



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:25 AM UTC

PDB ID : 6JLK / pdb_00006jlk
Title : XFEL structure of cyanobacterial photosystem II (1F state, dataset1)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2019-03-06
Resolution : 2.15 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

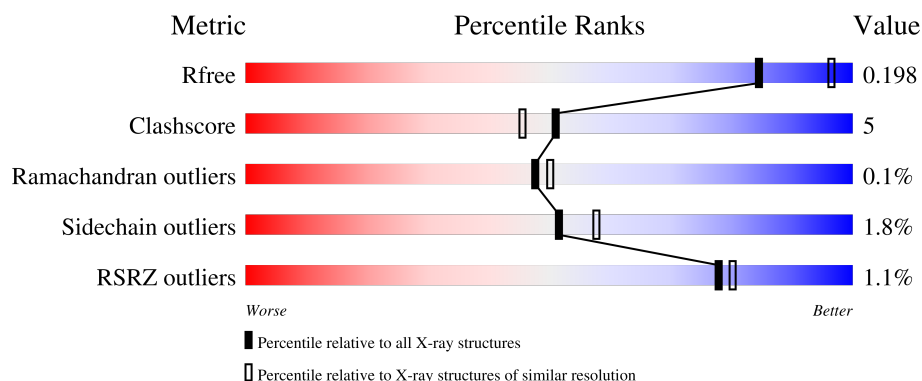
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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.



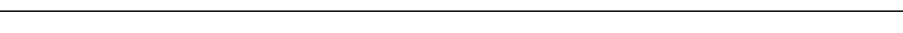
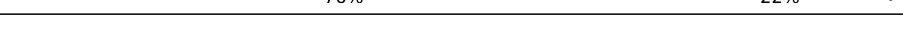
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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

Mol	Chain	Length	Quality of chain
1	A	344	90% 7% .
1	a	344	% 88% 8% ..
2	B	505	91% 9%
2	b	505	% 90% 10%
3	C	455	89% 10% .

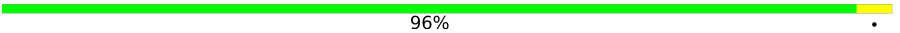
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Mol	Chain	Length	Quality of chain
3	c	455	 91% 8% .
4	D	342	 89% 11%
4	d	342	 93% 7%
5	E	84	 90% 6% .
5	e	84	 82% 14% .
6	F	44	 64% 14% 23%
6	f	44	 55% 18% 27%
7	H	65	 91% 8% .
7	h	65	 92% 8%
8	I	38	 79% 18% .
8	i	38	 87% 11% .
9	J	39	 90% 8% .
9	j	39	 95% 5%
10	K	37	 76% 24%
10	k	37	 76% 22% .
11	L	37	 92% 5% .
11	l	37	 89% 8% .
12	M	36	 67% 25% . 6%
12	m	36	 72% 19% . 6%
13	O	244	 92% 8%
13	o	244	 89% 9% .
14	T	32	 75% 16% . 6%
14	t	32	 84% 9% 6%
15	U	104	 87% 7% 7%
15	u	104	 90% . 7%

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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	34	

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	406	X	-	-	-
24	CLA	A	410	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	501	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	513	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	412	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	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	b	621	X	-	-	-
24	CLA	b	622	X	-	-	-
24	CLA	b	623	X	-	-	-
24	CLA	b	624	X	-	-	-
24	CLA	b	625	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	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	c	515	X	-	-	-
24	CLA	c	516	X	-	-	-
24	CLA	c	517	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 55631 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	53	0
			3019	1966	498	537	18			
1	a	334	Total	C	N	O	S	0	55	0
			3027	1973	498	538	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	See sequence details	UNP P51765
a	279	PRO	ARG	See sequence details	UNP P51765

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4021	2639	667	702	13			
2	b	503	Total	C	N	O	S	0	12	0
			4022	2644	664	701	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	7	0
			3518	2300	587	618	13			
3	c	455	Total	C	N	O	S	0	13	0
			3598	2356	599	629	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	See sequence details	UNP D0VWR7
C	20	SER	-	See sequence details	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	See sequence details	UNP D0VWR7
C	22	PHE	-	See sequence details	UNP D0VWR7
c	19	ASN	-	See sequence details	UNP D0VWR7
c	20	SER	-	See sequence details	UNP D0VWR7
c	21	ILE	-	See sequence details	UNP D0VWR7
c	22	PHE	-	See sequence details	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	16	0
			2849	1884	469	483	13			
4	d	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	2	0
			668	436	107	125			
5	e	81	Total	C	N	O	0	2	0
			670	439	107	124			

- 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	65	Total	C	N	O	S	0	1	0
			519	346	85	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			280	187	43	48	2			

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	See sequence details	UNP P19054
K	39	TRP	VAL	See sequence details	UNP P19054
k	33	LEU	PHE	See sequence details	UNP P19054
k	39	TRP	VAL	See sequence details	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	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	See sequence details	UNP P12312
m	8	LEU	PHE	See sequence details	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	8	0
			1903	1191	315	392	5			
13	o	243	Total	C	N	O	S	0	5	0
			1891	1183	315	388	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			
14	t	30	Total	C	N	O	S	0	1	0
			264	185	36	41	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	0	0
			774	491	129	154				
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	2	0
			1085	689	181	211	4			
16	v	137	Total	C	N	O	S	0	1	0
			1077	684	178	211	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	S	0	0	0
			287	191	46	50				
18	x	38	Total	C	N	O	S	0	0	0
			281	188	45	48				

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	30	Total	C	N	O	S	98	0	0
			239	163	41	35				

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

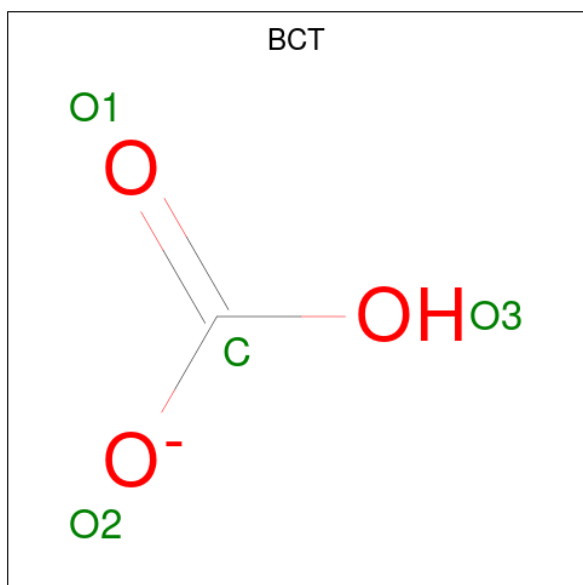
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		
22	U	1	Total	Cl	0	0
			1	1		

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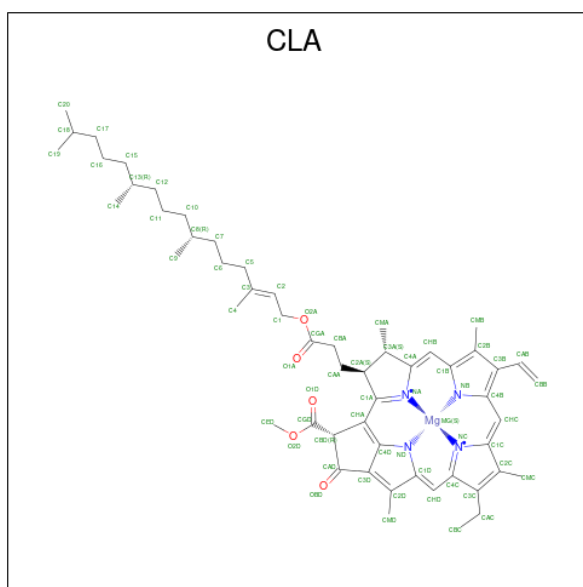
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	2	Total	Cl	0	2
			4	4		
22	v	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



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

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).

[illegible]

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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	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

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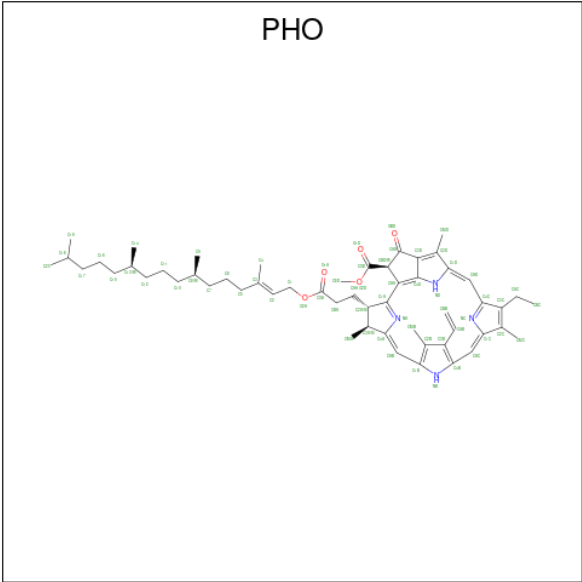
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

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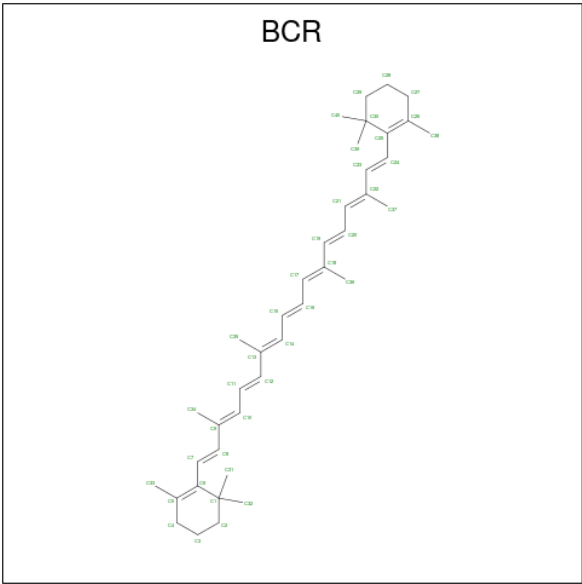
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 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: C₅₅H₇₄N₄O₅).



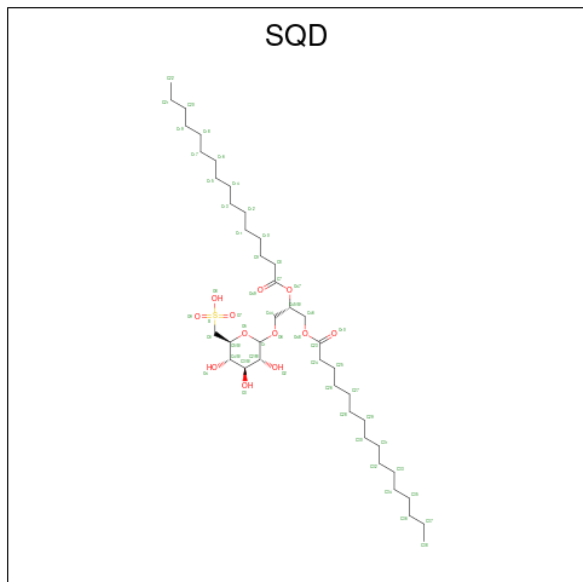
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	1
			128	110	8	10		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	1
			128	110	8	10		

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



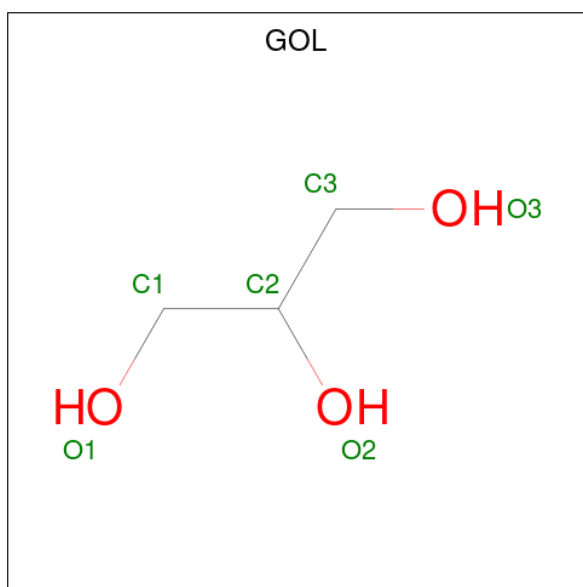
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total 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	d	1	Total C 40 40	0	0
26	h	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

- 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
			54	41	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
			43	30	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 28 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



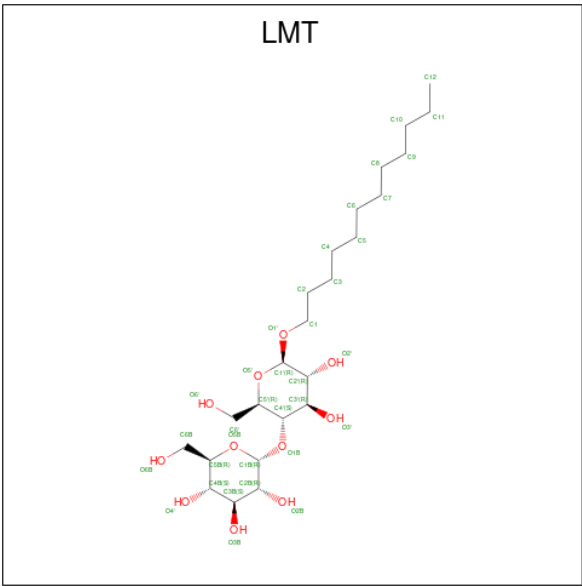
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total 6	C 3	O 3	0	0
28	T	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	c	1	Total 6	C 3	O 3	0	0
28	c	1	Total 6	C 3	O 3	0	0
28	o	1	Total 6	C 3	O 3	0	0
28	t	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0

- Molecule 29 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



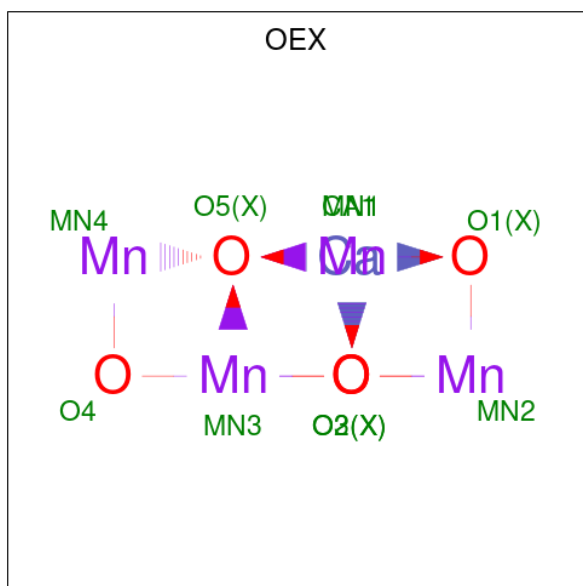
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			25	19	6		
29	C	1	Total	C	O	0	0
			35	24	11		
29	D	1	Total	C	O	0	0
			35	24	11		
29	F	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	T	1	Total	C	O	0	0
			25	19	6		
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		
29	f	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		

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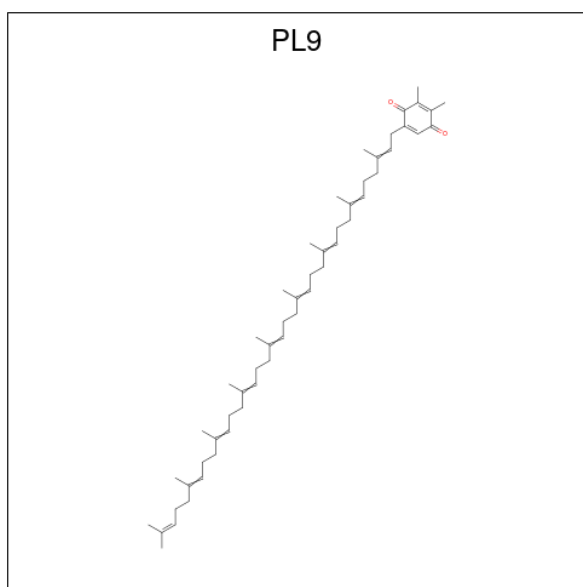
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	m	1	Total	C	O	0	0
			35	24	11		

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

- 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: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



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

- Molecule 32 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

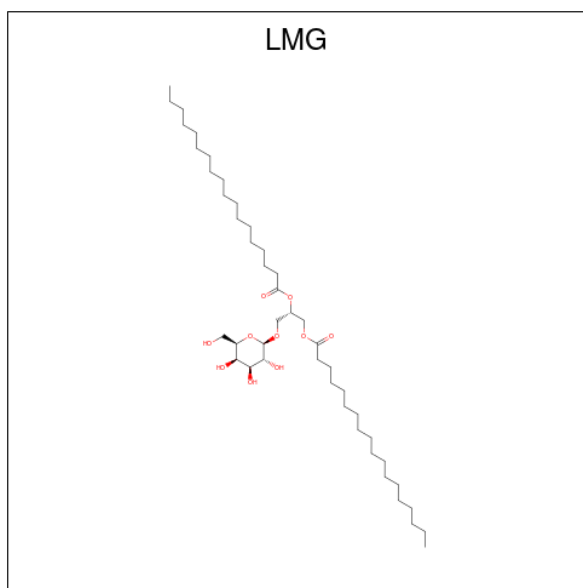
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			28	23	5		
32	B	1	Total	C	O	0	0
			33	28	5		
32	C	1	Total	C	O	0	0
			34	29	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	I	1	Total	C	O	0	0
			40	35	5		
32	J	1	Total	C		0	0
			10	10			
32	M	1	Total	C		0	0
			10	10			
32	X	1	Total	C	O	0	0
			18	16	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	a	1	Total	C	O	0	0
			30	25	5		
32	b	1	Total	C	O	0	0
			33	28	5		
32	c	1	Total	C	O	0	0
			32	27	5		
32	d	3	Total	C	O	0	0
			71	63	8		
32	i	1	Total	C	O	0	0
			40	35	5		
32	j	1	Total	C		0	0
			10	10			
32	m	1	Total	C		0	0
			10	10			

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

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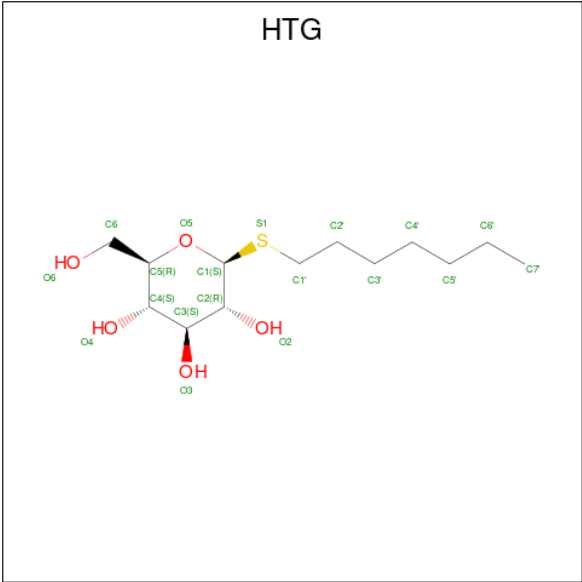
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	D	1	Total C O 51 41 10	0	0
33	Z	1	Total C O 37 27 10	0	0
33	b	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	d	1	Total C O 51 41 10	0	0
33	z	1	Total C O 39 29 10	0	0

- Molecule 34 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



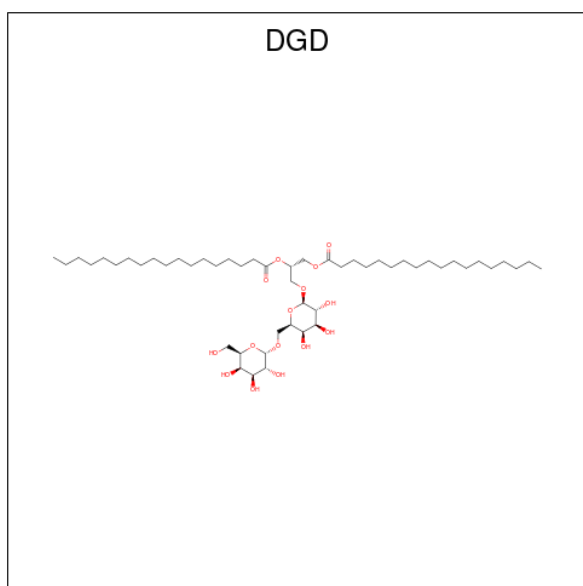
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19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

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

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



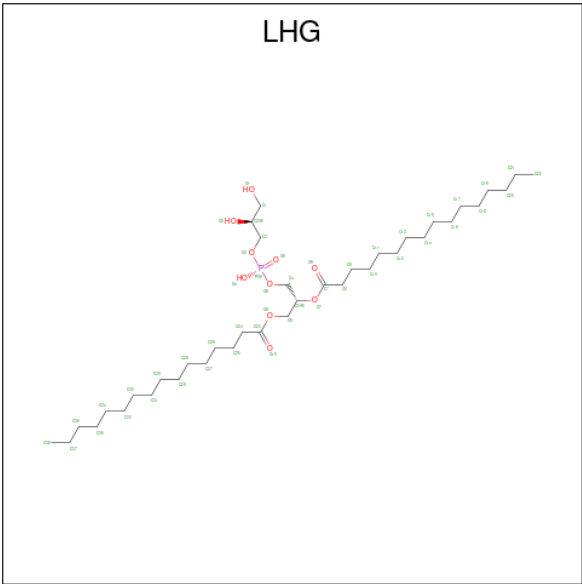
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	D	1	Total	C	O		0	0
			52	42	10			
36	H	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	e	1	Total	C	O	0	0
			62	47	15		
36	h	1	Total	C	O	0	0
			62	47	15		

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



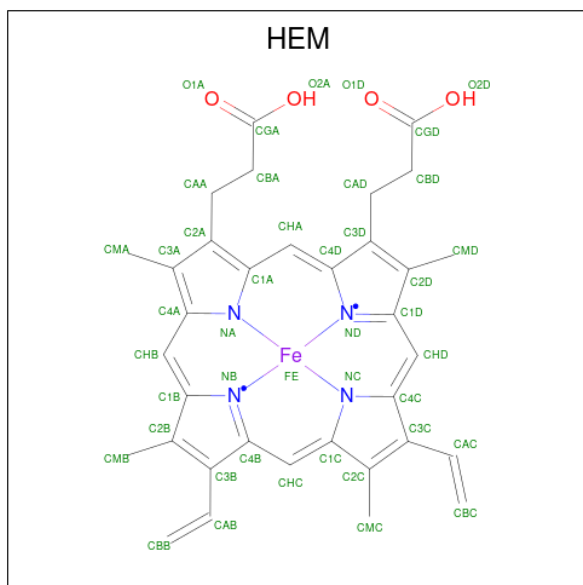
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	E	1	Total	C	O	P	0	0
			42	31	10	1		
37	L	1	Total	C	O	P	0	0
			49	38	10	1		
37	b	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0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

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

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

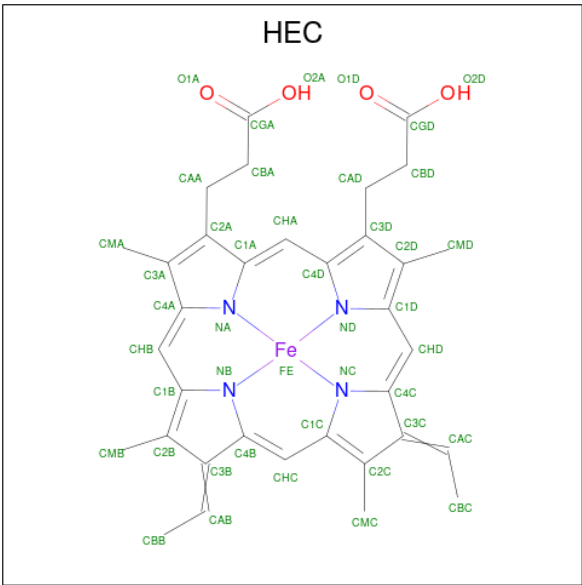


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	166	Total	O	0	15
			179	179		
41	B	289	Total	O	0	4
			293	293		
41	C	229	Total	O	0	6
			233	233		
41	D	146	Total	O	0	5
			151	151		
41	E	32	Total	O	0	1
			33	33		
41	F	8	Total	O	0	0
			8	8		
41	H	44	Total	O	0	0
			44	44		
41	I	5	Total	O	0	0
			5	5		
41	J	12	Total	O	0	0
			12	12		
41	K	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	18	Total O 19 19	0	1
41	M	19	Total O 19 19	0	0
41	O	175	Total O 177 177	0	2
41	T	16	Total O 17 17	0	1
41	U	82	Total O 82 82	0	0
41	V	113	Total O 115 115	0	2
41	Y	5	Total O 5 5	0	0
41	X	8	Total O 8 8	0	0
41	Z	1	Total O 1 1	0	0
41	a	155	Total O 167 167	0	14
41	b	259	Total O 262 262	0	3
41	c	202	Total O 207 207	0	7
41	d	134	Total O 137 137	0	3
41	e	16	Total O 16 16	0	0
41	f	7	Total O 7 7	0	0
41	h	42	Total O 42 42	0	0
41	i	5	Total O 5 5	0	0
41	j	7	Total O 7 7	0	0
41	k	7	Total O 7 7	0	0
41	l	9	Total O 9 9	0	0
41	m	16	Total O 16 16	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	o	157	Total 157	O 157	0	0
41	t	11	Total 11	O 11	0	0
41	u	93	Total 93	O 93	0	0
41	v	81	Total 82	O 82	0	1
41	y	2	Total 2	O 2	0	0
41	x	6	Total 6	O 6	0	0

3 Residue-property plots

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

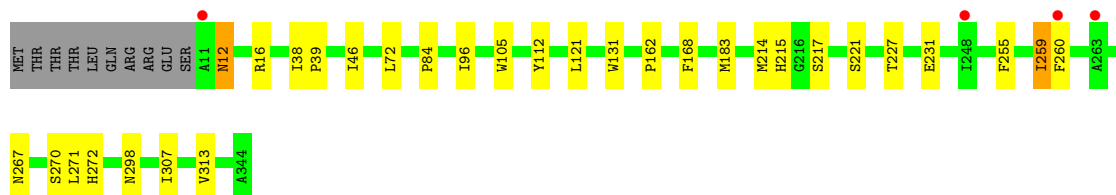
- Molecule 1: Photosystem II protein D1

Chain A: 



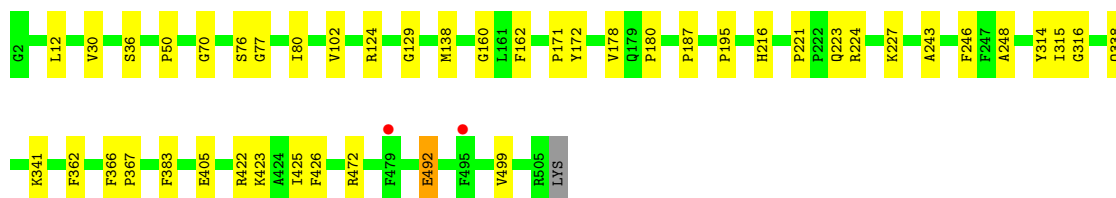
- Molecule 1: Photosystem II protein D1

Chain a: 



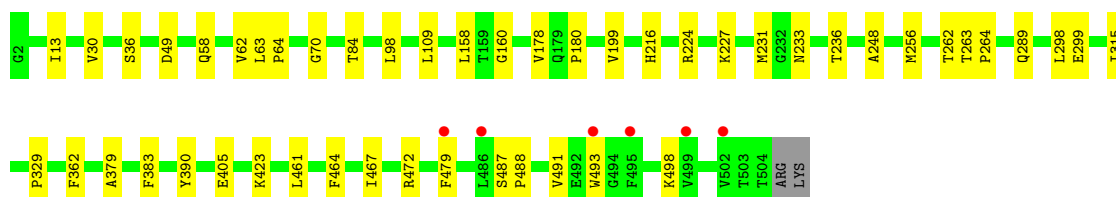
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 

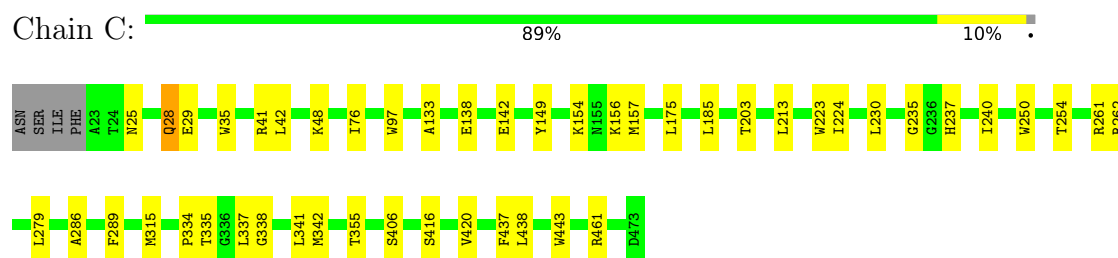


- Molecule 2: Photosystem II CP47 reaction center protein

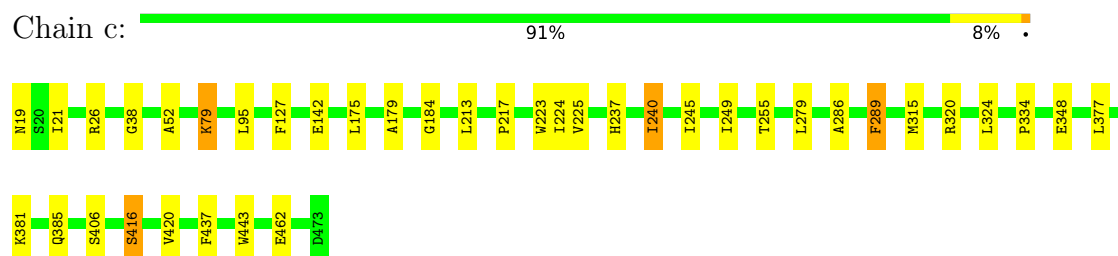
Chain b: 



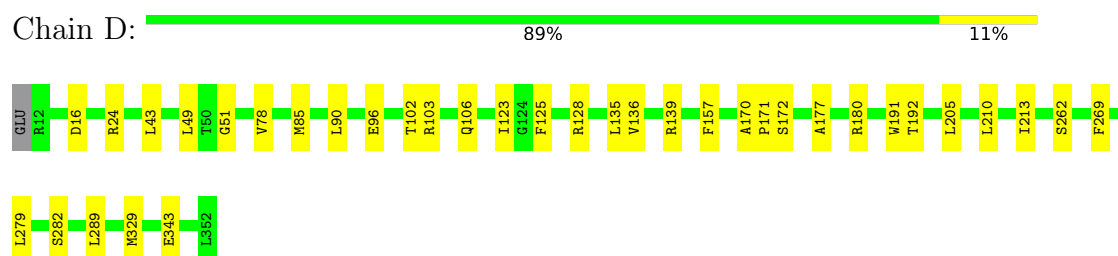
- Molecule 3: Photosystem II CP43 reaction center protein



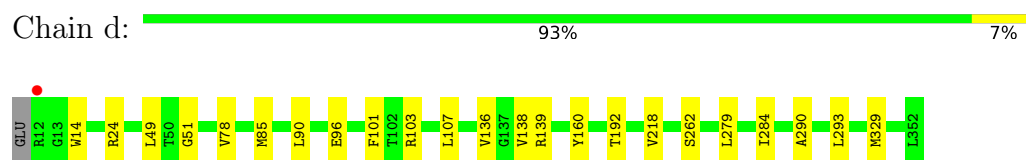
- Molecule 3: Photosystem II CP43 reaction center protein



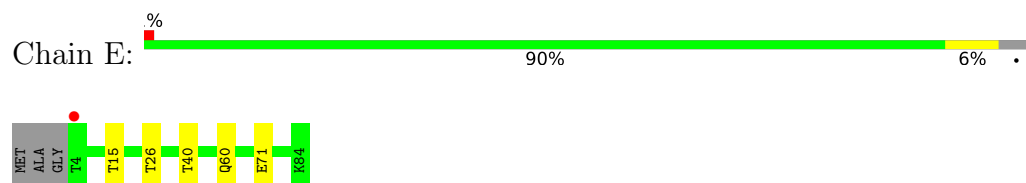
- Molecule 4: Photosystem II D2 protein



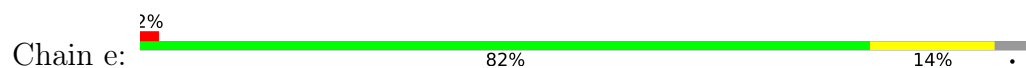
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha

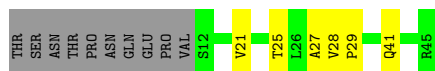


- Molecule 5: Cytochrome b559 subunit alpha

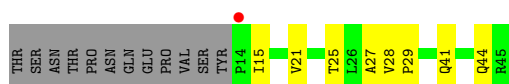




- Molecule 6: Cytochrome b559 subunit beta



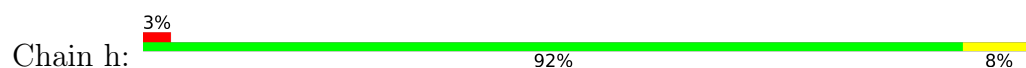
- Molecule 6: Cytochrome b559 subunit beta



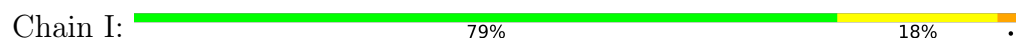
- Molecule 7: Photosystem II reaction center protein H



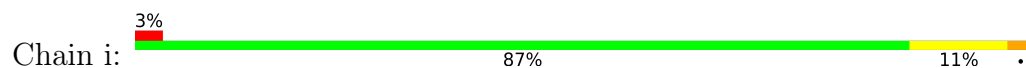
- Molecule 7: Photosystem II reaction center protein H



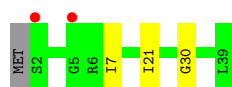
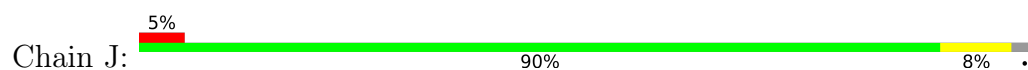
- Molecule 8: Photosystem II reaction center protein I



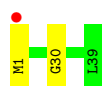
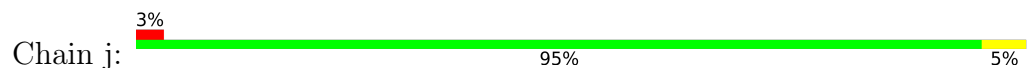
- Molecule 8: Photosystem II reaction center protein I



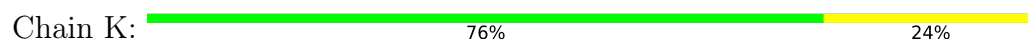
- Molecule 9: Photosystem II reaction center protein J



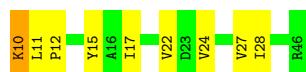
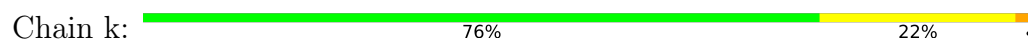
- Molecule 9: Photosystem II reaction center protein J



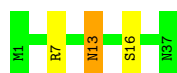
- Molecule 10: Photosystem II reaction center protein K



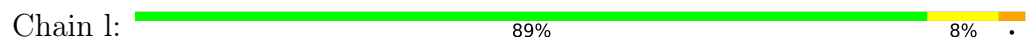
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

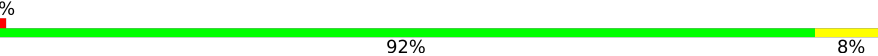


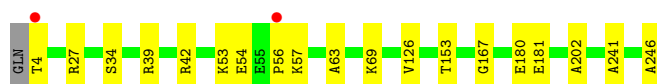
- Molecule 12: Photosystem II reaction center protein M

Chain m:  72% 19% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  92% 8%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  89% 9%



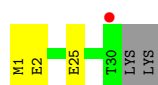
- Molecule 14: Photosystem II reaction center protein T

Chain T:  75% 16% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  84% 9% 6%



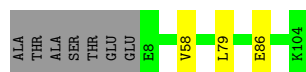
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  87% 7% 7%

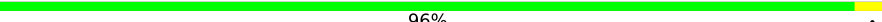


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  90% 7%



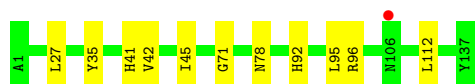
- Molecule 16: Cytochrome c-550

Chain V:  96% .



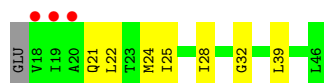
- Molecule 16: Cytochrome c-550

Chain v:  92% 8%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  10% 73% 23% .



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  10% 70% 23% . .



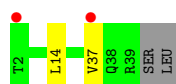
- Molecule 18: Photosystem II reaction center protein X

Chain X:  2% 88% 10% .



