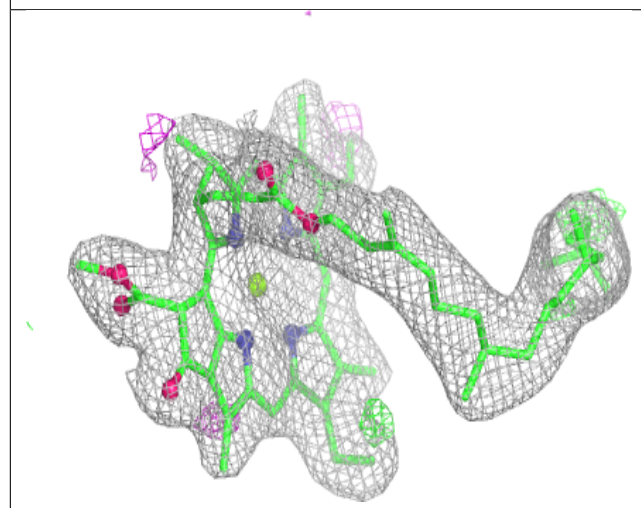
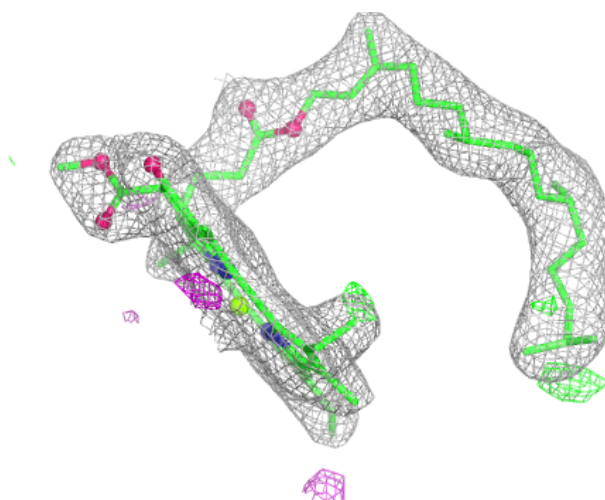
Electron density around CLA b 609:

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



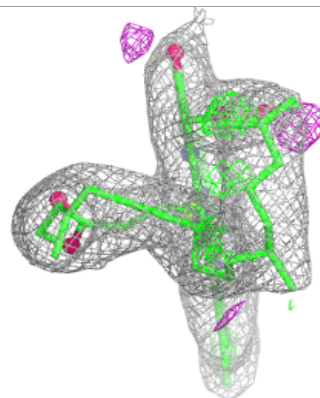
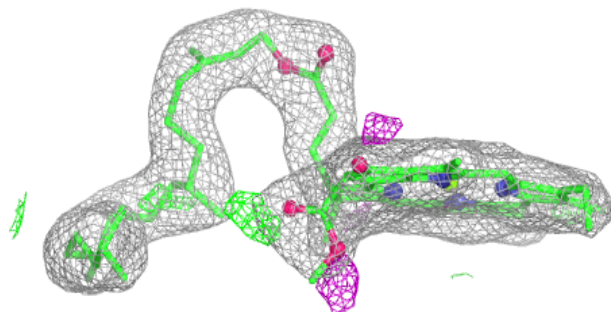
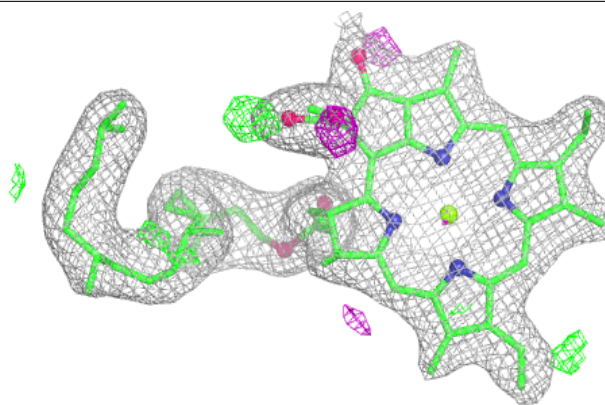
Electron density around CLA b 611:

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



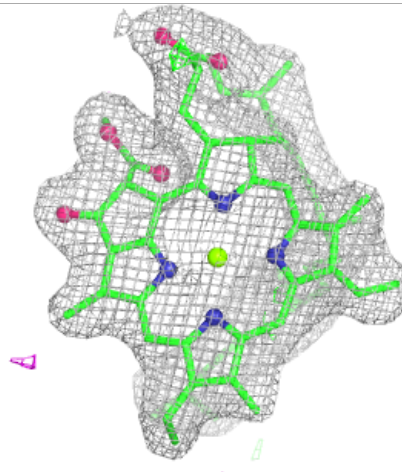
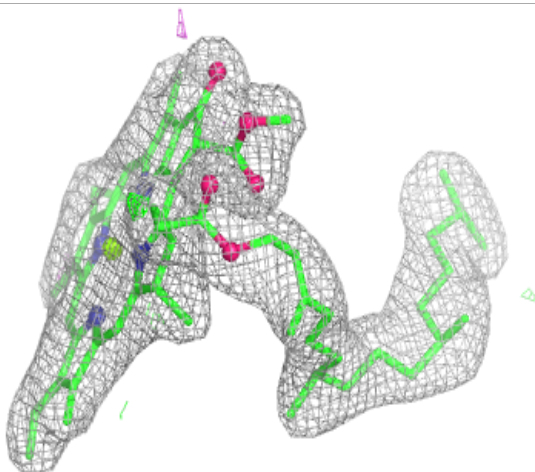
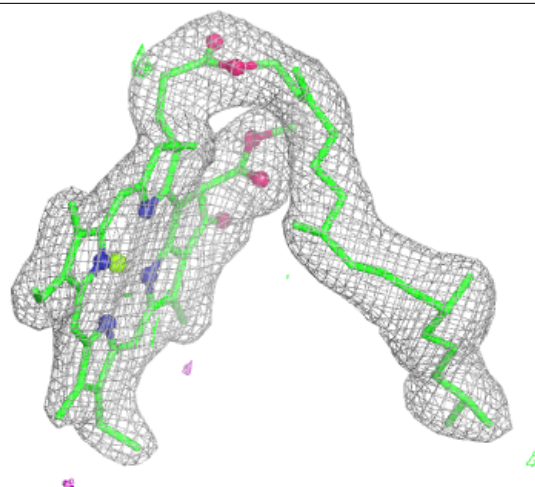
Electron density around CLA b 612:

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



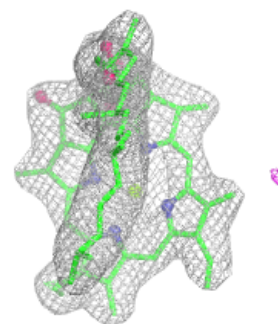
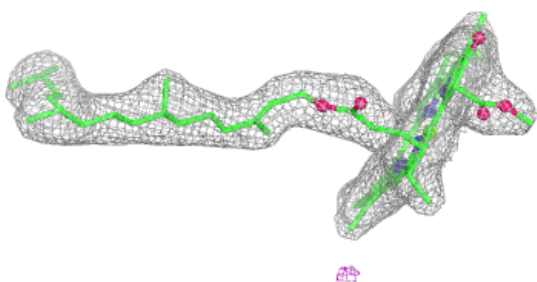
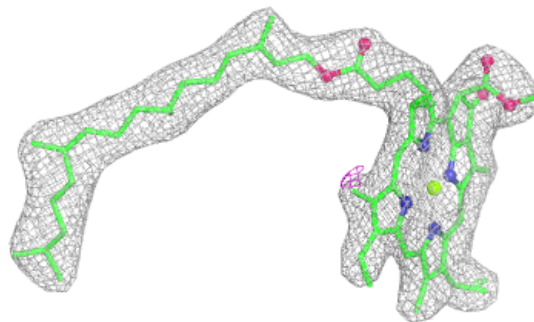
Electron density around CLA b 613:

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



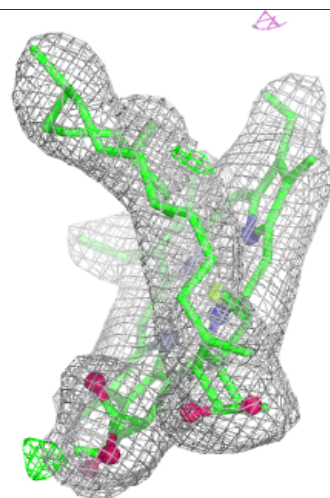
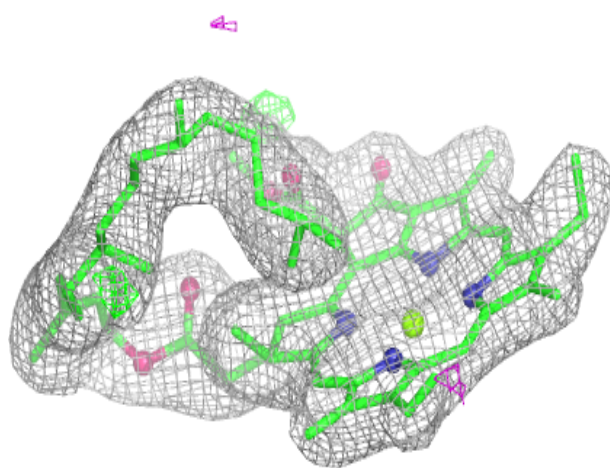
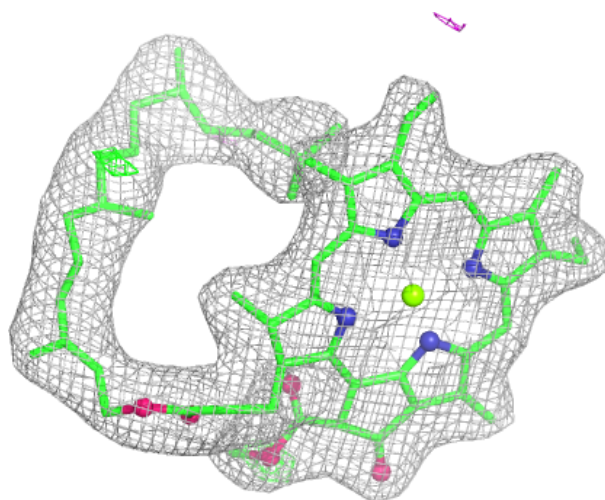
Electron density around CLA B 609:

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



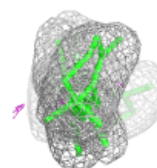
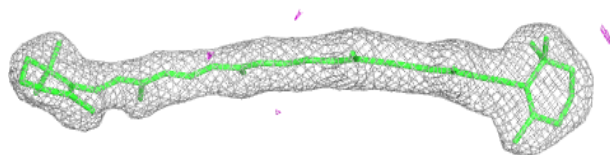
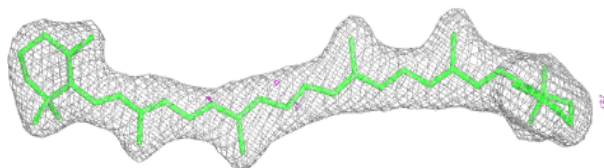
Electron density around CLA b 615:

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

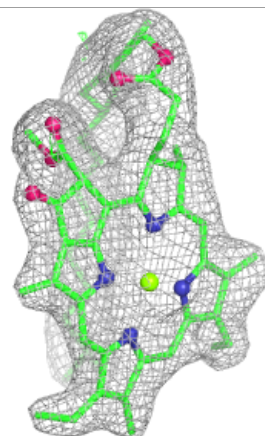
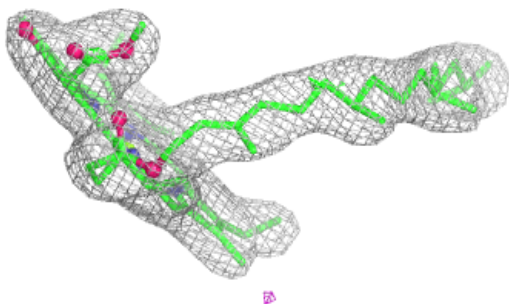
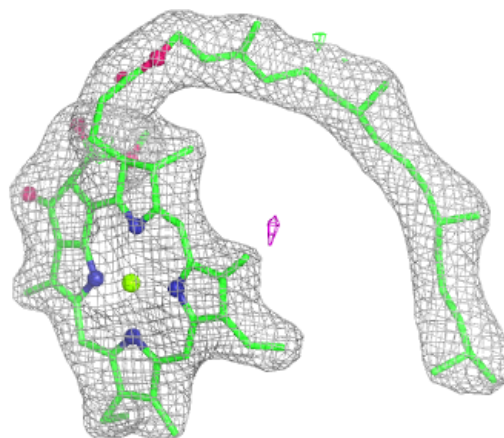


Electron density around BCR b 617:

