



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2026 – 08:22 AM JST

PDB ID : 8IRG / pdb_00008irg
Title : XFEL structure of cyanobacterial photosystem II following two flashes (2F)
with a 30-microsecond delay
Authors : Li, H.; Suga, M.; Shen, J.R.
Deposited on : 2023-03-17
Resolution : 2.30 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:

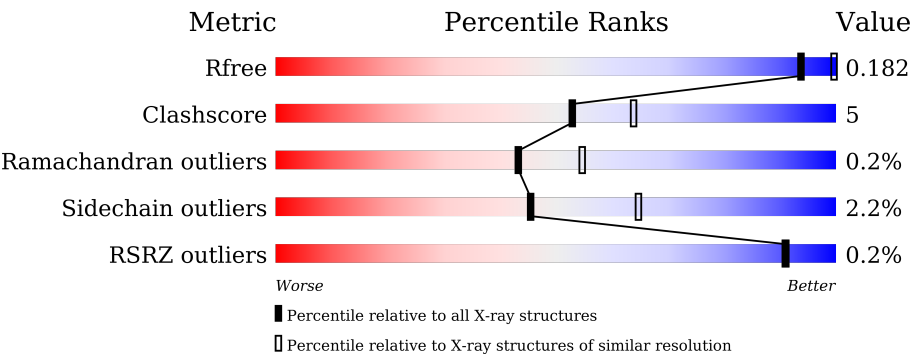
MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	344	88%9%
1	a	344	85%12%
2	B	505	92%7%
2	b	505	%91%8%
3	C	455	91%8%
3	c	455	89%10%

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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	 91% 9% .
17	X	40	 82% 12% 5%
17	x	40	 88% 8% 5%
18	Y	30	 87% 10% .
18	y	30	 50% 43% . .
19	Z	62	 87% 11% .
19	z	62	 76% 24%
20	R	34	 6% 74% 24% .

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
25	GOL	D	403	-	-	X	-
25	GOL	D	414	-	X	-	-
25	GOL	a	419	-	-	X	-
40	HEC	V	202	X	-	-	-
40	HEC	v	201	X	-	-	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 62602 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	222	0
			4338	2836	717	760	25			
1	a	334	Total	C	N	O	S	0	221	0
			4330	2830	716	759	25			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	20	0
			4146	2721	692	720	13			
2	b	504	Total	C	N	O	S	0	19	0
			4134	2718	687	716	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	97	0
			4260	2788	713	741	18			
3	c	455	Total	C	N	O	S	0	100	0
			4308	2821	719	750	18			

There are 8 discrepancies between the modelled and reference sequences:

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

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

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	114	0
			3620	2387	596	622	15			
4	d	341	Total	C	N	O	S	0	116	0
			3628	2391	599	623	15			

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	6	0
			311	213	48	48	2			
14	t	30	Total	C	N	O	S	0	5	0
			302	208	47	45	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O		0	4	0
			800	508	133	159				
15	u	97	Total	C	N	O		0	4	0
			807	513	134	160				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	6	0
			1120	711	185	220	4			
16	v	137	Total	C	N	O	S	0	6	0
			1117	712	185	216	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	1	0
			289	194	46	49			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

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

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

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

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

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

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

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

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

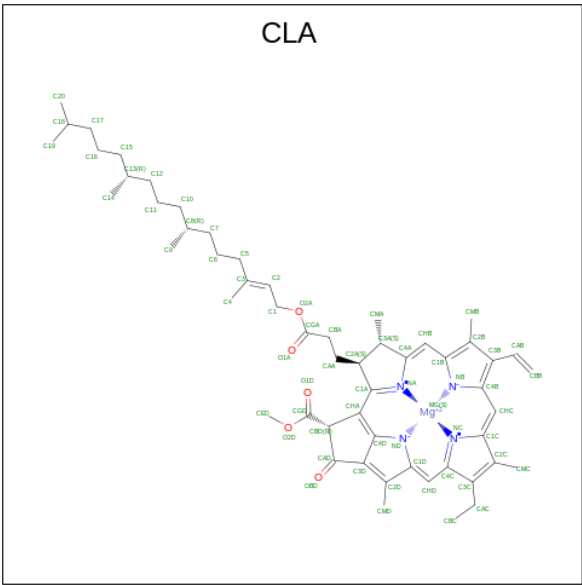
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		

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

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



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

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

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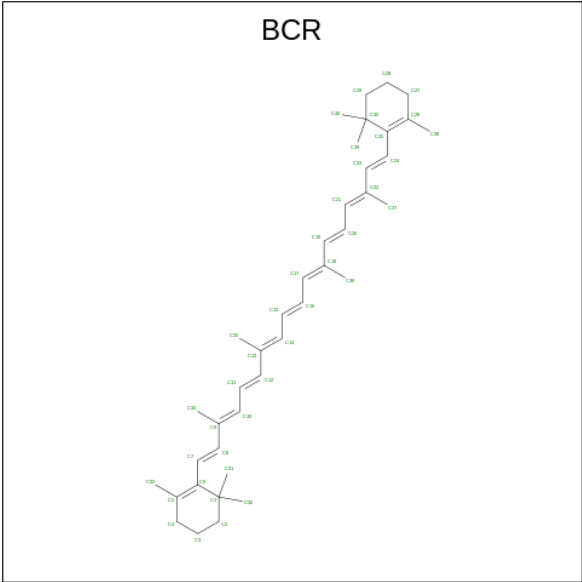
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 130	C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

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

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



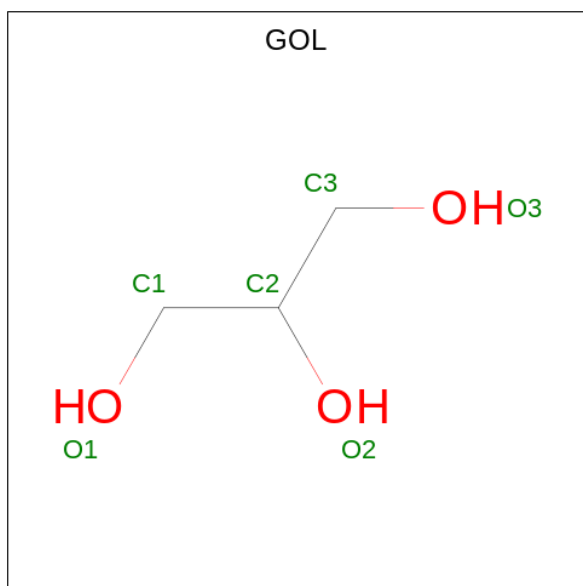
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	Y	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	d	1	Total C 40 40	0	0
24	h	1	Total C 40 40	0	0
24	k	1	Total C 40 40	0	0
24	t	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0

- Molecule 25 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



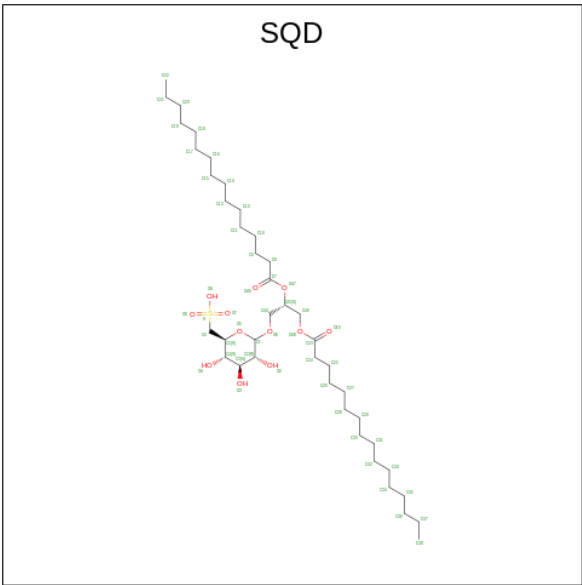
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 6 3 3	0	0
25	B	1	Total C O 6 3 3	0	0
25	B	1	Total C O 6 3 3	0	0

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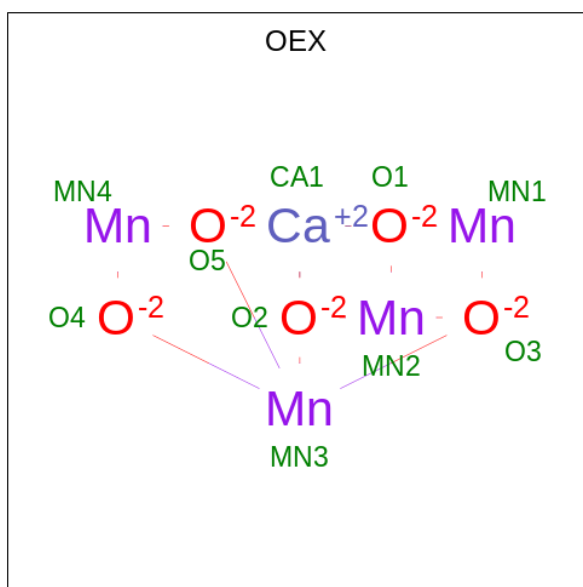
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			6	3	3		
25	C	1	Total	C	O	0	1
			12	6	6		
25	D	1	Total	C	O	0	0
			6	3	3		
25	D	1	Total	C	O	0	0
			6	3	3		
25	O	1	Total	C	O	0	0
			6	3	3		
25	O	1	Total	C	O	0	0
			6	3	3		
25	V	1	Total	C	O	0	1
			12	6	6		
25	a	1	Total	C	O	0	0
			6	3	3		
25	a	1	Total	C	O	0	0
			6	3	3		
25	b	1	Total	C	O	0	0
			6	3	3		
25	b	1	Total	C	O	0	0
			6	3	3		
25	c	1	Total	C	O	0	1
			12	6	6		
25	c	1	Total	C	O	0	0
			6	3	3		
25	c	1	Total	C	O	0	0
			6	3	3		
25	d	1	Total	C	O	0	0
			6	3	3		
25	l	1	Total	C	O	0	1
			12	6	6		
25	o	1	Total	C	O	0	0
			6	3	3		
25	v	1	Total	C	O	0	1
			12	6	6		

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



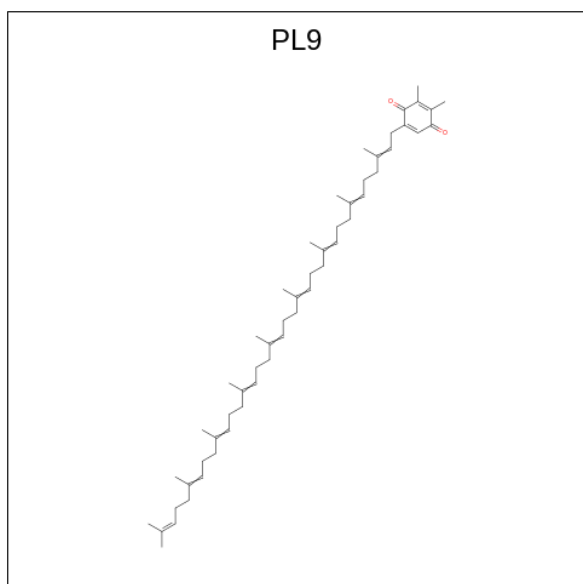
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			54	41	12	1		
26	C	1	Total	C	O	S	0	1
			108	82	24	2		
26	F	1	Total	C	O	S	0	0
			43	30	12	1		
26	a	1	Total	C	O	S	0	1
			108	82	24	2		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	b	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 27 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



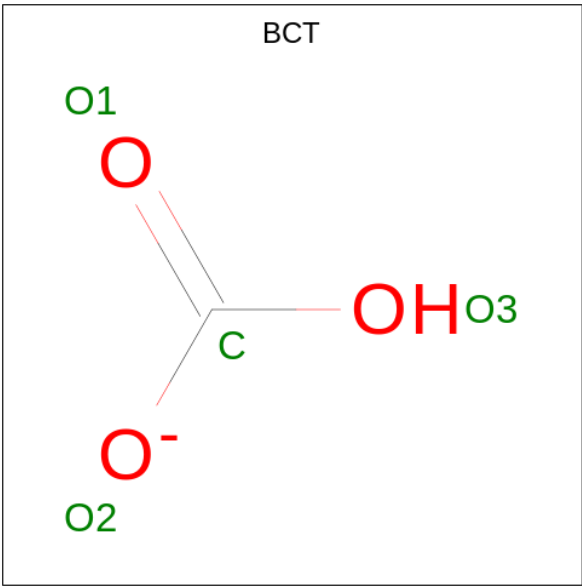
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	1
			110	106	4		
28	D	1	Total	C	O	0	1
			110	106	4		
28	a	1	Total	C	O	0	1
			110	106	4		
28	d	1	Total	C	O	0	1
			110	106	4		

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			28	23	5		
29	B	2	Total	C	O	0	0
			73	63	10		
29	D	2	Total	C	O	0	0
			57	51	6		
29	I	1	Total	C	O	0	0
			40	35	5		
29	J	1	Total	C		0	0
			10	10			
29	K	1	Total	C	O	0	1
			68	58	10		
29	M	1	Total	C		0	0
			10	10			
29	X	1	Total	C	O	0	0
			18	16	2		
29	a	1	Total	C	O	0	0
			30	25	5		
29	b	2	Total	C	O	0	0
			69	59	10		
29	c	1	Total	C	O	0	1
			64	54	10		
29	d	1	Total	C	O	0	0
			17	16	1		
29	j	1	Total	C		0	0
			10	10			
29	m	1	Total	C		0	0
			10	10			
29	x	1	Total	C	O	0	0
			18	16	2		

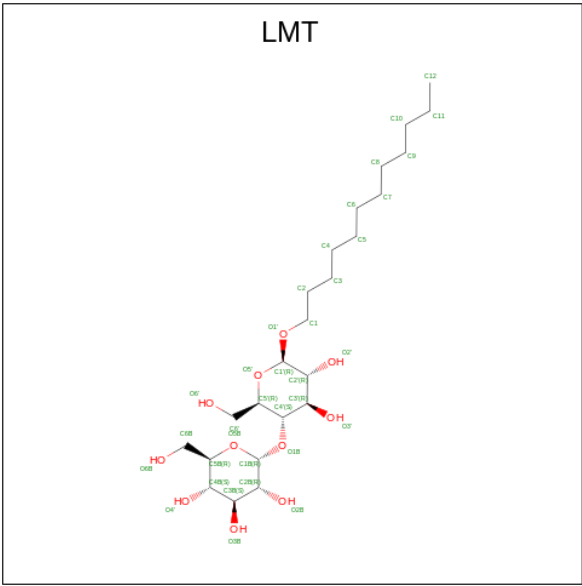
- Molecule 30 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand

of Interest" by depositor).



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

- Molecule 31 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



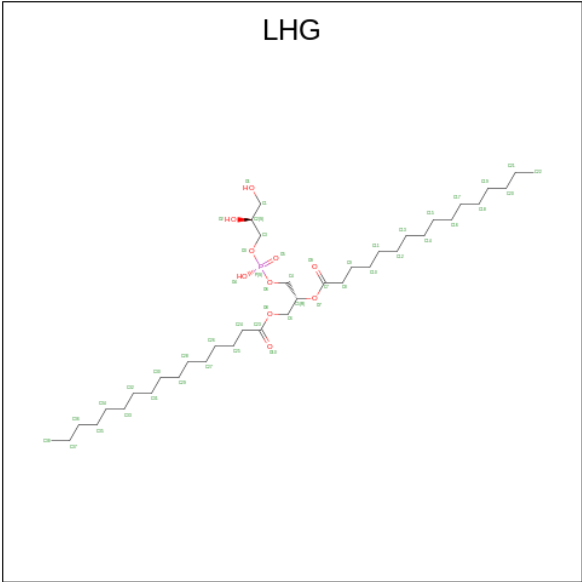
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			35	24	11		

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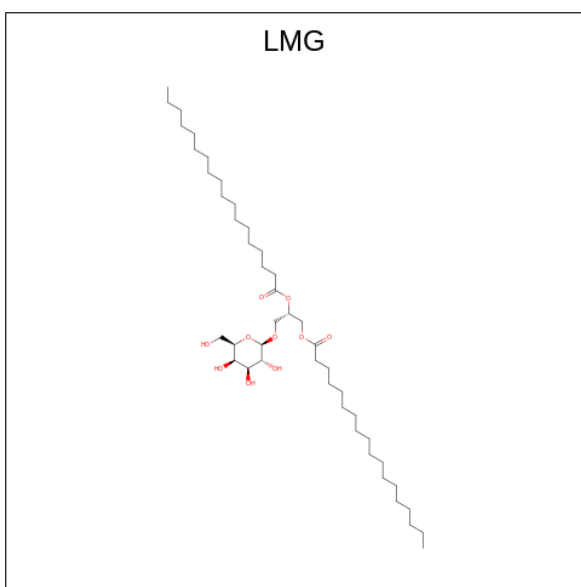
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	F	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	T	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C	O	0	0
			25	19	6		
31	b	1	Total	C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

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



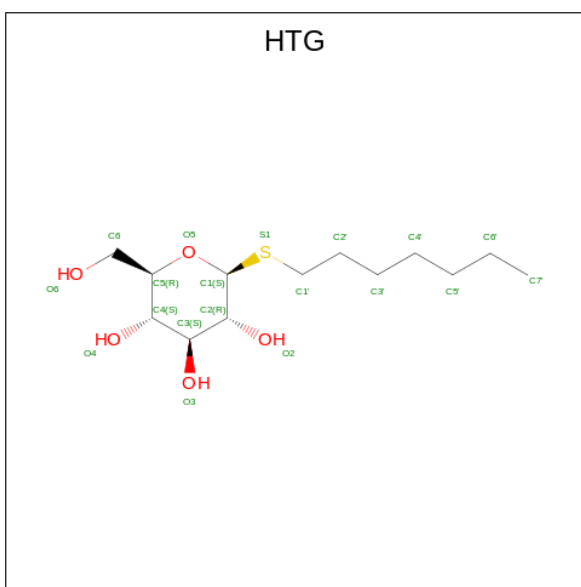
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	P	0	1
			98	76	20	2		
32	D	1	Total	C	O	P	0	1
			98	76	20	2		
32	D	1	Total	C	O	P	0	1
			98	76	20	2		
32	E	1	Total	C	O	P	0	1
			84	62	20	2		
32	L	1	Total	C	O	P	0	1
			98	76	20	2		
32	a	1	Total	C	O	P	0	1
			84	62	20	2		
32	d	1	Total	C	O	P	0	1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

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



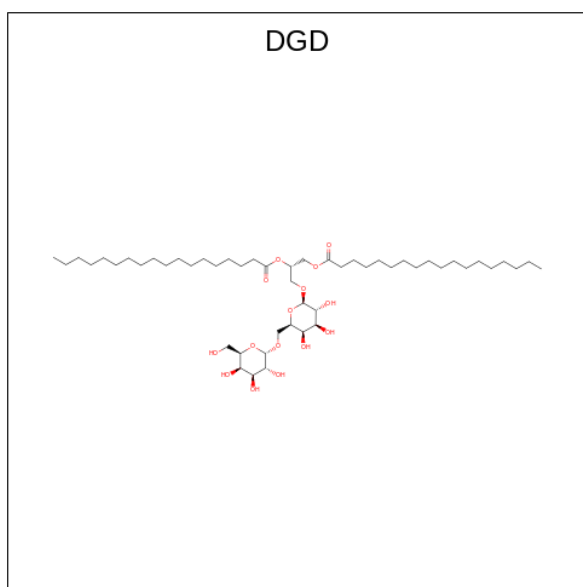
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			37	27	10		
33	D	1	Total	C	O	0	0
			51	41	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	d	1	Total	C	O	0	0
			51	41	10		
33	m	1	Total	C	O	0	0
			51	41	10		
33	z	1	Total	C	O	0	0
			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 19	C 13	O 5	S 1	0	0
34	B	1	Total 19	C 13	O 5	S 1	0	0
34	B	1	Total 19	C 13	O 5	S 1	0	0
34	C	1	Total 19	C 13	O 5	S 1	0	0
34	D	1	Total 16	C 10	O 5	S 1	0	0
34	V	1	Total 11	C 6	O 5		0	0
34	b	1	Total 19	C 13	O 5	S 1	0	0
34	b	1	Total 19	C 13	O 5	S 1	0	0
34	b	1	Total 19	C 13	O 5	S 1	0	0
34	c	1	Total 19	C 13	O 5	S 1	0	0
34	d	1	Total 16	C 10	O 5	S 1	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	C	1	Total	C	O	0	1
			124	94	30		
35	C	1	Total	C	O	0	1
			124	94	30		
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	1
			124	94	30		
35	c	1	Total	C	O	0	1
			124	94	30		
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).

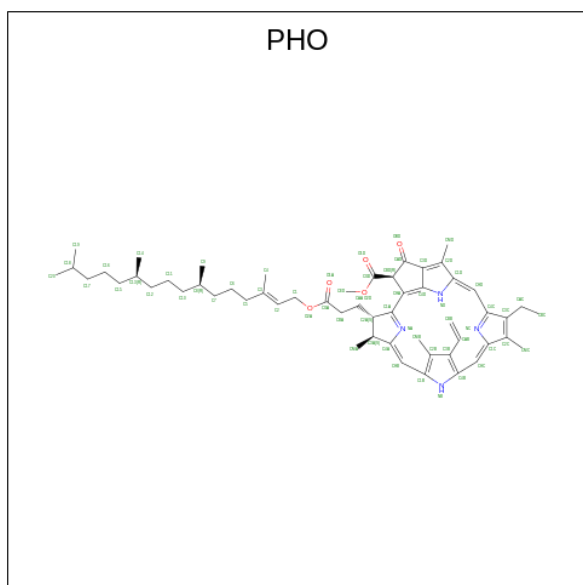
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	C	1	Total	Ca	0	0
			1	1		
36	O	1	Total	Ca	0	0
			1	1		
36	V	1	Total	Ca	0	0
			1	1		
36	c	2	Total	Ca	0	0
			2	2		

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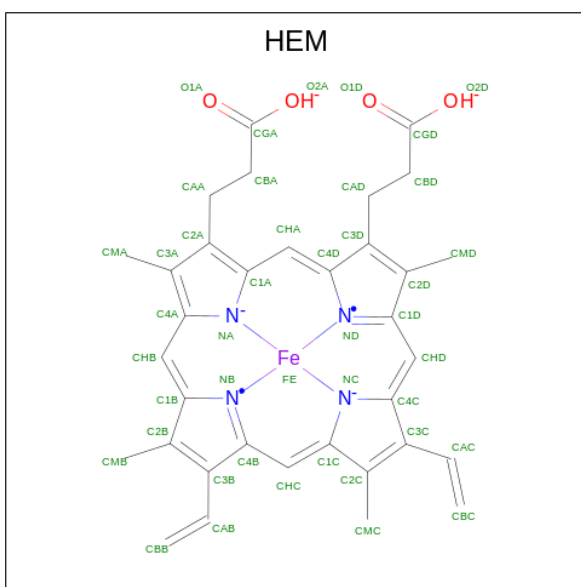
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	f	1	Total Ca 1 1	0	0
36	o	1	Total Ca 1 1	0	0

- Molecule 37 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

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

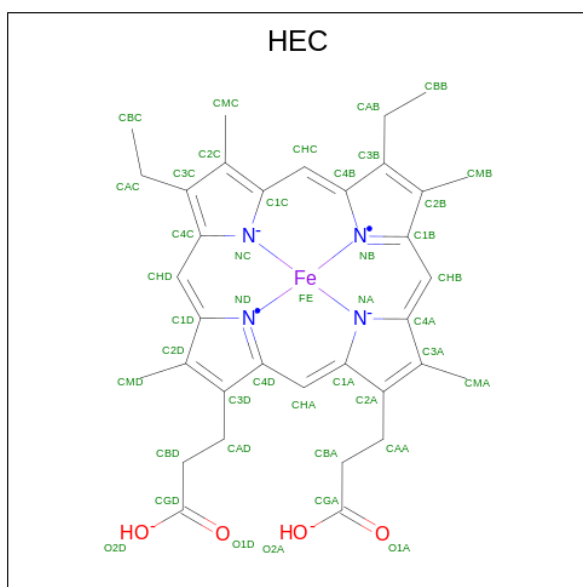


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	f	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 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: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



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	137	Total O 219 219	0	84
41	B	190	Total O 193 193	0	3
41	C	170	Total O 207 207	0	37
41	D	122	Total O 156 156	0	34
41	E	15	Total O 15 15	0	0
41	F	6	Total O 6 6	0	0
41	H	22	Total O 22 22	0	0
41	I	6	Total O 6 6	0	0
41	J	5	Total O 5 5	0	0
41	K	7	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	9	Total O 10 10	0	1
41	M	6	Total O 6 6	0	0
41	O	98	Total O 103 103	0	5
41	T	11	Total O 14 14	0	3
41	U	46	Total O 48 48	0	2
41	V	80	Total O 82 82	0	2
41	X	8	Total O 8 8	0	0
41	a	129	Total O 208 208	0	81
41	b	201	Total O 204 204	0	3
41	c	162	Total O 195 195	0	33
41	d	122	Total O 155 155	0	33
41	e	8	Total O 8 8	0	0
41	f	3	Total O 3 3	0	0
41	h	17	Total O 17 17	0	0
41	i	3	Total O 3 3	0	0
41	j	1	Total O 1 1	0	0
41	k	3	Total O 3 3	0	0
41	l	7	Total O 8 8	0	1
41	m	13	Total O 13 13	0	0
41	o	95	Total O 99 99	0	4
41	t	6	Total O 9 9	0	3

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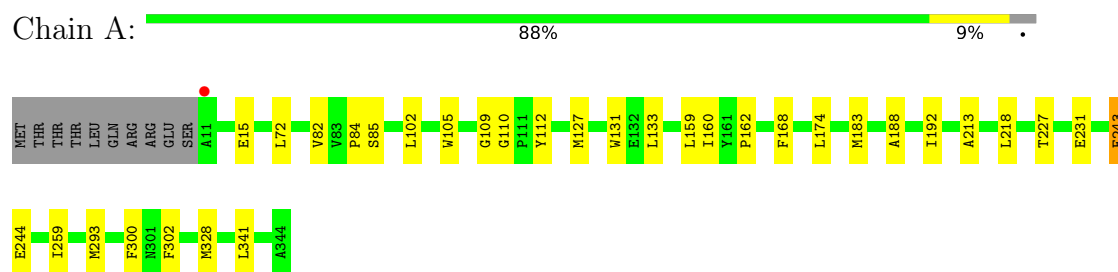
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	u	50	Total 51	O 51	0	1
41	v	57	Total 60	O 60	0	3
41	x	8	Total 8	O 8	0	0
41	y	2	Total 2	O 2	0	0

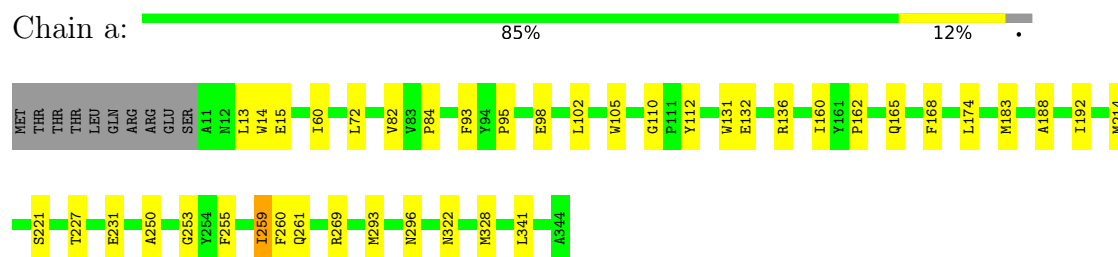
3 Residue-property plots

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

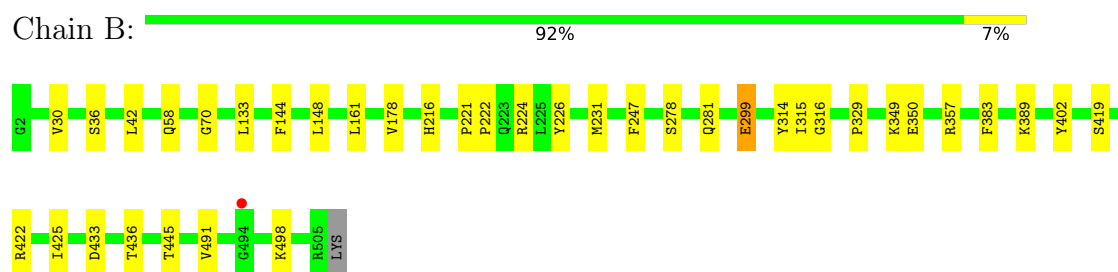
• Molecule 1: Photosystem II protein D1



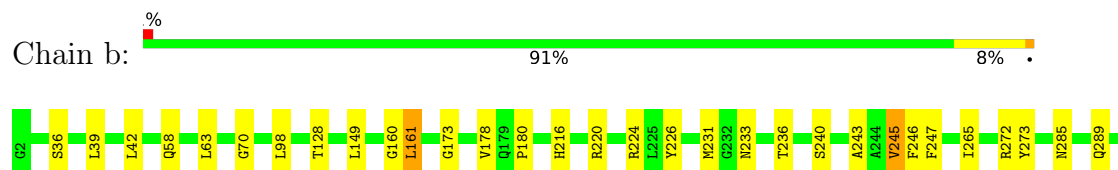
• Molecule 1: Photosystem II protein D1



• Molecule 2: Photosystem II CP47 reaction center protein



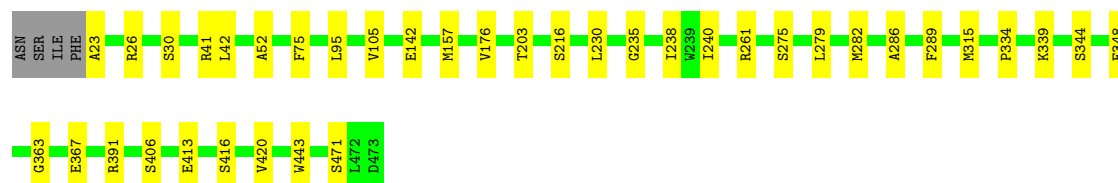
• Molecule 2: Photosystem II CP47 reaction center protein





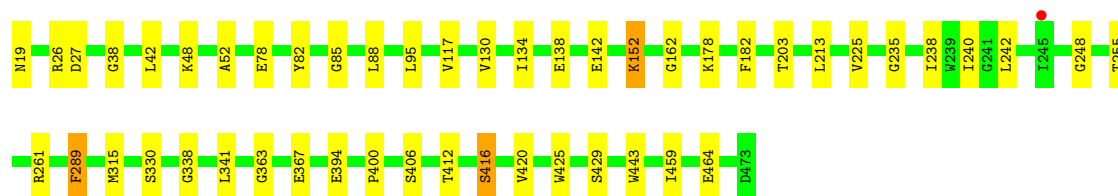
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 91% 8% .



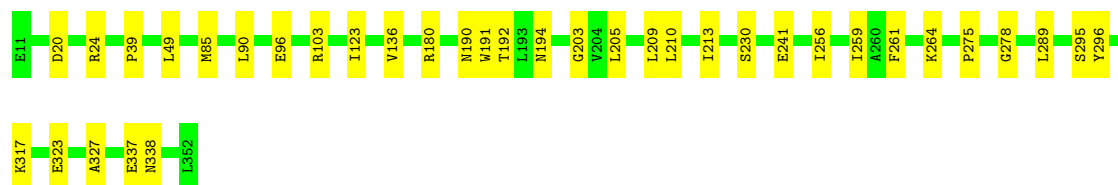
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 10% .



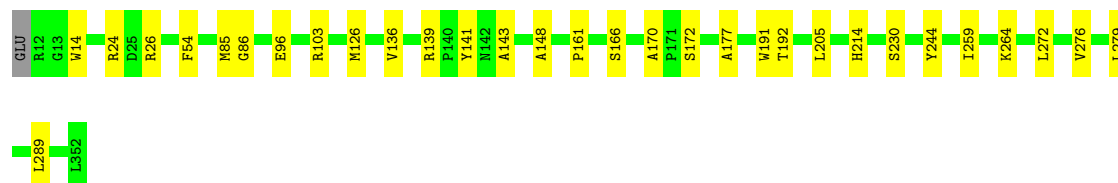
- Molecule 4: Photosystem II D2 protein

Chain D: 89% 11%



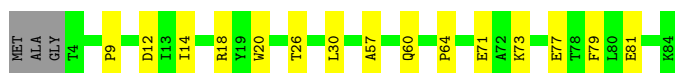
- Molecule 4: Photosystem II D2 protein

Chain d: 91% 9%

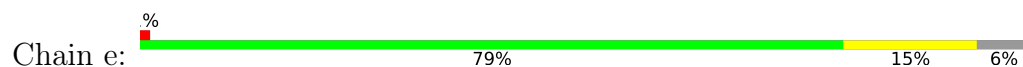


- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 79% 18% .



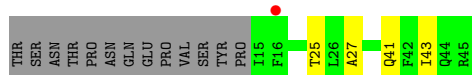
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



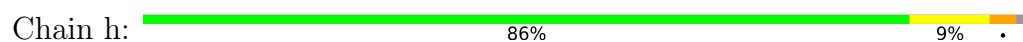
- Molecule 6: Cytochrome b559 subunit beta



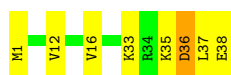
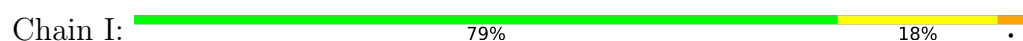
- Molecule 7: Photosystem II reaction center protein H



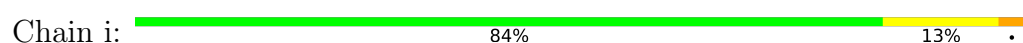
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I





- Molecule 9: Photosystem II reaction center protein J

Chain J: 82% 13% . .



- Molecule 9: Photosystem II reaction center protein J

Chain j: 92% 8%



- Molecule 10: Photosystem II reaction center protein K

Chain K: 81% 16% .



- Molecule 10: Photosystem II reaction center protein K

Chain k: 76% 19% 5%



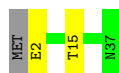
- Molecule 11: Photosystem II reaction center protein L

Chain L: 92% 5% .



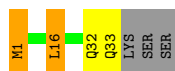
- Molecule 11: Photosystem II reaction center protein L

Chain l: 92% 5% .



- Molecule 12: Photosystem II reaction center protein M

Chain M: 81% 6% 6% 8%



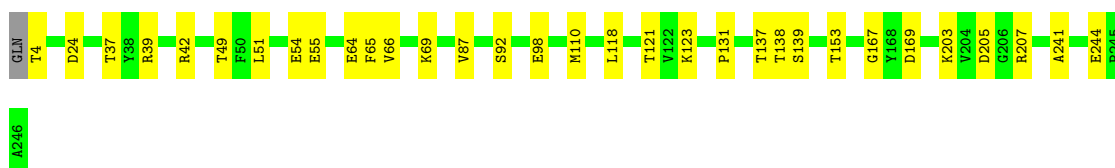
- Molecule 12: Photosystem II reaction center protein M

Chain m: 81% 11% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 86% 13%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 92% 7%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 84% 9% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 3% 81% 12% 6%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 85% 8% 8%

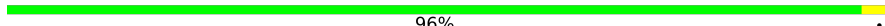


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  92% 7%



- Molecule 16: Cytochrome c-550

Chain V:  96%



- Molecule 16: Cytochrome c-550

Chain v:  91% 9%



- Molecule 17: Photosystem II reaction center protein X

Chain X:  82% 12% 5%



- Molecule 17: Photosystem II reaction center protein X

Chain x:  88% 8% 5%



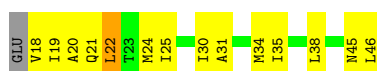
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  87% 10%

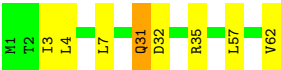
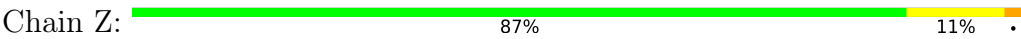


- Molecule 18: Photosystem II reaction center protein Ycf12

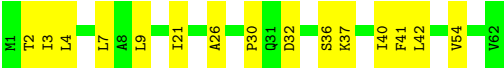
Chain y:  50% 43%



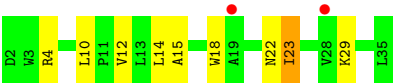
- Molecule 19: Photosystem II reaction center protein Z



• Molecule 19: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.77Å 231.76Å 288.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.30) 99.7 (19.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.30Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.141 , 0.180 0.142 , 0.182	Depositor DCC
R_{free} test set	28224 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 76.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	62602	wwPDB-VP
Average B, all atoms (Å ²)	65.0	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/4478	0.43	0/6098
1	a	0.25	0/4470	0.40	0/6087
2	B	0.38	0/4293	0.50	0/5851
2	b	0.34	0/4285	0.49	0/5841
3	C	0.30	0/4404	0.44	0/5997
3	c	0.28	0/4459	0.43	0/6071
4	D	0.34	0/3741	0.47	0/5095
4	d	0.31	0/3749	0.45	0/5106
5	E	0.35	0/681	0.52	0/928
5	e	0.30	0/690	0.48	0/939
6	F	0.35	0/284	0.45	0/387
6	f	0.29	0/269	0.47	0/365
7	H	0.35	0/519	0.53	0/708
7	h	0.31	0/530	0.46	0/722
8	I	0.30	0/311	0.46	0/419
8	i	0.35	0/311	0.45	0/419
9	J	0.32	0/278	0.40	0/376
9	j	0.28	0/283	0.40	0/383
10	K	0.34	0/303	0.48	0/416
10	k	0.33	0/303	0.47	0/416
11	L	0.37	0/318	0.47	0/433
11	l	0.37	0/318	0.45	0/433
12	M	0.38	0/261	0.54	0/357
12	m	0.39	0/279	0.47	0/380
13	O	0.36	0/1991	0.52	0/2698
13	o	0.34	0/1966	0.51	0/2665
14	T	0.34	0/310	0.43	0/419
14	t	0.32	0/301	0.42	0/406
15	U	0.38	0/811	0.54	0/1095
15	u	0.36	0/818	0.54	0/1105
16	V	0.36	0/1142	0.51	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.31	0/1139	0.48	0/1542
17	X	0.25	0/292	0.37	0/395
17	x	0.25	0/284	0.37	0/384
18	Y	0.25	0/216	0.47	0/289
18	y	0.24	0/216	0.39	0/289
19	Z	0.23	0/490	0.37	0/669
19	z	0.24	0/490	0.36	0/669
20	R	0.23	0/279	0.35	0/383
All	All	0.32	0/50562	0.46	0/68780

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4338	0	4142	28	0
1	a	4330	0	4132	40	0
2	B	4146	0	3983	25	0
2	b	4134	0	3976	40	0
3	C	4260	0	4123	27	0
3	c	4308	0	4172	36	0
4	D	3620	0	3484	37	0
4	d	3628	0	3490	22	0
5	E	662	0	648	12	0
5	e	670	0	655	9	0
6	F	275	0	282	5	0
6	f	261	0	269	5	0
7	H	506	0	529	3	0
7	h	517	0	541	8	0
8	I	314	0	328	5	0
8	i	314	0	328	3	0
9	J	272	0	279	7	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	311	0	320	3	0
11	l	311	0	320	2	0
12	M	268	0	285	6	0
12	m	286	0	305	7	0
13	O	1958	0	1920	15	0
13	o	1933	0	1900	9	0
14	T	311	0	318	1	0
14	t	302	0	311	3	0
15	U	800	0	796	5	0
15	u	807	0	805	1	0
16	V	1120	0	1122	3	0
16	v	1117	0	1131	8	0
17	X	289	0	322	4	0
17	x	281	0	312	3	0
18	Y	215	0	246	2	0
18	y	215	0	246	8	0
19	Z	479	0	516	3	0
19	z	479	0	516	5	0
20	R	273	0	305	5	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	4	0	0	0	0
22	a	4	0	0	0	0
23	A	455	0	504	14	0
23	B	1040	0	1152	26	0
23	C	845	0	936	37	0
23	D	195	0	216	7	0
23	a	455	0	504	15	0
23	b	1040	0	1152	30	0
23	c	845	0	936	32	0
23	d	195	0	216	7	0
24	A	40	0	56	1	0
24	B	120	0	168	4	0
24	C	80	0	112	0	0
24	D	40	0	56	2	0
24	H	40	0	56	2	0
24	K	40	0	56	1	0
24	T	40	0	56	6	0
24	Y	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	40	0	56	1	0
24	b	120	0	168	10	0
24	c	80	0	112	4	0
24	d	40	0	56	2	0
24	h	40	0	56	5	0
24	k	40	0	56	2	0
24	t	40	0	56	3	0
24	y	40	0	56	2	0
25	A	6	0	8	1	0
25	B	18	0	24	3	0
25	C	12	0	16	1	0
25	D	12	0	14	8	0
25	O	12	0	16	2	0
25	V	12	0	16	1	0
25	a	12	0	16	7	0
25	b	12	0	16	2	0
25	c	24	0	32	1	0
25	d	6	0	8	0	0
25	l	12	0	16	1	0
25	o	6	0	8	0	0
25	v	12	0	16	2	0
26	A	54	0	78	1	0
26	B	54	0	78	3	0
26	C	108	0	155	2	0
26	F	43	0	53	2	0
26	a	162	0	233	9	0
26	b	54	0	78	2	0
26	f	43	0	53	1	0
27	A	20	0	0	0	0
27	a	20	0	0	0	0
28	A	110	0	160	19	0
28	D	110	0	160	1	0
28	a	110	0	160	10	0
28	d	110	0	160	1	0
29	A	28	0	0	0	0
29	B	73	0	0	0	0
29	D	57	0	0	0	0
29	I	40	0	0	0	0
29	J	10	0	0	0	0
29	K	68	0	0	0	0
29	M	10	0	0	0	0
29	X	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	a	30	0	0	0	0
29	b	69	0	0	0	0
29	c	64	0	0	0	0
29	d	17	0	0	0	0
29	j	10	0	0	0	0
29	m	10	0	0	0	0
29	x	18	0	0	0	0
30	A	8	0	0	0	0
30	a	8	0	0	0	0
31	A	70	0	92	3	0
31	B	70	0	92	3	0
31	F	35	0	46	0	0
31	M	35	0	46	0	0
31	T	35	0	45	0	0
31	b	50	0	70	1	0
31	c	35	0	46	2	0
31	e	35	0	46	1	0
31	m	35	0	46	2	0
31	t	51	0	67	2	0
32	A	98	0	148	1	0
32	D	196	0	296	13	0
32	E	84	0	114	6	0
32	L	98	0	148	1	0
32	a	84	0	114	8	0
32	d	294	0	444	24	0
32	l	98	0	148	0	0
33	B	51	0	72	1	0
33	C	190	0	260	4	0
33	D	51	0	72	0	0
33	a	51	0	72	1	0
33	c	102	0	144	2	0
33	d	51	0	72	1	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	310	0	410	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	H	62	0	82	1	0
35	c	310	0	410	12	0
35	h	62	0	82	0	0
36	C	1	0	0	0	0
36	O	1	0	0	0	0
36	V	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	256	0	296	5	0
37	a	256	0	296	4	0
38	F	43	0	30	1	0
38	f	43	0	30	1	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	219	0	0	0	0
41	B	193	0	0	2	0
41	C	207	0	0	3	0
41	D	156	0	0	6	0
41	E	15	0	0	0	0
41	F	6	0	0	0	0
41	H	22	0	0	0	0
41	I	6	0	0	0	0
41	J	5	0	0	2	0
41	K	7	0	0	0	0
41	L	10	0	0	0	0
41	M	6	0	0	0	0
41	O	103	0	0	0	0
41	T	14	0	0	0	0
41	U	48	0	0	0	0
41	V	82	0	0	1	0
41	X	8	0	0	0	0
41	a	208	0	0	2	0
41	b	204	0	0	0	0
41	c	195	0	0	3	0
41	d	155	0	0	1	0
41	e	8	0	0	0	0
41	f	3	0	0	0	0
41	h	17	0	0	0	0
41	i	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	j	1	0	0	0	0
41	k	3	0	0	0	0
41	l	8	0	0	0	0
41	m	13	0	0	0	0
41	o	99	0	0	0	0
41	t	9	0	0	1	0
41	u	51	0	0	1	0
41	v	60	0	0	0	0
41	x	8	0	0	0	0
41	y	2	0	0	0	0
All	All	62602	0	61441	609	0

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

All (609) 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)
25:D:403:GOL:H11	12:M:1:FME:HG2	1.43	0.99
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.50	0.94
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.51	0.93
23:c:504:CLA:HBB1	23:c:513:CLA:H41	1.56	0.88
24:b:619:BCR:H331	24:b:619:BCR:HC8	1.60	0.84
23:B:601:CLA:H12	23:B:601:CLA:H71	1.65	0.78
4:d:192[B]:THR:HG23	23:d:401[B]:CLA:HBC2	1.66	0.78
4:d:192[A]:THR:HG23	23:d:401[A]:CLA:HBC2	1.66	0.77
23:A:406[A]:CLA:H152	28:A:412[A]:PL9:H252	1.67	0.76
23:B:604:CLA:H42	23:B:605:CLA:H2	1.67	0.75
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.68	0.74
23:c:506:CLA:HHC	23:c:506:CLA:HBB1	1.69	0.74
23:A:407:CLA:H193	23:C:508:CLA:H101	1.70	0.73
23:C:507:CLA:HHC	23:C:507:CLA:HBB1	1.70	0.73
23:A:406[B]:CLA:H152	28:A:412[B]:PL9:H252	1.71	0.73
23:c:503:CLA:H61	23:c:513:CLA:H42	1.71	0.71
32:D:409[B]:LHG:H382	32:D:409[B]:LHG:H112	1.73	0.71
23:a:409:CLA:H192	23:c:506:CLA:H142	1.71	0.71
25:D:403:GOL:O2	41:D:501:HOH:O	2.08	0.71
1:a:15:GLU:HB2	31:c:501:LMT:H6'2	1.73	0.70
23:a:409:CLA:H152	23:c:507:CLA:H142	1.73	0.70
2:b:98:LEU:HB2	34:b:622:HTG:H7'1	1.74	0.69
13:O:42:ARG:HH12	25:O:302:GOL:H12	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:253[A]:GLY:HA3	2:b:491[A]:VAL:HG12	1.75	0.69
1:a:253[B]:GLY:HA3	2:b:491[B]:VAL:HG12	1.75	0.69
23:C:508:CLA:H142	35:C:518[B]:DGD:HAF2	1.75	0.68
31:t:101:LMT:H6E	31:t:102:LMT:H6D	1.75	0.68
32:D:409[A]:LHG:H112	32:D:409[A]:LHG:H382	1.76	0.68
23:C:505:CLA:HBB1	23:C:514:CLA:H41	1.77	0.67
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.75	0.67
3:c:261:ARG:NH1	8:i:38:GLU:OE2	2.28	0.67
23:C:515:CLA:H202	33:C:522:LMG:H402	1.78	0.66
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.76	0.66
12:M:33:GLN:HB2	12:m:33:GLN:HG3	1.78	0.66
25:a:418:GOL:H32	12:m:1:FME:HG3	1.77	0.66
25:a:419:GOL:H11	12:m:1:FME:HE3	1.78	0.66
25:a:419:GOL:H31	12:m:1:FME:HG2	1.78	0.66
1:A:85[B]:SER:HA	1:A:109[B]:GLY:HA3	1.78	0.66
3:C:286:ALA:HB2	23:C:504:CLA:HMD1	1.77	0.66
24:y:101:BCR:H321	24:y:101:BCR:HC8	1.78	0.66
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.78	0.65
23:C:503:CLA:H193	23:C:509:CLA:HBB1	1.79	0.65
23:C:507:CLA:CMD	23:C:509:CLA:HAB	2.27	0.65
1:a:192[B]:ILE:HG13	1:a:293[B]:MET:HE1	1.77	0.65
3:c:213:LEU:HD13	23:c:507:CLA:H202	1.78	0.64
23:c:512:CLA:H191	33:z:101:LMG:H241	1.79	0.64
4:D:192[B]:THR:HG23	23:D:404[B]:CLA:HBC2	1.79	0.64
23:a:406[A]:CLA:HHC	23:a:406[A]:CLA:HBB1	1.80	0.64
1:A:102:LEU:HD12	34:b:625:HTG:H61	1.80	0.64
4:D:123:ILE:HD11	35:H:102:DGD:HAH2	1.80	0.64
26:a:411[A]:SQD:H321	23:c:509:CLA:H102	1.78	0.64
2:b:482[A]:ILE:HD12	2:b:486[A]:LEU:HD12	1.80	0.64
28:A:412[A]:PL9:H262	32:E:101[A]:LHG:H223	1.80	0.63
2:B:357[B]:ARG:NH2	4:D:337:GLU:O	2.29	0.63
23:C:512:CLA:HBC3	23:C:512:CLA:H192	1.81	0.63
13:O:39[B]:ARG:NH1	13:O:244:GLU:OE2	2.30	0.63
3:c:134[B]:ILE:HD13	23:c:512:CLA:H43	1.81	0.63
10:K:17:ILE:H	10:K:17:ILE:HD13	1.64	0.62
2:B:498:LYS:HE3	4:D:20:ASP:HA	1.80	0.62
3:c:78:GLU:OE2	16:v:106:ASN:ND2	2.32	0.62
26:a:411[A]:SQD:H152	32:d:406[A]:LHG:H172	1.82	0.62
3:C:261:ARG:NH1	8:I:38:GLU:OE2	2.32	0.62
13:O:169:ASP:OD1	25:O:303:GOL:H12	2.00	0.62
34:B:622:HTG:H4'1	31:B:630:LMT:H52	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:514:CLA:HBB1	24:c:515:BCR:H24C	1.80	0.62
23:C:508:CLA:H142	35:C:518[A]:DGD:HAF2	1.81	0.61
23:c:502:CLA:C4D	23:c:504:CLA:H2	2.30	0.61
35:c:518[B]:DGD:HAF1	35:c:518[B]:DGD:HA81	1.83	0.61
4:D:205[B]:LEU:HD13	37:D:401[B]:PHO:HAB	1.83	0.60
2:B:226:TYR:HA	2:B:231:MET:HG3	1.82	0.60
10:k:23:ASP:OD2	18:y:21:GLN:NE2	2.35	0.60
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.36	0.59
32:d:405[B]:LHG:HC62	11:l:15[B]:THR:HG23	1.85	0.59
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.84	0.59
24:t:103:BCR:H321	24:t:103:BCR:HC8	1.83	0.59
26:a:411[B]:SQD:H321	23:c:509:CLA:H102	1.82	0.59
26:a:411[A]:SQD:H141	32:d:406[A]:LHG:H152	1.84	0.59
23:c:506:CLA:CMD	23:c:508:CLA:HAB	2.33	0.59
28:A:412[B]:PL9:H262	32:E:101[B]:LHG:H223	1.84	0.58
23:C:510:CLA:HBC3	23:C:512:CLA:H71	1.84	0.58
1:a:214[B]:MET:HB3	28:a:414[B]:PL9:H103	1.86	0.58
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.33	0.58
2:b:285:ASN:O	2:b:289:GLN:HG2	2.03	0.58
10:k:17:ILE:HD13	10:k:17:ILE:H	1.69	0.58
13:o:58:ASN:HD22	13:o:61:GLN:HG3	1.67	0.58
23:b:601:CLA:H72	23:b:601:CLA:H2	1.86	0.57
25:D:403:GOL:H31	12:M:1:FME:HE3	1.85	0.57
4:D:192[A]:THR:HG23	23:D:404[A]:CLA:HBC2	1.87	0.57
23:A:407:CLA:H18	23:C:507:CLA:H142	1.87	0.57
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.87	0.57
23:a:407[A]:CLA:H191	32:a:420[A]:LHG:H111	1.85	0.57
37:a:416[A]:PHO:HBC3	4:d:279:LEU:HD22	1.86	0.56
19:Z:32:ASP:OD2	19:Z:35:ARG:HB3	2.06	0.56
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.85	0.56
4:D:323[A]:GLU:O	25:D:414:GOL:O2	2.23	0.56
26:a:411[B]:SQD:H141	32:d:406[B]:LHG:H152	1.86	0.56
35:c:517[A]:DGD:HG11	41:c:606[A]:HOH:O	2.06	0.56
5:E:57:ALA:H	5:E:60:GLN:HE21	1.51	0.56
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.87	0.56
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.19	0.55
32:D:408[B]:LHG:HC62	11:L:15[B]:THR:HG23	1.89	0.55
3:c:27:ASP:HB3	10:k:46:ARG:HG3	1.89	0.55
25:a:419:GOL:O2	41:a:501:HOH:O	2.09	0.55
10:k:24:VAL:HG22	18:y:25:ILE:HD13	1.89	0.55
4:D:327:ALA:HB2	25:D:414:GOL:H2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:86[B]:GLU:H	15:U:86[B]:GLU:CD	2.12	0.55
8:I:35:LYS:O	8:I:37:LEU:N	2.40	0.54
1:a:183[A]:MET:HA	23:a:405[A]:CLA:HMD1	1.89	0.54
16:v:134[A]:LYS:HE2	25:v:202[A]:GOL:H32	1.88	0.54
26:F:103:SQD:H102	17:X:31:ILE:HD11	1.90	0.54
32:D:409[A]:LHG:H382	32:D:409[A]:LHG:H132	1.89	0.54
25:b:628:GOL:O3	25:b:628:GOL:O1	2.21	0.54
3:C:406:SER:HA	3:C:420[B]:VAL:HG23	1.88	0.54
23:b:609:CLA:HMD1	7:h:27:THR:HB	1.88	0.54
3:c:406:SER:HA	3:c:420[B]:VAL:HG23	1.90	0.54
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.42	0.54
3:c:182:PHE:HA	34:c:522:HTG:H61	1.90	0.54
23:a:407[B]:CLA:H191	32:a:420[B]:LHG:H111	1.89	0.54
23:d:402:CLA:H162	7:h:37:LEU:HD21	1.90	0.54
28:A:412[A]:PL9:H253	23:D:404[A]:CLA:H141	1.89	0.54
23:B:601:CLA:HHC	23:B:601:CLA:HBB1	1.90	0.54
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.42	0.53
5:E:77:GLU:O	5:E:81:GLU:HG2	2.08	0.53
23:a:406[B]:CLA:HBB1	23:a:406[B]:CLA:HHC	1.90	0.53
2:b:216:HIS:HE1	23:b:609:CLA:C1A	2.21	0.53
4:D:317[B]:LYS:NZ	41:D:513[B]:HOH:O	2.38	0.53
23:a:405[B]:CLA:H152	37:a:408[B]:PHO:H52	1.89	0.53
16:V:126:LEU:HB3	16:V:129:LYS:HB2	1.89	0.53
3:c:338[B]:GLY:HA3	3:c:341[B]:LEU:O	2.08	0.53
24:Y:101:BCR:H321	24:Y:101:BCR:HC8	1.91	0.53
1:a:160[B]:ILE:HD11	35:c:517[B]:DGD:HBT1	1.89	0.53
1:a:192[A]:ILE:HG13	1:a:293[A]:MET:HE1	1.90	0.53
23:C:503:CLA:C3D	23:C:505:CLA:H2	2.39	0.53
25:l:801[A]:GOL:H32	14:t:25:GLU:HB2	1.89	0.53
2:b:245:VAL:HG22	23:b:612:CLA:H202	1.89	0.53
1:A:341[B]:LEU:HD13	25:C:524[B]:GOL:H31	1.90	0.53
23:B:615:CLA:H2	23:B:616:CLA:HBB2	1.90	0.52
23:B:607:CLA:HMB1	23:B:607:CLA:HBB1	1.91	0.52
3:c:225:VAL:HG13	3:c:289:PHE:HA	1.91	0.52
3:C:95:LEU:HD21	23:C:503:CLA:OBD	2.09	0.52
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.90	0.52
32:D:409[B]:LHG:H382	32:D:409[B]:LHG:H132	1.91	0.52
1:a:84[B]:PRO:HA	1:a:112[B]:TYR:CG	2.44	0.52
26:B:620:SQD:H381	31:m:103:LMT:H121	1.92	0.52
3:c:338[A]:GLY:HA3	3:c:341[A]:LEU:O	2.10	0.52
33:z:101:LMG:H302	33:z:101:LMG:H141	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84[A]:PRO:HA	1:A:112[A]:TYR:CG	2.44	0.52
2:B:36[B]:SER:OG	24:B:618:BCR:H362	2.09	0.52
35:c:519:DGD:HBH2	32:d:406[A]:LHG:H211	1.92	0.52
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.45	0.52
1:A:227[A]:THR:HB	1:A:231:GLU:HG3	1.91	0.51
23:A:404[B]:CLA:HBB1	23:D:404[B]:CLA:C4B	2.17	0.51
23:A:406[B]:CLA:HHC	23:A:406[B]:CLA:HBB1	1.91	0.51
10:k:19:ASP:HB3	10:k:20:PRO:HD3	1.93	0.51
1:A:227[B]:THR:HB	1:A:231:GLU:HG3	1.91	0.51
13:O:24:ASP:HA	13:O:203:LYS:HE2	1.93	0.51
1:a:214[B]:MET:HE2	1:a:255[B]:PHE:CE1	2.45	0.51
2:b:226:TYR:HA	2:b:231:MET:HG3	1.91	0.51
24:b:619:BCR:H331	24:b:619:BCR:C8	2.34	0.51
28:A:412[A]:PL9:H472	4:D:39:PRO:HD3	1.92	0.51
15:u:10[A]:VAL:HG12	41:u:246:HOH:O	2.09	0.51
23:B:609:CLA:HHC	23:B:609:CLA:HBB1	1.92	0.51
24:T:102:BCR:H321	24:T:102:BCR:HC8	1.93	0.51
32:a:420[A]:LHG:HC31	5:e:9:PRO:HA	1.92	0.51
23:c:509:CLA:H18	35:c:518[A]:DGD:HAT2	1.93	0.51
23:C:514:CLA:H143	23:C:515:CLA:H142	1.91	0.51
13:O:42:ARG:O	13:O:241:ALA:HA	2.11	0.51
16:v:134[B]:LYS:HE2	25:v:202[B]:GOL:H32	1.92	0.51
23:B:612:CLA:HBB1	23:B:612:CLA:HMB1	1.93	0.51
23:c:502:CLA:C3D	23:c:504:CLA:H2	2.41	0.51
24:h:101:BCR:H331	24:h:101:BCR:C8	2.40	0.51
25:D:403:GOL:H11	12:M:1:FME:CG	2.30	0.51
1:a:221[B]:SER:HB2	4:d:139[B]:ARG:O	2.11	0.51
23:B:615:CLA:H2	23:B:616:CLA:CBB	2.41	0.50
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.46	0.50
28:A:412[B]:PL9:H472	4:D:39:PRO:HD3	1.93	0.50
23:C:512:CLA:H52	32:D:409[A]:LHG:H371	1.92	0.50
28:A:412[B]:PL9:H253	23:D:404[B]:CLA:H141	1.91	0.50
3:C:176:VAL:HG21	3:C:238:ILE:HG13	1.93	0.50
4:D:85:MET:CE	4:D:96:GLU:HG2	2.42	0.50
3:c:363:GLY:O	3:c:367:GLU:HG2	2.12	0.50
6:f:27:ALA:HB1	38:f:101:HEM:HAC	1.92	0.50
23:b:616:CLA:HHC	23:b:616:CLA:HBB1	1.93	0.50
31:e:101:LMT:H6'1	6:f:43:ILE:HG12	1.92	0.50
23:A:406[B]:CLA:HED1	35:C:520:DGD:HAE2	1.93	0.50
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.46	0.50
4:d:85:MET:CE	4:d:96:GLU:HG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:606:CLA:H202	26:a:412:SQD:H302	1.94	0.50
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.12	0.50
26:a:411[B]:SQD:H271	32:d:406[B]:LHG:H141	1.92	0.50
3:c:117:VAL:HG12	33:c:521:LMG:H221	1.94	0.49
28:a:414[A]:PL9:H351	6:f:25:THR:OG1	2.12	0.49
1:a:221[A]:SER:HB2	4:d:139[A]:ARG:O	2.12	0.49
3:C:279:LEU:HD22	23:C:511:CLA:HED2	1.94	0.49
1:a:165[B]:GLN:OE1	41:a:518[B]:HOH:O	2.20	0.49
2:B:247:PHE:CE2	23:B:602:CLA:H102	2.47	0.49
13:O:137:THR:C	13:O:139:SER:H	2.19	0.49
23:a:405[A]:CLA:H201	32:d:405[A]:LHG:H161	1.95	0.49
18:y:20:ALA:O	18:y:24:MET:HG2	2.12	0.49
2:b:491[B]:VAL:HG13	4:d:136[B]:VAL:HG13	1.95	0.49
3:C:443[B]:TRP:CE2	23:C:510:CLA:HMD2	2.48	0.49
28:a:414[B]:PL9:H351	6:f:25:THR:OG1	2.13	0.49
4:d:14:TRP:CD1	34:d:408:HTG:H61	2.47	0.49
4:d:244[B]:TYR:OH	4:d:264[B]:LYS:HE3	2.12	0.49
32:d:405[A]:LHG:HC62	11:l:15[A]:THR:HG23	1.95	0.49
12:m:5[B]:GLN:H	12:m:5[B]:GLN:NE2	2.10	0.49
23:C:512:CLA:H52	32:D:409[B]:LHG:H371	1.95	0.49
13:O:205:ASP:OD1	13:O:207:ARG:HG3	2.12	0.49
23:C:513:CLA:HBB1	23:C:513:CLA:HMB3	1.94	0.48
25:D:403:GOL:H12	14:T:2:GLU:OE1	2.13	0.48
3:C:42:LEU:HD21	23:C:513:CLA:H2A	1.95	0.48
37:D:402[A]:PHO:H3A	23:D:404[A]:CLA:H142	1.94	0.48
3:c:425[A]:TRP:CD1	23:c:505:CLA:HMA2	2.48	0.48
32:d:406[A]:LHG:H122	32:d:406[A]:LHG:C38	2.44	0.48
2:b:36:SER:OG	24:b:618:BCR:H362	2.13	0.48
3:c:152:LYS:HD2	41:c:756:HOH:O	2.12	0.48
5:E:57:ALA:HB3	5:E:60:GLN:HG2	1.96	0.48
3:c:52:ALA:HB2	23:c:512:CLA:HMA2	1.94	0.48
31:t:102:LMT:H112	31:t:102:LMT:H81	1.46	0.48
3:C:157:MET:HE2	3:C:157:MET:HA	1.96	0.48
4:D:261[B]:PHE:CZ	32:D:408[B]:LHG:HC81	2.49	0.48
9:J:2:SER:N	41:J:201:HOH:O	2.46	0.48
2:b:482[B]:ILE:HD12	2:b:486[B]:LEU:HD12	1.95	0.48
34:B:622:HTG:O5	25:B:629:GOL:H12	2.14	0.48
32:a:420[B]:LHG:HC31	5:e:9:PRO:HA	1.94	0.48
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.96	0.48
4:D:24:ARG:HD3	17:X:37:VAL:HG22	1.95	0.48
37:a:408[B]:PHO:HAB	4:d:205[B]:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:B:621:LMG:H112	33:B:621:LMG:H141	1.71	0.48
32:D:408[A]:LHG:HC62	11:L:15[A]:THR:HG23	1.96	0.48
25:V:204[B]:GOL:H12	41:V:324[B]:HOH:O	2.12	0.48
2:b:383[B]:PHE:CZ	13:o:167:GLY:HA2	2.49	0.48
1:A:218[B]:LEU:HD12	28:A:412[B]:PL9:C3	2.44	0.47
4:D:264[B]:LYS:NZ	41:D:505[B]:HOH:O	2.46	0.47
26:b:620:SQD:H462	26:b:620:SQD:H1	1.95	0.47
24:t:103:BCR:H331	24:t:103:BCR:HC7	1.56	0.47
1:A:105:TRP:CE2	1:A:110[A]:GLY:HA3	2.50	0.47
3:C:203:THR:O	3:C:235:GLY:HA3	2.14	0.47
4:D:230[A]:SER:HB2	41:D:529:HOH:O	2.14	0.47
25:a:419:GOL:O3	14:t:2:GLU:OE1	2.28	0.47
4:D:180:ARG:HD3	4:D:180:ARG:C	2.40	0.47
23:B:604:CLA:HMD1	23:B:612:CLA:H203	1.96	0.47
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.97	0.47
35:c:517[B]:DGD:HG11	41:c:606[B]:HOH:O	2.15	0.47
10:k:21:LEU:HD13	18:y:24:MET:HE3	1.96	0.47
1:A:133:LEU:HD23	4:D:256[A]:ILE:HG12	1.97	0.47
23:C:512:CLA:H152	23:C:512:CLA:H112	1.51	0.47
1:a:84[A]:PRO:HA	1:a:112[A]:TYR:CG	2.49	0.47
1:a:214[A]:MET:HE2	1:a:255[A]:PHE:CE1	2.50	0.47
2:b:220:ARG:HG3	7:h:20:LYS:HG2	1.96	0.47
23:b:601:CLA:H92	24:h:101:BCR:H403	1.96	0.47
32:d:406[A]:LHG:H342	32:d:406[A]:LHG:H151	1.97	0.47
5:E:9:PRO:HA	32:E:101[A]:LHG:HC31	1.95	0.47
28:A:412[B]:PL9:H151	28:A:412[B]:PL9:H171	1.54	0.47
32:A:416[A]:LHG:H361	23:B:613:CLA:H51	1.97	0.47
26:C:501[B]:SQD:H361	10:K:34:ALA:HA	1.97	0.47
10:K:23:ASP:OD2	18:Y:21:GLN:NE2	2.48	0.47
35:c:519:DGD:HBH2	32:d:406[B]:LHG:H211	1.97	0.47
7:h:56:ASP:OD2	17:x:2:THR:OG1	2.32	0.47
9:j:6:ARG:NH1	9:j:6:ARG:HA	2.29	0.47
16:v:95:LEU:HD11	16:v:112:LEU:HD11	1.97	0.47
19:z:37:LYS:HE2	19:z:41:PHE:HE2	1.80	0.47
4:D:241[B]:GLU:CD	4:D:241[B]:GLU:H	2.23	0.47
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.97	0.47
32:d:406[A]:LHG:H302	32:d:406[A]:LHG:H332	1.67	0.47
2:B:58:GLN:C	2:B:329:PRO:HB3	2.40	0.47
15:U:53:ALA:HB1	15:U:54:PRO:HA	1.96	0.47
2:b:224:ARG:HH21	31:b:621:LMT:H1'	1.79	0.47
23:a:407[B]:CLA:HMB2	23:d:401[B]:CLA:H122	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:414[A]:PL9:H171	28:a:414[A]:PL9:H151	1.58	0.47
32:d:406[B]:LHG:H122	32:d:406[B]:LHG:C38	2.45	0.47
13:o:142:PHE:HB2	13:o:199:LEU:HB2	1.97	0.47
19:z:32:ASP:O	19:z:36:SER:OG	2.21	0.47
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.96	0.46
1:A:192[A]:ILE:HG13	1:A:293[A]:MET:HE1	1.97	0.46
3:C:443[B]:TRP:CD2	23:C:510:CLA:HMD2	2.50	0.46
23:a:405[B]:CLA:HBB1	23:d:401[B]:CLA:C4B	2.15	0.46
3:c:42:LEU:HD21	23:c:512:CLA:H2A	1.97	0.46
8:I:36:ASP:OD1	8:I:36:ASP:N	2.48	0.46
23:a:406[A]:CLA:HBA1	23:a:406[A]:CLA:C4A	2.45	0.46
25:A:409:GOL:O3	25:A:409:GOL:O1	2.32	0.46
1:a:14:TRP:HD1	31:c:501:LMT:H6'1	1.81	0.46
26:a:411[A]:SQD:H271	32:d:406[A]:LHG:H141	1.97	0.46
2:b:149[B]:LEU:HD11	23:b:604:CLA:H152	1.97	0.46
23:A:405[B]:CLA:H203	23:A:405[B]:CLA:H162	1.80	0.46
26:a:411[B]:SQD:H152	32:d:406[B]:LHG:H172	1.98	0.46
3:c:85:GLY:O	23:c:505:CLA:HED2	2.16	0.46
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.97	0.46
2:B:133:LEU:HB2	25:B:627:GOL:H31	1.98	0.46
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.97	0.46
32:d:406[A]:LHG:H331	32:d:406[A]:LHG:H361	1.46	0.46
18:y:34:MET:O	18:y:38:LEU:HG	2.15	0.46
23:B:612:CLA:H162	23:B:612:CLA:H122	1.79	0.46
13:O:92:SER:HB3	13:O:131:PRO:HA	1.97	0.46
24:T:102:BCR:HC7	24:T:102:BCR:H331	1.59	0.46
1:a:82[B]:VAL:HB	1:a:174[B]:LEU:HB2	1.97	0.46
28:a:414[B]:PL9:H171	28:a:414[B]:PL9:H151	1.53	0.46
24:d:403:BCR:C8	24:d:403:BCR:H331	2.45	0.46
24:t:103:BCR:H23C	24:t:103:BCR:H382	1.98	0.46
23:A:405[B]:CLA:C4A	23:A:405[B]:CLA:HBA1	2.45	0.46
24:B:619:BCR:H371	24:B:619:BCR:H24C	1.73	0.46
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.50	0.46
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.16	0.46
24:b:619:BCR:HC7	24:b:619:BCR:H311	1.60	0.46
23:d:402:CLA:H41	23:d:402:CLA:H61	1.64	0.46
26:A:410:SQD:H301	23:b:606:CLA:H202	1.98	0.45
3:C:41:ARG:NH1	23:C:513:CLA:HMD1	2.31	0.45
23:C:507:CLA:H111	23:C:507:CLA:H93	1.68	0.45
23:b:605:CLA:H41	23:b:605:CLA:H62	1.56	0.45
4:D:194:ASN:HA	4:D:295[B]:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:6:ARG:HG3	41:J:201:HOH:O	2.16	0.45
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.98	0.45
3:c:406:SER:HA	3:c:420[A]:VAL:HG23	1.98	0.45
33:c:520:LMG:H181	10:k:27:VAL:HG11	1.99	0.45
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.96	0.45
2:B:299:GLU:HG3	2:B:402:TYR:HD1	1.80	0.45
28:a:414[B]:PL9:H28	32:a:420[B]:LHG:H222	1.97	0.45
3:c:38:GLY:HA3	23:c:512:CLA:HMD2	1.98	0.45
23:B:614:CLA:H71	23:B:614:CLA:H112	1.48	0.45
23:C:508:CLA:H18	23:C:508:CLA:H152	1.43	0.45
23:b:614:CLA:H72	23:b:614:CLA:H112	1.58	0.45
2:B:30:VAL:HG12	23:B:605:CLA:HHD	1.98	0.45
4:D:261[A]:PHE:CZ	32:D:408[A]:LHG:HC81	2.52	0.45
5:E:20:TRP:CD1	9:J:7:ILE:HD12	2.52	0.45
12:M:32:GLN:HG2	31:m:103:LMT:H6'2	1.99	0.45
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.97	0.45
35:c:518[A]:DGD:HAT1	35:c:519:DGD:HB2	1.99	0.45
13:o:43:LEU:HB3	13:o:81:ILE:HB	1.99	0.45
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.52	0.45
32:d:406[A]:LHG:H142	32:d:406[A]:LHG:H372	1.97	0.45
1:a:341[B]:LEU:HD22	25:c:526[B]:GOL:H12	1.98	0.45
24:b:617:BCR:H24C	24:b:617:BCR:H371	1.77	0.45
2:B:445:THR:HA	41:B:712:HOH:O	2.16	0.45
24:T:102:BCR:H351	26:b:620:SQD:H211	1.99	0.45
2:b:233:ASN:O	2:b:236:THR:HG22	2.17	0.45
13:o:92:SER:HB3	13:o:131:PRO:HA	1.99	0.45
19:z:26:ALA:HB3	19:z:40:ILE:HD11	1.99	0.45
23:C:510:CLA:HBC2	32:D:409[A]:LHG:H351	2.00	0.45
32:E:101[A]:LHG:H241	32:E:101[A]:LHG:HC61	1.83	0.45
20:R:18:TRP:O	20:R:22:ASN:ND2	2.40	0.45
23:C:507:CLA:H101	23:C:507:CLA:H61	1.79	0.44
5:E:14:ILE:HD12	9:J:12:VAL:HG11	1.98	0.44
5:E:64:PRO:HB2	5:E:79:PHE:CD2	2.52	0.44
7:h:43:LEU:O	7:h:47:GLU:HG3	2.17	0.44
3:c:238:ILE:O	3:c:242:LEU:HG	2.17	0.44
35:c:518[B]:DGD:HAT1	35:c:519:DGD:HB2	1.99	0.44
28:A:412[A]:PL9:H151	28:A:412[A]:PL9:H171	1.55	0.44
28:A:412[A]:PL9:H301	28:A:412[A]:PL9:H322	1.76	0.44
3:C:23:ALA:HB1	3:C:26:ARG:HB2	1.98	0.44
3:C:334[B]:PRO:HA	13:O:153:THR:OG1	2.17	0.44
37:D:402[B]:PHO:HHD	37:D:402[B]:PHO:HBC2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:12:ASP:OD1	9:J:4:GLY:HA3	2.18	0.44
23:A:407:CLA:H61	23:A:407:CLA:H41	1.60	0.44
31:A:417:LMT:H6'2	31:A:417:LMT:O3'	2.18	0.44
5:E:30:LEU:HD23	20:R:12:VAL:HG22	2.00	0.44
13:O:66:VAL:HG21	13:O:110:MET:HE3	1.99	0.44
1:a:93[A]:PHE:CD2	1:a:95:PRO:HD3	2.53	0.44
28:a:414[A]:PL9:H503	17:x:24:THR:OG1	2.18	0.44
2:b:383[A]:PHE:CZ	13:o:167:GLY:HA2	2.52	0.44
4:d:214[B]:HIS:HA	28:d:404[B]:PL9:O2	2.17	0.44
5:e:68:ASP:O	5:e:72:ALA:HB2	2.17	0.44
28:A:412[B]:PL9:H351	6:F:25:THR:OG1	2.17	0.44
2:B:357[A]:ARG:HH12	25:B:624:GOL:C3	2.30	0.44
3:C:391[B]:ARG:HA	3:C:391[B]:ARG:HD3	1.78	0.44
23:C:503:CLA:C4D	23:C:505:CLA:H2	2.47	0.44
1:a:105:TRP:CE2	1:a:110[B]:GLY:HA3	2.52	0.44
23:b:615:CLA:H61	23:b:615:CLA:H92	1.65	0.44
4:D:230[B]:SER:HB2	41:D:529:HOH:O	2.18	0.44
1:a:214[A]:MET:HB3	28:a:414[A]:PL9:H103	1.98	0.44
16:V:28:GLU:CD	16:V:31:ARG:HH21	2.26	0.44
23:b:606:CLA:H142	23:b:606:CLA:H111	1.89	0.44
3:c:95:LEU:HD21	23:c:502:CLA:OBD	2.18	0.44
3:c:130:VAL:O	3:c:134[A]:ILE:HG12	2.18	0.44
3:c:330:SER:HB3	13:o:100:GLY:O	2.17	0.44
3:C:406:SER:HA	3:C:420[A]:VAL:HG23	1.99	0.44
2:b:298:LEU:HD12	2:b:298:LEU:HA	1.89	0.44
23:b:614:CLA:H8	24:b:617:BCR:H362	2.00	0.44
4:d:24:ARG:NH1	17:x:37:VAL:HG22	2.32	0.44
23:C:505:CLA:H101	23:C:505:CLA:H62	1.63	0.44
35:C:520:DGD:HBE2	35:C:520:DGD:HB81	1.75	0.44
8:I:38:GLU:HG2	8:I:38:GLU:OXT	2.18	0.44
2:b:433:ASP:OD2	2:b:436:THR:OG1	2.32	0.44
23:b:607:CLA:H112	23:b:607:CLA:H91	1.62	0.44
1:A:162[B]:PRO:HB3	1:A:168[B]:PHE:HA	2.00	0.43
37:D:402[B]:PHO:H3A	23:D:404[B]:CLA:H142	2.00	0.43
28:a:414[A]:PL9:H28	32:a:420[A]:LHG:H222	1.99	0.43
20:R:10:LEU:O	20:R:14:LEU:HG	2.18	0.43
31:B:628:LMT:H91	31:B:628:LMT:H62	1.59	0.43
6:F:15:ILE:HD13	20:R:23:ILE:HD11	1.99	0.43
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.00	0.43
1:a:259[A]:ILE:HG22	1:a:260[A]:PHE:CD1	2.53	0.43
18:y:31:ALA:O	18:y:35:ILE:HG13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:408:BCR:H24C	24:A:408:BCR:H371	1.76	0.43
3:C:275:SER:HB3	23:C:511:CLA:HED3	2.00	0.43
35:C:518[B]:DGD:HG11	41:C:601[B]:HOH:O	2.18	0.43
24:T:102:BCR:H19C	24:b:618:BCR:H363	1.99	0.43
1:a:131:TRP:CH2	23:c:506:CLA:HAA2	2.54	0.43
33:a:417:LMG:H172	33:a:417:LMG:H201	1.74	0.43
23:c:505:CLA:H151	23:c:509:CLA:H143	1.98	0.43
19:Z:4:LEU:HD22	19:Z:57:LEU:HD11	1.99	0.43
28:A:412[A]:PL9:H221	28:A:412[A]:PL9:H201	1.88	0.43
28:A:412[A]:PL9:HC2	28:A:412[A]:PL9:HC8	1.71	0.43
28:D:407[A]:PL9:H401	28:D:407[A]:PL9:H422	1.75	0.43
13:O:54:GLU:HG2	13:O:64:GLU:O	2.19	0.43
23:b:609:CLA:HHC	23:b:609:CLA:HBB1	2.00	0.43
2:B:422:ARG:O	2:B:425:ILE:HG12	2.17	0.43
35:C:518[B]:DGD:O1A	41:C:601[B]:HOH:O	2.21	0.43
24:T:102:BCR:H382	24:T:102:BCR:H23C	1.99	0.43
25:a:418:GOL:H12	41:t:201:HOH:O	2.18	0.43
1:A:131:TRP:CD2	1:A:131:TRP:C	2.95	0.43
14:t:2:GLU:HG2	14:t:3:THR:N	2.34	0.43
26:C:501[A]:SQD:H122	26:C:501[A]:SQD:H152	1.52	0.43
2:b:161:LEU:HD12	2:b:161:LEU:HA	1.85	0.43
35:c:518[B]:DGD:HBF2	35:c:518[B]:DGD:HBE1	1.87	0.43
4:d:126:MET:HE3	4:d:143[A]:ALA:O	2.18	0.43
2:B:278:SER:HB3	2:B:281:GLN:HB3	2.00	0.43
4:D:49:LEU:HD13	24:D:406:BCR:C15	2.48	0.43
1:a:227[A]:THR:HB	1:a:231:GLU:HG3	2.01	0.43
24:c:516:BCR:H24C	24:c:516:BCR:H371	1.85	0.43
4:d:148[B]:ALA:HB2	4:d:276[B]:VAL:HG13	2.00	0.43
5:E:26:THR:HG22	20:R:15:ALA:HB1	2.00	0.43
3:c:26:ARG:NH2	18:y:46:LEU:OXT	2.43	0.43
3:c:48:LYS:HG3	3:c:138:GLU:HG3	2.01	0.43
23:c:506:CLA:HAA1	23:c:506:CLA:HBD	2.01	0.43
23:B:602:CLA:H162	23:B:602:CLA:H203	1.64	0.42
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.84	0.42
3:C:344[A]:SER:OG	3:C:348:GLU:OE1	2.36	0.42
4:D:209[A]:LEU:C	4:D:209[A]:LEU:HD23	2.44	0.42
32:E:101[B]:LHG:H261	32:E:101[B]:LHG:H291	1.79	0.42
1:a:60[B]:ILE:HD12	1:a:84[B]:PRO:HD2	2.02	0.42
1:a:261[A]:GLN:HG3	2:b:493[A]:TRP:CH2	2.54	0.42
23:b:616:CLA:H92	23:b:616:CLA:H62	1.75	0.42
3:c:203:THR:O	3:c:235:GLY:HA3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:d:406[B]:LHG:H331	32:d:406[B]:LHG:H361	1.57	0.42
1:A:84[B]:PRO:HA	1:A:112[B]:TYR:CG	2.53	0.42
4:D:205[A]:LEU:HD13	37:D:401[A]:PHO:HAB	2.00	0.42
6:F:27:ALA:HB1	38:F:102:HEM:HAC	2.00	0.42
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.00	0.42
28:a:414[B]:PL9:H471	26:f:102:SQD:H292	2.01	0.42
2:b:247:PHE:CE2	23:b:602:CLA:H121	2.55	0.42
3:c:88:LEU:HD13	23:c:504:CLA:HED3	2.01	0.42
2:B:42:LEU:HD23	2:B:42:LEU:HA	1.91	0.42
23:B:616:CLA:H41	23:B:616:CLA:H61	1.69	0.42
26:B:620:SQD:H1	26:B:620:SQD:H462	2.01	0.42
1:a:296[B]:ASN:HB2	3:c:400[B]:PRO:O	2.19	0.42
23:b:607:CLA:H201	32:d:411[B]:LHG:H131	2.01	0.42
3:c:162:GLY:HA2	3:c:248:GLY:HA2	2.01	0.42
23:d:401[B]:CLA:HAA2	23:d:401[B]:CLA:HBD	2.01	0.42
23:A:405[A]:CLA:H203	23:A:405[A]:CLA:H162	1.76	0.42
35:C:519[B]:DGD:HBF2	35:C:519[B]:DGD:HBE2	1.79	0.42
24:D:406:BCR:H11C	24:D:406:BCR:H341	1.88	0.42
3:c:178:LYS:HA	3:c:182:PHE:HB2	2.02	0.42
1:A:127:MET:HE3	23:C:507:CLA:HMB2	2.01	0.42
34:D:412:HTG:H1'2	7:H:25:TRP:CE3	2.55	0.42
11:L:22:LEU:HD23	32:L:101[B]:LHG:H172	2.00	0.42
23:b:605:CLA:HAA1	23:b:605:CLA:HBD	2.01	0.42
1:A:82[A]:VAL:HB	1:A:174[A]:LEU:HB2	2.01	0.42
23:B:605:CLA:HAA1	23:B:605:CLA:HBD	2.02	0.42
23:B:613:CLA:H162	23:B:613:CLA:H121	1.78	0.42
3:C:230:LEU:HD23	3:C:230:LEU:HA	1.86	0.42
33:C:526:LMG:H141	33:C:526:LMG:H111	1.87	0.42
24:Y:101:BCR:H15C	24:Y:101:BCR:H351	1.84	0.42
1:a:269[B]:ARG:HB3	41:d:544[B]:HOH:O	2.20	0.42
24:y:101:BCR:H15C	24:y:101:BCR:H351	1.84	0.42
1:A:231:GLU:HB3	41:B:873:HOH:O	2.20	0.42
3:C:413[B]:GLU:OE2	41:C:612[B]:HOH:O	2.21	0.42
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.55	0.42
23:b:612:CLA:H122	23:b:612:CLA:H162	1.88	0.42
7:h:38:PHE:HB2	24:h:101:BCR:C10	2.49	0.42
23:A:404[A]:CLA:HBB1	23:A:404[A]:CLA:HMB3	2.02	0.42
1:a:105:TRP:CE2	1:a:110[A]:GLY:HA3	2.54	0.42
24:b:618:BCR:H24C	24:b:618:BCR:H371	1.83	0.42
8:i:32:PRO:C	8:i:33:LYS:HD2	2.44	0.42
1:A:72:LEU:HD23	1:A:72:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183[A]:MET:HA	23:A:404[A]:CLA:HMD1	2.01	0.42
1:A:300[B]:PHE:HB3	1:A:302:PHE:CE2	2.55	0.42
23:B:601:CLA:H62	23:B:601:CLA:H92	1.84	0.42
23:B:602:CLA:H141	23:B:602:CLA:H161	1.91	0.42
32:D:409[A]:LHG:H302	32:D:409[A]:LHG:H332	1.81	0.42
24:T:102:BCR:H24C	24:T:102:BCR:H371	1.85	0.42
24:a:410:BCR:H24C	24:a:410:BCR:H371	1.81	0.42
1:A:82[B]:VAL:HB	1:A:174[B]:LEU:HB2	2.02	0.42
24:B:618:BCR:H15C	24:B:618:BCR:H351	1.88	0.42
32:E:101[B]:LHG:H241	32:E:101[B]:LHG:HC61	1.80	0.42
8:I:12:VAL:O	8:I:16:VAL:HG23	2.19	0.42
24:K:102:BCR:H15C	24:K:102:BCR:H351	1.89	0.42
1:A:243[A]:GLU:CD	1:A:243[A]:GLU:H	2.27	0.41
3:C:279:LEU:HD12	3:C:282:MET:HE3	2.02	0.41
37:a:416[B]:PHO:HBC2	37:a:416[B]:PHO:HHD	2.02	0.41
23:b:616:CLA:H102	23:b:616:CLA:H13	1.72	0.41
23:c:502:CLA:H42	23:c:503:CLA:HMD3	2.02	0.41
24:k:101:BCR:H15C	24:k:101:BCR:H351	1.90	0.41
23:A:404[B]:CLA:CBD	23:A:405[B]:CLA:HAC2	2.50	0.41
23:C:504:CLA:HAA1	23:C:504:CLA:HBD	2.03	0.41
23:C:511:CLA:HMB1	23:C:511:CLA:HBB1	2.02	0.41
18:Y:20:ALA:O	18:Y:24:MET:HG2	2.20	0.41
2:b:58:GLN:C	2:b:329:PRO:HB3	2.45	0.41
2:b:173:GLY:HA3	2:b:265:ILE:HD11	2.02	0.41
23:b:609:CLA:NC	24:h:101:BCR:H332	2.35	0.41
1:A:213[B]:ALA:HB2	4:D:275[B]:PRO:HG2	2.02	0.41
3:C:363:GLY:O	3:C:367:GLU:HG2	2.20	0.41
32:a:420[A]:LHG:H241	32:a:420[A]:LHG:HC61	1.90	0.41
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.86	0.41
8:i:2:GLU:O	8:i:6:ILE:HG12	2.20	0.41
16:v:106:ASN:OD1	16:v:106:ASN:N	2.52	0.41
19:z:26:ALA:HB1	19:z:36:SER:HB3	2.01	0.41
1:A:160[B]:ILE:HD11	35:C:518[B]:DGD:HBT2	2.02	0.41
23:B:606:CLA:H122	23:B:606:CLA:H161	1.90	0.41
1:A:133:LEU:HD23	4:D:256[B]:ILE:HG12	2.01	0.41
3:C:52:ALA:HB2	23:C:513:CLA:HMA2	2.01	0.41
3:C:339[B]:LYS:NZ	15:U:99:ASN:O	2.51	0.41
4:D:264[B]:LYS:NZ	41:D:526[B]:HOH:O	2.53	0.41
24:H:101:BCR:H11C	24:H:101:BCR:H341	1.98	0.41
24:Y:101:BCR:HC7	24:Y:101:BCR:H331	1.84	0.41
1:a:132:GLU:O	1:a:136:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:322[B]:ASN:OD1	3:c:412[B]:THR:HA	2.20	0.41
23:a:406[A]:CLA:HHC	23:a:406[A]:CLA:CBB	2.48	0.41
25:a:419:GOL:C3	12:m:1:FME:HG2	2.47	0.41
3:c:443[B]:TRP:CZ2	23:c:509:CLA:HMD1	2.55	0.41
23:c:510:CLA:H43	23:c:510:CLA:H12	1.91	0.41
24:c:515:BCR:H11C	24:c:515:BCR:H341	1.78	0.41
32:d:411[B]:LHG:H211	12:m:18:PRO:HG3	2.03	0.41
18:y:22:LEU:HA	18:y:25:ILE:HG22	2.03	0.41
28:A:412[A]:PL9:H43	28:A:412[A]:PL9:H471	1.69	0.41
31:A:415:LMT:H71	2:b:39:LEU:HD13	2.02	0.41
23:C:504:CLA:H141	23:C:504:CLA:H161	1.86	0.41
23:a:406[B]:CLA:HBA1	23:a:406[B]:CLA:C4A	2.49	0.41
2:b:226:TYR:CD2	2:b:231:MET:HB2	2.55	0.41
23:b:603:CLA:H3A	23:b:603:CLA:CGA	2.50	0.41
32:d:406[A]:LHG:H131	32:d:406[A]:LHG:H102	1.91	0.41
23:B:603:CLA:HAB	23:B:605:CLA:H171	2.02	0.41
33:C:502:LMG:H201	33:C:502:LMG:H231	1.76	0.41
24:H:101:BCR:H331	24:H:101:BCR:C8	2.50	0.41
17:X:15[B]:LEU:HD23	17:X:15[B]:LEU:HA	1.92	0.41
3:c:459[B]:ILE:HG21	3:c:464[B]:GLU:HG3	2.03	0.41
23:c:507:CLA:HBA1	23:c:507:CLA:H3A	1.80	0.41
5:e:41:GLY:HA3	5:e:51[B]:ARG:HH22	1.86	0.41
5:e:80:LEU:HD23	5:e:80:LEU:HA	1.92	0.41
19:Z:7:LEU:HD23	19:Z:7:LEU:HA	1.88	0.41
1:A:192[B]:ILE:HG13	1:A:293[B]:MET:HE1	2.01	0.41
26:B:620:SQD:H332	26:B:620:SQD:H301	1.92	0.41
4:D:210[B]:LEU:HA	4:D:213[B]:ILE:HG22	2.03	0.41
28:A:412[A]:PL9:H503	26:F:103:SQD:H341	2.02	0.41
2:B:349:LYS:HG3	2:B:350:GLU:OE1	2.21	0.41
2:B:491[A]:VAL:HG12	4:D:136[A]:VAL:HG13	2.03	0.41
24:B:618:BCR:C8	24:B:618:BCR:H331	2.50	0.41
35:C:519[A]:DGD:HAE2	35:C:519[A]:DGD:HA81	1.91	0.41
32:D:409[B]:LHG:H332	32:D:409[B]:LHG:H302	1.92	0.41
6:F:21:VAL:O	6:F:25:THR:HG23	2.20	0.41
12:M:16[B]:LEU:HD22	12:M:16[B]:LEU:HA	1.95	0.41
1:a:162[A]:PRO:HB3	1:a:168[A]:PHE:HA	2.03	0.41
2:b:272:ARG:HG3	2:b:273:TYR:N	2.36	0.41
23:b:606:CLA:H72	24:b:619:BCR:HC7	2.03	0.41
23:b:613:CLA:H72	23:b:613:CLA:H111	1.89	0.41
24:b:619:BCR:H15C	24:b:619:BCR:H351	1.88	0.41
3:c:429:SER:HA	35:c:518[B]:DGD:HBW1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:505:CLA:H92	23:c:505:CLA:H61	1.77	0.41
4:d:54:PHE:HB3	5:e:47:PHE:CD2	2.55	0.41
4:d:103:ARG:HG3	5:e:73:LYS:HG3	2.01	0.41
4:d:161:PRO:HG3	4:d:170:ALA:HB2	2.03	0.41
28:A:412[A]:PL9:HC8	28:A:412[A]:PL9:H121	1.79	0.41
34:B:625:HTG:H61	1:a:102:LEU:HD12	2.03	0.41
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.95	0.41
4:D:203[B]:GLY:HA3	4:D:278[B]:GLY:HA3	2.03	0.41
17:X:24:THR:O	17:X:28:LEU:HG	2.21	0.41
23:b:615:CLA:HHC	23:b:615:CLA:HBB1	2.03	0.41
33:d:409:LMG:H221	33:d:409:LMG:H191	1.67	0.41
5:e:45:ASP:CG	5:e:51[A]:ARG:HH22	2.29	0.41
13:o:216:GLU:CD	13:o:234:LYS:HD2	2.46	0.41
16:v:41:HIS:HA	16:v:45[B]:ILE:O	2.21	0.41
3:C:216:SER:HB2	33:C:502:LMG:HC71	2.02	0.40
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.56	0.40
13:O:137:THR:C	13:O:139:SER:N	2.79	0.40
32:a:420[A]:LHG:H142	32:a:420[A]:LHG:H172	1.83	0.40
2:b:42:LEU:HD23	2:b:42:LEU:HA	1.92	0.40
24:k:101:BCR:H24C	24:k:101:BCR:H371	1.77	0.40
28:A:412[B]:PL9:H322	28:A:412[B]:PL9:H301	1.72	0.40
10:K:26:PRO:O	10:K:29:PRO:HD2	2.21	0.40
2:b:216:HIS:CE1	23:b:609:CLA:NA	2.88	0.40
23:b:616:CLA:H3A	23:b:616:CLA:HBA1	1.91	0.40
4:d:86:GLY:O	4:d:166:SER:HB2	2.20	0.40
32:d:406[A]:LHG:H242	32:d:406[A]:LHG:H272	1.92	0.40
13:o:58:ASN:ND2	13:o:61:GLN:HG3	2.33	0.40
1:A:159[B]:LEU:C	1:A:162[B]:PRO:HD2	2.46	0.40
2:B:221:PRO:HA	2:B:222:PRO:HD3	2.01	0.40
2:B:433:ASP:OD2	2:B:436:THR:OG1	2.34	0.40
23:C:506:CLA:H62	23:C:506:CLA:H41	1.74	0.40
13:O:121:THR:OG1	13:O:123:LYS:HG3	2.21	0.40
1:a:95:PRO:HD2	1:a:98:GLU:HG3	2.03	0.40
23:a:405[B]:CLA:H122	23:a:405[B]:CLA:H161	1.89	0.40
23:b:601:CLA:HAC1	24:h:101:BCR:H383	2.04	0.40
23:c:509:CLA:H162	23:c:509:CLA:H122	1.78	0.40
24:c:515:BCR:H351	24:c:515:BCR:H15C	1.82	0.40
4:d:141[B]:TYR:OH	32:d:411[B]:LHG:O4	2.29	0.40
32:d:406[B]:LHG:H372	32:d:406[B]:LHG:H142	2.03	0.40
1:A:15:GLU:HG2	31:A:417:LMT:O3B	2.22	0.40
2:B:144:PHE:CE2	2:B:148[A]:LEU:HD11	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:323[B]:GLU:O	25:D:414:GOL:O2	2.39	0.40
15:U:86[B]:GLU:OE1	15:U:86[B]:GLU:N	2.25	0.40
16:V:57:GLU:H	16:V:57:GLU:CD	2.29	0.40
1:a:261[A]:GLN:HG3	2:b:493[A]:TRP:CZ3	2.55	0.40
2:b:358:ARG:HB2	25:b:628:GOL:H31	2.02	0.40
2:b:497:GLN:HB2	2:b:504:THR:HB	2.03	0.40
23:c:506:CLA:HMD2	23:c:508:CLA:HAB	2.04	0.40
35:c:518[A]:DGD:HB2	35:c:518[A]:DGD:HBE1	1.91	0.40
31:B:630:LMT:H11	1:a:72:LEU:HD13	2.03	0.40
5:E:18:ARG:H	9:J:2:SER:N	2.20	0.40
3:c:82:TYR:OH	3:c:394[A]:GLU:OE2	2.31	0.40
24:d:403:BCR:H15C	24:d:403:BCR:H351	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/344 (161%)	548 (99%)	3 (0%)	2 (0%)	30	38
1	a	552/344 (160%)	545 (99%)	5 (1%)	2 (0%)	30	38
2	B	522/505 (103%)	515 (99%)	7 (1%)	0	100	100
2	b	521/505 (103%)	509 (98%)	12 (2%)	0	100	100
3	C	546/455 (120%)	540 (99%)	5 (1%)	1 (0%)	43	55
3	c	553/455 (122%)	540 (98%)	12 (2%)	1 (0%)	43	55
4	D	453/342 (132%)	437 (96%)	16 (4%)	0	100	100
4	d	454/342 (133%)	443 (98%)	11 (2%)	0	100	100
5	E	79/84 (94%)	77 (98%)	2 (2%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	62 (100%)	0	0	100	100
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	4	2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	251/244 (103%)	240 (96%)	10 (4%)	1 (0%)	30	38
13	o	249/244 (102%)	243 (98%)	6 (2%)	0	100	100
14	T	33/32 (103%)	33 (100%)	0	0	100	100
14	t	32/32 (100%)	32 (100%)	0	0	100	100
15	U	97/104 (93%)	92 (95%)	5 (5%)	0	100	100
15	u	98/104 (94%)	95 (97%)	3 (3%)	0	100	100
16	V	140/137 (102%)	137 (98%)	3 (2%)	0	100	100
16	v	140/137 (102%)	133 (95%)	7 (5%)	0	100	100
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	24 (89%)	3 (11%)	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	7
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	7
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	6171/5384 (115%)	6035 (98%)	126 (2%)	10 (0%)	43	55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP
3	c	416	SER
19	Z	31	GLN
13	O	138	THR
19	z	30	PRO
1	a	259[A]	ILE
1	a	259[B]	ILE
1	A	259[A]	ILE
1	A	259[B]	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	444/279 (159%)	440 (99%)	4 (1%)	70	84
1	a	443/279 (159%)	442 (100%)	1 (0%)	87	94
2	B	421/403 (104%)	416 (99%)	5 (1%)	63	79
2	b	420/403 (104%)	410 (98%)	10 (2%)	43	62
3	C	430/356 (121%)	424 (99%)	6 (1%)	59	76
3	c	436/356 (122%)	428 (98%)	8 (2%)	51	70
4	D	368/277 (133%)	365 (99%)	3 (1%)	73	86
4	d	369/277 (133%)	362 (98%)	7 (2%)	50	69
5	E	72/73 (99%)	71 (99%)	1 (1%)	59	76
5	e	72/73 (99%)	70 (97%)	2 (3%)	38	56
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%)	51 (94%)	3 (6%)	19	28
7	h	55/54 (102%)	53 (96%)	2 (4%)	31	47
8	I	34/34 (100%)	33 (97%)	1 (3%)	37	55
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	55
9	J	26/27 (96%)	25 (96%)	1 (4%)	29	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	44
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	9
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	9
11	L	36/35 (103%)	36 (100%)	0	100	100
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	56
12	M	30/32 (94%)	28 (93%)	2 (7%)	15	21
12	m	32/32 (100%)	30 (94%)	2 (6%)	16	23
13	O	216/207 (104%)	207 (96%)	9 (4%)	26	40
13	o	213/207 (103%)	206 (97%)	7 (3%)	33	50
14	T	32/28 (114%)	28 (88%)	4 (12%)	4	5
14	t	31/28 (111%)	31 (100%)	0	100	100
15	U	86/89 (97%)	84 (98%)	2 (2%)	44	63
15	u	87/89 (98%)	85 (98%)	2 (2%)	44	63
16	V	123/117 (105%)	123 (100%)	0	100	100
16	v	123/117 (105%)	119 (97%)	4 (3%)	33	50
17	X	32/33 (97%)	32 (100%)	0	100	100
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%)	17 (77%)	5 (23%)	1	1
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18	26
19	z	52/52 (100%)	46 (88%)	6 (12%)	5	6
20	R	29/29 (100%)	26 (90%)	3 (10%)	7	8
All	All	5103/4403 (116%)	4991 (98%)	112 (2%)	45	65

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243[A]	GLU
1	A	243[B]	GLU
1	A	244[A]	GLU
1	A	244[B]	GLU
2	B	161	LEU
2	B	299	GLU
2	B	315	ILE

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Mol	Chain	Res	Type
2	B	389	LYS
2	B	419	SER
3	C	30	SER
3	C	142	GLU
3	C	289	PHE
3	C	315[A]	MET
3	C	315[B]	MET
3	C	471	SER
4	D	259[A]	ILE
4	D	259[B]	ILE
4	D	338	ASN
5	E	71	GLU
7	H	12	ARG
7	H	43	LEU
7	H	52	THR
8	I	33	LYS
9	J	6	ARG
10	K	10	LYS
10	K	17	ILE
10	K	27	VAL
12	M	16[A]	LEU
12	M	16[B]	LEU
13	O	4	THR
13	O	37	THR
13	O	49	THR
13	O	55	GLU
13	O	69	LYS
13	O	87	VAL
13	O	98[A]	GLU
13	O	98[B]	GLU
13	O	118	LEU
14	T	25[A]	GLU
14	T	25[B]	GLU
14	T	30[A]	THR
14	T	30[B]	THR
15	U	10	VAL
15	U	70	ARG
1	a	13	LEU
2	b	63	LEU
2	b	128	THR
2	b	161	LEU
2	b	240	SER

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Mol	Chain	Res	Type
2	b	245	VAL
2	b	362	PHE
2	b	486[A]	LEU
2	b	486[B]	LEU
2	b	491[A]	VAL
2	b	491[B]	VAL
3	c	19	ASN
3	c	142	GLU
3	c	152	LYS
3	c	255	THR
3	c	289	PHE
3	c	315[A]	MET
3	c	315[B]	MET
3	c	416	SER
4	d	26	ARG
4	d	230[A]	SER
4	d	230[B]	SER
4	d	259[A]	ILE
4	d	259[B]	ILE
4	d	272[A]	LEU
4	d	272[B]	LEU
5	e	61	ARG
5	e	71	GLU
7	h	27	THR
7	h	43	LEU
8	i	33	LYS
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	24	VAL
11	l	2	GLU
12	m	16[A]	LEU
12	m	16[B]	LEU
13	o	25	THR
13	o	36	GLN
13	o	37	THR
13	o	58	ASN
13	o	69	LYS
13	o	118	LEU
13	o	194	LYS
15	u	10[A]	VAL
15	u	10[B]	VAL

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Mol	Chain	Res	Type
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	22	LEU
18	y	30	ILE
18	y	45	ASN
19	Z	3	ILE
19	Z	31	GLN
19	Z	62	VAL
20	R	4	ARG
20	R	23	ILE
20	R	29	LYS
19	z	2	THR
19	z	3	ILE
19	z	4	LEU
19	z	7	LEU
19	z	21	ILE
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
2	B	374	ASN
2	B	394	GLN
5	E	60	GLN
15	U	78	ASN
17	X	38	GLN
1	a	12	ASN
1	a	75	ASN
2	b	14	ASN
2	b	331	ASN
3	c	19	ASN
3	c	201	ASN
11	l	8	GLN
13	o	58	ASN
13	o	132	ASN
15	u	78	ASN
16	v	86	GLN
19	Z	31	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
14	FME	T	1	14	8,9,10	0.59	0	7,9,11	1.38	0
8	FME	I	1	8	8,9,10	0.65	0	7,9,11	1.10	1 (14%)
12	FME	m	1	12	8,9,10	0.48	0	7,9,11	1.42	2 (28%)
8	FME	i	1	8	8,9,10	0.66	0	7,9,11	1.32	1 (14%)
12	FME	M	1	12	8,9,10	0.70	0	7,9,11	1.41	2 (28%)
14	FME	t	1	14	8,9,10	0.79	0	7,9,11	1.46	1 (14%)

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	-	3/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	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	O-C-CA	-2.76	117.54	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1	FME	O-C-CA	-2.36	118.59	124.78
12	m	1	FME	O1-CN-N	-2.20	119.49	125.27
8	i	1	FME	O-C-CA	-2.17	119.08	124.78
12	M	1	FME	CA-N-CN	-2.17	119.48	122.82
12	M	1	FME	O-C-CA	-2.16	119.11	124.78
8	I	1	FME	O-C-CA	-2.05	119.41	124.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	4	0
12	M	1	FME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 274 ligands modelled in this entry, 21 are monoatomic and 20 are unknown - leaving 233 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	602	2	69,73,73	2.08	20 (28%)	83,113,113	2.82	32 (38%)
30	BCT	a	404[B]	21	2,3,3	0.64	0	2,3,3	0.91	0
25	GOL	a	418	-	5,5,5	1.31	2 (40%)	5,5,5	0.91	0
23	CLA	b	604	2	69,73,73	1.98	20 (28%)	83,113,113	2.75	29 (34%)
24	BCR	A	408	-	41,41,41	1.06	1 (2%)	56,56,56	1.46	8 (14%)
32	LHG	d	406[A]	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	3 (5%)
23	CLA	b	616	2	69,73,73	1.98	19 (27%)	83,113,113	2.94	31 (37%)
25	GOL	c	528	-	5,5,5	1.16	0	5,5,5	0.86	0
31	LMT	m	103	-	36,36,36	1.06	2 (5%)	47,47,47	1.16	4 (8%)
37	PHO	D	401[A]	-	58,69,69	2.66	12 (20%)	56,99,99	2.81	14 (25%)
23	CLA	a	409	1	69,73,73	1.99	19 (27%)	83,113,113	3.00	30 (36%)
23	CLA	D	404[A]	4	69,73,73	2.00	20 (28%)	83,113,113	2.86	32 (38%)
23	CLA	d	402	4	69,73,73	2.04	20 (28%)	83,113,113	2.84	30 (36%)
26	SQD	C	501[B]	-	53,54,54	0.95	3 (5%)	62,65,65	1.63	11 (17%)
26	SQD	a	412	-	53,54,54	1.09	3 (5%)	62,65,65	1.18	8 (12%)
25	GOL	o	302	-	5,5,5	1.24	1 (20%)	5,5,5	1.05	0
28	PL9	D	407[A]	-	55,55,55	0.63	1 (1%)	68,69,69	1.61	17 (25%)
35	DGD	c	518[A]	-	63,63,67	0.85	3 (4%)	77,77,81	0.97	3 (3%)
33	LMG	C	502	-	51,51,55	0.90	2 (3%)	59,59,63	1.60	10 (16%)
33	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.11	5 (10%)
25	GOL	D	414	-	5,5,5	1.82	2 (40%)	5,5,5	0.57	0
25	GOL	B	624	-	5,5,5	0.78	0	5,5,5	1.08	1 (20%)
32	LHG	D	409[B]	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
23	CLA	B	616	2	69,73,73	1.98	20 (28%)	83,113,113	2.88	30 (36%)
28	PL9	A	412[B]	-	55,55,55	0.63	2 (3%)	68,69,69	2.01	24 (35%)
23	CLA	B	610	41	69,73,73	2.03	19 (27%)	83,113,113	2.97	32 (38%)
23	CLA	b	603	2	69,73,73	1.98	20 (28%)	83,113,113	2.89	30 (36%)
23	CLA	c	503	3	69,73,73	1.97	19 (27%)	83,113,113	2.78	28 (33%)
37	PHO	a	408[A]	-	58,69,69	2.74	13 (22%)	56,99,99	2.81	14 (25%)
24	BCR	B	618	-	41,41,41	1.01	2 (4%)	56,56,56	1.32	7 (12%)
33	LMG	a	417	-	51,51,55	0.93	2 (3%)	59,59,63	1.19	6 (10%)
32	LHG	a	420[A]	-	41,41,48	1.06	2 (4%)	44,47,54	0.92	2 (4%)
25	GOL	B	627	-	5,5,5	0.99	0	5,5,5	0.96	0
25	GOL	v	202[A]	-	5,5,5	1.20	0	5,5,5	0.82	0
23	CLA	B	606	2	69,73,73	1.99	20 (28%)	83,113,113	2.90	32 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	GOL	b	624	-	5,5,5	1.17	1 (20%)	5,5,5	0.79	0
34	HTG	C	523	-	19,19,19	0.88	1 (5%)	23,24,24	1.39	2 (8%)
31	LMT	M	101	-	36,36,36	1.10	4 (11%)	47,47,47	1.24	5 (10%)
24	BCR	t	103	-	41,41,41	1.05	1 (2%)	56,56,56	1.55	11 (19%)
31	LMT	B	630	-	36,36,36	1.01	2 (5%)	47,47,47	1.18	4 (8%)
25	GOL	O	303	-	5,5,5	0.85	0	5,5,5	1.08	1 (20%)
23	CLA	c	511	3	69,73,73	2.02	20 (28%)	83,113,113	2.87	34 (40%)
23	CLA	B	607	41	69,73,73	1.92	22 (31%)	83,113,113	2.82	31 (37%)
30	BCT	A	414[A]	21	2,3,3	0.64	0	2,3,3	1.30	0
32	LHG	E	101[A]	-	41,41,48	1.08	2 (4%)	44,47,54	1.10	3 (6%)
25	GOL	C	524[A]	-	5,5,5	1.11	0	5,5,5	0.88	0
32	LHG	l	802[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.03	4 (7%)
34	HTG	D	412	-	16,16,19	1.02	1 (6%)	20,21,24	1.50	1 (5%)
34	HTG	b	622	-	19,19,19	1.22	2 (10%)	23,24,24	2.20	8 (34%)
32	LHG	L	101[A]	-	48,48,48	0.88	2 (4%)	51,54,54	1.15	4 (7%)
25	GOL	a	419	-	5,5,5	1.37	1 (20%)	5,5,5	1.01	0
23	CLA	A	405[A]	41	69,73,73	2.02	18 (26%)	83,113,113	2.85	33 (39%)
23	CLA	C	513	3	69,73,73	2.02	20 (28%)	83,113,113	2.67	27 (32%)
23	CLA	c	510	3	69,73,73	2.04	20 (28%)	83,113,113	2.94	33 (39%)
25	GOL	D	403	-	5,5,5	1.50	2 (40%)	5,5,5	0.84	0
26	SQD	A	410	-	53,54,54	1.06	3 (5%)	62,65,65	1.23	4 (6%)
27	OEX	a	413[B]	1,3,41	0,14,14	-	-	-	-	-
30	BCT	a	404[A]	21	2,3,3	0.59	0	2,3,3	1.49	0
37	PHO	a	416[B]	-	58,69,69	2.80	14 (24%)	56,99,99	2.92	16 (28%)
25	GOL	d	410	-	5,5,5	1.05	0	5,5,5	0.94	0
35	DGD	C	518[B]	-	63,63,67	0.84	2 (3%)	77,77,81	1.10	7 (9%)
24	BCR	B	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.34	7 (12%)
25	GOL	A	409	-	5,5,5	1.13	0	5,5,5	0.76	0
23	CLA	C	504	3	69,73,73	2.02	20 (28%)	83,113,113	2.67	28 (33%)
35	DGD	c	519	-	63,63,67	0.86	4 (6%)	77,77,81	1.12	6 (7%)
23	CLA	b	609	2	69,73,73	2.03	19 (27%)	83,113,113	2.84	31 (37%)
35	DGD	C	520	-	63,63,67	0.87	3 (4%)	77,77,81	1.02	4 (5%)
24	BCR	y	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.74	12 (21%)
23	CLA	c	508	41	69,73,73	1.99	18 (26%)	83,113,113	2.91	30 (36%)
33	LMG	c	520	-	51,51,55	0.92	2 (3%)	59,59,63	1.17	6 (10%)
31	LMT	F	101	-	36,36,36	1.05	1 (2%)	47,47,47	1.04	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	614	2	69,73,73	2.02	20 (28%)	83,113,113	3.02	30 (36%)
23	CLA	C	508	3	69,73,73	2.02	21 (30%)	83,113,113	2.86	32 (38%)
26	SQD	C	501[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.88	10 (16%)
23	CLA	C	512	3	69,73,73	2.01	21 (30%)	83,113,113	2.93	33 (39%)
25	GOL	V	204[B]	-	5,5,5	0.95	0	5,5,5	1.02	0
23	CLA	B	605	2	69,73,73	2.03	18 (26%)	83,113,113	2.98	28 (33%)
34	HTG	d	408	-	16,16,19	0.96	1 (6%)	20,21,24	1.55	2 (10%)
23	CLA	d	401[B]	4	69,73,73	2.00	20 (28%)	83,113,113	2.85	29 (34%)
32	LHG	D	409[A]	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
27	OEX	A	411[B]	1,3,41	0,14,14	-	-	-	-	-
24	BCR	c	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.44	11 (19%)
23	CLA	c	506	3	69,73,73	2.03	18 (26%)	83,113,113	2.77	27 (32%)
28	PL9	A	412[A]	-	55,55,55	0.69	2 (3%)	68,69,69	2.01	24 (35%)
24	BCR	C	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.49	7 (12%)
23	CLA	C	506	41	69,73,73	1.92	19 (27%)	83,113,113	2.82	31 (37%)
25	GOL	c	526[B]	-	5,5,5	0.93	0	5,5,5	0.96	0
33	LMG	d	409	39	51,51,55	0.91	2 (3%)	59,59,63	1.12	5 (8%)
23	CLA	c	513	3	69,73,73	2.08	19 (27%)	83,113,113	2.81	32 (38%)
35	DGD	h	102	-	63,63,67	0.86	3 (4%)	77,77,81	1.11	5 (6%)
24	BCR	K	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.43	11 (19%)
25	GOL	b	628	-	5,5,5	0.53	0	5,5,5	1.33	1 (20%)
24	BCR	b	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.27	9 (16%)
24	BCR	h	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.46	11 (19%)
23	CLA	b	601	41	69,73,73	2.06	18 (26%)	83,113,113	2.87	29 (34%)
26	SQD	a	411[B]	-	53,54,54	0.98	3 (5%)	62,65,65	1.55	12 (19%)
32	LHG	D	408[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.01	5 (9%)
32	LHG	d	411[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.06	3 (5%)
25	GOL	B	629	-	5,5,5	0.85	0	5,5,5	1.04	0
23	CLA	b	607	41	69,73,73	1.96	21 (30%)	83,113,113	2.77	28 (33%)
23	CLA	A	404[B]	1	69,73,73	2.07	19 (27%)	83,113,113	2.87	32 (38%)
23	CLA	b	610	41	69,73,73	2.01	19 (27%)	83,113,113	2.92	31 (37%)
23	CLA	C	507	3	69,73,73	2.01	19 (27%)	83,113,113	2.85	30 (36%)
32	LHG	l	802[A]	-	48,48,48	0.83	2 (4%)	51,54,54	1.04	4 (7%)
23	CLA	b	602	2	69,73,73	2.07	20 (28%)	83,113,113	3.05	33 (39%)
23	CLA	c	514	3	69,73,73	2.10	21 (30%)	83,113,113	2.88	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.79	15 (26%)
35	DGD	C	519[B]	-	63,63,67	0.87	3 (4%)	77,77,81	1.03	6 (7%)
40	HEC	v	201	16	50,50,50	1.78	8 (16%)	68,82,82	1.38	6 (8%)
27	OEX	a	413[A]	1,3,41	0,14,14	-	-	-		
23	CLA	c	502	3	69,73,73	2.02	21 (30%)	83,113,113	2.76	27 (32%)
37	PHO	a	416[A]	-	58,69,69	2.77	13 (22%)	56,99,99	2.94	17 (30%)
23	CLA	b	613	2	69,73,73	1.96	19 (27%)	83,113,113	2.84	31 (37%)
31	LMT	T	101	-	36,36,36	1.07	2 (5%)	47,47,47	1.11	3 (6%)
35	DGD	C	518[A]	-	63,63,67	0.83	2 (3%)	77,77,81	1.20	8 (10%)
38	HEM	F	102	5,6	50,50,50	1.52	7 (14%)	66,82,82	1.94	17 (25%)
31	LMT	t	101	-	25,25,36	0.90	1 (4%)	30,30,47	1.19	3 (10%)
26	SQD	f	102	-	42,43,54	1.20	3 (7%)	51,54,65	1.57	12 (23%)
23	CLA	c	505	41	69,73,73	2.04	20 (28%)	83,113,113	2.76	32 (38%)
23	CLA	b	615	2	69,73,73	2.01	17 (24%)	83,113,113	2.81	33 (39%)
34	HTG	B	622	-	19,19,19	1.17	2 (10%)	23,24,24	1.67	6 (26%)
34	HTG	c	522	-	19,19,19	0.91	1 (5%)	23,24,24	1.58	3 (13%)
34	HTG	b	623	-	19,19,19	1.06	1 (5%)	23,24,24	1.99	4 (17%)
24	BCR	b	617	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	5 (8%)
24	BCR	c	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.59	12 (21%)
25	GOL	V	204[A]	-	5,5,5	1.34	0	5,5,5	0.80	0
35	DGD	H	102	-	63,63,67	0.82	3 (4%)	77,77,81	1.11	9 (11%)
23	CLA	D	404[B]	4	69,73,73	2.00	20 (28%)	83,113,113	2.95	29 (34%)
31	LMT	c	501	-	36,36,36	0.99	2 (5%)	47,47,47	1.02	1 (2%)
23	CLA	b	614	2	69,73,73	2.03	20 (28%)	83,113,113	2.94	32 (38%)
23	CLA	d	401[A]	4	69,73,73	1.95	20 (28%)	83,113,113	2.76	32 (38%)
24	BCR	k	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.56	11 (19%)
27	OEX	A	411[A]	1,3,41	0,14,14	-	-	-		
23	CLA	a	406[B]	41	69,73,73	2.05	19 (27%)	83,113,113	2.81	31 (37%)
34	HTG	B	625	-	19,19,19	1.14	2 (10%)	23,24,24	1.25	3 (13%)
26	SQD	b	620	-	53,54,54	1.06	3 (5%)	62,65,65	1.69	11 (17%)
26	SQD	B	620	-	53,54,54	1.06	4 (7%)	62,65,65	1.73	12 (19%)
32	LHG	A	416[B]	-	48,48,48	0.86	2 (4%)	51,54,54	1.18	5 (9%)
33	LMG	D	413	39	51,51,55	0.83	2 (3%)	59,59,63	1.06	4 (6%)
23	CLA	b	606	2	69,73,73	1.99	19 (27%)	83,113,113	2.97	32 (38%)
32	LHG	d	405[B]	-	48,48,48	0.91	3 (6%)	51,54,54	1.04	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	GOL	c	526[A]	-	5,5,5	1.00	0	5,5,5	0.98	0
31	LMT	b	627	-	25,25,36	0.89	2 (8%)	30,30,47	1.10	2 (6%)
32	LHG	d	411[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.11	4 (7%)
25	GOL	c	527	-	5,5,5	1.20	1 (20%)	5,5,5	0.91	0
26	SQD	a	411[A]	-	53,54,54	0.96	3 (5%)	62,65,65	1.83	13 (20%)
32	LHG	D	408[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	3 (5%)
31	LMT	A	415	-	36,36,36	0.88	1 (2%)	47,47,47	1.10	2 (4%)
23	CLA	C	505	3	69,73,73	1.95	19 (27%)	83,113,113	2.82	28 (33%)
26	SQD	F	103	-	42,43,54	1.21	4 (9%)	51,54,65	2.07	14 (27%)
23	CLA	B	615	2	69,73,73	2.04	18 (26%)	83,113,113	2.91	32 (38%)
24	BCR	a	410	-	41,41,41	1.03	2 (4%)	56,56,56	1.36	9 (16%)
23	CLA	c	509	3	69,73,73	2.10	20 (28%)	83,113,113	2.75	30 (36%)
23	CLA	C	514	3	69,73,73	2.03	19 (27%)	83,113,113	2.81	31 (37%)
23	CLA	a	407[B]	41	69,73,73	2.04	19 (27%)	83,113,113	2.90	32 (38%)
24	BCR	C	517	-	41,41,41	1.05	2 (4%)	56,56,56	1.48	10 (17%)
37	PHO	D	402[B]	-	58,69,69	2.83	15 (25%)	56,99,99	2.85	15 (26%)
23	CLA	a	405[B]	1	69,73,73	2.04	20 (28%)	83,113,113	2.88	36 (43%)
35	DGD	c	517[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.03	5 (6%)
23	CLA	C	509	41	69,73,73	1.97	20 (28%)	83,113,113	2.94	32 (38%)
23	CLA	A	406[B]	41	69,73,73	2.11	20 (28%)	83,113,113	2.89	31 (37%)
35	DGD	C	519[A]	-	63,63,67	0.90	3 (4%)	77,77,81	1.03	5 (6%)
23	CLA	c	512	3	69,73,73	2.08	21 (30%)	83,113,113	2.84	33 (39%)
24	BCR	H	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.46	11 (19%)
33	LMG	m	101	-	51,51,55	0.86	2 (3%)	59,59,63	1.40	9 (15%)
23	CLA	B	608	2	69,73,73	1.92	21 (30%)	83,113,113	2.83	34 (40%)
28	PL9	a	414[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.94	22 (32%)
23	CLA	A	405[B]	41	69,73,73	2.00	21 (30%)	83,113,113	2.86	32 (38%)
23	CLA	C	510	3	69,73,73	2.07	20 (28%)	83,113,113	2.83	29 (34%)
25	GOL	l	801[B]	-	5,5,5	0.88	0	5,5,5	1.00	0
28	PL9	d	404[B]	-	55,55,55	0.63	1 (1%)	68,69,69	1.72	21 (30%)
25	GOL	O	302	-	5,5,5	1.00	0	5,5,5	0.88	0
23	CLA	b	605	2	69,73,73	1.95	19 (27%)	83,113,113	3.14	31 (37%)
33	LMG	C	522	-	51,51,55	1.08	3 (5%)	59,59,63	1.34	6 (10%)
34	HTG	b	625	-	19,19,19	1.02	2 (10%)	23,24,24	1.47	5 (21%)
34	HTG	V	203	-	11,11,19	0.35	0	15,15,24	1.33	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	608	2	69,73,73	2.02	21 (30%)	83,113,113	2.78	30 (36%)
32	LHG	d	406[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.01	4 (7%)
33	LMG	B	621	-	51,51,55	0.88	2 (3%)	59,59,63	1.32	5 (8%)
40	HEC	V	202	16	50,50,50	1.68	6 (12%)	68,82,82	1.44	9 (13%)
23	CLA	D	405	4	69,73,73	2.15	18 (26%)	83,113,113	2.74	30 (36%)
23	CLA	b	612	2	69,73,73	2.05	20 (28%)	83,113,113	2.77	31 (37%)
23	CLA	c	507	3	69,73,73	2.04	21 (30%)	83,113,113	2.73	30 (36%)
23	CLA	B	611	2	69,73,73	2.51	20 (28%)	83,113,113	3.91	30 (36%)
23	CLA	C	511	3	69,73,73	2.06	20 (28%)	83,113,113	2.84	29 (34%)
37	PHO	D	401[B]	-	58,69,69	2.71	16 (27%)	56,99,99	2.86	16 (28%)
23	CLA	a	406[A]	41	69,73,73	2.04	17 (24%)	83,113,113	2.86	32 (38%)
32	LHG	A	416[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.27	6 (11%)
24	BCR	b	619	-	41,41,41	1.05	1 (2%)	56,56,56	1.39	9 (16%)
24	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	7 (12%)
31	LMT	b	621	-	25,25,36	0.95	1 (4%)	30,30,47	1.15	2 (6%)
31	LMT	e	101	-	36,36,36	1.01	3 (8%)	47,47,47	1.02	1 (2%)
32	LHG	d	405[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.04	4 (7%)
28	PL9	D	407[B]	-	55,55,55	0.60	1 (1%)	68,69,69	1.70	17 (25%)
34	HTG	B	623	-	19,19,19	0.78	1 (5%)	23,24,24	1.56	1 (4%)
35	DGD	c	518[B]	-	63,63,67	0.87	2 (3%)	77,77,81	0.96	5 (6%)
31	LMT	B	628	-	36,36,36	1.14	3 (8%)	47,47,47	1.33	5 (10%)
23	CLA	B	612	2	69,73,73	1.98	19 (27%)	83,113,113	2.83	33 (39%)
23	CLA	B	601	41	69,73,73	2.09	21 (30%)	83,113,113	2.85	29 (34%)
23	CLA	C	503	3	69,73,73	2.01	19 (27%)	83,113,113	2.82	30 (36%)
23	CLA	B	604	2	69,73,73	2.05	21 (30%)	83,113,113	2.71	31 (37%)
37	PHO	a	408[B]	-	58,69,69	2.73	14 (24%)	56,99,99	2.77	16 (28%)
23	CLA	B	609	2	69,73,73	2.04	17 (24%)	83,113,113	2.82	30 (36%)
23	CLA	a	407[A]	41	69,73,73	1.98	19 (27%)	83,113,113	2.83	30 (36%)
31	LMT	A	417	-	36,36,36	1.04	2 (5%)	47,47,47	1.13	4 (8%)
32	LHG	a	420[B]	-	41,41,48	1.03	2 (4%)	44,47,54	0.92	2 (4%)
23	CLA	c	504	3	69,73,73	2.10	20 (28%)	83,113,113	2.93	28 (33%)
37	PHO	D	402[A]	-	58,69,69	2.79	15 (25%)	56,99,99	2.85	15 (26%)
23	CLA	a	405[A]	1	69,73,73	1.99	20 (28%)	83,113,113	2.87	33 (39%)
25	GOL	v	202[B]	-	5,5,5	1.02	0	5,5,5	0.91	0
35	DGD	c	517[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.10	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	HEM	f	101	5,6	50,50,50	1.50	6 (12%)	66,82,82	1.80	12 (18%)
23	CLA	A	406[A]	41	69,73,73	2.04	19 (27%)	83,113,113	2.85	32 (38%)
24	BCR	d	403	-	41,41,41	1.08	1 (2%)	56,56,56	1.92	16 (28%)
23	CLA	A	404[A]	1	69,73,73	2.00	20 (28%)	83,113,113	2.87	30 (36%)
23	CLA	A	407	1	69,73,73	1.95	20 (28%)	83,113,113	2.96	35 (42%)
23	CLA	B	603	2	69,73,73	1.98	19 (27%)	83,113,113	2.96	31 (37%)
23	CLA	b	611	2	69,73,73	1.95	20 (28%)	83,113,113	2.89	29 (34%)
24	BCR	D	406	-	41,41,41	1.08	1 (2%)	56,56,56	1.81	17 (30%)
31	LMT	t	102	-	26,26,36	0.95	2 (7%)	31,31,47	1.22	2 (6%)
23	CLA	C	515	3	69,73,73	2.03	19 (27%)	83,113,113	2.91	31 (37%)
30	BCT	A	414[B]	21	2,3,3	0.63	0	2,3,3	0.88	0
32	LHG	E	101[B]	-	41,41,48	1.04	2 (4%)	44,47,54	1.12	4 (9%)
28	PL9	a	414[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.01	22 (32%)
25	GOL	C	524[B]	-	5,5,5	1.20	0	5,5,5	0.82	0
33	LMG	C	526	-	37,37,55	1.01	2 (5%)	45,45,63	1.48	7 (15%)
23	CLA	B	613	2	69,73,73	2.02	20 (28%)	83,113,113	2.75	30 (36%)
33	LMG	c	521	-	51,51,55	1.02	2 (3%)	59,59,63	1.33	6 (10%)
32	LHG	L	101[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.05	4 (7%)
28	PL9	d	404[A]	-	55,55,55	0.70	1 (1%)	68,69,69	1.63	18 (26%)
25	GOL	l	801[A]	-	5,5,5	0.93	0	5,5,5	0.98	0
24	BCR	T	102	-	41,41,41	1.01	1 (2%)	56,56,56	1.55	11 (19%)
33	LMG	C	521	-	51,51,55	0.97	2 (3%)	59,59,63	1.16	4 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	602	2	-	12/39/115/115	-
25	GOL	a	418	-	-	2/4/4/4	-
23	CLA	b	604	2	-	12/39/115/115	-
24	BCR	A	408	-	-	0/29/63/63	0/2/2/2
32	LHG	d	406[A]	-	-	13/53/53/53	-
23	CLA	b	616	2	-	10/39/115/115	-
25	GOL	c	528	-	-	2/4/4/4	-
31	LMT	m	103	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PHO	D	401[A]	-	-	3/37/103/103	0/5/6/6
23	CLA	a	409	1	-	9/39/115/115	-
23	CLA	D	404[A]	4	-	2/39/115/115	-
23	CLA	d	402	4	-	8/39/115/115	-
26	SQD	C	501[B]	-	-	9/49/69/69	0/1/1/1
26	SQD	a	412	-	-	14/49/69/69	0/1/1/1
25	GOL	o	302	-	-	2/4/4/4	-
28	PL9	D	407[A]	-	-	6/53/73/73	0/1/1/1
35	DGD	c	518[A]	-	-	16/51/91/95	0/2/2/2
33	LMG	C	502	-	-	15/46/66/70	0/1/1/1
33	LMG	z	101	-	-	10/34/54/70	0/1/1/1
25	GOL	D	414	-	-	4/4/4/4	-
25	GOL	B	624	-	-	2/4/4/4	-
32	LHG	D	409[B]	-	-	13/53/53/53	-
23	CLA	B	616	2	-	7/39/115/115	-
28	PL9	A	412[B]	-	-	14/53/73/73	0/1/1/1
23	CLA	B	610	41	-	10/39/115/115	-
23	CLA	b	603	2	-	7/39/115/115	-
23	CLA	c	503	3	-	5/39/115/115	-
37	PHO	a	408[A]	-	-	6/37/103/103	0/5/6/6
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
33	LMG	a	417	-	-	14/46/66/70	0/1/1/1
32	LHG	a	420[A]	-	-	16/46/46/53	-
25	GOL	B	627	-	-	4/4/4/4	-
25	GOL	v	202[A]	-	-	2/4/4/4	-
23	CLA	B	606	2	-	6/39/115/115	-
25	GOL	b	624	-	-	2/4/4/4	-
34	HTG	C	523	-	-	0/10/30/30	0/1/1/1
31	LMT	M	101	-	-	5/21/61/61	0/2/2/2
24	BCR	t	103	-	-	1/29/63/63	0/2/2/2
31	LMT	B	630	-	-	11/21/61/61	0/2/2/2
25	GOL	O	303	-	-	2/4/4/4	-
23	CLA	c	511	3	-	12/39/115/115	-
23	CLA	B	607	41	-	3/39/115/115	-
32	LHG	E	101[A]	-	-	22/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	l	802[B]	-	-	15/53/53/53	-
25	GOL	C	524[A]	-	-	0/4/4/4	-
34	HTG	D	412	-	-	3/7/27/30	0/1/1/1
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1
32	LHG	L	101[A]	-	-	20/53/53/53	-
25	GOL	a	419	-	-	0/4/4/4	-
23	CLA	A	405[A]	41	-	3/39/115/115	-
23	CLA	C	513	3	-	4/39/115/115	-
23	CLA	c	510	3	-	15/39/115/115	-
25	GOL	D	403	-	-	2/4/4/4	-
26	SQD	A	410	-	-	15/49/69/69	0/1/1/1
37	PHO	a	416[B]	-	-	3/37/103/103	0/5/6/6
25	GOL	d	410	-	-	1/4/4/4	-
35	DGD	C	518[B]	-	-	14/51/91/95	0/2/2/2
24	BCR	B	617	-	-	2/29/63/63	0/2/2/2
25	GOL	A	409	-	-	2/4/4/4	-
23	CLA	C	504	3	-	8/39/115/115	-
35	DGD	c	519	-	-	11/51/91/95	0/2/2/2
23	CLA	b	609	2	-	1/39/115/115	-
35	DGD	C	520	-	-	23/51/91/95	0/2/2/2
24	BCR	y	101	-	-	6/29/63/63	0/2/2/2
23	CLA	c	508	41	-	8/39/115/115	-
33	LMG	c	520	-	-	11/46/66/70	0/1/1/1
31	LMT	F	101	-	-	8/21/61/61	0/2/2/2
23	CLA	B	614	2	-	15/39/115/115	-
23	CLA	C	508	3	-	11/39/115/115	-
26	SQD	C	501[A]	-	-	12/49/69/69	0/1/1/1
23	CLA	C	512	3	-	14/39/115/115	-
25	GOL	V	204[B]	-	-	3/4/4/4	-
23	CLA	B	605	2	-	6/39/115/115	-
34	HTG	d	408	-	-	1/7/27/30	0/1/1/1
23	CLA	d	401[B]	4	-	4/39/115/115	-
32	LHG	D	409[A]	-	-	14/53/53/53	-
24	BCR	c	516	-	-	2/29/63/63	0/2/2/2
23	CLA	c	506	3	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PL9	A	412[A]	-	-	15/53/73/73	0/1/1/1
24	BCR	C	516	-	-	2/29/63/63	0/2/2/2
23	CLA	C	506	41	-	8/39/115/115	-
25	GOL	c	526[B]	-	-	0/4/4/4	-
33	LMG	d	409	39	-	8/46/66/70	0/1/1/1
23	CLA	c	513	3	-	14/39/115/115	-
35	DGD	h	102	-	-	13/51/91/95	0/2/2/2
24	BCR	K	102	-	-	2/29/63/63	0/2/2/2
25	GOL	b	628	-	-	0/4/4/4	-
24	BCR	b	618	-	-	0/29/63/63	0/2/2/2
24	BCR	h	101	-	-	2/29/63/63	0/2/2/2
23	CLA	b	601	41	-	19/39/115/115	-
26	SQD	a	411[B]	-	-	9/49/69/69	0/1/1/1
32	LHG	D	408[B]	-	-	19/53/53/53	-
32	LHG	d	411[B]	-	-	15/53/53/53	-
25	GOL	B	629	-	-	4/4/4/4	-
23	CLA	b	607	41	-	4/39/115/115	-
23	CLA	A	404[B]	1	-	6/39/115/115	-
23	CLA	b	610	41	-	7/39/115/115	-
23	CLA	C	507	3	-	6/39/115/115	-
32	LHG	l	802[A]	-	-	14/53/53/53	-
23	CLA	b	602	2	-	5/39/115/115	-
23	CLA	c	514	3	-	11/39/115/115	-
24	BCR	Y	101	-	-	3/29/63/63	0/2/2/2
35	DGD	C	519[B]	-	-	11/51/91/95	0/2/2/2
40	HEC	v	201	16	1/1/3/7	6/14/54/54	-
23	CLA	c	502	3	-	8/39/115/115	-
37	PHO	a	416[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	b	613	2	-	3/39/115/115	-
31	LMT	T	101	-	-	8/21/61/61	0/2/2/2
35	DGD	C	518[A]	-	-	14/51/91/95	0/2/2/2
38	HEM	F	102	5,6	-	6/14/54/54	-
31	LMT	t	101	-	-	11/17/37/61	0/1/1/2
26	SQD	f	102	-	-	15/38/58/69	0/1/1/1
23	CLA	c	505	41	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	615	2	-	8/39/115/115	-
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
34	HTG	c	522	-	-	1/10/30/30	0/1/1/1
34	HTG	b	623	-	-	3/10/30/30	0/1/1/1
24	BCR	b	617	-	-	2/29/63/63	0/2/2/2
24	BCR	c	515	-	-	2/29/63/63	0/2/2/2
25	GOL	V	204[A]	-	-	2/4/4/4	-
35	DGD	H	102	-	-	9/51/91/95	0/2/2/2
23	CLA	D	404[B]	4	-	3/39/115/115	-
31	LMT	c	501	-	-	10/21/61/61	0/2/2/2
23	CLA	b	614	2	-	12/39/115/115	-
23	CLA	d	401[A]	4	-	4/39/115/115	-
24	BCR	k	101	-	-	0/29/63/63	0/2/2/2
23	CLA	a	406[B]	41	-	6/39/115/115	-
34	HTG	B	625	-	-	4/10/30/30	0/1/1/1
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
26	SQD	B	620	-	-	16/49/69/69	0/1/1/1
32	LHG	A	416[B]	-	-	11/53/53/53	-
33	LMG	D	413	39	-	10/46/66/70	0/1/1/1
23	CLA	b	606	2	-	14/39/115/115	-
32	LHG	d	405[B]	-	-	13/53/53/53	-
25	GOL	c	526[A]	-	-	0/4/4/4	-
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
32	LHG	d	411[A]	-	-	17/53/53/53	-
25	GOL	c	527	-	-	3/4/4/4	-
26	SQD	a	411[A]	-	-	9/49/69/69	0/1/1/1
32	LHG	D	408[A]	-	-	17/53/53/53	-
31	LMT	A	415	-	-	8/21/61/61	0/2/2/2
23	CLA	C	505	3	-	4/39/115/115	-
26	SQD	F	103	-	-	13/38/58/69	0/1/1/1
23	CLA	B	615	2	-	6/39/115/115	-
24	BCR	a	410	-	-	3/29/63/63	0/2/2/2
23	CLA	c	509	3	-	5/39/115/115	-
23	CLA	C	514	3	-	9/39/115/115	-
23	CLA	a	407[B]	41	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	C	517	-	-	0/29/63/63	0/2/2/2
37	PHO	D	402[B]	-	-	1/37/103/103	0/5/6/6
23	CLA	a	405[B]	1	-	9/39/115/115	-
35	DGD	c	517[B]	-	-	18/51/91/95	0/2/2/2
23	CLA	C	509	41	-	9/39/115/115	-
23	CLA	A	406[B]	41	-	4/39/115/115	-
35	DGD	C	519[A]	-	-	13/51/91/95	0/2/2/2
23	CLA	c	512	3	-	6/39/115/115	-
24	BCR	H	101	-	-	2/29/63/63	0/2/2/2
33	LMG	m	101	-	-	16/46/66/70	0/1/1/1
23	CLA	B	608	2	-	4/39/115/115	-
28	PL9	a	414[B]	-	-	16/53/73/73	0/1/1/1
23	CLA	A	405[B]	41	-	7/39/115/115	-
23	CLA	C	510	3	-	7/39/115/115	-
25	GOL	l	801[B]	-	-	0/4/4/4	-
28	PL9	d	404[B]	-	-	8/53/73/73	0/1/1/1
25	GOL	O	302	-	-	2/4/4/4	-
23	CLA	b	605	2	-	7/39/115/115	-
33	LMG	C	522	-	-	13/46/66/70	0/1/1/1
34	HTG	b	625	-	-	4/10/30/30	0/1/1/1
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
23	CLA	b	608	2	-	6/39/115/115	-
32	LHG	d	406[B]	-	-	13/53/53/53	-
33	LMG	B	621	-	-	21/46/66/70	0/1/1/1
40	HEC	V	202	16	1/1/3/7	6/14/54/54	-
23	CLA	D	405	4	-	13/39/115/115	-
23	CLA	b	612	2	-	6/39/115/115	-
23	CLA	c	507	3	-	9/39/115/115	-
23	CLA	B	611	2	-	4/39/115/115	-
23	CLA	C	511	3	-	5/39/115/115	-
37	PHO	D	401[B]	-	-	6/37/103/103	0/5/6/6
23	CLA	a	406[A]	41	-	8/39/115/115	-
32	LHG	A	416[A]	-	-	14/53/53/53	-
24	BCR	b	619	-	-	4/29/63/63	0/2/2/2
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	b	621	-	-	9/17/37/61	0/1/1/2
31	LMT	e	101	-	-	13/21/61/61	0/2/2/2
32	LHG	d	405[A]	-	-	13/53/53/53	-
28	PL9	D	407[B]	-	-	7/53/73/73	0/1/1/1
34	HTG	B	623	-	-	3/10/30/30	0/1/1/1
35	DGD	c	518[B]	-	-	15/51/91/95	0/2/2/2
31	LMT	B	628	-	-	12/21/61/61	0/2/2/2
23	CLA	B	612	2	-	4/39/115/115	-
23	CLA	B	601	41	-	13/39/115/115	-
23	CLA	C	503	3	-	4/39/115/115	-
23	CLA	B	604	2	-	5/39/115/115	-
37	PHO	a	408[B]	-	-	5/37/103/103	0/5/6/6
23	CLA	B	609	2	-	1/39/115/115	-
23	CLA	a	407[A]	41	-	8/39/115/115	-
31	LMT	A	417	-	-	16/21/61/61	0/2/2/2
32	LHG	a	420[B]	-	-	15/46/46/53	-
23	CLA	c	504	3	-	4/39/115/115	-
37	PHO	D	402[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	a	405[A]	1	-	4/39/115/115	-
25	GOL	v	202[B]	-	-	2/4/4/4	-
35	DGD	c	517[A]	-	-	18/51/91/95	0/2/2/2
38	HEM	f	101	5,6	-	8/14/54/54	-
23	CLA	A	406[A]	41	-	5/39/115/115	-
24	BCR	d	403	-	-	4/29/63/63	0/2/2/2
23	CLA	A	404[A]	1	-	3/39/115/115	-
23	CLA	A	407	1	-	8/39/115/115	-
23	CLA	B	603	2	-	3/39/115/115	-
23	CLA	b	611	2	-	2/39/115/115	-
24	BCR	D	406	-	-	5/29/63/63	0/2/2/2
31	LMT	t	102	-	-	9/17/38/61	0/1/1/2
23	CLA	C	515	3	-	7/39/115/115	-
32	LHG	E	101[B]	-	-	22/46/46/53	-
28	PL9	a	414[A]	-	-	14/53/73/73	0/1/1/1
25	GOL	C	524[B]	-	-	0/4/4/4	-
33	LMG	C	526	-	-	11/31/51/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	613	2	-	7/39/115/115	-
33	LMG	c	521	-	-	11/46/66/70	0/1/1/1
32	LHG	L	101[B]	-	-	18/53/53/53	-
28	PL9	d	404[A]	-	-	7/53/73/73	0/1/1/1
25	GOL	l	801[A]	-	-	1/4/4/4	-
24	BCR	T	102	-	-	1/29/63/63	0/2/2/2
33	LMG	C	521	-	-	10/46/66/70	0/1/1/1