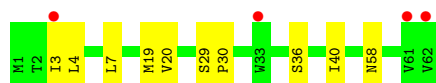
- Molecule 18: Photosystem II reaction center protein X

Chain x:  5% 90% 5% 5%

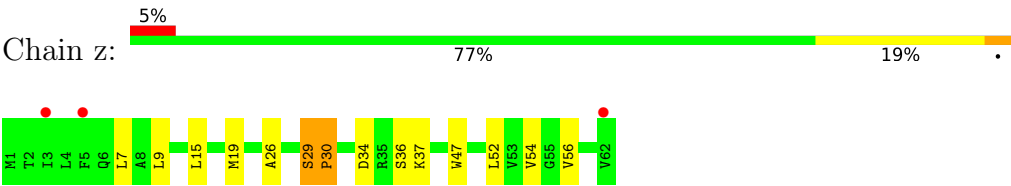


- Molecule 19: Photosystem II reaction center protein Z

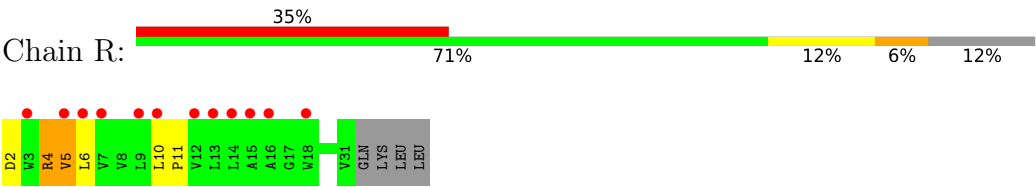
Chain Z:  6% 84% 16%



● 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	121.97Å 228.72Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.15 19.98 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.15) 99.8 (19.98-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.149 , 0.193 0.156 , 0.198	Depositor DCC
R_{free} test set	26831 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.629	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 77.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	55631	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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: MG, LMT, OEX, HEC, PHO, BCT, HEM, GOL, DGD, CA, BCR, CL, PL9, UNL, FE2, FME, LMG, CLA, HTG, SQD, LHG

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	0.55	0/3121	0.82	0/4250
1	a	0.56	0/3135	0.79	0/4269
2	B	0.55	0/4191	0.81	1/5709 (0.0%)
2	b	0.53	0/4198	0.81	1/5720 (0.0%)
3	C	0.50	0/3643	0.80	4/4958 (0.1%)
3	c	0.48	0/3731	0.79	2/5076 (0.0%)
4	D	0.60	0/2952	0.80	3/4021 (0.1%)
4	d	0.56	0/2952	0.77	1/4021 (0.0%)
5	E	0.46	0/693	0.78	0/944
5	e	0.44	0/695	0.80	0/948
6	F	0.57	0/284	0.79	0/387
6	f	0.54	0/265	0.77	0/360
7	H	0.44	0/535	0.87	0/728
7	h	0.43	0/524	0.76	0/713
8	I	0.43	0/311	0.74	0/419
8	i	0.47	0/311	0.81	0/419
9	J	0.46	0/278	0.76	0/376
9	j	0.44	0/286	0.76	0/386
10	K	0.47	0/303	0.79	0/416
10	k	0.53	0/303	0.86	0/416
11	L	0.58	0/319	0.69	0/433
11	l	0.50	0/319	0.74	0/433
12	M	0.60	0/270	0.84	0/368
12	m	0.57	0/262	0.84	0/357
13	O	0.46	0/1958	0.78	0/2654
13	o	0.44	0/1937	0.79	0/2625
14	T	0.57	0/266	0.72	0/362
14	t	0.57	0/266	0.74	0/362
15	U	0.49	0/785	0.74	0/1064
15	u	0.47	0/785	0.70	0/1064
16	V	0.51	0/1109	0.75	0/1502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.46	0/1098	0.80	2/1488 (0.1%)
17	Y	0.49	0/216	0.85	0/289
17	y	0.42	0/216	0.75	0/289
18	X	0.41	0/290	0.79	0/392
18	x	0.41	0/284	0.75	0/384
19	Z	0.38	0/490	0.76	0/669
19	z	0.34	0/490	0.80	0/669
20	R	0.35	0/245	0.67	0/338
All	All	0.51	0/44316	0.79	14/60278 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	76	ILE	CA-C-N	6.94	127.52	119.47
3	C	76	ILE	C-N-CA	6.94	127.52	119.47
4	D	170	ALA	CA-C-N	-6.39	113.37	119.76
4	D	170	ALA	C-N-CA	-6.39	113.37	119.76
3	C	133	ALA	CA-C-N	-5.38	116.12	122.36
3	C	133	ALA	C-N-CA	-5.38	116.12	122.36
3	c	385	GLN	CA-C-N	5.23	124.68	119.24
3	c	385	GLN	C-N-CA	5.23	124.68	119.24
4	D	262	SER	N-CA-C	-5.19	107.97	114.56
2	B	77	GLY	N-CA-C	5.07	121.52	114.92
16	v	92	HIS	CA-C-N	5.03	125.31	119.93
16	v	92	HIS	C-N-CA	5.03	125.31	119.93
4	d	262	SER	N-CA-C	-5.03	108.18	114.56
2	b	13	ILE	N-CA-C	5.01	115.73	110.62

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	3019	0	2872	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3027	0	2888	28	0
2	B	4021	0	3898	38	0
2	b	4022	0	3908	36	0
3	C	3518	0	3439	30	0
3	c	3598	0	3529	26	0
4	D	2849	0	2741	27	0
4	d	2849	0	2741	18	0
5	E	668	0	658	4	0
5	e	670	0	664	10	0
6	F	275	0	282	4	0
6	f	257	0	269	4	0
7	H	519	0	545	9	0
7	h	511	0	532	8	0
8	I	314	0	328	5	0
8	i	314	0	328	3	0
9	J	272	0	279	3	0
9	j	280	0	291	1	0
10	K	293	0	305	7	0
10	k	293	0	305	6	0
11	L	309	0	327	4	0
11	l	309	0	327	5	0
12	M	274	0	299	8	0
12	m	269	0	288	8	0
13	O	1903	0	1886	10	0
13	o	1891	0	1870	16	0
14	T	264	0	267	4	0
14	t	264	0	267	2	0
15	U	774	0	773	3	1
15	u	774	0	773	1	0
16	V	1085	0	1095	4	0
16	v	1077	0	1082	8	0
17	Y	215	0	246	5	0
17	y	215	0	246	5	0
18	X	287	0	317	3	0
18	x	281	0	312	2	0
19	Z	479	0	516	5	0
19	z	479	0	516	8	0
20	R	239	0	262	4	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	4	0	0	0	0
22	U	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	a	4	0	0	0	0
22	v	1	0	0	1	0
23	A	8	0	0	0	0
23	a	8	0	0	0	0
24	A	260	0	288	11	0
24	B	1040	0	1152	36	0
24	C	845	0	936	30	0
24	D	130	0	144	4	0
24	a	195	0	216	9	0
24	b	1040	0	1152	28	0
24	c	845	0	936	35	0
24	d	195	0	216	9	0
25	A	192	0	222	6	0
25	a	192	0	222	3	0
26	A	40	0	56	1	0
26	B	120	0	168	11	0
26	C	80	0	112	11	0
26	D	40	0	56	1	0
26	H	40	0	56	3	0
26	K	40	0	56	0	0
26	T	40	0	56	5	0
26	Y	40	0	56	4	0
26	a	40	0	56	1	0
26	b	120	0	168	10	0
26	c	80	0	112	5	0
26	d	40	0	56	3	0
26	h	40	0	56	4	0
26	k	40	0	56	1	0
26	t	40	0	56	5	0
26	y	40	0	56	2	0
27	A	108	0	156	7	0
27	B	54	0	78	3	0
27	F	43	0	53	2	0
27	L	54	0	78	3	0
27	a	108	0	156	3	0
27	f	43	0	53	1	1
28	A	24	0	32	1	0
28	B	42	0	56	1	0
28	C	12	0	16	0	0
28	O	6	0	8	0	0
28	T	12	0	16	3	0
28	V	24	0	32	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	a	18	0	23	2	0
28	b	30	0	40	0	0
28	c	12	0	16	2	0
28	o	6	0	8	0	0
28	t	6	0	8	1	0
28	v	18	0	24	1	0
29	A	35	0	46	2	0
29	B	25	0	35	0	0
29	C	35	0	46	1	0
29	D	35	0	46	1	0
29	F	35	0	46	0	0
29	M	70	0	92	4	0
29	T	25	0	35	0	0
29	a	70	0	92	2	0
29	b	25	0	35	3	0
29	f	35	0	46	1	0
29	m	70	0	92	3	0
30	A	20	0	0	0	0
30	a	20	0	0	0	0
31	A	110	0	160	9	0
31	D	110	0	160	1	0
31	a	110	0	160	14	0
31	d	110	0	160	0	0
32	A	28	0	0	0	0
32	B	33	0	0	0	0
32	C	34	0	0	0	0
32	D	57	0	0	0	0
32	I	40	0	0	0	0
32	J	10	0	0	0	0
32	M	10	0	0	0	0
32	X	18	0	0	0	0
32	a	30	0	0	0	0
32	b	33	0	0	0	0
32	c	32	0	0	0	0
32	d	71	0	0	0	0
32	i	40	0	0	0	0
32	j	10	0	0	0	0
32	m	10	0	0	0	0
33	A	51	0	72	4	0
33	B	51	0	72	1	0
33	C	102	0	144	7	0
33	D	51	0	72	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	Z	37	0	44	1	0
33	b	51	0	72	3	0
33	c	153	0	216	7	0
33	d	51	0	72	2	0
33	z	39	0	48	5	0
34	B	1	0	0	0	0
34	C	1	0	0	0	0
34	F	1	0	0	0	0
34	O	1	0	0	0	0
34	b	1	0	0	0	0
34	c	2	0	0	0	0
34	f	1	0	0	0	0
34	o	1	0	0	0	0
35	B	95	0	130	1	0
35	C	38	0	52	0	0
35	D	16	0	17	2	0
35	V	19	0	26	1	0
35	b	95	0	130	1	0
35	c	38	0	52	1	0
35	d	16	0	17	3	0
36	C	186	0	246	4	0
36	D	52	0	71	2	0
36	H	62	0	82	0	0
36	c	186	0	246	2	0
36	e	62	0	82	7	0
36	h	62	0	82	0	0
37	D	147	0	222	11	0
37	E	42	0	57	2	0
37	L	49	0	74	0	0
37	b	49	0	74	3	0
37	d	147	0	222	9	0
37	e	42	0	57	4	0
38	F	43	0	30	2	0
38	e	43	0	30	5	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	179	0	0	1	0
41	B	293	0	0	2	0
41	C	233	0	0	3	0
41	D	151	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	E	33	0	0	0	0
41	F	8	0	0	0	0
41	H	44	0	0	0	0
41	I	5	0	0	1	0
41	J	12	0	0	0	0
41	K	8	0	0	1	0
41	L	19	0	0	0	0
41	M	19	0	0	0	0
41	O	177	0	0	2	0
41	T	17	0	0	1	0
41	U	82	0	0	2	0
41	V	115	0	0	1	0
41	X	8	0	0	0	0
41	Y	5	0	0	0	0
41	Z	1	0	0	0	0
41	a	167	0	0	2	0
41	b	262	0	0	4	0
41	c	207	0	0	1	0
41	d	137	0	0	2	0
41	e	16	0	0	0	0
41	f	7	0	0	0	0
41	h	42	0	0	0	0
41	i	5	0	0	0	0
41	j	7	0	0	0	0
41	k	7	0	0	0	0
41	l	9	0	0	1	0
41	m	16	0	0	0	0
41	o	157	0	0	2	0
41	t	11	0	0	0	0
41	u	93	0	0	0	0
41	v	82	0	0	1	0
41	x	6	0	0	0	0
41	y	2	0	0	0	0
All	All	55631	0	54162	559	1

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

All (559) 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:214[B]:MET:HG2	31:A:419[B]:PL9:H102	1.48	0.93
1:A:214[A]:MET:HG2	31:A:419[A]:PL9:H102	1.50	0.93
24:B:616:CLA:H71	24:B:617:CLA:H192	1.52	0.92
24:c:518:CLA:HHC	24:c:518:CLA:HBB1	1.56	0.87
24:c:506:CLA:H202	24:c:512:CLA:HBB1	1.61	0.82
24:C:503:CLA:HBB1	24:C:512:CLA:H41	1.62	0.81
41:B:954:HOH:O	22:U:201:CL:CL	2.34	0.81
4:d:192:THR:HG23	24:d:402:CLA:HBC2	1.67	0.77
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.67	0.76
24:D:403:CLA:H171	18:X:15:LEU:HD13	1.68	0.75
33:b:629:LMG:H421	37:b:634:LHG:H371	1.69	0.75
1:a:298:ASN:ND2	41:a:501[A]:HOH:O	2.19	0.74
16:v:71:GLY:HA2	28:v:201:GOL:H31	1.68	0.74
24:C:505:CLA:CMD	24:C:507:CLA:HAB	2.18	0.74
24:b:624:CLA:HHC	24:b:624:CLA:HBB1	1.68	0.73
1:a:214[A]:MET:HG2	31:a:415[A]:PL9:H102	1.68	0.73
2:B:341:LYS:HA	2:B:405[A]:GLU:HG2	1.73	0.71
24:b:624:CLA:H2	24:b:625:CLA:HBB2	1.72	0.71
24:c:508:CLA:HHC	24:c:508:CLA:HBB1	1.72	0.71
24:a:410:CLA:H203	33:d:413:LMG:H412	1.73	0.70
31:A:419[B]:PL9:H261	37:E:101:LHG:H223	1.74	0.70
24:B:615:CLA:H18	33:B:622:LMG:H421	1.73	0.70
12:m:6:LEU:HD11	29:m:103:LMT:H11	1.73	0.70
1:a:215[B]:HIS:ND1	31:a:415[B]:PL9:O1	2.24	0.69
27:a:414:SQD:H271	37:d:408:LHG:H141	1.74	0.69
41:b:899:HOH:O	22:v:204:CL:CL	2.48	0.69
1:a:214[B]:MET:HG2	31:a:415[B]:PL9:H102	1.73	0.68
33:c:523:LMG:H181	10:k:27:VAL:HG11	1.75	0.68
15:U:51:LYS:NZ	41:U:301:HOH:O	2.27	0.66
31:A:419[A]:PL9:H261	37:E:101:LHG:H223	1.77	0.66
1:A:298:ASN:ND2	41:A:501[A]:HOH:O	2.29	0.65
24:C:506:CLA:HMC2	24:C:507:CLA:H102	1.78	0.65
37:D:409:LHG:H132	37:D:409:LHG:H372	1.79	0.65
3:C:286:ALA:HB2	24:C:502:CLA:HMD1	1.78	0.64
2:B:248:ALA:HA	24:B:604:CLA:H42	1.78	0.64
1:a:215[A]:HIS:ND1	31:a:415[A]:PL9:O1	2.28	0.64
2:B:124:ARG:O	7:H:12[A]:ARG:NH1	2.29	0.64
24:C:513:CLA:H171	26:C:514:BCR:H373	1.80	0.63
15:U:16:LYS:NZ	41:U:302:HOH:O	2.29	0.63
24:B:617:CLA:HED2	24:B:617:CLA:H43	1.81	0.63
31:a:415[B]:PL9:H28	37:e:102:LHG:H222	1.80	0.63
10:k:11:LEU:HD11	10:k:22:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:25[A]:GLU:HG3	28:T:101:GOL:H2	1.82	0.62
26:t:101:BCR:H321	26:t:101:BCR:HC8	1.79	0.62
24:C:513:CLA:HBB1	26:C:514:BCR:H24C	1.82	0.61
24:C:505:CLA:HMD3	24:C:507:CLA:HAB	1.82	0.61
26:B:619:BCR:H363	26:t:101:BCR:H19C	1.82	0.60
4:D:103:ARG:NH1	4:D:106:GLN:OE1	2.34	0.60
27:A:412:SQD:H251	37:D:409:LHG:H131	1.84	0.60
37:D:409:LHG:H112	37:D:409:LHG:H382	1.84	0.60
5:E:40:THR:HB	20:R:4:ARG:HG2	1.84	0.60
24:C:513:CLA:H202	33:C:520:LMG:H402	1.82	0.60
26:T:103:BCR:H321	26:T:103:BCR:HC8	1.82	0.60
12:M:33:GLN:HB2	12:m:33:GLN:HB2	1.84	0.59
8:I:37:LEU:O	41:I:201:HOH:O	2.16	0.59
1:A:72:LEU:HD13	29:A:417:LMT:H11	1.85	0.59
4:D:192:THR:HG23	24:D:402:CLA:HBC2	1.83	0.59
24:C:510:CLA:H43	37:D:409:LHG:H383	1.85	0.59
3:c:279:LEU:HD22	24:c:514:CLA:HED2	1.85	0.59
3:C:48:LYS:HG3	3:C:138:GLU:HG3	1.84	0.58
1:a:271:LEU:HD11	31:a:415[B]:PL9:HC8	1.85	0.58
24:c:517:CLA:O2D	24:c:518:CLA:HBB2	2.03	0.58
6:F:21:VAL:O	6:F:25:THR:HG23	2.04	0.58
11:L:13:ASN:ND2	11:L:16:SER:H	2.01	0.57
29:C:521:LMT:O3B	41:C:601:HOH:O	2.17	0.57
4:D:157:PHE:CE2	4:D:171:PRO:HG2	2.39	0.57
3:c:213[A]:LEU:HG	24:c:511:CLA:H202	1.86	0.57
24:c:509:CLA:H201	37:d:408:LHG:H352	1.86	0.57
2:B:171:PRO:HD3	7:H:66:GLY:HA2	1.87	0.57
2:b:248:ALA:HA	24:b:612:CLA:H42	1.86	0.57
28:a:420:GOL:H11	16:v:27:LEU:HD21	1.85	0.57
4:D:102:THR:OG1	36:D:406:DGD:HG31	2.04	0.57
2:B:472:ARG:NH2	41:B:703:HOH:O	2.30	0.56
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.87	0.56
24:C:513:CLA:HBB1	26:C:514:BCR:H371	1.86	0.56
1:a:271:LEU:HD11	31:a:415[A]:PL9:HC8	1.86	0.56
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.40	0.56
3:c:377:LEU:HG	3:c:381:LYS:HE3	1.87	0.56
26:y:101:BCR:H321	26:y:101:BCR:HC8	1.87	0.56
1:a:307[B]:ILE:HG22	1:a:313:VAL:HA	1.86	0.56
17:Y:28:ILE:HG23	26:Y:101:BCR:H10C	1.88	0.55
2:B:50:PRO:HB2	28:B:630:GOL:H12	1.88	0.55
24:b:610:CLA:H193	26:h:101:BCR:H353	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:35:TYR:OH	41:v:301:HOH:O	2.15	0.55
31:A:419[B]:PL9:H512	27:F:103:SQD:H301	1.88	0.55
24:c:518:CLA:H171	26:c:528:BCR:H373	1.89	0.55
25:A:409[A]:PHO:HBC3	4:D:279:LEU:HD22	1.89	0.55
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.89	0.55
3:c:320:ARG:HB2	28:c:503:GOL:H32	1.89	0.55
24:b:614:CLA:HHC	24:b:614:CLA:HBB1	1.87	0.55
24:b:622:CLA:H18	37:d:406:LHG:H202	1.88	0.55
5:e:9:PRO:HA	37:e:102:LHG:HC31	1.89	0.55
36:e:101:DGD:HAW1	27:f:101:SQD:H382	1.89	0.55
24:B:602:CLA:H91	26:H:101:BCR:H21C	1.88	0.54
2:B:216:HIS:HE1	24:B:610:CLA:C1A	2.20	0.54
1:A:257:ARG:NH2	2:B:492:GLU:O	2.40	0.54
31:a:415[A]:PL9:H28	37:e:102:LHG:H222	1.88	0.54
16:V:26:TYR:O	41:V:301:HOH:O	2.19	0.54
24:c:513:CLA:H201	33:c:523:LMG:H232	1.88	0.54
31:a:415[A]:PL9:HC2	31:a:415[A]:PL9:H103	1.90	0.54
27:A:412:SQD:H192	37:D:409:LHG:H201	1.89	0.54
2:B:12:LEU:HB2	24:B:613:CLA:HMC2	1.90	0.54
3:C:443:TRP:CZ2	24:C:508:CLA:HMD1	2.43	0.54
24:b:624:CLA:H2	24:b:625:CLA:CBB	2.36	0.53
24:c:513:CLA:H191	33:c:523:LMG:H232	1.89	0.53
24:c:506:CLA:C4D	24:c:508:CLA:H2	2.38	0.53
24:C:502:CLA:H61	24:C:512:CLA:H42	1.90	0.53
2:B:338:GLN:HA	13:o:57:LYS:HE3	1.89	0.53
36:D:406:DGD:O1B	36:D:406:DGD:O2D	2.26	0.53
11:L:13:ASN:C	11:L:13:ASN:HD22	2.17	0.53
33:c:501:LMG:H242	24:c:510:CLA:H92	1.91	0.53
24:c:513:CLA:HBC3	24:c:515:CLA:H71	1.90	0.53
29:f:102:LMT:O3'	29:f:102:LMT:O2B	2.24	0.53
31:a:415[B]:PL9:HC2	31:a:415[B]:PL9:H103	1.91	0.53
28:A:414:GOL:H11	12:M:1:FME:HG2	1.90	0.53
37:D:409:LHG:H352	37:D:409:LHG:H151	1.91	0.53
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.43	0.53
1:A:50:ILE:HG12	29:A:417:LMT:H102	1.89	0.53
3:C:42:LEU:HD21	24:C:511:CLA:H2A	1.91	0.53
24:c:507:CLA:H61	24:c:517:CLA:H42	1.90	0.52
25:A:408:PHO:HAB	4:D:205:LEU:HD13	1.91	0.52
20:R:2:ASP:HB3	20:R:5:VAL:HG23	1.91	0.52
2:B:30:VAL:HG12	24:B:606:CLA:HHD	1.91	0.52
36:e:101:DGD:HE3	36:e:101:DGD:HD4	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:179[A]:GLU:OE2	41:o:402:HOH:O	2.19	0.52
1:a:183:MET:HA	24:a:409:CLA:HMD1	1.92	0.52
28:c:503:GOL:H2	41:c:734:HOH:O	2.08	0.52
1:A:63:ILE:HB	3:C:335:THR:HG21	1.91	0.52
1:a:227:THR:HB	1:a:231:GLU:HG3	1.91	0.52
33:b:629:LMG:O2	41:b:701:HOH:O	2.19	0.52
1:A:183:MET:HA	24:A:405:CLA:HMD1	1.91	0.52
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.10	0.52
3:c:38:GLY:HA3	24:c:516:CLA:HMD2	1.90	0.52
24:C:501:CLA:C4D	24:C:503:CLA:H2	2.40	0.52
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.44	0.52
13:O:27:ARG:NH1	13:O:202:ALA:O	2.42	0.52
28:T:102:GOL:H12	29:m:103:LMT:H12	1.91	0.52
24:B:607:CLA:H191	26:B:620:BCR:H363	1.92	0.52
11:L:13:ASN:HD22	11:L:16:SER:H	1.58	0.51
1:a:162:PRO:HB3	1:a:168[B]:PHE:HA	1.93	0.51
24:b:619:CLA:OBD	24:b:619:CLA:H152	2.10	0.51
19:z:47:TRP:CE2	33:z:101:LMG:H241	2.45	0.51
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.92	0.51
3:C:149:TYR:HB2	3:C:157:MET:HE1	1.92	0.51
10:K:15:TYR:OH	19:Z:58:ASN:ND2	2.38	0.51
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.46	0.51
3:c:286:ALA:HB2	24:c:507:CLA:HMD1	1.92	0.51
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.46	0.51
16:v:95:LEU:HD11	16:v:112:LEU:HD11	1.92	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.46	0.51
25:A:409[A]:PHO:HMA2	31:A:419[A]:PL9:H221	1.93	0.51
3:C:438:LEU:HD11	24:C:505:CLA:HBB1	1.91	0.51
4:D:343:GLU:O	41:D:547[B]:HOH:O	2.19	0.51
24:a:410:CLA:H13	33:d:413:LMG:H242	1.93	0.51
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.92	0.51
24:C:511:CLA:H41	17:Y:39:LEU:HD13	1.93	0.51
29:M:101:LMT:H6D	11:l:9:PRO:HA	1.93	0.50
28:T:102:GOL:O1	41:T:201:HOH:O	2.19	0.50
2:b:498:LYS:HA	4:d:24:ARG:HA	1.94	0.50
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.44	0.50
24:B:616:CLA:H2	24:B:617:CLA:HBB2	1.92	0.50
24:A:410:CLA:H92	8:I:13:THR:HG23	1.94	0.50
24:b:613:CLA:H43	24:b:614:CLA:H2	1.92	0.50
3:C:406:SER:HA	3:C:420:VAL:HG23	1.94	0.50
1:a:214[A]:MET:HE2	1:a:255:PHE:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:214[B]:MET:HE2	1:a:255:PHE:CE1	2.47	0.50
24:c:518:CLA:HBB1	24:c:518:CLA:CHC	2.37	0.50
37:d:408:LHG:H342	37:d:408:LHG:H151	1.93	0.50
2:B:138:MET:HE3	24:B:616:CLA:CHD	2.41	0.50
2:B:195:PRO:HD2	7:H:65:LEU:HD11	1.93	0.50
24:A:410:CLA:H193	24:C:506:CLA:H93	1.93	0.50
3:C:334:PRO:HA	13:O:153:THR:OG1	2.12	0.50
24:b:622:CLA:HBB1	24:b:622:CLA:HMB1	1.93	0.50
25:A:409[B]:PHO:HBC3	4:D:279:LEU:HD22	1.93	0.49
2:B:405[B]:GLU:OE1	13:o:60:ARG:HD3	2.12	0.49
2:b:216:HIS:HE1	24:b:618:CLA:C1A	2.25	0.49
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.10	0.49
1:a:267[B]:ASN:HB3	1:a:270[B]:SER:OG	2.12	0.49
35:d:411:HTG:H1	7:h:25:TRP:CD1	2.47	0.49
33:D:413:LMG:H292	33:D:413:LMG:H152	1.95	0.49
2:b:224:ARG:HH11	29:b:630:LMT:H1'	1.77	0.49
12:M:20:VAL:HG22	12:m:20:VAL:HG11	1.94	0.49
33:A:421:LMG:C25	24:C:505:CLA:HBB2	2.42	0.49
33:C:519:LMG:H161	33:C:519:LMG:H292	1.94	0.49
29:a:419:LMT:O4'	41:a:502:HOH:O	2.20	0.49
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.93	0.49
13:O:180:GLU:CD	13:O:180:GLU:H	2.20	0.49
1:a:84:PRO:HA	1:a:112:TYR:CG	2.48	0.49
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.95	0.49
1:a:121[A]:LEU:HD11	24:c:510:CLA:H152	1.95	0.49
8:i:36:ASP:OD1	8:i:36:ASP:N	2.40	0.49
13:o:74[B]:GLU:OE1	41:o:401:HOH:O	2.18	0.49
19:z:26:ALA:HB1	19:z:36:SER:HB3	1.95	0.49
2:B:224:ARG:NH1	4:D:16:ASP:OD2	2.45	0.49
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.93	0.49
4:d:101:PHE:HB3	36:e:101:DGD:HG2	1.94	0.49
29:M:101:LMT:H6'2	11:l:9:PRO:HB3	1.93	0.49
33:c:524:LMG:H391	33:c:524:LMG:H232	1.95	0.48
12:M:27:VAL:HG12	12:m:28:GLN:HB3	1.95	0.48
24:b:620:CLA:H71	37:b:634:LHG:H311	1.96	0.48
3:c:443:TRP:CZ2	24:c:513:CLA:HMD1	2.48	0.48
1:a:72:LEU:HD11	29:a:404:LMT:H52	1.96	0.48
28:a:402:GOL:H2	5:e:63[A]:ILE:HD11	1.96	0.48
3:C:25:ASN:O	3:C:41:ARG:HD3	2.14	0.48
13:o:37:THR:HG22	13:o:246:ALA:HB3	1.95	0.48
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:409[B]:PHO:HMA2	31:A:419[B]:PL9:H221	1.96	0.48
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.95	0.48
26:T:103:BCR:H331	26:T:103:BCR:HC7	1.63	0.48
1:a:221[B]:SER:HB2	4:d:139:ARG:O	2.13	0.48
4:d:14:TRP:CD1	35:d:411:HTG:H61	2.49	0.48
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.94	0.47
24:B:611:CLA:HHC	24:B:611:CLA:HBB1	1.96	0.47
8:i:17:LEU:HD22	8:i:21:PHE:HE2	1.78	0.47
27:L:102:SQD:H1	27:L:102:SQD:H462	1.96	0.47
2:b:98:LEU:HB2	35:b:601:HTG:H7'1	1.97	0.47
3:c:223:TRP:CG	3:c:224:ILE:H	2.33	0.47
4:d:139:ARG:NH2	41:d:505:HOH:O	2.47	0.47
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.96	0.47
27:A:412:SQD:O7	3:C:28:GLN:NE2	2.46	0.47
31:a:415[A]:PL9:H221	31:a:415[A]:PL9:H201	1.68	0.47
24:b:619:CLA:HHC	24:b:619:CLA:HBB1	1.97	0.47
13:o:53:LYS:HE3	13:o:65:PHE:CE1	2.48	0.47
36:c:521:DGD:HB61	36:c:521:DGD:HB32	1.66	0.47
24:a:410:CLA:HMB2	24:d:402:CLA:H122	1.96	0.47
2:B:36[A]:SER:OG	26:B:619:BCR:H362	2.14	0.47
17:Y:32:GLY:HA3	26:Y:101:BCR:C15	2.45	0.47
10:k:10:LYS:HD2	10:k:10:LYS:N	2.30	0.47
24:c:513:CLA:H122	24:c:513:CLA:H162	1.64	0.47
5:e:26:THR:HB	38:e:103:HEM:HAB	1.96	0.47
3:C:223:TRP:CG	3:C:224:ILE:H	2.33	0.47
18:X:29:ILE:O	18:X:33:GLN:HG2	2.15	0.47
2:B:162:PHE:O	24:B:607:CLA:HHD	2.15	0.47
1:a:217[B]:SER:O	1:a:221[B]:SER:HB3	2.15	0.47
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.96	0.46
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.50	0.46
26:B:618:BCR:H383	27:B:621:SQD:H101	1.96	0.46
2:b:158:LEU:HB3	2:b:199:VAL:HG22	1.96	0.46
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.96	0.46
3:c:213[B]:LEU:HD11	26:c:519:BCR:H373	1.97	0.46
26:d:404:BCR:H313	36:e:101:DGD:HA91	1.96	0.46
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.97	0.46
24:B:614:CLA:HBB1	24:B:614:CLA:HMB1	1.97	0.46
26:C:514:BCR:H20C	26:C:514:BCR:H361	1.82	0.46
27:L:102:SQD:H101	26:b:626:BCR:H383	1.97	0.46
26:b:626:BCR:H12C	33:b:629:LMG:C43	2.46	0.46
37:d:408:LHG:H331	37:d:408:LHG:H361	1.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:t:101:BCR:H23C	26:t:101:BCR:H382	1.96	0.46
3:c:334:PRO:HA	13:o:153:THR:OG1	2.15	0.46
26:h:101:BCR:H331	26:h:101:BCR:C8	2.45	0.46
10:k:28:ILE:HD11	17:y:28:ILE:HD13	1.98	0.46
19:Z:7:LEU:HD23	19:Z:7:LEU:HA	1.85	0.46
1:a:162:PRO:HB3	1:a:168[A]:PHE:HA	1.97	0.46
24:c:511:CLA:HMC2	24:c:512:CLA:H102	1.98	0.46
2:B:76[B]:SER:HB2	35:B:623:HTG:HO6	1.81	0.46
3:C:213:LEU:HD21	26:C:515:BCR:C20	2.46	0.46
2:b:464:PHE:CZ	37:d:406:LHG:H252	2.50	0.46
26:t:101:BCR:H331	26:t:101:BCR:HC7	1.52	0.46
17:y:23:THR:O	17:y:27:MET:HG3	2.15	0.46
1:A:221[B]:SER:HB2	4:D:139:ARG:O	2.15	0.46
24:B:616:CLA:H112	24:B:616:CLA:H152	1.48	0.46
26:y:101:BCR:H15C	26:y:101:BCR:H351	1.84	0.46
24:B:607:CLA:H151	24:B:617:CLA:H122	1.98	0.45
24:A:410:CLA:H72	24:A:410:CLA:H112	1.75	0.45
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.51	0.45
24:B:603:CLA:H111	24:B:603:CLA:H151	1.79	0.45
10:K:25:LEU:HD22	26:Y:101:BCR:H332	1.98	0.45
37:d:408:LHG:H122	37:d:408:LHG:H381	1.98	0.45
7:h:38:PHE:HB2	26:h:101:BCR:C10	2.46	0.45
27:A:416:SQD:H272	2:b:109:LEU:HD13	1.98	0.45
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.50	0.45
4:D:16:ASP:OD2	29:D:401:LMT:O6'	2.34	0.45
10:K:11:LEU:HD11	10:K:22:VAL:HG21	1.98	0.45
2:b:299:GLU:HG3	41:b:911:HOH:O	2.16	0.45
6:F:27:ALA:HB1	38:F:102:HEM:HAC	1.98	0.45
24:b:610:CLA:H93	24:b:610:CLA:H111	1.73	0.45
24:A:405:CLA:CBD	24:A:406:CLA:HAC2	2.47	0.45
26:B:620:BCR:H331	26:B:620:BCR:C8	2.45	0.45
26:k:101:BCR:H371	26:k:101:BCR:H24C	1.62	0.45
25:A:409[A]:PHO:HMC2	4:D:279:LEU:HD21	1.98	0.45
3:C:185:LEU:HB2	3:C:230:LEU:HD13	1.99	0.45
3:C:279:LEU:HD22	24:C:509:CLA:HED2	1.98	0.45
33:C:519:LMG:H212	33:C:519:LMG:H331	1.97	0.45
24:c:513:CLA:H203	24:c:513:CLA:H161	1.78	0.45
20:R:6:LEU:O	20:R:10:LEU:HB2	2.17	0.45
2:b:224:ARG:NH1	29:b:630:LMT:H1'	2.32	0.45
24:c:518:CLA:H202	33:c:524:LMG:H402	1.98	0.45
24:A:407:CLA:HED1	36:C:518:DGD:HAE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:412:SQD:H122	27:A:412:SQD:H152	1.66	0.45
10:k:24:VAL:HG13	17:y:25:ILE:HD13	1.98	0.45
2:b:224:ARG:HG3	7:h:24:GLY:O	2.17	0.45
24:b:614:CLA:H62	24:b:614:CLA:H41	1.85	0.45
26:b:626:BCR:H15C	26:b:626:BCR:H351	1.86	0.45
24:c:514:CLA:H142	24:c:514:CLA:H112	1.78	0.45
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.99	0.45
1:a:12:ASN:O	1:a:16:ARG:HG3	2.17	0.44
24:d:403:CLA:H162	7:h:33:VAL:HG13	1.98	0.44
19:z:37:LYS:HZ2	33:z:101:LMG:HC4	1.82	0.44
2:B:499:VAL:HG12	4:D:135:LEU:HB3	2.00	0.44
3:C:35:TRP:CD1	10:K:45:PHE:HB3	2.52	0.44
26:H:101:BCR:H371	26:H:101:BCR:H24C	1.67	0.44
2:b:493:TRP:CD1	5:e:5:THR:HG22	2.52	0.44
26:d:404:BCR:H313	36:e:101:DGD:HAE1	1.99	0.44
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.53	0.44
24:B:615:CLA:H62	24:B:615:CLA:H41	1.72	0.44
24:C:513:CLA:CBB	26:C:514:BCR:H24C	2.46	0.44
36:C:517:DGD:HB51	33:C:519:LMG:H392	1.99	0.44
14:T:20:ALA:O	14:T:24:ARG:HB3	2.16	0.44
33:Z:101:LMG:HC8	33:Z:101:LMG:H111	1.63	0.44
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.76	0.44
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.99	0.44
4:D:85:MET:CE	4:D:96:GLU:HG2	2.47	0.44
5:E:26:THR:HB	38:F:102:HEM:HAB	1.99	0.44
1:a:259:ILE:HG22	1:a:260:PHE:CD1	2.52	0.44
26:b:626:BCR:H24C	26:b:626:BCR:H371	1.79	0.44
3:c:127:PHE:CE1	33:z:101:LMG:H152	2.52	0.44
24:c:510:CLA:HHC	24:c:510:CLA:HBB1	1.99	0.44
24:B:604:CLA:H3A	24:B:604:CLA:CGA	2.47	0.44
12:M:34:LYS:HG2	29:M:101:LMT:O3B	2.17	0.44
13:O:53:LYS:HE2	13:O:63:ALA:HB3	1.98	0.44
26:Y:101:BCR:H321	26:Y:101:BCR:HC8	1.98	0.44
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.53	0.44
26:b:628:BCR:H331	26:b:628:BCR:C8	2.47	0.44
26:T:103:BCR:H382	26:T:103:BCR:H23C	1.99	0.44
31:A:419[A]:PL9:H421	31:A:419[A]:PL9:H401	1.79	0.44
31:A:419[A]:PL9:H512	27:F:103:SQD:H301	1.98	0.44
3:C:262:ARG:HG2	8:I:38:GLU:HG2	1.98	0.44
8:I:2:GLU:O	8:I:6:ILE:HG12	2.17	0.44
24:a:409:CLA:H192	24:a:409:CLA:H161	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:256:MET:HA	2:b:263:THR:HG21	1.99	0.44
2:b:461:LEU:HD21	4:d:284:ILE:HD11	1.98	0.44
24:b:620:CLA:H142	37:b:634:LHG:H361	2.00	0.44
2:B:423:LYS:HE2	41:O:421:HOH:O	2.18	0.44
26:C:515:BCR:H11C	26:C:515:BCR:H341	1.87	0.44
4:D:269:PHE:CD2	37:D:407:LHG:HC11	2.53	0.44
3:c:245:ILE:O	3:c:249:ILE:HG13	2.18	0.44
36:e:101:DGD:HG2	36:e:101:DGD:HB21	1.84	0.44
35:D:412:HTG:H1'2	7:H:25:TRP:CD2	2.53	0.44
26:H:101:BCR:H331	26:H:101:BCR:C8	2.47	0.44
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	1.99	0.44
24:a:409:CLA:CBD	24:d:401:CLA:HAC2	2.48	0.44
25:a:418[A]:PHO:ND	25:a:418[A]:PHO:NC	2.66	0.44
26:c:519:BCR:H24C	26:c:519:BCR:H371	1.86	0.44
37:e:102:LHG:H171	37:e:102:LHG:H201	1.88	0.44
26:T:103:BCR:H19C	26:b:627:BCR:H363	1.99	0.43
24:c:510:CLA:HAA1	24:c:510:CLA:HBD	2.00	0.43
10:k:12:PRO:HB2	10:k:15:TYR:HD2	1.83	0.43
13:o:40:ILE:HD12	13:o:95:PHE:CD1	2.53	0.43
27:B:621:SQD:O8	11:L:7:ARG:HD3	2.18	0.43
26:C:515:BCR:H371	26:C:515:BCR:H24C	1.74	0.43
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.53	0.43
2:b:70:GLY:HA2	2:b:178:VAL:HG21	2.01	0.43
3:c:79:LYS:HD2	16:v:35:TYR:CE1	2.53	0.43
13:o:121:THR:OG1	13:o:123:LYS:HG3	2.17	0.43
8:I:33:LYS:HB3	8:I:34:ARG:H	1.55	0.43
2:b:62:VAL:HB	24:b:614:CLA:HED3	1.99	0.43
24:c:507:CLA:H193	35:c:525:HTG:H4'2	2.01	0.43
3:C:97:TRP:NE1	33:C:520:LMG:H131	2.33	0.43
31:a:415[B]:PL9:H171	31:a:415[B]:PL9:H151	1.70	0.43
2:b:227:LYS:NZ	29:b:630:LMT:O6'	2.51	0.43
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.83	0.43
3:c:348:GLU:OE1	13:o:11:VAL:HA	2.18	0.43
24:d:401:CLA:H162	24:d:401:CLA:H203	1.73	0.43
24:C:505:CLA:HAA1	24:C:505:CLA:HBD	2.00	0.43
31:a:415[A]:PL9:H171	31:a:415[A]:PL9:H151	1.75	0.43
25:a:418[A]:PHO:HBC3	4:d:279:LEU:HD22	2.00	0.43
2:b:231:MET:HE2	24:b:619:CLA:HMC2	2.00	0.43
3:c:175:LEU:HD23	3:c:237:HIS:CG	2.54	0.43
3:c:437:PHE:CE1	24:c:515:CLA:HMB2	2.54	0.43
24:B:615:CLA:H92	24:B:615:CLA:H61	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:616:CLA:H172	24:B:616:CLA:H13	1.85	0.43
27:B:621:SQD:H462	27:B:621:SQD:H1	2.00	0.43
1:a:131:TRP:CH2	24:c:510:CLA:HAA2	2.53	0.43
24:b:622:CLA:H72	24:b:622:CLA:H111	1.81	0.43
4:d:51:GLY:HA3	4:d:78:VAL:HG22	1.99	0.43
37:d:408:LHG:H251	37:d:408:LHG:H281	1.77	0.43
14:t:2:GLU:H	14:t:2:GLU:CD	2.26	0.43
19:z:37:LYS:NZ	33:z:101:LMG:HC4	2.33	0.43
3:C:437:PHE:CZ	24:C:510:CLA:HMB2	2.54	0.43
1:a:46:ILE:HD13	27:a:405:SQD:H371	2.00	0.43
1:a:215[B]:HIS:HA	31:a:415[B]:PL9:HC71	2.00	0.43
24:b:612:CLA:H3A	24:b:612:CLA:CGA	2.49	0.43
3:c:179:ALA:O	3:c:184:GLY:HA2	2.19	0.43
2:b:36:SER:OG	26:b:627:BCR:H362	2.18	0.43
2:B:223:GLN:NE2	2:B:227:LYS:HD3	2.34	0.43
33:C:519:LMG:H201	10:K:27:VAL:HG11	2.00	0.43
26:T:103:BCR:H11C	26:T:103:BCR:H341	1.81	0.43
24:a:412:CLA:H102	24:a:412:CLA:H61	1.65	0.43
2:b:30:VAL:HG12	24:b:614:CLA:HHD	2.00	0.43
2:b:233:ASN:O	2:b:236:THR:HG22	2.19	0.43
12:m:28:GLN:O	12:m:32:GLN:HG3	2.19	0.43
24:A:406:CLA:H203	24:A:406:CLA:H162	1.63	0.42
2:B:227:LYS:HE2	2:B:227:LYS:HB3	1.86	0.42
13:O:42:ARG:O	13:O:241:ALA:HA	2.19	0.42
2:b:487:SER:HA	2:b:488:PRO:HD3	1.79	0.42
24:b:614:CLA:HAA1	24:b:614:CLA:HBD	1.99	0.42
4:d:85:MET:HE1	4:d:96:GLU:HG2	2.01	0.42
3:C:337:LEU:HD22	3:C:342:MET:HE3	2.01	0.42
24:C:503:CLA:CBB	24:C:512:CLA:H41	2.41	0.42
16:V:12:LEU:HD12	16:V:69:ILE:HB	2.01	0.42
24:c:514:CLA:HBB1	24:c:514:CLA:HMB1	2.01	0.42
4:d:85:MET:CE	4:d:96:GLU:HG2	2.49	0.42
2:B:102:VAL:HA	26:B:619:BCR:C40	2.49	0.42
24:B:614:CLA:H162	24:B:614:CLA:H121	1.75	0.42
3:C:338:GLY:HA3	3:C:341:LEU:O	2.19	0.42
24:D:402:CLA:HAA2	24:D:402:CLA:HBD	2.01	0.42
13:O:57:LYS:NZ	2:b:49:ASP:OD1	2.48	0.42
24:a:409:CLA:HAA2	24:a:409:CLA:HBD	2.01	0.42
25:a:418[B]:PHO:NC	25:a:418[B]:PHO:ND	2.67	0.42
2:b:58:GLN:C	2:b:329:PRO:HB3	2.45	0.42
3:c:217:PRO:HB2	36:c:520:DGD:HA21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:401:CLA:HBA1	24:d:401:CLA:C4A	2.49	0.42
3:C:250:TRP:CZ3	3:C:254:THR:HG21	2.54	0.42
37:D:409:LHG:H272	37:D:409:LHG:H242	1.67	0.42
3:c:26:ARG:NH2	17:y:46:LEU:OXT	2.47	0.42
3:c:79:LYS:HD2	16:v:35:TYR:HE1	1.84	0.42
2:B:160:GLY:HA3	2:B:180:PRO:HB3	2.01	0.42
2:B:422:ARG:O	2:B:425:ILE:HG12	2.20	0.42
24:B:603:CLA:H41	7:H:46:LEU:HA	2.01	0.42
24:B:606:CLA:HAA1	24:B:606:CLA:HBD	2.01	0.42
3:C:203:THR:O	3:C:235:GLY:HA3	2.19	0.42
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.01	0.42
3:c:95:LEU:HD21	24:c:506:CLA:OBD	2.18	0.42
5:e:13:ILE:HG21	38:e:103:HEM:HAD2	2.01	0.42
5:e:60:GLN:HG2	5:e:61:ARG:N	2.34	0.42
24:B:607:CLA:C19	26:B:620:BCR:H16C	2.50	0.42
24:B:612:CLA:H192	24:B:612:CLA:H161	1.84	0.42
26:B:620:BCR:H15C	26:B:620:BCR:H351	1.83	0.42
19:Z:29:SER:HA	19:Z:30:PRO:HD3	1.87	0.42
24:b:620:CLA:HMA3	24:b:621:CLA:HMC2	2.02	0.42
26:c:528:BCR:H11C	26:c:528:BCR:H341	1.82	0.42
24:A:406:CLA:C4A	24:A:406:CLA:HBA1	2.50	0.42
24:B:617:CLA:H92	24:B:617:CLA:H61	1.87	0.42
3:c:406:SER:HA	3:c:420:VAL:HG23	2.01	0.42
4:d:49:LEU:HD13	26:d:404:BCR:C15	2.50	0.42
12:m:27:VAL:HG13	29:m:102:LMT:H11	2.01	0.42
1:A:214[A]:MET:HE2	1:A:255:PHE:CE1	2.55	0.42
3:C:156:LYS:HE3	41:C:771:HOH:O	2.19	0.42
24:C:509:CLA:H141	24:C:509:CLA:H161	1.86	0.42
33:C:520:LMG:H381	33:C:520:LMG:H411	1.83	0.42
27:a:414:SQD:H202	27:a:414:SQD:H171	1.90	0.42
24:d:401:CLA:HMB1	24:d:401:CLA:HBB1	2.01	0.42
24:d:402:CLA:HAA2	24:d:402:CLA:HBD	2.02	0.42
11:l:2:GLU:HB2	41:l:108:HOH:O	2.20	0.42
27:A:412:SQD:H291	24:C:508:CLA:H71	2.02	0.42
26:B:618:BCR:H11C	26:B:618:BCR:H341	1.88	0.42
36:C:517:DGD:HA81	36:C:517:DGD:HAE2	1.79	0.42
37:D:408:LHG:H192	14:T:17:PHE:HZ	1.85	0.42
16:V:126:LEU:HB3	16:V:129:LYS:HB2	2.02	0.42
20:R:10:LEU:HB3	20:R:11:PRO:HD3	2.02	0.42
1:a:38:ILE:HB	1:a:39:PRO:HD3	2.01	0.42
4:d:136:VAL:HG12	4:d:138:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:160:TYR:HA	4:d:290:ALA:HB2	2.01	0.42
19:z:29:SER:HA	19:z:30:PRO:HD3	1.85	0.42
1:A:187:GLN:HB2	24:A:405:CLA:HAC2	2.02	0.42
33:A:421:LMG:H242	33:A:421:LMG:H212	1.81	0.42
10:K:10:LYS:N	41:K:202:HOH:O	2.53	0.42
13:O:54:GLU:O	13:O:56:PRO:HD3	2.20	0.42
35:V:206:HTG:H6'2	35:V:206:HTG:H3'2	1.86	0.42
24:b:624:CLA:H91	24:b:624:CLA:H112	1.75	0.42
3:c:225:VAL:HG13	3:c:289:PHE:HA	2.01	0.42
41:d:619:HOH:O	28:t:102:GOL:H12	2.20	0.42
5:e:10:PHE:HE2	38:e:103:HEM:HBD2	1.84	0.42
19:z:15:LEU:O	19:z:19:MET:HG2	2.20	0.42
2:B:216:HIS:CE1	24:B:610:CLA:NA	2.88	0.41
24:B:617:CLA:H112	24:B:617:CLA:H91	1.80	0.41
2:b:405:GLU:OE1	41:b:702:HOH:O	2.21	0.41
24:b:623:CLA:H41	24:b:623:CLA:H62	1.66	0.41
3:c:52:ALA:HB2	24:c:516:CLA:HMA2	2.01	0.41
37:d:407:LHG:HC62	11:l:15:THR:HG23	2.02	0.41
17:y:30:ILE:HA	17:y:30:ILE:HD12	1.84	0.41
2:B:221:PRO:HA	24:B:610:CLA:HED3	2.02	0.41
24:B:609:CLA:HAB	4:D:123:ILE:HG12	2.02	0.41
26:b:628:BCR:H24C	26:b:628:BCR:H371	1.82	0.41
13:o:19:CYS:SG	13:o:46:GLN:HB2	2.59	0.41
1:A:162:PRO:HB3	1:A:168[B]:PHE:HA	2.03	0.41
27:A:412:SQD:H381	9:J:21:ILE:HD11	2.02	0.41
3:C:213:LEU:HD21	26:C:515:BCR:C19	2.50	0.41
13:O:39:ARG:HB2	13:O:246:ALA:HB2	2.01	0.41
13:o:51:LEU:HB3	13:o:65:PHE:HB3	2.01	0.41
24:B:616:CLA:H51	26:B:620:BCR:H341	2.03	0.41
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.88	0.41
24:C:508:CLA:H142	24:C:508:CLA:H111	1.84	0.41
4:D:51:GLY:HA3	4:D:78:VAL:HG22	2.02	0.41
24:a:412:CLA:H111	8:i:16:VAL:HG11	2.03	0.41
38:e:103:HEM:CAC	6:f:27:ALA:HB1	2.51	0.41
13:o:23:ASP:HB3	13:o:25:THR:HG23	2.03	0.41
1:A:309:ALA:HB3	16:V:1:ALA:O	2.21	0.41
33:A:421:LMG:H321	3:C:223:TRP:CD1	2.55	0.41
24:B:608:CLA:C4A	24:B:608:CLA:HBA2	2.51	0.41
26:C:515:BCR:H15C	26:C:515:BCR:H351	1.91	0.41
4:D:125:PHE:O	4:D:128:ARG:HB3	2.19	0.41
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:19:MET:HE3	19:Z:19:MET:HB3	1.98	0.41
19:z:9:LEU:HD13	19:z:54:VAL:HG11	2.02	0.41
26:A:411:BCR:H371	26:A:411:BCR:H24C	1.75	0.41
35:D:412:HTG:H1	7:H:25:TRP:CD1	2.56	0.41
12:M:6:LEU:HD11	29:M:103:LMT:H32	2.01	0.41
26:a:413:BCR:H24C	26:a:413:BCR:H371	1.83	0.41
24:c:507:CLA:H162	24:c:507:CLA:H141	1.86	0.41
13:o:42:ARG:O	13:o:241:ALA:HA	2.21	0.41
1:A:300:PHE:HB3	1:A:302:PHE:CE1	2.55	0.41
24:A:405:CLA:H192	24:A:405:CLA:H161	1.79	0.41
26:b:627:BCR:C8	26:b:627:BCR:H331	2.50	0.41
33:c:501:LMG:H182	33:c:501:LMG:H152	1.86	0.41
24:c:510:CLA:HBC2	26:c:519:BCR:H341	2.03	0.41
24:C:502:CLA:C6	24:C:512:CLA:H42	2.51	0.41
4:D:43:LEU:HD23	4:D:43:LEU:HA	1.88	0.41
5:e:10:PHE:CE2	38:e:103:HEM:HBD2	2.55	0.41
24:A:410:CLA:H162	24:A:410:CLA:H122	1.72	0.41
2:B:124:ARG:HD2	2:B:129:GLY:O	2.19	0.41
2:B:187:PRO:HD3	24:B:602:CLA:HMD2	2.02	0.41
26:B:618:BCR:H24C	26:B:618:BCR:H371	1.79	0.41
3:C:154:LYS:HE2	3:C:261:ARG:HG2	2.03	0.41
3:C:175:LEU:HD23	3:C:237:HIS:CG	2.55	0.41
4:D:49:LEU:HD13	26:D:404:BCR:C15	2.51	0.41
4:D:210:LEU:HA	4:D:213:ILE:HG22	2.02	0.41
13:O:126:VAL:O	41:O:401:HOH:O	2.22	0.41
24:b:613:CLA:HMD2	24:b:621:CLA:H203	2.03	0.41
24:b:624:CLA:H161	7:h:7:LEU:HD21	2.02	0.41
4:d:24:ARG:HD3	18:x:37:VAL:HG22	2.02	0.41
35:d:411:HTG:H1	7:h:25:TRP:CG	2.56	0.41
33:z:101:LMG:H142	33:z:101:LMG:H111	1.85	0.41
33:A:421:LMG:H221	36:C:516:DGD:HAE1	2.02	0.41
24:C:513:CLA:CBB	26:C:514:BCR:H371	2.49	0.41
26:b:628:BCR:H15C	26:b:628:BCR:H351	1.91	0.41
6:f:21:VAL:O	6:f:25:THR:HG23	2.21	0.41
26:t:101:BCR:H11C	26:t:101:BCR:H341	1.91	0.41
15:U:42:TYR:HA	15:U:43:PRO:HA	1.83	0.40
2:b:298:LEU:HD12	2:b:298:LEU:HA	1.94	0.40
36:e:101:DGD:O1B	36:e:101:DGD:O2D	2.39	0.40
13:o:180:GLU:H	13:o:180:GLU:CD	2.30	0.40
1:A:214[B]:MET:HE2	1:A:255:PHE:CE1	2.57	0.40
31:D:405[B]:PL9:H471	31:D:405[B]:PL9:H43	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:L:102:SQD:H62	11:l:7:ARG:NH1	2.37	0.40
12:M:28:GLN:HB3	12:m:27:VAL:HG12	2.02	0.40
19:Z:36:SER:O	19:Z:40:ILE:HG13	2.20	0.40
2:b:262:THR:C	2:b:264:PRO:HD3	2.46	0.40
24:c:510:CLA:CMD	24:c:512:CLA:HAB	2.52	0.40
2:B:172:TYR:OH	7:H:63:LYS:HE3	2.21	0.40
5:E:15:THR:HB	9:J:7:ILE:O	2.21	0.40
24:d:403:CLA:H2	18:x:14:LEU:HA	2.03	0.40
16:v:41:HIS:HA	16:v:45:ILE:O	2.22	0.40
24:B:615:CLA:HBD	24:B:615:CLA:HAA1	2.02	0.40
4:D:282:SER:OG	24:D:402:CLA:HED3	2.21	0.40
37:D:409:LHG:H112	37:D:409:LHG:C38	2.49	0.40
2:b:63:LEU:N	2:b:64:PRO:HD2	2.36	0.40
24:b:619:CLA:HHC	24:b:619:CLA:CBB	2.52	0.40
4:d:103:ARG:O	4:d:107:LEU:HG	2.21	0.40
19:z:52:LEU:O	19:z:56:VAL:HG23	2.21	0.40
24:B:614:CLA:H192	24:B:614:CLA:H161	1.95	0.40
3:C:461:ARG:NH2	41:C:615:HOH:O	2.53	0.40
24:C:510:CLA:C4	37:D:409:LHG:H383	2.49	0.40
1:a:272[A]:HIS:CD2	4:d:218:VAL:HG21	2.56	0.40
3:c:324:LEU:HD23	3:c:324:LEU:HA	1.91	0.40
26:h:101:BCR:H15C	26:h:101:BCR:H351	1.96	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:69:GLU:OE1	27:f:101:SQD:O3[2_554]	2.16	0.04

