



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 08:20 PM UTC

PDB ID : 8GN1 / pdb_00008gn1
Title : Crystal structure of DBBQ-bound photosystem II complex
Authors : Kamada, S.; Nakajima, Y.; Shen, J.-R.
Deposited on : 2022-08-22
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

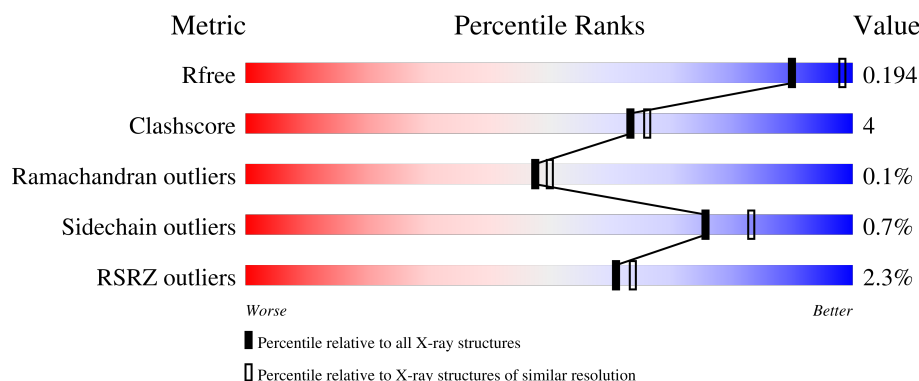
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



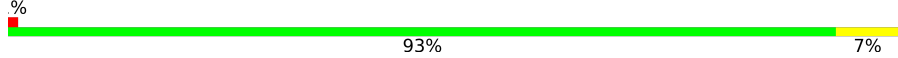
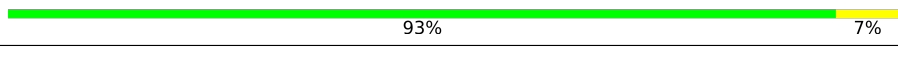
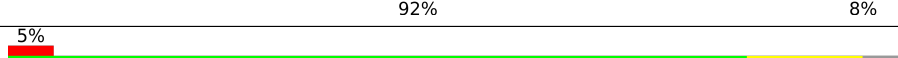
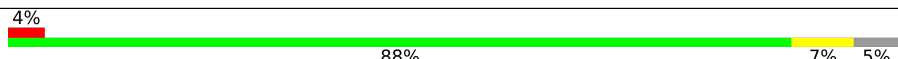
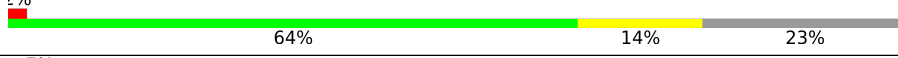
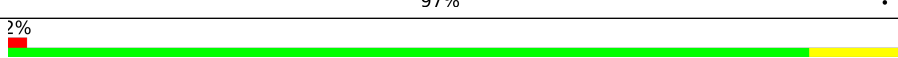
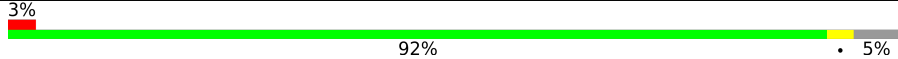
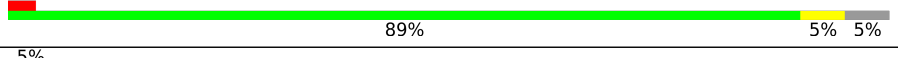
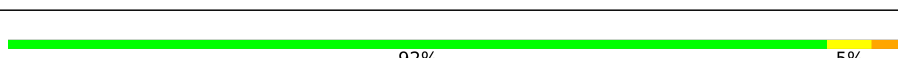
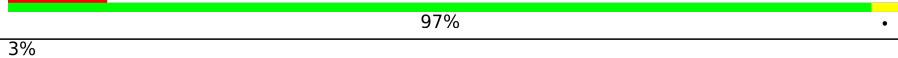
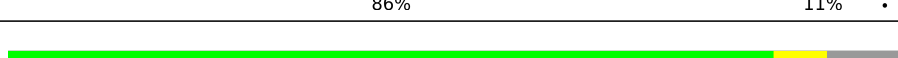
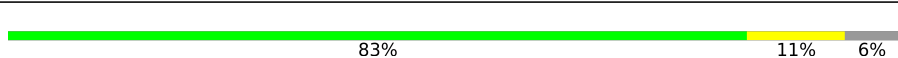
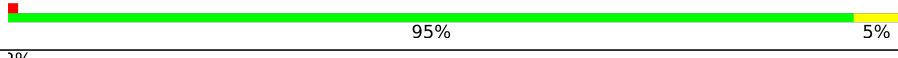
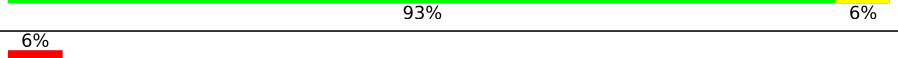
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	% 89% 8% .
1	a	344	2% 90% 8% .
2	B	505	2% 94% 6%
2	b	505	3% 91% 9%
3	C	455	% 91% 7% .

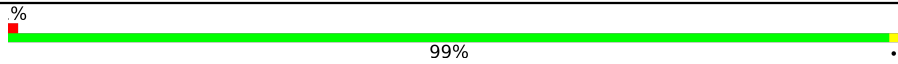
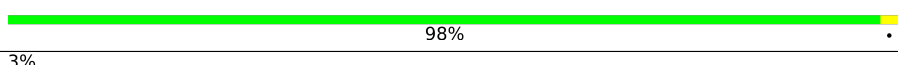
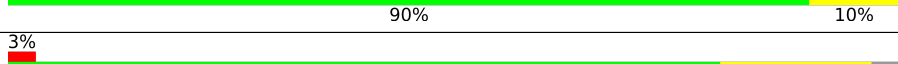
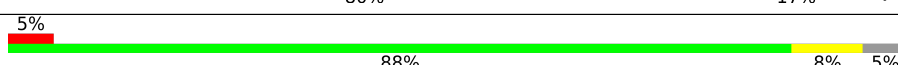
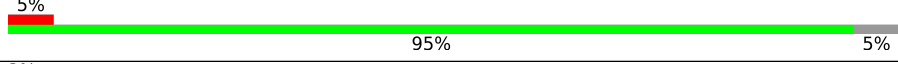
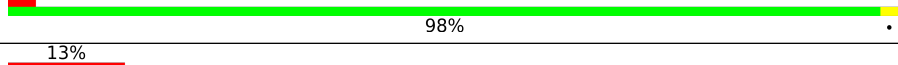
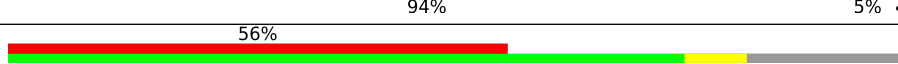
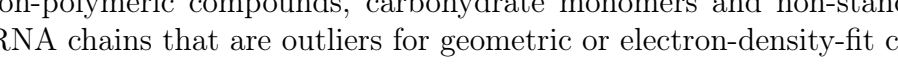
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Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	63	
7	h	63	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	41	

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
24	CLA	A	405	X	-	-	-
24	CLA	A	409	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	D	405	X	-	-	-
24	CLA	a	2109	X	-	-	-
24	CLA	a	2113	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 54282 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	3	0
			2610	1713	428	454	15			
1	a	334	Total	C	N	O	S	0	3	0
			2620	1717	431	457	15			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	5	0
			3997	2623	667	694	13			
2	b	503	Total	C	N	O	S	0	8	0
			3962	2601	660	688	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	2	0
			3494	2286	585	610	13			
3	c	455	Total	C	N	O	S	0	0	0
			3518	2303	589	613	13			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2726	1809	443	462	12			
4	d	342	Total	C	N	O	S	0	4	0
			2743	1819	447	464	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	80	Total	C	N	O		0	1	0
			649	425	103	121				
5	e	79	Total	C	N	O		0	0	0
			629	414	99	116				

- 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	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			293	198	45	49	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	39	Total	C	N	O	S	0	0	0
			271	182	40	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	1	0
			293	205	42	46			
10	k	37	Total	C	N	O	0	0	0
			286	198	42	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	37	Total	C	N	O	0	1	0
			298	202	45	51			
11	l	36	Total	C	N	O	0	2	0
			301	204	47	50			

- 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
			261	176	37	47	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	1	0
			270	182	39	48	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	244	Total	C	N	O	S	0	2	0
			1864	1167	313	379	5			
13	o	243	Total	C	N	O	S	0	3	0
			1865	1169	311	379	6			

- 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	0	0
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	1	0
			778	494	132	152				
15	u	97	Total	C	N	O		0	0	0
			774	491	129	154				

- 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	1	0
			1059	675	177	203	4			
16	v	137	Total	C	N	O	S	0	0	0
			1052	666	174	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	30	Total	C	N	O	S	0	0	0
			220	146	35	36	3			
17	y	29	Total	C	N	O	S	0	0	0
			212	139	37	33	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	0	0
			275	185	44	46				
18	x	38	Total	C	N	O		0	1	0
			278	188	44	46				

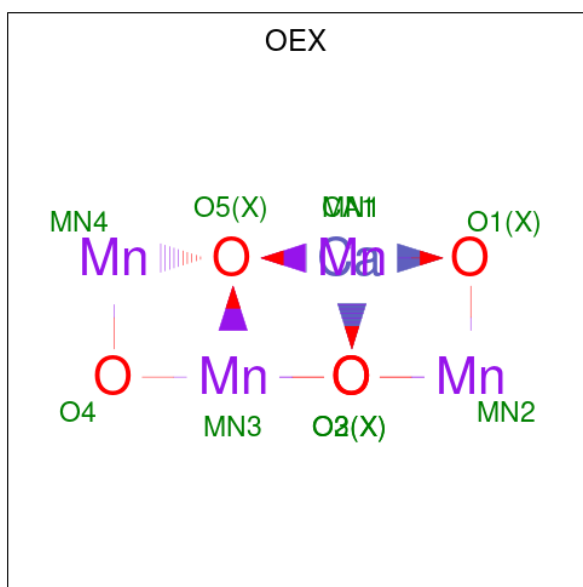
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			458	315	67	74	2			
19	z	61	Total	C	N	O	S	0	0	0
			453	309	70	72	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
			207	133	39	35				

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

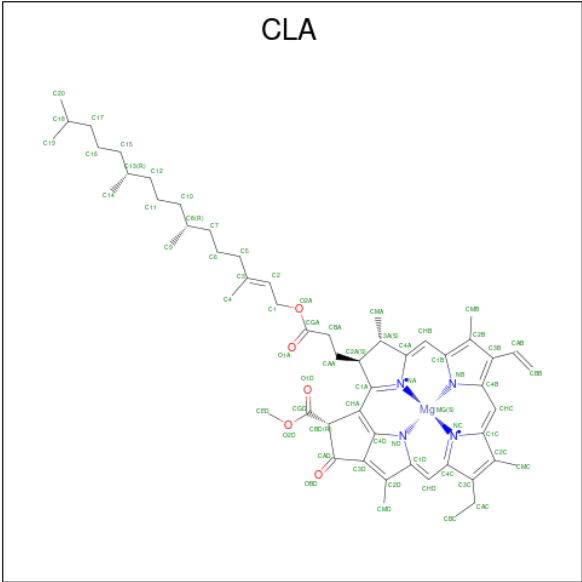
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	2	Total	Cl	0	0
			2	2		
23	a	2	Total	Cl	0	0
			2	2		

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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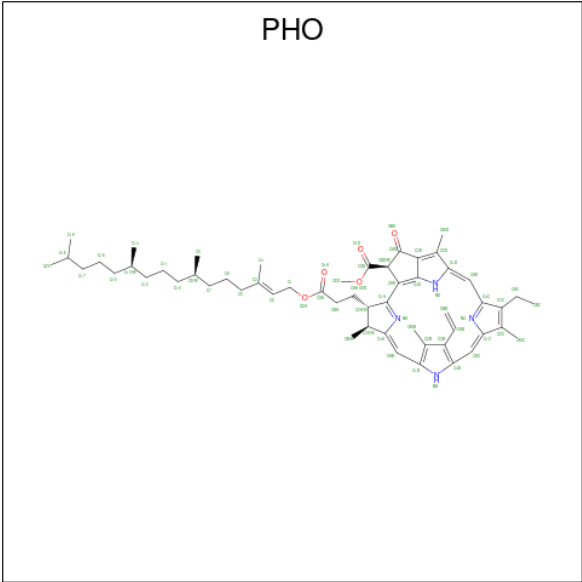
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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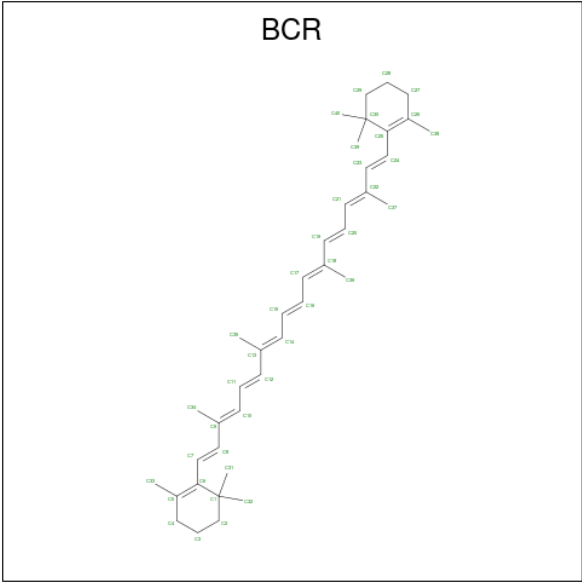
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N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

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



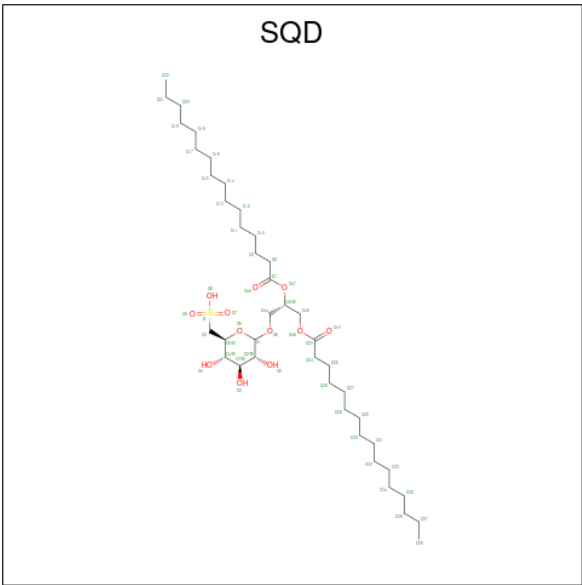
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



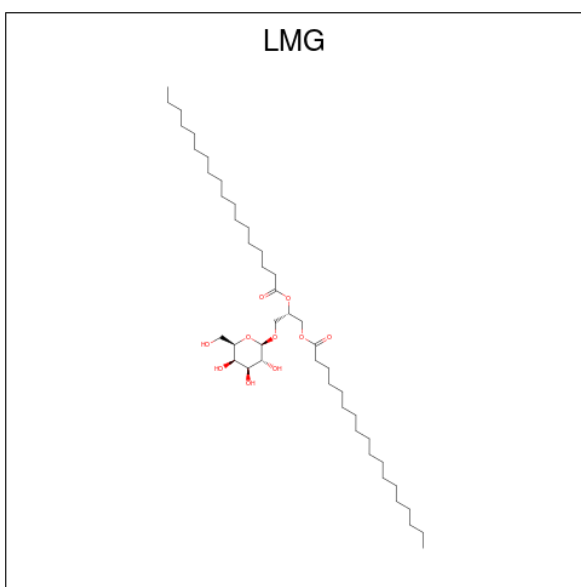
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total C 40 40	0	0
26	a	1	Total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

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



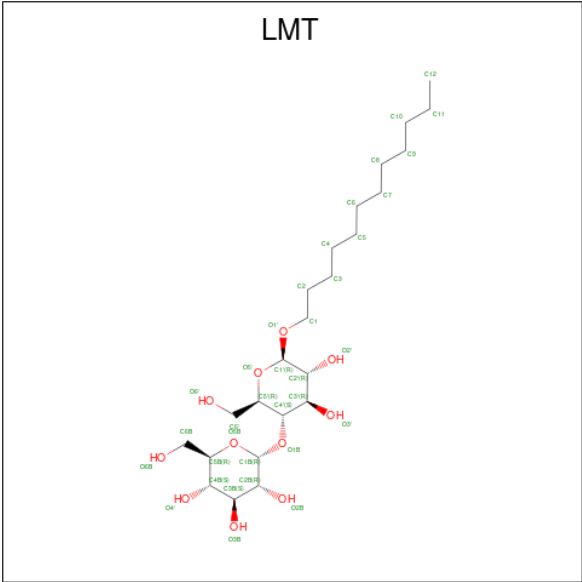
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			49	36	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			45	32	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			53	40	12	1		
27	a	1	Total	C	O	S	0	0
			47	34	12	1		
27	f	1	Total	C	O	S	0	0
			37	27	9	1		

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			51	41	10		
28	B	1	Total	C	O	0	0
			51	41	10		
28	C	1	Total	C	O	0	0
			51	41	10		
28	C	1	Total	C	O	0	0
			48	38	10		
28	D	1	Total	C	O	0	0
			44	34	10		
28	b	1	Total	C	O	0	0
			51	41	10		
28	c	1	Total	C	O	0	0
			49	39	10		
28	c	1	Total	C	O	0	0
			48	38	10		
28	d	1	Total	C	O	0	0
			48	38	10		
28	i	1	Total	C	O	0	0
			51	41	10		

- Molecule 29 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			34	23	11		
29	A	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			24	18	6		
29	E	1	Total	C	O	0	0
			24	18	6		
29	I	1	Total	C	O	0	0
			24	18	6		
29	J	1	Total	C	O	0	0
			24	18	6		
29	M	1	Total	C	O	0	0
			35	24	11		
29	T	1	Total	C	O	0	0
			24	18	6		
29	Z	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	b	1	Total	C	O	0	0
			25	19	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	f	1	Total	C	O	0	0
			24	18	6		
29	i	1	Total	C	O	0	0
			24	18	6		
29	j	1	Total	C	O	0	0
			23	17	6		
29	m	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		
29	z	1	Total	C	O	0	0
			33	22	11		

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

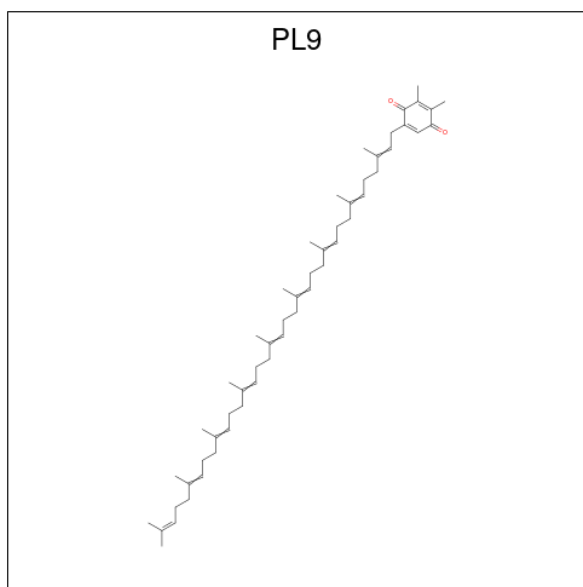
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	2	Total	C	O	0	0
			55	50	5		
30	B	5	Total	C	O	0	0
			74	68	6		
30	C	2	Total	C	O	0	0
			50	45	5		
30	D	3	Total	C	O	0	0
			65	60	5		
30	E	4	Total	C		0	0
			43	43			
30	I	2	Total	C		0	0
			29	29			
30	J	1	Total	C		0	0
			15	15			
30	M	1	Total	C	O	0	0
			15	13	2		
30	T	1	Total	C		0	0
			9	9			
30	Y	1	Total	C		0	0
			10	10			
30	X	1	Total	C	O	0	0
			18	16	2		
30	a	2	Total	C	O	0	0
			26	22	4		
30	b	4	Total	C	O	0	0
			56	52	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	c	2	Total C O 48 43 5	0	0
30	d	4	Total C O 82 75 7	0	0
30	e	1	Total C 15 15	0	0
30	h	2	Total C 23 23	0	0
30	i	2	Total C O 29 25 4	0	0
30	j	1	Total C 16 16	0	0
30	k	1	Total C 12 12	0	0
30	m	1	Total C 13 13	0	0
30	t	1	Total C 8 8	0	0

- Molecule 31 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).



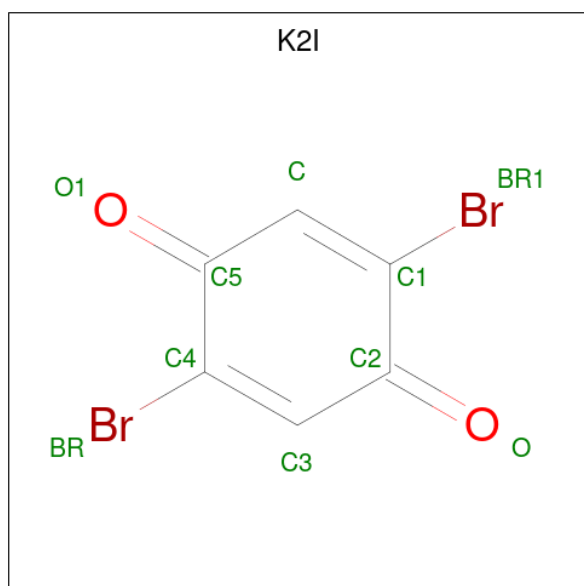
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C 39 39	0	0

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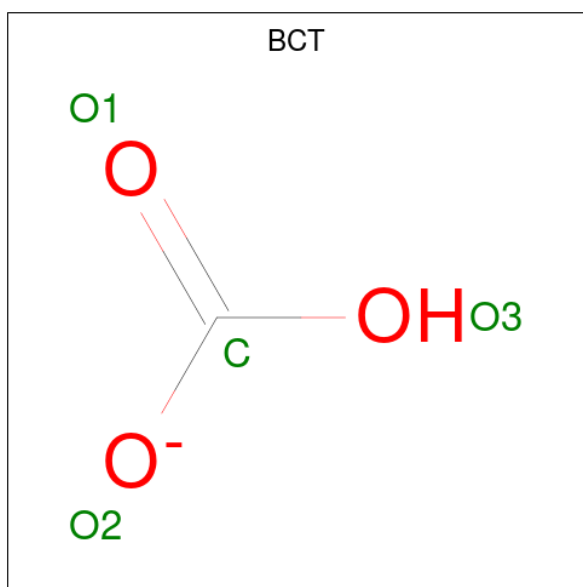
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	D	1	Total C O 55 53 2	0	0
31	d	1	Total C O 55 53 2	0	0
31	x	1	Total C 39 39	0	0

- Molecule 32 is 2,5-bis(bromanyl)cyclohexa-2,5-diene-1,4-dione (CCD ID: K2I) (formula: $C_6H_2Br_2O_2$) (labeled as "Ligand of Interest" by depositor).



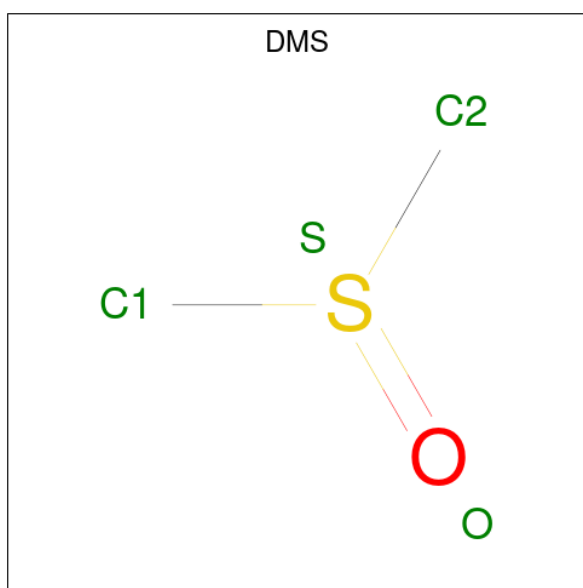
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total Br C O 20 4 12 4	0	1
32	A	1	Total Br C O 10 2 6 2	0	0
32	a	1	Total Br C O 20 4 12 4	0	1
32	a	1	Total Br C O 10 2 6 2	0	0

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 34 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	A	1	Total	C	O	S	0	0
			4	2	1	1		
34	A	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	A	1	Total 4	C 2	O 1	S 1	0	0
34	A	1	Total 4	C 2	O 1	S 1	0	0
34	A	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	B	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	C	1	Total 4	C 2	O 1	S 1	0	0
34	D	1	Total 4	C 2	O 1	S 1	0	0
34	D	1	Total 4	C 2	O 1	S 1	0	0
34	D	1	Total 4	C 2	O 1	S 1	0	0
34	D	1	Total 4	C 2	O 1	S 1	0	0
34	D	1	Total 4	C 2	O 1	S 1	0	0
34	E	1	Total 4	C 2	O 1	S 1	0	0
34	E	1	Total 4	C 2	O 1	S 1	0	0
34	F	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	O	1	Total 4	C 2	O 1	S 1	0	0
34	T	1	Total 4	C 2	O 1	S 1	0	0
34	T	1	Total 4	C 2	O 1	S 1	0	0
34	T	1	Total 4	C 2	O 1	S 1	0	0
34	U	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	V	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0
34	a	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	b	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	c	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	d	1	Total 4	C 2	O 1	S 1	0	0
34	e	1	Total 4	C 2	O 1	S 1	0	0
34	i	1	Total 4	C 2	O 1	S 1	0	0
34	j	1	Total 4	C 2	O 1	S 1	0	0
34	k	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0

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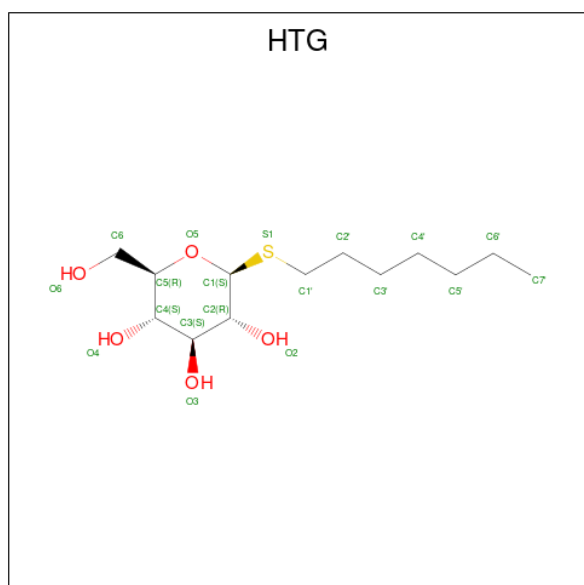
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	o	1	Total 4	C 2	O 1	S 1	0	0
34	t	1	Total 4	C 2	O 1	S 1	0	0
34	u	1	Total 4	C 2	O 1	S 1	0	0
34	u	1	Total 4	C 2	O 1	S 1	0	0
34	u	1	Total 4	C 2	O 1	S 1	0	0
34	u	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	v	1	Total 4	C 2	O 1	S 1	0	0
34	x	1	Total 4	C 2	O 1	S 1	0	0
34	z	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 35 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	B	1	Total	Ca	0	0
			1	1		
35	O	1	Total	Ca	0	0
			1	1		
35	b	1	Total	Ca	0	0
			1	1		
35	c	1	Total	Ca	0	0
			1	1		
35	o	1	Total	Ca	0	0
			1	1		

- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



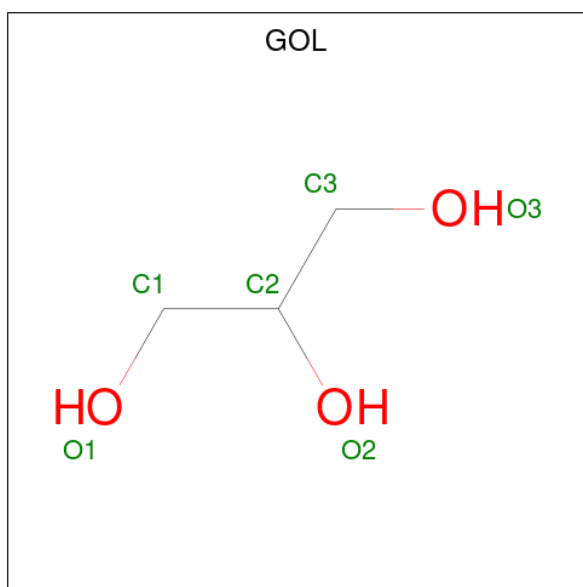
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	1
			38	26	10	2		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	D	1	Total	C	O	S	0	0
			19	13	5	1		
36	I	1	Total	C	O	S	0	0
			19	13	5	1		
36	O	1	Total	C	O	S	0	0
			19	13	5	1		
36	V	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			19	13	5	1		
36	i	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 37 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



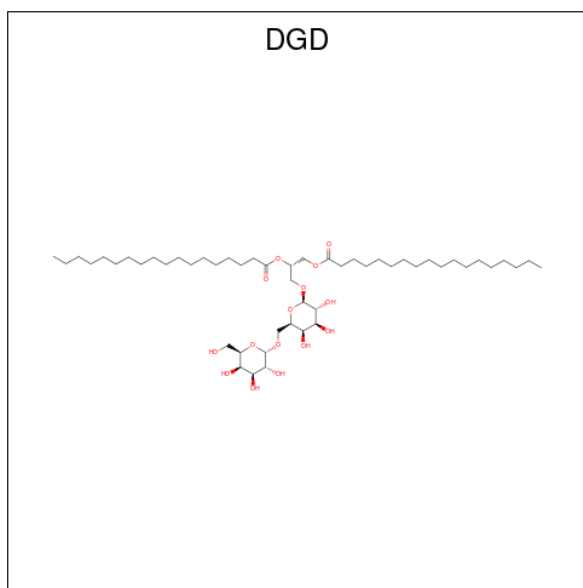
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	B	1	Total	C	O	0	0
			6	3	3		
37	B	1	Total	C	O	0	0
			6	3	3		
37	C	1	Total	C	O	0	0
			6	3	3		
37	C	1	Total	C	O	0	0
			6	3	3		
37	D	1	Total	C	O	0	0
			6	3	3		
37	H	1	Total	C	O	0	0
			6	3	3		
37	O	1	Total	C	O	0	0
			6	3	3		
37	U	1	Total	C	O	0	0
			6	3	3		
37	U	1	Total	C	O	0	0
			6	3	3		
37	V	1	Total	C	O	0	0
			6	3	3		
37	Z	1	Total	C	O	0	0
			6	3	3		
37	a	1	Total	C	O	0	0
			6	3	3		
37	b	1	Total	C	O	0	0
			6	3	3		
37	c	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	d	1	Total	C	O	0	0
			6	3	3		
37	k	1	Total	C	O	0	0
			6	3	3		
37	o	1	Total	C	O	0	0
			6	3	3		
37	o	1	Total	C	O	0	0
			6	3	3		
37	v	1	Total	C	O	0	0
			6	3	3		
37	v	1	Total	C	O	0	0
			6	3	3		
37	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 38 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



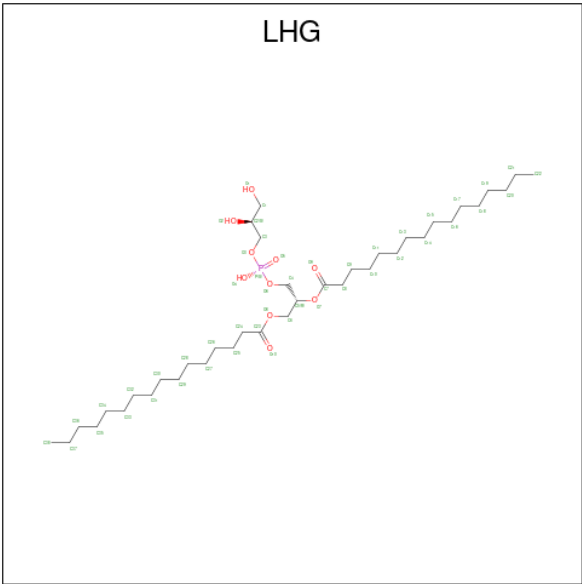
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	C	1	Total	C	O	0	0
			62	47	15		
38	C	1	Total	C	O	0	0
			62	47	15		
38	C	1	Total	C	O	0	0
			62	47	15		
38	D	1	Total	C	O	0	0
			46	35	11		

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

- Molecule 39 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



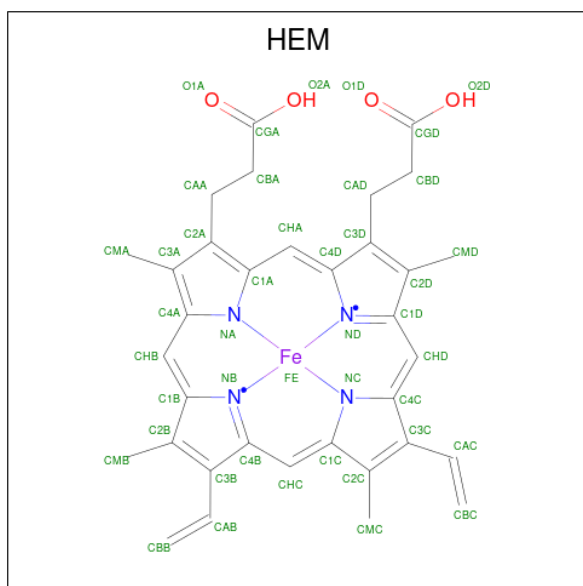
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
39	D	1	Total	C	O	P	0	0
			49	38	10	1		
39	D	1	Total	C	O	P	0	0
			49	38	10	1		
39	D	1	Total	C	O	P	0	0
			44	33	10	1		
39	E	1	Total	C	O	P	0	0
			49	38	10	1		
39	L	1	Total	C	O	P	0	0
			49	38	10	1		
39	d	1	Total	C	O	P	0	0
			49	38	10	1		

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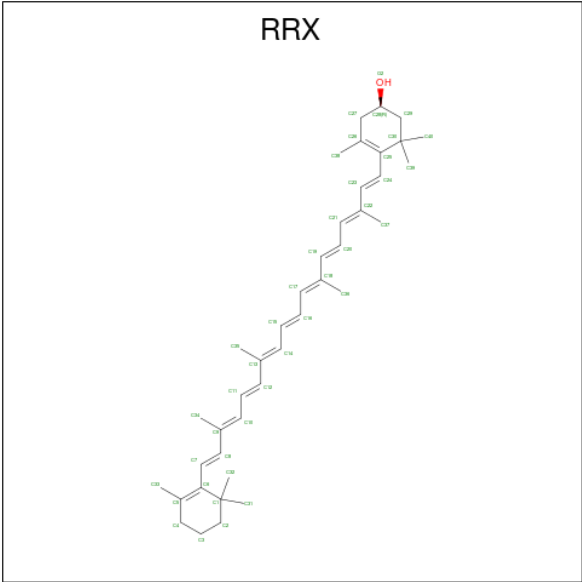
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
39	d	1	Total	C	O	P	0	0
			49	38	10	1		
39	d	1	Total	C	O	P	0	0
			36	25	10	1		
39	e	1	Total	C	O	P	0	0
			32	22	9	1		
39	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 40 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 41 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).

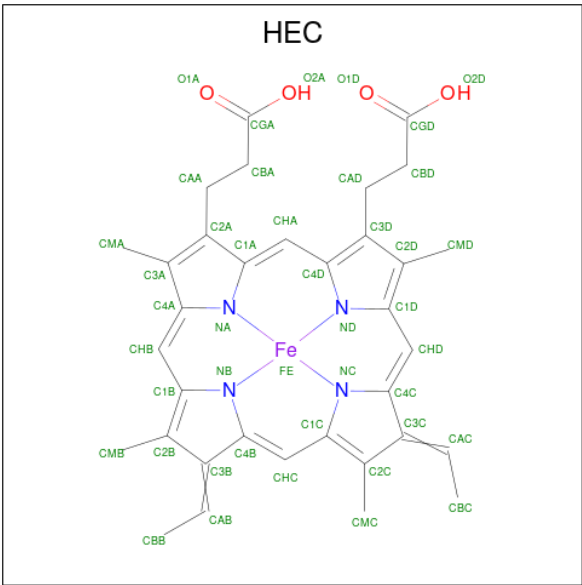


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
41	H	1	Total	C	O	0	0
			41	40	1		
41	h	1	Total	C	O	0	0
			41	40	1		

- Molecule 42 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 43 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

- Molecule 44 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
44	A	142	Total	O	0	0
			142	142		
44	B	291	Total	O	0	0
			291	291		
44	C	231	Total	O	0	0
			231	231		
44	D	140	Total	O	0	2
			142	142		
44	E	34	Total	O	0	0
			34	34		
44	F	6	Total	O	0	0
			6	6		
44	H	47	Total	O	0	0
			47	47		
44	I	11	Total	O	0	0
			11	11		
44	J	13	Total	O	0	0
			13	13		
44	K	12	Total	O	0	0
			12	12		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
44	L	19	Total 19	O 19	0	0
44	M	6	Total 6	O 6	0	0
44	O	148	Total 148	O 148	0	0
44	T	13	Total 13	O 13	0	0
44	U	80	Total 80	O 80	0	0
44	V	121	Total 121	O 121	0	0
44	Y	5	Total 5	O 5	0	0
44	X	14	Total 14	O 14	0	0
44	Z	1	Total 1	O 1	0	0
44	a	135	Total 135	O 135	0	0
44	b	265	Total 268	O 268	0	3
44	c	229	Total 229	O 229	0	0
44	d	135	Total 135	O 135	0	0
44	e	23	Total 23	O 23	0	0
44	f	9	Total 9	O 9	0	0
44	h	32	Total 32	O 32	0	0
44	i	12	Total 12	O 12	0	0
44	j	15	Total 15	O 15	0	0
44	k	8	Total 8	O 8	0	0
44	l	13	Total 14	O 14	0	1
44	m	9	Total 9	O 9	0	0

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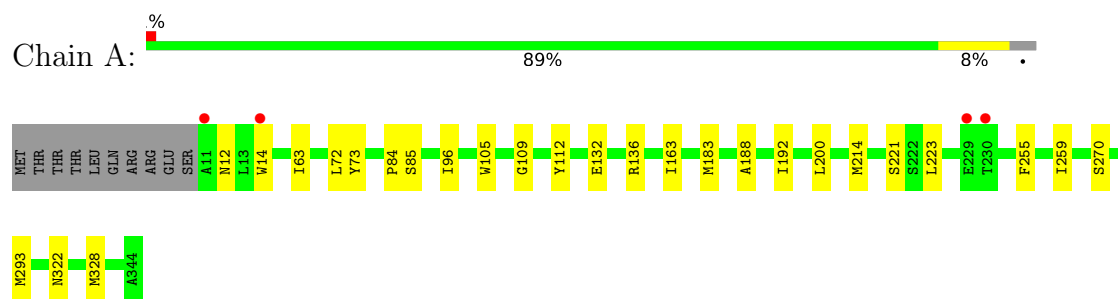
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
44	o	130	Total 131	O 131	0	1
44	t	11	Total 11	O 11	0	0
44	u	90	Total 91	O 91	0	1
44	v	98	Total 100	O 100	0	2
44	y	8	Total 8	O 8	0	0
44	x	12	Total 12	O 12	0	0
44	z	4	Total 4	O 4	0	0
44	R	1	Total 1	O 1	0	0

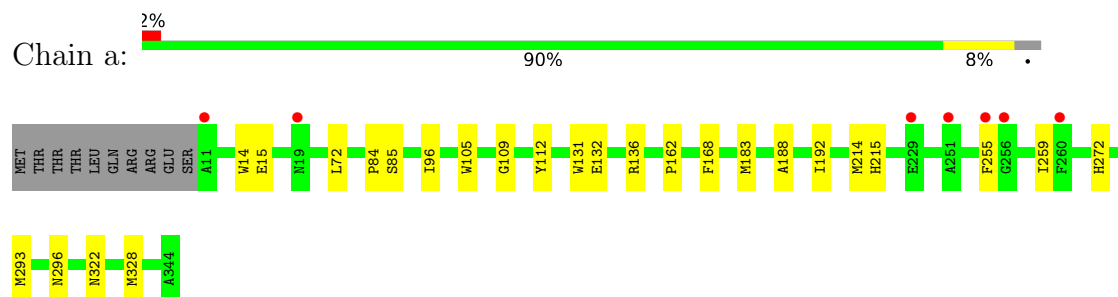
3 Residue-property plots [i](#)

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

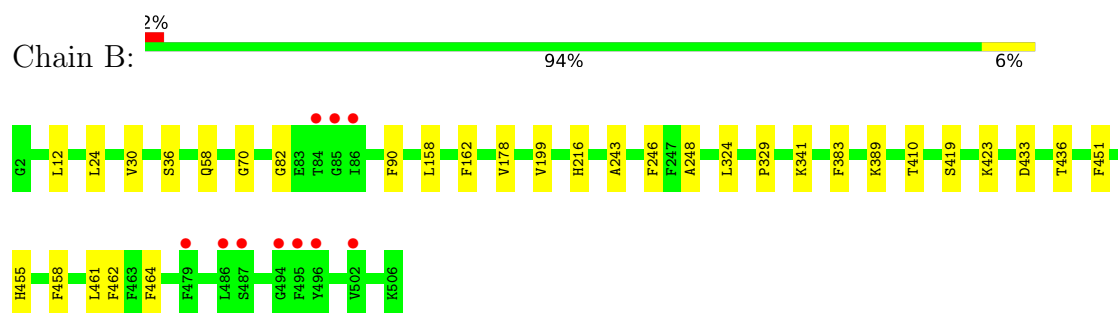
- Molecule 1: Photosystem II protein D1



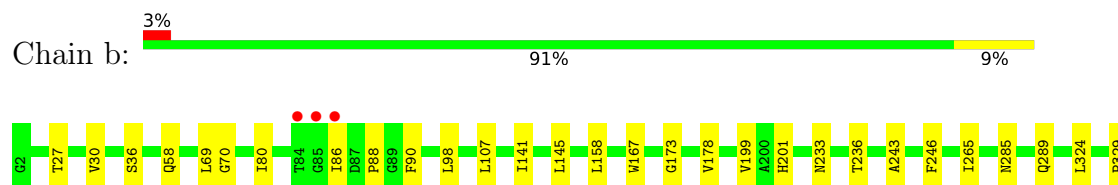
- Molecule 1: Photosystem II protein D1

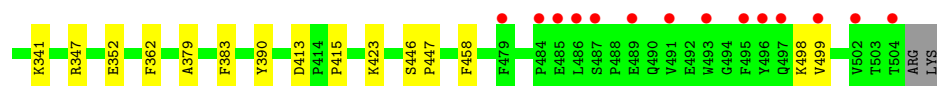


- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein





- Molecule 3: Photosystem II CP43 reaction center protein



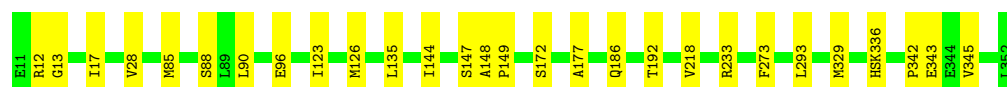
- Molecule 3: Photosystem II CP43 reaction center protein



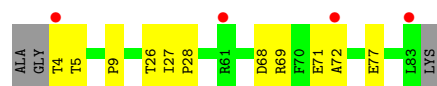
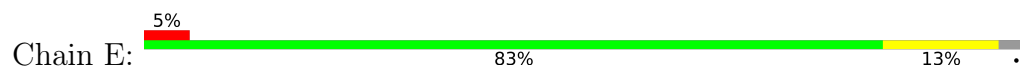
- Molecule 4: Photosystem II D2 protein



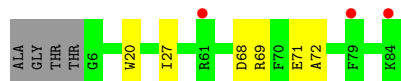
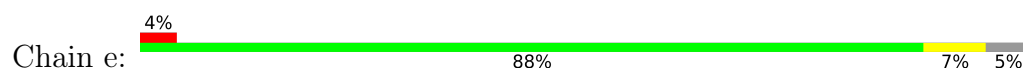
- Molecule 4: Photosystem II D2 protein



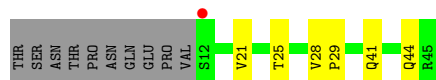
- Molecule 5: Cytochrome b559 subunit alpha



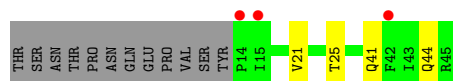
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



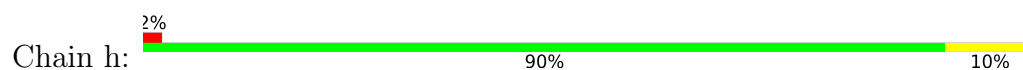
- Molecule 6: Cytochrome b559 subunit beta



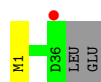
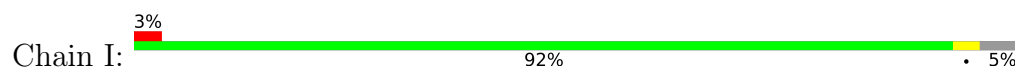
- Molecule 7: Photosystem II reaction center protein H



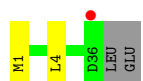
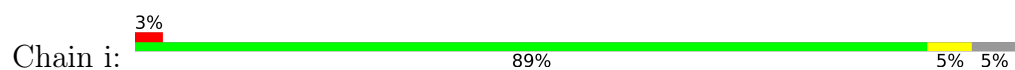
- Molecule 7: Photosystem II reaction center protein H



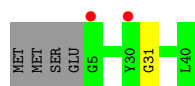
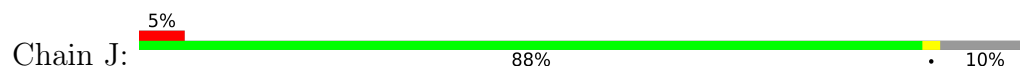
- Molecule 8: Photosystem II reaction center protein I



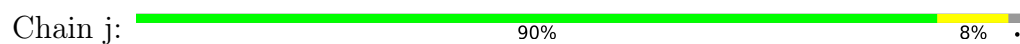
- Molecule 8: Photosystem II reaction center protein I



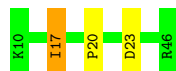
- Molecule 9: Photosystem II reaction center protein J



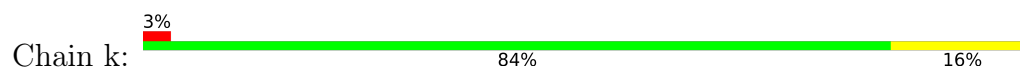
- Molecule 9: Photosystem II reaction center protein J



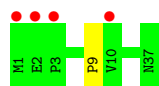
- Molecule 10: Photosystem II reaction center protein K



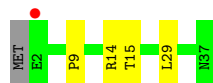
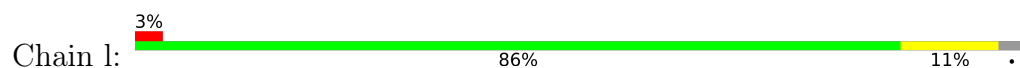
- Molecule 10: Photosystem II reaction center protein K



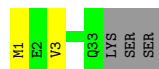
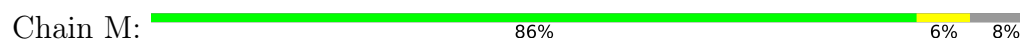
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

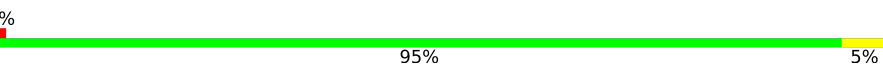


- Molecule 12: Photosystem II reaction center protein M

Chain m:  83% 11% 6%

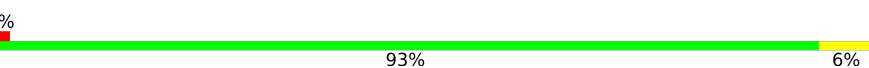


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  % 95% 5%



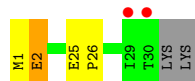
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  2% 93% 6%



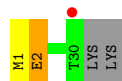
- Molecule 14: Photosystem II reaction center protein T

Chain T:  6% 81% 9% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 88% 6%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  87% 6% 7%



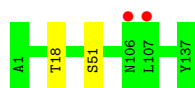
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  % 88% 5% 7%

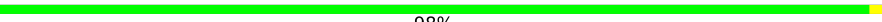


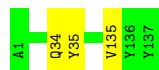
- Molecule 16: Cytochrome c-550

Chain V:  99%



- Molecule 16: Cytochrome c-550

Chain v:  98%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  90% 10%



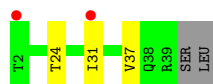
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  80% 17% 3%

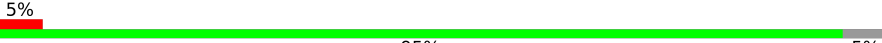


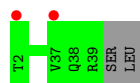
- Molecule 18: Photosystem II reaction center protein X

Chain X:  88% 8% 5%

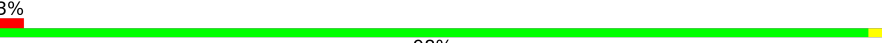


- Molecule 18: Photosystem II reaction center protein X

Chain x:  95% 5%

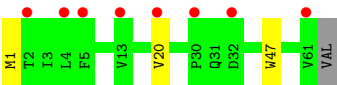
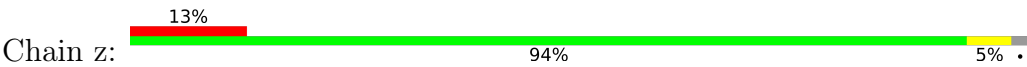


- Molecule 19: Photosystem II reaction center protein Z

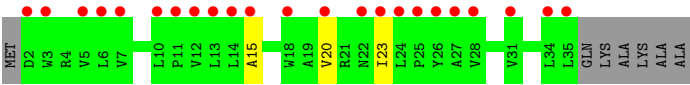
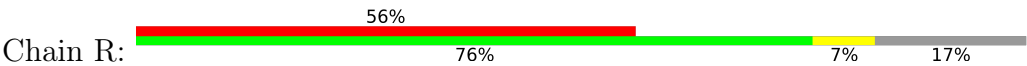
Chain Z:  98%



• 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	122.19Å 228.46Å 286.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.02 – 2.10 49.02 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.02-2.10) 88.1 (49.02-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.46 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.157 , 0.191 0.163 , 0.194	Depositor DCC
R_{free} test set	22959 reflections (3.68%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 71.2	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	0.97	EDS
Total number of atoms	54282	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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: SQD, DMS, LHG, CA, LMG, CL, OEX, LMT, BCR, CLA, K2I, HEM, UNL, HSK, PHO, MG, HTG, HEC, BCT, RRX, FE2, GOL, PL9, FME, DGD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/2704	0.53	0/3690
1	a	0.34	0/2713	0.52	0/3700
2	B	0.33	0/4149	0.49	0/5652
2	b	0.32	0/4123	0.47	0/5619
3	C	0.30	0/3613	0.46	0/4919
3	c	0.28	0/3632	0.46	0/4945
4	D	0.36	0/2804	0.50	0/3820
4	d	0.34	0/2827	0.48	0/3850
5	E	0.27	0/671	0.45	0/918
5	e	0.24	0/648	0.44	0/887
6	F	0.24	0/284	0.43	0/387
6	f	0.25	0/265	0.45	0/360
7	H	0.28	0/511	0.42	0/697
7	h	0.26	0/511	0.43	0/697
8	I	0.21	0/290	0.40	0/393
8	i	0.25	0/293	0.43	0/396
9	J	0.23	0/257	0.40	0/349
9	j	0.22	0/277	0.36	0/376
10	K	0.25	0/306	0.45	0/422
10	k	0.24	0/296	0.42	0/408
11	L	0.39	0/308	0.43	0/420
11	l	0.35	0/314	0.44	0/428
12	M	0.30	0/257	0.52	0/352
12	m	0.32	0/266	0.46	0/363
13	O	0.31	0/1901	0.50	0/2579
13	o	0.28	0/1905	0.49	0/2583
14	T	0.34	0/255	0.42	0/346
14	t	0.33	0/255	0.40	0/346
15	U	0.32	0/792	0.49	0/1073
15	u	0.31	0/785	0.47	0/1064
16	V	0.32	0/1083	0.46	0/1470

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.26	0/1073	0.44	0/1461
17	Y	0.22	0/221	0.37	0/296
17	y	0.24	0/213	0.40	0/285
18	X	0.21	0/278	0.34	0/376
18	x	0.20	0/284	0.35	0/384
19	Z	0.20	0/459	0.38	0/630
19	z	0.17	0/454	0.35	0/622
20	R	0.16	0/209	0.33	0/290
All	All	0.31	0/42486	0.47	0/57853

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	2610	0	2506	20	0
1	a	2620	0	2527	18	0
2	B	3997	0	3860	31	0
2	b	3962	0	3813	30	0
3	C	3494	0	3418	27	0
3	c	3518	0	3434	23	0
4	D	2726	0	2629	19	0
4	d	2743	0	2652	21	0
5	E	649	0	627	8	0
5	e	629	0	600	6	0
6	F	275	0	282	3	0
6	f	257	0	269	2	0
7	H	498	0	518	3	0
7	h	498	0	518	5	0
8	I	293	0	302	0	0
8	i	296	0	311	1	0
9	J	251	0	257	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	271	0	270	4	0
10	K	293	0	303	3	0
10	k	286	0	285	4	0
11	L	298	0	309	1	0
11	l	301	0	320	4	0
12	M	261	0	280	1	0
12	m	270	0	293	4	0
13	O	1864	0	1835	9	0
13	o	1865	0	1842	10	0
14	T	256	0	256	2	0
14	t	256	0	256	1	0
15	U	778	0	782	6	0
15	u	774	0	773	3	0
16	V	1059	0	1074	2	0
16	v	1052	0	1040	3	0
17	Y	220	0	245	3	0
17	y	212	0	237	4	0
18	X	275	0	301	3	0
18	x	278	0	305	0	0
19	Z	458	0	472	0	0
19	z	453	0	459	3	0
20	R	207	0	157	2	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	195	0	216	4	0
24	B	1040	0	1152	25	0
24	C	845	0	936	29	0
24	D	195	0	216	5	0
24	a	195	0	216	6	0
24	b	1040	0	1152	27	0
24	c	845	0	936	28	0
24	d	195	0	216	7	0
25	A	128	0	148	2	0
25	a	128	0	148	1	0
26	A	40	0	56	1	0
26	B	120	0	168	6	0
26	C	80	0	112	7	0
26	D	40	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	K	40	0	56	1	0
26	T	40	0	56	5	0
26	Y	40	0	56	3	0
26	a	40	0	56	1	0
26	b	120	0	168	6	0
26	c	120	0	168	6	0
26	d	40	0	56	1	0
26	k	40	0	56	1	0
26	t	40	0	56	6	0
27	A	103	0	143	2	0
27	B	54	0	78	3	0
27	F	45	0	57	2	0
27	L	54	0	78	1	0
27	a	100	0	131	2	0
27	f	37	0	45	1	0
28	A	51	0	72	1	0
28	B	51	0	72	2	0
28	C	99	0	138	2	0
28	D	44	0	58	0	0
28	b	51	0	72	1	0
28	c	97	0	134	1	0
28	d	48	0	66	0	0
28	i	51	0	72	2	0
29	A	69	0	87	3	0
29	B	94	0	127	2	0
29	E	24	0	35	0	0
29	I	24	0	35	0	0
29	J	24	0	35	1	0
29	M	35	0	46	2	0
29	T	24	0	35	0	0
29	Z	35	0	46	0	0
29	a	70	0	92	4	0
29	b	25	0	35	0	0
29	f	24	0	35	0	0
29	i	24	0	35	1	0
29	j	23	0	22	0	0
29	m	70	0	92	2	0
29	z	33	0	35	2	0
30	A	55	0	0	0	0
30	B	74	0	0	0	0
30	C	50	0	0	0	0
30	D	65	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	E	43	0	0	0	0
30	I	29	0	0	0	0
30	J	15	0	0	0	0
30	M	15	0	0	0	0
30	T	9	0	0	0	0
30	X	18	0	0	0	0
30	Y	10	0	0	0	0
30	a	26	0	0	0	0
30	b	56	0	0	0	0
30	c	48	0	0	0	0
30	d	82	0	0	0	0
30	e	15	0	0	0	0
30	h	23	0	0	0	0
30	i	29	0	0	0	0
30	j	16	0	0	0	0
30	k	12	0	0	0	0
30	m	13	0	0	0	0
30	t	8	0	0	0	0
31	A	39	0	59	2	0
31	D	55	0	80	0	0
31	d	55	0	80	1	0
31	x	39	0	59	1	0
32	A	30	0	0	3	0
32	a	30	0	0	3	0
33	A	4	0	0	0	0
33	a	4	0	0	0	0
34	A	20	0	30	0	0
34	B	52	0	78	2	0
34	C	52	0	78	3	0
34	D	20	0	30	0	0
34	E	8	0	12	0	0
34	F	4	0	6	0	0
34	O	44	0	66	2	0
34	T	12	0	18	0	0
34	U	4	0	6	2	0
34	V	28	0	42	1	0
34	a	16	0	24	0	0
34	b	48	0	72	2	0
34	c	56	0	84	2	0
34	d	28	0	42	3	0
34	e	4	0	6	0	0
34	i	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	j	4	0	6	0	0
34	k	4	0	6	0	0
34	o	36	0	54	1	0
34	t	4	0	6	0	0
34	u	16	0	24	0	0
34	v	40	0	60	1	0
34	x	4	0	6	0	0
34	z	4	0	6	0	0
35	B	1	0	0	0	0
35	O	1	0	0	0	0
35	b	1	0	0	0	0
35	c	1	0	0	0	0
35	o	1	0	0	0	0
36	B	114	0	156	8	0
36	C	38	0	52	0	0
36	D	19	0	26	3	0
36	I	19	0	26	1	0
36	O	19	0	26	1	0
36	V	19	0	26	0	0
36	b	76	0	104	7	0
36	c	57	0	78	0	0
36	d	38	0	52	2	0
36	i	19	0	26	0	0
37	B	12	0	16	2	0
37	C	12	0	16	0	0
37	D	6	0	8	1	0
37	H	6	0	8	0	0
37	O	6	0	8	0	0
37	U	12	0	16	0	0
37	V	6	0	8	0	0
37	Z	6	0	8	0	0
37	a	6	0	8	0	0
37	b	6	0	8	0	0
37	c	6	0	8	2	0
37	d	6	0	8	0	0
37	k	6	0	8	0	0
37	o	12	0	16	2	0
37	v	18	0	24	0	0
38	C	186	0	246	9	0
38	D	46	0	57	0	0
38	H	62	0	82	0	0
38	c	186	0	246	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	h	62	0	82	1	0
39	D	142	0	209	5	0
39	E	49	0	74	5	0
39	L	49	0	74	2	0
39	d	134	0	190	3	0
39	e	32	0	43	1	0
39	l	49	0	74	1	0
40	F	43	0	30	1	0
40	e	43	0	30	2	0
41	H	41	0	56	3	0
41	h	41	0	56	3	0
42	J	1	0	0	0	0
42	j	1	0	0	0	0
43	V	43	0	30	0	0
43	v	43	0	30	0	0
44	A	142	0	0	0	0
44	B	291	0	0	2	0
44	C	231	0	0	1	0
44	D	142	0	0	0	0
44	E	34	0	0	0	0
44	F	6	0	0	0	0
44	H	47	0	0	0	0
44	I	11	0	0	0	0
44	J	13	0	0	0	0
44	K	12	0	0	0	0
44	L	19	0	0	0	0
44	M	6	0	0	0	0
44	O	148	0	0	1	0
44	R	1	0	0	0	0
44	T	13	0	0	0	0
44	U	80	0	0	4	0
44	V	121	0	0	0	0
44	X	14	0	0	0	0
44	Y	5	0	0	0	0
44	Z	1	0	0	0	0
44	a	135	0	0	0	0
44	b	268	0	0	4	0
44	c	229	0	0	0	0
44	d	135	0	0	0	0
44	e	23	0	0	0	0
44	f	9	0	0	0	0
44	h	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	i	12	0	0	0	0
44	j	15	0	0	1	0
44	k	8	0	0	0	0
44	l	14	0	0	0	0
44	m	9	0	0	0	0
44	o	131	0	0	3	0
44	t	11	0	0	0	0
44	u	91	0	0	0	0
44	v	100	0	0	1	0
44	x	12	0	0	0	0
44	y	8	0	0	0	0
44	z	4	0	0	0	0
All	All	54282	0	52476	414	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (414) 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)
1:a:14:TRP:HD1	29:a:2120:LMT:H6B	0.98	0.91
1:a:14:TRP:CD1	29:a:2120:LMT:H6B	1.91	0.86
4:D:13:GLY:HA3	36:D:413:HTG:H62	1.62	0.82
4:d:192:THR:HG23	24:d:404:CLA:HBC2	1.68	0.76
24:b:618:CLA:H2	24:b:619:CLA:HBB2	1.71	0.73
3:C:315:MET:HG3	3:C:365:TRP:HZ3	1.55	0.72
2:B:410:THR:H	37:B:635:GOL:H2	1.53	0.72
2:B:248:ALA:HA	24:B:604:CLA:H42	1.73	0.70
4:d:13:GLY:HA3	36:d:403:HTG:H62	1.75	0.69
36:B:624:HTG:H1	29:a:2103:LMT:H21	1.74	0.69
36:b:601:HTG:O2	36:b:602:HTG:S1	2.48	0.68
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.75	0.68
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.74	0.68
24:c:513:CLA:H171	19:z:20:VAL:HA	1.76	0.67
2:B:90:PHE:H	36:B:628:HTG:H62	1.59	0.66
24:B:612:CLA:H142	39:L:101:LHG:H372	1.78	0.65
13:o:23:ASP:OD1	13:o:23:ASP:N	2.28	0.64
26:B:618:BCR:H383	27:B:621:SQD:H91	1.79	0.64
24:c:503:CLA:C4D	24:c:505:CLA:H2	2.27	0.64
4:d:233:ARG:NH2	34:d:423:DMS:S	2.71	0.64
3:C:315:MET:HG2	3:C:351:PHE:CZ	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:27:ILE:HG12	40:F:102:HEM:HMC3	1.79	0.63
25:A:408:PHO:HBC3	4:D:279:LEU:HD22	1.81	0.62
36:I:1202:HTG:H1	36:b:602:HTG:H1	1.80	0.61
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.82	0.61
38:c:518:DGD:HB52	28:i:101:LMG:H382	1.81	0.61
5:e:68:ASP:OD2	5:e:71:GLU:HB2	2.01	0.61
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.82	0.61
24:b:608:CLA:HHC	24:b:608:CLA:HBB1	1.82	0.61
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.83	0.61
4:D:192:THR:HG23	24:D:404:CLA:HBC2	1.83	0.60
11:L:9:PRO:HA	29:m:102:LMT:H6D	1.84	0.60
26:B:619:BCR:H363	26:t:102:BCR:H19C	1.84	0.59
1:a:183:MET:HA	24:a:2109:CLA:HMD1	1.83	0.59
20:R:20:VAL:HA	20:R:23:ILE:HG22	1.85	0.59
15:U:70[B]:ARG:NH1	44:U:603:HOH:O	2.34	0.59
3:c:286:ALA:HB2	24:c:504:CLA:HMD1	1.84	0.58
24:C:505:CLA:H42	38:C:518:DGD:HB52	1.86	0.58
24:B:611:CLA:HHC	24:B:611:CLA:HBB1	1.86	0.57
5:E:68:ASP:OD2	5:E:71:GLU:HB2	2.04	0.57
24:C:503:CLA:H61	24:C:513:CLA:H42	1.85	0.57
2:B:82:GLY:O	37:o:2601:GOL:O1	2.22	0.57
15:u:8:GLU:HG3	15:u:9:LEU:HD13	1.86	0.57
28:C:520:LMG:H172	17:Y:25:ILE:HG12	1.86	0.57
24:C:514:CLA:HAB	26:C:515:BCR:H24C	1.86	0.56
26:c:528:BCR:H321	26:c:528:BCR:HC8	1.87	0.56
36:d:403:HTG:H1	7:h:25:TRP:CD1	2.40	0.56
24:b:618:CLA:H2	24:b:619:CLA:CBB	2.35	0.56
1:A:183:MET:HA	24:A:405:CLA:HMD1	1.89	0.56
24:b:604:CLA:H72	24:b:604:CLA:H2	1.88	0.55
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.42	0.55
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.87	0.55
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.42	0.55
24:B:605:CLA:H43	24:B:606:CLA:H2	1.89	0.55
24:c:504:CLA:H61	24:c:514:CLA:H42	1.89	0.55
24:c:508:CLA:HMC2	24:c:509:CLA:H102	1.89	0.54
13:O:111:ALA:HB3	34:O:309:DMS:H12	1.89	0.54
1:a:215:HIS:ND1	32:a:2118[B]:K2I:O	2.30	0.54
24:C:514:CLA:H171	26:C:515:BCR:H373	1.90	0.54
24:B:603:CLA:H101	24:B:610:CLA:H193	1.90	0.54
24:C:510:CLA:HMB1	24:C:510:CLA:HBB1	1.90	0.54
15:U:81:HIS:HE1	44:U:670:HOH:O	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:502:CLA:C4D	24:C:504:CLA:H2	2.38	0.53
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.44	0.53
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.42	0.53
2:b:499:VAL:HG12	4:d:135:LEU:HB3	1.90	0.53
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.07	0.53
27:B:621:SQD:H242	11:l:14:ARG:HD3	1.90	0.53
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.73	0.53
3:c:60:ILE:HG22	24:c:505:CLA:HHD	1.91	0.53
3:c:52:ALA:HB2	24:c:513:CLA:HMA2	1.91	0.53
38:c:519:DGD:HAT2	38:c:520:DGD:HBN2	1.90	0.52
10:k:20:PRO:HB3	17:y:21:GLN:HG3	1.91	0.52
13:o:204:VAL:HG22	13:o:211:ILE:HG22	1.91	0.52
24:C:509:CLA:HBC3	24:C:511:CLA:H71	1.92	0.52
34:c:531:DMS:H11	34:v:205:DMS:H22	1.92	0.52
24:B:615:CLA:H18	28:B:622:LMG:H422	1.90	0.52
1:a:84:PRO:HA	1:a:112:TYR:CG	2.45	0.52
24:c:507:CLA:HAA1	24:c:507:CLA:HBD	1.92	0.52
13:O:194:LYS:HE2	44:O:534:HOH:O	2.10	0.51
2:B:162:PHE:O	24:B:607:CLA:HHD	2.11	0.51
9:j:2:MET:N	44:j:1701:HOH:O	2.43	0.51
13:o:180:GLU:CD	13:o:180:GLU:H	2.18	0.51
1:A:200:LEU:HG	38:C:519:DGD:HAT2	1.93	0.51
24:C:510:CLA:H141	24:C:513:CLA:HMD3	1.93	0.51
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.93	0.51
24:b:613:CLA:HHC	24:b:613:CLA:HBB1	1.93	0.51
3:C:279:LEU:HD22	24:C:510:CLA:HED2	1.93	0.51
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.10	0.50
24:b:607:CLA:H43	24:b:608:CLA:H2	1.93	0.50
2:B:341:LYS:NZ	36:B:625[B]:HTG:S1	2.83	0.50
26:T:101:BCR:H19C	26:b:621:BCR:H363	1.93	0.50
24:b:604:CLA:H122	24:b:604:CLA:C4B	2.42	0.50
28:B:622:LMG:H242	4:D:284:ILE:HD13	1.93	0.50
24:C:506:CLA:HBC2	26:C:516:BCR:H341	1.92	0.50
7:h:59:ASN:O	7:h:64:ALA:HB3	2.12	0.50
1:a:215:HIS:HA	32:a:2118[B]:K2I:O	2.12	0.50
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.94	0.50
17:y:20:ALA:O	17:y:24:MET:HG2	2.12	0.50
24:C:502:CLA:C3D	24:C:504:CLA:H2	2.42	0.49
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.48	0.49
34:U:503:DMS:H23	16:V:51:SER:HA	1.94	0.49
4:d:126[B]:MET:HE1	4:d:147:SER:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PRO:HA	1:A:112:TYR:CG	2.47	0.49
24:A:409:CLA:H172	24:C:507:CLA:H91	1.95	0.49
2:b:69:LEU:HD12	24:b:608:CLA:HBA1	1.93	0.49
2:b:233:ASN:O	2:b:236:THR:HG22	2.12	0.49
24:B:617:CLA:H101	24:B:617:CLA:H142	1.93	0.49
3:C:279:LEU:HD12	3:C:282:MET:HE3	1.93	0.49
3:C:338:GLY:HA3	3:C:341:LEU:O	2.12	0.49
3:c:41:ARG:NH1	24:c:513:CLA:HMD1	2.28	0.49
26:Y:302:BCR:H321	26:Y:302:BCR:HC8	1.93	0.49
10:K:17:ILE:H	10:K:17:ILE:HD13	1.78	0.49
26:T:101:BCR:HC7	26:T:101:BCR:H331	1.52	0.49
2:b:58:GLN:C	2:b:329:PRO:HB3	2.38	0.49
24:c:503:CLA:H202	24:c:509:CLA:HBB1	1.94	0.49
2:b:145:LEU:HB3	24:b:607:CLA:H162	1.95	0.48
36:b:625:HTG:H6'1	44:b:898:HOH:O	2.13	0.48
13:o:69:LYS:NZ	44:o:2705:HOH:O	2.45	0.48
1:A:255:PHE:CD2	32:A:418[B]:K2I:BR	3.22	0.48
3:C:266:TRP:CZ3	24:C:508:CLA:HAC2	2.48	0.48
24:c:503:CLA:C3D	24:c:505:CLA:H2	2.43	0.48
8:i:4:LEU:HD22	29:i:104:LMT:H61	1.96	0.48
17:y:18:VAL:HG22	17:y:20:ALA:H	1.79	0.48
16:V:18:THR:H	34:V:206:DMS:H13	1.78	0.48
3:c:79:LYS:HB3	3:c:84:GLN:NE2	2.27	0.48
2:b:36:SER:OG	26:b:621:BCR:H362	2.13	0.48
29:B:623:LMT:O6'	4:D:16:ASP:OD1	2.30	0.48
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.95	0.48
27:F:101:SQD:H321	18:X:24:THR:HA	1.96	0.48
34:B:643:DMS:H23	44:B:888:HOH:O	2.14	0.47
1:a:272:HIS:CD2	4:d:218:VAL:HG21	2.49	0.47
26:t:102:BCR:HC7	26:t:102:BCR:H331	1.54	0.47
1:A:63:ILE:HB	3:C:335:THR:HG21	1.96	0.47
3:C:286:ALA:HB2	24:C:503:CLA:HMD2	1.96	0.47
15:U:33:ALA:HB1	34:U:503:DMS:H22	1.95	0.47
24:b:618:CLA:H161	7:h:7:LEU:HD21	1.95	0.47
19:z:47:TRP:CE2	29:z:1801:LMT:H102	2.50	0.47
4:d:273:PHE:CZ	39:l:101:LHG:H101	2.49	0.47
24:c:510:CLA:HBC3	24:c:512:CLA:H71	1.95	0.47
2:B:30:VAL:HG12	24:B:606:CLA:HHD	1.96	0.47
2:b:446:SER:HB2	2:b:447:PRO:HD2	1.96	0.47
34:o:2606:DMS:H23	44:o:2751:HOH:O	2.15	0.47
2:B:341:LYS:NZ	36:B:625[A]:HTG:S1	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:347[A]:ARG:NH2	44:b:710:HOH:O	2.47	0.47
24:b:612:CLA:NC	41:h:702:RRX:H56	2.29	0.47
5:e:27:ILE:HG12	40:e:103:HEM:HMC3	1.97	0.47
26:Y:302:BCR:HC7	26:Y:302:BCR:H331	1.78	0.47
2:b:324:LEU:HA	4:d:293[A]:LEU:HG	1.96	0.47
3:c:387:TRP:CG	37:c:527:GOL:H2	2.49	0.47
5:e:20:TRP:HD1	9:j:8:ILE:HD12	1.79	0.47
13:o:42:ARG:O	13:o:241:ALA:HA	2.15	0.47
1:a:131:TRP:CH2	24:c:507:CLA:HAA2	2.49	0.47
24:b:610:CLA:H42	28:b:623:LMG:H311	1.97	0.47
2:B:389:LYS:NZ	37:D:403:GOL:O3	2.48	0.47
3:c:436:PHE:CE2	24:c:506:CLA:H152	2.50	0.47
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.50	0.47
2:b:498:LYS:NZ	44:b:713:HOH:O	2.48	0.46
2:B:24:LEU:HD21	24:B:617:CLA:CAB	2.45	0.46
3:c:387:TRP:CD2	37:c:527:GOL:H2	2.50	0.46
6:f:21:VAL:O	6:f:25:THR:HG23	2.15	0.46
4:D:273:PHE:CZ	39:L:101:LHG:H101	2.50	0.46
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.51	0.46
36:b:626:HTG:H1	34:b:643:DMS:S	2.56	0.46
24:c:513:CLA:HAA1	24:c:513:CLA:HBD	1.96	0.46
13:o:180:GLU:OE2	44:o:2701:HOH:O	2.21	0.46
24:B:602:CLA:H91	41:H:101:RRX:H25	1.98	0.46
24:C:504:CLA:HMC3	24:C:514:CLA:H191	1.96	0.46
13:O:39:ARG:HG2	13:O:246:ALA:HB2	1.96	0.46
24:c:511:CLA:HBB1	24:c:511:CLA:HMB1	1.98	0.46
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.98	0.46
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.98	0.46
31:A:417:PL9:H351	31:A:417:PL9:H372	1.44	0.46
5:E:68:ASP:O	5:E:72:ALA:HB2	2.15	0.46
26:T:101:BCR:H311	26:T:101:BCR:HC8	1.97	0.46
5:E:9:PRO:HA	39:E:101:LHG:HC31	1.97	0.46
3:c:362:ARG:HD3	34:c:532:DMS:O	2.16	0.46
4:d:12:ARG:HG3	4:d:17:ILE:HD11	1.97	0.46
3:C:406:SER:HA	3:C:420:VAL:HG23	1.98	0.45
24:c:508:CLA:H72	26:c:517:BCR:H10C	1.98	0.45
1:A:85:SER:HA	1:A:109:GLY:HA3	1.98	0.45
3:C:42:LEU:HD21	24:C:512:CLA:H2A	1.98	0.45
26:C:515:BCR:H11C	26:C:515:BCR:H341	1.84	0.45
2:B:36[A]:SER:OG	26:B:619:BCR:H362	2.16	0.45
4:D:85:MET:CE	4:D:96:GLU:HG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.99	0.45
2:B:423:LYS:HG3	36:B:625[B]:HTG:H1'1	1.99	0.45
24:D:401:CLA:H203	24:D:401:CLA:H162	1.70	0.45
3:c:334:PRO:HA	13:o:153:THR:OG1	2.16	0.45
4:d:343:GLU:HG2	16:v:135:VAL:HG11	1.98	0.45
34:B:647:DMS:O	44:B:701:HOH:O	2.21	0.45
4:d:342:PRO:O	4:d:345:VAL:HG22	2.17	0.45
40:e:103:HEM:HBB2	40:e:103:HEM:HMB2	1.98	0.45
1:A:132:GLU:O	1:A:136:ARG:HG2	2.17	0.45
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.97	0.45
24:b:604:CLA:H203	24:b:604:CLA:H162	1.82	0.45
24:B:615:CLA:H72	29:m:102:LMT:H92	1.99	0.45
4:D:103:ARG:NH1	4:D:106:GLN:OE1	2.46	0.45
2:b:201:HIS:HB2	24:b:605:CLA:CHB	2.47	0.45
27:f:102:SQD:H241	27:f:102:SQD:H272	1.66	0.45
26:C:516:BCR:H15C	26:C:516:BCR:H351	1.88	0.45
2:b:341:LYS:NZ	36:b:625:HTG:S1	2.89	0.45
26:c:516:BCR:H15C	26:c:516:BCR:H351	1.73	0.45
27:F:101:SQD:H242	18:X:31:ILE:HD13	1.99	0.44
24:a:2109:CLA:CBD	24:d:401:CLA:HAC2	2.46	0.44
26:c:516:BCR:H11C	26:c:516:BCR:H341	1.87	0.44
31:d:407:PL9:H411	11:l:29:LEU:HD23	1.98	0.44
1:A:255:PHE:CE2	32:A:418[B]:K2I:BR	3.26	0.44
24:B:617:CLA:H202	24:B:617:CLA:H162	1.79	0.44
24:c:506:CLA:H101	38:c:520:DGD:HBF2	1.99	0.44
7:h:38:PHE:HB2	41:h:702:RRX:C10	2.46	0.44
28:i:101:LMG:H161	28:i:101:LMG:H192	1.83	0.44
13:o:40:ILE:HD12	13:o:95:PHE:CD1	2.52	0.44
26:t:102:BCR:HC8	26:t:102:BCR:H311	1.99	0.44
26:t:102:BCR:HC8	26:t:102:BCR:H321	1.99	0.44
6:F:21:VAL:O	6:F:25:THR:HG23	2.16	0.44
1:A:14:TRP:NE1	29:A:420:LMT:H2B	2.32	0.44
1:A:221[A]:SER:HB2	4:D:139:ARG:O	2.18	0.44
26:Y:302:BCR:H15C	26:Y:302:BCR:H351	1.89	0.44
1:a:132:GLU:O	1:a:136:ARG:HG2	2.17	0.44
24:b:616:CLA:H72	24:b:616:CLA:H111	1.76	0.44
3:c:406:SER:HA	3:c:420:VAL:HG23	1.99	0.44
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.99	0.44
2:B:58:GLN:C	2:B:329:PRO:HB3	2.42	0.44
2:b:458:PHE:HB3	24:b:607:CLA:HBC2	1.99	0.44
24:d:401:CLA:H203	24:d:401:CLA:H162	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:SER:HB2	36:B:625[B]:HTG:H6'2	2.00	0.44
2:B:423:LYS:HG3	36:B:625[A]:HTG:H1'1	2.00	0.44
24:b:608:CLA:H41	24:b:608:CLA:H62	1.75	0.44
10:k:11:LEU:HD11	10:k:22:VAL:HG21	1.99	0.44
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.53	0.44
24:D:404:CLA:HAA2	24:D:404:CLA:HBD	2.00	0.44
24:b:619:CLA:H143	24:b:619:CLA:H162	1.83	0.43
24:c:506:CLA:H143	24:c:510:CLA:H143	1.98	0.43
2:B:462:PHE:CE2	24:B:614:CLA:HMB2	2.53	0.43
39:D:411:LHG:H223	39:D:411:LHG:H191	1.85	0.43
29:M:101:LMT:H6D	11:l:9:PRO:HA	1.99	0.43
13:O:180:GLU:H	13:O:180:GLU:CD	2.26	0.43
25:a:2112:PHO:ND	25:a:2112:PHO:NC	2.66	0.43
5:e:68:ASP:O	5:e:72:ALA:HB2	2.17	0.43
1:a:72:LEU:HD22	29:a:2103:LMT:O2'	2.17	0.43
24:a:2113:CLA:H161	24:a:2113:CLA:H122	1.73	0.43
24:b:616:CLA:H18	39:d:408:LHG:H202	1.99	0.43
26:b:620:BCR:H24C	26:b:620:BCR:H371	1.79	0.43
3:c:223:TRP:CG	3:c:224:ILE:H	2.36	0.43
38:c:519:DGD:HBF2	38:c:519:DGD:HBE2	1.72	0.43
25:A:408:PHO:NC	25:A:408:PHO:ND	2.67	0.43
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.52	0.43
24:B:610:CLA:NC	41:H:101:RRX:H56	2.33	0.43
3:C:50:LEU:HD11	24:C:514:CLA:HBB1	2.01	0.43
24:b:619:CLA:H61	24:b:619:CLA:H2	1.54	0.43
10:k:23:ASP:OD2	17:y:21:GLN:NE2	2.52	0.43
27:a:2115:SQD:H131	32:a:2119:K2I:BR1	2.73	0.43
24:b:609:CLA:H111	24:b:609:CLA:H142	1.79	0.43
24:c:504:CLA:H102	24:c:505:CLA:CHB	2.48	0.43
2:B:70:GLY:HA2	2:B:178:VAL:HG21	2.00	0.43
26:B:618:BCR:H24C	26:B:618:BCR:H371	1.83	0.43
24:b:609:CLA:H61	24:b:609:CLA:H102	1.60	0.43
26:c:517:BCR:H15C	26:c:517:BCR:H351	1.85	0.43
5:e:20:TRP:CD1	9:j:8:ILE:HD12	2.54	0.43
1:A:163:ILE:HD11	38:C:517:DGD:HA22	2.01	0.43
31:A:417:PL9:H201	39:E:101:LHG:H181	2.00	0.43
36:b:625:HTG:H6'2	36:b:625:HTG:H3'2	1.83	0.43
3:c:19:ASN:HB3	3:c:20:SER:H	1.64	0.43
39:d:409:LHG:HC62	11:l:15:THR:HG23	1.99	0.43
31:x:801:PL9:H272	31:x:801:PL9:H251	1.80	0.43
39:E:101:LHG:H172	39:E:101:LHG:H202	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:128:GLY:HA3	24:c:515:CLA:C3C	2.48	0.43
3:c:276:LEU:HD23	24:c:511:CLA:HED1	2.01	0.43
24:d:401:CLA:HBA1	24:d:401:CLA:C4A	2.47	0.43
15:u:58:VAL:HG12	15:u:79:LEU:HD22	2.00	0.43
2:B:458:PHE:HB3	24:B:605:CLA:HBC2	2.01	0.43
27:B:621:SQD:H312	27:B:621:SQD:H341	1.64	0.43
3:C:80:PRO:HG3	34:C:528:DMS:H11	2.00	0.43
38:C:518:DGD:HA41	29:J:102:LMT:H82	2.01	0.43
44:b:894:HOH:O	37:o:2603:GOL:H32	2.18	0.43
4:d:144:ILE:HD11	34:d:417:DMS:H21	2.01	0.43
27:A:411:SQD:H111	27:A:411:SQD:H141	1.75	0.43
36:D:413:HTG:H3'2	7:H:25:TRP:CZ3	2.54	0.43
27:L:102:SQD:H311	27:L:102:SQD:H341	1.72	0.43
1:a:85:SER:HA	1:a:109:GLY:HA3	2.01	0.43
26:a:2114:BCR:H15C	26:a:2114:BCR:H351	1.94	0.43
24:b:614:CLA:H112	24:b:614:CLA:H72	1.75	0.43
4:d:85:MET:CE	4:d:96:GLU:HG2	2.44	0.43
26:k:2003:BCR:H15C	26:k:2003:BCR:H351	1.89	0.43
24:B:605:CLA:H192	24:B:605:CLA:H162	1.92	0.42
3:C:52:ALA:HB2	24:C:512:CLA:HMA2	1.99	0.42
3:C:429:SER:HB3	38:C:518:DGD:HBT2	2.00	0.42
34:C:528:DMS:H23	34:C:529:DMS:H22	2.01	0.42
41:H:101:RRX:H43	41:H:101:RRX:H47	1.83	0.42
26:T:101:BCR:H11C	26:T:101:BCR:H341	1.90	0.42
2:b:141:ILE:HG21	24:b:618:CLA:HBB1	2.01	0.42
2:B:216:HIS:HE1	24:B:610:CLA:C1A	2.31	0.42
24:a:2110:CLA:HED1	38:c:520:DGD:HAE2	2.01	0.42
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.49	0.42
26:T:101:BCR:HC8	26:T:101:BCR:H321	2.02	0.42
24:c:506:CLA:HAA1	24:c:506:CLA:HBD	2.02	0.42
24:c:514:CLA:C1B	26:c:516:BCR:H401	2.49	0.42
26:K:101:BCR:H371	26:K:101:BCR:H24C	1.84	0.42
2:b:86:ILE:HD12	2:b:88:PRO:HD3	2.01	0.42
38:c:519:DGD:HB62	28:c:521:LMG:H401	2.01	0.42
39:e:101:LHG:H112	39:e:101:LHG:HC82	1.82	0.42
2:B:324:LEU:HA	4:D:293[A]:LEU:HG	2.01	0.42
24:C:504:CLA:C3B	28:C:526:LMG:H221	2.50	0.42
4:D:12:ARG:HB2	4:D:16:ASP:HB2	2.02	0.42
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.01	0.42
4:d:123:ILE:HD11	38:h:703:DGD:HAH1	2.02	0.42
3:C:77:PRO:HB2	34:C:534:DMS:H23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:C:518:DGD:HAT2	38:C:518:DGD:HA71	1.76	0.42
2:b:158:LEU:HB3	2:b:199:VAL:HG22	2.00	0.42
3:C:203:THR:O	3:C:235:GLY:HA3	2.19	0.42
2:b:30:VAL:HG12	24:b:608:CLA:HHD	2.01	0.42
24:b:608:CLA:HAA1	24:b:608:CLA:HBD	2.01	0.42
2:B:410:THR:O	37:B:635:GOL:H32	2.20	0.42
26:B:620:BCR:H15C	26:B:620:BCR:H351	1.95	0.42
26:C:516:BCR:H341	26:C:516:BCR:H11C	1.92	0.42
36:D:413:HTG:H1	7:H:25:TRP:CD1	2.55	0.42
1:a:162:PRO:HB3	1:a:168:PHE:HA	2.01	0.42
3:c:79:LYS:HD2	16:v:35:TYR:CE1	2.55	0.42
41:h:702:RRX:H32	41:h:702:RRX:H28	1.86	0.42
2:B:451:PHE:CE2	2:B:455:HIS:CE1	3.08	0.42
3:C:276:LEU:HD23	24:C:510:CLA:HED1	2.02	0.42
38:C:518:DGD:HAT2	38:C:518:DGD:HAH2	1.39	0.42
24:a:2113:CLA:H102	24:a:2113:CLA:H61	1.64	0.42
2:b:27:THR:HG22	2:b:107:LEU:HD13	2.02	0.42
3:C:223:TRP:CG	3:C:224:ILE:H	2.38	0.42
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.50	0.42
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.02	0.41
2:b:80:ILE:HD11	2:b:167:TRP:CZ3	2.55	0.41
2:b:285:ASN:O	2:b:289:GLN:HG2	2.20	0.41
3:c:167:VAL:HG13	24:c:514:CLA:H72	2.01	0.41
3:c:443:TRP:CZ2	24:c:510:CLA:HMD1	2.54	0.41
1:A:223:LEU:HD12	4:D:139:ARG:HH12	1.84	0.41
3:C:95:LEU:HD21	24:C:502:CLA:OBD	2.21	0.41
24:C:513:CLA:H203	24:C:513:CLA:H161	1.87	0.41
13:O:218:GLU:HG3	34:O:310:DMS:H13	2.01	0.41
24:a:2110:CLA:H142	24:a:2110:CLA:H112	1.85	0.41
16:v:34:GLN:NE2	44:v:305:HOH:O	2.50	0.41
24:B:606:CLA:H62	24:B:606:CLA:H41	1.80	0.41
24:C:513:CLA:H92	24:C:513:CLA:H62	1.81	0.41
38:C:518:DGD:HBF1	38:C:518:DGD:HBE2	1.78	0.41
4:D:126:MET:HE3	4:D:143:ALA:O	2.21	0.41
24:b:604:CLA:H141	24:b:604:CLA:H161	1.80	0.41
26:b:622:BCR:H15C	26:b:622:BCR:H351	1.92	0.41
24:A:405:CLA:CBD	24:D:401:CLA:HAC2	2.50	0.41
26:A:410:BCR:H15C	26:A:410:BCR:H351	1.92	0.41
24:D:405:CLA:H161	24:D:405:CLA:H141	1.87	0.41
13:O:42:ARG:O	13:O:241:ALA:HA	2.20	0.41
13:O:54:GLU:O	13:O:56:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:338:GLY:HA3	3:c:341:LEU:O	2.20	0.41
26:t:102:BCR:H11C	26:t:102:BCR:H341	1.94	0.41
2:B:419:SER:HB2	36:B:625[A]:HTG:H6'2	2.01	0.41
3:C:60:ILE:HG22	24:C:504:CLA:HHD	2.02	0.41
3:C:334:PRO:HA	13:O:153:THR:OG1	2.20	0.41
36:O:302:HTG:H7'3	2:b:98:LEU:HB2	2.02	0.41
15:U:76:ARG:NH1	44:U:609:HOH:O	2.53	0.41
24:B:616:CLA:H51	26:B:620:BCR:H341	2.02	0.41
3:C:94:THR:HG22	24:C:502:CLA:HED1	2.01	0.41
3:C:443:TRP:CZ2	24:C:509:CLA:HMD1	2.56	0.41
4:d:144:ILE:CD1	34:d:417:DMS:H21	2.51	0.41
2:B:461:LEU:HD22	39:D:409:LHG:H301	2.02	0.41
24:B:616:CLA:H161	7:H:7:LEU:HD21	2.03	0.41
39:d:408:LHG:H212	12:m:18:PRO:HG3	2.02	0.41
1:A:73:TYR:OH	29:A:414:LMT:H6E	2.21	0.41
2:b:90:PHE:H	36:b:602:HTG:H62	1.86	0.41
3:c:163:PHE:CD2	24:c:514:CLA:HAB	2.56	0.41
28:A:412:LMG:H182	28:A:412:LMG:H151	1.73	0.41
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.55	0.41
2:B:433:ASP:OD2	2:B:436:THR:OG1	2.36	0.41
24:C:514:CLA:CAB	26:C:515:BCR:H24C	2.51	0.41
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	2.02	0.41
15:U:16:LYS:NZ	44:U:608:HOH:O	2.53	0.41
34:b:633:DMS:H21	15:u:21:TYR:CZ	2.55	0.41
3:c:425:TRP:CD1	24:c:506:CLA:HMA3	2.55	0.41
4:d:186:GLN:HB2	24:d:404:CLA:HBC1	2.03	0.41
4:d:293[A]:LEU:HD12	4:d:293[A]:LEU:HA	1.91	0.41
10:k:24:VAL:O	10:k:27:VAL:HG22	2.21	0.41
13:o:193:THR:HG21	13:o:220:LEU:HD12	2.01	0.41
19:z:47:TRP:CD2	29:z:1801:LMT:H102	2.55	0.41
1:A:322:ASN:OD1	3:C:412:THR:HA	2.21	0.41
4:d:148:ALA:HB3	4:d:149:PRO:HD3	2.03	0.41
26:d:406:BCR:H15C	26:d:406:BCR:H351	1.90	0.41
24:C:508:CLA:H61	24:C:508:CLA:H92	1.83	0.40
44:C:604:HOH:O	39:E:101:LHG:H361	2.21	0.40
1:a:296:ASN:HB2	3:c:400:PRO:O	2.21	0.40
1:a:322:ASN:OD1	3:c:412:THR:HA	2.20	0.40
24:d:401:CLA:HMB1	24:d:401:CLA:HBB1	2.02	0.40
2:B:12:LEU:HB2	24:B:613:CLA:HMC2	2.03	0.40
24:B:606:CLA:C14	24:B:611:CLA:HED2	2.51	0.40
29:B:636:LMT:H81	12:m:8:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:464:GLU:OE2	4:D:245:SER:OG	2.27	0.40
5:E:26:THR:HA	20:R:15:ALA:HB1	2.04	0.40
26:b:621:BCR:H15C	26:b:621:BCR:H351	1.96	0.40
1:A:72:LEU:HD11	29:A:414:LMT:H52	2.02	0.40
24:A:406:CLA:H142	24:A:406:CLA:H112	1.90	0.40
24:B:610:CLA:HBA1	24:B:610:CLA:H3A	1.91	0.40
3:C:288:CYS:SG	38:C:517:DGD:HB32	2.61	0.40
39:D:409:LHG:H282	39:D:409:LHG:H312	1.83	0.40
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.82	0.40
24:d:405:CLA:H162	7:h:37:LEU:HD23	2.04	0.40
3:C:128:GLY:HA3	24:C:514:CLA:C3C	2.52	0.40
39:E:101:LHG:H321	39:E:101:LHG:H351	1.96	0.40
14:T:25:GLU:HA	14:T:26:PRO:HD3	1.97	0.40
27:a:2102:SQD:H141	26:t:102:BCR:HC41	2.04	0.40
2:b:379:ALA:HA	2:b:390:TYR:HB3	2.03	0.40
26:b:622:BCR:H24C	26:b:622:BCR:H371	1.88	0.40
1:A:270[B]:SER:OG	27:A:411:SQD:H3	2.22	0.40
32:A:419:K2I:BR1	39:D:411:LHG:H222	2.77	0.40
2:B:464:PHE:CZ	39:D:409:LHG:H252	2.57	0.40
24:B:603:CLA:H203	24:B:603:CLA:H162	1.92	0.40
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.54	0.40
29:M:101:LMT:H71	12:m:24:ILE:HD13	2.04	0.40
15:U:10:VAL:HG11	15:U:15:GLU:OE2	2.22	0.40
2:b:413:ASP:CG	2:b:415:PRO:HD2	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	335/344 (97%)	331 (99%)	3 (1%)	1 (0%)	36 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	335/344 (97%)	330 (98%)	4 (1%)	1 (0%)	36	36
2	B	508/505 (101%)	502 (99%)	6 (1%)	0	100	100
2	b	509/505 (101%)	503 (99%)	6 (1%)	0	100	100
3	C	451/455 (99%)	442 (98%)	8 (2%)	1 (0%)	43	44
3	c	453/455 (100%)	443 (98%)	9 (2%)	1 (0%)	43	44
4	D	339/342 (99%)	331 (98%)	8 (2%)	0	100	100
4	d	342/342 (100%)	335 (98%)	7 (2%)	0	100	100
5	E	79/83 (95%)	79 (100%)	0	0	100	100
5	e	77/83 (93%)	77 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
7	h	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	37/40 (92%)	37 (100%)	0	0	100	100
10	K	36/37 (97%)	36 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	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	33/36 (92%)	33 (100%)	0	0	100	100
13	O	244/244 (100%)	239 (98%)	5 (2%)	0	100	100
13	o	244/244 (100%)	239 (98%)	5 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	133 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	132 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	28/30 (93%)	28 (100%)	0	0	100	100
17	y	27/30 (90%)	27 (100%)	0	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
20	R	32/41 (78%)	32 (100%)	0	0	100	100
All	All	5244/5387 (97%)	5155 (98%)	85 (2%)	4 (0%)	48	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	c	416	SER
3	C	416	SER
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/279 (96%)	266 (100%)	1 (0%)	84	89
1	a	270/279 (97%)	269 (100%)	1 (0%)	84	89
2	B	405/403 (100%)	405 (100%)	0	100	100
2	b	398/403 (99%)	395 (99%)	3 (1%)	73	81
3	C	354/356 (99%)	351 (99%)	3 (1%)	73	81
3	c	355/356 (100%)	352 (99%)	3 (1%)	73	81
4	D	275/276 (100%)	273 (99%)	2 (1%)	76	83
4	d	278/276 (101%)	275 (99%)	3 (1%)	65	74
5	E	70/72 (97%)	68 (97%)	2 (3%)	37	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	66/72 (92%)	66 (100%)	0	100	100
6	F	28/38 (74%)	27 (96%)	1 (4%)	31	34
6	f	26/38 (68%)	25 (96%)	1 (4%)	29	32
7	H	53/53 (100%)	53 (100%)	0	100	100
7	h	53/53 (100%)	53 (100%)	0	100	100
8	I	31/34 (91%)	31 (100%)	0	100	100
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	30/30 (100%)	29 (97%)	1 (3%)	33	37
10	k	28/30 (93%)	28 (100%)	0	100	100
11	L	33/35 (94%)	33 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	205/207 (99%)	205 (100%)	0	100	100
13	o	206/207 (100%)	203 (98%)	3 (2%)	57	65
14	T	25/28 (89%)	24 (96%)	1 (4%)	28	29
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	29
15	U	84/89 (94%)	82 (98%)	2 (2%)	43	49
15	u	84/89 (94%)	82 (98%)	2 (2%)	43	49
16	V	115/117 (98%)	115 (100%)	0	100	100
16	v	114/117 (97%)	114 (100%)	0	100	100
17	Y	22/23 (96%)	21 (96%)	1 (4%)	24	25
17	y	21/23 (91%)	20 (95%)	1 (5%)	23	23
18	X	29/33 (88%)	29 (100%)	0	100	100
18	x	29/33 (88%)	29 (100%)	0	100	100
19	Z	45/51 (88%)	45 (100%)	0	100	100
19	z	43/51 (84%)	43 (100%)	0	100	100
20	R	11/33 (33%)	11 (100%)	0	100	100
All	All	4252/4401 (97%)	4220 (99%)	32 (1%)	76	81

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
3	C	255	THR
3	C	289	PHE
3	C	315	MET
4	D	90	LEU
4	D	329	MET
5	E	4	THR
5	E	5	THR
6	F	44	GLN
10	K	17	ILE
14	T	2	GLU
15	U	70[A]	ARG
15	U	70[B]	ARG
17	Y	30	ILE
1	a	15	GLU
2	b	352[A]	GLU
2	b	352[B]	GLU
2	b	362	PHE
3	c	255	THR
3	c	289	PHE
3	c	315	MET
4	d	28	VAL
4	d	90	LEU
4	d	329	MET
6	f	44	GLN
13	o	23	ASP
13	o	64	GLU
13	o	179	GLU
14	t	2	GLU
15	u	9	LEU
15	u	10	VAL
17	y	30	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	296	ASN
2	B	179	GLN
2	B	289	GLN
2	B	374	ASN

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Mol	Chain	Res	Type
3	C	44	ASN
4	D	186	GLN
4	D	255	GLN
5	E	60	GLN
13	O	61	GLN
13	O	155	ASN
15	U	37	GLN
15	U	78	ASN
1	a	165	GLN
1	a	296	ASN
2	b	282	GLN
2	b	289	GLN
2	b	331	ASN
3	c	385	GLN
4	d	186	GLN
4	d	255	GLN
4	d	301	GLN
16	v	118	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	$\# Z > 2$
19	FME	Z	1	19	8,9,10	0.66	0	8,9,11	1.51	2 (25%)
4	HSK	d	336[A]	-	10,10,12	4.04	2 (20%)	5,12,16	1.90	3 (60%)
14	FME	T	1	14	8,9,10	0.69	0	8,9,11	1.59	2 (25%)
4	HSK	D	336[B]	-	10,11,12	2.36	3 (30%)	5,14,16	3.73	4 (80%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	FME	z	1	19	8,9,10	0.65	0	8,9,11	1.43	3 (37%)
8	FME	i	1	8	8,9,10	0.60	0	8,9,11	1.45	2 (25%)
12	FME	m	1	12	8,9,10	0.59	0	8,9,11	1.12	0
8	FME	I	1	8	8,9,10	0.63	0	8,9,11	1.42	2 (25%)
14	FME	t	1	14	8,9,10	0.70	0	8,9,11	1.60	1 (12%)
4	HSK	D	336[A]	-	10,10,12	7.17	3 (30%)	5,12,16	2.17	2 (40%)
4	HSK	d	336[B]	-	10,11,12	2.29	3 (30%)	5,14,16	3.75	4 (80%)
12	FME	M	1	12	8,9,10	0.75	0	8,9,11	1.20	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	FME	Z	1	19	-	3/7/9/11	-
4	HSK	d	336[A]	-	-	0/5/6/8	0/1/1/1
14	FME	T	1	14	-	2/7/9/11	-
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
19	FME	z	1	19	-	4/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
4	HSK	D	336[A]	-	-	0/5/6/8	0/1/1/1
4	HSK	d	336[B]	-	-	0/5/6/8	0/1/1/1
12	FME	M	1	12	-	1/7/9/11	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[A]	HSK	OM-ND1	-21.90	0.97	1.38
4	d	336[A]	HSK	OM-ND1	-11.42	1.17	1.38
4	D	336[B]	HSK	CG-ND1	-5.72	1.33	1.40
4	d	336[B]	HSK	CG-ND1	-5.44	1.33	1.40
4	D	336[A]	HSK	CG-ND1	-4.93	1.34	1.40
4	d	336[A]	HSK	CG-ND1	-4.39	1.34	1.40
4	D	336[B]	HSK	OM-ND1	3.01	1.44	1.38
4	d	336[B]	HSK	OM-ND1	2.75	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[B]	HSK	CE1-ND1	-2.44	1.33	1.37
4	d	336[B]	HSK	CE1-ND1	-2.39	1.33	1.37
4	D	336[A]	HSK	CE1-ND1	-2.03	1.33	1.37

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	336[B]	HSK	ND1-CE1-NE2	-6.46	104.08	111.54
4	D	336[B]	HSK	ND1-CE1-NE2	-6.36	104.20	111.54
4	d	336[B]	HSK	CD2-NE2-CE1	3.35	109.63	105.24
4	D	336[B]	HSK	CD2-NE2-CE1	3.27	109.52	105.24
4	D	336[A]	HSK	ND1-CE1-NE2	-3.23	107.82	111.54
4	D	336[B]	HSK	CB-CG-ND1	3.05	128.04	122.89
4	d	336[B]	HSK	CE1-ND1-CG	2.92	114.88	108.87
4	D	336[B]	HSK	CE1-ND1-CG	2.79	114.61	108.87
4	d	336[B]	HSK	CB-CG-ND1	2.73	127.50	122.89
4	D	336[A]	HSK	CD2-NE2-CE1	2.69	108.76	105.24
14	t	1	FME	O-C-CA	-2.58	118.12	124.77
4	d	336[A]	HSK	ND1-CE1-NE2	-2.58	108.57	111.54
14	T	1	FME	O-C-CA	-2.38	118.65	124.77
4	d	336[A]	HSK	CD2-NE2-CE1	2.30	108.25	105.24
19	Z	1	FME	CA-N-CN	-2.25	119.36	122.82
14	T	1	FME	CB-CA-N	-2.19	106.52	110.52
19	z	1	FME	CA-N-CN	-2.12	119.57	122.82
8	I	1	FME	CA-N-CN	-2.09	119.61	122.82
19	z	1	FME	O-C-CA	-2.09	119.41	124.77
8	I	1	FME	O-C-CA	-2.06	119.46	124.77
4	d	336[A]	HSK	CB-CG-ND1	2.06	126.37	122.89
19	z	1	FME	O1-CN-N	-2.06	120.00	125.32
12	M	1	FME	CA-N-CN	-2.05	119.67	122.82
8	i	1	FME	O-C-CA	-2.04	119.51	124.77
8	i	1	FME	C-CA-N	2.04	113.43	109.50
19	Z	1	FME	O1-CN-N	-2.03	120.08	125.32

There are no chirality outliers.

All (16) 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
19	z	1	FME	N-CA-CB-CG
19	z	1	FME	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
19	Z	1	FME	CA-CB-CG-SD
19	z	1	FME	CA-CB-CG-SD
14	t	1	FME	CB-CG-SD-CE
14	T	1	FME	C-CA-CB-CG
14	t	1	FME	C-CA-CB-CG
14	T	1	FME	N-CA-CB-CG
8	I	1	FME	O1-CN-N-CA
12	M	1	FME	O1-CN-N-CA
19	Z	1	FME	O1-CN-N-CA
8	I	1	FME	CB-CA-N-CN
19	Z	1	FME	CB-CA-N-CN
19	z	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 399 ligands modelled in this entry, 13 are monoatomic and 44 are unknown - leaving 342 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	$\# Z > 2$
29	LMT	B	637	-	24,24,36	0.51	0	29,29,47	0.71	0
37	GOL	B	635	-	5,5,5	1.13	0	5,5,5	0.97	0
34	DMS	c	540	-	3,3,3	2.72	1 (33%)	3,3,3	0.53	0
34	DMS	o	2609	-	3,3,3	2.75	1 (33%)	3,3,3	0.61	0
33	BCT	a	2108	22	3,3,3	0.46	0	2,3,3	1.10	0
24	CLA	b	616	-	69,73,73	2.55	24 (34%)	82,113,113	2.40	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DMS	B	640	-	3,3,3	2.77	1 (33%)	3,3,3	0.58	0
36	HTG	c	524	-	19,19,19	0.99	2 (10%)	23,24,24	1.42	2 (8%)
34	DMS	d	417	-	3,3,3	2.75	1 (33%)	3,3,3	0.61	0
24	CLA	c	503	-	69,73,73	2.41	22 (31%)	82,113,113	2.51	27 (32%)
29	LMT	I	1201	-	24,24,36	0.44	0	29,29,47	1.13	3 (10%)
34	DMS	v	211	-	3,3,3	2.76	1 (33%)	3,3,3	0.59	0
26	BCR	Y	302	-	41,41,41	0.79	0	56,56,56	1.64	11 (19%)
24	CLA	C	503	-	69,73,73	2.64	24 (34%)	82,113,113	2.43	26 (31%)
27	SQD	A	413	-	52,54,54	0.98	2 (3%)	62,65,65	1.26	6 (9%)
37	GOL	b	631	-	5,5,5	0.90	0	5,5,5	1.06	0
34	DMS	C	530	-	3,3,3	2.75	1 (33%)	3,3,3	0.65	0
24	CLA	B	613	-	69,73,73	2.29	24 (34%)	82,113,113	2.45	26 (31%)
34	DMS	o	2607	-	3,3,3	2.73	1 (33%)	3,3,3	0.56	0
39	LHG	D	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.18	6 (11%)
24	CLA	B	615	-	69,73,73	2.29	21 (30%)	82,113,113	2.56	28 (34%)
37	GOL	k	2001	-	5,5,5	0.96	0	5,5,5	0.99	0
34	DMS	O	305	-	3,3,3	2.70	1 (33%)	3,3,3	0.53	0
24	CLA	B	605	-	69,73,73	2.52	23 (33%)	82,113,113	2.28	25 (30%)
36	HTG	B	625[A]	-	19,19,19	0.93	1 (5%)	23,24,24	1.13	2 (8%)
39	LHG	l	101	-	48,48,48	0.87	2 (4%)	51,54,54	1.14	4 (7%)
26	BCR	C	516	-	41,41,41	0.74	0	56,56,56	1.56	11 (19%)
34	DMS	B	646	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0
29	LMT	A	414	-	35,35,36	0.44	0	46,46,47	1.15	5 (10%)
37	GOL	d	415	-	5,5,5	0.94	0	5,5,5	1.07	0
26	BCR	B	618	-	41,41,41	0.75	0	56,56,56	1.40	8 (14%)
24	CLA	B	606	-	69,73,73	2.32	23 (33%)	82,113,113	2.40	27 (32%)
34	DMS	A	425	-	3,3,3	2.74	1 (33%)	3,3,3	0.57	0
34	DMS	e	104	-	3,3,3	2.74	1 (33%)	3,3,3	0.58	0
38	DGD	C	517	-	63,63,67	0.85	3 (4%)	77,77,81	1.08	6 (7%)
21	OEX	a	2104	1,44,3	0,15,15	-	-	-	-	-
26	BCR	a	2114	-	41,41,41	0.77	0	56,56,56	1.32	6 (10%)
40	HEM	e	103	6,5	50,50,50	1.94	10 (20%)	67,82,82	1.29	7 (10%)
34	DMS	a	2123	-	3,3,3	2.74	1 (33%)	3,3,3	0.54	0
26	BCR	A	410	-	41,41,41	0.85	1 (2%)	56,56,56	1.44	8 (14%)
34	DMS	T	105	-	3,3,3	2.72	1 (33%)	3,3,3	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	c	516	-	41,41,41	0.76	0	56,56,56	1.56	8 (14%)
34	DMS	o	2605	-	3,3,3	2.73	1 (33%)	3,3,3	0.59	0
27	SQD	B	621	-	52,54,54	1.01	3 (5%)	62,65,65	1.49	7 (11%)
29	LMT	j	1601	-	22,22,36	0.65	1 (4%)	26,26,47	1.18	2 (7%)
36	HTG	b	601	-	19,19,19	0.95	2 (10%)	23,24,24	1.47	4 (17%)
34	DMS	A	424	-	3,3,3	2.64	1 (33%)	3,3,3	0.49	0
34	DMS	v	208	-	3,3,3	2.74	1 (33%)	3,3,3	0.56	0
41	RRX	h	702	-	42,42,42	0.72	0	56,58,58	1.37	8 (14%)
34	DMS	u	201	-	3,3,3	2.72	1 (33%)	3,3,3	0.58	0
34	DMS	c	530	-	3,3,3	2.68	1 (33%)	3,3,3	0.48	0
27	SQD	a	2102	-	51,53,54	0.96	2 (3%)	61,64,65	1.19	5 (8%)
34	DMS	B	649	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
34	DMS	c	541	-	3,3,3	2.74	1 (33%)	3,3,3	0.49	0
24	CLA	b	610	44	69,73,73	2.66	24 (34%)	82,113,113	2.35	31 (37%)
37	GOL	v	204	-	5,5,5	0.83	0	5,5,5	1.02	0
36	HTG	B	627	-	19,19,19	0.95	2 (10%)	23,24,24	1.47	3 (13%)
34	DMS	b	636	-	3,3,3	2.81	1 (33%)	3,3,3	0.71	0
38	DGD	C	519	-	63,63,67	0.87	2 (3%)	77,77,81	1.18	7 (9%)
34	DMS	B	650	-	3,3,3	2.75	1 (33%)	3,3,3	0.55	0
26	BCR	C	515	-	41,41,41	0.78	0	56,56,56	1.46	7 (12%)
36	HTG	D	413	-	19,19,19	0.97	2 (10%)	23,24,24	1.19	2 (8%)
24	CLA	b	615	-	69,73,73	2.30	21 (30%)	82,113,113	2.52	26 (31%)
34	DMS	u	204	-	3,3,3	2.79	1 (33%)	3,3,3	0.66	0
43	HEC	v	201	16	46,50,50	2.04	8 (17%)	58,82,82	1.38	6 (10%)
37	GOL	V	203	-	5,5,5	1.00	0	5,5,5	0.96	0
34	DMS	C	527	-	3,3,3	2.76	1 (33%)	3,3,3	0.60	0
34	DMS	a	2124	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0
24	CLA	D	404	-	69,73,73	2.22	22 (31%)	82,113,113	2.62	30 (36%)
37	GOL	D	403	-	5,5,5	1.22	0	5,5,5	0.93	0
24	CLA	A	405	-	69,73,73	2.37	22 (31%)	82,113,113	2.35	31 (37%)
37	GOL	U	502	-	5,5,5	0.87	0	5,5,5	1.04	0
29	LMT	i	104	-	24,24,36	0.54	1 (4%)	29,29,47	1.39	3 (10%)
34	DMS	v	206	-	3,3,3	2.76	1 (33%)	3,3,3	0.65	0
26	BCR	d	406	-	41,41,41	0.89	1 (2%)	56,56,56	1.73	8 (14%)
24	CLA	c	508	-	69,73,73	2.46	24 (34%)	82,113,113	2.43	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DMS	b	643	-	3,3,3	2.74	1 (33%)	3,3,3	0.56	0
25	PHO	a	2111	-	58,69,69	2.57	10 (17%)	55,99,99	2.85	13 (23%)
26	BCR	c	517	-	41,41,41	0.80	0	56,56,56	1.53	9 (16%)
29	LMT	B	636	-	36,36,36	0.49	0	47,47,47	1.07	4 (8%)
34	DMS	o	2604	-	3,3,3	2.73	1 (33%)	3,3,3	0.51	0
24	CLA	d	404	-	69,73,73	2.39	23 (33%)	82,113,113	2.35	28 (34%)
34	DMS	O	311	-	3,3,3	2.76	1 (33%)	3,3,3	0.63	0
37	GOL	c	527	-	5,5,5	0.78	0	5,5,5	1.11	0
26	BCR	b	622	-	41,41,41	0.81	1 (2%)	56,56,56	1.42	7 (12%)
24	CLA	b	612	-	69,73,73	2.54	23 (33%)	82,113,113	2.38	30 (36%)
27	SQD	f	102	-	35,36,54	1.67	3 (8%)	39,41,65	1.37	5 (12%)
34	DMS	c	532	-	3,3,3	2.64	1 (33%)	3,3,3	0.36	0
34	DMS	B	647	-	3,3,3	2.75	1 (33%)	3,3,3	0.47	0
34	DMS	v	214	-	3,3,3	2.82	1 (33%)	3,3,3	0.79	0
24	CLA	C	507	-	69,73,73	2.70	21 (30%)	82,113,113	2.51	28 (34%)
24	CLA	B	602	44	69,73,73	2.45	25 (36%)	82,113,113	2.37	24 (29%)
28	LMG	b	623	-	51,51,55	0.94	2 (3%)	59,59,63	1.02	2 (3%)
24	CLA	b	611	-	69,73,73	2.50	25 (36%)	82,113,113	2.41	28 (34%)
24	CLA	c	510	-	69,73,73	2.50	22 (31%)	82,113,113	2.42	25 (30%)
34	DMS	E	108	-	3,3,3	2.75	1 (33%)	3,3,3	0.60	0
39	LHG	D	410	-	48,48,48	0.90	3 (6%)	51,54,54	0.93	3 (5%)
38	DGD	c	519	-	63,63,67	0.85	2 (3%)	77,77,81	1.07	5 (6%)
34	DMS	O	313	-	3,3,3	2.74	1 (33%)	3,3,3	0.56	0
36	HTG	C	521	-	19,19,19	0.94	2 (10%)	23,24,24	0.99	1 (4%)
29	LMT	E	105	-	24,24,36	0.52	1 (4%)	29,29,47	0.88	1 (3%)
29	LMT	T	102	-	24,24,36	0.41	0	29,29,47	0.95	1 (3%)
43	HEC	V	201	16	46,50,50	2.00	7 (15%)	58,82,82	1.41	5 (8%)
24	CLA	C	511	-	69,73,73	2.55	25 (36%)	82,113,113	2.36	30 (36%)
34	DMS	o	2610	-	3,3,3	2.72	1 (33%)	3,3,3	0.48	0
24	CLA	B	609	-	69,73,73	2.48	25 (36%)	82,113,113	2.32	28 (34%)
34	DMS	C	538	-	3,3,3	2.77	1 (33%)	3,3,3	0.55	0
24	CLA	b	613	44	69,73,73	2.41	24 (34%)	82,113,113	2.39	30 (36%)
29	LMT	b	624	-	25,25,36	0.44	0	30,30,47	1.17	3 (10%)
34	DMS	u	202	-	3,3,3	2.74	1 (33%)	3,3,3	0.73	0
34	DMS	D	417	-	3,3,3	2.75	1 (33%)	3,3,3	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DMS	O	309	-	3,3,3	2.75	1 (33%)	3,3,3	0.67	0
36	HTG	i	103	-	19,19,19	0.89	1 (5%)	23,24,24	1.14	1 (4%)
26	BCR	B	620	-	41,41,41	0.77	0	56,56,56	1.25	8 (14%)
24	CLA	b	614	-	69,73,73	2.59	25 (36%)	82,113,113	2.40	31 (37%)
24	CLA	c	512	-	69,73,73	2.40	22 (31%)	82,113,113	2.30	26 (31%)
27	SQD	F	101	-	43,45,54	1.06	2 (4%)	53,56,65	1.52	9 (16%)
34	DMS	b	639	-	3,3,3	2.69	1 (33%)	3,3,3	0.43	0
29	LMT	m	103	-	36,36,36	0.48	0	47,47,47	1.04	4 (8%)
34	DMS	c	538	-	3,3,3	2.78	1 (33%)	3,3,3	0.64	0
31	PL9	d	407	-	55,55,55	0.76	1 (1%)	68,69,69	1.55	13 (19%)
37	GOL	Z	102	-	5,5,5	1.02	0	5,5,5	0.89	0
26	BCR	k	2003	-	41,41,41	0.68	0	56,56,56	1.49	12 (21%)
34	DMS	C	537	-	3,3,3	2.73	1 (33%)	3,3,3	0.53	0
24	CLA	C	513	-	69,73,73	2.50	22 (31%)	82,113,113	2.46	32 (39%)
34	DMS	c	529	-	3,3,3	2.67	1 (33%)	3,3,3	0.36	0
24	CLA	C	510	-	69,73,73	2.58	24 (34%)	82,113,113	2.43	27 (32%)
27	SQD	A	411	-	47,49,54	0.95	2 (4%)	57,60,65	1.68	11 (19%)
24	CLA	C	504	-	69,73,73	2.54	21 (30%)	82,113,113	2.30	25 (30%)
33	BCT	A	421	22	3,3,3	0.49	0	2,3,3	1.00	0
34	DMS	V	207	-	3,3,3	2.71	1 (33%)	3,3,3	0.55	0
34	DMS	a	2121	-	3,3,3	2.57	1 (33%)	3,3,3	0.18	0
31	PL9	A	417	-	38,38,55	0.52	0	45,45,69	1.70	10 (22%)
34	DMS	o	2606	-	3,3,3	2.72	1 (33%)	3,3,3	0.58	0
34	DMS	V	210	-	3,3,3	2.72	1 (33%)	3,3,3	0.61	0
34	DMS	B	648	-	3,3,3	2.73	1 (33%)	3,3,3	0.37	0
34	DMS	v	210	-	3,3,3	2.73	1 (33%)	3,3,3	0.56	0
28	LMG	C	526	-	48,48,55	0.98	2 (4%)	56,56,63	1.26	6 (10%)
25	PHO	A	408	-	58,69,69	2.82	14 (24%)	55,99,99	3.01	14 (25%)
36	HTG	B	628	-	19,19,19	0.94	1 (5%)	23,24,24	1.50	4 (17%)
24	CLA	b	606	-	69,73,73	2.49	23 (33%)	82,113,113	2.44	32 (39%)
27	SQD	L	102	-	52,54,54	0.99	2 (3%)	62,65,65	1.56	9 (14%)
32	K2I	A	419	-	8,10,10	1.32	1 (12%)	10,14,14	1.53	3 (30%)
37	GOL	H	103	-	5,5,5	0.99	0	5,5,5	0.93	0
34	DMS	T	106	-	3,3,3	2.76	1 (33%)	3,3,3	0.58	0
34	DMS	C	529	-	3,3,3	2.73	1 (33%)	3,3,3	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DMS	b	632	-	3,3,3	2.51	1 (33%)	3,3,3	0.58	0
24	CLA	c	506	44	69,73,73	2.32	21 (30%)	82,113,113	2.48	32 (39%)
34	DMS	x	802	-	3,3,3	2.78	1 (33%)	3,3,3	0.67	0
37	GOL	O	303	-	5,5,5	0.98	0	5,5,5	0.99	0
24	CLA	C	505	44	69,73,73	2.51	24 (34%)	82,113,113	2.32	28 (34%)
34	DMS	o	2612	-	3,3,3	2.78	1 (33%)	3,3,3	0.67	0
36	HTG	C	522	-	19,19,19	0.90	1 (5%)	23,24,24	1.66	3 (13%)
34	DMS	O	314	-	3,3,3	2.73	1 (33%)	3,3,3	0.51	0
36	HTG	b	602	-	19,19,19	1.04	2 (10%)	23,24,24	1.70	4 (17%)
24	CLA	c	509	44	69,73,73	2.50	23 (33%)	82,113,113	2.48	29 (35%)
34	DMS	b	633	-	3,3,3	2.68	1 (33%)	3,3,3	0.60	0
24	CLA	C	508	44	69,73,73	2.59	22 (31%)	82,113,113	2.37	28 (34%)
37	GOL	C	525	-	5,5,5	0.98	0	5,5,5	1.03	0
24	CLA	b	619	-	69,73,73	2.44	22 (31%)	82,113,113	2.43	26 (31%)
34	DMS	k	2004	-	3,3,3	2.73	1 (33%)	3,3,3	0.53	0
24	CLA	b	604	44	69,73,73	2.46	24 (34%)	82,113,113	2.32	24 (29%)
24	CLA	B	610	-	69,73,73	2.57	21 (30%)	82,113,113	2.37	28 (34%)
29	LMT	B	623	-	36,36,36	0.39	0	47,47,47	1.33	7 (14%)
34	DMS	B	643	-	3,3,3	2.78	1 (33%)	3,3,3	0.62	0
34	DMS	d	422	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
34	DMS	O	312	-	3,3,3	2.72	1 (33%)	3,3,3	0.56	0
26	BCR	B	619	-	41,41,41	0.87	1 (2%)	56,56,56	1.12	5 (8%)
29	LMT	J	102	-	24,24,36	0.51	0	29,29,47	1.05	2 (6%)
34	DMS	d	421	-	3,3,3	2.75	1 (33%)	3,3,3	0.68	0
34	DMS	O	310	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0
24	CLA	B	614	-	69,73,73	2.28	22 (31%)	82,113,113	2.37	29 (35%)
37	GOL	o	2603	-	5,5,5	0.86	0	5,5,5	1.16	0
36	HTG	I	1202	-	19,19,19	1.05	2 (10%)	23,24,24	1.77	4 (17%)
24	CLA	B	603	-	69,73,73	2.44	23 (33%)	82,113,113	2.39	30 (36%)
29	LMT	A	420	-	36,36,36	0.56	1 (2%)	47,47,47	1.37	5 (10%)
29	LMT	z	1801	-	33,33,36	0.43	0	43,43,47	0.99	2 (4%)
34	DMS	C	532	-	3,3,3	2.71	1 (33%)	3,3,3	0.40	0
34	DMS	v	209	-	3,3,3	2.74	1 (33%)	3,3,3	0.64	0
34	DMS	c	539	-	3,3,3	2.75	1 (33%)	3,3,3	0.64	0
34	DMS	V	205	-	3,3,3	2.77	1 (33%)	3,3,3	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	GOL	C	524	-	5,5,5	0.92	0	5,5,5	1.05	0
24	CLA	b	618	-	69,73,73	2.36	21 (30%)	82,113,113	2.26	29 (35%)
32	K2I	a	2118[B]	-	8,10,10	1.39	1 (12%)	10,14,14	2.41	3 (30%)
34	DMS	i	106	-	3,3,3	2.70	1 (33%)	3,3,3	0.47	0
32	K2I	A	418[B]	-	8,10,10	1.37	2 (25%)	10,14,14	2.25	4 (40%)
39	LHG	D	411	-	43,43,48	0.93	2 (4%)	46,49,54	1.02	3 (6%)
40	HEM	F	102	6,5	50,50,50	1.88	9 (18%)	67,82,82	1.35	7 (10%)
37	GOL	v	202	-	5,5,5	1.02	0	5,5,5	1.00	0
34	DMS	D	418	-	3,3,3	2.71	1 (33%)	3,3,3	0.51	0
34	DMS	A	426	-	3,3,3	2.75	1 (33%)	3,3,3	0.62	0
29	LMT	a	2103	-	36,36,36	0.39	0	47,47,47	1.23	5 (10%)
34	DMS	T	104	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
34	DMS	B	644	-	3,3,3	2.74	1 (33%)	3,3,3	0.60	0
24	CLA	C	512	3	69,73,73	2.75	24 (34%)	82,113,113	2.32	30 (36%)
24	CLA	B	612	-	69,73,73	2.63	23 (33%)	82,113,113	2.45	29 (35%)
34	DMS	o	2608	-	3,3,3	2.71	1 (33%)	3,3,3	0.44	0
34	DMS	c	536	-	3,3,3	2.81	1 (33%)	3,3,3	0.63	0
34	DMS	b	634	-	3,3,3	2.78	1 (33%)	3,3,3	0.65	0
29	LMT	a	2120	-	36,36,36	0.48	0	47,47,47	1.20	6 (12%)
24	CLA	c	504	-	69,73,73	2.35	23 (33%)	82,113,113	2.31	25 (30%)
39	LHG	E	101	-	48,48,48	0.95	2 (4%)	51,54,54	1.07	4 (7%)
25	PHO	A	407	-	58,69,69	2.68	13 (22%)	55,99,99	2.96	16 (29%)
34	DMS	A	423	-	3,3,3	2.76	1 (33%)	3,3,3	0.57	0
24	CLA	b	609	-	69,73,73	2.43	25 (36%)	82,113,113	2.31	25 (30%)
36	HTG	B	625[B]	-	19,19,19	0.92	1 (5%)	23,24,24	1.36	3 (13%)
28	LMG	D	412	42	44,44,55	0.93	2 (4%)	52,52,63	0.90	4 (7%)
34	DMS	C	531	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
37	GOL	B	632	-	5,5,5	1.04	0	5,5,5	0.87	0
31	PL9	x	801	-	38,38,55	0.40	0	45,45,69	1.77	14 (31%)
34	DMS	b	640	-	3,3,3	2.73	1 (33%)	3,3,3	0.54	0
34	DMS	z	1802	-	3,3,3	2.74	1 (33%)	3,3,3	0.58	0
34	DMS	B	638	-	3,3,3	2.74	1 (33%)	3,3,3	0.50	0
34	DMS	c	533	-	3,3,3	2.74	1 (33%)	3,3,3	0.58	0
38	DGD	h	703	-	63,63,67	0.93	3 (4%)	77,77,81	1.06	6 (7%)
34	DMS	V	209	-	3,3,3	2.70	1 (33%)	3,3,3	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DMS	c	531	-	3,3,3	2.71	1 (33%)	3,3,3	0.42	0
34	DMS	V	202	-	3,3,3	2.73	1 (33%)	3,3,3	0.65	0
24	CLA	B	604	-	69,73,73	2.46	24 (34%)	82,113,113	2.40	29 (35%)
26	BCR	D	406	-	41,41,41	0.85	1 (2%)	56,56,56	1.63	8 (14%)
24	CLA	a	2110	44	69,73,73	2.32	20 (28%)	82,113,113	2.62	31 (37%)
34	DMS	C	535	-	3,3,3	2.73	1 (33%)	3,3,3	0.49	0
36	HTG	b	625	-	19,19,19	0.85	1 (5%)	23,24,24	1.71	6 (26%)
34	DMS	c	542	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
24	CLA	A	409	-	69,73,73	2.33	23 (33%)	82,113,113	2.44	32 (39%)
24	CLA	d	405	-	69,73,73	2.50	24 (34%)	82,113,113	2.36	32 (39%)
24	CLA	b	607	-	69,73,73	2.84	21 (30%)	82,113,113	2.43	31 (37%)
24	CLA	B	608	44	69,73,73	2.49	21 (30%)	82,113,113	2.32	31 (37%)
24	CLA	c	511	-	69,73,73	2.71	24 (34%)	82,113,113	2.31	28 (34%)
34	DMS	b	641	-	3,3,3	2.78	1 (33%)	3,3,3	0.61	0
34	DMS	B	642	-	3,3,3	2.72	1 (33%)	3,3,3	0.42	0
34	DMS	v	212	-	3,3,3	2.73	1 (33%)	3,3,3	0.59	0
34	DMS	C	534	-	3,3,3	2.72	1 (33%)	3,3,3	0.63	0
28	LMG	c	522	-	48,48,55	1.00	2 (4%)	56,56,63	1.26	6 (10%)
34	DMS	O	307	-	3,3,3	2.72	1 (33%)	3,3,3	0.57	0
24	CLA	b	605	-	69,73,73	2.49	24 (34%)	82,113,113	2.36	30 (36%)
34	DMS	v	207	-	3,3,3	2.70	1 (33%)	3,3,3	0.50	0
39	LHG	d	410	-	35,35,48	1.10	2 (5%)	38,41,54	1.03	3 (7%)
34	DMS	V	206	-	3,3,3	2.75	1 (33%)	3,3,3	0.59	0
34	DMS	b	637	-	3,3,3	2.74	1 (33%)	3,3,3	0.59	0
24	CLA	C	506	-	69,73,73	2.66	23 (33%)	82,113,113	2.22	27 (32%)
37	GOL	v	203	-	5,5,5	1.10	0	5,5,5	1.27	1 (20%)
36	HTG	c	526	-	19,19,19	0.99	2 (10%)	23,24,24	1.03	1 (4%)
37	GOL	U	501	-	5,5,5	1.18	0	5,5,5	0.96	0
34	DMS	D	419	-	3,3,3	2.74	1 (33%)	3,3,3	0.58	0
24	CLA	c	507	-	69,73,73	2.56	23 (33%)	82,113,113	2.34	25 (30%)
39	LHG	L	101	-	48,48,48	0.94	3 (6%)	51,54,54	1.06	3 (5%)
34	DMS	F	103	-	3,3,3	2.74	1 (33%)	3,3,3	0.73	0
34	DMS	d	418	-	3,3,3	2.73	1 (33%)	3,3,3	0.49	0
34	DMS	v	213	-	3,3,3	2.75	1 (33%)	3,3,3	0.61	0
37	GOL	o	2601	-	5,5,5	1.05	0	5,5,5	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMT	m	102	-	36,36,36	0.50	0	47,47,47	1.17	5 (10%)
34	DMS	C	539	-	3,3,3	2.82	1 (33%)	3,3,3	0.72	0
24	CLA	C	509	-	69,73,73	2.60	24 (34%)	82,113,113	2.32	21 (25%)
36	HTG	d	403	-	19,19,19	1.01	2 (10%)	23,24,24	0.99	2 (8%)
38	DGD	c	518	-	63,63,67	0.81	2 (3%)	77,77,81	1.20	7 (9%)
24	CLA	a	2109	-	69,73,73	2.60	24 (34%)	82,113,113	2.41	29 (35%)
39	LHG	d	409	-	48,48,48	0.81	2 (4%)	51,54,54	0.99	3 (5%)
26	BCR	t	102	-	41,41,41	0.74	0	56,56,56	1.58	16 (28%)
34	DMS	j	1604	-	3,3,3	2.72	1 (33%)	3,3,3	0.51	0
34	DMS	O	306	-	3,3,3	2.78	1 (33%)	3,3,3	0.57	0
37	GOL	a	2101	-	5,5,5	1.05	0	5,5,5	1.21	0
34	DMS	t	103	-	3,3,3	2.78	1 (33%)	3,3,3	0.62	0
34	DMS	C	536	-	3,3,3	2.75	1 (33%)	3,3,3	0.62	0
34	DMS	c	534	-	3,3,3	2.75	1 (33%)	3,3,3	0.58	0
24	CLA	a	2113	-	69,73,73	2.23	22 (31%)	82,113,113	2.50	29 (35%)
24	CLA	B	616	-	69,73,73	2.44	21 (30%)	82,113,113	2.46	31 (37%)
28	LMG	i	101	-	51,51,55	0.93	2 (3%)	59,59,63	1.12	4 (6%)
38	DGD	c	520	-	63,63,67	0.85	3 (4%)	77,77,81	0.98	5 (6%)
34	DMS	v	205	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
28	LMG	c	521	-	49,49,55	0.94	2 (4%)	57,57,63	1.13	5 (8%)
24	CLA	D	401	44	69,73,73	2.25	23 (33%)	82,113,113	2.62	32 (39%)
41	RRX	H	101	-	42,42,42	0.75	0	56,58,58	1.31	7 (12%)
36	HTG	d	414	-	19,19,19	0.93	2 (10%)	23,24,24	1.11	1 (4%)
24	CLA	c	505	-	69,73,73	2.81	23 (33%)	82,113,113	2.25	29 (35%)
38	DGD	H	102	-	63,63,67	0.89	3 (4%)	77,77,81	1.02	5 (6%)
38	DGD	D	408	-	46,46,67	1.03	2 (4%)	54,54,81	1.17	4 (7%)
24	CLA	b	617	-	69,73,73	2.44	23 (33%)	82,113,113	2.44	31 (37%)
36	HTG	c	523	-	19,19,19	0.92	1 (5%)	23,24,24	1.52	4 (17%)
38	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.07	5 (6%)
34	DMS	D	416	-	3,3,3	2.74	1 (33%)	3,3,3	0.60	0
29	LMT	M	101	-	36,36,36	0.40	0	47,47,47	1.11	5 (10%)
24	CLA	B	617	-	69,73,73	2.33	21 (30%)	82,113,113	2.51	28 (34%)
24	CLA	D	405	-	69,73,73	2.44	24 (34%)	82,113,113	2.38	29 (35%)
34	DMS	B	639	-	3,3,3	2.66	1 (33%)	3,3,3	0.62	0
34	DMS	E	107	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	513	3	69,73,73	2.45	23 (33%)	82,113,113	2.33	32 (39%)
24	CLA	B	607	-	69,73,73	2.47	23 (33%)	82,113,113	2.40	29 (35%)
34	DMS	D	420	-	3,3,3	2.74	1 (33%)	3,3,3	0.57	0
34	DMS	u	203	-	3,3,3	2.69	1 (33%)	3,3,3	0.61	0
34	DMS	B	641	-	3,3,3	2.61	1 (33%)	3,3,3	0.45	0
34	DMS	V	208	-	3,3,3	2.74	1 (33%)	3,3,3	0.62	0
24	CLA	A	406	44	69,73,73	2.23	23 (33%)	82,113,113	2.40	33 (40%)
34	DMS	A	422	-	3,3,3	2.59	1 (33%)	3,3,3	0.66	0
34	DMS	C	533	-	3,3,3	2.72	1 (33%)	3,3,3	0.53	0
21	OEX	A	401	1,44,3	0,15,15	-	-	-	-	-
39	LHG	e	101	-	31,31,48	0.89	1 (3%)	33,36,54	1.08	1 (3%)
29	LMT	Z	101	-	36,36,36	0.40	0	47,47,47	0.84	0
34	DMS	o	2611	-	3,3,3	2.71	1 (33%)	3,3,3	0.50	0
28	LMG	A	412	-	51,51,55	0.98	2 (3%)	59,59,63	1.13	4 (6%)
39	LHG	d	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.14	4 (7%)
34	DMS	c	537	-	3,3,3	2.75	1 (33%)	3,3,3	0.65	0
34	DMS	B	645	-	3,3,3	2.74	1 (33%)	3,3,3	0.49	0
26	BCR	b	621	-	41,41,41	0.86	0	56,56,56	1.19	7 (12%)
36	HTG	V	204	-	19,19,19	0.88	1 (5%)	23,24,24	1.75	4 (17%)
34	DMS	C	528	-	3,3,3	2.69	1 (33%)	3,3,3	0.46	0
34	DMS	b	642	-	3,3,3	2.77	1 (33%)	3,3,3	0.60	0
34	DMS	d	423	-	3,3,3	2.76	1 (33%)	3,3,3	0.58	0
27	SQD	a	2115	-	45,47,54	0.96	2 (4%)	55,58,65	1.75	11 (20%)
28	LMG	d	411	42	48,48,55	0.95	2 (4%)	56,56,63	1.04	2 (3%)
29	LMT	f	101	-	24,24,36	0.55	1 (4%)	29,29,47	0.91	1 (3%)
34	DMS	U	503	-	3,3,3	2.72	1 (33%)	3,3,3	0.55	0
36	HTG	B	626	-	19,19,19	1.00	1 (5%)	23,24,24	1.43	3 (13%)
24	CLA	d	401	44	69,73,73	2.40	21 (30%)	82,113,113	2.57	31 (37%)
24	CLA	b	608	-	69,73,73	2.22	24 (34%)	82,113,113	2.51	26 (31%)
34	DMS	b	638	-	3,3,3	2.75	1 (33%)	3,3,3	0.58	0
24	CLA	B	611	44	69,73,73	2.37	24 (34%)	82,113,113	2.44	31 (37%)
36	HTG	O	302	-	19,19,19	0.91	1 (5%)	23,24,24	0.91	1 (4%)
31	PL9	D	407	-	55,55,55	0.73	2 (3%)	68,69,69	1.55	14 (20%)
24	CLA	c	515	-	69,73,73	2.55	24 (34%)	82,113,113	2.30	25 (30%)
24	CLA	C	514	-	69,73,73	2.55	23 (33%)	82,113,113	2.35	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	HTG	B	624	-	19,19,19	1.01	1 (5%)	23,24,24	1.18	1 (4%)
34	DMS	O	304	-	3,3,3	2.73	1 (33%)	3,3,3	0.53	0
34	DMS	O	308	-	3,3,3	2.73	1 (33%)	3,3,3	0.54	0
34	DMS	b	635	-	3,3,3	2.72	1 (33%)	3,3,3	0.53	0
28	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.17	5 (8%)
34	DMS	a	2122	-	3,3,3	2.76	1 (33%)	3,3,3	0.57	0
36	HTG	b	626	-	19,19,19	1.00	2 (10%)	23,24,24	1.18	1 (4%)
26	BCR	b	620	-	41,41,41	0.81	0	56,56,56	1.39	5 (8%)
32	K2I	a	2119	-	8,10,10	1.39	2 (25%)	10,14,14	1.62	3 (30%)
34	DMS	d	419	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
34	DMS	c	535	-	3,3,3	2.74	1 (33%)	3,3,3	0.63	0
26	BCR	K	101	-	41,41,41	0.75	0	56,56,56	1.36	8 (14%)
34	DMS	d	420	-	3,3,3	2.76	1 (33%)	3,3,3	0.59	0
24	CLA	C	502	-	69,73,73	2.45	24 (34%)	82,113,113	2.26	25 (30%)
25	PHO	a	2112	-	58,69,69	2.75	12 (20%)	55,99,99	2.99	14 (25%)
28	LMG	B	622	-	51,51,55	0.94	2 (3%)	59,59,63	1.03	4 (6%)
26	BCR	c	528	-	41,41,41	0.74	0	56,56,56	1.47	10 (17%)
32	K2I	a	2118[A]	-	8,10,10	1.39	1 (12%)	10,14,14	2.54	4 (40%)
32	K2I	A	418[A]	-	8,10,10	1.36	2 (25%)	10,14,14	2.82	4 (40%)
24	CLA	c	514	-	69,73,73	2.61	23 (33%)	82,113,113	2.47	29 (35%)
26	BCR	T	101	-	41,41,41	0.73	0	56,56,56	1.69	16 (28%)

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
29	LMT	B	637	-	-	9/15/35/61	0/1/1/2
39	LHG	D	410	-	-	6/53/53/53	-
38	DGD	c	519	-	-	19/51/91/95	0/2/2/2
26	BCR	t	102	-	-	3/29/63/63	0/2/2/2
37	GOL	B	635	-	-	0/4/4/4	-
36	HTG	C	521	-	-	3/10/30/30	0/1/1/1
24	CLA	B	614	-	1/1/15/20	3/39/115/115	-
29	LMT	E	105	-	-	7/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	T	102	-	-	7/15/35/61	0/1/1/2
37	GOL	o	2603	-	-	3/4/4/4	-
37	GOL	a	2101	-	-	1/4/4/4	-
43	HEC	V	201	16	-	6/14/54/54	-
24	CLA	C	511	-	1/1/15/20	5/39/115/115	-
36	HTG	I	1202	-	-	3/10/30/30	0/1/1/1
24	CLA	b	616	-	1/1/15/20	4/39/115/115	-
24	CLA	B	603	-	1/1/15/20	2/39/115/115	-
29	LMT	A	420	-	-	6/21/61/61	0/2/2/2
29	LMT	z	1801	-	-	8/16/56/61	0/2/2/2
36	HTG	c	524	-	-	0/10/30/30	0/1/1/1
24	CLA	a	2113	-	1/1/15/20	8/39/115/115	-
24	CLA	B	616	-	1/1/15/20	11/39/115/115	-
24	CLA	B	609	-	-	1/39/115/115	-
24	CLA	c	503	-	-	1/39/115/115	-
28	LMG	i	101	-	-	11/46/66/70	0/1/1/1
29	LMT	I	1201	-	-	7/15/35/61	0/1/1/2
24	CLA	b	613	44	1/1/15/20	5/39/115/115	-
24	CLA	b	618	-	1/1/15/20	6/39/115/115	-
26	BCR	Y	302	-	-	4/29/63/63	0/2/2/2
37	GOL	C	524	-	-	0/4/4/4	-
24	CLA	C	503	-	1/1/15/20	4/39/115/115	-
27	SQD	A	413	-	-	12/49/69/69	0/1/1/1
32	K2I	a	2118[B]	-	-	-	0/1/1/1
29	LMT	b	624	-	-	5/17/37/61	0/1/1/2
37	GOL	b	631	-	-	2/4/4/4	-
32	K2I	A	418[B]	-	-	-	0/1/1/1
39	LHG	D	411	-	-	10/48/48/53	-
24	CLA	B	613	-	1/1/15/20	3/39/115/115	-
37	GOL	v	202	-	-	2/4/4/4	-
40	HEM	F	102	6,5	-	3/14/54/54	-
39	LHG	D	409	-	-	15/53/53/53	-
36	HTG	i	103	-	-	1/10/30/30	0/1/1/1
38	DGD	c	520	-	-	11/51/91/95	0/2/2/2
24	CLA	B	615	-	1/1/15/20	10/39/115/115	-
28	LMG	c	521	-	-	12/44/64/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	D	401	44	-	3/39/115/115	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
24	CLA	b	614	-	1/1/15/20	3/39/115/115	-
41	RRX	H	101	-	-	1/29/65/65	0/2/2/2
24	CLA	c	512	-	1/1/15/20	9/39/115/115	-
27	SQD	F	101	-	-	16/40/60/69	0/1/1/1
36	HTG	d	414	-	-	1/10/30/30	0/1/1/1
37	GOL	k	2001	-	-	2/4/4/4	-
36	HTG	B	625[A]	-	-	3/10/30/30	0/1/1/1
24	CLA	B	605	-	1/1/15/20	6/39/115/115	-
24	CLA	c	505	-	1/1/15/20	1/39/115/115	-
29	LMT	a	2103	-	-	11/21/61/61	0/2/2/2
38	DGD	H	102	-	-	10/51/91/95	0/2/2/2
38	DGD	D	408	-	-	17/40/61/95	0/1/1/2
24	CLA	b	617	-	1/1/15/20	10/39/115/115	-
24	CLA	C	512	3	1/1/15/20	3/39/115/115	-
24	CLA	B	612	-	1/1/15/20	4/39/115/115	-
39	LHG	l	101	-	-	16/53/53/53	-
29	LMT	m	103	-	-	1/21/61/61	0/2/2/2
26	BCR	C	516	-	-	0/29/63/63	0/2/2/2
36	HTG	c	523	-	-	0/10/30/30	0/1/1/1
38	DGD	C	518	-	-	19/51/91/95	0/2/2/2
29	LMT	A	414	-	-	6/20/60/61	0/2/2/2
31	PL9	d	407	-	-	3/53/73/73	0/1/1/1
37	GOL	d	415	-	-	2/4/4/4	-
37	GOL	Z	102	-	-	2/4/4/4	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
26	BCR	k	2003	-	-	0/29/63/63	0/2/2/2
24	CLA	B	606	-	1/1/15/20	5/39/115/115	-
29	LMT	a	2120	-	-	12/21/61/61	0/2/2/2
24	CLA	c	504	-	1/1/15/20	5/39/115/115	-
24	CLA	C	513	-	1/1/15/20	5/39/115/115	-
39	LHG	E	101	-	-	18/53/53/53	-
24	CLA	C	510	-	1/1/15/20	7/39/115/115	-
25	PHO	A	407	-	-	2/37/103/103	0/5/6/6
27	SQD	A	411	-	-	9/44/64/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	617	-	1/1/15/20	9/39/115/115	-
24	CLA	C	504	-	-	4/39/115/115	-
29	LMT	M	101	-	-	5/21/61/61	0/2/2/2
24	CLA	D	405	-	1/1/15/20	6/39/115/115	-
38	DGD	C	517	-	-	14/51/91/95	0/2/2/2
24	CLA	b	609	-	1/1/15/20	3/39/115/115	-
36	HTG	B	625[B]	-	-	2/10/30/30	0/1/1/1
28	LMG	D	412	42	-	9/39/59/70	0/1/1/1
24	CLA	c	513	3	-	3/39/115/115	-
37	GOL	B	632	-	-	0/4/4/4	-
24	CLA	B	607	-	1/1/15/20	8/39/115/115	-
26	BCR	a	2114	-	-	1/29/63/63	0/2/2/2
31	PL9	x	801	-	-	9/42/42/73	-
40	HEM	e	103	6,5	-	4/14/54/54	-
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
38	DGD	h	703	-	-	9/51/91/95	0/2/2/2
26	BCR	c	516	-	-	1/29/63/63	0/2/2/2
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
31	PL9	A	417	-	-	11/42/42/73	-
29	LMT	j	1601	-	-	5/11/31/61	0/1/1/2
36	HTG	b	601	-	-	2/10/30/30	0/1/1/1
41	RRX	h	702	-	-	1/29/65/65	0/2/2/2
24	CLA	B	604	-	1/1/15/20	1/39/115/115	-
24	CLA	A	406	44	-	5/39/115/115	-
26	BCR	D	406	-	-	6/29/63/63	0/2/2/2
24	CLA	a	2110	44	-	6/39/115/115	-
27	SQD	a	2102	-	-	13/48/68/69	0/1/1/1
28	LMG	C	526	-	-	11/43/63/70	0/1/1/1
39	LHG	e	101	-	-	15/35/35/53	-
29	LMT	Z	101	-	-	10/21/61/61	0/2/2/2
25	PHO	A	408	-	-	0/37/103/103	0/5/6/6
36	HTG	b	625	-	-	0/10/30/30	0/1/1/1
28	LMG	A	412	-	-	16/46/66/70	0/1/1/1
36	HTG	B	628	-	-	1/10/30/30	0/1/1/1
39	LHG	d	408	-	-	11/53/53/53	-
24	CLA	b	606	-	1/1/15/20	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	L	102	-	-	23/49/69/69	0/1/1/1
24	CLA	b	610	44	1/1/15/20	1/39/115/115	-
37	GOL	v	204	-	-	3/4/4/4	-
32	K2I	A	419	-	-	-	0/1/1/1
36	HTG	B	627	-	-	3/10/30/30	0/1/1/1
37	GOL	H	103	-	-	2/4/4/4	-
24	CLA	A	409	-	1/1/15/20	8/39/115/115	-
24	CLA	d	405	-	1/1/15/20	4/39/115/115	-
26	BCR	b	621	-	-	0/29/63/63	0/2/2/2
24	CLA	b	607	-	1/1/15/20	3/39/115/115	-
36	HTG	V	204	-	-	5/10/30/30	0/1/1/1
38	DGD	C	519	-	-	5/51/91/95	0/2/2/2
24	CLA	B	608	44	1/1/15/20	1/39/115/115	-
24	CLA	c	511	-	1/1/15/20	6/39/115/115	-
27	SQD	a	2115	-	-	12/42/62/69	0/1/1/1
28	LMG	d	411	42	-	6/43/63/70	0/1/1/1
26	BCR	C	515	-	-	1/29/63/63	0/2/2/2
29	LMT	f	101	-	-	6/15/35/61	0/1/1/2
24	CLA	c	506	44	1/1/15/20	8/39/115/115	-
36	HTG	B	626	-	-	3/10/30/30	0/1/1/1
36	HTG	D	413	-	-	2/10/30/30	0/1/1/1
24	CLA	d	401	44	1/1/15/20	2/39/115/115	-
24	CLA	b	608	-	1/1/15/20	4/39/115/115	-
24	CLA	b	615	-	1/1/15/20	3/39/115/115	-
37	GOL	O	303	-	-	4/4/4/4	-
43	HEC	v	201	16	-	6/14/54/54	-
28	LMG	c	522	-	-	9/43/63/70	0/1/1/1
24	CLA	B	611	44	1/1/15/20	8/39/115/115	-
37	GOL	V	203	-	-	4/4/4/4	-
36	HTG	O	302	-	-	5/10/30/30	0/1/1/1
24	CLA	C	505	44	1/1/15/20	4/39/115/115	-
31	PL9	D	407	-	-	3/53/73/73	0/1/1/1
24	CLA	c	515	-	1/1/15/20	6/39/115/115	-
24	CLA	C	514	-	1/1/15/20	2/39/115/115	-
36	HTG	C	522	-	-	2/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	605	-	1/1/15/20	2/39/115/115	-
36	HTG	B	624	-	-	3/10/30/30	0/1/1/1
39	LHG	d	410	-	-	5/40/40/53	-
24	CLA	C	506	-	1/1/15/20	3/39/115/115	-
37	GOL	v	203	-	-	1/4/4/4	-
24	CLA	D	404	-	1/1/15/20	2/39/115/115	-
37	GOL	D	403	-	-	0/4/4/4	-
24	CLA	A	405	-	1/1/15/20	5/39/115/115	-
37	GOL	U	502	-	-	2/4/4/4	-
36	HTG	c	526	-	-	2/10/30/30	0/1/1/1
37	GOL	U	501	-	-	2/4/4/4	-
29	LMT	i	104	-	-	11/15/35/61	0/1/1/2
28	LMG	C	520	-	-	14/46/66/70	0/1/1/1
26	BCR	d	406	-	-	6/29/63/63	0/2/2/2
24	CLA	c	508	-	1/1/15/20	8/39/115/115	-
36	HTG	b	626	-	-	5/10/30/30	0/1/1/1
26	BCR	b	620	-	-	2/29/63/63	0/2/2/2
36	HTG	b	602	-	-	3/10/30/30	0/1/1/1
25	PHO	a	2111	-	-	4/37/103/103	0/5/6/6
24	CLA	c	509	44	1/1/15/20	8/39/115/115	-
24	CLA	c	507	-	1/1/15/20	3/39/115/115	-
26	BCR	c	517	-	-	2/29/63/63	0/2/2/2
26	BCR	T	101	-	-	3/29/63/63	0/2/2/2
39	LHG	L	101	-	-	14/53/53/53	-
32	K2I	a	2119	-	-	-	0/1/1/1
29	LMT	B	636	-	-	8/21/61/61	0/2/2/2
24	CLA	C	508	44	1/1/15/20	7/39/115/115	-
24	CLA	d	404	-	1/1/15/20	2/39/115/115	-
37	GOL	c	527	-	-	1/4/4/4	-
37	GOL	C	525	-	-	2/4/4/4	-
26	BCR	b	622	-	-	2/29/63/63	0/2/2/2
24	CLA	b	612	-	1/1/15/20	4/39/115/115	-
24	CLA	b	619	-	1/1/15/20	8/39/115/115	-
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
24	CLA	C	502	-	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	GOL	o	2601	-	-	3/4/4/4	-
27	SQD	f	102	-	-	13/38/38/69	-
24	CLA	b	604	44	1/1/15/20	12/39/115/115	-
24	CLA	B	610	-	1/1/15/20	5/39/115/115	-
29	LMT	B	623	-	-	10/21/61/61	0/2/2/2
25	PHO	a	2112	-	-	2/37/103/103	0/5/6/6
24	CLA	C	507	-	1/1/15/20	12/39/115/115	-
24	CLA	B	602	44	1/1/15/20	11/39/115/115	-
28	LMG	b	623	-	-	11/46/66/70	0/1/1/1
28	LMG	B	622	-	-	12/46/66/70	0/1/1/1
26	BCR	c	528	-	-	4/29/63/63	0/2/2/2
29	LMT	m	102	-	-	6/21/61/61	0/2/2/2
32	K2I	a	2118[A]	-	-	-	0/1/1/1
24	CLA	C	509	-	1/1/15/20	5/39/115/115	-
24	CLA	b	611	-	-	1/39/115/115	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
29	LMT	J	102	-	-	6/15/35/61	0/1/1/2
24	CLA	a	2109	-	1/1/15/20	3/39/115/115	-
36	HTG	d	403	-	-	4/10/30/30	0/1/1/1
38	DGD	c	518	-	-	17/51/91/95	0/2/2/2
32	K2I	A	418[A]	-	-	-	0/1/1/1
24	CLA	c	514	-	1/1/15/20	4/39/115/115	-
24	CLA	c	510	-	1/1/15/20	3/39/115/115	-
39	LHG	d	409	-	-	11/53/53/53	-