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

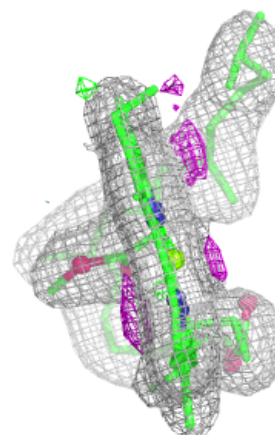
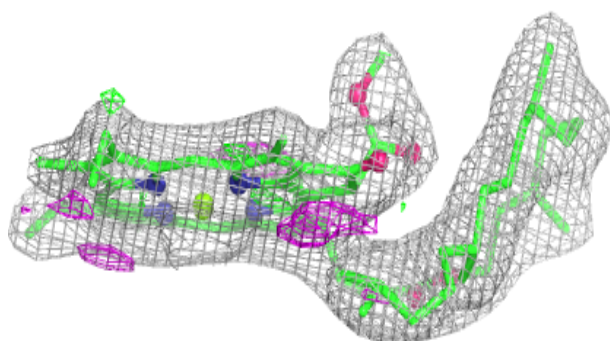
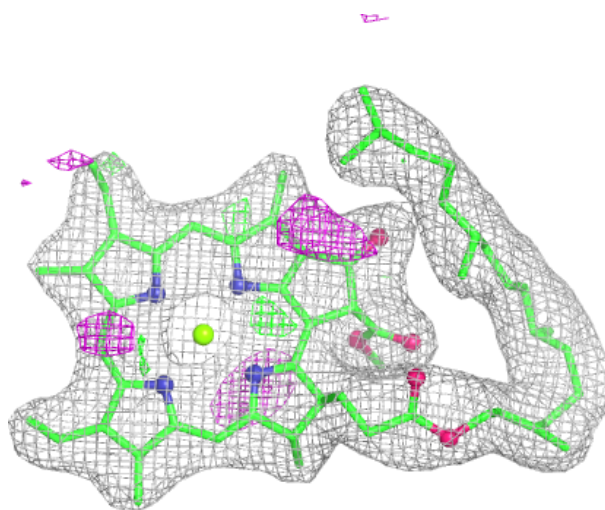
**Electron density around CLA C 508:**

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



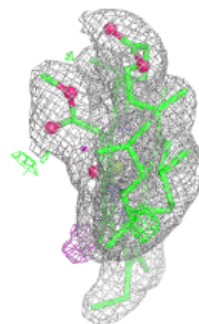
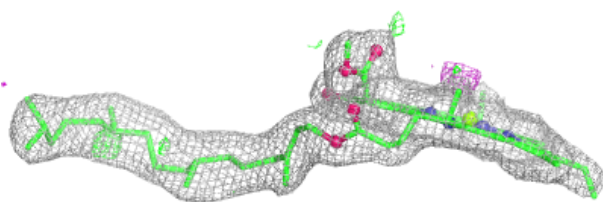
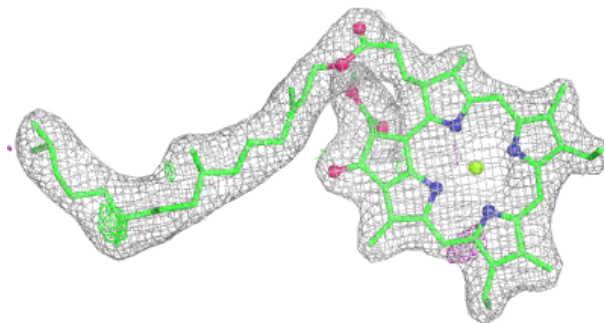
Electron density around CLA B 610:

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

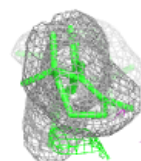
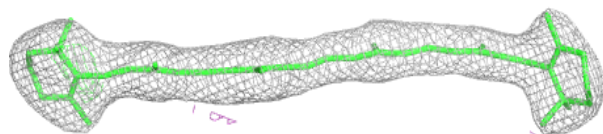
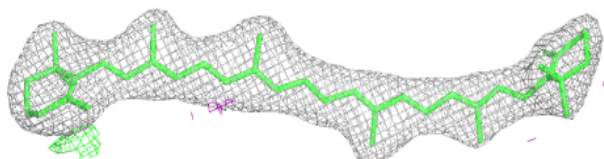


Electron density around CLA B 602:

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

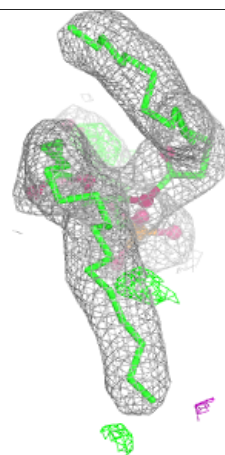
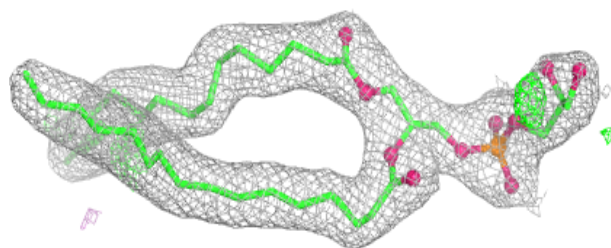
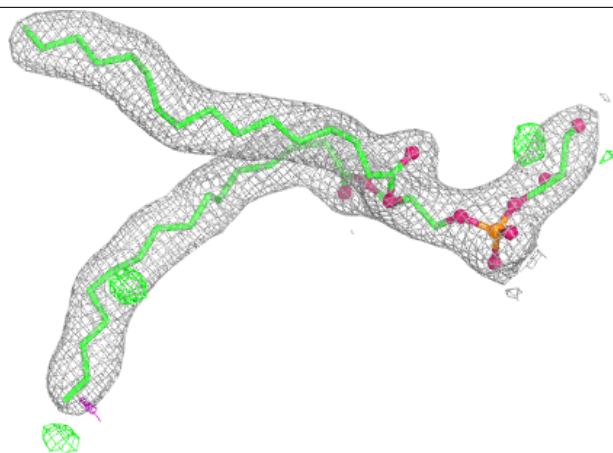
**Electron density around BCR c 516:**

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



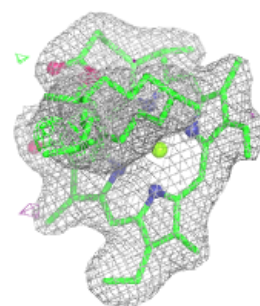
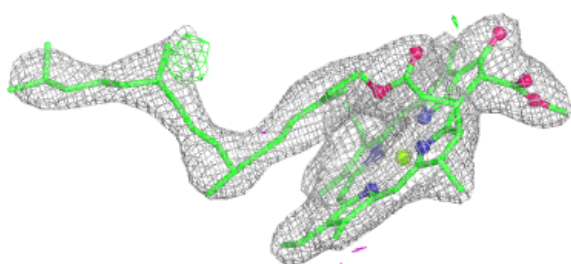
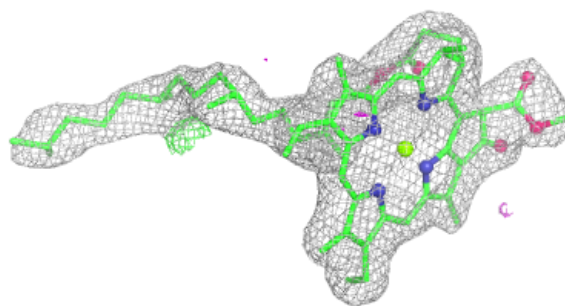
Electron density around LHG d 407:

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

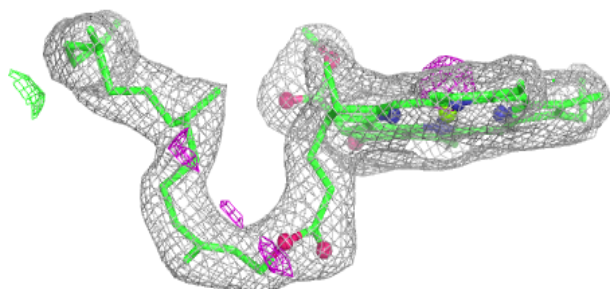
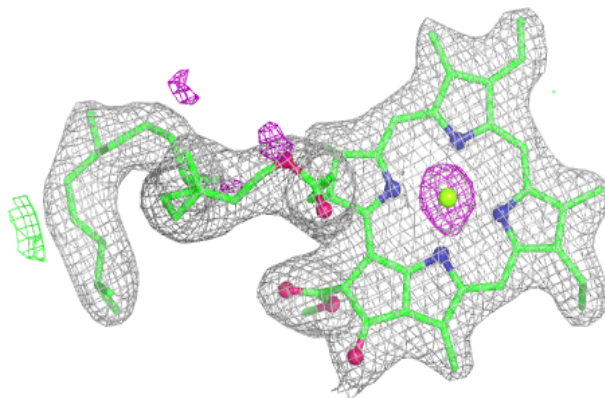


Electron density around CLA c 506:

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

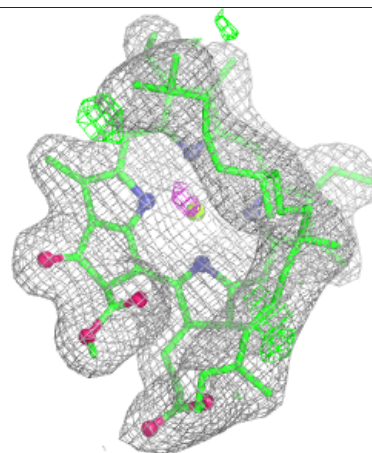
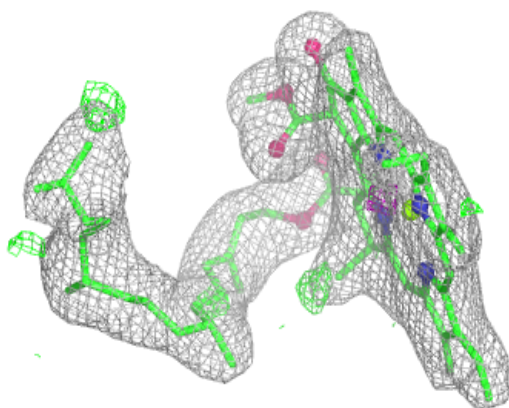
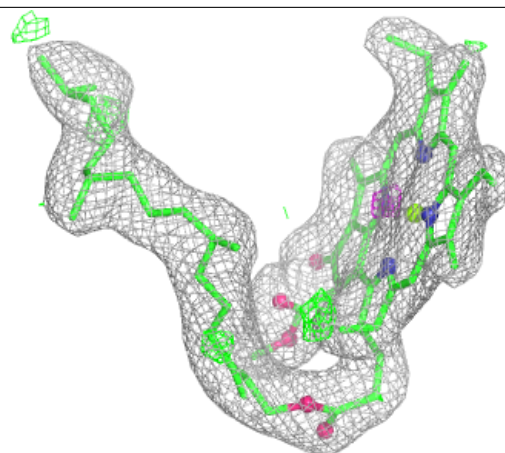
**Electron density around CLA B 612:**

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

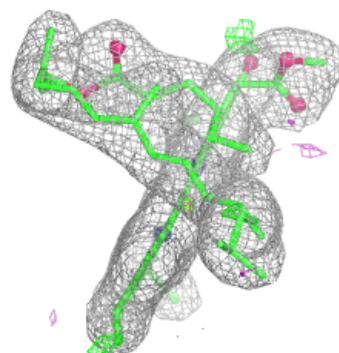
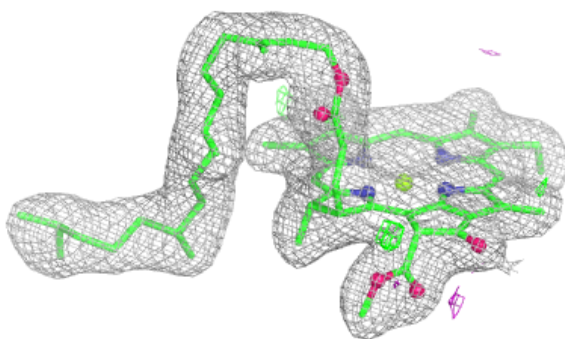
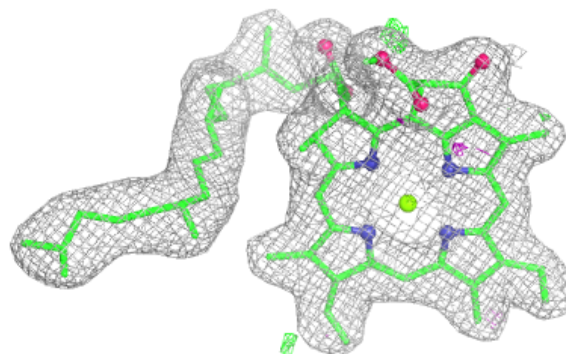


Electron density around CLA B 613:

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

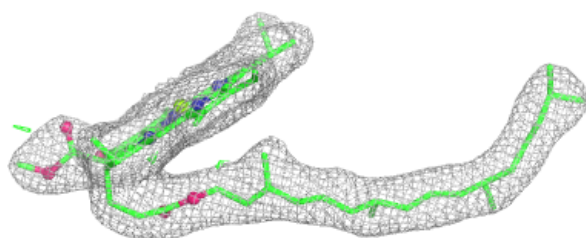
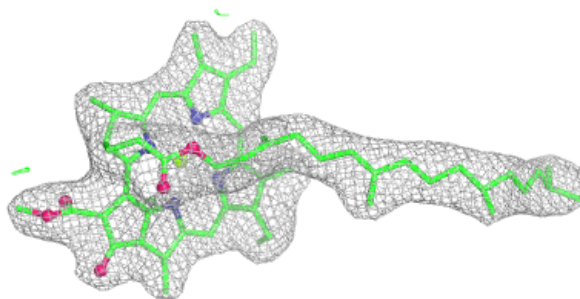
**Electron density around CLA A 405:**