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	384/344 (112%)	375 (98%)	8 (2%)	1 (0%)	36	34
1	a	386/344 (112%)	377 (98%)	8 (2%)	1 (0%)	36	34
2	B	512/505 (101%)	509 (99%)	3 (1%)	0	100	100
2	b	513/505 (102%)	504 (98%)	9 (2%)	0	100	100
3	C	456/455 (100%)	448 (98%)	6 (1%)	2 (0%)	30	26
3	c	466/455 (102%)	454 (97%)	10 (2%)	2 (0%)	30	26
4	D	355/342 (104%)	346 (98%)	9 (2%)	0	100	100
4	d	355/342 (104%)	346 (98%)	9 (2%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
6	F	32/44 (73%)	31 (97%)	1 (3%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	59 (92%)	5 (8%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	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	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	244 (98%)	5 (2%)	0	100	100
13	o	246/244 (101%)	240 (98%)	6 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	X	37/40 (92%)	37 (100%)	0	0	100	100
18	x	36/40 (90%)	36 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	2
20	R	28/34 (82%)	28 (100%)	0	0	100	100
All	All	5419/5384 (101%)	5300 (98%)	112 (2%)	7 (0%)	48	50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
1	a	259	ILE
19	z	30	PRO
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	312/279 (112%)	312 (100%)	0	100	100
1	a	314/279 (112%)	313 (100%)	1 (0%)	86	91
2	B	412/403 (102%)	409 (99%)	3 (1%)	76	82
2	b	413/403 (102%)	407 (98%)	6 (2%)	57	64
3	C	357/356 (100%)	351 (98%)	6 (2%)	53	60
3	c	367/356 (103%)	355 (97%)	12 (3%)	33	34
4	D	290/277 (105%)	287 (99%)	3 (1%)	68	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	290/277 (105%)	287 (99%)	3 (1%)	68	75
5	E	74/73 (101%)	73 (99%)	1 (1%)	59	66
5	e	74/73 (101%)	72 (97%)	2 (3%)	39	41
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	24 (92%)	2 (8%)	12	7
7	H	55/54 (102%)	54 (98%)	1 (2%)	51	58
7	h	54/54 (100%)	54 (100%)	0	100	100
8	I	34/34 (100%)	33 (97%)	1 (3%)	37	39
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	39
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	30	30
10	K	30/30 (100%)	29 (97%)	1 (3%)	33	34
10	k	30/30 (100%)	28 (93%)	2 (7%)	15	10
11	L	36/35 (103%)	35 (97%)	1 (3%)	38	40
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	40
12	M	31/32 (97%)	29 (94%)	2 (6%)	15	11
12	m	30/32 (94%)	29 (97%)	1 (3%)	33	34
13	O	214/207 (103%)	209 (98%)	5 (2%)	44	49
13	o	211/207 (102%)	203 (96%)	8 (4%)	29	29
14	T	27/28 (96%)	25 (93%)	2 (7%)	13	8
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	8
15	U	84/89 (94%)	82 (98%)	2 (2%)	43	47
15	u	84/89 (94%)	83 (99%)	1 (1%)	63	70
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	118/117 (101%)	117 (99%)	1 (1%)	73	79
17	Y	22/23 (96%)	21 (96%)	1 (4%)	24	22
17	y	22/23 (96%)	19 (86%)	3 (14%)	3	1
18	X	32/33 (97%)	32 (100%)	0	100	100
18	x	31/33 (94%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18	14
19	z	52/52 (100%)	49 (94%)	3 (6%)	18	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	R	25/29 (86%)	23 (92%)	2 (8%)	11 7
All	All	4500/4403 (102%)	4416 (98%)	84 (2%)	51 56

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	80	ILE
2	B	362	PHE
2	B	492	GLU
3	C	28	GLN
3	C	29	GLU
3	C	142	GLU
3	C	289	PHE
3	C	315	MET
3	C	355	THR
4	D	90	LEU
4	D	136	VAL
4	D	329	MET
5	E	71	GLU
7	H	65	LEU
8	I	38	GLU
10	K	17	ILE
11	L	13	ASN
12	M	5	GLN
12	M	9	ILE
13	O	4	THR
13	O	34	SER
13	O	69	LYS
13	O	181[A]	GLU
13	O	181[B]	GLU
14	T	25[A]	GLU
14	T	25[B]	GLU
15	U	59	GLU
15	U	70	ARG
17	Y	24	MET
19	Z	3	ILE
19	Z	4	LEU
19	Z	20	VAL
20	R	4	ARG
20	R	5	VAL
1	a	12	ASN
2	b	84	THR

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Mol	Chain	Res	Type
2	b	315	ILE
2	b	362	PHE
2	b	467	ILE
2	b	472	ARG
2	b	479	PHE
3	c	19	ASN
3	c	21	ILE
3	c	79	LYS
3	c	142	GLU
3	c	240	ILE
3	c	255	THR
3	c	289	PHE
3	c	315	MET
3	c	416[A]	SER
3	c	416[B]	SER
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	90	LEU
4	d	293	LEU
4	d	329	MET
5	e	16	SER
5	e	71	GLU
6	f	15	ILE
6	f	44	GLN
8	i	36	ASP
9	j	1	MET
10	k	10	LYS
10	k	17	ILE
11	l	15	THR
12	m	33	GLN
13	o	4	THR
13	o	23	ASP
13	o	25	THR
13	o	37	THR
13	o	57	LYS
13	o	69	LYS
13	o	141	ASP
13	o	194	LYS
14	t	25[A]	GLU
14	t	25[B]	GLU
15	u	86	GLU
16	v	42	VAL

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Mol	Chain	Res	Type
17	y	18	VAL
17	y	24	MET
17	y	30	ILE
19	z	7	LEU
19	z	29	SER
19	z	34	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	165	GLN
2	B	53	ASN
2	B	331	ASN
3	C	44	ASN
3	C	418	ASN
4	D	61	HIS
4	D	83	ASN
4	D	255	GLN
4	D	301	GLN
4	D	332	GLN
5	E	74	GLN
11	L	13	ASN
13	O	61	GLN
13	O	124	ASN
13	O	147	ASN
19	Z	58	ASN
1	a	12	ASN
1	a	165	GLN
1	a	315	ASN
2	b	53	ASN
2	b	331	ASN
3	c	28	GLN
3	c	44	ASN
3	c	201	ASN
3	c	311	GLN
3	c	373	ASN
4	d	83	ASN
4	d	301	GLN
4	d	332	GLN
5	e	74	GLN
10	k	40	GLN

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Mol	Chain	Res	Type
11	l	8	GLN
13	o	124	ASN
13	o	147	ASN
13	o	155	ASN
15	u	78	ASN
15	u	81	HIS
19	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.65	0	8,9,11	1.05	1 (12%)
12	FME	m	1	12	8,9,10	0.67	0	8,9,11	1.45	3 (37%)
14	FME	t	1	14	8,9,10	0.82	0	8,9,11	1.97	3 (37%)
14	FME	T	1	14	8,9,10	0.72	0	8,9,11	1.36	1 (12%)
12	FME	M	1	12	8,9,10	0.72	0	8,9,11	1.22	2 (25%)
8	FME	i	1	8	8,9,10	0.69	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
8	FME	I	1	8	-	2/7/9/11	-