All (1888) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	a	408[A]	PHO	C1B-C2B	9.21	1.49	1.39
37	a	416[B]	PHO	C1B-C2B	9.12	1.49	1.39
37	D	401[B]	PHO	C1D-C2D	9.09	1.49	1.39
37	D	402[B]	PHO	C1B-C2B	8.96	1.49	1.39
37	D	401[A]	PHO	C1D-C2D	8.89	1.49	1.39
37	a	408[B]	PHO	C1D-C2D	8.85	1.49	1.39
37	D	401[B]	PHO	C1B-C2B	8.77	1.49	1.39
37	a	408[B]	PHO	C1B-C2B	8.75	1.49	1.39
37	a	416[A]	PHO	C1B-C2B	8.69	1.49	1.39
37	a	416[B]	PHO	C1D-C2D	8.68	1.49	1.39
37	D	402[A]	PHO	C1B-C2B	8.65	1.49	1.39
37	a	416[A]	PHO	C1D-C2D	8.62	1.49	1.39
37	D	402[A]	PHO	C1D-C2D	8.53	1.49	1.39
37	D	401[A]	PHO	C1B-C2B	8.45	1.48	1.39
37	a	408[A]	PHO	C1D-C2D	8.40	1.48	1.39
37	D	402[B]	PHO	C1D-C2D	8.22	1.48	1.39
40	v	201	HEC	C3D-C2D	7.93	1.53	1.36
37	D	402[B]	PHO	C3B-C4B	7.72	1.50	1.41
37	a	416[A]	PHO	C3B-C4B	7.31	1.49	1.41
37	D	402[A]	PHO	C3B-C4B	7.11	1.49	1.41
40	V	202	HEC	C3D-C2D	7.02	1.51	1.36
23	B	611	CLA	CMB-C2B	6.75	1.65	1.50
23	B	611	CLA	C1B-C2B	6.71	1.59	1.43
37	a	408[A]	PHO	C3B-C4B	6.66	1.49	1.41
37	a	408[B]	PHO	C3B-C4B	6.64	1.49	1.41
37	a	416[B]	PHO	C3B-C4B	6.57	1.49	1.41
37	a	408[A]	PHO	C4D-CHA	6.54	1.50	1.39
23	B	611	CLA	C1D-ND	6.49	1.45	1.37
37	D	402[B]	PHO	C4D-CHA	6.42	1.49	1.39
37	a	416[B]	PHO	C4D-CHA	6.41	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	a	408[A]	PHO	C3B-C2B	6.39	1.49	1.40
37	D	401[B]	PHO	C3B-C4B	6.34	1.48	1.41
37	D	402[A]	PHO	C4D-CHA	6.27	1.49	1.39
37	D	401[B]	PHO	C4D-CHA	6.24	1.49	1.39
37	D	402[B]	PHO	C3B-C2B	6.24	1.49	1.40
37	D	402[B]	PHO	C3C-C2C	6.23	1.50	1.36
37	a	408[B]	PHO	C4D-CHA	6.21	1.49	1.39
37	a	416[B]	PHO	C3B-C2B	6.17	1.48	1.40
37	D	401[A]	PHO	C3B-C4B	6.16	1.48	1.41
37	D	401[A]	PHO	C4D-CHA	6.13	1.49	1.39
37	D	401[A]	PHO	C3B-C2B	6.13	1.48	1.40
37	a	408[B]	PHO	C3B-C2B	6.08	1.48	1.40
37	a	416[A]	PHO	C4D-CHA	6.05	1.49	1.39
37	a	416[B]	PHO	C3C-C2C	6.02	1.49	1.36
37	D	401[B]	PHO	C3B-C2B	5.97	1.48	1.40
37	D	402[A]	PHO	C3B-C2B	5.94	1.48	1.40
37	a	416[A]	PHO	C3B-C2B	5.88	1.48	1.40
37	a	416[A]	PHO	C3C-C2C	5.86	1.49	1.36
37	a	416[B]	PHO	C3D-C2D	5.82	1.49	1.39
23	B	611	CLA	C3C-C2C	5.81	1.49	1.36
23	B	605	CLA	C3C-C2C	5.80	1.49	1.36
37	D	402[A]	PHO	C3C-C2C	5.72	1.48	1.36
37	D	401[A]	PHO	C3C-C2C	5.71	1.48	1.36
23	b	605	CLA	C3C-C2C	5.67	1.48	1.36
23	c	513	CLA	C3C-C2C	5.65	1.48	1.36
23	A	404[B]	CLA	C1D-ND	5.64	1.44	1.37
23	C	514	CLA	C3C-C2C	5.60	1.48	1.36
37	D	402[B]	PHO	C3D-C2D	5.60	1.49	1.39
23	B	610	CLA	C3C-C2C	5.59	1.48	1.36
23	B	610	CLA	C1D-ND	5.59	1.44	1.37
23	c	509	CLA	O2D-CGD	5.59	1.46	1.33
23	C	512	CLA	C1D-ND	5.58	1.44	1.37
23	a	406[A]	CLA	C3C-C2C	5.58	1.48	1.36
23	b	601	CLA	C3C-C2C	5.57	1.48	1.36
23	a	406[B]	CLA	C3C-C2C	5.56	1.48	1.36
23	B	604	CLA	C3C-C2C	5.55	1.48	1.36
23	c	509	CLA	C3C-C2C	5.54	1.48	1.36
23	C	504	CLA	C1D-ND	5.53	1.44	1.37
37	a	408[B]	PHO	C3C-C2C	5.51	1.48	1.36
23	C	510	CLA	C3C-C2C	5.50	1.48	1.36
23	d	402	CLA	C3C-C2C	5.50	1.48	1.36
23	c	506	CLA	C3C-C2C	5.49	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D	401[B]	PHO	C3C-C2C	5.49	1.48	1.36
23	a	407[B]	CLA	C3C-C2C	5.49	1.48	1.36
23	c	504	CLA	C3C-C2C	5.48	1.48	1.36
23	d	402	CLA	C1D-ND	5.48	1.44	1.37
23	d	401[B]	CLA	C3C-C2C	5.48	1.48	1.36
23	C	511	CLA	C3C-C2C	5.47	1.48	1.36
23	a	405[B]	CLA	C3C-C2C	5.46	1.48	1.36
37	a	416[A]	PHO	C3D-C2D	5.46	1.49	1.39
23	b	601	CLA	C1D-ND	5.46	1.44	1.37
23	D	404[B]	CLA	C3C-C2C	5.46	1.48	1.36
37	a	408[A]	PHO	C3D-C2D	5.46	1.49	1.39
23	b	614	CLA	C3C-C2C	5.45	1.48	1.36
23	D	405	CLA	C3C-C2C	5.44	1.48	1.36
23	A	404[A]	CLA	C3C-C2C	5.43	1.48	1.36
23	b	607	CLA	C3C-C2C	5.42	1.48	1.36
23	a	406[A]	CLA	C1D-ND	5.42	1.44	1.37
23	a	406[B]	CLA	C1D-ND	5.41	1.44	1.37
23	b	615	CLA	C3C-C2C	5.40	1.48	1.36
23	c	505	CLA	C1D-ND	5.38	1.44	1.37
23	A	406[B]	CLA	C3C-C2C	5.38	1.48	1.36
23	c	511	CLA	O2D-CGD	5.38	1.46	1.33
23	b	612	CLA	C3C-C2C	5.37	1.48	1.36
23	c	514	CLA	C1D-ND	5.37	1.44	1.37
23	C	505	CLA	C3C-C2C	5.37	1.48	1.36
23	c	512	CLA	C1D-ND	5.37	1.44	1.37
23	B	602	CLA	C3C-C2C	5.36	1.48	1.36
37	a	408[A]	PHO	C3C-C2C	5.36	1.48	1.36
23	B	601	CLA	C3C-C2C	5.35	1.48	1.36
23	D	405	CLA	C1D-ND	5.35	1.44	1.37
23	b	609	CLA	O2D-CGD	5.35	1.46	1.33
23	b	616	CLA	C1D-ND	5.34	1.44	1.37
23	B	614	CLA	C3C-C2C	5.34	1.48	1.36
37	D	402[A]	PHO	C3D-C2D	5.33	1.49	1.39
23	a	409	CLA	C3C-C2C	5.32	1.48	1.36
23	c	514	CLA	C3C-C2C	5.32	1.48	1.36
23	a	407[A]	CLA	C3C-C2C	5.31	1.48	1.36
23	D	404[A]	CLA	C3C-C2C	5.30	1.48	1.36
37	a	416[A]	PHO	OBD-CAD	5.30	1.29	1.22
23	B	605	CLA	O2D-CGD	5.29	1.46	1.33
37	D	402[A]	PHO	OBD-CAD	5.28	1.29	1.22
23	c	504	CLA	C1D-ND	5.27	1.44	1.37
37	a	408[B]	PHO	C3D-C2D	5.27	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	405[B]	CLA	C1D-ND	5.26	1.44	1.37
23	B	609	CLA	CHC-C1C	5.26	1.49	1.38
23	b	603	CLA	C3C-C2C	5.26	1.47	1.36
23	C	509	CLA	CHC-C1C	5.24	1.49	1.38
23	b	606	CLA	C3C-C2C	5.24	1.47	1.36
37	a	408[A]	PHO	O2D-CGD	5.24	1.46	1.33
23	c	513	CLA	C1D-ND	5.23	1.44	1.37
23	A	404[B]	CLA	C3C-C2C	5.22	1.47	1.36
23	A	406[B]	CLA	C1D-ND	5.21	1.44	1.37
23	B	616	CLA	C3C-C2C	5.20	1.47	1.36
23	B	606	CLA	C1D-ND	5.20	1.44	1.37
23	b	602	CLA	C3C-C2C	5.19	1.47	1.36
23	b	610	CLA	C3C-C2C	5.19	1.47	1.36
23	c	510	CLA	C3C-C2C	5.18	1.47	1.36
23	A	405[B]	CLA	C1D-ND	5.18	1.44	1.37
23	C	515	CLA	C1D-ND	5.17	1.44	1.37
23	B	615	CLA	O2D-CGD	5.16	1.45	1.33
23	B	603	CLA	C3C-C2C	5.16	1.47	1.36
23	A	405[B]	CLA	C3C-C2C	5.16	1.47	1.36
23	c	512	CLA	C3C-C2C	5.15	1.47	1.36
23	A	405[A]	CLA	O2D-CGD	5.14	1.45	1.33
23	a	409	CLA	CHC-C1C	5.14	1.49	1.38
23	A	406[A]	CLA	C3C-C2C	5.13	1.47	1.36
23	b	603	CLA	O2D-CGD	5.13	1.45	1.33
23	a	405[A]	CLA	C1D-ND	5.13	1.44	1.37
23	A	404[A]	CLA	C1D-ND	5.13	1.44	1.37
23	c	511	CLA	C3C-C2C	5.12	1.47	1.36
23	C	515	CLA	C3C-C2C	5.12	1.47	1.36
23	b	610	CLA	CHC-C1C	5.12	1.48	1.38
23	b	602	CLA	CHC-C1C	5.12	1.48	1.38
23	b	609	CLA	C3C-C2C	5.11	1.47	1.36
23	c	511	CLA	C1D-ND	5.11	1.44	1.37
23	B	606	CLA	C3C-C2C	5.10	1.47	1.36
23	D	404[B]	CLA	O2D-CGD	5.09	1.45	1.33
23	C	512	CLA	C3C-C2C	5.09	1.47	1.36
23	d	401[A]	CLA	C3C-C2C	5.09	1.47	1.36
23	B	601	CLA	O2A-CGA	5.08	1.48	1.33
23	c	510	CLA	O2D-CGD	5.08	1.45	1.33
23	B	613	CLA	O2D-CGD	5.08	1.45	1.33
23	c	514	CLA	O2D-CGD	5.07	1.45	1.33
23	B	608	CLA	C3C-C2C	5.07	1.47	1.36
23	b	606	CLA	C1D-ND	5.06	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	f	101	HEM	FE-NB	5.06	2.10	1.94
23	C	508	CLA	C3C-C2C	5.05	1.47	1.36
23	b	616	CLA	C3C-C2C	5.05	1.47	1.36
23	c	503	CLA	C3C-C2C	5.05	1.47	1.36
23	B	606	CLA	CHC-C1C	5.05	1.48	1.38
24	C	516	BCR	C23-C22	-5.04	1.35	1.45
23	B	611	CLA	CHC-C1C	5.03	1.48	1.38
23	A	407	CLA	C3C-C2C	5.03	1.47	1.36
23	C	508	CLA	O2D-CGD	5.03	1.45	1.33
23	C	510	CLA	O2D-CGD	5.03	1.45	1.33
23	b	613	CLA	C3C-C2C	5.02	1.47	1.36
23	a	405[A]	CLA	C3C-C2C	5.02	1.47	1.36
23	C	504	CLA	O2D-CGD	5.02	1.45	1.33
23	b	613	CLA	C1D-ND	5.02	1.44	1.37
23	A	406[B]	CLA	O2D-CGD	5.02	1.45	1.33
23	b	605	CLA	O2D-CGD	5.01	1.45	1.33
23	c	503	CLA	C1D-ND	5.01	1.43	1.37
37	D	402[B]	PHO	O2D-CGD	5.01	1.45	1.33
23	C	507	CLA	C3C-C2C	5.01	1.47	1.36
38	F	102	HEM	FE-NB	5.01	2.10	1.94
23	C	510	CLA	C1D-ND	5.00	1.43	1.37
23	A	404[B]	CLA	CHC-C1C	5.00	1.48	1.38
23	B	601	CLA	O2D-CGD	5.00	1.45	1.33
23	C	513	CLA	O2D-CGD	5.00	1.45	1.33
23	C	509	CLA	C3C-C2C	4.99	1.47	1.36
23	C	503	CLA	C3C-C2C	4.99	1.47	1.36
23	B	609	CLA	C3C-C2C	4.99	1.47	1.36
23	B	611	CLA	C4B-NB	-4.98	1.31	1.37
23	c	507	CLA	C1D-ND	4.98	1.43	1.37
23	c	506	CLA	CHC-C1C	4.98	1.48	1.38
23	C	514	CLA	CHC-C1C	4.97	1.48	1.38
37	D	402[B]	PHO	OBD-CAD	4.97	1.29	1.22
23	B	602	CLA	C1D-ND	4.96	1.43	1.37
37	a	408[B]	PHO	O2D-CGD	4.96	1.45	1.33
23	A	405[A]	CLA	C3C-C2C	4.96	1.47	1.36
23	b	609	CLA	CHC-C1C	4.96	1.48	1.38
23	c	502	CLA	C3C-C2C	4.95	1.47	1.36
23	a	407[B]	CLA	CHC-C1C	4.95	1.48	1.38
23	a	406[A]	CLA	O2D-CGD	4.95	1.45	1.33
37	D	402[A]	PHO	O2D-CGD	4.95	1.45	1.33
23	D	405	CLA	CHD-C1D	4.95	1.48	1.38
23	A	406[A]	CLA	CHC-C1C	4.95	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	O2D-CGD	4.94	1.45	1.33
23	b	604	CLA	C3C-C2C	4.94	1.47	1.36
23	c	502	CLA	C1D-ND	4.94	1.43	1.37
23	c	513	CLA	CHC-C1C	4.94	1.48	1.38
37	a	416[B]	PHO	O2D-CGD	4.93	1.45	1.33
23	b	602	CLA	O2D-CGD	4.93	1.45	1.33
24	y	101	BCR	C23-C22	-4.93	1.35	1.45
23	b	614	CLA	C1D-ND	4.93	1.43	1.37
23	B	612	CLA	C3C-C2C	4.92	1.47	1.36
23	B	615	CLA	C3C-C2C	4.92	1.47	1.36
24	k	101	BCR	C23-C22	-4.92	1.35	1.45
23	b	601	CLA	O2D-CGD	4.92	1.45	1.33
24	d	403	BCR	C23-C22	-4.91	1.35	1.45
23	D	405	CLA	CHC-C1C	4.91	1.48	1.38
37	a	416[B]	PHO	OBD-CAD	4.91	1.29	1.22
23	C	511	CLA	O2D-CGD	4.91	1.45	1.33
23	A	404[B]	CLA	O2D-CGD	4.91	1.45	1.33
23	B	601	CLA	C1D-ND	4.91	1.43	1.37
37	D	401[A]	PHO	O2D-CGD	4.91	1.45	1.33
24	c	516	BCR	C23-C22	-4.90	1.35	1.45
23	a	405[B]	CLA	CHC-C1C	4.90	1.48	1.38
23	a	406[B]	CLA	O2D-CGD	4.90	1.45	1.33
40	v	201	HEC	FE-NB	4.89	2.10	1.94
23	B	613	CLA	C1D-ND	4.89	1.43	1.37
23	D	404[A]	CLA	O2D-CGD	4.88	1.45	1.33
23	A	406[B]	CLA	CHC-C1C	4.88	1.48	1.38
23	c	507	CLA	O2D-CGD	4.87	1.45	1.33
23	c	505	CLA	C3C-C2C	4.87	1.47	1.36
23	D	405	CLA	O2D-CGD	4.87	1.45	1.33
23	b	615	CLA	C1D-ND	4.87	1.43	1.37
23	C	514	CLA	C1D-ND	4.87	1.43	1.37
23	B	613	CLA	CHC-C1C	4.85	1.48	1.38
23	B	603	CLA	C1D-ND	4.85	1.43	1.37
23	C	503	CLA	CHC-C1C	4.85	1.48	1.38
23	c	509	CLA	CHC-C1C	4.85	1.48	1.38
23	c	505	CLA	O2D-CGD	4.85	1.45	1.33
23	b	615	CLA	O2D-CGD	4.84	1.45	1.33
37	a	416[A]	PHO	O2D-CGD	4.84	1.45	1.33
23	C	504	CLA	C3C-C2C	4.84	1.47	1.36
23	b	612	CLA	C1D-ND	4.84	1.43	1.37
23	c	504	CLA	CHC-C1C	4.84	1.48	1.38
23	c	504	CLA	CHD-C1D	4.84	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	408	BCR	C23-C22	-4.84	1.35	1.45
23	C	507	CLA	CHC-C1C	4.83	1.48	1.38
23	a	407[B]	CLA	O2D-CGD	4.83	1.45	1.33
24	K	102	BCR	C23-C22	-4.82	1.35	1.45
24	C	517	BCR	C23-C22	-4.82	1.35	1.45
23	B	615	CLA	C1D-ND	4.81	1.43	1.37
33	c	521	LMG	O7-C10	4.80	1.47	1.34
23	c	510	CLA	C1D-ND	4.80	1.43	1.37
23	B	610	CLA	CHC-C1C	4.79	1.48	1.38
37	D	401[A]	PHO	C3D-C2D	4.79	1.48	1.39
23	c	508	CLA	C3C-C2C	4.79	1.46	1.36
26	F	103	SQD	O47-C7	4.79	1.47	1.34
23	B	613	CLA	C3C-C2C	4.79	1.46	1.36
23	b	613	CLA	CHC-C1C	4.79	1.48	1.38
37	D	401[B]	PHO	C3D-C2D	4.79	1.48	1.39
23	b	616	CLA	O2D-CGD	4.79	1.44	1.33
23	B	605	CLA	C1D-ND	4.79	1.43	1.37
23	a	405[B]	CLA	O2D-CGD	4.78	1.44	1.33
23	C	515	CLA	O2D-CGD	4.78	1.44	1.33
23	b	616	CLA	CHC-C1C	4.78	1.48	1.38
23	A	407	CLA	O2D-CGD	4.78	1.44	1.33
23	c	509	CLA	C1D-ND	4.77	1.43	1.37
23	b	601	CLA	O2A-CGA	4.77	1.47	1.33
23	A	404[A]	CLA	O2D-CGD	4.77	1.44	1.33
23	b	611	CLA	C3C-C2C	4.77	1.46	1.36
23	B	601	CLA	CHC-C1C	4.77	1.48	1.38
23	b	608	CLA	O2D-CGD	4.76	1.44	1.33
37	D	401[B]	PHO	O2D-CGD	4.76	1.44	1.33
23	b	610	CLA	O2D-CGD	4.76	1.44	1.33
23	c	507	CLA	C3C-C2C	4.76	1.46	1.36
23	B	610	CLA	O2D-CGD	4.75	1.44	1.33
23	B	615	CLA	CHC-C1C	4.75	1.48	1.38
23	b	615	CLA	CHC-C1C	4.75	1.48	1.38
23	B	602	CLA	CHC-C1C	4.75	1.48	1.38
23	B	612	CLA	CHC-C1C	4.75	1.48	1.38
24	c	515	BCR	C23-C22	-4.75	1.35	1.45
23	C	512	CLA	CHC-C1C	4.73	1.48	1.38
23	A	406[A]	CLA	O2D-CGD	4.73	1.44	1.33
23	c	508	CLA	CHC-C1C	4.72	1.48	1.38
23	B	612	CLA	C1B-NB	-4.72	1.32	1.37
24	B	619	BCR	C23-C22	-4.72	1.35	1.45
37	D	401[B]	PHO	OBD-CAD	4.71	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401[B]	CLA	O2D-CGD	4.70	1.44	1.33
23	C	512	CLA	O2D-CGD	4.70	1.44	1.33
23	B	609	CLA	O2D-CGD	4.70	1.44	1.33
23	c	508	CLA	O2D-CGD	4.69	1.44	1.33
23	a	409	CLA	O2D-CGD	4.69	1.44	1.33
23	A	405[B]	CLA	CHC-C1C	4.69	1.48	1.38
23	b	602	CLA	CHD-C1D	4.67	1.47	1.38
23	b	614	CLA	CHC-C1C	4.67	1.48	1.38
23	C	507	CLA	C1D-ND	4.67	1.43	1.37
23	b	611	CLA	CHC-C1C	4.67	1.48	1.38
23	b	608	CLA	C3C-C2C	4.66	1.46	1.36
23	C	506	CLA	C3C-C2C	4.66	1.46	1.36
33	C	522	LMG	O7-C10	4.65	1.47	1.34
26	a	412	SQD	O48-C23	4.65	1.46	1.33
23	a	407[A]	CLA	O2D-CGD	4.65	1.44	1.33
24	T	102	BCR	C23-C22	-4.65	1.36	1.45
23	c	508	CLA	C1D-ND	4.64	1.43	1.37
23	a	405[A]	CLA	CHC-C1C	4.64	1.47	1.38
23	b	606	CLA	O2D-CGD	4.64	1.44	1.33
23	c	514	CLA	CHC-C1C	4.64	1.47	1.38
23	A	405[B]	CLA	O2D-CGD	4.63	1.44	1.33
23	d	402	CLA	CHC-C1C	4.63	1.47	1.38
24	b	619	BCR	C23-C22	-4.63	1.36	1.45
23	c	503	CLA	O2D-CGD	4.63	1.44	1.33
23	B	604	CLA	O2D-CGD	4.63	1.44	1.33
23	a	407[B]	CLA	C1D-ND	4.62	1.43	1.37
23	A	405[A]	CLA	CHC-C1C	4.61	1.47	1.38
23	C	505	CLA	CHC-C1C	4.61	1.47	1.38
23	a	407[A]	CLA	CHC-C1C	4.61	1.47	1.38
23	b	614	CLA	CHD-C1D	4.61	1.47	1.38
23	b	612	CLA	CHC-C1C	4.60	1.47	1.38
23	B	605	CLA	CHC-C1C	4.60	1.47	1.38
23	B	607	CLA	C3C-C2C	4.60	1.46	1.36
23	B	602	CLA	O2D-CGD	4.59	1.44	1.33
23	C	511	CLA	C1D-ND	4.59	1.43	1.37
23	C	514	CLA	O2D-CGD	4.59	1.44	1.33
23	d	401[A]	CLA	O2D-CGD	4.59	1.44	1.33
23	C	513	CLA	C3C-C2C	4.58	1.46	1.36
23	B	608	CLA	C1D-ND	4.58	1.43	1.37
23	B	602	CLA	CHD-C1D	4.58	1.47	1.38
23	b	601	CLA	CHC-C1C	4.58	1.47	1.38
23	B	603	CLA	O2D-CGD	4.58	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	t	103	BCR	C23-C22	-4.58	1.36	1.45
32	E	101[A]	LHG	O8-C23	4.57	1.46	1.33
33	z	101	LMG	O8-C28	4.57	1.46	1.33
37	a	408[B]	PHO	OBD-CAD	4.56	1.28	1.22
23	b	605	CLA	C1D-ND	4.56	1.43	1.37
23	c	514	CLA	CHD-C1D	4.56	1.47	1.38
23	A	405[A]	CLA	C1D-ND	4.55	1.43	1.37
23	b	611	CLA	C1D-ND	4.54	1.43	1.37
23	C	507	CLA	O2D-CGD	4.54	1.44	1.33
23	D	404[A]	CLA	CHC-C1C	4.54	1.47	1.38
23	c	512	CLA	CHD-C1D	4.54	1.47	1.38
24	h	101	BCR	C23-C22	-4.53	1.36	1.45
23	C	513	CLA	CHC-C1C	4.53	1.47	1.38
23	B	614	CLA	C1D-ND	4.52	1.43	1.37
23	c	507	CLA	CHD-C1D	4.52	1.47	1.38
23	B	616	CLA	CHC-C1C	4.52	1.47	1.38
23	b	602	CLA	C1D-ND	4.52	1.43	1.37
26	A	410	SQD	O48-C23	4.51	1.46	1.33
23	C	508	CLA	C1D-ND	4.51	1.43	1.37
23	B	604	CLA	CHD-C1D	4.51	1.47	1.38
23	C	504	CLA	CHC-C1C	4.51	1.47	1.38
23	B	615	CLA	CHD-C1D	4.51	1.47	1.38
32	a	420[A]	LHG	O8-C23	4.50	1.46	1.33
23	b	608	CLA	CHD-C1D	4.50	1.47	1.38
23	b	614	CLA	O2D-CGD	4.50	1.44	1.33
33	C	522	LMG	O8-C28	4.49	1.46	1.33
23	c	502	CLA	CHC-C1C	4.49	1.47	1.38
23	C	508	CLA	CHD-C1D	4.49	1.47	1.38
26	f	102	SQD	O47-C7	4.49	1.47	1.34
23	B	606	CLA	O2D-CGD	4.49	1.44	1.33
23	c	506	CLA	O2D-CGD	4.49	1.44	1.33
23	c	513	CLA	O2D-CGD	4.49	1.44	1.33
23	b	607	CLA	CHC-C1C	4.48	1.47	1.38
23	B	609	CLA	CHD-C1D	4.48	1.47	1.38
24	B	617	BCR	C23-C22	-4.48	1.36	1.45
23	b	607	CLA	C1B-NB	-4.48	1.32	1.37
23	b	606	CLA	CHC-C1C	4.48	1.47	1.38
23	b	605	CLA	CHC-C1C	4.48	1.47	1.38
23	a	407[A]	CLA	C1D-ND	4.48	1.43	1.37
23	C	509	CLA	O2D-CGD	4.48	1.44	1.33
23	A	404[A]	CLA	CHC-C1C	4.48	1.47	1.38
24	b	618	BCR	C23-C22	-4.48	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	C1D-ND	4.48	1.43	1.37
23	A	407	CLA	CHD-C1D	4.46	1.47	1.38
23	B	604	CLA	CHC-C1C	4.46	1.47	1.38
26	B	620	SQD	O47-C7	4.46	1.46	1.34
23	C	510	CLA	CHC-C1C	4.45	1.47	1.38
23	C	506	CLA	O2D-CGD	4.45	1.44	1.33
23	b	612	CLA	O2D-CGD	4.45	1.44	1.33
23	b	607	CLA	O2D-CGD	4.45	1.44	1.33
23	d	401[B]	CLA	CHC-C1C	4.45	1.47	1.38
23	C	503	CLA	C1D-ND	4.44	1.43	1.37
23	a	406[A]	CLA	CHC-C1C	4.44	1.47	1.38
23	C	506	CLA	CHC-C1C	4.44	1.47	1.38
23	c	502	CLA	CHD-C1D	4.44	1.47	1.38
26	b	620	SQD	O48-C23	4.43	1.46	1.33
23	c	514	CLA	O2A-CGA	4.43	1.46	1.33
23	a	406[B]	CLA	C3D-C2D	4.43	1.51	1.39
24	D	406	BCR	C23-C22	-4.42	1.36	1.45
23	D	404[B]	CLA	CHC-C1C	4.42	1.47	1.38
32	E	101[B]	LHG	O8-C23	4.42	1.46	1.33
23	c	512	CLA	CHB-C1B	4.42	1.49	1.39
26	b	620	SQD	O47-C7	4.41	1.46	1.34
23	B	604	CLA	CHB-C1B	4.41	1.49	1.39
24	b	617	BCR	C23-C22	-4.40	1.36	1.45
23	C	511	CLA	CHD-C1D	4.40	1.46	1.38
23	B	611	CLA	OBD-CAD	4.40	1.30	1.22
23	c	512	CLA	CHC-C1C	4.39	1.47	1.38
23	b	612	CLA	CHB-C1B	4.39	1.49	1.39
23	B	607	CLA	O2D-CGD	4.39	1.43	1.33
23	d	402	CLA	O2A-CGA	4.39	1.46	1.33
26	f	102	SQD	O48-C23	4.39	1.46	1.33
26	A	410	SQD	O47-C7	4.38	1.46	1.34
23	a	405[A]	CLA	O2D-CGD	4.38	1.43	1.33
23	B	616	CLA	O2D-CGD	4.38	1.43	1.33
23	B	604	CLA	C1D-ND	4.38	1.43	1.37
23	b	602	CLA	CHC-C4B	4.37	1.49	1.39
23	A	407	CLA	O2A-CGA	4.37	1.46	1.33
23	C	515	CLA	CHC-C1C	4.37	1.47	1.38
23	b	604	CLA	C1D-ND	4.37	1.43	1.37
23	C	505	CLA	O2D-CGD	4.37	1.43	1.33
23	C	503	CLA	CHD-C1D	4.36	1.46	1.38
32	a	420[B]	LHG	O8-C23	4.36	1.46	1.33
23	C	505	CLA	C1D-ND	4.36	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	CHC-C1C	4.35	1.47	1.38
23	a	406[B]	CLA	CHC-C1C	4.34	1.47	1.38
23	C	511	CLA	CHC-C1C	4.34	1.47	1.38
24	a	410	BCR	C23-C22	-4.34	1.36	1.45
23	b	603	CLA	CHC-C1C	4.34	1.47	1.38
23	A	406[A]	CLA	C1B-NB	-4.33	1.32	1.37
23	b	613	CLA	O2D-CGD	4.33	1.43	1.33
23	c	513	CLA	O2A-CGA	4.33	1.46	1.33
23	C	513	CLA	C1D-ND	4.33	1.43	1.37
33	C	521	LMG	O8-C28	4.33	1.46	1.33
23	d	402	CLA	CHD-C1D	4.33	1.46	1.38
40	V	202	HEC	FE-ND	4.33	2.08	1.94
23	c	510	CLA	CHD-C1D	4.33	1.46	1.38
23	a	409	CLA	O2A-CGA	4.32	1.46	1.33
24	H	101	BCR	C23-C22	-4.32	1.36	1.45
23	b	612	CLA	CHD-C1D	4.32	1.46	1.38
23	b	604	CLA	CHC-C1C	4.32	1.47	1.38
23	b	609	CLA	C1D-ND	4.32	1.43	1.37
23	b	609	CLA	OBD-CAD	4.31	1.29	1.22
23	B	614	CLA	CHC-C1C	4.31	1.47	1.38
23	c	505	CLA	CHC-C1C	4.31	1.47	1.38
23	a	406[A]	CLA	C3D-C2D	4.30	1.50	1.39
23	C	514	CLA	CHD-C1D	4.30	1.46	1.38
23	C	508	CLA	CHC-C1C	4.30	1.47	1.38
23	B	611	CLA	CHC-C4B	4.30	1.49	1.39
23	c	506	CLA	C1D-ND	4.29	1.43	1.37
23	B	616	CLA	C1D-ND	4.28	1.43	1.37
32	a	420[A]	LHG	O7-C7	4.28	1.46	1.34
23	B	611	CLA	CHD-C1D	4.28	1.46	1.38
23	A	406[B]	CLA	CHD-C1D	4.28	1.46	1.38
23	C	509	CLA	C1D-ND	4.28	1.43	1.37
23	B	611	CLA	O2D-CGD	4.28	1.43	1.33
23	A	405[B]	CLA	O2A-CGA	4.28	1.45	1.33
23	c	507	CLA	CHC-C1C	4.27	1.47	1.38
23	D	404[B]	CLA	O2A-CGA	4.27	1.45	1.33
33	c	521	LMG	O8-C28	4.27	1.45	1.33
23	A	407	CLA	CHC-C1C	4.27	1.47	1.38
23	b	607	CLA	CHD-C1D	4.26	1.46	1.38
23	c	513	CLA	CHD-C1D	4.26	1.46	1.38
23	b	611	CLA	O2D-CGD	4.26	1.43	1.33
23	C	504	CLA	C3D-C2D	4.26	1.50	1.39
23	c	508	CLA	CHD-C1D	4.26	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	O2A-CGA	4.25	1.45	1.33
23	C	510	CLA	C3D-C2D	4.25	1.50	1.39
23	D	404[A]	CLA	C1D-ND	4.25	1.43	1.37
23	d	401[B]	CLA	C1D-ND	4.25	1.43	1.37
23	b	611	CLA	O2A-CGA	4.24	1.45	1.33
23	d	401[B]	CLA	O2A-CGA	4.24	1.45	1.33
23	B	615	CLA	O2A-CGA	4.23	1.45	1.33
33	c	520	LMG	O7-C10	4.23	1.46	1.34
23	D	404[B]	CLA	C1D-ND	4.23	1.43	1.37
23	c	502	CLA	O2D-CGD	4.23	1.43	1.33
23	b	604	CLA	O2D-CGD	4.23	1.43	1.33
23	B	611	CLA	C1C-C2C	4.22	1.52	1.44
26	a	412	SQD	O47-C7	4.22	1.46	1.34
32	E	101[A]	LHG	O7-C7	4.22	1.46	1.34
23	d	401[A]	CLA	CHC-C1C	4.21	1.47	1.38
23	C	504	CLA	CHD-C1D	4.20	1.46	1.38
23	B	606	CLA	CHB-C1B	4.20	1.48	1.39
23	b	608	CLA	C1D-ND	4.20	1.42	1.37
23	C	512	CLA	CHD-C4C	4.20	1.48	1.39
32	d	406[A]	LHG	O8-C23	4.19	1.45	1.33
23	c	506	CLA	CHD-C4C	4.19	1.48	1.39
23	c	505	CLA	C3D-C2D	4.19	1.50	1.39
23	c	503	CLA	O2A-CGA	4.19	1.45	1.33
23	C	507	CLA	CHD-C1D	4.19	1.46	1.38
23	D	404[A]	CLA	CHD-C1D	4.19	1.46	1.38
23	a	406[B]	CLA	O2A-CGA	4.19	1.45	1.33
23	d	401[B]	CLA	CHD-C1D	4.19	1.46	1.38
33	m	101	LMG	O8-C28	4.18	1.45	1.33
23	c	514	CLA	CHD-C4C	4.18	1.48	1.39
23	b	609	CLA	CHD-C1D	4.18	1.46	1.38
23	b	610	CLA	C1D-ND	4.18	1.42	1.37
23	B	603	CLA	C1B-NB	-4.18	1.32	1.37
26	B	620	SQD	O48-C23	4.18	1.45	1.33
23	D	404[A]	CLA	O2A-CGA	4.18	1.45	1.33
23	C	515	CLA	CHD-C1D	4.18	1.46	1.38
23	c	506	CLA	CHD-C1D	4.18	1.46	1.38
35	C	520	DGD	O1G-C1A	4.17	1.45	1.33
32	d	406[B]	LHG	O8-C23	4.17	1.45	1.33
23	c	509	CLA	C3D-C2D	4.17	1.50	1.39
24	Y	101	BCR	C23-C22	-4.17	1.37	1.45
23	b	610	CLA	CHC-C4B	4.17	1.48	1.39
23	c	511	CLA	CHC-C1C	4.17	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	521	LMG	O7-C10	4.17	1.46	1.34
23	b	605	CLA	C1B-NB	-4.17	1.32	1.37
23	B	612	CLA	CHD-C1D	4.17	1.46	1.38
23	b	601	CLA	CHD-C1D	4.17	1.46	1.38
35	c	518[B]	DGD	O1G-C1A	4.16	1.45	1.33
23	C	515	CLA	O2A-CGA	4.16	1.45	1.33
23	B	601	CLA	CHC-C4B	4.16	1.48	1.39
23	b	602	CLA	CHD-C4C	4.16	1.48	1.39
26	a	411[B]	SQD	O47-C7	4.16	1.46	1.34
23	b	611	CLA	CHB-C1B	4.15	1.48	1.39
23	C	509	CLA	CHD-C1D	4.15	1.46	1.38
23	c	510	CLA	O2A-CGA	4.14	1.45	1.33
32	a	420[B]	LHG	O7-C7	4.14	1.46	1.34
33	B	621	LMG	O8-C28	4.14	1.45	1.33
35	c	519	DGD	O1G-C1A	4.14	1.45	1.33
23	B	614	CLA	CHC-C4B	4.13	1.48	1.39
35	C	518[A]	DGD	O2G-C1B	4.13	1.46	1.34
23	b	615	CLA	CHD-C1D	4.13	1.46	1.38
37	D	401[A]	PHO	OBD-CAD	4.13	1.28	1.22
23	a	405[B]	CLA	CHD-C1D	4.13	1.46	1.38
23	C	511	CLA	C4B-NB	-4.13	1.32	1.37
23	C	503	CLA	O2D-CGD	4.13	1.43	1.33
32	L	101[B]	LHG	O8-C23	4.13	1.45	1.33
23	B	614	CLA	O2D-CGD	4.13	1.43	1.33
23	a	406[B]	CLA	CHD-C1D	4.13	1.46	1.38
23	C	513	CLA	CHB-C1B	4.13	1.48	1.39
23	c	509	CLA	O2A-CGA	4.12	1.45	1.33
33	C	526	LMG	O7-C10	4.12	1.45	1.34
23	B	614	CLA	O2A-CGA	4.12	1.45	1.33
26	F	103	SQD	O48-C23	4.12	1.45	1.33
26	a	411[B]	SQD	O48-C23	4.12	1.45	1.33
23	b	608	CLA	CHB-C1B	4.12	1.48	1.39
23	a	406[A]	CLA	O2A-CGA	4.12	1.45	1.33
23	A	406[B]	CLA	O2A-CGA	4.12	1.45	1.33
23	b	603	CLA	OBD-CAD	4.12	1.29	1.22
23	c	504	CLA	CHD-C4C	4.12	1.48	1.39
23	B	608	CLA	CHC-C1C	4.11	1.46	1.38
23	A	406[B]	CLA	CHD-C4C	4.11	1.48	1.39
23	a	405[A]	CLA	CHD-C1D	4.11	1.46	1.38
23	B	602	CLA	CHB-C1B	4.11	1.48	1.39
23	a	407[B]	CLA	O2A-CGA	4.11	1.45	1.33
33	d	409	LMG	O8-C28	4.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	O2A-CGA	4.11	1.45	1.33
23	c	512	CLA	O2A-CGA	4.11	1.45	1.33
23	a	406[A]	CLA	C1B-NB	-4.11	1.32	1.37
38	F	102	HEM	FE-NC	4.11	2.09	1.95
35	c	517[B]	DGD	O2G-C1B	4.11	1.45	1.34
23	A	406[A]	CLA	CHD-C1D	4.10	1.46	1.38
23	A	407	CLA	C1D-ND	4.10	1.42	1.37
23	C	514	CLA	O2A-CGA	4.10	1.45	1.33
23	A	405[A]	CLA	C3D-C2D	4.10	1.50	1.39
38	f	101	HEM	FE-NC	4.10	2.09	1.95
32	D	409[B]	LHG	O7-C7	4.10	1.45	1.34
23	c	508	CLA	O2A-CGA	4.10	1.45	1.33
23	a	405[A]	CLA	CHD-C4C	4.10	1.48	1.39
23	c	504	CLA	O2D-CGD	4.09	1.43	1.33
23	D	405	CLA	CHB-C1B	4.09	1.48	1.39
33	c	520	LMG	O8-C28	4.09	1.45	1.33
23	A	406[A]	CLA	C1D-ND	4.09	1.42	1.37
23	C	512	CLA	CHB-C1B	4.09	1.48	1.39
23	c	513	CLA	CHB-C1B	4.09	1.48	1.39
23	C	513	CLA	CHD-C1D	4.09	1.46	1.38
23	A	405[B]	CLA	C3D-C2D	4.08	1.50	1.39
23	B	609	CLA	O2A-CGA	4.08	1.45	1.33
23	b	614	CLA	C3D-C2D	4.08	1.50	1.39
23	b	601	CLA	C3D-C2D	4.08	1.50	1.39
23	B	614	CLA	C4B-NB	-4.08	1.32	1.37
33	a	417	LMG	O7-C10	4.07	1.45	1.34
23	a	405[B]	CLA	CHD-C4C	4.07	1.48	1.39
23	A	405[A]	CLA	O2A-CGA	4.07	1.45	1.33
23	C	509	CLA	O2A-CGA	4.07	1.45	1.33
35	c	517[B]	DGD	O1G-C1A	4.07	1.45	1.33
32	E	101[B]	LHG	O7-C7	4.07	1.45	1.34
23	c	509	CLA	CHD-C1D	4.07	1.46	1.38
23	C	513	CLA	C3D-C2D	4.07	1.50	1.39
32	d	411[B]	LHG	O8-C23	4.07	1.45	1.33
23	a	409	CLA	CHD-C1D	4.06	1.46	1.38
23	D	405	CLA	C3D-C2D	4.06	1.50	1.39
23	D	405	CLA	CHC-C4B	4.06	1.48	1.39
23	C	507	CLA	CHB-C1B	4.06	1.48	1.39
23	C	507	CLA	CHC-C4B	4.06	1.48	1.39
23	c	513	CLA	CHC-C4B	4.05	1.48	1.39
23	C	508	CLA	O2A-CGA	4.05	1.45	1.33
23	C	510	CLA	O2A-CGA	4.05	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	411[A]	SQD	O47-C7	4.05	1.45	1.34
23	a	407[B]	CLA	CHD-C1D	4.05	1.46	1.38
23	b	616	CLA	O2A-CGA	4.04	1.45	1.33
23	B	609	CLA	CHC-C4B	4.04	1.48	1.39
23	c	507	CLA	CHD-C4C	4.04	1.48	1.39
23	B	610	CLA	C3D-C2D	4.04	1.50	1.39
23	B	616	CLA	C3D-C2D	4.04	1.50	1.39
23	B	613	CLA	C1B-NB	-4.04	1.32	1.37
23	B	610	CLA	OBD-CAD	4.04	1.29	1.22
23	b	606	CLA	CHD-C1D	4.04	1.46	1.38
33	a	417	LMG	O8-C28	4.03	1.45	1.33
23	B	604	CLA	OBD-CAD	4.03	1.29	1.22
23	b	604	CLA	CHD-C1D	4.03	1.46	1.38
23	B	611	CLA	C3B-C2B	4.03	1.54	1.41
23	A	406[B]	CLA	OBD-CAD	4.03	1.29	1.22
23	c	502	CLA	C3D-C2D	4.03	1.50	1.39
23	D	404[A]	CLA	CHB-C1B	4.02	1.48	1.39
23	c	509	CLA	CHD-C4C	4.02	1.48	1.39
23	B	612	CLA	CHB-C1B	4.02	1.48	1.39
23	C	515	CLA	C3D-C2D	4.02	1.50	1.39
32	d	405[B]	LHG	O7-C7	4.02	1.45	1.34
23	b	615	CLA	O2A-CGA	4.02	1.45	1.33
35	h	102	DGD	O2G-C1B	4.02	1.45	1.34
23	c	511	CLA	CHD-C4C	4.02	1.48	1.39
37	D	402[A]	PHO	O2A-CGA	4.02	1.45	1.33
23	b	608	CLA	CHC-C1C	4.02	1.46	1.38
23	B	611	CLA	O2A-CGA	4.02	1.45	1.33
23	a	405[A]	CLA	CHB-C1B	4.01	1.48	1.39
23	b	614	CLA	CHC-C4B	4.01	1.48	1.39
23	C	504	CLA	O2A-CGA	4.01	1.45	1.33
35	C	518[B]	DGD	O2G-C1B	4.01	1.45	1.34
23	C	503	CLA	C1B-NB	-4.01	1.32	1.37
35	c	518[A]	DGD	O1G-C1A	4.00	1.45	1.33
23	a	409	CLA	C1D-ND	4.00	1.42	1.37
23	A	404[B]	CLA	CHD-C1D	4.00	1.46	1.38
32	D	409[B]	LHG	O8-C23	4.00	1.45	1.33
23	C	505	CLA	CHD-C4C	4.00	1.48	1.39
23	b	601	CLA	CHD-C4C	4.00	1.48	1.39
23	c	510	CLA	CHD-C4C	4.00	1.48	1.39
23	b	609	CLA	O2A-CGA	4.00	1.45	1.33
23	C	513	CLA	CHD-C4C	4.00	1.48	1.39
23	c	511	CLA	CHB-C1B	4.00	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	C3D-C2D	3.99	1.50	1.39
23	b	610	CLA	CHB-C1B	3.99	1.48	1.39
23	d	401[A]	CLA	CHB-C1B	3.99	1.48	1.39
23	B	615	CLA	CHB-C1B	3.99	1.48	1.39
23	b	612	CLA	CHC-C4B	3.99	1.48	1.39
23	B	611	CLA	CHB-C1B	3.99	1.48	1.39
23	B	605	CLA	CHC-C4B	3.99	1.48	1.39
23	B	609	CLA	C3D-C2D	3.99	1.50	1.39
23	A	405[B]	CLA	CHD-C1D	3.98	1.46	1.38
23	b	608	CLA	O2A-CGA	3.98	1.45	1.33
23	B	613	CLA	CHB-C1B	3.98	1.48	1.39
23	B	601	CLA	CHD-C1D	3.98	1.46	1.38
23	b	615	CLA	C3D-C2D	3.98	1.50	1.39
23	C	506	CLA	C3D-C2D	3.98	1.50	1.39
23	A	405[A]	CLA	CHD-C1D	3.97	1.46	1.38
23	d	402	CLA	O2D-CGD	3.97	1.42	1.33
26	a	411[A]	SQD	O48-C23	3.97	1.44	1.33
23	b	608	CLA	C3D-C2D	3.97	1.50	1.39
23	C	503	CLA	O2A-CGA	3.97	1.44	1.33
23	c	502	CLA	CHD-C4C	3.97	1.48	1.39
23	C	503	CLA	CHD-C4C	3.96	1.48	1.39
23	b	604	CLA	CHC-C4B	3.96	1.48	1.39
23	a	407[A]	CLA	O2A-CGA	3.96	1.44	1.33
23	a	407[A]	CLA	C3D-C2D	3.96	1.49	1.39
26	C	501[B]	SQD	O48-C23	3.96	1.44	1.33
23	c	507	CLA	CHB-C1B	3.96	1.48	1.39
37	D	401[B]	PHO	O2A-CGA	3.96	1.44	1.33
23	d	401[A]	CLA	O2A-CGA	3.96	1.44	1.33
23	A	404[B]	CLA	CHD-C4C	3.96	1.48	1.39
23	C	514	CLA	CHC-C4B	3.96	1.48	1.39
35	c	518[B]	DGD	O2G-C1B	3.95	1.45	1.34
23	c	506	CLA	CHB-C1B	3.95	1.48	1.39
23	A	406[A]	CLA	OBD-CAD	3.95	1.29	1.22
23	B	602	CLA	CHC-C4B	3.95	1.48	1.39
34	B	625	HTG	C1'-S1	-3.95	1.76	1.81
23	A	406[A]	CLA	C3D-C2D	3.95	1.49	1.39
23	B	603	CLA	C3D-C2D	3.95	1.49	1.39
23	B	612	CLA	C1D-ND	3.95	1.42	1.37
23	c	504	CLA	CHB-C1B	3.94	1.48	1.39
23	c	504	CLA	CHC-C4B	3.94	1.48	1.39
23	c	503	CLA	C3D-C2D	3.94	1.49	1.39
23	b	608	CLA	OBD-CAD	3.93	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	C3D-C2D	3.93	1.49	1.39
37	D	402[B]	PHO	O2A-CGA	3.93	1.44	1.33
23	B	607	CLA	OBD-CAD	3.93	1.29	1.22
23	C	503	CLA	CHC-C4B	3.93	1.48	1.39
23	b	612	CLA	C3D-C2D	3.93	1.49	1.39
23	d	402	CLA	C3D-C2D	3.93	1.49	1.39
23	B	603	CLA	CHC-C1C	3.93	1.46	1.38
23	d	401[A]	CLA	CHD-C1D	3.93	1.46	1.38
23	B	608	CLA	O2D-CGD	3.92	1.42	1.33
23	B	602	CLA	CHD-C4C	3.92	1.48	1.39
23	B	606	CLA	CHD-C1D	3.92	1.46	1.38
23	C	513	CLA	C4B-NB	-3.92	1.33	1.37
33	C	502	LMG	O7-C10	3.92	1.45	1.34
23	c	513	CLA	CHD-C4C	3.92	1.48	1.39
32	L	101[A]	LHG	O8-C23	3.92	1.44	1.33
23	c	509	CLA	CHB-C1B	3.91	1.48	1.39
35	C	519[B]	DGD	O1G-C1A	3.91	1.44	1.33
23	a	407[B]	CLA	OBD-CAD	3.91	1.29	1.22
23	A	406[B]	CLA	CHC-C4B	3.91	1.48	1.39
23	c	506	CLA	CHC-C4B	3.91	1.48	1.39
33	z	101	LMG	O7-C10	3.91	1.45	1.34
32	D	409[A]	LHG	O8-C23	3.91	1.44	1.33
23	c	507	CLA	O2A-CGA	3.91	1.44	1.33
23	b	616	CLA	C3D-C2D	3.91	1.49	1.39
23	A	406[B]	CLA	C3D-C2D	3.90	1.49	1.39
23	A	404[B]	CLA	CHC-C4B	3.90	1.48	1.39
23	b	603	CLA	C1D-ND	3.90	1.42	1.37
24	B	618	BCR	C23-C22	-3.90	1.37	1.45
32	d	405[A]	LHG	O7-C7	3.90	1.45	1.34
23	c	502	CLA	O2A-CGA	3.89	1.44	1.33
32	D	409[A]	LHG	O7-C7	3.89	1.45	1.34
23	b	613	CLA	C3D-C2D	3.89	1.49	1.39
23	B	603	CLA	CHB-C1B	3.89	1.48	1.39
23	b	614	CLA	CHD-C4C	3.89	1.48	1.39
23	d	401[B]	CLA	CHD-C4C	3.89	1.48	1.39
23	b	609	CLA	CHC-C4B	3.89	1.48	1.39
23	C	510	CLA	CHD-C1D	3.89	1.45	1.38
23	c	505	CLA	CHB-C1B	3.89	1.48	1.39
23	D	404[B]	CLA	CHD-C1D	3.88	1.45	1.38
23	B	605	CLA	C3D-C2D	3.88	1.49	1.39
23	b	606	CLA	O2A-CGA	3.88	1.44	1.33
23	b	609	CLA	CHB-C1B	3.88	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	l	802[B]	LHG	O7-C7	3.88	1.45	1.34
23	c	503	CLA	CHD-C1D	3.88	1.45	1.38
23	B	605	CLA	O2A-CGA	3.88	1.44	1.33
33	C	502	LMG	O8-C28	3.87	1.44	1.33
37	a	408[A]	PHO	OBD-CAD	3.87	1.27	1.22
32	d	411[B]	LHG	O7-C7	3.87	1.45	1.34
23	B	609	CLA	CHD-C4C	3.87	1.48	1.39
23	C	505	CLA	CHD-C1D	3.87	1.45	1.38
32	D	408[B]	LHG	O7-C7	3.87	1.45	1.34
23	B	614	CLA	CHB-C1B	3.87	1.48	1.39
23	c	510	CLA	C1B-NB	-3.87	1.33	1.37
23	D	405	CLA	OBD-CAD	3.86	1.29	1.22
23	b	608	CLA	CHD-C4C	3.86	1.48	1.39
23	C	506	CLA	C1D-ND	3.86	1.42	1.37
23	c	503	CLA	CHC-C1C	3.86	1.46	1.38
23	B	608	CLA	C3D-C2D	3.86	1.49	1.39
23	B	603	CLA	CHC-C4B	3.86	1.48	1.39
23	c	514	CLA	CHB-C1B	3.85	1.48	1.39
23	b	603	CLA	CHD-C1D	3.85	1.45	1.38
23	a	407[B]	CLA	CHC-C4B	3.85	1.48	1.39
23	B	607	CLA	O2A-CGA	3.85	1.44	1.33
23	D	404[B]	CLA	CHD-C4C	3.85	1.48	1.39
32	A	416[B]	LHG	O8-C23	3.85	1.44	1.33
23	B	606	CLA	CHC-C4B	3.84	1.48	1.39
23	C	510	CLA	OBD-CAD	3.84	1.29	1.22
37	a	416[A]	PHO	O2A-CGA	3.84	1.44	1.33
23	C	514	CLA	C3D-C2D	3.84	1.49	1.39
35	C	519[A]	DGD	O2G-C1B	3.84	1.45	1.34
23	a	406[A]	CLA	OBD-CAD	3.84	1.29	1.22
23	C	512	CLA	O2A-CGA	3.84	1.44	1.33
33	d	409	LMG	O7-C10	3.84	1.45	1.34
23	C	509	CLA	CHC-C4B	3.84	1.48	1.39
23	B	606	CLA	O2A-CGA	3.84	1.44	1.33
35	C	519[B]	DGD	O2G-C1B	3.84	1.45	1.34
23	C	507	CLA	O2A-CGA	3.83	1.44	1.33
23	b	610	CLA	CHD-C1D	3.83	1.45	1.38
23	C	504	CLA	CHB-C1B	3.83	1.48	1.39
32	D	408[B]	LHG	O8-C23	3.83	1.44	1.33
32	d	406[B]	LHG	O7-C7	3.82	1.45	1.34
23	b	608	CLA	C1B-NB	-3.82	1.33	1.37
23	b	610	CLA	CHD-C4C	3.82	1.48	1.39
23	a	405[B]	CLA	C3D-C2D	3.82	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	CHB-C1B	3.82	1.48	1.39
23	c	503	CLA	CHD-C4C	3.81	1.47	1.39
37	a	416[B]	PHO	O2A-CGA	3.81	1.44	1.33
23	C	511	CLA	C3D-C2D	3.81	1.49	1.39
23	c	508	CLA	C3D-C2D	3.81	1.49	1.39
23	c	510	CLA	C3D-C2D	3.81	1.49	1.39
35	c	517[A]	DGD	O2G-C1B	3.81	1.45	1.34
23	C	508	CLA	C1B-NB	-3.81	1.33	1.37
23	B	613	CLA	OBD-CAD	3.81	1.29	1.22
23	B	615	CLA	OBD-CAD	3.81	1.29	1.22
37	a	408[B]	PHO	O2A-CGA	3.81	1.44	1.33
23	A	404[A]	CLA	C3D-C2D	3.81	1.49	1.39
23	B	615	CLA	C3D-C2D	3.80	1.49	1.39
23	C	504	CLA	CHC-C4B	3.80	1.47	1.39
23	a	407[B]	CLA	CHD-C4C	3.80	1.47	1.39
23	B	613	CLA	CHD-C1D	3.80	1.45	1.38
23	B	612	CLA	C4B-NB	-3.80	1.33	1.37
35	h	102	DGD	O1G-C1A	3.80	1.44	1.33
23	b	610	CLA	C3D-C2D	3.80	1.49	1.39
23	B	614	CLA	CHD-C1D	3.80	1.45	1.38
23	A	404[A]	CLA	CHB-C1B	3.80	1.47	1.39
23	c	506	CLA	O2A-CGA	3.80	1.44	1.33
23	A	406[B]	CLA	C1B-NB	-3.79	1.33	1.37
23	c	505	CLA	O2A-CGA	3.79	1.44	1.33
35	C	519[A]	DGD	O1G-C1A	3.79	1.44	1.33
23	c	511	CLA	CHD-C1D	3.79	1.45	1.38
23	b	615	CLA	CHB-C1B	3.79	1.47	1.39
23	A	405[A]	CLA	CHD-C4C	3.79	1.47	1.39
23	D	404[B]	CLA	OBD-CAD	3.79	1.29	1.22
23	b	605	CLA	CHD-C4C	3.79	1.47	1.39
23	b	604	CLA	C3D-C2D	3.79	1.49	1.39
23	C	506	CLA	CHB-C1B	3.79	1.47	1.39
23	a	407[A]	CLA	CHD-C4C	3.79	1.47	1.39
32	l	802[B]	LHG	O8-C23	3.78	1.44	1.33
23	B	610	CLA	CHB-C1B	3.78	1.47	1.39
35	c	517[A]	DGD	O1G-C1A	3.78	1.44	1.33
23	C	508	CLA	CHD-C4C	3.78	1.47	1.39
23	c	505	CLA	CHD-C1D	3.78	1.45	1.38
23	C	510	CLA	CHB-C1B	3.78	1.47	1.39
23	c	502	CLA	CHC-C4B	3.78	1.47	1.39
23	a	409	CLA	OBD-CAD	3.78	1.29	1.22
23	B	612	CLA	O2A-CGA	3.77	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	v	201	HEC	FE-ND	3.77	2.06	1.94
23	a	405[B]	CLA	OBD-CAD	3.77	1.29	1.22
23	B	614	CLA	CHD-C4C	3.77	1.47	1.39
37	D	401[A]	PHO	O2A-CGA	3.77	1.44	1.33
23	a	407[B]	CLA	C3D-C2D	3.77	1.49	1.39
23	B	616	CLA	CHC-C4B	3.77	1.47	1.39
23	b	602	CLA	OBD-CAD	3.77	1.29	1.22
23	A	405[A]	CLA	CHC-C4B	3.76	1.47	1.39
32	L	101[B]	LHG	O7-C7	3.76	1.44	1.34
23	b	615	CLA	CHD-C4C	3.76	1.47	1.39
23	c	510	CLA	C4B-NB	-3.76	1.33	1.37
23	b	616	CLA	CHC-C4B	3.76	1.47	1.39
23	b	613	CLA	CHB-C1B	3.76	1.47	1.39
23	B	610	CLA	CHD-C4C	3.76	1.47	1.39
26	C	501[A]	SQD	O48-C23	3.76	1.44	1.33
23	d	401[B]	CLA	CHB-C1B	3.76	1.47	1.39
23	a	409	CLA	CHC-C4B	3.76	1.47	1.39
23	b	615	CLA	CHC-C4B	3.75	1.47	1.39
23	C	507	CLA	CHD-C4C	3.75	1.47	1.39
23	b	604	CLA	C1B-NB	-3.75	1.33	1.37
23	c	512	CLA	C3D-C2D	3.75	1.49	1.39
23	a	406[B]	CLA	CHD-C4C	3.75	1.47	1.39
23	B	613	CLA	C3D-C2D	3.75	1.49	1.39
23	c	508	CLA	CHC-C4B	3.74	1.47	1.39
23	c	502	CLA	CHB-C1B	3.74	1.47	1.39
26	C	501[B]	SQD	O47-C7	3.74	1.44	1.34
23	B	603	CLA	CHD-C1D	3.74	1.45	1.38
23	C	515	CLA	CHD-C4C	3.74	1.47	1.39
35	C	518[B]	DGD	O1G-C1A	3.74	1.44	1.33
23	b	613	CLA	CHD-C1D	3.74	1.45	1.38
23	C	503	CLA	CHB-C1B	3.74	1.47	1.39
23	a	405[A]	CLA	OBD-CAD	3.74	1.28	1.22
23	c	503	CLA	OBD-CAD	3.74	1.28	1.22
33	B	621	LMG	O7-C10	3.74	1.44	1.34
23	c	514	CLA	C3D-C2D	3.74	1.49	1.39
23	B	616	CLA	O2A-CGA	3.74	1.44	1.33
23	b	612	CLA	O2A-CGA	3.74	1.44	1.33
23	c	511	CLA	C3D-C2D	3.73	1.49	1.39
23	b	613	CLA	CHC-C4B	3.73	1.47	1.39
23	b	606	CLA	C3D-C2D	3.73	1.49	1.39
23	A	406[A]	CLA	O2A-CGA	3.73	1.44	1.33
23	B	601	CLA	C3D-C2D	3.73	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	CHB-C1B	3.72	1.47	1.39
23	B	604	CLA	CHD-C4C	3.72	1.47	1.39
23	C	506	CLA	CHD-C4C	3.72	1.47	1.39
23	c	508	CLA	CHD-C4C	3.72	1.47	1.39
23	B	602	CLA	O2A-CGA	3.72	1.44	1.33
23	B	615	CLA	CHD-C4C	3.72	1.47	1.39
23	b	614	CLA	OBD-CAD	3.72	1.28	1.22
23	C	514	CLA	CHD-C4C	3.72	1.47	1.39
23	c	512	CLA	CHD-C4C	3.72	1.47	1.39
23	C	511	CLA	CHD-C4C	3.71	1.47	1.39
34	b	623	HTG	C1'-S1	-3.71	1.76	1.81
23	C	511	CLA	O2A-CGA	3.71	1.44	1.33
23	B	603	CLA	O2A-CGA	3.71	1.44	1.33
23	c	509	CLA	CHC-C4B	3.71	1.47	1.39
23	c	508	CLA	OBD-CAD	3.71	1.28	1.22
23	d	402	CLA	CHD-C4C	3.71	1.47	1.39
23	b	603	CLA	O2A-CGA	3.71	1.44	1.33
23	c	505	CLA	CHD-C4C	3.71	1.47	1.39
23	C	503	CLA	C3D-C2D	3.71	1.49	1.39
23	b	609	CLA	C3D-C2D	3.70	1.49	1.39
23	A	406[A]	CLA	CHD-C4C	3.70	1.47	1.39
23	d	402	CLA	CHB-C1B	3.70	1.47	1.39
23	B	616	CLA	CHD-C1D	3.70	1.45	1.38
23	B	605	CLA	CHD-C1D	3.70	1.45	1.38
34	B	622	HTG	C1'-S1	-3.70	1.76	1.81
23	C	512	CLA	CHD-C1D	3.70	1.45	1.38
23	b	612	CLA	CHD-C4C	3.70	1.47	1.39
23	C	515	CLA	OBD-CAD	3.70	1.28	1.22
23	A	404[A]	CLA	CHD-C1D	3.70	1.45	1.38
23	B	616	CLA	C4B-NB	-3.69	1.33	1.37
23	B	611	CLA	C3B-C4B	3.69	1.51	1.42
23	d	402	CLA	CHC-C4B	3.69	1.47	1.39
23	D	404[B]	CLA	CHB-C1B	3.69	1.47	1.39
23	C	508	CLA	C3D-C2D	3.68	1.49	1.39
23	c	513	CLA	OBD-CAD	3.68	1.28	1.22
23	d	401[B]	CLA	CHC-C4B	3.68	1.47	1.39
32	L	101[A]	LHG	O7-C7	3.68	1.44	1.34
23	b	607	CLA	CHB-C1B	3.68	1.47	1.39
26	C	501[A]	SQD	O47-C7	3.68	1.44	1.34
23	C	504	CLA	OBD-CAD	3.68	1.28	1.22
23	b	616	CLA	CHD-C1D	3.68	1.45	1.38
32	d	406[A]	LHG	O7-C7	3.68	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	CHB-C1B	3.68	1.47	1.39
23	c	510	CLA	CHC-C1C	3.67	1.46	1.38
23	a	405[A]	CLA	C3D-C2D	3.67	1.49	1.39
23	b	614	CLA	O2A-CGA	3.67	1.44	1.33
23	B	610	CLA	CHC-C4B	3.67	1.47	1.39
23	A	404[A]	CLA	CHD-C4C	3.67	1.47	1.39
23	A	404[B]	CLA	C1B-NB	-3.67	1.33	1.37
23	B	607	CLA	C3D-C2D	3.66	1.49	1.39
32	D	408[A]	LHG	O7-C7	3.66	1.44	1.34
23	C	509	CLA	CHD-C4C	3.66	1.47	1.39
23	b	609	CLA	CHD-C4C	3.66	1.47	1.39
23	b	608	CLA	C4B-NB	-3.65	1.33	1.37
23	b	606	CLA	CHB-C1B	3.65	1.47	1.39
23	b	601	CLA	CHB-C1B	3.65	1.47	1.39
35	C	518[A]	DGD	O1G-C1A	3.65	1.44	1.33
23	A	405[A]	CLA	CHB-C1B	3.65	1.47	1.39
23	c	505	CLA	C1B-NB	-3.65	1.33	1.37
23	a	406[A]	CLA	CHD-C1D	3.65	1.45	1.38
23	B	616	CLA	CHB-C1B	3.65	1.47	1.39
32	d	411[A]	LHG	O8-C23	3.64	1.44	1.33
23	D	404[A]	CLA	CHD-C4C	3.64	1.47	1.39
23	B	616	CLA	C1B-NB	-3.64	1.33	1.37
23	C	515	CLA	CHB-C1B	3.64	1.47	1.39
33	m	101	LMG	O7-C10	3.64	1.44	1.34
23	B	608	CLA	CHB-C1B	3.64	1.47	1.39
23	c	510	CLA	CHB-C1B	3.64	1.47	1.39
23	A	406[A]	CLA	CHC-C4B	3.64	1.47	1.39
23	D	405	CLA	O2A-CGA	3.64	1.44	1.33
23	B	606	CLA	CHD-C4C	3.64	1.47	1.39
23	B	607	CLA	CHD-C4C	3.64	1.47	1.39
23	a	406[B]	CLA	CHC-C4B	3.63	1.47	1.39
23	b	607	CLA	C3D-C2D	3.63	1.49	1.39
23	c	512	CLA	OBD-CAD	3.63	1.28	1.22
23	c	511	CLA	CHC-C4B	3.63	1.47	1.39
23	b	613	CLA	C1B-NB	-3.63	1.33	1.37
37	D	402[A]	PHO	CHA-CBD	-3.63	1.47	1.51
23	C	510	CLA	CHD-C4C	3.63	1.47	1.39
23	C	505	CLA	CHC-C4B	3.62	1.47	1.39
23	C	506	CLA	CHD-C1D	3.62	1.45	1.38
23	b	602	CLA	O2A-CGA	3.62	1.43	1.33
23	d	401[A]	CLA	C1D-ND	3.61	1.42	1.37
32	d	405[B]	LHG	O8-C23	3.61	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	O2D-CGD	3.61	1.42	1.33
23	a	407[A]	CLA	CHD-C1D	3.61	1.45	1.38
23	B	612	CLA	CHD-C4C	3.61	1.47	1.39
23	B	605	CLA	CHB-C1B	3.61	1.47	1.39
23	d	401[A]	CLA	OBD-CAD	3.61	1.28	1.22
23	b	616	CLA	CHD-C4C	3.61	1.47	1.39
23	A	407	CLA	C3D-C2D	3.61	1.49	1.39
32	l	802[A]	LHG	O7-C7	3.60	1.44	1.34
23	A	406[A]	CLA	CHB-C1B	3.60	1.47	1.39
23	D	404[B]	CLA	CHC-C4B	3.60	1.47	1.39
32	D	408[A]	LHG	O8-C23	3.60	1.43	1.33
23	b	602	CLA	C3D-C2D	3.60	1.49	1.39
23	d	401[A]	CLA	CHD-C4C	3.60	1.47	1.39
35	H	102	DGD	O1G-C1A	3.60	1.43	1.33
23	a	406[B]	CLA	C1B-NB	-3.60	1.33	1.37
32	A	416[A]	LHG	O7-C7	3.60	1.44	1.34
23	a	407[B]	CLA	CHB-C1B	3.60	1.47	1.39
23	D	405	CLA	CHD-C4C	3.59	1.47	1.39
23	b	603	CLA	C3D-C2D	3.59	1.48	1.39
23	c	509	CLA	OBD-CAD	3.59	1.28	1.22
23	A	405[B]	CLA	CHD-C4C	3.59	1.47	1.39
23	B	608	CLA	O2A-CGA	3.59	1.43	1.33
23	B	601	CLA	CHD-C4C	3.58	1.47	1.39
23	a	405[B]	CLA	O2A-CGA	3.58	1.43	1.33
23	B	602	CLA	C3D-C2D	3.58	1.48	1.39
32	d	405[A]	LHG	O8-C23	3.58	1.43	1.33
23	c	506	CLA	C1B-NB	-3.58	1.33	1.37
23	A	404[B]	CLA	C3D-C2D	3.58	1.48	1.39
23	c	507	CLA	OBD-CAD	3.58	1.28	1.22
23	C	511	CLA	CHB-C1B	3.58	1.47	1.39
23	B	607	CLA	CHB-C1B	3.57	1.47	1.39
23	b	606	CLA	CHD-C4C	3.57	1.47	1.39
23	C	507	CLA	OBD-CAD	3.57	1.28	1.22
23	b	606	CLA	C1B-NB	-3.57	1.33	1.37
23	b	604	CLA	CHD-C4C	3.57	1.47	1.39
23	c	508	CLA	CHB-C1B	3.57	1.47	1.39
23	a	409	CLA	CHD-C4C	3.56	1.47	1.39
23	C	511	CLA	OBD-CAD	3.56	1.28	1.22
23	c	505	CLA	C4B-NB	-3.56	1.33	1.37
23	b	602	CLA	C3B-C4B	3.56	1.51	1.42
23	b	605	CLA	CHD-C1D	3.56	1.45	1.38
23	A	404[A]	CLA	C4B-NB	-3.56	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404[B]	CLA	C3D-C2D	3.56	1.48	1.39
23	B	611	CLA	CHD-C4C	3.56	1.47	1.39
23	b	603	CLA	CHD-C4C	3.55	1.47	1.39
23	a	405[A]	CLA	CHC-C4B	3.55	1.47	1.39
23	C	511	CLA	CHC-C4B	3.55	1.47	1.39
23	C	508	CLA	OBD-CAD	3.55	1.28	1.22
23	c	507	CLA	C1B-NB	-3.55	1.33	1.37
23	a	407[A]	CLA	CHB-C1B	3.55	1.47	1.39
23	D	404[A]	CLA	C3D-C2D	3.55	1.48	1.39
23	B	608	CLA	CHD-C1D	3.54	1.45	1.38
23	B	605	CLA	CHD-C4C	3.54	1.47	1.39
23	B	601	CLA	OBD-CAD	3.54	1.28	1.22
35	c	518[A]	DGD	O2G-C1B	3.54	1.44	1.34
23	d	401[A]	CLA	C3D-C2D	3.53	1.48	1.39
23	B	601	CLA	CHB-C1B	3.53	1.47	1.39
23	b	603	CLA	C4B-NB	-3.53	1.33	1.37
23	A	404[B]	CLA	O2A-CGA	3.53	1.43	1.33
23	A	405[B]	CLA	CHC-C4B	3.52	1.47	1.39
23	a	406[A]	CLA	CHD-C4C	3.52	1.47	1.39
23	B	609	CLA	C1B-NB	-3.52	1.33	1.37
23	b	611	CLA	CHD-C4C	3.52	1.47	1.39
23	C	505	CLA	C3D-C2D	3.52	1.48	1.39
23	B	607	CLA	C1B-NB	-3.52	1.33	1.37
23	d	401[B]	CLA	OBD-CAD	3.52	1.28	1.22
23	b	602	CLA	CHB-C1B	3.51	1.47	1.39
23	C	509	CLA	C3D-C2D	3.51	1.48	1.39
23	B	612	CLA	C3D-C2D	3.51	1.48	1.39
32	d	411[A]	LHG	O7-C7	3.50	1.44	1.34
23	A	407	CLA	CHD-C4C	3.50	1.47	1.39
23	a	406[B]	CLA	CHB-C1B	3.50	1.47	1.39
23	b	612	CLA	OBD-CAD	3.50	1.28	1.22
23	A	404[B]	CLA	CHB-C1B	3.50	1.47	1.39
23	c	505	CLA	OBD-CAD	3.50	1.28	1.22
23	D	404[A]	CLA	CHC-C4B	3.50	1.47	1.39
23	a	407[A]	CLA	OBD-CAD	3.50	1.28	1.22
32	A	416[A]	LHG	O8-C23	3.49	1.43	1.33
23	D	405	CLA	C3B-C4B	3.49	1.50	1.42
38	f	101	HEM	C4D-ND	-3.49	1.34	1.40
23	C	515	CLA	CHC-C4B	3.49	1.47	1.39
23	c	506	CLA	C3D-C2D	3.49	1.48	1.39
23	B	606	CLA	C3D-C2D	3.49	1.48	1.39
23	B	607	CLA	C1D-ND	3.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	409	CLA	CHB-C1B	3.49	1.47	1.39
23	b	613	CLA	O2A-CGA	3.48	1.43	1.33
23	A	405[A]	CLA	C1B-NB	-3.48	1.33	1.37
23	C	512	CLA	OBD-CAD	3.48	1.28	1.22
23	b	606	CLA	CHC-C4B	3.48	1.47	1.39
23	C	506	CLA	O2A-CGA	3.48	1.43	1.33
23	A	404[B]	CLA	OBD-CAD	3.48	1.28	1.22
23	a	406[A]	CLA	CHB-C1B	3.48	1.47	1.39
23	B	609	CLA	C3B-C4B	3.48	1.50	1.42
23	b	611	CLA	C1B-NB	-3.48	1.33	1.37
23	b	611	CLA	CHD-C1D	3.47	1.45	1.38
23	b	605	CLA	C3D-C2D	3.47	1.48	1.39
23	b	604	CLA	OBD-CAD	3.47	1.28	1.22
23	B	615	CLA	CHC-C4B	3.47	1.47	1.39
23	B	613	CLA	CHD-C4C	3.47	1.47	1.39
23	c	511	CLA	O2A-CGA	3.47	1.43	1.33
23	A	407	CLA	C4B-NB	-3.47	1.33	1.37
23	b	605	CLA	CHB-C1B	3.47	1.47	1.39
23	C	512	CLA	C3D-C2D	3.46	1.48	1.39
23	a	406[B]	CLA	OBD-CAD	3.46	1.28	1.22
23	D	404[B]	CLA	C4B-NB	-3.46	1.33	1.37
23	a	405[B]	CLA	C1B-NB	-3.46	1.33	1.37
32	A	416[B]	LHG	O7-C7	3.45	1.44	1.34
23	C	514	CLA	CHB-C1B	3.45	1.47	1.39
23	c	503	CLA	CHB-C1B	3.44	1.47	1.39
23	c	502	CLA	OBD-CAD	3.44	1.28	1.22
23	C	511	CLA	C1B-NB	-3.44	1.33	1.37
23	c	514	CLA	CHC-C4B	3.44	1.47	1.39
34	b	622	HTG	C1'-S1	-3.44	1.77	1.81
23	b	604	CLA	CHB-C1B	3.44	1.47	1.39
23	c	504	CLA	OBD-CAD	3.44	1.28	1.22
23	C	507	CLA	C3D-C2D	3.43	1.48	1.39
23	B	602	CLA	C1C-C2C	3.43	1.51	1.44
23	a	405[B]	CLA	C3B-C4B	3.43	1.50	1.42
23	C	509	CLA	CHB-C1B	3.43	1.47	1.39
23	B	608	CLA	CHC-C4B	3.42	1.47	1.39
23	B	608	CLA	CHD-C4C	3.42	1.47	1.39
23	a	405[B]	CLA	CHC-C4B	3.41	1.47	1.39
23	C	504	CLA	CHD-C4C	3.41	1.47	1.39
23	c	503	CLA	CHC-C4B	3.41	1.47	1.39
23	d	401[A]	CLA	C1B-NB	-3.41	1.33	1.37
23	A	406[B]	CLA	C3B-C4B	3.41	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	OBD-CAD	3.40	1.28	1.22
23	D	405	CLA	C1B-NB	-3.40	1.33	1.37
23	c	514	CLA	OBD-CAD	3.40	1.28	1.22
23	b	605	CLA	CHC-C4B	3.40	1.47	1.39
23	C	514	CLA	OBD-CAD	3.40	1.28	1.22
23	A	406[B]	CLA	CHB-C1B	3.40	1.47	1.39
23	B	613	CLA	O2A-CGA	3.40	1.43	1.33
23	b	610	CLA	OBD-CAD	3.40	1.28	1.22
23	D	405	CLA	C1C-C2C	3.40	1.51	1.44
23	B	604	CLA	CHC-C4B	3.39	1.47	1.39
32	l	802[A]	LHG	O8-C23	3.39	1.43	1.33
23	b	616	CLA	CHB-C1B	3.39	1.47	1.39
23	b	611	CLA	C3D-C2D	3.39	1.48	1.39
33	D	413	LMG	O7-C10	3.39	1.43	1.34
23	d	401[B]	CLA	C1B-NB	-3.38	1.33	1.37
23	b	611	CLA	CHC-C4B	3.38	1.47	1.39
23	c	507	CLA	C4B-NB	-3.38	1.33	1.37
23	C	513	CLA	CHC-C4B	3.38	1.47	1.39
23	d	401[A]	CLA	CHC-C4B	3.38	1.47	1.39
23	B	603	CLA	CHD-C4C	3.37	1.46	1.39
23	A	405[B]	CLA	OBD-CAD	3.37	1.28	1.22
23	B	607	CLA	CHC-C4B	3.37	1.47	1.39
23	b	601	CLA	OBD-CAD	3.37	1.28	1.22
23	A	406[A]	CLA	C3B-C4B	3.36	1.50	1.42
23	C	510	CLA	CHC-C4B	3.36	1.47	1.39
23	b	611	CLA	OBD-CAD	3.36	1.28	1.22
23	A	405[A]	CLA	OBD-CAD	3.36	1.28	1.22
23	C	508	CLA	CHB-C1B	3.36	1.46	1.39
23	b	603	CLA	CHB-C1B	3.35	1.46	1.39
23	B	604	CLA	O2A-CGA	3.35	1.43	1.33
23	B	604	CLA	C3D-C2D	3.35	1.48	1.39
23	B	614	CLA	C3D-C2D	3.35	1.48	1.39
37	a	408[A]	PHO	O2A-CGA	3.35	1.43	1.33
23	b	607	CLA	O2A-CGA	3.35	1.43	1.33
23	b	606	CLA	OBD-CAD	3.35	1.28	1.22
23	C	506	CLA	CHC-C4B	3.35	1.46	1.39
23	b	603	CLA	CHC-C4B	3.35	1.46	1.39
23	A	404[B]	CLA	C3B-C4B	3.35	1.50	1.42
23	c	512	CLA	C1B-C2B	3.34	1.51	1.43
23	b	601	CLA	CHC-C4B	3.34	1.46	1.39
35	H	102	DGD	O2G-C1B	3.34	1.43	1.34
23	C	514	CLA	C3B-C4B	3.34	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	413	LMG	O8-C28	3.33	1.43	1.33
23	A	407	CLA	OBD-CAD	3.33	1.28	1.22
23	B	605	CLA	C3B-C4B	3.33	1.50	1.42
23	A	404[A]	CLA	OBD-CAD	3.33	1.28	1.22
35	c	519	DGD	O2G-C1B	3.32	1.43	1.34
23	d	401[B]	CLA	C4B-NB	-3.32	1.33	1.37
23	B	602	CLA	C1B-NB	-3.32	1.33	1.37
23	C	508	CLA	C4B-NB	-3.31	1.33	1.37
23	B	612	CLA	CHC-C4B	3.31	1.46	1.39
23	b	615	CLA	OBD-CAD	3.30	1.28	1.22
23	b	607	CLA	C1D-ND	3.30	1.41	1.37
38	f	101	HEM	C1B-NB	-3.29	1.34	1.40
23	A	407	CLA	CHC-C4B	3.29	1.46	1.39
23	C	508	CLA	CHC-C4B	3.29	1.46	1.39
23	c	505	CLA	CHC-C4B	3.29	1.46	1.39
23	b	604	CLA	O2A-CGA	3.29	1.43	1.33
23	C	515	CLA	C1B-NB	-3.29	1.33	1.37
23	A	405[B]	CLA	CHB-C1B	3.29	1.46	1.39
23	b	610	CLA	C1B-NB	-3.29	1.33	1.37
23	b	615	CLA	C1B-NB	-3.28	1.33	1.37
23	A	404[A]	CLA	O2A-CGA	3.28	1.42	1.33
23	b	613	CLA	CHD-C4C	3.28	1.46	1.39
23	C	505	CLA	OBD-CAD	3.27	1.28	1.22
23	C	509	CLA	C1B-NB	-3.27	1.33	1.37
34	D	412	HTG	C1'-S1	-3.27	1.77	1.81
23	b	605	CLA	O2A-CGA	3.27	1.42	1.33
23	a	407[A]	CLA	CHC-C4B	3.27	1.46	1.39
23	B	607	CLA	C4B-NB	-3.26	1.33	1.37
23	c	504	CLA	C3D-C2D	3.25	1.48	1.39
23	b	607	CLA	CHC-C4B	3.25	1.46	1.39
23	b	614	CLA	C1B-NB	-3.25	1.33	1.37
40	V	202	HEC	FE-NB	3.25	2.04	1.94
23	b	607	CLA	CHD-C4C	3.25	1.46	1.39
23	c	504	CLA	C3B-C4B	3.25	1.50	1.42
23	C	505	CLA	O2A-CGA	3.24	1.42	1.33
23	B	607	CLA	CHD-C1D	3.24	1.44	1.38
23	b	616	CLA	OBD-CAD	3.24	1.28	1.22
23	B	609	CLA	OBD-CAD	3.24	1.28	1.22
23	b	603	CLA	C1B-NB	-3.24	1.33	1.37
23	D	404[A]	CLA	OBD-CAD	3.24	1.28	1.22
23	B	611	CLA	C3D-C2D	3.24	1.48	1.39
23	a	406[A]	CLA	CHC-C4B	3.23	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401[B]	CLA	C3D-C2D	3.23	1.47	1.39
23	c	507	CLA	CHC-C4B	3.23	1.46	1.39
38	F	102	HEM	C4D-ND	-3.23	1.34	1.40
23	c	514	CLA	C4B-NB	-3.23	1.33	1.37
23	c	512	CLA	CHC-C4B	3.23	1.46	1.39
23	B	616	CLA	C1B-C2B	3.22	1.50	1.43
23	c	511	CLA	OBD-CAD	3.21	1.28	1.22
23	c	504	CLA	C4B-NB	-3.21	1.33	1.37
23	D	405	CLA	C4C-C3C	3.20	1.50	1.45
23	B	602	CLA	OBD-CAD	3.20	1.28	1.22
23	D	404[A]	CLA	C1B-NB	-3.20	1.33	1.37
23	c	503	CLA	C4B-NB	-3.20	1.33	1.37
38	F	102	HEM	C1B-NB	-3.19	1.34	1.40
23	b	602	CLA	C1C-C2C	3.19	1.50	1.44
23	a	405[A]	CLA	O2A-CGA	3.19	1.42	1.33
23	C	507	CLA	C1B-C2B	3.19	1.50	1.43
23	C	509	CLA	OBD-CAD	3.18	1.28	1.22
40	V	202	HEC	FE-NC	3.18	2.05	1.95
23	c	510	CLA	C4C-C3C	3.18	1.50	1.45
23	c	506	CLA	C3B-C4B	3.18	1.50	1.42
23	b	613	CLA	C4B-NB	-3.18	1.33	1.37
23	B	610	CLA	CHD-C1D	3.18	1.44	1.38
23	B	606	CLA	OBD-CAD	3.17	1.27	1.22
23	A	405[A]	CLA	C3B-C4B	3.17	1.50	1.42
23	b	609	CLA	C3B-C4B	3.17	1.50	1.42
23	A	407	CLA	CHB-C1B	3.17	1.46	1.39
23	B	610	CLA	O2A-CGA	3.17	1.42	1.33
23	C	503	CLA	C1B-C2B	3.17	1.50	1.43
23	c	504	CLA	C1B-NB	-3.17	1.33	1.37
23	C	506	CLA	OBD-CAD	3.16	1.27	1.22
23	a	409	CLA	C3D-C2D	3.16	1.47	1.39
23	B	604	CLA	C1B-C2B	3.15	1.50	1.43
23	C	509	CLA	C1C-C2C	3.15	1.50	1.44
23	B	601	CLA	C1C-C2C	3.15	1.50	1.44
23	B	601	CLA	C3B-C4B	3.15	1.50	1.42
23	a	409	CLA	C3B-C4B	3.14	1.50	1.42
23	B	605	CLA	C1B-C2B	3.14	1.50	1.43
23	A	405[B]	CLA	C3B-C4B	3.14	1.50	1.42
23	B	615	CLA	C1B-NB	-3.14	1.33	1.37
23	d	402	CLA	OBD-CAD	3.14	1.27	1.22
23	B	603	CLA	OBD-CAD	3.13	1.27	1.22
23	B	614	CLA	C1B-NB	-3.13	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	C4B-NB	-3.12	1.33	1.37
35	C	520	DGD	O2G-C1B	3.12	1.43	1.34
23	C	510	CLA	C4B-NB	-3.12	1.33	1.37
23	B	610	CLA	C1B-NB	-3.12	1.33	1.37
23	b	616	CLA	C3B-C4B	3.12	1.50	1.42
23	C	506	CLA	C1B-NB	-3.11	1.34	1.37
23	C	507	CLA	C3B-C4B	3.10	1.50	1.42
34	d	408	HTG	C1'-S1	-3.10	1.77	1.81
23	a	405[B]	CLA	CHB-C1B	3.10	1.46	1.39
23	b	601	CLA	C3B-C4B	3.10	1.50	1.42
23	B	612	CLA	C1C-C2C	3.10	1.50	1.44
23	A	404[A]	CLA	C1B-NB	-3.09	1.34	1.37
23	B	613	CLA	CHC-C4B	3.09	1.46	1.39
23	A	405[B]	CLA	C1B-NB	-3.09	1.34	1.37
23	d	401[A]	CLA	C4B-NB	-3.09	1.34	1.37
23	C	512	CLA	CHC-C4B	3.09	1.46	1.39
23	B	608	CLA	C4B-NB	-3.09	1.34	1.37
23	B	614	CLA	C3B-C4B	3.08	1.50	1.42
23	B	604	CLA	C1C-C2C	3.08	1.50	1.44
23	B	612	CLA	OBD-CAD	3.08	1.27	1.22
23	B	601	CLA	C1B-NB	-3.08	1.34	1.37
23	c	514	CLA	C1B-NB	-3.07	1.34	1.37
23	c	513	CLA	C3B-C4B	3.07	1.49	1.42
23	c	510	CLA	OBD-CAD	3.07	1.27	1.22
23	b	610	CLA	O2A-CGA	3.07	1.42	1.33
23	c	514	CLA	C3B-C4B	3.06	1.49	1.42
23	b	608	CLA	CHC-C4B	3.06	1.46	1.39
23	c	511	CLA	C1B-C2B	3.06	1.50	1.43
23	a	405[A]	CLA	C1B-NB	-3.06	1.34	1.37
23	C	509	CLA	C1B-C2B	3.05	1.50	1.43
23	c	503	CLA	C1B-C2B	3.05	1.50	1.43
23	a	405[A]	CLA	C4B-NB	-3.05	1.34	1.37
23	C	515	CLA	C4B-NB	-3.04	1.34	1.37
23	a	407[A]	CLA	C1B-NB	-3.04	1.34	1.37
23	B	612	CLA	C1B-C2B	3.04	1.50	1.43
23	D	404[B]	CLA	C1B-NB	-3.04	1.34	1.37
23	c	508	CLA	C1B-NB	-3.04	1.34	1.37
23	c	508	CLA	C4B-NB	-3.04	1.34	1.37
34	b	625	HTG	C1'-S1	-3.04	1.77	1.81
23	C	505	CLA	C3B-C4B	3.04	1.49	1.42
23	b	612	CLA	C1B-C2B	3.04	1.50	1.43
23	a	409	CLA	C1C-C2C	3.03	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	C3B-C4B	3.03	1.49	1.42
23	b	614	CLA	C1B-C2B	3.02	1.50	1.43
23	a	407[B]	CLA	C3B-C4B	3.01	1.49	1.42
23	C	515	CLA	C1B-C2B	3.01	1.50	1.43
23	A	404[A]	CLA	CHC-C4B	3.01	1.46	1.39
23	b	607	CLA	C4B-NB	-3.00	1.34	1.37
23	B	613	CLA	C1C-C2C	3.00	1.50	1.44
23	C	513	CLA	C4D-CHA	2.99	1.49	1.38
23	a	407[B]	CLA	C4B-NB	-2.99	1.34	1.37
23	B	604	CLA	C1B-NB	-2.99	1.34	1.37
23	b	605	CLA	OBD-CAD	2.99	1.27	1.22
23	C	503	CLA	OBD-CAD	2.99	1.27	1.22
23	B	601	CLA	C4B-NB	-2.99	1.34	1.37
23	a	407[A]	CLA	C3B-C4B	2.98	1.49	1.42
23	B	605	CLA	C1C-C2C	2.98	1.50	1.44
23	B	608	CLA	C1B-C2B	2.98	1.50	1.43
23	c	502	CLA	C1B-NB	-2.98	1.34	1.37
34	C	523	HTG	C1'-S1	-2.98	1.77	1.81
23	B	615	CLA	C3B-C4B	2.97	1.49	1.42
23	B	615	CLA	C1C-C2C	2.97	1.50	1.44
23	B	616	CLA	OBD-CAD	2.97	1.27	1.22
23	c	512	CLA	C4B-NB	-2.96	1.34	1.37
23	C	513	CLA	C1C-C2C	2.96	1.50	1.44
23	b	616	CLA	C1B-NB	-2.96	1.34	1.37
23	A	406[A]	CLA	C1B-C2B	2.96	1.50	1.43
23	b	604	CLA	C1B-C2B	2.96	1.50	1.43
23	B	615	CLA	C1B-C2B	2.96	1.50	1.43
23	a	409	CLA	C1B-C2B	2.96	1.50	1.43
23	b	613	CLA	OBD-CAD	2.96	1.27	1.22
23	a	409	CLA	C1B-NB	-2.95	1.34	1.37
23	b	604	CLA	C4D-CHA	2.94	1.48	1.38
23	c	510	CLA	C4D-CHA	2.94	1.48	1.38
23	C	508	CLA	C4C-C3C	2.93	1.50	1.45
23	C	503	CLA	C3B-C4B	2.93	1.49	1.42
23	b	612	CLA	C1C-C2C	2.93	1.50	1.44
23	B	605	CLA	C1B-NB	-2.93	1.34	1.37
23	c	505	CLA	C1B-C2B	2.93	1.50	1.43
23	C	507	CLA	C1C-C2C	2.92	1.50	1.44
23	C	514	CLA	C1C-C2C	2.92	1.50	1.44
23	d	402	CLA	C3B-C4B	2.92	1.49	1.42
34	b	625	HTG	C1-S1	-2.91	1.76	1.80
23	a	407[A]	CLA	C1C-C2C	2.91	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	C1B-NB	-2.91	1.34	1.37
23	C	506	CLA	C1C-C2C	2.90	1.50	1.44
23	B	603	CLA	C4B-NB	-2.90	1.34	1.37
23	c	509	CLA	C3B-C4B	2.89	1.49	1.42
23	c	511	CLA	C4B-NB	-2.89	1.34	1.37
23	C	512	CLA	C1B-NB	-2.88	1.34	1.37
34	b	622	HTG	O5-C1	2.88	1.46	1.42
23	c	510	CLA	CHC-C4B	2.88	1.45	1.39
23	C	506	CLA	C1B-C2B	2.88	1.50	1.43
23	B	614	CLA	C4D-CHA	2.88	1.48	1.38
23	C	511	CLA	C1C-C2C	2.88	1.50	1.44
23	B	614	CLA	OBD-CAD	2.88	1.27	1.22
23	C	506	CLA	C4B-NB	-2.87	1.34	1.37
23	d	402	CLA	C1B-NB	-2.87	1.34	1.37
23	B	604	CLA	C4D-CHA	2.87	1.48	1.38
23	b	607	CLA	C1B-C2B	2.87	1.50	1.43
23	D	404[A]	CLA	C4B-NB	-2.86	1.34	1.37
23	C	510	CLA	C1B-C2B	2.86	1.50	1.43
23	b	610	CLA	C3D-C4D	-2.86	1.37	1.44
23	B	614	CLA	C1B-C2B	2.85	1.50	1.43
23	c	509	CLA	C4D-CHA	2.85	1.48	1.38
23	C	510	CLA	C1B-NB	-2.85	1.34	1.37
23	b	609	CLA	C1B-NB	-2.84	1.34	1.37
23	A	404[A]	CLA	C4C-C3C	2.84	1.49	1.45
23	B	616	CLA	C1C-C2C	2.84	1.50	1.44
23	C	503	CLA	C1C-C2C	2.84	1.50	1.44
23	b	602	CLA	C4B-NB	-2.84	1.34	1.37
23	a	406[A]	CLA	C3B-C4B	2.84	1.49	1.42
23	C	512	CLA	C1B-C2B	2.84	1.49	1.43
23	b	612	CLA	C1B-NB	-2.84	1.34	1.37
26	C	501[B]	SQD	C6-S	-2.83	1.66	1.77
23	B	609	CLA	C1C-C2C	2.83	1.50	1.44
23	B	606	CLA	C1B-NB	-2.83	1.34	1.37
23	b	607	CLA	C1C-C2C	2.83	1.50	1.44
23	B	616	CLA	CHD-C4C	2.83	1.45	1.39
23	b	603	CLA	C3B-C4B	2.81	1.49	1.42
23	C	507	CLA	C1B-NB	-2.81	1.34	1.37
23	C	511	CLA	C3B-C4B	2.81	1.49	1.42
28	A	412[A]	PL9	C6-C5	2.81	1.49	1.35
23	B	606	CLA	C1C-C2C	2.81	1.50	1.44
23	B	610	CLA	C1B-C2B	2.81	1.49	1.43
23	B	604	CLA	C4B-NB	-2.81	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	C1B-C2B	2.81	1.49	1.43
23	b	604	CLA	C4B-NB	-2.81	1.34	1.37
23	c	509	CLA	C4B-NB	-2.80	1.34	1.37
23	c	510	CLA	C1B-C2B	2.80	1.49	1.43
23	b	610	CLA	C3B-C4B	2.80	1.49	1.42
23	c	508	CLA	C4D-CHA	2.80	1.48	1.38
26	a	411[B]	SQD	C6-S	-2.80	1.67	1.77
34	c	522	HTG	C1'-S1	-2.80	1.77	1.81
23	D	404[A]	CLA	C1B-C2B	2.79	1.49	1.43
23	d	401[A]	CLA	C4C-C3C	2.79	1.49	1.45
23	b	616	CLA	C1C-C2C	2.79	1.50	1.44
23	c	511	CLA	C4D-CHA	2.79	1.48	1.38
23	C	503	CLA	C4D-CHA	2.79	1.48	1.38
23	B	606	CLA	C3B-C4B	2.79	1.49	1.42
23	C	504	CLA	C1C-C2C	2.79	1.50	1.44
23	d	402	CLA	C4B-NB	-2.79	1.34	1.37
23	A	407	CLA	C1B-NB	-2.78	1.34	1.37
23	c	503	CLA	C1B-NB	-2.78	1.34	1.37
23	a	406[B]	CLA	C3B-C4B	2.78	1.49	1.42
35	C	520	DGD	O2G-C2G	-2.78	1.39	1.46
23	A	406[B]	CLA	C4B-NB	-2.78	1.34	1.37
23	b	615	CLA	C4D-CHA	2.78	1.48	1.38
23	c	511	CLA	C3B-C4B	2.78	1.49	1.42
23	B	613	CLA	C1B-C2B	2.78	1.49	1.43
23	c	511	CLA	C1C-C2C	2.78	1.49	1.44
23	A	404[B]	CLA	C1C-C2C	2.78	1.49	1.44
23	c	514	CLA	C1B-C2B	2.78	1.49	1.43
23	c	505	CLA	C4D-CHA	2.77	1.48	1.38
23	a	407[B]	CLA	C1C-C2C	2.77	1.49	1.44
23	C	511	CLA	C4D-CHA	2.77	1.48	1.38
23	b	611	CLA	C1B-C2B	2.77	1.49	1.43
23	A	404[A]	CLA	C1B-C2B	2.76	1.49	1.43
37	D	401[A]	PHO	CBD-CGD	-2.76	1.48	1.52
23	B	613	CLA	C4B-NB	-2.76	1.34	1.37
23	B	602	CLA	C1B-C2B	2.76	1.49	1.43
26	C	501[A]	SQD	C6-S	-2.76	1.67	1.77
23	C	506	CLA	C4D-CHA	2.75	1.48	1.38
25	a	419	GOL	C1-C2	2.75	1.63	1.51
23	c	508	CLA	C1B-C2B	2.75	1.49	1.43
23	b	610	CLA	C4B-NB	-2.75	1.34	1.37
23	c	506	CLA	C1B-C2B	2.75	1.49	1.43
23	C	504	CLA	C4B-NB	-2.75	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	407[A]	CLA	C4B-NB	-2.74	1.34	1.37
23	a	407[B]	CLA	C1B-NB	-2.74	1.34	1.37
28	a	414[A]	PL9	C6-C5	2.74	1.49	1.35
23	B	612	CLA	C4D-CHA	2.74	1.48	1.38
23	b	608	CLA	C3B-C4B	2.74	1.49	1.42
23	C	510	CLA	C3B-C2B	2.74	1.50	1.41
23	B	614	CLA	C3D-C4D	-2.74	1.38	1.44
23	b	615	CLA	C3B-C4B	2.74	1.49	1.42
23	b	601	CLA	C4B-NB	-2.74	1.34	1.37
23	c	512	CLA	C4D-CHA	2.74	1.48	1.38
23	C	513	CLA	OBD-CAD	2.73	1.27	1.22
26	a	411[A]	SQD	C6-S	-2.73	1.67	1.77
33	C	526	LMG	O8-C28	2.73	1.46	1.33
23	C	510	CLA	C1C-C2C	2.73	1.49	1.44
23	b	613	CLA	C1C-C2C	2.73	1.49	1.44
23	a	406[A]	CLA	C4B-NB	-2.73	1.34	1.37
23	A	405[A]	CLA	C1C-C2C	2.73	1.49	1.44
23	b	605	CLA	C4D-CHA	2.73	1.48	1.38
25	D	414	GOL	O2-C2	-2.72	1.35	1.43
23	A	405[A]	CLA	C4B-NB	-2.72	1.34	1.37
23	B	602	CLA	C4B-NB	-2.71	1.34	1.37
23	C	512	CLA	C4C-C3C	2.71	1.49	1.45
23	c	502	CLA	C1B-C2B	2.71	1.49	1.43
34	B	625	HTG	C1-S1	-2.71	1.76	1.80
23	b	605	CLA	C1C-C2C	2.71	1.49	1.44
23	b	606	CLA	C3B-C4B	2.70	1.49	1.42
23	c	504	CLA	C3D-C4D	-2.70	1.38	1.44
23	c	513	CLA	C4D-CHA	2.70	1.48	1.38
28	a	414[B]	PL9	C6-C5	2.70	1.49	1.35
23	B	607	CLA	C1B-C2B	2.70	1.49	1.43
23	c	502	CLA	C4B-NB	-2.70	1.34	1.37
23	A	405[A]	CLA	C1B-C2B	2.69	1.49	1.43
23	b	615	CLA	C1B-C2B	2.69	1.49	1.43
23	C	512	CLA	C4B-NB	-2.69	1.34	1.37
23	b	611	CLA	C3B-C4B	2.69	1.49	1.42
23	A	405[A]	CLA	C4D-CHA	2.69	1.48	1.38
31	t	102	LMT	O3'-C3'	-2.69	1.36	1.43
23	B	603	CLA	C4D-CHA	2.69	1.47	1.38
23	b	614	CLA	C3B-C4B	2.69	1.49	1.42
23	A	405[B]	CLA	C1B-C2B	2.69	1.49	1.43
23	B	613	CLA	C4D-CHA	2.69	1.47	1.38
23	C	509	CLA	C4D-CHA	2.69	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C4D-CHA	2.68	1.47	1.38
23	c	503	CLA	C3B-C4B	2.67	1.49	1.42
26	f	102	SQD	C6-S	-2.67	1.67	1.77
23	a	407[A]	CLA	C4D-CHA	2.67	1.47	1.38
23	B	613	CLA	C4C-C3C	2.67	1.49	1.45
23	a	407[A]	CLA	C1B-C2B	2.67	1.49	1.43
23	D	405	CLA	C1B-C2B	2.67	1.49	1.43
23	d	402	CLA	C1C-C2C	2.67	1.49	1.44
23	a	409	CLA	C4B-NB	-2.67	1.34	1.37
23	C	515	CLA	C1C-C2C	2.67	1.49	1.44
23	b	609	CLA	C4D-CHA	2.66	1.47	1.38
23	a	406[A]	CLA	C1B-C2B	2.66	1.49	1.43
23	B	602	CLA	C3D-C4D	-2.66	1.38	1.44
23	d	401[B]	CLA	C4C-C3C	2.66	1.49	1.45
23	C	514	CLA	C1B-NB	-2.65	1.34	1.37
23	c	506	CLA	C4D-CHA	2.65	1.47	1.38
23	B	602	CLA	C3B-C4B	2.65	1.49	1.42
23	b	612	CLA	C4C-C3C	2.64	1.49	1.45
23	B	610	CLA	C1C-C2C	2.64	1.49	1.44
23	C	508	CLA	C1C-C2C	2.64	1.49	1.44
40	V	202	HEC	CAC-C3C	2.64	1.57	1.51
23	c	507	CLA	C4C-C3C	2.64	1.49	1.45
26	a	412	SQD	C6-S	-2.64	1.67	1.77
23	b	609	CLA	C1C-C2C	2.64	1.49	1.44
23	B	607	CLA	C4D-CHA	2.64	1.47	1.38
23	C	510	CLA	C4D-CHA	2.64	1.47	1.38
23	C	505	CLA	C1B-NB	-2.64	1.34	1.37
23	b	610	CLA	C1C-C2C	2.64	1.49	1.44
31	t	101	LMT	O3'-C3'	-2.64	1.36	1.43
23	c	502	CLA	C1C-C2C	2.63	1.49	1.44
23	c	505	CLA	C4C-C3C	2.63	1.49	1.45
23	b	613	CLA	C4D-CHA	2.63	1.47	1.38
23	c	508	CLA	C1C-C2C	2.63	1.49	1.44
23	c	504	CLA	C1C-C2C	2.63	1.49	1.44
23	c	513	CLA	C1C-C2C	2.63	1.49	1.44
23	B	604	CLA	C3D-C4D	-2.63	1.38	1.44
26	A	410	SQD	C6-S	-2.63	1.67	1.77
23	c	502	CLA	C3B-C4B	2.63	1.48	1.42
23	c	505	CLA	C1C-C2C	2.63	1.49	1.44
23	b	608	CLA	C4D-CHA	2.63	1.47	1.38
23	a	405[B]	CLA	C4D-CHA	2.62	1.47	1.38
23	b	606	CLA	C4B-NB	-2.62	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	C3D-C4D	-2.62	1.38	1.44
23	B	607	CLA	C1C-C2C	2.62	1.49	1.44
23	B	610	CLA	C3B-C4B	2.62	1.48	1.42
23	a	405[B]	CLA	C1C-C2C	2.62	1.49	1.44
23	c	512	CLA	C1B-NB	-2.62	1.34	1.37
23	c	514	CLA	C1C-C2C	2.62	1.49	1.44
23	c	504	CLA	C4D-CHA	2.62	1.47	1.38
23	B	603	CLA	C4C-C3C	2.61	1.49	1.45
28	A	412[B]	PL9	C6-C5	2.61	1.48	1.35
23	D	404[A]	CLA	C4D-CHA	2.61	1.47	1.38
23	B	610	CLA	C4D-CHA	2.61	1.47	1.38
23	b	606	CLA	C4D-CHA	2.61	1.47	1.38
23	a	406[B]	CLA	C4D-CHA	2.61	1.47	1.38
31	T	101	LMT	O3'-C3'	-2.61	1.36	1.43
23	C	507	CLA	C4C-C3C	2.61	1.49	1.45
23	c	502	CLA	C4C-C3C	2.61	1.49	1.45
23	A	405[B]	CLA	C4D-CHA	2.60	1.47	1.38
23	d	401[A]	CLA	C4D-CHA	2.60	1.47	1.38
23	b	613	CLA	C1B-C2B	2.60	1.49	1.43
23	C	505	CLA	C4B-NB	-2.60	1.34	1.37
23	C	505	CLA	C4D-CHA	2.60	1.47	1.38
23	b	606	CLA	C1B-C2B	2.60	1.49	1.43
23	b	607	CLA	C4D-CHA	2.60	1.47	1.38
23	c	506	CLA	C4C-C3C	2.60	1.49	1.45
23	c	513	CLA	C4B-NB	-2.60	1.34	1.37
23	c	502	CLA	C4D-CHA	2.60	1.47	1.38
23	B	608	CLA	C1B-NB	-2.60	1.34	1.37
23	b	604	CLA	C1C-C2C	2.59	1.49	1.44
23	b	611	CLA	C3D-C4D	-2.59	1.38	1.44
23	b	612	CLA	C3B-C4B	2.59	1.48	1.42
23	c	509	CLA	C1B-C2B	2.59	1.49	1.43
23	c	507	CLA	C4D-CHA	2.59	1.47	1.38
23	C	513	CLA	C3B-C4B	2.59	1.48	1.42
23	c	509	CLA	C1C-C2C	2.59	1.49	1.44
23	b	601	CLA	C1B-NB	-2.59	1.34	1.37
23	b	603	CLA	C4D-CHA	2.59	1.47	1.38
23	C	504	CLA	C1B-NB	-2.59	1.34	1.37
23	b	603	CLA	C1B-C2B	2.58	1.49	1.43
34	B	622	HTG	O5-C1	2.58	1.46	1.42
23	d	401[B]	CLA	C1B-C2B	2.58	1.49	1.43
23	A	405[B]	CLA	C4B-NB	-2.58	1.34	1.37
38	f	101	HEM	C1C-C2C	-2.58	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	C4D-CHA	2.58	1.47	1.38
23	A	406[A]	CLA	C4D-CHA	2.58	1.47	1.38
23	B	602	CLA	C4C-C3C	2.58	1.49	1.45
37	a	408[A]	PHO	CBD-CGD	-2.58	1.49	1.52
23	b	601	CLA	C4D-CHA	2.57	1.47	1.38
23	B	611	CLA	MG-NB	2.57	2.10	2.05
23	C	515	CLA	C3B-C4B	2.57	1.48	1.42
23	B	609	CLA	C4D-CHA	2.57	1.47	1.38
23	b	607	CLA	C4C-C3C	2.57	1.49	1.45
23	b	603	CLA	C1C-C2C	2.57	1.49	1.44
28	d	404[B]	PL9	C6-C5	2.57	1.48	1.35
37	D	402[B]	PHO	CHA-CBD	-2.57	1.48	1.51
23	b	602	CLA	C4D-CHA	2.57	1.47	1.38
23	c	507	CLA	C1B-C2B	2.56	1.49	1.43
23	C	513	CLA	C1B-C2B	2.56	1.49	1.43
23	d	402	CLA	C4D-CHA	2.56	1.47	1.38
23	B	608	CLA	OBD-CAD	2.56	1.26	1.22
23	B	605	CLA	C4D-CHA	2.56	1.47	1.38
23	C	508	CLA	C1B-C2B	2.56	1.49	1.43
23	C	505	CLA	C1C-C2C	2.56	1.49	1.44
23	a	405[A]	CLA	C4D-CHA	2.55	1.47	1.38
26	F	103	SQD	C6-S	-2.55	1.68	1.77
23	d	401[A]	CLA	C1C-C2C	2.55	1.49	1.44
23	b	601	CLA	C1C-C2C	2.55	1.49	1.44
35	H	102	DGD	O5D-C1E	2.55	1.44	1.40
23	A	406[A]	CLA	C4B-NB	-2.55	1.34	1.37
23	c	511	CLA	C1B-NB	-2.55	1.34	1.37
23	A	407	CLA	C3B-C4B	2.55	1.48	1.42
23	C	504	CLA	C3B-C2B	2.55	1.49	1.41
23	a	407[B]	CLA	C4D-CHA	2.55	1.47	1.38
23	B	605	CLA	OBD-CAD	2.54	1.26	1.22
23	A	404[A]	CLA	C4D-CHA	2.54	1.47	1.38
23	b	612	CLA	C4D-CHA	2.54	1.47	1.38
23	c	510	CLA	C1C-C2C	2.54	1.49	1.44
23	B	606	CLA	C1B-C2B	2.54	1.49	1.43
23	b	610	CLA	C4D-CHA	2.54	1.47	1.38
23	c	512	CLA	C1C-C2C	2.53	1.49	1.44
23	C	506	CLA	C3B-C4B	2.53	1.48	1.42
23	B	609	CLA	C1B-C2B	2.53	1.49	1.43
23	b	605	CLA	C3B-C4B	2.53	1.48	1.42
23	C	504	CLA	C1B-C2B	2.53	1.49	1.43
23	C	508	CLA	C3B-C4B	2.53	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	C3D-C4D	-2.53	1.38	1.44
23	A	404[B]	CLA	C4D-CHA	2.53	1.47	1.38
23	b	604	CLA	C3B-C4B	2.53	1.48	1.42
23	c	513	CLA	C1B-C2B	2.53	1.49	1.43
23	c	514	CLA	C4D-CHA	2.53	1.47	1.38
23	C	505	CLA	C3D-C4D	-2.52	1.38	1.44
23	A	406[B]	CLA	C1C-C2C	2.52	1.49	1.44
23	A	406[B]	CLA	C4D-CHA	2.52	1.47	1.38
23	a	407[B]	CLA	C1B-C2B	2.52	1.49	1.43
23	a	406[A]	CLA	C4D-CHA	2.52	1.47	1.38
37	a	416[A]	PHO	C3A-C2A	-2.52	1.52	1.54
23	a	406[B]	CLA	C1B-C2B	2.52	1.49	1.43
23	C	503	CLA	C3D-C4D	-2.51	1.38	1.44
23	b	616	CLA	C4B-NB	-2.51	1.34	1.37
23	c	504	CLA	C4C-C3C	2.51	1.49	1.45
23	B	604	CLA	C3B-C4B	2.51	1.48	1.42
23	B	601	CLA	C1B-C2B	2.51	1.49	1.43
23	d	401[A]	CLA	C1B-C2B	2.51	1.49	1.43
23	D	404[B]	CLA	C4D-CHA	2.51	1.47	1.38
23	B	616	CLA	C4D-CHA	2.51	1.47	1.38
23	C	506	CLA	C3B-C2B	2.51	1.49	1.41
23	b	602	CLA	C4C-C3C	2.50	1.49	1.45
23	B	614	CLA	C1C-C2C	2.50	1.49	1.44
23	C	514	CLA	C4D-CHA	2.50	1.47	1.38
23	C	507	CLA	C4D-CHA	2.50	1.47	1.38
23	c	506	CLA	C1C-C2C	2.50	1.49	1.44
23	A	407	CLA	C4D-CHA	2.50	1.47	1.38
28	D	407[A]	PL9	C6-C5	2.50	1.48	1.35
26	b	620	SQD	C6-S	-2.49	1.68	1.77
25	o	302	GOL	C1-C2	2.49	1.62	1.51
31	B	630	LMT	O2'-C2'	-2.49	1.37	1.43
23	A	407	CLA	C3B-C2B	2.49	1.49	1.41
23	C	512	CLA	C1C-C2C	2.49	1.49	1.44
23	B	605	CLA	C3D-C4D	-2.48	1.38	1.44
33	C	522	LMG	O1-C1	2.48	1.44	1.40
23	d	402	CLA	C1B-C2B	2.48	1.49	1.43
23	b	611	CLA	C1C-C2C	2.48	1.49	1.44
23	c	509	CLA	C3D-C4D	-2.48	1.38	1.44
23	B	608	CLA	C4D-CHA	2.48	1.47	1.38
25	D	414	GOL	C3-C2	2.48	1.61	1.51
23	B	616	CLA	C1C-NC	-2.48	1.34	1.37
37	D	402[A]	PHO	C3D-C4D	-2.48	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	C3B-C4B	2.48	1.48	1.42
23	B	604	CLA	C4C-C3C	2.48	1.49	1.45
23	C	505	CLA	C1B-C2B	2.48	1.49	1.43
31	m	103	LMT	C3'-C2'	2.47	1.58	1.52
37	D	402[B]	PHO	C3A-C2A	-2.47	1.52	1.54
23	a	405[A]	CLA	C1C-C2C	2.47	1.49	1.44
23	a	405[A]	CLA	C1B-C2B	2.47	1.49	1.43
23	b	609	CLA	C1B-C2B	2.47	1.49	1.43
23	C	515	CLA	C4D-CHA	2.47	1.47	1.38
23	B	616	CLA	C3B-C2B	2.47	1.49	1.41
23	C	512	CLA	C4D-CHA	2.47	1.47	1.38
23	D	404[A]	CLA	C1C-C2C	2.46	1.49	1.44
23	B	603	CLA	C1C-C2C	2.46	1.49	1.44
23	B	601	CLA	C4D-CHA	2.46	1.47	1.38
23	A	407	CLA	C1B-C2B	2.46	1.49	1.43
23	D	404[B]	CLA	C3D-C4D	-2.46	1.38	1.44
23	B	608	CLA	C3D-C4D	-2.46	1.38	1.44
23	C	504	CLA	C3B-C4B	2.46	1.48	1.42
23	b	616	CLA	C4D-CHA	2.45	1.47	1.38
26	B	620	SQD	C6-S	-2.45	1.68	1.77
23	a	405[B]	CLA	C3B-C2B	2.45	1.49	1.41
23	c	514	CLA	C4C-C3C	2.45	1.49	1.45
23	b	612	CLA	C3B-C2B	2.45	1.49	1.41
37	a	416[B]	PHO	C3A-C2A	-2.45	1.52	1.54
23	B	606	CLA	C3D-C4D	-2.45	1.38	1.44
23	B	606	CLA	C4D-CHA	2.45	1.47	1.38
23	C	510	CLA	C3B-C4B	2.45	1.48	1.42
23	d	401[A]	CLA	C3D-C4D	-2.45	1.38	1.44
31	B	628	LMT	C3'-C2'	2.44	1.58	1.52
23	b	614	CLA	C4B-NB	-2.44	1.34	1.37
23	C	505	CLA	C4C-C3C	2.44	1.49	1.45
31	A	417	LMT	O3'-C3'	-2.43	1.37	1.43
23	b	611	CLA	C4B-NB	-2.43	1.34	1.37
23	d	401[B]	CLA	C3B-C4B	2.43	1.48	1.42
23	A	404[A]	CLA	C3B-C4B	2.43	1.48	1.42
23	D	404[A]	CLA	C3D-C4D	-2.43	1.38	1.44
23	D	405	CLA	C4D-CHA	2.43	1.47	1.38
23	b	601	CLA	C1B-C2B	2.43	1.49	1.43
28	D	407[B]	PL9	C6-C5	2.43	1.48	1.35
23	A	404[B]	CLA	C1B-C2B	2.43	1.49	1.43
23	b	607	CLA	C3B-C4B	2.42	1.48	1.42
23	C	509	CLA	C3B-C4B	2.42	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	C4B-NB	-2.42	1.34	1.37
23	A	404[A]	CLA	C1C-C2C	2.42	1.49	1.44
23	B	612	CLA	C3B-C2B	2.42	1.49	1.41
23	C	511	CLA	C3B-C2B	2.42	1.49	1.41
23	b	606	CLA	C3D-C4D	-2.41	1.38	1.44
23	B	603	CLA	C3B-C2B	2.41	1.49	1.41
23	d	401[A]	CLA	C3B-C4B	2.41	1.48	1.42
23	B	610	CLA	C4C-C3C	2.41	1.49	1.45
23	C	513	CLA	C1B-NB	-2.40	1.34	1.37
23	c	503	CLA	C3B-C2B	2.40	1.49	1.41
37	a	416[A]	PHO	C4B-NB	-2.40	1.34	1.38
23	C	508	CLA	C4D-CHA	2.40	1.46	1.38
23	C	506	CLA	C3D-C4D	-2.40	1.38	1.44
23	B	605	CLA	C4B-NB	-2.39	1.34	1.37
23	C	513	CLA	C3D-C4D	-2.39	1.38	1.44
37	a	408[A]	PHO	C4B-NB	-2.39	1.34	1.38
23	A	406[A]	CLA	C1C-C2C	2.39	1.49	1.44
31	M	101	LMT	O2'-C2'	-2.39	1.37	1.43
23	D	404[A]	CLA	C3B-C2B	2.38	1.49	1.41
31	t	102	LMT	O2'-C2'	-2.38	1.37	1.43
23	C	513	CLA	C3B-C2B	2.38	1.49	1.41
25	D	403	GOL	O2-C2	-2.38	1.36	1.43
23	c	512	CLA	C3B-C4B	2.38	1.48	1.42
38	f	101	HEM	C1D-ND	-2.38	1.33	1.38
23	c	510	CLA	C3B-C4B	2.38	1.48	1.42
23	b	616	CLA	C3D-C4D	-2.38	1.38	1.44
23	a	407[B]	CLA	C4C-C3C	2.38	1.49	1.45
37	D	402[A]	PHO	C4B-NB	-2.38	1.34	1.38
23	B	607	CLA	C3D-C4D	-2.38	1.38	1.44
23	C	504	CLA	C3D-C4D	-2.37	1.38	1.44
23	C	515	CLA	C3B-C2B	2.37	1.49	1.41
35	h	102	DGD	O5D-C1E	2.37	1.44	1.40
23	C	514	CLA	C1B-C2B	2.37	1.48	1.43
23	C	511	CLA	C1B-C2B	2.37	1.48	1.43
23	c	509	CLA	C1B-NB	-2.37	1.34	1.37
23	a	407[A]	CLA	C3D-C4D	-2.36	1.38	1.44
37	D	402[A]	PHO	C3A-C2A	-2.36	1.52	1.54
23	C	514	CLA	C3D-C4D	-2.36	1.38	1.44
23	b	605	CLA	C3D-C4D	-2.36	1.38	1.44
23	b	610	CLA	C1B-C2B	2.36	1.48	1.43
23	B	604	CLA	C1A-CHA	2.36	1.52	1.43
23	a	405[A]	CLA	C4C-C3C	2.36	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	C1B-C2B	2.36	1.48	1.43
23	B	608	CLA	C3B-C2B	2.36	1.49	1.41
23	b	607	CLA	OBD-CAD	2.36	1.26	1.22
23	c	509	CLA	C3B-C2B	2.35	1.49	1.41
23	C	510	CLA	C4C-C3C	2.35	1.49	1.45
23	d	401[B]	CLA	C1C-C2C	2.35	1.49	1.44
31	b	621	LMT	C3'-C2'	2.35	1.58	1.52
23	C	507	CLA	C3D-C4D	-2.35	1.38	1.44
23	A	406[B]	CLA	C1B-C2B	2.35	1.48	1.43
38	F	102	HEM	C1C-C2C	-2.35	1.40	1.45
23	b	611	CLA	C4D-CHA	2.34	1.46	1.38
23	C	513	CLA	C4C-C3C	2.34	1.49	1.45
23	c	514	CLA	C3D-C4D	-2.34	1.38	1.44
23	d	401[B]	CLA	C4D-CHA	2.34	1.46	1.38
23	b	615	CLA	C3D-C4D	-2.34	1.38	1.44
40	v	201	HEC	CMC-C2C	2.33	1.55	1.50
37	a	408[B]	PHO	C4B-NB	-2.33	1.34	1.38
23	B	616	CLA	C3B-C4B	2.33	1.48	1.42
23	c	512	CLA	C3B-C2B	2.33	1.49	1.41
23	B	611	CLA	C4D-CHA	2.33	1.46	1.38
23	b	610	CLA	C4C-C3C	2.33	1.49	1.45
28	d	404[A]	PL9	C6-C5	2.33	1.47	1.35
23	A	404[B]	CLA	C3B-C2B	2.32	1.49	1.41
34	B	623	HTG	C1'-S1	-2.32	1.78	1.81
23	b	614	CLA	C1C-C2C	2.31	1.49	1.44
23	c	502	CLA	C3D-C4D	-2.31	1.39	1.44
23	a	406[B]	CLA	C4B-NB	-2.31	1.34	1.37
23	b	616	CLA	C1B-C2B	2.31	1.48	1.43
37	a	416[B]	PHO	CHA-CBD	-2.31	1.48	1.51
23	c	507	CLA	C3B-C4B	2.31	1.48	1.42
23	C	503	CLA	C4C-C3C	2.31	1.49	1.45
23	D	404[B]	CLA	C1B-C2B	2.31	1.48	1.43
23	a	409	CLA	C4D-CHA	2.30	1.46	1.38
23	D	404[B]	CLA	C3B-C2B	2.30	1.49	1.41
23	b	614	CLA	C4D-CHA	2.30	1.46	1.38
24	B	619	BCR	C30-C25	-2.30	1.50	1.53
31	c	501	LMT	O2'-C2'	-2.30	1.37	1.43
23	a	409	CLA	C1D-C2D	2.30	1.49	1.45
23	B	608	CLA	C1C-C2C	2.30	1.49	1.44
23	C	512	CLA	C1D-C2D	2.29	1.49	1.45
38	F	102	HEM	C3B-C4B	2.29	1.49	1.44
23	B	611	CLA	C3D-C4D	-2.29	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	628	LMT	O3'-C3'	-2.29	1.37	1.43
23	d	402	CLA	C4C-C3C	2.29	1.49	1.45
23	b	601	CLA	C3B-C2B	2.29	1.48	1.41
23	d	401[B]	CLA	C3B-C2B	2.28	1.48	1.41
37	a	416[B]	PHO	C4B-NB	-2.28	1.34	1.38
40	v	201	HEC	CAC-C3C	2.28	1.57	1.51
23	b	604	CLA	C3B-C2B	2.28	1.48	1.41
23	c	511	CLA	C4C-C3C	2.28	1.49	1.45
23	B	612	CLA	C4C-C3C	2.28	1.49	1.45
23	D	404[B]	CLA	C3B-C4B	2.28	1.48	1.42
23	B	602	CLA	C3B-C2B	2.28	1.48	1.41
23	A	407	CLA	C4C-C3C	2.27	1.49	1.45
23	C	512	CLA	C3B-C4B	2.27	1.48	1.42
23	b	613	CLA	C3B-C2B	2.27	1.48	1.41
23	B	601	CLA	C4C-C3C	2.27	1.49	1.45
31	e	101	LMT	O3'-C3'	-2.27	1.37	1.43
23	b	613	CLA	C3B-C4B	2.27	1.48	1.42
23	b	602	CLA	C1B-NB	-2.27	1.35	1.37
23	b	614	CLA	C4C-C3C	2.27	1.48	1.45
23	b	604	CLA	MG-NA	2.26	2.11	2.06
23	A	405[B]	CLA	C3D-C4D	-2.26	1.39	1.44
23	c	510	CLA	C3B-C2B	2.26	1.48	1.41
23	C	514	CLA	C4B-NB	-2.26	1.35	1.37
23	B	603	CLA	C3B-C4B	2.26	1.48	1.42
23	C	507	CLA	C4B-NB	-2.26	1.35	1.37
23	d	401[B]	CLA	C3D-C4D	-2.26	1.39	1.44
23	c	513	CLA	C4C-C3C	2.26	1.48	1.45
23	c	512	CLA	C4C-C3C	2.25	1.48	1.45
23	a	406[B]	CLA	C1C-C2C	2.25	1.48	1.44
23	A	405[A]	CLA	C3D-C4D	-2.25	1.39	1.44
23	C	508	CLA	C3D-C4D	-2.25	1.39	1.44
37	a	408[A]	PHO	C1D-ND	-2.25	1.34	1.38
23	a	405[B]	CLA	C1B-C2B	2.25	1.48	1.43
23	D	405	CLA	C3D-C4D	-2.25	1.39	1.44
23	b	603	CLA	C3B-C2B	2.25	1.48	1.41
23	b	606	CLA	C3B-C2B	2.25	1.48	1.41
23	B	613	CLA	C3D-C4D	-2.25	1.39	1.44
23	c	505	CLA	C1C-NC	-2.25	1.34	1.37
23	A	404[B]	CLA	C4C-C3C	2.24	1.48	1.45
26	F	103	SQD	O6-C1	2.24	1.44	1.40
23	b	614	CLA	C3B-C2B	2.24	1.48	1.41
23	B	608	CLA	C4C-C3C	2.24	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C3B-C2B	2.24	1.48	1.41
23	B	606	CLA	C4B-NB	-2.24	1.35	1.37
23	B	609	CLA	C3D-C4D	-2.23	1.39	1.44
23	b	611	CLA	C4C-C3C	2.23	1.48	1.45
23	b	608	CLA	C3B-C2B	2.23	1.48	1.41
25	D	403	GOL	C3-C2	2.23	1.60	1.51
23	a	405[B]	CLA	C4C-C3C	2.23	1.48	1.45
23	b	602	CLA	C3D-C4D	-2.23	1.39	1.44
23	C	509	CLA	C3B-C2B	2.22	1.48	1.41
35	c	519	DGD	O5D-C1E	2.22	1.44	1.40
35	C	519[A]	DGD	O5D-C1E	2.22	1.44	1.40
23	a	407[B]	CLA	C3D-C4D	-2.22	1.39	1.44
23	A	405[B]	CLA	C1C-C2C	2.22	1.48	1.44
23	c	509	CLA	C4C-C3C	2.22	1.48	1.45
23	C	514	CLA	C3B-C2B	2.22	1.48	1.41
23	c	503	CLA	C4D-CHA	2.22	1.46	1.38
31	M	101	LMT	O3'-C3'	-2.22	1.37	1.43
23	B	610	CLA	C3D-C4D	-2.22	1.39	1.44
23	d	402	CLA	C1D-C2D	2.22	1.49	1.45
31	M	101	LMT	C1B-C2B	2.22	1.58	1.52
23	A	407	CLA	C1C-NC	-2.21	1.34	1.37
37	D	401[B]	PHO	CBD-CGD	-2.21	1.49	1.52
23	c	508	CLA	C3D-C4D	-2.21	1.39	1.44
40	v	201	HEC	FE-NC	2.21	2.02	1.95
23	C	508	CLA	C1D-C2D	2.21	1.49	1.45
37	D	402[B]	PHO	C4B-NB	-2.21	1.34	1.38
23	c	503	CLA	C3D-C4D	-2.21	1.39	1.44
23	A	404[A]	CLA	C3B-C2B	2.20	1.48	1.41
23	A	406[B]	CLA	C3D-C4D	-2.20	1.39	1.44
23	B	603	CLA	C1B-C2B	2.20	1.48	1.43
40	V	202	HEC	CMB-C2B	2.20	1.55	1.50
23	b	615	CLA	C4B-NB	-2.20	1.35	1.37
23	B	601	CLA	C1C-NC	-2.19	1.34	1.37
23	C	504	CLA	C4D-CHA	2.19	1.46	1.38
23	B	614	CLA	C3B-C2B	2.19	1.48	1.41
23	c	511	CLA	C3B-C2B	2.19	1.48	1.41
23	a	405[A]	CLA	C3B-C4B	2.19	1.47	1.42
24	B	618	BCR	C19-C18	2.19	1.50	1.45
37	a	416[B]	PHO	C1B-NB	-2.19	1.34	1.38
23	B	607	CLA	C3B-C2B	2.19	1.48	1.41
23	B	604	CLA	MG-NA	2.19	2.11	2.06
23	c	512	CLA	MG-NA	2.18	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D	402[A]	PHO	C1D-ND	-2.18	1.34	1.38
23	D	404[A]	CLA	C4C-C3C	2.18	1.48	1.45
23	b	608	CLA	C1B-C2B	2.18	1.48	1.43
23	C	512	CLA	C3D-C4D	-2.18	1.39	1.44
23	c	505	CLA	C3D-C4D	-2.17	1.39	1.44
23	c	507	CLA	C3D-C4D	-2.17	1.39	1.44
23	b	608	CLA	C3D-C4D	-2.17	1.39	1.44
31	m	103	LMT	O2B-C2B	-2.17	1.37	1.43
23	c	514	CLA	C3B-C2B	2.17	1.48	1.41
23	D	404[B]	CLA	C1C-C2C	2.17	1.48	1.44
23	b	609	CLA	C3D-C4D	-2.16	1.39	1.44
23	a	405[A]	CLA	C3B-C2B	2.16	1.48	1.41
23	B	606	CLA	C4C-C3C	2.16	1.48	1.45
31	F	101	LMT	O3'-C3'	-2.16	1.37	1.43
23	b	611	CLA	C3B-C2B	2.16	1.48	1.41
23	D	404[A]	CLA	C3B-C4B	2.15	1.47	1.42
23	b	608	CLA	C4C-C3C	2.15	1.48	1.45
24	a	410	BCR	C19-C18	2.15	1.50	1.45
37	D	402[B]	PHO	C1D-ND	-2.15	1.34	1.38
23	b	614	CLA	C3D-C4D	-2.15	1.39	1.44
37	a	408[B]	PHO	C3A-C2A	-2.15	1.52	1.54
23	B	601	CLA	C3D-C4D	-2.15	1.39	1.44
31	B	630	LMT	O3B-C3B	-2.15	1.37	1.43
23	C	503	CLA	C3B-C2B	2.14	1.48	1.41
23	c	513	CLA	C3D-C4D	-2.14	1.39	1.44
25	b	624	GOL	C3-C2	2.14	1.60	1.51
23	B	607	CLA	C1C-NC	-2.14	1.34	1.37
23	C	515	CLA	C3D-C4D	-2.14	1.39	1.44
23	B	615	CLA	C4B-NB	-2.14	1.35	1.37
23	b	612	CLA	C3D-C4D	-2.14	1.39	1.44
23	b	606	CLA	C1C-C2C	2.14	1.48	1.44
23	c	514	CLA	C1D-C2D	2.13	1.49	1.45
31	A	417	LMT	O2'-C2'	-2.13	1.38	1.43
37	D	401[B]	PHO	C1D-ND	-2.13	1.34	1.38
23	c	507	CLA	C3B-C2B	2.13	1.48	1.41
23	B	614	CLA	C4C-C3C	2.13	1.48	1.45
23	C	509	CLA	C3D-C4D	-2.13	1.39	1.44
23	C	510	CLA	C1C-NC	-2.13	1.34	1.37
35	c	519	DGD	O2G-C2G	-2.12	1.41	1.46
37	D	402[B]	PHO	C3D-C4D	-2.12	1.38	1.41
23	a	405[B]	CLA	C3D-C4D	-2.12	1.39	1.44
23	B	601	CLA	C3B-C2B	2.12	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	C4C-C3C	2.12	1.48	1.45
31	b	627	LMT	O3'-C3'	-2.12	1.38	1.43
28	a	414[A]	PL9	C2-C3	2.12	1.40	1.34
23	b	602	CLA	C1B-C2B	2.12	1.48	1.43
23	a	406[A]	CLA	C1C-C2C	2.12	1.48	1.44
23	A	406[A]	CLA	C1C-NC	-2.12	1.34	1.37
37	D	401[B]	PHO	CHA-CBD	-2.11	1.49	1.51
31	c	501	LMT	O3'-C3'	-2.11	1.38	1.43
23	B	610	CLA	C4B-NB	-2.11	1.35	1.37
23	A	406[A]	CLA	C3D-C4D	-2.11	1.39	1.44
23	a	406[B]	CLA	C3D-C4D	-2.11	1.39	1.44
24	C	517	BCR	C1-C6	-2.11	1.50	1.53
38	F	102	HEM	C3C-C4C	-2.11	1.42	1.46
23	b	604	CLA	C4C-C3C	2.11	1.48	1.45
37	D	401[B]	PHO	C1B-NB	-2.11	1.34	1.38
23	b	616	CLA	C3B-C2B	2.10	1.48	1.41
23	C	511	CLA	C4C-C3C	2.10	1.48	1.45
23	c	503	CLA	C4C-C3C	2.10	1.48	1.45
31	T	101	LMT	O3B-C3B	-2.10	1.38	1.43
40	v	201	HEC	CAB-C3B	2.10	1.56	1.51
37	a	408[B]	PHO	C1D-ND	-2.10	1.34	1.38
23	C	504	CLA	C4C-C3C	2.10	1.48	1.45
23	a	405[A]	CLA	C3D-C4D	-2.10	1.39	1.44
23	a	407[A]	CLA	C4C-C3C	2.10	1.48	1.45
40	v	201	HEC	CMD-C2D	2.10	1.55	1.50
23	C	508	CLA	C3B-C2B	2.10	1.48	1.41
23	b	608	CLA	C1C-C2C	2.10	1.48	1.44
23	B	613	CLA	C3B-C2B	2.09	1.48	1.41
23	c	505	CLA	C3B-C2B	2.09	1.48	1.41
28	a	414[B]	PL9	C2-C3	2.09	1.40	1.34
23	D	404[B]	CLA	C4C-C3C	2.09	1.48	1.45
26	B	620	SQD	O6-C1	2.09	1.43	1.40
23	c	506	CLA	C4B-NB	-2.09	1.35	1.37
23	d	401[A]	CLA	C3B-C2B	2.09	1.48	1.41
37	a	416[A]	PHO	C1B-NB	-2.08	1.34	1.38
23	B	606	CLA	C3B-C2B	2.08	1.48	1.41
23	a	406[B]	CLA	C3B-C2B	2.08	1.48	1.41
23	b	607	CLA	C3B-C2B	2.08	1.48	1.41
37	D	401[B]	PHO	C4B-NB	-2.08	1.34	1.38
23	b	602	CLA	C1D-C2D	2.08	1.49	1.45
23	A	406[B]	CLA	C4C-C3C	2.08	1.48	1.45
23	B	608	CLA	C1C-NC	-2.08	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	C1C-NC	-2.07	1.34	1.37
23	B	607	CLA	C4C-C3C	2.07	1.48	1.45
35	c	518[A]	DGD	O2G-C2G	-2.07	1.41	1.46
25	c	527	GOL	C3-C2	2.07	1.60	1.51
23	c	510	CLA	C1C-NC	-2.07	1.34	1.37
23	a	409	CLA	C3B-C2B	2.06	1.48	1.41
23	c	502	CLA	C1C-NC	-2.06	1.34	1.37
31	M	101	LMT	O2B-C2B	-2.06	1.38	1.43
23	b	613	CLA	C4C-C3C	2.06	1.48	1.45
23	A	406[B]	CLA	C1D-C2D	2.05	1.49	1.45
25	a	418	GOL	C1-C2	2.05	1.60	1.51
37	D	401[A]	PHO	C1B-NB	-2.05	1.34	1.38
31	b	627	LMT	O2'-C2'	-2.04	1.38	1.43
23	A	407	CLA	C3D-C4D	-2.04	1.39	1.44
31	A	415	LMT	O2'-C2'	-2.04	1.38	1.43
24	b	617	BCR	C19-C18	2.04	1.50	1.45
23	a	405[B]	CLA	C4B-NB	-2.04	1.35	1.37
25	a	418	GOL	C3-C2	2.04	1.60	1.51
23	B	607	CLA	C3B-C4B	2.04	1.47	1.42
28	A	412[A]	PL9	C2-C1	-2.04	1.39	1.44
32	d	405[B]	LHG	O7-C5	-2.04	1.41	1.46
23	A	404[B]	CLA	C3D-C4D	-2.04	1.39	1.44
23	b	603	CLA	C4C-C3C	2.04	1.48	1.45
23	b	607	CLA	C1A-CHA	2.03	1.51	1.43
23	d	402	CLA	C3D-C4D	-2.03	1.39	1.44
23	B	613	CLA	C1C-NC	-2.03	1.34	1.37
37	a	408[B]	PHO	C1B-NB	-2.03	1.34	1.38
31	e	101	LMT	O2B-C2B	-2.03	1.38	1.43
31	e	101	LMT	O2'-C2'	-2.03	1.38	1.43
23	A	404[A]	CLA	C3D-C4D	-2.03	1.39	1.44
23	B	616	CLA	C3D-C4D	-2.03	1.39	1.44
23	C	509	CLA	C4B-NB	-2.02	1.35	1.37
23	B	607	CLA	C1A-CHA	2.02	1.51	1.43
23	c	507	CLA	C1C-NC	-2.02	1.34	1.37
23	b	609	CLA	C3B-C2B	2.02	1.48	1.41
23	A	405[B]	CLA	C4C-C3C	2.02	1.48	1.45
23	A	405[B]	CLA	C1D-C2D	2.02	1.49	1.45
31	B	628	LMT	O5'-C5'	-2.02	1.39	1.44
23	b	609	CLA	C4B-NB	-2.02	1.35	1.37
23	b	605	CLA	C3B-C2B	2.02	1.48	1.41
23	A	405[B]	CLA	C3B-C2B	2.02	1.48	1.41
28	A	412[B]	PL9	C2-C3	2.02	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	519[B]	DGD	O5D-C1E	2.01	1.43	1.40
23	b	603	CLA	C3D-C4D	-2.01	1.39	1.44
23	c	507	CLA	C1D-C2D	2.01	1.49	1.45
23	c	512	CLA	C1C-NC	-2.01	1.34	1.37
23	C	511	CLA	C3D-C4D	-2.01	1.39	1.44
23	c	504	CLA	MG-NA	2.01	2.11	2.06
23	B	615	CLA	C4C-C3C	2.00	1.48	1.45
23	B	612	CLA	C3B-C4B	2.00	1.47	1.42
37	D	401[B]	PHO	C3D-C4D	-2.00	1.38	1.41
23	c	502	CLA	C3B-C2B	2.00	1.48	1.41