All (1953) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	505	CLA	MG-NA	11.53	2.33	2.06
24	C	512	CLA	MG-NA	11.41	2.33	2.06
24	C	508	CLA	MG-NA	10.32	2.30	2.06
24	C	506	CLA	MG-NA	9.69	2.29	2.06
24	C	504	CLA	MG-NA	9.53	2.28	2.06
24	a	2109	CLA	MG-ND	-9.47	1.87	2.05
24	B	607	CLA	MG-NA	9.40	2.28	2.06
24	b	607	CLA	MG-NA	9.38	2.28	2.06
24	b	607	CLA	MG-ND	-9.16	1.87	2.05
24	C	507	CLA	MG-ND	-9.13	1.87	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	513	CLA	MG-NA	9.13	2.27	2.06
24	b	607	CLA	MG-NC	9.11	2.27	2.06
25	a	2112	PHO	C1D-C2D	9.04	1.49	1.39
24	b	610	CLA	MG-ND	-8.96	1.88	2.05
25	A	408	PHO	C1B-C2B	8.92	1.49	1.39
24	c	511	CLA	MG-NA	8.92	2.27	2.06
24	B	612	CLA	MG-NA	8.89	2.27	2.06
25	a	2112	PHO	C1B-C2B	8.84	1.49	1.39
25	A	407	PHO	C1D-C2D	8.80	1.49	1.39
24	C	503	CLA	MG-NA	8.79	2.27	2.06
24	c	514	CLA	MG-ND	-8.66	1.88	2.05
25	a	2111	PHO	C1D-C2D	8.62	1.49	1.39
25	A	407	PHO	C1B-C2B	8.59	1.48	1.39
24	b	612	CLA	MG-NA	8.52	2.26	2.06
24	c	514	CLA	MG-NA	8.47	2.26	2.06
25	A	408	PHO	C1D-C2D	8.44	1.48	1.39
24	B	605	CLA	MG-NC	8.37	2.26	2.06
24	B	612	CLA	MG-ND	-8.36	1.89	2.05
24	C	503	CLA	MG-ND	-8.32	1.89	2.05
25	A	408	PHO	C3B-C4B	8.31	1.49	1.41
24	c	507	CLA	MG-NA	8.29	2.26	2.06
24	c	511	CLA	MG-ND	-8.29	1.89	2.05
24	c	509	CLA	MG-NA	8.28	2.25	2.06
24	B	608	CLA	MG-NA	8.25	2.25	2.06
24	C	513	CLA	MG-NA	8.20	2.25	2.06
24	c	506	CLA	MG-NA	8.20	2.25	2.06
24	C	512	CLA	MG-ND	-8.19	1.89	2.05
25	a	2112	PHO	C3B-C4B	8.18	1.49	1.41
24	B	617	CLA	MG-NA	8.17	2.25	2.06
24	b	614	CLA	MG-ND	-8.15	1.89	2.05
24	b	611	CLA	MG-ND	-8.00	1.89	2.05
24	b	619	CLA	MG-NA	7.90	2.25	2.06
24	c	508	CLA	MG-ND	-7.89	1.90	2.05
24	C	507	CLA	MG-NC	7.87	2.25	2.06
24	b	618	CLA	MG-NA	7.83	2.24	2.06
24	C	505	CLA	MG-NC	7.79	2.24	2.06
25	a	2111	PHO	C1B-C2B	7.78	1.48	1.39
24	C	510	CLA	MG-NA	7.76	2.24	2.06
24	C	507	CLA	MG-NA	7.74	2.24	2.06
40	e	103	HEM	C3D-C2D	7.71	1.53	1.36
24	C	509	CLA	MG-ND	-7.66	1.90	2.05
24	B	610	CLA	MG-ND	-7.63	1.90	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	514	CLA	MG-ND	-7.61	1.90	2.05
24	c	505	CLA	MG-NC	7.60	2.24	2.06
24	C	514	CLA	MG-NA	7.57	2.24	2.06
24	B	602	CLA	MG-NA	7.57	2.24	2.06
24	c	515	CLA	MG-NC	7.57	2.24	2.06
24	d	405	CLA	MG-NA	7.55	2.24	2.06
24	b	605	CLA	MG-NA	7.48	2.24	2.06
24	d	404	CLA	MG-NC	7.46	2.24	2.06
40	F	102	HEM	C3D-C2D	7.43	1.52	1.36
24	B	615	CLA	MG-NA	7.38	2.23	2.06
25	A	407	PHO	C3B-C4B	7.38	1.49	1.41
24	B	610	CLA	MG-NA	7.36	2.23	2.06
24	C	509	CLA	MG-NC	7.28	2.23	2.06
24	B	613	CLA	MG-NA	7.22	2.23	2.06
24	d	401	CLA	MG-ND	-7.19	1.91	2.05
24	b	604	CLA	MG-NC	7.18	2.23	2.06
25	A	408	PHO	C4D-CHA	7.13	1.50	1.39
24	B	603	CLA	MG-NA	7.12	2.23	2.06
24	C	502	CLA	MG-NC	7.12	2.23	2.06
24	B	609	CLA	MG-ND	-7.11	1.91	2.05
24	B	610	CLA	MG-NC	7.09	2.23	2.06
27	f	102	SQD	C6-S	-7.05	1.67	1.77
24	B	606	CLA	MG-NA	7.05	2.23	2.06
24	c	503	CLA	MG-ND	-7.03	1.91	2.05
24	B	616	CLA	MG-ND	-7.01	1.91	2.05
24	c	510	CLA	MG-NC	6.96	2.22	2.06
24	C	510	CLA	MG-ND	-6.92	1.92	2.05
24	B	604	CLA	MG-NA	6.92	2.22	2.06
24	c	503	CLA	MG-NA	6.90	2.22	2.06
24	B	616	CLA	MG-NA	6.88	2.22	2.06
25	A	408	PHO	C3B-C2B	6.87	1.49	1.40
24	a	2110	CLA	MG-NA	6.86	2.22	2.06
25	a	2111	PHO	C3B-C2B	6.82	1.49	1.40
24	B	609	CLA	MG-NA	6.80	2.22	2.06
24	b	606	CLA	MG-NC	6.77	2.22	2.06
24	b	612	CLA	MG-NC	6.75	2.22	2.06
24	b	614	CLA	MG-NA	6.73	2.22	2.06
24	b	616	CLA	MG-ND	-6.73	1.92	2.05
24	B	605	CLA	MG-ND	-6.72	1.92	2.05
24	c	507	CLA	MG-ND	-6.70	1.92	2.05
24	b	619	CLA	MG-ND	-6.69	1.92	2.05
24	C	506	CLA	MG-ND	-6.69	1.92	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	MG-NC	6.68	2.22	2.06
24	b	616	CLA	MG-NA	6.67	2.22	2.06
24	d	404	CLA	MG-NA	6.65	2.22	2.06
24	C	511	CLA	MG-NA	6.65	2.22	2.06
24	C	504	CLA	MG-NC	6.63	2.22	2.06
25	a	2112	PHO	C4D-CHA	6.62	1.49	1.39
24	a	2109	CLA	MG-NA	6.61	2.22	2.06
25	A	407	PHO	C4D-CHA	6.61	1.49	1.39
24	C	511	CLA	MG-NC	6.60	2.21	2.06
24	b	610	CLA	MG-NC	6.58	2.21	2.06
24	c	505	CLA	MG-ND	-6.56	1.92	2.05
24	B	604	CLA	MG-NC	6.53	2.21	2.06
43	V	201	HEC	CAB-C3B	6.51	1.56	1.35
24	C	511	CLA	MG-ND	-6.51	1.92	2.05
24	A	405	CLA	MG-ND	-6.49	1.92	2.05
24	a	2110	CLA	MG-ND	-6.46	1.93	2.05
24	D	405	CLA	MG-NA	6.46	2.21	2.06
24	D	405	CLA	MG-NC	6.45	2.21	2.06
24	c	511	CLA	MG-NC	6.45	2.21	2.06
24	b	617	CLA	MG-ND	-6.45	1.93	2.05
43	v	201	HEC	CAC-C3C	6.44	1.55	1.35
24	b	609	CLA	MG-NC	6.43	2.21	2.06
24	C	505	CLA	MG-NA	6.43	2.21	2.06
43	V	201	HEC	CAC-C3C	6.43	1.55	1.35
24	b	616	CLA	MG-NC	6.39	2.21	2.06
24	b	606	CLA	MG-ND	-6.37	1.93	2.05
24	C	506	CLA	MG-NC	6.37	2.21	2.06
24	b	610	CLA	MG-NA	6.34	2.21	2.06
24	c	510	CLA	MG-ND	-6.33	1.93	2.05
24	c	515	CLA	MG-NA	6.33	2.21	2.06
25	A	407	PHO	C3B-C2B	6.32	1.48	1.40
25	a	2111	PHO	C4D-CHA	6.31	1.49	1.39
24	D	404	CLA	MG-NA	6.31	2.21	2.06
24	b	605	CLA	MG-NC	6.28	2.21	2.06
43	v	201	HEC	CAB-C3B	6.28	1.55	1.35
24	b	609	CLA	MG-NA	6.23	2.21	2.06
24	B	605	CLA	MG-NA	6.18	2.21	2.06
24	c	509	CLA	MG-NC	6.16	2.20	2.06
24	b	604	CLA	MG-NA	6.16	2.20	2.06
24	b	613	CLA	MG-NA	6.12	2.20	2.06
24	b	617	CLA	MG-NA	6.12	2.20	2.06
24	b	606	CLA	MG-NA	6.10	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	515	CLA	MG-ND	-6.09	1.93	2.05
24	B	603	CLA	MG-ND	-6.08	1.93	2.05
24	A	409	CLA	MG-NC	6.07	2.20	2.06
24	B	611	CLA	MG-NC	6.06	2.20	2.06
25	a	2111	PHO	C3B-C4B	6.05	1.47	1.41
24	D	405	CLA	C3C-C2C	6.04	1.49	1.36
24	B	612	CLA	MG-NC	6.01	2.20	2.06
24	b	607	CLA	C1D-ND	6.01	1.45	1.37
24	C	513	CLA	MG-ND	-5.99	1.93	2.05
24	C	502	CLA	MG-NA	5.96	2.20	2.06
24	b	611	CLA	MG-NC	5.93	2.20	2.06
24	C	503	CLA	C1D-ND	5.92	1.45	1.37
24	C	509	CLA	C3C-C2C	5.89	1.49	1.36
24	c	512	CLA	MG-NC	5.88	2.20	2.06
24	A	405	CLA	MG-NA	5.87	2.20	2.06
24	C	510	CLA	MG-NC	5.86	2.20	2.06
24	c	510	CLA	C3C-C2C	5.86	1.49	1.36
24	B	604	CLA	C3C-C2C	5.83	1.49	1.36
24	b	615	CLA	MG-NA	5.82	2.20	2.06
40	e	103	HEM	FE-ND	5.82	2.12	1.94
24	a	2113	CLA	C3C-C2C	5.81	1.49	1.36
24	C	508	CLA	MG-ND	-5.81	1.94	2.05
24	c	515	CLA	C1D-ND	5.80	1.45	1.37
24	B	611	CLA	C3C-C2C	5.80	1.49	1.36
25	a	2112	PHO	C3B-C2B	5.80	1.48	1.40
24	b	613	CLA	C3C-C2C	5.78	1.49	1.36
24	B	608	CLA	MG-NC	5.78	2.20	2.06
24	d	401	CLA	C3C-C2C	5.77	1.49	1.36
24	C	507	CLA	C1D-ND	5.77	1.45	1.37
24	C	502	CLA	C1D-ND	5.76	1.45	1.37
24	B	610	CLA	C1D-ND	5.76	1.45	1.37
24	C	510	CLA	C3C-C2C	5.76	1.49	1.36
24	c	511	CLA	C1D-ND	5.76	1.45	1.37
24	c	515	CLA	C3C-C2C	5.75	1.49	1.36
24	b	604	CLA	C3C-C2C	5.75	1.49	1.36
40	F	102	HEM	FE-ND	5.73	2.12	1.94
24	c	505	CLA	C1D-ND	5.70	1.45	1.37
24	c	512	CLA	C3C-C2C	5.70	1.49	1.36
24	C	514	CLA	C3C-C2C	5.69	1.49	1.36
24	b	606	CLA	C3C-C2C	5.69	1.49	1.36
24	B	603	CLA	C3C-C2C	5.67	1.49	1.36
24	A	405	CLA	C3C-C2C	5.66	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	514	CLA	MG-NC	5.66	2.19	2.06
24	c	508	CLA	MG-NC	5.66	2.19	2.06
24	B	602	CLA	C3C-C2C	5.65	1.49	1.36
24	c	514	CLA	C3C-C2C	5.65	1.48	1.36
24	c	508	CLA	C1D-ND	5.64	1.45	1.37
24	c	504	CLA	C3C-C2C	5.63	1.48	1.36
24	b	612	CLA	C1D-ND	5.62	1.45	1.37
24	C	506	CLA	C3C-C2C	5.61	1.48	1.36
24	b	610	CLA	C3C-C2C	5.60	1.48	1.36
24	a	2113	CLA	MG-NC	5.59	2.19	2.06
24	c	504	CLA	MG-NA	5.58	2.19	2.06
24	A	409	CLA	C3C-C2C	5.58	1.48	1.36
24	B	613	CLA	CHC-C1C	5.57	1.49	1.38
24	C	504	CLA	C1D-ND	5.55	1.45	1.37
24	C	502	CLA	C3C-C2C	5.55	1.48	1.36
24	C	513	CLA	C3C-C2C	5.55	1.48	1.36
24	c	508	CLA	C3C-C2C	5.54	1.48	1.36
24	C	503	CLA	C3C-C2C	5.54	1.48	1.36
24	C	514	CLA	C1D-ND	5.54	1.45	1.37
24	A	406	CLA	C3C-C2C	5.52	1.48	1.36
43	v	201	HEC	C3D-C2D	5.52	1.53	1.38
24	C	504	CLA	C3C-C2C	5.52	1.48	1.36
24	C	507	CLA	C3C-C2C	5.52	1.48	1.36
24	b	605	CLA	C3C-C2C	5.51	1.48	1.36
24	b	612	CLA	C3C-C2C	5.49	1.48	1.36
24	B	607	CLA	C3C-C2C	5.49	1.48	1.36
24	c	512	CLA	MG-ND	-5.48	1.94	2.05
24	b	614	CLA	MG-NC	5.48	2.19	2.06
24	b	608	CLA	C3C-C2C	5.48	1.48	1.36
24	C	505	CLA	C3C-C2C	5.48	1.48	1.36
24	c	505	CLA	C3C-C2C	5.47	1.48	1.36
24	b	617	CLA	MG-NC	5.47	2.19	2.06
24	c	511	CLA	C3C-C2C	5.47	1.48	1.36
24	c	514	CLA	C1D-ND	5.46	1.45	1.37
24	b	614	CLA	MG-NB	5.46	2.16	2.05
43	V	201	HEC	C3D-C2D	5.45	1.53	1.38
24	c	509	CLA	C3C-C2C	5.45	1.48	1.36
24	B	614	CLA	C3C-C2C	5.44	1.48	1.36
24	b	616	CLA	C3C-C2C	5.44	1.48	1.36
24	D	401	CLA	C3C-C2C	5.44	1.48	1.36
24	b	618	CLA	C3C-C2C	5.42	1.48	1.36
24	b	617	CLA	C3C-C2C	5.42	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C3C-C2C	5.41	1.48	1.36
24	a	2109	CLA	C3C-C2C	5.41	1.48	1.36
24	C	511	CLA	C3C-C2C	5.40	1.48	1.36
24	b	611	CLA	C3C-C2C	5.39	1.48	1.36
24	B	609	CLA	C3C-C2C	5.39	1.48	1.36
24	B	602	CLA	CHC-C1C	5.38	1.49	1.38
24	d	405	CLA	MG-ND	-5.37	1.95	2.05
24	C	510	CLA	C1D-ND	5.37	1.44	1.37
24	b	609	CLA	C1D-ND	5.37	1.44	1.37
24	B	608	CLA	C3C-C2C	5.37	1.48	1.36
25	a	2112	PHO	C3D-C2D	5.37	1.48	1.39
25	A	407	PHO	C3D-C2D	5.37	1.48	1.39
24	D	401	CLA	MG-ND	-5.36	1.95	2.05
24	b	616	CLA	C1D-ND	5.36	1.44	1.37
24	b	608	CLA	CHC-C1C	5.35	1.49	1.38
24	d	405	CLA	C3C-C2C	5.35	1.48	1.36
24	B	612	CLA	C1D-ND	5.35	1.44	1.37
24	b	604	CLA	C1D-ND	5.35	1.44	1.37
24	B	609	CLA	C1D-ND	5.35	1.44	1.37
24	d	401	CLA	C1D-ND	5.35	1.44	1.37
24	c	508	CLA	MG-NA	5.34	2.19	2.06
24	B	610	CLA	C3C-C2C	5.34	1.48	1.36
24	C	508	CLA	C1D-ND	5.33	1.44	1.37
24	b	617	CLA	C1D-ND	5.33	1.44	1.37
24	c	504	CLA	MG-ND	-5.32	1.95	2.05
24	c	507	CLA	C1D-ND	5.32	1.44	1.37
24	B	602	CLA	C1D-ND	5.32	1.44	1.37
24	c	513	CLA	C3C-C2C	5.32	1.48	1.36
24	C	507	CLA	O2D-CGD	5.32	1.46	1.33
24	b	609	CLA	MG-ND	-5.31	1.95	2.05
24	b	609	CLA	C3C-C2C	5.31	1.48	1.36
24	C	512	CLA	C3C-C2C	5.30	1.48	1.36
24	A	409	CLA	C1D-ND	5.30	1.44	1.37
24	c	506	CLA	C3C-C2C	5.29	1.48	1.36
24	b	613	CLA	CHC-C1C	5.29	1.49	1.38
24	b	611	CLA	C1D-ND	5.29	1.44	1.37
24	B	615	CLA	C3C-C2C	5.29	1.48	1.36
24	b	612	CLA	O2D-CGD	5.28	1.46	1.33
24	d	404	CLA	C3C-C2C	5.27	1.48	1.36
24	a	2110	CLA	C3C-C2C	5.25	1.48	1.36
25	A	408	PHO	C3D-C2D	5.25	1.48	1.39
24	D	404	CLA	C3C-C2C	5.25	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	C1D-ND	5.25	1.44	1.37
24	b	613	CLA	C1D-ND	5.25	1.44	1.37
24	c	506	CLA	O2D-CGD	5.24	1.46	1.33
24	b	614	CLA	C1D-ND	5.23	1.44	1.37
24	C	513	CLA	CHC-C1C	5.23	1.49	1.38
24	C	512	CLA	CHC-C1C	5.22	1.48	1.38
24	B	612	CLA	C3C-C2C	5.21	1.48	1.36
25	a	2111	PHO	C3D-C2D	5.21	1.48	1.39
24	b	615	CLA	MG-ND	-5.20	1.95	2.05
24	b	617	CLA	CHC-C1C	5.20	1.48	1.38
24	B	605	CLA	C3C-C2C	5.20	1.48	1.36
24	B	613	CLA	C3C-C2C	5.20	1.48	1.36
24	b	608	CLA	MG-NA	5.20	2.18	2.06
24	c	503	CLA	C3C-C2C	5.19	1.48	1.36
24	B	617	CLA	C3C-C2C	5.19	1.48	1.36
24	b	619	CLA	C3C-C2C	5.19	1.48	1.36
24	b	607	CLA	C3C-C2C	5.19	1.48	1.36
24	C	505	CLA	C1D-ND	5.18	1.44	1.37
24	B	616	CLA	C3C-C2C	5.18	1.47	1.36
24	B	614	CLA	MG-NA	5.17	2.18	2.06
24	C	511	CLA	C1D-ND	5.17	1.44	1.37
24	b	614	CLA	O2D-CGD	5.16	1.45	1.33
24	b	613	CLA	MG-ND	-5.16	1.95	2.05
24	B	608	CLA	MG-ND	-5.16	1.95	2.05
24	C	511	CLA	CHC-C1C	5.16	1.48	1.38
24	B	616	CLA	C1D-ND	5.15	1.44	1.37
24	B	616	CLA	O2D-CGD	5.15	1.45	1.33
24	B	609	CLA	MG-NC	5.15	2.18	2.06
24	B	614	CLA	C1D-ND	5.15	1.44	1.37
24	b	614	CLA	C3C-C2C	5.14	1.47	1.36
24	B	604	CLA	MG-ND	-5.14	1.95	2.05
24	c	513	CLA	CHC-C1C	5.14	1.48	1.38
24	B	604	CLA	C1D-ND	5.14	1.44	1.37
24	b	611	CLA	MG-NA	5.14	2.18	2.06
24	c	504	CLA	O2D-CGD	5.14	1.45	1.33
24	C	509	CLA	CHC-C1C	5.13	1.48	1.38
24	b	618	CLA	CHC-C1C	5.13	1.48	1.38
24	b	615	CLA	C3C-C2C	5.13	1.47	1.36
24	c	512	CLA	C1D-ND	5.12	1.44	1.37
25	a	2111	PHO	O2D-CGD	5.12	1.45	1.33
24	b	606	CLA	O2D-CGD	5.11	1.45	1.33
24	c	510	CLA	CHC-C1C	5.11	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	611	CLA	O2D-CGD	5.11	1.45	1.33
24	b	610	CLA	CHC-C1C	5.11	1.48	1.38
24	c	506	CLA	CHC-C1C	5.10	1.48	1.38
24	D	405	CLA	CHC-C1C	5.10	1.48	1.38
24	B	607	CLA	MG-NC	5.10	2.18	2.06
24	c	512	CLA	MG-NA	5.10	2.18	2.06
24	b	606	CLA	C1D-ND	5.10	1.44	1.37
24	B	607	CLA	C1D-ND	5.09	1.44	1.37
24	B	606	CLA	C3C-C2C	5.08	1.47	1.36
24	b	605	CLA	O2D-CGD	5.08	1.45	1.33
24	c	513	CLA	C1D-ND	5.08	1.44	1.37
24	C	506	CLA	CHD-C1D	5.07	1.48	1.38
24	B	603	CLA	CHC-C1C	5.06	1.48	1.38
24	c	504	CLA	C1D-ND	5.05	1.44	1.37
24	b	618	CLA	C1D-ND	5.05	1.44	1.37
24	b	619	CLA	O2D-CGD	5.05	1.45	1.33
24	c	505	CLA	CHC-C1C	5.05	1.48	1.38
24	B	611	CLA	CHC-C1C	5.04	1.48	1.38
24	c	508	CLA	O2D-CGD	5.04	1.45	1.33
24	B	605	CLA	C1D-ND	5.04	1.44	1.37
24	D	405	CLA	C1D-ND	5.03	1.44	1.37
24	D	401	CLA	O2D-CGD	5.03	1.45	1.33
24	b	604	CLA	CHC-C1C	5.03	1.48	1.38
24	C	506	CLA	CHC-C1C	5.03	1.48	1.38
24	b	610	CLA	O2D-CGD	5.02	1.45	1.33
24	d	401	CLA	O2D-CGD	5.02	1.45	1.33
24	C	510	CLA	CHC-C1C	5.02	1.48	1.38
24	c	515	CLA	CHC-C1C	5.02	1.48	1.38
24	b	612	CLA	CHD-C1D	5.02	1.48	1.38
24	B	612	CLA	CHC-C1C	5.01	1.48	1.38
24	c	514	CLA	MG-NC	5.01	2.18	2.06
24	C	505	CLA	CHC-C1C	5.00	1.48	1.38
24	c	504	CLA	CHC-C1C	5.00	1.48	1.38
24	B	611	CLA	C1D-ND	5.00	1.44	1.37
24	B	617	CLA	O2D-CGD	5.00	1.45	1.33
24	C	514	CLA	O2D-CGD	4.99	1.45	1.33
24	B	611	CLA	MG-NA	4.98	2.18	2.06
24	c	507	CLA	C3C-C2C	4.98	1.47	1.36
24	b	608	CLA	O2D-CGD	4.98	1.45	1.33
24	C	511	CLA	CHB-C1B	4.98	1.50	1.39
24	B	608	CLA	CHC-C1C	4.97	1.48	1.38
24	d	405	CLA	CHC-C1C	4.97	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	404	CLA	CHC-C1C	4.97	1.48	1.38
24	B	614	CLA	MG-NC	4.97	2.18	2.06
24	b	605	CLA	C1D-ND	4.97	1.44	1.37
24	a	2109	CLA	C1D-ND	4.97	1.44	1.37
24	a	2113	CLA	O2D-CGD	4.97	1.45	1.33
24	B	617	CLA	MG-ND	-4.97	1.95	2.05
24	c	503	CLA	CHC-C1C	4.97	1.48	1.38
24	C	502	CLA	CHC-C1C	4.96	1.48	1.38
24	B	616	CLA	CHC-C1C	4.96	1.48	1.38
24	A	409	CLA	CHC-C1C	4.96	1.48	1.38
24	B	610	CLA	O2D-CGD	4.95	1.45	1.33
24	B	604	CLA	CHC-C1C	4.95	1.48	1.38
24	c	511	CLA	CHC-C1C	4.95	1.48	1.38
24	B	606	CLA	O2D-CGD	4.95	1.45	1.33
24	A	406	CLA	CHC-C1C	4.95	1.48	1.38
24	b	615	CLA	CHC-C1C	4.95	1.48	1.38
24	b	616	CLA	O2D-CGD	4.95	1.45	1.33
24	b	604	CLA	O2D-CGD	4.94	1.45	1.33
24	b	615	CLA	O2D-CGD	4.94	1.45	1.33
24	C	512	CLA	C1D-ND	4.93	1.44	1.37
24	b	616	CLA	CHC-C1C	4.93	1.48	1.38
24	C	509	CLA	C1D-ND	4.93	1.44	1.37
24	d	401	CLA	MG-NA	4.92	2.18	2.06
24	C	510	CLA	O2D-CGD	4.91	1.45	1.33
24	C	514	CLA	CHC-C1C	4.91	1.48	1.38
24	b	607	CLA	CHC-C1C	4.91	1.48	1.38
24	c	515	CLA	CHD-C1D	4.91	1.48	1.38
24	c	503	CLA	MG-NC	4.91	2.17	2.06
24	B	609	CLA	CHC-C1C	4.90	1.48	1.38
24	B	613	CLA	O2D-CGD	4.90	1.45	1.33
24	B	606	CLA	CHC-C1C	4.90	1.48	1.38
24	b	609	CLA	CHC-C1C	4.90	1.48	1.38
24	b	605	CLA	CHC-C1C	4.89	1.48	1.38
24	b	607	CLA	O2D-CGD	4.89	1.45	1.33
24	D	405	CLA	O2D-CGD	4.89	1.45	1.33
24	B	607	CLA	CHC-C1C	4.88	1.48	1.38
24	C	505	CLA	MG-ND	-4.88	1.96	2.05
24	C	513	CLA	C1D-ND	4.88	1.44	1.37
24	A	406	CLA	CHD-C1D	4.87	1.47	1.38
24	d	405	CLA	MG-NC	4.87	2.17	2.06
24	D	401	CLA	MG-NA	4.87	2.17	2.06
24	A	406	CLA	MG-NC	4.86	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	513	CLA	CHD-C1D	4.86	1.47	1.38
24	C	504	CLA	CHC-C1C	4.86	1.48	1.38
24	B	614	CLA	CHC-C1C	4.86	1.48	1.38
24	c	504	CLA	MG-NC	4.86	2.17	2.06
24	B	609	CLA	CHD-C1D	4.86	1.47	1.38
24	c	511	CLA	CHB-C1B	4.85	1.50	1.39
24	c	512	CLA	CHC-C1C	4.85	1.48	1.38
24	C	509	CLA	O2D-CGD	4.84	1.45	1.33
25	A	408	PHO	O2D-CGD	4.84	1.45	1.33
24	B	614	CLA	O2D-CGD	4.84	1.45	1.33
24	c	509	CLA	C1D-ND	4.84	1.44	1.37
24	c	505	CLA	CHD-C1D	4.83	1.47	1.38
24	B	606	CLA	C1D-ND	4.83	1.44	1.37
24	B	602	CLA	O2D-CGD	4.83	1.45	1.33
24	d	405	CLA	C1D-ND	4.83	1.44	1.37
24	C	503	CLA	CHC-C1C	4.82	1.48	1.38
24	c	510	CLA	C1D-ND	4.81	1.44	1.37
24	C	502	CLA	CHD-C1D	4.80	1.47	1.38
24	A	405	CLA	O2D-CGD	4.79	1.45	1.33
24	b	619	CLA	C1D-ND	4.78	1.44	1.37
24	b	618	CLA	MG-NC	4.78	2.17	2.06
24	c	511	CLA	O2D-CGD	4.78	1.45	1.33
24	b	604	CLA	CHD-C1D	4.78	1.47	1.38
24	b	610	CLA	CHD-C1D	4.77	1.47	1.38
24	a	2109	CLA	MG-NC	4.77	2.17	2.06
40	e	103	HEM	FE-NB	4.77	2.09	1.94
24	a	2113	CLA	CHC-C1C	4.76	1.48	1.38
24	B	611	CLA	MG-ND	-4.76	1.96	2.05
24	C	508	CLA	CHD-C1D	4.76	1.47	1.38
24	b	617	CLA	O2D-CGD	4.76	1.44	1.33
24	b	607	CLA	CHD-C1D	4.76	1.47	1.38
24	B	610	CLA	CHC-C1C	4.75	1.48	1.38
24	D	401	CLA	C1D-ND	4.75	1.44	1.37
24	b	618	CLA	O2D-CGD	4.75	1.44	1.33
24	a	2109	CLA	CHC-C1C	4.75	1.48	1.38
25	A	407	PHO	O2D-CGD	4.74	1.44	1.33
24	b	605	CLA	CHD-C1D	4.74	1.47	1.38
24	B	603	CLA	MG-NC	4.74	2.17	2.06
24	b	606	CLA	CHD-C1D	4.74	1.47	1.38
24	c	507	CLA	CHD-C1D	4.74	1.47	1.38
34	C	539	DMS	O-S	4.74	1.81	1.50
24	A	405	CLA	C1D-ND	4.73	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	2112	PHO	OBD-CAD	4.73	1.28	1.22
24	C	505	CLA	O2D-CGD	4.73	1.44	1.33
24	C	514	CLA	CHD-C1D	4.73	1.47	1.38
24	C	508	CLA	CHC-C1C	4.73	1.48	1.38
24	b	614	CLA	CHC-C1C	4.73	1.48	1.38
24	C	507	CLA	CHC-C1C	4.72	1.47	1.38
24	c	507	CLA	CHC-C1C	4.72	1.47	1.38
34	v	214	DMS	O-S	4.72	1.81	1.50
24	c	509	CLA	MG-ND	-4.72	1.96	2.05
24	C	508	CLA	O2D-CGD	4.72	1.44	1.33
24	B	613	CLA	CHB-C1B	4.72	1.50	1.39
24	C	513	CLA	MG-NB	4.71	2.15	2.05
24	c	514	CLA	O2D-CGD	4.71	1.44	1.33
24	b	611	CLA	CHC-C1C	4.71	1.47	1.38
24	B	611	CLA	O2D-CGD	4.71	1.44	1.33
34	c	536	DMS	O-S	4.70	1.81	1.50
24	B	612	CLA	O2D-CGD	4.70	1.44	1.33
24	B	607	CLA	O2D-CGD	4.70	1.44	1.33
24	C	503	CLA	O2D-CGD	4.70	1.44	1.33
24	C	506	CLA	O2D-CGD	4.70	1.44	1.33
34	b	636	DMS	O-S	4.70	1.81	1.50
24	B	604	CLA	O2D-CGD	4.70	1.44	1.33
24	B	617	CLA	C1D-ND	4.69	1.44	1.37
24	c	512	CLA	O2D-CGD	4.69	1.44	1.33
24	c	511	CLA	CHD-C1D	4.69	1.47	1.38
24	B	603	CLA	C1D-ND	4.69	1.44	1.37
24	b	609	CLA	O2D-CGD	4.69	1.44	1.33
24	b	610	CLA	C1D-ND	4.68	1.44	1.37
24	c	515	CLA	O2D-CGD	4.68	1.44	1.33
24	d	405	CLA	O2D-CGD	4.68	1.44	1.33
24	C	509	CLA	MG-NB	4.68	2.15	2.05
34	d	417	DMS	O-S	4.68	1.81	1.50
24	D	404	CLA	CHB-C1B	4.68	1.49	1.39
34	u	204	DMS	O-S	4.67	1.81	1.50
25	a	2112	PHO	O2D-CGD	4.67	1.44	1.33
24	D	404	CLA	MG-NB	-4.67	1.96	2.05
34	O	306	DMS	O-S	4.67	1.81	1.50
34	V	205	DMS	O-S	4.67	1.81	1.50
34	b	641	DMS	O-S	4.66	1.81	1.50
24	A	409	CLA	O2D-CGD	4.66	1.44	1.33
34	b	634	DMS	O-S	4.66	1.81	1.50
34	x	802	DMS	O-S	4.66	1.81	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	643	DMS	O-S	4.66	1.81	1.50
24	B	603	CLA	CHD-C1D	4.66	1.47	1.38
24	A	406	CLA	O2D-CGD	4.66	1.44	1.33
34	t	103	DMS	O-S	4.66	1.81	1.50
34	c	538	DMS	O-S	4.66	1.81	1.50
34	o	2612	DMS	O-S	4.66	1.80	1.50
34	b	642	DMS	O-S	4.65	1.80	1.50
24	b	610	CLA	MG-NB	4.65	2.15	2.05
24	B	615	CLA	C1D-ND	4.65	1.44	1.37
24	c	510	CLA	O2D-CGD	4.65	1.44	1.33
24	b	615	CLA	C1D-ND	4.65	1.44	1.37
34	C	538	DMS	O-S	4.65	1.80	1.50
24	B	608	CLA	C1D-ND	4.64	1.44	1.37
34	v	206	DMS	O-S	4.64	1.80	1.50
24	c	510	CLA	CHD-C1D	4.64	1.47	1.38
34	B	640	DMS	O-S	4.64	1.80	1.50
24	B	608	CLA	O2D-CGD	4.64	1.44	1.33
24	a	2110	CLA	O2D-CGD	4.63	1.44	1.33
34	d	420	DMS	O-S	4.63	1.80	1.50
34	a	2122	DMS	O-S	4.63	1.80	1.50
24	c	506	CLA	MG-ND	-4.63	1.96	2.05
34	A	423	DMS	O-S	4.63	1.80	1.50
24	c	509	CLA	O2D-CGD	4.63	1.44	1.33
24	c	514	CLA	CHC-C1C	4.63	1.47	1.38
24	B	605	CLA	O2D-CGD	4.63	1.44	1.33
24	B	614	CLA	MG-ND	-4.63	1.96	2.05
34	O	311	DMS	O-S	4.63	1.80	1.50
34	T	106	DMS	O-S	4.63	1.80	1.50
34	b	638	DMS	O-S	4.62	1.80	1.50
34	C	527	DMS	O-S	4.62	1.80	1.50
34	d	423	DMS	O-S	4.62	1.80	1.50
34	B	650	DMS	O-S	4.62	1.80	1.50
34	B	647	DMS	O-S	4.62	1.80	1.50
24	C	505	CLA	CHD-C1D	4.62	1.47	1.38
24	c	508	CLA	CHD-C1D	4.62	1.47	1.38
24	C	513	CLA	O2D-CGD	4.62	1.44	1.33
34	B	645	DMS	O-S	4.62	1.80	1.50
24	a	2113	CLA	C1D-ND	4.62	1.43	1.37
34	c	539	DMS	O-S	4.62	1.80	1.50
34	A	426	DMS	O-S	4.62	1.80	1.50
34	d	421	DMS	O-S	4.62	1.80	1.50
34	C	530	DMS	O-S	4.62	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	211	DMS	O-S	4.62	1.80	1.50
34	C	536	DMS	O-S	4.62	1.80	1.50
24	C	511	CLA	O2D-CGD	4.61	1.44	1.33
24	b	606	CLA	CHC-C1C	4.61	1.47	1.38
34	a	2124	DMS	O-S	4.61	1.80	1.50
24	B	602	CLA	O2A-CGA	4.61	1.46	1.33
34	D	417	DMS	O-S	4.61	1.80	1.50
34	V	206	DMS	O-S	4.61	1.80	1.50
34	E	108	DMS	O-S	4.61	1.80	1.50
34	A	425	DMS	O-S	4.61	1.80	1.50
34	o	2609	DMS	O-S	4.61	1.80	1.50
34	D	419	DMS	O-S	4.60	1.80	1.50
34	c	534	DMS	O-S	4.60	1.80	1.50
24	D	404	CLA	O2D-CGD	4.60	1.44	1.33
24	c	510	CLA	MG-NA	4.60	2.17	2.06
34	c	541	DMS	O-S	4.60	1.80	1.50
34	a	2123	DMS	O-S	4.60	1.80	1.50
34	e	104	DMS	O-S	4.60	1.80	1.50
24	C	503	CLA	MG-NC	4.60	2.17	2.06
24	C	512	CLA	O2D-CGD	4.60	1.44	1.33
34	v	208	DMS	O-S	4.60	1.80	1.50
34	O	309	DMS	O-S	4.60	1.80	1.50
34	O	310	DMS	O-S	4.60	1.80	1.50
34	b	637	DMS	O-S	4.60	1.80	1.50
34	c	535	DMS	O-S	4.60	1.80	1.50
34	D	416	DMS	O-S	4.60	1.80	1.50
34	c	537	DMS	O-S	4.60	1.80	1.50
34	O	313	DMS	O-S	4.60	1.80	1.50
24	B	605	CLA	CHC-C1C	4.60	1.47	1.38
24	B	603	CLA	O2D-CGD	4.60	1.44	1.33
34	O	314	DMS	O-S	4.60	1.80	1.50
34	b	643	DMS	O-S	4.60	1.80	1.50
34	v	213	DMS	O-S	4.60	1.80	1.50
34	z	1802	DMS	O-S	4.60	1.80	1.50
24	c	512	CLA	CHB-C1B	4.59	1.49	1.39
34	B	638	DMS	O-S	4.59	1.80	1.50
34	C	535	DMS	O-S	4.59	1.80	1.50
34	c	533	DMS	O-S	4.59	1.80	1.50
24	c	503	CLA	C1D-ND	4.59	1.43	1.37
24	a	2109	CLA	MG-NB	4.59	2.14	2.05
24	b	619	CLA	CHC-C1C	4.59	1.47	1.38
34	B	646	DMS	O-S	4.59	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	210	DMS	O-S	4.59	1.80	1.50
34	d	418	DMS	O-S	4.59	1.80	1.50
34	C	537	DMS	O-S	4.59	1.80	1.50
34	v	209	DMS	O-S	4.59	1.80	1.50
24	b	613	CLA	O2D-CGD	4.59	1.44	1.33
34	T	104	DMS	O-S	4.59	1.80	1.50
34	d	422	DMS	O-S	4.59	1.80	1.50
34	D	420	DMS	O-S	4.59	1.80	1.50
34	F	103	DMS	O-S	4.59	1.80	1.50
24	d	401	CLA	CHC-C1C	4.59	1.47	1.38
34	O	304	DMS	O-S	4.59	1.80	1.50
24	c	503	CLA	O2D-CGD	4.59	1.44	1.33
34	C	529	DMS	O-S	4.59	1.80	1.50
34	B	649	DMS	O-S	4.58	1.80	1.50
24	C	502	CLA	O2D-CGD	4.58	1.44	1.33
34	O	308	DMS	O-S	4.58	1.80	1.50
34	k	2004	DMS	O-S	4.58	1.80	1.50
34	o	2604	DMS	O-S	4.58	1.80	1.50
34	V	208	DMS	O-S	4.58	1.80	1.50
34	U	503	DMS	O-S	4.58	1.80	1.50
27	B	621	SQD	O47-C7	4.58	1.47	1.34
34	o	2605	DMS	O-S	4.58	1.80	1.50
34	B	644	DMS	O-S	4.58	1.80	1.50
24	c	505	CLA	CHB-C1B	4.58	1.49	1.39
34	v	212	DMS	O-S	4.58	1.80	1.50
24	B	615	CLA	CHC-C1C	4.58	1.47	1.38
34	B	642	DMS	O-S	4.58	1.80	1.50
34	o	2607	DMS	O-S	4.58	1.80	1.50
34	u	202	DMS	O-S	4.57	1.80	1.50
34	o	2606	DMS	O-S	4.57	1.80	1.50
34	V	202	DMS	O-S	4.57	1.80	1.50
34	B	648	DMS	O-S	4.57	1.80	1.50
24	c	507	CLA	O2D-CGD	4.57	1.44	1.33
24	C	509	CLA	MG-NA	4.57	2.17	2.06
34	D	418	DMS	O-S	4.57	1.80	1.50
34	j	1604	DMS	O-S	4.57	1.80	1.50
34	C	534	DMS	O-S	4.57	1.80	1.50
24	b	604	CLA	O2A-CGA	4.57	1.46	1.33
24	b	609	CLA	CHD-C1D	4.56	1.47	1.38
34	o	2610	DMS	O-S	4.56	1.80	1.50
34	O	307	DMS	O-S	4.56	1.80	1.50
34	b	640	DMS	O-S	4.56	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	605	CLA	MG-ND	-4.56	1.96	2.05
34	c	531	DMS	O-S	4.56	1.80	1.50
34	c	540	DMS	O-S	4.56	1.80	1.50
34	b	635	DMS	O-S	4.56	1.80	1.50
34	E	107	DMS	O-S	4.56	1.80	1.50
34	O	312	DMS	O-S	4.56	1.80	1.50
34	T	105	DMS	O-S	4.56	1.80	1.50
34	u	201	DMS	O-S	4.56	1.80	1.50
24	B	610	CLA	CHD-C1D	4.56	1.47	1.38
34	d	419	DMS	O-S	4.56	1.80	1.50
34	o	2608	DMS	O-S	4.56	1.80	1.50
24	D	405	CLA	CHD-C1D	4.56	1.47	1.38
34	C	533	DMS	O-S	4.56	1.80	1.50
24	B	615	CLA	CHB-C1B	4.55	1.49	1.39
34	V	210	DMS	O-S	4.55	1.80	1.50
24	c	508	CLA	CHC-C1C	4.55	1.47	1.38
24	c	503	CLA	CHB-C1B	4.55	1.49	1.39
34	o	2611	DMS	O-S	4.54	1.80	1.50
24	B	610	CLA	CHB-C1B	4.54	1.49	1.39
34	b	633	DMS	O-S	4.54	1.80	1.50
34	c	542	DMS	O-S	4.54	1.80	1.50
34	C	532	DMS	O-S	4.54	1.80	1.50
24	d	405	CLA	CHB-C1B	4.53	1.49	1.39
34	i	106	DMS	O-S	4.53	1.80	1.50
34	V	209	DMS	O-S	4.53	1.80	1.50
24	A	409	CLA	MG-ND	-4.53	1.96	2.05
34	v	207	DMS	O-S	4.53	1.80	1.50
24	b	608	CLA	C1D-ND	4.53	1.43	1.37
34	V	207	DMS	O-S	4.53	1.80	1.50
24	B	615	CLA	MG-ND	-4.53	1.96	2.05
24	C	511	CLA	CHD-C1D	4.53	1.47	1.38
24	C	512	CLA	CHB-C1B	4.53	1.49	1.39
24	a	2110	CLA	C1D-ND	4.52	1.43	1.37
34	C	528	DMS	O-S	4.52	1.80	1.50
24	A	409	CLA	CHD-C1D	4.52	1.47	1.38
34	v	205	DMS	O-S	4.52	1.80	1.50
24	B	602	CLA	CHD-C1D	4.52	1.47	1.38
34	O	305	DMS	O-S	4.52	1.80	1.50
34	u	203	DMS	O-S	4.51	1.80	1.50
24	b	617	CLA	CHD-C1D	4.51	1.47	1.38
34	b	639	DMS	O-S	4.51	1.80	1.50
28	c	522	LMG	O7-C10	4.51	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	O2A-CGA	4.51	1.46	1.33
24	A	405	CLA	MG-NC	4.51	2.17	2.06
24	C	509	CLA	CHD-C1D	4.51	1.47	1.38
27	f	102	SQD	O47-C7	4.50	1.47	1.34
24	b	612	CLA	CHB-C1B	4.50	1.49	1.39
24	a	2110	CLA	CHC-C1C	4.50	1.47	1.38
24	B	606	CLA	CHD-C1D	4.50	1.47	1.38
34	c	529	DMS	O-S	4.50	1.79	1.50
24	b	619	CLA	CHD-C1D	4.50	1.47	1.38
34	B	639	DMS	O-S	4.50	1.79	1.50
24	d	404	CLA	O2A-CGA	4.49	1.46	1.33
24	b	615	CLA	CHB-C1B	4.49	1.49	1.39
24	c	505	CLA	O2D-CGD	4.49	1.44	1.33
34	c	530	DMS	O-S	4.49	1.79	1.50
24	C	504	CLA	CHD-C1D	4.49	1.47	1.38
24	b	614	CLA	CHD-C1D	4.49	1.47	1.38
24	D	405	CLA	MG-ND	-4.49	1.96	2.05
28	C	526	LMG	O7-C10	4.48	1.46	1.34
24	b	618	CLA	CHD-C1D	4.48	1.47	1.38
27	A	413	SQD	O48-C23	4.48	1.46	1.33
24	b	612	CLA	CHC-C1C	4.48	1.47	1.38
24	b	607	CLA	CHB-C1B	4.48	1.49	1.39
24	C	510	CLA	CHD-C1D	4.48	1.47	1.38
24	A	406	CLA	C1D-ND	4.47	1.43	1.37
34	C	531	DMS	O-S	4.46	1.79	1.50
24	B	611	CLA	CHD-C1D	4.46	1.47	1.38
24	B	608	CLA	CHB-C1B	4.45	1.49	1.39
24	b	619	CLA	CHB-C1B	4.45	1.49	1.39
24	a	2110	CLA	CHB-C1B	4.44	1.49	1.39
24	d	404	CLA	O2D-CGD	4.44	1.44	1.33
24	C	504	CLA	O2D-CGD	4.44	1.44	1.33
24	D	405	CLA	CHB-C1B	4.44	1.49	1.39
27	A	413	SQD	O47-C7	4.44	1.46	1.34
28	A	412	LMG	O7-C10	4.44	1.46	1.34
24	B	606	CLA	MG-ND	-4.44	1.97	2.05
24	A	409	CLA	CHB-C1B	4.44	1.49	1.39
24	C	503	CLA	CHB-C1B	4.44	1.49	1.39
24	D	401	CLA	O2A-CGA	4.43	1.46	1.33
38	D	408	DGD	O1G-C1A	4.43	1.46	1.33
24	B	617	CLA	CHC-C1C	4.43	1.47	1.38
24	c	513	CLA	O2D-CGD	4.43	1.44	1.33
24	C	506	CLA	CHB-C1B	4.43	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	604	CLA	CHC-C4B	4.42	1.49	1.39
34	c	532	DMS	O-S	4.42	1.79	1.50
24	c	507	CLA	CHB-C1B	4.42	1.49	1.39
24	C	509	CLA	O2A-CGA	4.41	1.46	1.33
24	B	608	CLA	CHC-C4B	4.41	1.49	1.39
24	c	512	CLA	CHD-C1D	4.41	1.47	1.38
24	C	512	CLA	MG-NB	4.41	2.14	2.05
24	c	509	CLA	CHC-C1C	4.41	1.47	1.38
24	C	504	CLA	CHB-C1B	4.41	1.49	1.39
24	b	611	CLA	CHD-C1D	4.40	1.47	1.38
28	b	623	LMG	O8-C28	4.40	1.46	1.33
24	C	508	CLA	MG-NC	4.40	2.16	2.06
24	c	514	CLA	CHD-C1D	4.40	1.47	1.38
34	A	424	DMS	O-S	4.40	1.79	1.50
24	b	608	CLA	CHC-C4B	4.39	1.49	1.39
24	b	616	CLA	MG-NB	4.39	2.14	2.05
34	B	641	DMS	O-S	4.39	1.79	1.50
24	C	512	CLA	CHD-C1D	4.39	1.47	1.38
24	A	405	CLA	CHC-C1C	4.38	1.47	1.38
24	b	614	CLA	CHB-C1B	4.38	1.49	1.39
24	b	606	CLA	O2A-CGA	4.38	1.46	1.33
28	C	520	LMG	O8-C28	4.37	1.46	1.33
24	B	607	CLA	CHD-C1D	4.37	1.46	1.38
38	C	519	DGD	O1G-C1A	4.37	1.46	1.33
24	C	507	CLA	CHD-C1D	4.36	1.46	1.38
24	C	503	CLA	CHD-C1D	4.36	1.46	1.38
24	B	605	CLA	CHD-C1D	4.36	1.46	1.38
24	c	510	CLA	CHC-C4B	4.36	1.49	1.39
39	E	101	LHG	O8-C23	4.35	1.46	1.33
38	D	408	DGD	O2G-C1B	4.35	1.46	1.34
24	c	506	CLA	C1D-ND	4.35	1.43	1.37
24	c	504	CLA	CHD-C1D	4.35	1.46	1.38
24	d	405	CLA	CHD-C1D	4.35	1.46	1.38
24	B	603	CLA	CHB-C1B	4.34	1.49	1.39
24	B	606	CLA	MG-NC	4.34	2.16	2.06
24	B	615	CLA	O2D-CGD	4.34	1.43	1.33
24	B	608	CLA	CHD-C1D	4.34	1.46	1.38
25	a	2111	PHO	OBD-CAD	4.33	1.28	1.22
39	d	408	LHG	O8-C23	4.33	1.46	1.33
24	B	604	CLA	CHD-C1D	4.33	1.46	1.38
24	a	2109	CLA	O2D-CGD	4.33	1.43	1.33
24	a	2113	CLA	O2A-CGA	4.32	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	A	422	DMS	O-S	4.32	1.78	1.50
24	B	607	CLA	MG-ND	-4.32	1.97	2.05
24	B	611	CLA	CHC-C4B	4.32	1.49	1.39
24	B	614	CLA	CHC-C4B	4.32	1.49	1.39
24	C	504	CLA	CHC-C4B	4.32	1.49	1.39
24	C	502	CLA	CHB-C1B	4.32	1.49	1.39
28	i	101	LMG	O8-C28	4.31	1.45	1.33
28	A	412	LMG	O8-C28	4.31	1.45	1.33
24	B	602	CLA	CHC-C4B	4.31	1.49	1.39
24	d	405	CLA	CHC-C4B	4.31	1.49	1.39
24	c	509	CLA	O2A-CGA	4.31	1.45	1.33
24	C	508	CLA	OBD-CAD	4.30	1.29	1.22
28	B	622	LMG	O8-C28	4.30	1.45	1.33
24	b	616	CLA	CHB-C1B	4.30	1.49	1.39
24	c	515	CLA	O2A-CGA	4.30	1.45	1.33
24	c	513	CLA	OBD-CAD	4.30	1.29	1.22
24	b	613	CLA	CHD-C1D	4.29	1.46	1.38
34	a	2121	DMS	O-S	4.29	1.78	1.50
24	C	510	CLA	CHB-C1B	4.29	1.49	1.39
24	B	612	CLA	CHB-C1B	4.29	1.49	1.39
27	a	2102	SQD	O48-C23	4.29	1.45	1.33
39	e	101	LHG	O7-C7	4.29	1.46	1.34
24	c	510	CLA	MG-NB	4.29	2.14	2.05
27	L	102	SQD	O47-C7	4.28	1.46	1.34
27	a	2102	SQD	O47-C7	4.28	1.46	1.34
24	d	401	CLA	CHD-C1D	4.28	1.46	1.38
24	d	404	CLA	CHD-C1D	4.28	1.46	1.38
24	B	605	CLA	CHB-C1B	4.28	1.49	1.39
24	C	513	CLA	CHB-C1B	4.28	1.49	1.39
24	C	512	CLA	O2A-CGA	4.27	1.45	1.33
27	F	101	SQD	O47-C7	4.27	1.46	1.34
24	b	611	CLA	CHB-C1B	4.27	1.49	1.39
24	c	509	CLA	CHD-C1D	4.27	1.46	1.38
24	c	504	CLA	CHB-C1B	4.26	1.49	1.39
24	D	401	CLA	CHC-C1C	4.26	1.47	1.38
24	C	503	CLA	O2A-CGA	4.25	1.45	1.33
24	b	609	CLA	CHB-C1B	4.25	1.48	1.39
27	F	101	SQD	O48-C23	4.25	1.45	1.33
24	c	515	CLA	CHB-C1B	4.24	1.48	1.39
24	b	615	CLA	CHC-C4B	4.24	1.48	1.39
24	C	505	CLA	CHD-C4C	4.24	1.48	1.39
24	d	405	CLA	O2A-CGA	4.23	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	605	CLA	CHB-C1B	4.23	1.48	1.39
24	B	617	CLA	CHD-C1D	4.22	1.46	1.38
24	C	502	CLA	CHD-C4C	4.22	1.48	1.39
24	c	511	CLA	O2A-CGA	4.22	1.45	1.33
24	D	404	CLA	O2A-CGA	4.22	1.45	1.33
24	b	609	CLA	O2A-CGA	4.22	1.45	1.33
24	C	507	CLA	CHB-C1B	4.21	1.48	1.39
24	C	514	CLA	CHB-C1B	4.21	1.48	1.39
25	A	408	PHO	OBD-CAD	4.21	1.27	1.22
34	b	632	DMS	O-S	4.21	1.78	1.50
24	B	609	CLA	O2D-CGD	4.21	1.43	1.33
24	d	404	CLA	CHB-C1B	4.21	1.48	1.39
24	A	406	CLA	OBD-CAD	4.20	1.29	1.22
24	b	605	CLA	O2A-CGA	4.20	1.45	1.33
38	h	703	DGD	O1G-C1A	4.20	1.45	1.33
24	B	614	CLA	CHD-C1D	4.20	1.46	1.38
24	C	502	CLA	CHC-C4B	4.20	1.48	1.39
24	B	604	CLA	CHB-C1B	4.20	1.48	1.39
24	B	617	CLA	CHB-C1B	4.20	1.48	1.39
24	b	612	CLA	O2A-CGA	4.20	1.45	1.33
24	B	606	CLA	CHB-C1B	4.20	1.48	1.39
24	b	618	CLA	CHB-C1B	4.20	1.48	1.39
24	a	2109	CLA	CHB-C1B	4.20	1.48	1.39
24	C	513	CLA	CHD-C1D	4.19	1.46	1.38
24	b	619	CLA	O2A-CGA	4.19	1.45	1.33
24	D	405	CLA	CHC-C4B	4.19	1.48	1.39
24	b	613	CLA	CHB-C1B	4.18	1.48	1.39
24	B	613	CLA	CHD-C1D	4.17	1.46	1.38
28	c	522	LMG	O8-C28	4.17	1.45	1.33
24	B	615	CLA	CHD-C1D	4.17	1.46	1.38
27	A	411	SQD	O48-C23	4.17	1.45	1.33
24	B	602	CLA	MG-NC	4.17	2.16	2.06
39	E	101	LHG	O7-C7	4.17	1.46	1.34
24	b	614	CLA	O2A-CGA	4.17	1.45	1.33
24	c	508	CLA	O2A-CGA	4.17	1.45	1.33
24	d	401	CLA	CHB-C1B	4.16	1.48	1.39
27	f	102	SQD	O48-C23	4.16	1.45	1.33
24	C	513	CLA	O2A-CGA	4.16	1.45	1.33
24	B	612	CLA	CHC-C4B	4.16	1.48	1.39
24	a	2113	CLA	CHB-C1B	4.16	1.48	1.39
24	b	617	CLA	CHB-C1B	4.16	1.48	1.39
24	B	611	CLA	CHB-C1B	4.16	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	401	CLA	O2A-CGA	4.16	1.45	1.33
24	b	608	CLA	O2A-CGA	4.16	1.45	1.33
24	b	604	CLA	CHB-C1B	4.16	1.48	1.39
24	C	506	CLA	CHC-C4B	4.15	1.48	1.39
24	D	404	CLA	CHC-C1C	4.15	1.46	1.38
24	b	605	CLA	CHC-C4B	4.15	1.48	1.39
24	B	602	CLA	CHB-C1B	4.15	1.48	1.39
24	B	602	CLA	MG-ND	-4.15	1.97	2.05
24	c	513	CLA	CHB-C1B	4.14	1.48	1.39
24	b	608	CLA	CHD-C1D	4.14	1.46	1.38
28	d	411	LMG	O8-C28	4.14	1.45	1.33
39	d	410	LHG	O8-C23	4.14	1.45	1.33
24	a	2109	CLA	CHD-C1D	4.14	1.46	1.38
38	H	102	DGD	O1G-C1A	4.14	1.45	1.33
24	b	616	CLA	O2A-CGA	4.14	1.45	1.33
24	b	607	CLA	CHC-C4B	4.13	1.48	1.39
24	B	602	CLA	CHD-C4C	4.13	1.48	1.39
24	a	2110	CLA	O2A-CGA	4.13	1.45	1.33
27	L	102	SQD	O48-C23	4.13	1.45	1.33
24	B	604	CLA	CHC-C4B	4.13	1.48	1.39
24	b	613	CLA	CHC-C4B	4.13	1.48	1.39
24	B	605	CLA	CHC-C4B	4.13	1.48	1.39
24	C	511	CLA	CHC-C4B	4.13	1.48	1.39
24	B	610	CLA	O2A-CGA	4.12	1.45	1.33
24	b	610	CLA	CHB-C1B	4.12	1.48	1.39
24	b	610	CLA	CHC-C4B	4.12	1.48	1.39
25	A	408	PHO	O2A-CGA	4.11	1.45	1.33
24	b	604	CLA	C3D-C2D	4.11	1.50	1.39
24	b	618	CLA	O2A-CGA	4.11	1.45	1.33
24	A	406	CLA	CHD-C4C	4.11	1.48	1.39
24	B	614	CLA	CHB-C1B	4.11	1.48	1.39
24	C	514	CLA	O2A-CGA	4.10	1.45	1.33
24	c	510	CLA	CHB-C1B	4.10	1.48	1.39
39	D	409	LHG	O8-C23	4.10	1.45	1.33
24	C	509	CLA	CHB-C1B	4.10	1.48	1.39
24	c	506	CLA	CHD-C1D	4.10	1.46	1.38
24	c	507	CLA	CHC-C4B	4.10	1.48	1.39
24	c	512	CLA	CHC-C4B	4.10	1.48	1.39
24	b	617	CLA	CHC-C4B	4.09	1.48	1.39
28	c	521	LMG	O8-C28	4.09	1.45	1.33
24	c	514	CLA	O2A-CGA	4.09	1.45	1.33
24	B	616	CLA	OBD-CAD	4.09	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	CHD-C1D	4.09	1.46	1.38
24	b	611	CLA	O2A-CGA	4.09	1.45	1.33
24	b	604	CLA	CHD-C4C	4.09	1.48	1.39
28	c	521	LMG	O7-C10	4.08	1.45	1.34
24	B	608	CLA	O2A-CGA	4.08	1.45	1.33
24	A	405	CLA	CHD-C1D	4.08	1.46	1.38
24	C	505	CLA	CHB-C1B	4.08	1.48	1.39
28	C	526	LMG	O8-C28	4.08	1.45	1.33
24	C	505	CLA	CHC-C4B	4.08	1.48	1.39
24	B	604	CLA	O2A-CGA	4.08	1.45	1.33
24	A	405	CLA	C1B-NB	-4.08	1.32	1.37
28	i	101	LMG	O7-C10	4.07	1.45	1.34
24	c	510	CLA	O2A-CGA	4.07	1.45	1.33
24	c	509	CLA	CHB-C1B	4.07	1.48	1.39
24	C	503	CLA	C3D-C2D	4.07	1.50	1.39
25	A	407	PHO	OBD-CAD	4.07	1.27	1.22
24	b	606	CLA	CHB-C1B	4.07	1.48	1.39
24	B	603	CLA	CHC-C4B	4.07	1.48	1.39
24	c	504	CLA	CHC-C4B	4.07	1.48	1.39
24	B	603	CLA	O2A-CGA	4.07	1.45	1.33
24	d	405	CLA	OBD-CAD	4.07	1.29	1.22
24	b	618	CLA	C3D-C2D	4.07	1.50	1.39
24	B	607	CLA	CHC-C4B	4.06	1.48	1.39
38	C	517	DGD	O2G-C1B	4.06	1.45	1.34
24	c	504	CLA	C3D-C2D	4.06	1.50	1.39
24	a	2110	CLA	OBD-CAD	4.06	1.29	1.22
39	d	410	LHG	O7-C7	4.05	1.45	1.34
24	C	505	CLA	C3D-C2D	4.05	1.50	1.39
24	C	502	CLA	OBD-CAD	4.05	1.29	1.22
24	c	513	CLA	O2A-CGA	4.05	1.45	1.33
28	b	623	LMG	O7-C10	4.05	1.45	1.34
25	A	407	PHO	O2A-CGA	4.05	1.45	1.33
24	b	605	CLA	CHD-C4C	4.04	1.48	1.39
24	b	607	CLA	O2A-CGA	4.04	1.45	1.33
24	b	619	CLA	MG-NC	4.03	2.15	2.06
24	D	404	CLA	C1D-ND	4.03	1.43	1.37
24	b	613	CLA	MG-NB	4.03	2.13	2.05
24	A	406	CLA	MG-NA	4.03	2.15	2.06
24	b	613	CLA	CHD-C4C	4.03	1.48	1.39
24	c	503	CLA	O2A-CGA	4.03	1.45	1.33
24	D	404	CLA	CHC-C4B	4.03	1.48	1.39
24	a	2109	CLA	CHC-C4B	4.03	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	510	CLA	OBD-CAD	4.03	1.29	1.22
24	A	409	CLA	CHC-C4B	4.03	1.48	1.39
24	C	507	CLA	O2A-CGA	4.03	1.45	1.33
24	B	606	CLA	CHC-C4B	4.02	1.48	1.39
24	C	510	CLA	OBD-CAD	4.02	1.29	1.22
24	C	508	CLA	O2A-CGA	4.02	1.45	1.33
24	b	608	CLA	MG-NC	4.01	2.15	2.06
24	c	509	CLA	OBD-CAD	4.01	1.29	1.22
24	D	405	CLA	CHD-C4C	4.01	1.48	1.39
24	C	509	CLA	CHC-C4B	4.01	1.48	1.39
24	b	618	CLA	CHD-C4C	4.01	1.48	1.39
24	C	508	CLA	CHB-C1B	4.01	1.48	1.39
27	B	621	SQD	O48-C23	4.01	1.45	1.33
24	a	2113	CLA	CHD-C1D	4.01	1.46	1.38
24	d	405	CLA	CHD-C4C	4.00	1.48	1.39
39	L	101	LHG	O8-C23	4.00	1.45	1.33
24	b	613	CLA	MG-NC	4.00	2.15	2.06
24	C	510	CLA	C3D-C2D	4.00	1.49	1.39
24	B	612	CLA	CHD-C1D	4.00	1.46	1.38
24	B	617	CLA	MG-NC	4.00	2.15	2.06
24	C	511	CLA	CHD-C4C	3.99	1.48	1.39
24	B	610	CLA	CHC-C4B	3.99	1.48	1.39
28	B	622	LMG	O7-C10	3.99	1.45	1.34
24	C	502	CLA	O2A-CGA	3.99	1.45	1.33
43	v	201	HEC	CBC-CAC	-3.99	1.34	1.49
28	C	520	LMG	O7-C10	3.99	1.45	1.34
24	C	513	CLA	CHC-C4B	3.99	1.48	1.39
24	B	615	CLA	C3D-C2D	3.99	1.49	1.39
24	B	607	CLA	CHB-C1B	3.99	1.48	1.39
24	b	615	CLA	MG-NC	3.99	2.15	2.06
24	a	2113	CLA	MG-ND	-3.98	1.97	2.05
24	C	509	CLA	OBD-CAD	3.98	1.29	1.22
24	c	514	CLA	CHB-C1B	3.98	1.48	1.39
24	c	503	CLA	CHC-C4B	3.98	1.48	1.39
24	B	617	CLA	O2A-CGA	3.98	1.45	1.33
24	c	513	CLA	MG-ND	-3.98	1.97	2.05
24	B	609	CLA	CHB-C1B	3.98	1.48	1.39
24	c	513	CLA	MG-NC	3.98	2.15	2.06
24	D	404	CLA	MG-NC	3.98	2.15	2.06
25	a	2112	PHO	O2A-CGA	3.97	1.44	1.33
24	B	616	CLA	C3D-C2D	3.97	1.49	1.39
24	B	616	CLA	CHD-C1D	3.97	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	405	CLA	CHB-C1B	3.97	1.48	1.39
24	c	506	CLA	CHB-C1B	3.97	1.48	1.39
24	B	605	CLA	O2A-CGA	3.97	1.44	1.33
24	b	610	CLA	O2A-CGA	3.96	1.44	1.33
24	B	608	CLA	CHD-C4C	3.96	1.48	1.39
24	C	509	CLA	C3D-C2D	3.96	1.49	1.39
24	B	603	CLA	OBD-CAD	3.96	1.29	1.22
24	C	510	CLA	CHC-C4B	3.96	1.48	1.39
24	c	511	CLA	OBD-CAD	3.95	1.29	1.22
24	C	507	CLA	CHC-C4B	3.95	1.48	1.39
24	C	502	CLA	MG-ND	-3.95	1.98	2.05
24	b	608	CLA	CHB-C1B	3.95	1.48	1.39
24	b	606	CLA	CHD-C4C	3.95	1.48	1.39
24	c	512	CLA	C3D-C2D	3.95	1.49	1.39
24	b	610	CLA	C3D-C2D	3.95	1.49	1.39
24	c	513	CLA	CHC-C4B	3.95	1.48	1.39
24	C	511	CLA	MG-NB	3.94	2.13	2.05
24	b	615	CLA	O2A-CGA	3.94	1.44	1.33
39	L	101	LHG	O7-C7	3.94	1.45	1.34
24	b	615	CLA	CHD-C1D	3.93	1.46	1.38
24	A	409	CLA	O2A-CGA	3.93	1.44	1.33
24	b	617	CLA	O2A-CGA	3.93	1.44	1.33
24	B	608	CLA	OBD-CAD	3.93	1.29	1.22
24	c	514	CLA	C3D-C2D	3.93	1.49	1.39
24	c	505	CLA	CHC-C4B	3.93	1.48	1.39
24	c	515	CLA	CHC-C4B	3.93	1.48	1.39
24	B	609	CLA	O2A-CGA	3.93	1.44	1.33
24	B	616	CLA	O2A-CGA	3.93	1.44	1.33
24	C	504	CLA	O2A-CGA	3.92	1.44	1.33
24	A	405	CLA	C3D-C2D	3.92	1.49	1.39
24	B	616	CLA	CHC-C4B	3.92	1.48	1.39
24	B	603	CLA	CHD-C4C	3.92	1.48	1.39
24	A	409	CLA	CHD-C4C	3.92	1.48	1.39
24	b	616	CLA	CHC-C4B	3.92	1.48	1.39
28	D	412	LMG	O8-C28	3.91	1.44	1.33
24	c	503	CLA	CHD-C1D	3.91	1.46	1.38
24	B	613	CLA	O2A-CGA	3.91	1.44	1.33
24	B	609	CLA	C3D-C2D	3.91	1.49	1.39
24	c	509	CLA	CHD-C4C	3.91	1.48	1.39
38	h	703	DGD	O2G-C1B	3.91	1.45	1.34
24	C	513	CLA	C3D-C2D	3.91	1.49	1.39
24	B	609	CLA	CHC-C4B	3.91	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	506	CLA	C3D-C2D	3.91	1.49	1.39
39	D	410	LHG	O8-C23	3.91	1.44	1.33
27	a	2115	SQD	O48-C23	3.90	1.44	1.33
24	C	509	CLA	CHD-C4C	3.90	1.48	1.39
24	B	612	CLA	OBD-CAD	3.90	1.29	1.22
24	B	616	CLA	CHB-C1B	3.90	1.48	1.39
24	b	606	CLA	CHC-C4B	3.90	1.48	1.39
24	C	506	CLA	O2A-CGA	3.90	1.44	1.33
24	c	511	CLA	CHC-C4B	3.90	1.48	1.39
39	l	101	LHG	O8-C23	3.90	1.44	1.33
24	b	617	CLA	CHD-C4C	3.89	1.48	1.39
24	B	612	CLA	O2A-CGA	3.89	1.44	1.33
24	b	612	CLA	CHD-C4C	3.89	1.48	1.39
24	B	615	CLA	CHD-C4C	3.89	1.48	1.39
24	C	503	CLA	CHC-C4B	3.89	1.48	1.39
24	B	607	CLA	O2A-CGA	3.89	1.44	1.33
24	A	406	CLA	CHB-C1B	3.89	1.48	1.39
24	c	510	CLA	CHD-C4C	3.89	1.48	1.39
27	a	2115	SQD	O47-C7	3.89	1.45	1.34
24	B	608	CLA	C3D-C2D	3.88	1.49	1.39
24	c	513	CLA	CHD-C4C	3.88	1.48	1.39
24	D	401	CLA	OBD-CAD	3.88	1.29	1.22
24	d	405	CLA	C3D-C2D	3.88	1.49	1.39
24	b	604	CLA	OBD-CAD	3.88	1.29	1.22
24	B	610	CLA	C3D-C2D	3.88	1.49	1.39
24	C	502	CLA	C3D-C2D	3.88	1.49	1.39
24	B	615	CLA	CHC-C4B	3.88	1.48	1.39
24	b	612	CLA	MG-ND	-3.88	1.98	2.05
38	c	520	DGD	O1G-C1A	3.87	1.44	1.33
24	c	509	CLA	C3D-C2D	3.87	1.49	1.39
24	b	614	CLA	CHC-C4B	3.87	1.48	1.39
24	b	605	CLA	C3D-C2D	3.87	1.49	1.39
24	c	509	CLA	CHC-C4B	3.87	1.48	1.39
25	a	2111	PHO	O2A-CGA	3.87	1.44	1.33
38	c	519	DGD	O2G-C1B	3.87	1.45	1.34
43	V	201	HEC	CBC-CAC	-3.86	1.35	1.49
24	B	606	CLA	O2A-CGA	3.86	1.44	1.33
24	C	508	CLA	CHC-C4B	3.86	1.48	1.39
24	A	409	CLA	C3D-C2D	3.86	1.49	1.39
24	b	616	CLA	CHD-C4C	3.86	1.48	1.39
24	a	2110	CLA	C3D-C2D	3.86	1.49	1.39
24	c	508	CLA	CHD-C4C	3.86	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	c	518	DGD	O2G-C1B	3.86	1.45	1.34
24	c	505	CLA	O2A-CGA	3.86	1.44	1.33
27	A	411	SQD	O47-C7	3.86	1.45	1.34
24	d	401	CLA	C3D-C2D	3.86	1.49	1.39
36	B	624	HTG	C1'-S1	-3.86	1.76	1.81
24	c	511	CLA	C3D-C2D	3.86	1.49	1.39
24	C	514	CLA	CHD-C4C	3.85	1.48	1.39
24	B	612	CLA	CHD-C4C	3.85	1.48	1.39
24	D	405	CLA	O2A-CGA	3.85	1.44	1.33
24	B	614	CLA	OBD-CAD	3.85	1.29	1.22
24	b	611	CLA	OBD-CAD	3.85	1.29	1.22
24	C	503	CLA	OBD-CAD	3.85	1.29	1.22
24	C	506	CLA	OBD-CAD	3.85	1.29	1.22
24	c	503	CLA	OBD-CAD	3.85	1.29	1.22
24	B	614	CLA	CHD-C4C	3.85	1.48	1.39
24	A	406	CLA	O2A-CGA	3.84	1.44	1.33
38	c	519	DGD	O1G-C1A	3.84	1.44	1.33
24	d	404	CLA	CHC-C4B	3.84	1.48	1.39
24	B	611	CLA	C3D-C2D	3.83	1.49	1.39
24	c	507	CLA	O2A-CGA	3.83	1.44	1.33
24	B	607	CLA	CHD-C4C	3.83	1.47	1.39
24	b	613	CLA	C1B-NB	-3.83	1.32	1.37
43	v	201	HEC	CBB-CAB	-3.83	1.35	1.49
24	C	512	CLA	CHD-C4C	3.82	1.47	1.39
24	B	610	CLA	OBD-CAD	3.82	1.29	1.22
24	A	406	CLA	CHC-C4B	3.82	1.48	1.39
40	F	102	HEM	FE-NC	3.82	2.07	1.95
24	B	613	CLA	OBD-CAD	3.82	1.29	1.22
24	A	405	CLA	CHC-C4B	3.82	1.48	1.39
39	D	411	LHG	O8-C23	3.82	1.44	1.33
24	d	401	CLA	OBD-CAD	3.82	1.29	1.22
24	c	509	CLA	MG-NB	-3.81	1.98	2.05
24	c	504	CLA	CHD-C4C	3.81	1.47	1.39
25	A	408	PHO	CHA-CBD	-3.81	1.47	1.51
24	c	514	CLA	CHD-C4C	3.81	1.47	1.39
24	C	512	CLA	C3D-C2D	3.81	1.49	1.39
24	D	401	CLA	C3D-C2D	3.81	1.49	1.39
24	C	512	CLA	CHC-C4B	3.80	1.47	1.39
24	b	618	CLA	CHC-C4B	3.80	1.47	1.39
24	b	609	CLA	CHC-C4B	3.80	1.47	1.39
24	D	401	CLA	CHC-C4B	3.80	1.47	1.39
24	c	508	CLA	CHB-C1B	3.80	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	2109	CLA	OBD-CAD	3.80	1.29	1.22
24	C	514	CLA	CHC-C4B	3.80	1.47	1.39
24	c	515	CLA	CHD-C4C	3.79	1.47	1.39
24	C	505	CLA	O2A-CGA	3.79	1.44	1.33
24	B	613	CLA	C1B-NB	-3.79	1.32	1.37
24	C	513	CLA	CHD-C4C	3.79	1.47	1.39
24	b	615	CLA	C3D-C2D	3.79	1.49	1.39
38	C	518	DGD	O1G-C1A	3.79	1.44	1.33
38	C	519	DGD	O2G-C1B	3.78	1.45	1.34
24	d	401	CLA	CHC-C4B	3.78	1.47	1.39
24	C	511	CLA	C3D-C2D	3.78	1.49	1.39
24	c	513	CLA	C3D-C2D	3.78	1.49	1.39
24	D	405	CLA	C3D-C2D	3.78	1.49	1.39
24	b	613	CLA	O2A-CGA	3.78	1.44	1.33
28	d	411	LMG	O7-C10	3.78	1.44	1.34
24	c	512	CLA	CHD-C4C	3.78	1.47	1.39
24	c	515	CLA	C3D-C2D	3.77	1.49	1.39
24	d	404	CLA	CHD-C4C	3.77	1.47	1.39
24	c	504	CLA	O2A-CGA	3.77	1.44	1.33
24	B	617	CLA	C3D-C2D	3.77	1.49	1.39
24	a	2113	CLA	C3D-C2D	3.76	1.49	1.39
24	A	405	CLA	OBD-CAD	3.76	1.29	1.22
24	C	506	CLA	CHD-C4C	3.76	1.47	1.39
24	d	401	CLA	CHD-C4C	3.76	1.47	1.39
39	D	411	LHG	O7-C7	3.75	1.44	1.34
24	A	409	CLA	OBD-CAD	3.75	1.28	1.22
24	C	504	CLA	CHD-C4C	3.75	1.47	1.39
24	C	510	CLA	CHD-C4C	3.75	1.47	1.39
24	c	506	CLA	CHC-C4B	3.75	1.47	1.39
24	c	512	CLA	OBD-CAD	3.75	1.28	1.22
24	c	511	CLA	CHD-C4C	3.75	1.47	1.39
24	c	514	CLA	OBD-CAD	3.75	1.28	1.22
24	a	2110	CLA	CHD-C4C	3.74	1.47	1.39
24	d	404	CLA	C3D-C2D	3.74	1.49	1.39
24	B	615	CLA	O2A-CGA	3.74	1.44	1.33
24	a	2113	CLA	CHC-C4B	3.74	1.47	1.39
24	b	614	CLA	CHD-C4C	3.74	1.47	1.39
24	b	613	CLA	C3D-C2D	3.73	1.49	1.39
24	B	616	CLA	MG-NB	3.73	2.13	2.05
38	c	518	DGD	O1G-C1A	3.73	1.44	1.33
24	c	505	CLA	C3D-C2D	3.73	1.49	1.39
24	A	405	CLA	CHD-C4C	3.73	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C3D-C2D	3.73	1.49	1.39
38	C	518	DGD	O2G-C1B	3.73	1.44	1.34
24	B	615	CLA	OBD-CAD	3.73	1.28	1.22
24	B	603	CLA	C3D-C2D	3.72	1.49	1.39
24	c	515	CLA	OBD-CAD	3.72	1.28	1.22
24	B	605	CLA	CHD-C4C	3.72	1.47	1.39
24	c	507	CLA	CHD-C4C	3.71	1.47	1.39
38	H	102	DGD	O2G-C1B	3.71	1.44	1.34
24	C	504	CLA	C3D-C2D	3.71	1.49	1.39
24	b	616	CLA	C3D-C2D	3.71	1.49	1.39
24	c	504	CLA	OBD-CAD	3.71	1.28	1.22
24	B	617	CLA	CHC-C4B	3.71	1.47	1.39
24	B	612	CLA	C3D-C2D	3.71	1.49	1.39
24	D	401	CLA	CHB-C1B	3.71	1.47	1.39
24	D	401	CLA	CHD-C1D	3.70	1.45	1.38
24	c	510	CLA	C3D-C2D	3.70	1.49	1.39
24	B	602	CLA	C3D-C2D	3.70	1.49	1.39
24	C	503	CLA	CHD-C4C	3.70	1.47	1.39
38	c	520	DGD	O2G-C1B	3.70	1.44	1.34
24	b	611	CLA	CHC-C4B	3.70	1.47	1.39
24	c	506	CLA	CHD-C4C	3.69	1.47	1.39
24	b	610	CLA	CHD-C4C	3.69	1.47	1.39
24	d	405	CLA	MG-NB	3.69	2.13	2.05
24	c	505	CLA	CHD-C4C	3.69	1.47	1.39
24	D	405	CLA	OBD-CAD	3.69	1.28	1.22
24	b	605	CLA	OBD-CAD	3.68	1.28	1.22
24	A	405	CLA	O2A-CGA	3.68	1.44	1.33
24	b	618	CLA	OBD-CAD	3.68	1.28	1.22
24	B	606	CLA	C3D-C2D	3.68	1.49	1.39
24	C	513	CLA	MG-NC	3.68	2.15	2.06
38	C	517	DGD	O1G-C1A	3.68	1.44	1.33
24	b	612	CLA	CHC-C4B	3.67	1.47	1.39
24	b	617	CLA	C3D-C2D	3.67	1.49	1.39
24	a	2109	CLA	CHD-C4C	3.67	1.47	1.39
36	I	1202	HTG	C1'-S1	-3.67	1.76	1.81
24	b	608	CLA	CHD-C4C	3.67	1.47	1.39
39	D	410	LHG	O7-C7	3.67	1.44	1.34
24	B	615	CLA	C4B-NB	-3.67	1.33	1.37
24	B	614	CLA	O2A-CGA	3.66	1.44	1.33
24	C	507	CLA	CHD-C4C	3.66	1.47	1.39
24	C	512	CLA	C4B-NB	-3.65	1.33	1.37
24	A	406	CLA	C3D-C2D	3.65	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	OBD-CAD	3.65	1.28	1.22
24	c	505	CLA	OBD-CAD	3.65	1.28	1.22
24	c	512	CLA	O2A-CGA	3.65	1.44	1.33
24	b	609	CLA	CHD-C4C	3.64	1.47	1.39
24	c	514	CLA	CHC-C4B	3.64	1.47	1.39
24	a	2110	CLA	CHD-C1D	3.63	1.45	1.38
24	b	614	CLA	C3D-C2D	3.63	1.48	1.39
24	c	508	CLA	C3D-C2D	3.63	1.48	1.39
24	c	508	CLA	CHC-C4B	3.62	1.47	1.39
24	c	506	CLA	O2A-CGA	3.62	1.43	1.33
24	B	604	CLA	C3D-C2D	3.62	1.48	1.39
24	b	612	CLA	C3D-C2D	3.62	1.48	1.39
24	D	401	CLA	CHD-C4C	3.62	1.47	1.39
24	D	404	CLA	CHD-C4C	3.62	1.47	1.39
24	b	609	CLA	C3D-C2D	3.61	1.48	1.39
24	C	514	CLA	C3D-C2D	3.61	1.48	1.39
24	C	507	CLA	C3D-C2D	3.61	1.48	1.39
24	B	602	CLA	OBD-CAD	3.61	1.28	1.22
24	c	508	CLA	OBD-CAD	3.61	1.28	1.22
24	b	619	CLA	CHC-C4B	3.61	1.47	1.39
39	l	101	LHG	O7-C7	3.60	1.44	1.34
24	B	613	CLA	MG-ND	-3.60	1.98	2.05
24	b	611	CLA	C3D-C2D	3.59	1.48	1.39
24	B	614	CLA	C3D-C2D	3.59	1.48	1.39
24	C	511	CLA	O2A-CGA	3.59	1.43	1.33
24	B	606	CLA	CHD-C4C	3.58	1.47	1.39
24	B	604	CLA	CHD-C4C	3.58	1.47	1.39
24	B	613	CLA	C3D-C2D	3.58	1.48	1.39
24	c	503	CLA	C3D-C2D	3.56	1.48	1.39
24	C	507	CLA	OBD-CAD	3.56	1.28	1.22
24	b	606	CLA	OBD-CAD	3.56	1.28	1.22
24	b	611	CLA	CHD-C4C	3.56	1.47	1.39
24	D	404	CLA	C3D-C2D	3.56	1.48	1.39
24	B	605	CLA	C3D-C2D	3.55	1.48	1.39
24	B	616	CLA	CHD-C4C	3.55	1.47	1.39
36	c	524	HTG	C1'-S1	-3.55	1.76	1.81
24	C	508	CLA	CHD-C4C	3.54	1.47	1.39
36	b	626	HTG	C1'-S1	-3.54	1.76	1.81
24	a	2109	CLA	O2A-CGA	3.54	1.43	1.33
24	a	2113	CLA	CHD-C4C	3.53	1.47	1.39
24	b	613	CLA	OBD-CAD	3.53	1.28	1.22
24	b	607	CLA	CHD-C4C	3.53	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	C3D-C2D	3.52	1.48	1.39
24	d	404	CLA	C1D-ND	3.52	1.42	1.37
24	B	611	CLA	O2A-CGA	3.52	1.43	1.33
24	C	513	CLA	OBD-CAD	3.52	1.28	1.22
24	B	605	CLA	OBD-CAD	3.52	1.28	1.22
24	C	511	CLA	OBD-CAD	3.51	1.28	1.22
24	b	607	CLA	C3D-C2D	3.51	1.48	1.39
36	B	625[B]	HTG	C1'-S1	-3.51	1.76	1.81
24	b	615	CLA	OBD-CAD	3.51	1.28	1.22
36	B	625[A]	HTG	C1'-S1	-3.51	1.76	1.81
24	B	613	CLA	C1D-ND	3.50	1.42	1.37
24	d	401	CLA	C1B-NB	-3.50	1.33	1.37
24	B	610	CLA	CHD-C4C	3.50	1.47	1.39
24	A	406	CLA	C1B-NB	-3.50	1.33	1.37
24	c	503	CLA	CHD-C4C	3.49	1.47	1.39
24	B	611	CLA	OBD-CAD	3.49	1.28	1.22
24	B	613	CLA	MG-NC	3.49	2.14	2.06
24	B	611	CLA	CHD-C4C	3.49	1.47	1.39
24	b	619	CLA	C3D-C2D	3.49	1.48	1.39
36	b	602	HTG	C1'-S1	-3.48	1.76	1.81
39	d	408	LHG	O7-C7	3.48	1.44	1.34
24	c	505	CLA	C4D-CHA	3.48	1.50	1.38
24	B	613	CLA	CHD-C4C	3.47	1.47	1.39
24	C	508	CLA	C4D-CHA	3.47	1.50	1.38
24	C	514	CLA	OBD-CAD	3.46	1.28	1.22
24	B	609	CLA	CHD-C4C	3.46	1.47	1.39
24	b	608	CLA	C3D-C2D	3.46	1.48	1.39
24	c	506	CLA	OBD-CAD	3.45	1.28	1.22
28	D	412	LMG	O7-C10	3.45	1.44	1.34
36	B	626	HTG	C1'-S1	-3.45	1.76	1.81
24	B	616	CLA	C1B-NB	-3.44	1.33	1.37
36	O	302	HTG	C1'-S1	-3.44	1.76	1.81
24	C	512	CLA	OBD-CAD	3.44	1.28	1.22
24	B	613	CLA	CHC-C4B	3.43	1.47	1.39
43	V	201	HEC	CBB-CAB	-3.43	1.36	1.49
24	b	614	CLA	OBD-CAD	3.43	1.28	1.22
36	D	413	HTG	C1'-S1	-3.43	1.76	1.81
24	b	616	CLA	OBD-CAD	3.43	1.28	1.22
24	b	607	CLA	C4D-CHA	3.42	1.50	1.38
24	B	606	CLA	OBD-CAD	3.42	1.28	1.22
24	b	619	CLA	OBD-CAD	3.42	1.28	1.22
24	C	505	CLA	OBD-CAD	3.41	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	C3D-C2D	3.41	1.48	1.39
24	B	609	CLA	OBD-CAD	3.40	1.28	1.22
24	a	2113	CLA	MG-NA	3.39	2.14	2.06
24	c	507	CLA	C3D-C2D	3.38	1.48	1.39
24	B	607	CLA	OBD-CAD	3.37	1.28	1.22
24	a	2109	CLA	C3D-C2D	3.37	1.48	1.39
39	d	409	LHG	O7-C7	3.36	1.43	1.34
24	a	2109	CLA	C1B-NB	-3.35	1.33	1.37
24	c	507	CLA	OBD-CAD	3.35	1.28	1.22
24	d	404	CLA	OBD-CAD	3.35	1.28	1.22
24	C	506	CLA	C3D-C2D	3.34	1.48	1.39
24	B	617	CLA	CHD-C4C	3.34	1.46	1.39
24	C	512	CLA	C4D-CHA	3.33	1.49	1.38
24	C	504	CLA	MG-ND	-3.33	1.99	2.05
24	B	611	CLA	C1B-NB	-3.33	1.33	1.37
36	c	526	HTG	C1'-S1	-3.32	1.76	1.81
36	d	403	HTG	C1'-S1	-3.32	1.76	1.81
24	B	608	CLA	C4D-CHA	3.32	1.49	1.38
24	d	401	CLA	MG-NB	3.31	2.12	2.05
24	B	604	CLA	OBD-CAD	3.31	1.28	1.22
39	d	409	LHG	O8-C23	3.30	1.43	1.33
24	D	401	CLA	C4B-NB	-3.30	1.33	1.37
24	b	619	CLA	C4B-NB	-3.30	1.33	1.37
24	d	401	CLA	MG-NC	3.30	2.14	2.06
24	C	504	CLA	OBD-CAD	3.29	1.28	1.22
24	b	607	CLA	OBD-CAD	3.29	1.28	1.22
24	C	508	CLA	MG-NB	-3.28	1.99	2.05
36	b	601	HTG	C1'-S1	-3.28	1.76	1.81
24	b	610	CLA	C1B-C2B	3.28	1.50	1.43
39	D	409	LHG	O7-C7	3.28	1.43	1.34
24	c	509	CLA	C4D-CHA	3.27	1.49	1.38
24	D	404	CLA	CHD-C1D	3.27	1.44	1.38
24	b	615	CLA	C1B-NB	-3.26	1.33	1.37
24	B	605	CLA	C4D-CHA	3.26	1.49	1.38
24	c	511	CLA	C4D-CHA	3.24	1.49	1.38
36	B	628	HTG	C1'-S1	-3.23	1.76	1.81
24	b	611	CLA	C1B-NB	-3.23	1.33	1.37
36	b	625	HTG	C1'-S1	-3.22	1.76	1.81
24	B	616	CLA	C4B-NB	-3.22	1.33	1.37
36	B	627	HTG	C1'-S1	-3.21	1.76	1.81
24	D	404	CLA	MG-ND	-3.21	1.99	2.05
24	b	619	CLA	C1B-C2B	3.21	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	510	CLA	C1B-NB	-3.21	1.33	1.37
24	B	617	CLA	C4D-CHA	3.21	1.49	1.38
24	b	608	CLA	OBD-CAD	3.21	1.28	1.22
24	C	513	CLA	C4D-CHA	3.20	1.49	1.38
24	d	405	CLA	C1B-NB	-3.20	1.33	1.37
24	B	607	CLA	C4D-CHA	3.19	1.49	1.38
24	C	506	CLA	C4D-CHA	3.18	1.49	1.38
24	D	401	CLA	C1B-NB	-3.18	1.33	1.37
36	C	521	HTG	C1'-S1	-3.18	1.77	1.81
24	c	506	CLA	C4D-CHA	3.17	1.49	1.38
36	d	414	HTG	C1'-S1	-3.17	1.77	1.81
24	b	609	CLA	C4D-CHA	3.17	1.49	1.38
24	a	2110	CLA	C4B-NB	-3.17	1.33	1.37
24	b	607	CLA	C1B-C2B	3.16	1.50	1.43
24	A	409	CLA	C1B-C2B	3.16	1.50	1.43
24	b	619	CLA	CHD-C4C	3.16	1.46	1.39
24	C	510	CLA	C4B-NB	-3.16	1.33	1.37
24	b	617	CLA	MG-NB	3.16	2.12	2.05
36	c	523	HTG	C1'-S1	-3.16	1.77	1.81
24	b	618	CLA	C4D-CHA	3.15	1.49	1.38
24	C	510	CLA	C4D-CHA	3.14	1.49	1.38
24	a	2110	CLA	C1B-C2B	3.14	1.50	1.43
24	B	605	CLA	C1B-C2B	3.14	1.50	1.43
24	B	611	CLA	C4D-CHA	3.14	1.49	1.38
24	b	613	CLA	C4D-CHA	3.13	1.49	1.38
24	C	511	CLA	C4D-CHA	3.13	1.49	1.38
24	b	615	CLA	CHD-C4C	3.13	1.46	1.39
24	C	503	CLA	C4D-CHA	3.12	1.49	1.38
36	V	204	HTG	C1'-S1	-3.12	1.77	1.81
24	b	610	CLA	C1B-NB	-3.12	1.33	1.37
24	B	614	CLA	C4D-CHA	3.12	1.49	1.38
24	c	514	CLA	C4D-CHA	3.12	1.49	1.38
24	B	603	CLA	C1B-NB	-3.11	1.33	1.37
24	B	615	CLA	C4D-CHA	3.11	1.49	1.38
24	C	507	CLA	C4D-CHA	3.11	1.49	1.38
24	c	508	CLA	C1B-NB	-3.10	1.33	1.37
24	b	610	CLA	OBD-CAD	3.10	1.27	1.22
24	B	609	CLA	C4D-CHA	3.10	1.49	1.38
24	B	602	CLA	C4D-CHA	3.09	1.49	1.38
24	B	612	CLA	C4D-CHA	3.09	1.49	1.38
24	b	617	CLA	C1B-NB	-3.09	1.33	1.37
24	c	512	CLA	C1B-NB	-3.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	C4D-CHA	3.09	1.49	1.38
24	b	615	CLA	C4B-NB	-3.09	1.33	1.37
40	F	102	HEM	CAB-C3B	3.08	1.55	1.47
24	D	405	CLA	C1B-C2B	3.08	1.50	1.43
24	B	608	CLA	C1B-C2B	3.08	1.50	1.43
24	a	2110	CLA	CHC-C4B	3.08	1.46	1.39
24	a	2113	CLA	C1B-C2B	3.08	1.50	1.43
24	C	506	CLA	C1B-C2B	3.07	1.50	1.43
24	a	2113	CLA	C1B-NB	-3.07	1.33	1.37
24	d	401	CLA	C1B-C2B	3.07	1.50	1.43
24	C	506	CLA	C1B-NB	-3.06	1.33	1.37
24	C	502	CLA	C4D-CHA	3.05	1.48	1.38
24	c	507	CLA	C1B-C2B	3.05	1.50	1.43
24	C	504	CLA	C4D-CHA	3.05	1.48	1.38
24	c	512	CLA	C4D-CHA	3.04	1.48	1.38
24	B	609	CLA	C1B-NB	-3.04	1.33	1.37
24	b	618	CLA	C1B-C2B	3.04	1.50	1.43
24	b	605	CLA	C4D-CHA	3.04	1.48	1.38
24	d	404	CLA	C1C-NC	-3.04	1.33	1.37
40	e	103	HEM	CAB-C3B	3.04	1.55	1.47
36	i	103	HTG	C1'-S1	-3.03	1.77	1.81
24	d	404	CLA	C1B-C2B	3.03	1.50	1.43
36	C	522	HTG	C1'-S1	-3.03	1.77	1.81
24	C	505	CLA	C4D-CHA	3.03	1.48	1.38
24	C	511	CLA	C1B-NB	-3.02	1.33	1.37
24	b	611	CLA	MG-NB	3.02	2.11	2.05
24	b	616	CLA	C1B-C2B	3.02	1.50	1.43
24	b	619	CLA	C4D-CHA	3.02	1.48	1.38
24	B	617	CLA	OBD-CAD	3.02	1.27	1.22
24	D	404	CLA	C1B-C2B	3.01	1.50	1.43
24	b	612	CLA	C1C-NC	-3.01	1.33	1.37
24	D	401	CLA	MG-NC	3.01	2.13	2.06
24	b	616	CLA	C4D-CHA	3.01	1.48	1.38
24	c	515	CLA	C4D-CHA	3.01	1.48	1.38
24	b	604	CLA	C4D-CHA	3.01	1.48	1.38
24	B	615	CLA	C1B-C2B	3.00	1.50	1.43
40	F	102	HEM	CAC-C3C	3.00	1.55	1.47
24	c	511	CLA	C1B-C2B	3.00	1.50	1.43
24	C	505	CLA	C1B-NB	-2.99	1.33	1.37
24	D	401	CLA	C4D-CHA	2.98	1.48	1.38
24	B	609	CLA	C4B-NB	-2.98	1.34	1.37
24	D	405	CLA	C4D-CHA	2.98	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	C1B-C2B	2.97	1.50	1.43
24	b	612	CLA	C4D-CHA	2.97	1.48	1.38
24	a	2110	CLA	C4D-CHA	2.97	1.48	1.38
40	e	103	HEM	CAC-C3C	2.97	1.55	1.47
24	b	614	CLA	C4D-CHA	2.96	1.48	1.38
24	b	619	CLA	C1C-NC	-2.96	1.33	1.37
24	b	608	CLA	MG-ND	-2.96	1.99	2.05
24	b	611	CLA	C4D-CHA	2.96	1.48	1.38
24	b	617	CLA	C1B-C2B	2.96	1.50	1.43
24	C	510	CLA	C1B-NB	-2.96	1.34	1.37
24	B	607	CLA	MG-NB	-2.96	1.99	2.05
24	b	619	CLA	C1B-NB	-2.95	1.34	1.37
24	A	409	CLA	MG-NA	2.95	2.13	2.06
24	d	404	CLA	C4D-CHA	2.95	1.48	1.38
24	d	405	CLA	C1B-C2B	2.95	1.50	1.43
24	b	617	CLA	OBD-CAD	2.95	1.27	1.22
24	b	610	CLA	C4D-CHA	2.95	1.48	1.38
24	c	505	CLA	C1B-C2B	2.94	1.50	1.43
24	D	404	CLA	OBD-CAD	2.94	1.27	1.22
24	b	612	CLA	C1B-C2B	2.94	1.50	1.43
24	B	610	CLA	C4D-CHA	2.94	1.48	1.38
24	B	604	CLA	C1B-C2B	2.94	1.50	1.43
24	c	509	CLA	C1B-C2B	2.94	1.50	1.43
24	d	404	CLA	C1B-NB	-2.94	1.34	1.37
24	c	512	CLA	C1B-C2B	2.94	1.50	1.43
24	B	617	CLA	C4B-NB	-2.93	1.34	1.37
24	B	606	CLA	C4D-CHA	2.93	1.48	1.38
24	a	2110	CLA	C1B-NB	-2.93	1.34	1.37
24	C	514	CLA	C4D-CHA	2.92	1.48	1.38
24	a	2113	CLA	OBD-CAD	2.92	1.27	1.22
24	B	616	CLA	C1B-C2B	2.92	1.50	1.43
24	A	409	CLA	C4D-CHA	2.92	1.48	1.38
24	c	509	CLA	C4B-NB	-2.92	1.34	1.37
24	c	513	CLA	C4D-CHA	2.92	1.48	1.38
24	A	409	CLA	MG-NB	2.91	2.11	2.05
24	c	504	CLA	C1B-C2B	2.91	1.50	1.43
24	B	608	CLA	C1B-NB	-2.91	1.34	1.37
24	a	2113	CLA	C4B-NB	-2.91	1.34	1.37
24	c	513	CLA	C1B-NB	-2.91	1.34	1.37
24	b	615	CLA	C4D-CHA	2.91	1.48	1.38
24	B	612	CLA	C1B-C2B	2.91	1.50	1.43
24	d	405	CLA	C4B-NB	-2.91	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	C4D-CHA	2.90	1.48	1.38
24	B	613	CLA	C1B-C2B	2.90	1.49	1.43
24	c	504	CLA	C1B-NB	-2.90	1.34	1.37
24	b	615	CLA	C1B-C2B	2.90	1.49	1.43
24	a	2109	CLA	C4D-CHA	2.90	1.48	1.38
24	B	616	CLA	MG-NC	2.89	2.13	2.06
24	c	504	CLA	C4D-CHA	2.88	1.48	1.38
24	c	512	CLA	C4B-NB	-2.88	1.34	1.37
24	b	609	CLA	OBD-CAD	2.88	1.27	1.22
24	c	507	CLA	C4B-NB	-2.87	1.34	1.37
24	A	405	CLA	C4D-CHA	2.87	1.48	1.38
24	B	603	CLA	C4D-CHA	2.87	1.48	1.38
24	D	404	CLA	C4D-CHA	2.86	1.48	1.38
24	C	511	CLA	C1C-C2C	2.86	1.50	1.44
24	a	2113	CLA	C4D-CHA	2.85	1.48	1.38
24	b	606	CLA	C4D-CHA	2.85	1.48	1.38
24	C	514	CLA	C1B-C2B	2.85	1.49	1.43
24	c	503	CLA	C1B-NB	-2.85	1.34	1.37
24	b	609	CLA	C1B-C2B	2.85	1.49	1.43
24	C	502	CLA	C1B-NB	-2.84	1.34	1.37
24	C	503	CLA	C4B-NB	-2.84	1.34	1.37
24	C	513	CLA	C4B-NB	-2.84	1.34	1.37
24	C	507	CLA	C1C-NC	-2.84	1.33	1.37
24	c	505	CLA	C1C-NC	-2.84	1.33	1.37
24	B	616	CLA	C4D-CHA	2.84	1.48	1.38
24	b	617	CLA	C4D-CHA	2.84	1.48	1.38
24	c	506	CLA	C4B-NB	-2.84	1.34	1.37
24	d	401	CLA	C4D-CHA	2.84	1.48	1.38
24	C	504	CLA	C1B-C2B	2.83	1.49	1.43
24	d	405	CLA	C4D-CHA	2.83	1.48	1.38
24	C	502	CLA	C1B-C2B	2.83	1.49	1.43
24	b	607	CLA	C1C-NC	-2.82	1.33	1.37
24	C	512	CLA	C1B-C2B	2.82	1.49	1.43
24	B	603	CLA	C1B-C2B	2.82	1.49	1.43
24	b	611	CLA	C4B-NB	-2.81	1.34	1.37
24	C	505	CLA	C4B-NB	-2.81	1.34	1.37
24	c	515	CLA	C1B-C2B	2.81	1.49	1.43
24	c	505	CLA	C4B-NB	-2.80	1.34	1.37
25	A	407	PHO	C4B-NB	-2.80	1.33	1.38
24	b	615	CLA	C1C-NC	-2.80	1.33	1.37
26	b	622	BCR	C30-C25	-2.80	1.50	1.53
24	a	2109	CLA	C4B-NB	-2.80	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	C1B-C2B	2.79	1.49	1.43
25	a	2112	PHO	C4B-NB	-2.79	1.33	1.38
24	c	503	CLA	C4D-CHA	2.79	1.48	1.38
24	b	605	CLA	C1B-C2B	2.79	1.49	1.43
24	C	508	CLA	C4B-NB	-2.79	1.34	1.37
24	b	614	CLA	C1B-C2B	2.78	1.49	1.43
40	F	102	HEM	FE-NB	2.77	2.03	1.94
24	b	608	CLA	C4D-CHA	2.77	1.47	1.38
24	B	610	CLA	C1B-C2B	2.77	1.49	1.43
24	B	617	CLA	C1B-C2B	2.77	1.49	1.43
24	C	508	CLA	C1B-C2B	2.77	1.49	1.43
24	B	602	CLA	MG-NB	2.76	2.11	2.05
24	c	514	CLA	C1B-C2B	2.76	1.49	1.43
24	c	508	CLA	C4D-CHA	2.76	1.47	1.38
24	b	609	CLA	C1B-NB	-2.76	1.34	1.37
24	b	616	CLA	C1B-NB	-2.76	1.34	1.37
24	b	608	CLA	C3B-C4B	2.76	1.50	1.42
31	d	407	PL9	C6-C5	2.76	1.48	1.35
24	B	602	CLA	C1B-C2B	2.76	1.49	1.43
40	e	103	HEM	FE-NA	2.75	2.04	1.95
24	C	510	CLA	C1B-C2B	2.75	1.49	1.43
24	D	401	CLA	C1B-C2B	2.75	1.49	1.43
24	b	608	CLA	C1B-NB	-2.75	1.34	1.37
24	C	504	CLA	C1C-C2C	2.75	1.50	1.44
24	a	2109	CLA	C1B-C2B	2.74	1.49	1.43
24	d	404	CLA	MG-ND	-2.74	2.00	2.05
24	B	607	CLA	C1B-NB	-2.74	1.34	1.37
24	A	409	CLA	C4C-C3C	2.73	1.49	1.45
24	B	613	CLA	C4D-CHA	2.73	1.47	1.38
24	C	513	CLA	C1B-C2B	2.73	1.49	1.43
24	A	406	CLA	C4D-CHA	2.73	1.47	1.38
24	b	606	CLA	C4B-NB	-2.73	1.34	1.37
24	B	615	CLA	C1B-NB	-2.73	1.34	1.37
24	B	604	CLA	C1C-C2C	2.73	1.50	1.44
24	B	602	CLA	C4B-NB	-2.72	1.34	1.37
24	C	505	CLA	C1C-NC	-2.72	1.33	1.37
24	d	405	CLA	C4C-C3C	2.71	1.49	1.45
24	B	614	CLA	C1B-NB	-2.71	1.34	1.37
24	c	513	CLA	C1B-C2B	2.71	1.49	1.43
24	C	506	CLA	C1C-NC	-2.71	1.33	1.37
24	d	401	CLA	C4B-NB	-2.71	1.34	1.37
24	C	509	CLA	C4D-CHA	2.71	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	C1B-NB	-2.71	1.34	1.37
24	B	607	CLA	C1B-C2B	2.70	1.49	1.43
24	c	506	CLA	C1B-C2B	2.70	1.49	1.43
24	b	605	CLA	C4C-C3C	2.70	1.49	1.45
24	b	604	CLA	C1B-C2B	2.69	1.49	1.43
24	A	409	CLA	C1B-NB	-2.69	1.34	1.37
24	C	511	CLA	C1B-C2B	2.69	1.49	1.43
24	b	614	CLA	C4B-NB	-2.69	1.34	1.37
24	A	406	CLA	MG-ND	-2.69	2.00	2.05
24	D	405	CLA	C4B-NB	-2.68	1.34	1.37
24	C	513	CLA	C1C-C2C	2.68	1.50	1.44
24	b	612	CLA	MG-NB	-2.67	2.00	2.05
24	c	514	CLA	C1B-NB	-2.67	1.34	1.37
24	C	505	CLA	C1B-C2B	2.67	1.49	1.43
38	h	703	DGD	O5D-C1E	2.67	1.44	1.40
24	c	506	CLA	C1B-NB	-2.67	1.34	1.37
24	C	513	CLA	C1B-NB	-2.66	1.34	1.37
24	c	505	CLA	C1C-C2C	2.66	1.49	1.44
31	D	407	PL9	C6-C5	2.66	1.48	1.35
24	b	609	CLA	MG-NB	2.65	2.11	2.05
36	d	403	HTG	C1-S1	-2.65	1.76	1.80
25	A	408	PHO	C3D-C4D	-2.65	1.37	1.41
24	c	511	CLA	C1C-NC	-2.65	1.33	1.37
24	b	606	CLA	C1B-C2B	2.64	1.49	1.43
24	b	605	CLA	C4B-NB	-2.64	1.34	1.37
24	B	609	CLA	C4C-C3C	2.64	1.49	1.45
24	B	617	CLA	C1C-NC	-2.64	1.33	1.37
24	c	507	CLA	C1C-C2C	2.64	1.49	1.44
24	C	511	CLA	C4B-NB	-2.63	1.34	1.37
24	A	409	CLA	C4B-NB	-2.63	1.34	1.37
24	B	609	CLA	C1B-C2B	2.63	1.49	1.43
24	B	602	CLA	C1C-C2C	2.63	1.49	1.44
24	C	509	CLA	C1B-NB	-2.62	1.34	1.37
24	B	612	CLA	C4B-NB	-2.62	1.34	1.37
24	b	616	CLA	C4B-NB	-2.62	1.34	1.37
25	a	2112	PHO	C3A-C2A	-2.62	1.52	1.54
24	B	603	CLA	C4C-C3C	2.62	1.49	1.45
43	V	201	HEC	CMC-C2C	2.62	1.56	1.50
24	B	606	CLA	C1B-NB	-2.62	1.34	1.37
24	b	608	CLA	C1B-C2B	2.61	1.49	1.43
25	A	408	PHO	C1D-ND	-2.61	1.33	1.38
24	c	514	CLA	C4C-C3C	2.61	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	604	CLA	C1B-NB	-2.61	1.34	1.37
24	b	609	CLA	C4B-NB	-2.61	1.34	1.37
24	d	404	CLA	C3D-C4D	-2.61	1.38	1.44
24	c	509	CLA	C4C-C3C	2.61	1.49	1.45
24	C	514	CLA	C1C-NC	-2.61	1.33	1.37
24	C	509	CLA	C3B-C4B	2.60	1.50	1.42
24	C	504	CLA	C1C-NC	-2.60	1.33	1.37
24	c	504	CLA	C4B-NB	-2.60	1.34	1.37
24	c	513	CLA	C4B-NB	-2.59	1.34	1.37
24	b	613	CLA	C4B-NB	-2.59	1.34	1.37
24	C	506	CLA	C4C-C3C	2.58	1.49	1.45
24	C	507	CLA	C1B-NB	-2.58	1.34	1.37
24	c	511	CLA	C1C-C2C	2.58	1.49	1.44
24	a	2113	CLA	C1C-NC	-2.58	1.33	1.37
24	b	613	CLA	C1B-C2B	2.57	1.49	1.43
31	D	407	PL9	C2-C3	2.57	1.41	1.34
25	a	2111	PHO	C4B-NB	-2.57	1.34	1.38
24	c	509	CLA	C1C-NC	-2.57	1.33	1.37
24	B	606	CLA	C3B-C4B	2.57	1.50	1.42
24	b	605	CLA	C1B-NB	-2.56	1.34	1.37
24	C	503	CLA	C3B-C2B	2.56	1.49	1.41
24	c	510	CLA	C1B-C2B	2.56	1.49	1.43
24	c	515	CLA	C4B-NB	-2.56	1.34	1.37
24	C	507	CLA	C4B-NB	-2.56	1.34	1.37
24	b	604	CLA	C1C-C2C	2.56	1.49	1.44
24	C	503	CLA	C4C-C3C	2.56	1.49	1.45
24	a	2110	CLA	C1C-NC	-2.55	1.33	1.37
24	b	608	CLA	MG-NB	2.55	2.10	2.05
24	c	511	CLA	C3B-C2B	2.55	1.49	1.41
24	D	401	CLA	C1C-C2C	2.55	1.49	1.44
24	B	609	CLA	C1C-C2C	2.55	1.49	1.44
24	D	405	CLA	C1B-NB	-2.55	1.34	1.37
24	c	515	CLA	C1C-C2C	2.54	1.49	1.44
24	c	507	CLA	C1C-NC	-2.54	1.33	1.37
24	B	611	CLA	C4B-NB	-2.54	1.34	1.37
24	C	509	CLA	C4B-NB	-2.54	1.34	1.37
24	A	405	CLA	C4C-C3C	2.54	1.49	1.45
24	c	503	CLA	C1B-C2B	2.53	1.49	1.43
24	c	510	CLA	C4D-CHA	2.53	1.47	1.38
24	B	613	CLA	C1C-C2C	2.53	1.49	1.44
24	b	608	CLA	C1C-C2C	2.53	1.49	1.44
24	c	510	CLA	C1C-C2C	2.53	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	C4C-C3C	2.53	1.49	1.45
24	c	511	CLA	C1B-NB	-2.52	1.34	1.37
24	b	611	CLA	C1B-C2B	2.52	1.49	1.43
24	b	610	CLA	C4B-NB	-2.52	1.34	1.37
24	B	611	CLA	C1C-C2C	2.51	1.49	1.44
24	b	618	CLA	C1B-NB	-2.51	1.34	1.37
24	b	612	CLA	C4B-NB	-2.51	1.34	1.37
24	b	604	CLA	MG-ND	-2.51	2.00	2.05
24	B	614	CLA	C4B-NB	-2.51	1.34	1.37
24	b	606	CLA	C4C-C3C	2.51	1.49	1.45
24	b	616	CLA	C1C-NC	-2.50	1.34	1.37
24	B	611	CLA	C1B-C2B	2.50	1.49	1.43
24	A	405	CLA	C1C-C2C	2.50	1.49	1.44
24	B	604	CLA	C1B-NB	-2.50	1.34	1.37
26	d	406	BCR	C30-C25	-2.50	1.50	1.53
24	d	405	CLA	C1C-C2C	2.50	1.49	1.44
24	B	606	CLA	C1C-C2C	2.50	1.49	1.44
24	c	508	CLA	C1B-C2B	2.50	1.49	1.43
24	b	605	CLA	C1C-C2C	2.50	1.49	1.44
43	v	201	HEC	CMC-C2C	2.50	1.55	1.50
27	B	621	SQD	O6-C1	2.49	1.44	1.40
24	b	605	CLA	C1C-NC	-2.49	1.34	1.37
24	C	503	CLA	C1C-C2C	2.49	1.49	1.44
36	c	526	HTG	C1-S1	-2.48	1.76	1.80
24	c	507	CLA	C4C-C3C	2.48	1.49	1.45
24	c	512	CLA	MG-NB	2.47	2.10	2.05
24	C	505	CLA	C3B-C2B	2.47	1.49	1.41
24	b	615	CLA	C1C-C2C	2.47	1.49	1.44
24	b	616	CLA	C1C-C2C	2.47	1.49	1.44
24	B	611	CLA	MG-NB	2.47	2.10	2.05
24	b	604	CLA	C3B-C4B	2.47	1.49	1.42
24	C	509	CLA	C1B-C2B	2.47	1.48	1.43
24	a	2113	CLA	C3B-C4B	2.47	1.49	1.42
24	C	512	CLA	C1B-NB	-2.47	1.34	1.37
24	c	508	CLA	C1C-NC	-2.47	1.34	1.37
24	b	604	CLA	C1C-NC	-2.47	1.34	1.37
24	b	618	CLA	C3B-C4B	2.46	1.49	1.42
24	A	406	CLA	C3B-C4B	2.46	1.49	1.42
24	b	616	CLA	C4C-C3C	2.46	1.49	1.45
24	b	607	CLA	C4B-NB	-2.46	1.34	1.37
24	b	614	CLA	C3B-C2B	2.46	1.49	1.41
25	A	408	PHO	C4B-NB	-2.46	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	404	CLA	MG-NB	-2.46	2.00	2.05
24	B	610	CLA	C1C-NC	-2.46	1.34	1.37
24	C	507	CLA	C1C-C2C	2.46	1.49	1.44
24	b	617	CLA	C1C-C2C	2.46	1.49	1.44
38	H	102	DGD	O5D-C1E	2.45	1.44	1.40
24	b	606	CLA	C1C-C2C	2.45	1.49	1.44
24	c	510	CLA	C3B-C4B	2.45	1.49	1.42
24	C	504	CLA	C4B-NB	-2.45	1.34	1.37
24	c	505	CLA	C4C-C3C	2.45	1.49	1.45
24	b	610	CLA	C1C-C2C	2.44	1.49	1.44
24	b	605	CLA	C3B-C2B	2.44	1.49	1.41
24	C	502	CLA	C1C-C2C	2.44	1.49	1.44
24	c	503	CLA	C4B-NB	-2.44	1.34	1.37
24	C	502	CLA	C1C-NC	-2.44	1.34	1.37
24	C	510	CLA	C4C-C3C	2.44	1.49	1.45
24	c	503	CLA	MG-NB	2.43	2.10	2.05
24	B	613	CLA	C4B-NB	-2.43	1.34	1.37
24	B	604	CLA	C4B-NB	-2.43	1.34	1.37
24	c	511	CLA	C4B-NB	-2.42	1.34	1.37
24	c	510	CLA	C3B-C2B	2.42	1.49	1.41
24	B	614	CLA	C1B-C2B	2.42	1.48	1.43
24	a	2109	CLA	C1C-C2C	2.42	1.49	1.44
24	C	508	CLA	C1C-NC	-2.42	1.34	1.37
24	A	405	CLA	C3B-C2B	2.42	1.49	1.41
24	C	512	CLA	C3B-C2B	2.42	1.49	1.41
24	d	404	CLA	C4B-NB	-2.42	1.34	1.37
25	A	407	PHO	CBD-CGD	-2.42	1.49	1.52
24	A	406	CLA	C1B-C2B	2.42	1.48	1.43
24	D	404	CLA	C1C-C2C	2.42	1.49	1.44
24	b	618	CLA	C1C-C2C	2.42	1.49	1.44
24	b	615	CLA	C3B-C2B	2.41	1.49	1.41
24	A	409	CLA	C3B-C2B	2.41	1.49	1.41
24	B	611	CLA	C3B-C4B	2.41	1.49	1.42
24	b	610	CLA	C3B-C4B	2.41	1.49	1.42
24	c	514	CLA	C4B-NB	-2.40	1.34	1.37
43	v	201	HEC	CMD-C2D	2.40	1.55	1.50
24	c	515	CLA	C1C-NC	-2.40	1.34	1.37
24	b	619	CLA	C3B-C2B	2.40	1.49	1.41
24	c	505	CLA	C1B-NB	-2.40	1.34	1.37
24	c	515	CLA	C1B-NB	-2.40	1.34	1.37
24	C	514	CLA	C3B-C2B	2.40	1.49	1.41
24	b	616	CLA	C3B-C2B	2.40	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	MG-NB	2.40	2.10	2.05
38	c	520	DGD	O2G-C2G	-2.39	1.41	1.46
24	B	602	CLA	C3B-C4B	2.39	1.49	1.42
24	b	607	CLA	C4C-C3C	2.39	1.49	1.45
24	B	611	CLA	C4C-C3C	2.39	1.49	1.45
24	B	614	CLA	C3B-C2B	2.39	1.49	1.41
24	B	609	CLA	MG-NB	2.39	2.10	2.05
24	c	515	CLA	C3B-C2B	2.38	1.49	1.41
24	C	508	CLA	C3B-C2B	2.38	1.49	1.41
24	C	506	CLA	C4B-NB	-2.38	1.34	1.37
24	b	609	CLA	C3B-C2B	2.38	1.49	1.41
24	B	604	CLA	C4C-C3C	2.38	1.49	1.45
24	c	506	CLA	MG-NC	2.38	2.11	2.06
24	B	609	CLA	C1C-NC	-2.38	1.34	1.37
32	a	2119	K2I	C-C5	-2.38	1.38	1.44
24	B	606	CLA	C4B-NB	-2.37	1.34	1.37
24	C	509	CLA	C3B-C2B	2.37	1.49	1.41
24	b	613	CLA	C3B-C2B	2.37	1.49	1.41
24	c	514	CLA	C3B-C2B	2.37	1.49	1.41
24	b	614	CLA	C4C-C3C	2.37	1.49	1.45
24	a	2109	CLA	C1C-NC	-2.37	1.34	1.37
24	b	611	CLA	C1C-NC	-2.37	1.34	1.37
29	j	1601	LMT	O1'-C1'	2.36	1.44	1.40
29	A	420	LMT	O1'-C1'	2.36	1.44	1.40
24	C	514	CLA	C1C-C2C	2.36	1.49	1.44
24	a	2109	CLA	C3B-C2B	2.36	1.49	1.41
24	B	602	CLA	C1C-NC	-2.36	1.34	1.37
24	c	508	CLA	C4B-NB	-2.36	1.34	1.37
24	B	606	CLA	C1C-NC	-2.36	1.34	1.37
24	C	508	CLA	C1C-C2C	2.35	1.49	1.44
24	B	605	CLA	C3B-C4B	2.35	1.49	1.42
24	A	405	CLA	C4B-NB	-2.35	1.34	1.37
36	B	627	HTG	C1-S1	-2.35	1.76	1.80
24	C	510	CLA	C1C-NC	-2.35	1.34	1.37
24	b	617	CLA	C4B-NB	-2.35	1.34	1.37
24	C	503	CLA	MG-NB	2.35	2.10	2.05
24	B	604	CLA	C1C-NC	-2.34	1.34	1.37
24	b	607	CLA	C1C-C2C	2.34	1.49	1.44
24	b	609	CLA	C1C-C2C	2.34	1.49	1.44
24	B	603	CLA	C1C-C2C	2.34	1.49	1.44
24	a	2113	CLA	C3B-C2B	2.34	1.49	1.41
24	a	2110	CLA	C4C-C3C	2.33	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	C4C-C3C	2.33	1.49	1.45
24	B	612	CLA	C1B-NB	-2.33	1.34	1.37
24	C	512	CLA	C1C-C2C	2.33	1.49	1.44
24	c	508	CLA	C3D-C4D	-2.33	1.38	1.44
24	B	607	CLA	C4B-NB	-2.33	1.34	1.37
24	a	2109	CLA	C4C-C3C	2.33	1.49	1.45
24	c	512	CLA	C1C-NC	-2.33	1.34	1.37
24	B	610	CLA	C1B-NB	-2.33	1.34	1.37
40	e	103	HEM	CMC-C2C	2.33	1.55	1.50
24	D	405	CLA	C1C-NC	-2.33	1.34	1.37
25	A	407	PHO	C1D-ND	-2.32	1.34	1.38
24	d	405	CLA	C3B-C2B	2.32	1.49	1.41
24	b	605	CLA	C3B-C4B	2.32	1.49	1.42
24	d	404	CLA	C3B-C2B	2.32	1.49	1.41
26	D	406	BCR	C30-C25	-2.32	1.50	1.53
24	C	514	CLA	C4B-NB	-2.32	1.34	1.37
24	B	605	CLA	C1C-C2C	2.32	1.49	1.44
36	b	602	HTG	C1-S1	-2.32	1.76	1.80
24	c	508	CLA	C3B-C2B	2.32	1.49	1.41
24	c	503	CLA	C1C-C2C	2.31	1.49	1.44
24	B	617	CLA	C3B-C2B	2.31	1.49	1.41
24	B	614	CLA	C1C-C2C	2.31	1.49	1.44
24	C	510	CLA	C1C-C2C	2.31	1.49	1.44
24	A	405	CLA	C1B-C2B	2.31	1.48	1.43
24	A	406	CLA	C4B-NB	-2.31	1.34	1.37
24	b	606	CLA	C1C-NC	-2.31	1.34	1.37
24	c	515	CLA	C4C-C3C	2.31	1.49	1.45
24	b	610	CLA	C3D-C4D	-2.30	1.39	1.44
24	c	504	CLA	C3D-C4D	-2.30	1.39	1.44
24	b	617	CLA	C4C-C3C	2.30	1.48	1.45
24	B	603	CLA	C4B-NB	-2.30	1.34	1.37
24	b	614	CLA	C3D-C4D	-2.30	1.39	1.44
24	c	507	CLA	C3B-C2B	2.30	1.48	1.41
24	c	509	CLA	C3B-C2B	2.29	1.48	1.41
24	b	611	CLA	C1C-C2C	2.29	1.49	1.44
24	b	613	CLA	C3B-C4B	2.29	1.49	1.42
24	b	608	CLA	C4B-NB	-2.29	1.34	1.37
24	C	514	CLA	C3B-C4B	2.29	1.49	1.42
24	c	503	CLA	C3B-C2B	2.29	1.48	1.41
24	c	503	CLA	C1C-NC	-2.28	1.34	1.37
24	C	502	CLA	C3B-C4B	2.28	1.49	1.42
24	c	507	CLA	C1B-NB	-2.28	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	C1B-C2B	2.28	1.48	1.43
24	b	614	CLA	C3B-C4B	2.28	1.49	1.42
24	C	506	CLA	C1C-C2C	2.28	1.49	1.44
24	A	406	CLA	C3D-C4D	-2.28	1.39	1.44
24	B	616	CLA	C1C-NC	-2.28	1.34	1.37
24	B	602	CLA	C1B-NB	-2.28	1.34	1.37
24	C	513	CLA	C3B-C4B	2.27	1.49	1.42
24	b	619	CLA	C3D-C4D	-2.27	1.39	1.44
24	c	509	CLA	C1C-C2C	2.27	1.49	1.44
36	b	601	HTG	C1-S1	-2.27	1.76	1.80
24	B	608	CLA	C3B-C2B	2.27	1.48	1.41
24	c	506	CLA	C1C-C2C	2.27	1.49	1.44
24	C	504	CLA	C3B-C2B	2.27	1.48	1.41
24	C	512	CLA	C4C-C3C	2.27	1.48	1.45
24	b	611	CLA	C3B-C2B	2.26	1.48	1.41
24	c	510	CLA	C4B-NB	-2.26	1.34	1.37
24	C	509	CLA	C1C-C2C	2.26	1.49	1.44
24	b	613	CLA	C1C-C2C	2.26	1.49	1.44
24	b	610	CLA	C3B-C2B	2.25	1.48	1.41
24	C	511	CLA	C1C-NC	-2.25	1.34	1.37
24	A	409	CLA	C1C-C2C	2.25	1.49	1.44
24	D	404	CLA	C3B-C2B	2.25	1.48	1.41
24	C	513	CLA	C3B-C2B	2.25	1.48	1.41
24	d	405	CLA	C1D-C2D	2.25	1.49	1.45
24	C	504	CLA	C1B-NB	-2.25	1.34	1.37
24	c	514	CLA	C1C-C2C	2.25	1.49	1.44
24	B	613	CLA	C1C-NC	-2.25	1.34	1.37
24	A	406	CLA	C1C-C2C	2.24	1.49	1.44
24	C	511	CLA	C4C-C3C	2.24	1.48	1.45
24	D	404	CLA	C3D-C4D	-2.24	1.39	1.44
24	d	404	CLA	C4C-C3C	2.24	1.48	1.45
24	B	613	CLA	C3D-C4D	-2.24	1.39	1.44
24	B	613	CLA	C4C-C3C	2.24	1.48	1.45
24	b	617	CLA	C3B-C2B	2.24	1.48	1.41
24	D	405	CLA	C3B-C2B	2.24	1.48	1.41
24	B	604	CLA	C3D-C4D	-2.24	1.39	1.44
24	b	609	CLA	C3B-C4B	2.24	1.49	1.42
24	C	509	CLA	C1C-NC	-2.24	1.34	1.37
24	B	607	CLA	C1C-C2C	2.24	1.49	1.44
24	B	605	CLA	C3B-C2B	2.24	1.48	1.41
24	D	401	CLA	C4C-C3C	2.24	1.48	1.45
24	c	504	CLA	C3B-C4B	2.23	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C4C-C3C	2.23	1.48	1.45
24	B	602	CLA	C3B-C2B	2.23	1.48	1.41
24	D	404	CLA	C1B-NB	-2.23	1.34	1.37
24	B	602	CLA	C4C-C3C	2.23	1.48	1.45
24	C	511	CLA	C3B-C2B	2.23	1.48	1.41
24	b	606	CLA	C3D-C4D	-2.23	1.39	1.44
24	B	612	CLA	C3B-C2B	2.23	1.48	1.41
24	C	503	CLA	C1B-NB	-2.23	1.34	1.37
24	b	612	CLA	C1D-C2D	2.22	1.49	1.45
24	b	606	CLA	C3B-C4B	2.22	1.49	1.42
24	D	401	CLA	C3B-C2B	2.22	1.48	1.41
29	f	101	LMT	O1'-C1'	2.22	1.43	1.40
24	c	513	CLA	C3B-C2B	2.22	1.48	1.41
24	b	611	CLA	C3B-C4B	2.22	1.49	1.42
24	d	401	CLA	C3B-C2B	2.22	1.48	1.41
24	C	502	CLA	C3D-C4D	-2.22	1.39	1.44
24	C	510	CLA	C3D-C4D	-2.22	1.39	1.44
40	F	102	HEM	FE-NA	2.22	2.02	1.95
24	B	605	CLA	C1C-NC	-2.22	1.34	1.37
24	b	612	CLA	C1B-NB	-2.21	1.35	1.37
24	B	612	CLA	C3B-C4B	2.21	1.49	1.42
32	a	2118[B]	K2I	C3-C2	-2.21	1.38	1.44
24	B	606	CLA	C4C-C3C	2.21	1.48	1.45
24	C	511	CLA	C3D-C4D	-2.21	1.39	1.44
24	b	607	CLA	C3B-C2B	2.21	1.48	1.41
24	c	512	CLA	C3B-C4B	2.21	1.49	1.42
24	C	505	CLA	C1C-C2C	2.21	1.49	1.44
36	b	626	HTG	C1-S1	-2.21	1.77	1.80
24	C	506	CLA	C3B-C2B	2.20	1.48	1.41
24	b	614	CLA	C1C-C2C	2.20	1.49	1.44
32	A	418[B]	K2I	C3-C2	-2.20	1.39	1.44
24	D	405	CLA	C3B-C4B	2.20	1.49	1.42
24	b	617	CLA	C3D-C4D	-2.20	1.39	1.44
24	C	502	CLA	C4B-NB	-2.20	1.35	1.37
24	B	604	CLA	C3B-C4B	2.20	1.49	1.42
24	C	512	CLA	C3B-C4B	2.19	1.49	1.42
24	b	605	CLA	C3D-C4D	-2.19	1.39	1.44
24	b	604	CLA	C3B-C2B	2.19	1.48	1.41
24	B	608	CLA	C4B-NB	-2.19	1.35	1.37
24	D	405	CLA	C1C-C2C	2.19	1.49	1.44
24	c	505	CLA	C3B-C2B	2.19	1.48	1.41
32	a	2119	K2I	C3-C2	-2.19	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	C3B-C4B	2.19	1.49	1.42
24	c	504	CLA	C1C-C2C	2.19	1.49	1.44
24	c	515	CLA	C3D-C4D	-2.18	1.39	1.44
24	c	513	CLA	C1C-C2C	2.18	1.48	1.44
24	c	504	CLA	C1C-NC	-2.18	1.34	1.37
24	B	615	CLA	MG-NC	2.18	2.11	2.06
24	C	510	CLA	C3B-C2B	2.18	1.48	1.41
24	b	618	CLA	C1C-NC	-2.18	1.34	1.37
24	B	615	CLA	C3D-C4D	-2.18	1.39	1.44
24	b	613	CLA	C3D-C4D	-2.18	1.39	1.44
24	b	609	CLA	C4C-C3C	2.17	1.48	1.45
24	c	506	CLA	C3B-C2B	2.17	1.48	1.41
24	B	603	CLA	C3B-C2B	2.17	1.48	1.41
24	B	610	CLA	C1C-C2C	2.17	1.48	1.44
24	b	604	CLA	C4B-NB	-2.17	1.35	1.37
24	B	607	CLA	C3D-C4D	-2.17	1.39	1.44
24	b	608	CLA	C3B-C2B	2.17	1.48	1.41
24	B	604	CLA	C3B-C2B	2.17	1.48	1.41
24	c	514	CLA	C3D-C4D	-2.16	1.39	1.44
24	b	610	CLA	C4C-C3C	2.16	1.48	1.45
24	b	606	CLA	C3B-C2B	2.16	1.48	1.41
25	a	2112	PHO	CHA-CBD	-2.16	1.49	1.51
36	C	521	HTG	C1-S1	-2.16	1.77	1.80
24	c	513	CLA	C3B-C4B	2.15	1.49	1.42
24	c	504	CLA	C3B-C2B	2.15	1.48	1.41
24	B	615	CLA	C4C-C3C	2.15	1.48	1.45
24	B	605	CLA	C1B-NB	-2.15	1.35	1.37
24	C	507	CLA	C3D-C4D	-2.15	1.39	1.44
24	B	617	CLA	C3D-C4D	-2.15	1.39	1.44
24	B	611	CLA	C1C-NC	-2.14	1.34	1.37
24	B	607	CLA	C4C-C3C	2.14	1.48	1.45
24	b	618	CLA	MG-ND	-2.14	2.01	2.05
24	B	612	CLA	C3D-C4D	-2.14	1.39	1.44
24	B	605	CLA	C4B-NB	-2.14	1.35	1.37
26	A	410	BCR	C30-C25	-2.14	1.51	1.53
24	b	604	CLA	C3D-C4D	-2.14	1.39	1.44
24	B	612	CLA	C4C-C3C	2.14	1.48	1.45
24	c	508	CLA	C4C-C3C	2.14	1.48	1.45
24	b	618	CLA	C3B-C2B	2.14	1.48	1.41
24	C	502	CLA	C4C-C3C	2.14	1.48	1.45
24	a	2110	CLA	C3B-C2B	2.14	1.48	1.41
24	C	506	CLA	C3D-C4D	-2.13	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	511	CLA	C4C-C3C	2.13	1.48	1.45
40	e	103	HEM	FE-NC	2.13	2.02	1.95
24	A	405	CLA	C1C-NC	-2.13	1.34	1.37
24	a	2113	CLA	C1C-C2C	2.13	1.48	1.44
24	C	505	CLA	C3D-C4D	-2.13	1.39	1.44
24	D	401	CLA	C3B-C4B	2.13	1.48	1.42
24	D	405	CLA	C4C-C3C	2.12	1.48	1.45
24	c	507	CLA	C3B-C4B	2.12	1.48	1.42
24	B	608	CLA	C3B-C4B	2.12	1.48	1.42
24	C	514	CLA	C3D-C4D	-2.12	1.39	1.44
40	F	102	HEM	CMB-C2B	2.12	1.55	1.50
36	c	524	HTG	C1-S1	-2.12	1.77	1.80
24	c	512	CLA	C3B-C2B	2.12	1.48	1.41
36	I	1202	HTG	C1-S1	-2.12	1.77	1.80
24	D	401	CLA	C1C-NC	-2.12	1.34	1.37
24	B	607	CLA	C3B-C2B	2.12	1.48	1.41
24	B	609	CLA	C3B-C2B	2.12	1.48	1.41
24	A	406	CLA	C1C-NC	-2.12	1.34	1.37
24	C	512	CLA	MG-NC	2.11	2.11	2.06
43	v	201	HEC	CMB-C2B	2.11	1.55	1.50
24	c	513	CLA	C1C-NC	-2.11	1.34	1.37
25	A	408	PHO	CBD-CGD	-2.11	1.49	1.52
40	e	103	HEM	CMA-C3A	2.11	1.55	1.50
32	a	2118[A]	K2I	C-C5	-2.11	1.39	1.44
24	B	613	CLA	C3B-C2B	2.11	1.48	1.41
38	C	517	DGD	O5D-C1E	2.11	1.43	1.40
24	d	401	CLA	C1C-C2C	2.11	1.48	1.44
24	B	609	CLA	C3B-C4B	2.10	1.48	1.42
29	i	104	LMT	O1'-C1'	2.10	1.43	1.40
24	C	512	CLA	C1C-NC	-2.10	1.34	1.37
32	A	419	K2I	C-C5	-2.10	1.39	1.44
24	b	612	CLA	C3D-C4D	-2.10	1.39	1.44
24	c	509	CLA	C1B-NB	-2.10	1.35	1.37
40	e	103	HEM	CMB-C2B	2.10	1.55	1.50
24	B	603	CLA	C3D-C4D	-2.10	1.39	1.44
24	B	616	CLA	C3B-C4B	2.09	1.48	1.42
24	b	612	CLA	C4C-C3C	2.09	1.48	1.45
24	C	503	CLA	C3B-C4B	2.09	1.48	1.42
24	C	508	CLA	C4C-C3C	2.09	1.48	1.45
24	C	511	CLA	C3B-C4B	2.09	1.48	1.42
24	C	505	CLA	C3B-C4B	2.08	1.48	1.42
24	B	602	CLA	C3D-C4D	-2.08	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	506	CLA	C1C-NC	-2.08	1.34	1.37
29	E	105	LMT	O1'-C1'	2.08	1.43	1.40
24	b	604	CLA	C4C-C3C	2.08	1.48	1.45
24	B	610	CLA	C3D-C4D	-2.08	1.39	1.44
24	C	510	CLA	C3B-C4B	2.08	1.48	1.42
24	b	609	CLA	C1C-NC	-2.08	1.34	1.37
24	A	409	CLA	C3B-C4B	2.08	1.48	1.42
24	c	515	CLA	C3B-C4B	2.08	1.48	1.42
36	d	414	HTG	C1-S1	-2.07	1.77	1.80
24	B	609	CLA	C3D-C4D	-2.07	1.39	1.44
32	A	418[B]	K2I	C-C5	-2.07	1.39	1.44
24	C	505	CLA	C4C-C3C	2.07	1.48	1.45
36	D	413	HTG	C1-S1	-2.07	1.77	1.80
32	A	418[A]	K2I	C-C5	-2.06	1.39	1.44
24	B	603	CLA	C3B-C4B	2.06	1.48	1.42
32	A	418[A]	K2I	C3-C2	-2.06	1.39	1.44
24	A	406	CLA	C4C-C3C	2.06	1.48	1.45
24	B	610	CLA	C3B-C2B	2.05	1.48	1.41
24	B	611	CLA	C3B-C2B	2.05	1.48	1.41
25	A	407	PHO	CHA-CBD	-2.05	1.49	1.51
43	V	201	HEC	CMA-C3A	2.05	1.55	1.50
24	c	508	CLA	C1C-C2C	2.05	1.48	1.44
24	b	611	CLA	C3D-C4D	-2.05	1.39	1.44
24	B	615	CLA	C3B-C2B	2.04	1.48	1.41
24	B	613	CLA	C3B-C4B	2.04	1.48	1.42
24	b	608	CLA	C1C-NC	-2.04	1.34	1.37
24	b	614	CLA	C1C-NC	-2.04	1.34	1.37
24	C	503	CLA	C1C-NC	-2.04	1.34	1.37
24	D	404	CLA	C3B-C4B	2.04	1.48	1.42
24	b	609	CLA	C3D-C4D	-2.04	1.39	1.44
24	B	608	CLA	C1C-C2C	2.04	1.48	1.44
24	D	405	CLA	C3D-C4D	-2.03	1.39	1.44
24	C	502	CLA	C3B-C2B	2.03	1.48	1.41
24	b	608	CLA	C3D-C4D	-2.03	1.39	1.44
24	B	617	CLA	C1C-C2C	2.03	1.48	1.44
24	b	611	CLA	C4C-C3C	2.03	1.48	1.45
39	D	410	LHG	O7-C5	-2.03	1.41	1.46
26	B	619	BCR	C19-C18	2.03	1.50	1.46
24	c	511	CLA	C3B-C4B	2.03	1.48	1.42
39	L	101	LHG	O7-C5	-2.02	1.41	1.46
24	b	616	CLA	C3B-C4B	2.02	1.48	1.42
24	c	514	CLA	C1C-NC	-2.02	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C1C-NC	-2.02	1.34	1.37
24	d	405	CLA	C3B-C4B	2.02	1.48	1.42
24	c	513	CLA	C1A-CHA	2.01	1.51	1.43
24	B	606	CLA	C3B-C2B	2.01	1.47	1.41
24	c	505	CLA	C1A-CHA	2.01	1.51	1.43
40	F	102	HEM	CMC-C2C	2.00	1.54	1.50
24	a	2109	CLA	C3D-C4D	-2.00	1.39	1.44
24	c	511	CLA	C3D-C4D	-2.00	1.39	1.44
24	b	613	CLA	C4C-C3C	2.00	1.48	1.45
24	C	514	CLA	C1B-NB	-2.00	1.35	1.37
24	b	619	CLA	C1C-C2C	2.00	1.48	1.44