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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-3.45	117.52	122.82
14	t	1	FME	O-C-CA	-2.49	118.37	124.77
14	T	1	FME	O-C-CA	-2.49	118.38	124.77
14	t	1	FME	C-CA-N	2.44	114.20	109.50
12	m	1	FME	CA-N-CN	-2.29	119.30	122.82
12	m	1	FME	O-C-CA	-2.26	118.97	124.77
12	m	1	FME	O1-CN-N	-2.23	119.56	125.32
8	I	1	FME	O-C-CA	-2.19	119.13	124.77
8	i	1	FME	O-C-CA	-2.15	119.25	124.77
12	M	1	FME	CA-N-CN	-2.01	119.73	122.82
12	M	1	FME	O-C-CA	-2.00	119.62	124.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 267 ligands modelled in this entry, 25 are monoatomic and 18 are unknown - leaving 224 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
24	CLA	B	608	41	69,73,73	1.91	20 (28%)	82,113,113	2.64	34 (41%)
36	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.16	8 (10%)
36	DGD	c	522	-	63,63,67	0.90	2 (3%)	77,77,81	1.02	5 (6%)
24	CLA	b	615	-	69,73,73	1.97	19 (27%)	82,113,113	2.73	30 (36%)
24	CLA	b	618	-	69,73,73	2.00	18 (26%)	82,113,113	2.67	31 (37%)
28	GOL	o	301	-	5,5,5	0.39	0	5,5,5	0.25	0
28	GOL	a	402	-	5,5,5	0.38	0	5,5,5	0.28	0
27	SQD	L	102	-	52,54,54	0.98	2 (3%)	62,65,65	1.54	10 (16%)
24	CLA	b	623	-	69,73,73	2.01	19 (27%)	82,113,113	2.69	33 (40%)
24	CLA	b	611	-	69,73,73	2.00	20 (28%)	82,113,113	2.76	31 (37%)
35	HTG	c	525	-	19,19,19	0.96	2 (10%)	23,24,24	1.38	1 (4%)
36	DGD	C	517	-	63,63,67	0.87	2 (3%)	77,77,81	1.06	5 (6%)
24	CLA	b	624	-	69,73,73	1.98	20 (28%)	82,113,113	2.64	30 (36%)
40	HEC	V	205	16	46,50,50	1.75	9 (19%)	58,82,82	1.59	11 (18%)
24	CLA	A	410	-	69,73,73	2.03	20 (28%)	82,113,113	2.64	35 (42%)
35	HTG	b	632	-	19,19,19	1.03	2 (10%)	23,24,24	1.60	3 (13%)
27	SQD	A	412	-	52,54,54	0.92	2 (3%)	62,65,65	1.50	11 (17%)
24	CLA	C	509	-	69,73,73	2.09	20 (28%)	82,113,113	2.65	29 (35%)
28	GOL	a	420	34	5,5,5	0.34	0	5,5,5	0.44	0
33	LMG	C	519	-	51,51,55	0.96	2 (3%)	59,59,63	1.00	4 (6%)
24	CLA	b	620	-	69,73,73	1.98	19 (27%)	82,113,113	2.67	31 (37%)
27	SQD	f	101	-	41,43,54	1.11	2 (4%)	51,54,65	1.44	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	GOL	v	202	-	5,5,5	0.35	0	5,5,5	0.29	0
28	GOL	b	604	-	5,5,5	0.39	0	5,5,5	0.27	0
24	CLA	b	619	41	69,73,73	2.02	22 (31%)	82,113,113	2.68	31 (37%)
24	CLA	C	513	-	69,73,73	2.04	20 (28%)	82,113,113	2.62	31 (37%)
24	CLA	b	614	-	69,73,73	1.99	19 (27%)	82,113,113	2.80	32 (39%)
24	CLA	b	621	-	69,73,73	2.02	20 (28%)	82,113,113	2.63	32 (39%)
35	HTG	c	526	-	19,19,19	0.93	2 (10%)	23,24,24	1.34	2 (8%)
24	CLA	A	407	41	69,73,73	2.04	20 (28%)	82,113,113	2.73	33 (40%)
24	CLA	c	512	41	69,73,73	1.96	19 (27%)	82,113,113	2.69	29 (35%)
24	CLA	C	502	-	69,73,73	1.99	20 (28%)	82,113,113	2.63	30 (36%)
25	PHO	A	408	-	58,69,69	2.73	12 (20%)	55,99,99	2.89	13 (23%)
24	CLA	b	613	-	69,73,73	1.99	19 (27%)	82,113,113	2.60	29 (35%)
27	SQD	a	405	-	52,54,54	1.01	2 (3%)	62,65,65	1.17	5 (8%)
26	BCR	T	103	-	41,41,41	1.09	1 (2%)	56,56,56	1.56	14 (25%)
26	BCR	Y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.61	10 (17%)
28	GOL	B	628	-	5,5,5	0.35	0	5,5,5	0.58	0
25	PHO	A	409[B]	-	58,69,69	2.78	15 (25%)	55,99,99	2.92	15 (27%)
26	BCR	B	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.31	7 (12%)
26	BCR	b	628	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	6 (10%)
30	OEX	a	416[B]	41,3,1	0,15,15	-	-	-	-	-
31	PL9	d	405[B]	-	55,55,55	0.67	2 (3%)	68,69,69	1.55	13 (19%)
31	PL9	D	405[A]	-	55,55,55	0.67	2 (3%)	68,69,69	1.74	22 (32%)
36	DGD	e	101	-	63,63,67	0.93	2 (3%)	77,77,81	1.19	7 (9%)
24	CLA	C	507	41	69,73,73	2.02	20 (28%)	82,113,113	2.56	32 (39%)
36	DGD	c	521	-	63,63,67	0.88	2 (3%)	77,77,81	0.95	6 (7%)
24	CLA	C	511	3	69,73,73	2.04	19 (27%)	82,113,113	2.60	31 (37%)
31	PL9	A	419[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.79	21 (30%)
26	BCR	h	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.45	7 (12%)
28	GOL	V	203	-	5,5,5	0.39	0	5,5,5	0.30	0
28	GOL	c	503	-	5,5,5	0.40	0	5,5,5	0.64	0
24	CLA	c	513	-	69,73,73	2.05	20 (28%)	82,113,113	2.61	29 (35%)
24	CLA	c	516	3	69,73,73	1.99	19 (27%)	82,113,113	2.59	31 (37%)
28	GOL	V	204	-	5,5,5	0.36	0	5,5,5	0.36	0
28	GOL	C	525	-	5,5,5	0.35	0	5,5,5	0.51	0
35	HTG	b	631	-	19,19,19	0.75	1 (5%)	23,24,24	1.28	2 (8%)
29	LMT	M	103	-	36,36,36	0.53	1 (2%)	47,47,47	0.98	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	GOL	O	301	-	5,5,5	0.35	0	5,5,5	0.42	0
23	BCT	A	404[A]	21	3,3,3	0.47	0	2,3,3	1.28	0
35	HTG	B	624	-	19,19,19	0.72	1 (5%)	23,24,24	1.53	3 (13%)
37	LHG	d	406	-	48,48,48	0.91	3 (6%)	51,54,54	1.05	4 (7%)
24	CLA	B	613	-	69,73,73	1.96	18 (26%)	82,113,113	2.77	31 (37%)
24	CLA	B	615	-	69,73,73	2.01	19 (27%)	82,113,113	2.70	31 (37%)
37	LHG	D	407	-	48,48,48	0.85	2 (4%)	51,54,54	1.16	5 (9%)
29	LMT	a	419	-	36,36,36	0.45	0	47,47,47	0.79	1 (2%)
33	LMG	b	629	-	51,51,55	0.90	2 (3%)	59,59,63	1.08	5 (8%)
26	BCR	B	619	-	41,41,41	1.05	1 (2%)	56,56,56	1.45	9 (16%)
29	LMT	T	104	-	25,25,36	0.50	0	30,30,47	0.97	1 (3%)
24	CLA	B	610	-	69,73,73	2.01	19 (27%)	82,113,113	2.62	31 (37%)
26	BCR	C	514	-	41,41,41	1.06	1 (2%)	56,56,56	1.51	9 (16%)
37	LHG	D	408	-	48,48,48	0.94	2 (4%)	51,54,54	0.87	3 (5%)
35	HTG	B	625	-	19,19,19	0.97	1 (5%)	23,24,24	1.70	4 (17%)
24	CLA	B	605	-	69,73,73	1.96	20 (28%)	82,113,113	2.64	32 (39%)
24	CLA	c	518	-	69,73,73	2.05	19 (27%)	82,113,113	2.69	32 (39%)
29	LMT	b	630	-	25,25,36	0.52	0	30,30,47	0.66	0
38	HEM	F	102	6,5	50,50,50	1.57	6 (12%)	67,82,82	1.73	12 (17%)
28	GOL	b	606	-	5,5,5	0.37	0	5,5,5	0.30	0
27	SQD	a	414	-	52,54,54	0.91	2 (3%)	62,65,65	1.58	12 (19%)
35	HTG	B	623	-	19,19,19	0.95	1 (5%)	23,24,24	1.08	1 (4%)
37	LHG	d	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.03	2 (3%)
25	PHO	a	418[B]	-	58,69,69	2.77	13 (22%)	55,99,99	3.03	15 (27%)
36	DGD	C	518	-	63,63,67	0.87	2 (3%)	77,77,81	0.90	4 (5%)
28	GOL	C	524	-	5,5,5	0.37	0	5,5,5	0.80	0
24	CLA	C	503	-	69,73,73	2.04	19 (27%)	82,113,113	2.58	28 (34%)
28	GOL	A	415	-	5,5,5	0.41	0	5,5,5	0.25	0
26	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.46	8 (14%)
35	HTG	b	607	-	19,19,19	0.91	2 (10%)	23,24,24	1.11	1 (4%)
35	HTG	b	608	-	19,19,19	0.97	2 (10%)	23,24,24	1.19	3 (13%)
35	HTG	D	412	-	16,16,19	1.03	2 (12%)	20,21,24	1.32	1 (5%)
29	LMT	C	521	-	36,36,36	0.48	0	47,47,47	1.23	3 (6%)
30	OEX	A	418[B]	41,3,1	0,15,15	-	-	-	-	-
33	LMG	c	524	-	51,51,55	0.96	2 (3%)	59,59,63	1.25	7 (11%)
24	CLA	C	501	-	69,73,73	2.01	19 (27%)	82,113,113	2.70	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	611	41	69,73,73	2.07	21 (30%)	82,113,113	2.66	34 (41%)
36	DGD	H	102	-	63,63,67	0.91	3 (4%)	77,77,81	1.01	7 (9%)
23	BCT	a	417[A]	21	3,3,3	0.51	0	2,3,3	0.77	0
28	GOL	A	413	-	5,5,5	0.30	0	5,5,5	0.42	0
28	GOL	A	414	-	5,5,5	0.45	0	5,5,5	0.53	0
35	HTG	C	522	-	19,19,19	0.94	2 (10%)	23,24,24	1.41	2 (8%)
24	CLA	c	517	-	69,73,73	2.05	20 (28%)	82,113,113	2.76	33 (40%)
29	LMT	A	417	-	36,36,36	0.60	1 (2%)	47,47,47	1.27	4 (8%)
31	PL9	a	415[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.94	21 (30%)
24	CLA	c	510	-	69,73,73	1.99	20 (28%)	82,113,113	2.60	29 (35%)
25	PHO	a	411	-	58,69,69	2.81	13 (22%)	55,99,99	2.86	17 (30%)
28	GOL	T	102	-	5,5,5	0.40	0	5,5,5	0.30	0
24	CLA	B	607	-	69,73,73	1.99	20 (28%)	82,113,113	2.77	33 (40%)
24	CLA	b	617	-	69,73,73	2.06	20 (28%)	82,113,113	2.55	32 (39%)
24	CLA	b	612	-	69,73,73	2.03	20 (28%)	82,113,113	2.72	32 (39%)
24	CLA	B	614	-	69,73,73	2.01	18 (26%)	82,113,113	2.58	34 (41%)
26	BCR	A	411	-	41,41,41	1.00	1 (2%)	56,56,56	1.14	6 (10%)
30	OEX	a	416[A]	41,3,1	0,15,15	-	-	-	-	-
25	PHO	A	409[A]	-	58,69,69	2.83	14 (24%)	55,99,99	2.86	13 (23%)
24	CLA	b	616	41	69,73,73	1.97	18 (26%)	82,113,113	2.69	30 (36%)
26	BCR	b	626	-	41,41,41	1.04	1 (2%)	56,56,56	1.44	7 (12%)
37	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.07	5 (9%)
24	CLA	d	402	-	69,73,73	1.99	18 (26%)	82,113,113	2.68	32 (39%)
28	GOL	B	631	-	5,5,5	0.40	0	5,5,5	0.33	0
24	CLA	a	409	-	69,73,73	2.01	19 (27%)	82,113,113	2.64	31 (37%)
28	GOL	B	627	-	5,5,5	0.34	0	5,5,5	0.52	0
28	GOL	c	502	-	5,5,5	0.28	0	5,5,5	0.50	0
26	BCR	b	627	-	41,41,41	1.02	1 (2%)	56,56,56	1.26	4 (7%)
29	LMT	B	635	-	25,25,36	0.52	1 (4%)	30,30,47	0.84	1 (3%)
37	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.09	4 (9%)
26	BCR	t	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.64	15 (26%)
26	BCR	C	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.49	11 (19%)
24	CLA	c	514	-	69,73,73	2.07	19 (27%)	82,113,113	2.64	30 (36%)
24	CLA	d	401	41	69,73,73	2.04	19 (27%)	82,113,113	2.69	34 (41%)
24	CLA	B	609	-	69,73,73	2.00	20 (28%)	82,113,113	2.64	33 (40%)
24	CLA	c	509	41	69,73,73	2.01	19 (27%)	82,113,113	2.75	35 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SQD	B	621	-	52,54,54	0.97	2 (3%)	62,65,65	1.45	7 (11%)
35	HTG	d	411	-	16,16,19	1.05	2 (12%)	20,21,24	1.52	2 (10%)
28	GOL	B	629	-	5,5,5	0.33	0	5,5,5	0.40	0
33	LMG	B	622	-	51,51,55	0.93	2 (3%)	59,59,63	1.07	5 (8%)
24	CLA	C	512	-	69,73,73	2.00	20 (28%)	82,113,113	2.70	30 (36%)
36	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.98	4 (5%)
24	CLA	A	406	41	69,73,73	1.95	19 (27%)	82,113,113	2.76	34 (41%)
38	HEM	e	103	6,5	50,50,50	1.55	8 (16%)	67,82,82	1.65	15 (22%)
24	CLA	D	402	-	69,73,73	1.97	19 (27%)	82,113,113	2.74	31 (37%)
36	DGD	c	520	-	63,63,67	0.84	2 (3%)	77,77,81	1.11	5 (6%)
28	GOL	v	203	-	5,5,5	0.40	0	5,5,5	0.24	0
24	CLA	B	612	-	69,73,73	1.98	18 (26%)	82,113,113	2.71	32 (39%)
24	CLA	C	510	-	69,73,73	2.05	20 (28%)	82,113,113	2.60	30 (36%)
23	BCT	A	404[B]	21	3,3,3	0.51	0	2,3,3	1.09	0
26	BCR	K	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.46	11 (19%)
28	GOL	V	201	-	5,5,5	0.40	0	5,5,5	0.34	0
24	CLA	a	410	41	69,73,73	1.98	20 (28%)	82,113,113	2.75	33 (40%)
33	LMG	c	523	-	51,51,55	0.90	2 (3%)	59,59,63	1.13	4 (6%)
37	LHG	e	102	-	41,41,48	1.03	2 (4%)	44,47,54	0.97	2 (4%)
28	GOL	v	201	-	5,5,5	0.33	0	5,5,5	0.24	0
35	HTG	C	523	-	19,19,19	0.92	1 (5%)	23,24,24	1.68	4 (17%)
37	LHG	D	409	-	48,48,48	0.98	2 (4%)	51,54,54	1.04	3 (5%)
24	CLA	D	403	-	69,73,73	2.03	20 (28%)	82,113,113	2.66	31 (37%)
28	GOL	b	605	-	5,5,5	0.36	0	5,5,5	0.34	0
29	LMT	D	401	-	36,36,36	0.43	0	47,47,47	1.06	1 (2%)
36	DGD	D	406	-	52,52,67	1.02	3 (5%)	60,60,81	1.18	5 (8%)
24	CLA	B	604	-	69,73,73	2.04	19 (27%)	82,113,113	2.72	32 (39%)
25	PHO	a	418[A]	-	58,69,69	2.77	13 (22%)	55,99,99	3.07	15 (27%)
28	GOL	T	101	-	5,5,5	0.46	0	5,5,5	0.16	0
28	GOL	V	202	-	5,5,5	0.40	0	5,5,5	0.39	0
29	LMT	M	101	-	36,36,36	0.40	0	47,47,47	0.91	0
29	LMT	f	102	-	36,36,36	0.47	0	47,47,47	0.92	1 (2%)
28	GOL	b	602	-	5,5,5	0.43	0	5,5,5	0.53	0
28	GOL	b	603	-	5,5,5	0.34	0	5,5,5	0.13	0
29	LMT	a	404	-	36,36,36	0.46	0	47,47,47	1.11	3 (6%)
29	LMT	m	103	-	36,36,36	0.47	0	47,47,47	1.01	3 (6%)
24	CLA	B	606	-	69,73,73	2.01	19 (27%)	82,113,113	2.77	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SQD	A	416	-	52,54,54	0.97	2 (3%)	62,65,65	1.12	3 (4%)
33	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.13	3 (5%)
30	OEX	A	418[A]	41,3,1	0,15,15	-	-	-		
26	BCR	D	404	-	41,41,41	1.05	1 (2%)	56,56,56	1.71	10 (17%)
33	LMG	D	413	39	51,51,55	0.87	2 (3%)	59,59,63	1.00	5 (8%)
28	GOL	A	422	34	5,5,5	0.35	0	5,5,5	0.24	0
26	BCR	c	519	-	41,41,41	1.04	1 (2%)	56,56,56	1.45	7 (12%)
26	BCR	B	620	-	41,41,41	1.07	1 (2%)	56,56,56	1.45	6 (10%)
24	CLA	b	625	-	69,73,73	1.99	18 (26%)	82,113,113	2.72	32 (39%)
24	CLA	C	504	41	69,73,73	2.04	20 (28%)	82,113,113	2.69	29 (35%)
31	PL9	d	405[A]	-	55,55,55	0.71	2 (3%)	68,69,69	1.52	15 (22%)
37	LHG	d	407	-	48,48,48	0.88	2 (4%)	51,54,54	1.01	4 (7%)
24	CLA	C	506	-	69,73,73	2.04	19 (27%)	82,113,113	2.55	31 (37%)
24	CLA	B	602	41	69,73,73	2.05	20 (28%)	82,113,113	2.69	29 (35%)
26	BCR	c	528	-	41,41,41	1.05	1 (2%)	56,56,56	1.47	6 (10%)
33	LMG	Z	101	-	37,37,55	0.97	2 (5%)	45,45,63	1.39	6 (13%)
24	CLA	c	507	-	69,73,73	2.03	21 (30%)	82,113,113	2.55	27 (32%)
31	PL9	a	415[A]	-	55,55,55	0.65	2 (3%)	68,69,69	1.93	20 (29%)
31	PL9	A	419[A]	-	55,55,55	0.66	2 (3%)	68,69,69	1.80	22 (32%)
24	CLA	c	515	-	69,73,73	2.02	19 (27%)	82,113,113	2.63	31 (37%)
28	GOL	B	636	-	5,5,5	0.41	0	5,5,5	0.49	0
23	BCT	a	417[B]	21	3,3,3	0.53	0	2,3,3	0.85	0
35	HTG	B	632	-	19,19,19	0.96	2 (10%)	23,24,24	1.29	3 (13%)
31	PL9	D	405[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.67	19 (27%)
24	CLA	C	505	-	69,73,73	1.99	20 (28%)	82,113,113	2.57	28 (34%)
24	CLA	b	622	-	69,73,73	2.02	20 (28%)	82,113,113	2.56	29 (35%)
24	CLA	B	616	-	69,73,73	1.97	18 (26%)	82,113,113	2.67	29 (35%)
33	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.10	3 (6%)
27	SQD	F	103	-	41,43,54	1.09	2 (4%)	51,54,65	1.56	11 (21%)
24	CLA	B	603	-	69,73,73	2.04	20 (28%)	82,113,113	2.72	32 (39%)
24	CLA	a	412	-	69,73,73	2.01	19 (27%)	82,113,113	2.71	32 (39%)
24	CLA	c	508	-	69,73,73	2.04	19 (27%)	82,113,113	2.69	28 (34%)
33	LMG	A	421	-	51,51,55	0.94	2 (3%)	59,59,63	1.11	4 (6%)
37	LHG	b	634	-	48,48,48	0.92	2 (4%)	51,54,54	1.02	4 (7%)
24	CLA	A	405	-	69,73,73	2.02	20 (28%)	82,113,113	2.61	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.50	8 (14%)
35	HTG	V	206	-	19,19,19	0.93	2 (10%)	23,24,24	1.23	3 (13%)
28	GOL	a	401	-	5,5,5	0.45	0	5,5,5	0.52	0
28	GOL	B	626	-	5,5,5	0.44	0	5,5,5	0.40	0
24	CLA	B	617	-	69,73,73	2.01	19 (27%)	82,113,113	2.69	29 (35%)
33	LMG	c	501	-	51,51,55	0.90	2 (3%)	59,59,63	1.17	5 (8%)
26	BCR	a	413	-	41,41,41	1.04	1 (2%)	56,56,56	1.13	6 (10%)
28	GOL	t	102	-	5,5,5	0.49	0	5,5,5	0.11	0
33	LMG	d	413	39	51,51,55	0.93	2 (3%)	59,59,63	0.94	3 (5%)
26	BCR	d	404	-	41,41,41	1.13	1 (2%)	56,56,56	1.71	12 (21%)
35	HTG	b	601	-	19,19,19	0.90	1 (5%)	23,24,24	1.02	2 (8%)
24	CLA	b	610	41	69,73,73	2.05	20 (28%)	82,113,113	2.66	29 (35%)
24	CLA	C	508	-	69,73,73	2.06	20 (28%)	82,113,113	2.63	26 (31%)
24	CLA	c	506	-	69,73,73	1.98	19 (27%)	82,113,113	2.62	29 (35%)
29	LMT	m	102	-	36,36,36	0.47	0	47,47,47	0.85	1 (2%)
24	CLA	c	511	-	69,73,73	2.00	19 (27%)	82,113,113	2.63	32 (39%)
35	HTG	B	633	-	19,19,19	0.92	1 (5%)	23,24,24	1.28	1 (4%)
40	HEC	v	205	16	46,50,50	1.71	10 (21%)	58,82,82	1.63	12 (20%)
28	GOL	B	630	-	5,5,5	0.41	0	5,5,5	0.27	0
29	LMT	F	101	-	36,36,36	0.47	0	47,47,47	0.95	1 (2%)
24	CLA	d	403	-	69,73,73	2.01	21 (30%)	82,113,113	2.72	32 (39%)
26	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.42	9 (16%)

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
24	CLA	B	608	41	1/1/15/20	5/39/115/115	-
36	DGD	C	516	-	-	13/51/91/95	0/2/2/2
36	DGD	c	522	-	-	14/51/91/95	0/2/2/2
24	CLA	b	615	-	1/1/15/20	7/39/115/115	-
24	CLA	b	618	-	1/1/15/20	5/39/115/115	-
28	GOL	o	301	-	-	4/4/4/4	-
28	GOL	a	402	-	-	2/4/4/4	-
27	SQD	L	102	-	-	23/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	623	-	1/1/15/20	20/39/115/115	-
24	CLA	b	611	-	1/1/15/20	5/39/115/115	-
35	HTG	c	525	-	-	3/10/30/30	0/1/1/1
36	DGD	C	517	-	-	14/51/91/95	0/2/2/2
24	CLA	b	624	-	1/1/15/20	3/39/115/115	-
40	HEC	V	205	16	-	6/14/54/54	-
24	CLA	A	410	-	1/1/15/20	10/39/115/115	-
35	HTG	b	632	-	-	6/10/30/30	0/1/1/1
27	SQD	A	412	-	-	12/49/69/69	0/1/1/1
24	CLA	C	509	-	1/1/15/20	13/39/115/115	-
28	GOL	a	420	34	-	3/4/4/4	-
33	LMG	C	519	-	-	10/46/66/70	0/1/1/1
24	CLA	b	620	-	1/1/15/20	3/39/115/115	-
27	SQD	f	101	-	-	13/38/58/69	0/1/1/1
28	GOL	v	202	-	-	2/4/4/4	-
28	GOL	b	604	-	-	2/4/4/4	-
24	CLA	b	619	41	1/1/15/20	5/39/115/115	-
24	CLA	C	513	-	1/1/15/20	6/39/115/115	-
24	CLA	b	614	-	1/1/15/20	5/39/115/115	-
24	CLA	b	621	-	1/1/15/20	2/39/115/115	-
35	HTG	c	526	-	-	0/10/30/30	0/1/1/1
24	CLA	A	407	41	-	3/39/115/115	-
24	CLA	c	512	41	1/1/15/20	7/39/115/115	-
24	CLA	C	502	-	-	6/39/115/115	-
25	PHO	A	408	-	-	3/37/103/103	0/5/6/6
24	CLA	b	613	-	1/1/15/20	3/39/115/115	-
27	SQD	a	405	-	-	15/49/69/69	0/1/1/1
26	BCR	T	103	-	-	1/29/63/63	0/2/2/2
26	BCR	Y	101	-	-	3/29/63/63	0/2/2/2
28	GOL	B	628	-	-	2/4/4/4	-
25	PHO	A	409[B]	-	-	0/37/103/103	0/5/6/6
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
26	BCR	b	628	-	-	0/29/63/63	0/2/2/2
31	PL9	d	405[B]	-	-	8/53/73/73	0/1/1/1
31	PL9	D	405[A]	-	-	7/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DGD	e	101	-	-	27/51/91/95	0/2/2/2
24	CLA	C	507	41	1/1/15/20	8/39/115/115	-
36	DGD	c	521	-	-	15/51/91/95	0/2/2/2
24	CLA	C	511	3	1/1/15/20	3/39/115/115	-
31	PL9	A	419[B]	-	-	10/53/73/73	0/1/1/1
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
28	GOL	V	203	-	-	1/4/4/4	-
28	GOL	c	503	-	-	1/4/4/4	-
24	CLA	c	513	-	1/1/15/20	3/39/115/115	-
24	CLA	c	516	3	1/1/15/20	5/39/115/115	-
28	GOL	V	204	-	-	0/4/4/4	-
28	GOL	C	525	-	-	0/4/4/4	-
35	HTG	b	631	-	-	2/10/30/30	0/1/1/1
29	LMT	M	103	-	-	9/21/61/61	0/2/2/2
28	GOL	O	301	-	-	2/4/4/4	-
35	HTG	B	624	-	-	5/10/30/30	0/1/1/1
37	LHG	d	406	-	-	11/53/53/53	-
24	CLA	B	613	-	1/1/15/20	3/39/115/115	-
24	CLA	B	615	-	1/1/15/20	12/39/115/115	-
37	LHG	D	407	-	-	11/53/53/53	-
29	LMT	a	419	-	-	4/21/61/61	0/2/2/2
33	LMG	b	629	-	-	11/46/66/70	0/1/1/1
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
29	LMT	T	104	-	-	7/17/37/61	0/1/1/2
24	CLA	B	610	-	1/1/15/20	4/39/115/115	-
26	BCR	C	514	-	-	2/29/63/63	0/2/2/2
37	LHG	D	408	-	-	7/53/53/53	-
35	HTG	B	625	-	-	4/10/30/30	0/1/1/1
24	CLA	B	605	-	1/1/15/20	4/39/115/115	-
24	CLA	c	518	-	-	5/39/115/115	-
29	LMT	b	630	-	-	4/17/37/61	0/1/1/2
38	HEM	F	102	6,5	-	8/14/54/54	-
28	GOL	b	606	-	-	1/4/4/4	-
27	SQD	a	414	-	-	15/49/69/69	0/1/1/1
35	HTG	B	623	-	-	3/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LHG	d	408	-	-	10/53/53/53	-
25	PHO	a	418[B]	-	-	1/37/103/103	0/5/6/6
36	DGD	C	518	-	-	10/51/91/95	0/2/2/2
28	GOL	C	524	-	-	2/4/4/4	-
24	CLA	C	503	-	1/1/15/20	1/39/115/115	-
28	GOL	A	415	-	-	2/4/4/4	-
26	BCR	H	101	-	-	0/29/63/63	0/2/2/2
35	HTG	b	607	-	-	1/10/30/30	0/1/1/1
35	HTG	b	608	-	-	0/10/30/30	0/1/1/1
35	HTG	D	412	-	-	0/7/27/30	0/1/1/1
29	LMT	C	521	-	-	9/21/61/61	0/2/2/2
33	LMG	c	524	-	-	4/46/66/70	0/1/1/1
24	CLA	C	501	-	1/1/15/20	4/39/115/115	-
24	CLA	B	611	41	1/1/15/20	3/39/115/115	-
36	DGD	H	102	-	-	12/51/91/95	0/2/2/2
28	GOL	A	413	-	-	0/4/4/4	-
28	GOL	A	414	-	-	2/4/4/4	-
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
24	CLA	c	517	-	1/1/15/20	11/39/115/115	-
29	LMT	A	417	-	-	5/21/61/61	0/2/2/2
31	PL9	a	415[B]	-	-	14/53/73/73	0/1/1/1
24	CLA	c	510	-	1/1/15/20	1/39/115/115	-
25	PHO	a	411	-	-	3/37/103/103	0/5/6/6
28	GOL	T	102	-	-	2/4/4/4	-
24	CLA	B	607	-	1/1/15/20	2/39/115/115	-
24	CLA	b	617	-	-	1/39/115/115	-
24	CLA	b	612	-	1/1/15/20	3/39/115/115	-
24	CLA	B	614	-	1/1/15/20	3/39/115/115	-
26	BCR	A	411	-	-	0/29/63/63	0/2/2/2
25	PHO	A	409[A]	-	-	0/37/103/103	0/5/6/6
24	CLA	b	616	41	1/1/15/20	2/39/115/115	-
26	BCR	b	626	-	-	2/29/63/63	0/2/2/2
37	LHG	L	101	-	-	14/53/53/53	-
24	CLA	d	402	-	1/1/15/20	4/39/115/115	-
28	GOL	B	631	-	-	0/4/4/4	-
24	CLA	a	409	-	1/1/15/20	4/39/115/115	-
28	GOL	B	627	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	c	502	-	-	0/4/4/4	-
26	BCR	b	627	-	-	0/29/63/63	0/2/2/2
29	LMT	B	635	-	-	7/17/37/61	0/1/1/2
37	LHG	E	101	-	-	23/46/46/53	-
26	BCR	t	101	-	-	1/29/63/63	0/2/2/2
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
24	CLA	c	514	-	1/1/15/20	15/39/115/115	-
24	CLA	d	401	41	1/1/15/20	4/39/115/115	-
24	CLA	c	509	41	1/1/15/20	4/39/115/115	-
24	CLA	B	609	-	-	1/39/115/115	-
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
35	HTG	d	411	-	-	1/7/27/30	0/1/1/1
28	GOL	B	629	-	-	2/4/4/4	-
33	LMG	B	622	-	-	6/46/66/70	0/1/1/1
24	CLA	C	512	-	1/1/15/20	9/39/115/115	-
36	DGD	h	102	-	-	12/51/91/95	0/2/2/2
24	CLA	A	406	41	1/1/15/20	2/39/115/115	-
38	HEM	e	103	6,5	-	10/14/54/54	-
24	CLA	D	402	-	1/1/15/20	0/39/115/115	-
36	DGD	c	520	-	-	14/51/91/95	0/2/2/2
28	GOL	v	203	-	-	2/4/4/4	-
24	CLA	B	612	-	1/1/15/20	3/39/115/115	-
24	CLA	C	510	-	1/1/15/20	7/39/115/115	-
26	BCR	K	101	-	-	2/29/63/63	0/2/2/2
28	GOL	V	201	-	-	2/4/4/4	-
24	CLA	a	410	41	-	6/39/115/115	-
33	LMG	c	523	-	-	13/46/66/70	0/1/1/1
37	LHG	e	102	-	-	16/46/46/53	-
28	GOL	v	201	-	-	2/4/4/4	-
35	HTG	C	523	-	-	2/10/30/30	0/1/1/1
37	LHG	D	409	-	-	10/53/53/53	-
24	CLA	D	403	-	1/1/15/20	4/39/115/115	-
28	GOL	b	605	-	-	2/4/4/4	-
29	LMT	D	401	-	-	9/21/61/61	0/2/2/2
36	DGD	D	406	-	-	23/47/67/95	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	604	-	1/1/15/20	1/39/115/115	-
25	PHO	a	418[A]	-	-	0/37/103/103	0/5/6/6
28	GOL	T	101	-	-	0/4/4/4	-
28	GOL	V	202	-	-	2/4/4/4	-
29	LMT	M	101	-	-	4/21/61/61	0/2/2/2
29	LMT	f	102	-	-	10/21/61/61	0/2/2/2
28	GOL	b	602	-	-	0/4/4/4	-
28	GOL	b	603	-	-	0/4/4/4	-
29	LMT	a	404	-	-	9/21/61/61	0/2/2/2
29	LMT	m	103	-	-	7/21/61/61	0/2/2/2
24	CLA	B	606	-	1/1/15/20	4/39/115/115	-
27	SQD	A	416	-	-	16/49/69/69	0/1/1/1
33	LMG	C	520	-	-	10/46/66/70	0/1/1/1
33	LMG	D	413	39	-	8/46/66/70	0/1/1/1
26	BCR	D	404	-	-	8/29/63/63	0/2/2/2
28	GOL	A	422	34	-	2/4/4/4	-
26	BCR	c	519	-	-	1/29/63/63	0/2/2/2
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
24	CLA	b	625	-	1/1/15/20	8/39/115/115	-
24	CLA	C	504	41	1/1/15/20	3/39/115/115	-
31	PL9	d	405[A]	-	-	5/53/73/73	0/1/1/1
37	LHG	d	407	-	-	7/53/53/53	-
24	CLA	C	506	-	1/1/15/20	6/39/115/115	-
24	CLA	B	602	41	1/1/15/20	13/39/115/115	-
26	BCR	c	528	-	-	0/29/63/63	0/2/2/2
33	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
24	CLA	c	507	-	1/1/15/20	6/39/115/115	-
31	PL9	a	415[A]	-	-	17/53/73/73	0/1/1/1
31	PL9	A	419[A]	-	-	14/53/73/73	0/1/1/1
24	CLA	c	515	-	1/1/15/20	8/39/115/115	-
28	GOL	B	636	-	-	0/4/4/4	-
35	HTG	B	632	-	-	3/10/30/30	0/1/1/1
31	PL9	D	405[B]	-	-	7/53/73/73	0/1/1/1
24	CLA	C	505	-	1/1/15/20	6/39/115/115	-
24	CLA	b	622	-	1/1/15/20	2/39/115/115	-
24	CLA	B	616	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	z	101	-	-	15/34/54/70	0/1/1/1
27	SQD	F	103	-	-	16/38/58/69	0/1/1/1
24	CLA	B	603	-	1/1/15/20	2/39/115/115	-
24	CLA	a	412	-	1/1/15/20	11/39/115/115	-
24	CLA	c	508	-	-	1/39/115/115	-
33	LMG	A	421	-	-	19/46/66/70	0/1/1/1
37	LHG	b	634	-	-	15/53/53/53	-
24	CLA	A	405	-	1/1/15/20	4/39/115/115	-
26	BCR	y	101	-	-	2/29/63/63	0/2/2/2
35	HTG	V	206	-	-	2/10/30/30	0/1/1/1
28	GOL	a	401	-	-	1/4/4/4	-
28	GOL	B	626	-	-	2/4/4/4	-
24	CLA	B	617	-	1/1/15/20	6/39/115/115	-
33	LMG	c	501	-	-	16/46/66/70	0/1/1/1
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
28	GOL	t	102	-	-	0/4/4/4	-
33	LMG	d	413	39	-	11/46/66/70	0/1/1/1
26	BCR	d	404	-	-	6/29/63/63	0/2/2/2
35	HTG	b	601	-	-	3/10/30/30	0/1/1/1
24	CLA	b	610	41	1/1/15/20	17/39/115/115	-
24	CLA	C	508	-	1/1/15/20	2/39/115/115	-
24	CLA	c	506	-	1/1/15/20	3/39/115/115	-
29	LMT	m	102	-	-	8/21/61/61	0/2/2/2
24	CLA	c	511	-	1/1/15/20	11/39/115/115	-
35	HTG	B	633	-	-	0/10/30/30	0/1/1/1
40	HEC	v	205	16	-	6/14/54/54	-
28	GOL	B	630	-	-	4/4/4/4	-
29	LMT	F	101	-	-	5/21/61/61	0/2/2/2
24	CLA	d	403	-	1/1/15/20	5/39/115/115	-
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2