All (3365) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C2B-C1B-NB	16.09	121.02	110.23
23	B	611	CLA	C3B-C2B-C1B	-13.14	91.30	107.16
37	D	401[A]	PHO	C2D-C1D-ND	11.89	117.73	109.53
37	a	416[A]	PHO	C2D-C1D-ND	11.37	117.38	109.53
37	a	416[B]	PHO	C2D-C1D-ND	11.27	117.31	109.53
37	D	401[B]	PHO	C2D-C1D-ND	11.26	117.30	109.53
37	a	408[A]	PHO	C2D-C1D-ND	11.17	117.24	109.53
23	B	611	CLA	C1D-ND-C4D	-11.15	98.41	106.33
23	a	409	CLA	C1D-ND-C4D	-11.14	98.42	106.33
37	D	402[B]	PHO	C2D-C1D-ND	10.95	117.09	109.53
37	D	402[A]	PHO	C2D-C1D-ND	10.94	117.08	109.53
37	a	408[B]	PHO	C2D-C1D-ND	10.66	116.88	109.53
23	B	611	CLA	CHB-C1B-NB	-10.60	113.03	124.26
23	b	605	CLA	C1D-ND-C4D	-10.37	98.97	106.33
23	a	409	CLA	C2D-C1D-ND	10.25	117.66	110.10
23	B	615	CLA	C1D-ND-C4D	-10.07	99.18	106.33
23	B	606	CLA	C1D-ND-C4D	-10.06	99.19	106.33
23	a	407[B]	CLA	C1D-ND-C4D	-10.03	99.21	106.33
23	B	610	CLA	C2D-C1D-ND	9.91	117.41	110.10
23	A	407	CLA	C1D-ND-C4D	-9.91	99.30	106.33
23	B	601	CLA	C1D-ND-C4D	-9.91	99.30	106.33
23	c	504	CLA	C1D-ND-C4D	-9.85	99.34	106.33
23	b	605	CLA	C2D-C1D-ND	9.75	117.29	110.10
23	d	401[B]	CLA	C1D-ND-C4D	-9.73	99.42	106.33
23	C	512	CLA	C1D-ND-C4D	-9.72	99.43	106.33
23	A	406[B]	CLA	C1D-ND-C4D	-9.69	99.45	106.33
23	C	506	CLA	C2D-C1D-ND	9.66	117.22	110.10
23	c	512	CLA	C1D-ND-C4D	-9.65	99.48	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	C1D-ND-C4D	-9.64	99.48	106.33
23	B	615	CLA	C2D-C1D-ND	9.63	117.20	110.10
23	b	602	CLA	C1D-ND-C4D	-9.62	99.50	106.33
23	b	614	CLA	C1D-ND-C4D	-9.60	99.52	106.33
23	B	610	CLA	C1D-ND-C4D	-9.57	99.54	106.33
23	C	515	CLA	C1D-ND-C4D	-9.57	99.54	106.33
23	b	601	CLA	C1D-ND-C4D	-9.56	99.54	106.33
23	a	405[B]	CLA	C1D-ND-C4D	-9.54	99.56	106.33
23	C	505	CLA	C1D-ND-C4D	-9.50	99.58	106.33
23	D	404[B]	CLA	C1D-ND-C4D	-9.48	99.60	106.33
23	B	614	CLA	C1D-ND-C4D	-9.47	99.61	106.33
23	c	510	CLA	C1D-ND-C4D	-9.47	99.61	106.33
23	C	507	CLA	C1D-ND-C4D	-9.46	99.61	106.33
23	B	612	CLA	C1D-ND-C4D	-9.45	99.62	106.33
23	A	405[B]	CLA	C1D-ND-C4D	-9.45	99.62	106.33
23	b	603	CLA	C1D-ND-C4D	-9.44	99.63	106.33
23	A	404[B]	CLA	C1D-ND-C4D	-9.43	99.63	106.33
23	b	609	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	b	613	CLA	C2D-C1D-ND	9.31	116.96	110.10
23	B	611	CLA	C2D-C1D-ND	9.30	116.96	110.10
23	b	611	CLA	C1D-ND-C4D	-9.30	99.73	106.33
23	B	605	CLA	C1D-ND-C4D	-9.28	99.74	106.33
23	d	402	CLA	C1D-ND-C4D	-9.28	99.74	106.33
23	c	514	CLA	C1D-ND-C4D	-9.26	99.76	106.33
23	C	506	CLA	C1D-ND-C4D	-9.25	99.77	106.33
23	b	606	CLA	C1D-ND-C4D	-9.24	99.77	106.33
23	B	607	CLA	C1D-ND-C4D	-9.22	99.78	106.33
23	a	407[A]	CLA	C1D-ND-C4D	-9.17	99.82	106.33
23	b	610	CLA	C1D-ND-C4D	-9.17	99.82	106.33
23	b	614	CLA	C2D-C1D-ND	9.16	116.86	110.10
23	D	404[A]	CLA	C1D-ND-C4D	-9.16	99.83	106.33
23	A	407	CLA	C2D-C1D-ND	9.11	116.81	110.10
23	B	607	CLA	C2D-C1D-ND	9.10	116.81	110.10
23	d	401[A]	CLA	C1D-ND-C4D	-9.09	99.88	106.33
23	A	406[A]	CLA	C1D-ND-C4D	-9.08	99.89	106.33
23	a	406[A]	CLA	C1D-ND-C4D	-9.04	99.91	106.33
23	C	511	CLA	C1D-ND-C4D	-9.04	99.91	106.33
23	B	608	CLA	C1D-ND-C4D	-8.99	99.95	106.33
23	C	508	CLA	C1D-ND-C4D	-8.98	99.95	106.33
23	b	616	CLA	C1D-ND-C4D	-8.95	99.98	106.33
23	B	612	CLA	C2D-C1D-ND	8.94	116.69	110.10
23	b	615	CLA	C1D-ND-C4D	-8.94	99.98	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	C2D-C1D-ND	8.94	116.69	110.10
23	a	406[B]	CLA	C1D-ND-C4D	-8.92	100.00	106.33
23	B	605	CLA	C2D-C1D-ND	8.91	116.67	110.10
23	A	405[A]	CLA	C1D-ND-C4D	-8.91	100.01	106.33
23	B	609	CLA	C1D-ND-C4D	-8.91	100.01	106.33
23	B	603	CLA	C1D-ND-C4D	-8.87	100.03	106.33
23	B	602	CLA	C1D-ND-C4D	-8.83	100.06	106.33
23	a	405[A]	CLA	C1D-ND-C4D	-8.83	100.06	106.33
23	c	502	CLA	C1D-ND-C4D	-8.83	100.06	106.33
23	b	601	CLA	C2D-C1D-ND	8.77	116.56	110.10
23	c	513	CLA	C1D-ND-C4D	-8.76	100.11	106.33
23	a	406[A]	CLA	C2D-C1D-ND	8.75	116.56	110.10
23	B	606	CLA	C2D-C1D-ND	8.75	116.55	110.10
23	D	404[B]	CLA	C2D-C1D-ND	8.74	116.55	110.10
23	C	503	CLA	C1D-ND-C4D	-8.72	100.14	106.33
23	C	509	CLA	C1D-ND-C4D	-8.72	100.14	106.33
23	B	613	CLA	C1D-ND-C4D	-8.71	100.15	106.33
23	B	614	CLA	C2D-C1D-ND	8.69	116.51	110.10
23	a	407[A]	CLA	C2D-C1D-ND	8.65	116.48	110.10
23	b	612	CLA	C1D-ND-C4D	-8.63	100.21	106.33
23	B	616	CLA	C2D-C1D-ND	8.61	116.45	110.10
23	C	514	CLA	C1D-ND-C4D	-8.61	100.22	106.33
23	b	607	CLA	C1D-ND-C4D	-8.59	100.23	106.33
23	c	507	CLA	C1D-ND-C4D	-8.55	100.26	106.33
23	c	512	CLA	C2D-C1D-ND	8.55	116.40	110.10
23	c	510	CLA	C2D-C1D-ND	8.51	116.38	110.10
23	D	404[A]	CLA	C2D-C1D-ND	8.50	116.37	110.10
23	A	404[A]	CLA	C1D-ND-C4D	-8.50	100.30	106.33
23	b	603	CLA	C2D-C1D-ND	8.48	116.36	110.10
23	c	508	CLA	C1D-ND-C4D	-8.48	100.31	106.33
23	a	407[B]	CLA	C2D-C1D-ND	8.44	116.32	110.10
23	B	601	CLA	C2D-C1D-ND	8.43	116.32	110.10
23	c	503	CLA	C1D-ND-C4D	-8.41	100.36	106.33
23	A	405[B]	CLA	C2D-C1D-ND	8.39	116.29	110.10
23	a	406[B]	CLA	C2D-C1D-ND	8.39	116.28	110.10
23	C	510	CLA	C1D-ND-C4D	-8.38	100.38	106.33
23	b	608	CLA	C1D-ND-C4D	-8.38	100.38	106.33
23	C	504	CLA	C1D-ND-C4D	-8.37	100.39	106.33
23	C	515	CLA	C2D-C1D-ND	8.35	116.26	110.10
23	b	611	CLA	C2D-C1D-ND	8.35	116.26	110.10
23	b	616	CLA	C2D-C1D-ND	8.34	116.25	110.10
23	b	613	CLA	C1D-ND-C4D	-8.31	100.43	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	C2D-C1D-ND	8.31	116.23	110.10
23	a	405[B]	CLA	C2B-C1B-NB	8.31	115.80	110.23
23	c	511	CLA	C1D-ND-C4D	-8.29	100.45	106.33
23	c	508	CLA	C2D-C1D-ND	8.28	116.20	110.10
23	b	602	CLA	C4A-NA-C1A	-8.26	102.99	106.71
23	A	405[A]	CLA	C2D-C1D-ND	8.25	116.18	110.10
23	A	406[B]	CLA	C2B-C1B-NB	8.23	115.75	110.23
23	C	505	CLA	C2D-C1D-ND	8.22	116.16	110.10
23	b	609	CLA	C2D-C1D-ND	8.22	116.16	110.10
23	C	510	CLA	C2D-C1D-ND	8.22	116.16	110.10
23	B	616	CLA	C1D-ND-C4D	-8.22	100.50	106.33
23	b	606	CLA	C2D-C1D-ND	8.18	116.14	110.10
23	B	608	CLA	C2D-C1D-ND	8.18	116.13	110.10
23	B	609	CLA	C2D-C1D-ND	8.17	116.12	110.10
23	c	505	CLA	C1D-ND-C4D	-8.16	100.54	106.33
23	A	406[A]	CLA	C2D-C1D-ND	8.15	116.11	110.10
23	b	615	CLA	C2D-C1D-ND	8.15	116.11	110.10
23	d	402	CLA	C2D-C1D-ND	8.15	116.11	110.10
37	a	408[A]	PHO	O2D-CGD-CBD	8.14	121.31	111.00
23	b	602	CLA	C2B-C1B-NB	8.10	115.66	110.23
23	C	509	CLA	C2D-C1D-ND	8.09	116.07	110.10
23	A	404[B]	CLA	C2D-C1D-ND	8.07	116.05	110.10
23	c	503	CLA	C2D-C1D-ND	8.05	116.03	110.10
23	c	513	CLA	C2D-C1D-ND	8.04	116.03	110.10
23	c	505	CLA	C2D-C1D-ND	8.04	116.03	110.10
23	D	404[B]	CLA	C4A-NA-C1A	-8.03	103.10	106.71
23	c	514	CLA	C2B-C1B-NB	8.03	115.61	110.23
23	c	509	CLA	C1D-ND-C4D	-8.02	100.64	106.33
23	C	511	CLA	C2D-C1D-ND	8.02	116.01	110.10
23	c	513	CLA	C2B-C1B-NB	7.97	115.57	110.23
23	A	406[B]	CLA	C2D-C1D-ND	7.94	115.96	110.10
23	b	607	CLA	C2D-C1D-ND	7.93	115.94	110.10
23	b	606	CLA	C2B-C1B-NB	7.92	115.54	110.23
23	c	504	CLA	C2D-C1D-ND	7.90	115.93	110.10
37	a	408[B]	PHO	O2D-CGD-CBD	7.88	120.98	111.00
23	B	609	CLA	C4A-NA-C1A	-7.87	103.17	106.71
23	C	514	CLA	C2B-C1B-NB	7.87	115.51	110.23
37	D	402[B]	PHO	O2D-CGD-CBD	7.87	120.97	111.00
34	b	623	HTG	C1'-S1-C1	7.86	114.79	100.09
23	b	610	CLA	C2D-C1D-ND	7.84	115.88	110.10
23	d	401[B]	CLA	C2D-C1D-ND	7.83	115.88	110.10
37	a	416[A]	PHO	O2D-CGD-CBD	7.83	120.91	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D	401[B]	PHO	O2D-CGD-CBD	7.83	120.91	111.00
23	d	401[A]	CLA	C2D-C1D-ND	7.82	115.87	110.10
23	c	509	CLA	C2D-C1D-ND	7.81	115.86	110.10
23	a	405[B]	CLA	C2D-C1D-ND	7.81	115.86	110.10
23	C	515	CLA	C2B-C1B-NB	7.80	115.46	110.23
23	c	502	CLA	C2D-C1D-ND	7.77	115.83	110.10
23	C	513	CLA	C1D-ND-C4D	-7.76	100.82	106.33
23	a	407[B]	CLA	C2B-C1B-NB	7.76	115.43	110.23
23	b	602	CLA	C2D-C1D-ND	7.74	115.81	110.10
37	a	416[B]	PHO	O2D-CGD-CBD	7.70	120.75	111.00
23	C	503	CLA	C2D-C1D-ND	7.68	115.76	110.10
23	A	407	CLA	C2B-C1B-NB	7.67	115.37	110.23
23	C	513	CLA	C2D-C1D-ND	7.66	115.75	110.10
23	A	404[A]	CLA	C2D-C1D-ND	7.64	115.73	110.10
23	c	514	CLA	C2D-C1D-ND	7.64	115.73	110.10
23	C	504	CLA	C2D-C1D-ND	7.63	115.73	110.10
23	c	506	CLA	C2D-C1D-ND	7.62	115.72	110.10
23	C	512	CLA	CMD-C2D-C1D	7.60	138.12	124.71
23	C	512	CLA	C2D-C1D-ND	7.60	115.71	110.10
23	C	507	CLA	C2D-C1D-ND	7.60	115.70	110.10
23	B	602	CLA	C2D-C1D-ND	7.59	115.69	110.10
23	B	611	CLA	CHD-C4C-C3C	-7.54	113.75	124.84
23	A	406[A]	CLA	C2B-C1B-NB	7.52	115.27	110.23
23	d	402	CLA	C2B-C1B-NB	7.51	115.27	110.23
23	D	405	CLA	C1D-ND-C4D	-7.49	101.02	106.33
37	D	402[A]	PHO	C2B-C1B-NB	7.46	114.68	109.53
37	D	402[A]	PHO	O2D-CGD-CBD	7.46	120.44	111.00
23	B	614	CLA	C2B-C1B-NB	7.45	115.23	110.23
23	C	509	CLA	O2D-CGD-CBD	7.44	124.49	111.27
23	b	604	CLA	C1D-ND-C4D	-7.44	101.05	106.33
23	c	503	CLA	C2B-C1B-NB	7.43	115.21	110.23
23	c	504	CLA	C4A-NA-C1A	-7.40	103.38	106.71
23	c	504	CLA	CMD-C2D-C1D	7.38	137.72	124.71
23	a	409	CLA	C2B-C1B-NB	7.38	115.18	110.23
23	b	603	CLA	C2B-C1B-NB	7.36	115.17	110.23
23	C	508	CLA	C2D-C1D-ND	7.36	115.53	110.10
23	c	511	CLA	C2B-C1B-NB	7.36	115.17	110.23
23	B	601	CLA	C2B-C1B-NB	7.36	115.17	110.23
23	b	604	CLA	C2D-C1D-ND	7.35	115.52	110.10
37	D	401[A]	PHO	C4D-ND-C1D	-7.35	101.35	108.83
23	B	611	CLA	CMB-C2B-C1B	7.35	136.56	125.37
23	c	504	CLA	C2B-C1B-NB	7.33	115.15	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	C2D-C1D-ND	7.33	115.50	110.10
23	a	405[A]	CLA	C2D-C1D-ND	7.32	115.50	110.10
23	C	505	CLA	C4A-NA-C1A	-7.31	103.42	106.71
23	D	405	CLA	C4A-NA-C1A	-7.31	103.42	106.71
23	B	604	CLA	C1D-ND-C4D	-7.31	101.14	106.33
23	C	514	CLA	C2D-C1D-ND	7.31	115.49	110.10
23	b	605	CLA	CHD-C4C-C3C	-7.27	114.16	124.84
23	A	404[B]	CLA	C2B-C1B-NB	7.25	115.09	110.23
23	b	608	CLA	C2D-C1D-ND	7.24	115.44	110.10
23	D	404[A]	CLA	C4A-NA-C1A	-7.21	103.46	106.71
23	b	615	CLA	C4A-NA-C1A	-7.18	103.48	106.71
23	b	616	CLA	C2B-C1B-NB	7.17	115.04	110.23
23	b	616	CLA	O2D-CGD-CBD	7.16	123.99	111.27
23	A	405[A]	CLA	C2B-C1B-NB	7.15	115.03	110.23
23	b	614	CLA	C2B-C1B-NB	7.15	115.03	110.23
23	B	616	CLA	O2D-CGD-CBD	7.15	123.97	111.27
23	C	509	CLA	CMD-C2D-C1D	7.14	137.30	124.71
23	C	508	CLA	C2B-C1B-NB	7.14	115.02	110.23
23	b	612	CLA	C2D-C1D-ND	7.12	115.35	110.10
23	b	605	CLA	C2B-C1B-NB	7.12	115.00	110.23
23	C	511	CLA	C2B-C1B-NB	7.09	114.99	110.23
37	D	402[B]	PHO	C2B-C1B-NB	7.09	114.42	109.53
23	B	614	CLA	CMD-C2D-C1D	7.07	137.17	124.71
23	B	605	CLA	CHD-C4C-C3C	-7.06	114.46	124.84
23	b	616	CLA	C4A-NA-C1A	-7.04	103.54	106.71
23	C	505	CLA	C2B-C1B-NB	7.04	114.95	110.23
23	b	608	CLA	C2B-C1B-NB	7.04	114.95	110.23
23	B	616	CLA	CHD-C4C-C3C	-7.03	114.50	124.84
23	b	605	CLA	CHD-C1D-ND	-7.03	117.99	124.45
23	B	605	CLA	C2B-C1B-NB	7.01	114.93	110.23
23	c	508	CLA	O2D-CGD-CBD	7.01	123.72	111.27
23	B	610	CLA	O2D-CGD-CBD	7.00	123.72	111.27
23	d	402	CLA	CMD-C2D-C1D	6.99	137.04	124.71
23	b	615	CLA	C2B-C1B-NB	6.99	114.92	110.23
23	A	405[B]	CLA	C2B-C1B-NB	6.98	114.91	110.23
23	a	407[A]	CLA	C2B-C1B-NB	6.94	114.89	110.23
23	a	406[A]	CLA	C2B-C1B-NB	6.94	114.88	110.23
23	c	502	CLA	C2B-C1B-NB	6.94	114.88	110.23
37	D	401[B]	PHO	C4D-ND-C1D	-6.93	101.78	108.83
23	B	606	CLA	CMD-C2D-C1D	6.92	136.91	124.71
37	a	416[A]	PHO	C2B-C1B-NB	6.92	114.30	109.53
23	c	514	CLA	CMD-C2D-C1D	6.92	136.90	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	C2B-C1B-NB	6.91	114.87	110.23
23	b	604	CLA	C2B-C1B-NB	6.91	114.86	110.23
23	C	513	CLA	C2B-C1B-NB	6.89	114.85	110.23
23	c	511	CLA	C2D-C1D-ND	6.86	115.16	110.10
23	b	610	CLA	CHD-C4C-C3C	-6.85	114.77	124.84
23	c	510	CLA	C2B-C1B-NB	6.84	114.82	110.23
23	b	601	CLA	C2B-C1B-NB	6.83	114.81	110.23
23	B	603	CLA	O2D-CGD-CBD	6.83	123.40	111.27
26	F	103	SQD	O6-C1-C2	6.82	118.95	108.30
23	D	405	CLA	C2B-C1B-NB	6.82	114.80	110.23
23	C	508	CLA	CMD-C2D-C1D	6.82	136.73	124.71
23	C	510	CLA	C2B-C1B-NB	6.81	114.80	110.23
23	c	508	CLA	CMD-C2D-C1D	6.80	136.70	124.71
23	B	616	CLA	C2B-C1B-NB	6.80	114.79	110.23
23	b	605	CLA	CMD-C2D-C1D	6.79	136.67	124.71
23	d	401[B]	CLA	CMD-C2D-C1D	6.77	136.65	124.71
23	C	514	CLA	CHD-C4C-C3C	-6.77	114.89	124.84
23	B	608	CLA	C2B-C1B-NB	6.76	114.77	110.23
23	b	606	CLA	C4A-NA-C1A	-6.74	103.67	106.71
23	a	405[A]	CLA	C2B-C1B-NB	6.74	114.75	110.23
23	b	601	CLA	CHD-C4C-C3C	-6.74	114.93	124.84
23	b	616	CLA	CHD-C4C-C3C	-6.74	114.94	124.84
23	b	610	CLA	C2B-C1B-NB	6.73	114.75	110.23
37	a	416[A]	PHO	C4D-ND-C1D	-6.72	101.99	108.83
23	C	503	CLA	O2D-CGD-CBD	6.72	123.20	111.27
23	C	508	CLA	CHD-C1D-ND	-6.71	118.28	124.45
23	A	404[A]	CLA	CMD-C2D-C1D	6.70	136.53	124.71
23	C	512	CLA	CHD-C1D-ND	-6.70	118.30	124.45
23	A	404[B]	CLA	CMD-C2D-C1D	6.70	136.52	124.71
23	a	407[B]	CLA	CHD-C1D-ND	-6.69	118.30	124.45
23	c	508	CLA	CHD-C1D-ND	-6.69	118.31	124.45
23	a	406[B]	CLA	C2B-C1B-NB	6.69	114.71	110.23
23	d	402	CLA	CHD-C1D-ND	-6.68	118.31	124.45
23	C	509	CLA	C2B-C1B-NB	6.66	114.69	110.23
23	A	404[A]	CLA	C2B-C1B-NB	6.65	114.69	110.23
37	a	408[B]	PHO	C1C-C2C-C3C	-6.64	103.09	108.61
37	D	401[B]	PHO	C1C-C2C-C3C	-6.62	103.10	108.61
37	a	408[B]	PHO	C2B-C1B-NB	6.62	114.10	109.53
23	b	611	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	a	406[A]	CLA	CHD-C4C-C3C	-6.61	115.12	124.84
23	b	613	CLA	C2B-C1B-NB	6.61	114.66	110.23
23	b	606	CLA	CHD-C4C-C3C	-6.61	115.13	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	a	416[B]	PHO	C4D-ND-C1D	-6.60	102.11	108.83
23	D	405	CLA	C2D-C1D-ND	6.60	114.97	110.10
23	b	601	CLA	O2D-CGD-CBD	6.58	122.95	111.27
37	a	416[B]	PHO	C2B-C1B-NB	6.57	114.06	109.53
23	b	609	CLA	CHD-C4C-C3C	-6.57	115.19	124.84
23	c	503	CLA	C2C-C1C-NC	6.56	116.12	109.97
23	b	603	CLA	CHD-C4C-C3C	-6.55	115.21	124.84
23	b	607	CLA	CHD-C1D-ND	-6.54	118.44	124.45
23	c	508	CLA	C2B-C1B-NB	6.54	114.62	110.23
23	b	611	CLA	C2B-C1B-NB	6.54	114.61	110.23
23	B	611	CLA	CMD-C2D-C1D	6.53	136.22	124.71
37	a	416[B]	PHO	C1C-C2C-C3C	-6.53	103.18	108.61
23	B	604	CLA	C2B-C1B-NB	6.51	114.59	110.23
23	d	401[A]	CLA	C2C-C1C-NC	6.49	116.05	109.97
37	a	408[A]	PHO	C2B-C1B-NB	6.49	114.01	109.53
23	D	404[B]	CLA	C2B-C1B-NB	6.48	114.58	110.23
37	a	408[A]	PHO	C1C-C2C-C3C	-6.48	103.22	108.61
23	c	514	CLA	CHD-C1D-ND	-6.48	118.50	124.45
23	b	607	CLA	CMD-C2D-C1D	6.48	136.12	124.71
23	b	602	CLA	O2D-CGD-CBD	6.46	122.75	111.27
23	c	505	CLA	C2B-C1B-NB	6.46	114.56	110.23
23	C	514	CLA	C4A-NA-C1A	-6.44	103.81	106.71
23	A	404[A]	CLA	C4A-NA-C1A	-6.44	103.81	106.71
26	C	501[A]	SQD	O6-C1-C2	6.44	118.36	108.30
23	A	406[B]	CLA	CMD-C2D-C1D	6.44	136.06	124.71
37	D	402[A]	PHO	C1C-C2C-C3C	-6.44	103.26	108.61
23	D	404[B]	CLA	CHD-C1D-ND	-6.43	118.54	124.45
23	C	512	CLA	C2B-C1B-NB	6.43	114.54	110.23
37	D	402[A]	PHO	C4D-ND-C1D	-6.43	102.29	108.83
23	B	606	CLA	CHD-C4C-C3C	-6.42	115.40	124.84
23	D	404[B]	CLA	CMD-C2D-C1D	6.42	136.03	124.71
23	c	502	CLA	CMD-C2D-C1D	6.41	136.00	124.71
23	b	613	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
23	B	615	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
23	a	407[A]	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
23	C	507	CLA	CHD-C4C-C3C	-6.39	115.44	124.84
23	c	507	CLA	C2B-C1B-NB	6.38	114.51	110.23
23	B	613	CLA	CMD-C2D-C1D	6.38	135.95	124.71
23	B	603	CLA	CHD-C4C-C3C	-6.38	115.47	124.84
23	d	401[B]	CLA	C2B-C1B-NB	6.37	114.50	110.23
23	B	610	CLA	CMD-C2D-C1D	6.37	135.94	124.71
23	B	601	CLA	CHD-C4C-C3C	-6.37	115.47	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	C2B-C1B-NB	6.37	114.50	110.23
23	C	510	CLA	C2C-C1C-NC	6.37	115.94	109.97
23	B	605	CLA	CMD-C2D-C1D	6.36	135.93	124.71
23	c	506	CLA	C2B-C1B-NB	6.36	114.50	110.23
23	c	511	CLA	C4A-NA-C1A	-6.35	103.85	106.71
37	a	408[B]	PHO	C4D-ND-C1D	-6.35	102.37	108.83
23	C	509	CLA	CHD-C4C-C3C	-6.34	115.51	124.84
23	c	512	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
23	A	406[B]	CLA	CHD-C1D-ND	-6.34	118.63	124.45
23	c	504	CLA	CHD-C1D-ND	-6.34	118.63	124.45
23	b	609	CLA	C2B-C1B-NB	6.34	114.48	110.23
23	c	507	CLA	C2C-C1C-NC	6.34	115.91	109.97
23	B	602	CLA	C2B-C1B-NB	6.33	114.48	110.23
23	b	607	CLA	C2B-C1B-NB	6.33	114.47	110.23
23	B	606	CLA	CHD-C1D-ND	-6.32	118.65	124.45
37	a	416[A]	PHO	C1C-C2C-C3C	-6.32	103.36	108.61
23	B	615	CLA	C2B-C1B-NB	6.31	114.46	110.23
23	d	401[B]	CLA	C4A-NA-C1A	-6.31	103.87	106.71
23	b	604	CLA	C2C-C1C-NC	6.30	115.88	109.97
23	a	409	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
23	c	513	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
23	B	603	CLA	C2B-C1B-NB	6.28	114.44	110.23
23	b	610	CLA	O2D-CGD-CBD	6.25	122.38	111.27
23	C	511	CLA	CHD-C1D-ND	-6.25	118.71	124.45
23	B	603	CLA	C2C-C1C-NC	6.25	115.83	109.97
23	b	605	CLA	C4A-NA-C1A	-6.24	103.90	106.71
23	B	614	CLA	CHD-C1D-ND	-6.24	118.72	124.45
23	c	502	CLA	CHD-C1D-ND	-6.24	118.72	124.45
23	C	508	CLA	C2C-C1C-NC	6.24	115.81	109.97
37	D	401[B]	PHO	C2B-C1B-NB	6.24	113.83	109.53
23	B	609	CLA	C2B-C1B-NB	6.23	114.41	110.23
37	D	401[A]	PHO	O2D-CGD-CBD	6.23	118.89	111.00
23	c	510	CLA	C2C-C1C-NC	6.23	115.81	109.97
34	D	412	HTG	C1'-S1-C1	6.23	111.74	100.09
23	c	506	CLA	C4A-NA-C1A	-6.23	103.91	106.71
37	D	402[B]	PHO	C4D-ND-C1D	-6.23	102.49	108.83
34	B	623	HTG	C1'-S1-C1	6.22	111.73	100.09
23	A	404[B]	CLA	CHD-C4C-C3C	-6.22	115.69	124.84
23	B	609	CLA	CHD-C4C-C3C	-6.22	115.69	124.84
26	F	103	SQD	O47-C7-C8	6.22	124.91	111.50
23	b	611	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	B	609	CLA	CHD-C1D-ND	-6.22	118.74	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
37	D	401[A]	PHO	C1C-C2C-C3C	-6.21	103.45	108.61
23	b	606	CLA	CMD-C2D-C1D	6.21	135.66	124.71
23	a	405[A]	CLA	C2C-C1C-NC	6.21	115.79	109.97
34	c	522	HTG	C1'-S1-C1	6.21	111.70	100.09
23	a	406[B]	CLA	CHD-C4C-C3C	-6.20	115.72	124.84
23	b	602	CLA	CHD-C1D-ND	-6.20	118.76	124.45
23	B	610	CLA	CHD-C4C-C3C	-6.20	115.73	124.84
23	B	607	CLA	C2C-C1C-NC	6.19	115.77	109.97
23	b	606	CLA	CHD-C1D-ND	-6.19	118.77	124.45
23	C	515	CLA	CHD-C4C-C3C	-6.19	115.75	124.84
23	C	510	CLA	O2D-CGD-CBD	6.19	122.26	111.27
40	v	201	HEC	C1D-ND-C4D	6.18	111.46	105.07
23	a	405[A]	CLA	C4A-NA-C1A	-6.18	103.93	106.71
23	C	504	CLA	CHD-C4C-C3C	-6.18	115.76	124.84
23	B	606	CLA	O2D-CGD-CBD	6.18	122.25	111.27
23	C	513	CLA	CHD-C4C-C3C	-6.18	115.76	124.84
23	B	605	CLA	CHD-C1D-ND	-6.17	118.78	124.45
23	c	511	CLA	CMD-C2D-C1D	6.17	135.59	124.71
23	C	506	CLA	C2C-C1C-NC	6.17	115.75	109.97
23	a	407[A]	CLA	C4A-NA-C1A	-6.17	103.93	106.71
23	b	612	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
23	C	515	CLA	CHD-C1D-ND	-6.16	118.79	124.45
23	B	604	CLA	CMD-C2D-C1D	6.16	135.57	124.71
23	a	407[B]	CLA	CMD-C2D-C1D	6.15	135.55	124.71
23	C	505	CLA	CMD-C2D-C1D	6.15	135.55	124.71
23	b	610	CLA	CMD-C2D-C1D	6.15	135.54	124.71
23	B	602	CLA	CHD-C4C-C3C	-6.14	115.81	124.84
23	A	406[A]	CLA	CHD-C1D-ND	-6.14	118.81	124.45
23	b	605	CLA	O2D-CGD-CBD	6.14	122.18	111.27
37	D	401[A]	PHO	C2B-C1B-NB	6.14	113.77	109.53
23	a	407[A]	CLA	CHD-C1D-ND	-6.14	118.81	124.45
23	d	401[B]	CLA	CHD-C1D-ND	-6.13	118.82	124.45
23	B	604	CLA	C2C-C1C-NC	6.13	115.71	109.97
23	C	509	CLA	CHD-C1D-ND	-6.12	118.83	124.45
23	B	601	CLA	CMD-C2D-C1D	6.12	135.49	124.71
23	A	404[A]	CLA	CHD-C1D-ND	-6.11	118.83	124.45
23	C	504	CLA	C2B-C1B-NB	6.11	114.33	110.23
23	c	511	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
23	c	509	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
23	B	604	CLA	C2D-C1D-ND	6.10	114.60	110.10
23	C	511	CLA	CMD-C2D-C1D	6.10	135.47	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	404[A]	CLA	CMD-C2D-C1D	6.10	135.47	124.71
23	b	612	CLA	C2B-C1B-NB	6.10	114.32	110.23
23	b	608	CLA	C4A-NA-C1A	-6.09	103.97	106.71
23	A	407	CLA	CHD-C4C-C3C	-6.09	115.88	124.84
23	A	405[B]	CLA	CHD-C1D-ND	-6.08	118.86	124.45
23	D	405	CLA	CMD-C2D-C1D	6.08	135.43	124.71
23	c	509	CLA	C2B-C1B-NB	6.08	114.31	110.23
23	a	405[B]	CLA	CHD-C4C-C3C	-6.07	115.91	124.84
23	a	405[A]	CLA	CMD-C2D-C1D	6.07	135.41	124.71
23	B	609	CLA	CMD-C2D-C1D	6.05	135.38	124.71
23	a	407[B]	CLA	CHD-C4C-C3C	-6.05	115.94	124.84
37	a	408[A]	PHO	C4D-ND-C1D	-6.05	102.68	108.83
23	b	601	CLA	CMD-C2D-C1D	6.04	135.35	124.71
23	B	614	CLA	C4A-NA-C1A	-6.02	104.00	106.71
23	C	511	CLA	CHD-C4C-C3C	-6.02	116.00	124.84
23	d	401[A]	CLA	C2B-C1B-NB	6.01	114.26	110.23
23	b	609	CLA	C4A-NA-C1A	-6.01	104.00	106.71
26	B	620	SQD	O6-C1-C2	6.01	117.69	108.30
23	b	602	CLA	CMD-C2D-C1D	6.01	135.30	124.71
23	c	509	CLA	C4A-NA-C1A	-6.00	104.01	106.71
23	C	512	CLA	C2C-C1C-NC	6.00	115.59	109.97
23	B	615	CLA	CHD-C1D-ND	-6.00	118.94	124.45
23	B	603	CLA	C4A-NA-C1A	-6.00	104.01	106.71
23	a	405[B]	CLA	CMD-C2D-C1D	5.99	135.28	124.71
23	c	505	CLA	CMD-C2D-C1D	5.99	135.27	124.71
23	B	614	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
23	D	404[B]	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
23	B	615	CLA	C4A-NA-C1A	-5.99	104.02	106.71
23	b	601	CLA	CHD-C1D-ND	-5.98	118.96	124.45
23	b	608	CLA	C2C-C1C-NC	5.97	115.57	109.97
23	c	508	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
23	A	404[B]	CLA	CHD-C1D-ND	-5.95	118.98	124.45
23	C	511	CLA	C4A-NA-C1A	-5.95	104.03	106.71
23	b	609	CLA	CMD-C2D-C1D	5.95	135.20	124.71
38	F	102	HEM	CAD-CBD-CGD	5.95	126.40	113.60
23	B	616	CLA	C3C-C4C-NC	5.93	117.23	110.57
37	D	402[B]	PHO	C1C-C2C-C3C	-5.93	103.68	108.61
23	a	406[A]	CLA	CMD-C2D-C1D	5.93	135.16	124.71
23	C	505	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
23	A	407	CLA	CHD-C1D-ND	-5.92	119.01	124.45
23	A	406[A]	CLA	C4A-NA-C1A	-5.91	104.05	106.71
23	D	404[A]	CLA	CHD-C1D-ND	-5.91	119.02	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406[B]	CLA	C4A-NA-C1A	-5.91	104.05	106.71
23	b	602	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
23	B	607	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
23	A	406[A]	CLA	CMD-C2D-C1D	5.89	135.10	124.71
23	b	607	CLA	C2C-C1C-NC	5.89	115.49	109.97
23	C	510	CLA	CHD-C4C-C3C	-5.89	116.19	124.84
23	D	404[A]	CLA	C2C-C1C-NC	5.88	115.48	109.97
23	B	608	CLA	CMD-C2D-C1D	5.87	135.06	124.71
23	c	509	CLA	C2C-C1C-NC	5.87	115.47	109.97
23	c	507	CLA	CHD-C1D-ND	-5.87	119.06	124.45
23	c	506	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
23	A	406[A]	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
23	B	610	CLA	C3D-C2D-C1D	-5.84	97.86	105.83
23	A	404[A]	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	604	CLA	O2D-CGD-CBD	5.83	121.64	111.27
23	B	601	CLA	O2D-CGD-CBD	5.83	121.63	111.27
23	b	613	CLA	C2C-C1C-NC	5.83	115.44	109.97
23	C	503	CLA	C4A-NA-C1A	-5.83	104.08	106.71
23	A	407	CLA	CMD-C2D-C1D	5.83	134.99	124.71
23	B	603	CLA	CHD-C1D-ND	-5.83	119.10	124.45
23	C	507	CLA	CMD-C2D-C1D	5.82	134.97	124.71
23	b	609	CLA	CHD-C1D-ND	-5.82	119.11	124.45
23	B	613	CLA	C2B-C1B-NB	5.81	114.13	110.23
23	B	608	CLA	CHD-C1D-ND	-5.81	119.12	124.45
23	B	614	CLA	C2C-C1C-NC	5.80	115.41	109.97
23	b	616	CLA	CMD-C2D-C1D	5.80	134.93	124.71
23	b	614	CLA	CHD-C1D-ND	-5.79	119.13	124.45
23	B	602	CLA	CMD-C2D-C1D	5.79	134.92	124.71
23	c	507	CLA	CMD-C2D-C1D	5.78	134.89	124.71
23	b	614	CLA	CHD-C4C-C3C	-5.77	116.35	124.84
23	a	406[B]	CLA	CHD-C1D-ND	-5.77	119.15	124.45
23	A	405[A]	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
23	B	612	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
23	C	506	CLA	C2B-C1B-NB	5.77	114.10	110.23
23	A	406[B]	CLA	CHD-C4C-C3C	-5.77	116.37	124.84
23	c	512	CLA	CMD-C2D-C1D	5.76	134.87	124.71
23	C	503	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
23	d	401[B]	CLA	C2C-C1C-NC	5.75	115.36	109.97
23	b	611	CLA	O2D-CGD-CBD	5.75	121.48	111.27
23	C	505	CLA	CHD-C1D-ND	-5.74	119.18	124.45
23	c	505	CLA	CHD-C1D-ND	-5.73	119.19	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	C2C-C1C-NC	5.73	115.34	109.97
23	b	615	CLA	CMD-C2D-C1D	5.72	134.80	124.71
23	A	407	CLA	C2C-C1C-NC	5.72	115.33	109.97
23	c	509	CLA	CMD-C2D-C1D	5.71	134.78	124.71
23	c	510	CLA	O2D-CGD-CBD	5.71	121.42	111.27
23	B	610	CLA	C2B-C1B-NB	5.71	114.06	110.23
23	b	614	CLA	O2D-CGD-CBD	5.71	121.41	111.27
23	C	507	CLA	C2C-C1C-NC	5.71	115.32	109.97
23	c	504	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
23	c	510	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
23	C	512	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
26	a	411[A]	SQD	O6-C1-C2	5.69	117.19	108.30
23	B	611	CLA	O2D-CGD-CBD	5.69	121.38	111.27
23	b	607	CLA	C4A-NA-C1A	-5.69	104.15	106.71
23	c	503	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
23	B	605	CLA	C4A-NA-C1A	-5.69	104.15	106.71
23	c	510	CLA	C1-C2-C3	-5.68	116.22	126.04
26	C	501[B]	SQD	O6-C1-C2	5.67	117.16	108.30
23	A	405[B]	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
33	C	502	LMG	C7-O1-C1	-5.67	102.67	113.74
23	C	515	CLA	CMD-C2D-C1D	5.66	134.69	124.71
23	B	612	CLA	C2B-C1B-NB	5.66	114.02	110.23
23	b	615	CLA	CHD-C1D-ND	-5.65	119.26	124.45
26	b	620	SQD	O6-C1-C2	5.65	117.12	108.30
23	D	404[B]	CLA	C2C-C1C-NC	5.65	115.27	109.97
23	B	601	CLA	CHD-C1D-ND	-5.65	119.26	124.45
23	a	406[B]	CLA	C2C-C1C-NC	5.65	115.26	109.97
23	c	507	CLA	C4A-NA-C1A	-5.65	104.17	106.71
23	c	512	CLA	C2B-C1B-NB	5.64	114.02	110.23
26	C	501[A]	SQD	C1-O5-C5	-5.64	102.61	113.69
23	B	604	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
23	b	605	CLA	C3D-C2D-C1D	-5.64	98.14	105.83
23	c	505	CLA	C2C-C1C-NC	5.64	115.25	109.97
23	b	614	CLA	CMD-C2D-C1D	5.63	134.64	124.71
23	B	605	CLA	O2D-CGD-CBD	5.63	121.28	111.27
23	c	506	CLA	O2D-CGD-CBD	5.62	121.26	111.27
23	C	504	CLA	CMD-C2D-C1D	5.62	134.62	124.71
23	b	611	CLA	C4A-NA-C1A	-5.62	104.18	106.71
23	b	604	CLA	O2D-CGD-CBD	5.62	121.25	111.27
23	b	615	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
23	a	409	CLA	O2D-CGD-CBD	5.61	121.24	111.27
23	a	407[B]	CLA	C4A-NA-C1A	-5.61	104.18	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	CMD-C2D-C1D	5.61	134.59	124.71
23	a	405[B]	CLA	CHD-C1D-ND	-5.61	119.30	124.45
23	A	405[B]	CLA	CMD-C2D-C1D	5.60	134.59	124.71
23	b	603	CLA	C2C-C1C-NC	5.60	115.22	109.97
23	C	513	CLA	C2C-C1C-NC	5.60	115.22	109.97
23	c	512	CLA	CHD-C1D-ND	-5.60	119.31	124.45
23	C	507	CLA	O2D-CGD-CBD	5.58	121.19	111.27
23	B	606	CLA	C4A-NA-C1A	-5.58	104.20	106.71
40	V	202	HEC	C1D-ND-C4D	5.57	110.83	105.07
26	B	620	SQD	O47-C7-C8	5.56	123.49	111.50
34	d	408	HTG	C1'-S1-C1	5.55	110.47	100.09
23	b	613	CLA	C3D-C2D-C1D	-5.54	98.26	105.83
23	A	405[A]	CLA	C2C-C1C-NC	5.54	115.17	109.97
23	C	506	CLA	CHD-C1D-ND	-5.54	119.36	124.45
23	B	612	CLA	O2D-CGD-CBD	5.54	121.11	111.27
23	D	404[A]	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
23	d	402	CLA	CHD-C4C-C3C	-5.53	116.70	124.84
23	B	603	CLA	CMD-C2D-C1D	5.53	134.46	124.71
23	B	610	CLA	CHD-C1D-ND	-5.53	119.38	124.45
23	C	511	CLA	C2C-C1C-NC	5.53	115.15	109.97
23	c	508	CLA	C2C-C1C-NC	5.53	115.15	109.97
23	C	514	CLA	CMD-C2D-C1D	5.52	134.45	124.71
23	c	506	CLA	CMD-C2D-C1D	5.52	134.45	124.71
23	A	405[B]	CLA	C2C-C1C-NC	5.52	115.15	109.97
23	C	504	CLA	C2C-C1C-NC	5.52	115.14	109.97
23	c	514	CLA	C4A-NA-C1A	-5.51	104.23	106.71
23	B	613	CLA	CHD-C1D-ND	-5.51	119.39	124.45
24	D	406	BCR	C7-C8-C9	-5.51	117.91	126.23
23	a	405[A]	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
23	c	513	CLA	O2D-CGD-CBD	5.51	121.05	111.27
23	a	406[A]	CLA	C2C-C1C-NC	5.50	115.13	109.97
23	b	601	CLA	C4A-NA-C1A	-5.50	104.23	106.71
23	C	508	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
23	d	401[A]	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
23	B	613	CLA	C2C-C1C-NC	5.50	115.12	109.97
23	b	606	CLA	O2D-CGD-CBD	5.49	121.03	111.27
23	a	406[A]	CLA	CHD-C1D-ND	-5.49	119.41	124.45
23	a	407[A]	CLA	CMD-C2D-C1D	5.49	134.38	124.71
23	b	612	CLA	C2C-C1C-NC	5.47	115.10	109.97
23	B	606	CLA	C2B-C1B-NB	5.47	113.90	110.23
23	D	404[A]	CLA	C2B-C1B-NB	5.47	113.90	110.23
23	a	405[B]	CLA	C4A-NA-C1A	-5.46	104.25	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	CMD-C2D-C1D	5.46	134.33	124.71
23	C	506	CLA	C3D-C2D-C1D	-5.45	98.39	105.83
23	B	611	CLA	C3D-C2D-C1D	-5.45	98.40	105.83
23	b	611	CLA	C2C-C1C-NC	5.44	115.07	109.97
26	a	411[B]	SQD	O47-C7-C8	5.44	123.22	111.50
23	b	608	CLA	CMD-C2D-C1D	5.44	134.30	124.71
23	D	405	CLA	O2D-CGD-CBD	5.44	120.93	111.27
23	b	608	CLA	CHD-C1D-ND	-5.44	119.46	124.45
23	d	401[A]	CLA	CMD-C2D-C1D	5.44	134.30	124.71
23	c	503	CLA	C3B-C2B-C1B	-5.44	100.60	107.16
23	C	515	CLA	C2C-C1C-NC	5.43	115.06	109.97
23	c	511	CLA	C2C-C1C-NC	5.43	115.06	109.97
23	c	508	CLA	C4A-NA-C1A	-5.43	104.27	106.71
34	b	622	HTG	C1-O5-C5	5.43	122.59	112.58
23	B	602	CLA	C2C-C1C-NC	5.43	115.06	109.97
23	C	506	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
23	A	405[A]	CLA	CHD-C1D-ND	-5.41	119.48	124.45
23	b	607	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
23	c	506	CLA	C2C-C1C-NC	5.40	115.03	109.97
23	D	405	CLA	CHD-C4C-C3C	-5.40	116.91	124.84
23	a	409	CLA	CHD-C1D-ND	-5.40	119.49	124.45
23	b	604	CLA	CHD-C4C-C3C	-5.40	116.91	124.84
23	B	616	CLA	C2C-C1C-NC	5.39	115.03	109.97
37	a	416[A]	PHO	C1-C2-C3	-5.39	116.72	126.04
23	B	612	CLA	CHD-C1D-ND	-5.38	119.51	124.45
23	A	405[A]	CLA	C4A-NA-C1A	-5.38	104.29	106.71
23	c	505	CLA	CHD-C4C-C3C	-5.38	116.94	124.84
23	B	614	CLA	C3D-C2D-C1D	-5.37	98.51	105.83
34	C	523	HTG	C1'-S1-C1	5.36	110.12	100.09
23	c	502	CLA	C2C-C1C-NC	5.36	114.99	109.97
23	b	611	CLA	CHD-C1D-ND	-5.36	119.53	124.45
23	B	604	CLA	C3C-C4C-NC	5.35	116.58	110.57
23	B	605	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
23	d	401[B]	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
23	a	406[B]	CLA	CMD-C2D-C1D	5.35	134.14	124.71
26	C	501[A]	SQD	C1-C2-C3	-5.35	98.86	110.00
23	C	510	CLA	C3C-C4C-NC	5.34	116.56	110.57
23	a	405[A]	CLA	CHD-C1D-ND	-5.34	119.55	124.45
37	D	401[A]	PHO	C3D-C4D-ND	5.34	115.00	107.72
23	b	610	CLA	CHD-C1D-ND	-5.33	119.56	124.45
23	B	615	CLA	C2C-C1C-NC	5.33	114.96	109.97
23	b	614	CLA	C4A-NA-C1A	-5.33	104.31	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	101	BCR	C33-C5-C6	-5.33	118.55	124.53
23	c	506	CLA	CHD-C1D-ND	-5.33	119.56	124.45
23	d	402	CLA	O2D-CGD-CBD	5.32	120.73	111.27
23	C	503	CLA	CMD-C2D-C1D	5.32	134.09	124.71
23	B	602	CLA	C4A-NA-C1A	-5.32	104.31	106.71
23	c	514	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
23	b	603	CLA	O2D-CGD-CBD	5.31	120.70	111.27
23	B	604	CLA	C1-C2-C3	-5.31	116.86	126.04
23	B	613	CLA	CHD-C4C-C3C	-5.28	117.07	124.84
23	B	607	CLA	CHD-C1D-ND	-5.28	119.60	124.45
24	d	403	BCR	C7-C8-C9	-5.28	118.26	126.23
23	c	509	CLA	O2D-CGD-CBD	5.28	120.64	111.27
23	C	515	CLA	C3B-C2B-C1B	-5.26	100.81	107.16
23	C	513	CLA	O2D-CGD-CBD	5.26	120.62	111.27
24	y	101	BCR	C33-C5-C6	-5.25	118.63	124.53
23	B	612	CLA	CMD-C2D-C1D	5.25	133.96	124.71
23	C	513	CLA	C3B-C2B-C1B	-5.24	100.83	107.16
23	b	602	CLA	C3B-C2B-C1B	-5.24	100.83	107.16
23	c	502	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
23	B	603	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
23	c	505	CLA	O2D-CGD-CBD	5.23	120.56	111.27
23	c	504	CLA	O2D-CGD-CBD	5.22	120.55	111.27
37	a	416[B]	PHO	C1-C2-C3	-5.22	117.02	126.04
23	C	508	CLA	C4A-NA-C1A	-5.22	104.36	106.71
23	C	504	CLA	CHD-C1D-ND	-5.20	119.68	124.45
23	B	614	CLA	O2D-CGD-CBD	5.20	120.50	111.27
23	c	513	CLA	C4A-NA-C1A	-5.19	104.37	106.71
23	C	512	CLA	O2D-CGD-CBD	5.19	120.50	111.27
37	D	401[B]	PHO	C3D-C4D-ND	5.19	114.80	107.72
23	b	606	CLA	C2C-C1C-NC	5.19	114.84	109.97
37	a	416[A]	PHO	C3D-C4D-ND	5.19	114.79	107.72
23	d	401[A]	CLA	CHD-C1D-ND	-5.18	119.69	124.45
23	b	610	CLA	C4A-NA-C1A	-5.18	104.38	106.71
23	C	513	CLA	CMD-C2D-C1D	5.18	133.84	124.71
26	b	620	SQD	O47-C7-C8	5.18	122.66	111.50
23	A	407	CLA	C3B-C2B-C1B	-5.17	100.92	107.16
23	d	402	CLA	C4A-NA-C1A	-5.16	104.38	106.71
23	B	608	CLA	C2C-C1C-NC	5.16	114.81	109.97
23	b	611	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
23	b	612	CLA	CMD-C2D-C1D	5.16	133.81	124.71
37	a	416[B]	PHO	C3D-C4D-ND	5.16	114.75	107.72
23	C	505	CLA	C2C-C1C-NC	5.16	114.81	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	CHD-C1D-ND	-5.15	119.72	124.45
23	b	608	CLA	CHD-C4C-C3C	-5.13	117.29	124.84
23	C	505	CLA	O2D-CGD-CBD	5.13	120.39	111.27
23	C	509	CLA	C3B-C2B-C1B	-5.13	100.96	107.16
23	A	404[A]	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
23	b	616	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
23	B	606	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
23	B	607	CLA	C3D-C2D-C1D	-5.13	98.84	105.83
23	b	615	CLA	C2C-C1C-NC	5.12	114.77	109.97
24	t	103	BCR	C33-C5-C6	-5.12	118.78	124.53
23	b	607	CLA	C3C-C4C-NC	5.12	116.31	110.57
23	C	506	CLA	CMD-C2D-C1D	5.12	133.74	124.71
23	C	506	CLA	O2D-CGD-CBD	5.12	120.36	111.27
23	b	614	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
23	b	603	CLA	C4A-NA-C1A	-5.11	104.41	106.71
23	b	614	CLA	C2C-C1C-NC	5.10	114.75	109.97
23	c	513	CLA	C3B-C2B-C1B	-5.10	101.01	107.16
23	c	504	CLA	C2C-C1C-NC	5.10	114.75	109.97
23	B	613	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
23	b	604	CLA	CMD-C2D-C1D	5.09	133.69	124.71
23	B	615	CLA	CMD-C2D-C1D	5.09	133.69	124.71
23	c	512	CLA	O2D-CGD-CBD	5.09	120.31	111.27
23	B	615	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
23	b	603	CLA	CMD-C2D-C1D	5.09	133.68	124.71
23	B	608	CLA	O2D-CGD-CBD	5.09	120.31	111.27
26	a	411[A]	SQD	O47-C7-C8	5.08	122.45	111.50
23	C	513	CLA	C3C-C4C-NC	5.08	116.27	110.57
23	a	406[A]	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
23	B	606	CLA	C2C-C1C-NC	5.07	114.73	109.97
23	C	503	CLA	CHD-C1D-ND	-5.07	119.79	124.45
23	d	401[B]	CLA	O2D-CGD-CBD	5.07	120.28	111.27
38	f	101	HEM	CHC-C4B-NB	5.07	129.93	124.42
23	D	404[A]	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
23	C	507	CLA	CHD-C1D-ND	-5.06	119.80	124.45
23	c	511	CLA	C3B-C2B-C1B	-5.06	101.05	107.16
23	B	612	CLA	C3C-C4C-NC	5.05	116.24	110.57
23	C	503	CLA	O2D-CGD-O1D	-5.05	113.97	123.84
23	A	405[B]	CLA	O2D-CGD-CBD	5.05	120.23	111.27
23	A	404[B]	CLA	C4A-NA-C1A	-5.04	104.44	106.71
23	b	604	CLA	C4A-NA-C1A	-5.04	104.44	106.71
23	B	616	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
23	A	405[B]	CLA	C3D-C2D-C1D	-5.04	98.96	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	C3C-C4C-NC	5.03	116.21	110.57
23	c	513	CLA	CMD-C2D-C1D	5.02	133.55	124.71
23	A	405[A]	CLA	O2D-CGD-CBD	5.01	120.17	111.27
23	a	407[B]	CLA	C3B-C2B-C1B	-5.01	101.12	107.16
23	C	514	CLA	O2D-CGD-CBD	5.00	120.16	111.27
23	c	508	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
23	D	404[A]	CLA	C3C-C4C-NC	5.00	116.18	110.57
23	B	616	CLA	C3B-C4B-NB	5.00	115.15	110.52
23	B	614	CLA	C3B-C2B-C1B	-4.99	101.13	107.16
23	a	407[B]	CLA	O2D-CGD-CBD	4.99	120.14	111.27
23	D	404[B]	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
23	B	612	CLA	C3B-C2B-C1B	-4.99	101.14	107.16
23	B	607	CLA	O2D-CGD-CBD	4.99	120.14	111.27
23	b	614	CLA	C3B-C2B-C1B	-4.99	101.14	107.16
23	c	510	CLA	CHD-C1D-ND	-4.99	119.87	124.45
23	C	507	CLA	C4A-NA-C1A	-4.98	104.47	106.71
23	c	504	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
37	a	408[B]	PHO	C3D-C4D-ND	4.98	114.51	107.72
23	c	511	CLA	O2D-CGD-CBD	4.98	120.12	111.27
23	c	509	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
23	b	604	CLA	C1-C2-C3	-4.98	117.43	126.04
28	a	414[A]	PL9	C7-C8-C9	-4.98	118.50	126.79
23	c	505	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
23	A	406[B]	CLA	C2C-C1C-NC	4.98	114.63	109.97
23	C	506	CLA	C1C-C2C-C3C	-4.97	101.73	106.96
23	d	402	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
23	b	603	CLA	CHD-C1D-ND	-4.97	119.89	124.45
23	c	505	CLA	C3B-C2B-C1B	-4.96	101.17	107.16
23	a	407[A]	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
37	D	402[A]	PHO	C3D-C4D-ND	4.96	114.48	107.72
23	b	613	CLA	C3C-C4C-NC	4.96	116.13	110.57
23	c	506	CLA	C3C-C4C-NC	4.96	116.13	110.57
23	b	608	CLA	O2D-CGD-CBD	4.96	120.07	111.27
23	C	509	CLA	C3C-C4C-NC	4.96	116.13	110.57
23	b	612	CLA	C3C-C4C-NC	4.95	116.13	110.57
23	C	515	CLA	O2D-CGD-CBD	4.95	120.07	111.27
23	c	503	CLA	CMD-C2D-C1D	4.95	133.44	124.71
23	a	406[B]	CLA	C4A-NA-C1A	-4.95	104.48	106.71
23	B	616	CLA	C4A-NA-C1A	-4.94	104.48	106.71
28	A	412[A]	PL9	C7-C8-C9	-4.94	118.56	126.79
23	C	509	CLA	C4A-NA-C1A	-4.94	104.48	106.71
23	C	514	CLA	CHD-C1D-ND	-4.94	119.92	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	407	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
23	B	609	CLA	C2C-C1C-NC	4.93	114.59	109.97
23	c	514	CLA	C3B-C2B-C1B	-4.93	101.21	107.16
23	c	514	CLA	C2C-C1C-NC	4.93	114.59	109.97
23	a	406[B]	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
23	c	508	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
26	a	411[A]	SQD	C1-O5-C5	-4.91	104.05	113.69
23	D	405	CLA	C2C-C1C-NC	4.91	114.57	109.97
23	C	507	CLA	C3C-C4C-NC	4.90	116.07	110.57
23	C	509	CLA	C2C-C1C-NC	4.90	114.56	109.97
23	b	611	CLA	C3C-C4C-NC	4.90	116.06	110.57
23	A	404[B]	CLA	C2C-C1C-NC	4.90	114.56	109.97
23	b	605	CLA	C2C-C1C-NC	4.89	114.56	109.97
23	d	401[A]	CLA	C4A-NA-C1A	-4.89	104.51	106.71
23	b	603	CLA	C3B-C2B-C1B	-4.89	101.26	107.16
23	b	609	CLA	C3C-C4C-NC	4.89	116.06	110.57
23	a	409	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	c	507	CLA	CHD-C4C-C3C	-4.89	117.65	124.84
26	f	102	SQD	O47-C7-C8	4.89	122.03	111.50
23	c	514	CLA	O2D-CGD-CBD	4.88	119.94	111.27
23	C	509	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
23	C	504	CLA	C3C-C4C-NC	4.87	116.03	110.57
23	b	612	CLA	C4A-NA-C1A	-4.86	104.52	106.71
23	B	608	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	B	611	CLA	CHD-C1D-ND	-4.86	119.99	124.45
23	c	502	CLA	C4A-NA-C1A	-4.85	104.52	106.71
23	C	514	CLA	C3B-C2B-C1B	-4.85	101.30	107.16
23	C	503	CLA	C2C-C1C-NC	4.85	114.51	109.97
23	b	607	CLA	C3D-C2D-C1D	-4.84	99.22	105.83
24	b	617	BCR	C33-C5-C6	-4.84	119.09	124.53
23	B	604	CLA	C4A-NA-C1A	-4.84	104.53	106.71
23	D	404[B]	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
23	B	611	CLA	CMC-C2C-C1C	4.83	132.40	125.04
23	b	601	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
23	A	406[A]	CLA	C2C-C1C-NC	4.83	114.50	109.97
23	a	407[A]	CLA	C2C-C1C-NC	4.82	114.49	109.97
23	B	603	CLA	O2D-CGD-O1D	-4.82	114.41	123.84
23	b	615	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
37	D	402[B]	PHO	C3D-C4D-ND	4.82	114.29	107.72
23	B	610	CLA	C2C-C1C-NC	4.82	114.49	109.97
23	c	511	CLA	CHD-C1D-ND	-4.82	120.03	124.45
23	b	606	CLA	C3D-C2D-C1D	-4.82	99.26	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	C4A-NA-C1A	-4.82	104.54	106.71
23	c	510	CLA	C4A-NA-C1A	-4.82	104.54	106.71
23	C	510	CLA	C1-C2-C3	-4.81	117.72	126.04
23	B	602	CLA	C3C-C4C-NC	4.81	115.97	110.57
23	a	409	CLA	C3C-C4C-NC	4.81	115.96	110.57
23	a	409	CLA	C2C-C1C-NC	4.81	114.47	109.97
23	b	610	CLA	C2C-C1C-NC	4.80	114.47	109.97
23	C	511	CLA	C3B-C2B-C1B	-4.80	101.36	107.16
23	c	512	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
23	C	504	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
23	c	503	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	b	604	CLA	C3C-C4C-NC	4.79	115.94	110.57
23	c	503	CLA	C1C-C2C-C3C	-4.79	101.92	106.96
23	b	609	CLA	C1-C2-C3	-4.79	117.76	126.04
23	D	405	CLA	CHD-C1D-ND	-4.78	120.06	124.45
23	b	616	CLA	CHD-C1D-ND	-4.78	120.06	124.45
23	A	405[A]	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	b	605	CLA	O2D-CGD-O1D	-4.78	114.50	123.84
23	B	607	CLA	C2B-C1B-NB	4.77	113.43	110.23
23	A	405[A]	CLA	CMD-C2D-C1D	4.77	133.12	124.71
23	B	616	CLA	C3B-C2B-C1B	-4.77	101.41	107.16
23	C	504	CLA	C4A-NA-C1A	-4.76	104.56	106.71
23	a	405[B]	CLA	C2C-C1C-NC	4.76	114.43	109.97
23	c	509	CLA	CHD-C1D-ND	-4.76	120.08	124.45
23	b	602	CLA	C3D-C4D-ND	4.76	117.94	110.24
23	b	611	CLA	C1-C2-C3	-4.76	117.81	126.04
23	A	406[B]	CLA	C3D-C4D-ND	4.76	117.93	110.24
23	a	407[B]	CLA	C3D-C4D-ND	4.76	117.93	110.24
23	B	609	CLA	C3C-C4C-NC	4.75	115.90	110.57
23	C	505	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	a	409	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
23	c	502	CLA	O2D-CGD-CBD	4.74	119.70	111.27
23	c	503	CLA	O2D-CGD-CBD	4.74	119.70	111.27
23	b	609	CLA	C2C-C1C-NC	4.74	114.41	109.97
23	a	409	CLA	C3D-C4D-ND	4.74	117.90	110.24
23	B	605	CLA	C3C-C4C-NC	4.73	115.88	110.57
23	B	605	CLA	C2C-C1C-NC	4.73	114.40	109.97
23	B	607	CLA	C1C-C2C-C3C	-4.73	101.99	106.96
23	B	611	CLA	C3C-C4C-NC	4.72	115.87	110.57
23	C	510	CLA	CMD-C2D-C1D	4.72	133.03	124.71
26	b	620	SQD	C1-O5-C5	-4.72	104.43	113.69
23	b	601	CLA	C2C-C1C-NC	4.72	114.39	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	C1-C2-C3	-4.72	117.89	126.04
23	c	513	CLA	C3D-C2D-C1D	-4.72	99.40	105.83
23	A	407	CLA	C3C-C4C-NC	4.71	115.85	110.57
23	a	405[A]	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
23	B	609	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
23	c	506	CLA	C3D-C4D-ND	4.71	117.86	110.24
23	B	611	CLA	C1D-CHD-C4C	-4.71	115.90	126.06
23	b	603	CLA	C3C-C4C-NC	4.71	115.85	110.57
23	b	606	CLA	C3B-C2B-C1B	-4.70	101.49	107.16
23	c	511	CLA	C1-C2-C3	-4.70	117.92	126.04
23	B	601	CLA	C3B-C2B-C1B	-4.70	101.49	107.16
23	d	402	CLA	C3B-C2B-C1B	-4.69	101.49	107.16
23	c	510	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
23	b	605	CLA	C3C-C4C-NC	4.69	115.83	110.57
23	B	615	CLA	C3C-C4C-NC	4.69	115.83	110.57
23	B	602	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
23	b	613	CLA	C4A-NA-C1A	-4.68	104.60	106.71
23	C	512	CLA	C3D-C4D-ND	4.68	117.80	110.24
23	c	505	CLA	C4A-NA-C1A	-4.67	104.61	106.71
23	B	607	CLA	CMD-C2D-C1D	4.67	132.95	124.71
23	B	607	CLA	C3C-C4C-NC	4.67	115.81	110.57
23	B	602	CLA	CHD-C1D-ND	-4.67	120.16	124.45
23	A	407	CLA	O2D-CGD-CBD	4.67	119.57	111.27
23	c	502	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
23	c	514	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
23	C	510	CLA	C3B-C2B-C1B	-4.66	101.53	107.16
23	C	504	CLA	C3B-C2B-C1B	-4.66	101.53	107.16
23	B	613	CLA	C1-C2-C3	-4.66	117.99	126.04
23	C	512	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
23	C	510	CLA	CHD-C1D-ND	-4.65	120.18	124.45
33	C	502	LMG	O1-C1-C2	4.65	115.57	108.30
23	b	610	CLA	C3C-C4C-NC	4.65	115.79	110.57
23	d	401[B]	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
23	b	603	CLA	C1D-CHD-C4C	-4.65	116.03	126.06
37	a	408[A]	PHO	C3D-C4D-ND	4.64	114.04	107.72
23	C	504	CLA	O2D-CGD-CBD	4.64	119.51	111.27
23	C	512	CLA	C1C-C2C-C3C	-4.64	102.08	106.96
23	C	515	CLA	C3D-C2D-C1D	-4.64	99.51	105.83
23	C	511	CLA	C3C-C4C-NC	4.63	115.77	110.57
28	A	412[B]	PL9	C7-C8-C9	-4.63	119.08	126.79
23	c	509	CLA	C3C-C4C-NC	4.63	115.77	110.57
23	B	615	CLA	CMB-C2B-C1B	4.63	132.43	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	406[A]	CLA	O2D-CGD-CBD	4.63	119.49	111.27
23	A	404[B]	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
23	B	610	CLA	C3C-C4C-NC	4.63	115.76	110.57
23	B	612	CLA	C2C-C1C-NC	4.63	114.31	109.97
33	m	101	LMG	O7-C10-C11	4.62	121.47	111.50
23	c	510	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
23	C	514	CLA	C3C-C4C-NC	4.61	115.75	110.57
23	C	511	CLA	C1-C2-C3	-4.61	118.07	126.04
24	a	410	BCR	C38-C26-C25	-4.61	119.35	124.53
23	b	612	CLA	CAC-C3C-C4C	4.59	130.77	124.81
23	A	404[A]	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
23	B	605	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
23	C	508	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
23	B	601	CLA	C3C-C4C-NC	4.58	115.71	110.57
23	a	407[B]	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	c	513	CLA	CHD-C1D-ND	-4.58	120.25	124.45
23	C	506	CLA	C3C-C4C-NC	4.58	115.70	110.57
23	C	513	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	B	613	CLA	C4A-NA-C1A	-4.58	104.65	106.71
23	B	616	CLA	O2D-CGD-O1D	-4.57	114.89	123.84
23	A	404[A]	CLA	C3B-C2B-C1B	-4.57	101.64	107.16
23	B	604	CLA	C3B-C2B-C1B	-4.57	101.64	107.16
23	A	405[A]	CLA	C1C-C2C-C3C	-4.57	102.15	106.96
23	a	406[B]	CLA	O2D-CGD-CBD	4.57	119.38	111.27
23	C	505	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
23	d	401[B]	CLA	C3D-C4D-ND	4.56	117.61	110.24
23	B	612	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
23	A	405[B]	CLA	C3D-C4D-ND	4.55	117.60	110.24
23	A	407	CLA	C3D-C4D-ND	4.54	117.59	110.24
23	B	613	CLA	C3C-C4C-NC	4.54	115.66	110.57
23	B	601	CLA	C3D-C4D-ND	4.54	117.58	110.24
23	d	401[A]	CLA	C3C-C4C-NC	4.54	115.66	110.57
24	H	101	BCR	C38-C26-C25	-4.54	119.43	124.53
26	F	103	SQD	C1-O5-C5	-4.53	104.79	113.69
23	A	406[B]	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
23	A	406[A]	CLA	CMB-C2B-C1B	4.53	132.27	125.37
23	a	409	CLA	C4A-NA-C1A	-4.53	104.67	106.71
23	C	510	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	A	406[A]	CLA	C3D-C4D-ND	4.53	117.56	110.24
23	B	601	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	a	409	CLA	CMD-C2D-C1D	4.53	132.69	124.71
23	C	508	CLA	C3D-C4D-ND	4.53	117.56	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	C2C-C1C-NC	4.52	114.21	109.97
23	b	610	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
23	a	405[B]	CLA	C3D-C4D-ND	4.52	117.55	110.24
23	B	610	CLA	O2A-CGA-CBA	4.52	126.08	111.91
23	C	515	CLA	C4A-NA-C1A	-4.52	104.68	106.71
23	b	612	CLA	C3B-C2B-C1B	-4.51	101.71	107.16
23	A	406[A]	CLA	O2D-CGD-CBD	4.51	119.28	111.27
23	B	612	CLA	O2D-CGD-O1D	-4.51	115.02	123.84
23	a	406[B]	CLA	C1C-C2C-C3C	-4.50	102.22	106.96
33	B	621	LMG	O7-C10-C11	4.50	121.20	111.50
23	b	616	CLA	O2D-CGD-O1D	-4.50	115.04	123.84
23	C	512	CLA	C4A-NA-C1A	-4.50	104.69	106.71
23	C	514	CLA	C2C-C1C-NC	4.49	114.18	109.97
23	b	604	CLA	CHD-C1D-ND	-4.49	120.33	124.45
23	d	401[A]	CLA	C3D-C4D-ND	4.49	117.50	110.24
23	C	503	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
23	A	405[B]	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
23	b	610	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
23	d	402	CLA	C2C-C1C-NC	4.48	114.17	109.97
23	c	503	CLA	CHD-C1D-ND	-4.48	120.34	124.45
23	C	515	CLA	C3D-C4D-ND	4.47	117.48	110.24
23	b	605	CLA	C3B-C2B-C1B	-4.47	101.76	107.16
23	b	613	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
23	b	616	CLA	C3C-C4C-NC	4.47	115.58	110.57
23	A	406[B]	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
23	c	502	CLA	C3B-C2B-C1B	-4.46	101.77	107.16
23	b	613	CLA	C1-C2-C3	-4.46	118.33	126.04
23	b	609	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
23	B	606	CLA	C3C-C4C-NC	4.46	115.57	110.57
23	a	407[B]	CLA	C2C-C1C-NC	4.45	114.14	109.97
23	c	504	CLA	C3D-C4D-ND	4.45	117.44	110.24
37	D	402[B]	PHO	C1-C2-C3	-4.45	118.35	126.04
23	b	612	CLA	CHD-C1D-ND	-4.45	120.36	124.45
23	B	601	CLA	C2C-C1C-NC	4.45	114.14	109.97
28	A	412[B]	PL9	C7-C3-C4	4.45	120.49	116.88
23	B	608	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
23	a	407[A]	CLA	O2D-CGD-CBD	4.44	119.17	111.27
23	b	616	CLA	C1D-CHD-C4C	-4.44	116.47	126.06
23	c	512	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
23	c	502	CLA	O2D-CGD-O1D	-4.44	115.15	123.84
23	D	405	CLA	C3C-C4C-NC	4.44	115.55	110.57
23	A	404[B]	CLA	O2D-CGD-CBD	4.43	119.14	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
23	B	607	CLA	C4A-NA-C1A	-4.43	104.72	106.71
23	B	611	CLA	C3D-C4D-ND	4.42	117.39	110.24
26	F	103	SQD	O8-S-C6	4.42	112.78	105.74
23	B	602	CLA	O2D-CGD-O1D	-4.42	115.19	123.84
26	f	102	SQD	C1-O5-C5	4.42	122.36	113.69
23	C	507	CLA	C3B-C2B-C1B	-4.42	101.83	107.16
23	A	406[B]	CLA	O2D-CGD-CBD	4.42	119.12	111.27
23	c	507	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
23	a	405[B]	CLA	C1D-CHD-C4C	-4.41	116.54	126.06
23	b	614	CLA	C3D-C4D-ND	4.41	117.37	110.24
23	c	510	CLA	C1D-CHD-C4C	-4.41	116.55	126.06
23	C	512	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
23	A	404[B]	CLA	C1D-CHD-C4C	-4.40	116.56	126.06
23	b	603	CLA	C3D-C4D-ND	4.40	117.36	110.24
23	a	405[A]	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
23	b	609	CLA	C3D-C4D-ND	4.39	117.34	110.24
23	C	510	CLA	C3B-C4B-NB	4.39	114.59	110.52
23	a	406[A]	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
24	k	101	BCR	C29-C30-C25	4.39	117.24	110.48
23	b	604	CLA	C3B-C2B-C1B	-4.39	101.87	107.16
23	C	507	CLA	C3D-C4D-ND	4.39	117.33	110.24
23	B	616	CLA	CMD-C2D-C1D	4.39	132.44	124.71
23	B	608	CLA	C4A-NA-C1A	-4.38	104.73	106.71
23	B	613	CLA	O2D-CGD-CBD	4.38	119.06	111.27
23	c	508	CLA	C1C-C2C-C3C	-4.38	102.35	106.96
23	b	610	CLA	C3D-C4D-ND	4.38	117.32	110.24
23	a	406[A]	CLA	C4A-NA-C1A	-4.38	104.74	106.71
28	A	412[B]	PL9	C32-C33-C34	-4.38	117.12	127.66
23	b	601	CLA	C3C-C4C-NC	4.37	115.48	110.57
23	C	515	CLA	C3C-C4C-NC	4.37	115.47	110.57
23	b	612	CLA	C1-C2-C3	-4.37	118.48	126.04
23	C	513	CLA	C1D-CHD-C4C	-4.37	116.63	126.06
23	A	406[A]	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
23	b	616	CLA	C3B-C2B-C1B	-4.36	101.89	107.16
23	A	405[A]	CLA	C3D-C4D-ND	4.36	117.30	110.24
23	C	505	CLA	C3D-C4D-ND	4.36	117.30	110.24
33	a	417	LMG	O7-C10-C11	4.36	120.90	111.50
23	C	511	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
23	d	402	CLA	C3D-C4D-ND	4.36	117.29	110.24
32	E	101[A]	LHG	O7-C7-C8	4.36	120.90	111.50
23	b	605	CLA	C3D-C4D-ND	4.36	117.29	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407[A]	CLA	C3B-C2B-C1B	-4.36	101.90	107.16
23	b	601	CLA	C3D-C4D-ND	4.36	117.28	110.24
23	c	514	CLA	C3D-C4D-ND	4.36	117.28	110.24
23	C	508	CLA	O2D-CGD-CBD	4.35	119.00	111.27
23	a	407[A]	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	C	503	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	b	602	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
23	b	608	CLA	C3D-C4D-ND	4.34	117.27	110.24
23	b	601	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
23	d	401[A]	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
23	C	508	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
26	A	410	SQD	O8-S-C6	4.34	112.65	105.74
23	C	510	CLA	O2D-CGD-O1D	-4.34	115.36	123.84
23	b	611	CLA	C3B-C4B-NB	4.33	114.54	110.52
23	C	507	CLA	CMB-C2B-C1B	4.33	131.97	125.37
28	a	414[B]	PL9	C32-C33-C34	-4.33	117.24	127.66
23	b	614	CLA	O2D-CGD-O1D	-4.33	115.37	123.84
23	b	604	CLA	C3B-C4B-NB	4.32	114.53	110.52
23	c	507	CLA	C3B-C2B-C1B	-4.32	101.94	107.16
33	C	522	LMG	O6-C5-C4	4.32	117.55	109.69
23	b	610	CLA	O2A-CGA-CBA	4.32	125.47	111.91
23	b	607	CLA	C3D-C4D-ND	4.32	117.22	110.24
23	B	615	CLA	C3D-C4D-ND	4.31	117.22	110.24
23	a	405[B]	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
23	c	504	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
23	b	606	CLA	C3C-C4C-NC	4.31	115.41	110.57
23	c	513	CLA	C3C-C4C-NC	4.31	115.41	110.57
32	E	101[B]	LHG	O7-C7-C8	4.31	120.79	111.50
23	D	404[B]	CLA	C3C-C4C-NC	4.31	115.41	110.57
23	B	612	CLA	CAC-C3C-C4C	4.31	130.40	124.81
23	b	604	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
23	b	602	CLA	C2C-C1C-NC	4.31	114.01	109.97
26	a	411[A]	SQD	C1-C2-C3	-4.31	101.02	110.00
23	c	502	CLA	C3D-C4D-ND	4.31	117.21	110.24
23	C	506	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
23	c	507	CLA	C3D-C4D-ND	4.30	117.20	110.24
38	F	102	HEM	CHC-C4B-NB	4.30	129.09	124.42
23	b	607	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
23	c	510	CLA	C3D-C4D-ND	4.30	117.19	110.24
28	A	412[A]	PL9	C32-C33-C34	-4.30	117.31	127.66
23	B	602	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
23	a	406[B]	CLA	C3D-C4D-ND	4.29	117.18	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	102	BCR	C7-C8-C9	-4.29	119.75	126.23
23	a	407[A]	CLA	C3D-C4D-ND	4.29	117.17	110.24
33	C	526	LMG	O7-C10-C11	4.29	120.74	111.50
23	c	508	CLA	CMC-C2C-C1C	4.29	131.57	125.04
23	b	602	CLA	C3C-C4C-NC	4.28	115.38	110.57
23	a	405[A]	CLA	C3D-C4D-ND	4.28	117.17	110.24
23	A	405[A]	CLA	C3B-C2B-C1B	-4.28	102.00	107.16
23	b	612	CLA	C3D-C4D-ND	4.28	117.16	110.24
24	C	517	BCR	C32-C1-C6	-4.27	103.37	110.30
26	a	411[A]	SQD	O9-S-C6	4.27	112.01	106.94
23	C	514	CLA	C1D-CHD-C4C	-4.27	116.85	126.06
23	D	404[B]	CLA	C1-C2-C3	-4.27	118.66	126.04
23	d	401[B]	CLA	C3C-C4C-NC	4.26	115.35	110.57
23	a	405[A]	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	B	609	CLA	C3D-C4D-ND	4.26	117.13	110.24
23	c	512	CLA	C1D-CHD-C4C	-4.26	116.87	126.06
23	b	606	CLA	O2D-CGD-O1D	-4.26	115.52	123.84
23	b	602	CLA	CMC-C2C-C1C	4.26	131.52	125.04
23	D	405	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	A	405[B]	CLA	C3B-C2B-C1B	-4.26	102.03	107.16
23	c	504	CLA	C3C-C4C-NC	4.25	115.34	110.57
23	b	604	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
23	B	614	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
23	B	606	CLA	C3D-C4D-ND	4.25	117.11	110.24
23	B	603	CLA	C3B-C2B-C1B	-4.24	102.04	107.16
23	c	503	CLA	C4A-NA-C1A	-4.24	104.80	106.71
23	b	616	CLA	C2C-C1C-NC	4.24	113.94	109.97
23	C	508	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
23	b	615	CLA	C3B-C2B-C1B	-4.23	102.05	107.16
23	c	508	CLA	C3C-C4C-NC	4.23	115.32	110.57
23	C	514	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
23	C	505	CLA	C3C-C4C-NC	4.23	115.31	110.57
23	d	401[A]	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
38	F	102	HEM	C1B-NB-C4B	4.22	109.43	105.07
26	B	620	SQD	O7-S-C6	4.22	111.96	106.94
23	A	405[B]	CLA	C4A-NA-C1A	-4.22	104.81	106.71
23	c	510	CLA	C3B-C4B-NB	4.22	114.43	110.52
23	b	603	CLA	CAA-C2A-C3A	-4.22	101.23	112.78
23	c	507	CLA	O2D-CGD-CBD	4.21	118.76	111.27
23	a	406[A]	CLA	C3C-C4C-NC	4.21	115.29	110.57
23	C	511	CLA	C3D-C4D-ND	4.21	117.05	110.24
23	C	514	CLA	C3D-C4D-ND	4.21	117.05	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	C3D-C4D-ND	4.20	117.03	110.24
23	B	607	CLA	C3B-C2B-C1B	-4.20	102.10	107.16
23	C	504	CLA	C3D-C4D-ND	4.19	117.02	110.24
23	A	407	CLA	C4A-NA-C1A	-4.19	104.82	106.71
32	A	416[A]	LHG	O8-C23-O10	-4.18	113.04	123.59
23	B	607	CLA	C3D-C4D-ND	4.18	117.00	110.24
23	c	512	CLA	C3C-C4C-NC	4.17	115.25	110.57
38	F	102	HEM	C4C-NC-C1C	4.17	109.43	105.35
33	c	521	LMG	O6-C5-C4	4.17	117.27	109.69
23	d	401[B]	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
23	A	404[A]	CLA	C3B-C4B-NB	4.17	114.38	110.52
23	c	512	CLA	O2D-CGD-O1D	-4.16	115.70	123.84
33	d	409	LMG	O7-C10-C11	4.16	120.47	111.50
23	b	609	CLA	O2D-CGD-CBD	4.16	118.66	111.27
23	c	512	CLA	C3B-C4B-NB	4.16	114.37	110.52
23	b	611	CLA	C3D-C4D-ND	4.16	116.96	110.24
23	B	608	CLA	C3C-C4C-NC	4.15	115.22	110.57
23	A	406[A]	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
23	c	512	CLA	C3D-C4D-ND	4.15	116.95	110.24
23	c	509	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
23	C	515	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
23	B	613	CLA	C3B-C4B-NB	4.15	114.36	110.52
23	D	404[A]	CLA	C3B-C2B-C1B	-4.15	102.16	107.16
23	b	602	CLA	O2D-CGD-O1D	-4.14	115.73	123.84
23	a	405[A]	CLA	C1D-CHD-C4C	-4.14	117.12	126.06
23	C	511	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
23	D	405	CLA	O2D-CGD-O1D	-4.14	115.75	123.84
23	C	509	CLA	O2D-CGD-O1D	-4.14	115.75	123.84
23	D	404[B]	CLA	C3D-C4D-ND	4.14	116.93	110.24
23	c	511	CLA	C3D-C2D-C1D	-4.14	100.19	105.83
23	c	514	CLA	C1D-CHD-C4C	-4.14	117.14	126.06
24	C	516	BCR	C33-C5-C6	-4.13	119.89	124.53
28	a	414[A]	PL9	C7-C3-C4	4.13	120.24	116.88
23	c	511	CLA	C1D-CHD-C4C	-4.13	117.15	126.06
24	c	515	BCR	C11-C10-C9	-4.13	121.42	127.31
23	D	405	CLA	CAC-C3C-C4C	4.13	130.17	124.81
23	c	505	CLA	C3C-C4C-NC	4.13	115.20	110.57
23	a	406[A]	CLA	C3D-C4D-ND	4.12	116.91	110.24
23	c	508	CLA	CMB-C2B-C1B	4.12	131.65	125.37
23	A	404[B]	CLA	C3C-C4C-NC	4.12	115.19	110.57
23	b	608	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
23	C	503	CLA	C3D-C4D-ND	4.11	116.89	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	C4-C3-C5	4.11	122.18	115.27
38	F	102	HEM	CHD-C4C-NC	4.11	128.88	124.44
34	b	622	HTG	C1'-S1-C1	4.10	107.76	100.09
23	b	608	CLA	C3B-C4B-NB	4.10	114.32	110.52
23	B	615	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
23	D	404[B]	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
23	C	503	CLA	C3B-C2B-C1B	-4.10	102.22	107.16
23	C	513	CLA	CHD-C1D-ND	-4.10	120.69	124.45
28	a	414[B]	PL9	C7-C8-C9	-4.09	119.98	126.79
24	C	516	BCR	C15-C14-C13	-4.09	121.47	127.31
23	a	406[A]	CLA	CMB-C2B-C1B	4.09	131.60	125.37
23	d	401[A]	CLA	O2D-CGD-CBD	4.09	118.53	111.27
23	d	401[A]	CLA	C3B-C2B-C1B	-4.09	102.23	107.16
23	C	508	CLA	C3C-C4C-NC	4.09	115.15	110.57
23	a	406[A]	CLA	CAA-C2A-C3A	-4.09	101.59	112.78
23	b	613	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
23	B	614	CLA	CAC-C3C-C4C	4.08	130.11	124.81
23	B	602	CLA	C3D-C4D-ND	4.08	116.84	110.24
23	c	510	CLA	C3C-C4C-NC	4.08	115.15	110.57
23	b	606	CLA	C3D-C4D-ND	4.08	116.84	110.24
23	b	606	CLA	C1D-CHD-C4C	-4.08	117.26	126.06
23	c	513	CLA	C1D-CHD-C4C	-4.08	117.26	126.06
37	D	401[A]	PHO	C1A-C2A-C3A	-4.08	98.96	102.84
23	c	511	CLA	C3C-C4C-NC	4.08	115.14	110.57
24	T	102	BCR	C15-C16-C17	-4.08	115.13	123.47
23	B	613	CLA	C3B-C2B-C1B	-4.07	102.24	107.16
24	d	403	BCR	C15-C14-C13	-4.07	121.50	127.31
23	A	404[B]	CLA	C3D-C4D-ND	4.07	116.82	110.24
23	D	404[A]	CLA	C3D-C4D-ND	4.07	116.82	110.24
24	Y	101	BCR	C15-C14-C13	-4.07	121.50	127.31
37	D	402[A]	PHO	C1-C2-C3	-4.07	119.00	126.04
23	B	616	CLA	CHD-C1D-ND	-4.07	120.72	124.45
23	D	404[A]	CLA	O2D-CGD-CBD	4.06	118.49	111.27
23	b	601	CLA	C1D-CHD-C4C	-4.06	117.29	126.06
23	a	405[A]	CLA	CAA-C2A-C3A	-4.06	101.65	112.78
23	a	406[A]	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
23	c	511	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
23	c	502	CLA	C3C-C4C-NC	4.06	115.12	110.57
23	a	406[A]	CLA	C1D-CHD-C4C	-4.06	117.30	126.06
23	B	608	CLA	C3D-C4D-ND	4.05	116.80	110.24
23	B	614	CLA	C3C-C4C-NC	4.05	115.11	110.57
23	c	504	CLA	C1D-CHD-C4C	-4.05	117.32	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	406[B]	CLA	C3C-C4C-NC	4.05	115.11	110.57
23	C	510	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
23	B	615	CLA	C3B-C2B-C1B	-4.04	102.28	107.16
23	c	507	CLA	C1C-C2C-C3C	-4.04	102.70	106.96
33	c	521	LMG	O7-C10-C11	4.04	120.22	111.50
23	C	506	CLA	C3D-C4D-ND	4.04	116.78	110.24
26	a	411[A]	SQD	C44-O6-C1	-4.04	105.84	113.74
23	B	605	CLA	C3D-C4D-ND	4.04	116.77	110.24
23	b	608	CLA	C3B-C2B-C1B	-4.04	102.29	107.16
24	d	403	BCR	C29-C30-C25	4.04	116.70	110.48
33	c	521	LMG	C3-C4-C5	4.04	117.44	110.24
23	b	608	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
38	f	101	HEM	CAD-CBD-CGD	4.03	122.28	113.60
23	C	512	CLA	C3B-C4B-NB	4.03	114.26	110.52
23	b	610	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
23	B	616	CLA	C4C-C3C-C2C	-4.03	101.02	106.90
23	B	614	CLA	CMC-C2C-C1C	4.03	131.18	125.04
23	A	404[A]	CLA	C3D-C4D-ND	4.03	116.75	110.24
23	a	405[A]	CLA	C3C-C4C-NC	4.03	115.09	110.57
28	a	414[A]	PL9	C32-C33-C34	-4.03	117.96	127.66
23	b	610	CLA	C1-C2-C3	-4.03	119.08	126.04
23	b	616	CLA	C3D-C4D-ND	4.03	116.75	110.24
23	B	602	CLA	C1D-CHD-C4C	-4.02	117.38	126.06
23	A	404[B]	CLA	C3B-C4B-NB	4.02	114.24	110.52
23	B	601	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
32	l	802[B]	LHG	O7-C7-C8	4.02	120.16	111.50
33	C	502	LMG	O7-C10-C11	4.02	120.16	111.50
23	B	603	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
23	c	509	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
23	B	612	CLA	C3D-C4D-ND	4.01	116.72	110.24
23	A	404[A]	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
23	a	406[B]	CLA	C3B-C2B-C1B	-4.01	102.33	107.16
23	B	614	CLA	C3D-C4D-ND	4.00	116.72	110.24
35	C	519[A]	DGD	O2G-C1B-C2B	4.00	120.12	111.50
23	C	513	CLA	C4A-NA-C1A	-4.00	104.91	106.71
23	b	612	CLA	O2D-CGD-CBD	4.00	118.37	111.27
23	C	507	CLA	C3D-C2D-C1D	-4.00	100.38	105.83
38	f	101	HEM	C4C-NC-C1C	3.99	109.25	105.35
26	A	410	SQD	O47-C7-C8	3.98	120.08	111.50
33	c	520	LMG	O7-C10-C11	3.97	120.06	111.50
31	t	102	LMT	C3'-C4'-C5'	-3.97	101.82	110.93
23	D	404[B]	CLA	O2D-CGD-CBD	3.97	118.32	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	C3D-C4D-ND	3.97	116.66	110.24
35	C	518[A]	DGD	O2G-C1B-C2B	3.97	120.05	111.50
23	B	605	CLA	C1-C2-C3	-3.97	119.19	126.04
23	A	406[A]	CLA	C3C-C4C-NC	3.96	115.02	110.57
23	b	608	CLA	C1-C2-C3	-3.96	119.19	126.04
23	b	613	CLA	O2A-CGA-O1A	-3.96	113.60	123.59
23	a	405[B]	CLA	C3B-C2B-C1B	-3.96	102.39	107.16
26	C	501[A]	SQD	O9-S-C6	3.96	111.64	106.94
23	A	406[B]	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
23	C	507	CLA	CMC-C2C-C1C	3.95	131.06	125.04
23	B	611	CLA	O2D-CGD-O1D	-3.95	116.12	123.84
24	C	516	BCR	C7-C8-C9	-3.94	120.28	126.23
23	C	514	CLA	C1-C2-C3	-3.94	119.22	126.04
23	c	513	CLA	C3D-C4D-ND	3.94	116.61	110.24
23	A	405[A]	CLA	CMC-C2C-C1C	3.94	131.04	125.04
23	b	612	CLA	CMC-C2C-C1C	3.94	131.04	125.04
23	b	602	CLA	CAA-C2A-C3A	-3.94	101.99	112.78
37	D	401[B]	PHO	C1A-C2A-C3A	-3.93	99.10	102.84
23	a	405[B]	CLA	C3B-C4B-NB	3.93	114.16	110.52
23	A	404[A]	CLA	C3C-C4C-NC	3.93	114.98	110.57
23	c	511	CLA	CMC-C2C-C1C	3.93	131.02	125.04
23	c	509	CLA	C3D-C4D-ND	3.93	116.59	110.24
23	A	405[B]	CLA	CBC-CAC-C3C	-3.92	101.62	112.43
23	b	608	CLA	CAC-C3C-C4C	3.92	129.90	124.81
34	V	203	HTG	C1-O5-C5	3.92	117.50	112.19
23	B	611	CLA	CHD-C4C-NC	3.92	130.38	124.20
23	c	503	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
23	c	511	CLA	C3D-C4D-ND	3.91	116.57	110.24
24	B	618	BCR	C29-C30-C25	3.91	116.50	110.48
23	b	612	CLA	C4-C3-C5	3.91	121.84	115.27
23	b	614	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
24	h	101	BCR	C38-C26-C25	-3.90	120.15	124.53
23	d	402	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
23	B	606	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
23	b	604	CLA	CMC-C2C-C1C	3.90	130.98	125.04
23	c	509	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
23	d	402	CLA	C3C-C4C-NC	3.90	114.94	110.57
23	c	503	CLA	C3D-C4D-ND	3.90	116.55	110.24
23	B	608	CLA	C3B-C4B-NB	3.90	114.13	110.52
33	C	526	LMG	C1-C2-C3	3.90	118.11	110.00
23	b	615	CLA	C3C-C4C-NC	3.90	114.94	110.57
23	C	507	CLA	C1D-CHD-C4C	-3.89	117.66	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
23	a	407[B]	CLA	C3C-C4C-NC	3.89	114.94	110.57
23	A	406[A]	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
23	C	510	CLA	C3D-C4D-ND	3.89	116.53	110.24
23	a	405[A]	CLA	O2D-CGD-CBD	3.88	118.16	111.27
28	a	414[B]	PL9	C7-C3-C4	3.88	120.03	116.88
23	c	512	CLA	C4A-NA-C1A	-3.87	104.97	106.71
23	B	606	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
26	C	501[B]	SQD	C1-O5-C5	-3.87	106.09	113.69
33	C	521	LMG	O7-C10-C11	3.87	119.84	111.50
23	b	605	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
23	B	604	CLA	C1D-CHD-C4C	-3.86	117.72	126.06
23	a	406[B]	CLA	C1D-CHD-C4C	-3.86	117.72	126.06
35	C	518[B]	DGD	O2G-C1B-C2B	3.86	119.83	111.50
23	B	610	CLA	C3B-C2B-C1B	-3.86	102.50	107.16
23	b	610	CLA	O2A-CGA-O1A	-3.86	113.86	123.59
23	B	608	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
23	c	507	CLA	C3B-C4B-NB	3.85	114.09	110.52
23	C	503	CLA	C1D-CHD-C4C	-3.85	117.76	126.06
23	B	614	CLA	O2D-CGD-O1D	-3.85	116.32	123.84
23	b	613	CLA	C3B-C4B-NB	3.84	114.08	110.52
23	c	509	CLA	C1-C2-C3	-3.84	119.40	126.04
23	C	505	CLA	C1D-CHD-C4C	-3.84	117.77	126.06
23	b	608	CLA	C1D-CHD-C4C	-3.84	117.77	126.06
23	a	409	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
24	A	408	BCR	C15-C14-C13	-3.84	121.83	127.31
23	b	615	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
23	C	509	CLA	CMB-C2B-C1B	3.84	131.21	125.37
23	b	614	CLA	C3C-C4C-NC	3.84	114.87	110.57
23	C	509	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
23	B	613	CLA	C3D-C4D-ND	3.83	116.44	110.24
26	B	620	SQD	C3-C4-C5	3.83	117.07	110.24
28	A	412[A]	PL9	C7-C3-C4	3.83	119.99	116.88
28	d	404[B]	PL9	C7-C8-C9	-3.83	120.42	126.79
23	A	404[A]	CLA	CAA-C2A-C3A	-3.83	102.30	112.78
33	C	522	LMG	C3-C4-C5	3.83	117.06	110.24
23	A	405[A]	CLA	C3C-C4C-NC	3.83	114.86	110.57
23	b	607	CLA	O2D-CGD-CBD	3.82	118.06	111.27
33	C	522	LMG	O7-C10-C11	3.82	119.74	111.50
23	B	615	CLA	CMC-C2C-C1C	3.82	130.85	125.04
23	D	405	CLA	C3D-C4D-ND	3.81	116.40	110.24
23	B	604	CLA	C3B-C4B-NB	3.81	114.05	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	C3D-C2D-C1D	-3.81	100.64	105.83
23	c	505	CLA	C3D-C4D-ND	3.80	116.39	110.24
23	C	511	CLA	O2D-CGD-CBD	3.80	118.02	111.27
23	b	611	CLA	C3B-C2B-C1B	-3.80	102.58	107.16
23	B	610	CLA	C3D-C4D-ND	3.80	116.38	110.24
23	A	407	CLA	CAA-C2A-C3A	-3.80	102.39	112.78
24	d	403	BCR	C40-C30-C25	-3.79	104.14	110.30
23	a	405[B]	CLA	C3C-C4C-NC	3.79	114.83	110.57
23	A	404[A]	CLA	O2A-CGA-CBA	3.79	123.81	111.91
23	B	605	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
23	B	608	CLA	O2D-CGD-O1D	-3.79	116.43	123.84
23	B	603	CLA	C3D-C4D-ND	3.79	116.36	110.24
23	C	504	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
23	B	616	CLA	C3D-C4D-ND	3.78	116.35	110.24
23	A	404[A]	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
23	a	405[B]	CLA	CAA-C2A-C3A	-3.77	102.44	112.78
28	A	412[B]	PL9	C22-C23-C24	-3.77	118.58	127.66
23	D	404[A]	CLA	C3B-C4B-NB	3.77	114.01	110.52
23	B	606	CLA	C3B-C2B-C1B	-3.77	102.61	107.16
23	b	612	CLA	C3D-C2D-C1D	-3.77	100.69	105.83
23	b	612	CLA	C3B-C4B-NB	3.76	114.01	110.52
28	a	414[A]	PL9	C15-C14-C16	3.76	121.60	115.27
23	B	606	CLA	O2D-CGD-O1D	-3.76	116.48	123.84
23	C	507	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
34	b	622	HTG	O2-C2-C1	3.76	117.17	110.27
23	D	404[A]	CLA	C1-C2-C3	-3.76	119.54	126.04
23	c	506	CLA	C3B-C2B-C1B	-3.76	102.62	107.16
23	c	502	CLA	CAC-C3C-C4C	3.76	129.68	124.81
38	F	102	HEM	CBD-CAD-C3D	-3.75	102.19	112.63
23	B	615	CLA	C4-C3-C5	3.75	121.58	115.27
23	c	505	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
26	C	501[B]	SQD	O47-C7-C8	3.75	119.59	111.50
23	A	405[A]	CLA	CBC-CAC-C3C	-3.75	102.10	112.43
28	a	414[B]	PL9	C15-C14-C16	3.75	121.57	115.27
23	c	505	CLA	C3B-C4B-NB	3.74	113.99	110.52
23	B	613	CLA	C4-C3-C5	3.74	121.56	115.27
23	C	508	CLA	C1-C2-C3	-3.74	119.57	126.04
28	D	407[B]	PL9	C42-C43-C44	-3.74	118.67	127.66
23	d	401[B]	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
32	d	411[A]	LHG	O8-C23-O10	-3.73	114.17	123.59
23	C	507	CLA	CAC-C3C-C4C	3.73	129.65	124.81
23	B	610	CLA	C1D-CHD-C4C	-3.73	118.02	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
23	c	506	CLA	C3D-C2D-C1D	-3.72	100.75	105.83
23	b	612	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
23	C	513	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
23	C	506	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
23	A	404[A]	CLA	O2D-CGD-CBD	3.72	117.88	111.27
23	c	506	CLA	C4C-C3C-C2C	-3.72	101.48	106.90
23	b	613	CLA	O2A-CGA-CBA	3.72	123.57	111.91
23	c	503	CLA	C3C-C4C-NC	3.72	114.74	110.57
23	b	607	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
23	b	603	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
32	L	101[A]	LHG	O7-C7-C8	3.71	119.50	111.50
24	c	516	BCR	C7-C8-C9	-3.71	120.63	126.23
28	a	414[A]	PL9	C7-C3-C2	-3.71	118.42	123.30
33	C	521	LMG	O8-C28-C29	3.70	123.53	111.91
34	b	625	HTG	C1-O5-C5	3.70	119.41	112.58
23	D	405	CLA	CMB-C2B-C1B	3.70	131.01	125.37
23	B	613	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
23	b	609	CLA	C3B-C2B-C1B	-3.70	102.70	107.16
23	B	609	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
23	C	512	CLA	C1D-CHD-C4C	-3.70	118.09	126.06
23	B	605	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
34	B	622	HTG	C1'-S1-C1	3.69	107.00	100.09
40	V	202	HEC	CBD-CAD-C3D	-3.69	102.37	112.63
23	B	604	CLA	CHD-C1D-ND	-3.69	121.06	124.45
23	C	515	CLA	C3B-C4B-NB	3.69	113.94	110.52
23	B	609	CLA	O2D-CGD-CBD	3.69	117.82	111.27
23	D	405	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
23	b	604	CLA	CAC-C3C-C4C	3.69	129.59	124.81
23	a	405[B]	CLA	O2D-CGD-CBD	3.69	117.82	111.27
23	B	603	CLA	C1D-CHD-C4C	-3.69	118.11	126.06
28	A	412[B]	PL9	C7-C3-C2	-3.68	118.45	123.30
26	a	411[B]	SQD	O6-C1-C2	3.68	114.05	108.30
23	c	510	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
23	b	605	CLA	CHD-C4C-NC	3.68	130.01	124.20
23	a	409	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
31	A	415	LMT	O5B-C5B-C4B	3.68	116.38	109.69
23	b	606	CLA	C3B-C4B-NB	3.68	113.93	110.52
23	A	405[B]	CLA	CAA-C2A-C3A	-3.68	102.71	112.78
23	B	616	CLA	C1D-CHD-C4C	-3.68	118.13	126.06
26	C	501[A]	SQD	C44-O6-C1	-3.67	106.57	113.74
28	a	414[A]	PL9	C30-C29-C31	3.67	121.44	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	407[A]	PL9	C42-C43-C44	-3.67	118.83	127.66
23	c	504	CLA	CMB-C2B-C1B	3.67	130.95	125.37
23	B	615	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
23	D	404[A]	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
23	B	610	CLA	CAA-C2A-C3A	-3.66	102.76	112.78
23	B	609	CLA	CMB-C2B-C1B	3.65	130.94	125.37
23	c	508	CLA	O2D-CGD-O1D	-3.65	116.69	123.84
23	B	611	CLA	C1-C2-C3	-3.65	119.72	126.04
23	b	616	CLA	O2A-CGA-CBA	3.65	123.37	111.91
28	A	412[A]	PL9	C15-C14-C16	3.65	121.41	115.27
35	C	519[B]	DGD	O2G-C1B-C2B	3.65	119.37	111.50
23	b	607	CLA	C3B-C4B-NB	3.65	113.90	110.52
35	c	518[B]	DGD	O2G-C1B-C2B	3.64	119.35	111.50
23	b	603	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
23	a	407[A]	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
23	c	507	CLA	CAC-C3C-C4C	3.64	129.53	124.81
35	c	517[A]	DGD	O2G-C1B-C2B	3.64	119.34	111.50
23	D	405	CLA	C4-C3-C5	3.64	121.39	115.27
23	A	407	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
23	B	614	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
23	a	407[A]	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
23	B	602	CLA	CAA-C2A-C3A	-3.63	102.84	112.78
24	b	617	BCR	C7-C8-C9	-3.63	120.75	126.23
38	f	101	HEM	CHA-C4D-ND	3.63	128.85	124.37
23	c	513	CLA	C1-C2-C3	-3.63	119.77	126.04
23	A	406[B]	CLA	C3C-C4C-NC	3.63	114.64	110.57
23	B	607	CLA	O2D-CGD-O1D	-3.62	116.75	123.84
23	c	508	CLA	C3D-C4D-ND	3.62	116.10	110.24
23	c	507	CLA	C1-C2-C3	-3.62	119.78	126.04
24	B	617	BCR	C33-C5-C6	-3.62	120.46	124.53
23	a	405[A]	CLA	O2A-CGA-O1A	-3.62	114.47	123.59
23	B	612	CLA	C4C-C3C-C2C	-3.61	101.64	106.90
23	C	513	CLA	C3D-C4D-ND	3.61	116.08	110.24
23	A	406[B]	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
23	c	509	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
23	C	508	CLA	C3B-C4B-NB	3.61	113.86	110.52
23	c	510	CLA	CAC-C3C-C4C	3.61	129.49	124.81
23	a	406[B]	CLA	CAA-C2A-C3A	-3.60	102.91	112.78
31	B	628	LMT	C1'-O5'-C5'	-3.60	106.62	113.69
32	d	411[A]	LHG	O8-C23-C24	3.60	123.21	111.91
23	C	506	CLA	CMC-C2C-C1C	3.60	130.52	125.04
23	b	615	CLA	C1C-C2C-C3C	-3.59	103.18	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
28	D	407[B]	PL9	C25-C24-C26	3.59	121.31	115.27
23	B	614	CLA	C3B-C4B-NB	3.59	113.85	110.52
23	c	505	CLA	C1-O2A-CGA	3.59	125.86	116.44
28	d	404[A]	PL9	C42-C43-C44	-3.59	119.02	127.66
23	c	507	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
23	c	502	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
23	c	514	CLA	C3B-C4B-NB	3.58	113.84	110.52
23	c	507	CLA	C3C-C4C-NC	3.58	114.59	110.57
23	C	510	CLA	C4A-NA-C1A	-3.58	105.10	106.71
23	b	614	CLA	C1-C2-C3	-3.58	119.85	126.04
28	a	414[B]	PL9	C27-C28-C29	-3.58	119.04	127.66
23	B	610	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
23	B	604	CLA	C1C-C2C-C3C	-3.58	103.20	106.96
23	C	515	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
26	F	103	SQD	C44-O6-C1	-3.58	106.75	113.74
28	A	412[A]	PL9	C22-C23-C24	-3.57	119.05	127.66
23	C	515	CLA	CMC-C2C-C1C	3.57	130.48	125.04
23	c	514	CLA	C3C-C4C-NC	3.57	114.58	110.57
28	d	404[A]	PL9	C40-C39-C41	3.57	121.28	115.27
23	b	612	CLA	C4C-C3C-C2C	-3.57	101.69	106.90
35	c	518[A]	DGD	O2G-C1B-C2B	3.57	119.19	111.50
23	b	604	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
32	d	411[B]	LHG	O7-C7-C8	3.57	119.19	111.50
23	B	610	CLA	O2A-CGA-O1A	-3.57	114.59	123.59
32	D	409[B]	LHG	O7-C7-C8	3.57	119.19	111.50
23	a	407[B]	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
23	A	407	CLA	C4C-C3C-C2C	-3.56	101.70	106.90
23	C	512	CLA	C4-C3-C5	3.56	121.27	115.27
28	A	412[B]	PL9	C15-C14-C16	3.56	121.26	115.27
23	B	604	CLA	C3D-C4D-ND	3.56	116.00	110.24
23	C	506	CLA	C1-O2A-CGA	3.56	125.78	116.44
23	c	506	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
23	A	405[A]	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
23	B	603	CLA	CAA-C2A-C3A	-3.56	103.04	112.78
23	b	605	CLA	O2A-CGA-O1A	-3.55	114.62	123.59
26	C	501[A]	SQD	O47-C7-C8	3.55	119.16	111.50
33	D	413	LMG	O7-C10-C11	3.55	119.16	111.50
23	B	605	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
28	A	412[A]	PL9	C7-C3-C2	-3.55	118.63	123.30
23	c	503	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
24	k	101	BCR	C7-C8-C9	-3.54	120.88	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	L	101[B]	LHG	O7-C7-C8	3.54	119.14	111.50
23	b	611	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
23	A	406[A]	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
23	A	404[B]	CLA	CAA-C2A-C3A	-3.54	103.09	112.78
24	D	406	BCR	C29-C30-C25	3.53	115.92	110.48
23	b	608	CLA	C3C-C4C-NC	3.53	114.53	110.57
23	b	602	CLA	C1-C2-C3	-3.53	119.94	126.04
23	D	405	CLA	CMC-C2C-C1C	3.53	130.42	125.04
23	B	601	CLA	C4C-C3C-C2C	-3.53	101.75	106.90
23	C	510	CLA	C4C-C3C-C2C	-3.53	101.75	106.90
38	f	101	HEM	CHD-C1D-ND	3.53	128.25	124.42
23	c	510	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
23	c	513	CLA	CMB-C2B-C1B	3.53	130.74	125.37
23	A	407	CLA	C1-C2-C3	-3.53	119.94	126.04
23	b	611	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
23	A	405[A]	CLA	CAA-C2A-C3A	-3.52	103.13	112.78
23	A	404[B]	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
23	a	405[B]	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
23	B	611	CLA	CHB-C4A-NA	3.52	129.38	124.51
23	B	602	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
23	B	612	CLA	C1-C2-C3	-3.51	119.97	126.04
38	F	102	HEM	CHD-C1D-ND	3.50	128.22	124.42
32	A	416[A]	LHG	O7-C7-C8	3.50	119.04	111.50
23	a	409	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
26	a	412	SQD	O47-C7-C8	3.49	119.03	111.50
23	A	404[B]	CLA	C3B-C2B-C1B	-3.49	102.95	107.16
23	b	607	CLA	C4C-C3C-C2C	-3.49	101.81	106.90
23	a	407[B]	CLA	C1D-CHD-C4C	-3.49	118.54	126.06
23	c	504	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
23	c	504	CLA	C3B-C4B-NB	3.48	113.75	110.52
38	f	101	HEM	C4D-ND-C1D	3.48	108.67	105.07
23	c	514	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
23	c	502	CLA	CMB-C2B-C1B	3.48	130.67	125.37
23	b	605	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
23	d	401[A]	CLA	O2A-CGA-CBA	3.48	122.83	111.91
24	A	408	BCR	C24-C23-C22	-3.48	120.98	126.23
33	B	621	LMG	O8-C28-C29	3.48	122.81	111.91
32	D	408[B]	LHG	O7-C7-C8	3.47	118.99	111.50
23	b	616	CLA	CMC-C2C-C1C	3.47	130.33	125.04
23	B	605	CLA	O2A-CGA-O1A	-3.47	114.83	123.59
23	b	601	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
23	d	401[A]	CLA	C3B-C4B-NB	3.47	113.73	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	CMB-C2B-C1B	3.47	130.65	125.37
23	b	610	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
23	C	506	CLA	C3B-C4B-NB	3.47	113.73	110.52
37	D	402[A]	PHO	C1A-C2A-C3A	-3.46	99.54	102.84
28	d	404[A]	PL9	C37-C38-C39	-3.46	119.33	127.66
23	B	605	CLA	CHD-C4C-NC	3.46	129.66	124.20
23	A	405[B]	CLA	C1D-CHD-C4C	-3.46	118.60	126.06
23	c	505	CLA	C1D-CHD-C4C	-3.46	118.60	126.06
23	b	616	CLA	CMB-C2B-C1B	3.45	130.63	125.37
23	B	614	CLA	C1-C2-C3	-3.45	120.07	126.04
23	C	507	CLA	C1-C2-C3	-3.45	120.08	126.04
23	A	404[A]	CLA	O2A-CGA-O1A	-3.45	114.89	123.59
23	B	607	CLA	C4-C3-C5	3.45	121.07	115.27
23	c	502	CLA	C3B-C4B-NB	3.45	113.71	110.52
23	b	615	CLA	CMB-C2B-C1B	3.45	130.62	125.37
23	D	405	CLA	C3B-C2B-C1B	-3.44	103.00	107.16
23	b	604	CLA	C3D-C4D-ND	3.44	115.81	110.24
24	A	408	BCR	C40-C30-C25	-3.44	104.72	110.30
28	A	412[B]	PL9	C37-C38-C39	-3.43	119.39	127.66
23	C	509	CLA	CBC-CAC-C3C	-3.43	102.97	112.43
37	a	416[B]	PHO	O2D-CGD-O1D	-3.43	117.13	123.84
23	B	611	CLA	C4C-C3C-C2C	-3.43	101.90	106.90
23	C	503	CLA	C3B-C4B-NB	3.43	113.70	110.52
23	A	405[B]	CLA	C3C-C4C-NC	3.43	114.42	110.57
26	C	501[B]	SQD	C1-C2-C3	-3.43	102.86	110.00
37	a	408[A]	PHO	C1A-C2A-C3A	-3.43	99.58	102.84
35	c	517[B]	DGD	O2G-C1B-C2B	3.43	118.88	111.50
23	b	609	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
23	c	506	CLA	CMB-C2B-C1B	3.42	130.59	125.37
23	B	607	CLA	CAA-C2A-C3A	-3.42	103.40	112.78
37	D	402[B]	PHO	C1A-C2A-C3A	-3.42	99.58	102.84
23	B	615	CLA	O2D-CGD-CBD	3.42	117.35	111.27
34	b	622	HTG	O5-C5-C4	3.42	115.91	109.69
23	B	609	CLA	C3B-C2B-C1B	-3.42	103.03	107.16
23	c	511	CLA	C3B-C4B-NB	3.42	113.69	110.52
23	C	509	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
23	b	601	CLA	CHD-C4C-NC	3.42	129.59	124.20
23	B	610	CLA	CMB-C2B-C1B	3.42	130.57	125.37
32	d	406[A]	LHG	O7-C7-C8	3.42	118.86	111.50
23	b	610	CLA	C4C-C3C-C2C	-3.42	101.92	106.90
23	a	406[A]	CLA	CHD-C4C-NC	3.41	129.58	124.20
23	C	510	CLA	C1D-CHD-C4C	-3.41	118.71	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	a	408[A]	PHO	O1D-CGD-CBD	-3.41	119.07	124.74
23	c	503	CLA	CBC-CAC-C3C	-3.40	103.06	112.43
23	b	610	CLA	CAA-C2A-C3A	-3.40	103.47	112.78
23	B	610	CLA	C4C-C3C-C2C	-3.39	101.95	106.90
23	B	605	CLA	C4-C3-C5	3.39	120.98	115.27
23	B	616	CLA	CAC-C3C-C4C	3.39	129.21	124.81
23	c	512	CLA	C4-C3-C5	3.39	120.97	115.27
23	d	401[B]	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
23	c	505	CLA	CMB-C2B-C1B	3.39	130.53	125.37
23	B	604	CLA	CMB-C2B-C1B	3.39	130.53	125.37
24	d	403	BCR	C37-C22-C23	3.39	123.41	118.08
23	d	401[B]	CLA	C1D-CHD-C4C	-3.38	118.76	126.06
24	B	617	BCR	C7-C8-C9	-3.38	121.12	126.23
23	A	407	CLA	C3B-C4B-NB	3.38	113.65	110.52
23	b	612	CLA	O2A-CGA-O1A	-3.38	115.06	123.59
23	a	406[A]	CLA	C3B-C4B-NB	3.38	113.65	110.52
23	b	613	CLA	O2D-CGD-CBD	3.38	117.27	111.27
23	b	615	CLA	O2D-CGD-CBD	3.38	117.27	111.27
28	a	414[A]	PL9	C27-C28-C29	-3.38	119.53	127.66
23	B	610	CLA	CAA-CBA-CGA	-3.38	103.39	113.25
28	A	412[A]	PL9	C37-C38-C39	-3.37	119.54	127.66
23	D	405	CLA	C4C-C3C-C2C	-3.37	101.98	106.90
38	f	101	HEM	C1B-NB-C4B	3.37	108.56	105.07
23	c	507	CLA	CHC-C1C-C2C	-3.37	117.37	126.73
23	b	606	CLA	C1-C2-C3	-3.37	120.21	126.04
24	y	101	BCR	C15-C14-C13	-3.37	122.50	127.31
23	B	613	CLA	CAC-C3C-C4C	3.37	129.18	124.81
23	C	505	CLA	CMB-C2B-C1B	3.36	130.49	125.37
23	C	508	CLA	C1D-CHD-C4C	-3.36	118.80	126.06
23	B	609	CLA	C1D-CHD-C4C	-3.36	118.80	126.06
28	A	412[A]	PL9	C27-C28-C29	-3.36	119.56	127.66
23	b	611	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
23	a	405[A]	CLA	O2A-CGA-CBA	3.36	122.45	111.91
23	b	604	CLA	C1D-CHD-C4C	-3.36	118.82	126.06
23	b	602	CLA	C1D-CHD-C4C	-3.36	118.82	126.06
23	B	604	CLA	C4C-C3C-C2C	-3.36	102.01	106.90
23	D	404[A]	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
23	B	612	CLA	CMC-C2C-C1C	3.35	130.15	125.04
23	B	602	CLA	C3B-C4B-NB	3.35	113.63	110.52
23	b	614	CLA	CMB-C2B-C1B	3.35	130.47	125.37
23	C	513	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
23	B	615	CLA	CED-O2D-CGD	3.35	123.51	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	515	BCR	C15-C14-C13	-3.35	122.53	127.31
23	B	610	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
23	C	514	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
23	D	405	CLA	CAA-C2A-C3A	-3.35	103.61	112.78
23	A	404[A]	CLA	CAC-C3C-C4C	3.35	129.15	124.81
32	l	802[A]	LHG	O7-C7-C8	3.35	118.72	111.50
32	A	416[B]	LHG	C5-O7-C7	-3.35	109.55	117.79
23	b	616	CLA	CHD-C4C-NC	3.35	129.48	124.20
35	c	519	DGD	O2G-C1B-C2B	3.35	118.71	111.50
37	a	416[A]	PHO	C4-C3-C5	3.35	120.90	115.27
23	B	607	CLA	CMC-C2C-C1C	3.34	130.13	125.04
23	b	609	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
23	c	507	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
23	C	513	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
34	B	625	HTG	C1'-S1-C1	3.34	106.34	100.09
23	d	401[A]	CLA	C4-C3-C5	3.34	120.89	115.27
26	C	501[B]	SQD	C44-O6-C1	-3.34	107.22	113.74
23	b	613	CLA	C3D-C4D-ND	3.34	115.64	110.24
23	c	506	CLA	C1D-CHD-C4C	-3.34	118.86	126.06
23	B	608	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
23	a	405[A]	CLA	C1-C2-C3	-3.33	120.28	126.04
23	b	606	CLA	CHD-C4C-NC	3.33	129.46	124.20
23	A	404[A]	CLA	CAA-C2A-C1A	-3.33	101.05	111.97
32	A	416[B]	LHG	O7-C7-C8	3.33	118.68	111.50
23	C	515	CLA	CBC-CAC-C3C	-3.33	103.24	112.43
28	d	404[B]	PL9	C10-C9-C11	3.33	120.87	115.27
23	B	609	CLA	CBC-CAC-C3C	-3.33	103.25	112.43
23	C	505	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
23	c	513	CLA	O2A-CGA-CBA	3.33	122.35	111.91
23	A	406[B]	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
23	c	510	CLA	CHC-C1C-C2C	-3.32	117.50	126.73
23	b	610	CLA	CHD-C4C-NC	3.32	129.44	124.20
23	b	601	CLA	C1C-C2C-C3C	-3.32	103.46	106.96
23	B	601	CLA	CAC-C3C-C4C	3.32	129.12	124.81
23	C	512	CLA	CHD-C4C-NC	3.32	129.44	124.20
28	a	414[B]	PL9	C7-C3-C2	-3.32	118.93	123.30
23	a	405[A]	CLA	CAA-C2A-C1A	-3.32	101.10	111.97
23	C	510	CLA	CAC-C3C-C4C	3.32	129.12	124.81
24	A	408	BCR	C16-C17-C18	-3.32	122.58	127.31
23	A	405[B]	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
23	b	611	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
23	A	405[B]	CLA	CMB-C2B-C1B	3.31	130.41	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	d	406[B]	LHG	O7-C7-C8	3.31	118.63	111.50
34	B	622	HTG	O5-C1-C2	3.31	114.47	110.31
23	b	610	CLA	CMB-C2B-C1B	3.31	130.40	125.37
23	b	612	CLA	O2A-CGA-CBA	3.30	122.28	111.91
23	B	612	CLA	C1D-CHD-C4C	-3.30	118.93	126.06
32	A	416[A]	LHG	O8-C23-C24	3.30	122.28	111.91
28	a	414[A]	PL9	C37-C38-C39	-3.30	119.71	127.66
23	b	605	CLA	C4-C3-C5	3.30	120.83	115.27
23	c	508	CLA	C4-C3-C5	3.30	120.83	115.27
23	A	407	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
23	B	603	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
23	a	405[A]	CLA	C3B-C4B-NB	3.30	113.58	110.52
23	C	514	CLA	CMC-C2C-C1C	3.30	130.06	125.04
23	d	401[A]	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
23	B	614	CLA	O2A-CGA-O1A	-3.29	115.28	123.59
28	D	407[A]	PL9	C25-C24-C26	3.29	120.81	115.27
23	b	612	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
23	c	504	CLA	C1-C2-C3	-3.29	120.35	126.04
37	a	408[B]	PHO	CMA-C3A-C4A	-3.29	107.17	114.38
37	D	402[B]	PHO	C4-C3-C5	3.29	120.80	115.27
23	a	409	CLA	O2A-CGA-CBA	3.29	122.22	111.91
23	A	406[A]	CLA	C3B-C4B-NB	3.29	113.56	110.52
28	D	407[B]	PL9	C7-C8-C9	-3.29	121.32	126.79
23	b	613	CLA	C1D-CHD-C4C	-3.28	118.97	126.06
23	A	406[A]	CLA	CAA-C2A-C3A	-3.28	103.78	112.78
23	c	513	CLA	C4-C3-C5	3.28	120.79	115.27
24	C	517	BCR	C7-C8-C9	-3.28	121.28	126.23
23	C	503	CLA	C1-C2-C3	-3.28	120.37	126.04
24	D	406	BCR	C38-C26-C25	-3.28	120.85	124.53
23	a	405[A]	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
23	c	511	CLA	CAC-C3C-C4C	3.28	129.06	124.81
28	a	414[B]	PL9	C30-C29-C31	3.28	120.78	115.27
23	C	514	CLA	CHD-C4C-NC	3.28	129.37	124.20
23	B	607	CLA	CBC-CAC-C3C	-3.27	103.40	112.43
23	C	511	CLA	O2A-CGA-O1A	-3.27	115.33	123.59
23	d	402	CLA	C1D-CHD-C4C	-3.27	119.00	126.06
23	b	612	CLA	C2A-C1A-CHA	-3.27	118.14	123.86
26	a	412	SQD	O48-C23-C24	3.27	122.17	111.91
23	B	603	CLA	O2A-CGA-O1A	-3.27	115.35	123.59
28	A	412[B]	PL9	C17-C18-C19	-3.26	119.80	127.66
35	C	520	DGD	O1G-C1A-C2A	3.26	122.14	111.91
23	c	508	CLA	C1D-CHD-C4C	-3.26	119.02	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	515	CLA	C1-C2-C3	-3.26	120.41	126.04
24	Y	101	BCR	C28-C27-C26	-3.26	108.26	114.08
23	D	404[B]	CLA	O2A-CGA-CBA	3.26	122.13	111.91
23	b	601	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
33	C	526	LMG	O6-C1-C2	3.26	117.24	110.35
23	c	513	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
23	b	608	CLA	CHC-C1C-C2C	-3.25	117.70	126.73
23	C	511	CLA	C3B-C4B-NB	3.25	113.53	110.52
23	D	404[B]	CLA	O2A-CGA-O1A	-3.25	115.39	123.59
33	c	520	LMG	O1-C7-C8	-3.25	103.06	110.90
23	C	506	CLA	C1D-CHD-C4C	-3.25	119.06	126.06
23	d	401[A]	CLA	C1-C2-C3	-3.24	120.43	126.04
24	C	517	BCR	C33-C5-C6	-3.24	120.89	124.53
31	b	627	LMT	C3'-C4'-C5'	-3.24	103.49	110.93
23	D	404[B]	CLA	C1D-CHD-C4C	-3.24	119.06	126.06
37	a	416[B]	PHO	C4-C3-C5	3.24	120.72	115.27
24	b	618	BCR	C37-C22-C21	-3.24	118.39	122.92
23	C	504	CLA	C1D-CHD-C4C	-3.24	119.07	126.06
23	c	511	CLA	C4-C3-C5	3.24	120.72	115.27
23	C	512	CLA	CHC-C1C-C2C	-3.23	117.75	126.73
24	y	101	BCR	C38-C26-C25	-3.23	120.90	124.53
31	B	628	LMT	C4B-C3B-C2B	3.23	116.46	110.82
37	D	402[B]	PHO	O2D-CGD-O1D	-3.23	117.52	123.84
23	b	602	CLA	CAC-C3C-C4C	3.23	129.00	124.81
23	a	409	CLA	C4-C3-C5	3.23	120.70	115.27
23	a	406[B]	CLA	C3B-C4B-NB	3.23	113.51	110.52
23	A	406[A]	CLA	O2A-CGA-O1A	-3.23	115.45	123.59
23	c	513	CLA	C4C-C3C-C2C	-3.23	102.20	106.90
28	d	404[B]	PL9	C37-C38-C39	-3.23	119.89	127.66
23	b	605	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
23	B	614	CLA	O2A-CGA-CBA	3.22	122.02	111.91
23	b	609	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
23	b	608	CLA	CMC-C2C-C1C	3.22	129.95	125.04
23	C	506	CLA	C4A-NA-C1A	-3.22	105.26	106.71
31	B	630	LMT	O1'-C1'-C2'	3.22	113.33	108.30
23	c	504	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
23	B	606	CLA	CMC-C2C-C1C	3.22	129.94	125.04
23	B	605	CLA	CMB-C2B-C1B	3.22	130.27	125.37
23	d	401[B]	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
23	c	506	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
26	a	411[A]	SQD	C45-O47-C7	-3.21	109.88	117.79
23	A	404[B]	CLA	O2A-CGA-CBA	3.21	121.99	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	C3B-C4B-NB	3.21	113.49	110.52
23	b	603	CLA	C3B-C4B-NB	3.21	113.49	110.52
23	d	401[B]	CLA	C4-C3-C5	3.21	120.67	115.27
28	a	414[A]	PL9	C17-C18-C19	-3.21	119.94	127.66
32	d	411[B]	LHG	O8-C23-C24	3.21	121.97	111.91
23	d	401[B]	CLA	C1-C2-C3	-3.20	120.50	126.04
23	C	511	CLA	C1D-CHD-C4C	-3.20	119.15	126.06
37	a	408[A]	PHO	O2A-CGA-O1A	-3.20	115.51	123.59
23	b	602	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
23	C	504	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
23	b	610	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
28	a	414[A]	PL9	C25-C24-C26	3.20	120.65	115.27
28	D	407[A]	PL9	C17-C18-C19	-3.20	119.96	127.66
24	D	406	BCR	C11-C10-C9	-3.20	122.75	127.31
23	a	405[B]	CLA	CHD-C4C-NC	3.20	129.24	124.20
23	c	510	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
23	c	505	CLA	CAC-C3C-C4C	3.19	128.95	124.81
23	A	407	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
37	D	402[A]	PHO	C4-C3-C5	3.19	120.64	115.27
23	d	402	CLA	C1C-C2C-C3C	-3.19	103.60	106.96
26	b	620	SQD	C3-C4-C5	3.19	115.93	110.24
23	B	608	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
23	C	509	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
33	c	521	LMG	C9-C8-C7	-3.18	104.26	111.79
23	c	504	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
23	c	512	CLA	CHD-C4C-NC	3.18	129.22	124.20
23	C	503	CLA	CAC-C3C-C4C	3.18	128.94	124.81
23	b	603	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
23	B	613	CLA	O2A-CGA-O1A	-3.18	115.57	123.59
23	C	514	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
23	d	401[A]	CLA	O2A-CGA-O1A	-3.18	115.57	123.59
23	b	614	CLA	CMC-C2C-C1C	3.18	129.88	125.04
23	a	407[B]	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
38	f	101	HEM	CBD-CAD-C3D	-3.18	103.80	112.63
26	a	411[B]	SQD	C45-O47-C7	-3.17	109.98	117.79
23	B	602	CLA	C4C-C3C-C2C	-3.17	102.27	106.90
23	b	616	CLA	C4C-C3C-C2C	-3.17	102.27	106.90
34	b	625	HTG	O5-C5-C4	3.17	115.45	109.69
23	A	406[B]	CLA	CMB-C2B-C1B	3.17	130.20	125.37
23	B	609	CLA	O2A-CGA-CBA	3.17	121.85	111.91
26	b	620	SQD	O7-S-C6	3.16	110.70	106.94
23	A	405[A]	CLA	CMB-C2B-C1B	3.16	130.18	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	405	CLA	C3B-C4B-NB	3.16	113.45	110.52
23	b	601	CLA	C4-C3-C5	3.16	120.58	115.27
23	B	605	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
23	b	611	CLA	CHC-C1C-C2C	-3.15	117.97	126.73
23	B	610	CLA	C4A-NA-C1A	-3.15	105.29	106.71
23	a	407[B]	CLA	CMC-C2C-C1C	3.15	129.84	125.04
23	C	507	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
23	a	406[B]	CLA	CHD-C4C-NC	3.15	129.17	124.20
23	a	405[A]	CLA	C4-C3-C5	3.15	120.57	115.27
28	D	407[B]	PL9	C53-C6-C1	3.15	121.43	114.99
23	A	406[B]	CLA	CBC-CAC-C3C	-3.15	103.75	112.43
23	b	609	CLA	CBC-CAC-C3C	-3.15	103.76	112.43
28	a	414[B]	PL9	C25-C24-C26	3.15	120.56	115.27
24	Y	101	BCR	C16-C17-C18	-3.14	122.82	127.31
23	C	505	CLA	C4-C3-C5	3.14	120.56	115.27
23	C	507	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
23	d	401[B]	CLA	O2A-CGA-CBA	3.14	121.76	111.91
23	C	508	CLA	C4-C3-C5	3.14	120.55	115.27
23	C	512	CLA	C3C-C4C-NC	3.14	114.09	110.57
23	c	509	CLA	C3B-C4B-NB	3.14	113.42	110.52
23	B	607	CLA	C1D-CHD-C4C	-3.14	119.29	126.06
23	B	612	CLA	O2A-CGA-CBA	3.14	121.75	111.91
24	b	619	BCR	C24-C23-C22	-3.14	121.50	126.23
32	d	405[B]	LHG	O7-C7-C8	3.13	118.25	111.50
24	T	102	BCR	C11-C10-C9	-3.13	122.84	127.31
23	b	612	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
23	A	404[A]	CLA	C1-C2-C3	-3.13	120.63	126.04
23	c	512	CLA	C1-O2A-CGA	3.13	124.65	116.44
23	c	514	CLA	CAC-C3C-C4C	3.13	128.87	124.81
23	B	613	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
23	A	405[B]	CLA	C3B-C4B-NB	3.13	113.42	110.52
23	C	503	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
37	a	416[B]	PHO	C1A-C2A-C3A	-3.13	99.87	102.84
23	a	407[A]	CLA	CMB-C2B-C1B	3.12	130.12	125.37
26	a	411[B]	SQD	C1-O5-C5	-3.12	107.56	113.69
33	m	101	LMG	C8-O7-C10	-3.12	110.11	117.79
23	A	405[A]	CLA	CAC-C3C-C4C	3.12	128.86	124.81
23	c	503	CLA	CMC-C2C-C1C	3.12	129.79	125.04
28	D	407[B]	PL9	C10-C9-C11	3.12	120.52	115.27
23	A	404[B]	CLA	CHD-C4C-NC	3.12	129.12	124.20
23	a	407[A]	CLA	CHD-C4C-NC	3.12	129.12	124.20
23	c	503	CLA	CHC-C1C-C2C	-3.12	118.07	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	102	SQD	O5-C1-C2	3.12	116.95	110.35
33	a	417	LMG	C7-O1-C1	-3.11	107.65	113.74
23	a	407[B]	CLA	CHD-C4C-NC	3.11	129.11	124.20
31	M	101	LMT	C3'-C4'-C5'	-3.11	103.79	110.93
28	A	412[B]	PL9	C27-C28-C29	-3.11	120.17	127.66
28	a	414[B]	PL9	C17-C18-C19	-3.11	120.17	127.66
23	c	510	CLA	O2A-CGA-CBA	3.11	121.67	111.91
23	D	404[A]	CLA	C1D-CHD-C4C	-3.11	119.36	126.06
28	a	414[A]	PL9	C35-C34-C36	3.10	120.49	115.27
23	C	503	CLA	C4C-C3C-C2C	-3.10	102.37	106.90
32	D	409[A]	LHG	O7-C7-C8	3.10	118.19	111.50
23	c	509	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
24	a	410	BCR	C7-C8-C9	-3.10	121.55	126.23
23	c	506	CLA	CAC-C3C-C4C	3.10	128.83	124.81
37	a	408[A]	PHO	O2A-CGA-CBA	3.10	121.63	111.91
33	C	526	LMG	C4-C3-C2	3.10	116.23	110.82
28	A	412[B]	PL9	C53-C6-C1	3.10	121.33	114.99
23	a	406[B]	CLA	C1-C2-C3	-3.10	120.68	126.04
23	C	514	CLA	C4-C3-C5	3.10	120.48	115.27
23	B	616	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
23	A	404[B]	CLA	CMC-C2C-C1C	3.10	129.75	125.04
23	A	405[B]	CLA	CHD-C4C-NC	3.09	129.08	124.20
23	a	407[A]	CLA	CAA-C2A-C3A	-3.09	104.31	112.78
23	b	614	CLA	O2A-CGA-O1A	-3.09	115.79	123.59
23	C	511	CLA	O2A-CGA-CBA	3.09	121.60	111.91
23	B	608	CLA	CHD-C4C-NC	3.09	129.07	124.20
26	f	102	SQD	C4-C3-C2	-3.09	105.43	110.82
23	B	601	CLA	CMB-C2B-C1B	3.08	130.07	125.37
23	a	409	CLA	CAA-C2A-C3A	-3.08	104.33	112.78
32	D	408[A]	LHG	O8-C23-O10	-3.08	115.82	123.59
24	d	403	BCR	C38-C26-C25	-3.08	121.07	124.53
23	a	406[B]	CLA	CMB-C2B-C1B	3.08	130.06	125.37
23	C	506	CLA	CBC-CAC-C3C	-3.08	103.95	112.43
23	b	613	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
23	b	603	CLA	O2A-CGA-CBA	3.08	121.56	111.91
23	b	615	CLA	C11-C10-C8	-3.08	105.98	115.92
23	a	407[A]	CLA	C3B-C4B-NB	3.07	113.37	110.52
34	b	622	HTG	O5-C1-C2	3.07	114.18	110.31
23	b	615	CLA	C4-C3-C5	3.07	120.44	115.27
23	C	508	CLA	CHC-C1C-C2C	-3.07	118.20	126.73
23	a	406[B]	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
23	c	503	CLA	C1-C2-C3	-3.07	120.73	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	CAC-C3C-C4C	3.07	128.79	124.81
28	a	414[B]	PL9	C42-C43-C44	-3.07	120.27	127.66
33	m	101	LMG	O8-C28-C29	3.07	121.53	111.91
23	b	609	CLA	CMC-C2C-C1C	3.07	129.71	125.04
33	C	522	LMG	O8-C28-C29	3.06	121.53	111.91
23	a	406[B]	CLA	CBC-CAC-C3C	-3.06	103.98	112.43
23	C	509	CLA	O2A-CGA-CBA	3.06	121.53	111.91
23	c	504	CLA	C4-C3-C5	3.06	120.42	115.27
23	c	503	CLA	C3B-C4B-NB	3.06	113.36	110.52
23	b	608	CLA	CBC-CAC-C3C	-3.06	103.99	112.43
23	B	608	CLA	CMA-C3A-C4A	-3.06	103.55	111.77
28	a	414[B]	PL9	C35-C34-C36	3.06	120.42	115.27
23	B	603	CLA	O2A-CGA-CBA	3.06	121.50	111.91
23	B	603	CLA	CHC-C1C-C2C	-3.06	118.24	126.73
23	C	511	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
23	B	606	CLA	CHD-C4C-NC	3.05	129.02	124.20
32	a	420[A]	LHG	O7-C7-C8	3.05	118.08	111.50
23	b	612	CLA	CHB-C1B-NB	-3.05	121.02	124.26
26	b	620	SQD	O8-S-C6	3.05	110.60	105.74
23	c	502	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
23	A	404[A]	CLA	CMC-C2C-C1C	3.05	129.68	125.04
32	D	409[A]	LHG	O8-C23-C24	3.05	121.46	111.91
28	A	412[A]	PL9	O1-C4-C3	-3.05	117.37	120.72
23	d	402	CLA	CAC-C3C-C4C	3.04	128.76	124.81
23	c	505	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
28	a	414[A]	PL9	C10-C9-C11	3.04	120.39	115.27
37	D	401[B]	PHO	CBC-CAC-C3C	-3.04	108.42	112.88
28	d	404[B]	PL9	C40-C39-C41	3.04	120.39	115.27
33	z	101	LMG	O8-C28-C29	3.04	121.45	111.91
23	A	406[B]	CLA	CHD-C4C-NC	3.04	129.00	124.20
24	D	406	BCR	C37-C22-C23	3.04	122.87	118.08
23	a	407[B]	CLA	CMB-C2B-C1B	3.04	130.00	125.37
28	A	412[A]	PL9	C20-C19-C21	3.04	120.38	115.27
23	C	504	CLA	C1-C2-C3	-3.04	120.79	126.04
23	c	510	CLA	C4-C3-C5	3.04	120.38	115.27
32	d	411[A]	LHG	O7-C7-C8	3.03	118.04	111.50
23	B	606	CLA	O2A-CGA-O1A	-3.03	115.94	123.59
23	c	511	CLA	CHD-C4C-NC	3.03	128.98	124.20
37	a	416[B]	PHO	CMB-C2B-C3B	3.03	130.35	124.68
23	a	409	CLA	CMB-C2B-C1B	3.03	129.99	125.37
26	F	103	SQD	O7-S-C6	3.03	110.54	106.94
23	c	513	CLA	CHD-C4C-NC	3.03	128.98	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
23	a	405[B]	CLA	CHC-C1C-C2C	-3.03	118.32	126.73
35	h	102	DGD	O2G-C1B-C2B	3.03	118.02	111.50
23	d	401[B]	CLA	C3B-C4B-NB	3.02	113.32	110.52
23	B	609	CLA	CMC-C2C-C1C	3.02	129.65	125.04
23	A	405[B]	CLA	CHC-C1C-C2C	-3.02	118.34	126.73
23	A	405[A]	CLA	C3B-C4B-NB	3.02	113.32	110.52
38	f	101	HEM	CHD-C4C-NC	3.02	127.71	124.44
28	D	407[B]	PL9	C27-C28-C29	-3.02	120.39	127.66
23	B	610	CLA	CMA-C3A-C4A	-3.02	103.66	111.77
28	D	407[B]	PL9	C17-C18-C19	-3.02	120.40	127.66
37	a	416[A]	PHO	CBA-CAA-C2A	-3.02	105.00	113.81
23	B	601	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
23	c	513	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
23	c	502	CLA	C1D-CHD-C4C	-3.01	119.56	126.06
23	C	505	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
23	B	610	CLA	C3B-C4B-NB	3.01	113.31	110.52
23	A	406[A]	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
32	D	409[A]	LHG	O8-C23-O10	-3.01	115.99	123.59
23	B	614	CLA	CHC-C1C-C2C	-3.01	118.37	126.73
23	C	511	CLA	CMC-C2C-C1C	3.01	129.62	125.04
28	A	412[B]	PL9	C35-C34-C36	3.01	120.33	115.27
37	a	416[A]	PHO	CMB-C2B-C3B	3.01	130.30	124.68
23	a	409	CLA	C3B-C4B-NB	3.01	113.30	110.52
23	a	407[B]	CLA	C4-C3-C5	3.00	120.32	115.27
28	D	407[A]	PL9	C53-C6-C1	3.00	121.13	114.99
28	d	404[A]	PL9	C22-C23-C24	-3.00	120.44	127.66
23	b	603	CLA	CHD-C4C-NC	3.00	128.93	124.20
28	d	404[A]	PL9	C36-C34-C33	-3.00	115.05	121.12
33	z	101	LMG	O7-C10-C11	3.00	117.96	111.50
23	a	407[A]	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
23	B	602	CLA	CMC-C2C-C1C	2.99	129.60	125.04
23	C	515	CLA	CMB-C2B-C1B	2.99	129.93	125.37
28	A	412[A]	PL9	C17-C18-C19	-2.99	120.45	127.66
23	C	513	CLA	CAC-C3C-C4C	2.99	128.69	124.81
23	a	405[A]	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
23	A	406[B]	CLA	CAA-C2A-C3A	-2.99	104.60	112.78
23	B	612	CLA	C3B-C4B-NB	2.99	113.29	110.52
23	a	406[B]	CLA	CHC-C1C-C2C	-2.98	118.44	126.73
23	d	401[A]	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	a	405[A]	CLA	CMA-C3A-C4A	-2.98	103.77	111.77
23	A	406[A]	CLA	CMC-C2C-C1C	2.98	129.57	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	C3B-C4B-NB	2.98	113.28	110.52
23	b	614	CLA	CAC-C3C-C4C	2.97	128.67	124.81
35	C	518[A]	DGD	C2G-O2G-C1B	-2.97	110.47	117.79
23	d	401[A]	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
28	a	414[A]	PL9	C42-C43-C44	-2.97	120.50	127.66
23	a	405[A]	CLA	CMC-C2C-C1C	2.97	129.56	125.04
23	a	409	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
28	a	414[B]	PL9	C37-C38-C39	-2.97	120.51	127.66
28	d	404[A]	PL9	C10-C9-C11	2.97	120.27	115.27
23	a	405[B]	CLA	O2A-CGA-CBA	2.97	121.22	111.91
35	C	518[B]	DGD	C2G-O2G-C1B	-2.97	110.49	117.79
23	b	602	CLA	CMB-C2B-C1B	2.97	129.88	125.37
23	B	608	CLA	C1-C2-C3	-2.96	120.92	126.04
26	C	501[A]	SQD	O8-S-C6	2.96	110.46	105.74
24	d	403	BCR	C21-C20-C19	-2.96	113.97	123.22
23	B	611	CLA	C2A-C1A-CHA	-2.96	118.68	123.86
23	C	508	CLA	CMC-C2C-C1C	2.96	129.55	125.04
23	b	610	CLA	CMC-C2C-C1C	2.96	129.55	125.04
23	b	614	CLA	CBC-CAC-C3C	-2.96	104.26	112.43
37	a	416[A]	PHO	O2D-CGD-O1D	-2.96	118.05	123.84
24	D	406	BCR	C10-C11-C12	-2.96	113.98	123.22
23	b	606	CLA	CHC-C1C-C2C	-2.96	118.51	126.73
24	H	101	BCR	C37-C22-C21	-2.96	118.78	122.92
23	b	609	CLA	CAC-C3C-C4C	2.96	128.65	124.81
23	B	612	CLA	O2A-CGA-O1A	-2.96	116.13	123.59
23	c	507	CLA	O2A-CGA-O1A	-2.96	116.13	123.59
23	A	404[B]	CLA	C1-C2-C3	-2.96	120.93	126.04
28	A	412[B]	PL9	C20-C19-C21	2.95	120.24	115.27
32	a	420[B]	LHG	O7-C7-C8	2.95	117.86	111.50
23	D	404[A]	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
23	C	505	CLA	O2A-CGA-O1A	-2.95	116.14	123.59
23	B	607	CLA	C3B-C4B-NB	2.95	113.25	110.52
38	f	101	HEM	CHB-C1B-NB	2.95	128.01	124.37
23	B	615	CLA	C3B-C4B-NB	2.95	113.25	110.52
24	h	101	BCR	C16-C15-C14	-2.95	117.43	123.47
23	b	615	CLA	CHC-C1C-C2C	-2.95	118.54	126.73
23	b	607	CLA	CAA-C2A-C3A	-2.95	104.71	112.78
23	c	512	CLA	CHC-C1C-C2C	-2.95	118.55	126.73
35	h	102	DGD	O1G-C1A-O1A	-2.95	116.16	123.59
23	C	512	CLA	CMB-C2B-C1B	2.94	129.85	125.37
40	V	202	HEC	C4B-NB-C1B	2.94	108.11	105.07
23	b	602	CLA	C1C-C2C-C3C	-2.94	103.86	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	CMC-C2C-C1C	2.94	129.52	125.04
23	C	510	CLA	CHC-C1C-C2C	-2.94	118.56	126.73
24	b	619	BCR	C15-C14-C13	-2.94	123.11	127.31
23	A	404[B]	CLA	C2A-C1A-CHA	-2.94	118.72	123.86
23	b	608	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
23	c	509	CLA	C4-C3-C5	2.94	120.21	115.27
23	a	405[B]	CLA	C1-C2-C3	-2.94	120.96	126.04
23	D	404[B]	CLA	C4-C3-C5	2.94	120.21	115.27
24	k	101	BCR	C15-C14-C13	-2.94	123.12	127.31
24	t	103	BCR	C11-C10-C9	-2.94	123.12	127.31
23	c	512	CLA	CMB-C2B-C1B	2.93	129.84	125.37
23	C	513	CLA	CMC-C2C-C1C	2.93	129.51	125.04
23	b	601	CLA	C1-O2A-CGA	2.93	124.14	116.44
24	Y	101	BCR	C37-C22-C23	2.93	122.70	118.08
24	H	101	BCR	C16-C15-C14	-2.93	117.47	123.47
28	D	407[A]	PL9	C10-C9-C11	2.93	120.20	115.27
23	B	613	CLA	C1D-CHD-C4C	-2.93	119.74	126.06
23	A	405[A]	CLA	CMA-C3A-C4A	-2.93	103.90	111.77
23	B	601	CLA	CHD-C4C-NC	2.93	128.82	124.20
23	c	505	CLA	CHC-C1C-C2C	-2.93	118.60	126.73
23	c	512	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
23	b	614	CLA	C3B-C4B-NB	2.93	113.23	110.52
23	a	409	CLA	CMC-C2C-C1C	2.92	129.49	125.04
23	A	404[A]	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
23	a	406[A]	CLA	CMA-C3A-C2A	-2.92	102.03	113.83
23	D	405	CLA	C1C-C2C-C3C	-2.92	103.88	106.96
37	a	408[B]	PHO	C1A-C2A-C3A	-2.92	100.06	102.84
23	A	404[B]	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
23	b	604	CLA	C6-C5-C3	-2.92	105.80	113.45
23	C	507	CLA	C4-C3-C5	2.92	120.19	115.27
33	a	417	LMG	C8-O7-C10	-2.92	110.60	117.79
23	c	509	CLA	O2A-CGA-CBA	2.92	121.07	111.91
35	h	102	DGD	O1G-C1A-C2A	2.92	121.07	111.91
23	B	614	CLA	CHD-C4C-NC	2.92	128.80	124.20
23	B	601	CLA	C1C-C2C-C3C	-2.92	103.89	106.96
32	E	101[A]	LHG	O8-C23-C24	2.92	121.06	111.91
23	b	609	CLA	C16-C15-C13	-2.92	106.50	115.92
23	b	616	CLA	C1C-C2C-C3C	-2.91	103.89	106.96
23	D	404[A]	CLA	C4-C3-C5	2.91	120.17	115.27
24	Y	101	BCR	C10-C11-C12	-2.91	114.13	123.22
23	b	602	CLA	C2A-C1A-CHA	-2.91	118.77	123.86
23	A	404[A]	CLA	C2A-C1A-CHA	-2.91	118.77	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	515	CLA	C4-C3-C5	2.91	120.16	115.27
23	B	614	CLA	CBC-CAC-C3C	-2.91	104.42	112.43
28	d	404[B]	PL9	C15-C14-C16	2.91	120.16	115.27
23	b	614	CLA	CHC-C1C-C2C	-2.91	118.66	126.73
23	C	515	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
31	e	101	LMT	O1'-C1'-C2'	2.90	112.84	108.30
23	C	515	CLA	CHD-C4C-NC	2.90	128.78	124.20
23	A	405[A]	CLA	CHD-C4C-NC	2.90	128.78	124.20
23	c	503	CLA	CHD-C4C-NC	2.90	128.78	124.20
23	C	504	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
24	T	102	BCR	C7-C8-C9	-2.90	121.85	126.23
23	b	606	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	D	404[A]	CLA	O2A-CGA-CBA	2.90	121.00	111.91
23	c	502	CLA	CHC-C1C-C2C	-2.90	118.68	126.73
23	b	614	CLA	CHD-C4C-NC	2.90	128.77	124.20
37	D	401[B]	PHO	C1-C2-C3	-2.90	121.04	126.04
23	C	513	CLA	C4-C3-C5	2.89	120.14	115.27
23	C	503	CLA	O2A-CGA-O1A	-2.89	116.29	123.59
35	C	518[B]	DGD	O3G-C3G-C2G	-2.89	103.92	110.90
23	b	615	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
23	C	509	CLA	C4-C3-C5	2.89	120.13	115.27
23	D	404[B]	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
23	d	401[A]	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
26	C	501[B]	SQD	O7-S-C6	2.89	110.37	106.94
23	b	605	CLA	C1-C2-C3	-2.89	121.05	126.04
23	C	511	CLA	C16-C15-C13	-2.89	106.59	115.92
23	c	503	CLA	O2A-CGA-CBA	2.89	120.96	111.91
23	a	405[B]	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
23	A	407	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
28	A	412[B]	PL9	C30-C29-C31	2.88	120.12	115.27
31	A	417	LMT	O5B-C5B-C4B	2.88	114.93	109.69
32	d	405[A]	LHG	O7-C7-C8	2.88	117.71	111.50
23	b	609	CLA	CHD-C4C-NC	2.88	128.75	124.20
23	D	404[A]	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
23	b	616	CLA	CAC-C3C-C4C	2.88	128.55	124.81
24	D	406	BCR	C28-C27-C26	-2.88	108.94	114.08
23	C	503	CLA	O2A-CGA-CBA	2.88	120.94	111.91
23	B	615	CLA	CHD-C4C-NC	2.88	128.74	124.20
37	a	416[A]	PHO	C4A-C3A-C2A	-2.88	100.10	102.84
23	B	611	CLA	C3B-C4B-NB	2.88	113.18	110.52
23	A	406[A]	CLA	CHD-C4C-NC	2.88	128.73	124.20
26	a	411[A]	SQD	O47-C7-O49	-2.87	116.75	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
37	D	402[A]	PHO	O2D-CGD-O1D	-2.87	118.22	123.84
23	a	407[B]	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
23	a	405[A]	CLA	CAC-C3C-C4C	2.87	128.53	124.81
32	A	416[A]	LHG	C5-O7-C7	-2.87	110.73	117.79
23	B	609	CLA	O2A-CGA-O1A	-2.87	116.36	123.59
23	C	506	CLA	CAC-C3C-C4C	2.86	128.52	124.81
23	B	608	CLA	O2A-CGA-O1A	-2.86	116.37	123.59
23	c	505	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
28	D	407[A]	PL9	C51-C49-C50	2.86	120.92	114.60
23	b	607	CLA	C4-C3-C5	2.86	120.08	115.27
23	a	407[B]	CLA	C1-C2-C3	-2.86	121.10	126.04
24	H	101	BCR	C7-C8-C9	-2.86	121.92	126.23
23	c	506	CLA	CHC-C1C-C2C	-2.86	118.79	126.73
23	B	609	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
23	A	404[B]	CLA	C4-C3-C5	2.86	120.07	115.27
23	a	406[A]	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
24	h	101	BCR	C20-C21-C22	-2.85	123.24	127.31
28	a	414[A]	PL9	C53-C6-C1	2.85	120.82	114.99
33	c	520	LMG	O8-C28-C29	2.85	120.85	111.91
31	t	101	LMT	C3'-C4'-C5'	-2.85	104.39	110.93
23	A	407	CLA	O2A-CGA-CBA	2.85	120.84	111.91
33	C	521	LMG	O8-C28-O10	-2.85	116.41	123.59
23	c	510	CLA	CMB-C2B-C1B	2.85	129.70	125.37
23	c	514	CLA	O2A-CGA-CBA	2.85	120.84	111.91
35	C	518[A]	DGD	O6D-C1D-O3G	-2.85	103.24	109.97
23	D	404[B]	CLA	CHC-C1C-C2C	-2.84	118.83	126.73
23	d	401[B]	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
26	C	501[A]	SQD	O48-C23-C24	2.84	120.82	111.91
23	B	614	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
23	B	607	CLA	O2A-CGA-O1A	-2.84	116.42	123.59
23	B	611	CLA	C2C-C1C-NC	2.84	112.63	109.97
23	C	504	CLA	CHC-C1C-C2C	-2.84	118.85	126.73
28	d	404[B]	PL9	C42-C43-C44	-2.84	120.83	127.66
23	C	514	CLA	O2A-CGA-CBA	2.84	120.81	111.91
23	a	407[A]	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
33	C	502	LMG	C8-O7-C10	-2.83	110.81	117.79
23	A	406[A]	CLA	O2A-CGA-CBA	2.83	120.80	111.91
28	a	414[B]	PL9	C53-C6-C1	2.83	120.78	114.99
23	a	406[B]	CLA	C4-C3-C5	2.83	120.03	115.27
26	f	102	SQD	O8-S-C6	2.83	110.25	105.74
32	E	101[B]	LHG	O8-C23-C24	2.83	120.79	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
23	A	406[B]	CLA	C3B-C4B-NB	2.83	113.14	110.52
23	C	509	CLA	O2A-CGA-O1A	-2.83	116.45	123.59
28	D	407[A]	PL9	C37-C38-C39	-2.83	120.85	127.66
23	c	506	CLA	C3B-C4B-NB	2.83	113.14	110.52
23	B	609	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
32	d	405[B]	LHG	O8-C23-O10	-2.82	116.46	123.59
33	D	413	LMG	O8-C28-O10	-2.82	116.46	123.59
38	F	102	HEM	CHB-C1B-NB	2.82	127.86	124.37
28	d	404[B]	PL9	C17-C18-C19	-2.82	120.86	127.66
23	c	514	CLA	CMB-C2B-C1B	2.82	129.67	125.37
28	a	414[B]	PL9	C22-C23-C24	-2.82	120.87	127.66
26	B	620	SQD	O48-C23-C24	2.82	120.76	111.91
23	B	604	CLA	CHC-C1C-C2C	-2.82	118.90	126.73
28	A	412[A]	PL9	C35-C34-C36	2.82	120.01	115.27
23	C	504	CLA	CAC-C3C-C4C	2.82	128.47	124.81
32	L	101[A]	LHG	O8-C23-C24	2.82	120.75	111.91
23	A	404[A]	CLA	CHC-C1C-C2C	-2.81	118.92	126.73
23	A	406[A]	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
38	F	102	HEM	O2A-CGA-CBA	2.81	123.06	114.03
23	a	409	CLA	O2A-CGA-O1A	-2.81	116.50	123.59
24	y	101	BCR	C34-C9-C8	2.81	122.50	118.08
24	h	101	BCR	C7-C8-C9	-2.81	121.99	126.23
23	b	607	CLA	CBC-CAC-C3C	-2.81	104.69	112.43
32	A	416[B]	LHG	O8-C23-O10	-2.81	116.50	123.59
23	A	406[A]	CLA	C4-C3-C5	2.81	119.99	115.27
23	C	505	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
23	c	514	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
28	A	412[A]	PL9	C30-C29-C31	2.81	119.99	115.27
26	F	103	SQD	O48-C23-C24	2.81	120.72	111.91
23	a	405[B]	CLA	CMA-C3A-C4A	-2.80	104.25	111.77
28	a	414[A]	PL9	C22-C23-C24	-2.80	120.92	127.66
23	b	609	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
23	D	405	CLA	O2A-CGA-O1A	-2.80	116.53	123.59
23	A	407	CLA	C4-C3-C5	2.80	119.97	115.27
32	d	411[B]	LHG	O8-C23-O10	-2.80	116.53	123.59
23	b	616	CLA	O2A-CGA-O1A	-2.79	116.54	123.59
23	A	405[A]	CLA	CHC-C1C-C2C	-2.79	118.97	126.73
24	t	103	BCR	C36-C18-C19	2.79	122.47	118.08
26	a	411[B]	SQD	C1-C2-C3	-2.79	104.19	110.00
23	C	513	CLA	C3B-C4B-NB	2.79	113.10	110.52
23	a	407[A]	CLA	CHC-C1C-C2C	-2.79	118.98	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	D	409[B]	LHG	O8-C23-C24	2.79	120.66	111.91
23	d	401[B]	CLA	CAC-C3C-C4C	2.79	128.43	124.81
24	C	516	BCR	C16-C17-C18	-2.79	123.33	127.31
23	c	508	CLA	CHD-C4C-NC	2.79	128.59	124.20
24	k	101	BCR	C39-C30-C25	-2.79	105.78	110.30
23	C	503	CLA	CMB-C2B-C1B	2.79	129.61	125.37
23	d	402	CLA	C3B-C4B-NB	2.78	113.10	110.52
26	a	412	SQD	O7-S-C6	2.78	110.25	106.94
23	b	605	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
26	A	410	SQD	C4-C3-C2	-2.78	105.97	110.82
32	A	416[B]	LHG	O8-C23-C24	2.78	120.64	111.91
23	b	604	CLA	C4-C3-C5	2.78	119.95	115.27
23	C	505	CLA	CHC-C1C-C2C	-2.78	119.01	126.73
23	B	615	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
23	B	612	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
38	F	102	HEM	CBA-CAA-C2A	-2.78	104.91	112.63
23	A	406[B]	CLA	CHC-C1C-C2C	-2.78	119.01	126.73
23	c	514	CLA	CAA-C2A-C3A	-2.78	105.17	112.78
24	T	102	BCR	C33-C5-C6	-2.78	121.41	124.53
23	b	613	CLA	CHC-C1C-C2C	-2.78	119.02	126.73
31	B	628	LMT	O1'-C1'-C2'	2.77	112.64	108.30
37	a	408[B]	PHO	O2D-CGD-O1D	-2.77	118.41	123.84
26	a	411[B]	SQD	C44-O6-C1	-2.77	108.32	113.74
23	B	612	CLA	C4A-NA-C1A	-2.77	105.46	106.71
35	H	102	DGD	O3G-C3G-C2G	-2.77	104.21	110.90
23	C	507	CLA	CHC-C1C-C2C	-2.77	119.03	126.73
23	B	604	CLA	CAC-C3C-C4C	2.77	128.41	124.81
23	A	405[A]	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
23	b	605	CLA	O2A-C1-C2	-2.77	101.35	108.64
23	B	601	CLA	C1-O2A-CGA	2.77	123.71	116.44
28	d	404[B]	PL9	C25-C24-C26	2.77	119.93	115.27
37	a	408[A]	PHO	CMB-C2B-C3B	2.77	129.86	124.68
24	d	403	BCR	C10-C11-C12	-2.77	114.57	123.22
38	F	102	HEM	C4A-NA-C1A	2.77	108.06	105.35
23	B	606	CLA	O2A-CGA-CBA	2.77	120.59	111.91
23	c	514	CLA	CHC-C1C-C2C	-2.77	119.04	126.73
23	B	604	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
23	b	609	CLA	C3B-C4B-NB	2.77	113.08	110.52
23	a	406[A]	CLA	O2A-CGA-CBA	2.76	120.58	111.91
23	c	514	CLA	CBC-CAC-C3C	-2.76	104.82	112.43
35	H	102	DGD	O1G-C1A-C2A	2.76	120.58	111.91
23	D	404[B]	CLA	CHD-C4C-NC	2.76	128.56	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F	103	SQD	C1-C2-C3	-2.76	104.25	110.00
23	C	504	CLA	C4-C3-C5	2.76	119.92	115.27
23	a	407[A]	CLA	O2A-CGA-O1A	-2.76	116.62	123.59
23	b	605	CLA	CMB-C2B-C1B	2.76	129.57	125.37
23	D	404[B]	CLA	CAA-C2A-C3A	-2.76	105.23	112.78
23	C	503	CLA	C4-C3-C5	2.76	119.91	115.27
23	b	604	CLA	C4C-C3C-C2C	-2.75	102.88	106.90
32	D	408[A]	LHG	O7-C7-C8	2.75	117.44	111.50
23	C	503	CLA	CHC-C1C-C2C	-2.75	119.08	126.73
23	C	505	CLA	CHD-C4C-NC	2.75	128.54	124.20
23	B	608	CLA	C11-C12-C13	-2.75	107.03	115.92
24	h	101	BCR	C37-C22-C21	-2.75	119.07	122.92
23	B	611	CLA	CAC-C3C-C4C	2.75	128.38	124.81
23	C	515	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
23	b	604	CLA	CMB-C2B-C1B	2.75	129.55	125.37
23	c	504	CLA	CAC-C3C-C4C	2.75	128.37	124.81
23	c	502	CLA	CMC-C2C-C1C	2.75	129.22	125.04
23	a	409	CLA	CBC-CAC-C3C	-2.75	104.86	112.43
37	D	401[B]	PHO	O1D-CGD-CBD	-2.75	120.17	124.74
23	c	511	CLA	O2A-CGA-O1A	-2.75	116.66	123.59
23	b	607	CLA	C1D-CHD-C4C	-2.74	120.14	126.06
28	d	404[A]	PL9	C36-C37-C38	-2.74	102.86	111.88
35	C	519[B]	DGD	C2G-O2G-C1B	-2.74	111.04	117.79
23	b	615	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
23	B	608	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	b	601	CLA	C3B-C4B-NB	2.74	113.06	110.52
24	T	102	BCR	C12-C13-C14	-2.74	114.73	118.94
31	T	101	LMT	C1'-O5'-C5'	-2.74	108.31	113.69
33	C	502	LMG	C6-C5-C4	2.74	119.42	113.00
28	D	407[B]	PL9	C20-C19-C21	2.74	119.88	115.27
23	B	613	CLA	O2A-CGA-CBA	2.74	120.49	111.91
23	d	402	CLA	O2A-CGA-CBA	2.73	120.49	111.91
26	f	102	SQD	O5-C5-C4	2.73	114.66	109.69
23	B	610	CLA	CHD-C4C-NC	2.73	128.51	124.20
24	Y	101	BCR	C34-C9-C8	2.73	122.38	118.08
32	d	406[B]	LHG	O8-C23-C24	2.73	120.48	111.91
23	A	407	CLA	C1-O2A-CGA	2.73	123.61	116.44
23	B	607	CLA	CMB-C2B-C1B	2.73	129.53	125.37
23	C	508	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
31	B	628	LMT	C2'-C3'-C4'	2.73	115.91	109.68
23	c	513	CLA	CHC-C1C-C2C	-2.73	119.16	126.73
24	t	103	BCR	C28-C27-C26	-2.73	109.21	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
23	C	507	CLA	C3B-C4B-NB	2.72	113.04	110.52
23	b	602	CLA	C1-O2A-CGA	2.72	123.59	116.44
40	v	201	HEC	CHA-C4D-ND	2.72	127.38	124.42
28	a	414[B]	PL9	C40-C39-C41	2.72	119.85	115.27
23	B	616	CLA	C1-O2A-CGA	2.72	123.59	116.44
28	d	404[A]	PL9	C27-C28-C29	-2.72	121.11	127.66
23	a	405[B]	CLA	C4-C3-C5	2.72	119.84	115.27
23	d	402	CLA	C2A-C1A-CHA	-2.72	119.11	123.86
23	B	610	CLA	CHC-C1C-C2C	-2.72	119.19	126.73
24	C	517	BCR	C11-C10-C9	-2.72	123.43	127.31
28	D	407[B]	PL9	C40-C39-C41	2.72	119.84	115.27
28	D	407[B]	PL9	C45-C44-C46	2.72	119.84	115.27
23	b	616	CLA	C2A-C1A-CHA	-2.71	119.11	123.86
23	C	507	CLA	CHD-C4C-NC	2.71	128.48	124.20
23	b	603	CLA	CHC-C1C-C2C	-2.71	119.19	126.73
23	A	405[B]	CLA	CMC-C2C-C1C	2.71	129.17	125.04
23	b	609	CLA	O2A-CGA-O1A	-2.71	116.74	123.59
23	c	513	CLA	CAC-C3C-C4C	2.71	128.33	124.81
23	C	504	CLA	CMC-C2C-C1C	2.71	129.17	125.04
28	a	414[B]	PL9	C20-C19-C21	2.71	119.83	115.27
23	c	509	CLA	CAA-C2A-C3A	-2.71	105.35	112.78
23	B	602	CLA	O2A-CGA-CBA	2.71	120.42	111.91
24	c	515	BCR	C16-C17-C18	-2.71	123.44	127.31
23	B	616	CLA	CMC-C2C-C1C	2.71	129.17	125.04
28	A	412[B]	PL9	C42-C43-C44	-2.71	121.14	127.66
23	C	508	CLA	C2A-C1A-CHA	-2.71	119.12	123.86
23	A	404[B]	CLA	CHC-C1C-C2C	-2.71	119.21	126.73
23	b	615	CLA	CHD-C4C-NC	2.71	128.47	124.20
23	B	604	CLA	C4-C3-C5	2.71	119.82	115.27
24	k	101	BCR	C11-C10-C9	-2.71	123.45	127.31
23	b	602	CLA	CHD-C4C-NC	2.71	128.47	124.20
24	d	403	BCR	C16-C17-C18	-2.70	123.45	127.31
23	C	515	CLA	CHB-C1B-NB	-2.70	121.39	124.26
23	A	406[B]	CLA	C1-C2-C3	-2.70	121.37	126.04
23	c	505	CLA	O2A-CGA-O1A	-2.70	116.77	123.59
23	b	607	CLA	CAC-C3C-C4C	2.70	128.32	124.81
23	b	607	CLA	O2A-CGA-O1A	-2.70	116.77	123.59
28	d	404[B]	PL9	C20-C19-C21	2.70	119.81	115.27
31	T	101	LMT	C3'-C4'-C5'	-2.70	104.73	110.93
23	C	512	CLA	CBC-CAC-C3C	-2.70	104.99	112.43
23	B	607	CLA	C4C-C3C-C2C	-2.70	102.96	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	CGD-CBD-CAD	-2.70	101.99	110.73
26	C	501[B]	SQD	O48-C23-C24	2.70	120.38	111.91
23	B	604	CLA	C11-C12-C13	-2.70	107.20	115.92
23	C	515	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
23	B	603	CLA	C4-C3-C5	2.70	119.81	115.27
23	B	606	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
31	M	101	LMT	C1'-O5'-C5'	-2.70	108.40	113.69
23	b	605	CLA	C2A-C1A-CHA	-2.70	119.15	123.86
23	A	405[B]	CLA	C4-C3-C5	2.69	119.80	115.27
26	B	620	SQD	C4-C3-C2	2.69	115.53	110.82
23	A	406[B]	CLA	O2A-CGA-CBA	2.69	120.36	111.91
23	a	405[A]	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
23	b	613	CLA	CED-O2D-CGD	2.69	122.03	115.94
23	D	405	CLA	O2A-CGA-CBA	2.69	120.36	111.91
26	f	102	SQD	O48-C23-C24	2.69	120.36	111.91
37	D	401[B]	PHO	CMA-C3A-C4A	-2.69	108.48	114.38
23	C	506	CLA	CHB-C1B-NB	-2.69	121.41	124.26
24	y	101	BCR	C24-C23-C22	-2.69	122.17	126.23
32	L	101[A]	LHG	O8-C23-O10	-2.69	116.80	123.59
23	B	610	CLA	O1D-CGD-CBD	-2.69	118.98	124.48
23	D	404[A]	CLA	CAC-C3C-C4C	2.69	128.30	124.81
23	b	613	CLA	CHD-C4C-NC	2.69	128.44	124.20
23	d	402	CLA	C4-C3-C5	2.69	119.79	115.27
23	b	607	CLA	CHC-C1C-C2C	-2.69	119.27	126.73
23	B	604	CLA	C6-C7-C8	-2.69	107.24	115.92
26	C	501[B]	SQD	O8-S-C6	2.69	110.02	105.74
23	A	406[B]	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
23	A	404[B]	CLA	CAC-C3C-C4C	2.68	128.29	124.81
23	d	402	CLA	CMB-C2B-C1B	2.68	129.46	125.37
28	A	412[B]	PL9	C40-C39-C41	2.68	119.78	115.27
23	b	608	CLA	CMA-C3A-C4A	-2.68	104.56	111.77
32	l	802[A]	LHG	O8-C23-C24	2.68	120.32	111.91
23	B	609	CLA	C16-C15-C13	-2.68	107.26	115.92
23	B	612	CLA	C11-C12-C13	-2.68	107.27	115.92
23	a	409	CLA	CHD-C4C-NC	2.68	128.42	124.20
23	B	604	CLA	O2A-CGA-O1A	-2.68	116.84	123.59
23	b	614	CLA	C2A-C1A-CHA	-2.67	119.18	123.86
23	A	406[B]	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
23	c	507	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
23	B	602	CLA	OBD-CAD-C3D	-2.67	122.09	128.52
23	D	404[B]	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
23	A	404[A]	CLA	CMA-C3A-C2A	-2.67	103.05	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	514	CLA	CMB-C2B-C1B	2.67	129.44	125.37
26	B	620	SQD	O9-S-C6	2.67	110.11	106.94
23	d	401[B]	CLA	CHC-C1C-C2C	-2.67	119.31	126.73
24	D	406	BCR	C16-C17-C18	-2.67	123.50	127.31
23	c	514	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
23	C	506	CLA	O2A-CGA-CBA	2.67	120.28	111.91
23	B	616	CLA	O2A-CGA-CBA	2.67	120.27	111.91
23	a	406[A]	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
23	D	404[B]	CLA	C3B-C4B-NB	2.66	112.99	110.52
34	B	622	HTG	C1-O5-C5	2.66	117.49	112.58
23	C	503	CLA	CMC-C2C-C1C	2.66	129.09	125.04
24	H	101	BCR	C16-C17-C18	-2.66	123.51	127.31
23	B	606	CLA	CHC-C1C-C2C	-2.66	119.34	126.73
32	a	420[A]	LHG	O8-C23-C24	2.66	120.25	111.91
23	B	609	CLA	CHD-C4C-NC	2.66	128.39	124.20
23	b	604	CLA	CHC-C1C-C2C	-2.66	119.35	126.73
23	c	507	CLA	C4-C3-C5	2.66	119.74	115.27
23	c	514	CLA	CHD-C4C-NC	2.66	128.39	124.20
37	D	401[A]	PHO	C1-C2-C3	-2.66	121.45	126.04
23	c	511	CLA	CBC-CAC-C3C	-2.66	105.11	112.43
23	c	510	CLA	CHD-C4C-NC	2.66	128.39	124.20
24	c	515	BCR	C20-C21-C22	-2.65	123.52	127.31
23	B	602	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
23	D	404[A]	CLA	CHC-C1C-C2C	-2.65	119.36	126.73
23	C	504	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
23	b	609	CLA	CHC-C1C-C2C	-2.65	119.36	126.73
35	c	517[B]	DGD	O3G-C3G-C2G	-2.65	104.50	110.90
23	a	406[A]	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
23	d	401[A]	CLA	CAC-C3C-C4C	2.65	128.25	124.81
35	C	519[A]	DGD	O1G-C1A-O1A	-2.65	116.90	123.59
23	B	608	CLA	CHC-C1C-C2C	-2.65	119.37	126.73
23	d	401[A]	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
23	A	405[A]	CLA	C4-C3-C5	2.65	119.73	115.27
23	A	404[B]	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
28	a	414[A]	PL9	C40-C39-C41	2.65	119.72	115.27
23	b	604	CLA	O2A-CGA-O1A	-2.64	116.92	123.59
23	D	404[A]	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
23	d	402	CLA	CHC-C1C-C2C	-2.64	119.39	126.73
32	D	408[A]	LHG	O8-C23-C24	2.64	120.20	111.91
23	c	509	CLA	CHD-C4C-NC	2.64	128.37	124.20
24	A	408	BCR	C33-C5-C6	-2.64	121.56	124.53
23	b	616	CLA	C4-C3-C5	2.64	119.71	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	514	CLA	CMC-C2C-C1C	2.64	129.06	125.04
28	d	404[B]	PL9	C22-C23-C24	-2.64	121.30	127.66
35	C	520	DGD	O2G-C1B-C2B	2.64	117.19	111.50
35	c	517[B]	DGD	C3G-C2G-C1G	-2.64	105.55	111.79
23	B	608	CLA	CMC-C2C-C1C	2.64	129.06	125.04
23	b	609	CLA	CMB-C2B-C1B	2.64	129.39	125.37
24	c	515	BCR	C37-C22-C21	-2.64	119.23	122.92
24	t	103	BCR	C21-C20-C19	-2.64	114.99	123.22
23	b	608	CLA	O2A-CGA-O1A	-2.64	116.94	123.59
28	d	404[B]	PL9	C7-C3-C4	2.64	119.02	116.88
23	C	507	CLA	O2A-CGA-CBA	2.64	120.18	111.91
23	C	511	CLA	CHC-C1C-C2C	-2.64	119.41	126.73
23	C	509	CLA	CHD-C4C-NC	2.63	128.35	124.20
24	K	102	BCR	C36-C18-C19	2.63	122.23	118.08
23	c	509	CLA	CMB-C2B-C1B	2.63	129.38	125.37
28	A	412[A]	PL9	C40-C39-C41	2.63	119.70	115.27
23	b	614	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
23	b	611	CLA	CAC-C3C-C4C	2.63	128.22	124.81
23	d	402	CLA	CHD-C4C-NC	2.63	128.35	124.20
23	B	613	CLA	CMC-C2C-C1C	2.63	129.04	125.04
23	C	506	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
32	d	405[B]	LHG	C6-C5-C4	-2.63	105.57	111.79
23	B	614	CLA	C4C-C3C-C2C	-2.63	103.07	106.90
23	b	609	CLA	C7-C6-C5	-2.63	106.22	113.36
23	B	606	CLA	C2A-C1A-CHA	-2.62	119.27	123.86
24	B	619	BCR	C7-C8-C9	-2.62	122.27	126.23
23	A	407	CLA	CAC-C3C-C4C	2.62	128.21	124.81
31	c	501	LMT	C3'-C4'-C5'	-2.62	104.92	110.93
32	a	420[B]	LHG	O8-C23-C24	2.62	120.13	111.91
24	H	101	BCR	C10-C11-C12	-2.62	115.04	123.22
23	D	404[B]	CLA	CBC-CAC-C3C	-2.62	105.21	112.43
24	k	101	BCR	C10-C11-C12	-2.62	115.05	123.22
23	c	510	CLA	CHB-C1B-NB	-2.62	121.49	124.26
23	B	606	CLA	C3B-C4B-NB	2.62	112.94	110.52
23	B	603	CLA	CHD-C4C-NC	2.61	128.32	124.20
26	B	620	SQD	C1-O5-C5	-2.61	108.56	113.69
23	A	407	CLA	CMB-C2B-C1B	2.61	129.35	125.37
28	a	414[A]	PL9	C47-C48-C49	-2.61	118.83	127.75
23	a	407[A]	CLA	O2A-CGA-CBA	2.61	120.10	111.91
32	d	406[A]	LHG	O8-C23-C24	2.61	120.09	111.91
23	C	512	CLA	C4-C3-C2	-2.61	116.99	123.68
24	B	619	BCR	C24-C23-C22	-2.61	122.29	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	O2A-CGA-CBA	2.61	120.09	111.91
24	d	403	BCR	C28-C27-C26	-2.61	109.42	114.08
24	K	102	BCR	C29-C30-C25	2.61	114.49	110.48
24	b	619	BCR	C16-C17-C18	-2.61	123.59	127.31
37	a	416[B]	PHO	O2A-CGA-CBA	2.60	120.08	111.91
24	B	619	BCR	C21-C20-C19	-2.60	115.10	123.22
28	d	404[B]	PL9	C12-C13-C14	-2.60	121.39	127.66
23	A	405[A]	CLA	CMA-C3A-C2A	-2.60	103.33	113.83
23	C	512	CLA	O2A-CGA-CBA	2.60	120.07	111.91
26	a	411[B]	SQD	O47-C7-O49	-2.60	117.42	123.70
28	a	414[A]	PL9	C10-C9-C8	-2.60	117.01	123.68
23	b	610	CLA	C4-C3-C5	2.60	119.64	115.27
32	A	416[B]	LHG	O7-C7-O9	-2.60	117.43	123.70
23	a	407[A]	CLA	CMC-C2C-C1C	2.60	128.99	125.04
23	c	509	CLA	CMC-C2C-C1C	2.60	128.99	125.04
24	c	516	BCR	C32-C1-C6	-2.60	106.09	110.30
23	b	601	CLA	C2A-C1A-CHA	-2.60	119.32	123.86
24	T	102	BCR	C15-C14-C13	2.60	131.01	127.31
23	a	407[B]	CLA	CAC-C3C-C4C	2.60	128.18	124.81
37	D	401[A]	PHO	O2A-CGA-CBA	2.59	120.05	111.91
26	F	103	SQD	O47-C7-O49	-2.59	117.43	123.70
23	A	407	CLA	CMA-C3A-C2A	-2.59	103.36	113.83
35	H	102	DGD	O1G-C1A-O1A	-2.59	117.05	123.59
23	b	608	CLA	O2A-CGA-CBA	2.59	120.04	111.91
23	c	513	CLA	O2A-CGA-O1A	-2.59	117.05	123.59
23	b	610	CLA	CAA-CBA-CGA	-2.59	105.68	113.25
24	a	410	BCR	C29-C30-C25	2.59	114.47	110.48
23	B	608	CLA	CAC-C3C-C4C	2.59	128.17	124.81
23	a	407[B]	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
23	a	406[A]	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
23	d	402	CLA	CAA-C2A-C3A	-2.58	105.70	112.78
23	c	508	CLA	O2A-CGA-CBA	2.58	120.01	111.91
24	b	618	BCR	C29-C30-C25	2.58	114.46	110.48
23	B	608	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
33	c	521	LMG	O8-C28-C29	2.58	120.00	111.91
23	B	609	CLA	CHC-C1C-C2C	-2.58	119.56	126.73
28	a	414[B]	PL9	C10-C9-C11	2.58	119.61	115.27
23	c	504	CLA	CHC-C1C-C2C	-2.58	119.57	126.73
23	b	615	CLA	CAC-C3C-C4C	2.58	128.16	124.81
23	A	406[A]	CLA	CHC-C1C-C2C	-2.58	119.57	126.73
23	C	512	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
23	c	509	CLA	CHC-C1C-C2C	-2.58	119.57	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	404[B]	PL9	C51-C49-C50	2.58	120.30	114.60
24	b	619	BCR	C16-C15-C14	-2.58	118.20	123.47
23	A	405[A]	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
23	C	509	CLA	CHC-C1C-C2C	-2.57	119.58	126.73
23	B	615	CLA	CHC-C1C-C2C	-2.57	119.58	126.73
23	A	407	CLA	CHD-C4C-NC	2.57	128.26	124.20
23	a	405[B]	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
40	V	202	HEC	CAD-CBD-CGD	-2.57	108.07	113.60
23	D	404[A]	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
34	b	622	HTG	O2-C2-C3	-2.57	104.40	110.35
23	B	616	CLA	CHD-C4C-NC	2.57	128.26	124.20
37	D	401[A]	PHO	O1D-CGD-CBD	-2.57	120.46	124.74
28	D	407[B]	PL9	C51-C49-C50	2.57	120.28	114.60
26	C	501[A]	SQD	O48-C23-O10	-2.57	117.11	123.59
28	A	412[B]	PL9	C10-C9-C11	2.57	119.59	115.27
37	D	401[A]	PHO	O2A-CGA-O1A	-2.57	117.12	123.59
24	K	102	BCR	C15-C14-C13	-2.57	123.65	127.31
33	c	520	LMG	C8-O7-C10	-2.57	111.47	117.79
23	b	601	CLA	CHC-C1C-C2C	-2.56	119.61	126.73
23	b	603	CLA	C4-C3-C5	2.56	119.58	115.27
24	K	102	BCR	C24-C23-C22	-2.56	122.36	126.23
35	c	519	DGD	O1G-C1A-C2A	2.56	119.95	111.91
23	C	508	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
28	A	412[A]	PL9	C10-C9-C8	-2.56	117.11	123.68
31	A	417	LMT	O5'-C5'-C6'	2.56	112.80	106.44
23	B	601	CLA	O2A-CGA-CBA	2.56	119.94	111.91
40	V	202	HEC	CBC-CAC-C3C	2.56	119.49	112.43
24	t	103	BCR	C29-C28-C27	-2.56	105.66	111.38
23	b	611	CLA	CHD-C4C-NC	2.56	128.23	124.20
24	b	619	BCR	C11-C10-C9	-2.56	123.66	127.31
23	C	511	CLA	CHD-C4C-NC	2.56	128.23	124.20
23	A	404[B]	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
24	D	406	BCR	C40-C30-C25	-2.56	106.15	110.30
23	c	511	CLA	C4C-C3C-C2C	-2.56	103.17	106.90
33	D	413	LMG	O8-C28-C29	2.56	119.93	111.91
23	c	507	CLA	CAA-C2A-C3A	-2.55	105.79	112.78
23	b	616	CLA	OBD-CAD-C3D	-2.55	122.38	128.52
23	C	504	CLA	C3B-C4B-NB	2.55	112.88	110.52
23	a	405[B]	CLA	CAA-C2A-C1A	-2.55	103.61	111.97
31	m	103	LMT	C1'-O5'-C5'	-2.55	108.68	113.69
23	B	602	CLA	CHD-C4C-NC	2.55	128.22	124.20
24	B	617	BCR	C37-C22-C23	2.55	122.09	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	O2A-CGA-CBA	2.55	119.90	111.91
23	b	605	CLA	C3B-C4B-NB	2.55	112.88	110.52
23	B	605	CLA	CHC-C1C-C2C	-2.55	119.66	126.73
24	b	617	BCR	C29-C30-C25	2.55	114.40	110.48
23	A	405[A]	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
26	f	102	SQD	O47-C7-O49	-2.54	117.55	123.70
28	D	407[B]	PL9	C12-C13-C14	-2.54	121.53	127.66
23	d	401[A]	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
24	C	517	BCR	C36-C18-C19	2.54	122.09	118.08
28	A	412[A]	PL9	C47-C48-C49	-2.54	119.05	127.75
23	B	613	CLA	CHC-C1C-C2C	-2.54	119.66	126.73
23	b	606	CLA	CMB-C2B-C1B	2.54	129.24	125.37
24	h	101	BCR	C24-C23-C22	-2.54	122.39	126.23
23	b	615	CLA	O2A-CGA-CBA	2.54	119.89	111.91
23	a	407[B]	CLA	C2A-C1A-CHA	-2.54	119.41	123.86
23	c	513	CLA	CBA-CAA-C2A	-2.54	106.36	113.86
23	a	407[B]	CLA	CHC-C1C-C2C	-2.54	119.67	126.73
23	b	614	CLA	CHB-C1B-NB	-2.54	121.57	124.26
23	C	512	CLA	CMC-C2C-C1C	2.54	128.90	125.04
23	C	504	CLA	CHD-C4C-NC	2.54	128.20	124.20
23	c	504	CLA	CHD-C4C-NC	2.53	128.20	124.20
35	C	520	DGD	O3G-C3G-C2G	-2.53	104.78	110.90
26	b	620	SQD	O48-C23-C24	2.53	119.86	111.91
23	A	405[B]	CLA	C2A-C1A-CHA	-2.53	119.43	123.86
23	a	407[B]	CLA	CBC-CAC-C3C	-2.53	105.45	112.43
23	C	504	CLA	CMB-C2B-C1B	2.53	129.23	125.37
23	A	406[B]	CLA	O2A-CGA-O1A	-2.53	117.20	123.59
23	c	514	CLA	CHB-C1B-NB	-2.53	121.58	124.26
23	B	610	CLA	CAC-C3C-C4C	2.53	128.09	124.81
24	T	102	BCR	C2-C1-C6	2.53	114.37	110.48
23	a	406[B]	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
26	A	410	SQD	O48-C23-C24	2.53	119.84	111.91
31	m	103	LMT	C3'-C4'-C5'	-2.53	105.13	110.93
23	b	613	CLA	CMA-C3A-C4A	-2.52	104.99	111.77
26	B	620	SQD	O5-C1-C2	-2.52	105.01	110.35
23	B	602	CLA	CAC-C3C-C4C	2.52	128.08	124.81
23	C	508	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
23	b	612	CLA	CHC-C1C-C2C	-2.52	119.73	126.73
23	c	512	CLA	CMC-C2C-C1C	2.52	128.88	125.04
32	D	408[B]	LHG	O8-C23-C24	2.52	119.81	111.91
23	b	608	CLA	CHD-C4C-NC	2.52	128.17	124.20
34	c	522	HTG	O5-C1-C2	2.52	113.48	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C7-C6-C5	-2.52	106.52	113.36
23	C	515	CLA	O2A-CGA-CBA	2.52	119.81	111.91
23	C	503	CLA	CHD-C4C-NC	2.52	128.17	124.20
23	a	405[B]	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
37	D	401[B]	PHO	O2D-CGD-O1D	-2.52	118.92	123.84
37	a	408[B]	PHO	O2A-CGA-CBA	2.52	119.80	111.91
23	b	613	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
37	D	402[B]	PHO	CED-O2D-CGD	2.52	121.63	115.94
32	D	409[B]	LHG	O8-C23-O10	-2.51	117.25	123.59
23	b	602	CLA	CHB-C1B-C2B	-2.51	120.14	127.24
23	a	406[A]	CLA	CAA-CBA-CGA	2.51	120.59	113.25
34	B	625	HTG	O5-C5-C4	2.51	114.26	109.69
31	B	630	LMT	O5'-C5'-C6'	2.51	112.68	106.44
33	B	621	LMG	O8-C28-O10	-2.51	117.26	123.59
23	d	401[A]	CLA	CMC-C2C-C1C	2.51	128.86	125.04
23	C	513	CLA	CHC-C1C-C2C	-2.51	119.76	126.73
35	c	518[B]	DGD	O1G-C1A-C2A	2.51	119.78	111.91
23	A	406[A]	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
23	a	405[A]	CLA	CHD-C4C-NC	2.51	128.15	124.20
23	b	609	CLA	O2A-CGA-CBA	2.51	119.78	111.91
23	b	613	CLA	CMC-C2C-C1C	2.51	128.85	125.04
23	B	605	CLA	C3B-C4B-NB	2.51	112.84	110.52
23	C	509	CLA	C1-C2-C3	-2.50	121.71	126.04
23	B	601	CLA	C3B-C4B-NB	2.50	112.84	110.52
23	a	409	CLA	C2A-C1A-CHA	-2.50	119.48	123.86
23	c	505	CLA	CBC-CAC-C3C	-2.50	105.53	112.43
28	D	407[A]	PL9	C42-C41-C39	-2.50	104.75	112.98
24	k	101	BCR	C2-C1-C6	2.50	114.33	110.48
32	d	405[B]	LHG	O8-C23-C24	2.50	119.75	111.91
23	B	612	CLA	C6-C5-C3	-2.50	106.91	113.45
35	h	102	DGD	O3G-C1D-C2D	2.50	112.20	108.30
35	c	518[A]	DGD	O1G-C1A-C2A	2.50	119.74	111.91
23	c	508	CLA	CBC-CAC-C3C	-2.50	105.55	112.43
28	d	404[B]	PL9	C53-C6-C1	2.50	120.09	114.99
23	B	616	CLA	CHC-C1C-C2C	-2.49	119.80	126.73
26	a	411[B]	SQD	C3-C4-C5	2.49	114.69	110.24
37	D	401[B]	PHO	O2A-CGA-CBA	2.49	119.74	111.91
23	a	405[A]	CLA	C4C-C3C-C2C	-2.49	103.26	106.90
23	b	606	CLA	C1-O2A-CGA	2.49	122.99	116.44
37	a	408[B]	PHO	O1D-CGD-CBD	-2.49	120.59	124.74
23	D	405	CLA	C1-C2-C3	-2.49	121.73	126.04
23	D	405	CLA	CHC-C1C-C2C	-2.49	119.81	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	C1-O2A-CGA	2.49	122.98	116.44
37	a	408[B]	PHO	CMB-C2B-C3B	2.49	129.34	124.68
23	b	605	CLA	CMC-C2C-C1C	2.49	128.83	125.04
28	A	412[B]	PL9	C12-C13-C14	-2.49	121.66	127.66
26	a	411[B]	SQD	O9-S-C6	2.49	109.90	106.94
23	c	504	CLA	C2A-C1A-CHA	-2.49	119.51	123.86
35	c	519	DGD	O2G-C1B-O1B	-2.49	117.69	123.70
23	B	613	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	B	607	CLA	CHC-C1C-C2C	-2.49	119.82	126.73
23	a	409	CLA	CMA-C3A-C2A	-2.49	103.80	113.83
23	a	405[B]	CLA	C2A-C1A-CHA	-2.49	119.51	123.86
28	A	412[B]	PL9	C45-C44-C46	2.49	119.45	115.27
26	a	411[A]	SQD	O8-S-C6	2.49	109.70	105.74
23	C	507	CLA	O2A-CGA-O1A	-2.48	117.32	123.59
23	b	608	CLA	C4C-C3C-C2C	-2.48	103.28	106.90
24	H	101	BCR	C20-C21-C22	-2.48	123.77	127.31
24	k	101	BCR	C24-C23-C22	-2.48	122.48	126.23
24	T	102	BCR	C16-C17-C18	-2.48	123.77	127.31
23	a	406[A]	CLA	CBC-CAC-C3C	-2.48	105.59	112.43
24	C	517	BCR	C15-C14-C13	-2.48	123.77	127.31
23	c	505	CLA	CED-O2D-CGD	2.48	121.55	115.94
23	a	405[B]	CLA	C7-C6-C5	-2.48	106.62	113.36
24	c	515	BCR	C38-C26-C25	-2.48	121.74	124.53
23	B	607	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
24	b	618	BCR	C37-C22-C23	2.48	121.98	118.08
23	A	407	CLA	C2A-C1A-CHA	-2.48	119.53	123.86
23	b	607	CLA	C2A-C1A-CHA	-2.48	119.53	123.86
23	C	510	CLA	CMB-C2B-C1B	2.48	129.14	125.37
24	c	516	BCR	C33-C5-C6	-2.48	121.75	124.53
24	Y	101	BCR	C29-C30-C25	2.47	114.29	110.48
23	b	601	CLA	CMB-C2B-C1B	2.47	129.14	125.37
28	D	407[A]	PL9	C20-C19-C21	2.47	119.43	115.27
33	m	101	LMG	O7-C10-O9	-2.47	117.72	123.70
40	V	202	HEC	CHA-C4D-ND	2.47	127.11	124.42
31	b	621	LMT	C1'-O5'-C5'	-2.47	108.83	113.69
35	c	517[A]	DGD	C2G-O2G-C1B	-2.47	111.70	117.79
23	B	606	CLA	CMB-C2B-C1B	2.47	129.13	125.37
23	c	506	CLA	O2A-CGA-CBA	2.47	119.66	111.91
24	d	403	BCR	C16-C15-C14	-2.47	118.42	123.47
23	B	614	CLA	CMA-C3A-C2A	-2.47	103.87	113.83
24	B	618	BCR	C38-C26-C25	-2.47	121.75	124.53
23	a	407[B]	CLA	C3B-C4B-NB	2.47	112.81	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	102	SQD	O7-S-C6	2.47	109.87	106.94
23	a	407[B]	CLA	O2A-CGA-CBA	2.47	119.65	111.91
23	b	612	CLA	CHD-C4C-NC	2.47	128.09	124.20
23	A	407	CLA	CBC-CAC-C3C	-2.47	105.63	112.43
26	b	620	SQD	O47-C7-O49	-2.46	117.75	123.70
23	C	508	CLA	CHD-C4C-NC	2.46	128.09	124.20
23	B	611	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
37	D	401[A]	PHO	CMB-C2B-C3B	2.46	129.29	124.68
24	k	101	BCR	C20-C21-C22	-2.46	123.80	127.31
23	c	508	CLA	C3B-C4B-NB	2.46	112.80	110.52
23	C	512	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
31	F	101	LMT	C1'-O5'-C5'	-2.46	108.86	113.69
23	b	613	CLA	C4-C3-C5	2.46	119.41	115.27
23	D	404[B]	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
23	b	603	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
35	H	102	DGD	C3E-C4E-C5E	-2.46	105.85	110.24
23	B	612	CLA	CHC-C1C-C2C	-2.46	119.90	126.73
24	t	103	BCR	C35-C13-C12	2.46	121.95	118.08
23	c	502	CLA	C1-C2-C3	-2.46	121.79	126.04
23	a	406[B]	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
23	C	511	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
23	B	602	CLA	CHC-C1C-C2C	-2.45	119.92	126.73
31	A	417	LMT	O1'-C1'-C2'	2.45	112.13	108.30
23	C	503	CLA	C2A-C1A-CHA	-2.45	119.57	123.86
24	c	516	BCR	C20-C21-C22	-2.45	123.81	127.31
23	c	508	CLA	CHC-C1C-C2C	-2.45	119.92	126.73
23	c	514	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
23	c	508	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
23	A	404[A]	CLA	CAA-CBA-CGA	-2.45	106.09	113.25
33	C	502	LMG	O6-C1-O1	-2.45	104.17	109.97
23	B	602	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
28	D	407[A]	PL9	C40-C39-C41	2.45	119.39	115.27
23	C	514	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	B	603	CLA	CMA-C3A-C2A	-2.44	103.98	113.83
31	B	630	LMT	O5'-C5'-C4'	2.44	114.90	109.75
25	b	628	GOL	C3-C2-C1	-2.44	102.22	111.70
23	B	611	CLA	C4A-NA-C1A	-2.44	105.61	106.71
23	b	611	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
23	b	615	CLA	CMC-C2C-C1C	2.44	128.75	125.04
23	B	605	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
23	A	406[B]	CLA	C4-C3-C5	2.44	119.37	115.27
24	Y	101	BCR	C3-C4-C5	-2.44	109.73	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	l	802[B]	LHG	O8-C23-C24	2.43	119.55	111.91
23	A	407	CLA	CHB-C4A-NA	2.43	127.88	124.51
28	d	404[B]	PL9	C27-C28-C29	-2.43	121.80	127.66
23	b	602	CLA	CAA-CBA-CGA	-2.43	106.14	113.25
23	a	406[B]	CLA	O2A-CGA-CBA	2.43	119.54	111.91
23	c	507	CLA	O2A-CGA-CBA	2.43	119.53	111.91
35	C	519[B]	DGD	O1G-C1A-C2A	2.43	119.53	111.91
23	b	602	CLA	CMA-C3A-C2A	-2.43	104.03	113.83
23	B	607	CLA	CHD-C4C-NC	2.43	128.03	124.20
23	C	515	CLA	CHC-C1C-C2C	-2.43	119.98	126.73
24	K	102	BCR	C20-C21-C22	-2.43	123.85	127.31
23	c	511	CLA	CMB-C2B-C1B	2.42	129.06	125.37
33	z	101	LMG	C7-O1-C1	-2.42	109.00	113.74
23	A	405[A]	CLA	CAA-CBA-CGA	2.42	120.34	113.25
23	c	508	CLA	O1D-CGD-CBD	-2.42	119.52	124.48
23	b	603	CLA	C7-C6-C5	-2.42	106.78	113.36
23	B	610	CLA	CHB-C4A-NA	2.42	127.86	124.51
23	b	606	CLA	CMC-C2C-C1C	2.42	128.72	125.04
23	b	615	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
23	c	512	CLA	CHB-C1B-NB	-2.42	121.70	124.26
24	K	102	BCR	C38-C26-C25	-2.42	121.81	124.53
23	A	406[A]	CLA	C1-C2-C3	-2.42	121.86	126.04
23	B	609	CLA	C3B-C4B-NB	2.42	112.76	110.52
23	C	513	CLA	O2A-CGA-CBA	2.42	119.49	111.91
28	D	407[A]	PL9	C7-C8-C9	-2.41	122.77	126.79
33	z	101	LMG	C8-O7-C10	-2.41	111.85	117.79
32	A	416[A]	LHG	O7-C7-O9	-2.41	117.87	123.70
23	c	513	CLA	CMC-C2C-C1C	2.41	128.71	125.04
28	a	414[B]	PL9	C45-C44-C46	2.41	119.33	115.27
23	B	607	CLA	CED-O2D-CGD	2.41	121.39	115.94
37	D	401[B]	PHO	CMB-C2B-C3B	2.41	129.19	124.68
23	C	508	CLA	CMB-C2B-C1B	2.41	129.04	125.37
32	L	101[B]	LHG	O8-C23-C24	2.41	119.47	111.91
23	B	603	CLA	C7-C6-C5	-2.41	106.82	113.36
23	b	602	CLA	C11-C12-C13	-2.41	108.13	115.92
37	D	401[A]	PHO	CMA-C3A-C4A	-2.41	109.11	114.38
24	h	101	BCR	C11-C10-C9	-2.41	123.88	127.31
23	b	611	CLA	OBD-CAD-C3D	-2.41	122.73	128.52
23	B	609	CLA	C7-C6-C5	-2.41	106.83	113.36
23	A	406[B]	CLA	CMC-C2C-C1C	2.41	128.70	125.04
23	c	503	CLA	O2A-CGA-O1A	-2.40	117.52	123.59
24	b	618	BCR	C33-C5-C6	-2.40	121.83	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	502	CLA	CBC-CAC-C3C	-2.40	105.80	112.43
40	v	201	HEC	CBD-CAD-C3D	-2.40	105.95	112.63
23	c	510	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
34	C	523	HTG	C1-O5-C5	2.40	117.01	112.58
24	b	619	BCR	C7-C6-C5	2.40	127.28	121.46
23	b	615	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
32	l	802[A]	LHG	O8-C23-O10	-2.40	117.53	123.59
28	A	412[B]	PL9	C10-C9-C8	-2.40	117.52	123.68
23	b	606	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
37	D	401[B]	PHO	C4-C3-C5	2.40	119.31	115.27
23	c	511	CLA	CED-O2D-CGD	2.40	121.36	115.94
24	b	618	BCR	C15-C14-C13	-2.40	123.89	127.31
32	d	406[A]	LHG	O8-C23-O10	-2.40	117.54	123.59
28	d	404[A]	PL9	C17-C18-C19	-2.40	121.89	127.66
40	v	201	HEC	CHA-C1A-NA	2.40	127.03	124.44
23	b	610	CLA	CHC-C1C-C2C	-2.40	120.07	126.73
23	B	601	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
23	c	503	CLA	C4C-C3C-C2C	-2.40	103.40	106.90
23	B	605	CLA	O2A-CGA-CBA	2.40	119.43	111.91
37	a	408[B]	PHO	C4A-C3A-C2A	-2.40	100.56	102.84
23	C	514	CLA	CHC-C1C-C2C	-2.39	120.08	126.73
23	b	616	CLA	C3B-C4B-NB	2.39	112.74	110.52
24	B	618	BCR	C2-C1-C6	2.39	114.17	110.48
23	b	608	CLA	C11-C12-C13	-2.39	108.18	115.92
28	d	404[A]	PL9	C7-C8-C9	-2.39	122.81	126.79
23	D	405	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
23	b	605	CLA	O2A-CGA-CBA	2.39	119.41	111.91
23	C	509	CLA	CMC-C2C-C1C	2.39	128.68	125.04
23	b	609	CLA	CMA-C3A-C4A	-2.39	105.35	111.77
24	t	103	BCR	C1-C6-C7	2.39	122.54	115.78
28	D	407[B]	PL9	C22-C23-C24	-2.39	121.90	127.66
24	c	515	BCR	C33-C5-C6	-2.39	121.84	124.53
23	C	513	CLA	CHD-C4C-NC	2.39	127.97	124.20
23	d	402	CLA	CMA-C3A-C2A	-2.39	104.19	113.83
23	c	508	CLA	C4C-C3C-C2C	-2.39	103.42	106.90
23	B	615	CLA	C11-C10-C8	-2.39	108.20	115.92
24	B	618	BCR	C15-C14-C13	-2.39	123.90	127.31
23	B	602	CLA	C11-C12-C13	-2.39	108.20	115.92
23	C	508	CLA	O2A-CGA-CBA	2.39	119.40	111.91
31	t	101	LMT	O1'-C1'-C2'	2.39	112.03	108.30
23	B	608	CLA	CMA-C3A-C2A	-2.39	104.20	113.83
34	b	625	HTG	C1'-S1-C1	2.38	104.55	100.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	404[A]	CLA	CMC-C2C-C1C	2.38	128.67	125.04
23	d	401[A]	CLA	CMB-C2B-C1B	2.38	129.00	125.37
23	a	405[A]	CLA	CMA-C3A-C2A	-2.38	104.22	113.83
40	V	202	HEC	C3B-C4B-NB	-2.38	107.51	110.17
23	c	512	CLA	C1-C2-C3	-2.38	121.92	126.04
28	a	414[A]	PL9	C20-C19-C21	2.38	119.28	115.27
23	c	503	CLA	CHB-C1B-NB	-2.38	121.74	124.26
23	C	503	CLA	C11-C12-C13	-2.38	108.22	115.92
23	b	607	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
28	D	407[A]	PL9	C36-C37-C38	-2.38	104.07	111.88
23	b	611	CLA	CMB-C2B-C1B	2.38	128.99	125.37
23	d	402	CLA	CMC-C2C-C1C	2.37	128.66	125.04
24	c	515	BCR	C36-C18-C17	-2.37	119.60	122.92
24	c	516	BCR	C21-C20-C19	-2.37	115.81	123.22
23	c	507	CLA	CMC-C2C-C1C	2.37	128.65	125.04
24	Y	101	BCR	C1-C6-C7	2.37	122.49	115.78
23	A	406[A]	CLA	CAC-C3C-C4C	2.37	127.89	124.81
35	C	519[B]	DGD	O1G-C1A-O1A	-2.37	117.61	123.59
23	B	615	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
24	D	406	BCR	C39-C30-C25	-2.37	106.45	110.30
23	d	401[B]	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
24	c	515	BCR	C28-C27-C26	-2.37	109.85	114.08
40	V	202	HEC	CMD-C2D-C1D	2.37	128.64	125.04
32	D	408[B]	LHG	O8-C23-O10	-2.37	117.62	123.59
31	M	101	LMT	O1B-C1B-C2B	2.37	114.23	108.10
38	F	102	HEM	CHA-C4D-ND	2.37	127.29	124.37
37	D	402[A]	PHO	C4D-CHA-CBD	2.37	109.59	108.52
24	B	617	BCR	C15-C14-C13	-2.36	123.94	127.31
28	D	407[B]	PL9	C37-C38-C39	-2.36	121.97	127.66
24	B	617	BCR	C16-C17-C18	-2.36	123.94	127.31
23	c	514	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
37	a	416[A]	PHO	C1A-C2A-C3A	-2.36	100.59	102.84
23	C	507	CLA	CHB-C1B-NB	-2.36	121.76	124.26
23	c	502	CLA	C1-O2A-CGA	2.36	122.64	116.44
23	B	611	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
24	h	101	BCR	C16-C17-C18	-2.36	123.94	127.31
23	C	514	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
35	c	517[A]	DGD	C3G-C2G-C1G	-2.36	106.21	111.79
23	B	608	CLA	C11-C10-C8	-2.36	108.29	115.92
24	D	406	BCR	C21-C20-C19	-2.36	115.86	123.22
23	b	616	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
31	m	103	LMT	C3B-C4B-C5B	-2.36	106.03	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	412	SQD	O5-C5-C4	2.36	113.97	109.69
28	d	404[A]	PL9	C12-C13-C14	-2.36	121.99	127.66
23	B	603	CLA	C2A-C1A-CHA	-2.35	119.74	123.86
23	A	404[B]	CLA	CAA-C2A-C1A	-2.35	104.26	111.97
23	A	404[B]	CLA	CAA-CBA-CGA	-2.35	106.38	113.25
23	c	513	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
23	a	405[B]	CLA	CHB-C1B-C2B	-2.35	120.59	127.24
23	C	503	CLA	CHB-C1B-NB	-2.35	121.77	124.26
23	a	407[A]	CLA	C1-C2-C3	-2.35	121.98	126.04
26	a	411[B]	SQD	O48-C23-C24	2.35	119.28	111.91
23	c	511	CLA	C4-C3-C2	-2.35	117.65	123.68
35	c	519	DGD	O3G-C1D-C2D	-2.35	104.64	108.30
28	A	412[A]	PL9	C45-C44-C46	2.35	119.22	115.27
26	F	103	SQD	O5-C1-O6	2.35	115.54	109.97
26	F	103	SQD	O48-C23-O10	-2.35	117.67	123.59
26	a	412	SQD	C3-C4-C5	2.35	114.42	110.24
23	B	607	CLA	CMA-C3A-C2A	-2.35	104.36	113.83
23	C	509	CLA	CHB-C1B-NB	-2.35	121.77	124.26
35	H	102	DGD	O2G-C1B-C2B	2.34	116.55	111.50
37	D	402[B]	PHO	C6-C5-C3	-2.34	107.31	113.45
23	a	407[B]	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
23	C	515	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
23	A	406[A]	CLA	CMA-C3A-C2A	-2.34	104.38	113.83
24	y	101	BCR	C1-C6-C7	2.34	122.40	115.78
34	b	623	HTG	O5-C1-C2	2.34	113.25	110.31
28	A	412[A]	PL9	C42-C43-C44	-2.34	122.03	127.66
23	c	505	CLA	CMC-C2C-C1C	2.34	128.60	125.04
35	C	518[B]	DGD	O1G-C1A-O1A	-2.34	117.70	123.59
37	D	401[B]	PHO	C4A-C3A-C2A	-2.34	100.62	102.84
24	k	101	BCR	C36-C18-C19	2.33	121.76	118.08
23	b	602	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
32	d	405[A]	LHG	C6-C5-C4	-2.33	106.27	111.79
28	d	404[A]	PL9	C20-C19-C21	2.33	119.20	115.27
26	a	412	SQD	O8-S-C6	2.33	109.46	105.74
23	C	506	CLA	C4C-C3C-C2C	-2.33	103.50	106.90
33	m	101	LMG	O3-C3-C2	-2.33	104.96	110.35
23	D	404[A]	CLA	CMB-C2B-C1B	2.33	128.92	125.37
28	D	407[B]	PL9	C7-C3-C4	2.33	118.77	116.88
26	b	620	SQD	C44-O6-C1	-2.33	109.19	113.74
33	m	101	LMG	C1-O6-C5	-2.33	109.12	113.69
23	C	513	CLA	C1-O2A-CGA	2.33	122.55	116.44
23	b	612	CLA	CMA-C3A-C2A	-2.33	104.44	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	515	BCR	C34-C9-C10	-2.33	119.67	122.92
24	d	403	BCR	C39-C30-C25	-2.32	106.53	110.30
23	a	406[B]	CLA	O2A-CGA-O1A	-2.32	117.72	123.59
23	a	405[B]	CLA	CMC-C2C-C1C	2.32	128.58	125.04
28	d	404[B]	PL9	C45-C44-C46	2.32	119.18	115.27
23	b	601	CLA	CAC-C3C-C2C	2.32	131.50	127.53
26	a	412	SQD	C1-O5-C5	2.32	118.25	113.69
23	C	510	CLA	C4-C3-C5	2.32	119.18	115.27
23	b	612	CLA	C6-C7-C8	-2.32	108.42	115.92
23	c	505	CLA	CHD-C4C-NC	2.32	127.86	124.20
23	b	615	CLA	C6-C7-C8	-2.32	108.42	115.92
23	C	513	CLA	C1-C2-C3	-2.32	122.03	126.04
24	Y	101	BCR	C36-C18-C19	2.32	121.73	118.08
23	b	614	CLA	O2A-CGA-CBA	2.32	119.18	111.91
23	B	601	CLA	CHC-C1C-C2C	-2.32	120.29	126.73
23	b	611	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
23	a	409	CLA	CHB-C4A-NA	2.32	127.72	124.51
34	B	625	HTG	C3-C4-C5	2.32	114.37	110.24
23	C	513	CLA	CMB-C2B-C1B	2.32	128.90	125.37
23	b	601	CLA	O2A-CGA-CBA	2.32	119.17	111.91
23	C	506	CLA	C2A-C1A-CHA	-2.31	119.81	123.86
24	c	516	BCR	C2-C1-C6	2.31	114.04	110.48
23	D	404[B]	CLA	CMC-C2C-C1C	2.31	128.56	125.04
24	c	516	BCR	C37-C22-C23	2.31	121.72	118.08
23	a	406[A]	CLA	CMC-C2C-C1C	2.31	128.56	125.04
23	b	604	CLA	O2A-CGA-CBA	2.31	119.16	111.91
23	C	509	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
23	C	512	CLA	CHB-C4A-NA	2.31	127.70	124.51
23	B	615	CLA	CHB-C1B-NB	-2.31	121.81	124.26
35	C	519[A]	DGD	C2G-O2G-C1B	-2.31	112.11	117.79
35	C	518[A]	DGD	O6E-C5E-C4E	2.30	113.88	109.69
38	F	102	HEM	C4C-CHD-C1D	-2.30	121.09	126.06
23	B	604	CLA	C6-C5-C3	-2.30	107.42	113.45
23	A	406[B]	CLA	CAC-C3C-C4C	2.30	127.80	124.81
23	C	504	CLA	O2A-CGA-CBA	2.30	119.12	111.91
23	B	607	CLA	OBD-CAD-C3D	-2.30	122.99	128.52
24	y	101	BCR	C16-C17-C18	-2.30	124.03	127.31
23	A	407	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
23	c	514	CLA	C1-O2A-CGA	2.30	122.47	116.44
26	a	411[A]	SQD	O48-C23-C24	2.30	119.11	111.91
24	B	617	BCR	C29-C30-C25	2.30	114.02	110.48
23	B	606	CLA	C1-C2-C3	-2.29	122.07	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
23	c	508	CLA	CAC-C3C-C4C	2.29	127.78	124.81
23	B	611	CLA	CMB-C2B-C3B	2.29	132.13	126.59
24	B	618	BCR	C37-C22-C23	2.29	121.68	118.08
23	B	604	CLA	CMC-C2C-C1C	2.29	128.52	125.04
24	d	403	BCR	C37-C22-C21	-2.29	119.72	122.92
23	c	511	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
23	d	401[B]	CLA	CMB-C2B-C1B	2.29	128.85	125.37
35	C	518[A]	DGD	C3G-C2G-C1G	-2.29	106.38	111.79
32	d	406[B]	LHG	O8-C23-O10	-2.29	117.82	123.59
23	B	605	CLA	CAC-C3C-C2C	2.28	131.44	127.53
23	b	607	CLA	C1-O2A-CGA	2.28	122.44	116.44
23	c	504	CLA	CMC-C2C-C1C	2.28	128.51	125.04
23	C	506	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
23	C	506	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
23	b	606	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
23	c	505	CLA	CHB-C1B-NB	-2.28	121.84	124.26
23	c	512	CLA	C4-C3-C2	-2.28	117.83	123.68
33	C	521	LMG	C8-O7-C10	-2.28	112.18	117.79
28	d	404[B]	PL9	C36-C37-C38	-2.28	104.39	111.88
33	C	522	LMG	O1-C1-C2	2.28	111.86	108.30
23	b	616	CLA	CHC-C1C-C2C	-2.28	120.40	126.73
23	C	512	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
23	c	509	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
28	d	404[A]	PL9	C51-C49-C50	2.28	119.63	114.60
23	b	613	CLA	CBC-CAC-C3C	-2.28	106.16	112.43
26	a	411[B]	SQD	O7-S-C6	2.28	109.64	106.94
23	b	610	CLA	CHB-C4A-NA	2.28	127.66	124.51
33	m	101	LMG	O8-C28-O10	-2.27	117.85	123.59
24	y	101	BCR	C11-C10-C9	-2.27	124.06	127.31
26	C	501[B]	SQD	O9-S-C6	2.27	109.64	106.94
24	D	406	BCR	C15-C16-C17	-2.27	118.82	123.47
23	b	606	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
23	c	512	CLA	CAC-C3C-C4C	2.27	127.76	124.81
23	b	612	CLA	CMB-C2B-C1B	2.27	128.83	125.37
23	c	512	CLA	CMA-C3A-C4A	2.27	117.88	111.77
24	b	617	BCR	C32-C1-C6	-2.27	106.62	110.30
24	C	516	BCR	C38-C26-C25	-2.27	121.98	124.53
37	a	416[A]	PHO	O2A-CGA-CBA	2.27	119.03	111.91
24	y	101	BCR	C21-C20-C19	-2.27	116.14	123.22
23	C	510	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
31	M	101	LMT	O5B-C5B-C6B	2.27	112.07	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	412[A]	PL9	C35-C34-C33	-2.27	117.86	123.68
26	B	620	SQD	O48-C23-O10	-2.27	117.87	123.59
23	a	405[A]	CLA	C7-C6-C5	-2.27	107.20	113.36
32	E	101[B]	LHG	O7-C7-O9	-2.27	118.23	123.70
24	K	102	BCR	C2-C1-C6	2.27	113.97	110.48
23	c	513	CLA	CHB-C4A-NA	2.26	127.64	124.51
37	a	416[B]	PHO	C4A-C3A-C2A	-2.26	100.68	102.84
23	c	510	CLA	O2A-C1-C2	2.26	114.59	108.64
23	B	602	CLA	C11-C10-C8	-2.26	108.60	115.92
23	C	512	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
23	B	615	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
24	A	408	BCR	C8-C7-C6	-2.26	120.85	127.20
23	A	404[B]	CLA	CHB-C1B-C2B	-2.26	120.85	127.24
24	C	516	BCR	C40-C30-C25	-2.26	106.63	110.30
23	b	603	CLA	C5-C3-C2	-2.26	116.54	121.12
35	C	519[A]	DGD	O2G-C1B-O1B	-2.26	118.24	123.70
23	B	610	CLA	CMA-C3A-C2A	-2.26	104.71	113.83
23	c	511	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
23	b	611	CLA	CBC-CAC-C3C	-2.26	106.20	112.43
33	B	621	LMG	C12-C11-C10	-2.26	105.41	113.62
26	F	103	SQD	C46-C45-C44	-2.26	106.45	111.79
37	a	408[B]	PHO	CBA-CAA-C2A	-2.26	107.22	113.81
23	b	615	CLA	C1-C2-C3	-2.26	122.14	126.04
23	C	510	CLA	CMC-C2C-C1C	2.25	128.47	125.04
24	b	619	BCR	C38-C26-C25	-2.25	122.00	124.53
23	b	601	CLA	CAA-C2A-C3A	-2.25	106.60	112.78
23	c	507	CLA	CHD-C4C-NC	2.25	127.76	124.20
33	d	409	LMG	O8-C28-C29	2.25	118.98	111.91
37	D	401[A]	PHO	C4-C3-C5	2.25	119.06	115.27
23	B	606	CLA	C4-C3-C5	2.25	119.06	115.27
23	c	506	CLA	C1-C2-C3	-2.25	122.15	126.04
23	D	404[A]	CLA	CED-O2D-CGD	2.25	121.03	115.94
23	C	511	CLA	CAC-C3C-C4C	2.25	127.73	124.81
23	C	514	CLA	CAC-C3C-C4C	2.25	127.73	124.81
23	C	505	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
37	a	408[A]	PHO	CMA-C3A-C4A	-2.25	109.45	114.38
40	v	201	HEC	C1D-C2D-C3D	-2.25	104.59	106.96
23	a	406[A]	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
23	C	505	CLA	C3B-C4B-NB	2.25	112.60	110.52
23	A	405[B]	CLA	C1-C2-C3	-2.25	122.15	126.04
35	C	518[B]	DGD	O1G-C1A-C2A	2.25	118.96	111.91
23	B	612	CLA	C4-C3-C5	2.25	119.05	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	630	LMT	O5B-C5B-C6B	2.25	112.02	106.44
24	a	410	BCR	C38-C26-C27	2.25	117.93	113.62
33	C	526	LMG	C1-O6-C5	2.25	118.09	113.69
35	c	517[A]	DGD	O3G-C3G-C2G	-2.24	105.48	110.90
23	b	610	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
23	B	601	CLA	CHB-C4A-NA	2.24	127.61	124.51
28	d	404[A]	PL9	C47-C48-C49	-2.24	120.08	127.75
23	B	616	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
31	B	628	LMT	C1B-C2B-C3B	2.24	114.66	110.00
33	d	409	LMG	O7-C10-O9	-2.24	118.29	123.70
23	c	502	CLA	CHD-C4C-NC	2.24	127.73	124.20
23	c	507	CLA	CMB-C2B-C1B	2.24	128.78	125.37
26	f	102	SQD	C44-O6-C1	-2.24	109.37	113.74
28	A	412[B]	PL9	C35-C34-C33	-2.24	117.94	123.68
23	B	612	CLA	CMB-C2B-C1B	2.24	128.77	125.37
32	E	101[B]	LHG	C5-O7-C7	-2.23	112.29	117.79
23	b	605	CLA	OBD-CAD-C3D	-2.23	123.14	128.52
23	B	609	CLA	C2A-C1A-CHA	-2.23	119.95	123.86
23	C	511	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
38	F	102	HEM	CHA-C1A-NA	2.23	127.95	123.85
28	a	414[A]	PL9	C35-C34-C33	-2.23	117.95	123.68
33	C	502	LMG	C9-C8-C7	-2.23	106.51	111.79
23	B	604	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
23	c	505	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
23	B	606	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
23	c	503	CLA	CAC-C3C-C4C	2.23	127.70	124.81
24	h	101	BCR	C36-C18-C17	-2.23	119.80	122.92
23	b	602	CLA	C4-C3-C5	2.23	119.02	115.27
37	a	416[B]	PHO	O2A-CGA-O1A	-2.23	117.97	123.59
31	t	101	LMT	O5'-C5'-C4'	2.23	114.45	109.75
24	y	101	BCR	C37-C22-C23	2.23	121.59	118.08
35	C	520	DGD	O1G-C1A-O1A	-2.23	117.97	123.59
35	H	102	DGD	O6E-C5E-C6E	2.23	111.98	106.44
35	h	102	DGD	C3B-C2B-C1B	-2.23	105.52	113.62
28	A	412[A]	PL9	C25-C24-C26	2.23	119.02	115.27
32	D	408[B]	LHG	C5-O7-C7	-2.23	112.31	117.79
33	C	502	LMG	C12-C11-C10	-2.23	105.52	113.62
23	b	615	CLA	C2A-C1A-CHA	-2.23	119.97	123.86
28	A	412[A]	PL9	C12-C13-C14	-2.23	122.30	127.66
34	B	622	HTG	C2'-C1'-S1	-2.22	105.21	112.40
31	A	415	LMT	O1'-C1'-C2'	2.22	111.78	108.30
23	A	405[B]	CLA	O2A-CGA-CBA	2.22	118.89	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D	402[A]	PHO	CED-O2D-CGD	2.22	120.97	115.94
28	A	412[A]	PL9	C53-C6-C1	2.22	119.54	114.99
26	C	501[A]	SQD	O9-S-O7	-2.22	106.25	113.95
23	A	404[A]	CLA	CHD-C4C-NC	2.22	127.71	124.20
23	b	606	CLA	CBC-CAC-C3C	-2.22	106.30	112.43
37	a	416[A]	PHO	O1D-CGD-CBD	-2.22	121.04	124.74
23	A	405[A]	CLA	C4C-C3C-C2C	-2.22	103.66	106.90
23	B	613	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
33	B	621	LMG	C8-O7-C10	-2.22	112.32	117.79
32	d	405[A]	LHG	O8-C23-O10	-2.22	117.99	123.59
23	b	603	CLA	CMB-C2B-C1B	2.22	128.75	125.37
23	c	504	CLA	O2A-CGA-CBA	2.22	118.86	111.91
23	a	409	CLA	CHC-C1C-C2C	-2.22	120.58	126.73
23	C	505	CLA	CAC-C3C-C4C	2.22	127.68	124.81
23	a	406[B]	CLA	CMA-C3A-C2A	-2.21	104.89	113.83
23	C	507	CLA	C11-C10-C8	-2.21	108.76	115.92
23	c	509	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
28	a	414[B]	PL9	C51-C49-C50	2.21	119.49	114.60
23	D	404[A]	CLA	CMA-C3A-C4A	-2.21	105.82	111.77
31	A	417	LMT	O5'-C5'-C4'	2.21	114.42	109.75
24	y	101	BCR	C34-C9-C10	-2.21	119.82	122.92
23	B	605	CLA	CMC-C2C-C1C	2.21	128.40	125.04
23	C	505	CLA	CMC-C2C-C1C	2.21	128.40	125.04
23	A	405[B]	CLA	C4C-C3C-C2C	-2.21	103.68	106.90
24	B	617	BCR	C21-C20-C19	-2.21	116.33	123.22
32	E	101[A]	LHG	O7-C7-O9	-2.21	118.37	123.70
23	d	401[B]	CLA	CAA-C2A-C3A	-2.21	106.74	112.78
23	c	505	CLA	O2A-CGA-CBA	2.21	118.83	111.91
23	c	514	CLA	C4-C3-C5	2.21	118.98	115.27
23	B	613	CLA	C4-C3-C2	-2.20	118.02	123.68
23	B	602	CLA	CAA-CBA-CGA	-2.20	106.82	113.25
23	c	508	CLA	OBD-CAD-C3D	-2.20	123.22	128.52
35	C	518[A]	DGD	O3G-C3G-C2G	-2.20	105.59	110.90
35	C	518[B]	DGD	C3G-C2G-C1G	-2.20	106.58	111.79
35	H	102	DGD	C3G-C2G-C1G	-2.20	106.58	111.79
26	a	411[A]	SQD	O9-S-O7	-2.20	106.34	113.95
24	H	101	BCR	C31-C1-C6	-2.20	106.73	110.30
34	B	622	HTG	O5-C5-C6	2.20	111.90	106.44
23	d	401[B]	CLA	CHD-C4C-NC	2.20	127.67	124.20
28	A	412[B]	PL9	C47-C48-C49	-2.20	120.24	127.75
38	f	101	HEM	CMD-C2D-C1D	2.20	128.38	125.04
23	C	512	CLA	C4C-C3C-C2C	-2.19	103.70	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	CMA-C3A-C2A	-2.19	104.98	113.83
23	C	514	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
23	A	407	CLA	C11-C12-C13	-2.19	108.83	115.92
23	B	603	CLA	CMC-C2C-C1C	2.19	128.38	125.04
35	c	518[A]	DGD	O1G-C1A-O1A	-2.19	118.06	123.59
23	b	601	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
24	h	101	BCR	C36-C18-C19	2.19	121.53	118.08
24	k	101	BCR	C34-C9-C8	2.19	121.53	118.08
32	l	802[B]	LHG	O7-C7-O9	-2.19	118.40	123.70
23	B	609	CLA	CHA-C1A-NA	-2.19	121.38	126.40
24	B	619	BCR	C39-C30-C25	-2.19	106.74	110.30
23	B	616	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
23	C	510	CLA	O2A-CGA-CBA	2.19	118.78	111.91
23	B	601	CLA	C4-C3-C5	2.19	118.96	115.27
23	c	512	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
24	y	101	BCR	C10-C11-C12	-2.19	116.39	123.22
24	B	618	BCR	C36-C18-C17	-2.19	119.86	122.92
37	a	416[A]	PHO	C4-C3-C2	-2.19	118.07	123.68
31	T	101	LMT	C3B-C4B-C5B	-2.18	106.34	110.24
23	A	407	CLA	CMC-C2C-C1C	2.18	128.36	125.04
33	c	521	LMG	O8-C28-O10	-2.18	118.08	123.59
23	B	614	CLA	OBD-CAD-C3D	-2.18	123.27	128.52
23	c	506	CLA	C4-C3-C5	2.18	118.94	115.27
32	l	802[B]	LHG	C5-O7-C7	-2.18	112.42	117.79
24	t	103	BCR	C7-C6-C5	-2.18	116.18	121.46
26	a	411[B]	SQD	O8-S-C6	2.18	109.21	105.74
34	b	622	HTG	C6-C5-C4	-2.18	107.90	113.00
23	c	507	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
24	A	408	BCR	C31-C1-C6	-2.18	106.77	110.30
23	C	514	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
24	C	516	BCR	C29-C30-C25	2.18	113.83	110.48
24	a	410	BCR	C40-C30-C25	-2.17	106.77	110.30
23	a	406[B]	CLA	CAC-C3C-C2C	2.17	131.25	127.53
24	T	102	BCR	C21-C20-C19	-2.17	116.44	123.22
23	a	407[A]	CLA	C4-C3-C5	2.17	118.92	115.27
32	L	101[B]	LHG	O8-C23-O10	-2.17	118.11	123.59
33	D	413	LMG	O7-C10-O9	-2.17	118.45	123.70
23	b	603	CLA	CMC-C2C-C1C	2.17	128.35	125.04
24	C	517	BCR	C38-C26-C25	-2.17	122.09	124.53
23	c	506	CLA	CHD-C4C-NC	2.17	127.62	124.20
32	A	416[A]	LHG	O4-P-O5	2.17	122.96	112.24
23	A	405[B]	CLA	CHB-C4A-NA	2.17	127.51	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	O2A-CGA-CBA	2.17	118.71	111.91
23	A	406[B]	CLA	CHB-C1B-C2B	-2.17	121.11	127.24
38	F	102	HEM	O2D-CGD-CBD	2.17	120.99	114.03
23	C	507	CLA	CHA-C1A-NA	-2.17	121.43	126.40
23	B	613	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
23	b	608	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
23	C	504	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
28	D	407[B]	PL9	C30-C29-C31	2.17	118.91	115.27
23	c	512	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
24	b	617	BCR	C16-C17-C18	-2.17	124.22	127.31
23	b	610	CLA	C3B-C4B-NB	2.16	112.52	110.52
28	a	414[A]	PL9	C45-C44-C46	2.16	118.91	115.27
33	C	502	LMG	C1-O6-C5	-2.16	109.44	113.69
23	A	405[B]	CLA	CED-O2D-CGD	2.16	120.83	115.94
23	B	614	CLA	CMB-C2B-C1B	2.16	128.66	125.37
23	C	510	CLA	CHB-C1B-NB	-2.16	121.97	124.26
23	c	510	CLA	C4-C3-C2	-2.16	118.13	123.68
23	C	506	CLA	C4-C3-C5	2.16	118.91	115.27
23	B	606	CLA	CAC-C3C-C4C	2.16	127.61	124.81
23	A	405[A]	CLA	O2A-CGA-CBA	2.16	118.68	111.91
23	c	504	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
37	a	408[A]	PHO	O2D-CGD-O1D	-2.16	119.62	123.84
23	c	510	CLA	CMC-C2C-C1C	2.16	128.32	125.04
24	Y	101	BCR	C7-C6-C5	-2.16	116.24	121.46
28	a	414[B]	PL9	C47-C48-C49	-2.15	120.39	127.75
26	a	412	SQD	O48-C23-O10	-2.15	118.16	123.59
23	a	405[B]	CLA	CMA-C3A-C2A	-2.15	105.15	113.83
23	C	505	CLA	O2A-CGA-CBA	2.15	118.66	111.91
23	B	611	CLA	OBD-CAD-C3D	-2.15	123.34	128.52
24	d	403	BCR	C40-C30-C39	2.15	115.13	108.53
28	D	407[A]	PL9	C12-C13-C14	-2.15	122.48	127.66
23	a	406[B]	CLA	C1-O2A-CGA	2.15	122.08	116.44
32	d	411[A]	LHG	O7-C7-O9	-2.15	118.51	123.70
23	a	405[B]	CLA	CAA-CBA-CGA	-2.15	106.97	113.25
33	d	409	LMG	O8-C28-O10	-2.15	118.17	123.59
33	C	522	LMG	C9-C8-C7	-2.15	106.71	111.79
34	b	623	HTG	O5-C5-C6	2.15	111.78	106.44
32	D	408[B]	LHG	O7-C7-O9	-2.15	118.51	123.70
23	B	603	CLA	OBD-CAD-C3D	-2.15	123.35	128.52
24	b	619	BCR	C21-C20-C19	-2.15	116.52	123.22
34	d	408	HTG	C4-C3-C2	-2.15	107.08	110.82
24	a	410	BCR	C8-C7-C6	-2.15	121.18	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	404[B]	PL9	C36-C34-C33	-2.15	116.78	121.12
23	B	609	CLA	C1-C2-C3	-2.15	122.33	126.04
23	c	513	CLA	OBD-CAD-C3D	-2.14	123.36	128.52
28	A	412[B]	PL9	C51-C49-C50	2.14	119.34	114.60
23	b	605	CLA	C1-O2A-CGA	2.14	122.07	116.44
23	b	614	CLA	CED-O2D-CGD	2.14	120.78	115.94
28	d	404[A]	PL9	C45-C44-C46	2.14	118.87	115.27
23	D	404[A]	CLA	OBD-CAD-C3D	-2.14	123.37	128.52
24	D	406	BCR	C3-C4-C5	-2.14	110.25	114.08
23	C	509	CLA	C3B-C4B-NB	2.14	112.50	110.52
37	D	402[B]	PHO	CMA-C3A-C4A	-2.14	109.69	114.38
26	f	102	SQD	O48-C23-O10	-2.14	118.19	123.59
23	B	615	CLA	CAC-C3C-C4C	2.14	127.59	124.81
23	c	506	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
24	H	101	BCR	C11-C10-C9	-2.14	124.26	127.31
23	B	612	CLA	CHB-C1B-NB	-2.14	121.99	124.26
23	b	614	CLA	CMA-C3A-C2A	-2.14	105.20	113.83
26	C	501[B]	SQD	O6-C44-C45	-2.14	105.74	110.90
23	B	613	CLA	C7-C6-C5	-2.14	107.56	113.36
23	c	511	CLA	C11-C10-C8	-2.14	109.01	115.92
23	C	514	CLA	CBA-CAA-C2A	-2.14	107.56	113.86
23	b	606	CLA	CHB-C1B-C2B	-2.14	121.20	127.24
24	K	102	BCR	C16-C17-C18	-2.13	124.26	127.31
35	H	102	DGD	C3B-C2B-C1B	-2.13	105.86	113.62
23	C	512	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
23	B	616	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
23	B	615	CLA	O2A-CGA-CBA	2.13	118.60	111.91
24	c	515	BCR	C31-C1-C6	-2.13	106.84	110.30
35	C	519[B]	DGD	C6D-C5D-C4D	2.13	116.54	112.09
31	t	102	LMT	C1-O1'-C1'	2.13	117.38	113.84
34	B	622	HTG	O2-C2-C3	-2.13	105.42	110.35
23	C	515	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
24	C	517	BCR	C24-C23-C22	-2.13	123.02	126.23
35	c	517[A]	DGD	O6D-C1D-O3G	-2.13	104.93	109.97
23	A	406[A]	CLA	CHB-C4A-NA	2.13	127.46	124.51
23	b	607	CLA	CAA-CBA-CGA	2.13	119.48	113.25
23	B	602	CLA	CMA-C3A-C2A	-2.13	105.24	113.83
35	C	518[A]	DGD	O5D-C6D-C5D	-2.13	105.11	109.05
37	a	416[B]	PHO	C4-C3-C2	-2.13	118.22	123.68
32	d	405[A]	LHG	O8-C23-C24	2.13	118.59	111.91
24	K	102	BCR	C10-C11-C12	-2.13	116.58	123.22
23	B	606	CLA	CHB-C1B-C2B	-2.13	121.23	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D	402[B]	PHO	O2A-CGA-CBA	2.13	118.58	111.91
23	c	512	CLA	O2A-CGA-CBA	2.13	118.58	111.91
23	B	608	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
23	a	407[A]	CLA	CBC-CAC-C3C	-2.12	106.57	112.43
23	B	611	CLA	C7-C6-C5	-2.12	107.59	113.36
23	C	514	CLA	CHB-C1B-C2B	-2.12	121.24	127.24
23	d	401[A]	CLA	CHD-C4C-NC	2.12	127.55	124.20
23	b	613	CLA	CAC-C3C-C4C	2.12	127.56	124.81
23	A	405[B]	CLA	CAC-C3C-C4C	2.12	127.56	124.81
24	a	410	BCR	C37-C22-C21	-2.12	119.95	122.92
23	A	405[A]	CLA	CHB-C4A-NA	2.12	127.44	124.51
26	F	103	SQD	C3-C4-C5	2.12	114.02	110.24
23	c	512	CLA	O2A-C1-C2	-2.12	103.06	108.64
23	b	604	CLA	CHA-C1A-NA	-2.12	121.54	126.40
23	A	404[B]	CLA	CMA-C3A-C2A	-2.12	105.28	113.83
24	T	102	BCR	C7-C6-C5	-2.12	116.33	121.46
23	D	405	CLA	CHD-C4C-NC	2.12	127.54	124.20
33	C	526	LMG	C9-C8-C7	-2.12	106.78	111.79
24	D	406	BCR	C36-C18-C17	-2.12	119.96	122.92
24	a	410	BCR	C24-C23-C22	-2.12	123.04	126.23
28	D	407[B]	PL9	C7-C3-C2	-2.12	120.52	123.30
23	c	502	CLA	O2A-CGA-CBA	2.11	118.54	111.91
35	c	517[A]	DGD	O1G-C1A-O1A	-2.11	118.26	123.59
23	a	406[A]	CLA	CHB-C4A-NA	2.11	127.43	124.51
28	A	412[B]	PL9	C25-C24-C26	2.11	118.82	115.27
24	c	516	BCR	C15-C16-C17	-2.11	119.15	123.47
23	d	401[A]	CLA	CMA-C3A-C2A	-2.11	105.31	113.83
35	C	519[A]	DGD	O1G-C1A-C2A	2.11	118.53	111.91
26	b	620	SQD	C1-C2-C3	-2.11	105.60	110.00
26	a	411[A]	SQD	C3-C4-C5	2.11	114.00	110.24
23	b	615	CLA	CHA-C1A-NA	-2.11	121.57	126.40
40	V	202	HEC	CBA-CAA-C2A	-2.11	106.77	112.63
24	B	619	BCR	C31-C1-C6	-2.11	106.88	110.30
23	B	615	CLA	C1-O2A-CGA	2.11	121.97	116.44
31	b	621	LMT	C2'-C3'-C4'	2.11	114.49	109.68
23	B	604	CLA	CHA-C1A-NA	-2.11	121.58	126.40
24	b	618	BCR	C2-C1-C6	2.11	113.72	110.48
23	b	602	CLA	O2A-CGA-CBA	2.10	118.51	111.91
28	d	404[A]	PL9	C31-C32-C33	-2.10	104.97	111.88
23	B	607	CLA	C6-C7-C8	-2.10	109.12	115.92
23	a	406[A]	CLA	CAC-C3C-C2C	2.10	131.13	127.53
31	F	101	LMT	C2'-C3'-C4'	2.10	114.49	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	CBC-CAC-C3C	-2.10	106.63	112.43
28	a	414[A]	PL9	C51-C49-C50	2.10	119.25	114.60
23	A	404[A]	CLA	C7-C6-C5	-2.10	107.65	113.36
23	C	508	CLA	CED-O2D-CGD	2.10	120.69	115.94
37	D	402[B]	PHO	CMB-C2B-C3B	2.10	128.61	124.68
23	b	610	CLA	CAC-C3C-C2C	2.10	131.12	127.53
24	b	618	BCR	C28-C27-C26	-2.10	110.33	114.08
23	B	616	CLA	CMB-C2B-C3B	2.10	131.67	126.59
23	c	509	CLA	CHA-C1A-NA	-2.10	121.60	126.40
35	c	519	DGD	C6B-C5B-C4B	-2.10	103.78	114.42
23	C	511	CLA	C11-C12-C13	-2.10	109.14	115.92
31	b	627	LMT	C1'-O5'-C5'	-2.10	109.58	113.69
32	L	101[B]	LHG	C5-O7-C7	-2.10	112.63	117.79
24	Y	101	BCR	C39-C30-C25	-2.09	106.90	110.30
26	b	620	SQD	C4-C3-C2	2.09	114.48	110.82
28	A	412[A]	PL9	C51-C49-C50	2.09	119.22	114.60
23	C	509	CLA	CAC-C3C-C4C	2.09	127.53	124.81
24	C	517	BCR	C2-C1-C6	2.09	113.70	110.48
37	a	408[B]	PHO	CBC-CAC-C3C	-2.09	109.82	112.88
23	B	603	CLA	C6-C7-C8	-2.09	109.16	115.92
24	c	516	BCR	C38-C26-C25	-2.09	122.18	124.53
23	B	603	CLA	C5-C3-C2	-2.09	116.89	121.12
24	c	516	BCR	C15-C14-C13	-2.09	124.33	127.31
24	H	101	BCR	C24-C23-C22	-2.09	123.08	126.23
26	f	102	SQD	O6-C1-C2	2.09	111.56	108.30
23	C	509	CLA	C6-C7-C8	-2.09	109.17	115.92
23	a	405[B]	CLA	CHB-C4A-NA	2.09	127.40	124.51
37	D	402[A]	PHO	OBD-CAD-C3D	-2.09	124.52	127.98
28	a	414[B]	PL9	C35-C34-C33	-2.09	118.33	123.68
23	a	407[A]	CLA	CAC-C3C-C4C	2.08	127.52	124.81
23	b	608	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
23	a	406[A]	CLA	CHB-C1B-NB	-2.08	122.05	124.26
33	C	526	LMG	C3-C4-C5	2.08	113.95	110.24
28	d	404[B]	PL9	C7-C3-C2	-2.08	120.56	123.30
23	b	606	CLA	C4-C3-C2	-2.08	118.34	123.68
24	b	618	BCR	C8-C7-C6	-2.08	121.36	127.20
28	A	412[B]	PL9	C37-C36-C34	-2.08	106.13	112.98
28	d	404[B]	PL9	C35-C34-C36	2.08	118.77	115.27
26	C	501[B]	SQD	O48-C23-O10	-2.08	118.34	123.59
23	c	513	CLA	C3B-C4B-NB	2.08	112.44	110.52
35	c	517[B]	DGD	O6D-C1D-O3G	-2.08	105.05	109.97
23	d	401[B]	CLA	CMC-C2C-C1C	2.08	128.20	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	412[A]	PL9	C10-C9-C11	2.08	118.77	115.27
24	B	619	BCR	C29-C30-C25	2.08	113.68	110.48
24	b	618	BCR	C15-C16-C17	-2.08	119.22	123.47
23	c	508	CLA	CHA-C1A-NA	-2.08	121.64	126.40
23	B	612	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
23	B	613	CLA	CMA-C3A-C4A	-2.08	106.19	111.77
23	C	509	CLA	CHA-C1A-NA	-2.08	121.64	126.40
33	c	520	LMG	O7-C10-O9	-2.08	118.69	123.70
23	D	404[A]	CLA	CBC-CAC-C3C	-2.07	106.71	112.43
40	v	201	HEC	C4B-NB-C1B	2.07	107.22	105.07
35	c	518[B]	DGD	C2G-O2G-C1B	-2.07	112.69	117.79
24	K	102	BCR	C33-C5-C6	-2.07	122.20	124.53
23	a	405[B]	CLA	CBB-CAB-C3B	-2.07	117.31	127.62
23	B	612	CLA	OBD-CAD-C3D	-2.07	123.53	128.52
23	d	402	CLA	C1-O2A-CGA	2.07	121.88	116.44
23	b	602	CLA	C11-C10-C8	-2.07	109.22	115.92
23	b	611	CLA	C7-C6-C5	-2.07	107.73	113.36
28	d	404[A]	PL9	C40-C39-C38	-2.07	118.37	123.68
23	B	610	CLA	C1-C2-C3	-2.07	122.46	126.04
23	d	401[A]	CLA	CBB-CAB-C3B	-2.07	117.32	127.62
23	b	606	CLA	CMA-C3A-C2A	-2.07	105.48	113.83
34	c	522	HTG	C1-O5-C5	2.07	116.40	112.58
23	B	606	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
24	B	619	BCR	C10-C11-C12	-2.07	116.77	123.22
23	A	407	CLA	CMA-C3A-C4A	-2.07	106.22	111.77
32	d	406[B]	LHG	C5-O7-C7	-2.07	112.70	117.79
23	B	615	CLA	CHA-C1A-NA	-2.07	121.67	126.40
33	a	417	LMG	O7-C10-O9	-2.07	118.71	123.70
23	B	616	CLA	C4-C3-C2	-2.06	118.38	123.68
24	d	403	BCR	C29-C28-C27	-2.06	106.76	111.38
23	C	515	CLA	CAC-C3C-C4C	2.06	127.49	124.81
23	b	615	CLA	C11-C12-C13	-2.06	109.25	115.92
35	c	519	DGD	O4D-C4D-C3D	-2.06	105.58	110.35
24	T	102	BCR	C1-C6-C7	2.06	121.61	115.78
23	B	602	CLA	CMB-C2B-C1B	2.06	128.51	125.37
24	h	101	BCR	C10-C11-C12	-2.06	116.78	123.22
23	c	505	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
23	A	405[B]	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
28	d	404[B]	PL9	C31-C32-C33	-2.06	105.11	111.88
23	d	401[A]	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
23	B	615	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
24	D	406	BCR	C29-C28-C27	-2.06	106.78	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	c	517[B]	DGD	O1G-C1A-C2A	2.06	118.37	111.91
23	B	608	CLA	C6-C7-C8	-2.06	109.27	115.92
24	C	517	BCR	C37-C22-C23	2.06	121.32	118.08
28	D	407[A]	PL9	C27-C28-C29	-2.06	122.71	127.66
24	t	103	BCR	C37-C22-C23	2.06	121.32	118.08
24	a	410	BCR	C33-C5-C6	-2.06	122.22	124.53
24	t	103	BCR	C15-C16-C17	-2.06	119.26	123.47
23	B	606	CLA	C7-C6-C5	-2.06	107.78	113.36
23	D	405	CLA	CHB-C4A-NA	2.06	127.35	124.51
23	c	507	CLA	CAA-CBA-CGA	2.05	119.25	113.25
28	d	404[A]	PL9	O2-C1-C6	-2.05	117.04	120.59
23	c	505	CLA	OBD-CAD-C3D	-2.05	123.58	128.52
33	z	101	LMG	O8-C28-O10	-2.05	118.41	123.59
23	b	614	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
23	C	512	CLA	CAC-C3C-C4C	2.05	127.47	124.81
26	B	620	SQD	C44-O6-C1	-2.05	109.73	113.74
23	b	616	CLA	C11-C12-C13	-2.05	109.29	115.92
37	D	402[A]	PHO	O1D-CGD-CBD	-2.05	121.33	124.74
28	D	407[A]	PL9	C45-C44-C46	2.05	118.72	115.27
31	M	101	LMT	O6'-C6'-C5'	-2.05	104.26	111.29
24	Y	101	BCR	C37-C22-C21	-2.05	120.05	122.92
23	C	510	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
32	L	101[A]	LHG	O4-P-O5	2.05	122.36	112.24
33	a	417	LMG	O6-C5-C4	2.05	113.41	109.69
23	B	610	CLA	CMC-C2C-C1C	2.05	128.16	125.04
23	a	405[A]	CLA	CMB-C2B-C3B	2.05	131.54	126.59
23	A	406[A]	CLA	CBC-CAC-C3C	-2.04	106.79	112.43
24	d	403	BCR	C3-C4-C5	-2.04	110.43	114.08
23	c	511	CLA	OBD-CAD-C3D	-2.04	123.60	128.52
33	a	417	LMG	O8-C28-C29	2.04	118.32	111.91
24	c	516	BCR	C39-C30-C25	-2.04	106.99	110.30
23	D	404[B]	CLA	CBB-CAB-C3B	-2.04	117.46	127.62
33	d	409	LMG	O3-C3-C2	-2.04	105.63	110.35
37	a	416[A]	PHO	O2A-CGA-O1A	-2.04	118.44	123.59
38	F	102	HEM	C4D-ND-C1D	2.04	107.18	105.07
34	b	622	HTG	C3-C4-C5	2.04	113.88	110.24
37	a	408[A]	PHO	C1-C2-C3	-2.04	122.51	126.04
33	m	101	LMG	C3-C4-C5	2.04	113.88	110.24
32	l	802[A]	LHG	O7-C7-O9	-2.04	118.77	123.70
23	c	506	CLA	C1-O2A-CGA	2.04	121.79	116.44
35	c	518[B]	DGD	O1G-C1A-O1A	-2.04	118.45	123.59
24	Y	101	BCR	C15-C16-C17	-2.04	119.30	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407[B]	CLA	CHB-C1B-C2B	-2.04	121.48	127.24
24	D	406	BCR	C30-C25-C24	2.04	121.54	115.78
34	b	625	HTG	C1-C2-C3	-2.03	106.58	110.59
28	D	407[A]	PL9	C47-C48-C49	-2.03	120.81	127.75
28	D	407[A]	PL9	C21-C22-C23	-2.03	105.21	111.88
35	c	518[B]	DGD	C1D-O6D-C5D	2.03	117.67	113.69
37	a	408[B]	PHO	C1-C2-C3	-2.03	122.53	126.04
23	B	612	CLA	CHD-C4C-NC	2.03	127.40	124.20
23	b	609	CLA	CGD-CBD-CAD	-2.03	104.16	110.73
25	B	624	GOL	C3-C2-C1	-2.03	103.82	111.70
23	c	513	CLA	CHA-C1A-NA	-2.03	121.75	126.40
24	c	515	BCR	C21-C20-C19	-2.03	116.89	123.22
33	C	502	LMG	O8-C28-C29	2.03	118.27	111.91
24	H	101	BCR	C37-C22-C23	2.03	121.27	118.08
33	m	101	LMG	O1-C7-C8	-2.03	106.01	110.90
23	B	616	CLA	OBD-CAD-C3D	-2.02	123.65	128.52
28	a	414[B]	PL9	C12-C13-C14	-2.02	122.78	127.66
23	c	509	CLA	CAC-C3C-C4C	2.02	127.44	124.81
31	m	103	LMT	O5B-C5B-C6B	2.02	111.47	106.44
23	C	511	CLA	CMB-C2B-C3B	2.02	131.48	126.59
23	a	407[A]	CLA	CHA-C1A-NA	-2.02	121.77	126.40
23	B	601	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
35	H	102	DGD	C1E-O6E-C5E	-2.02	109.72	113.69
23	b	601	CLA	CMC-C2C-C1C	2.02	128.11	125.04
26	F	103	SQD	O5-C1-C2	-2.02	106.08	110.35
24	b	619	BCR	C1-C6-C5	-2.02	119.77	122.61
26	a	411[A]	SQD	O4-C4-C3	-2.02	105.68	110.35
23	C	506	CLA	CHD-C4C-NC	2.02	127.38	124.20
23	b	613	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
24	B	618	BCR	C37-C22-C21	-2.01	120.10	122.92
34	b	623	HTG	C1-C2-C3	2.01	114.57	110.59
24	A	408	BCR	C11-C10-C9	-2.01	124.44	127.31
35	c	517[A]	DGD	O1G-C1A-C2A	2.01	118.23	111.91
23	B	604	CLA	CHC-C4B-NB	2.01	126.39	124.26
23	C	510	CLA	CHB-C4A-NA	2.01	127.30	124.51
23	b	604	CLA	C1-O2A-CGA	2.01	121.72	116.44
23	c	510	CLA	CHB-C4A-NA	2.01	127.29	124.51
23	c	510	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
23	d	402	CLA	C6-C7-C8	-2.01	109.42	115.92
26	B	620	SQD	O9-S-O7	-2.01	107.00	113.95
24	D	406	BCR	C40-C30-C39	2.01	114.69	108.53
23	b	605	CLA	C6-C7-C8	-2.01	109.43	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	f	101	HEM	O2A-CGA-CBA	2.01	120.48	114.03
23	C	514	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
34	b	625	HTG	O5-C1-S1	-2.01	105.03	109.82
23	b	607	CLA	CMB-C2B-C1B	2.01	128.42	125.37
23	b	613	CLA	C16-C15-C13	-2.00	109.44	115.92
23	C	506	CLA	OBD-CAD-C3D	-2.00	123.70	128.52
35	C	519[B]	DGD	O2G-C1B-O1B	-2.00	118.86	123.70
25	O	303	GOL	C3-C2-C1	-2.00	103.91	111.70
37	D	402[A]	PHO	CMB-C2B-C3B	2.00	128.43	124.68
23	a	405[B]	CLA	CHC-C1C-NC	2.00	127.24	124.20
23	C	505	CLA	C2A-C1A-CHA	-2.00	120.36	123.86
23	a	407[B]	CLA	CHB-C4A-NA	2.00	127.28	124.51
23	B	608	CLA	C16-C15-C13	-2.00	109.44	115.92
23	b	616	CLA	C1-C2-C3	-2.00	122.58	126.04
38	F	102	HEM	O2A-CGA-O1A	-2.00	118.31	123.30
35	C	518[A]	DGD	C4E-C3E-C2E	-2.00	107.33	110.82
33	c	520	LMG	O8-C28-O10	-2.00	118.54	123.59
35	C	518[B]	DGD	O6E-C5E-C4E	2.00	113.33	109.69
37	a	416[B]	PHO	C4D-CHA-CBD	2.00	109.42	108.52