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



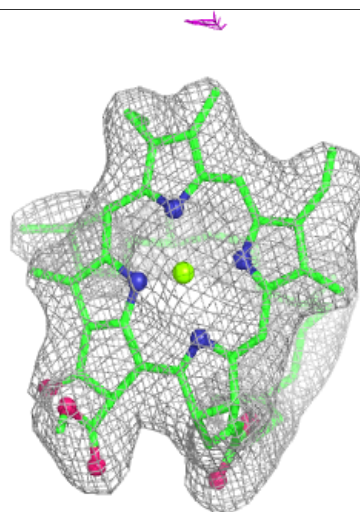
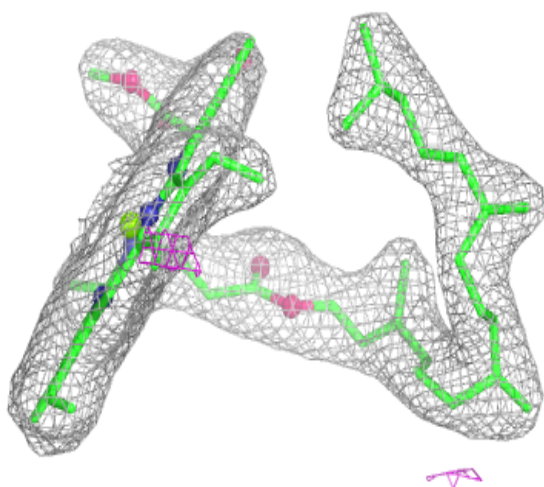
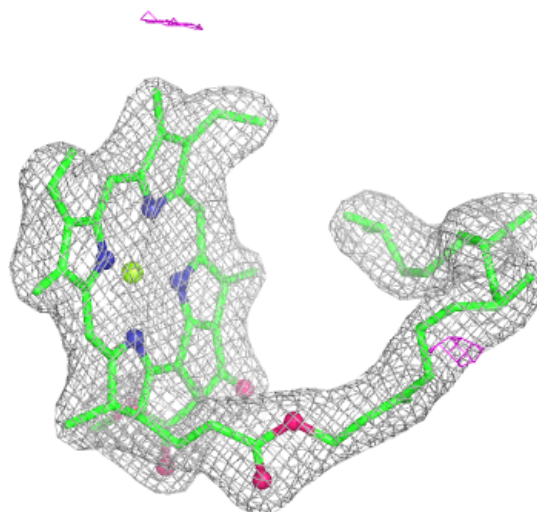
Electron density around CLA b 608:

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



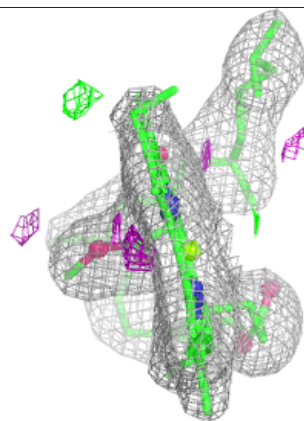
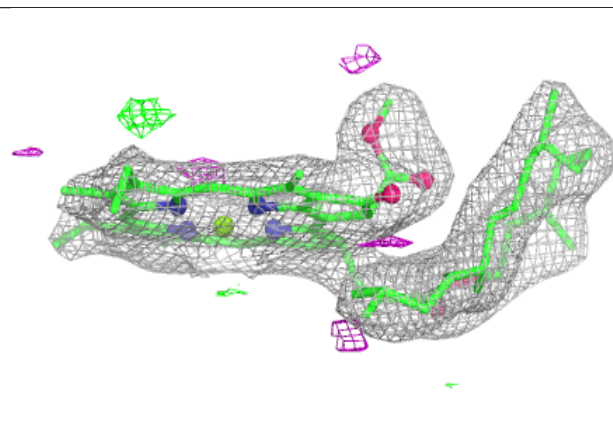
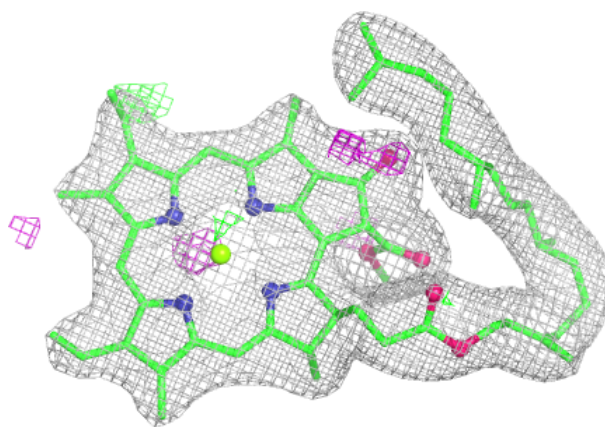
Electron density around CLA C 504:

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



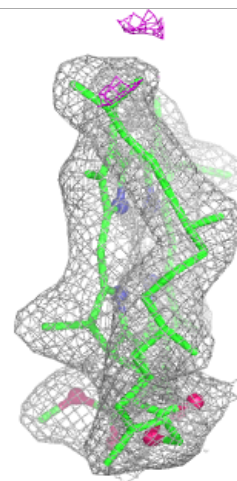
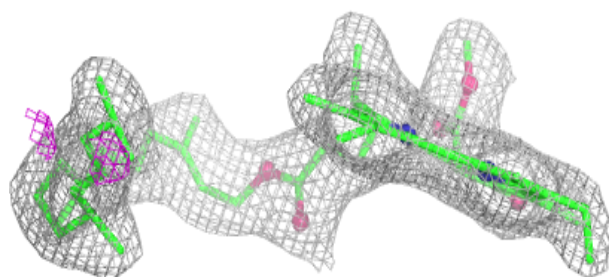
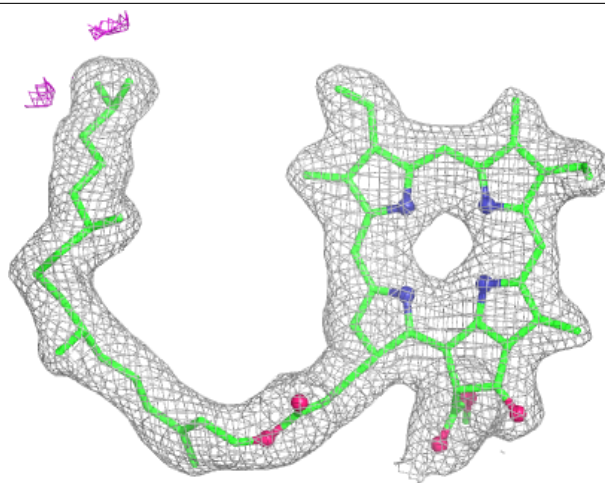
Electron density around CLA b 610:

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



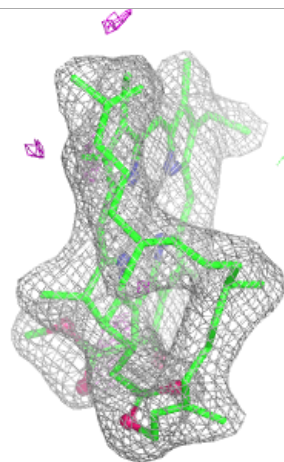
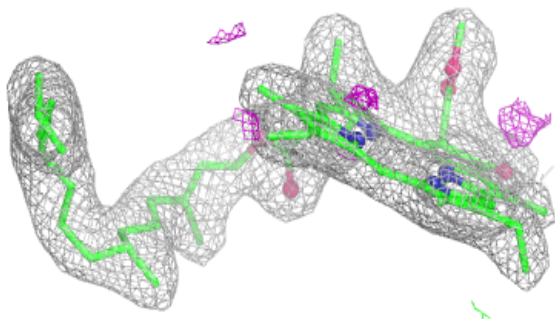
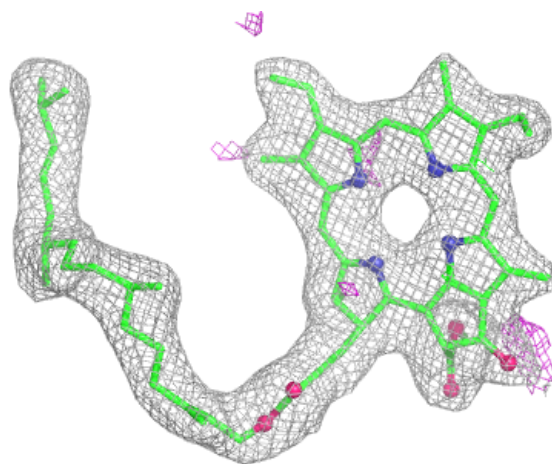
Electron density around PHO A 407:

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



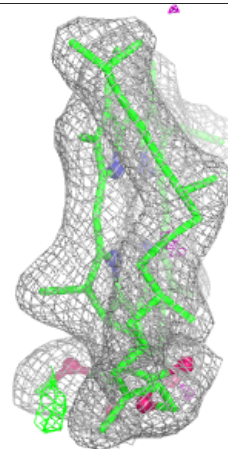
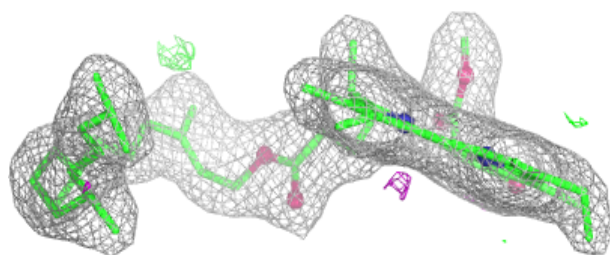
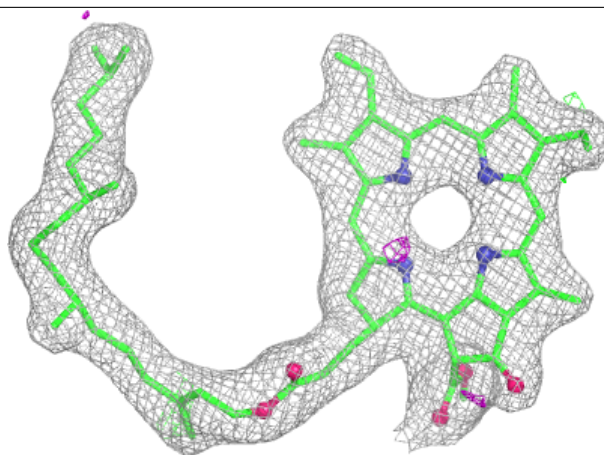
Electron density around PHO A 353:

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



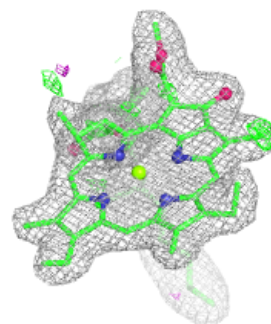
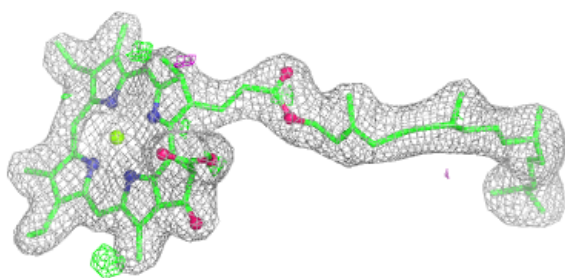
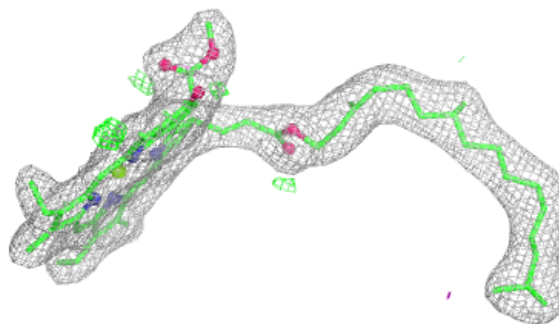
Electron density around PHO a 408:

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

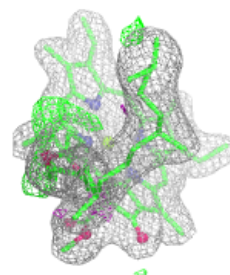
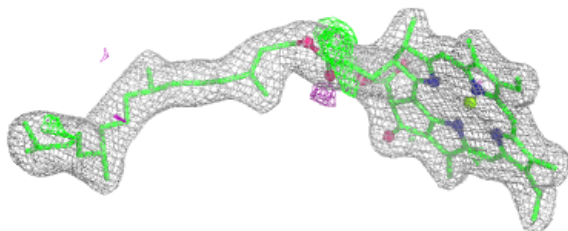
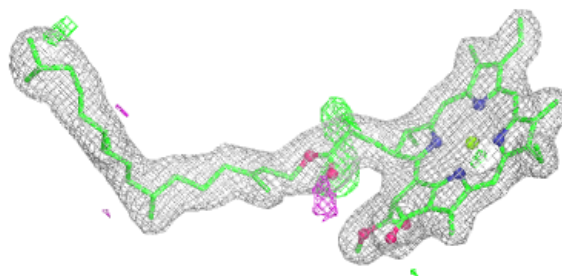


Electron density around CLA D 405:

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

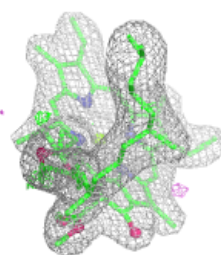
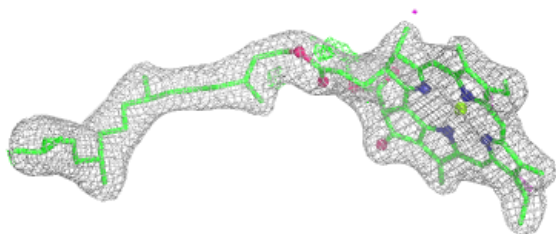
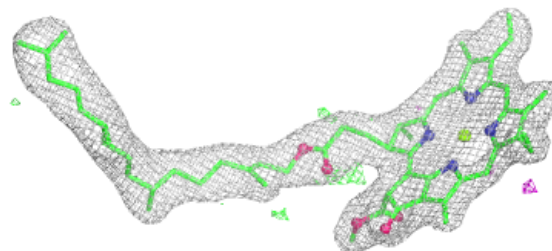
**Electron density around CLA A 404:**