All (1627) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	418[A]	PHO	C1B-C2B	9.33	1.49	1.39
25	A	408	PHO	C1D-C2D	9.28	1.49	1.39
25	A	408	PHO	C1B-C2B	9.22	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	411	PHO	C1D-C2D	9.13	1.49	1.39
25	A	409[A]	PHO	C1D-C2D	9.13	1.49	1.39
25	a	418[B]	PHO	C1D-C2D	8.87	1.49	1.39
25	a	411	PHO	C1B-C2B	8.81	1.49	1.39
25	a	418[A]	PHO	C1D-C2D	8.81	1.49	1.39
25	a	418[B]	PHO	C1B-C2B	8.77	1.49	1.39
25	A	409[A]	PHO	C1B-C2B	8.63	1.49	1.39
25	A	409[B]	PHO	C1D-C2D	8.63	1.49	1.39
25	A	409[B]	PHO	C1B-C2B	8.44	1.48	1.39
25	a	411	PHO	C3B-C4B	8.25	1.49	1.41
25	A	409[A]	PHO	C3B-C4B	8.18	1.49	1.41
25	A	409[B]	PHO	C3B-C4B	8.12	1.49	1.41
25	a	418[A]	PHO	C3B-C4B	8.11	1.49	1.41
25	a	418[B]	PHO	C3B-C4B	7.99	1.49	1.41
25	A	409[A]	PHO	C4D-CHA	7.21	1.50	1.39
25	A	409[B]	PHO	C4D-CHA	6.93	1.49	1.39
25	A	408	PHO	C4D-CHA	6.92	1.49	1.39
25	a	418[B]	PHO	C4D-CHA	6.81	1.49	1.39
25	a	411	PHO	C4D-CHA	6.66	1.49	1.39
25	A	409[B]	PHO	C3B-C2B	6.61	1.49	1.40
25	a	418[A]	PHO	C4D-CHA	6.60	1.49	1.39
25	A	409[A]	PHO	C3B-C2B	6.51	1.49	1.40
25	A	408	PHO	C3B-C4B	6.37	1.48	1.41
25	A	408	PHO	C3B-C2B	6.30	1.48	1.40
25	a	411	PHO	C3B-C2B	6.26	1.48	1.40
25	a	418[B]	PHO	C3B-C2B	6.24	1.48	1.40
25	A	409[A]	PHO	C3D-C2D	5.89	1.49	1.39
25	a	418[A]	PHO	C3B-C2B	5.86	1.48	1.40
25	a	418[A]	PHO	C3D-C2D	5.81	1.49	1.39
25	a	418[B]	PHO	C3D-C2D	5.73	1.49	1.39
25	a	411	PHO	C3D-C2D	5.62	1.49	1.39
24	C	508	CLA	C3C-C2C	5.59	1.48	1.36
24	b	610	CLA	C3C-C2C	5.54	1.48	1.36
25	A	408	PHO	C3D-C2D	5.52	1.49	1.39
25	A	409[B]	PHO	C3D-C2D	5.51	1.49	1.39
24	b	614	CLA	C3C-C2C	5.46	1.48	1.36
24	B	611	CLA	C3C-C2C	5.41	1.48	1.36
24	b	619	CLA	C3C-C2C	5.40	1.48	1.36
24	B	606	CLA	O2D-CGD	5.40	1.46	1.33
24	C	510	CLA	C3C-C2C	5.35	1.48	1.36
24	C	513	CLA	C3C-C2C	5.34	1.48	1.36
24	B	604	CLA	C3C-C2C	5.34	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	C3C-C2C	5.34	1.48	1.36
24	c	518	CLA	C3C-C2C	5.32	1.48	1.36
24	b	623	CLA	C3C-C2C	5.32	1.48	1.36
24	B	603	CLA	C3C-C2C	5.32	1.48	1.36
24	D	402	CLA	C3C-C2C	5.31	1.48	1.36
24	A	407	CLA	C3C-C2C	5.29	1.48	1.36
24	b	622	CLA	C3C-C2C	5.28	1.48	1.36
24	C	503	CLA	C3C-C2C	5.27	1.48	1.36
25	a	411	PHO	OBD-CAD	5.27	1.29	1.22
24	D	403	CLA	C3C-C2C	5.27	1.48	1.36
24	b	611	CLA	C3C-C2C	5.26	1.48	1.36
24	C	512	CLA	C3C-C2C	5.26	1.48	1.36
24	c	513	CLA	C3C-C2C	5.26	1.48	1.36
24	c	515	CLA	C3C-C2C	5.23	1.48	1.36
24	b	617	CLA	C3C-C2C	5.22	1.48	1.36
24	b	621	CLA	C3C-C2C	5.21	1.48	1.36
24	a	412	CLA	C3C-C2C	5.21	1.48	1.36
24	d	401	CLA	C3C-C2C	5.21	1.48	1.36
24	D	403	CLA	C1D-ND	5.20	1.44	1.37
26	b	628	BCR	C23-C22	-5.20	1.34	1.46
24	C	509	CLA	C1D-ND	5.20	1.44	1.37
26	B	620	BCR	C23-C22	-5.19	1.34	1.46
24	c	507	CLA	C3C-C2C	5.19	1.48	1.36
24	B	602	CLA	C3C-C2C	5.19	1.48	1.36
24	B	615	CLA	C3C-C2C	5.18	1.47	1.36
24	c	508	CLA	CHC-C1C	5.17	1.48	1.38
24	b	623	CLA	O2D-CGD	5.17	1.45	1.33
24	B	614	CLA	C1D-ND	5.17	1.44	1.37
25	a	411	PHO	O2D-CGD	5.17	1.45	1.33
25	A	408	PHO	OBD-CAD	5.17	1.29	1.22
24	b	615	CLA	C3C-C2C	5.16	1.47	1.36
24	c	509	CLA	O2D-CGD	5.15	1.45	1.33
24	C	507	CLA	C3C-C2C	5.15	1.47	1.36
24	d	403	CLA	C3C-C2C	5.14	1.47	1.36
24	B	610	CLA	C3C-C2C	5.14	1.47	1.36
24	a	409	CLA	C3C-C2C	5.14	1.47	1.36
24	c	511	CLA	C3C-C2C	5.14	1.47	1.36
24	c	517	CLA	C3C-C2C	5.13	1.47	1.36
38	F	102	HEM	FE-NB	5.13	2.10	1.94
24	B	603	CLA	O2D-CGD	5.13	1.45	1.33
24	b	622	CLA	C1D-ND	5.13	1.44	1.37
38	e	103	HEM	FE-NB	5.12	2.10	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	k	101	BCR	C23-C22	-5.12	1.35	1.46
24	B	617	CLA	C1D-ND	5.12	1.44	1.37
24	b	616	CLA	C3C-C2C	5.11	1.47	1.36
24	c	513	CLA	O2D-CGD	5.11	1.45	1.33
24	C	503	CLA	CHC-C1C	5.10	1.48	1.38
24	b	622	CLA	O2D-CGD	5.08	1.45	1.33
24	C	502	CLA	C3C-C2C	5.07	1.47	1.36
24	B	603	CLA	CHC-C1C	5.07	1.48	1.38
24	B	612	CLA	C3C-C2C	5.07	1.47	1.36
24	c	508	CLA	C3C-C2C	5.07	1.47	1.36
24	c	512	CLA	C3C-C2C	5.07	1.47	1.36
24	c	514	CLA	C1D-ND	5.06	1.44	1.37
25	A	409[B]	PHO	O2D-CGD	5.06	1.45	1.33
24	b	620	CLA	C3C-C2C	5.06	1.47	1.36
24	C	505	CLA	C3C-C2C	5.06	1.47	1.36
24	B	607	CLA	O2D-CGD	5.06	1.45	1.33
24	d	401	CLA	O2D-CGD	5.05	1.45	1.33
26	T	103	BCR	C23-C22	-5.04	1.35	1.46
24	b	613	CLA	C3C-C2C	5.04	1.47	1.36
24	B	604	CLA	CHC-C1C	5.04	1.48	1.38
24	B	607	CLA	C3C-C2C	5.03	1.47	1.36
24	c	517	CLA	O2D-CGD	5.03	1.45	1.33
24	c	514	CLA	C3C-C2C	5.03	1.47	1.36
24	B	608	CLA	C3C-C2C	5.03	1.47	1.36
24	c	507	CLA	O2D-CGD	5.02	1.45	1.33
24	B	609	CLA	C3C-C2C	5.02	1.47	1.36
24	b	618	CLA	C3C-C2C	5.02	1.47	1.36
24	C	511	CLA	C3C-C2C	5.01	1.47	1.36
24	A	406	CLA	C3C-C2C	5.01	1.47	1.36
24	b	621	CLA	O2D-CGD	5.01	1.45	1.33
24	B	614	CLA	C3C-C2C	5.01	1.47	1.36
24	B	602	CLA	C1D-ND	5.00	1.44	1.37
24	b	625	CLA	O2D-CGD	5.00	1.45	1.33
24	d	403	CLA	O2D-CGD	5.00	1.45	1.33
24	c	509	CLA	C3C-C2C	5.00	1.47	1.36
24	C	508	CLA	O2D-CGD	5.00	1.45	1.33
24	c	506	CLA	C3C-C2C	5.00	1.47	1.36
24	c	516	CLA	C3C-C2C	4.99	1.47	1.36
24	c	518	CLA	C1D-ND	4.99	1.44	1.37
24	C	504	CLA	C3C-C2C	4.99	1.47	1.36
24	c	514	CLA	O2D-CGD	4.99	1.45	1.33
24	b	618	CLA	O2D-CGD	4.99	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	O2D-CGD	4.99	1.45	1.33
24	c	517	CLA	CHC-C1C	4.98	1.48	1.38
24	C	506	CLA	C3C-C2C	4.98	1.47	1.36
24	c	518	CLA	O2D-CGD	4.98	1.45	1.33
25	A	409[A]	PHO	O2D-CGD	4.97	1.45	1.33
24	C	501	CLA	CHC-C1C	4.97	1.48	1.38
24	B	616	CLA	O2D-CGD	4.97	1.45	1.33
24	C	513	CLA	O2D-CGD	4.96	1.45	1.33
24	B	606	CLA	C3C-C2C	4.96	1.47	1.36
24	C	509	CLA	O2D-CGD	4.96	1.45	1.33
24	b	624	CLA	C3C-C2C	4.96	1.47	1.36
24	B	614	CLA	O2D-CGD	4.95	1.45	1.33
24	B	606	CLA	CHC-C1C	4.95	1.48	1.38
25	a	418[B]	PHO	O2D-CGD	4.94	1.45	1.33
24	A	410	CLA	C3C-C2C	4.93	1.47	1.36
24	B	602	CLA	O2D-CGD	4.93	1.45	1.33
24	B	605	CLA	C1D-ND	4.93	1.44	1.37
24	B	617	CLA	O2D-CGD	4.93	1.45	1.33
24	b	617	CLA	C1D-ND	4.93	1.44	1.37
26	C	514	BCR	C23-C22	-4.93	1.35	1.46
24	b	616	CLA	O2D-CGD	4.93	1.45	1.33
24	c	511	CLA	O2D-CGD	4.93	1.45	1.33
24	C	505	CLA	CHC-C1C	4.92	1.48	1.38
24	b	610	CLA	O2D-CGD	4.92	1.45	1.33
24	C	510	CLA	C1D-ND	4.92	1.44	1.37
24	b	614	CLA	O2D-CGD	4.92	1.45	1.33
24	A	407	CLA	CHC-C1C	4.91	1.48	1.38
24	a	409	CLA	C1D-ND	4.91	1.44	1.37
24	b	620	CLA	O2D-CGD	4.91	1.45	1.33
24	C	510	CLA	O2D-CGD	4.91	1.45	1.33
24	b	612	CLA	C3C-C2C	4.90	1.47	1.36
24	C	504	CLA	CHC-C1C	4.90	1.48	1.38
26	d	404	BCR	C23-C22	-4.90	1.35	1.46
24	C	506	CLA	C1D-ND	4.90	1.44	1.37
24	d	402	CLA	CHC-C1C	4.90	1.48	1.38
24	C	506	CLA	O2D-CGD	4.90	1.45	1.33
24	c	510	CLA	C3C-C2C	4.90	1.47	1.36
24	C	508	CLA	CHC-C1C	4.90	1.48	1.38
24	C	513	CLA	CHC-C1C	4.90	1.48	1.38
24	A	407	CLA	O2D-CGD	4.89	1.45	1.33
24	d	401	CLA	C1D-ND	4.89	1.44	1.37
24	A	405	CLA	CHC-C1C	4.89	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	C1D-ND	4.87	1.44	1.37
24	d	403	CLA	CHC-C1C	4.87	1.48	1.38
24	B	615	CLA	C1D-ND	4.86	1.44	1.37
24	a	410	CLA	CHC-C1C	4.86	1.48	1.38
24	d	402	CLA	C3C-C2C	4.86	1.47	1.36
24	C	512	CLA	O2D-CGD	4.85	1.45	1.33
24	c	515	CLA	C1D-ND	4.85	1.44	1.37
26	h	101	BCR	C23-C22	-4.85	1.35	1.46
24	B	612	CLA	O2D-CGD	4.84	1.45	1.33
24	C	502	CLA	CHC-C1C	4.84	1.48	1.38
24	B	605	CLA	C3C-C2C	4.83	1.47	1.36
24	C	501	CLA	C3C-C2C	4.83	1.47	1.36
24	c	510	CLA	CHC-C1C	4.83	1.48	1.38
24	A	410	CLA	O2D-CGD	4.83	1.45	1.33
24	b	619	CLA	O2D-CGD	4.82	1.45	1.33
24	C	511	CLA	C1D-ND	4.82	1.44	1.37
26	K	101	BCR	C23-C22	-4.82	1.35	1.46
24	C	507	CLA	CHC-C1C	4.82	1.48	1.38
24	a	412	CLA	O2D-CGD	4.82	1.45	1.33
24	b	620	CLA	C1D-ND	4.81	1.44	1.37
24	b	610	CLA	C1D-ND	4.81	1.44	1.37
24	b	624	CLA	O2D-CGD	4.80	1.45	1.33
24	B	602	CLA	O2A-CGA	4.80	1.47	1.33
24	C	509	CLA	CHC-C1C	4.80	1.48	1.38
26	H	101	BCR	C23-C22	-4.80	1.35	1.46
24	B	616	CLA	CHC-C1C	4.79	1.48	1.38
24	b	614	CLA	CHC-C1C	4.79	1.48	1.38
26	C	515	BCR	C23-C22	-4.79	1.35	1.46
24	D	403	CLA	O2D-CGD	4.79	1.45	1.33
26	y	101	BCR	C23-C22	-4.79	1.35	1.46
24	A	410	CLA	C1D-ND	4.78	1.44	1.37
24	b	611	CLA	CHC-C1C	4.78	1.48	1.38
24	b	618	CLA	C1D-ND	4.78	1.44	1.37
24	c	515	CLA	O2D-CGD	4.78	1.45	1.33
24	C	511	CLA	O2D-CGD	4.77	1.45	1.33
24	A	405	CLA	C3C-C2C	4.77	1.47	1.36
24	b	615	CLA	O2D-CGD	4.76	1.44	1.33
24	a	409	CLA	O2D-CGD	4.76	1.44	1.33
24	B	615	CLA	CHC-C1C	4.75	1.48	1.38
24	C	512	CLA	CHC-C1C	4.75	1.48	1.38
24	B	612	CLA	C1D-ND	4.75	1.44	1.37
24	A	405	CLA	O2D-CGD	4.74	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	501	CLA	O2D-CGD	4.74	1.44	1.33
24	B	610	CLA	CHC-C1C	4.74	1.48	1.38
24	b	623	CLA	CHC-C1C	4.74	1.48	1.38
24	B	617	CLA	C3C-C2C	4.73	1.47	1.36
24	c	507	CLA	CHC-C1C	4.73	1.48	1.38
24	B	613	CLA	O2D-CGD	4.73	1.44	1.33
24	a	410	CLA	C3C-C2C	4.73	1.47	1.36
24	B	602	CLA	CHC-C1C	4.73	1.48	1.38
24	C	502	CLA	C1D-ND	4.73	1.44	1.37
24	b	623	CLA	C1D-ND	4.73	1.44	1.37
24	C	501	CLA	C1D-ND	4.72	1.44	1.37
24	c	509	CLA	CHC-C1C	4.72	1.47	1.38
25	a	418[A]	PHO	O2D-CGD	4.72	1.44	1.33
24	c	518	CLA	CHC-C1C	4.72	1.47	1.38
24	C	504	CLA	C1D-ND	4.71	1.44	1.37
24	B	605	CLA	CHC-C1C	4.71	1.47	1.38
24	b	617	CLA	O2D-CGD	4.71	1.44	1.33
24	b	612	CLA	CHC-C1C	4.71	1.47	1.38
24	c	516	CLA	CHC-C1C	4.70	1.47	1.38
24	B	610	CLA	O2D-CGD	4.70	1.44	1.33
24	b	616	CLA	CHC-C1C	4.69	1.47	1.38
24	c	511	CLA	C1D-ND	4.69	1.44	1.37
24	c	506	CLA	O2D-CGD	4.69	1.44	1.33
24	b	617	CLA	CHC-C1C	4.68	1.47	1.38
24	B	617	CLA	CHC-C1C	4.68	1.47	1.38
24	b	618	CLA	CHC-C1C	4.68	1.47	1.38
24	B	616	CLA	C3C-C2C	4.67	1.46	1.36
27	a	405	SQD	O48-C23	4.67	1.47	1.33
26	c	528	BCR	C23-C22	-4.67	1.36	1.46
24	B	609	CLA	O2D-CGD	4.67	1.44	1.33
26	Y	101	BCR	C23-C22	-4.67	1.36	1.46
24	B	611	CLA	C1D-ND	4.67	1.44	1.37
24	c	508	CLA	O2D-CGD	4.66	1.44	1.33
24	b	611	CLA	C1D-ND	4.66	1.44	1.37
24	b	613	CLA	C1D-ND	4.66	1.44	1.37
24	c	513	CLA	O2A-CGA	4.65	1.46	1.33
26	t	101	BCR	C23-C22	-4.64	1.36	1.46
24	b	610	CLA	CHC-C1C	4.64	1.47	1.38
24	B	613	CLA	C3C-C2C	4.64	1.46	1.36
24	C	513	CLA	C1D-ND	4.64	1.44	1.37
24	c	510	CLA	O2D-CGD	4.64	1.44	1.33
24	b	624	CLA	C1D-ND	4.63	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	513	CLA	C1D-ND	4.62	1.43	1.37
24	c	508	CLA	C1D-ND	4.62	1.43	1.37
24	C	510	CLA	CHC-C1C	4.62	1.47	1.38
24	B	611	CLA	O2D-CGD	4.62	1.44	1.33
24	b	611	CLA	O2D-CGD	4.62	1.44	1.33
24	A	410	CLA	CHC-C1C	4.61	1.47	1.38
27	A	416	SQD	O48-C23	4.61	1.46	1.33
24	c	509	CLA	C1D-ND	4.61	1.43	1.37
24	C	506	CLA	CHC-C1C	4.61	1.47	1.38
24	C	507	CLA	O2D-CGD	4.61	1.44	1.33
24	b	619	CLA	C1D-ND	4.60	1.43	1.37
24	b	617	CLA	CHD-C1D	4.60	1.47	1.38
24	B	607	CLA	CHC-C1C	4.60	1.47	1.38
24	c	506	CLA	C1D-ND	4.59	1.43	1.37
24	c	514	CLA	CHC-C1C	4.59	1.47	1.38
24	b	625	CLA	C3C-C2C	4.59	1.46	1.36
24	C	507	CLA	C1D-ND	4.59	1.43	1.37
24	c	517	CLA	C1D-ND	4.59	1.43	1.37
24	D	402	CLA	O2D-CGD	4.59	1.44	1.33
24	C	508	CLA	C1D-ND	4.59	1.43	1.37
24	B	608	CLA	O2D-CGD	4.59	1.44	1.33
25	A	408	PHO	O2D-CGD	4.58	1.44	1.33
24	B	606	CLA	C1D-ND	4.57	1.43	1.37
24	C	504	CLA	O2D-CGD	4.57	1.44	1.33
24	a	410	CLA	O2D-CGD	4.57	1.44	1.33
24	c	512	CLA	O2D-CGD	4.57	1.44	1.33
24	d	403	CLA	C1D-ND	4.56	1.43	1.37
27	f	101	SQD	O47-C7	4.56	1.47	1.34
24	D	403	CLA	CHC-C1C	4.56	1.47	1.38
24	C	505	CLA	O2D-CGD	4.56	1.44	1.33
24	b	615	CLA	C1D-ND	4.55	1.43	1.37
24	b	614	CLA	C1D-ND	4.55	1.43	1.37
24	B	610	CLA	O2A-CGA	4.55	1.46	1.33
24	C	506	CLA	CHD-C1D	4.55	1.47	1.38
26	D	404	BCR	C23-C22	-4.55	1.36	1.46
36	D	406	DGD	O1G-C1A	4.55	1.46	1.33
24	c	512	CLA	CHC-C1C	4.55	1.47	1.38
26	a	413	BCR	C23-C22	-4.55	1.36	1.46
24	C	502	CLA	O2D-CGD	4.55	1.44	1.33
24	A	407	CLA	C1D-ND	4.55	1.43	1.37
24	b	613	CLA	CHC-C1C	4.54	1.47	1.38
24	c	516	CLA	C1D-ND	4.53	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	406	CLA	C1D-ND	4.53	1.43	1.37
24	B	615	CLA	O2D-CGD	4.53	1.44	1.33
24	B	605	CLA	O2D-CGD	4.53	1.44	1.33
26	b	626	BCR	C23-C22	-4.52	1.36	1.46
24	c	516	CLA	O2D-CGD	4.51	1.44	1.33
24	b	613	CLA	O2D-CGD	4.51	1.44	1.33
24	b	612	CLA	C1D-ND	4.51	1.43	1.37
24	c	511	CLA	CHC-C1C	4.51	1.47	1.38
40	V	205	HEC	CAC-C3C	4.50	1.49	1.35
25	A	409[B]	PHO	OBD-CAD	4.50	1.28	1.22
24	b	615	CLA	CHC-C1C	4.49	1.47	1.38
24	c	507	CLA	C1D-ND	4.49	1.43	1.37
26	B	618	BCR	C23-C22	-4.49	1.36	1.46
24	B	612	CLA	CHC-C1C	4.48	1.47	1.38
27	F	103	SQD	O47-C7	4.48	1.46	1.34
24	C	509	CLA	O2A-CGA	4.48	1.46	1.33
24	c	517	CLA	CHD-C1D	4.48	1.47	1.38
25	A	409[A]	PHO	OBD-CAD	4.48	1.28	1.22
24	b	622	CLA	CHC-C1C	4.48	1.47	1.38
33	C	519	LMG	O8-C28	4.47	1.46	1.33
24	b	621	CLA	C1D-ND	4.47	1.43	1.37
26	c	519	BCR	C23-C22	-4.47	1.36	1.46
33	z	101	LMG	O8-C28	4.46	1.46	1.33
24	a	409	CLA	CHD-C1D	4.46	1.47	1.38
24	A	405	CLA	C1D-ND	4.45	1.43	1.37
24	c	515	CLA	CHC-C1C	4.45	1.47	1.38
24	d	402	CLA	O2D-CGD	4.45	1.44	1.33
24	b	621	CLA	CHC-C1C	4.45	1.47	1.38
24	a	412	CLA	CHC-C1C	4.45	1.47	1.38
24	C	503	CLA	O2D-CGD	4.44	1.44	1.33
24	B	608	CLA	CHC-C1C	4.43	1.47	1.38
24	B	609	CLA	C1D-ND	4.42	1.43	1.37
24	B	604	CLA	O2D-CGD	4.42	1.44	1.33
24	d	402	CLA	O2A-CGA	4.42	1.46	1.33
38	e	103	HEM	FE-NC	4.42	2.09	1.95
24	b	610	CLA	CHD-C1D	4.42	1.47	1.38
24	d	401	CLA	CHD-C1D	4.42	1.47	1.38
24	C	512	CLA	O2A-CGA	4.42	1.46	1.33
24	C	508	CLA	O2A-CGA	4.41	1.46	1.33
24	B	613	CLA	CHC-C1C	4.41	1.47	1.38
24	C	506	CLA	O2A-CGA	4.41	1.46	1.33
24	b	624	CLA	CHC-C1C	4.41	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	O2A-CGA	4.41	1.46	1.33
25	a	418[B]	PHO	OBD-CAD	4.41	1.28	1.22
24	B	616	CLA	C1D-ND	4.41	1.43	1.37
36	D	406	DGD	O2G-C1B	4.40	1.46	1.34
26	A	411	BCR	C23-C22	-4.40	1.36	1.46
24	b	623	CLA	CHD-C1D	4.39	1.47	1.38
24	b	610	CLA	O2A-CGA	4.39	1.46	1.33
24	b	624	CLA	O2A-CGA	4.39	1.46	1.33
24	b	625	CLA	CHC-C1C	4.39	1.47	1.38
24	C	511	CLA	CHC-C1C	4.38	1.47	1.38
24	c	516	CLA	O2A-CGA	4.38	1.46	1.33
24	B	609	CLA	CHD-C1D	4.38	1.47	1.38
37	E	101	LHG	O8-C23	4.38	1.46	1.33
24	c	514	CLA	CHD-C1D	4.38	1.47	1.38
24	c	514	CLA	O2A-CGA	4.37	1.46	1.33
24	c	515	CLA	CHD-C1D	4.37	1.46	1.38
26	b	627	BCR	C23-C22	-4.37	1.36	1.46
24	c	513	CLA	CHC-C1C	4.37	1.47	1.38
24	B	614	CLA	CHC-C1C	4.37	1.47	1.38
24	C	507	CLA	CHD-C1D	4.37	1.46	1.38
36	e	101	DGD	O2G-C1B	4.37	1.46	1.34
24	B	611	CLA	CHC-C1C	4.36	1.47	1.38
24	b	620	CLA	CHC-C1C	4.36	1.47	1.38
24	b	619	CLA	CHC-C1C	4.36	1.47	1.38
24	A	407	CLA	CHD-C1D	4.35	1.46	1.38
24	B	604	CLA	C1D-ND	4.35	1.43	1.37
24	C	508	CLA	CHD-C1D	4.35	1.46	1.38
24	a	410	CLA	O2A-CGA	4.35	1.46	1.33
24	C	512	CLA	C1D-ND	4.34	1.43	1.37
33	A	421	LMG	O7-C10	4.33	1.46	1.34
27	a	405	SQD	O47-C7	4.33	1.46	1.34
33	C	520	LMG	O7-C10	4.32	1.46	1.34
24	D	403	CLA	CHD-C1D	4.31	1.46	1.38
24	B	610	CLA	C1D-ND	4.31	1.43	1.37
27	B	621	SQD	O47-C7	4.31	1.46	1.34
24	B	607	CLA	C1D-ND	4.31	1.43	1.37
36	e	101	DGD	O1G-C1A	4.31	1.45	1.33
37	D	409	LHG	O7-C7	4.31	1.46	1.34
24	a	412	CLA	C1D-ND	4.31	1.43	1.37
24	c	506	CLA	CHC-C1C	4.31	1.47	1.38
24	C	507	CLA	O2A-CGA	4.31	1.45	1.33
24	B	602	CLA	CHD-C1D	4.30	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	CHD-C1D	4.30	1.46	1.38
40	v	205	HEC	CAC-C3C	4.29	1.48	1.35
24	B	603	CLA	C1D-ND	4.29	1.43	1.37
24	A	410	CLA	CHD-C1D	4.29	1.46	1.38
24	C	511	CLA	O2A-CGA	4.29	1.45	1.33
24	C	513	CLA	CHD-C1D	4.29	1.46	1.38
24	B	603	CLA	CHD-C1D	4.28	1.46	1.38
40	v	205	HEC	CBC-CAC	-4.28	1.33	1.49
24	C	510	CLA	CHD-C1D	4.28	1.46	1.38
24	B	611	CLA	CHD-C1D	4.28	1.46	1.38
40	V	205	HEC	CAB-C3B	4.28	1.48	1.35
24	c	510	CLA	CHD-C1D	4.28	1.46	1.38
24	c	513	CLA	C3D-C2D	4.28	1.50	1.39
24	b	612	CLA	O2A-CGA	4.28	1.45	1.33
33	c	524	LMG	O7-C10	4.27	1.46	1.34
37	e	102	LHG	O8-C23	4.27	1.45	1.33
24	C	510	CLA	CHB-C1B	4.27	1.49	1.39
36	H	102	DGD	O1G-C1A	4.27	1.45	1.33
37	b	634	LHG	O8-C23	4.27	1.45	1.33
24	c	512	CLA	C1D-ND	4.26	1.43	1.37
24	d	401	CLA	O2A-CGA	4.26	1.45	1.33
24	C	501	CLA	O2A-CGA	4.26	1.45	1.33
24	B	617	CLA	CHD-C1D	4.26	1.46	1.38
24	c	511	CLA	CHD-C1D	4.26	1.46	1.38
24	B	609	CLA	O2A-CGA	4.25	1.45	1.33
24	c	514	CLA	CHB-C1B	4.25	1.48	1.39
25	a	418[B]	PHO	O2A-CGA	4.25	1.45	1.33
24	C	509	CLA	CHD-C1D	4.24	1.46	1.38
24	c	512	CLA	O2A-CGA	4.24	1.45	1.33
27	f	101	SQD	O48-C23	4.24	1.45	1.33
24	c	516	CLA	CHD-C1D	4.24	1.46	1.38
24	B	610	CLA	C3D-C2D	4.23	1.50	1.39
24	c	518	CLA	CHD-C1D	4.23	1.46	1.38
24	C	509	CLA	C3D-C2D	4.23	1.50	1.39
24	a	409	CLA	CHC-C1C	4.23	1.47	1.38
24	c	518	CLA	O2A-CGA	4.23	1.45	1.33
24	b	618	CLA	CHD-C1D	4.23	1.46	1.38
33	B	622	LMG	O8-C28	4.22	1.45	1.33
33	A	421	LMG	O8-C28	4.22	1.45	1.33
24	b	613	CLA	CHD-C1D	4.22	1.46	1.38
27	L	102	SQD	O47-C7	4.22	1.46	1.34
33	C	520	LMG	O8-C28	4.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	C1D-ND	4.21	1.43	1.37
24	B	616	CLA	O2A-CGA	4.21	1.45	1.33
33	c	524	LMG	O8-C28	4.21	1.45	1.33
24	c	517	CLA	O2A-CGA	4.21	1.45	1.33
24	c	510	CLA	C1D-ND	4.20	1.43	1.37
24	C	513	CLA	O2A-CGA	4.20	1.45	1.33
24	B	606	CLA	O2A-CGA	4.20	1.45	1.33
24	a	412	CLA	CHD-C4C	4.19	1.48	1.39
24	C	511	CLA	CHD-C1D	4.19	1.46	1.38
24	C	503	CLA	CHD-C1D	4.19	1.46	1.38
24	C	506	CLA	CHD-C4C	4.19	1.48	1.39
24	B	609	CLA	CHC-C1C	4.19	1.46	1.38
37	d	408	LHG	O8-C23	4.19	1.45	1.33
36	c	522	DGD	O1G-C1A	4.18	1.45	1.33
24	C	501	CLA	CHD-C1D	4.18	1.46	1.38
24	A	406	CLA	O2D-CGD	4.18	1.43	1.33
24	D	402	CLA	C1D-ND	4.18	1.43	1.37
24	c	513	CLA	CHD-C1D	4.18	1.46	1.38
24	d	401	CLA	CHC-C1C	4.18	1.46	1.38
40	v	205	HEC	CAB-C3B	4.18	1.48	1.35
24	b	618	CLA	O2A-CGA	4.18	1.45	1.33
24	b	625	CLA	C1D-ND	4.18	1.43	1.37
24	c	506	CLA	CHD-C1D	4.17	1.46	1.38
24	D	402	CLA	CHC-C1C	4.17	1.46	1.38
24	B	617	CLA	O2A-CGA	4.17	1.45	1.33
24	B	611	CLA	OBD-CAD	4.17	1.29	1.22
38	F	102	HEM	FE-NC	4.17	2.08	1.95
33	b	629	LMG	O8-C28	4.17	1.45	1.33
37	e	102	LHG	O7-C7	4.16	1.46	1.34
24	B	615	CLA	O2A-CGA	4.16	1.45	1.33
24	d	402	CLA	CHD-C1D	4.16	1.46	1.38
24	b	617	CLA	O2A-CGA	4.16	1.45	1.33
25	a	418[A]	PHO	OBD-CAD	4.16	1.27	1.22
24	C	503	CLA	CHD-C4C	4.16	1.48	1.39
24	b	625	CLA	C3D-C2D	4.16	1.50	1.39
36	C	518	DGD	O1G-C1A	4.15	1.45	1.33
33	d	413	LMG	O7-C10	4.15	1.46	1.34
33	c	501	LMG	O8-C28	4.15	1.45	1.33
24	B	616	CLA	CHC-C4B	4.15	1.48	1.39
24	C	511	CLA	C3D-C2D	4.15	1.50	1.39
24	b	623	CLA	C3D-C2D	4.15	1.50	1.39
24	A	407	CLA	CHC-C4B	4.14	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	L	102	SQD	O48-C23	4.14	1.45	1.33
24	B	607	CLA	CHD-C1D	4.14	1.46	1.38
33	c	523	LMG	O8-C28	4.14	1.45	1.33
37	d	408	LHG	O7-C7	4.14	1.46	1.34
24	b	611	CLA	O2A-CGA	4.13	1.45	1.33
25	a	418[A]	PHO	O2A-CGA	4.13	1.45	1.33
27	a	414	SQD	O48-C23	4.13	1.45	1.33
24	B	607	CLA	O2A-CGA	4.13	1.45	1.33
24	b	623	CLA	O2A-CGA	4.13	1.45	1.33
36	C	517	DGD	O1G-C1A	4.13	1.45	1.33
25	A	409[B]	PHO	O2A-CGA	4.12	1.45	1.33
24	c	518	CLA	CHD-C4C	4.12	1.48	1.39
33	Z	101	LMG	O7-C10	4.12	1.45	1.34
24	A	410	CLA	O2A-CGA	4.12	1.45	1.33
24	c	507	CLA	CHD-C1D	4.12	1.46	1.38
24	c	508	CLA	O2A-CGA	4.12	1.45	1.33
24	b	624	CLA	CHD-C1D	4.12	1.46	1.38
24	C	501	CLA	CHD-C4C	4.12	1.48	1.39
37	E	101	LHG	O7-C7	4.12	1.45	1.34
24	b	625	CLA	CHD-C1D	4.11	1.46	1.38
24	A	406	CLA	O2A-CGA	4.11	1.45	1.33
24	B	612	CLA	CHB-C1B	4.11	1.48	1.39
24	b	617	CLA	CHD-C4C	4.11	1.48	1.39
24	b	625	CLA	O2A-CGA	4.11	1.45	1.33
24	A	407	CLA	CHD-C4C	4.11	1.48	1.39
24	C	502	CLA	CHD-C1D	4.11	1.46	1.38
24	c	508	CLA	CHD-C1D	4.11	1.46	1.38
36	c	521	DGD	O1G-C1A	4.11	1.45	1.33
24	b	617	CLA	CHB-C1B	4.10	1.48	1.39
24	C	506	CLA	C3D-C2D	4.10	1.50	1.39
36	h	102	DGD	O1G-C1A	4.10	1.45	1.33
24	C	510	CLA	O2A-CGA	4.10	1.45	1.33
24	C	505	CLA	CHC-C4B	4.10	1.48	1.39
24	c	516	CLA	C3D-C2D	4.10	1.50	1.39
24	C	510	CLA	CHD-C4C	4.10	1.48	1.39
24	B	613	CLA	C1B-NB	-4.10	1.32	1.37
24	B	612	CLA	C3D-C2D	4.09	1.50	1.39
24	C	504	CLA	C3D-C2D	4.09	1.50	1.39
33	z	101	LMG	O7-C10	4.09	1.45	1.34
24	b	610	CLA	C3D-C2D	4.09	1.50	1.39
37	D	408	LHG	O7-C7	4.09	1.45	1.34
24	B	615	CLA	CHB-C1B	4.09	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	C3D-C2D	4.09	1.50	1.39
24	d	402	CLA	CHD-C4C	4.09	1.48	1.39
24	b	621	CLA	CHD-C1D	4.09	1.46	1.38
24	c	507	CLA	CHD-C4C	4.09	1.48	1.39
24	C	503	CLA	CHC-C4B	4.08	1.48	1.39
40	V	205	HEC	CBC-CAC	-4.08	1.34	1.49
24	C	505	CLA	CHD-C1D	4.08	1.46	1.38
24	B	604	CLA	CHD-C1D	4.08	1.46	1.38
24	c	515	CLA	CHB-C1B	4.07	1.48	1.39
27	F	103	SQD	O48-C23	4.07	1.45	1.33
24	c	506	CLA	O2A-CGA	4.07	1.45	1.33
26	B	619	BCR	C23-C22	-4.07	1.37	1.46
24	C	511	CLA	CHD-C4C	4.07	1.48	1.39
24	a	410	CLA	CHD-C1D	4.07	1.46	1.38
24	C	511	CLA	CHB-C1B	4.06	1.48	1.39
24	b	620	CLA	CHD-C1D	4.06	1.46	1.38
24	C	512	CLA	CHD-C1D	4.06	1.46	1.38
24	d	403	CLA	O2A-CGA	4.06	1.45	1.33
24	a	409	CLA	CHD-C4C	4.06	1.48	1.39
24	B	605	CLA	CHD-C1D	4.06	1.46	1.38
24	c	509	CLA	CHD-C1D	4.06	1.46	1.38
27	A	416	SQD	O47-C7	4.05	1.45	1.34
24	A	407	CLA	OBD-CAD	4.05	1.29	1.22
24	A	407	CLA	O2A-CGA	4.05	1.45	1.33
37	D	409	LHG	O8-C23	4.05	1.45	1.33
24	b	624	CLA	C3D-C2D	4.05	1.50	1.39
40	v	205	HEC	CBB-CAB	-4.05	1.34	1.49
25	A	408	PHO	O2A-CGA	4.05	1.45	1.33
24	d	401	CLA	CHD-C4C	4.05	1.48	1.39
24	a	410	CLA	OBD-CAD	4.05	1.29	1.22
24	B	606	CLA	CHC-C4B	4.05	1.48	1.39
27	B	621	SQD	O48-C23	4.05	1.45	1.33
24	b	619	CLA	O2A-CGA	4.04	1.45	1.33
24	b	612	CLA	CHD-C1D	4.04	1.46	1.38
24	B	614	CLA	CHB-C1B	4.04	1.48	1.39