All (2654) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	407	PHO	C2D-C1D-ND	12.10	118.17	109.43
25	A	408	PHO	C2D-C1D-ND	12.05	118.14	109.43
25	a	2111	PHO	C2D-C1D-ND	11.51	117.75	109.43
24	c	503	CLA	C1D-ND-C4D	-10.98	98.61	106.31
24	D	404	CLA	C1D-ND-C4D	-10.66	98.83	106.31
24	a	2110	CLA	C1D-ND-C4D	-10.54	98.92	106.31
24	b	615	CLA	C1D-ND-C4D	-10.23	99.14	106.31
24	c	510	CLA	C1D-ND-C4D	-10.10	99.23	106.31
25	a	2112	PHO	C2D-C1D-ND	10.09	116.72	109.43
24	a	2109	CLA	C1D-ND-C4D	-10.08	99.24	106.31
24	b	608	CLA	C1D-ND-C4D	-9.99	99.30	106.31
24	B	612	CLA	C1D-ND-C4D	-9.93	99.34	106.31
24	D	401	CLA	C1D-ND-C4D	-9.93	99.35	106.31
24	d	401	CLA	C1D-ND-C4D	-9.88	99.38	106.31
24	B	613	CLA	C1D-ND-C4D	-9.87	99.38	106.31
24	B	606	CLA	C1D-ND-C4D	-9.87	99.39	106.31
24	b	611	CLA	C1D-ND-C4D	-9.77	99.46	106.31
24	a	2113	CLA	C1D-ND-C4D	-9.61	99.57	106.31
24	B	616	CLA	C1D-ND-C4D	-9.55	99.61	106.31
24	C	509	CLA	C1D-ND-C4D	-9.50	99.64	106.31
24	C	514	CLA	C1D-ND-C4D	-9.46	99.67	106.31
24	B	614	CLA	C1D-ND-C4D	-9.44	99.69	106.31
24	B	610	CLA	C1D-ND-C4D	-9.43	99.70	106.31
24	B	604	CLA	C1D-ND-C4D	-9.36	99.74	106.31
24	c	504	CLA	C1D-ND-C4D	-9.36	99.74	106.31
24	B	615	CLA	C1D-ND-C4D	-9.33	99.76	106.31
24	d	405	CLA	C1D-ND-C4D	-9.33	99.77	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	506	CLA	C1D-ND-C4D	-9.31	99.78	106.31
24	c	508	CLA	C1D-ND-C4D	-9.31	99.78	106.31
24	A	409	CLA	C1D-ND-C4D	-9.29	99.79	106.31
24	b	614	CLA	C1D-ND-C4D	-9.23	99.84	106.31
24	B	609	CLA	C1D-ND-C4D	-9.20	99.86	106.31
24	b	619	CLA	C1D-ND-C4D	-9.17	99.88	106.31
24	C	511	CLA	C1D-ND-C4D	-9.13	99.91	106.31
24	C	507	CLA	C1D-ND-C4D	-9.12	99.91	106.31
24	A	406	CLA	C1D-ND-C4D	-9.12	99.91	106.31
24	b	617	CLA	C1D-ND-C4D	-9.07	99.95	106.31
24	b	616	CLA	C1D-ND-C4D	-9.02	99.98	106.31
24	c	512	CLA	C1D-ND-C4D	-9.02	99.99	106.31
25	a	2112	PHO	O2D-CGD-CBD	8.99	120.82	110.95
24	C	503	CLA	C1D-ND-C4D	-8.98	100.01	106.31
24	D	405	CLA	C1D-ND-C4D	-8.97	100.02	106.31
24	A	405	CLA	C1D-ND-C4D	-8.94	100.04	106.31
24	B	617	CLA	C1D-ND-C4D	-8.93	100.05	106.31
24	B	603	CLA	C1D-ND-C4D	-8.92	100.05	106.31
24	c	507	CLA	C1D-ND-C4D	-8.92	100.06	106.31
24	C	513	CLA	C1D-ND-C4D	-8.88	100.08	106.31
24	b	606	CLA	C1D-ND-C4D	-8.87	100.09	106.31
25	a	2111	PHO	O2D-CGD-CBD	8.86	120.68	110.95
24	b	610	CLA	C1D-ND-C4D	-8.83	100.11	106.31
24	B	607	CLA	C1D-ND-C4D	-8.82	100.12	106.31
24	C	502	CLA	C1D-ND-C4D	-8.81	100.13	106.31
24	c	511	CLA	C1D-ND-C4D	-8.81	100.13	106.31
24	C	512	CLA	C1D-ND-C4D	-8.81	100.13	106.31
24	C	510	CLA	C1D-ND-C4D	-8.78	100.15	106.31
24	b	613	CLA	C1D-ND-C4D	-8.77	100.16	106.31
24	c	515	CLA	C1D-ND-C4D	-8.77	100.16	106.31
24	B	605	CLA	C1D-ND-C4D	-8.70	100.21	106.31
24	c	514	CLA	C1D-ND-C4D	-8.70	100.21	106.31
24	b	607	CLA	C1D-ND-C4D	-8.65	100.24	106.31
24	b	612	CLA	C1D-ND-C4D	-8.64	100.25	106.31
25	A	407	PHO	C3B-C4B-NB	8.61	113.08	107.46
24	B	602	CLA	C1D-ND-C4D	-8.57	100.30	106.31
24	c	509	CLA	C1D-ND-C4D	-8.56	100.30	106.31
25	a	2112	PHO	C3B-C4B-NB	8.52	113.02	107.46
24	C	505	CLA	C1D-ND-C4D	-8.51	100.34	106.31
24	B	608	CLA	C1D-ND-C4D	-8.44	100.39	106.31
24	b	609	CLA	C1D-ND-C4D	-8.38	100.43	106.31
24	b	618	CLA	C1D-ND-C4D	-8.34	100.46	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	CLA	C1D-ND-C4D	-8.30	100.49	106.31
24	b	605	CLA	C1D-ND-C4D	-8.29	100.49	106.31
24	d	404	CLA	C1D-ND-C4D	-8.28	100.50	106.31
24	b	604	CLA	C1D-ND-C4D	-8.26	100.52	106.31
24	B	611	CLA	C1D-ND-C4D	-8.09	100.64	106.31
24	C	504	CLA	C1D-ND-C4D	-7.96	100.73	106.31
24	c	505	CLA	C1D-ND-C4D	-7.91	100.76	106.31
24	C	508	CLA	C1D-ND-C4D	-7.84	100.81	106.31
24	C	506	CLA	C1D-ND-C4D	-7.81	100.83	106.31
25	A	408	PHO	O2D-CGD-CBD	7.60	119.29	110.95
25	a	2112	PHO	C2B-C1B-NB	7.55	114.89	109.43
25	A	408	PHO	C3B-C4B-NB	7.48	112.34	107.46
24	C	507	CLA	C1-C2-C3	-7.27	114.28	126.20
24	c	509	CLA	O2D-CGD-CBD	7.27	123.93	111.23
24	D	404	CLA	C2D-C1D-ND	7.12	117.17	110.13
24	c	503	CLA	C2D-C1D-ND	7.08	117.13	110.13
24	D	401	CLA	C2D-C1D-ND	7.03	117.08	110.13
24	a	2110	CLA	C2D-C1D-ND	6.98	117.03	110.13
24	b	615	CLA	C2D-C1D-ND	6.91	116.97	110.13
25	A	407	PHO	C2B-C1B-NB	6.84	114.37	109.43
24	b	608	CLA	CMD-C2D-C1D	6.82	136.73	124.73
24	c	514	CLA	O2D-CGD-CBD	6.82	123.15	111.23
25	A	408	PHO	C2B-C1B-NB	6.76	114.31	109.43
24	B	602	CLA	CMD-C2D-C1D	6.74	136.60	124.73
24	B	605	CLA	CMD-C2D-C1D	6.72	136.56	124.73
24	b	612	CLA	CMD-C2D-C1D	6.72	136.56	124.73
24	B	607	CLA	CMD-C2D-C1D	6.69	136.50	124.73
24	a	2113	CLA	C2D-C1D-ND	6.62	116.67	110.13
24	c	508	CLA	CMD-C2D-C1D	6.59	136.34	124.73
25	A	407	PHO	O2D-CGD-CBD	6.58	118.17	110.95
24	b	617	CLA	CMD-C2D-C1D	6.53	136.23	124.73
24	C	504	CLA	CMD-C2D-C1D	6.45	136.09	124.73
24	b	613	CLA	CMD-C2D-C1D	6.44	136.07	124.73
24	c	506	CLA	C2D-C1D-ND	6.44	116.50	110.13
24	b	616	CLA	CMD-C2D-C1D	6.42	136.03	124.73
25	a	2111	PHO	C3B-C4B-NB	6.41	111.64	107.46
24	B	612	CLA	C2D-C1D-ND	6.40	116.46	110.13
25	a	2111	PHO	C2B-C1B-NB	6.39	114.05	109.43
24	C	507	CLA	CMD-C2D-C1D	6.39	135.98	124.73
24	d	401	CLA	C2D-C1D-ND	6.39	116.45	110.13
24	b	604	CLA	O2D-CGD-CBD	6.39	122.40	111.23
24	B	617	CLA	C2D-C1D-ND	6.38	116.44	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608	CLA	C2D-C1D-ND	6.38	116.44	110.13
24	d	404	CLA	CMD-C2D-C1D	6.37	135.94	124.73
24	c	515	CLA	CMD-C2D-C1D	6.37	135.94	124.73
24	B	602	CLA	O2D-CGD-CBD	6.36	122.35	111.23
24	B	615	CLA	C2D-C1D-ND	6.36	116.42	110.13
24	B	614	CLA	CMD-C2D-C1D	6.35	135.90	124.73
24	A	409	CLA	C2D-C1D-ND	6.33	116.39	110.13
24	B	615	CLA	O2D-CGD-CBD	6.31	122.27	111.23
24	B	612	CLA	CMD-C2D-C1D	6.27	135.77	124.73
24	B	616	CLA	C2D-C1D-ND	6.26	116.32	110.13
24	B	606	CLA	C2D-C1D-ND	6.25	116.31	110.13
24	B	613	CLA	C2D-C1D-ND	6.18	116.24	110.13
24	C	513	CLA	C2D-C1D-ND	6.18	116.24	110.13
24	A	406	CLA	CMD-C2D-C1D	6.18	135.60	124.73
24	C	502	CLA	CMD-C2D-C1D	6.14	135.54	124.73
24	C	506	CLA	CMD-C2D-C1D	6.14	135.54	124.73
24	b	606	CLA	CMD-C2D-C1D	6.14	135.54	124.73
24	C	512	CLA	C2D-C1D-ND	6.14	116.20	110.13
24	b	611	CLA	C2D-C1D-ND	6.12	116.19	110.13
24	B	614	CLA	C2D-C1D-ND	6.12	116.18	110.13
24	B	613	CLA	O2D-CGD-CBD	6.12	121.92	111.23
24	b	607	CLA	CMD-C2D-C1D	6.11	135.48	124.73
24	a	2109	CLA	C2D-C1D-ND	6.11	116.17	110.13
27	a	2115	SQD	O6-C1-C2	6.10	117.54	108.27
25	A	407	PHO	C4D-ND-C1D	-6.09	101.58	108.87
24	C	510	CLA	O2D-CGD-CBD	6.08	121.87	111.23
25	A	408	PHO	C4D-ND-C1D	-6.07	101.59	108.87
24	C	503	CLA	C2D-C1D-ND	6.07	116.14	110.13
24	C	511	CLA	O2D-CGD-CBD	6.07	121.85	111.23
24	c	510	CLA	C2D-C1D-ND	6.07	116.13	110.13
24	b	616	CLA	C2D-C1D-ND	6.06	116.13	110.13
24	C	510	CLA	CMD-C2D-C1D	6.05	135.39	124.73
24	B	617	CLA	O2D-CGD-CBD	6.04	121.78	111.23
24	b	619	CLA	C2D-C1D-ND	6.02	116.09	110.13
24	d	405	CLA	C2D-C1D-ND	6.00	116.06	110.13
24	D	404	CLA	CMD-C2D-C1D	5.99	135.28	124.73
24	C	512	CLA	CMD-C2D-C1D	5.99	135.28	124.73
24	b	605	CLA	O2D-CGD-CBD	5.99	121.70	111.23
24	b	614	CLA	C2D-C1D-ND	5.99	116.05	110.13
24	C	505	CLA	CMD-C2D-C1D	5.97	135.25	124.73
25	a	2111	PHO	C4D-ND-C1D	-5.97	101.72	108.87
24	C	503	CLA	O2D-CGD-CBD	5.97	121.66	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	609	CLA	CMD-C2D-C1D	5.97	135.24	124.73
24	b	613	CLA	C2D-C1D-ND	5.96	116.03	110.13
24	B	608	CLA	C2D-C1D-ND	5.95	116.02	110.13
24	C	508	CLA	O2D-CGD-CBD	5.95	121.62	111.23
24	b	610	CLA	C2D-C1D-ND	5.94	116.01	110.13
24	C	514	CLA	CMD-C2D-C1D	5.93	135.16	124.73
24	D	405	CLA	O2D-CGD-CBD	5.92	121.58	111.23
24	c	507	CLA	CMD-C2D-C1D	5.91	135.13	124.73
24	D	405	CLA	CMD-C2D-C1D	5.88	135.08	124.73
24	B	609	CLA	C2D-C1D-ND	5.87	115.94	110.13
24	B	607	CLA	C2D-C1D-ND	5.87	115.94	110.13
24	B	610	CLA	CMD-C2D-C1D	5.87	135.06	124.73
24	b	614	CLA	CMD-C2D-C1D	5.86	135.04	124.73
24	B	604	CLA	O2D-CGD-CBD	5.83	121.42	111.23
24	c	513	CLA	CMD-C2D-C1D	5.83	135.00	124.73
24	B	611	CLA	CMD-C2D-C1D	5.83	134.99	124.73
24	d	405	CLA	CMD-C2D-C1D	5.83	134.99	124.73
36	I	1202	HTG	C1'-S1-C1	5.83	113.03	100.45
24	b	605	CLA	CMD-C2D-C1D	5.82	134.97	124.73
24	B	610	CLA	C2D-C1D-ND	5.80	115.87	110.13
24	c	507	CLA	O2D-CGD-CBD	5.80	121.37	111.23
24	C	508	CLA	CMD-C2D-C1D	5.79	134.93	124.73
24	d	401	CLA	CMD-C2D-C1D	5.78	134.91	124.73
24	C	513	CLA	O2D-CGD-CBD	5.78	121.33	111.23
24	C	509	CLA	C2D-C1D-ND	5.76	115.83	110.13
24	B	604	CLA	CMD-C2D-C1D	5.76	134.88	124.73
24	b	618	CLA	C2D-C1D-ND	5.76	115.83	110.13
24	b	604	CLA	CMD-C2D-C1D	5.76	134.88	124.73
24	D	401	CLA	CMD-C2D-C1D	5.75	134.86	124.73
24	b	619	CLA	O2D-CGD-CBD	5.75	121.28	111.23
24	b	619	CLA	CMD-C2D-C1D	5.74	134.84	124.73
24	c	505	CLA	C2D-C1D-ND	5.73	115.80	110.13
24	a	2109	CLA	CMD-C2D-C1D	5.73	134.81	124.73
24	c	511	CLA	CMD-C2D-C1D	5.72	134.80	124.73
24	b	611	CLA	CMD-C2D-C1D	5.72	134.79	124.73
26	D	406	BCR	C7-C8-C9	-5.72	117.78	126.23
24	b	617	CLA	C2D-C1D-ND	5.70	115.77	110.13
24	B	604	CLA	C2D-C1D-ND	5.70	115.76	110.13
24	B	611	CLA	C1-C2-C3	-5.69	116.88	126.20
24	b	609	CLA	O2D-CGD-CBD	5.67	121.14	111.23
24	c	509	CLA	C2D-C1D-ND	5.67	115.74	110.13
24	C	502	CLA	O2D-CGD-CBD	5.67	121.14	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	607	CLA	C2D-C1D-ND	5.67	115.73	110.13
24	c	504	CLA	C2D-C1D-ND	5.65	115.72	110.13
24	c	506	CLA	CMD-C2D-C1D	5.65	134.68	124.73
24	B	617	CLA	CMD-C2D-C1D	5.64	134.66	124.73
25	a	2112	PHO	C4D-ND-C1D	-5.63	102.12	108.87
25	A	408	PHO	C1-C2-C3	-5.63	116.98	126.20
24	c	511	CLA	C2D-C1D-ND	5.62	115.69	110.13
24	c	514	CLA	C2D-C1D-ND	5.60	115.67	110.13
24	C	511	CLA	CMD-C2D-C1D	5.59	134.57	124.73
25	A	407	PHO	C3D-C4D-ND	5.59	114.87	107.71
24	b	613	CLA	O2D-CGD-CBD	5.59	121.00	111.23
24	A	405	CLA	CMD-C2D-C1D	5.58	134.56	124.73
24	B	611	CLA	C2D-C1D-ND	5.58	115.64	110.13
24	C	509	CLA	O2D-CGD-CBD	5.57	120.98	111.23
24	C	507	CLA	C2D-C1D-ND	5.57	115.64	110.13
24	c	506	CLA	O2D-CGD-CBD	5.57	120.96	111.23
24	B	603	CLA	CMD-C2D-C1D	5.55	134.51	124.73
24	A	409	CLA	CMD-C2D-C1D	5.55	134.50	124.73
24	B	608	CLA	CMD-C2D-C1D	5.55	134.50	124.73
25	a	2111	PHO	C3D-C4D-ND	5.55	114.82	107.71
24	B	606	CLA	CMD-C2D-C1D	5.53	134.47	124.73
24	c	503	CLA	O2D-CGD-CBD	5.51	120.87	111.23
24	b	614	CLA	O2D-CGD-CBD	5.51	120.86	111.23
24	C	504	CLA	C2D-C1D-ND	5.51	115.58	110.13
24	C	510	CLA	C1-C2-C3	-5.50	117.19	126.20
24	A	405	CLA	C2D-C1D-ND	5.47	115.54	110.13
27	A	411	SQD	O6-C1-C2	5.46	116.57	108.27
24	C	514	CLA	C2D-C1D-ND	5.45	115.52	110.13
24	b	618	CLA	CMD-C2D-C1D	5.43	134.29	124.73
24	c	503	CLA	CMD-C2D-C1D	5.42	134.28	124.73
25	a	2112	PHO	C3D-C4D-ND	5.42	114.66	107.71
24	B	603	CLA	C2D-C1D-ND	5.42	115.49	110.13
25	A	408	PHO	C3D-C4D-ND	5.41	114.65	107.71
24	b	606	CLA	O2D-CGD-CBD	5.41	120.69	111.23
24	D	405	CLA	C2D-C1D-ND	5.41	115.48	110.13
24	c	514	CLA	CMD-C2D-C1D	5.38	134.20	124.73
24	B	615	CLA	CMD-C2D-C1D	5.37	134.19	124.73
24	B	613	CLA	CMD-C2D-C1D	5.37	134.18	124.73
24	b	609	CLA	C2D-C1D-ND	5.37	115.44	110.13
24	b	615	CLA	O2D-CGD-CBD	5.36	120.60	111.23
24	B	616	CLA	CMD-C2D-C1D	5.36	134.16	124.73
24	C	513	CLA	CMD-C2D-C1D	5.36	134.16	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	511	CLA	C2D-C1D-ND	5.35	115.42	110.13
24	C	510	CLA	C2D-C1D-ND	5.34	115.41	110.13
24	b	608	CLA	CHD-C4C-C3C	-5.33	117.00	124.77
36	c	523	HTG	C1'-S1-C1	5.33	111.97	100.45
24	C	508	CLA	C2D-C1D-ND	5.33	115.40	110.13
26	d	406	BCR	C38-C26-C25	-5.32	118.68	124.48
24	B	603	CLA	O2D-CGD-CBD	5.31	120.52	111.23
24	c	508	CLA	C2D-C1D-ND	5.30	115.38	110.13
28	C	526	LMG	O7-C10-C11	5.29	122.93	111.48
24	B	612	CLA	O2D-CGD-CBD	5.28	120.45	111.23
24	A	406	CLA	C2D-C1D-ND	5.27	115.34	110.13
24	b	610	CLA	CMD-C2D-C1D	5.27	134.00	124.73
24	B	611	CLA	O2D-CGD-CBD	5.26	120.43	111.23
24	B	602	CLA	C2D-C1D-ND	5.26	115.33	110.13
24	c	513	CLA	C2D-C1D-ND	5.25	115.32	110.13
24	c	512	CLA	C2D-C1D-ND	5.24	115.31	110.13
24	C	503	CLA	CMD-C2D-C1D	5.22	133.91	124.73
24	b	617	CLA	O2D-CGD-CBD	5.21	120.34	111.23
24	c	505	CLA	CMD-C2D-C1D	5.21	133.90	124.73
24	B	605	CLA	C2D-C1D-ND	5.21	115.28	110.13
24	d	404	CLA	O2D-CGD-CBD	5.21	120.33	111.23
24	C	508	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
24	C	505	CLA	O2D-CGD-CBD	5.19	120.30	111.23
24	C	505	CLA	C2D-C1D-ND	5.18	115.26	110.13
24	D	404	CLA	CHD-C4C-C3C	-5.17	117.23	124.77
24	b	607	CLA	C1-C2-C3	-5.17	117.73	126.20
24	D	401	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
24	c	509	CLA	CMD-C2D-C1D	5.15	133.79	124.73
32	A	418[A]	K2I	C3-C4-C5	-5.15	119.22	123.59
24	D	401	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
24	a	2110	CLA	CMD-C2D-C1D	5.14	133.78	124.73
24	B	607	CLA	O2D-CGD-CBD	5.14	120.21	111.23
29	A	420	LMT	C1'-O5'-C5'	5.13	123.74	113.72
27	B	621	SQD	O47-C7-C8	5.12	122.55	111.48
24	b	612	CLA	C2D-C1D-ND	5.09	115.17	110.13
24	a	2113	CLA	O2D-CGD-CBD	5.09	120.12	111.23
24	C	502	CLA	C2D-C1D-ND	5.09	115.16	110.13
24	b	615	CLA	CHD-C4C-C3C	-5.07	117.38	124.77
24	c	507	CLA	C2D-C1D-ND	5.07	115.14	110.13
24	b	613	CLA	C3D-C2D-C1D	-5.05	98.95	105.83
24	C	503	CLA	C1-C2-C3	-5.02	117.98	126.20
27	L	102	SQD	O6-C1-C2	5.02	115.89	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	515	CLA	C2D-C1D-ND	5.02	115.09	110.13
24	b	605	CLA	C2D-C1D-ND	5.01	115.08	110.13
24	C	509	CLA	CMD-C2D-C1D	5.01	133.55	124.73
24	d	401	CLA	C3B-C2B-C1B	-5.01	101.27	107.17
27	f	102	SQD	O47-C7-C8	5.00	122.30	111.48
36	c	524	HTG	C1'-S1-C1	5.00	111.25	100.45
27	B	621	SQD	C1-O5-C5	5.00	123.48	113.72
24	c	509	CLA	C3B-C2B-C1B	-4.99	101.28	107.17
24	B	605	CLA	O2D-CGD-CBD	4.99	119.95	111.23
27	L	102	SQD	O47-C7-C8	4.98	122.25	111.48
24	b	604	CLA	C2D-C1D-ND	4.97	115.05	110.13
24	c	510	CLA	CMD-C2D-C1D	4.96	133.47	124.73
24	b	606	CLA	C2D-C1D-ND	4.95	115.03	110.13
24	B	608	CLA	O2D-CGD-CBD	4.93	119.85	111.23
32	a	2118[A]	K2I	C3-C4-C5	-4.92	119.41	123.59
24	B	609	CLA	CMD-C2D-C1D	4.91	133.38	124.73
24	A	409	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
25	a	2112	PHO	C1-C2-C3	-4.89	118.18	126.20
24	c	504	CLA	O2D-CGD-CBD	4.89	119.78	111.23
38	c	518	DGD	O2G-C1B-C2B	4.88	122.03	111.48
24	c	512	CLA	CMD-C2D-C1D	4.87	133.31	124.73
24	c	509	CLA	C1C-C2C-C3C	-4.87	101.86	106.98
24	C	513	CLA	CHD-C4C-C3C	-4.86	117.69	124.77
24	D	404	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
40	e	103	HEM	C4D-ND-C1D	4.84	110.93	105.21
24	b	607	CLA	O2D-CGD-CBD	4.84	119.68	111.23
24	b	616	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
24	d	404	CLA	C2D-C1D-ND	4.83	114.91	110.13
24	b	610	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
40	F	102	HEM	C4D-ND-C1D	4.82	110.92	105.21
24	B	617	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
24	C	504	CLA	C1-C2-C3	-4.82	118.30	126.20
24	A	409	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
24	a	2113	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
24	D	404	CLA	C2C-C1C-NC	4.80	115.02	109.98
24	b	608	CLA	C3D-C2D-C1D	-4.80	99.29	105.83
24	d	401	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
24	B	616	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
24	B	612	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
24	a	2110	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
28	c	522	LMG	O7-C10-C11	4.78	121.82	111.48
24	B	616	CLA	CHD-C4C-C3C	-4.77	117.82	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	411	SQD	C1-O5-C5	-4.76	104.42	113.72
24	B	615	CLA	C3B-C2B-C1B	-4.76	101.56	107.17
43	V	201	HEC	CBB-CAB-C3B	-4.75	117.93	127.43
24	c	504	CLA	CHD-C4C-C3C	-4.75	117.84	124.77
24	D	401	CLA	O2D-CGD-CBD	4.74	119.52	111.23
29	i	104	LMT	C1'-O5'-C5'	4.74	122.98	113.72
36	C	522	HTG	C1'-S1-C1	4.74	110.68	100.45
24	c	507	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
24	C	506	CLA	O2D-CGD-CBD	4.73	119.49	111.23
26	k	2003	BCR	C24-C23-C22	-4.72	119.25	126.23
24	c	510	CLA	C3D-C4D-ND	4.72	117.66	109.99
24	c	511	CLA	O2D-CGD-CBD	4.72	119.48	111.23
24	C	513	CLA	C3B-C2B-C1B	-4.70	101.62	107.17
24	c	503	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
24	B	611	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
31	d	407	PL9	C7-C8-C9	-4.69	118.75	126.83
24	c	505	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
24	B	610	CLA	O2D-CGD-CBD	4.68	119.41	111.23
27	A	413	SQD	O47-C7-C8	4.67	121.59	111.48
24	B	614	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
24	b	614	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
26	b	622	BCR	C24-C23-C22	-4.67	119.32	126.23
24	C	514	CLA	C3B-C2B-C1B	-4.67	101.66	107.17
24	C	513	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
24	c	506	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
24	c	510	CLA	O2D-CGD-CBD	4.67	119.39	111.23
24	d	401	CLA	CHD-C4C-C3C	-4.65	117.99	124.77
24	C	512	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
24	b	606	CLA	C1C-C2C-C3C	-4.64	102.10	106.98
24	c	504	CLA	CMD-C2D-C1D	4.64	132.89	124.73
24	a	2113	CLA	CMD-C2D-C1D	4.63	132.89	124.73
24	B	607	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
24	D	405	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
24	A	406	CLA	C3D-C4D-ND	4.62	117.50	109.99
24	B	617	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
24	B	606	CLA	CHD-C4C-C3C	-4.62	118.04	124.77
24	c	509	CLA	C2C-C1C-NC	4.61	114.83	109.98
24	c	504	CLA	C3B-C2B-C1B	-4.61	101.73	107.17
24	a	2110	CLA	C3D-C4D-ND	4.61	117.48	109.99
24	b	617	CLA	C3B-C2B-C1B	-4.61	101.74	107.17
24	b	619	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
24	C	504	CLA	C3D-C2D-C1D	-4.59	99.56	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	617	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
24	b	610	CLA	O2D-CGD-CBD	4.59	119.26	111.23
24	c	515	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
24	C	509	CLA	C3D-C4D-ND	4.59	117.44	109.99
24	C	512	CLA	C3D-C2D-C1D	-4.58	99.57	105.83
24	b	619	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
24	c	503	CLA	C3D-C4D-ND	4.57	117.42	109.99
24	D	401	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
24	b	611	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
24	a	2113	CLA	C1-C2-C3	-4.57	118.72	126.20
24	b	618	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
24	b	608	CLA	C3B-C2B-C1B	-4.56	101.80	107.17
24	B	617	CLA	CHD-C4C-C3C	-4.55	118.14	124.77
24	c	503	CLA	O2D-CGD-O1D	-4.55	114.99	123.85
36	B	627	HTG	C1'-S1-C1	4.55	110.27	100.45
24	B	608	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
24	C	510	CLA	C3B-C2B-C1B	-4.54	101.82	107.17
32	A	418[A]	K2I	C-C1-C2	-4.54	119.74	123.59
24	C	503	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
26	T	101	BCR	C33-C5-C6	-4.53	119.54	124.48
36	C	522	HTG	C1-O5-C5	4.53	120.68	112.56
24	D	404	CLA	C3D-C4D-ND	4.52	117.34	109.99
24	D	401	CLA	CBC-CAC-C3C	-4.52	100.16	112.42
24	B	615	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
24	a	2110	CLA	C3B-C4B-NB	4.52	114.56	110.53
24	B	609	CLA	O2D-CGD-CBD	4.52	119.13	111.23
24	b	611	CLA	O2D-CGD-CBD	4.51	119.12	111.23
26	c	516	BCR	C15-C14-C13	-4.51	120.96	127.28
24	b	615	CLA	C3D-C2D-C1D	-4.50	99.68	105.83
24	b	607	CLA	CAC-C3C-C4C	4.50	130.65	124.79
24	B	614	CLA	C3B-C2B-C1B	-4.49	101.87	107.17
24	b	605	CLA	C3B-C2B-C1B	-4.49	101.87	107.17
24	B	613	CLA	C3D-C4D-ND	4.49	117.28	109.99
24	D	404	CLA	C1C-C2C-C3C	-4.49	102.26	106.98
24	D	401	CLA	C2C-C1C-NC	4.49	114.69	109.98
24	B	615	CLA	CHD-C4C-C3C	-4.49	118.23	124.77
39	e	101	LHG	O7-C7-C8	4.49	121.19	111.48
24	b	617	CLA	C1-C2-C3	-4.49	118.85	126.20
24	d	405	CLA	O2D-CGD-CBD	4.48	119.06	111.23
24	C	503	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
24	B	606	CLA	O2D-CGD-CBD	4.47	119.05	111.23
24	b	615	CLA	CMD-C2D-C1D	4.47	132.61	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	609	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
24	c	515	CLA	O2D-CGD-CBD	4.47	119.05	111.23
24	B	606	CLA	C3D-C4D-ND	4.47	117.26	109.99
24	d	405	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
24	B	616	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
26	d	406	BCR	C24-C23-C22	-4.46	119.64	126.23
24	a	2113	CLA	CHD-C4C-C3C	-4.46	118.27	124.77
26	C	516	BCR	C7-C8-C9	-4.46	119.64	126.23
24	B	606	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
27	F	101	SQD	O47-C7-C8	4.46	121.12	111.48
24	c	514	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
24	C	504	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
24	b	608	CLA	C3D-C4D-ND	4.45	117.22	109.99
24	b	608	CLA	O2D-CGD-CBD	4.44	119.00	111.23
24	b	604	CLA	C3B-C2B-C1B	-4.44	101.93	107.17
24	B	602	CLA	C3B-C2B-C1B	-4.44	101.94	107.17
24	c	504	CLA	C3D-C4D-ND	4.44	117.20	109.99
24	c	512	CLA	C3D-C4D-ND	4.44	117.20	109.99
24	D	401	CLA	CHD-C4C-C3C	-4.43	118.31	124.77
28	A	412	LMG	O7-C10-C11	4.43	121.06	111.48
26	b	620	BCR	C7-C8-C9	-4.42	119.69	126.23
32	a	2118[B]	K2I	BR-C4-C5	4.42	121.23	116.06
26	C	515	BCR	C33-C5-C6	-4.41	119.67	124.48
24	B	607	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
24	B	609	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
24	C	507	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
24	b	606	CLA	C3B-C2B-C1B	-4.40	101.99	107.17
24	c	508	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
26	B	618	BCR	C33-C5-C6	-4.39	119.69	124.48
24	d	401	CLA	C1C-C2C-C3C	-4.39	102.36	106.98
26	D	406	BCR	C24-C23-C22	-4.39	119.74	126.23
24	B	615	CLA	O2D-CGD-O1D	-4.39	115.31	123.85
24	c	506	CLA	CHD-C4C-C3C	-4.38	118.38	124.77
24	B	613	CLA	CHD-C4C-C3C	-4.38	118.38	124.77
39	E	101	LHG	O7-C7-C8	4.38	120.96	111.48
24	B	603	CLA	CAA-C2A-C3A	-4.38	101.16	113.00
24	b	612	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
24	b	610	CLA	C3B-C2B-C1B	-4.38	102.01	107.17
24	d	405	CLA	C3B-C2B-C1B	-4.38	102.01	107.17
36	b	602	HTG	C1-O5-C5	4.37	120.41	112.56
24	b	607	CLA	C3B-C2B-C1B	-4.37	102.01	107.17
24	B	614	CLA	CHD-C4C-C3C	-4.37	118.40	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	C3B-C2B-C1B	-4.37	102.02	107.17
36	V	204	HTG	C1-C2-C3	-4.36	102.02	110.55
24	C	503	CLA	O2D-CGD-O1D	-4.36	115.36	123.85
24	C	506	CLA	C2D-C1D-ND	4.36	114.44	110.13
24	B	610	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
24	a	2109	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
24	b	607	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
24	D	404	CLA	O2D-CGD-CBD	4.35	118.83	111.23
24	B	609	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
24	C	509	CLA	C3B-C2B-C1B	-4.34	102.05	107.17
40	F	102	HEM	CBD-CAD-C3D	-4.34	100.53	112.53
24	d	404	CLA	C3D-C4D-ND	4.34	117.04	109.99
24	b	619	CLA	CHD-C4C-C3C	-4.34	118.45	124.77
24	c	505	CLA	C3B-C2B-C1B	-4.33	102.06	107.17
26	D	406	BCR	C38-C26-C25	-4.33	119.76	124.48
24	B	616	CLA	O2D-CGD-CBD	4.33	118.80	111.23
24	B	602	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
24	C	504	CLA	CHD-C4C-C3C	-4.33	118.47	124.77
24	b	609	CLA	C3B-C2B-C1B	-4.33	102.07	107.17
24	a	2110	CLA	C2C-C1C-NC	4.32	114.52	109.98
24	B	615	CLA	C2C-C1C-NC	4.32	114.52	109.98
24	b	616	CLA	C1-C2-C3	-4.32	119.12	126.20
24	d	401	CLA	C3D-C4D-ND	4.31	117.00	109.99
24	C	514	CLA	O2D-CGD-CBD	4.31	118.77	111.23
26	t	102	BCR	C33-C5-C6	-4.31	119.78	124.48
27	F	101	SQD	O6-C1-C2	4.31	114.81	108.27
24	b	615	CLA	C3D-C4D-ND	4.30	116.98	109.99
24	c	508	CLA	C3D-C4D-ND	4.30	116.97	109.99
24	d	405	CLA	C3D-C4D-ND	4.29	116.97	109.99
38	C	519	DGD	O2G-C1B-C2B	4.29	120.75	111.48
24	c	514	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
24	c	513	CLA	C3B-C2B-C1B	-4.28	102.12	107.17
24	a	2109	CLA	C3D-C4D-ND	4.28	116.95	109.99
24	a	2110	CLA	C3B-C2B-C1B	-4.28	102.12	107.17
24	b	615	CLA	C3B-C2B-C1B	-4.28	102.13	107.17
24	d	404	CLA	C1C-C2C-C3C	-4.28	102.48	106.98
27	L	102	SQD	C3-C4-C5	4.27	117.98	110.23
24	C	507	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
24	d	404	CLA	C1-C2-C3	-4.27	119.20	126.20
29	B	623	LMT	C1-O1'-C1'	-4.27	106.39	113.68
24	C	511	CLA	C3D-C4D-ND	4.27	116.93	109.99
24	A	405	CLA	C3D-C4D-ND	4.26	116.91	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	C1C-C2C-C3C	-4.25	102.51	106.98
24	B	604	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
24	b	613	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
24	A	406	CLA	O2D-CGD-CBD	4.25	118.66	111.23
24	b	611	CLA	C3D-C4D-ND	4.25	116.90	109.99
24	c	506	CLA	C3B-C2B-C1B	-4.24	102.17	107.17
24	d	401	CLA	CBC-CAC-C3C	-4.24	100.92	112.42
24	c	515	CLA	C1-C2-C3	-4.24	119.25	126.20
26	c	528	BCR	C33-C5-C6	-4.24	119.86	124.48
24	b	612	CLA	C3B-C2B-C1B	-4.24	102.17	107.17
24	B	612	CLA	C3B-C2B-C1B	-4.24	102.17	107.17
24	b	612	CLA	CBC-CAC-C3C	-4.24	100.93	112.42
24	B	602	CLA	CHD-C4C-C3C	-4.24	118.60	124.77
28	i	101	LMG	O7-C10-C11	4.23	120.63	111.48
24	b	618	CLA	C3B-C2B-C1B	-4.23	102.19	107.17
24	c	511	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
24	C	507	CLA	O2D-CGD-CBD	4.22	118.61	111.23
24	a	2109	CLA	C3B-C2B-C1B	-4.22	102.19	107.17
24	a	2113	CLA	C3B-C2B-C1B	-4.22	102.19	107.17
24	a	2110	CLA	O2D-CGD-CBD	4.22	118.61	111.23
24	B	616	CLA	C1D-CHD-C4C	-4.22	117.05	126.02
24	c	510	CLA	C1-C2-C3	-4.22	119.29	126.20
24	B	606	CLA	C3B-C2B-C1B	-4.22	102.20	107.17
38	D	408	DGD	O2G-C1B-C2B	4.22	120.60	111.48
24	b	618	CLA	CHD-C4C-C3C	-4.21	118.63	124.77
24	C	510	CLA	O2D-CGD-O1D	-4.21	115.65	123.85
24	b	614	CLA	C3B-C2B-C1B	-4.21	102.21	107.17
24	c	510	CLA	C3B-C2B-C1B	-4.21	102.21	107.17
24	C	506	CLA	C3B-C2B-C1B	-4.20	102.22	107.17
24	B	604	CLA	C1C-C2C-C3C	-4.20	102.56	106.98
24	b	613	CLA	CHD-C4C-C3C	-4.20	118.65	124.77
24	C	508	CLA	C3D-C2D-C1D	-4.20	100.11	105.83
36	d	414	HTG	C1'-S1-C1	4.19	109.51	100.45
24	c	510	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
24	C	514	CLA	C3D-C4D-ND	4.19	116.79	109.99
38	c	519	DGD	O2G-C1B-C2B	4.18	120.52	111.48
24	b	608	CLA	CHD-C1D-ND	-4.18	118.92	124.80
24	C	505	CLA	C1C-C2C-C3C	-4.17	102.59	106.98
24	c	512	CLA	O2D-CGD-CBD	4.17	118.53	111.23
24	d	405	CLA	C1C-C2C-C3C	-4.17	102.59	106.98
38	C	517	DGD	O2G-C1B-C2B	4.17	120.50	111.48
26	Y	302	BCR	C33-C5-C6	-4.17	119.94	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	406	BCR	C33-C5-C6	-4.17	119.94	124.48
24	B	603	CLA	C3B-C2B-C1B	-4.17	102.26	107.17
24	c	503	CLA	C1C-C2C-C3C	-4.16	102.60	106.98
24	A	406	CLA	C2B-C1B-NB	4.16	114.64	110.33
24	c	514	CLA	C1C-C2C-C3C	-4.16	102.61	106.98
24	B	603	CLA	C3D-C4D-ND	4.16	116.74	109.99
26	A	410	BCR	C33-C5-C6	-4.16	119.95	124.48
24	b	606	CLA	C3D-C4D-ND	4.15	116.74	109.99
24	C	505	CLA	C3D-C2D-C1D	-4.15	100.16	105.83
24	C	505	CLA	C3D-C4D-ND	4.15	116.74	109.99
24	a	2113	CLA	C3D-C4D-ND	4.15	116.73	109.99
36	b	626	HTG	C1'-S1-C1	4.15	109.40	100.45
24	c	513	CLA	C4-C3-C5	4.14	122.41	115.23
24	C	514	CLA	C3D-C2D-C1D	-4.14	100.19	105.83
24	C	510	CLA	C1C-C2C-C3C	-4.14	102.63	106.98
24	B	604	CLA	C3D-C4D-ND	4.14	116.71	109.99
24	D	405	CLA	C3D-C4D-ND	4.13	116.71	109.99
24	b	605	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
24	C	509	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
28	C	520	LMG	O7-C10-C11	4.13	120.41	111.48
24	D	401	CLA	C3D-C4D-ND	4.13	116.69	109.99
32	a	2118[B]	K2I	C3-C4-C5	-4.13	120.09	123.59
27	a	2115	SQD	C1-C2-C3	-4.12	101.33	110.01
24	C	514	CLA	C1-C2-C3	-4.12	119.45	126.20
24	B	611	CLA	CHD-C4C-C3C	-4.12	118.77	124.77
24	B	609	CLA	C3D-C4D-ND	4.11	116.67	109.99
24	B	613	CLA	C3D-C2D-C1D	-4.11	100.23	105.83
24	B	608	CLA	C1C-C2C-C3C	-4.10	102.67	106.98
24	B	604	CLA	C3B-C2B-C1B	-4.10	102.34	107.17
24	c	504	CLA	C3D-C2D-C1D	-4.10	100.24	105.83
24	C	502	CLA	C3D-C4D-ND	4.10	116.65	109.99
24	B	615	CLA	O2A-CGA-O1A	-4.10	113.38	123.63
24	d	401	CLA	C2C-C1C-NC	4.09	114.28	109.98
24	b	612	CLA	O2D-CGD-CBD	4.09	118.38	111.23
32	a	2118[A]	K2I	C-C1-C2	-4.09	120.12	123.59
24	c	506	CLA	C1C-C2C-C3C	-4.08	102.69	106.98
24	d	404	CLA	C2C-C1C-NC	4.08	114.27	109.98
24	c	509	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
24	d	404	CLA	C3B-C2B-C1B	-4.08	102.36	107.17
24	c	514	CLA	CBA-CAA-C2A	-4.08	101.66	113.79
24	c	513	CLA	CHD-C4C-C3C	-4.07	118.84	124.77
24	B	603	CLA	C3D-C2D-C1D	-4.07	100.28	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	508	CLA	CHD-C4C-C3C	-4.07	118.84	124.77
24	a	2113	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
24	B	613	CLA	C3B-C2B-C1B	-4.06	102.38	107.17
24	D	405	CLA	C3D-C2D-C1D	-4.06	100.29	105.83
24	B	605	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
24	c	506	CLA	C3D-C4D-ND	4.06	116.59	109.99
24	b	619	CLA	C1D-CHD-C4C	-4.06	117.39	126.02
24	b	609	CLA	CHD-C4C-C3C	-4.06	118.86	124.77
39	d	408	LHG	O8-C23-C24	4.06	124.20	111.83
24	b	612	CLA	C1C-C2C-C3C	-4.06	102.72	106.98
36	b	602	HTG	C1'-S1-C1	4.05	109.21	100.45
24	B	616	CLA	C3D-C4D-ND	4.05	116.58	109.99
32	A	418[A]	K2I	BR-C4-C5	4.05	120.81	116.06
24	b	616	CLA	C3B-C2B-C1B	-4.05	102.40	107.17
24	c	515	CLA	C3D-C2D-C1D	-4.05	100.31	105.83
24	A	406	CLA	C3B-C2B-C1B	-4.04	102.41	107.17
26	c	516	BCR	C33-C5-C6	-4.03	120.08	124.48
24	B	610	CLA	C3D-C4D-ND	4.03	116.53	109.99
24	D	401	CLA	C2B-C1B-NB	4.03	114.50	110.33
24	C	513	CLA	C1-C2-C3	-4.03	119.60	126.20
36	B	628	HTG	C1-O5-C5	4.03	119.78	112.56
24	b	610	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
24	b	604	CLA	C3D-C4D-ND	4.01	116.51	109.99
24	c	512	CLA	C3B-C2B-C1B	-4.01	102.44	107.17
24	B	614	CLA	C3D-C4D-ND	4.01	116.50	109.99
31	D	407	PL9	C40-C39-C41	4.01	122.18	115.23
24	b	606	CLA	C2C-C1C-NC	4.00	114.19	109.98
24	B	612	CLA	C3D-C4D-ND	4.00	116.49	109.99
24	A	409	CLA	C3D-C4D-ND	4.00	116.49	109.99
24	C	502	CLA	C3D-C2D-C1D	-4.00	100.37	105.83
26	b	620	BCR	C33-C5-C6	-4.00	120.12	124.48
24	c	514	CLA	C1-O2A-CGA	4.00	126.33	116.65
24	b	604	CLA	C3D-C2D-C1D	-4.00	100.38	105.83
24	c	515	CLA	C3D-C4D-ND	3.99	116.48	109.99
24	B	605	CLA	C3D-C2D-C1D	-3.99	100.39	105.83
36	B	626	HTG	C1'-S1-C1	3.98	109.06	100.45
24	b	617	CLA	C3D-C4D-ND	3.98	116.46	109.99
24	b	612	CLA	C2C-C1C-NC	3.98	114.17	109.98
24	b	611	CLA	C3B-C2B-C1B	-3.98	102.48	107.17
27	a	2102	SQD	O47-C7-C8	3.98	120.08	111.48
26	T	101	BCR	C15-C16-C17	-3.98	115.39	123.52
24	c	510	CLA	CHD-C4C-C3C	-3.97	118.98	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	C1C-C2C-C3C	-3.97	102.80	106.98
27	a	2115	SQD	O47-C7-C8	3.97	120.07	111.48
29	A	420	LMT	O1B-C4'-C3'	3.97	117.32	107.23
24	B	615	CLA	C3D-C4D-ND	3.97	116.44	109.99
24	a	2110	CLA	C1C-C2C-C3C	-3.97	102.81	106.98
43	v	201	HEC	CBB-CAB-C3B	-3.96	119.51	127.43
24	C	510	CLA	C3D-C2D-C1D	-3.96	100.42	105.83
24	c	513	CLA	C3D-C2D-C1D	-3.96	100.42	105.83
25	a	2111	PHO	O1D-CGD-CBD	-3.96	118.72	124.72
24	a	2110	CLA	CHD-C4C-C3C	-3.96	119.00	124.77
24	d	401	CLA	C2B-C1B-NB	3.96	114.43	110.33
26	Y	302	BCR	C38-C26-C25	-3.96	120.17	124.48
31	A	417	PL9	C27-C28-C29	-3.96	118.57	127.62
24	d	401	CLA	C1D-CHD-C4C	-3.95	117.62	126.02
24	B	605	CLA	C3B-C2B-C1B	-3.95	102.51	107.17
24	c	507	CLA	C2C-C1C-NC	3.95	114.13	109.98
24	B	614	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
24	A	406	CLA	C3D-C2D-C1D	-3.95	100.45	105.83
36	V	204	HTG	O5-C1-C2	-3.94	104.88	110.32
24	B	612	CLA	CAC-C3C-C4C	3.94	129.92	124.79
24	B	605	CLA	C3D-C4D-ND	3.94	116.39	109.99
36	b	601	HTG	C1'-S1-C1	3.94	108.96	100.45
24	D	404	CLA	C1-C2-C3	-3.93	119.75	126.20
24	b	605	CLA	C3D-C4D-ND	3.93	116.38	109.99
24	c	510	CLA	C1C-C2C-C3C	-3.92	102.85	106.98
24	b	610	CLA	C3D-C4D-ND	3.92	116.36	109.99
24	A	405	CLA	CAA-C2A-C3A	-3.92	102.40	113.00
24	C	508	CLA	C1C-C2C-C3C	-3.92	102.86	106.98
24	A	405	CLA	C3D-C2D-C1D	-3.92	100.48	105.83
24	c	507	CLA	C1C-C2C-C3C	-3.92	102.86	106.98
24	A	409	CLA	C1C-C2C-C3C	-3.91	102.86	106.98
26	c	516	BCR	C16-C17-C18	-3.91	121.79	127.28
24	B	611	CLA	C3B-C2B-C1B	-3.91	102.56	107.17
24	A	409	CLA	O2D-CGD-CBD	3.91	118.06	111.23
24	c	508	CLA	C3B-C2B-C1B	-3.91	102.56	107.17
24	c	507	CLA	C3D-C4D-ND	3.91	116.34	109.99
24	b	604	CLA	O2D-CGD-O1D	-3.90	116.25	123.85
26	d	406	BCR	C7-C8-C9	-3.90	120.46	126.23
24	b	612	CLA	C3D-C4D-ND	3.90	116.33	109.99
24	c	511	CLA	C3B-C2B-C1B	-3.90	102.57	107.17
24	B	608	CLA	CAA-C2A-C3A	-3.90	102.45	113.00
24	b	604	CLA	CHD-C4C-C3C	-3.90	119.09	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608	CLA	C2B-C1B-NB	3.90	114.37	110.33
36	c	526	HTG	C1'-S1-C1	3.89	108.85	100.45
24	c	511	CLA	O2D-CGD-O1D	-3.89	116.28	123.85
24	C	510	CLA	C3D-C4D-ND	3.89	116.31	109.99
24	b	614	CLA	C3D-C4D-ND	3.89	116.31	109.99
24	B	608	CLA	C3B-C2B-C1B	-3.88	102.59	107.17
24	b	619	CLA	C4C-C3C-C2C	-3.88	101.24	106.89
24	c	503	CLA	C3B-C2B-C1B	-3.88	102.60	107.17
24	b	616	CLA	O2D-CGD-CBD	3.88	118.01	111.23
24	b	607	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
24	C	507	CLA	C3B-C2B-C1B	-3.88	102.60	107.17
24	c	503	CLA	CHD-C4C-C3C	-3.87	119.13	124.77
24	b	616	CLA	C3D-C4D-ND	3.87	116.28	109.99
24	b	613	CLA	C3D-C4D-ND	3.87	116.27	109.99
24	B	602	CLA	C3D-C4D-ND	3.86	116.27	109.99
24	b	606	CLA	C3D-C2D-C1D	-3.86	100.56	105.83
43	V	201	HEC	C4D-ND-C1D	3.86	112.11	105.82
24	d	401	CLA	O2D-CGD-CBD	3.86	117.97	111.23
26	a	2114	BCR	C33-C5-C6	-3.85	120.28	124.48
24	C	503	CLA	C3D-C4D-ND	3.85	116.25	109.99
24	c	514	CLA	C2C-C1C-NC	3.85	114.03	109.98
24	b	610	CLA	C4-C3-C5	3.85	121.91	115.23
24	c	508	CLA	C2C-C1C-NC	3.84	114.02	109.98
41	H	101	RRX	C24-C23-C22	-3.84	120.55	126.23
24	c	508	CLA	C1C-C2C-C3C	-3.84	102.94	106.98
24	C	507	CLA	C3D-C4D-ND	3.84	116.22	109.99
24	d	401	CLA	CAA-C2A-C3A	-3.84	102.63	113.00
24	A	406	CLA	CHD-C4C-C3C	-3.83	119.18	124.77
24	b	615	CLA	C1-C2-C3	-3.83	119.92	126.20
24	b	615	CLA	C3C-C4C-NC	3.83	115.34	110.43
24	c	514	CLA	C3D-C4D-ND	3.82	116.20	109.99
24	c	505	CLA	C4A-NA-C1A	3.82	108.42	106.68
24	C	513	CLA	C1C-C2C-C3C	-3.82	102.96	106.98
24	B	616	CLA	C2B-C1B-NB	3.82	114.29	110.33
24	C	511	CLA	C3D-C2D-C1D	-3.82	100.62	105.83
27	A	411	SQD	C1-C2-C3	-3.81	101.99	110.01
36	B	625[B]	HTG	C1'-S1-C1	3.81	108.68	100.45
24	c	513	CLA	C3D-C4D-ND	3.81	116.17	109.99
24	a	2109	CLA	CAA-C2A-C1A	-3.80	99.51	111.97
24	B	617	CLA	C1C-C2C-C3C	-3.80	102.98	106.98
24	B	607	CLA	CHD-C4C-C3C	-3.80	119.23	124.77
24	B	613	CLA	O2D-CGD-O1D	-3.80	116.46	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	t	102	BCR	C15-C16-C17	-3.80	115.75	123.52
24	b	604	CLA	C4-C3-C5	3.79	121.81	115.23
24	C	504	CLA	O2D-CGD-CBD	3.79	117.86	111.23
36	V	204	HTG	C1'-S1-C1	3.79	108.64	100.45
31	x	801	PL9	C27-C28-C29	-3.79	118.95	127.62
24	c	512	CLA	CHD-C4C-C3C	-3.79	119.25	124.77
24	c	507	CLA	C1-O2A-CGA	3.79	125.83	116.65
24	C	513	CLA	CBC-CAC-C3C	-3.79	102.15	112.42
24	c	508	CLA	O2D-CGD-CBD	3.79	117.86	111.23
28	C	520	LMG	O8-C28-C29	3.79	123.39	111.83
24	C	508	CLA	C2B-C1B-NB	3.79	114.25	110.33
24	C	508	CLA	C1-C2-C3	-3.79	120.00	126.20
24	B	617	CLA	C1D-CHD-C4C	-3.78	117.98	126.02
24	c	513	CLA	C1-O2A-CGA	3.78	125.81	116.65
24	B	608	CLA	CBC-CAC-C3C	-3.77	102.19	112.42
24	b	604	CLA	C2B-C1B-NB	3.77	114.24	110.33
24	C	513	CLA	C3D-C4D-ND	3.77	116.12	109.99
28	b	623	LMG	O7-C10-C11	3.77	119.64	111.48
24	c	509	CLA	C3D-C4D-ND	3.76	116.10	109.99
24	B	615	CLA	C4-C3-C5	3.76	121.75	115.23
24	A	409	CLA	C2C-C1C-NC	3.76	113.93	109.98
24	C	511	CLA	C3B-C2B-C1B	-3.75	102.74	107.17
24	b	618	CLA	C3D-C4D-ND	3.75	116.09	109.99
24	B	612	CLA	O2D-CGD-O1D	-3.75	116.55	123.85
24	b	619	CLA	C3D-C4D-ND	3.75	116.08	109.99
32	a	2118[B]	K2I	C-C1-C2	-3.75	120.41	123.59
24	a	2113	CLA	C2C-C1C-NC	3.75	113.92	109.98
24	A	406	CLA	C1C-C2C-C3C	-3.75	103.04	106.98
24	A	405	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
24	b	619	CLA	C3B-C4B-NB	3.74	113.87	110.53
24	B	617	CLA	C2C-C1C-NC	3.74	113.91	109.98
24	c	510	CLA	C2B-C1B-NB	3.74	114.20	110.33
24	C	507	CLA	C2C-C1C-NC	3.74	113.91	109.98
27	A	411	SQD	O47-C7-C8	3.73	119.56	111.48
24	b	609	CLA	C1D-CHD-C4C	-3.73	118.08	126.02
24	b	611	CLA	CHD-C4C-C3C	-3.73	119.33	124.77
24	a	2109	CLA	C1D-CHD-C4C	-3.73	118.09	126.02
24	B	609	CLA	CMA-C3A-C4A	-3.73	101.75	111.77
24	A	405	CLA	C3B-C2B-C1B	-3.73	102.77	107.17
24	C	503	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
24	b	606	CLA	C1D-CHD-C4C	-3.73	118.10	126.02
24	B	608	CLA	C3D-C4D-ND	3.72	116.04	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	C1-C2-C3	-3.72	120.10	126.20
24	d	404	CLA	C3D-C2D-C1D	-3.72	100.76	105.83
24	D	404	CLA	C3C-C4C-NC	3.72	115.19	110.43
24	b	605	CLA	C2B-C1B-NB	3.72	114.18	110.33
43	v	201	HEC	C4D-ND-C1D	3.71	111.88	105.82
25	A	407	PHO	CBC-CAC-C3C	-3.71	107.56	112.87
24	A	409	CLA	CMA-C3A-C4A	-3.71	101.80	111.77
24	c	509	CLA	CMB-C2B-C1B	3.71	131.06	125.42
24	D	404	CLA	O2D-CGD-O1D	-3.70	116.65	123.85
24	C	508	CLA	C2C-C1C-NC	3.70	113.86	109.98
24	B	617	CLA	CBC-CAC-C3C	-3.70	102.40	112.42
24	D	405	CLA	O2D-CGD-O1D	-3.70	116.66	123.85
24	B	605	CLA	C2C-C1C-NC	3.69	113.86	109.98
24	c	513	CLA	O2D-CGD-CBD	3.69	117.69	111.23
24	c	507	CLA	C3D-C2D-C1D	-3.69	100.79	105.83
38	C	518	DGD	O2G-C1B-C2B	3.69	119.47	111.48
24	C	514	CLA	C2B-C1B-NB	3.69	114.15	110.33
24	b	606	CLA	C2B-C1B-NB	3.69	114.15	110.33
32	A	418[B]	K2I	C-C1-C2	-3.69	120.46	123.59
24	b	617	CLA	O2D-CGD-O1D	-3.69	116.67	123.85
24	c	514	CLA	CBC-CAC-C3C	-3.69	102.43	112.42
24	c	505	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
26	c	517	BCR	C33-C5-C6	-3.68	120.47	124.48
26	c	517	BCR	C38-C26-C25	-3.68	120.47	124.48
24	c	505	CLA	C2C-C1C-NC	3.68	113.84	109.98
24	A	405	CLA	O2D-CGD-CBD	3.67	117.65	111.23
24	A	405	CLA	C2C-C1C-NC	3.67	113.84	109.98
32	A	418[B]	K2I	C3-C4-C5	-3.67	120.47	123.59
24	B	602	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
24	b	608	CLA	O2D-CGD-O1D	-3.67	116.71	123.85
24	B	615	CLA	C1D-CHD-C4C	-3.66	118.24	126.02
29	b	624	LMT	O5'-C5'-C4'	3.66	117.29	109.72
24	a	2109	CLA	C2C-C1C-NC	3.66	113.83	109.98
24	c	508	CLA	C2B-C1B-NB	3.66	114.12	110.33
24	C	509	CLA	C2B-C1B-NB	3.66	114.12	110.33
24	D	405	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
24	c	508	CLA	C1D-CHD-C4C	-3.66	118.25	126.02
26	b	622	BCR	C38-C26-C25	-3.65	120.50	124.48
36	I	1202	HTG	C1-O5-C5	3.65	119.11	112.56
24	A	409	CLA	C2B-C1B-NB	3.65	114.11	110.33
36	B	626	HTG	O5-C1-C2	3.65	115.35	110.32
26	c	517	BCR	C7-C8-C9	-3.65	120.84	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	i	103	HTG	C1'-S1-C1	3.65	108.33	100.45
24	c	504	CLA	C2B-C1B-NB	3.65	114.11	110.33
24	B	611	CLA	C3D-C4D-ND	3.64	115.91	109.99
24	B	610	CLA	C3B-C2B-C1B	-3.64	102.88	107.17
31	x	801	PL9	C32-C33-C34	-3.64	119.30	127.62
32	A	418[B]	K2I	BR-C4-C5	3.64	120.32	116.06
24	c	505	CLA	C1D-CHD-C4C	-3.63	118.30	126.02
24	c	510	CLA	CAA-C2A-C3A	-3.63	103.18	113.00
24	b	616	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
26	C	515	BCR	C7-C8-C9	-3.63	120.87	126.23
24	C	513	CLA	C1D-CHD-C4C	-3.63	118.31	126.02
24	c	508	CLA	CBC-CAC-C3C	-3.62	102.59	112.42
25	a	2112	PHO	O2D-CGD-O1D	-3.62	116.80	123.85
24	c	504	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
24	b	607	CLA	C2C-C1C-NC	3.61	113.77	109.98
24	c	511	CLA	C3D-C4D-ND	3.61	115.85	109.99
26	C	516	BCR	C33-C5-C6	-3.61	120.55	124.48
24	C	508	CLA	C1D-CHD-C4C	-3.60	118.36	126.02
24	b	618	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
24	b	609	CLA	C3D-C4D-ND	3.60	115.84	109.99
24	C	502	CLA	C3B-C2B-C1B	-3.60	102.93	107.17
24	C	510	CLA	C2B-C1B-NB	3.60	114.06	110.33
24	A	409	CLA	C1-C2-C3	-3.60	120.31	126.20
24	B	610	CLA	CHD-C4C-C3C	-3.59	119.53	124.77
24	b	610	CLA	CBC-CAC-C3C	-3.59	102.68	112.42
24	c	509	CLA	O2D-CGD-O1D	-3.59	116.85	123.85
27	L	102	SQD	O7-S-C6	3.59	112.11	106.76
26	T	101	BCR	C7-C8-C9	-3.58	120.93	126.23
24	C	507	CLA	CBC-CAC-C3C	-3.58	102.71	112.42
24	b	611	CLA	C1D-CHD-C4C	-3.58	118.41	126.02
24	B	617	CLA	C3D-C4D-ND	3.58	115.81	109.99
24	B	604	CLA	C2C-C1C-NC	3.58	113.74	109.98
38	h	703	DGD	O2G-C1B-C2B	3.58	119.22	111.48
24	D	401	CLA	C3B-C4B-NB	3.58	113.72	110.53
24	b	619	CLA	C3C-C4C-NC	3.58	115.01	110.43
24	C	511	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
26	B	618	BCR	C24-C23-C22	-3.57	120.95	126.23
24	c	511	CLA	C1D-CHD-C4C	-3.57	118.44	126.02
24	b	605	CLA	C1C-C2C-C3C	-3.57	103.23	106.98
24	c	514	CLA	C1D-CHD-C4C	-3.56	118.44	126.02
24	c	512	CLA	C3D-C2D-C1D	-3.56	100.97	105.83
24	B	607	CLA	C1C-C2C-C3C	-3.56	103.23	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	C4C-C3C-C2C	-3.56	101.71	106.89
24	a	2109	CLA	CAA-C2A-C3A	-3.56	103.38	113.00
24	C	510	CLA	C2C-C1C-NC	3.56	113.72	109.98
24	B	602	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
24	C	514	CLA	C1D-CHD-C4C	-3.56	118.46	126.02
24	d	401	CLA	C3B-C4B-NB	3.55	113.70	110.53
24	B	604	CLA	O2D-CGD-O1D	-3.55	116.93	123.85
24	C	502	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
24	A	405	CLA	C4B-C3B-C2B	-3.55	102.89	107.30
24	c	503	CLA	CBC-CAC-C3C	-3.55	102.81	112.42
24	a	2113	CLA	CBC-CAC-C3C	-3.55	102.81	112.42
24	C	503	CLA	C2C-C1C-NC	3.54	113.70	109.98
24	a	2109	CLA	C1C-C2C-C3C	-3.54	103.25	106.98
25	A	408	PHO	C1A-C2A-C3A	-3.54	99.47	102.84
39	d	408	LHG	O8-C23-O10	-3.54	114.78	123.63
24	C	514	CLA	CHD-C4C-C3C	-3.54	119.62	124.77
24	c	506	CLA	CBC-CAC-C3C	-3.53	102.84	112.42
24	a	2110	CLA	C2B-C1B-NB	3.53	113.99	110.33
31	A	417	PL9	C12-C13-C14	-3.53	119.54	127.62
24	C	511	CLA	C1-C2-C3	-3.53	120.41	126.20
27	a	2115	SQD	C1-O5-C5	-3.53	106.83	113.72
24	b	617	CLA	CBC-CAC-C3C	-3.53	102.85	112.42
24	d	405	CLA	CHD-C1D-ND	-3.53	119.84	124.80
24	b	612	CLA	CMB-C2B-C1B	3.53	130.79	125.42
24	B	607	CLA	C3D-C4D-ND	3.53	115.72	109.99
24	C	513	CLA	C2B-C1B-NB	3.53	113.98	110.33
24	b	618	CLA	C1D-CHD-C4C	-3.52	118.54	126.02
24	b	615	CLA	C1D-CHD-C4C	-3.52	118.55	126.02
24	a	2113	CLA	C2B-C1B-NB	3.51	113.97	110.33
28	c	521	LMG	O7-C10-C11	3.51	119.08	111.48
24	b	613	CLA	C2B-C1B-NB	3.51	113.97	110.33
24	B	611	CLA	CAA-C2A-C3A	-3.51	103.51	113.00
31	x	801	PL9	C37-C38-C39	-3.51	119.59	127.62
24	b	608	CLA	C1C-C2C-C3C	-3.51	103.29	106.98
24	c	504	CLA	C1D-CHD-C4C	-3.51	118.56	126.02
24	C	503	CLA	C1D-CHD-C4C	-3.51	118.56	126.02
24	A	406	CLA	C4-C3-C5	3.51	121.31	115.23
24	b	607	CLA	C1D-CHD-C4C	-3.50	118.57	126.02
24	b	606	CLA	O2A-CGA-CBA	3.50	122.52	111.83
36	B	628	HTG	C1'-S1-C1	3.50	108.02	100.45
24	B	610	CLA	C1D-CHD-C4C	-3.50	118.58	126.02
24	b	604	CLA	C1C-C2C-C3C	-3.50	103.30	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
24	c	515	CLA	C2B-C1B-NB	3.50	113.95	110.33
24	B	609	CLA	CAC-C3C-C4C	3.50	129.34	124.79
24	D	401	CLA	CHD-C1D-ND	-3.49	119.88	124.80
38	C	518	DGD	O1G-C1A-C2A	3.49	122.49	111.83
24	B	612	CLA	CMC-C2C-C1C	3.49	130.49	125.03
36	b	602	HTG	O5-C1-C2	3.49	115.13	110.32
24	C	512	CLA	C3D-C4D-ND	3.49	115.66	109.99
24	c	511	CLA	C1-C2-C3	-3.49	120.48	126.20
24	C	503	CLA	CHD-C4C-C3C	-3.49	119.69	124.77
24	c	506	CLA	CHD-C1D-ND	-3.49	119.90	124.80
24	B	614	CLA	C2C-C1C-NC	3.48	113.64	109.98
24	c	514	CLA	O2D-CGD-O1D	-3.48	117.07	123.85
24	b	606	CLA	O2A-CGA-O1A	-3.48	114.92	123.63
24	C	506	CLA	C3D-C4D-ND	3.48	115.65	109.99
24	c	508	CLA	CHD-C4C-C3C	-3.48	119.70	124.77
24	b	617	CLA	CHD-C4C-C3C	-3.48	119.70	124.77
25	A	407	PHO	C1A-C2A-C3A	-3.48	99.53	102.84
24	a	2110	CLA	C4-C3-C5	3.48	121.26	115.23
24	b	611	CLA	C2B-C1B-NB	3.48	113.93	110.33
24	b	604	CLA	C1-O2A-CGA	3.47	125.06	116.65
24	D	404	CLA	C3B-C2B-C1B	-3.47	103.08	107.17
24	B	611	CLA	C4C-C3C-C2C	-3.47	101.84	106.89
24	b	618	CLA	O2D-CGD-CBD	3.47	117.30	111.23
36	b	625	HTG	C1'-S1-C1	3.47	107.95	100.45
24	b	615	CLA	C4C-C3C-C2C	-3.47	101.84	106.89
24	C	502	CLA	C1D-CHD-C4C	-3.47	118.65	126.02
24	b	615	CLA	O2A-CGA-CBA	3.47	122.41	111.83
24	b	616	CLA	C2C-C1C-NC	3.47	113.62	109.98
24	B	617	CLA	O2D-CGD-O1D	-3.46	117.10	123.85
24	d	405	CLA	C2C-C1C-NC	3.46	113.62	109.98
24	A	406	CLA	CMB-C2B-C1B	3.46	130.69	125.42
24	B	611	CLA	CMB-C2B-C1B	3.46	130.69	125.42
24	B	606	CLA	C4C-C3C-C2C	-3.46	101.86	106.89
24	b	614	CLA	CAC-C3C-C4C	3.46	129.29	124.79
31	x	801	PL9	C22-C23-C24	-3.46	119.71	127.62
24	C	505	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
36	B	625[A]	HTG	C1'-S1-C1	3.45	107.91	100.45
24	C	502	CLA	O2D-CGD-O1D	-3.45	117.12	123.85
24	C	506	CLA	C3D-C2D-C1D	-3.45	101.12	105.83
24	C	506	CLA	CAC-C3C-C4C	3.45	129.28	124.79
24	B	612	CLA	C1C-C2C-C3C	-3.45	103.35	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	411	LMG	O7-C10-C11	3.45	118.94	111.48
24	c	508	CLA	CAA-C2A-C3A	-3.45	103.68	113.00
24	B	608	CLA	C2C-C1C-NC	3.45	113.60	109.98
24	b	614	CLA	C1-C2-C3	-3.45	120.55	126.20
24	c	506	CLA	C2C-C1C-NC	3.45	113.60	109.98
24	c	513	CLA	C1D-CHD-C4C	-3.44	118.70	126.02
24	B	613	CLA	C2B-C1B-NB	3.44	113.89	110.33
24	c	512	CLA	C1C-C2C-C3C	-3.44	103.36	106.98
27	A	413	SQD	O48-C23-C24	3.44	122.32	111.83
24	c	503	CLA	CMC-C2C-C1C	3.44	130.41	125.03
24	B	607	CLA	C1D-CHD-C4C	-3.44	118.72	126.02
32	A	418[A]	K2I	BR1-C1-C2	3.44	120.08	116.06
29	A	414	LMT	C1'-O5'-C5'	3.43	120.43	113.72
24	C	507	CLA	C1D-CHD-C4C	-3.43	118.72	126.02
24	c	506	CLA	C1D-CHD-C4C	-3.43	118.72	126.02
24	c	504	CLA	C1C-C2C-C3C	-3.43	103.37	106.98
24	C	508	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
24	c	513	CLA	C1C-C2C-C3C	-3.43	103.37	106.98
24	c	505	CLA	C1-C2-C3	-3.43	120.58	126.20
41	H	101	RRX	C16-C17-C18	-3.43	122.47	127.28
24	C	509	CLA	C1C-C2C-C3C	-3.42	103.38	106.98
24	c	511	CLA	C1C-C2C-C3C	-3.42	103.38	106.98
24	C	512	CLA	CAC-C3C-C4C	3.42	129.24	124.79
38	c	518	DGD	C2G-O2G-C1B	-3.42	109.61	117.80
24	C	502	CLA	CMB-C2B-C1B	3.42	130.63	125.42
24	b	619	CLA	O2A-CGA-CBA	3.42	122.27	111.83
24	A	406	CLA	CBC-CAC-C3C	-3.42	103.15	112.42
29	j	1601	LMT	C1'-C2'-C3'	3.42	117.20	110.01
24	C	505	CLA	C2C-C1C-NC	3.42	113.57	109.98
24	b	611	CLA	C1C-C2C-C3C	-3.42	103.39	106.98
24	B	609	CLA	C2B-C1B-NB	3.41	113.87	110.33
24	B	604	CLA	O2A-CGA-CBA	3.41	122.25	111.83
24	c	513	CLA	C2B-C1B-NB	3.41	113.87	110.33
29	a	2103	LMT	C1'-O5'-C5'	3.41	120.39	113.72
24	B	615	CLA	C2B-C1B-NB	3.41	113.86	110.33
24	b	617	CLA	C2B-C1B-NB	3.41	113.86	110.33
24	B	603	CLA	C2C-C1C-NC	3.41	113.56	109.98
24	b	605	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
24	B	603	CLA	C1C-C2C-C3C	-3.41	103.39	106.98
24	D	405	CLA	C2B-C1B-NB	3.41	113.86	110.33
24	B	606	CLA	C3C-C4C-NC	3.41	114.80	110.43
27	f	102	SQD	O7-S-C6	3.40	111.87	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	D	409	LHG	C5-O7-C7	-3.40	109.65	117.80
24	c	505	CLA	O2D-CGD-CBD	3.40	117.18	111.23
24	B	616	CLA	CMB-C2B-C1B	3.40	130.60	125.42
24	b	617	CLA	C1C-C2C-C3C	-3.40	103.40	106.98
24	c	507	CLA	C1D-CHD-C4C	-3.40	118.80	126.02
24	c	514	CLA	C2B-C1B-NB	3.39	113.84	110.33
24	C	504	CLA	C4A-NA-C1A	3.39	108.23	106.68
24	C	506	CLA	C1-C2-C3	-3.39	120.64	126.20
24	c	512	CLA	C1D-CHD-C4C	-3.39	118.82	126.02
24	c	508	CLA	C4-C3-C5	3.38	121.10	115.23
24	b	617	CLA	C1D-CHD-C4C	-3.38	118.83	126.02
24	c	505	CLA	CHA-C1A-NA	-3.38	118.73	126.39
24	c	511	CLA	CHD-C4C-C3C	-3.38	119.84	124.77
24	C	505	CLA	C2B-C1B-NB	3.38	113.83	110.33
27	a	2115	SQD	O48-C23-C24	3.38	122.14	111.83
24	B	613	CLA	C4-C3-C5	3.38	121.09	115.23
31	A	417	PL9	C17-C18-C19	-3.38	119.89	127.62
24	a	2113	CLA	C1D-CHD-C4C	-3.38	118.84	126.02
24	b	607	CLA	C6-C5-C3	-3.37	105.25	113.47
24	D	401	CLA	CAA-C2A-C3A	-3.37	103.88	113.00
24	c	511	CLA	C4A-NA-C1A	3.37	108.22	106.68
24	C	504	CLA	C1D-CHD-C4C	-3.37	118.85	126.02
24	B	607	CLA	C2B-C1B-NB	3.37	113.82	110.33
24	b	609	CLA	C2B-C1B-NB	3.37	113.82	110.33
24	b	618	CLA	C2B-C1B-NB	3.37	113.82	110.33
31	d	407	PL9	C42-C43-C44	-3.37	119.92	127.62
24	B	617	CLA	CMB-C2B-C1B	3.37	130.55	125.42
24	c	509	CLA	C2B-C1B-NB	3.37	113.82	110.33
24	b	611	CLA	C2C-C1C-NC	3.37	113.52	109.98
24	b	609	CLA	C1C-C2C-C3C	-3.36	103.44	106.98
24	c	515	CLA	C1D-CHD-C4C	-3.36	118.87	126.02
27	a	2102	SQD	O48-C23-C24	3.36	122.09	111.83
24	a	2110	CLA	C3C-C4C-NC	3.36	114.74	110.43
24	c	515	CLA	C1C-C2C-C3C	-3.36	103.44	106.98
24	B	614	CLA	C2B-C1B-NB	3.36	113.81	110.33
24	c	507	CLA	C2B-C1B-NB	3.36	113.81	110.33
24	C	506	CLA	C2C-C1C-NC	3.36	113.51	109.98
25	A	408	PHO	C4-C3-C5	3.36	121.06	115.23
24	C	506	CLA	CHA-C1A-NA	-3.36	118.79	126.39
24	B	610	CLA	CMB-C2B-C1B	3.36	130.53	125.42
24	B	606	CLA	CMB-C2B-C1B	3.35	130.53	125.42
24	C	506	CLA	C1D-CHD-C4C	-3.35	118.89	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	CHD-C4C-C3C	-3.35	119.89	124.77
39	l	101	LHG	O7-C7-C8	3.35	118.72	111.48
24	A	406	CLA	C1-C2-C3	-3.35	120.71	126.20
24	b	606	CLA	CHD-C4C-C3C	-3.35	119.89	124.77
24	B	603	CLA	C1D-CHD-C4C	-3.34	118.91	126.02
36	b	625	HTG	C6-C5-C4	-3.34	104.81	113.02
24	C	512	CLA	CHD-C4C-C3C	-3.34	119.90	124.77
24	D	405	CLA	C4-C3-C5	3.34	121.03	115.23
24	A	409	CLA	CHD-C4C-C3C	-3.34	119.90	124.77
24	B	609	CLA	C4C-C3C-C2C	-3.34	102.03	106.89
24	B	602	CLA	C2B-C1B-NB	3.34	113.79	110.33
24	c	508	CLA	C4B-C3B-C2B	-3.34	103.15	107.30
24	b	614	CLA	C1D-CHD-C4C	-3.33	118.93	126.02
24	B	611	CLA	C3C-C4C-NC	3.33	114.70	110.43
24	C	511	CLA	CHD-C4C-C3C	-3.33	119.92	124.77
24	B	615	CLA	C3B-C4B-NB	3.33	113.50	110.53
24	c	510	CLA	C1D-CHD-C4C	-3.33	118.94	126.02
24	B	607	CLA	C2C-C1C-NC	3.33	113.48	109.98
24	a	2113	CLA	C3C-C4C-NC	3.32	114.69	110.43
24	b	605	CLA	C2C-C1C-NC	3.32	113.47	109.98
24	a	2113	CLA	CAA-C2A-C3A	-3.32	104.02	113.00
24	b	606	CLA	CAA-C2A-C3A	-3.32	104.03	113.00
24	B	616	CLA	C4C-C3C-C2C	-3.32	102.06	106.89
24	a	2110	CLA	C1-C2-C3	-3.31	120.77	126.20
24	C	514	CLA	C1C-C2C-C3C	-3.31	103.50	106.98
24	b	614	CLA	C2C-C1C-NC	3.31	113.46	109.98
24	c	506	CLA	C2B-C1B-NB	3.31	113.76	110.33
26	C	515	BCR	C11-C10-C9	-3.31	122.63	127.28
36	b	625	HTG	C1-C2-C3	3.31	117.02	110.55
27	B	621	SQD	C4-C3-C2	-3.31	105.02	110.83
24	B	606	CLA	C2B-C1B-NB	3.31	113.75	110.33
24	C	512	CLA	C1D-CHD-C4C	-3.31	119.00	126.02
24	B	611	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
24	b	605	CLA	CAA-C2A-C3A	-3.30	104.07	113.00
24	c	503	CLA	C2C-C1C-NC	3.30	113.45	109.98
24	B	603	CLA	C2B-C1B-NB	3.30	113.75	110.33
26	C	515	BCR	C38-C26-C25	-3.30	120.88	124.48
29	m	103	LMT	C1'-O5'-C5'	3.30	120.16	113.72
24	c	509	CLA	CHD-C4C-C3C	-3.30	119.96	124.77
24	c	504	CLA	O2A-CGA-CBA	3.30	121.89	111.83
39	d	409	LHG	O8-C23-O10	-3.30	115.38	123.63
24	a	2110	CLA	C4B-C3B-C2B	-3.29	103.20	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	V	201	HEC	CBC-CAC-C3C	-3.29	120.85	127.43
26	A	410	BCR	C38-C26-C25	-3.29	120.89	124.48
24	B	606	CLA	C4-C3-C5	3.29	120.94	115.23
24	b	619	CLA	CAC-C3C-C4C	3.29	129.07	124.79
24	B	610	CLA	C4C-C3C-C2C	-3.29	102.10	106.89
32	a	2118[A]	K2I	BR-C4-C5	3.29	119.91	116.06
24	C	509	CLA	CHD-C4C-C3C	-3.29	119.98	124.77
24	a	2109	CLA	C3C-C4C-NC	3.28	114.64	110.43
24	c	513	CLA	C4A-NA-C1A	3.28	108.17	106.68
24	c	509	CLA	CBC-CAC-C3C	-3.28	103.53	112.42
24	D	404	CLA	CHD-C1D-ND	-3.28	120.19	124.80
24	a	2109	CLA	O2A-CGA-CBA	3.28	121.82	111.83
24	b	607	CLA	C3D-C4D-ND	3.27	115.31	109.99
24	C	512	CLA	O2D-CGD-CBD	3.27	116.95	111.23
24	B	613	CLA	C1C-C2C-C3C	-3.27	103.54	106.98
24	b	614	CLA	C1C-C2C-C3C	-3.27	103.54	106.98
24	c	507	CLA	C3C-C4C-NC	3.27	114.61	110.43
24	B	604	CLA	CHD-C4C-C3C	-3.27	120.01	124.77
24	c	507	CLA	CHD-C4C-C3C	-3.27	120.01	124.77
24	B	611	CLA	O2A-CGA-CBA	3.26	121.79	111.83
24	b	605	CLA	C1D-CHD-C4C	-3.26	119.08	126.02
24	b	613	CLA	C1D-CHD-C4C	-3.26	119.08	126.02
24	B	606	CLA	C1D-CHD-C4C	-3.26	119.09	126.02
24	a	2110	CLA	O2A-CGA-O1A	-3.26	115.47	123.63
28	C	526	LMG	C9-C8-C7	-3.26	104.18	111.78
24	A	406	CLA	C2C-C1C-NC	3.26	113.41	109.98
24	B	609	CLA	C1D-CHD-C4C	-3.26	119.09	126.02
24	c	505	CLA	C3C-C4C-NC	3.26	114.61	110.43
24	A	406	CLA	CAA-C2A-C3A	-3.26	104.20	113.00
24	B	616	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
24	A	406	CLA	C1D-CHD-C4C	-3.25	119.11	126.02
24	c	514	CLA	CHD-C4C-C3C	-3.25	120.04	124.77
24	B	606	CLA	CMC-C2C-C1C	3.25	130.11	125.03
24	C	511	CLA	CBC-CAC-C3C	-3.25	103.61	112.42
24	c	512	CLA	C2B-C1B-NB	3.25	113.69	110.33
24	b	604	CLA	C1D-CHD-C4C	-3.24	119.12	126.02
24	C	502	CLA	CHD-C4C-C3C	-3.24	120.04	124.77
27	A	411	SQD	O9-S-C6	3.24	111.60	106.76
24	b	612	CLA	C2B-C1B-NB	3.24	113.68	110.33
24	c	505	CLA	C4C-C3C-C2C	-3.24	102.18	106.89
26	K	101	BCR	C33-C5-C6	-3.24	120.95	124.48
38	C	518	DGD	O1G-C1A-O1A	-3.24	115.54	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	614	CLA	CMA-C3A-C4A	-3.23	103.08	111.77
39	L	101	LHG	O8-C23-C24	3.23	121.69	111.83
24	B	604	CLA	O2A-CGA-O1A	-3.23	115.54	123.63
24	b	619	CLA	C2B-C1B-NB	3.23	113.68	110.33
24	B	602	CLA	O2A-CGA-CBA	3.23	121.69	111.83
24	C	504	CLA	CBC-CAC-C3C	-3.23	103.66	112.42
24	B	616	CLA	C11-C10-C8	-3.23	105.22	115.97
24	d	401	CLA	C3C-C4C-NC	3.23	114.57	110.43
24	B	604	CLA	C1D-CHD-C4C	-3.23	119.15	126.02
24	A	405	CLA	CAA-C2A-C1A	-3.23	101.40	111.97
24	b	612	CLA	C1-C2-C3	-3.23	120.91	126.20
24	B	617	CLA	C4-C3-C5	3.22	120.83	115.23
24	c	512	CLA	CBC-CAC-C3C	-3.22	103.68	112.42
31	D	407	PL9	C25-C24-C26	3.22	120.82	115.23
24	b	612	CLA	CHD-C4C-C3C	-3.22	120.08	124.77
24	C	503	CLA	CBC-CAC-C3C	-3.22	103.69	112.42
24	b	618	CLA	CMB-C2B-C1B	3.22	130.32	125.42
24	a	2110	CLA	CHD-C1D-ND	-3.22	120.27	124.80
24	B	613	CLA	CMC-C2C-C1C	3.22	130.07	125.03
39	D	409	LHG	O7-C7-C8	3.22	118.45	111.48
24	C	509	CLA	C1-C2-C3	-3.22	120.92	126.20
24	C	512	CLA	C1-C2-C3	-3.22	120.92	126.20
25	a	2112	PHO	C1A-C2A-C3A	-3.22	99.78	102.84
24	A	405	CLA	C2B-C1B-NB	3.22	113.66	110.33
24	C	512	CLA	C2B-C1B-NB	3.22	113.66	110.33
24	a	2109	CLA	C2B-C1B-NB	3.22	113.66	110.33
24	D	405	CLA	CHD-C4C-C3C	-3.22	120.08	124.77
24	C	509	CLA	C4C-C3C-C2C	-3.21	102.22	106.89
24	B	612	CLA	C2C-C1C-NC	3.21	113.36	109.98
24	d	401	CLA	CMA-C3A-C2A	-3.21	101.57	113.98
24	b	607	CLA	CMC-C2C-C1C	3.21	130.05	125.03
41	h	702	RRX	C11-C10-C9	-3.20	122.78	127.28
24	D	404	CLA	C1D-CHD-C4C	-3.20	119.21	126.02
24	C	504	CLA	C3D-C4D-ND	3.20	115.19	109.99
24	B	616	CLA	C2C-C1C-NC	3.20	113.34	109.98
24	b	611	CLA	C3C-C4C-NC	3.20	114.53	110.43
24	B	617	CLA	C2B-C1B-NB	3.20	113.64	110.33
38	D	408	DGD	O1G-C1A-C2A	3.20	121.59	111.83
24	C	502	CLA	CBC-CAC-C3C	-3.20	103.75	112.42
24	C	510	CLA	C1D-CHD-C4C	-3.20	119.22	126.02
24	b	614	CLA	CHD-C4C-C3C	-3.20	120.11	124.77
24	b	607	CLA	CMB-C2B-C1B	3.19	130.28	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	615	CLA	C4-C3-C5	3.19	120.77	115.23
24	b	615	CLA	C1C-C2C-C3C	-3.19	103.62	106.98
29	m	102	LMT	O1'-C1'-C2'	3.19	113.12	108.27
43	v	201	HEC	CBC-CAC-C3C	-3.19	121.05	127.43
24	b	611	CLA	C4B-C3B-C2B	-3.19	103.33	107.30
24	C	503	CLA	C2B-C1B-NB	3.19	113.64	110.33
24	c	511	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
24	b	610	CLA	CAA-C2A-C3A	-3.19	104.39	113.00
24	B	607	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
24	B	611	CLA	CAA-CBA-CGA	-3.18	104.17	113.21
24	b	616	CLA	CHD-C4C-C3C	-3.18	120.14	124.77
24	c	505	CLA	CMB-C2B-C1B	3.18	130.26	125.42
24	c	515	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
24	c	504	CLA	C3C-C4C-NC	3.18	114.50	110.43
24	c	510	CLA	C4-C3-C5	3.18	120.74	115.23
24	b	613	CLA	C1C-C2C-C3C	-3.18	103.64	106.98
24	b	615	CLA	CMC-C2C-C1C	3.18	130.00	125.03
29	a	2120	LMT	C1'-O5'-C5'	3.18	119.92	113.72
24	C	512	CLA	C1C-C2C-C3C	-3.17	103.64	106.98
24	b	611	CLA	O2A-CGA-CBA	3.17	121.50	111.83
24	B	604	CLA	C2B-C1B-NB	3.17	113.61	110.33
24	C	507	CLA	C2B-C1B-NB	3.17	113.61	110.33
24	c	512	CLA	C3B-C4B-NB	3.17	113.36	110.53
24	B	609	CLA	CHD-C4C-C3C	-3.17	120.16	124.77
24	a	2113	CLA	C4B-C3B-C2B	-3.17	103.37	107.30
27	F	101	SQD	C1-C2-C3	-3.16	103.35	110.01
24	a	2109	CLA	C4C-C3C-C2C	-3.16	102.29	106.89
29	J	102	LMT	C1'-O5'-C5'	3.16	119.90	113.72
26	Y	302	BCR	C15-C14-C13	-3.16	122.84	127.28
24	b	607	CLA	CHA-C1A-NA	-3.16	119.23	126.39
24	B	609	CLA	C3C-C4C-NC	3.16	114.48	110.43
24	B	609	CLA	C2C-C1C-NC	3.16	113.30	109.98
38	C	519	DGD	O1G-C1A-C2A	3.15	121.45	111.83
24	b	610	CLA	C2B-C1B-NB	3.15	113.59	110.33
24	B	617	CLA	C1-C2-C3	-3.15	121.03	126.20
24	A	405	CLA	C3B-C4B-NB	3.15	113.34	110.53
24	b	610	CLA	CHD-C4C-C3C	-3.15	120.18	124.77
24	b	616	CLA	C4C-C3C-C2C	-3.15	102.31	106.89
24	c	509	CLA	C4A-NA-C1A	3.15	108.11	106.68
24	C	506	CLA	C3C-C4C-NC	3.15	114.46	110.43
38	c	520	DGD	O3G-C3G-C2G	-3.15	103.17	110.82
24	B	610	CLA	C3C-C4C-NC	3.14	114.46	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	101	BCR	C20-C21-C22	-3.14	122.87	127.28
26	b	620	BCR	C24-C23-C22	-3.14	121.59	126.23
24	c	511	CLA	C3C-C4C-NC	3.14	114.45	110.43
24	b	616	CLA	C3C-C4C-NC	3.14	114.45	110.43
39	D	409	LHG	O8-C23-O10	-3.13	115.79	123.63
39	D	409	LHG	O8-C23-C24	3.13	121.39	111.83
29	a	2103	LMT	C2'-C3'-C4'	-3.13	102.57	109.68
24	C	508	CLA	C3D-C4D-ND	3.13	115.08	109.99
24	B	616	CLA	CAC-C3C-C4C	3.13	128.86	124.79
29	f	101	LMT	O1'-C1'-C2'	3.13	113.03	108.27
24	a	2110	CLA	C4C-C3C-C2C	-3.13	102.34	106.89
24	a	2109	CLA	O2A-CGA-O1A	-3.13	115.80	123.63
24	B	610	CLA	CAC-C3C-C4C	3.13	128.86	124.79
24	c	503	CLA	CHD-C1D-ND	-3.13	120.40	124.80
24	a	2113	CLA	C3B-C4B-NB	3.12	113.32	110.53
31	A	417	PL9	C20-C19-C21	3.12	120.64	115.23
26	k	2003	BCR	C33-C5-C6	-3.12	121.08	124.48
24	B	613	CLA	C4B-C3B-C2B	-3.12	103.42	107.30
24	b	611	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
24	d	404	CLA	CHD-C4C-C3C	-3.12	120.23	124.77
24	A	406	CLA	CHD-C1D-ND	-3.12	120.42	124.80
24	c	512	CLA	C2C-C1C-NC	3.11	113.25	109.98
24	b	618	CLA	C1-O2A-CGA	3.11	124.19	116.65
24	b	608	CLA	C4-C3-C5	3.11	120.63	115.23
27	a	2102	SQD	O8-S-C6	3.11	111.97	105.97
24	B	614	CLA	CBC-CAC-C3C	-3.11	104.00	112.42
24	c	511	CLA	C2C-C1C-NC	3.11	113.24	109.98
39	L	101	LHG	O7-C7-C8	3.11	118.20	111.48
24	b	605	CLA	CBC-CAC-C3C	-3.10	104.00	112.42
24	a	2109	CLA	CAC-C3C-C4C	3.10	128.83	124.79
38	h	703	DGD	O1G-C1A-C2A	3.10	121.30	111.83
24	B	605	CLA	C1-C2-C3	-3.10	121.11	126.20
24	c	512	CLA	C4B-C3B-C2B	-3.10	103.44	107.30
24	C	510	CLA	CHD-C4C-C3C	-3.10	120.25	124.77
24	B	605	CLA	O2A-CGA-CBA	3.10	121.29	111.83
24	B	613	CLA	CHD-C1D-ND	-3.10	120.44	124.80
24	C	509	CLA	CAA-C2A-C3A	-3.10	104.62	113.00
24	B	609	CLA	C1C-C2C-C3C	-3.10	103.72	106.98
38	H	102	DGD	O1G-C1A-C2A	3.09	121.27	111.83
39	d	410	LHG	O7-C7-C8	3.09	118.17	111.48
24	a	2110	CLA	C1D-CHD-C4C	-3.09	119.45	126.02
24	B	611	CLA	C2C-C1C-NC	3.09	113.23	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	508	CLA	C3B-C4B-NB	3.09	113.29	110.53
29	M	101	LMT	C1'-O5'-C5'	-3.09	107.68	113.72
24	B	602	CLA	C4C-C3C-C2C	-3.09	102.39	106.89
24	b	614	CLA	C2B-C1B-NB	3.09	113.53	110.33
24	c	507	CLA	CHA-C1A-NA	-3.09	119.40	126.39
24	d	405	CLA	C2B-C1B-NB	3.09	113.53	110.33
24	B	609	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
24	b	616	CLA	C3B-C4B-NB	3.09	113.28	110.53
25	a	2112	PHO	CMB-C2B-C3B	3.09	130.85	124.68
24	A	405	CLA	CHD-C1D-ND	-3.08	120.46	124.80
24	C	514	CLA	C4C-C3C-C2C	-3.08	102.41	106.89
28	b	623	LMG	O8-C28-C29	3.08	121.23	111.83
24	c	513	CLA	O2A-CGA-CBA	3.08	121.22	111.83
24	A	405	CLA	CHD-C4C-C3C	-3.08	120.29	124.77
24	B	611	CLA	CAC-C3C-C4C	3.08	128.79	124.79
24	B	611	CLA	C2B-C1B-NB	3.08	113.52	110.33
24	C	506	CLA	CHD-C4C-C3C	-3.07	120.29	124.77
27	B	621	SQD	O7-S-C6	3.07	111.34	106.76
24	c	504	CLA	C4C-C3C-C2C	-3.07	102.42	106.89
24	C	502	CLA	C2C-C1C-NC	3.07	113.21	109.98
24	B	617	CLA	C3C-C4C-NC	3.07	114.36	110.43
24	D	401	CLA	C4B-C3B-C2B	-3.07	103.49	107.30
24	B	611	CLA	C1D-CHD-C4C	-3.07	119.50	126.02
24	C	508	CLA	C3C-C4C-NC	3.06	114.36	110.43
24	B	606	CLA	CAC-C3C-C4C	3.06	128.78	124.79
24	c	510	CLA	C2C-C1C-NC	3.06	113.20	109.98
24	d	405	CLA	CHD-C4C-C3C	-3.06	120.31	124.77
24	B	613	CLA	C4C-C3C-C2C	-3.06	102.43	106.89
24	C	512	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
24	B	605	CLA	C2B-C1B-NB	3.06	113.50	110.33
29	a	2120	LMT	C1B-O5B-C5B	3.06	119.70	113.72
24	B	616	CLA	C3C-C4C-NC	3.06	114.35	110.43
24	B	612	CLA	C2B-C1B-NB	3.06	113.50	110.33
24	B	613	CLA	C3B-C4B-NB	3.06	113.26	110.53
24	b	610	CLA	C1D-CHD-C4C	-3.06	119.53	126.02
29	i	104	LMT	O5'-C1'-C2'	3.05	116.65	110.37
24	b	615	CLA	C2C-C1C-NC	3.05	113.19	109.98
24	c	512	CLA	C6-C7-C8	-3.05	105.81	115.97
24	c	513	CLA	C2C-C1C-NC	3.05	113.19	109.98
41	H	101	RRX	C7-C8-C9	-3.05	121.72	126.23
24	c	515	CLA	CAA-C2A-C3A	-3.05	104.75	113.00
24	D	404	CLA	O2A-CGA-CBA	3.05	121.14	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	O2A-CGA-CBA	3.05	121.14	111.83
24	D	401	CLA	C1D-CHD-C4C	-3.05	119.54	126.02
24	A	405	CLA	C3C-C4C-NC	3.05	114.33	110.43
24	b	619	CLA	C2C-C1C-NC	3.04	113.18	109.98
24	B	607	CLA	CBC-CAC-C3C	-3.04	104.18	112.42
24	b	607	CLA	C3B-C4B-NB	3.04	113.24	110.53
24	c	506	CLA	C4-C3-C5	3.04	120.50	115.23
24	C	507	CLA	CHD-C4C-C3C	-3.04	120.34	124.77
24	C	507	CLA	C3C-C4C-NC	3.04	114.32	110.43
24	b	614	CLA	CMA-C3A-C4A	-3.04	103.61	111.77
24	d	404	CLA	O2A-CGA-CBA	3.04	121.10	111.83
24	C	504	CLA	C2C-C1C-NC	3.04	113.17	109.98
24	C	512	CLA	C2C-C1C-NC	3.04	113.17	109.98
28	c	521	LMG	O8-C28-C29	3.04	121.10	111.83
24	B	605	CLA	CAC-C3C-C4C	3.04	128.74	124.79
24	c	504	CLA	C2C-C1C-NC	3.04	113.17	109.98
24	b	614	CLA	C3C-C4C-NC	3.04	114.32	110.43
31	d	407	PL9	C37-C38-C39	-3.03	120.68	127.62
24	A	409	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
24	b	614	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
24	C	506	CLA	C1C-C2C-C3C	-3.03	103.79	106.98
24	c	512	CLA	C1-C2-C3	-3.03	121.23	126.20
24	c	507	CLA	CBC-CAC-C3C	-3.03	104.21	112.42
24	b	613	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
24	c	515	CLA	C2C-C1C-NC	3.03	113.16	109.98
24	a	2113	CLA	C4C-C3C-C2C	-3.02	102.49	106.89
24	b	612	CLA	C3B-C4B-NB	3.02	113.23	110.53
24	c	509	CLA	C4-C3-C5	3.02	120.48	115.23
24	B	614	CLA	C1D-CHD-C4C	-3.02	119.59	126.02
24	D	404	CLA	CMC-C2C-C1C	3.02	129.76	125.03
24	c	507	CLA	CMC-C2C-C1C	3.02	129.76	125.03
38	C	518	DGD	O2G-C1B-O1B	-3.02	116.64	123.70
24	c	513	CLA	CBC-CAC-C3C	-3.02	104.23	112.42
24	C	504	CLA	CMB-C2B-C1B	3.02	130.02	125.42
24	B	610	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
38	C	517	DGD	O3G-C3G-C2G	-3.02	103.47	110.82
24	B	603	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
24	b	615	CLA	O2A-CGA-O1A	-3.02	116.08	123.63
24	b	610	CLA	C2C-C1C-NC	3.02	113.15	109.98
24	a	2109	CLA	CHD-C4C-C3C	-3.02	120.37	124.77
24	c	504	CLA	O2A-CGA-O1A	-3.01	116.09	123.63
24	b	607	CLA	C4A-NA-C1A	3.01	108.05	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
24	d	405	CLA	CAC-C3C-C4C	3.01	128.71	124.79
24	C	505	CLA	CBC-CAC-C3C	-3.01	104.26	112.42
24	c	515	CLA	CHD-C4C-C3C	-3.01	120.39	124.77
24	A	409	CLA	CMA-C3A-C2A	-3.01	102.35	113.98
38	c	519	DGD	C3B-C2B-C1B	-3.01	102.68	113.69
24	C	504	CLA	C1-O2A-CGA	3.01	123.93	116.65
24	b	608	CLA	C3C-C4C-NC	3.01	114.28	110.43
24	c	511	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
43	v	201	HEC	CMD-C2D-C1D	3.00	129.99	125.42
24	C	509	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
36	B	627	HTG	C3-C4-C5	3.00	115.67	110.23
24	B	607	CLA	CHD-C1D-ND	-3.00	120.59	124.80
41	h	702	RRX	C10-C11-C12	-3.00	114.52	123.20
24	b	616	CLA	C4B-C3B-C2B	-3.00	103.58	107.30
24	c	505	CLA	C3D-C4D-ND	2.99	114.86	109.99
24	A	405	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
24	B	605	CLA	C1D-CHD-C4C	-2.99	119.66	126.02
24	C	511	CLA	C4-C3-C5	2.99	120.42	115.23
39	l	101	LHG	O8-C23-C24	2.99	120.95	111.83
24	B	606	CLA	O2A-CGA-O1A	-2.99	116.15	123.63
24	C	511	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
24	C	505	CLA	CHD-C1D-ND	-2.99	120.60	124.80
27	a	2115	SQD	O8-S-C6	2.99	111.74	105.97
24	C	513	CLA	O2A-CGA-CBA	2.99	120.94	111.83
24	c	515	CLA	C3C-C4C-NC	2.99	114.25	110.43
26	Y	302	BCR	C37-C22-C23	2.99	122.65	118.09
24	B	610	CLA	C1C-C2C-C3C	-2.98	103.84	106.98
29	a	2103	LMT	O1B-C4'-C3'	2.98	114.81	107.23
24	d	404	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
26	K	101	BCR	C7-C8-C9	-2.98	121.82	126.23
24	C	512	CLA	C4-C3-C5	2.98	120.40	115.23
24	C	514	CLA	CBC-CAC-C3C	-2.98	104.34	112.42
24	B	604	CLA	CMC-C2C-C1C	2.98	129.69	125.03
24	b	608	CLA	CMC-C2C-C1C	2.98	129.69	125.03
24	d	404	CLA	C3B-C4B-NB	2.98	113.19	110.53
24	c	512	CLA	C4C-C3C-C2C	-2.98	102.56	106.89
24	a	2110	CLA	CBC-CAC-C3C	-2.98	104.36	112.42
24	C	512	CLA	C3C-C4C-NC	2.97	114.24	110.43
24	b	617	CLA	C2C-C1C-NC	2.97	113.10	109.98
24	A	405	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
24	D	404	CLA	CBC-CAC-C3C	-2.97	104.37	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	512	CLA	CBC-CAC-C3C	-2.97	104.37	112.42
41	h	702	RRX	C16-C17-C18	-2.97	123.11	127.28
26	t	102	BCR	C3-C4-C5	-2.97	108.76	114.06
24	b	608	CLA	C1D-CHD-C4C	-2.97	119.71	126.02
24	C	511	CLA	C11-C10-C8	-2.97	106.09	115.97
27	a	2115	SQD	C44-O6-C1	-2.97	107.43	113.80
24	B	613	CLA	C3C-C4C-NC	2.97	114.23	110.43
24	c	509	CLA	C1-C2-C3	-2.97	121.34	126.20
24	B	605	CLA	O2A-CGA-O1A	-2.96	116.22	123.63
26	D	406	BCR	C33-C5-C6	-2.96	121.25	124.48
24	b	618	CLA	C2C-C1C-NC	2.96	113.09	109.98
24	a	2109	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
24	b	613	CLA	CHD-C1D-ND	-2.96	120.64	124.80
24	C	507	CLA	O2A-CGA-CBA	2.96	120.85	111.83
24	d	404	CLA	CAA-C2A-C3A	-2.96	105.01	113.00
24	b	614	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
26	b	621	BCR	C8-C7-C6	-2.95	119.13	127.00
24	C	503	CLA	CHA-C1A-NA	-2.95	119.72	126.39
24	a	2110	CLA	O2A-CGA-CBA	2.94	120.81	111.83
24	B	607	CLA	C3C-C4C-NC	2.94	114.20	110.43
24	C	512	CLA	CHA-C1A-NA	-2.94	119.73	126.39
24	B	602	CLA	CHD-C1D-ND	-2.94	120.66	124.80
24	d	405	CLA	CMC-C2C-C1C	2.94	129.63	125.03
24	b	615	CLA	C3B-C4B-NB	2.94	113.16	110.53
24	B	608	CLA	C4B-C3B-C2B	-2.94	103.65	107.30
25	A	408	PHO	CMA-C3A-C4A	-2.94	108.28	114.61
41	h	702	RRX	C24-C23-C22	-2.94	121.89	126.23
32	A	419	K2I	C-C1-C2	-2.94	121.09	123.59
24	b	604	CLA	C2C-C1C-NC	2.94	113.07	109.98
32	a	2118[A]	K2I	BR1-C1-C2	2.94	119.50	116.06
24	b	609	CLA	C2C-C1C-NC	2.94	113.07	109.98
24	b	615	CLA	C2B-C1B-NB	2.94	113.37	110.33
24	c	507	CLA	C4C-C3C-C2C	-2.94	102.62	106.89
24	c	506	CLA	C3B-C4B-NB	2.93	113.15	110.53
24	C	505	CLA	C1-O2A-CGA	2.93	123.75	116.65
24	B	608	CLA	CHD-C4C-C3C	-2.93	120.50	124.77
24	b	619	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
24	b	609	CLA	O2A-CGA-O1A	-2.93	116.29	123.63
24	b	609	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
36	B	624	HTG	C1'-S1-C1	2.93	106.78	100.45
39	D	411	LHG	O7-C7-C8	2.93	117.82	111.48
24	b	610	CLA	O2A-CGA-O1A	-2.93	116.30	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	615	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
24	b	618	CLA	C4-C3-C5	2.93	120.31	115.23
24	d	404	CLA	C3C-C4C-NC	2.93	114.18	110.43
24	C	507	CLA	O2A-CGA-O1A	-2.93	116.30	123.63
24	d	404	CLA	C4-C3-C5	2.93	120.31	115.23
24	B	605	CLA	CMB-C2B-C1B	2.93	129.88	125.42
24	B	611	CLA	C1C-C2C-C3C	-2.93	103.90	106.98
24	B	602	CLA	C1C-C2C-C3C	-2.92	103.90	106.98
36	B	627	HTG	O5-C5-C4	2.92	114.97	109.70
24	B	617	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
24	B	615	CLA	CBC-CAC-C3C	-2.92	104.50	112.42
24	C	504	CLA	CMC-C2C-C1C	2.92	129.60	125.03
24	B	617	CLA	C3B-C4B-NB	2.92	113.14	110.53
27	a	2115	SQD	O9-S-C6	2.92	111.12	106.76
24	C	503	CLA	C3C-C4C-NC	2.92	114.17	110.43
26	C	516	BCR	C37-C22-C23	2.92	122.55	118.09
24	A	405	CLA	CMA-C3A-C4A	-2.92	103.93	111.77
24	b	607	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
26	T	101	BCR	C11-C10-C9	-2.92	123.19	127.28
24	b	605	CLA	CHD-C4C-C3C	-2.92	120.52	124.77
26	k	2003	BCR	C38-C26-C25	-2.92	121.30	124.48
24	B	607	CLA	C4-C3-C5	2.92	120.29	115.23
25	a	2112	PHO	C4-C3-C5	2.91	120.28	115.23
24	b	616	CLA	C2B-C1B-NB	2.91	113.35	110.33
27	F	101	SQD	O48-C23-C24	2.91	120.71	111.83
24	d	404	CLA	C2B-C1B-NB	2.91	113.34	110.33
24	d	404	CLA	CMB-C2B-C1B	2.91	129.85	125.42
24	b	612	CLA	C1D-CHD-C4C	-2.91	119.84	126.02
24	C	505	CLA	C4A-NA-C1A	2.91	108.00	106.68
27	A	411	SQD	O48-C23-C24	2.91	120.69	111.83
38	C	519	DGD	C2G-O2G-C1B	-2.90	110.85	117.80
31	d	407	PL9	C40-C39-C41	2.90	120.26	115.23
24	B	602	CLA	CMB-C2B-C1B	2.90	129.84	125.42
24	D	405	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
24	B	603	CLA	C3C-C4C-NC	2.90	114.15	110.43
29	A	420	LMT	O5'-C5'-C4'	2.90	115.72	109.72
26	c	517	BCR	C21-C20-C19	-2.90	114.80	123.20
24	c	510	CLA	C4B-C3B-C2B	-2.90	103.70	107.30
26	c	517	BCR	C15-C14-C13	-2.90	123.22	127.28
24	A	406	CLA	C4B-C3B-C2B	-2.90	103.70	107.30
24	C	503	CLA	C4C-C3C-C2C	-2.90	102.68	106.89
24	c	513	CLA	O2A-CGA-O1A	-2.89	116.39	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	102	SQD	C4-C3-C2	2.89	115.91	110.83
28	c	522	LMG	O8-C28-C29	2.89	120.66	111.83
24	b	608	CLA	CHD-C4C-NC	2.89	128.72	124.23
24	C	508	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
24	b	605	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
24	B	604	CLA	C3C-C4C-NC	2.89	114.13	110.43
27	L	102	SQD	O48-C23-C24	2.89	120.65	111.83
24	B	615	CLA	CHD-C1D-ND	-2.89	120.73	124.80
24	b	618	CLA	CHD-C1D-ND	-2.89	120.74	124.80
24	b	604	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
24	c	508	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
24	d	404	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
24	C	513	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
24	b	616	CLA	C4A-NA-C1A	2.88	108.00	106.68
24	c	508	CLA	O2A-CGA-O1A	-2.88	116.41	123.63
24	C	505	CLA	CHD-C4C-C3C	-2.88	120.57	124.77
24	C	513	CLA	C3C-C4C-NC	2.88	114.12	110.43
24	b	613	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
36	b	625	HTG	C1-O5-C5	2.88	117.73	112.56
24	C	507	CLA	CAA-C2A-C3A	-2.88	105.21	113.00
24	C	509	CLA	C2C-C1C-NC	2.88	113.01	109.98
24	a	2113	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
36	C	522	HTG	O5-C5-C4	2.88	114.89	109.70
24	C	506	CLA	C2B-C1B-NB	2.88	113.31	110.33
24	c	507	CLA	CAC-C3C-C4C	2.88	128.53	124.79
24	b	618	CLA	CED-O2D-CGD	2.87	122.44	115.92
36	c	524	HTG	C1-O5-C5	2.87	117.72	112.56
24	b	607	CLA	C2B-C1B-NB	2.87	113.31	110.33
24	B	603	CLA	C1-C2-C3	-2.87	121.49	126.20
24	A	409	CLA	C3B-C4B-NB	2.87	113.09	110.53
24	C	509	CLA	C3C-C4C-NC	2.87	114.11	110.43
29	B	623	LMT	C1B-O5B-C5B	2.87	119.32	113.72
24	C	511	CLA	C1D-CHD-C4C	-2.87	119.92	126.02
26	c	516	BCR	C11-C10-C9	-2.87	123.25	127.28
24	c	509	CLA	C3B-C4B-NB	2.87	113.09	110.53
24	b	609	CLA	C4C-C3C-C2C	-2.87	102.72	106.89
24	b	618	CLA	CBC-CAC-C3C	-2.86	104.66	112.42
24	b	614	CLA	O2A-CGA-CBA	2.86	120.56	111.83
27	F	101	SQD	O7-S-C6	2.86	111.03	106.76
24	b	606	CLA	C3B-C4B-NB	2.86	113.08	110.53
26	K	101	BCR	C11-C10-C9	-2.86	123.27	127.28
24	D	404	CLA	C4B-C3B-C2B	-2.86	103.75	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	CLA	C4B-C3B-C2B	-2.86	103.75	107.30
24	B	616	CLA	C1C-C2C-C3C	-2.86	103.97	106.98
24	C	507	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
24	B	610	CLA	C2C-C1C-NC	2.86	112.98	109.98
24	b	609	CLA	CBC-CAC-C3C	-2.86	104.67	112.42
24	C	508	CLA	CHA-C1A-NA	-2.86	119.92	126.39
31	x	801	PL9	C35-C34-C36	2.86	120.19	115.23
31	D	407	PL9	C42-C43-C44	-2.86	121.09	127.62
24	b	611	CLA	C3B-C4B-NB	2.86	113.08	110.53
24	B	612	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
24	C	505	CLA	C1D-CHD-C4C	-2.85	119.95	126.02
24	A	406	CLA	O2A-CGA-O1A	-2.85	116.49	123.63
26	K	101	BCR	C24-C23-C22	-2.85	122.02	126.23
24	C	507	CLA	CMC-C2C-C1C	2.85	129.49	125.03
24	c	510	CLA	C3C-C4C-NC	2.85	114.08	110.43
24	c	515	CLA	O2A-CGA-CBA	2.85	120.53	111.83
26	C	515	BCR	C23-C24-C25	-2.85	119.38	127.00
24	c	503	CLA	C3C-C4C-NC	2.85	114.08	110.43
24	B	608	CLA	C1D-CHD-C4C	-2.85	119.96	126.02
24	d	401	CLA	CAA-CBA-CGA	2.85	121.29	113.21
31	D	407	PL9	C10-C9-C11	2.85	120.17	115.23
24	C	514	CLA	C2C-C1C-NC	2.85	112.97	109.98
24	b	613	CLA	C3C-C4C-NC	2.85	114.08	110.43
24	a	2109	CLA	C3B-C4B-NB	2.85	113.07	110.53
24	c	508	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
24	A	409	CLA	CHD-C1D-ND	-2.84	120.80	124.80
27	F	101	SQD	O9-S-C6	2.84	111.00	106.76
24	c	511	CLA	C3B-C4B-NB	2.84	113.07	110.53
26	B	618	BCR	C7-C8-C9	-2.84	122.03	126.23
24	D	405	CLA	C2C-C1C-NC	2.84	112.96	109.98
24	C	505	CLA	C4B-C3B-C2B	-2.84	103.77	107.30
24	b	611	CLA	CMA-C3A-C4A	-2.84	104.15	111.77
24	C	504	CLA	C2B-C1B-NB	2.84	113.27	110.33
28	c	521	LMG	C8-O7-C10	-2.83	111.01	117.80
24	C	509	CLA	O2A-CGA-CBA	2.83	120.47	111.83
38	H	102	DGD	O1G-C1A-O1A	-2.83	116.54	123.63
24	B	607	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
24	a	2113	CLA	CMB-C2B-C1B	2.83	129.73	125.42
24	c	508	CLA	C3C-C4C-NC	2.83	114.06	110.43
24	b	613	CLA	C2C-C1C-NC	2.83	112.96	109.98
24	d	405	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
24	B	612	CLA	CHD-C4C-C3C	-2.83	120.64	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	614	CLA	C3C-C4C-NC	2.83	114.06	110.43
43	V	201	HEC	CBD-CAD-C3D	-2.83	104.71	112.53
26	c	528	BCR	C24-C23-C22	-2.83	122.06	126.23
24	B	613	CLA	CAC-C3C-C4C	2.83	128.47	124.79
24	a	2113	CLA	CMA-C3A-C2A	-2.82	103.06	113.98
24	b	607	CLA	CHC-C4B-NB	2.82	128.28	124.05
24	d	404	CLA	CHD-C1D-ND	-2.82	120.83	124.80
24	B	613	CLA	O2A-CGA-CBA	2.82	120.43	111.83
27	a	2115	SQD	O48-C23-O10	-2.82	116.58	123.63
41	H	101	RRX	C10-C11-C12	-2.82	115.04	123.20
39	d	408	LHG	O7-C7-C8	2.82	117.58	111.48
24	C	502	CLA	C4B-C3B-C2B	-2.81	103.80	107.30
24	c	509	CLA	C3C-C4C-NC	2.81	114.03	110.43
24	C	510	CLA	C3B-C4B-NB	2.81	113.04	110.53
31	d	407	PL9	C15-C14-C16	2.81	120.11	115.23
24	B	608	CLA	C2B-C1B-NB	2.81	113.24	110.33
24	C	513	CLA	CMA-C3A-C4A	-2.81	104.21	111.77
24	b	609	CLA	CAC-C3C-C4C	2.81	128.45	124.79
39	d	410	LHG	O8-C23-C24	2.81	120.41	111.83
24	c	515	CLA	CAC-C3C-C4C	2.81	128.45	124.79
24	B	603	CLA	CAC-C3C-C4C	2.81	128.45	124.79
24	B	605	CLA	C3B-C4B-NB	2.81	113.04	110.53
24	b	608	CLA	CMB-C2B-C1B	2.81	129.70	125.42
24	B	609	CLA	C1-C2-C3	-2.81	121.59	126.20
29	B	623	LMT	O1B-C4'-C5'	-2.81	102.11	109.48
31	A	417	PL9	C22-C23-C24	-2.81	121.19	127.62
29	T	102	LMT	C1-O1'-C1'	-2.81	108.88	113.68
24	d	405	CLA	C1-C2-C3	-2.81	121.60	126.20
24	c	514	CLA	CAA-C2A-C3A	-2.81	105.41	113.00
24	C	507	CLA	CHA-C1A-NA	-2.81	120.03	126.39
24	B	606	CLA	C2C-C1C-NC	2.81	112.93	109.98
24	b	611	CLA	C1-C2-C3	-2.81	121.60	126.20
29	j	1601	LMT	O5'-C1'-C2'	2.80	116.13	110.37
28	C	526	LMG	O8-C28-C29	2.80	120.38	111.83
24	b	605	CLA	CMA-C3A-C4A	-2.80	104.24	111.77
24	c	507	CLA	CMB-C2B-C1B	2.80	129.69	125.42
24	C	508	CLA	C4A-NA-C1A	2.80	107.96	106.68
24	B	610	CLA	CBC-CAC-C3C	-2.80	104.83	112.42
24	C	503	CLA	C1-O2A-CGA	2.80	123.42	116.65
26	c	528	BCR	C15-C14-C13	-2.80	123.36	127.28
24	C	509	CLA	C1D-CHD-C4C	-2.80	120.08	126.02
24	b	615	CLA	O2D-CGD-O1D	-2.79	118.42	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	604	CLA	CAA-CBA-CGA	-2.79	105.28	113.21
36	I	1202	HTG	O5-C1-C2	2.79	114.16	110.32
24	B	612	CLA	C3C-C4C-NC	2.79	114.00	110.43
24	b	613	CLA	O2A-CGA-CBA	2.79	120.34	111.83
24	B	604	CLA	CAA-C2A-C3A	-2.79	105.47	113.00
24	c	514	CLA	C1-C2-C3	-2.79	121.63	126.20
24	b	611	CLA	CBC-CAC-C3C	-2.79	104.86	112.42
24	b	613	CLA	CHA-C1A-NA	-2.78	120.08	126.39
24	c	504	CLA	CMB-C2B-C1B	2.78	129.66	125.42
26	d	406	BCR	C21-C20-C19	-2.78	115.13	123.20
24	b	608	CLA	O2A-CGA-O1A	-2.78	116.67	123.63
24	B	604	CLA	C4C-C3C-C2C	-2.78	102.84	106.89
24	B	610	CLA	CMA-C3A-C4A	-2.78	104.30	111.77
24	b	616	CLA	CMB-C2B-C1B	2.78	129.65	125.42
24	D	401	CLA	CED-O2D-CGD	2.78	122.22	115.92
24	C	513	CLA	C2C-C1C-NC	2.78	112.90	109.98
24	a	2113	CLA	C4-C3-C5	2.77	120.04	115.23
24	c	506	CLA	O2A-CGA-O1A	-2.77	116.69	123.63
31	d	407	PL9	C10-C9-C11	2.77	120.04	115.23
24	B	606	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
24	C	514	CLA	C3C-C4C-NC	2.77	113.98	110.43
24	b	612	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
26	C	516	BCR	C38-C26-C25	-2.77	121.46	124.48
24	D	401	CLA	C3C-C4C-NC	2.77	113.98	110.43
27	f	102	SQD	O48-C23-C24	2.77	120.28	111.83
24	b	608	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
24	c	509	CLA	C1D-CHD-C4C	-2.77	120.14	126.02
27	B	621	SQD	O5-C1-C2	2.77	116.05	110.37
24	B	605	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
24	C	510	CLA	C4C-C3C-C2C	-2.77	102.87	106.89
31	D	407	PL9	C22-C23-C24	-2.77	121.29	127.62
24	C	511	CLA	C4A-NA-C1A	2.76	107.94	106.68
24	B	612	CLA	C1D-CHD-C4C	-2.76	120.15	126.02
24	b	609	CLA	C4-C3-C5	2.76	120.02	115.23
24	C	511	CLA	CMC-C2C-C1C	2.76	129.35	125.03
24	b	606	CLA	CMC-C2C-C1C	2.76	129.35	125.03
24	D	405	CLA	C1-C2-C3	-2.76	121.67	126.20
24	b	608	CLA	O2A-CGA-CBA	2.76	120.25	111.83
24	B	603	CLA	C4-C3-C5	2.76	120.02	115.23
24	A	409	CLA	CBC-CAC-C3C	-2.76	104.94	112.42
39	D	410	LHG	O8-C23-C24	2.76	120.25	111.83
24	B	608	CLA	C3B-C4B-NB	2.76	112.99	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	C3B-C4B-NB	2.76	112.99	110.53
24	B	614	CLA	C4C-C3C-C2C	-2.76	102.88	106.89
36	c	523	HTG	C1-O5-C5	2.76	117.50	112.56
24	b	608	CLA	CBC-CAC-C3C	-2.75	104.95	112.42
24	C	506	CLA	CMB-C2B-C1B	2.75	129.61	125.42
26	C	516	BCR	C15-C14-C13	-2.75	123.42	127.28
24	c	503	CLA	C4B-C3B-C2B	-2.75	103.89	107.30
24	C	514	CLA	CMB-C2B-C1B	2.75	129.60	125.42
26	t	102	BCR	C21-C20-C19	-2.74	115.25	123.20
24	b	607	CLA	C3C-C4C-NC	2.74	113.94	110.43
24	b	614	CLA	CMC-C2C-C1C	2.74	129.32	125.03
36	b	601	HTG	C3-C4-C5	2.74	115.20	110.23
24	c	510	CLA	C4C-C3C-C2C	-2.74	102.90	106.89
24	B	616	CLA	CBC-CAC-C3C	-2.74	104.99	112.42
38	H	102	DGD	O2G-C1B-C2B	2.74	117.41	111.48
24	B	608	CLA	C4-C3-C5	2.74	119.98	115.23
31	d	407	PL9	C25-C24-C26	2.74	119.98	115.23
28	c	522	LMG	O6-C5-C4	2.74	114.63	109.70
24	c	514	CLA	CHA-C1A-NA	-2.74	120.19	126.39
26	D	406	BCR	C10-C11-C12	-2.74	115.28	123.20
24	b	606	CLA	CBC-CAC-C3C	-2.73	105.01	112.42
24	B	604	CLA	C3B-C4B-NB	2.73	112.97	110.53
24	B	617	CLA	C1-O2A-CGA	2.73	123.27	116.65
26	T	101	BCR	C35-C13-C12	2.73	122.26	118.09
24	d	405	CLA	C4-C3-C5	2.73	119.97	115.23
24	a	2110	CLA	CED-O2D-CGD	2.73	122.11	115.92
24	b	611	CLA	O2A-CGA-O1A	-2.73	116.80	123.63
24	C	510	CLA	O2A-CGA-CBA	2.73	120.16	111.83
24	D	405	CLA	CHD-C1D-ND	-2.73	120.96	124.80
24	A	409	CLA	C4-C3-C5	2.73	119.96	115.23
24	b	612	CLA	C4-C3-C5	2.73	119.96	115.23
24	B	603	CLA	CMA-C3A-C2A	-2.73	103.44	113.98
24	B	614	CLA	CHD-C1D-ND	-2.73	120.97	124.80
24	c	506	CLA	C4B-C3B-C2B	-2.73	103.91	107.30
24	C	502	CLA	C4C-C3C-C2C	-2.72	102.93	106.89
39	L	101	LHG	O8-C23-O10	-2.72	116.82	123.63
24	C	511	CLA	C2B-C1B-NB	2.72	113.15	110.33
24	b	609	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
24	b	614	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
24	A	405	CLA	O2A-CGA-CBA	2.72	120.13	111.83
24	b	616	CLA	O2A-CGA-CBA	2.72	120.13	111.83
24	c	503	CLA	C2B-C1B-NB	2.72	113.14	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	517	BCR	C3-C4-C5	-2.72	109.21	114.06
24	B	608	CLA	CMC-C2C-C1C	2.72	129.28	125.03
24	D	404	CLA	C4C-C3C-C2C	-2.72	102.94	106.89
24	B	611	CLA	CMA-C3A-C4A	-2.72	104.47	111.77
38	c	518	DGD	O2G-C1B-O1B	-2.72	117.36	123.70
24	B	603	CLA	CMA-C3A-C4A	-2.71	104.48	111.77
31	D	407	PL9	C53-C6-C1	2.71	120.84	115.28
24	b	617	CLA	C4C-C3C-C2C	-2.71	102.94	106.89
24	B	613	CLA	C2C-C1C-NC	2.71	112.83	109.98
24	B	611	CLA	O2A-CGA-O1A	-2.71	116.84	123.63
24	c	505	CLA	C2B-C1B-NB	2.71	113.14	110.33
24	B	604	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
24	c	513	CLA	C4C-C3C-C2C	-2.71	102.95	106.89
24	b	617	CLA	C3C-C4C-NC	2.71	113.90	110.43
24	b	607	CLA	O2A-CGA-CBA	2.71	120.09	111.83
24	c	509	CLA	CHC-C4B-NB	2.71	128.11	124.05
38	C	517	DGD	C3G-C2G-C1G	-2.70	105.48	111.78
24	B	612	CLA	CBC-CAC-C3C	-2.70	105.09	112.42
24	C	502	CLA	C2B-C1B-NB	2.70	113.13	110.33
24	b	614	CLA	O2A-CGA-O1A	-2.70	116.88	123.63
36	D	413	HTG	C3-C4-C5	2.70	115.13	110.23
31	x	801	PL9	C12-C13-C14	-2.70	121.45	127.62
24	D	404	CLA	C3B-C4B-NB	2.70	112.94	110.53
24	A	405	CLA	CMA-C3A-C2A	-2.70	103.55	113.98
24	b	605	CLA	C4B-C3B-C2B	-2.70	103.95	107.30
27	F	101	SQD	C44-O6-C1	-2.69	108.02	113.80
24	c	509	CLA	O1D-CGD-CBD	-2.69	119.21	124.52
24	d	405	CLA	C4B-C3B-C2B	-2.69	103.95	107.30
24	D	405	CLA	CAA-C2A-C3A	-2.69	105.73	113.00
26	t	102	BCR	C1-C6-C7	2.69	122.95	115.65
24	C	513	CLA	CBA-CAA-C2A	-2.69	105.79	113.79
28	C	520	LMG	C8-O7-C10	-2.69	111.36	117.80
38	h	703	DGD	O1G-C1A-O1A	-2.69	116.90	123.63
24	B	605	CLA	CMC-C2C-C1C	2.69	129.23	125.03
25	A	408	PHO	O2D-CGD-O1D	-2.69	118.62	123.85
24	D	404	CLA	CAA-C2A-C3A	-2.69	105.74	113.00
24	d	401	CLA	CHD-C1D-ND	-2.69	121.02	124.80
24	A	405	CLA	C1D-CHD-C4C	-2.69	120.31	126.02
24	B	610	CLA	C2B-C1B-NB	2.68	113.11	110.33
26	C	516	BCR	C2-C1-C6	2.68	114.34	110.44
24	C	509	CLA	O2A-CGA-O1A	-2.68	116.91	123.63
24	c	512	CLA	C3C-C4C-NC	2.68	113.87	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	512	CLA	CHD-C1D-ND	-2.68	121.03	124.80
24	a	2113	CLA	O2A-CGA-CBA	2.68	120.02	111.83
24	B	608	CLA	CAC-C3C-C4C	2.68	128.28	124.79
24	b	613	CLA	CMA-C3A-C4A	-2.68	104.57	111.77
24	B	603	CLA	C4B-C3B-C2B	-2.68	103.97	107.30
31	D	407	PL9	C37-C38-C39	-2.68	121.49	127.62
24	C	512	CLA	C1-O2A-CGA	2.68	123.14	116.65
39	D	411	LHG	O8-C23-C24	2.68	120.00	111.83
24	B	607	CLA	CHA-C1A-NA	-2.68	120.33	126.39
24	B	611	CLA	C4-C3-C5	2.68	119.87	115.23
24	b	609	CLA	C3C-C4C-NC	2.68	113.86	110.43
24	B	609	CLA	O2A-CGA-O1A	-2.67	116.94	123.63
26	b	621	BCR	C28-C27-C26	-2.67	109.29	114.06
24	B	607	CLA	O2A-CGA-CBA	2.67	119.98	111.83
25	A	407	PHO	C1-C2-C3	-2.67	121.82	126.20
36	b	601	HTG	O5-C5-C4	2.67	114.51	109.70
36	D	413	HTG	C4-C3-C2	2.67	115.52	110.83
24	c	511	CLA	O2A-CGA-CBA	2.67	119.98	111.83
26	Y	302	BCR	C10-C11-C12	-2.67	115.47	123.20
24	c	506	CLA	C3C-C4C-NC	2.67	113.85	110.43
24	C	510	CLA	C4B-C3B-C2B	-2.67	103.98	107.30
40	e	103	HEM	CHC-C1C-NC	2.67	127.36	124.45
24	C	504	CLA	O2A-CGA-CBA	2.67	119.97	111.83
28	B	622	LMG	O7-C10-C11	2.67	117.25	111.48
24	B	609	CLA	O2A-CGA-CBA	2.66	119.96	111.83
29	z	1801	LMT	C1B-O1B-C4'	-2.66	111.67	117.98
24	C	512	CLA	C4A-NA-C1A	2.66	107.89	106.68
24	B	606	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
24	D	405	CLA	O2A-CGA-O1A	-2.66	116.97	123.63
24	B	614	CLA	O2D-CGD-CBD	2.66	115.88	111.23
38	c	520	DGD	O1G-C1A-C2A	2.66	119.94	111.83
36	b	625	HTG	C2'-C1'-S1	-2.66	103.41	112.36
24	c	511	CLA	CMC-C2C-C1C	2.66	129.19	125.03
24	b	605	CLA	C1-C2-C3	-2.66	121.84	126.20
24	B	602	CLA	C3C-C4C-NC	2.66	113.83	110.43
24	C	511	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
40	e	103	HEM	CBD-CAD-C3D	-2.66	105.19	112.53
24	A	409	CLA	C1D-CHD-C4C	-2.66	120.38	126.02
36	b	602	HTG	O5-C5-C4	2.65	114.48	109.70
24	c	507	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
24	c	511	CLA	CBC-CAC-C3C	-2.65	105.23	112.42
24	d	401	CLA	CHC-C1C-C2C	-2.65	119.41	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	101	BCR	C15-C14-C13	2.65	131.00	127.28
25	A	407	PHO	O1D-CGD-CBD	-2.65	120.70	124.72
24	b	613	CLA	CAA-C2A-C3A	-2.65	105.83	113.00
24	C	504	CLA	O2A-CGA-O1A	-2.65	117.00	123.63
24	b	611	CLA	CHA-C1A-NA	-2.65	120.39	126.39
24	D	405	CLA	C1D-CHD-C4C	-2.65	120.39	126.02
24	B	610	CLA	C4B-C3B-C2B	-2.65	104.01	107.30
24	c	513	CLA	C4B-C3B-C2B	-2.65	104.01	107.30
24	b	617	CLA	O2A-CGA-O1A	-2.65	117.01	123.63
24	C	508	CLA	CBC-CAC-C3C	-2.65	105.24	112.42
31	d	407	PL9	C20-C19-C21	2.65	119.82	115.23
24	b	610	CLA	CAA-CBA-CGA	2.65	120.72	113.21
24	c	505	CLA	C4-C3-C5	2.65	119.82	115.23
39	D	410	LHG	O8-C23-O10	-2.65	117.01	123.63
24	B	615	CLA	C3C-C4C-NC	2.64	113.82	110.43
24	b	604	CLA	C3C-C4C-NC	2.64	113.82	110.43
24	C	507	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
24	c	511	CLA	CHA-C1A-NA	-2.64	120.41	126.39
24	C	511	CLA	C4C-C3C-C2C	-2.64	103.05	106.89
26	c	517	BCR	C31-C1-C6	-2.64	106.10	110.24
26	T	101	BCR	C12-C13-C14	-2.64	114.85	119.01
28	c	522	LMG	C8-O7-C10	-2.64	111.47	117.80
32	a	2119	K2I	BR-C4-C5	2.64	119.15	116.06
24	b	612	CLA	CHD-C1D-ND	-2.64	121.09	124.80
31	x	801	PL9	C20-C19-C21	2.64	119.81	115.23
24	c	514	CLA	C4C-C3C-C2C	-2.64	103.05	106.89
24	B	616	CLA	C3B-C4B-NB	2.64	112.89	110.53
25	A	407	PHO	CMA-C3A-C4A	-2.64	108.93	114.61
24	b	619	CLA	CBC-CAC-C3C	-2.64	105.27	112.42
24	C	506	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
24	B	602	CLA	CBC-CAC-C3C	-2.63	105.28	112.42
24	B	611	CLA	C4B-C3B-C2B	-2.63	104.03	107.30
24	b	617	CLA	CAC-C3C-C4C	2.63	128.21	124.79
24	B	616	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
26	A	410	BCR	C31-C1-C6	-2.63	106.12	110.24
24	C	514	CLA	CAA-C2A-C3A	-2.63	105.90	113.00
24	B	606	CLA	CHD-C1D-ND	-2.63	121.11	124.80
24	a	2110	CLA	CAA-C2A-C3A	-2.63	105.90	113.00
31	D	407	PL9	C7-C8-C9	-2.63	122.31	126.83
24	a	2109	CLA	CMA-C3A-C2A	-2.62	103.84	113.98
36	B	628	HTG	O5-C5-C4	2.62	114.43	109.70
24	b	604	CLA	CMB-C2B-C1B	2.62	129.41	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	C3C-C4C-NC	2.62	113.79	110.43
24	b	612	CLA	CED-O2D-CGD	2.62	121.86	115.92
25	A	407	PHO	CMB-C2B-C3B	2.62	129.92	124.68
24	C	507	CLA	C4B-C3B-C2B	-2.62	104.04	107.30
24	B	613	CLA	C1D-CHD-C4C	-2.62	120.45	126.02
24	B	615	CLA	CHC-C1C-C2C	-2.62	119.50	126.95
24	B	611	CLA	CHA-C1A-NA	-2.62	120.46	126.39
24	b	616	CLA	C1D-CHD-C4C	-2.62	120.46	126.02
24	b	605	CLA	C3B-C4B-NB	2.62	112.86	110.53
24	B	612	CLA	CHA-C1A-NA	-2.62	120.47	126.39
24	D	405	CLA	CMA-C3A-C4A	-2.62	104.74	111.77
24	C	513	CLA	CMB-C2B-C1B	2.62	129.40	125.42
24	C	507	CLA	C4-C3-C5	2.61	119.77	115.23
24	c	506	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
24	c	514	CLA	C3B-C4B-NB	2.61	112.86	110.53
24	B	607	CLA	C1-O2A-CGA	2.61	122.97	116.65
24	C	513	CLA	CHD-C1D-ND	-2.61	121.13	124.80
43	v	201	HEC	CBD-CAD-C3D	-2.61	105.32	112.53
31	A	417	PL9	C37-C38-C39	-2.61	121.65	127.62
29	b	624	LMT	C3'-C4'-C5'	2.61	116.71	110.93
26	c	528	BCR	C10-C11-C12	-2.61	115.64	123.20
24	c	511	CLA	C2B-C1B-NB	2.61	113.03	110.33
24	A	409	CLA	C4C-C3C-C2C	-2.61	103.10	106.89
24	B	614	CLA	CMA-C3A-C2A	-2.61	103.90	113.98
26	C	516	BCR	C21-C20-C19	-2.61	115.65	123.20
24	b	610	CLA	C4B-C3B-C2B	-2.61	104.06	107.30
27	L	102	SQD	C44-O6-C1	-2.61	108.21	113.80
24	c	505	CLA	CAC-C3C-C4C	2.61	128.18	124.79
24	B	616	CLA	CBA-CAA-C2A	-2.61	106.04	113.79
24	b	614	CLA	CMB-C2B-C1B	2.60	129.38	125.42
26	k	2003	BCR	C20-C21-C22	-2.60	123.63	127.28
24	B	610	CLA	CHA-C1A-NA	-2.60	120.50	126.39
36	d	403	HTG	C1'-S1-C1	2.60	106.07	100.45
24	b	616	CLA	CHA-C1A-NA	-2.60	120.50	126.39
24	C	504	CLA	C4C-C3C-C2C	-2.60	103.11	106.89
24	D	404	CLA	C4-C3-C5	2.60	119.74	115.23
24	C	514	CLA	C4-C3-C5	2.60	119.74	115.23
24	C	511	CLA	C1-O2A-CGA	2.60	122.94	116.65
24	b	609	CLA	O2A-CGA-CBA	2.60	119.75	111.83
24	b	610	CLA	CMC-C2C-C1C	2.59	129.09	125.03
24	b	618	CLA	C4C-C3C-C2C	-2.59	103.11	106.89
24	c	508	CLA	CGD-CBD-CAD	-2.59	102.45	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	511	CLA	O1D-CGD-CBD	-2.59	119.40	124.52
24	c	505	CLA	CHD-C4C-C3C	-2.59	120.99	124.77
24	c	503	CLA	C4C-C3C-C2C	-2.59	103.12	106.89
31	d	407	PL9	O1-C4-C3	-2.59	118.00	120.73
26	B	619	BCR	C38-C26-C25	-2.59	121.66	124.48
24	B	607	CLA	CMC-C2C-C1C	2.59	129.08	125.03
24	c	508	CLA	CHA-C1A-NA	-2.59	120.53	126.39
24	c	509	CLA	C4C-C3C-C2C	-2.59	103.13	106.89
24	c	513	CLA	C3C-C4C-NC	2.58	113.74	110.43
24	C	505	CLA	C3B-C4B-NB	2.58	112.84	110.53
24	B	616	CLA	CHA-C1A-NA	-2.58	120.54	126.39
24	c	514	CLA	CMA-C3A-C4A	-2.58	104.83	111.77
31	d	407	PL9	C12-C13-C14	-2.58	121.72	127.62
26	B	620	BCR	C38-C26-C25	-2.58	121.67	124.48
24	C	505	CLA	C4C-C3C-C2C	-2.58	103.14	106.89
24	B	605	CLA	C3C-C4C-NC	2.58	113.73	110.43
24	D	401	CLA	CHC-C1C-C2C	-2.58	119.63	126.95
24	C	504	CLA	CHA-C1A-NA	-2.57	120.56	126.39
24	C	506	CLA	C4B-C3B-C2B	-2.57	104.10	107.30
24	b	605	CLA	CHD-C1D-ND	-2.57	121.18	124.80
24	c	505	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
26	B	618	BCR	C21-C20-C19	-2.57	115.75	123.20
24	B	605	CLA	C4C-C3C-C2C	-2.57	103.15	106.89
24	c	509	CLA	CHA-C1A-NA	-2.57	120.57	126.39
24	C	508	CLA	C4-C3-C5	2.57	119.69	115.23
24	a	2109	CLA	O2D-CGD-CBD	2.57	115.72	111.23
24	C	513	CLA	C4C-C3C-C2C	-2.57	103.15	106.89
24	b	613	CLA	C1-C2-C3	-2.57	121.98	126.20
24	C	513	CLA	C4A-NA-C1A	2.57	107.85	106.68
24	b	615	CLA	CMB-C2B-C1B	2.57	129.33	125.42
24	b	617	CLA	O2A-CGA-CBA	2.57	119.66	111.83
24	B	607	CLA	C3B-C4B-NB	2.57	112.82	110.53
24	c	512	CLA	C4-C3-C5	2.56	119.68	115.23
24	C	503	CLA	C4B-C3B-C2B	-2.56	104.12	107.30
24	b	619	CLA	CHA-C1A-NA	-2.56	120.59	126.39
29	b	624	LMT	C1'-O5'-C5'	2.56	118.72	113.72
24	b	606	CLA	C1-O2A-CGA	2.56	122.84	116.65
26	T	101	BCR	C21-C20-C19	-2.56	115.79	123.20
24	C	514	CLA	O2A-CGA-CBA	2.56	119.63	111.83
24	C	506	CLA	C4A-NA-C1A	2.56	107.84	106.68
24	C	513	CLA	CHA-C1A-NA	-2.55	120.61	126.39
24	b	616	CLA	CAC-C3C-C4C	2.55	128.11	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	616	CLA	CHD-C1D-ND	-2.55	121.21	124.80
24	A	405	CLA	CAC-C3C-C4C	2.55	128.11	124.79
24	C	504	CLA	C3C-C4C-NC	2.55	113.70	110.43
24	c	514	CLA	C3C-C4C-NC	2.55	113.70	110.43
24	C	512	CLA	C4B-C3B-C2B	-2.55	104.13	107.30
28	c	522	LMG	C3-C4-C5	2.55	114.85	110.23
24	c	513	CLA	CMC-C2C-C1C	2.55	129.01	125.03
24	C	514	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
24	C	512	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
24	d	405	CLA	C3B-C4B-NB	2.55	112.80	110.53
26	Y	302	BCR	C32-C1-C6	-2.54	106.25	110.24
24	B	605	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
24	b	616	CLA	CED-O2D-CGD	2.54	121.69	115.92
24	a	2110	CLA	CHC-C1C-C2C	-2.54	119.72	126.95
24	c	506	CLA	CMC-C2C-C1C	2.54	129.01	125.03
24	C	509	CLA	C4B-C3B-C2B	-2.54	104.14	107.30
24	b	612	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
24	d	405	CLA	CAA-C2A-C3A	-2.54	106.14	113.00
24	b	606	CLA	CMA-C3A-C2A	-2.54	104.16	113.98
29	i	104	LMT	O5'-C5'-C4'	2.54	114.28	109.70
24	b	619	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
26	t	102	BCR	C7-C8-C9	-2.54	122.48	126.23
26	C	515	BCR	C20-C21-C22	-2.54	123.72	127.28
24	C	506	CLA	C3B-C4B-NB	2.54	112.80	110.53
24	C	505	CLA	C4-C3-C5	2.54	119.63	115.23
24	b	608	CLA	CED-O2D-CGD	2.54	121.67	115.92
36	C	521	HTG	C1'-S1-C1	2.54	105.93	100.45
24	B	605	CLA	CHA-C1A-NA	-2.54	120.65	126.39
29	B	623	LMT	O5B-C5B-C4B	2.53	114.27	109.70
24	c	512	CLA	C11-C10-C8	-2.53	107.55	115.97
24	b	613	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
36	B	625[B]	HTG	C6-C5-C4	-2.53	106.80	113.02
26	c	528	BCR	C21-C20-C19	-2.53	115.86	123.20
24	A	409	CLA	C3C-C4C-NC	2.53	113.67	110.43
26	Y	302	BCR	C1-C6-C7	2.53	122.52	115.65
24	B	602	CLA	C2C-C1C-NC	2.53	112.64	109.98
24	A	409	CLA	CAA-C2A-C3A	-2.53	106.16	113.00
24	B	613	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
24	b	604	CLA	CBC-CAC-C3C	-2.53	105.56	112.42
24	b	605	CLA	CMA-C3A-C2A	-2.53	104.20	113.98
24	C	512	CLA	C3B-C4B-NB	2.53	112.79	110.53
31	x	801	PL9	C15-C14-C16	2.53	119.62	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	C	517	DGD	O1G-C1A-O1A	-2.53	117.30	123.63
24	b	612	CLA	CMA-C3A-C4A	-2.53	104.98	111.77
41	h	702	RRX	C7-C8-C9	-2.53	122.50	126.23
26	T	101	BCR	C16-C17-C18	-2.53	123.73	127.28
39	D	409	LHG	O7-C7-O9	-2.53	117.80	123.70
24	C	511	CLA	C2C-C1C-NC	2.53	112.64	109.98
24	b	610	CLA	C3C-C4C-NC	2.52	113.66	110.43
28	B	622	LMG	O8-C28-C29	2.52	119.53	111.83
36	B	628	HTG	C4-C3-C2	-2.52	106.40	110.83
24	C	508	CLA	CHB-C1B-C2B	-2.52	120.10	127.43
26	t	102	BCR	C15-C14-C13	2.52	130.82	127.28
38	c	518	DGD	O6D-C1D-O3G	-2.52	104.08	110.04
24	d	401	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
24	B	604	CLA	CAA-C2A-C1A	-2.52	103.72	111.97
24	c	513	CLA	CHD-C1D-ND	-2.52	121.26	124.80
24	b	606	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
26	c	528	BCR	C1-C6-C7	2.52	122.48	115.65
24	B	608	CLA	O2A-CGA-CBA	2.52	119.51	111.83
24	C	503	CLA	C3B-C4B-NB	2.52	112.78	110.53
24	b	616	CLA	C4-C3-C5	2.52	119.60	115.23
27	A	411	SQD	O48-C23-O10	-2.52	117.33	123.63
24	B	610	CLA	C1-O2A-CGA	2.52	122.74	116.65
24	c	503	CLA	C1D-CHD-C4C	-2.51	120.67	126.02
24	b	606	CLA	C4B-C3B-C2B	-2.51	104.17	107.30
24	d	401	CLA	C4C-C3C-C2C	-2.51	103.23	106.89
27	L	102	SQD	O47-C7-O49	-2.51	117.83	123.70
24	b	618	CLA	C3C-C4C-NC	2.51	113.65	110.43
24	D	401	CLA	CMA-C3A-C4A	-2.51	105.02	111.77
24	B	612	CLA	C4-C3-C5	2.51	119.59	115.23
24	c	514	CLA	C11-C12-C13	-2.51	107.62	115.97
24	b	618	CLA	CMC-C2C-C1C	2.51	128.96	125.03
28	D	412	LMG	O7-C10-C11	2.51	116.91	111.48
24	b	605	CLA	C3C-C4C-NC	2.51	113.64	110.43
24	B	609	CLA	C4B-C3B-C2B	-2.51	104.19	107.30
24	b	607	CLA	CHD-C1D-C2D	-2.51	120.27	125.49
28	i	101	LMG	C8-O7-C10	-2.50	111.80	117.80
24	C	510	CLA	CBC-CAC-C3C	-2.50	105.63	112.42
24	B	605	CLA	CHD-C4C-C3C	-2.50	121.12	124.77
24	b	617	CLA	CHD-C1D-ND	-2.50	121.28	124.80
26	b	622	BCR	C15-C14-C13	-2.50	123.77	127.28
24	B	604	CLA	CBC-CAC-C3C	-2.50	105.64	112.42
24	C	506	CLA	CMA-C3A-C4A	-2.50	105.05	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	609	CLA	C3B-C4B-NB	2.50	112.76	110.53
26	k	2003	BCR	C15-C14-C13	-2.50	123.78	127.28
24	c	514	CLA	C4B-C3B-C2B	-2.50	104.20	107.30
24	D	404	CLA	C2B-C1B-NB	2.50	112.92	110.33
24	B	603	CLA	C3B-C4B-NB	2.49	112.76	110.53
38	H	102	DGD	C3G-O3G-C1D	-2.49	108.45	113.80
24	c	504	CLA	CMC-C2C-C1C	2.49	128.93	125.03
24	b	612	CLA	C3C-C4C-NC	2.49	113.62	110.43
29	B	636	LMT	O5'-C5'-C4'	2.49	114.87	109.72
24	c	508	CLA	O2A-CGA-CBA	2.49	119.43	111.83
24	B	611	CLA	O2A-C1-C2	2.49	117.69	108.11
32	a	2119	K2I	C3-C4-C5	-2.49	121.47	123.59
24	C	505	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
24	b	605	CLA	O2A-CGA-CBA	2.49	119.42	111.83
27	A	411	SQD	C45-O47-C7	-2.49	111.84	117.80
24	D	404	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
24	C	512	CLA	O2A-CGA-CBA	2.49	119.42	111.83
26	c	516	BCR	C7-C8-C9	-2.49	122.56	126.23
24	c	505	CLA	O2A-CGA-O1A	-2.48	117.41	123.63
26	t	102	BCR	C2-C1-C6	2.48	114.05	110.44
24	B	614	CLA	C4-C3-C5	2.48	119.54	115.23
38	c	519	DGD	C5B-C4B-C3B	-2.48	101.82	114.37
24	B	615	CLA	CMB-C2B-C1B	2.48	129.20	125.42
24	C	513	CLA	CHD-C4C-NC	2.48	128.08	124.23
24	B	612	CLA	C1-C2-C3	-2.48	122.13	126.20
24	c	510	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
24	A	409	CLA	CMB-C2B-C1B	2.48	129.20	125.42
40	F	102	HEM	C3B-C2B-C1B	2.48	108.27	106.41
31	A	417	PL9	C40-C39-C41	2.48	119.53	115.23
26	c	528	BCR	C38-C26-C25	-2.48	121.78	124.48
24	B	615	CLA	C4B-C3B-C2B	-2.48	104.22	107.30
24	b	610	CLA	C4C-C3C-C2C	-2.48	103.29	106.89
24	D	405	CLA	O2A-CGA-CBA	2.48	119.38	111.83
24	C	511	CLA	C3C-C4C-NC	2.47	113.60	110.43
24	c	505	CLA	C3B-C4B-NB	2.47	112.74	110.53
28	C	520	LMG	O8-C28-O10	-2.47	117.45	123.63
24	B	603	CLA	CHD-C1D-ND	-2.47	121.33	124.80
24	C	511	CLA	C3B-C4B-NB	2.47	112.73	110.53
24	B	603	CLA	CHA-C1A-NA	-2.47	120.80	126.39
24	A	409	CLA	CHB-C4A-NA	2.46	127.96	124.40
24	B	604	CLA	CAC-C3C-C4C	2.46	128.00	124.79
26	t	102	BCR	C7-C6-C5	-2.46	115.88	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	612	CLA	C4B-C3B-C2B	-2.46	104.24	107.30
24	B	609	CLA	CMC-C2C-C1C	2.46	128.88	125.03
24	b	608	CLA	C2C-C1C-NC	2.46	112.57	109.98
24	B	612	CLA	C7-C6-C5	-2.46	106.70	113.26
24	A	406	CLA	C4C-C3C-C2C	-2.46	103.31	106.89
24	c	503	CLA	C3B-C4B-NB	2.46	112.72	110.53
24	D	405	CLA	C3C-C4C-NC	2.46	113.58	110.43
24	d	405	CLA	C3C-C4C-NC	2.46	113.58	110.43
24	b	617	CLA	CMC-C2C-C1C	2.46	128.88	125.03
28	D	412	LMG	O8-C28-O10	-2.46	117.48	123.63
24	c	514	CLA	CMB-C2B-C1B	2.46	129.16	125.42
41	H	101	RRX	C38-C26-C25	-2.46	121.80	124.48
24	c	513	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
24	b	609	CLA	CMC-C2C-C1C	2.45	128.87	125.03
24	b	610	CLA	O2A-CGA-CBA	2.45	119.31	111.83
24	A	406	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
26	D	406	BCR	C15-C14-C13	-2.45	123.84	127.28
24	C	502	CLA	C3C-C4C-NC	2.45	113.57	110.43
24	c	503	CLA	CAC-C3C-C4C	2.45	127.98	124.79
24	c	507	CLA	C3B-C4B-NB	2.45	112.72	110.53
29	I	1201	LMT	C1'-O5'-C5'	2.45	118.50	113.72
24	b	605	CLA	CAC-C3C-C4C	2.45	127.97	124.79
24	A	409	CLA	C4B-C3B-C2B	-2.45	104.26	107.30
27	a	2102	SQD	O48-C23-O10	-2.45	117.51	123.63
24	c	515	CLA	C3B-C4B-NB	2.44	112.71	110.53
24	B	608	CLA	C3C-C4C-NC	2.44	113.56	110.43
25	a	2111	PHO	CMB-C2B-C3B	2.44	129.56	124.68
24	c	513	CLA	C6-C5-C3	-2.44	107.52	113.47
24	B	616	CLA	C4B-C3B-C2B	-2.44	104.27	107.30
24	c	506	CLA	C4C-C3C-C2C	-2.44	103.34	106.89
24	A	406	CLA	CAC-C3C-C4C	2.44	127.97	124.79
26	c	517	BCR	C2-C1-C6	2.44	113.98	110.44
27	A	413	SQD	O8-S-C6	2.44	110.68	105.97
26	K	101	BCR	C38-C26-C25	-2.44	121.83	124.48
31	D	407	PL9	C40-C39-C38	-2.43	117.38	123.63
31	A	417	PL9	C25-C24-C26	2.43	119.45	115.23
31	x	801	PL9	C25-C24-C26	2.43	119.45	115.23
24	b	614	CLA	CBC-CAC-C3C	-2.43	105.83	112.42
24	C	503	CLA	O2A-CGA-CBA	2.43	119.25	111.83
24	C	508	CLA	CMB-C2B-C1B	2.43	129.12	125.42
24	A	406	CLA	CMC-C2C-C1C	2.43	128.83	125.03
24	b	617	CLA	C3B-C4B-NB	2.43	112.70	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	617	CLA	CHA-C1A-NA	-2.43	120.89	126.39
24	b	605	CLA	C4-C3-C5	2.43	119.44	115.23
24	B	608	CLA	C1-O2A-CGA	2.43	122.53	116.65
24	B	610	CLA	C4-C3-C5	2.43	119.44	115.23
26	C	516	BCR	C20-C21-C22	-2.43	123.88	127.28
24	D	405	CLA	CMA-C3A-C2A	-2.42	104.61	113.98
24	b	618	CLA	CHA-C1A-NA	-2.42	120.90	126.39
39	d	409	LHG	O8-C23-C24	2.42	119.23	111.83
24	d	405	CLA	C4C-C3C-C2C	-2.42	103.36	106.89
24	B	604	CLA	C4-C3-C5	2.42	119.43	115.23
24	A	405	CLA	CMB-C2B-C3B	2.42	132.25	126.55
27	A	411	SQD	O8-S-C6	2.42	110.65	105.97
24	B	602	CLA	CMC-C2C-C1C	2.42	128.82	125.03
24	B	612	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
26	T	101	BCR	C29-C28-C27	-2.42	105.95	111.28
24	b	617	CLA	CAA-C2A-C3A	-2.42	106.46	113.00
24	a	2110	CLA	CHA-C1A-NA	-2.42	120.92	126.39
24	b	607	CLA	CHD-C4C-C3C	-2.42	121.25	124.77
38	c	519	DGD	O2G-C1B-O1B	-2.42	118.06	123.70
26	A	410	BCR	C7-C8-C9	-2.42	122.66	126.23
24	B	612	CLA	CHD-C1D-ND	-2.41	121.40	124.80
32	A	419	K2I	C3-C4-C5	-2.41	121.54	123.59
24	C	510	CLA	CHA-C1A-NA	-2.41	120.93	126.39
26	C	515	BCR	C8-C7-C6	-2.41	120.55	127.00
25	a	2111	PHO	C1A-C2A-C3A	-2.41	100.54	102.84
24	b	605	CLA	CHB-C1B-C2B	-2.41	120.43	127.43
24	B	614	CLA	C3B-C4B-NB	2.41	112.68	110.53
24	D	405	CLA	C3B-C4B-NB	2.41	112.68	110.53
24	b	610	CLA	CED-O2D-CGD	2.41	121.38	115.92
26	c	516	BCR	C38-C26-C25	-2.41	121.86	124.48
24	b	612	CLA	C4B-C3B-C2B	-2.41	104.31	107.30
24	A	406	CLA	C3B-C4B-NB	2.41	112.68	110.53
29	m	102	LMT	C1B-O5B-C5B	2.41	118.42	113.72
38	C	517	DGD	C2G-O2G-C1B	-2.41	112.03	117.80
24	b	613	CLA	C4-C3-C5	2.41	119.41	115.23
26	b	621	BCR	C29-C28-C27	-2.41	105.99	111.28
24	B	606	CLA	O2A-CGA-CBA	2.41	119.17	111.83
24	C	503	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
24	B	608	CLA	CHD-C1D-ND	-2.40	121.42	124.80
24	c	512	CLA	CMA-C3A-C4A	-2.40	105.31	111.77
24	c	514	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
24	B	604	CLA	CMB-C2B-C1B	2.40	129.07	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	d	409	LHG	O7-C7-C8	2.40	116.67	111.48
40	e	103	HEM	CBA-CAA-C2A	-2.40	105.90	112.53
26	c	516	BCR	C20-C21-C22	-2.40	123.92	127.28
31	D	407	PL9	C27-C28-C29	-2.40	122.14	127.62
24	B	615	CLA	CHD-C4C-NC	2.39	127.94	124.23
24	c	514	CLA	CHC-C1C-C2C	-2.39	120.15	126.95
26	T	101	BCR	C1-C6-C7	2.39	122.14	115.65
24	b	612	CLA	CHA-C1A-NA	-2.39	120.97	126.39
24	b	614	CLA	CHA-C1A-NA	-2.39	120.97	126.39
24	d	405	CLA	CBC-CAC-C3C	-2.39	105.94	112.42
24	c	515	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
24	C	505	CLA	C3C-C4C-NC	2.39	113.49	110.43
24	D	401	CLA	CMA-C3A-C2A	-2.39	104.75	113.98
24	b	616	CLA	CMA-C3A-C4A	-2.39	105.36	111.77
24	b	619	CLA	O1D-CGD-CBD	-2.38	119.81	124.52
24	c	513	CLA	C3B-C4B-NB	2.38	112.66	110.53
24	C	507	CLA	CHB-C1B-C2B	-2.38	120.51	127.43
24	B	614	CLA	C4B-C3B-C2B	-2.38	104.34	107.30
26	c	528	BCR	C34-C9-C8	2.38	121.73	118.09
24	C	502	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
24	B	608	CLA	C4C-C3C-C2C	-2.38	103.42	106.89
31	D	407	PL9	C20-C19-C21	2.38	119.36	115.23
39	E	101	LHG	O8-C23-C24	2.38	119.09	111.83
29	A	420	LMT	O5'-C1'-C2'	2.38	115.26	110.37
24	B	609	CLA	CMA-C3A-C2A	-2.38	104.78	113.98
24	B	614	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
24	b	615	CLA	CAC-C3C-C4C	2.38	127.89	124.79
38	C	519	DGD	O2G-C1B-O1B	-2.38	118.15	123.70
24	B	607	CLA	CAC-C3C-C4C	2.37	127.88	124.79
24	C	505	CLA	CAA-C2A-C3A	-2.37	106.59	113.00
26	T	101	BCR	C7-C6-C5	-2.37	116.09	121.56
24	c	515	CLA	C4B-C3B-C2B	-2.37	104.35	107.30
39	E	101	LHG	C5-O7-C7	-2.37	112.12	117.80
24	b	619	CLA	C4-C3-C5	2.37	119.34	115.23
24	A	409	CLA	C7-C6-C5	-2.37	106.95	113.26
24	a	2110	CLA	CAA-CBA-CGA	2.37	119.93	113.21
32	A	418[B]	K2I	BR1-C1-C2	2.36	118.83	116.06
26	B	620	BCR	C23-C24-C25	-2.36	120.68	127.00
36	b	601	HTG	C1-O5-C5	2.36	116.80	112.56
24	c	507	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
24	c	508	CLA	CHC-C1C-C2C	-2.36	120.24	126.95
24	C	507	CLA	C3B-C4B-NB	2.36	112.64	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	2109	CLA	CHC-C1C-C2C	-2.36	120.24	126.95
24	b	612	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
26	t	102	BCR	C28-C27-C26	-2.36	109.85	114.06
24	C	511	CLA	CAA-CBA-CGA	-2.36	106.51	113.21
25	a	2111	PHO	CBA-CAA-C2A	-2.36	106.84	113.78
24	A	409	CLA	CHC-C1C-C2C	-2.36	120.25	126.95
24	C	512	CLA	CMC-C2C-C1C	2.35	128.71	125.03
24	c	513	CLA	CHA-C1A-NA	-2.35	121.06	126.39
24	D	405	CLA	CMB-C2B-C1B	2.35	129.00	125.42
31	D	407	PL9	C12-C13-C14	-2.35	122.24	127.62
24	b	611	CLA	CAC-C3C-C4C	2.35	127.85	124.79
24	b	607	CLA	C6-C7-C8	-2.35	108.15	115.97
26	D	406	BCR	C21-C20-C19	-2.35	116.39	123.20
27	B	621	SQD	O47-C7-O49	-2.35	118.21	123.70
28	d	411	LMG	O8-C28-O10	-2.35	117.75	123.63
24	A	406	CLA	O2A-CGA-CBA	2.35	119.00	111.83
24	b	619	CLA	OBD-CAD-C3D	-2.35	122.93	128.42
24	b	619	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
26	C	516	BCR	C23-C24-C25	-2.35	120.73	127.00
26	a	2114	BCR	C15-C14-C13	-2.35	123.99	127.28
24	C	508	CLA	C1-O2A-CGA	2.34	122.32	116.65
31	x	801	PL9	C17-C18-C19	-2.34	122.26	127.62
26	T	101	BCR	C23-C24-C25	-2.34	120.75	127.00
24	b	606	CLA	CAC-C3C-C4C	2.34	127.83	124.79
24	c	504	CLA	C4B-C3B-C2B	-2.34	104.39	107.30
24	a	2109	CLA	CMA-C3A-C4A	-2.34	105.49	111.77
24	b	617	CLA	C4B-C3B-C2B	-2.34	104.40	107.30
36	b	625	HTG	O6-C6-C5	-2.34	103.38	111.33
29	a	2103	LMT	O5'-C1'-O1'	-2.34	104.53	110.04
24	b	618	CLA	C4B-C3B-C2B	-2.34	104.40	107.30
28	A	412	LMG	O6-C5-C4	2.34	113.91	109.70
24	a	2113	CLA	OBD-CAD-C3D	-2.34	122.96	128.42
38	C	519	DGD	C4A-C3A-C2A	-2.33	104.55	113.13
40	F	102	HEM	C2A-C1A-NA	-2.33	107.56	110.15
26	k	2003	BCR	C16-C17-C18	-2.33	124.00	127.28
24	b	606	CLA	CHB-C1B-C2B	-2.33	120.65	127.43
24	C	512	CLA	CHC-C1C-C2C	-2.33	120.32	126.95
24	b	606	CLA	C4C-C3C-C2C	-2.33	103.50	106.89
26	Y	302	BCR	C21-C20-C19	-2.33	116.44	123.20
24	B	615	CLA	OBD-CAD-C3D	-2.33	122.96	128.42
24	B	602	CLA	CAC-C3C-C4C	2.33	127.83	124.79
24	b	611	CLA	CMC-C2C-C1C	2.33	128.68	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	508	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
24	A	405	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
24	C	513	CLA	CMC-C2C-C1C	2.33	128.68	125.03
24	b	604	CLA	CHD-C1D-ND	-2.33	121.52	124.80
28	C	520	LMG	O7-C10-O9	-2.33	118.26	123.70
24	c	504	CLA	CHD-C1D-ND	-2.33	121.52	124.80
27	A	413	SQD	C44-O6-C1	-2.33	108.80	113.80
24	b	618	CLA	C11-C10-C8	-2.33	108.22	115.97
26	t	102	BCR	C23-C24-C25	-2.33	120.78	127.00
26	t	102	BCR	C11-C10-C9	-2.33	124.01	127.28
25	a	2112	PHO	C4A-C3A-C2A	-2.33	100.62	102.84
24	B	606	CLA	C4B-C3B-C2B	-2.33	104.41	107.30
24	a	2110	CLA	C11-C10-C8	-2.33	108.23	115.97
24	b	619	CLA	C1C-C2C-C3C	-2.33	104.53	106.98
26	a	2114	BCR	C31-C1-C6	-2.33	106.59	110.24
24	C	510	CLA	C1-O2A-CGA	2.33	122.28	116.65
24	b	610	CLA	CMB-C2B-C1B	2.32	128.96	125.42
24	c	506	CLA	CHC-C1C-C2C	-2.32	120.34	126.95
24	B	606	CLA	CED-O2D-CGD	2.32	121.18	115.92
24	B	607	CLA	C4B-C3B-C2B	-2.32	104.41	107.30
24	B	617	CLA	C4B-C3B-C2B	-2.32	104.42	107.30
38	c	518	DGD	O4D-C4D-C3D	-2.32	104.90	110.38
24	B	615	CLA	C4C-C3C-C2C	-2.32	103.51	106.89
24	c	503	CLA	C1-C2-C3	-2.32	122.40	126.20
36	c	523	HTG	O5-C5-C4	2.32	113.88	109.70
24	b	617	CLA	C4-C3-C5	2.32	119.25	115.23
24	c	513	CLA	CMB-C2B-C1B	2.32	128.95	125.42
24	c	505	CLA	CMC-C2C-C1C	2.32	128.66	125.03
24	B	612	CLA	C3B-C4B-NB	2.32	112.60	110.53
24	C	505	CLA	CMA-C3A-C4A	-2.32	105.55	111.77
31	d	407	PL9	C22-C23-C24	-2.31	122.33	127.62
27	a	2115	SQD	O47-C7-O49	-2.31	118.30	123.70
24	d	401	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
26	A	410	BCR	C20-C21-C22	-2.31	124.03	127.28
24	d	405	CLA	O2A-CGA-CBA	2.31	118.88	111.83
24	B	607	CLA	CHB-C1B-C2B	-2.31	120.72	127.43
24	C	506	CLA	C4-C3-C5	2.31	119.24	115.23
24	B	616	CLA	C1-O2A-CGA	2.31	122.24	116.65
24	D	405	CLA	C4B-C3B-C2B	-2.31	104.43	107.30
24	b	614	CLA	CHC-C1C-C2C	-2.31	120.39	126.95
24	B	612	CLA	O2A-CGA-CBA	2.31	118.87	111.83
27	A	413	SQD	O48-C23-O10	-2.31	117.86	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	CMC-C2C-C1C	2.31	128.64	125.03
24	B	607	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
24	b	614	CLA	CHD-C1D-ND	-2.31	121.56	124.80
24	B	614	CLA	CMB-C2B-C1B	2.30	128.93	125.42
24	B	612	CLA	C4A-NA-C1A	2.30	107.73	106.68
24	c	515	CLA	CMB-C2B-C1B	2.30	128.93	125.42
24	B	613	CLA	CBC-CAC-C3C	-2.30	106.18	112.42
26	d	406	BCR	C15-C14-C13	-2.30	124.05	127.28
24	b	607	CLA	C4B-C3B-C2B	-2.30	104.44	107.30
28	D	412	LMG	O8-C28-C29	2.30	118.84	111.83
38	h	703	DGD	C2G-O2G-C1B	-2.29	112.31	117.80
24	a	2109	CLA	CHD-C1D-ND	-2.29	121.58	124.80
24	d	404	CLA	C1D-CHD-C4C	-2.29	121.15	126.02
24	b	604	CLA	C4B-C3B-C2B	-2.29	104.45	107.30
24	b	605	CLA	CHA-C1A-NA	-2.29	121.21	126.39
28	c	522	LMG	O7-C10-O9	-2.29	118.36	123.70
24	c	503	CLA	C4-C3-C5	2.29	119.20	115.23
26	b	621	BCR	C20-C21-C22	-2.29	124.07	127.28
24	D	404	CLA	CHC-C4B-NB	2.29	127.48	124.05
24	B	615	CLA	CMC-C2C-C1C	2.29	128.61	125.03
24	B	603	CLA	CAA-CBA-CGA	-2.29	106.71	113.21
24	A	405	CLA	CHC-C1C-C2C	-2.29	120.45	126.95
39	d	410	LHG	O8-C23-O10	-2.29	117.91	123.63
24	A	405	CLA	CMC-C2C-C1C	2.28	128.60	125.03
26	b	622	BCR	C21-C20-C19	-2.28	116.59	123.20
24	c	515	CLA	C4-C3-C5	2.28	119.19	115.23
24	c	512	CLA	CMB-C2B-C1B	2.28	128.89	125.42
24	C	511	CLA	CAC-C3C-C4C	2.28	127.76	124.79
24	c	513	CLA	CAC-C3C-C4C	2.28	127.76	124.79
24	d	401	CLA	CMB-C2B-C1B	2.28	128.89	125.42
24	C	502	CLA	CHD-C1D-ND	-2.28	121.59	124.80
26	t	102	BCR	C35-C13-C12	2.28	121.57	118.09
24	C	508	CLA	C3B-C4B-NB	2.28	112.56	110.53
24	c	505	CLA	C4B-C3B-C2B	-2.28	104.47	107.30
24	B	617	CLA	CHC-C1C-C2C	-2.28	120.48	126.95
24	d	405	CLA	C1D-CHD-C4C	-2.28	121.18	126.02
24	C	506	CLA	O2A-CGA-CBA	2.27	118.77	111.83
24	A	406	CLA	C3C-C4C-NC	2.27	113.34	110.43
27	f	102	SQD	O47-C7-O49	-2.27	118.39	123.70
24	C	502	CLA	C1-O2A-CGA	2.27	122.15	116.65
27	a	2115	SQD	C45-O47-C7	-2.27	112.36	117.80
25	a	2111	PHO	O2A-CGA-CBA	2.27	118.76	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414	LMT	O5'-C1'-O1'	-2.27	104.67	110.04
24	D	404	CLA	CMA-C3A-C2A	-2.27	105.20	113.98
24	B	608	CLA	CAA-C2A-C1A	-2.27	104.54	111.97
41	h	702	RRX	C20-C21-C22	-2.27	124.09	127.28
24	B	603	CLA	O2A-CGA-CBA	2.27	118.75	111.83
25	A	407	PHO	CBA-CAA-C2A	-2.27	107.10	113.78
25	A	408	PHO	C4A-C3A-C2A	-2.27	100.68	102.84
24	C	511	CLA	C6-C7-C8	-2.27	108.43	115.97
24	b	607	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
24	B	610	CLA	O2A-CGA-CBA	2.27	118.75	111.83
24	C	504	CLA	CHD-C1D-ND	-2.26	121.61	124.80
24	c	513	CLA	C1-C2-C3	-2.26	122.49	126.20
24	c	509	CLA	C1-O2A-CGA	2.26	122.13	116.65
24	B	604	CLA	CHD-C1D-ND	-2.26	121.62	124.80
24	b	612	CLA	O2A-CGA-CBA	2.26	118.73	111.83
24	b	613	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
24	B	607	CLA	CHC-C4B-NB	2.26	127.44	124.05
24	B	609	CLA	C3B-C4B-NB	2.26	112.55	110.53
24	b	615	CLA	CHD-C1D-ND	-2.26	121.62	124.80
24	B	604	CLA	CMA-C3A-C2A	-2.26	105.24	113.98
24	d	401	CLA	CED-O2D-CGD	2.26	121.04	115.92
26	B	620	BCR	C10-C11-C12	-2.26	116.66	123.20
24	c	512	CLA	O2A-CGA-CBA	2.26	118.72	111.83
29	A	414	LMT	O1B-C4'-C3'	2.26	112.97	107.23
43	V	201	HEC	C2A-C1A-NA	-2.26	108.15	110.32
24	c	512	CLA	CHC-C1C-C2C	-2.25	120.54	126.95
24	C	503	CLA	CMB-C2B-C1B	2.25	128.85	125.42
24	B	608	CLA	CHA-C1A-NA	-2.25	121.29	126.39
24	b	618	CLA	CHD-C4C-NC	2.25	127.72	124.23
24	D	401	CLA	CAA-CBA-CGA	2.25	119.59	113.21
29	M	101	LMT	O5B-C5B-C4B	2.25	113.75	109.70
24	b	611	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
40	e	103	HEM	CHD-C4C-NC	2.25	126.90	124.45
24	A	405	CLA	C4-C3-C5	2.25	119.13	115.23
24	d	405	CLA	CHA-C1A-NA	-2.25	121.30	126.39
24	A	406	CLA	CMA-C3A-C2A	-2.25	105.29	113.98
26	a	2114	BCR	C7-C8-C9	-2.25	122.91	126.23
37	v	203	GOL	C3-C2-C1	-2.25	103.55	111.80
24	d	404	CLA	CAC-C3C-C4C	2.25	127.71	124.79
24	C	514	CLA	C11-C10-C8	-2.25	108.50	115.97
24	B	602	CLA	C4B-C3B-C2B	-2.25	104.51	107.30
24	c	505	CLA	O2A-CGA-CBA	2.24	118.68	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	606	CLA	C3C-C4C-NC	2.24	113.31	110.43
39	D	410	LHG	O7-C7-C8	2.24	116.34	111.48
36	I	1202	HTG	C3-C4-C5	2.24	114.30	110.23
24	D	401	CLA	CHD-C4C-NC	2.24	127.70	124.23
24	b	618	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
39	D	411	LHG	O8-C23-O10	-2.24	118.03	123.63
24	D	401	CLA	O2D-CGD-O1D	-2.24	119.50	123.85
24	B	603	CLA	CHC-C1C-C2C	-2.24	120.60	126.95
24	A	409	CLA	C2A-C1A-CHA	-2.23	119.99	123.87
24	d	404	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
28	A	412	LMG	O8-C28-C29	2.23	118.64	111.83
24	c	503	CLA	CMB-C2B-C1B	2.23	128.82	125.42
24	D	401	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
24	c	506	CLA	CHD-C4C-NC	2.23	127.69	124.23
24	c	504	CLA	C3B-C4B-NB	2.23	112.52	110.53
24	B	611	CLA	CHD-C1D-ND	-2.23	121.67	124.80
28	B	622	LMG	O1-C7-C8	-2.22	105.41	110.82
24	b	606	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
24	b	616	CLA	CBC-CAC-C3C	-2.22	106.39	112.42
24	D	401	CLA	CMC-C2C-C1C	2.22	128.50	125.03
24	C	506	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
24	C	514	CLA	CMC-C2C-C1C	2.22	128.50	125.03
24	C	509	CLA	CHD-C1D-ND	-2.22	121.68	124.80
38	c	520	DGD	O2G-C1B-C2B	2.22	116.28	111.48
24	a	2110	CLA	CAC-C3C-C4C	2.22	127.68	124.79
41	H	101	RRX	C11-C10-C9	-2.22	124.17	127.28
24	B	608	CLA	C4A-NA-C1A	2.22	107.69	106.68
24	d	401	CLA	O2A-CGA-CBA	2.22	118.59	111.83
27	A	411	SQD	C44-O6-C1	-2.22	109.04	113.80
24	c	506	CLA	O1D-CGD-CBD	-2.22	120.15	124.52
24	C	510	CLA	CMC-C2C-C1C	2.22	128.50	125.03
24	C	511	CLA	CHD-C1D-ND	-2.22	121.69	124.80
26	T	101	BCR	C3-C4-C5	-2.21	110.11	114.06
24	b	613	CLA	CAC-C3C-C4C	2.21	127.67	124.79
24	D	405	CLA	CMC-C2C-C1C	2.21	128.49	125.03
26	c	528	BCR	C16-C17-C18	-2.21	124.18	127.28
43	v	201	HEC	C2A-C1A-NA	-2.21	108.19	110.32
29	M	101	LMT	C3'-C4'-C5'	-2.21	106.03	110.93
24	B	617	CLA	CHD-C1D-ND	-2.21	121.69	124.80
24	a	2110	CLA	CMA-C3A-C2A	-2.21	105.44	113.98
24	B	611	CLA	CMC-C2C-C1C	2.21	128.48	125.03
27	F	101	SQD	O47-C7-O49	-2.21	118.55	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	619	BCR	C29-C28-C27	-2.21	106.42	111.28
24	c	506	CLA	C11-C10-C8	-2.21	108.63	115.97
29	a	2120	LMT	O5B-C5B-C4B	2.20	113.67	109.70
24	c	507	CLA	C4B-C3B-C2B	-2.20	104.56	107.30
29	B	636	LMT	C1B-C2B-C3B	2.20	114.65	110.01
24	C	514	CLA	C4B-C3B-C2B	-2.20	104.56	107.30
24	C	514	CLA	C3B-C4B-NB	2.20	112.50	110.53
31	D	407	PL9	C51-C49-C50	2.20	119.66	114.59
24	C	510	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
24	b	616	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
24	b	614	CLA	CHB-C4A-NA	2.20	127.58	124.40
24	a	2109	CLA	CHA-C1A-NA	-2.20	121.41	126.39
26	B	619	BCR	C15-C16-C17	-2.20	119.02	123.52
24	c	508	CLA	CAA-CBA-CGA	2.20	119.45	113.21
24	d	404	CLA	CMA-C3A-C2A	-2.20	105.48	113.98
28	c	521	LMG	O1-C7-C8	-2.20	105.47	110.82
24	c	510	CLA	CHA-C1A-NA	-2.20	121.42	126.39
24	B	608	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
29	m	103	LMT	C1B-O1B-C4'	-2.20	112.77	117.98
38	C	518	DGD	O6E-C5E-C6E	2.20	111.88	106.44
24	c	511	CLA	CAC-C3C-C4C	2.20	127.65	124.79
26	d	406	BCR	C10-C11-C12	-2.19	116.84	123.20
24	d	401	CLA	C1-O2A-CGA	2.19	121.96	116.65
26	b	620	BCR	C15-C14-C13	-2.19	124.20	127.28
25	A	407	PHO	C4-C3-C5	2.19	119.03	115.23
26	k	2003	BCR	C21-C20-C19	-2.19	116.85	123.20
24	b	610	CLA	C3B-C4B-NB	2.19	112.49	110.53
24	b	614	CLA	C3B-C4B-NB	2.19	112.49	110.53
24	c	509	CLA	CMC-C2C-C1C	2.19	128.46	125.03
26	c	517	BCR	C16-C17-C18	-2.19	124.21	127.28
26	A	410	BCR	C15-C16-C17	-2.19	119.05	123.52
29	B	636	LMT	O5B-C5B-C6B	2.19	111.86	106.44
24	B	612	CLA	CMB-C2B-C1B	2.19	128.75	125.42
26	b	621	BCR	C37-C22-C21	-2.19	119.28	122.82
24	b	610	CLA	CHC-C1C-C2C	-2.19	120.74	126.95
27	B	621	SQD	O5-C5-C4	2.18	113.64	109.70
28	A	412	LMG	O1-C1-C2	2.18	111.59	108.27
26	K	101	BCR	C10-C11-C12	-2.18	116.87	123.20
24	c	508	CLA	CHD-C1D-ND	-2.18	121.73	124.80
24	b	613	CLA	CMC-C2C-C1C	2.18	128.45	125.03
31	d	407	PL9	C47-C48-C49	-2.18	120.36	127.64
24	C	505	CLA	C1-C2-C3	-2.18	122.62	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	d	408	LHG	O7-C7-O9	-2.18	118.60	123.70
40	F	102	HEM	CBA-CAA-C2A	-2.18	106.50	112.53
24	B	616	CLA	C11-C12-C13	-2.18	108.71	115.97
24	b	610	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
24	C	508	CLA	CBA-CAA-C2A	-2.18	107.30	113.79
24	d	404	CLA	CHA-C1A-NA	-2.18	121.45	126.39
26	b	622	BCR	C3-C4-C5	-2.18	110.17	114.06
38	D	408	DGD	O2G-C1B-O1B	-2.18	118.61	123.70
29	I	1201	LMT	C3'-C4'-C5'	2.18	114.18	110.23
24	B	614	CLA	O2A-CGA-CBA	2.18	118.48	111.83
24	b	606	CLA	CAA-C2A-C1A	-2.18	104.83	111.97
26	B	620	BCR	C16-C17-C18	-2.18	124.22	127.28
25	A	408	PHO	C4-C3-C2	-2.18	118.03	123.63
24	d	405	CLA	CMB-C2B-C1B	2.18	128.73	125.42
24	c	508	CLA	CHB-C1B-C2B	-2.17	121.12	127.43
29	m	102	LMT	O5'-C1'-O1'	-2.17	104.91	110.04
26	b	622	BCR	C2-C3-C4	-2.17	106.50	111.28
24	c	513	CLA	CHC-C1C-C2C	-2.17	120.77	126.95
29	B	623	LMT	O5'-C5'-C4'	2.17	114.21	109.72
24	b	617	CLA	CED-O2D-CGD	2.17	120.84	115.92
24	b	617	CLA	CHC-C1C-C2C	-2.17	120.78	126.95
24	C	514	CLA	CHA-C1A-NA	-2.17	121.48	126.39
41	h	702	RRX	C15-C16-C17	-2.17	119.08	123.52
24	d	404	CLA	CMC-C2C-C1C	2.17	128.42	125.03
24	C	514	CLA	CAC-C3C-C4C	2.17	127.61	124.79
26	c	516	BCR	C37-C22-C23	2.17	121.40	118.09
28	B	622	LMG	C9-C8-C7	-2.17	106.73	111.78
24	C	504	CLA	CHD-C4C-NC	2.17	127.59	124.23
24	b	611	CLA	CAA-C2A-C3A	-2.17	107.15	113.00
24	C	513	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
31	D	407	PL9	O2-C1-C6	-2.16	117.04	120.48
24	b	613	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
24	d	401	CLA	CHA-C1A-NA	-2.16	121.49	126.39
29	A	420	LMT	C2'-C3'-C4'	-2.16	104.77	109.68
24	C	513	CLA	CAC-C3C-C2C	2.16	131.53	127.56
31	x	801	PL9	C46-C44-C45	2.16	119.56	114.59
24	b	607	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
24	b	608	CLA	CMA-C3A-C4A	-2.16	105.97	111.77
24	c	512	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
29	M	101	LMT	O1B-C1B-O5B	-2.16	105.02	110.69
31	x	801	PL9	C27-C26-C24	-2.16	106.04	113.19
24	b	618	CLA	C6-C7-C8	-2.16	108.80	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	C3B-C4B-NB	2.16	112.45	110.53
24	D	404	CLA	CHD-C4C-NC	2.16	127.57	124.23
24	B	615	CLA	CHA-C1A-NA	-2.15	121.51	126.39
38	C	519	DGD	O6E-C1E-O5D	-2.15	104.95	110.04
31	x	801	PL9	C30-C29-C31	2.15	118.96	115.23
24	c	505	CLA	CHD-C1D-C2D	-2.15	121.01	125.49
24	C	503	CLA	CAC-C3C-C4C	2.15	127.59	124.79
24	A	405	CLA	C1-C2-C3	-2.15	122.67	126.20
24	B	602	CLA	CHD-C4C-NC	2.15	127.57	124.23
24	c	510	CLA	CHD-C1D-ND	-2.15	121.78	124.80
26	k	2003	BCR	C8-C7-C6	-2.15	121.25	127.00
24	b	605	CLA	CED-O2D-CGD	2.15	120.79	115.92
29	B	623	LMT	O5B-C1B-C2B	2.15	114.79	110.37
24	B	609	CLA	CHA-C1A-NA	-2.15	121.52	126.39
29	I	1201	LMT	C1-O1'-C1'	-2.15	110.01	113.68
36	c	523	HTG	C6-C5-C4	-2.15	107.74	113.02
24	B	609	CLA	C11-C12-C13	-2.15	108.82	115.97
24	b	619	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
24	c	508	CLA	CAC-C3C-C4C	2.15	127.58	124.79
24	B	606	CLA	C1-C2-C3	-2.15	122.68	126.20
24	C	513	CLA	CHC-C1C-C2C	-2.15	120.85	126.95
24	b	606	CLA	CMB-C2B-C1B	2.15	128.69	125.42
24	D	401	CLA	C4C-C3C-C2C	-2.15	103.77	106.89
24	d	405	CLA	CHC-C1C-C2C	-2.15	120.85	126.95
24	c	515	CLA	CMC-C2C-C1C	2.15	128.39	125.03
26	t	102	BCR	C12-C13-C14	-2.15	115.63	119.01
41	h	702	RRX	C38-C26-C25	-2.15	122.14	124.48
24	b	609	CLA	CHC-C1C-C2C	-2.14	120.85	126.95
29	E	105	LMT	O2'-C2'-C3'	-2.14	105.32	110.38
24	b	615	CLA	CED-O2D-CGD	2.14	120.78	115.92
26	A	410	BCR	C8-C7-C6	-2.14	121.27	127.00
36	B	625[B]	HTG	C1-C2-C3	2.14	114.74	110.55
31	d	407	PL9	C53-C6-C1	2.14	119.67	115.28
24	C	512	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
24	B	614	CLA	CHB-C4A-NA	2.14	127.49	124.40
24	B	608	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
31	A	417	PL9	C30-C29-C28	-2.14	118.13	123.63
26	b	621	BCR	C38-C26-C25	-2.14	122.15	124.48
24	C	503	CLA	CHC-C1C-C2C	-2.14	120.87	126.95
24	b	617	CLA	CMB-C2B-C1B	2.14	128.68	125.42
26	k	2003	BCR	C3-C4-C5	-2.14	110.24	114.06
24	D	405	CLA	C11-C10-C8	-2.14	108.86	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	619	BCR	C33-C5-C6	-2.14	122.15	124.48
38	h	703	DGD	C3G-O3G-C1D	-2.14	109.22	113.80
38	C	519	DGD	O6D-C1D-O3G	-2.14	105.00	110.04
24	c	509	CLA	O2A-CGA-CBA	2.13	118.34	111.83
24	B	617	CLA	CMA-C3A-C4A	-2.13	106.04	111.77
24	A	406	CLA	CAA-CBA-CGA	2.13	119.27	113.21
24	A	405	CLA	CHB-C1B-C2B	-2.13	121.23	127.43
28	i	101	LMG	C7-O1-C1	-2.13	109.23	113.80
24	C	513	CLA	C4B-C3B-C2B	-2.13	104.65	107.30
24	c	510	CLA	CAC-C3C-C2C	2.13	131.47	127.56
24	b	611	CLA	CHC-C1C-C2C	-2.13	120.89	126.95
24	b	606	CLA	C4-C3-C5	2.13	118.93	115.23
24	c	515	CLA	CHA-C1A-NA	-2.13	121.57	126.39
24	b	617	CLA	OBD-CAD-C3D	-2.13	123.44	128.42
27	F	101	SQD	O48-C23-O10	-2.13	118.30	123.63
24	b	614	CLA	C7-C6-C5	-2.13	107.59	113.26
24	c	506	CLA	CMB-C2B-C1B	2.13	128.66	125.42
38	c	518	DGD	O6D-C5D-C6D	2.13	110.91	106.69
24	D	401	CLA	CHB-C4A-NA	2.13	127.47	124.40
29	B	623	LMT	O1B-C4'-C3'	2.13	112.63	107.23
27	A	413	SQD	O9-S-C6	2.13	109.93	106.76
29	a	2120	LMT	C1-O1'-C1'	-2.13	110.05	113.68
24	b	606	CLA	C7-C6-C5	-2.13	107.60	113.26
26	b	621	BCR	C29-C30-C25	2.13	113.53	110.44
32	a	2119	K2I	C5-C-C1	-2.12	118.30	121.24
24	A	406	CLA	CHB-C1B-C2B	-2.12	121.26	127.43
26	k	2003	BCR	C11-C10-C9	-2.12	124.30	127.28
28	D	412	LMG	C9-C8-C7	-2.12	106.83	111.78
25	a	2112	PHO	O2A-CGA-CBA	2.12	118.30	111.83
26	b	622	BCR	C2-C1-C6	2.12	113.52	110.44
29	m	103	LMT	O5'-C5'-C6'	2.12	111.69	106.44
24	b	604	CLA	CAA-C2A-C3A	-2.12	107.27	113.00
41	H	101	RRX	C40-C30-C25	-2.12	106.92	110.24
24	b	609	CLA	C1-O2A-CGA	2.12	121.78	116.65
28	c	521	LMG	O8-C28-O10	-2.12	118.33	123.63
24	a	2109	CLA	C1-C2-C3	-2.12	122.73	126.20
29	z	1801	LMT	C1'-O5'-C5'	2.12	117.85	113.72
24	B	609	CLA	CHB-C4A-NA	2.12	127.45	124.40
24	D	405	CLA	C6-C7-C8	-2.11	108.94	115.97
24	c	504	CLA	CHD-C4C-NC	2.11	127.51	124.23
24	c	506	CLA	CED-O2D-CGD	2.11	120.70	115.92
25	a	2111	PHO	CMA-C3A-C4A	-2.11	110.06	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	401	CLA	O2D-CGD-O1D	-2.11	119.74	123.85
24	a	2113	CLA	CHC-C1C-C2C	-2.11	120.95	126.95
29	m	102	LMT	O5B-C5B-C4B	2.11	113.50	109.70
24	B	602	CLA	CHA-C1A-NA	-2.11	121.62	126.39
24	C	507	CLA	CMB-C2B-C1B	2.11	128.63	125.42
24	C	511	CLA	CHA-C1A-NA	-2.11	121.62	126.39
24	C	507	CLA	CAC-C3C-C4C	2.11	127.53	124.79
24	B	614	CLA	CMC-C2C-C1C	2.11	128.32	125.03
40	F	102	HEM	C1D-C2D-C3D	-2.11	104.77	106.98
36	B	626	HTG	C1-C2-C3	2.11	114.67	110.55
24	C	510	CLA	CAC-C3C-C4C	2.11	127.53	124.79
24	c	503	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
24	d	405	CLA	CMA-C3A-C2A	-2.10	105.84	113.98
24	c	506	CLA	CAA-C2A-C1A	-2.10	105.08	111.97
39	l	101	LHG	C9-C8-C7	-2.10	105.98	113.69
26	B	618	BCR	C10-C11-C12	-2.10	117.11	123.20
24	A	406	CLA	CHC-C1C-C2C	-2.10	120.97	126.95
26	B	620	BCR	C15-C14-C13	-2.10	124.33	127.28
24	b	613	CLA	CHC-C1C-C2C	-2.10	120.97	126.95
24	C	512	CLA	CMB-C2B-C1B	2.10	128.62	125.42
24	d	405	CLA	C6-C7-C8	-2.10	108.98	115.97
24	C	513	CLA	C6-C7-C8	-2.10	108.98	115.97
25	A	408	PHO	CMB-C2B-C3B	2.10	128.88	124.68
24	b	608	CLA	C4B-C3B-C2B	-2.10	104.69	107.30
24	C	505	CLA	CMC-C2C-C1C	2.10	128.32	125.03
26	d	406	BCR	C3-C4-C5	-2.10	110.31	114.06
24	c	510	CLA	C3B-C4B-NB	2.10	112.40	110.53
29	a	2120	LMT	O5'-C5'-C4'	2.10	114.06	109.72
24	c	508	CLA	C11-C12-C13	-2.10	108.99	115.97
24	c	505	CLA	CBC-CAC-C3C	-2.10	106.74	112.42
26	Y	302	BCR	C3-C4-C5	-2.10	110.32	114.06
24	c	503	CLA	O2A-CGA-CBA	2.10	118.23	111.83
26	a	2114	BCR	C10-C11-C12	-2.10	117.13	123.20
24	B	616	CLA	CHD-C1D-ND	-2.10	121.85	124.80
24	b	612	CLA	C4A-NA-C1A	2.10	107.64	106.68
24	b	613	CLA	CMA-C3A-C2A	-2.09	105.88	113.98
26	Y	302	BCR	C16-C17-C18	-2.09	124.34	127.28
25	A	407	PHO	C4A-C3A-C2A	-2.09	100.85	102.84
29	m	103	LMT	O5'-C5'-C4'	2.09	114.05	109.72
24	B	614	CLA	C1-C2-C3	-2.09	122.77	126.20
24	A	409	CLA	O2A-CGA-CBA	2.09	118.21	111.83
24	A	406	CLA	CHD-C4C-NC	2.09	127.47	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	2112	PHO	C4D-CHA-CBD	2.09	109.46	108.45
24	c	506	CLA	O2A-CGA-CBA	2.09	118.21	111.83
31	x	801	PL9	C40-C39-C41	2.09	118.86	115.23
24	a	2109	CLA	CMC-C2C-C1C	2.09	128.30	125.03
24	B	611	CLA	CHC-C1C-C2C	-2.09	121.01	126.95
26	k	2003	BCR	C10-C11-C12	-2.09	117.14	123.20
24	d	401	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
25	a	2111	PHO	C4A-C3A-C2A	-2.09	100.85	102.84
26	t	102	BCR	C29-C28-C27	-2.09	106.69	111.28
26	D	406	BCR	C16-C17-C18	-2.09	124.35	127.28
24	c	509	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
29	A	414	LMT	O5B-C5B-C6B	2.09	111.61	106.44
24	b	607	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
38	c	520	DGD	O1G-C1A-O1A	-2.08	118.41	123.63
28	i	101	LMG	O8-C28-C29	2.08	118.19	111.83
24	b	606	CLA	CHC-C1C-C2C	-2.08	121.03	126.95
24	a	2110	CLA	O2D-CGD-O1D	-2.08	119.80	123.85
26	k	2003	BCR	C34-C9-C8	2.08	121.27	118.09
24	C	514	CLA	CHD-C1D-ND	-2.08	121.87	124.80
24	B	608	CLA	CMB-C2B-C1B	2.08	128.59	125.42
29	a	2103	LMT	O5B-C5B-C6B	2.08	111.59	106.44
39	D	409	LHG	C25-C24-C23	-2.08	106.07	113.69
38	D	408	DGD	O6D-C5D-C6D	2.08	110.82	106.69
24	B	611	CLA	C16-C17-C18	-2.08	106.66	115.94
24	b	618	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
29	m	102	LMT	C1-O1'-C1'	-2.08	110.13	113.68
28	C	526	LMG	C12-C11-C10	-2.08	106.08	113.69
24	b	610	CLA	CHA-C1A-NA	-2.08	121.69	126.39
36	O	302	HTG	O2-C2-C3	-2.08	105.48	110.38
24	C	513	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
38	h	703	DGD	C6D-C5D-C4D	2.08	116.42	112.07
24	B	610	CLA	CED-O2D-CGD	2.07	120.62	115.92
26	C	516	BCR	C11-C10-C9	-2.07	124.37	127.28
28	C	526	LMG	O7-C10-O9	-2.07	118.86	123.70
24	b	616	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
24	d	401	CLA	CHD-C4C-NC	2.07	127.44	124.23
26	B	620	BCR	C21-C20-C19	-2.07	117.19	123.20
24	b	604	CLA	CMC-C2C-C1C	2.07	128.27	125.03
24	c	510	CLA	CHC-C1C-C2C	-2.07	121.06	126.95
31	A	417	PL9	C10-C9-C11	2.07	120.65	114.96
27	f	102	SQD	O48-C23-O10	-2.07	118.45	123.63
24	D	404	CLA	CHA-C1A-NA	-2.07	121.71	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	O2A-CGA-CBA	2.07	118.14	111.83
24	B	613	CLA	C11-C10-C8	-2.07	109.09	115.97
24	B	616	CLA	C4-C3-C5	2.07	118.82	115.23
24	d	405	CLA	C4A-NA-C1A	2.07	107.62	106.68
24	B	614	CLA	CHC-C1C-C2C	-2.07	121.08	126.95
29	M	101	LMT	O1B-C1B-C2B	2.06	113.17	108.09
38	C	517	DGD	O6D-C5D-C6D	2.06	110.79	106.69
24	C	508	CLA	CHC-C4B-NB	2.06	127.14	124.05
24	b	610	CLA	CAA-C2A-C1A	-2.06	105.21	111.97
27	A	411	SQD	O9-S-O7	-2.06	107.11	113.82
38	c	520	DGD	C2G-O2G-C1B	-2.06	112.86	117.80
27	a	2102	SQD	C44-O6-C1	-2.06	109.38	113.80
29	J	102	LMT	O5'-C5'-C4'	2.06	113.41	109.70
40	e	103	HEM	C1B-NB-C4B	2.06	107.64	105.21
24	b	612	CLA	CHC-C1C-C2C	-2.06	121.10	126.95
24	D	404	CLA	CMB-C2B-C1B	2.06	128.55	125.42
24	b	607	CLA	CHC-C4B-C3B	-2.05	118.45	127.37
24	c	504	CLA	CHA-C1A-NA	-2.05	121.74	126.39
24	D	401	CLA	O2A-CGA-CBA	2.05	118.09	111.83
24	B	603	CLA	CBC-CAC-C3C	-2.05	106.86	112.42
24	a	2113	CLA	CMA-C3A-C4A	-2.05	106.26	111.77
24	c	504	CLA	CHC-C1C-C2C	-2.05	121.12	126.95
24	A	409	CLA	CAC-C3C-C4C	2.05	127.46	124.79
26	B	620	BCR	C15-C16-C17	-2.05	119.32	123.52
24	c	514	CLA	C4-C3-C5	2.05	118.79	115.23
38	H	102	DGD	C6D-C5D-C4D	2.05	116.37	112.07
24	c	511	CLA	C4-C3-C5	2.05	118.78	115.23
29	a	2120	LMT	O5'-C5'-C6'	2.05	111.52	106.44
26	K	101	BCR	C2-C3-C4	-2.05	106.77	111.28
39	E	101	LHG	O7-C7-O9	-2.05	118.92	123.70
24	c	506	CLA	C1-O2A-CGA	2.05	121.61	116.65
24	C	510	CLA	CMB-C2B-C1B	2.05	128.53	125.42
26	B	620	BCR	C7-C8-C9	-2.05	123.21	126.23
24	c	511	CLA	CHD-C1D-C2D	-2.04	121.24	125.49
24	B	609	CLA	CAA-C2A-C3A	-2.04	107.48	113.00
24	C	508	CLA	CAC-C3C-C2C	2.04	131.31	127.56
24	b	611	CLA	C4-C3-C5	2.04	118.77	115.23
24	b	605	CLA	CMC-C2C-C1C	2.04	128.22	125.03
36	V	204	HTG	C4-C3-C2	-2.04	107.25	110.83
24	b	617	CLA	C1-O2A-CGA	2.04	121.58	116.65
24	C	505	CLA	O2A-CGA-CBA	2.04	118.05	111.83
24	c	503	CLA	C1-O2A-CGA	2.04	121.58	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	d	403	HTG	O5-C5-C4	2.04	113.37	109.70
24	B	607	CLA	C1-C2-C3	-2.04	122.86	126.20
24	B	606	CLA	CHA-C1A-NA	-2.04	121.78	126.39
26	A	410	BCR	C29-C30-C25	2.04	113.40	110.44
24	B	616	CLA	CED-O2D-CGD	2.03	120.53	115.92
26	T	101	BCR	C36-C18-C19	2.03	121.19	118.09
24	b	612	CLA	C7-C6-C5	-2.03	107.85	113.26
26	a	2114	BCR	C8-C7-C6	-2.03	121.57	127.00
24	c	513	CLA	CHD-C4C-NC	2.03	127.38	124.23
24	b	610	CLA	CAC-C3C-C4C	2.03	127.43	124.79
24	a	2113	CLA	CHB-C4A-NA	2.03	127.33	124.40
26	B	618	BCR	C28-C27-C26	-2.03	110.44	114.06
24	B	614	CLA	CHA-C1A-NA	-2.03	121.80	126.39
24	C	510	CLA	C4-C3-C2	-2.03	118.42	123.63
24	b	610	CLA	CMA-C3A-C2A	-2.03	106.14	113.98
24	c	511	CLA	CMB-C2B-C1B	2.03	128.50	125.42
24	B	617	CLA	O2A-CGA-CBA	2.03	118.01	111.83
26	c	528	BCR	C7-C6-C5	-2.03	116.89	121.56
24	B	616	CLA	C7-C6-C5	-2.02	107.87	113.26
24	B	605	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
36	B	625[A]	HTG	C1-C2-C3	2.02	114.50	110.55
24	D	401	CLA	C1-O2A-CGA	2.02	121.54	116.65
26	B	618	BCR	C34-C9-C10	-2.02	119.54	122.82
26	b	620	BCR	C40-C30-C25	-2.02	107.07	110.24
40	F	102	HEM	C1B-NB-C4B	2.02	107.60	105.21
32	A	419	K2I	C2-C3-C4	-2.02	118.44	121.24
38	c	519	DGD	O1G-C1A-C2A	2.02	117.99	111.83
28	C	526	LMG	O8-C28-O10	-2.02	118.58	123.63
27	L	102	SQD	O48-C23-O10	-2.02	118.58	123.63
26	T	101	BCR	C2-C1-C6	2.02	113.37	110.44
24	B	616	CLA	CHD-C4C-NC	2.01	127.36	124.23
38	c	518	DGD	O1G-C1A-O1A	-2.01	118.59	123.63
24	c	511	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
24	A	406	CLA	CHA-C1A-NA	-2.01	121.84	126.39
24	C	502	CLA	CMC-C2C-C1C	2.01	128.18	125.03
24	B	606	CLA	CMA-C3A-C2A	-2.01	106.21	113.98
24	B	613	CLA	CMA-C3A-C2A	-2.01	106.21	113.98
24	C	506	CLA	CMC-C2C-C1C	2.01	128.18	125.03
24	c	509	CLA	CHD-C1D-ND	-2.01	121.97	124.80
24	A	409	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
24	B	617	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
24	c	505	CLA	C6-C7-C8	-2.01	109.28	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414	LMT	O5'-C1'-C2'	2.01	114.50	110.37
24	a	2109	CLA	C7-C6-C5	-2.01	107.91	113.26
24	B	603	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
25	A	407	PHO	O2A-CGA-CBA	2.01	117.96	111.83
24	d	405	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
26	B	619	BCR	C11-C10-C9	-2.01	124.46	127.28
24	b	613	CLA	C11-C12-C13	-2.01	109.29	115.97
26	C	516	BCR	C15-C16-C17	-2.01	119.41	123.52
26	t	102	BCR	C16-C15-C14	2.01	127.62	123.52
24	D	401	CLA	C4-C3-C5	2.01	118.71	115.23
24	b	618	CLA	CMA-C3A-C4A	-2.00	106.39	111.77
26	B	618	BCR	C34-C9-C8	2.00	121.15	118.09
24	B	608	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
24	B	604	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
24	b	614	CLA	C11-C12-C13	-2.00	109.31	115.97
26	Y	302	BCR	C7-C6-C5	-2.00	116.94	121.56
29	B	636	LMT	C1-O1'-C1'	-2.00	110.26	113.68
24	C	502	CLA	CHA-C1A-NA	-2.00	121.86	126.39
24	c	506	CLA	CHA-C1A-NA	-2.00	121.86	126.39
40	e	103	HEM	C2A-C1A-NA	-2.00	107.93	110.15
39	l	101	LHG	O4-P-O5	2.00	121.75	112.44
24	a	2113	CLA	CHD-C1D-C2D	-2.00	121.33	125.49
24	c	507	CLA	CMA-C3A-C4A	-2.00	106.40	111.77