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	202	HEC	NA
40	v	201	HEC	NA

All (1722) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	404[B]	CLA	C2B-C3B-CAB-CBB
23	A	404[B]	CLA	C4B-C3B-CAB-CBB
23	A	407	CLA	C2-C3-C5-C6
23	A	407	CLA	C4-C3-C5-C6
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	506	CLA	C2-C3-C5-C6
23	C	506	CLA	C4-C3-C5-C6
23	C	509	CLA	C2B-C3B-CAB-CBB
23	C	509	CLA	C4B-C3B-CAB-CBB
23	C	509	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	C	510	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O2D
23	a	405[B]	CLA	C2B-C3B-CAB-CBB
23	a	405[B]	CLA	C4B-C3B-CAB-CBB
23	a	407[B]	CLA	C2B-C3B-CAB-CBB
23	a	407[B]	CLA	C4B-C3B-CAB-CBB
23	a	409	CLA	C2-C3-C5-C6
23	a	409	CLA	C4-C3-C5-C6
23	b	604	CLA	C6-C7-C8-C9
23	b	605	CLA	C4-C3-C5-C6
23	b	606	CLA	C2B-C3B-CAB-CBB
23	b	606	CLA	C4B-C3B-CAB-CBB
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	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	402	CLA	C2-C3-C5-C6
23	d	402	CLA	C4-C3-C5-C6
24	T	102	BCR	C13-C14-C15-C16
24	Y	101	BCR	C5-C6-C7-C8
24	a	410	BCR	C23-C24-C25-C30
24	b	619	BCR	C5-C6-C7-C8
24	y	101	BCR	C1-C6-C7-C8
24	y	101	BCR	C5-C6-C7-C8
25	A	409	GOL	O1-C1-C2-O2
25	A	409	GOL	O1-C1-C2-C3
25	B	624	GOL	C1-C2-C3-O3
25	B	629	GOL	O1-C1-C2-C3
25	B	629	GOL	C1-C2-C3-O3
25	D	403	GOL	O1-C1-C2-C3
25	D	414	GOL	C1-C2-C3-O3
25	V	204[A]	GOL	C1-C2-C3-O3
25	V	204[B]	GOL	C1-C2-C3-O3
25	a	418	GOL	O1-C1-C2-O2
25	a	418	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	b	624	GOL	C1-C2-C3-O3
25	c	527	GOL	C1-C2-C3-O3
25	c	528	GOL	C1-C2-C3-O3
25	o	302	GOL	C1-C2-C3-O3
25	v	202[B]	GOL	O1-C1-C2-O2
26	A	410	SQD	O6-C44-C45-O47
26	B	620	SQD	O5-C1-O6-C44
26	B	620	SQD	O49-C7-O47-C45
26	B	620	SQD	C8-C7-O47-C45
26	C	501[B]	SQD	C8-C7-O47-C45
26	F	103	SQD	C2-C1-O6-C44
26	F	103	SQD	O49-C7-O47-C45
26	F	103	SQD	C8-C7-O47-C45
26	a	412	SQD	O6-C44-C45-O47
26	a	412	SQD	C5-C6-S-O7
26	a	412	SQD	C5-C6-S-O8
26	a	412	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
28	A	412[A]	PL9	C9-C11-C12-C13
28	A	412[A]	PL9	C15-C14-C16-C17
28	A	412[A]	PL9	C14-C16-C17-C18
28	A	412[B]	PL9	C9-C11-C12-C13
28	A	412[B]	PL9	C14-C16-C17-C18
28	a	414[A]	PL9	C9-C11-C12-C13
28	a	414[A]	PL9	C14-C16-C17-C18
28	a	414[A]	PL9	C23-C24-C26-C27
28	a	414[A]	PL9	C25-C24-C26-C27
28	a	414[B]	PL9	C9-C11-C12-C13
28	a	414[B]	PL9	C14-C16-C17-C18
28	a	414[B]	PL9	C30-C29-C31-C32
31	A	415	LMT	C2'-C1'-O1'-C1
31	A	415	LMT	O5'-C1'-O1'-C1
31	A	417	LMT	C2'-C1'-O1'-C1
31	A	417	LMT	O5'-C1'-O1'-C1
31	A	417	LMT	C2-C1-O1'-C1'
31	B	630	LMT	C2'-C1'-O1'-C1
31	F	101	LMT	C2'-C1'-O1'-C1
31	F	101	LMT	O5'-C1'-O1'-C1
31	T	101	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
31	b	627	LMT	C2'-C1'-O1'-C1
31	b	627	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	C2-C1-O1'-C1'
31	t	102	LMT	O5'-C1'-O1'-C1
31	t	102	LMT	C2-C1-O1'-C1'
32	D	408[A]	LHG	O2-C2-C3-O3
32	D	408[A]	LHG	C3-O3-P-O4
32	D	408[A]	LHG	C3-O3-P-O5
32	D	408[A]	LHG	C3-O3-P-O6
32	D	408[A]	LHG	C4-O6-P-O4
32	D	408[B]	LHG	C3-O3-P-O4
32	D	408[B]	LHG	C4-O6-P-O3
32	D	408[B]	LHG	C4-O6-P-O4
32	D	408[B]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C3-O3-P-O4
32	E	101[A]	LHG	C3-O3-P-O5
32	E	101[A]	LHG	O10-C23-O8-C6
32	E	101[A]	LHG	C24-C23-O8-C6
32	E	101[B]	LHG	C3-O3-P-O4
32	E	101[B]	LHG	C3-O3-P-O5
32	E	101[B]	LHG	C4-O6-P-O3
32	E	101[B]	LHG	C4-O6-P-O5
32	E	101[B]	LHG	O10-C23-O8-C6
32	E	101[B]	LHG	C24-C23-O8-C6
32	L	101[A]	LHG	C4-O6-P-O4
32	L	101[A]	LHG	C4-O6-P-O5
32	L	101[B]	LHG	C4-O6-P-O3
32	L	101[B]	LHG	C4-O6-P-O4
32	L	101[B]	LHG	C4-O6-P-O5
32	a	420[A]	LHG	C3-O3-P-O4
32	a	420[A]	LHG	C4-O6-P-O5
32	a	420[A]	LHG	O10-C23-O8-C6
32	a	420[A]	LHG	C24-C23-O8-C6
32	a	420[B]	LHG	C3-O3-P-O4
32	a	420[B]	LHG	C4-O6-P-O4
32	a	420[B]	LHG	C4-O6-P-O5
32	a	420[B]	LHG	O10-C23-O8-C6
32	a	420[B]	LHG	C24-C23-O8-C6
32	d	405[A]	LHG	C3-O3-P-O4
32	d	405[A]	LHG	C3-O3-P-O5
32	d	405[A]	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
32	d	405[B]	LHG	O2-C2-C3-O3
32	d	405[B]	LHG	C3-O3-P-O4
32	d	405[B]	LHG	C4-O6-P-O4
32	d	411[A]	LHG	C3-O3-P-O5
32	d	411[B]	LHG	C1-C2-C3-O3
32	d	411[B]	LHG	C3-O3-P-O5
32	l	802[A]	LHG	C4-O6-P-O4
32	l	802[A]	LHG	C4-O6-P-O5
32	l	802[B]	LHG	C4-O6-P-O4
32	l	802[B]	LHG	C4-O6-P-O5
33	C	522	LMG	C11-C10-O7-C8
33	C	526	LMG	O9-C10-O7-C8
33	C	526	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	O6-C1-O1-C7
33	z	101	LMG	C11-C10-O7-C8
34	B	622	HTG	C2'-C1'-S1-C1
38	F	102	HEM	C2C-C3C-CAC-CBC
38	F	102	HEM	C4C-C3C-CAC-CBC
38	f	101	HEM	C4C-C3C-CAC-CBC
31	A	417	LMT	O5B-C1B-O1B-C4'
23	D	405	CLA	CBD-CGD-O2D-CED
26	C	501[A]	SQD	O49-C7-O47-C45
26	C	501[B]	SQD	O49-C7-O47-C45
26	b	620	SQD	O49-C7-O47-C45
33	z	101	LMG	O9-C10-O7-C8
23	D	405	CLA	C3-C5-C6-C7
23	c	513	CLA	C3-C5-C6-C7
23	d	402	CLA	C3-C5-C6-C7
31	F	101	LMT	O5'-C5'-C6'-O6'
23	c	505	CLA	C4-C3-C5-C6
28	A	412[A]	PL9	C20-C19-C21-C22
28	A	412[B]	PL9	C30-C29-C31-C32
28	a	414[B]	PL9	C25-C24-C26-C27
31	B	630	LMT	C4'-C5'-C6'-O6'
23	b	605	CLA	C2-C3-C5-C6
23	c	508	CLA	C2-C3-C5-C6
28	A	412[A]	PL9	C18-C19-C21-C22
28	a	414[B]	PL9	C23-C24-C26-C27
28	a	414[B]	PL9	C28-C29-C31-C32
23	B	606	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	B	614	CLA	C3-C5-C6-C7
23	b	616	CLA	C3-C5-C6-C7
23	c	502	CLA	CBD-CGD-O2D-CED
34	B	625	HTG	S1-C1'-C2'-C3'
33	C	522	LMG	O9-C10-O7-C8
31	T	101	LMT	C4B-C5B-C6B-O6B
31	B	630	LMT	O5B-C5B-C6B-O6B
31	B	630	LMT	O5'-C5'-C6'-O6'
31	T	101	LMT	O5'-C5'-C6'-O6'
31	b	621	LMT	O5'-C5'-C6'-O6'
31	c	501	LMT	O5B-C5B-C6B-O6B
23	B	605	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CBD-CGD-O2D-CED
32	d	405[A]	LHG	O2-C2-C3-O3
31	A	417	LMT	O5B-C5B-C6B-O6B
31	b	627	LMT	O5'-C5'-C6'-O6'
33	C	522	LMG	O6-C5-C6-O5
34	D	412	HTG	C4-C5-C6-O6
26	C	501[A]	SQD	C8-C7-O47-C45
23	c	514	CLA	CBD-CGD-O2D-CED
34	D	412	HTG	O5-C5-C6-O6
34	b	625	HTG	O5-C5-C6-O6
31	m	103	LMT	C4B-C5B-C6B-O6B
34	b	625	HTG	S1-C1'-C2'-C3'
31	B	628	LMT	O5B-C5B-C6B-O6B
31	t	101	LMT	O5'-C5'-C6'-O6'
31	T	101	LMT	C4'-C5'-C6'-O6'
31	b	621	LMT	C4'-C5'-C6'-O6'
31	e	101	LMT	C4'-C5'-C6'-O6'
33	B	621	LMG	C39-C40-C41-C42
31	A	417	LMT	O5'-C5'-C6'-O6'
31	T	101	LMT	O5B-C5B-C6B-O6B
23	B	605	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
28	A	412[B]	PL9	C15-C14-C16-C17
28	A	412[B]	PL9	C20-C19-C21-C22
28	a	414[A]	PL9	C15-C14-C16-C17
28	a	414[A]	PL9	C30-C29-C31-C32
28	a	414[B]	PL9	C15-C14-C16-C17
31	B	628	LMT	C4'-C5'-C6'-O6'
23	B	605	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	C	509	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
28	A	412[A]	PL9	C13-C14-C16-C17
28	A	412[B]	PL9	C13-C14-C16-C17
28	A	412[B]	PL9	C18-C19-C21-C22
28	a	414[A]	PL9	C13-C14-C16-C17
28	a	414[A]	PL9	C28-C29-C31-C32
28	a	414[B]	PL9	C13-C14-C16-C17
23	b	606	CLA	C2A-CAA-CBA-CGA
33	c	521	LMG	C4-C5-C6-O5
28	A	412[A]	PL9	C44-C46-C47-C48
28	D	407[A]	PL9	C39-C41-C42-C43
23	a	405[B]	CLA	CBD-CGD-O2D-CED
40	v	201	HEC	C2C-C3C-CAC-CBC
31	B	630	LMT	C4B-C5B-C6B-O6B
31	B	628	LMT	C6-C7-C8-C9
32	d	405[A]	LHG	C1-C2-C3-O3
32	d	405[B]	LHG	C1-C2-C3-O3
23	A	407	CLA	C3-C5-C6-C7
23	c	510	CLA	CBA-CGA-O2A-C1
23	b	614	CLA	C8-C10-C11-C12
23	C	510	CLA	C10-C11-C12-C13
31	F	101	LMT	C4'-C5'-C6'-O6'
31	c	501	LMT	C4B-C5B-C6B-O6B
40	V	202	HEC	C2C-C3C-CAC-CBC
31	b	627	LMT	C4'-C5'-C6'-O6'
31	t	101	LMT	C4'-C5'-C6'-O6'
23	b	611	CLA	C8-C10-C11-C12
31	b	621	LMT	C2'-C1'-O1'-C1
31	t	101	LMT	C2'-C1'-O1'-C1
31	t	102	LMT	C2'-C1'-O1'-C1
31	A	415	LMT	O5B-C5B-C6B-O6B
28	A	412[A]	PL9	C30-C29-C31-C32
23	c	505	CLA	C2-C3-C5-C6
23	B	602	CLA	C6-C7-C8-C9
23	C	508	CLA	C14-C13-C15-C16
23	b	601	CLA	C11-C10-C8-C9
23	b	616	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C12-C13-C14
23	c	513	CLA	C6-C7-C8-C9
23	C	505	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
35	h	102	DGD	C6B-C7B-C8B-C9B
23	B	601	CLA	C10-C11-C12-C13
24	b	619	BCR	C7-C8-C9-C34
24	c	516	BCR	C7-C8-C9-C34
34	b	622	HTG	S1-C1'-C2'-C3'
24	b	619	BCR	C7-C8-C9-C10
31	m	103	LMT	O5B-C5B-C6B-O6B
26	b	620	SQD	C18-C19-C20-C21
31	B	628	LMT	C4B-C5B-C6B-O6B
26	B	620	SQD	C7-C8-C9-C10
32	E	101[A]	LHG	C23-C24-C25-C26
31	B	628	LMT	O5'-C5'-C6'-O6'
31	M	101	LMT	O5'-C5'-C6'-O6'
31	A	417	LMT	C4B-C5B-C6B-O6B
23	A	407	CLA	C5-C6-C7-C8
23	B	615	CLA	C10-C11-C12-C13
23	b	611	CLA	C15-C16-C17-C18
31	B	628	LMT	C5'-C4'-O1B-C1B
23	B	602	CLA	C13-C15-C16-C17
23	B	606	CLA	C10-C11-C12-C13
23	b	601	CLA	C10-C11-C12-C13
23	b	604	CLA	C8-C10-C11-C12
25	O	302	GOL	O1-C1-C2-O2
33	C	526	LMG	C10-C11-C12-C13
35	c	518[A]	DGD	C1B-C2B-C3B-C4B
35	c	518[B]	DGD	C1B-C2B-C3B-C4B
23	B	601	CLA	C5-C6-C7-C8
23	b	614	CLA	C10-C11-C12-C13
26	b	620	SQD	C31-C32-C33-C34
31	c	501	LMT	C4'-C5'-C6'-O6'
32	D	409[A]	LHG	C33-C34-C35-C36
23	c	513	CLA	C15-C16-C17-C18
26	F	103	SQD	C23-C24-C25-C26
32	D	409[B]	LHG	C33-C34-C35-C36
31	e	101	LMT	O5'-C5'-C6'-O6'
23	C	514	CLA	C11-C10-C8-C7
23	b	606	CLA	C12-C13-C15-C16
23	C	513	CLA	C3-C5-C6-C7
23	b	610	CLA	C2A-CAA-CBA-CGA
26	F	103	SQD	O5-C1-O6-C44
31	B	630	LMT	O5'-C1'-O1'-C1
31	b	621	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
31	e	101	LMT	O5'-C1'-O1'-C1
23	a	405[A]	CLA	C15-C16-C17-C18
28	A	412[B]	PL9	C44-C46-C47-C48
28	D	407[B]	PL9	C39-C41-C42-C43
28	d	404[A]	PL9	C39-C41-C42-C43
28	d	404[B]	PL9	C39-C41-C42-C43
33	B	621	LMG	C15-C16-C17-C18
40	V	202	HEC	C4C-C3C-CAC-CBC
23	D	405	CLA	C10-C11-C12-C13
23	c	514	CLA	C10-C11-C12-C13
31	A	415	LMT	O1'-C1-C2-C3
35	C	520	DGD	C6B-C7B-C8B-C9B
23	c	510	CLA	O1A-CGA-O2A-C1
23	A	405[B]	CLA	C15-C16-C17-C18
23	b	604	CLA	C5-C6-C7-C8
23	b	606	CLA	C10-C11-C12-C13
23	b	606	CLA	C13-C15-C16-C17
23	b	606	CLA	C15-C16-C17-C18
23	c	513	CLA	C13-C15-C16-C17
31	c	501	LMT	O1'-C1-C2-C3
31	c	501	LMT	O5'-C5'-C6'-O6'
23	D	405	CLA	O1D-CGD-O2D-CED
33	B	621	LMG	C37-C38-C39-C40
23	C	509	CLA	C5-C6-C7-C8
32	D	408[B]	LHG	C3-O3-P-O6
32	E	101[A]	LHG	C3-O3-P-O6
32	E	101[A]	LHG	C4-O6-P-O3
32	E	101[B]	LHG	C3-O3-P-O6
32	L	101[A]	LHG	C4-O6-P-O3
32	a	420[A]	LHG	C3-O3-P-O6
32	a	420[A]	LHG	C4-O6-P-O3
32	a	420[B]	LHG	C3-O3-P-O6
32	a	420[B]	LHG	C4-O6-P-O3
32	d	405[A]	LHG	C3-O3-P-O6
32	d	405[B]	LHG	C3-O3-P-O6
32	l	802[A]	LHG	C4-O6-P-O3
32	l	802[B]	LHG	C4-O6-P-O3
26	C	501[A]	SQD	C7-C8-C9-C10
32	D	409[B]	LHG	C24-C23-O8-C6
34	B	622	HTG	C1'-C2'-C3'-C4'
34	b	623	HTG	C1'-C2'-C3'-C4'
31	A	417	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
31	t	102	LMT	C11-C10-C9-C8
23	B	614	CLA	C10-C11-C12-C13
33	c	520	LMG	C4-C5-C6-O5
35	c	517[B]	DGD	O6D-C5D-C6D-O5D
31	A	417	LMT	O1'-C1-C2-C3
35	C	520	DGD	C2B-C3B-C4B-C5B
34	D	412	HTG	S1-C1'-C2'-C3'
32	D	408[A]	LHG	C1-C2-C3-O3
23	c	506	CLA	C4-C3-C5-C6
26	C	501[A]	SQD	C12-C13-C14-C15
40	v	201	HEC	C2B-C3B-CAB-CBB
23	a	409	CLA	CBA-CGA-O2A-C1
31	e	101	LMT	O5B-C5B-C6B-O6B
31	A	417	LMT	C4'-C5'-C6'-O6'
35	c	519	DGD	CBB-CCB-CDB-CEB
26	F	103	SQD	C30-C31-C32-C33
26	f	102	SQD	C32-C33-C34-C35
31	b	627	LMT	C7-C8-C9-C10
31	e	101	LMT	C4-C5-C6-C7
32	D	408[B]	LHG	C12-C13-C14-C15
32	L	101[A]	LHG	C15-C16-C17-C18
32	L	101[A]	LHG	C17-C18-C19-C20
32	L	101[B]	LHG	C17-C18-C19-C20
33	C	522	LMG	C18-C19-C20-C21
33	c	520	LMG	C34-C35-C36-C37
35	c	517[A]	DGD	C9A-CAA-CBA-CCA
35	c	518[A]	DGD	C9A-CAA-CBA-CCA
23	a	409	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C20
23	c	509	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C20
23	d	402	CLA	C16-C17-C18-C20
40	v	201	HEC	C4C-C3C-CAC-CBC
26	A	410	SQD	C17-C18-C19-C20
26	B	620	SQD	C30-C31-C32-C33
26	C	501[B]	SQD	C15-C16-C17-C18
26	a	412	SQD	C25-C26-C27-C28
32	D	408[B]	LHG	C16-C17-C18-C19
32	d	411[A]	LHG	C16-C17-C18-C19
33	C	502	LMG	C17-C18-C19-C20
33	D	413	LMG	C19-C20-C21-C22
33	B	621	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
26	C	501[B]	SQD	C11-C10-C9-C8
35	c	518[B]	DGD	C9A-CAA-CBA-CCA
35	h	102	DGD	C7B-C8B-C9B-CAB
31	b	627	LMT	C3-C4-C5-C6
32	D	408[A]	LHG	C16-C17-C18-C19
32	D	409[B]	LHG	C32-C33-C34-C35
32	d	411[A]	LHG	C32-C33-C34-C35
33	C	502	LMG	C12-C13-C14-C15
35	C	518[A]	DGD	C5B-C6B-C7B-C8B
31	A	417	LMT	C5-C6-C7-C8
31	B	628	LMT	C5-C6-C7-C8
31	t	101	LMT	O1'-C1-C2-C3
31	t	101	LMT	C11-C10-C9-C8
32	a	420[A]	LHG	C26-C27-C28-C29
35	C	518[B]	DGD	C5B-C6B-C7B-C8B
35	c	517[A]	DGD	C5A-C6A-C7A-C8A
35	c	518[A]	DGD	CBA-CCA-CDA-CEA
23	B	616	CLA	C3-C5-C6-C7
23	c	510	CLA	C3-C5-C6-C7
33	c	520	LMG	C10-C11-C12-C13
23	c	502	CLA	O1D-CGD-O2D-CED
31	e	101	LMT	C2'-C1'-O1'-C1
35	C	519[A]	DGD	C2E-C1E-O5D-C6D
33	B	621	LMG	C17-C18-C19-C20
35	C	518[A]	DGD	C4B-C5B-C6B-C7B
35	c	517[A]	DGD	C2B-C3B-C4B-C5B
35	c	518[A]	DGD	CAA-CBA-CCA-CDA
35	h	102	DGD	C9A-CAA-CBA-CCA
23	B	608	CLA	C16-C17-C18-C20
23	b	602	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C20
37	a	416[B]	PHO	C2C-C3C-CAC-CBC
32	L	101[A]	LHG	C13-C14-C15-C16
32	a	420[B]	LHG	C26-C27-C28-C29
32	l	802[B]	LHG	C12-C13-C14-C15
33	a	417	LMG	C34-C35-C36-C37
34	b	622	HTG	C2'-C3'-C4'-C5'
35	H	102	DGD	C9B-CAB-CBB-CCB
35	c	518[B]	DGD	CBA-CCA-CDA-CEA
23	a	407[A]	CLA	C11-C12-C13-C14
23	a	407[B]	CLA	C11-C12-C13-C14
23	b	606	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	b	610	CLA	C11-C12-C13-C14
35	C	518[B]	DGD	O6D-C5D-C6D-O5D
26	C	501[A]	SQD	C15-C16-C17-C18
26	a	412	SQD	C16-C17-C18-C19
31	B	630	LMT	C2-C3-C4-C5
31	e	101	LMT	C5-C6-C7-C8
33	B	621	LMG	C34-C35-C36-C37
35	C	519[A]	DGD	CCB-CDB-CEB-CFB
35	c	517[B]	DGD	C9A-CAA-CBA-CCA
25	B	627	GOL	C1-C2-C3-O3
25	D	414	GOL	O1-C1-C2-C3
25	O	302	GOL	O1-C1-C2-C3
25	O	303	GOL	O1-C1-C2-C3
25	v	202[A]	GOL	O1-C1-C2-C3
25	v	202[B]	GOL	O1-C1-C2-C3
34	B	625	HTG	O5-C5-C6-O6
23	c	507	CLA	C15-C16-C17-C18
33	B	621	LMG	C11-C10-O7-C8
32	D	409[A]	LHG	C32-C33-C34-C35
32	l	802[A]	LHG	C14-C15-C16-C17
33	D	413	LMG	C35-C36-C37-C38
33	C	502	LMG	C10-C11-C12-C13
33	a	417	LMG	C10-C11-C12-C13
31	t	101	LMT	C3-C4-C5-C6
32	A	416[B]	LHG	C34-C35-C36-C37
32	L	101[A]	LHG	C12-C13-C14-C15
32	L	101[B]	LHG	C12-C13-C14-C15
32	d	411[A]	LHG	C29-C30-C31-C32
32	d	411[B]	LHG	C16-C17-C18-C19
33	C	502	LMG	C36-C37-C38-C39
33	C	522	LMG	C13-C14-C15-C16
33	C	522	LMG	C17-C18-C19-C20
34	B	623	HTG	C3'-C4'-C5'-C6'
23	B	602	CLA	C4B-C3B-CAB-CBB
23	c	502	CLA	C4B-C3B-CAB-CBB
23	B	615	CLA	C16-C17-C18-C19
23	B	615	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C19
23	d	401[A]	CLA	C16-C17-C18-C20
23	A	405[A]	CLA	C15-C16-C17-C18
23	B	614	CLA	C8-C10-C11-C12
23	B	615	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	B	620	SQD	C11-C10-C9-C8
31	b	621	LMT	C11-C10-C9-C8
32	l	802[A]	LHG	C16-C17-C18-C19
33	C	521	LMG	C16-C17-C18-C19
33	a	417	LMG	C30-C31-C32-C33
35	H	102	DGD	C7A-C8A-C9A-CAA
35	H	102	DGD	C5B-C6B-C7B-C8B
35	c	518[B]	DGD	CAA-CBA-CCA-CDA
35	c	517[B]	DGD	C4D-C5D-C6D-O5D
31	c	501	LMT	C1-C2-C3-C4
32	D	408[B]	LHG	C10-C11-C12-C13
32	L	101[B]	LHG	C13-C14-C15-C16
33	m	101	LMG	C39-C40-C41-C42
35	c	517[B]	DGD	CAA-CBA-CCA-CDA
23	B	614	CLA	C5-C6-C7-C8
31	t	102	LMT	C4-C5-C6-C7
31	t	102	LMT	C7-C8-C9-C10
33	C	521	LMG	C17-C18-C19-C20
35	C	518[B]	DGD	C4B-C5B-C6B-C7B
23	B	605	CLA	O1D-CGD-O2D-CED
32	d	406[A]	LHG	C27-C28-C29-C30
35	C	518[A]	DGD	C9A-CAA-CBA-CCA
35	C	519[B]	DGD	CCB-CDB-CEB-CFB
31	F	101	LMT	C2-C1-O1'-C1'
32	E	101[A]	LHG	C24-C25-C26-C27
32	d	406[B]	LHG	C27-C28-C29-C30
32	l	802[B]	LHG	C17-C18-C19-C20
33	D	413	LMG	C12-C13-C14-C15
33	a	417	LMG	C29-C30-C31-C32
33	m	101	LMG	C35-C36-C37-C38
35	C	520	DGD	CAA-CBA-CCA-CDA
35	H	102	DGD	CCA-CDA-CEA-CFA
23	a	409	CLA	O1A-CGA-O2A-C1
32	D	409[B]	LHG	O10-C23-O8-C6
23	B	608	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C19
23	d	402	CLA	C16-C17-C18-C19
32	E	101[B]	LHG	C24-C25-C26-C27
32	L	101[A]	LHG	C25-C26-C27-C28
32	d	411[B]	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
35	c	517[B]	DGD	C2B-C3B-C4B-C5B
26	A	410	SQD	C26-C27-C28-C29
32	l	802[A]	LHG	C27-C28-C29-C30
35	c	517[B]	DGD	C5A-C6A-C7A-C8A
35	c	517[A]	DGD	O6D-C5D-C6D-O5D
31	A	417	LMT	C1-C2-C3-C4
35	H	102	DGD	CCB-CDB-CEB-CFB
23	C	512	CLA	C4-C3-C5-C6
37	a	408[B]	PHO	C4-C3-C5-C6
23	C	512	CLA	C2-C3-C5-C6
23	c	506	CLA	C2-C3-C5-C6
28	A	412[A]	PL9	C12-C11-C9-C8
28	A	412[B]	PL9	C12-C11-C9-C8
28	D	407[A]	PL9	C13-C14-C16-C17
28	d	404[B]	PL9	C28-C29-C31-C32
37	a	408[B]	PHO	C2-C3-C5-C6
33	m	101	LMG	C11-C10-O7-C8
35	C	518[B]	DGD	C4D-C5D-C6D-O5D
26	b	620	SQD	C13-C14-C15-C16
25	B	624	GOL	O2-C2-C3-O3
25	B	629	GOL	O1-C1-C2-O2
25	D	403	GOL	O1-C1-C2-O2
25	D	414	GOL	O2-C2-C3-O3
25	O	303	GOL	O1-C1-C2-O2
25	V	204[A]	GOL	O2-C2-C3-O3
25	V	204[B]	GOL	O2-C2-C3-O3
25	b	624	GOL	O2-C2-C3-O3
25	o	302	GOL	O2-C2-C3-O3
26	F	103	SQD	C24-C25-C26-C27
31	T	101	LMT	C3-C4-C5-C6
32	d	411[A]	LHG	C24-C25-C26-C27
32	l	802[B]	LHG	C27-C28-C29-C30
33	c	520	LMG	C31-C32-C33-C34
23	B	603	CLA	C16-C17-C18-C19
23	a	409	CLA	C16-C17-C18-C20
31	e	101	LMT	C1-C2-C3-C4
23	B	602	CLA	C2B-C3B-CAB-CBB
23	c	502	CLA	C2B-C3B-CAB-CBB
32	E	101[A]	LHG	O2-C2-C3-O3
32	D	408[A]	LHG	C12-C13-C14-C15
31	B	630	LMT	C5-C6-C7-C8
33	C	502	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
23	B	616	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C1-O2A-CGA
35	C	518[A]	DGD	O6D-C5D-C6D-O5D
33	c	520	LMG	C30-C31-C32-C33
33	d	409	LMG	C29-C30-C31-C32
35	c	519	DGD	CBA-CCA-CDA-CEA
26	F	103	SQD	C29-C30-C31-C32
26	f	102	SQD	C25-C26-C27-C28
32	A	416[A]	LHG	C34-C35-C36-C37
32	D	409[B]	LHG	C17-C18-C19-C20
23	B	610	CLA	C16-C17-C18-C19
32	E	101[B]	LHG	C23-C24-C25-C26
33	C	522	LMG	C10-C11-C12-C13
24	B	617	BCR	C1-C6-C7-C8
24	Y	101	BCR	C1-C6-C7-C8
24	a	410	BCR	C23-C24-C25-C26
24	b	617	BCR	C1-C6-C7-C8
24	b	617	BCR	C5-C6-C7-C8
24	b	619	BCR	C1-C6-C7-C8
31	B	628	LMT	C3'-C4'-O1B-C1B
33	C	522	LMG	C12-C13-C14-C15
35	c	517[A]	DGD	C7A-C8A-C9A-CAA
23	A	406[B]	CLA	C13-C15-C16-C17
23	c	511	CLA	C10-C11-C12-C13
26	b	620	SQD	C28-C29-C30-C31
32	d	406[A]	LHG	C29-C30-C31-C32
32	d	405[A]	LHG	C34-C35-C36-C37
35	c	518[A]	DGD	C6A-C7A-C8A-C9A
26	b	620	SQD	C27-C28-C29-C30
28	A	412[A]	PL9	C45-C44-C46-C47
28	a	414[A]	PL9	C12-C11-C9-C10
28	a	414[B]	PL9	C12-C11-C9-C10
28	d	404[B]	PL9	C15-C14-C16-C17
23	A	407	CLA	C12-C13-C15-C16
23	B	602	CLA	C11-C12-C13-C15
23	B	606	CLA	C11-C10-C8-C7
23	C	506	CLA	C12-C13-C15-C16
23	C	507	CLA	C2-C3-C5-C6
23	C	512	CLA	C11-C12-C13-C15
23	D	405	CLA	C11-C10-C8-C7
23	a	407[A]	CLA	C11-C12-C13-C15
23	a	407[B]	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	c	505	CLA	C12-C13-C15-C16
28	d	404[A]	PL9	C13-C14-C16-C17
37	D	402[B]	PHO	C2C-C3C-CAC-CBC
26	a	412	SQD	C31-C32-C33-C34
32	A	416[A]	LHG	C12-C13-C14-C15
33	C	502	LMG	C39-C40-C41-C42
33	C	521	LMG	C34-C35-C36-C37
35	c	518[A]	DGD	C4A-C5A-C6A-C7A
33	c	521	LMG	C29-C28-O8-C9
31	m	103	LMT	C7-C8-C9-C10
31	t	101	LMT	C4-C5-C6-C7
35	C	518[B]	DGD	C8A-C9A-CAA-CBA
23	c	507	CLA	C10-C11-C12-C13
35	h	102	DGD	CAB-CBB-CCB-CDB
26	a	411[B]	SQD	C12-C13-C14-C15
26	b	620	SQD	C14-C15-C16-C17
32	d	406[A]	LHG	C25-C26-C27-C28
33	m	101	LMG	C38-C39-C40-C41
23	C	513	CLA	C8-C10-C11-C12
32	D	409[A]	LHG	C13-C14-C15-C16
35	c	517[A]	DGD	CAA-CBA-CCA-CDA
38	f	101	HEM	C2C-C3C-CAC-CBC
32	d	411[B]	LHG	C33-C34-C35-C36
33	c	521	LMG	O6-C5-C6-O5
35	C	519[A]	DGD	O6E-C1E-O5D-C6D
35	c	517[B]	DGD	O6E-C1E-O5D-C6D
23	a	405[B]	CLA	C15-C16-C17-C18
23	c	511	CLA	O1D-CGD-O2D-CED
31	M	101	LMT	C3-C4-C5-C6
32	D	409[A]	LHG	C15-C16-C17-C18
33	C	502	LMG	C11-C12-C13-C14
33	c	520	LMG	C33-C34-C35-C36
35	c	518[B]	DGD	C6A-C7A-C8A-C9A
31	B	630	LMT	C6-C7-C8-C9
23	B	604	CLA	CBD-CGD-O2D-CED
33	C	522	LMG	C19-C20-C21-C22
32	d	411[B]	LHG	O2-C2-C3-O3
33	m	101	LMG	O9-C10-O7-C8
35	c	519	DGD	C1A-C2A-C3A-C4A
31	b	627	LMT	C5-C6-C7-C8
32	D	409[B]	LHG	C13-C14-C15-C16
35	c	518[B]	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
26	A	410	SQD	C2-C1-O6-C44
26	C	501[A]	SQD	O6-C44-C45-O47
26	C	501[B]	SQD	O6-C44-C45-O47
33	C	526	LMG	O6-C5-C6-O5
31	b	621	LMT	C3-C4-C5-C6
32	d	406[A]	LHG	C34-C35-C36-C37
32	d	411[A]	LHG	C25-C26-C27-C28
23	c	512	CLA	CBD-CGD-O2D-CED
23	B	610	CLA	C16-C17-C18-C20
33	d	409	LMG	O6-C5-C6-O5
23	C	507	CLA	C4-C3-C5-C6
28	D	407[B]	PL9	C15-C14-C16-C17
31	b	621	LMT	C3'-C4'-O1B-C1B
23	B	602	CLA	C11-C12-C13-C14
23	B	606	CLA	C11-C10-C8-C9
23	B	611	CLA	C11-C12-C13-C14
23	C	504	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C9
23	D	405	CLA	C14-C13-C15-C16
23	c	505	CLA	C14-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C14
35	C	518[B]	DGD	C3B-C4B-C5B-C6B
35	c	518[A]	DGD	C2B-C3B-C4B-C5B
23	a	405[B]	CLA	C2C-C3C-CAC-CBC
32	L	101[B]	LHG	C24-C25-C26-C27
23	A	406[A]	CLA	C13-C15-C16-C17
23	C	508	CLA	C15-C16-C17-C18
33	c	521	LMG	O10-C28-O8-C9
23	C	503	CLA	C1A-C2A-CAA-CBA
23	B	603	CLA	C16-C17-C18-C20
23	c	509	CLA	C16-C17-C18-C20
26	a	411[A]	SQD	C9-C10-C11-C12
32	A	416[A]	LHG	C26-C27-C28-C29
23	B	615	CLA	C5-C6-C7-C8
23	C	504	CLA	C15-C16-C17-C18
32	D	408[A]	LHG	C4-O6-P-O3
26	f	102	SQD	C34-C35-C36-C37
35	H	102	DGD	CAB-CBB-CCB-CDB
35	h	102	DGD	C9B-CAB-CBB-CCB
40	V	202	HEC	C2B-C3B-CAB-CBB
31	m	103	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
23	b	607	CLA	C3-C5-C6-C7
26	F	103	SQD	C34-C35-C36-C37
26	b	620	SQD	C11-C10-C9-C8
31	e	101	LMT	C3-C4-C5-C6
31	A	417	LMT	C3'-C4'-O1B-C1B
32	d	406[A]	LHG	C28-C29-C30-C31
23	B	611	CLA	C8-C10-C11-C12
23	b	601	CLA	C13-C15-C16-C17
32	d	406[B]	LHG	C34-C35-C36-C37
31	A	417	LMT	C3-C4-C5-C6
23	C	510	CLA	CBD-CGD-O2D-CED
35	C	518[A]	DGD	C8A-C9A-CAA-CBA
35	c	517[A]	DGD	C4D-C5D-C6D-O5D
26	b	620	SQD	C24-C23-O48-C46
23	D	405	CLA	C4-C3-C5-C6
23	c	514	CLA	C4-C3-C5-C6
33	a	417	LMG	C4-C5-C6-O5
35	h	102	DGD	CAA-CBA-CCA-CDA
35	C	520	DGD	C8A-C9A-CAA-CBA
35	c	518[B]	DGD	C2B-C3B-C4B-C5B
32	D	408[A]	LHG	C10-C11-C12-C13
32	l	802[B]	LHG	C13-C14-C15-C16
23	d	401[A]	CLA	C16-C17-C18-C19
34	b	623	HTG	O5-C5-C6-O6
26	A	410	SQD	O6-C44-C45-C46
26	C	501[B]	SQD	O6-C44-C45-C46
26	a	411[A]	SQD	O6-C44-C45-C46
26	a	412	SQD	O6-C44-C45-C46
26	b	620	SQD	C44-C45-C46-O48
26	f	102	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
32	E	101[A]	LHG	C4-C5-C6-O8
32	a	420[B]	LHG	C4-C5-C6-O8
35	C	519[A]	DGD	CDA-CEA-CFA-CGA
35	C	519[B]	DGD	CDA-CEA-CFA-CGA
35	C	520	DGD	CDB-CEB-CFB-CGB
23	c	514	CLA	O1D-CGD-O2D-CED
23	B	605	CLA	C5-C6-C7-C8
31	b	627	LMT	C1-C2-C3-C4
31	B	628	LMT	C7-C8-C9-C10
35	C	518[B]	DGD	C9A-CAA-CBA-CCA
35	C	520	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
35	C	519[A]	DGD	C2G-C3G-O3G-C1D
35	C	519[B]	DGD	C5D-C6D-O5D-C1E
35	c	518[A]	DGD	C2G-C3G-O3G-C1D
35	c	518[A]	DGD	C5D-C6D-O5D-C1E
31	t	102	LMT	O1'-C1-C2-C3
32	d	406[B]	LHG	C9-C10-C11-C12
32	l	802[A]	LHG	C9-C10-C11-C12
32	D	409[A]	LHG	C29-C30-C31-C32
34	B	622	HTG	C2'-C3'-C4'-C5'
23	a	406[B]	CLA	C2C-C3C-CAC-CBC
32	d	411[A]	LHG	C33-C34-C35-C36
33	D	413	LMG	O6-C5-C6-O5
25	B	629	GOL	O2-C2-C3-O3
25	D	414	GOL	O1-C1-C2-O2
25	c	528	GOL	O2-C2-C3-O3
33	a	417	LMG	C21-C22-C23-C24
34	B	625	HTG	C4'-C5'-C6'-C7'
35	C	518[A]	DGD	O6E-C5E-C6E-O5E
35	C	518[B]	DGD	O6E-C5E-C6E-O5E
35	c	517[A]	DGD	O6E-C5E-C6E-O5E
28	d	404[B]	PL9	C45-C44-C46-C47
23	a	405[B]	CLA	O1D-CGD-O2D-CED
23	a	406[A]	CLA	C2C-C3C-CAC-CBC
35	h	102	DGD	CDB-CEB-CFB-CGB
26	B	620	SQD	C46-C45-O47-C7
26	b	620	SQD	C46-C45-O47-C7
35	c	517[B]	DGD	O6E-C5E-C6E-O5E
23	B	602	CLA	C15-C16-C17-C18
35	c	519	DGD	O6D-C5D-C6D-O5D
26	a	411[A]	SQD	C12-C13-C14-C15
33	z	101	LMG	C14-C15-C16-C17
23	C	514	CLA	C10-C11-C12-C13
33	C	521	LMG	C11-C12-C13-C14
33	z	101	LMG	C13-C14-C15-C16
35	c	517[A]	DGD	C2A-C1A-O1G-C1G
32	D	409[A]	LHG	C17-C18-C19-C20
32	D	409[B]	LHG	C27-C28-C29-C30
26	C	501[A]	SQD	C11-C10-C9-C8
32	A	416[A]	LHG	O2-C2-C3-O3
31	b	621	LMT	C7-C8-C9-C10
31	c	501	LMT	C2-C3-C4-C5
35	C	518[B]	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
34	b	622	HTG	C1'-C2'-C3'-C4'
23	C	512	CLA	C10-C11-C12-C13
23	c	504	CLA	C8-C10-C11-C12
35	C	519[B]	DGD	C2E-C1E-O5D-C6D
35	c	517[B]	DGD	C2E-C1E-O5D-C6D
32	E	101[A]	LHG	C25-C26-C27-C28
32	d	406[A]	LHG	C33-C34-C35-C36
35	C	520	DGD	C6A-C7A-C8A-C9A
35	h	102	DGD	CBA-CCA-CDA-CEA
31	b	627	LMT	O1'-C1-C2-C3
32	E	101[A]	LHG	C13-C14-C15-C16
33	D	413	LMG	C30-C31-C32-C33
33	z	101	LMG	C20-C21-C22-C23
23	A	404[A]	CLA	C13-C15-C16-C17
23	b	604	CLA	C15-C16-C17-C18
23	b	610	CLA	C15-C16-C17-C18
23	b	616	CLA	C5-C6-C7-C8
32	d	411[B]	LHG	C25-C26-C27-C28
33	m	101	LMG	C11-C12-C13-C14
23	B	610	CLA	C12-C13-C15-C16
23	B	614	CLA	C11-C10-C8-C7
23	C	507	CLA	C11-C12-C13-C15
23	C	515	CLA	C11-C10-C8-C7
23	D	405	CLA	C12-C13-C15-C16
23	b	601	CLA	C11-C10-C8-C7
23	b	606	CLA	C11-C10-C8-C7
23	c	506	CLA	C11-C12-C13-C15
23	c	510	CLA	C11-C10-C8-C7
28	D	407[B]	PL9	C13-C14-C16-C17
28	d	404[B]	PL9	C13-C14-C16-C17
32	A	416[B]	LHG	C12-C13-C14-C15
32	E	101[B]	LHG	C25-C26-C27-C28
23	B	610	CLA	C14-C13-C15-C16
23	C	507	CLA	C11-C12-C13-C14
23	C	508	CLA	C6-C7-C8-C9
23	C	515	CLA	C11-C10-C8-C9
23	D	405	CLA	C11-C10-C8-C9
23	b	601	CLA	C6-C7-C8-C9
23	b	606	CLA	C11-C10-C8-C9
26	F	103	SQD	C7-C8-C9-C10
32	d	405[B]	LHG	C34-C35-C36-C37
23	d	402	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	D	409[B]	LHG	C15-C16-C17-C18
32	E	101[B]	LHG	C17-C18-C19-C20
33	m	101	LMG	C37-C38-C39-C40
23	C	505	CLA	O1D-CGD-O2D-CED
24	y	101	BCR	C37-C22-C23-C24
35	c	519	DGD	C2B-C3B-C4B-C5B
25	l	801[A]	GOL	O1-C1-C2-C3
26	A	410	SQD	C27-C28-C29-C30
33	d	409	LMG	C35-C36-C37-C38
32	L	101[B]	LHG	C25-C26-C27-C28
23	b	616	CLA	CBA-CGA-O2A-C1
23	c	513	CLA	CBA-CGA-O2A-C1
33	C	502	LMG	C20-C21-C22-C23
32	a	420[A]	LHG	C23-C24-C25-C26
31	c	501	LMT	C3-C4-C5-C6
32	D	409[B]	LHG	C10-C11-C12-C13
35	c	517[B]	DGD	C8B-C9B-CAB-CBB
23	D	404[B]	CLA	C4B-C3B-CAB-CBB
23	a	407[A]	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C4B-C3B-CAB-CBB
23	C	508	CLA	C5-C6-C7-C8
23	b	615	CLA	C5-C6-C7-C8
32	L	101[B]	LHG	O6-C4-C5-C6
28	A	412[A]	PL9	C39-C41-C42-C43
26	a	412	SQD	C18-C19-C20-C21
33	C	522	LMG	C35-C36-C37-C38
31	t	102	LMT	O5'-C5'-C6'-O6'
23	B	616	CLA	C4-C3-C5-C6
23	C	508	CLA	C4-C3-C5-C6
28	D	407[A]	PL9	C45-C44-C46-C47
26	C	501[B]	SQD	C7-C8-C9-C10
23	c	513	CLA	C10-C11-C12-C13
26	b	620	SQD	O10-C23-O48-C46
33	m	101	LMG	C14-C15-C16-C17
35	c	518[A]	DGD	CBB-CCB-CDB-CEB
35	h	102	DGD	C2B-C3B-C4B-C5B
23	b	606	CLA	C16-C17-C18-C20
23	d	401[B]	CLA	C16-C17-C18-C20
23	B	601	CLA	CBA-CGA-O2A-C1
23	C	512	CLA	CBA-CGA-O2A-C1
35	c	519	DGD	C2A-C1A-O1G-C1G
32	a	420[B]	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
35	C	518[A]	DGD	CCA-CDA-CEA-CFA
23	c	507	CLA	C3A-C2A-CAA-CBA
32	a	420[A]	LHG	C10-C11-C12-C13
31	B	628	LMT	C2-C1-O1'-C1'
31	b	627	LMT	C2-C1-O1'-C1'
31	m	103	LMT	C2-C1-O1'-C1'
33	d	409	LMG	C10-C11-C12-C13
32	A	416[B]	LHG	C11-C12-C13-C14
23	C	514	CLA	CBA-CGA-O2A-C1
26	A	410	SQD	C24-C23-O48-C46
35	c	517[B]	DGD	C2A-C1A-O1G-C1G
33	C	526	LMG	C11-C12-C13-C14
26	C	501[A]	SQD	O6-C44-C45-C46
32	E	101[B]	LHG	C4-C5-C6-O8
32	a	420[A]	LHG	C4-C5-C6-O8
33	C	502	LMG	C7-C8-C9-O8
33	a	417	LMG	C7-C8-C9-O8
32	L	101[A]	LHG	C27-C28-C29-C30
35	C	518[A]	DGD	C1B-C2B-C3B-C4B
23	d	402	CLA	O1A-CGA-O2A-C1
35	C	520	DGD	CBA-CCA-CDA-CEA
32	d	411[B]	LHG	C24-C25-C26-C27
35	c	517[A]	DGD	O1A-C1A-O1G-C1G
23	a	406[B]	CLA	C15-C16-C17-C18
28	D	407[A]	PL9	C15-C14-C16-C17
28	D	407[A]	PL9	C43-C44-C46-C47
35	C	518[A]	DGD	C4D-C5D-C6D-O5D
32	L	101[B]	LHG	C26-C27-C28-C29
32	l	802[B]	LHG	C14-C15-C16-C17
35	C	518[A]	DGD	C7A-C8A-C9A-CAA
23	b	608	CLA	C13-C15-C16-C17
32	d	405[B]	LHG	C4-O6-P-O3
32	d	411[A]	LHG	C3-O3-P-O6
35	c	519	DGD	O6E-C5E-C6E-O5E
33	B	621	LMG	C21-C22-C23-C24
25	c	527	GOL	O2-C2-C3-O3
25	v	202[A]	GOL	O1-C1-C2-O2
33	d	409	LMG	C19-C20-C21-C22
35	C	518[A]	DGD	C3B-C4B-C5B-C6B
23	A	406[A]	CLA	C16-C17-C18-C20
23	b	606	CLA	C16-C17-C18-C19
32	L	101[B]	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
35	H	102	DGD	O2G-C1B-C2B-C3B
23	a	407[A]	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
32	A	416[B]	LHG	O2-C2-C3-O3
32	D	408[B]	LHG	O2-C2-C3-O3
26	B	620	SQD	C34-C35-C36-C37
26	b	620	SQD	C26-C27-C28-C29
32	l	802[B]	LHG	C25-C26-C27-C28
26	a	411[A]	SQD	O6-C44-C45-O47
26	b	620	SQD	O47-C45-C46-O48
35	c	517[B]	DGD	C4B-C5B-C6B-C7B
26	a	411[B]	SQD	C35-C36-C37-C38
26	A	410	SQD	O5-C1-O6-C44
35	c	517[A]	DGD	O6E-C1E-O5D-C6D
28	a	414[A]	PL9	C24-C26-C27-C28
32	A	416[A]	LHG	C1-C2-C3-O3
32	A	416[B]	LHG	C1-C2-C3-O3
23	b	614	CLA	C2-C1-O2A-CGA
28	a	414[B]	PL9	C12-C11-C9-C8
32	d	406[B]	LHG	C25-C26-C27-C28
33	B	621	LMG	O8-C28-C29-C30
23	b	605	CLA	C11-C10-C8-C9
23	c	514	CLA	C6-C7-C8-C9
23	d	402	CLA	C11-C12-C13-C14
26	a	411[B]	SQD	C27-C28-C29-C30
31	B	630	LMT	C3-C4-C5-C6
32	d	411[B]	LHG	C29-C30-C31-C32
23	c	510	CLA	C8-C10-C11-C12
26	a	412	SQD	C15-C16-C17-C18
32	D	409[A]	LHG	C27-C28-C29-C30
32	l	802[A]	LHG	C34-C35-C36-C37
24	B	617	BCR	C5-C6-C7-C8
24	D	406	BCR	C23-C24-C25-C26
24	D	406	BCR	C23-C24-C25-C30
24	H	101	BCR	C23-C24-C25-C26
24	H	101	BCR	C23-C24-C25-C30
24	d	403	BCR	C23-C24-C25-C26
24	d	403	BCR	C23-C24-C25-C30
24	h	101	BCR	C23-C24-C25-C26
26	a	411[B]	SQD	C9-C10-C11-C12
31	A	415	LMT	C9-C10-C11-C12
33	c	521	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
24	D	406	BCR	C37-C22-C23-C24
23	b	616	CLA	O1A-CGA-O2A-C1
24	D	406	BCR	C21-C22-C23-C24
24	c	516	BCR	C7-C8-C9-C10
24	d	403	BCR	C21-C22-C23-C24
24	y	101	BCR	C21-C22-C23-C24
31	B	628	LMT	C1-C2-C3-C4
32	L	101[A]	LHG	C11-C10-C9-C8
35	c	518[B]	DGD	CBB-CCB-CDB-CEB
32	D	409[B]	LHG	C29-C30-C31-C32
26	C	501[A]	SQD	C18-C19-C20-C21
32	a	420[A]	LHG	C7-C8-C9-C10
35	C	519[A]	DGD	C5B-C6B-C7B-C8B
32	l	802[A]	LHG	C13-C14-C15-C16
34	b	622	HTG	C3'-C4'-C5'-C6'
23	A	404[B]	CLA	C13-C15-C16-C17
23	b	605	CLA	C5-C6-C7-C8
32	D	408[B]	LHG	O6-C4-C5-C6
32	L	101[A]	LHG	O6-C4-C5-C6
32	d	405[B]	LHG	C13-C14-C15-C16
35	C	519[A]	DGD	C8B-C9B-CAB-CBB
34	b	625	HTG	C4-C5-C6-O6
23	B	614	CLA	C12-C13-C15-C16
23	C	508	CLA	C6-C7-C8-C10
23	C	512	CLA	C12-C13-C15-C16
23	a	409	CLA	C11-C10-C8-C7
23	b	601	CLA	C6-C7-C8-C10
23	b	604	CLA	C6-C7-C8-C10
23	c	505	CLA	C11-C12-C13-C15
23	c	506	CLA	C12-C13-C15-C16
23	d	401[B]	CLA	C11-C12-C13-C15
28	a	414[A]	PL9	C12-C11-C9-C8
32	D	408[A]	LHG	C11-C10-C9-C8
32	d	406[B]	LHG	C29-C30-C31-C32
35	c	517[A]	DGD	CCB-CDB-CEB-CFB
23	C	509	CLA	C13-C15-C16-C17
26	a	411[A]	SQD	C27-C28-C29-C30
32	L	101[A]	LHG	C24-C25-C26-C27
32	a	420[B]	LHG	C10-C11-C12-C13
32	D	409[A]	LHG	C10-C11-C12-C13
32	d	405[A]	LHG	C13-C14-C15-C16
35	C	518[B]	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
23	a	405[B]	CLA	C2A-CAA-CBA-CGA
33	D	413	LMG	C36-C37-C38-C39
35	C	519[A]	DGD	C7A-C8A-C9A-CAA
35	c	517[B]	DGD	CAB-CBB-CCB-CDB
23	b	601	CLA	CBA-CGA-O2A-C1
31	c	501	LMT	C9-C10-C11-C12
31	e	101	LMT	C9-C10-C11-C12
23	b	604	CLA	C10-C11-C12-C13
26	b	620	SQD	C35-C36-C37-C38
23	B	610	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
37	D	401[B]	PHO	CAD-CBD-CGD-O2D
37	a	408[A]	PHO	CAD-CBD-CGD-O2D
37	a	416[B]	PHO	CAD-CBD-CGD-O2D
38	F	102	HEM	C2B-C3B-CAB-CBB
38	f	101	HEM	C2B-C3B-CAB-CBB
31	F	101	LMT	C4-C5-C6-C7
33	c	520	LMG	C29-C30-C31-C32
23	B	601	CLA	C15-C16-C17-C18
23	b	601	CLA	C8-C10-C11-C12
33	a	417	LMG	C35-C36-C37-C38
28	d	404[A]	PL9	C45-C44-C46-C47
26	a	411[A]	SQD	C34-C35-C36-C37
32	d	405[B]	LHG	C16-C17-C18-C19
35	C	519[B]	DGD	O6E-C1E-O5D-C6D
35	c	518[A]	DGD	O6E-C1E-O5D-C6D
28	d	404[B]	PL9	C43-C44-C46-C47
28	a	414[B]	PL9	C24-C26-C27-C28
26	B	620	SQD	C44-C45-C46-O48
32	D	409[B]	LHG	C2-C3-O3-P
23	C	512	CLA	O1A-CGA-O2A-C1
40	v	201	HEC	C4B-C3B-CAB-CBB
32	E	101[A]	LHG	O6-C4-C5-O7
32	L	101[A]	LHG	O6-C4-C5-O7
32	L	101[B]	LHG	O6-C4-C5-O7
33	C	526	LMG	C29-C28-O8-C9
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	C	504	CLA	CHA-CBD-CGD-O1D
23	C	506	CLA	CHA-CBD-CGD-O1D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O1D
23	c	503	CLA	CHA-CBD-CGD-O1D
23	c	503	CLA	CHA-CBD-CGD-O2D
23	c	505	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	O1A-CGA-O2A-C1
23	C	514	CLA	O1A-CGA-O2A-C1
23	c	513	CLA	O1A-CGA-O2A-C1
35	c	519	DGD	O1A-C1A-O1G-C1G
35	c	517[A]	DGD	C2E-C1E-O5D-C6D
35	c	518[A]	DGD	C2E-C1E-O5D-C6D
32	A	416[A]	LHG	C32-C33-C34-C35
26	B	620	SQD	O47-C45-C46-O48
26	f	102	SQD	O47-C45-C46-O48
32	E	101[B]	LHG	O7-C5-C6-O8
32	a	420[A]	LHG	O7-C5-C6-O8
32	a	420[B]	LHG	O7-C5-C6-O8
33	C	502	LMG	O7-C8-C9-O8
26	C	501[A]	SQD	C34-C35-C36-C37
32	d	405[B]	LHG	C9-C10-C11-C12
26	A	410	SQD	O10-C23-O48-C46
23	A	406[B]	CLA	C16-C17-C18-C20
25	B	627	GOL	O1-C1-C2-O2
25	c	527	GOL	O1-C1-C2-O2
32	d	405[A]	LHG	C11-C10-C9-C8
32	d	406[A]	LHG	C9-C10-C11-C12
33	C	502	LMG	C13-C14-C15-C16
35	c	518[B]	DGD	C9B-CAB-CBB-CCB
35	c	517[B]	DGD	O1A-C1A-O1G-C1G
26	B	620	SQD	C12-C13-C14-C15
23	C	512	CLA	C14-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C9
23	a	405[B]	CLA	C4C-C3C-CAC-CBC
26	b	620	SQD	C30-C31-C32-C33
23	b	601	CLA	O1A-CGA-O2A-C1
33	m	101	LMG	C28-C29-C30-C31
23	B	610	CLA	C2A-CAA-CBA-CGA
23	b	601	CLA	CAA-CBA-CGA-O2A
35	C	520	DGD	C4A-C5A-C6A-C7A
25	B	627	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	d	410	GOL	O1-C1-C2-C3
23	B	602	CLA	C3-C5-C6-C7
32	d	406[B]	LHG	C28-C29-C30-C31
32	d	411[A]	LHG	C18-C19-C20-C21
23	B	604	CLA	C1A-C2A-CAA-CBA
23	C	513	CLA	C1A-C2A-CAA-CBA
23	a	406[A]	CLA	C1A-C2A-CAA-CBA
23	a	406[B]	CLA	C1A-C2A-CAA-CBA
32	d	405[A]	LHG	C16-C17-C18-C19
26	F	103	SQD	C32-C33-C34-C35
26	a	411[A]	SQD	C35-C36-C37-C38
31	F	101	LMT	C2-C3-C4-C5
23	c	511	CLA	C4-C3-C5-C6
32	D	409[A]	LHG	C2-C3-O3-P
32	d	406[B]	LHG	C2-C3-O3-P
23	D	405	CLA	C2-C3-C5-C6
26	B	620	SQD	C9-C10-C11-C12
23	c	508	CLA	C4B-C3B-CAB-CBB
32	D	408[A]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C4-O6-P-O5
32	a	420[A]	LHG	C4-O6-P-O4
32	d	405[B]	LHG	C4-O6-P-O5
23	C	503	CLA	C16-C17-C18-C20
33	C	521	LMG	C37-C38-C39-C40
35	c	518[B]	DGD	O6E-C1E-O5D-C6D
32	E	101[A]	LHG	O6-C4-C5-C6
23	C	510	CLA	O1D-CGD-O2D-CED
31	M	101	LMT	O1'-C1-C2-C3
23	B	601	CLA	C2A-CAA-CBA-CGA
33	c	520	LMG	O6-C5-C6-O5
32	L	101[A]	LHG	C26-C27-C28-C29
23	d	401[B]	CLA	C16-C17-C18-C19
35	c	518[A]	DGD	C7B-C8B-C9B-CAB
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	C	506	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
31	c	501	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
35	C	518[A]	DGD	C6A-C7A-C8A-C9A
31	B	628	LMT	C9-C10-C11-C12
33	C	522	LMG	C4-C5-C6-O5
26	f	102	SQD	C7-C8-C9-C10
32	d	411[B]	LHG	C18-C19-C20-C21
31	b	627	LMT	C6-C7-C8-C9
23	A	406[A]	CLA	C12-C13-C15-C16
23	A	406[B]	CLA	C12-C13-C15-C16
23	B	601	CLA	C11-C12-C13-C15
23	B	616	CLA	C12-C13-C15-C16
23	C	509	CLA	C11-C12-C13-C15
23	b	601	CLA	C11-C12-C13-C15
23	b	608	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C7
23	c	510	CLA	C6-C7-C8-C10
23	d	401[A]	CLA	C11-C12-C13-C15
32	D	408[B]	LHG	O6-C4-C5-O7
26	C	501[A]	SQD	C13-C14-C15-C16
32	d	406[B]	LHG	C33-C34-C35-C36
33	C	522	LMG	C38-C39-C40-C41
23	C	511	CLA	C3-C5-C6-C7
32	D	408[A]	LHG	C34-C35-C36-C37
35	C	519[B]	DGD	C1A-C2A-C3A-C4A
35	C	520	DGD	CDA-CEA-CFA-CGA
33	d	409	LMG	C11-C12-C13-C14
35	c	518[A]	DGD	C5A-C6A-C7A-C8A
23	b	602	CLA	C10-C11-C12-C13
23	B	607	CLA	C3-C5-C6-C7
31	A	415	LMT	C7-C8-C9-C10
33	B	621	LMG	C36-C37-C38-C39
26	F	103	SQD	O47-C45-C46-O48
32	E	101[A]	LHG	O7-C5-C6-O8
33	a	417	LMG	O7-C8-C9-O8
32	d	406[A]	LHG	C32-C33-C34-C35
35	C	519[A]	DGD	C8A-C9A-CAA-CBA
32	L	101[B]	LHG	C33-C34-C35-C36
35	C	519[A]	DGD	C5D-C6D-O5D-C1E
35	c	518[B]	DGD	C5D-C6D-O5D-C1E
23	B	612	CLA	C10-C11-C12-C13
23	D	404[B]	CLA	C8-C10-C11-C12
23	B	604	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
32	d	406[A]	LHG	C2-C3-O3-P
35	H	102	DGD	CDB-CEB-CFB-CGB
32	D	408[B]	LHG	O10-C23-O8-C6
28	D	407[B]	PL9	C45-C44-C46-C47
33	d	409	LMG	C40-C41-C42-C43
32	d	411[A]	LHG	C34-C35-C36-C37
23	B	602	CLA	C8-C10-C11-C12
23	B	614	CLA	C14-C13-C15-C16
23	a	409	CLA	C11-C10-C8-C9
23	d	401[B]	CLA	C11-C12-C13-C14
32	D	408[A]	LHG	C26-C27-C28-C29
28	A	412[B]	PL9	C39-C41-C42-C43
25	B	627	GOL	O2-C2-C3-O3
23	C	504	CLA	C13-C15-C16-C17
35	C	519[A]	DGD	C7B-C8B-C9B-CAB
26	a	411[B]	SQD	C11-C12-C13-C14
32	d	411[A]	LHG	C11-C12-C13-C14
26	a	411[B]	SQD	C34-C35-C36-C37
23	D	404[A]	CLA	C2B-C3B-CAB-CBB
23	D	404[B]	CLA	C2B-C3B-CAB-CBB
23	c	505	CLA	C2B-C3B-CAB-CBB
23	c	508	CLA	C2B-C3B-CAB-CBB
23	c	511	CLA	O1A-CGA-O2A-C1
23	b	612	CLA	C10-C11-C12-C13
32	D	409[B]	LHG	C28-C29-C30-C31
33	C	502	LMG	C18-C19-C20-C21
28	D	407[B]	PL9	C28-C29-C31-C32
28	a	414[A]	PL9	C43-C44-C46-C47
28	a	414[B]	PL9	C43-C44-C46-C47
32	L	101[A]	LHG	C23-C24-C25-C26
32	D	408[A]	LHG	C13-C14-C15-C16
32	d	406[B]	LHG	C11-C10-C9-C8
32	l	802[A]	LHG	C28-C29-C30-C31
33	C	502	LMG	C29-C30-C31-C32
23	A	404[B]	CLA	C2A-CAA-CBA-CGA
26	A	410	SQD	C30-C31-C32-C33
23	A	407	CLA	C2-C1-O2A-CGA
23	B	613	CLA	C2-C1-O2A-CGA
23	C	511	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CAA-CBA-CGA-O2A
31	A	417	LMT	C4-C5-C6-C7
32	D	408[B]	LHG	C13-C14-C15-C16
33	z	101	LMG	C19-C20-C21-C22
33	C	522	LMG	C11-C12-C13-C14
23	c	511	CLA	CBA-CGA-O2A-C1
32	D	408[B]	LHG	C24-C23-O8-C6
32	l	802[B]	LHG	C16-C17-C18-C19
23	c	505	CLA	C5-C6-C7-C8
23	c	510	CLA	C15-C16-C17-C18
28	a	414[B]	PL9	C45-C44-C46-C47
28	d	404[B]	PL9	C30-C29-C31-C32
24	C	516	BCR	C1-C6-C7-C8
24	h	101	BCR	C23-C24-C25-C30
24	y	101	BCR	C23-C24-C25-C26
24	y	101	BCR	C23-C24-C25-C30
23	c	511	CLA	C2-C3-C5-C6
23	c	514	CLA	C2-C3-C5-C6
28	A	412[A]	PL9	C28-C29-C31-C32
32	d	406[A]	LHG	C10-C11-C12-C13
23	C	508	CLA	C16-C17-C18-C20
35	C	518[B]	DGD	O6E-C1E-O5D-C6D
34	B	622	HTG	C4'-C5'-C6'-C7'
23	c	508	CLA	C5-C6-C7-C8
33	B	621	LMG	C2-C1-O1-C7
35	C	518[B]	DGD	C2E-C1E-O5D-C6D
35	c	518[B]	DGD	C2E-C1E-O5D-C6D
35	h	102	DGD	C6A-C7A-C8A-C9A
35	h	102	DGD	C3B-C4B-C5B-C6B
32	d	411[B]	LHG	C3-O3-P-O6
26	C	501[B]	SQD	C12-C13-C14-C15
23	B	604	CLA	O1D-CGD-O2D-CED
31	F	101	LMT	C6-C7-C8-C9
26	C	501[A]	SQD	C16-C17-C18-C19
23	c	513	CLA	O1D-CGD-O2D-CED
23	B	614	CLA	C4-C3-C5-C6
35	C	520	DGD	C7A-C8A-C9A-CAA
37	D	401[B]	PHO	C2-C3-C5-C6
23	a	406[A]	CLA	C4C-C3C-CAC-CBC
32	D	408[B]	LHG	C11-C10-C9-C8
23	A	406[A]	CLA	C14-C13-C15-C16
23	A	406[B]	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	b	615	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C9
23	d	401[A]	CLA	C11-C12-C13-C14
23	B	610	CLA	C13-C15-C16-C17
23	b	603	CLA	C5-C6-C7-C8
32	D	408[A]	LHG	C28-C29-C30-C31
37	a	408[A]	PHO	C2C-C3C-CAC-CBC
32	E	101[B]	LHG	C13-C14-C15-C16
23	b	610	CLA	C13-C15-C16-C17
33	D	413	LMG	C18-C19-C20-C21
26	B	620	SQD	C29-C30-C31-C32
26	f	102	SQD	C23-C24-C25-C26
32	d	406[B]	LHG	O10-C23-O8-C6
23	B	613	CLA	C13-C15-C16-C17
32	A	416[A]	LHG	O1-C1-C2-C3
33	B	621	LMG	C18-C19-C20-C21
23	a	406[A]	CLA	C15-C16-C17-C18
23	c	510	CLA	C13-C15-C16-C17
33	m	101	LMG	C32-C33-C34-C35
28	A	412[B]	PL9	C45-C44-C46-C47
32	d	406[B]	LHG	C24-C23-O8-C6
26	a	411[A]	SQD	C11-C12-C13-C14
26	a	412	SQD	C19-C20-C21-C22
35	C	518[B]	DGD	CDB-CEB-CFB-CGB
23	C	512	CLA	C8-C10-C11-C12
35	C	520	DGD	O6D-C5D-C6D-O5D
32	D	409[A]	LHG	O10-C23-O8-C6
23	A	405[B]	CLA	CBD-CGD-O2D-CED
32	D	409[A]	LHG	C24-C23-O8-C6
31	M	101	LMT	C2-C3-C4-C5
23	B	610	CLA	C4B-C3B-CAB-CBB
23	D	404[A]	CLA	C4B-C3B-CAB-CBB
23	c	505	CLA	C4B-C3B-CAB-CBB
23	C	503	CLA	C2A-CAA-CBA-CGA
33	B	621	LMG	O6-C1-O1-C7
32	l	802[B]	LHG	O6-C4-C5-C6
32	D	408[B]	LHG	C23-C24-C25-C26
23	C	510	CLA	C5-C6-C7-C8
26	f	102	SQD	C11-C10-C9-C8
38	F	102	HEM	C4B-C3B-CAB-CBB
38	f	101	HEM	C4B-C3B-CAB-CBB
37	D	401[B]	PHO	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
37	a	408[A]	PHO	C4-C3-C5-C6
23	c	512	CLA	O1D-CGD-O2D-CED
37	a	408[A]	PHO	C2-C3-C5-C6
23	c	512	CLA	C8-C10-C11-C12
35	h	102	DGD	O2G-C1B-C2B-C3B
23	b	608	CLA	C16-C17-C18-C20
23	a	406[B]	CLA	C4C-C3C-CAC-CBC
23	c	513	CLA	CBD-CGD-O2D-CED
31	t	102	LMT	C2-C3-C4-C5
33	d	409	LMG	C36-C37-C38-C39
35	c	517[A]	DGD	C4B-C5B-C6B-C7B
33	B	621	LMG	O6-C5-C6-O5
33	C	521	LMG	C36-C37-C38-C39
23	C	508	CLA	C3A-C2A-CAA-CBA
26	a	412	SQD	C28-C29-C30-C31
32	d	405[A]	LHG	C9-C10-C11-C12
23	B	608	CLA	C13-C15-C16-C17
32	D	408[A]	LHG	C17-C18-C19-C20
33	C	521	LMG	C29-C30-C31-C32
28	A	412[B]	PL9	C28-C29-C31-C32
28	A	412[B]	PL9	C4-C3-C7-C8
28	a	414[A]	PL9	C4-C3-C7-C8
28	a	414[B]	PL9	C4-C3-C7-C8
28	d	404[B]	PL9	C4-C3-C7-C8
32	a	420[B]	LHG	C24-C25-C26-C27
23	A	407	CLA	C11-C12-C13-C14
23	B	601	CLA	C11-C12-C13-C14
23	B	610	CLA	C11-C12-C13-C14
23	B	613	CLA	C11-C12-C13-C14
23	B	614	CLA	C6-C7-C8-C9
23	a	407[A]	CLA	C14-C13-C15-C16
23	a	407[B]	CLA	C6-C7-C8-C9
23	b	602	CLA	C6-C7-C8-C9
23	b	603	CLA	C11-C10-C8-C9
23	b	608	CLA	C14-C13-C15-C16
23	b	616	CLA	C11-C10-C8-C9
33	B	621	LMG	C20-C21-C22-C23
35	c	519	DGD	C4D-C5D-C6D-O5D
32	l	802[B]	LHG	C11-C12-C13-C14
33	a	417	LMG	C33-C34-C35-C36
32	l	802[A]	LHG	C10-C11-C12-C13
33	c	520	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
32	d	411[A]	LHG	C1-C2-C3-O3
35	H	102	DGD	O1G-C1G-C2G-C3G
23	b	603	CLA	C2A-CAA-CBA-CGA
26	a	411[A]	SQD	C10-C11-C12-C13
32	E	101[A]	LHG	C12-C13-C14-C15
35	c	518[B]	DGD	C5A-C6A-C7A-C8A
23	A	407	CLA	C16-C17-C18-C19
23	B	602	CLA	O2A-C1-C2-C3
37	D	401[A]	PHO	O2A-C1-C2-C3
37	a	408[A]	PHO	O2A-C1-C2-C3
37	a	408[B]	PHO	O2A-C1-C2-C3
37	D	402[A]	PHO	C2C-C3C-CAC-CBC
35	c	517[A]	DGD	CBA-CCA-CDA-CEA
24	K	102	BCR	C7-C8-C9-C34
24	d	403	BCR	C37-C22-C23-C24
26	B	620	SQD	C33-C34-C35-C36
33	m	101	LMG	C29-C30-C31-C32
35	C	519[B]	DGD	C8A-C9A-CAA-CBA
31	e	101	LMT	C2B-C1B-O1B-C4'
28	a	414[A]	PL9	C45-C44-C46-C47
23	B	611	CLA	C1A-C2A-CAA-CBA
23	a	407[A]	CLA	C1A-C2A-CAA-CBA
23	B	602	CLA	C6-C7-C8-C10
23	B	613	CLA	C11-C10-C8-C7
23	B	616	CLA	C2-C3-C5-C6
23	C	515	CLA	C11-C12-C13-C15
23	b	603	CLA	C11-C10-C8-C7
23	b	604	CLA	C11-C12-C13-C15
23	b	615	CLA	C11-C12-C13-C15
23	b	616	CLA	C6-C7-C8-C10
23	c	509	CLA	C12-C13-C15-C16
23	c	513	CLA	C6-C7-C8-C10
34	B	623	HTG	C1'-C2'-C3'-C4'
32	A	416[A]	LHG	C29-C30-C31-C32
32	L	101[A]	LHG	C10-C11-C12-C13
35	C	519[B]	DGD	C5B-C6B-C7B-C8B
35	c	517[B]	DGD	C7B-C8B-C9B-CAB
23	b	605	CLA	C3-C5-C6-C7
23	c	508	CLA	C2A-CAA-CBA-CGA
23	c	507	CLA	C13-C15-C16-C17
33	C	521	LMG	O6-C5-C6-O5
38	F	102	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
35	C	520	DGD	C2A-C1A-O1G-C1G
23	b	601	CLA	C4-C3-C5-C6
23	B	610	CLA	C2B-C3B-CAB-CBB
23	C	506	CLA	C2B-C3B-CAB-CBB
32	E	101[B]	LHG	O2-C2-C3-O3
26	a	411[B]	SQD	C10-C11-C12-C13
35	h	102	DGD	CCA-CDA-CEA-CFA
35	C	520	DGD	O1A-C1A-O1G-C1G
23	C	510	CLA	C13-C15-C16-C17
26	a	411[B]	SQD	O6-C44-C45-O47
33	c	521	LMG	O1-C7-C8-O7
32	A	416[B]	LHG	C9-C10-C11-C12
32	a	420[A]	LHG	C24-C25-C26-C27
32	d	411[A]	LHG	C27-C28-C29-C30
23	A	406[A]	CLA	C16-C17-C18-C19
32	d	411[A]	LHG	C17-C18-C19-C20
33	c	521	LMG	C30-C31-C32-C33
40	V	202	HEC	CAD-CBD-CGD-O1D
32	d	405[A]	LHG	C25-C26-C27-C28
35	C	519[B]	DGD	C7A-C8A-C9A-CAA
23	C	515	CLA	C8-C10-C11-C12
23	A	404[B]	CLA	C2-C1-O2A-CGA
23	a	405[A]	CLA	C2-C1-O2A-CGA
23	a	405[B]	CLA	C2-C1-O2A-CGA
28	D	407[B]	PL9	C43-C44-C46-C47
28	d	404[A]	PL9	C43-C44-C46-C47
40	V	202	HEC	C4B-C3B-CAB-CBB
23	b	605	CLA	C13-C15-C16-C17
35	c	517[B]	DGD	C7A-C8A-C9A-CAA
35	c	518[B]	DGD	C7B-C8B-C9B-CAB
31	t	101	LMT	C1-C2-C3-C4
23	C	512	CLA	C15-C16-C17-C18
31	A	417	LMT	C7-C8-C9-C10
32	L	101[B]	LHG	C11-C10-C9-C8
33	C	526	LMG	C21-C22-C23-C24
23	B	615	CLA	C8-C10-C11-C12
31	t	101	LMT	C2-C3-C4-C5
35	C	520	DGD	CCA-CDA-CEA-CFA
23	c	512	CLA	O1A-CGA-O2A-C1
24	c	515	BCR	C23-C24-C25-C30
23	B	613	CLA	C15-C16-C17-C18
32	D	408[B]	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
32	d	411[B]	LHG	C34-C35-C36-C37
25	V	204[B]	GOL	O1-C1-C2-C3
33	m	101	LMG	C30-C31-C32-C33
24	K	102	BCR	C7-C8-C9-C10
32	d	411[A]	LHG	C9-C10-C11-C12
35	C	520	DGD	C3B-C4B-C5B-C6B
28	A	412[A]	PL9	C43-C44-C46-C47
26	A	410	SQD	C7-C8-C9-C10
35	c	517[B]	DGD	C5D-C6D-O5D-C1E
35	c	518[B]	DGD	C2G-C3G-O3G-C1D
32	A	416[A]	LHG	C17-C18-C19-C20
26	A	410	SQD	C16-C17-C18-C19
40	V	202	HEC	CAD-CBD-CGD-O2D
33	a	417	LMG	O8-C28-C29-C30
33	B	621	LMG	C14-C15-C16-C17
26	f	102	SQD	C26-C27-C28-C29
35	c	517[A]	DGD	CDB-CEB-CFB-CGB
23	D	405	CLA	C8-C10-C11-C12
23	a	409	CLA	C15-C16-C17-C18
23	c	504	CLA	C2A-CAA-CBA-CGA
33	C	502	LMG	C31-C32-C33-C34
32	d	411[B]	LHG	C27-C28-C29-C30
23	C	506	CLA	C4B-C3B-CAB-CBB
23	B	612	CLA	C13-C15-C16-C17
35	C	520	DGD	C2A-C3A-C4A-C5A
35	c	518[A]	DGD	C1A-C2A-C3A-C4A
28	D	407[A]	PL9	C35-C34-C36-C37
23	C	505	CLA	C6-C7-C8-C10
23	C	508	CLA	C2-C3-C5-C6
26	a	412	SQD	C24-C25-C26-C27
24	t	103	BCR	C13-C14-C15-C16
33	m	101	LMG	C2-C1-O1-C7
32	l	802[A]	LHG	C25-C26-C27-C28
23	D	405	CLA	O1A-CGA-O2A-C1
31	T	101	LMT	C7-C8-C9-C10
23	C	505	CLA	C5-C6-C7-C8
23	C	514	CLA	CAA-CBA-CGA-O2A
32	A	416[A]	LHG	O8-C23-C24-C25
32	E	101[B]	LHG	C12-C13-C14-C15
34	B	625	HTG	C2'-C1'-S1-C1
23	B	613	CLA	CAA-CBA-CGA-O2A
32	l	802[B]	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	A	412[A]	PL9	C25-C24-C26-C27
28	a	414[B]	PL9	C35-C34-C36-C37
23	B	612	CLA	C8-C10-C11-C12
34	B	623	HTG	C2'-C3'-C4'-C5'
33	C	526	LMG	O10-C28-O8-C9
31	A	415	LMT	C4B-C5B-C6B-O6B
23	c	511	CLA	CAA-CBA-CGA-O2A
35	C	520	DGD	O1G-C1A-C2A-C3A
23	B	616	CLA	C14-C13-C15-C16
23	C	512	CLA	C11-C12-C13-C14
23	C	515	CLA	C6-C7-C8-C9
23	D	405	CLA	C6-C7-C8-C9
23	a	407[A]	CLA	C6-C7-C8-C9
23	a	407[B]	CLA	C14-C13-C15-C16
23	b	601	CLA	C11-C12-C13-C14
23	b	604	CLA	C11-C12-C13-C14
23	c	506	CLA	C14-C13-C15-C16
23	c	511	CLA	C11-C10-C8-C9
23	C	504	CLA	C3-C5-C6-C7
31	B	630	LMT	C7-C8-C9-C10
38	F	102	HEM	CAD-CBD-CGD-O2D
23	b	613	CLA	CAA-CBA-CGA-O2A
32	E	101[B]	LHG	O7-C7-C8-C9
32	a	420[A]	LHG	O8-C23-C24-C25
32	a	420[B]	LHG	O8-C23-C24-C25
23	C	515	CLA	CBD-CGD-O2D-CED
23	A	404[B]	CLA	CAD-CBD-CGD-O2D
23	B	603	CLA	CAD-CBD-CGD-O2D
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	612	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	CAD-CBD-CGD-O2D
23	C	514	CLA	CAD-CBD-CGD-O2D
23	b	603	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	607	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O2D
37	D	401[A]	PHO	CAD-CBD-CGD-O2D
37	a	408[B]	PHO	CAD-CBD-CGD-O2D
32	d	411[B]	LHG	C7-C8-C9-C10
23	b	610	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	C	509	CLA	C2A-CAA-CBA-CGA
23	C	515	CLA	C2-C1-O2A-CGA
38	f	101	HEM	CAA-CBA-CGA-O2A
32	L	101[A]	LHG	C11-C12-C13-C14
23	c	513	CLA	CAA-CBA-CGA-O2A
32	L	101[A]	LHG	O7-C7-C8-C9
33	C	502	LMG	C38-C39-C40-C41
23	b	604	CLA	C13-C15-C16-C17
23	b	616	CLA	C4-C3-C5-C6
31	A	415	LMT	C2B-C1B-O1B-C4'
38	f	101	HEM	CAD-CBD-CGD-O1D
40	v	201	HEC	CAD-CBD-CGD-O2D
23	b	601	CLA	C2-C3-C5-C6
32	l	802[A]	LHG	O7-C7-C8-C9
33	c	520	LMG	O7-C10-C11-C12
33	z	101	LMG	O7-C10-C11-C12
32	A	416[B]	LHG	C18-C19-C20-C21
32	A	416[B]	LHG	C27-C28-C29-C30
35	C	520	DGD	C5B-C6B-C7B-C8B
24	Y	101	BCR	C21-C22-C23-C24
26	B	620	SQD	C14-C15-C16-C17
35	C	520	DGD	CCB-CDB-CEB-CFB
26	F	103	SQD	C44-C45-C46-O48
33	B	621	LMG	O1-C7-C8-C9
37	D	401[B]	PHO	CBA-CGA-O2A-C1
32	L	101[B]	LHG	O7-C7-C8-C9
33	C	526	LMG	O7-C10-C11-C12
32	d	411[B]	LHG	C11-C10-C9-C8
23	C	511	CLA	O2A-C1-C2-C3
37	D	401[B]	PHO	O2A-C1-C2-C3
23	c	502	CLA	C2A-CAA-CBA-CGA
32	A	416[B]	LHG	O8-C23-C24-C25
38	f	101	HEM	CAD-CBD-CGD-O2D
40	v	201	HEC	CAD-CBD-CGD-O1D
23	a	405[A]	CLA	C2C-C3C-CAC-CBC
23	b	608	CLA	C16-C17-C18-C19
23	b	610	CLA	C16-C17-C18-C19
23	A	404[A]	CLA	C2C-C3C-CAC-CBC
26	b	620	SQD	C12-C13-C14-C15
33	a	417	LMG	C14-C15-C16-C17
23	A	405[A]	CLA	CHA-CBD-CGD-O1D
23	A	405[A]	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	A	405[B]	CLA	CHA-CBD-CGD-O2D
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	C	504	CLA	CHA-CBD-CGD-O2D
23	C	511	CLA	CHA-CBD-CGD-O1D
23	C	511	CLA	CHA-CBD-CGD-O2D
23	C	512	CLA	CHA-CBD-CGD-O2D
23	a	406[A]	CLA	CHA-CBD-CGD-O1D
23	a	406[A]	CLA	CHA-CBD-CGD-O2D
23	a	406[B]	CLA	CHA-CBD-CGD-O1D
23	a	406[B]	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	c	505	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-O1D
23	c	510	CLA	CHA-CBD-CGD-O2D
38	f	101	HEM	CAA-CBA-CGA-O1A
23	b	616	CLA	C2-C3-C5-C6
32	E	101[B]	LHG	C11-C10-C9-C8
33	m	101	LMG	O6-C5-C6-O5
35	C	520	DGD	C9A-CAA-CBA-CCA
26	a	411[B]	SQD	O47-C7-C8-C9
23	c	512	CLA	C3-C5-C6-C7
31	T	101	LMT	C9-C10-C11-C12
32	A	416[A]	LHG	O1-C1-C2-O2
37	D	401[A]	PHO	CHA-CBD-CGD-O2D
37	a	408[A]	PHO	CHA-CBD-CGD-O1D
35	c	519	DGD	C3B-C4B-C5B-C6B
33	D	413	LMG	O7-C10-C11-C12
32	l	802[B]	LHG	C9-C10-C11-C12
34	c	522	HTG	C4'-C5'-C6'-C7'
23	B	614	CLA	C2-C3-C5-C6
23	C	508	CLA	C12-C13-C15-C16
23	a	406[A]	CLA	C11-C12-C13-C15
23	a	407[B]	CLA	C6-C7-C8-C10
23	b	607	CLA	C12-C13-C15-C16
23	c	503	CLA	C11-C12-C13-C15
23	c	514	CLA	C12-C13-C15-C16
23	c	507	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	A	412[A]	PL9	C4-C3-C7-C8
37	a	416[A]	PHO	C2C-C3C-CAC-CBC
23	C	512	CLA	CAA-CBA-CGA-O2A
32	d	411[A]	LHG	C30-C31-C32-C33
35	c	517[B]	DGD	C6B-C7B-C8B-C9B
23	C	509	CLA	C11-C12-C13-C14
23	b	607	CLA	C14-C13-C15-C16
23	c	514	CLA	C14-C13-C15-C16
28	d	404[A]	PL9	C34-C36-C37-C38
33	B	621	LMG	C30-C31-C32-C33
23	b	612	CLA	C2B-C3B-CAB-CBB
32	A	416[B]	LHG	C30-C31-C32-C33
34	b	623	HTG	C4'-C5'-C6'-C7'
26	A	410	SQD	C15-C16-C17-C18
33	B	621	LMG	O10-C28-C29-C30
23	a	405[A]	CLA	C4C-C3C-CAC-CBC
23	C	513	CLA	O1A-CGA-O2A-C1
23	B	602	CLA	C2A-CAA-CBA-CGA
28	D	407[B]	PL9	C11-C12-C13-C14
31	e	101	LMT	C2-C3-C4-C5
23	b	612	CLA	C13-C15-C16-C17
31	m	103	LMT	C11-C10-C9-C8
33	m	101	LMG	C40-C41-C42-C43
23	C	508	CLA	C16-C17-C18-C19
34	b	622	HTG	O5-C5-C6-O6
32	L	101[B]	LHG	C15-C16-C17-C18
23	c	513	CLA	CAA-CBA-CGA-O1A
23	c	512	CLA	CBA-CGA-O2A-C1
23	c	504	CLA	C5-C6-C7-C8
23	A	405[B]	CLA	C1A-C2A-CAA-CBA
23	c	507	CLA	C1A-C2A-CAA-CBA
32	L	101[B]	LHG	C11-C12-C13-C14
34	b	625	HTG	C4'-C5'-C6'-C7'
32	L	101[B]	LHG	O9-C7-C8-C9
32	l	802[A]	LHG	O9-C7-C8-C9
35	C	520	DGD	O1A-C1A-C2A-C3A
33	z	101	LMG	C15-C16-C17-C18
28	a	414[B]	PL9	C21-C22-C23-C24
23	B	608	CLA	C2-C1-O2A-CGA
23	A	404[A]	CLA	C4C-C3C-CAC-CBC
32	A	416[A]	LHG	O10-C23-C24-C25
32	L	101[A]	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	a	420[A]	LHG	O10-C23-C24-C25
32	a	420[B]	LHG	O10-C23-C24-C25
32	d	405[B]	LHG	C11-C10-C9-C8
35	C	518[A]	DGD	C3A-C4A-C5A-C6A
32	E	101[A]	LHG	O7-C7-C8-C9
33	a	417	LMG	C31-C32-C33-C34
23	C	503	CLA	C16-C17-C18-C19
23	B	613	CLA	CAA-CBA-CGA-O1A
23	C	514	CLA	CAA-CBA-CGA-O1A
23	c	511	CLA	CAA-CBA-CGA-O1A
32	E	101[B]	LHG	O9-C7-C8-C9
32	l	802[B]	LHG	O9-C7-C8-C9
23	b	602	CLA	C8-C10-C11-C12
23	b	615	CLA	C13-C15-C16-C17
26	f	102	SQD	C28-C29-C30-C31
33	C	526	LMG	C2-C1-O1-C7
23	b	615	CLA	C10-C11-C12-C13
23	C	514	CLA	C4B-C3B-CAB-CBB
32	d	405[A]	LHG	C4-O6-P-O5
33	B	621	LMG	O1-C7-C8-O7
32	d	405[B]	LHG	C25-C26-C27-C28
35	C	520	DGD	C8B-C9B-CAB-CBB
33	c	520	LMG	O9-C10-C11-C12
24	C	516	BCR	C5-C6-C7-C8
24	c	515	BCR	C23-C24-C25-C26
35	C	518[B]	DGD	C6A-C7A-C8A-C9A
37	a	408[B]	PHO	C8-C10-C11-C12
23	b	613	CLA	CAA-CBA-CGA-O1A
32	A	416[B]	LHG	O10-C23-C24-C25
33	C	526	LMG	O9-C10-C11-C12
31	b	621	LMT	C5'-C4'-O1B-C1B
33	B	621	LMG	O7-C10-C11-C12
32	d	406[A]	LHG	O10-C23-O8-C6
32	D	408[B]	LHG	C31-C32-C33-C34
32	D	408[B]	LHG	C26-C27-C28-C29
32	A	416[A]	LHG	C18-C19-C20-C21
35	C	519[B]	DGD	C3B-C4B-C5B-C6B
28	d	404[A]	PL9	C15-C14-C16-C17
32	d	406[A]	LHG	C30-C31-C32-C33
28	A	412[B]	PL9	C46-C47-C48-C49
28	d	404[A]	PL9	C11-C12-C13-C14
35	c	518[A]	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
23	A	405[B]	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	611	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
26	f	102	SQD	O5-C5-C6-S
37	D	401[B]	PHO	O1A-CGA-O2A-C1
32	E	101[A]	LHG	O8-C23-C24-C25
35	C	519[A]	DGD	O2G-C1B-C2B-C3B
23	B	614	CLA	C11-C10-C8-C9
23	a	406[A]	CLA	C11-C12-C13-C14
23	c	503	CLA	C11-C12-C13-C14
26	B	620	SQD	C11-C12-C13-C14
32	A	416[A]	LHG	C30-C31-C32-C33
32	D	409[A]	LHG	C28-C29-C30-C31
23	c	502	CLA	CAA-CBA-CGA-O2A
32	d	406[B]	LHG	O8-C23-C24-C25
35	C	519[B]	DGD	O2G-C1B-C2B-C3B
33	D	413	LMG	C38-C39-C40-C41
34	d	408	HTG	S1-C1'-C2'-C3'
26	A	410	SQD	C25-C26-C27-C28
33	z	101	LMG	C17-C18-C19-C20
35	C	518[A]	DGD	CBA-CCA-CDA-CEA
32	L	101[A]	LHG	C32-C33-C34-C35
32	d	406[B]	LHG	C32-C33-C34-C35
26	a	412	SQD	O48-C23-C24-C25
32	D	409[A]	LHG	O8-C23-C24-C25
32	E	101[B]	LHG	O8-C23-C24-C25
23	B	601	CLA	C13-C15-C16-C17
23	b	612	CLA	O1A-CGA-O2A-C1
31	M	101	LMT	C4'-C5'-C6'-O6'
23	C	504	CLA	C12-C13-C15-C16
23	a	407[A]	CLA	C6-C7-C8-C10
23	b	614	CLA	C11-C10-C8-C7
23	c	511	CLA	C11-C10-C8-C7
23	c	513	CLA	C12-C13-C15-C16
32	E	101[B]	LHG	O6-C4-C5-O7
23	C	512	CLA	CAA-CBA-CGA-O1A
23	c	502	CLA	CAA-CBA-CGA-O1A
32	E	101[A]	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	E	101[A]	LHG	O10-C23-C24-C25
33	D	413	LMG	O9-C10-C11-C12
32	D	409[B]	LHG	O8-C23-C24-C25
33	C	521	LMG	O7-C10-C11-C12
33	c	521	LMG	O7-C10-C11-C12
35	c	517[A]	DGD	O2G-C1B-C2B-C3B
24	D	406	BCR	C7-C8-C9-C10
32	D	409[A]	LHG	O10-C23-C24-C25
32	E	101[B]	LHG	O10-C23-C24-C25
35	c	517[A]	DGD	O1B-C1B-C2B-C3B
24	a	410	BCR	C19-C20-C21-C22
23	A	405[B]	CLA	C2C-C3C-CAC-CBC
31	e	101	LMT	C2-C1-O1'-C1'
33	m	101	LMG	O6-C1-O1-C7
33	a	417	LMG	C13-C14-C15-C16
35	c	519	DGD	C3A-C4A-C5A-C6A
33	c	521	LMG	O9-C10-C11-C12
35	C	519[A]	DGD	O1B-C1B-C2B-C3B
23	A	405[B]	CLA	O1D-CGD-O2D-CED
32	d	411[A]	LHG	C31-C32-C33-C34
23	C	507	CLA	CAA-CBA-CGA-O2A
33	C	521	LMG	O9-C10-C11-C12
23	b	612	CLA	C8-C10-C11-C12
37	a	416[B]	PHO	C8-C10-C11-C12
23	b	601	CLA	C3-C5-C6-C7
26	C	501[B]	SQD	C18-C19-C20-C21
32	E	101[A]	LHG	C11-C10-C9-C8
26	A	410	SQD	O48-C23-C24-C25
32	d	406[A]	LHG	O8-C23-C24-C25

There are no ring outliers.

183 monomers are involved in 358 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	602	CLA	3	0
25	a	418	GOL	2	0
23	b	604	CLA	1	0
24	A	408	BCR	1	0
32	d	406[A]	LHG	11	0
23	b	616	CLA	4	0
31	m	103	LMT	2	0
37	D	401[A]	PHO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	a	409	CLA	2	0
23	D	404[A]	CLA	3	0
23	d	402	CLA	2	0
26	C	501[B]	SQD	1	0
26	a	412	SQD	1	0
28	D	407[A]	PL9	1	0
35	c	518[A]	DGD	3	0
33	C	502	LMG	2	0
33	z	101	LMG	2	0
25	D	414	GOL	3	0
25	B	624	GOL	1	0
32	D	409[B]	LHG	4	0
23	B	616	CLA	4	0
28	A	412[B]	PL9	8	0
23	b	603	CLA	1	0
23	c	503	CLA	2	0
24	B	618	BCR	3	0
33	a	417	LMG	1	0
32	a	420[A]	LHG	5	0
25	B	627	GOL	1	0
25	v	202[A]	GOL	1	0
23	B	606	CLA	2	0
24	t	103	BCR	3	0
31	B	630	LMT	2	0
25	O	303	GOL	1	0
23	B	607	CLA	1	0
32	E	101[A]	LHG	3	0
34	D	412	HTG	1	0
34	b	622	HTG	1	0
25	a	419	GOL	5	0
23	A	405[A]	CLA	1	0
23	C	513	CLA	4	0
23	c	510	CLA	1	0
25	D	403	GOL	5	0
26	A	410	SQD	1	0
37	a	416[B]	PHO	1	0
35	C	518[B]	DGD	4	0
25	A	409	GOL	1	0
23	C	504	CLA	3	0
35	c	519	DGD	4	0
23	b	609	CLA	5	0
35	C	520	DGD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	y	101	BCR	2	0
23	c	508	CLA	2	0
33	c	520	LMG	1	0
23	B	614	CLA	1	0
23	C	508	CLA	4	0
26	C	501[A]	SQD	1	0
23	C	512	CLA	5	0
25	V	204[B]	GOL	1	0
23	B	605	CLA	4	0
34	d	408	HTG	1	0
23	d	401[B]	CLA	4	0
32	D	409[A]	LHG	5	0
24	c	516	BCR	1	0
23	c	506	CLA	6	0
28	A	412[A]	PL9	11	0
23	C	506	CLA	1	0
25	c	526[B]	GOL	1	0
33	d	409	LMG	1	0
23	c	513	CLA	2	0
24	K	102	BCR	1	0
25	b	628	GOL	2	0
24	b	618	BCR	3	0
24	h	101	BCR	5	0
23	b	601	CLA	3	0
26	a	411[B]	SQD	4	0
32	D	408[B]	LHG	2	0
32	d	411[B]	LHG	3	0
25	B	629	GOL	1	0
23	b	607	CLA	2	0
23	A	404[B]	CLA	2	0
23	C	507	CLA	6	0
23	b	602	CLA	1	0
23	c	514	CLA	1	0
24	Y	101	BCR	3	0
35	C	519[B]	DGD	1	0
23	c	502	CLA	4	0
37	a	416[A]	PHO	1	0
23	b	613	CLA	1	0
35	C	518[A]	DGD	1	0
38	F	102	HEM	1	0
31	t	101	LMT	1	0
26	f	102	SQD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	505	CLA	4	0
23	b	615	CLA	2	0
34	B	622	HTG	2	0
34	c	522	HTG	1	0
24	b	617	BCR	2	0
24	c	515	BCR	3	0
35	H	102	DGD	1	0
23	D	404[B]	CLA	4	0
31	c	501	LMT	2	0
23	b	614	CLA	2	0
23	d	401[A]	CLA	1	0
24	k	101	BCR	2	0
23	a	406[B]	CLA	2	0
34	B	625	HTG	1	0
26	b	620	SQD	2	0
26	B	620	SQD	3	0
23	b	606	CLA	3	0
32	d	405[B]	LHG	1	0
26	a	411[A]	SQD	4	0
32	D	408[A]	LHG	2	0
31	A	415	LMT	1	0
23	C	505	CLA	4	0
26	F	103	SQD	2	0
23	B	615	CLA	2	0
24	a	410	BCR	1	0
23	c	509	CLA	6	0
23	C	514	CLA	2	0
23	a	407[B]	CLA	2	0
37	D	402[B]	PHO	2	0
23	a	405[B]	CLA	3	0
35	c	517[B]	DGD	2	0
23	C	509	CLA	2	0
23	A	406[B]	CLA	3	0
35	C	519[A]	DGD	1	0
23	c	512	CLA	5	0
24	H	101	BCR	2	0
28	a	414[B]	PL9	5	0
23	A	405[B]	CLA	3	0
23	C	510	CLA	4	0
28	d	404[B]	PL9	1	0
25	O	302	GOL	1	0
23	b	605	CLA	3	0

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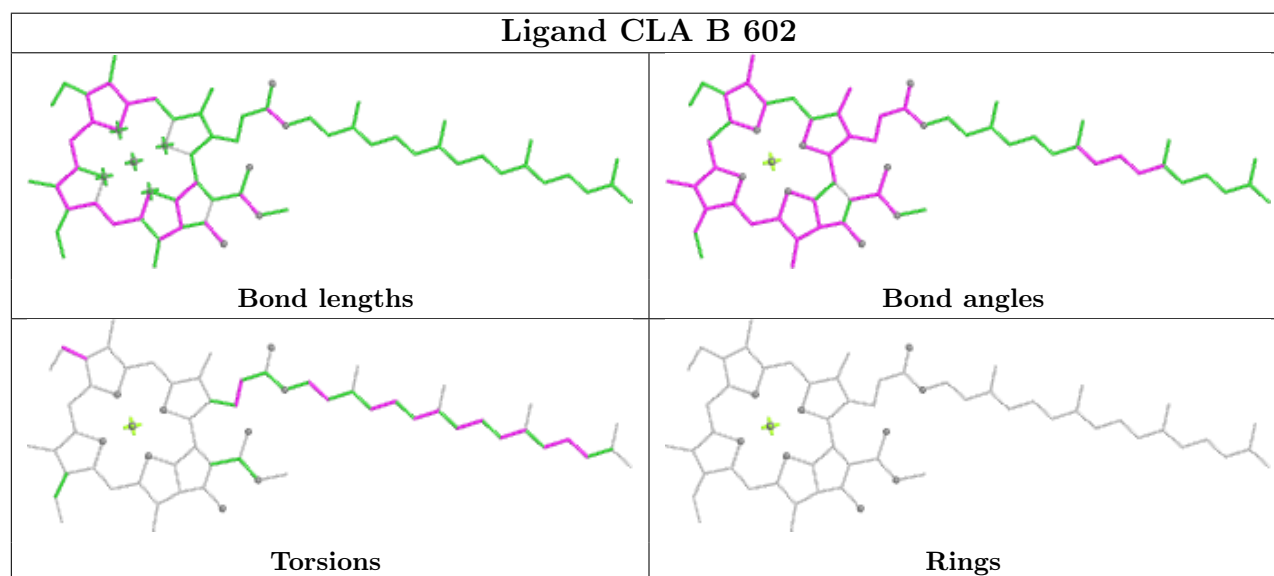
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33	C	522	LMG	1	0
34	b	625	HTG	1	0
32	d	406[B]	LHG	7	0
33	B	621	LMG	1	0
23	b	612	CLA	2	0
23	c	507	CLA	3	0
23	C	511	CLA	3	0
37	D	401[B]	PHO	1	0
23	a	406[A]	CLA	3	0
32	A	416[A]	LHG	1	0
24	b	619	BCR	5	0
24	B	619	BCR	1	0
31	b	621	LMT	1	0
31	e	101	LMT	1	0
32	d	405[A]	LHG	2	0
35	c	518[B]	DGD	4	0
31	B	628	LMT	1	0
23	B	612	CLA	3	0
23	B	601	CLA	3	0
23	C	503	CLA	4	0
23	B	604	CLA	2	0
37	a	408[B]	PHO	2	0
23	B	609	CLA	2	0
23	a	407[A]	CLA	1	0
31	A	417	LMT	2	0
32	a	420[B]	LHG	3	0
23	c	504	CLA	4	0
37	D	402[A]	PHO	1	0
23	a	405[A]	CLA	2	0
25	v	202[B]	GOL	1	0
35	c	517[A]	DGD	1	0
38	f	101	HEM	1	0
23	A	406[A]	CLA	1	0
24	d	403	BCR	2	0
23	A	404[A]	CLA	2	0
23	A	407	CLA	3	0
23	B	603	CLA	1	0
24	D	406	BCR	2	0
31	t	102	LMT	2	0
23	C	515	CLA	2	0
32	E	101[B]	LHG	3	0
28	a	414[A]	PL9	5	0

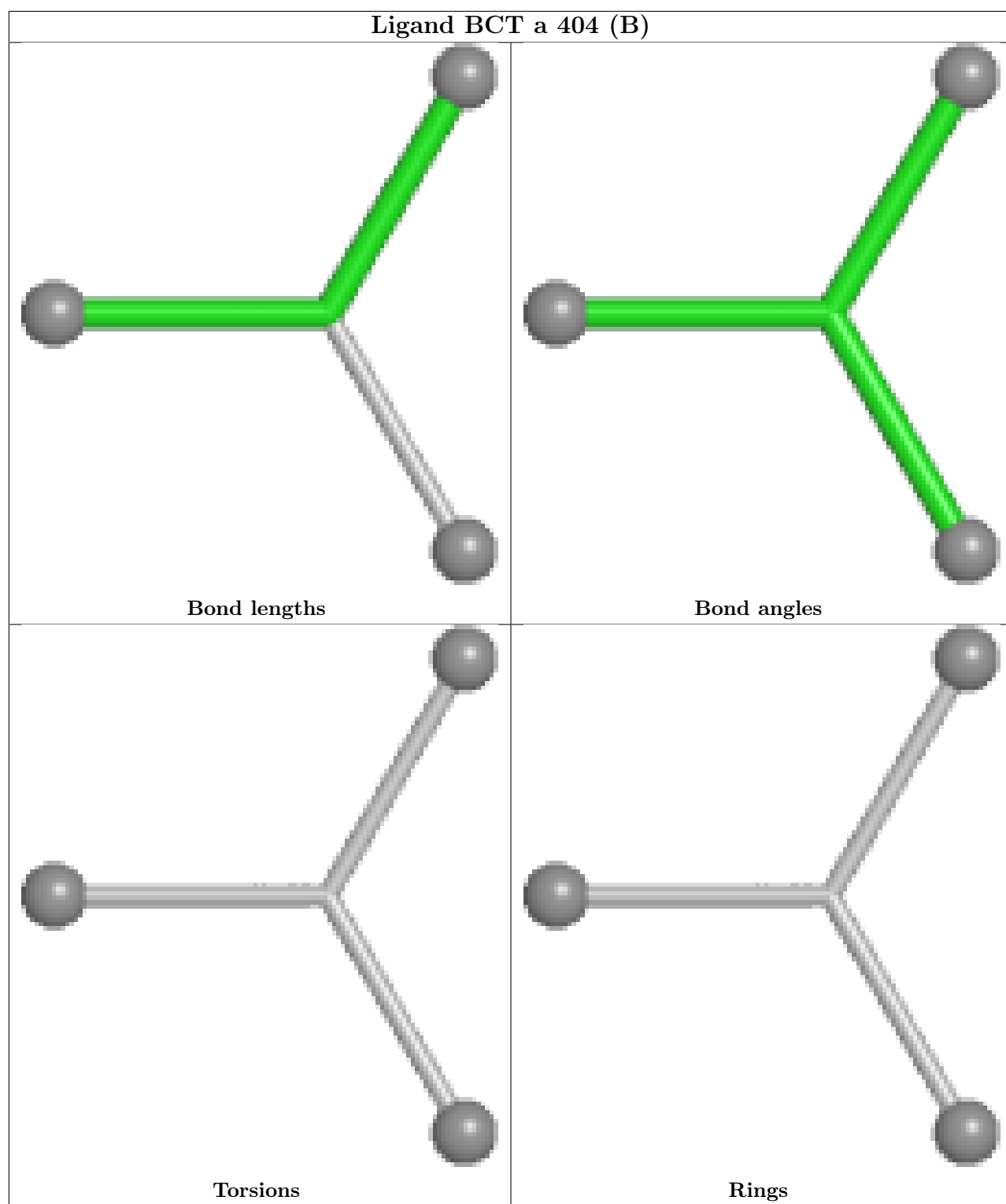
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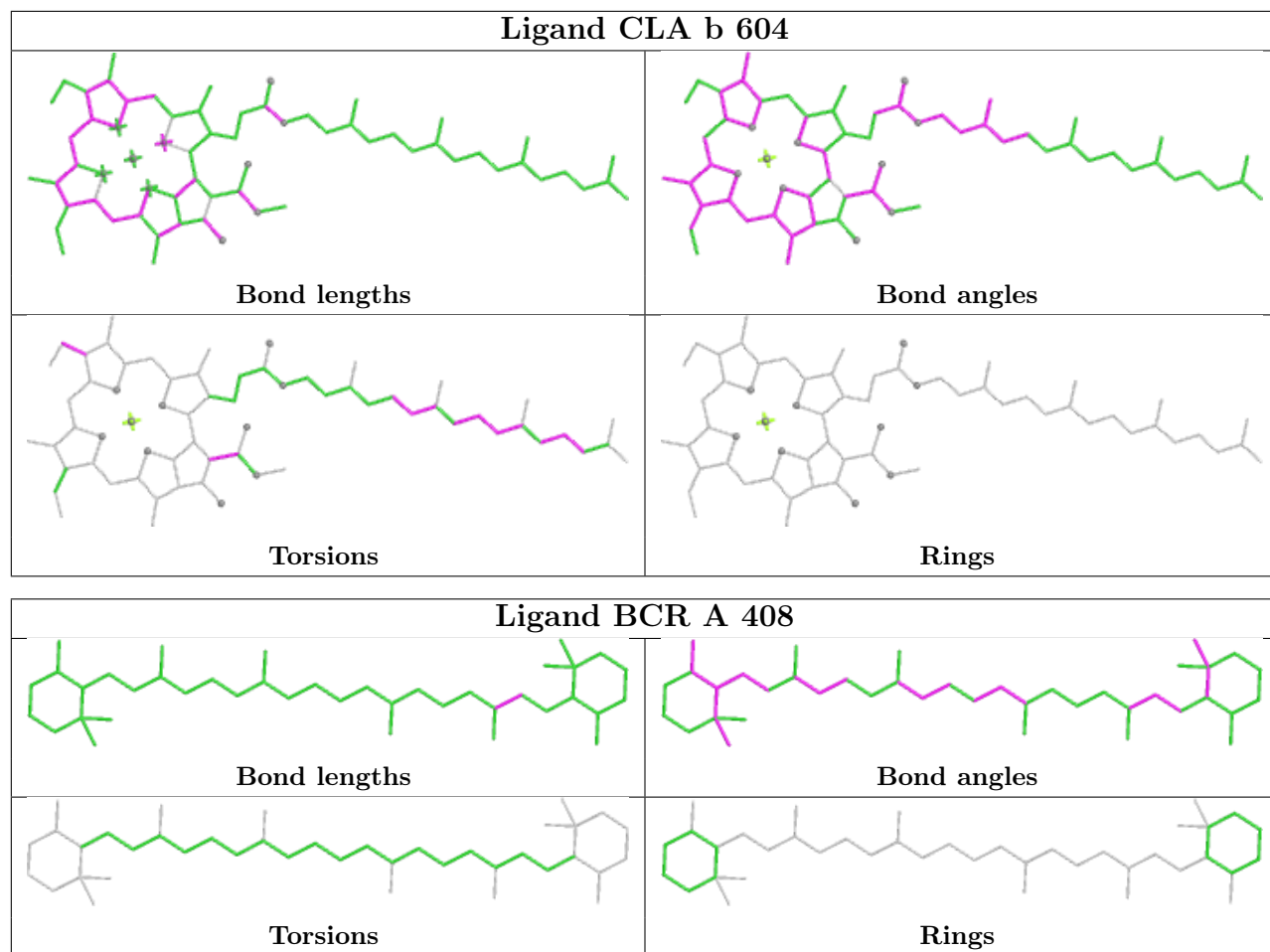
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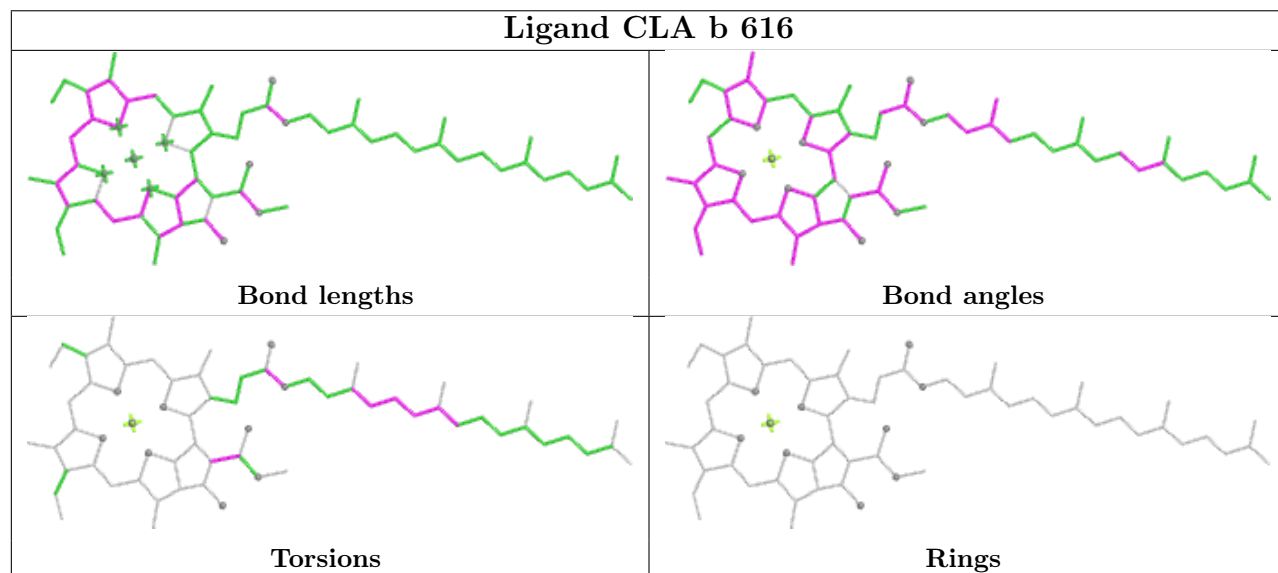
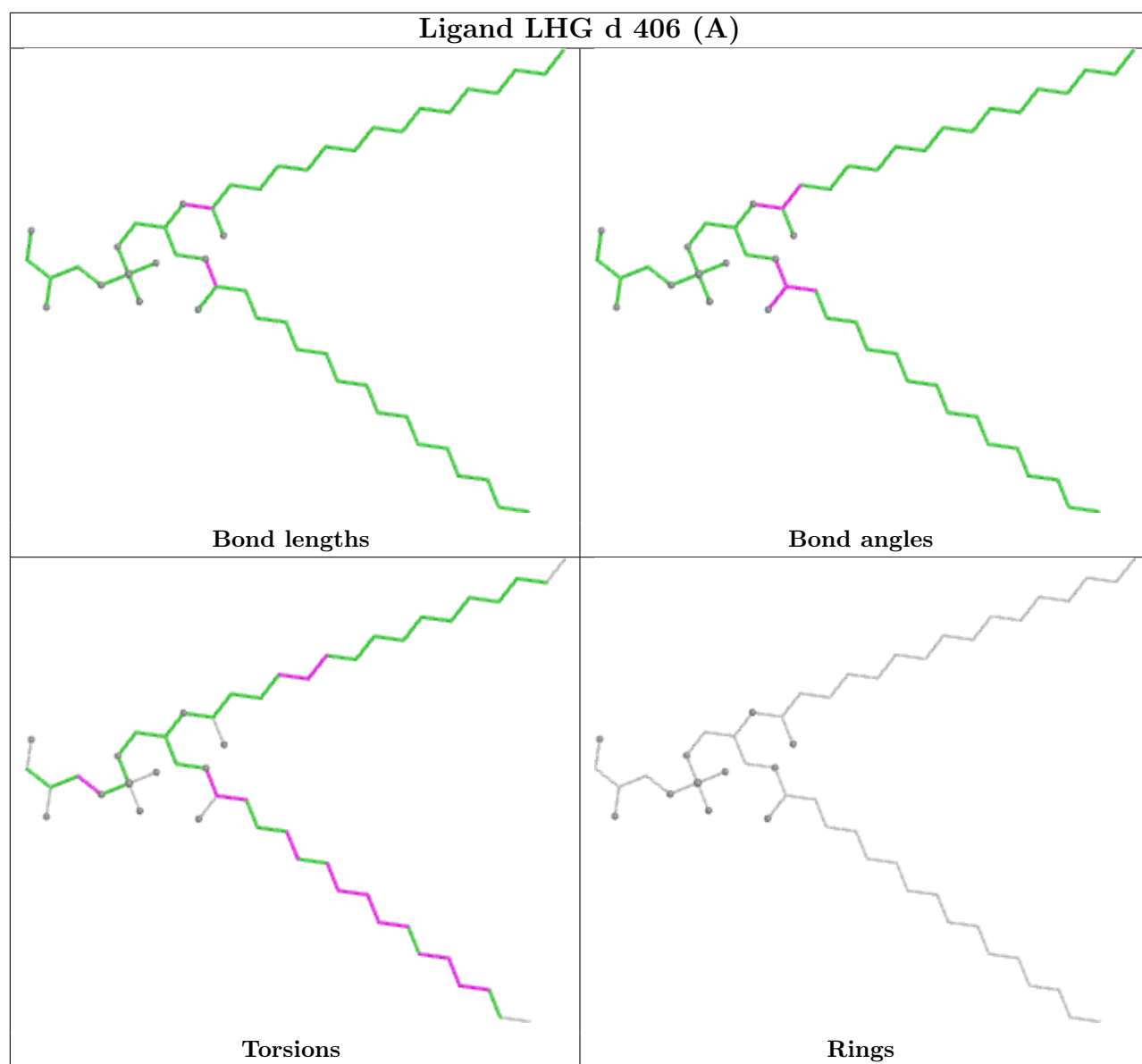
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	524[B]	GOL	1	0
33	C	526	LMG	1	0
23	B	613	CLA	3	0
33	c	521	LMG	1	0
32	L	101[B]	LHG	1	0
25	l	801[A]	GOL	1	0
24	T	102	BCR	6	0

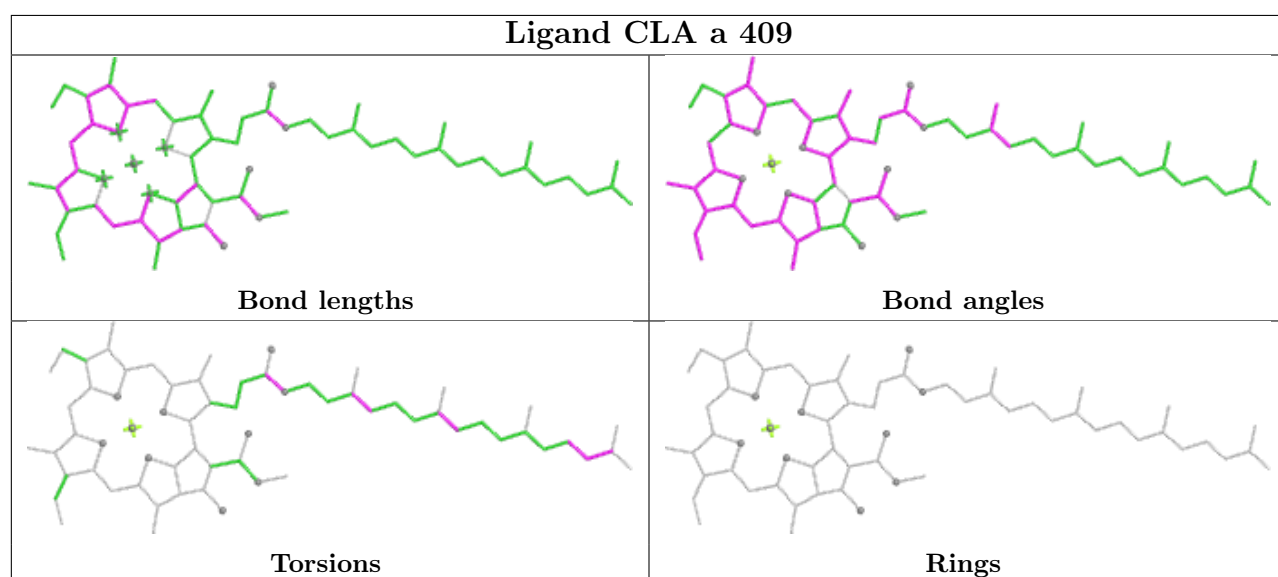
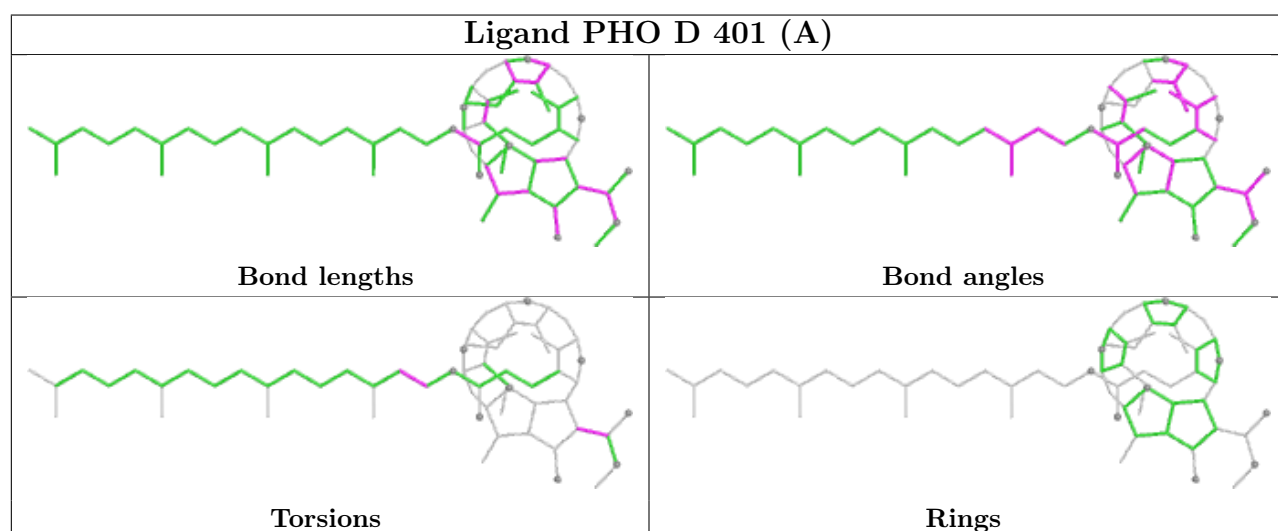
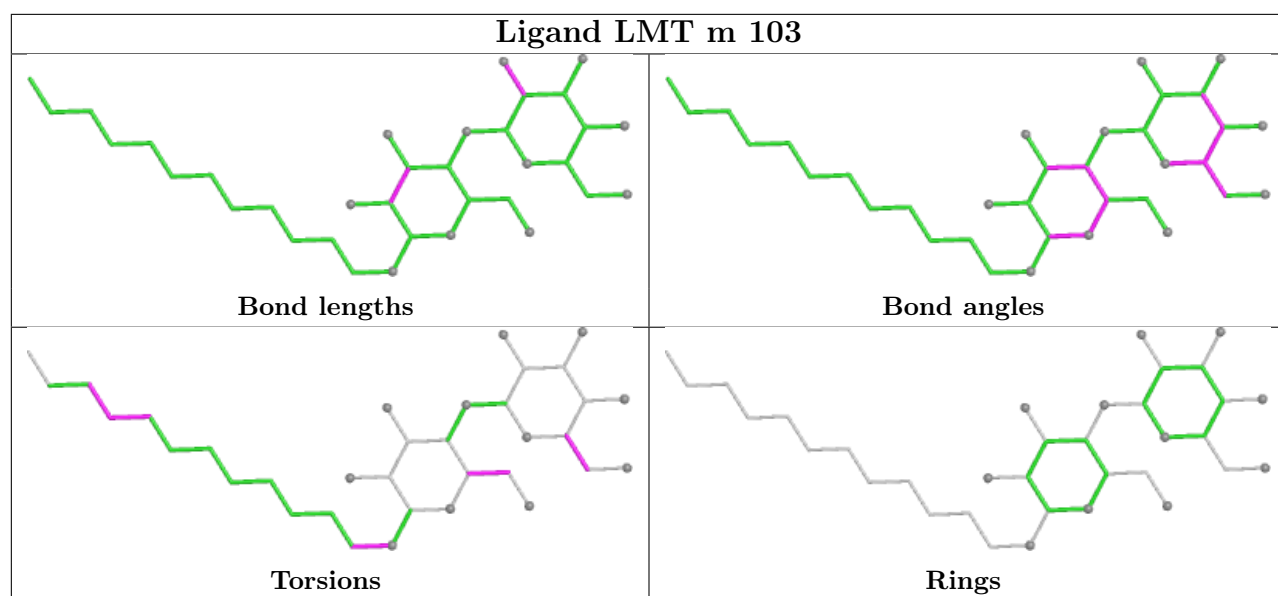
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



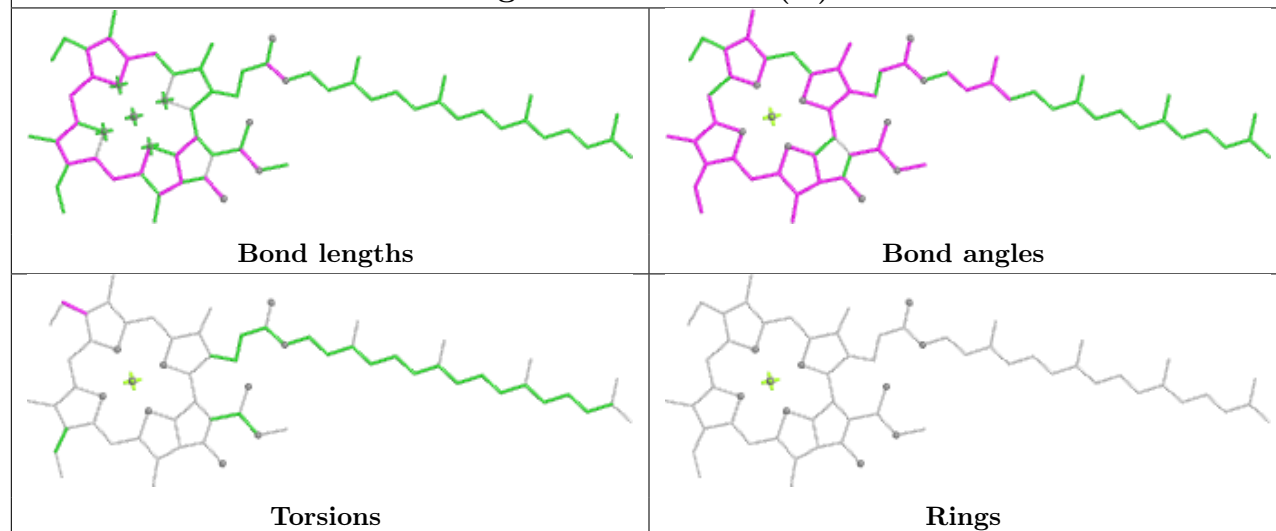




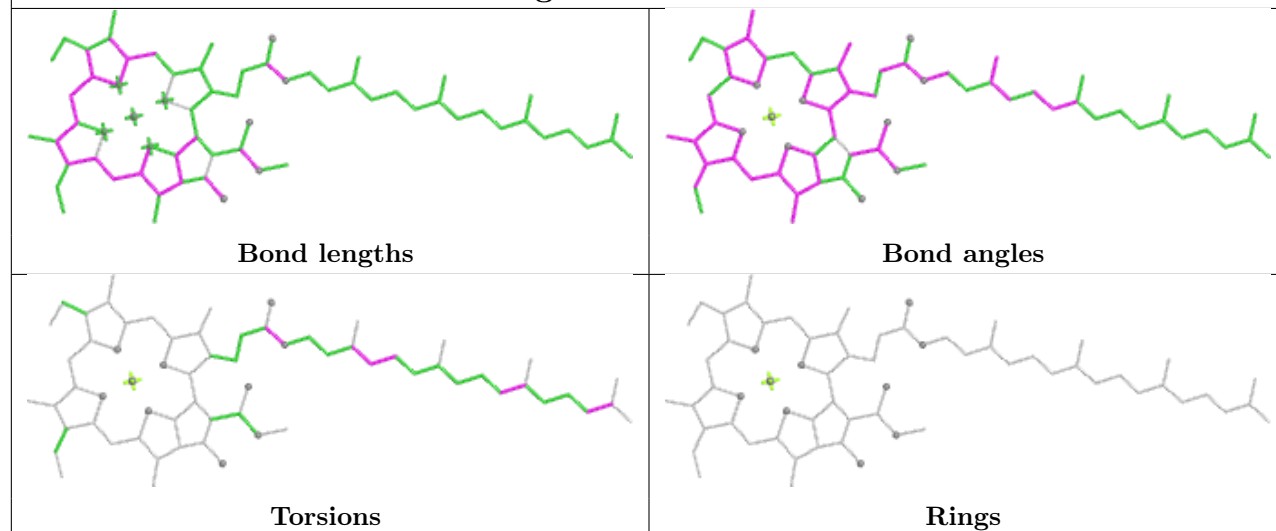


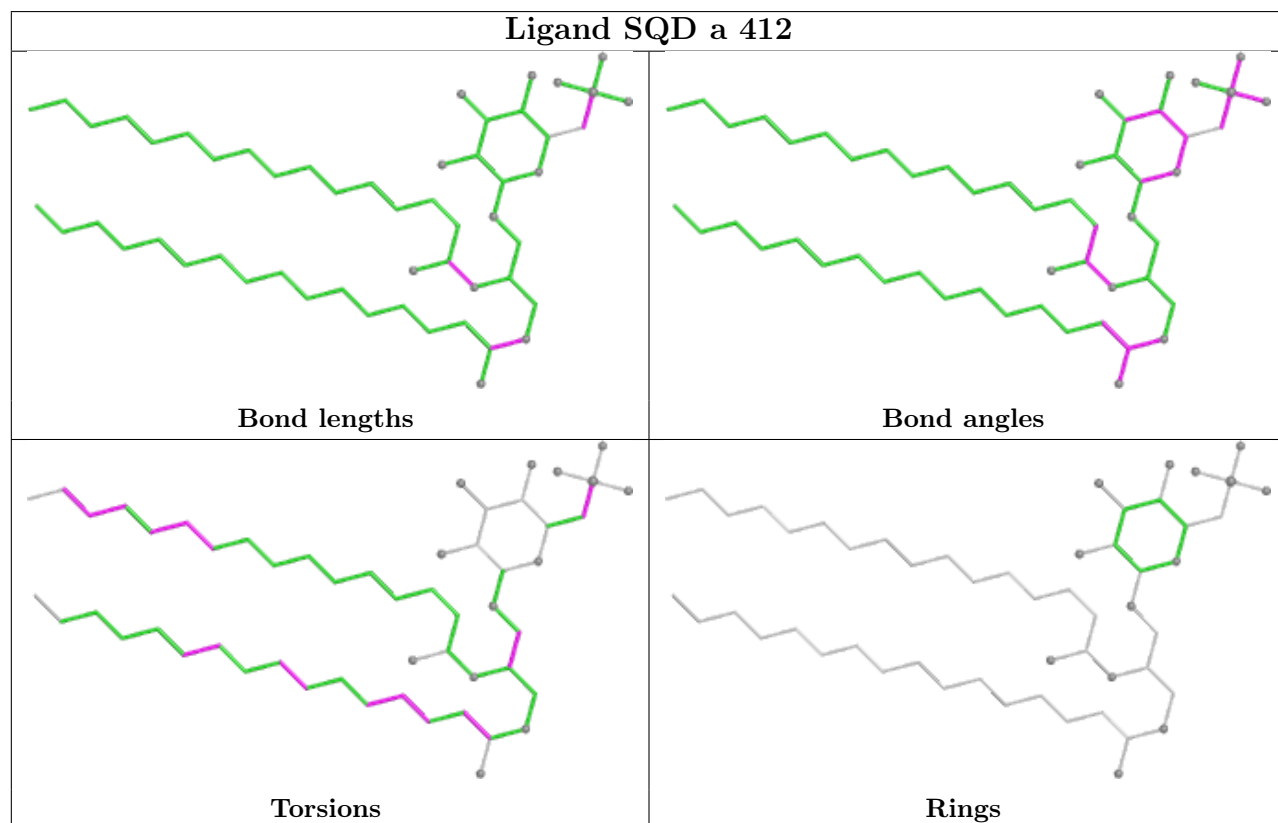
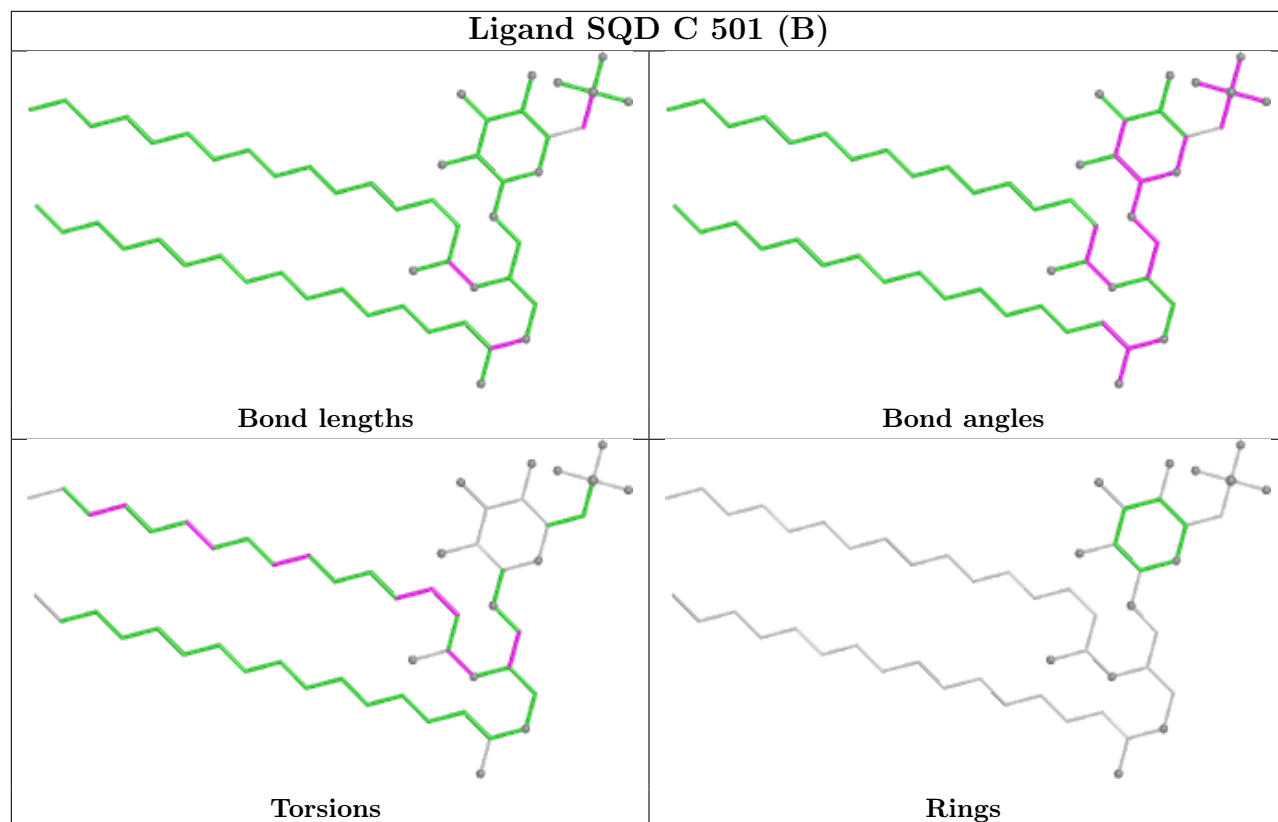


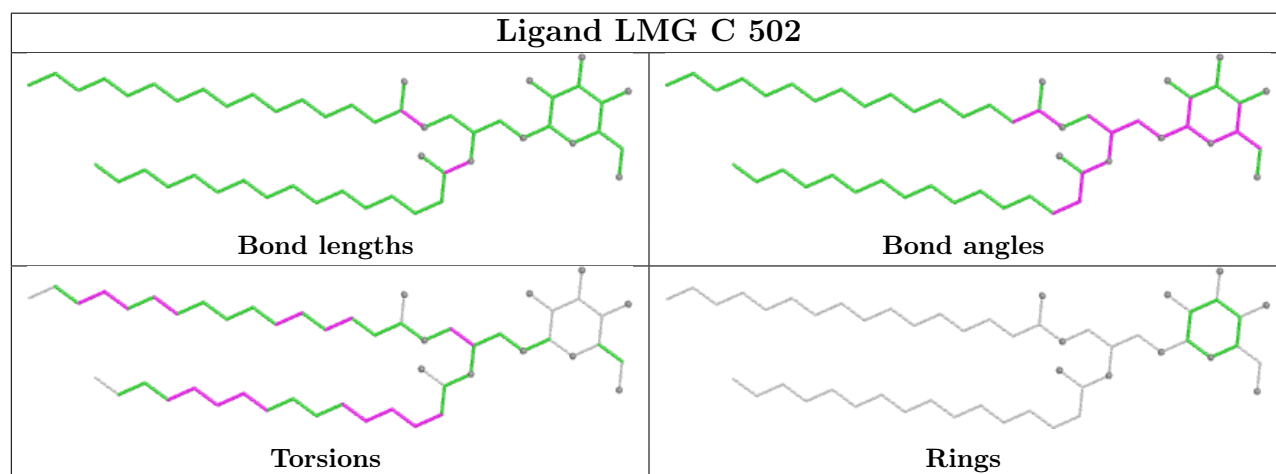
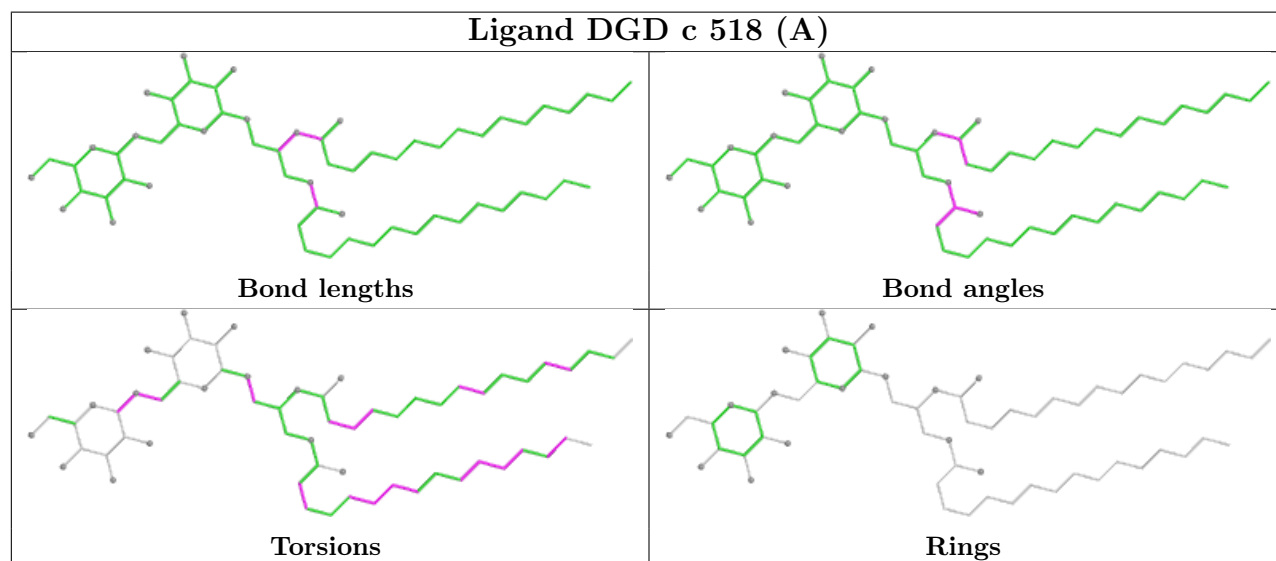
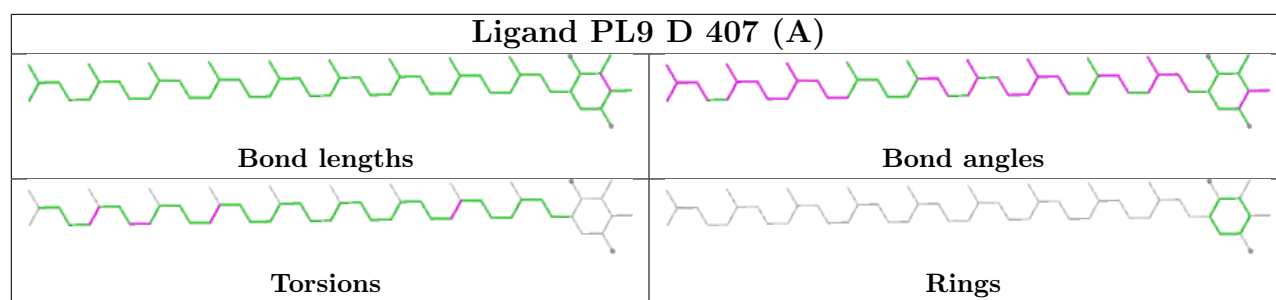
Ligand CLA D 404 (A)

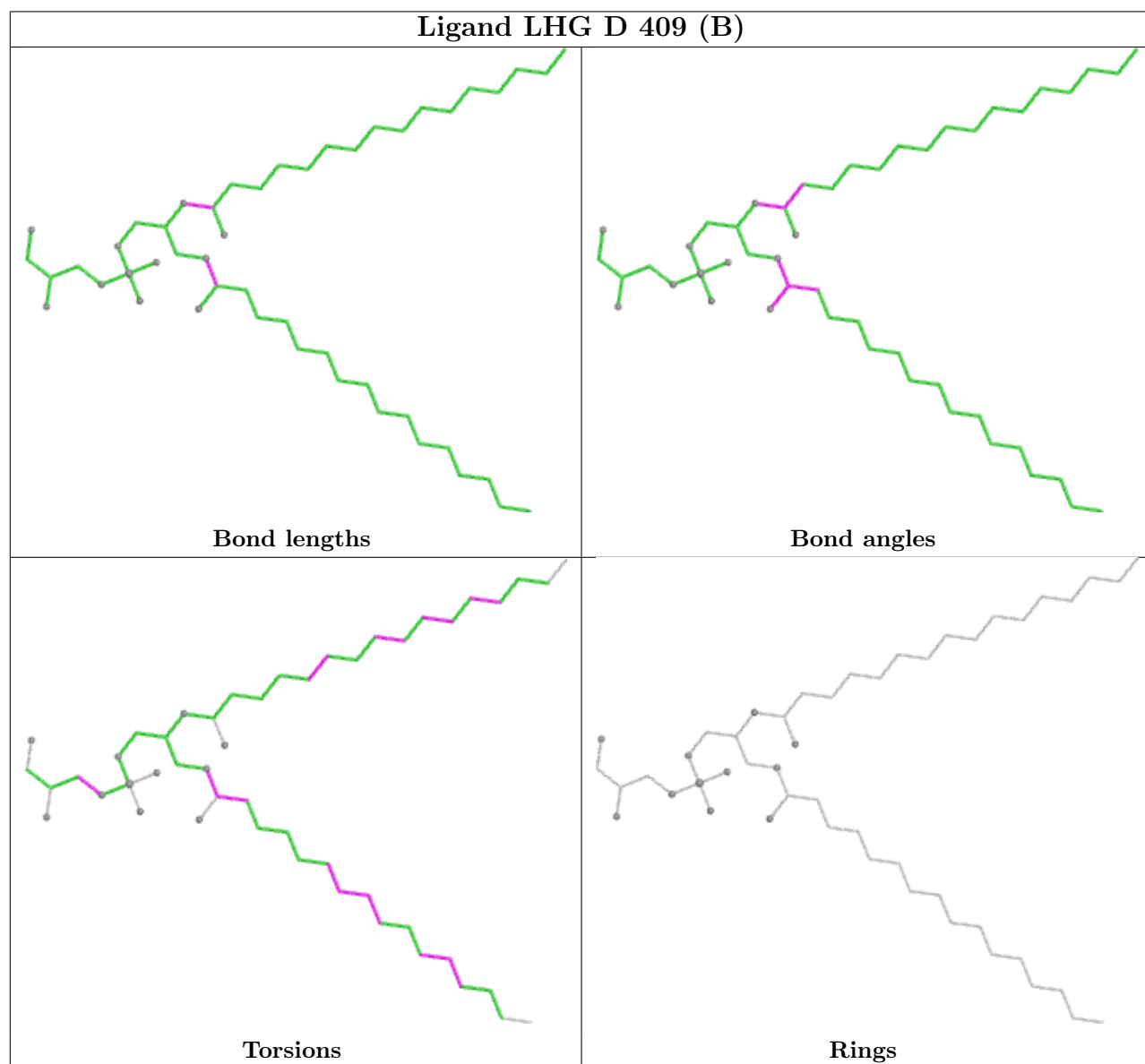
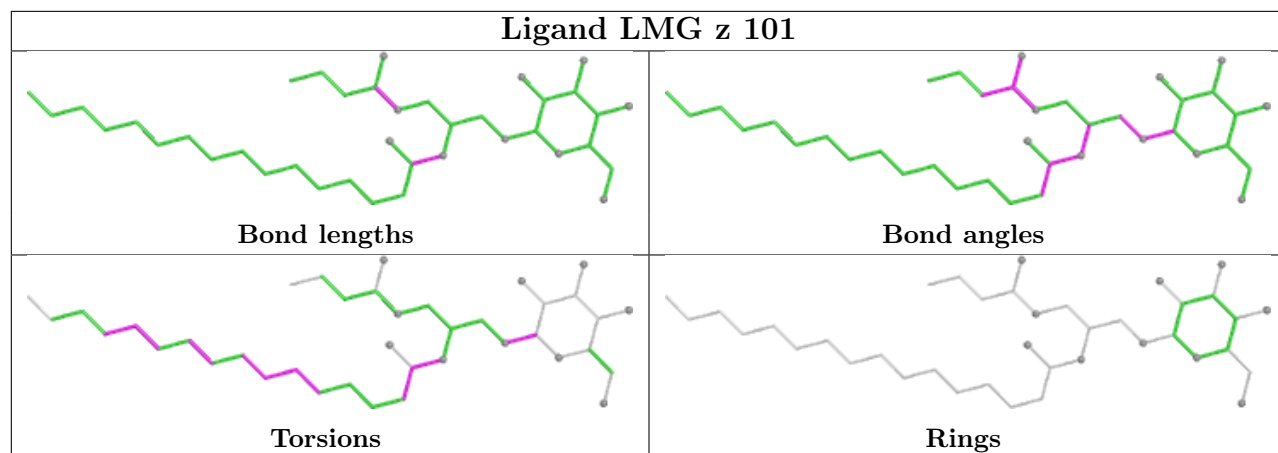


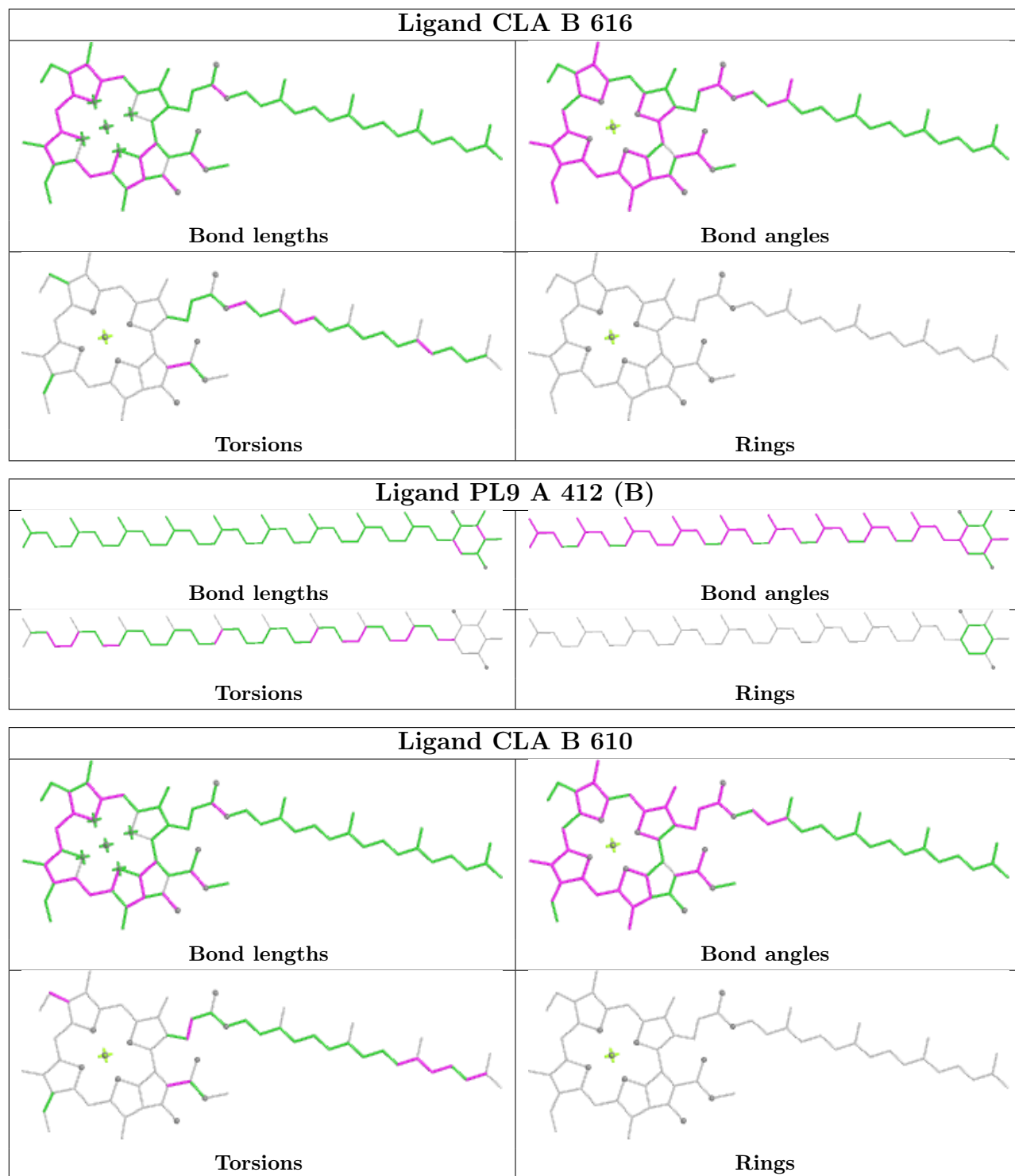
Ligand CLA d 402

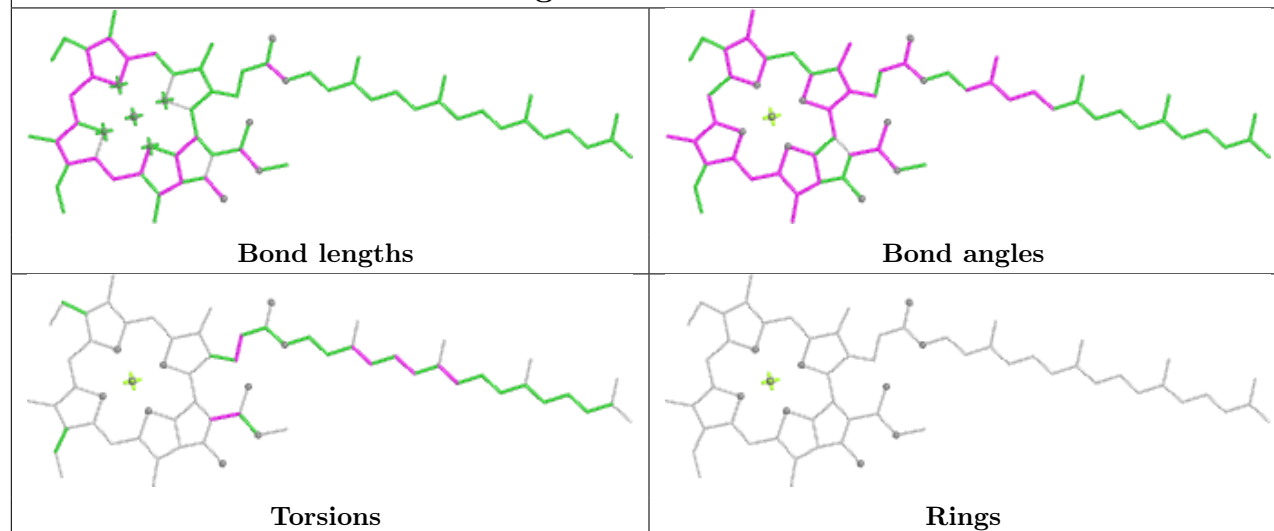
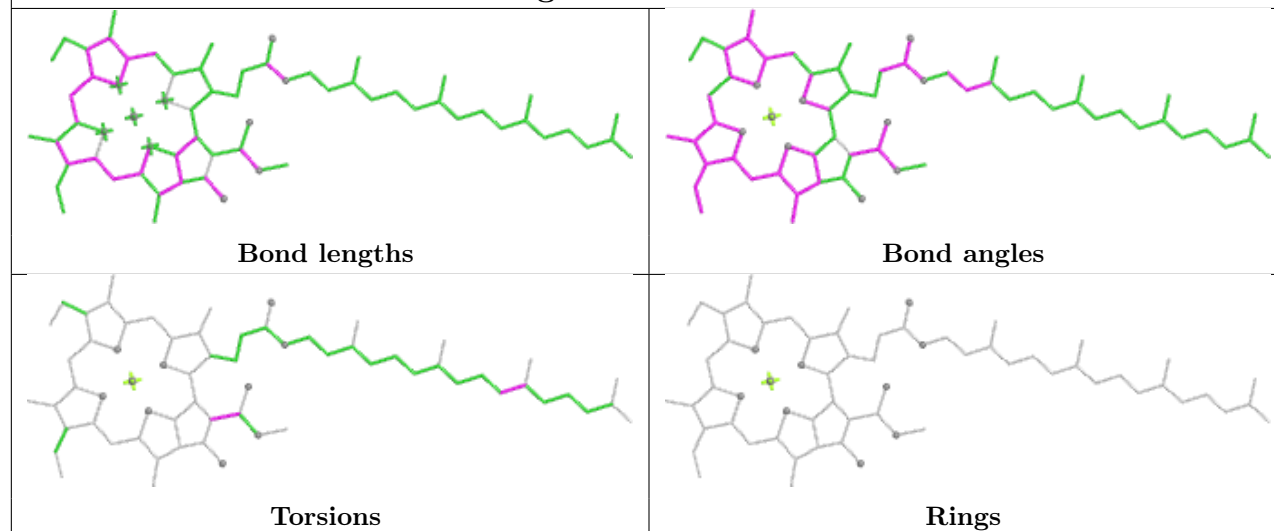
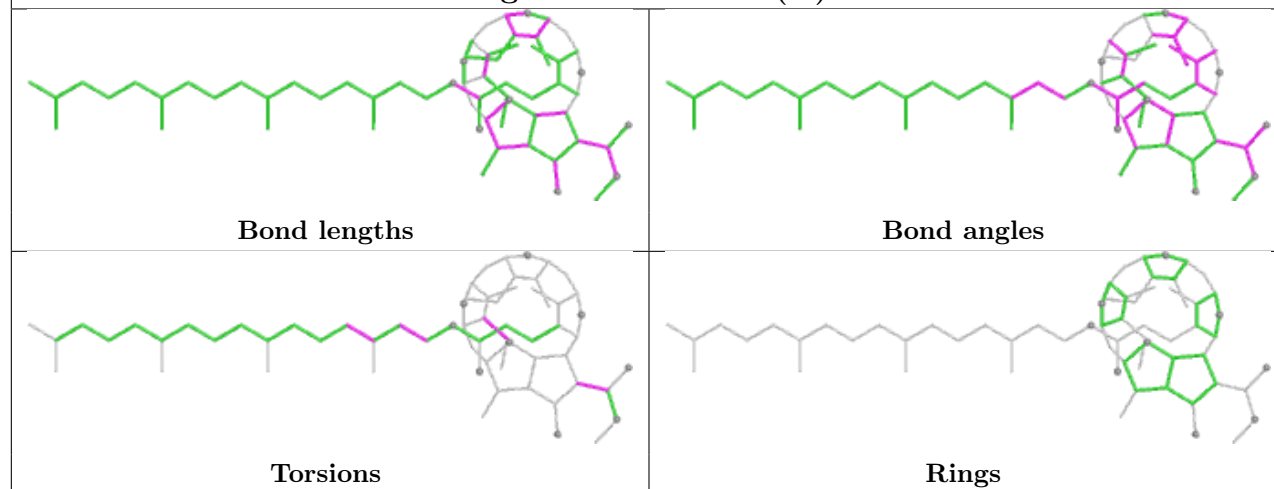


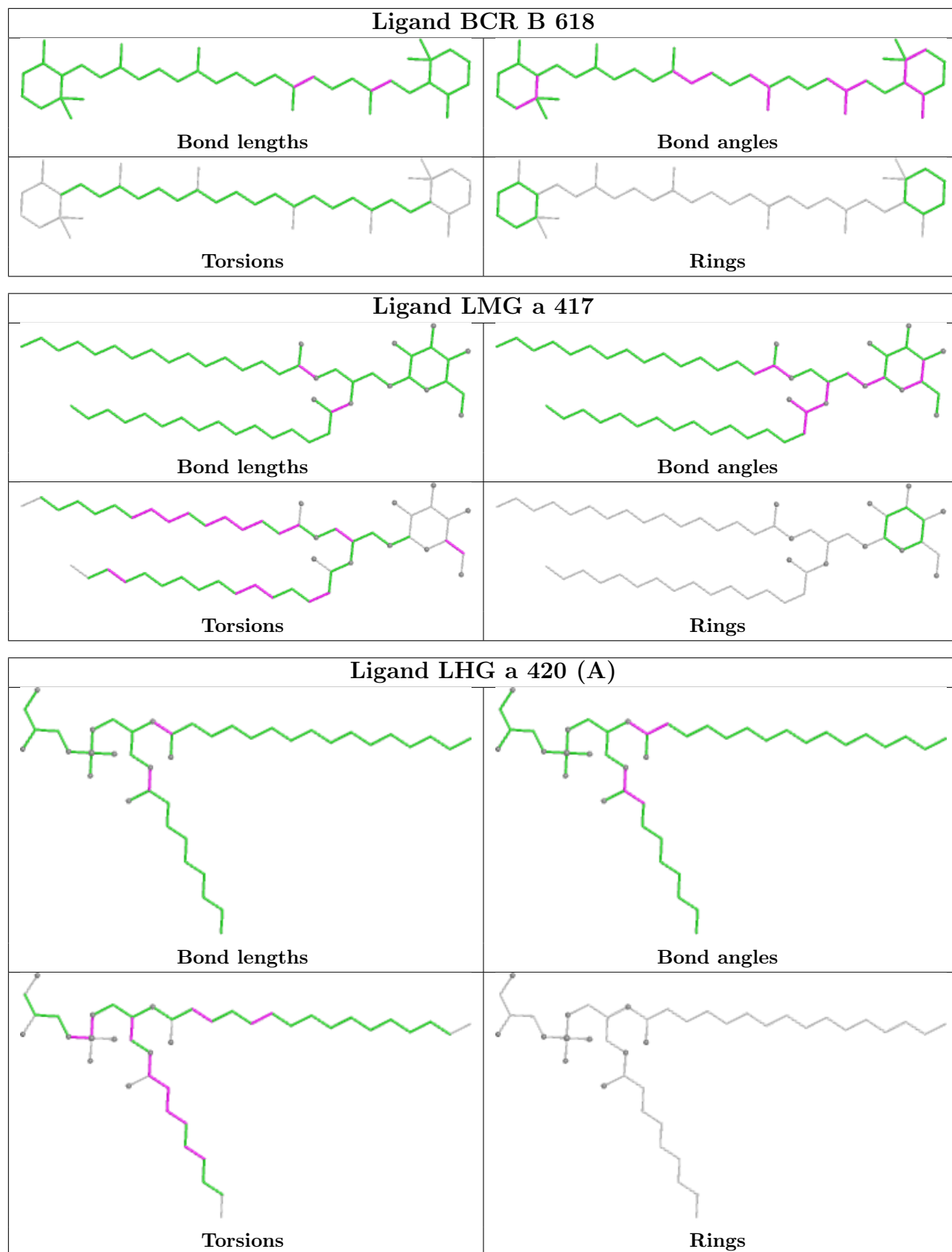


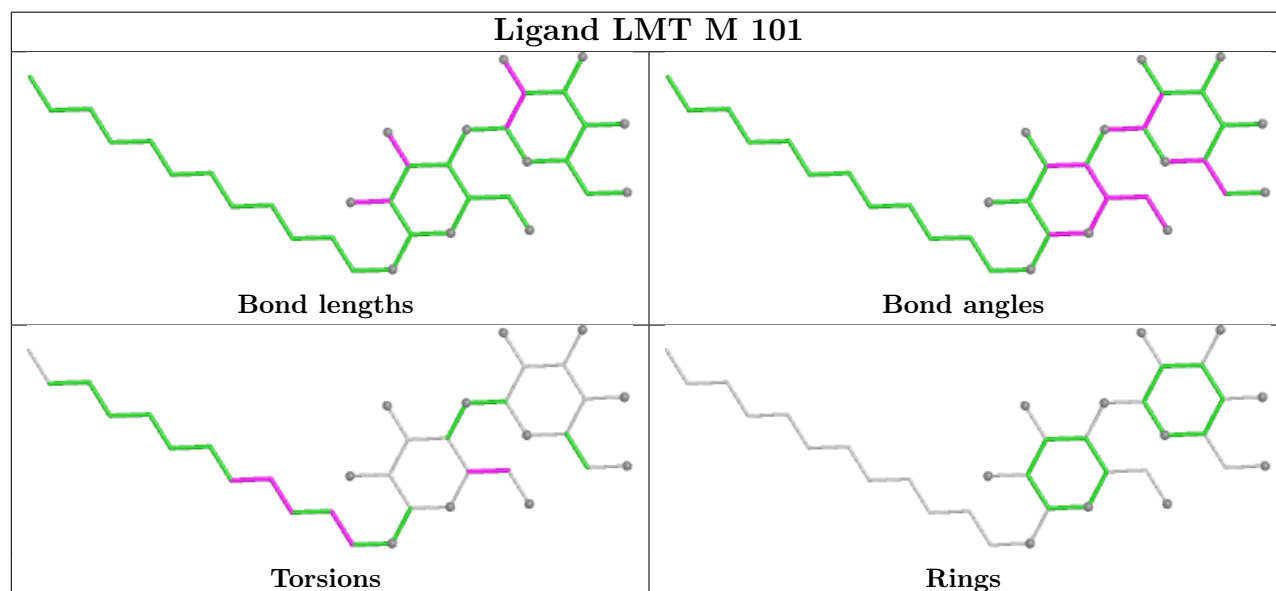
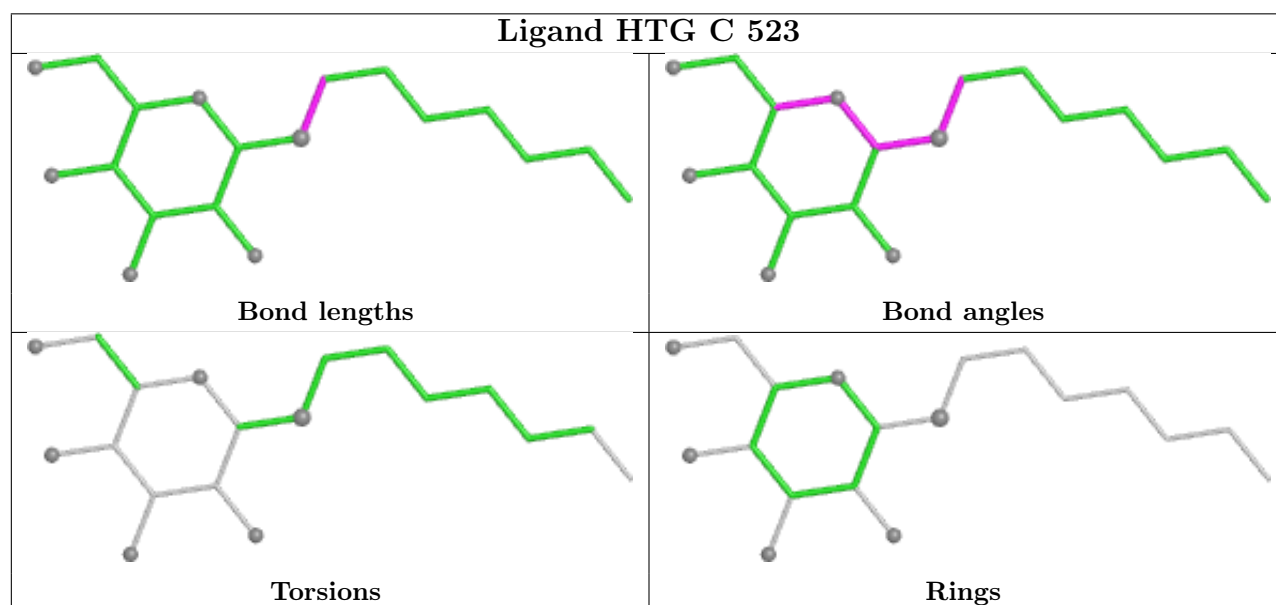
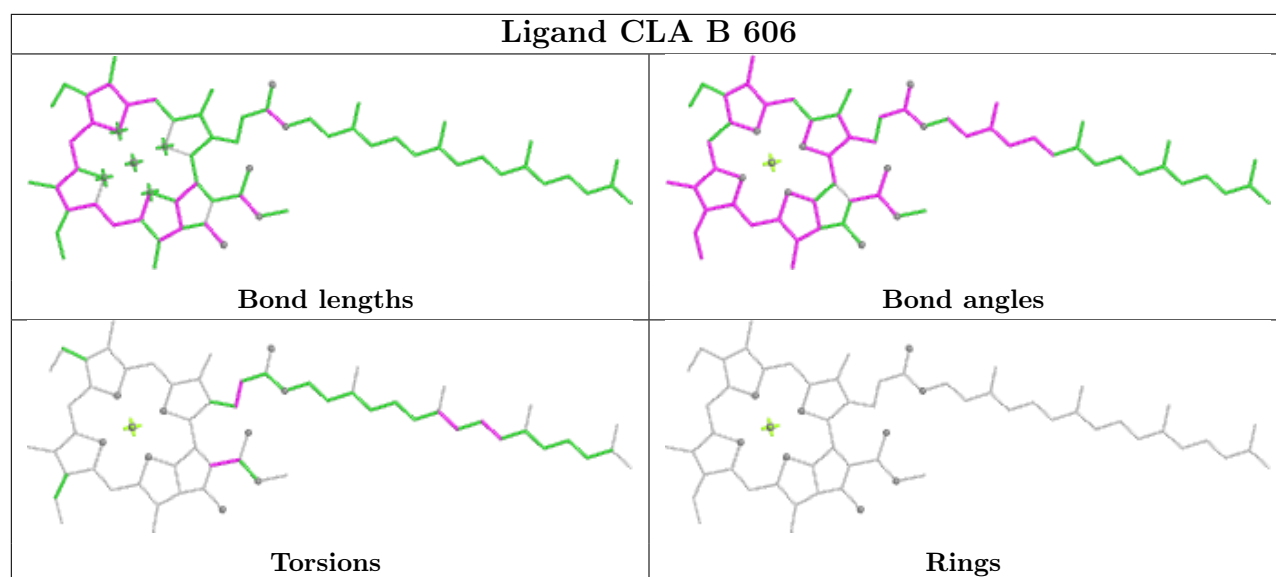


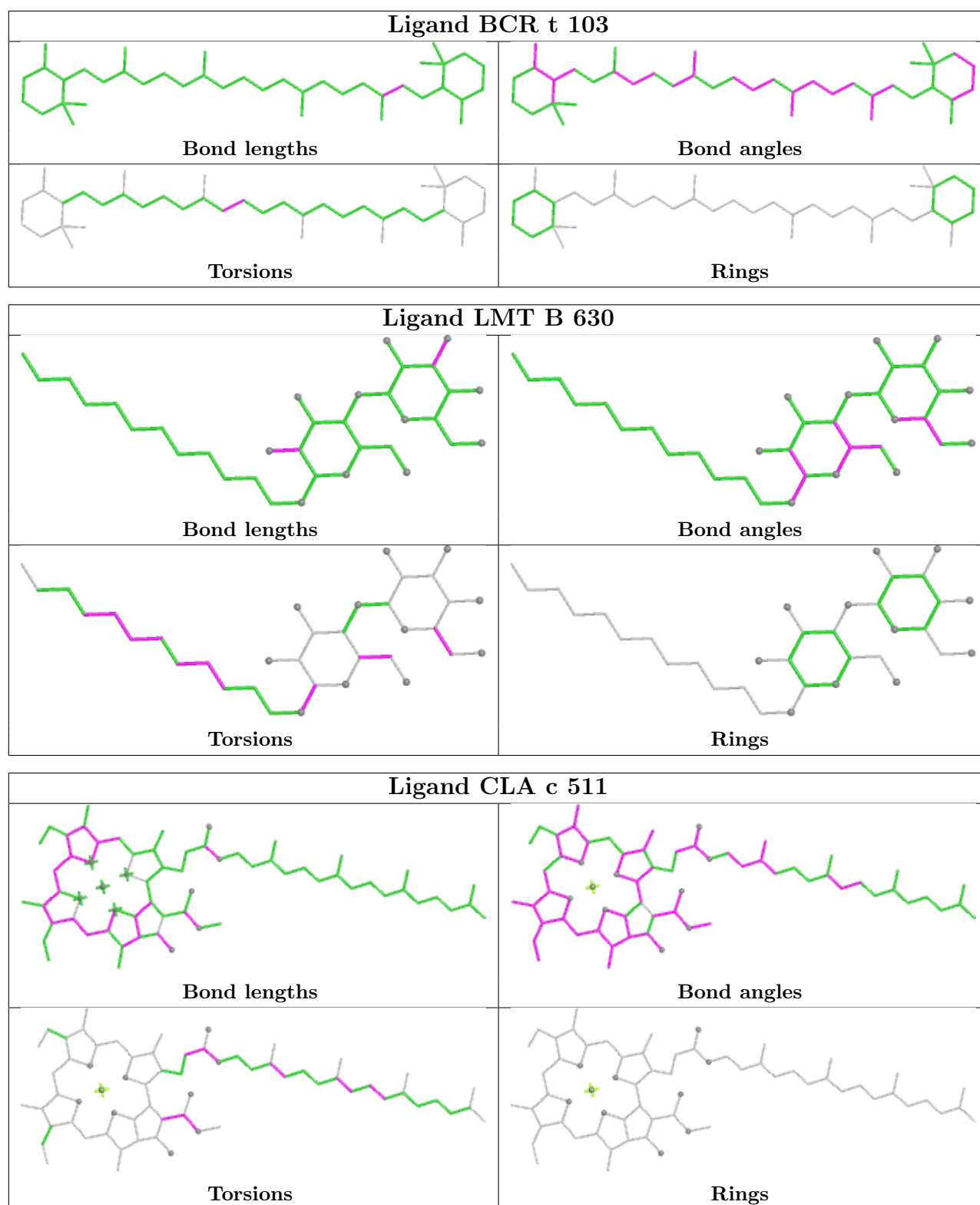


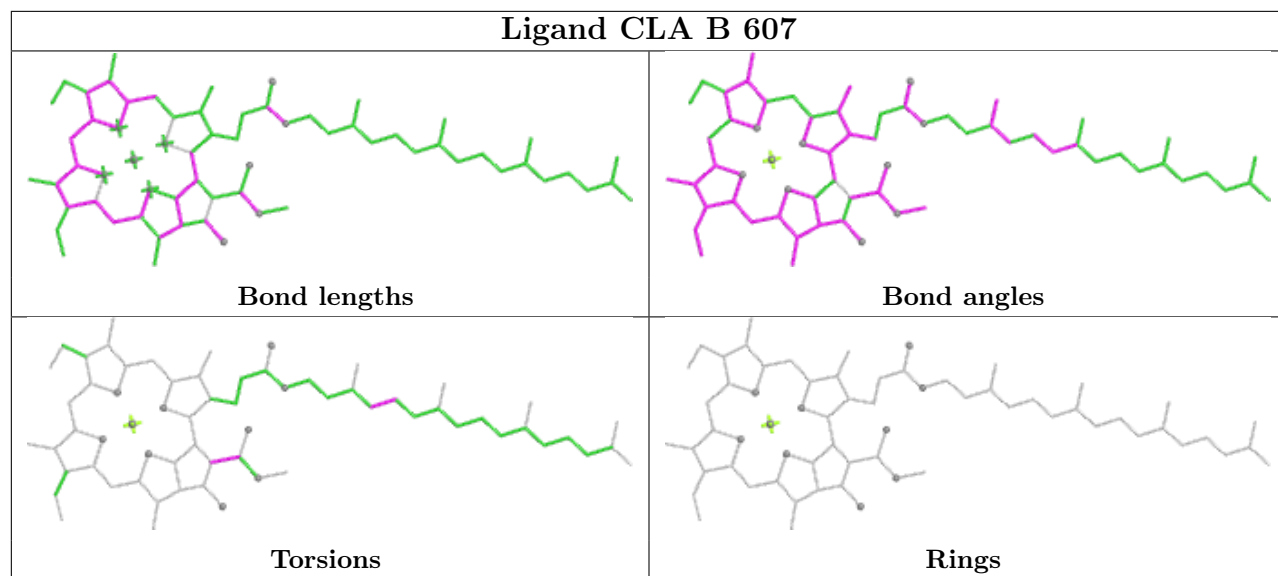


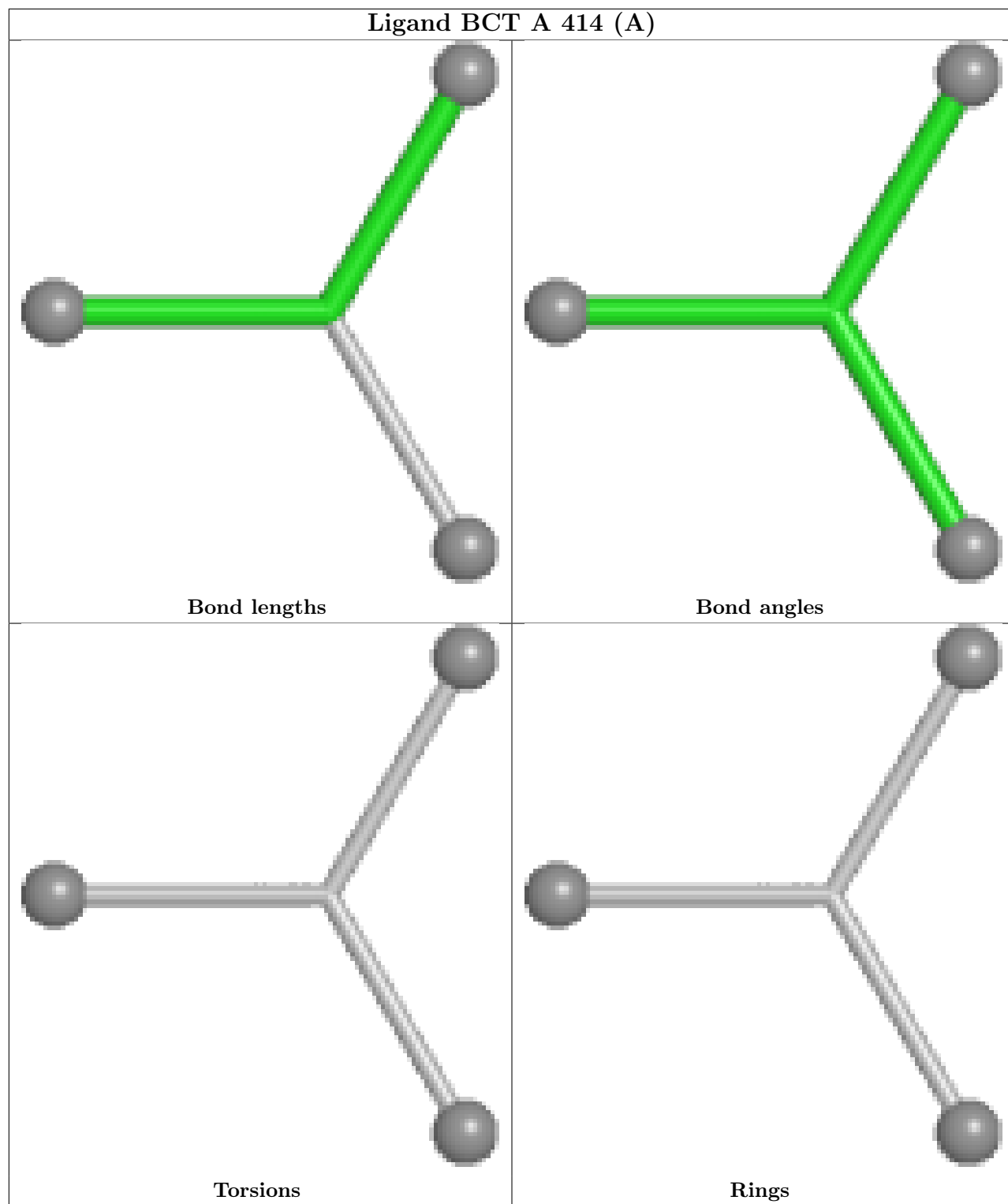
Ligand CLA b 603**Ligand CLA c 503****Ligand PHO a 408 (A)**

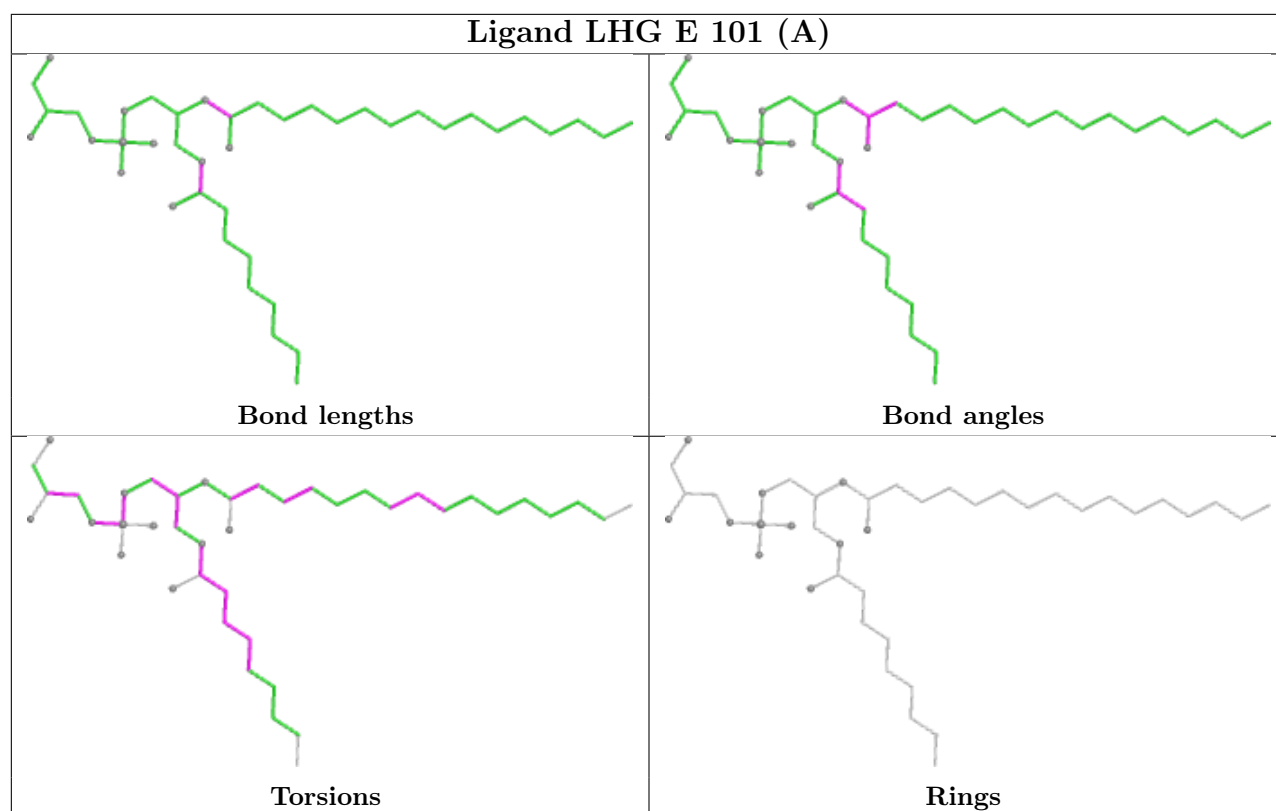


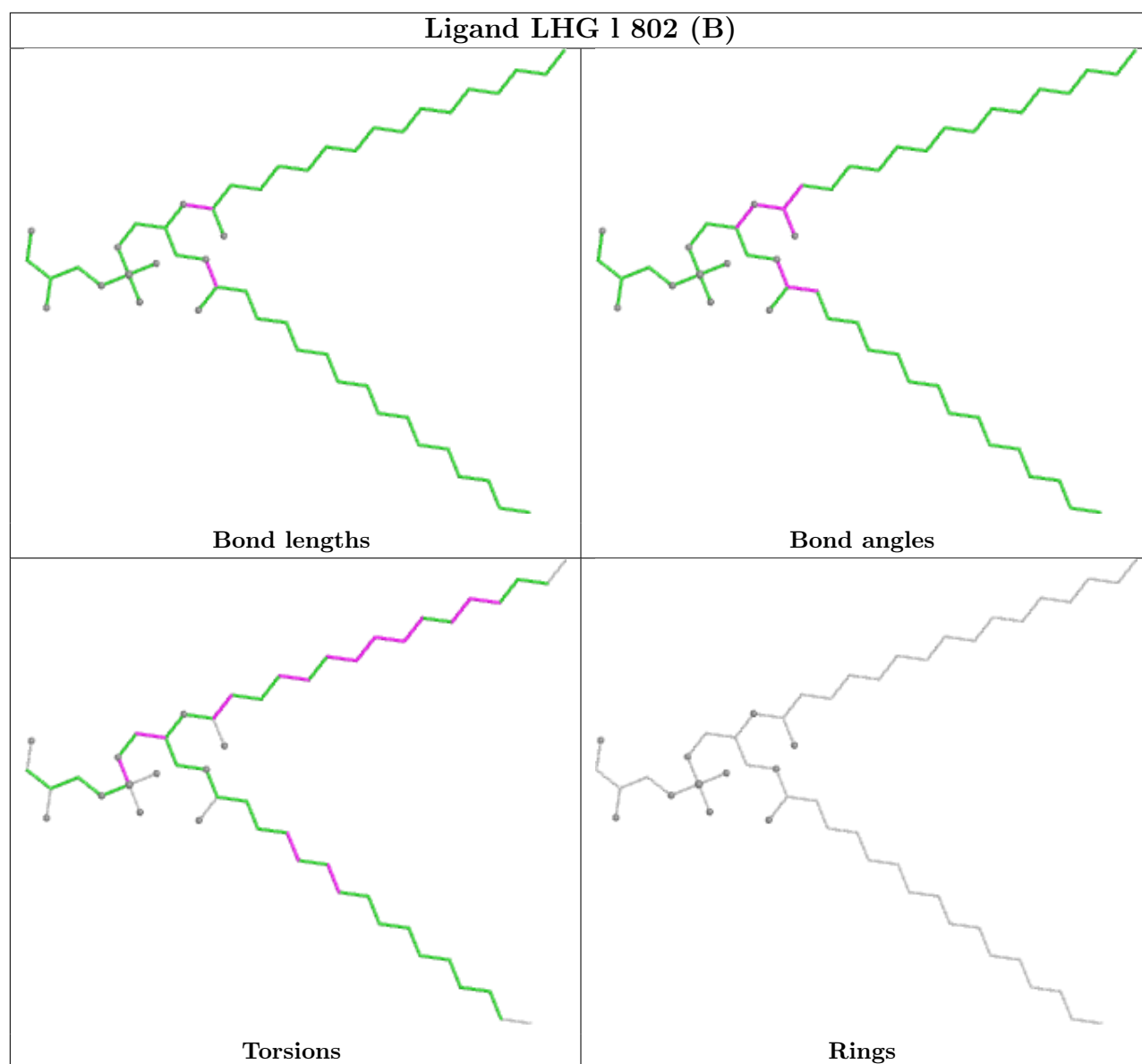


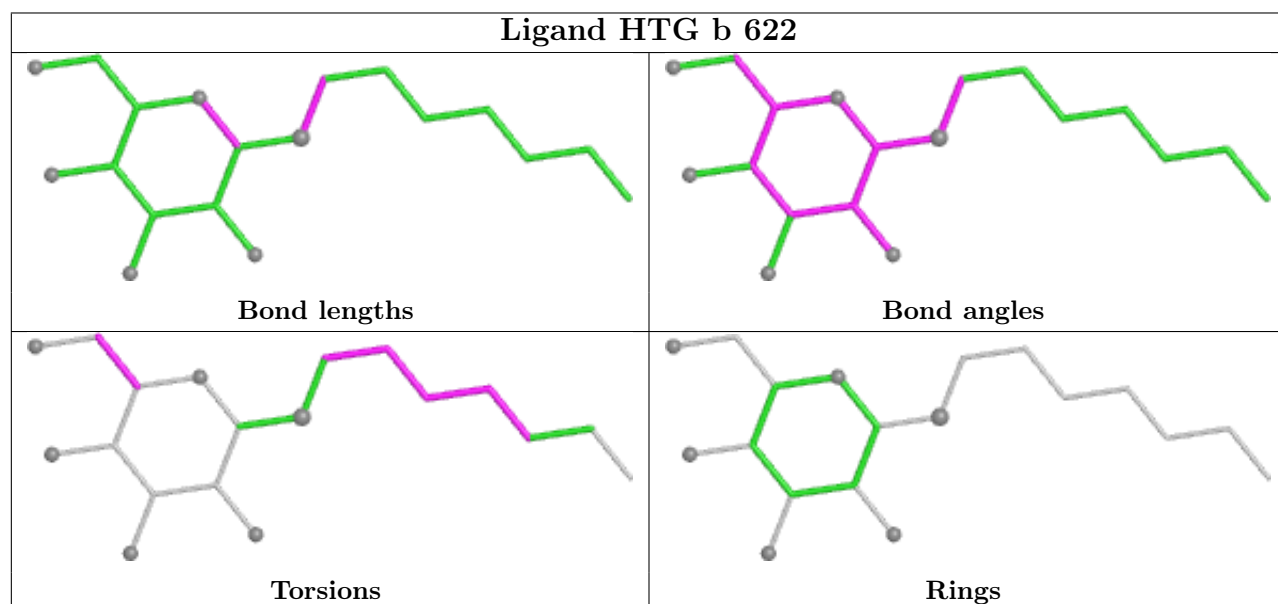
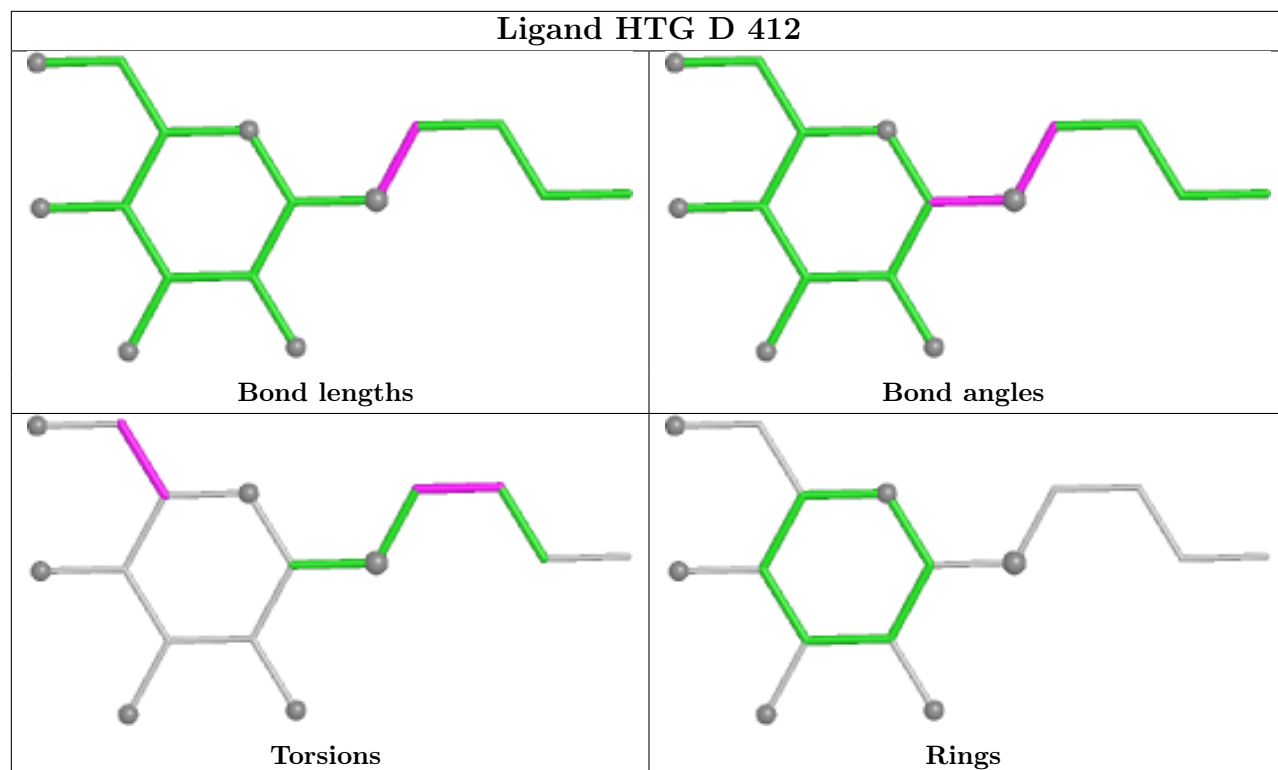




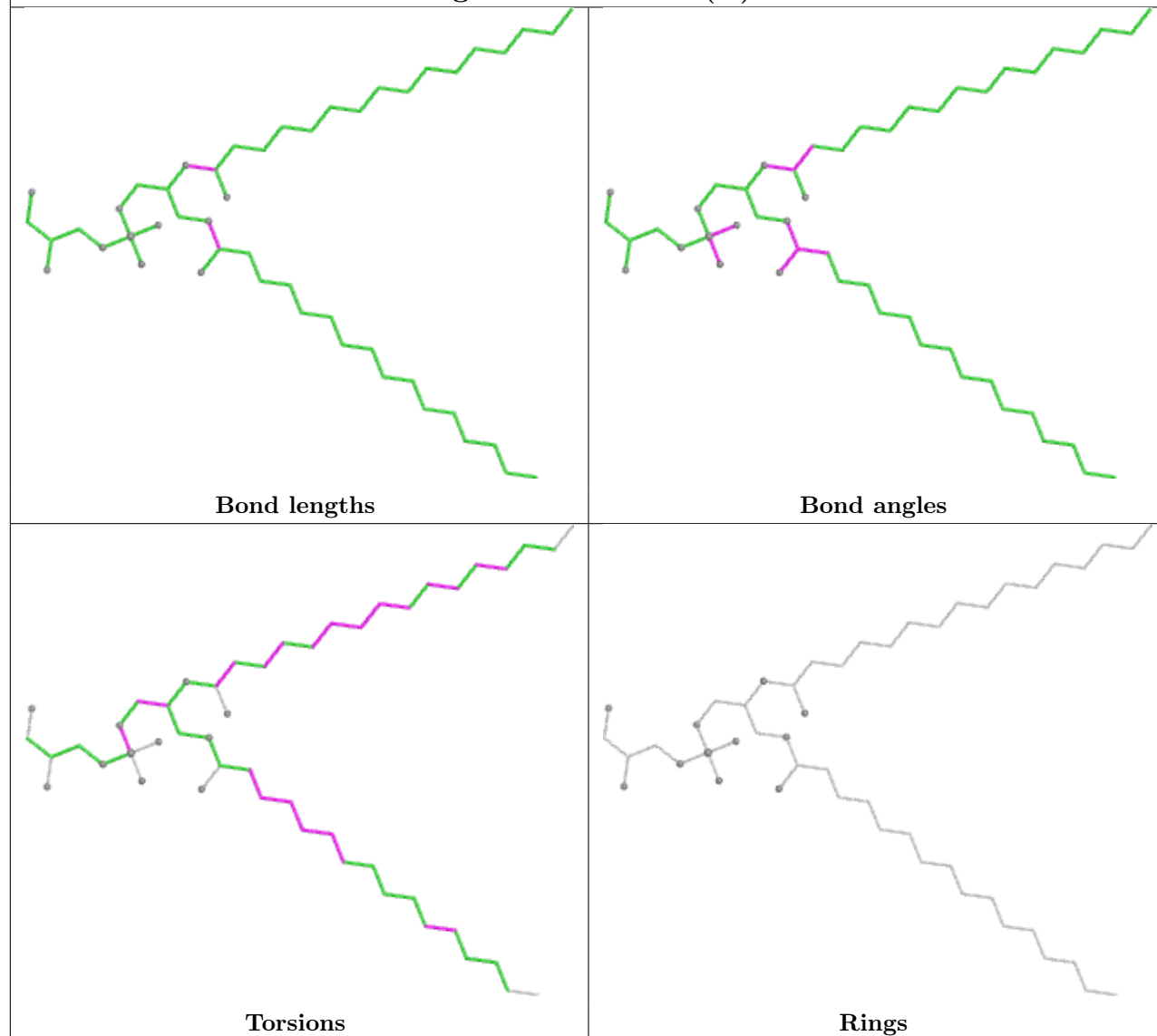




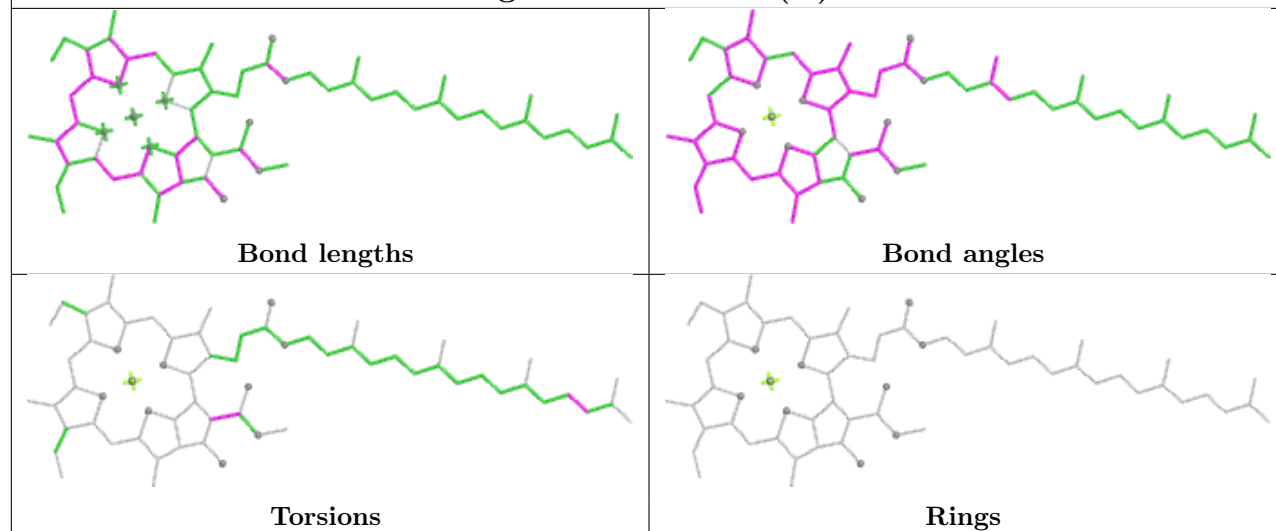


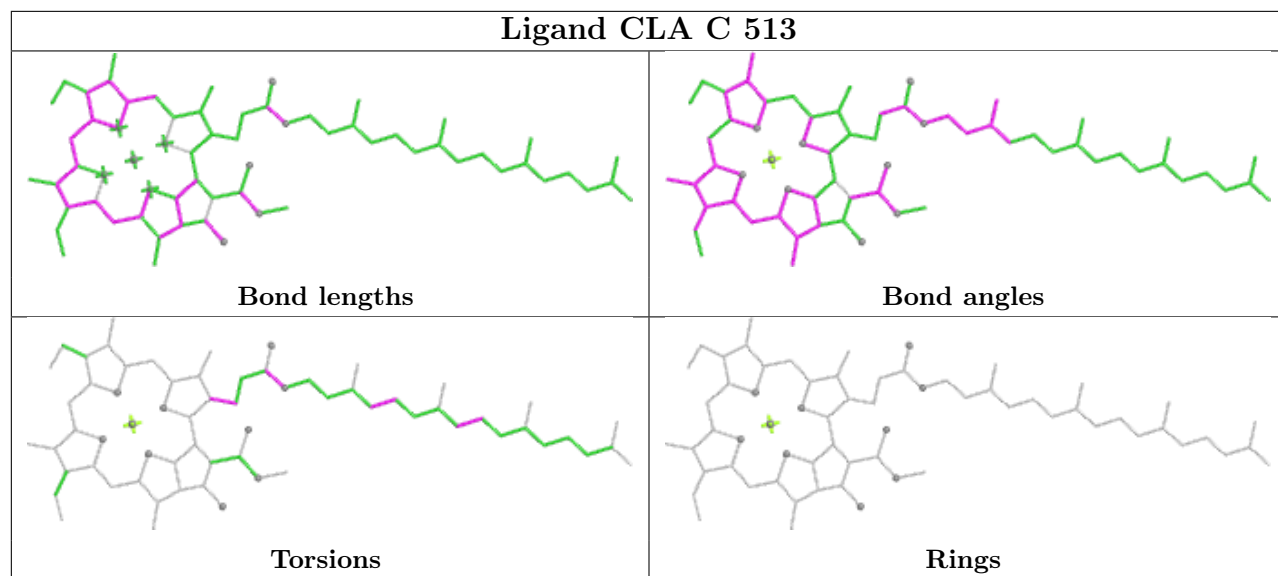
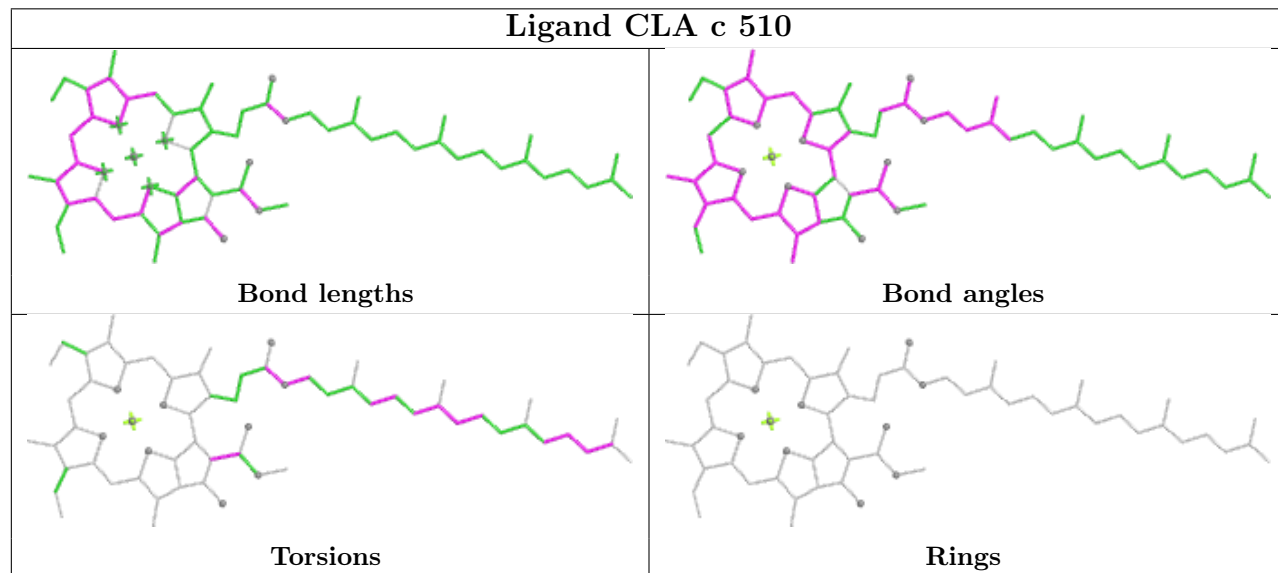


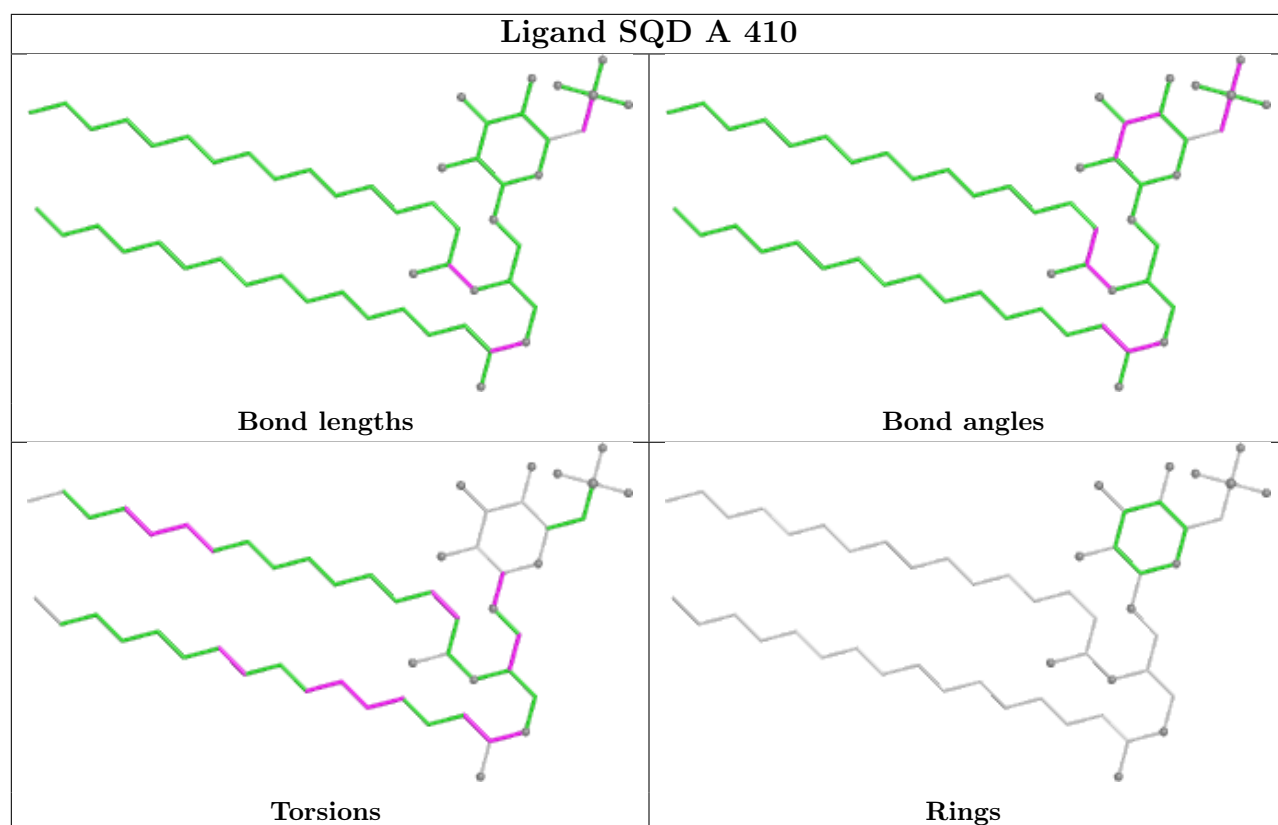
Ligand LHG L 101 (A)



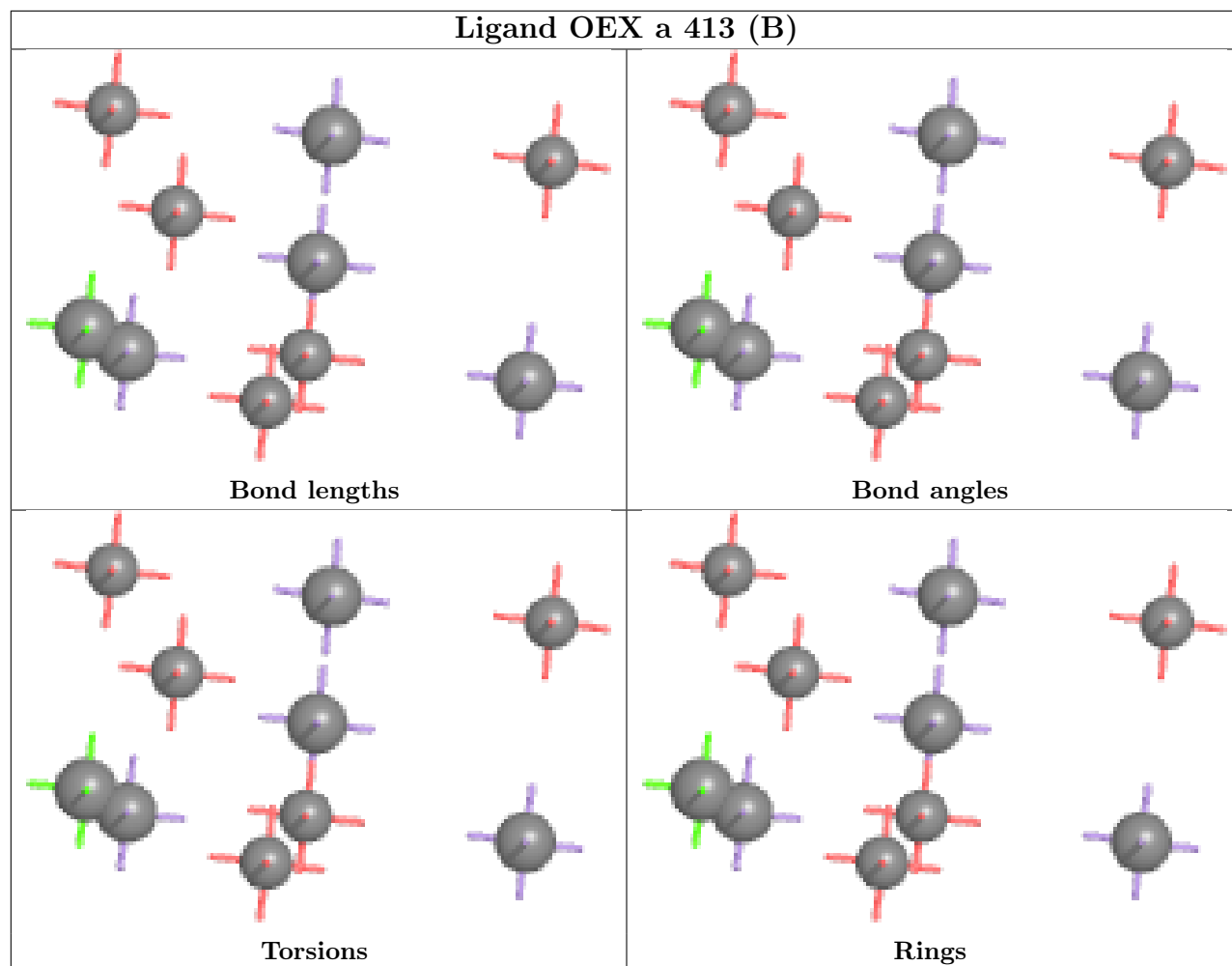
Ligand CLA A 405 (A)

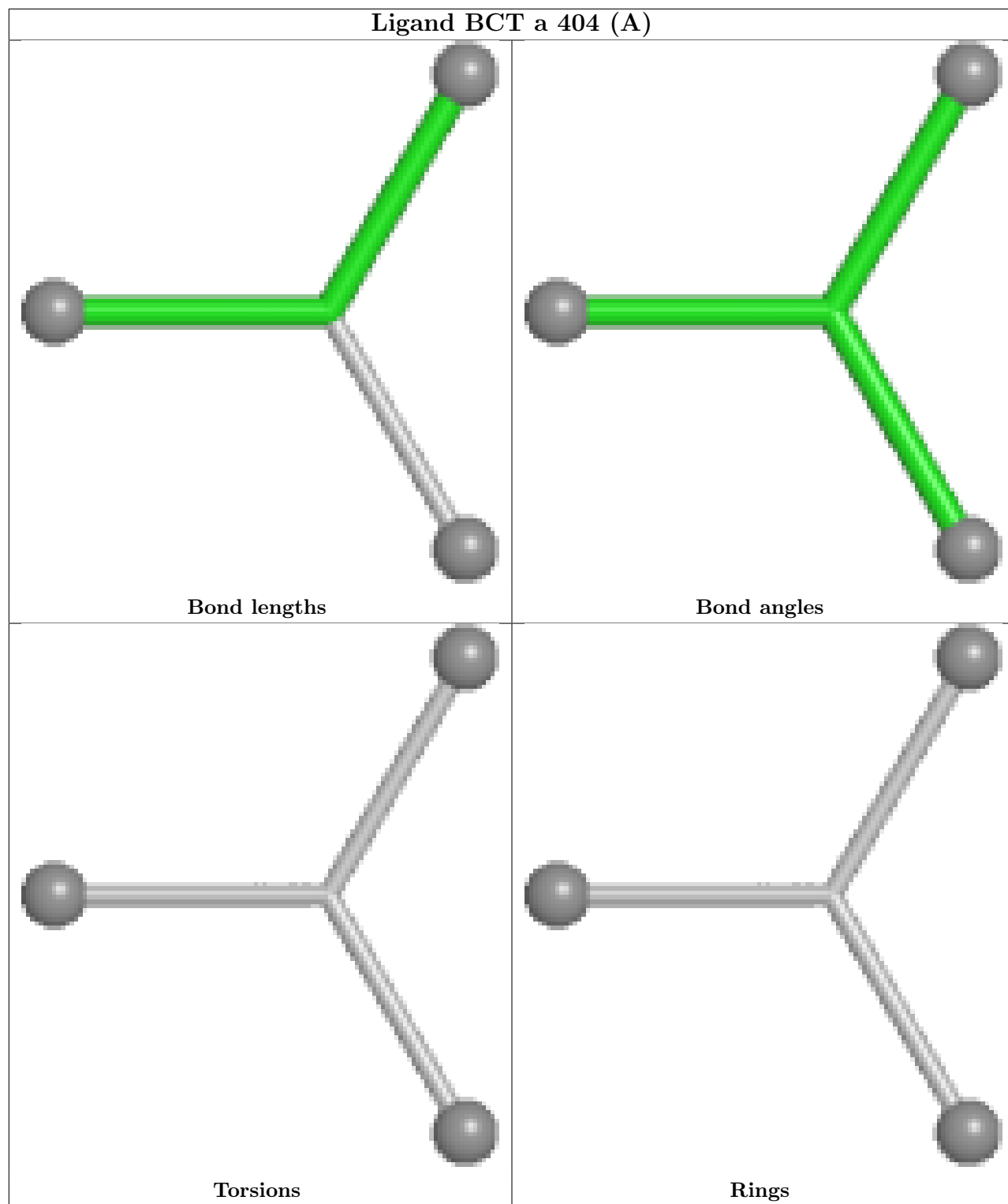


Ligand CLA C 513**Ligand CLA c 510**

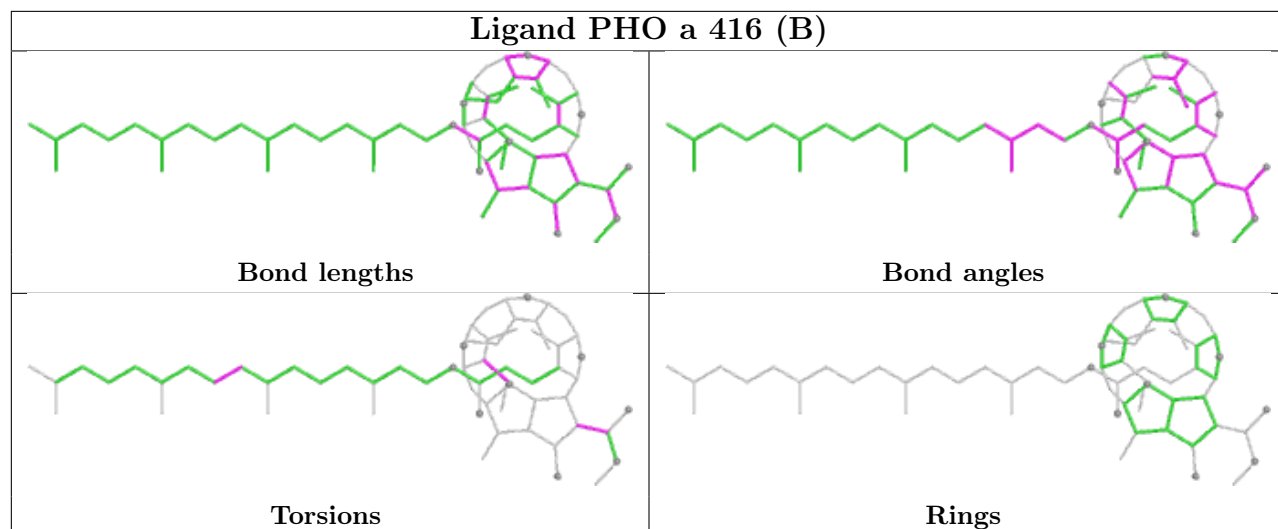


Ligand OEX a 413 (B)