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

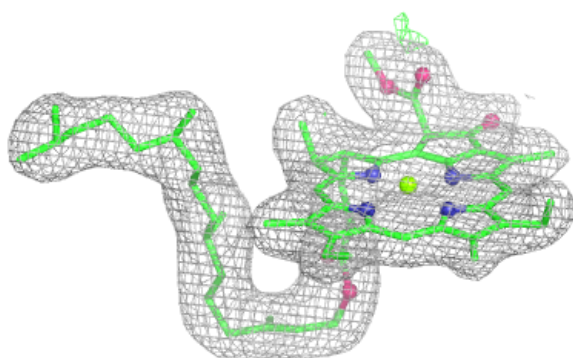
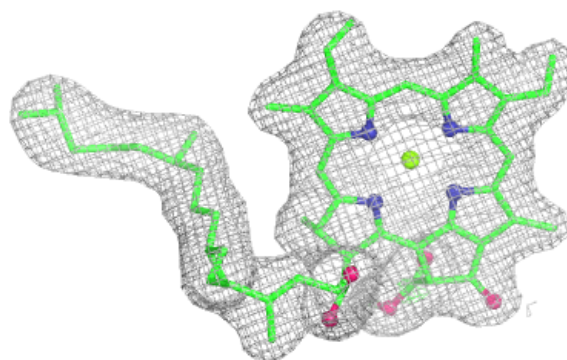


Electron density around CLA a 405:

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

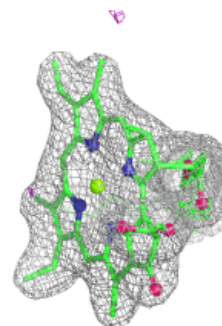
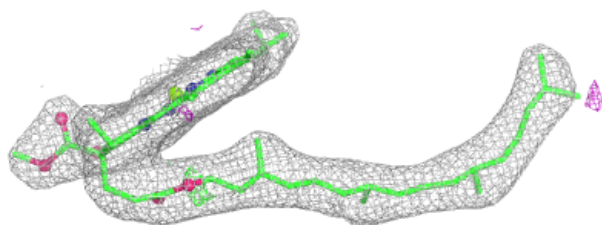
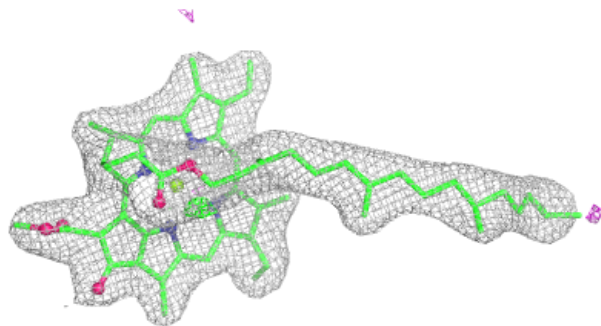
**Electron density around CLA a 406:**

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

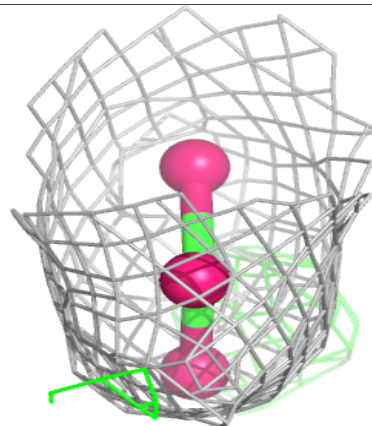
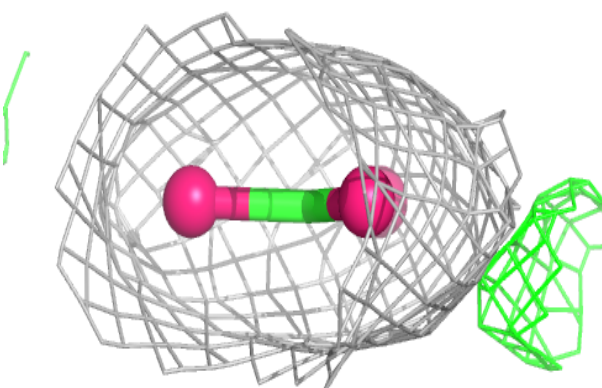
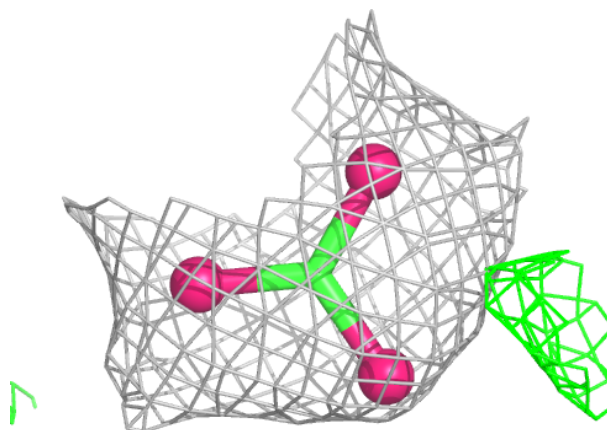


Electron density around CLA B 608:

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

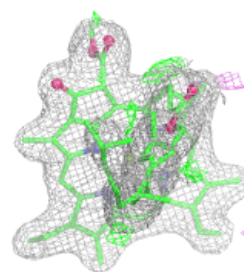
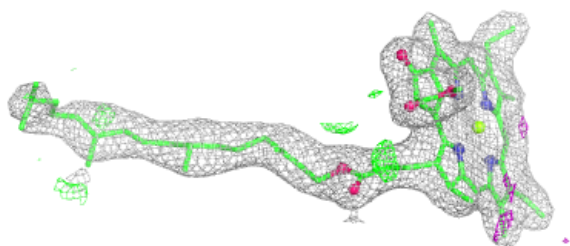
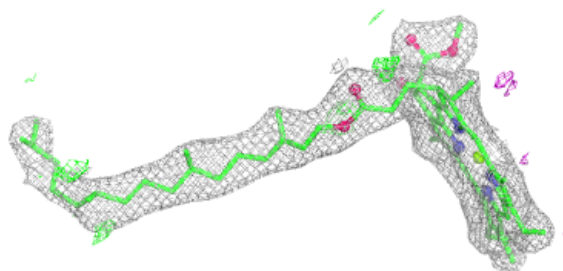
**Electron density around BCT A 348:**

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



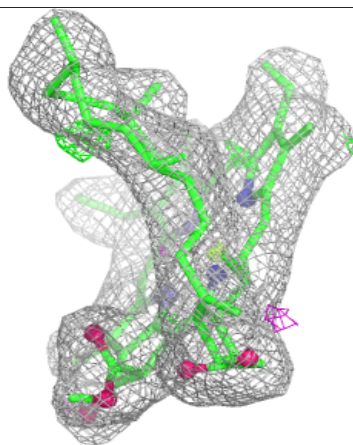
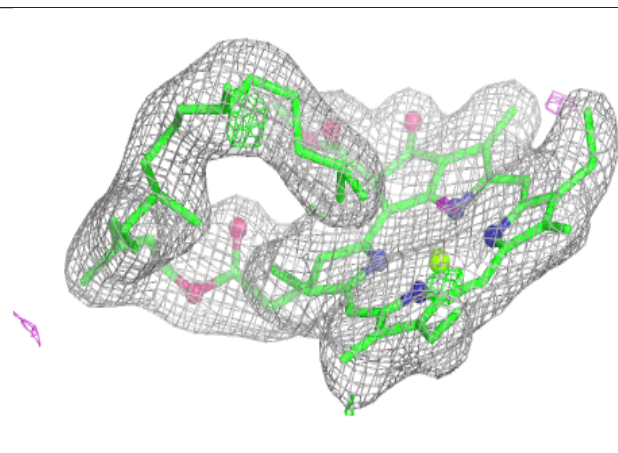
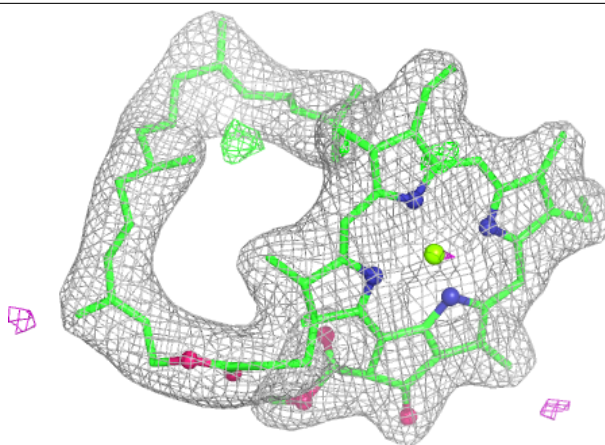
Electron density around CLA B 604:

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



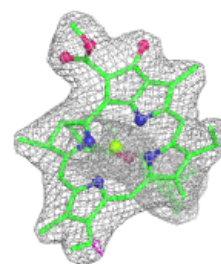
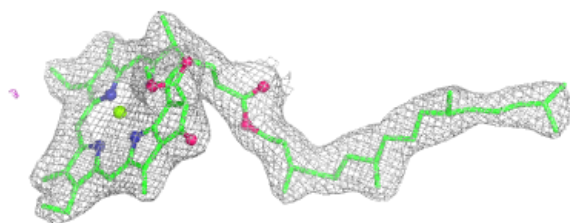
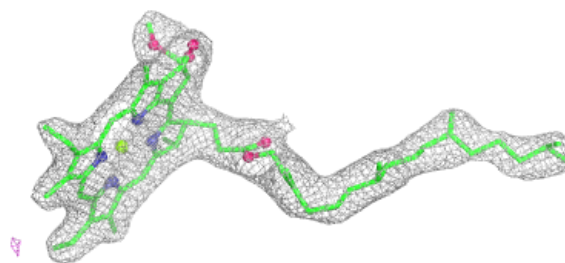
Electron density around CLA B 615:

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



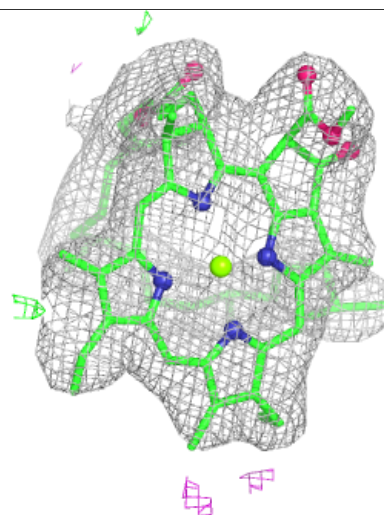
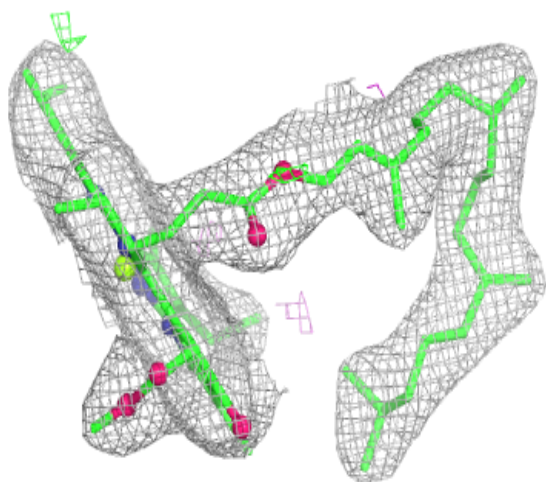
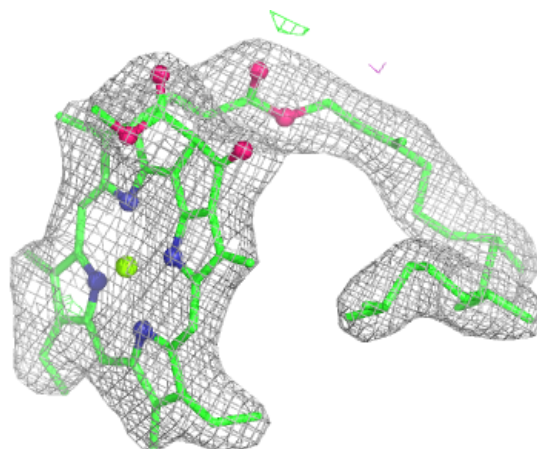
Electron density around CLA c 503:

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



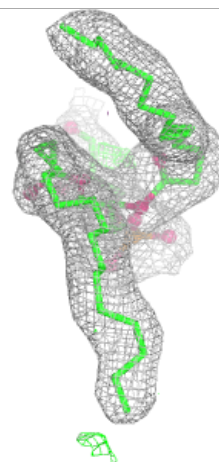
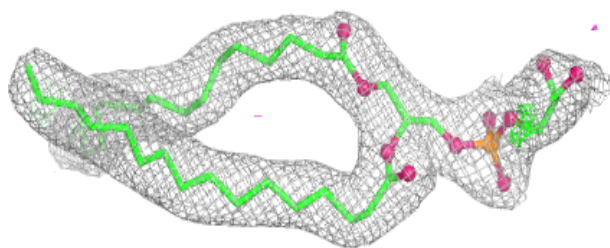
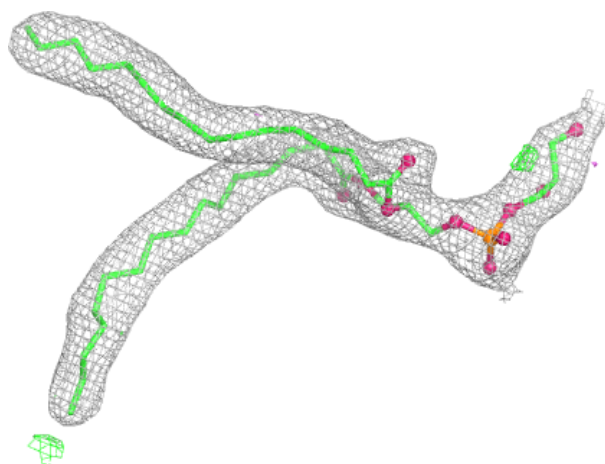
Electron density around CLA c 504:

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



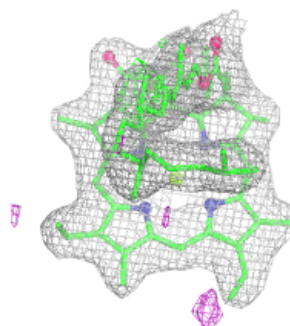
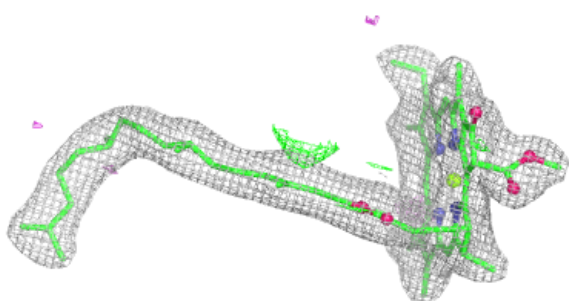
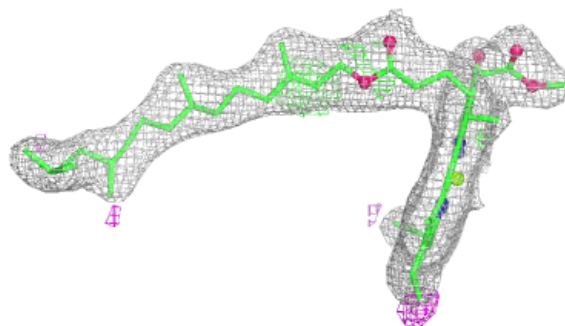
Electron density around LHG D 410:

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



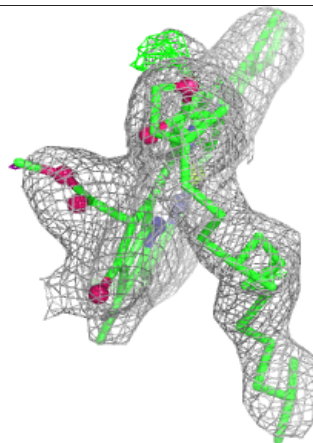
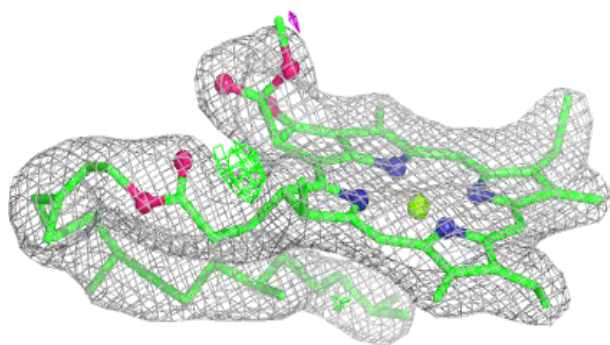
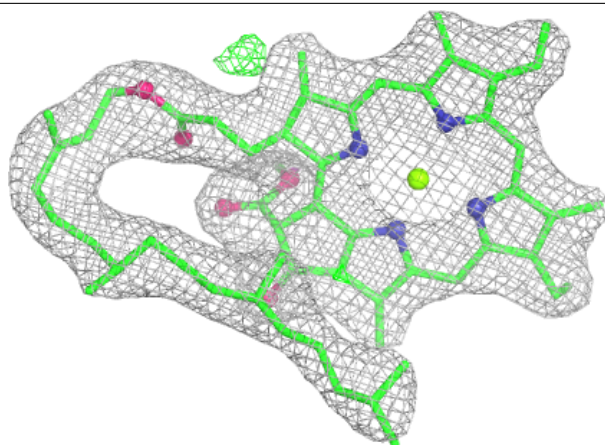
Electron density around CLA B 605:

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



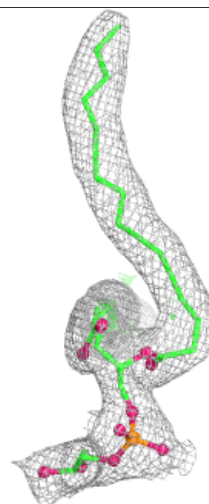
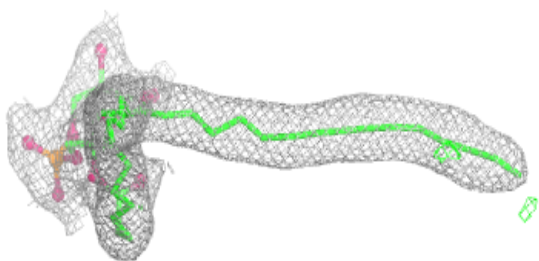
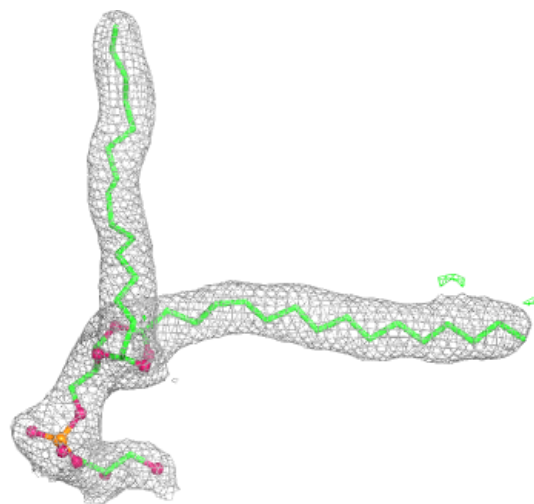
Electron density around CLA C 510:

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



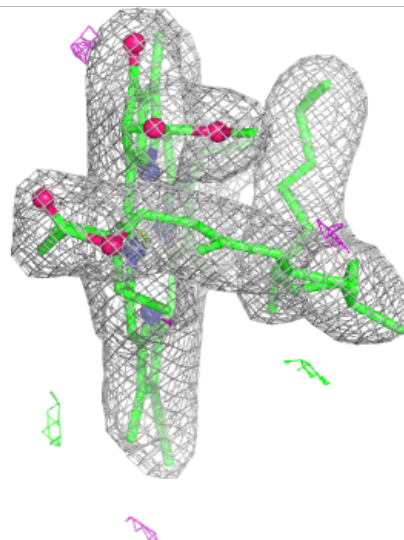
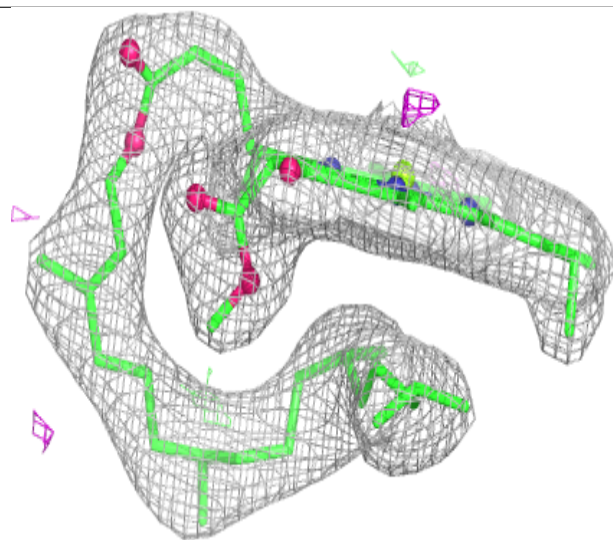
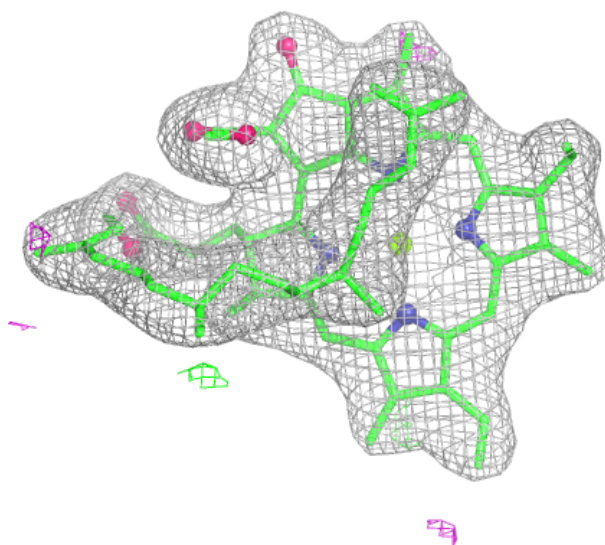
Electron density around LHG L 101:

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



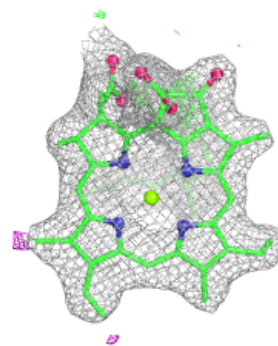
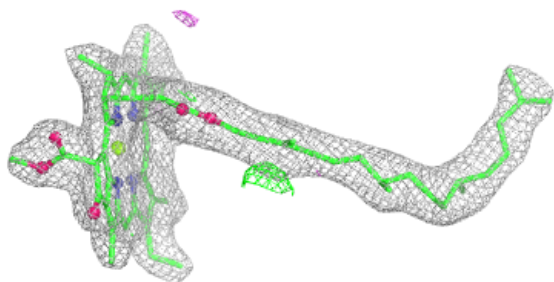
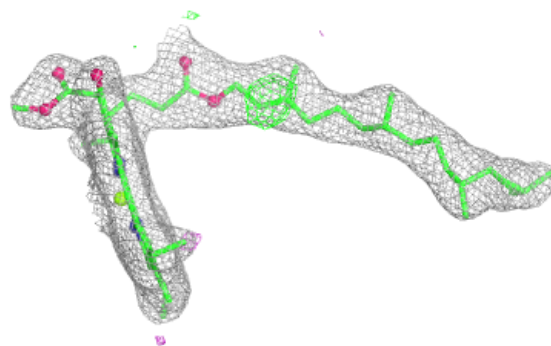
Electron density around CLA C 511:

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

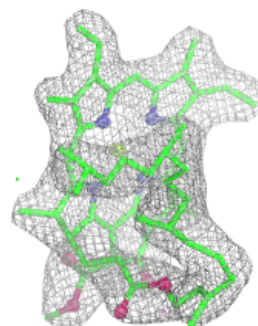
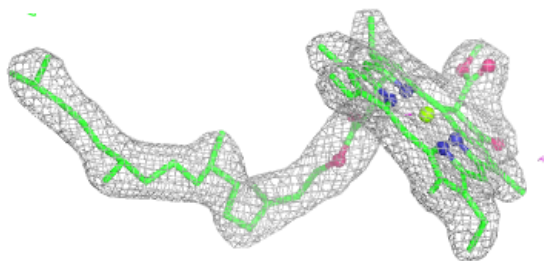
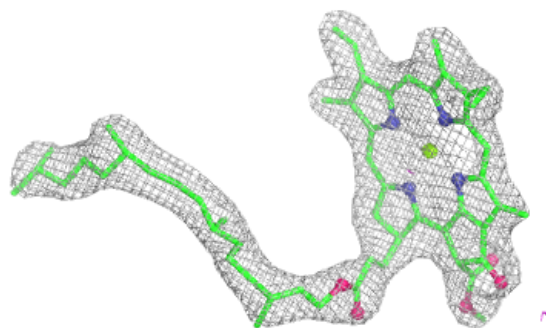


Electron density around CLA b 605:

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

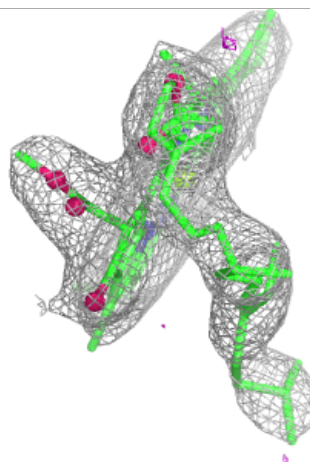
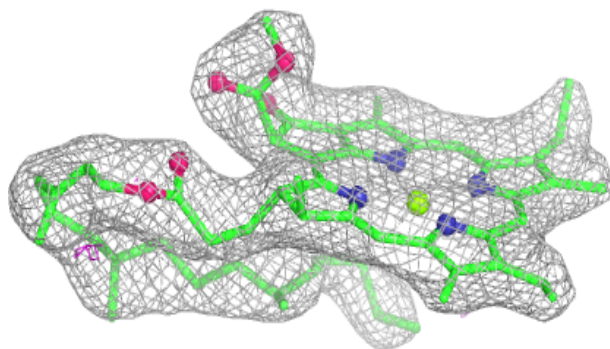
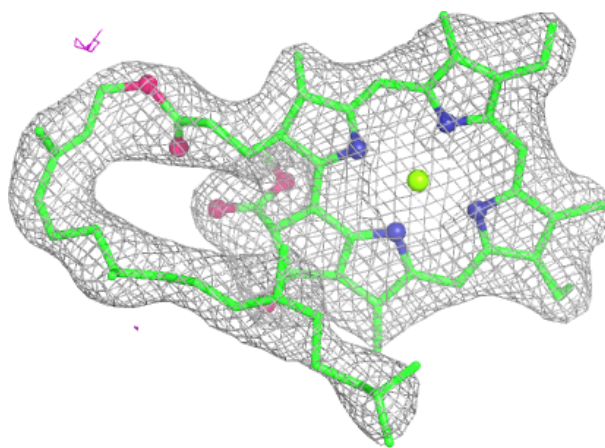
**Electron density around CLA C 512:**