All (62) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	409	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND
24	B	606	CLA	ND
24	B	607	CLA	ND
24	B	608	CLA	ND
24	B	610	CLA	ND
24	B	611	CLA	ND
24	B	612	CLA	ND
24	B	613	CLA	ND
24	B	614	CLA	ND
24	B	615	CLA	ND

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Mol	Chain	Res	Type	Atom
24	B	616	CLA	ND
24	B	617	CLA	ND
24	C	502	CLA	ND
24	C	503	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	507	CLA	ND
24	C	508	CLA	ND
24	C	509	CLA	ND
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	C	514	CLA	ND
24	D	404	CLA	ND
24	D	405	CLA	ND
24	a	2109	CLA	ND
24	a	2113	CLA	ND
24	b	604	CLA	ND
24	b	605	CLA	ND
24	b	606	CLA	ND
24	b	607	CLA	ND
24	b	608	CLA	ND
24	b	609	CLA	ND
24	b	610	CLA	ND
24	b	612	CLA	ND
24	b	613	CLA	ND
24	b	614	CLA	ND
24	b	615	CLA	ND
24	b	616	CLA	ND
24	b	617	CLA	ND
24	b	618	CLA	ND
24	b	619	CLA	ND
24	c	504	CLA	ND
24	c	505	CLA	ND
24	c	506	CLA	ND
24	c	507	CLA	ND
24	c	508	CLA	ND
24	c	509	CLA	ND
24	c	510	CLA	ND
24	c	511	CLA	ND
24	c	512	CLA	ND

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Mol	Chain	Res	Type	Atom
24	c	514	CLA	ND
24	c	515	CLA	ND
24	d	401	CLA	ND
24	d	404	CLA	ND
24	d	405	CLA	ND

All (1142) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	C	510	CLA	CHA-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O2D
24	b	617	CLA	CAD-CBD-CGD-O1D
24	b	617	CLA	CAD-CBD-CGD-O2D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
26	D	406	BCR	C21-C22-C23-C24
26	T	101	BCR	C13-C14-C15-C16
26	d	406	BCR	C21-C22-C23-C24
26	t	102	BCR	C13-C14-C15-C16
27	A	413	SQD	O6-C44-C45-O47
27	B	621	SQD	O5-C1-O6-C44
27	B	621	SQD	O49-C7-O47-C45
27	B	621	SQD	C8-C7-O47-C45
27	B	621	SQD	C5-C6-S-O7
27	B	621	SQD	C5-C6-S-O8
27	B	621	SQD	C5-C6-S-O9
27	F	101	SQD	C8-C7-O47-C45
27	L	102	SQD	O5-C1-O6-C44
27	L	102	SQD	O49-C7-O47-C45
27	L	102	SQD	C5-C6-S-O7
27	a	2102	SQD	O5-C5-C6-S
27	f	102	SQD	C8-C7-O47-C45
27	f	102	SQD	C5-C6-S-O7
28	C	526	LMG	O9-C10-O7-C8
28	C	526	LMG	C11-C10-O7-C8
28	i	101	LMG	C11-C10-O7-C8
29	A	420	LMT	C3'-C4'-O1B-C1B
29	A	420	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
29	E	105	LMT	O5'-C1'-O1'-C1
29	I	1201	LMT	C2'-C1'-O1'-C1
29	f	101	LMT	O5'-C1'-O1'-C1
29	i	104	LMT	O5'-C1'-O1'-C1
29	j	1601	LMT	O5'-C1'-O1'-C1
31	A	417	PL9	C12-C11-C9-C8
31	A	417	PL9	C12-C11-C9-C10
31	A	417	PL9	C33-C34-C36-C37
31	A	417	PL9	C35-C34-C36-C37
36	B	626	HTG	O5-C1-S1-C1'
36	I	1202	HTG	O5-C1-S1-C1'
36	V	204	HTG	O5-C1-S1-C1'
36	b	626	HTG	O5-C1-S1-C1'
37	C	525	GOL	C1-C2-C3-O3
37	C	525	GOL	O2-C2-C3-O3
37	H	103	GOL	C1-C2-C3-O3
37	U	501	GOL	C1-C2-C3-O3
37	Z	102	GOL	O2-C2-C3-O3
37	b	631	GOL	C1-C2-C3-O3
37	k	2001	GOL	O1-C1-C2-C3
37	o	2603	GOL	C1-C2-C3-O3
37	v	202	GOL	C1-C2-C3-O3
38	D	408	DGD	O1B-C1B-O2G-C2G
38	D	408	DGD	C2D-C1D-O3G-C3G
38	D	408	DGD	O6D-C1D-O3G-C3G
39	D	410	LHG	C4-O6-P-O4
39	E	101	LHG	O2-C2-C3-O3
39	E	101	LHG	C3-O3-P-O4
39	E	101	LHG	C3-O3-P-O5
39	E	101	LHG	C3-O3-P-O6
39	L	101	LHG	C4-O6-P-O3
39	L	101	LHG	C4-O6-P-O4
39	L	101	LHG	C4-O6-P-O5
39	d	408	LHG	C1-C2-C3-O3
39	d	409	LHG	C1-C2-C3-O3
39	d	409	LHG	C3-O3-P-O4
39	d	409	LHG	C3-O3-P-O5
39	d	409	LHG	C3-O3-P-O6
39	e	101	LHG	O2-C2-C3-O3
39	e	101	LHG	C4-O6-P-O5
39	l	101	LHG	C4-O6-P-O3
39	l	101	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
39	l	101	LHG	C4-O6-P-O5
43	V	201	HEC	C2B-C3B-CAB-CBB
43	V	201	HEC	C4B-C3B-CAB-CBB
43	V	201	HEC	C2C-C3C-CAC-CBC
43	V	201	HEC	C4C-C3C-CAC-CBC
43	v	201	HEC	C2B-C3B-CAB-CBB
43	v	201	HEC	C4B-C3B-CAB-CBB
43	v	201	HEC	C2C-C3C-CAC-CBC
43	v	201	HEC	C4C-C3C-CAC-CBC
27	F	101	SQD	O10-C23-O48-C46
27	F	101	SQD	O49-C7-O47-C45
27	f	102	SQD	O49-C7-O47-C45
28	A	412	LMG	O9-C10-O7-C8
28	i	101	LMG	O9-C10-O7-C8
24	B	605	CLA	C3-C5-C6-C7
24	b	619	CLA	C3-C5-C6-C7
27	L	102	SQD	C8-C7-O47-C45
38	D	408	DGD	C2B-C1B-O2G-C2G
24	B	606	CLA	C4-C3-C5-C6
24	c	509	CLA	C4-C3-C5-C6
27	F	101	SQD	C24-C23-O48-C46
29	i	104	LMT	C4'-C5'-C6'-O6'
24	B	615	CLA	C3-C5-C6-C7
39	d	408	LHG	O2-C2-C3-O3
39	d	409	LHG	O2-C2-C3-O3
28	A	412	LMG	C11-C10-O7-C8
29	m	102	LMT	O5B-C5B-C6B-O6B
24	B	602	CLA	C3-C5-C6-C7
29	T	102	LMT	O5'-C5'-C6'-O6'
36	O	302	HTG	S1-C1'-C2'-C3'
24	b	617	CLA	C4-C3-C5-C6
24	B	606	CLA	C2-C3-C5-C6
24	b	617	CLA	C2-C3-C5-C6
24	c	509	CLA	C2-C3-C5-C6
29	a	2120	LMT	O5B-C5B-C6B-O6B
29	z	1801	LMT	O5B-C5B-C6B-O6B
36	B	626	HTG	O5-C5-C6-O6
31	A	417	PL9	C19-C21-C22-C23
31	A	417	PL9	C29-C31-C32-C33
29	Z	101	LMT	O5B-C1B-O1B-C4'
29	B	637	LMT	O5'-C1'-O1'-C1
29	I	1201	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
29	Z	101	LMT	O5'-C1'-O1'-C1
29	z	1801	LMT	O5'-C1'-O1'-C1
29	B	637	LMT	O5'-C5'-C6'-O6'
29	i	104	LMT	O5'-C5'-C6'-O6'
36	b	602	HTG	O5-C5-C6-O6
36	b	626	HTG	O5-C5-C6-O6
24	B	612	CLA	C8-C10-C11-C12
28	C	526	LMG	C29-C28-O8-C9
24	C	504	CLA	CBD-CGD-O2D-CED
36	b	626	HTG	C4-C5-C6-O6
29	a	2103	LMT	C3'-C4'-O1B-C1B
24	c	508	CLA	C13-C15-C16-C17
38	C	518	DGD	CAA-CBA-CCA-CDA
24	B	615	CLA	C4-C3-C5-C6
24	b	608	CLA	C4-C3-C5-C6
24	B	615	CLA	C2-C3-C5-C6
24	b	608	CLA	C2-C3-C5-C6
24	B	602	CLA	C11-C10-C8-C9
24	B	611	CLA	C14-C13-C15-C16
24	C	505	CLA	C11-C12-C13-C14
24	C	510	CLA	C11-C10-C8-C9
24	b	604	CLA	C14-C13-C15-C16
24	b	613	CLA	C11-C12-C13-C14
24	c	506	CLA	C14-C13-C15-C16
29	B	637	LMT	C4'-C5'-C6'-O6'
29	B	637	LMT	C2'-C1'-O1'-C1
29	Z	101	LMT	C2'-C1'-O1'-C1
29	a	2120	LMT	C2'-C1'-O1'-C1
29	z	1801	LMT	C2'-C1'-O1'-C1
39	D	409	LHG	C28-C29-C30-C31
26	D	406	BCR	C37-C22-C23-C24
26	d	406	BCR	C37-C22-C23-C24
36	C	522	HTG	S1-C1'-C2'-C3'
38	C	518	DGD	C3A-C4A-C5A-C6A
27	a	2102	SQD	O6-C44-C45-O47
24	B	611	CLA	C15-C16-C17-C18
24	b	609	CLA	C10-C11-C12-C13
28	C	526	LMG	O6-C5-C6-O5
37	d	415	GOL	O2-C2-C3-O3
24	b	616	CLA	C11-C12-C13-C15
38	c	518	DGD	CAA-CBA-CCA-CDA
29	i	104	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
29	Z	101	LMT	C2B-C1B-O1B-C4'
24	b	604	CLA	C10-C11-C12-C13
31	A	417	PL9	C14-C16-C17-C18
31	D	407	PL9	C39-C41-C42-C43
31	d	407	PL9	C39-C41-C42-C43
31	x	801	PL9	C14-C16-C17-C18
36	b	602	HTG	C4-C5-C6-O6
24	a	2109	CLA	C15-C16-C17-C18
29	b	624	LMT	C3'-C4'-O1B-C1B
38	D	408	DGD	C1B-C2B-C3B-C4B
39	e	101	LHG	C7-C8-C9-C10
24	B	605	CLA	CBD-CGD-O2D-CED
24	B	602	CLA	C10-C11-C12-C13
24	C	505	CLA	C15-C16-C17-C18
24	D	405	CLA	C8-C10-C11-C12
24	c	514	CLA	C15-C16-C17-C18
29	m	102	LMT	C4B-C5B-C6B-O6B
29	z	1801	LMT	C4B-C5B-C6B-O6B
24	B	614	CLA	C15-C16-C17-C18
24	d	405	CLA	C8-C10-C11-C12
28	C	526	LMG	O10-C28-O8-C9
29	a	2120	LMT	O5'-C1'-O1'-C1
29	b	624	LMT	O5'-C1'-O1'-C1
24	b	604	CLA	C15-C16-C17-C18
24	b	607	CLA	C15-C16-C17-C18
38	C	518	DGD	C7A-C8A-C9A-CAA
29	T	102	LMT	C4'-C5'-C6'-O6'
24	C	507	CLA	C8-C10-C11-C12
27	L	102	SQD	C31-C32-C33-C34
24	A	406	CLA	C13-C15-C16-C17
24	B	615	CLA	C5-C6-C7-C8
36	B	626	HTG	C4-C5-C6-O6
27	F	101	SQD	C23-C24-C25-C26
28	b	623	LMG	C10-C11-C12-C13
24	B	602	CLA	CBA-CGA-O2A-C1
27	B	621	SQD	C24-C23-O48-C46
24	C	502	CLA	CBD-CGD-O2D-CED
39	E	101	LHG	C1-C2-C3-O3
39	e	101	LHG	C1-C2-C3-O3
24	B	607	CLA	C2A-CAA-CBA-CGA
39	e	101	LHG	C11-C10-C9-C8
24	a	2113	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	b	618	CLA	C10-C11-C12-C13
29	b	624	LMT	O1'-C1-C2-C3
27	B	621	SQD	C23-C24-C25-C26
24	c	515	CLA	C10-C11-C12-C13
24	B	617	CLA	C5-C6-C7-C8
24	C	507	CLA	C5-C6-C7-C8
24	b	619	CLA	C8-C10-C11-C12
28	d	411	LMG	O6-C5-C6-O5
27	A	413	SQD	C2-C1-O6-C44
29	A	420	LMT	C2'-C1'-O1'-C1
29	J	102	LMT	C2'-C1'-O1'-C1
29	a	2103	LMT	C2'-C1'-O1'-C1
29	b	624	LMT	C2'-C1'-O1'-C1
29	m	102	LMT	C2'-C1'-O1'-C1
24	b	619	CLA	C13-C15-C16-C17
28	C	526	LMG	C28-C29-C30-C31
29	A	420	LMT	O1'-C1-C2-C3
36	I	1202	HTG	C1'-C2'-C3'-C4'
29	A	414	LMT	C5'-C4'-O1B-C1B
28	c	522	LMG	O6-C5-C6-O5
26	D	406	BCR	C7-C8-C9-C34
26	Y	302	BCR	C37-C22-C23-C24
29	B	623	LMT	O1'-C1-C2-C3
24	b	606	CLA	C5-C6-C7-C8
24	c	512	CLA	C8-C10-C11-C12
37	O	303	GOL	C1-C2-C3-O3
37	U	502	GOL	O1-C1-C2-C3
37	V	203	GOL	O1-C1-C2-C3
37	V	203	GOL	C1-C2-C3-O3
37	Z	102	GOL	C1-C2-C3-O3
37	d	415	GOL	C1-C2-C3-O3
37	o	2601	GOL	C1-C2-C3-O3
37	v	204	GOL	O1-C1-C2-C3
39	D	411	LHG	O1-C1-C2-C3
39	d	408	LHG	O1-C1-C2-C3
39	d	409	LHG	O1-C1-C2-C3
36	d	403	HTG	C4-C5-C6-O6
38	c	519	DGD	CBB-CCB-CDB-CEB
39	E	101	LHG	C17-C18-C19-C20
24	B	602	CLA	O1A-CGA-O2A-C1
27	B	621	SQD	O10-C23-O48-C46
27	A	413	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
29	B	636	LMT	O5'-C1'-O1'-C1
29	J	102	LMT	O5'-C1'-O1'-C1
29	m	102	LMT	O5'-C1'-O1'-C1
29	A	414	LMT	C3'-C4'-O1B-C1B
24	C	513	CLA	CBA-CGA-O2A-C1
38	C	518	DGD	C1B-C2B-C3B-C4B
29	J	102	LMT	O5'-C5'-C6'-O6'
24	C	510	CLA	C2-C1-O2A-CGA
24	b	604	CLA	C2-C1-O2A-CGA
29	J	102	LMT	C11-C10-C9-C8
29	Z	101	LMT	C4-C5-C6-C7
39	D	409	LHG	C29-C30-C31-C32
29	J	102	LMT	C7-C8-C9-C10
36	C	522	HTG	O5-C5-C6-O6
29	J	102	LMT	C5-C6-C7-C8
29	a	2103	LMT	C2-C3-C4-C5
38	D	408	DGD	C8A-C9A-CAA-CBA
36	B	627	HTG	C2'-C3'-C4'-C5'
29	Z	101	LMT	C2-C1-O1'-C1'
37	H	103	GOL	O2-C2-C3-O3
37	U	501	GOL	O2-C2-C3-O3
37	o	2601	GOL	O2-C2-C3-O3
37	o	2603	GOL	O2-C2-C3-O3
37	v	204	GOL	O1-C1-C2-O2
24	B	616	CLA	C4B-C3B-CAB-CBB
24	C	514	CLA	C4B-C3B-CAB-CBB
24	c	514	CLA	C4B-C3B-CAB-CBB
39	l	101	LHG	C7-C8-C9-C10
28	c	521	LMG	C33-C34-C35-C36
27	F	101	SQD	C26-C27-C28-C29
28	b	623	LMG	C35-C36-C37-C38
24	a	2113	CLA	C10-C11-C12-C13
24	B	617	CLA	C12-C13-C15-C16
27	a	2102	SQD	C32-C33-C34-C35
28	C	526	LMG	C11-C12-C13-C14
28	i	101	LMG	C11-C12-C13-C14
39	L	101	LHG	C7-C8-C9-C10
24	b	607	CLA	C13-C15-C16-C17
24	c	508	CLA	C15-C16-C17-C18
28	C	526	LMG	C29-C30-C31-C32
29	z	1801	LMT	C7-C8-C9-C10
24	C	513	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	D	412	LMG	C12-C13-C14-C15
28	b	623	LMG	C20-C21-C22-C23
29	B	637	LMT	C6-C7-C8-C9
38	C	517	DGD	C4B-C5B-C6B-C7B
39	E	101	LHG	C18-C19-C20-C21
29	E	105	LMT	O5'-C5'-C6'-O6'
28	c	522	LMG	C35-C36-C37-C38
24	b	619	CLA	C5-C6-C7-C8
24	C	507	CLA	C16-C17-C18-C20
24	b	618	CLA	C16-C17-C18-C19
24	b	618	CLA	C16-C17-C18-C20
29	a	2120	LMT	C4B-C5B-C6B-O6B
28	c	521	LMG	C18-C19-C20-C21
39	E	101	LHG	C26-C27-C28-C29
28	c	522	LMG	C10-C11-C12-C13
39	E	101	LHG	C7-C8-C9-C10
28	C	520	LMG	C21-C22-C23-C24
28	c	521	LMG	C32-C33-C34-C35
38	C	518	DGD	C4B-C5B-C6B-C7B
39	D	409	LHG	C25-C26-C27-C28
28	A	412	LMG	C36-C37-C38-C39
39	d	408	LHG	C29-C30-C31-C32
27	L	102	SQD	C27-C28-C29-C30
27	A	413	SQD	C19-C20-C21-C22
27	A	411	SQD	C11-C12-C13-C14
28	D	412	LMG	C35-C36-C37-C38
28	b	623	LMG	C21-C22-C23-C24
28	c	521	LMG	C16-C17-C18-C19
29	Z	101	LMT	O1'-C1-C2-C3
27	B	621	SQD	C11-C10-C9-C8
28	A	412	LMG	C15-C16-C17-C18
29	B	637	LMT	C9-C10-C11-C12
28	C	520	LMG	C31-C32-C33-C34
38	C	517	DGD	CCA-CDA-CEA-CFA
28	B	622	LMG	C28-C29-C30-C31
28	c	522	LMG	C36-C37-C38-C39
38	C	517	DGD	C5B-C6B-C7B-C8B
24	c	512	CLA	C11-C12-C13-C14
38	H	102	DGD	C7A-C8A-C9A-CAA
38	c	518	DGD	C4B-C5B-C6B-C7B
38	c	520	DGD	C8B-C9B-CAB-CBB
39	l	101	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
24	a	2113	CLA	C8-C10-C11-C12
28	c	521	LMG	C15-C16-C17-C18
29	f	101	LMT	C5-C6-C7-C8
39	E	101	LHG	C25-C26-C27-C28
29	M	101	LMT	O5'-C1'-O1'-C1
29	a	2103	LMT	O5'-C1'-O1'-C1
28	A	412	LMG	C12-C13-C14-C15
39	D	409	LHG	C32-C33-C34-C35
29	B	636	LMT	C2'-C1'-O1'-C1
29	E	105	LMT	C2'-C1'-O1'-C1
29	f	101	LMT	C2'-C1'-O1'-C1
38	C	518	DGD	C9A-CAA-CBA-CCA
27	L	102	SQD	C29-C30-C31-C32
27	A	413	SQD	C33-C34-C35-C36
39	D	411	LHG	C27-C28-C29-C30
24	b	614	CLA	C16-C17-C18-C19
28	c	522	LMG	C28-C29-C30-C31
39	E	101	LHG	C9-C10-C11-C12
29	B	623	LMT	C3'-C4'-O1B-C1B
24	A	409	CLA	C15-C16-C17-C18
24	B	615	CLA	C10-C11-C12-C13
27	B	621	SQD	C27-C28-C29-C30
38	h	703	DGD	C7A-C8A-C9A-CAA
29	B	623	LMT	C5'-C4'-O1B-C1B
36	b	626	HTG	C1'-C2'-C3'-C4'
24	D	405	CLA	C13-C15-C16-C17
29	T	102	LMT	C4-C5-C6-C7
38	C	518	DGD	C2G-C3G-O3G-C1D
38	c	519	DGD	C5D-C6D-O5D-C1E
39	L	101	LHG	C11-C10-C9-C8
24	a	2109	CLA	C2C-C3C-CAC-CBC
29	i	104	LMT	C2-C3-C4-C5
28	b	623	LMG	C19-C20-C21-C22
28	i	101	LMG	C36-C37-C38-C39
28	B	622	LMG	C16-C17-C18-C19
24	a	2110	CLA	C15-C16-C17-C18
24	b	619	CLA	C15-C16-C17-C18
39	d	408	LHG	C27-C28-C29-C30
38	C	517	DGD	O6E-C5E-C6E-O5E
38	c	518	DGD	O6E-C5E-C6E-O5E
28	A	412	LMG	C13-C14-C15-C16
38	c	519	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
39	E	101	LHG	C33-C34-C35-C36
31	x	801	PL9	C19-C21-C22-C23
39	e	101	LHG	C17-C18-C19-C20
29	f	101	LMT	C1-C2-C3-C4
28	C	520	LMG	C10-C11-C12-C13
27	f	102	SQD	C25-C26-C27-C28
28	C	520	LMG	C14-C15-C16-C17
29	i	104	LMT	C7-C8-C9-C10
38	c	520	DGD	CBA-CCA-CDA-CEA
36	B	627	HTG	O5-C5-C6-O6
28	c	521	LMG	C14-C15-C16-C17
39	L	101	LHG	C33-C34-C35-C36
24	d	405	CLA	C13-C15-C16-C17
27	L	102	SQD	C28-C29-C30-C31
36	V	204	HTG	C2'-C3'-C4'-C5'
24	B	617	CLA	C2-C1-O2A-CGA
24	B	609	CLA	C13-C15-C16-C17
28	B	622	LMG	C37-C38-C39-C40
38	C	517	DGD	C2A-C3A-C4A-C5A
27	F	101	SQD	C24-C25-C26-C27
27	F	101	SQD	C33-C34-C35-C36
29	m	103	LMT	O5'-C5'-C6'-O6'
28	A	412	LMG	C19-C20-C21-C22
39	d	409	LHG	C32-C33-C34-C35
29	a	2103	LMT	C4B-C5B-C6B-O6B
24	b	616	CLA	C8-C10-C11-C12
38	c	518	DGD	C9A-CAA-CBA-CCA
28	D	412	LMG	C30-C31-C32-C33
37	b	631	GOL	O2-C2-C3-O3
37	k	2001	GOL	O1-C1-C2-O2
38	D	408	DGD	C5A-C6A-C7A-C8A
24	c	510	CLA	C1A-C2A-CAA-CBA
29	j	1601	LMT	C2-C3-C4-C5
29	M	101	LMT	C4B-C5B-C6B-O6B
24	c	511	CLA	C8-C10-C11-C12
29	I	1201	LMT	O5'-C5'-C6'-O6'
36	B	628	HTG	O5-C5-C6-O6
27	f	102	SQD	C26-C27-C28-C29
28	B	622	LMG	C36-C37-C38-C39
28	d	411	LMG	C12-C13-C14-C15
24	A	409	CLA	C11-C12-C13-C15
24	B	614	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	B	615	CLA	C12-C13-C15-C16
24	c	513	CLA	C11-C12-C13-C15
36	b	601	HTG	O5-C5-C6-O6
27	f	102	SQD	C30-C31-C32-C33
29	m	102	LMT	C6-C7-C8-C9
39	D	410	LHG	C32-C33-C34-C35
24	B	616	CLA	C10-C11-C12-C13
24	B	605	CLA	C6-C7-C8-C9
24	B	607	CLA	C11-C12-C13-C14
29	B	636	LMT	C4B-C5B-C6B-O6B
24	D	401	CLA	C2C-C3C-CAC-CBC
29	A	420	LMT	O5B-C5B-C6B-O6B
29	j	1601	LMT	C2'-C1'-O1'-C1
29	z	1801	LMT	O5'-C5'-C6'-O6'
27	A	411	SQD	O6-C44-C45-C46
27	A	413	SQD	O6-C44-C45-C46
27	a	2102	SQD	O6-C44-C45-C46
27	a	2115	SQD	O6-C44-C45-C46
38	C	518	DGD	C3B-C4B-C5B-C6B
39	E	101	LHG	C11-C10-C9-C8
29	B	636	LMT	C5-C6-C7-C8
39	d	408	LHG	C32-C33-C34-C35
38	C	517	DGD	C1B-C2B-C3B-C4B
28	D	412	LMG	O6-C5-C6-O5
36	I	1202	HTG	O5-C5-C6-O6
38	c	518	DGD	C8A-C9A-CAA-CBA
24	C	511	CLA	C8-C10-C11-C12
28	C	520	LMG	C32-C33-C34-C35
39	D	411	LHG	C14-C15-C16-C17
28	A	412	LMG	C21-C22-C23-C24
24	C	511	CLA	C2-C3-C5-C6
39	l	101	LHG	C13-C14-C15-C16
39	L	101	LHG	C13-C14-C15-C16
28	c	522	LMG	C4-C5-C6-O5
24	C	507	CLA	C16-C17-C18-C19
26	Y	302	BCR	C21-C22-C23-C24
24	B	604	CLA	C5-C6-C7-C8
38	c	519	DGD	C9A-CAA-CBA-CCA
38	c	519	DGD	C1A-C2A-C3A-C4A
27	L	102	SQD	C24-C23-O48-C46
27	B	621	SQD	C46-C45-O47-C7
27	A	411	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
38	c	520	DGD	CCB-CDB-CEB-CFB
29	a	2103	LMT	C5'-C4'-O1B-C1B
27	A	413	SQD	C34-C35-C36-C37
29	A	414	LMT	C1-C2-C3-C4
28	d	411	LMG	C19-C20-C21-C22
38	C	518	DGD	CBB-CCB-CDB-CEB
38	c	519	DGD	C4B-C5B-C6B-C7B
29	E	105	LMT	C1-C2-C3-C4
29	A	414	LMT	O1'-C1-C2-C3
38	c	518	DGD	C3B-C4B-C5B-C6B
31	x	801	PL9	C25-C24-C26-C27
36	C	521	HTG	C2'-C3'-C4'-C5'
28	c	521	LMG	C11-C12-C13-C14
29	B	623	LMT	C6-C7-C8-C9
29	E	105	LMT	C6-C7-C8-C9
29	Z	101	LMT	C3-C4-C5-C6
38	D	408	DGD	C6B-C7B-C8B-C9B
38	c	519	DGD	CAA-CBA-CCA-CDA
39	e	101	LHG	C19-C20-C21-C22
27	L	102	SQD	O47-C45-C46-O48
39	d	410	LHG	C28-C29-C30-C31
38	h	703	DGD	C9A-CAA-CBA-CCA
29	a	2120	LMT	C1-C2-C3-C4
36	B	625[B]	HTG	C1'-C2'-C3'-C4'
39	e	101	LHG	C8-C7-O7-C5
28	c	521	LMG	C28-C29-C30-C31
39	D	409	LHG	C7-C8-C9-C10
38	c	519	DGD	C5B-C6B-C7B-C8B
24	a	2113	CLA	C16-C17-C18-C20
27	f	102	SQD	C24-C25-C26-C27
27	a	2115	SQD	C34-C35-C36-C37
29	B	637	LMT	C3-C4-C5-C6
29	B	623	LMT	C2-C1-O1'-C1'
29	I	1201	LMT	C2-C1-O1'-C1'
37	U	502	GOL	O1-C1-C2-O2
37	V	203	GOL	O1-C1-C2-O2
37	v	202	GOL	O2-C2-C3-O3
24	C	509	CLA	C11-C10-C8-C9
24	a	2113	CLA	C11-C12-C13-C14
24	b	604	CLA	C11-C10-C8-C9
24	c	509	CLA	C11-C10-C8-C9
38	H	102	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
39	e	101	LHG	C2-C3-O3-P
24	B	607	CLA	C4B-C3B-CAB-CBB
24	B	610	CLA	C4B-C3B-CAB-CBB
24	b	612	CLA	C4B-C3B-CAB-CBB
27	L	102	SQD	C12-C13-C14-C15
27	a	2115	SQD	C24-C25-C26-C27
28	B	622	LMG	C15-C16-C17-C18
38	C	518	DGD	C2E-C1E-O5D-C6D
39	D	410	LHG	C16-C17-C18-C19
39	e	101	LHG	C12-C13-C14-C15
39	D	409	LHG	C13-C14-C15-C16
24	A	409	CLA	C11-C10-C8-C7
24	B	605	CLA	C6-C7-C8-C10
24	B	607	CLA	C11-C12-C13-C15
24	B	611	CLA	C12-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C7
24	a	2110	CLA	C11-C10-C8-C7
24	a	2113	CLA	C11-C12-C13-C15
24	c	509	CLA	C11-C10-C8-C7
24	d	405	CLA	C6-C7-C8-C10
24	C	512	CLA	C8-C10-C11-C12
38	C	517	DGD	O6D-C5D-C6D-O5D
28	i	101	LMG	C40-C41-C42-C43
29	I	1201	LMT	C9-C10-C11-C12
24	B	610	CLA	C3A-C2A-CAA-CBA
24	c	512	CLA	C4-C3-C5-C6
24	c	512	CLA	C2-C3-C5-C6
38	C	519	DGD	C9A-CAA-CBA-CCA
39	D	411	LHG	C24-C23-O8-C6
28	C	520	LMG	C39-C40-C41-C42
28	c	522	LMG	C34-C35-C36-C37
29	B	637	LMT	C4-C5-C6-C7
28	C	520	LMG	C11-C12-C13-C14
27	L	102	SQD	O10-C23-O48-C46
27	A	411	SQD	C30-C31-C32-C33
36	B	624	HTG	C4-C5-C6-O6
24	b	604	CLA	C8-C10-C11-C12
27	a	2102	SQD	C13-C14-C15-C16
28	i	101	LMG	C30-C31-C32-C33
27	f	102	SQD	O6-C1-O5-C5
27	L	102	SQD	C30-C31-C32-C33
28	A	412	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	a	2115	SQD	C28-C29-C30-C31
39	d	408	LHG	C30-C31-C32-C33
39	d	408	LHG	C33-C34-C35-C36
38	c	518	DGD	C7A-C8A-C9A-CAA
24	C	511	CLA	C4-C3-C5-C6
25	A	407	PHO	C2-C3-C5-C6
24	c	515	CLA	C3-C5-C6-C7
39	d	410	LHG	C29-C30-C31-C32
36	d	403	HTG	C3'-C4'-C5'-C6'
24	C	503	CLA	C16-C17-C18-C20
24	a	2113	CLA	C16-C17-C18-C19
24	c	504	CLA	C16-C17-C18-C20
39	l	101	LHG	C33-C34-C35-C36
26	B	618	BCR	C1-C6-C7-C8
26	C	515	BCR	C1-C6-C7-C8
26	Y	302	BCR	C5-C6-C7-C8
26	b	620	BCR	C1-C6-C7-C8
26	c	517	BCR	C1-C6-C7-C8
26	c	528	BCR	C5-C6-C7-C8
27	A	411	SQD	C8-C7-O47-C45
27	f	102	SQD	C34-C35-C36-C37
38	c	518	DGD	C8B-C9B-CAB-CBB
36	D	413	HTG	C4'-C5'-C6'-C7'
24	c	511	CLA	C13-C15-C16-C17
27	L	102	SQD	C11-C10-C9-C8
24	b	614	CLA	C16-C17-C18-C20
27	A	411	SQD	O6-C44-C45-O47
27	F	101	SQD	O47-C45-C46-O48
27	a	2115	SQD	O6-C44-C45-O47
28	A	412	LMG	O1-C7-C8-O7
36	b	602	HTG	O5-C1-S1-C1'
36	d	403	HTG	O5-C5-C6-O6
25	A	407	PHO	C4-C3-C5-C6
29	a	2120	LMT	O1'-C1-C2-C3
27	a	2115	SQD	C12-C13-C14-C15
38	C	518	DGD	C8B-C9B-CAB-CBB
38	h	703	DGD	C5B-C6B-C7B-C8B
39	l	101	LHG	C27-C28-C29-C30
29	f	101	LMT	C6-C7-C8-C9
38	H	102	DGD	C5B-C6B-C7B-C8B
24	A	409	CLA	C8-C10-C11-C12
39	D	411	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
24	A	409	CLA	C14-C13-C15-C16
24	B	615	CLA	C14-C13-C15-C16
24	c	504	CLA	C14-C13-C15-C16
24	d	405	CLA	C6-C7-C8-C9
24	b	604	CLA	CAA-CBA-CGA-O2A
38	C	518	DGD	O6E-C1E-O5D-C6D
29	B	636	LMT	O5'-C5'-C6'-O6'
25	a	2112	PHO	C2C-C3C-CAC-CBC
29	i	104	LMT	C2'-C1'-O1'-C1
24	C	507	CLA	C15-C16-C17-C18
27	B	621	SQD	C7-C8-C9-C10
24	d	401	CLA	C2C-C3C-CAC-CBC
24	B	611	CLA	C8-C10-C11-C12
36	D	413	HTG	C1'-C2'-C3'-C4'
27	a	2102	SQD	C26-C27-C28-C29
24	c	508	CLA	C5-C6-C7-C8
37	V	203	GOL	O2-C2-C3-O3
37	a	2101	GOL	O2-C2-C3-O3
37	v	204	GOL	O2-C2-C3-O3
39	D	410	LHG	O1-C1-C2-O2
39	d	408	LHG	O1-C1-C2-O2
39	d	409	LHG	O1-C1-C2-O2
25	a	2111	PHO	C4-C3-C5-C6
38	h	703	DGD	O2G-C1B-C2B-C3B
28	B	622	LMG	C40-C41-C42-C43
24	C	506	CLA	C2-C3-C5-C6
25	a	2111	PHO	C2-C3-C5-C6
24	b	617	CLA	C16-C17-C18-C19
29	A	414	LMT	C2-C3-C4-C5
24	C	502	CLA	O1D-CGD-O2D-CED
38	C	519	DGD	C1B-C2B-C3B-C4B
28	B	622	LMG	C34-C35-C36-C37
24	B	606	CLA	C8-C10-C11-C12
39	D	409	LHG	C1-C2-C3-O3
28	D	412	LMG	C36-C37-C38-C39
28	b	623	LMG	C37-C38-C39-C40
24	A	406	CLA	C16-C17-C18-C20
24	b	613	CLA	C15-C16-C17-C18
28	D	412	LMG	C34-C35-C36-C37
38	c	520	DGD	CBB-CCB-CDB-CEB
24	B	602	CLA	C11-C10-C8-C7
24	C	505	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	C	510	CLA	C11-C10-C8-C7
24	D	405	CLA	C6-C7-C8-C10
24	c	515	CLA	C12-C13-C15-C16
27	F	101	SQD	C25-C26-C27-C28
27	L	102	SQD	C24-C25-C26-C27
28	i	101	LMG	C34-C35-C36-C37
39	D	409	LHG	C17-C18-C19-C20
24	B	617	CLA	C3-C5-C6-C7
24	A	405	CLA	C13-C15-C16-C17
24	B	603	CLA	C13-C15-C16-C17
24	b	619	CLA	CBA-CGA-O2A-C1
24	c	513	CLA	CBA-CGA-O2A-C1
29	a	2120	LMT	C2B-C1B-O1B-C4'
28	C	526	LMG	C8-C7-O1-C1
28	c	522	LMG	C8-C7-O1-C1
38	C	518	DGD	C5D-C6D-O5D-C1E
38	c	520	DGD	CDB-CEB-CFB-CGB
28	C	520	LMG	C37-C38-C39-C40
29	B	623	LMT	C7-C8-C9-C10
36	d	414	HTG	S1-C1'-C2'-C3'
38	C	518	DGD	CAB-CBB-CCB-CDB
27	a	2115	SQD	C30-C31-C32-C33
38	D	408	DGD	C2B-C3B-C4B-C5B
24	c	513	CLA	O1A-CGA-O2A-C1
36	O	302	HTG	C4-C5-C6-O6
27	f	102	SQD	C28-C29-C30-C31
29	A	420	LMT	C3-C4-C5-C6
24	B	614	CLA	C13-C15-C16-C17
27	A	411	SQD	O49-C7-O47-C45
29	A	414	LMT	C7-C8-C9-C10
28	A	412	LMG	O1-C7-C8-C9
36	B	625[A]	HTG	C1'-C2'-C3'-C4'
38	D	408	DGD	C3B-C4B-C5B-C6B
24	B	617	CLA	C4-C3-C5-C6
36	V	204	HTG	C2-C1-S1-C1'
24	C	508	CLA	C5-C6-C7-C8
36	O	302	HTG	O5-C5-C6-O6
38	D	408	DGD	O1G-C1G-C2G-O2G
24	C	507	CLA	C14-C13-C15-C16
24	c	515	CLA	C6-C7-C8-C9
24	B	611	CLA	C16-C17-C18-C20
39	e	101	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
39	l	101	LHG	C9-C10-C11-C12
24	C	512	CLA	O1A-CGA-O2A-C1
28	c	521	LMG	C39-C40-C41-C42
27	f	102	SQD	C5-C6-S-O8
24	B	605	CLA	O1D-CGD-O2D-CED
24	C	508	CLA	C2-C1-O2A-CGA
29	M	101	LMT	C2'-C1'-O1'-C1
29	I	1201	LMT	C6-C7-C8-C9
38	C	517	DGD	C4D-C5D-C6D-O5D
38	H	102	DGD	O2G-C1B-C2B-C3B
24	C	504	CLA	C15-C16-C17-C18
28	D	412	LMG	C32-C33-C34-C35
36	d	403	HTG	C4'-C5'-C6'-C7'
29	B	623	LMT	C1-C2-C3-C4
27	a	2102	SQD	C4-C5-C6-S
39	L	101	LHG	C9-C10-C11-C12
24	b	613	CLA	C16-C17-C18-C19
29	z	1801	LMT	C2-C1-O1'-C1'
39	d	410	LHG	C10-C11-C12-C13
24	C	509	CLA	C1A-C2A-CAA-CBA
24	c	508	CLA	C1A-C2A-CAA-CBA
24	c	515	CLA	C1A-C2A-CAA-CBA
24	a	2109	CLA	C4C-C3C-CAC-CBC
26	c	528	BCR	C21-C22-C23-C24
38	C	517	DGD	C4A-C5A-C6A-C7A
24	b	610	CLA	C3-C5-C6-C7
39	D	411	LHG	C30-C31-C32-C33
29	B	623	LMT	O5B-C1B-O1B-C4'
24	b	618	CLA	C13-C15-C16-C17
24	b	604	CLA	C12-C13-C15-C16
24	c	506	CLA	C11-C10-C8-C7
24	c	508	CLA	C11-C12-C13-C15
24	c	508	CLA	C12-C13-C15-C16
27	a	2115	SQD	C25-C26-C27-C28
24	b	604	CLA	C16-C17-C18-C20
24	b	613	CLA	C16-C17-C18-C20
24	c	510	CLA	C15-C16-C17-C18
36	V	204	HTG	C3'-C4'-C5'-C6'
39	D	409	LHG	O2-C2-C3-O3
39	L	101	LHG	C16-C17-C18-C19
27	L	102	SQD	C11-C12-C13-C14
38	C	518	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
24	b	619	CLA	O1A-CGA-O2A-C1
39	d	410	LHG	C2-C3-O3-P
24	C	507	CLA	C3A-C2A-CAA-CBA
31	d	407	PL9	C15-C14-C16-C17
24	A	409	CLA	C11-C10-C8-C9
24	D	405	CLA	C6-C7-C8-C9
24	b	616	CLA	C11-C12-C13-C14
24	c	508	CLA	C14-C13-C15-C16
24	c	511	CLA	C6-C7-C8-C9
24	c	515	CLA	C14-C13-C15-C16
39	l	101	LHG	C16-C17-C18-C19
29	a	2120	LMT	C4-C5-C6-C7
24	B	613	CLA	C8-C10-C11-C12
28	d	411	LMG	C29-C30-C31-C32
27	L	102	SQD	C44-C45-C46-O48
38	D	408	DGD	O1G-C1G-C2G-C3G
31	x	801	PL9	C23-C24-C26-C27
39	L	101	LHG	C27-C28-C29-C30
24	B	602	CLA	CAD-CBD-CGD-O2D
24	B	606	CLA	CAD-CBD-CGD-O2D
24	B	608	CLA	CAD-CBD-CGD-O2D
24	B	610	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	C	507	CLA	CAD-CBD-CGD-O2D
24	b	608	CLA	CAD-CBD-CGD-O2D
24	c	504	CLA	CAD-CBD-CGD-O2D
24	c	507	CLA	CAD-CBD-CGD-O2D
29	z	1801	LMT	C6-C7-C8-C9
29	a	2120	LMT	O5B-C1B-O1B-C4'
27	A	413	SQD	C24-C23-O48-C46
24	b	611	CLA	C13-C15-C16-C17
27	A	413	SQD	O10-C23-O48-C46
24	B	612	CLA	C15-C16-C17-C18
38	C	519	DGD	C8B-C9B-CAB-CBB
38	c	518	DGD	CAB-CBB-CCB-CDB
27	B	621	SQD	C28-C29-C30-C31
24	B	602	CLA	CAD-CBD-CGD-O1D
24	B	606	CLA	CAD-CBD-CGD-O1D
24	B	610	CLA	CAD-CBD-CGD-O1D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	507	CLA	CAD-CBD-CGD-O1D
24	b	608	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	b	612	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D
27	f	102	SQD	C5-C6-S-O9
39	D	410	LHG	C4-O6-P-O3
39	E	101	LHG	C4-O6-P-O5
39	e	101	LHG	C3-O3-P-O4
39	e	101	LHG	C3-O3-P-O5
39	e	101	LHG	C3-O3-P-O6
36	C	521	HTG	C1'-C2'-C3'-C4'
24	B	610	CLA	C2B-C3B-CAB-CBB
24	B	616	CLA	C2B-C3B-CAB-CBB
24	C	514	CLA	C2B-C3B-CAB-CBB
24	c	514	CLA	C2B-C3B-CAB-CBB
26	d	406	BCR	C23-C24-C25-C30
27	L	102	SQD	C33-C34-C35-C36
27	A	413	SQD	C32-C33-C34-C35
38	h	703	DGD	CCA-CDA-CEA-CFA
24	B	607	CLA	C13-C15-C16-C17
26	c	528	BCR	C37-C22-C23-C24
26	d	406	BCR	C7-C8-C9-C34
39	D	411	LHG	C2-C3-O3-P
38	H	102	DGD	CCA-CDA-CEA-CFA
27	a	2102	SQD	C24-C25-C26-C27
28	B	622	LMG	C10-C11-C12-C13
27	L	102	SQD	C46-C45-O47-C7
27	a	2102	SQD	C12-C13-C14-C15
29	E	105	LMT	C9-C10-C11-C12
38	c	518	DGD	C4D-C5D-C6D-O5D
24	B	602	CLA	C8-C10-C11-C12
27	a	2102	SQD	C14-C15-C16-C17
24	B	607	CLA	C16-C17-C18-C20
24	B	616	CLA	C16-C17-C18-C20
29	I	1201	LMT	C11-C10-C9-C8
24	a	2110	CLA	C11-C10-C8-C9
24	c	508	CLA	C11-C12-C13-C14
24	b	618	CLA	C5-C6-C7-C8
38	c	520	DGD	O1A-C1A-O1G-C1G
28	A	412	LMG	O6-C1-O1-C7
24	c	507	CLA	C16-C17-C18-C19
28	B	622	LMG	C13-C14-C15-C16
28	c	521	LMG	C36-C37-C38-C39
24	c	512	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	f	101	LMT	C9-C10-C11-C12
24	B	603	CLA	C15-C16-C17-C18
24	A	406	CLA	C16-C17-C18-C19
25	a	2111	PHO	C8-C10-C11-C12
24	b	617	CLA	C8-C10-C11-C12
38	H	102	DGD	C9B-CAB-CBB-CCB
38	c	519	DGD	C9B-CAB-CBB-CCB
38	c	520	DGD	C2A-C1A-O1G-C1G
38	C	519	DGD	C2A-C3A-C4A-C5A
27	B	621	SQD	C32-C33-C34-C35
24	c	506	CLA	C15-C16-C17-C18
28	A	412	LMG	C10-C11-C12-C13
24	b	609	CLA	C2A-CAA-CBA-CGA
24	B	616	CLA	C16-C17-C18-C19
24	C	503	CLA	C16-C17-C18-C19
27	F	101	SQD	C44-C45-C46-O48
31	x	801	PL9	C9-C11-C12-C13
27	F	101	SQD	C28-C29-C30-C31
39	D	409	LHG	C31-C32-C33-C34
24	C	510	CLA	C15-C16-C17-C18
29	Z	101	LMT	C1-C2-C3-C4
38	C	517	DGD	C5D-C6D-O5D-C1E
38	c	519	DGD	C2G-C3G-O3G-C1D
27	F	101	SQD	C34-C35-C36-C37
24	B	611	CLA	C2A-CAA-CBA-CGA
41	H	101	RRX	C9-C10-C11-C12
41	h	702	RRX	C9-C10-C11-C12
24	b	617	CLA	C16-C17-C18-C20
28	C	520	LMG	C33-C34-C35-C36
31	d	407	PL9	C13-C14-C16-C17
39	D	411	LHG	C25-C26-C27-C28
24	b	617	CLA	C10-C11-C12-C13
29	T	102	LMT	C2-C1-O1'-C1'
28	D	412	LMG	C10-C11-C12-C13
24	B	617	CLA	C14-C13-C15-C16
36	B	624	HTG	C3'-C4'-C5'-C6'
24	c	512	CLA	CBA-CGA-O2A-C1
39	d	409	LHG	C24-C23-O8-C6
29	B	636	LMT	O5B-C5B-C6B-O6B
24	c	504	CLA	C16-C17-C18-C19
24	c	507	CLA	C16-C17-C18-C20
27	a	2102	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
24	C	512	CLA	CBA-CGA-O2A-C1
24	B	617	CLA	C2-C3-C5-C6
38	c	518	DGD	O6D-C5D-C6D-O5D
39	l	101	LHG	O6-C4-C5-C6
28	B	622	LMG	C14-C15-C16-C17
36	V	204	HTG	C4-C5-C6-O6
24	b	607	CLA	C11-C12-C13-C15
24	c	510	CLA	C12-C13-C15-C16
28	b	623	LMG	C30-C31-C32-C33
38	D	408	DGD	CAB-CBB-CCB-CDB
24	B	613	CLA	C13-C15-C16-C17
29	B	636	LMT	C3-C4-C5-C6
29	i	104	LMT	C6-C7-C8-C9
27	B	621	SQD	O47-C45-C46-O48
27	B	621	SQD	C29-C30-C31-C32
27	a	2115	SQD	C33-C34-C35-C36
29	a	2120	LMT	C9-C10-C11-C12
29	i	104	LMT	C3-C4-C5-C6
27	a	2115	SQD	C13-C14-C15-C16
28	b	623	LMG	O9-C10-O7-C8
29	a	2120	LMT	C6-C7-C8-C9
27	L	102	SQD	C15-C16-C17-C18
26	T	101	BCR	C11-C12-C13-C35
26	b	622	BCR	C37-C22-C23-C24
26	t	102	BCR	C11-C12-C13-C35
29	a	2103	LMT	O1'-C1-C2-C3
36	i	103	HTG	O5-C5-C6-O6
26	D	406	BCR	C7-C8-C9-C10
24	B	605	CLA	C13-C15-C16-C17
38	h	703	DGD	C9B-CAB-CBB-CCB
36	B	624	HTG	O5-C5-C6-O6
24	c	506	CLA	C11-C10-C8-C9
38	C	517	DGD	C5A-C6A-C7A-C8A
37	O	303	GOL	O1-C1-C2-C3
37	o	2601	GOL	O1-C1-C2-C3
38	C	517	DGD	C3B-C4B-C5B-C6B
27	a	2115	SQD	C11-C12-C13-C14
36	B	625[A]	HTG	C4'-C5'-C6'-C7'
27	F	101	SQD	C46-C45-O47-C7
27	B	621	SQD	C26-C27-C28-C29
24	C	507	CLA	C4-C3-C5-C6
28	b	623	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
37	O	303	GOL	O1-C1-C2-O2
37	O	303	GOL	O2-C2-C3-O3
36	B	627	HTG	C1'-C2'-C3'-C4'
24	b	617	CLA	C2A-CAA-CBA-CGA
28	c	521	LMG	C37-C38-C39-C40
24	B	607	CLA	C2B-C3B-CAB-CBB
24	c	506	CLA	C2B-C3B-CAB-CBB
24	d	404	CLA	C2B-C3B-CAB-CBB
26	B	618	BCR	C5-C6-C7-C8
26	D	406	BCR	C23-C24-C25-C30
26	Y	302	BCR	C1-C6-C7-C8
26	b	620	BCR	C5-C6-C7-C8
26	c	517	BCR	C5-C6-C7-C8
26	c	528	BCR	C1-C6-C7-C8
26	d	406	BCR	C23-C24-C25-C26
24	b	604	CLA	C4-C3-C5-C6
31	D	407	PL9	C15-C14-C16-C17
31	x	801	PL9	C15-C14-C16-C17
31	x	801	PL9	C40-C39-C41-C42
28	C	520	LMG	C40-C41-C42-C43
29	B	623	LMT	C9-C10-C11-C12
38	c	518	DGD	C6A-C7A-C8A-C9A
39	L	101	LHG	O6-C4-C5-C6
24	b	604	CLA	C2-C3-C5-C6
24	B	616	CLA	C11-C10-C8-C7
24	B	616	CLA	C12-C13-C15-C16
24	C	508	CLA	C12-C13-C15-C16
24	c	511	CLA	C12-C13-C15-C16
24	B	615	CLA	C2A-CAA-CBA-CGA
38	H	102	DGD	O1G-C1G-C2G-O2G
24	c	505	CLA	C10-C11-C12-C13
29	j	1601	LMT	C3-C4-C5-C6
39	l	101	LHG	C10-C11-C12-C13
40	F	102	HEM	CAD-CBD-CGD-O1D
40	e	103	HEM	CAD-CBD-CGD-O1D
28	C	520	LMG	C16-C17-C18-C19
28	d	411	LMG	C30-C31-C32-C33
24	B	607	CLA	C16-C17-C18-C19
31	A	417	PL9	C40-C39-C41-C42
29	a	2103	LMT	C1-C2-C3-C4
31	A	417	PL9	C13-C14-C16-C17
31	D	407	PL9	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
24	C	509	CLA	C13-C15-C16-C17
39	d	409	LHG	O10-C23-O8-C6
24	B	617	CLA	C11-C10-C8-C9
27	L	102	SQD	C9-C10-C11-C12
28	i	101	LMG	C33-C34-C35-C36
24	C	502	CLA	C13-C15-C16-C17
24	C	504	CLA	C10-C11-C12-C13
40	F	102	HEM	CAD-CBD-CGD-O2D
36	O	302	HTG	C4'-C5'-C6'-C7'
24	B	616	CLA	C4-C3-C5-C6
24	B	617	CLA	C10-C11-C12-C13
29	j	1601	LMT	O1'-C1-C2-C3
31	x	801	PL9	C38-C39-C41-C42
38	c	519	DGD	C1B-C2B-C3B-C4B
36	C	521	HTG	C4'-C5'-C6'-C7'
39	L	101	LHG	C10-C11-C12-C13
28	C	526	LMG	O1-C7-C8-C9
40	e	103	HEM	CAD-CBD-CGD-O2D
24	b	614	CLA	C8-C10-C11-C12
28	d	411	LMG	C10-C11-C12-C13
39	L	101	LHG	O6-C4-C5-O7
39	l	101	LHG	O6-C4-C5-O7
40	e	103	HEM	CAA-CBA-CGA-O1A
28	C	520	LMG	C17-C18-C19-C20
39	D	411	LHG	C28-C29-C30-C31
39	D	409	LHG	C30-C31-C32-C33
24	D	404	CLA	C4B-C3B-CAB-CBB
24	c	506	CLA	C4B-C3B-CAB-CBB
24	d	404	CLA	C4B-C3B-CAB-CBB
38	C	518	DGD	C6A-C7A-C8A-C9A
24	B	602	CLA	CAA-CBA-CGA-O2A
29	Z	101	LMT	C5-C6-C7-C8
39	L	101	LHG	C17-C18-C19-C20
38	C	517	DGD	CAA-CBA-CCA-CDA
38	D	408	DGD	C7B-C8B-C9B-CAB
24	A	405	CLA	C16-C17-C18-C19
25	a	2111	PHO	CHA-CBD-CGD-O1D
24	c	511	CLA	C3-C5-C6-C7
40	e	103	HEM	CAA-CBA-CGA-O2A
24	C	506	CLA	C4-C3-C5-C6
29	a	2103	LMT	O5B-C5B-C6B-O6B
29	a	2103	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
36	c	526	HTG	C1'-C2'-C3'-C4'
24	C	510	CLA	C13-C15-C16-C17
24	A	406	CLA	C11-C10-C8-C7
24	a	2110	CLA	C12-C13-C15-C16
43	V	201	HEC	CAD-CBD-CGD-O2D
43	v	201	HEC	CAD-CBD-CGD-O2D
24	D	401	CLA	C4C-C3C-CAC-CBC
24	B	612	CLA	C11-C10-C8-C9
24	C	507	CLA	C11-C12-C13-C14
24	D	405	CLA	C11-C10-C8-C9
24	a	2110	CLA	C6-C7-C8-C9
24	c	511	CLA	C14-C13-C15-C16
27	F	101	SQD	C45-C44-O6-C1
27	L	102	SQD	C5-C6-S-O8
38	c	518	DGD	C5D-C6D-O5D-C1E
28	A	412	LMG	C30-C31-C32-C33
43	V	201	HEC	CAD-CBD-CGD-O1D
24	b	613	CLA	C2A-CAA-CBA-CGA
24	c	503	CLA	C2A-CAA-CBA-CGA
24	b	617	CLA	C2-C1-O2A-CGA
36	B	625[B]	HTG	C4'-C5'-C6'-C7'
24	C	509	CLA	C5-C6-C7-C8
31	A	417	PL9	C15-C14-C16-C17
28	i	101	LMG	O8-C28-C29-C30
43	v	201	HEC	CAD-CBD-CGD-O1D
39	l	101	LHG	C17-C18-C19-C20
28	A	412	LMG	C2-C1-O1-C7
27	F	101	SQD	C44-C45-O47-C7
24	c	509	CLA	C2A-CAA-CBA-CGA
24	B	616	CLA	C5-C6-C7-C8
29	B	623	LMT	C2B-C1B-O1B-C4'
24	b	615	CLA	C8-C10-C11-C12
28	A	412	LMG	C29-C30-C31-C32
29	B	636	LMT	C6-C7-C8-C9
27	B	621	SQD	C44-C45-C46-O48
31	x	801	PL9	C34-C36-C37-C38
36	c	526	HTG	C2'-C3'-C4'-C5'
39	D	409	LHG	C33-C34-C35-C36
37	c	527	GOL	O2-C2-C3-O3
37	v	203	GOL	O2-C2-C3-O3
38	D	408	DGD	C7A-C8A-C9A-CAA
29	M	101	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
29	i	104	LMT	C5-C6-C7-C8
29	E	105	LMT	O1'-C1-C2-C3
39	d	408	LHG	C34-C35-C36-C37
38	C	518	DGD	C5A-C6A-C7A-C8A
24	d	401	CLA	C4C-C3C-CAC-CBC
28	B	622	LMG	C30-C31-C32-C33
39	D	411	LHG	C16-C17-C18-C19
27	A	413	SQD	C28-C29-C30-C31
28	C	520	LMG	C30-C31-C32-C33
39	l	101	LHG	C25-C26-C27-C28
38	h	703	DGD	O1G-C1G-C2G-O2G
38	D	408	DGD	C2A-C3A-C4A-C5A
24	A	409	CLA	C6-C7-C8-C9
39	D	409	LHG	C11-C12-C13-C14
39	D	409	LHG	C15-C16-C17-C18
39	l	101	LHG	C30-C31-C32-C33
39	D	410	LHG	C14-C15-C16-C17
24	A	409	CLA	C6-C7-C8-C10
24	B	612	CLA	C11-C10-C8-C7
24	a	2110	CLA	C6-C7-C8-C10
24	b	609	CLA	C11-C10-C8-C7
24	c	512	CLA	C11-C12-C13-C15
24	D	404	CLA	C2B-C3B-CAB-CBB
24	b	612	CLA	C2B-C3B-CAB-CBB
26	D	406	BCR	C23-C24-C25-C26
26	a	2114	BCR	C1-C6-C7-C8
26	c	516	BCR	C1-C6-C7-C8
28	b	623	LMG	C11-C10-O7-C8
38	c	520	DGD	C3B-C4B-C5B-C6B
24	B	611	CLA	C2-C1-O2A-CGA
39	d	409	LHG	C11-C10-C9-C8
27	a	2102	SQD	C31-C32-C33-C34
31	A	417	PL9	C34-C36-C37-C38
38	c	518	DGD	O6E-C1E-O5D-C6D
27	f	102	SQD	C11-C10-C9-C8
38	c	519	DGD	C8A-C9A-CAA-CBA
39	e	101	LHG	C10-C11-C12-C13
24	C	511	CLA	CAA-CBA-CGA-O2A
27	A	411	SQD	O47-C7-C8-C9
28	B	622	LMG	O8-C28-C29-C30
36	O	302	HTG	C2'-C1'-S1-C1
36	b	626	HTG	C2'-C1'-S1-C1

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Mol	Chain	Res	Type	Atoms
39	E	101	LHG	C10-C11-C12-C13
38	c	518	DGD	C5A-C6A-C7A-C8A
24	A	405	CLA	C2C-C3C-CAC-CBC
38	C	518	DGD	O2G-C1B-C2B-C3B
39	d	408	LHG	C13-C14-C15-C16
24	C	507	CLA	C2-C3-C5-C6
29	T	102	LMT	C3-C4-C5-C6
24	b	604	CLA	CAA-CBA-CGA-O1A
29	B	637	LMT	C2-C3-C4-C5
29	a	2120	LMT	C3-C4-C5-C6
24	C	508	CLA	C14-C13-C15-C16
24	C	513	CLA	CAA-CBA-CGA-O2A
38	c	519	DGD	O2G-C1B-C2B-C3B
39	D	409	LHG	O8-C23-C24-C25
24	B	602	CLA	C4B-C3B-CAB-CBB
24	C	502	CLA	C4B-C3B-CAB-CBB
24	C	506	CLA	C4B-C3B-CAB-CBB
29	M	101	LMT	C6-C7-C8-C9
39	E	101	LHG	C34-C35-C36-C37
38	c	519	DGD	O6E-C1E-O5D-C6D
28	c	522	LMG	O7-C8-C9-O8
26	b	622	BCR	C21-C22-C23-C24
26	d	406	BCR	C7-C8-C9-C10
24	b	615	CLA	O1A-CGA-O2A-C1
38	c	518	DGD	O2G-C1B-C2B-C3B
39	E	101	LHG	O8-C23-C24-C25
29	m	102	LMT	C5-C6-C7-C8
38	C	519	DGD	C8A-C9A-CAA-CBA
28	C	520	LMG	C34-C35-C36-C37
24	C	504	CLA	O1D-CGD-O2D-CED
38	h	703	DGD	O1B-C1B-C2B-C3B
27	L	102	SQD	C5-C6-S-O9
37	o	2603	GOL	O1-C1-C2-C3
24	c	512	CLA	CAA-CBA-CGA-O2A
24	A	406	CLA	C12-C13-C15-C16
24	C	505	CLA	C6-C7-C8-C10
24	D	405	CLA	C11-C10-C8-C7
24	c	506	CLA	C12-C13-C15-C16
28	b	623	LMG	C15-C16-C17-C18
29	a	2103	LMT	C11-C10-C9-C8
24	c	514	CLA	O2A-C1-C2-C3
28	i	101	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
24	c	509	CLA	C5-C6-C7-C8
38	D	408	DGD	C4A-C5A-C6A-C7A
24	b	605	CLA	C2A-CAA-CBA-CGA
29	T	102	LMT	C6-C7-C8-C9
40	F	102	HEM	CAA-CBA-CGA-O2A
24	a	2113	CLA	C4-C3-C5-C6
24	D	401	CLA	C15-C16-C17-C18
38	c	519	DGD	CBA-CCA-CDA-CEA
39	d	410	LHG	C11-C12-C13-C14
28	c	521	LMG	C17-C18-C19-C20
38	c	519	DGD	C2A-C3A-C4A-C5A
28	i	101	LMG	C22-C23-C24-C25
27	A	411	SQD	O49-C7-C8-C9
28	C	526	LMG	C4-C5-C6-O5
24	A	405	CLA	C4C-C3C-CAC-CBC
24	B	616	CLA	C14-C13-C15-C16
38	H	102	DGD	O1B-C1B-C2B-C3B
36	B	625[A]	HTG	C2'-C3'-C4'-C5'
24	A	405	CLA	C15-C16-C17-C18
28	D	412	LMG	C18-C19-C20-C21
27	B	621	SQD	C31-C32-C33-C34
24	C	513	CLA	CAA-CBA-CGA-O1A
27	A	413	SQD	O5-C5-C6-S
24	c	512	CLA	CAA-CBA-CGA-O1A
38	c	520	DGD	C9A-CAA-CBA-CCA
27	a	2115	SQD	C31-C32-C33-C34
26	T	101	BCR	C11-C12-C13-C14
26	t	102	BCR	C11-C12-C13-C14
27	a	2102	SQD	C45-C44-O6-C1
24	B	613	CLA	CAA-CBA-CGA-O2A
25	a	2112	PHO	C8-C10-C11-C12
38	c	519	DGD	C8B-C9B-CAB-CBB
36	b	601	HTG	C2'-C3'-C4'-C5'
29	T	102	LMT	C2-C3-C4-C5
38	H	102	DGD	O1G-C1G-C2G-C3G
24	C	511	CLA	CAA-CBA-CGA-O1A
39	E	101	LHG	O10-C23-C24-C25
24	B	611	CLA	C10-C11-C12-C13
24	B	616	CLA	C13-C15-C16-C17
24	C	513	CLA	C15-C16-C17-C18
24	b	616	CLA	CAA-CBA-CGA-O2A
38	c	520	DGD	O1G-C1A-C2A-C3A

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Mol	Chain	Res	Type	Atoms
38	C	518	DGD	O1B-C1B-C2B-C3B
29	b	624	LMT	C5'-C4'-O1B-C1B
38	c	519	DGD	O6D-C5D-C6D-O5D
24	b	612	CLA	CAD-CBD-CGD-O2D
24	b	619	CLA	CAD-CBD-CGD-O2D
24	c	506	CLA	CAD-CBD-CGD-O2D
24	b	618	CLA	C8-C10-C11-C12
24	C	508	CLA	C15-C16-C17-C18
24	b	615	CLA	CBA-CGA-O2A-C1
24	b	605	CLA	C16-C17-C18-C19
38	H	102	DGD	C3B-C4B-C5B-C6B
38	c	519	DGD	CDA-CEA-CFA-CGA
29	i	104	LMT	C9-C10-C11-C12
38	h	703	DGD	C3B-C4B-C5B-C6B
38	C	517	DGD	O2G-C1B-C2B-C3B
38	c	518	DGD	O1B-C1B-C2B-C3B
38	c	520	DGD	O1A-C1A-C2A-C3A

There are no ring outliers.

170 monomers are involved in 279 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	B	635	GOL	2	0
24	b	616	CLA	2	0
34	d	417	DMS	2	0
24	c	503	CLA	3	0
26	Y	302	BCR	3	0
24	C	503	CLA	2	0
24	B	613	CLA	1	0
39	D	409	LHG	3	0
24	B	615	CLA	2	0
24	B	605	CLA	3	0
36	B	625[A]	HTG	3	0
39	l	101	LHG	1	0
26	C	516	BCR	3	0
29	A	414	LMT	2	0
26	B	618	BCR	2	0
24	B	606	CLA	4	0
38	C	517	DGD	2	0
26	a	2114	BCR	1	0
40	e	103	HEM	2	0
26	A	410	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	516	BCR	3	0
27	B	621	SQD	3	0
36	b	601	HTG	1	0
41	h	702	RRX	3	0
27	a	2102	SQD	1	0
24	b	610	CLA	1	0
38	C	519	DGD	1	0
26	C	515	BCR	4	0
36	D	413	HTG	3	0
24	D	404	CLA	2	0
37	D	403	GOL	1	0
24	A	405	CLA	2	0
29	i	104	LMT	1	0
26	d	406	BCR	1	0
24	c	508	CLA	2	0
34	b	643	DMS	1	0
26	c	517	BCR	2	0
29	B	636	LMT	1	0
24	d	404	CLA	2	0
37	c	527	GOL	2	0
26	b	622	BCR	2	0
24	b	612	CLA	1	0
27	f	102	SQD	1	0
34	c	532	DMS	1	0
34	B	647	DMS	1	0
24	C	507	CLA	1	0
24	B	602	CLA	1	0
28	b	623	LMG	1	0
24	c	510	CLA	3	0
38	c	519	DGD	3	0
24	C	511	CLA	1	0
24	b	613	CLA	1	0
34	O	309	DMS	1	0
26	B	620	BCR	2	0
24	b	614	CLA	1	0
24	c	512	CLA	1	0
27	F	101	SQD	2	0
31	d	407	PL9	1	0
26	k	2003	BCR	1	0
24	C	513	CLA	4	0
24	C	510	CLA	4	0
27	A	411	SQD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	504	CLA	5	0
31	A	417	PL9	2	0
34	o	2606	DMS	1	0
28	C	526	LMG	1	0
25	A	408	PHO	2	0
36	B	628	HTG	1	0
27	L	102	SQD	1	0
32	A	419	K2I	1	0
34	C	529	DMS	1	0
24	c	506	CLA	5	0
24	C	505	CLA	1	0
36	b	602	HTG	3	0
24	c	509	CLA	2	0
34	b	633	DMS	1	0
24	C	508	CLA	2	0
24	b	619	CLA	4	0
24	b	604	CLA	4	0
24	B	610	CLA	4	0
29	B	623	LMT	1	0
34	B	643	DMS	1	0
26	B	619	BCR	2	0
29	J	102	LMT	1	0
34	O	310	DMS	1	0
24	B	614	CLA	1	0
37	o	2603	GOL	1	0
36	I	1202	HTG	1	0
24	B	603	CLA	2	0
29	A	420	LMT	1	0
29	z	1801	LMT	2	0
24	b	618	CLA	4	0
32	a	2118[B]	K2I	2	0
32	A	418[B]	K2I	2	0
39	D	411	LHG	2	0
40	F	102	HEM	1	0
29	a	2103	LMT	2	0
24	C	512	CLA	2	0
24	B	612	CLA	1	0
29	a	2120	LMT	2	0
24	c	504	CLA	3	0
39	E	101	LHG	5	0
24	b	609	CLA	2	0
36	B	625[B]	HTG	3	0

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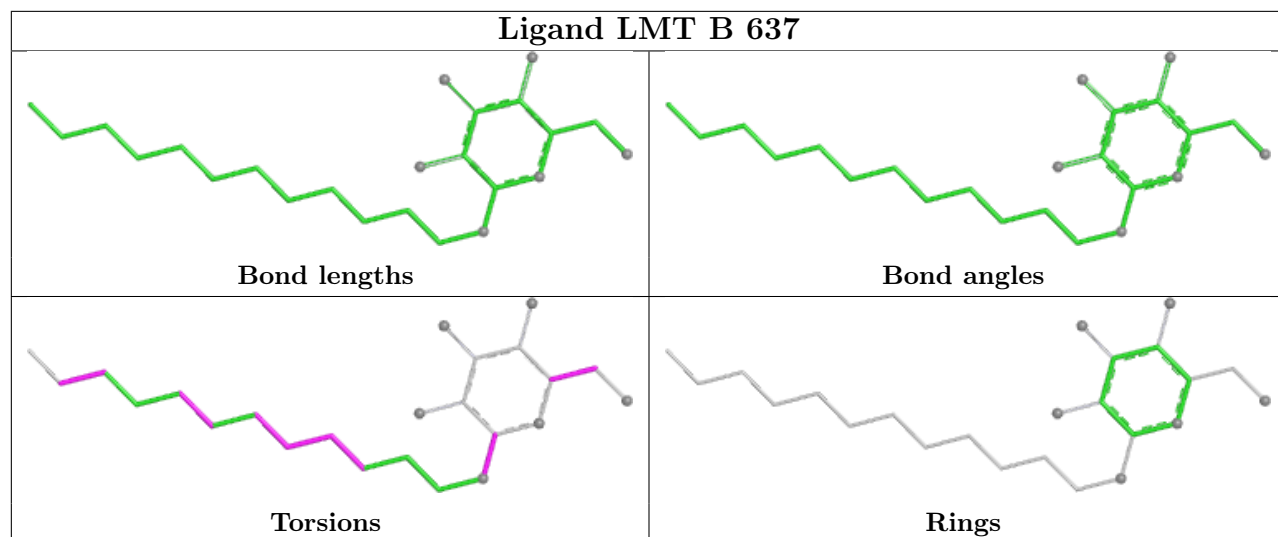
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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38	h	703	DGD	1	0
34	c	531	DMS	1	0
24	B	604	CLA	1	0
24	a	2110	CLA	2	0
36	b	625	HTG	3	0
24	A	409	CLA	1	0
24	d	405	CLA	1	0
24	b	607	CLA	3	0
24	c	511	CLA	2	0
34	C	534	DMS	1	0
24	b	605	CLA	1	0
34	V	206	DMS	1	0
24	C	506	CLA	1	0
24	c	507	CLA	2	0
39	L	101	LHG	2	0
37	o	2601	GOL	1	0
29	m	102	LMT	2	0
24	C	509	CLA	2	0
36	d	403	HTG	2	0
38	c	518	DGD	1	0
24	a	2109	CLA	2	0
39	d	409	LHG	1	0
26	t	102	BCR	6	0
24	a	2113	CLA	2	0
24	B	616	CLA	2	0
28	i	101	LMG	2	0
38	c	520	DGD	3	0
34	v	205	DMS	1	0
28	c	521	LMG	1	0
24	D	401	CLA	2	0
41	H	101	RRX	3	0
24	c	505	CLA	4	0
38	C	518	DGD	6	0
29	M	101	LMT	2	0
24	B	617	CLA	3	0
24	D	405	CLA	1	0
24	c	513	CLA	4	0
24	B	607	CLA	1	0
24	A	406	CLA	1	0
39	e	101	LHG	1	0
28	A	412	LMG	1	0

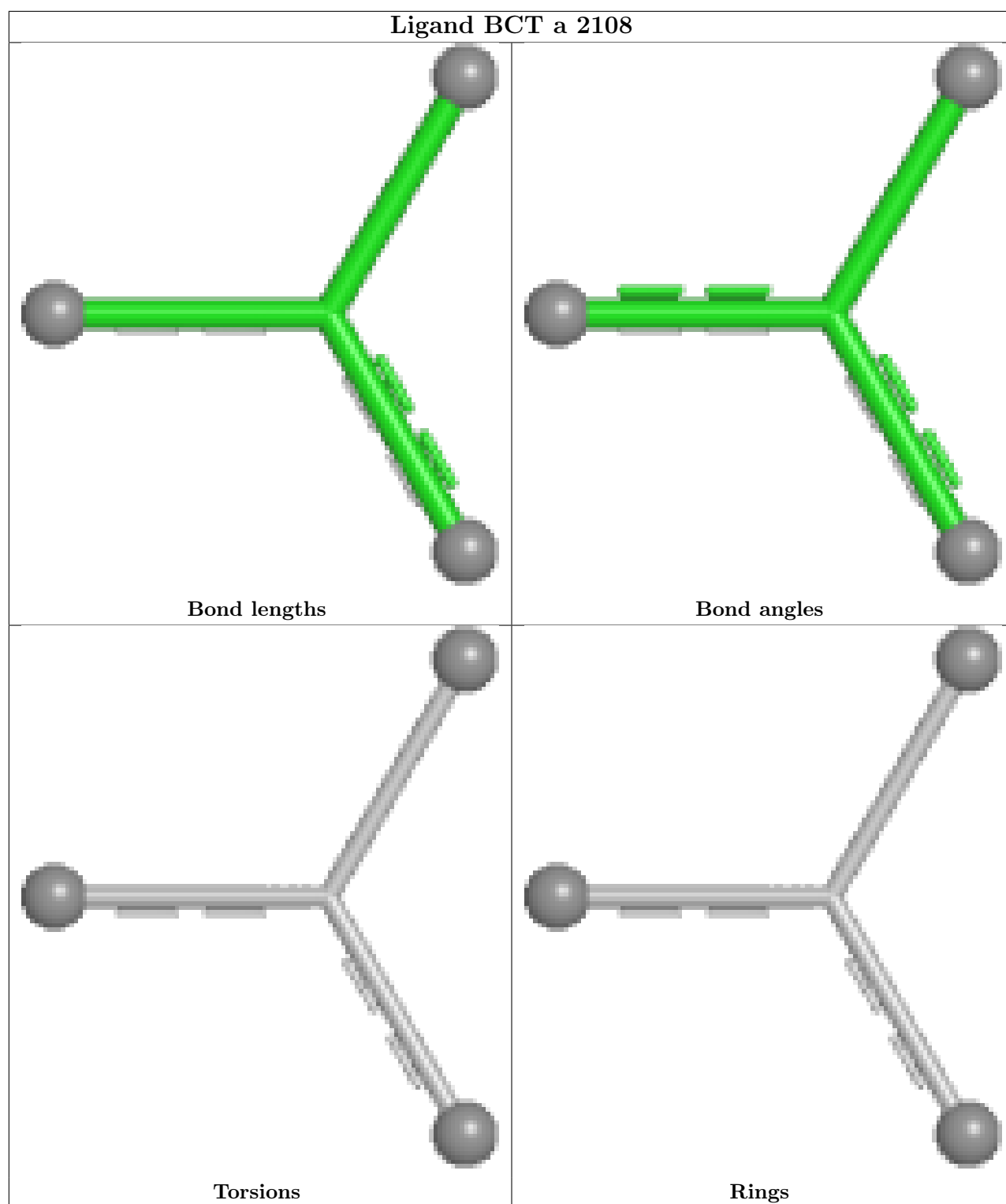
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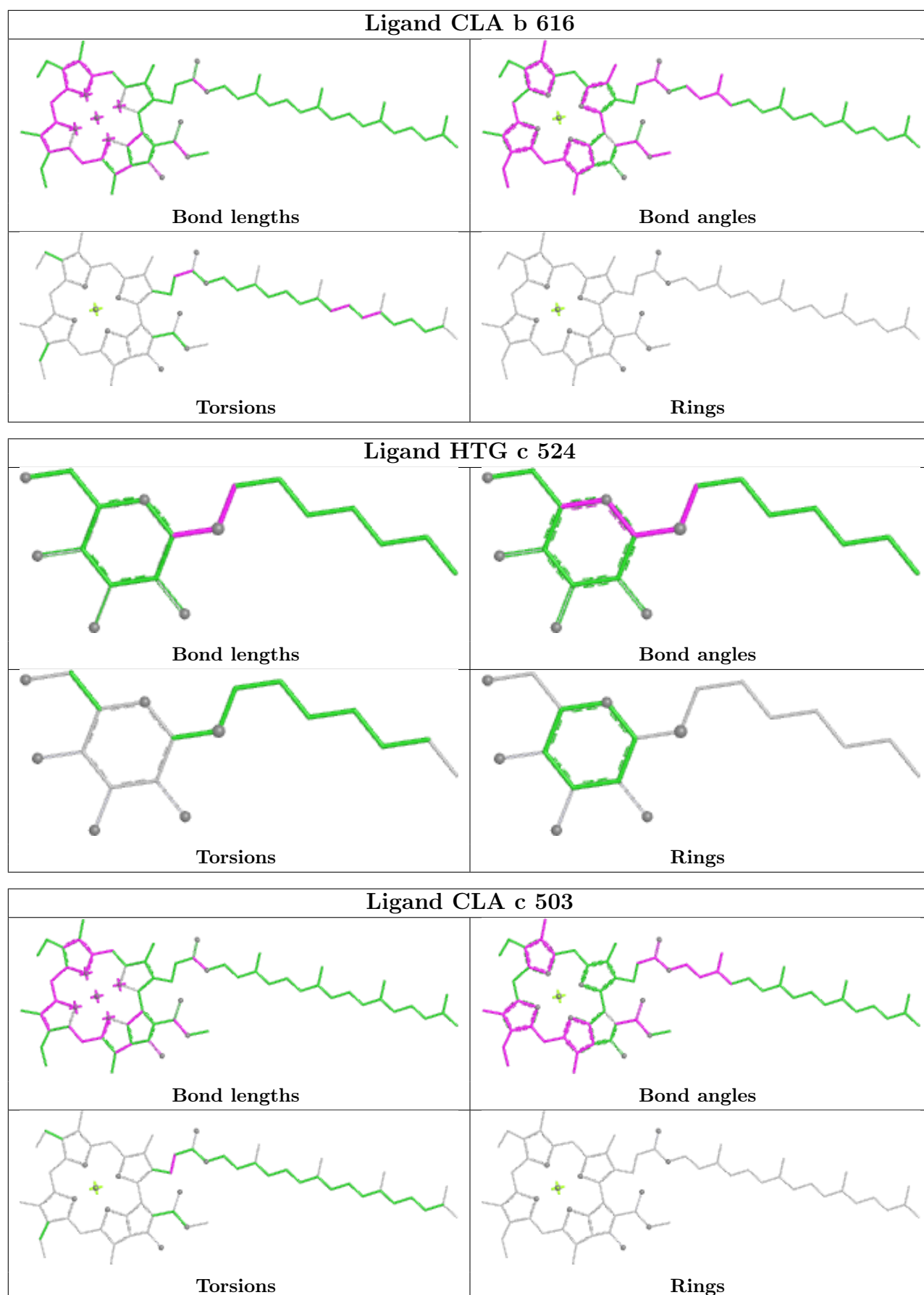
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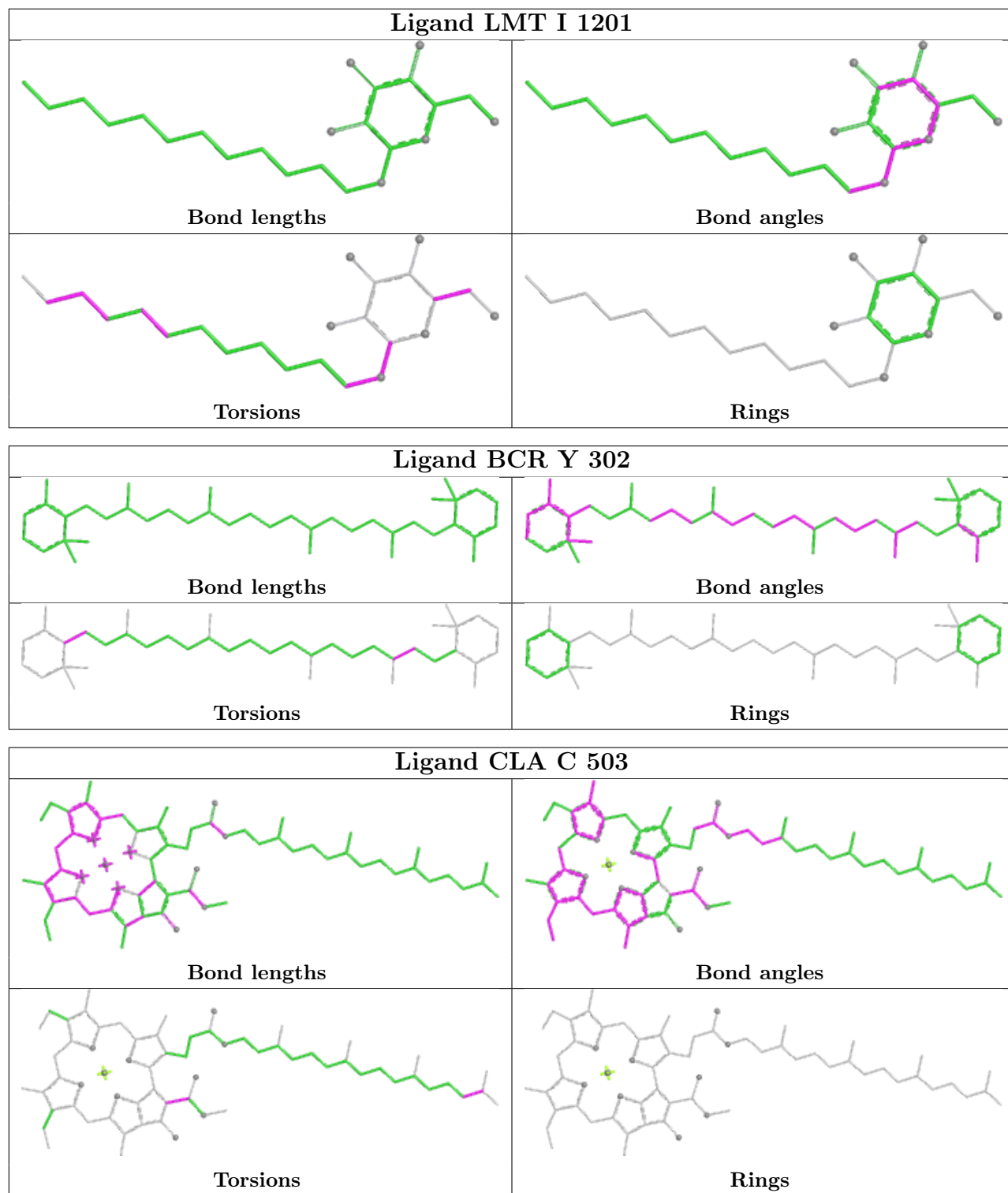
Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	d	408	LHG	2	0
26	b	621	BCR	3	0
34	C	528	DMS	2	0
34	d	423	DMS	1	0
27	a	2115	SQD	1	0
34	U	503	DMS	2	0
24	d	401	CLA	4	0
24	b	608	CLA	6	0
24	B	611	CLA	2	0
36	O	302	HTG	1	0
24	c	515	CLA	1	0
24	C	514	CLA	6	0
36	B	624	HTG	1	0
28	C	520	LMG	1	0
36	b	626	HTG	1	0
26	b	620	BCR	1	0
32	a	2119	K2I	1	0
26	K	101	BCR	1	0
24	C	502	CLA	4	0
25	a	2112	PHO	1	0
28	B	622	LMG	2	0
26	c	528	BCR	1	0
24	c	514	CLA	4	0
26	T	101	BCR	5	0

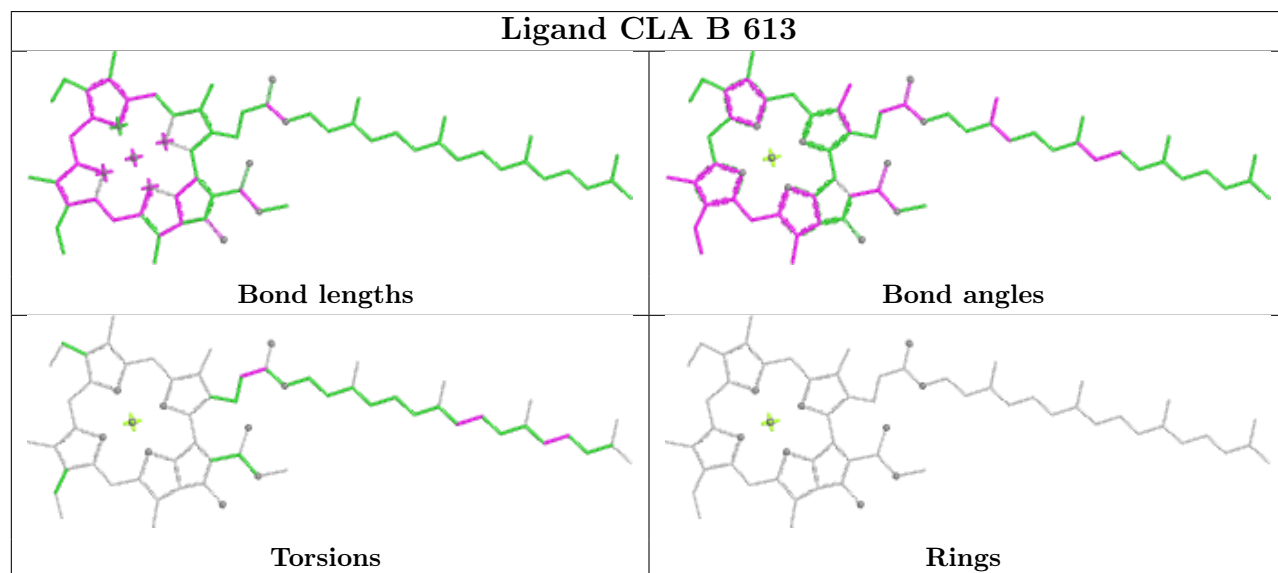
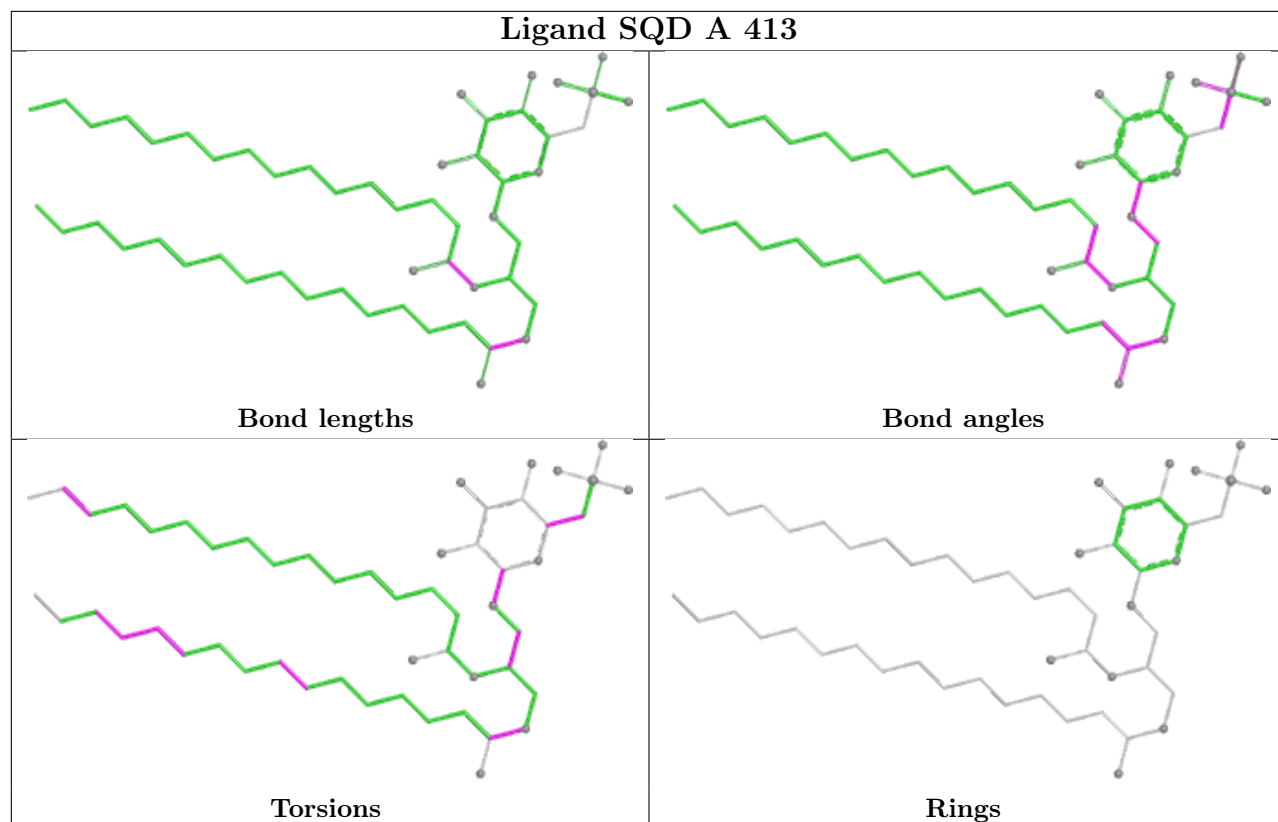
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

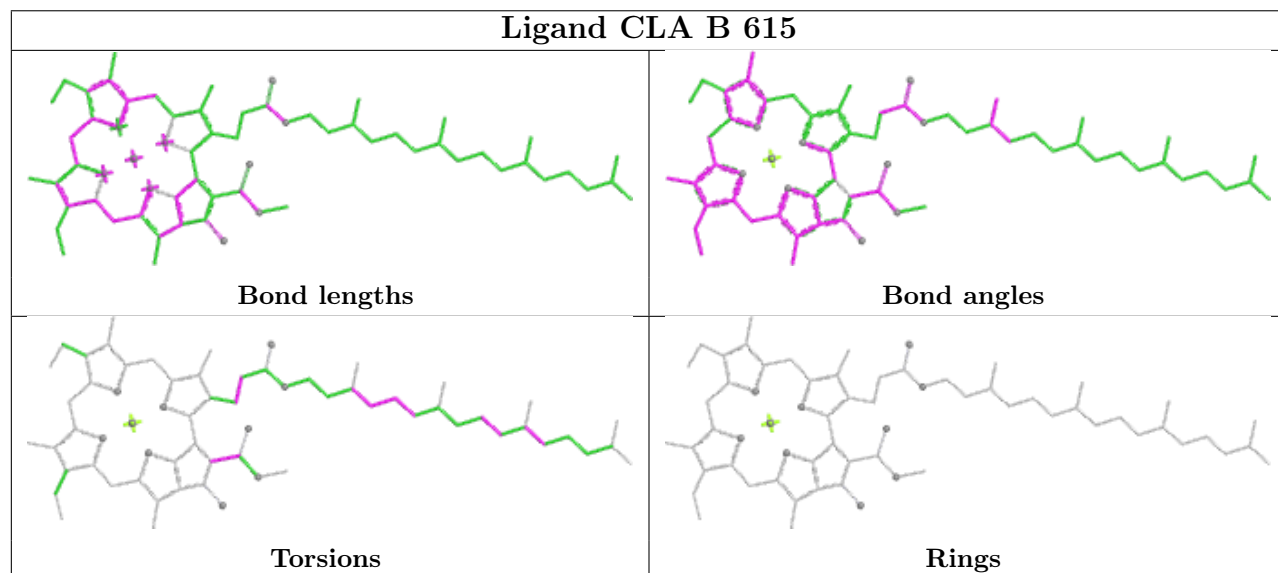
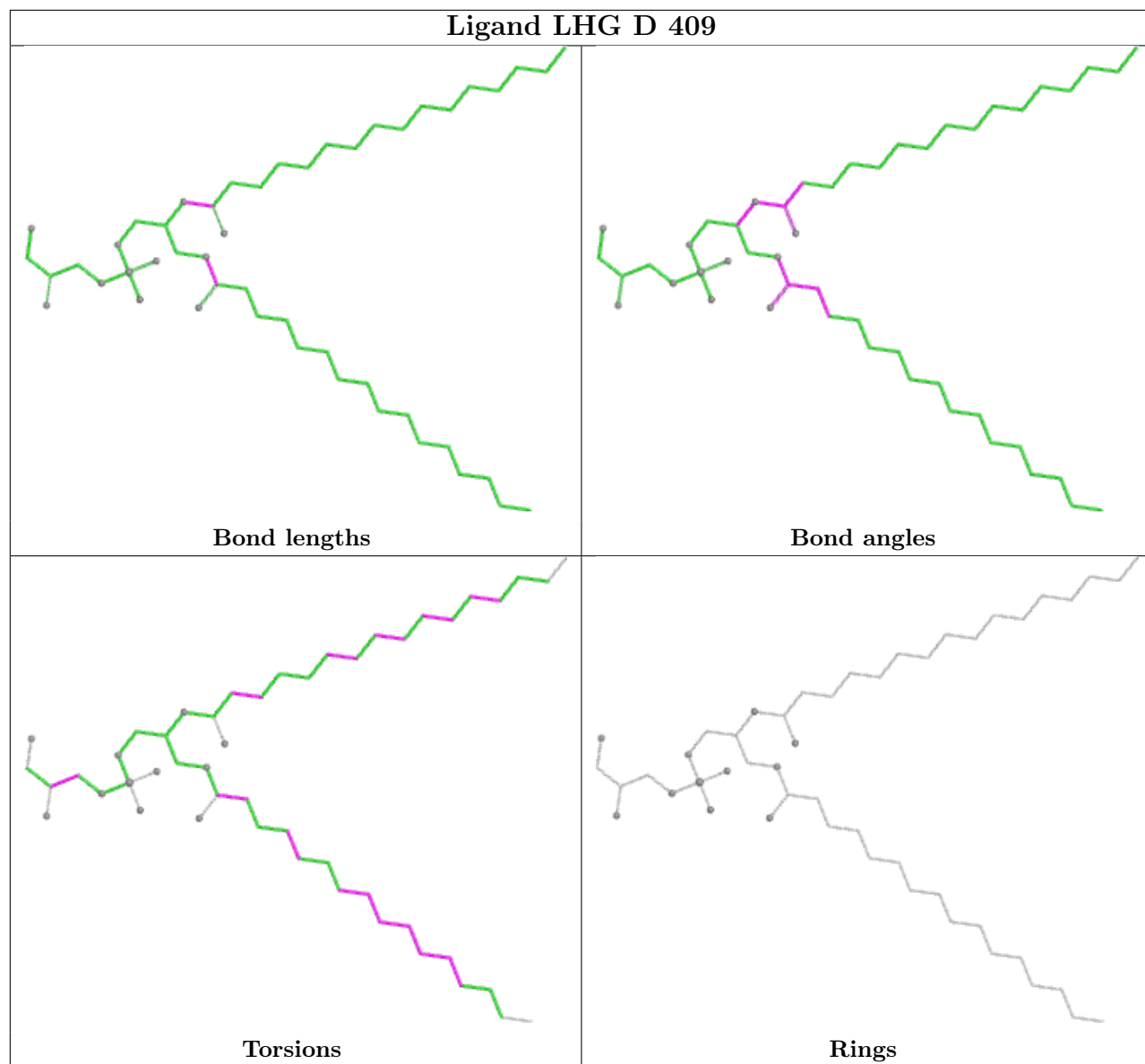


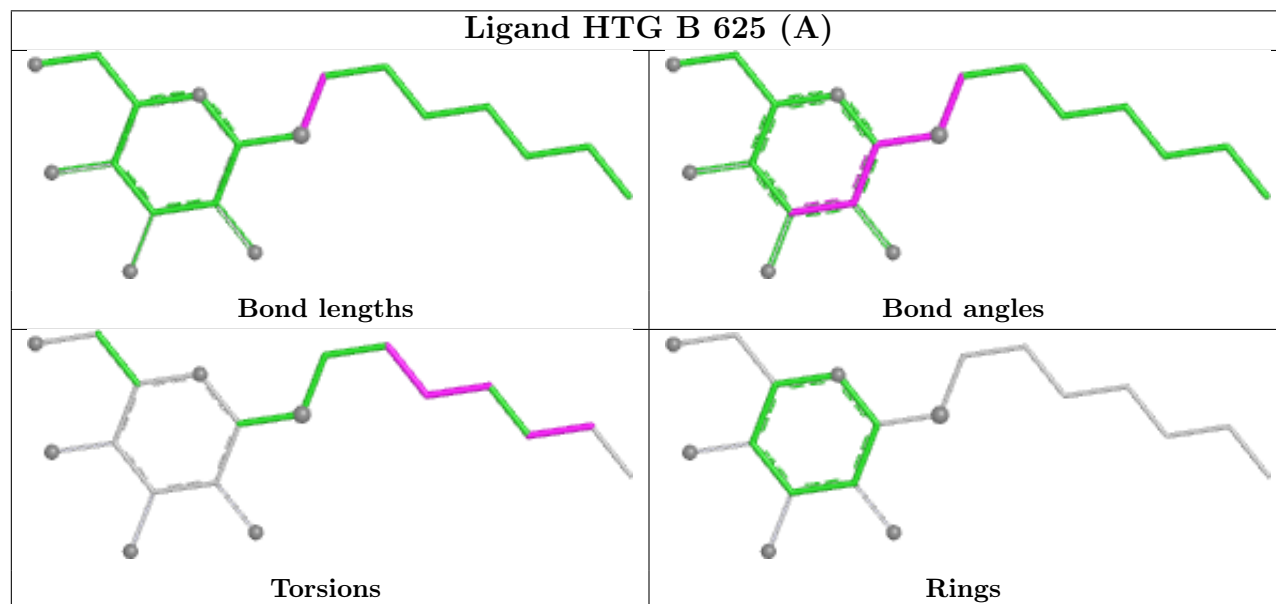
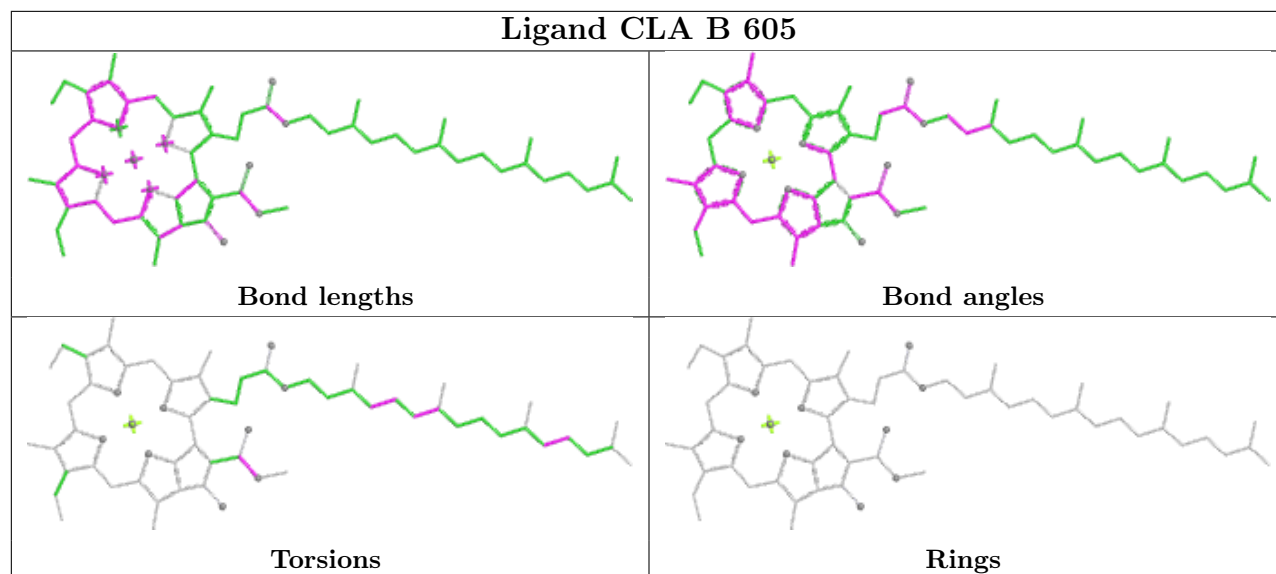


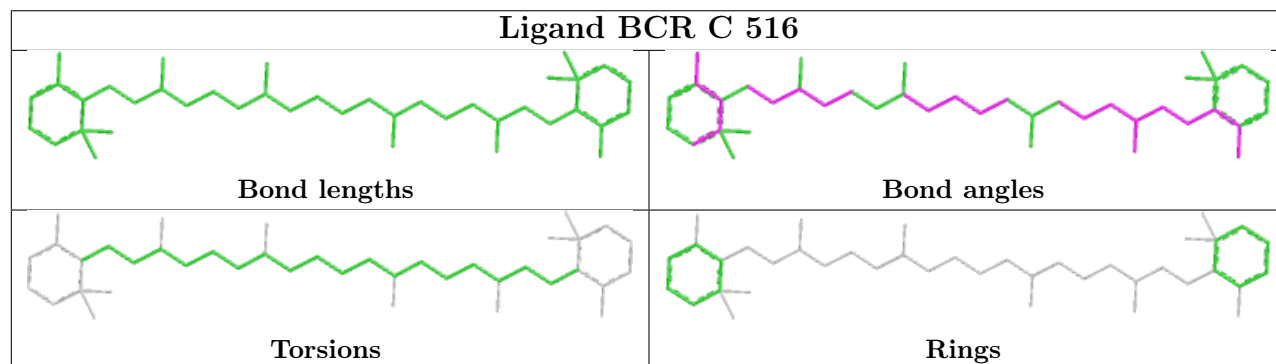
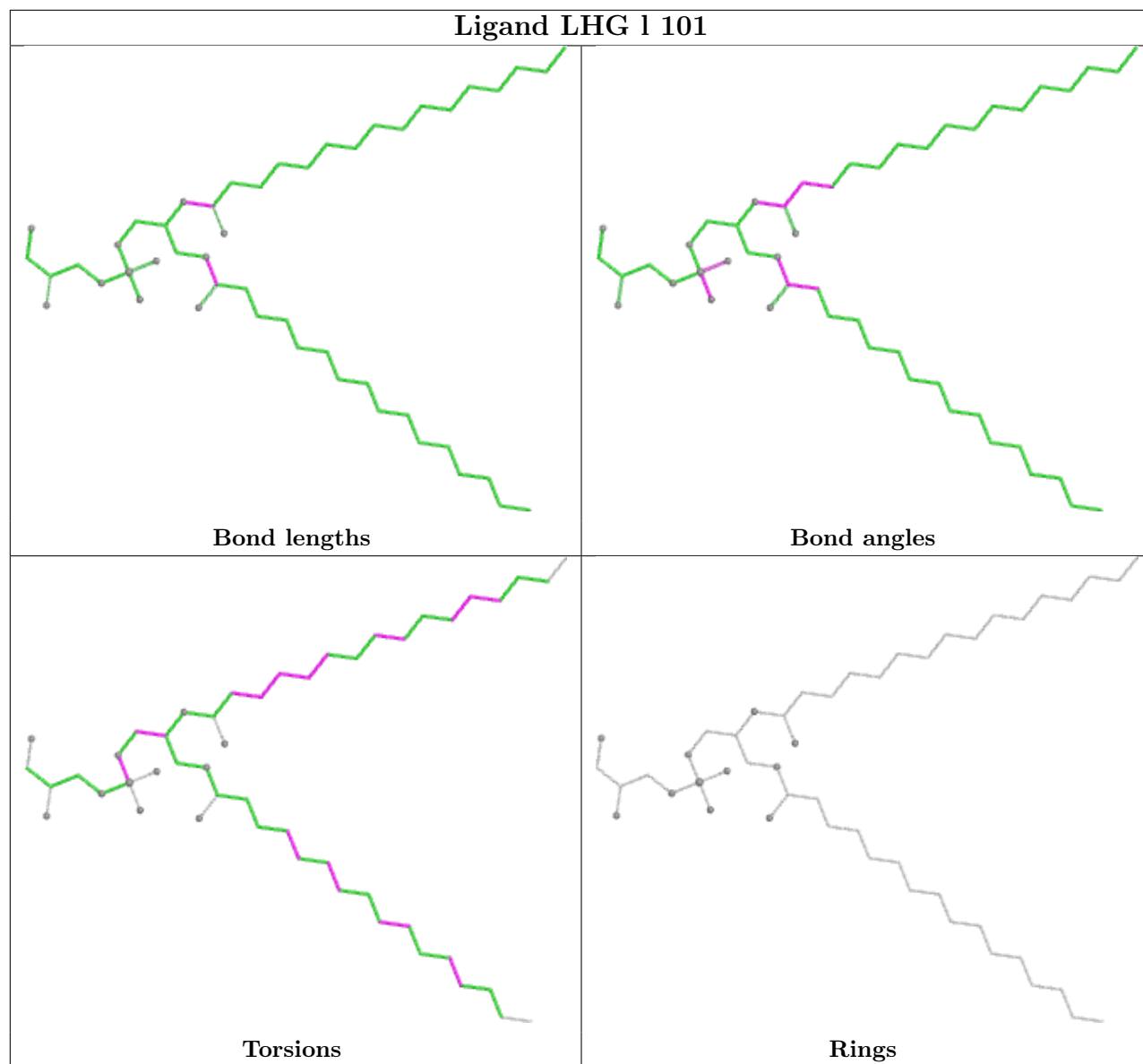


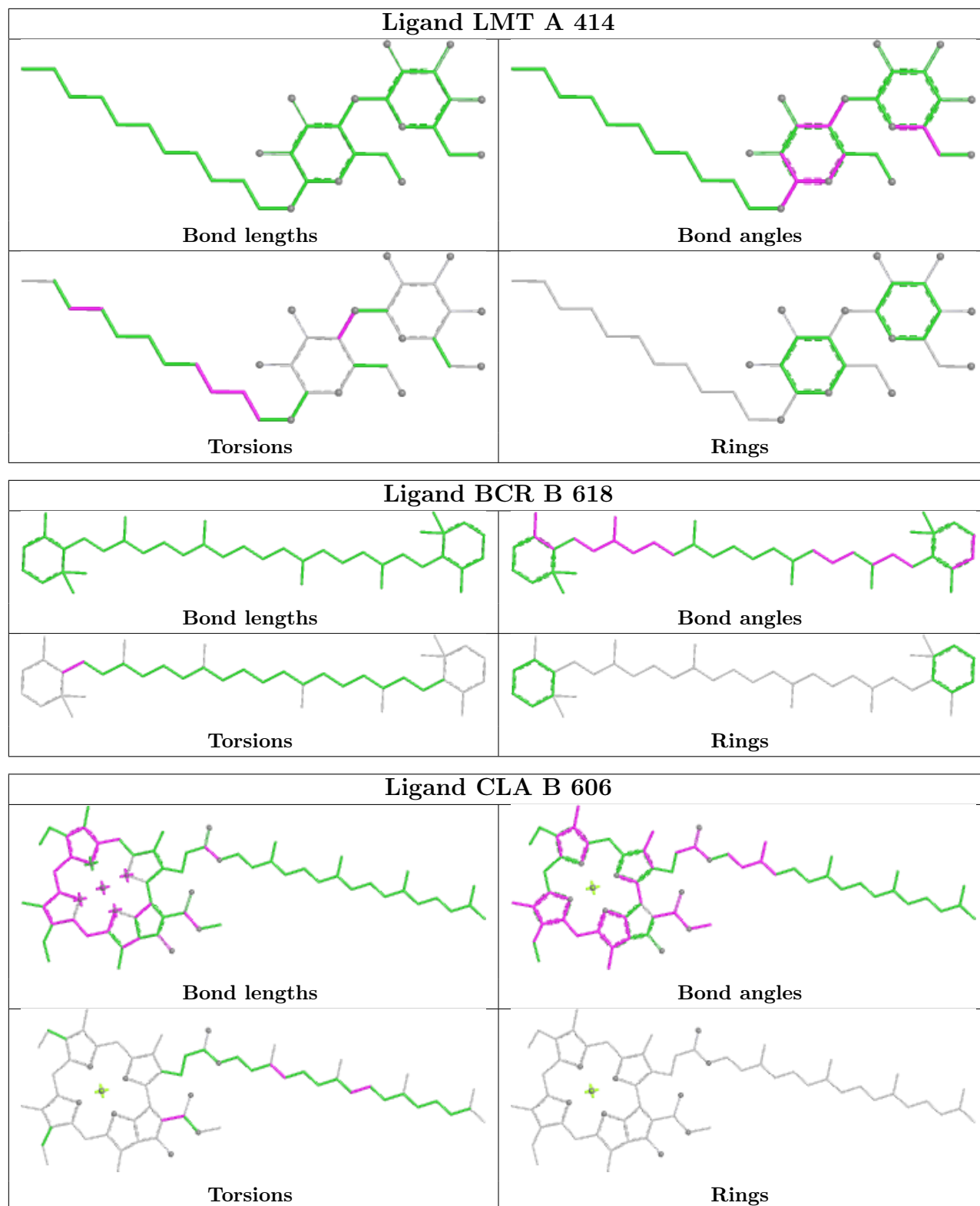


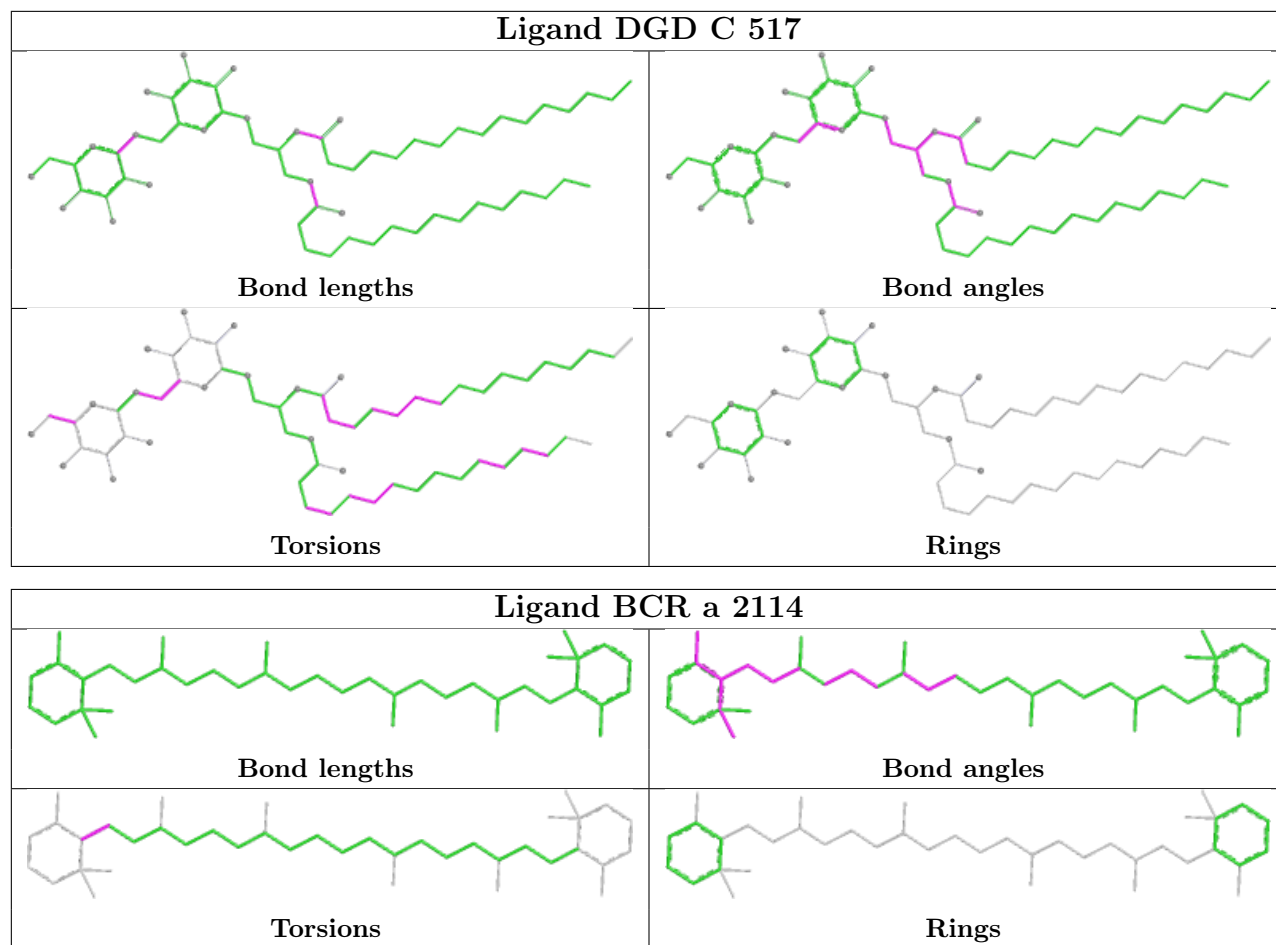




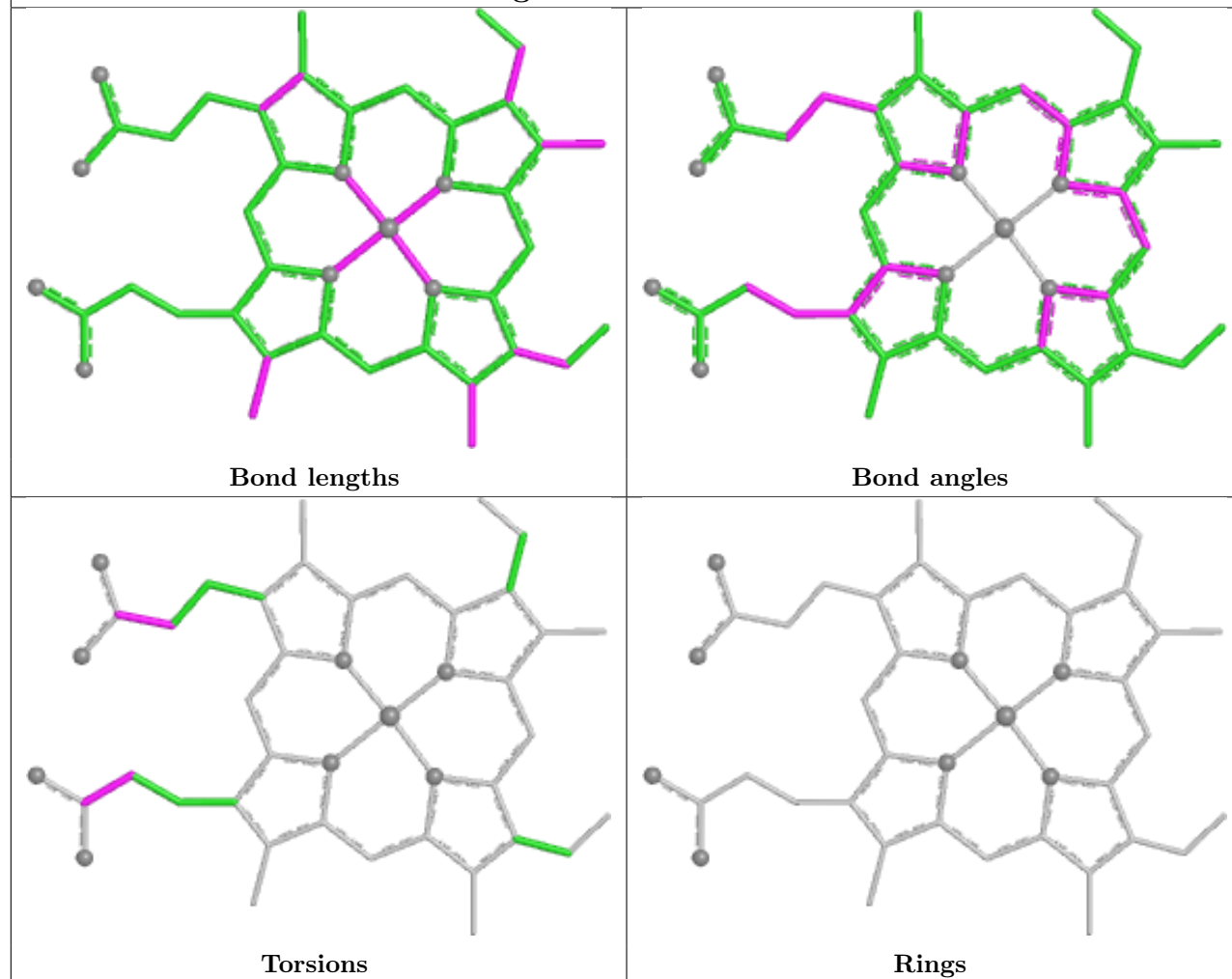




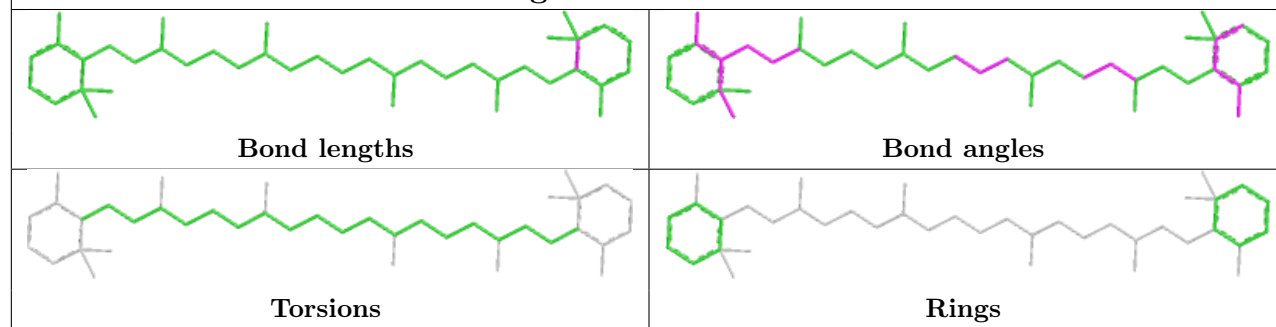




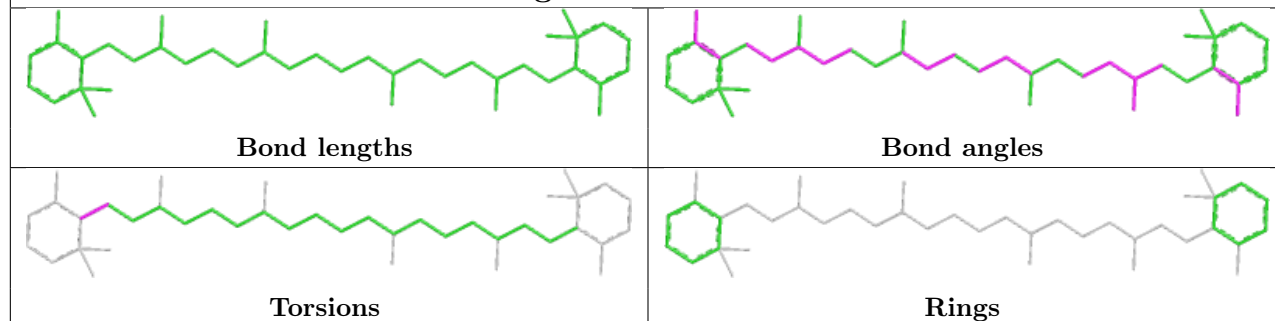
Ligand HEM e 103



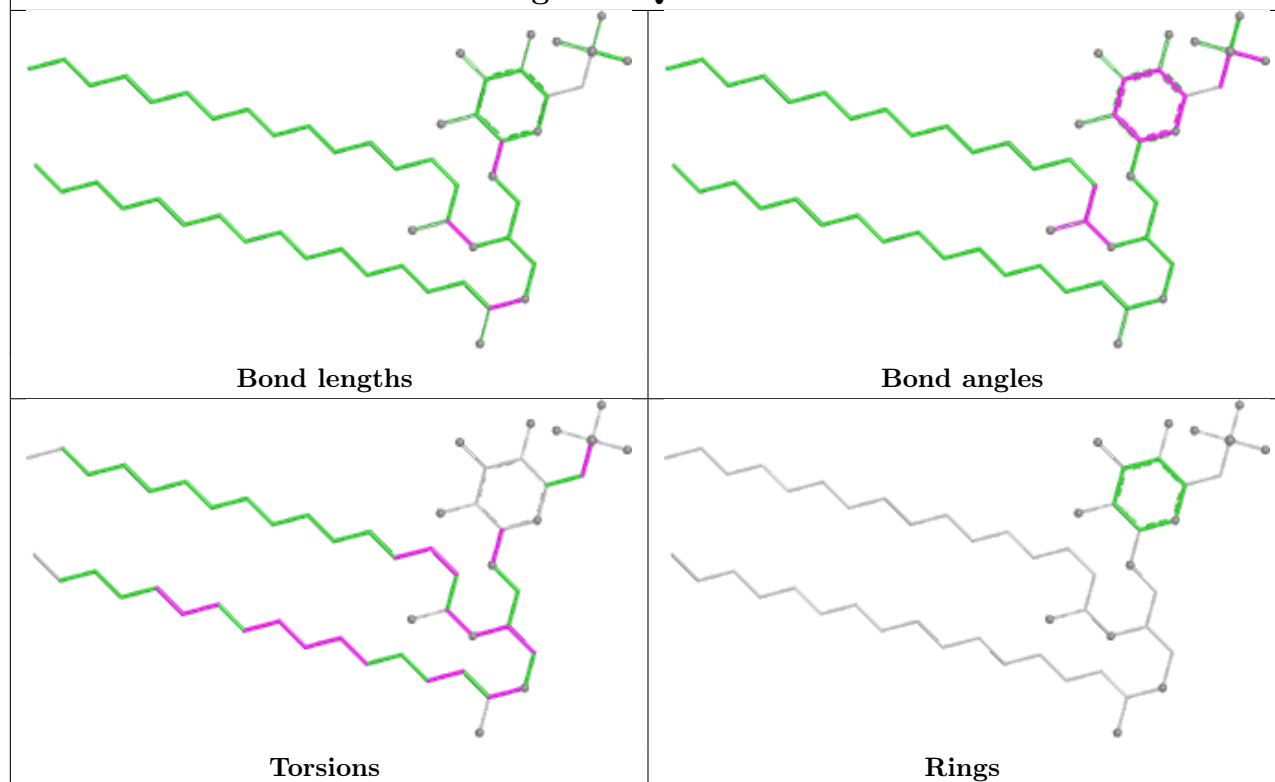
Ligand BCR A 410



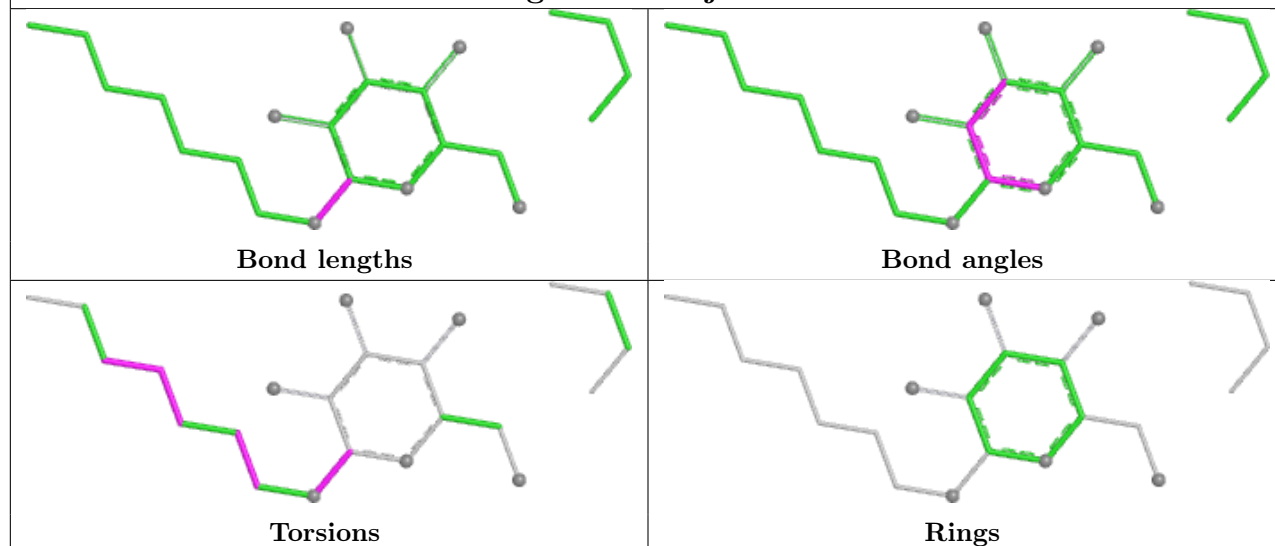
Ligand BCR c 516

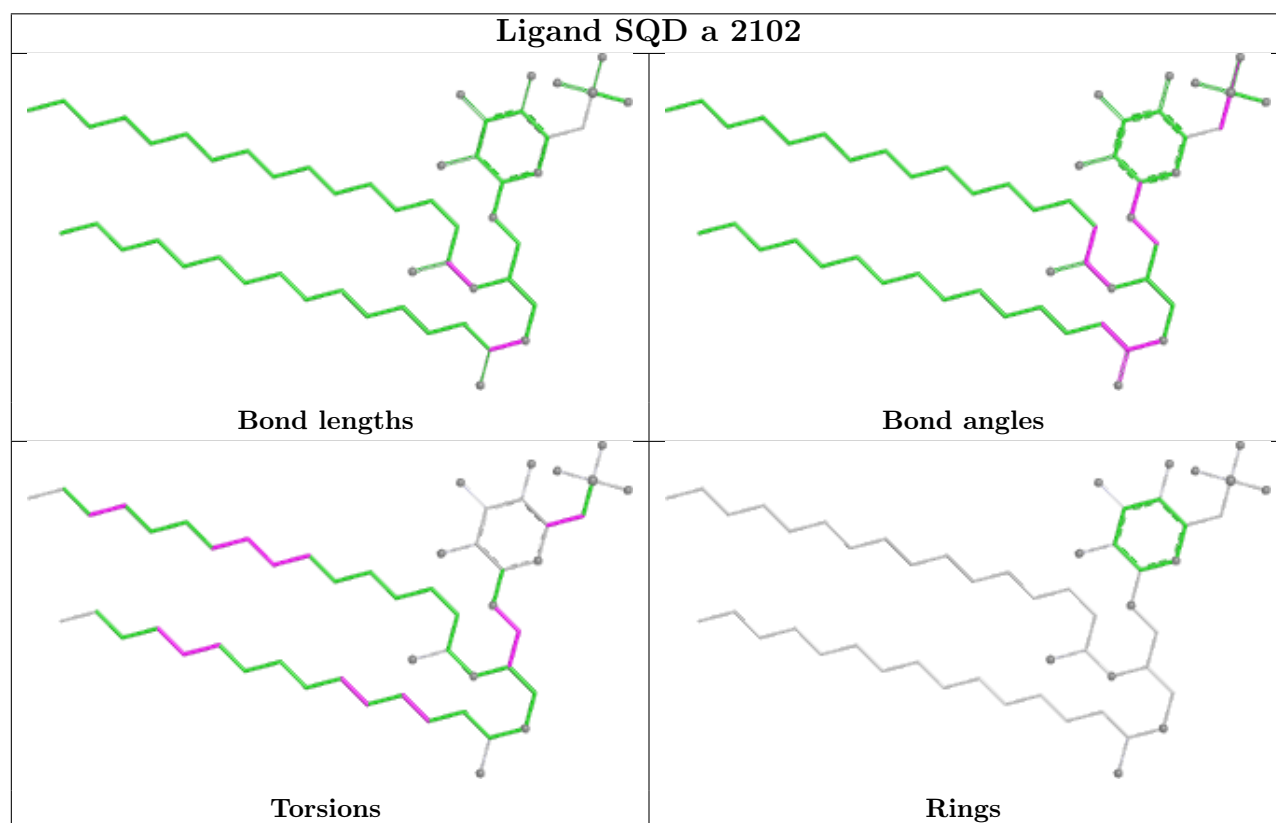
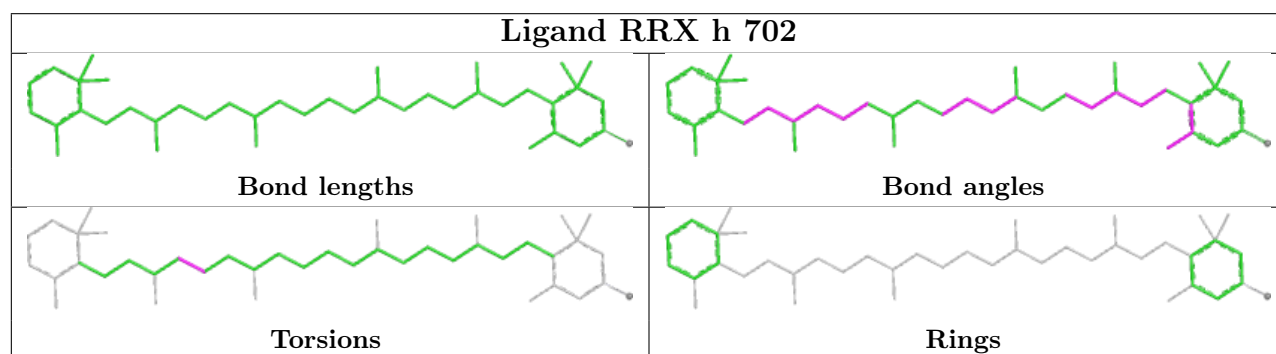
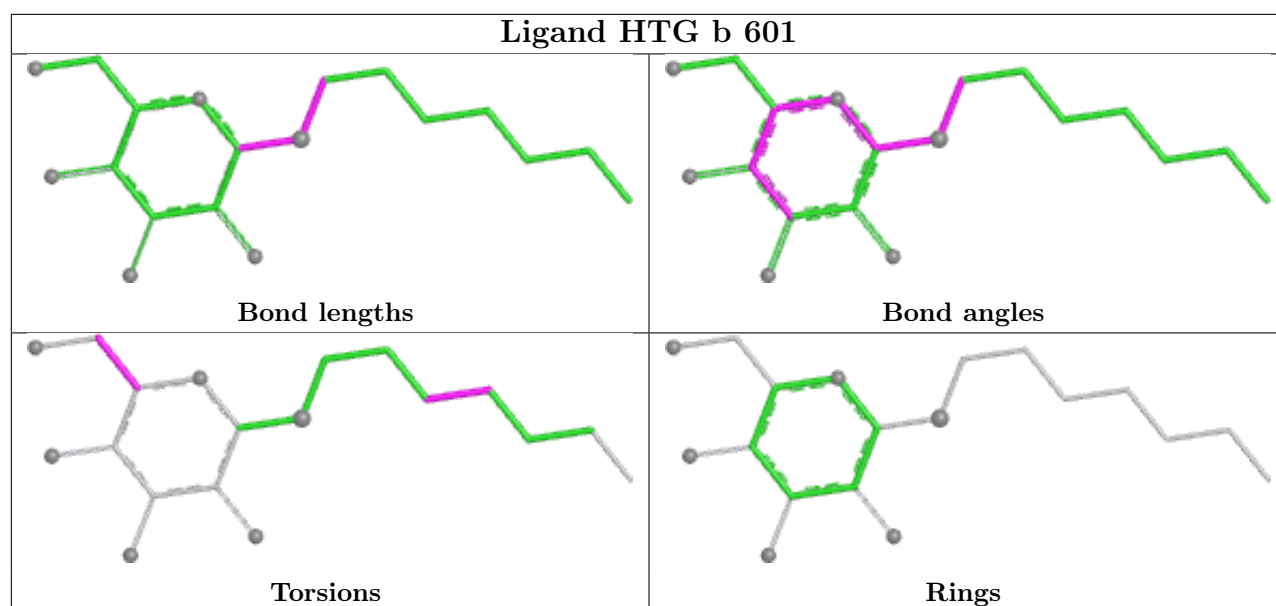


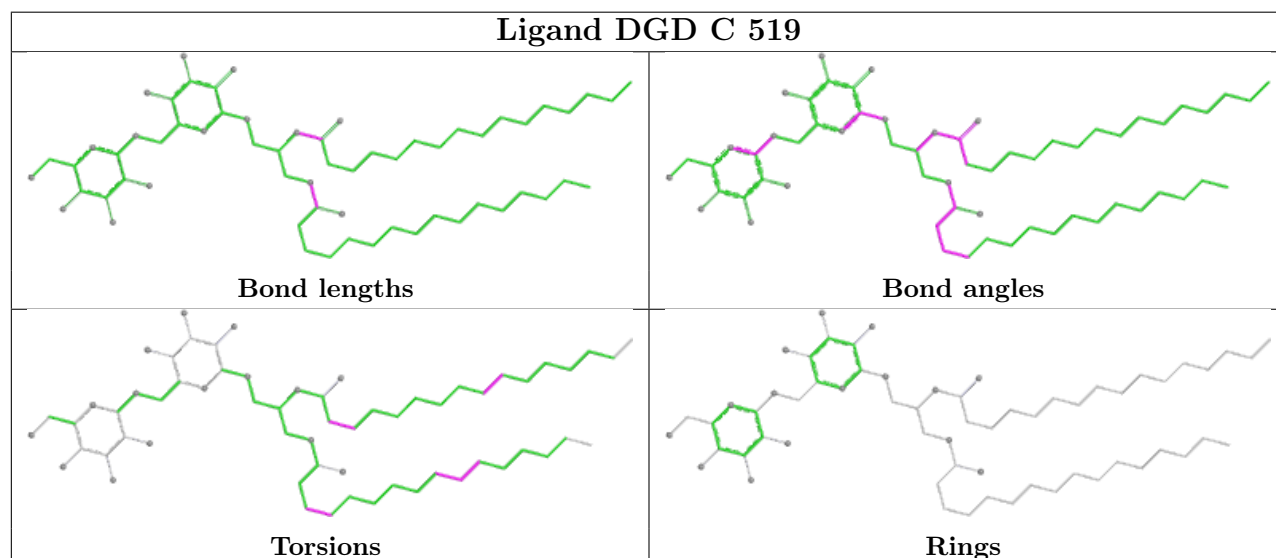
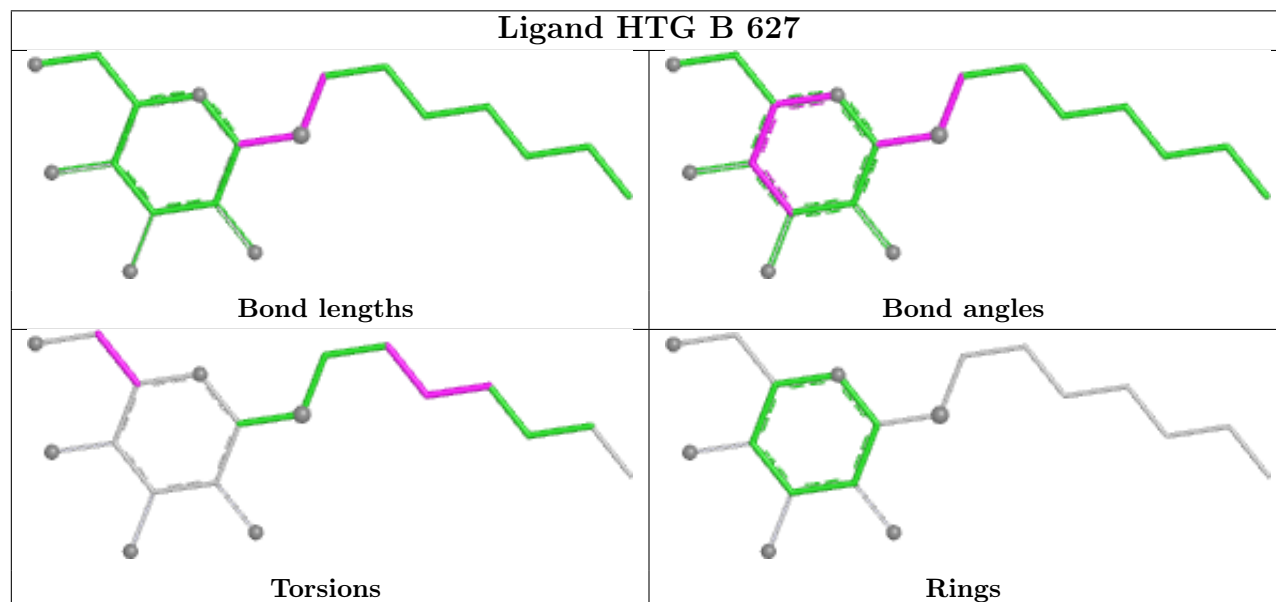
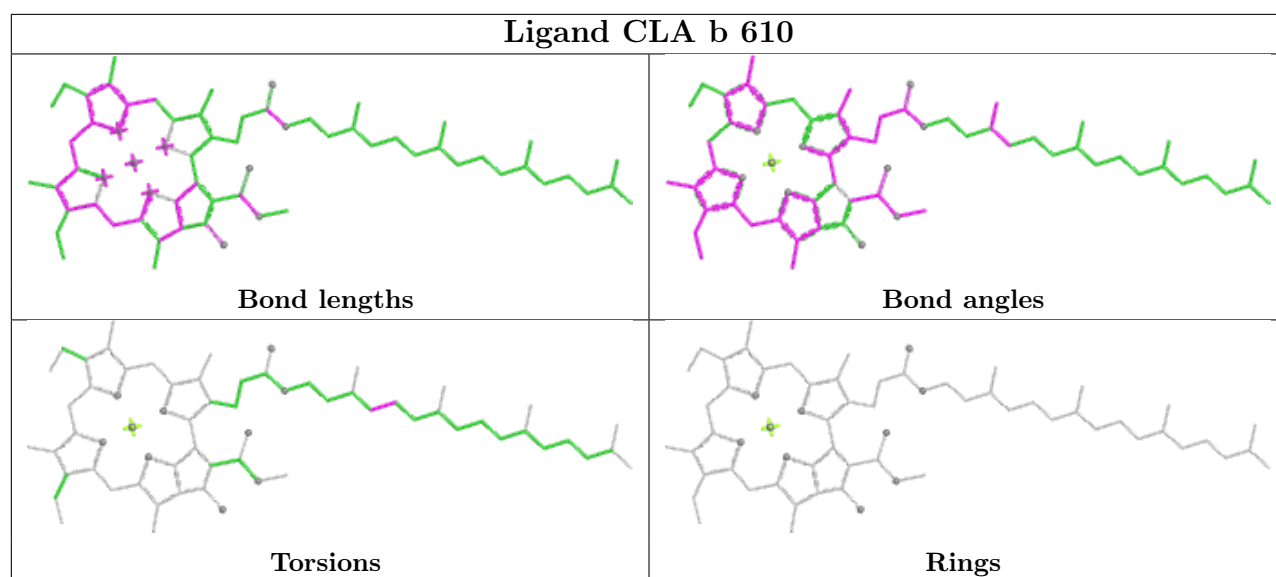
Ligand SQD B 621

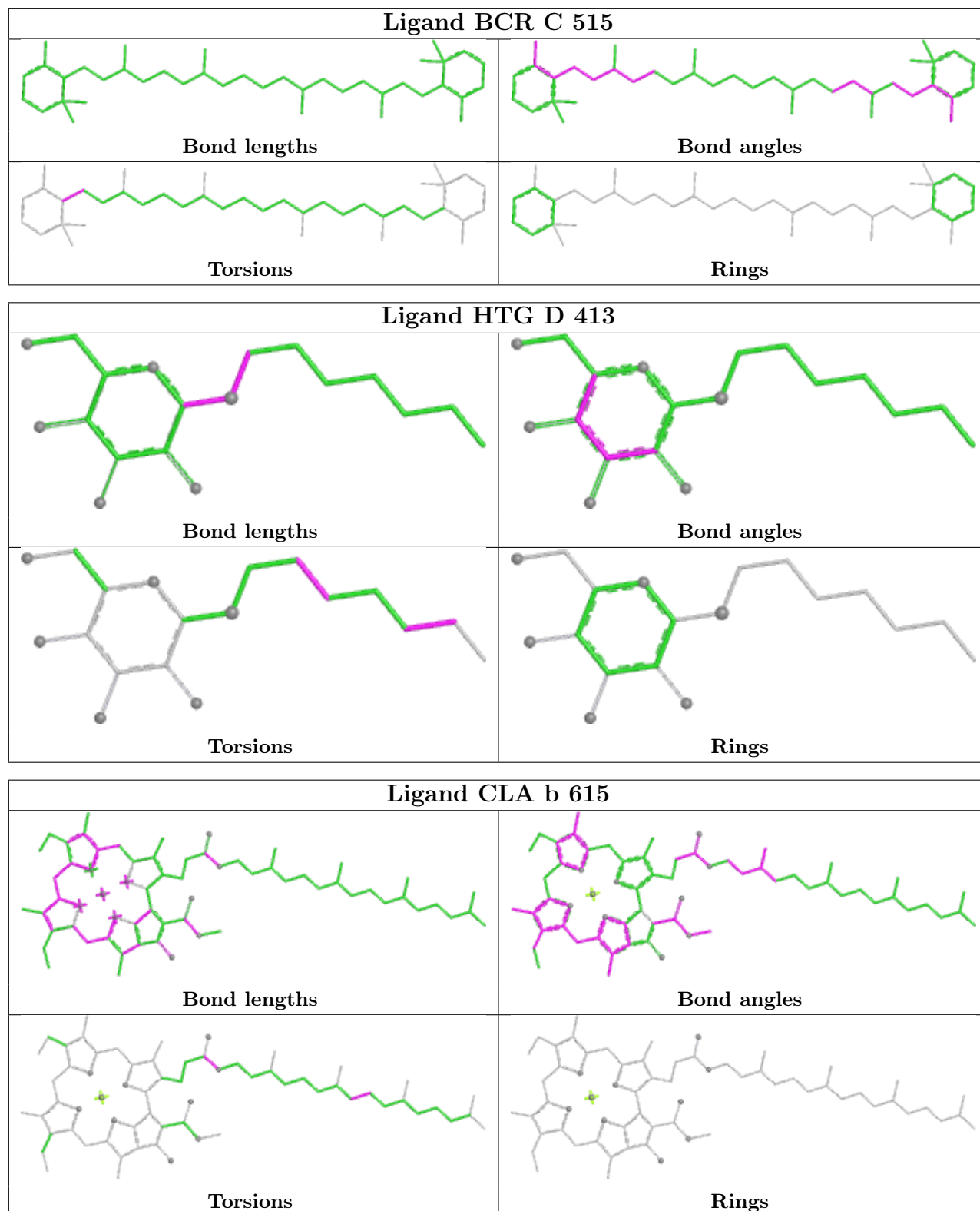


Ligand LMT j 1601

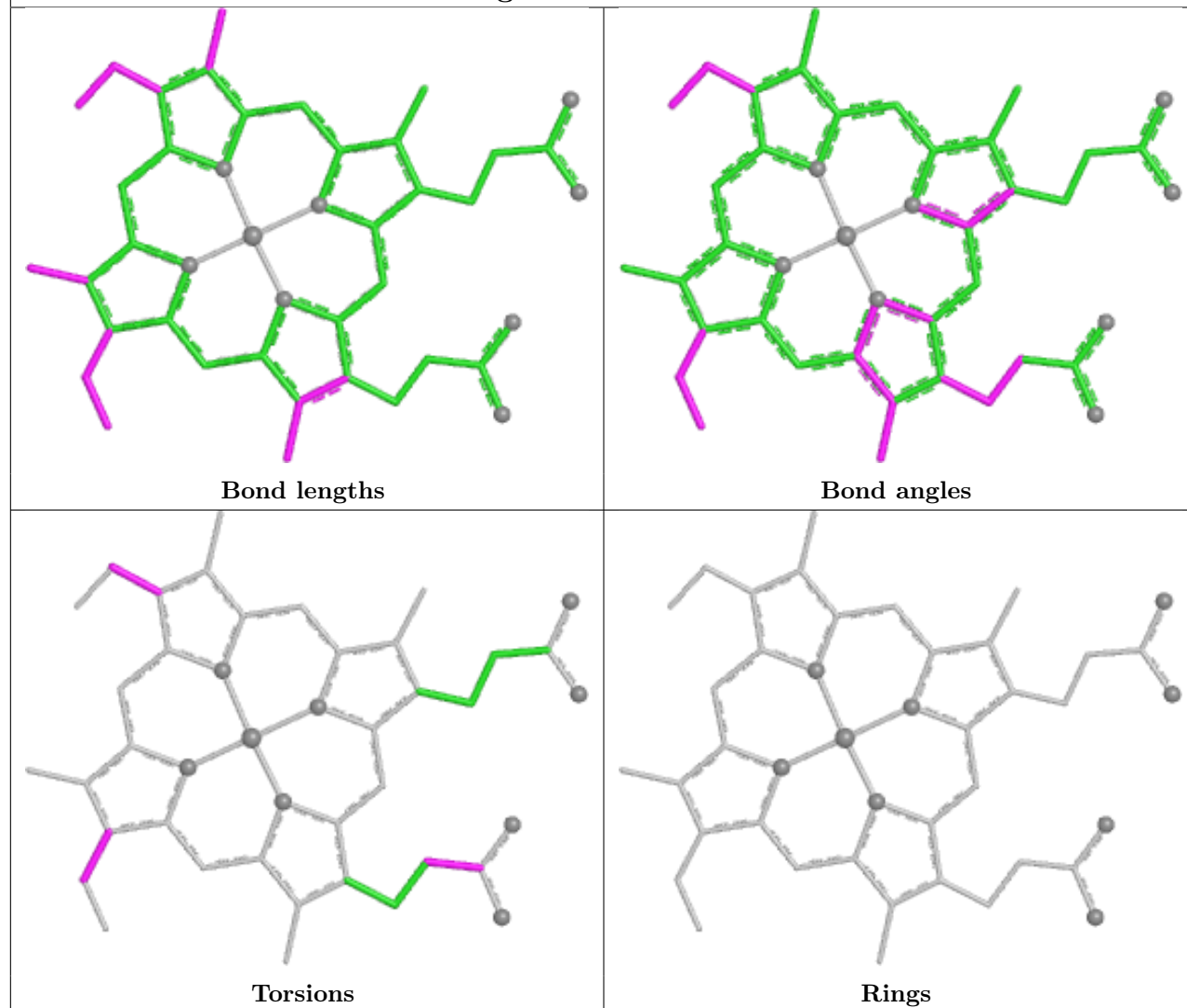




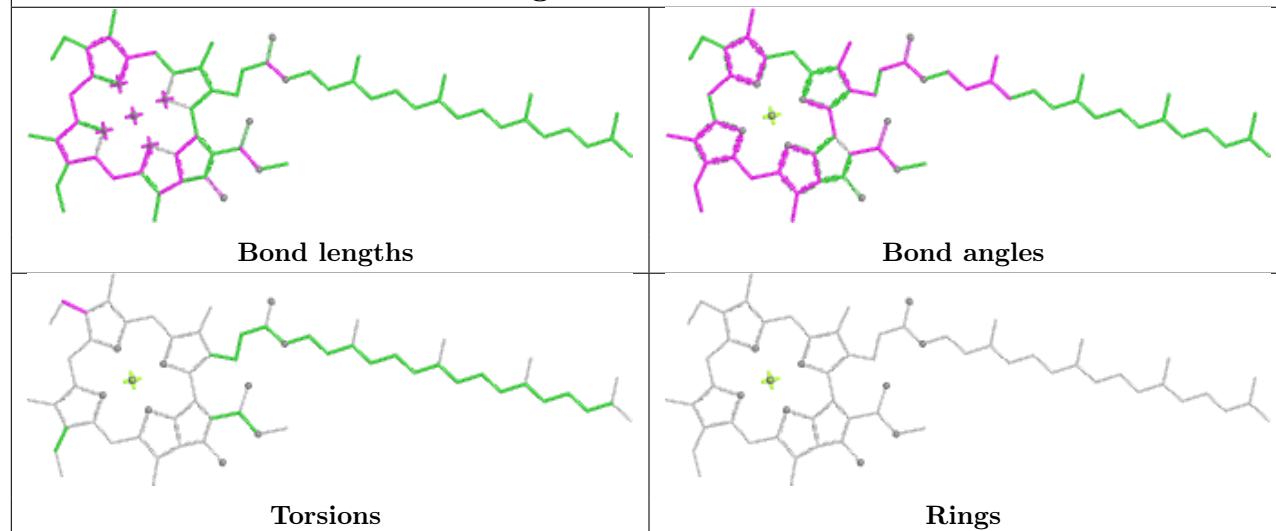


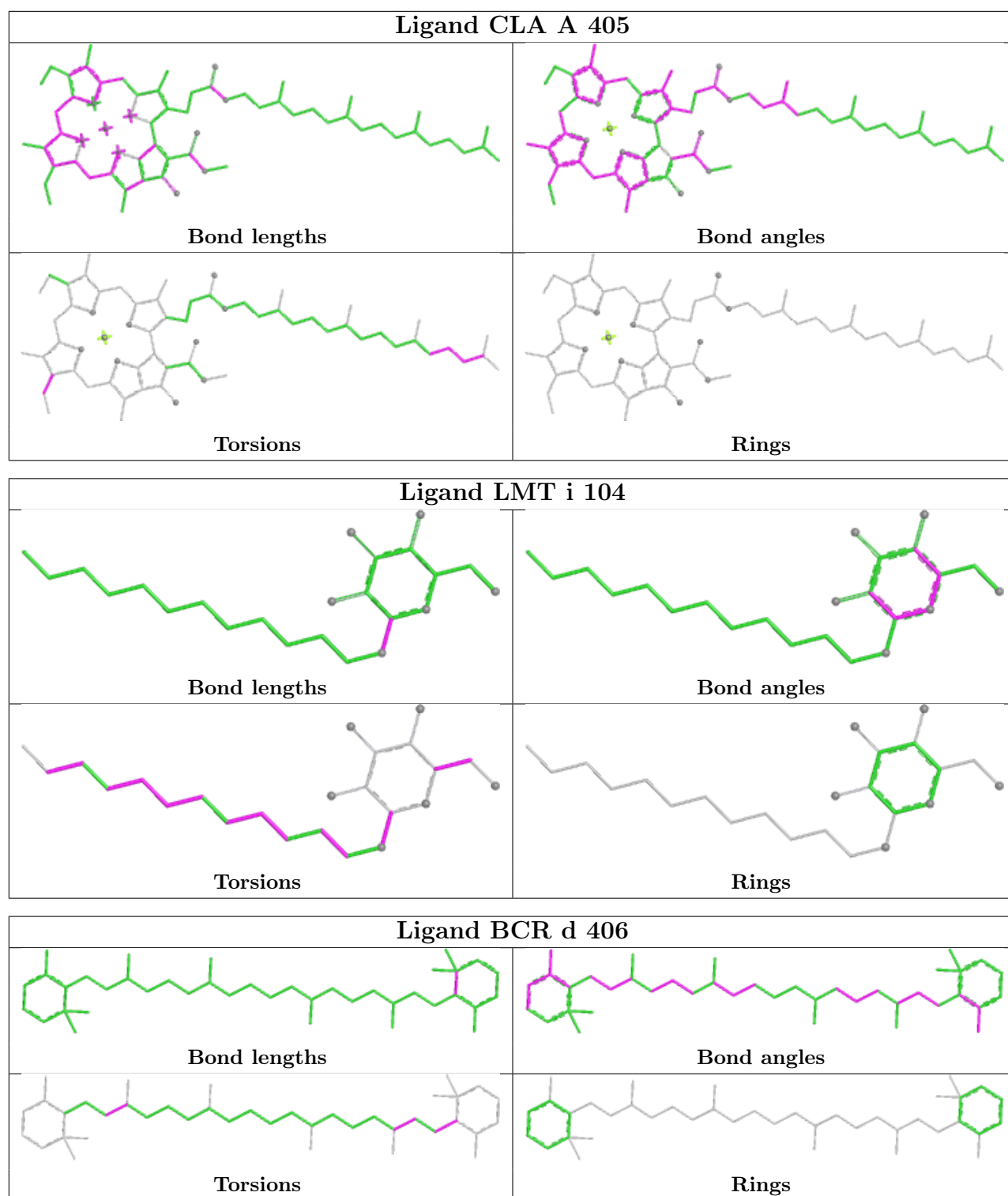


Ligand HEC v 201

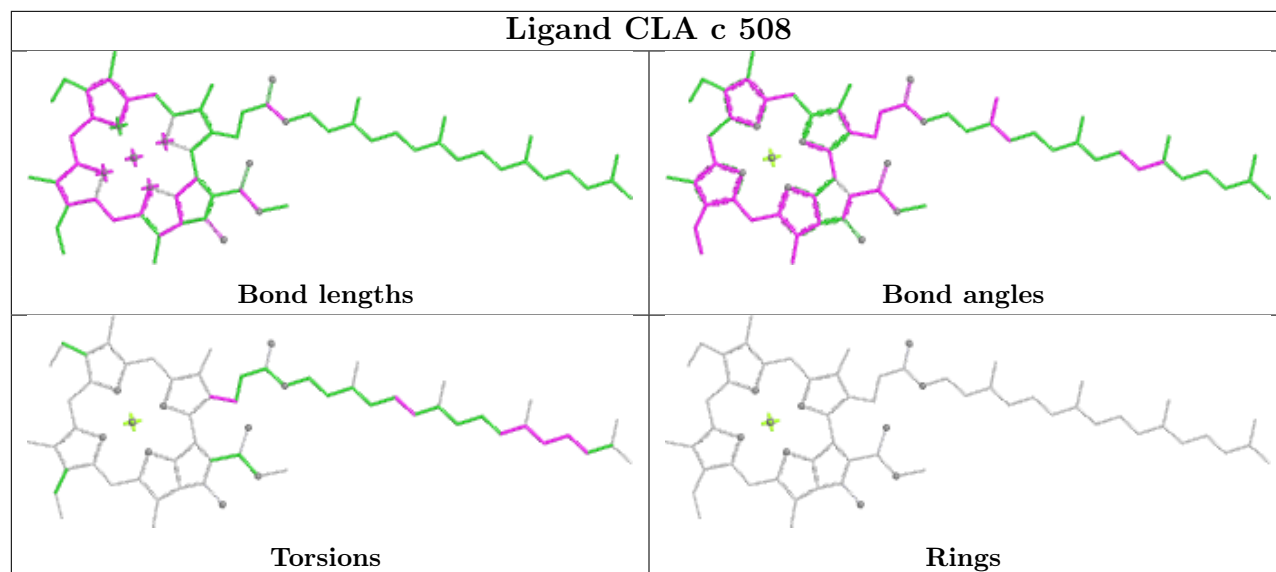


Ligand CLA D 404

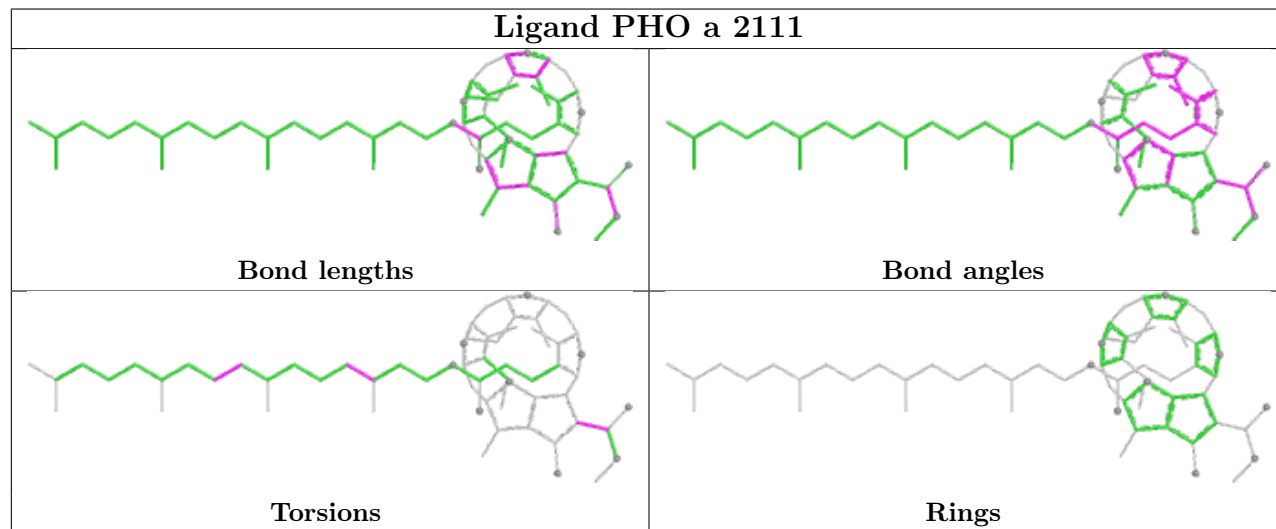




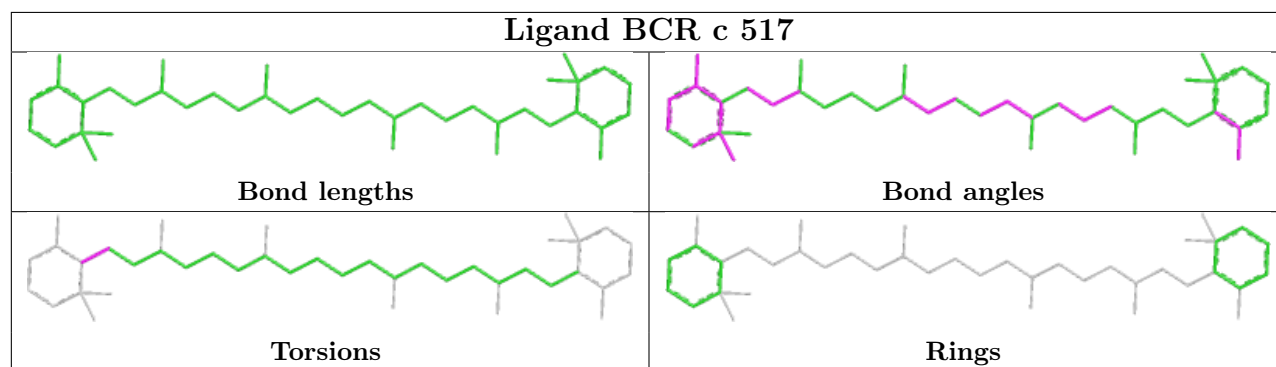
Ligand CLA c 508

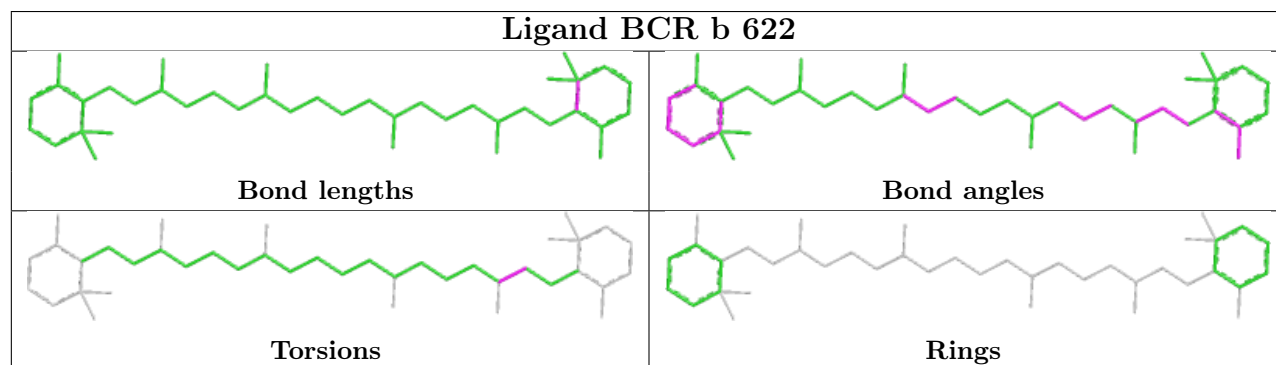
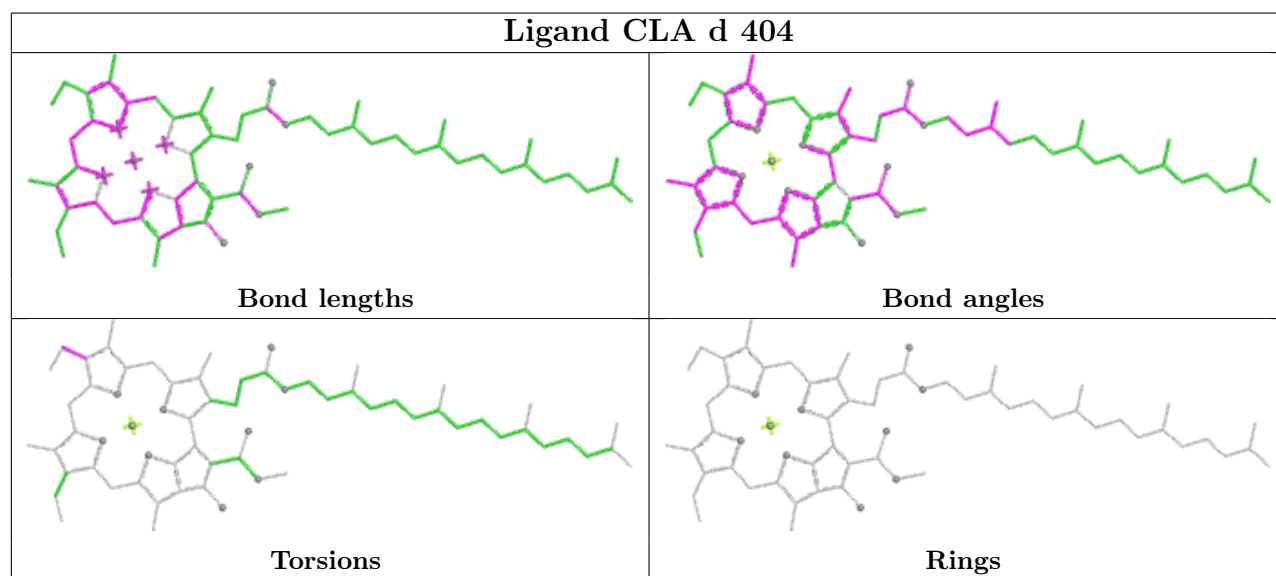
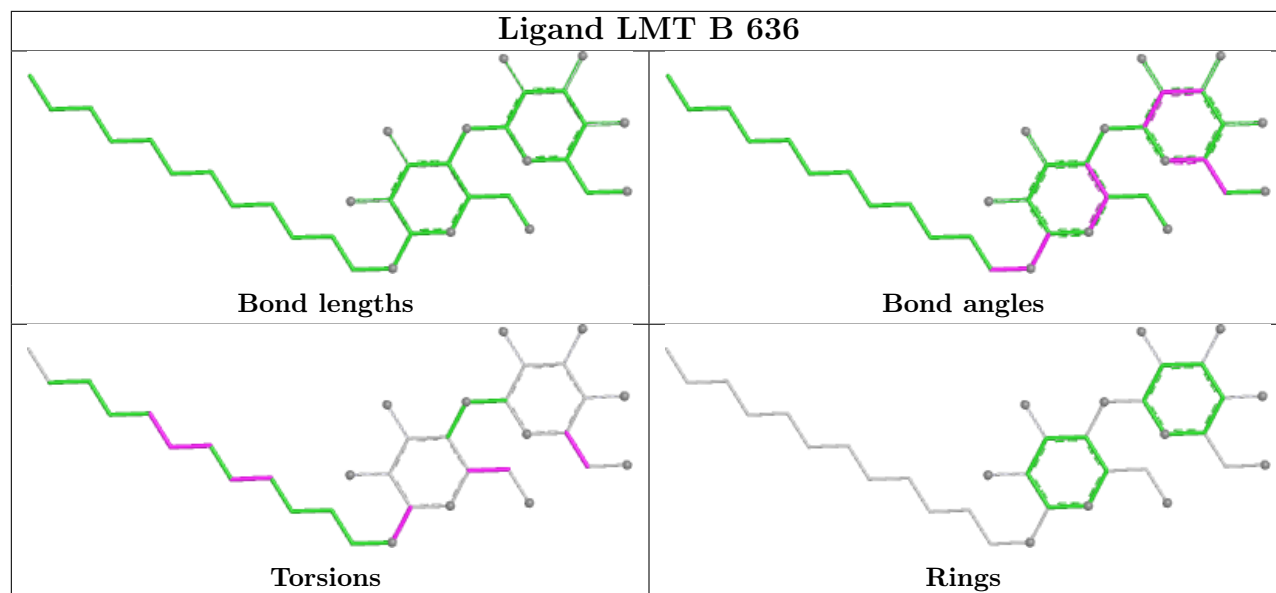