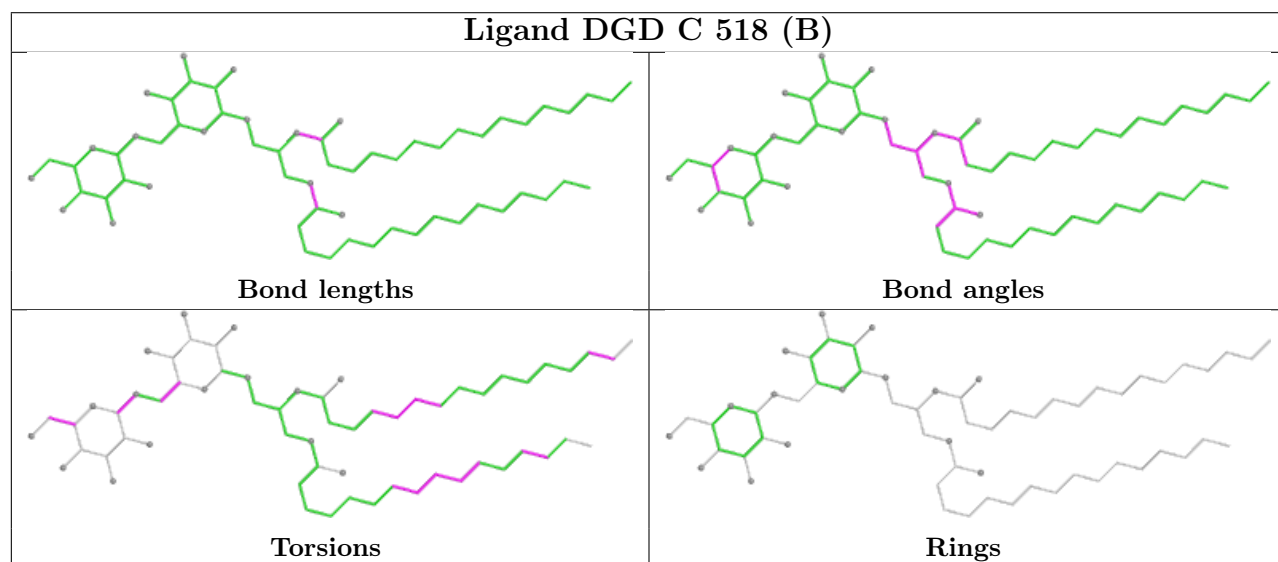




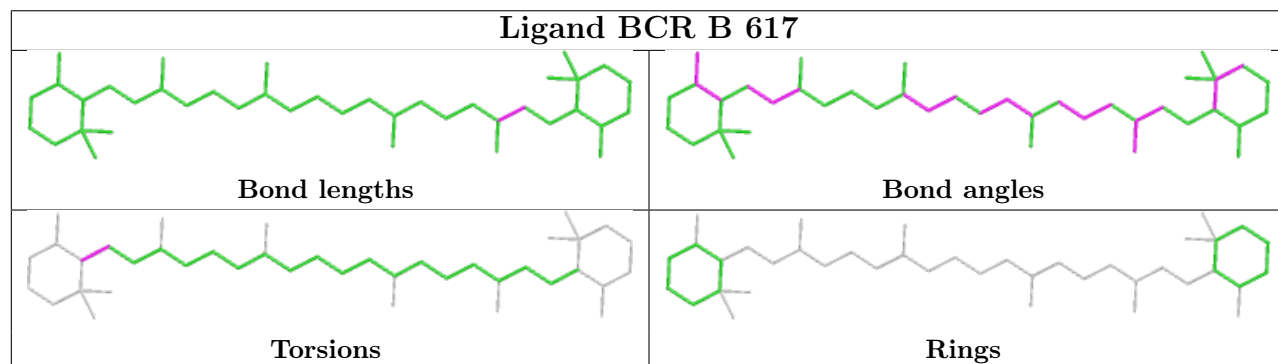
Ligand PHO a 416 (B)

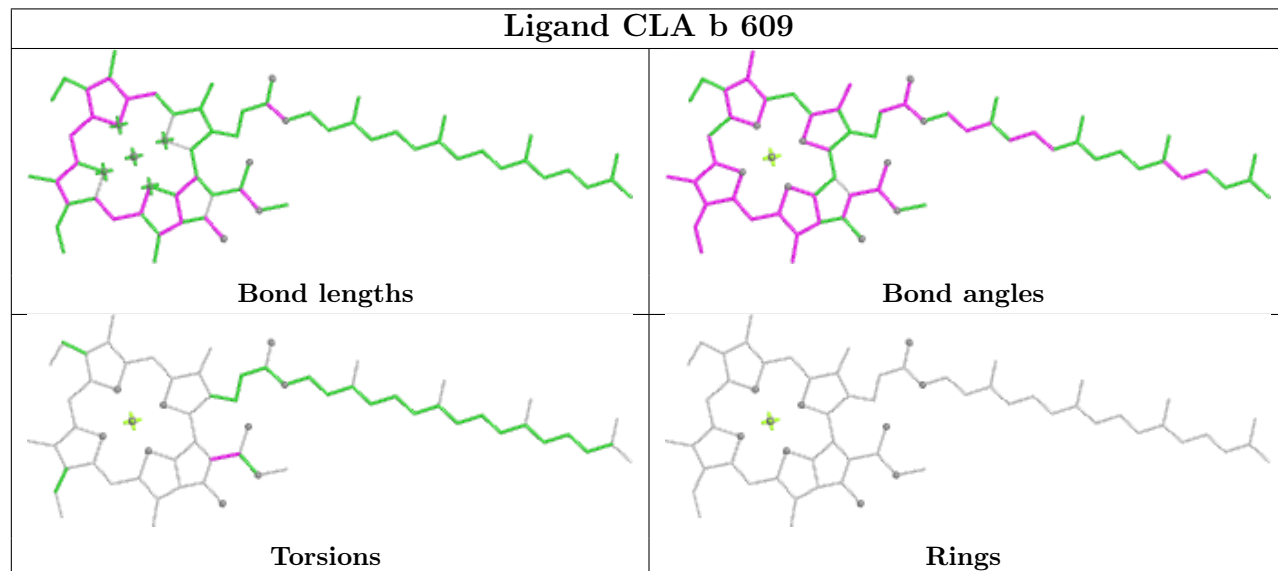
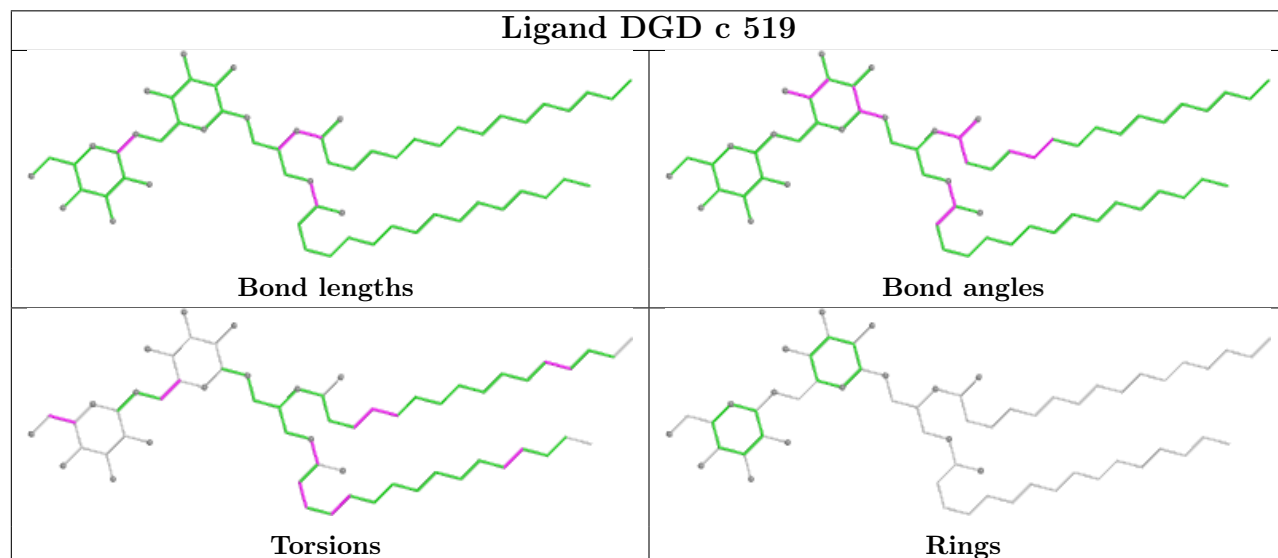
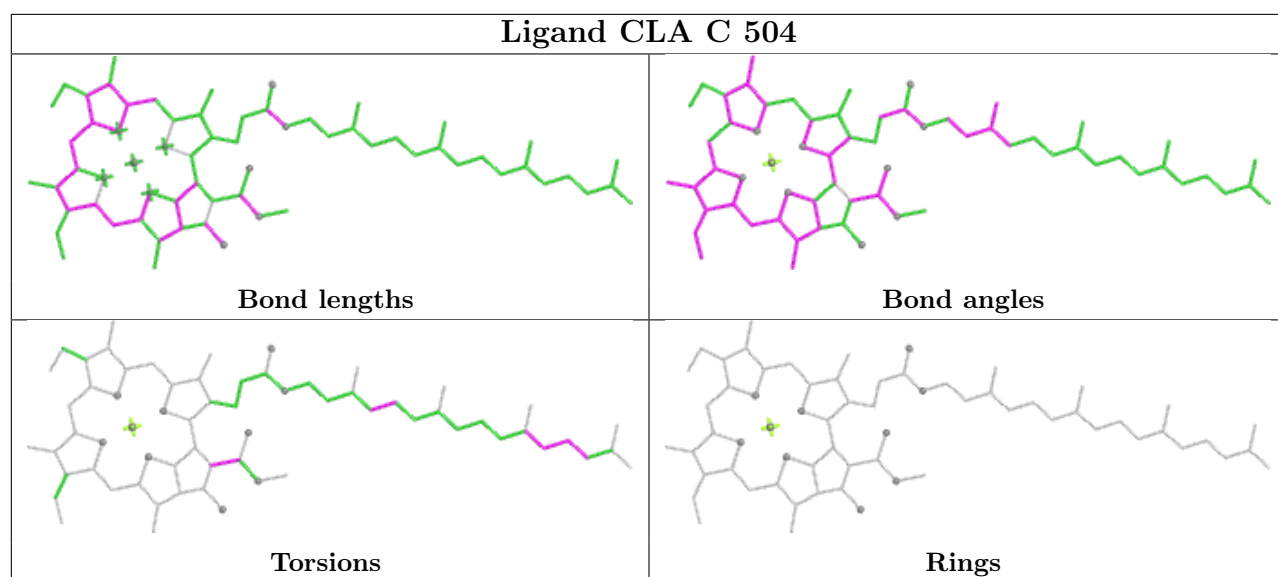


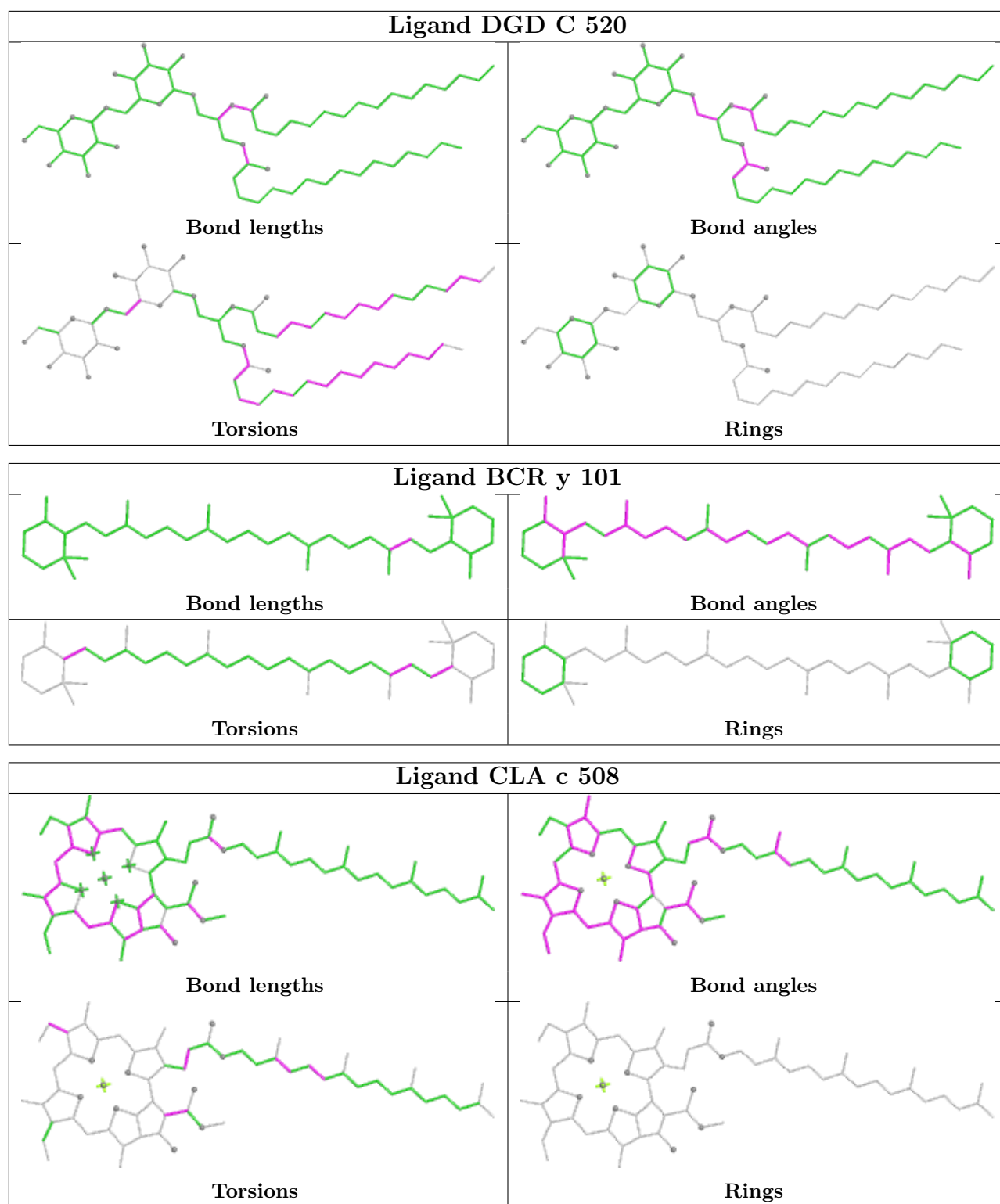
Ligand DGD C 518 (B)

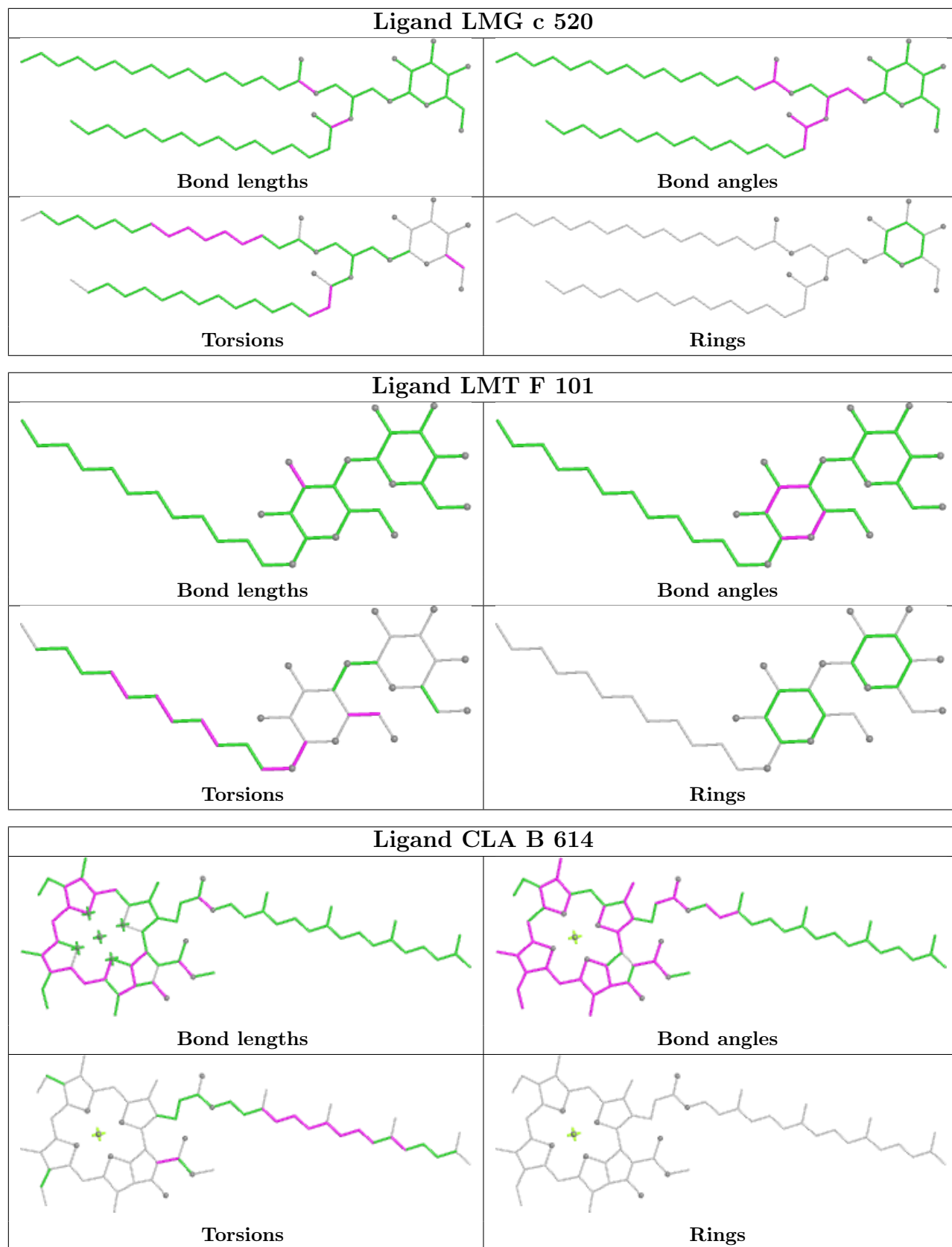


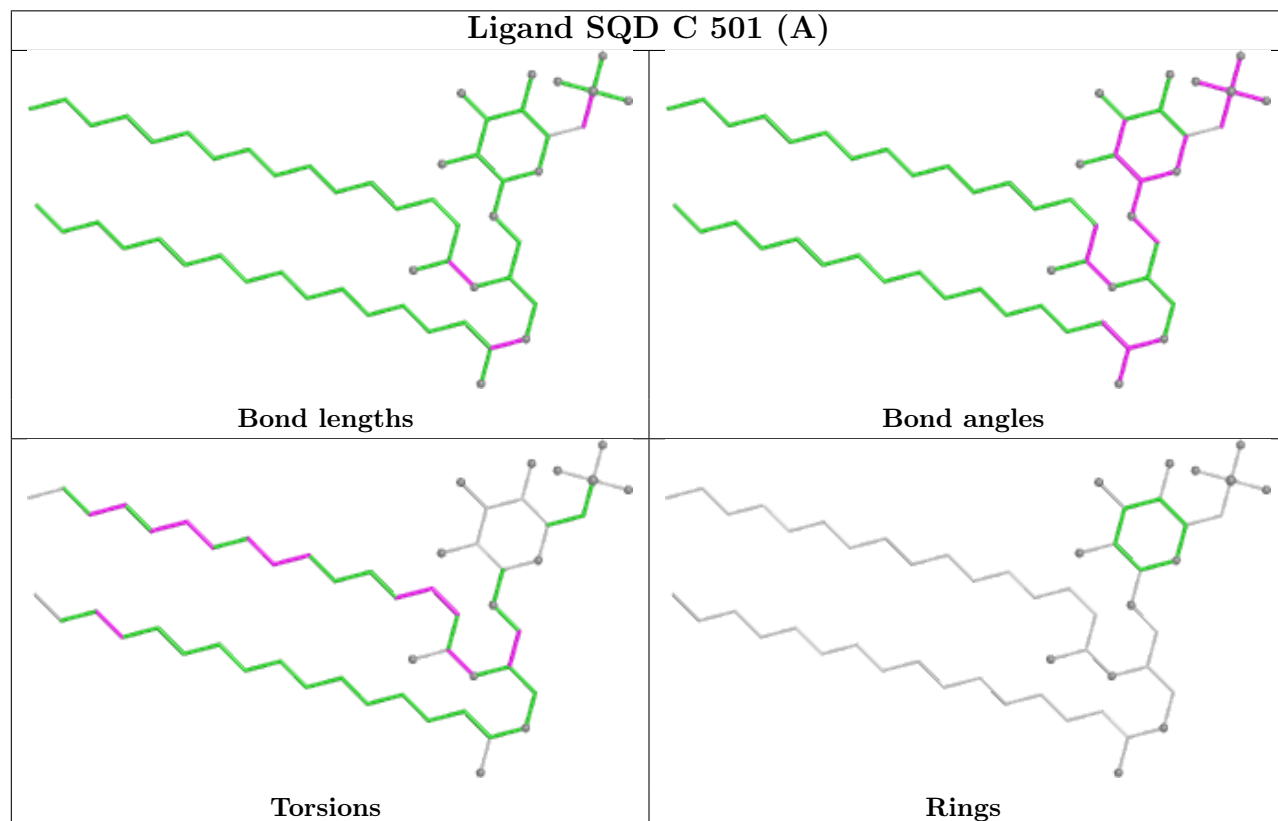
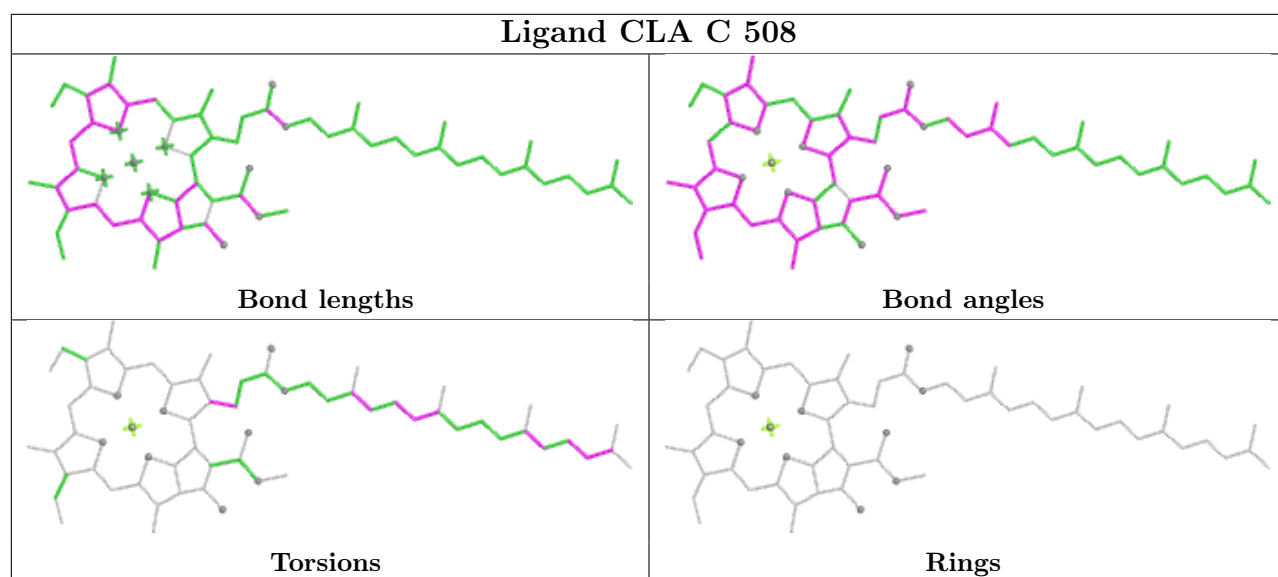
Ligand BCR B 617

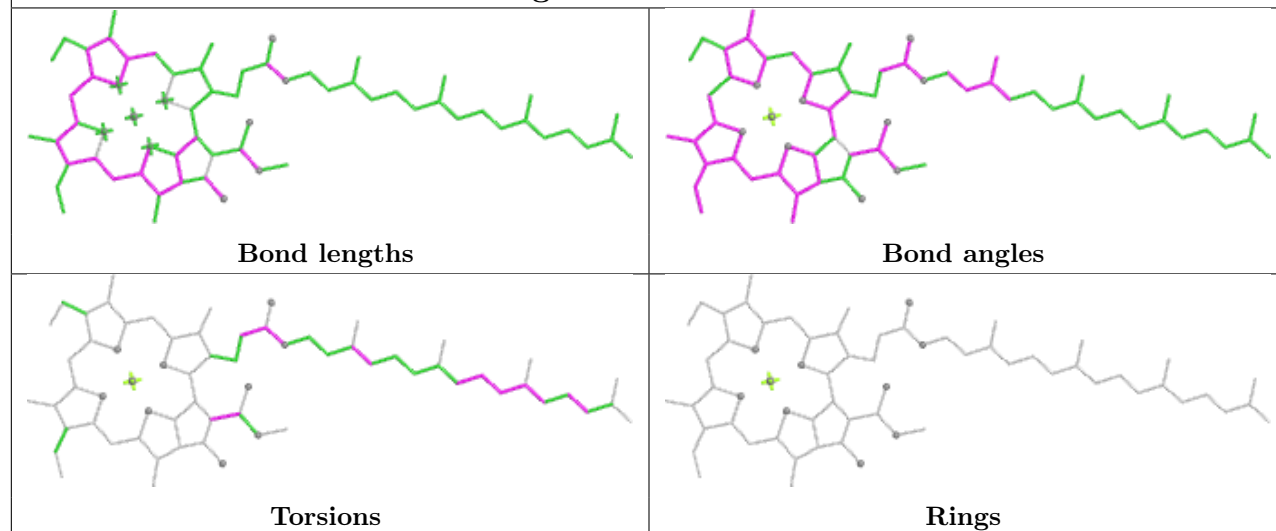
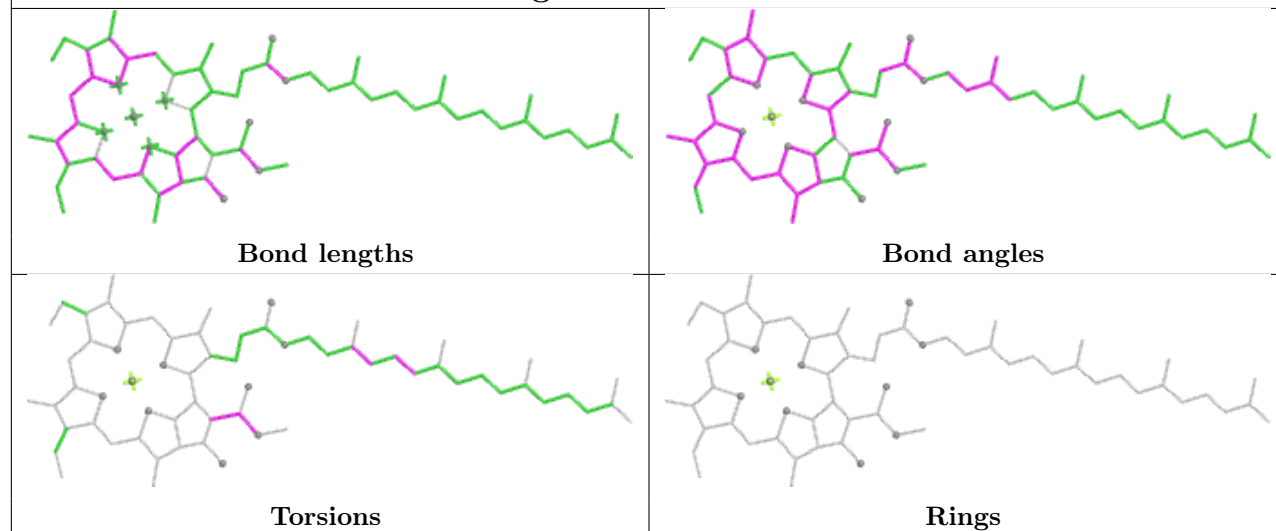


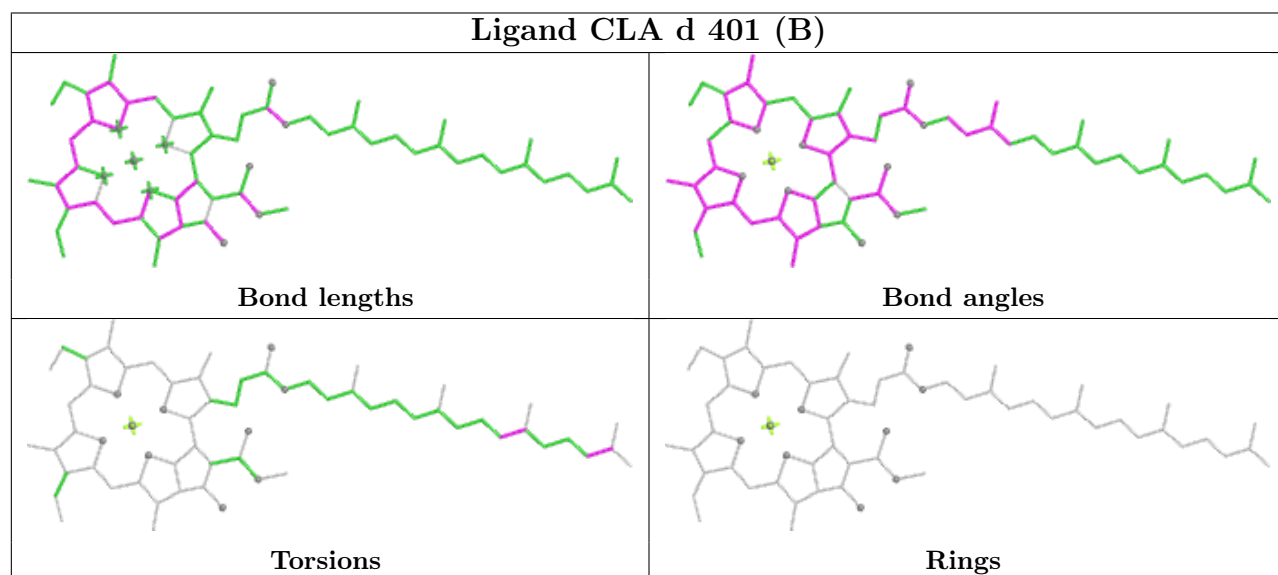
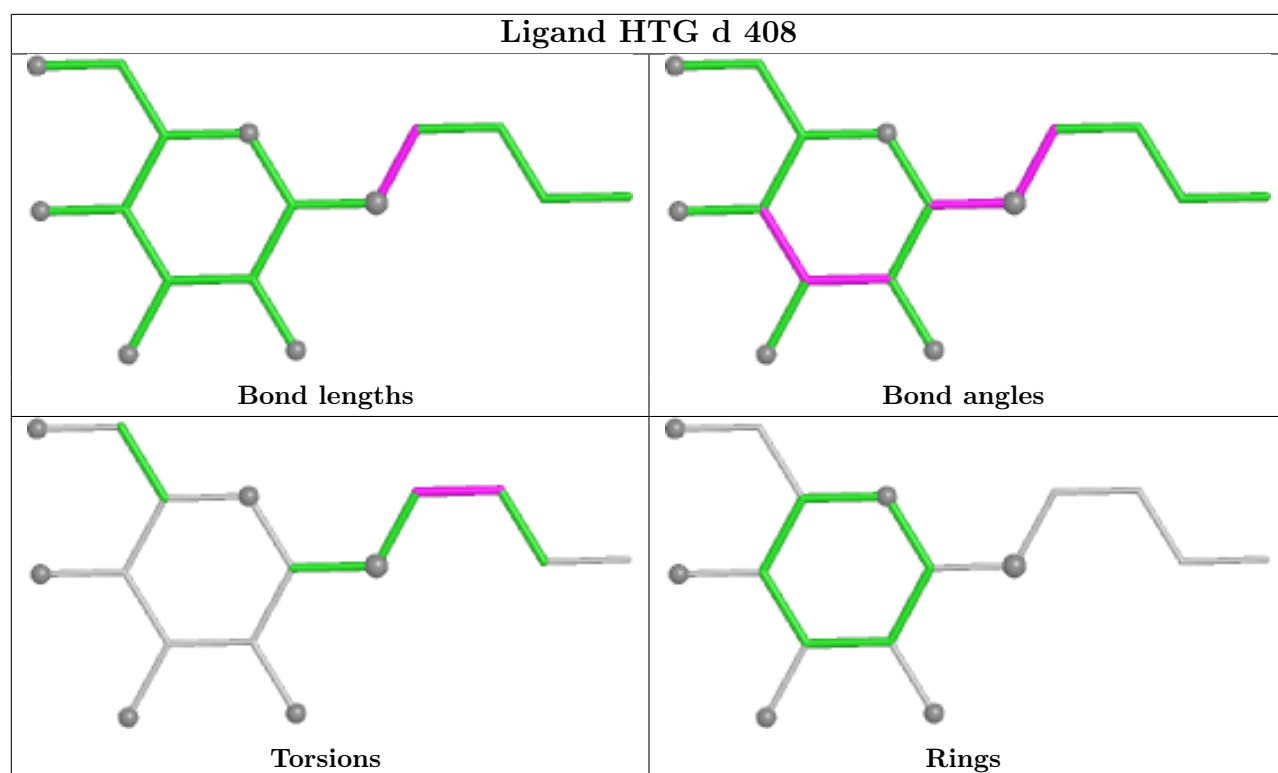


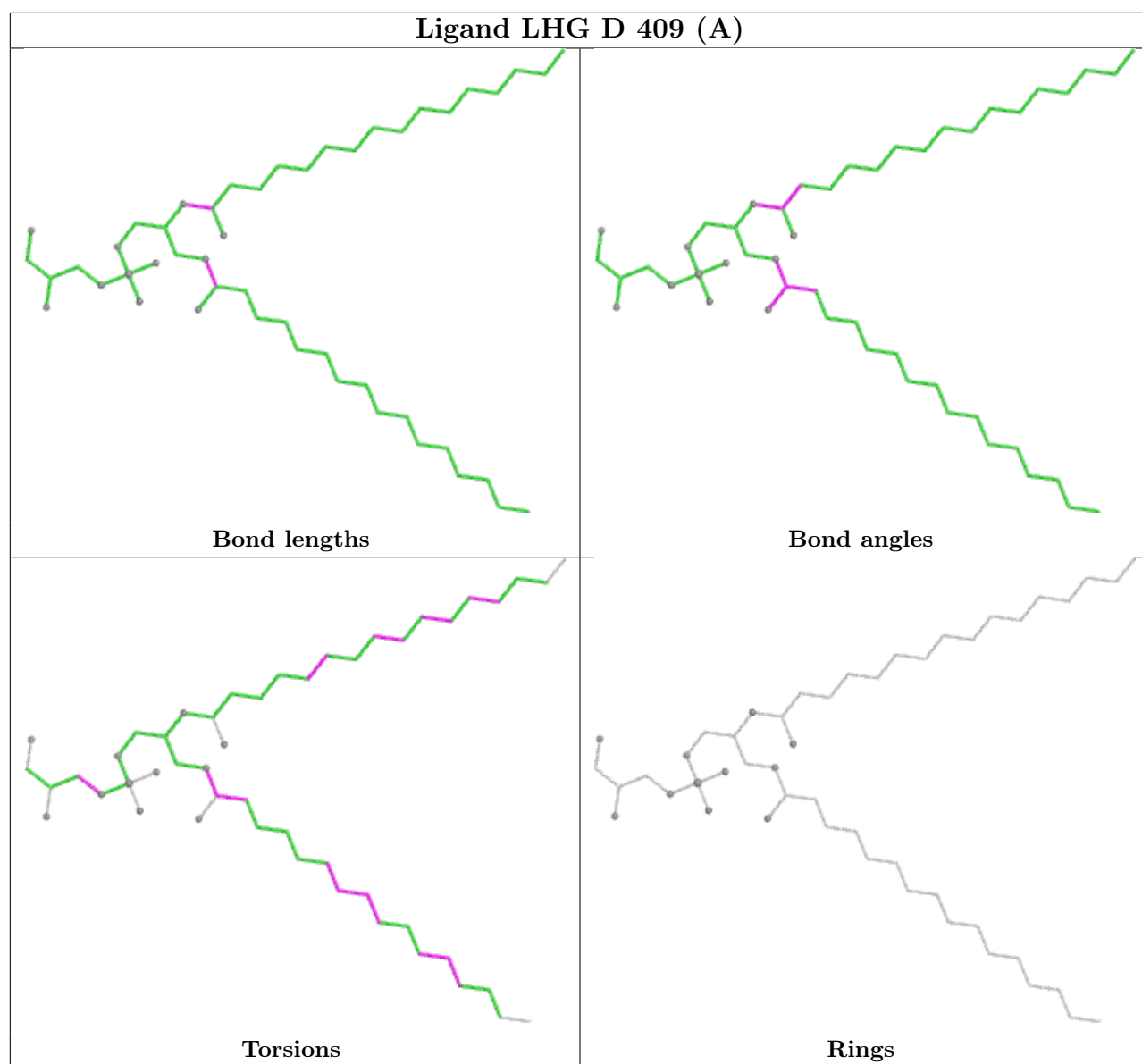




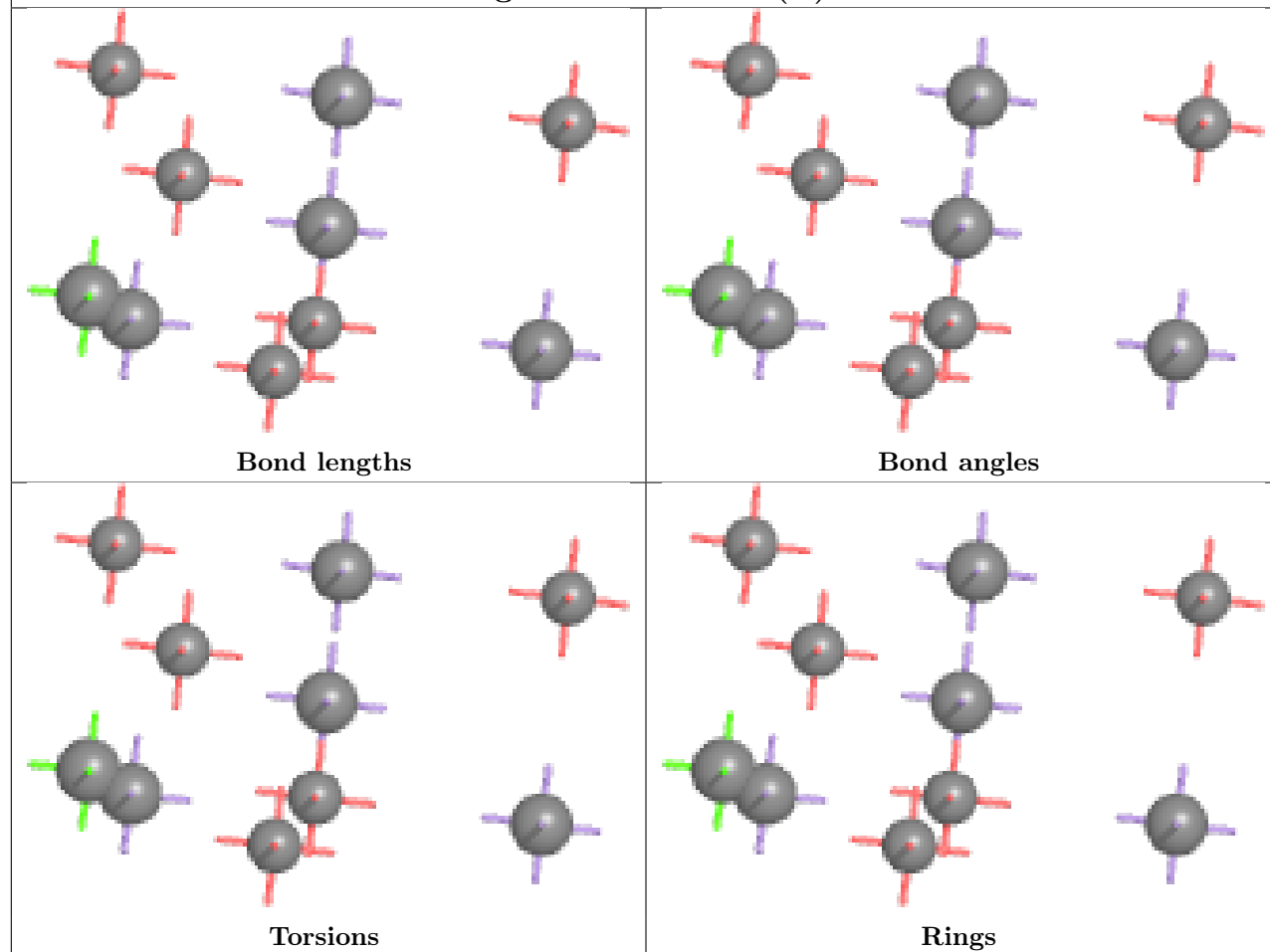


Ligand CLA C 512**Ligand CLA B 605**

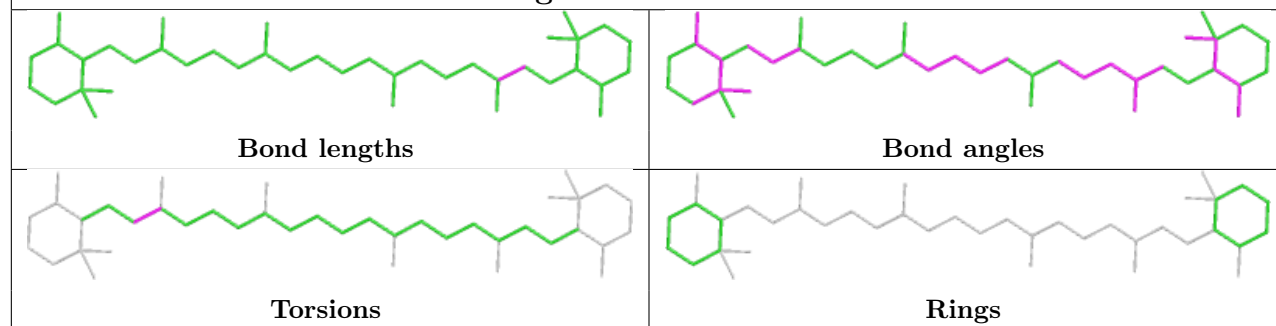


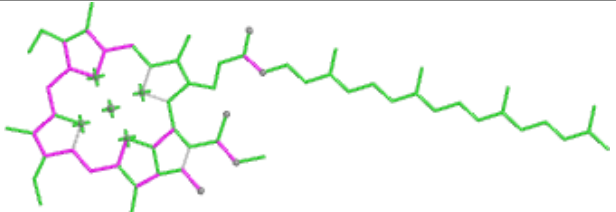
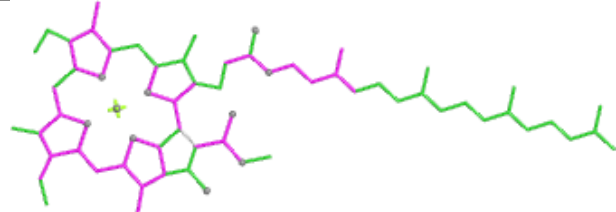
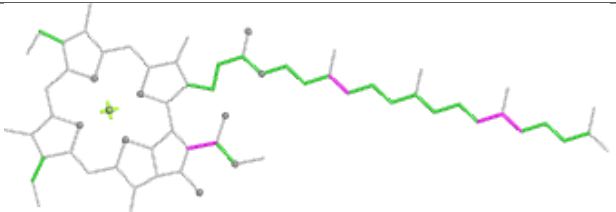
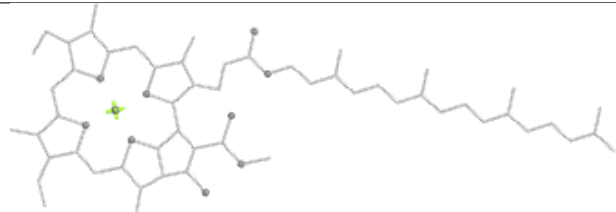


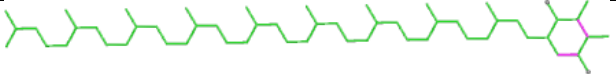
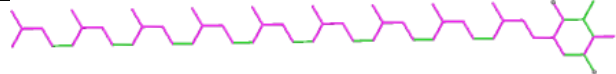
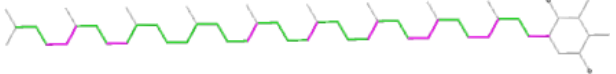
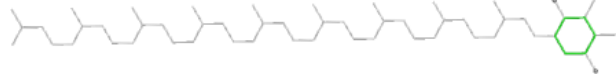
Ligand OEX A 411 (B)

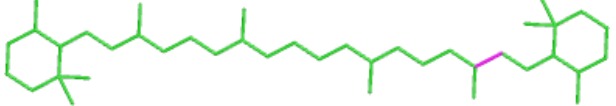
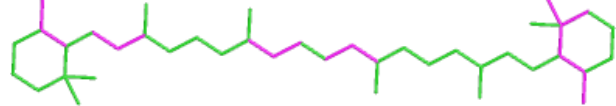
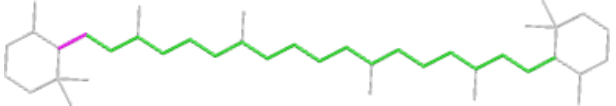
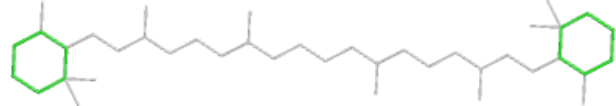


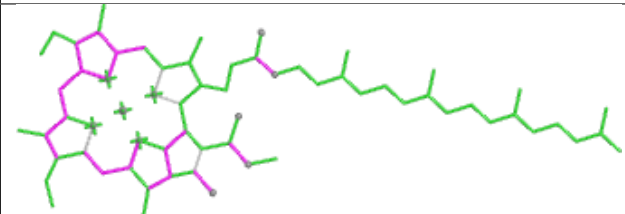
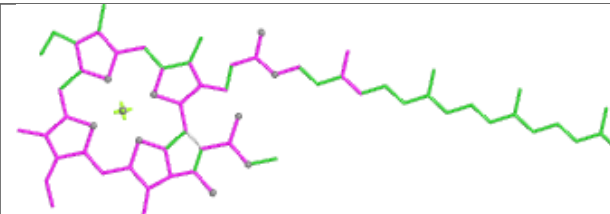
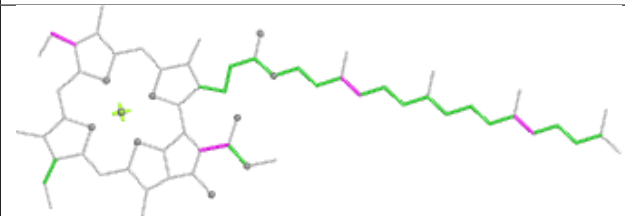
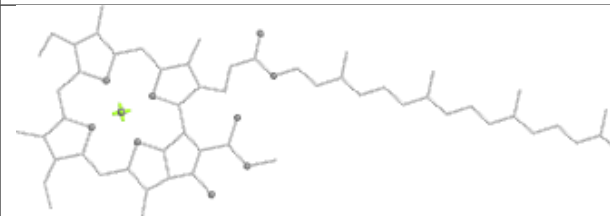
Ligand BCR c 516

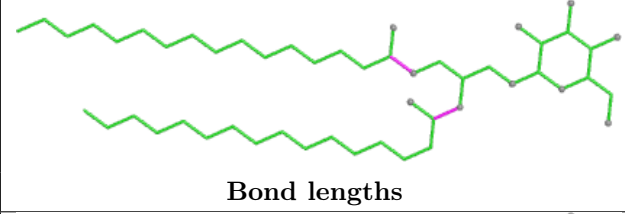
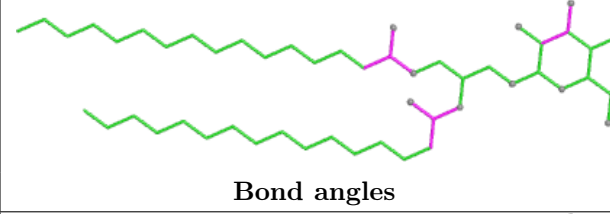
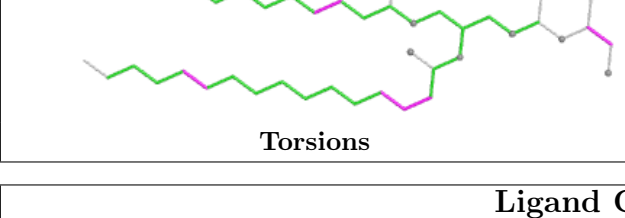


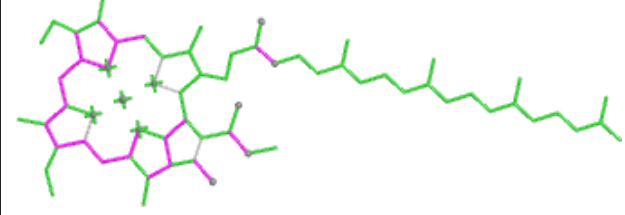
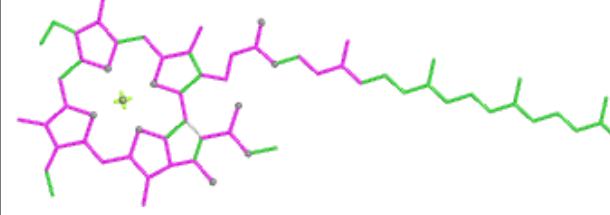
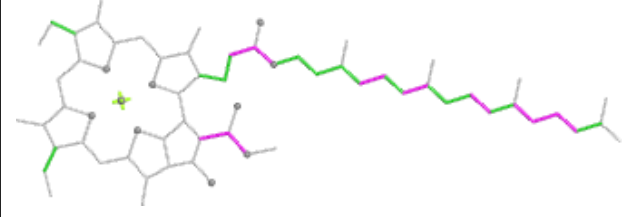
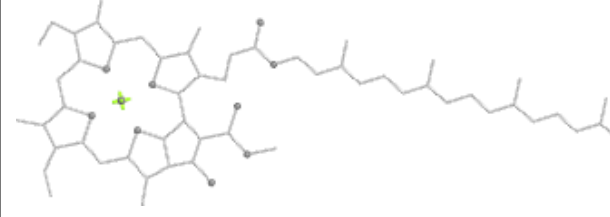
Ligand CLA c 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

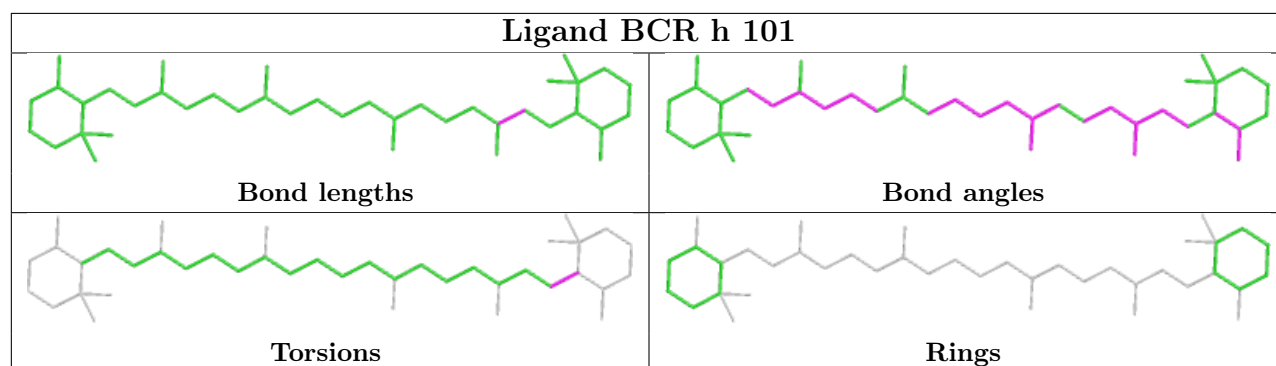
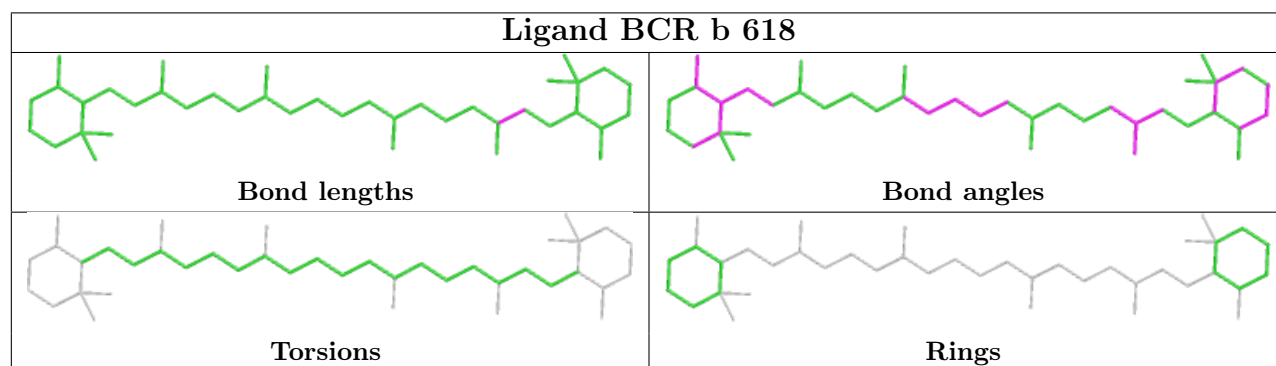
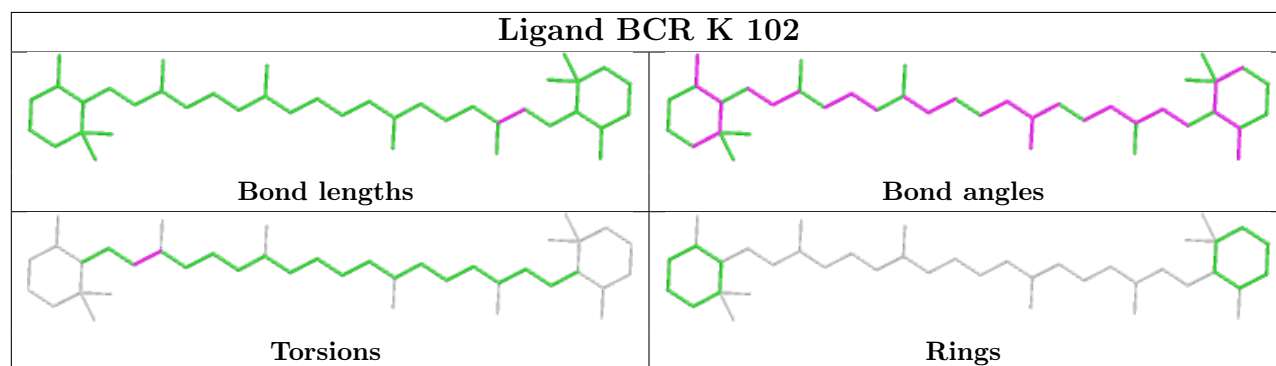
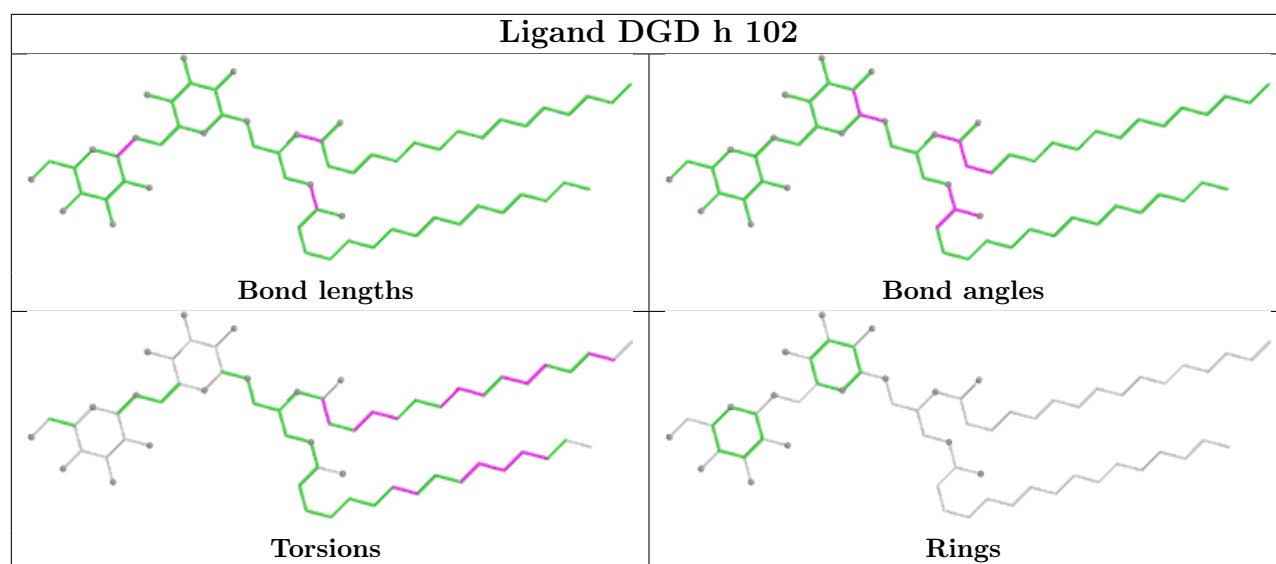
Ligand PL9 A 412 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

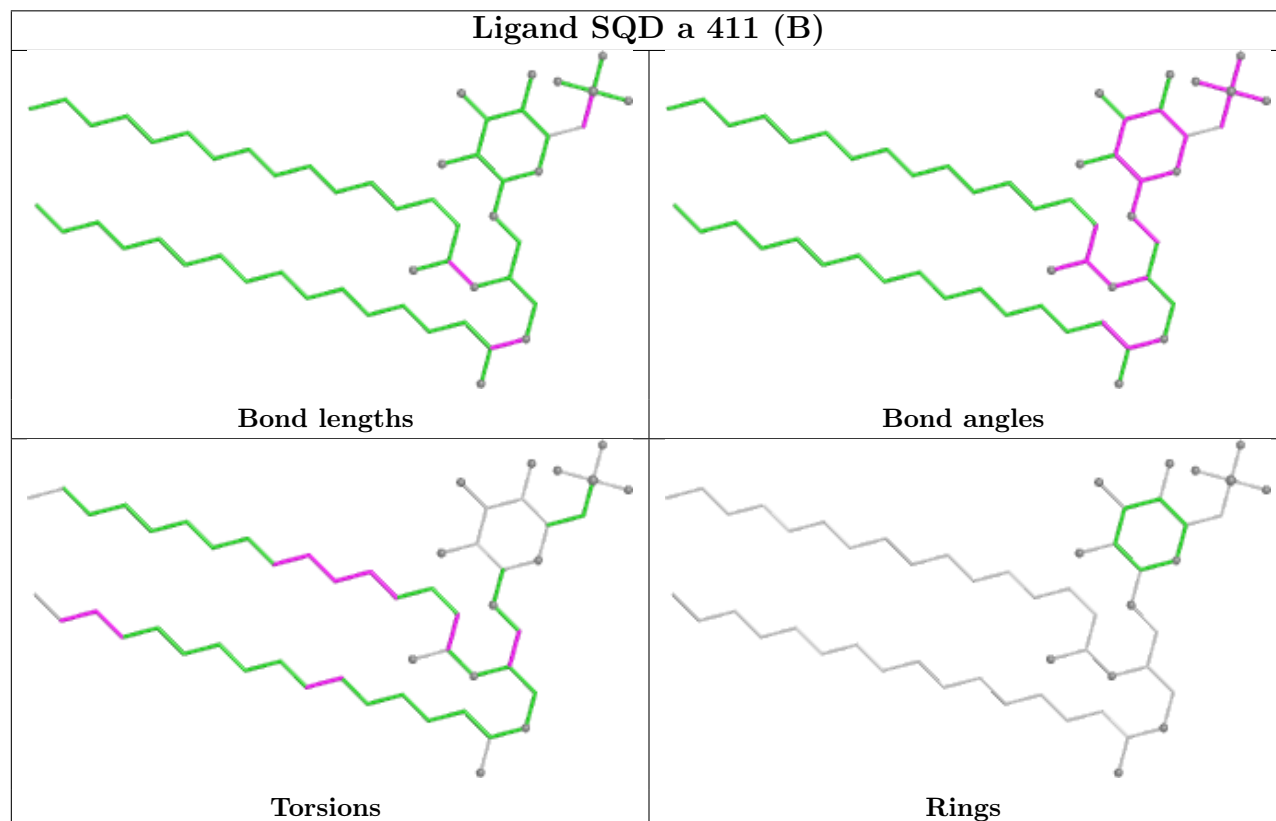
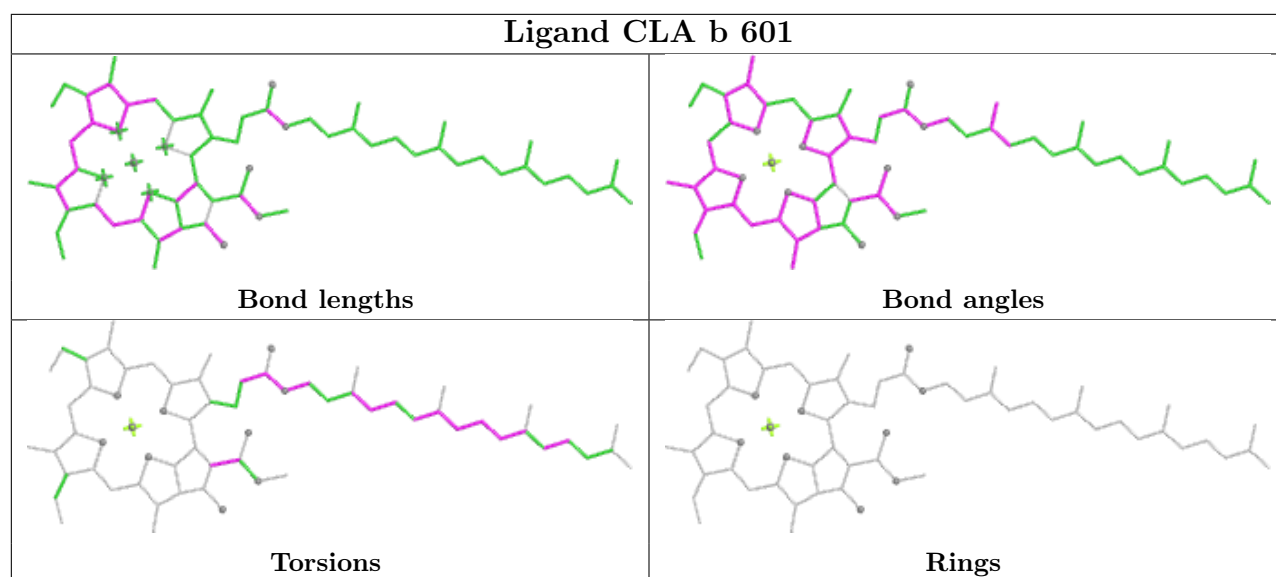
Ligand BCR C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

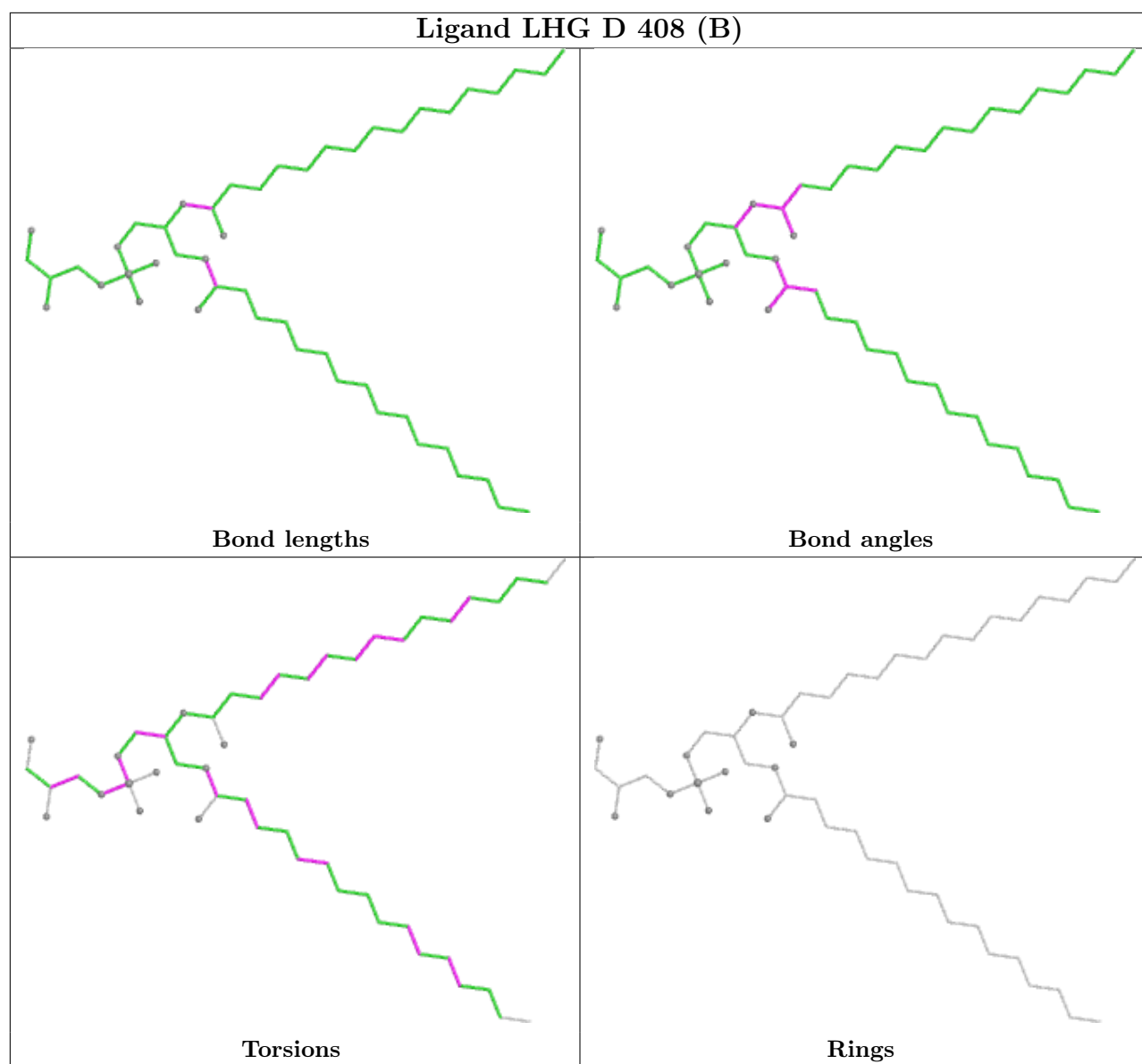
Ligand CLA C 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

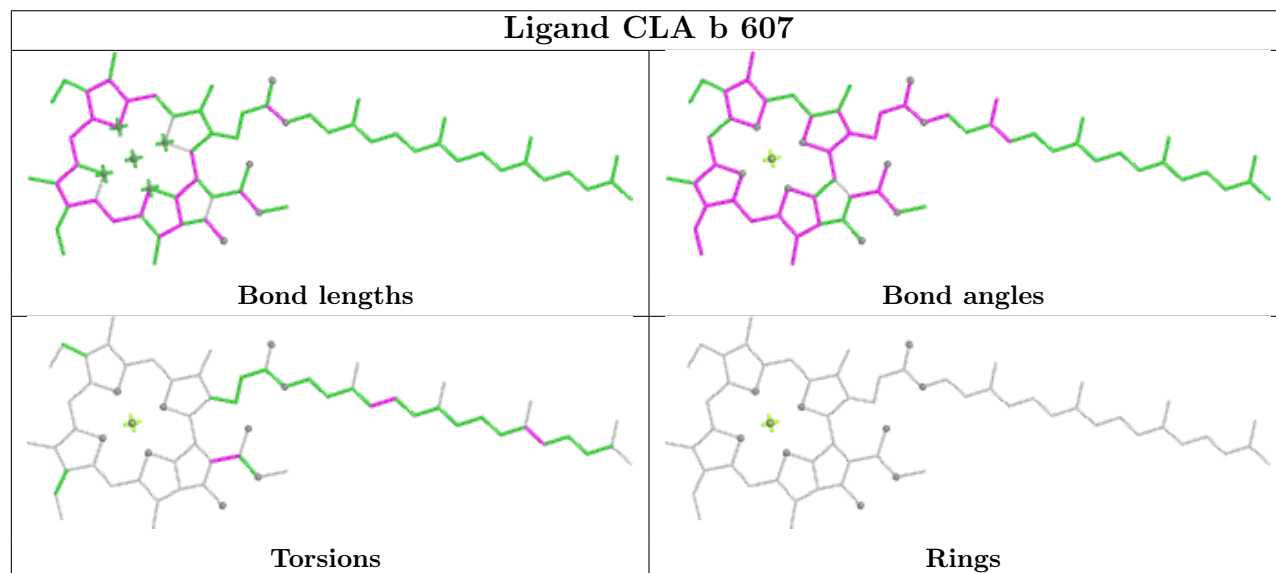
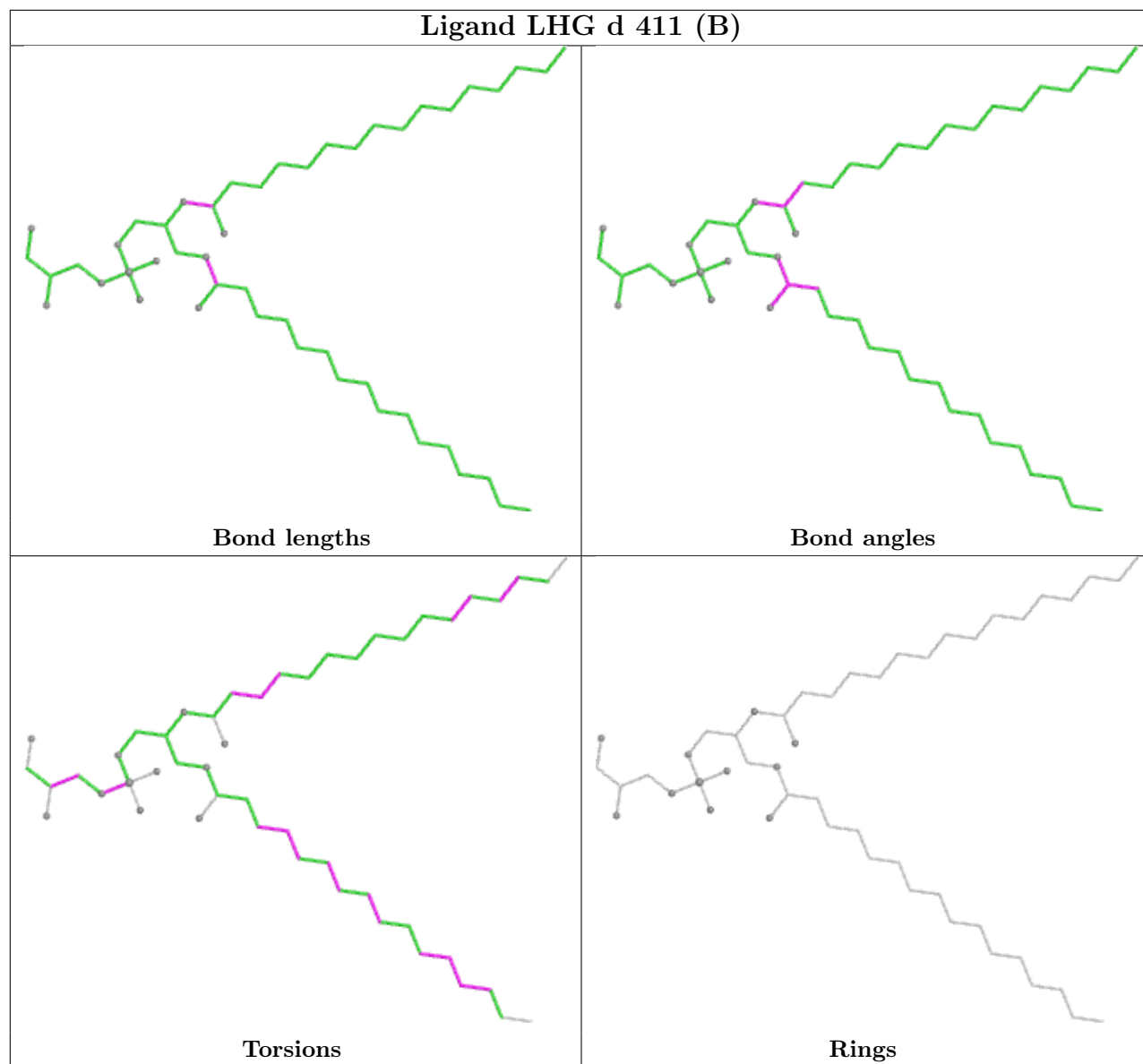
Ligand LMG d 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

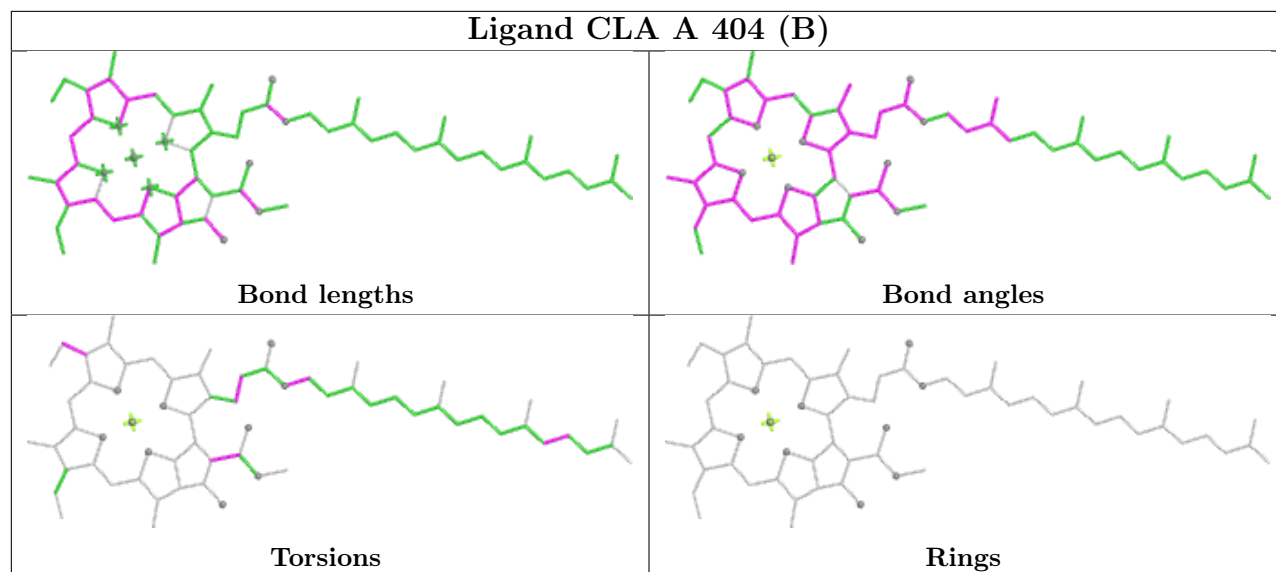




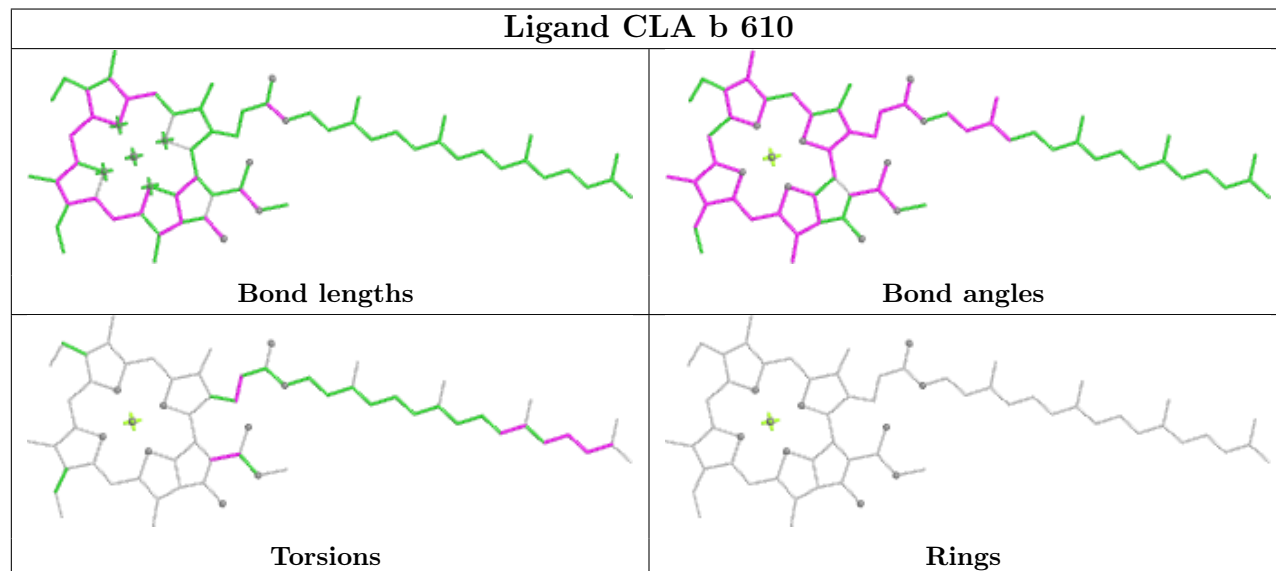




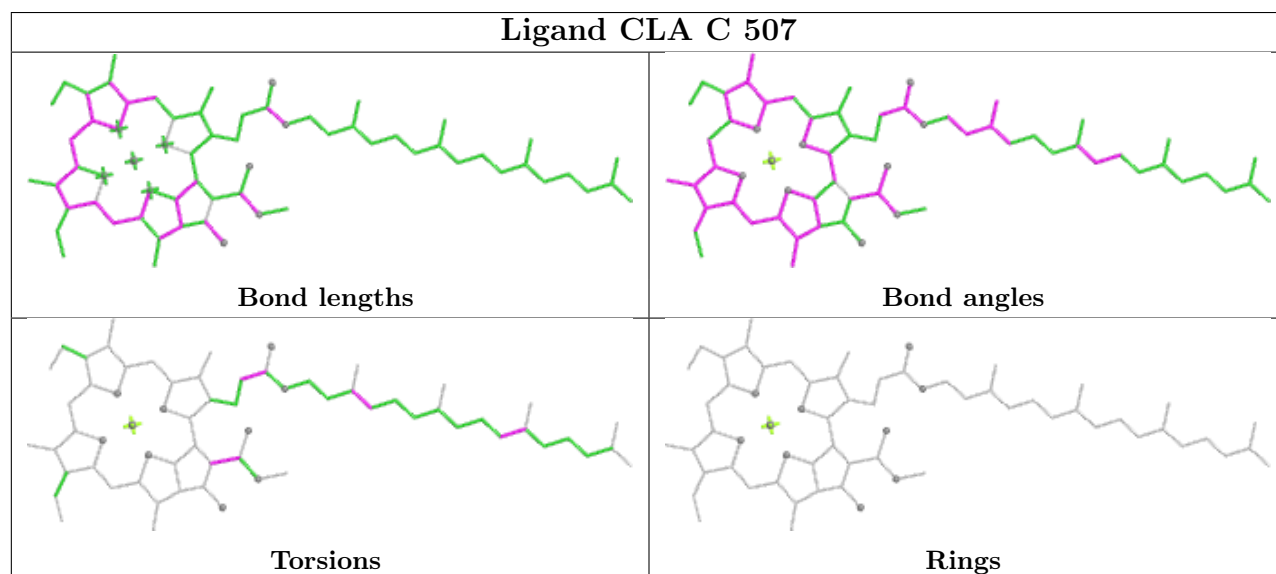
Ligand CLA A 404 (B)

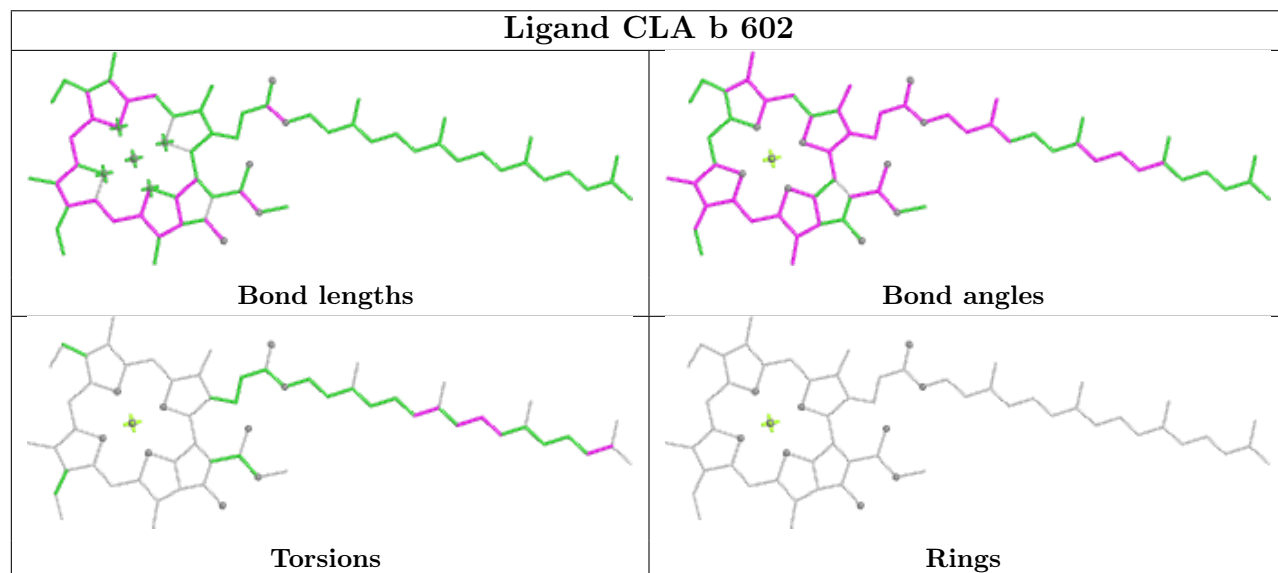
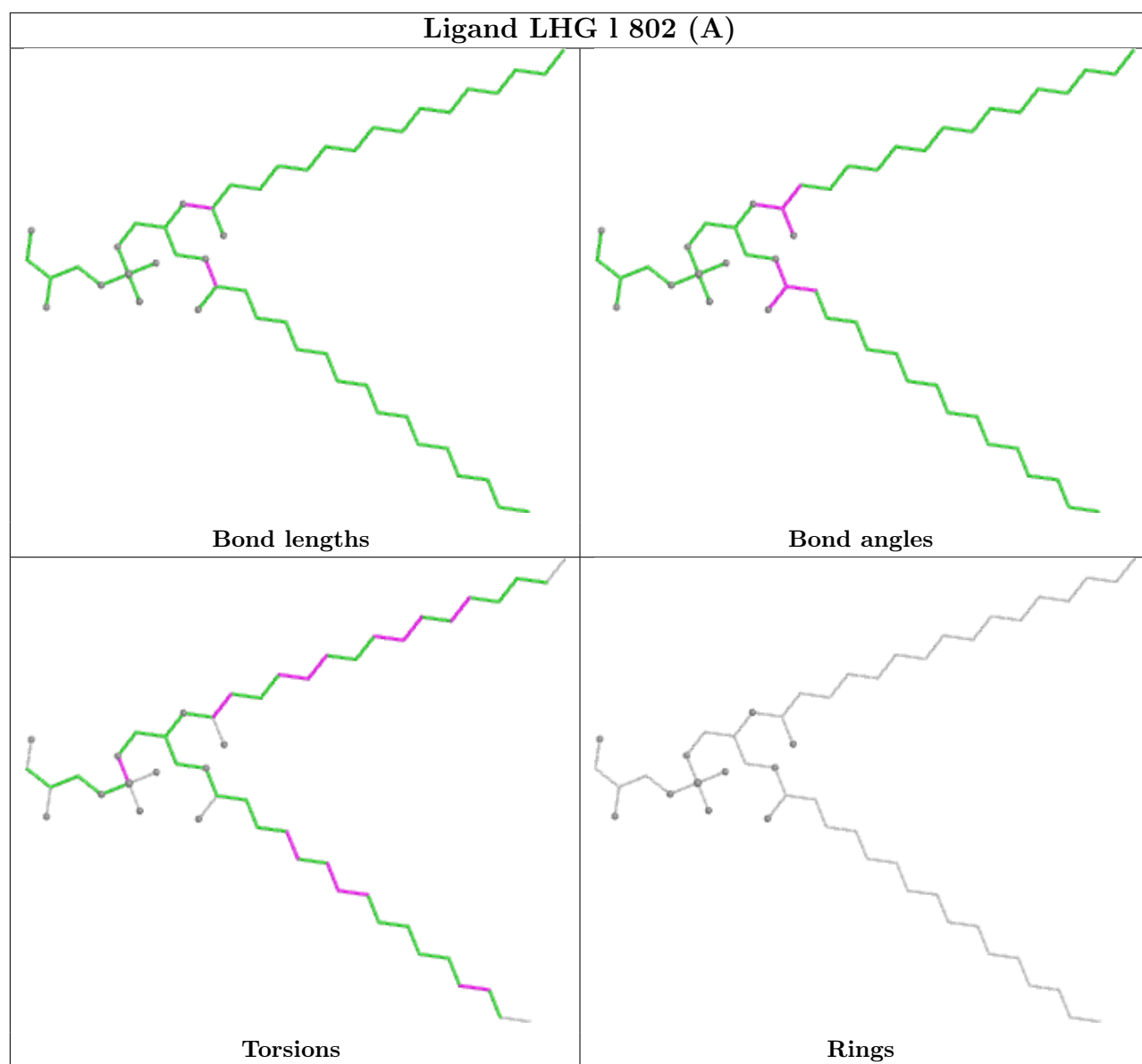


Ligand CLA b 610

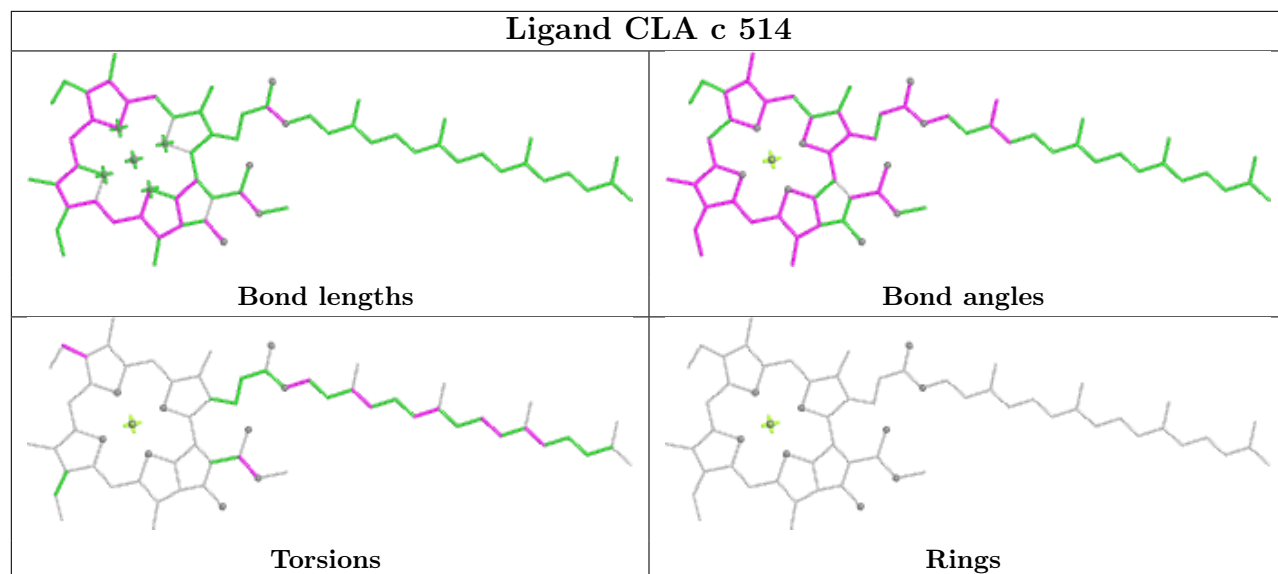


Ligand CLA C 507

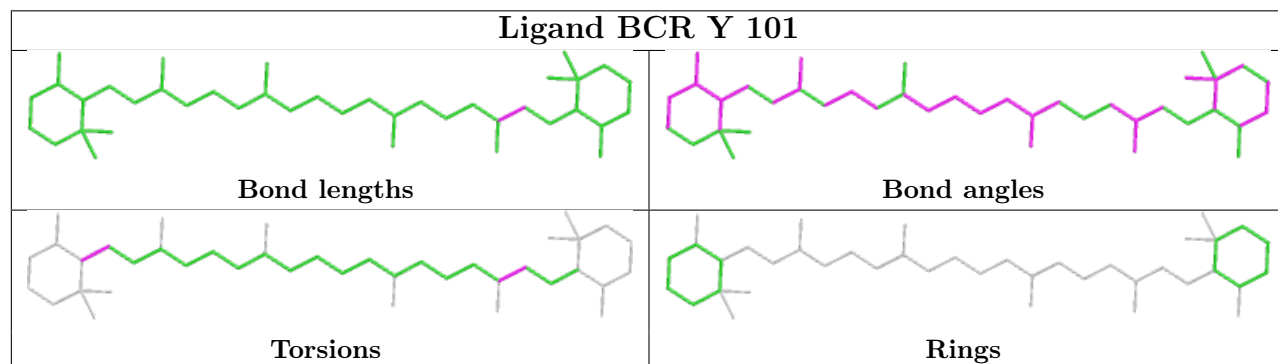




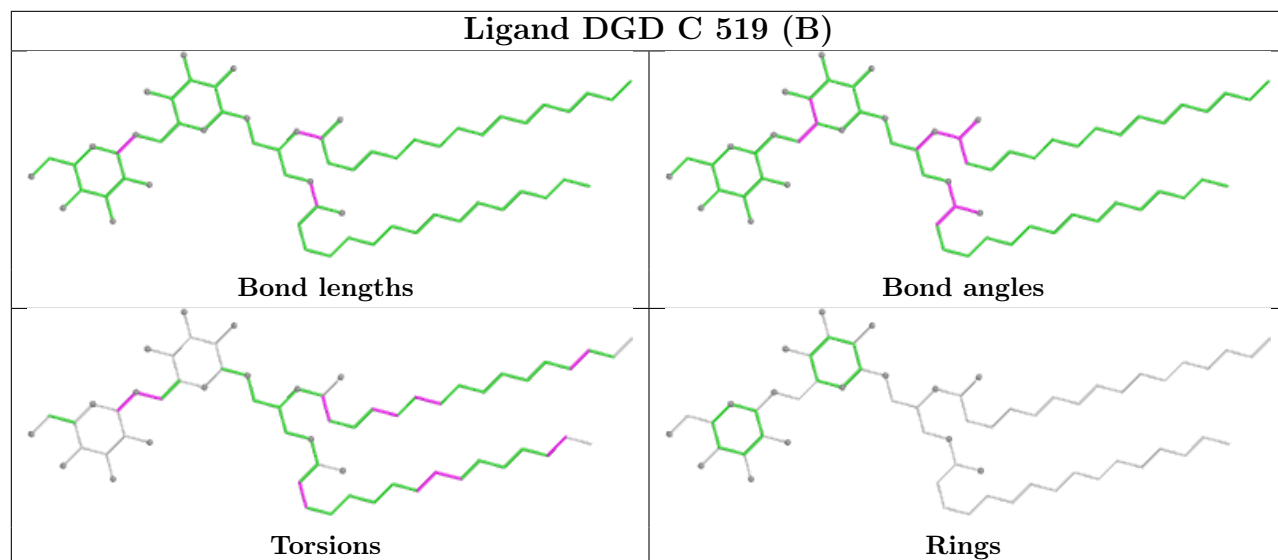
Ligand CLA c 514



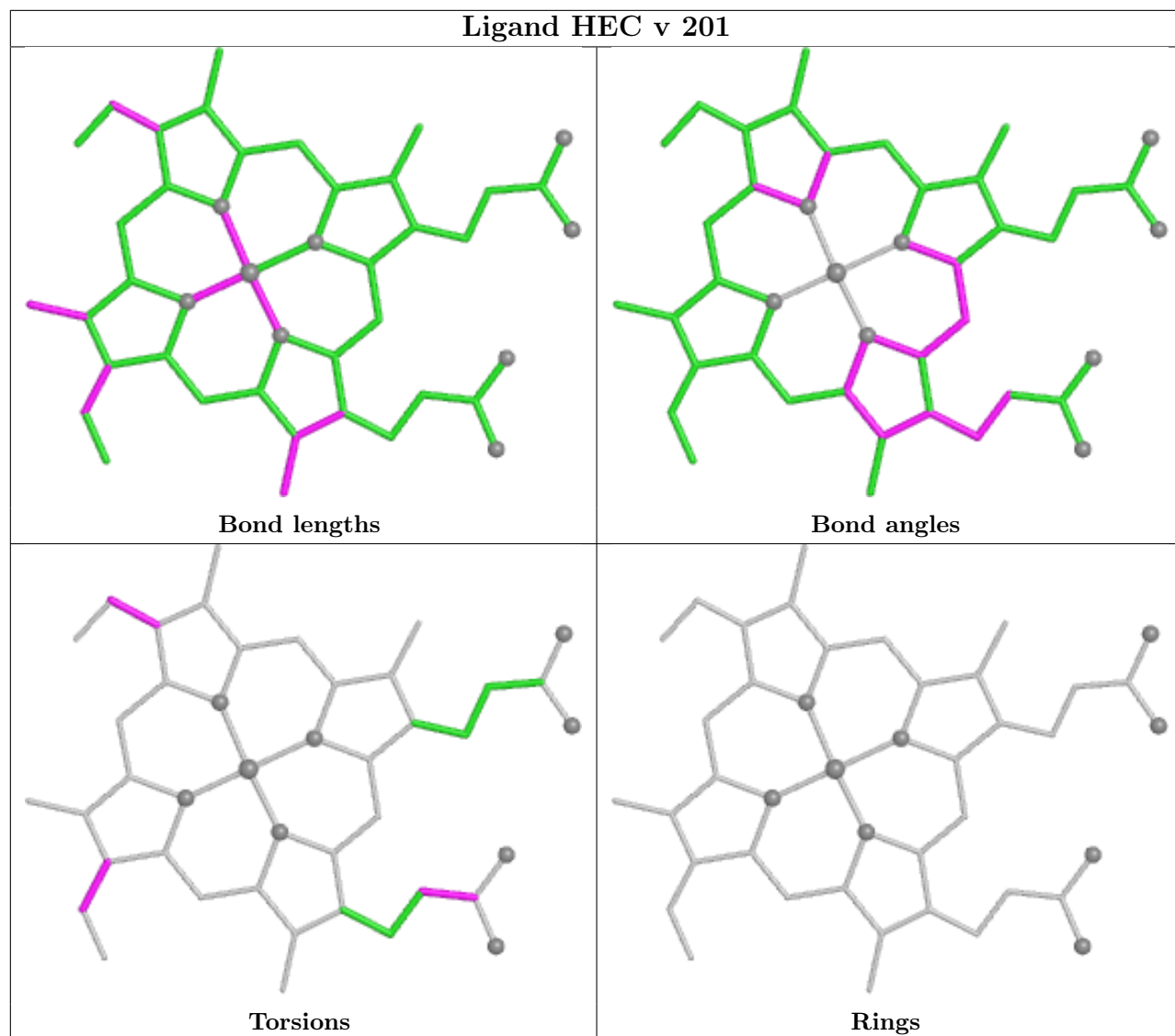
Ligand BCR Y 101



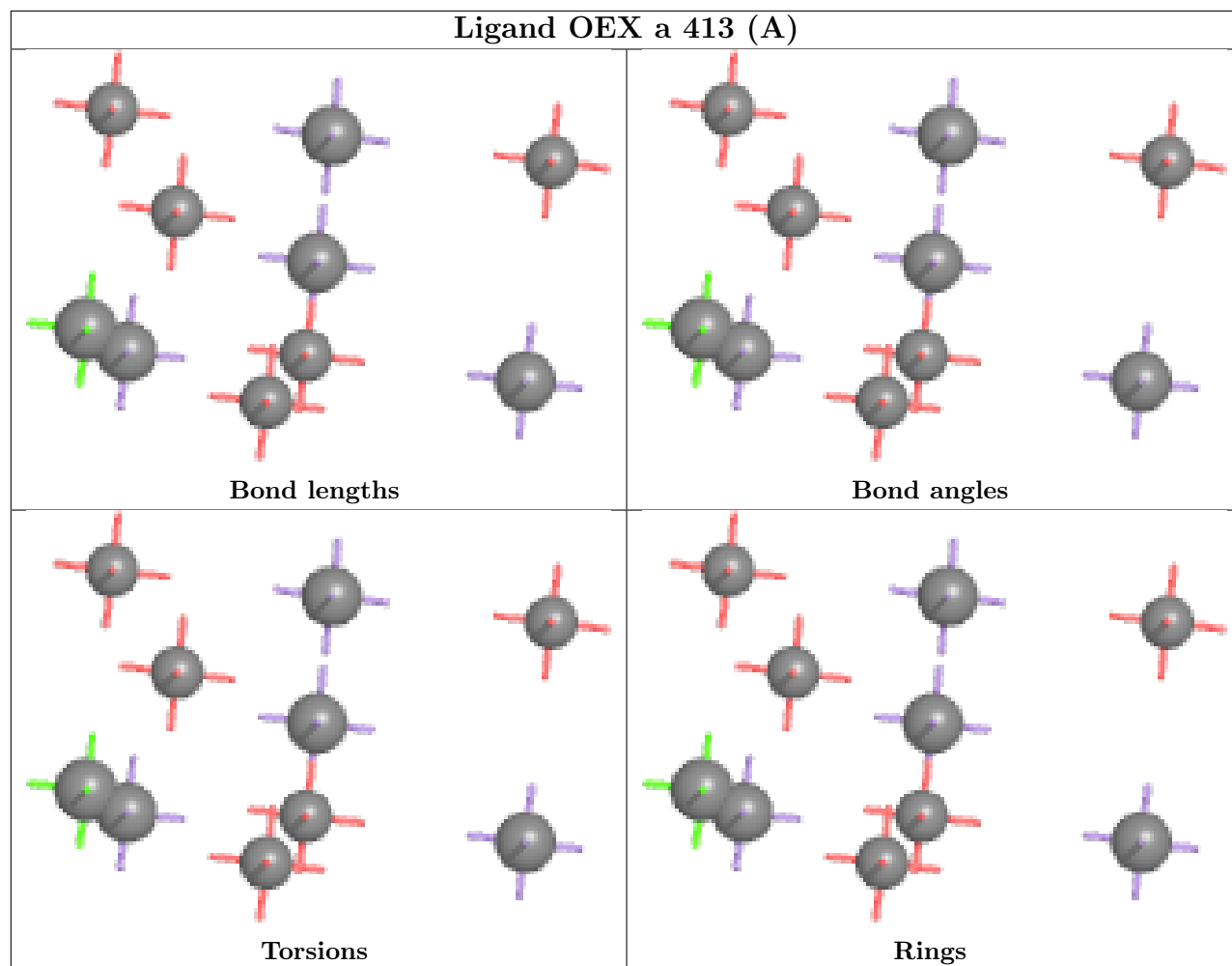
Ligand DGD C 519 (B)



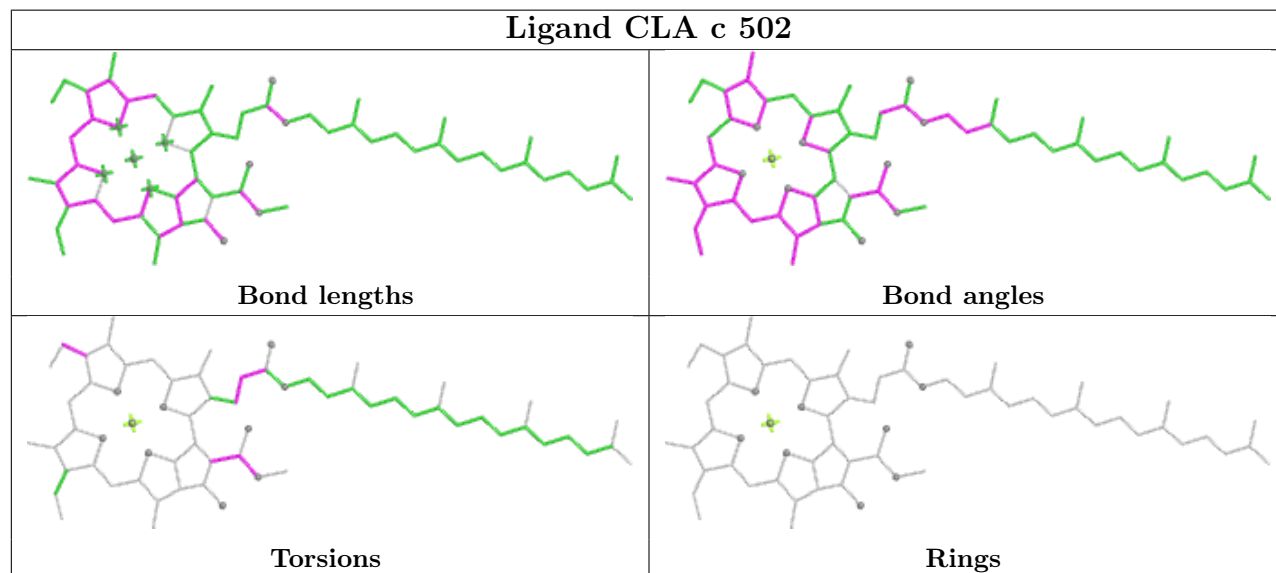
Ligand HEC v 201

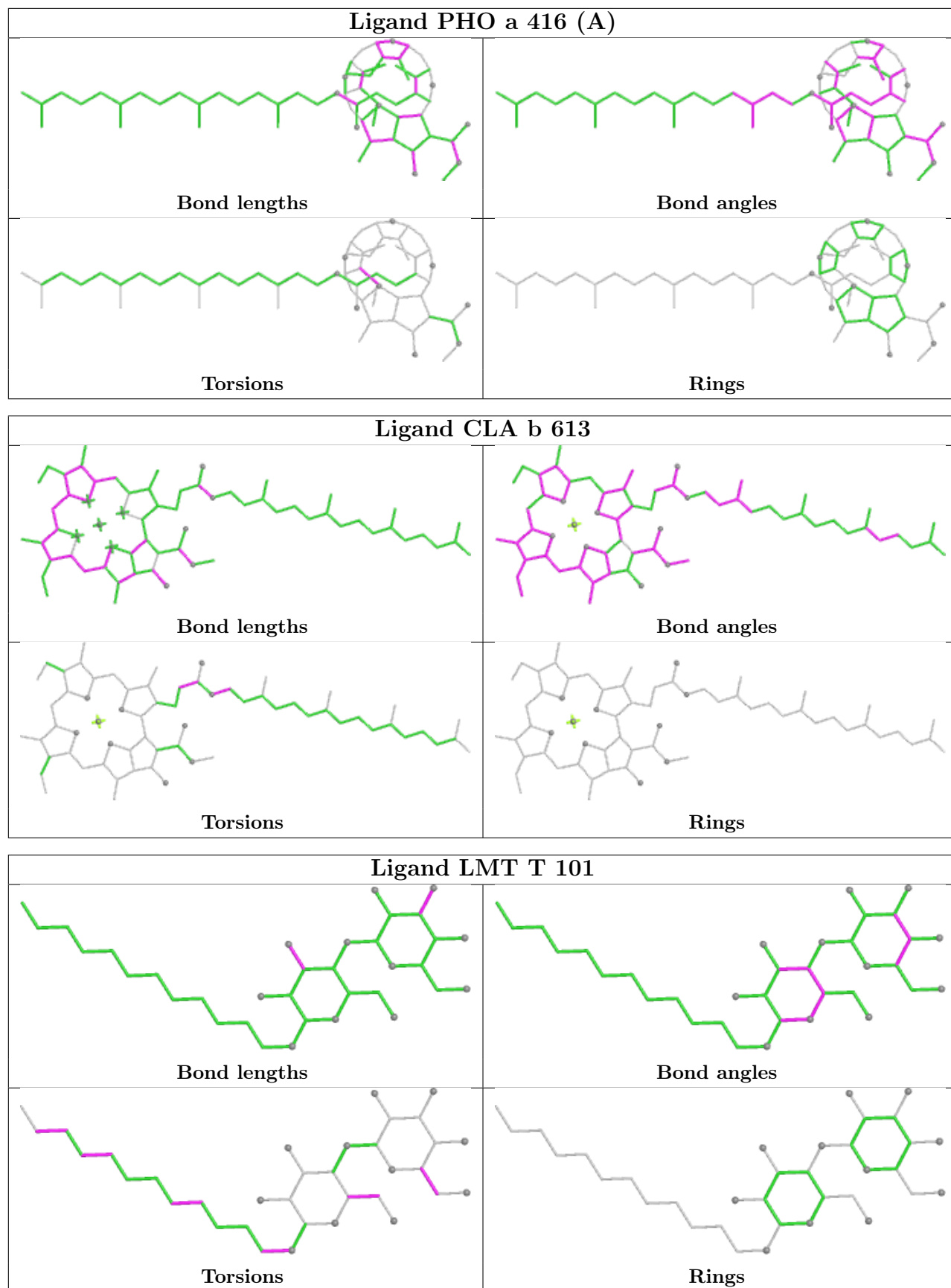


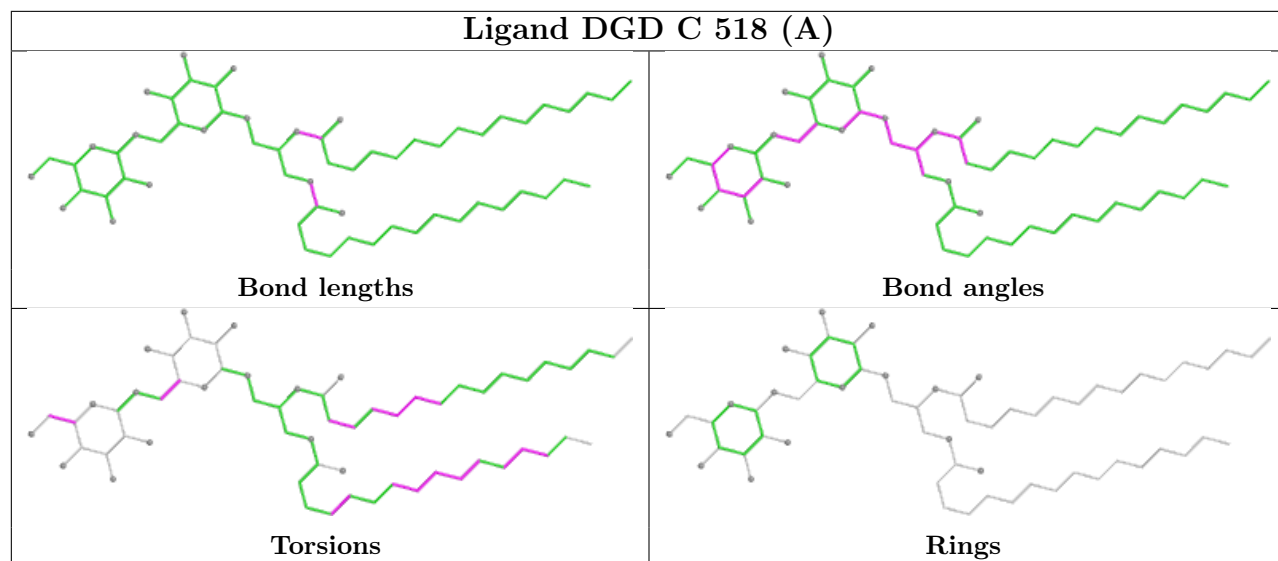
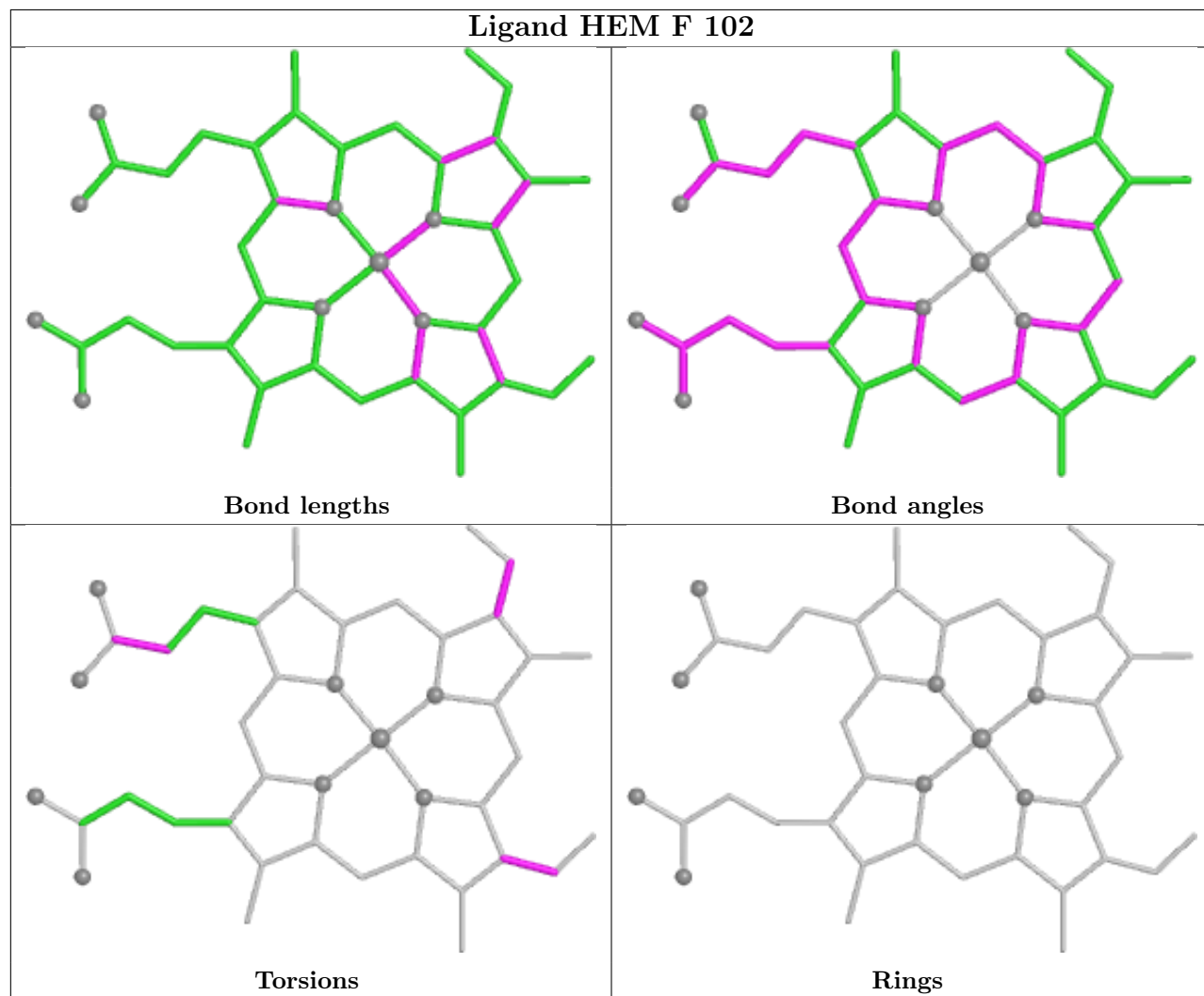
Ligand OEX a 413 (A)

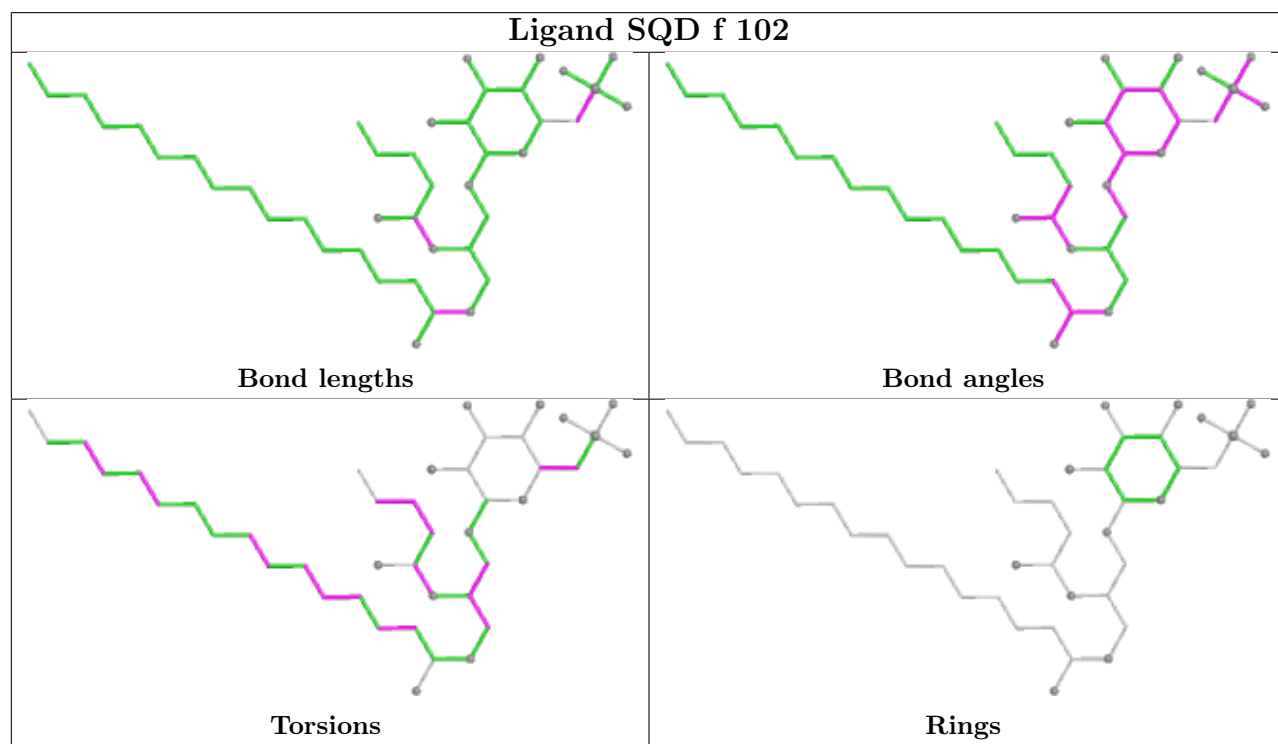
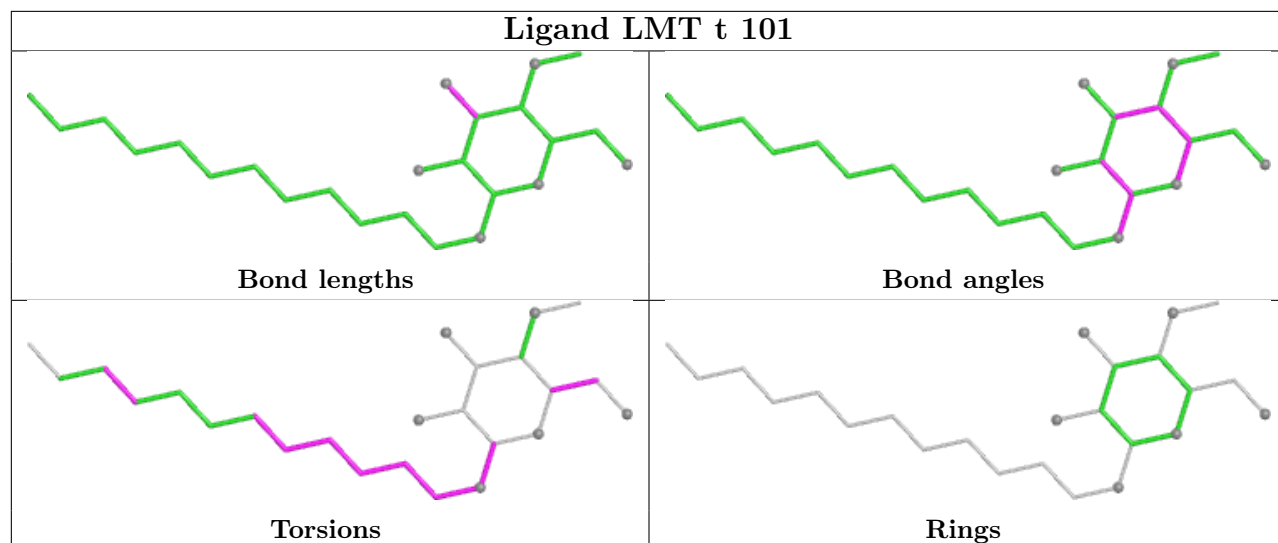


Ligand CLA c 502

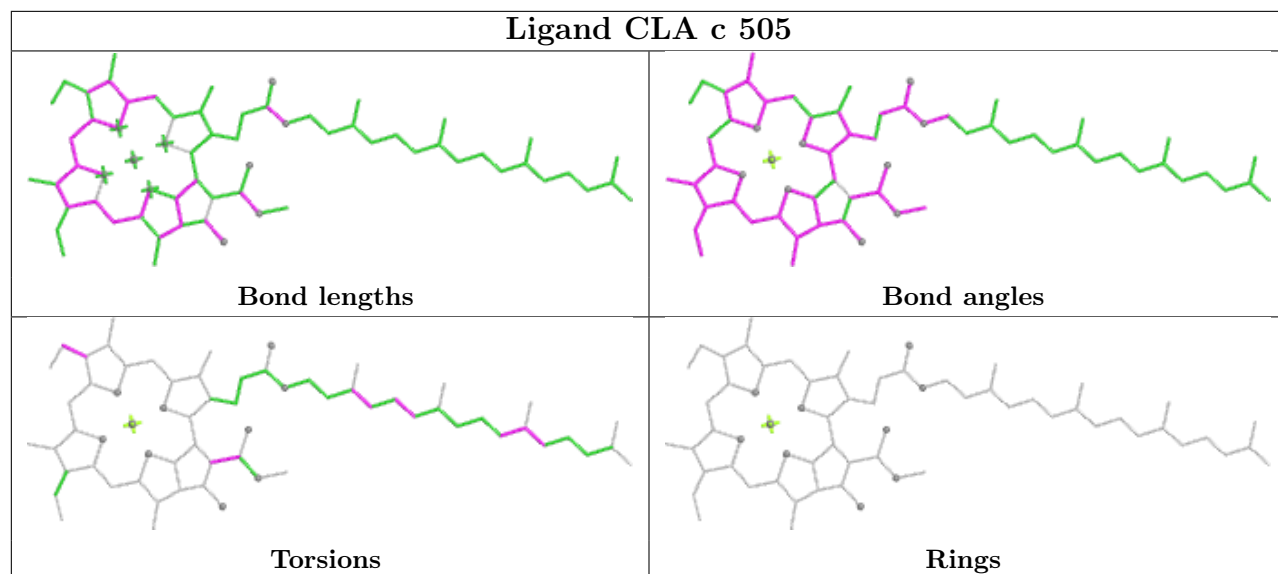




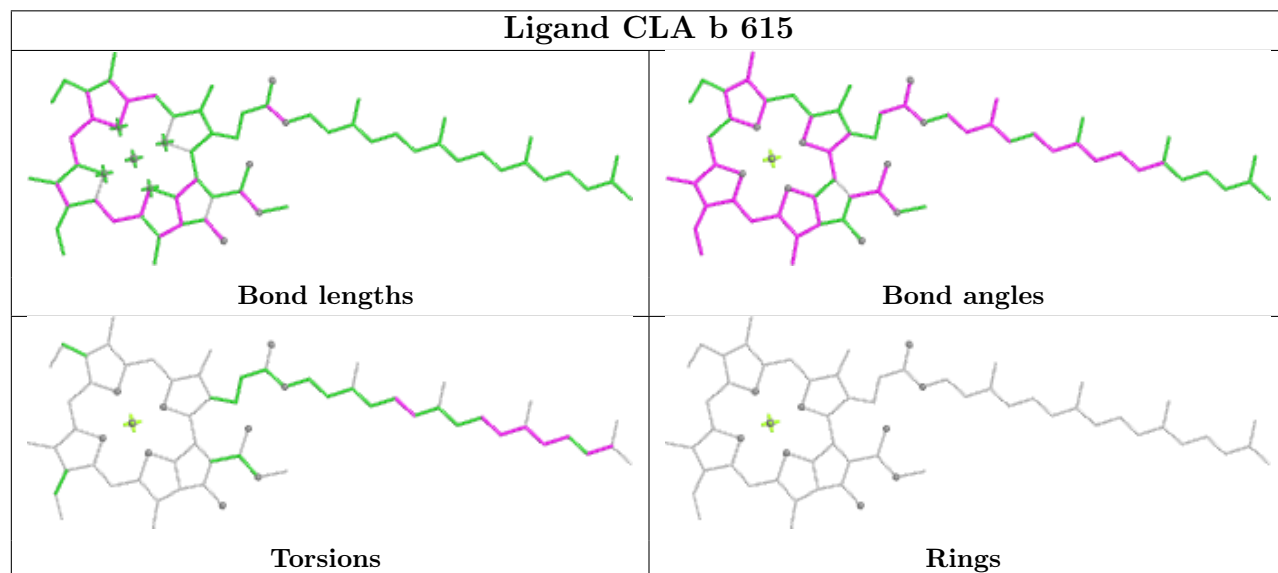
Ligand DGD C 518 (A)**Ligand HEM F 102**



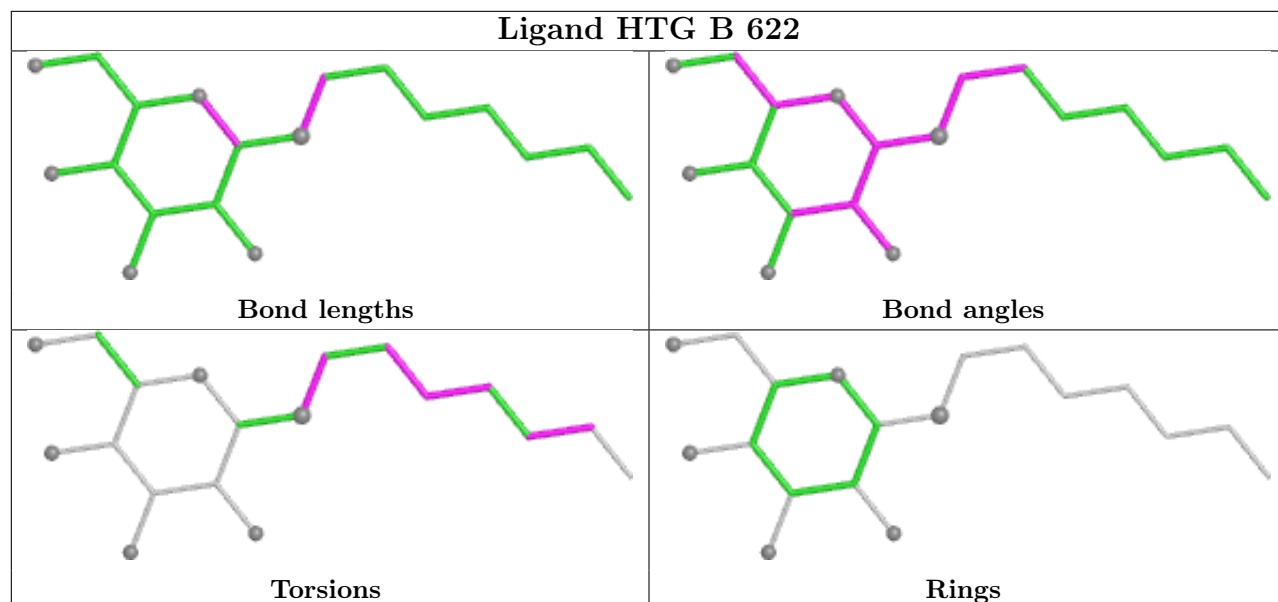
Ligand CLA c 505

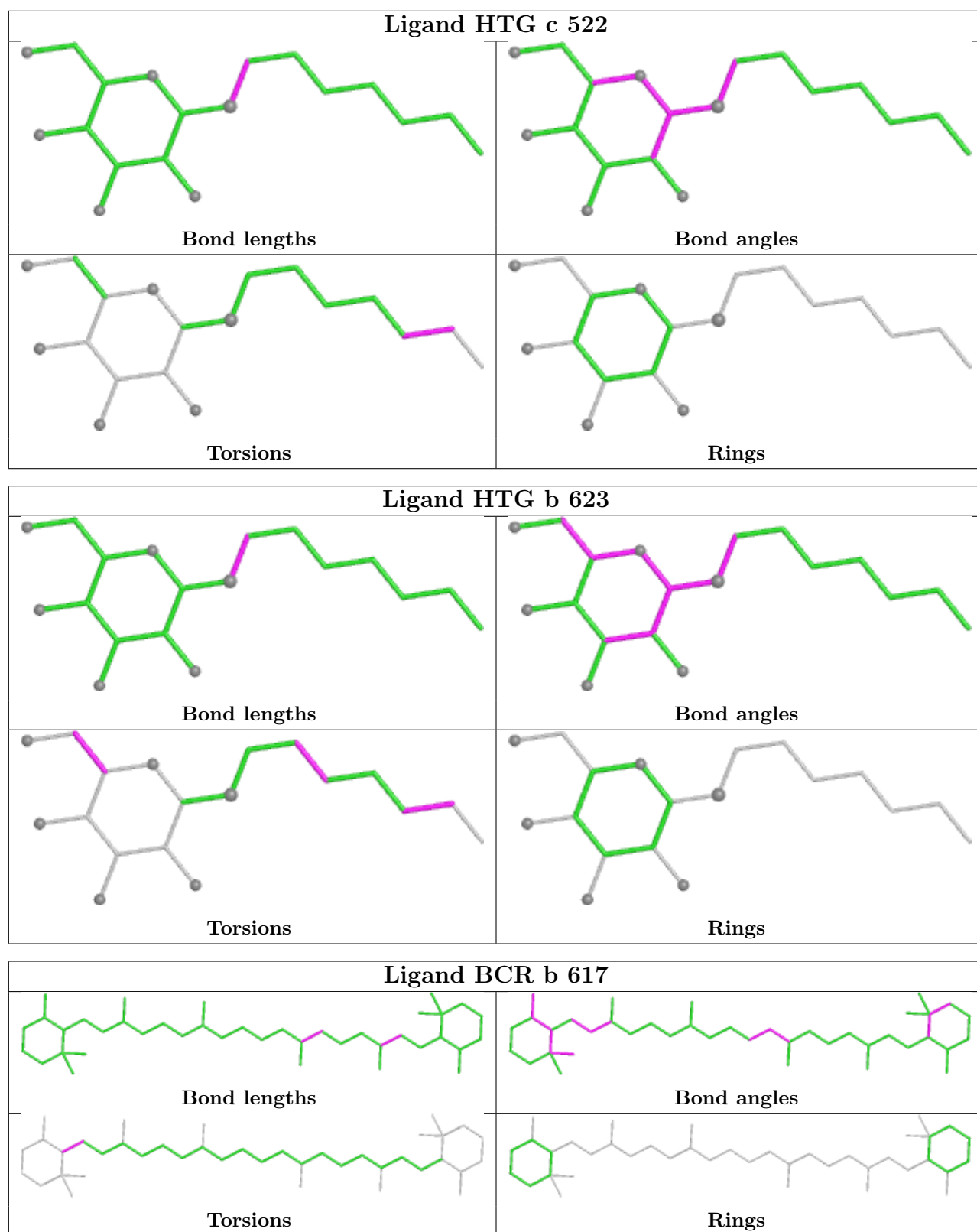


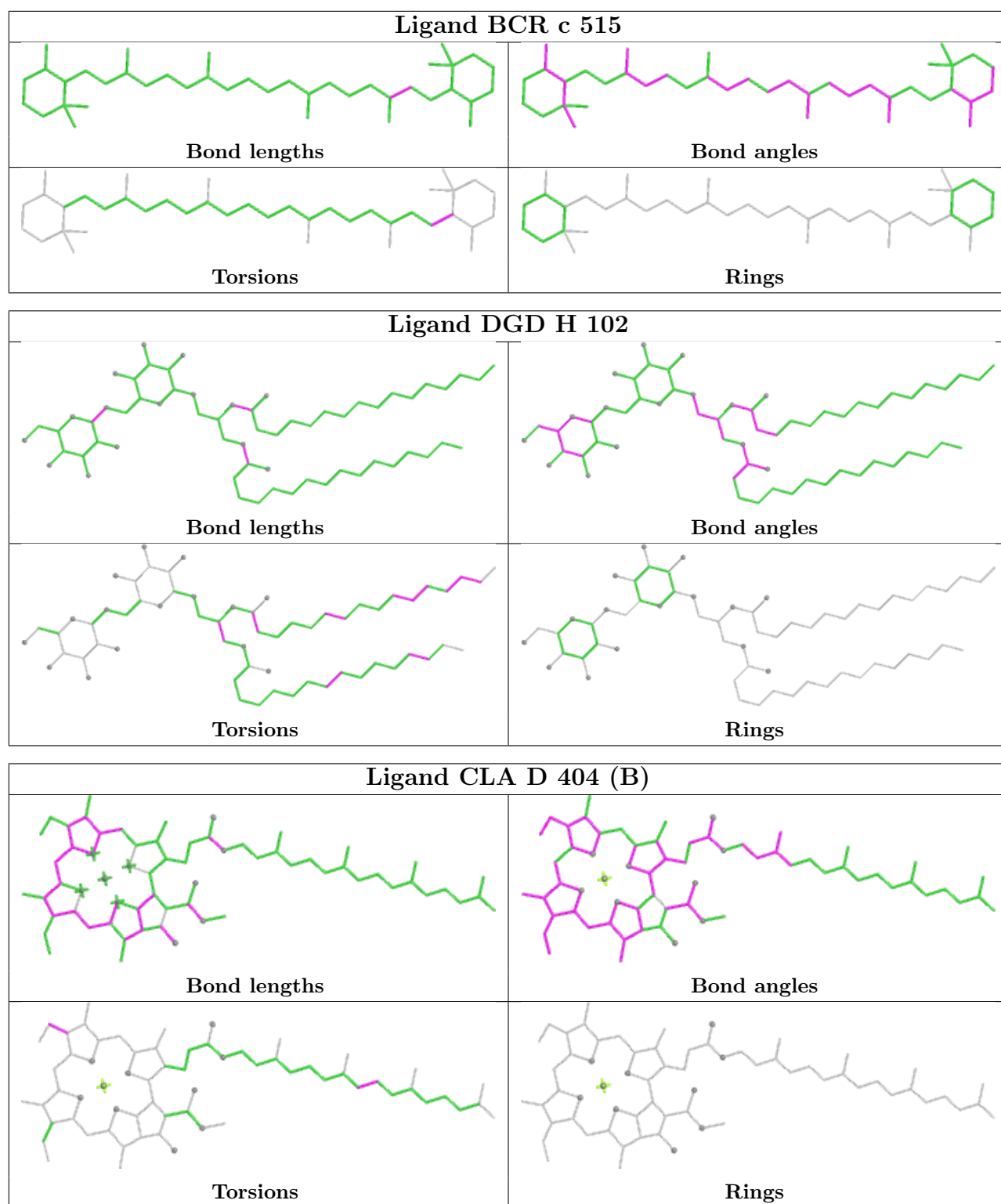
Ligand CLA b 615

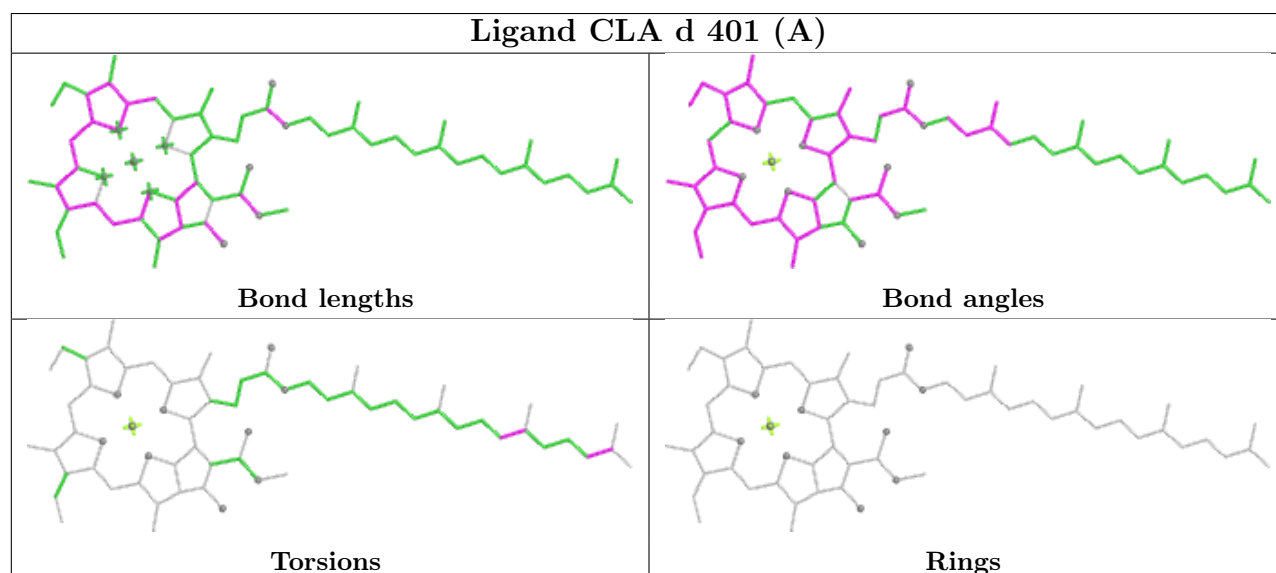
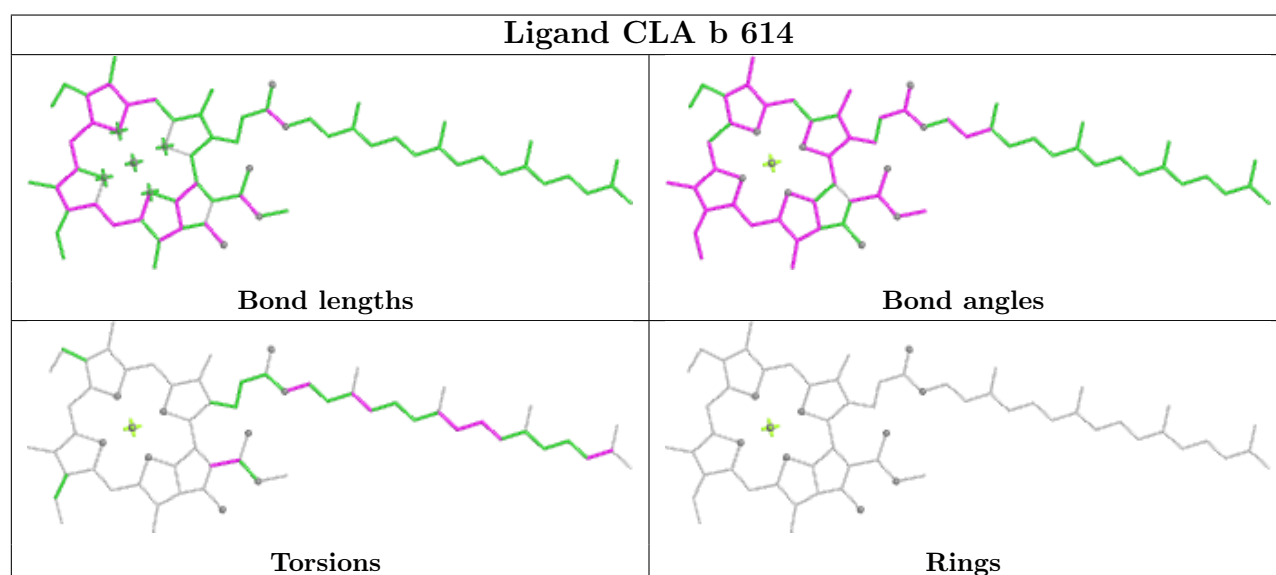
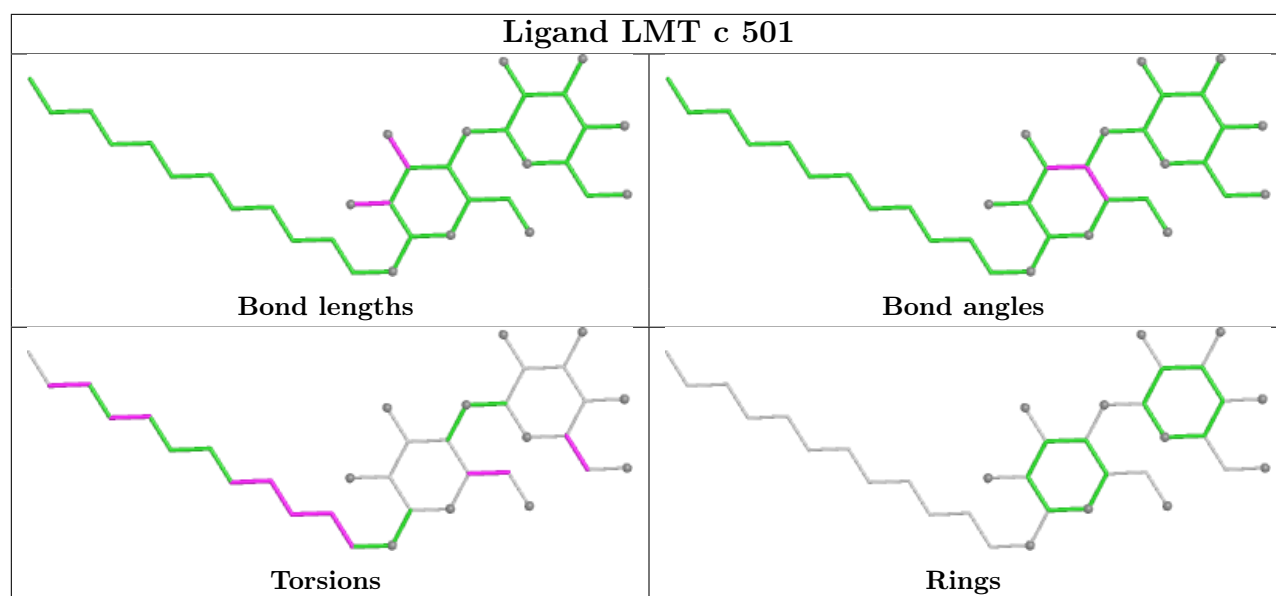


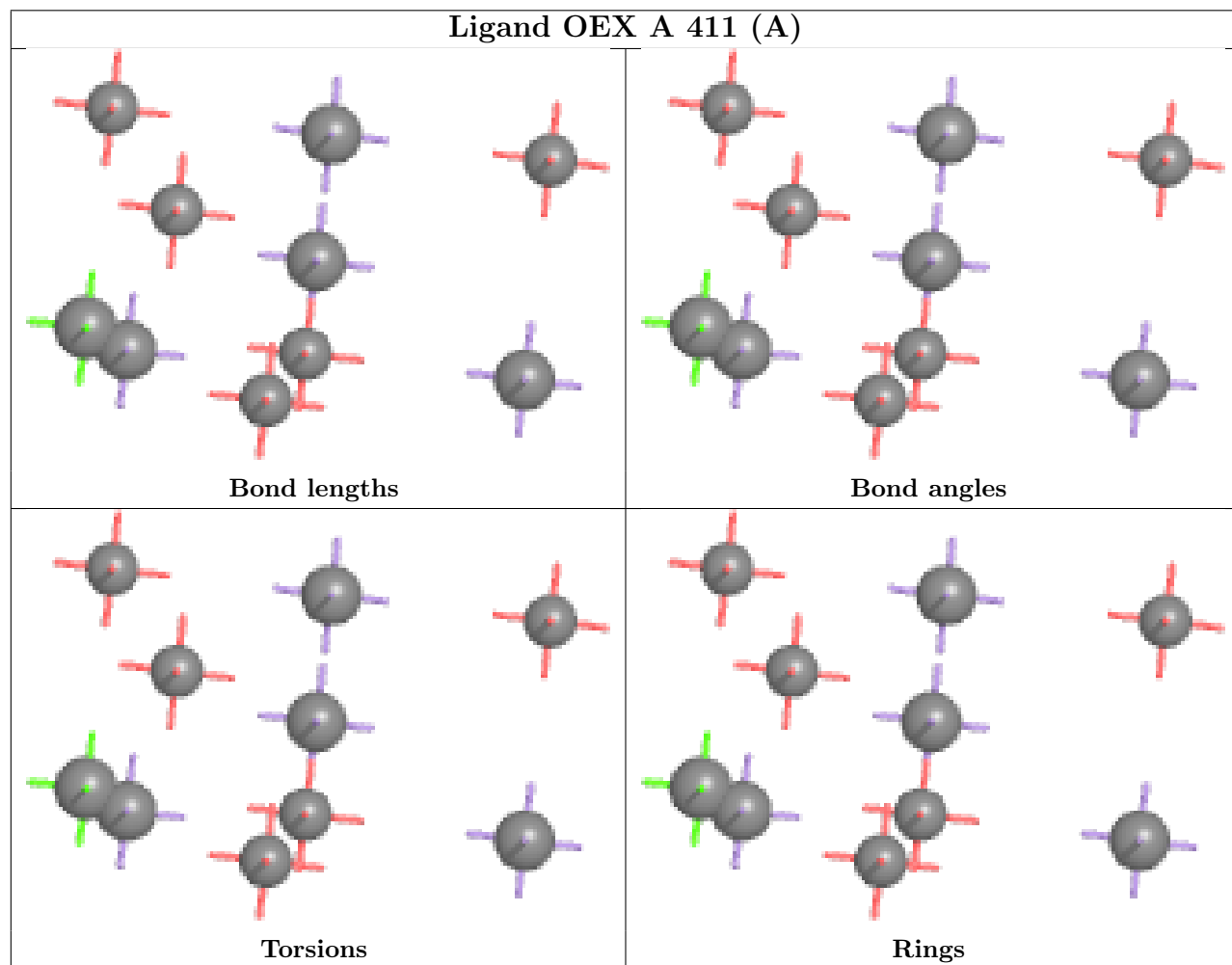
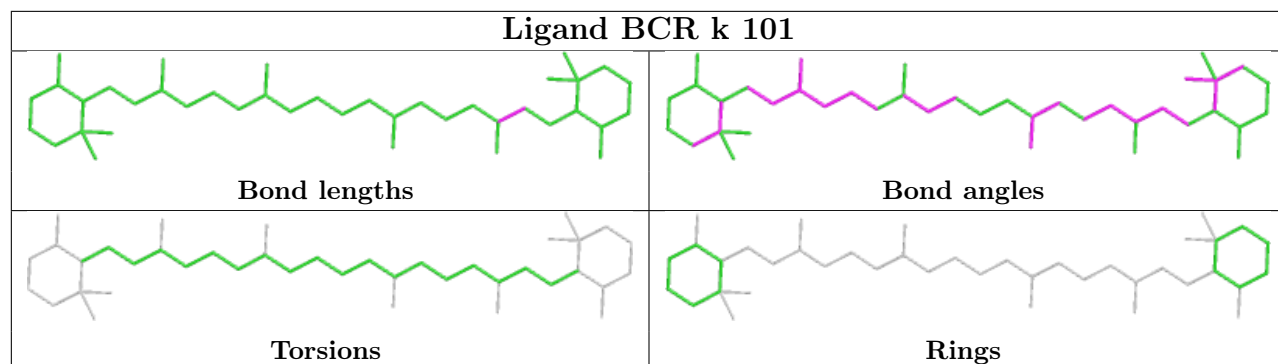
Ligand HTG B 622



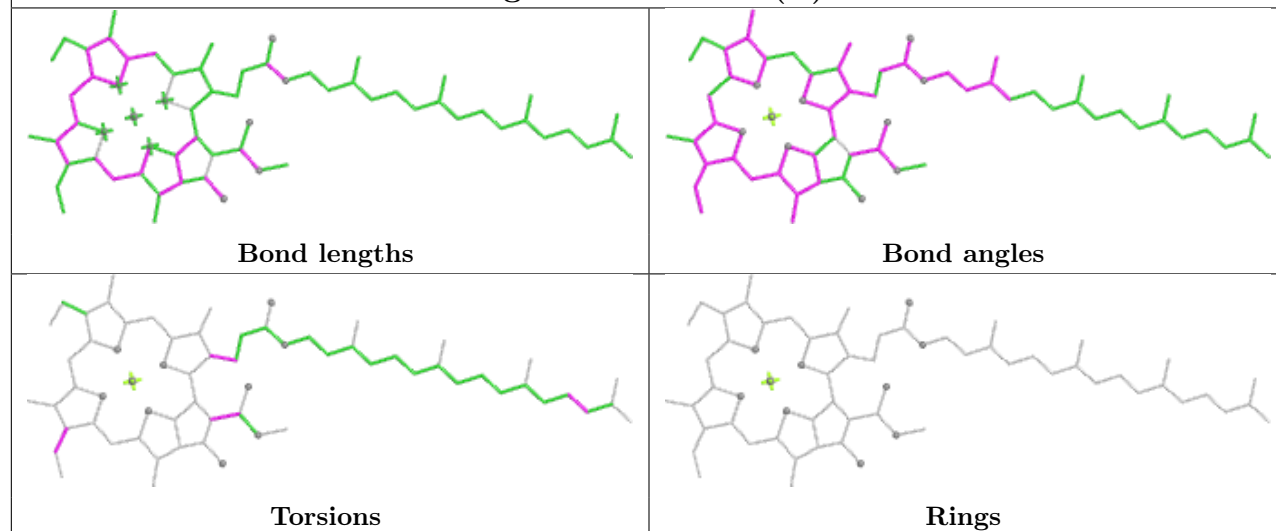




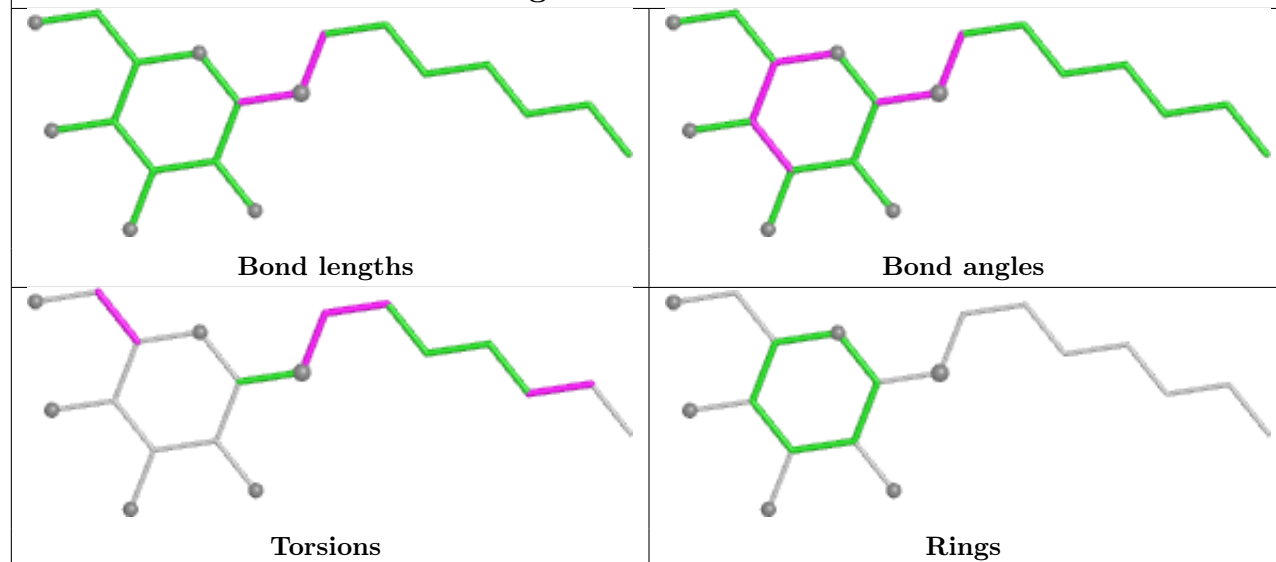


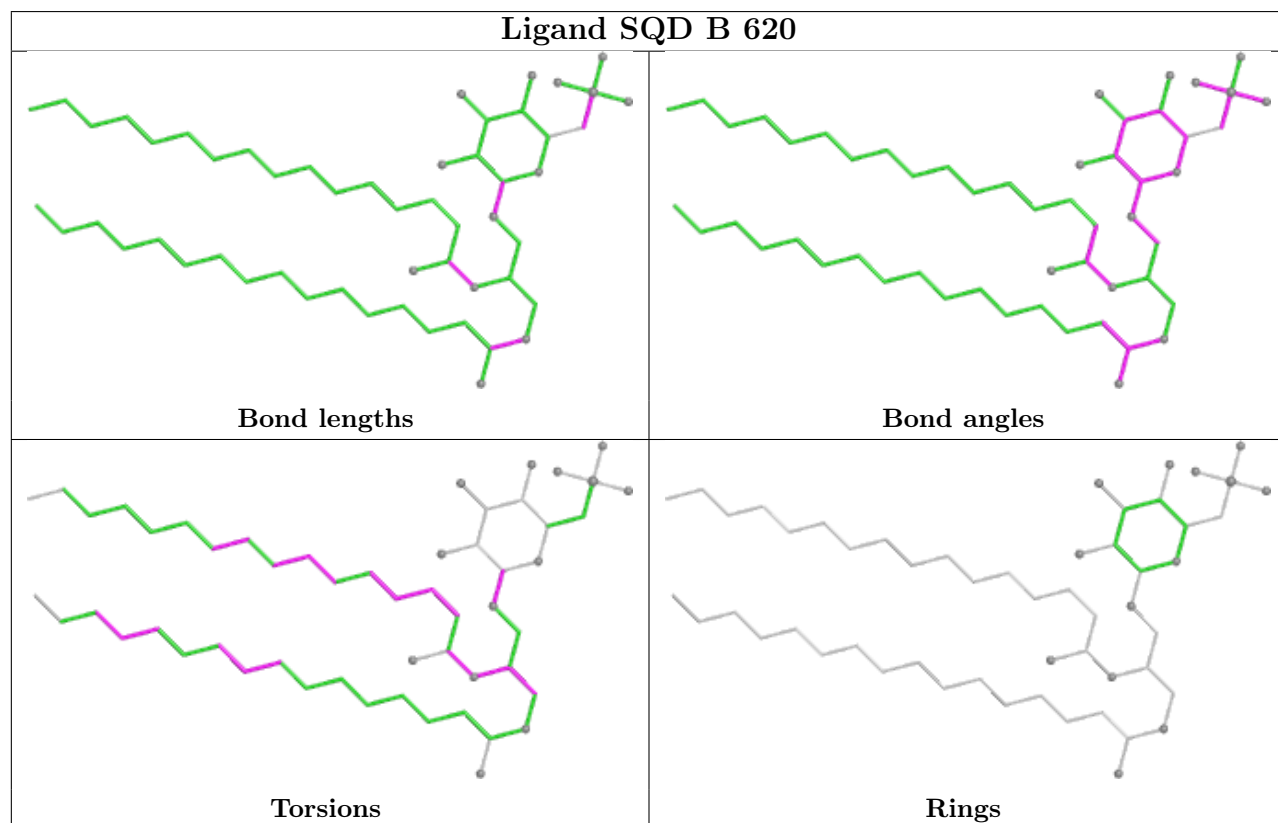
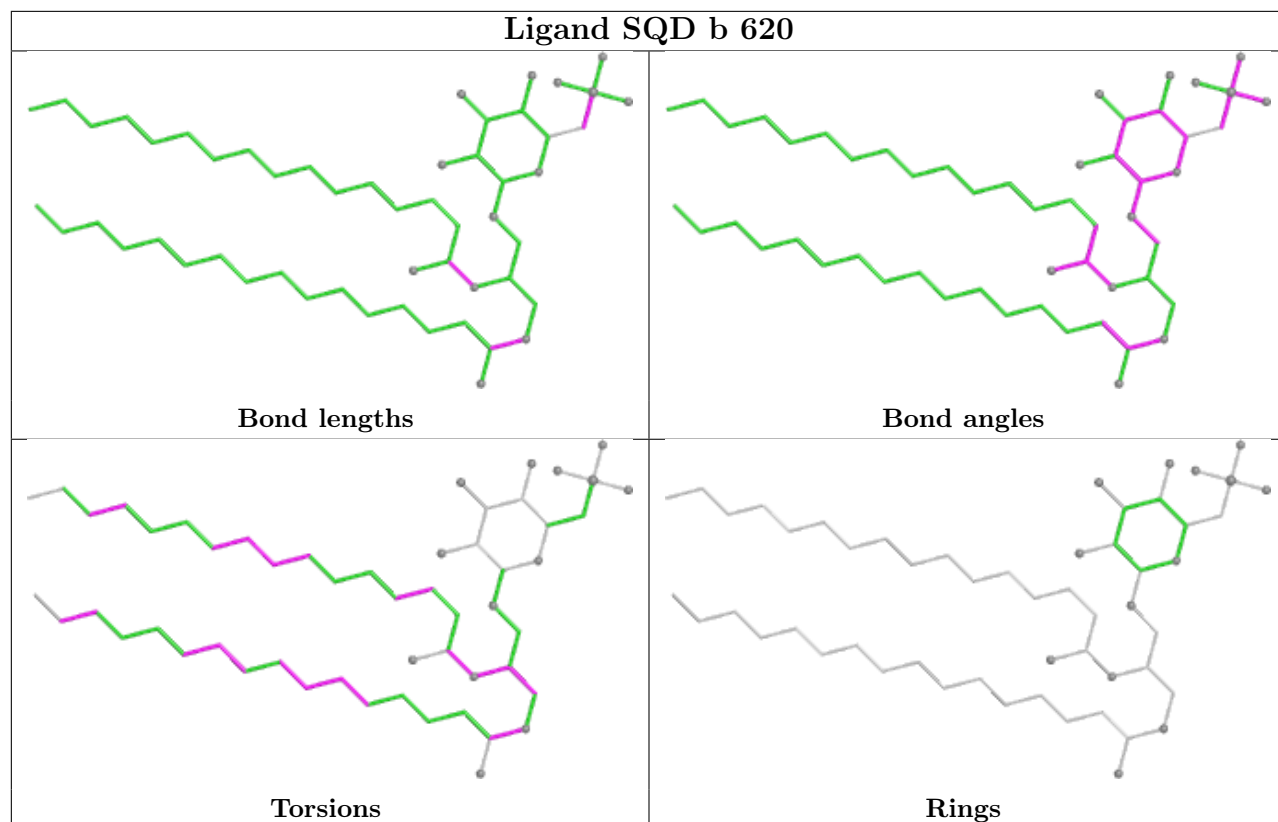


Ligand CLA a 406 (B)

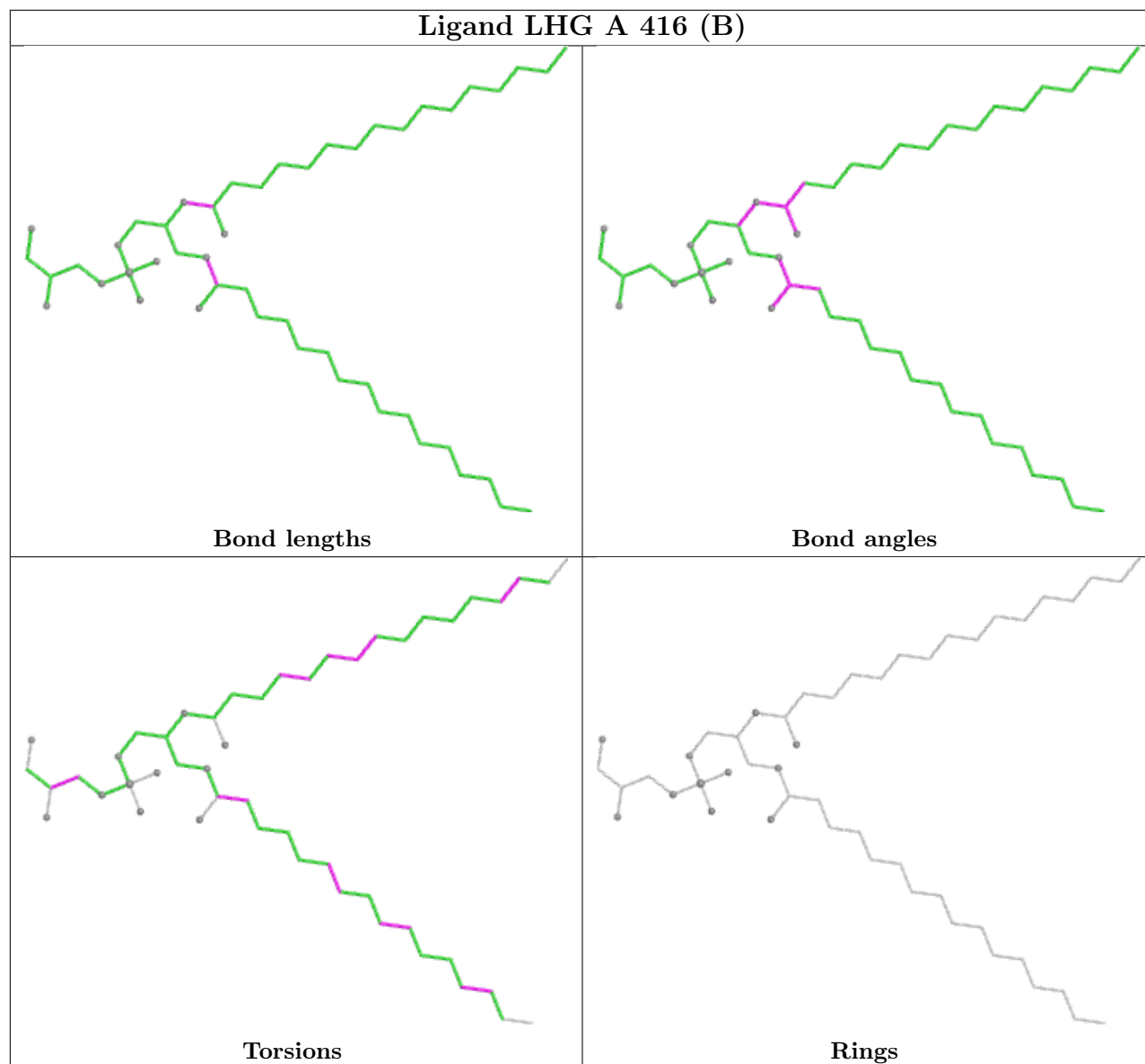


Ligand HTG B 625

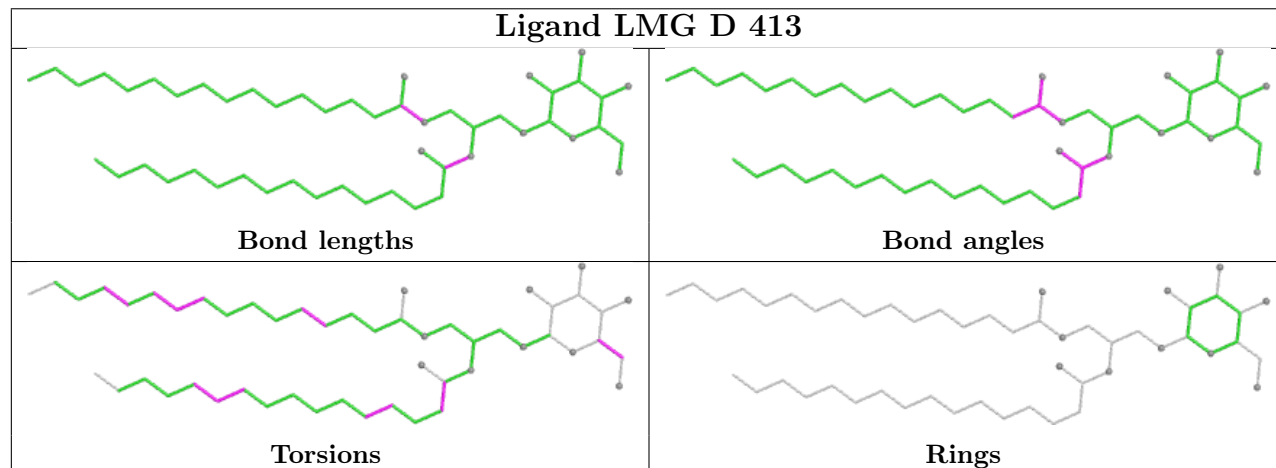


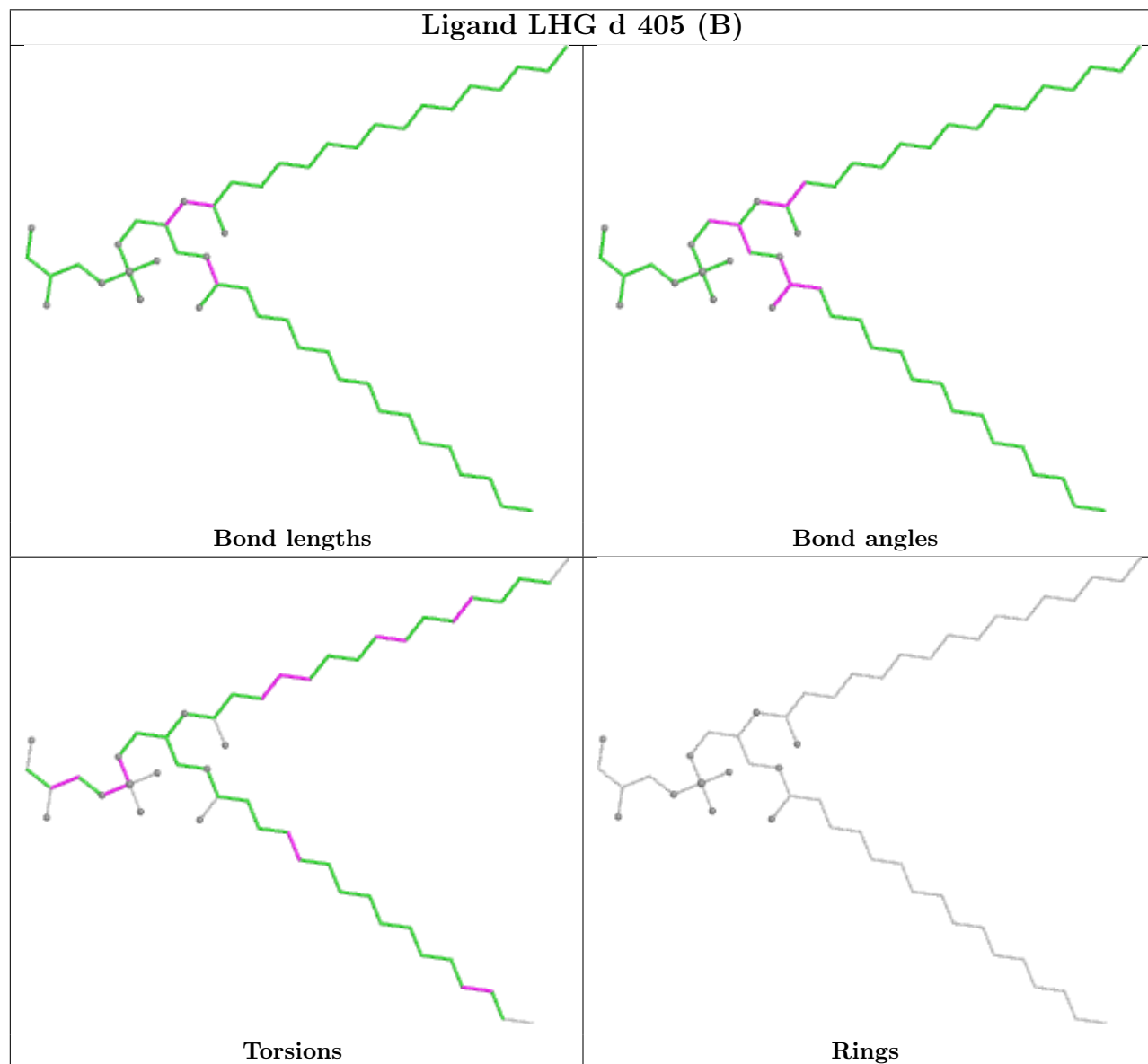
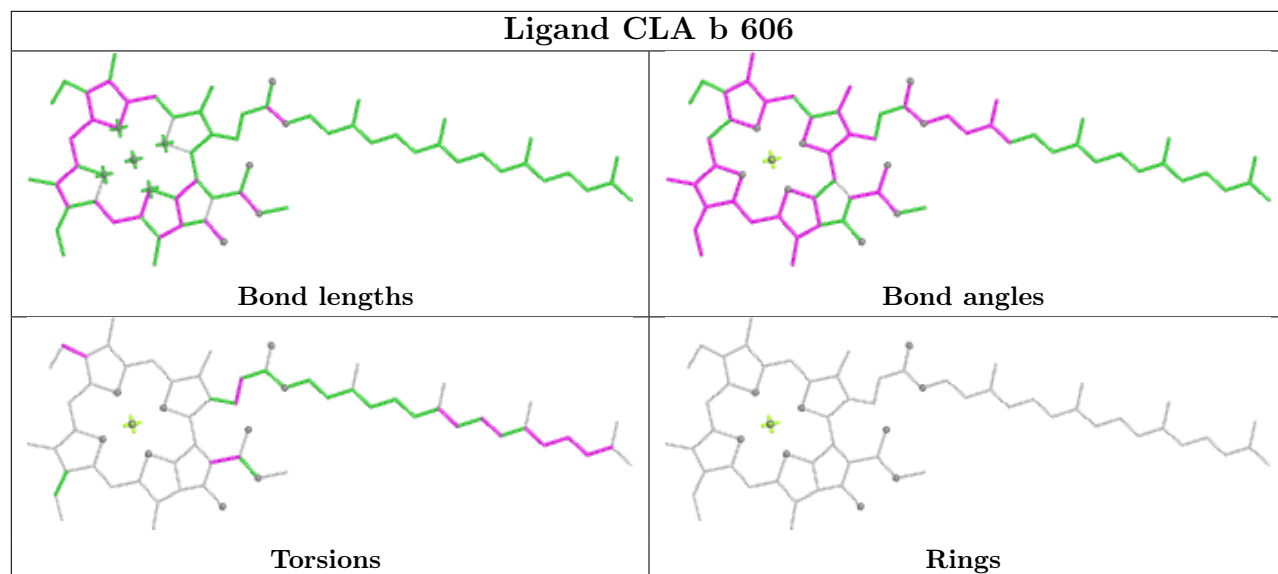


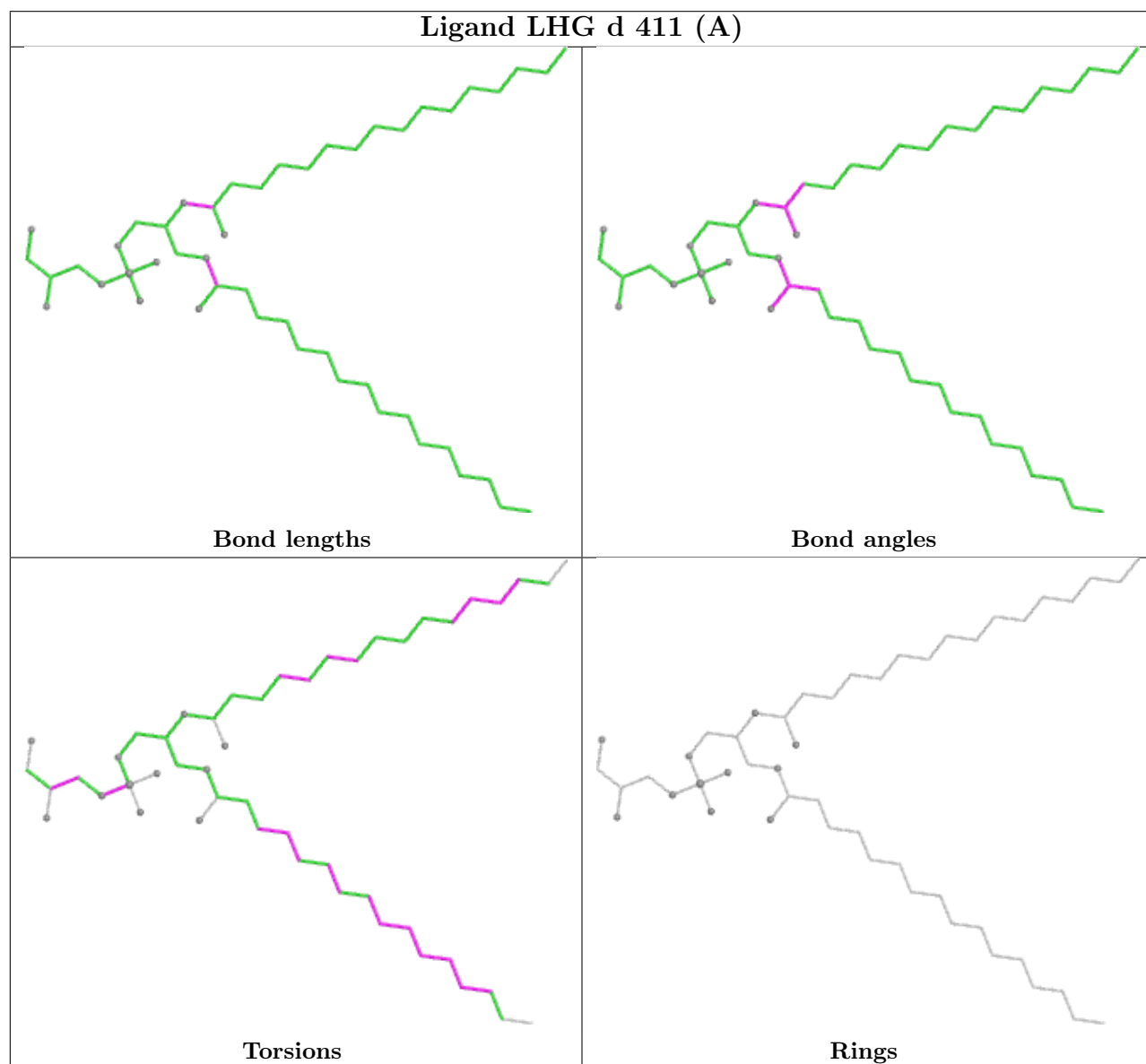
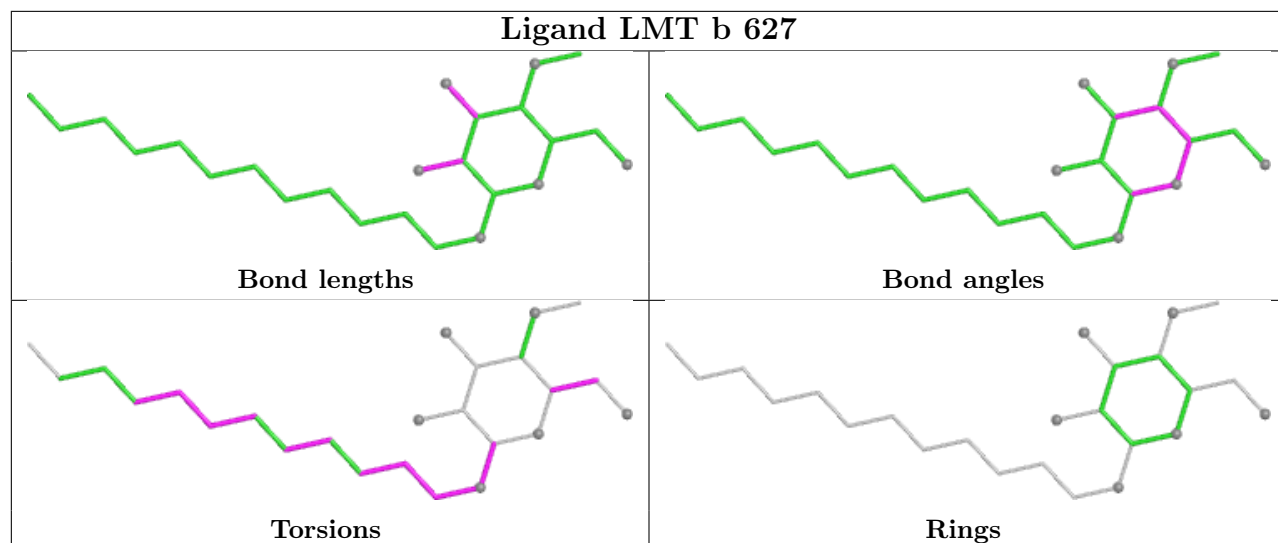
Ligand LHG A 416 (B)

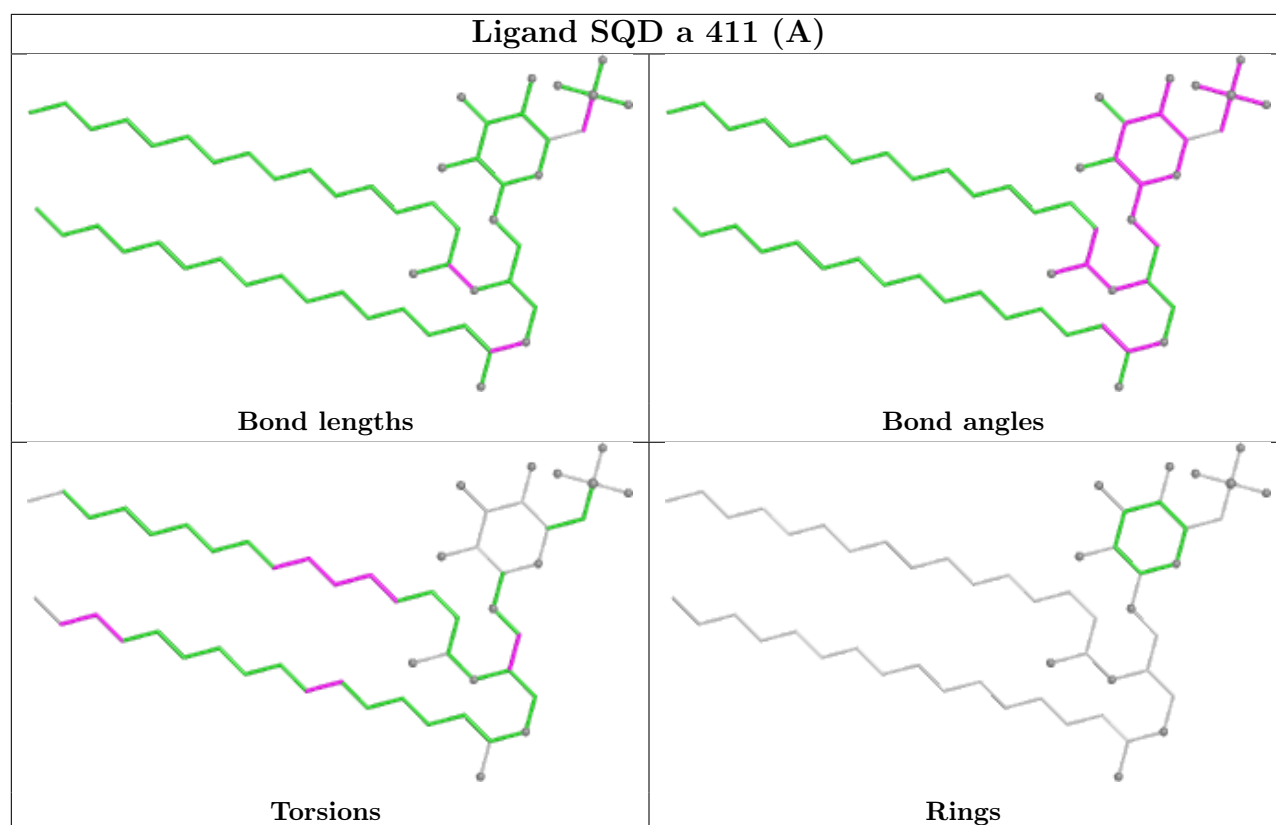


Ligand LMG D 413

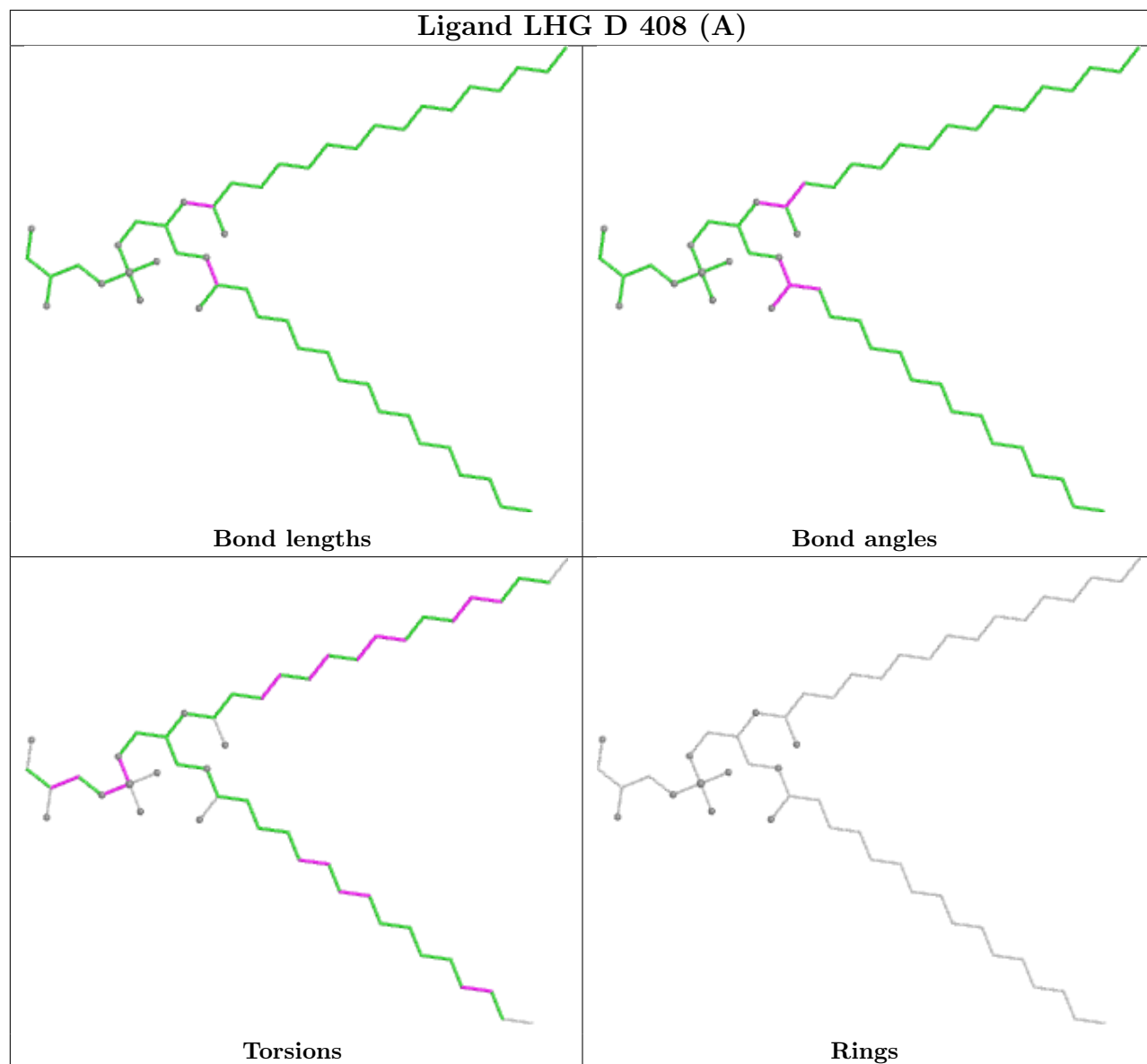




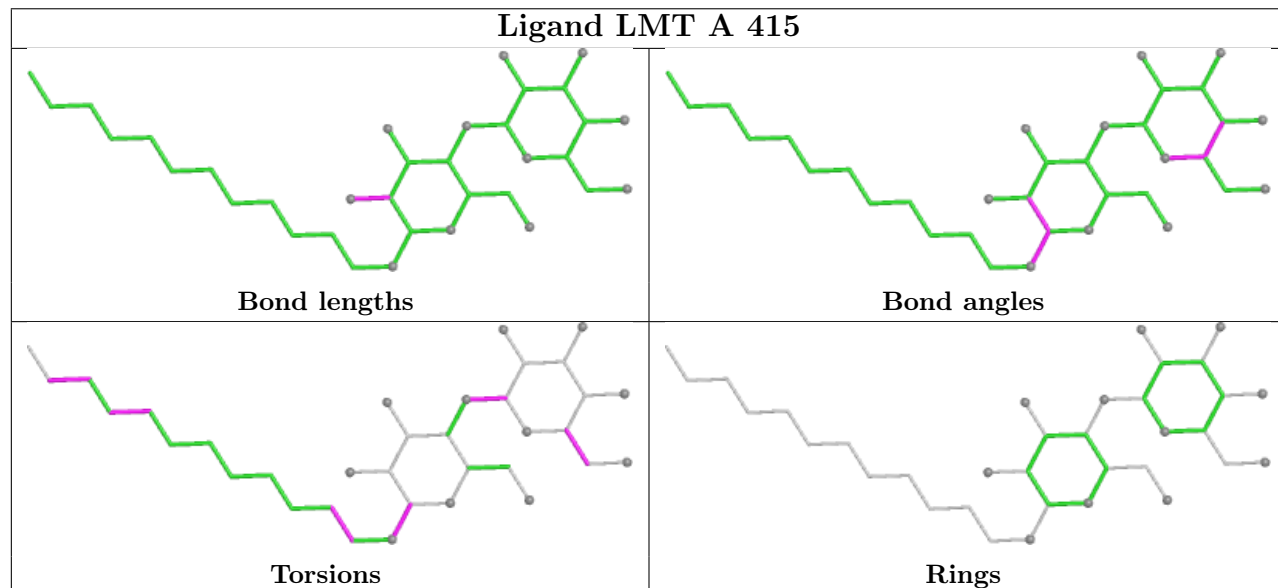


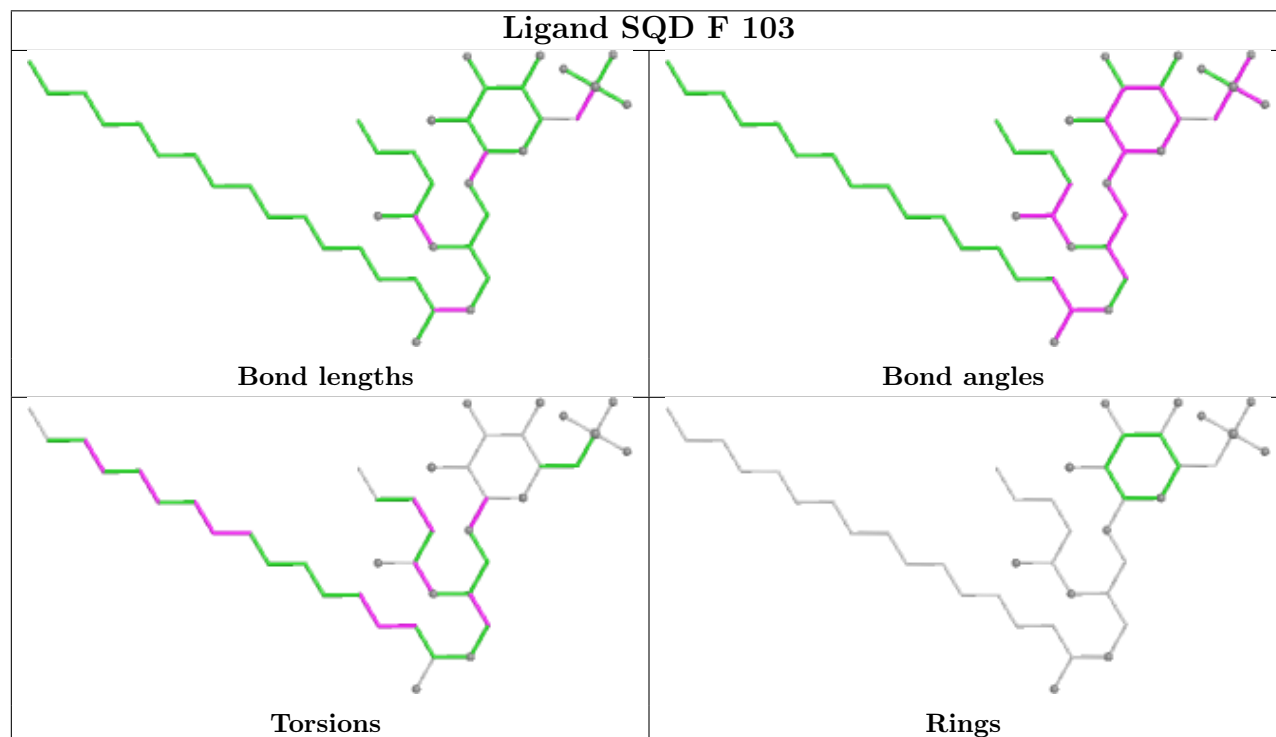
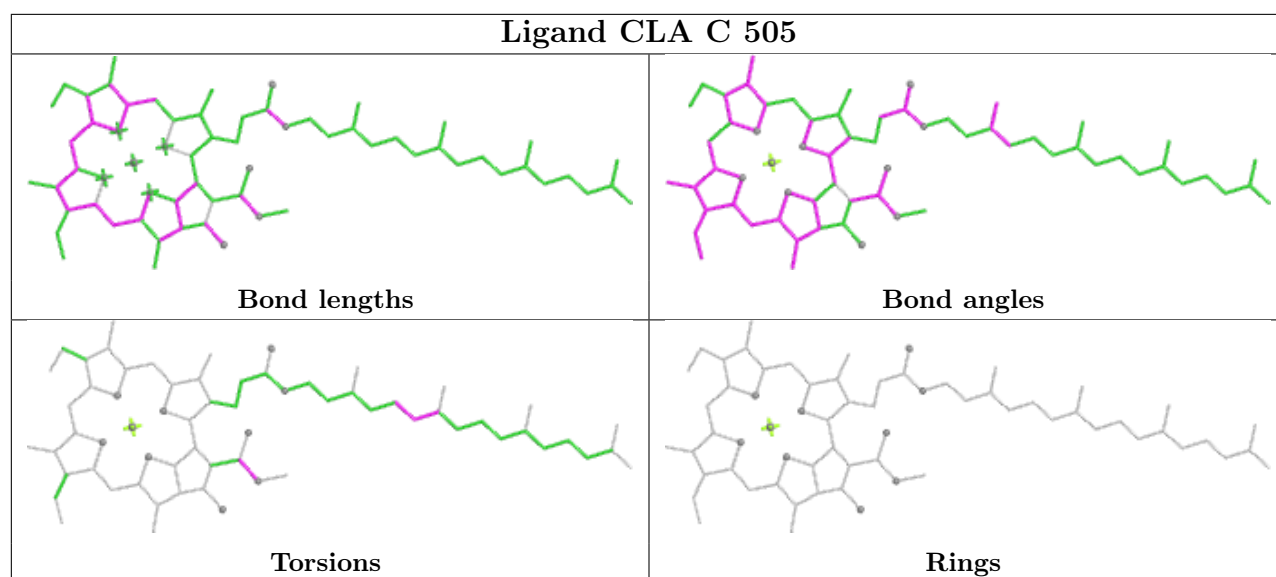