24	B	612	CLA	CHD-C1D	4.04	1.46	1.38
24	c	514	CLA	OBD-CAD	4.04	1.29	1.22
24	b	612	CLA	OBD-CAD	4.04	1.29	1.22
24	A	406	CLA	C3D-C2D	4.04	1.50	1.39
36	c	522	DGD	O2G-C1B	4.04	1.45	1.34
24	C	505	CLA	O2A-CGA	4.04	1.45	1.33
24	d	402	CLA	C1D-ND	4.04	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	OBD-CAD	4.04	1.29	1.22
36	c	520	DGD	O1G-C1A	4.03	1.45	1.33
24	B	604	CLA	O2A-CGA	4.03	1.45	1.33
24	B	613	CLA	O2A-CGA	4.03	1.45	1.33
37	L	101	LHG	O8-C23	4.03	1.45	1.33
24	C	505	CLA	C1D-ND	4.03	1.43	1.37
24	C	509	CLA	CHD-C4C	4.03	1.48	1.39
24	d	401	CLA	C3D-C2D	4.03	1.50	1.39
24	d	403	CLA	CHD-C1D	4.03	1.46	1.38
24	b	625	CLA	CHB-C1B	4.02	1.48	1.39
24	c	508	CLA	CHC-C4B	4.02	1.48	1.39
24	C	512	CLA	C3D-C2D	4.02	1.50	1.39
24	C	504	CLA	O2A-CGA	4.02	1.45	1.33
24	B	611	CLA	C3D-C2D	4.02	1.50	1.39
24	B	602	CLA	CHD-C4C	4.02	1.48	1.39
33	d	413	LMG	O8-C28	4.02	1.45	1.33
24	B	613	CLA	CHB-C1B	4.02	1.48	1.39
24	a	412	CLA	O2A-CGA	4.02	1.45	1.33
24	C	504	CLA	CHB-C1B	4.01	1.48	1.39
24	D	403	CLA	C3D-C2D	4.01	1.49	1.39
37	D	408	LHG	O8-C23	4.01	1.45	1.33
24	b	616	CLA	CHD-C1D	4.01	1.46	1.38
24	c	507	CLA	O2A-CGA	4.01	1.45	1.33
24	c	517	CLA	C3D-C2D	4.01	1.49	1.39
24	C	508	CLA	CHD-C4C	4.01	1.48	1.39
24	b	614	CLA	CHB-C1B	4.00	1.48	1.39
24	b	621	CLA	C3D-C2D	4.00	1.49	1.39
24	C	513	CLA	CHD-C4C	3.99	1.48	1.39
24	a	412	CLA	C3D-C2D	3.99	1.49	1.39
24	b	614	CLA	CHD-C1D	3.99	1.46	1.38
24	B	614	CLA	O2A-CGA	3.99	1.45	1.33
24	b	622	CLA	CHD-C1D	3.99	1.46	1.38
24	C	503	CLA	C3D-C2D	3.98	1.49	1.39
24	C	504	CLA	CHD-C1D	3.98	1.46	1.38
24	b	612	CLA	CHB-C1B	3.98	1.48	1.39
24	b	616	CLA	C1D-ND	3.98	1.43	1.37
24	b	615	CLA	CHB-C1B	3.98	1.48	1.39
24	D	403	CLA	CHD-C4C	3.98	1.48	1.39
24	b	611	CLA	CHD-C1D	3.98	1.46	1.38
27	A	412	SQD	O47-C7	3.98	1.45	1.34
24	b	620	CLA	O2A-CGA	3.98	1.44	1.33
24	b	613	CLA	CHB-C1B	3.97	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	OBD-CAD	3.97	1.29	1.22
24	A	405	CLA	O2A-CGA	3.96	1.44	1.33
24	c	517	CLA	CHD-C4C	3.96	1.48	1.39
24	D	402	CLA	O2A-CGA	3.96	1.44	1.33
24	b	619	CLA	CHD-C1D	3.96	1.46	1.38
24	C	504	CLA	CHD-C4C	3.96	1.48	1.39
24	b	621	CLA	O2A-CGA	3.96	1.44	1.33
36	H	102	DGD	O2G-C1B	3.96	1.45	1.34
24	a	412	CLA	CHD-C1D	3.96	1.46	1.38
33	c	523	LMG	O7-C10	3.96	1.45	1.34
24	A	405	CLA	OBD-CAD	3.96	1.29	1.22
25	A	409[A]	PHO	O2A-CGA	3.96	1.44	1.33
40	V	205	HEC	CBB-CAB	-3.96	1.34	1.49
24	c	515	CLA	CHD-C4C	3.96	1.48	1.39
24	c	511	CLA	CHD-C4C	3.95	1.48	1.39
24	c	514	CLA	C3D-C2D	3.95	1.49	1.39
33	D	413	LMG	O8-C28	3.95	1.44	1.33
24	c	508	CLA	CHD-C4C	3.95	1.48	1.39
24	c	510	CLA	CHB-C1B	3.95	1.48	1.39
24	b	623	CLA	CHD-C4C	3.95	1.48	1.39
24	c	511	CLA	O2A-CGA	3.95	1.44	1.33
24	B	614	CLA	OBD-CAD	3.94	1.29	1.22
24	b	615	CLA	CHD-C1D	3.94	1.46	1.38
24	b	610	CLA	CHD-C4C	3.94	1.48	1.39
33	B	622	LMG	O7-C10	3.94	1.45	1.34
24	c	513	CLA	OBD-CAD	3.94	1.29	1.22
24	c	512	CLA	C3D-C2D	3.94	1.49	1.39
24	a	410	CLA	C1D-ND	3.93	1.43	1.37
33	C	519	LMG	O7-C10	3.93	1.45	1.34
24	B	603	CLA	CHD-C4C	3.93	1.48	1.39
24	B	611	CLA	O2A-CGA	3.93	1.44	1.33
24	B	602	CLA	C3D-C2D	3.93	1.49	1.39
36	C	516	DGD	O1G-C1A	3.93	1.44	1.33
24	b	615	CLA	O2A-CGA	3.93	1.44	1.33
24	b	615	CLA	CHD-C4C	3.93	1.48	1.39
24	C	508	CLA	C3D-C2D	3.93	1.49	1.39
24	C	513	CLA	CHC-C4B	3.93	1.48	1.39
24	c	506	CLA	CHD-C4C	3.93	1.48	1.39
24	b	618	CLA	OBD-CAD	3.93	1.29	1.22
24	B	605	CLA	O2A-CGA	3.92	1.44	1.33
24	B	609	CLA	CHD-C4C	3.92	1.48	1.39
24	B	602	CLA	CHC-C4B	3.92	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	C3D-C2D	3.92	1.49	1.39
24	c	514	CLA	CHD-C4C	3.92	1.48	1.39
24	B	611	CLA	CHD-C4C	3.92	1.48	1.39
24	B	606	CLA	CHD-C4C	3.91	1.48	1.39
24	d	403	CLA	CHC-C4B	3.91	1.48	1.39
24	A	405	CLA	CHD-C4C	3.91	1.48	1.39
24	c	517	CLA	OBD-CAD	3.91	1.29	1.22
24	c	509	CLA	C3D-C2D	3.91	1.49	1.39
24	a	410	CLA	CHB-C1B	3.91	1.48	1.39
24	c	509	CLA	CHB-C1B	3.91	1.48	1.39
24	B	617	CLA	CHB-C1B	3.91	1.48	1.39
24	A	406	CLA	CHC-C1C	3.91	1.46	1.38
24	D	402	CLA	C3D-C2D	3.91	1.49	1.39
24	c	509	CLA	CHD-C4C	3.91	1.48	1.39
24	B	605	CLA	CHB-C1B	3.90	1.48	1.39
24	B	604	CLA	CHB-C1B	3.90	1.48	1.39
24	a	410	CLA	CHD-C4C	3.90	1.48	1.39
24	A	410	CLA	C3D-C2D	3.90	1.49	1.39
24	b	616	CLA	CHC-C4B	3.90	1.48	1.39
24	B	609	CLA	C3D-C2D	3.90	1.49	1.39
24	B	606	CLA	OBD-CAD	3.90	1.29	1.22
24	c	509	CLA	O2A-CGA	3.89	1.44	1.33
24	C	507	CLA	C3D-C2D	3.89	1.49	1.39
24	B	614	CLA	C3D-C2D	3.89	1.49	1.39
24	B	610	CLA	OBD-CAD	3.89	1.29	1.22
24	c	515	CLA	OBD-CAD	3.89	1.29	1.22
24	A	407	CLA	C3D-C2D	3.89	1.49	1.39
24	b	622	CLA	CHB-C1B	3.88	1.48	1.39
24	B	603	CLA	OBD-CAD	3.88	1.29	1.22
24	C	502	CLA	O2A-CGA	3.88	1.44	1.33
24	A	410	CLA	CHC-C4B	3.88	1.48	1.39
24	b	619	CLA	CHB-C1B	3.88	1.48	1.39
24	D	403	CLA	O2A-CGA	3.88	1.44	1.33
24	B	606	CLA	C3D-C2D	3.88	1.49	1.39
27	A	412	SQD	O48-C23	3.88	1.44	1.33
24	C	501	CLA	OBD-CAD	3.87	1.29	1.22
24	B	603	CLA	O2A-CGA	3.87	1.44	1.33
24	b	614	CLA	O2A-CGA	3.87	1.44	1.33
24	A	410	CLA	OBD-CAD	3.87	1.29	1.22
24	c	513	CLA	CHD-C4C	3.87	1.48	1.39
24	B	604	CLA	CHC-C4B	3.87	1.48	1.39
36	h	102	DGD	O2G-C1B	3.87	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	CLA	C1B-NB	-3.87	1.32	1.37
24	A	410	CLA	CHB-C1B	3.87	1.48	1.39
33	b	629	LMG	O7-C10	3.86	1.45	1.34
24	B	608	CLA	CHD-C1D	3.86	1.45	1.38
24	c	517	CLA	CHC-C4B	3.86	1.48	1.39
24	B	608	CLA	O2A-CGA	3.85	1.44	1.33
24	B	604	CLA	C3D-C2D	3.85	1.49	1.39
37	d	407	LHG	O7-C7	3.85	1.45	1.34
24	c	512	CLA	CHD-C1D	3.85	1.45	1.38
24	b	617	CLA	CHC-C4B	3.84	1.48	1.39
24	b	622	CLA	C3D-C2D	3.84	1.49	1.39
24	C	507	CLA	CHD-C4C	3.84	1.47	1.39
24	a	412	CLA	OBD-CAD	3.84	1.29	1.22
24	c	518	CLA	C3D-C2D	3.84	1.49	1.39
24	b	613	CLA	O2A-CGA	3.84	1.44	1.33
24	b	613	CLA	C3D-C2D	3.84	1.49	1.39
24	d	401	CLA	CHB-C1B	3.84	1.48	1.39
24	A	405	CLA	CHD-C1D	3.84	1.45	1.38
24	C	502	CLA	C3D-C2D	3.83	1.49	1.39
24	B	603	CLA	CHC-C4B	3.83	1.48	1.39
24	c	511	CLA	C3D-C2D	3.83	1.49	1.39
37	D	407	LHG	O8-C23	3.83	1.44	1.33
33	c	501	LMG	O7-C10	3.83	1.45	1.34
24	b	618	CLA	CHD-C4C	3.83	1.47	1.39
24	b	614	CLA	CHD-C4C	3.83	1.47	1.39
24	C	501	CLA	C3D-C2D	3.83	1.49	1.39
24	D	402	CLA	CHD-C1D	3.82	1.45	1.38
24	B	603	CLA	C3D-C2D	3.82	1.49	1.39
24	B	604	CLA	CHD-C4C	3.82	1.47	1.39
24	d	403	CLA	CHD-C4C	3.82	1.47	1.39
36	C	518	DGD	O2G-C1B	3.82	1.45	1.34
24	b	619	CLA	CHC-C4B	3.82	1.48	1.39
24	b	610	CLA	CHC-C4B	3.82	1.48	1.39
24	b	624	CLA	CHD-C4C	3.82	1.47	1.39
24	c	506	CLA	CHB-C1B	3.82	1.48	1.39
24	C	502	CLA	CHD-C4C	3.82	1.47	1.39
24	B	616	CLA	CHD-C1D	3.82	1.45	1.38
24	C	502	CLA	CHB-C1B	3.82	1.48	1.39
36	C	516	DGD	O2G-C1B	3.81	1.45	1.34
37	b	634	LHG	O7-C7	3.81	1.45	1.34
24	b	622	CLA	O2A-CGA	3.81	1.44	1.33
24	C	505	CLA	CHD-C4C	3.81	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	CHC-C4B	3.81	1.48	1.39
24	b	615	CLA	C3D-C2D	3.81	1.49	1.39
24	B	606	CLA	CHB-C1B	3.80	1.47	1.39
24	c	509	CLA	CHC-C4B	3.80	1.47	1.39
27	a	414	SQD	O47-C7	3.80	1.45	1.34
24	c	518	CLA	CHC-C4B	3.80	1.47	1.39
24	C	513	CLA	C3D-C2D	3.79	1.49	1.39
24	D	402	CLA	CHD-C4C	3.79	1.47	1.39
24	b	614	CLA	CHC-C4B	3.79	1.47	1.39
24	b	618	CLA	CHB-C1B	3.79	1.47	1.39
24	B	607	CLA	CHD-C4C	3.79	1.47	1.39
24	c	506	CLA	C3D-C2D	3.79	1.49	1.39
24	B	612	CLA	CHD-C4C	3.79	1.47	1.39
24	B	613	CLA	C1D-ND	3.79	1.42	1.37
24	b	617	CLA	OBD-CAD	3.78	1.29	1.22
24	B	606	CLA	CHD-C1D	3.78	1.45	1.38
24	b	621	CLA	CHB-C1B	3.78	1.47	1.39
24	d	402	CLA	C3D-C2D	3.78	1.49	1.39
24	d	403	CLA	CHB-C1B	3.78	1.47	1.39
36	c	521	DGD	O2G-C1B	3.77	1.44	1.34
24	B	612	CLA	O2A-CGA	3.77	1.44	1.33
24	B	617	CLA	C3D-C2D	3.77	1.49	1.39
24	c	515	CLA	O2A-CGA	3.77	1.44	1.33
36	C	517	DGD	O2G-C1B	3.77	1.44	1.34
24	b	616	CLA	CHD-C4C	3.77	1.47	1.39
24	b	620	CLA	CHD-C4C	3.77	1.47	1.39
24	B	614	CLA	CHC-C4B	3.76	1.47	1.39
24	b	618	CLA	C3D-C2D	3.76	1.49	1.39
24	D	403	CLA	CHB-C1B	3.76	1.47	1.39
24	B	602	CLA	CHB-C1B	3.76	1.47	1.39
24	b	620	CLA	CHB-C1B	3.76	1.47	1.39
37	d	406	LHG	O8-C23	3.76	1.44	1.33
24	C	512	CLA	OBD-CAD	3.76	1.29	1.22
24	b	619	CLA	CHD-C4C	3.75	1.47	1.39
24	B	609	CLA	OBD-CAD	3.75	1.28	1.22
24	b	611	CLA	OBD-CAD	3.75	1.28	1.22
24	A	406	CLA	CHD-C1D	3.75	1.45	1.38
24	c	510	CLA	O2A-CGA	3.75	1.44	1.33
24	a	412	CLA	CHB-C1B	3.75	1.47	1.39
24	c	510	CLA	CHC-C4B	3.75	1.47	1.39
24	C	509	CLA	CHB-C1B	3.74	1.47	1.39
24	C	505	CLA	CHB-C1B	3.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	501	CLA	CHC-C4B	3.74	1.47	1.39
24	B	610	CLA	CHB-C1B	3.74	1.47	1.39
24	B	613	CLA	OBD-CAD	3.74	1.28	1.22
24	c	511	CLA	CHB-C1B	3.74	1.47	1.39
24	B	607	CLA	CHC-C4B	3.74	1.47	1.39
24	b	611	CLA	CHD-C4C	3.74	1.47	1.39
24	C	512	CLA	CHD-C4C	3.74	1.47	1.39
24	C	512	CLA	CHC-C4B	3.73	1.47	1.39
24	C	512	CLA	CHB-C1B	3.73	1.47	1.39
24	A	406	CLA	CHD-C4C	3.73	1.47	1.39
24	b	614	CLA	C3D-C2D	3.73	1.49	1.39
24	C	506	CLA	CHB-C1B	3.72	1.47	1.39
24	b	612	CLA	CHC-C4B	3.72	1.47	1.39
24	c	513	CLA	CHB-C1B	3.72	1.47	1.39
24	B	617	CLA	CHD-C4C	3.72	1.47	1.39
24	B	613	CLA	C3D-C2D	3.72	1.49	1.39
24	B	613	CLA	CHC-C4B	3.72	1.47	1.39
24	C	504	CLA	CHC-C4B	3.72	1.47	1.39
24	B	611	CLA	CHB-C1B	3.72	1.47	1.39
24	b	619	CLA	OBD-CAD	3.72	1.28	1.22
24	B	615	CLA	CHC-C4B	3.71	1.47	1.39
24	b	625	CLA	CHD-C4C	3.71	1.47	1.39
24	B	611	CLA	CHC-C4B	3.71	1.47	1.39
24	b	621	CLA	OBD-CAD	3.71	1.28	1.22
24	B	609	CLA	CHB-C1B	3.71	1.47	1.39
24	a	409	CLA	CHC-C4B	3.70	1.47	1.39
37	L	101	LHG	O7-C7	3.70	1.44	1.34
24	B	610	CLA	CHD-C4C	3.70	1.47	1.39
24	b	616	CLA	O2A-CGA	3.70	1.44	1.33
24	C	508	CLA	OBD-CAD	3.70	1.28	1.22
24	c	515	CLA	C3D-C2D	3.70	1.49	1.39
36	c	520	DGD	O2G-C1B	3.69	1.44	1.34
24	B	614	CLA	CHD-C1D	3.69	1.45	1.38
24	D	402	CLA	CHB-C1B	3.69	1.47	1.39
24	B	615	CLA	C3D-C2D	3.69	1.49	1.39
24	b	621	CLA	CHC-C4B	3.69	1.47	1.39
24	d	402	CLA	OBD-CAD	3.69	1.28	1.22
24	B	613	CLA	CHD-C1D	3.69	1.45	1.38
24	B	604	CLA	OBD-CAD	3.69	1.28	1.22
24	d	402	CLA	CHB-C1B	3.69	1.47	1.39
24	C	510	CLA	CHC-C4B	3.69	1.47	1.39
24	c	512	CLA	CHD-C4C	3.69	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	CHB-C1B	3.68	1.47	1.39
24	C	501	CLA	CHB-C1B	3.68	1.47	1.39
24	b	620	CLA	CHC-C4B	3.68	1.47	1.39
24	c	507	CLA	CHB-C1B	3.68	1.47	1.39
24	b	611	CLA	C3D-C2D	3.68	1.49	1.39
24	C	511	CLA	OBD-CAD	3.68	1.28	1.22
24	b	623	CLA	OBD-CAD	3.68	1.28	1.22
24	C	510	CLA	C3D-C2D	3.68	1.49	1.39
24	B	608	CLA	CHD-C4C	3.68	1.47	1.39
38	F	102	HEM	C4D-ND	-3.67	1.33	1.40
24	A	406	CLA	C1B-NB	-3.67	1.33	1.37
33	D	413	LMG	O7-C10	3.67	1.44	1.34
24	C	509	CLA	CHC-C4B	3.67	1.47	1.39
24	B	608	CLA	CHC-C4B	3.67	1.47	1.39
24	c	512	CLA	CHB-C1B	3.67	1.47	1.39
24	b	620	CLA	C3D-C2D	3.67	1.49	1.39
24	d	403	CLA	C3D-C2D	3.67	1.49	1.39
24	B	612	CLA	CHC-C4B	3.67	1.47	1.39
24	c	510	CLA	CHD-C4C	3.66	1.47	1.39
24	A	410	CLA	CHD-C4C	3.66	1.47	1.39
24	a	412	CLA	C4B-NB	-3.66	1.33	1.37
24	B	615	CLA	CHD-C4C	3.65	1.47	1.39
37	d	407	LHG	O8-C23	3.65	1.44	1.33
24	c	516	CLA	OBD-CAD	3.65	1.28	1.22
24	b	624	CLA	CHB-C1B	3.65	1.47	1.39
24	a	410	CLA	C3D-C2D	3.65	1.48	1.39
24	B	607	CLA	C1B-NB	-3.65	1.33	1.37
24	B	616	CLA	C3D-C2D	3.64	1.48	1.39
24	b	616	CLA	C3D-C2D	3.64	1.48	1.39
24	C	502	CLA	CHC-C4B	3.63	1.47	1.39
24	B	605	CLA	CHC-C4B	3.63	1.47	1.39
24	b	622	CLA	CHD-C4C	3.63	1.47	1.39
24	B	616	CLA	CHB-C1B	3.63	1.47	1.39
24	B	605	CLA	CHD-C4C	3.63	1.47	1.39
24	c	518	CLA	OBD-CAD	3.63	1.28	1.22
24	B	608	CLA	C3D-C2D	3.62	1.48	1.39
37	d	406	LHG	O7-C7	3.62	1.44	1.34
24	a	412	CLA	CHC-C4B	3.62	1.47	1.39
24	c	510	CLA	C3D-C2D	3.62	1.48	1.39
24	B	616	CLA	OBD-CAD	3.62	1.28	1.22
24	D	402	CLA	CHC-C4B	3.62	1.47	1.39
24	d	402	CLA	C1B-NB	-3.61	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	405	CLA	C3D-C2D	3.61	1.48	1.39
24	b	619	CLA	C3D-C2D	3.61	1.48	1.39
24	b	612	CLA	C3D-C2D	3.61	1.48	1.39
35	b	632	HTG	C1'-S1	-3.61	1.76	1.81
24	B	614	CLA	CHD-C4C	3.61	1.47	1.39
24	b	620	CLA	OBD-CAD	3.60	1.28	1.22
24	B	617	CLA	CHC-C4B	3.60	1.47	1.39
24	c	516	CLA	CHC-C4B	3.60	1.47	1.39
24	C	503	CLA	OBD-CAD	3.60	1.28	1.22
24	B	615	CLA	CHD-C1D	3.59	1.45	1.38
24	c	516	CLA	CHD-C4C	3.59	1.47	1.39
24	c	507	CLA	OBD-CAD	3.58	1.28	1.22
24	B	608	CLA	CHB-C1B	3.58	1.47	1.39
24	b	621	CLA	CHD-C4C	3.57	1.47	1.39
24	B	610	CLA	CHC-C4B	3.57	1.47	1.39
24	b	613	CLA	CHC-C4B	3.57	1.47	1.39
24	a	409	CLA	O2A-CGA	3.57	1.43	1.33
35	B	623	HTG	C1'-S1	-3.57	1.76	1.81
24	C	509	CLA	OBD-CAD	3.56	1.28	1.22
24	A	405	CLA	CHC-C4B	3.56	1.47	1.39
24	c	508	CLA	C3D-C2D	3.56	1.48	1.39
24	a	409	CLA	OBD-CAD	3.56	1.28	1.22
24	b	618	CLA	CHC-C4B	3.55	1.47	1.39
24	b	624	CLA	OBD-CAD	3.55	1.28	1.22
24	B	616	CLA	CHD-C4C	3.54	1.47	1.39
24	C	503	CLA	CHB-C1B	3.54	1.47	1.39
24	d	401	CLA	C4B-NB	-3.54	1.33	1.37
24	c	507	CLA	CHC-C4B	3.53	1.47	1.39
24	A	405	CLA	CHB-C1B	3.53	1.47	1.39
24	B	607	CLA	CHB-C1B	3.53	1.47	1.39
24	a	409	CLA	C3D-C2D	3.53	1.48	1.39
24	B	603	CLA	CHB-C1B	3.53	1.47	1.39
24	b	611	CLA	CHC-C4B	3.52	1.47	1.39
24	D	403	CLA	CHC-C4B	3.52	1.47	1.39
24	B	607	CLA	C3D-C2D	3.52	1.48	1.39
24	d	403	CLA	OBD-CAD	3.52	1.28	1.22
24	b	612	CLA	CHD-C4C	3.52	1.47	1.39
24	B	615	CLA	OBD-CAD	3.51	1.28	1.22
24	c	516	CLA	CHB-C1B	3.51	1.47	1.39
24	c	508	CLA	CHB-C1B	3.51	1.47	1.39
24	d	403	CLA	C1B-NB	-3.51	1.33	1.37
24	d	401	CLA	OBD-CAD	3.49	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	624	CLA	CHC-C4B	3.49	1.47	1.39
24	C	507	CLA	OBD-CAD	3.49	1.28	1.22
35	B	632	HTG	C1'-S1	-3.48	1.76	1.81
24	C	513	CLA	OBD-CAD	3.48	1.28	1.22
24	b	622	CLA	OBD-CAD	3.48	1.28	1.22
24	d	401	CLA	CHC-C4B	3.48	1.47	1.39
24	b	616	CLA	CHB-C1B	3.48	1.47	1.39
24	c	518	CLA	CHB-C1B	3.48	1.47	1.39
24	c	511	CLA	C1B-NB	-3.48	1.33	1.37
24	C	513	CLA	CHB-C1B	3.47	1.47	1.39
24	d	402	CLA	CHC-C4B	3.47	1.47	1.39
24	c	514	CLA	CHC-C4B	3.47	1.47	1.39
24	c	509	CLA	OBD-CAD	3.46	1.28	1.22
24	C	504	CLA	C1B-NB	-3.46	1.33	1.37
24	C	510	CLA	OBD-CAD	3.46	1.28	1.22
24	c	515	CLA	CHC-C4B	3.46	1.47	1.39
24	b	623	CLA	CHC-C4B	3.46	1.47	1.39
24	D	403	CLA	OBD-CAD	3.45	1.28	1.22
24	b	625	CLA	OBD-CAD	3.45	1.28	1.22
24	b	611	CLA	CHB-C1B	3.45	1.47	1.39
24	c	512	CLA	CHC-C4B	3.44	1.47	1.39
24	B	602	CLA	OBD-CAD	3.44	1.28	1.22
24	A	406	CLA	CHC-C4B	3.44	1.47	1.39
24	B	617	CLA	OBD-CAD	3.44	1.28	1.22
24	B	612	CLA	OBD-CAD	3.43	1.28	1.22
24	b	623	CLA	CHB-C1B	3.42	1.47	1.39
24	C	506	CLA	C1B-NB	-3.42	1.33	1.37
24	B	605	CLA	C3D-C2D	3.42	1.48	1.39
24	b	616	CLA	C1B-NB	-3.41	1.33	1.37
24	b	625	CLA	CHC-C4B	3.40	1.47	1.39
24	B	611	CLA	C1B-NB	-3.40	1.33	1.37
24	C	505	CLA	C3D-C2D	3.39	1.48	1.39
24	c	511	CLA	CHC-C4B	3.38	1.47	1.39
24	a	409	CLA	CHB-C1B	3.37	1.47	1.39
24	C	508	CLA	CHC-C4B	3.37	1.47	1.39
24	C	506	CLA	CHC-C4B	3.37	1.47	1.39
24	b	610	CLA	CHB-C1B	3.37	1.47	1.39
24	A	406	CLA	CHB-C1B	3.37	1.47	1.39
24	C	505	CLA	C1B-NB	-3.36	1.33	1.37
24	c	512	CLA	OBD-CAD	3.36	1.28	1.22
35	V	206	HTG	C1'-S1	-3.36	1.76	1.81
24	B	615	CLA	C1B-NB	-3.36	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	OBD-CAD	3.35	1.28	1.22
24	c	510	CLA	OBD-CAD	3.35	1.28	1.22
24	C	511	CLA	C1B-C2B	3.35	1.51	1.43
35	d	411	HTG	C1'-S1	-3.34	1.76	1.81
24	c	511	CLA	OBD-CAD	3.34	1.28	1.22
24	c	506	CLA	CHC-C4B	3.34	1.46	1.39
24	B	609	CLA	C4B-NB	-3.34	1.33	1.37
38	F	102	HEM	C1B-NB	-3.34	1.34	1.40
24	b	610	CLA	OBD-CAD	3.34	1.28	1.22
38	e	103	HEM	C4D-ND	-3.33	1.34	1.40
24	b	615	CLA	OBD-CAD	3.33	1.28	1.22
24	b	613	CLA	C1B-NB	-3.33	1.33	1.37
35	B	625	HTG	C1'-S1	-3.33	1.76	1.81
24	a	410	CLA	CHC-C4B	3.33	1.46	1.39
24	C	508	CLA	CHB-C1B	3.32	1.46	1.39
24	B	611	CLA	C4B-NB	-3.32	1.33	1.37
35	D	412	HTG	C1'-S1	-3.32	1.76	1.81
35	b	608	HTG	C1'-S1	-3.31	1.76	1.81
24	c	506	CLA	OBD-CAD	3.30	1.28	1.22
24	B	603	CLA	C1B-NB	-3.30	1.33	1.37
24	C	506	CLA	OBD-CAD	3.30	1.28	1.22
24	A	407	CLA	CHB-C1B	3.30	1.46	1.39
24	B	609	CLA	CHC-C4B	3.30	1.46	1.39
24	c	517	CLA	CHB-C1B	3.29	1.46	1.39
24	b	625	CLA	C4B-NB	-3.29	1.33	1.37
24	B	604	CLA	C1B-NB	-3.29	1.33	1.37
24	c	513	CLA	CHC-C4B	3.28	1.46	1.39
35	c	525	HTG	C1'-S1	-3.28	1.76	1.81
24	b	613	CLA	CHD-C4C	3.28	1.46	1.39
24	A	406	CLA	C4B-NB	-3.27	1.33	1.37
24	C	509	CLA	C1B-NB	-3.27	1.33	1.37
24	c	506	CLA	C1B-NB	-3.26	1.33	1.37
37	D	407	LHG	O7-C7	3.26	1.43	1.34
24	b	615	CLA	CHC-C4B	3.24	1.46	1.39
24	b	618	CLA	C1B-NB	-3.24	1.33	1.37
24	B	613	CLA	C1C-C2C	3.24	1.51	1.44
35	c	526	HTG	C1'-S1	-3.23	1.76	1.81
24	b	616	CLA	C1B-C2B	3.22	1.50	1.43
24	C	508	CLA	C4C-C3C	3.21	1.50	1.45
35	B	633	HTG	C1'-S1	-3.20	1.76	1.81
24	c	516	CLA	C4B-NB	-3.20	1.33	1.37
24	B	610	CLA	C1B-NB	-3.20	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	522	HTG	C1'-S1	-3.19	1.76	1.81
25	a	411	PHO	O2A-CGA	3.19	1.42	1.33
24	b	616	CLA	OBD-CAD	3.18	1.28	1.22
24	B	613	CLA	CHD-C4C	3.18	1.46	1.39
38	e	103	HEM	C1B-NB	-3.18	1.34	1.40
24	b	614	CLA	OBD-CAD	3.17	1.27	1.22
24	b	613	CLA	OBD-CAD	3.16	1.27	1.22
24	B	607	CLA	OBD-CAD	3.16	1.27	1.22
24	C	511	CLA	CHC-C4B	3.16	1.46	1.39
35	C	523	HTG	C1'-S1	-3.16	1.77	1.81
24	b	610	CLA	C1B-NB	-3.15	1.33	1.37
24	c	514	CLA	C1B-NB	-3.15	1.33	1.37
24	C	501	CLA	C1B-NB	-3.15	1.33	1.37
24	C	505	CLA	OBD-CAD	3.14	1.27	1.22
35	b	601	HTG	C1'-S1	-3.14	1.77	1.81
24	c	514	CLA	C1B-C2B	3.14	1.50	1.43
24	b	625	CLA	C1B-C2B	3.13	1.50	1.43
24	A	405	CLA	C4C-C3C	3.13	1.50	1.45
35	b	607	HTG	C1'-S1	-3.13	1.77	1.81
24	b	611	CLA	C1B-NB	-3.12	1.33	1.37
24	c	512	CLA	C4D-CHA	3.11	1.49	1.38
24	B	607	CLA	C4B-NB	-3.10	1.33	1.37
24	b	619	CLA	C4B-NB	-3.10	1.33	1.37
24	b	619	CLA	C1B-NB	-3.09	1.33	1.37
24	b	622	CLA	CHC-C4B	3.09	1.46	1.39
24	B	615	CLA	C4B-NB	-3.09	1.33	1.37
24	b	613	CLA	C1B-C2B	3.09	1.50	1.43
24	b	611	CLA	C4B-NB	-3.08	1.33	1.37
24	A	406	CLA	OBD-CAD	3.08	1.27	1.22
24	B	605	CLA	C1B-C2B	3.07	1.50	1.43
24	b	615	CLA	C1B-NB	-3.07	1.33	1.37
24	C	513	CLA	C1B-NB	-3.06	1.33	1.37
24	A	405	CLA	C4B-NB	-3.06	1.33	1.37
24	c	507	CLA	C4B-NB	-3.06	1.33	1.37
24	c	510	CLA	C1B-NB	-3.06	1.33	1.37
40	V	205	HEC	C1B-NB	-3.05	1.33	1.39
24	b	622	CLA	C1B-C2B	3.05	1.50	1.43
24	c	509	CLA	C1B-NB	-3.04	1.33	1.37
24	b	613	CLA	C4D-CHA	3.04	1.48	1.38
24	c	517	CLA	C1B-NB	-3.03	1.33	1.37
24	C	502	CLA	C1B-NB	-3.02	1.33	1.37
24	c	508	CLA	C1C-C2C	3.02	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	C1B-C2B	3.02	1.50	1.43
24	B	610	CLA	C1B-C2B	3.02	1.50	1.43
24	b	625	CLA	C1B-NB	-3.02	1.33	1.37
24	A	410	CLA	C4B-NB	-3.02	1.33	1.37
24	C	508	CLA	C1B-NB	-3.01	1.33	1.37
40	V	205	HEC	C4D-ND	-3.01	1.33	1.39
24	c	510	CLA	C1B-C2B	3.01	1.50	1.43
24	C	505	CLA	C1B-C2B	3.01	1.50	1.43
24	c	517	CLA	C4B-NB	-3.01	1.33	1.37
24	c	506	CLA	C4B-NB	-3.00	1.33	1.37
24	c	513	CLA	C1B-NB	-3.00	1.33	1.37
24	b	621	CLA	C1B-NB	-2.99	1.33	1.37
24	c	509	CLA	C4B-NB	-2.99	1.33	1.37
24	c	515	CLA	C1B-C2B	2.99	1.50	1.43
24	C	511	CLA	C4C-C3C	2.98	1.50	1.45
24	C	507	CLA	C1B-NB	-2.98	1.33	1.37
24	C	510	CLA	C1B-NB	-2.98	1.33	1.37
24	b	615	CLA	C1B-C2B	2.98	1.50	1.43
24	C	510	CLA	C1B-C2B	2.98	1.50	1.43
24	c	512	CLA	C1B-C2B	2.98	1.50	1.43
24	b	621	CLA	C4B-NB	-2.98	1.33	1.37
24	a	409	CLA	C4C-C3C	2.98	1.50	1.45
24	D	403	CLA	C4B-NB	-2.97	1.34	1.37
24	a	410	CLA	C1B-NB	-2.97	1.34	1.37
24	B	612	CLA	C1B-C2B	2.97	1.50	1.43
24	c	515	CLA	C1B-NB	-2.97	1.34	1.37
24	b	624	CLA	C1B-NB	-2.96	1.34	1.37
24	c	514	CLA	C4B-NB	-2.96	1.34	1.37
24	b	622	CLA	C4B-NB	-2.96	1.34	1.37
24	C	511	CLA	C4B-NB	-2.96	1.34	1.37
24	B	616	CLA	C1B-C2B	2.96	1.50	1.43
24	b	620	CLA	C1B-NB	-2.95	1.34	1.37
24	b	621	CLA	C4D-CHA	2.95	1.48	1.38
24	B	606	CLA	C1C-C2C	2.94	1.50	1.44
25	A	409[A]	PHO	CHA-CBD	-2.94	1.48	1.51
24	C	509	CLA	C1B-C2B	2.93	1.50	1.43
24	a	409	CLA	C1B-NB	-2.93	1.34	1.37
24	A	405	CLA	C1B-NB	-2.92	1.34	1.37
24	c	512	CLA	C4B-NB	-2.92	1.34	1.37
24	C	512	CLA	C1B-C2B	2.92	1.50	1.43
24	b	623	CLA	C1B-NB	-2.91	1.34	1.37
24	b	612	CLA	C1B-C2B	2.91	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	C4D-CHA	2.90	1.48	1.38
24	c	506	CLA	C1B-C2B	2.90	1.49	1.43
24	c	516	CLA	C1B-NB	-2.90	1.34	1.37
25	a	418[A]	PHO	C3A-C2A	-2.90	1.52	1.54
24	c	514	CLA	C4D-CHA	2.90	1.48	1.38
24	B	608	CLA	C1B-C2B	2.90	1.49	1.43
24	a	409	CLA	C4B-NB	-2.90	1.34	1.37
24	B	613	CLA	C4B-NB	-2.90	1.34	1.37
24	c	513	CLA	C1B-C2B	2.89	1.49	1.43
24	b	625	CLA	C4D-CHA	2.89	1.48	1.38
24	c	507	CLA	C1B-C2B	2.89	1.49	1.43
24	b	612	CLA	C4B-NB	-2.89	1.34	1.37
24	C	510	CLA	C4D-CHA	2.88	1.48	1.38
24	c	515	CLA	C4B-NB	-2.88	1.34	1.37
24	B	605	CLA	C4D-CHA	2.88	1.48	1.38
24	C	505	CLA	C4B-NB	-2.87	1.34	1.37
24	C	511	CLA	C4D-CHA	2.87	1.48	1.38
24	A	406	CLA	C4D-CHA	2.87	1.48	1.38
24	B	612	CLA	C1B-NB	-2.87	1.34	1.37
24	b	624	CLA	C1B-C2B	2.87	1.49	1.43
24	B	617	CLA	C4B-NB	-2.86	1.34	1.37
24	A	410	CLA	C1B-NB	-2.86	1.34	1.37
24	b	617	CLA	C1B-C2B	2.86	1.49	1.43
24	A	405	CLA	C1B-C2B	2.86	1.49	1.43
24	B	609	CLA	C1B-C2B	2.85	1.49	1.43
24	B	608	CLA	C1B-NB	-2.85	1.34	1.37
24	A	406	CLA	C1B-C2B	2.85	1.49	1.43
24	B	616	CLA	C1B-NB	-2.85	1.34	1.37
24	b	622	CLA	C4C-C3C	2.84	1.49	1.45
24	b	621	CLA	C1B-C2B	2.84	1.49	1.43
24	B	605	CLA	C1B-NB	-2.84	1.34	1.37
24	c	506	CLA	C4D-CHA	2.84	1.48	1.38
24	C	507	CLA	C4D-CHA	2.83	1.48	1.38
24	C	512	CLA	C1B-NB	-2.83	1.34	1.37