Ligand PHO a 2111

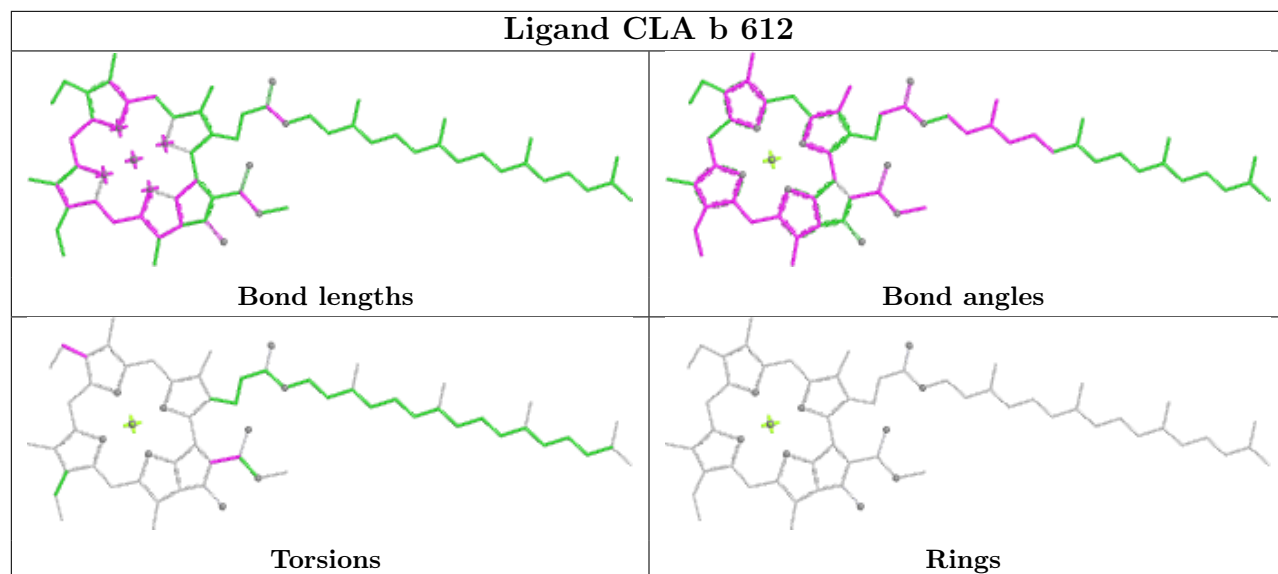


Ligand BCR c 517

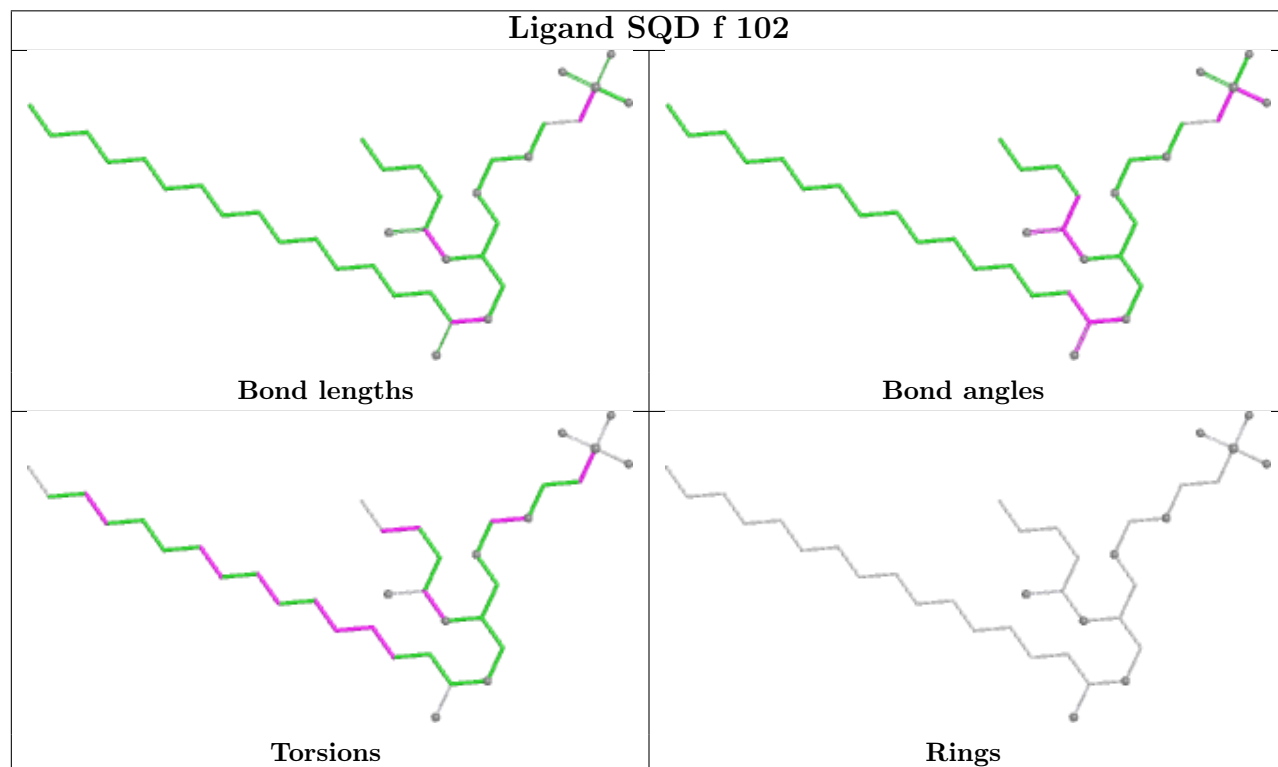


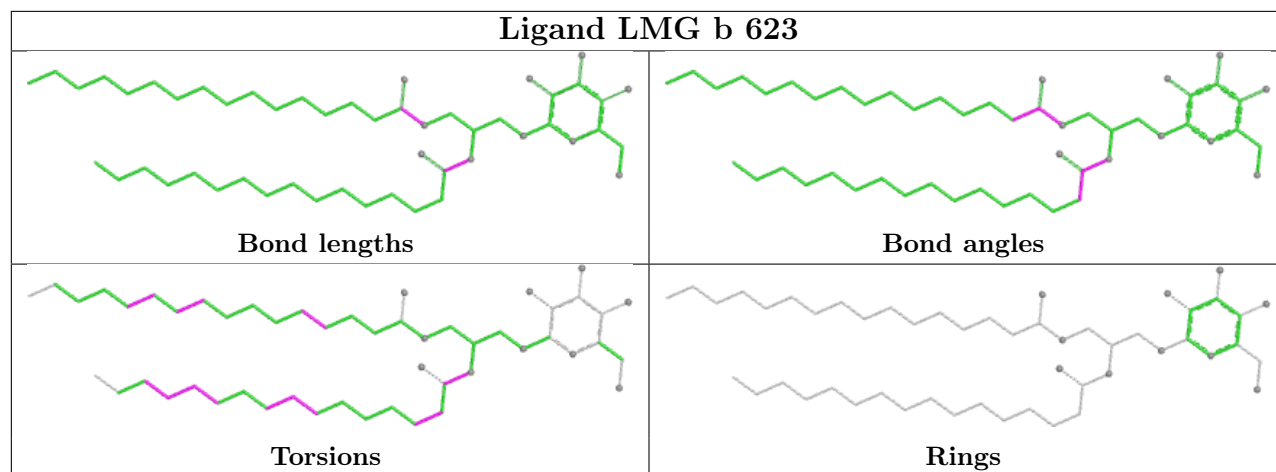
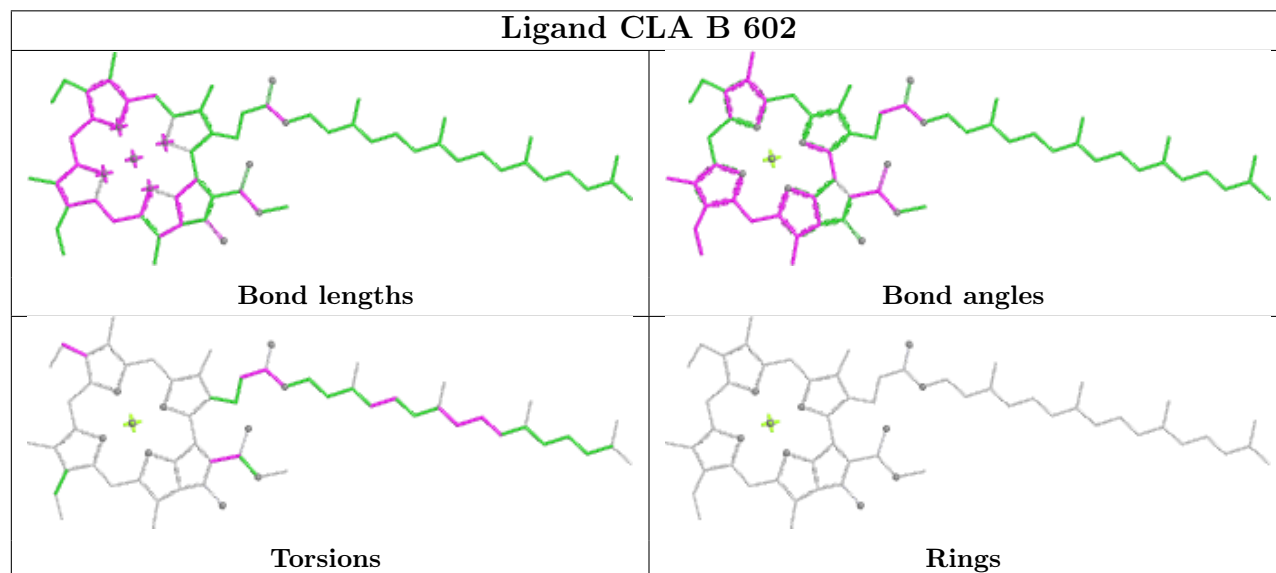
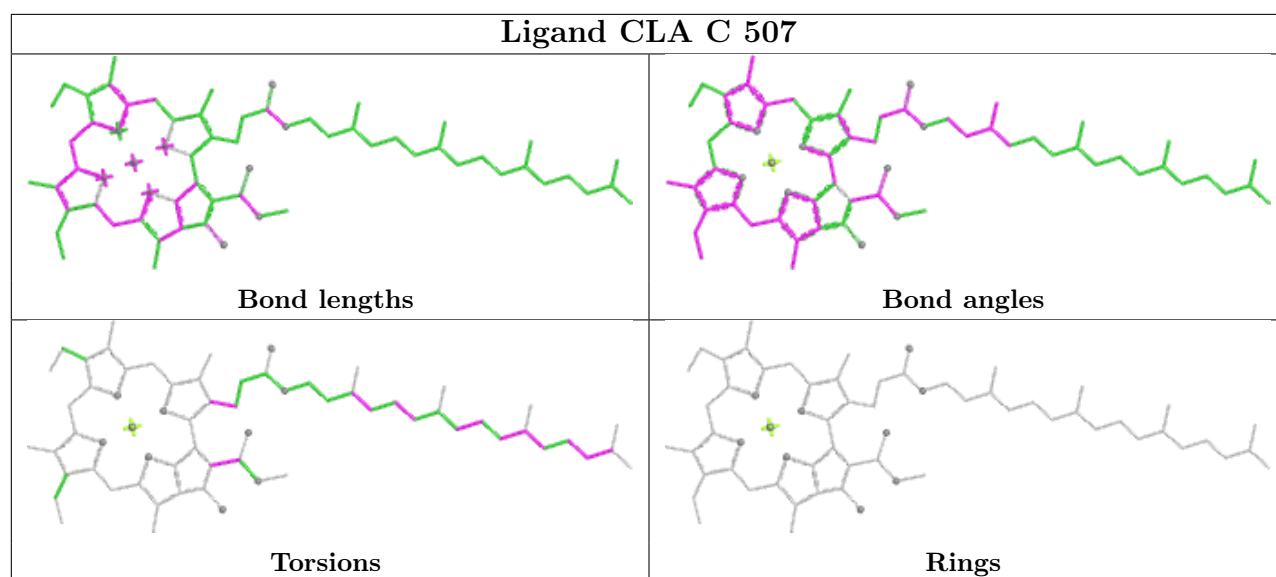


Ligand CLA b 612

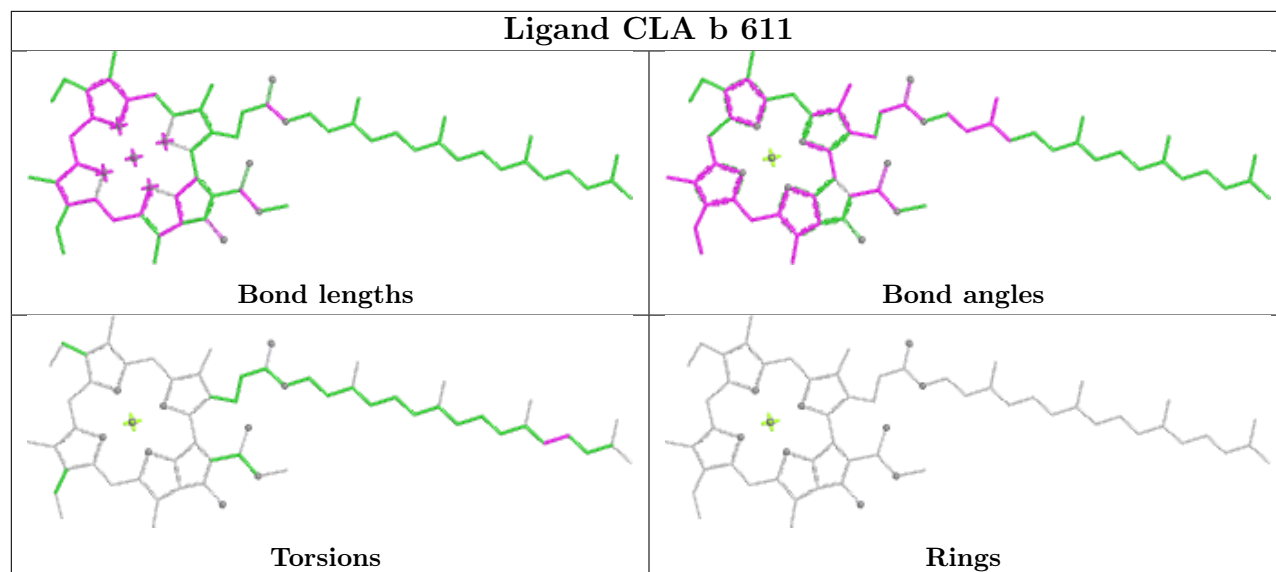


Ligand SQD f 102

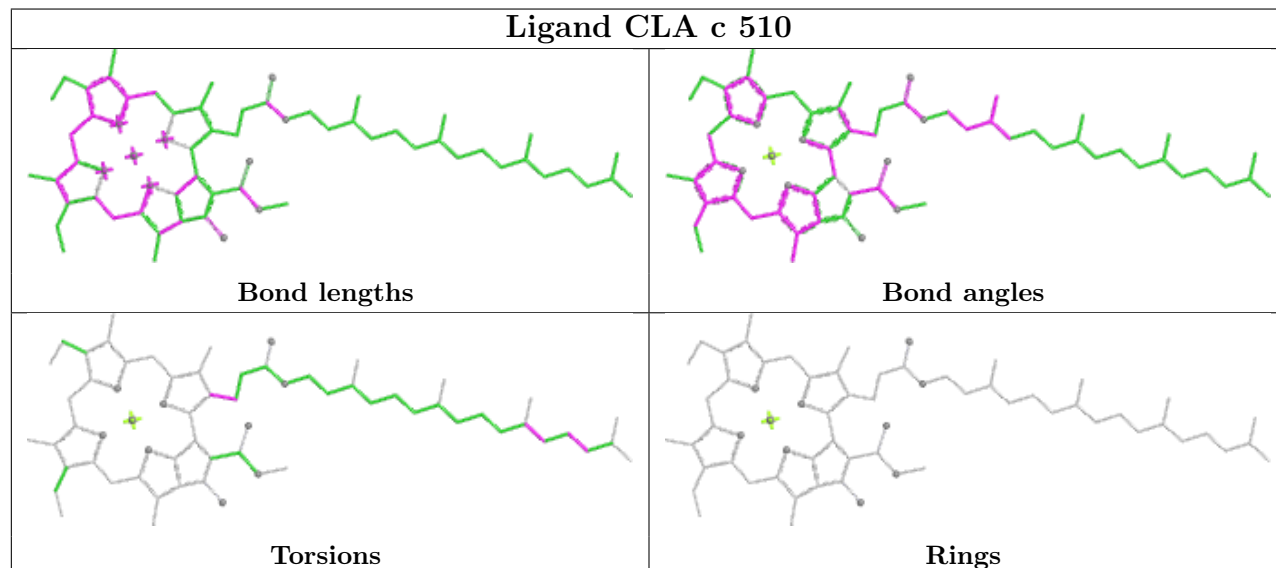


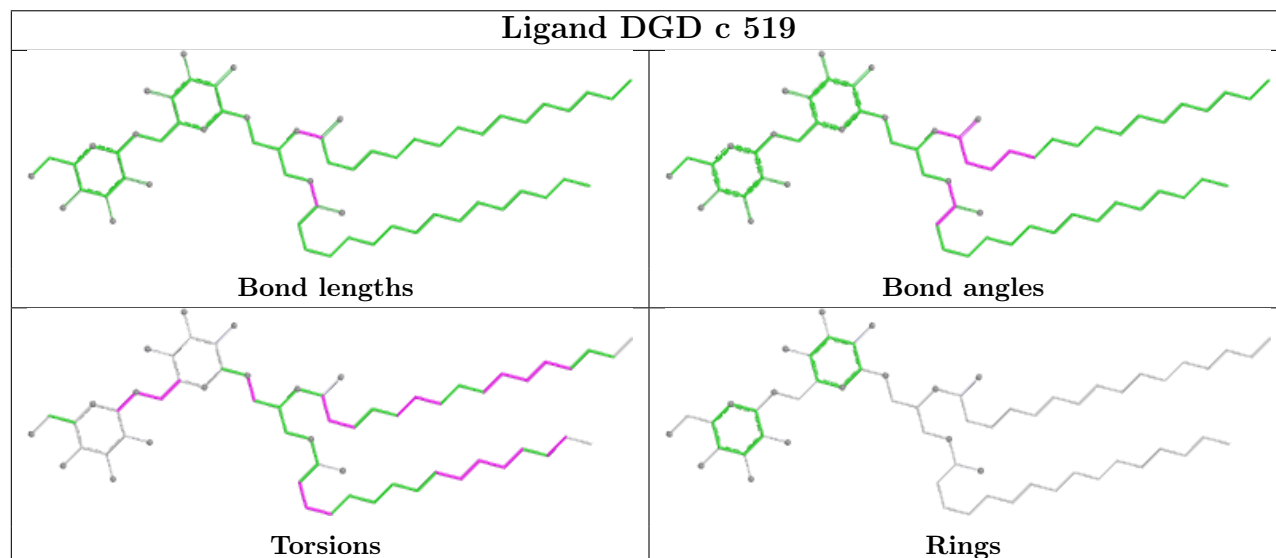
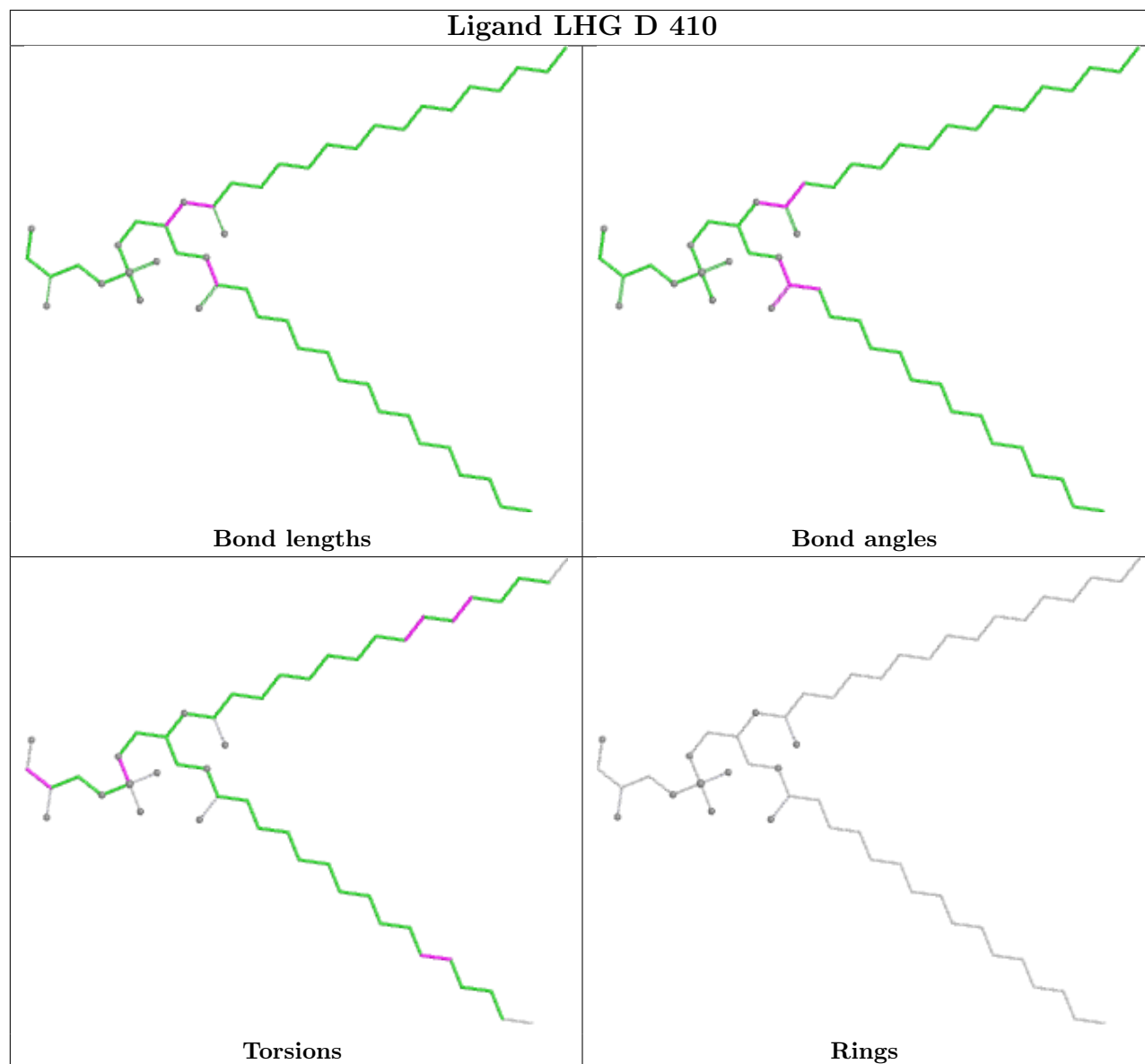


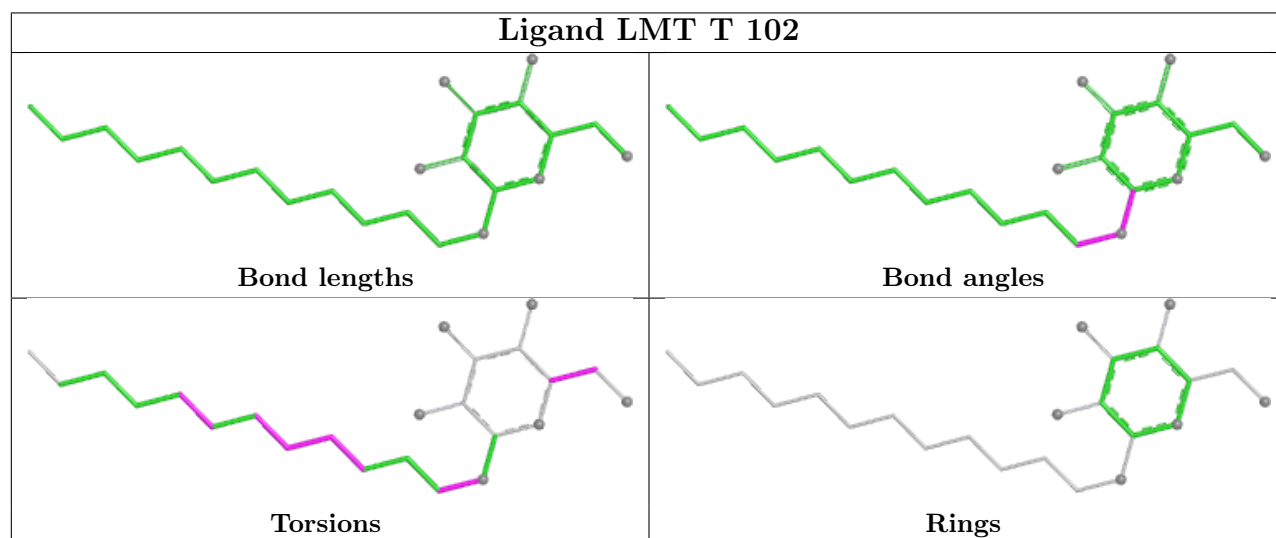
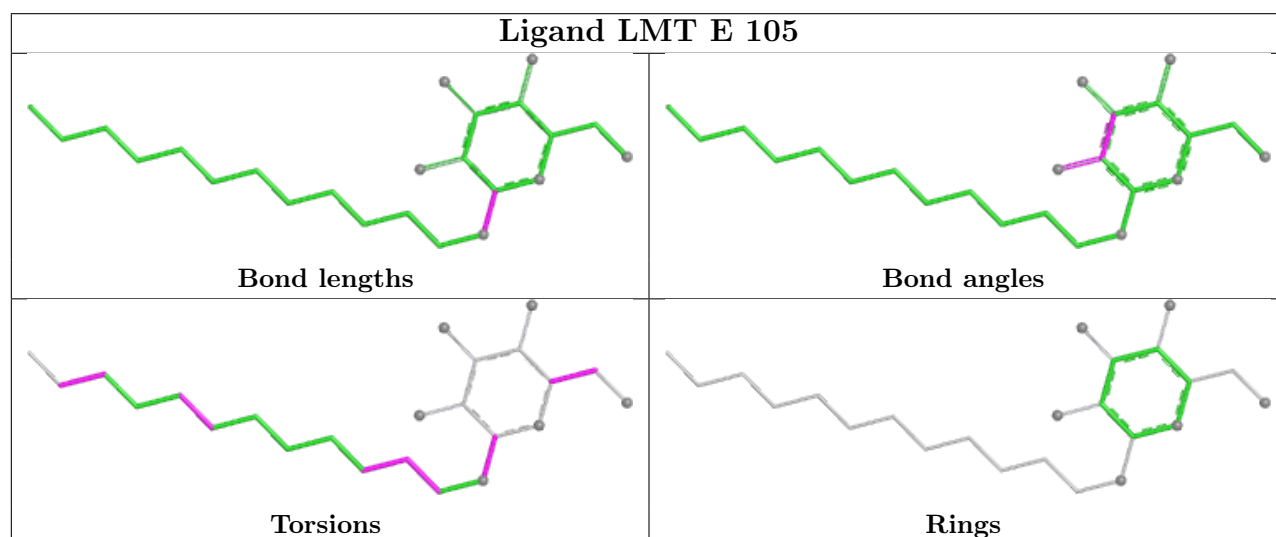
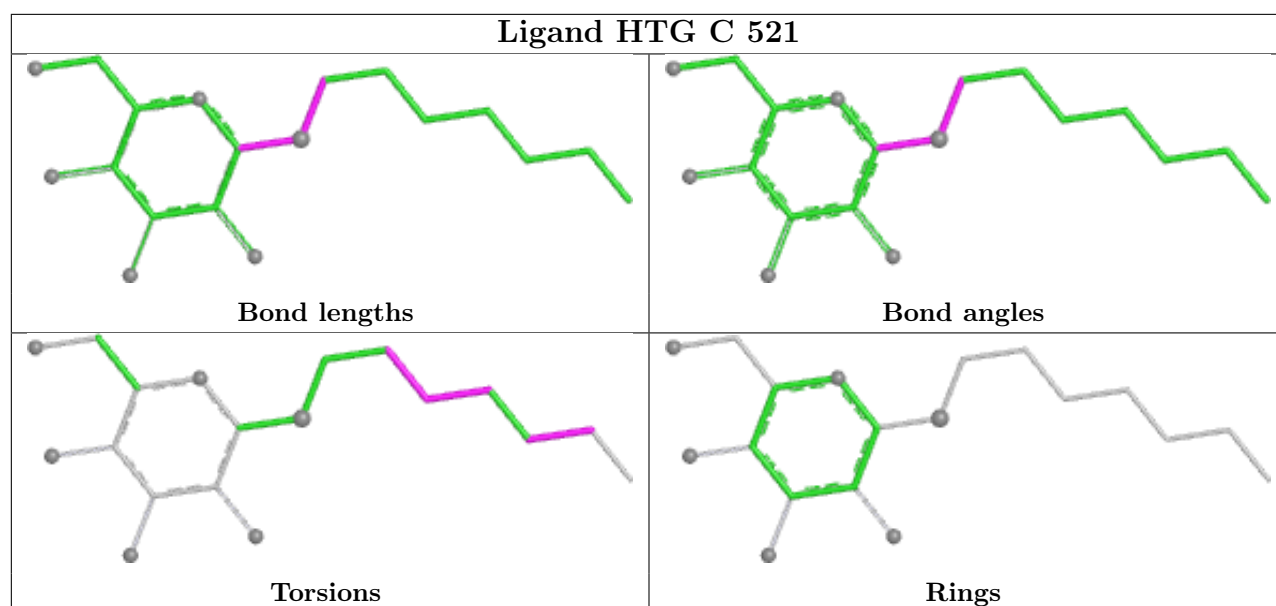
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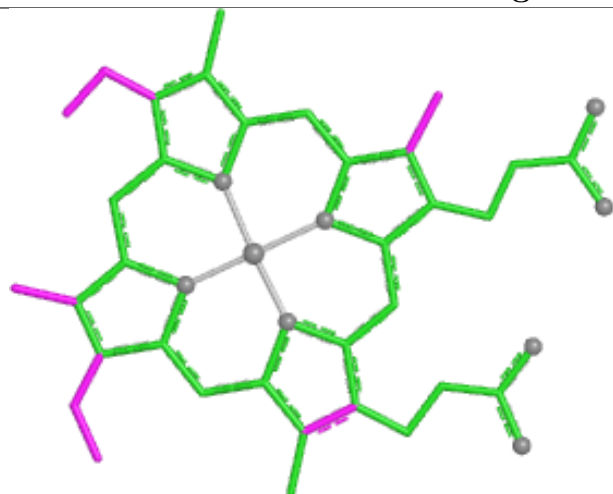
Ligand CLA c 510



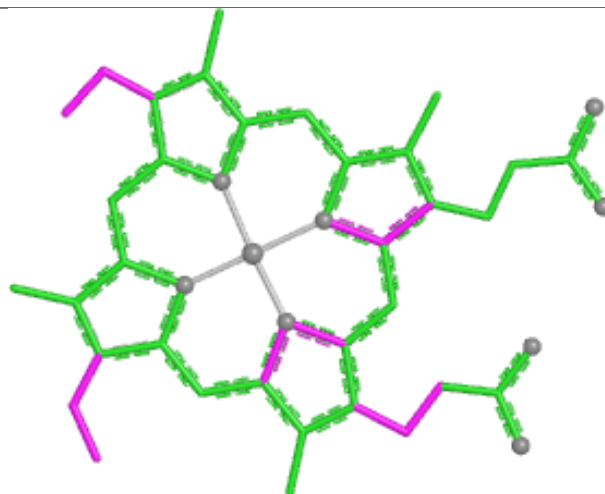




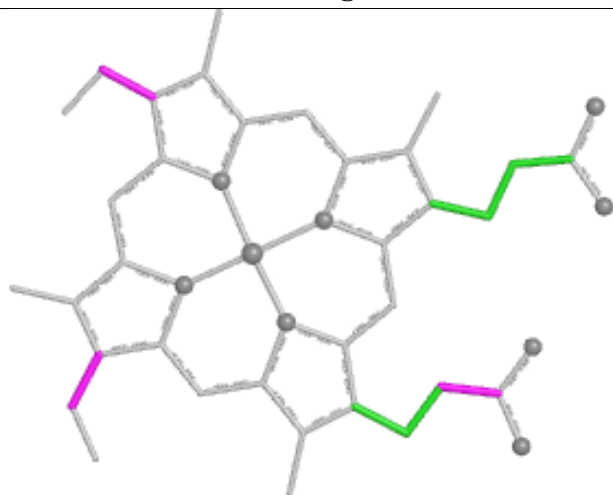
Ligand HEC V 201



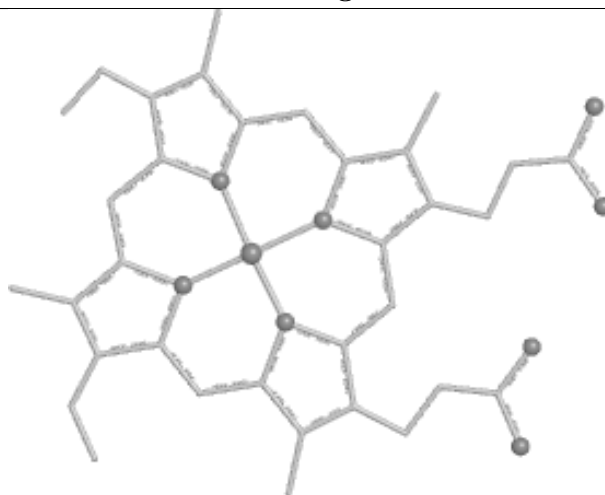
Bond lengths



Bond angles

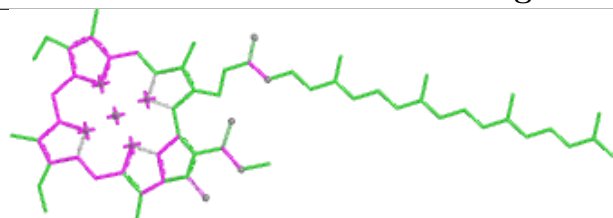


Torsions

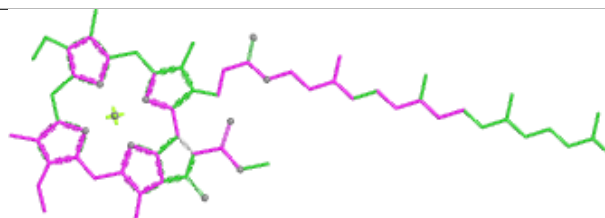


Rings

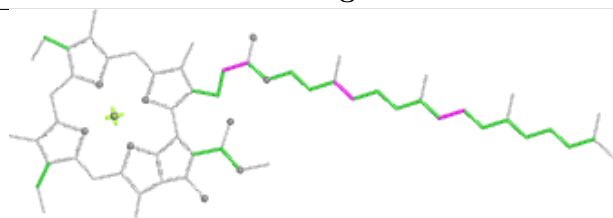
Ligand CLA C 511



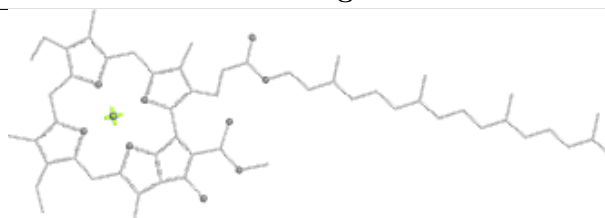
Bond lengths



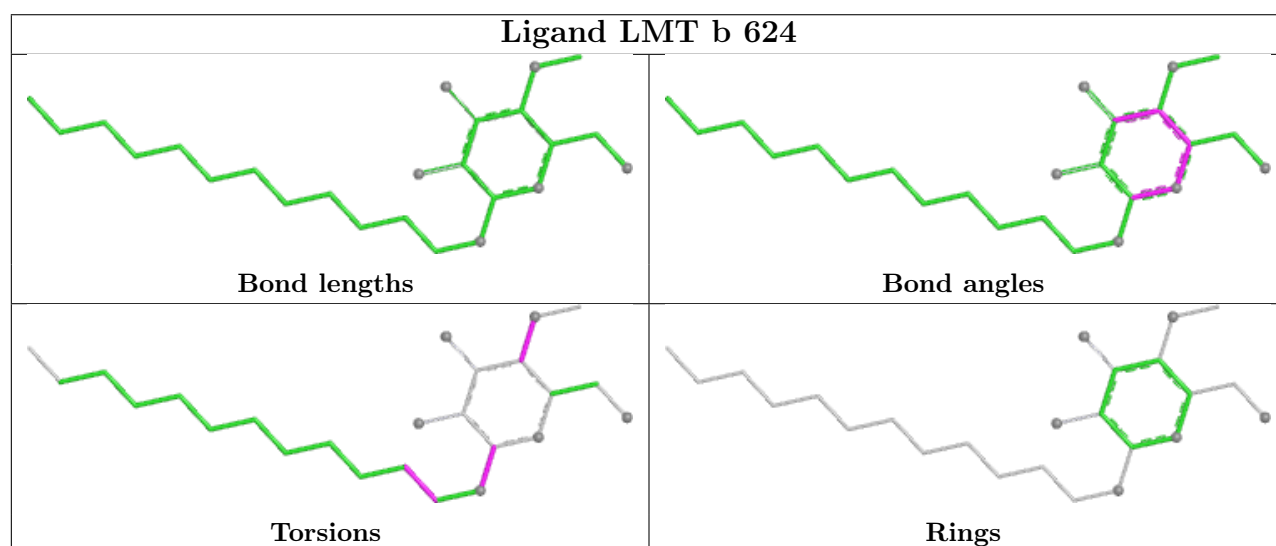
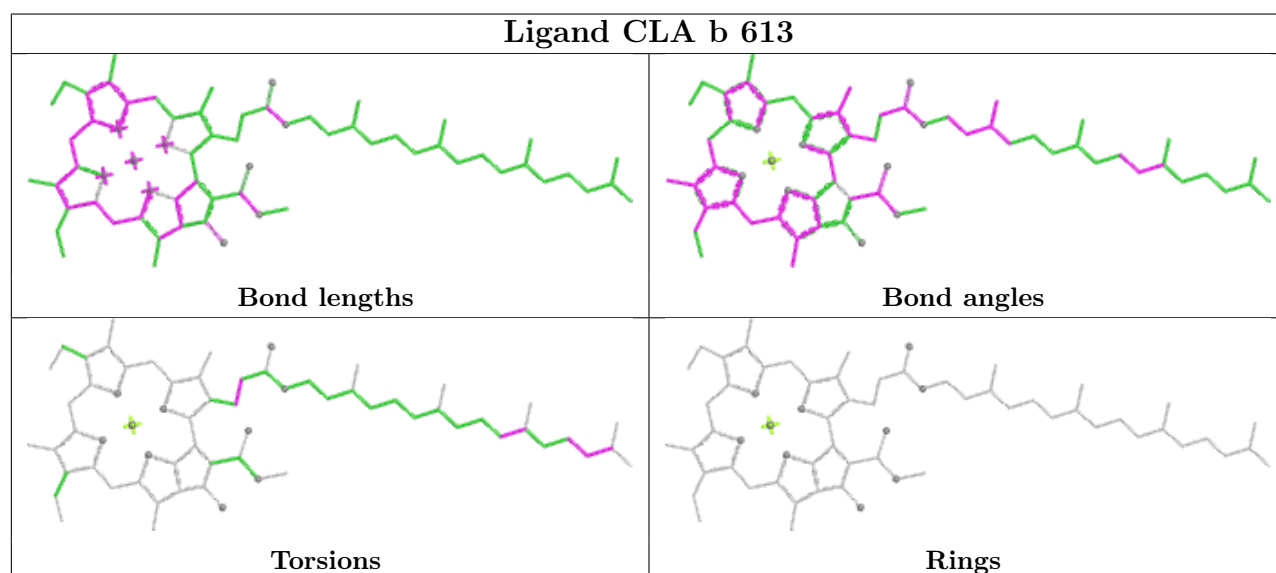
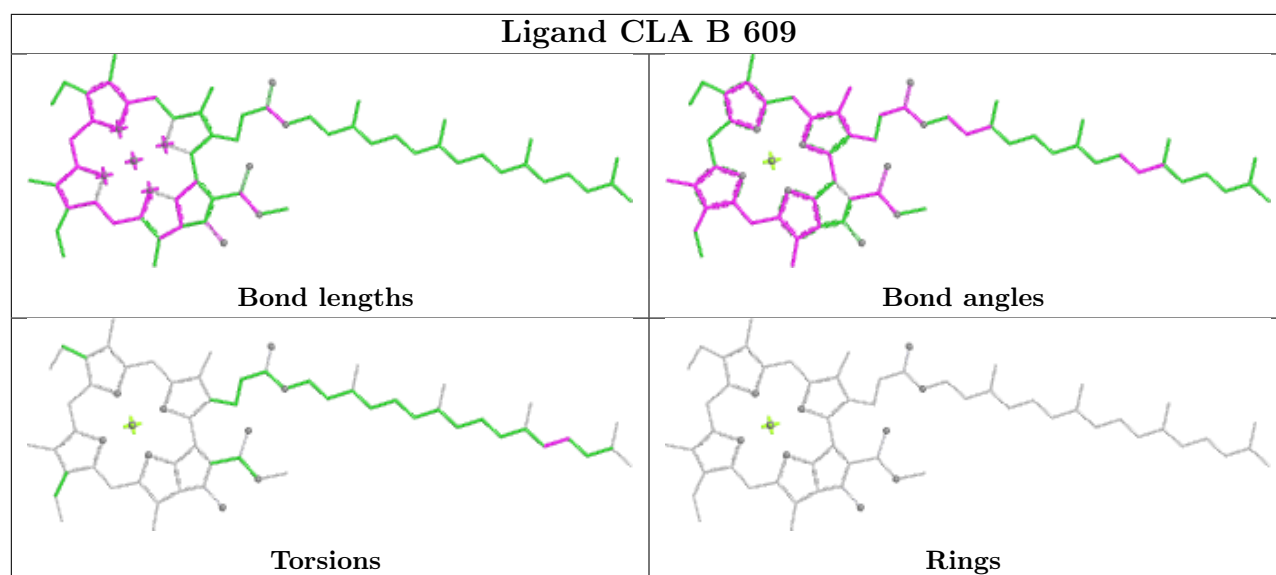
Bond angles

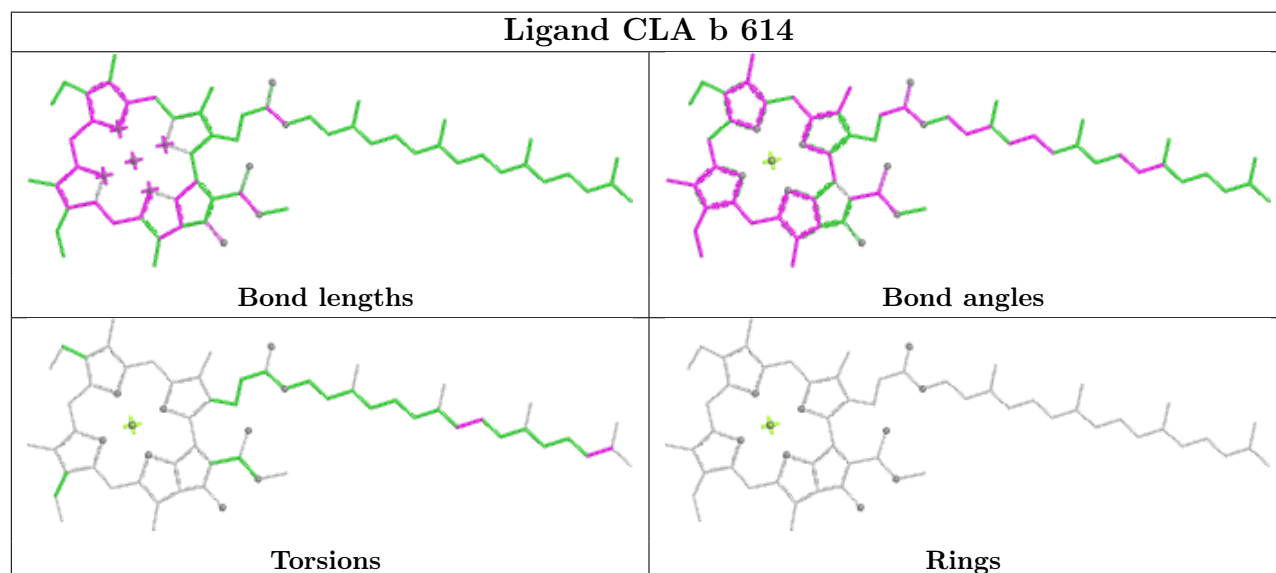
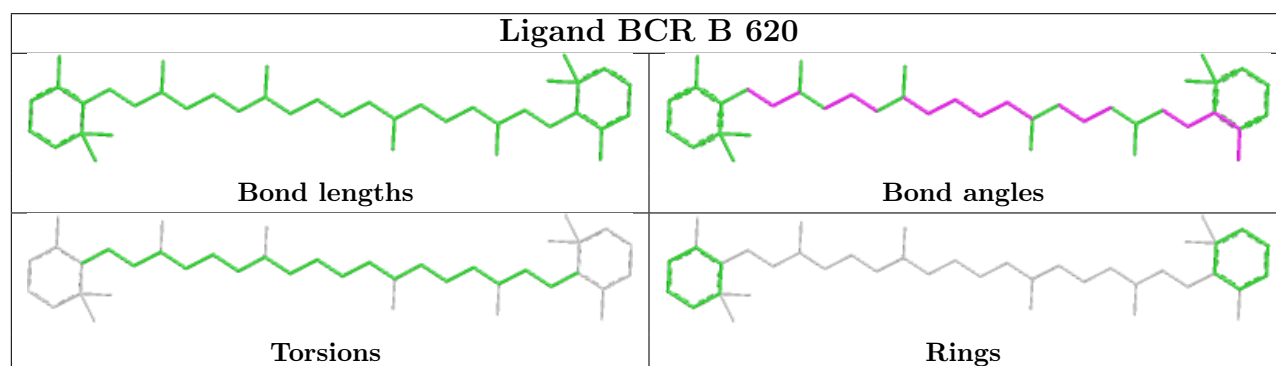
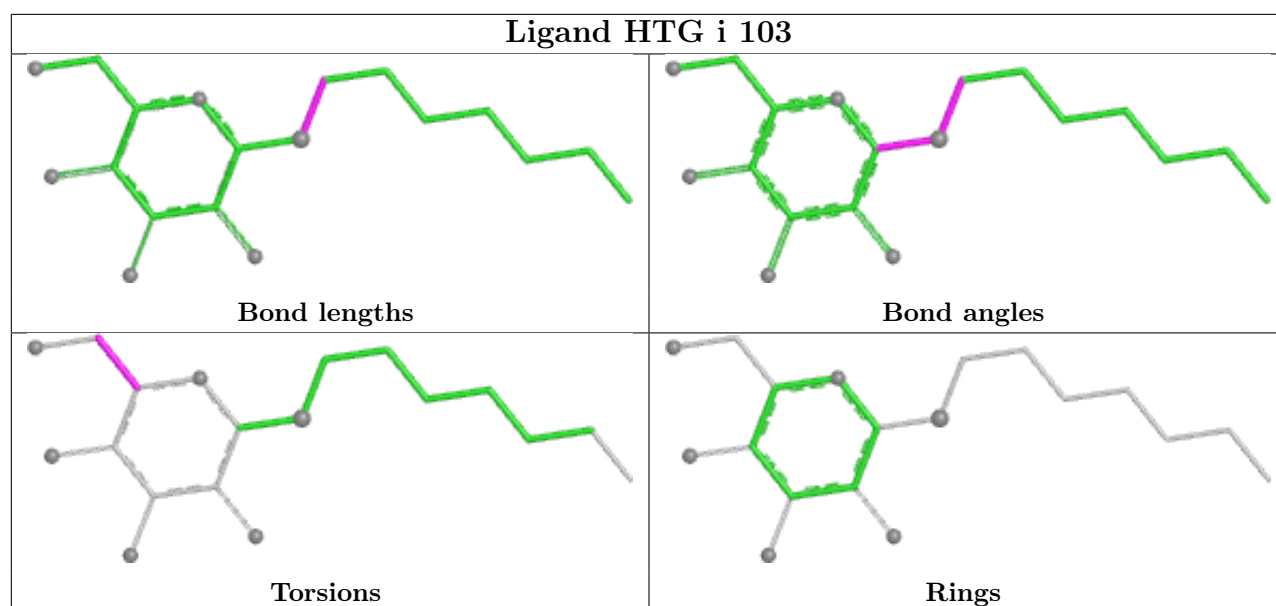


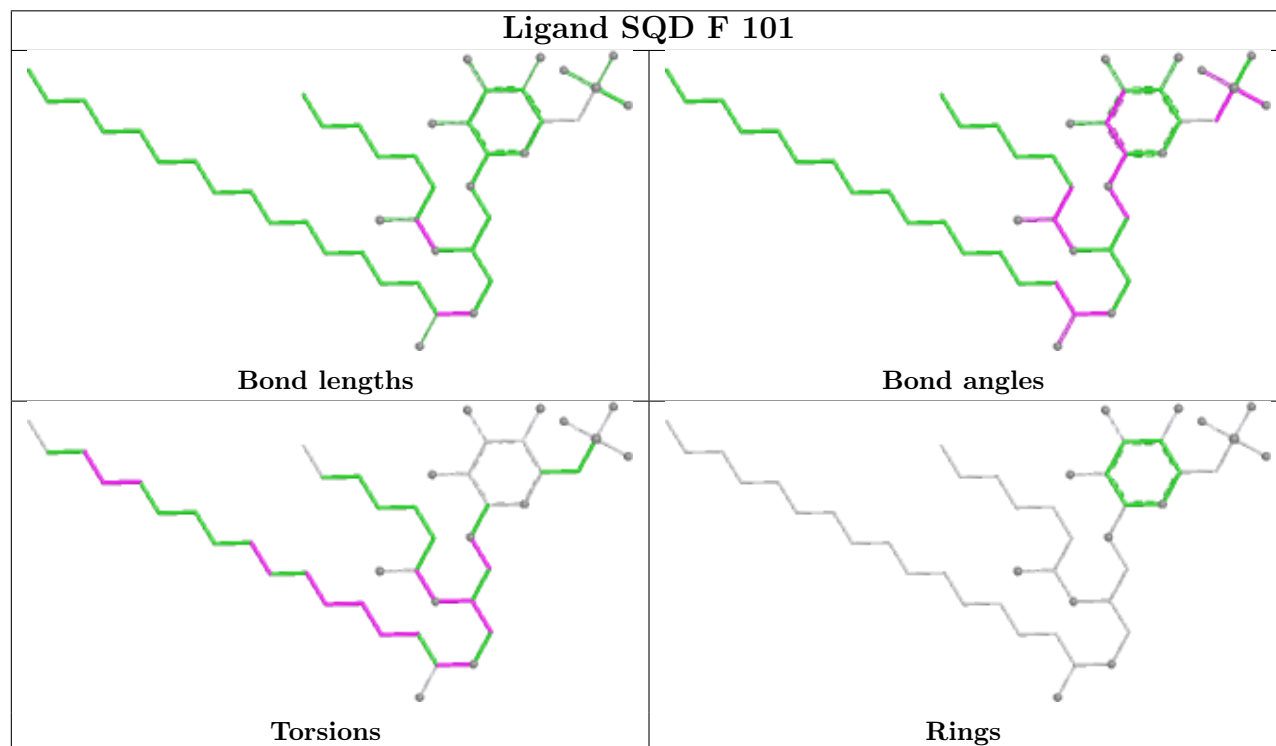
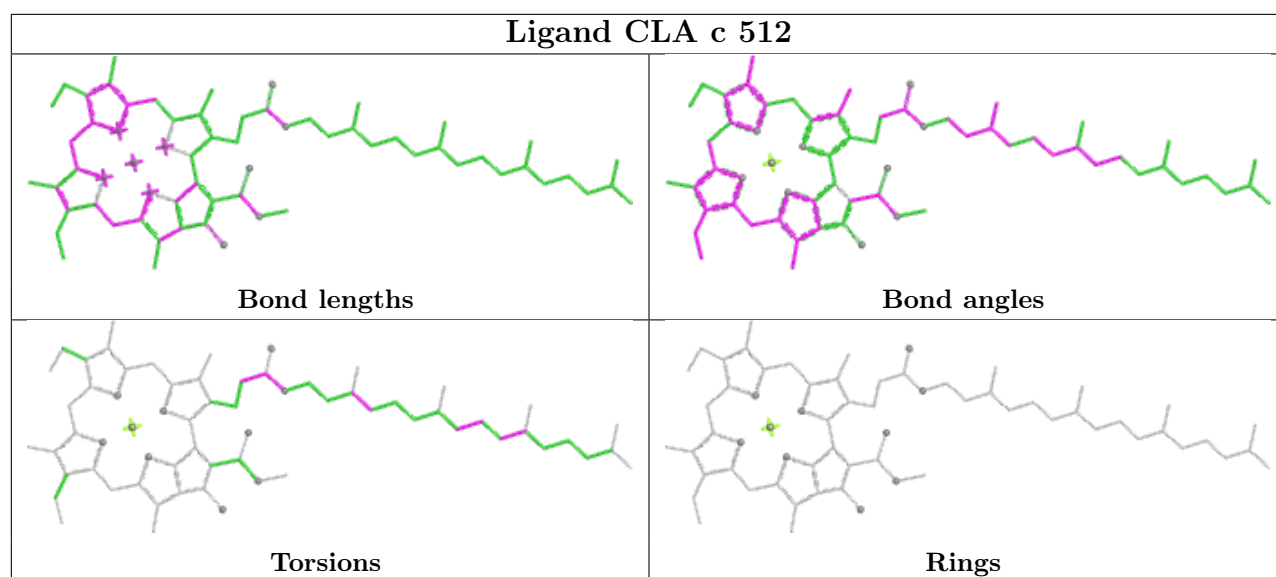
Torsions

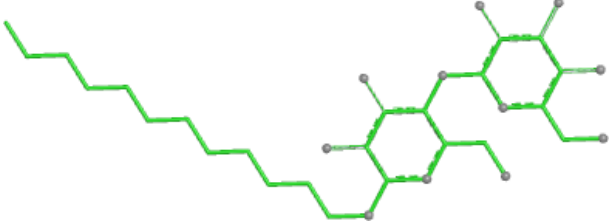
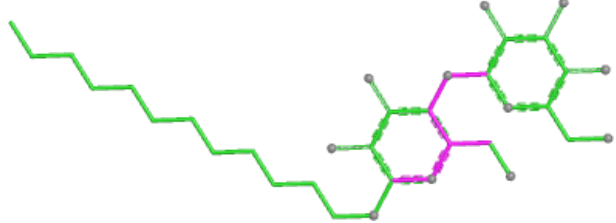
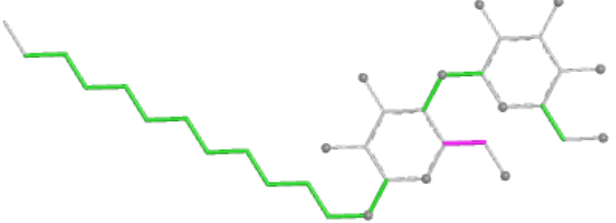
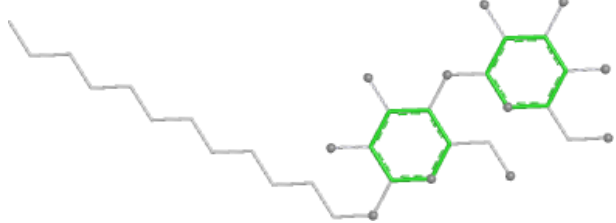
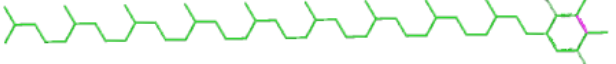
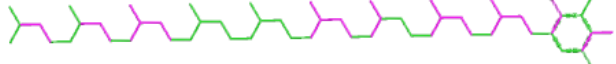
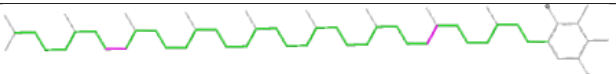
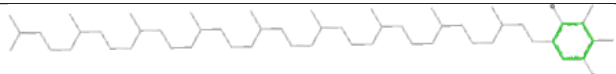
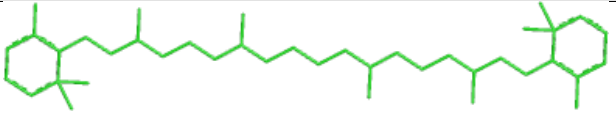
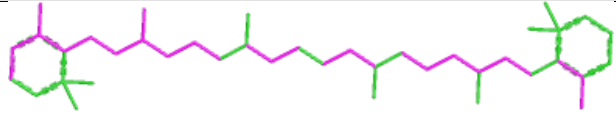
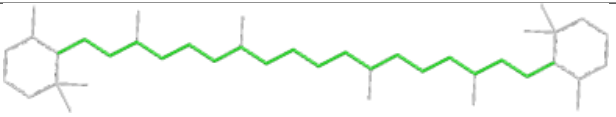
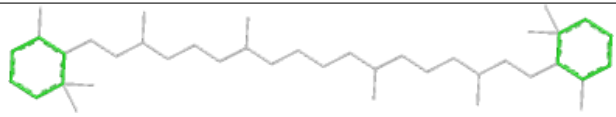


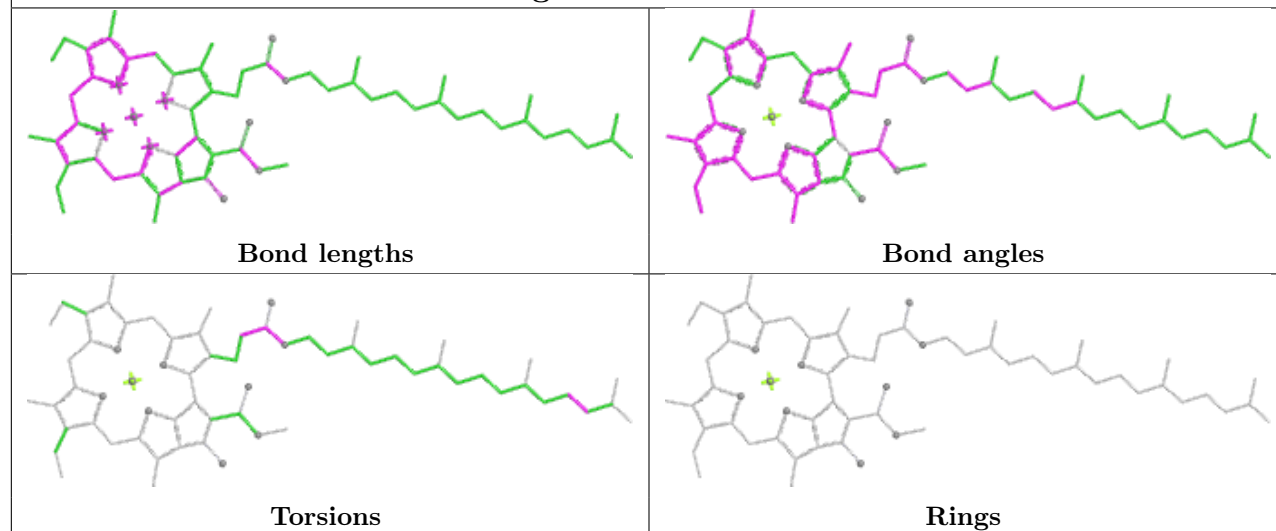
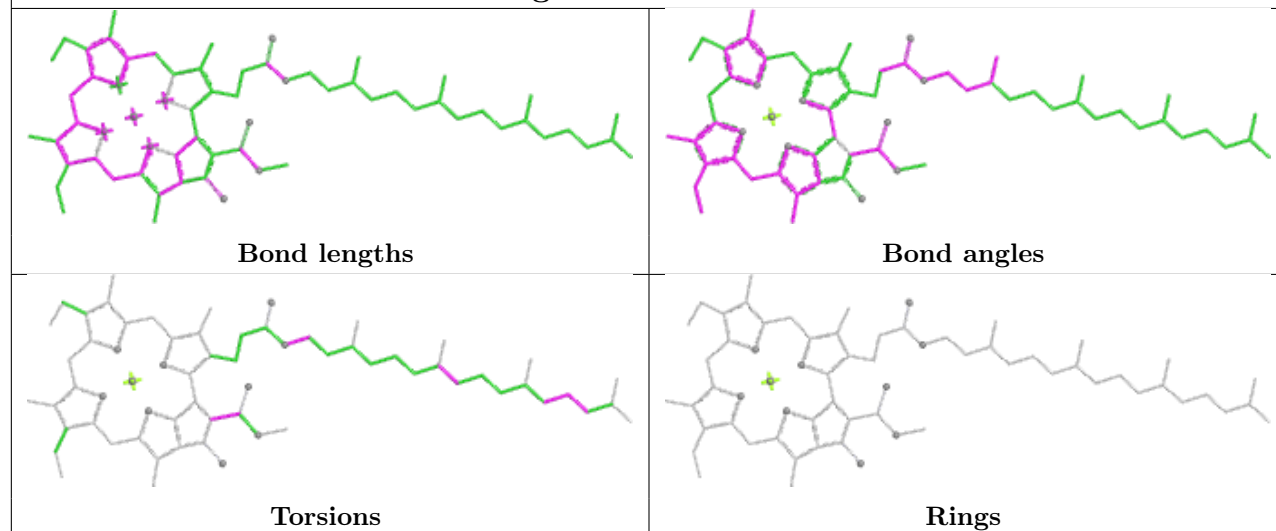
Rings

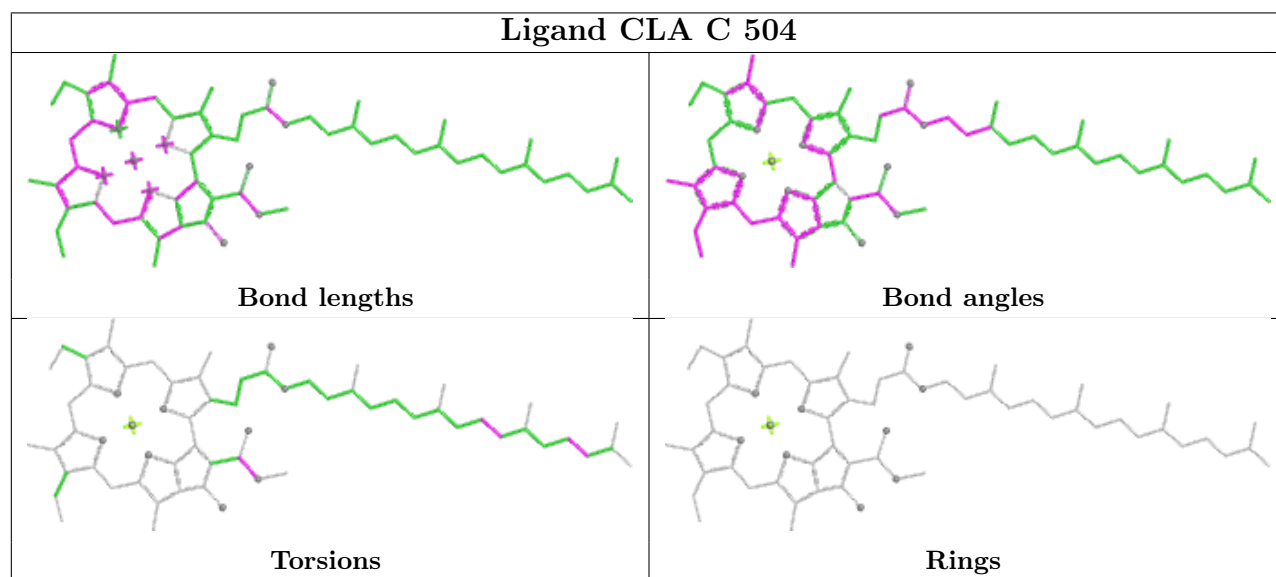
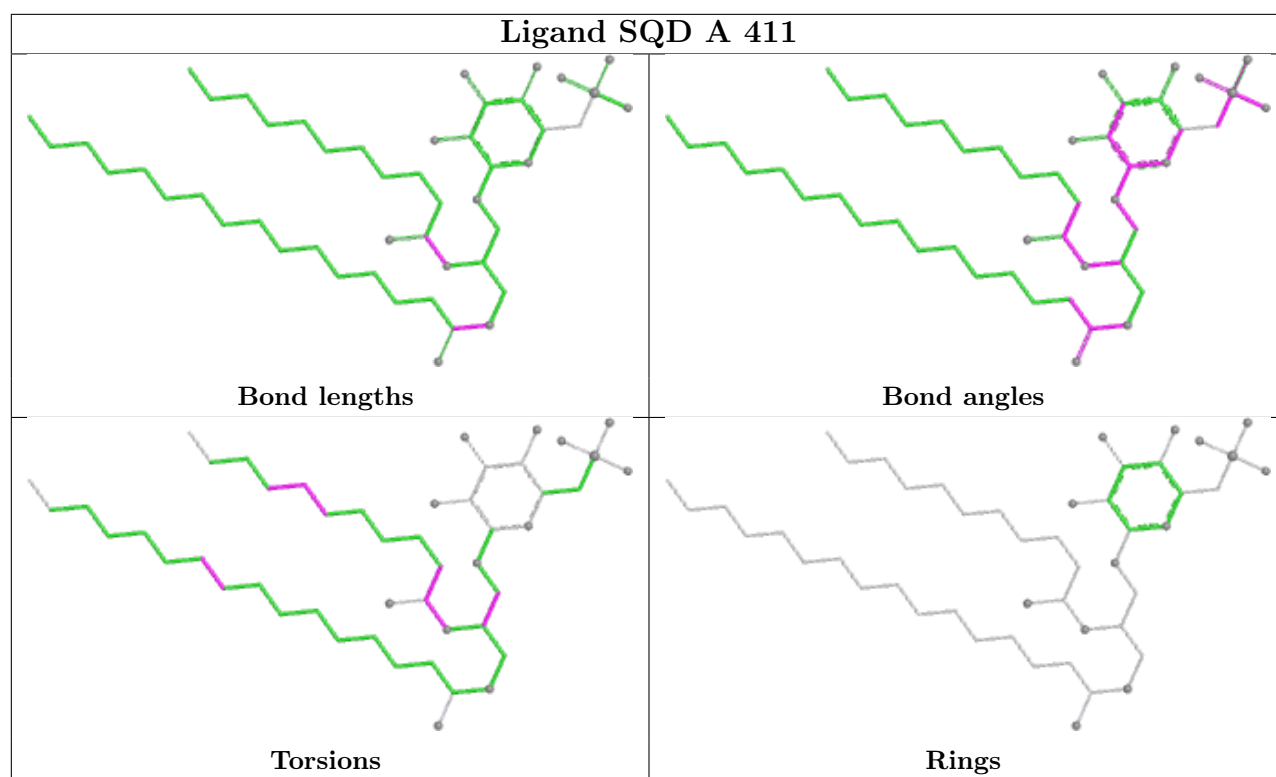


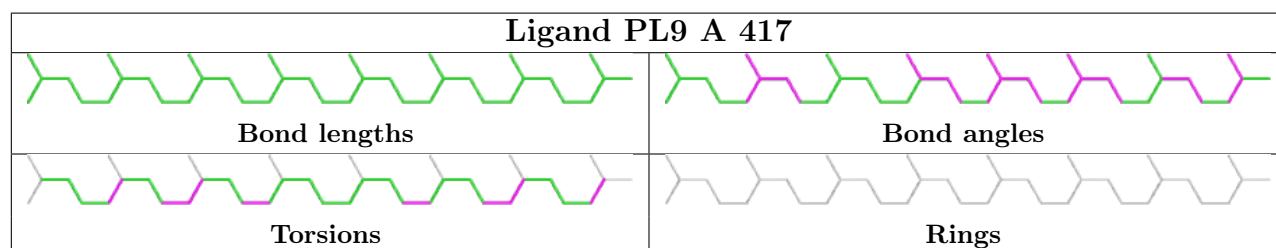
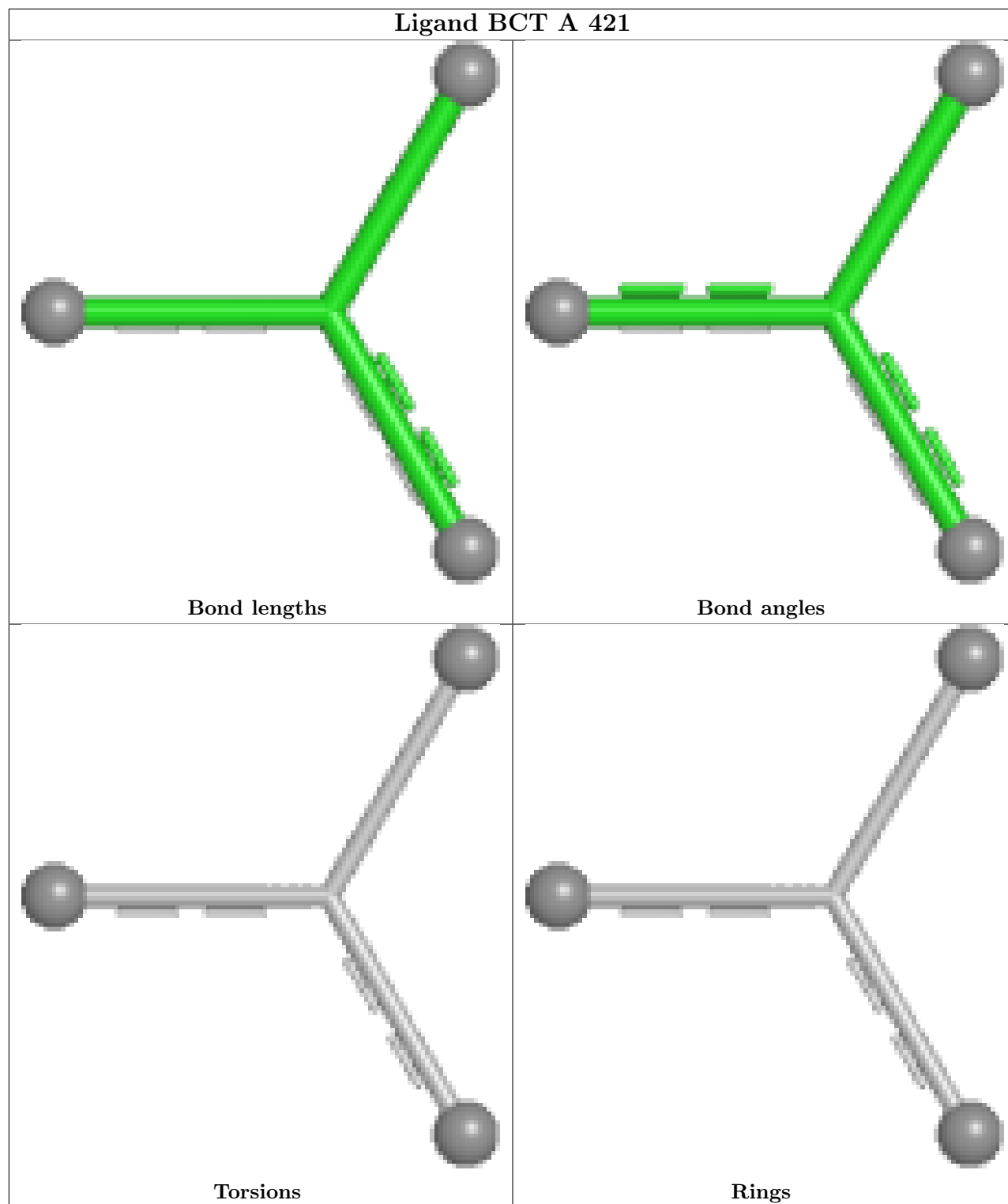


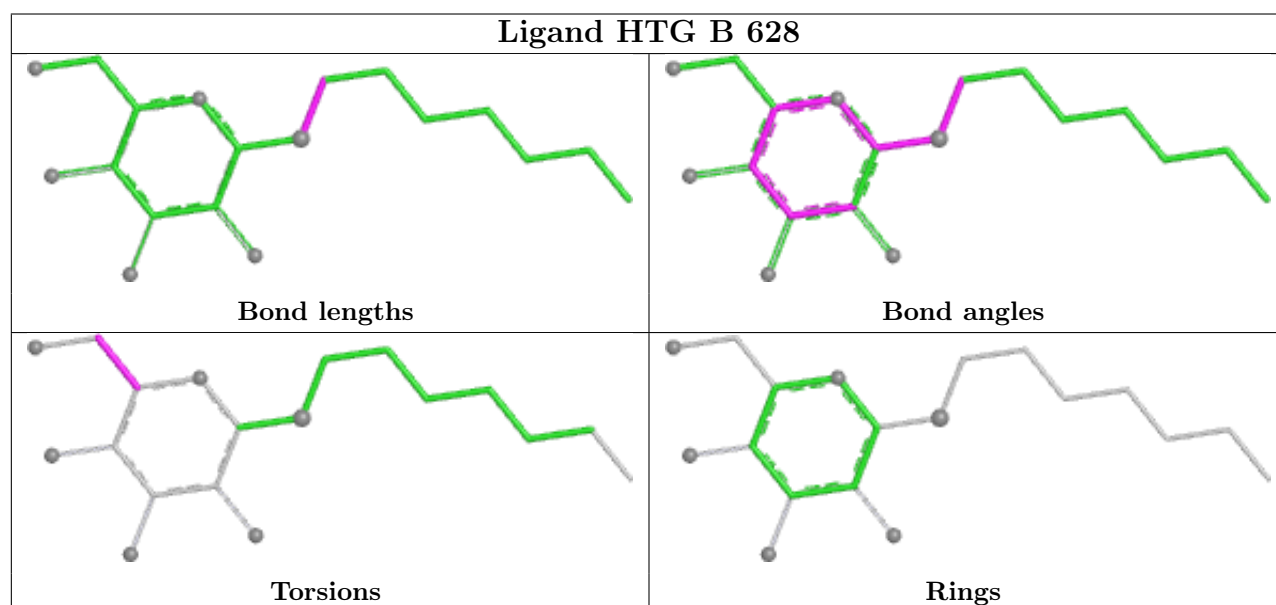
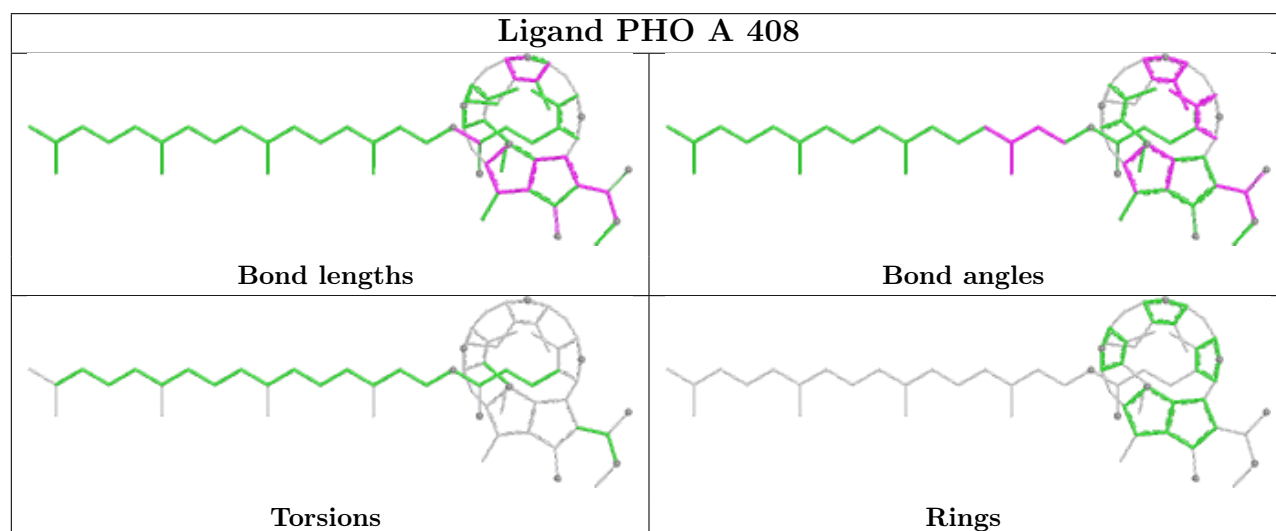
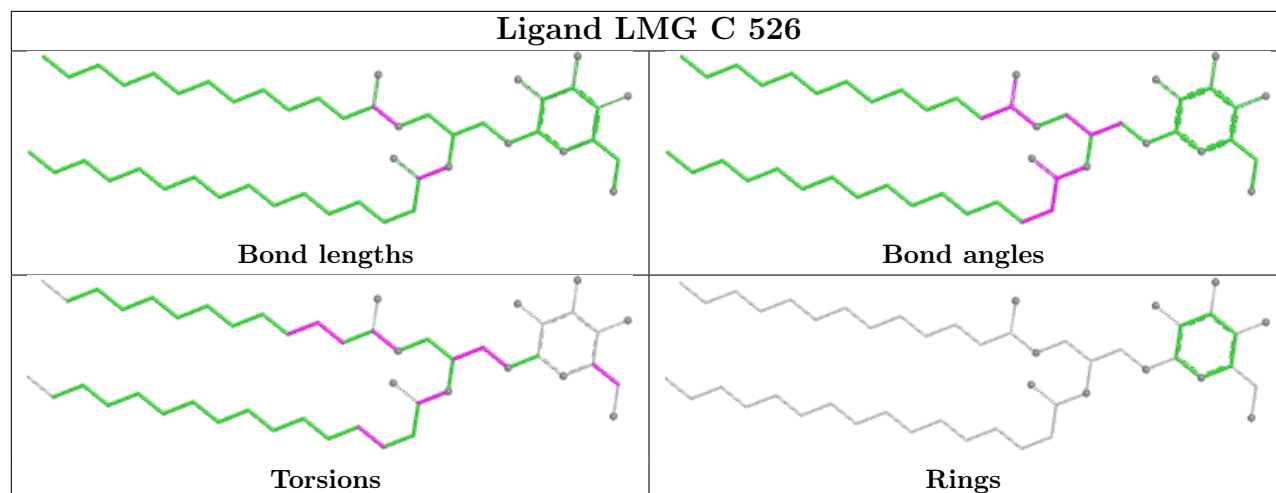


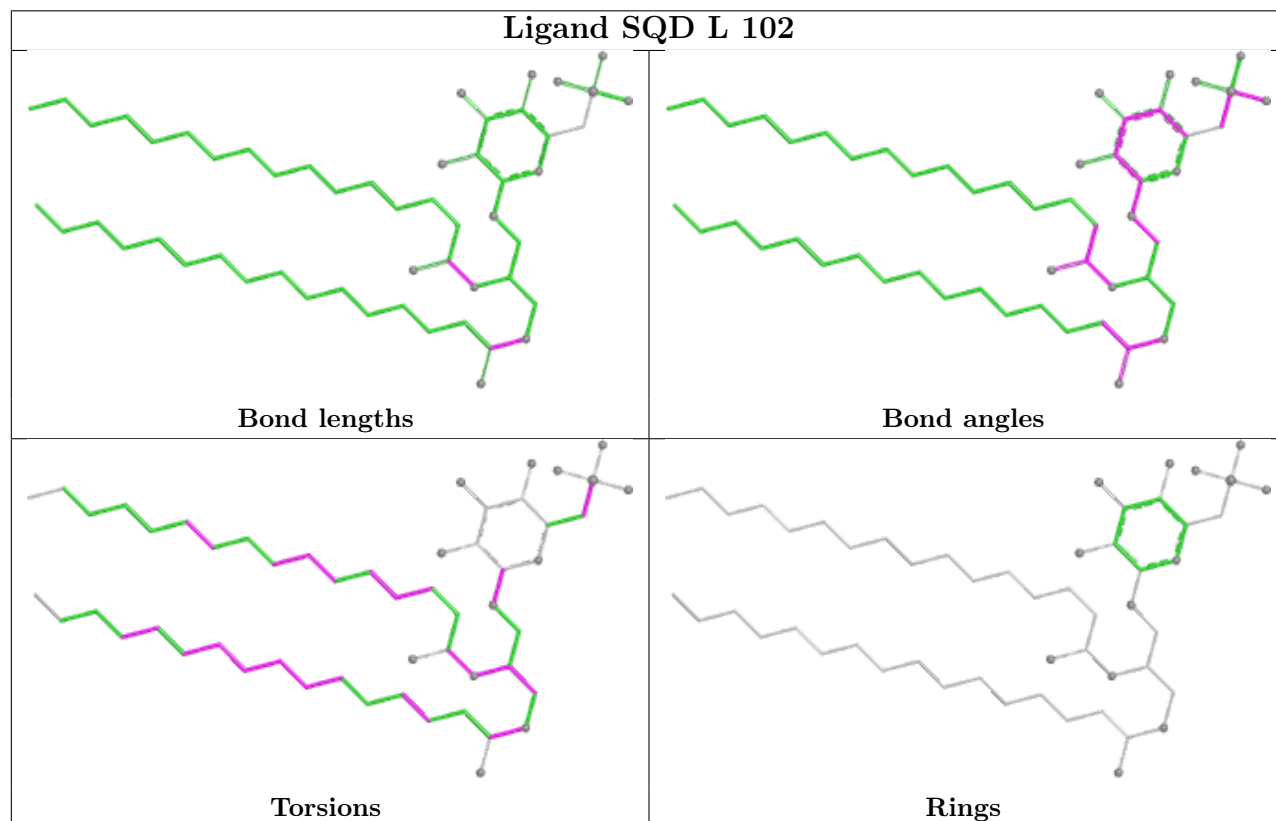
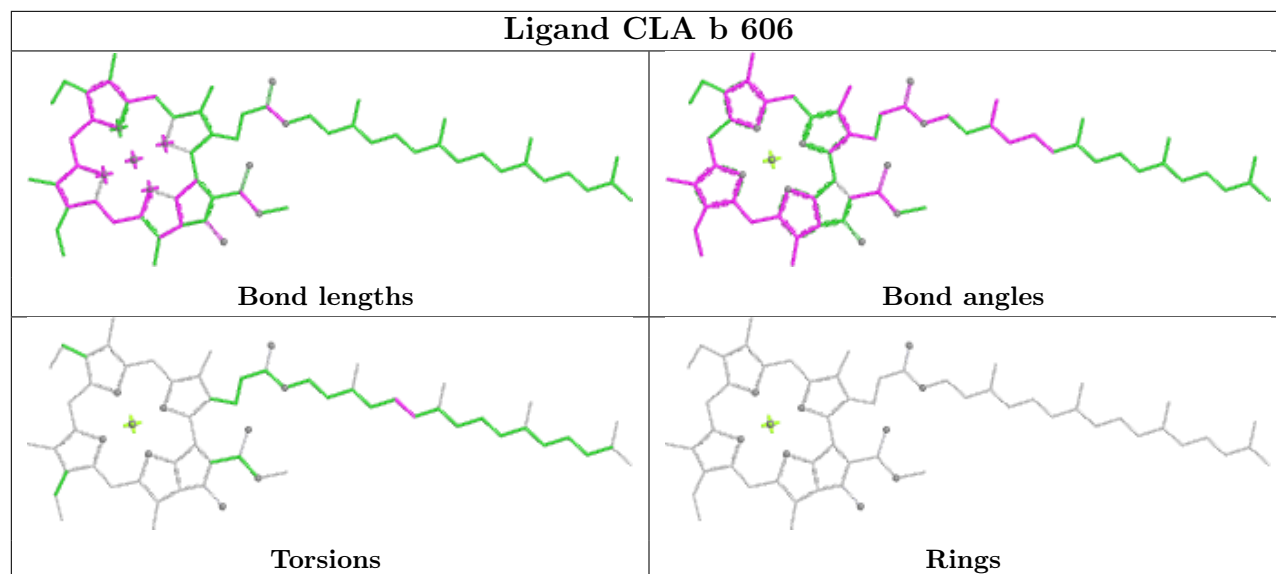
Ligand LMT m 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 d 407	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR k 2003	
 Bond lengths	 Bond angles
 Torsions	 Rings

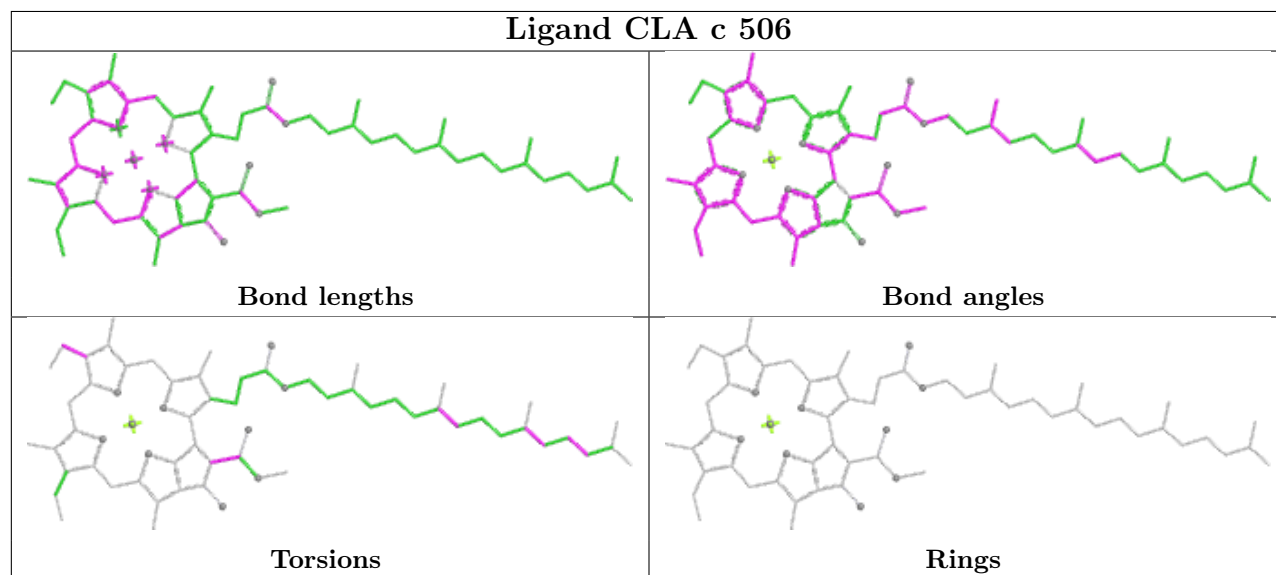
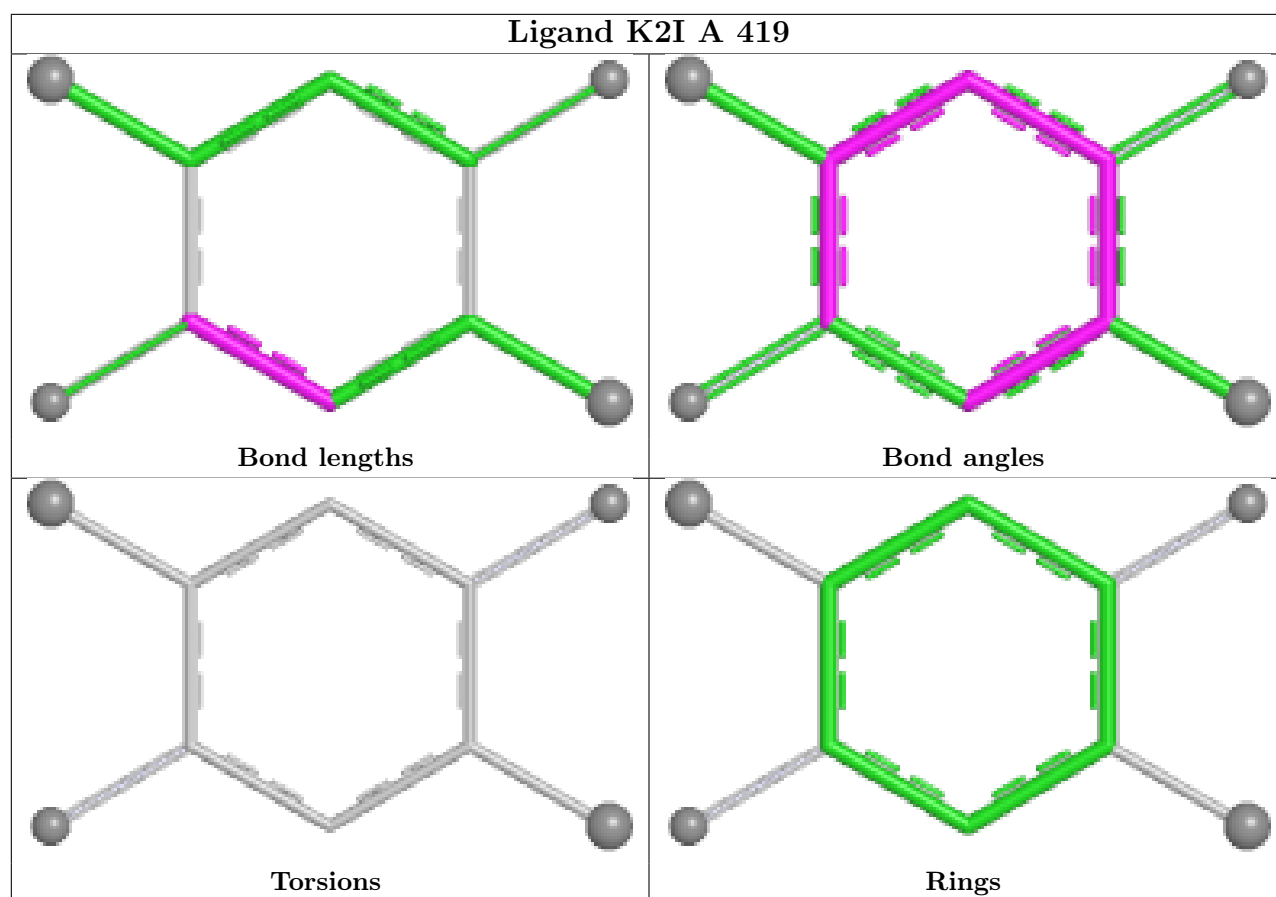
Ligand CLA C 513**Ligand CLA C 510**

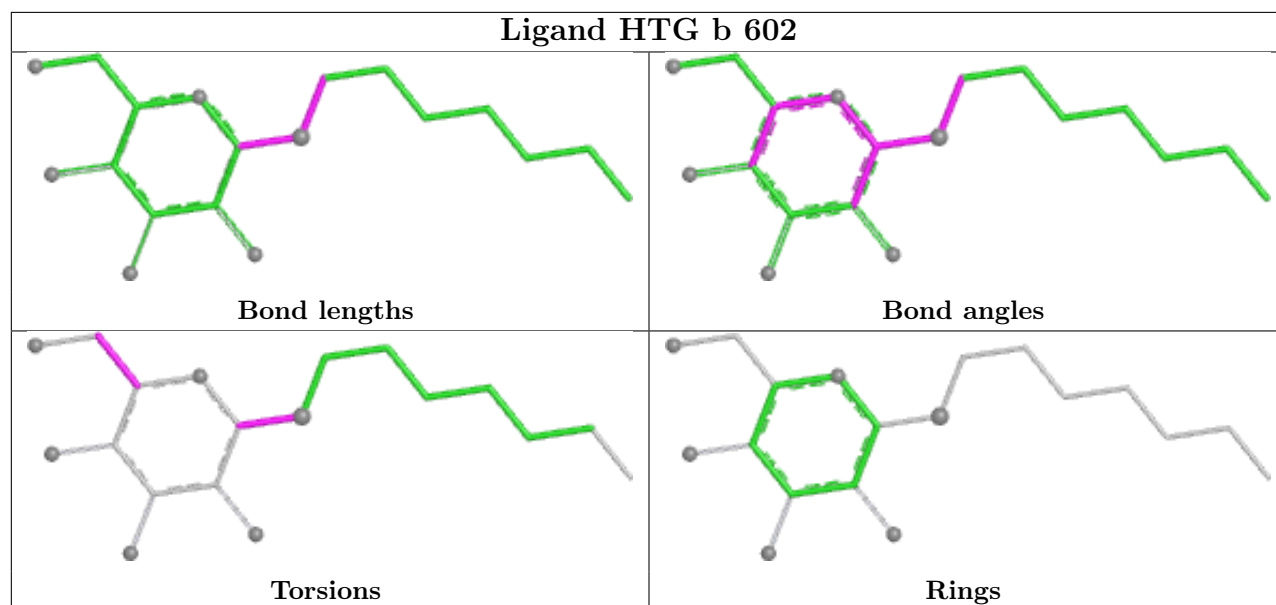
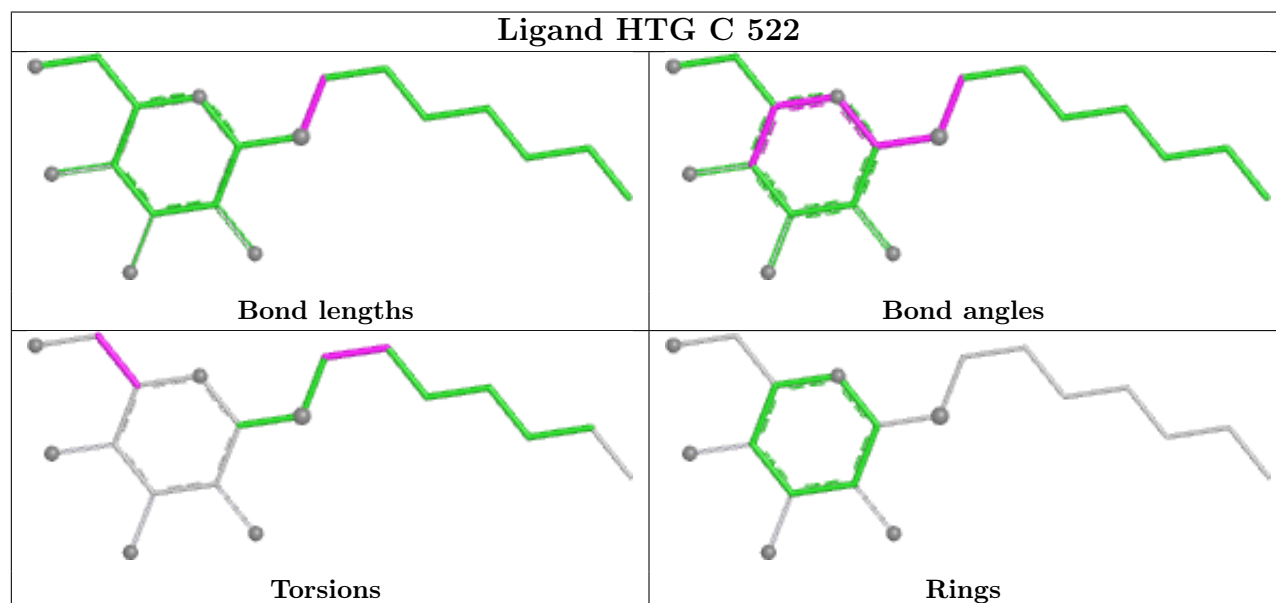
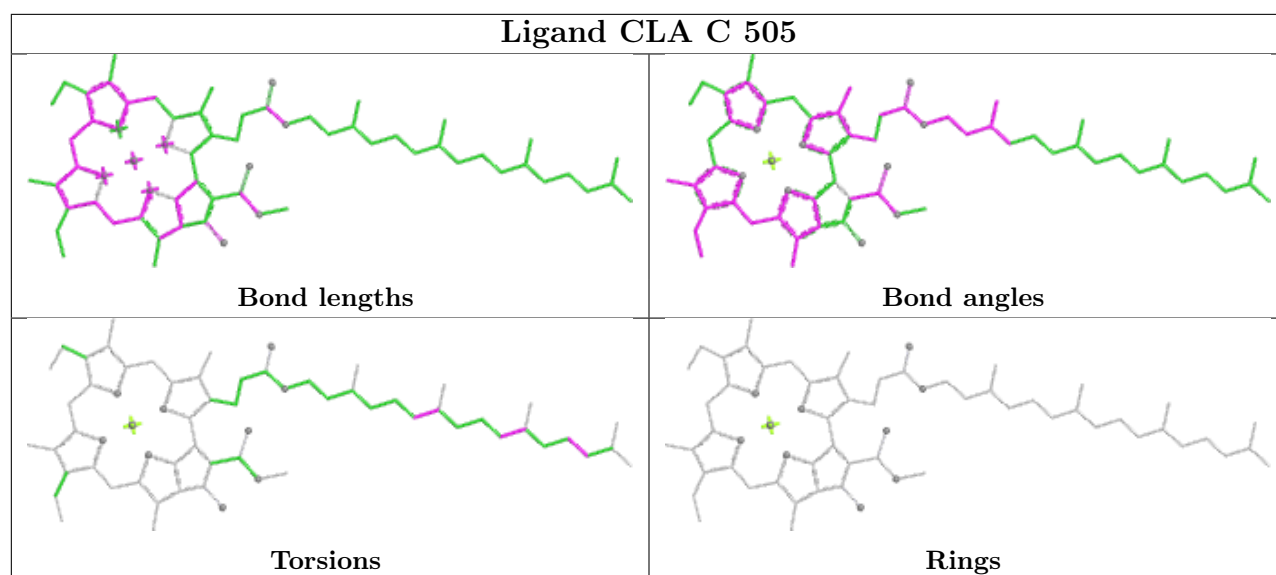




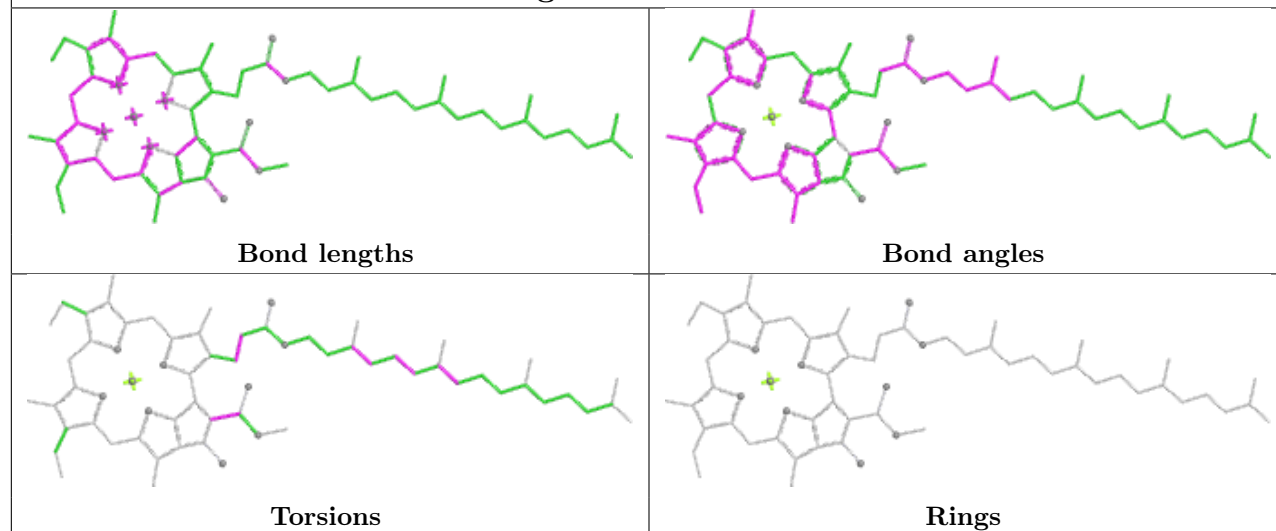




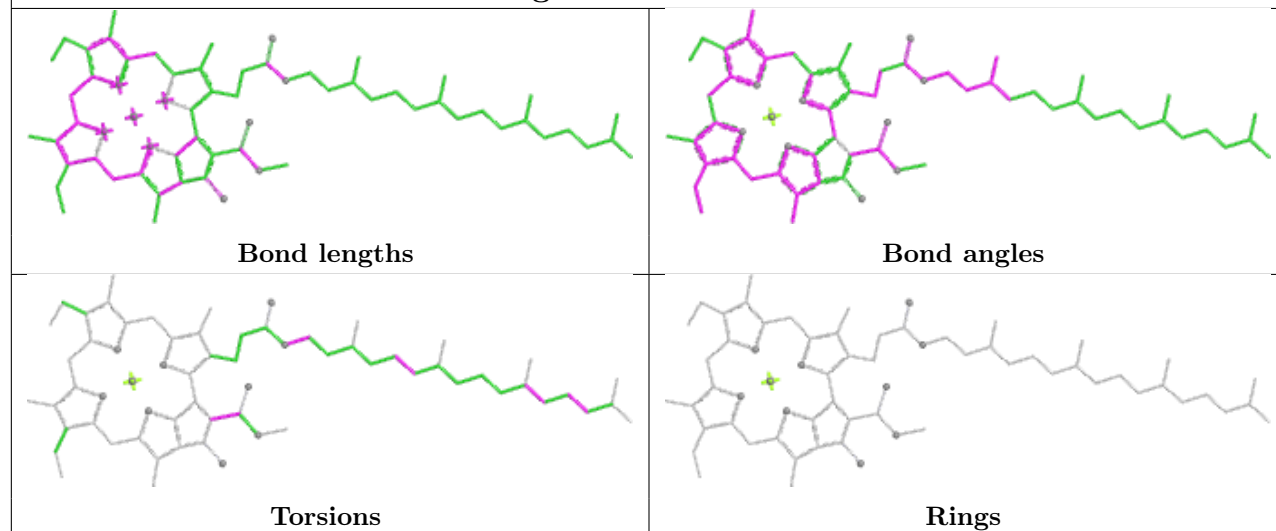




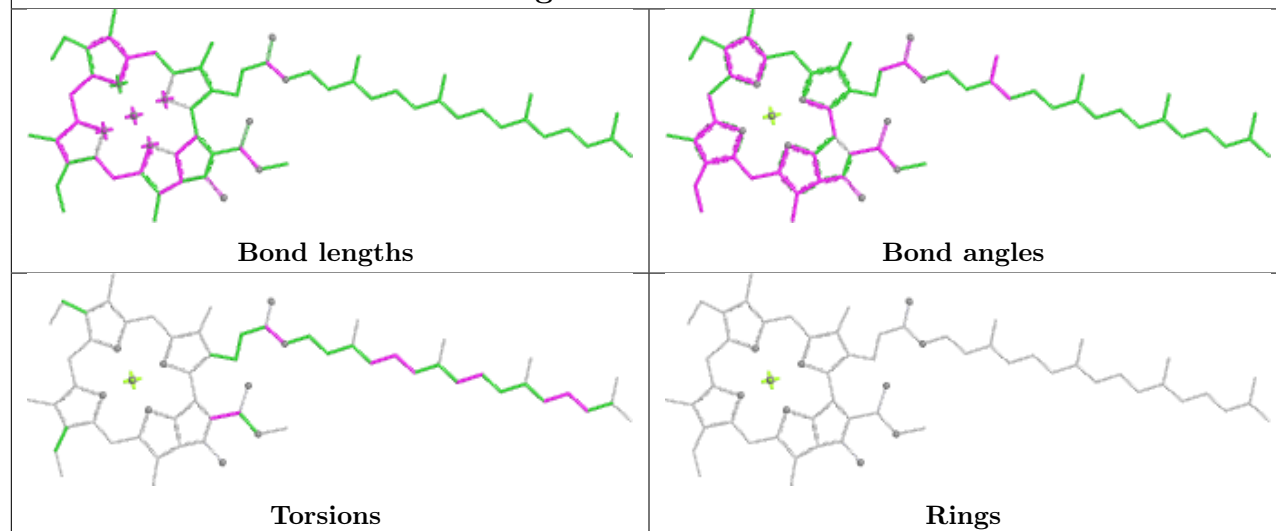
Ligand CLA c 509

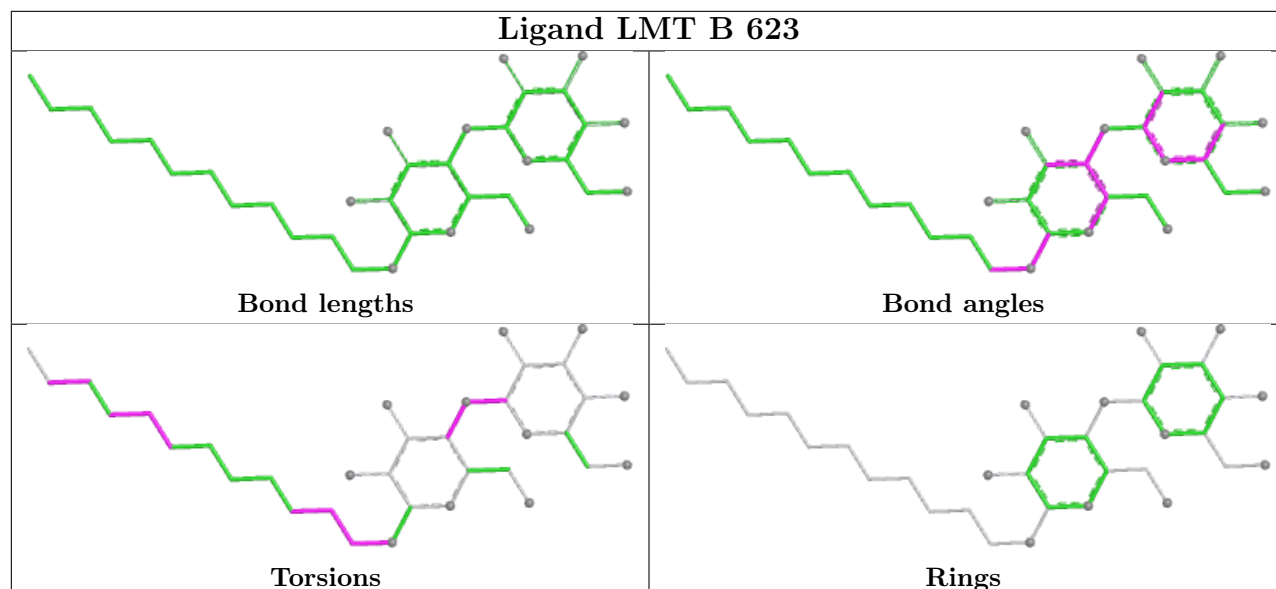
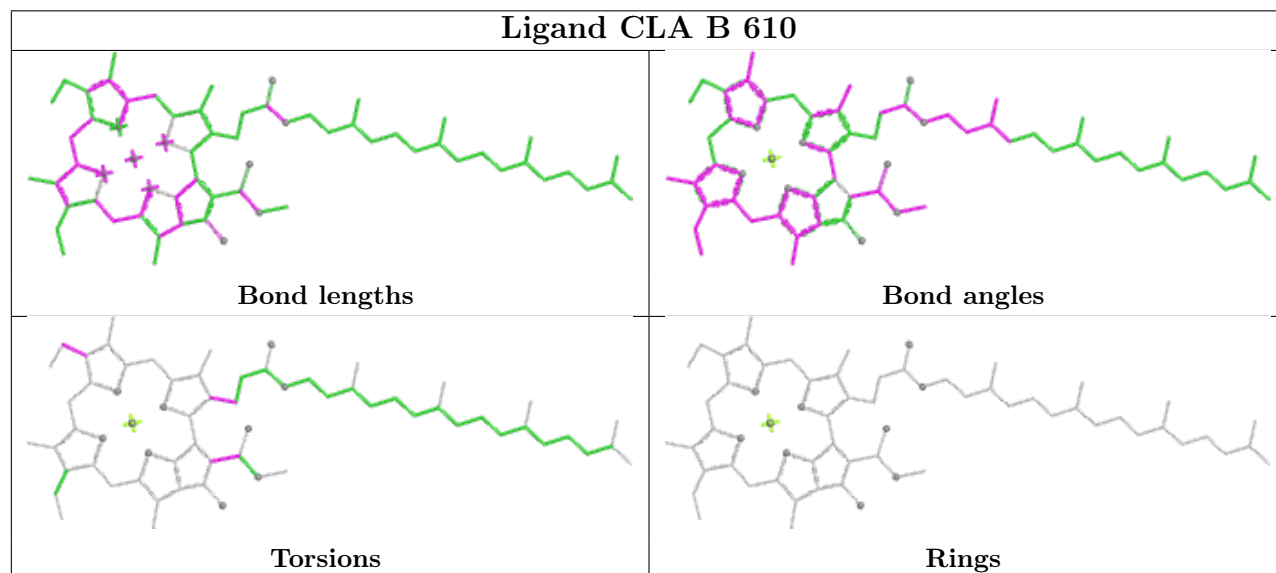
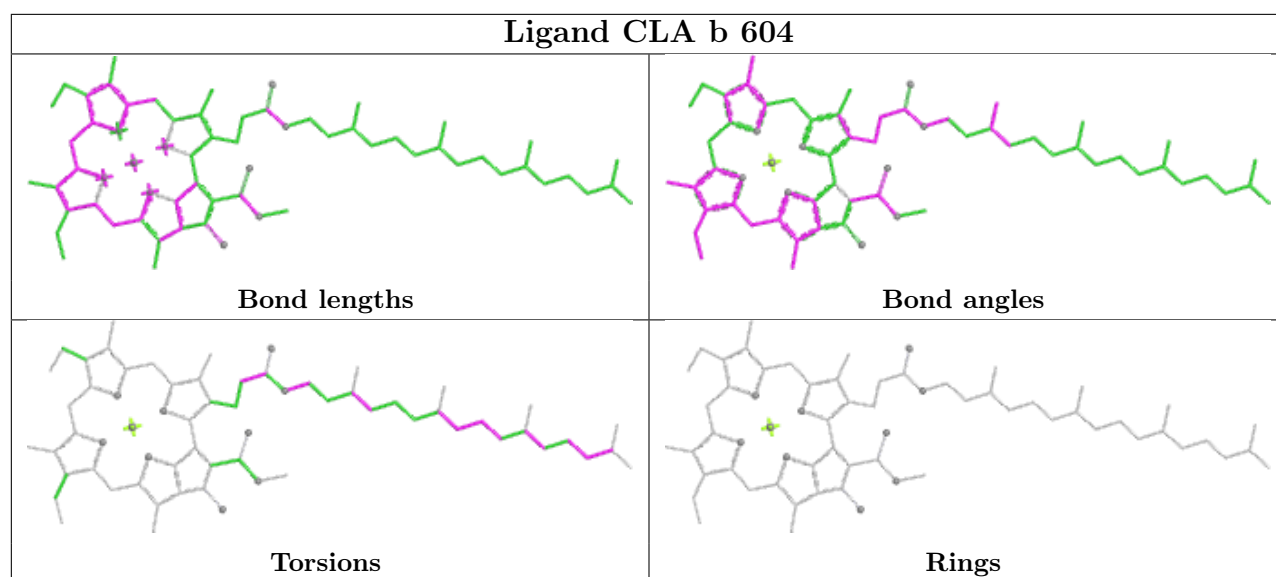


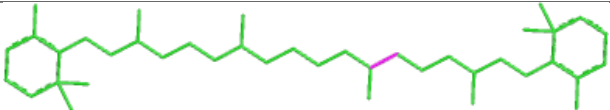
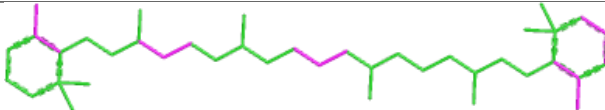
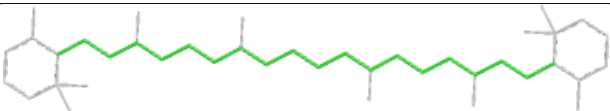
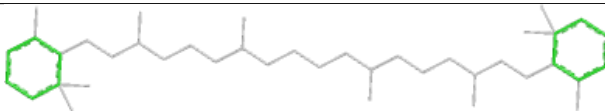
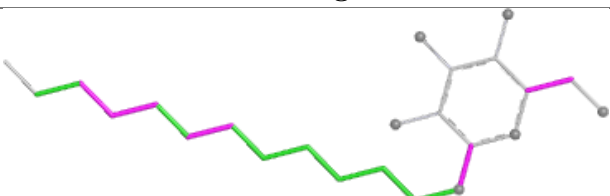
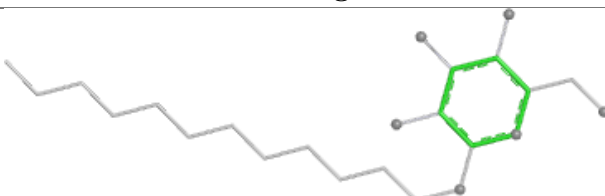
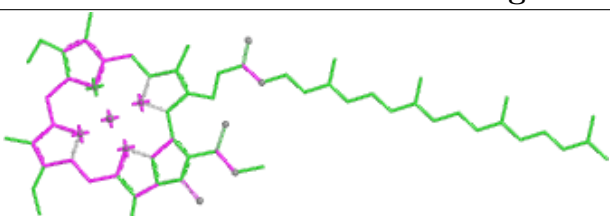
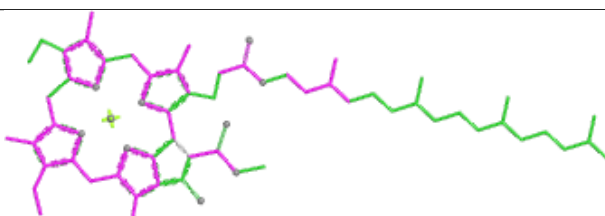
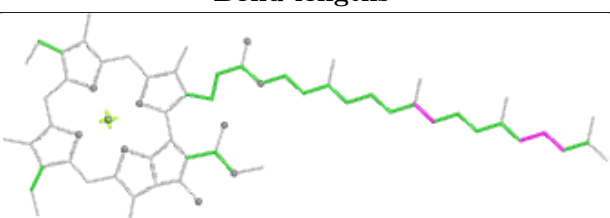
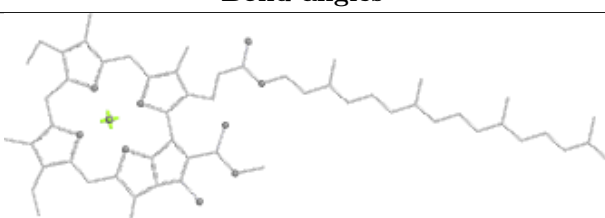
Ligand CLA C 508

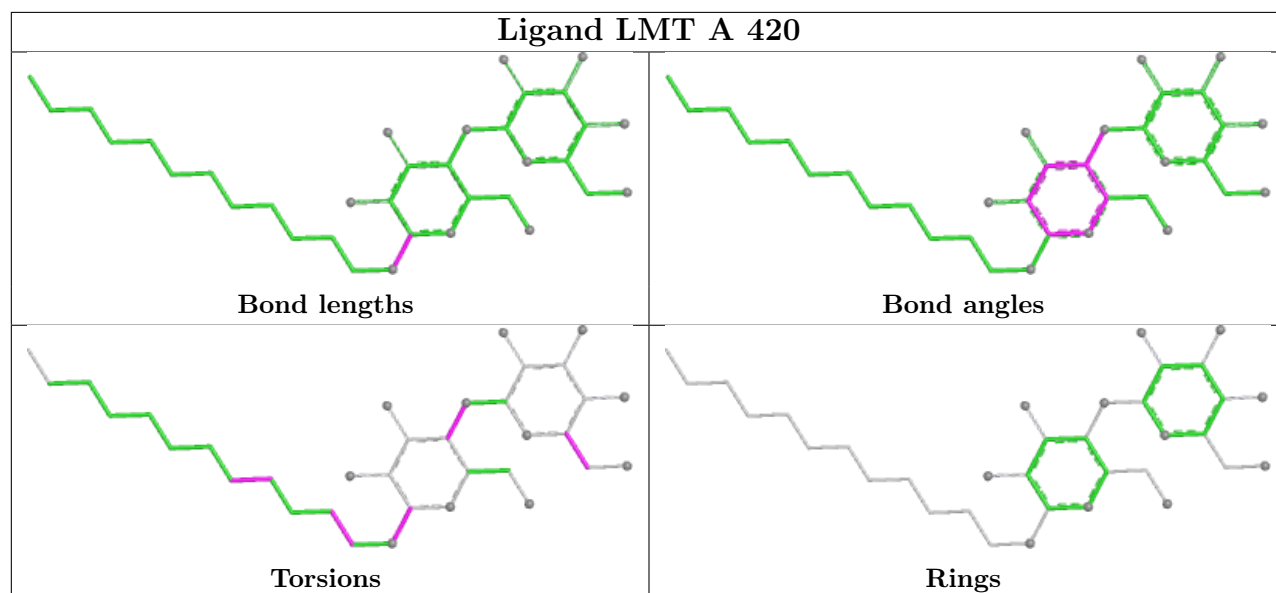
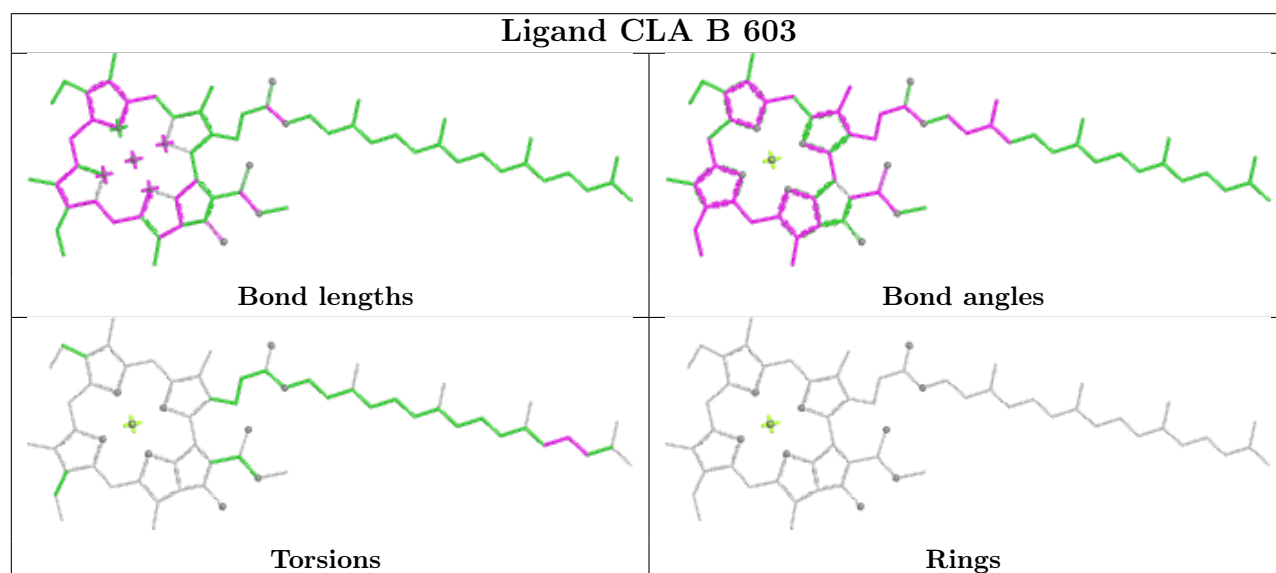
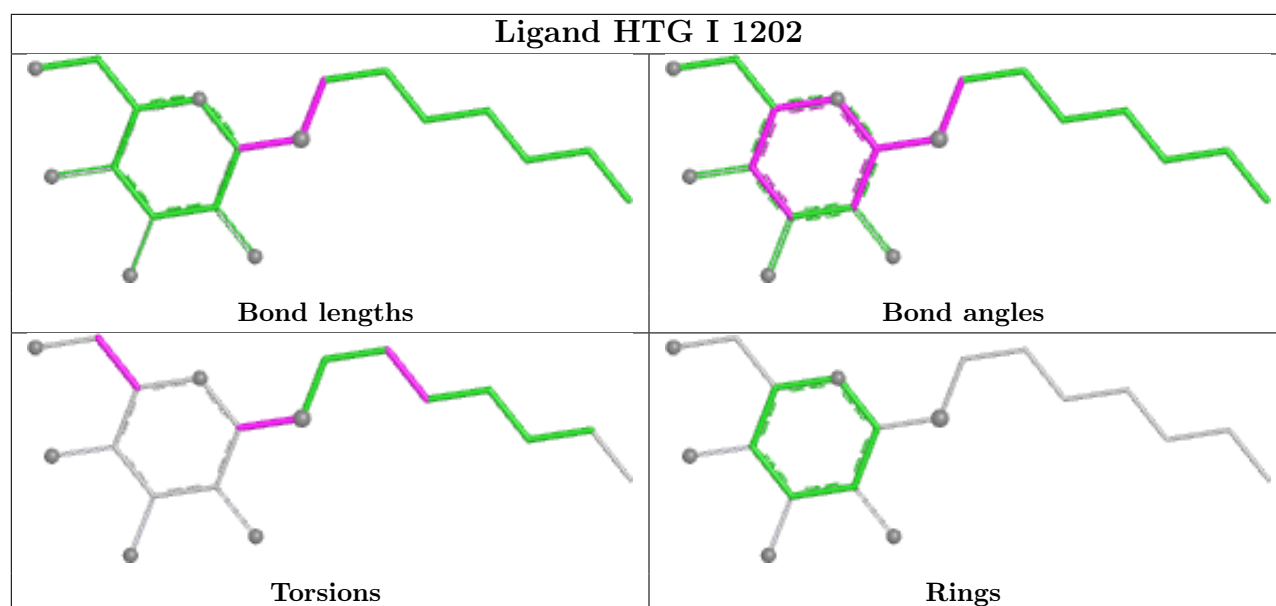


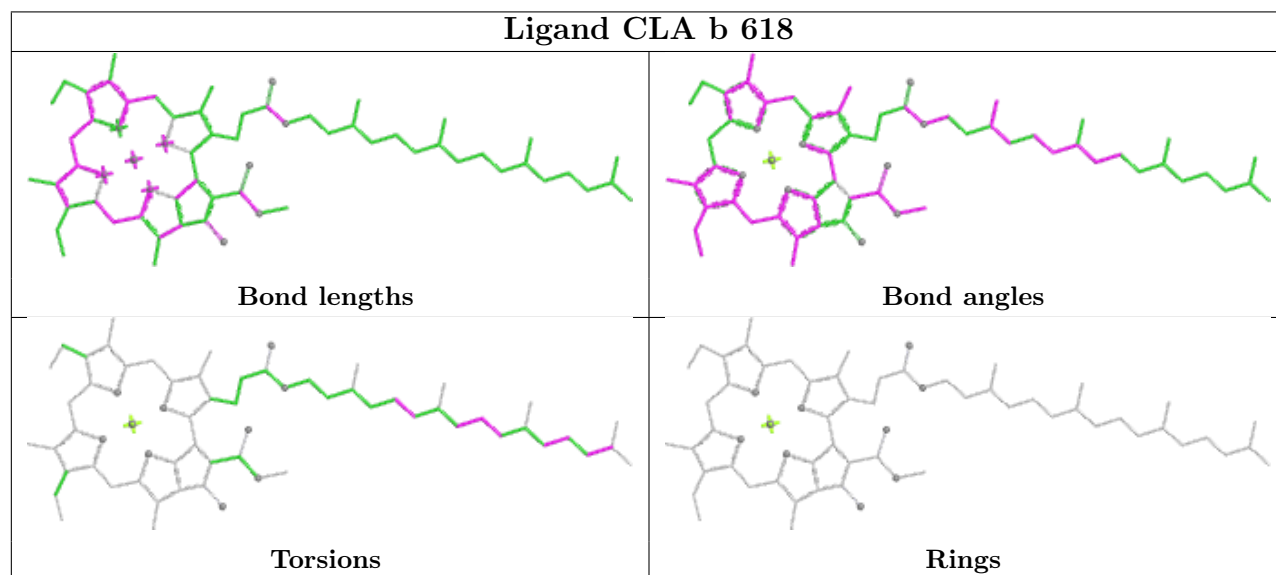
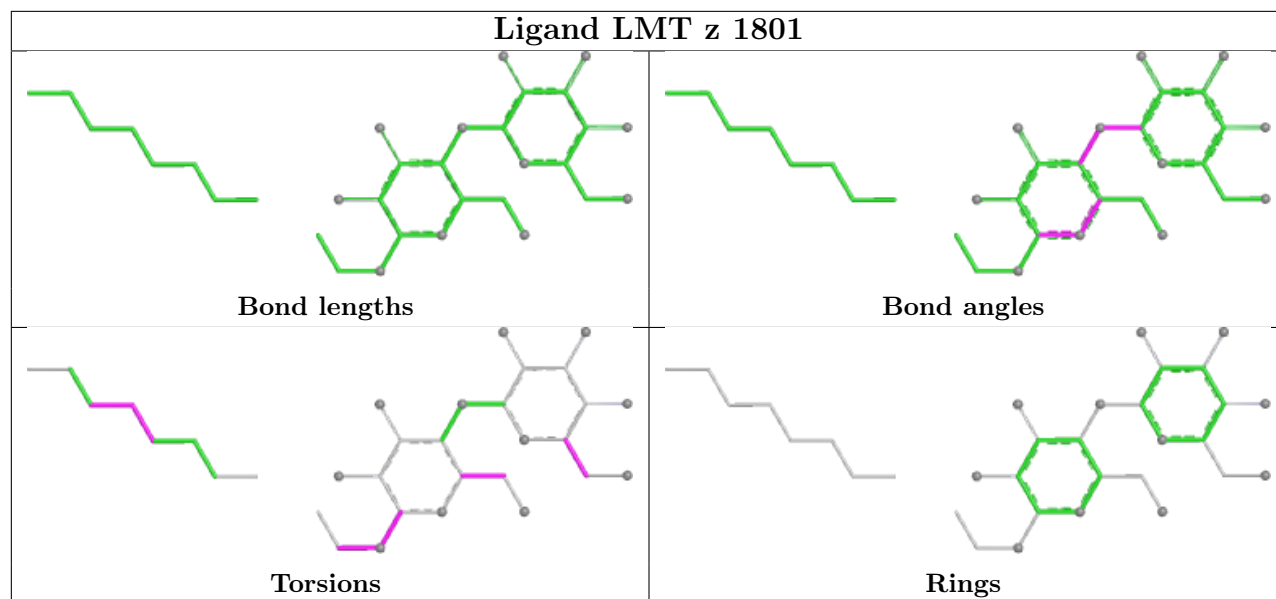
Ligand CLA b 619

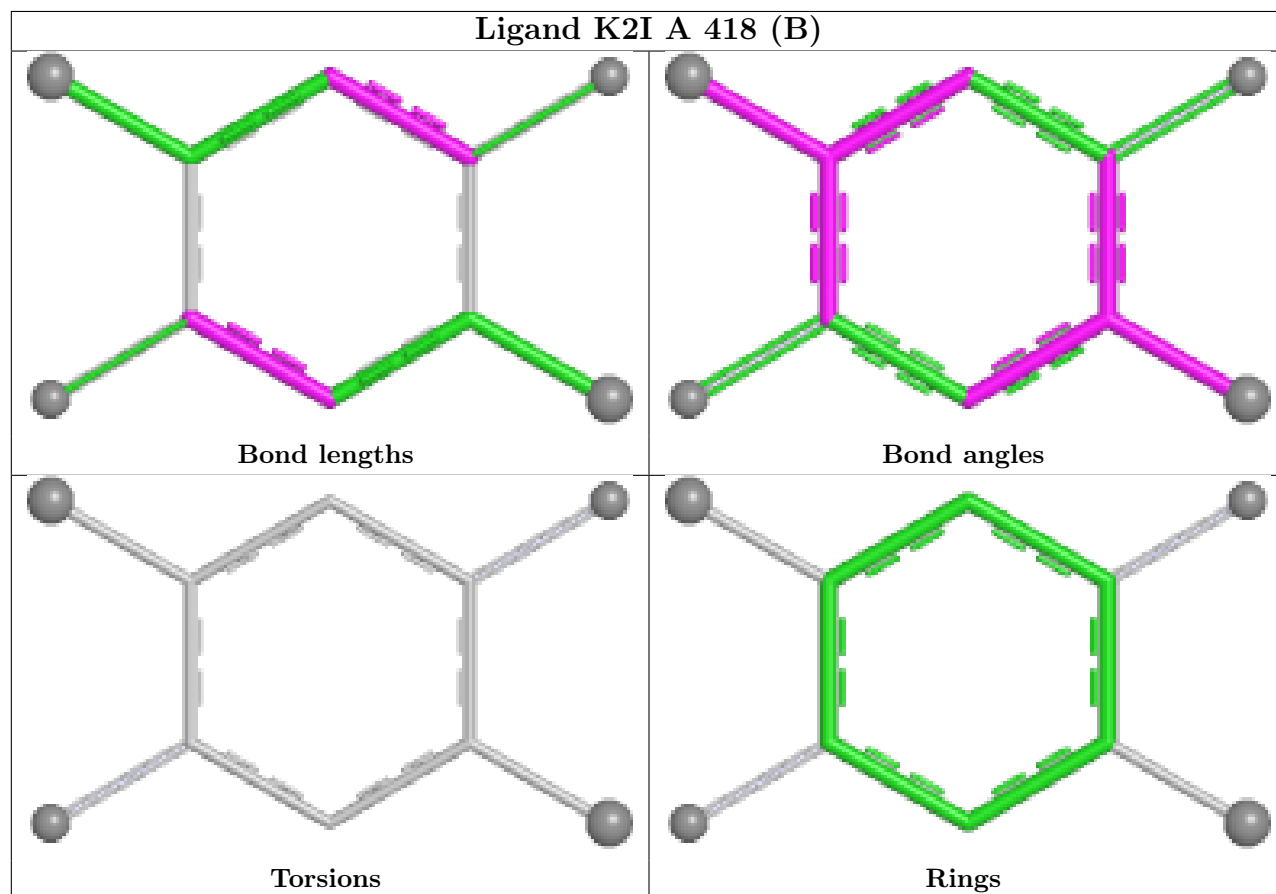
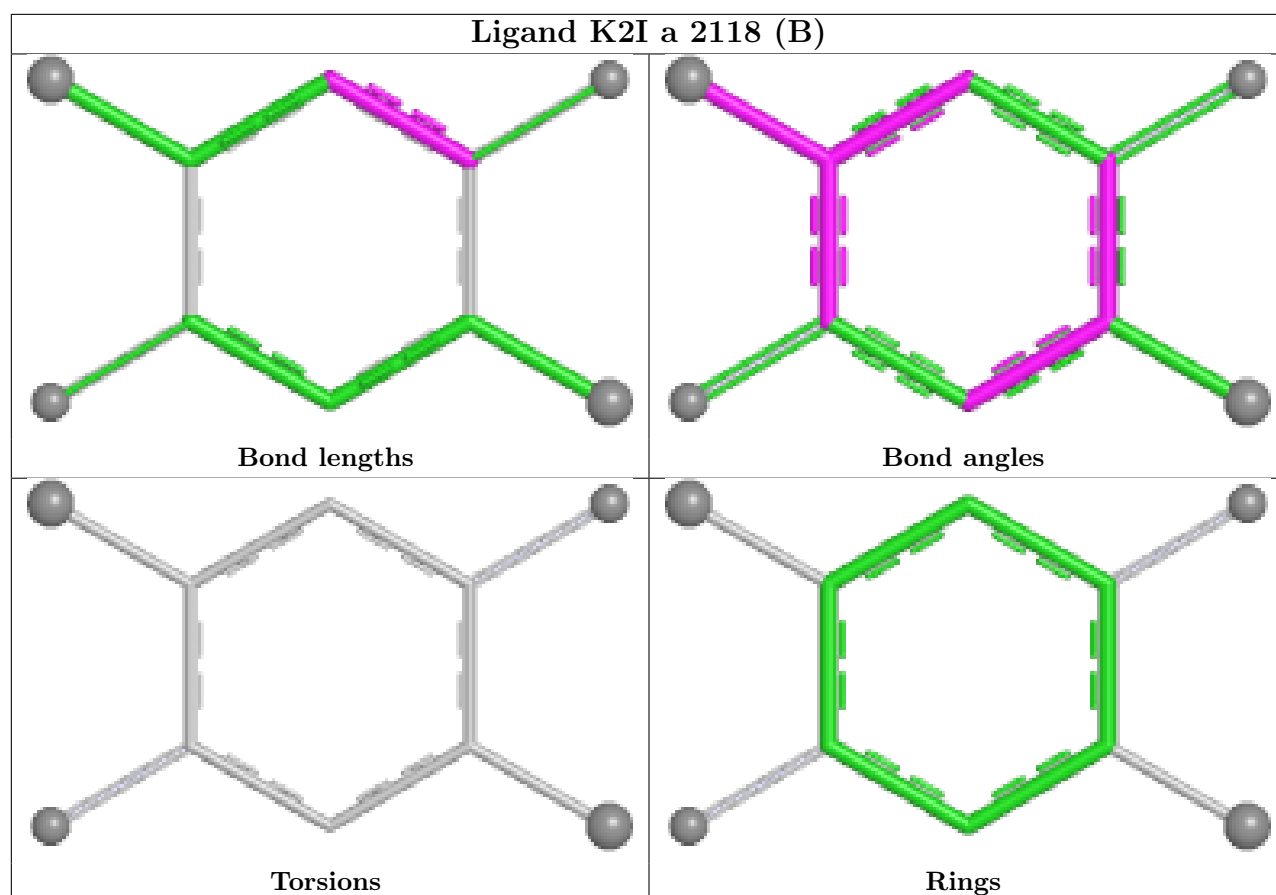


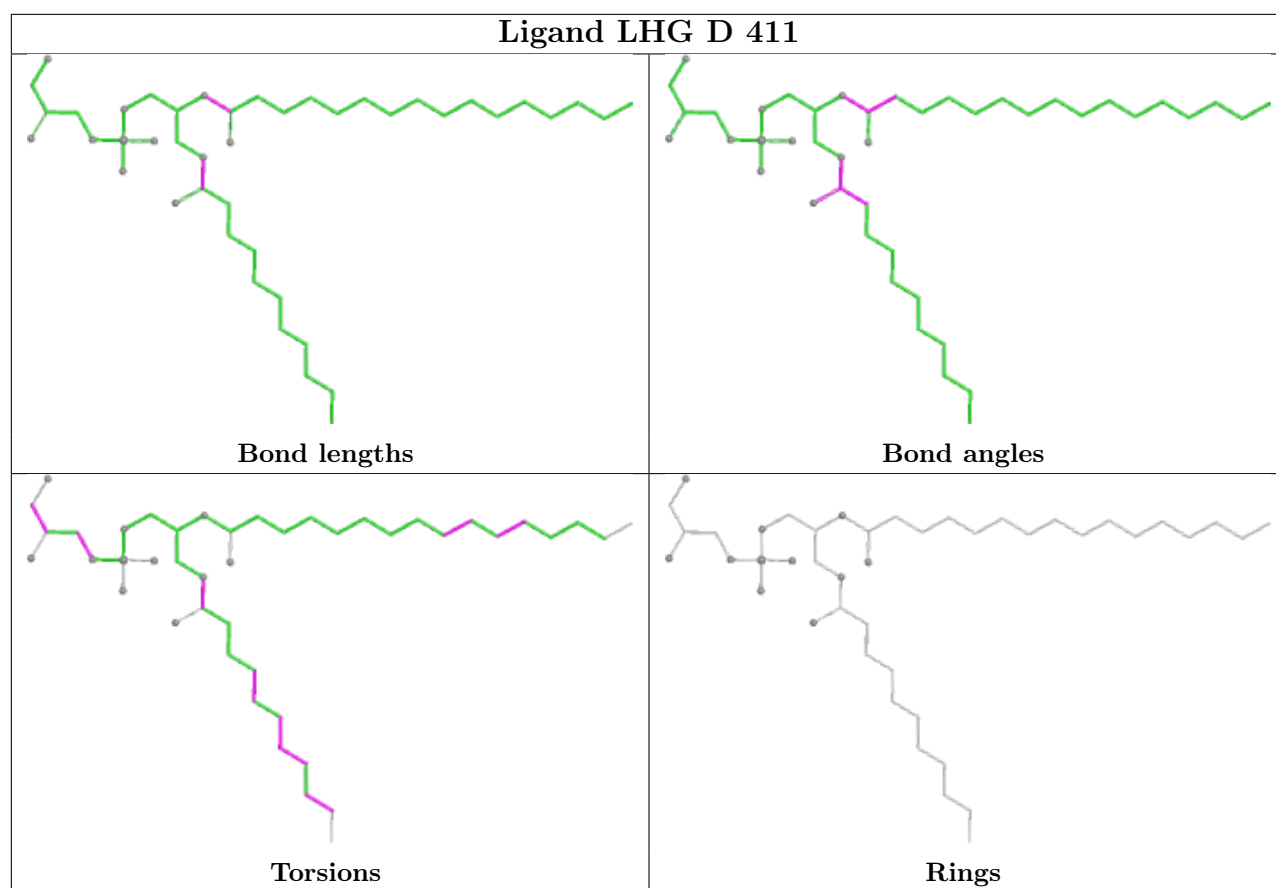


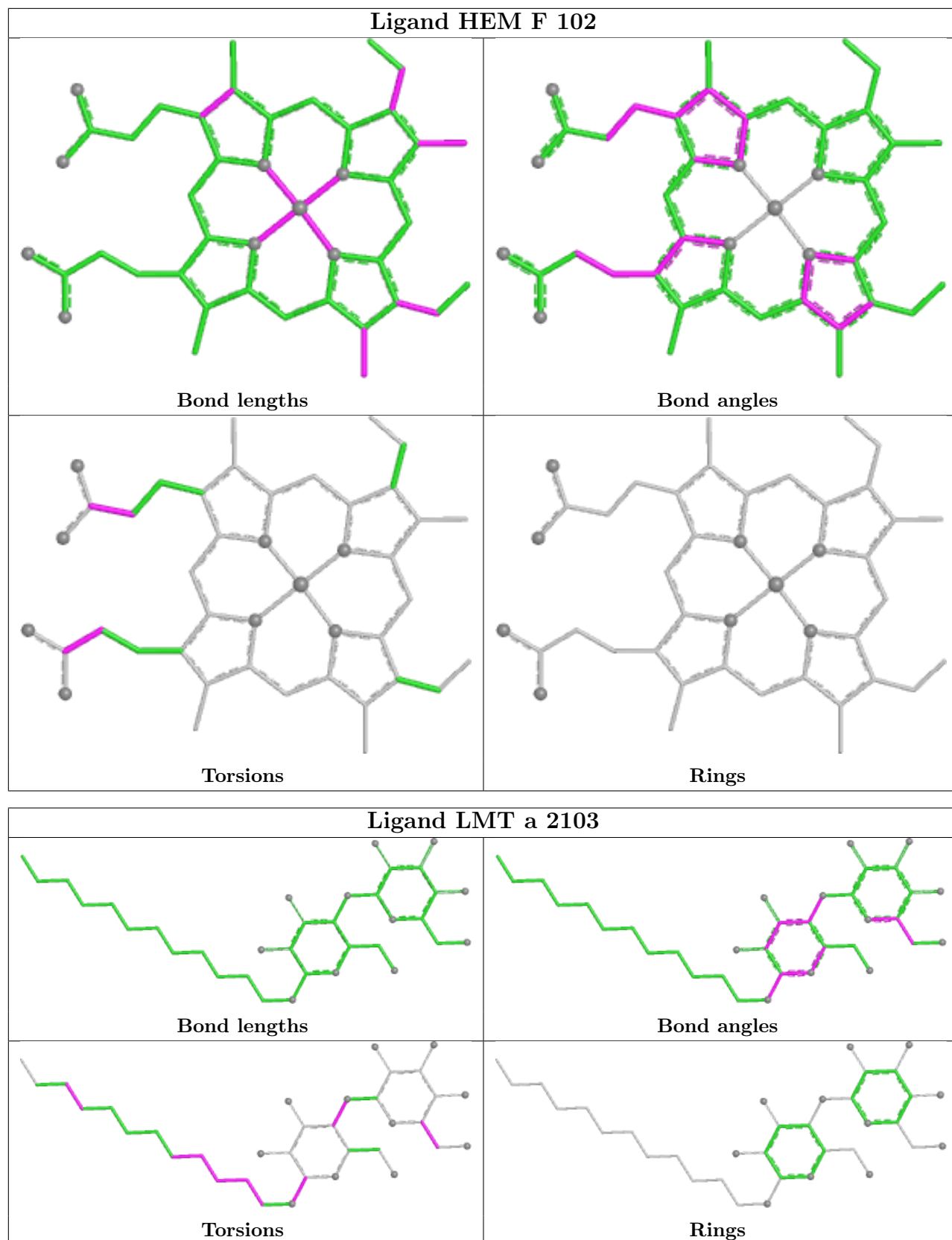
Ligand BCR B 619	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

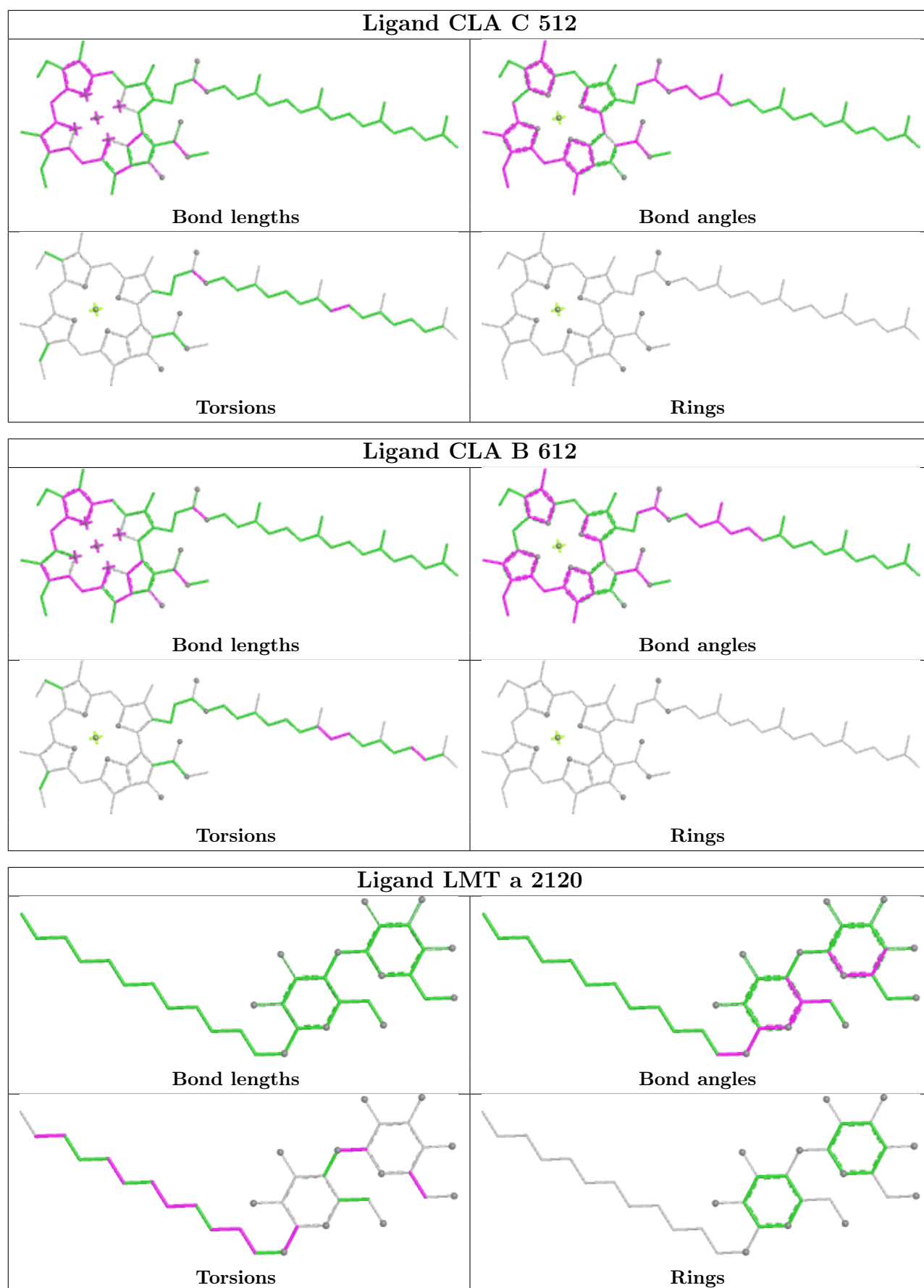


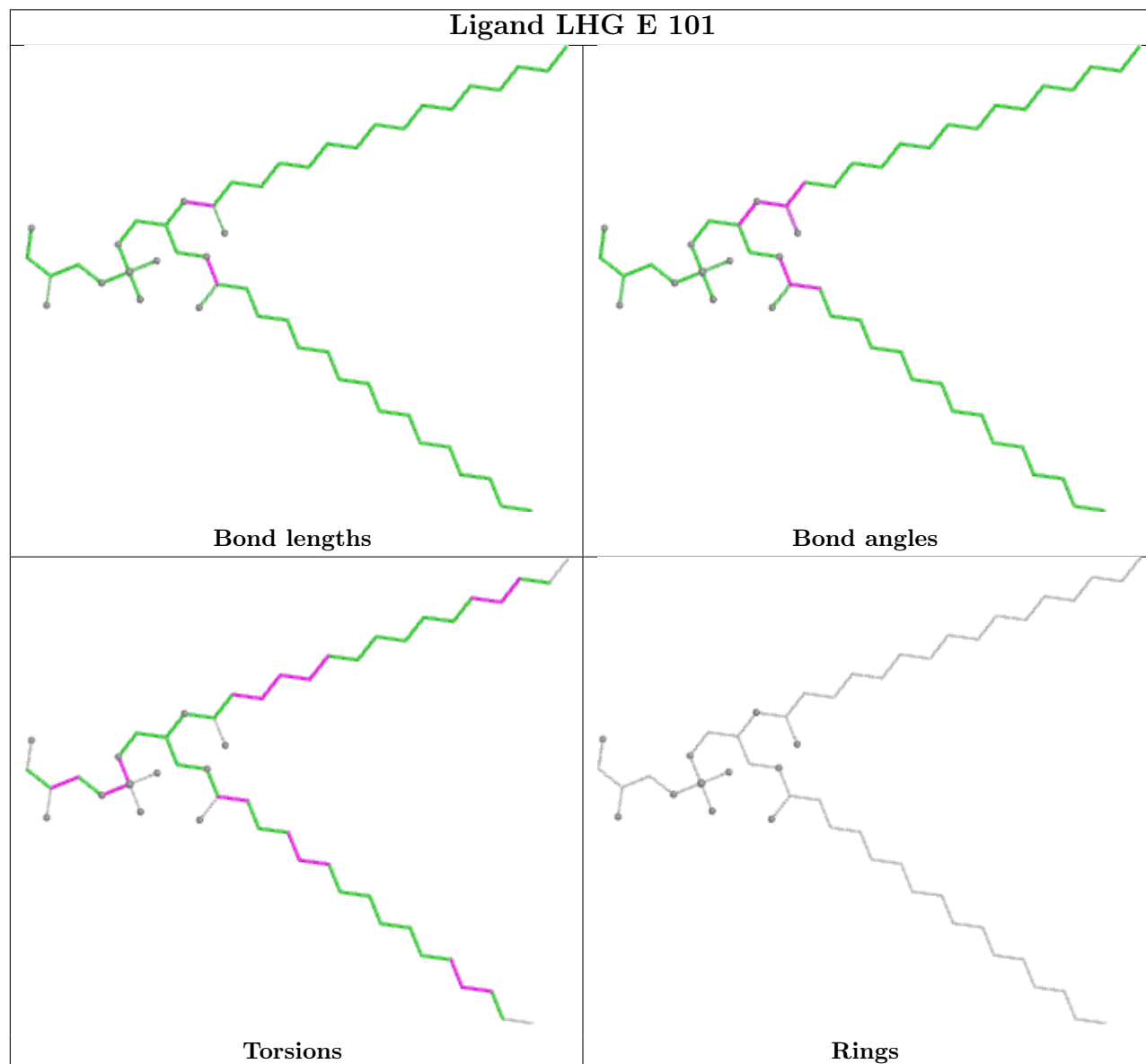
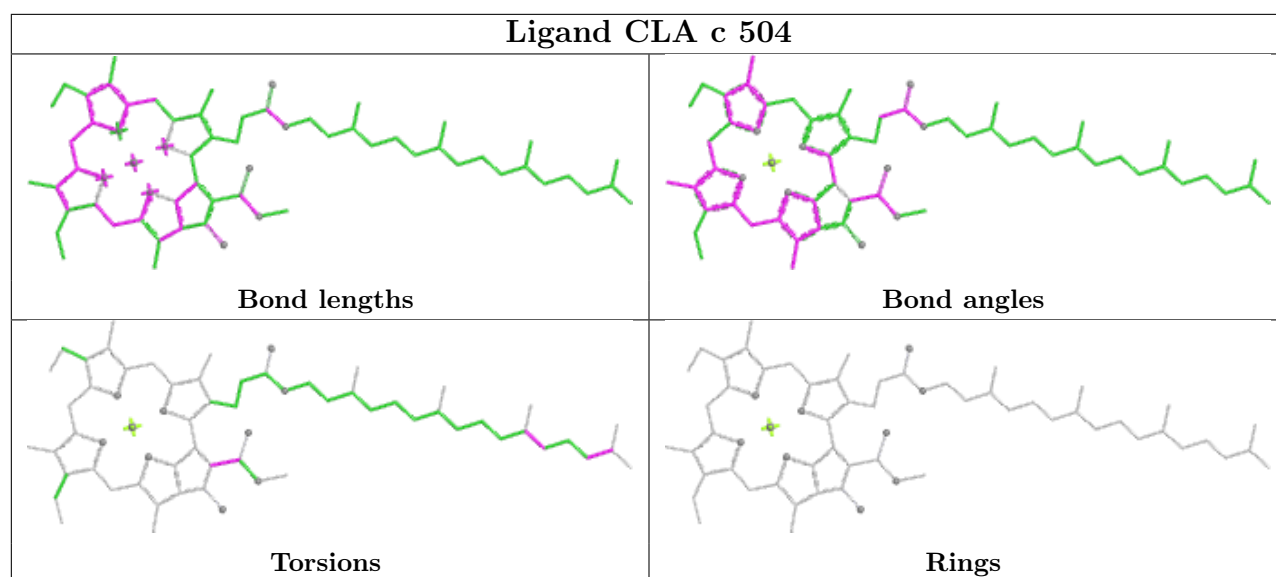


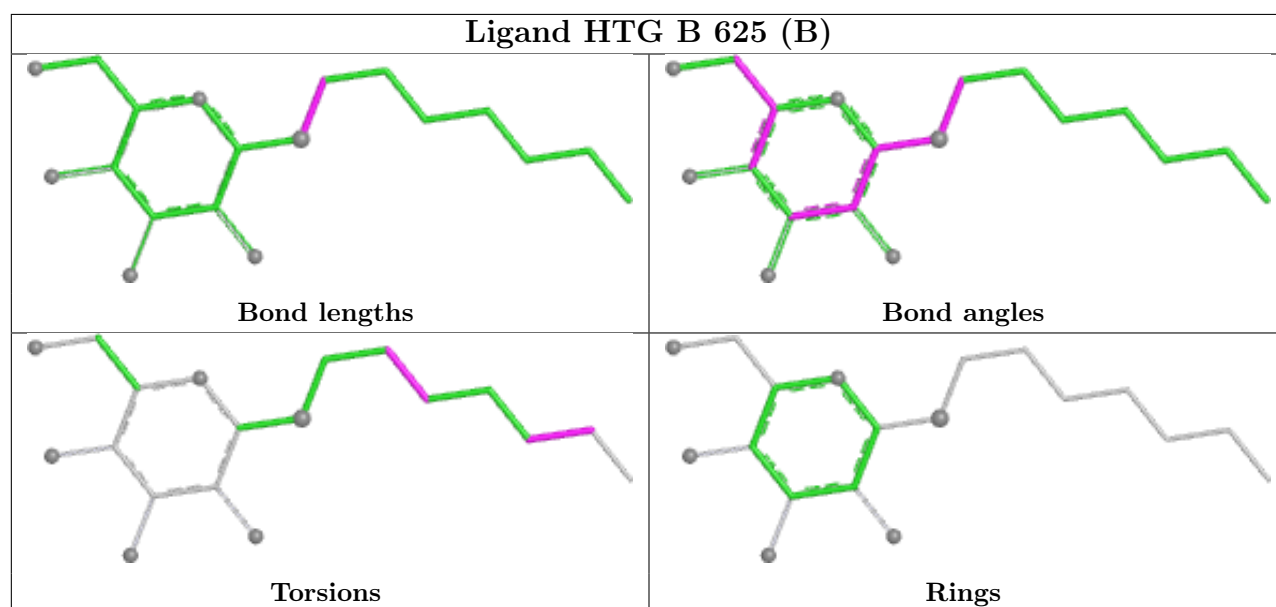
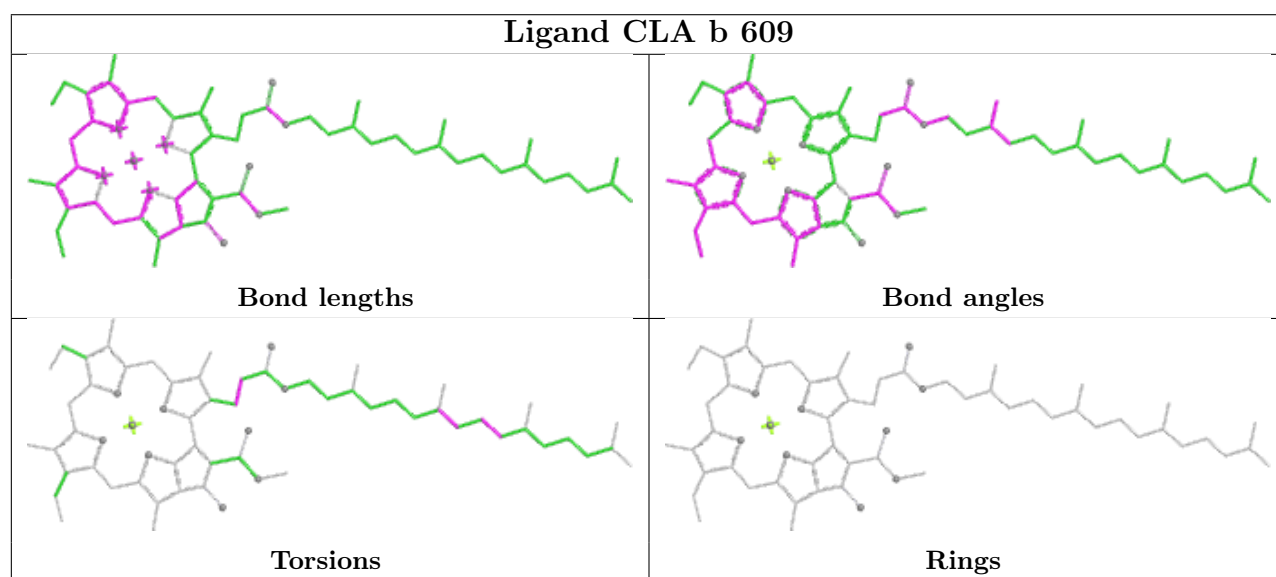
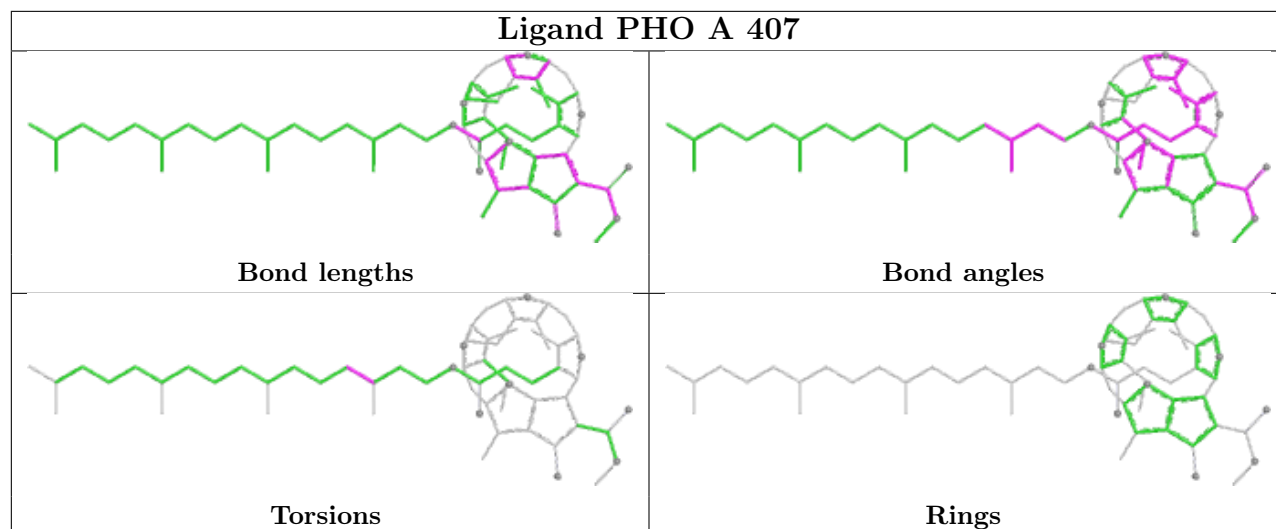


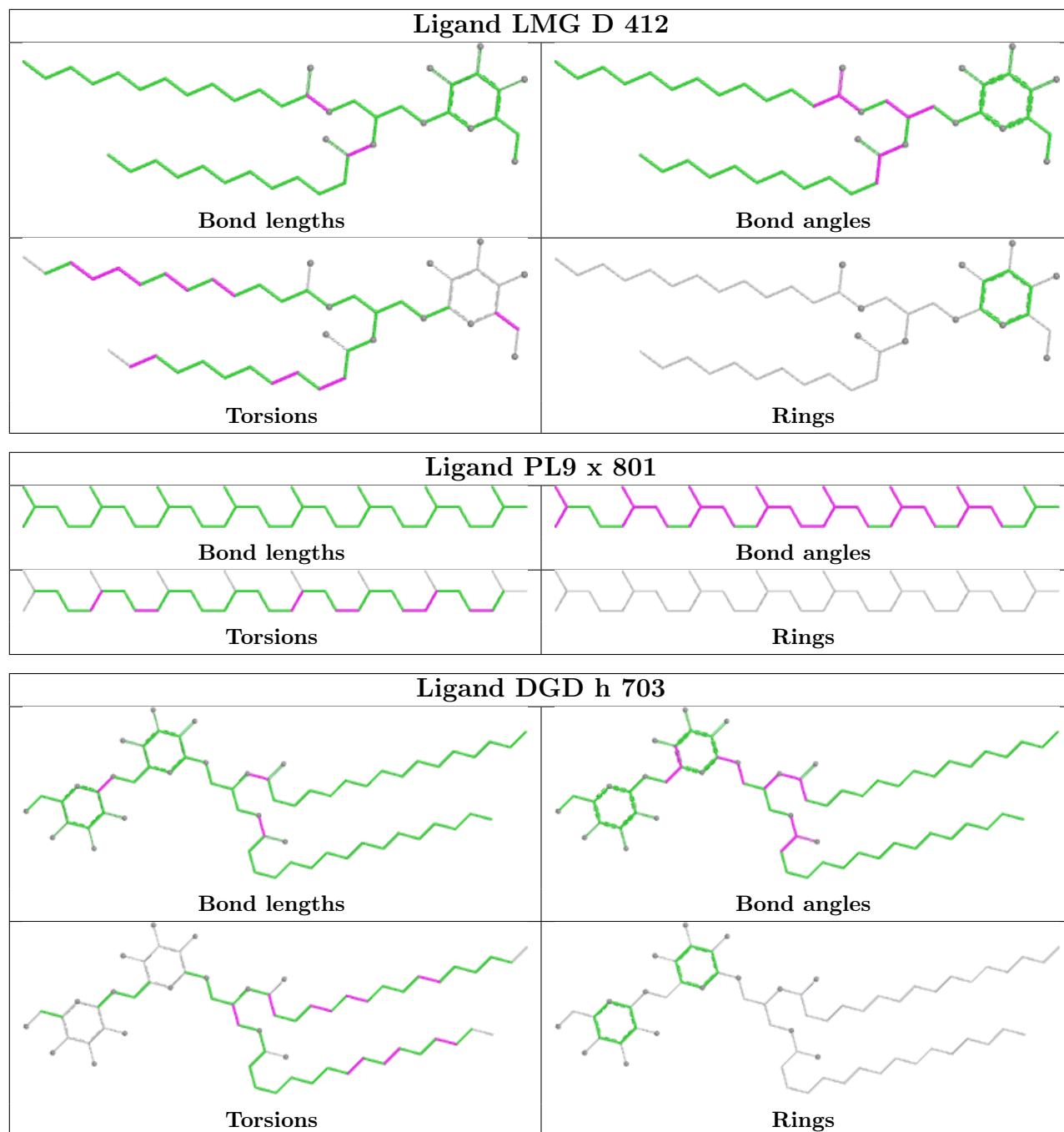


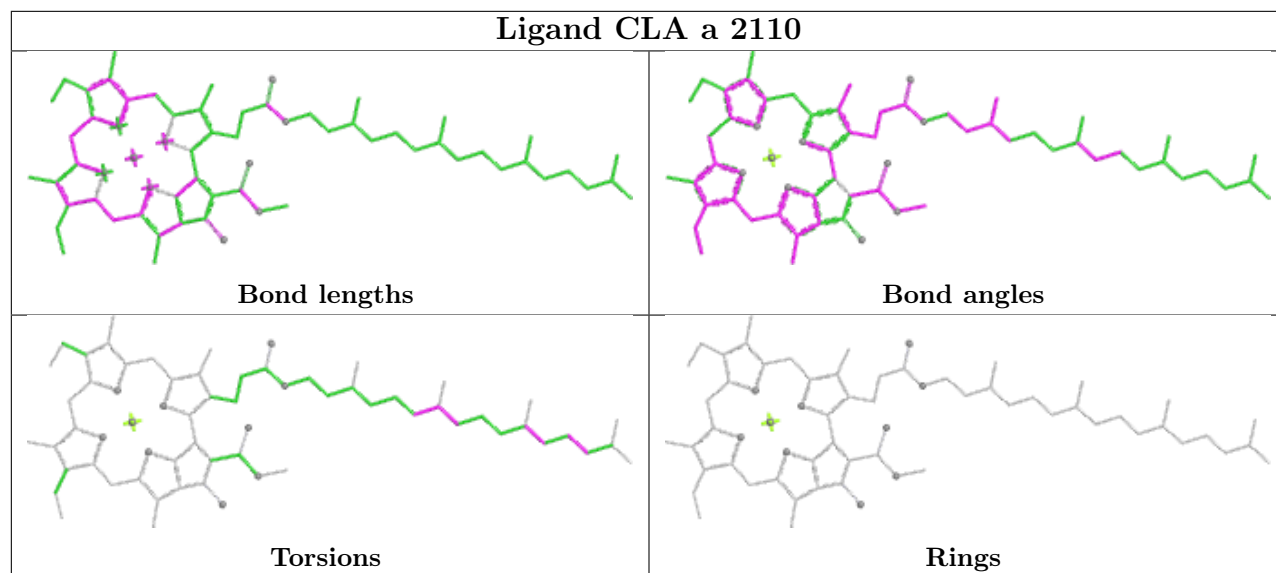
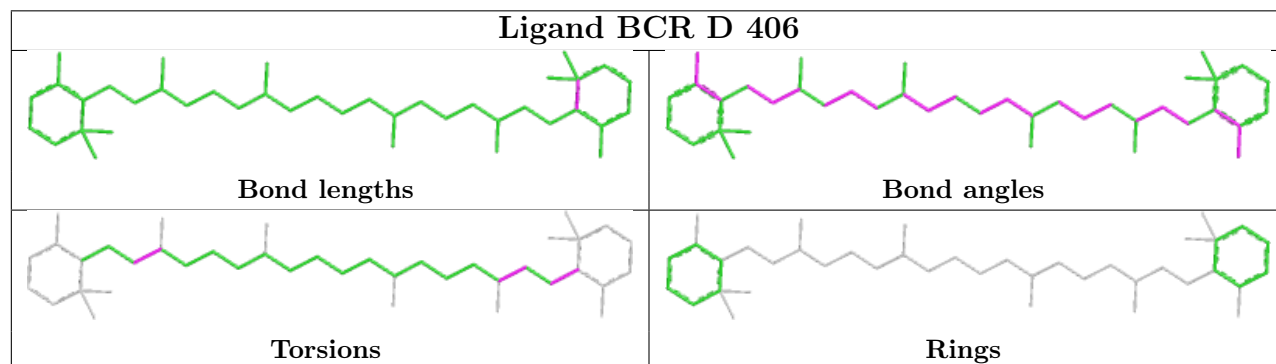
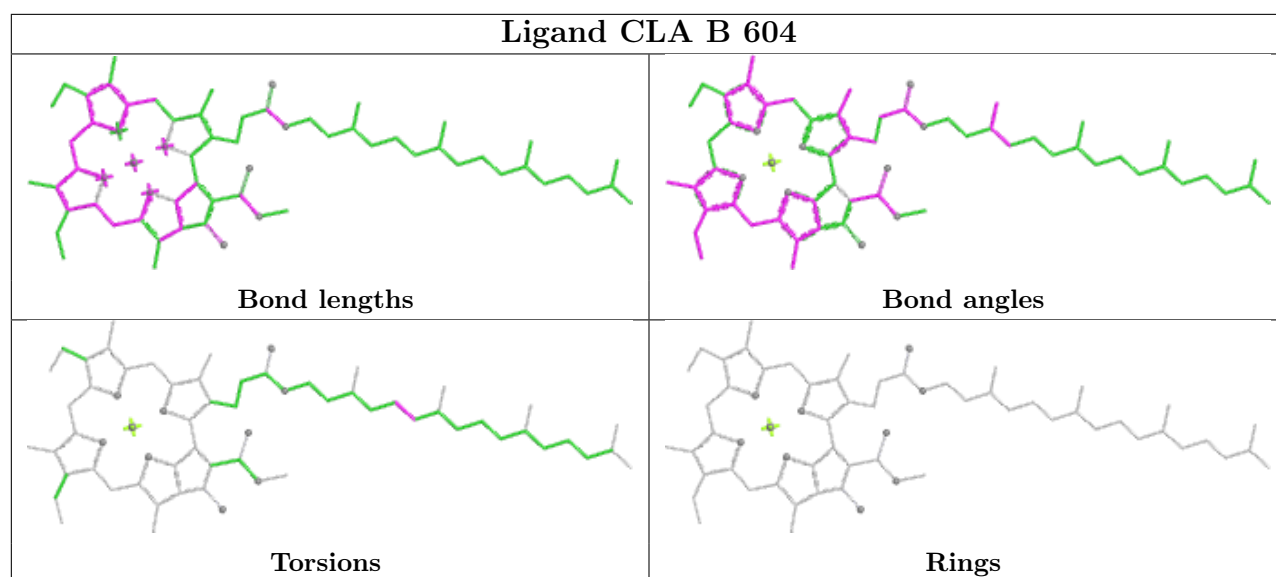