Ligand LHG D 408 (A)

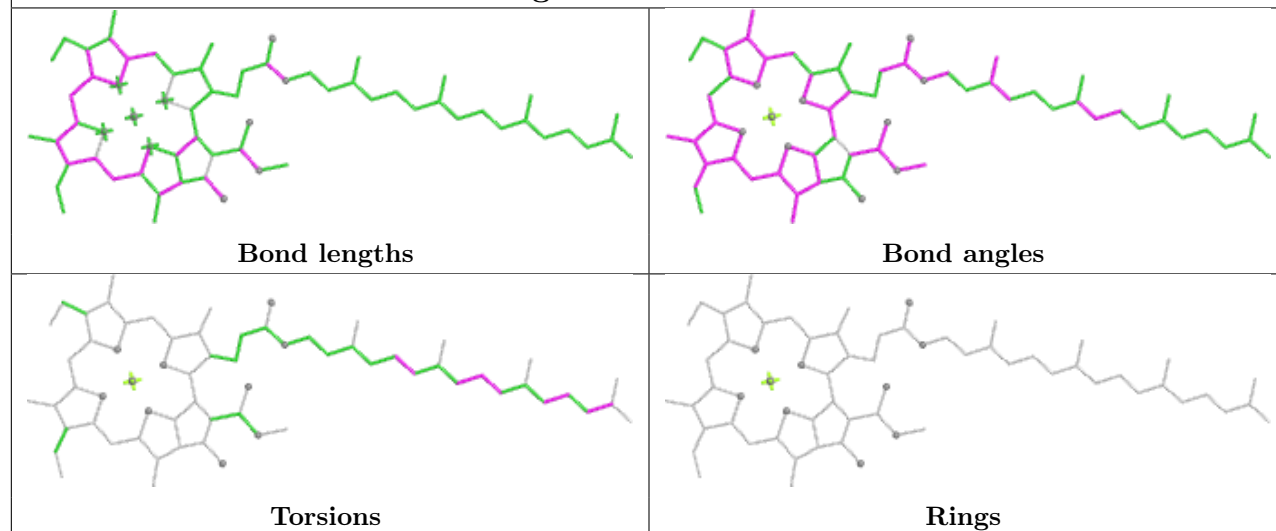


Ligand LMT A 415

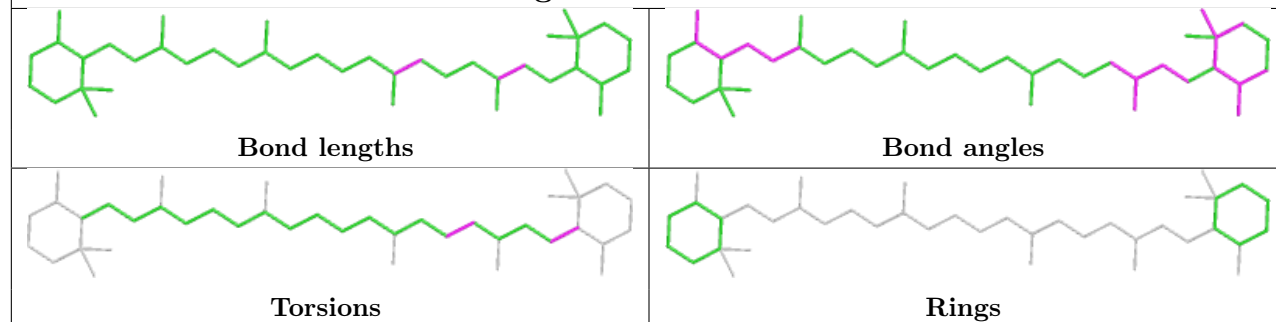




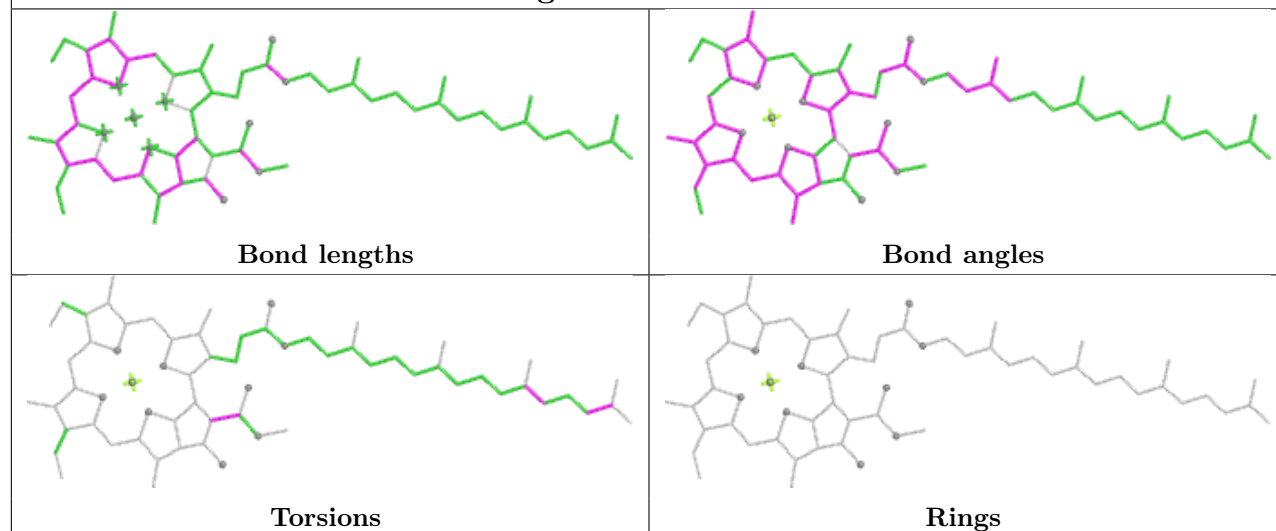
Ligand CLA B 615

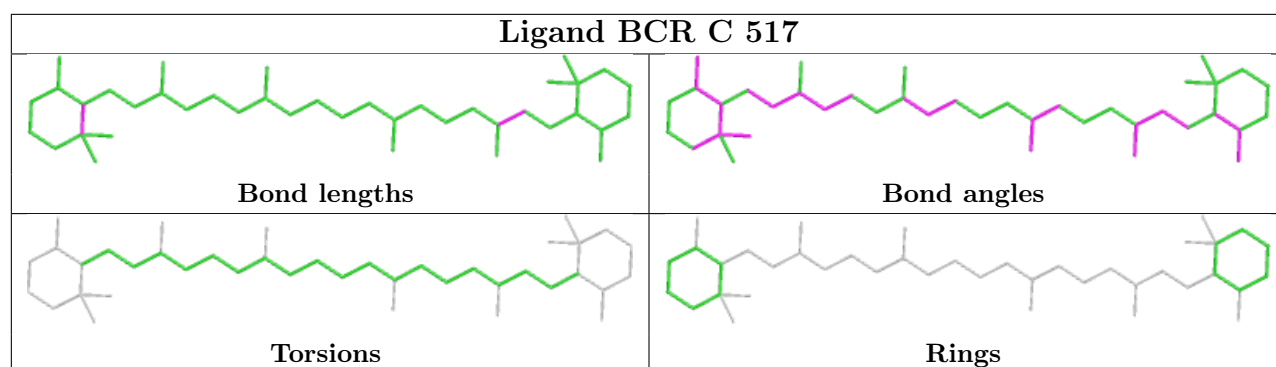
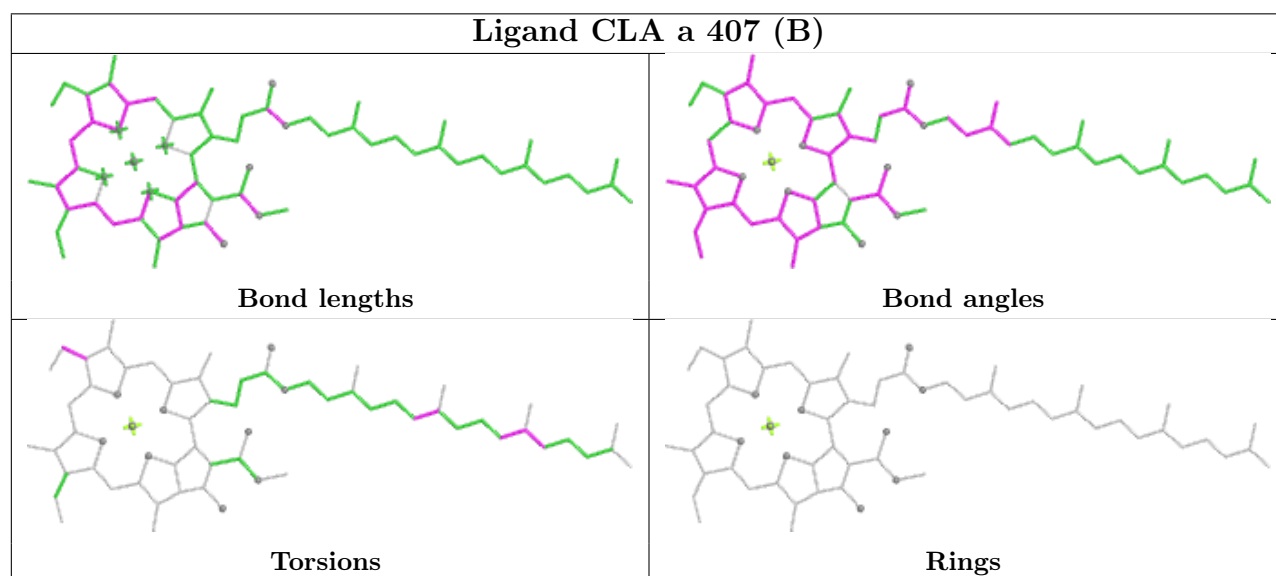
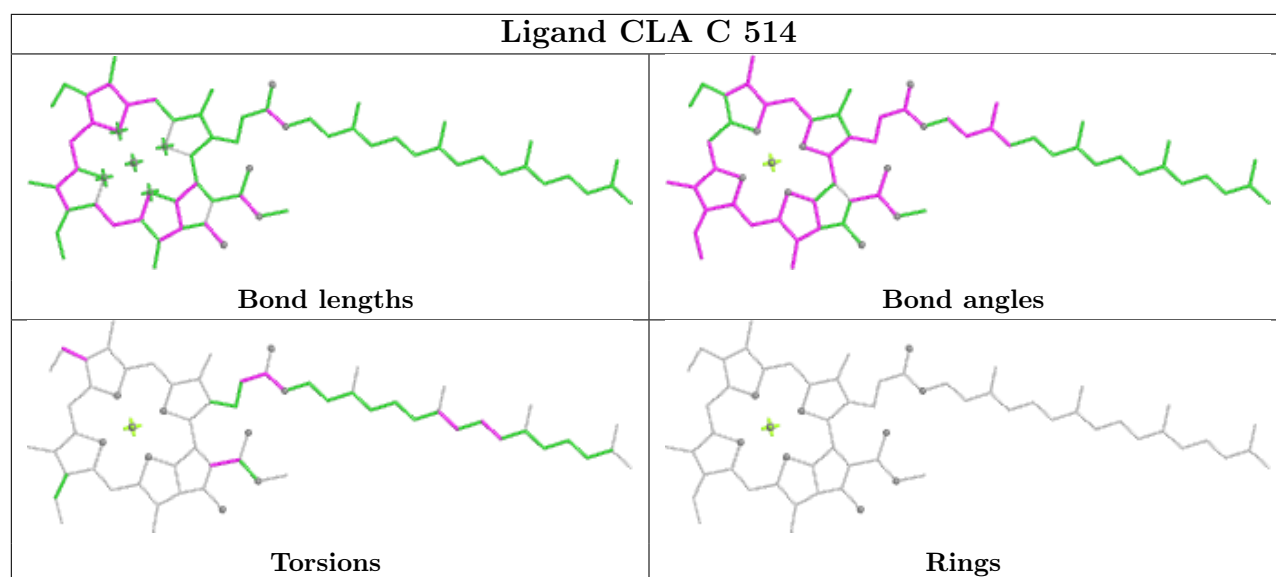


Ligand BCR a 410

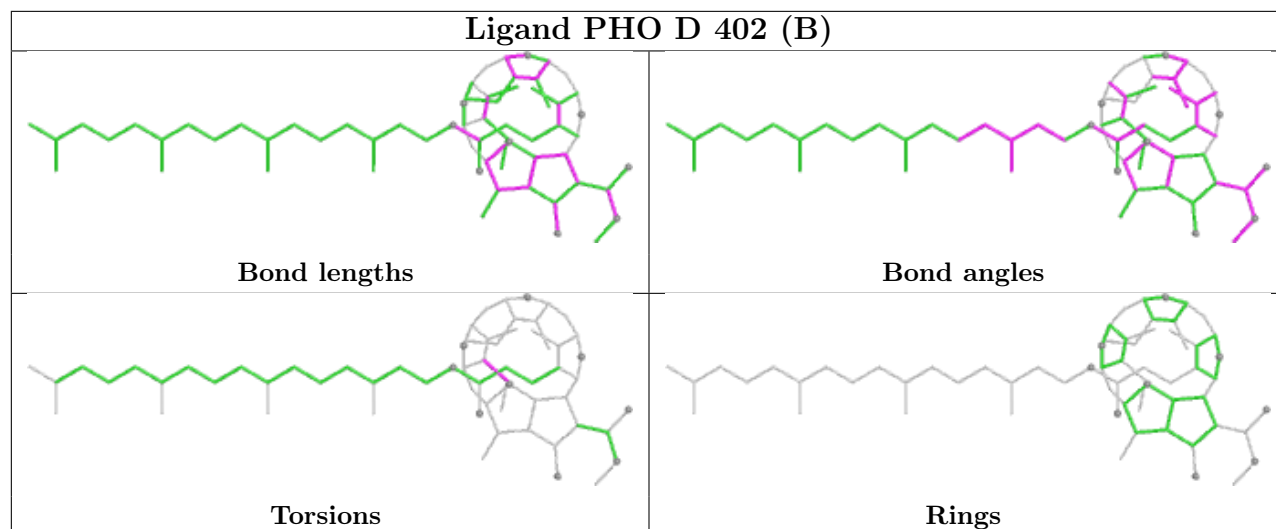


Ligand CLA c 509

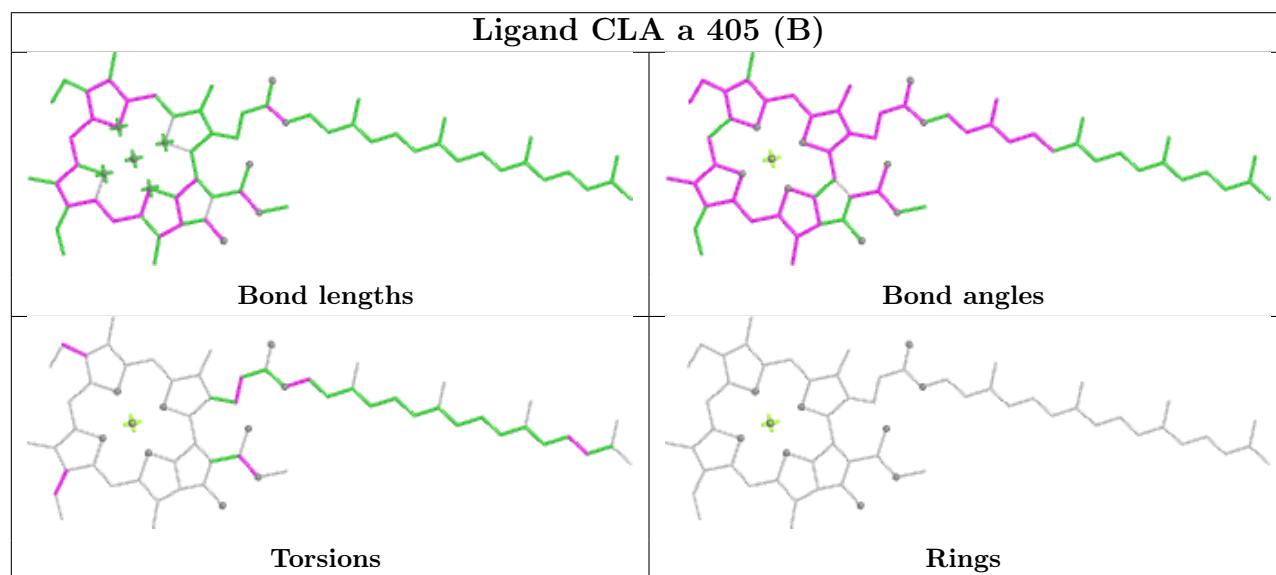




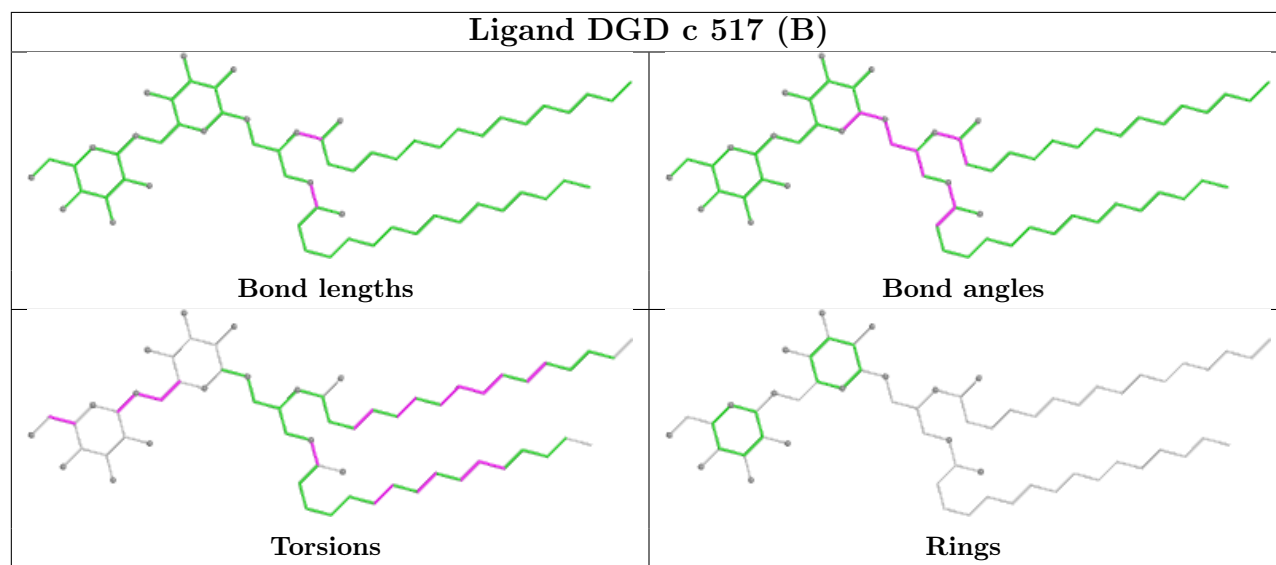
Ligand PHO D 402 (B)

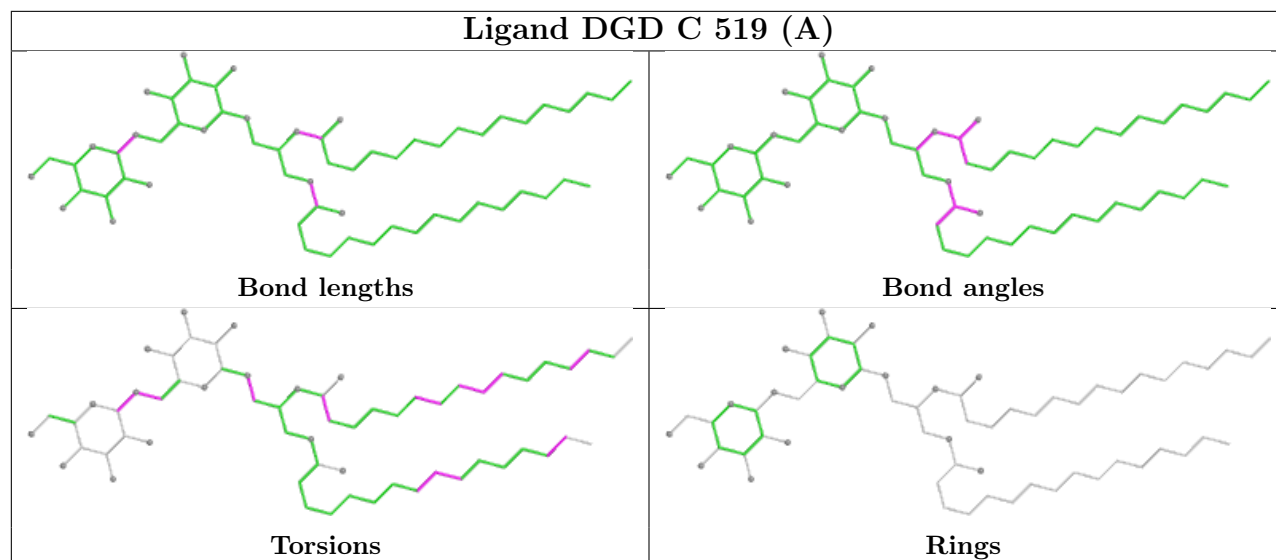
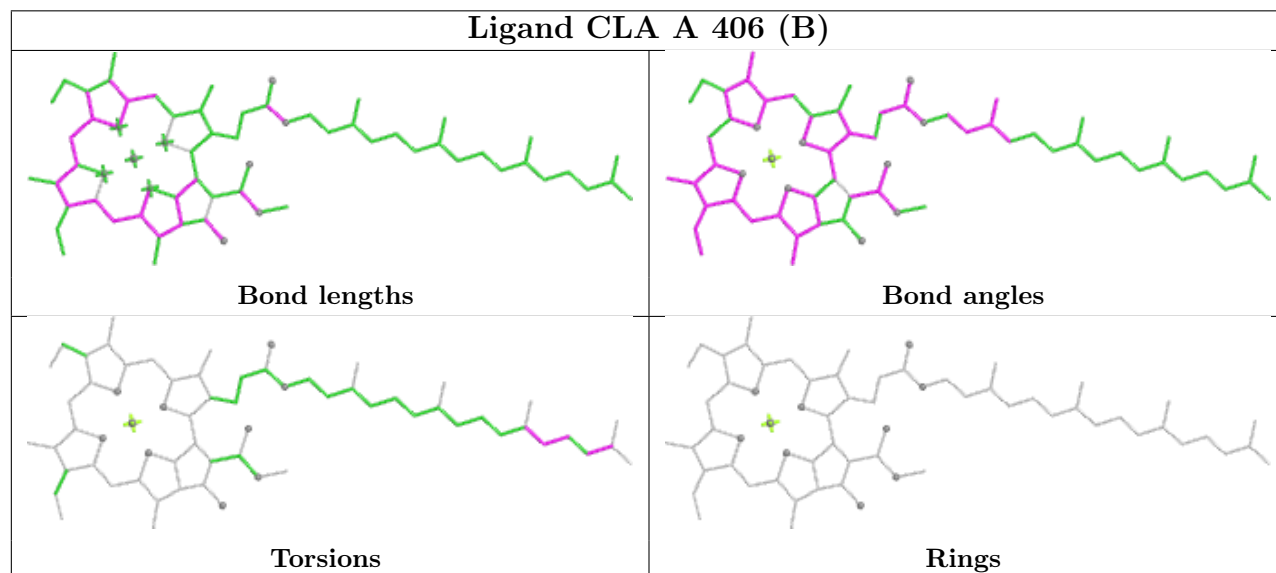
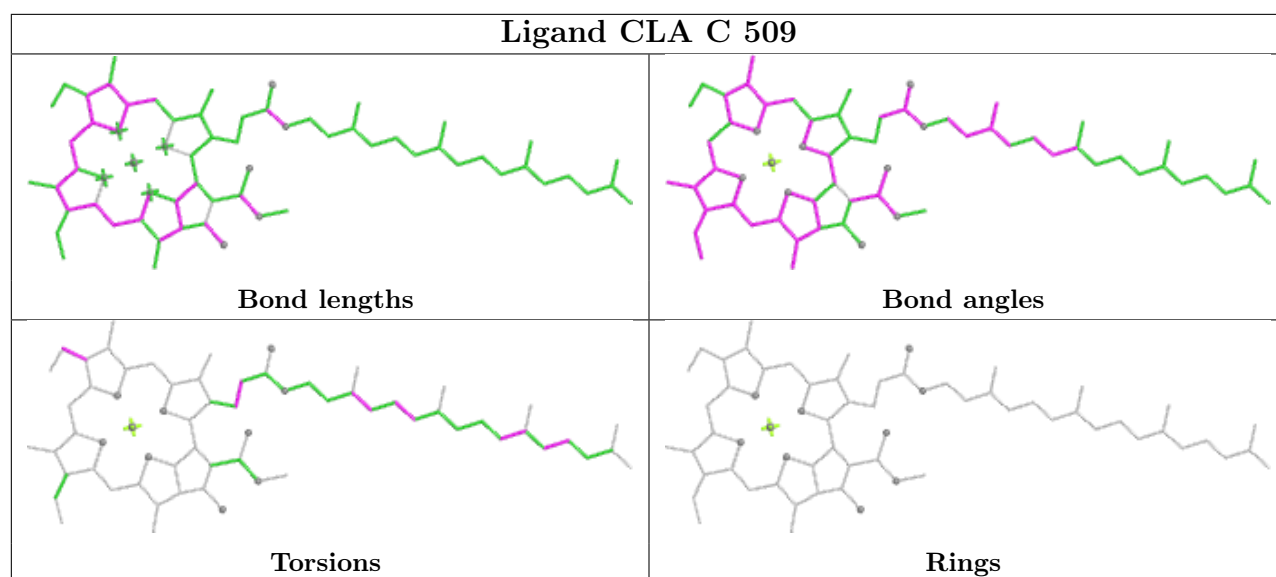


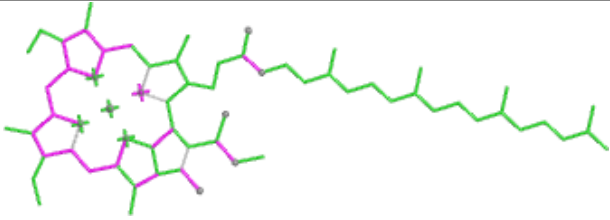
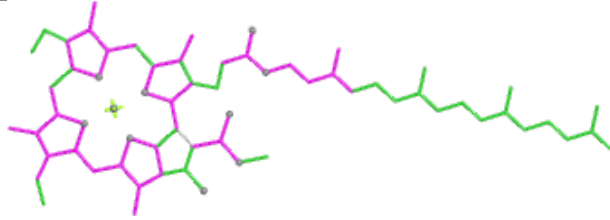
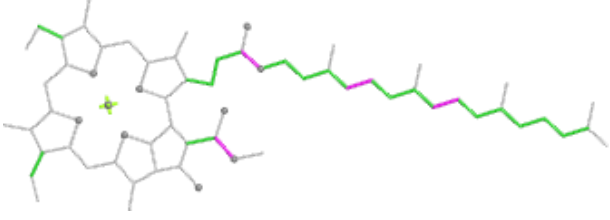
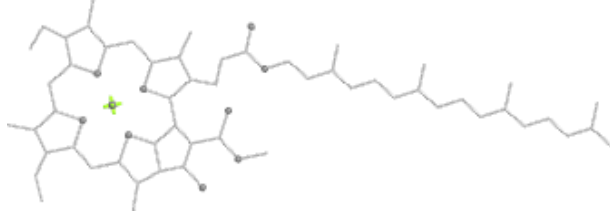
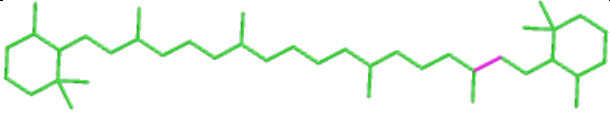
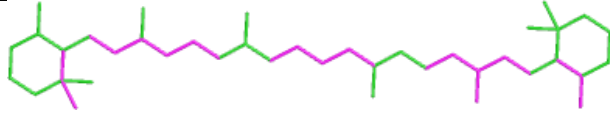
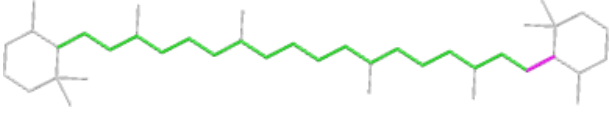
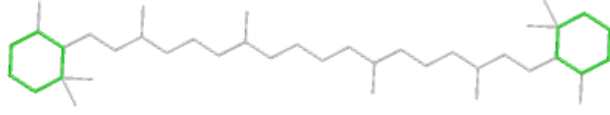
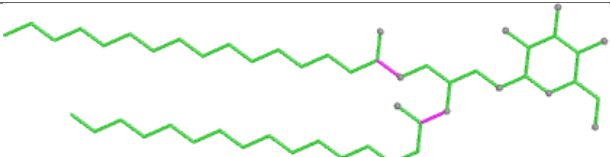
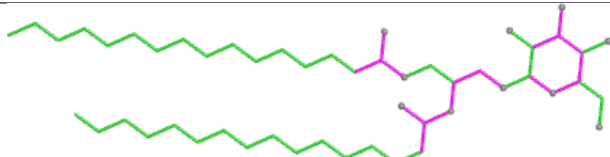
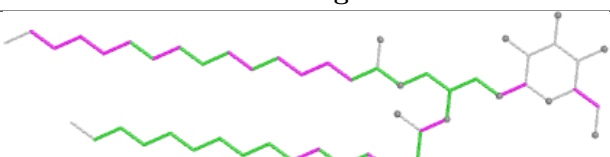
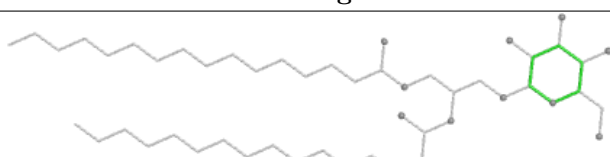
Ligand CLA a 405 (B)

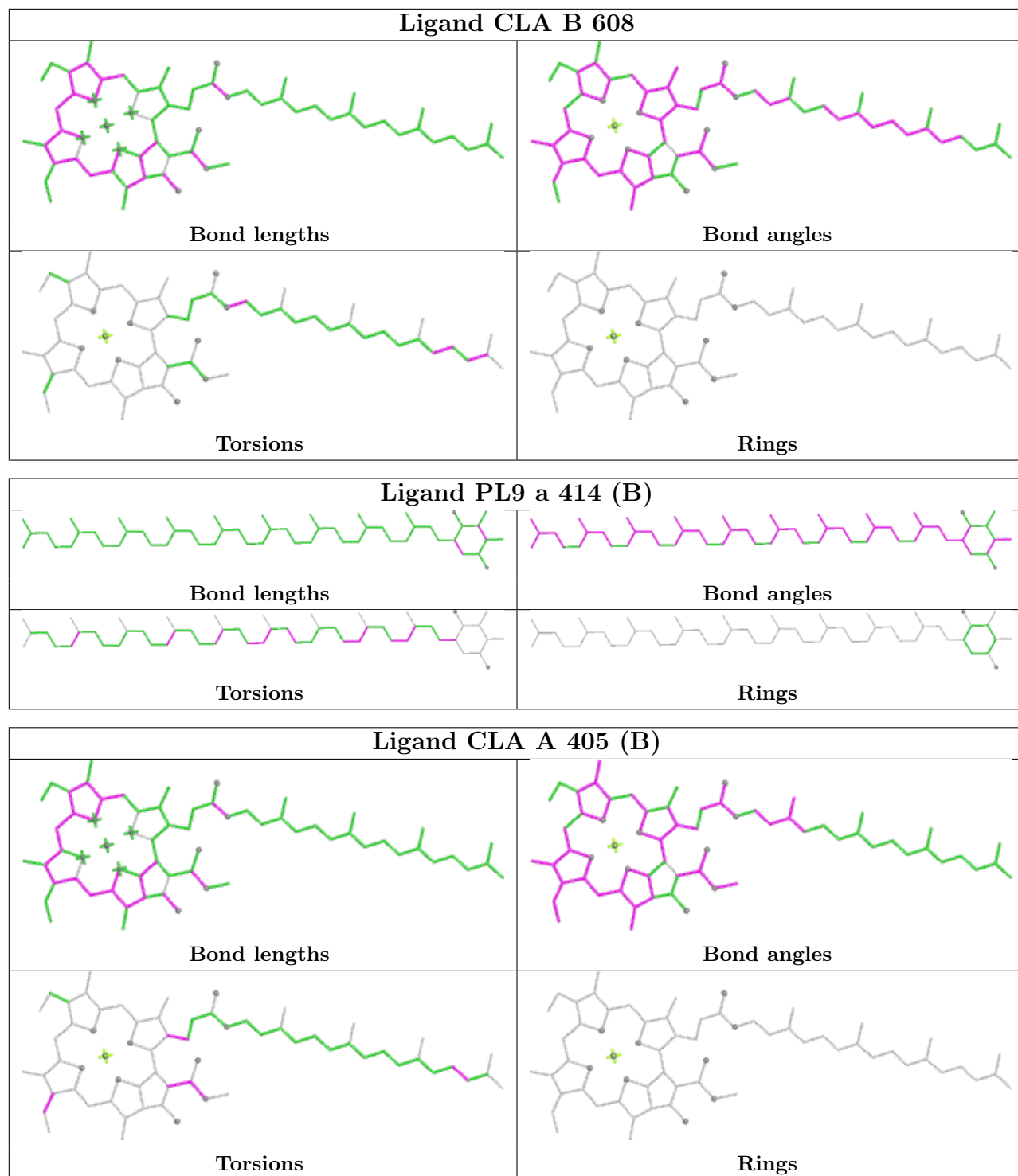


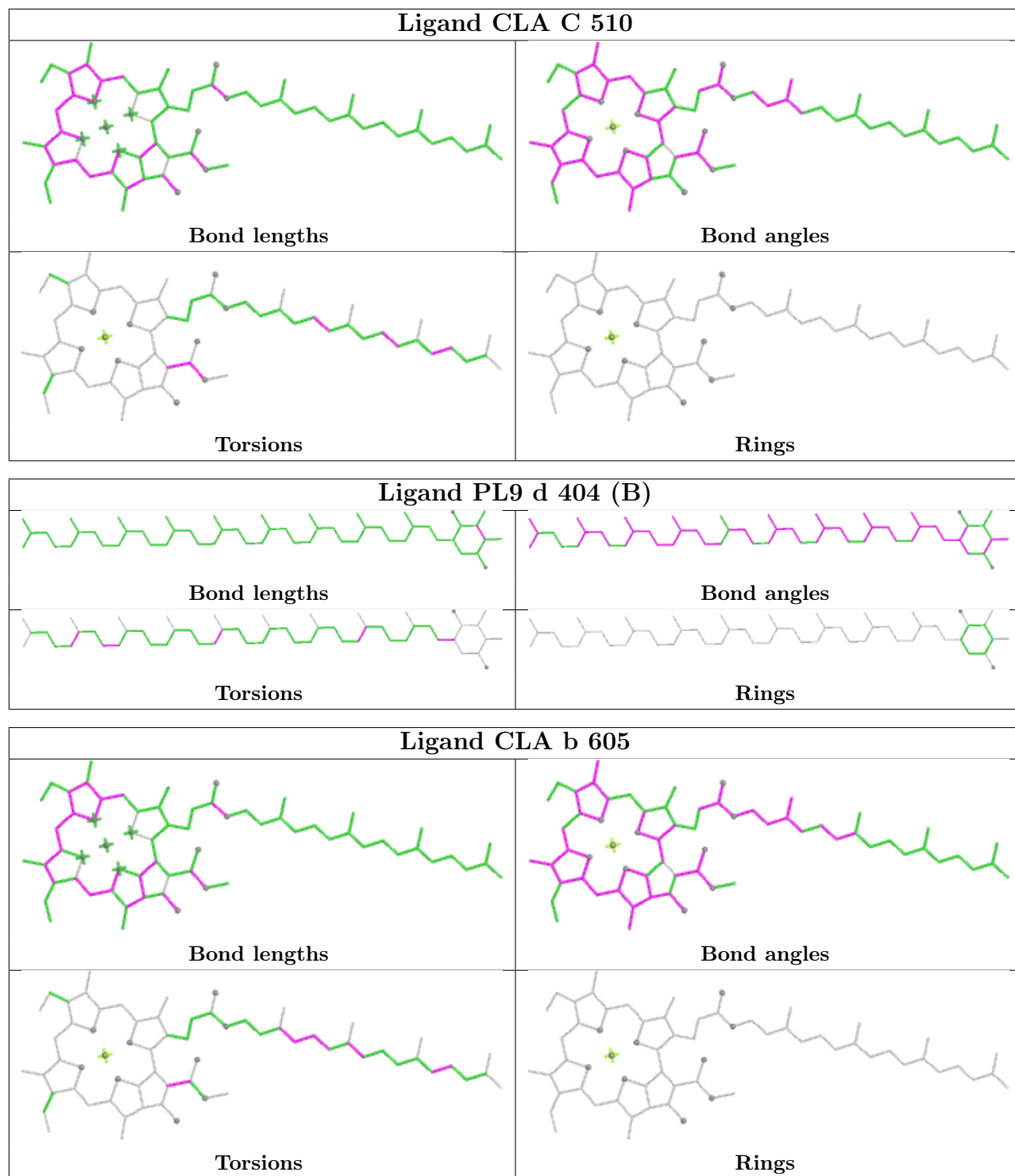
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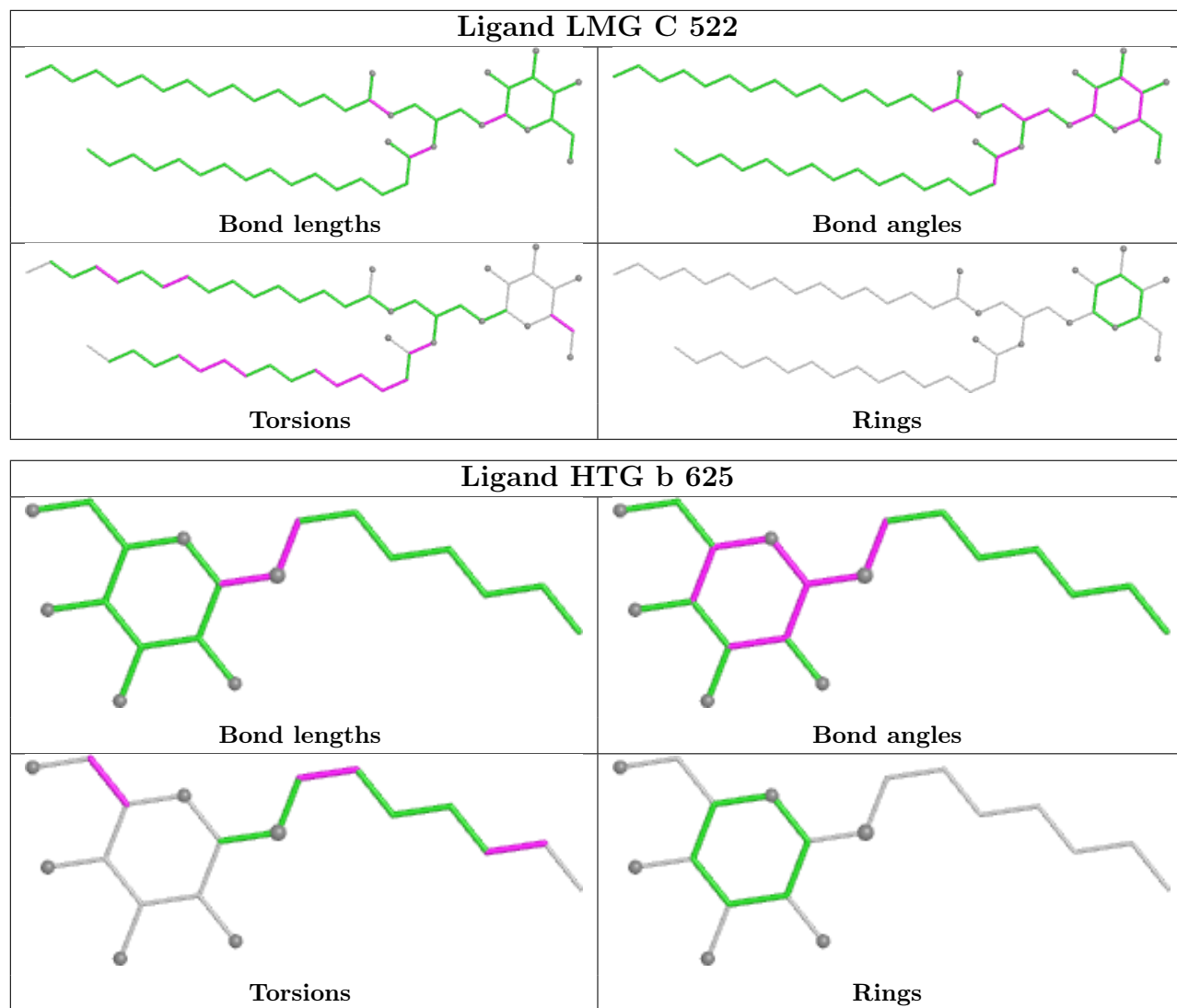


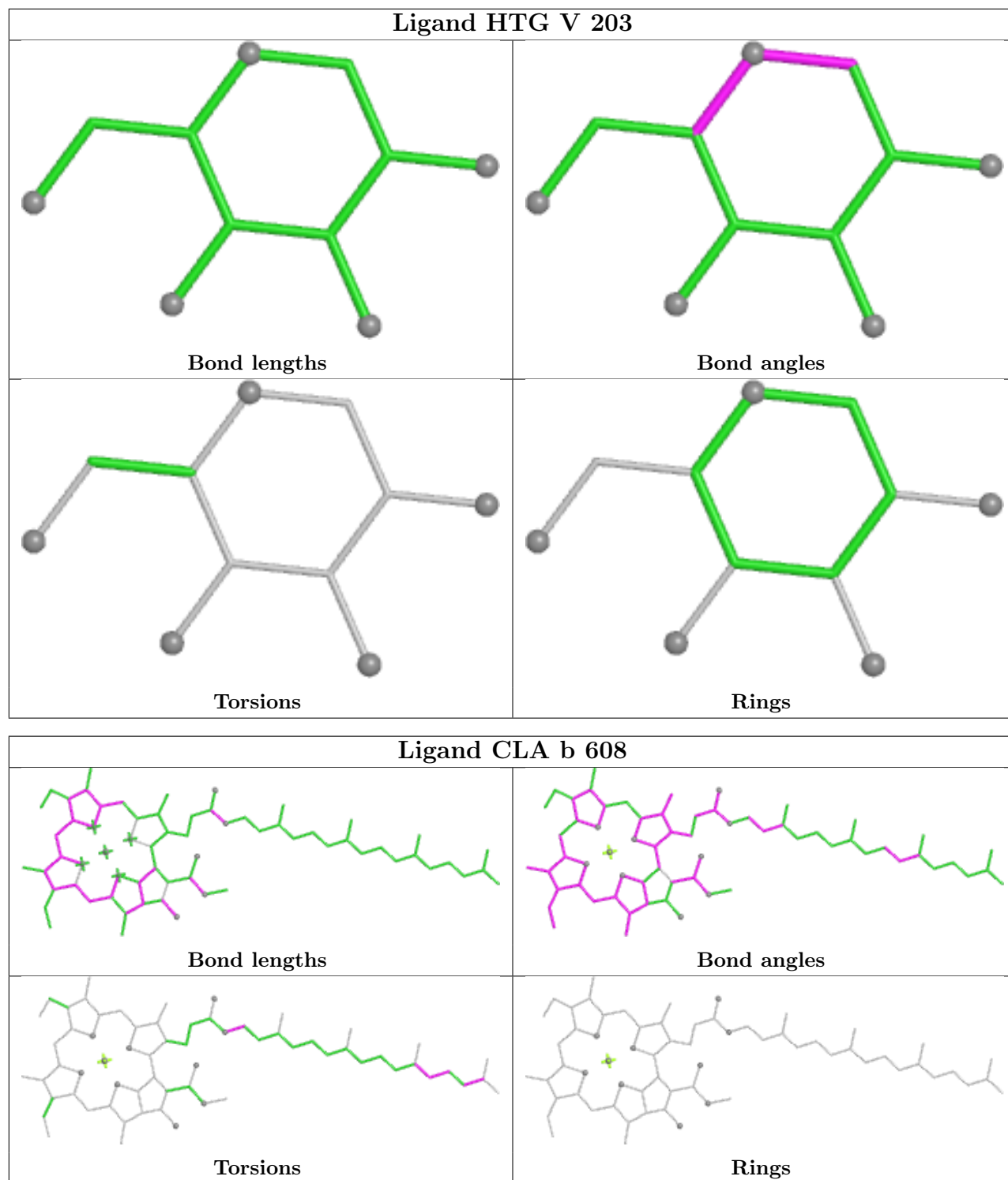


Ligand CLA c 512	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR H 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG m 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

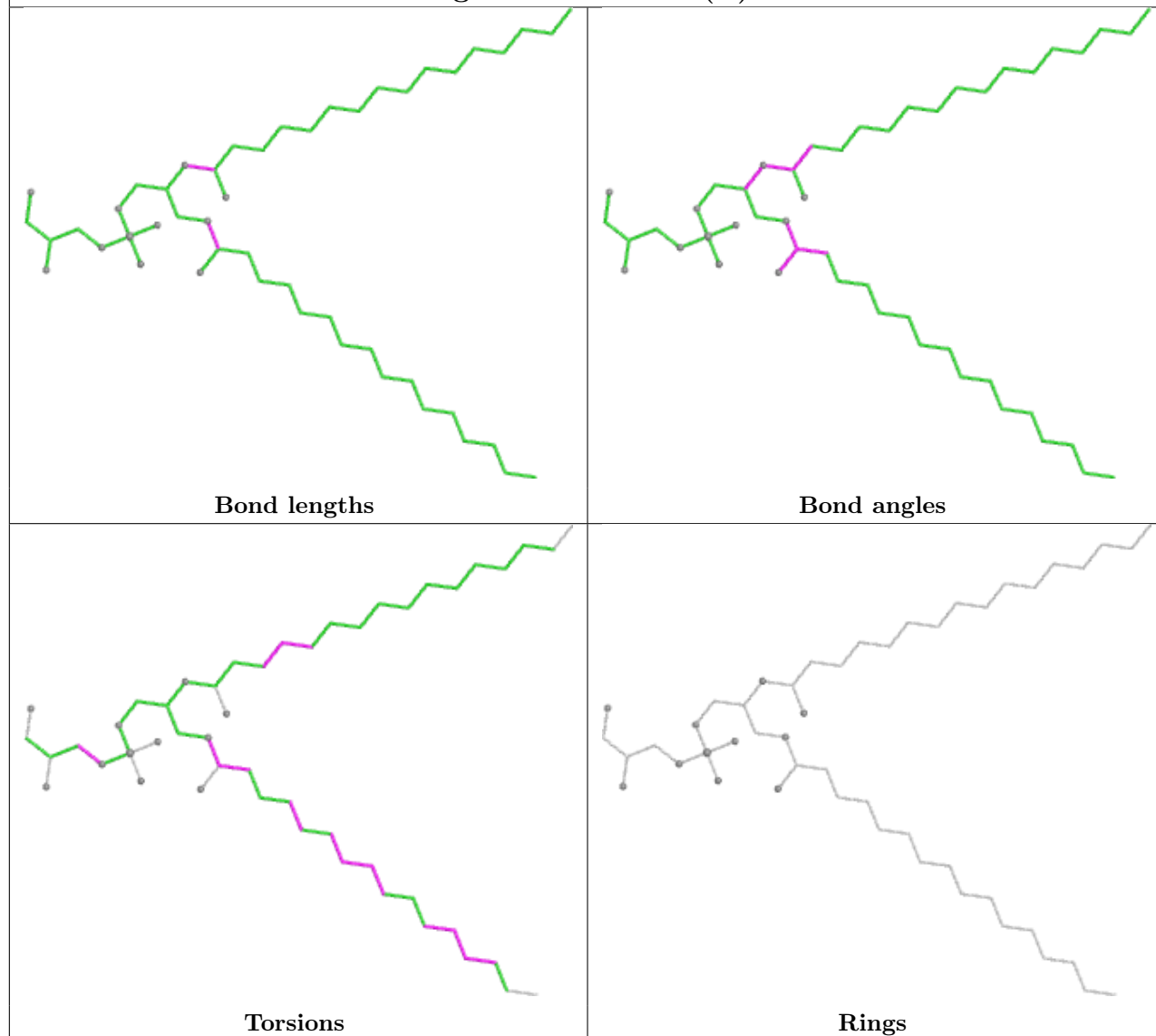




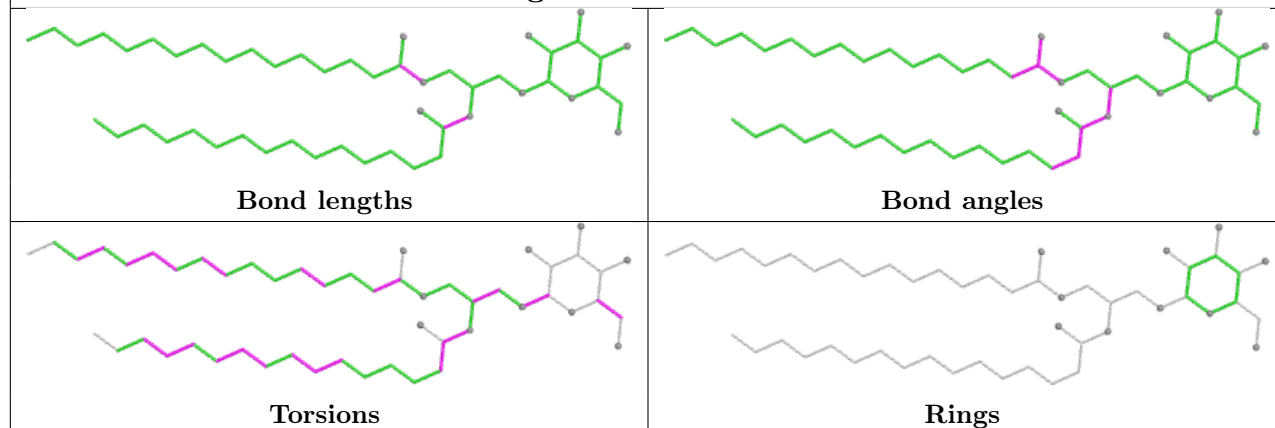




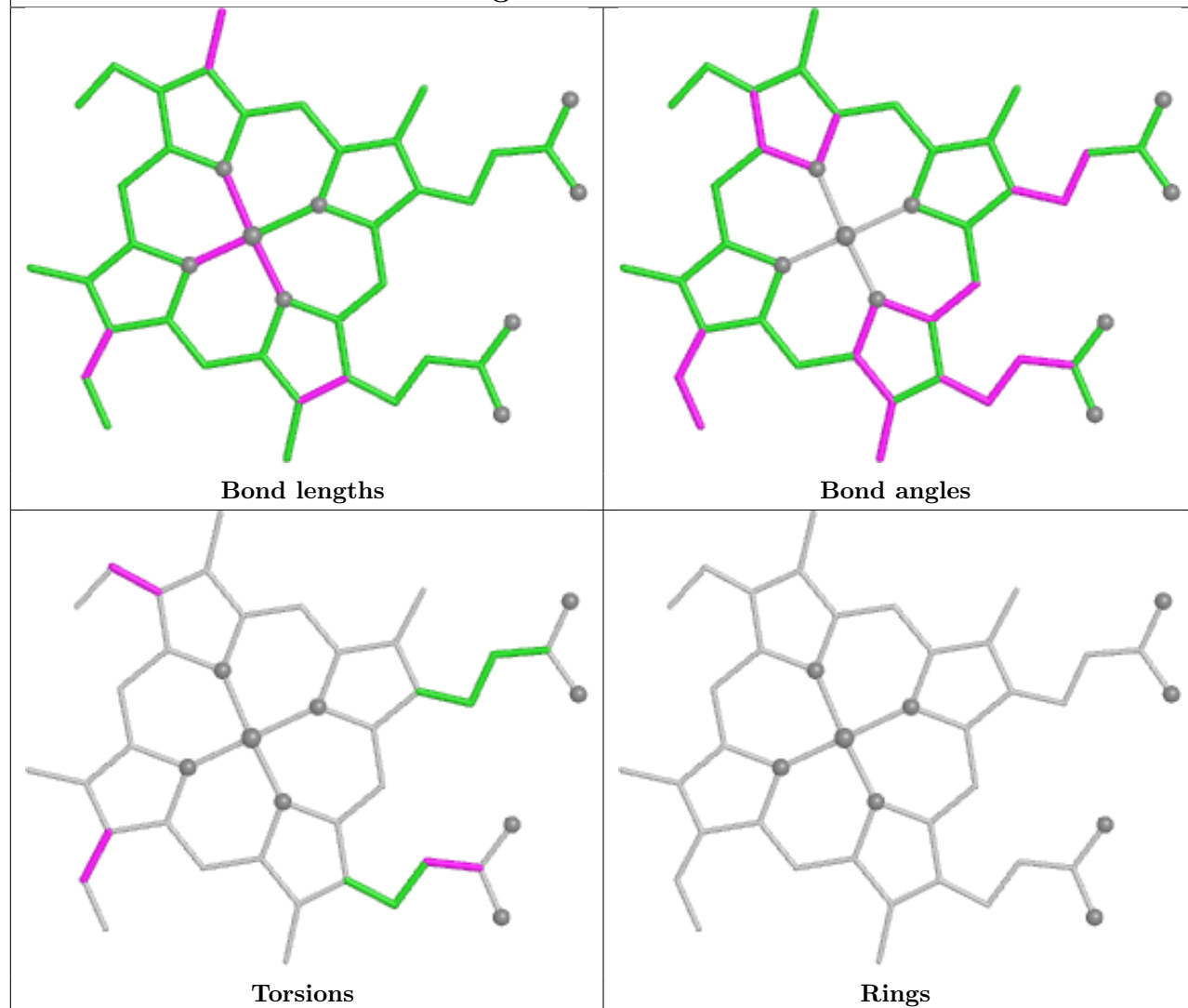
Ligand LHG d 406 (B)



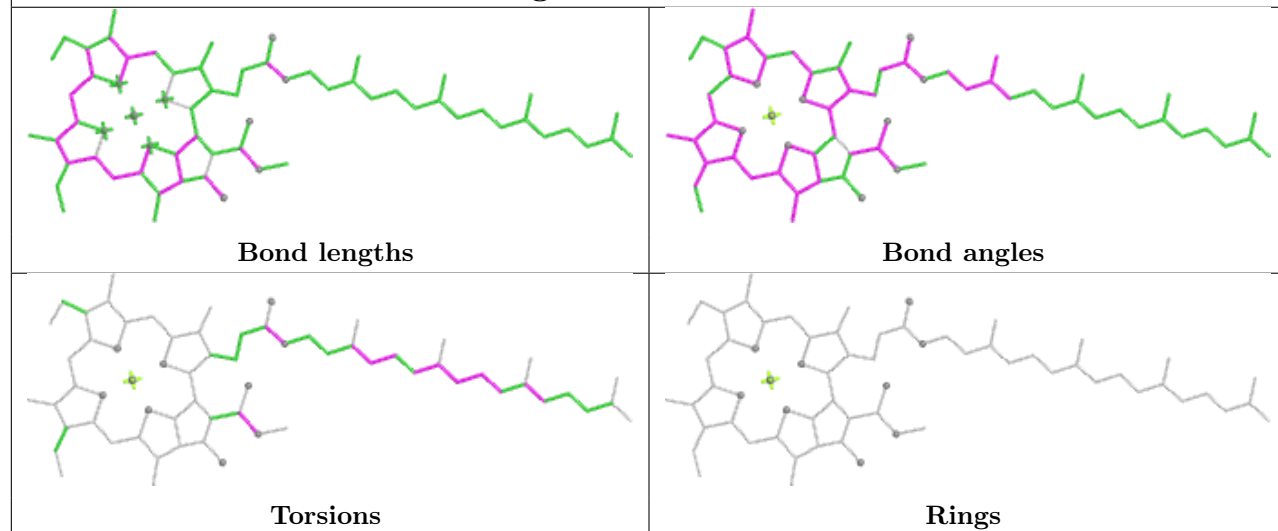
Ligand LMG B 621



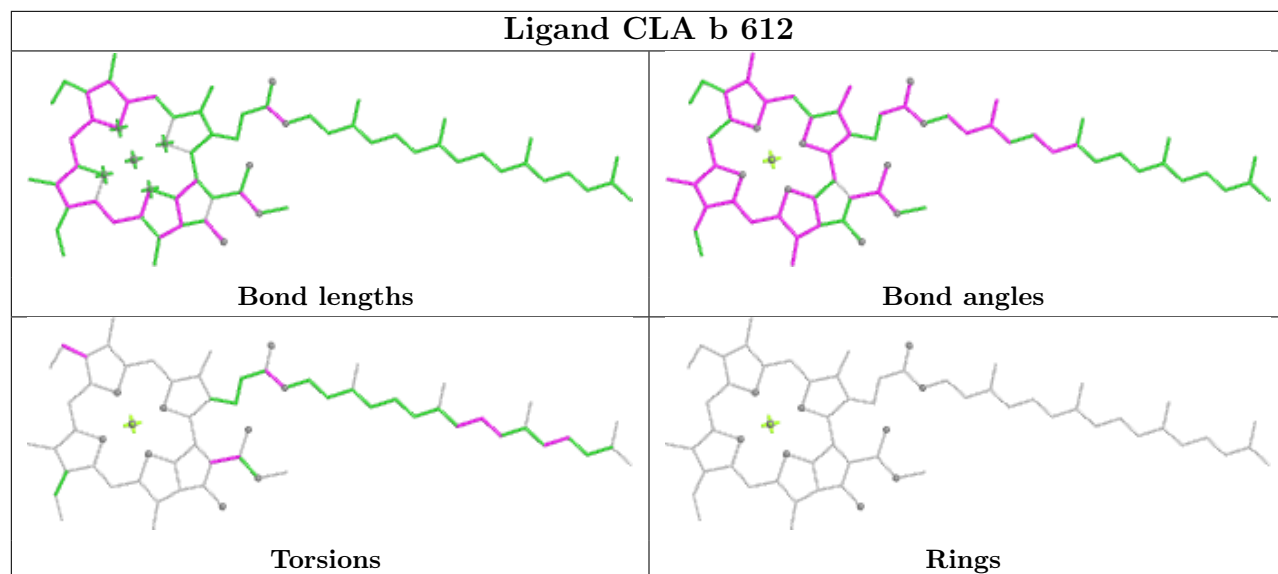
Ligand HEC V 202



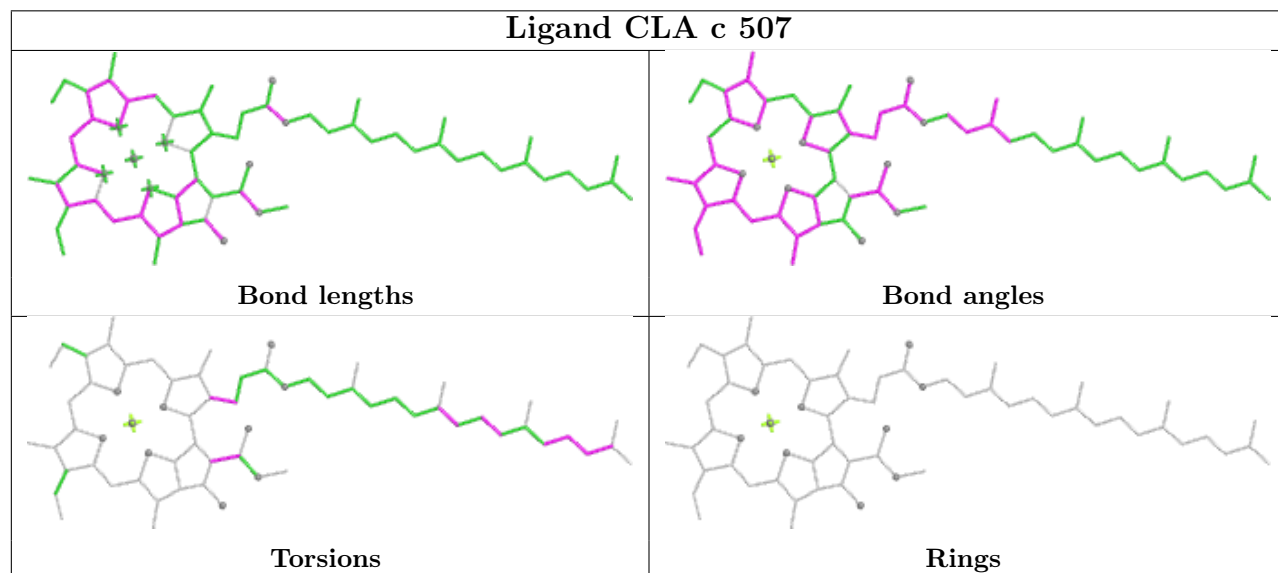
Ligand CLA D 405



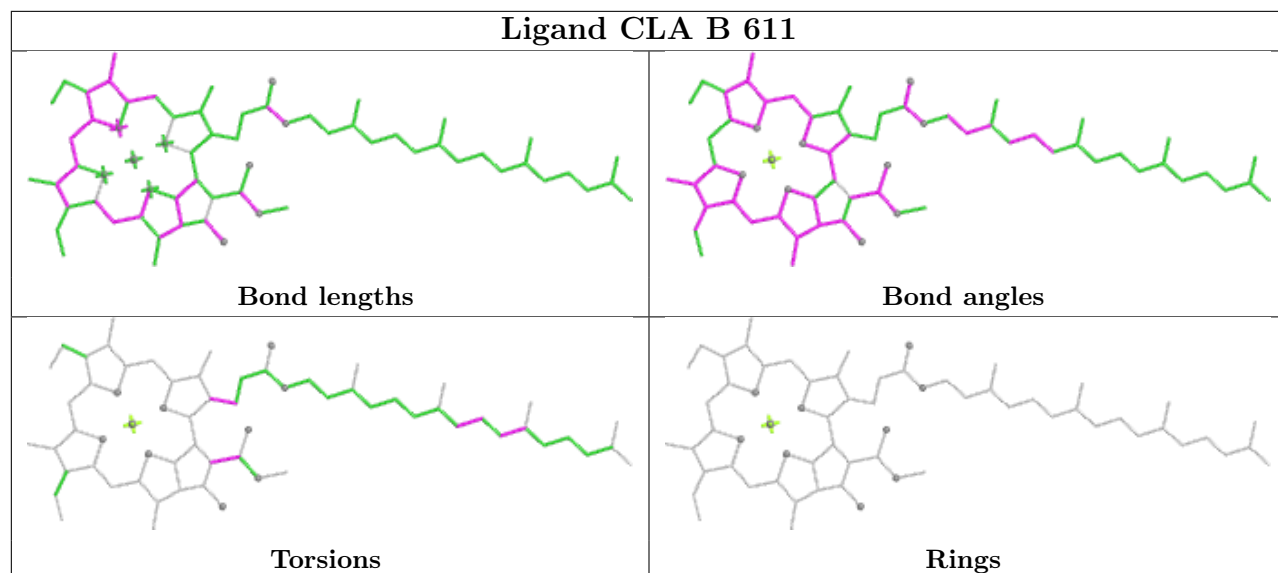
Ligand CLA b 612

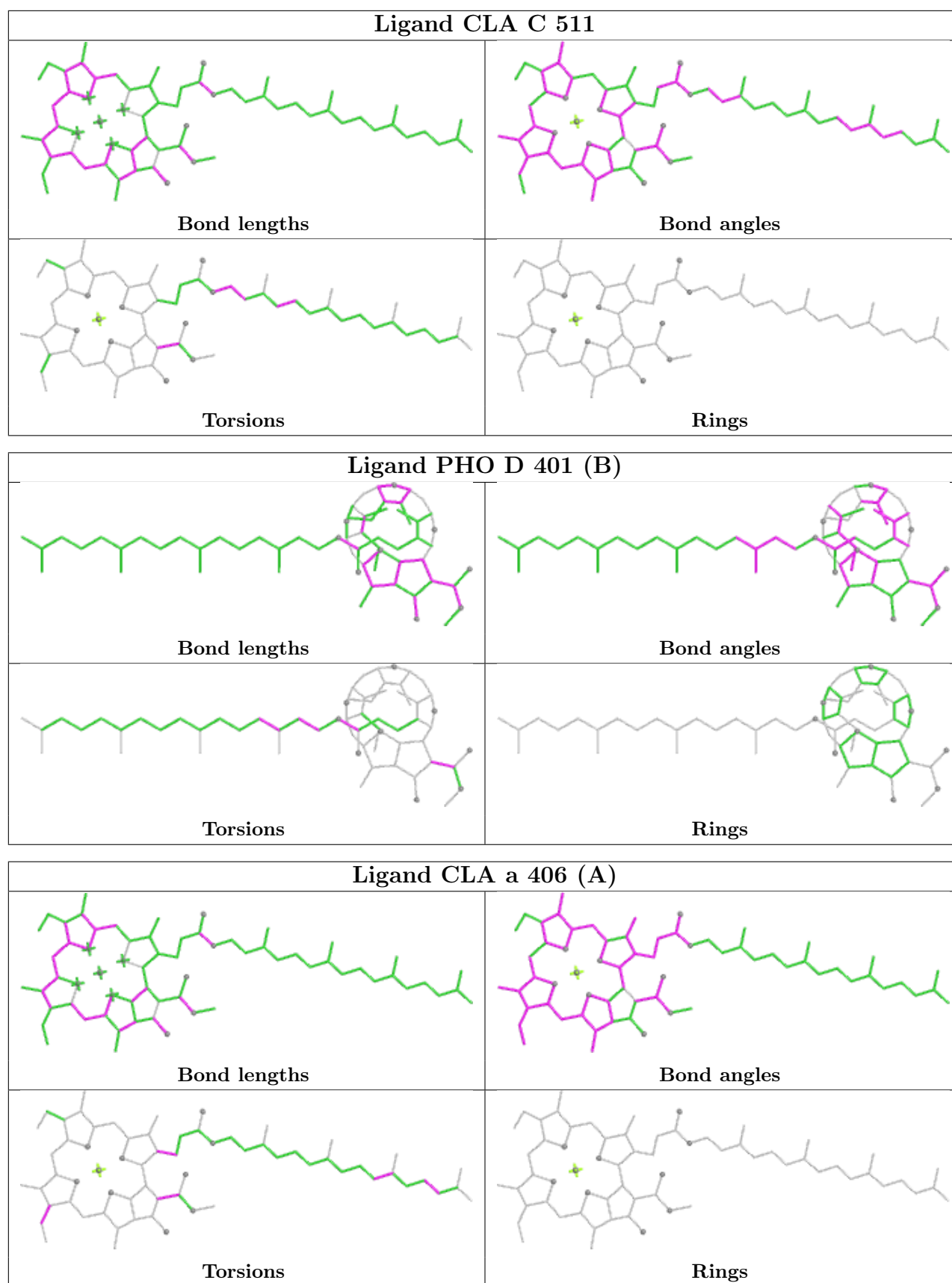


Ligand CLA c 507

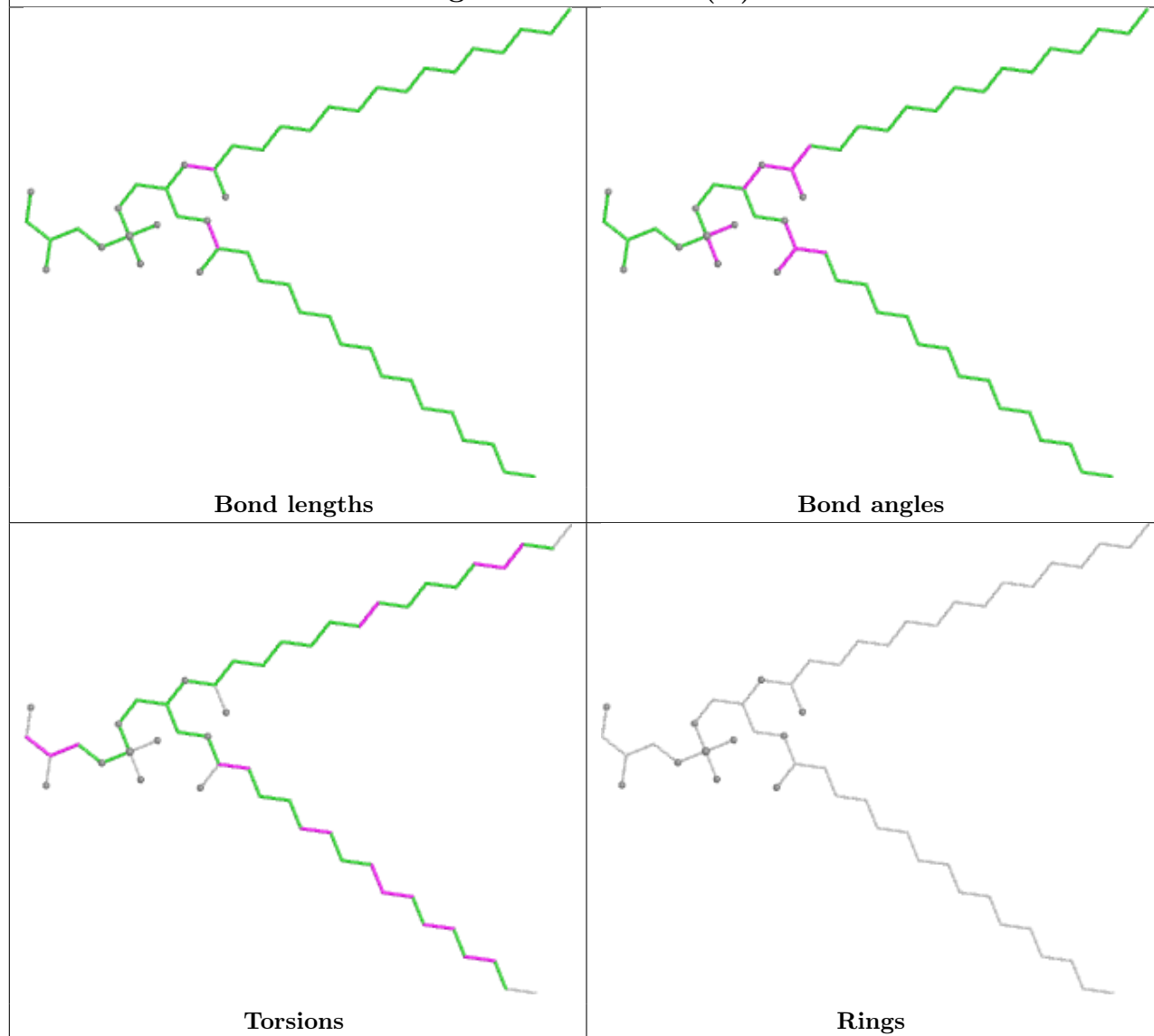


Ligand CLA B 611

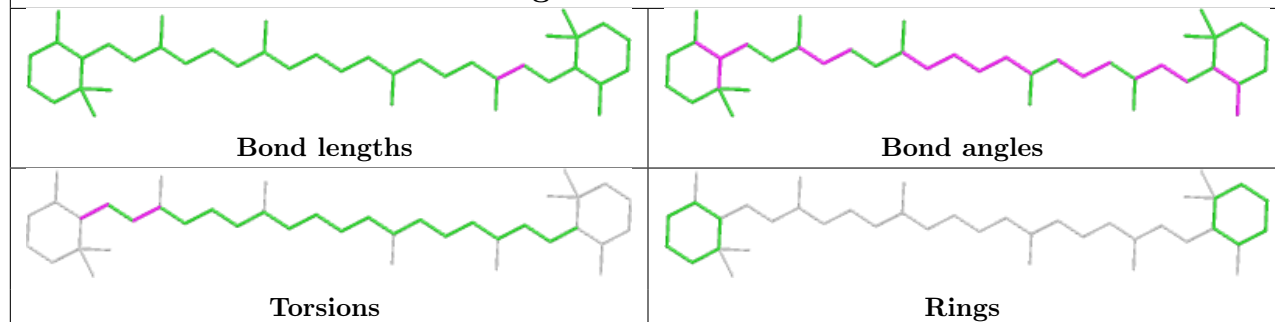


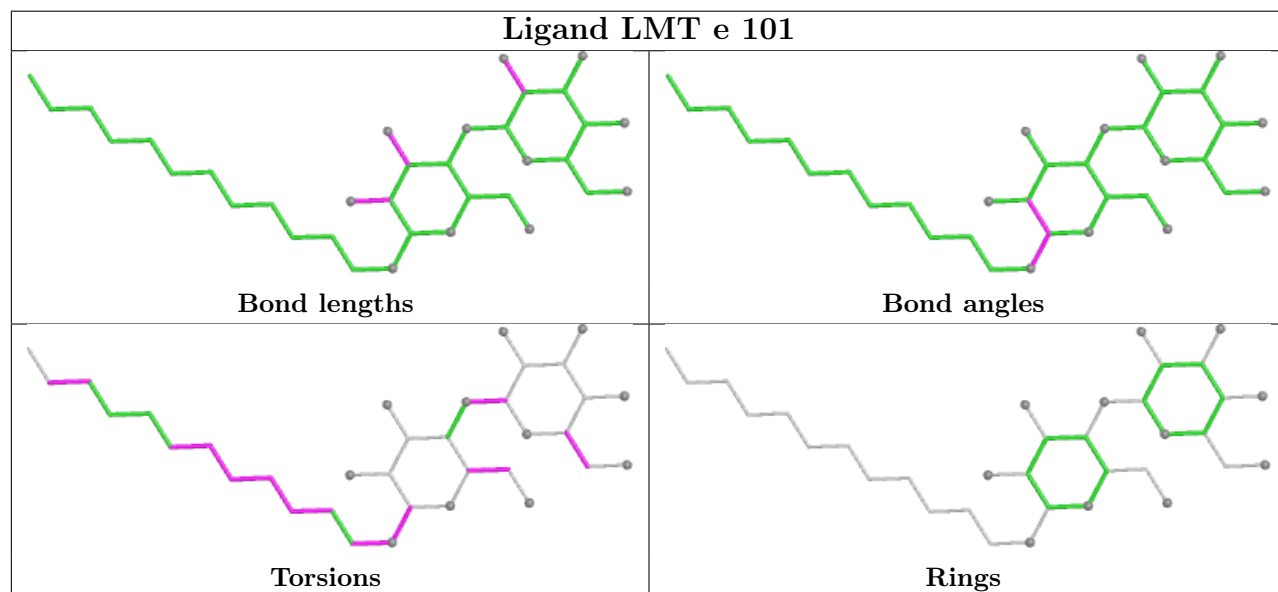
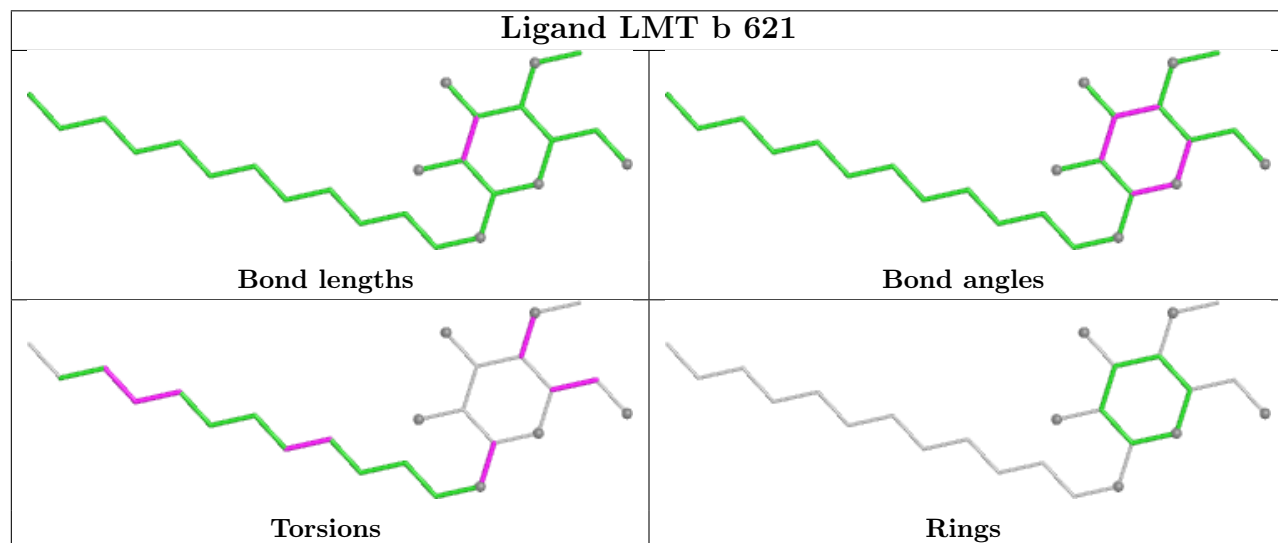
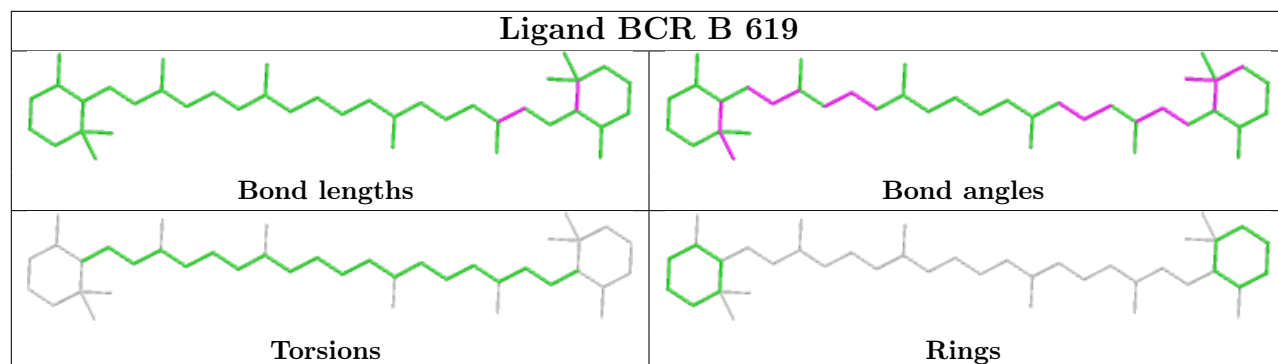


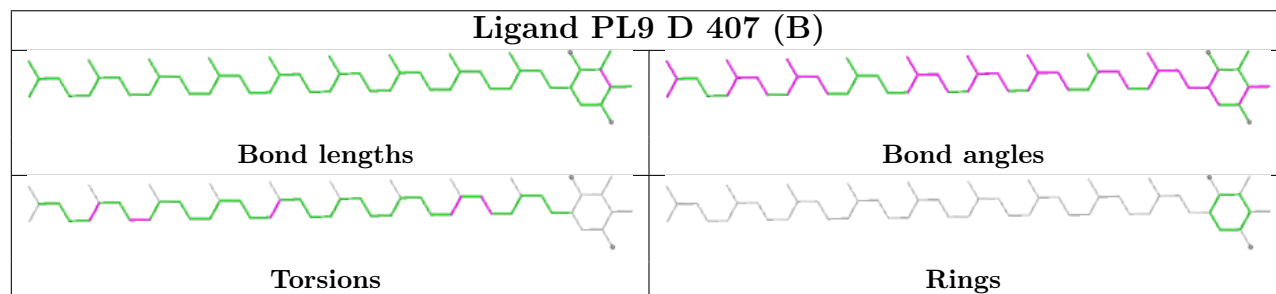
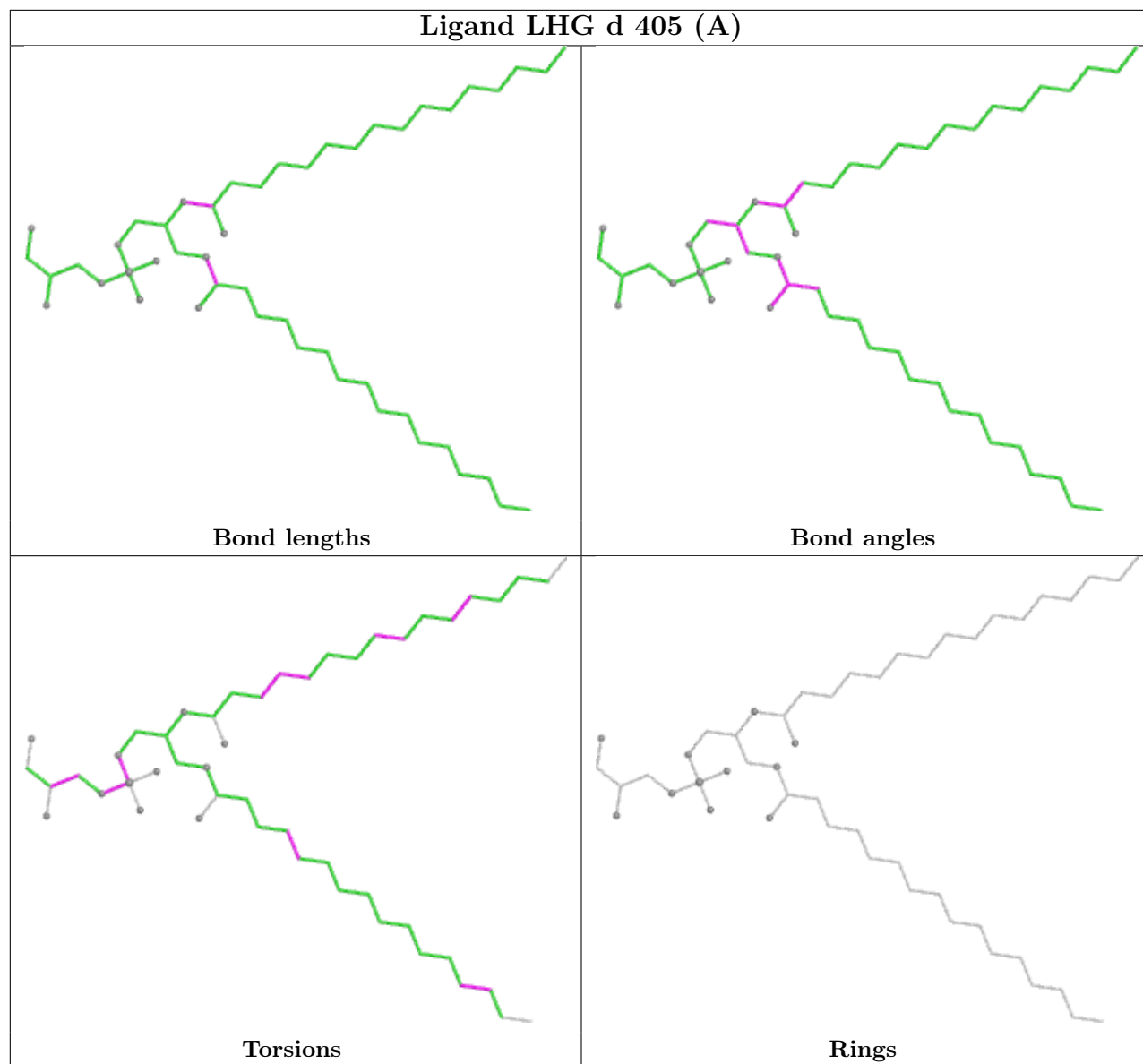
Ligand LHG A 416 (A)

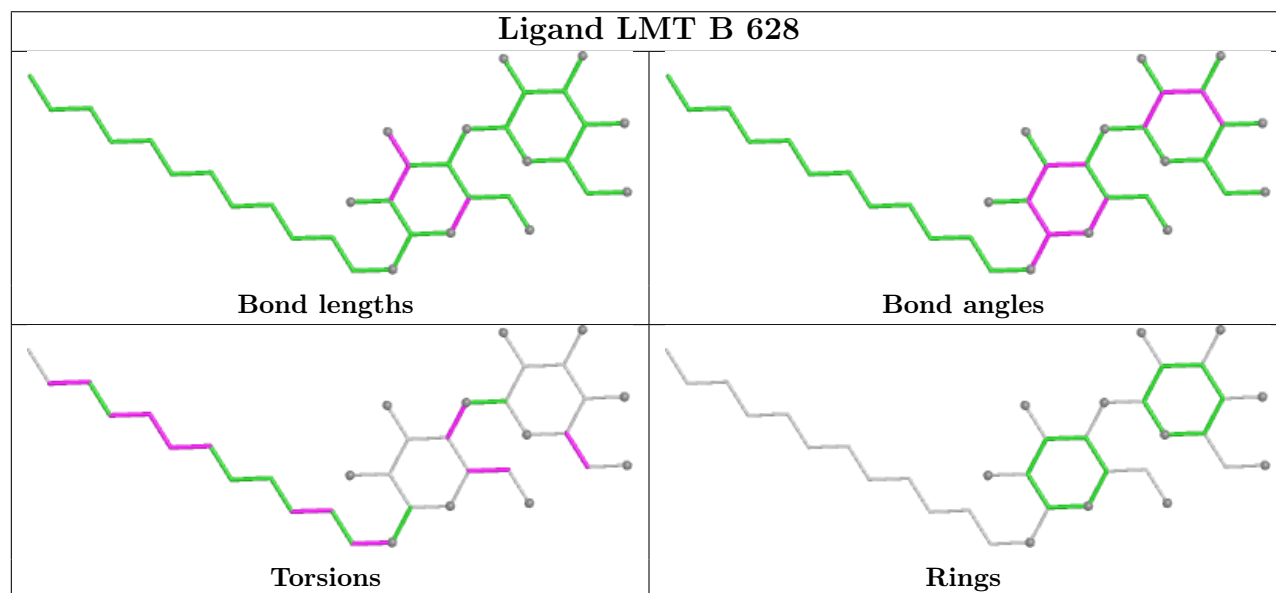
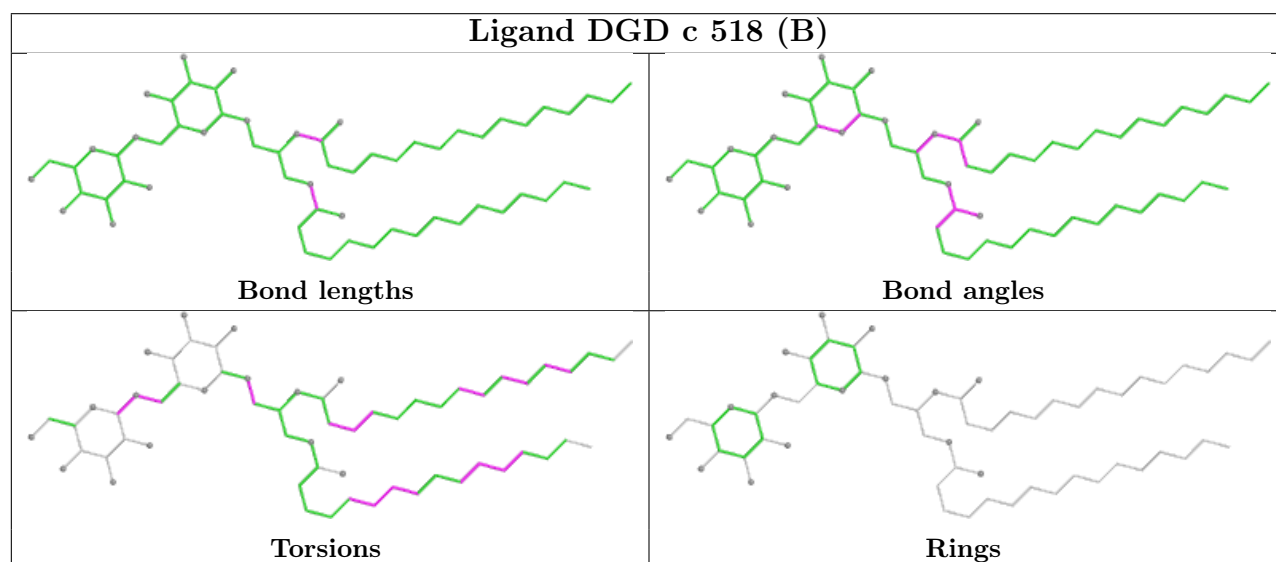
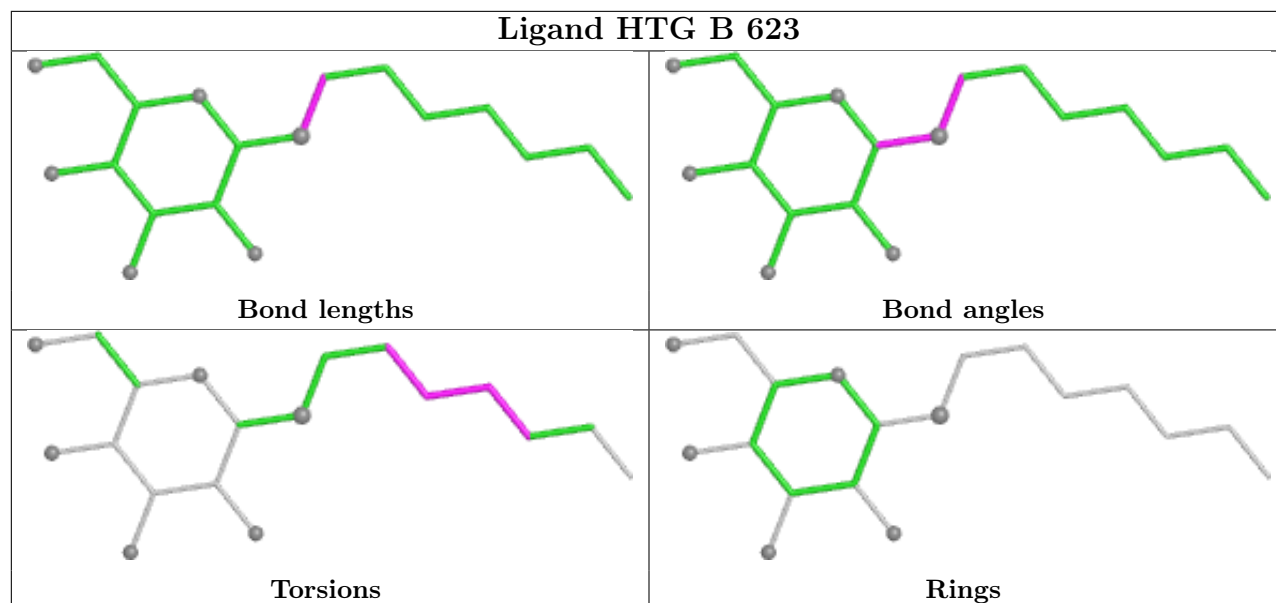


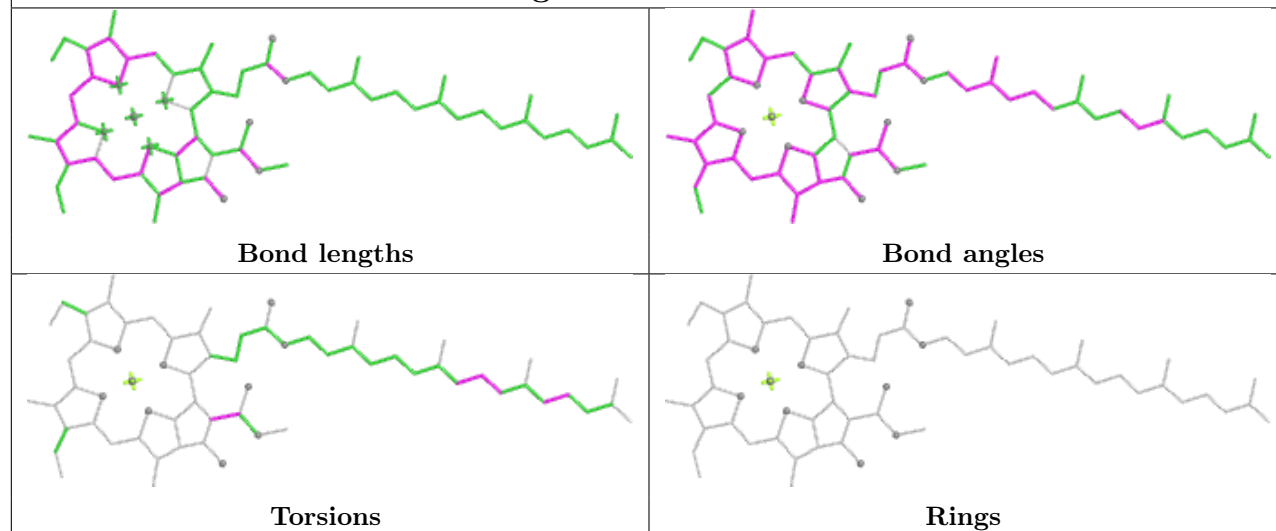
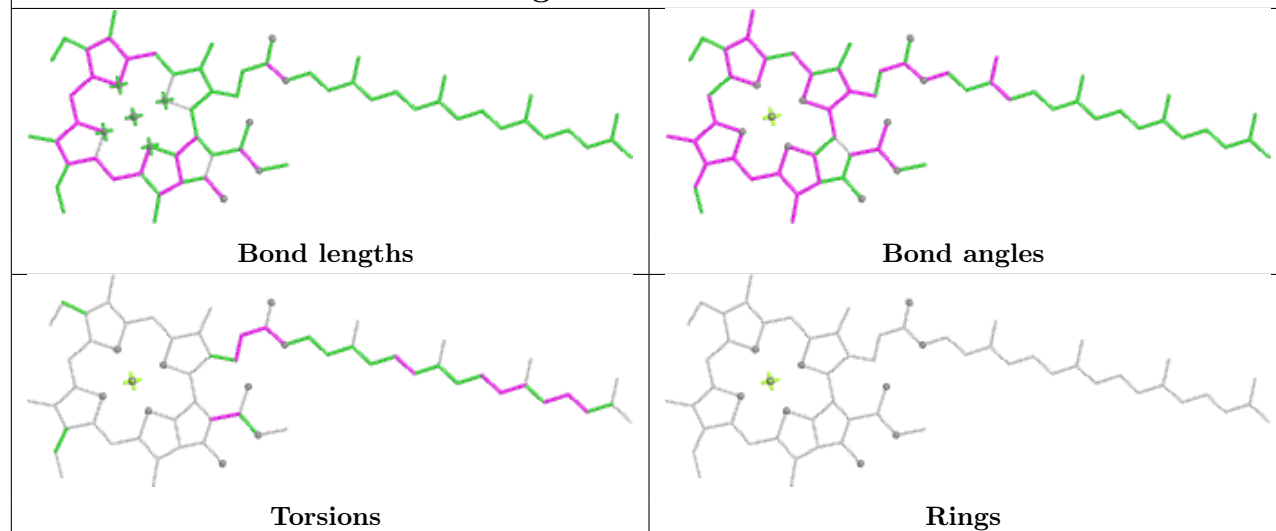
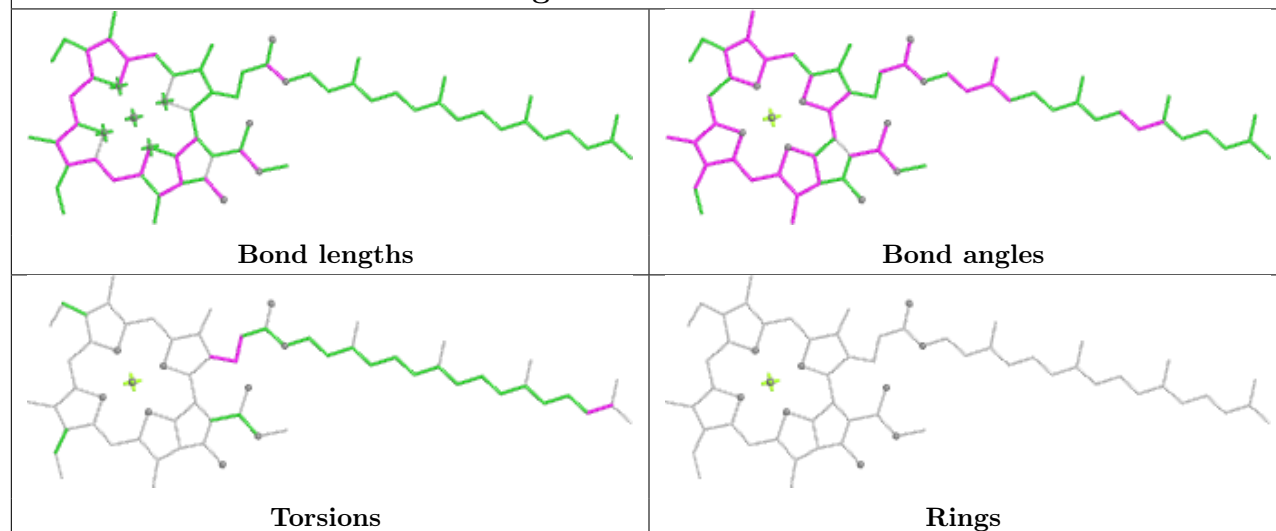
Ligand BCR b 619

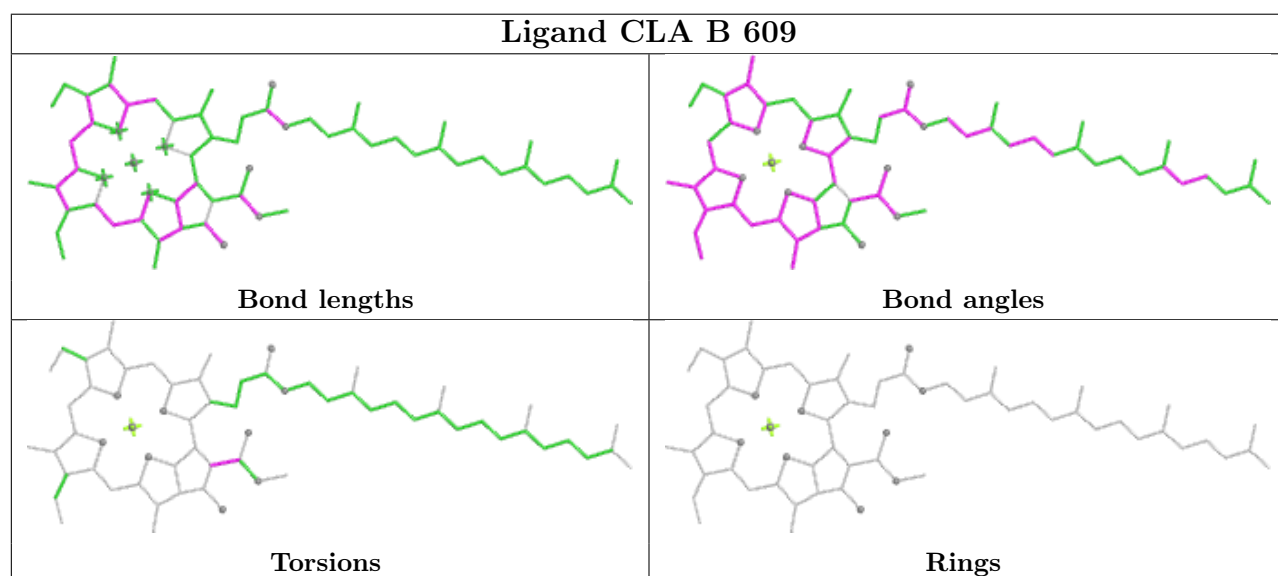
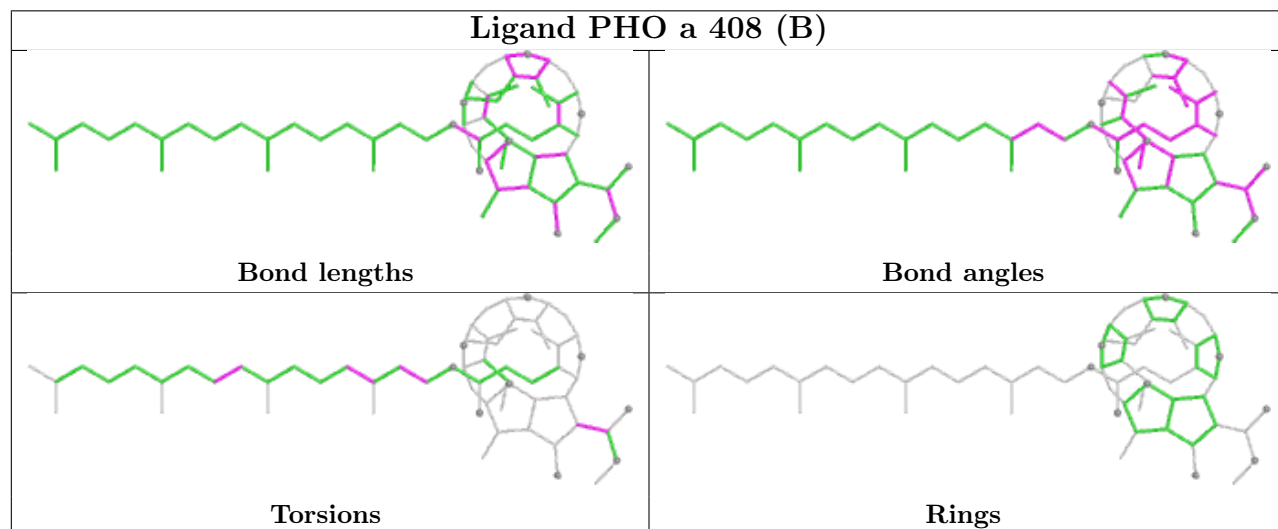
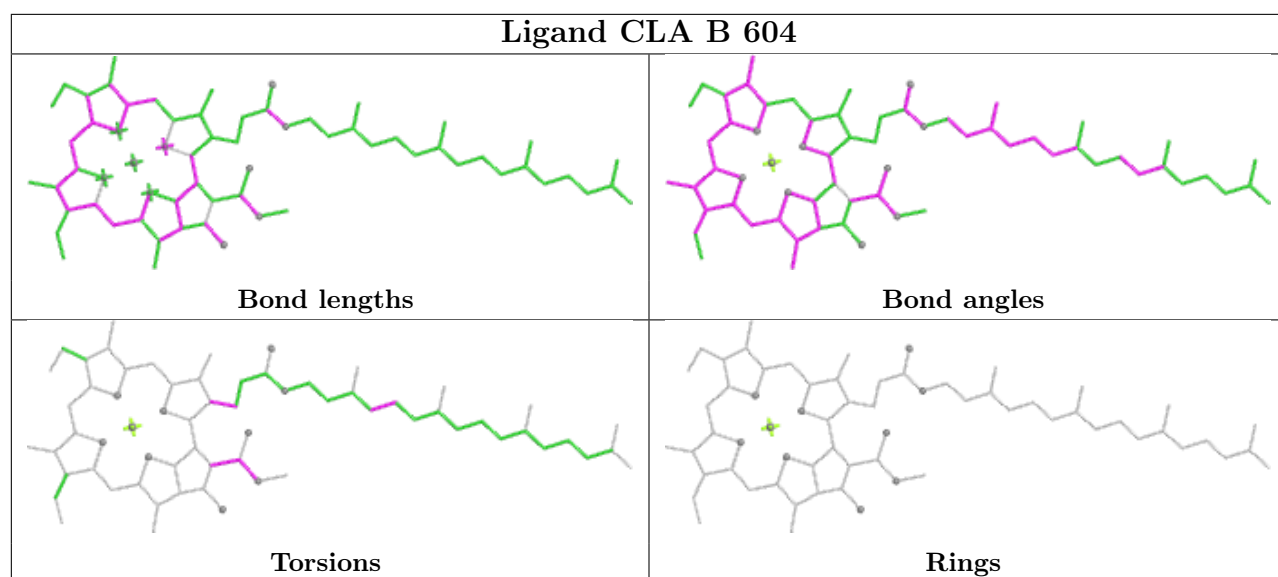


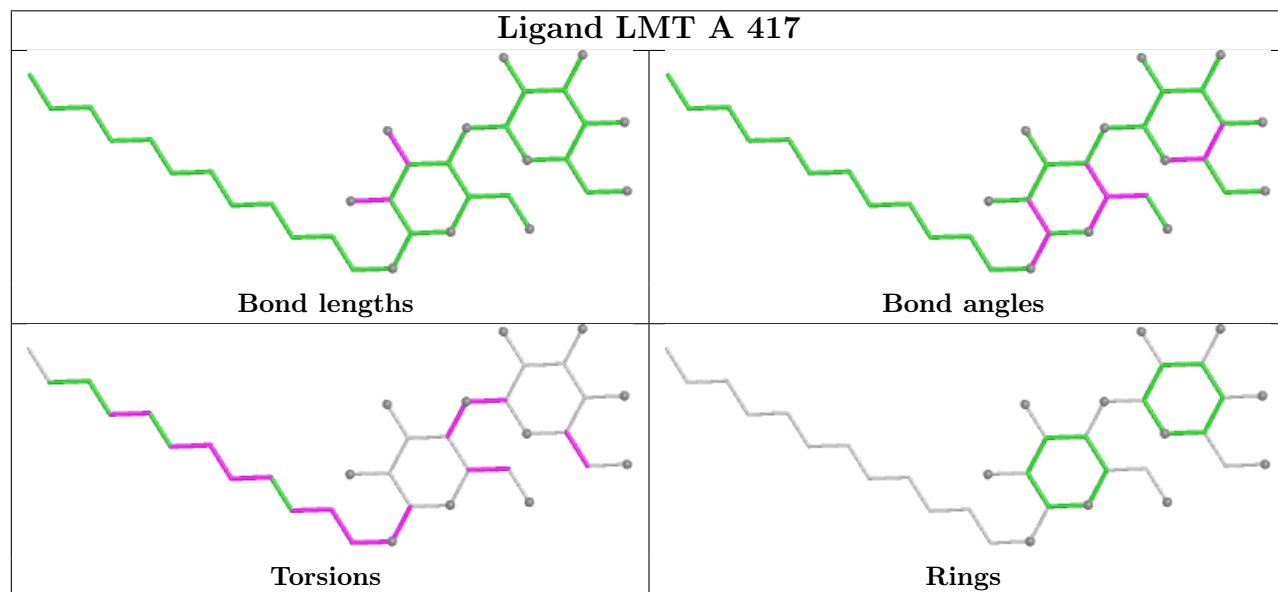
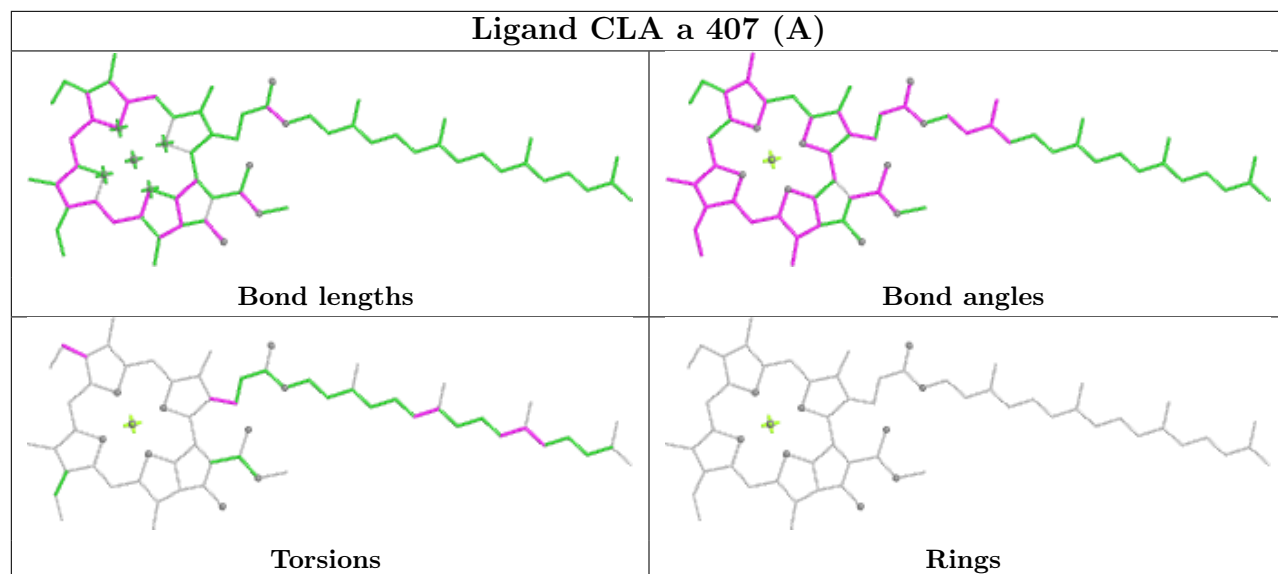


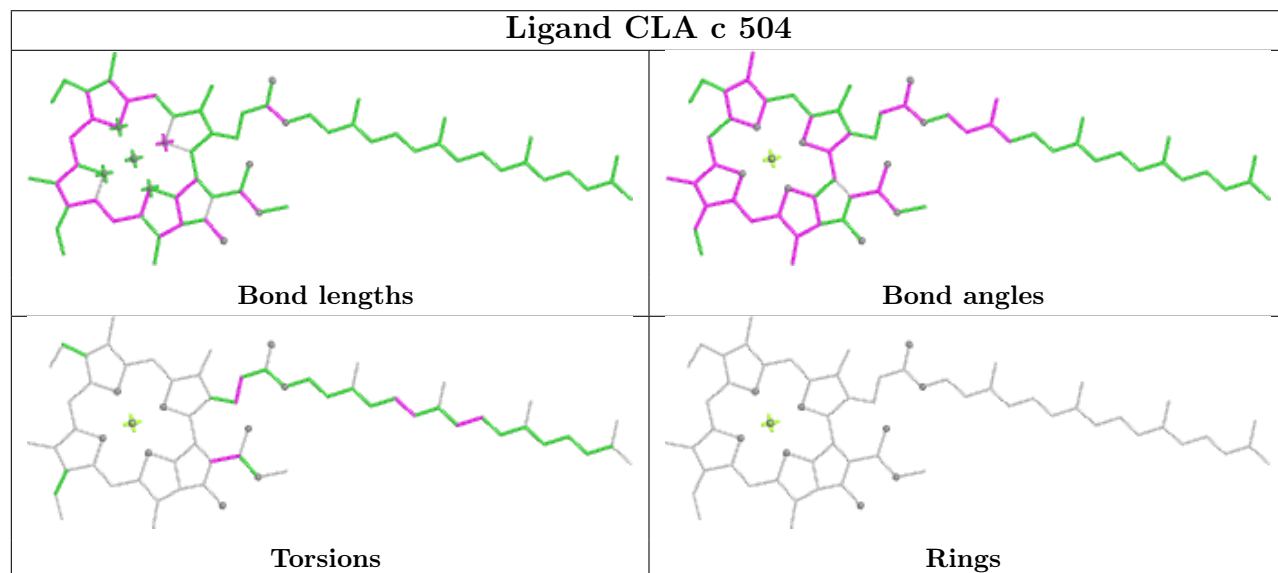
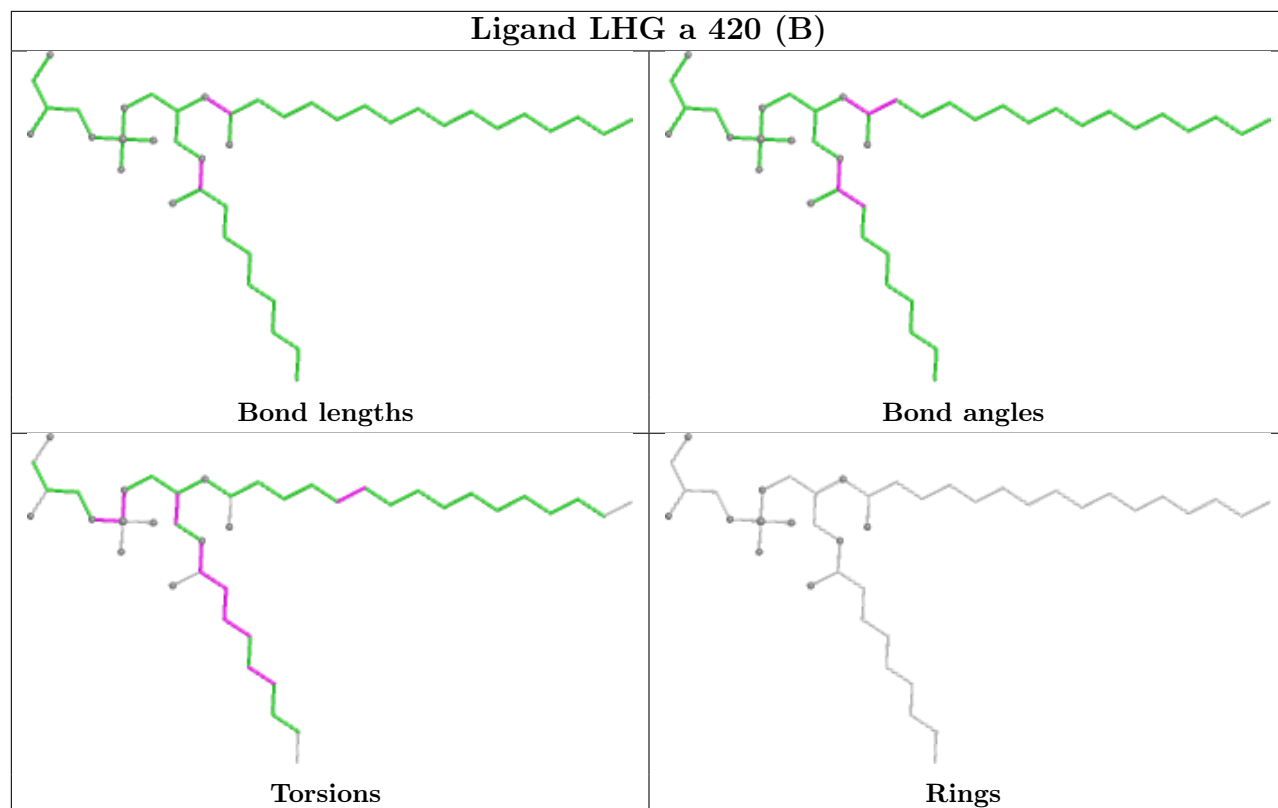


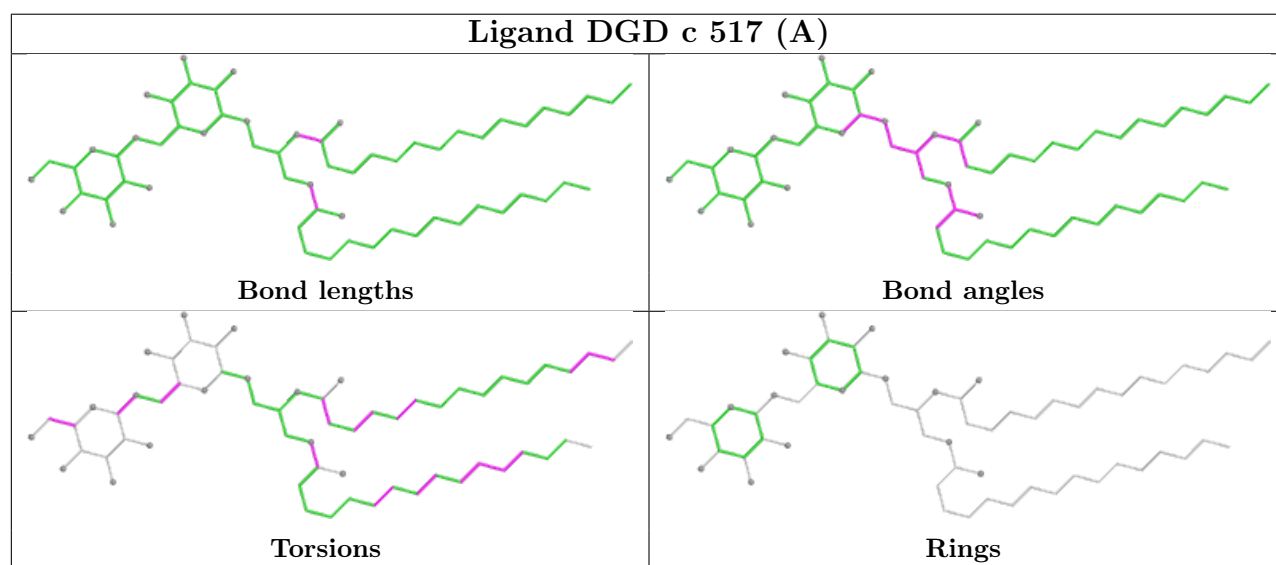
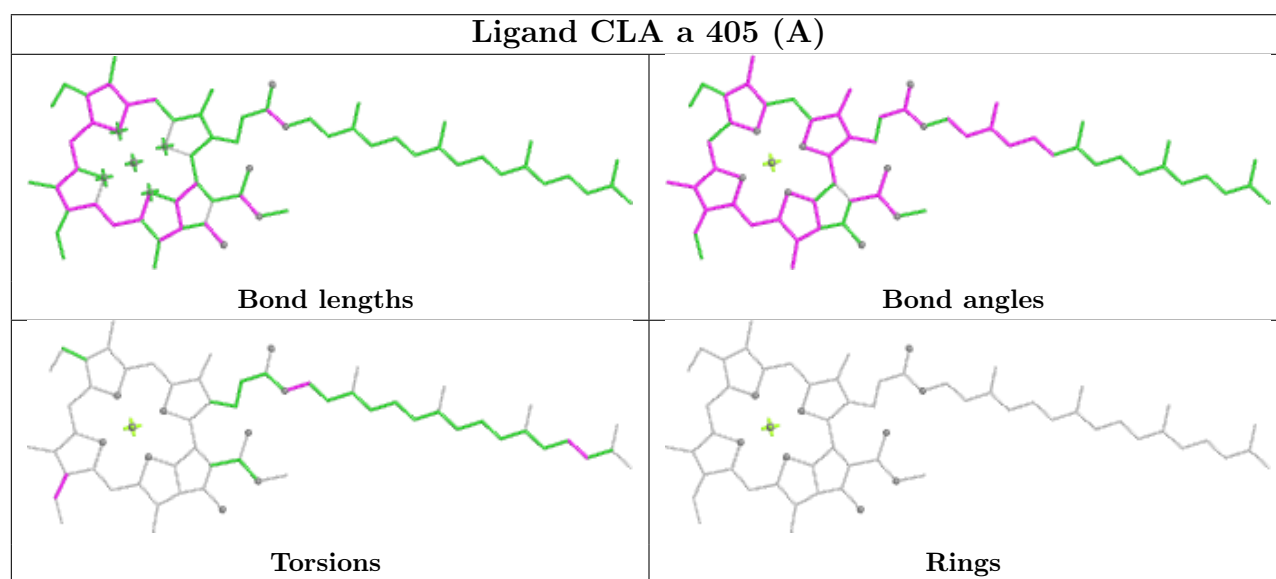
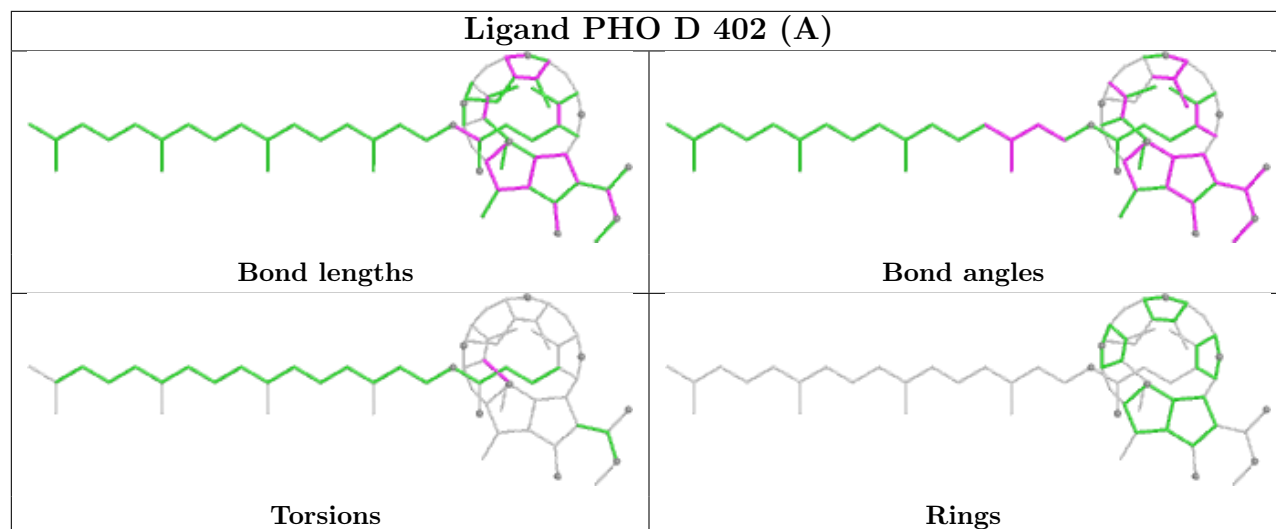


Ligand CLA B 612**Ligand CLA B 601****Ligand CLA C 503**

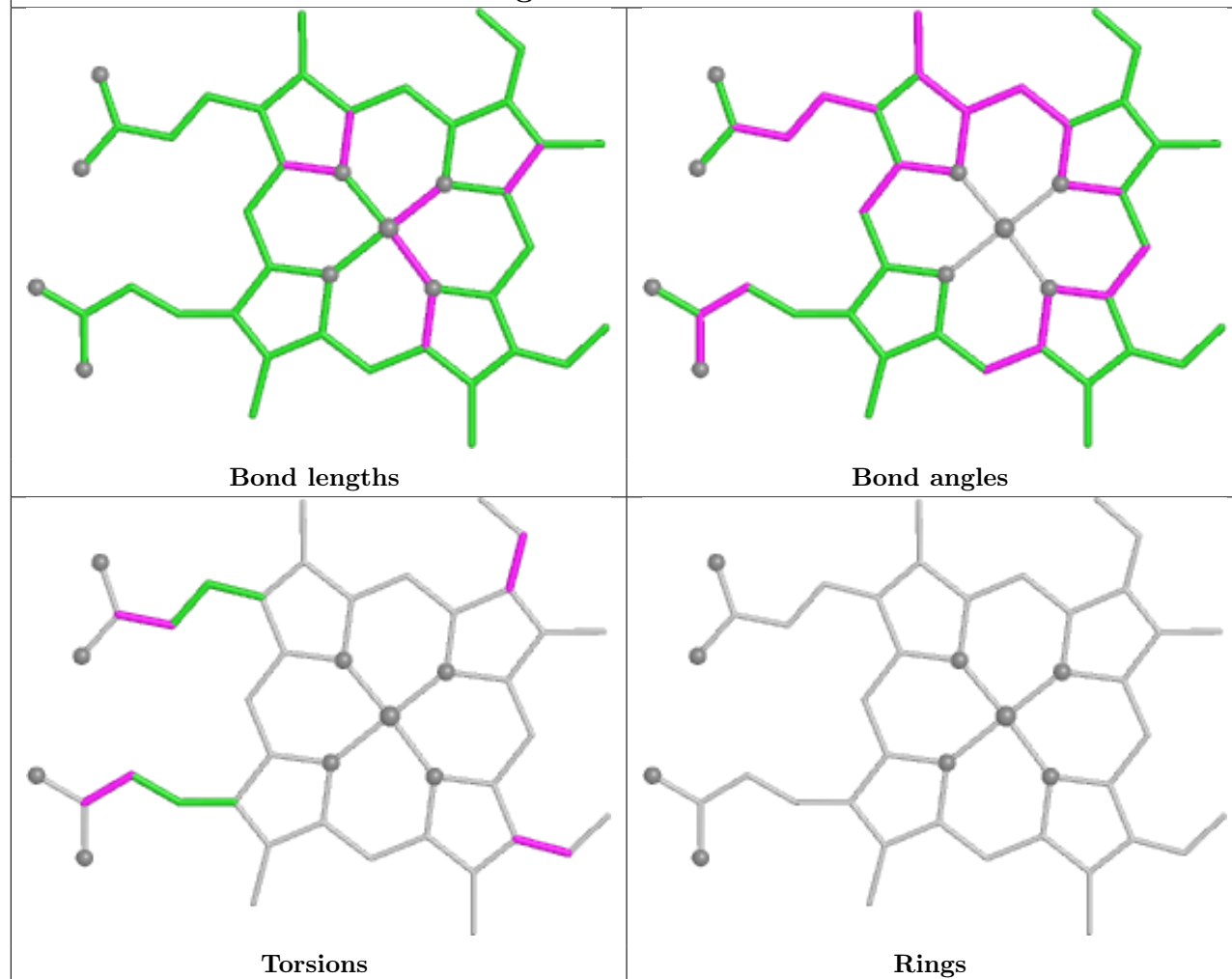




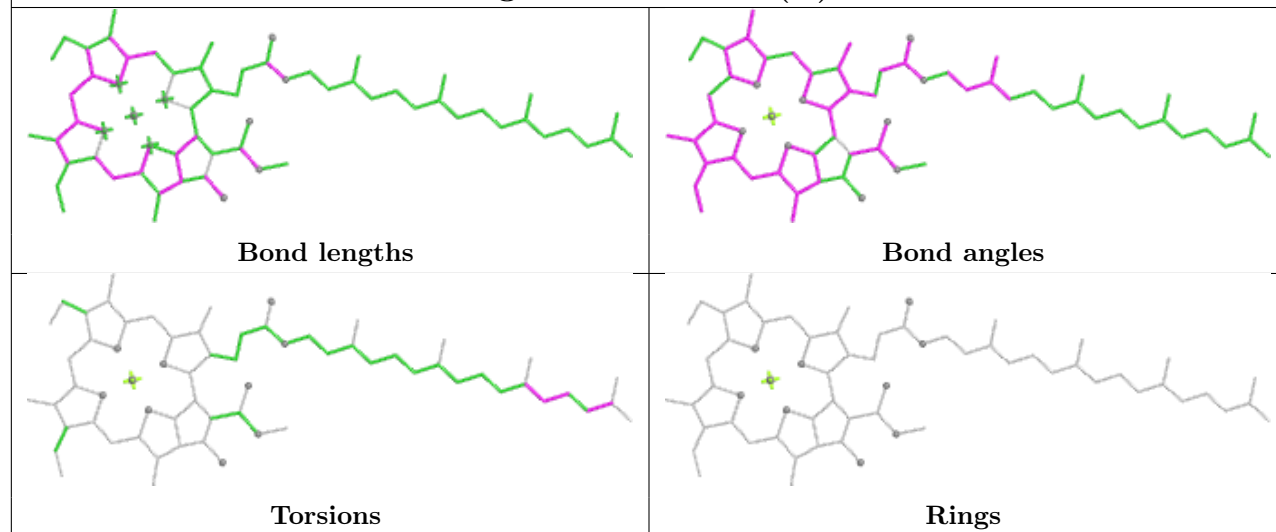


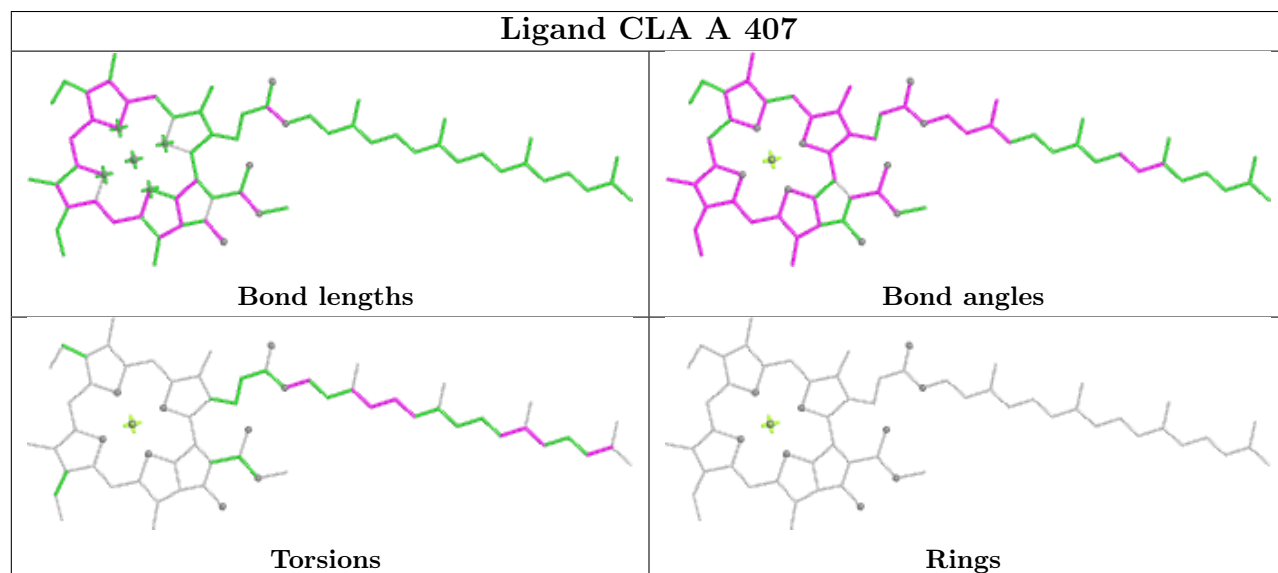
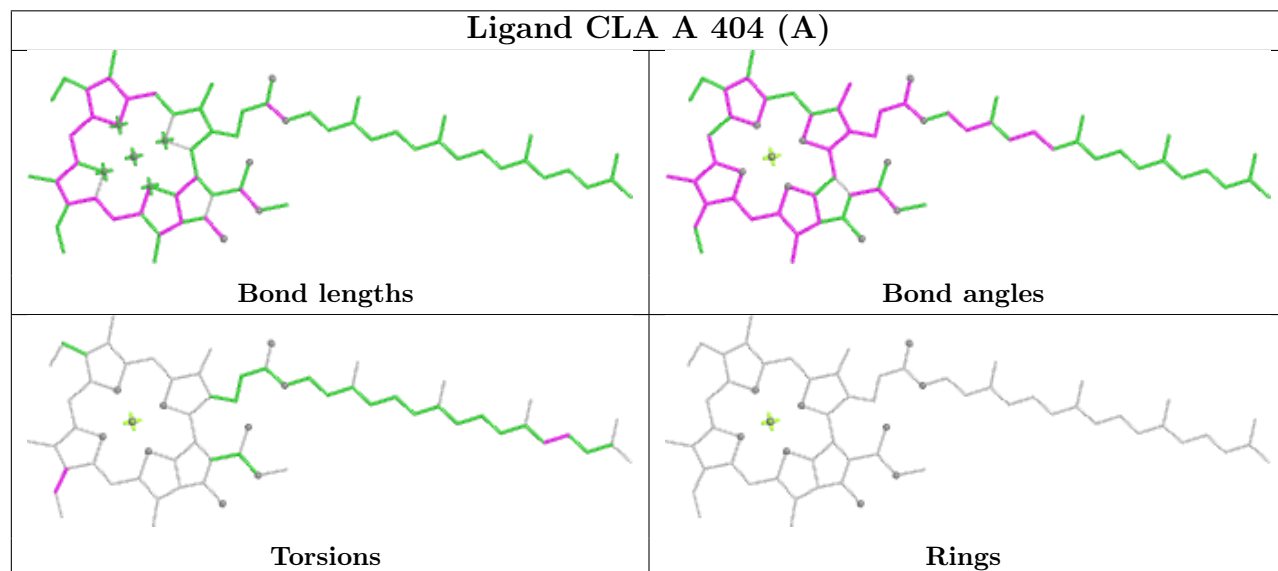
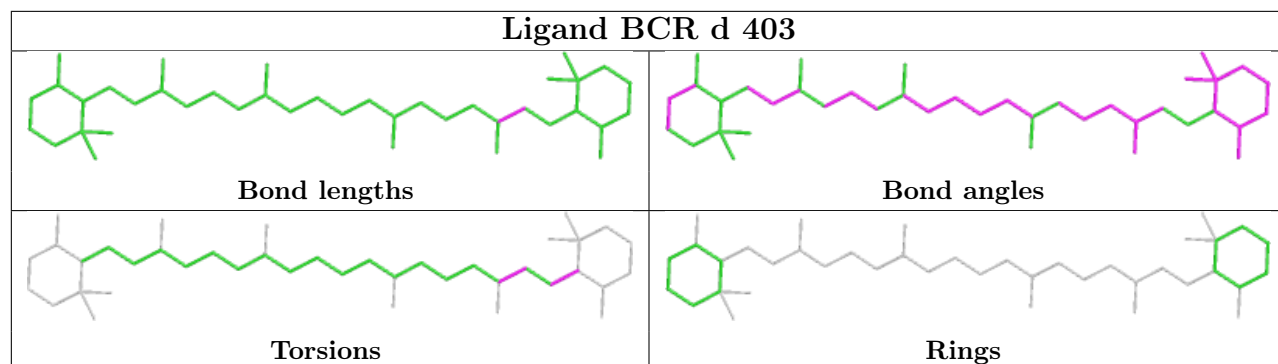


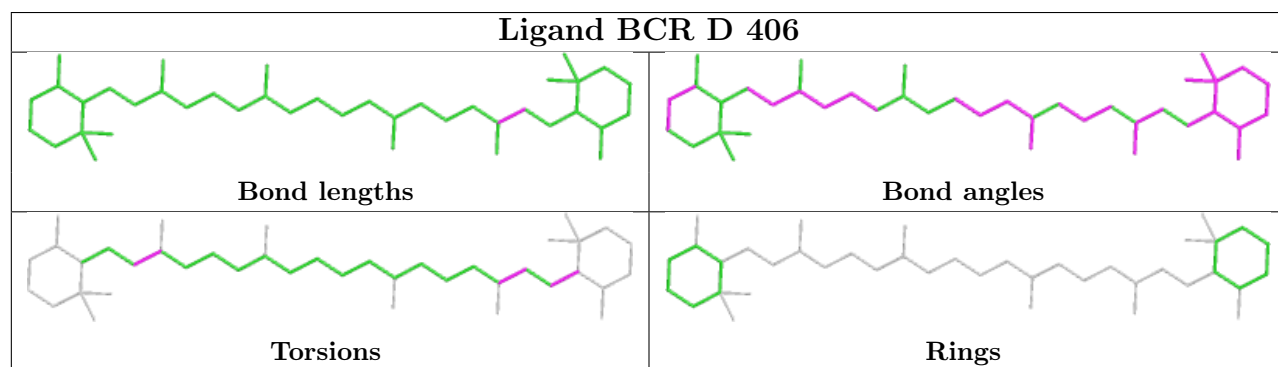
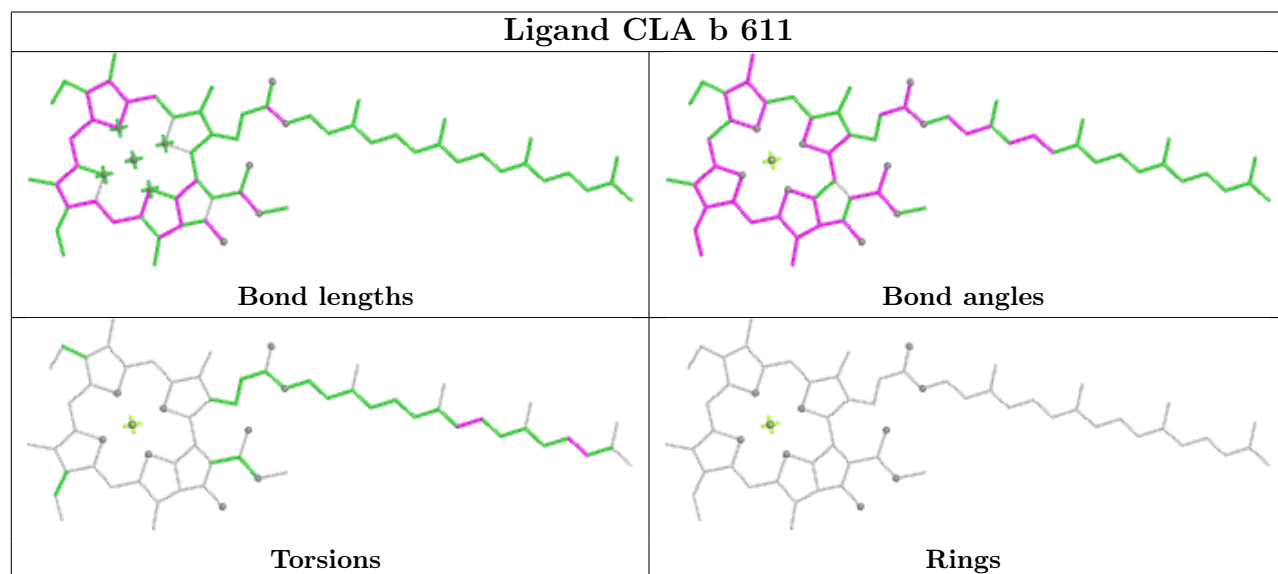
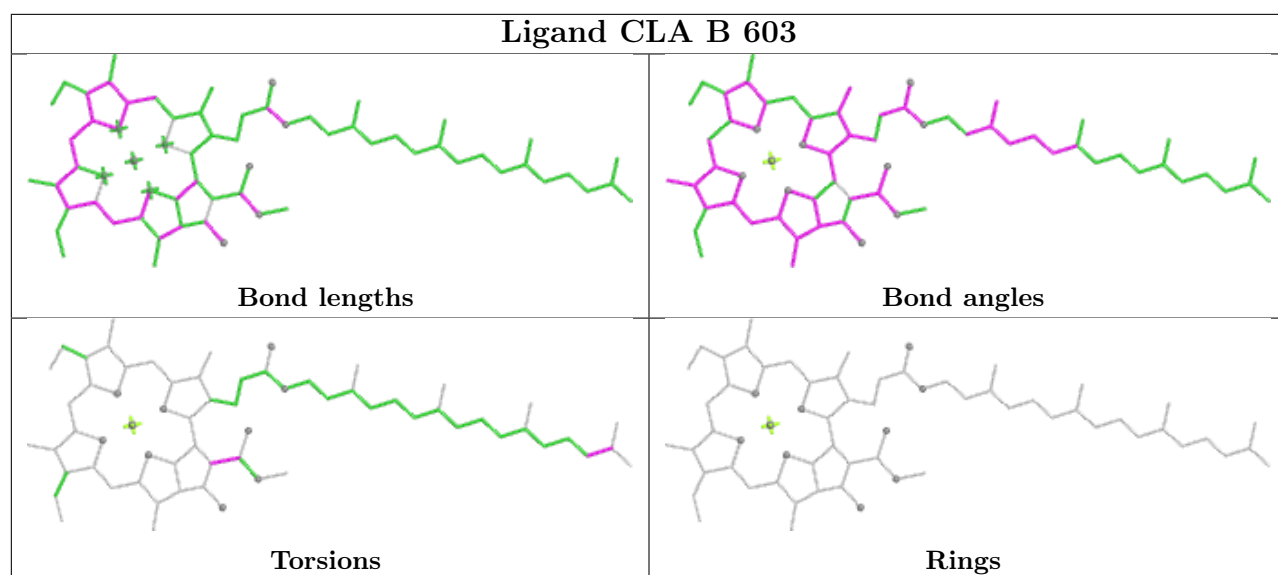
Ligand HEM f 101

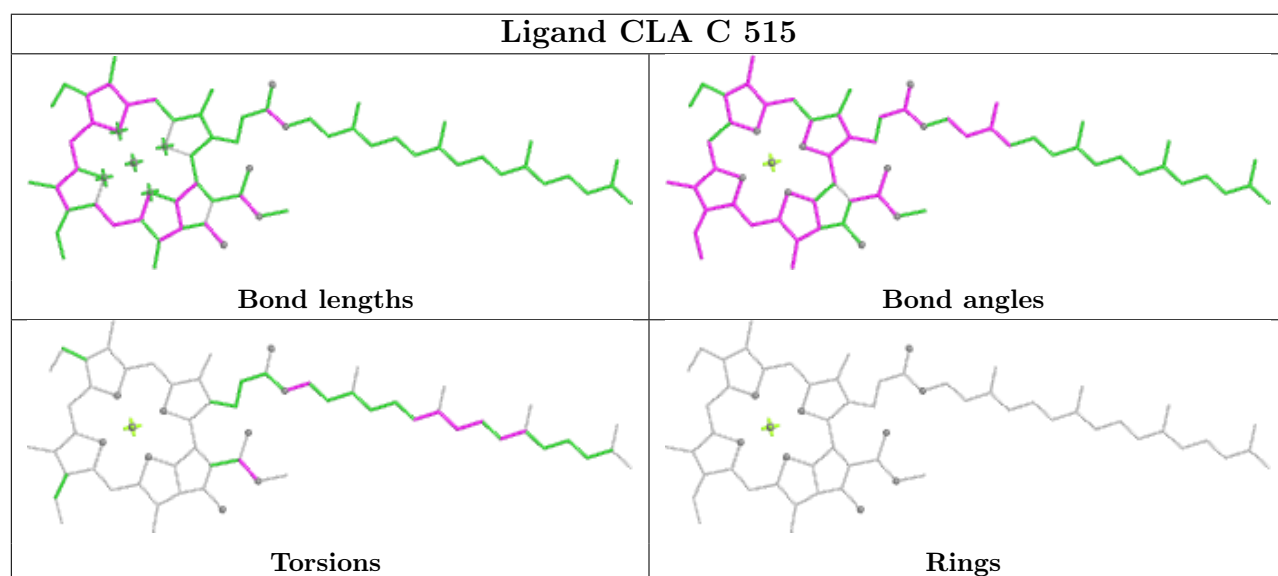
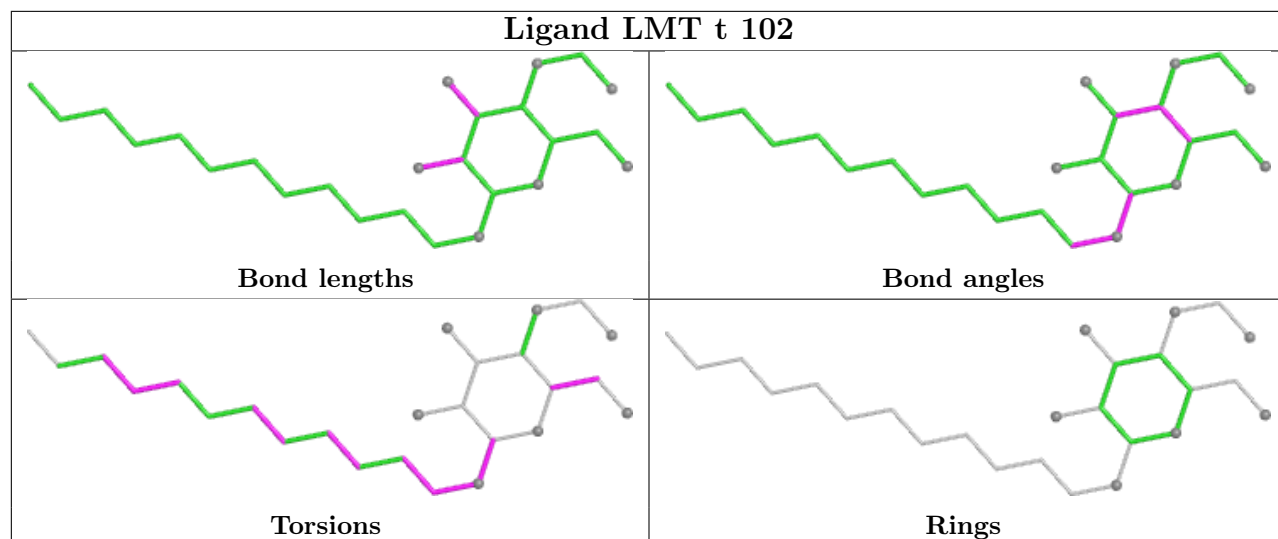


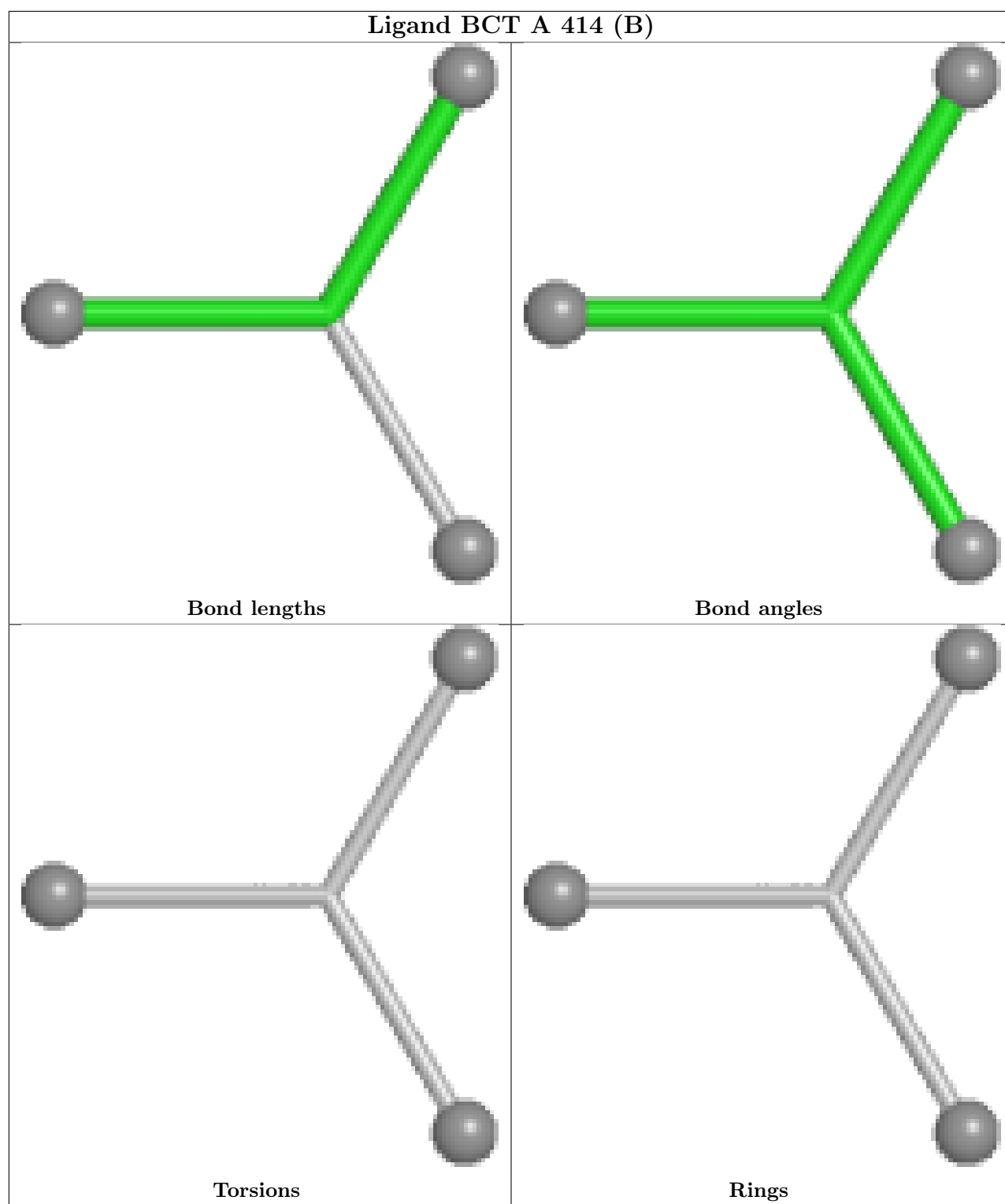
Ligand CLA A 406 (A)



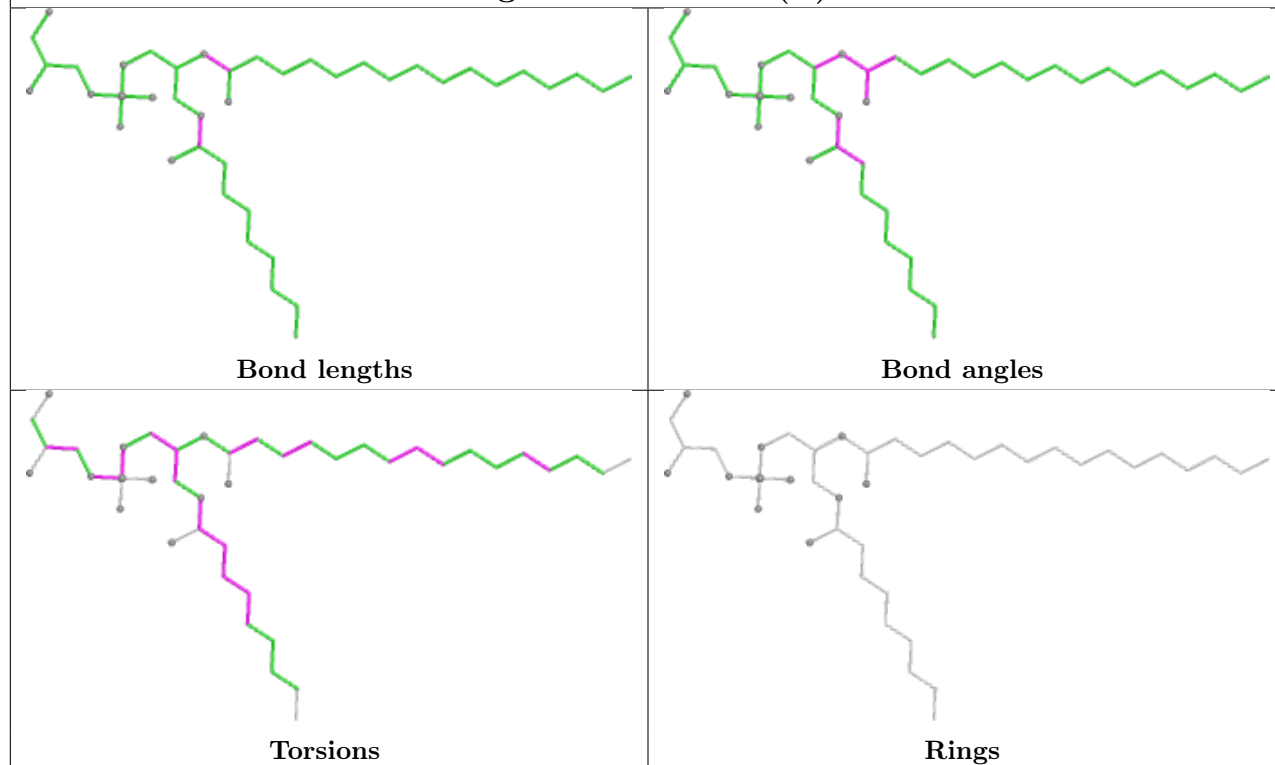




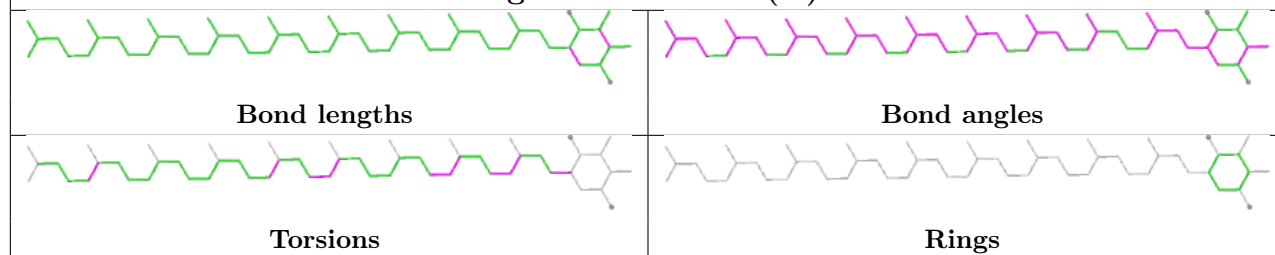




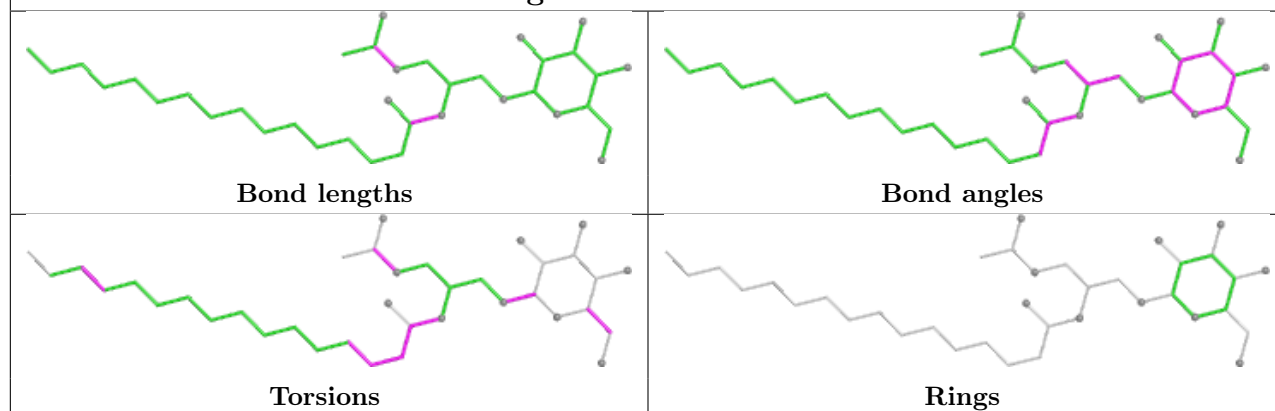
Ligand LHG E 101 (B)

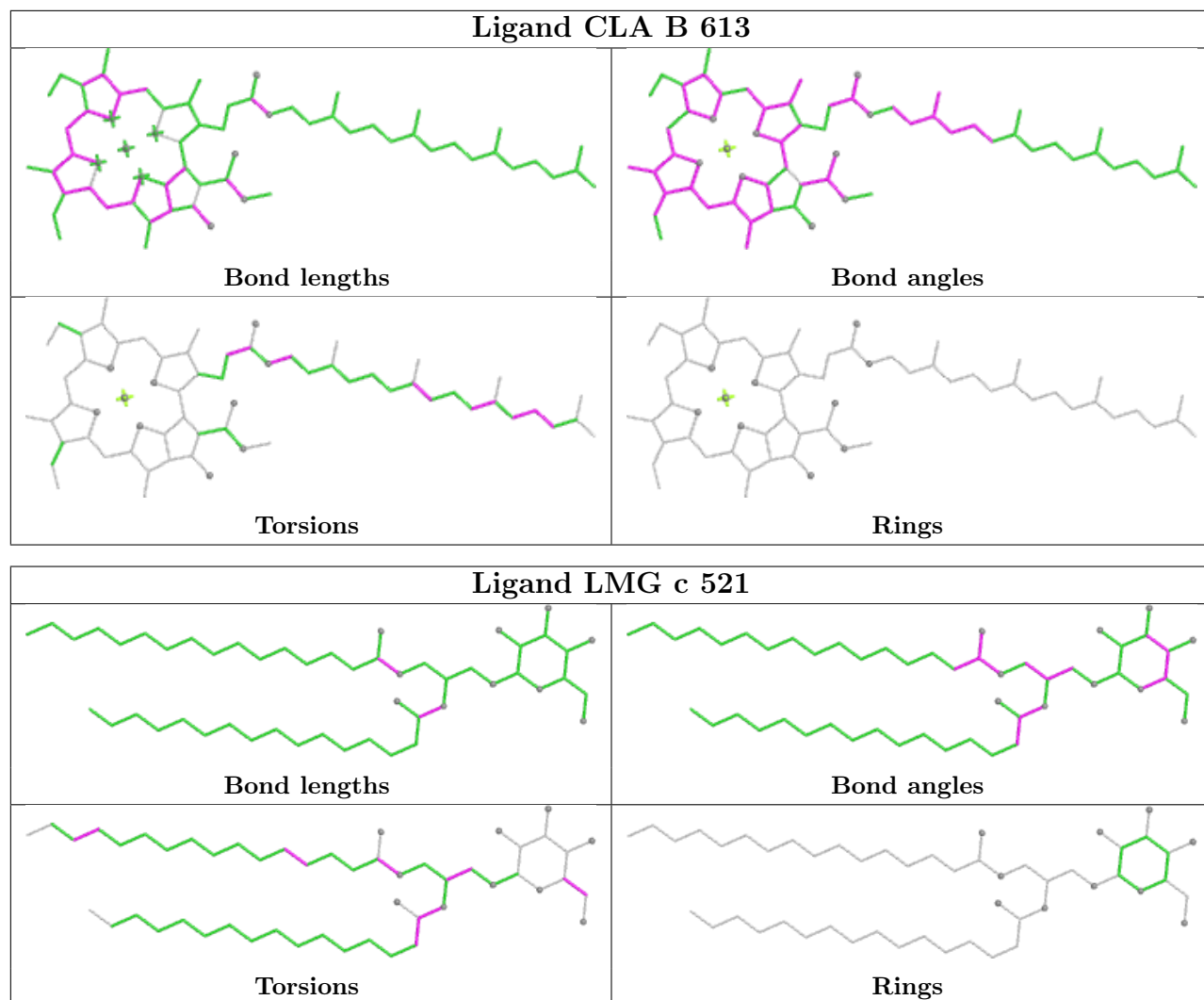


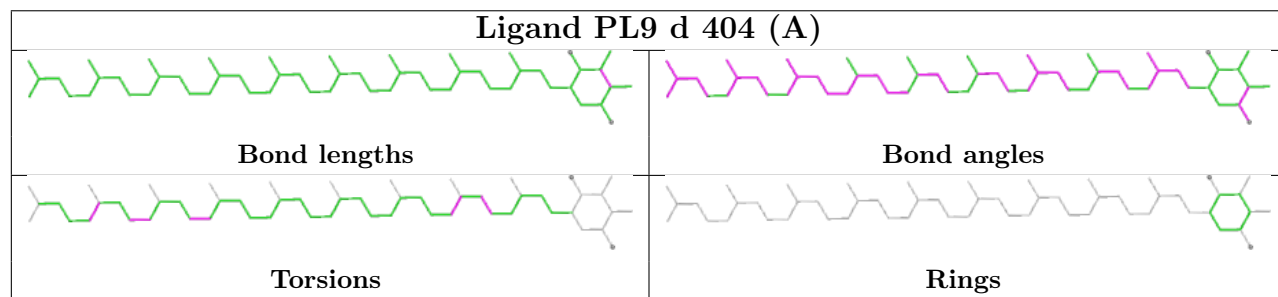
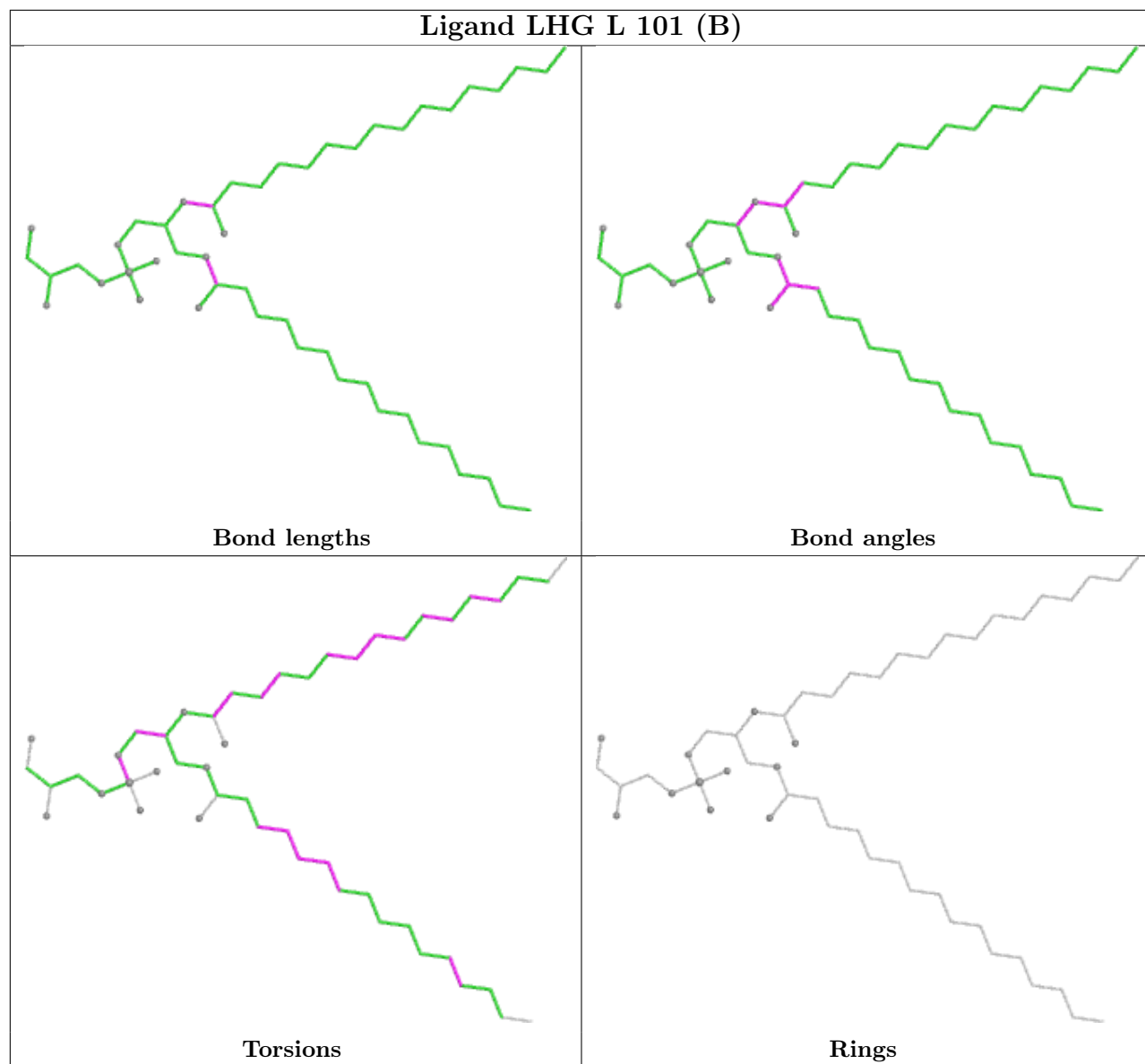
Ligand PL9 a 414 (A)

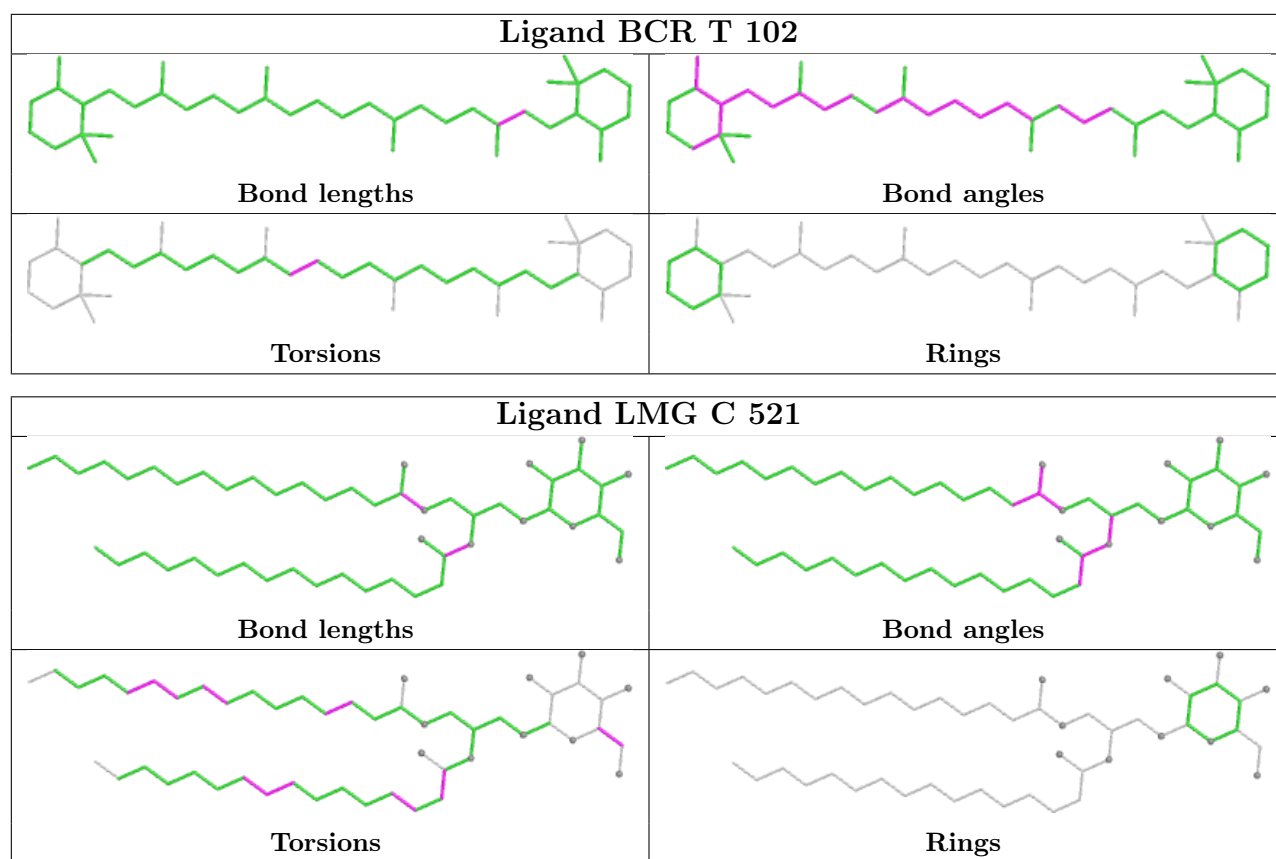


Ligand LMG C 526









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.69	1 (0%) 90 90	20, 26, 61, 122	222 (66%)
1	a	334/344 (97%)	-0.63	0 100 100	21, 29, 65, 126	221 (66%)
2	B	504/505 (99%)	-0.61	1 (0%) 91 91	23, 54, 84, 113	20 (3%)
2	b	504/505 (99%)	-0.48	3 (0%) 85 86	24, 58, 95, 154	19 (3%)
3	C	451/455 (99%)	-0.56	0 100 100	22, 61, 84, 136	97 (21%)
3	c	455/455 (100%)	-0.47	1 (0%) 91 91	25, 67, 88, 125	100 (21%)
4	D	342/342 (100%)	-0.72	0 100 100	20, 46, 66, 129	114 (33%)
4	d	341/342 (99%)	-0.71	0 100 100	22, 51, 76, 130	116 (34%)
5	E	81/84 (96%)	-0.39	0 100 100	53, 71, 98, 147	0
5	e	79/84 (94%)	-0.32	1 (1%) 75 76	33, 76, 116, 143	2 (2%)
6	F	34/44 (77%)	-0.57	0 100 100	55, 61, 89, 113	0
6	f	31/44 (70%)	-0.35	1 (3%) 50 52	55, 69, 94, 138	1 (3%)
7	H	64/65 (98%)	-0.35	1 (1%) 70 72	54, 65, 89, 105	0
7	h	64/65 (98%)	-0.36	0 100 100	40, 73, 96, 101	1 (1%)
8	I	37/38 (97%)	-0.26	0 100 100	58, 66, 123, 146	0
8	i	37/38 (97%)	-0.29	0 100 100	56, 66, 115, 134	0
9	J	38/39 (97%)	-0.47	0 100 100	49, 70, 119, 153	0
9	j	39/39 (100%)	-0.30	0 100 100	58, 78, 129, 151	0
10	K	37/37 (100%)	-0.63	0 100 100	54, 68, 88, 110	0
10	k	37/37 (100%)	-0.52	0 100 100	65, 75, 98, 112	0
11	L	36/37 (97%)	-0.70	0 100 100	23, 46, 112, 127	2 (5%)
11	l	36/37 (97%)	-0.67	0 100 100	23, 47, 105, 115	2 (5%)
12	M	32/36 (88%)	-0.67	0 100 100	27, 50, 75, 131	1 (3%)
12	m	33/36 (91%)	-0.63	0 100 100	25, 49, 71, 140	2 (6%)

Continued on next page...