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



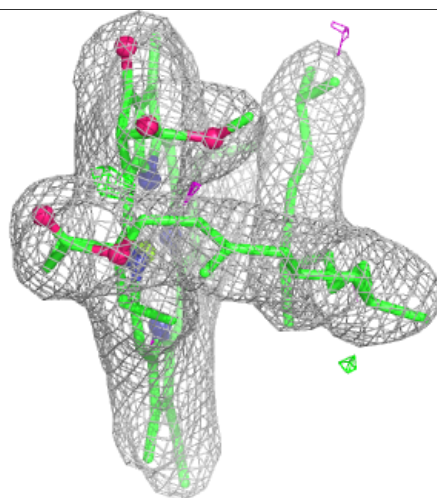
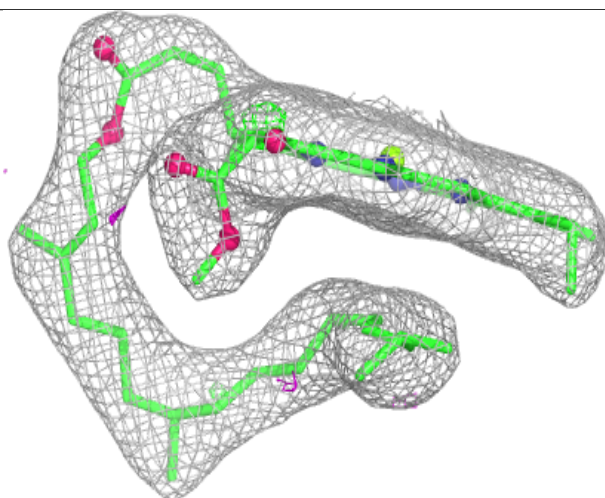
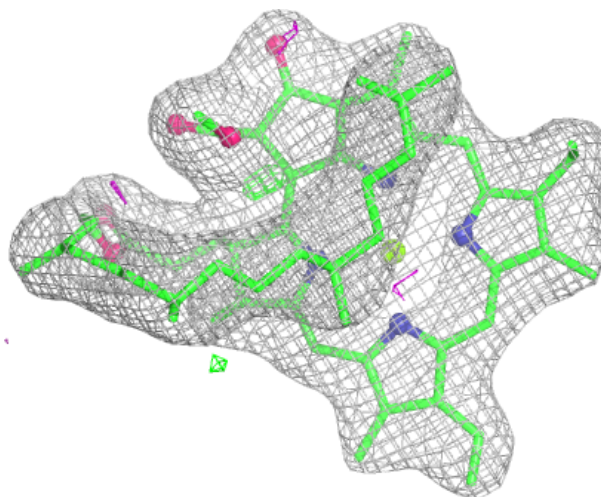
Electron density around CLA c 510:

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



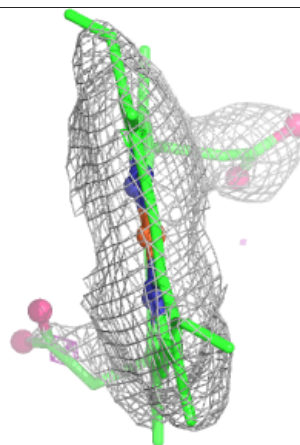
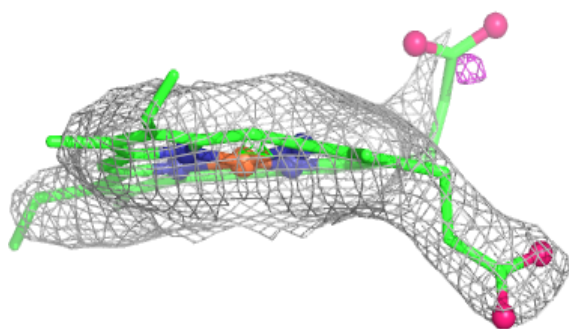
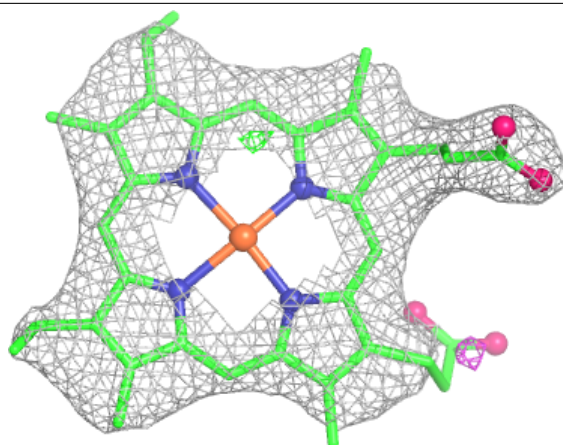
Electron density around CLA c 511:

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



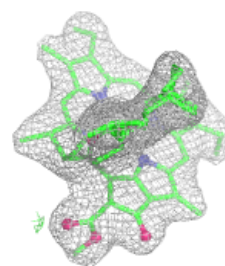
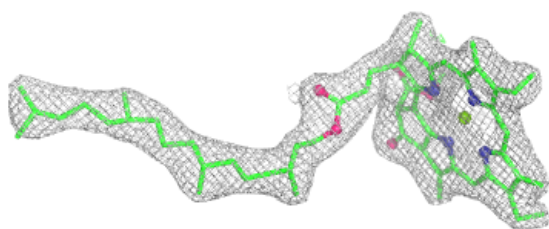
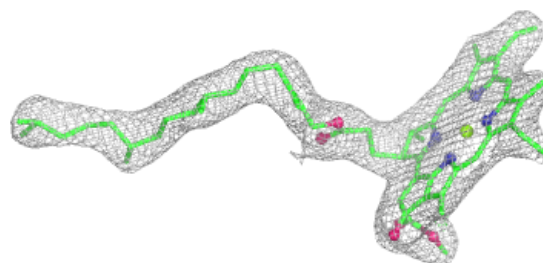
Electron density around HEM e 87:

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



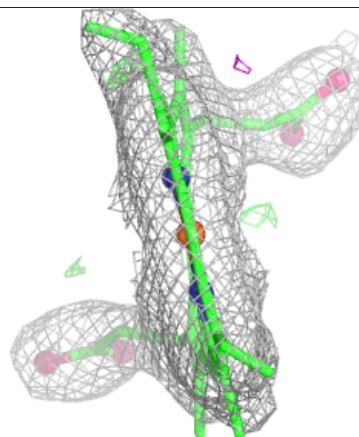
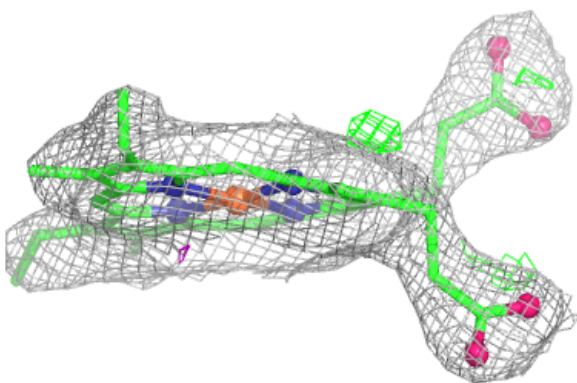
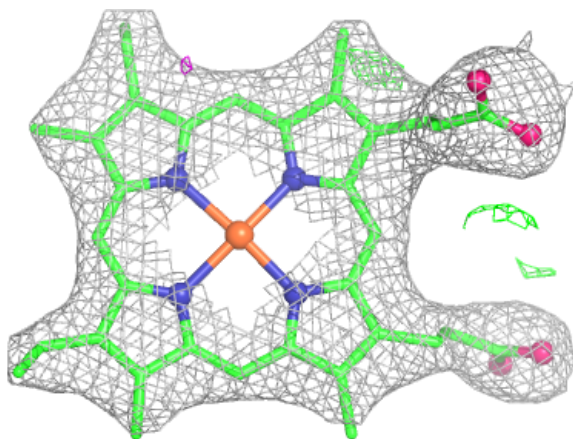
Electron density around CLA C 503:

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



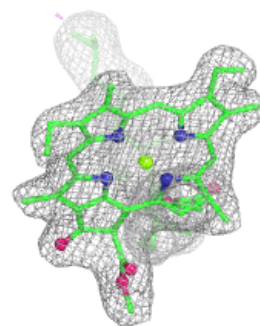
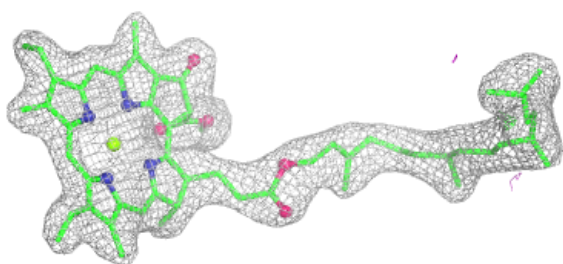
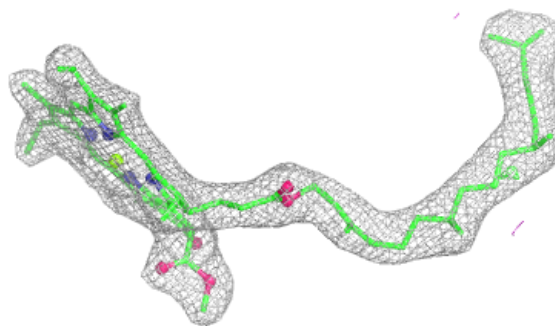
Electron density around HEM E 103:

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



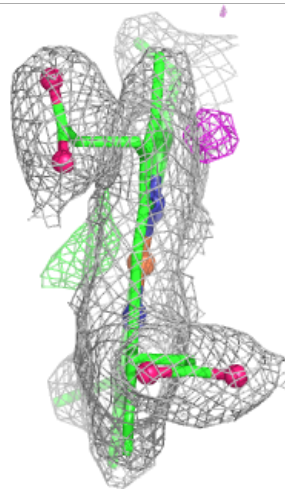
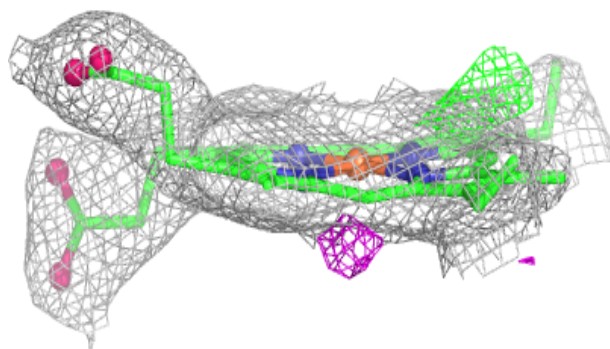
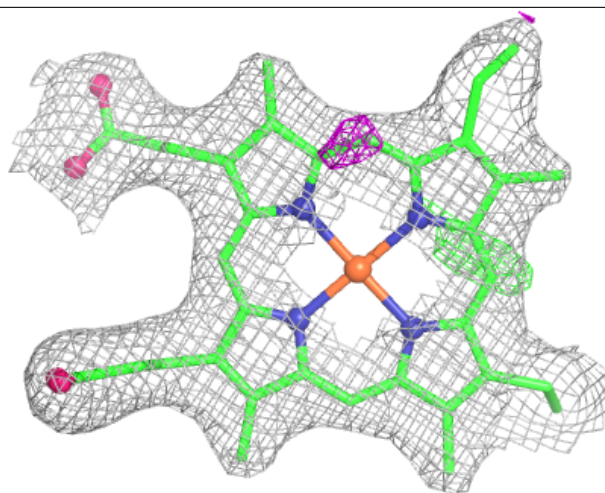
Electron density around CLA d 402:

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



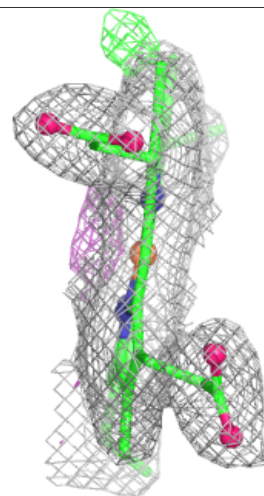
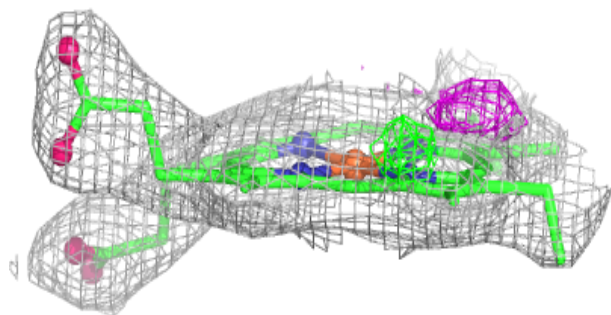
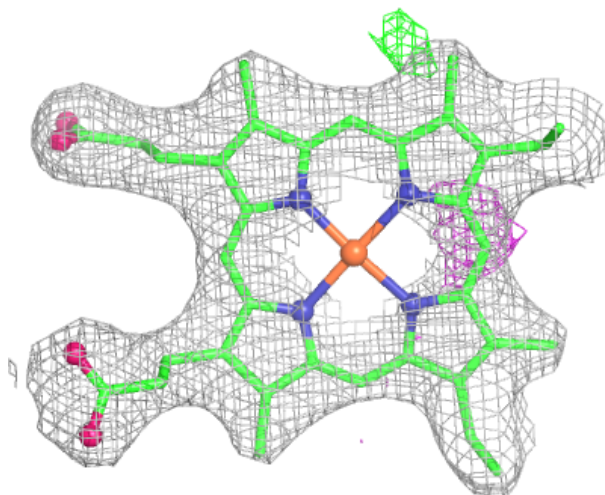
Electron density around HEC V 202:

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



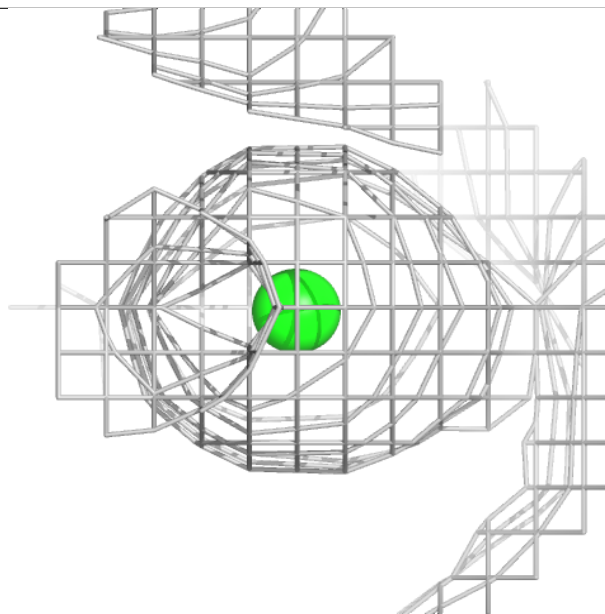
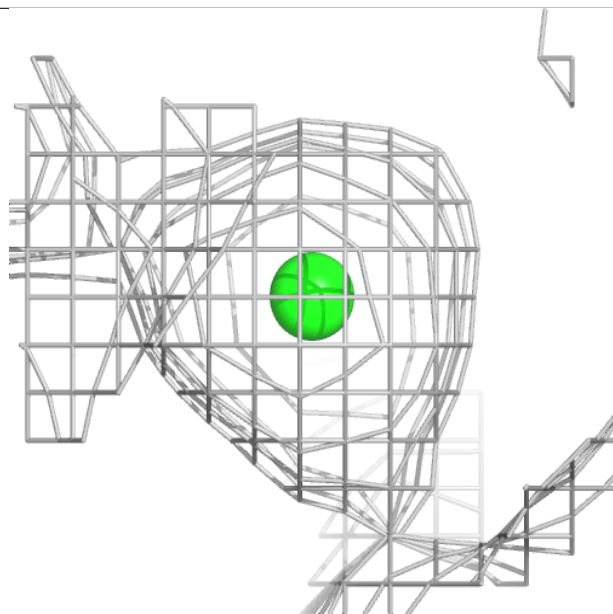
Electron density around HEC v 202:

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



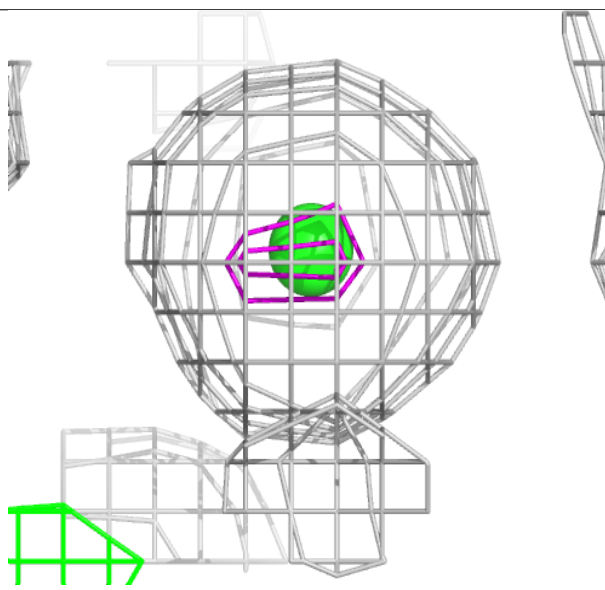
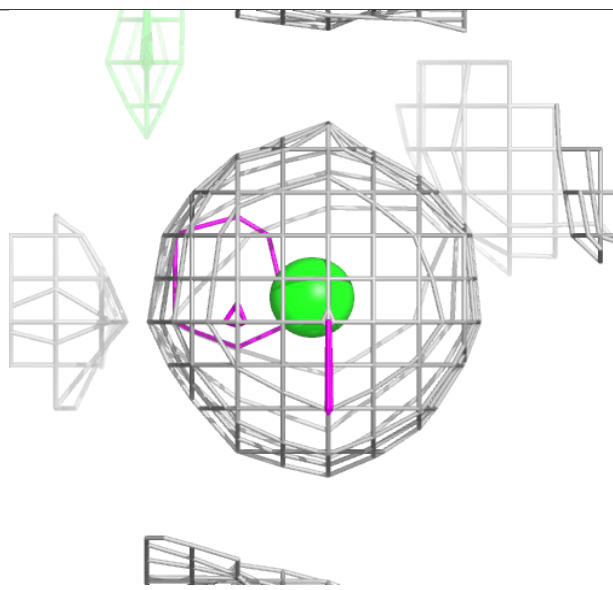
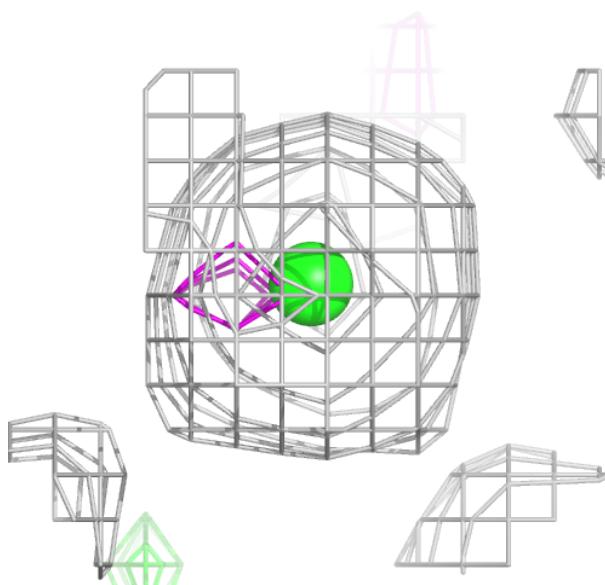
Electron density around CL a 403:

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



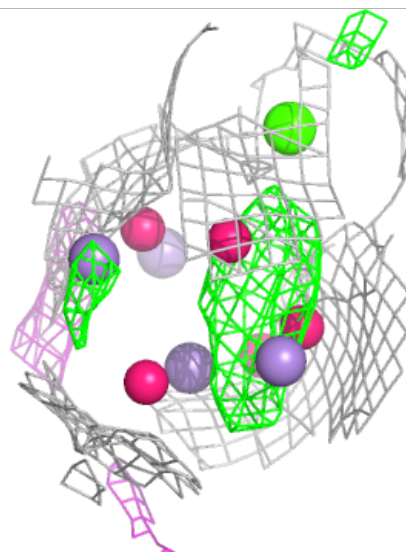
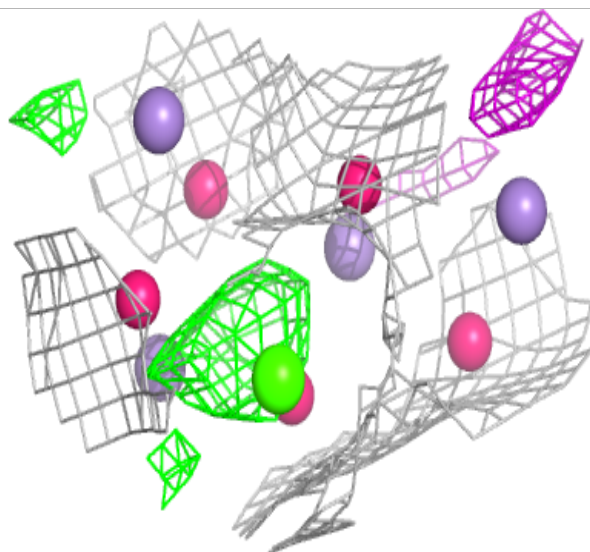
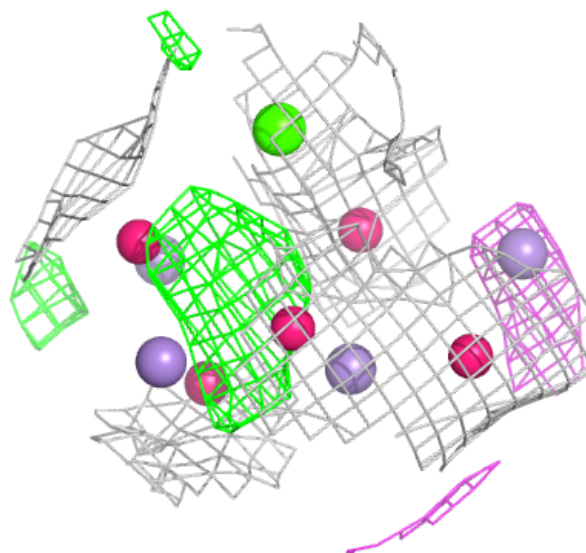
Electron density around CL A 402:

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



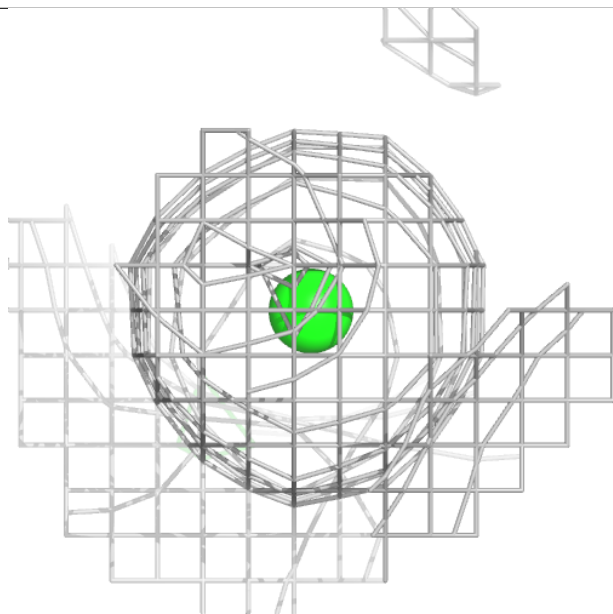
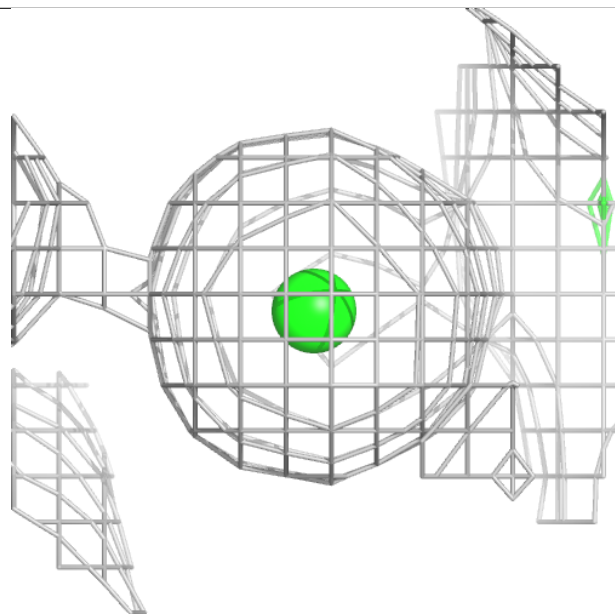
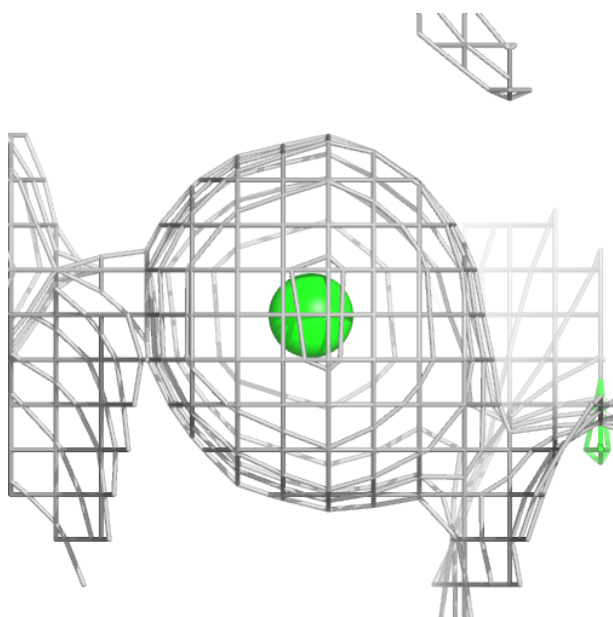
Electron density around OEX A 413:

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



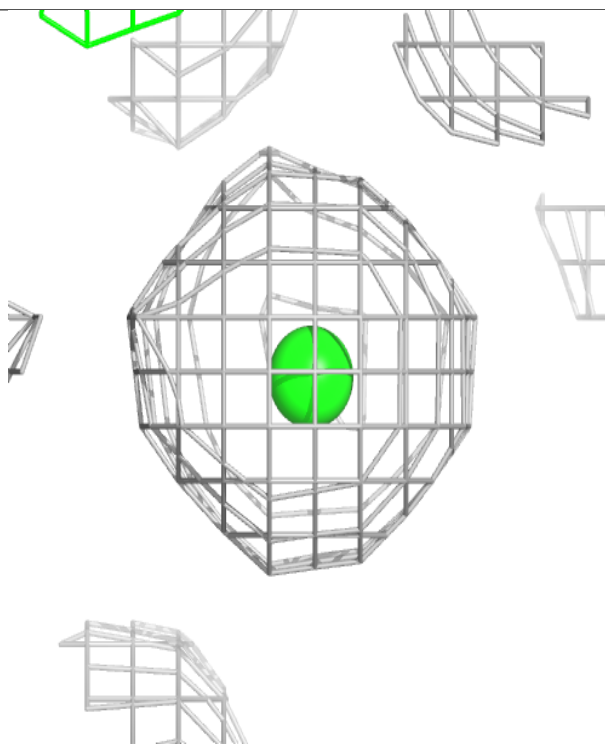
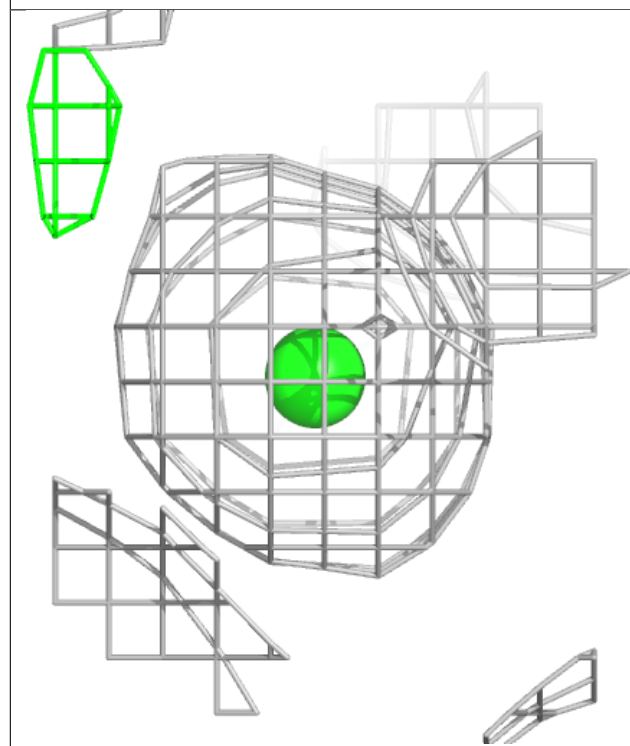
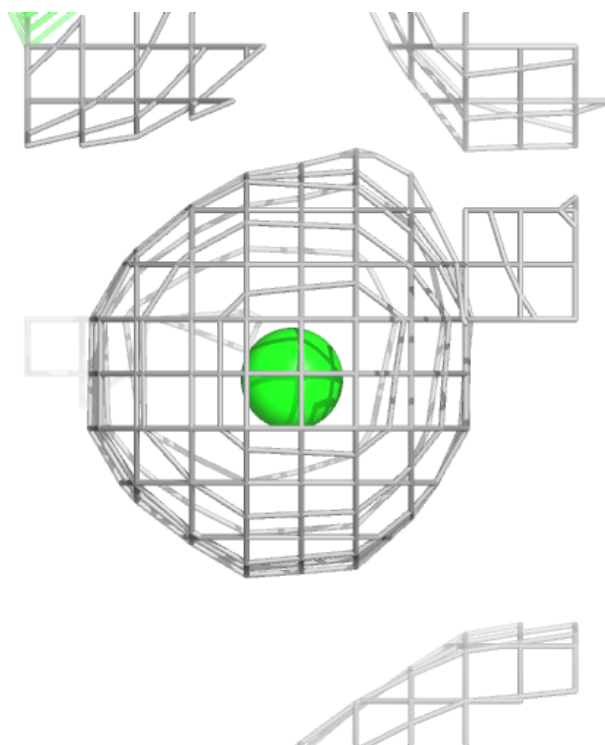
Electron density around CL A 403:

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



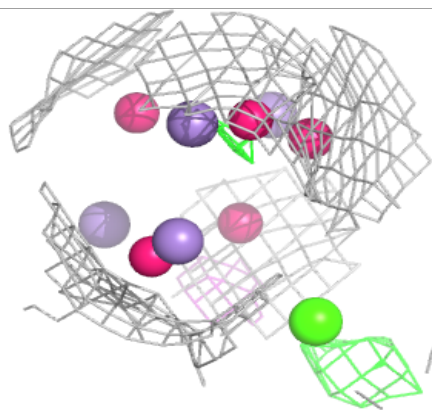
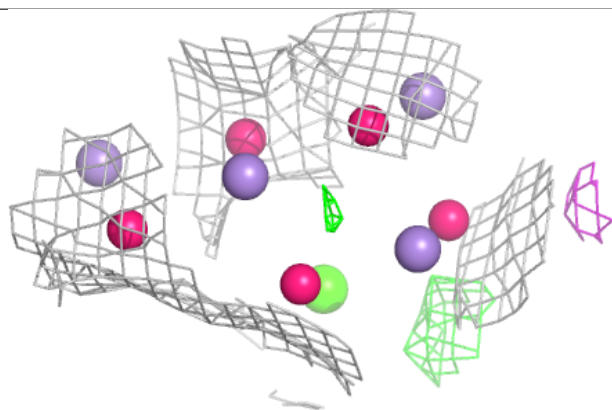
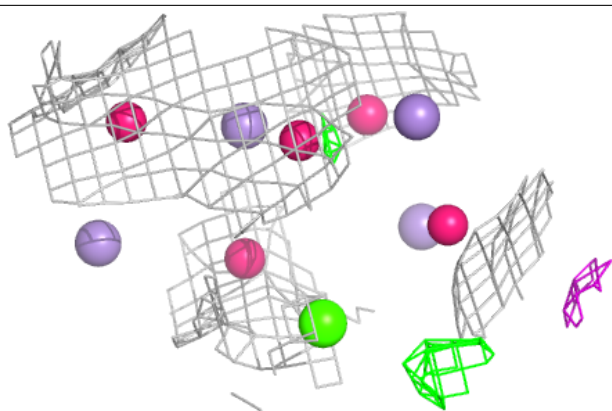
Electron density around CL a 402:

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



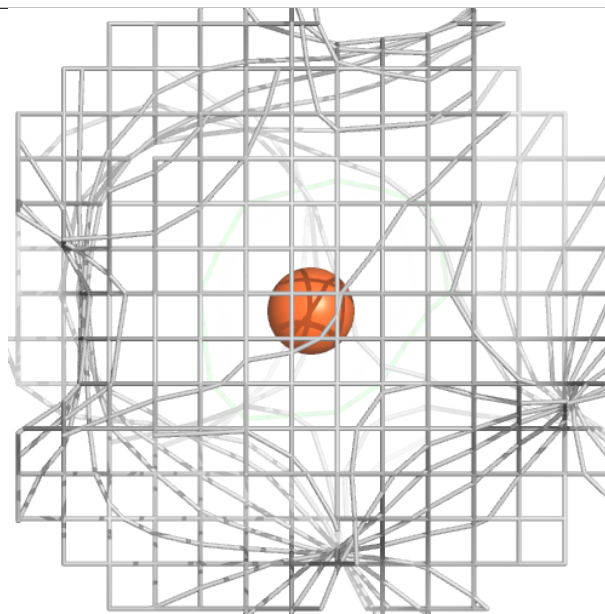
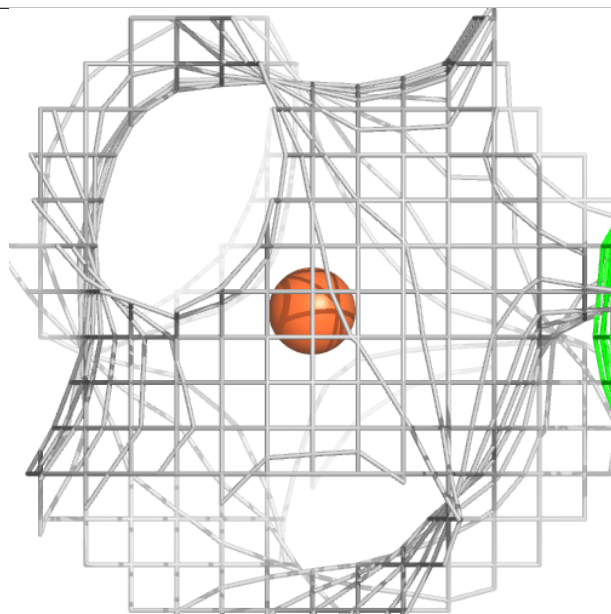
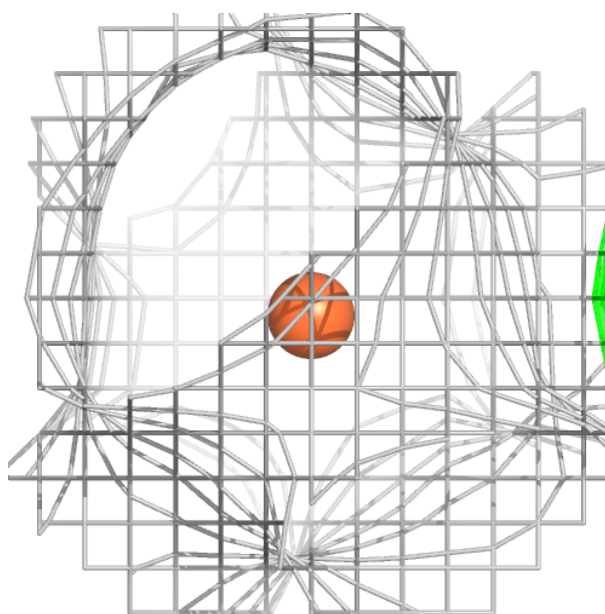
Electron density around OEX a 415:

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



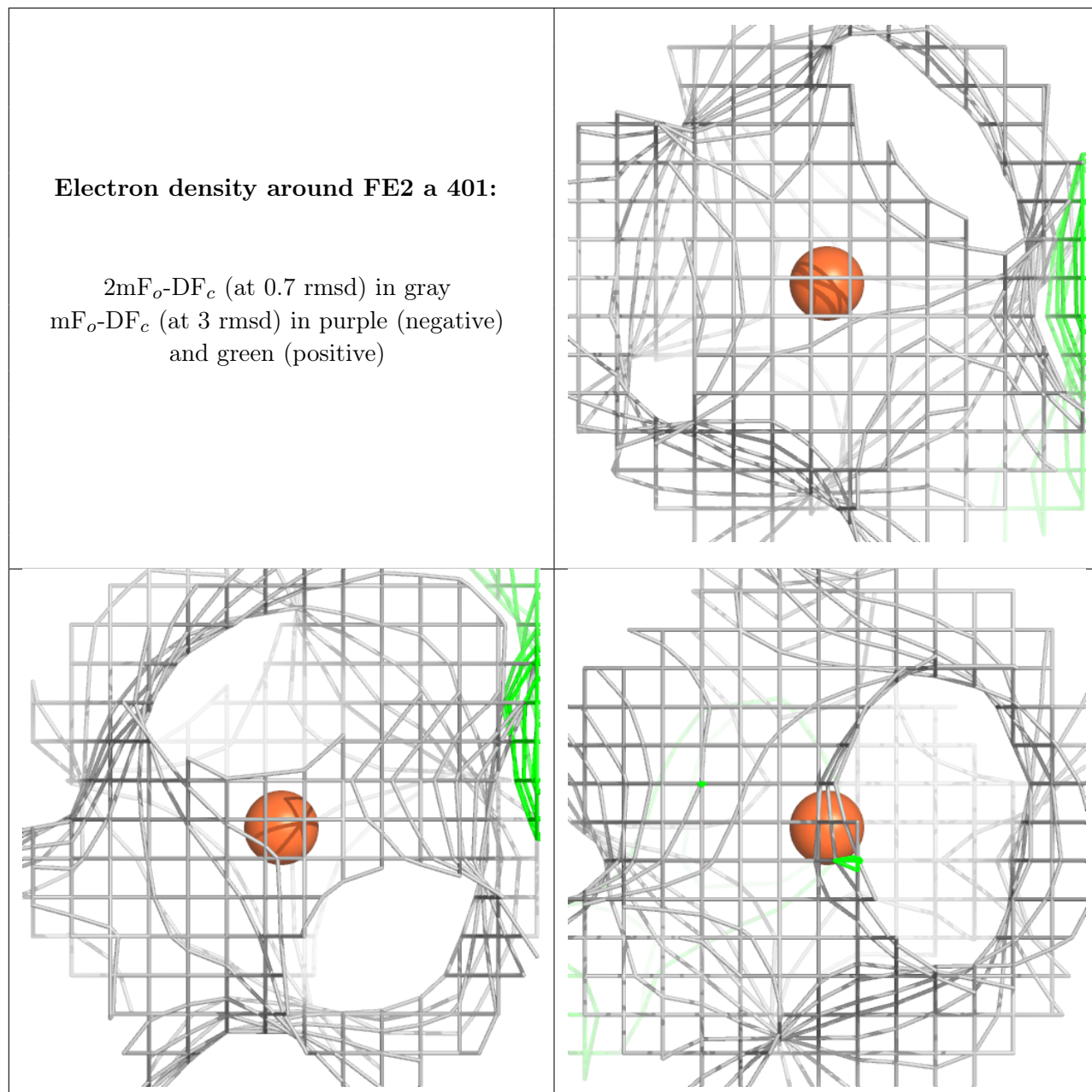
Electron density around FE2 A 401:

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



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 ⓘ

There are no such residues in this entry.