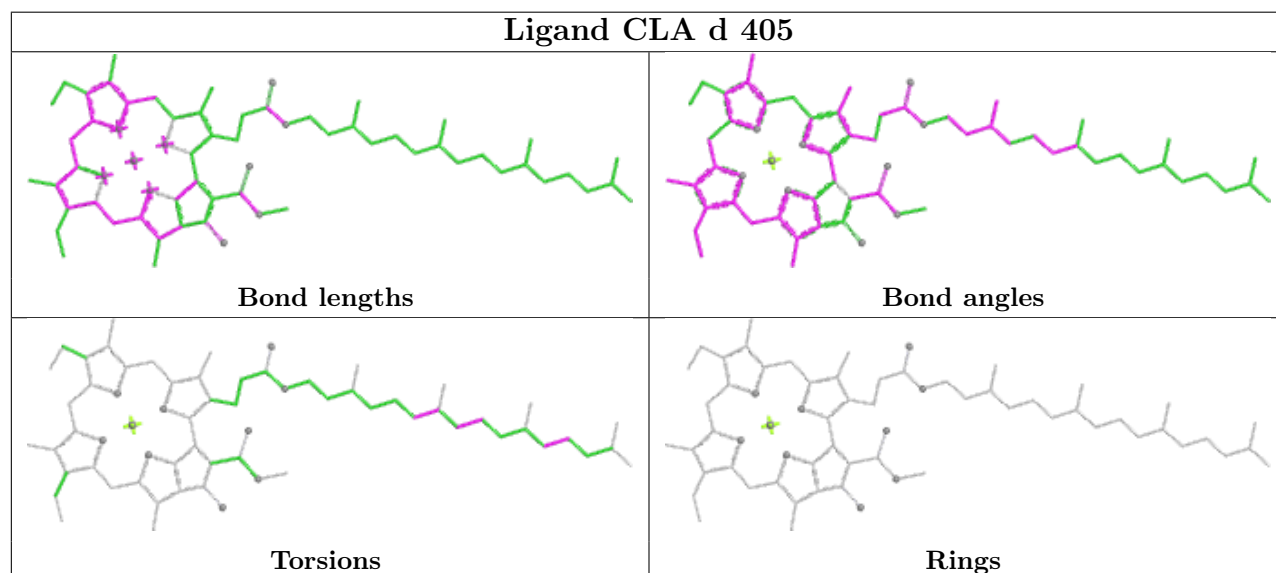
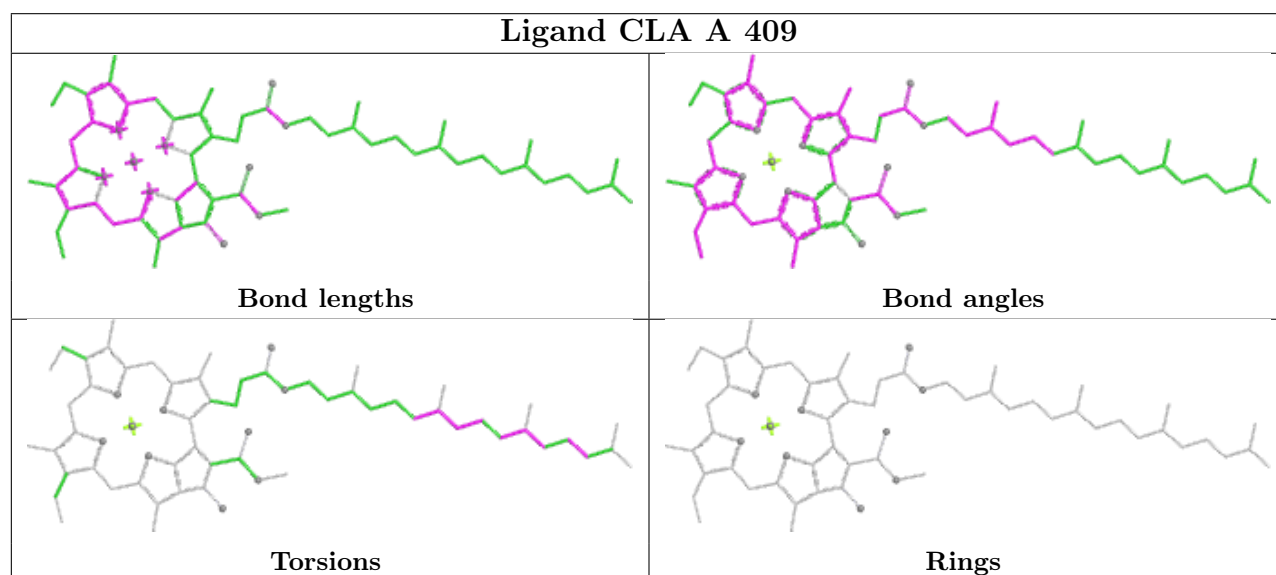
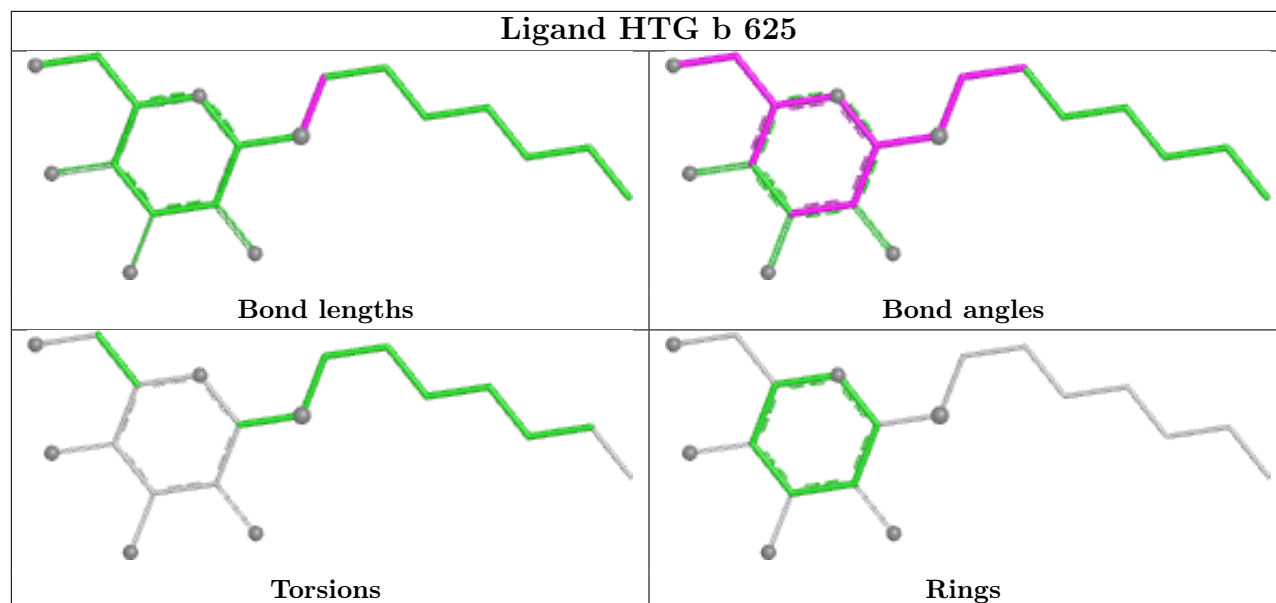




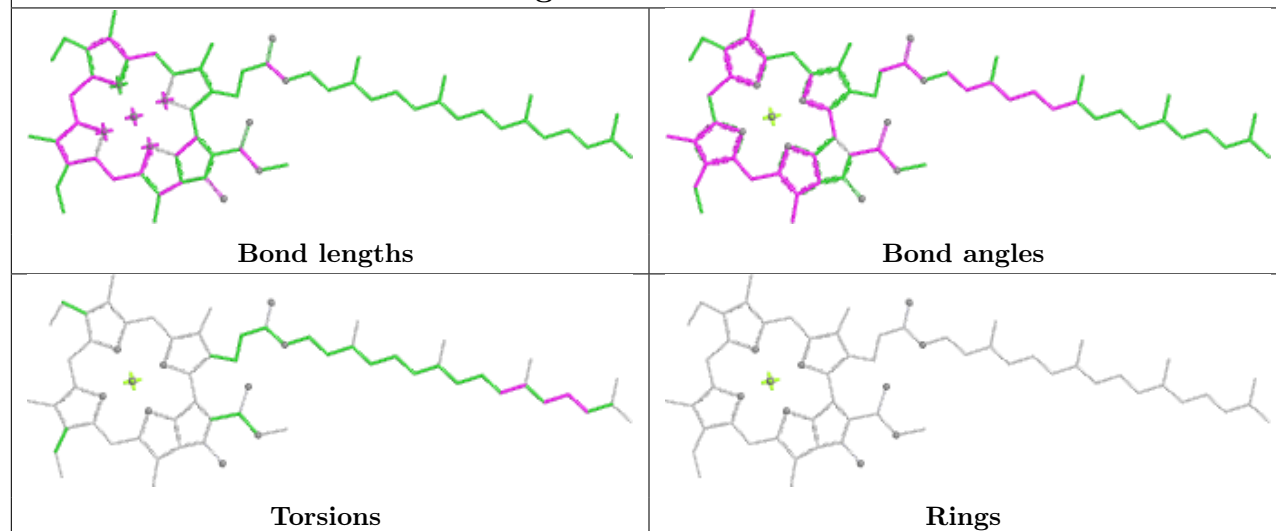




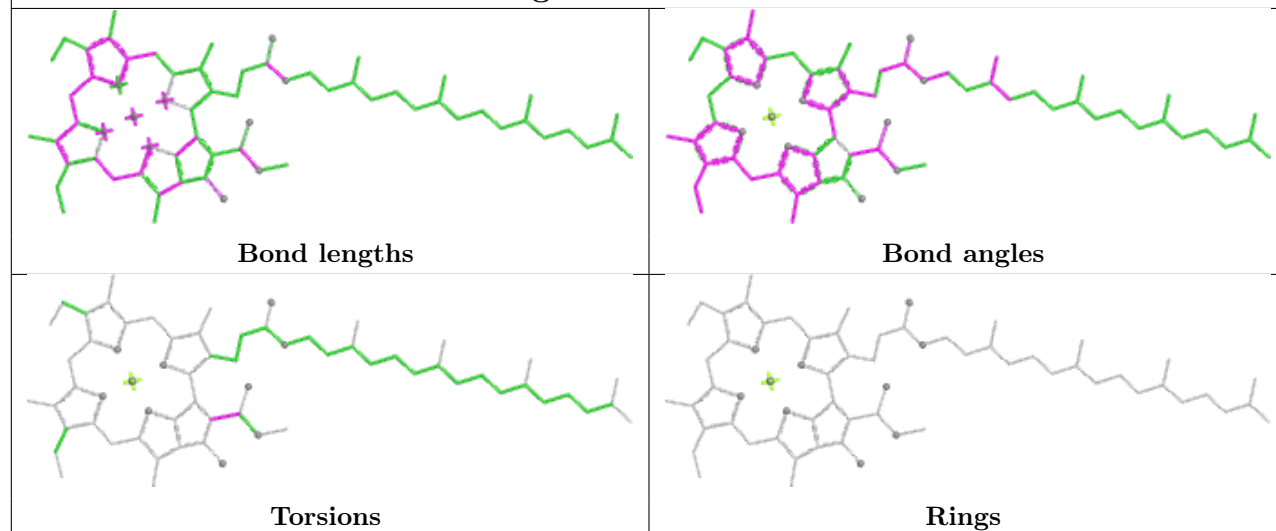




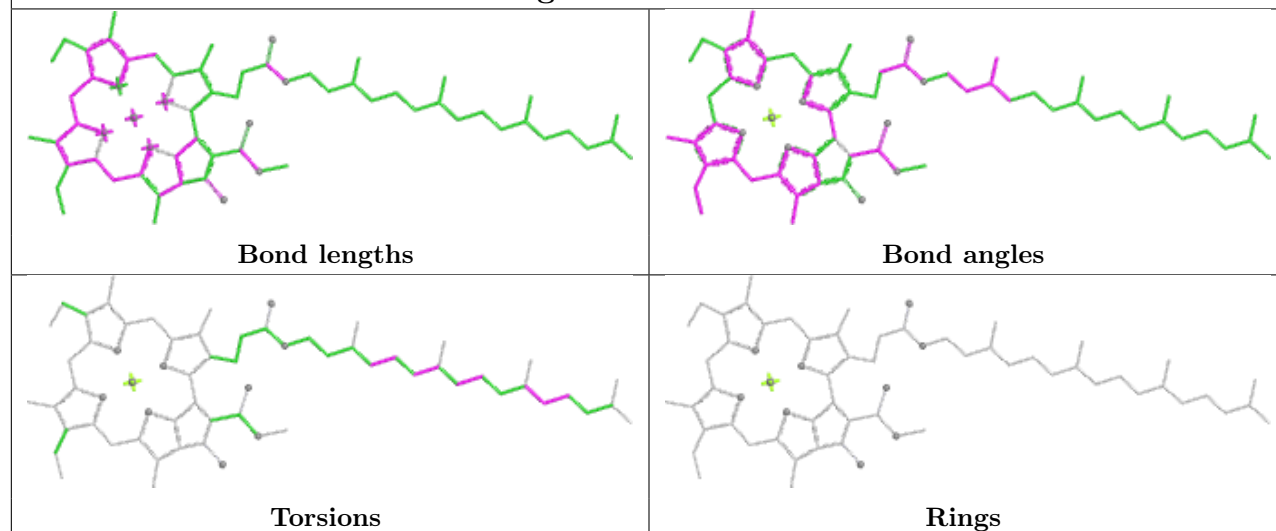
Ligand CLA b 607

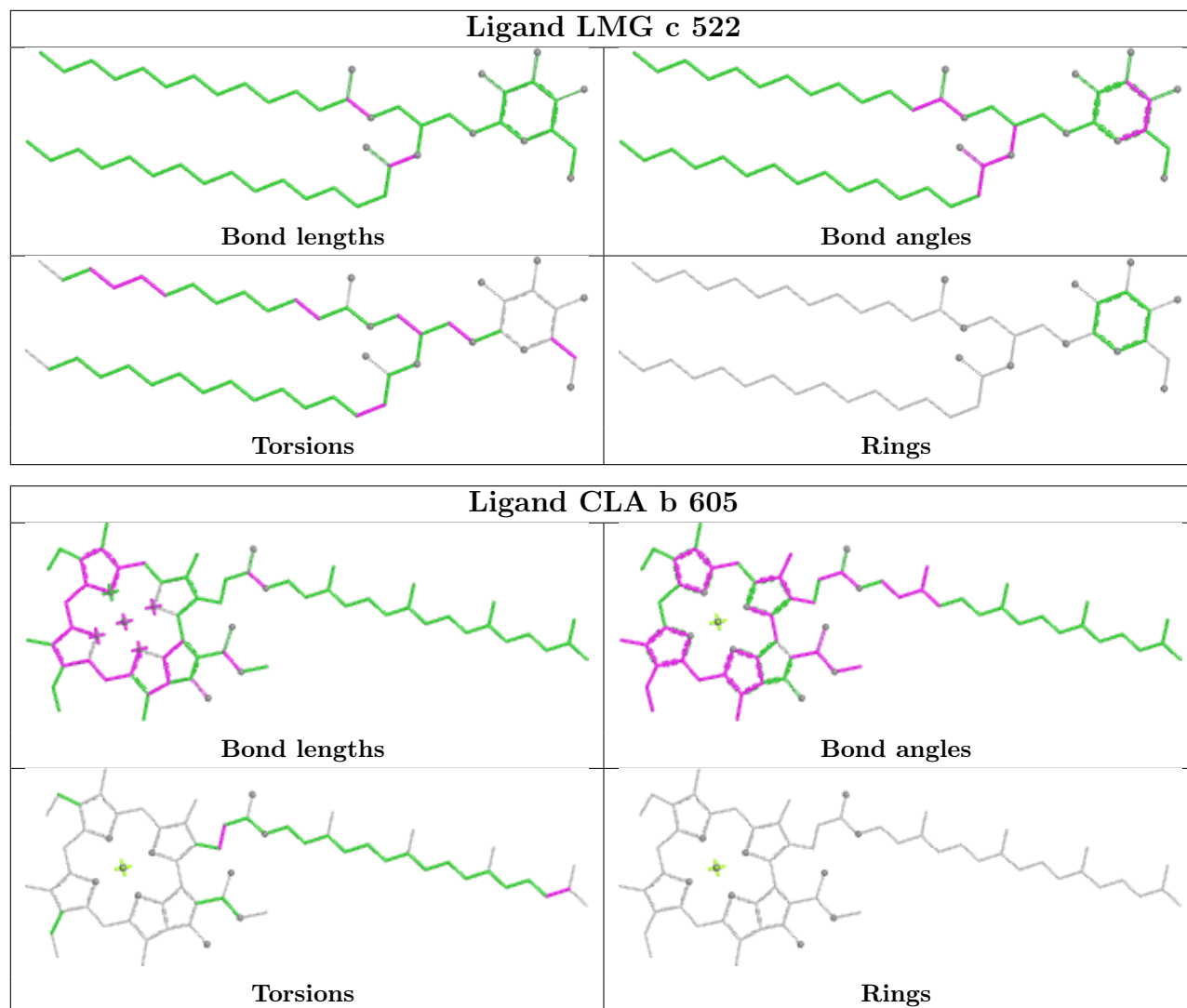


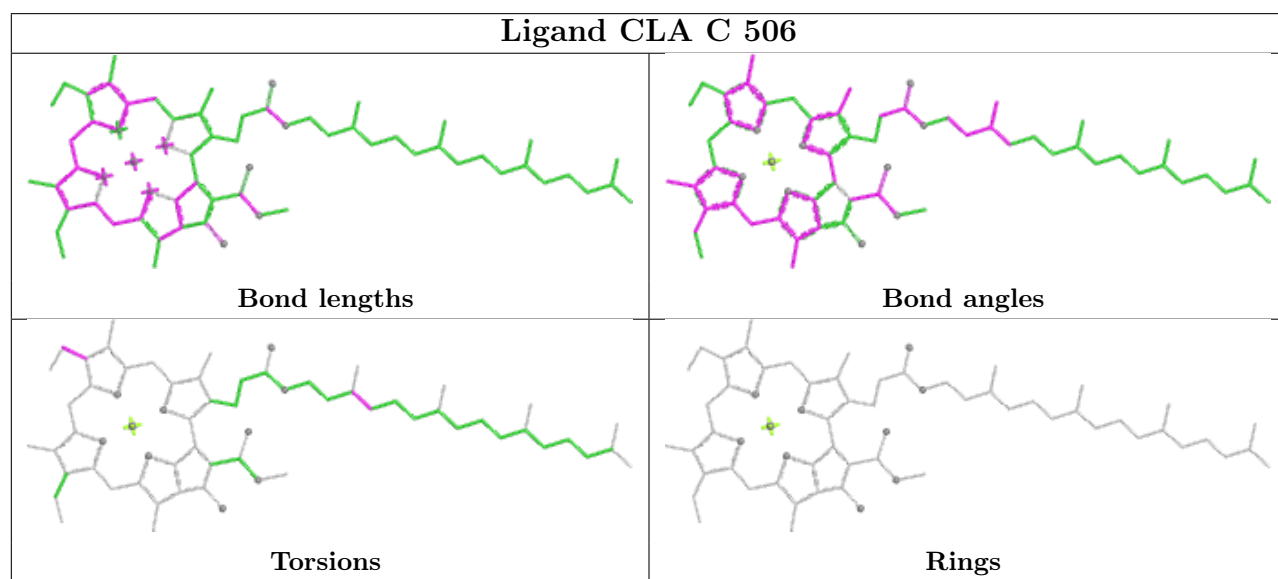
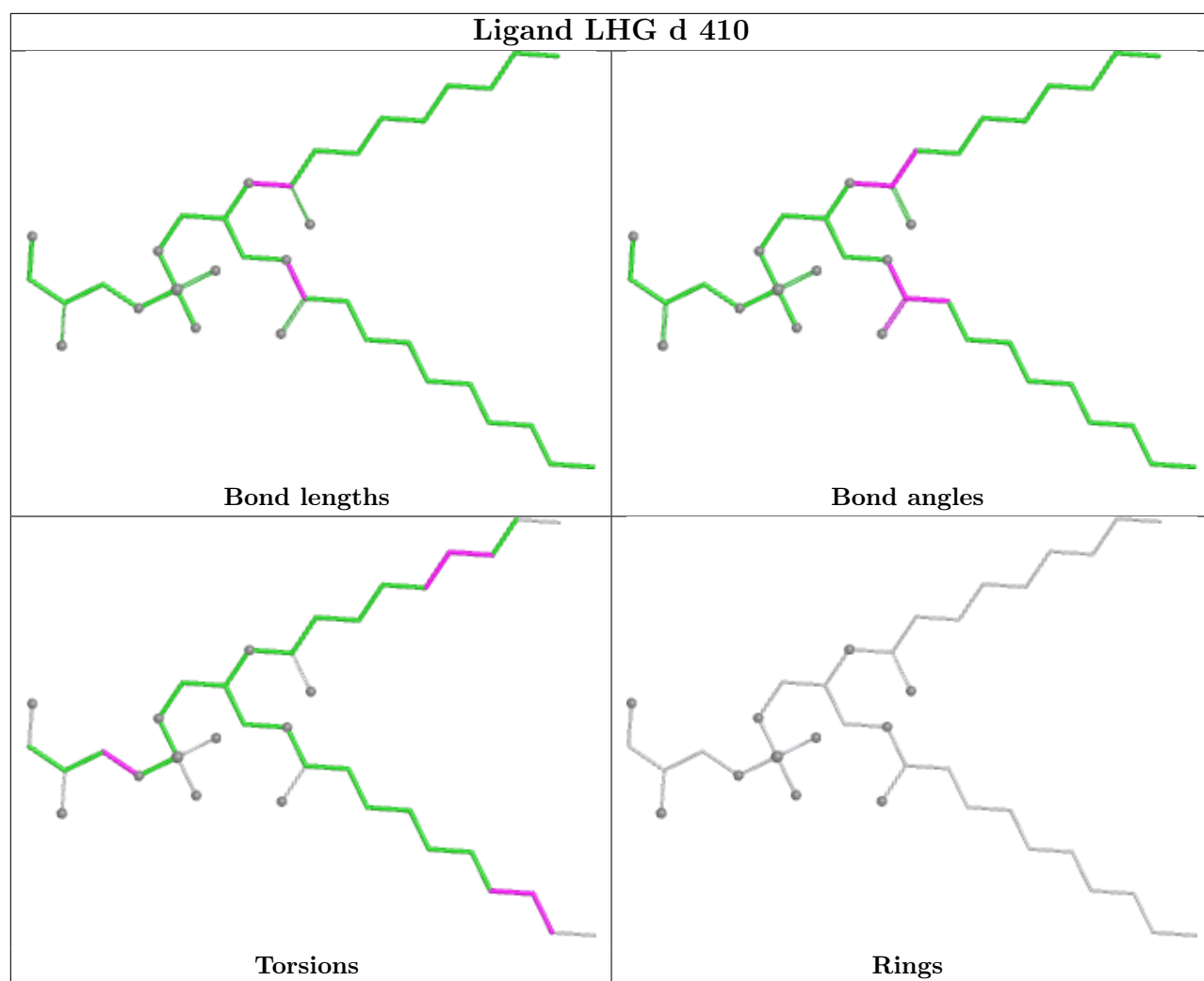
Ligand CLA B 608

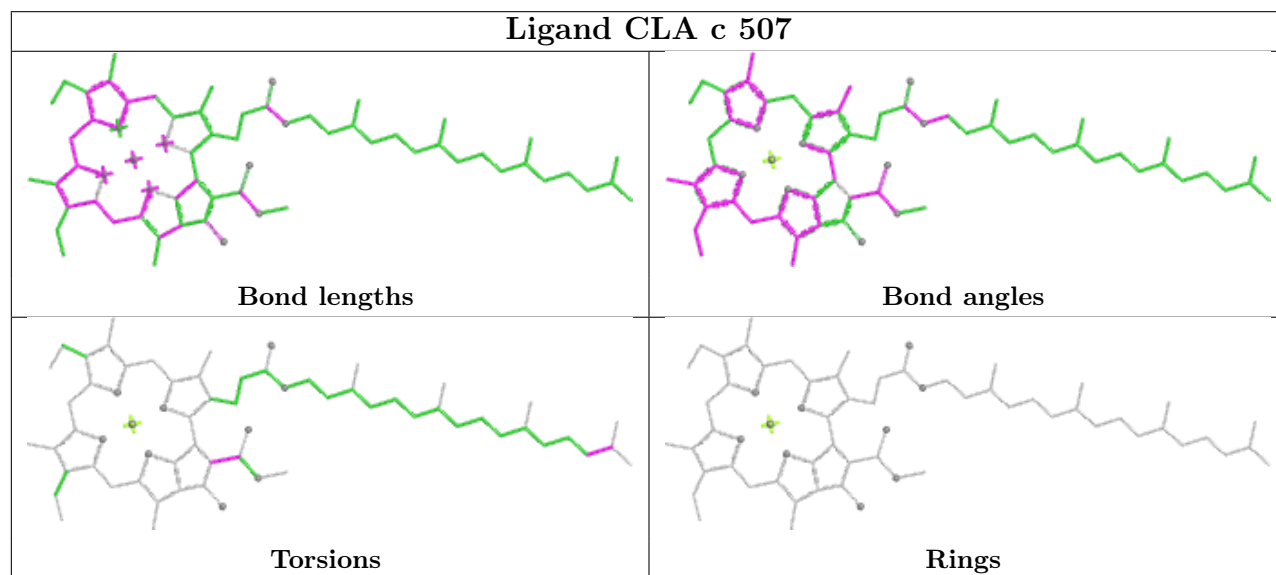
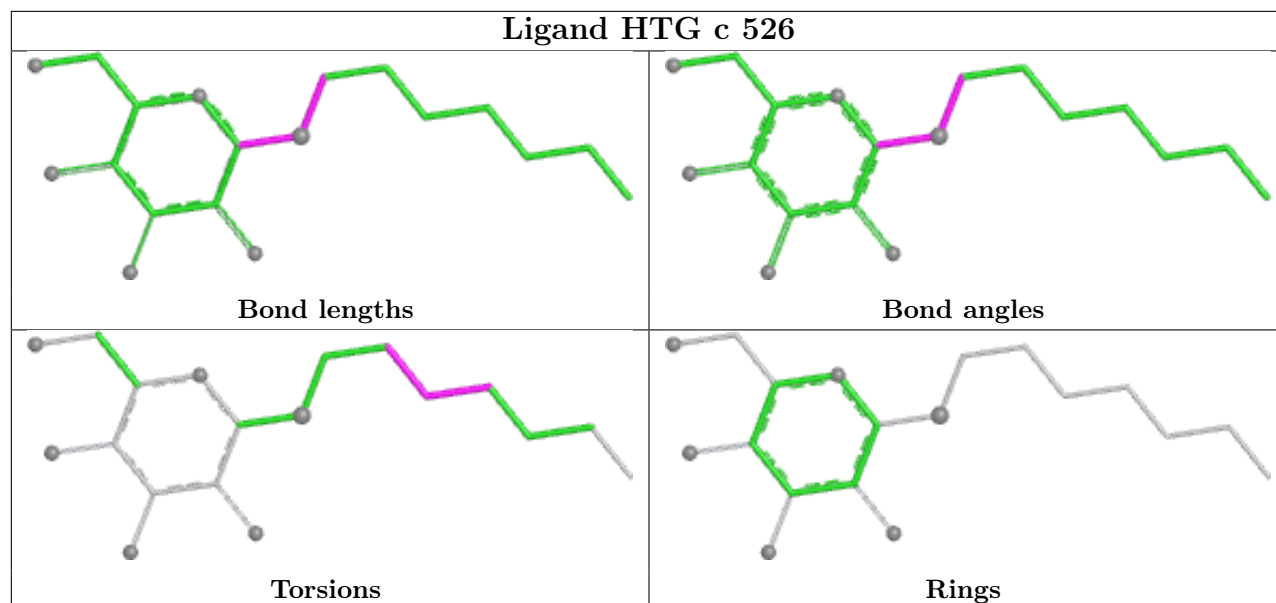


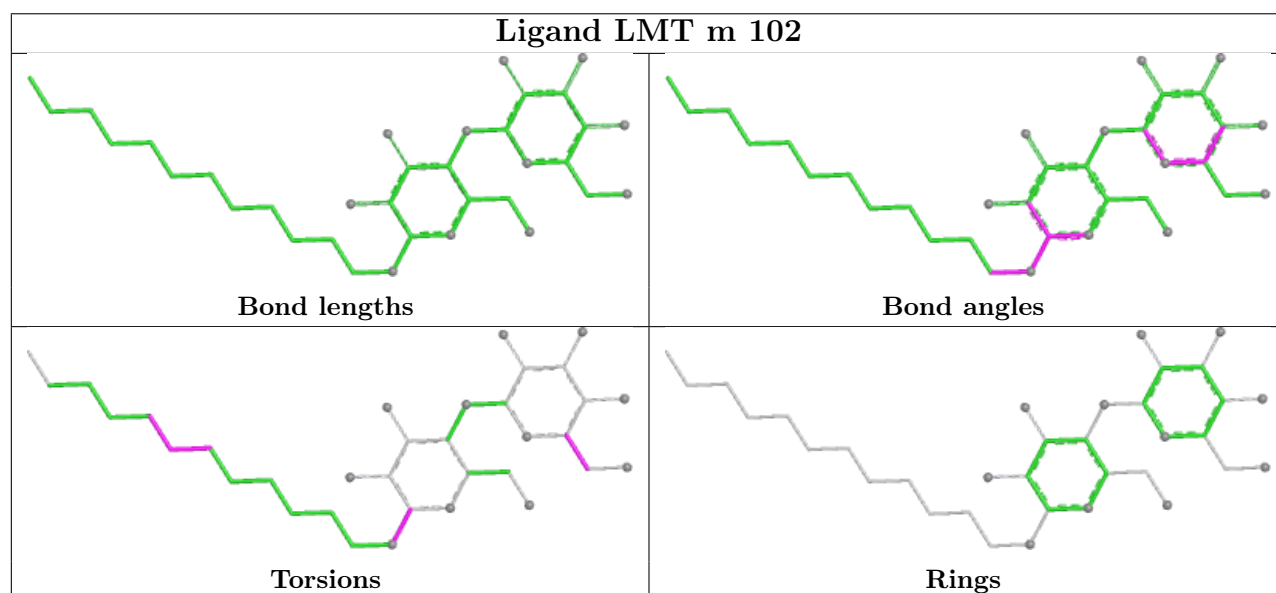
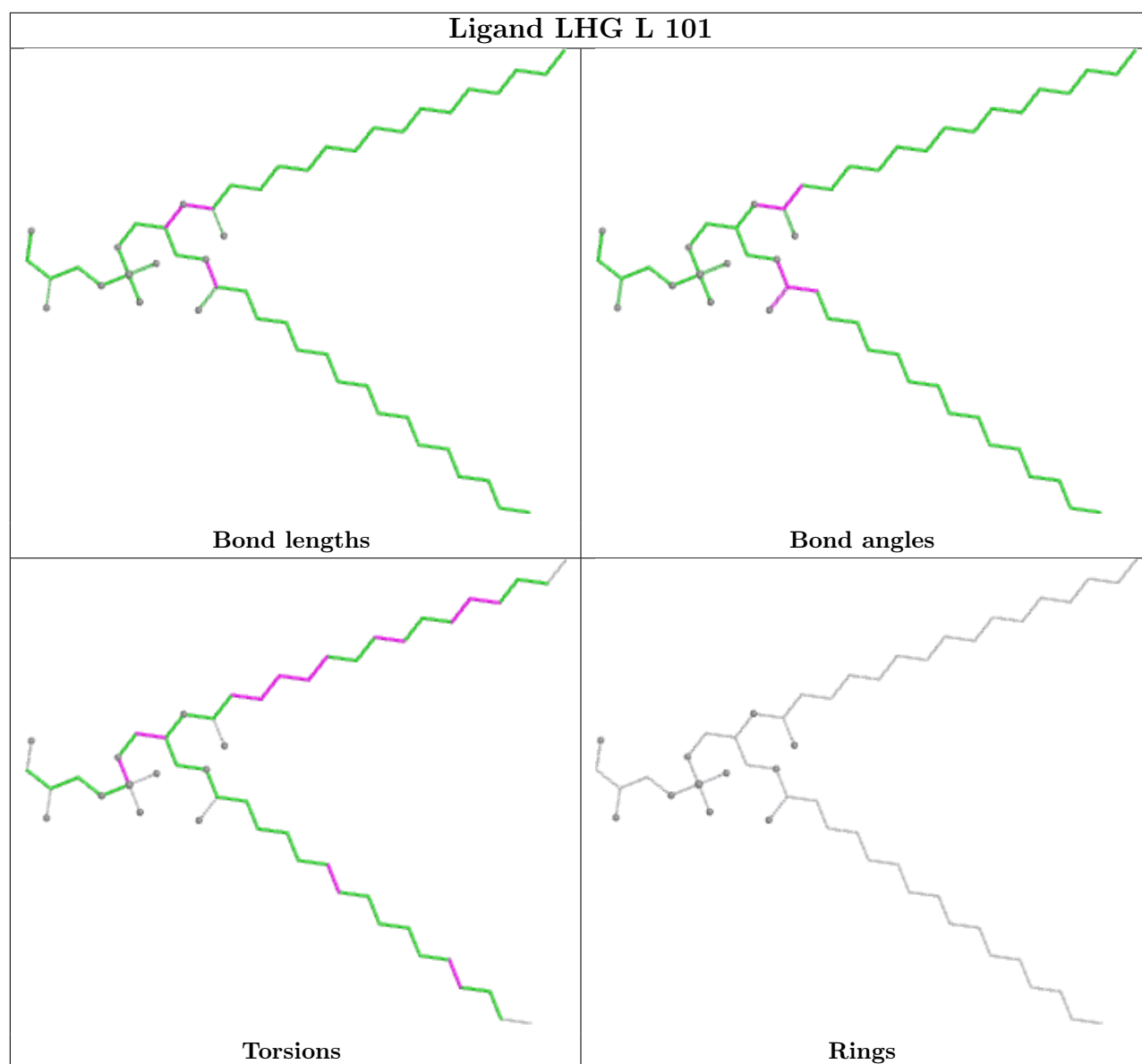
Ligand CLA c 511

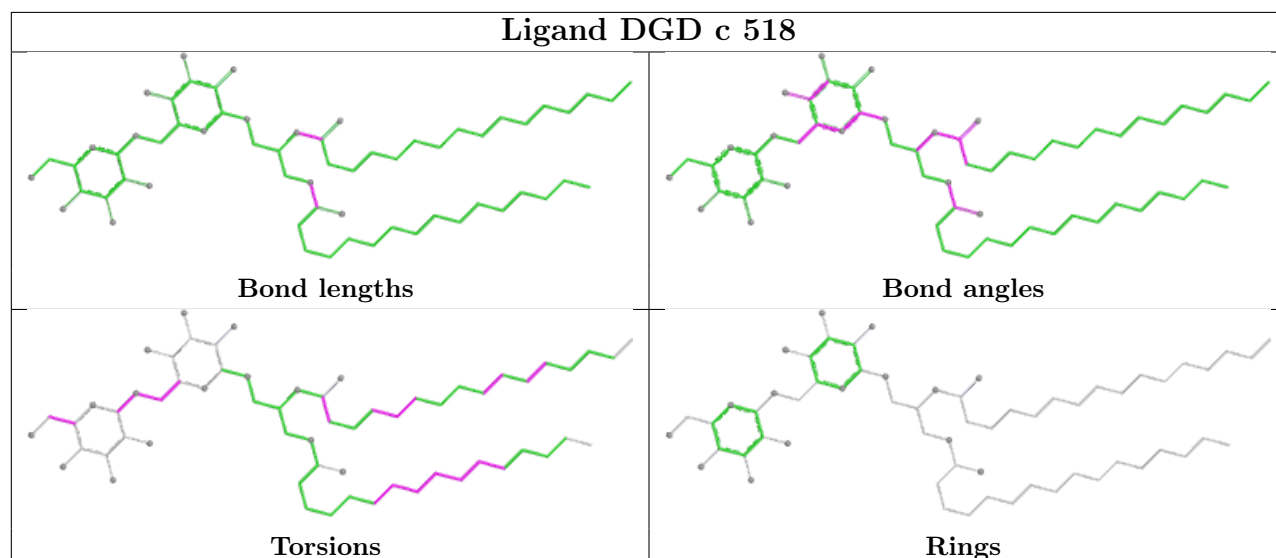
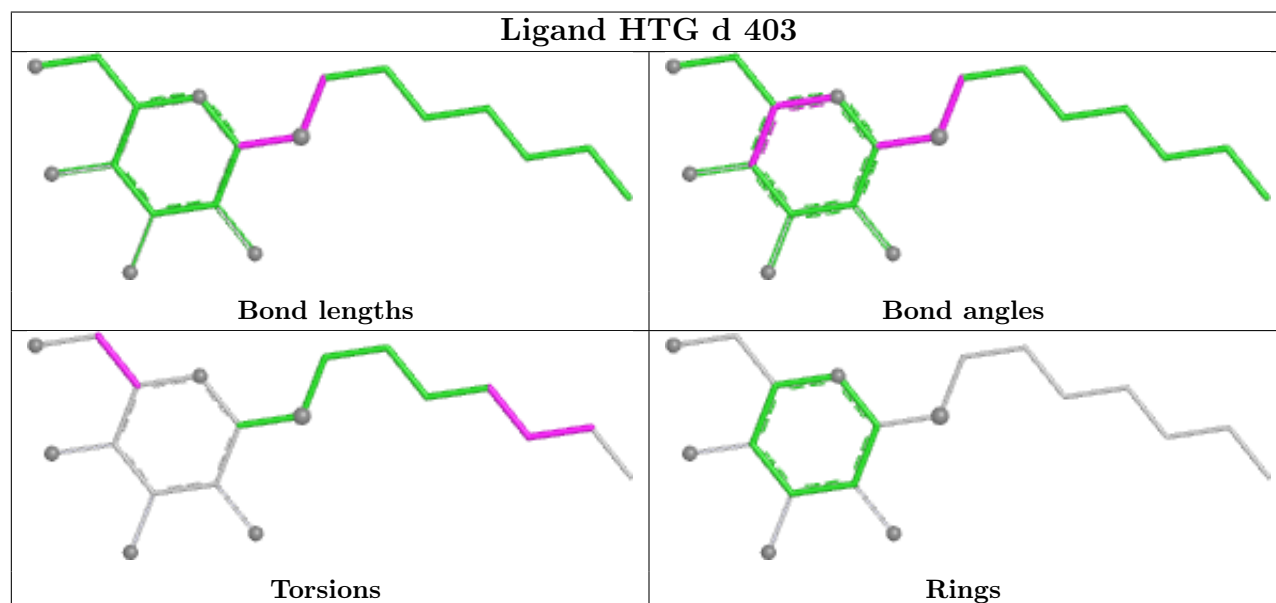
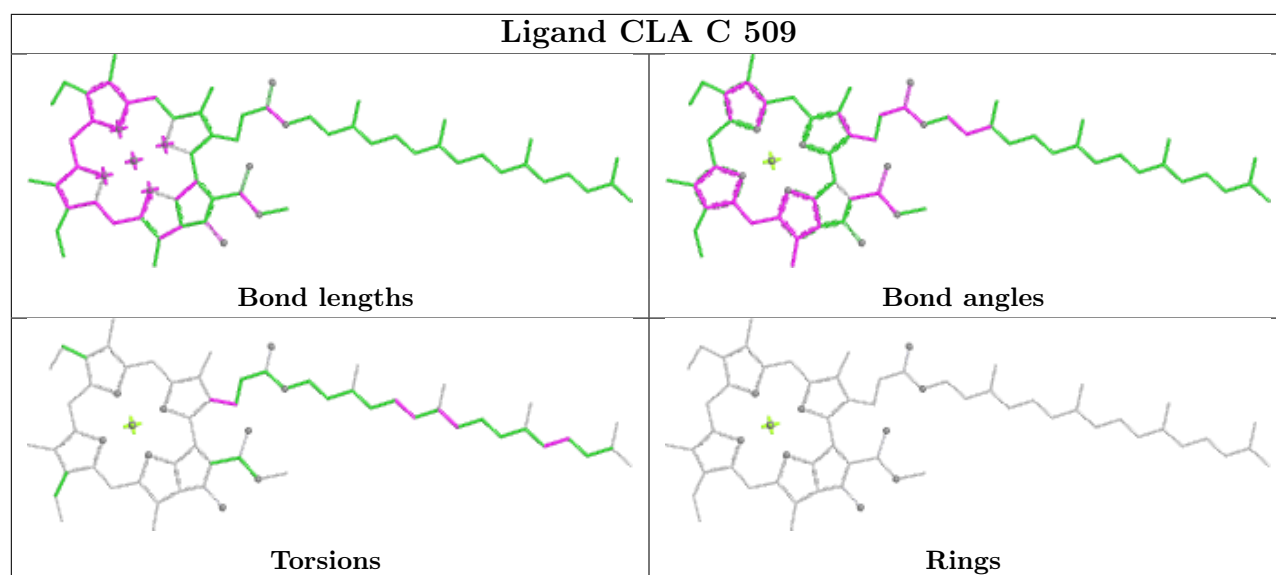


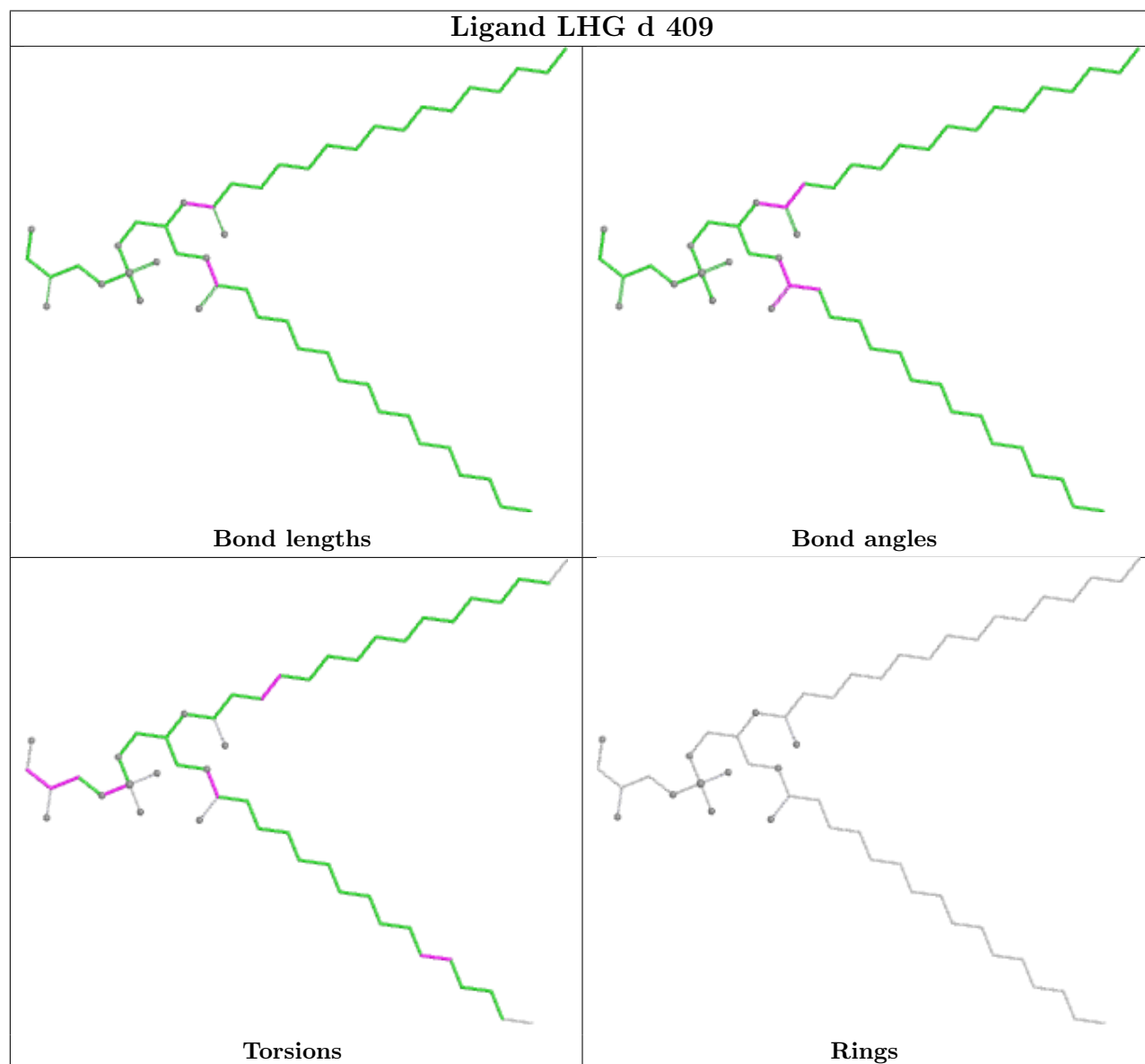
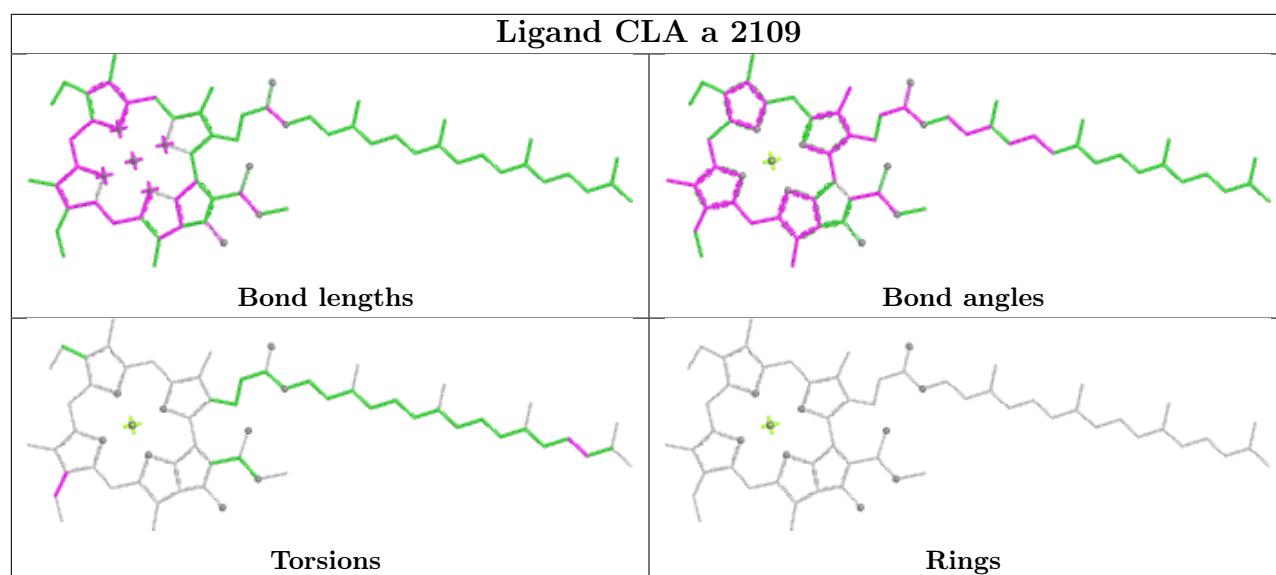




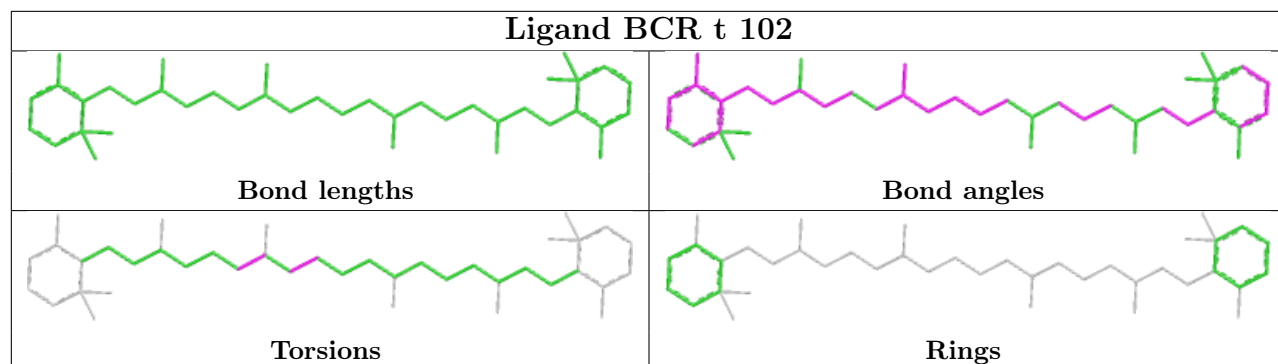




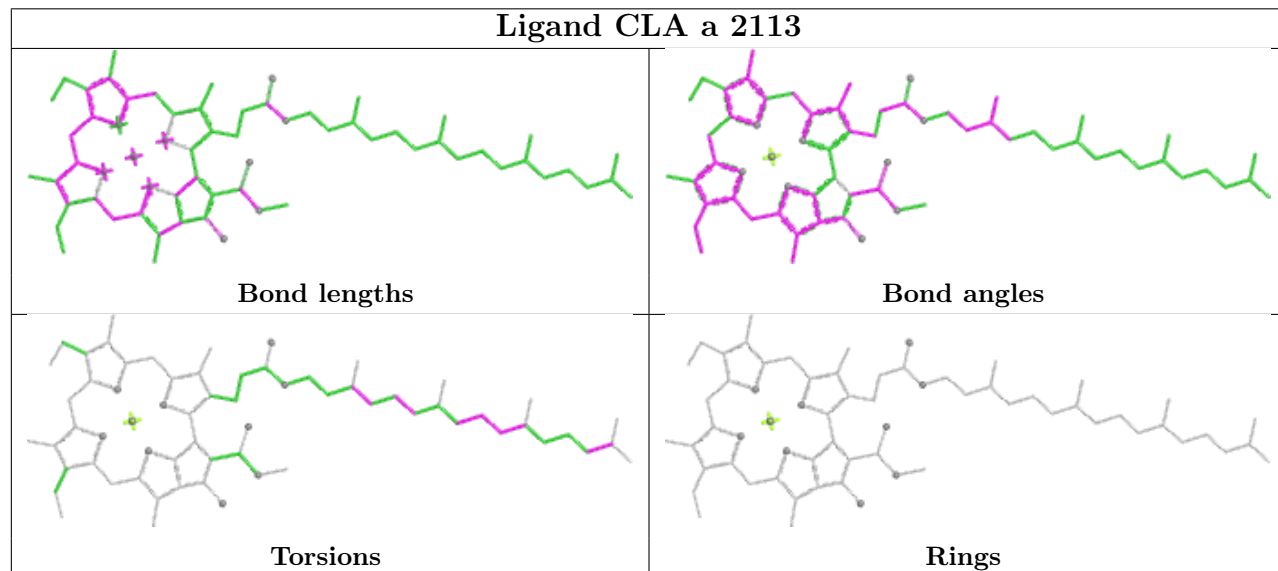




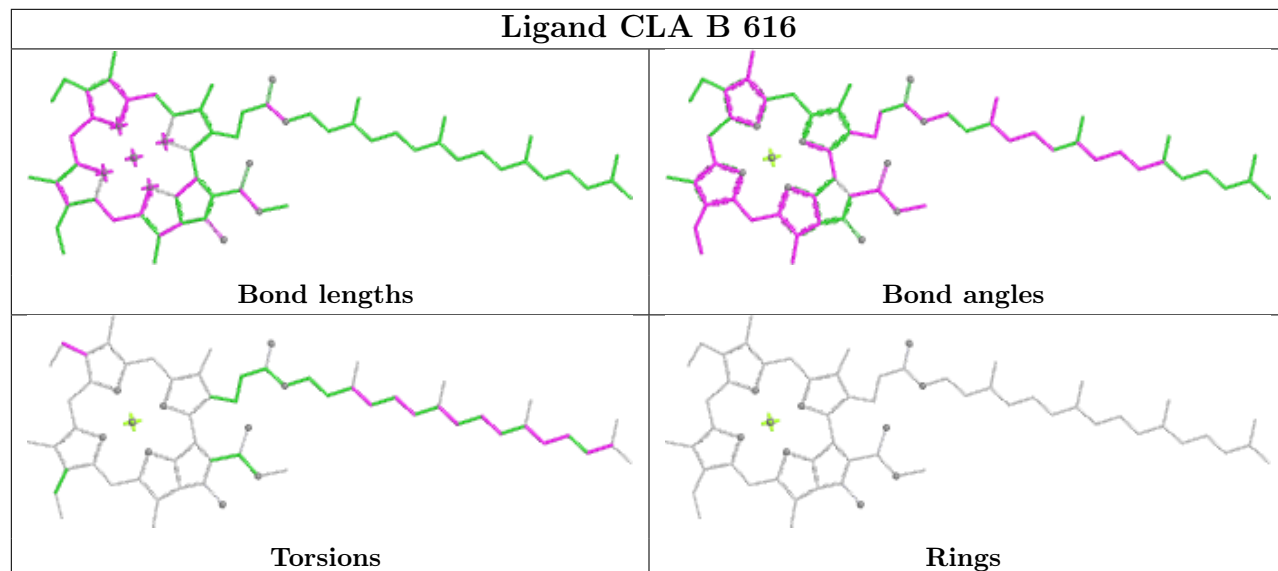
Ligand BCR t 102

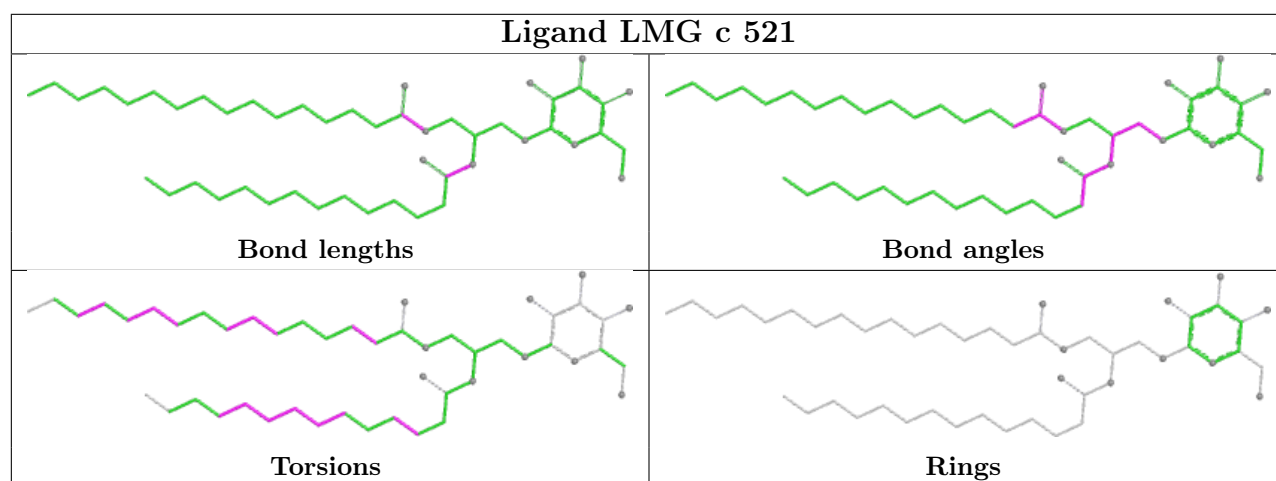
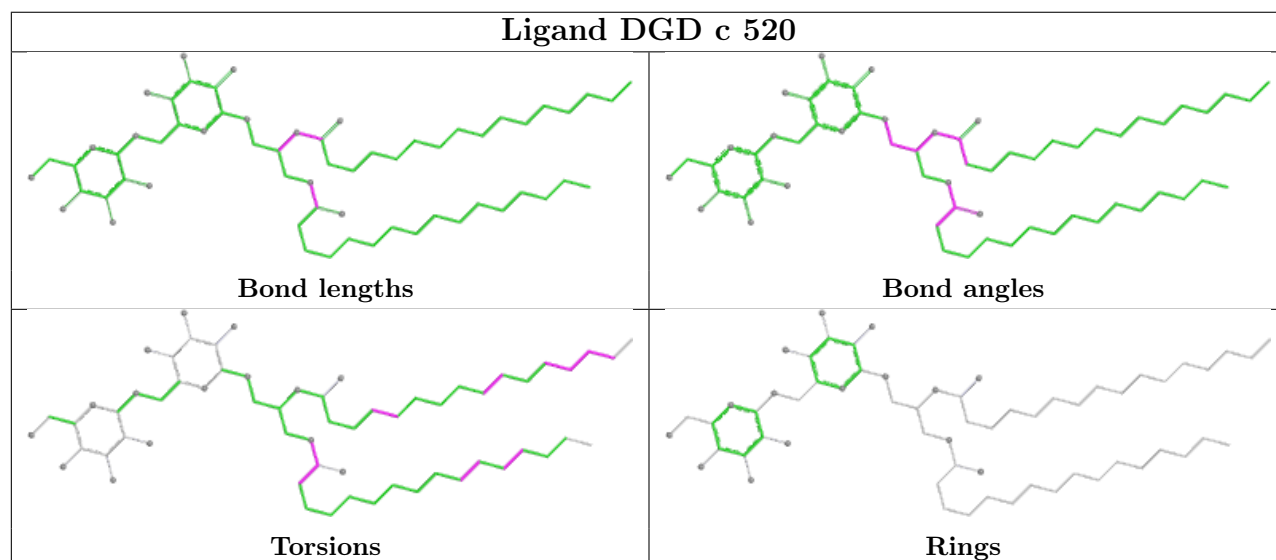
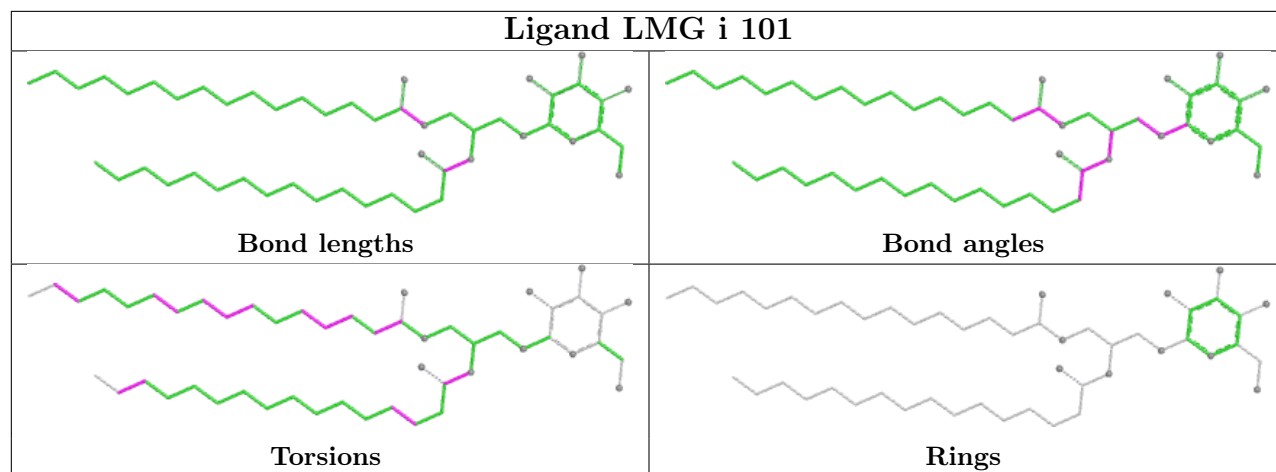


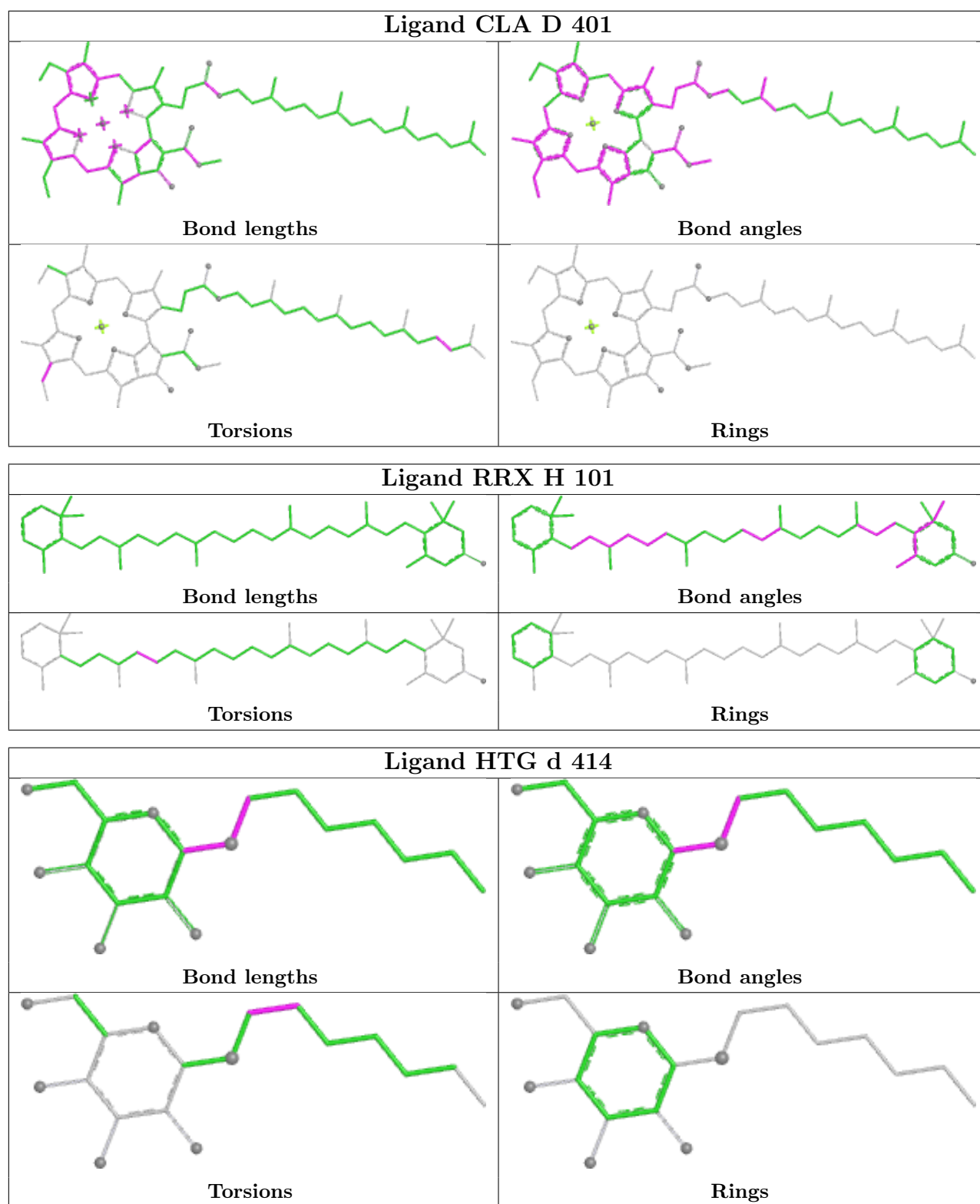
Ligand CLA a 2113

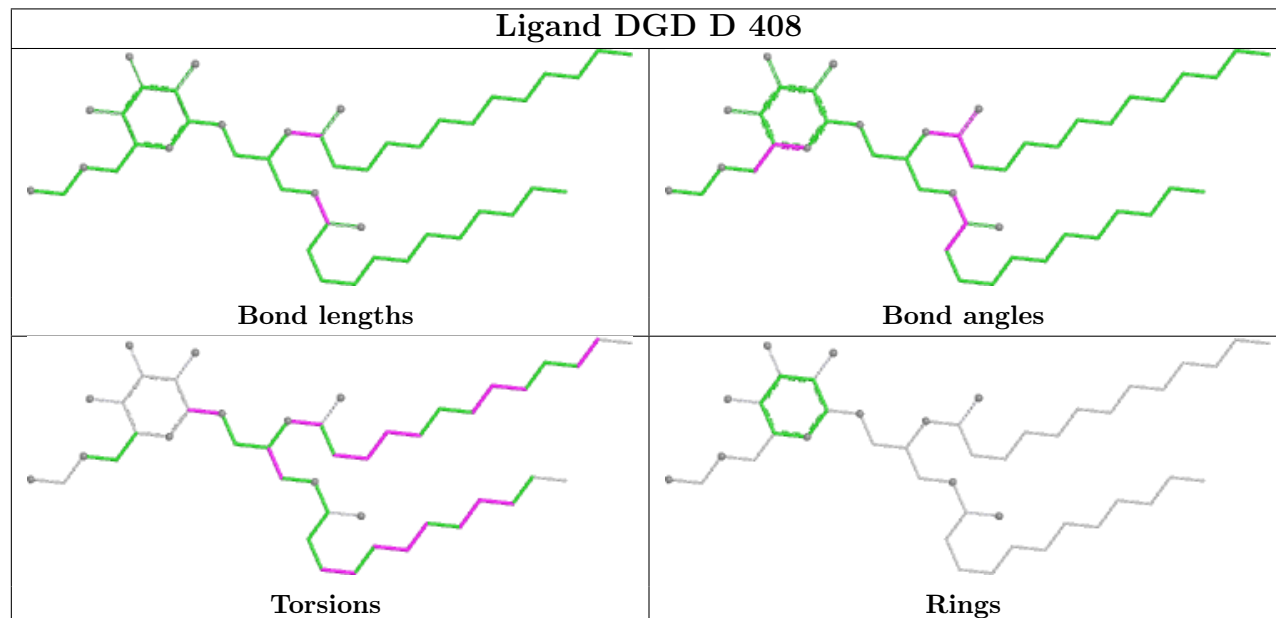
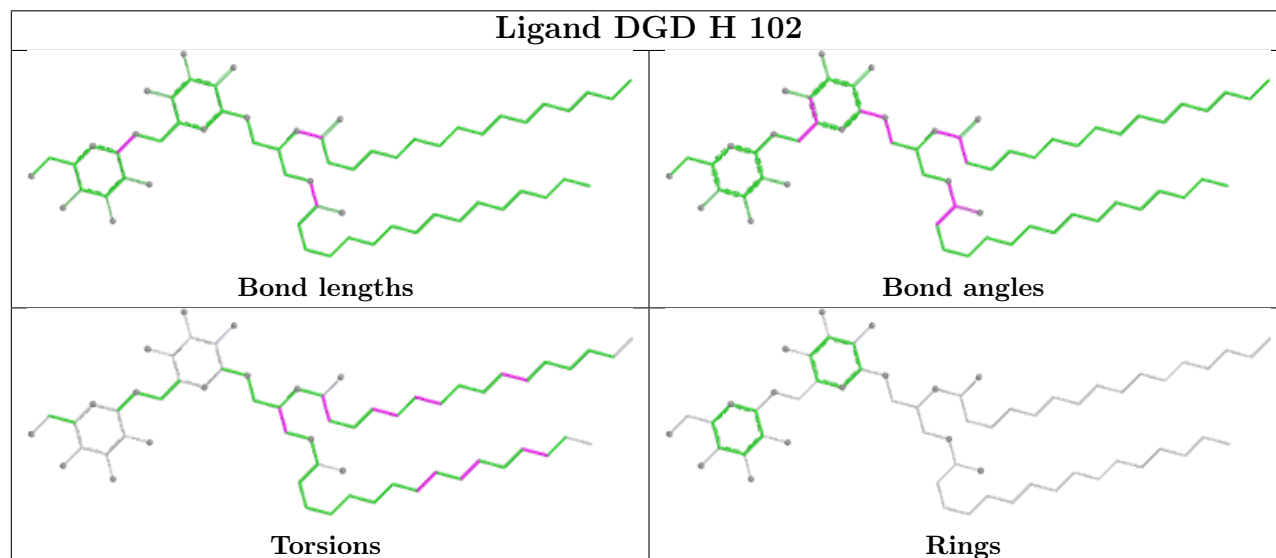
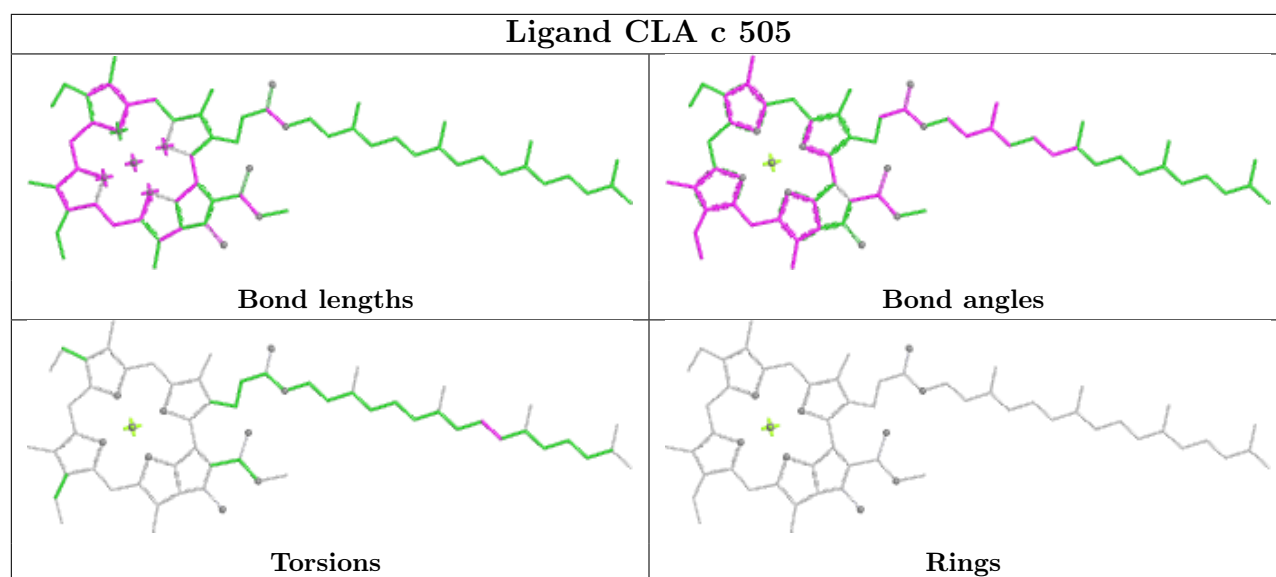


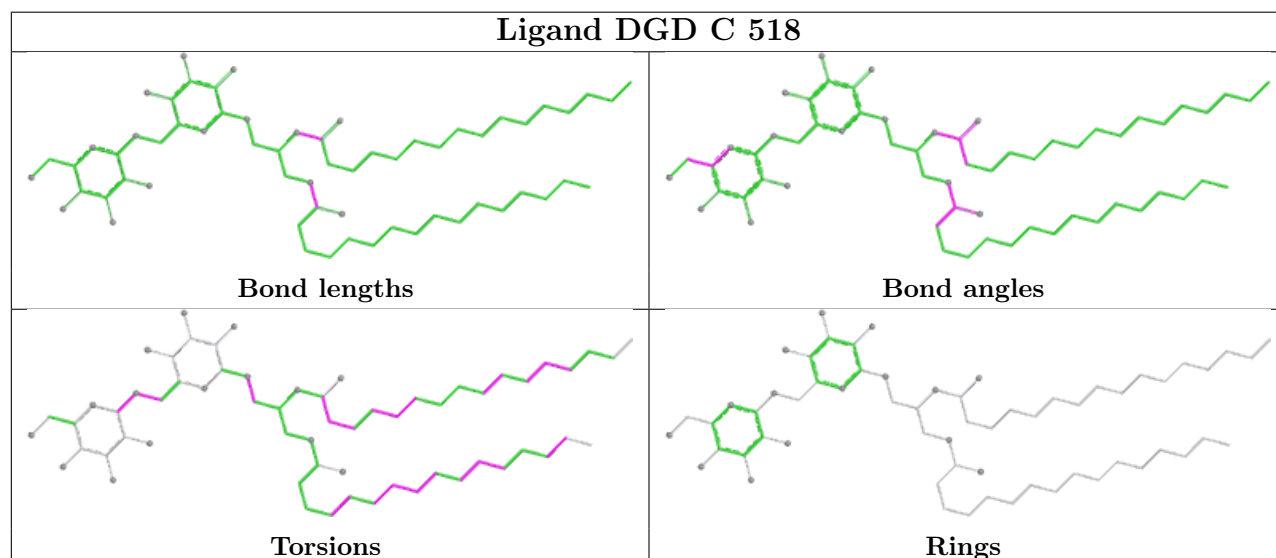
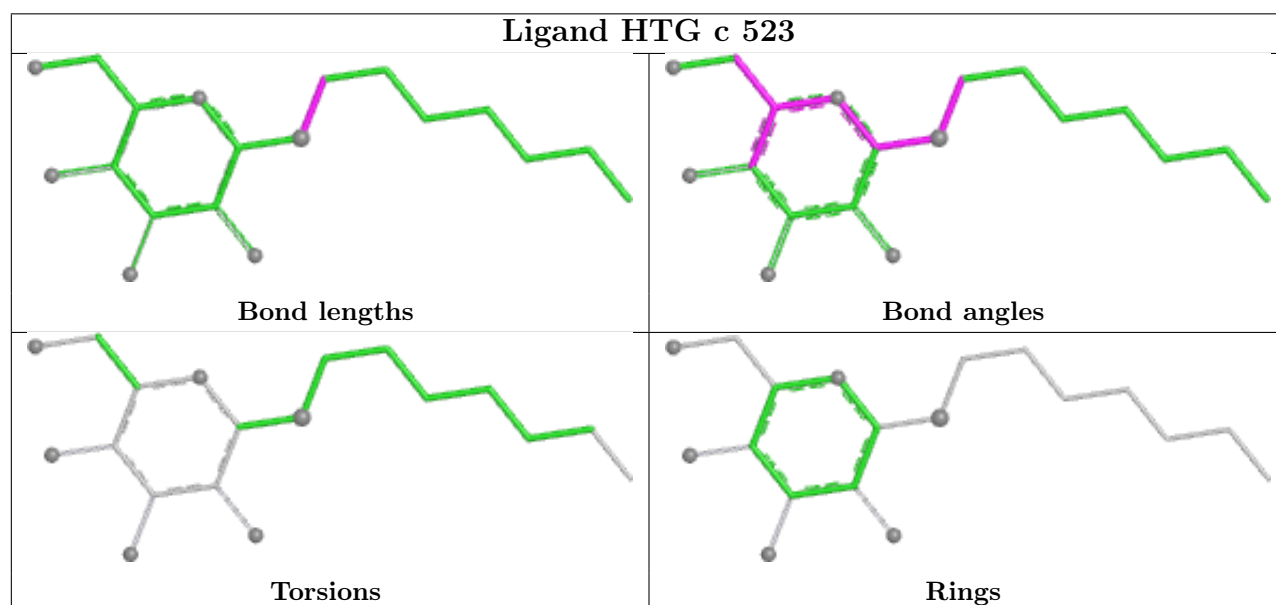
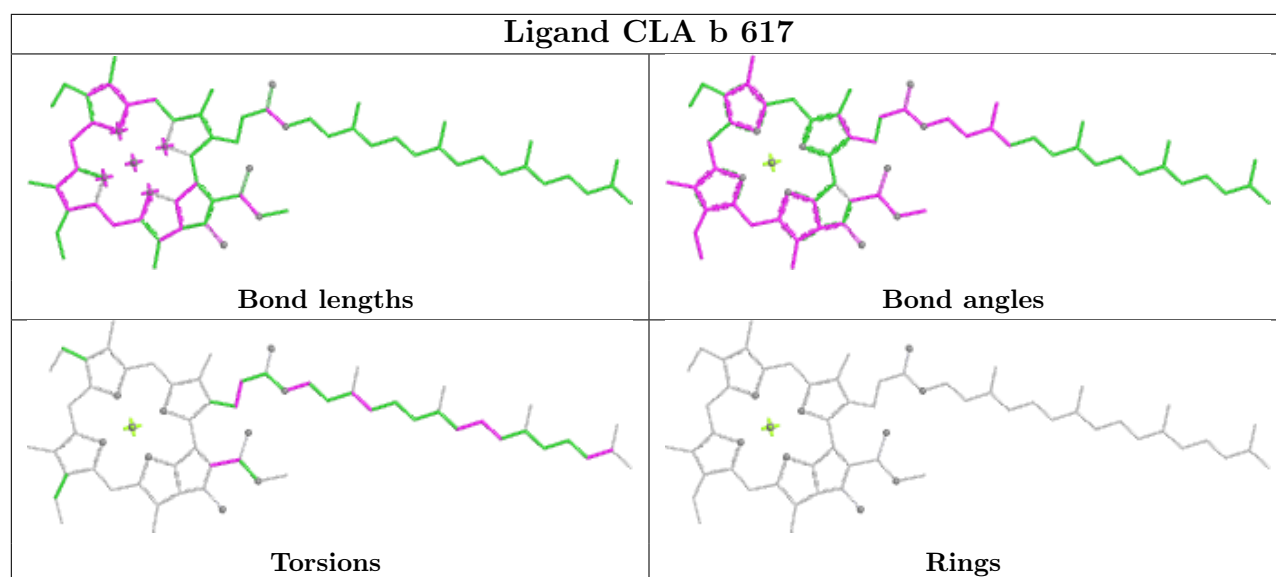
Ligand CLA B 616

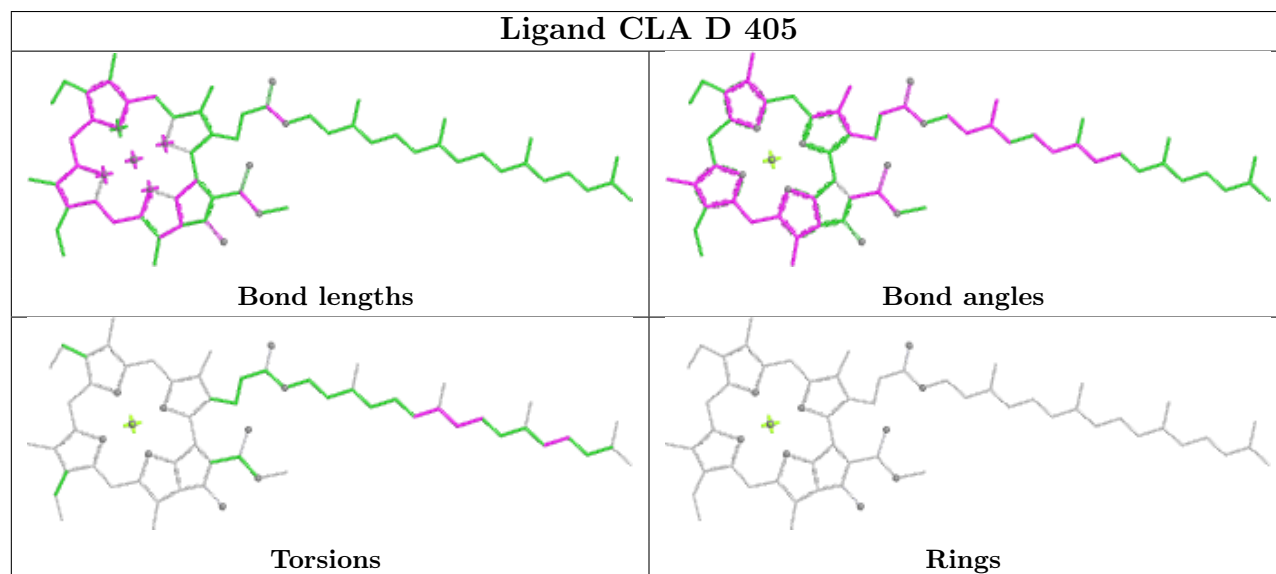
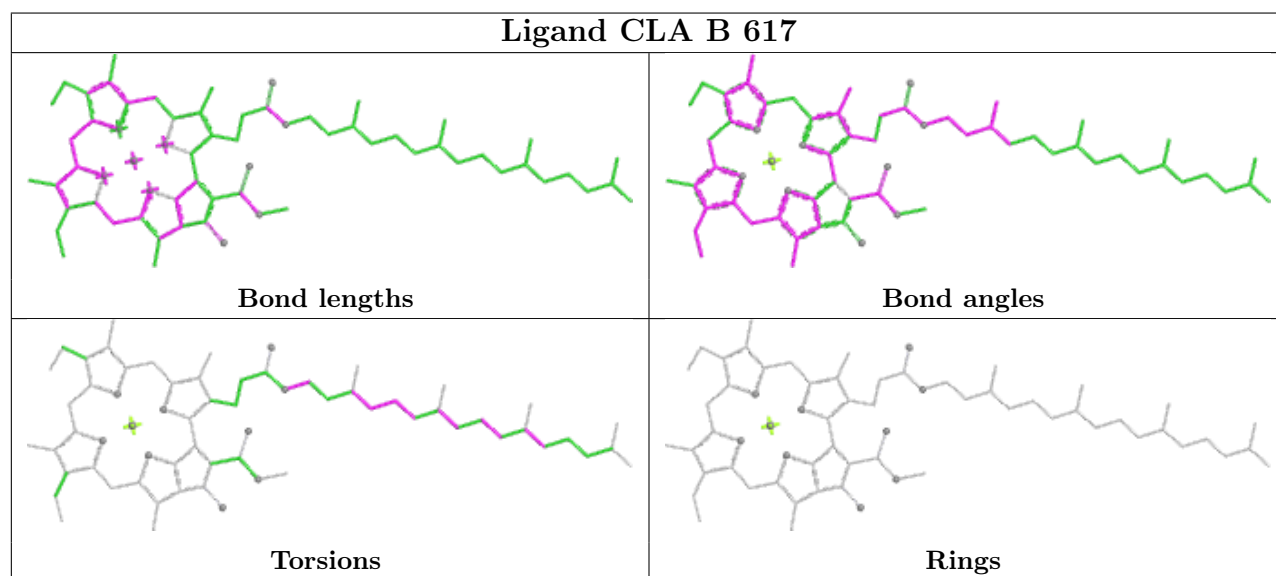
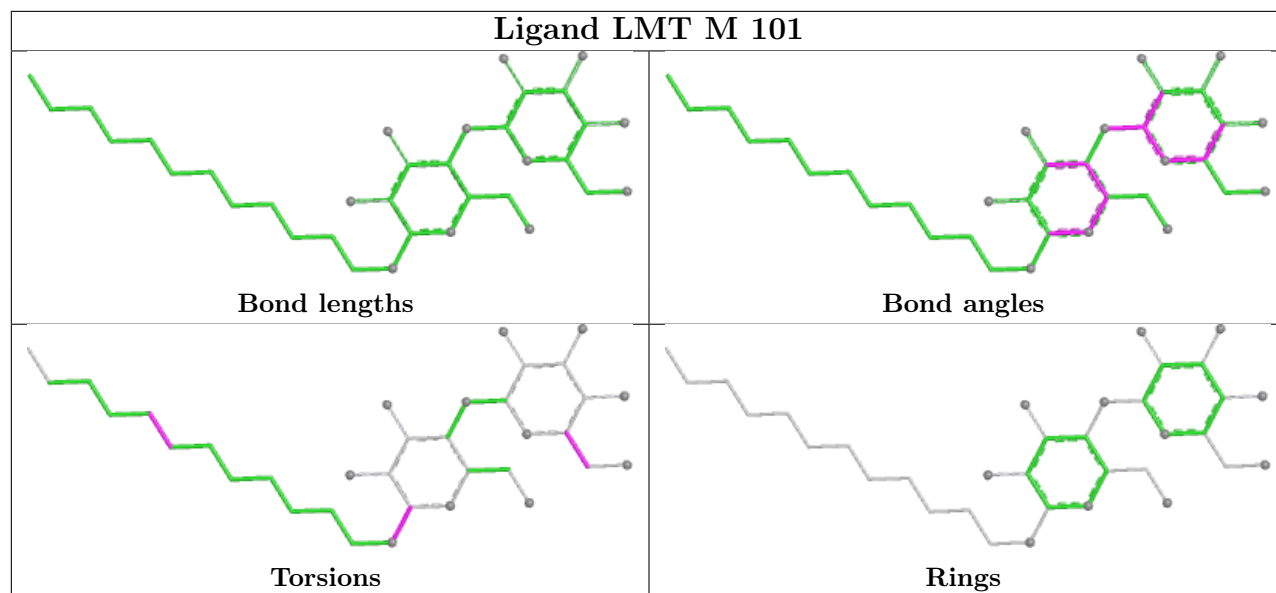




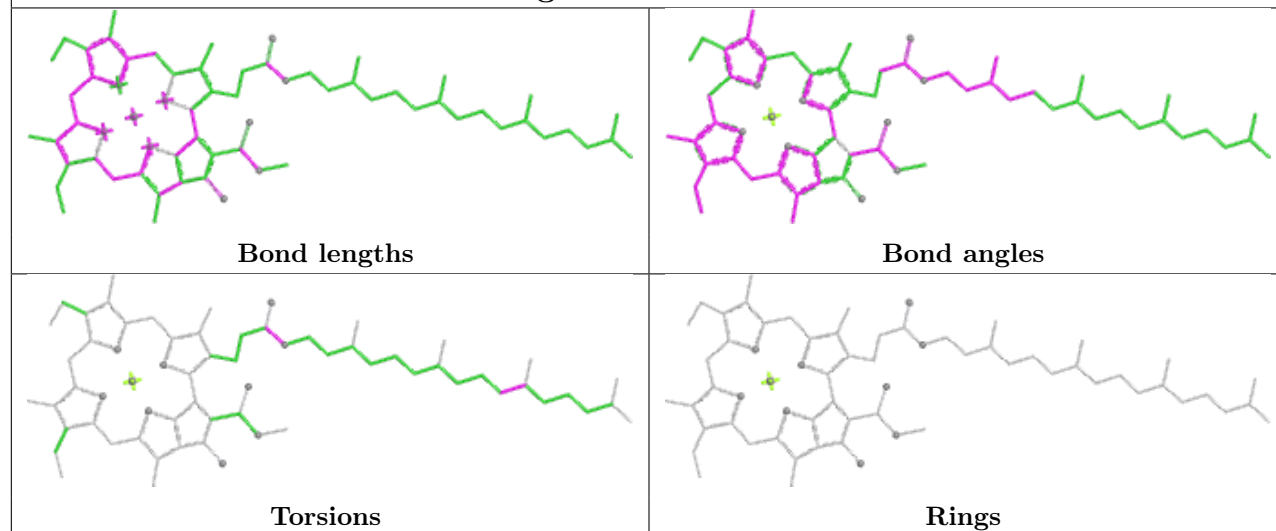




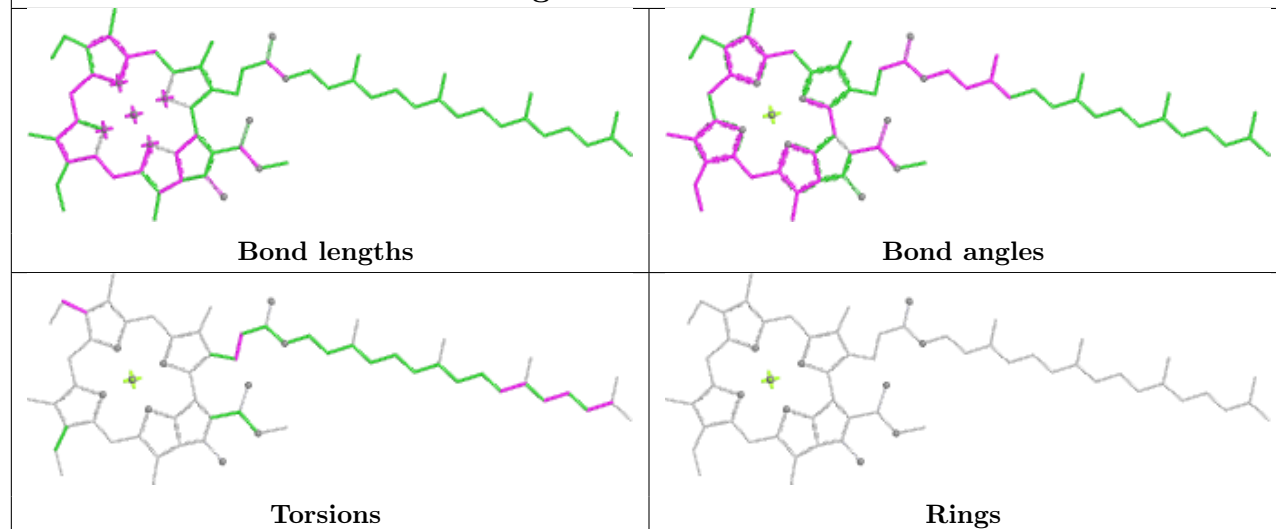




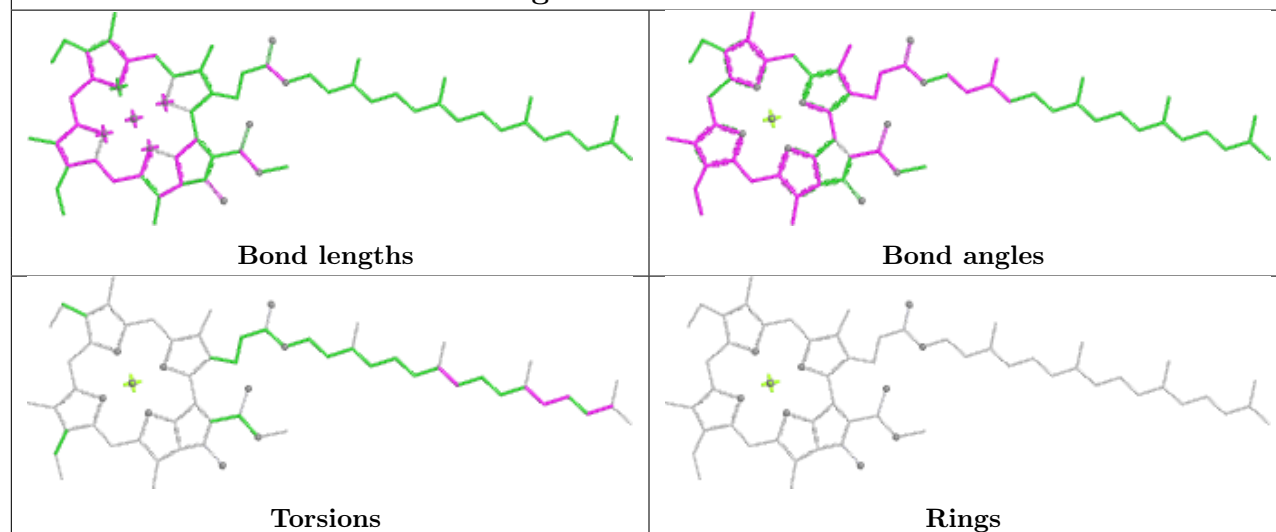
Ligand CLA c 513



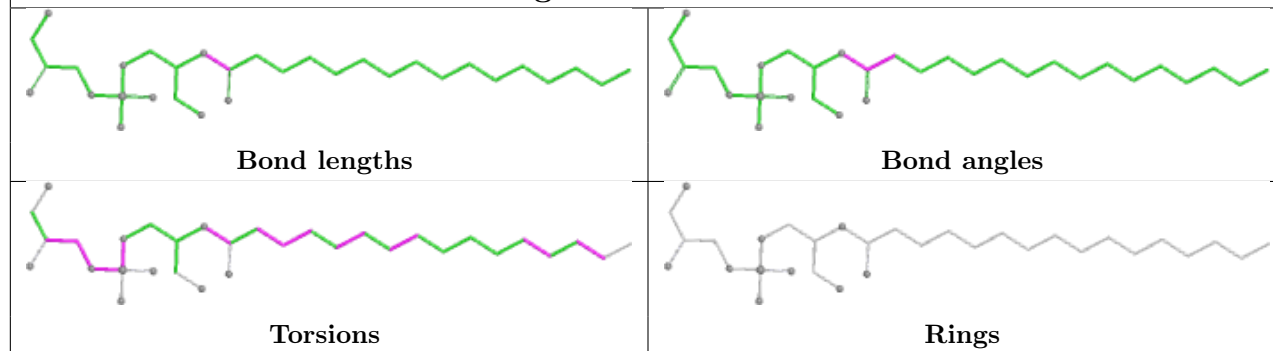
Ligand CLA B 607



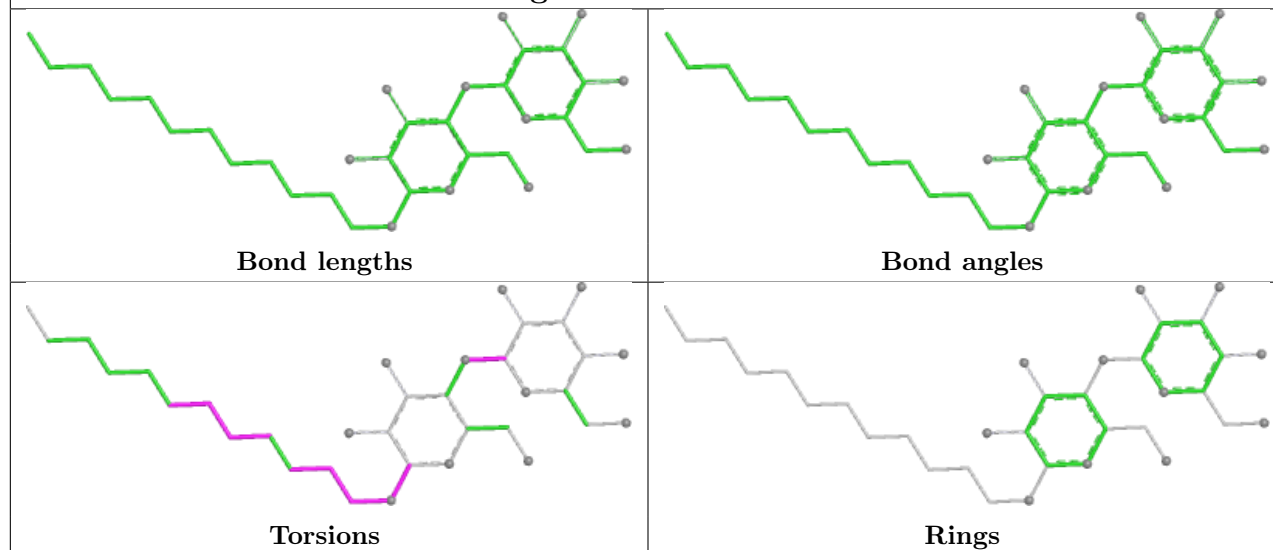
Ligand CLA A 406



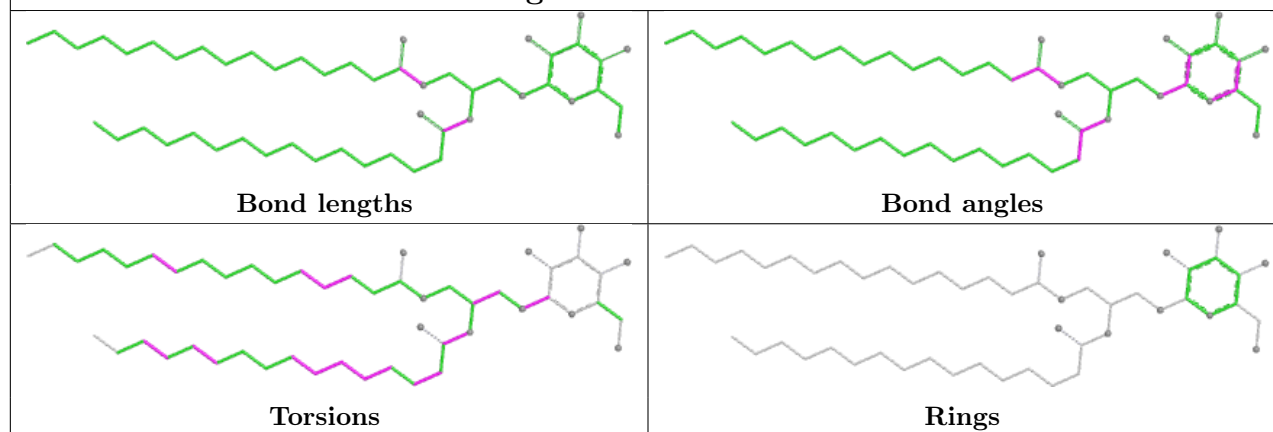
Ligand LHG e 101

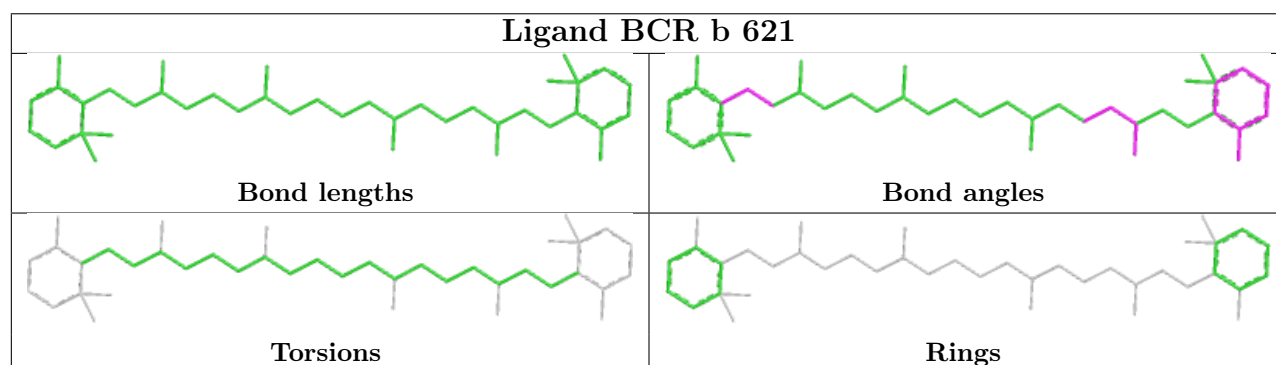
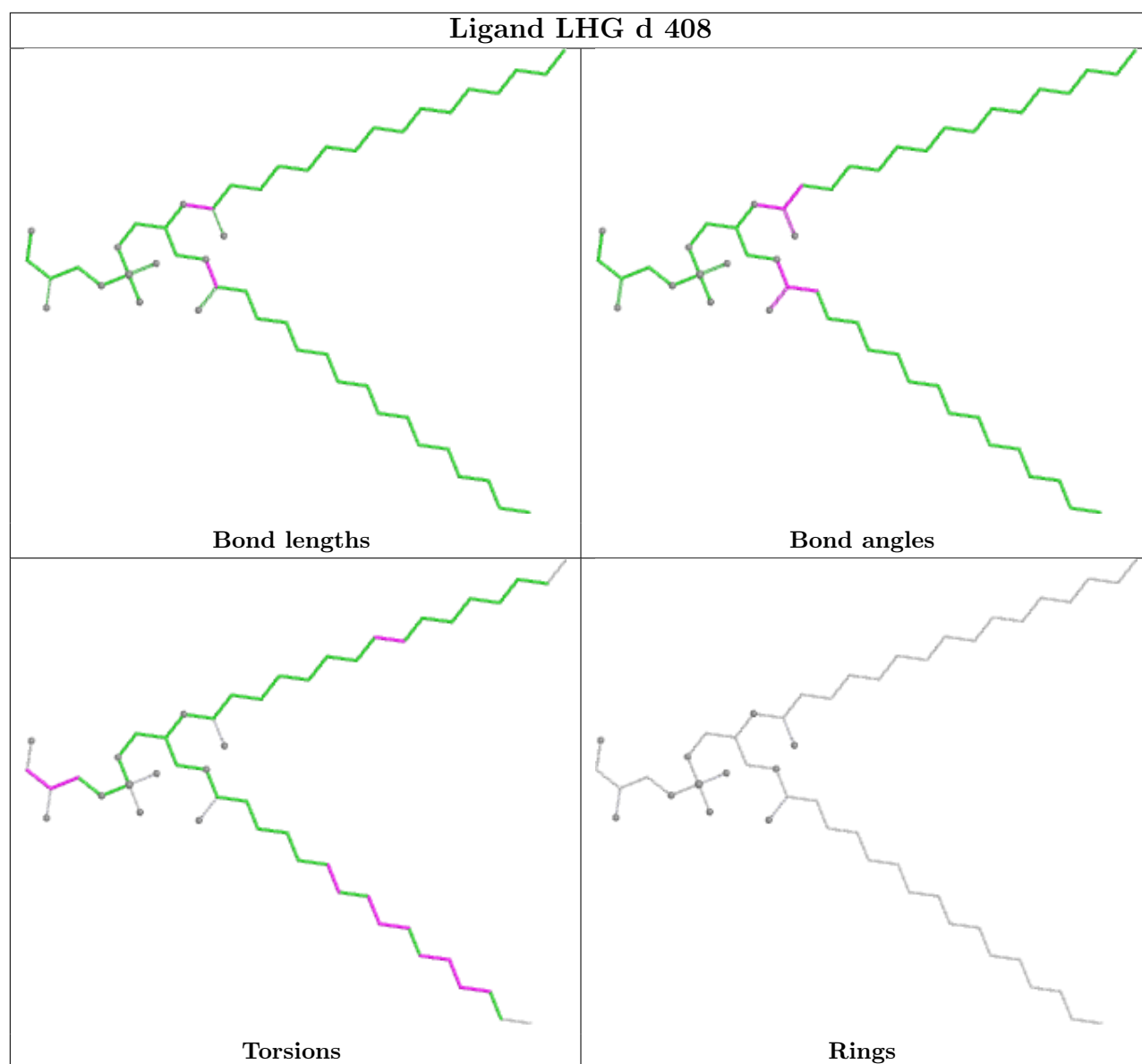


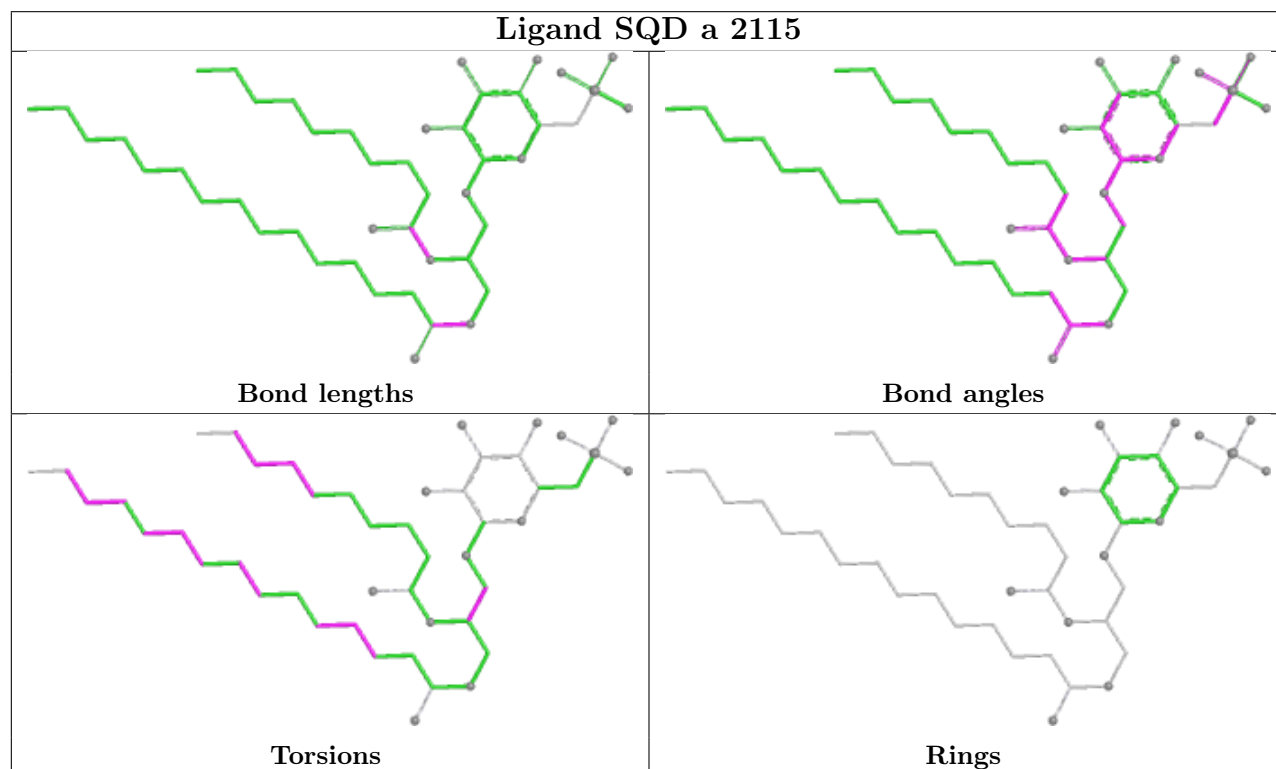
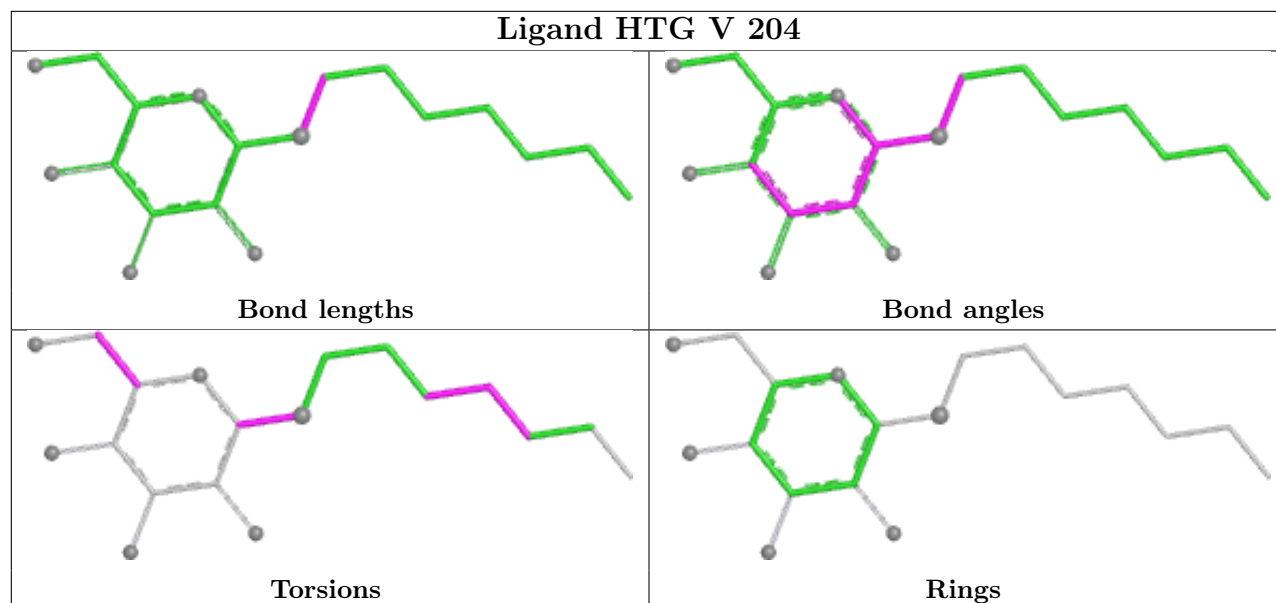
Ligand LMT Z 101

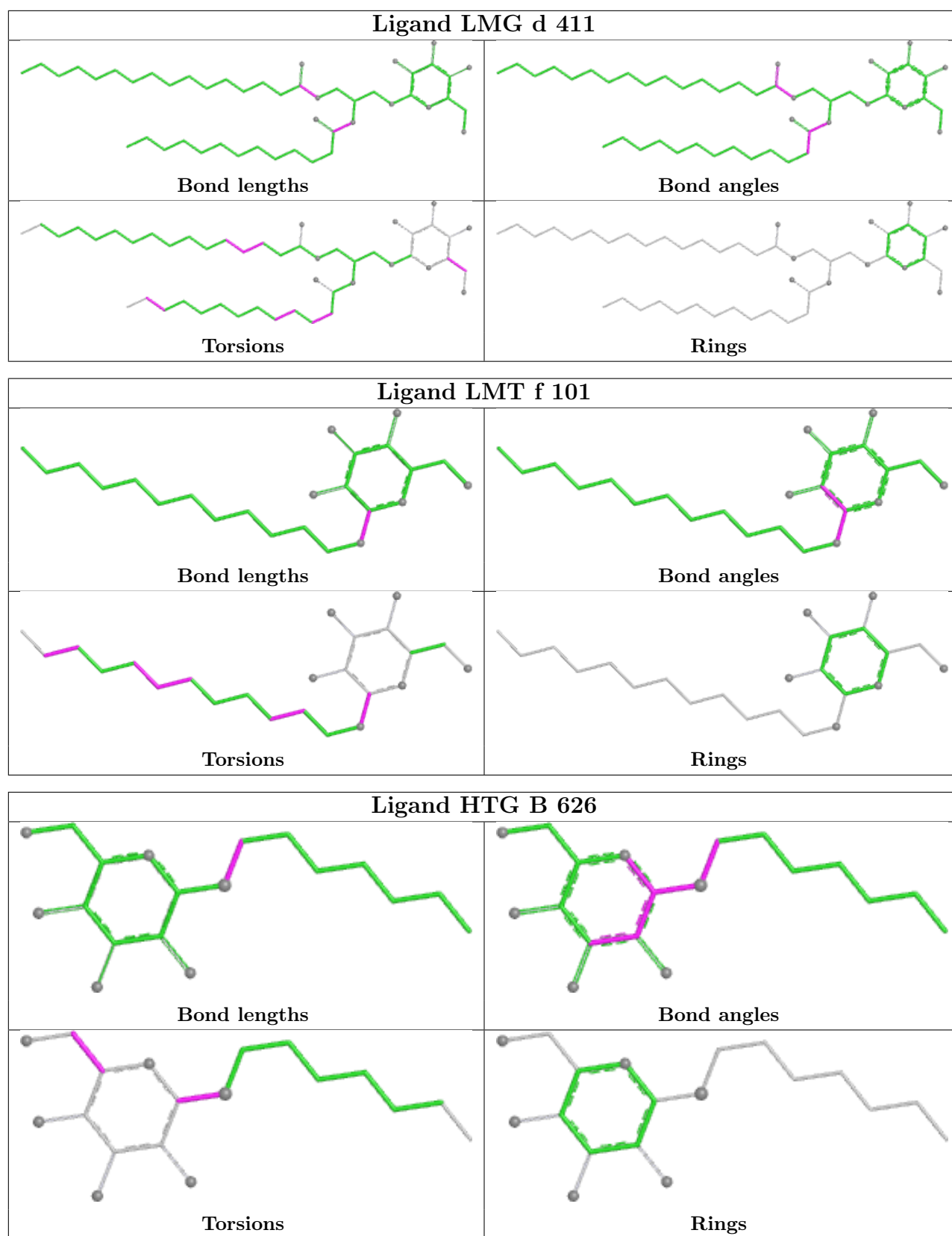


Ligand LMG A 412

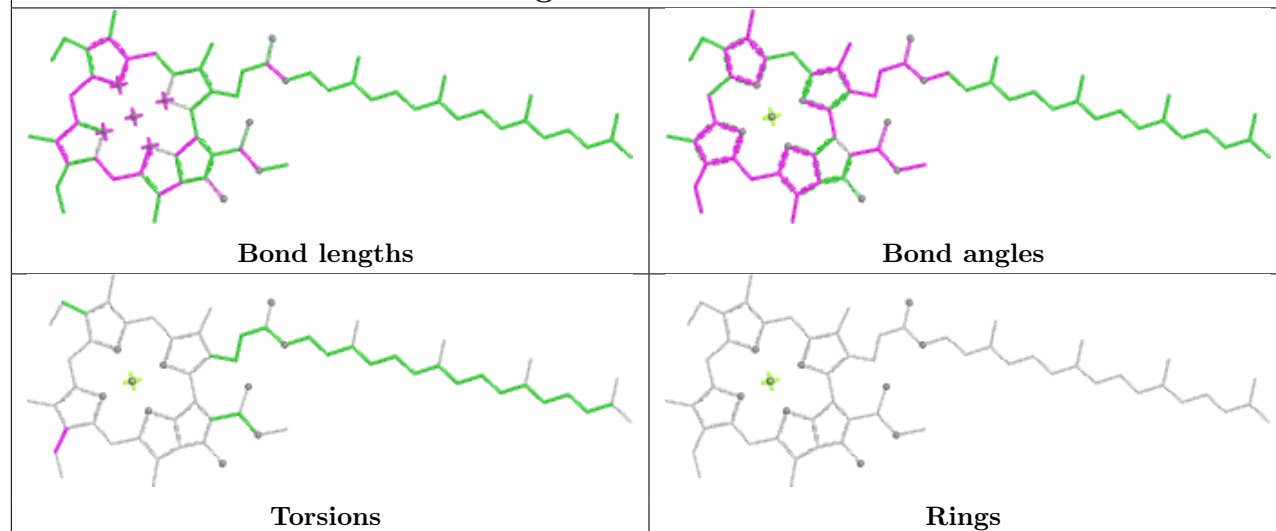




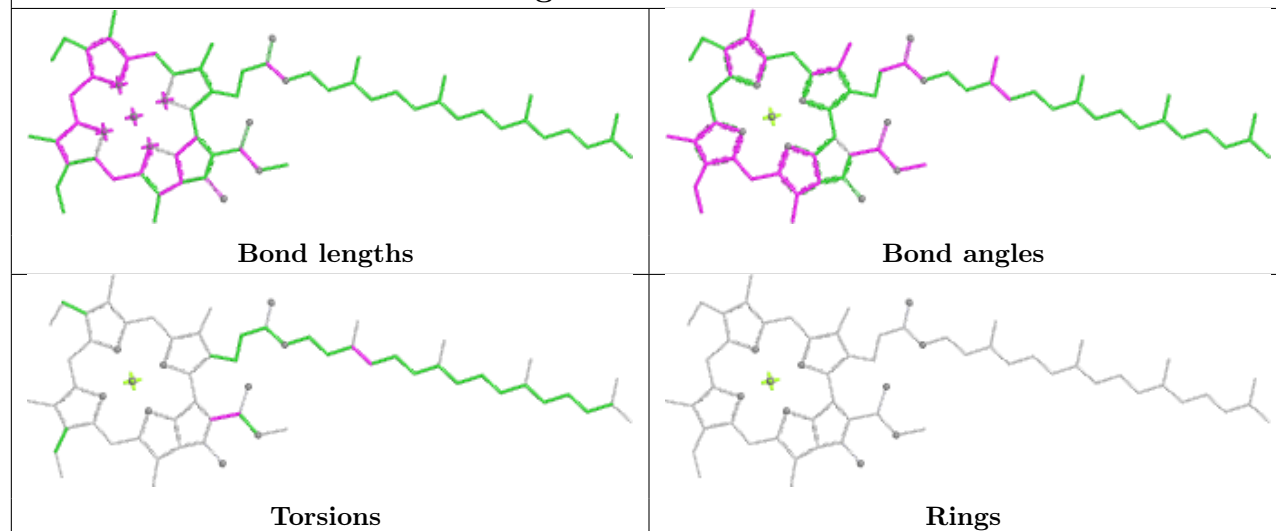




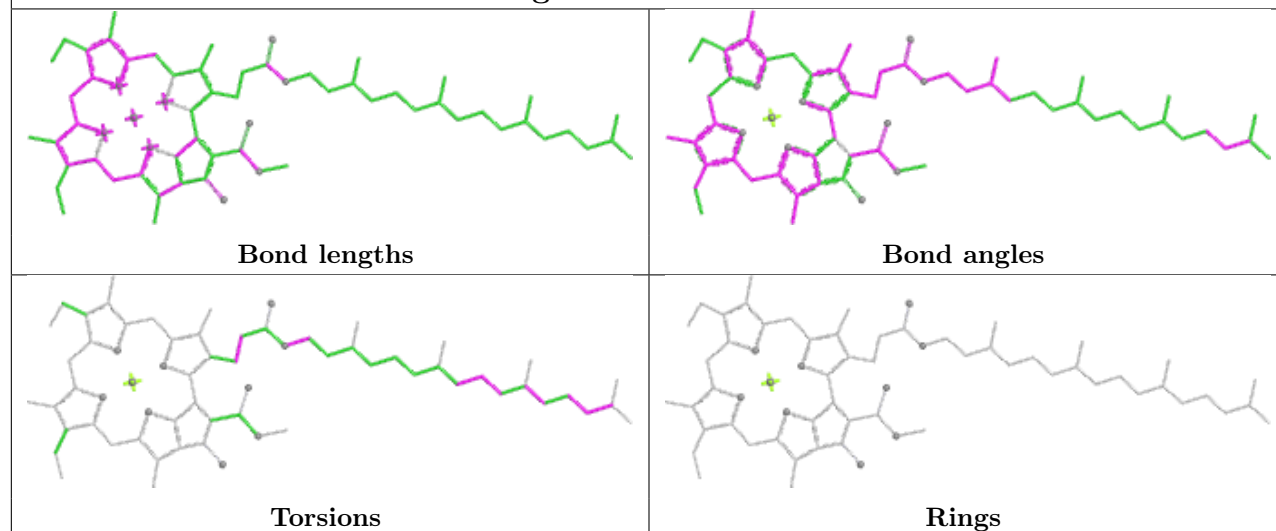
Ligand CLA d 401

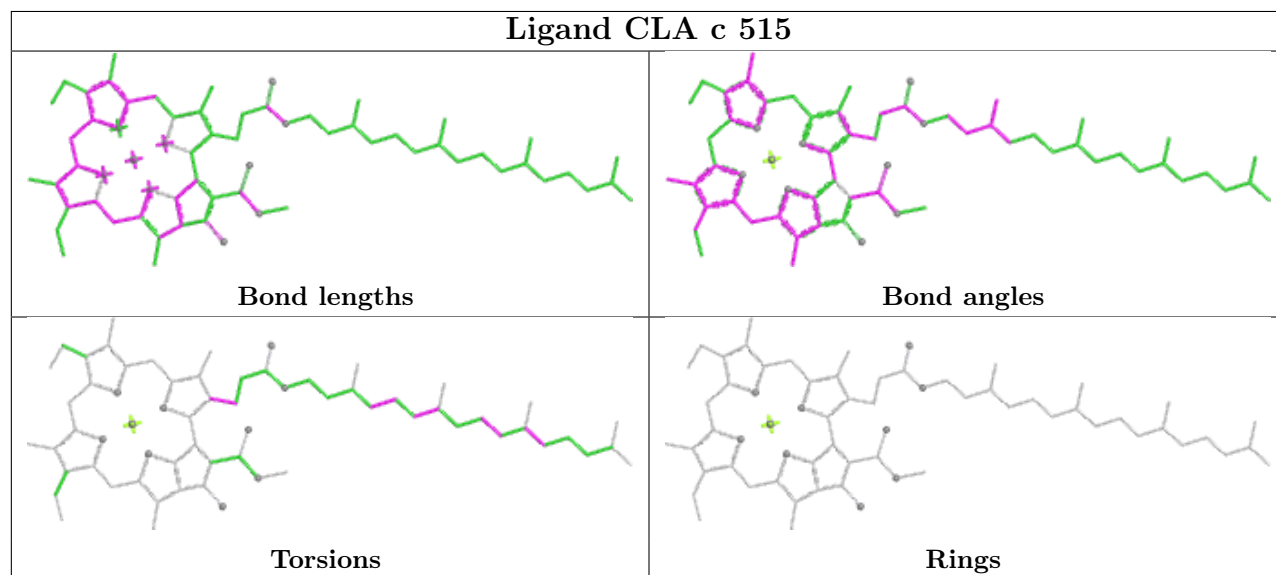
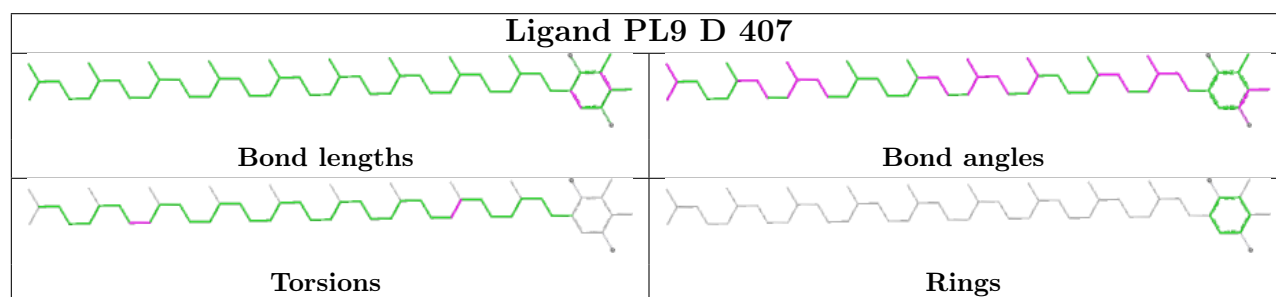
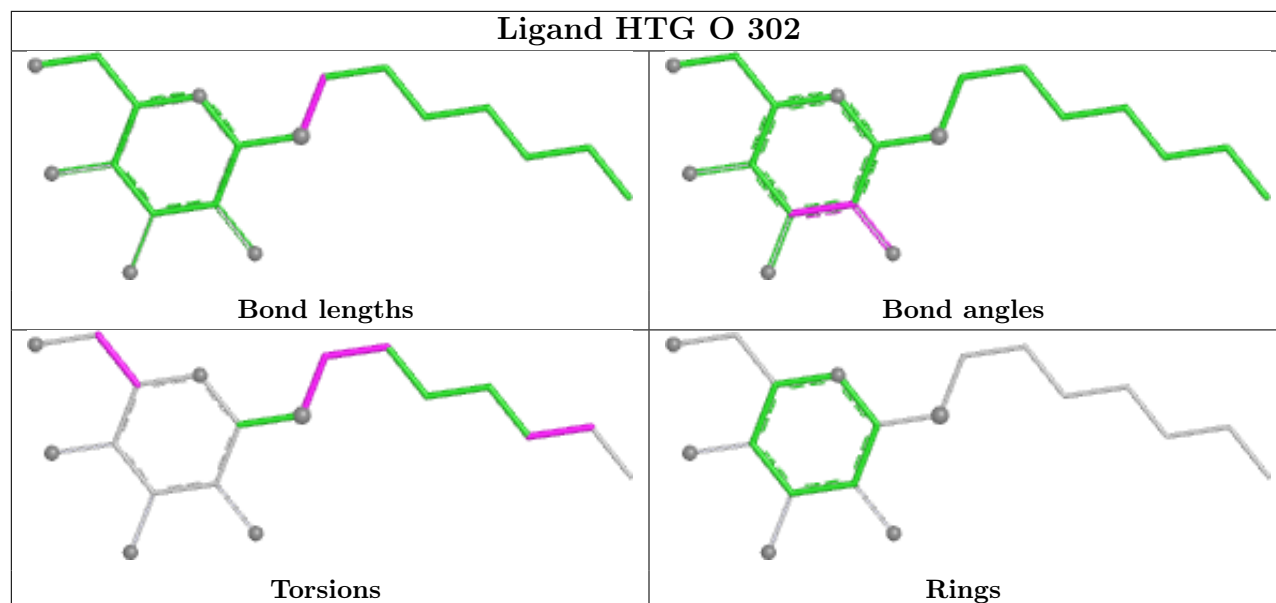


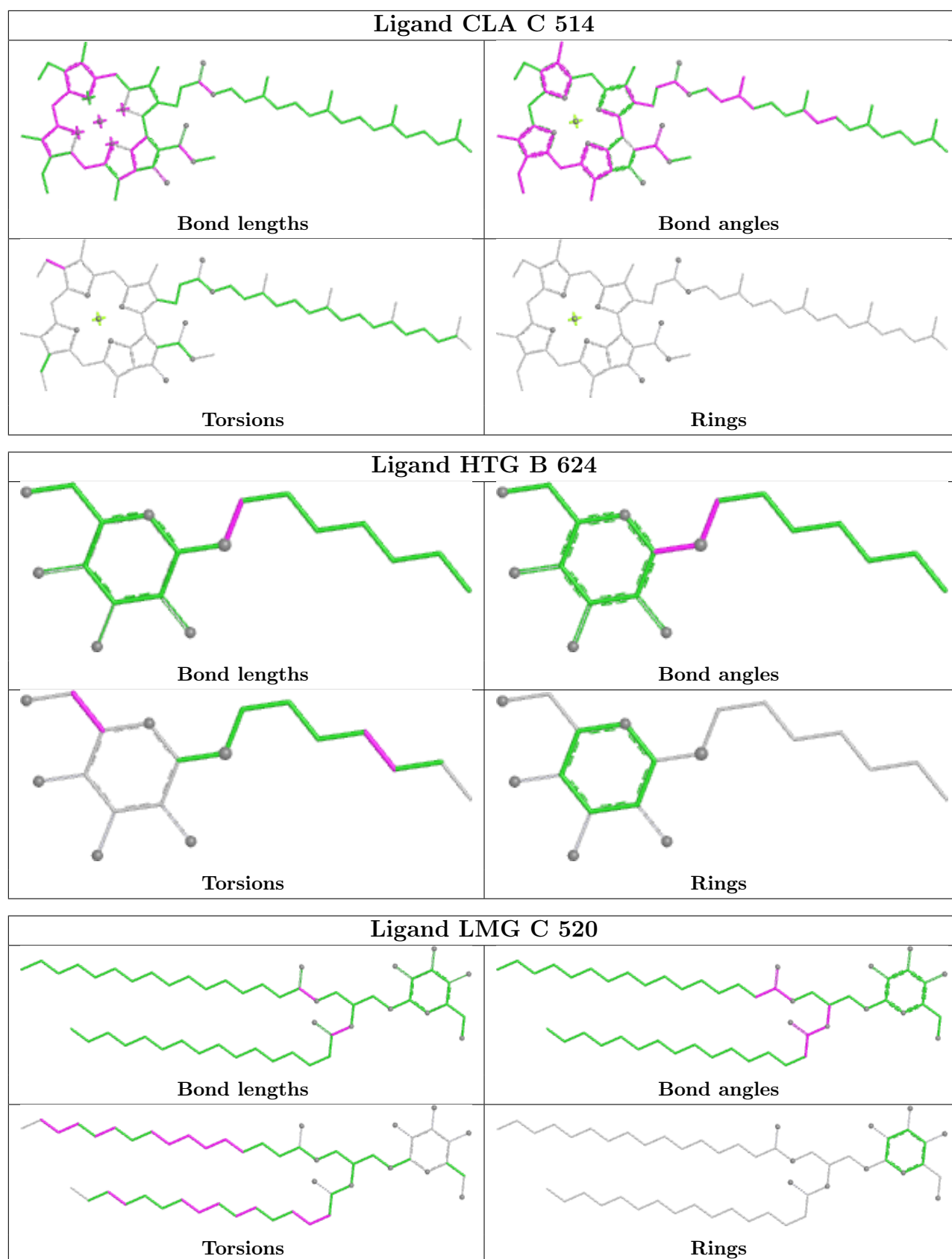
Ligand CLA b 608

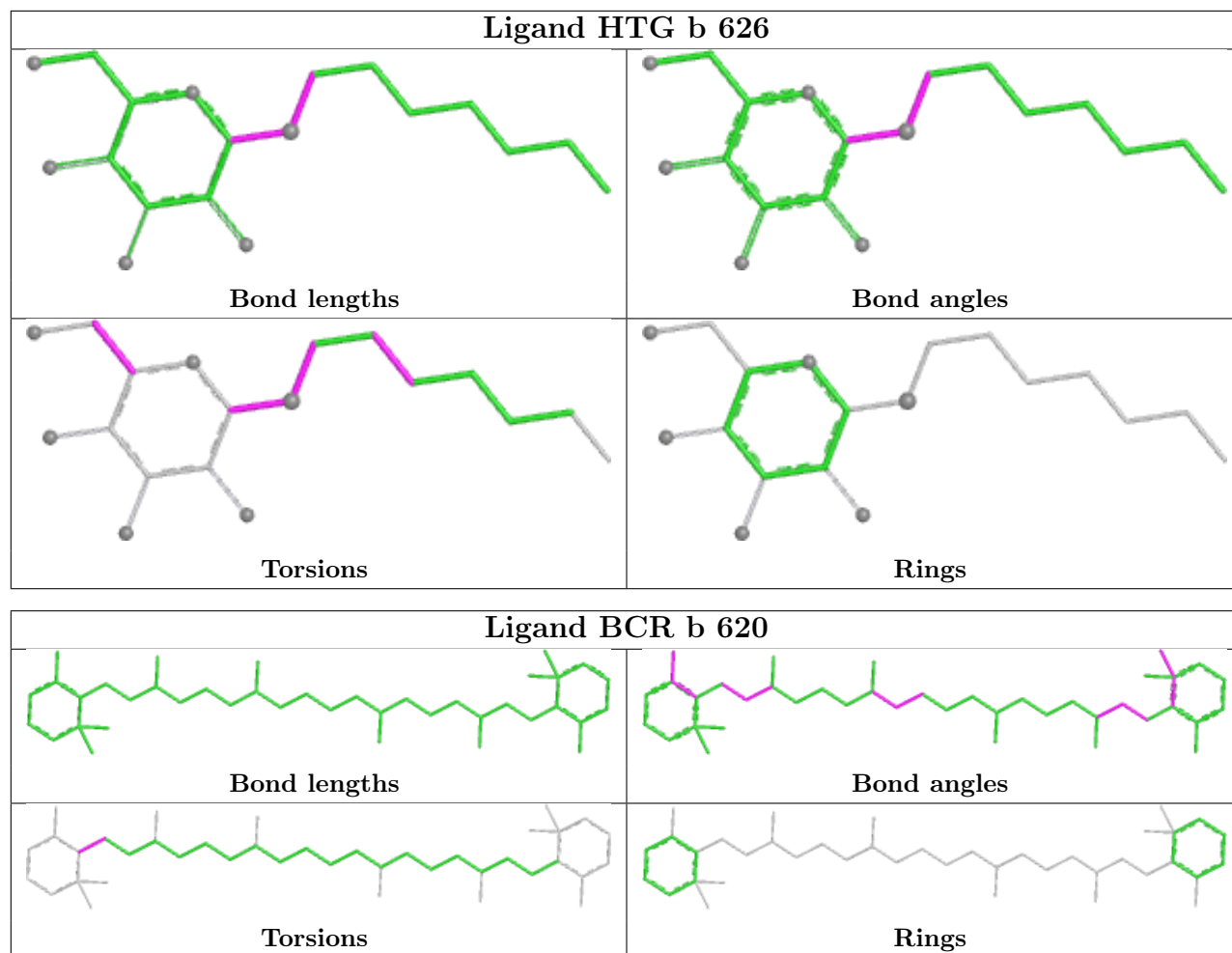


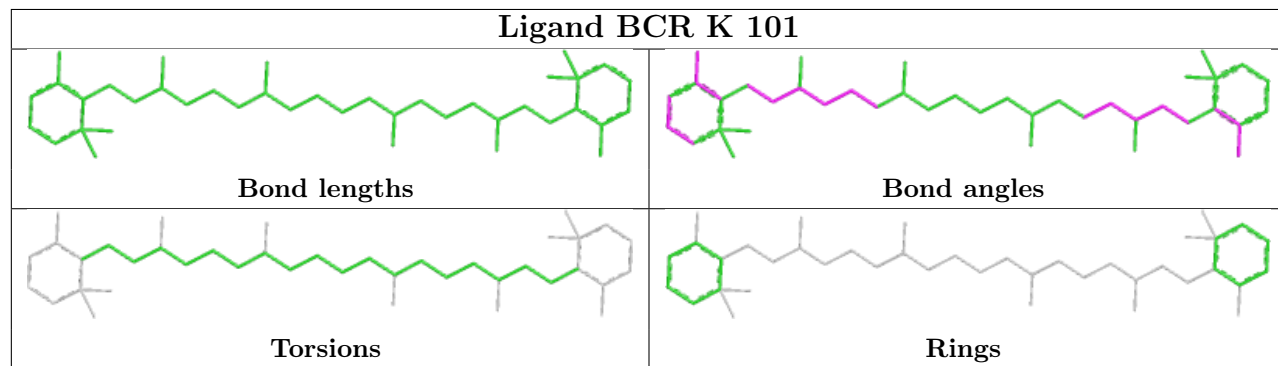
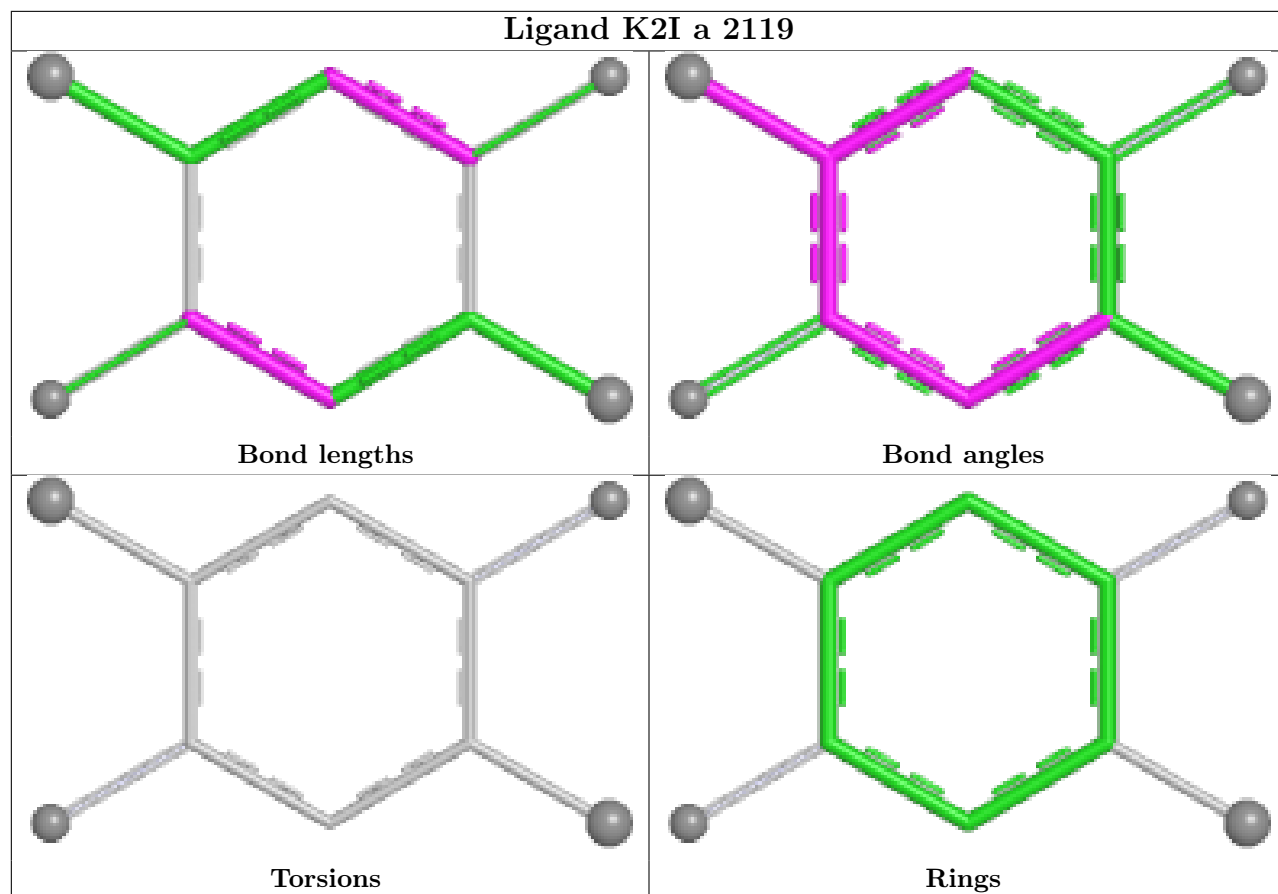
Ligand CLA B 611

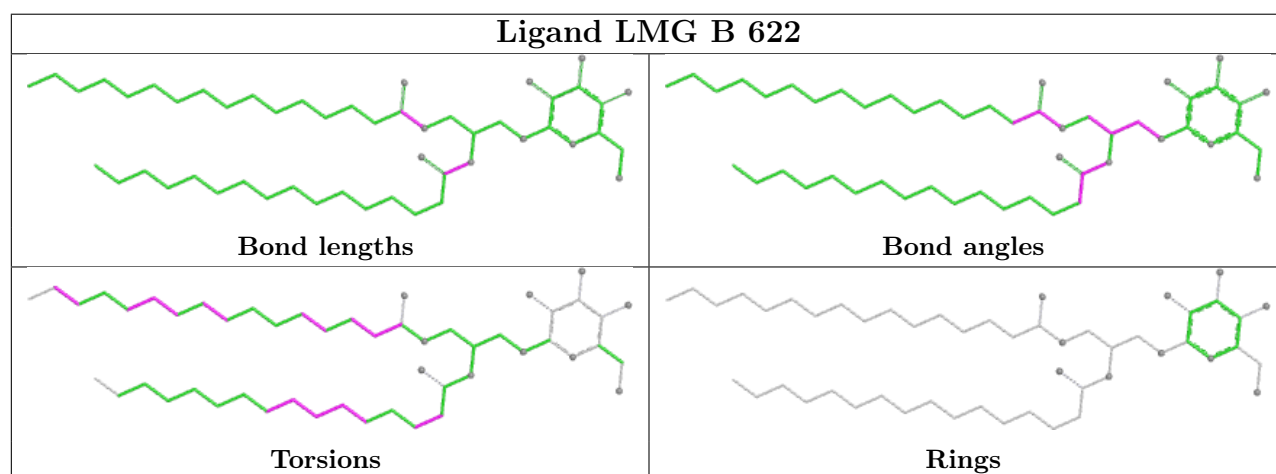
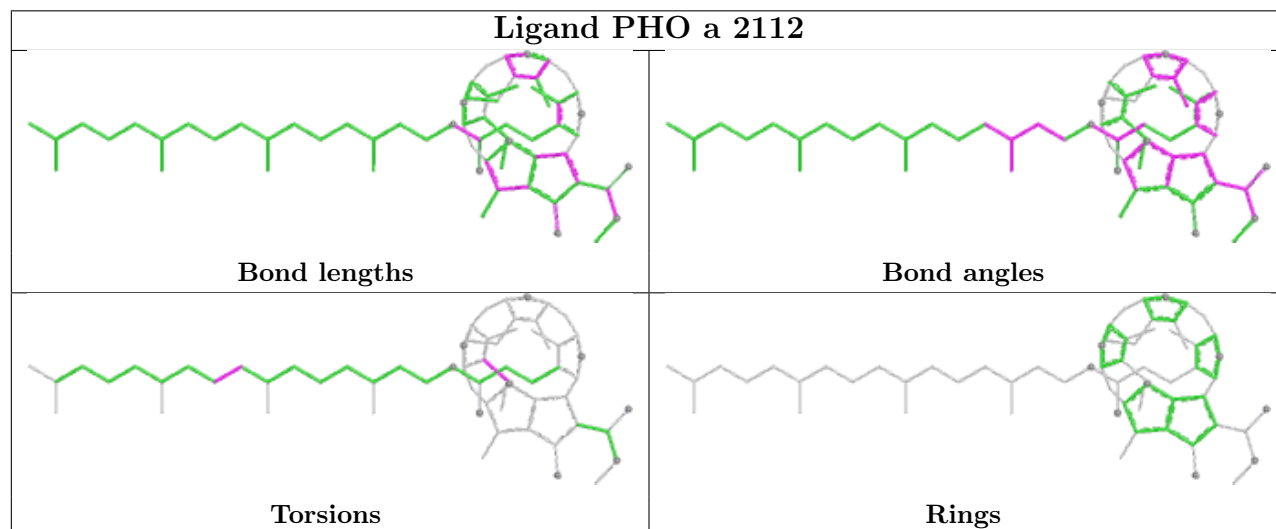
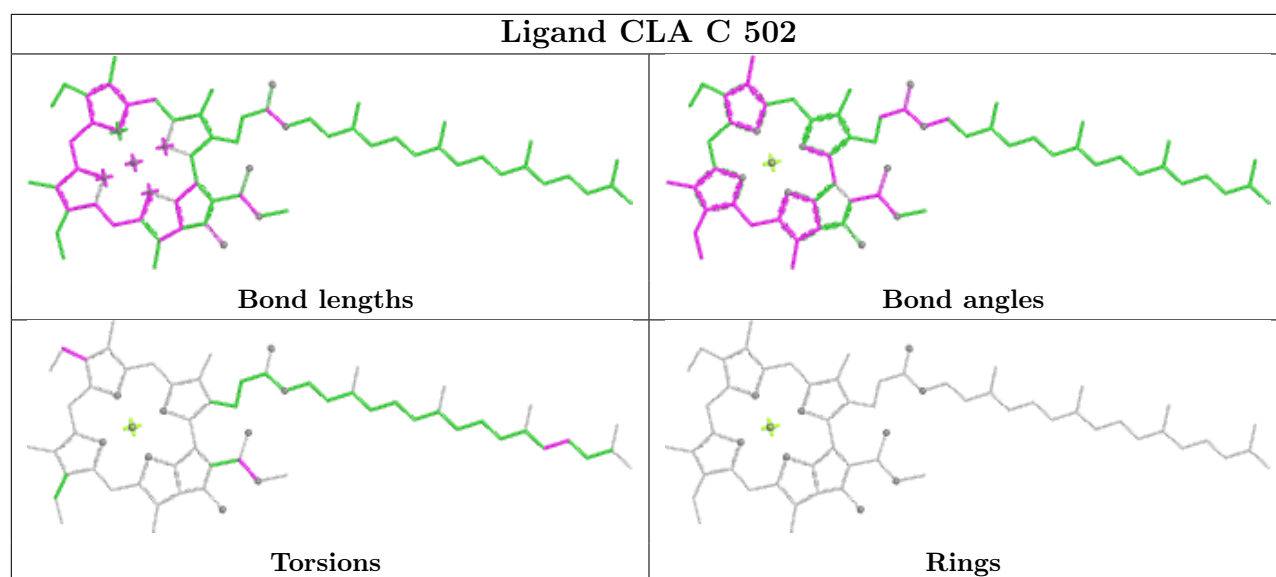


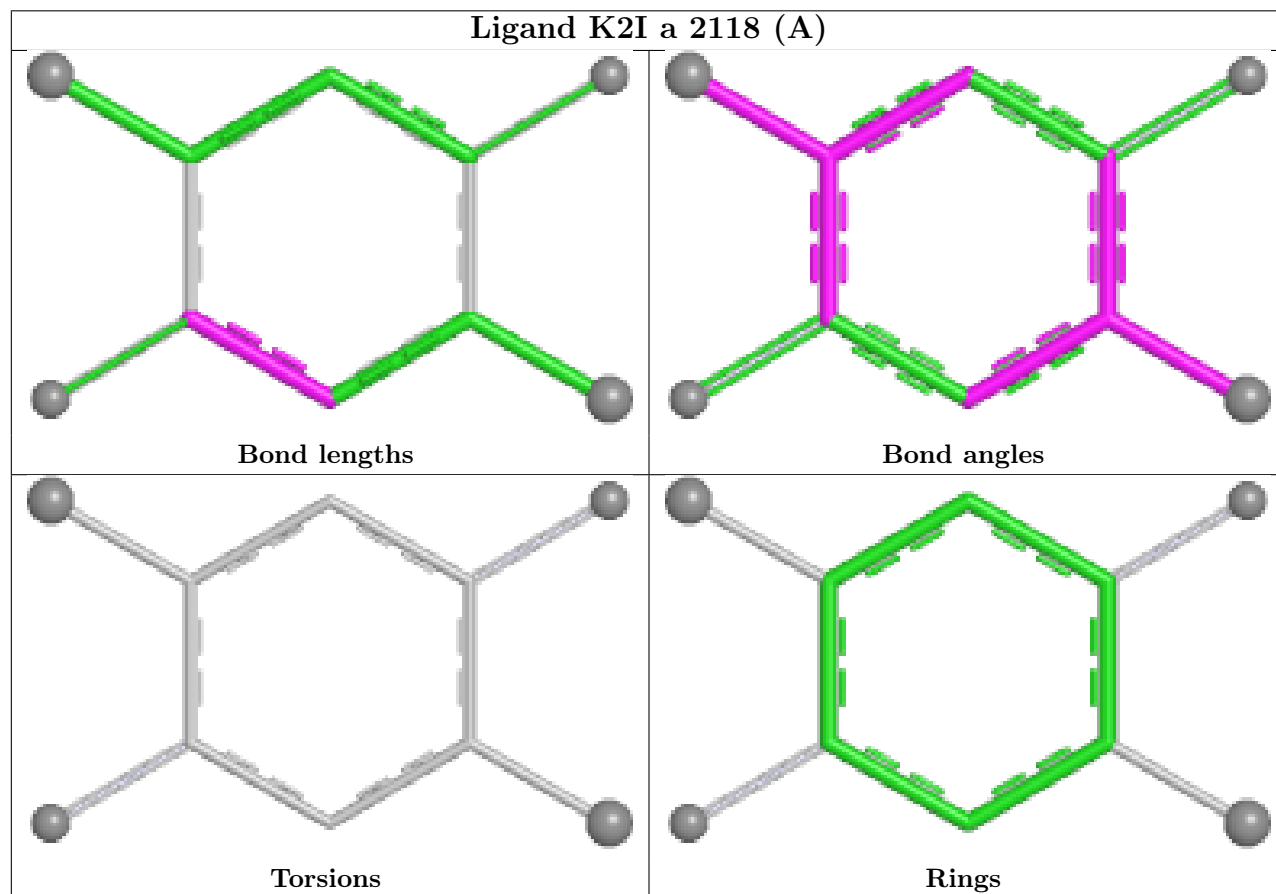
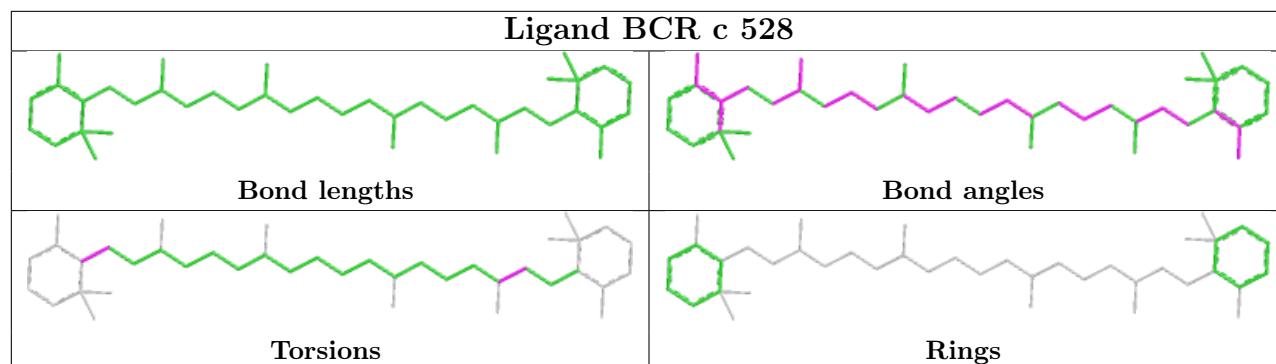


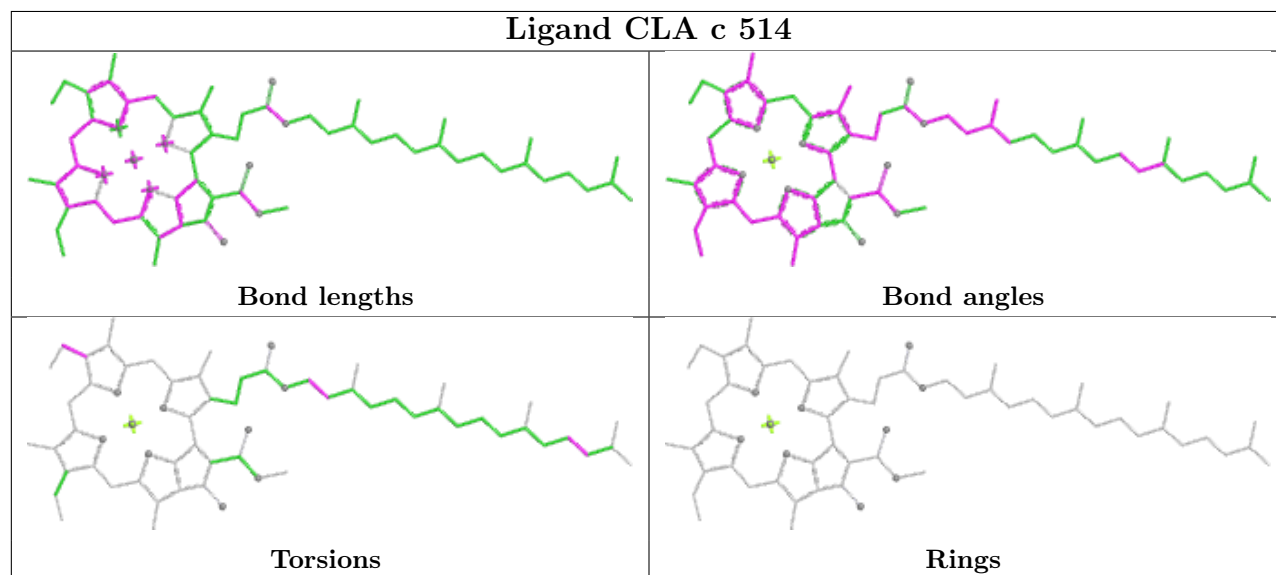
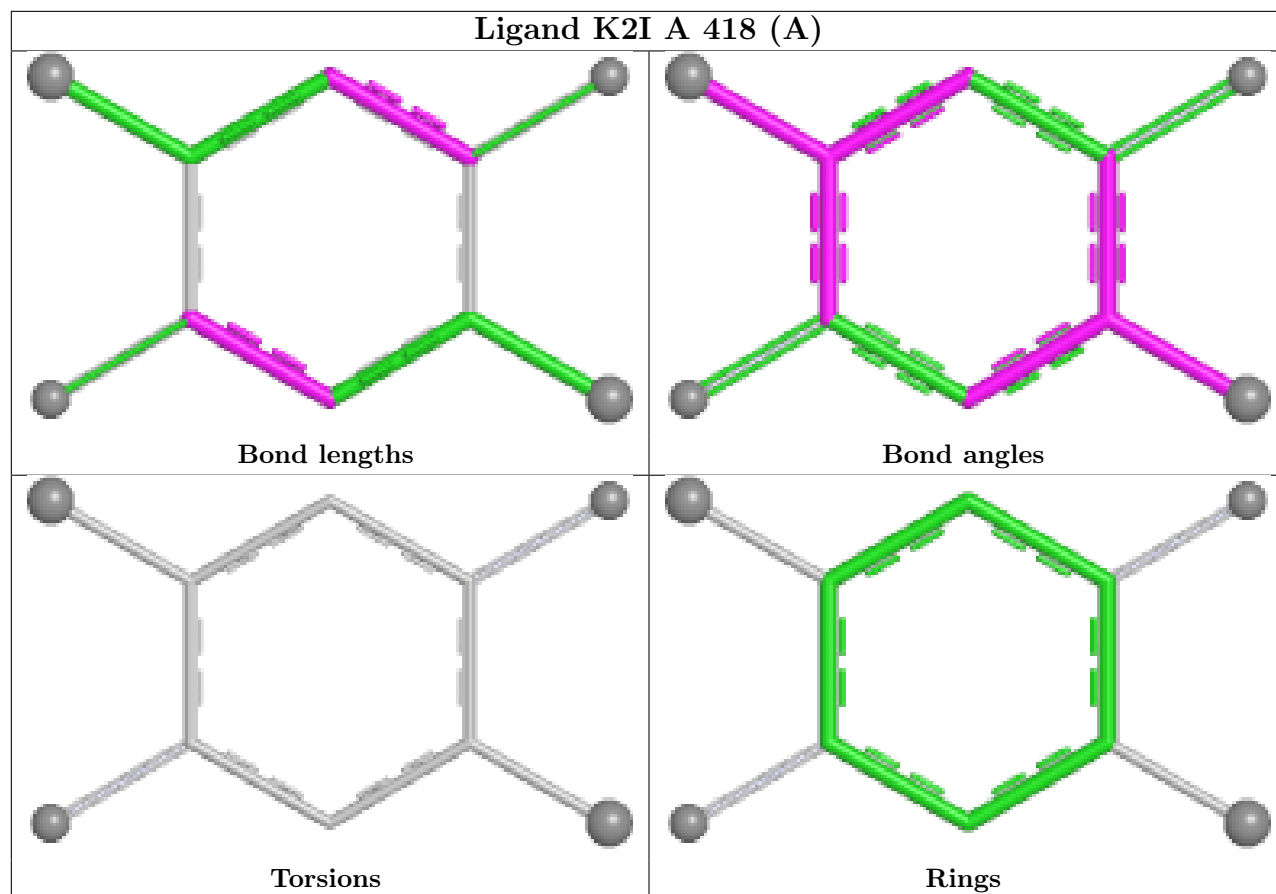