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.52	0 100 100	21, 66, 119, 161	10 (4%)
13	o	243/244 (99%)	-0.45	0 100 100	23, 68, 125, 155	8 (3%)
14	T	29/32 (90%)	-0.63	0 100 100	27, 47, 56, 66	6 (20%)
14	t	29/32 (90%)	-0.71	1 (3%) 48 50	27, 47, 61, 72	5 (17%)
15	U	96/104 (92%)	-0.63	0 100 100	25, 58, 93, 100	4 (4%)
15	u	97/104 (93%)	-0.68	0 100 100	28, 62, 81, 120	4 (4%)
16	V	137/137 (100%)	-0.75	0 100 100	24, 58, 81, 109	6 (4%)
16	v	137/137 (100%)	-0.55	0 100 100	27, 72, 102, 128	6 (4%)
17	X	38/40 (95%)	-0.20	0 100 100	37, 74, 97, 114	1 (2%)
17	x	38/40 (95%)	-0.04	0 100 100	69, 82, 131, 154	0
18	Y	29/30 (96%)	-0.08	0 100 100	68, 85, 113, 123	0
18	y	29/30 (96%)	-0.24	0 100 100	78, 91, 109, 115	0
19	Z	62/62 (100%)	-0.30	0 100 100	68, 83, 130, 153	0
19	z	62/62 (100%)	0.10	0 100 100	80, 95, 144, 168	0
20	R	34/34 (100%)	0.59	2 (5%) 28 30	85, 111, 136, 142	0
All	All	5283/5384 (98%)	-0.54	12 (0%) 91 91	20, 59, 101, 168	970 (18%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	3.4
5	e	79[A]	PHE	3.4
6	f	16[A]	PHE	3.2
20	R	19	ALA	2.5
1	A	11	ALA	2.5
20	R	28	VAL	2.5
3	c	245[A]	ILE	2.4
2	b	499	VAL	2.3
14	t	30[A]	THR	2.3
2	b	502	VAL	2.1
2	B	494	GLY	2.1
2	b	486[A]	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.95	0.07	67,71,79,85	0
14	FME	T	1	10/11	0.95	0.07	43,53,62,73	0
8	FME	i	1	10/11	0.97	0.07	54,75,84,86	0
12	FME	m	1	10/11	0.97	0.07	48,63,87,111	0
14	FME	t	1	10/11	0.97	0.06	44,48,61,77	0
12	FME	M	1	10/11	0.98	0.06	46,62,94,98	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
25	GOL	a	418	6/6	0.59	0.17	74,98,100,102	0
29	UNL	A	413	28/-	0.67	0.15	80,110,132,143	0
31	LMT	A	417	35/35	0.68	0.13	97,127,153,163	0
31	LMT	F	101	35/35	0.68	0.15	88,126,165,171	0
31	LMT	e	101	35/35	0.68	0.15	98,140,176,179	0
31	LMT	B	630	35/35	0.69	0.15	65,111,140,146	0
29	UNL	J	101	10/-	0.70	0.22	69,80,87,101	0
29	UNL	K	101[A]	34/-	0.71	0.14	76,104,114,118	34
29	UNL	K	101[B]	34/-	0.71	0.14	75,104,114,118	34
29	UNL	a	415	30/-	0.71	0.12	85,113,133,140	0
31	LMT	A	415	35/35	0.71	0.13	61,109,130,134	0
29	UNL	m	102	10/-	0.72	0.20	68,75,102,103	0
34	HTG	C	523	19/19	0.73	0.13	100,124,139,139	0
31	LMT	c	501	35/35	0.74	0.13	103,128,147,150	0
29	UNL	I	101	40/-	0.74	0.15	73,102,150,162	0
34	HTG	B	623	19/19	0.74	0.16	61,95,108,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	SQD	f	102	43/54	0.74	0.13	101,124,167,183	0
25	GOL	o	302	6/6	0.75	0.16	82,89,96,104	0
25	GOL	O	302	6/6	0.76	0.12	81,90,105,109	0
34	HTG	D	412	16/19	0.76	0.12	93,103,134,149	0
29	UNL	j	101	10/-	0.77	0.15	73,90,97,98	0
32	LHG	a	420[A]	42/49	0.78	0.12	88,131,146,154	42
32	LHG	a	420[B]	42/49	0.78	0.12	87,131,146,154	42
29	UNL	c	525[B]	32/-	0.78	0.14	86,106,118,127	32
25	GOL	B	627	6/6	0.78	0.14	75,86,96,114	0
29	UNL	c	525[A]	32/-	0.78	0.14	86,106,118,127	32
34	HTG	c	522	19/19	0.78	0.10	109,124,142,145	0
33	LMG	C	522	51/55	0.79	0.11	61,115,156,161	0
29	UNL	M	102	10/-	0.80	0.15	63,77,98,100	0
29	UNL	B	631	40/-	0.80	0.13	74,103,154,159	0
29	UNL	b	626	33/-	0.80	0.13	67,98,162,171	0
29	UNL	D	411	40/-	0.80	0.13	63,88,138,150	0
29	UNL	b	629	36/-	0.81	0.11	68,96,134,143	0
25	GOL	c	528	6/6	0.81	0.16	82,104,109,121	0
36	CA	V	201	1/1	0.81	0.24	129,129,129,129	0
31	LMT	T	101	35/35	0.82	0.10	65,121,165,169	0
31	LMT	b	621	25/35	0.82	0.11	77,114,158,164	0
25	GOL	A	409	6/6	0.82	0.13	60,77,80,83	0
25	GOL	b	624	6/6	0.82	0.15	93,96,104,113	0
28	PL9	a	414[B]	55/55	0.83	0.14	75,97,111,114	55
25	GOL	d	410	6/6	0.83	0.23	51,69,79,86	0
28	PL9	A	412[A]	55/55	0.83	0.13	60,88,103,106	55
31	LMT	B	628	35/35	0.83	0.11	63,102,135,149	0
34	HTG	b	622	19/19	0.83	0.13	63,85,118,119	0
28	PL9	A	412[B]	55/55	0.83	0.13	60,88,103,106	55
28	PL9	a	414[A]	55/55	0.83	0.14	75,97,111,114	55
29	UNL	B	626	33/-	0.84	0.14	60,106,142,146	0
25	GOL	O	303	6/6	0.84	0.13	76,91,93,95	0
34	HTG	V	203	11/19	0.84	0.09	81,111,125,126	0
26	SQD	a	412	54/54	0.84	0.10	66,93,140,149	0
34	HTG	b	623	19/19	0.84	0.10	85,129,154,161	0
33	LMG	c	521	51/55	0.84	0.10	78,131,161,183	0
31	LMT	t	102	26/35	0.84	0.11	67,101,137,148	0
31	LMT	t	101	25/35	0.85	0.12	54,81,132,154	0
26	SQD	A	410	54/54	0.85	0.10	66,89,130,150	0
25	GOL	c	527	6/6	0.85	0.16	96,97,106,110	0
33	LMG	z	101	39/55	0.85	0.12	74,126,151,164	0
31	LMT	b	627	25/35	0.86	0.11	58,93,140,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	HTG	B	622	19/19	0.86	0.12	69,85,110,123	0
33	LMG	C	526	37/55	0.87	0.12	70,124,146,160	0
34	HTG	d	408	16/19	0.87	0.10	89,116,139,152	0
31	LMT	m	103	35/35	0.87	0.10	62,92,105,108	0
25	GOL	l	801[A]	6/6	0.88	0.17	67,93,96,98	6
25	GOL	l	801[B]	6/6	0.88	0.17	68,93,96,98	6
25	GOL	V	204[B]	6/6	0.88	0.13	59,70,77,78	6
31	LMT	M	101	35/35	0.88	0.10	59,96,115,122	0
25	GOL	v	202[A]	6/6	0.88	0.11	70,80,83,86	6
25	GOL	v	202[B]	6/6	0.88	0.11	70,80,83,86	6
25	GOL	V	204[A]	6/6	0.88	0.13	62,72,77,78	6
32	LHG	E	101[A]	42/49	0.89	0.11	74,100,113,119	42
32	LHG	E	101[B]	42/49	0.89	0.11	74,100,113,119	42
26	SQD	b	620	54/54	0.89	0.09	61,94,119,129	0
26	SQD	B	620	54/54	0.89	0.09	59,92,137,145	0
26	SQD	F	103	43/54	0.89	0.11	77,107,129,137	0
25	GOL	B	629	6/6	0.89	0.11	71,78,90,91	0
25	GOL	a	419	6/6	0.90	0.25	54,76,81,87	0
23	CLA	b	601	65/65	0.90	0.10	63,89,128,157	0
33	LMG	a	417	51/55	0.90	0.09	71,93,110,118	0
33	LMG	c	520	51/55	0.91	0.09	65,89,136,153	0
23	CLA	c	514	65/65	0.91	0.09	69,94,127,149	0
33	LMG	C	502	51/55	0.91	0.09	64,87,110,124	0
29	UNL	D	410	17/-	0.91	0.10	59,78,106,113	0
23	CLA	B	601	65/65	0.91	0.09	59,81,115,150	0
34	HTG	B	625	19/19	0.91	0.08	65,81,97,104	0
25	GOL	D	414	6/6	0.91	0.16	43,62,69,85	0
36	CA	f	103	1/1	0.91	0.13	120,120,120,120	0
36	CA	o	301	1/1	0.91	0.06	116,116,116,116	0
33	LMG	B	621	51/55	0.92	0.07	49,68,87,107	0
25	GOL	c	526[B]	6/6	0.92	0.09	68,70,75,77	6
33	LMG	C	521	51/55	0.92	0.09	55,85,119,129	0
33	LMG	m	101	51/55	0.92	0.09	51,73,100,110	0
25	GOL	D	403	6/6	0.92	0.28	50,72,82,83	0
25	GOL	c	526[A]	6/6	0.92	0.09	68,70,75,77	6
33	LMG	D	413	51/55	0.93	0.08	47,67,125,131	0
29	UNL	d	407	17/-	0.93	0.09	67,79,113,114	0
26	SQD	C	501[A]	54/54	0.93	0.09	57,79,116,121	54
26	SQD	C	501[B]	54/54	0.93	0.09	57,80,116,121	54
33	LMG	d	409	51/55	0.93	0.08	53,76,118,148	0
23	CLA	c	513	65/65	0.93	0.09	61,84,127,139	0
23	CLA	C	515	65/65	0.93	0.08	64,87,116,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	LHG	A	416[A]	49/49	0.93	0.09	48,61,83,86	49
32	LHG	A	416[B]	49/49	0.93	0.09	48,61,83,86	49
24	BCR	T	102	40/40	0.93	0.07	48,59,70,75	0
23	CLA	B	614	65/65	0.94	0.08	39,52,102,126	0
24	BCR	Y	101	40/40	0.94	0.08	54,67,83,93	0
24	BCR	c	515	40/40	0.94	0.08	70,83,97,99	0
24	BCR	d	403	40/40	0.94	0.08	54,67,98,107	0
24	BCR	t	103	40/40	0.94	0.06	43,59,74,78	0
24	BCR	y	101	40/40	0.94	0.07	60,72,86,98	0
23	CLA	a	409	65/65	0.94	0.10	43,59,139,154	0
23	CLA	C	506	65/65	0.94	0.08	44,58,101,133	0
23	CLA	b	614	65/65	0.94	0.07	43,54,101,107	0
25	GOL	C	524[A]	6/6	0.94	0.09	59,62,66,70	6
25	GOL	C	524[B]	6/6	0.94	0.09	61,61,68,70	6
23	CLA	c	505	65/65	0.94	0.07	52,62,111,132	0
23	CLA	c	507	65/65	0.94	0.08	55,70,119,137	0
23	CLA	C	508	65/65	0.94	0.08	54,72,122,143	0
23	CLA	C	514	65/65	0.94	0.08	62,77,112,128	0
24	BCR	C	516	40/40	0.94	0.08	62,77,88,93	0
26	SQD	a	411[A]	54/54	0.94	0.09	61,81,115,120	54
32	LHG	D	409[A]	49/49	0.94	0.09	51,60,109,116	49
32	LHG	D	409[B]	49/49	0.94	0.09	51,61,109,116	49
26	SQD	a	411[B]	54/54	0.94	0.09	61,81,115,120	54
34	HTG	b	625	19/19	0.94	0.07	63,82,95,106	0
24	BCR	D	406	40/40	0.94	0.08	45,59,102,109	0
24	BCR	H	101	40/40	0.94	0.08	52,69,86,91	0
35	DGD	C	519[A]	62/66	0.94	0.08	48,66,110,113	62
35	DGD	C	519[B]	62/66	0.94	0.08	48,65,110,113	62
35	DGD	c	517[A]	62/66	0.94	0.08	51,66,102,113	62
35	DGD	c	517[B]	62/66	0.94	0.08	51,66,102,113	62
35	DGD	c	518[A]	62/66	0.94	0.08	53,70,120,136	62
35	DGD	c	518[B]	62/66	0.94	0.08	53,70,120,136	62
24	BCR	K	102	40/40	0.94	0.09	57,65,75,81	0
32	LHG	d	411[A]	49/49	0.94	0.08	51,66,80,89	49
32	LHG	d	411[B]	49/49	0.94	0.08	51,66,80,89	49
24	BCR	A	408	40/40	0.95	0.07	40,53,65,68	0
24	BCR	B	619	40/40	0.95	0.07	50,61,96,102	0
23	CLA	b	606	65/65	0.95	0.07	47,62,122,131	0
28	PL9	D	407[A]	55/55	0.95	0.06	36,49,57,68	55
28	PL9	D	407[B]	55/55	0.95	0.06	36,49,57,68	55
23	CLA	D	405	65/65	0.95	0.08	49,60,123,131	0
23	CLA	b	616	65/65	0.95	0.08	52,65,133,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	a	407[A]	65/65	0.95	0.07	41,52,121,129	65
32	LHG	d	406[A]	49/49	0.95	0.09	54,64,115,127	49
32	LHG	d	406[B]	49/49	0.95	0.09	54,64,115,127	49
23	CLA	a	407[B]	65/65	0.95	0.07	41,52,121,129	65
23	CLA	c	508	65/65	0.95	0.09	53,70,87,94	0
24	BCR	b	619	40/40	0.95	0.07	51,64,86,91	0
23	CLA	c	509	65/65	0.95	0.07	45,64,127,142	0
24	BCR	c	516	40/40	0.95	0.07	55,68,84,92	0
35	DGD	C	520	62/66	0.95	0.07	44,58,92,112	0
35	DGD	H	102	62/66	0.95	0.08	46,61,74,83	0
23	CLA	A	407	65/65	0.95	0.08	40,54,129,145	0
24	BCR	h	101	40/40	0.95	0.09	58,72,98,100	0
24	BCR	k	101	40/40	0.95	0.09	60,74,90,92	0
25	GOL	b	628	6/6	0.95	0.08	80,82,87,90	0
35	DGD	c	519	62/66	0.95	0.07	51,65,109,131	0
35	DGD	h	102	62/66	0.95	0.08	51,65,79,84	0
29	UNL	X	101	18/-	0.95	0.10	64,76,108,112	0
23	CLA	C	510	65/65	0.95	0.07	44,57,120,146	0
23	CLA	d	402	65/65	0.95	0.09	55,68,126,147	0
23	CLA	B	611	65/65	0.96	0.06	33,45,65,86	0
23	CLA	A	406[A]	65/65	0.96	0.06	38,47,111,118	65
24	BCR	B	617	40/40	0.96	0.05	42,52,64,65	0
29	UNL	x	101	18/-	0.96	0.10	68,81,119,137	0
24	BCR	B	618	40/40	0.96	0.05	37,57,69,76	0
23	CLA	B	616	65/65	0.96	0.08	45,61,131,138	0
23	CLA	b	602	65/65	0.96	0.07	52,63,84,91	0
24	BCR	C	517	40/40	0.96	0.07	52,67,79,90	0
23	CLA	C	503	65/65	0.96	0.07	50,62,76,89	0
23	CLA	b	607	65/65	0.96	0.06	39,48,84,93	0
23	CLA	b	612	65/65	0.96	0.07	47,56,66,78	0
23	CLA	A	406[B]	65/65	0.96	0.06	38,47,111,119	65
28	PL9	d	404[A]	55/55	0.96	0.06	39,51,61,68	55
28	PL9	d	404[B]	55/55	0.96	0.06	39,50,61,68	55
23	CLA	A	404[A]	65/65	0.96	0.06	38,42,60,67	65
24	BCR	a	410	40/40	0.96	0.06	46,54,66,68	0
24	BCR	b	617	40/40	0.96	0.06	44,54,66,67	0
24	BCR	b	618	40/40	0.96	0.06	43,59,78,89	0
23	CLA	c	502	65/65	0.96	0.07	54,69,80,87	0
23	CLA	c	504	65/65	0.96	0.07	55,71,85,90	0
32	LHG	D	408[A]	49/49	0.96	0.07	46,54,66,76	49
32	LHG	D	408[B]	49/49	0.96	0.07	46,55,66,77	49
23	CLA	C	509	65/65	0.96	0.07	52,66,83,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	DGD	C	518[A]	62/66	0.96	0.07	47,60,102,111	62
35	DGD	C	518[B]	62/66	0.96	0.07	47,60,102,111	62
23	CLA	c	506	65/65	0.96	0.06	51,65,94,103	0
23	CLA	A	404[B]	65/65	0.96	0.06	38,43,63,67	65
23	CLA	B	602	65/65	0.96	0.07	50,59,73,91	0
23	CLA	B	603	65/65	0.96	0.07	44,54,75,85	0
23	CLA	c	511	65/65	0.96	0.06	49,65,80,90	0
32	LHG	d	405[A]	49/49	0.96	0.07	48,55,70,76	49
32	LHG	d	405[B]	49/49	0.96	0.07	47,56,70,77	49
23	CLA	c	512	65/65	0.96	0.07	59,70,86,96	0
25	GOL	B	624	6/6	0.96	0.11	67,78,81,82	0
23	CLA	B	606	65/65	0.96	0.07	43,58,110,134	0
36	CA	O	301	1/1	0.96	0.04	105,105,105,105	0
23	CLA	B	609	65/65	0.96	0.07	46,61,72,83	0
32	LHG	l	802[A]	49/49	0.96	0.07	48,58,72,91	49
32	LHG	l	802[B]	49/49	0.96	0.07	48,57,72,91	49
37	PHO	D	402[A]	64/64	0.96	0.06	41,50,55,59	64
37	PHO	D	402[B]	64/64	0.96	0.06	40,50,55,60	64
37	PHO	a	416[A]	64/64	0.96	0.07	47,57,62,67	64
37	PHO	a	416[B]	64/64	0.96	0.07	47,57,62,66	64
23	CLA	a	406[B]	65/65	0.97	0.05	37,44,64,72	65
23	CLA	A	405[A]	65/65	0.97	0.05	35,43,53,64	65
23	CLA	d	401[A]	65/65	0.97	0.06	40,47,73,94	65
23	CLA	d	401[B]	65/65	0.97	0.06	40,47,73,94	65
23	CLA	B	607	65/65	0.97	0.06	33,48,76,83	0
23	CLA	C	505	65/65	0.97	0.06	48,65,73,84	0
23	CLA	A	405[B]	65/65	0.97	0.05	35,43,53,64	65
23	CLA	C	507	65/65	0.97	0.06	49,63,99,114	0
23	CLA	b	603	65/65	0.97	0.06	45,60,85,98	0
23	CLA	b	604	65/65	0.97	0.06	42,54,100,119	0
23	CLA	b	605	65/65	0.97	0.07	37,52,74,80	0
23	CLA	B	610	65/65	0.97	0.07	40,56,71,84	0
23	CLA	B	604	65/65	0.97	0.06	36,47,108,129	0
23	CLA	b	609	65/65	0.97	0.07	53,68,83,102	0
23	CLA	b	610	65/65	0.97	0.07	48,59,73,78	0
23	CLA	b	611	65/65	0.97	0.06	37,48,71,88	0
23	CLA	B	612	65/65	0.97	0.06	35,50,63,71	0
32	LHG	L	101[A]	49/49	0.97	0.06	47,55,68,87	49
32	LHG	L	101[B]	49/49	0.97	0.06	47,56,68,87	49
23	CLA	b	613	65/65	0.97	0.06	42,52,90,108	0
23	CLA	C	511	65/65	0.97	0.07	50,59,84,91	0
23	CLA	b	615	65/65	0.97	0.07	48,64,87,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	C	512	65/65	0.97	0.06	48,59,78,84	0
23	CLA	C	513	65/65	0.97	0.07	51,65,81,83	0
23	CLA	c	503	65/65	0.97	0.06	46,60,90,109	0
23	CLA	B	613	65/65	0.97	0.06	38,47,90,106	0
23	CLA	B	605	65/65	0.97	0.05	40,50,67,84	0
23	CLA	D	404[A]	65/65	0.97	0.06	36,44,67,75	65
36	CA	C	525	1/1	0.97	0.06	79,79,79,79	0
23	CLA	D	404[B]	65/65	0.97	0.06	36,44,67,76	65
30	BCT	a	404[A]	4/4	0.97	0.05	57,59,65,72	4
36	CA	c	523	1/1	0.97	0.05	78,78,78,78	0
30	BCT	a	404[B]	4/4	0.97	0.05	56,59,65,72	4
23	CLA	B	615	65/65	0.97	0.06	43,55,75,89	0
37	PHO	D	401[A]	64/64	0.97	0.04	39,46,52,56	64
37	PHO	D	401[B]	64/64	0.97	0.04	39,46,52,56	64
23	CLA	a	405[A]	65/65	0.97	0.06	36,46,63,76	65
23	CLA	c	510	65/65	0.97	0.07	45,62,86,94	0
37	PHO	a	408[A]	64/64	0.97	0.05	42,48,53,57	64
37	PHO	a	408[B]	64/64	0.97	0.05	42,48,53,57	64
23	CLA	a	405[B]	65/65	0.97	0.06	39,46,63,76	65
23	CLA	a	406[A]	65/65	0.97	0.05	37,43,63,72	65
23	CLA	B	608	65/65	0.98	0.05	41,52,70,84	0
22	CL	a	403[A]	1/1	0.98	0.09	53,53,53,53	1
22	CL	a	403[B]	1/1	0.98	0.09	53,53,53,53	1
30	BCT	A	414[A]	4/4	0.98	0.06	54,55,61,67	4
30	BCT	A	414[B]	4/4	0.98	0.06	54,55,61,67	4
22	CL	a	402[A]	1/1	0.98	0.05	49,49,49,49	1
23	CLA	b	608	65/65	0.98	0.05	44,57,80,96	0
22	CL	a	402[B]	1/1	0.98	0.05	49,49,49,49	1
23	CLA	C	504	65/65	0.98	0.06	43,55,83,93	0
38	HEM	f	101	43/43	0.98	0.08	69,88,123,141	0
40	HEC	v	201	43/43	0.98	0.06	54,64,74,80	0
22	CL	A	403[B]	1/1	0.99	0.04	47,47,47,47	1
27	OEX	A	411[A]	10/10	0.99	0.03	39,46,50,51	10
27	OEX	A	411[B]	10/10	0.99	0.03	40,46,50,52	10
22	CL	A	402[A]	1/1	0.99	0.06	43,43,43,43	1
38	HEM	F	102	43/43	0.99	0.06	57,72,84,91	0
22	CL	A	402[B]	1/1	0.99	0.06	42,42,42,42	1
39	MG	J	102	1/1	0.99	0.03	60,60,60,60	0
39	MG	j	102	1/1	0.99	0.03	67,67,67,67	0
40	HEC	V	202	43/43	0.99	0.06	37,51,58,60	0
22	CL	A	403[A]	1/1	0.99	0.04	48,48,48,48	1
27	OEX	a	413[B]	10/10	1.00	0.02	46,50,55,56	10

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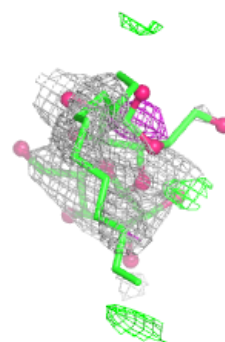
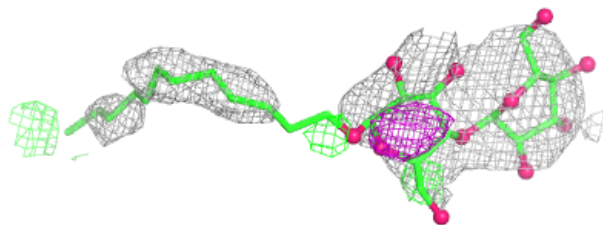
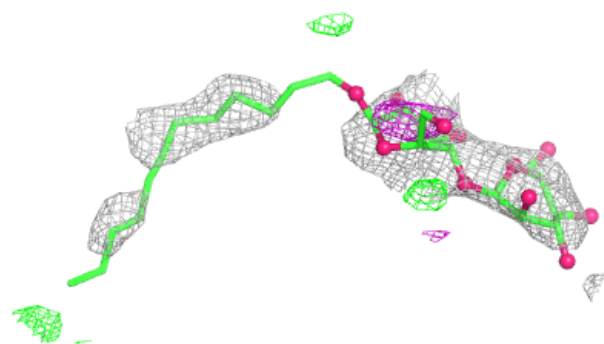
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	FE2	a	401[A]	1/1	1.00	0.01	53,53,53,53	1
21	FE2	a	401[B]	1/1	1.00	0.01	53,53,53,53	1
21	FE2	A	401[A]	1/1	1.00	0.01	51,51,51,51	1
36	CA	c	524	1/1	1.00	0.04	80,80,80,80	0
21	FE2	A	401[B]	1/1	1.00	0.01	51,51,51,51	1
27	OEX	a	413[A]	10/10	1.00	0.02	46,50,55,56	10

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

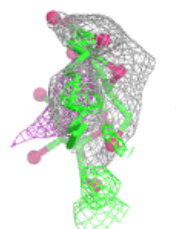
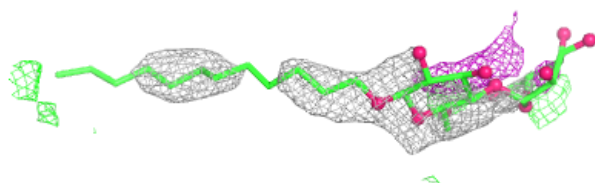
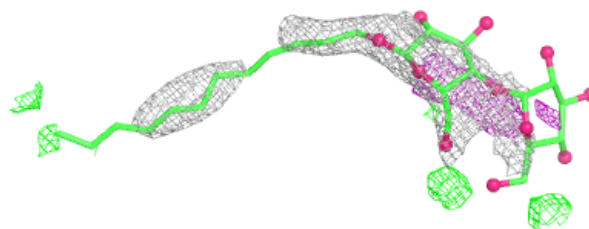
Electron density around LMT A 417:

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

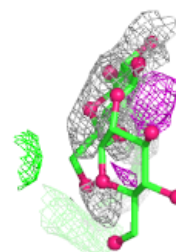
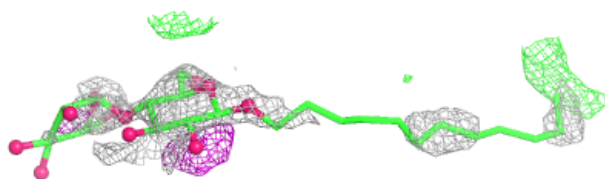
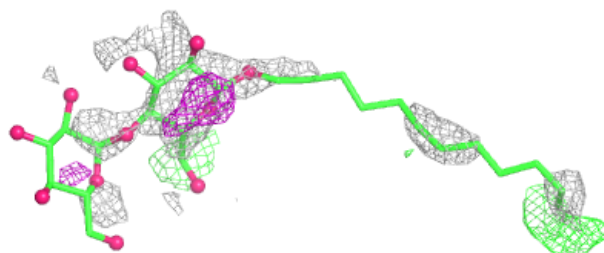


Electron density around LMT F 101:

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

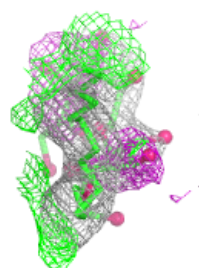
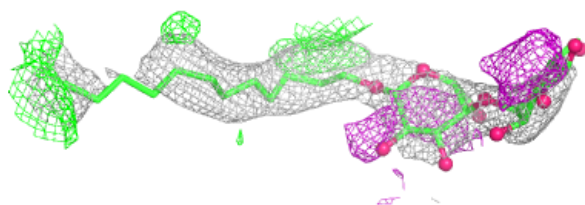
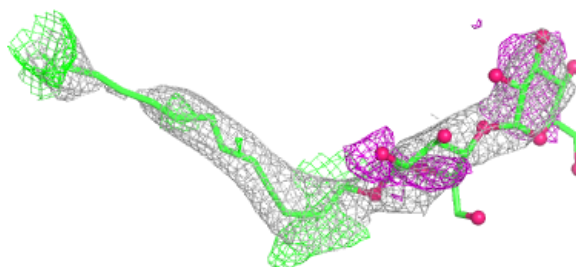
**Electron density around LMT e 101:**

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

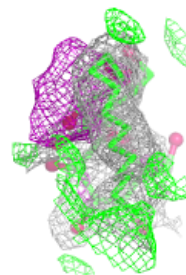
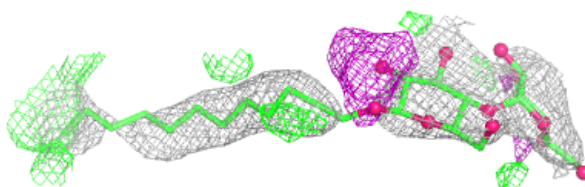
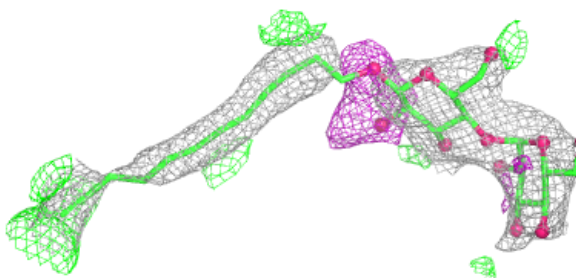


Electron density around LMT B 630:

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

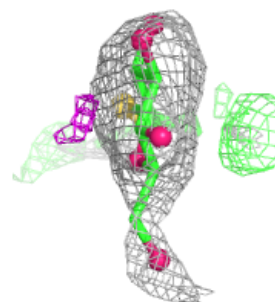
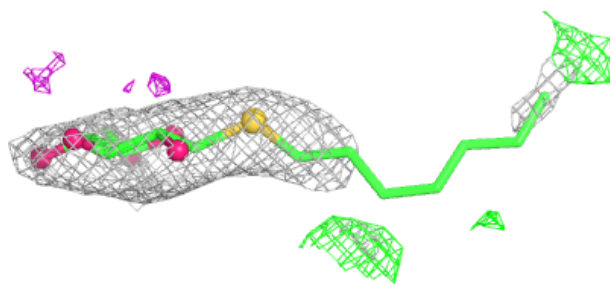
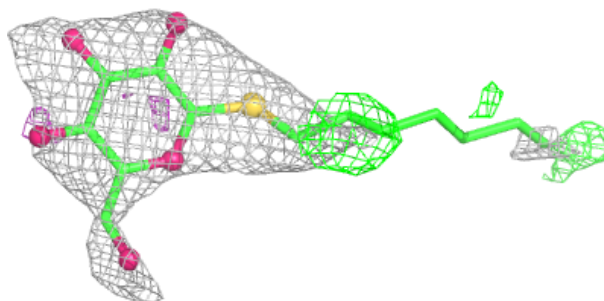
**Electron density around LMT A 415:**

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

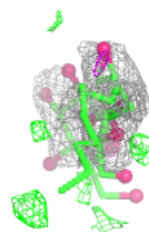
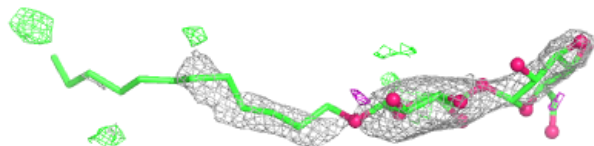
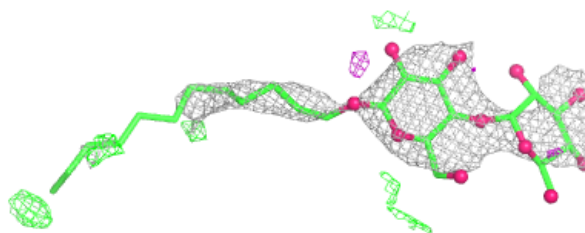


Electron density around HTG C 523:

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

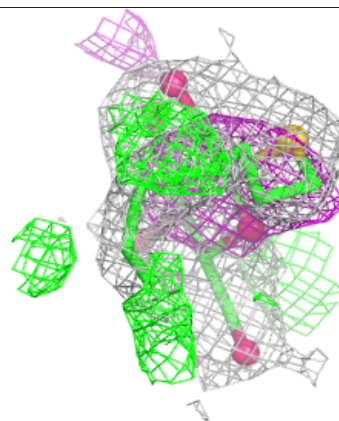
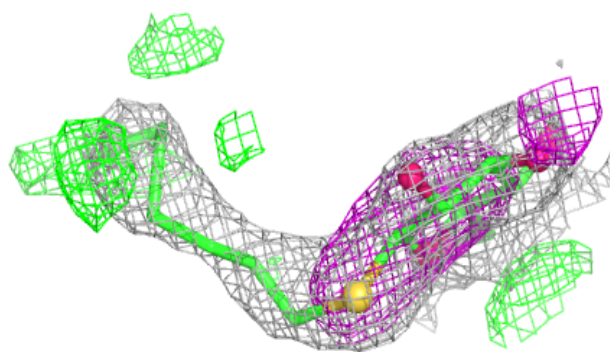
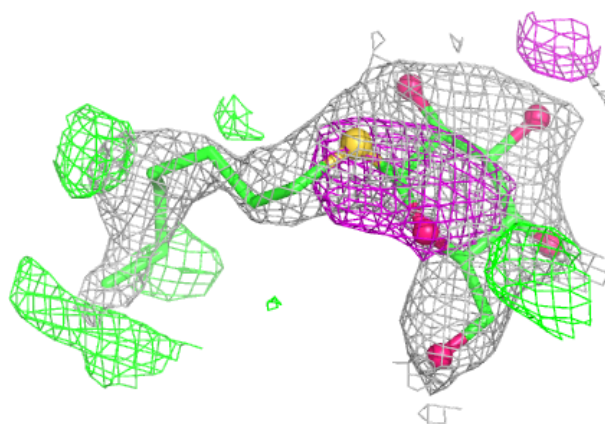
**Electron density around LMT c 501:**

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

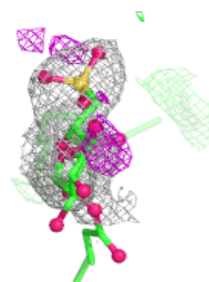
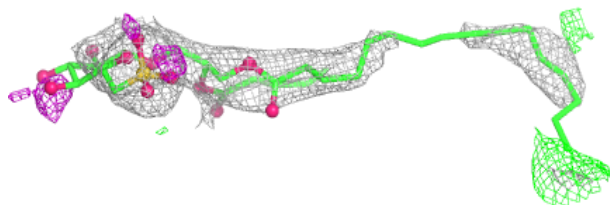
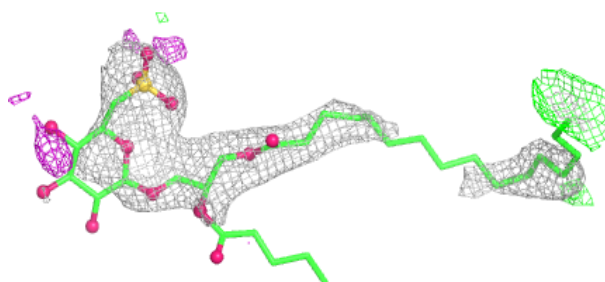


Electron density around HTG B 623:

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

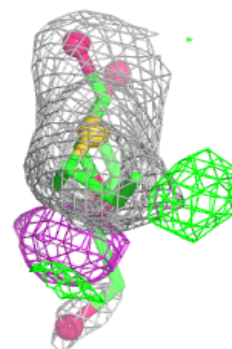
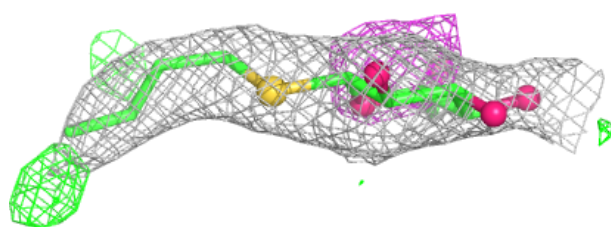
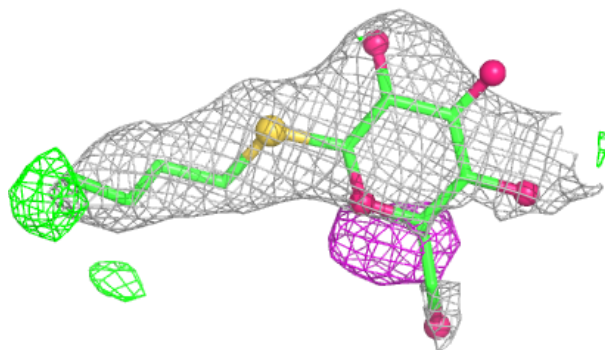
**Electron density around SQD f 102:**

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and green (positive)

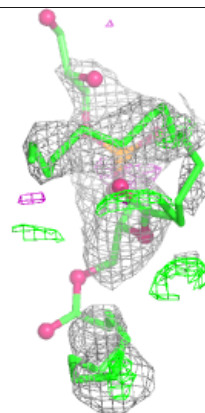
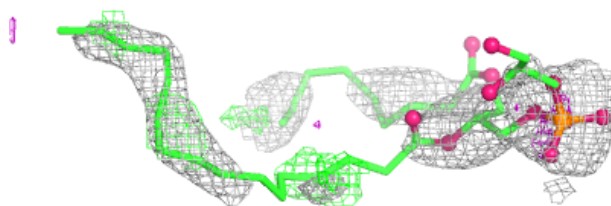
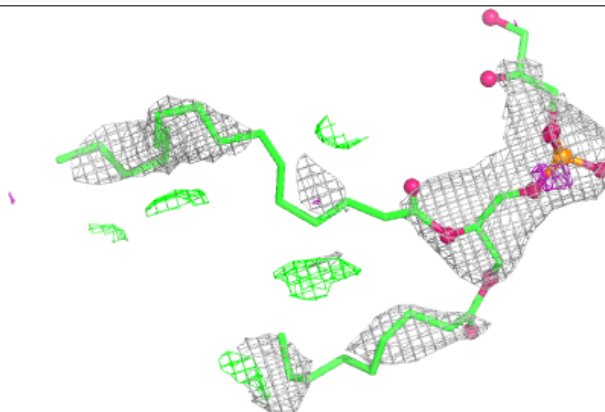


Electron density around HTG D 412:

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

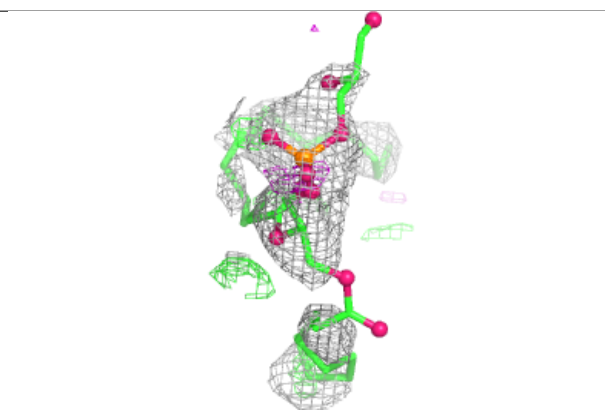
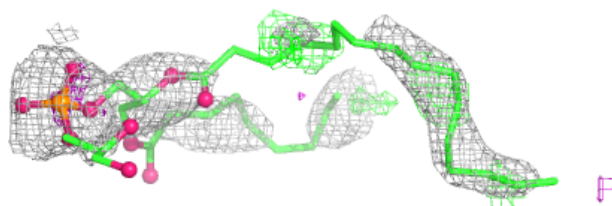
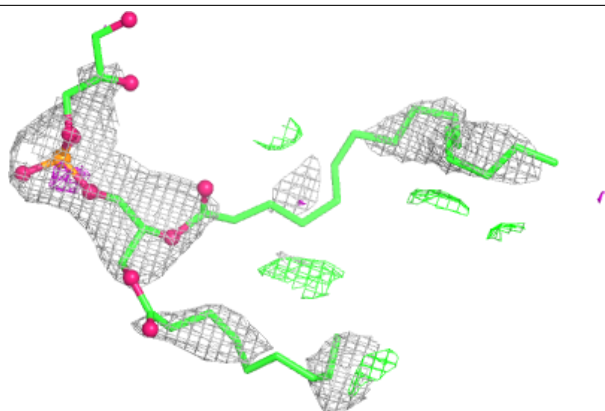
**Electron density around LHG a 420 (A):**

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

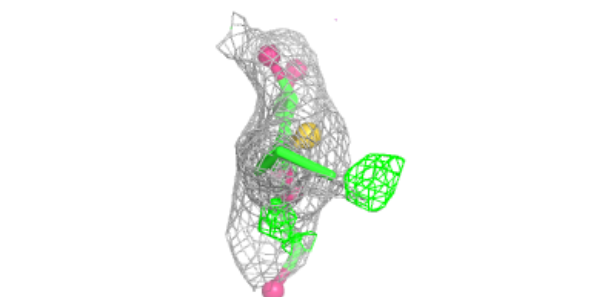
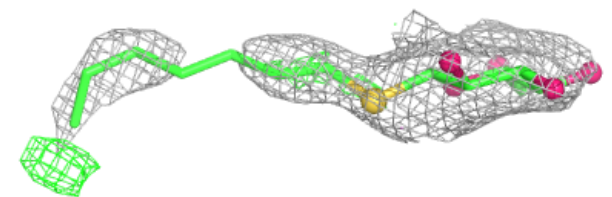
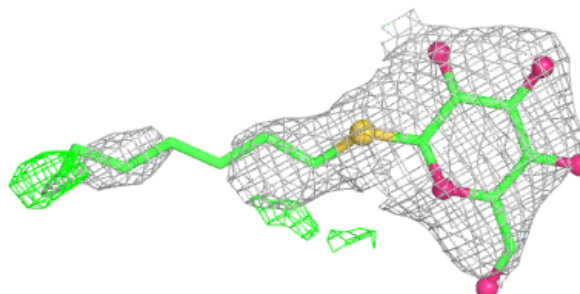


Electron density around LHG a 420 (B):

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

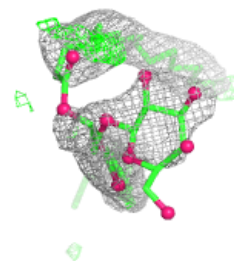
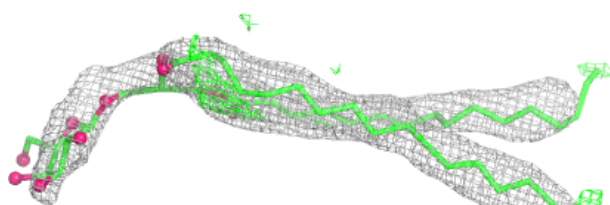
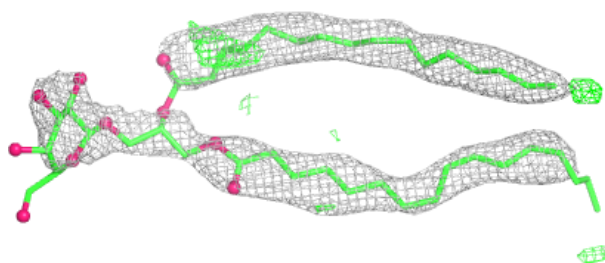
**Electron density around HTG c 522:**

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

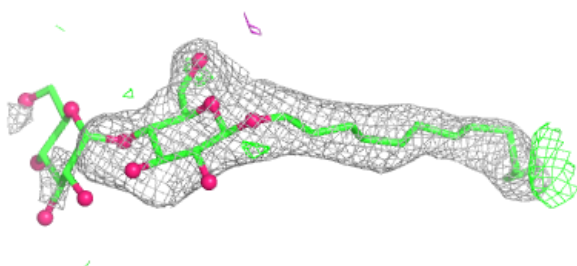
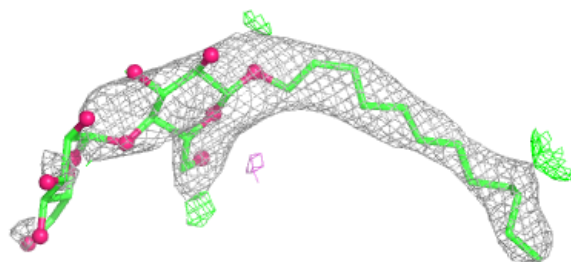


Electron density around LMG C 522:

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

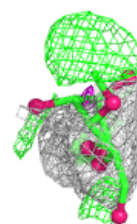
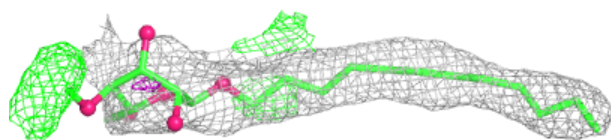
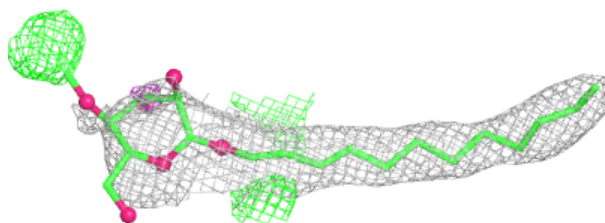
**Electron density around LMT T 101:**

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and green (positive)

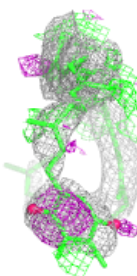
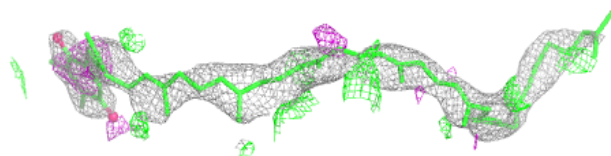
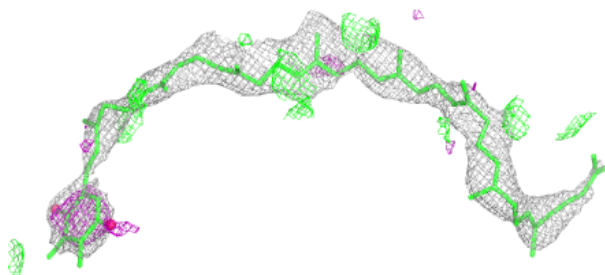


Electron density around LMT b 621:

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

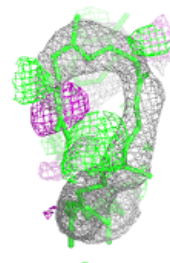
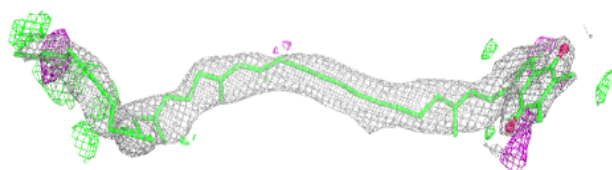
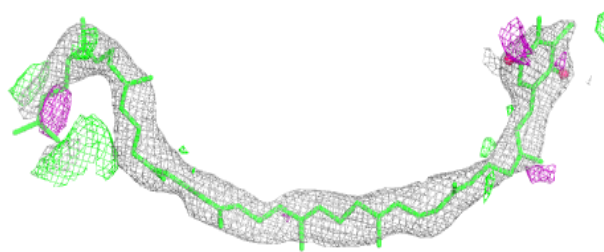
**Electron density around PL9 a 414 (B):**

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and green (positive)

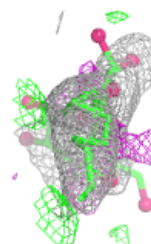
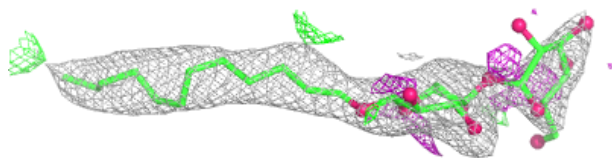
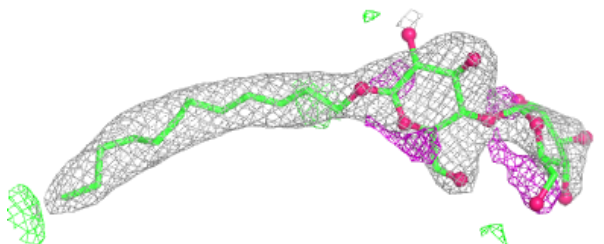


Electron density around PL9 A 412 (A):

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

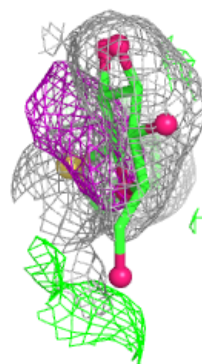
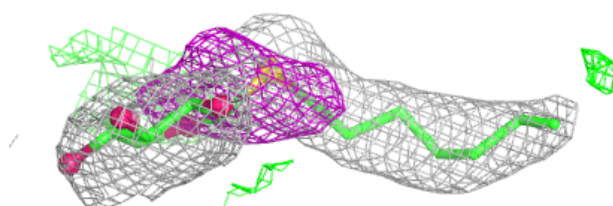
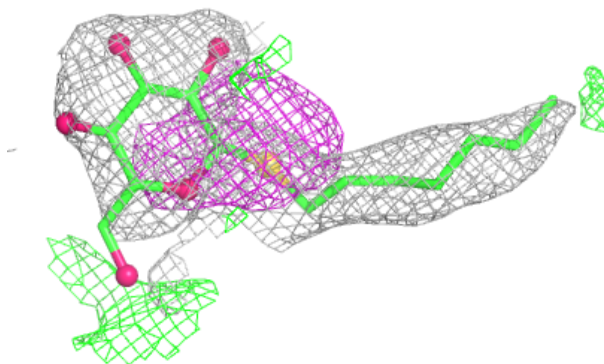
**Electron density around LMT B 628:**

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and green (positive)

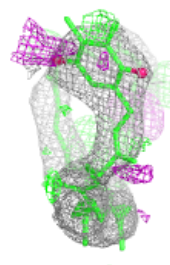
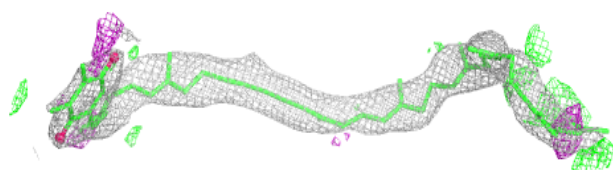
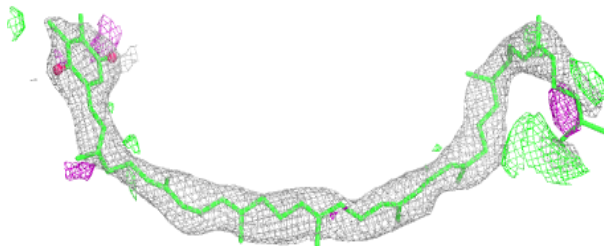


Electron density around HTG b 622:

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

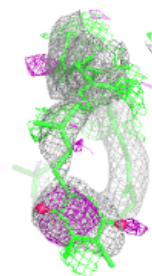
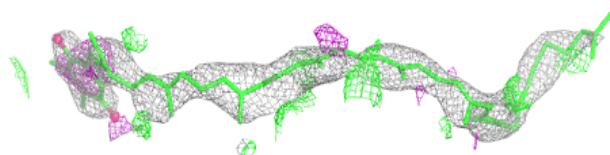
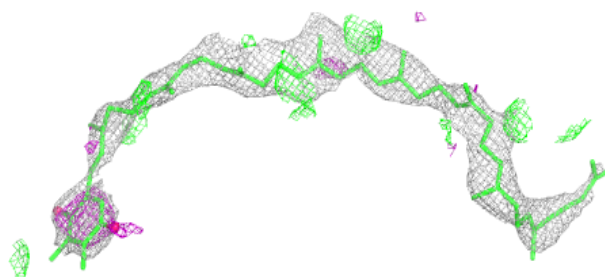
**Electron density around PL9 A 412 (B):**

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



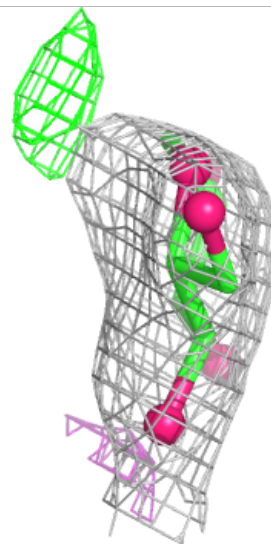
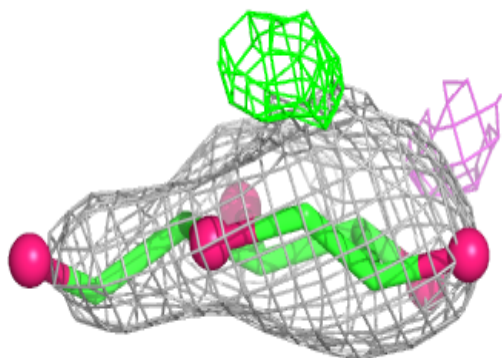
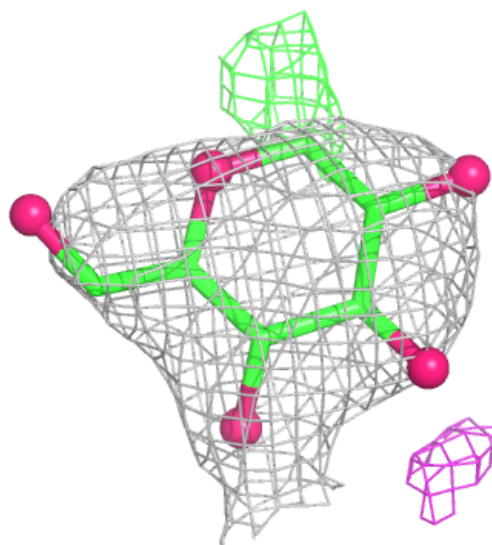
Electron density around PL9 a 414 (A):

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



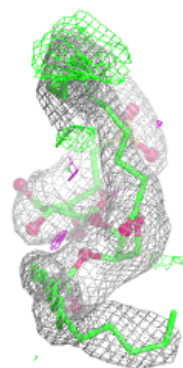
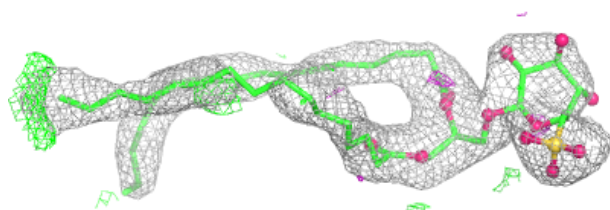
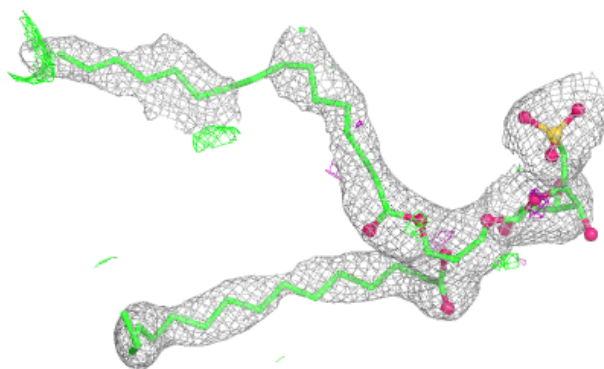
Electron density around HTG V 203:

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

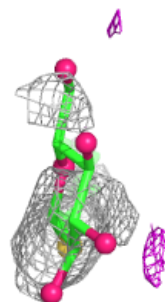
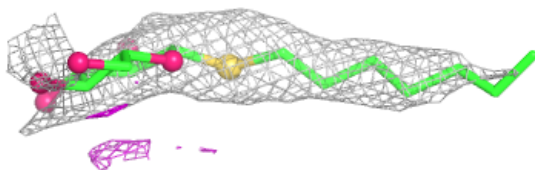
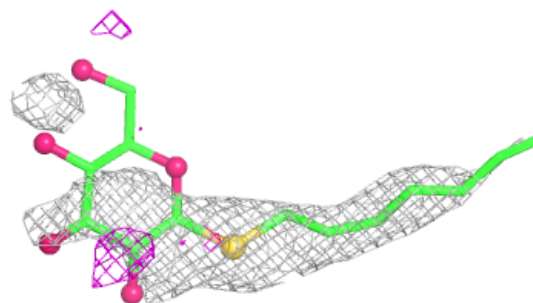


Electron density around SQD a 412:

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

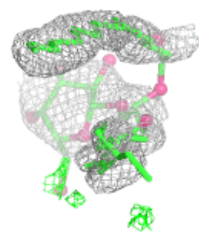
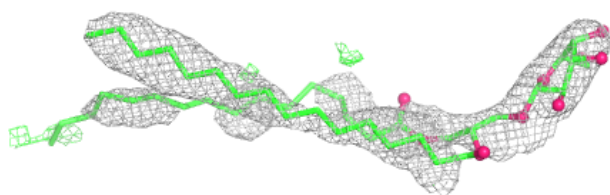
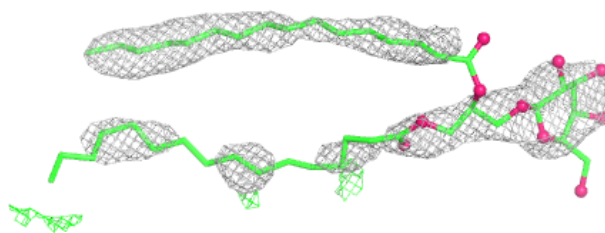
**Electron density around HTG b 623:**

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

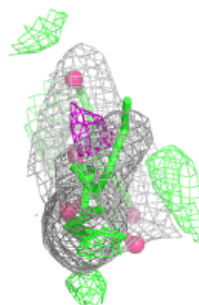
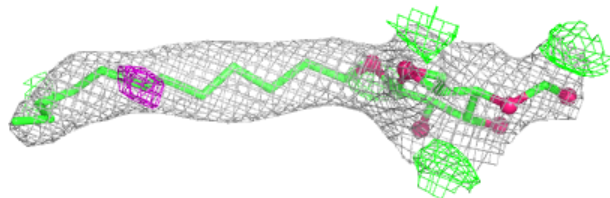
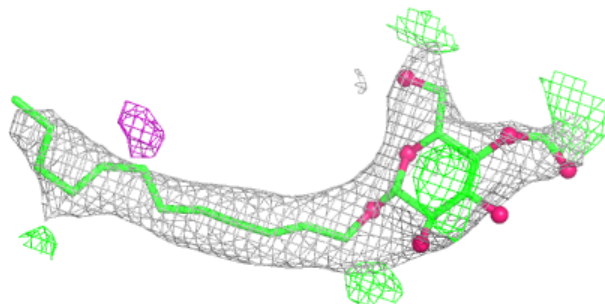


Electron density around LMG c 521:

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

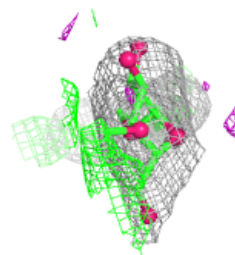
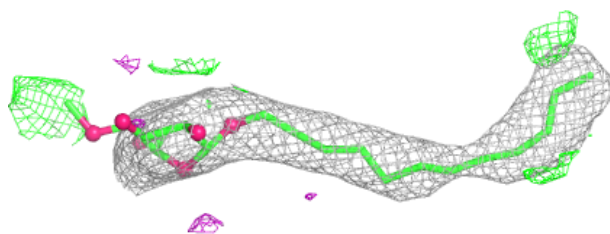
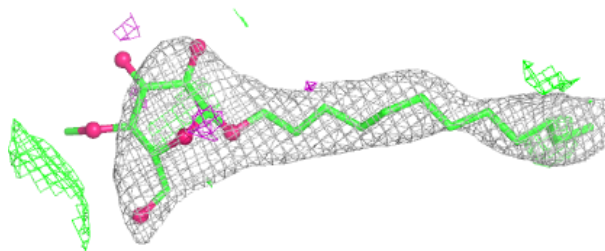
**Electron density around LMT t 102:**

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

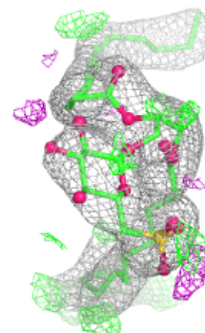
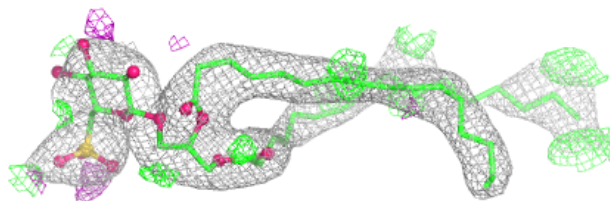
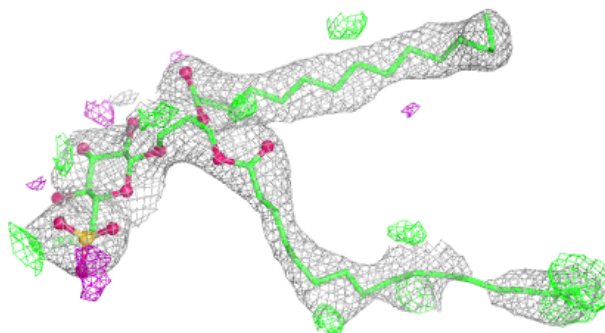


Electron density around LMT t 101:

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

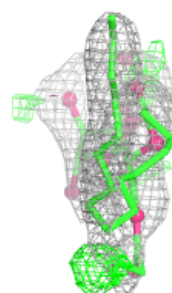
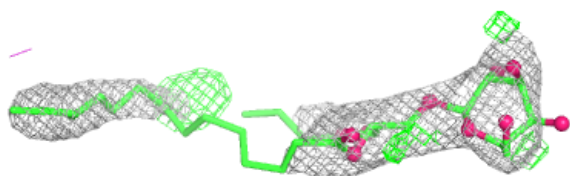
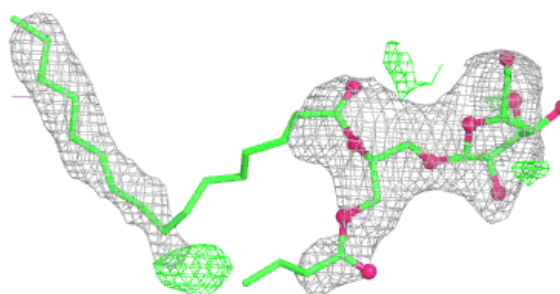
**Electron density around SQD A 410:**

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

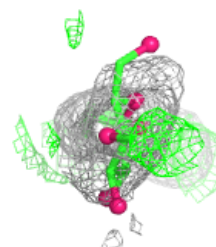
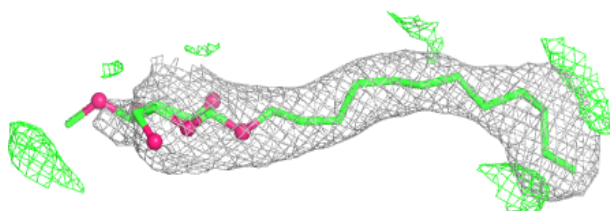
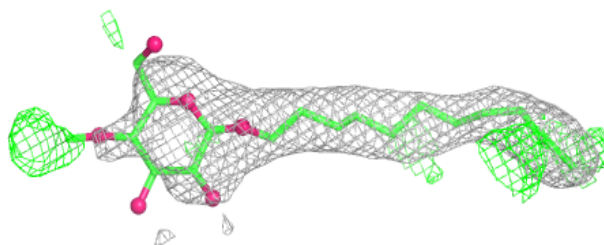


Electron density around LMG z 101:

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

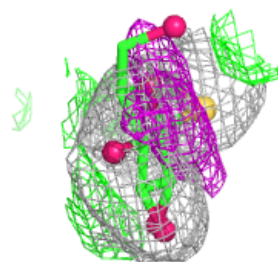
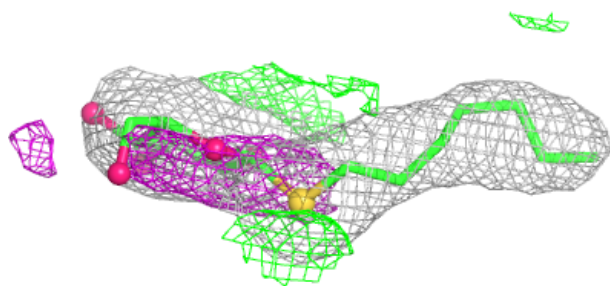
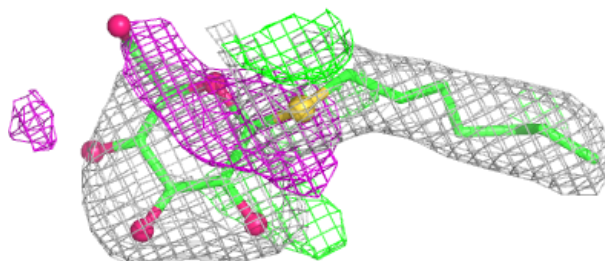
**Electron density around LMT b 627:**

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

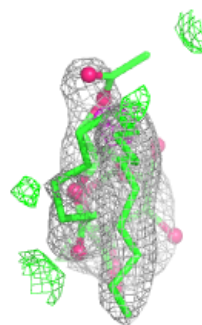
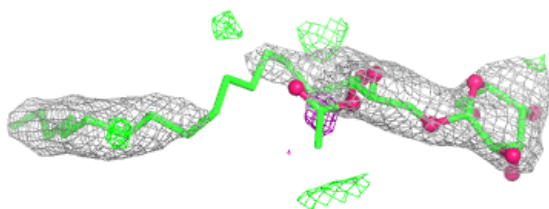
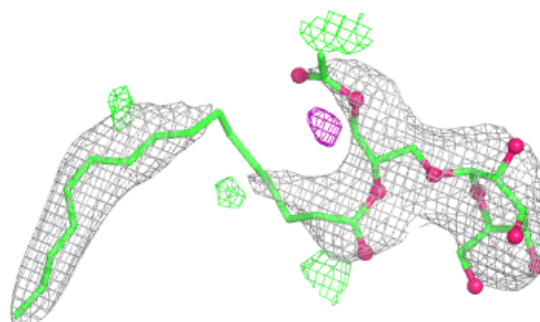


Electron density around HTG B 622:

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

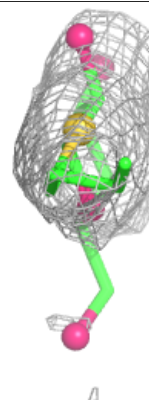
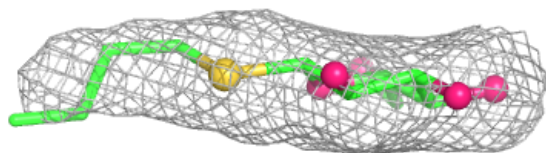
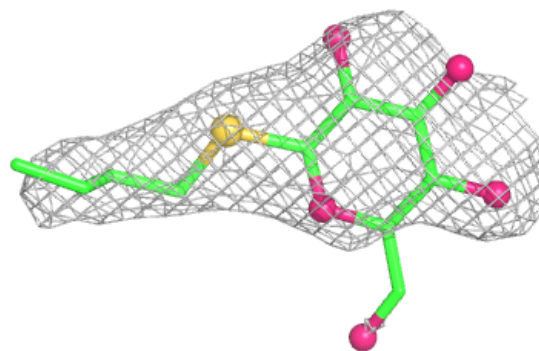
**Electron density around LMG C 526:**

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

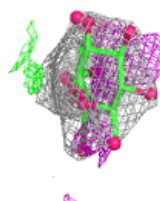
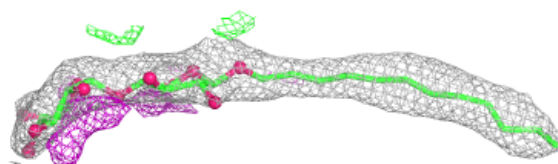
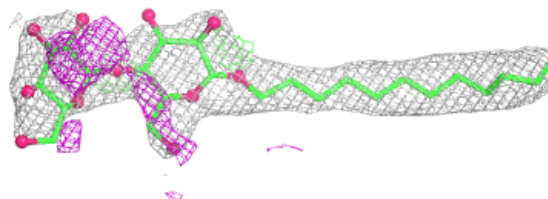


Electron density around HTG d 408:

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

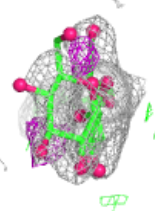
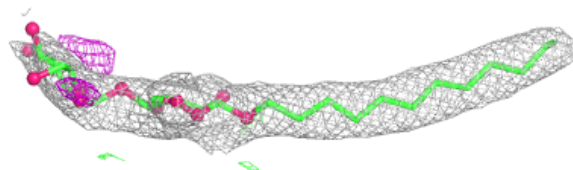
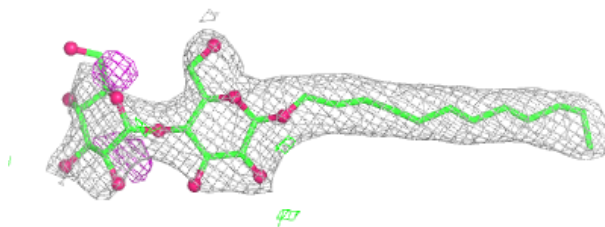
**Electron density around LMT m 103:**

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

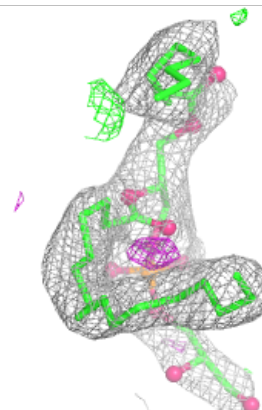
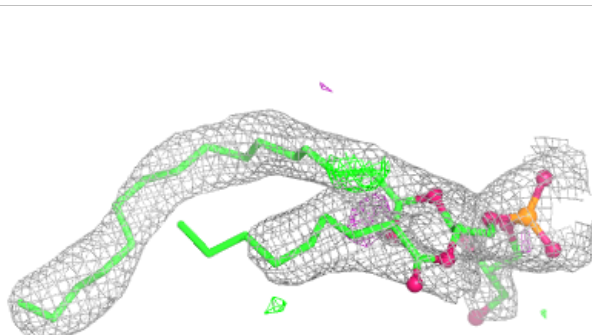
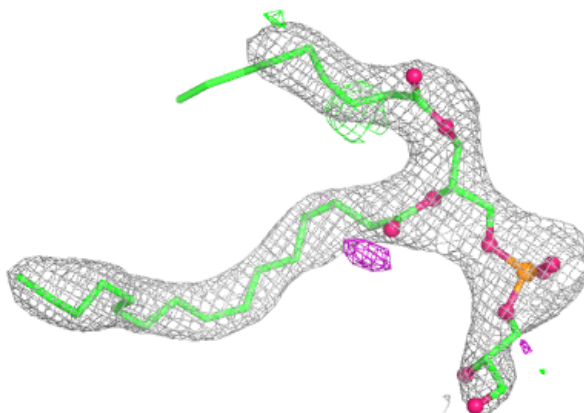


Electron density around LMT M 101:

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

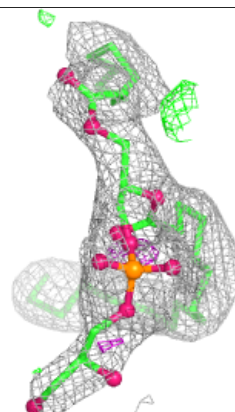
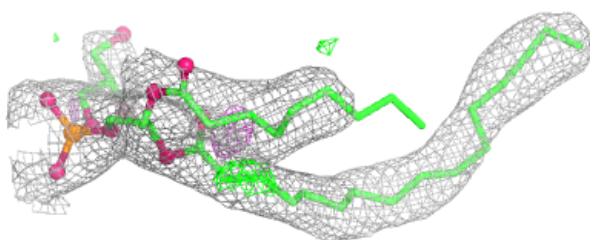
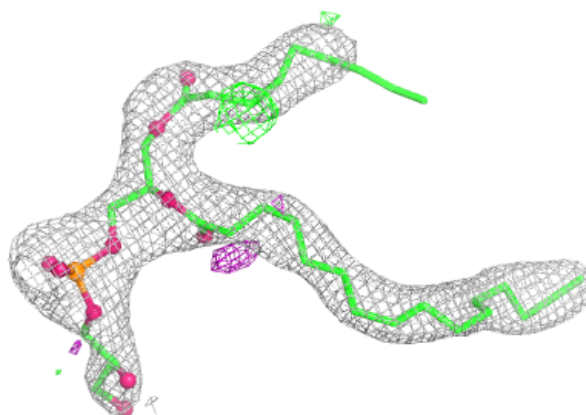
**Electron density around LHG E 101 (A):**

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

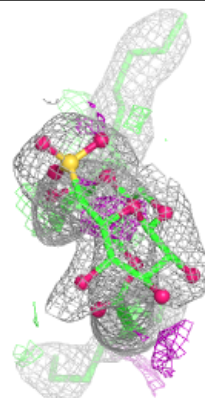
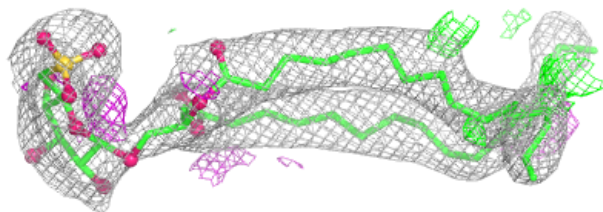
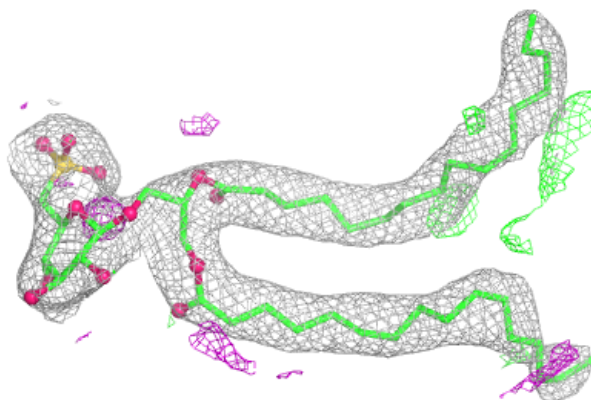


Electron density around LHG E 101 (B):

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

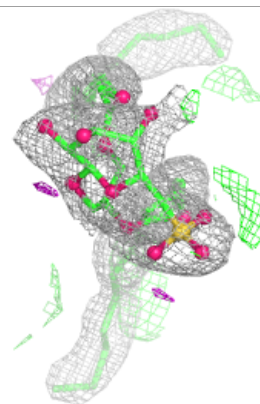
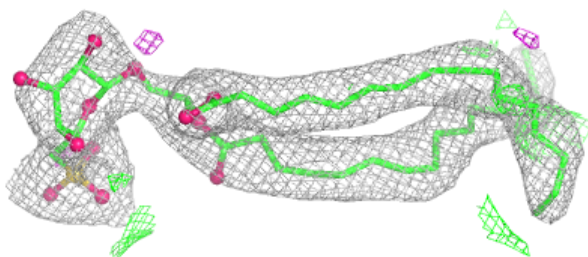
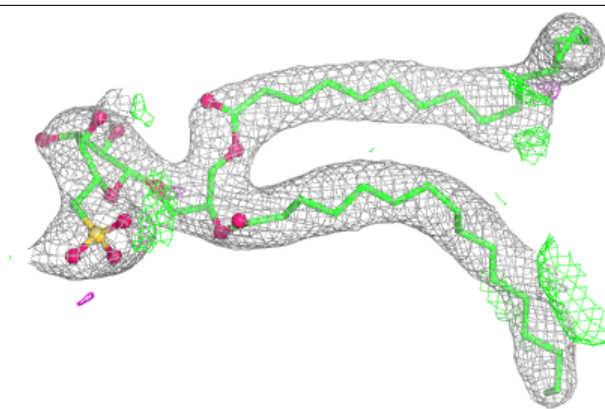
**Electron density around SQD b 620:**

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

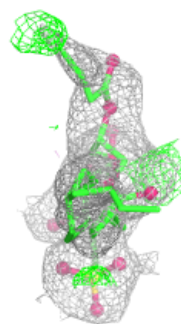
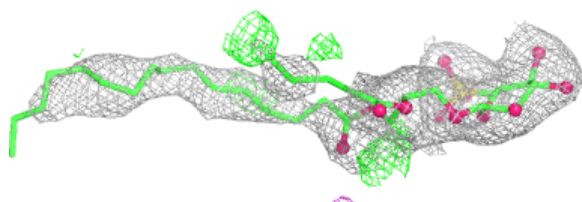
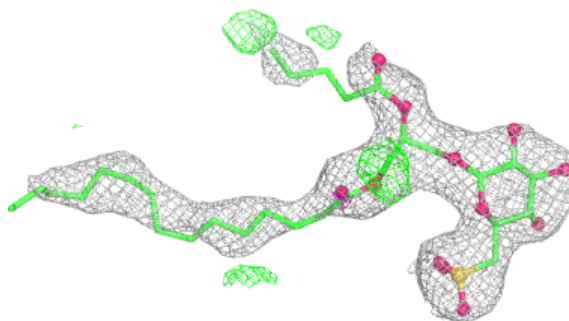


Electron density around SQD B 620:

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

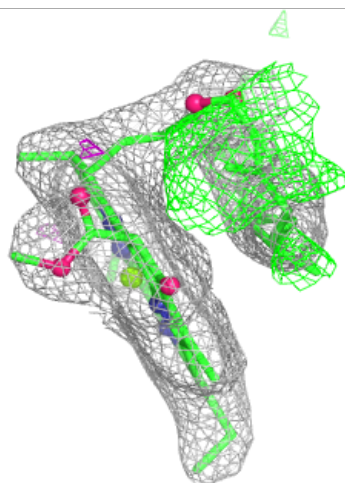
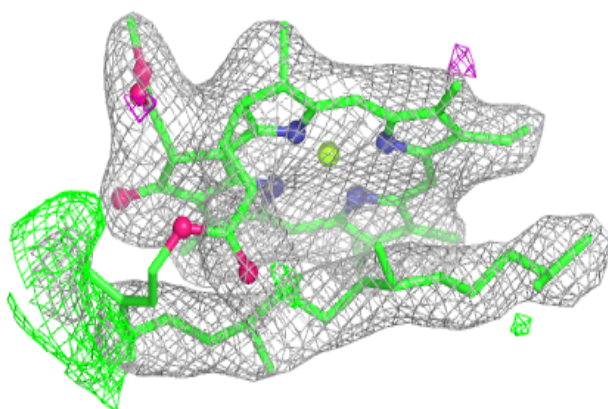
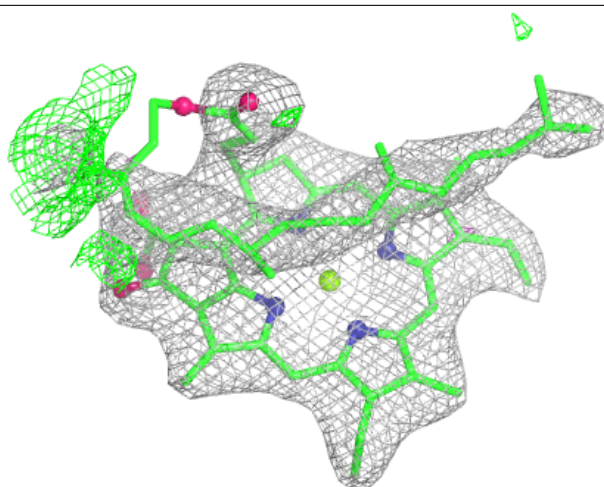
**Electron density around SQD F 103:**

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



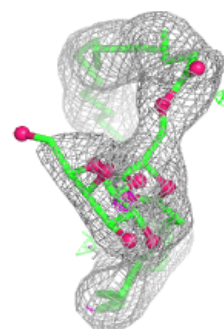
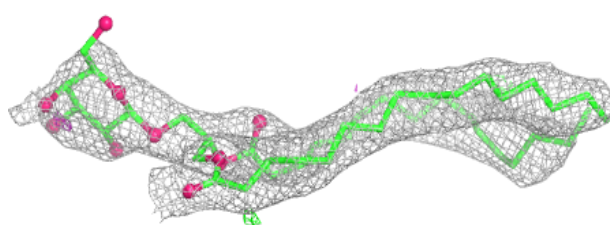
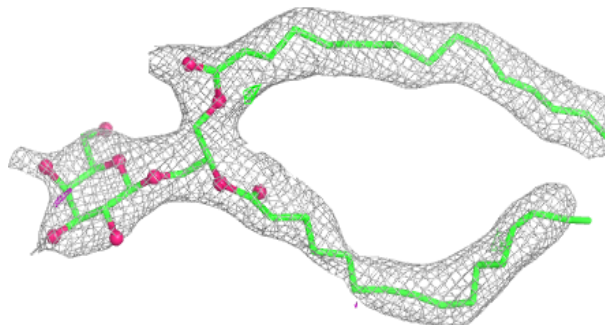
Electron density around CLA b 601:

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

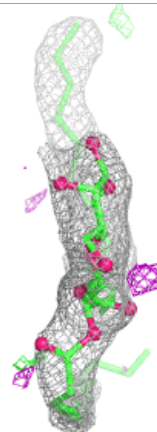
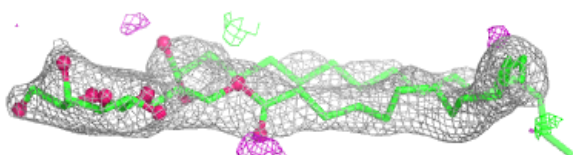
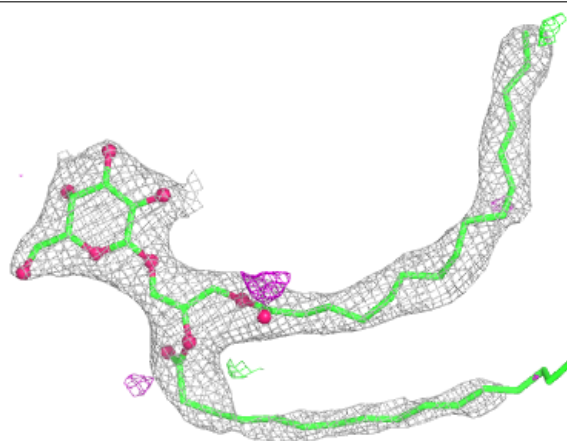


Electron density around LMG a 417:

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

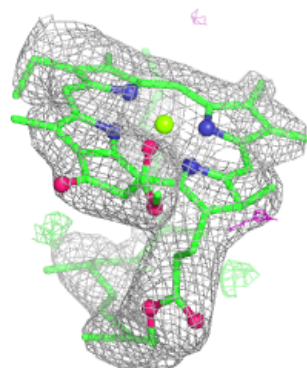
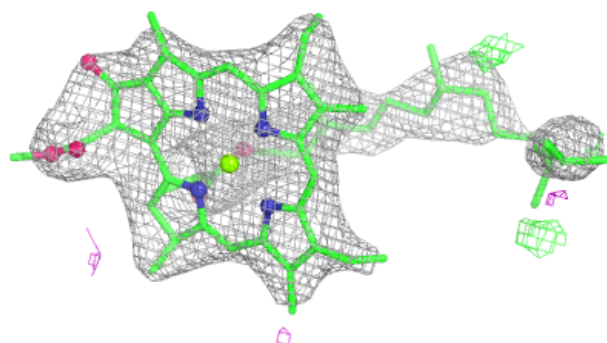
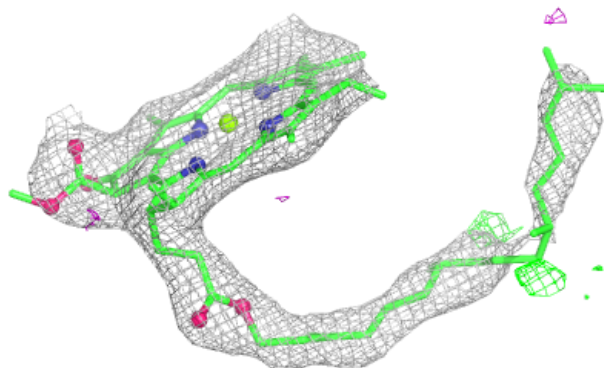
**Electron density around LMG c 520:**

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

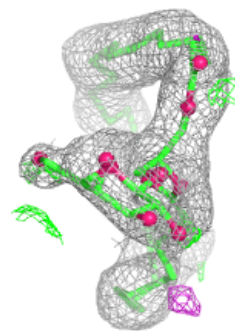
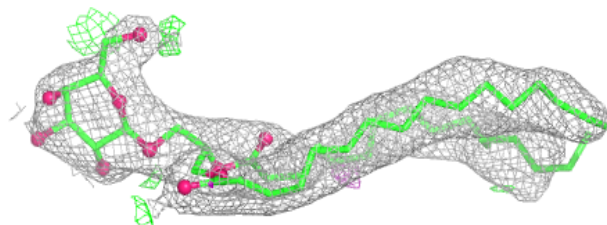
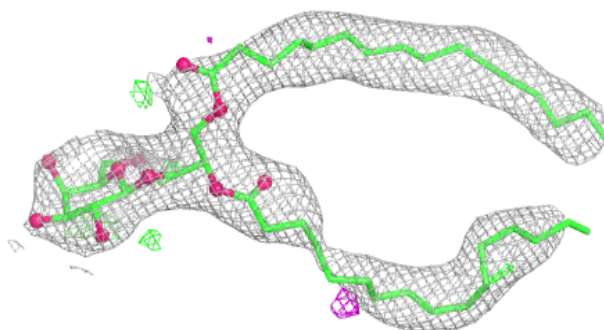


Electron density around CLA c 514:

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

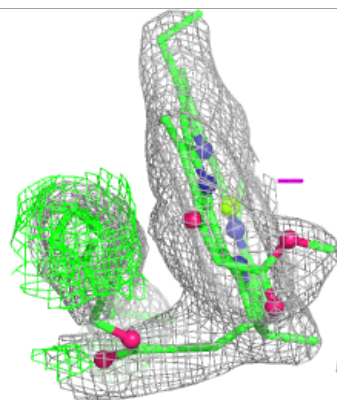
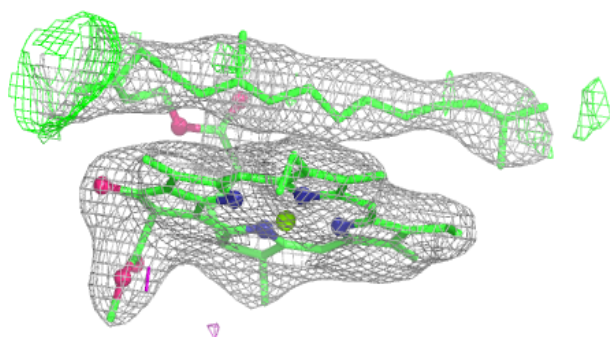
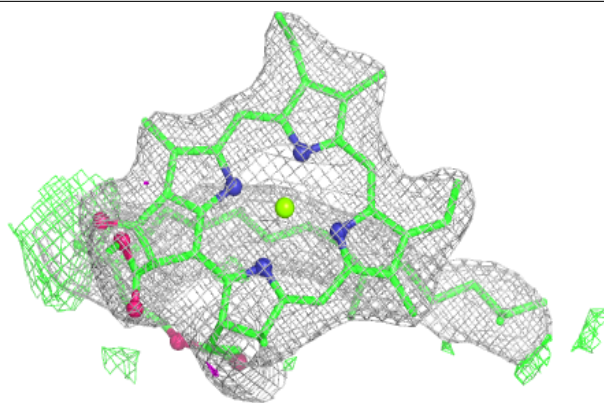
**Electron density around LMG C 502:**

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

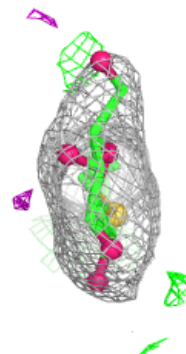
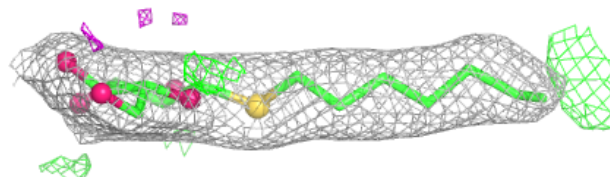
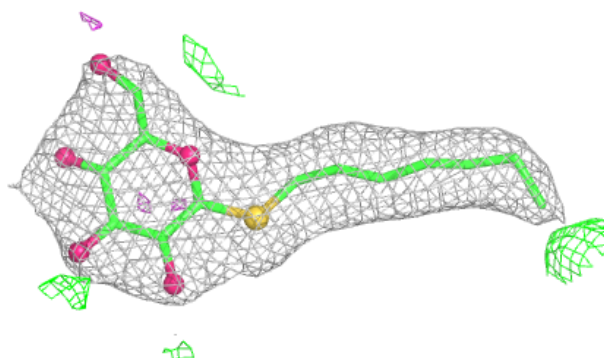


Electron density around CLA B 601:

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

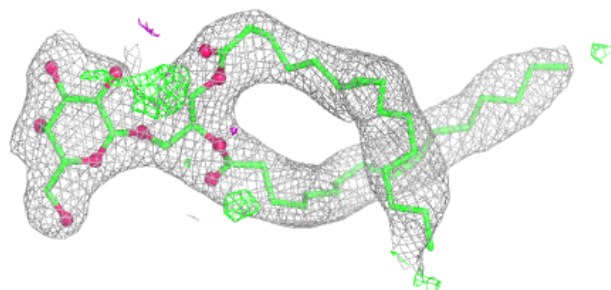
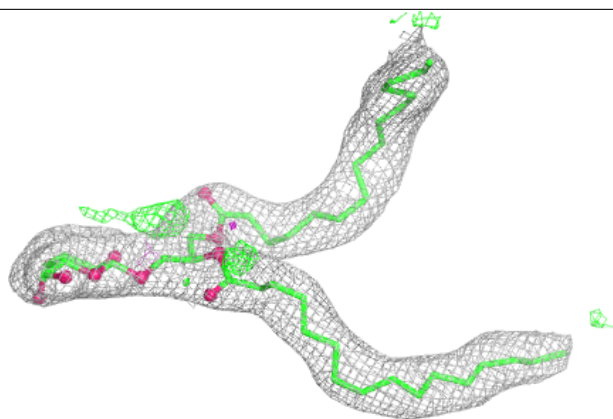
**Electron density around HTG B 625:**

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

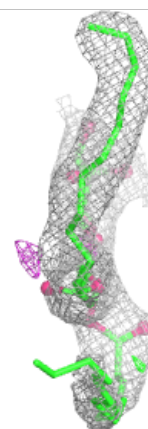
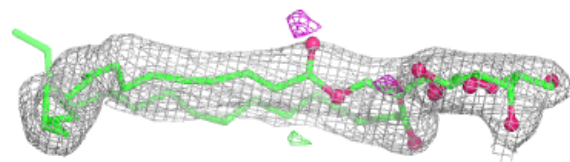
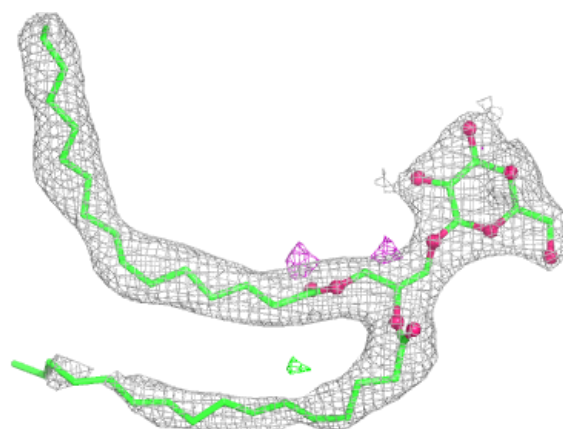


Electron density around LMG B 621:

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

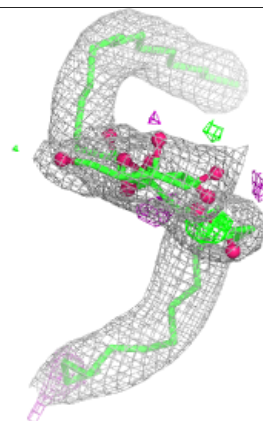
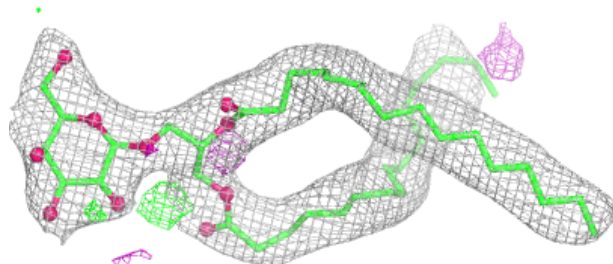
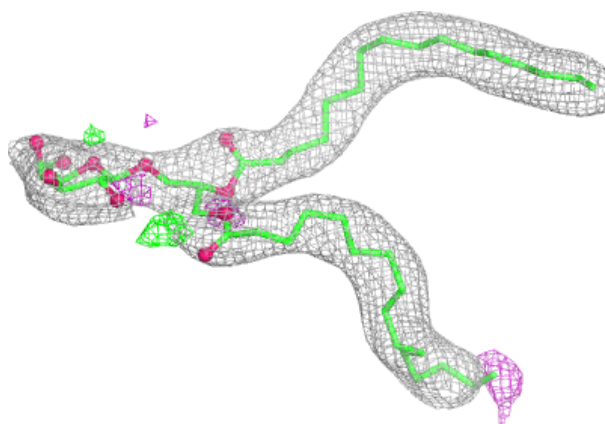
**Electron density around LMG C 521:**

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

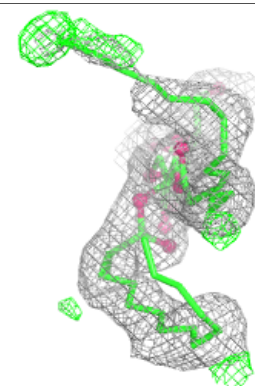
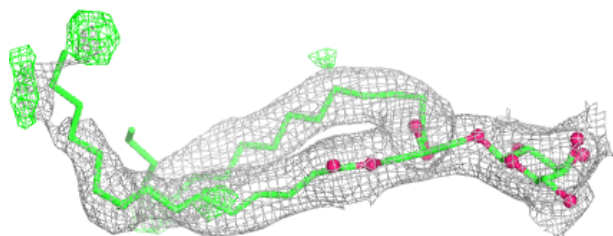
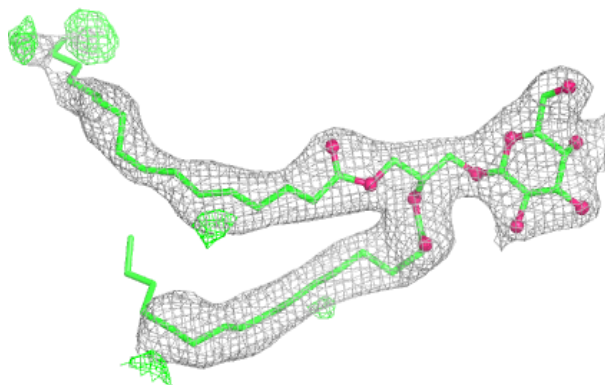


Electron density around LMG m 101:

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

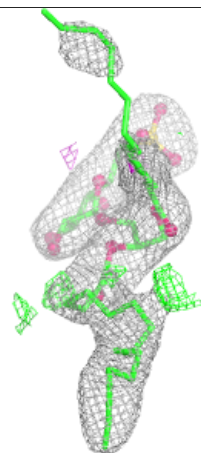
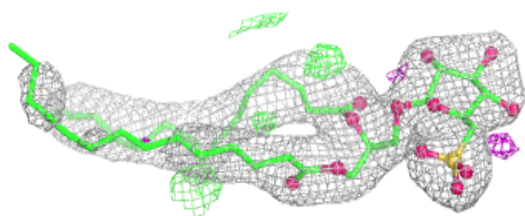
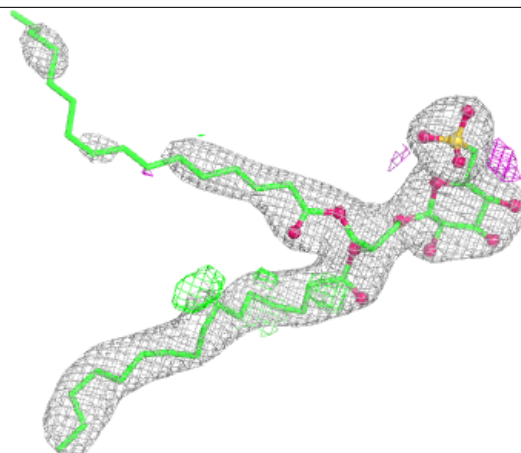
**Electron density around LMG D 413:**

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



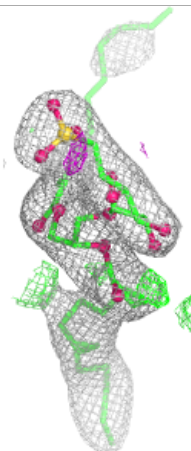
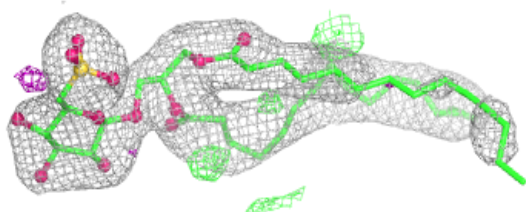
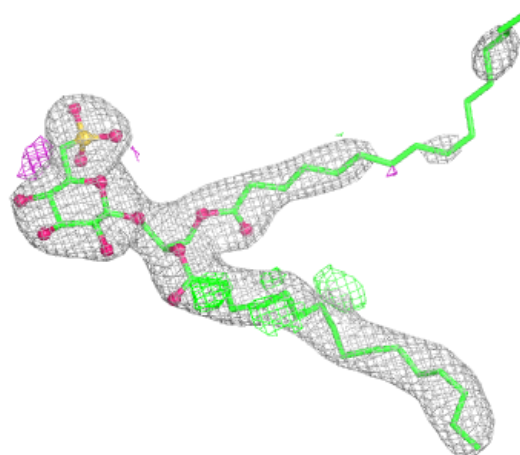
Electron density around SQD C 501 (A):

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



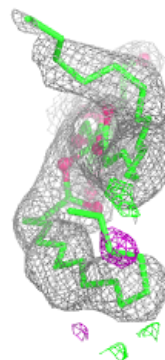
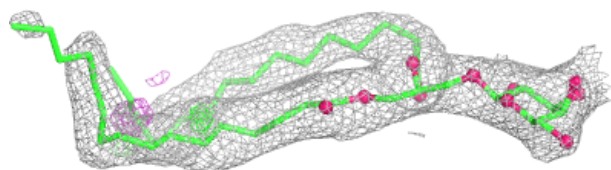
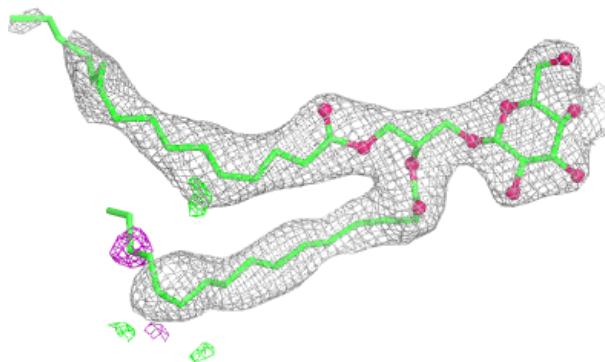
Electron density around SQD C 501 (B):

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



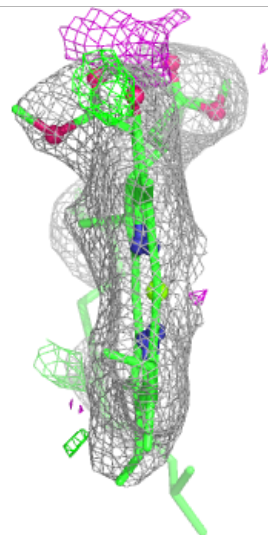
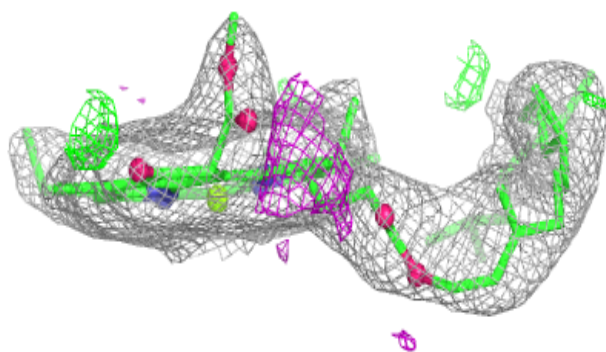
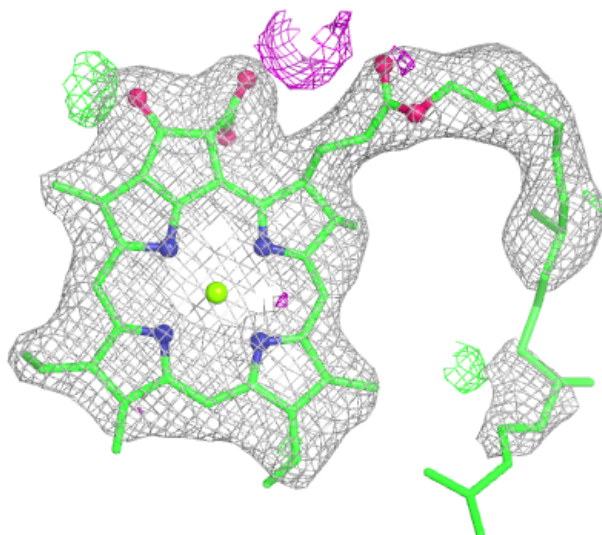
Electron density around LMG d 409:

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



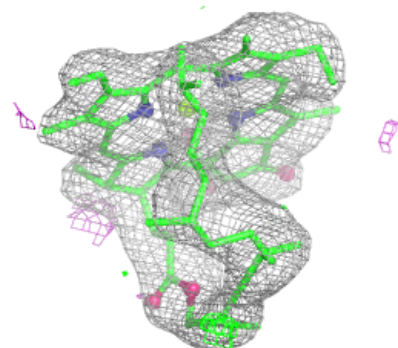
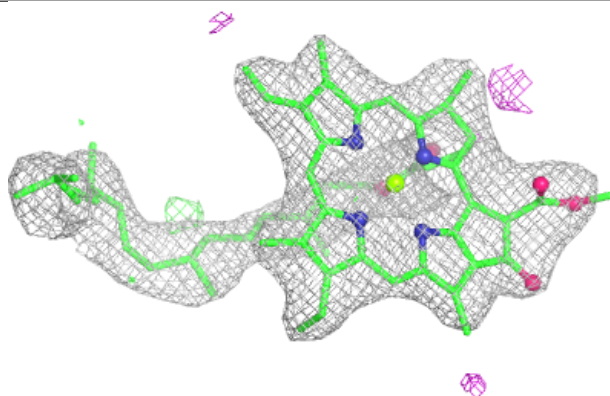
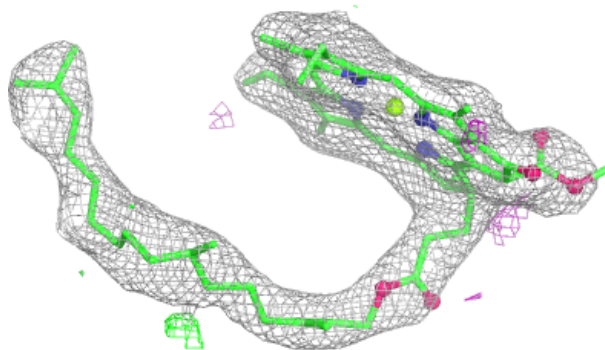
Electron density around CLA c 513:

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

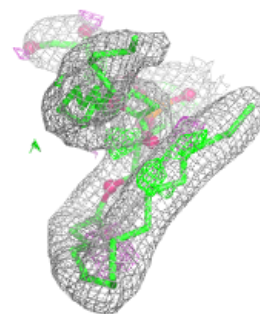
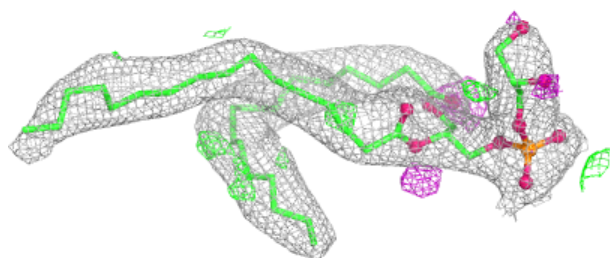
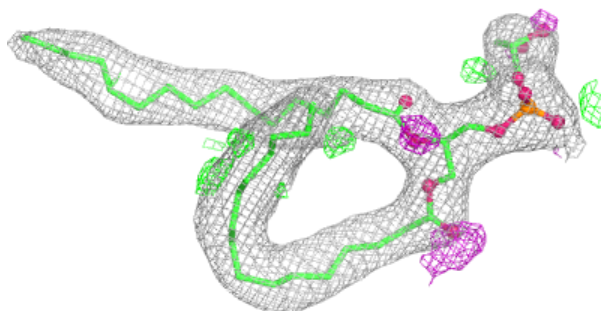


Electron density around CLA C 515:

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

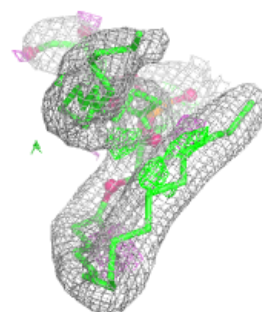
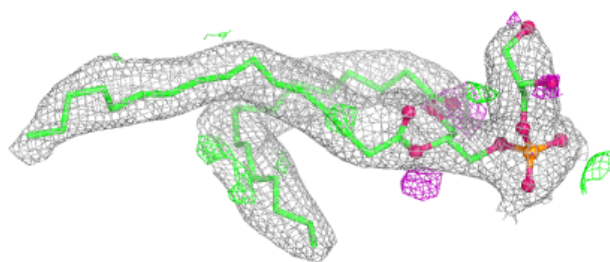
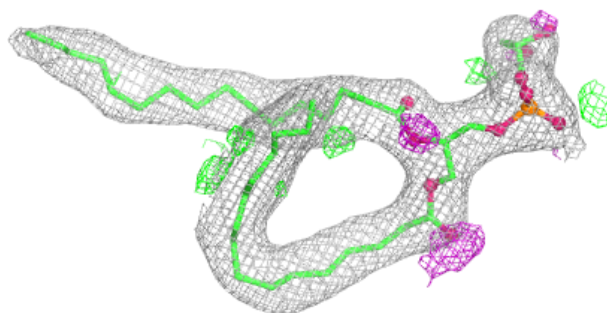
**Electron density around LHG A 416 (A):**

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

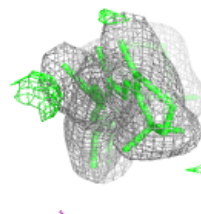
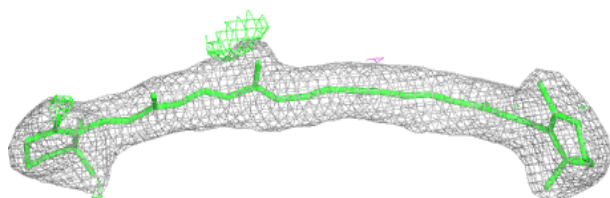
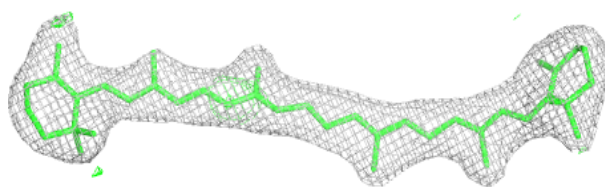


Electron density around LHG A 416 (B):

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

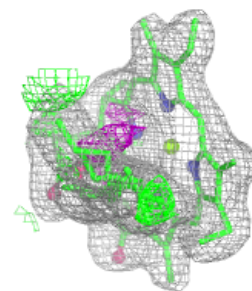
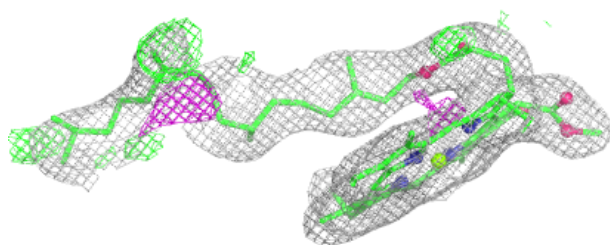
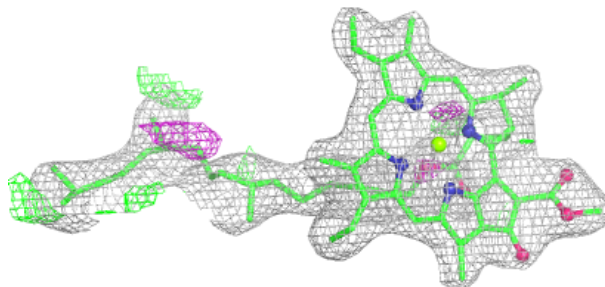
**Electron density around BCR T 102:**

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

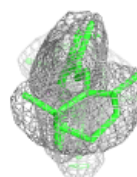
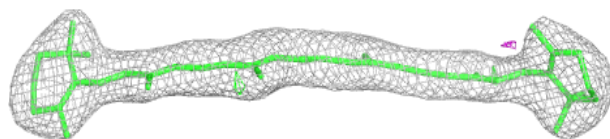
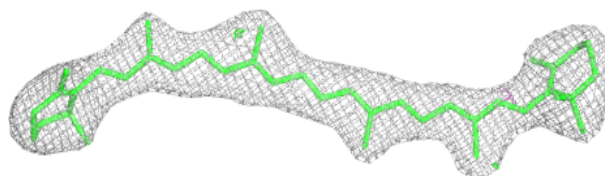


Electron density around CLA B 614:

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

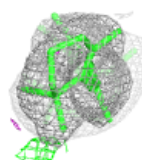
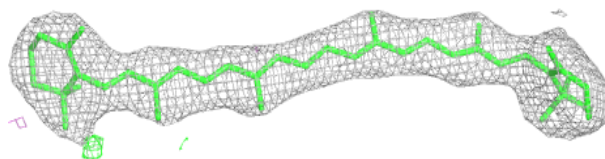
**Electron density around BCR Y 101:**

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

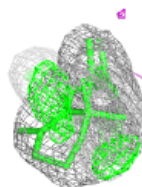
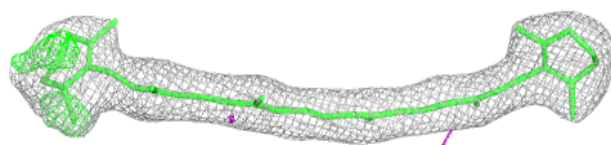
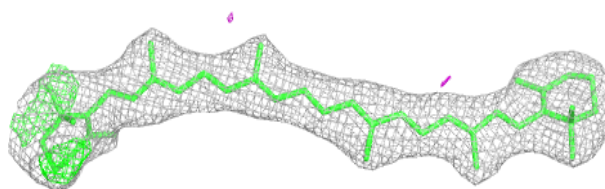


Electron density around BCR c 515:

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

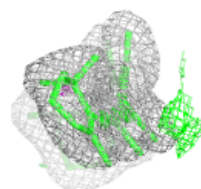
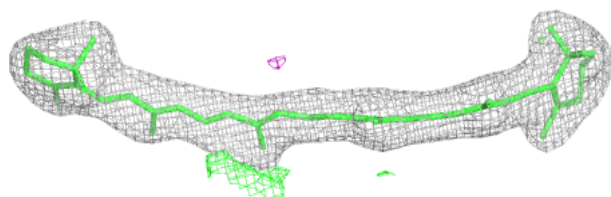
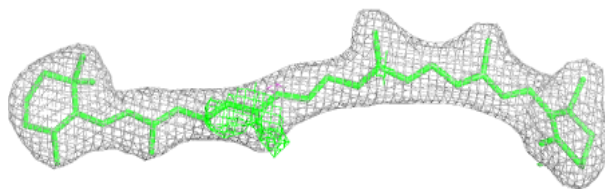
**Electron density around BCR d 403:**

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

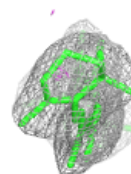
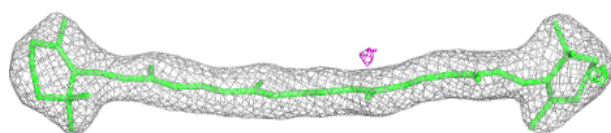
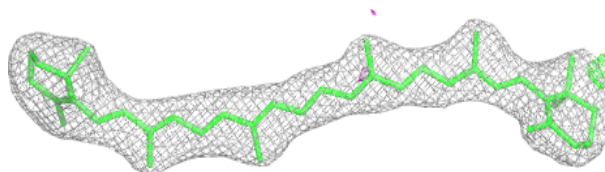


Electron density around BCR t 103:

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

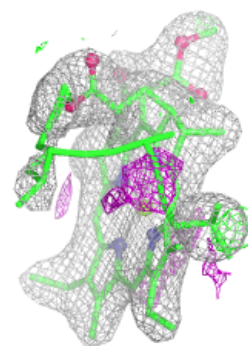
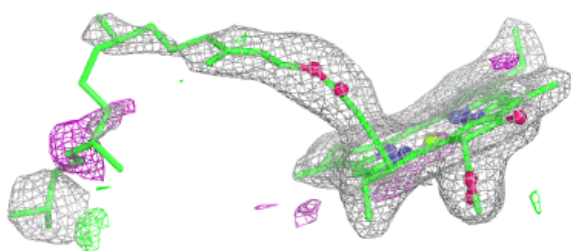
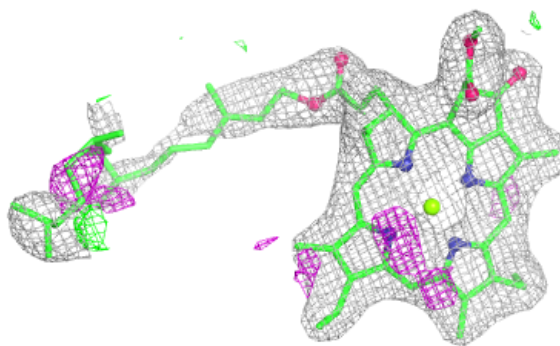
**Electron density around BCR y 101:**

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

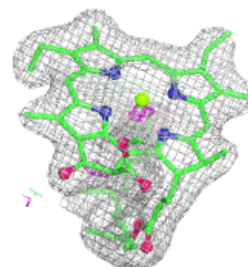
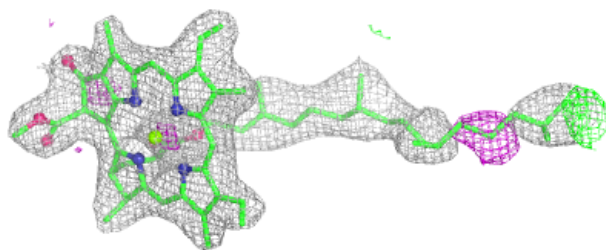
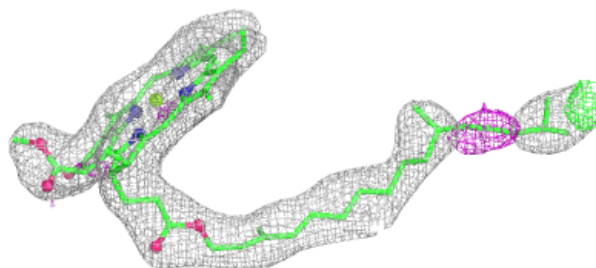


Electron density around CLA a 409:

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

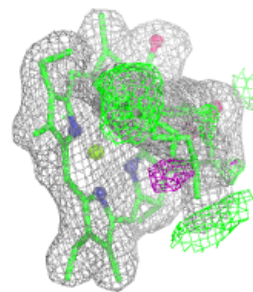
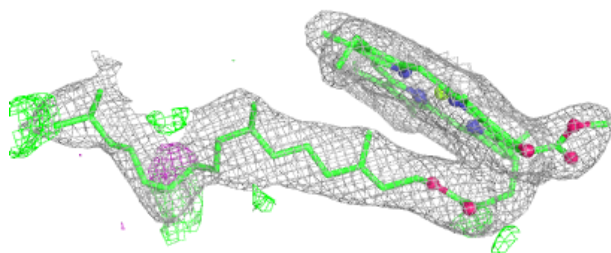
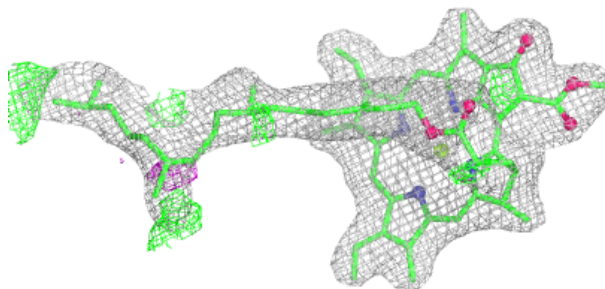
**Electron density around CLA C 506:**

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

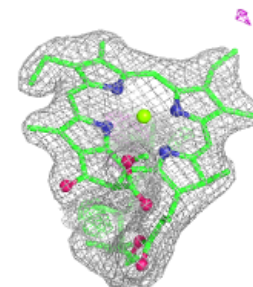
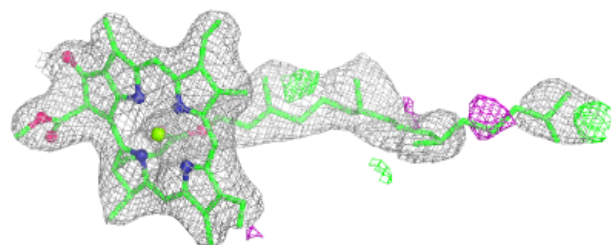
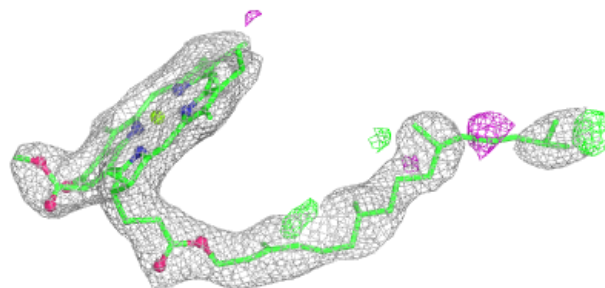


Electron density around CLA b 614:

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

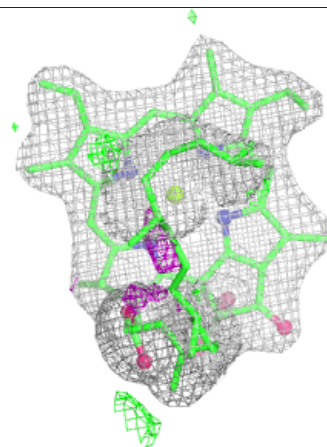
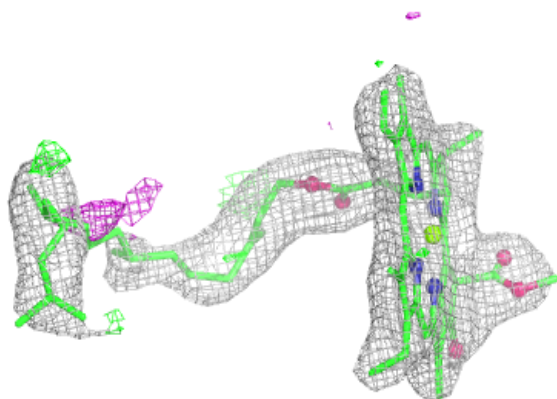
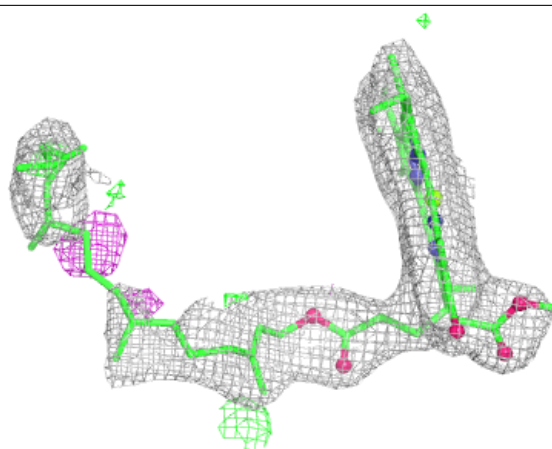
**Electron density around CLA c 505:**

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



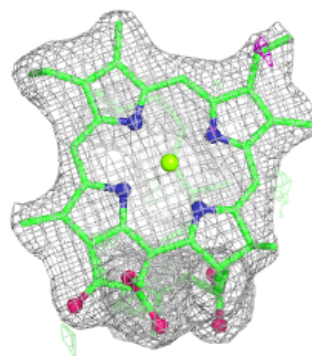
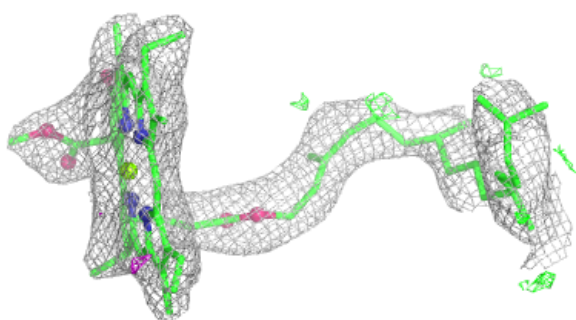
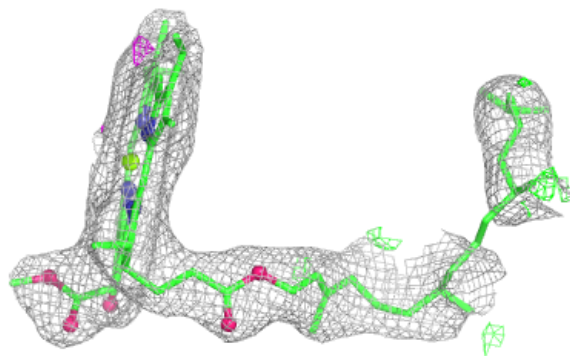
Electron density around CLA c 507:

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



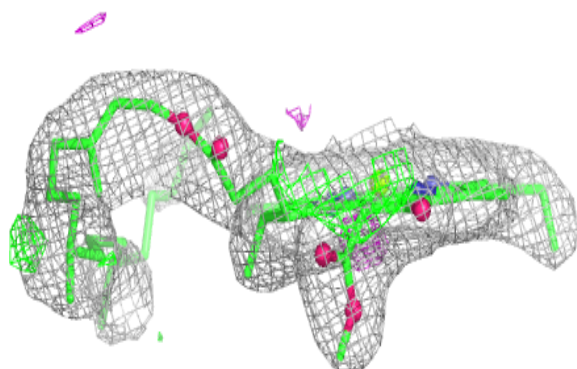
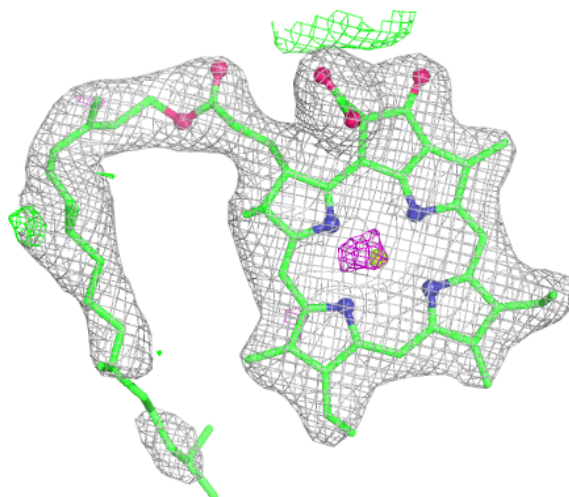
Electron density around CLA C 508:

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



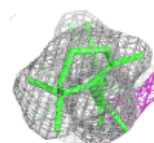
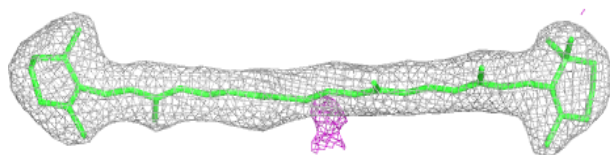
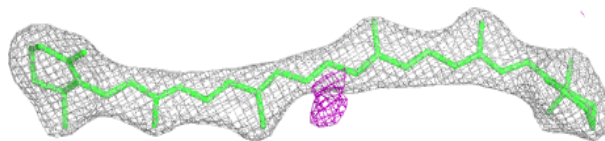
Electron density around CLA C 514:

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



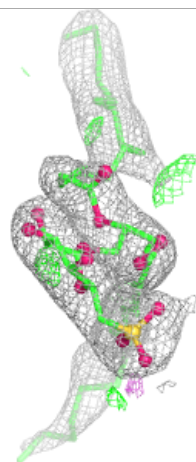
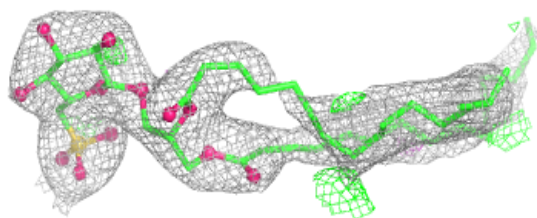
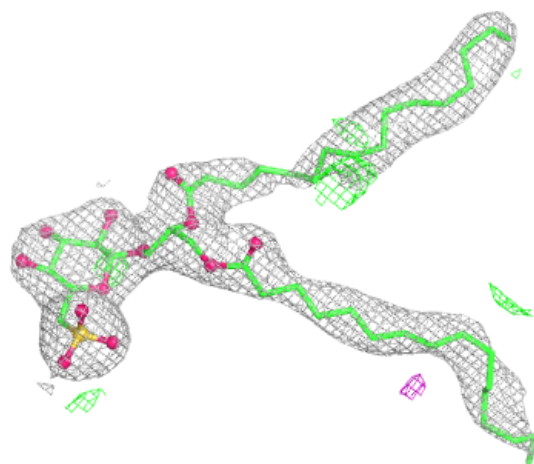
Electron density around BCR C 516:

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



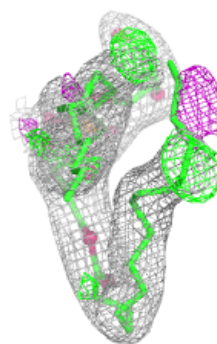
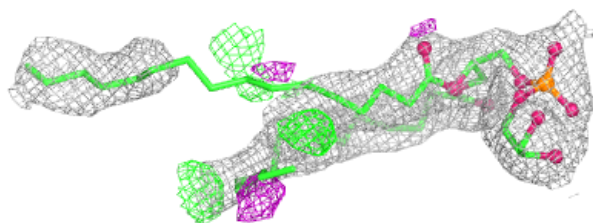
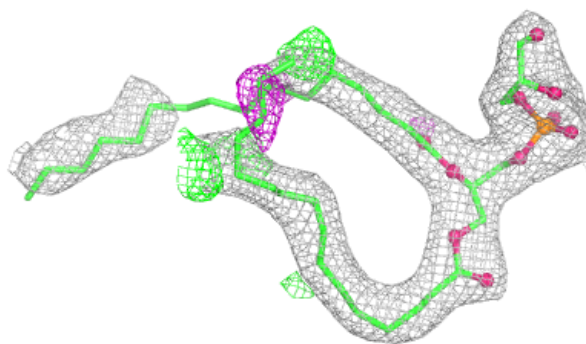
Electron density around SQD a 411 (A):

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

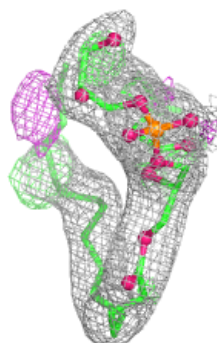
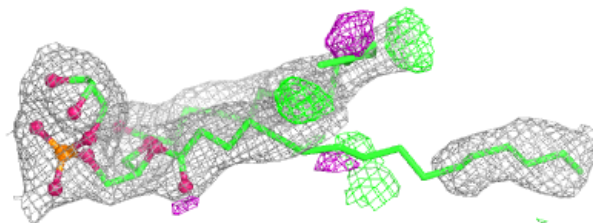
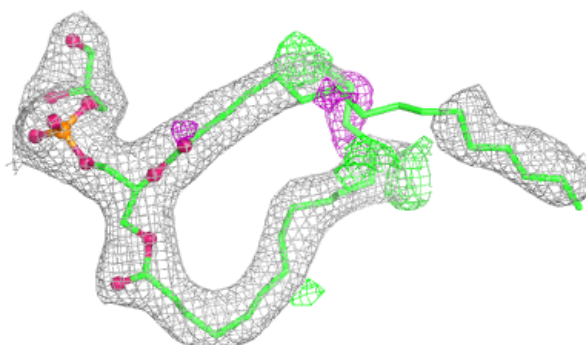


Electron density around LHG D 409 (A):

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

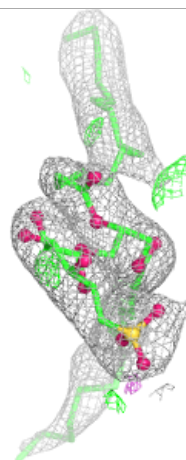
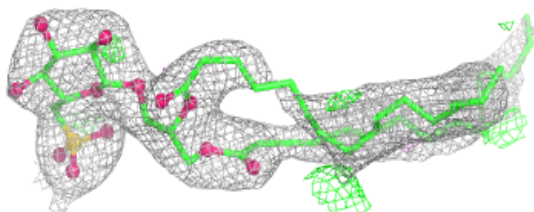
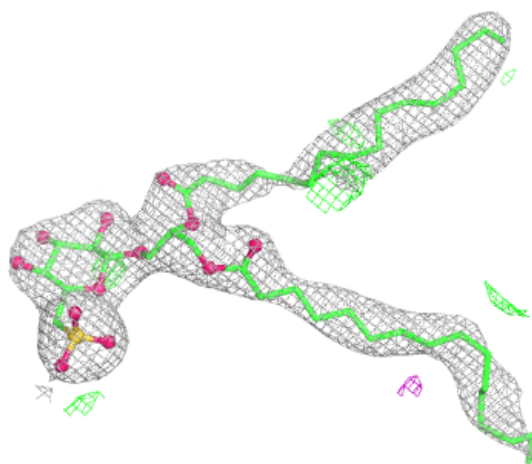
**Electron density around LHG D 409 (B):**

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



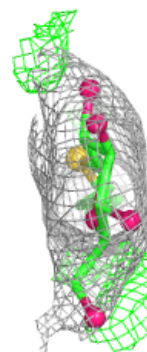
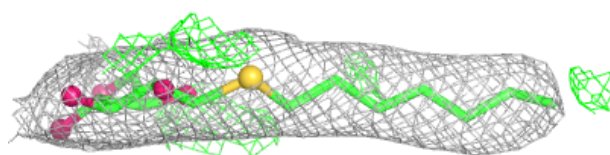
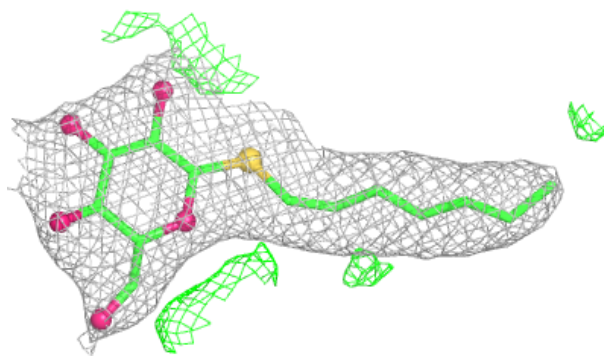
Electron density around SQD a 411 (B):

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

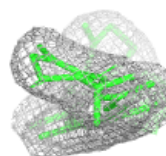
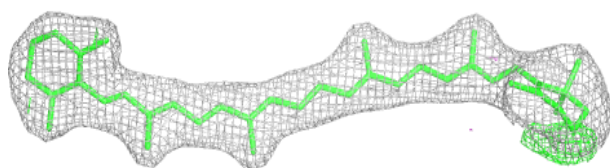
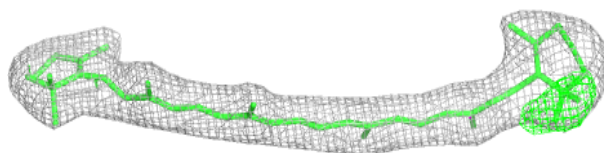


Electron density around HTG b 625:

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

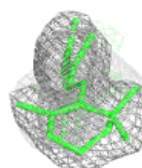
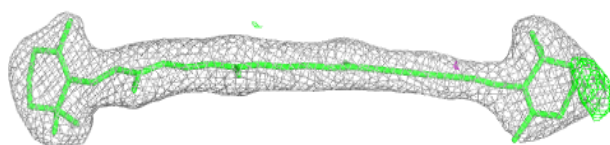
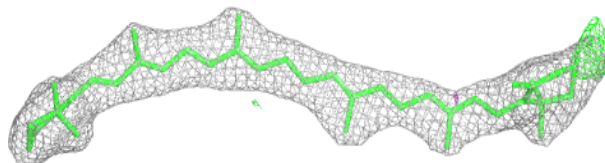
**Electron density around BCR D 406:**

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

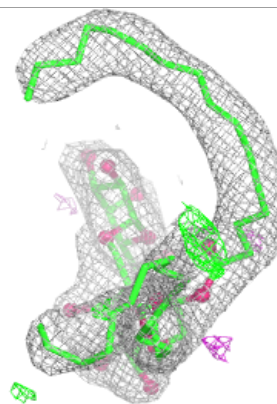
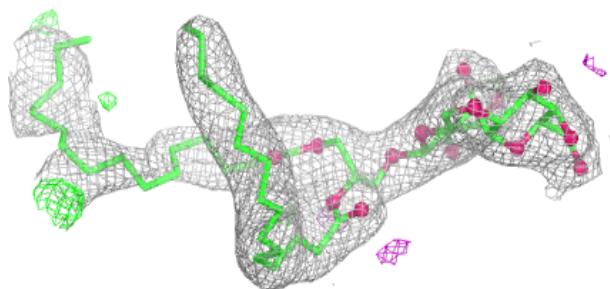
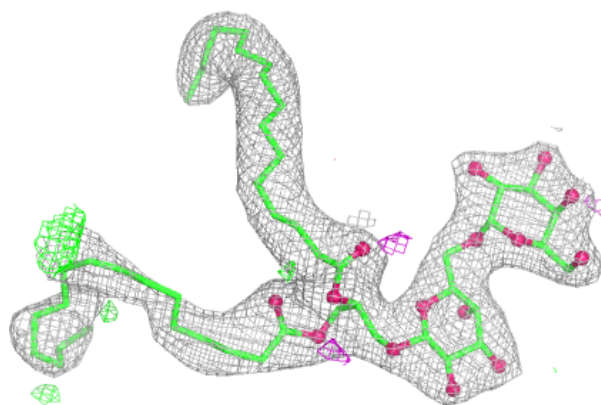


Electron density around BCR H 101:

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

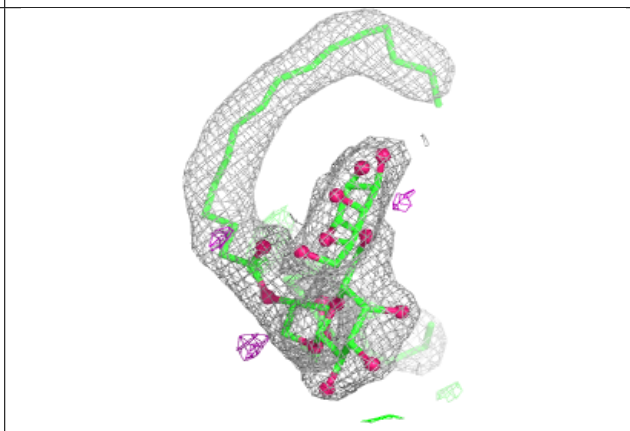
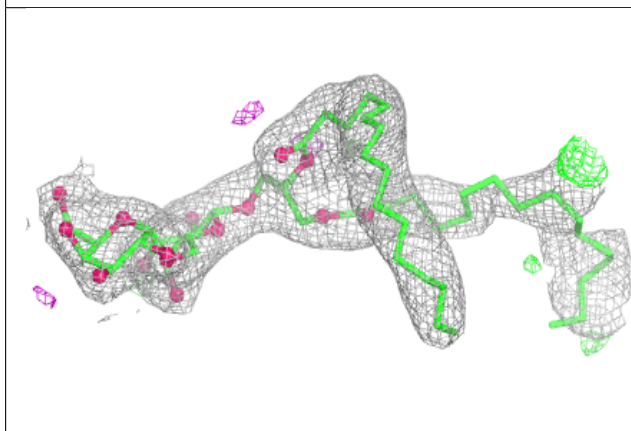
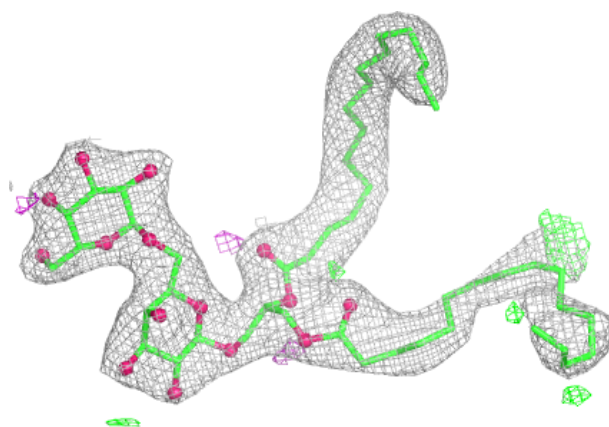
**Electron density around DGD C 519 (A):**

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

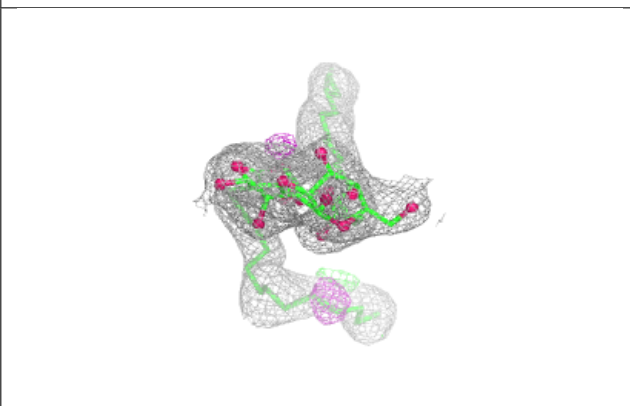
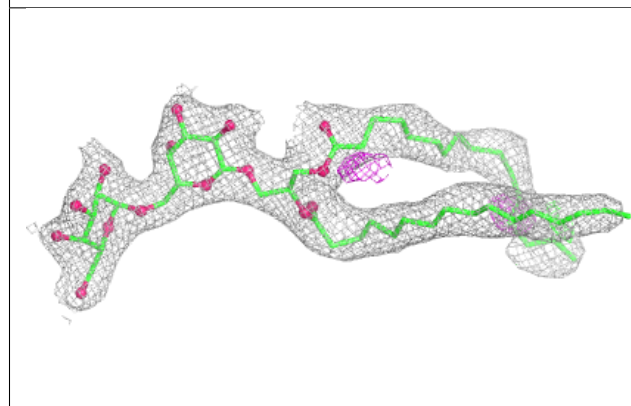
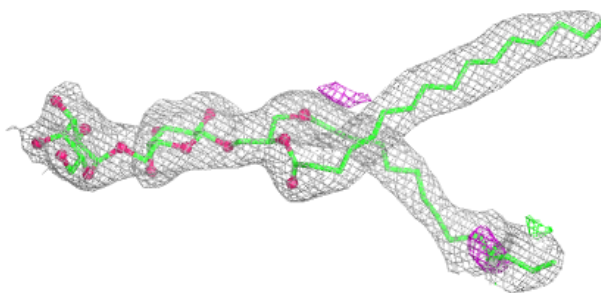


Electron density around DGD C 519 (B):

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

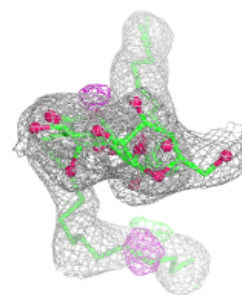
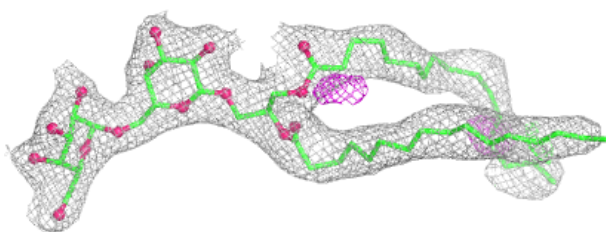
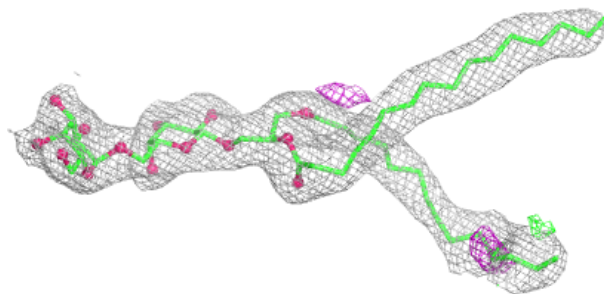
**Electron density around DGD c 517 (A):**

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

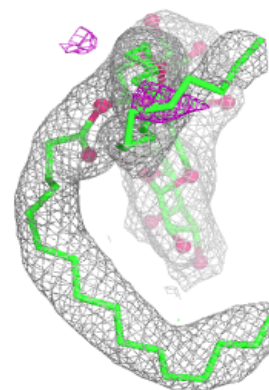
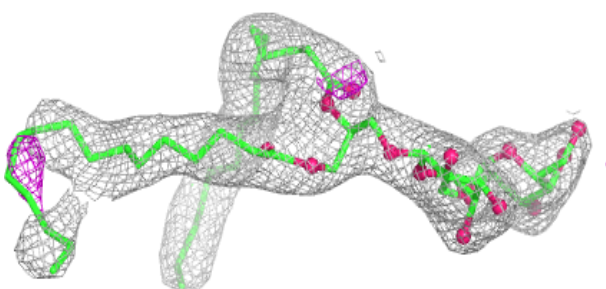
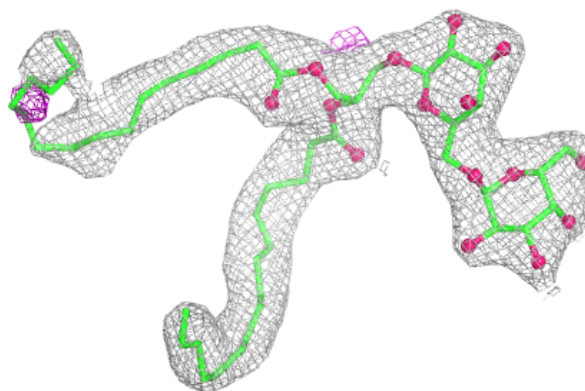


Electron density around DGD c 517 (B):

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

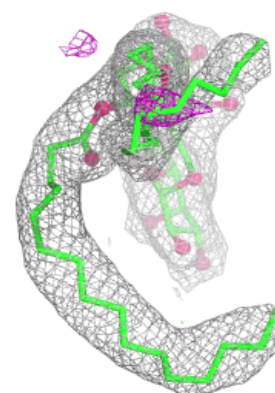
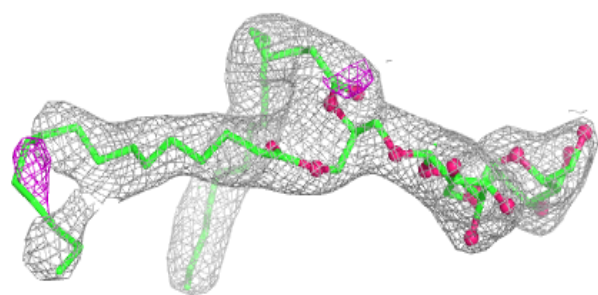
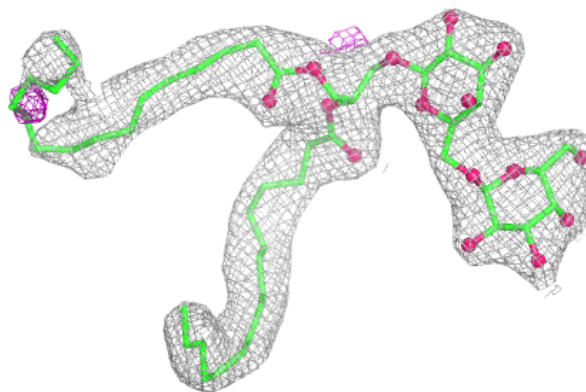
**Electron density around DGD c 518 (A):**

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

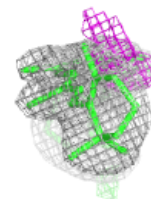
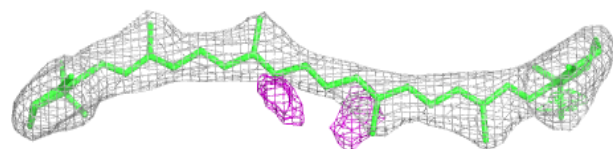
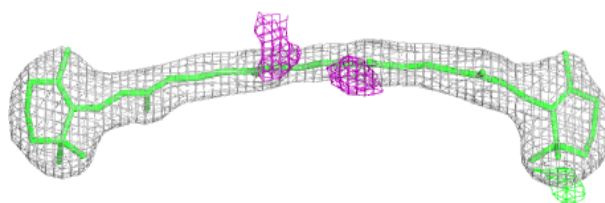


Electron density around DGD c 518 (B):

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

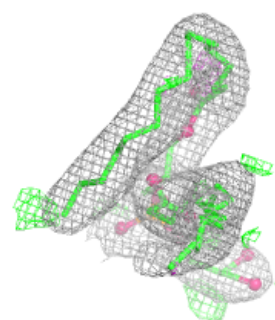
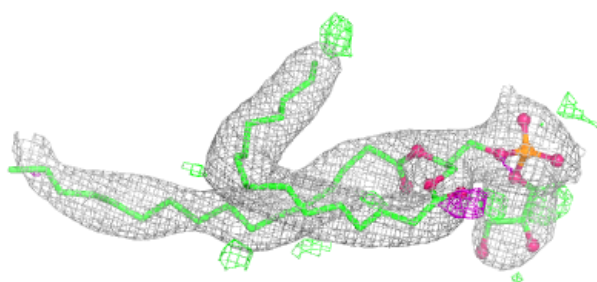
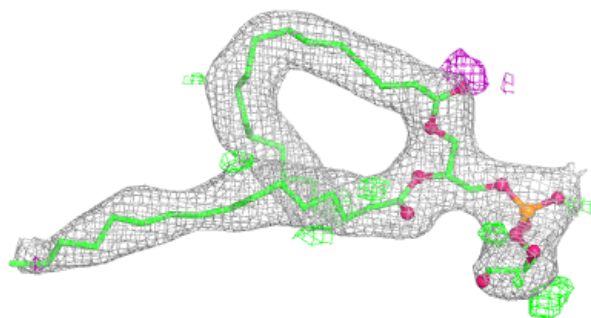
**Electron density around BCR K 102:**

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

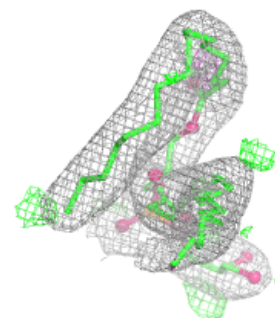
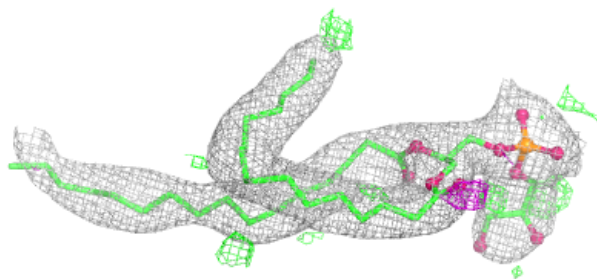
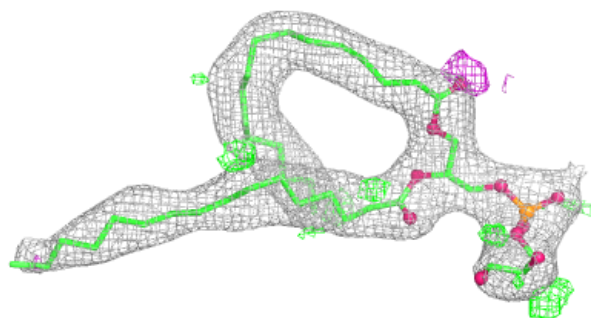


Electron density around LHG d 411 (A):

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

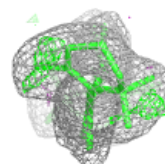
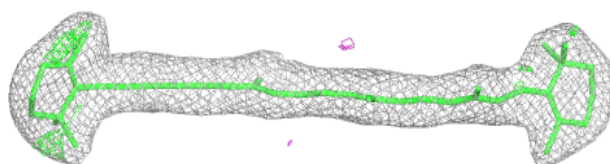
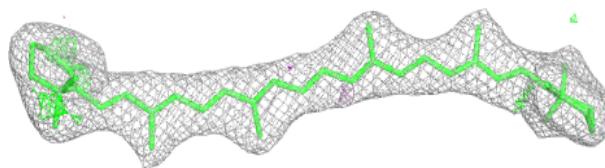
**Electron density around LHG d 411 (B):**

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

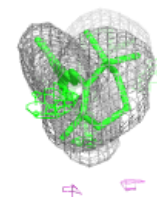
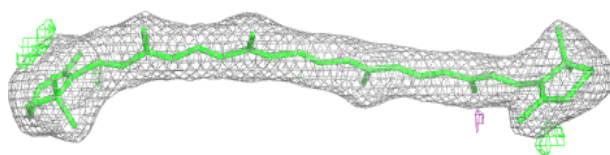
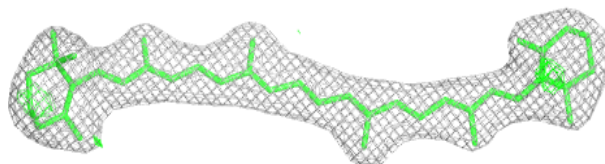


Electron density around BCR A 408:

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

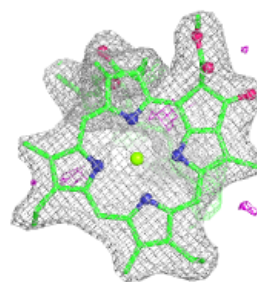
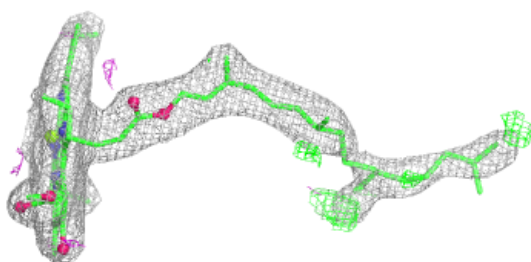
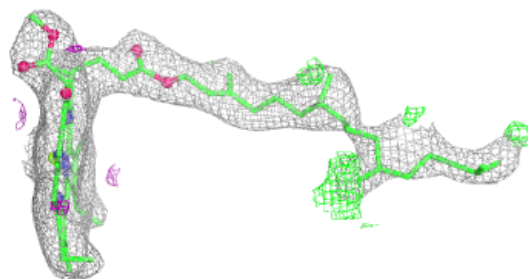
**Electron density around BCR B 619:**

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

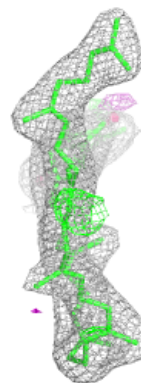
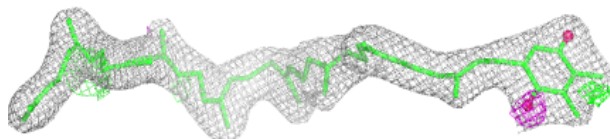
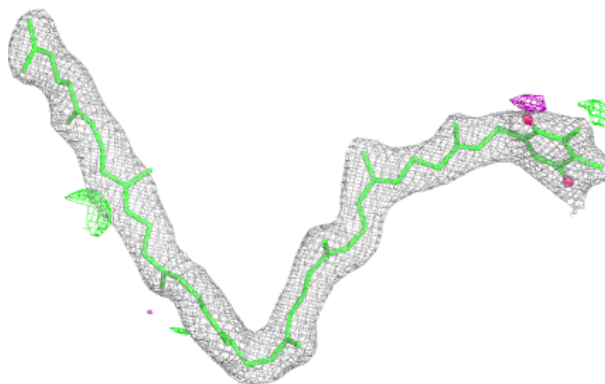


Electron density around CLA b 606:

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

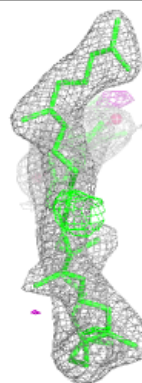
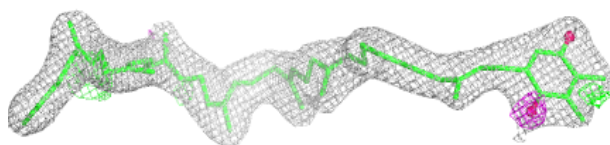
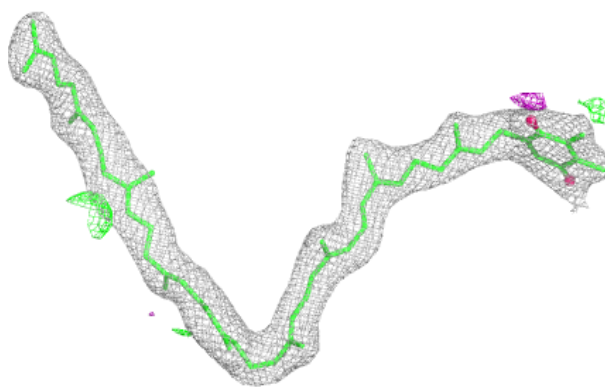
**Electron density around PL9 D 407 (A):**

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

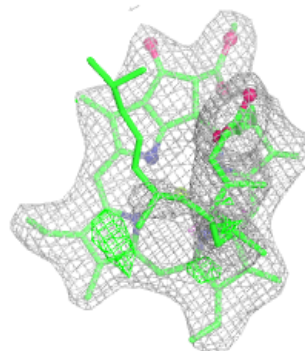
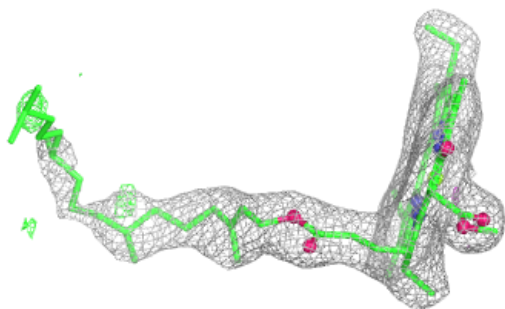
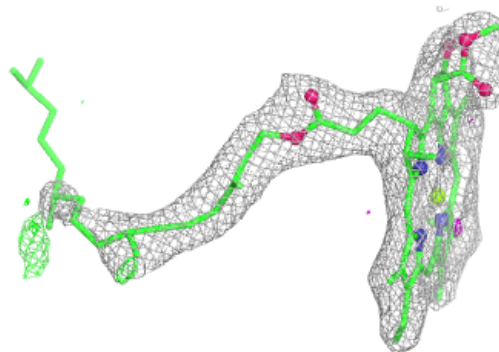


Electron density around PL9 D 407 (B):

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

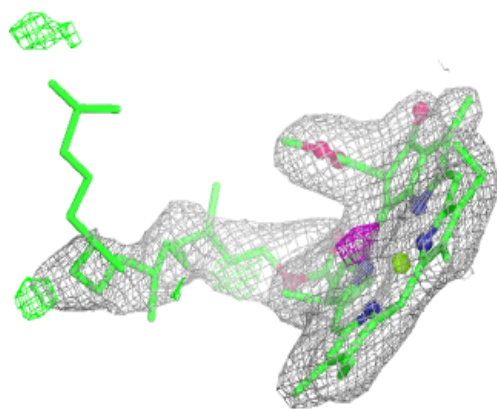
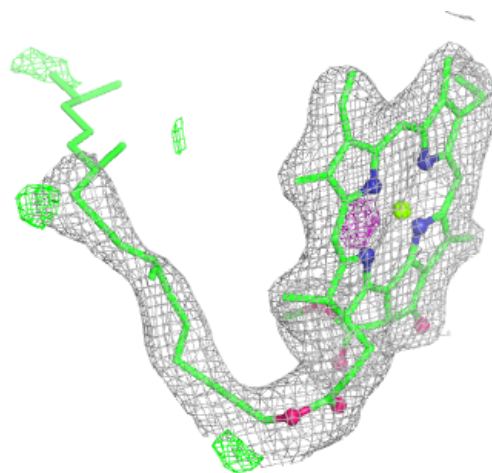
**Electron density around CLA D 405:**

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



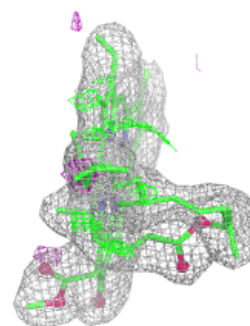
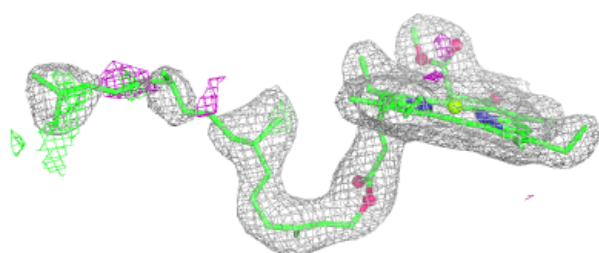
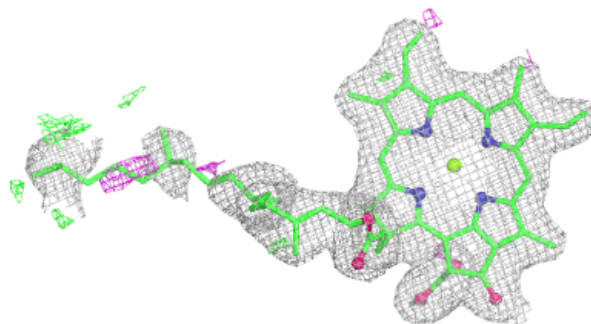
Electron density around CLA b 616:

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

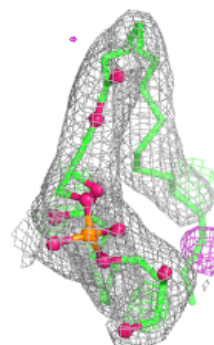
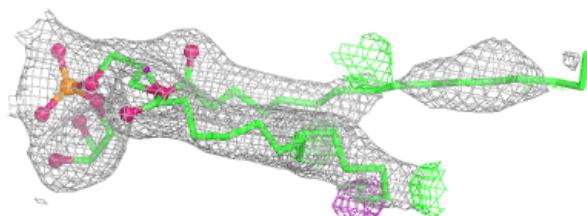
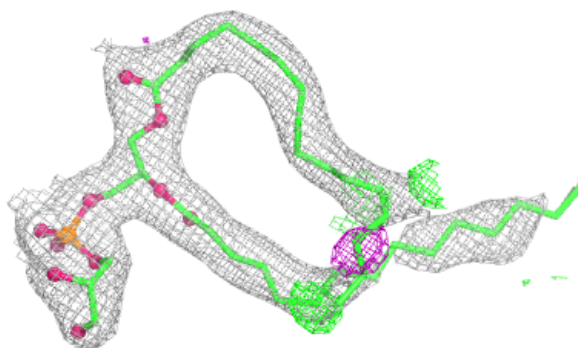


Electron density around CLA a 407 (A):

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

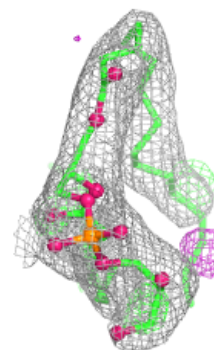
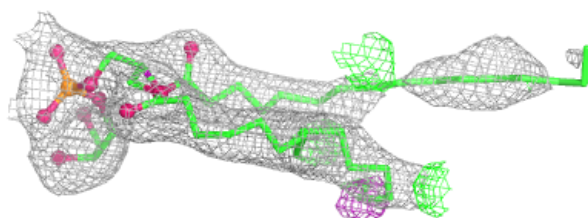
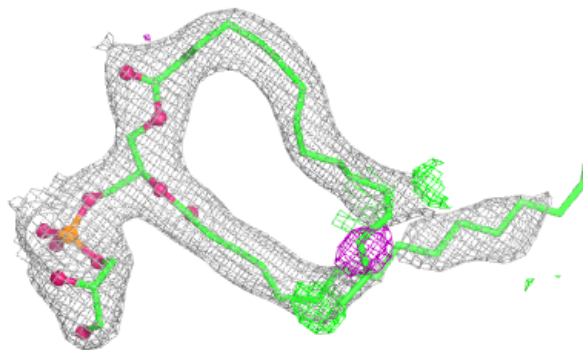
**Electron density around LHG d 406 (A):**

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

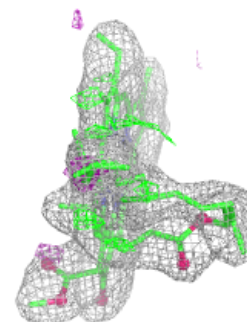
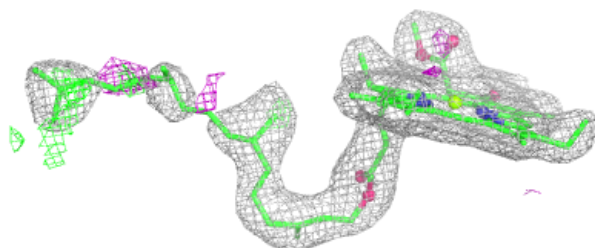
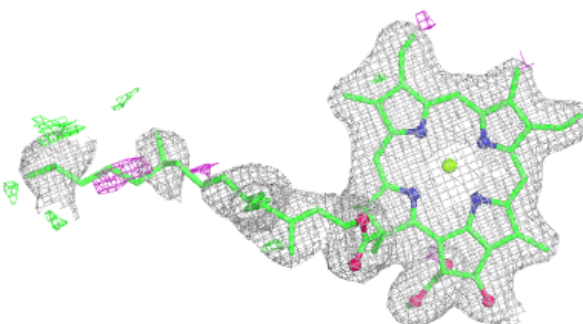


Electron density around LHG d 406 (B):

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

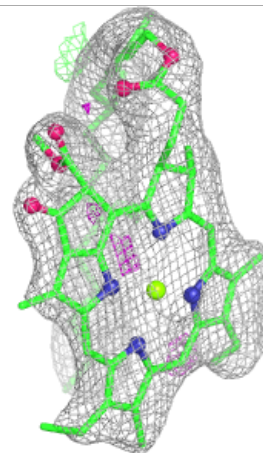
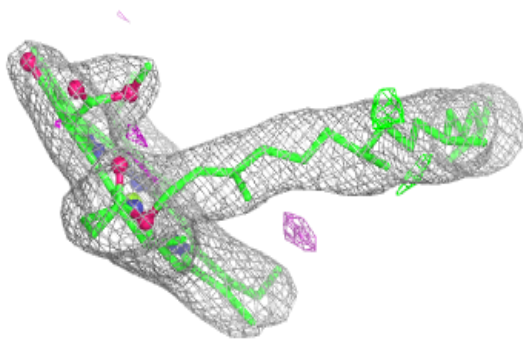
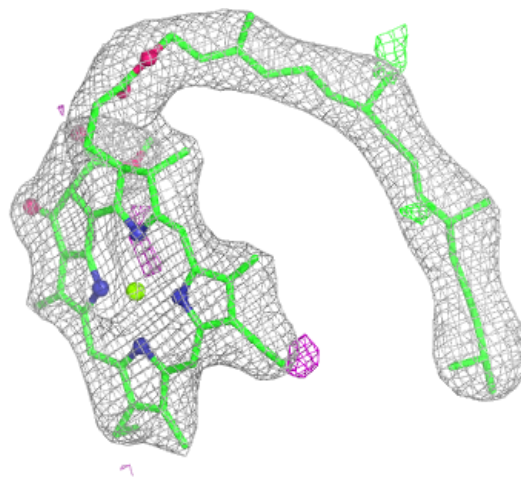
**Electron density around CLA a 407 (B):**

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



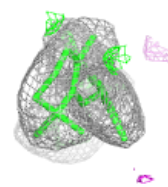
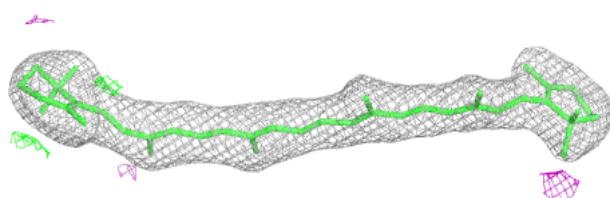
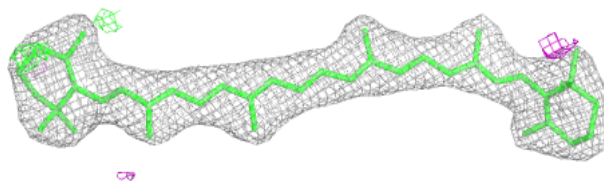
Electron density around CLA c 508:

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

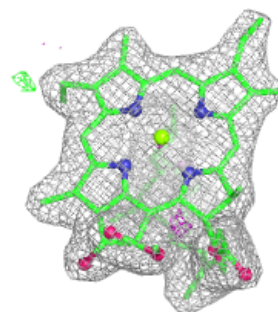
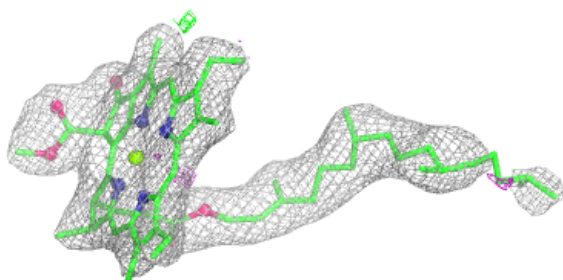
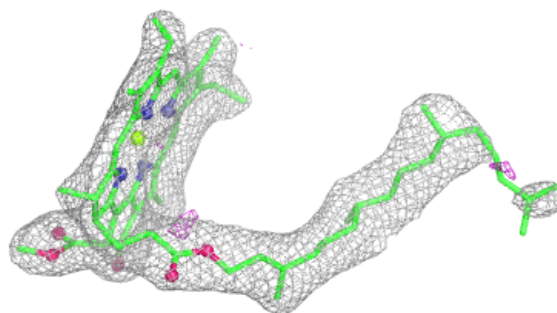


Electron density around BCR b 619:

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

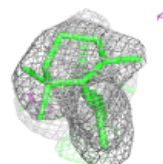
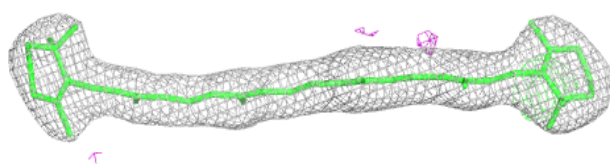
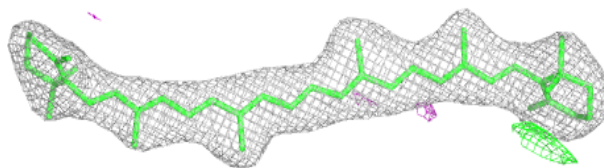
**Electron density around CLA c 509:**

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

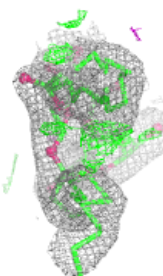
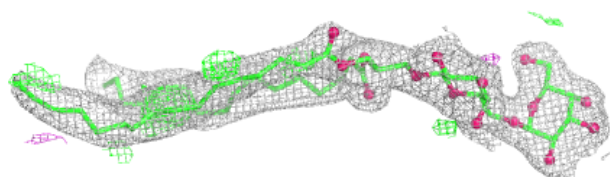
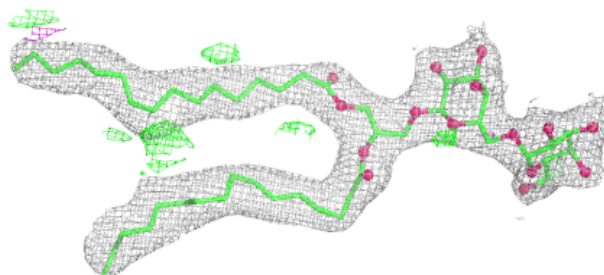


Electron density around BCR c 516:

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

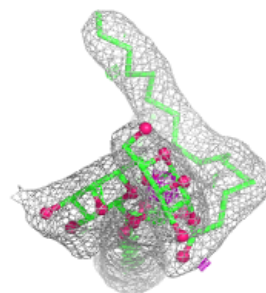
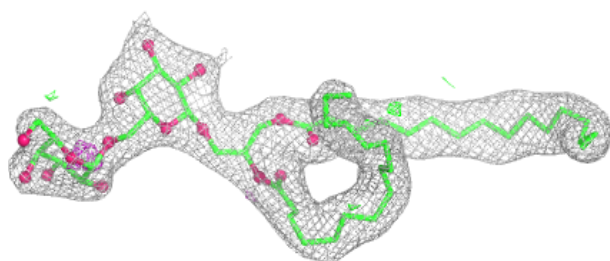
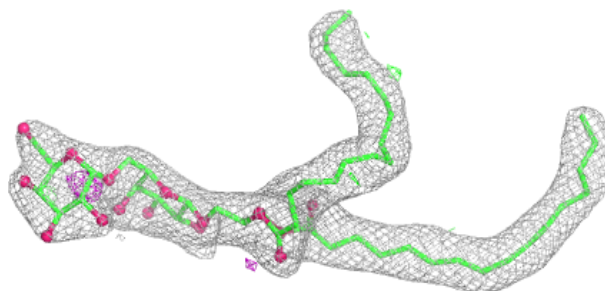
**Electron density around DGD C 520:**

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

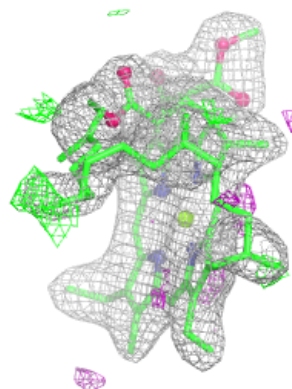
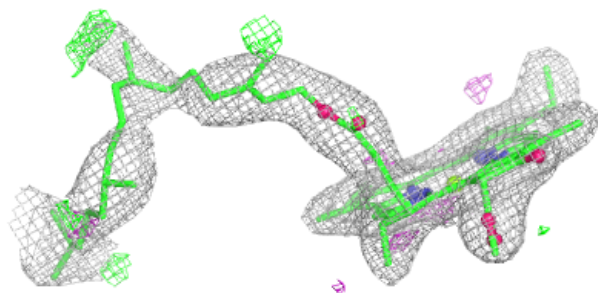
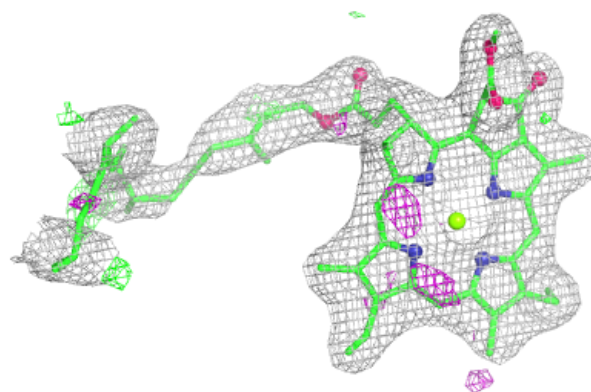


Electron density around DGD H 102:

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

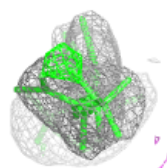
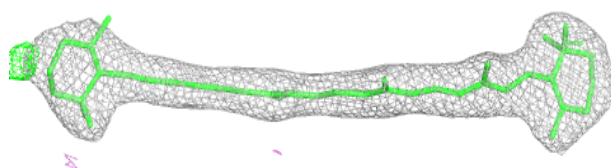
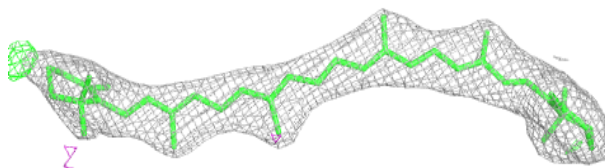
**Electron density around CLA A 407:**

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

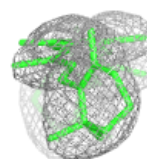
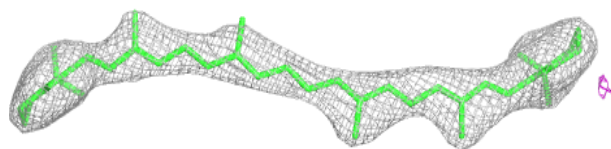
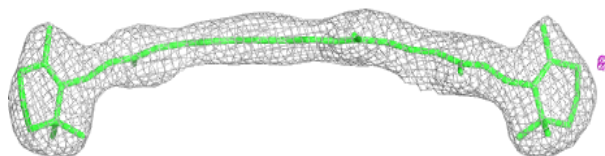


Electron density around BCR h 101:

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

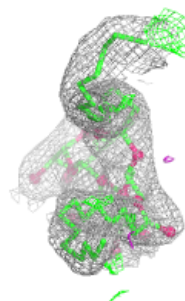
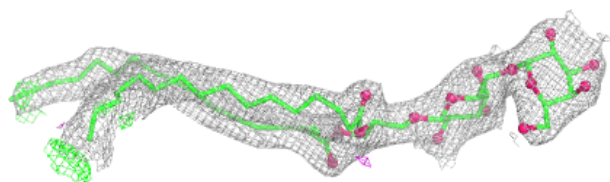
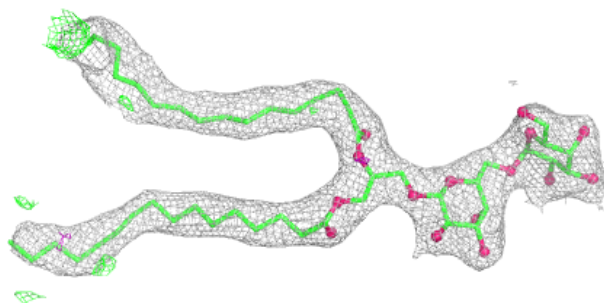
**Electron density around BCR k 101:**

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

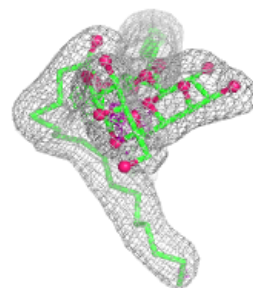
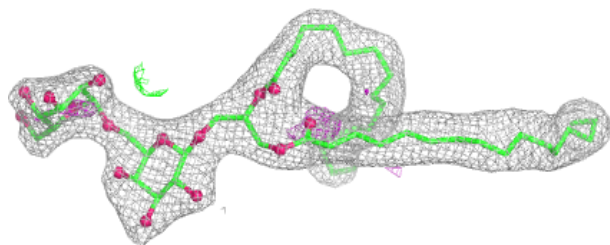
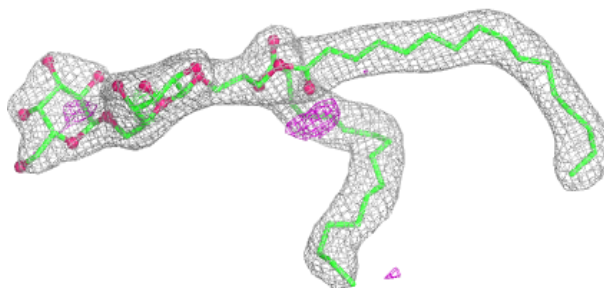


Electron density around DGD c 519:

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

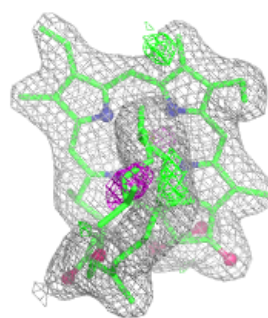
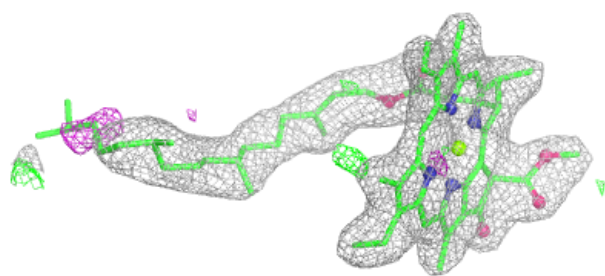
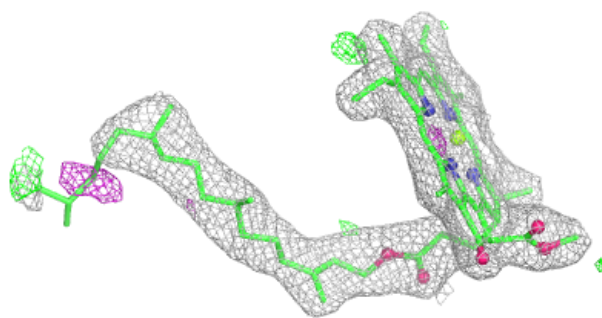
**Electron density around DGD h 102:**

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

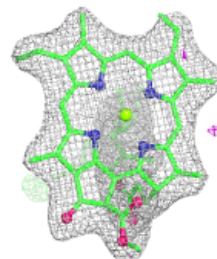
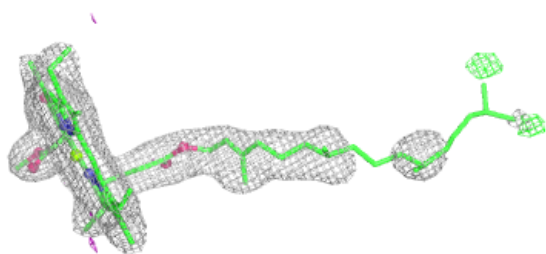
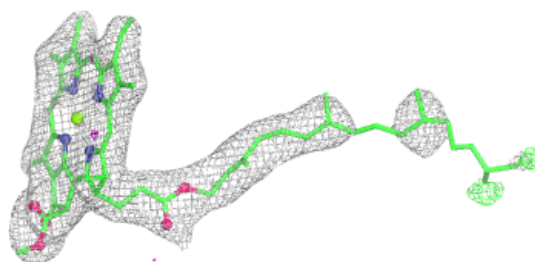


Electron density around CLA C 510:

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

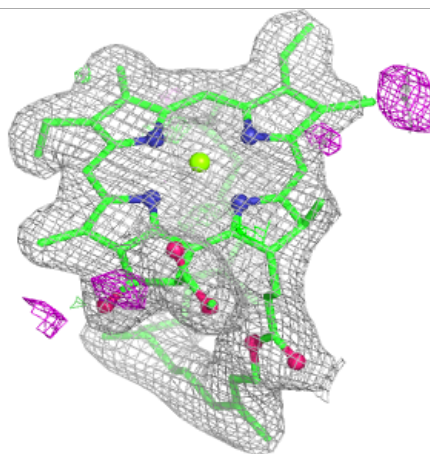
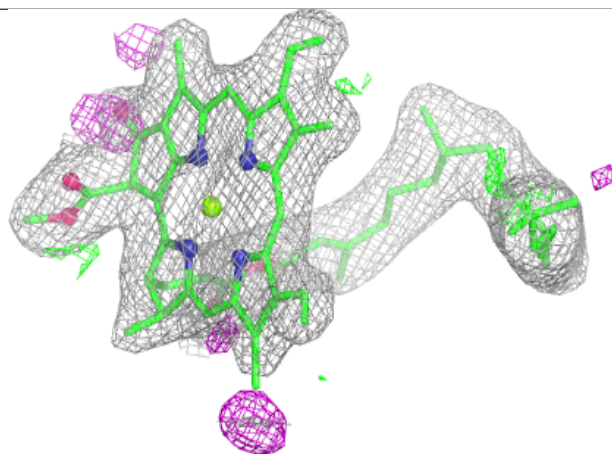
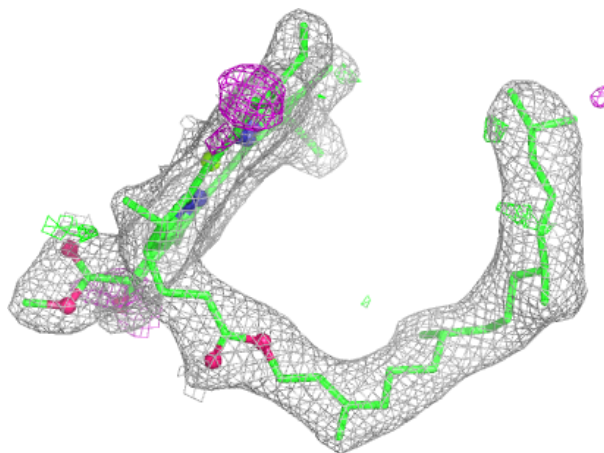
**Electron density around CLA d 402:**

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



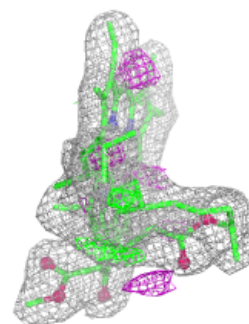
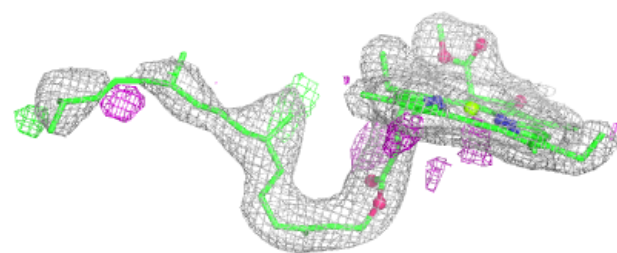
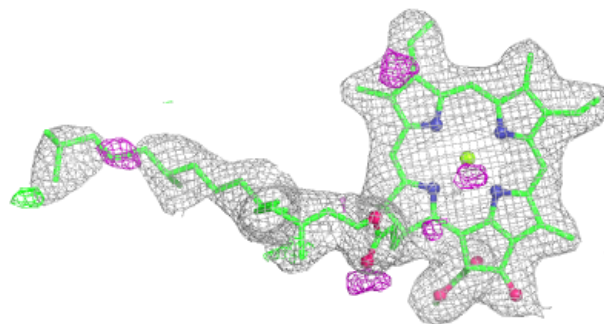
Electron density around CLA B 611:

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

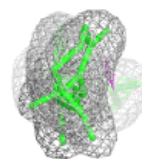
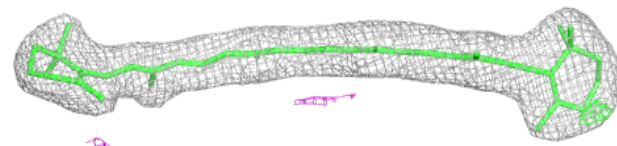
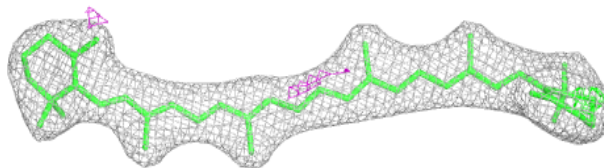


Electron density around CLA A 406 (A):

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

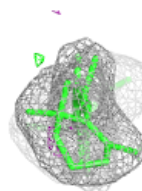
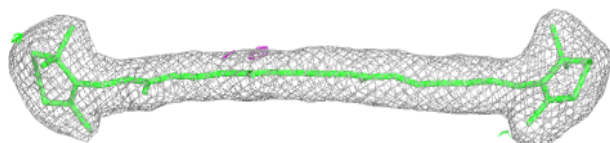
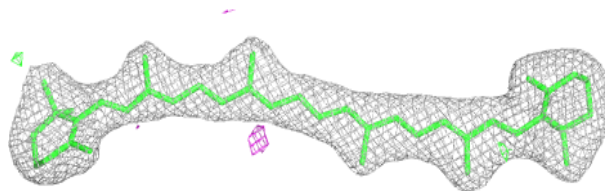
**Electron density around BCR B 617:**

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



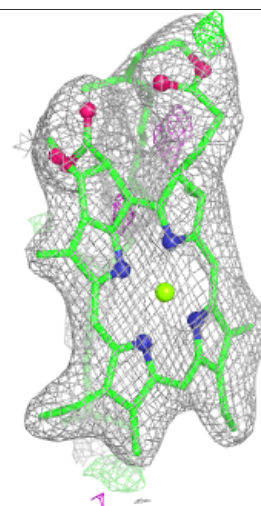
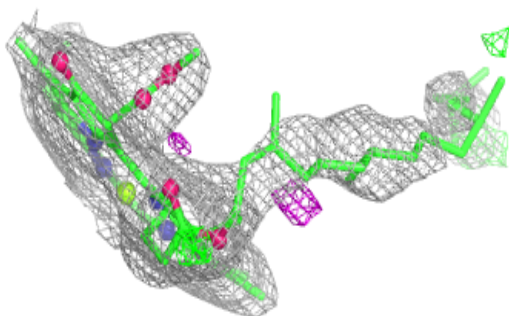
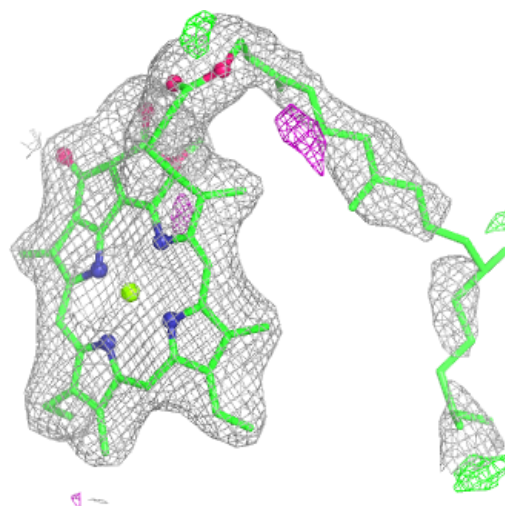
Electron density around BCR B 618:

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



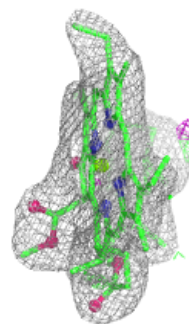
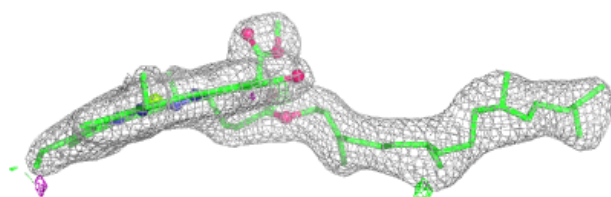
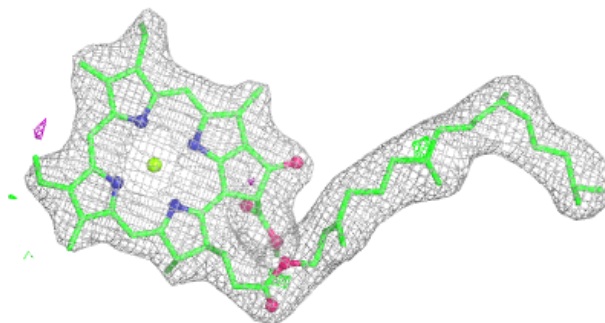
Electron density around CLA B 616:

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

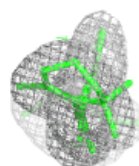
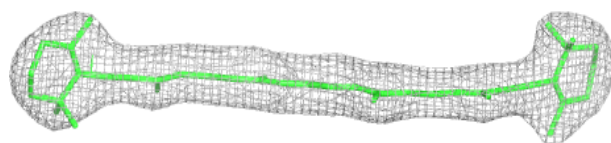
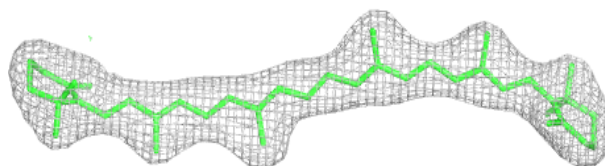


Electron density around CLA b 602:

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

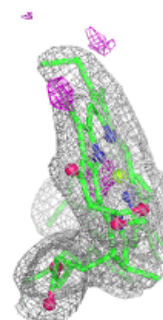
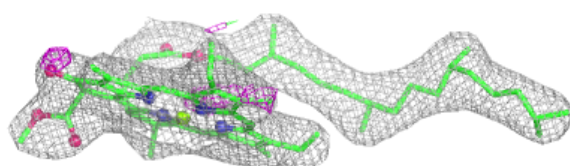
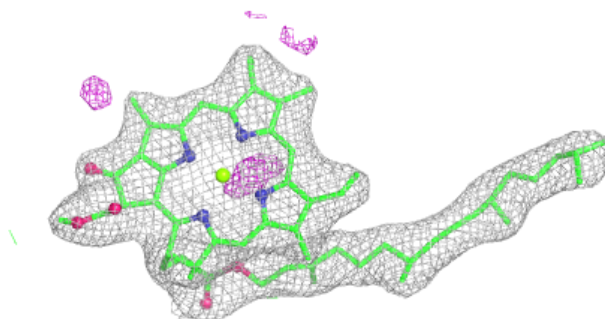
**Electron density around BCR C 517:**

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

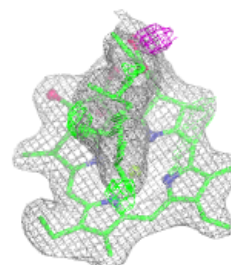
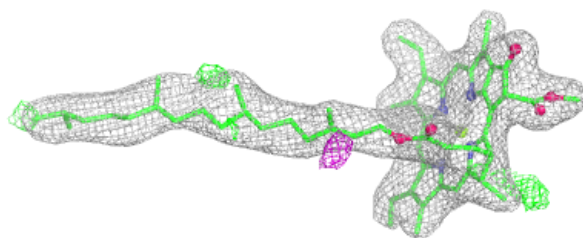
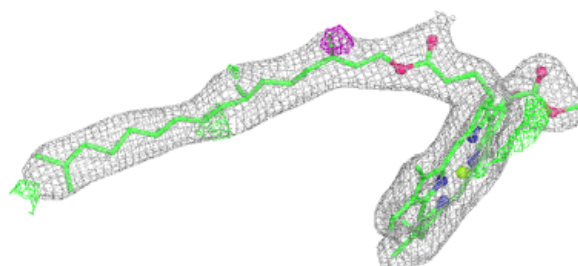


Electron density around CLA C 503:

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

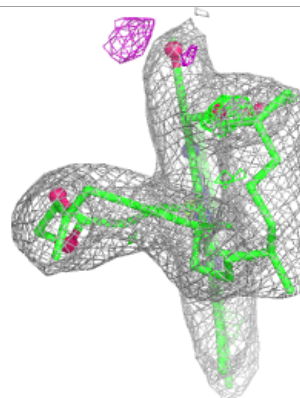
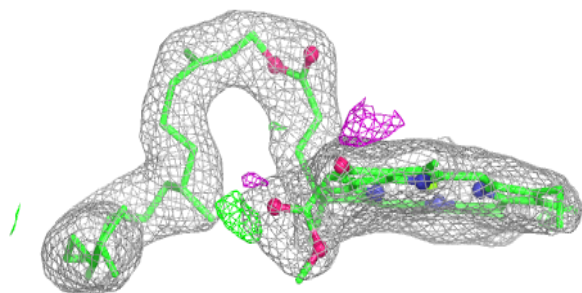
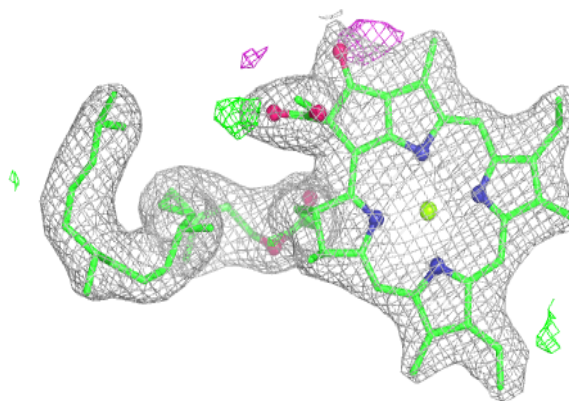
**Electron density around CLA b 607:**

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

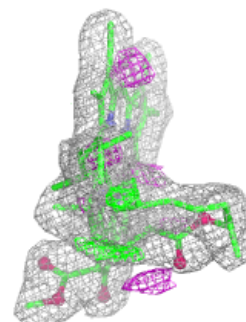
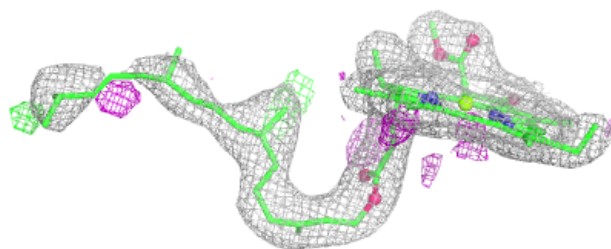
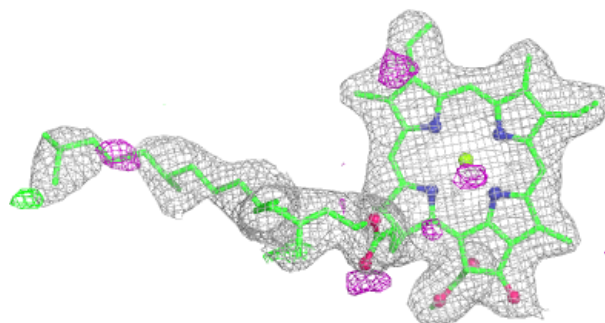


Electron density around CLA b 612:

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

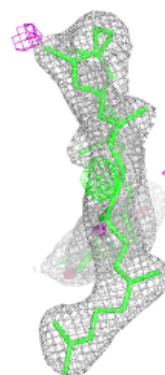
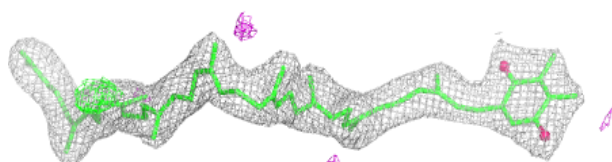
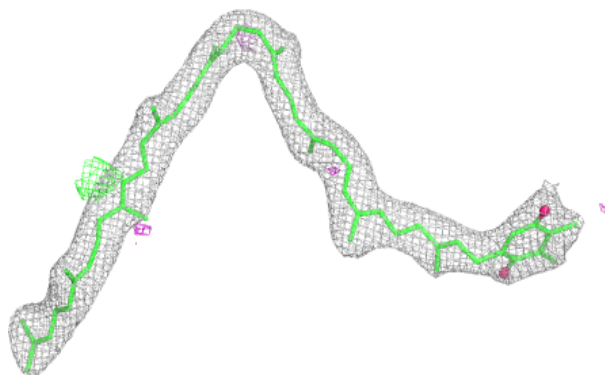
**Electron density around CLA A 406 (B):**