24	A	407	CLA	C1B-NB	-2.83	1.34	1.37
24	B	614	CLA	C4C-C3C	2.83	1.49	1.45
24	D	403	CLA	C1B-C2B	2.83	1.49	1.43
24	D	402	CLA	C1B-C2B	2.83	1.49	1.43
24	c	518	CLA	C4B-NB	-2.82	1.34	1.37
40	V	205	HEC	C1D-ND	-2.81	1.34	1.39
24	B	614	CLA	C4D-CHA	2.81	1.48	1.38
24	c	518	CLA	C1B-NB	-2.80	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	C1B-NB	-2.80	1.34	1.37
24	C	506	CLA	C4B-NB	-2.80	1.34	1.37
24	B	608	CLA	OBD-CAD	2.79	1.27	1.22
24	B	613	CLA	C1B-C2B	2.79	1.49	1.43
24	B	602	CLA	C4B-NB	-2.79	1.34	1.37
24	b	620	CLA	C1B-C2B	2.79	1.49	1.43
24	c	508	CLA	C1B-NB	-2.79	1.34	1.37
24	D	402	CLA	OBD-CAD	2.78	1.27	1.22
24	B	604	CLA	C1B-C2B	2.78	1.49	1.43
24	b	617	CLA	C4D-CHA	2.78	1.47	1.38
24	C	504	CLA	C4B-NB	-2.78	1.34	1.37
24	C	509	CLA	C4B-NB	-2.78	1.34	1.37
24	d	401	CLA	C1B-NB	-2.78	1.34	1.37
24	C	509	CLA	C4D-CHA	2.78	1.47	1.38
24	B	604	CLA	C1C-C2C	2.77	1.50	1.44
24	C	504	CLA	C1B-C2B	2.77	1.49	1.43
24	B	617	CLA	C1B-C2B	2.77	1.49	1.43
24	b	610	CLA	C4B-NB	-2.77	1.34	1.37
24	b	622	CLA	C1B-NB	-2.77	1.34	1.37
24	C	507	CLA	C1C-C2C	2.76	1.50	1.44
24	c	516	CLA	C1B-C2B	2.76	1.49	1.43
24	b	623	CLA	C1B-C2B	2.76	1.49	1.43
24	B	607	CLA	C4D-CHA	2.75	1.47	1.38
24	C	502	CLA	C4D-CHA	2.75	1.47	1.38
24	b	624	CLA	C4D-CHA	2.75	1.47	1.38
31	a	415[B]	PL9	C6-C5	2.75	1.48	1.35
24	A	410	CLA	C1B-C2B	2.74	1.49	1.43
31	a	415[A]	PL9	C6-C5	2.74	1.48	1.35
24	C	504	CLA	C4D-CHA	2.74	1.47	1.38
24	C	506	CLA	C4D-CHA	2.74	1.47	1.38
24	c	511	CLA	C1B-C2B	2.74	1.49	1.43
24	b	615	CLA	C4B-NB	-2.74	1.34	1.37
24	b	620	CLA	C4D-CHA	2.74	1.47	1.38
29	A	417	LMT	O1'-C1'	2.74	1.44	1.40
24	c	513	CLA	C4B-NB	-2.73	1.34	1.37
24	b	612	CLA	C1C-C2C	2.73	1.50	1.44
24	B	611	CLA	C4D-CHA	2.73	1.47	1.38
24	b	613	CLA	C4B-NB	-2.73	1.34	1.37
24	B	607	CLA	C1B-C2B	2.73	1.49	1.43
24	b	614	CLA	C1B-NB	-2.73	1.34	1.37
38	F	102	HEM	C1C-C2C	-2.73	1.39	1.45
31	D	405[B]	PL9	C6-C5	2.73	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	609	CLA	C1B-NB	-2.72	1.34	1.37
24	d	401	CLA	C1B-C2B	2.72	1.49	1.43
24	B	612	CLA	C4D-CHA	2.72	1.47	1.38
31	A	419[B]	PL9	C6-C5	2.72	1.48	1.35
24	B	605	CLA	OBD-CAD	2.72	1.27	1.22
24	B	614	CLA	C1C-C2C	2.72	1.50	1.44
24	B	616	CLA	C4B-NB	-2.71	1.34	1.37
24	c	518	CLA	C1C-C2C	2.71	1.50	1.44
24	C	503	CLA	C1B-NB	-2.71	1.34	1.37
24	B	617	CLA	C1B-NB	-2.71	1.34	1.37
24	B	617	CLA	C4D-CHA	2.71	1.47	1.38
31	A	419[A]	PL9	C6-C5	2.71	1.48	1.35
24	b	610	CLA	C3B-C4B	2.71	1.50	1.42
24	a	412	CLA	C1B-C2B	2.71	1.49	1.43
24	C	501	CLA	C1B-C2B	2.71	1.49	1.43
24	b	622	CLA	C4D-CHA	2.70	1.47	1.38
24	a	412	CLA	C4D-CHA	2.70	1.47	1.38
25	A	409[B]	PHO	CHA-CBD	-2.70	1.48	1.51
31	d	405[A]	PL9	C6-C5	2.70	1.48	1.35
31	d	405[B]	PL9	C6-C5	2.70	1.48	1.35
24	c	511	CLA	C4B-NB	-2.70	1.34	1.37
24	B	610	CLA	C4D-CHA	2.70	1.47	1.38
24	B	607	CLA	C1C-C2C	2.69	1.50	1.44
24	c	512	CLA	C1B-NB	-2.69	1.34	1.37
24	C	513	CLA	C4D-CHA	2.69	1.47	1.38
35	b	631	HTG	C1'-S1	-2.69	1.77	1.81
24	c	506	CLA	C4C-C3C	2.69	1.49	1.45
24	B	604	CLA	C4B-NB	-2.69	1.34	1.37
24	A	410	CLA	C4D-CHA	2.69	1.47	1.38
24	C	512	CLA	C4D-CHA	2.69	1.47	1.38
24	B	614	CLA	C1B-C2B	2.68	1.49	1.43
24	D	403	CLA	C4C-C3C	2.68	1.49	1.45
24	D	402	CLA	C1C-C2C	2.68	1.50	1.44
24	b	610	CLA	C4D-CHA	2.68	1.47	1.38
24	B	606	CLA	C1B-C2B	2.68	1.49	1.43
24	c	510	CLA	C4D-CHA	2.67	1.47	1.38
24	C	513	CLA	C1B-C2B	2.67	1.49	1.43
24	C	503	CLA	C1C-C2C	2.67	1.49	1.44
24	c	515	CLA	C4D-CHA	2.67	1.47	1.38
24	b	615	CLA	C4D-CHA	2.67	1.47	1.38
33	Z	101	LMG	O8-C28	2.67	1.46	1.33
24	b	616	CLA	C4D-CHA	2.66	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	619	CLA	C1B-C2B	2.66	1.49	1.43
24	B	614	CLA	C4B-NB	-2.66	1.34	1.37
24	B	611	CLA	C1B-C2B	2.66	1.49	1.43
24	C	510	CLA	C4B-NB	-2.66	1.34	1.37
25	a	418[A]	PHO	C4B-NB	-2.66	1.33	1.38
24	C	504	CLA	C1C-C2C	2.66	1.49	1.44
40	v	205	HEC	C1D-ND	-2.65	1.34	1.39
24	B	608	CLA	C4D-CHA	2.65	1.47	1.38
24	C	508	CLA	C4D-CHA	2.65	1.47	1.38
24	c	513	CLA	C4D-CHA	2.65	1.47	1.38
24	c	509	CLA	C4D-CHA	2.65	1.47	1.38
24	b	620	CLA	C4C-C3C	2.64	1.49	1.45
24	C	502	CLA	C4B-NB	-2.64	1.34	1.37
24	B	603	CLA	C4D-CHA	2.64	1.47	1.38
24	c	518	CLA	C4C-C3C	2.64	1.49	1.45
25	a	411	PHO	CHA-CBD	-2.64	1.48	1.51
24	B	615	CLA	C1B-C2B	2.64	1.49	1.43
24	C	509	CLA	C4C-C3C	2.64	1.49	1.45
24	A	405	CLA	C4D-CHA	2.64	1.47	1.38
24	B	602	CLA	C4D-CHA	2.63	1.47	1.38
24	A	407	CLA	C3B-C4B	2.63	1.50	1.42
24	c	509	CLA	C1C-C2C	2.63	1.49	1.44
35	B	624	HTG	C1'-S1	-2.63	1.77	1.81
24	B	603	CLA	C4C-C3C	2.63	1.49	1.45
24	C	505	CLA	C4D-CHA	2.62	1.47	1.38
24	d	402	CLA	C1B-C2B	2.62	1.49	1.43
24	b	618	CLA	C4D-CHA	2.62	1.47	1.38
24	a	410	CLA	C1B-C2B	2.62	1.49	1.43
24	B	609	CLA	C4D-CHA	2.61	1.47	1.38
24	B	615	CLA	C4D-CHA	2.61	1.47	1.38
24	d	403	CLA	C1C-C2C	2.61	1.49	1.44
24	b	611	CLA	C1B-C2B	2.60	1.49	1.43
24	B	604	CLA	C4D-CHA	2.60	1.47	1.38
24	A	410	CLA	C1C-C2C	2.60	1.49	1.44
24	d	403	CLA	C1B-C2B	2.60	1.49	1.43
24	C	507	CLA	C1B-C2B	2.60	1.49	1.43
24	C	513	CLA	C3B-C4B	2.60	1.50	1.42
24	C	505	CLA	C1C-C2C	2.60	1.49	1.44
24	b	614	CLA	C1C-C2C	2.60	1.49	1.44
24	B	612	CLA	C4B-NB	-2.59	1.34	1.37
24	a	409	CLA	C4D-CHA	2.59	1.47	1.38
24	b	620	CLA	C4B-NB	-2.59	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	602	CLA	C1B-C2B	2.59	1.49	1.43
24	B	613	CLA	C4D-CHA	2.59	1.47	1.38
24	b	611	CLA	C4D-CHA	2.58	1.47	1.38
24	C	513	CLA	C4B-NB	-2.58	1.34	1.37
31	D	405[A]	PL9	C6-C5	2.58	1.47	1.35
24	B	609	CLA	C4C-C3C	2.58	1.49	1.45
24	c	517	CLA	C1C-C2C	2.58	1.49	1.44
40	v	205	HEC	C1B-NB	-2.58	1.34	1.39
24	B	617	CLA	C4C-C3C	2.58	1.49	1.45
24	b	617	CLA	C1C-C2C	2.57	1.49	1.44
24	c	516	CLA	C4D-CHA	2.57	1.47	1.38
24	c	517	CLA	C4D-CHA	2.57	1.47	1.38
24	c	512	CLA	C1C-C2C	2.57	1.49	1.44
24	a	410	CLA	C1C-C2C	2.57	1.49	1.44
24	c	510	CLA	C4C-C3C	2.56	1.49	1.45
24	c	509	CLA	C1B-C2B	2.56	1.49	1.43
24	B	615	CLA	C1C-C2C	2.56	1.49	1.44
24	d	403	CLA	C4B-NB	-2.56	1.34	1.37
24	C	509	CLA	C1C-C2C	2.56	1.49	1.44
24	c	518	CLA	C3B-C4B	2.55	1.50	1.42
24	D	402	CLA	C4B-NB	-2.55	1.34	1.37
24	c	508	CLA	C3B-C4B	2.55	1.50	1.42
24	B	616	CLA	C4D-CHA	2.55	1.47	1.38
24	C	506	CLA	C4C-C3C	2.55	1.49	1.45
24	C	510	CLA	C4C-C3C	2.55	1.49	1.45
24	b	612	CLA	C4D-CHA	2.55	1.47	1.38
24	b	615	CLA	C1C-C2C	2.55	1.49	1.44
24	C	511	CLA	C1B-NB	-2.55	1.34	1.37
24	c	518	CLA	C1B-C2B	2.55	1.49	1.43
24	a	412	CLA	C1B-NB	-2.54	1.34	1.37
24	c	508	CLA	C3D-C4D	-2.54	1.38	1.44
24	C	503	CLA	C3B-C4B	2.54	1.50	1.42
24	d	403	CLA	C4D-CHA	2.53	1.47	1.38
24	c	518	CLA	C4D-CHA	2.53	1.47	1.38
24	D	403	CLA	C4D-CHA	2.53	1.47	1.38
24	d	401	CLA	C4D-CHA	2.52	1.47	1.38
24	D	402	CLA	C4C-C3C	2.52	1.49	1.45
24	C	501	CLA	C4D-CHA	2.52	1.47	1.38
24	b	616	CLA	C3B-C4B	2.52	1.50	1.42
24	c	508	CLA	C4B-NB	-2.52	1.34	1.37
24	b	617	CLA	C1B-NB	-2.51	1.34	1.37
25	a	418[B]	PHO	C4B-NB	-2.51	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	C1C-C2C	2.51	1.49	1.44
24	c	511	CLA	C4D-CHA	2.51	1.47	1.38
24	b	621	CLA	C3B-C2B	2.51	1.49	1.41
24	B	605	CLA	C3B-C2B	2.51	1.49	1.41
24	C	508	CLA	C1C-C2C	2.51	1.49	1.44
24	C	508	CLA	C3B-C4B	2.50	1.50	1.42
24	c	508	CLA	C4D-CHA	2.50	1.47	1.38
24	B	603	CLA	C1B-C2B	2.50	1.49	1.43
24	B	602	CLA	C3B-C4B	2.50	1.50	1.42
24	C	508	CLA	C1B-C2B	2.50	1.49	1.43
24	c	515	CLA	C4C-C3C	2.50	1.49	1.45
24	D	402	CLA	C4D-CHA	2.50	1.47	1.38
24	A	410	CLA	C4C-C3C	2.50	1.49	1.45
24	c	507	CLA	C1B-NB	-2.49	1.34	1.37
24	d	402	CLA	C4D-CHA	2.49	1.47	1.38
24	C	508	CLA	C4B-NB	-2.49	1.34	1.37
24	C	501	CLA	C4B-NB	-2.49	1.34	1.37
25	A	409[B]	PHO	C3A-C2A	-2.49	1.52	1.54
24	d	403	CLA	C4C-C3C	2.49	1.49	1.45
24	A	407	CLA	C1C-C2C	2.49	1.49	1.44
24	c	510	CLA	C3B-C4B	2.49	1.50	1.42
24	B	616	CLA	C1C-C2C	2.49	1.49	1.44
24	A	407	CLA	C4D-CHA	2.48	1.46	1.38
24	C	503	CLA	C4D-CHA	2.48	1.46	1.38
24	b	619	CLA	C4D-CHA	2.48	1.46	1.38
25	a	418[B]	PHO	C3A-C2A	-2.48	1.52	1.54
40	V	205	HEC	C4B-NB	-2.48	1.34	1.39
24	A	407	CLA	C1B-C2B	2.48	1.48	1.43
24	B	606	CLA	C4D-CHA	2.48	1.46	1.38
24	b	622	CLA	C1C-C2C	2.47	1.49	1.44
24	b	617	CLA	C4B-NB	-2.47	1.34	1.37
24	C	512	CLA	C1C-C2C	2.47	1.49	1.44
24	b	614	CLA	C4D-CHA	2.47	1.46	1.38
24	c	510	CLA	C1C-C2C	2.47	1.49	1.44
24	C	505	CLA	C3D-C4D	-2.47	1.38	1.44
24	c	511	CLA	C3D-C4D	-2.47	1.38	1.44
24	b	614	CLA	C3D-C4D	-2.47	1.38	1.44
24	b	614	CLA	C3B-C4B	2.46	1.49	1.42
24	C	506	CLA	C1B-C2B	2.45	1.48	1.43
24	B	612	CLA	C1C-C2C	2.45	1.49	1.44
24	a	410	CLA	C3B-C4B	2.45	1.49	1.42
38	e	103	HEM	C3C-C4C	-2.44	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	409	CLA	C1B-C2B	2.44	1.48	1.43
24	B	611	CLA	C4C-C3C	2.44	1.49	1.45
24	B	617	CLA	C3D-C4D	-2.44	1.38	1.44
24	D	403	CLA	C1B-NB	-2.44	1.34	1.37
24	c	517	CLA	C3B-C4B	2.44	1.49	1.42
38	F	102	HEM	C1D-ND	-2.43	1.34	1.38
24	B	603	CLA	C3D-C4D	-2.43	1.38	1.44
40	v	205	HEC	C4D-ND	-2.43	1.35	1.39
24	b	622	CLA	C3D-C4D	-2.43	1.38	1.44
24	d	402	CLA	C3D-C4D	-2.43	1.38	1.44
24	b	618	CLA	C3D-C4D	-2.42	1.38	1.44
24	a	409	CLA	C1C-C2C	2.42	1.49	1.44
24	A	405	CLA	C1C-C2C	2.42	1.49	1.44
24	a	410	CLA	C4D-CHA	2.42	1.46	1.38
24	C	503	CLA	C1B-C2B	2.41	1.48	1.43
24	b	614	CLA	C4B-NB	-2.41	1.34	1.37
24	C	504	CLA	C4C-C3C	2.41	1.49	1.45
24	B	607	CLA	C4C-C3C	2.41	1.49	1.45
24	C	504	CLA	C3B-C2B	2.41	1.49	1.41
25	A	409[A]	PHO	C1B-NB	-2.41	1.34	1.38
24	B	606	CLA	C1B-NB	-2.40	1.34	1.37
24	b	611	CLA	C3B-C4B	2.40	1.49	1.42
24	c	507	CLA	C4C-C3C	2.40	1.49	1.45
24	d	402	CLA	C4B-NB	-2.40	1.34	1.37
24	C	509	CLA	C3B-C2B	2.39	1.49	1.41
25	a	411	PHO	C4B-NB	-2.39	1.34	1.38
24	B	608	CLA	C4B-NB	-2.39	1.34	1.37
24	B	608	CLA	C4C-C3C	2.39	1.49	1.45
24	c	513	CLA	C3B-C2B	2.39	1.49	1.41
24	C	510	CLA	C1C-C2C	2.39	1.49	1.44
24	C	506	CLA	C3D-C4D	-2.39	1.38	1.44
36	D	406	DGD	O3G-C1D	2.39	1.44	1.40
24	B	603	CLA	C4B-NB	-2.39	1.34	1.37
25	A	409[A]	PHO	C3A-C2A	-2.39	1.52	1.54
24	C	507	CLA	C3B-C4B	2.38	1.49	1.42
24	B	614	CLA	C1B-NB	-2.38	1.34	1.37
24	C	501	CLA	C1C-C2C	2.38	1.49	1.44
24	b	610	CLA	C1B-C2B	2.38	1.48	1.43
24	c	508	CLA	C4C-C3C	2.38	1.49	1.45
24	A	406	CLA	C3D-C4D	-2.38	1.38	1.44
24	B	615	CLA	C3D-C4D	-2.38	1.38	1.44
24	a	410	CLA	C4B-NB	-2.38	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	625	CLA	C1C-NC	-2.37	1.34	1.37
24	C	512	CLA	C4B-NB	-2.37	1.34	1.37
24	B	617	CLA	C3B-C2B	2.37	1.49	1.41
24	B	603	CLA	C1C-C2C	2.37	1.49	1.44
24	B	611	CLA	C3B-C4B	2.37	1.49	1.42
24	b	621	CLA	C1C-C2C	2.37	1.49	1.44
24	C	513	CLA	C3D-C4D	-2.36	1.38	1.44
24	c	510	CLA	C3D-C4D	-2.36	1.38	1.44
24	C	501	CLA	C3B-C4B	2.36	1.49	1.42
24	C	513	CLA	C4C-C3C	2.36	1.49	1.45
24	B	613	CLA	C3B-C2B	2.36	1.49	1.41
24	b	618	CLA	C4B-NB	-2.36	1.34	1.37
24	b	617	CLA	C4C-C3C	2.35	1.49	1.45
24	C	507	CLA	C4B-NB	-2.35	1.34	1.37
24	c	508	CLA	C1B-C2B	2.35	1.48	1.43
24	c	507	CLA	C1C-C2C	2.35	1.49	1.44
24	B	610	CLA	C3B-C4B	2.35	1.49	1.42
24	D	403	CLA	C3D-C4D	-2.35	1.38	1.44
24	c	511	CLA	C3B-C2B	2.35	1.49	1.41
24	b	611	CLA	C4C-C3C	2.35	1.49	1.45
24	B	614	CLA	C3B-C2B	2.35	1.49	1.41
24	b	614	CLA	C1B-C2B	2.35	1.48	1.43
24	C	502	CLA	C4C-C3C	2.34	1.49	1.45
24	B	615	CLA	C4C-C3C	2.34	1.49	1.45
25	A	409[B]	PHO	C1B-NB	-2.34	1.34	1.38
24	b	617	CLA	C3B-C4B	2.34	1.49	1.42
24	B	610	CLA	C4C-C3C	2.34	1.49	1.45
24	d	402	CLA	C4C-C3C	2.34	1.49	1.45
24	B	609	CLA	C1C-C2C	2.34	1.49	1.44
24	b	621	CLA	C1C-NC	-2.34	1.34	1.37
24	b	612	CLA	C3B-C4B	2.33	1.49	1.42
24	b	616	CLA	C3D-C4D	-2.33	1.38	1.44
24	c	512	CLA	C4C-C3C	2.33	1.49	1.45
24	c	515	CLA	C3B-C2B	2.33	1.49	1.41
24	a	412	CLA	C3B-C4B	2.33	1.49	1.42
24	D	403	CLA	C1C-C2C	2.33	1.49	1.44
24	c	515	CLA	C1C-C2C	2.33	1.49	1.44
24	C	513	CLA	C1C-C2C	2.33	1.49	1.44
24	b	619	CLA	C3B-C2B	2.32	1.49	1.41
24	b	611	CLA	C1C-C2C	2.32	1.49	1.44
24	b	623	CLA	C4C-C3C	2.32	1.49	1.45
24	C	511	CLA	C1C-C2C	2.32	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	C4C-C3C	2.32	1.49	1.45
24	c	509	CLA	C3D-C4D	-2.32	1.39	1.44
24	b	616	CLA	C1C-C2C	2.32	1.49	1.44
24	b	618	CLA	C1B-C2B	2.32	1.48	1.43
25	A	409[B]	PHO	C4B-NB	-2.32	1.34	1.38
36	h	102	DGD	O5D-C1E	2.31	1.44	1.40
24	A	405	CLA	C3B-C2B	2.31	1.49	1.41
40	v	205	HEC	C1D-C2D	2.31	1.48	1.43
24	c	517	CLA	C1B-C2B	2.31	1.48	1.43
24	C	508	CLA	C3B-C2B	2.31	1.49	1.41
24	C	505	CLA	C4C-C3C	2.31	1.49	1.45
24	B	605	CLA	C1C-C2C	2.31	1.49	1.44
24	c	515	CLA	C3D-C4D	-2.30	1.39	1.44
24	B	608	CLA	C1C-C2C	2.30	1.49	1.44
24	b	624	CLA	C3B-C4B	2.30	1.49	1.42
24	c	514	CLA	C4C-C3C	2.30	1.48	1.45
25	a	418[A]	PHO	CHA-CBD	-2.30	1.49	1.51
24	b	613	CLA	C4C-C3C	2.30	1.48	1.45
24	b	613	CLA	C1C-C2C	2.30	1.49	1.44
24	C	501	CLA	C4C-C3C	2.30	1.48	1.45
24	C	503	CLA	C4C-C3C	2.30	1.48	1.45
24	c	514	CLA	C1C-C2C	2.30	1.49	1.44
24	B	609	CLA	C3D-C4D	-2.29	1.39	1.44
24	b	624	CLA	C4C-C3C	2.29	1.48	1.45
24	C	504	CLA	C3D-C4D	-2.29	1.39	1.44
24	B	611	CLA	C1C-NC	-2.29	1.34	1.37
24	B	606	CLA	C3B-C4B	2.29	1.49	1.42
25	A	409[A]	PHO	C4B-NB	-2.29	1.34	1.38
24	C	510	CLA	C3D-C4D	-2.29	1.39	1.44
24	a	409	CLA	C3B-C2B	2.29	1.48	1.41
24	C	507	CLA	C4C-C3C	2.29	1.48	1.45
24	D	402	CLA	C3B-C2B	2.29	1.48	1.41
24	B	602	CLA	C1B-NB	-2.29	1.34	1.37
24	b	622	CLA	C3B-C2B	2.29	1.48	1.41
24	b	617	CLA	C3D-C4D	-2.28	1.39	1.44
24	c	513	CLA	C3D-C4D	-2.28	1.39	1.44
24	C	505	CLA	C3B-C4B	2.28	1.49	1.42
24	b	617	CLA	C3B-C2B	2.28	1.48	1.41
37	d	406	LHG	O7-C5	-2.28	1.41	1.46
24	b	616	CLA	C4B-NB	-2.27	1.34	1.37
24	c	518	CLA	C3D-C4D	-2.27	1.39	1.44
24	C	509	CLA	C3B-C4B	2.27	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	619	CLA	C4C-C3C	2.27	1.48	1.45
24	b	619	CLA	C3B-C4B	2.27	1.49	1.42
24	B	602	CLA	C1C-C2C	2.27	1.49	1.44
24	c	517	CLA	C4C-C3C	2.27	1.48	1.45
24	D	402	CLA	C3D-C4D	-2.27	1.39	1.44
24	C	502	CLA	C3B-C4B	2.27	1.49	1.42
24	b	610	CLA	C1C-C2C	2.26	1.49	1.44
24	C	512	CLA	C3B-C4B	2.26	1.49	1.42
24	B	606	CLA	C3D-C4D	-2.26	1.39	1.44
24	b	619	CLA	C3D-C4D	-2.26	1.39	1.44
24	b	615	CLA	C3B-C2B	2.26	1.48	1.41
24	B	609	CLA	C3B-C4B	2.26	1.49	1.42
24	b	620	CLA	C3D-C4D	-2.26	1.39	1.44
24	c	516	CLA	C4C-C3C	2.26	1.48	1.45
24	B	606	CLA	C4B-NB	-2.26	1.34	1.37
24	b	618	CLA	C1C-C2C	2.26	1.49	1.44
24	c	507	CLA	C3B-C4B	2.26	1.49	1.42
24	B	607	CLA	C3D-C4D	-2.25	1.39	1.44
24	c	512	CLA	C3B-C2B	2.25	1.48	1.41
24	A	410	CLA	C3D-C4D	-2.25	1.39	1.44
24	c	514	CLA	C3B-C2B	2.24	1.48	1.41
24	a	412	CLA	C4C-C3C	2.24	1.48	1.45
25	a	418[B]	PHO	CHA-CBD	-2.24	1.49	1.51
24	b	625	CLA	C3B-C2B	2.24	1.48	1.41
24	b	612	CLA	C3D-C4D	-2.24	1.39	1.44
24	B	605	CLA	C4C-C3C	2.24	1.48	1.45
24	a	410	CLA	C3D-C4D	-2.24	1.39	1.44
25	a	411	PHO	C3A-C2A	-2.24	1.52	1.54
24	B	616	CLA	C3B-C4B	2.24	1.49	1.42
24	c	509	CLA	C3B-C2B	2.23	1.48	1.41
24	d	403	CLA	C3D-C4D	-2.23	1.39	1.44
24	C	509	CLA	C3D-C4D	-2.23	1.39	1.44
40	v	205	HEC	C4B-NB	-2.23	1.35	1.39
24	A	406	CLA	C3B-C2B	2.23	1.48	1.41
24	d	401	CLA	C3B-C2B	2.23	1.48	1.41
24	B	611	CLA	C3D-C4D	-2.23	1.39	1.44
24	c	506	CLA	C3D-C4D	-2.23	1.39	1.44
24	C	508	CLA	C3D-C4D	-2.23	1.39	1.44
35	b	607	HTG	C1-S1	-2.23	1.77	1.80
24	C	510	CLA	C3B-C2B	2.22	1.48	1.41
25	A	408	PHO	C4B-NB	-2.22	1.34	1.38
24	B	610	CLA	C3D-C4D	-2.22	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	CLA	C4B-NB	-2.22	1.34	1.37
24	b	612	CLA	C3B-C2B	2.22	1.48	1.41
24	c	516	CLA	C3B-C4B	2.22	1.49	1.42
24	C	507	CLA	C3D-C4D	-2.22	1.39	1.44
24	B	604	CLA	C3D-C4D	-2.22	1.39	1.44
24	a	410	CLA	C4C-C3C	2.22	1.48	1.45
24	b	620	CLA	C3B-C2B	2.22	1.48	1.41
24	c	510	CLA	C4B-NB	-2.22	1.34	1.37
24	a	409	CLA	C3D-C4D	-2.22	1.39	1.44
24	b	610	CLA	C3D-C4D	-2.22	1.39	1.44
25	a	411	PHO	CBD-CGD	-2.21	1.49	1.52
24	a	412	CLA	C1C-C2C	2.21	1.49	1.44
24	c	506	CLA	C3B-C2B	2.21	1.48	1.41
24	C	503	CLA	C3D-C4D	-2.21	1.39	1.44
24	A	407	CLA	C4C-C3C	2.21	1.48	1.45
24	c	516	CLA	C3B-C2B	2.21	1.48	1.41
31	d	405[A]	PL9	C2-C3	2.21	1.40	1.34
38	e	103	HEM	C1C-C2C	-2.21	1.41	1.45
25	a	418[B]	PHO	C1B-NB	-2.20	1.34	1.38
24	c	512	CLA	C3D-C4D	-2.20	1.39	1.44
24	c	517	CLA	C3D-C4D	-2.20	1.39	1.44
35	c	525	HTG	C1-S1	-2.20	1.77	1.80
31	a	415[A]	PL9	C2-C3	2.20	1.40	1.34
24	A	407	CLA	C3D-C4D	-2.20	1.39	1.44
24	B	607	CLA	C3B-C2B	2.20	1.48	1.41
25	A	408	PHO	C1B-NB	-2.19	1.34	1.38
25	A	409[A]	PHO	C1D-ND	-2.19	1.34	1.38
24	B	603	CLA	C3B-C2B	2.19	1.48	1.41
24	b	624	CLA	C1C-C2C	2.19	1.49	1.44
24	c	514	CLA	C3D-C4D	-2.19	1.39	1.44
24	c	511	CLA	C4C-C3C	2.19	1.48	1.45
24	b	623	CLA	C4D-CHA	2.19	1.45	1.38
24	b	624	CLA	C3D-C4D	-2.19	1.39	1.44
24	D	403	CLA	C3B-C4B	2.19	1.49	1.42
24	b	610	CLA	C3B-C2B	2.19	1.48	1.41
24	b	612	CLA	C4C-C3C	2.19	1.48	1.45
24	b	613	CLA	C3B-C2B	2.19	1.48	1.41
24	B	616	CLA	C3D-C4D	-2.19	1.39	1.44
24	d	401	CLA	C1C-NC	-2.18	1.34	1.37
25	A	408	PHO	C3A-C2A	-2.18	1.52	1.54
24	b	623	CLA	C3D-C4D	-2.18	1.39	1.44
24	b	621	CLA	C4C-C3C	2.18	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	C3D-C4D	-2.17	1.39	1.44
35	D	412	HTG	C1-S1	-2.17	1.77	1.80
24	D	403	CLA	C3B-C2B	2.17	1.48	1.41
35	b	632	HTG	C1-S1	-2.17	1.77	1.80
24	b	620	CLA	C3B-C4B	2.17	1.49	1.42
24	B	602	CLA	C3B-C2B	2.17	1.48	1.41
25	A	409[B]	PHO	C3D-C4D	-2.17	1.38	1.41
24	A	410	CLA	C3B-C2B	2.17	1.48	1.41
24	b	625	CLA	C3D-C4D	-2.16	1.39	1.44
24	C	502	CLA	C3B-C2B	2.16	1.48	1.41
24	C	507	CLA	C3B-C2B	2.16	1.48	1.41
31	D	405[B]	PL9	C2-C3	2.16	1.40	1.34
24	B	603	CLA	C3B-C4B	2.16	1.49	1.42
35	d	411	HTG	C1-S1	-2.16	1.77	1.80
38	e	103	HEM	C1D-ND	-2.16	1.34	1.38
24	B	612	CLA	C4C-C3C	2.16	1.48	1.45
24	A	410	CLA	C3B-C4B	2.16	1.49	1.42
31	A	419[A]	PL9	C2-C3	2.16	1.40	1.34
24	c	517	CLA	C3B-C2B	2.15	1.48	1.41
24	b	624	CLA	C4B-NB	-2.15	1.35	1.37
24	B	604	CLA	C3B-C2B	2.15	1.48	1.41
24	c	513	CLA	C4C-C3C	2.15	1.48	1.45
24	b	623	CLA	C1C-C2C	2.15	1.48	1.44
24	B	611	CLA	C1C-C2C	2.15	1.48	1.44
24	b	621	CLA	C3B-C4B	2.15	1.49	1.42
24	d	403	CLA	C3B-C4B	2.15	1.49	1.42
31	d	405[B]	PL9	C2-C3	2.15	1.40	1.34
24	C	501	CLA	C3D-C4D	-2.14	1.39	1.44
35	b	608	HTG	C1-S1	-2.14	1.77	1.80
24	c	507	CLA	C3D-C4D	-2.14	1.39	1.44
26	b	628	BCR	C30-C25	-2.14	1.51	1.53
24	b	623	CLA	C3B-C2B	2.14	1.48	1.41
35	C	522	HTG	C1-S1	-2.14	1.77	1.80
24	A	406	CLA	C1C-C2C	2.14	1.48	1.44
24	d	401	CLA	C1C-C2C	2.13	1.48	1.44
31	a	415[B]	PL9	C2-C3	2.13	1.40	1.34
24	C	511	CLA	C3B-C2B	2.13	1.48	1.41
24	A	407	CLA	C3B-C2B	2.13	1.48	1.41
24	b	611	CLA	C3D-C4D	-2.13	1.39	1.44
24	b	615	CLA	C3B-C4B	2.13	1.48	1.42
24	b	615	CLA	C3D-C4D	-2.12	1.39	1.44
40	v	205	HEC	C4A-C3A	-2.12	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	619	CLA	C1C-C2C	2.12	1.48	1.44
24	c	513	CLA	C1C-C2C	2.12	1.48	1.44
24	C	506	CLA	C1C-C2C	2.12	1.48	1.44
24	c	513	CLA	C3B-C4B	2.12	1.48	1.42
24	B	605	CLA	C3D-C4D	-2.12	1.39	1.44
24	B	605	CLA	C1A-CHA	2.12	1.51	1.43
24	a	412	CLA	C3D-C4D	-2.12	1.39	1.44
24	b	614	CLA	C3B-C2B	2.12	1.48	1.41
25	a	418[A]	PHO	C1B-NB	-2.11	1.34	1.38
24	C	504	CLA	C3B-C4B	2.11	1.48	1.42
24	c	507	CLA	C3B-C2B	2.11	1.48	1.41
29	M	103	LMT	O1'-C1'	2.11	1.43	1.40
24	c	510	CLA	C3B-C2B	2.11	1.48	1.41
24	b	618	CLA	C4C-C3C	2.11	1.48	1.45
24	d	403	CLA	C3B-C2B	2.11	1.48	1.41
24	b	610	CLA	C4C-C3C	2.11	1.48	1.45
24	b	619	CLA	C1C-NC	-2.11	1.34	1.37
24	B	613	CLA	C3D-C4D	-2.10	1.39	1.44
24	c	506	CLA	C1C-C2C	2.10	1.48	1.44
24	B	602	CLA	C1D-C2D	2.10	1.49	1.45
24	C	512	CLA	C3B-C2B	2.09	1.48	1.41
24	C	513	CLA	C3B-C2B	2.09	1.48	1.41
24	c	516	CLA	C1C-C2C	2.09	1.48	1.44
24	C	512	CLA	C4C-C3C	2.09	1.48	1.45
24	B	612	CLA	C3B-C2B	2.08	1.48	1.41
38	e	103	HEM	C3B-C4B	2.08	1.49	1.44
24	C	510	CLA	C3B-C4B	2.08	1.48	1.42
24	c	509	CLA	C4C-C3C	2.08	1.48	1.45
24	c	511	CLA	C1C-C2C	2.08	1.48	1.44
24	A	405	CLA	C3B-C4B	2.08	1.48	1.42
36	H	102	DGD	O5D-C1E	2.08	1.43	1.40
24	B	617	CLA	C1C-C2C	2.08	1.48	1.44
24	b	611	CLA	C3B-C2B	2.08	1.48	1.41
31	A	419[B]	PL9	C2-C3	2.07	1.39	1.34
35	c	526	HTG	C1-S1	-2.07	1.77	1.80
24	b	613	CLA	C3B-C4B	2.07	1.48	1.42
24	C	505	CLA	C3B-C2B	2.07	1.48	1.41
24	B	608	CLA	C3B-C4B	2.07	1.48	1.42
24	B	607	CLA	C3B-C4B	2.07	1.48	1.42
24	d	401	CLA	C3D-C4D	-2.06	1.39	1.44
24	C	511	CLA	C3D-C4D	-2.06	1.39	1.44
24	c	507	CLA	C1C-NC	-2.06	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	402	CLA	C3B-C2B	2.05	1.48	1.41
24	B	602	CLA	C3D-C4D	-2.05	1.39	1.44
24	B	608	CLA	C3B-C2B	2.04	1.48	1.41
24	A	406	CLA	C4C-C3C	2.04	1.48	1.45
35	B	632	HTG	C1-S1	-2.04	1.77	1.80
24	B	606	CLA	C4C-C3C	2.04	1.48	1.45
35	V	206	HTG	C1-S1	-2.04	1.77	1.80
24	B	605	CLA	C3B-C4B	2.04	1.48	1.42
24	a	410	CLA	C3B-C2B	2.04	1.48	1.41
24	B	610	CLA	C4B-NB	-2.03	1.35	1.37
25	A	409[B]	PHO	C1D-ND	-2.03	1.34	1.38
31	D	405[A]	PL9	C2-C3	2.03	1.39	1.34
24	B	610	CLA	C1C-C2C	2.03	1.48	1.44
24	b	623	CLA	C4B-NB	-2.03	1.35	1.37
24	A	405	CLA	C3D-C4D	-2.03	1.39	1.44
40	V	205	HEC	C1D-C2D	2.03	1.47	1.43
24	C	506	CLA	C3B-C2B	2.02	1.48	1.41
24	C	502	CLA	C3D-C4D	-2.02	1.39	1.44
24	b	624	CLA	C3B-C2B	2.02	1.48	1.41
24	B	615	CLA	C3B-C4B	2.02	1.48	1.42
29	B	635	LMT	O1'-C1'	2.01	1.43	1.40
24	C	512	CLA	C3D-C4D	-2.01	1.39	1.44
24	B	609	CLA	C3B-C2B	2.01	1.47	1.41
24	C	503	CLA	C3B-C2B	2.01	1.47	1.41
24	B	611	CLA	C3B-C2B	2.01	1.47	1.41
24	b	619	CLA	C1D-C2D	2.00	1.49	1.45
24	d	403	CLA	C1D-C2D	2.00	1.49	1.45
24	b	622	CLA	C3B-C4B	2.00	1.48	1.42