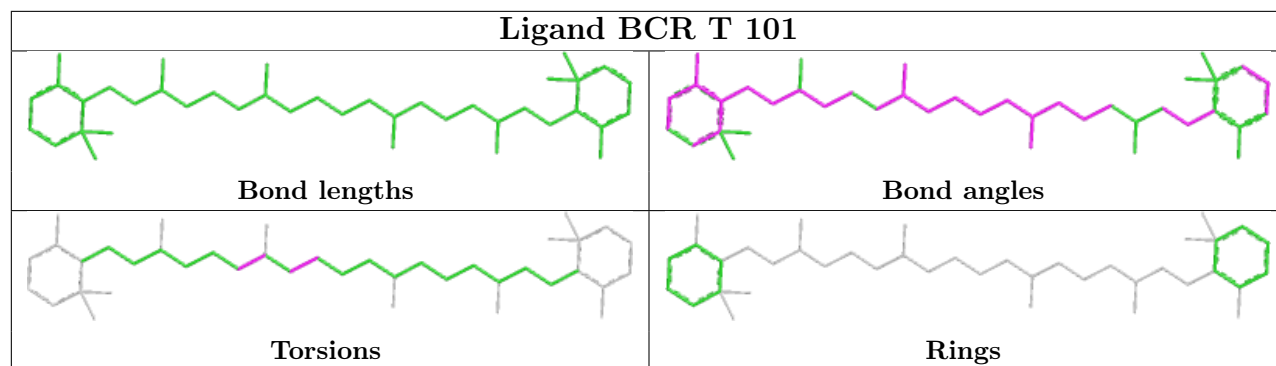












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.22	4 (1%) 76 78	27, 43, 72, 128	3 (0%)
1	a	334/344 (97%)	-0.07	7 (2%) 63 66	27, 45, 84, 116	3 (0%)
2	B	505/505 (100%)	-0.13	10 (1%) 65 67	27, 48, 79, 117	5 (0%)
2	b	503/505 (99%)	-0.05	17 (3%) 48 50	31, 50, 88, 168	8 (1%)
3	C	451/455 (99%)	-0.13	5 (1%) 78 80	35, 52, 71, 138	2 (0%)
3	c	455/455 (100%)	-0.00	4 (0%) 81 83	43, 57, 75, 119	0
4	D	340/342 (99%)	-0.25	1 (0%) 90 91	22, 44, 64, 107	1 (0%)
4	d	341/342 (99%)	-0.28	0 100 100	25, 46, 70, 114	3 (0%)
5	E	80/83 (96%)	0.28	4 (5%) 34 36	44, 66, 108, 118	1 (1%)
5	e	79/83 (95%)	0.29	3 (3%) 44 46	52, 67, 101, 124	0
6	F	34/44 (77%)	-0.20	1 (2%) 53 56	48, 56, 86, 104	0
6	f	32/44 (72%)	0.19	3 (9%) 14 14	49, 58, 104, 129	0
7	H	63/63 (100%)	0.15	1 (1%) 70 73	45, 57, 74, 103	0
7	h	63/63 (100%)	0.29	1 (1%) 70 73	46, 61, 80, 102	0
8	I	35/38 (92%)	0.61	1 (2%) 53 56	47, 63, 114, 124	0
8	i	35/38 (92%)	0.29	1 (2%) 53 56	47, 62, 109, 130	0
9	J	36/40 (90%)	-0.03	2 (5%) 30 32	45, 60, 95, 109	0
9	j	39/40 (97%)	-0.03	0 100 100	51, 62, 86, 108	0
10	K	37/37 (100%)	-0.07	0 100 100	38, 59, 73, 88	1 (2%)
10	k	37/37 (100%)	0.28	1 (2%) 56 59	54, 64, 85, 100	0
11	L	37/37 (100%)	-0.12	4 (10%) 11 11	22, 42, 94, 127	1 (2%)
11	l	36/37 (97%)	-0.24	1 (2%) 55 57	23, 43, 101, 128	2 (5%)
12	M	32/36 (88%)	-0.25	0 100 100	25, 44, 63, 86	1 (3%)
12	m	33/36 (91%)	-0.06	0 100 100	26, 45, 82, 105	1 (3%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	0.02	3 (1%) 76 78	32, 55, 89, 169	2 (0%)
13	o	243/244 (99%)	0.00	4 (1%) 70 73	29, 57, 101, 138	3 (1%)
14	T	29/32 (90%)	-0.01	2 (6%) 23 24	36, 43, 72, 147	0
14	t	29/32 (90%)	-0.06	1 (3%) 48 50	37, 43, 76, 98	0
15	U	97/104 (93%)	-0.14	0 100 100	37, 52, 79, 92	1 (1%)
15	u	97/104 (93%)	-0.10	1 (1%) 79 81	46, 56, 75, 124	0
16	V	137/137 (100%)	-0.19	2 (1%) 72 74	32, 50, 68, 98	1 (0%)
16	v	137/137 (100%)	-0.13	0 100 100	48, 63, 87, 99	0
17	Y	30/30 (100%)	0.40	1 (3%) 49 51	59, 74, 114, 121	0
17	y	29/30 (96%)	0.51	1 (3%) 48 50	64, 78, 100, 113	0
18	X	38/40 (95%)	0.13	2 (5%) 32 34	53, 66, 85, 92	0
18	x	38/40 (95%)	0.34	2 (5%) 32 34	37, 66, 123, 143	1 (2%)
19	Z	61/62 (98%)	0.39	2 (3%) 49 51	58, 69, 110, 130	0
19	z	60/62 (96%)	0.64	8 (13%) 7 7	66, 79, 125, 142	0
20	R	34/41 (82%)	2.52	23 (67%) 0 0	99, 139, 163, 165	0
All	All	5274/5387 (97%)	-0.04	123 (2%) 61 64	22, 52, 89, 169	40 (0%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	28	VAL	5.7
14	T	30	THR	5.3
20	R	26	TYR	4.8
7	H	64	ALA	4.7
1	a	260	PHE	4.7
18	x	37	VAL	4.5
2	b	495	PHE	4.4
2	b	499	VAL	4.2
7	h	64	ALA	3.9
2	b	493	TRP	3.6
2	b	487	SER	3.5
20	R	22	ASN	3.5
10	k	18	PHE	3.5
2	b	491	VAL	3.5
2	B	86	ILE	3.4
2	B	479	PHE	3.4
2	b	484	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	b	496	TYR	3.3
9	J	5	GLY	3.3
17	y	18	VAL	3.3
20	R	18	TRP	3.3
5	E	4	THR	3.3
3	c	183	GLY	3.3
20	R	35	LEU	3.3
14	t	30	THR	3.2
2	B	486	LEU	3.2
1	a	251	ALA	3.2
20	R	23	ILE	3.2
20	R	25	PRO	3.2
2	B	487	SER	3.1
20	R	31	VAL	3.1
20	R	6	LEU	3.1
20	R	34	LEU	3.1
20	R	3	TRP	3.0
2	b	486	LEU	3.0
1	A	229	GLU	3.0
1	a	11	ALA	3.0
19	z	61	VAL	3.0
8	i	36	ASP	2.9
2	B	495	PHE	2.9
13	O	58	ASN	2.8
2	b	485	GLU	2.8
2	b	479	PHE	2.8
20	R	2	ASP	2.8
20	R	10	LEU	2.8
20	R	24	LEU	2.8
18	x	2	THR	2.8
1	A	11	ALA	2.8
3	C	143	TYR	2.7
20	R	20	VAL	2.7
2	B	84	THR	2.7
13	o	61	GLN	2.6
11	l	2	GLU	2.6
13	o	58	ASN	2.6
20	R	13	LEU	2.6
4	D	12	ARG	2.6
5	E	61	ARG	2.6
2	B	85	GLY	2.6
1	a	19	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
19	z	2	THR	2.6
3	c	143	TYR	2.6
2	b	84	THR	2.6
6	f	14	PRO	2.6
11	L	2	GLU	2.5
17	Y	18	VAL	2.5
20	R	7	VAL	2.5
19	z	32	ASP	2.5
20	R	5	VAL	2.5
20	R	27	ALA	2.5
2	b	502	VAL	2.5
3	c	19	ASN	2.5
3	C	24	THR	2.4
13	o	62	GLU	2.4
5	E	72	ALA	2.4
1	a	229	GLU	2.4
2	b	489	GLU	2.4
11	L	10	VAL	2.3
2	B	496	TYR	2.3
5	e	61	ARG	2.3
3	c	147	PHE	2.3
18	X	31	ILE	2.3
5	e	84	LYS	2.3
13	O	65	PHE	2.3
15	u	70	ARG	2.3
1	A	230	THR	2.2
19	Z	32	ASP	2.2
3	C	260	ALA	2.2
1	A	14	TRP	2.2
2	b	497	GLN	2.2
13	o	4	THR	2.2
18	X	2	THR	2.2
2	B	502	VAL	2.2
20	R	12	VAL	2.2
11	L	1	MET	2.2
20	R	15	ALA	2.2
20	R	14	LEU	2.2
13	O	30	TYR	2.2
2	b	86	ILE	2.2
2	b	504	THR	2.2
19	z	13	VAL	2.2
19	z	4	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	262	ARG	2.2
16	V	106	ASN	2.2
20	R	11	PRO	2.1
19	Z	62	VAL	2.1
2	B	494	GLY	2.1
5	E	83	LEU	2.1
1	a	255	PHE	2.1
1	a	256	GLY	2.1
16	V	107	LEU	2.1
8	I	36	ASP	2.1
2	b	85	GLY	2.1
14	T	29	ILE	2.1
19	z	5	PHE	2.1
19	z	20	VAL	2.1
19	z	30	PRO	2.1
6	f	15	ILE	2.1
6	f	42	PHE	2.1
3	C	259	TRP	2.1
6	F	12	SER	2.1
11	L	3	PRO	2.0
5	e	79	PHE	2.0
9	J	30	TYR	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
19	FME	Z	1	10/11	0.87	0.13	86,100,112,113	0
19	FME	z	1	10/11	0.87	0.11	108,131,143,145	0
14	FME	T	1	10/11	0.94	0.09	45,52,78,79	0
14	FME	t	1	10/11	0.95	0.08	41,47,73,76	0
12	FME	M	1	10/11	0.95	0.09	42,48,82,86	0
4	HSK	d	336[A]	10/12	0.96	0.08	48,51,53,55	7
4	HSK	d	336[B]	11/12	0.96	0.08	48,51,55,59	8
12	FME	m	1	10/11	0.96	0.08	38,54,81,85	0
4	HSK	D	336[B]	11/12	0.96	0.08	45,48,49,50	8
4	HSK	D	336[A]	10/12	0.96	0.08	45,48,50,50	7
8	FME	I	1	10/11	0.97	0.06	45,54,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	FME	i	1	10/11	0.98	0.07	41,53,56,56	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($\text{\AA}^2$)	Q<0.9
34	DMS	O	314	4/4	0.56	0.17	133,135,136,138	0
34	DMS	k	2004	4/4	0.57	0.23	147,149,149,150	0
29	LMT	A	420	35/35	0.62	0.17	91,129,142,147	0
30	UNL	D	415	9/-	0.62	0.25	89,92,97,98	0
37	GOL	Z	102	6/6	0.62	0.16	105,121,124,124	0
30	UNL	B	630	9/-	0.63	0.35	80,89,103,103	0
37	GOL	v	202	6/6	0.63	0.13	100,106,107,107	0
37	GOL	o	2603	6/6	0.66	0.27	76,86,87,90	0
34	DMS	C	536	4/4	0.66	0.22	109,110,113,114	0
34	DMS	o	2604	4/4	0.67	0.28	124,124,125,126	0
34	DMS	E	108	4/4	0.67	0.21	115,118,120,120	0
34	DMS	b	643	4/4	0.68	0.17	149,150,151,151	0
37	GOL	k	2001	6/6	0.68	0.15	86,107,121,126	0
30	UNL	i	105	10/-	0.69	0.21	85,95,98,99	0
34	DMS	B	647	4/4	0.69	0.20	106,110,112,116	0
34	DMS	c	539	4/4	0.69	0.20	120,122,123,123	0
34	DMS	T	106	4/4	0.70	0.31	121,124,125,126	0
34	DMS	O	306	4/4	0.70	0.21	114,121,122,124	0
30	UNL	b	627	11/-	0.70	0.24	91,97,103,103	0
34	DMS	C	527	4/4	0.71	0.26	111,114,115,117	0
34	DMS	o	2610	4/4	0.71	0.20	131,131,131,133	0
34	DMS	z	1802	4/4	0.72	0.17	139,141,144,144	0
34	DMS	B	650	4/4	0.72	0.26	130,131,132,134	0
34	DMS	B	646	4/4	0.72	0.21	111,111,113,115	0
29	LMT	a	2120	35/35	0.72	0.15	101,133,144,145	0
34	DMS	v	214	4/4	0.72	0.21	127,132,134,135	0
34	DMS	C	535	4/4	0.73	0.29	121,122,124,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	DMS	o	2612	4/4	0.73	0.23	94,95,103,105	0
30	UNL	B	634	10/-	0.74	0.18	81,96,108,108	0
34	DMS	a	2124	4/4	0.74	0.20	128,130,130,131	0
34	DMS	B	649	4/4	0.74	0.15	124,124,125,126	0
34	DMS	D	420	4/4	0.74	0.24	124,124,126,126	0
30	UNL	A	415	40/-	0.74	0.20	80,111,132,143	0
30	UNL	E	102	15/-	0.74	0.24	96,102,109,111	0
34	DMS	C	533	4/4	0.74	0.18	120,121,121,122	0
34	DMS	o	2607	4/4	0.75	0.21	140,140,141,142	0
34	DMS	o	2609	4/4	0.75	0.24	110,119,119,121	0
30	UNL	h	701	11/-	0.75	0.23	85,89,97,98	0
34	DMS	O	309	4/4	0.75	0.26	98,101,104,109	0
30	UNL	e	102	15/-	0.75	0.20	76,82,95,98	0
30	UNL	E	104	6/-	0.76	0.24	67,78,88,89	0
34	DMS	b	640	4/4	0.76	0.21	103,108,109,111	0
30	UNL	a	2116	17/-	0.76	0.17	85,96,115,118	0
34	DMS	c	536	4/4	0.76	0.25	83,86,90,95	0
34	DMS	c	537	4/4	0.76	0.25	109,111,112,114	0
34	DMS	D	417	4/4	0.76	0.21	74,86,91,95	0
30	UNL	I	1203	16/-	0.77	0.20	88,99,102,103	0
34	DMS	C	539	4/4	0.77	0.25	75,90,91,96	0
30	UNL	j	1602	16/-	0.77	0.21	80,88,100,101	0
34	DMS	d	419	4/4	0.77	0.20	100,101,102,104	0
36	HTG	B	625[A]	19/19	0.77	0.19	57,70,80,83	19
36	HTG	B	625[B]	19/19	0.77	0.19	57,70,80,83	19
34	DMS	B	644	4/4	0.77	0.31	116,119,120,121	0
37	GOL	d	415	6/6	0.77	0.15	94,106,109,110	0
30	UNL	I	1204	13/-	0.77	0.18	80,87,94,95	0
37	GOL	o	2601	6/6	0.77	0.15	89,94,98,103	0
34	DMS	b	642	4/4	0.77	0.20	135,136,137,138	0
29	LMT	B	636	35/35	0.77	0.18	66,146,168,168	0
38	DGD	D	408	46/66	0.77	0.19	77,106,140,148	0
29	LMT	m	103	35/35	0.78	0.17	75,143,152,155	0
30	UNL	B	631	15/-	0.78	0.29	87,100,112,114	0
34	DMS	B	640	4/4	0.78	0.22	119,120,122,123	0
34	DMS	O	311	4/4	0.78	0.23	103,108,112,113	0
34	DMS	o	2605	4/4	0.78	0.28	111,114,114,122	0
34	DMS	b	639	4/4	0.79	0.19	93,94,94,99	0
30	UNL	B	629	18/-	0.79	0.17	78,85,103,105	0
34	DMS	d	422	4/4	0.79	0.19	113,118,118,121	0
34	DMS	O	312	4/4	0.79	0.23	112,116,117,118	0
30	UNL	E	106	16/-	0.79	0.27	93,104,113,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	LMT	f	101	24/35	0.79	0.15	93,112,125,126	0
30	UNL	b	628	15/-	0.79	0.22	85,97,105,106	0
34	DMS	x	802	4/4	0.80	0.21	110,115,116,118	0
34	DMS	O	304	4/4	0.80	0.28	129,133,136,141	0
34	DMS	b	635	4/4	0.80	0.19	102,104,106,108	0
30	UNL	c	525	12/-	0.80	0.24	88,97,118,118	0
36	HTG	B	626	19/19	0.80	0.15	53,114,123,126	19
36	HTG	B	628	19/19	0.80	0.14	56,128,134,137	0
36	HTG	I	1202	19/19	0.80	0.13	72,116,134,134	0
37	GOL	B	635	6/6	0.80	0.12	70,80,94,97	0
37	GOL	D	403	6/6	0.80	0.16	74,79,84,85	0
34	DMS	C	538	4/4	0.80	0.18	121,122,124,126	0
30	UNL	d	413	10/-	0.80	0.17	85,88,96,100	0
29	LMT	E	105	24/35	0.80	0.16	89,104,131,136	0
29	LMT	a	2103	35/35	0.80	0.18	60,100,116,118	0
34	DMS	T	104	4/4	0.80	0.24	118,127,127,129	0
34	DMS	c	538	4/4	0.80	0.18	111,113,114,116	0
30	UNL	J	103	15/-	0.80	0.24	86,93,99,99	0
29	LMT	j	1601	23/35	0.81	0.16	77,104,149,151	0
34	DMS	d	420	4/4	0.81	0.27	117,117,120,122	0
34	DMS	b	637	4/4	0.81	0.24	131,135,135,137	0
34	DMS	d	423	4/4	0.81	0.19	143,144,144,145	0
34	DMS	e	104	4/4	0.81	0.20	117,119,120,120	0
30	UNL	Y	301	10/-	0.81	0.21	93,101,108,109	0
36	HTG	d	414	19/19	0.81	0.17	76,99,110,110	19
30	UNL	k	2002	12/-	0.81	0.24	84,93,114,115	0
34	DMS	O	313	4/4	0.81	0.16	99,102,104,111	0
37	GOL	U	501	6/6	0.81	0.24	86,95,97,103	0
30	UNL	A	416	15/-	0.81	0.20	70,89,101,102	0
34	DMS	c	533	4/4	0.81	0.21	110,116,116,117	0
34	DMS	O	305	4/4	0.81	0.21	101,101,103,112	0
30	UNL	h	704	12/-	0.81	0.23	83,89,104,106	0
34	DMS	v	208	4/4	0.81	0.20	115,115,120,124	0
34	DMS	a	2122	4/4	0.81	0.16	128,128,129,129	0
37	GOL	v	204	6/6	0.81	0.15	85,89,93,97	0
34	DMS	O	307	4/4	0.81	0.20	119,120,120,120	0
39	LHG	e	101	32/49	0.81	0.17	77,130,154,158	0
30	UNL	i	102	19/-	0.82	0.16	86,96,114,114	0
30	UNL	C	501	40/-	0.82	0.19	75,102,126,129	0
34	DMS	c	534	4/4	0.82	0.15	120,120,122,123	0
37	GOL	b	631	6/6	0.82	0.15	94,99,103,109	0
36	HTG	C	522	19/19	0.82	0.13	66,115,134,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
36	HTG	D	413	19/19	0.82	0.15	74,106,124,127	0
34	DMS	V	206	4/4	0.82	0.16	88,96,102,105	0
36	HTG	b	626	19/19	0.82	0.14	96,137,142,142	0
36	HTG	d	403	19/19	0.82	0.14	83,114,127,128	0
30	UNL	C	523	10/-	0.82	0.21	81,88,98,100	0
37	GOL	B	632	6/6	0.82	0.18	95,101,103,106	0
39	LHG	E	101	49/49	0.82	0.17	77,108,122,123	0
29	LMT	A	414	34/35	0.82	0.17	68,107,122,131	0
30	UNL	b	629	9/-	0.83	0.20	76,90,96,96	0
37	GOL	H	103	6/6	0.83	0.17	85,97,100,102	0
30	UNL	E	103	6/-	0.83	0.16	82,82,84,85	0
37	GOL	V	203	6/6	0.83	0.15	84,103,106,107	0
34	DMS	j	1604	4/4	0.83	0.23	126,129,130,133	0
34	DMS	t	103	4/4	0.83	0.19	109,112,116,117	0
34	DMS	u	204	4/4	0.83	0.21	106,108,109,110	0
30	UNL	d	402	40/-	0.83	0.23	61,88,130,131	0
34	DMS	v	210	4/4	0.83	0.17	122,123,124,125	0
34	DMS	v	211	4/4	0.83	0.18	95,111,113,114	0
34	DMS	v	213	4/4	0.83	0.18	108,108,109,109	0
34	DMS	A	424	4/4	0.83	0.16	78,84,87,89	0
36	HTG	i	103	19/19	0.83	0.14	74,133,147,148	0
34	DMS	T	105	4/4	0.83	0.24	134,134,135,135	0
29	LMT	I	1201	24/35	0.83	0.17	56,96,144,148	0
34	DMS	c	540	4/4	0.84	0.15	118,124,125,128	0
34	DMS	A	423	4/4	0.84	0.22	113,115,117,121	0
34	DMS	C	537	4/4	0.84	0.17	112,114,116,118	0
36	HTG	b	602	19/19	0.84	0.14	68,120,134,138	0
34	DMS	o	2611	4/4	0.84	0.18	96,99,99,99	0
36	HTG	c	523	19/19	0.84	0.14	95,110,115,116	0
36	HTG	c	524	19/19	0.84	0.15	73,97,108,110	19
34	DMS	B	642	4/4	0.84	0.23	109,111,113,115	0
34	DMS	E	107	4/4	0.84	0.19	124,128,129,133	0
37	GOL	c	527	6/6	0.85	0.18	81,86,93,93	0
29	LMT	Z	101	35/35	0.85	0.15	60,125,151,156	0
27	SQD	L	102	54/54	0.85	0.17	55,78,119,123	0
34	DMS	B	638	4/4	0.85	0.20	124,124,126,126	0
29	LMT	J	102	24/35	0.85	0.16	76,101,135,137	0
37	GOL	O	303	6/6	0.85	0.12	91,94,95,96	0
37	GOL	v	203	6/6	0.85	0.14	78,80,83,87	0
30	UNL	b	630	21/-	0.85	0.14	61,79,105,107	0
34	DMS	C	534	4/4	0.85	0.22	119,119,120,121	0
30	UNL	c	501	36/-	0.85	0.19	80,98,127,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	UNL	m	101	13/-	0.85	0.21	70,75,95,99	0
34	DMS	v	212	4/4	0.86	0.17	119,121,122,124	0
29	LMT	z	1801	33/35	0.86	0.14	74,116,131,136	0
27	SQD	F	101	45/54	0.86	0.14	69,97,121,132	0
37	GOL	C	525	6/6	0.86	0.15	83,98,100,101	0
34	DMS	A	425	4/4	0.86	0.19	93,96,96,98	0
34	DMS	u	201	4/4	0.86	0.26	104,109,110,111	0
34	DMS	b	636	4/4	0.86	0.15	69,96,97,100	0
29	LMT	m	102	35/35	0.86	0.13	49,82,99,101	0
36	HTG	c	526	19/19	0.86	0.12	97,131,146,149	0
30	UNL	a	2117	9/-	0.86	0.17	72,79,83,84	0
28	LMG	C	526	48/55	0.86	0.16	63,111,128,134	0
36	HTG	V	204	19/19	0.87	0.13	67,84,115,118	0
34	DMS	B	645	4/4	0.87	0.13	86,91,92,93	0
29	LMT	b	624	25/35	0.87	0.17	80,110,138,139	0
29	LMT	B	623	35/35	0.87	0.13	74,104,121,122	0
34	DMS	C	529	4/4	0.87	0.24	123,124,124,127	0
30	UNL	D	402	40/-	0.88	0.18	60,82,118,122	0
29	LMT	M	101	35/35	0.88	0.12	57,89,104,107	0
27	SQD	B	621	54/54	0.88	0.14	48,87,130,133	0
34	DMS	c	535	4/4	0.88	0.17	95,103,106,106	0
36	HTG	b	625	19/19	0.88	0.16	46,69,88,89	19
27	SQD	f	102	37/54	0.88	0.15	73,101,129,134	0
30	UNL	M	102	15/-	0.88	0.17	58,68,108,113	0
30	UNL	T	103	9/-	0.88	0.21	78,85,93,95	0
29	LMT	i	104	24/35	0.88	0.15	64,103,141,147	0
34	DMS	V	208	4/4	0.88	0.14	81,91,94,96	0
34	DMS	c	541	4/4	0.88	0.14	104,106,106,106	0
31	PL9	A	417	39/55	0.89	0.18	73,85,102,105	0
34	DMS	b	641	4/4	0.89	0.14	67,70,72,74	0
34	DMS	V	207	4/4	0.89	0.14	92,93,99,100	0
34	DMS	C	530	4/4	0.89	0.15	88,93,97,99	0
34	DMS	c	530	4/4	0.89	0.20	121,122,122,126	0
31	PL9	x	801	39/55	0.89	0.19	71,91,119,122	0
28	LMG	i	101	51/55	0.89	0.15	65,82,94,101	0
34	DMS	b	634	4/4	0.89	0.17	96,98,98,104	0
37	GOL	C	524	6/6	0.89	0.12	91,98,103,105	0
27	SQD	A	413	54/54	0.89	0.13	62,81,122,128	0
30	UNL	B	633	22/-	0.89	0.13	61,84,112,113	0
34	DMS	O	310	4/4	0.89	0.15	102,103,103,107	0
34	DMS	o	2606	4/4	0.89	0.18	109,111,111,111	0
34	DMS	V	202	4/4	0.89	0.17	96,97,99,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	LMG	c	522	48/55	0.90	0.14	55,110,127,139	0
34	DMS	v	209	4/4	0.90	0.14	82,93,93,101	0
34	DMS	d	421	4/4	0.90	0.20	85,92,95,96	0
34	DMS	o	2608	4/4	0.90	0.12	102,107,110,114	0
34	DMS	V	209	4/4	0.90	0.16	87,103,104,110	0
24	CLA	B	602	65/65	0.90	0.10	45,68,113,120	0
29	LMT	B	637	24/35	0.90	0.13	50,77,118,128	0
34	DMS	U	503	4/4	0.90	0.20	95,109,110,112	0
34	DMS	B	648	4/4	0.90	0.14	63,65,67,80	0
28	LMG	C	520	51/55	0.90	0.15	48,81,101,108	0
34	DMS	u	203	4/4	0.90	0.14	76,85,86,89	0
27	SQD	a	2102	53/54	0.90	0.13	52,80,111,115	0
26	BCR	t	102	40/40	0.91	0.10	42,55,75,77	0
24	CLA	C	507	65/65	0.91	0.13	50,69,110,117	0
36	HTG	B	627	19/19	0.91	0.13	59,90,110,116	0
29	LMT	T	102	24/35	0.91	0.15	48,79,108,114	0
36	HTG	C	521	19/19	0.91	0.13	90,106,113,116	0
34	DMS	v	207	4/4	0.91	0.15	96,97,99,100	0
34	DMS	A	426	4/4	0.91	0.18	79,80,80,84	0
34	DMS	a	2123	4/4	0.91	0.19	113,115,118,123	0
36	HTG	B	624	19/19	0.91	0.13	60,69,74,76	0
34	DMS	d	417	4/4	0.91	0.22	84,87,87,90	0
30	UNL	D	414	16/-	0.92	0.16	55,70,85,89	0
28	LMG	B	622	51/55	0.92	0.13	51,70,83,92	0
34	DMS	b	633	4/4	0.92	0.16	79,80,81,92	0
32	K2I	A	418[A]	10/10	0.92	0.14	94,96,102,105	10
32	K2I	A	418[B]	10/10	0.92	0.14	74,95,100,112	10
26	BCR	C	516	40/40	0.92	0.11	48,56,69,72	0
34	DMS	u	202	4/4	0.92	0.14	79,80,89,90	0
26	BCR	T	101	40/40	0.92	0.09	39,52,71,75	0
34	DMS	D	419	4/4	0.92	0.15	88,95,95,104	0
28	LMG	b	623	51/55	0.92	0.13	56,70,83,100	0
36	HTG	b	601	19/19	0.92	0.11	63,84,94,98	0
30	UNL	X	801	18/-	0.92	0.12	65,71,96,98	0
34	DMS	C	528	4/4	0.92	0.17	88,96,97,98	0
34	DMS	i	106	4/4	0.92	0.15	95,96,97,98	0
34	DMS	F	103	4/4	0.92	0.13	77,78,79,88	0
24	CLA	b	604	65/65	0.92	0.11	52,73,118,121	0
28	LMG	A	412	51/55	0.92	0.13	57,79,100,104	0
30	UNL	t	101	8/-	0.92	0.16	75,81,88,89	0
34	DMS	B	643	4/4	0.92	0.17	81,85,90,91	0
34	DMS	V	210	4/4	0.92	0.15	87,96,98,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	DMS	O	308	4/4	0.92	0.18	102,105,106,108	0
32	K2I	a	2118[A]	10/10	0.93	0.10	103,106,111,114	10
37	GOL	a	2101	6/6	0.93	0.13	66,76,77,80	0
32	K2I	a	2118[B]	10/10	0.93	0.10	82,105,107,112	10
30	UNL	d	412	14/-	0.93	0.17	56,73,79,82	0
34	DMS	b	638	4/4	0.93	0.14	81,85,89,94	0
26	BCR	c	516	40/40	0.93	0.12	63,76,81,85	0
36	HTG	O	302	19/19	0.93	0.11	51,68,78,81	0
30	UNL	d	416	18/-	0.93	0.11	59,74,105,105	0
24	CLA	c	508	65/65	0.93	0.11	51,67,102,107	0
24	CLA	a	2113	65/65	0.93	0.11	40,46,116,121	0
34	DMS	c	542	4/4	0.93	0.11	113,114,117,118	0
27	SQD	a	2115	47/54	0.93	0.13	59,80,97,104	0
38	DGD	c	518	62/66	0.93	0.12	42,54,95,100	0
24	CLA	B	617	65/65	0.93	0.11	40,52,119,123	0
28	LMG	c	521	49/55	0.93	0.14	53,88,105,108	0
27	SQD	A	411	49/54	0.94	0.12	66,82,98,99	0
24	CLA	b	619	65/65	0.94	0.11	43,56,119,121	0
34	DMS	D	416	4/4	0.94	0.12	61,76,81,82	0
33	BCT	A	421	4/4	0.94	0.09	51,56,61,64	0
33	BCT	a	2108	4/4	0.94	0.10	55,57,63,68	0
24	CLA	C	514	65/65	0.94	0.09	54,65,95,98	0
24	CLA	c	514	65/65	0.94	0.10	56,64,100,102	0
24	CLA	c	515	65/65	0.94	0.10	55,68,98,106	0
34	DMS	d	418	4/4	0.94	0.14	69,73,81,88	0
24	CLA	d	405	65/65	0.94	0.09	46,55,105,115	0
24	CLA	B	615	65/65	0.94	0.10	35,45,99,107	0
34	DMS	C	531	4/4	0.94	0.14	63,70,77,78	0
24	CLA	C	513	65/65	0.94	0.10	51,65,107,110	0
26	BCR	a	2114	40/40	0.94	0.08	35,45,51,53	0
24	CLA	b	609	65/65	0.94	0.09	39,50,86,88	0
34	DMS	v	206	4/4	0.94	0.14	78,93,93,98	0
39	LHG	D	409	49/49	0.94	0.11	48,59,70,74	0
26	BCR	c	517	40/40	0.94	0.10	47,59,75,78	0
24	CLA	b	617	65/65	0.94	0.11	36,45,100,113	0
41	RRX	H	101	41/41	0.94	0.09	45,59,68,78	0
41	RRX	h	702	41/41	0.94	0.10	46,59,81,93	0
24	CLA	B	607	65/65	0.95	0.09	37,46,74,84	0
26	BCR	D	406	40/40	0.95	0.09	42,52,85,86	0
26	BCR	K	101	40/40	0.95	0.09	50,57,63,67	0
24	CLA	D	405	65/65	0.95	0.09	42,52,106,112	0
26	BCR	Y	302	40/40	0.95	0.07	48,56,62,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	c	505	65/65	0.95	0.09	43,57,63,70	0
26	BCR	b	622	40/40	0.95	0.09	45,57,71,76	0
24	CLA	c	506	65/65	0.95	0.10	44,52,86,90	0
24	CLA	B	611	65/65	0.95	0.08	41,49,57,68	0
28	LMG	d	411	48/55	0.95	0.10	47,56,86,95	0
26	BCR	c	528	40/40	0.95	0.09	48,58,68,69	0
26	BCR	d	406	40/40	0.95	0.09	47,55,75,82	0
24	CLA	c	510	65/65	0.95	0.09	41,51,114,126	0
24	CLA	C	511	65/65	0.95	0.09	37,51,59,70	0
34	DMS	c	531	4/4	0.95	0.14	97,99,101,106	0
38	DGD	C	517	62/66	0.95	0.10	40,51,93,96	0
38	DGD	C	518	62/66	0.95	0.10	41,54,109,119	0
38	DGD	C	519	62/66	0.95	0.10	39,51,92,103	0
24	CLA	A	409	65/65	0.95	0.11	35,45,117,121	0
38	DGD	H	102	62/66	0.95	0.10	45,54,66,70	0
24	CLA	b	610	65/65	0.95	0.08	31,43,58,62	0
38	DGD	c	519	62/66	0.95	0.10	47,59,107,117	0
38	DGD	h	703	62/66	0.95	0.10	46,57,74,79	0
26	BCR	B	618	40/40	0.95	0.08	38,47,54,55	0
26	BCR	B	620	40/40	0.95	0.08	42,52,63,67	0
39	LHG	d	408	49/49	0.95	0.10	45,58,73,78	0
26	BCR	C	515	40/40	0.95	0.08	47,65,74,79	0
39	LHG	l	101	49/49	0.95	0.10	43,52,71,79	0
31	PL9	D	407	55/55	0.95	0.08	34,43,50,55	0
31	PL9	d	407	55/55	0.95	0.09	33,44,55,60	0
24	CLA	A	406	65/65	0.96	0.09	34,42,100,104	0
24	CLA	c	507	65/65	0.96	0.08	42,52,66,74	0
24	CLA	C	508	65/65	0.96	0.09	47,56,73,77	0
24	CLA	c	509	65/65	0.96	0.09	45,56,77,79	0
24	CLA	C	509	65/65	0.96	0.08	38,50,106,117	0
24	CLA	c	511	65/65	0.96	0.09	43,55,79,90	0
24	CLA	c	513	65/65	0.96	0.08	45,59,70,79	0
24	CLA	C	510	65/65	0.96	0.09	46,54,74,77	0
28	LMG	D	412	44/55	0.96	0.09	44,53,80,83	0
24	CLA	B	608	65/65	0.96	0.08	33,42,57,67	0
24	CLA	C	512	65/65	0.96	0.07	41,56,65,69	0
34	DMS	v	205	4/4	0.96	0.13	75,76,84,85	0
25	PHO	A	407	64/64	0.96	0.07	33,39,48,49	0
37	GOL	U	502	6/6	0.96	0.09	69,78,90,95	0
25	PHO	A	408	64/64	0.96	0.07	34,45,52,55	0
24	CLA	B	610	65/65	0.96	0.07	42,49,58,60	0
34	DMS	c	532	4/4	0.96	0.11	72,72,73,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	BCR	B	619	40/40	0.96	0.07	40,50,62,67	0
24	CLA	B	603	65/65	0.96	0.08	41,48,57,58	0
24	CLA	B	614	65/65	0.96	0.07	34,41,79,93	0
24	CLA	a	2110	65/65	0.96	0.10	35,44,106,111	0
24	CLA	B	604	65/65	0.96	0.07	36,45,57,63	0
24	CLA	B	606	65/65	0.96	0.07	34,43,59,64	0
24	CLA	b	608	65/65	0.96	0.07	37,45,58,61	0
24	CLA	C	502	65/65	0.96	0.08	43,52,68,88	0
34	DMS	B	641	4/4	0.96	0.12	63,65,69,71	0
24	CLA	C	503	65/65	0.96	0.07	39,48,62,66	0
26	BCR	b	620	40/40	0.96	0.08	40,49,58,59	0
26	BCR	b	621	40/40	0.96	0.08	39,51,63,71	0
24	CLA	b	612	65/65	0.96	0.08	43,52,62,70	0
24	CLA	b	613	65/65	0.96	0.08	42,50,57,64	0
24	CLA	b	615	65/65	0.96	0.07	37,45,52,56	0
24	CLA	b	616	65/65	0.96	0.08	37,41,80,84	0
38	DGD	c	520	62/66	0.96	0.10	44,57,80,88	0
34	DMS	V	205	4/4	0.96	0.11	66,69,70,75	0
24	CLA	C	504	65/65	0.96	0.07	42,52,59,67	0
39	LHG	D	410	49/49	0.96	0.09	41,47,65,81	0
39	LHG	D	411	44/49	0.96	0.10	44,53,90,98	0
26	BCR	k	2003	40/40	0.96	0.09	50,60,69,71	0
24	CLA	b	618	65/65	0.96	0.09	41,51,70,78	0
39	LHG	d	409	49/49	0.96	0.09	40,46,72,84	0
39	LHG	d	410	36/49	0.96	0.08	46,54,79,85	0
24	CLA	C	505	65/65	0.96	0.09	41,49,81,86	0
24	CLA	c	503	65/65	0.96	0.09	44,55,68,73	0
24	CLA	c	504	65/65	0.96	0.08	40,50,64,81	0
24	CLA	C	506	65/65	0.96	0.09	45,52,70,76	0
25	PHO	a	2112	64/64	0.97	0.06	36,46,54,56	0
26	BCR	A	410	40/40	0.97	0.06	37,45,50,52	0
24	CLA	D	401	65/65	0.97	0.06	33,39,49,59	0
24	CLA	D	404	65/65	0.97	0.06	31,38,59,65	0
24	CLA	b	611	65/65	0.97	0.07	42,49,57,63	0
24	CLA	B	616	65/65	0.97	0.08	39,50,70,78	0
24	CLA	a	2109	65/65	0.97	0.07	33,40,51,74	0
24	CLA	b	614	65/65	0.97	0.07	34,44,61,64	0
24	CLA	B	612	65/65	0.97	0.07	35,44,57,68	0
24	CLA	c	512	65/65	0.97	0.08	42,52,62,74	0
34	DMS	D	418	4/4	0.97	0.11	77,82,88,90	0
24	CLA	B	613	65/65	0.97	0.06	34,43,50,53	0
34	DMS	c	529	4/4	0.97	0.15	57,60,62,63	0

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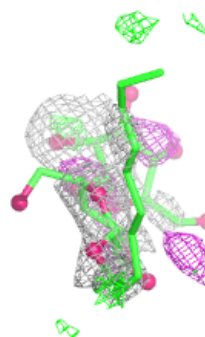
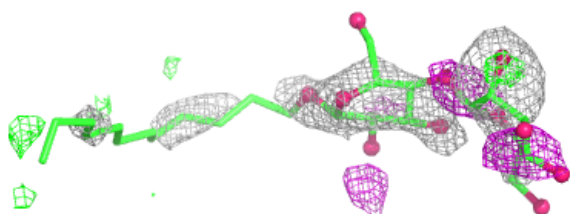
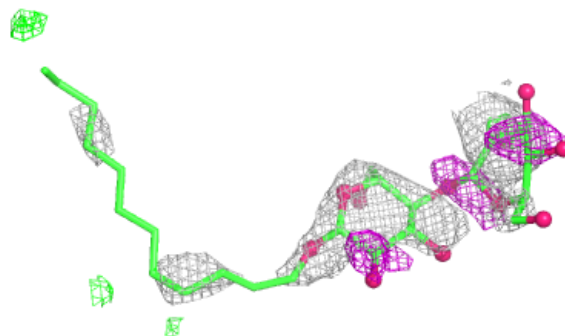
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	B	605	65/65	0.97	0.08	31,42,75,81	0
39	LHG	L	101	49/49	0.97	0.08	44,51,68,70	0
24	CLA	b	605	65/65	0.97	0.07	40,51,62,65	0
24	CLA	d	401	65/65	0.97	0.06	34,39,47,55	0
24	CLA	d	404	65/65	0.97	0.07	31,41,59,71	0
24	CLA	b	606	65/65	0.97	0.07	38,48,60,64	0
24	CLA	b	607	65/65	0.97	0.08	34,44,84,89	0
40	HEM	e	103	43/43	0.97	0.09	52,63,90,105	0
24	CLA	B	609	65/65	0.97	0.06	40,48,58,61	0
25	PHO	a	2111	64/64	0.97	0.06	33,41,47,55	0
35	CA	o	2602	1/1	0.98	0.04	71,71,71,71	0
34	DMS	b	632	4/4	0.98	0.07	47,48,54,58	0
24	CLA	A	405	65/65	0.98	0.06	30,38,50,72	0
34	DMS	C	532	4/4	0.98	0.07	62,63,63,67	0
32	K2I	A	419	10/10	0.98	0.09	43,52,58,64	10
34	DMS	A	422	4/4	0.98	0.08	45,48,53,55	0
32	K2I	a	2119	10/10	0.98	0.08	48,57,64,73	10
34	DMS	B	639	4/4	0.98	0.08	42,46,47,58	0
40	HEM	F	102	43/43	0.98	0.07	52,62,73,90	0
35	CA	B	601	1/1	0.98	0.05	64,64,64,64	0
35	CA	O	301	1/1	0.98	0.04	72,72,72,72	0
35	CA	b	603	1/1	0.98	0.04	72,72,72,72	0
42	MG	J	101	1/1	0.98	0.09	53,53,53,53	0
43	HEC	V	201	43/43	0.98	0.06	37,45,50,53	0
43	HEC	v	201	43/43	0.98	0.07	45,55,61,64	0
23	CL	A	404	1/1	0.99	0.03	41,41,41,41	0
23	CL	a	2106	1/1	0.99	0.07	47,47,47,47	0
34	DMS	a	2121	4/4	0.99	0.06	42,48,52,52	0
23	CL	a	2107	1/1	0.99	0.04	46,46,46,46	0
21	OEX	A	401	10/10	0.99	0.03	39,42,46,48	0
42	MG	j	1603	1/1	0.99	0.08	57,57,57,57	0
23	CL	A	403	1/1	0.99	0.08	42,42,42,42	0
35	CA	c	502	1/1	0.99	0.05	66,66,66,66	0
22	FE2	a	2105	1/1	1.00	0.02	47,47,47,47	0
21	OEX	a	2104	10/10	1.00	0.02	38,43,49,52	0
22	FE2	A	402	1/1	1.00	0.01	48,48,48,48	0

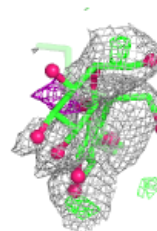
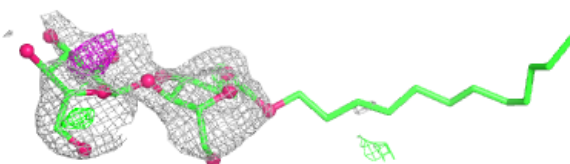
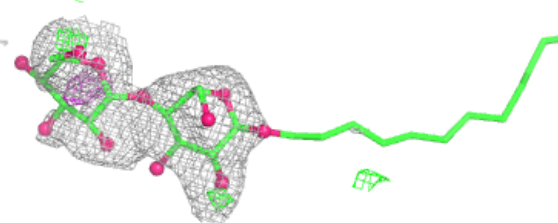
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT A 420:

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

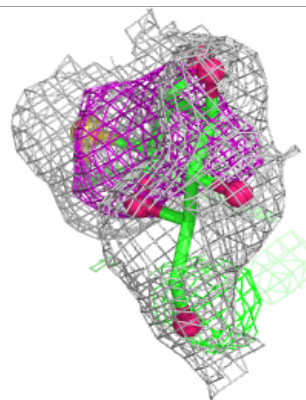
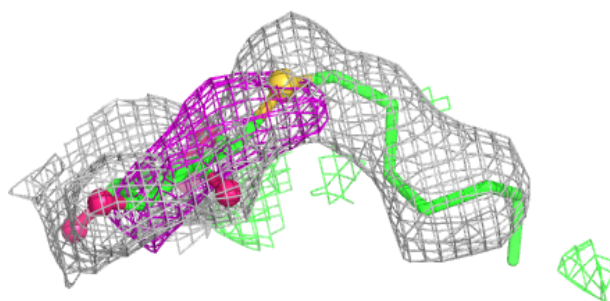
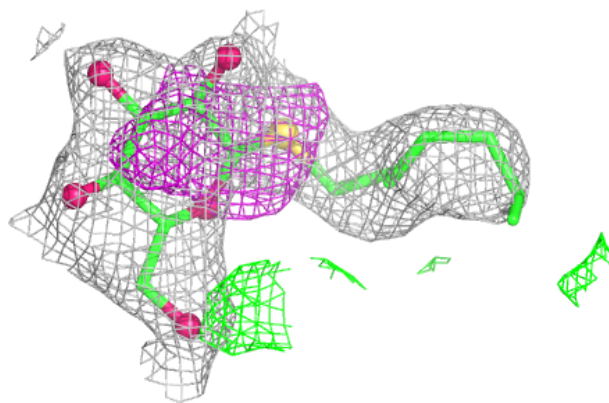
**Electron density around LMT a 2120:**

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

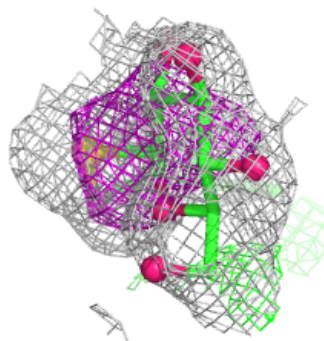
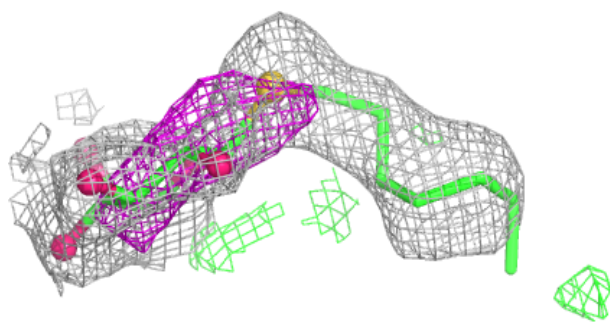
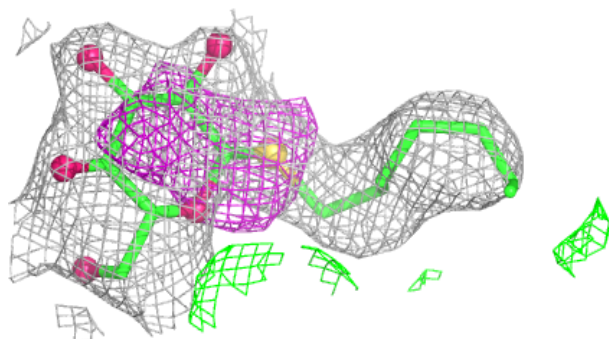


Electron density around HTG B 625 (A):

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

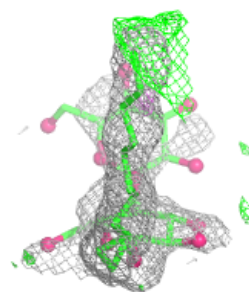
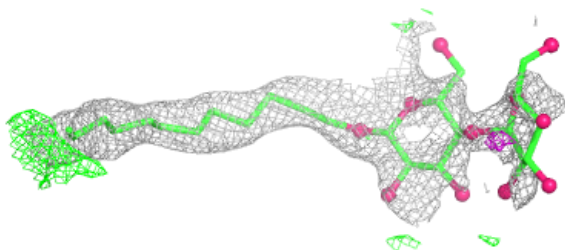
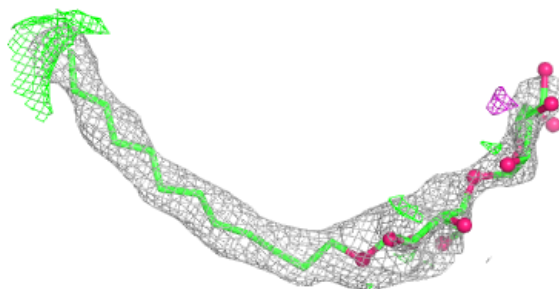
**Electron density around HTG B 625 (B):**

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

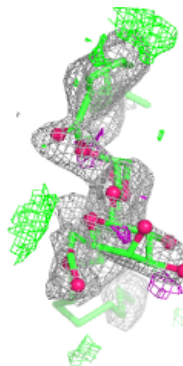
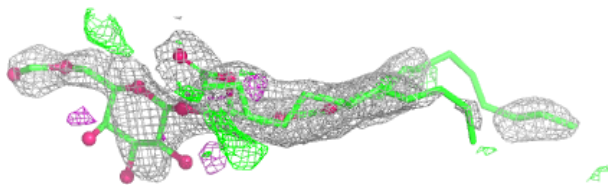
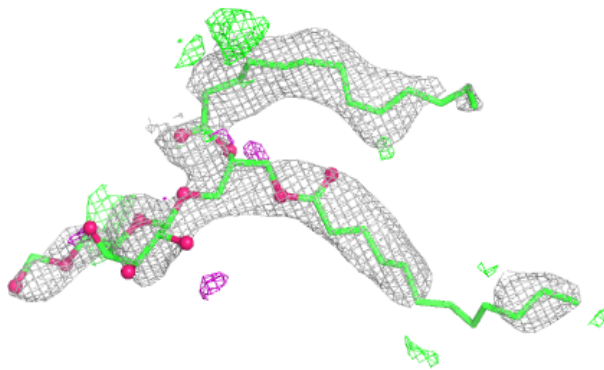


Electron density around LMT B 636:

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

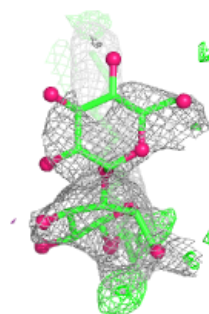
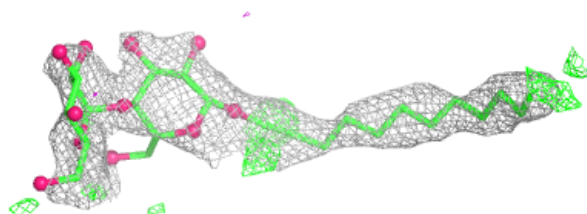
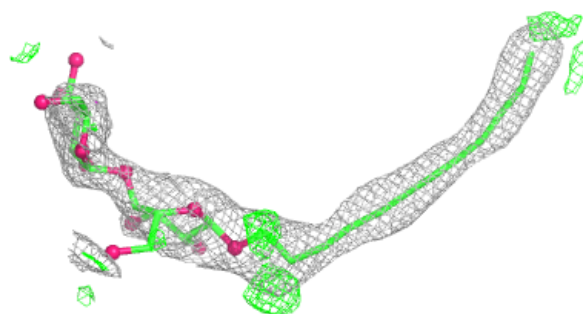
**Electron density around DGD D 408:**

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

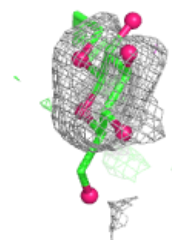
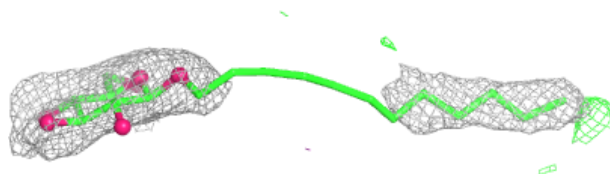
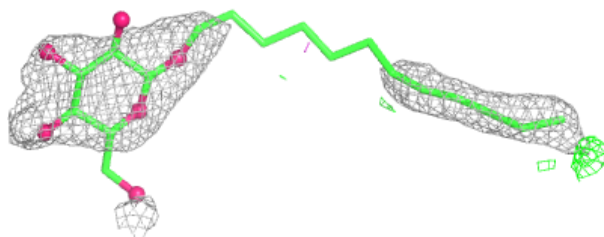


Electron density around LMT m 103:

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

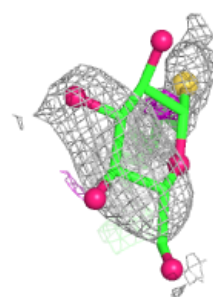
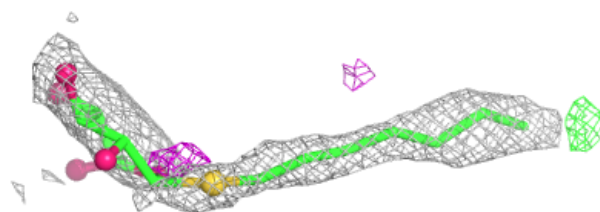
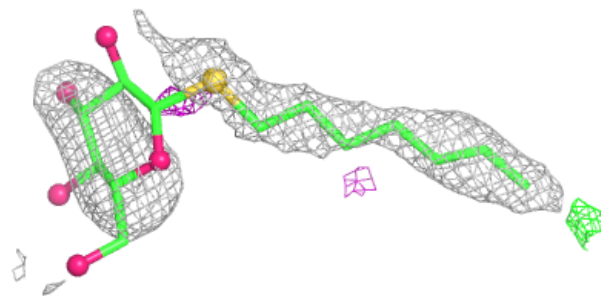
**Electron density around LMT f 101:**

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

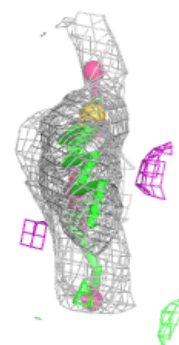
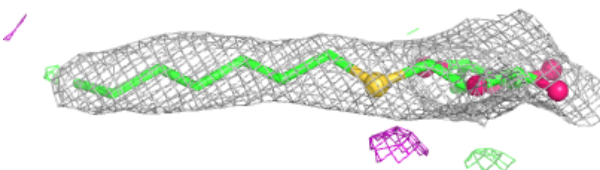
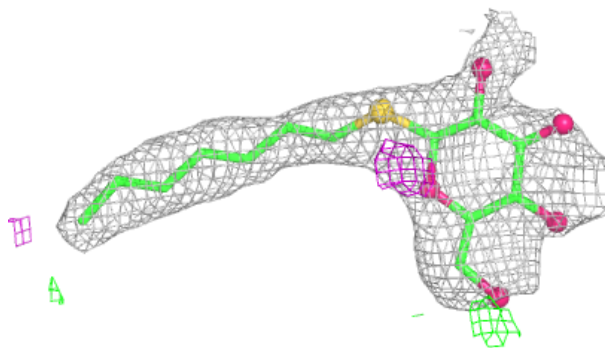


Electron density around HTG B 626:

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

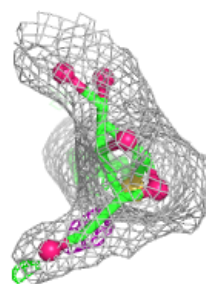
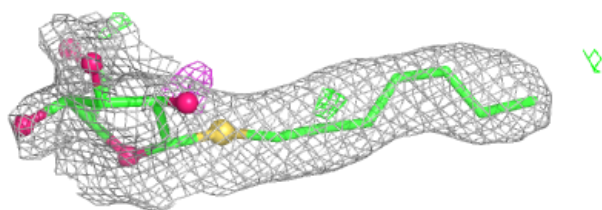
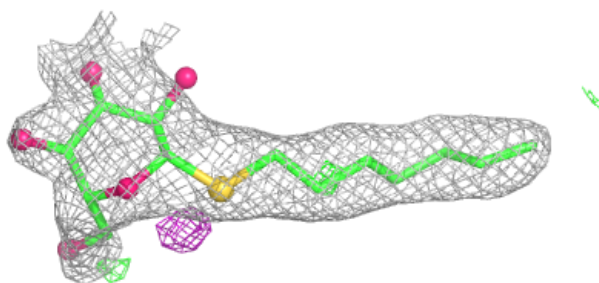
**Electron density around HTG B 628:**

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

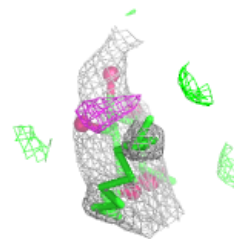
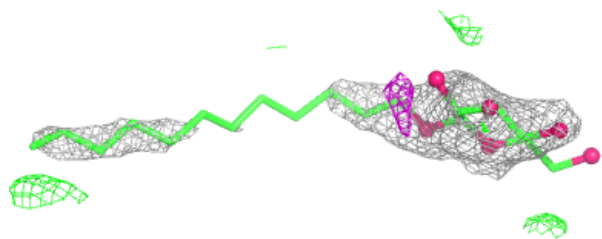
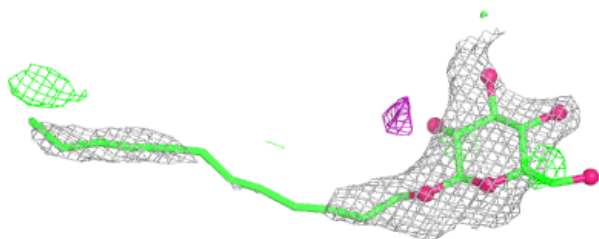


Electron density around HTG I 1202:

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

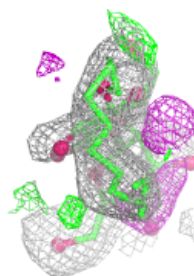
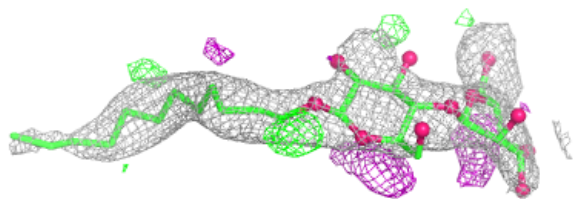
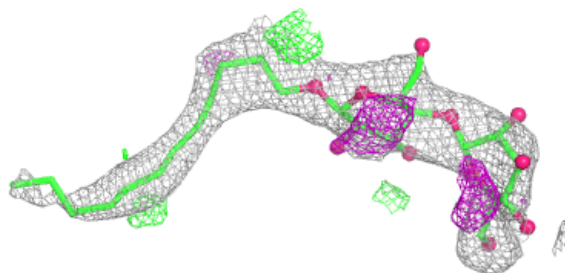
**Electron density around LMT E 105:**

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

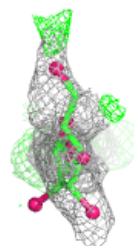
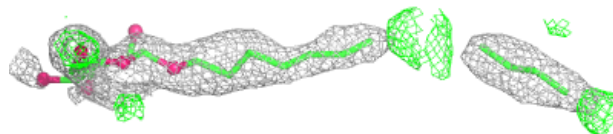
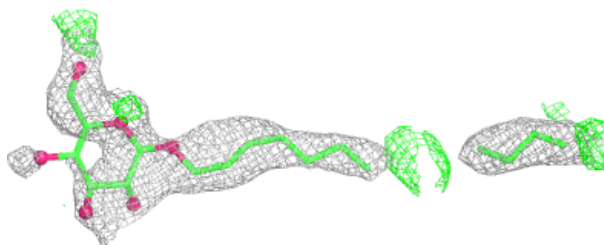


Electron density around LMT a 2103:

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

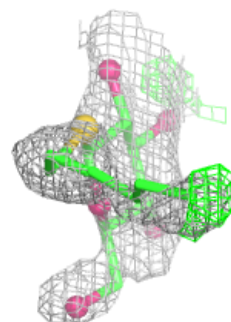
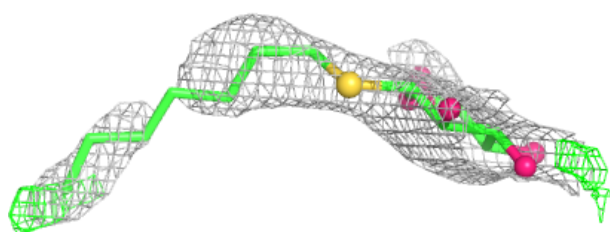
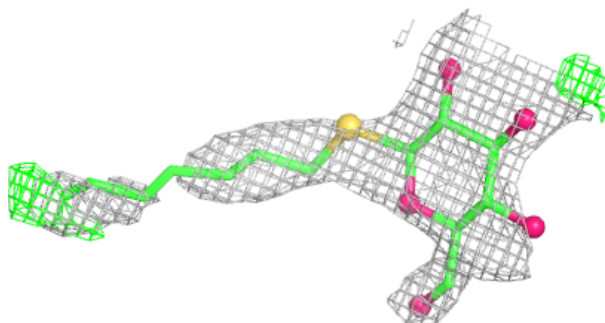
**Electron density around LMT j 1601:**

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

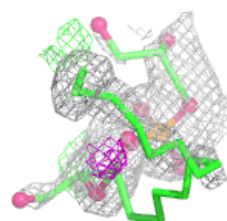
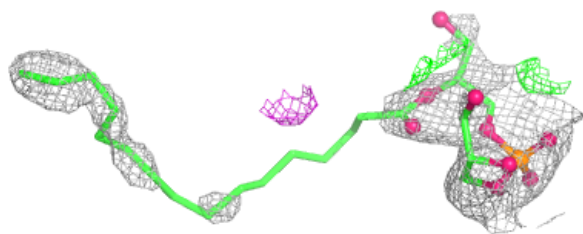
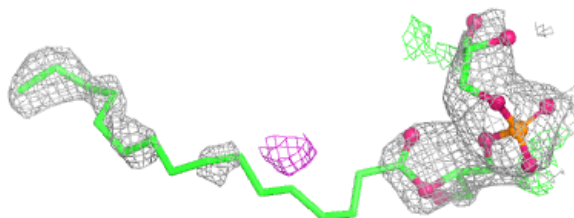


Electron density around HTG d 414:

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

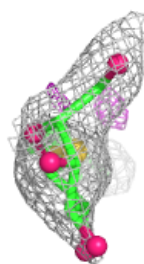
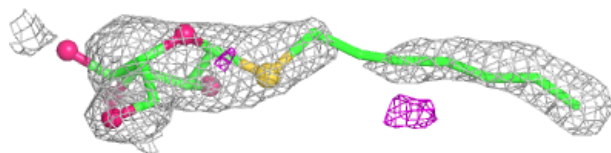
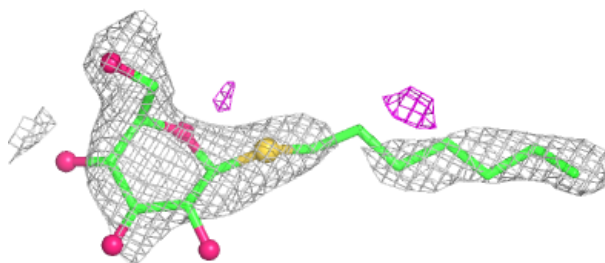
**Electron density around LHG e 101:**

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

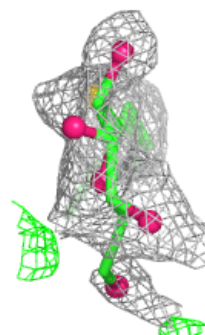
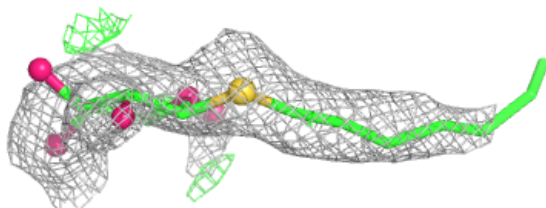
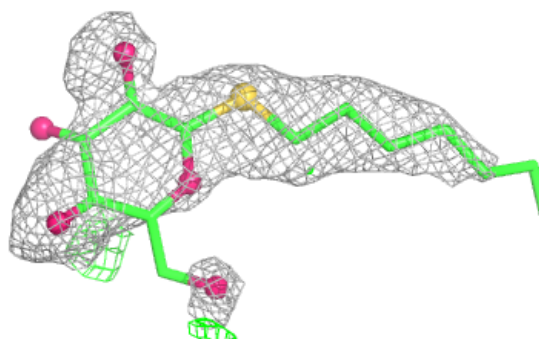


Electron density around HTG C 522:

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

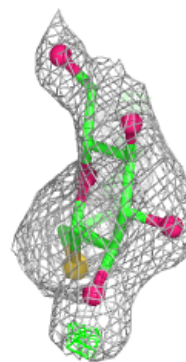
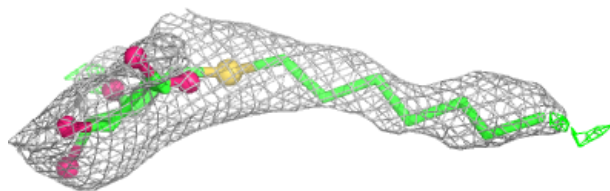
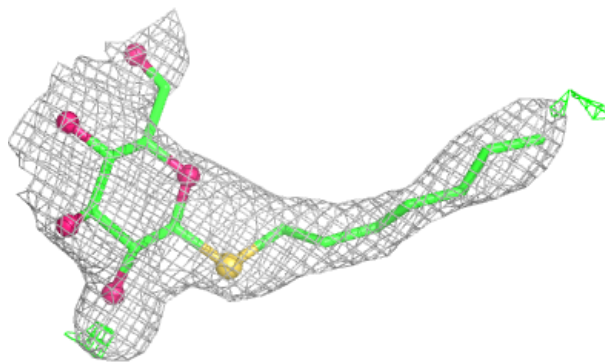
**Electron density around HTG D 413:**

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

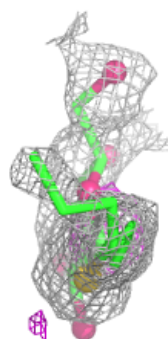
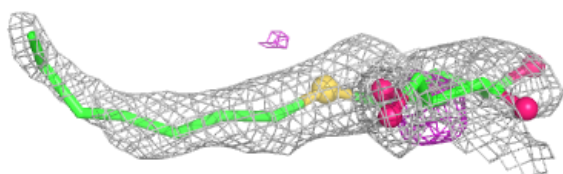
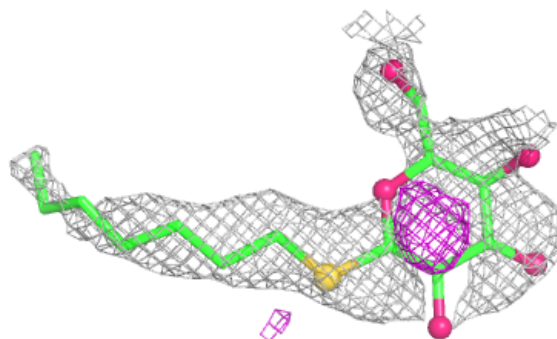


Electron density around HTG b 626:

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

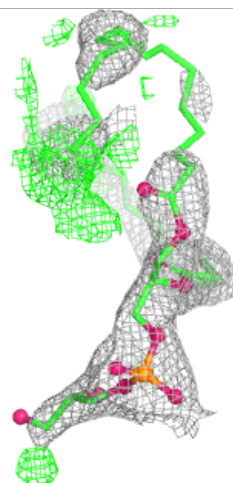
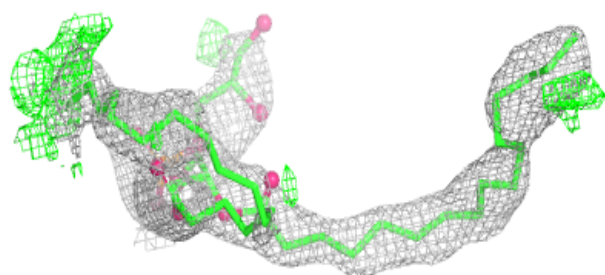
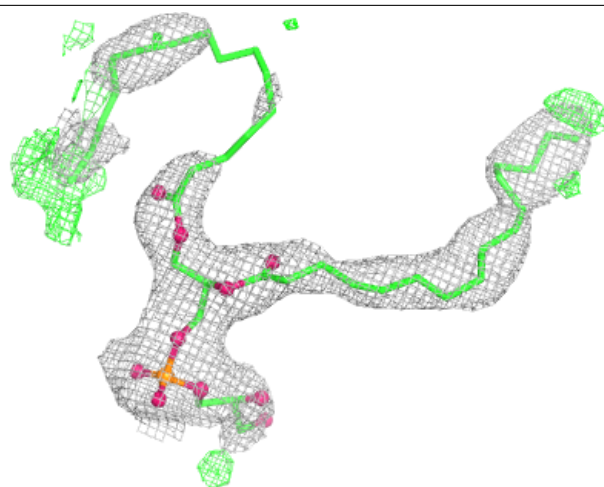
**Electron density around HTG d 403:**

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



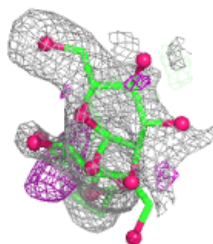
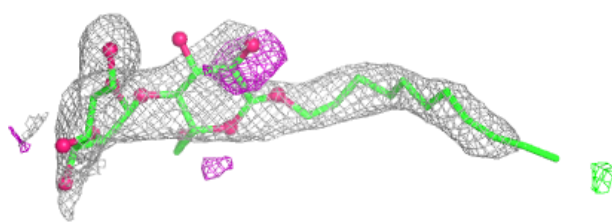
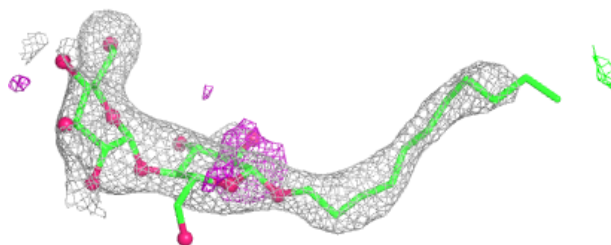
Electron density around LHG E 101:

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

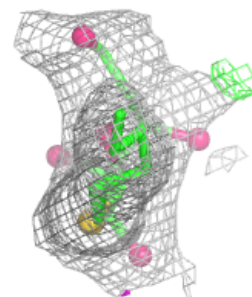
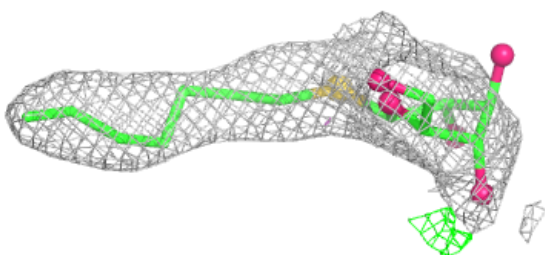
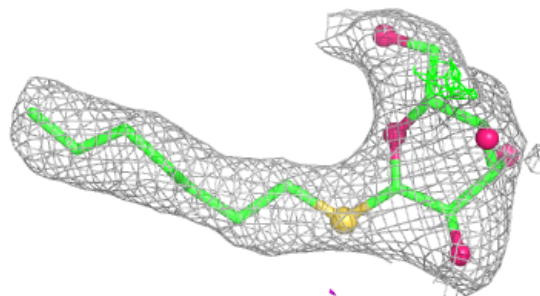


Electron density around LMT A 414:

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

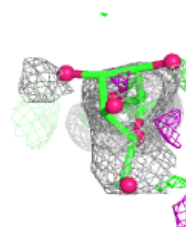
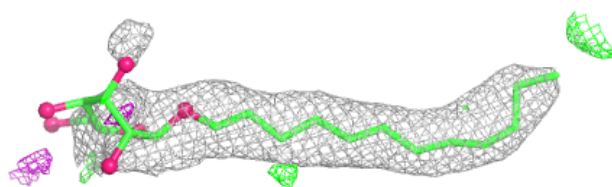
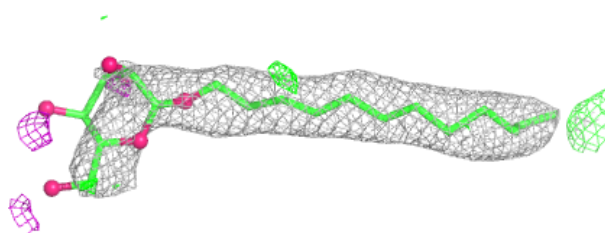
**Electron density around HTG i 103:**

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

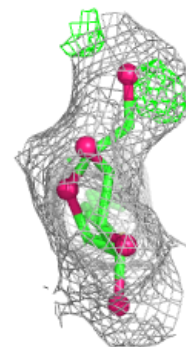
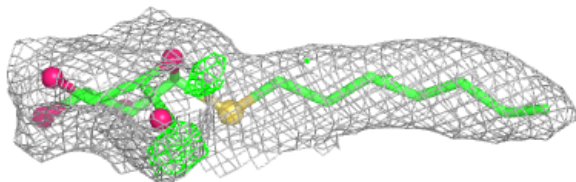
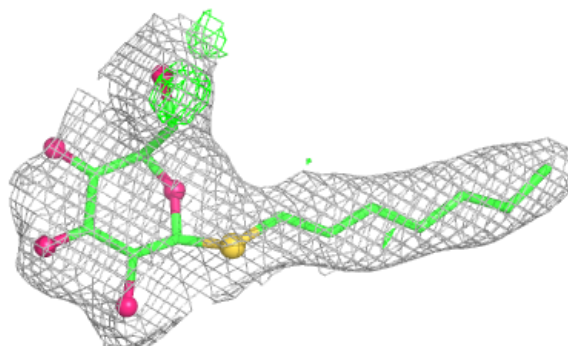


Electron density around LMT I 1201:

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

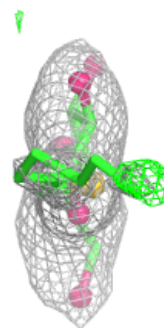
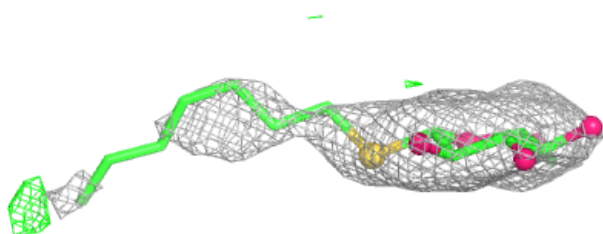
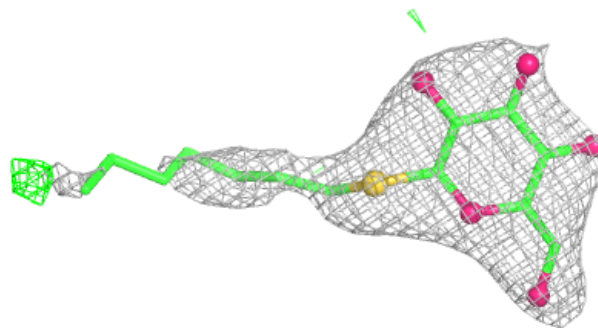
**Electron density around HTG b 602:**

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

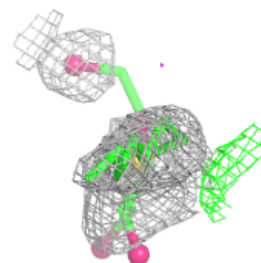
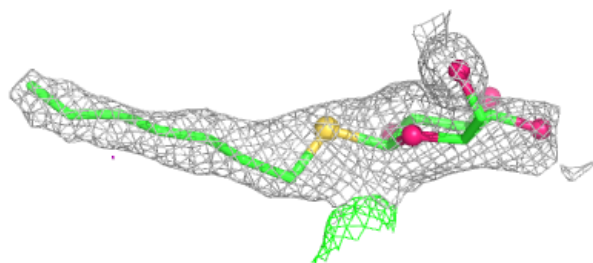
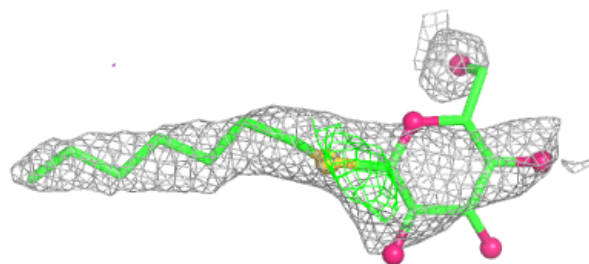


Electron density around HTG c 523:

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

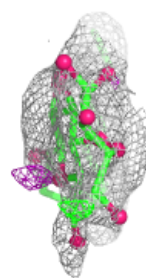
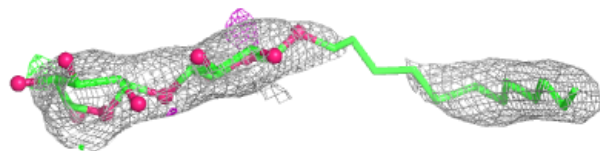
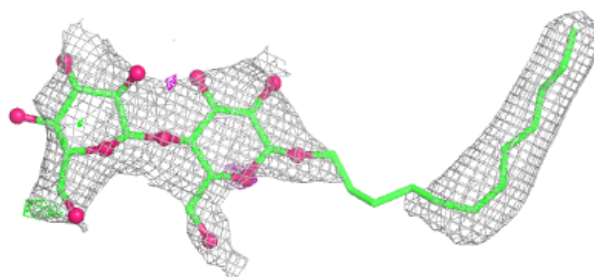
**Electron density around HTG c 524:**

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

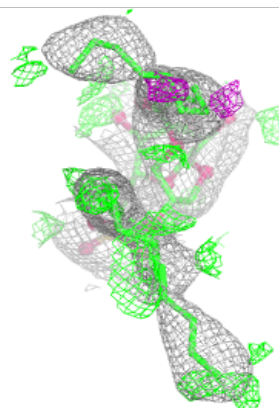
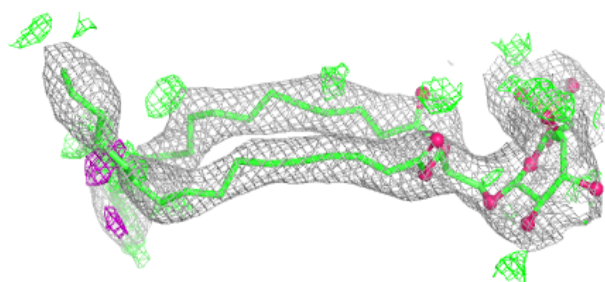
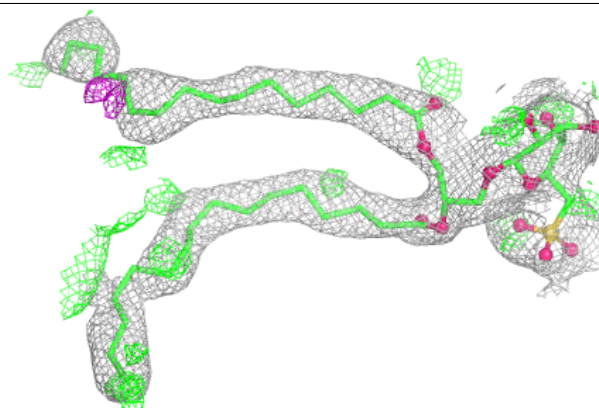


Electron density around LMT Z 101:

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

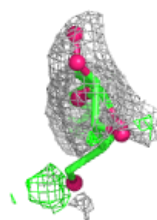
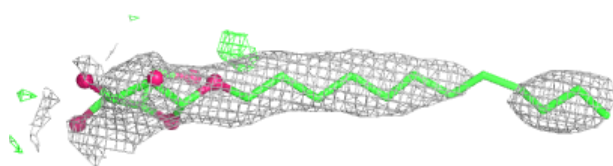
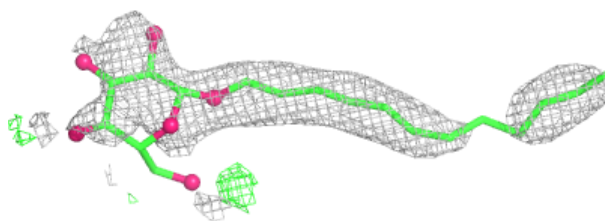
**Electron density around SQD L 102:**

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

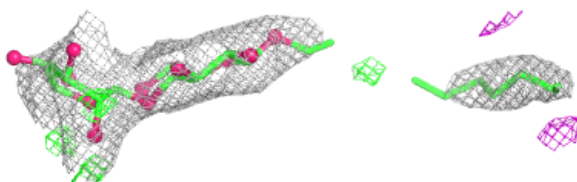
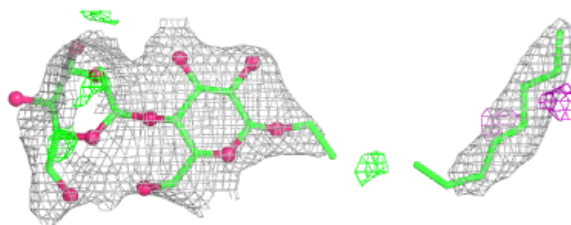


Electron density around LMT J 102:

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

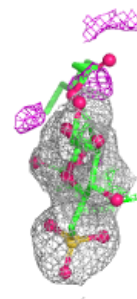
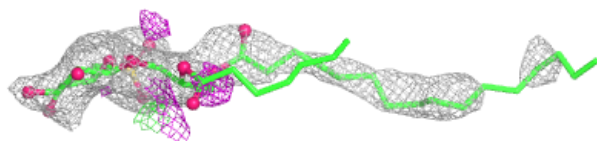
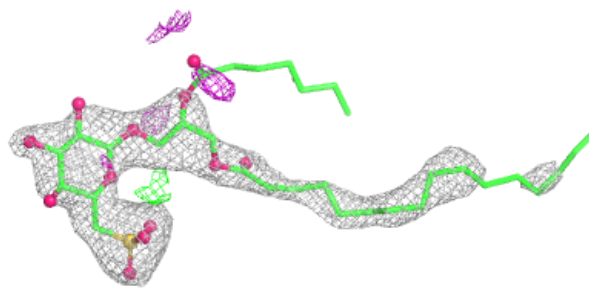
**Electron density around LMT z 1801:**

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

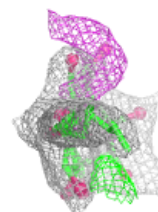
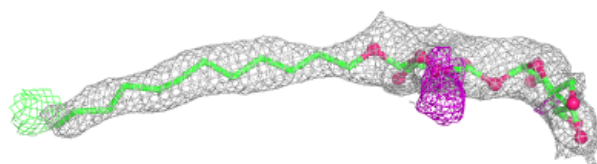
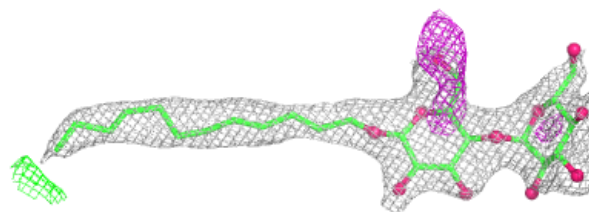


Electron density around SQD F 101:

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

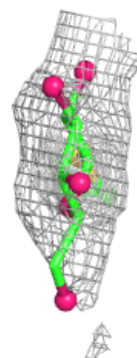
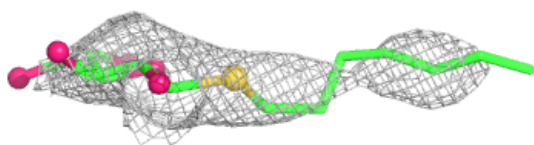
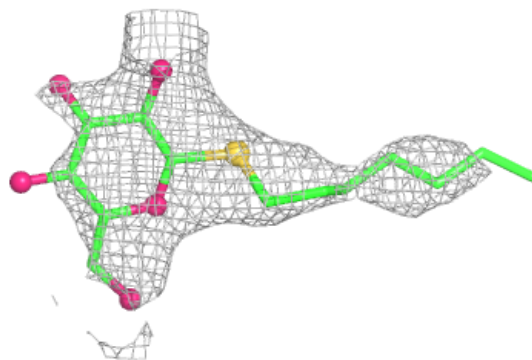
**Electron density around LMT m 102:**

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

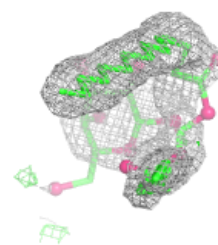
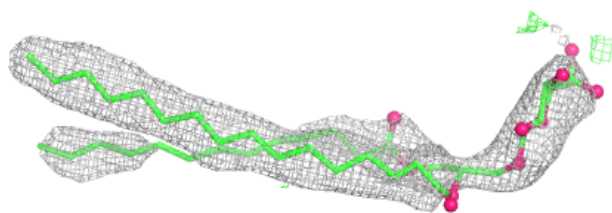
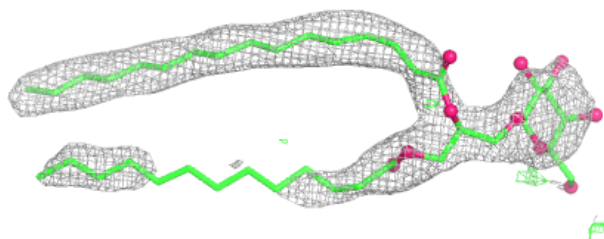


Electron density around HTG c 526:

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

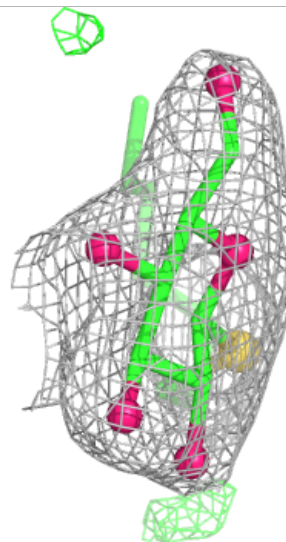
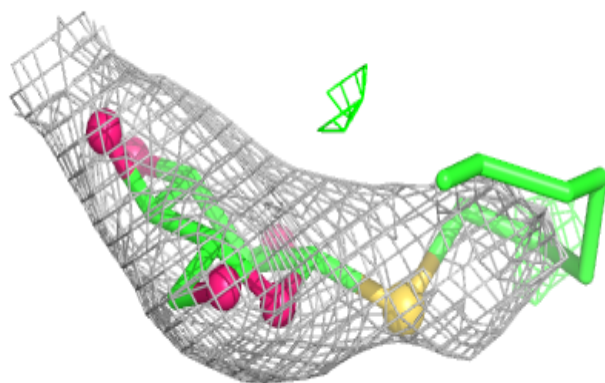
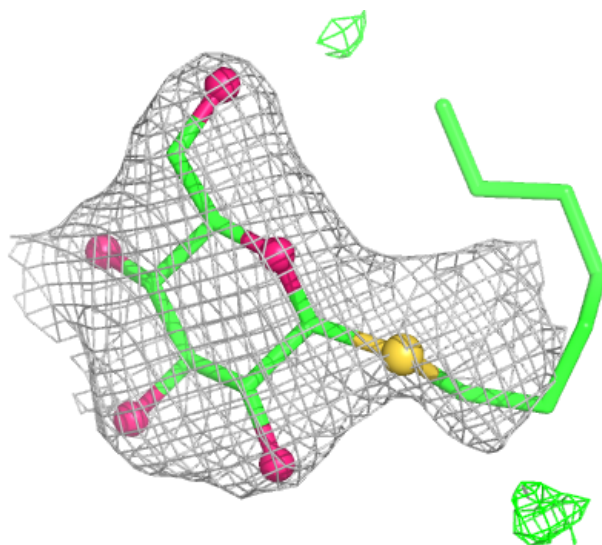
**Electron density around LMG C 526:**

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



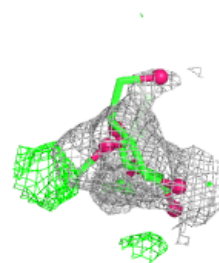
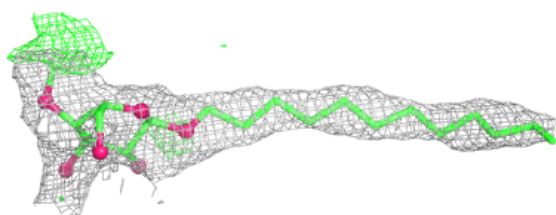
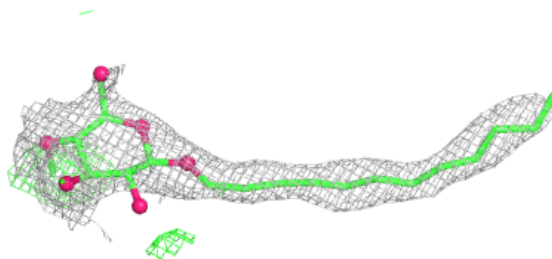
Electron density around HTG V 204:

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

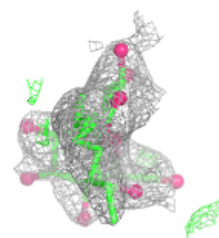
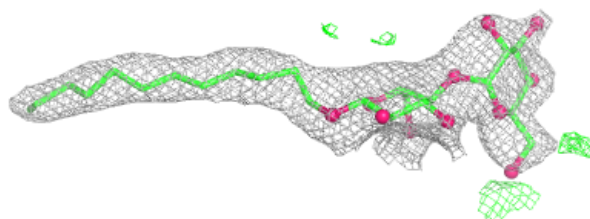
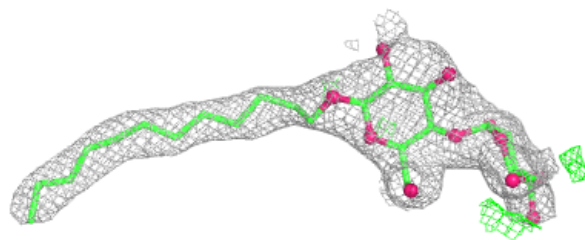


Electron density around LMT b 624:

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

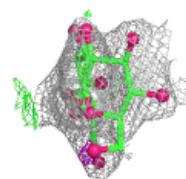
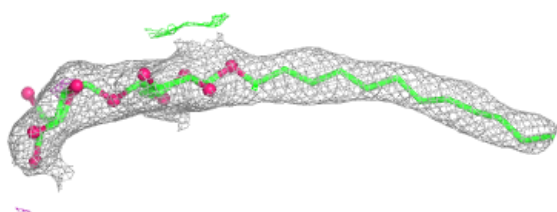
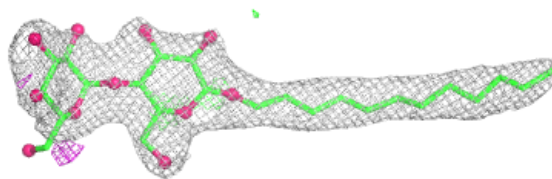
**Electron density around LMT B 623:**

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

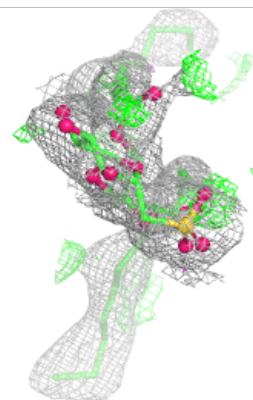
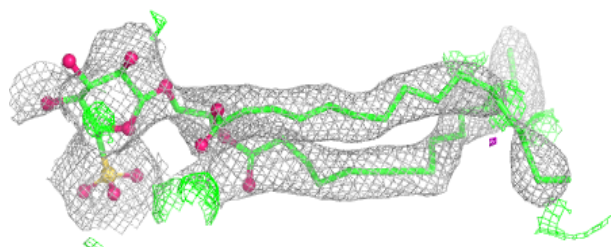
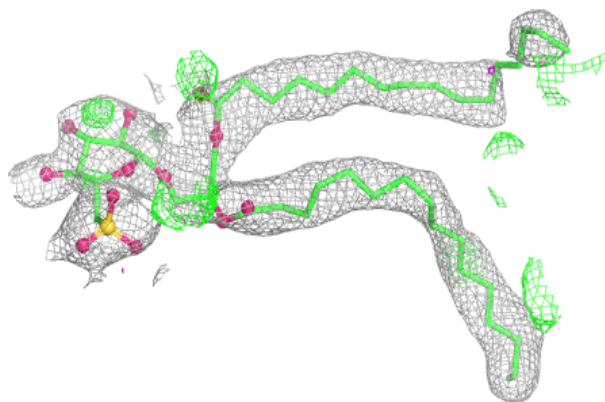


Electron density around LMT M 101:

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

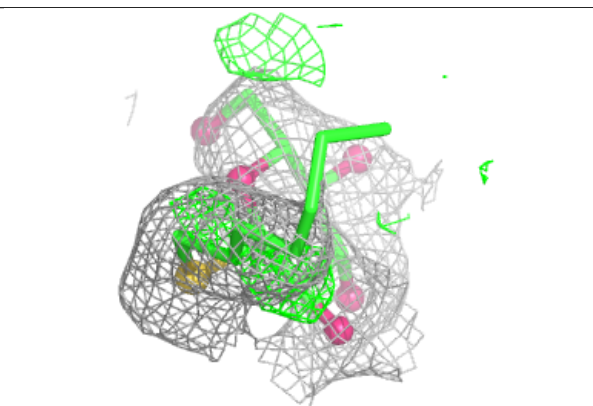
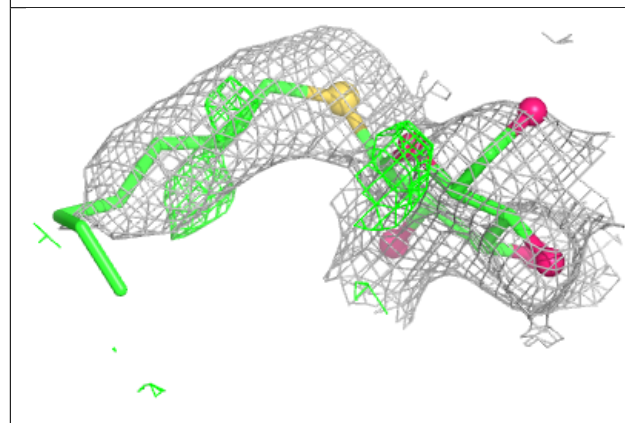
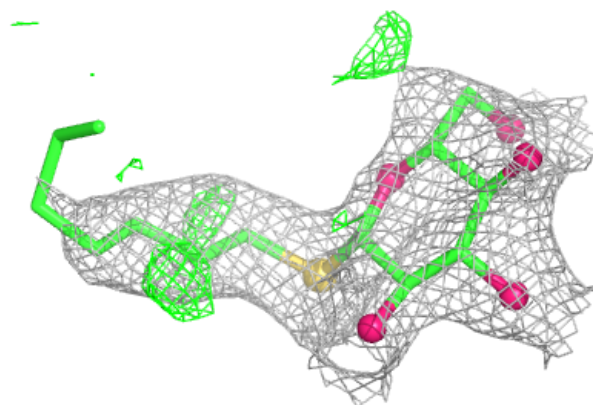
**Electron density around SQD B 621:**

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

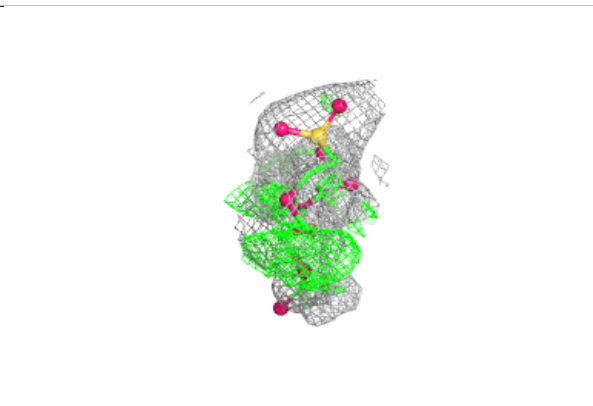
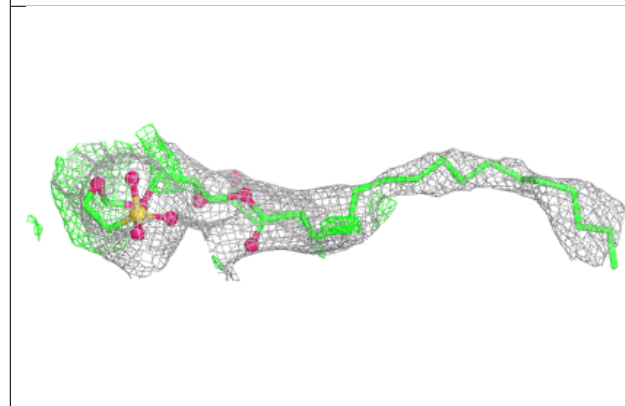
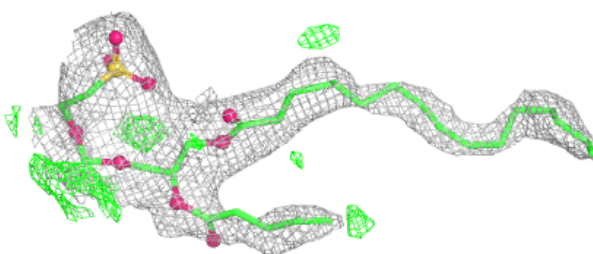


Electron density around HTG b 625:

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

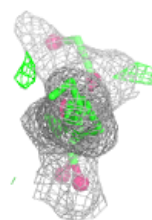
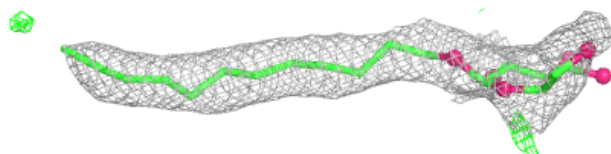
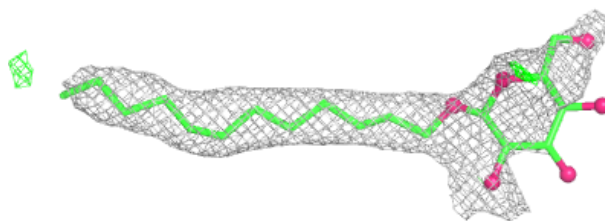
**Electron density around SQD f 102:**

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

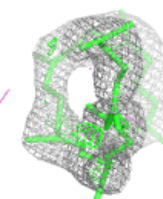
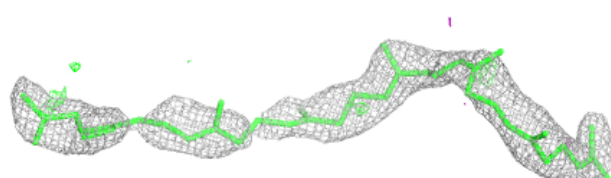
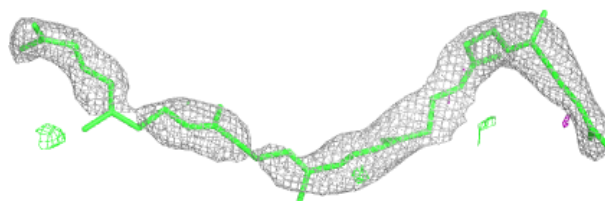


Electron density around LMT i 104:

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

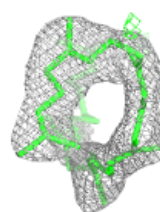
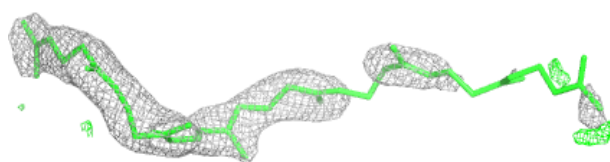
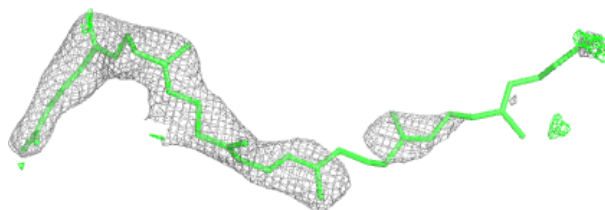
**Electron density around PL9 A 417:**

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

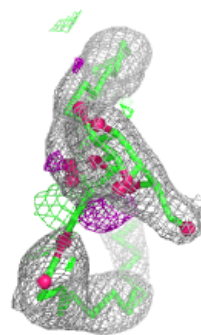
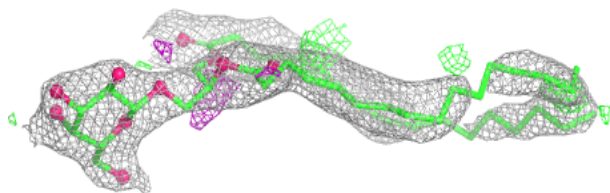
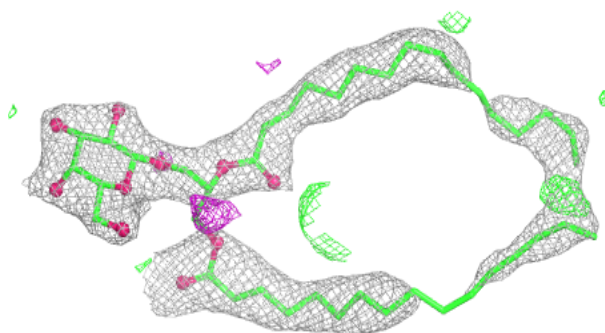


Electron density around PL9 x 801:

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

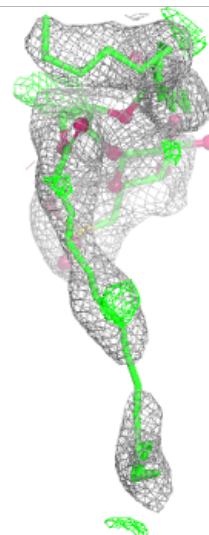
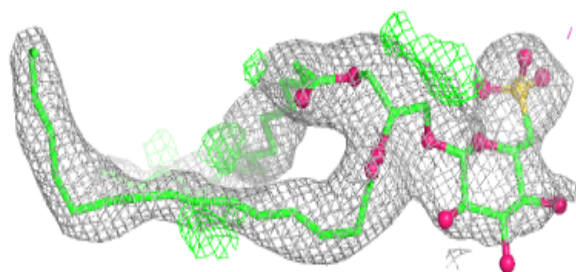
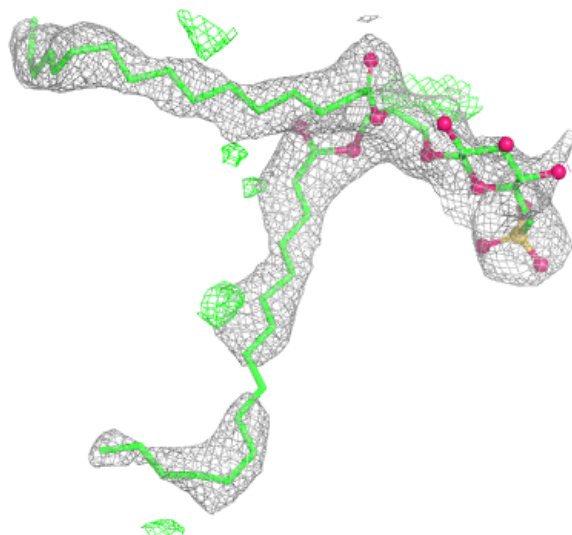
**Electron density around LMG i 101:**

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



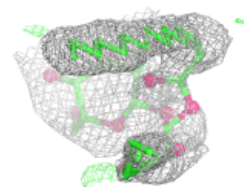
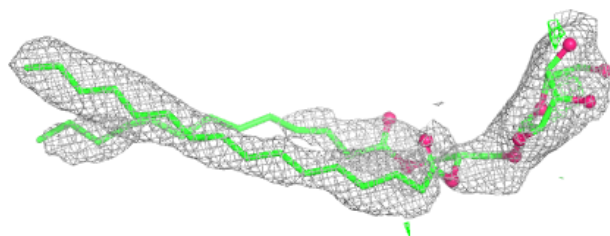
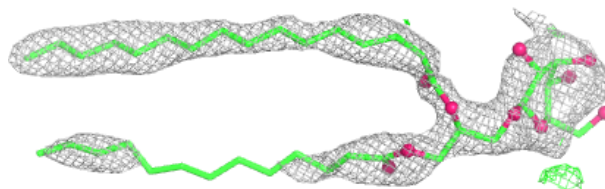
Electron density around SQD A 413:

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

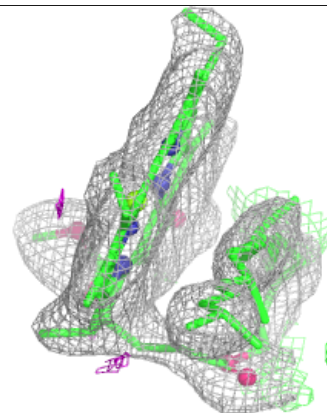
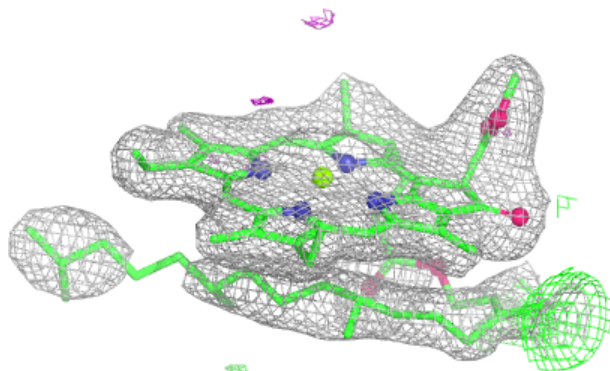
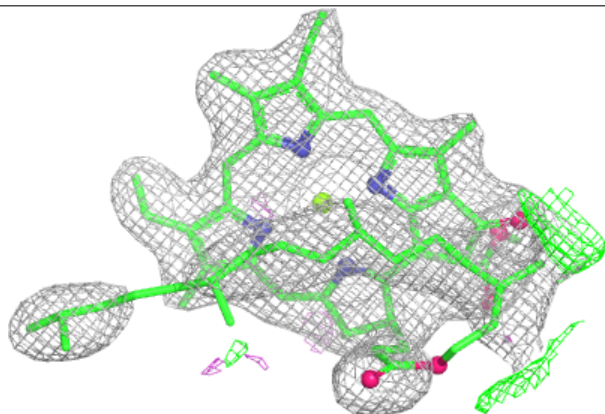


Electron density around LMG c 522:

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

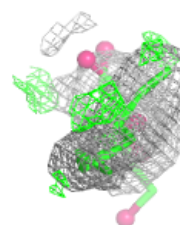
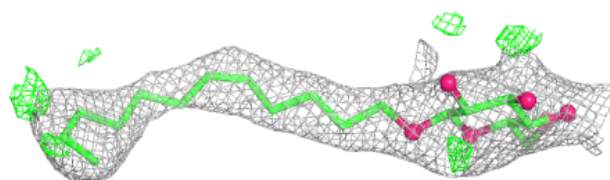
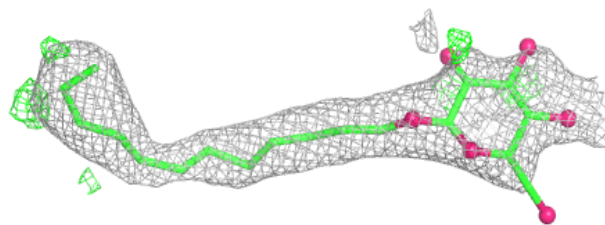
**Electron density around CLA B 602:**

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



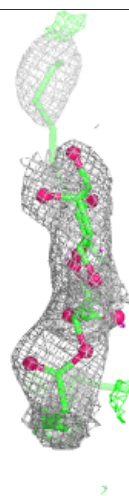
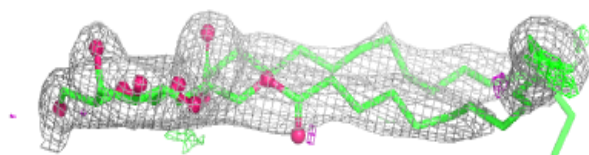
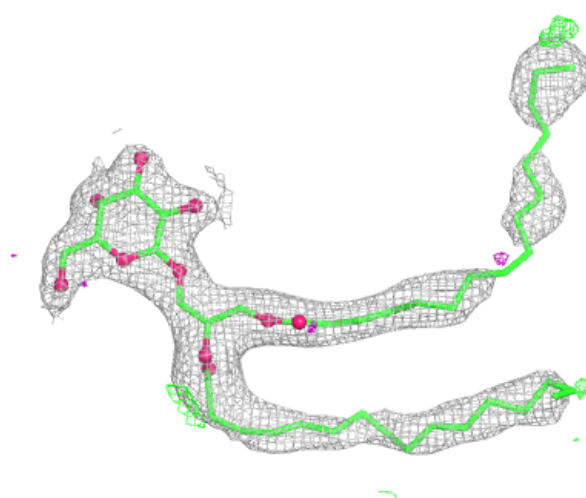
Electron density around LMT B 637:

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



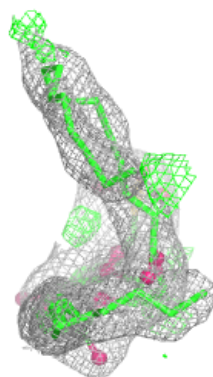
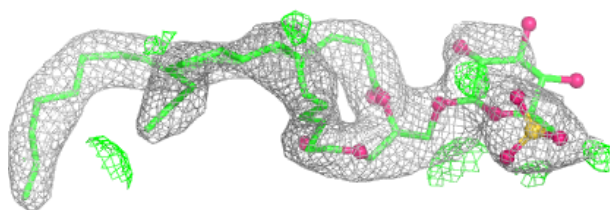
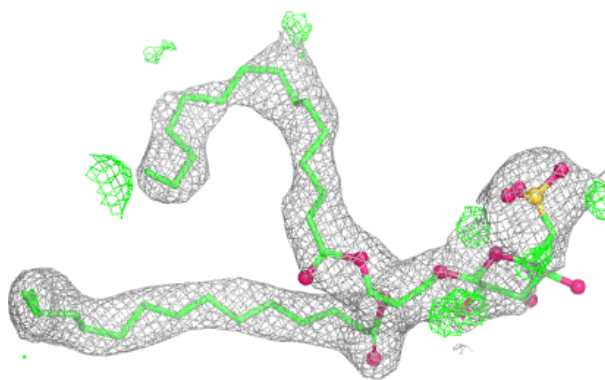
Electron density around LMG C 520:

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

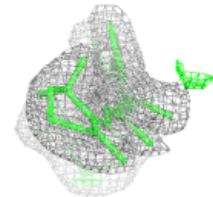
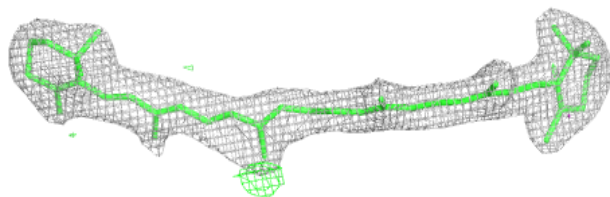
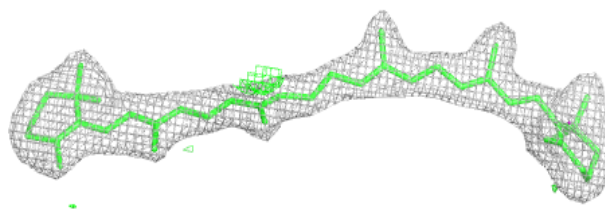


Electron density around SQD a 2102:

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

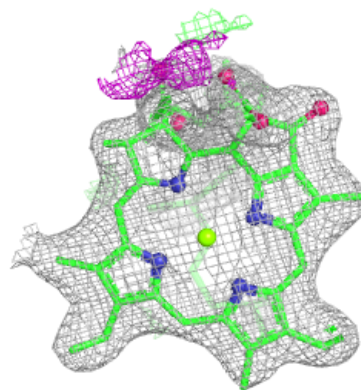
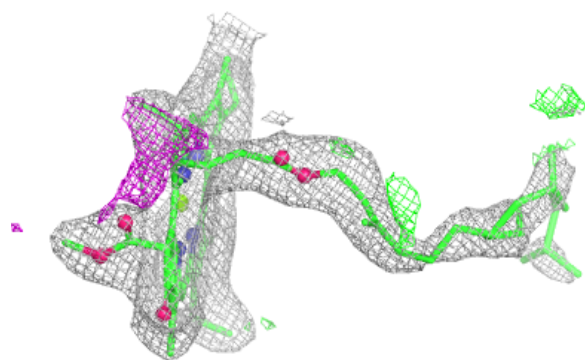
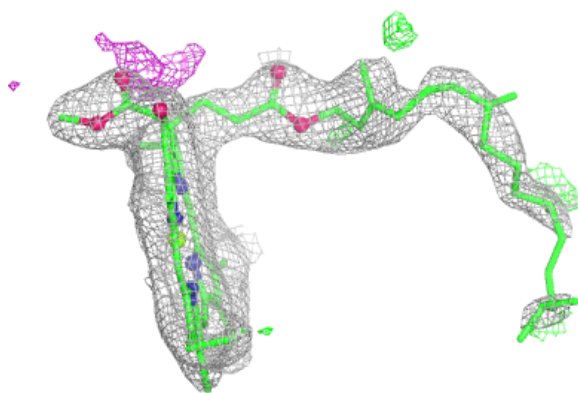
**Electron density around BCR t 102:**

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

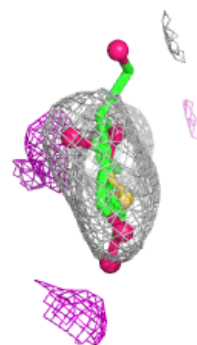
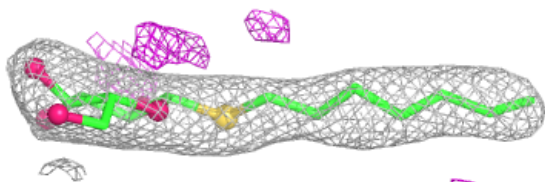
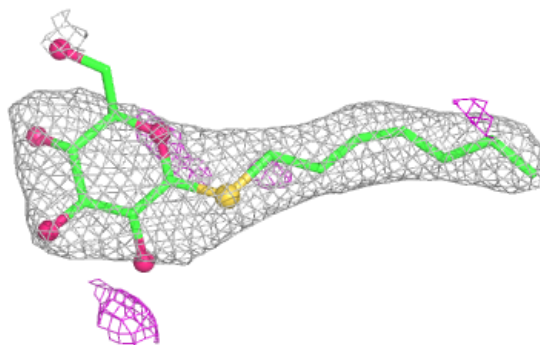


Electron density around CLA C 507:

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

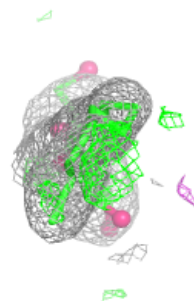
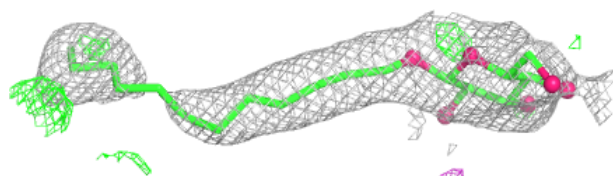
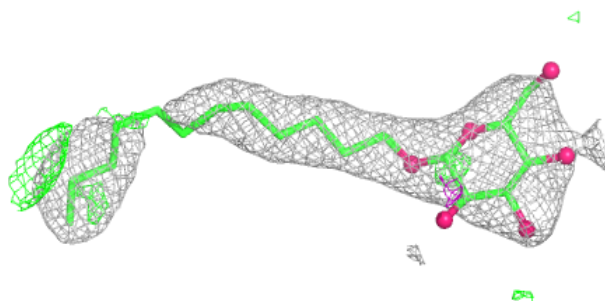
**Electron density around HTG B 627:**

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

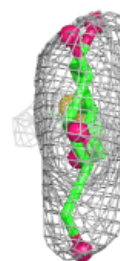
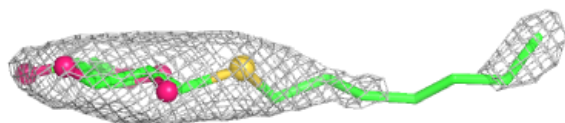
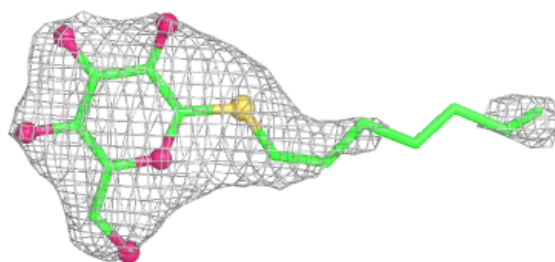


Electron density around LMT T 102:

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

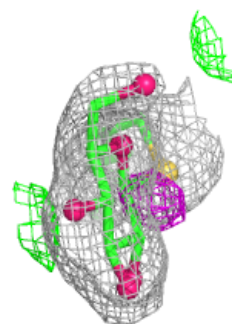
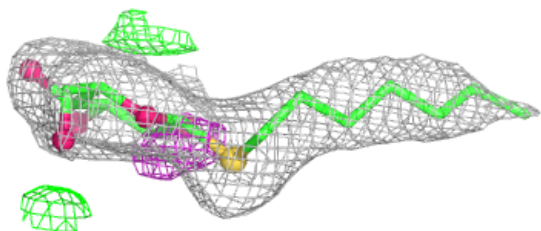
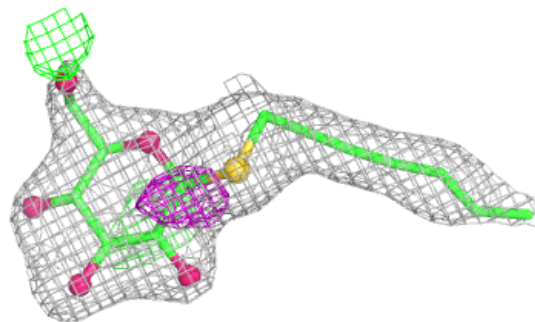
**Electron density around HTG C 521:**

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

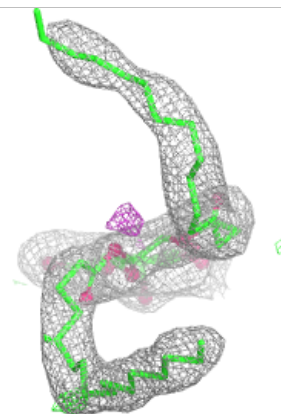
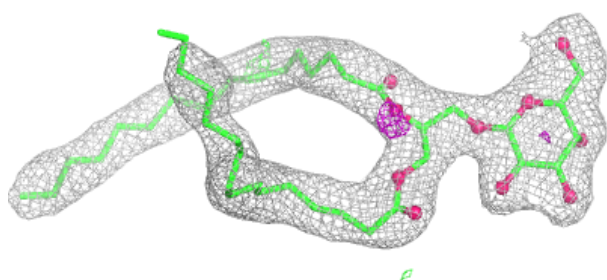
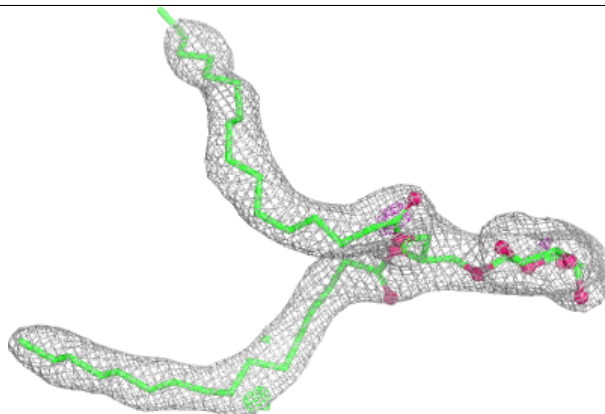


Electron density around HTG B 624:

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

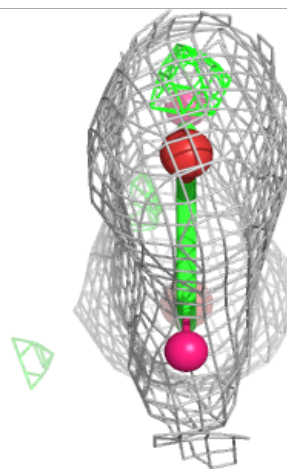
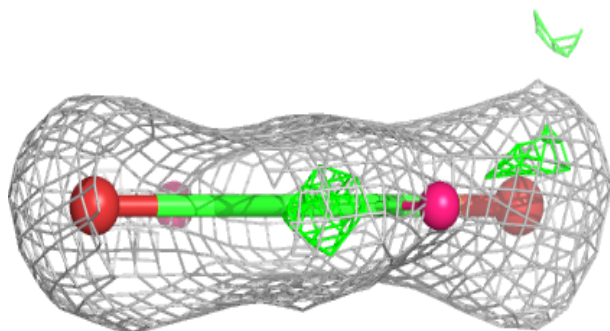
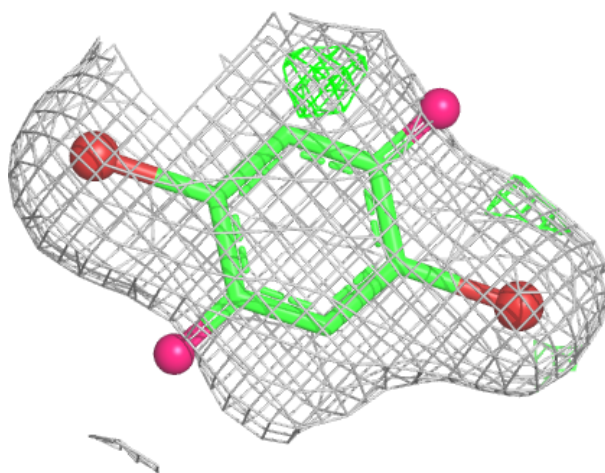
**Electron density around LMG B 622:**

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



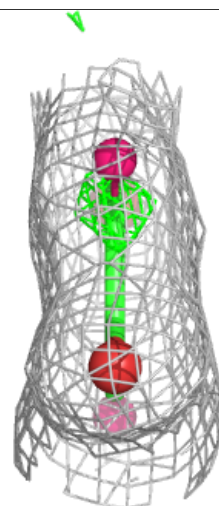
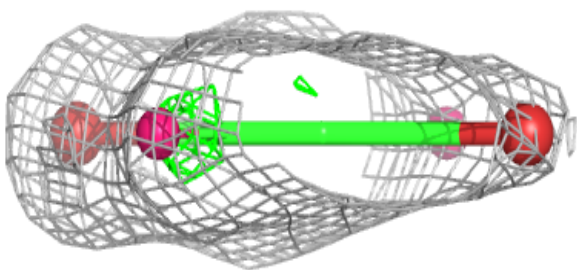
Electron density around K2I A 418 (A):

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



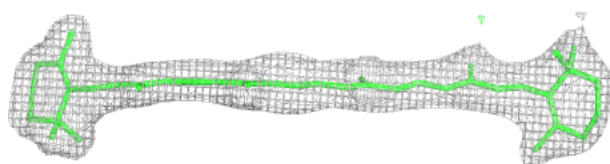
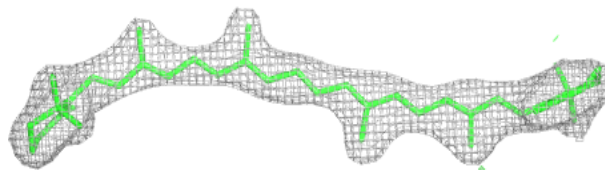
Electron density around K2I A 418 (B):

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

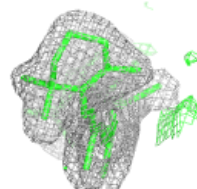
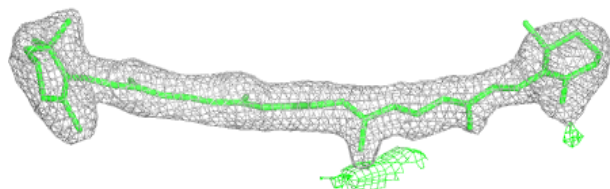
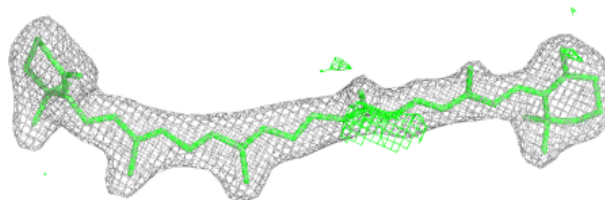


Electron density around BCR C 516:

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

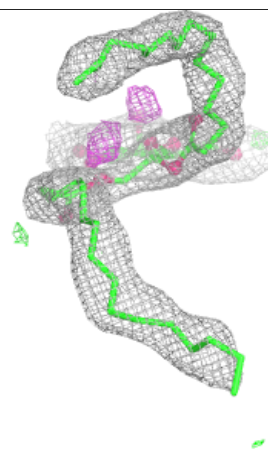
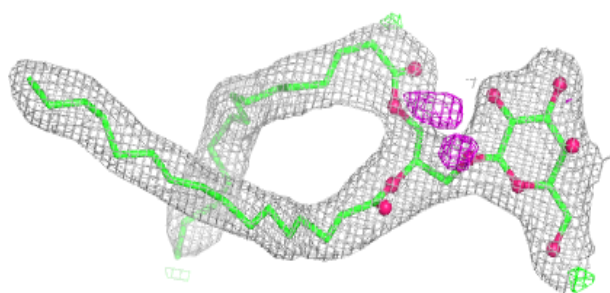
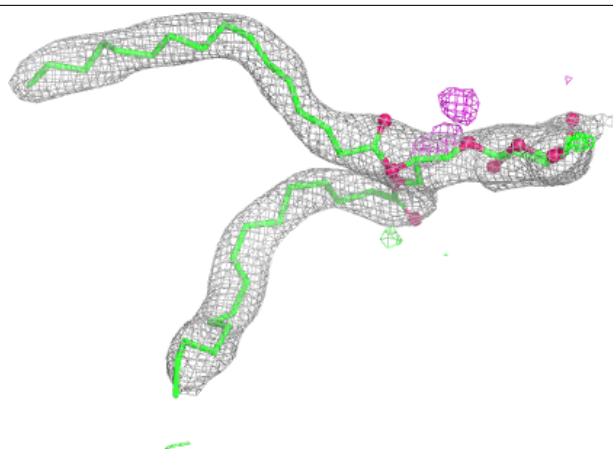
**Electron density around BCR T 101:**

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



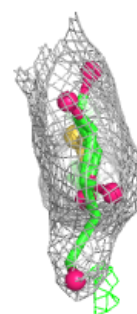
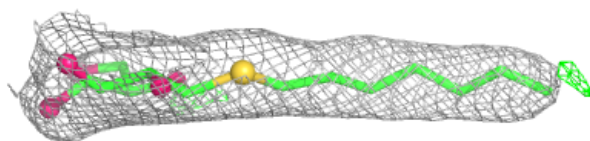
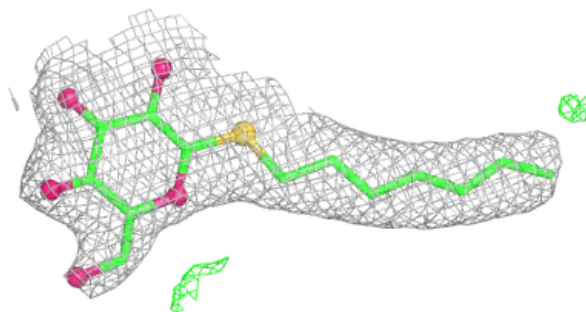
Electron density around LMG b 623:

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



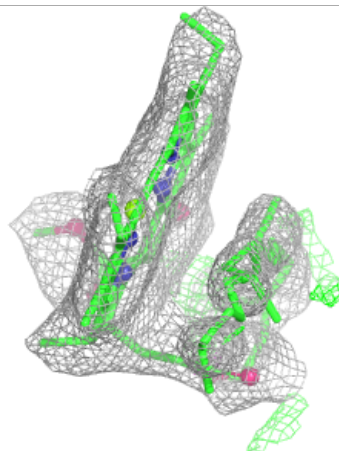
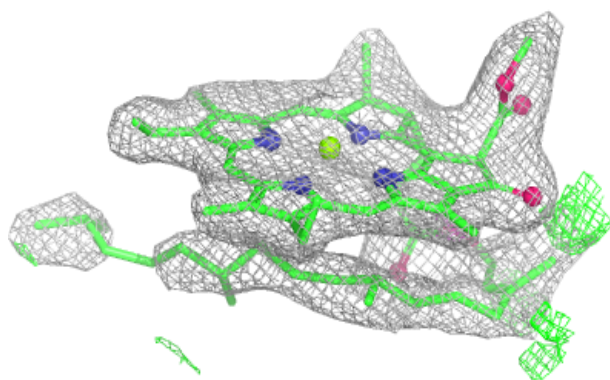
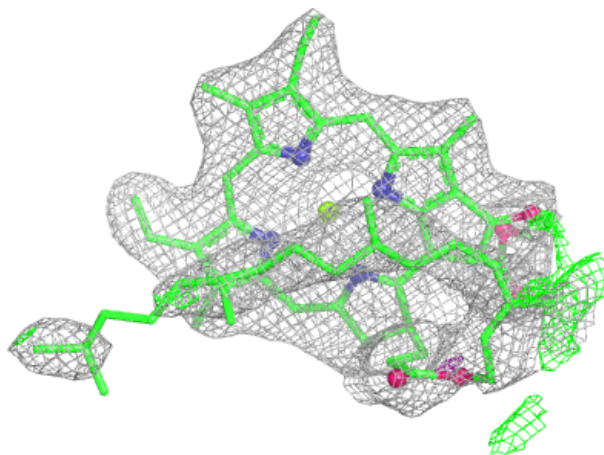
Electron density around HTG b 601:

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



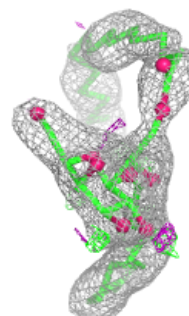
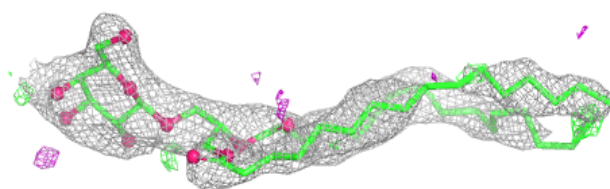
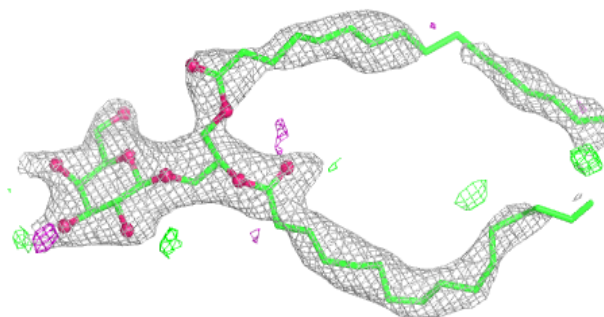
Electron density around CLA b 604:

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

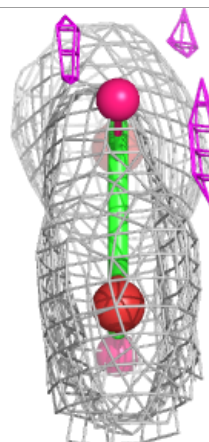
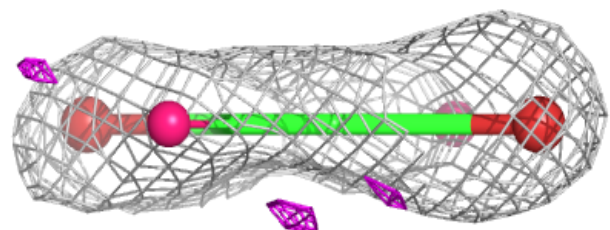
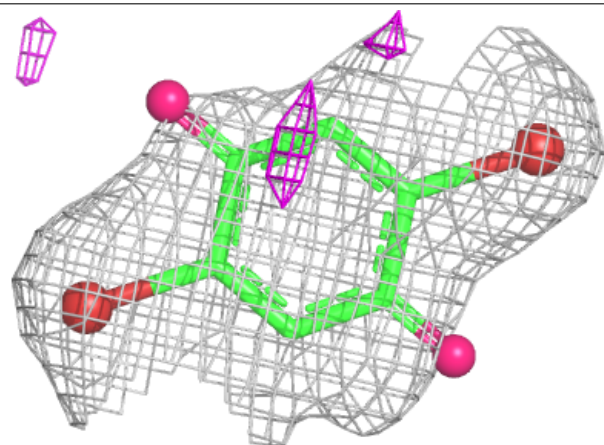


Electron density around LMG A 412:

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

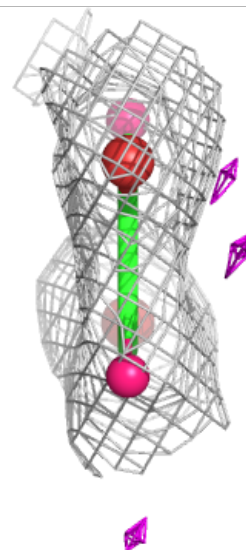
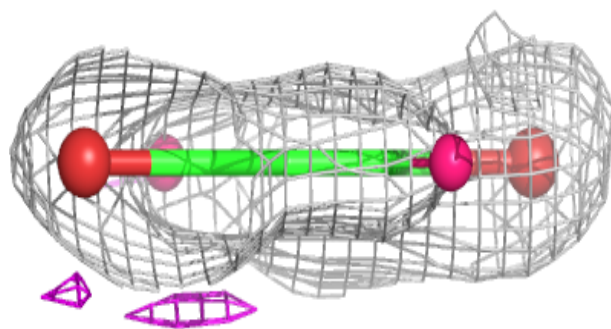
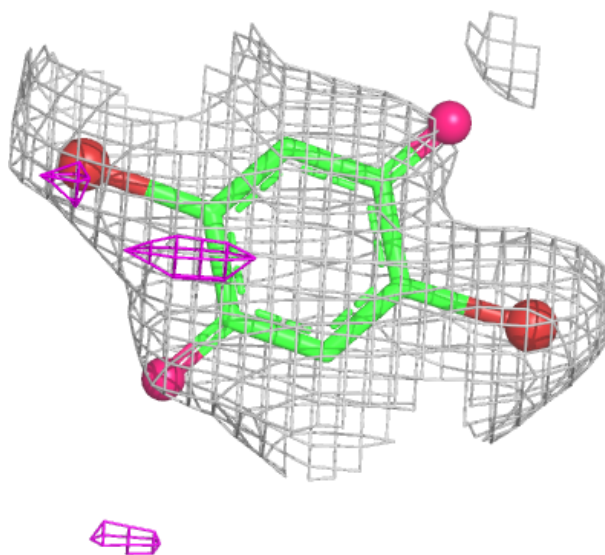
**Electron density around K2I a 2118 (A):**

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



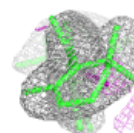
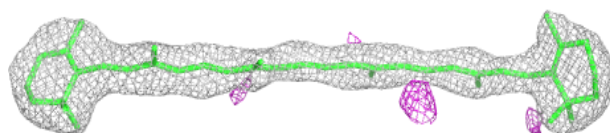
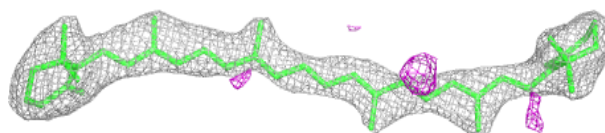
Electron density around K2I a 2118 (B):

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

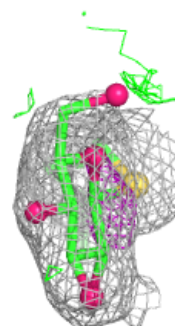
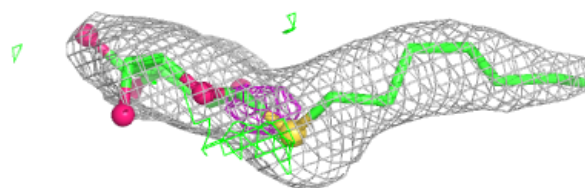
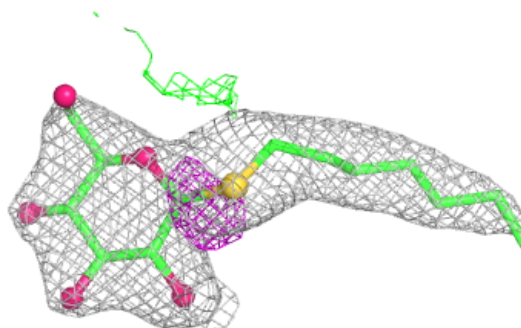


Electron density around BCR c 516:

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

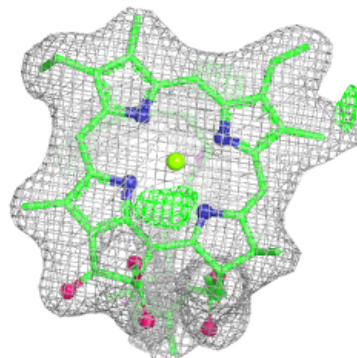
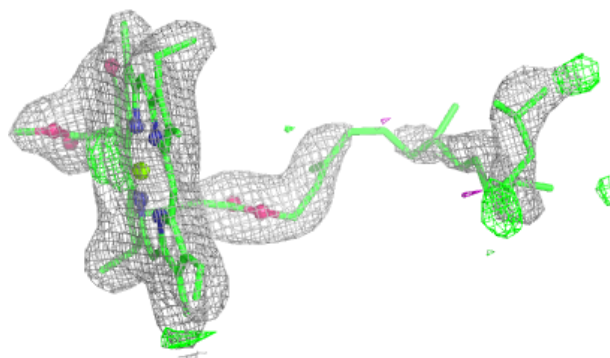
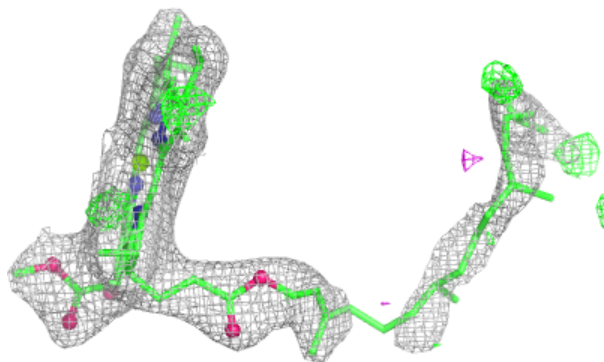
**Electron density around HTG O 302:**

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

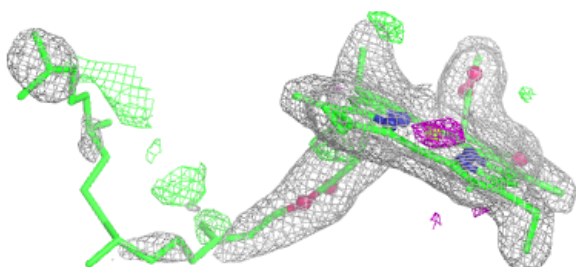
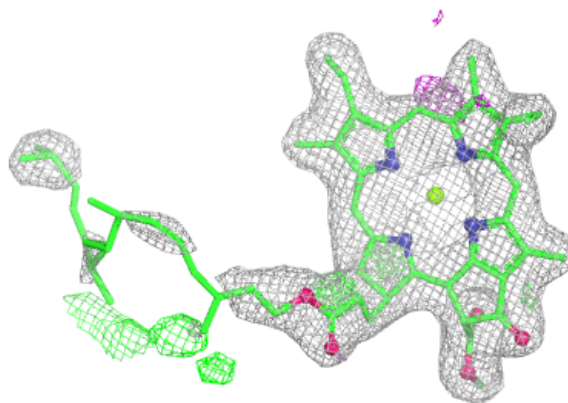


Electron density around CLA c 508:

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

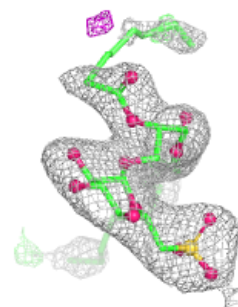
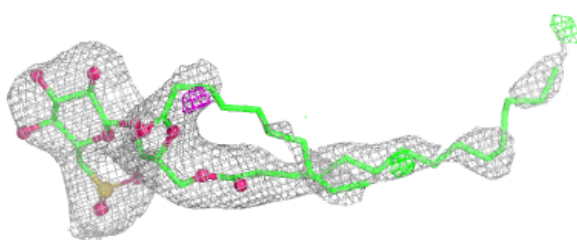
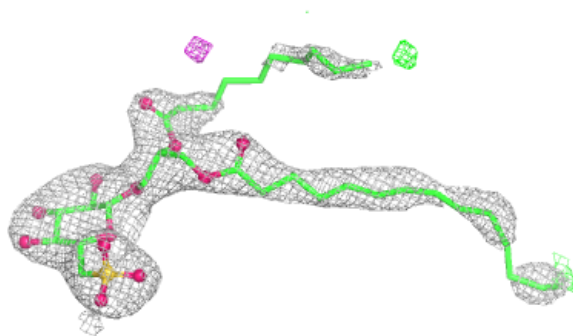
**Electron density around CLA a 2113:**

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

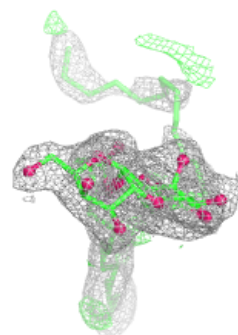
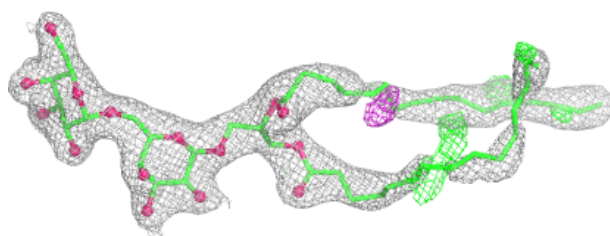
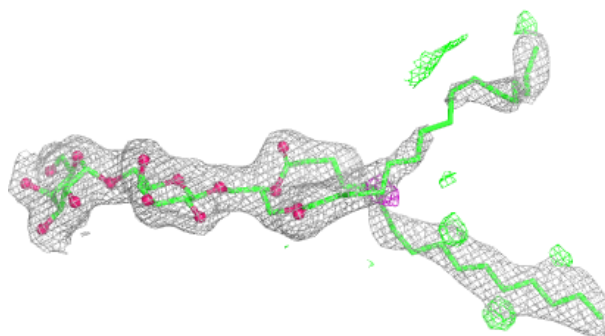


Electron density around SQD a 2115:

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

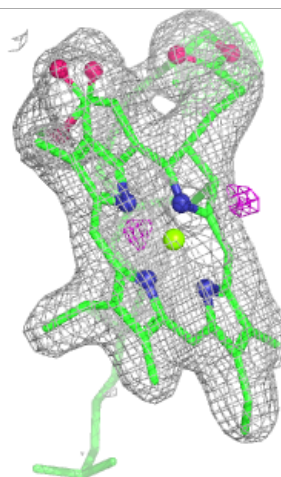
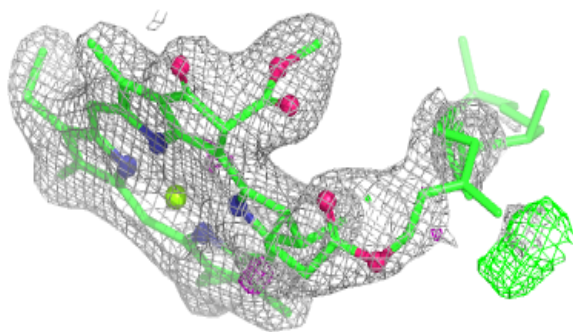
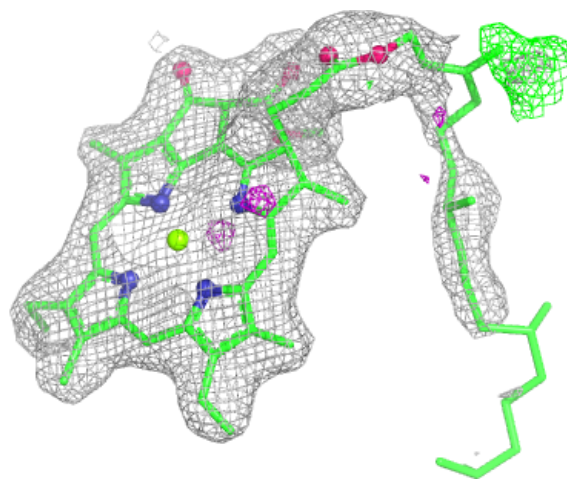
**Electron density around DGD c 518:**

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



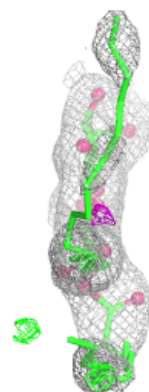
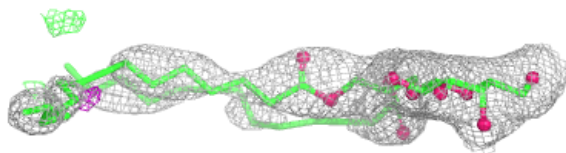
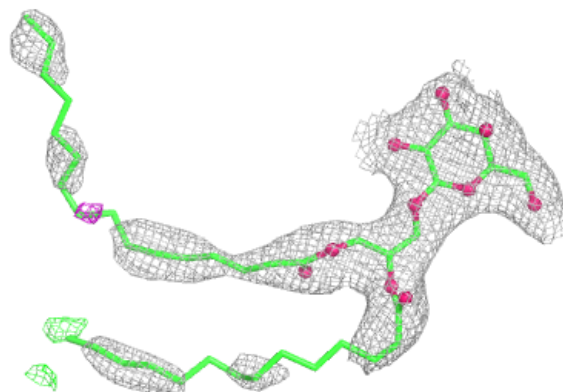
Electron density around CLA B 617:

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

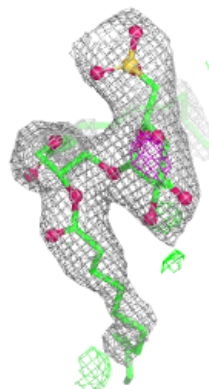
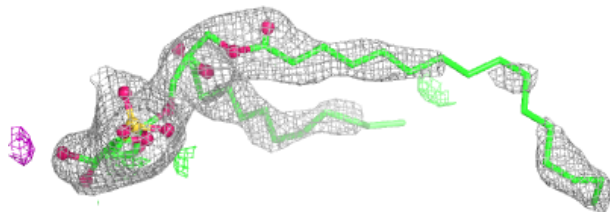
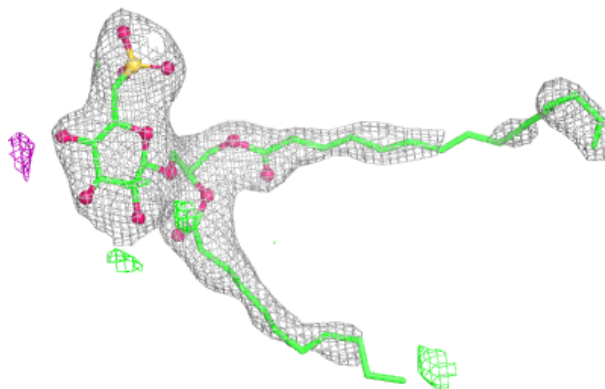


Electron density around LMG c 521:

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

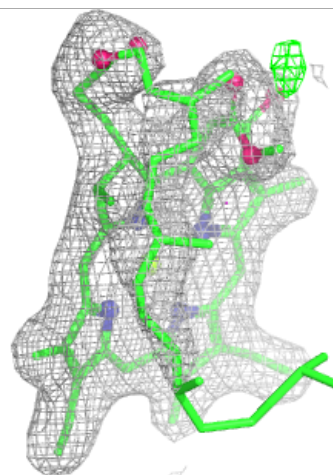
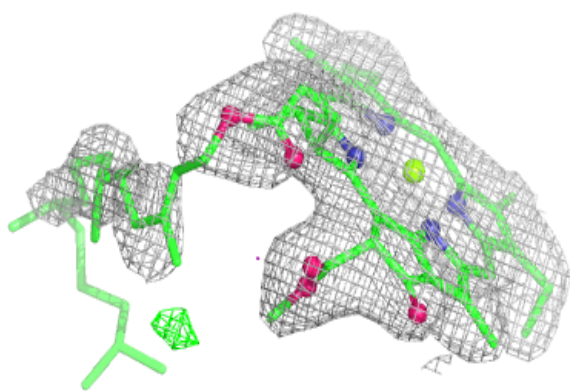
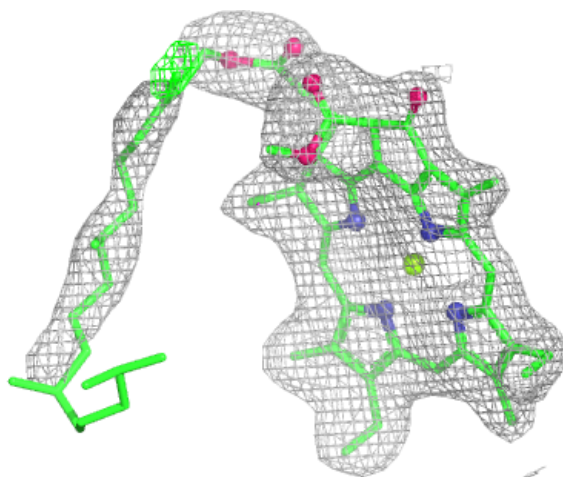
**Electron density around SQD A 411:**

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



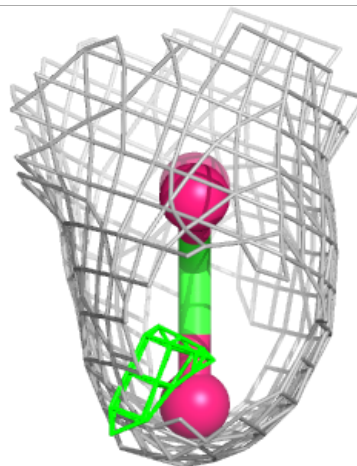
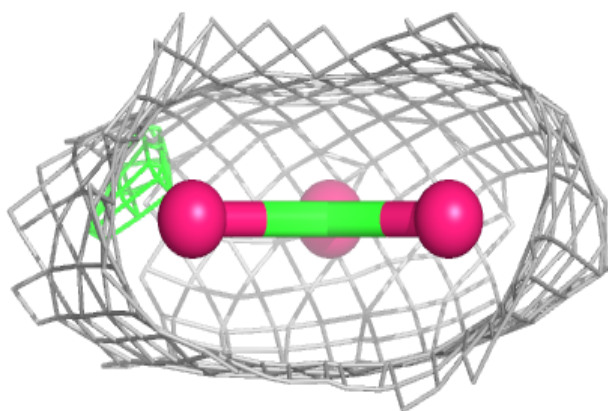
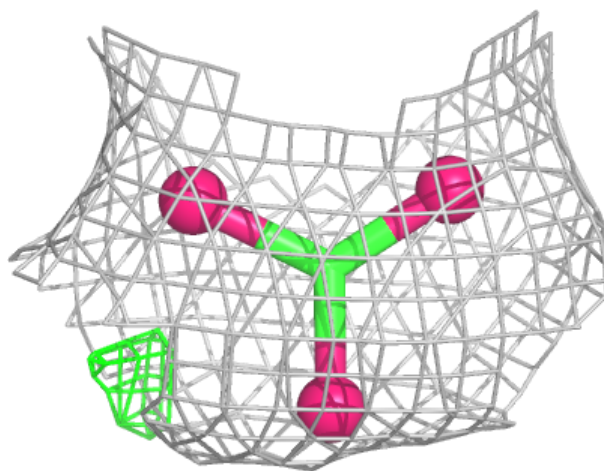
Electron density around CLA b 619:

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



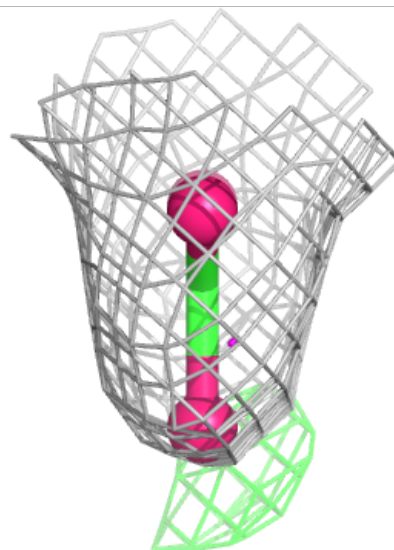
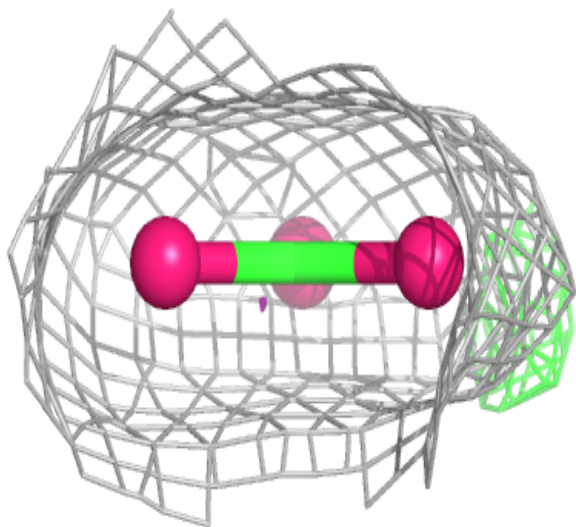
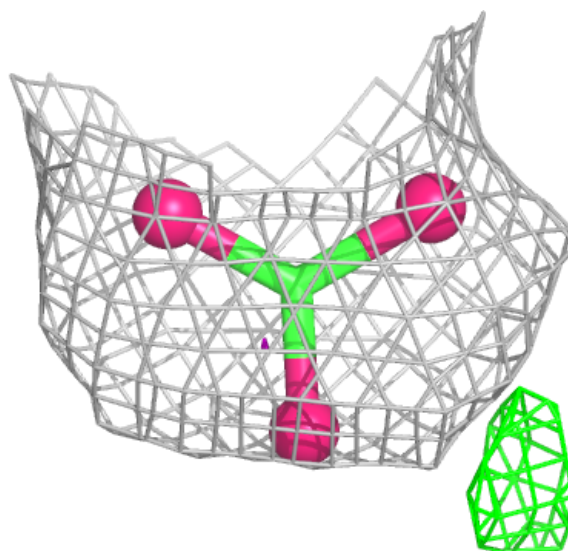
Electron density around BCT A 421:

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



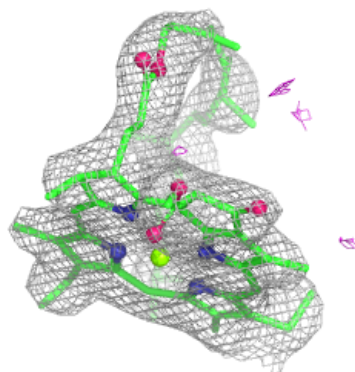
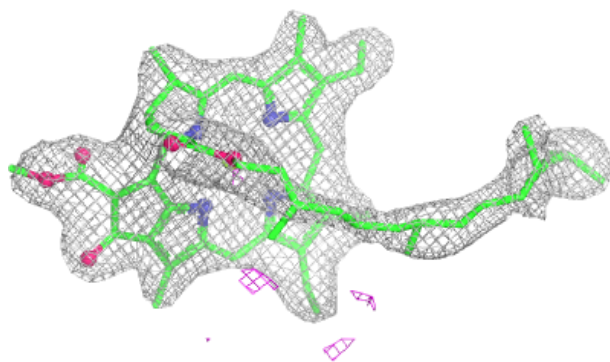
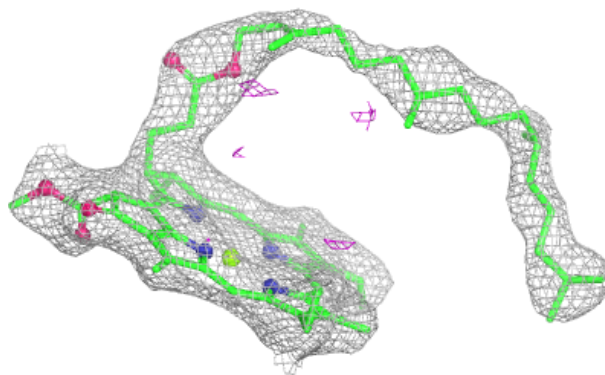
Electron density around BCT a 2108:

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



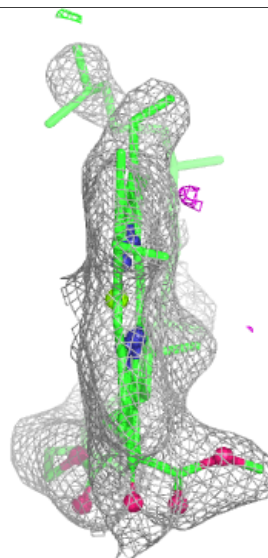
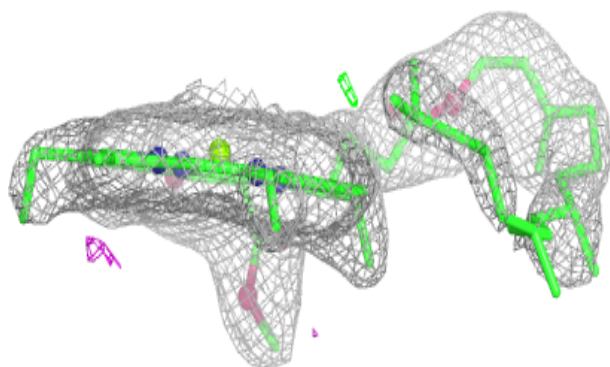
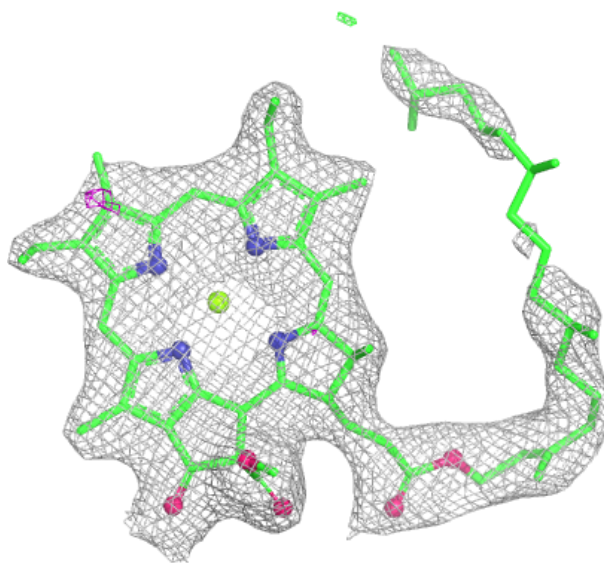
Electron density around CLA C 514:

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



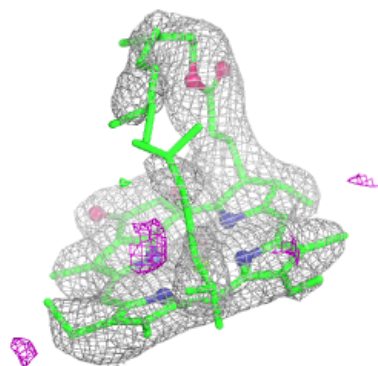
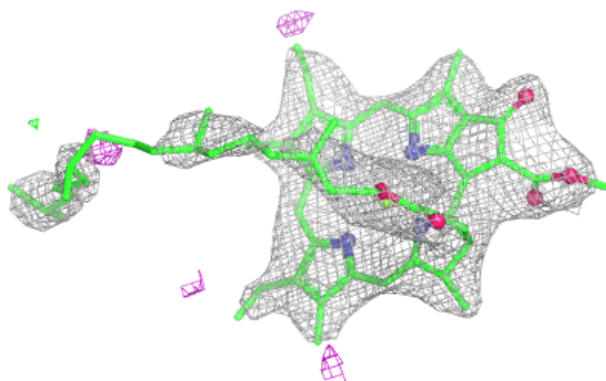
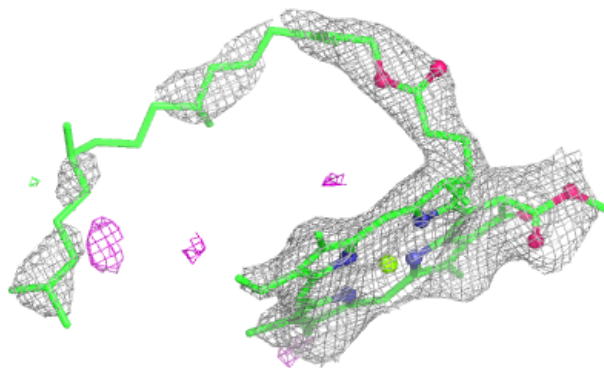
Electron density around CLA c 514:

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

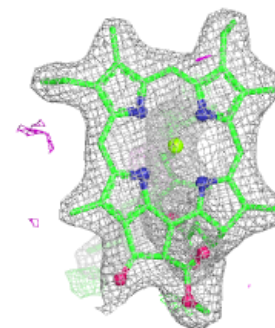
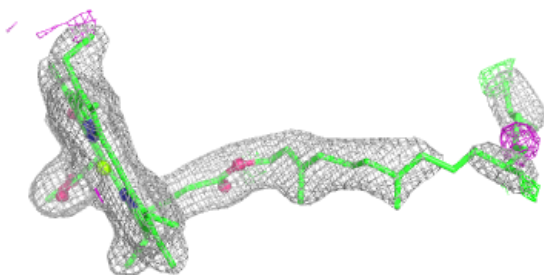
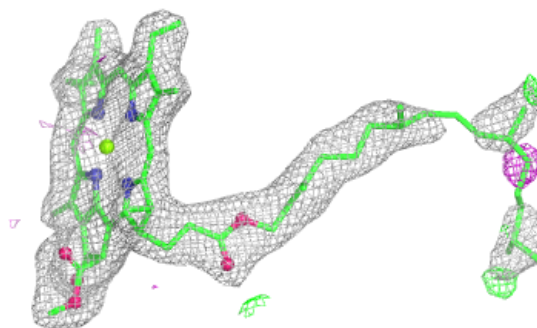


Electron density around CLA c 515:

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

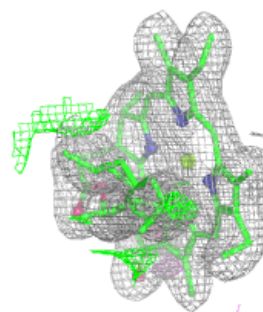
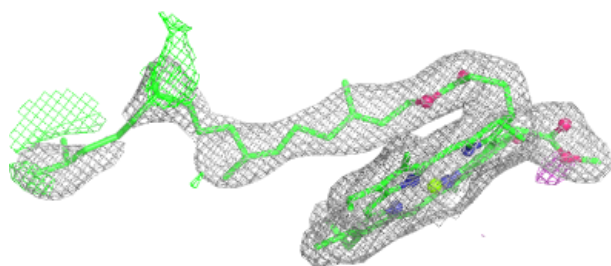
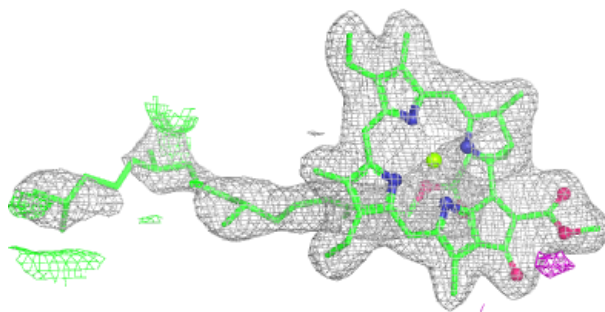
**Electron density around CLA d 405:**

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



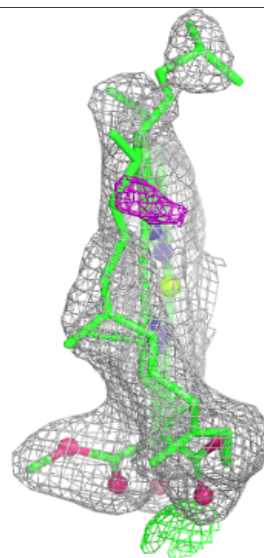
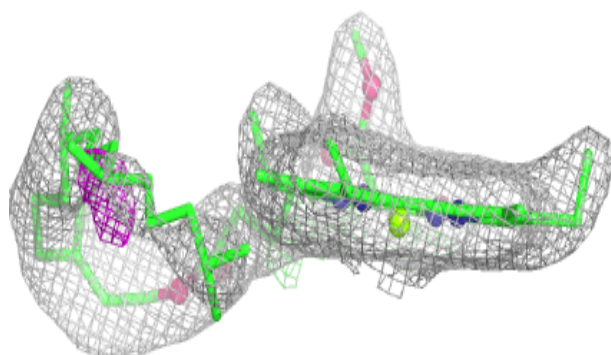
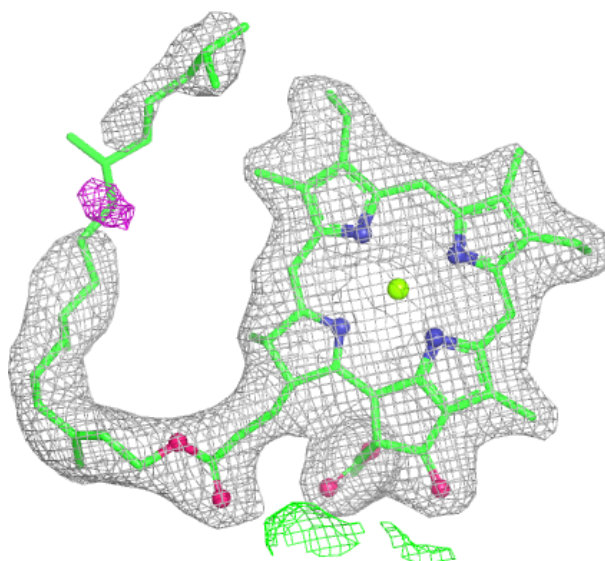
Electron density around CLA B 615:

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



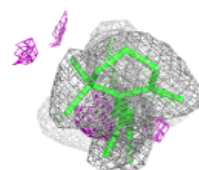
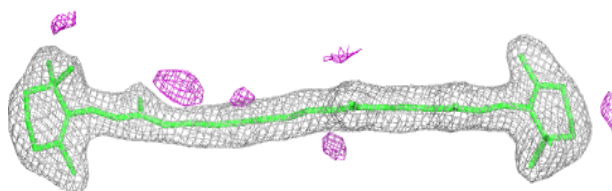
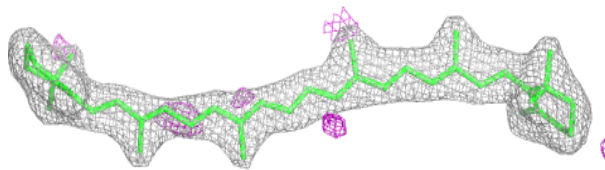
Electron density around CLA C 513:

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



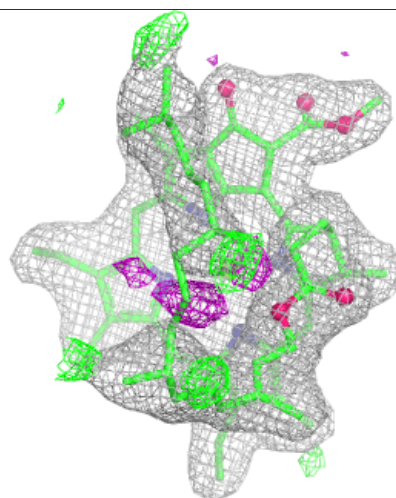
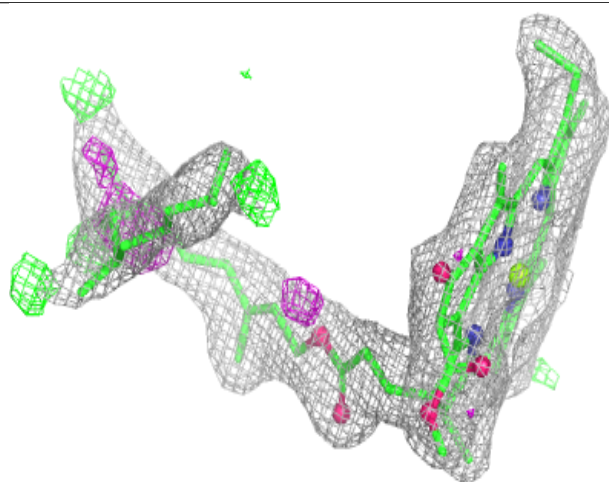
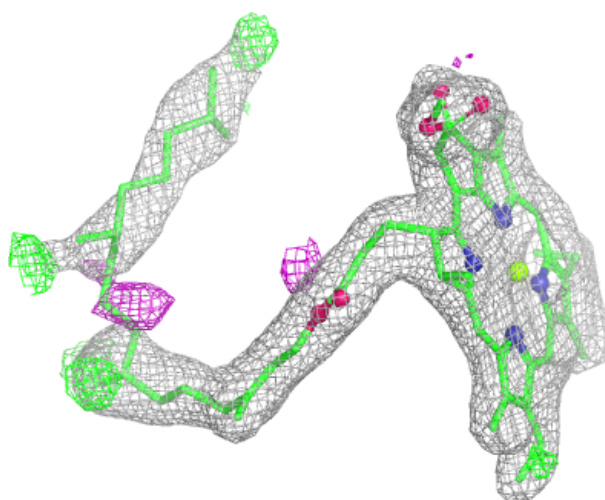
Electron density around BCR a 2114:

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



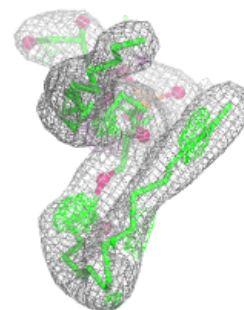
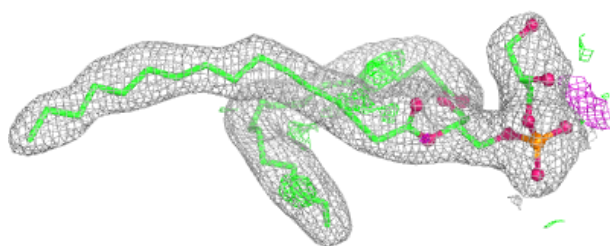
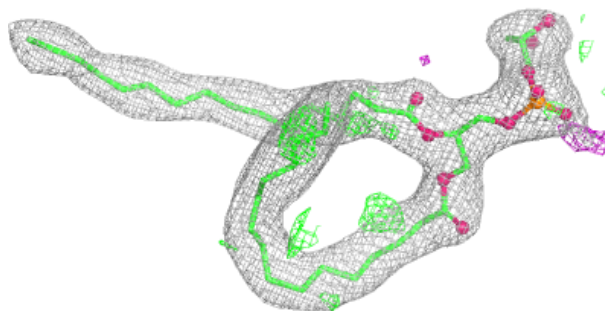
Electron density around CLA b 609:

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

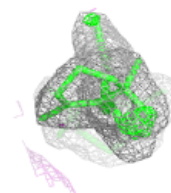
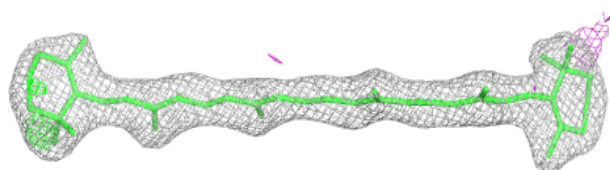
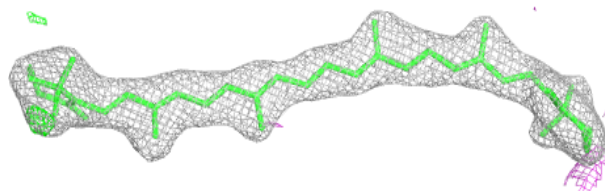


Electron density around LHG D 409:

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

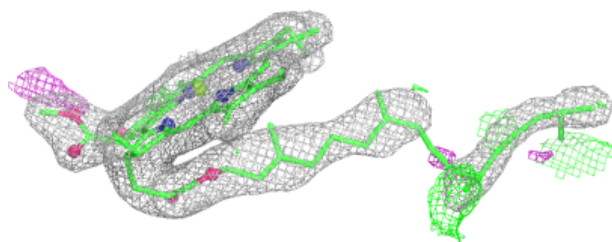
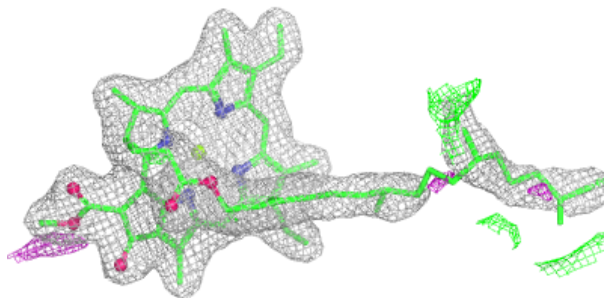
**Electron density around BCR c 517:**

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

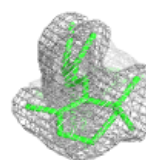
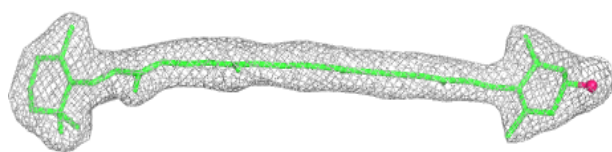
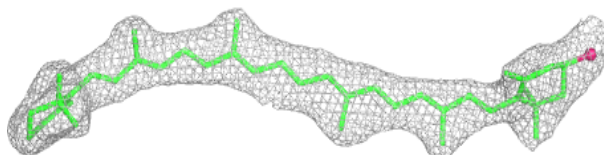


Electron density around CLA b 617:

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

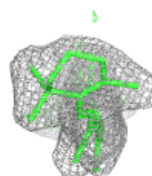
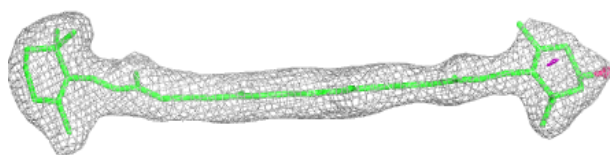
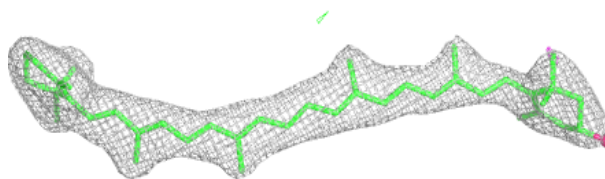
**Electron density around RRX H 101:**

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



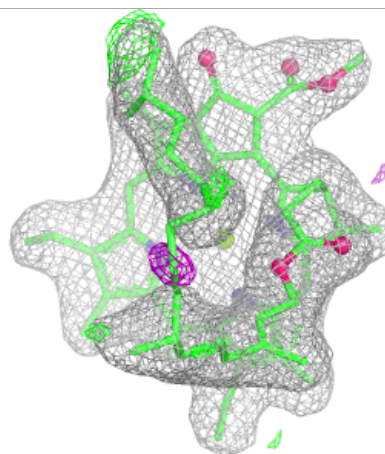
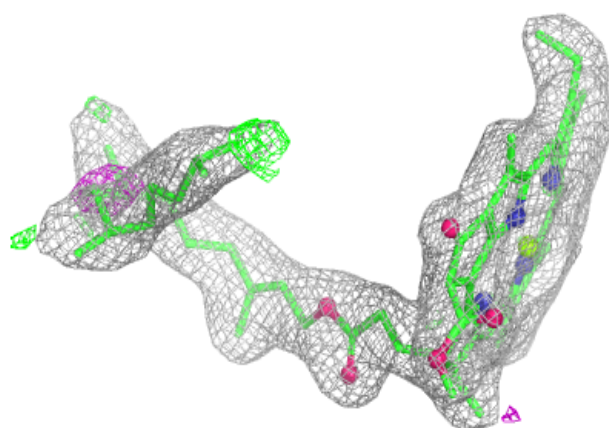
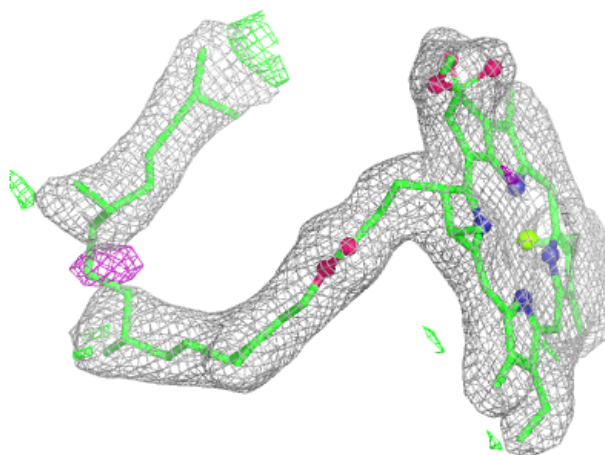
Electron density around RRX h 702:

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



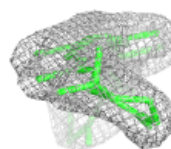
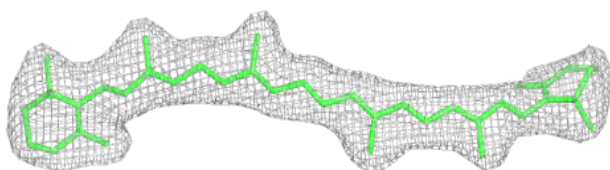
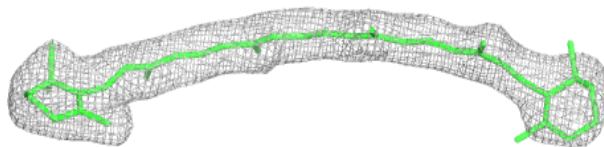
Electron density around CLA B 607:

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

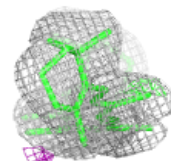
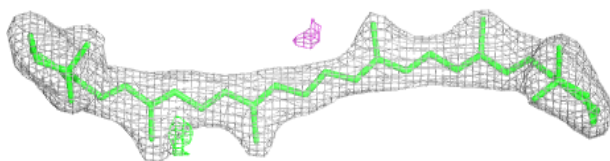
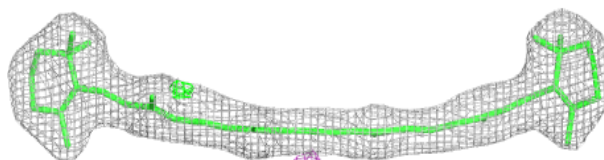


Electron density around BCR D 406:

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

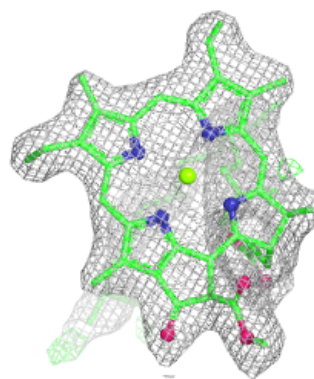
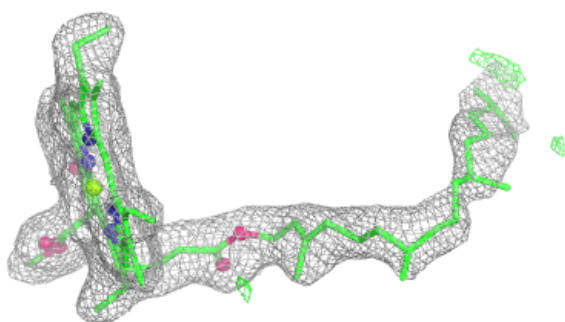
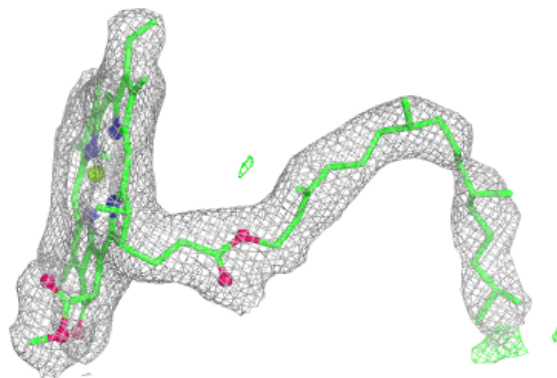
**Electron density around BCR K 101:**

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

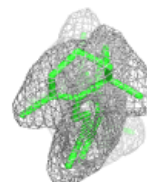
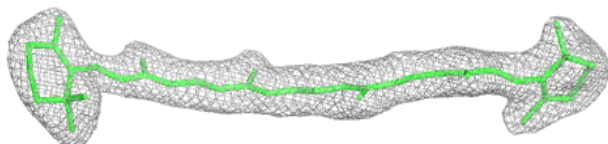
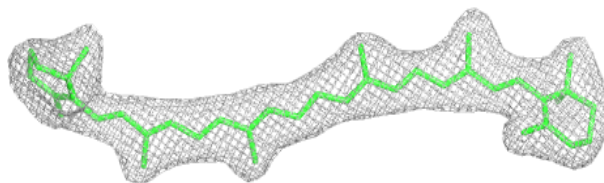


Electron density around CLA D 405:

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

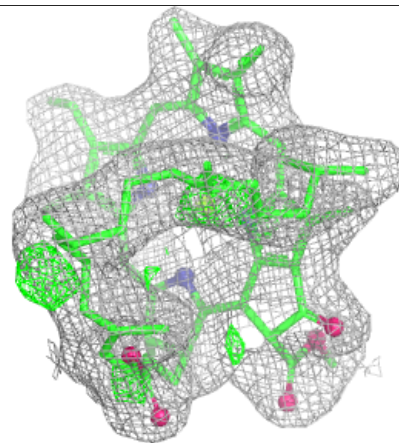
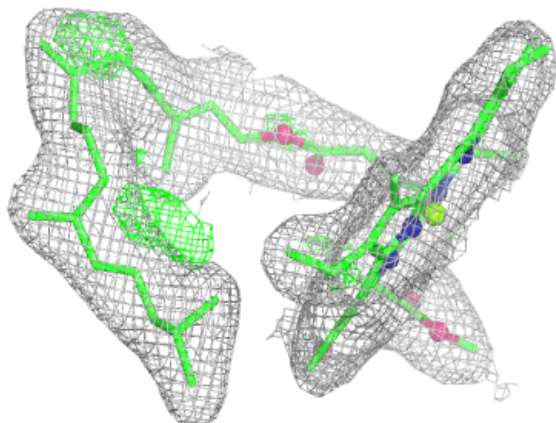
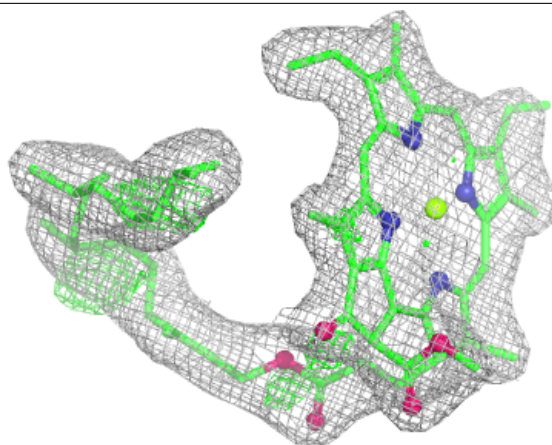
**Electron density around BCR Y 302:**

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

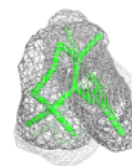
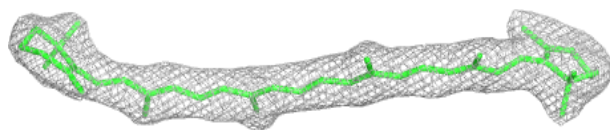
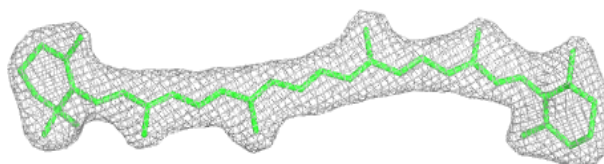


Electron density around CLA c 505:

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

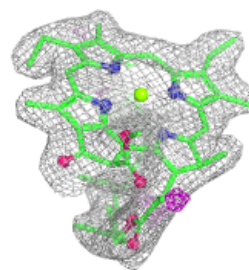
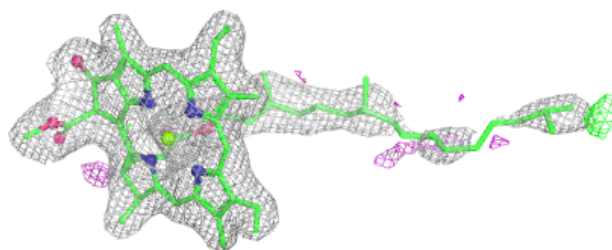
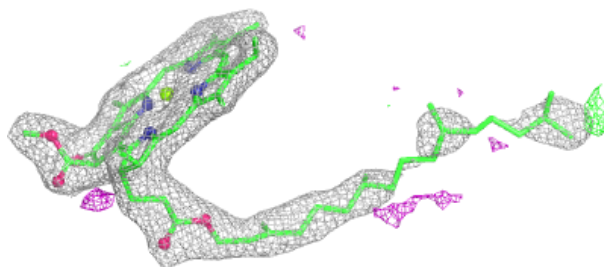
**Electron density around BCR b 622:**

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

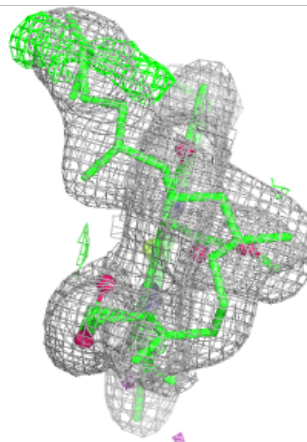
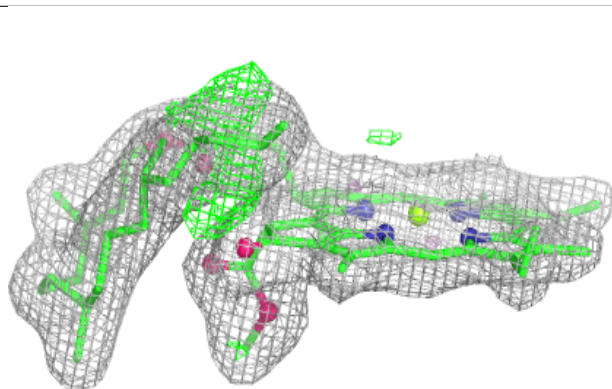
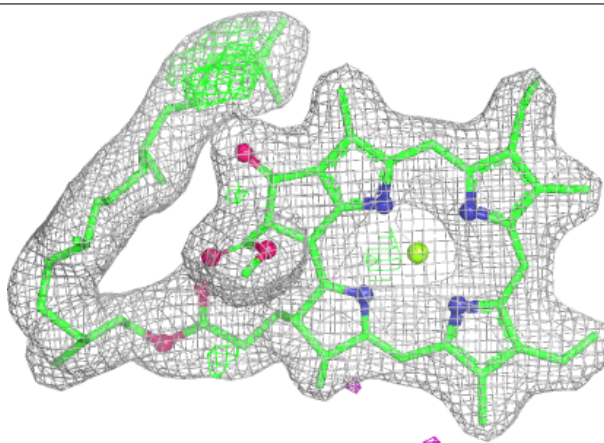


Electron density around CLA c 506:

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

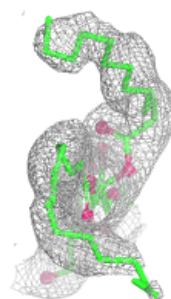
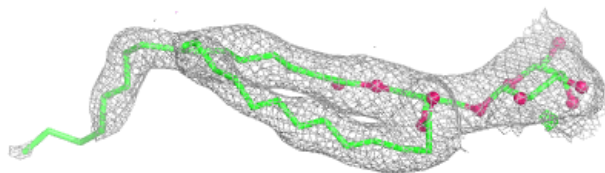
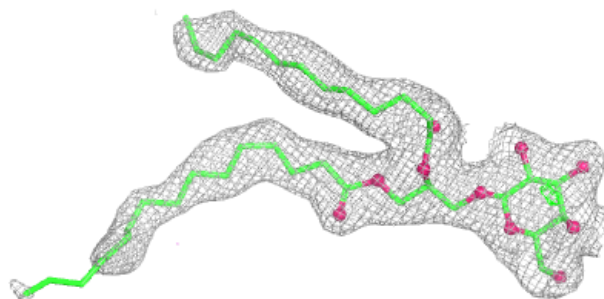
**Electron density around CLA B 611:**

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

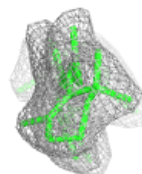
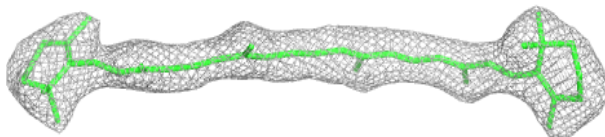
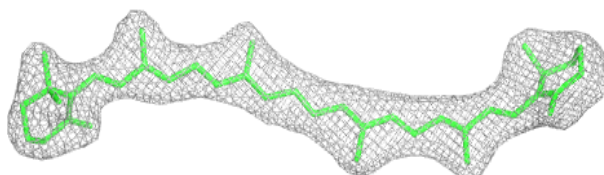


Electron density around LMG d 411:

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

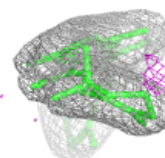
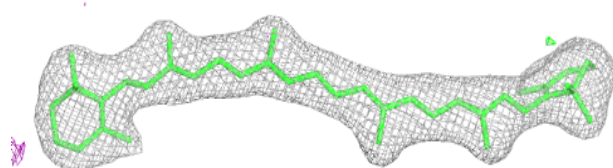
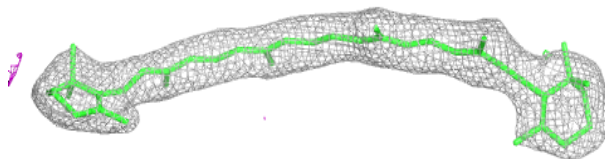
**Electron density around BCR c 528:**

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

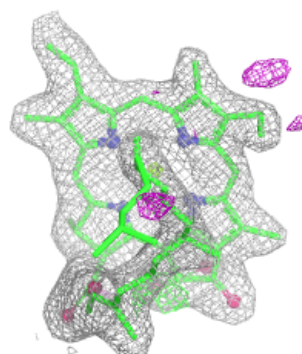
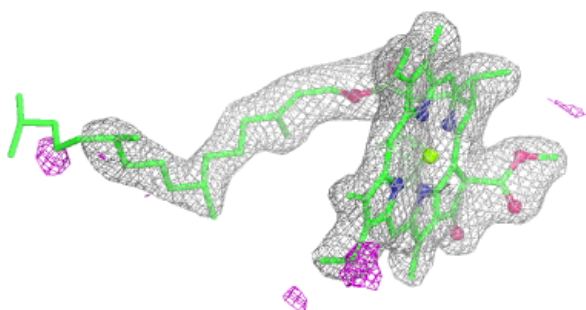
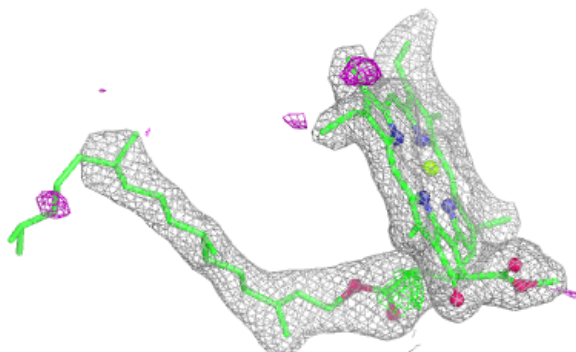


Electron density around BCR d 406:

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

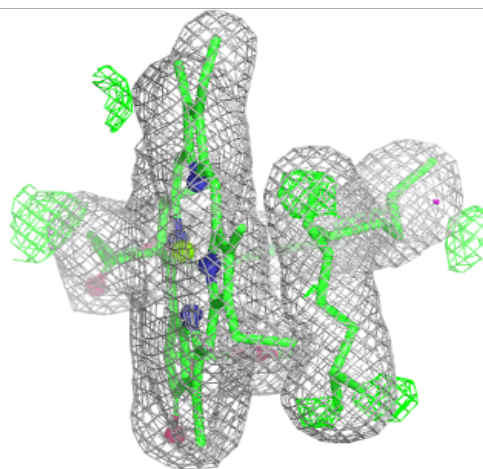
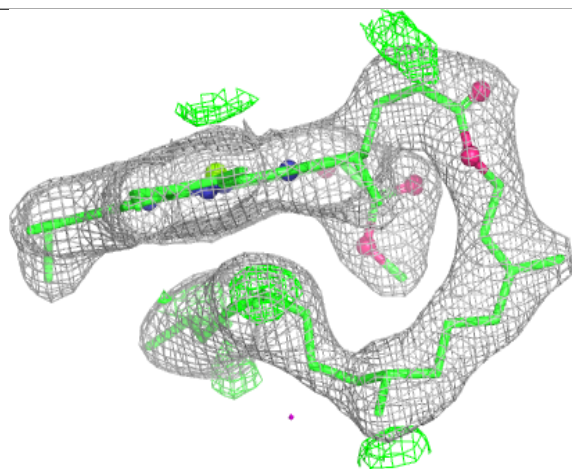
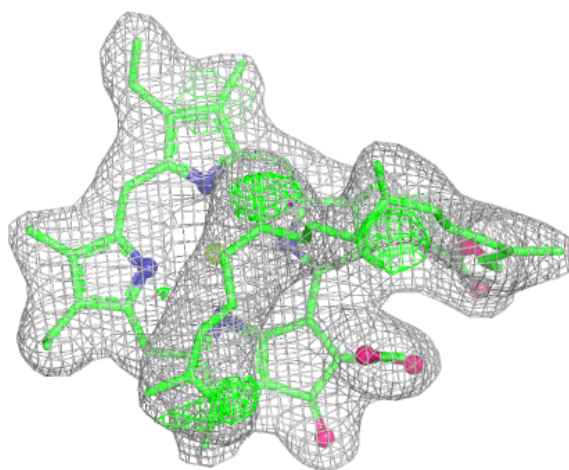
**Electron density around CLA c 510:**

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



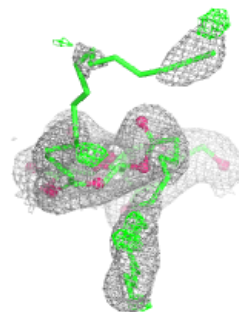
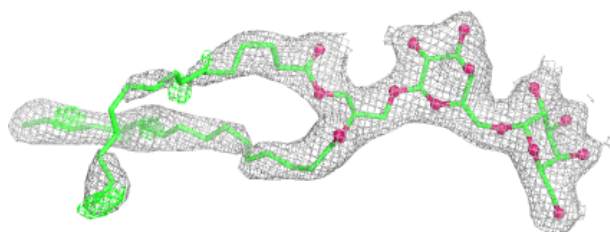
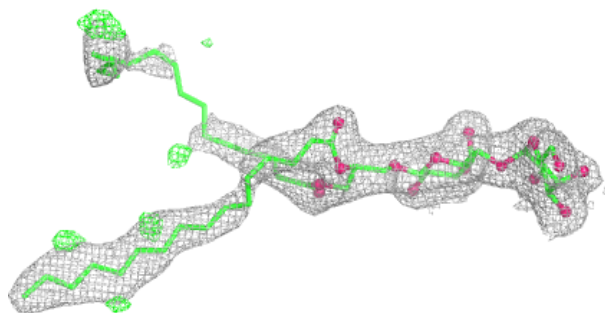
Electron density around CLA C 511:

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

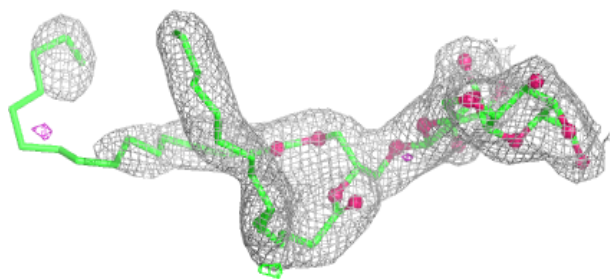
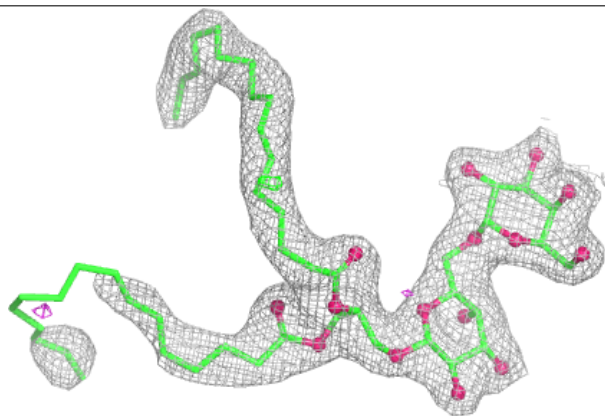


Electron density around DGD C 517:

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

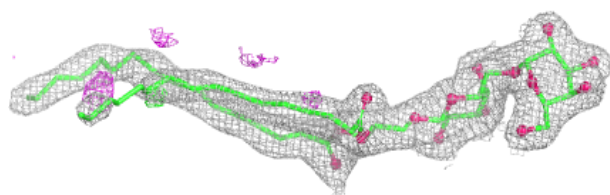
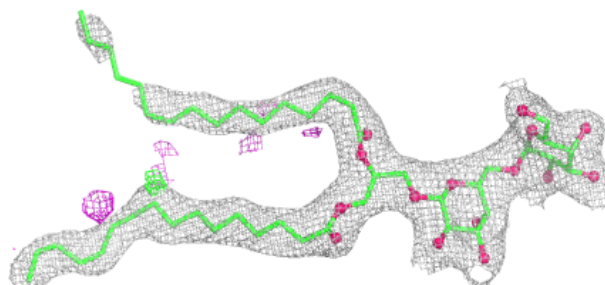
**Electron density around DGD C 518:**

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

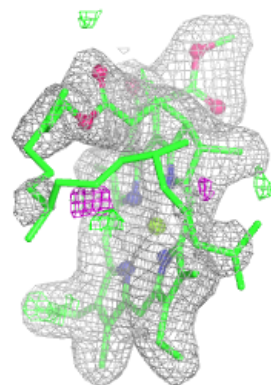
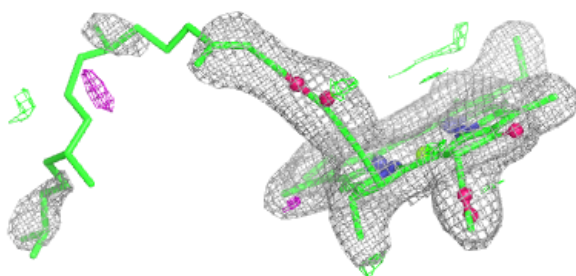
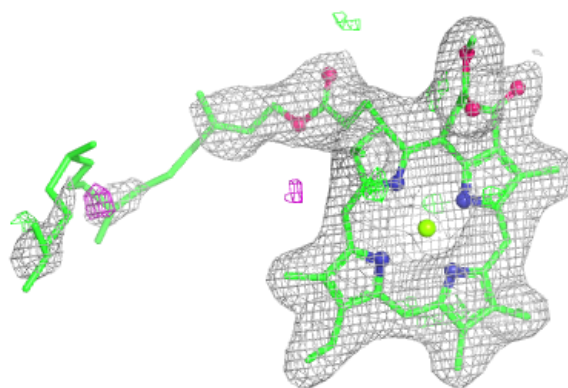


Electron density around DGD C 519:

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

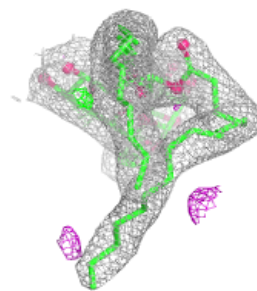
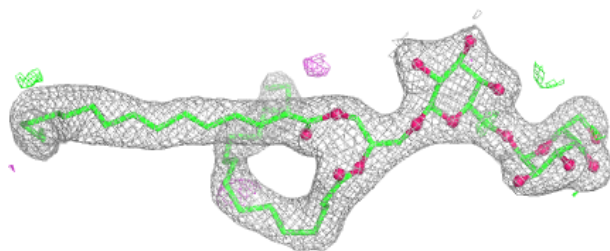
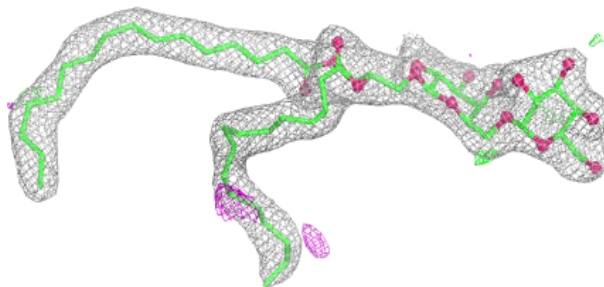
**Electron density around CLA A 409:**

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

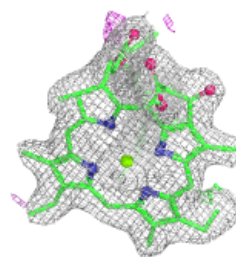
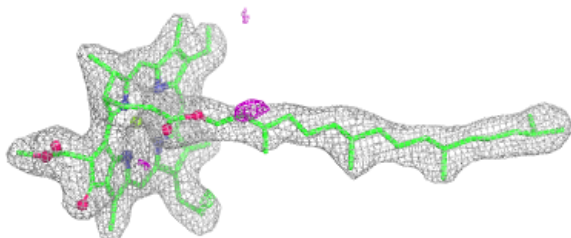
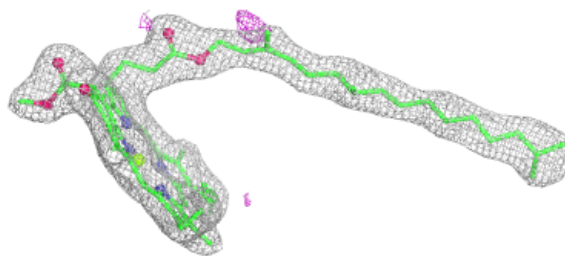


Electron density around DGD H 102:

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

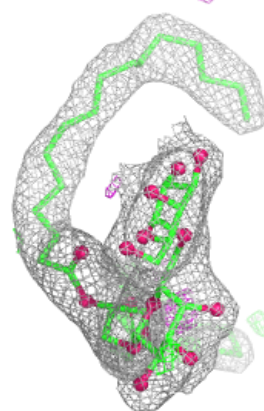
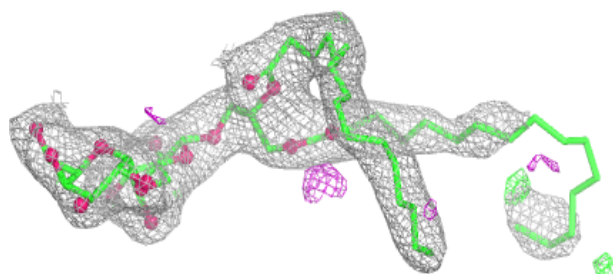
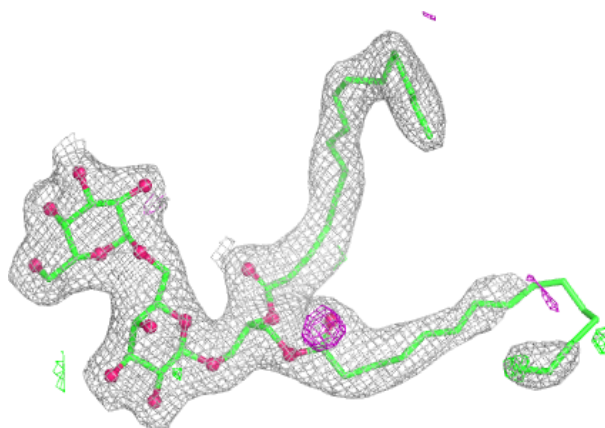
**Electron density around CLA b 610:**

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

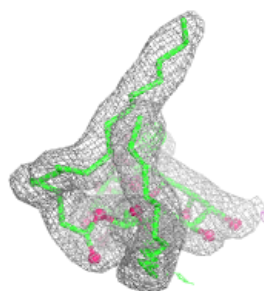
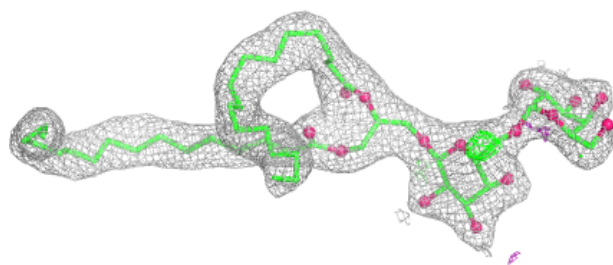
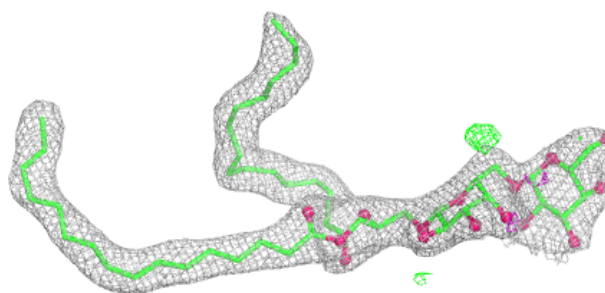


Electron density around DGD c 519:

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

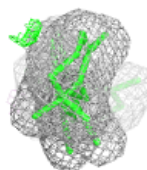
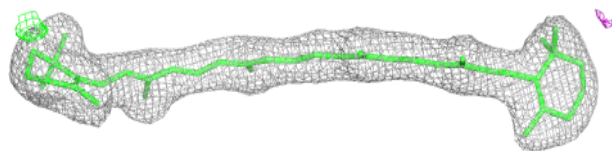
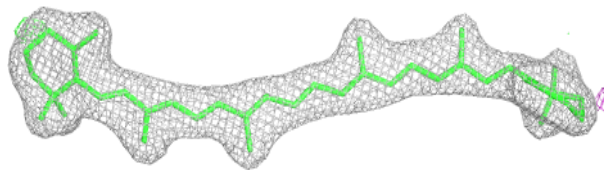
**Electron density around DGD h 703:**

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

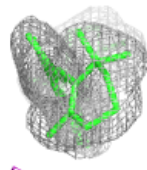
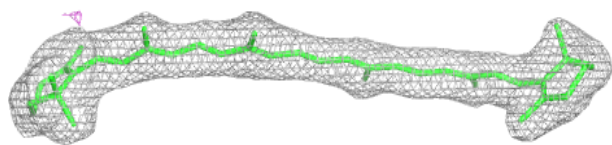
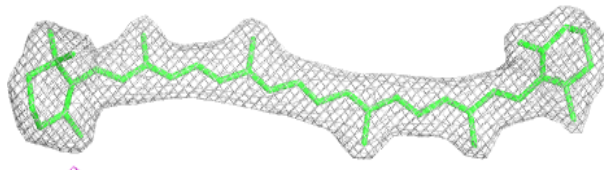


Electron density around BCR B 618:

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

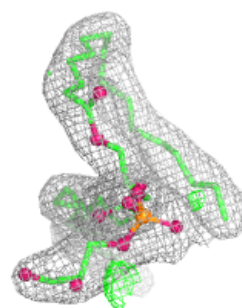
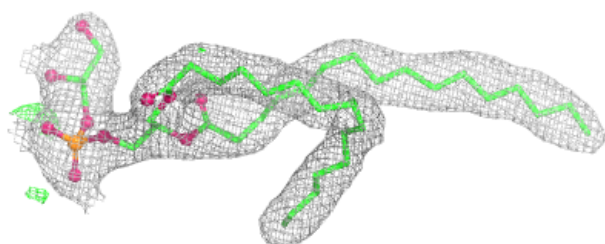
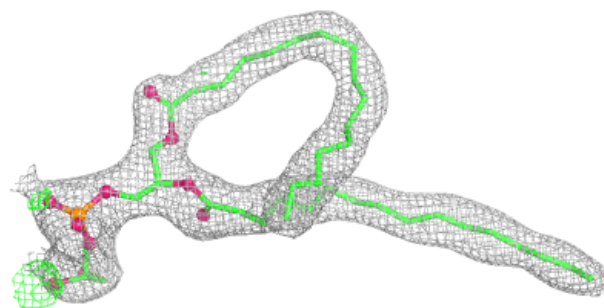
**Electron density around BCR B 620:**

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

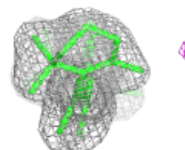
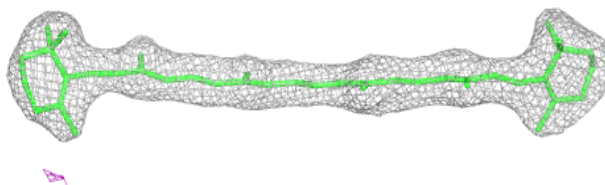
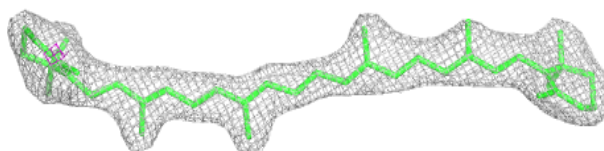


Electron density around LHG d 408:

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

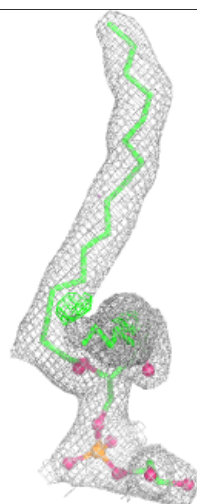
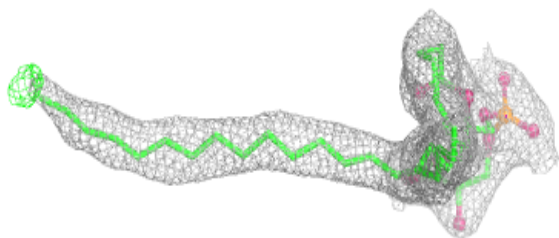
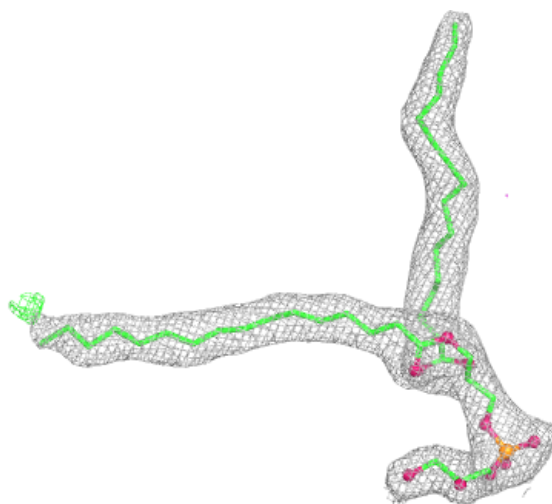
**Electron density around BCR C 515:**

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



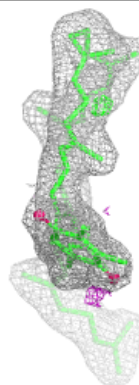
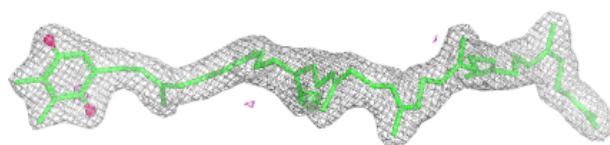
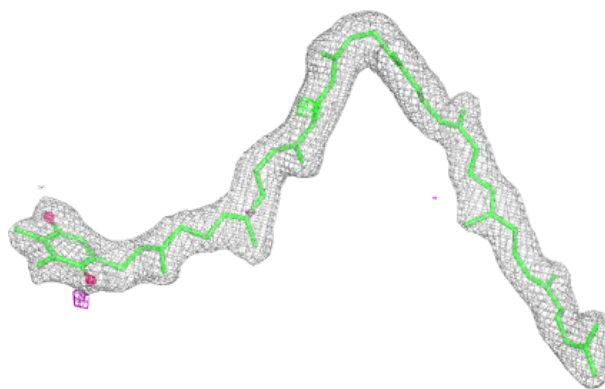
Electron density around LHG 1 101:

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

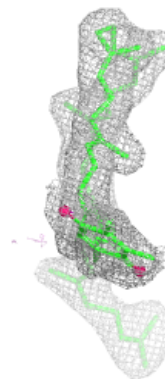
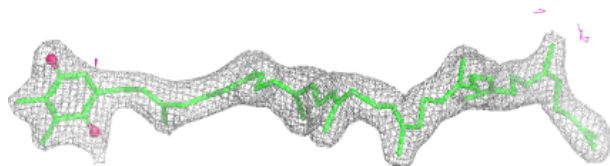
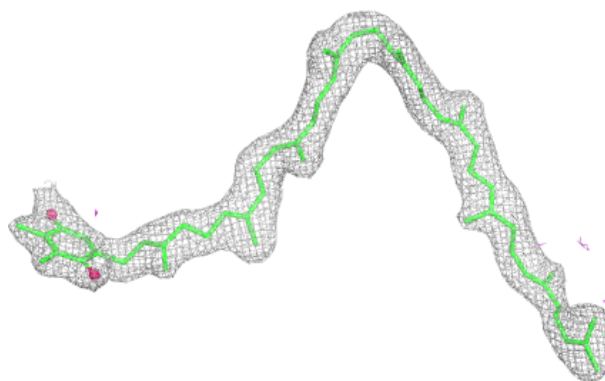


Electron density around PL9 D 407:

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

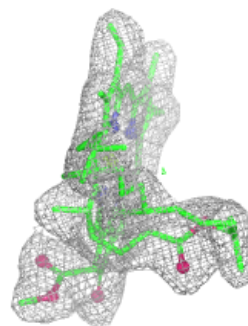
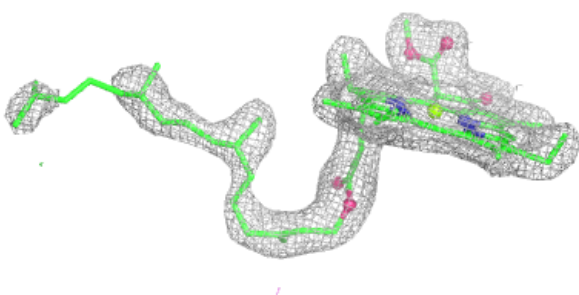
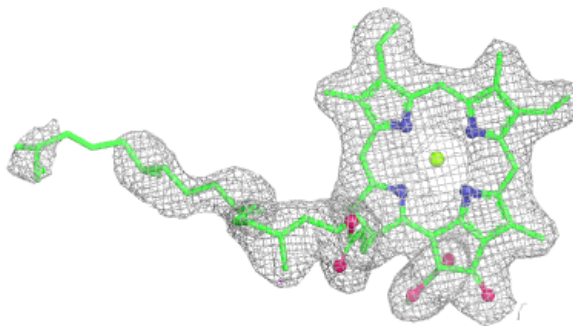
**Electron density around PL9 d 407:**

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

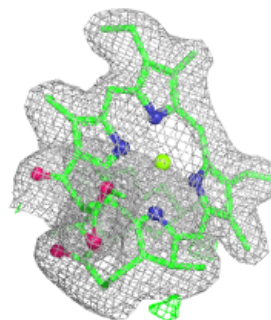
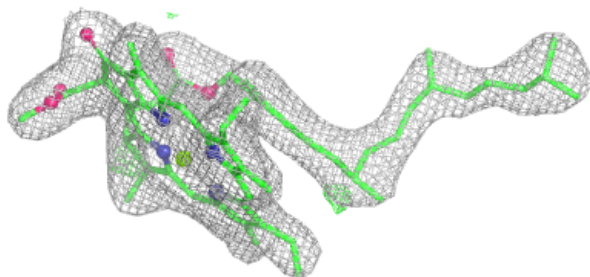
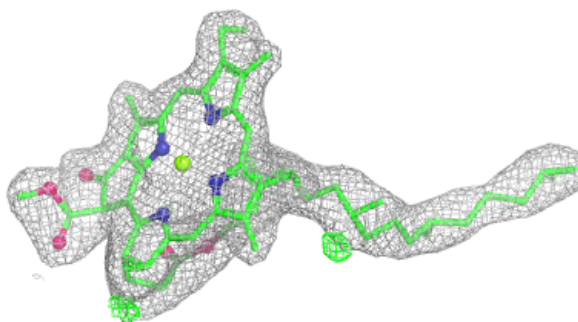


Electron density around CLA A 406:

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

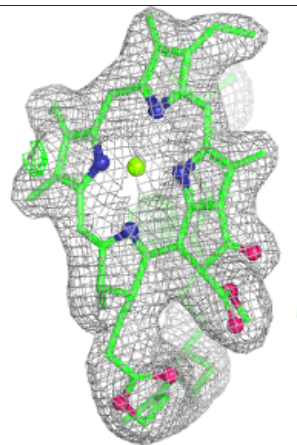
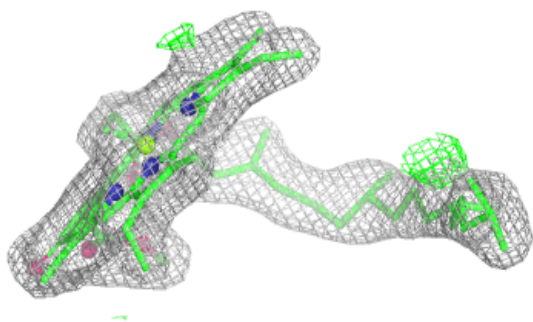
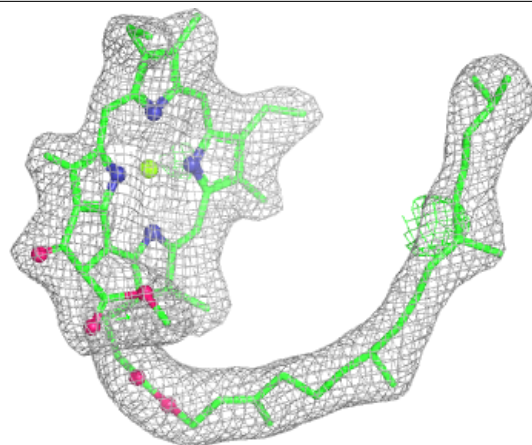
**Electron density around CLA c 507:**

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



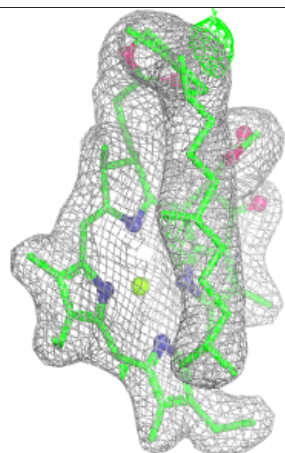
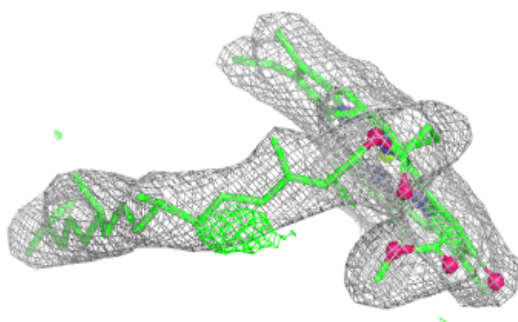
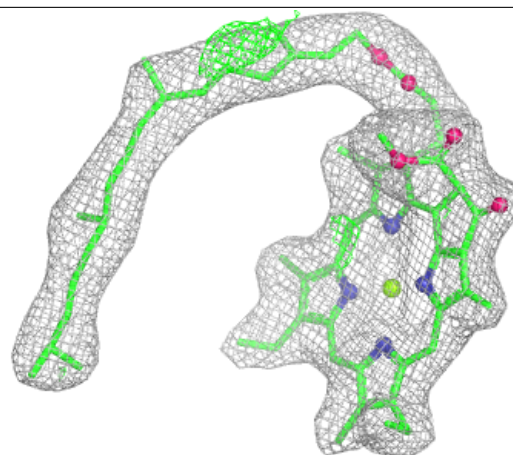
Electron density around CLA C 508:

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



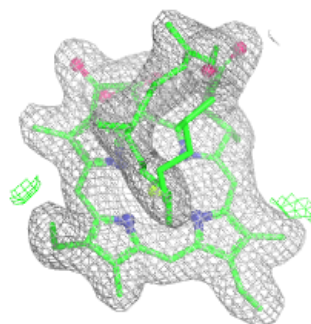
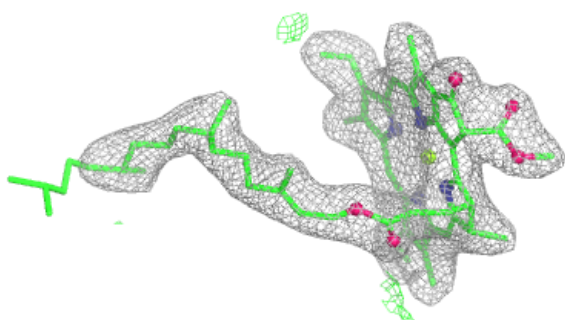
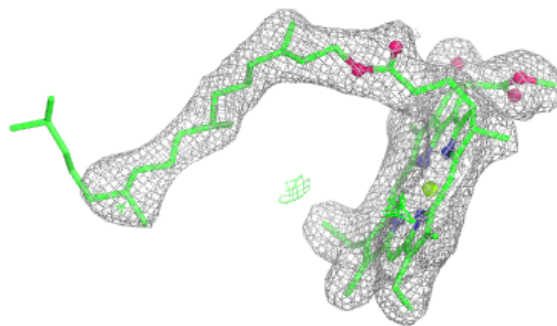
Electron density around CLA c 509:

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



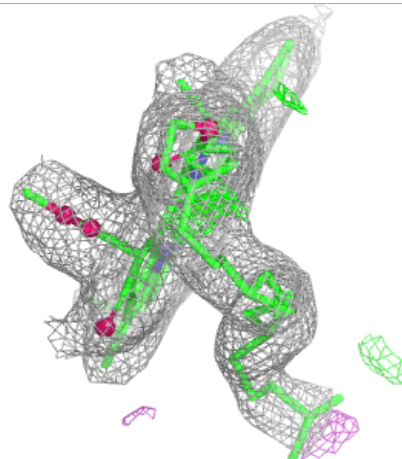
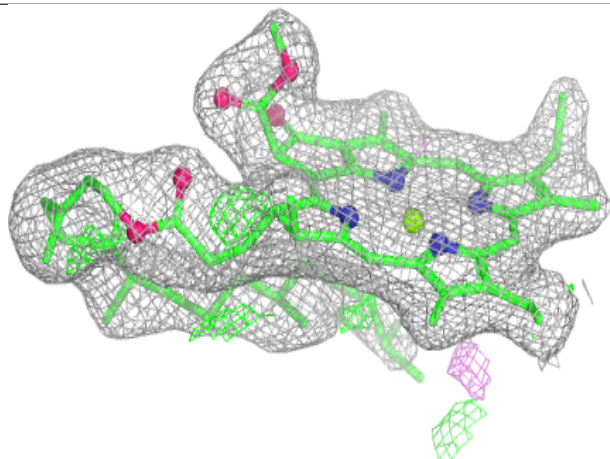
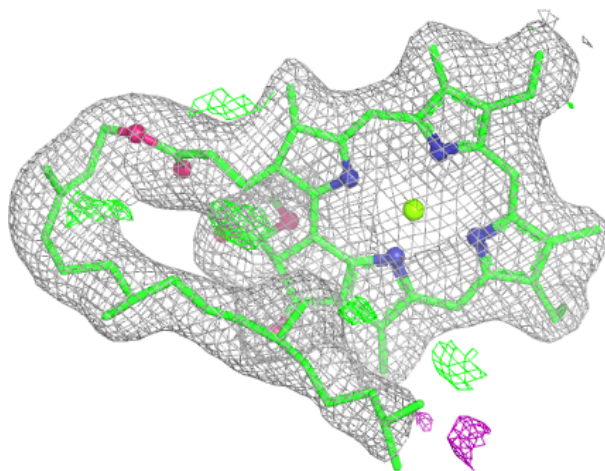
Electron density around CLA C 509:

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



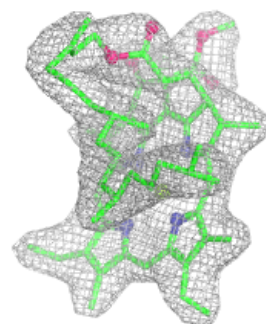
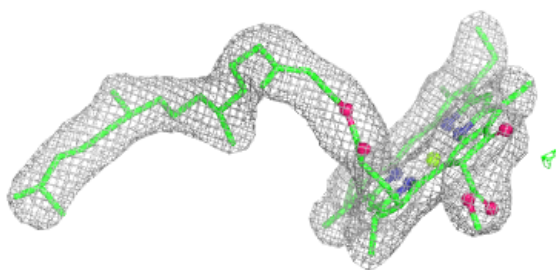
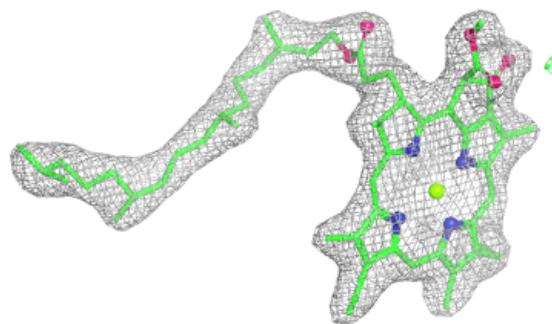
Electron density around CLA c 511:

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



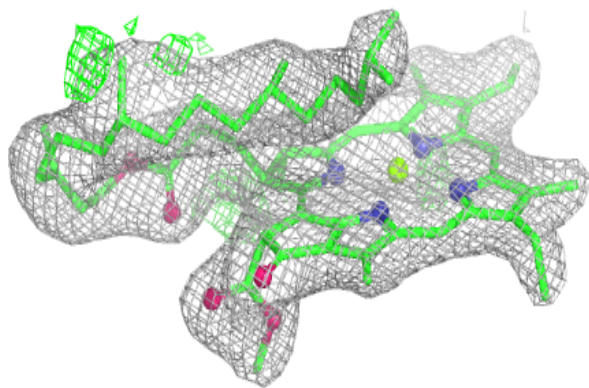
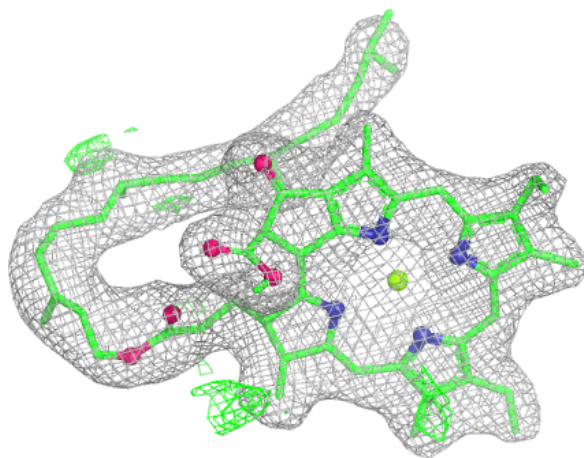
Electron density around CLA c 513:

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



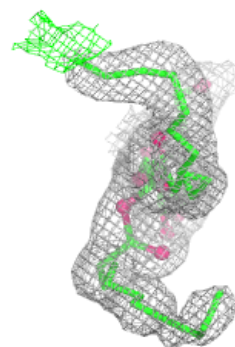
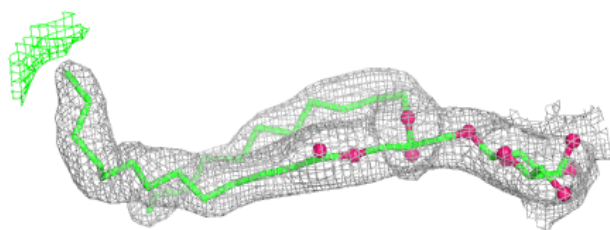
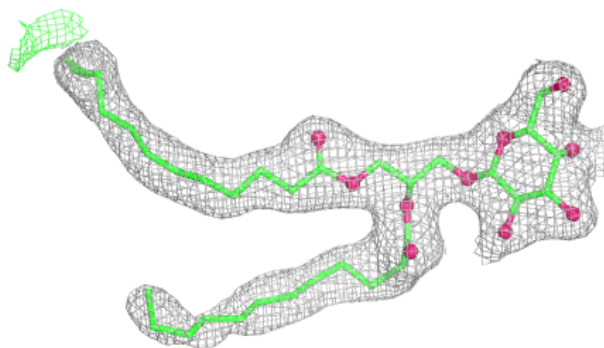
Electron density around CLA C 510:

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

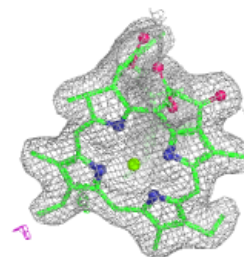
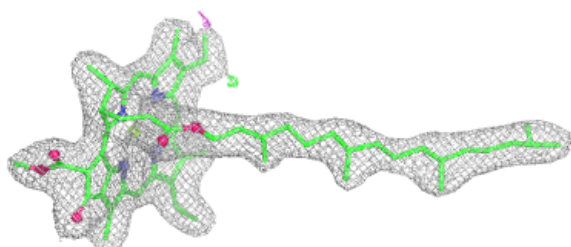
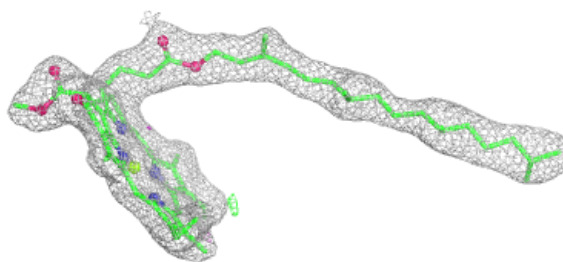


Electron density around LMG D 412:

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

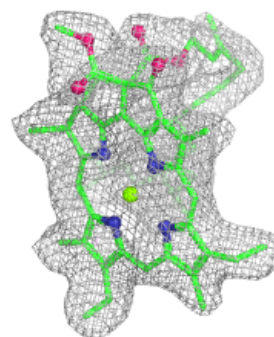
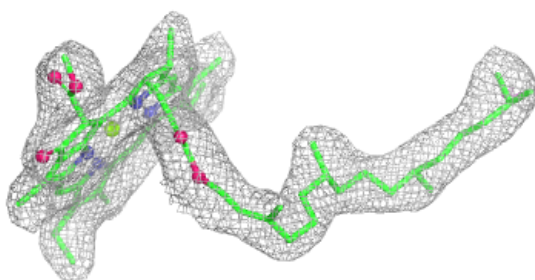
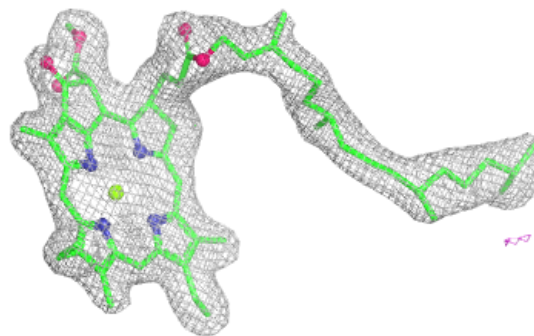
**Electron density around CLA B 608:**

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



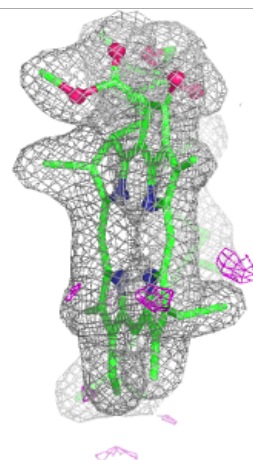
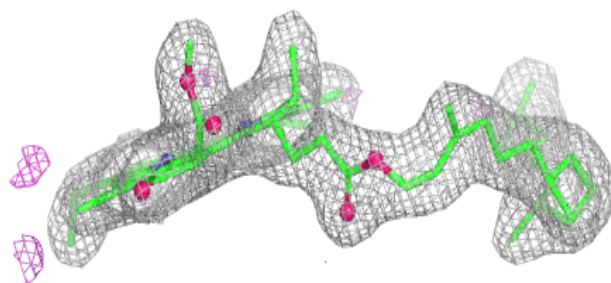
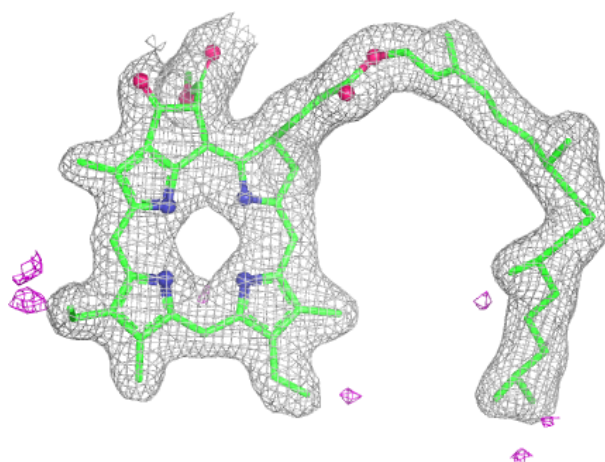
Electron density around CLA C 512:

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



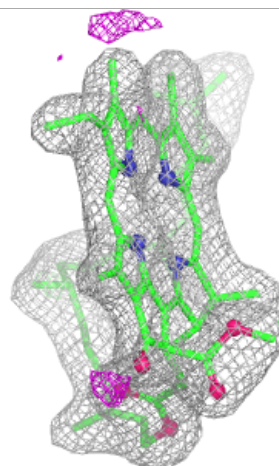
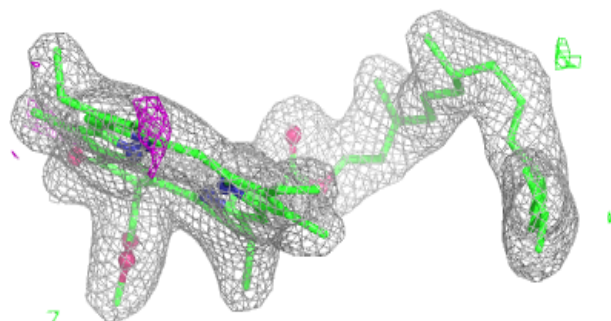
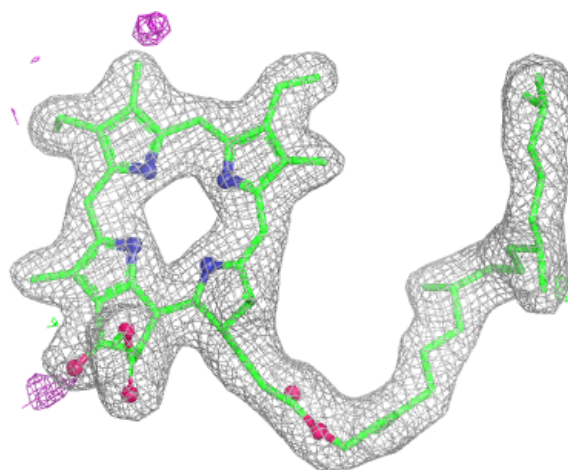
Electron density around PHO A 407:

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



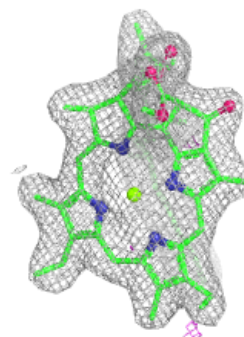
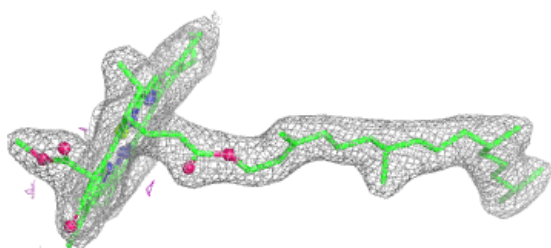
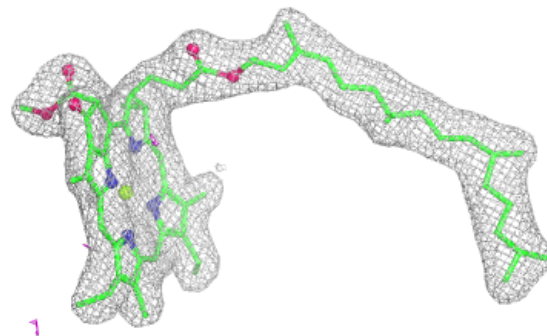
Electron density around PHO A 408:

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

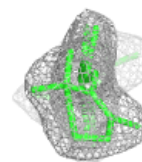
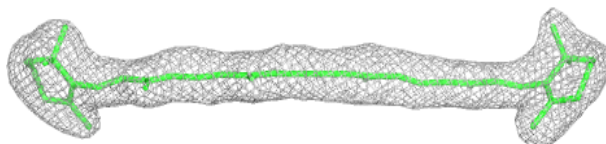
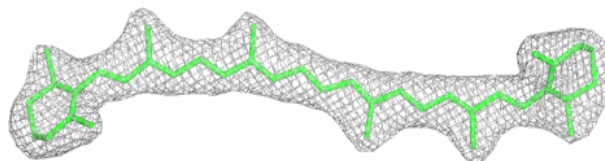


Electron density around CLA B 610:

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

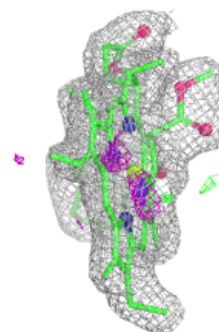
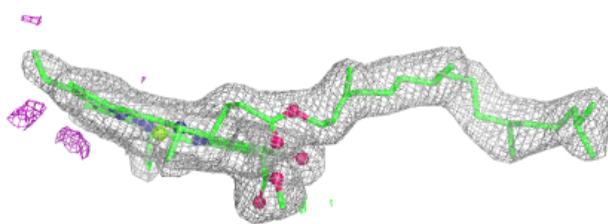
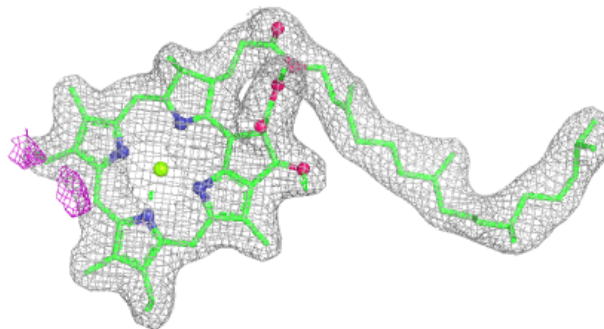
**Electron density around BCR B 619:**

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

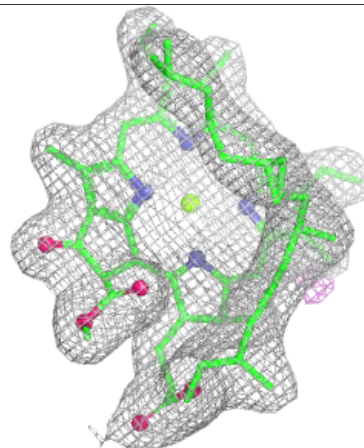
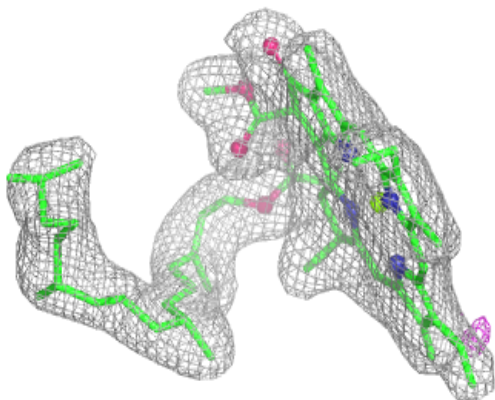
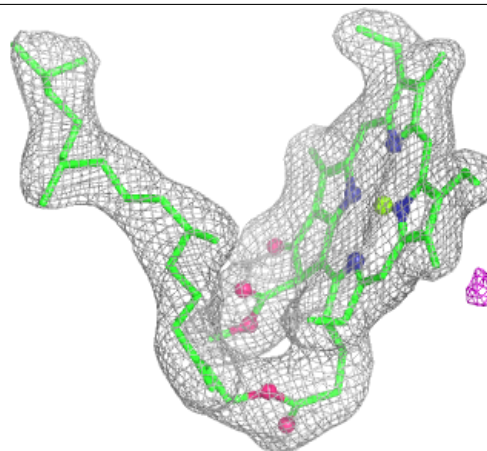


Electron density around CLA B 603:

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

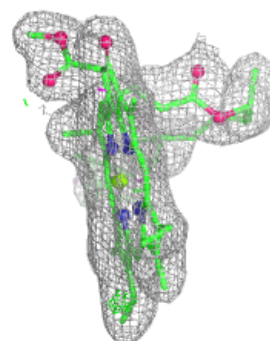
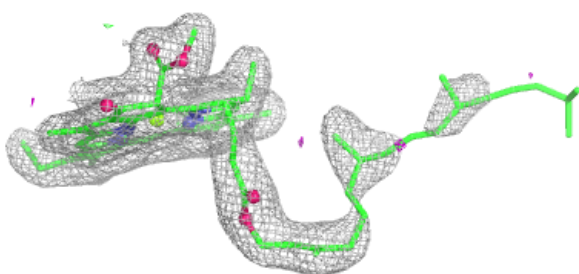
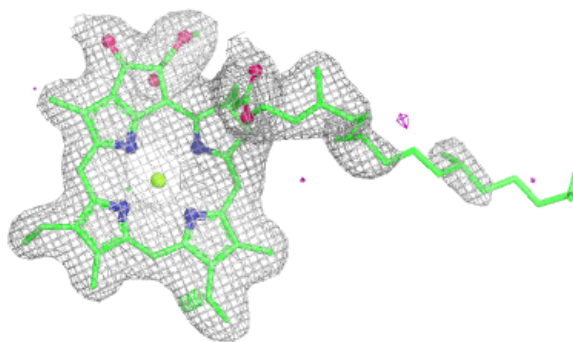
**Electron density around CLA B 614:**

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

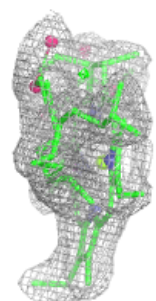
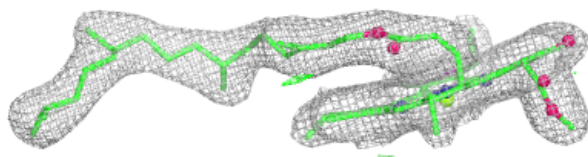
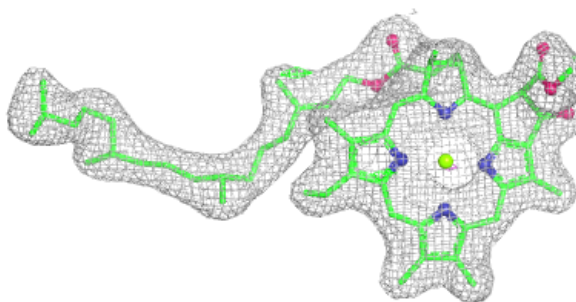


Electron density around CLA a 2110:

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

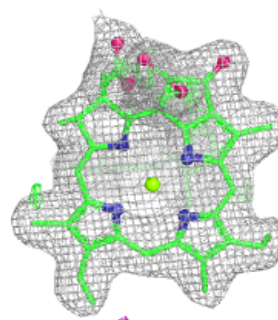
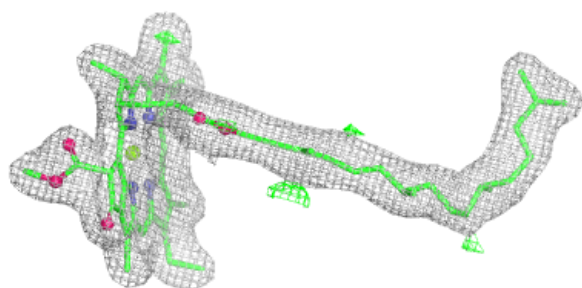
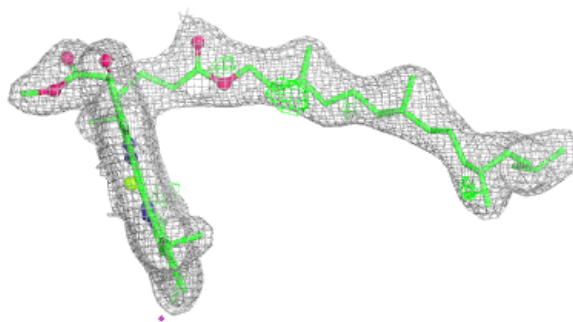
**Electron density around CLA B 604:**

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

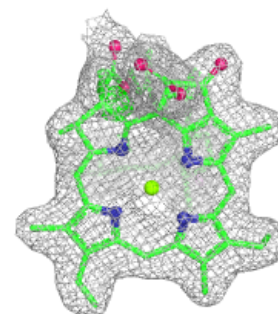
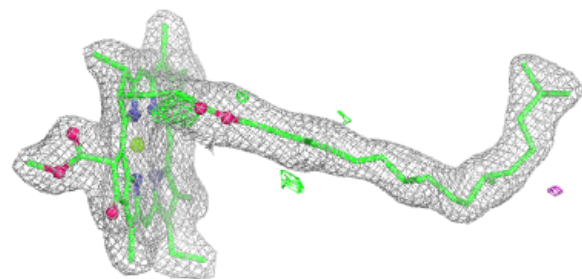
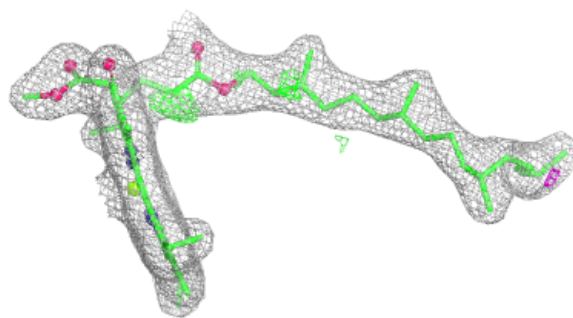


Electron density around CLA B 606:

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

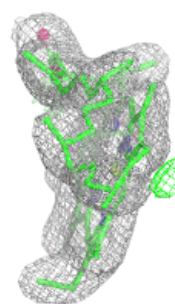
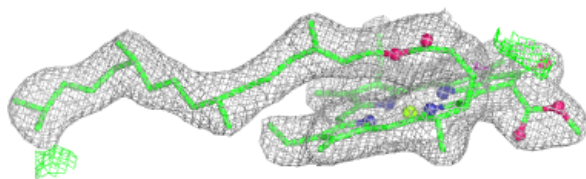
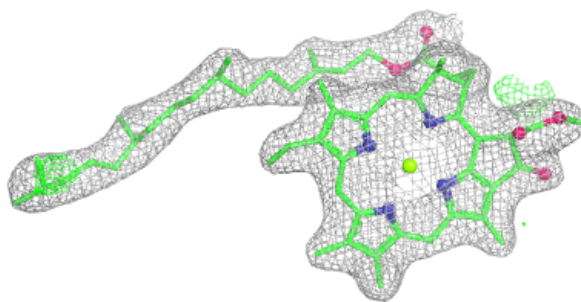
**Electron density around CLA b 608:**

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

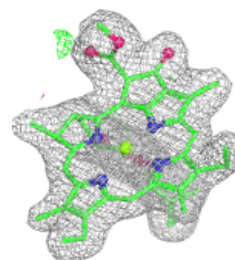
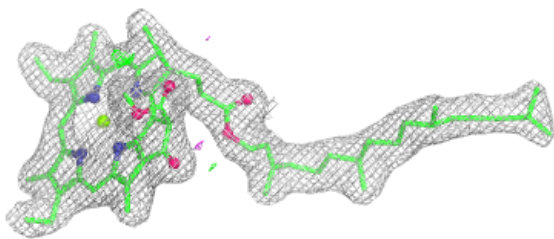
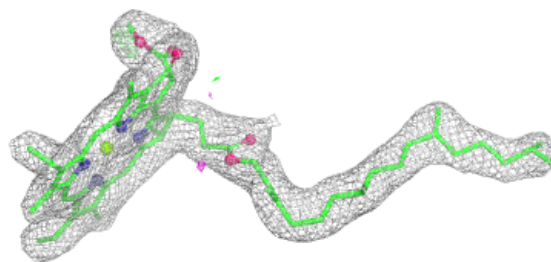


Electron density around CLA C 502:

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

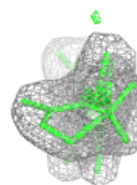
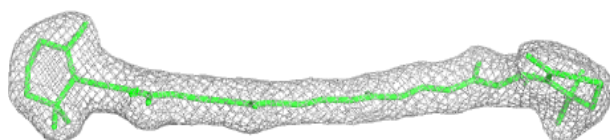
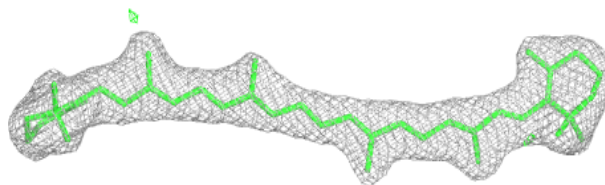
**Electron density around CLA C 503:**

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

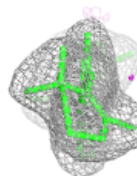
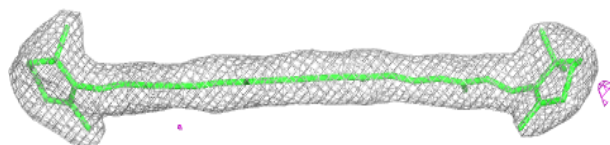
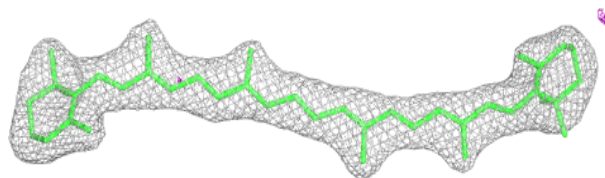


Electron density around BCR b 620:

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

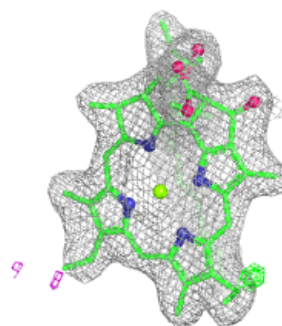
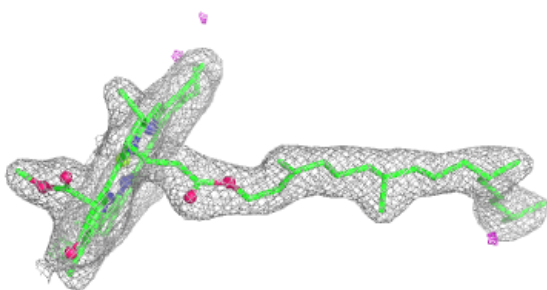
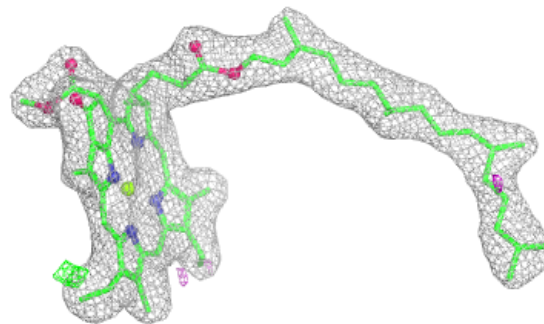
**Electron density around BCR b 621:**

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



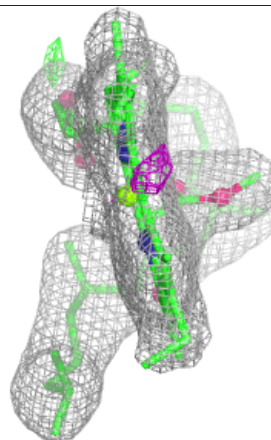
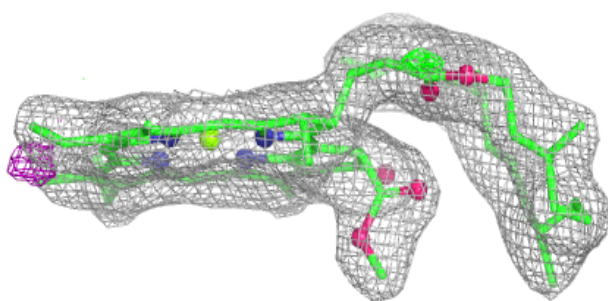
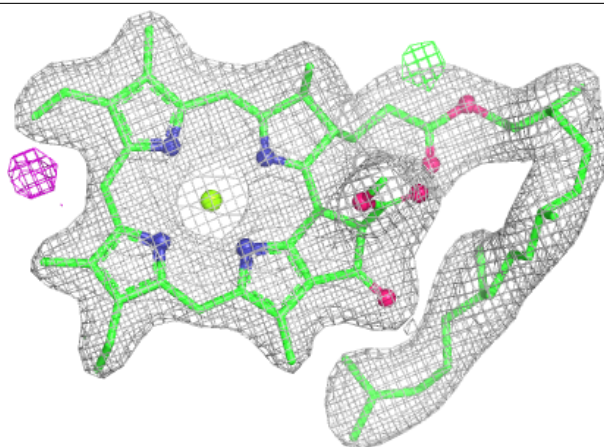
Electron density around CLA b 612:

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

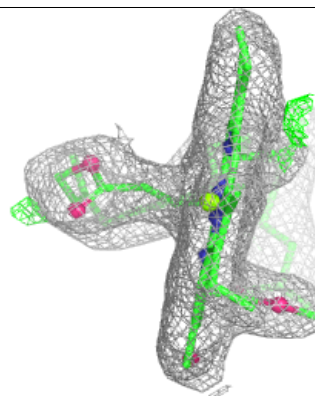
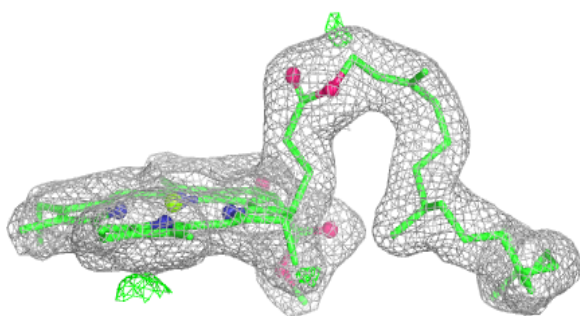
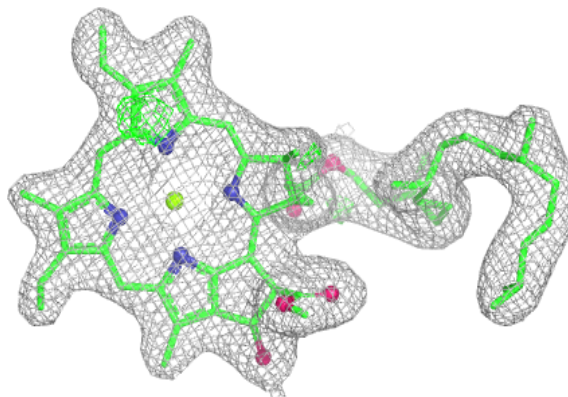


Electron density around CLA b 613:

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

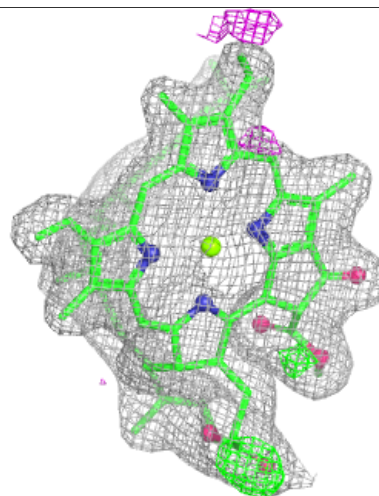
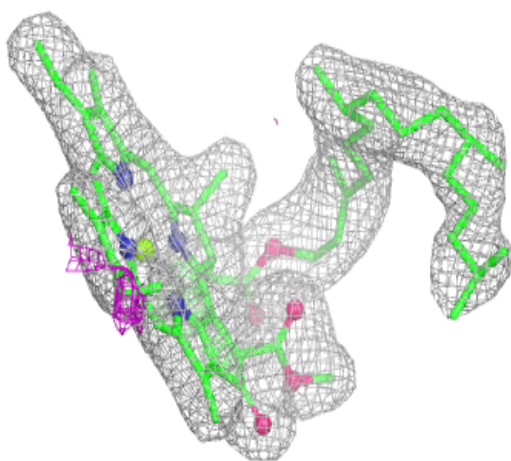
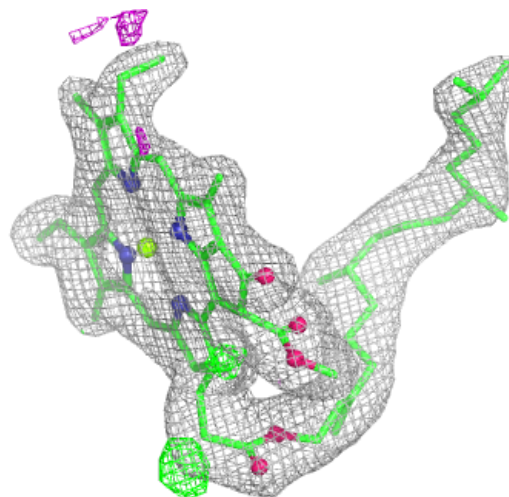
**Electron density around CLA b 615:**

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



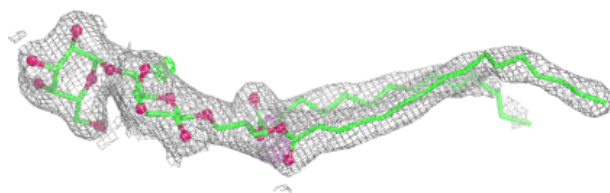
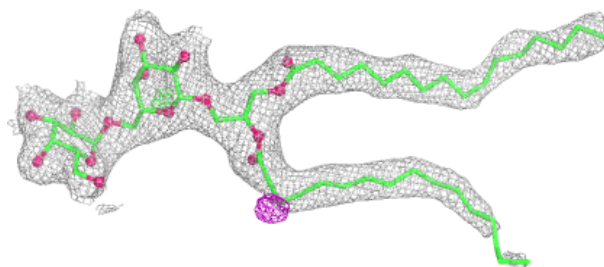
Electron density around CLA b 616:

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



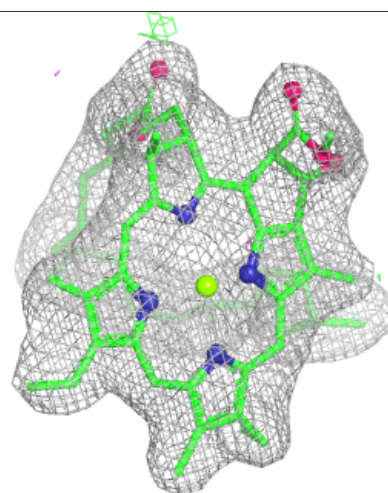
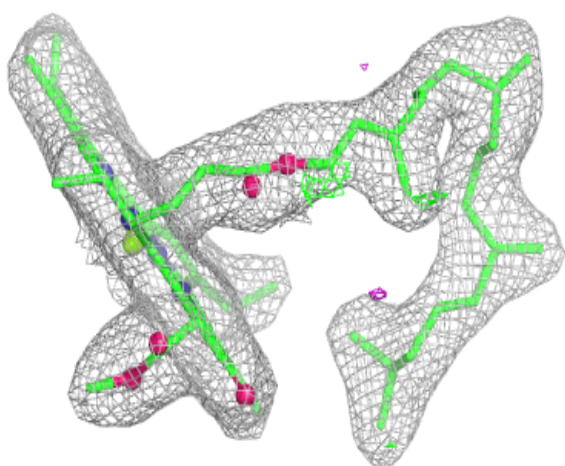
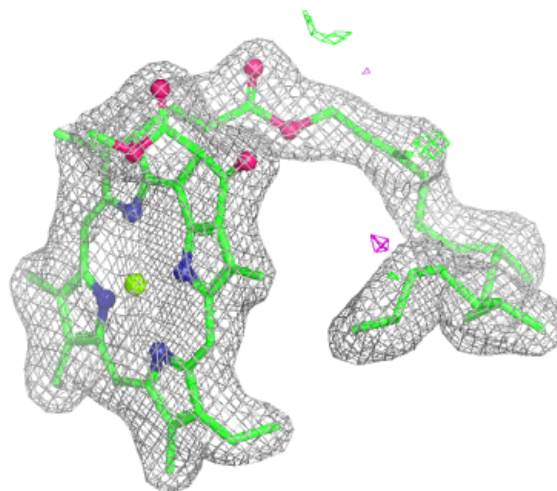
Electron density around DGD c 520:

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



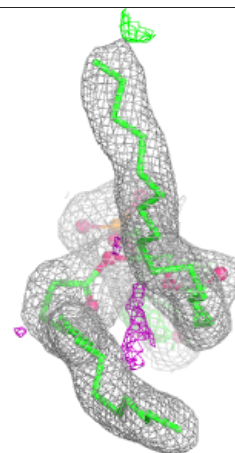
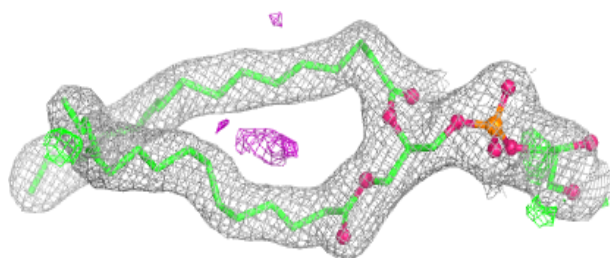
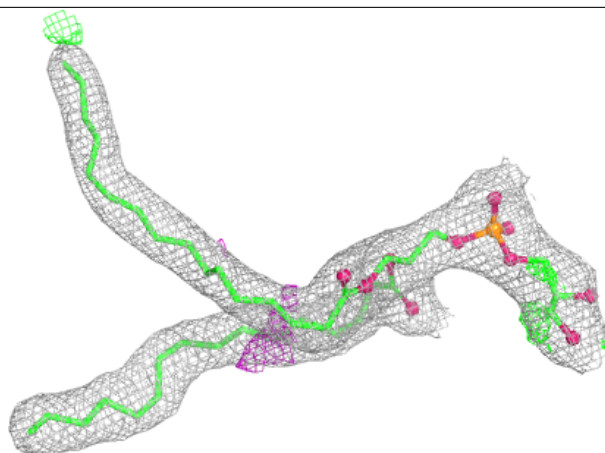
Electron density around CLA C 504:

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



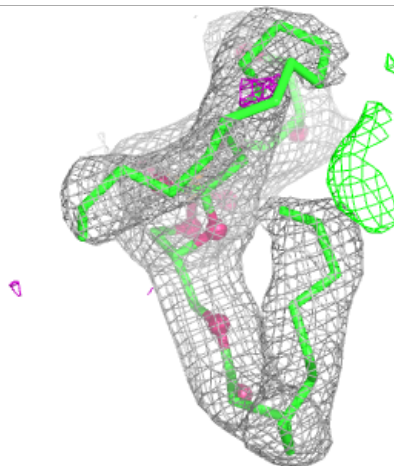
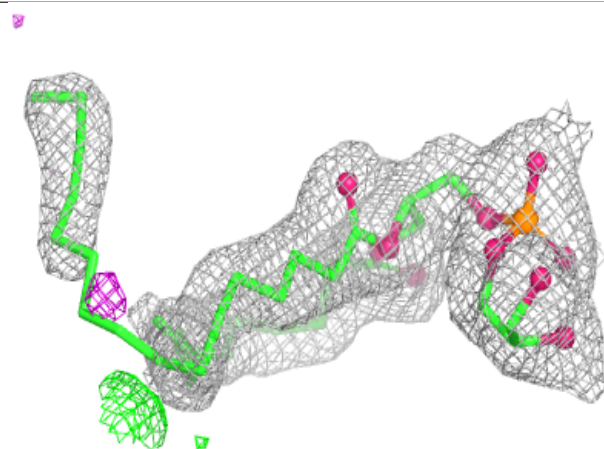
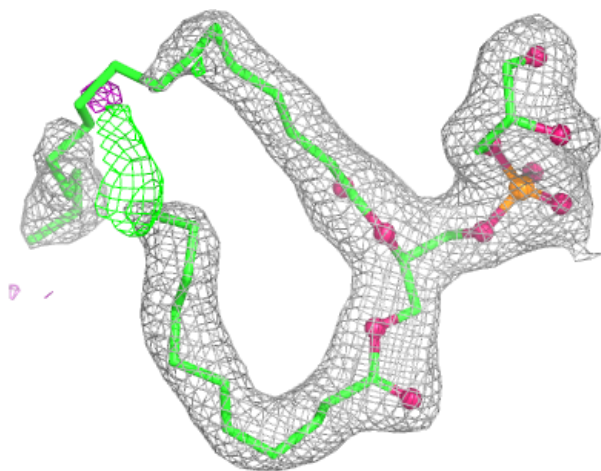
Electron density around LHG D 410:

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



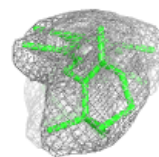
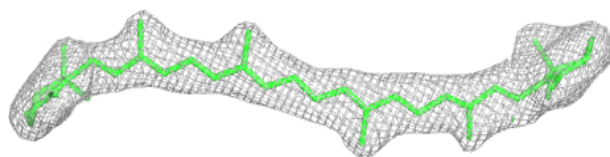
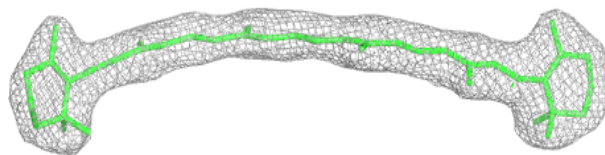
Electron density around LHG D 411:

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



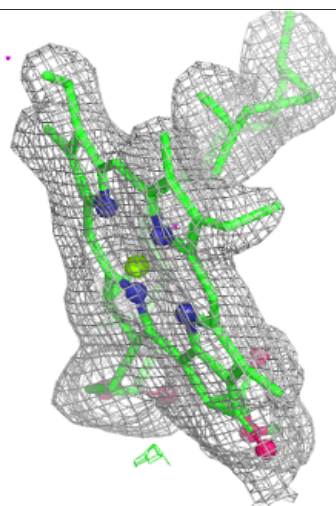
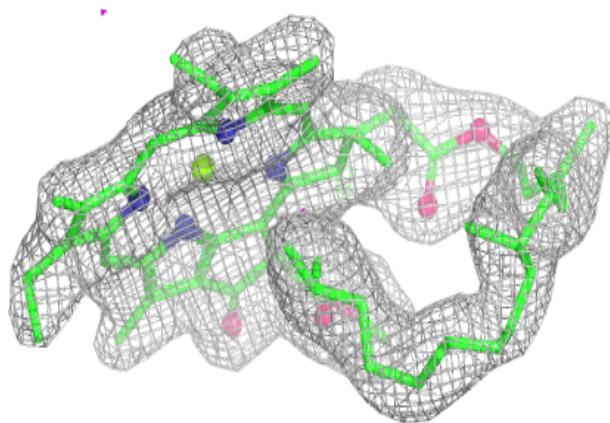
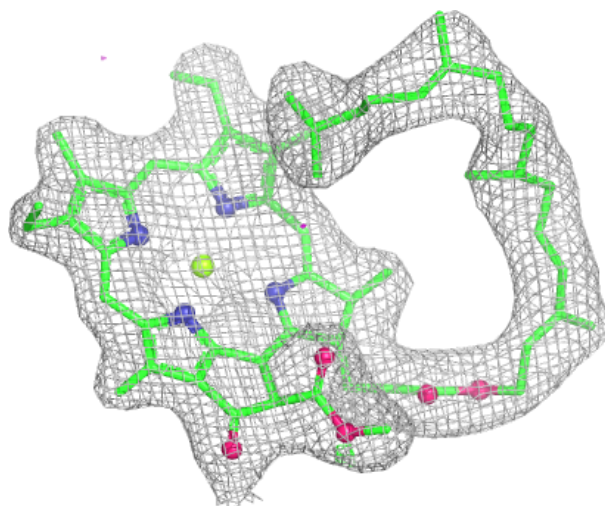
Electron density around BCR k 2003:

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



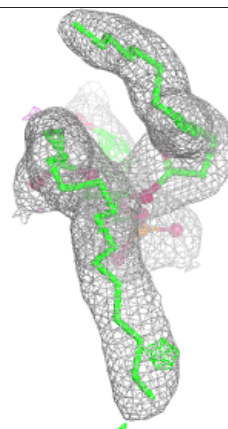
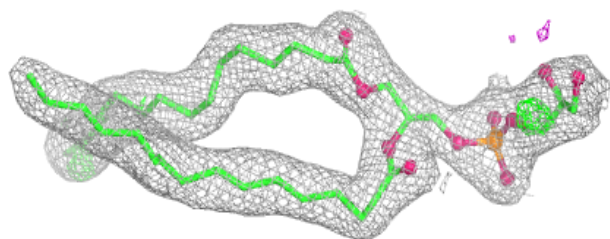
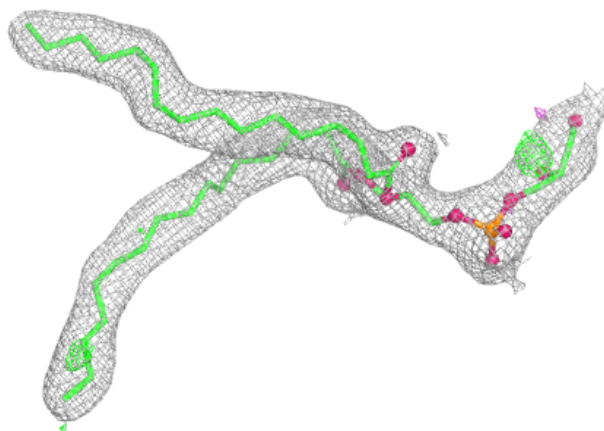
Electron density around CLA b 618:

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



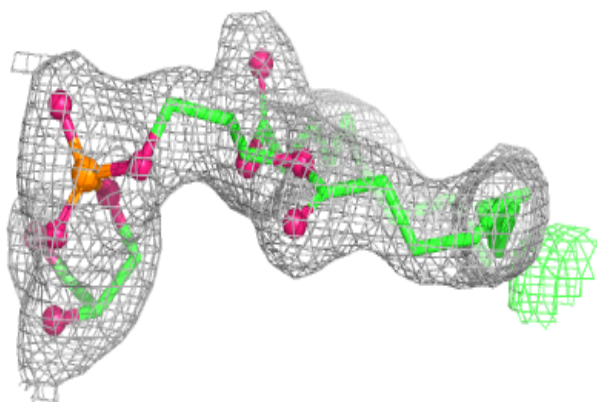
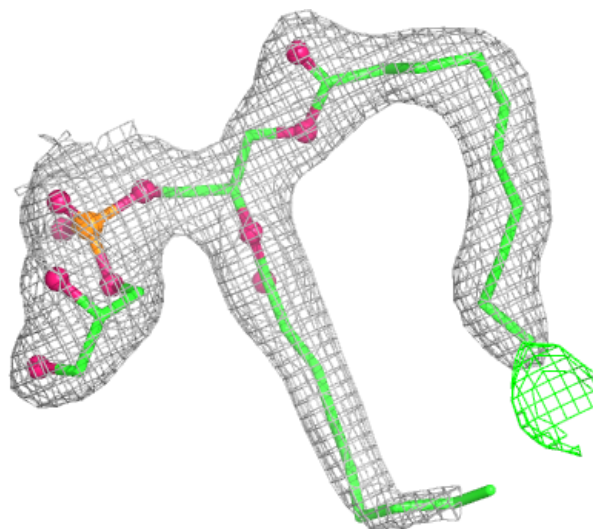
Electron density around LHG d 409:

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



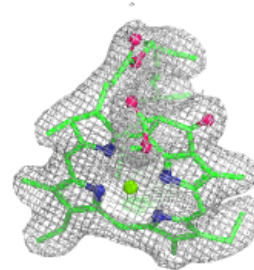
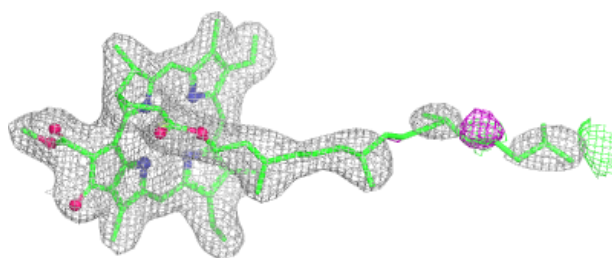
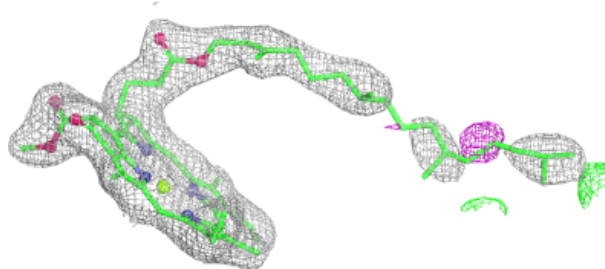
Electron density around LHG d 410:

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

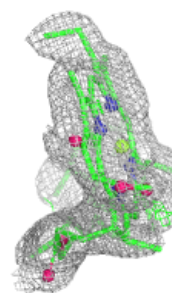
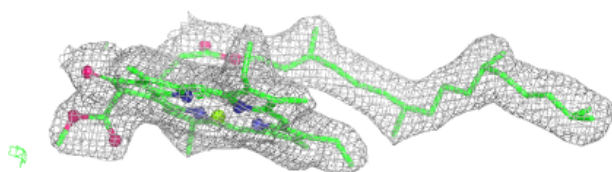
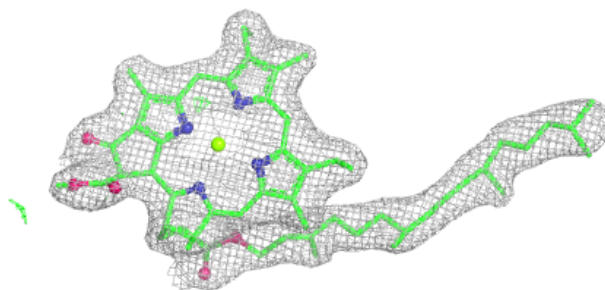


Electron density around CLA C 505:

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

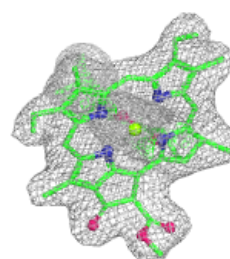
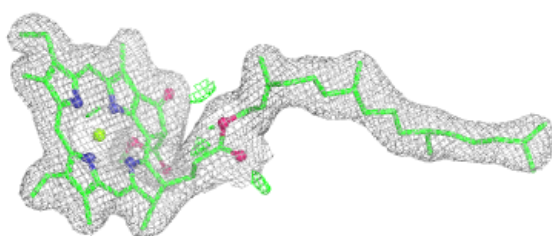
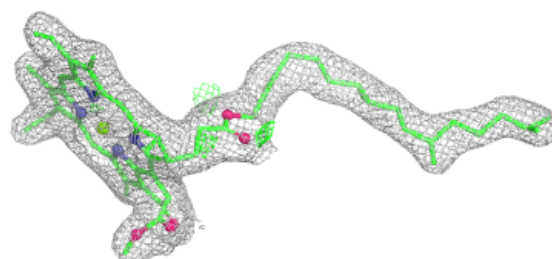
**Electron density around CLA c 503:**

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

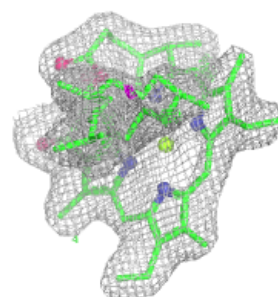
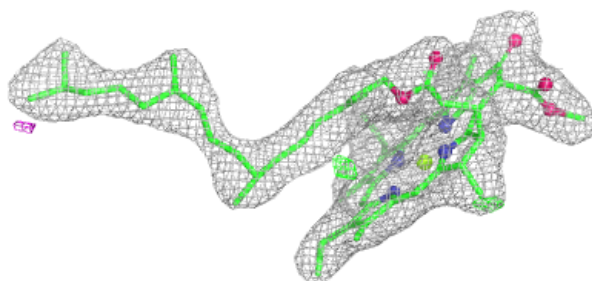
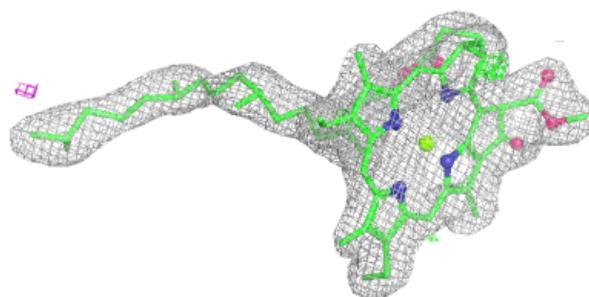


Electron density around CLA c 504:

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

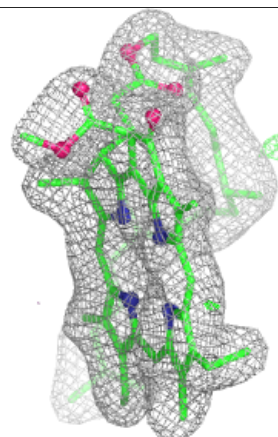
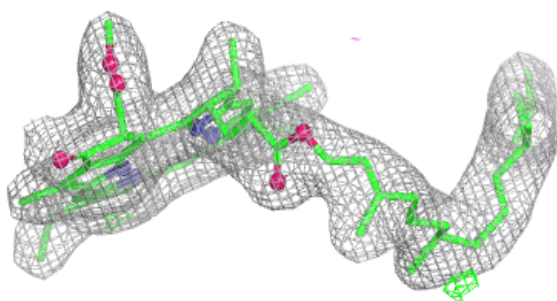
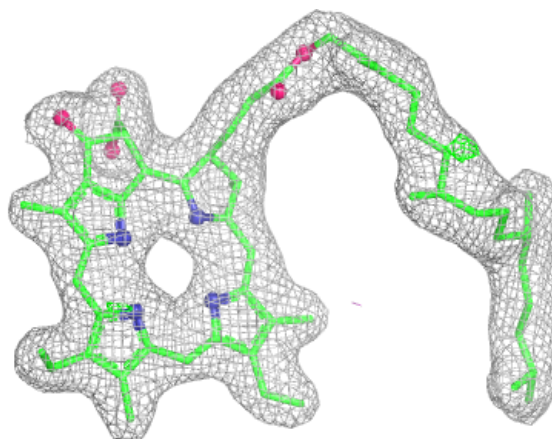
**Electron density around CLA C 506:**

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

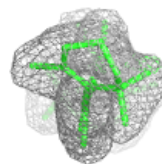
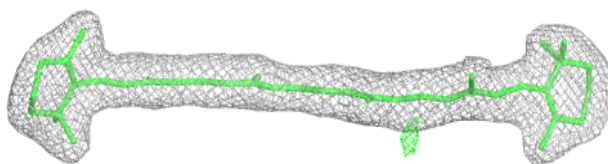
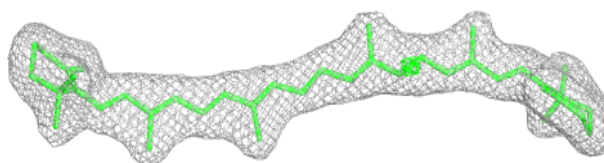


Electron density around PHO a 2112:

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

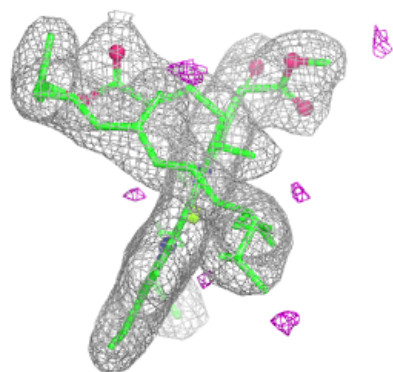
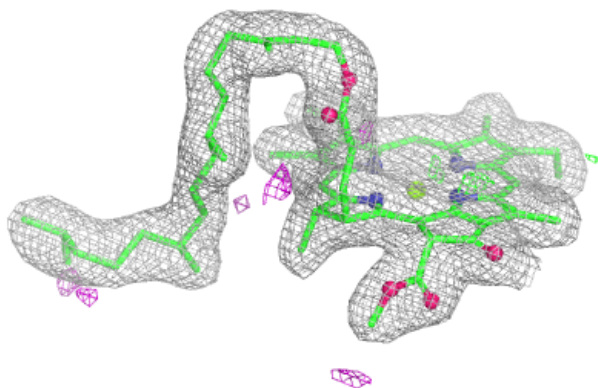
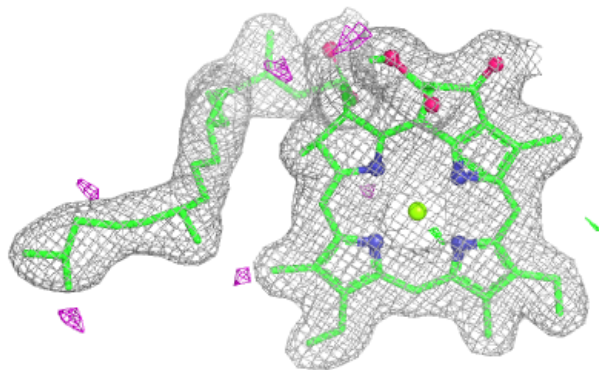
**Electron density around BCR A 410:**

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

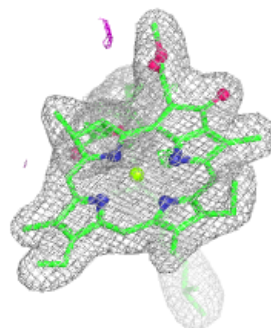
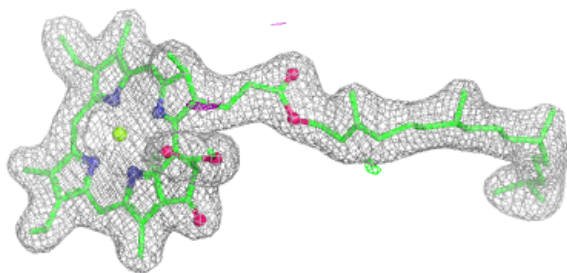
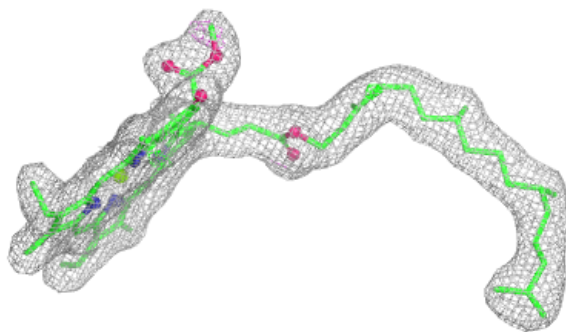


Electron density around CLA D 401:

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

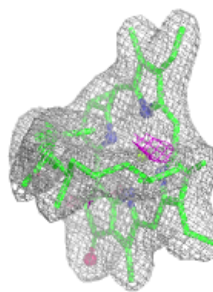
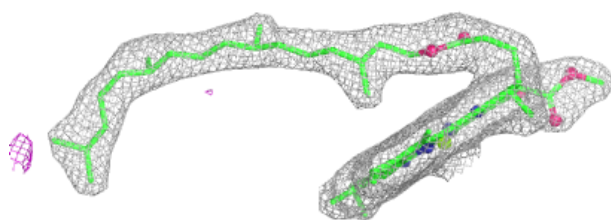
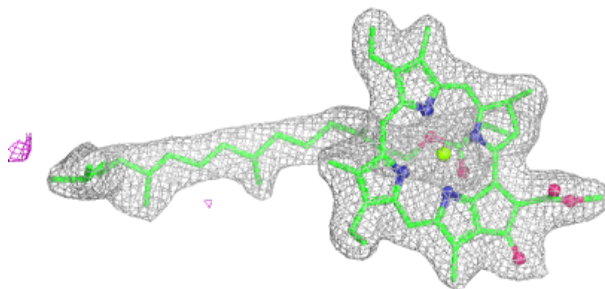
**Electron density around CLA D 404:**

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



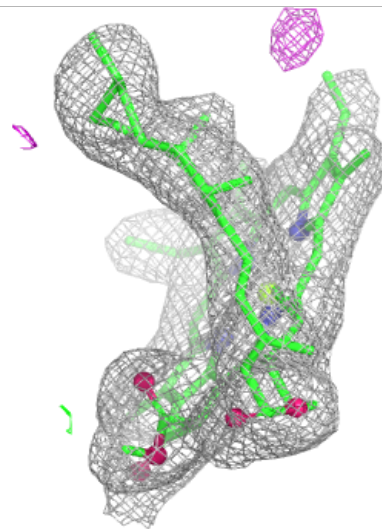
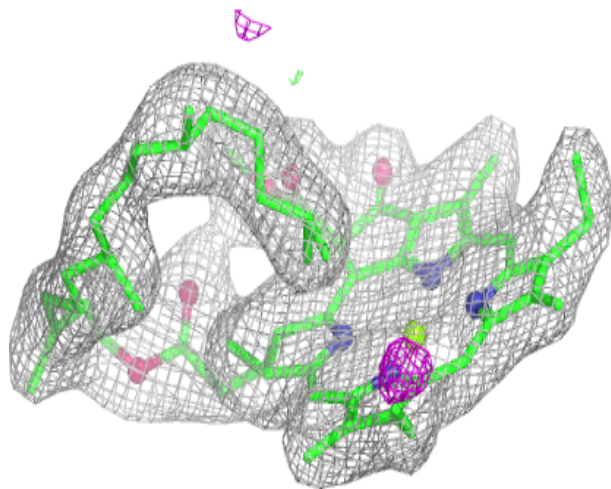
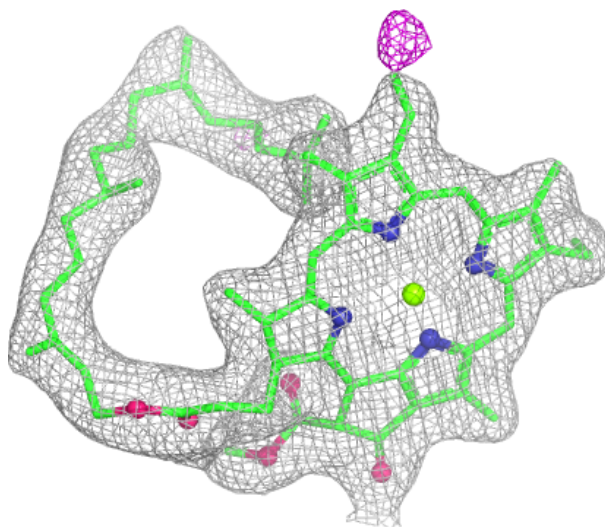
Electron density around CLA b 611:

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



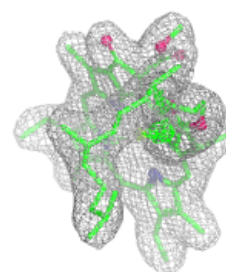
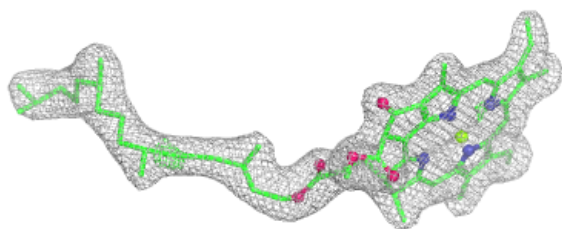
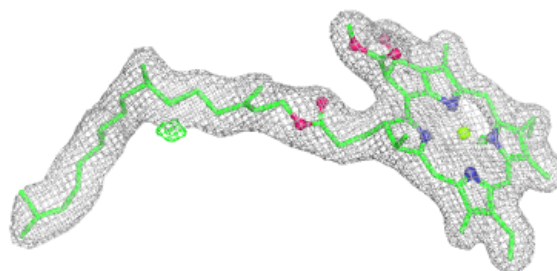
Electron density around CLA B 616:

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



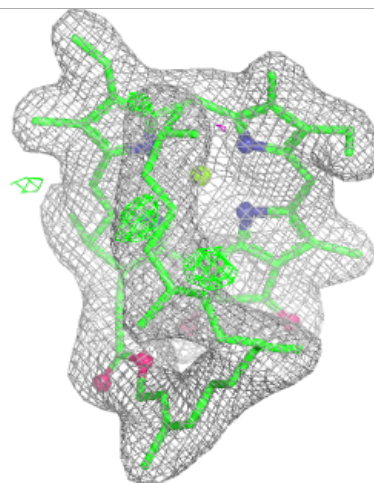
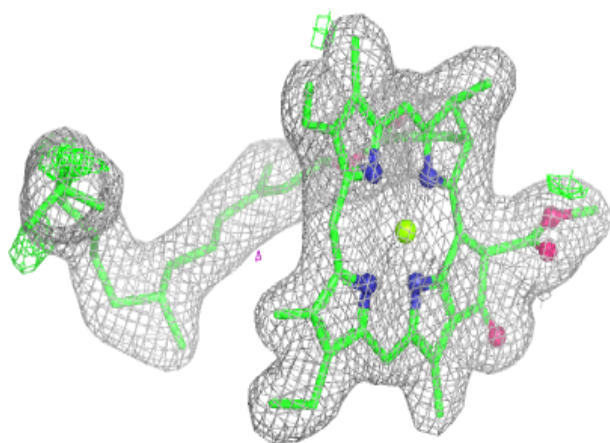
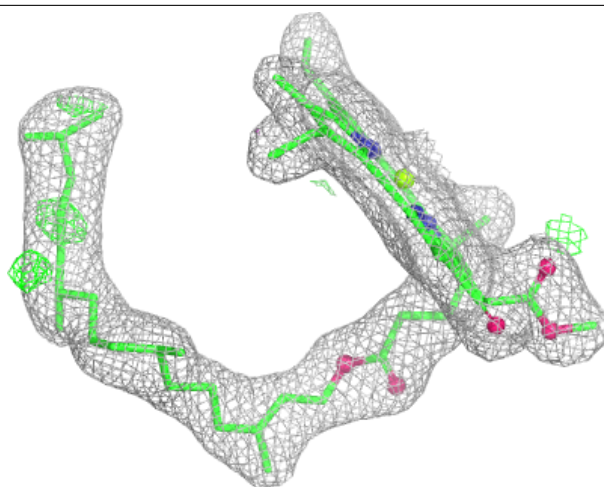
Electron density around CLA a 2109:

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



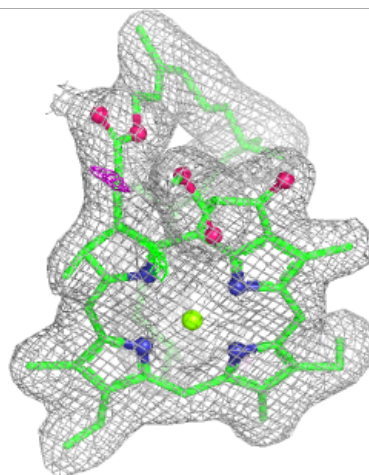
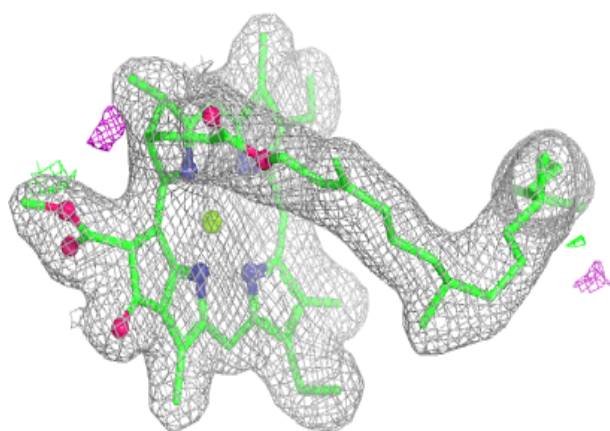
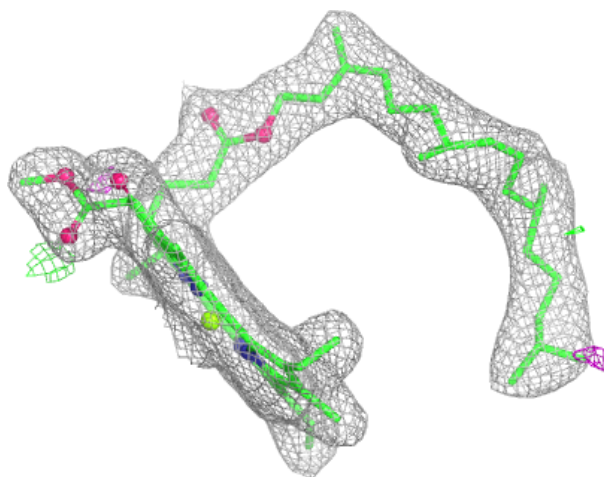
Electron density around CLA b 614:

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



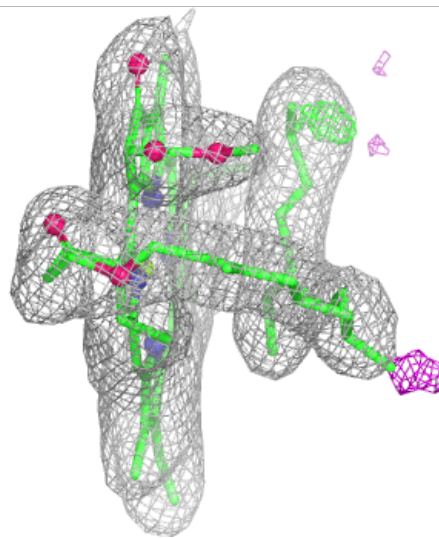
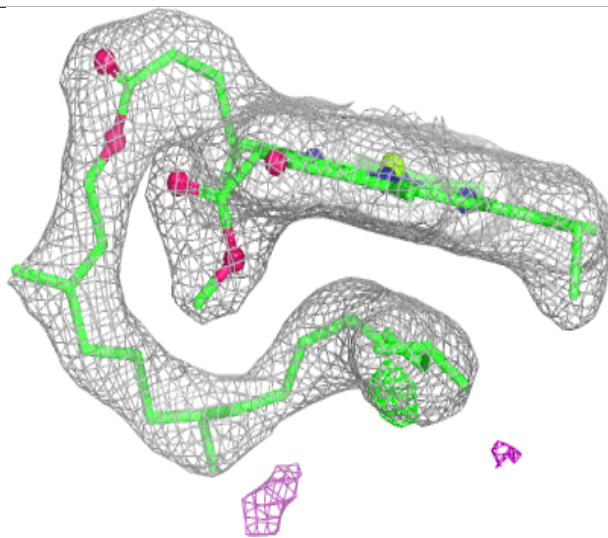
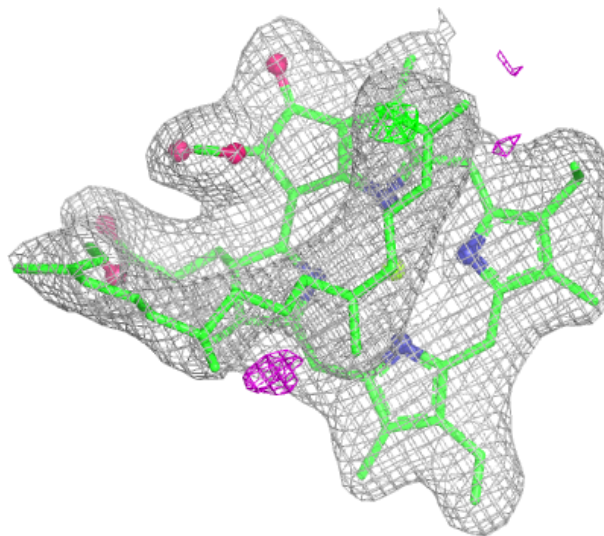
Electron density around CLA B 612:

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



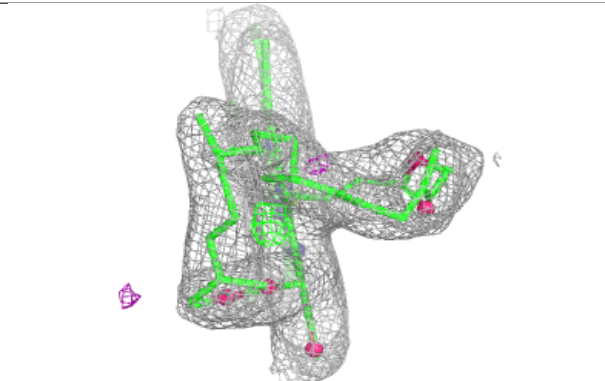
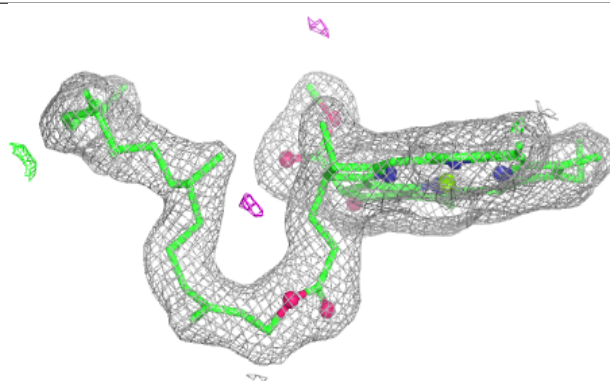
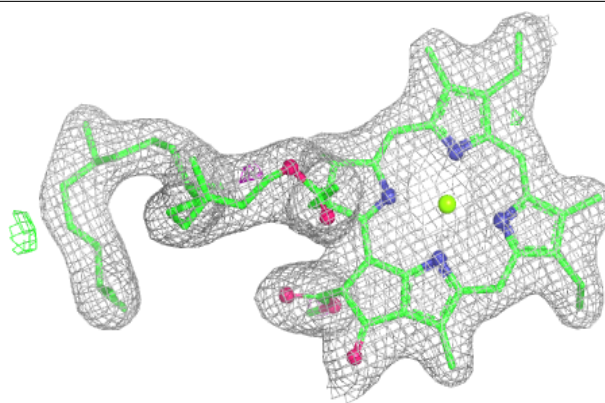
Electron density around CLA c 512:

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

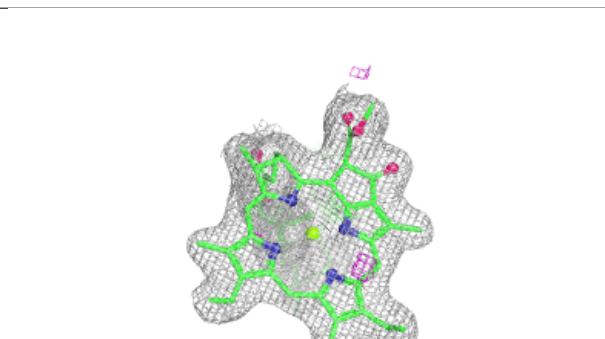
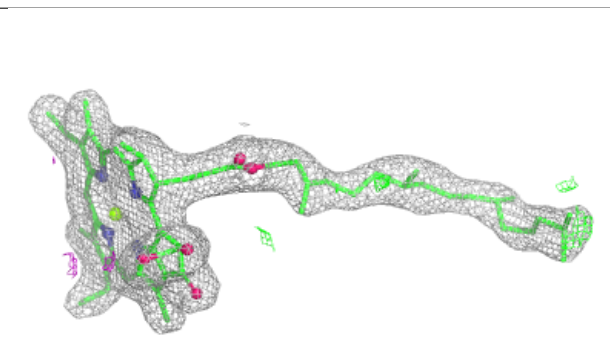
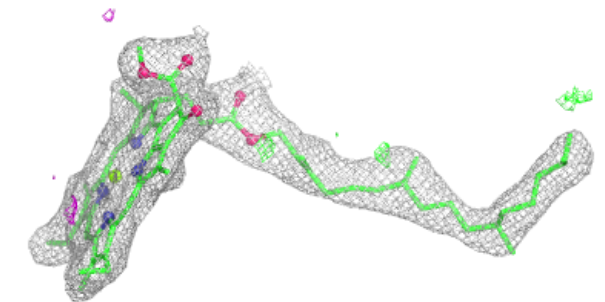


Electron density around CLA B 613:

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

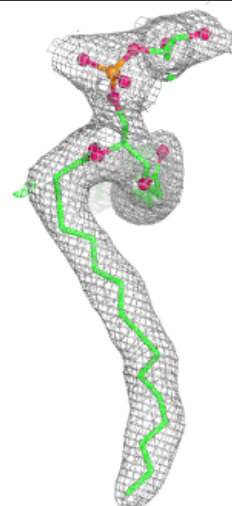
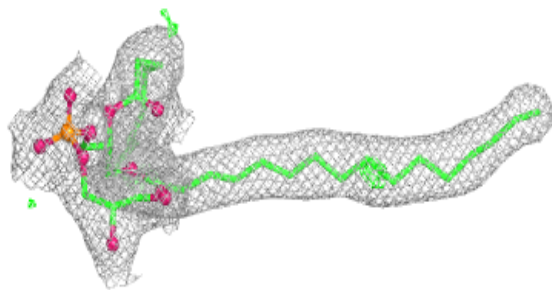
**Electron density around CLA B 605:**

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



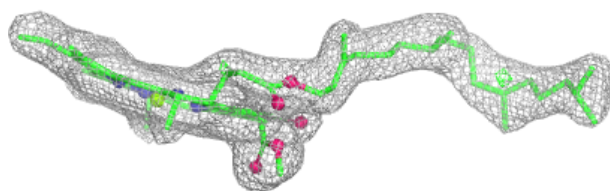
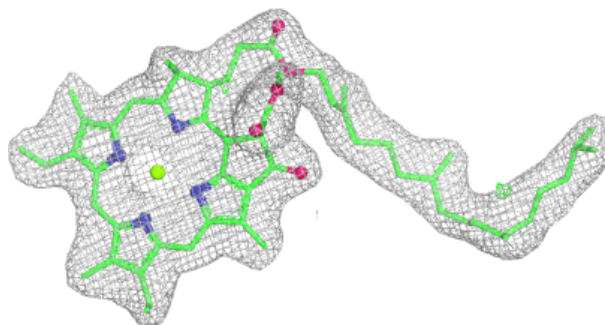
Electron density around LHG L 101:

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

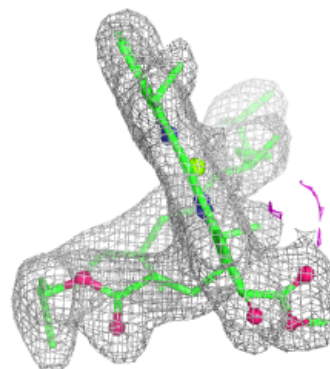
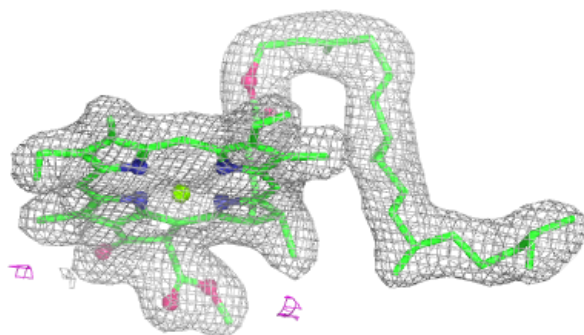
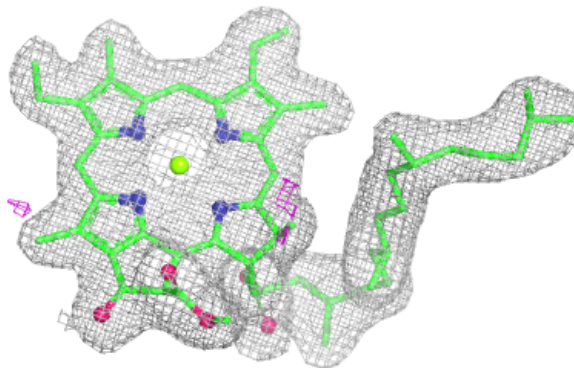


Electron density around CLA b 605:

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

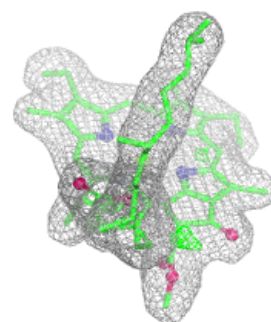
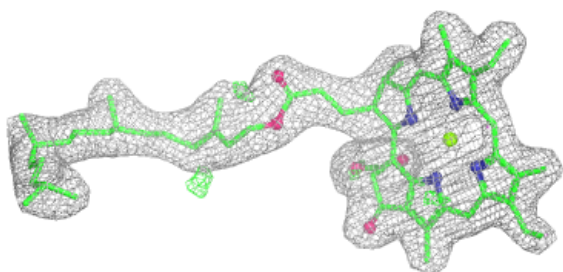
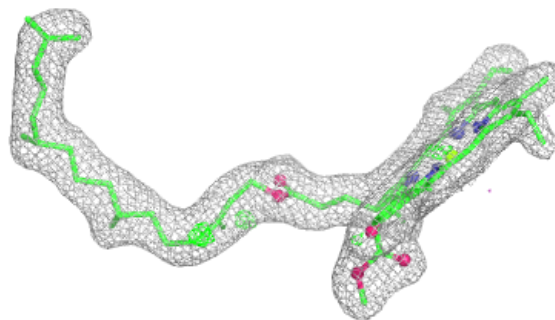
**Electron density around CLA d 401:**

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

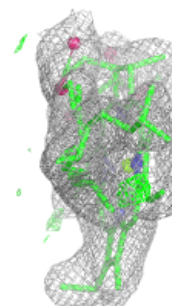
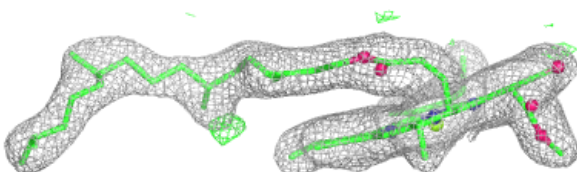
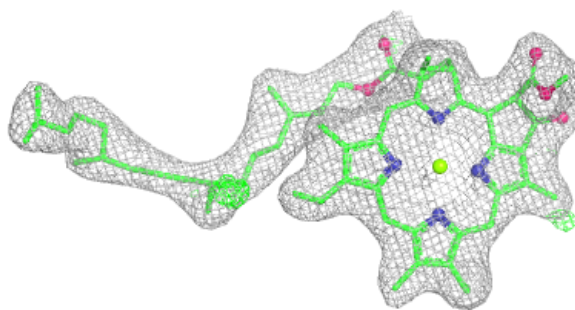


Electron density around CLA d 404:

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

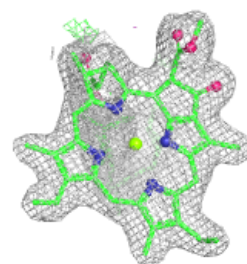
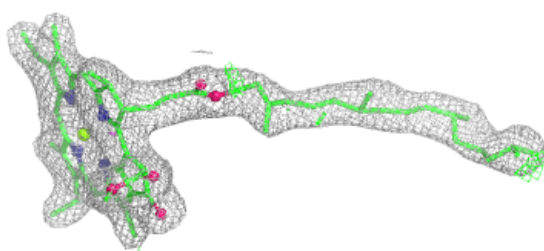
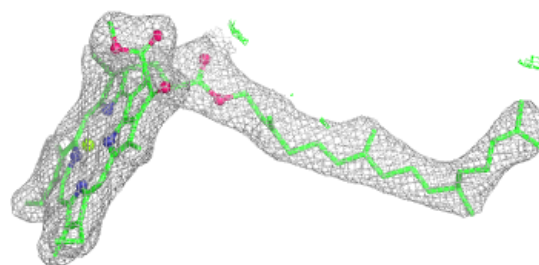
**Electron density around CLA b 606:**

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



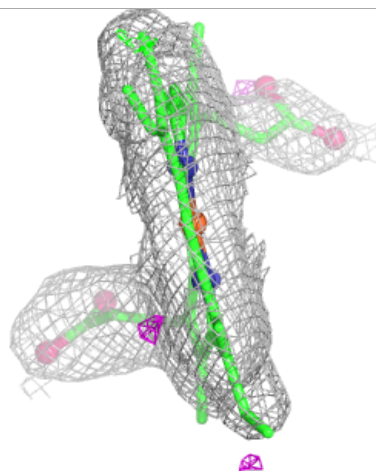
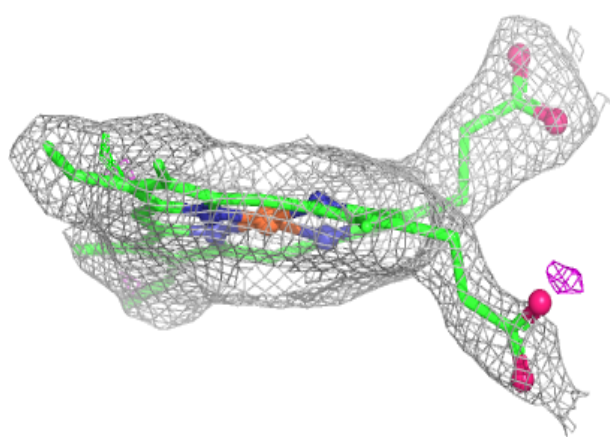
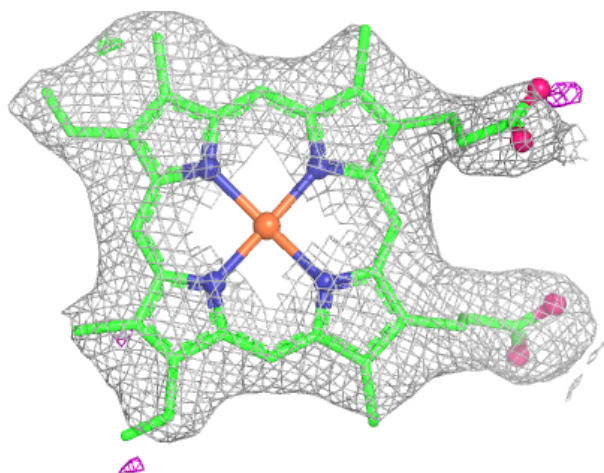
Electron density around CLA b 607:

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



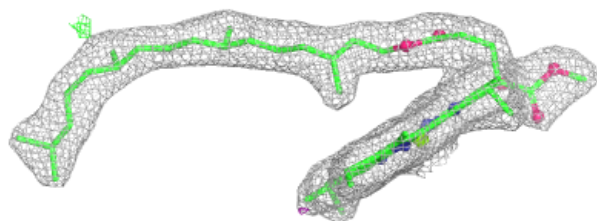
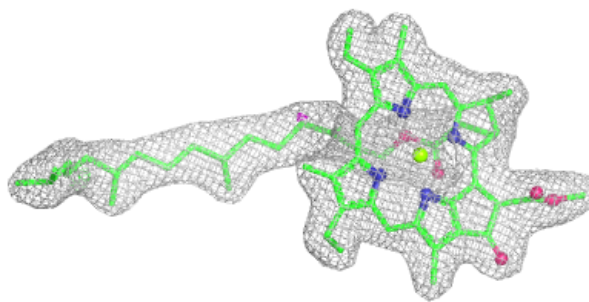
Electron density around HEM e 103:

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



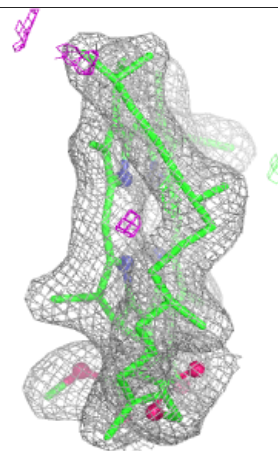
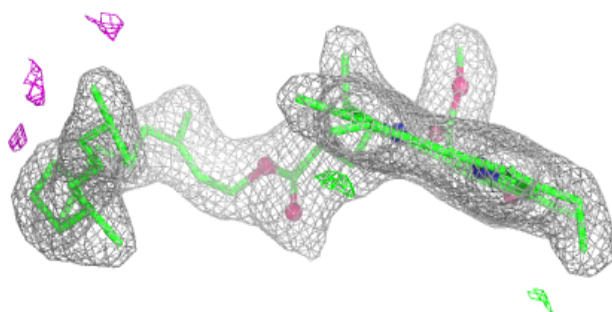
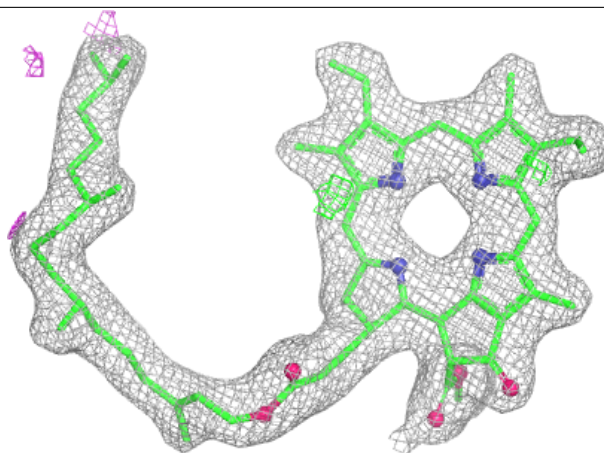
Electron density around CLA B 609:

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



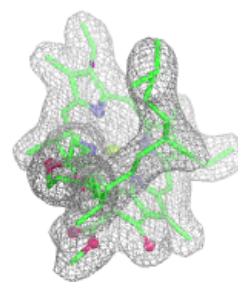
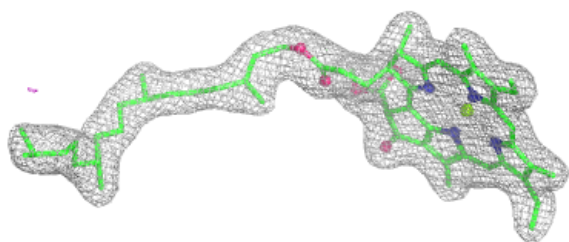
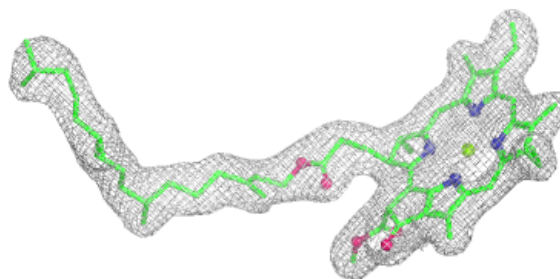
Electron density around PHO a 2111:

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



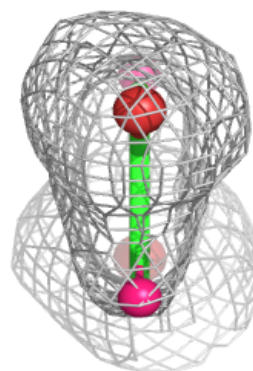
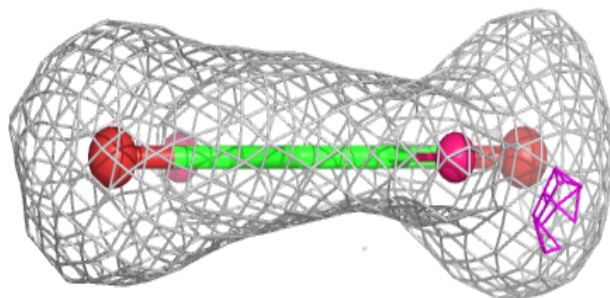
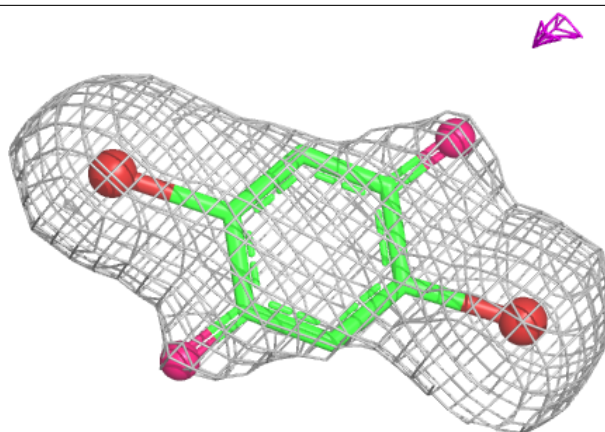
Electron density around CLA A 405:

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



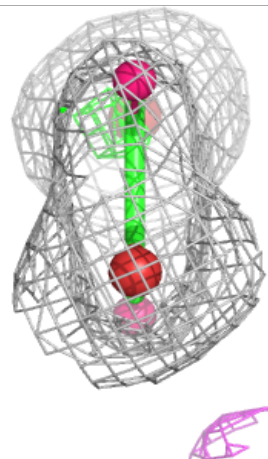
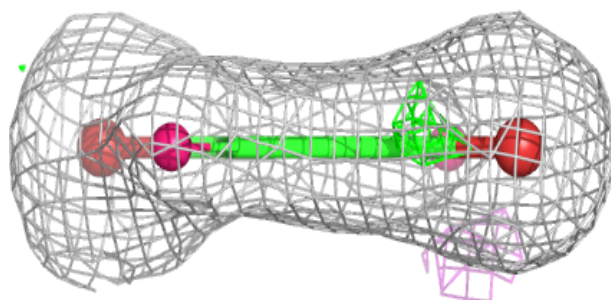
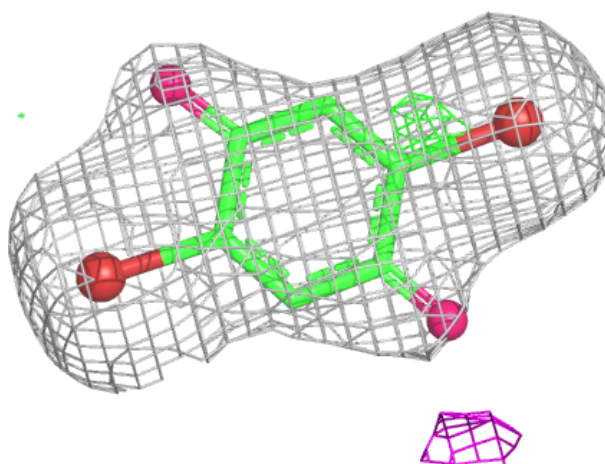
Electron density around K2I A 419:

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



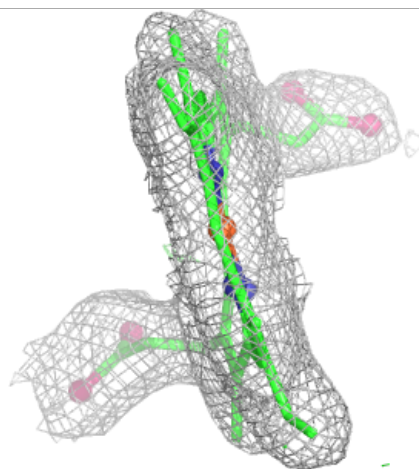
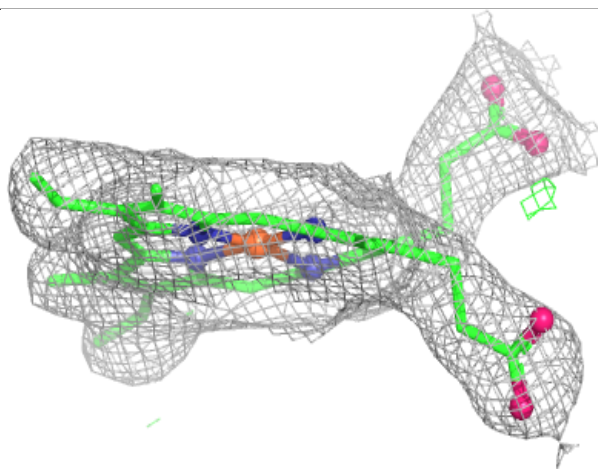
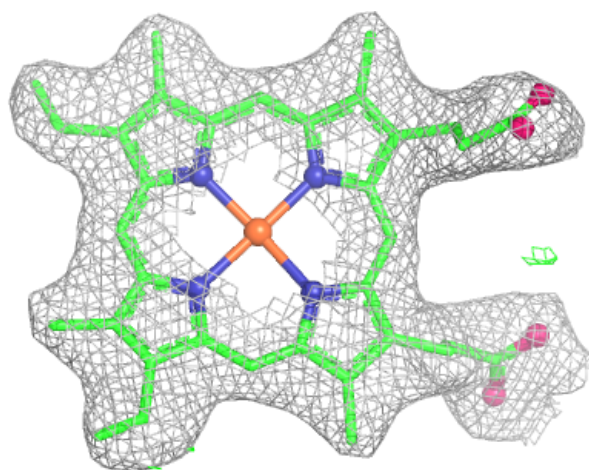
Electron density around K2I a 2119:

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



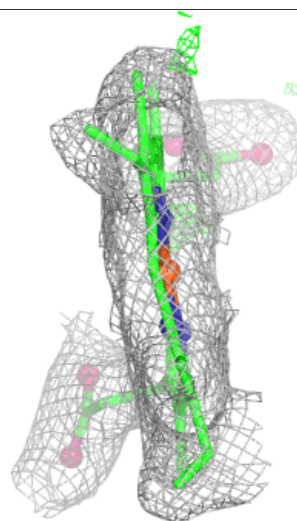
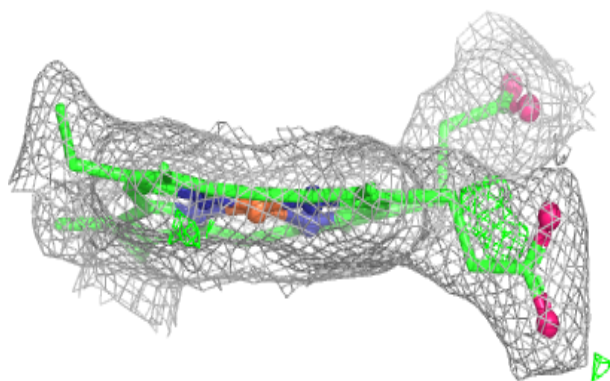
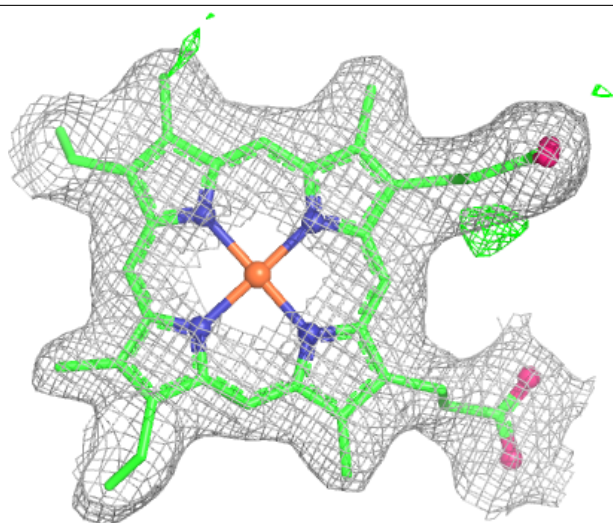
Electron density around HEM F 102:

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



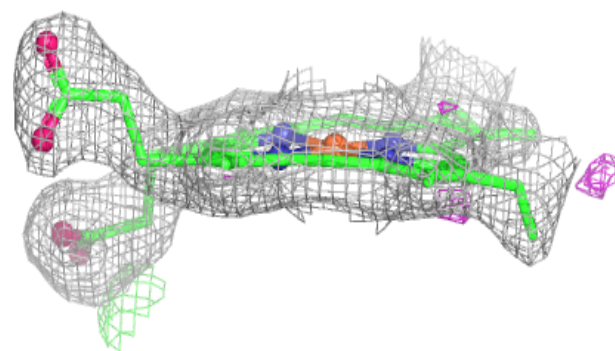
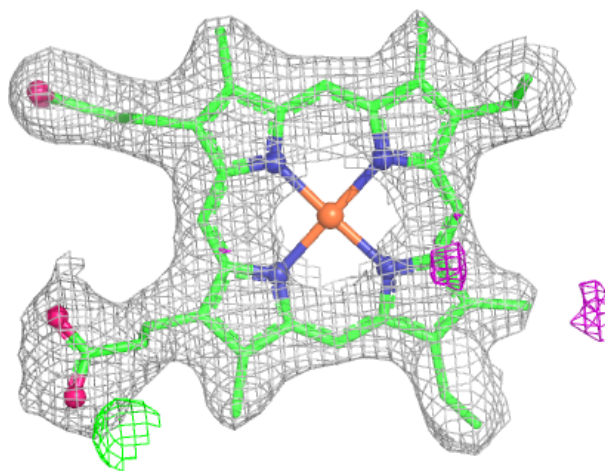
Electron density around HEC V 201:

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



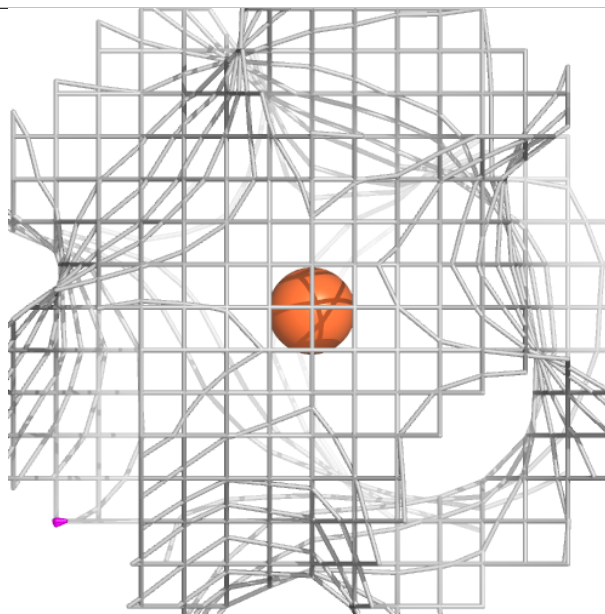
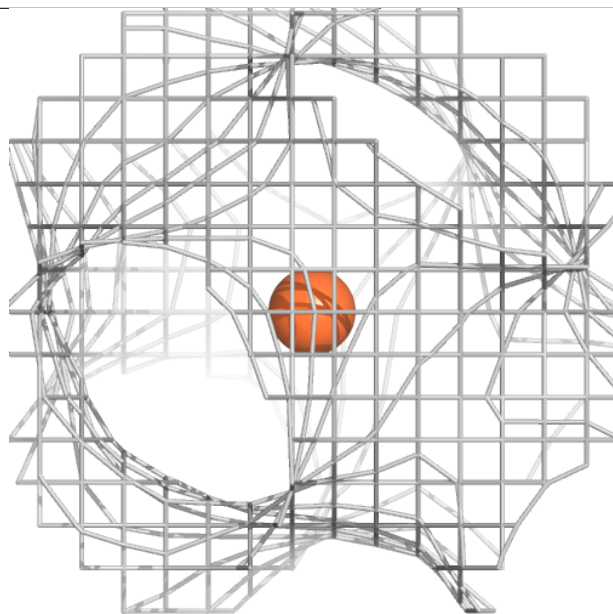
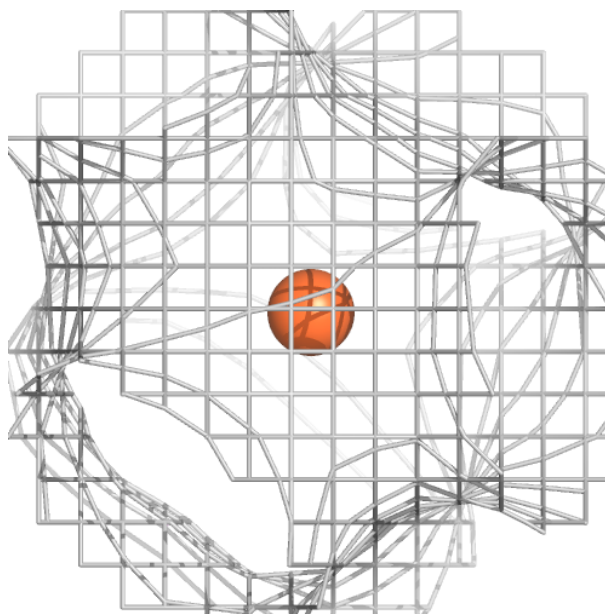
Electron density around HEC v 201:

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



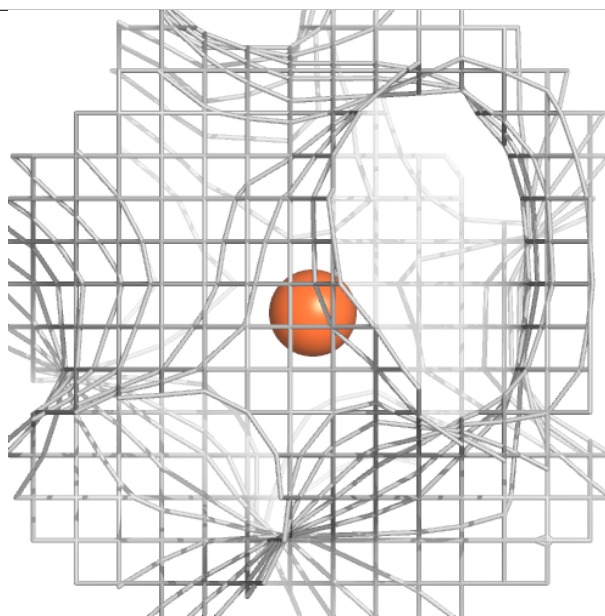
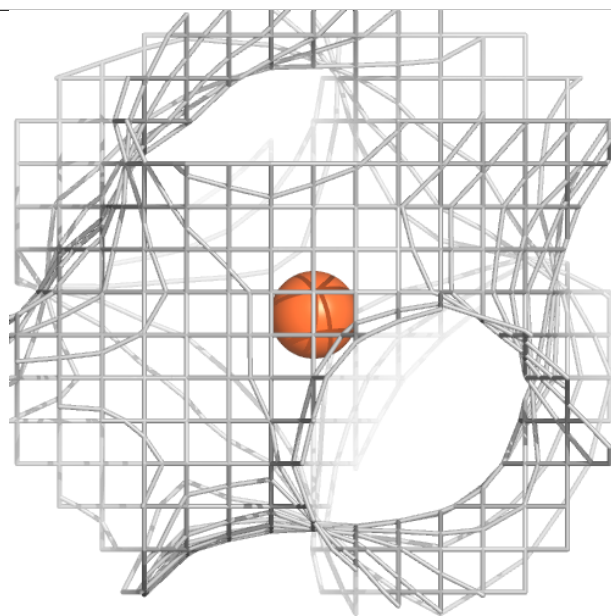
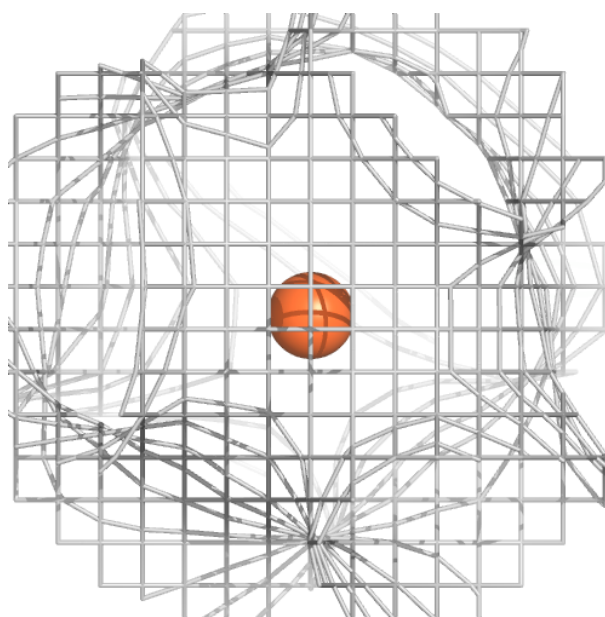
Electron density around FE2 a 2105:

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



Electron density around FE2 A 402:

$2mF_o-DF_c$ (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.