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

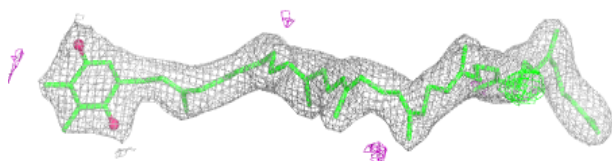
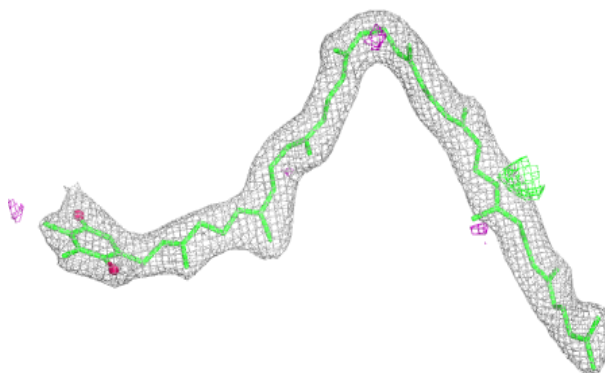


Electron density around PL9 d 404 (A):

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

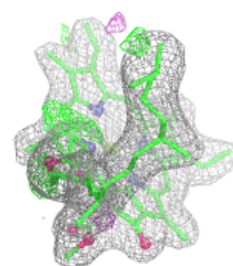
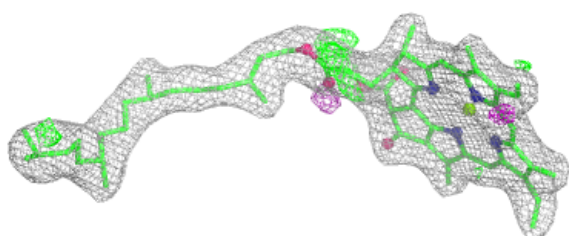
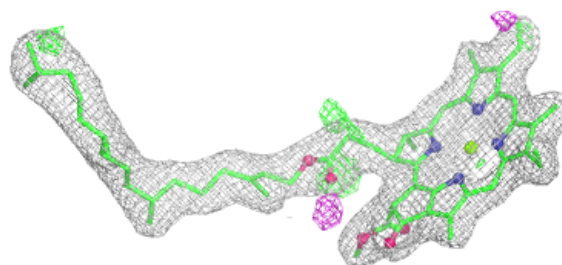
**Electron density around PL9 d 404 (B):**

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

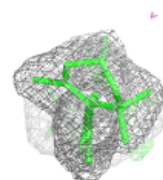
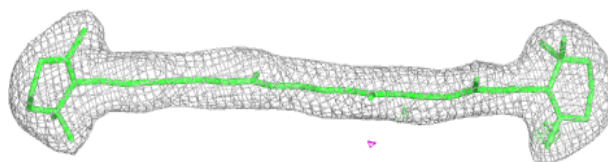
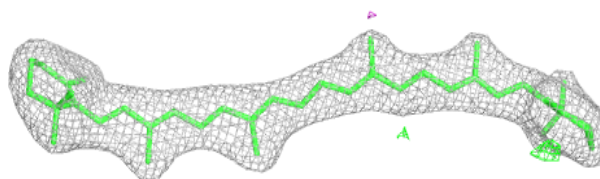


Electron density around CLA A 404 (A):

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

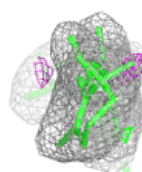
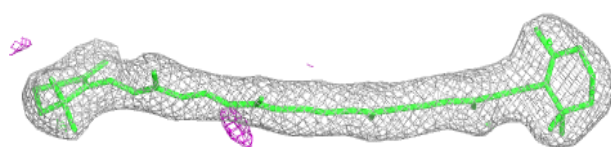
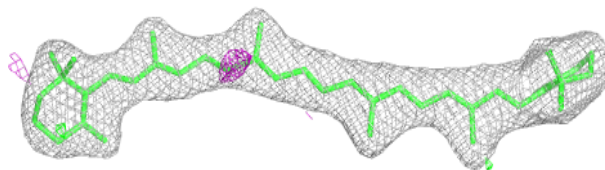
**Electron density around BCR a 410:**

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

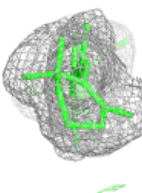
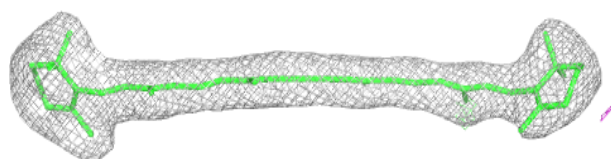
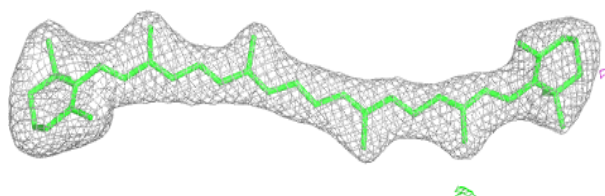


Electron density around BCR b 617:

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

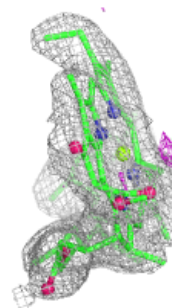
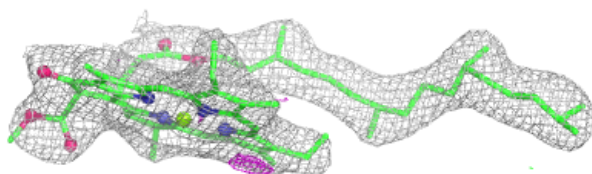
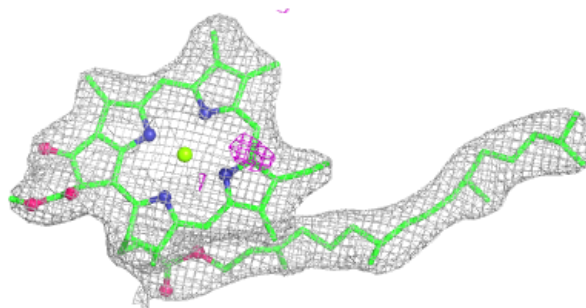
**Electron density around BCR b 618:**

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



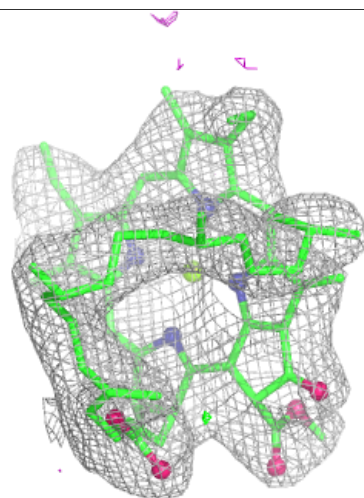
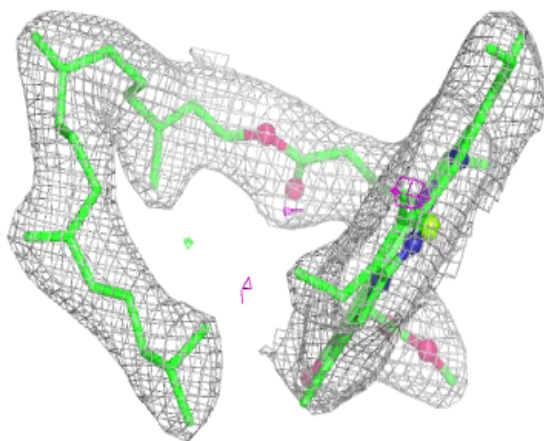
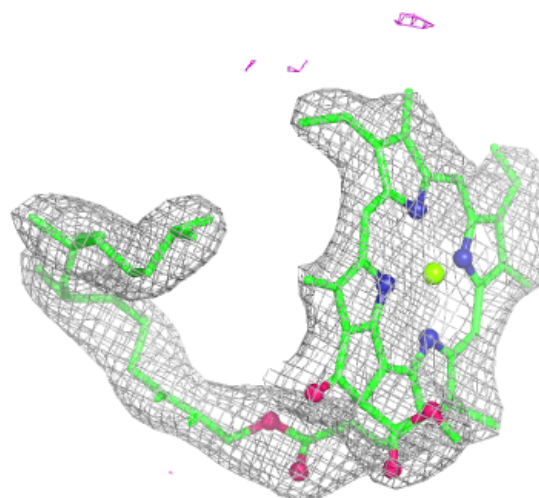
Electron density around CLA c 502:

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



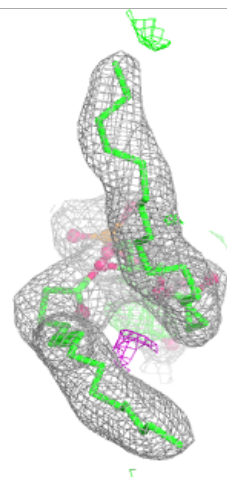
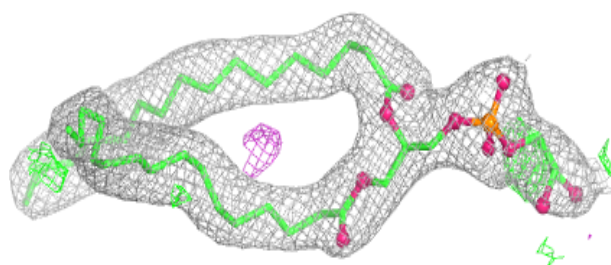
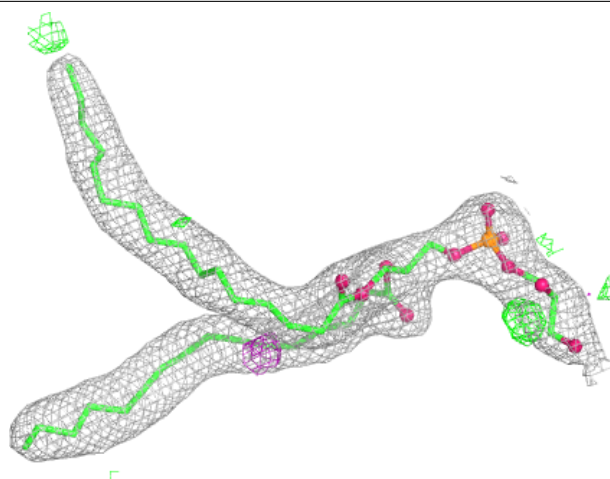
Electron density around CLA c 504:

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



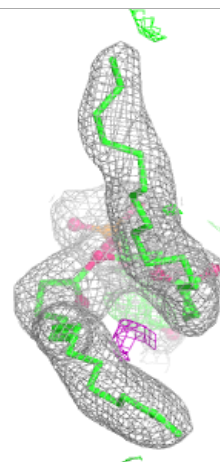
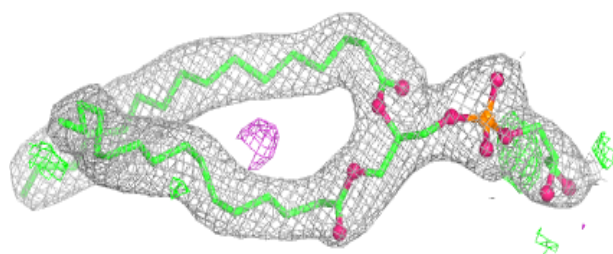
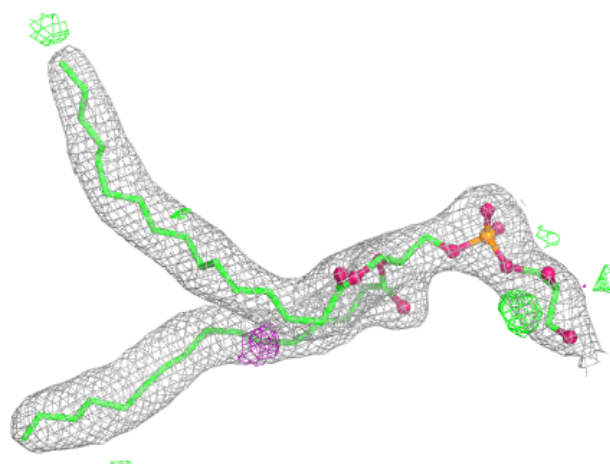
Electron density around LHG D 408 (A):

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



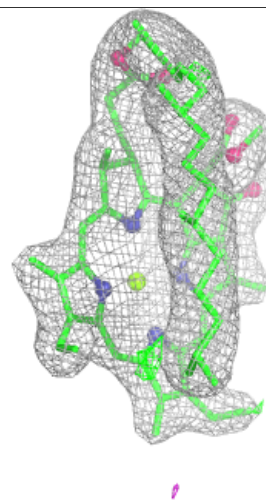
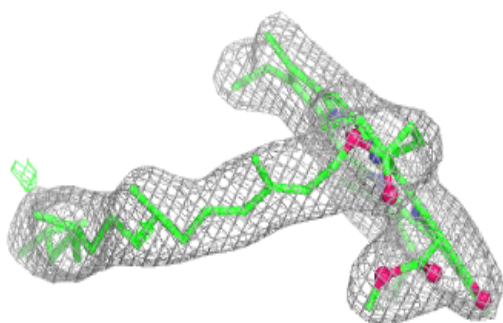
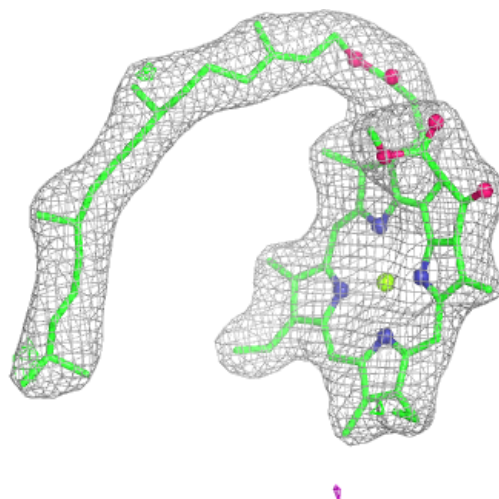
Electron density around LHG D 408 (B):

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



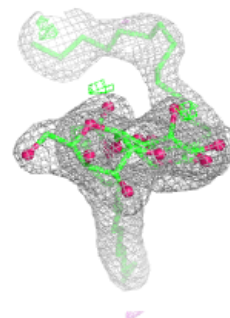
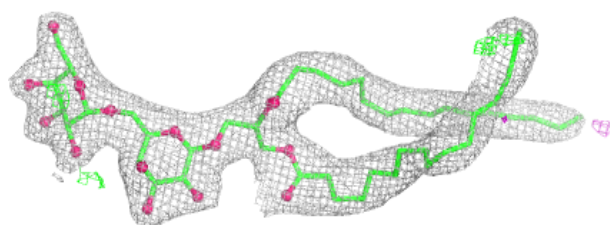
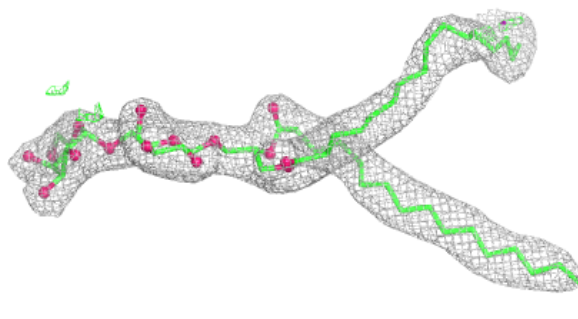
Electron density around CLA C 509:

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

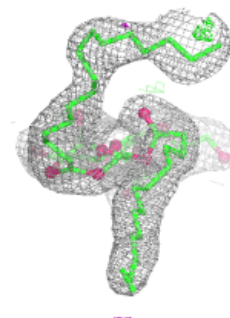
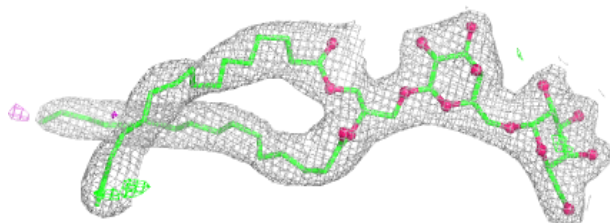
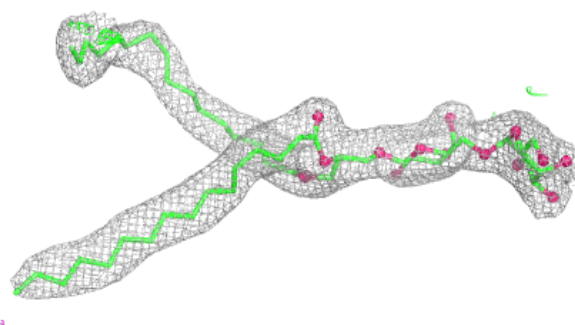


Electron density around DGD C 518 (A):

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

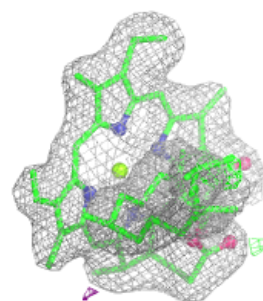
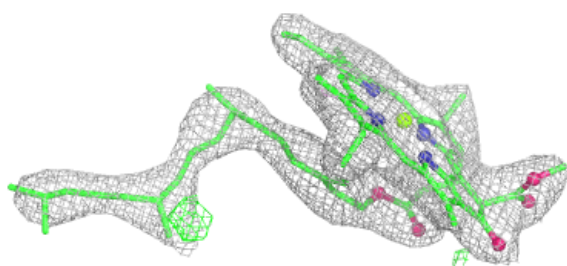
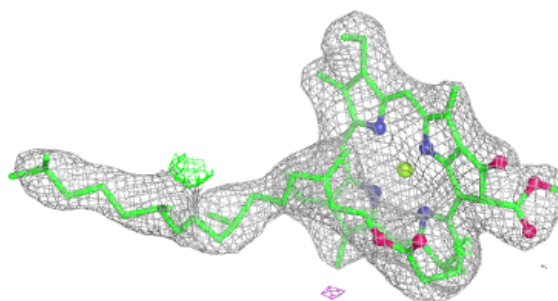
**Electron density around DGD C 518 (B):**

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

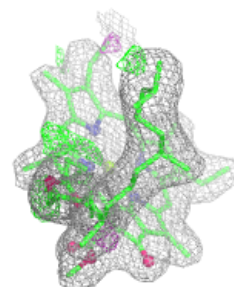
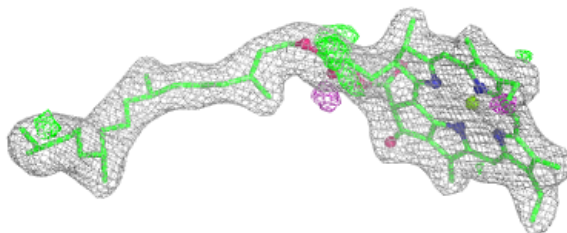
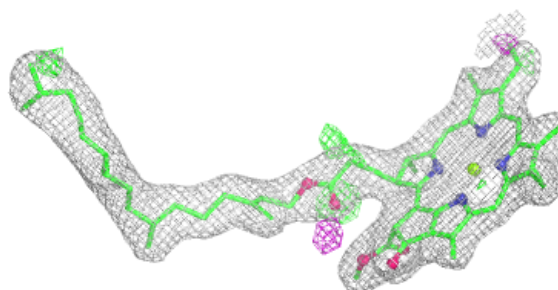


Electron density around CLA c 506:

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

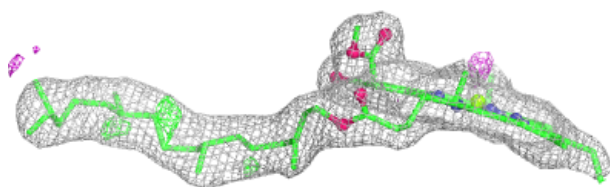
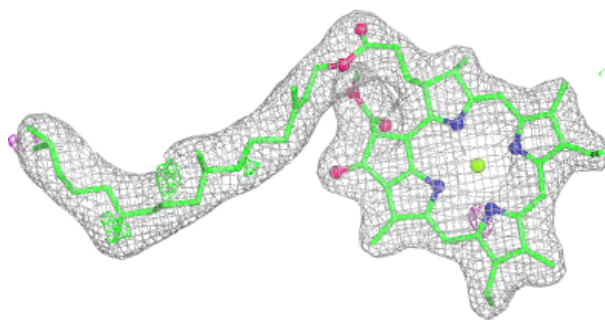
**Electron density around CLA A 404 (B):**

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

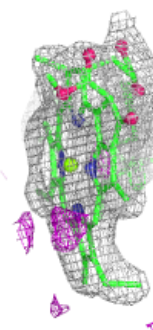
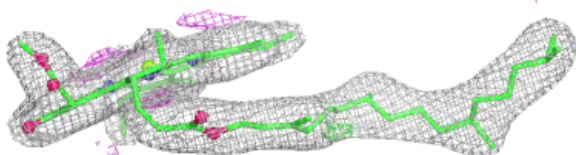
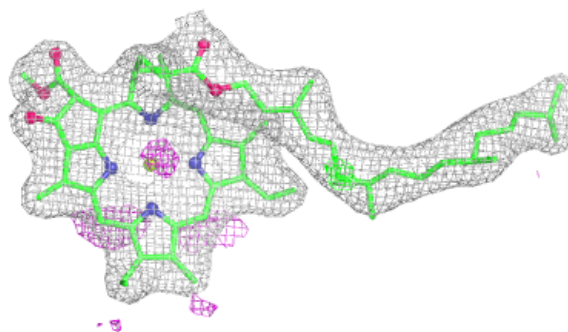


Electron density around CLA B 602:

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

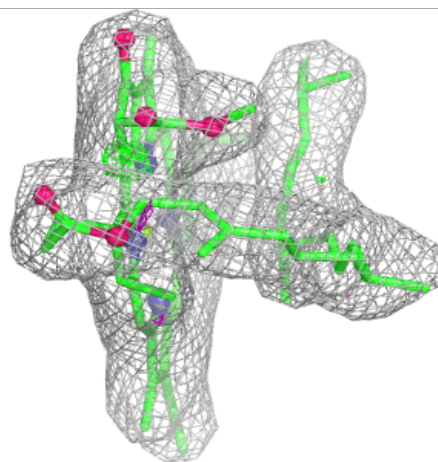
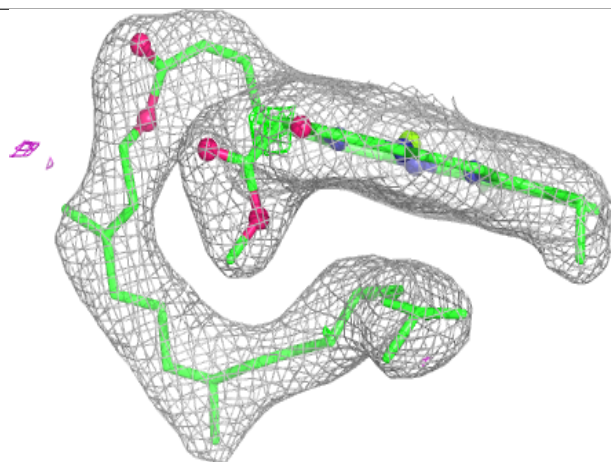
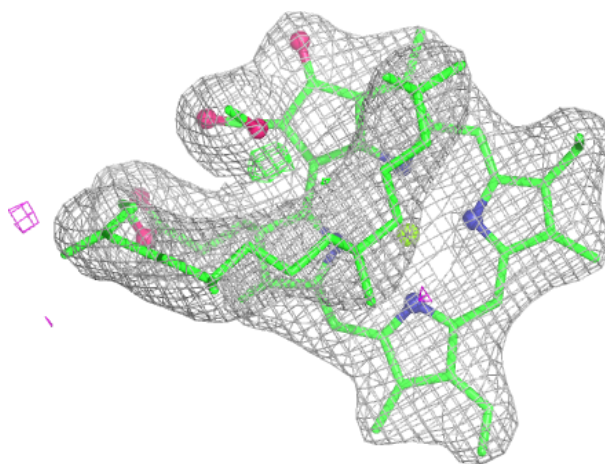
**Electron density around CLA B 603:**

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



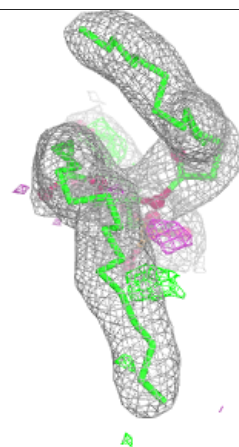
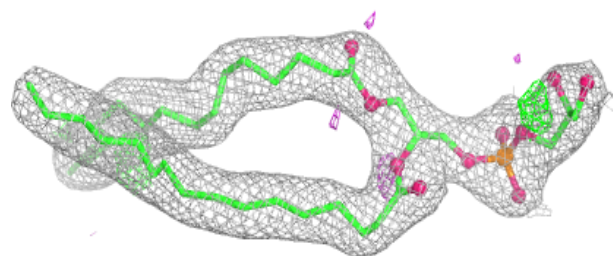
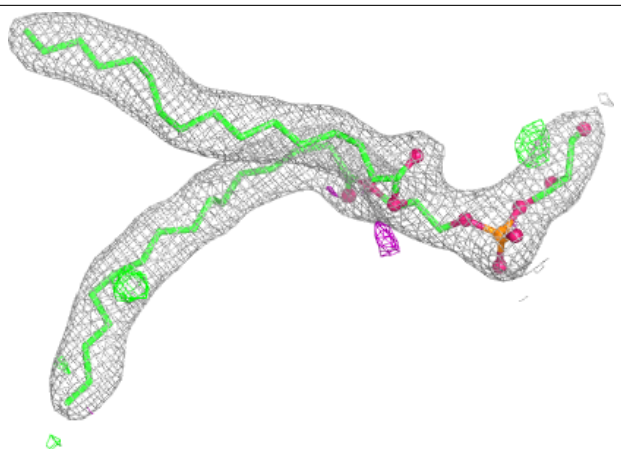
Electron density around CLA c 511:

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



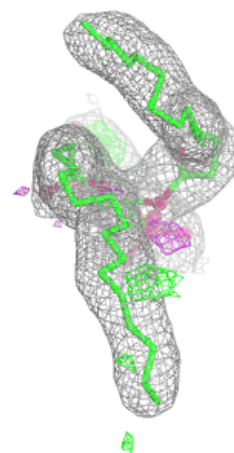
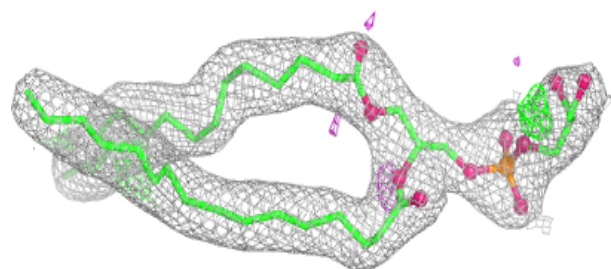
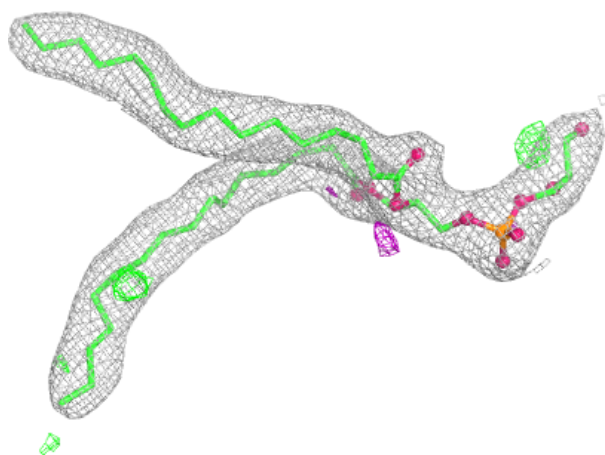
Electron density around LHG d 405 (A):

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



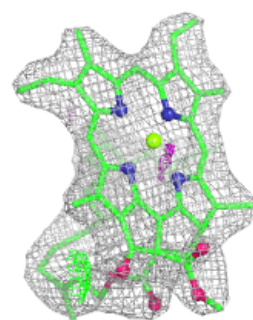
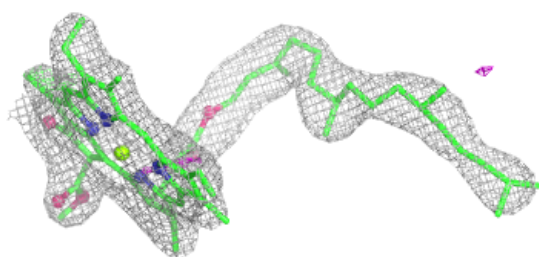
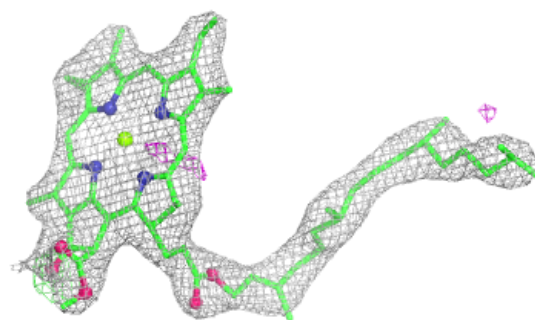
Electron density around LHG d 405 (B):

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

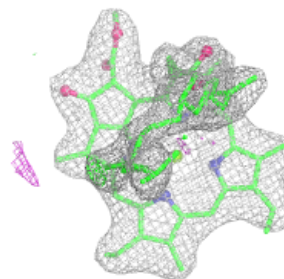
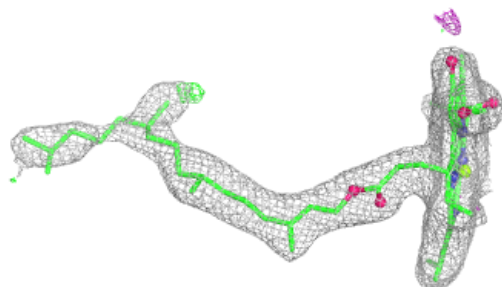
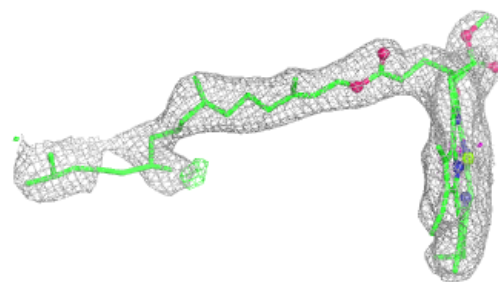


Electron density around CLA c 512:

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

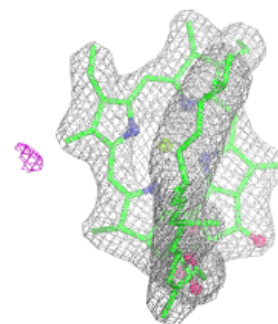
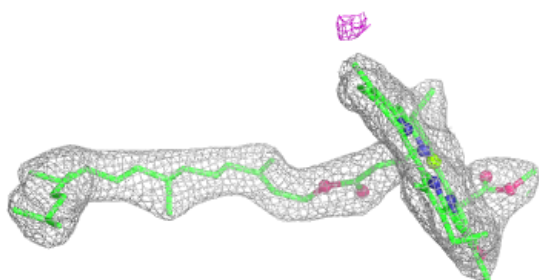
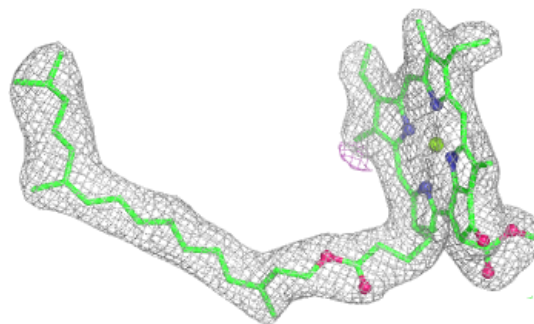
**Electron density around CLA B 606:**

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



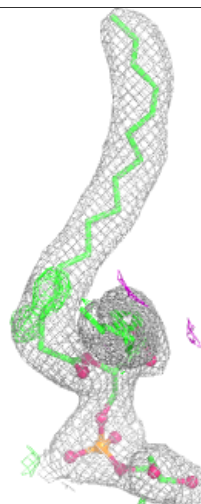
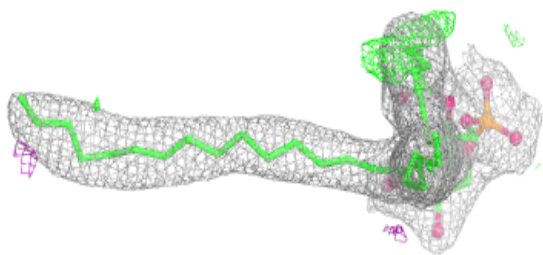
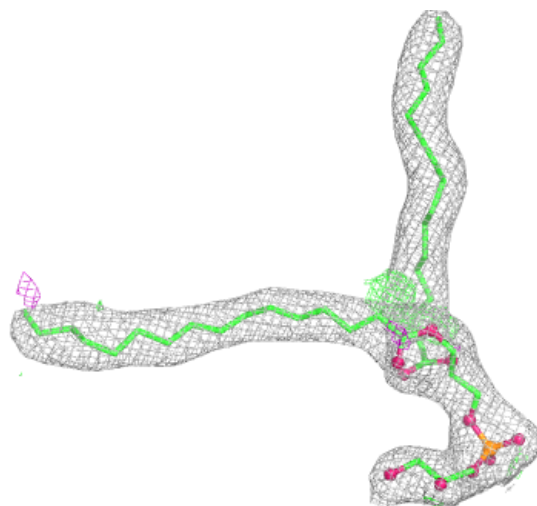
Electron density around CLA B 609:

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



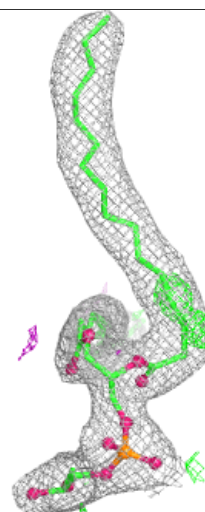
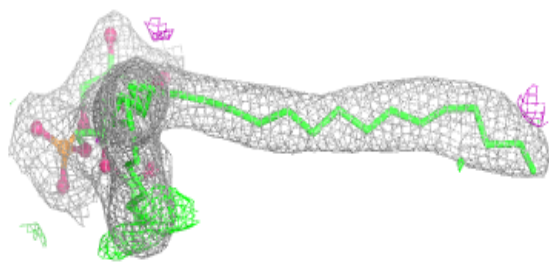
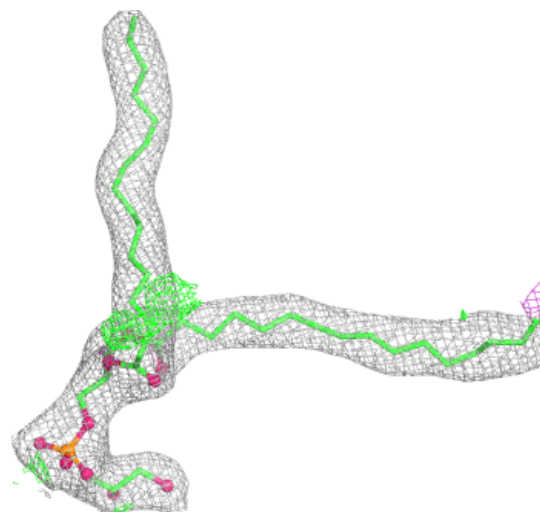
Electron density around LHG 1 802 (A):

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



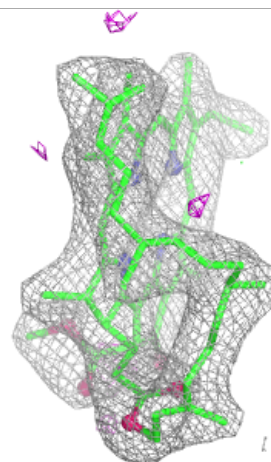
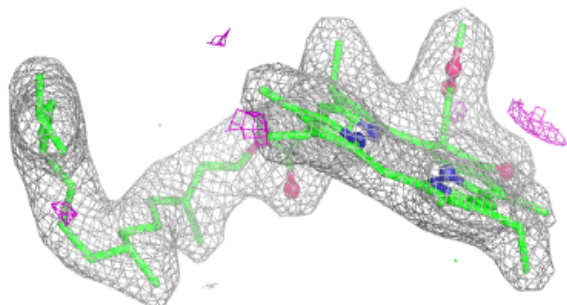
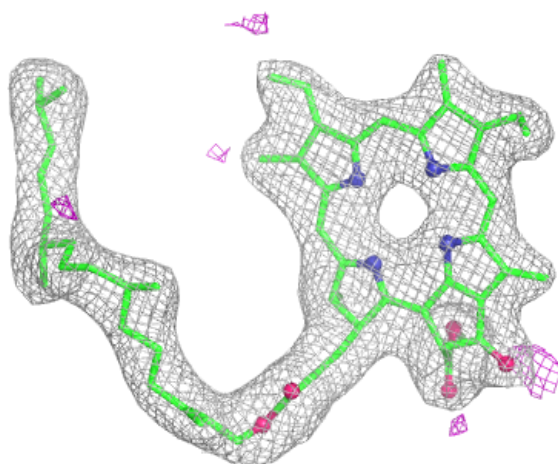
Electron density around LHG 1 802 (B):

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



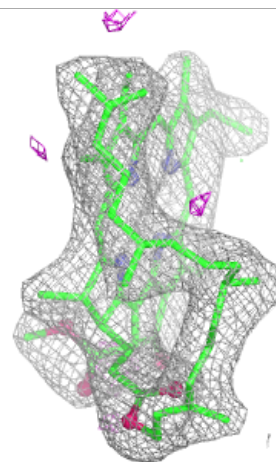
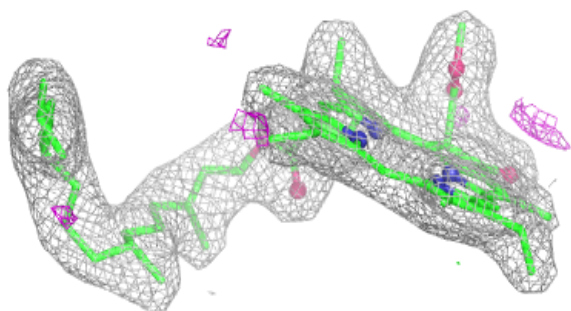
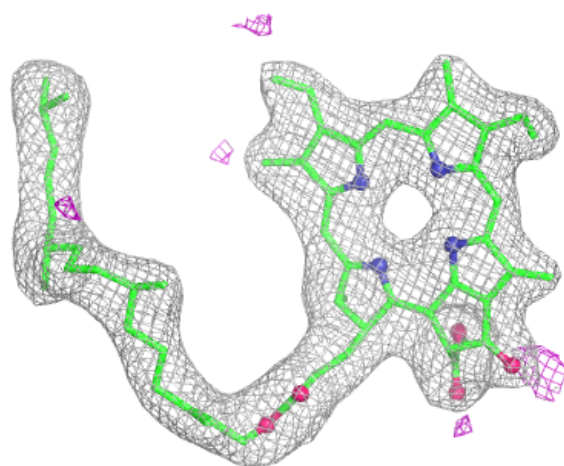
Electron density around PHO D 402 (A):

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



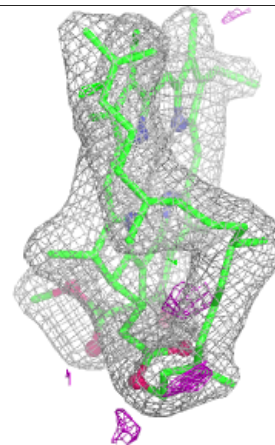
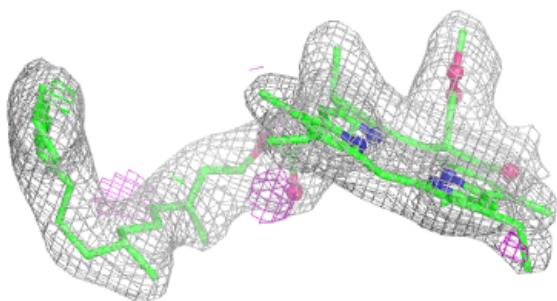
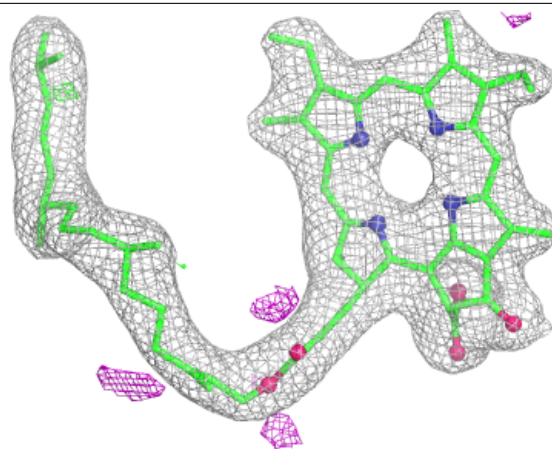
Electron density around PHO D 402 (B):

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



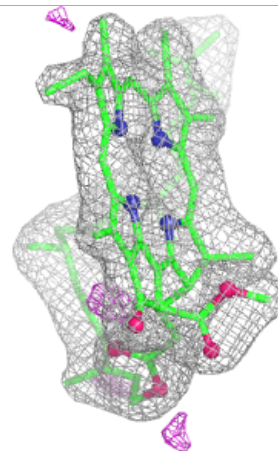
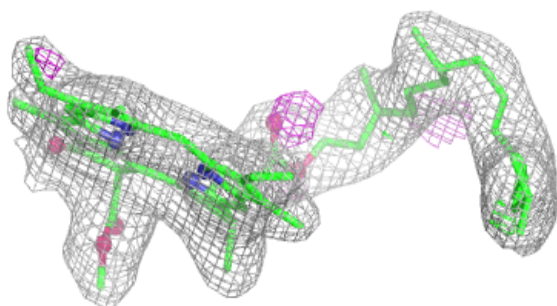
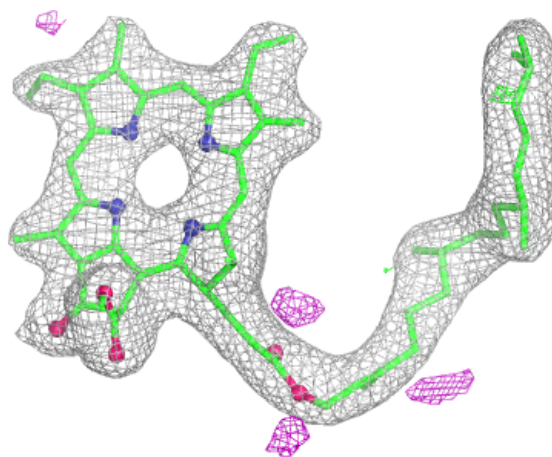
Electron density around PHO a 416 (A):

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



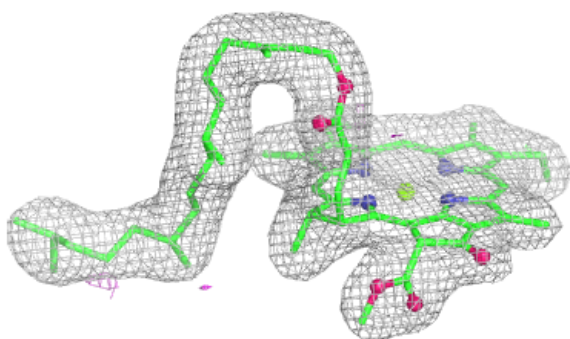
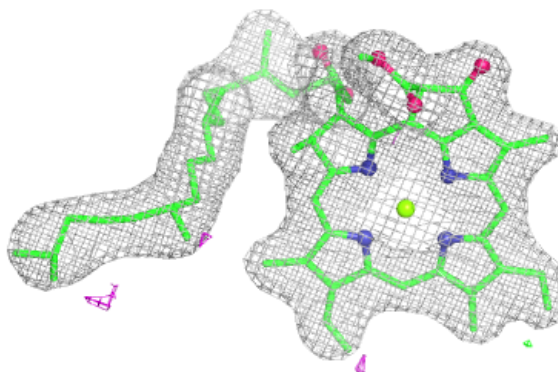
Electron density around PHO a 416 (B):

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

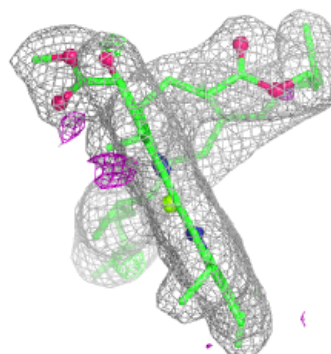
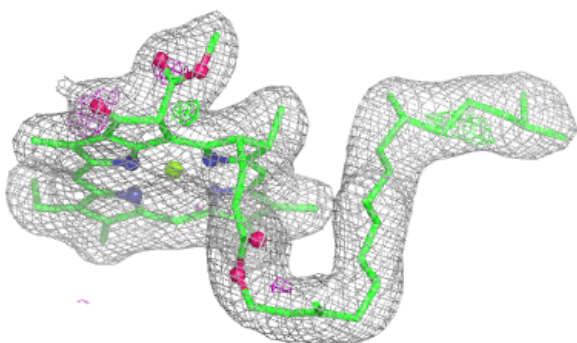
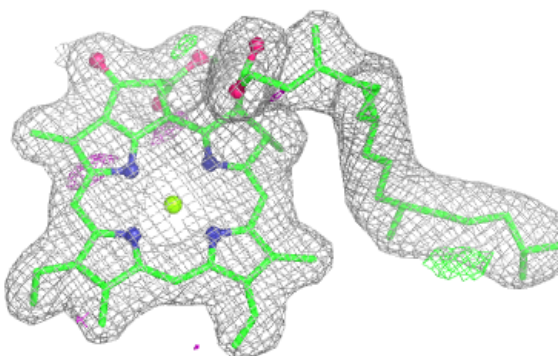


Electron density around CLA a 406 (B):

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

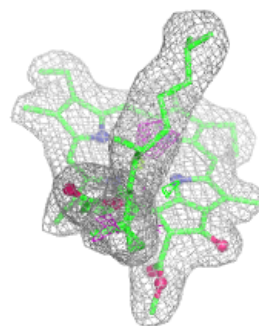
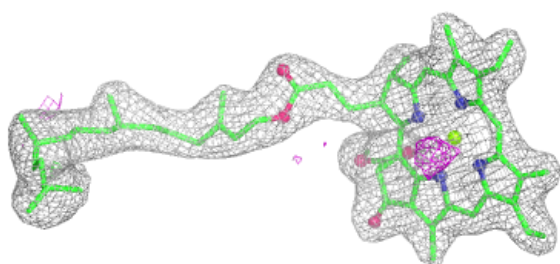
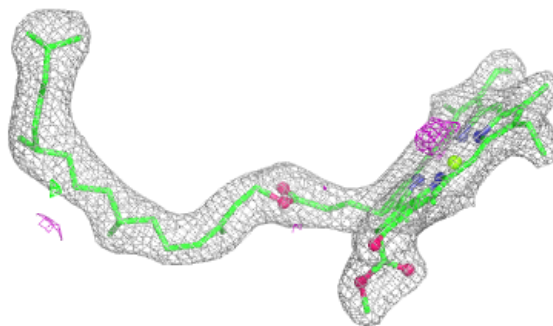
**Electron density around CLA A 405 (A):**

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

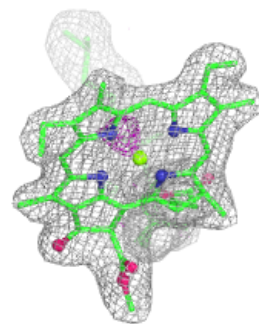
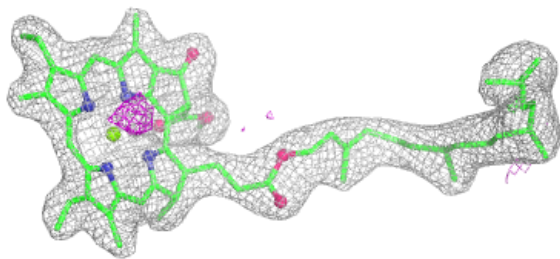
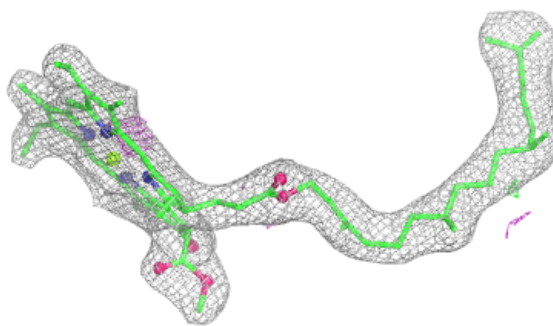


Electron density around CLA d 401 (A):

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

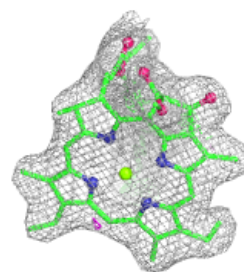
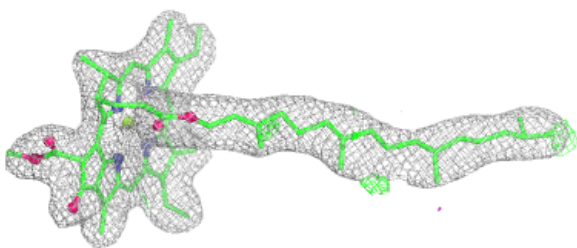
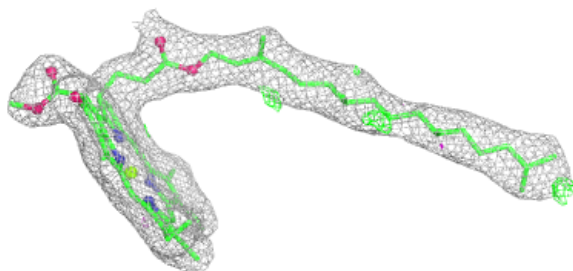
**Electron density around CLA d 401 (B):**

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



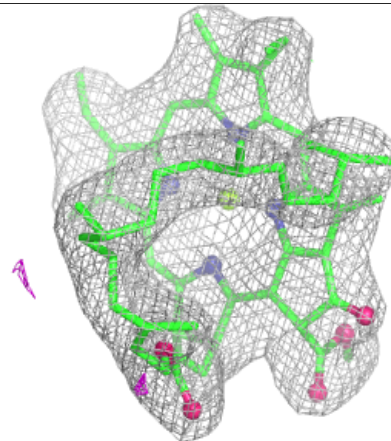
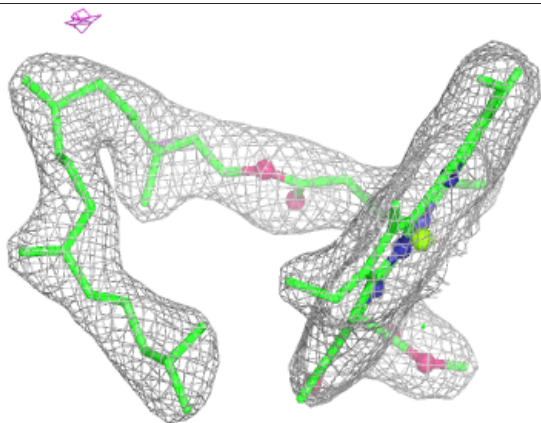
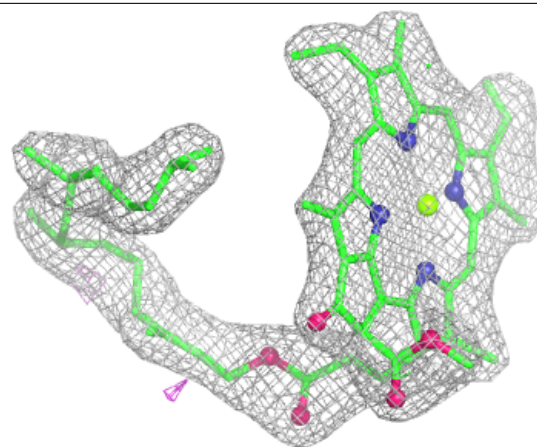
Electron density around CLA B 607:

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



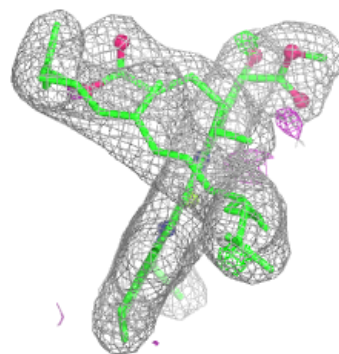
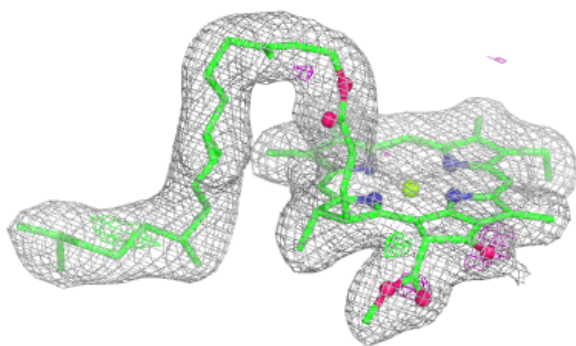
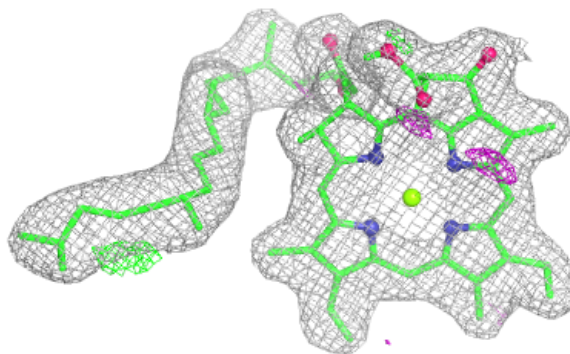
Electron density around CLA C 505:

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

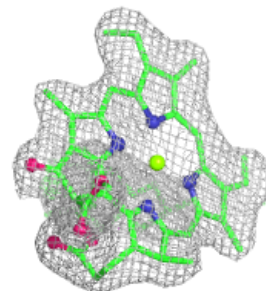
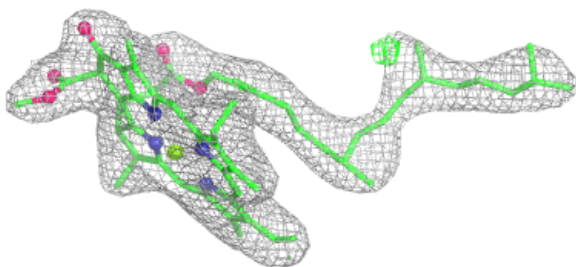
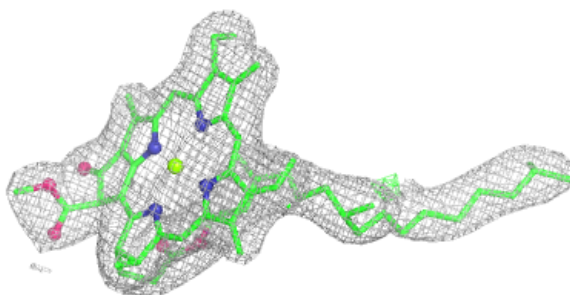


Electron density around CLA A 405 (B):

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

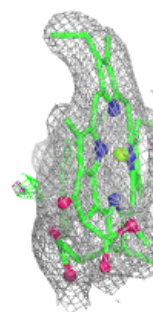
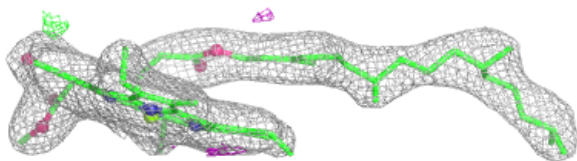
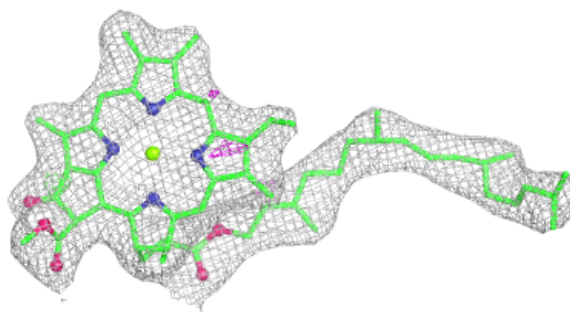
**Electron density around CLA C 507:**

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

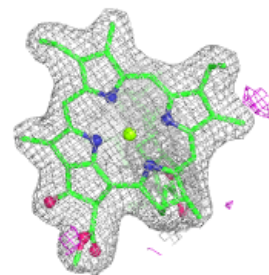
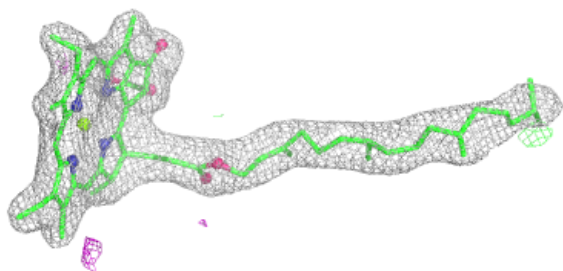
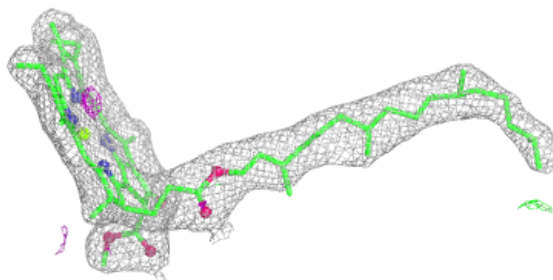


Electron density around CLA b 603:

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

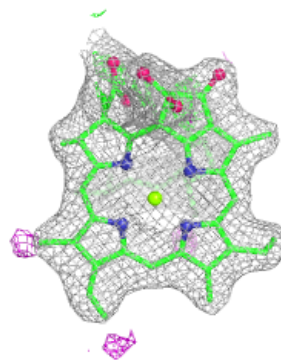
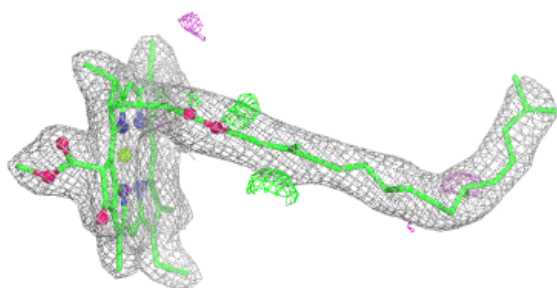
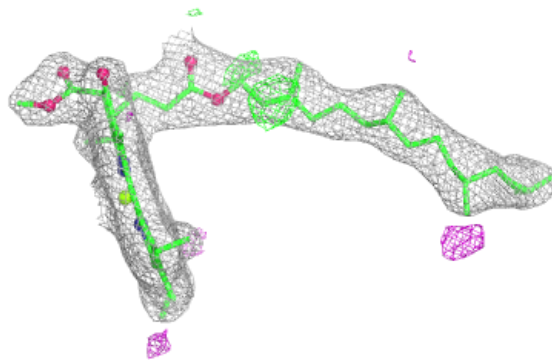
**Electron density around CLA b 604:**

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



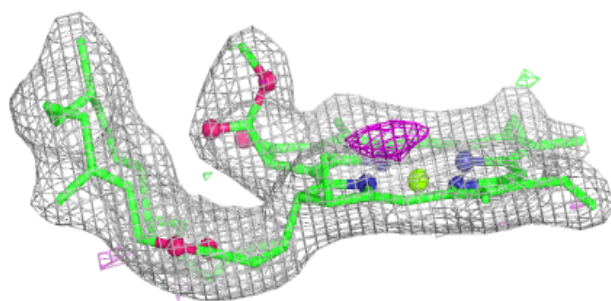
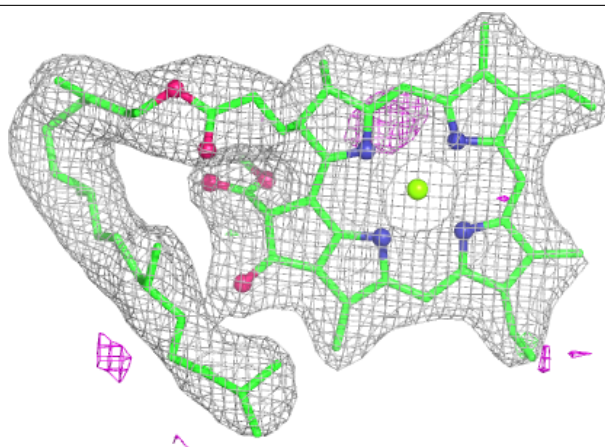
Electron density around CLA b 605:

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



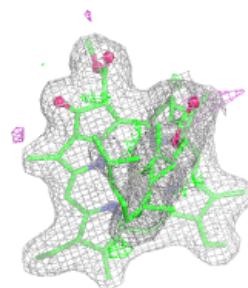
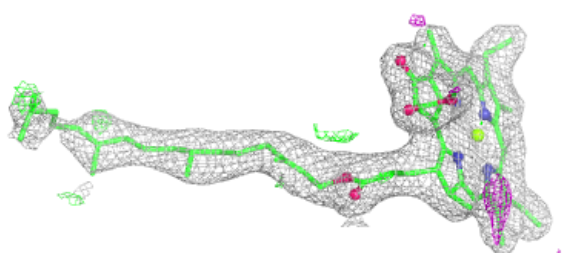
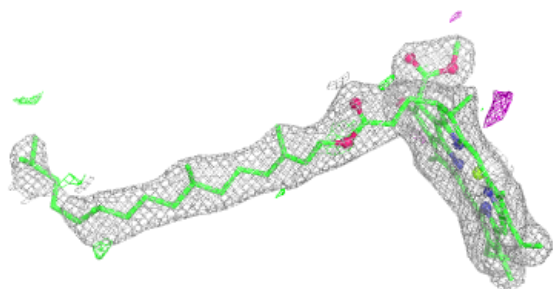
Electron density around CLA B 610:

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

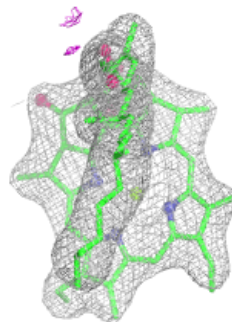
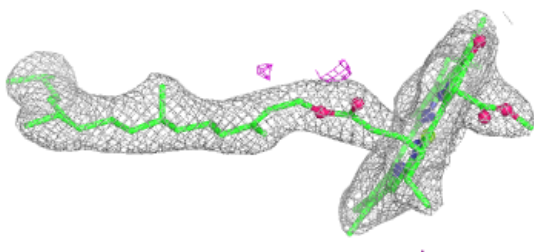
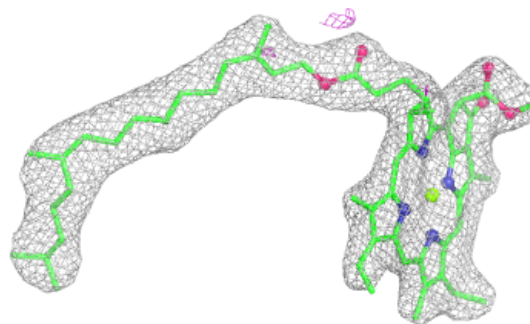


Electron density around CLA B 604:

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

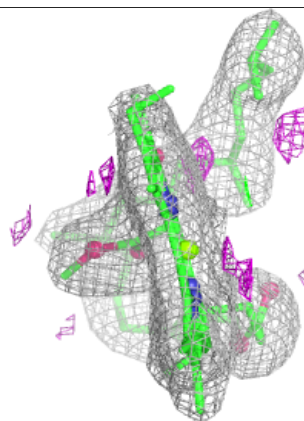
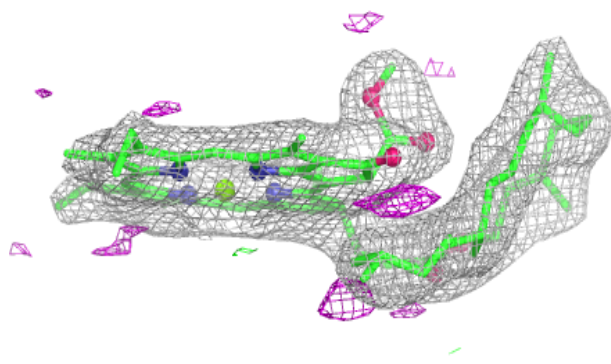
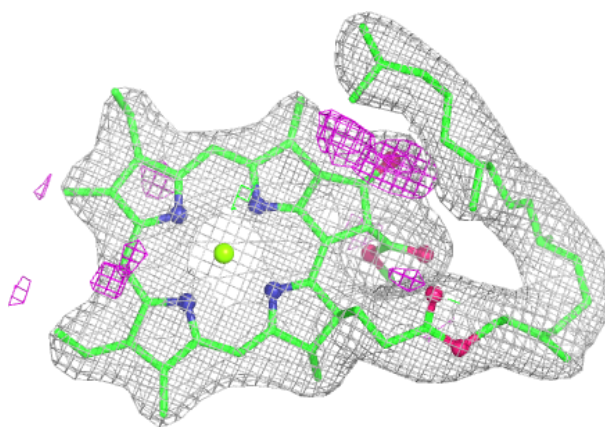
**Electron density around CLA b 609:**

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



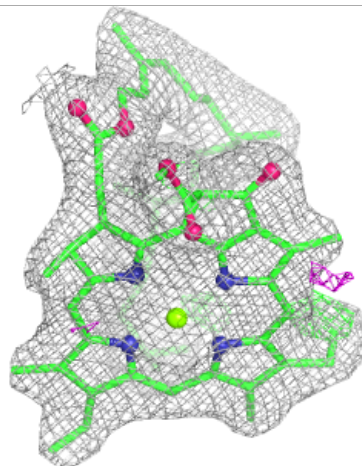
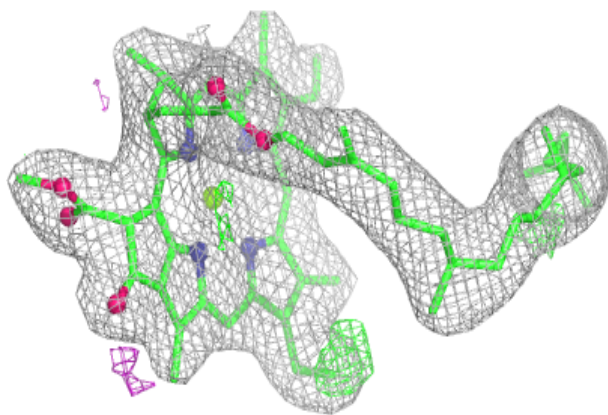
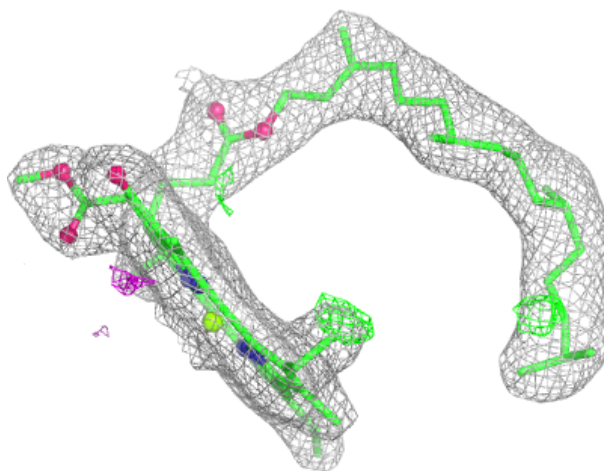
Electron density around CLA b 610:

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



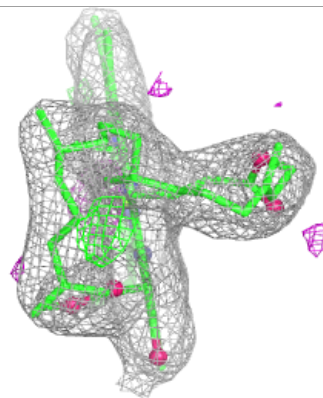
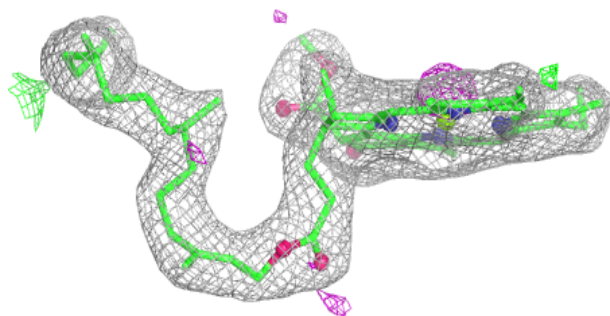
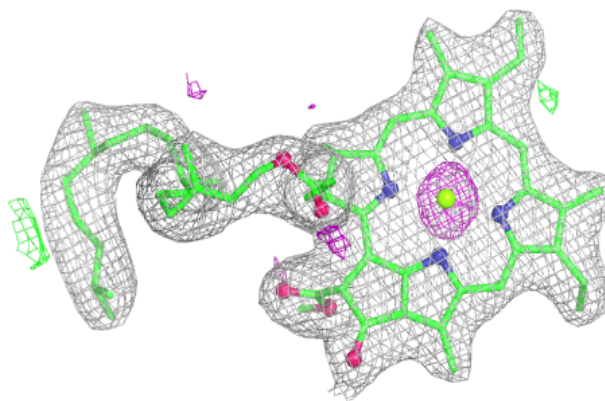
Electron density around CLA b 611:

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



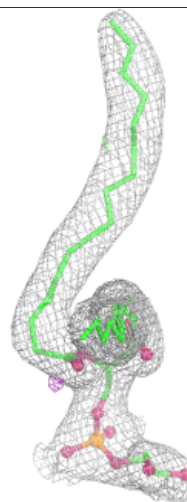
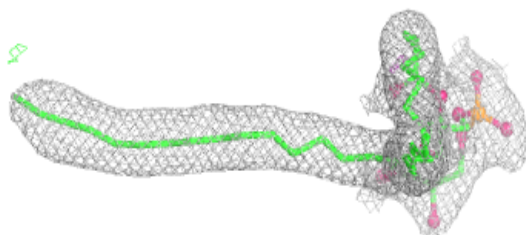
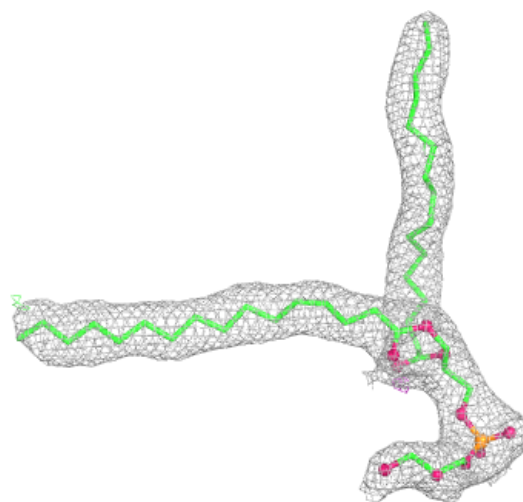
Electron density around CLA B 612:

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



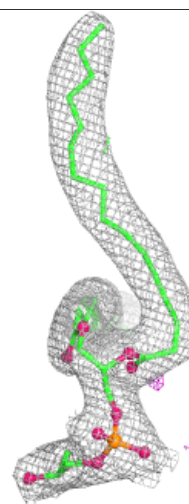
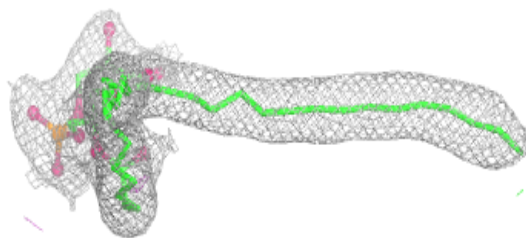
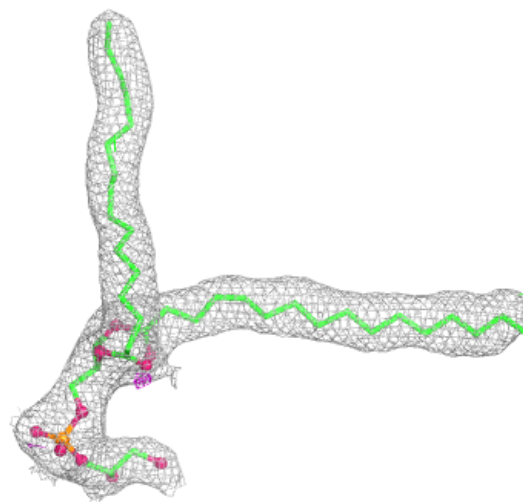
Electron density around LHG L 101 (A):

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



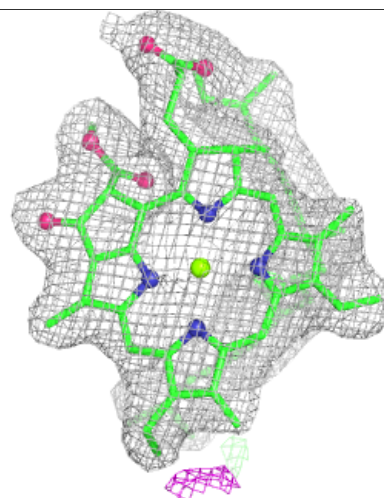
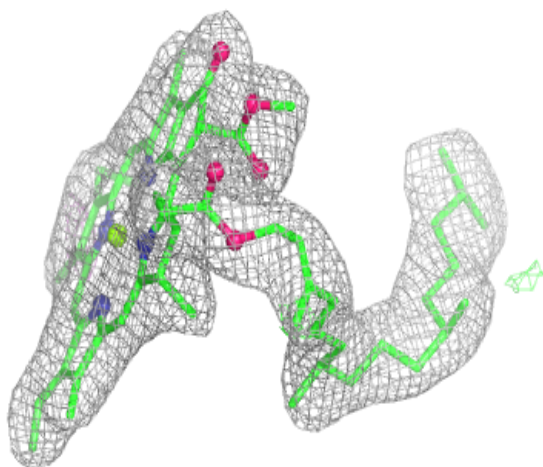
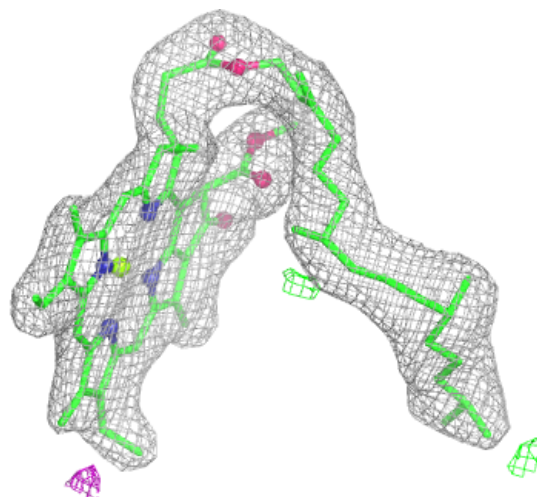
Electron density around LHG L 101 (B):

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



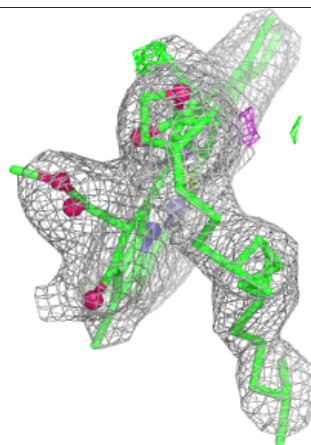
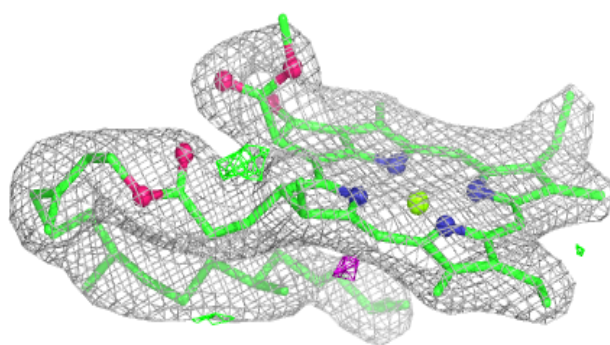
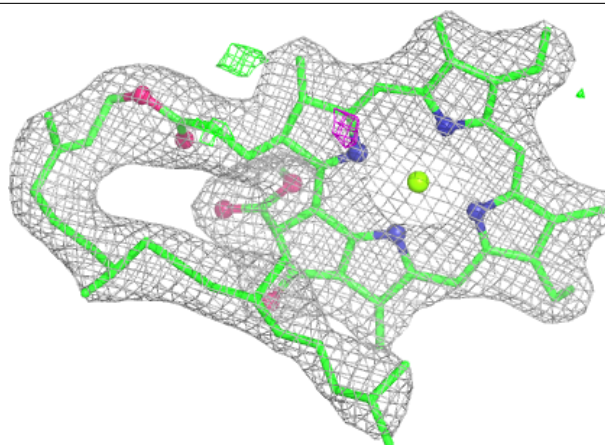
Electron density around CLA b 613:

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



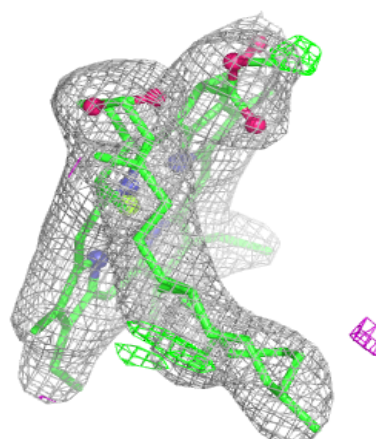
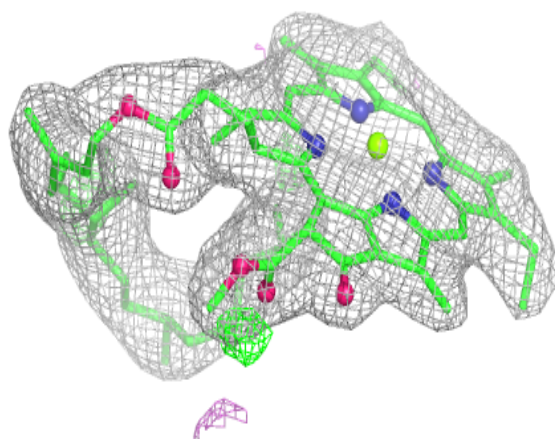
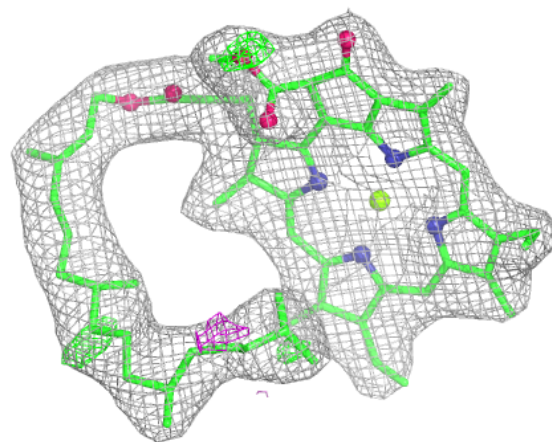
Electron density around CLA C 511:

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



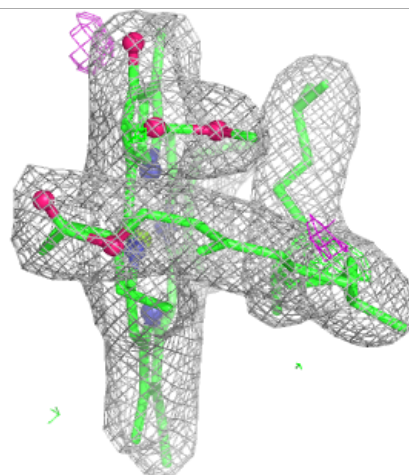
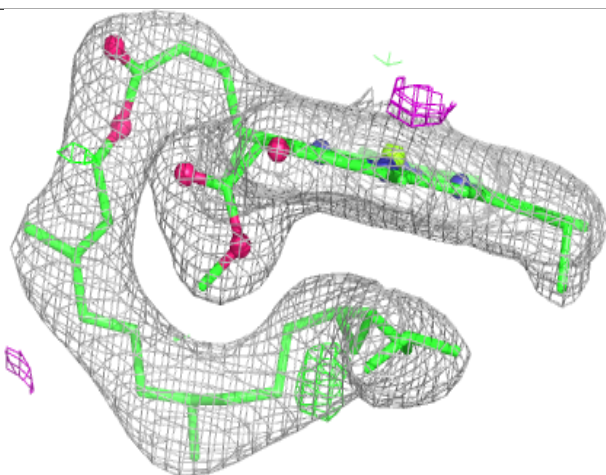
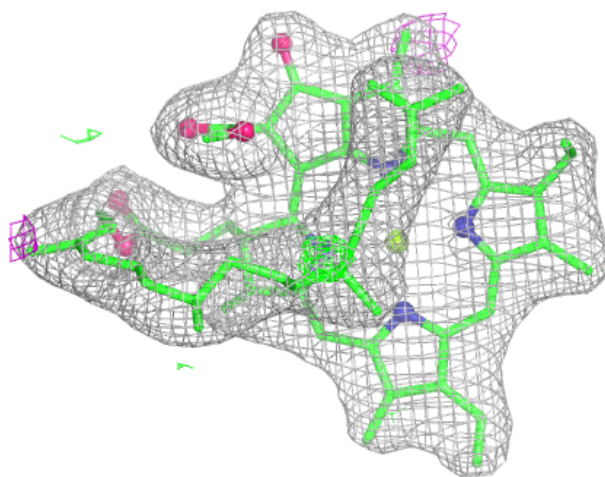
Electron density around CLA b 615:

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



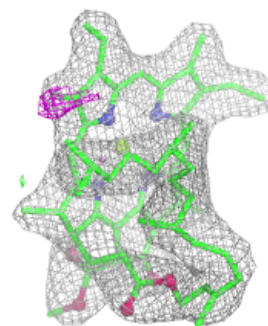
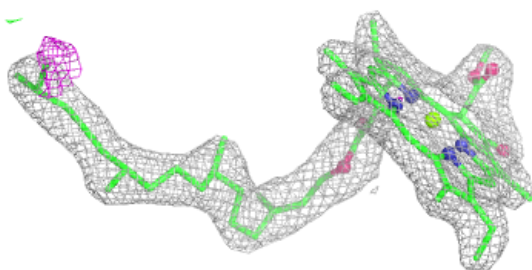
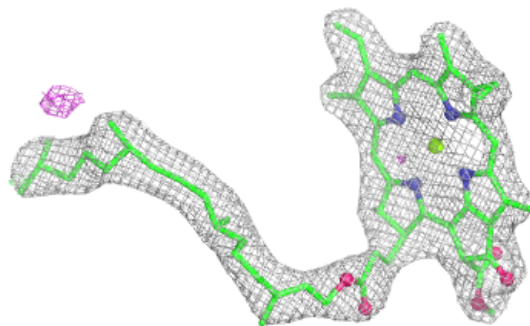
Electron density around CLA C 512:

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

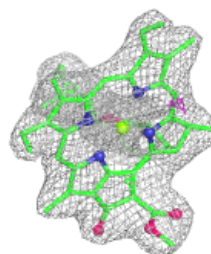
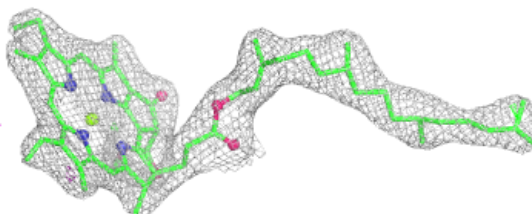
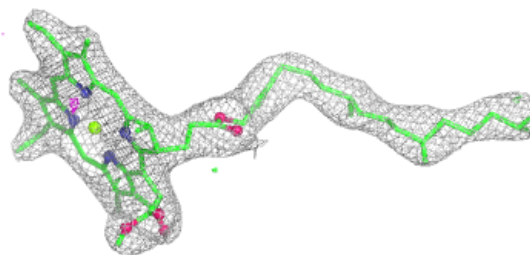


Electron density around CLA C 513:

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

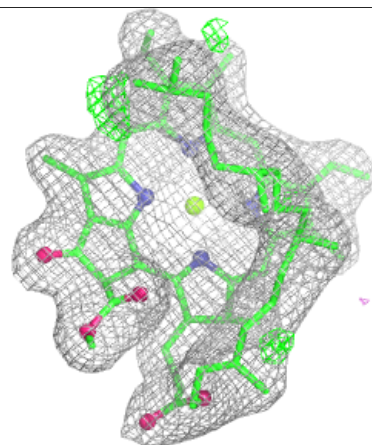
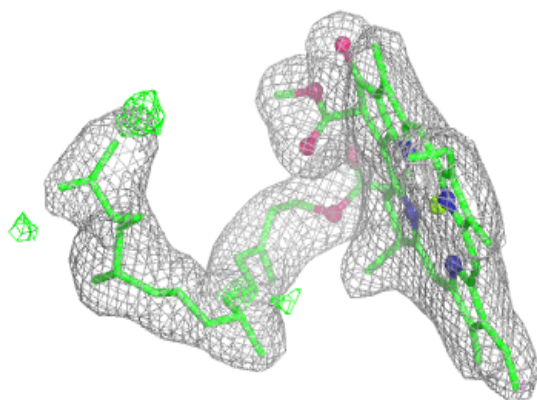
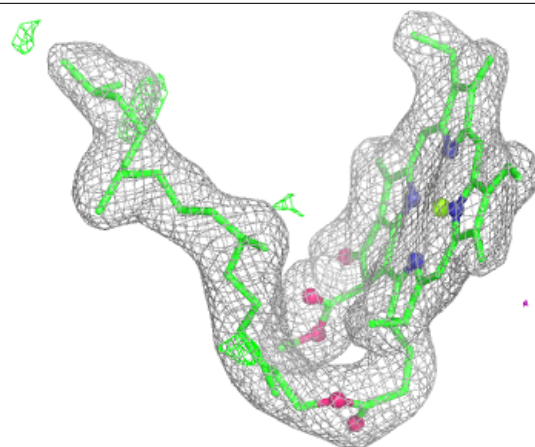
**Electron density around CLA c 503:**

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



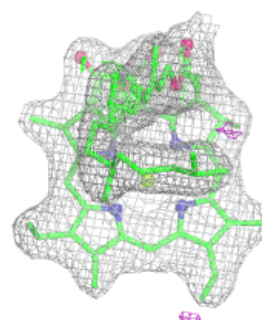
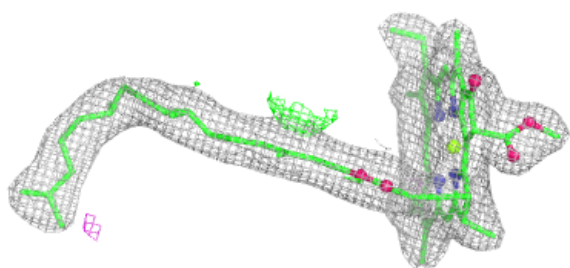
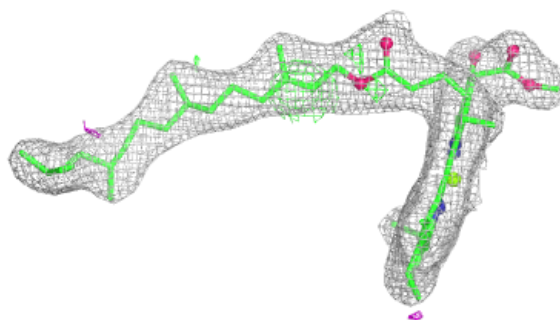
Electron density around CLA B 613:

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

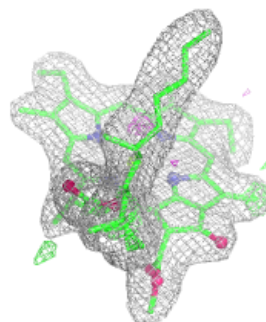
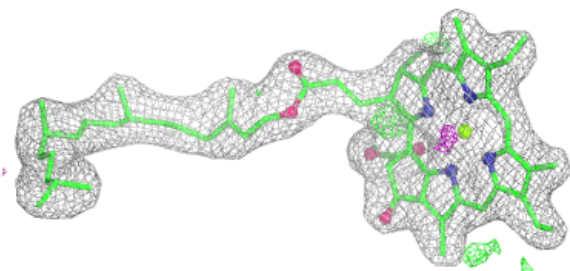
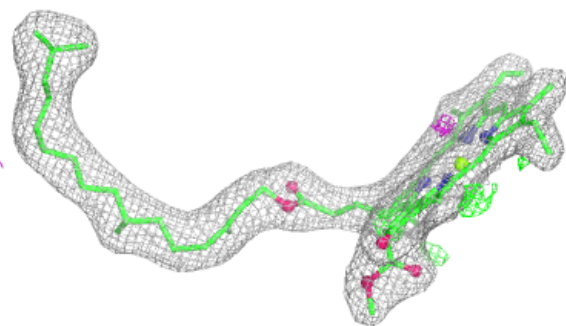


Electron density around CLA B 605:

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

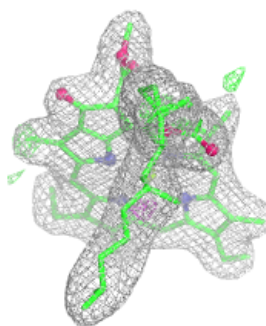
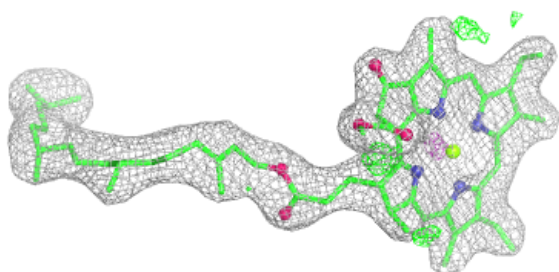
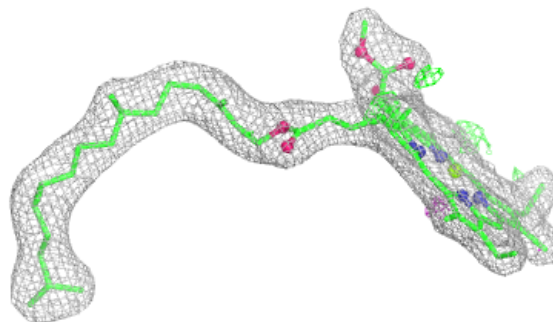
**Electron density around CLA D 404 (A):**

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

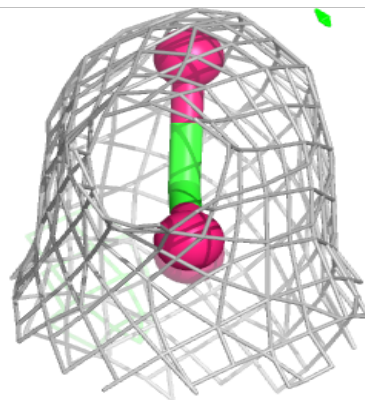
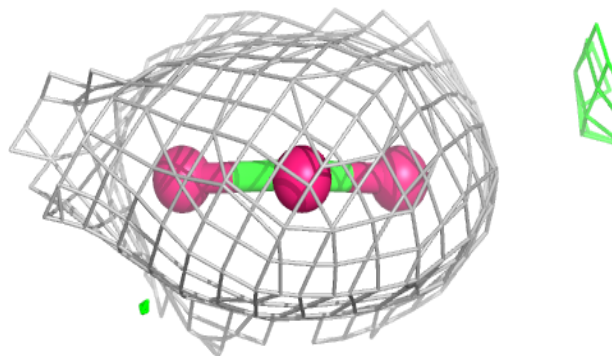
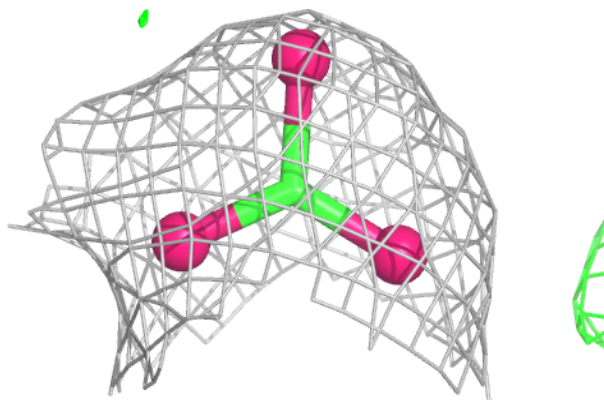


Electron density around CLA D 404 (B):

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

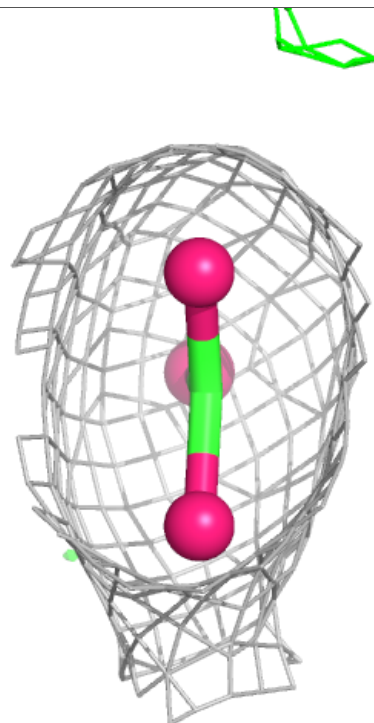
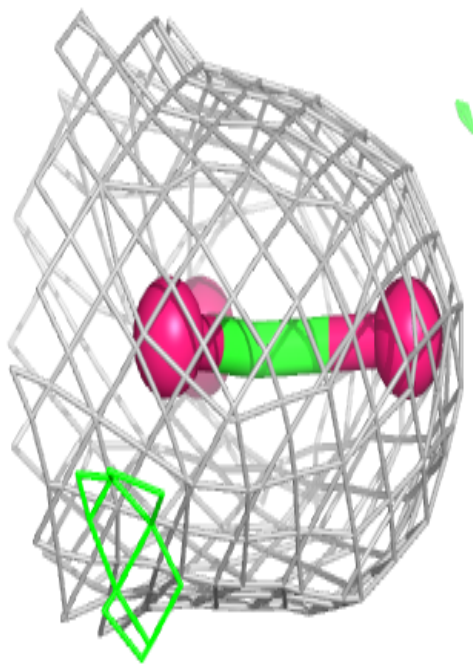
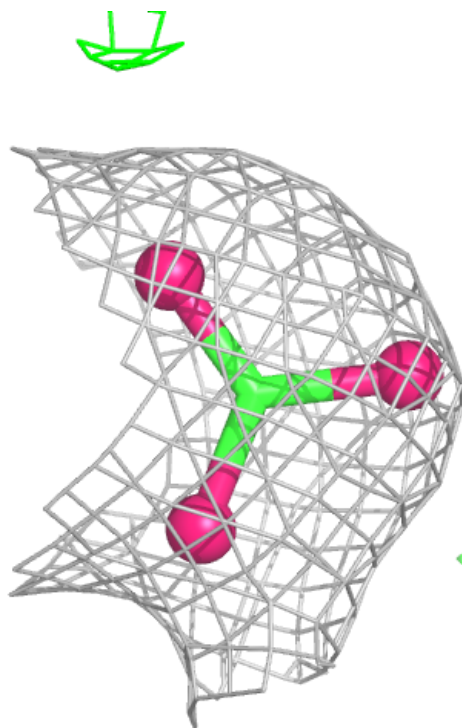
**Electron density around BCT a 404 (A):**

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



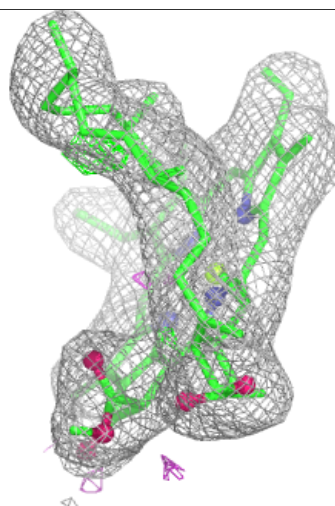
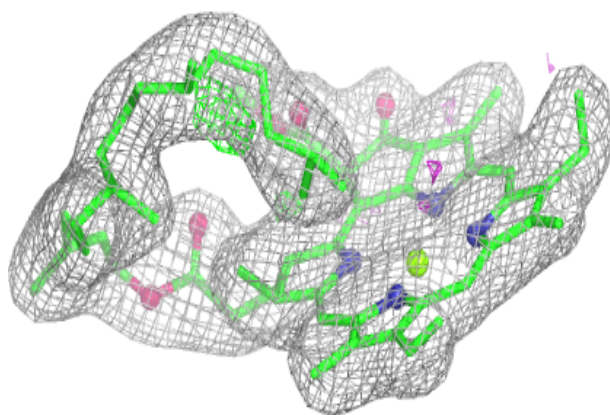
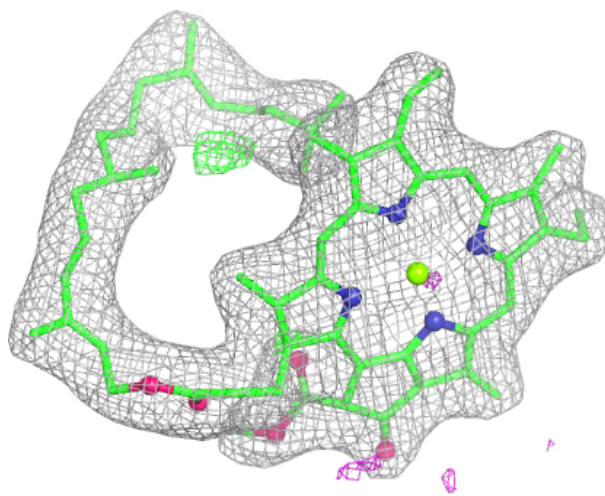
Electron density around BCT a 404 (B):

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



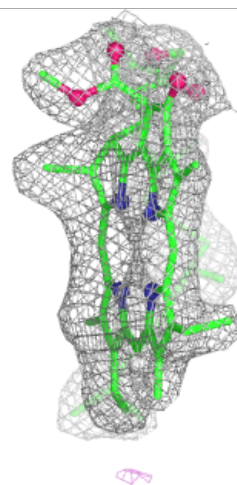
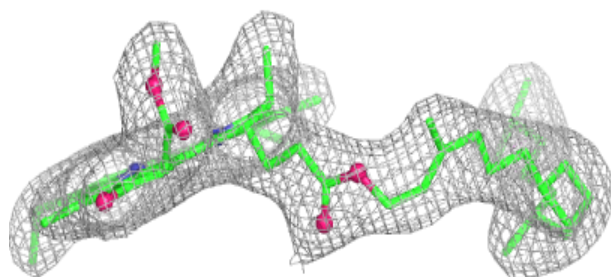
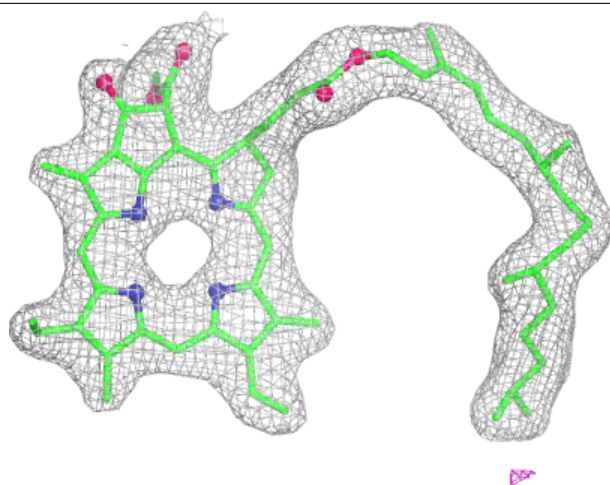
Electron density around CLA B 615:

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



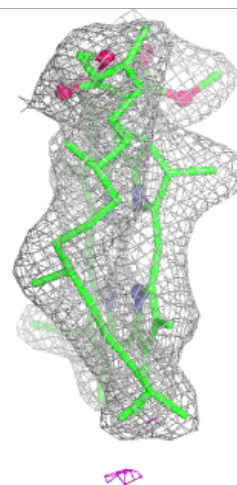
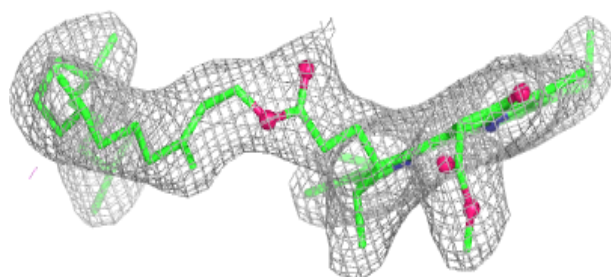
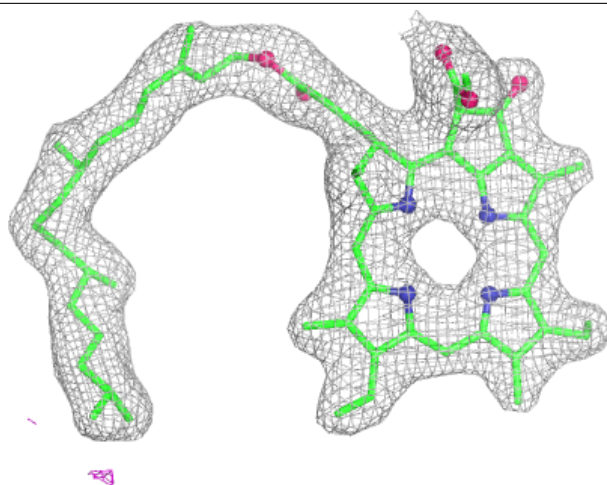
Electron density around PHO D 401 (A):

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



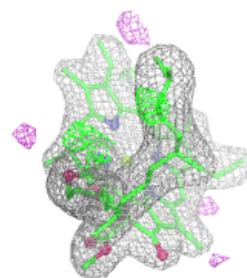
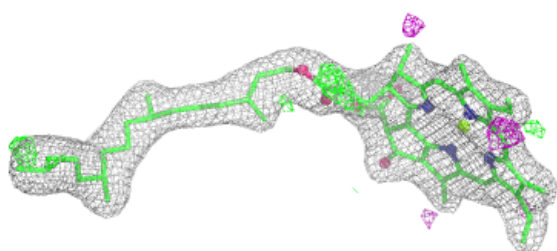
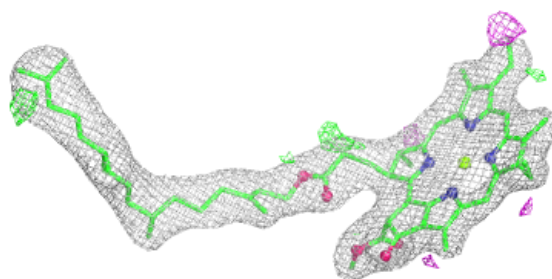
Electron density around PHO D 401 (B):

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



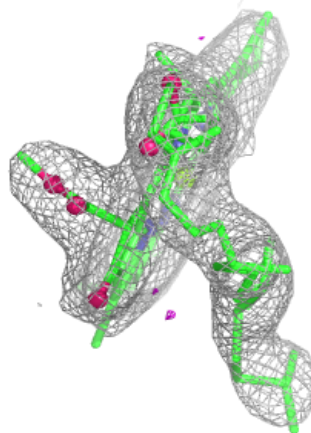
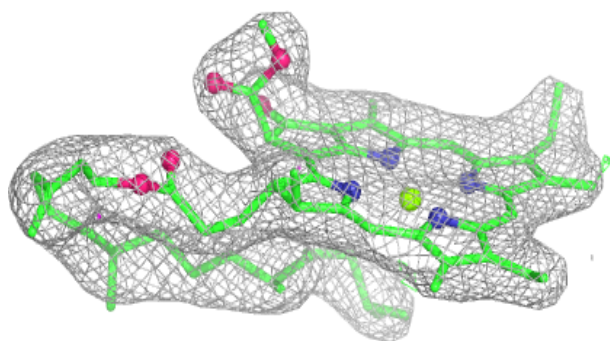
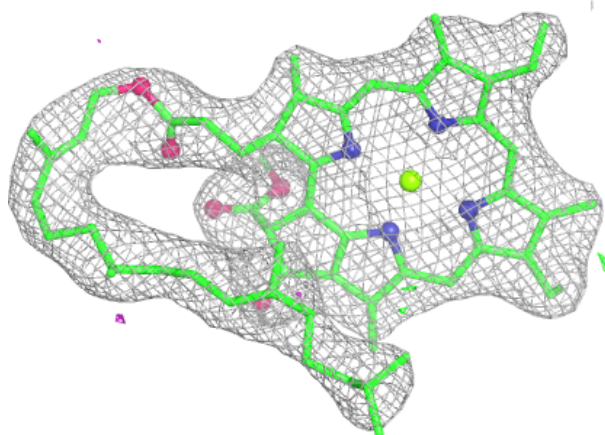
Electron density around CLA a 405 (A):

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



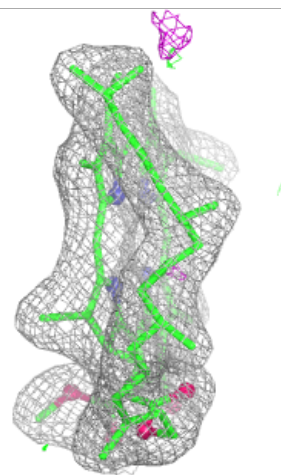
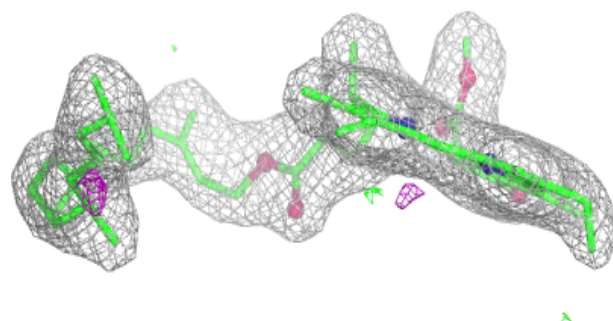
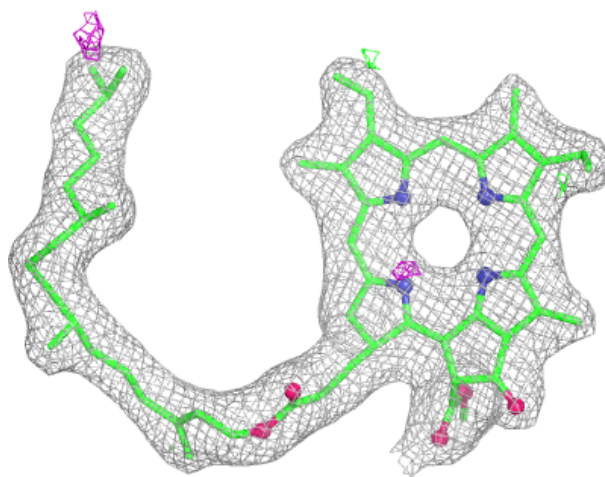
Electron density around CLA c 510:

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



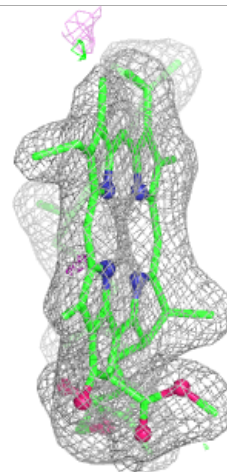
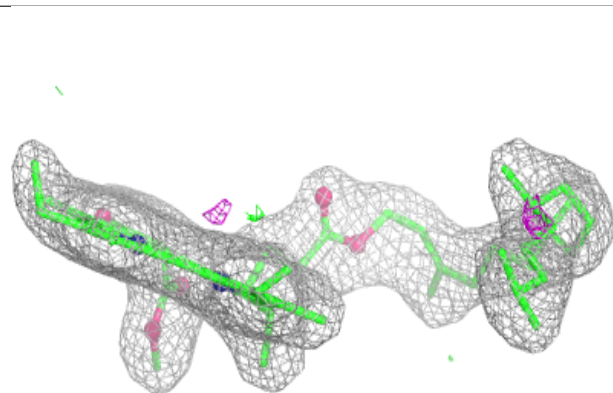
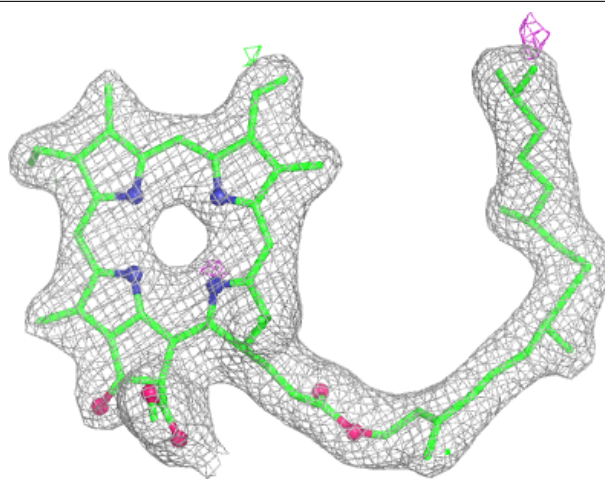
Electron density around PHO a 408 (A):

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



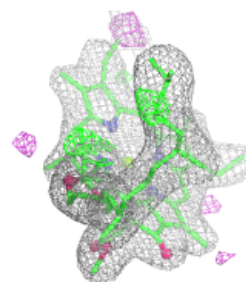
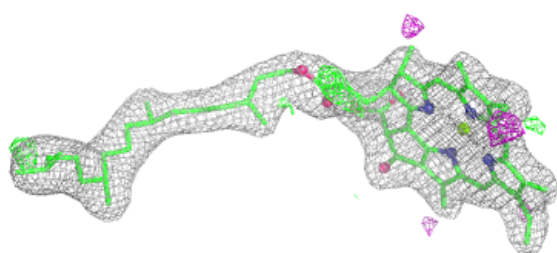
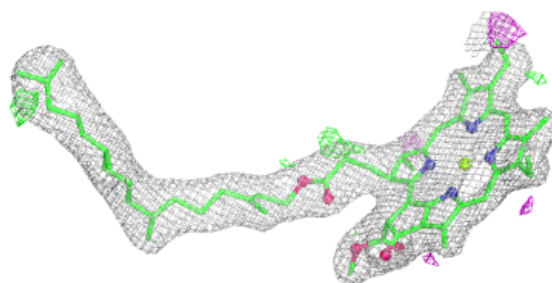
Electron density around PHO a 408 (B):

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

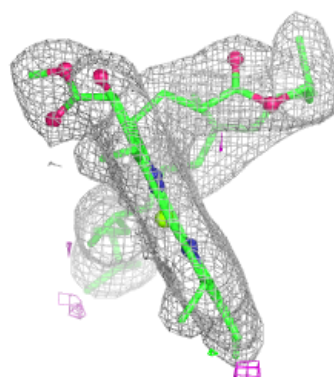
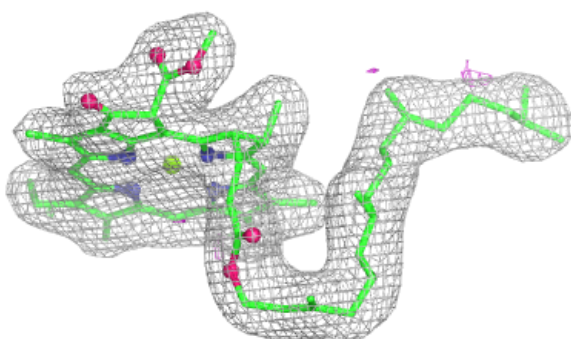
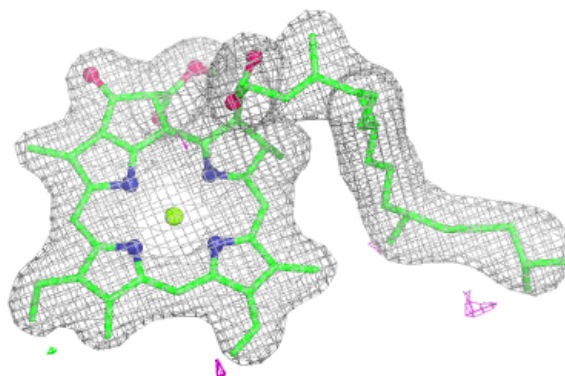


Electron density around CLA a 405 (B):

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

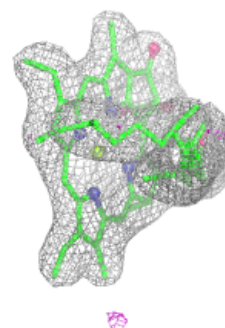
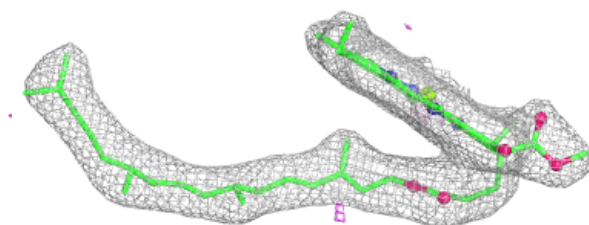
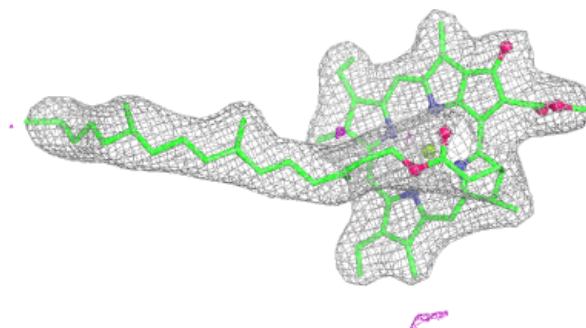
**Electron density around CLA a 406 (A):**

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



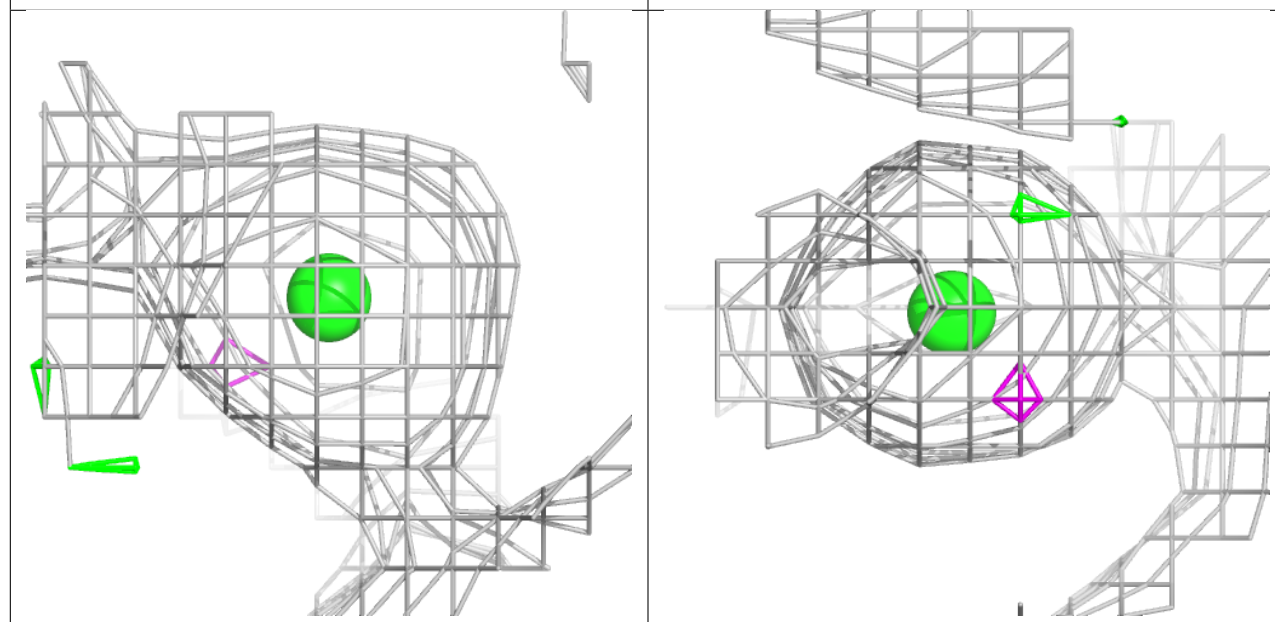
Electron density around CLA B 608:

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



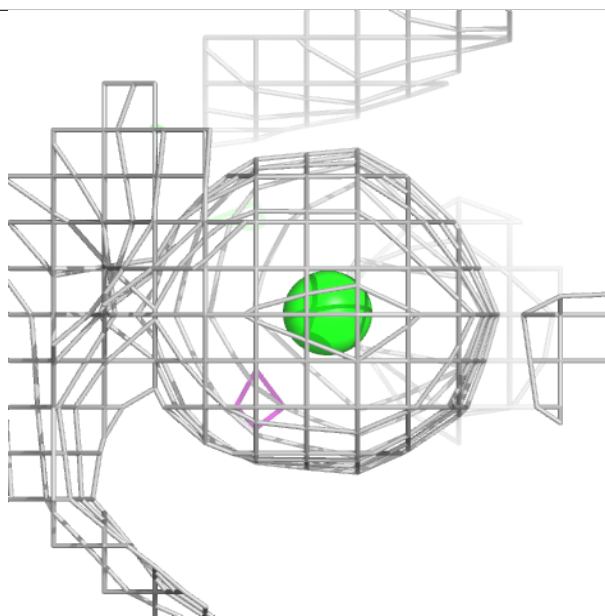
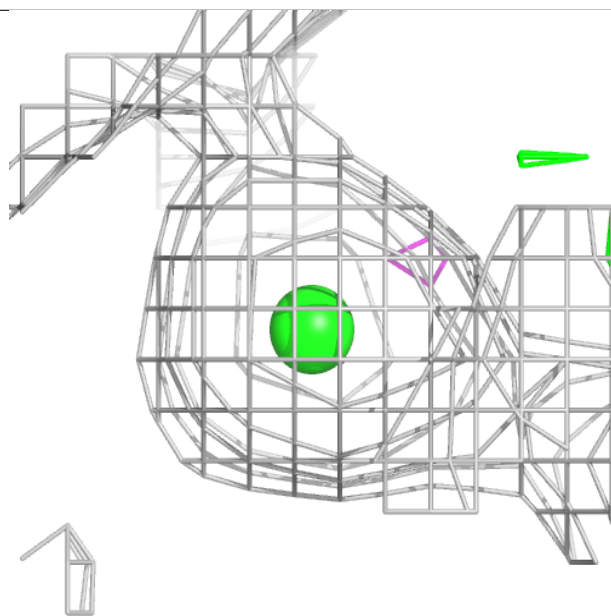
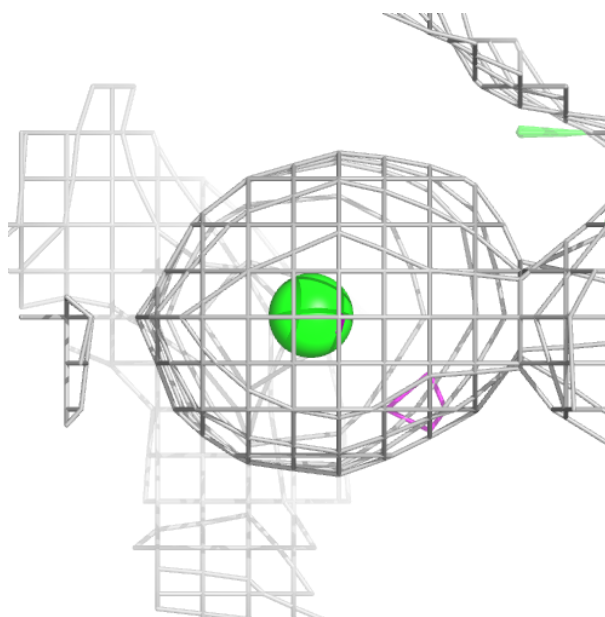
Electron density around CL a 403 (A):

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



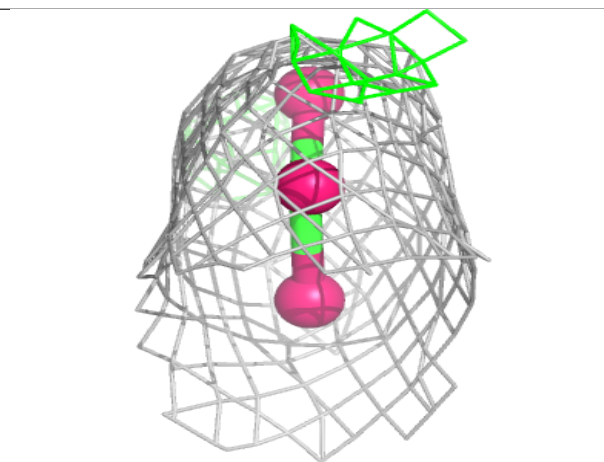
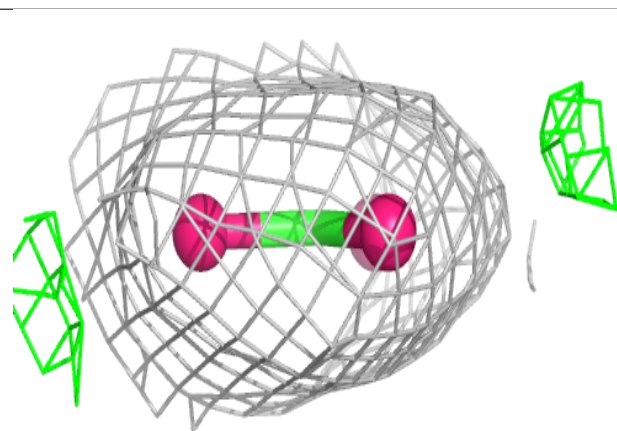
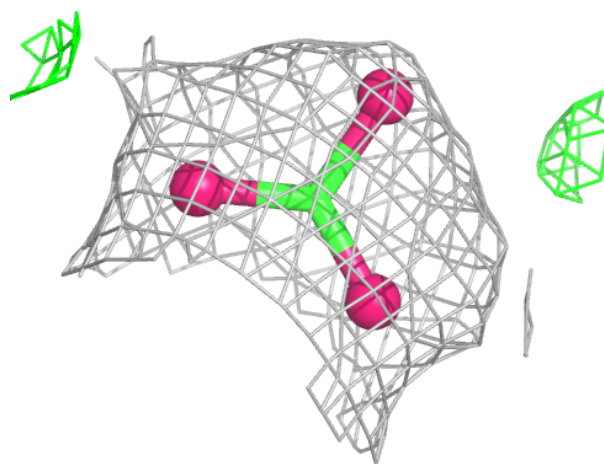
Electron density around CL a 403 (B):

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



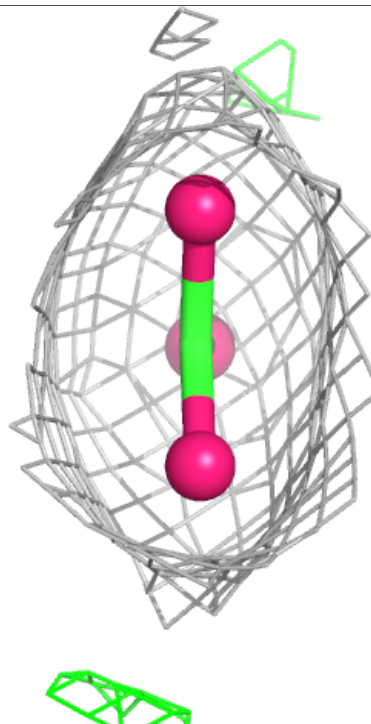
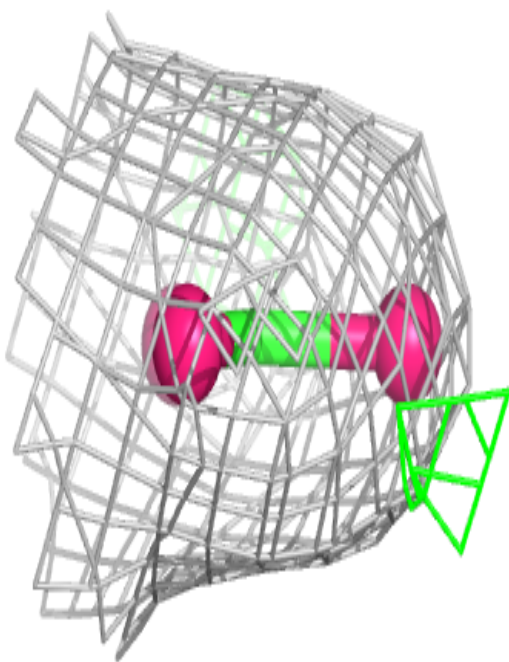
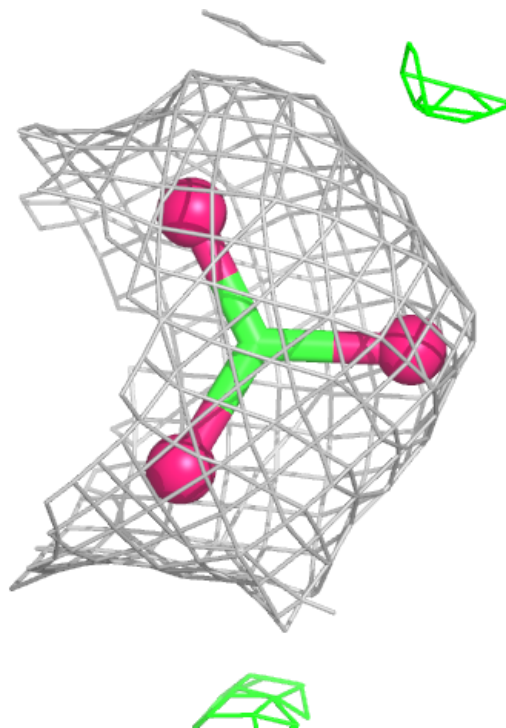
Electron density around BCT A 414 (A):

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



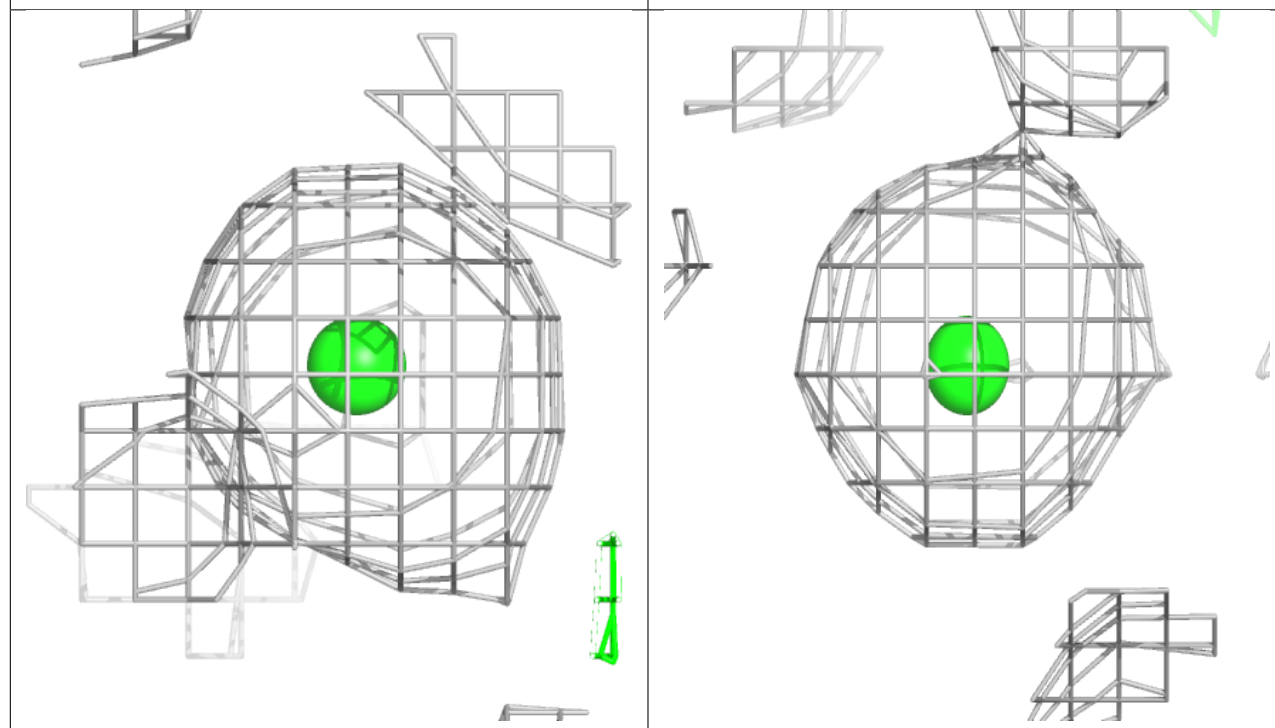
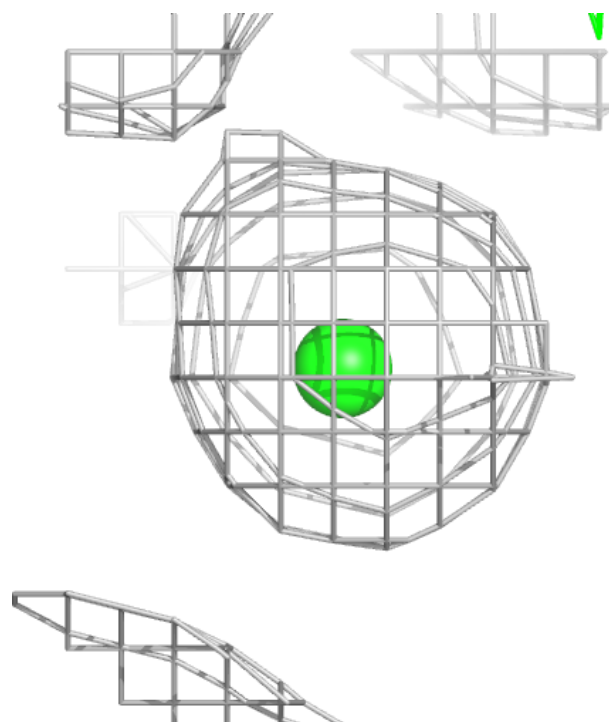
Electron density around BCT A 414 (B):

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



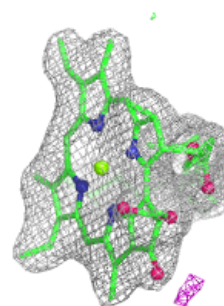
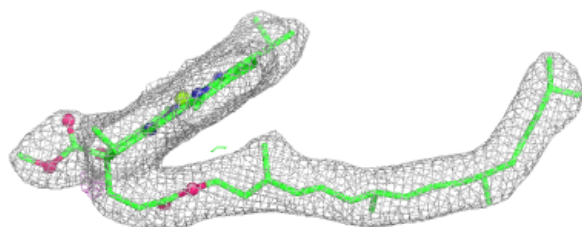
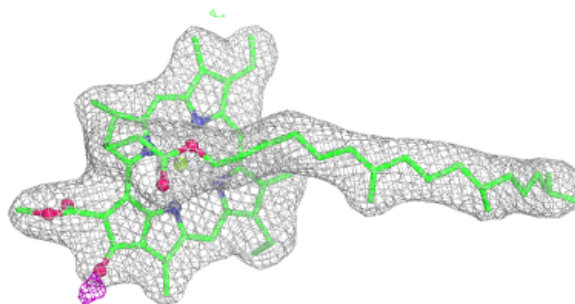
Electron density around CL a 402 (A):

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



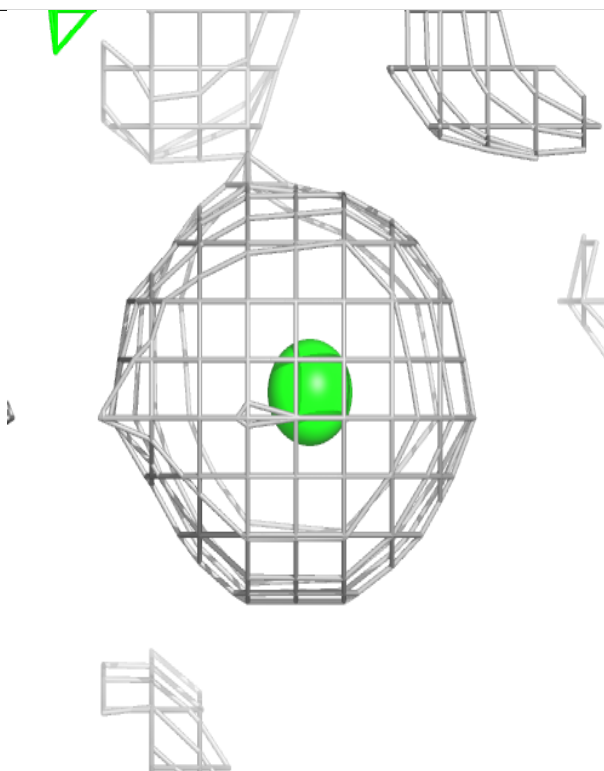
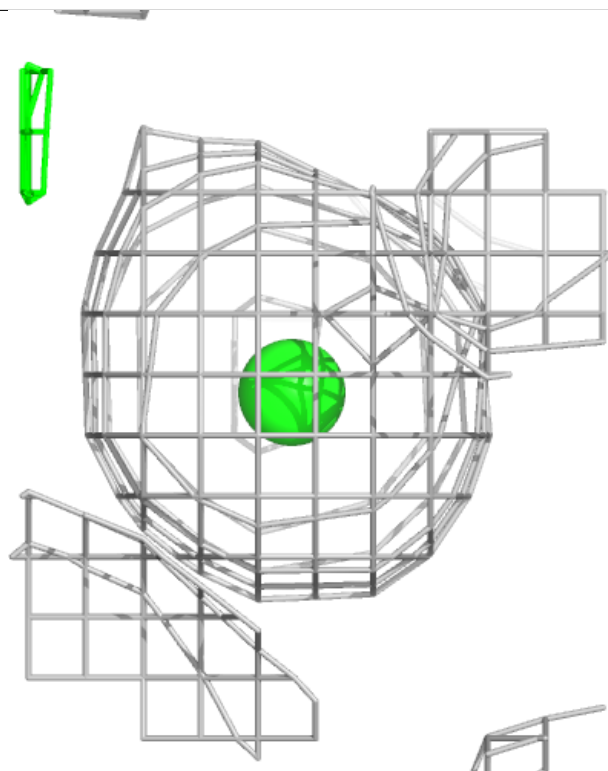
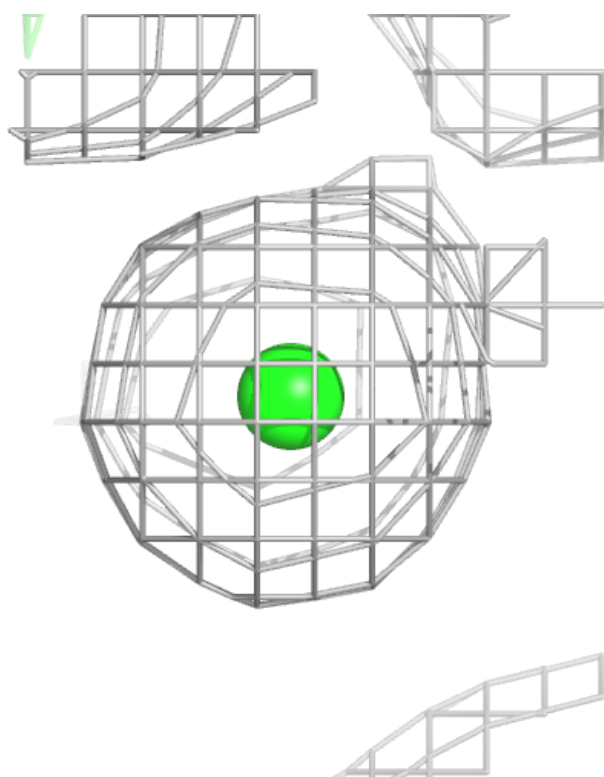
Electron density around CLA b 608:

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



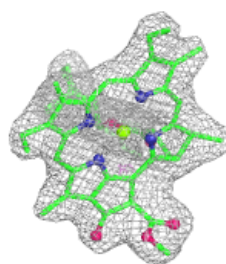
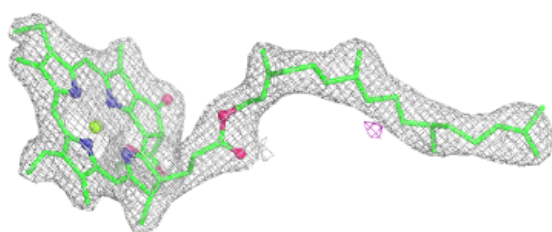
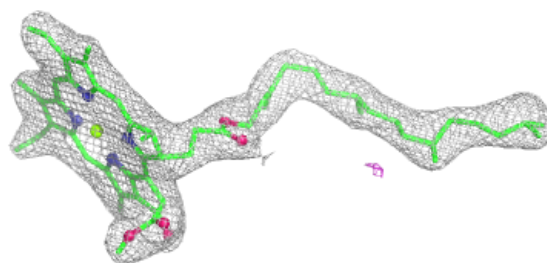
Electron density around CL a 402 (B):

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



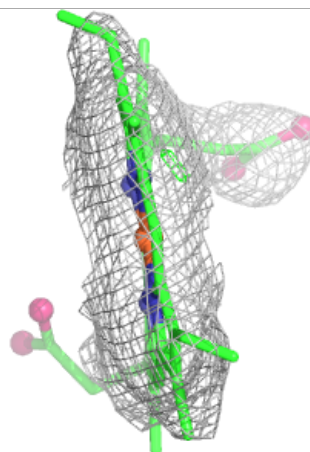
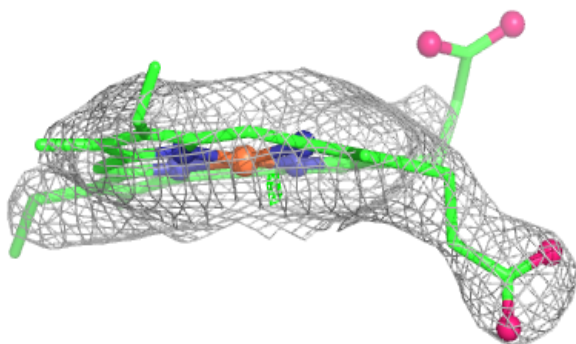
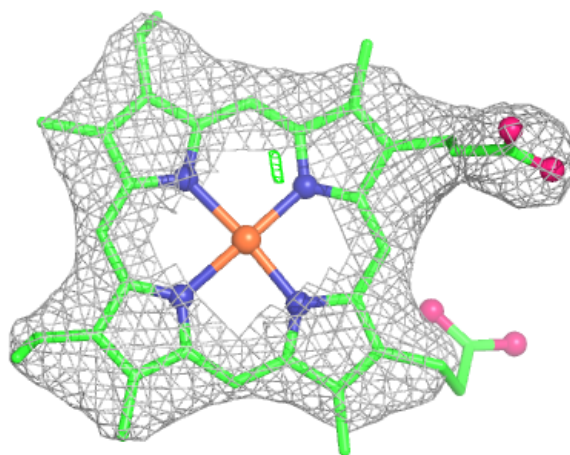
Electron density around CLA C 504:

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



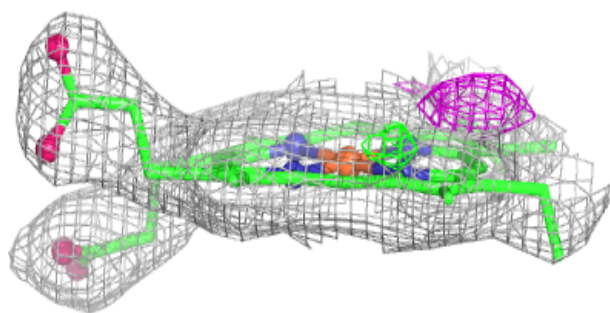
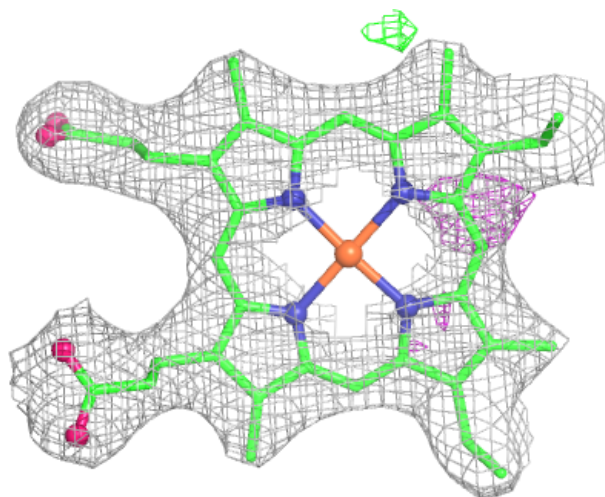
Electron density around HEM f 101:

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



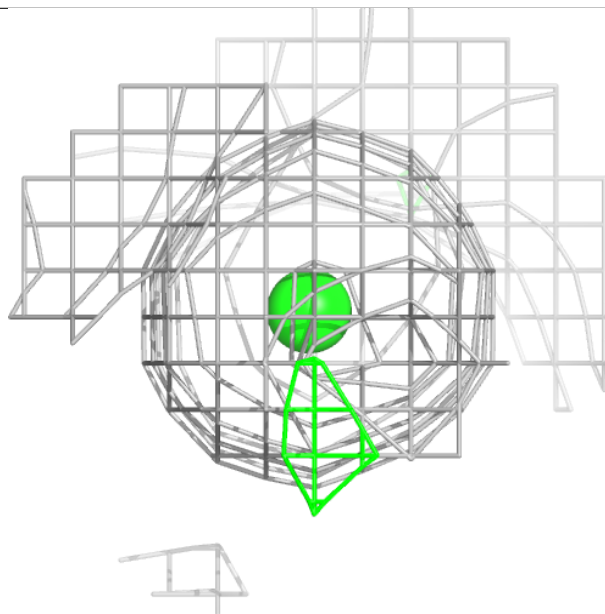
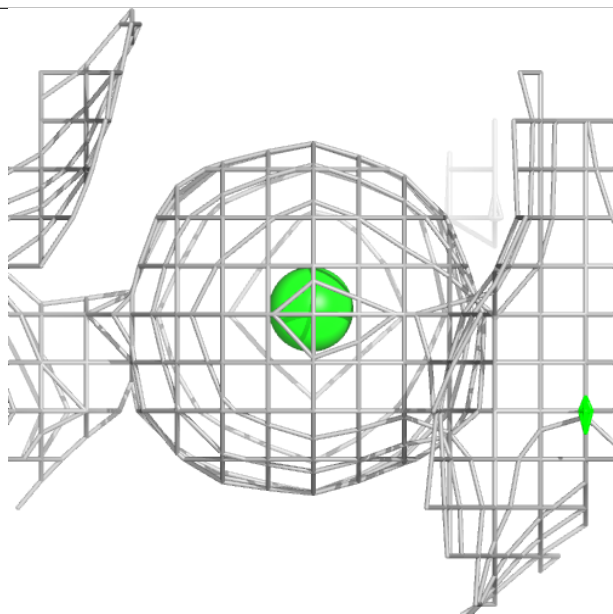
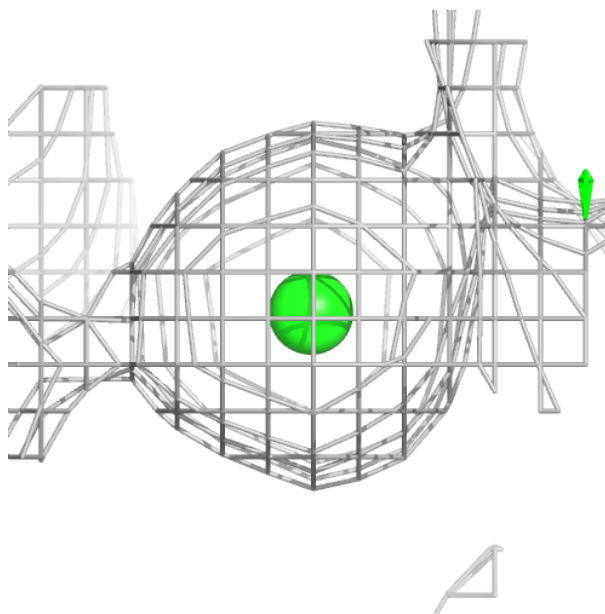
Electron density around HEC v 201:

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



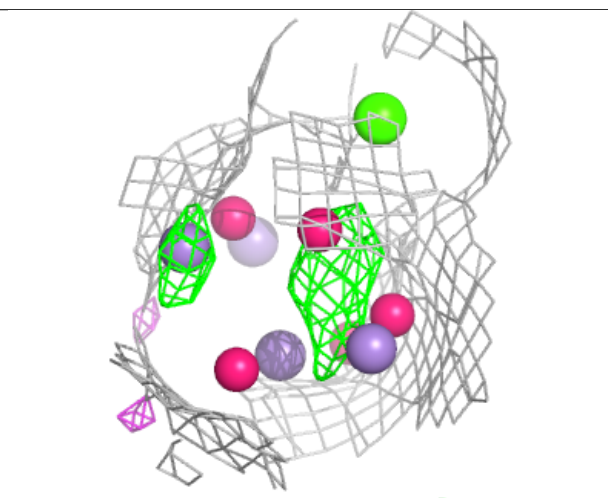
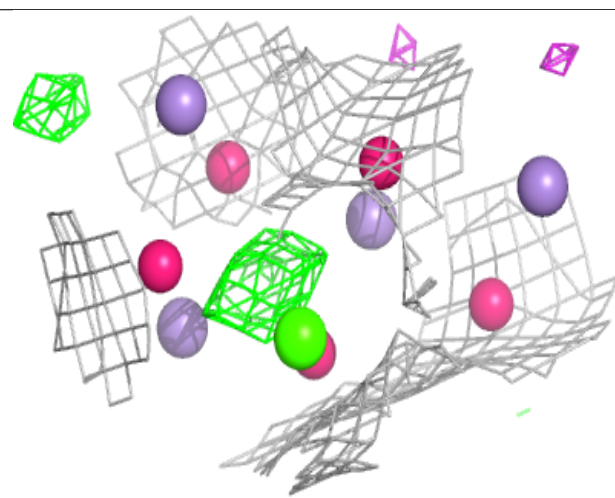
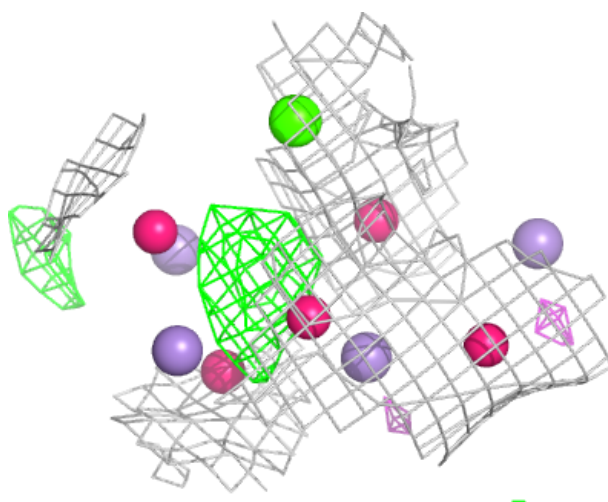
Electron density around CL A 403 (B):

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



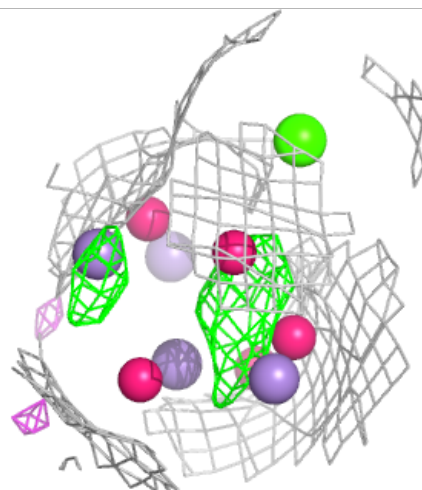
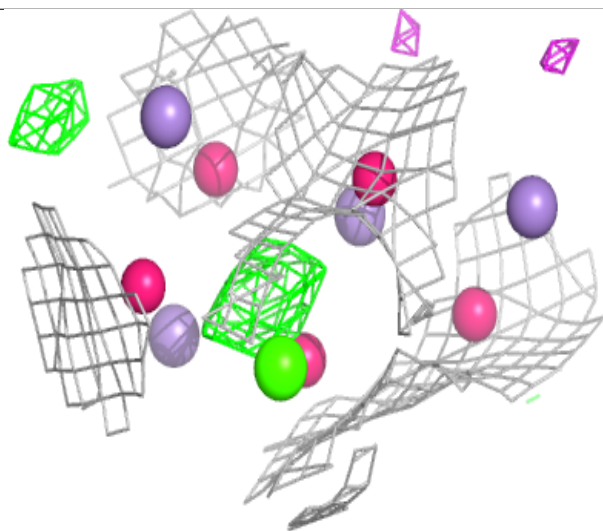
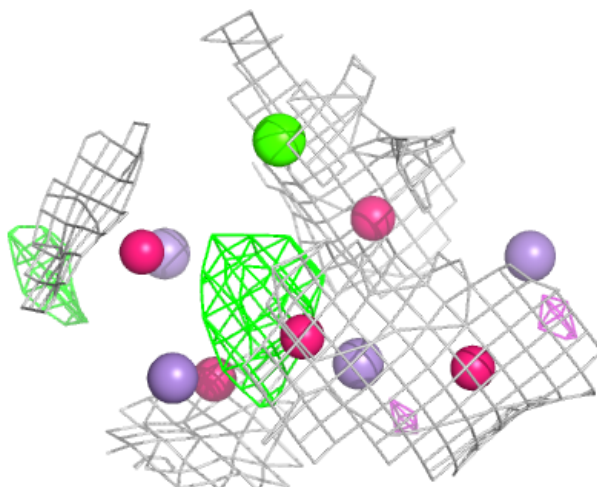
Electron density around OEX A 411 (A):

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



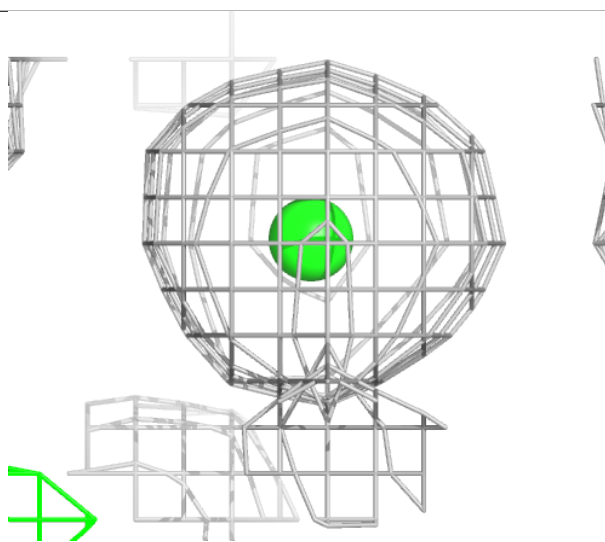
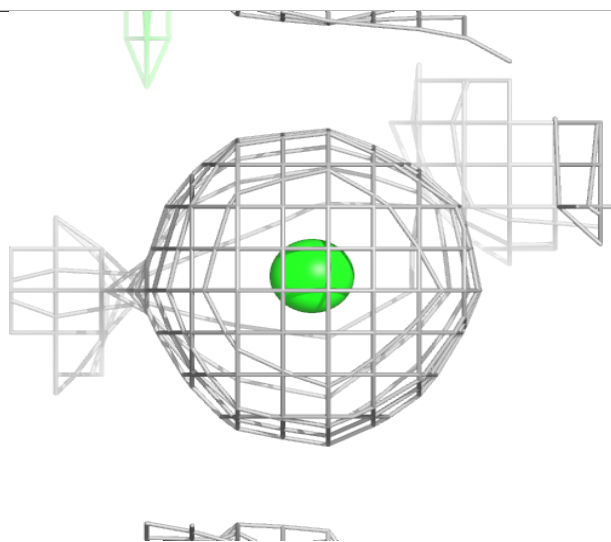
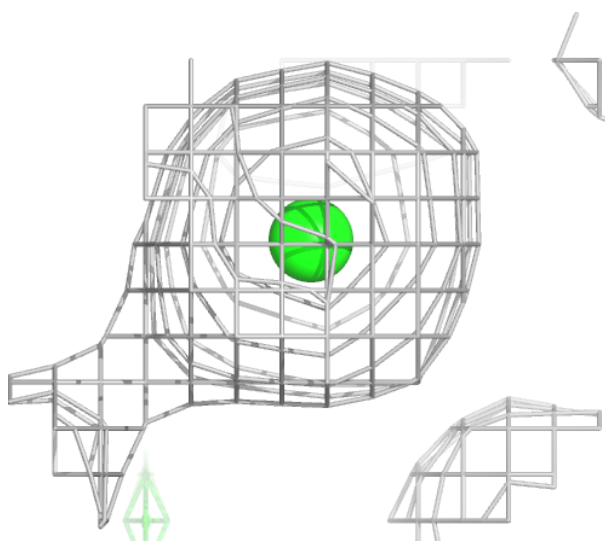
Electron density around OEX A 411 (B):

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



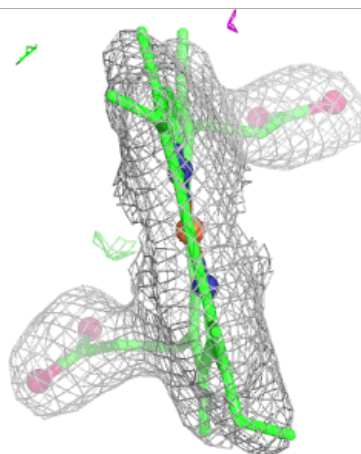
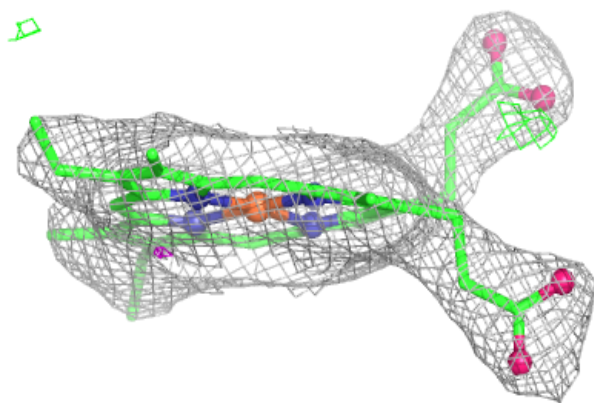
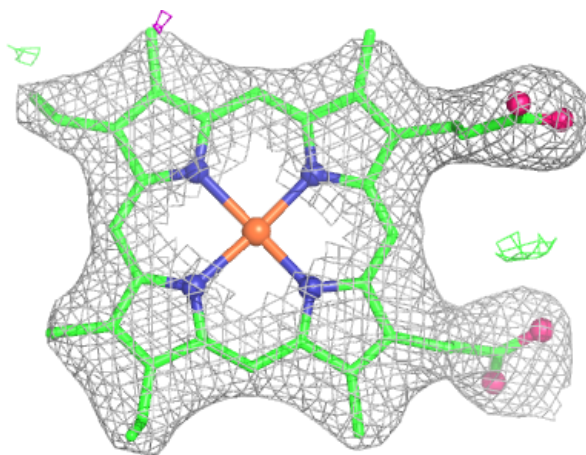
Electron density around CL A 402 (A):

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



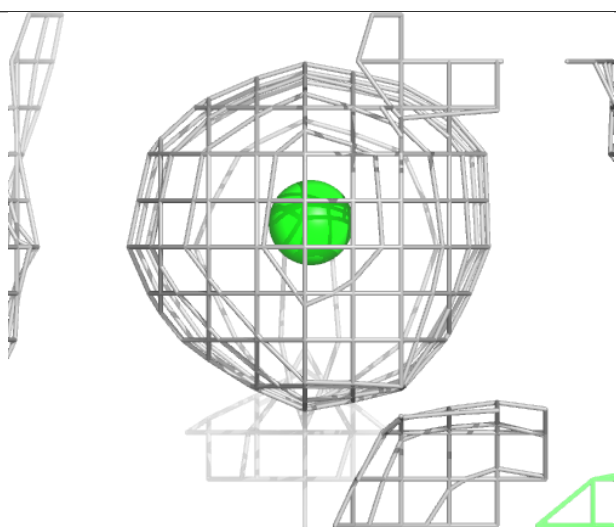
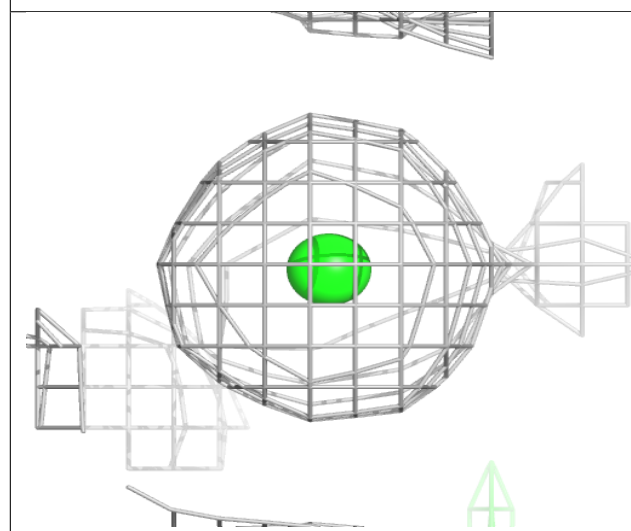
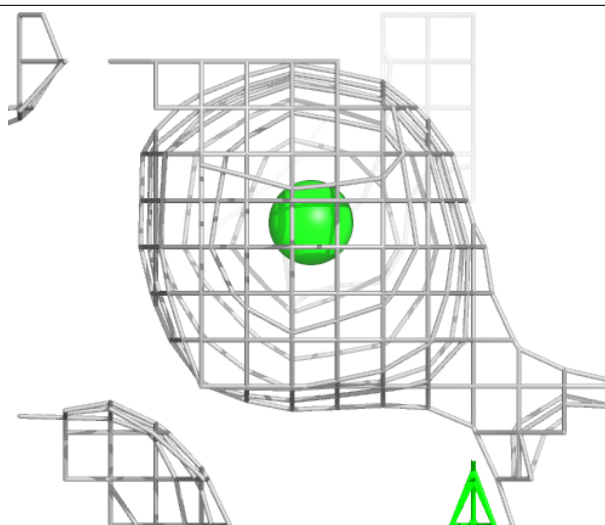
Electron density around HEM F 102:

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



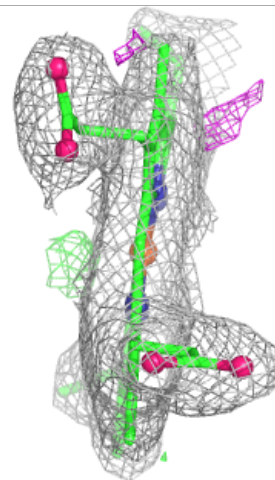
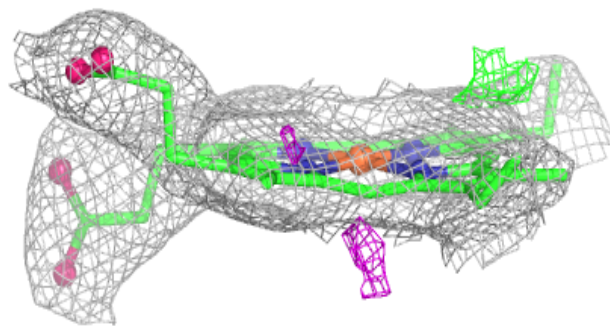
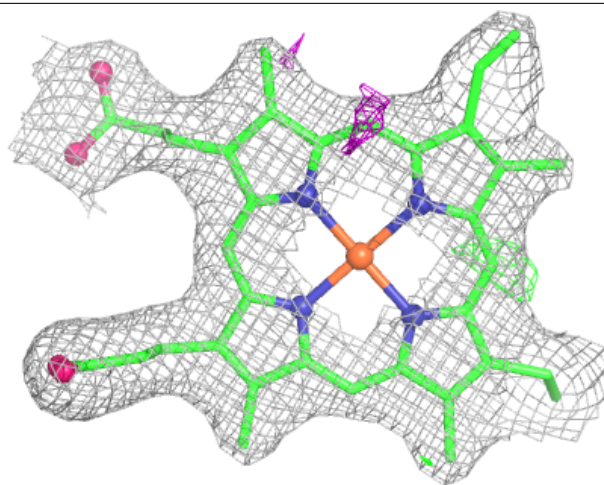
Electron density around CL A 402 (B):

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



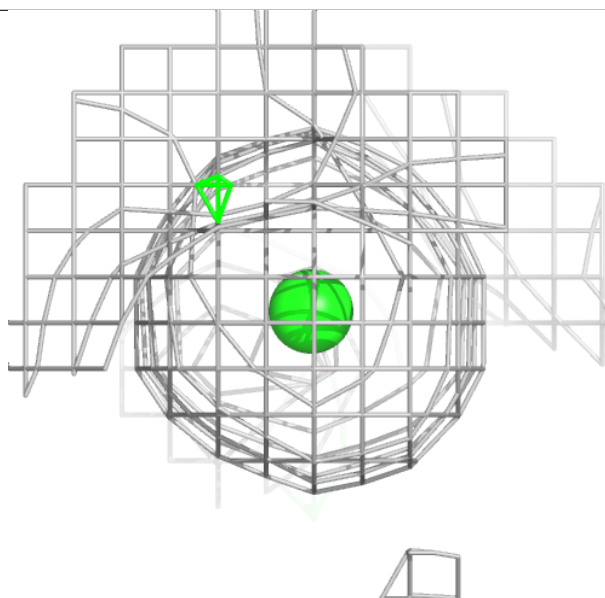
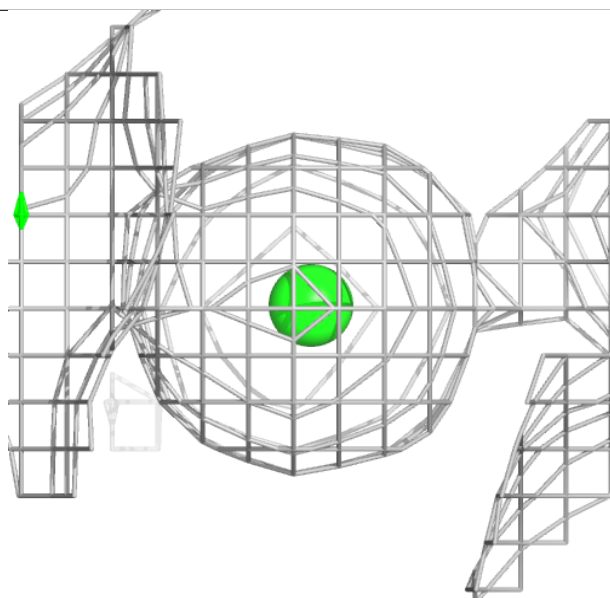
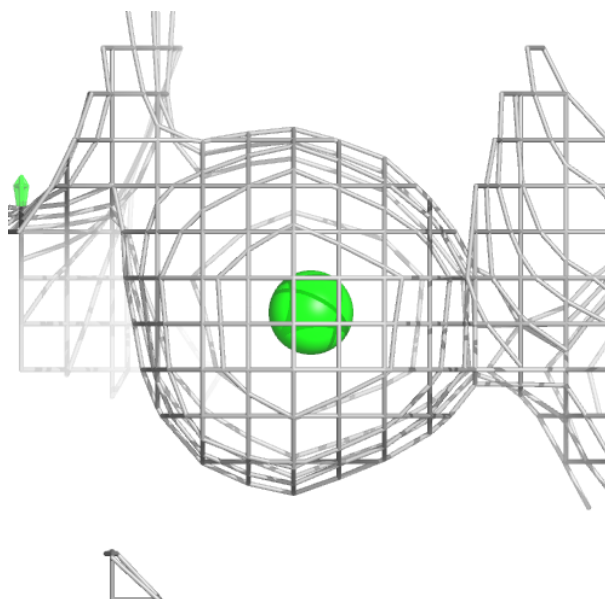
Electron density around HEC V 202:

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



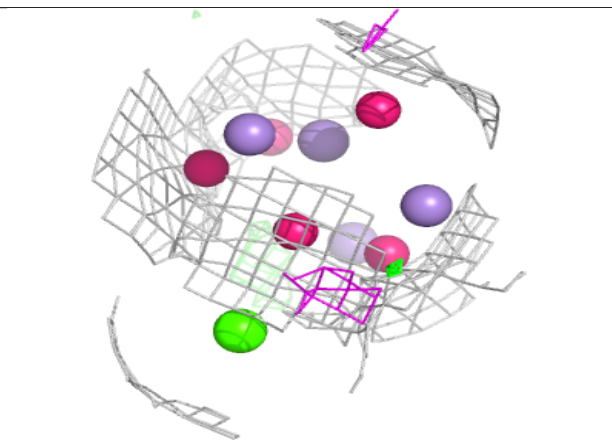
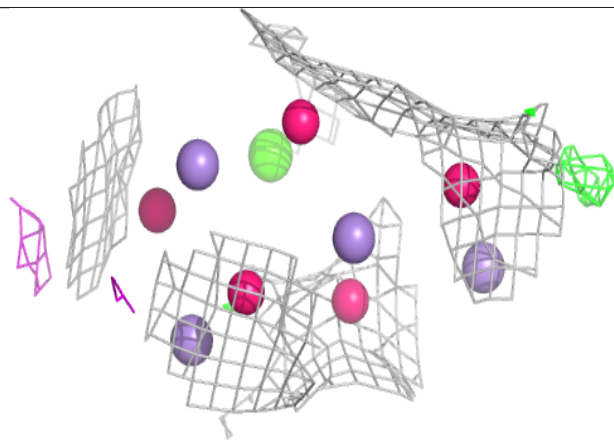
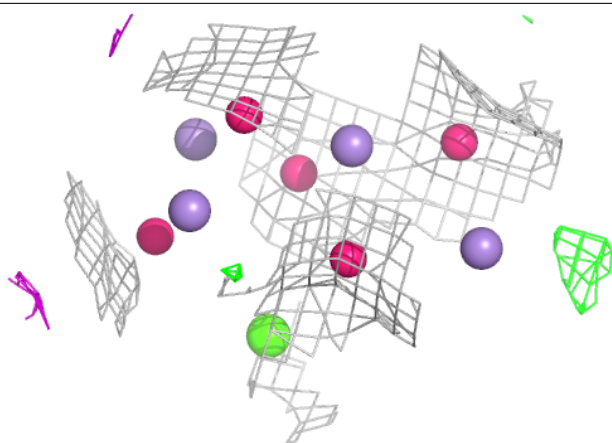
Electron density around CL A 403 (A):

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



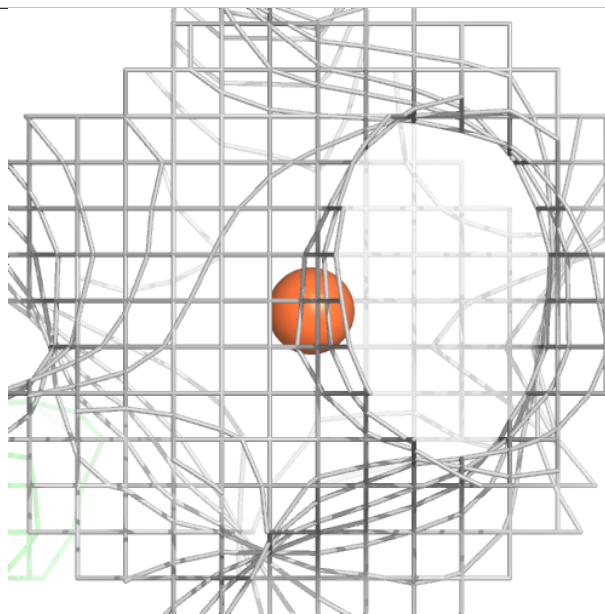
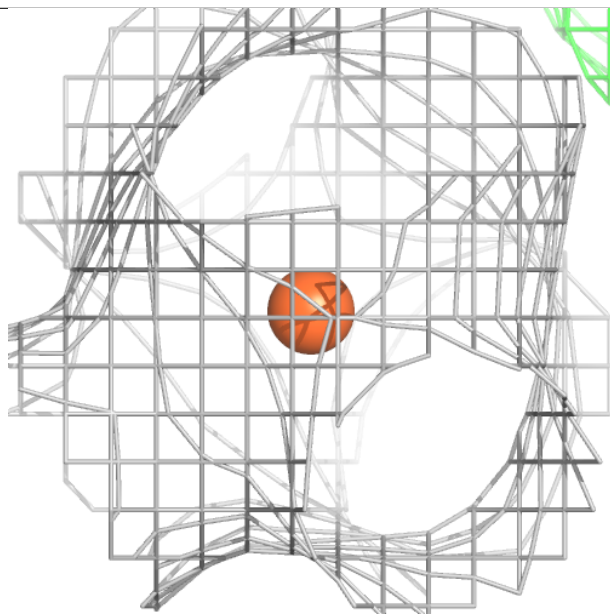
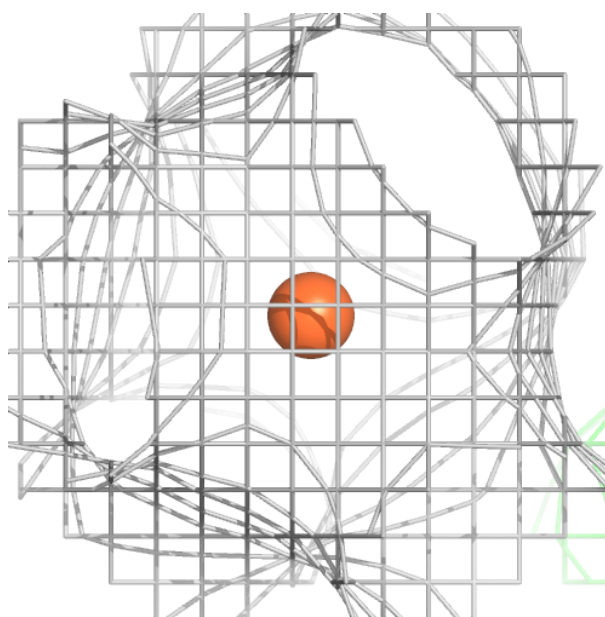
Electron density around OEX a 413 (B):

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



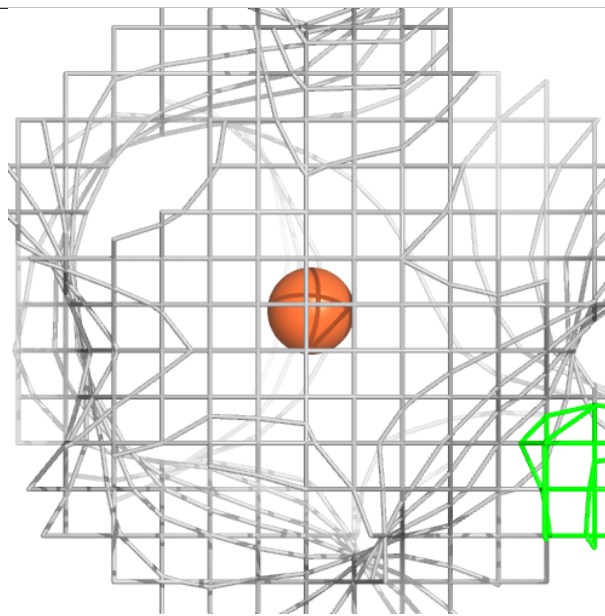
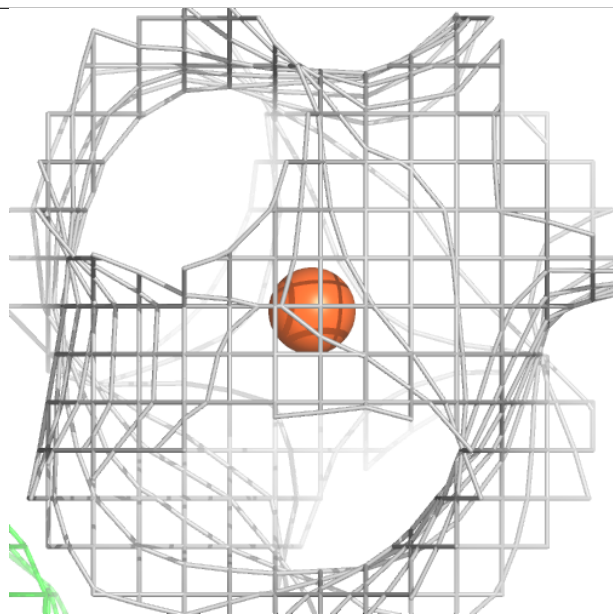
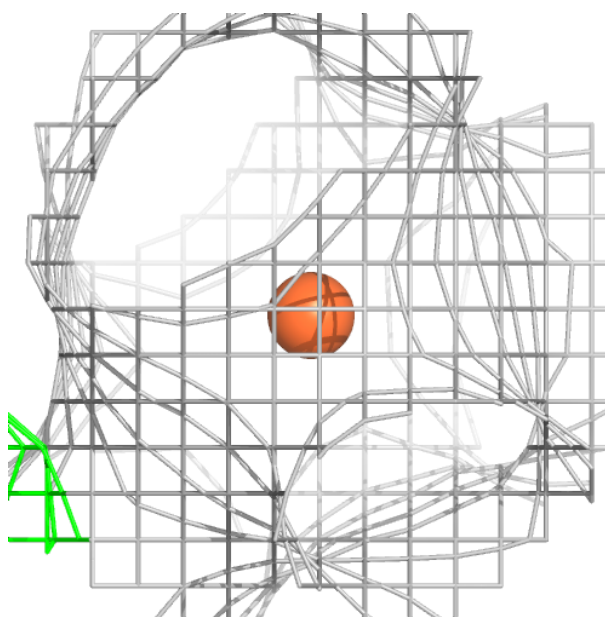
Electron density around FE2 a 401 (A):

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



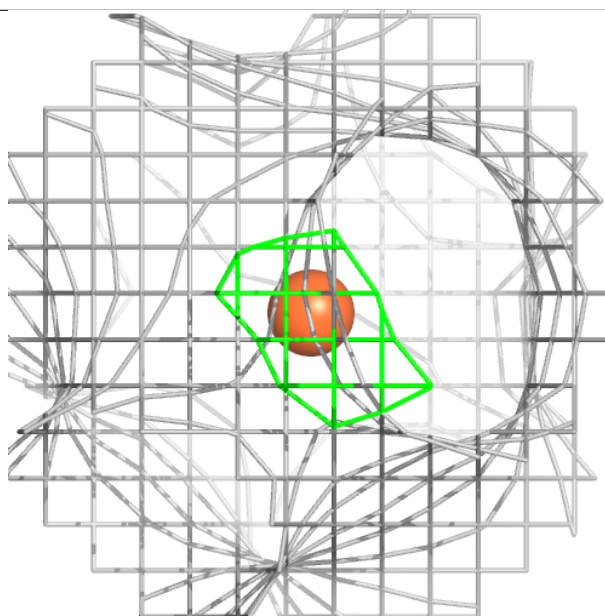
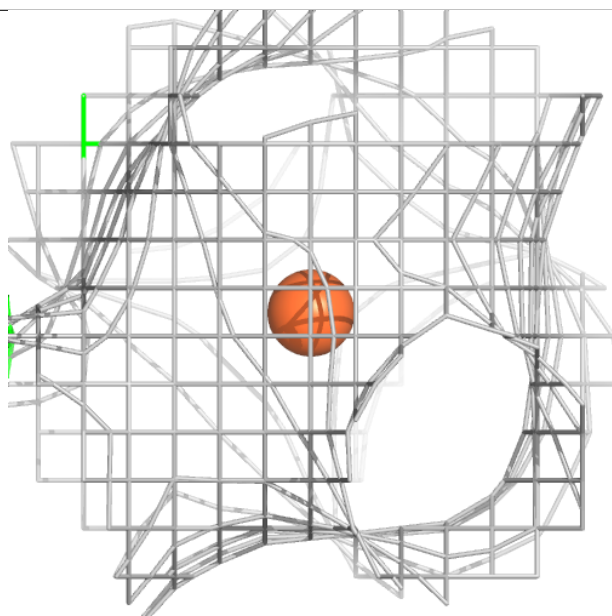
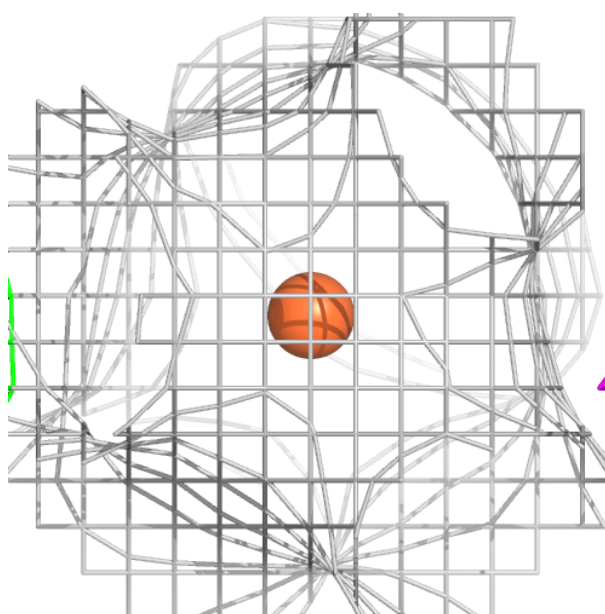
Electron density around FE2 a 401 (B):

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



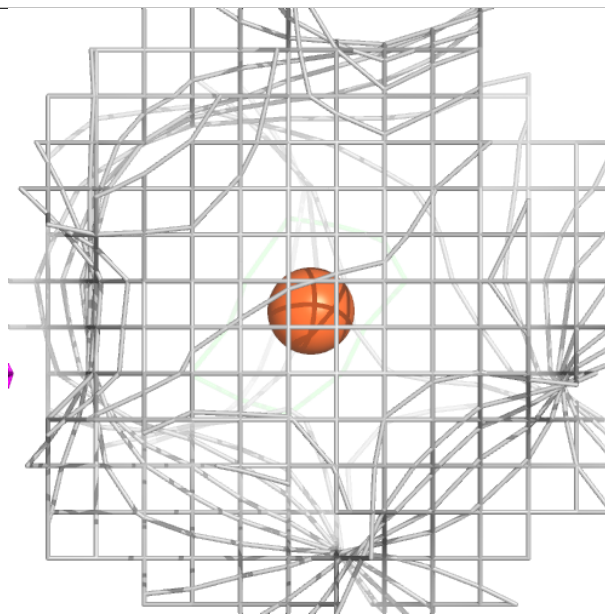
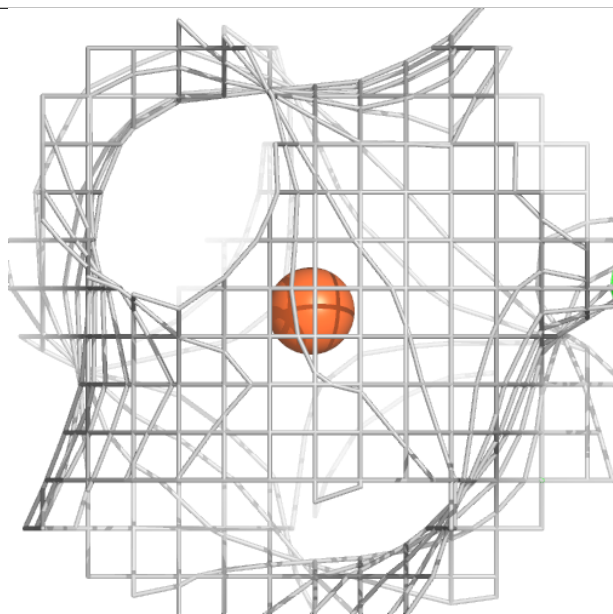
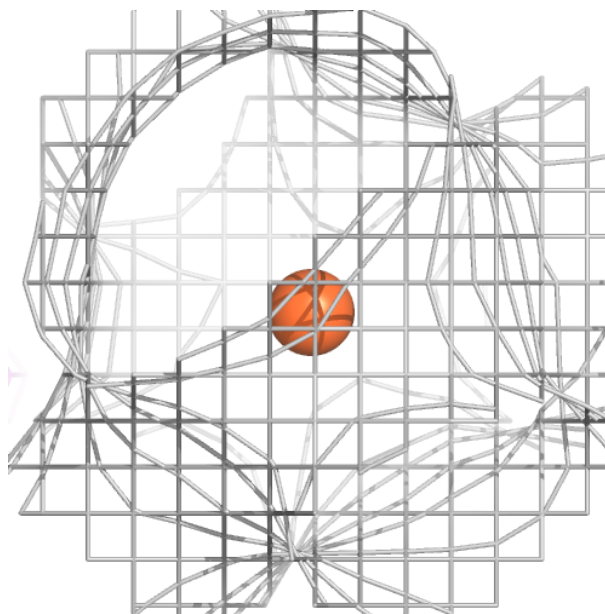
Electron density around FE2 A 401 (A):

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



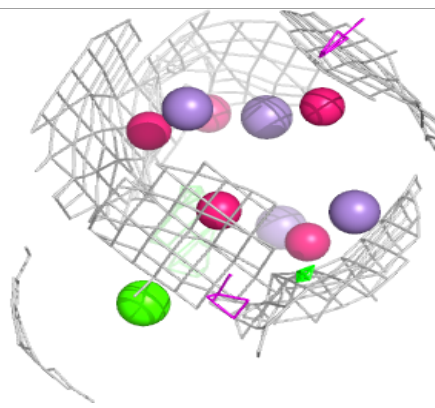
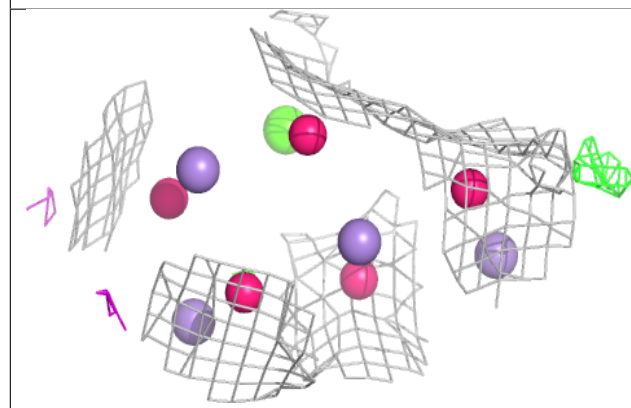
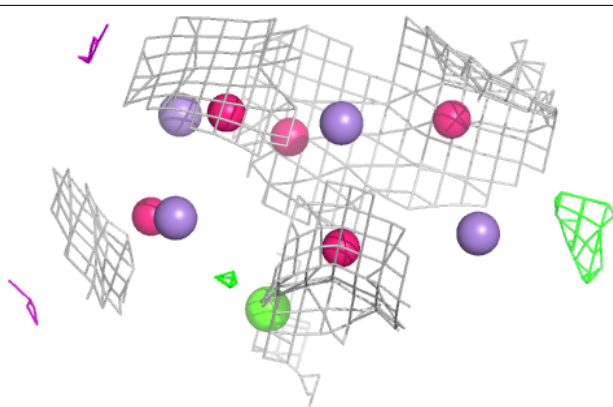
Electron density around FE2 A 401 (B):

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



Electron density around OEX a 413 (A):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.