All (2921) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	409[B]	PHO	C2D-C1D-ND	11.23	117.55	109.43
25	A	409[A]	PHO	C2D-C1D-ND	11.13	117.47	109.43
25	A	408	PHO	C2D-C1D-ND	11.01	117.39	109.43
25	a	418[A]	PHO	C2D-C1D-ND	10.87	117.29	109.43
24	B	613	CLA	C1D-ND-C4D	-10.81	98.72	106.31
25	a	418[B]	PHO	C2D-C1D-ND	10.80	117.24	109.43
24	a	410	CLA	C1D-ND-C4D	-10.65	98.84	106.31
24	b	614	CLA	C1D-ND-C4D	-10.45	98.98	106.31
24	A	407	CLA	C1D-ND-C4D	-10.30	99.08	106.31
25	a	411	PHO	C2D-C1D-ND	10.26	116.84	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	C1D-ND-C4D	-10.16	99.18	106.31
24	c	508	CLA	C1D-ND-C4D	-10.04	99.27	106.31
24	B	616	CLA	C1D-ND-C4D	-9.92	99.35	106.31
24	C	503	CLA	C1D-ND-C4D	-9.84	99.41	106.31
24	C	501	CLA	C1D-ND-C4D	-9.82	99.42	106.31
24	c	516	CLA	C1D-ND-C4D	-9.78	99.45	106.31
24	b	618	CLA	C1D-ND-C4D	-9.75	99.47	106.31
24	C	502	CLA	C1D-ND-C4D	-9.72	99.49	106.31
24	d	403	CLA	C1D-ND-C4D	-9.70	99.51	106.31
24	b	620	CLA	C1D-ND-C4D	-9.68	99.52	106.31
24	B	602	CLA	C1D-ND-C4D	-9.64	99.55	106.31
25	A	408	PHO	C3B-C4B-NB	9.56	113.70	107.46
24	D	402	CLA	C1D-ND-C4D	-9.56	99.61	106.31
24	c	518	CLA	C1D-ND-C4D	-9.55	99.61	106.31
24	c	509	CLA	C1D-ND-C4D	-9.53	99.62	106.31
24	B	612	CLA	C1D-ND-C4D	-9.50	99.65	106.31
24	a	412	CLA	C1D-ND-C4D	-9.48	99.66	106.31
24	b	619	CLA	C1D-ND-C4D	-9.39	99.72	106.31
24	b	615	CLA	C1D-ND-C4D	-9.39	99.72	106.31
24	B	615	CLA	C1D-ND-C4D	-9.37	99.73	106.31
24	C	513	CLA	C1D-ND-C4D	-9.34	99.76	106.31
24	d	402	CLA	C1D-ND-C4D	-9.33	99.77	106.31
24	C	512	CLA	C1D-ND-C4D	-9.32	99.78	106.31
24	b	624	CLA	C1D-ND-C4D	-9.27	99.81	106.31
24	b	612	CLA	C1D-ND-C4D	-9.26	99.81	106.31
24	c	517	CLA	C1D-ND-C4D	-9.24	99.83	106.31
24	b	611	CLA	C1D-ND-C4D	-9.24	99.83	106.31
24	B	608	CLA	C1D-ND-C4D	-9.22	99.84	106.31
24	C	511	CLA	C1D-ND-C4D	-9.17	99.88	106.31
24	b	621	CLA	C1D-ND-C4D	-9.17	99.88	106.31
24	A	410	CLA	C1D-ND-C4D	-9.17	99.88	106.31
24	b	623	CLA	C1D-ND-C4D	-9.15	99.89	106.31
24	B	607	CLA	C1D-ND-C4D	-9.13	99.91	106.31
24	B	603	CLA	C1D-ND-C4D	-9.11	99.92	106.31
24	B	611	CLA	C1D-ND-C4D	-9.08	99.94	106.31
24	A	406	CLA	C1D-ND-C4D	-9.03	99.97	106.31
24	C	504	CLA	C1D-ND-C4D	-9.03	99.98	106.31
24	C	510	CLA	C1D-ND-C4D	-9.02	99.98	106.31
24	b	625	CLA	C1D-ND-C4D	-9.00	100.00	106.31
24	B	609	CLA	C1D-ND-C4D	-8.97	100.02	106.31
24	B	617	CLA	C1D-ND-C4D	-8.95	100.03	106.31
24	B	614	CLA	C1D-ND-C4D	-8.95	100.03	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	418[A]	PHO	O2D-CGD-CBD	8.93	120.76	110.95
24	b	616	CLA	C1D-ND-C4D	-8.92	100.05	106.31
24	c	514	CLA	C1D-ND-C4D	-8.92	100.05	106.31
25	a	418[B]	PHO	O2D-CGD-CBD	8.91	120.74	110.95
24	c	512	CLA	C1D-ND-C4D	-8.91	100.06	106.31
24	B	604	CLA	C1D-ND-C4D	-8.88	100.08	106.31
24	C	508	CLA	C1D-ND-C4D	-8.88	100.08	106.31
24	B	610	CLA	C1D-ND-C4D	-8.84	100.11	106.31
24	a	409	CLA	C1D-ND-C4D	-8.82	100.13	106.31
24	d	401	CLA	C1D-ND-C4D	-8.80	100.14	106.31
24	C	507	CLA	C1D-ND-C4D	-8.79	100.14	106.31
24	c	511	CLA	C1D-ND-C4D	-8.78	100.15	106.31
24	c	506	CLA	C1D-ND-C4D	-8.78	100.15	106.31
24	C	509	CLA	C1D-ND-C4D	-8.77	100.16	106.31
25	a	411	PHO	O2D-CGD-CBD	8.77	120.58	110.95
24	b	610	CLA	C1D-ND-C4D	-8.74	100.18	106.31
24	c	507	CLA	C1D-ND-C4D	-8.71	100.20	106.31
24	D	403	CLA	C1D-ND-C4D	-8.69	100.21	106.31
24	B	605	CLA	C1D-ND-C4D	-8.66	100.24	106.31
24	b	617	CLA	C1D-ND-C4D	-8.60	100.28	106.31
24	c	515	CLA	C1D-ND-C4D	-8.59	100.28	106.31
24	c	513	CLA	C1D-ND-C4D	-8.58	100.29	106.31
24	C	505	CLA	C1D-ND-C4D	-8.46	100.37	106.31
24	c	510	CLA	C1D-ND-C4D	-8.31	100.48	106.31
24	A	405	CLA	C1D-ND-C4D	-8.12	100.61	106.31
24	b	622	CLA	C1D-ND-C4D	-8.06	100.66	106.31
24	C	506	CLA	C1D-ND-C4D	-8.00	100.70	106.31
25	a	418[A]	PHO	C3B-C4B-NB	7.99	112.67	107.46
25	a	418[B]	PHO	C3B-C4B-NB	7.74	112.51	107.46
25	A	409[B]	PHO	O2D-CGD-CBD	7.53	119.22	110.95
25	a	411	PHO	C3B-C4B-NB	7.51	112.36	107.46
25	A	409[A]	PHO	O2D-CGD-CBD	7.45	119.14	110.95
24	B	613	CLA	C2D-C1D-ND	7.43	117.47	110.13
24	B	605	CLA	CMD-C2D-C1D	7.39	137.74	124.73
25	A	408	PHO	O2D-CGD-CBD	7.32	118.99	110.95
25	a	418[B]	PHO	C2B-C1B-NB	7.21	114.64	109.43
25	A	409[B]	PHO	C3B-C4B-NB	7.20	112.16	107.46
24	b	613	CLA	C1D-ND-C4D	-7.20	101.26	106.31
24	B	606	CLA	CHD-C4C-C3C	-7.18	114.30	124.77
25	A	409[A]	PHO	C3B-C4B-NB	7.16	112.13	107.46
24	d	403	CLA	CMD-C2D-C1D	6.97	137.00	124.73
24	C	510	CLA	CMD-C2D-C1D	6.94	136.96	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	616	CLA	CMD-C2D-C1D	6.91	136.90	124.73
24	b	614	CLA	CHD-C4C-C3C	-6.90	114.71	124.77
25	a	411	PHO	C2B-C1B-NB	6.90	114.42	109.43
24	c	512	CLA	O2D-CGD-CBD	6.89	123.28	111.23
24	c	517	CLA	C4A-NA-C1A	-6.86	103.55	106.68
25	a	418[A]	PHO	C2B-C1B-NB	6.82	114.36	109.43
24	a	409	CLA	CMD-C2D-C1D	6.82	136.74	124.73
24	b	610	CLA	O2D-CGD-CBD	6.77	123.06	111.23
24	c	508	CLA	CMD-C2D-C1D	6.76	136.64	124.73
24	b	611	CLA	CMD-C2D-C1D	6.74	136.60	124.73
24	B	613	CLA	CHD-C4C-C3C	-6.73	114.96	124.77
24	c	518	CLA	CMD-C2D-C1D	6.72	136.56	124.73
25	A	409[B]	PHO	C2B-C1B-NB	6.71	114.28	109.43
24	B	603	CLA	C4A-NA-C1A	-6.67	103.64	106.68
24	d	402	CLA	CMD-C2D-C1D	6.66	136.45	124.73
25	A	409[A]	PHO	C2B-C1B-NB	6.65	114.23	109.43
24	c	509	CLA	CMD-C2D-C1D	6.65	136.43	124.73
24	b	619	CLA	CMD-C2D-C1D	6.64	136.42	124.73
24	b	614	CLA	C4A-NA-C1A	-6.63	103.66	106.68
24	a	410	CLA	C2D-C1D-ND	6.63	116.68	110.13
24	B	612	CLA	CHD-C4C-C3C	-6.58	115.17	124.77
24	C	501	CLA	CMD-C2D-C1D	6.57	136.30	124.73
24	C	513	CLA	CMD-C2D-C1D	6.57	136.29	124.73
24	b	612	CLA	CMD-C2D-C1D	6.57	136.29	124.73
24	d	402	CLA	C4A-NA-C1A	-6.55	103.69	106.68
24	D	402	CLA	C2D-C1D-ND	6.54	116.60	110.13
24	b	613	CLA	CMD-C2D-C1D	6.54	136.24	124.73
24	C	504	CLA	CMD-C2D-C1D	6.54	136.24	124.73
24	B	602	CLA	CMD-C2D-C1D	6.53	136.23	124.73
24	B	614	CLA	CMD-C2D-C1D	6.52	136.21	124.73
24	c	515	CLA	CMD-C2D-C1D	6.49	136.15	124.73
24	B	606	CLA	C2D-C1D-ND	6.48	116.54	110.13
24	B	612	CLA	C2D-C1D-ND	6.48	116.54	110.13
24	B	603	CLA	CMD-C2D-C1D	6.47	136.12	124.73
24	D	403	CLA	CMD-C2D-C1D	6.47	136.12	124.73
24	B	604	CLA	O2D-CGD-CBD	6.45	122.50	111.23
24	b	620	CLA	CMD-C2D-C1D	6.45	136.08	124.73
24	c	508	CLA	CHD-C4C-C3C	-6.45	115.38	124.77
24	C	512	CLA	C2D-C1D-ND	6.44	116.50	110.13
24	C	502	CLA	C2D-C1D-ND	6.44	116.50	110.13
24	B	614	CLA	C2D-C1D-ND	6.44	116.50	110.13
24	b	623	CLA	O2D-CGD-CBD	6.43	122.48	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	CHD-C4C-C3C	-6.43	115.39	124.77
24	b	614	CLA	CMD-C2D-C1D	6.43	136.04	124.73
24	B	617	CLA	O2D-CGD-CBD	6.42	122.46	111.23
24	b	614	CLA	C2D-C1D-ND	6.42	116.48	110.13
24	c	512	CLA	CHD-C4C-C3C	-6.42	115.41	124.77
24	c	511	CLA	CMD-C2D-C1D	6.40	136.01	124.73
24	B	607	CLA	CMD-C2D-C1D	6.39	135.98	124.73
24	b	621	CLA	C2D-C1D-ND	6.39	116.45	110.13
24	c	512	CLA	C2D-C1D-ND	6.39	116.45	110.13
24	B	617	CLA	CMD-C2D-C1D	6.38	135.96	124.73
24	B	608	CLA	CMD-C2D-C1D	6.37	135.94	124.73
24	B	604	CLA	CHD-C4C-C3C	-6.36	115.50	124.77
24	B	608	CLA	C2D-C1D-ND	6.35	116.41	110.13
24	C	512	CLA	CHD-C4C-C3C	-6.34	115.52	124.77
24	c	510	CLA	C4A-NA-C1A	-6.34	103.79	106.68
24	B	616	CLA	CMD-C2D-C1D	6.33	135.88	124.73
24	C	503	CLA	CHD-C4C-C3C	-6.33	115.55	124.77
24	c	509	CLA	C2D-C1D-ND	6.30	116.36	110.13
24	C	505	CLA	CHD-C4C-C3C	-6.30	115.59	124.77
24	C	501	CLA	O2D-CGD-CBD	6.30	122.23	111.23
24	C	504	CLA	C2D-C1D-ND	6.27	116.33	110.13
24	b	615	CLA	CHD-C4C-C3C	-6.25	115.66	124.77
24	c	508	CLA	C2D-C1D-ND	6.25	116.31	110.13
24	C	507	CLA	CMD-C2D-C1D	6.24	135.72	124.73
24	b	621	CLA	CHD-C4C-C3C	-6.24	115.68	124.77
24	A	406	CLA	C2D-C1D-ND	6.23	116.29	110.13
24	b	622	CLA	CMD-C2D-C1D	6.23	135.69	124.73
24	b	612	CLA	CHD-C4C-C3C	-6.23	115.70	124.77
24	B	607	CLA	C2D-C1D-ND	6.22	116.28	110.13
24	b	616	CLA	CHD-C4C-C3C	-6.22	115.71	124.77
24	a	412	CLA	C2D-C1D-ND	6.20	116.26	110.13
24	b	611	CLA	C4A-NA-C1A	-6.20	103.85	106.68
24	C	508	CLA	CMD-C2D-C1D	6.19	135.63	124.73
24	c	516	CLA	C2D-C1D-ND	6.19	116.25	110.13
24	c	508	CLA	C4A-NA-C1A	-6.19	103.85	106.68
24	c	517	CLA	O2D-CGD-CBD	6.18	122.04	111.23
24	B	616	CLA	C2D-C1D-ND	6.18	116.24	110.13
24	d	403	CLA	C2D-C1D-ND	6.18	116.24	110.13
24	d	403	CLA	CHD-C4C-C3C	-6.17	115.78	124.77
24	C	505	CLA	C4A-NA-C1A	-6.17	103.86	106.68
24	b	618	CLA	CHD-C4C-C3C	-6.16	115.79	124.77
24	B	606	CLA	CMD-C2D-C1D	6.16	135.57	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	CMD-C2D-C1D	6.15	135.56	124.73
24	c	510	CLA	CHD-C4C-C3C	-6.14	115.82	124.77
24	b	613	CLA	O2D-CGD-CBD	6.14	121.96	111.23
24	b	618	CLA	CMD-C2D-C1D	6.14	135.53	124.73
24	b	615	CLA	C2D-C1D-ND	6.13	116.19	110.13
24	C	507	CLA	CHD-C4C-C3C	-6.13	115.84	124.77
24	B	609	CLA	CMD-C2D-C1D	6.13	135.52	124.73
24	A	407	CLA	C2D-C1D-ND	6.12	116.19	110.13
24	b	624	CLA	CHD-C4C-C3C	-6.11	115.86	124.77
24	a	410	CLA	CHD-C4C-C3C	-6.11	115.86	124.77
24	b	625	CLA	O2D-CGD-CBD	6.11	121.91	111.23
24	b	616	CLA	C2D-C1D-ND	6.11	116.17	110.13
24	b	610	CLA	CHD-C4C-C3C	-6.10	115.88	124.77
24	C	509	CLA	CMD-C2D-C1D	6.10	135.47	124.73
24	C	505	CLA	CMD-C2D-C1D	6.10	135.47	124.73
24	D	402	CLA	C4A-NA-C1A	-6.09	103.90	106.68
24	b	620	CLA	C2D-C1D-ND	6.09	116.16	110.13
24	C	501	CLA	C2D-C1D-ND	6.09	116.15	110.13
24	c	509	CLA	CHD-C4C-C3C	-6.07	115.92	124.77
24	b	610	CLA	CMD-C2D-C1D	6.07	135.42	124.73
24	C	503	CLA	CMD-C2D-C1D	6.06	135.41	124.73
24	b	625	CLA	CHD-C4C-C3C	-6.06	115.94	124.77
24	b	624	CLA	CMD-C2D-C1D	6.04	135.37	124.73
24	b	625	CLA	C2D-C1D-ND	6.04	116.11	110.13
24	b	623	CLA	C2D-C1D-ND	6.04	116.10	110.13
24	c	506	CLA	CMD-C2D-C1D	6.03	135.35	124.73
24	b	615	CLA	C4A-NA-C1A	-6.03	103.93	106.68
24	B	602	CLA	CHD-C4C-C3C	-6.02	116.00	124.77
24	B	607	CLA	CHD-C4C-C3C	-6.02	116.00	124.77
24	B	617	CLA	CHD-C4C-C3C	-6.01	116.02	124.77
24	D	402	CLA	CHD-C4C-C3C	-6.01	116.02	124.77
24	A	407	CLA	CHD-C4C-C3C	-6.00	116.03	124.77
24	B	602	CLA	C2D-C1D-ND	5.98	116.05	110.13
24	d	401	CLA	CHD-C4C-C3C	-5.97	116.07	124.77
24	b	617	CLA	CMD-C2D-C1D	5.97	135.24	124.73
24	C	510	CLA	CHD-C4C-C3C	-5.96	116.08	124.77
24	B	615	CLA	CMD-C2D-C1D	5.96	135.22	124.73
24	c	514	CLA	CHD-C4C-C3C	-5.96	116.08	124.77
24	A	406	CLA	CHD-C4C-C3C	-5.95	116.09	124.77
25	a	418[A]	PHO	C4D-ND-C1D	-5.95	101.74	108.87
24	c	517	CLA	C2D-C1D-ND	5.95	116.02	110.13
24	B	615	CLA	O2D-CGD-CBD	5.95	121.62	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	405	CLA	CMD-C2D-C1D	5.95	135.20	124.73
24	C	511	CLA	C2D-C1D-ND	5.94	116.01	110.13
24	B	602	CLA	O2D-CGD-CBD	5.94	121.62	111.23
24	A	410	CLA	CMD-C2D-C1D	5.94	135.19	124.73
24	A	407	CLA	CMD-C2D-C1D	5.94	135.19	124.73
24	b	624	CLA	C4A-NA-C1A	-5.94	103.97	106.68
24	C	502	CLA	CHD-C4C-C3C	-5.93	116.12	124.77
24	C	503	CLA	C2D-C1D-ND	5.93	116.00	110.13
24	B	614	CLA	CHD-C4C-C3C	-5.93	116.12	124.77
24	B	610	CLA	C2D-C1D-ND	5.93	115.99	110.13
24	c	507	CLA	CHD-C4C-C3C	-5.93	116.13	124.77
24	b	618	CLA	C2D-C1D-ND	5.92	115.99	110.13
24	c	506	CLA	C2D-C1D-ND	5.92	115.99	110.13
24	B	611	CLA	CMD-C2D-C1D	5.92	135.16	124.73
24	B	610	CLA	CHD-C4C-C3C	-5.92	116.14	124.77
24	c	514	CLA	CMD-C2D-C1D	5.92	135.15	124.73
24	B	615	CLA	C2D-C1D-ND	5.91	115.98	110.13
24	C	512	CLA	O2D-CGD-CBD	5.91	121.57	111.23
24	c	510	CLA	O2D-CGD-CBD	5.91	121.57	111.23
24	B	615	CLA	CHD-C4C-C3C	-5.90	116.17	124.77
24	B	610	CLA	CMD-C2D-C1D	5.90	135.12	124.73
25	A	408	PHO	C4D-ND-C1D	-5.90	101.80	108.87
24	b	625	CLA	CMD-C2D-C1D	5.89	135.11	124.73
24	A	410	CLA	C2D-C1D-ND	5.89	115.96	110.13
25	A	409[B]	PHO	C4D-ND-C1D	-5.89	101.82	108.87
24	B	604	CLA	CMD-C2D-C1D	5.89	135.10	124.73
24	b	624	CLA	C2D-C1D-ND	5.88	115.94	110.13
24	a	410	CLA	CMD-C2D-C1D	5.87	135.06	124.73
24	C	507	CLA	C2D-C1D-ND	5.86	115.93	110.13
24	B	605	CLA	C2D-C1D-ND	5.85	115.92	110.13
24	b	615	CLA	CMD-C2D-C1D	5.85	135.03	124.73
24	d	401	CLA	CMD-C2D-C1D	5.85	135.03	124.73
24	b	611	CLA	CHD-C4C-C3C	-5.85	116.25	124.77
24	A	410	CLA	CHD-C4C-C3C	-5.84	116.26	124.77
25	a	418[B]	PHO	C4D-ND-C1D	-5.83	101.89	108.87
24	d	401	CLA	C2D-C1D-ND	5.83	115.90	110.13
24	b	617	CLA	CHD-C4C-C3C	-5.82	116.28	124.77
24	c	517	CLA	CHD-C4C-C3C	-5.82	116.28	124.77
24	B	610	CLA	C4A-NA-C1A	-5.81	104.03	106.68
24	B	617	CLA	C2D-C1D-ND	5.81	115.88	110.13
24	b	611	CLA	C2D-C1D-ND	5.80	115.86	110.13
24	B	605	CLA	CHD-C4C-C3C	-5.79	116.33	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	508	CLA	C2D-C1D-ND	5.79	115.86	110.13
24	b	619	CLA	CHD-C4C-C3C	-5.79	116.33	124.77
24	c	518	CLA	C4A-NA-C1A	-5.78	104.04	106.68
24	A	406	CLA	CMD-C2D-C1D	5.78	134.91	124.73
24	B	616	CLA	C4A-NA-C1A	-5.77	104.05	106.68
24	a	412	CLA	CHD-C4C-C3C	-5.76	116.37	124.77
24	c	514	CLA	C2D-C1D-ND	5.76	115.82	110.13
24	B	603	CLA	CHD-C4C-C3C	-5.74	116.40	124.77
24	c	510	CLA	CMD-C2D-C1D	5.73	134.83	124.73
24	b	618	CLA	C4A-NA-C1A	-5.73	104.06	106.68
24	c	516	CLA	CHD-C4C-C3C	-5.73	116.42	124.77
24	c	518	CLA	CHD-C4C-C3C	-5.73	116.42	124.77
24	B	609	CLA	C2D-C1D-ND	5.72	115.78	110.13
24	b	620	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
24	b	619	CLA	C2D-C1D-ND	5.70	115.77	110.13
24	b	612	CLA	O2D-CGD-CBD	5.70	121.19	111.23
24	C	511	CLA	CHD-C4C-C3C	-5.68	116.49	124.77
24	C	513	CLA	C2D-C1D-ND	5.68	115.74	110.13
24	C	502	CLA	CMD-C2D-C1D	5.67	134.72	124.73
24	b	613	CLA	C2C-C1C-NC	5.67	115.94	109.98
24	B	617	CLA	C4A-NA-C1A	-5.67	104.09	106.68
24	B	608	CLA	CHD-C4C-C3C	-5.67	116.51	124.77
24	c	512	CLA	CMD-C2D-C1D	5.65	134.68	124.73
24	B	611	CLA	C2D-C1D-ND	5.65	115.72	110.13
24	c	518	CLA	C2D-C1D-ND	5.65	115.72	110.13
24	c	513	CLA	CHD-C4C-C3C	-5.65	116.54	124.77
25	A	408	PHO	C3D-C4D-ND	5.64	114.94	107.71
24	A	405	CLA	C4A-NA-C1A	-5.64	104.11	106.68
24	C	509	CLA	CHD-C4C-C3C	-5.64	116.55	124.77
24	b	612	CLA	C2D-C1D-ND	5.63	115.70	110.13
24	c	507	CLA	C2D-C1D-ND	5.63	115.69	110.13
24	c	511	CLA	CHD-C4C-C3C	-5.62	116.57	124.77
24	b	613	CLA	C2D-C1D-ND	5.62	115.69	110.13
24	c	515	CLA	CHD-C4C-C3C	-5.61	116.60	124.77
24	b	610	CLA	C4A-NA-C1A	-5.60	104.12	106.68
24	C	509	CLA	C2D-C1D-ND	5.60	115.67	110.13
24	A	407	CLA	C4A-NA-C1A	-5.60	104.12	106.68
24	C	508	CLA	O2D-CGD-CBD	5.60	121.01	111.23
24	c	513	CLA	C2D-C1D-ND	5.60	115.67	110.13
24	c	511	CLA	C2D-C1D-ND	5.58	115.65	110.13
24	b	623	CLA	CHD-C4C-C3C	-5.58	116.64	124.77
24	c	517	CLA	C2B-C1B-NB	5.58	116.11	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	623	CLA	CMD-C2D-C1D	5.57	134.54	124.73
24	C	504	CLA	CHD-C4C-C3C	-5.57	116.66	124.77
24	B	604	CLA	C2D-C1D-ND	5.57	115.64	110.13
24	D	402	CLA	CMD-C2D-C1D	5.56	134.52	124.73
24	b	617	CLA	C4A-NA-C1A	-5.56	104.14	106.68
24	B	607	CLA	O2D-CGD-CBD	5.55	120.94	111.23
24	b	622	CLA	C2D-C1D-ND	5.55	115.62	110.13
24	D	403	CLA	C4A-NA-C1A	-5.55	104.15	106.68
24	B	603	CLA	C2D-C1D-ND	5.55	115.61	110.13
26	Y	101	BCR	C33-C5-C6	-5.54	118.44	124.48
24	C	510	CLA	C2D-C1D-ND	5.54	115.61	110.13
24	b	613	CLA	CHD-C4C-C3C	-5.54	116.70	124.77
25	A	408	PHO	C2B-C1B-NB	5.53	113.43	109.43
24	D	403	CLA	C2D-C1D-ND	5.52	115.59	110.13
24	a	409	CLA	C2C-C1C-NC	5.52	115.78	109.98
24	B	607	CLA	C4A-NA-C1A	-5.51	104.16	106.68
24	b	610	CLA	C2D-C1D-ND	5.51	115.58	110.13
24	C	511	CLA	C2C-C1C-NC	5.51	115.77	109.98
24	d	401	CLA	C2C-C1C-NC	5.50	115.75	109.98
24	C	503	CLA	C4A-NA-C1A	-5.49	104.17	106.68
24	C	513	CLA	CHD-C4C-C3C	-5.49	116.77	124.77
24	b	617	CLA	C2D-C1D-ND	5.48	115.55	110.13
24	C	509	CLA	C1-C2-C3	-5.48	117.22	126.20
24	c	507	CLA	C4A-NA-C1A	-5.48	104.18	106.68
25	a	418[A]	PHO	C1-C2-C3	-5.48	117.22	126.20
24	B	611	CLA	CHD-C4C-C3C	-5.48	116.79	124.77
24	c	506	CLA	O2D-CGD-CBD	5.47	120.80	111.23
24	d	403	CLA	C4A-NA-C1A	-5.47	104.18	106.68
24	B	605	CLA	C2C-C1C-NC	5.47	115.72	109.98
24	b	622	CLA	CHD-C4C-C3C	-5.47	116.80	124.77
24	B	609	CLA	CHD-C4C-C3C	-5.46	116.81	124.77
25	A	409[A]	PHO	C4D-ND-C1D	-5.45	102.35	108.87
24	C	511	CLA	CMD-C2D-C1D	5.44	134.31	124.73
38	F	102	HEM	CHC-C4B-NB	5.44	130.28	124.42
25	a	418[B]	PHO	C3D-C4D-ND	5.43	114.67	107.71
35	d	411	HTG	C1'-S1-C1	5.43	112.18	100.45
24	C	507	CLA	O2D-CGD-CBD	5.43	120.72	111.23
27	L	102	SQD	O6-C1-C2	5.42	116.50	108.27
24	B	609	CLA	C2C-C1C-NC	5.41	115.67	109.98
24	B	613	CLA	O2D-CGD-CBD	5.41	120.69	111.23
26	D	404	BCR	C7-C8-C9	-5.41	118.23	126.23
25	A	409[A]	PHO	C1-C2-C3	-5.40	117.34	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	501	CLA	CHD-C4C-C3C	-5.40	116.90	124.77
24	c	509	CLA	O2D-CGD-CBD	5.40	120.67	111.23
24	c	517	CLA	CMD-C2D-C1D	5.40	134.24	124.73
24	d	402	CLA	C2D-C1D-ND	5.40	115.47	110.13
24	c	517	CLA	C3B-C2B-C1B	-5.40	100.81	107.17
24	c	512	CLA	C2C-C1C-NC	5.38	115.63	109.98
24	B	612	CLA	CMD-C2D-C1D	5.37	134.19	124.73
27	f	101	SQD	O47-C7-C8	5.37	123.10	111.48
24	B	603	CLA	O2D-CGD-CBD	5.37	120.62	111.23
35	C	522	HTG	C1'-S1-C1	5.37	112.04	100.45
24	D	403	CLA	CHD-C4C-C3C	-5.36	116.96	124.77
24	a	412	CLA	O2D-CGD-CBD	5.35	120.58	111.23
25	a	418[A]	PHO	C3D-C4D-ND	5.34	114.56	107.71
24	C	508	CLA	C2B-C1B-NB	5.34	115.87	110.33
24	A	406	CLA	O2D-CGD-CBD	5.34	120.56	111.23
25	A	409[B]	PHO	C1-C2-C3	-5.34	117.45	126.20
24	c	506	CLA	C2C-C1C-NC	5.34	115.59	109.98
24	a	410	CLA	C4A-NA-C1A	-5.34	104.24	106.68
24	b	615	CLA	O2D-CGD-CBD	5.34	120.56	111.23
24	b	619	CLA	C4A-NA-C1A	-5.34	104.25	106.68
24	b	622	CLA	C2C-C1C-NC	5.33	115.58	109.98
24	c	510	CLA	C2C-C1C-NC	5.33	115.58	109.98
25	a	411	PHO	C4D-ND-C1D	-5.31	102.50	108.87
24	c	506	CLA	CHD-C4C-C3C	-5.31	117.02	124.77
24	D	402	CLA	C2C-C1C-NC	5.31	115.56	109.98
24	c	513	CLA	O2D-CGD-CBD	5.31	120.51	111.23
24	C	506	CLA	CHD-C4C-C3C	-5.30	117.04	124.77
24	C	508	CLA	CHD-C4C-C3C	-5.30	117.05	124.77
24	b	625	CLA	C4A-NA-C1A	-5.29	104.27	106.68
24	A	407	CLA	O2D-CGD-CBD	5.28	120.46	111.23
27	a	414	SQD	O6-C1-C2	5.27	116.28	108.27
24	B	604	CLA	C4A-NA-C1A	-5.27	104.28	106.68
24	a	409	CLA	C2D-C1D-ND	5.25	115.33	110.13
24	c	515	CLA	C2C-C1C-NC	5.25	115.50	109.98
24	a	412	CLA	CMD-C2D-C1D	5.25	133.98	124.73
24	C	512	CLA	CMD-C2D-C1D	5.25	133.97	124.73
24	b	612	CLA	C4A-NA-C1A	-5.23	104.29	106.68
24	A	406	CLA	C2C-C1C-NC	5.23	115.48	109.98
24	C	506	CLA	C2D-C1D-ND	5.23	115.30	110.13
25	A	409[B]	PHO	C3D-C4D-ND	5.23	114.41	107.71
24	B	612	CLA	C2C-C1C-NC	5.22	115.47	109.98
24	b	610	CLA	C2B-C1B-NB	5.21	115.72	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	611	CLA	O2D-CGD-CBD	5.21	120.33	111.23
24	C	506	CLA	C2C-C1C-NC	5.20	115.44	109.98
24	d	402	CLA	C2C-C1C-NC	5.19	115.43	109.98
24	c	516	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
24	b	620	CLA	C2C-C1C-NC	5.18	115.42	109.98
24	c	516	CLA	CMD-C2D-C1D	5.17	133.83	124.73
24	b	611	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
24	A	405	CLA	C2C-C1C-NC	5.16	115.40	109.98
24	b	616	CLA	C2C-C1C-NC	5.15	115.40	109.98
24	b	611	CLA	C2B-C1B-NB	5.15	115.66	110.33
24	C	510	CLA	O2D-CGD-CBD	5.14	120.22	111.23
25	a	418[B]	PHO	C1-C2-C3	-5.14	117.78	126.20
25	a	411	PHO	C3D-C4D-ND	5.14	114.30	107.71
24	b	619	CLA	O2D-CGD-CBD	5.13	120.19	111.23
24	B	611	CLA	C3B-C2B-C1B	-5.13	101.13	107.17
24	B	613	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
24	a	409	CLA	CHD-C4C-C3C	-5.12	117.30	124.77
24	c	511	CLA	C2C-C1C-NC	5.12	115.36	109.98
27	F	103	SQD	O47-C7-C8	5.12	122.56	111.48
27	B	621	SQD	O6-C1-C2	5.11	116.03	108.27
24	a	412	CLA	C2C-C1C-NC	5.11	115.35	109.98
24	c	507	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
24	C	505	CLA	O2D-CGD-CBD	5.11	120.16	111.23
24	B	606	CLA	C4A-NA-C1A	-5.10	104.35	106.68
24	D	403	CLA	C2C-C1C-NC	5.10	115.34	109.98
24	C	505	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
24	A	407	CLA	C3D-C4D-ND	5.09	118.26	109.99
24	b	616	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
24	C	504	CLA	O2D-CGD-CBD	5.09	120.12	111.23
24	A	405	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
24	D	403	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
24	c	513	CLA	C4A-NA-C1A	-5.08	104.36	106.68
24	D	403	CLA	O2D-CGD-CBD	5.08	120.11	111.23
25	A	409[A]	PHO	C3D-C4D-ND	5.08	114.22	107.71
24	B	607	CLA	C3B-C2B-C1B	-5.08	101.19	107.17
24	B	608	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
24	b	616	CLA	O2D-CGD-CBD	5.07	120.09	111.23
24	B	613	CLA	CMD-C2D-C1D	5.07	133.65	124.73
24	B	614	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
24	c	515	CLA	C2D-C1D-ND	5.06	115.14	110.13
24	c	509	CLA	C2C-C1C-NC	5.06	115.29	109.98
35	C	523	HTG	C1-O5-C5	5.05	121.62	112.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
24	C	504	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
24	b	613	CLA	C4A-NA-C1A	-5.03	104.39	106.68
24	a	410	CLA	C3D-C4D-ND	5.03	118.16	109.99
24	A	410	CLA	C3B-C2B-C1B	-5.03	101.25	107.17
24	B	609	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
24	C	512	CLA	C4A-NA-C1A	-5.02	104.39	106.68
24	a	409	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
24	c	513	CLA	C2C-C1C-NC	5.01	115.24	109.98
24	c	513	CLA	CMD-C2D-C1D	5.01	133.55	124.73
24	B	607	CLA	C2C-C1C-NC	5.01	115.24	109.98
24	A	405	CLA	C2D-C1D-ND	5.00	115.08	110.13
24	B	611	CLA	C2B-C1B-NB	5.00	115.51	110.33
24	c	512	CLA	C3B-C2B-C1B	-5.00	101.28	107.17
24	B	614	CLA	C2C-C1C-NC	5.00	115.23	109.98
24	C	505	CLA	C2D-C1D-ND	5.00	115.07	110.13
24	c	518	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
24	C	513	CLA	C2B-C1B-NB	4.97	115.48	110.33
24	c	514	CLA	O2D-CGD-CBD	4.97	119.91	111.23
24	c	512	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
24	a	409	CLA	C4A-NA-C1A	-4.96	104.42	106.68
24	b	622	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
35	c	525	HTG	C1'-S1-C1	4.95	111.14	100.45
24	B	607	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
24	B	605	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
24	A	406	CLA	C3B-C2B-C1B	-4.95	101.33	107.17
27	B	621	SQD	O47-C7-C8	4.95	122.18	111.48
24	C	508	CLA	C2C-C1C-NC	4.94	115.17	109.98
24	b	624	CLA	C2C-C1C-NC	4.94	115.17	109.98
24	C	513	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
24	c	506	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
24	B	602	CLA	C4A-NA-C1A	-4.93	104.43	106.68
24	c	514	CLA	C2C-C1C-NC	4.93	115.16	109.98
24	C	509	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
24	b	615	CLA	C2C-C1C-NC	4.93	115.16	109.98
24	d	402	CLA	C3D-C4D-ND	4.93	118.00	109.99
24	B	609	CLA	O2D-CGD-CBD	4.93	119.84	111.23
24	B	610	CLA	C2C-C1C-NC	4.93	115.16	109.98
24	A	406	CLA	C2B-C1B-NB	4.93	115.44	110.33
24	b	613	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
24	b	623	CLA	C2C-C1C-NC	4.92	115.15	109.98
24	B	608	CLA	O2D-CGD-CBD	4.91	119.82	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	508	CLA	C3D-C2D-C1D	-4.91	99.14	105.83
24	B	611	CLA	C4A-NA-C1A	-4.91	104.44	106.68
24	c	509	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
24	c	518	CLA	C2B-C1B-NB	4.90	115.41	110.33
24	B	616	CLA	C3B-C2B-C1B	-4.90	101.40	107.17
24	C	513	CLA	C4A-NA-C1A	-4.89	104.45	106.68
24	d	403	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
24	a	412	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
24	B	617	CLA	C2C-C1C-NC	4.89	115.12	109.98
24	c	507	CLA	CMD-C2D-C1D	4.89	133.33	124.73
24	B	606	CLA	O2D-CGD-CBD	4.88	119.76	111.23
24	c	516	CLA	C3D-C4D-ND	4.88	117.92	109.99
24	B	605	CLA	O2D-CGD-CBD	4.88	119.76	111.23
24	B	611	CLA	C2C-C1C-NC	4.87	115.10	109.98
24	B	607	CLA	C2B-C1B-NB	4.85	115.36	110.33
35	B	633	HTG	C1'-S1-C1	4.85	110.93	100.45
24	b	614	CLA	C3D-C4D-ND	4.85	117.87	109.99
24	C	507	CLA	C3B-C2B-C1B	-4.85	101.46	107.17
25	a	411	PHO	O1D-CGD-CBD	-4.84	117.38	124.72
26	b	626	BCR	C33-C5-C6	-4.84	119.20	124.48
24	C	504	CLA	C2C-C1C-NC	4.84	115.06	109.98
36	C	516	DGD	O2G-C1B-C2B	4.84	121.94	111.48
24	b	619	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
24	A	405	CLA	C2B-C1B-NB	4.83	115.34	110.33
24	C	502	CLA	C1-C2-C3	-4.83	118.29	126.20
24	C	512	CLA	C3B-C2B-C1B	-4.82	101.48	107.17
24	B	604	CLA	C2C-C1C-NC	4.82	115.04	109.98
24	C	509	CLA	C2C-C1C-NC	4.82	115.04	109.98
24	a	410	CLA	O2D-CGD-CBD	4.81	119.65	111.23
24	A	407	CLA	C2B-C1B-NB	4.81	115.31	110.33
24	c	513	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
24	C	508	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
24	d	403	CLA	O2D-CGD-CBD	4.80	119.63	111.23
24	c	516	CLA	C2B-C1B-NB	4.80	115.31	110.33
24	d	401	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
27	A	412	SQD	O47-C7-C8	4.80	121.86	111.48
24	A	410	CLA	C2C-C1C-NC	4.79	115.02	109.98
24	C	505	CLA	C2C-C1C-NC	4.79	115.01	109.98
24	b	621	CLA	O2D-CGD-CBD	4.79	119.60	111.23
24	A	405	CLA	CAC-C3C-C4C	4.79	131.02	124.79
24	c	506	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
24	b	625	CLA	C3B-C2B-C1B	-4.79	101.53	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	511	CLA	C3B-C4B-NB	4.78	114.80	110.53
24	b	617	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
24	B	613	CLA	C3C-C4C-NC	4.78	116.56	110.43
24	B	612	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
24	D	402	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
24	b	618	CLA	C2C-C1C-NC	4.77	115.00	109.98
26	t	101	BCR	C33-C5-C6	-4.77	119.28	124.48
24	B	609	CLA	C2B-C1B-NB	4.76	115.26	110.33
24	D	403	CLA	C2B-C1B-NB	4.76	115.26	110.33
24	A	406	CLA	C3B-C4B-NB	4.76	114.78	110.53
35	D	412	HTG	C1'-S1-C1	4.76	110.72	100.45
24	d	401	CLA	C4A-NA-C1A	-4.75	104.51	106.68
24	B	602	CLA	C3B-C2B-C1B	-4.75	101.57	107.17
24	C	502	CLA	C3D-C2D-C1D	-4.75	99.34	105.83
24	b	619	CLA	C2C-C1C-NC	4.75	114.97	109.98
24	b	612	CLA	C2C-C1C-NC	4.75	114.97	109.98
24	b	617	CLA	C2C-C1C-NC	4.75	114.97	109.98
24	B	612	CLA	O2D-CGD-CBD	4.74	119.53	111.23
24	b	622	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
24	b	614	CLA	O2D-CGD-CBD	4.74	119.52	111.23
24	b	623	CLA	C4A-NA-C1A	-4.74	104.52	106.68
24	B	613	CLA	C3D-C4D-ND	4.74	117.69	109.99
24	B	610	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
24	C	503	CLA	C3D-C4D-ND	4.73	117.68	109.99
24	B	605	CLA	C4A-NA-C1A	-4.73	104.52	106.68
24	c	515	CLA	O2D-CGD-CBD	4.73	119.50	111.23
24	b	615	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
24	c	511	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
24	C	510	CLA	C2C-C1C-NC	4.72	114.94	109.98
29	A	417	LMT	C1'-O5'-C5'	4.72	122.94	113.72
24	B	606	CLA	C3D-C4D-ND	4.72	117.65	109.99
24	d	402	CLA	CHD-C4C-C3C	-4.72	117.90	124.77
24	C	512	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
24	d	401	CLA	C3B-C4B-NB	4.71	114.74	110.53
24	B	615	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
24	c	518	CLA	C3D-C4D-ND	4.70	117.64	109.99
24	c	514	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
24	B	603	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
24	D	403	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
24	b	614	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
24	C	509	CLA	C2B-C1B-NB	4.69	115.19	110.33
24	b	615	CLA	C3D-C2D-C1D	-4.69	99.43	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	501	CLA	C2C-C1C-NC	4.69	114.91	109.98
24	c	507	CLA	C2C-C1C-NC	4.69	114.91	109.98
24	B	617	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
24	d	401	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
24	d	403	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
24	B	615	CLA	C4A-NA-C1A	-4.68	104.54	106.68
24	b	621	CLA	C3B-C2B-C1B	-4.68	101.66	107.17
24	C	501	CLA	C3D-C4D-ND	4.67	117.58	109.99
24	A	407	CLA	C3B-C2B-C1B	-4.67	101.66	107.17
24	c	510	CLA	C2D-C1D-ND	4.67	114.75	110.13
24	C	508	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
24	b	621	CLA	C2C-C1C-NC	4.66	114.88	109.98
27	L	102	SQD	O47-C7-C8	4.66	121.56	111.48
35	B	625	HTG	C1'-S1-C1	4.66	110.51	100.45
24	B	603	CLA	C2B-C1B-NB	4.66	115.16	110.33
24	c	513	CLA	C2B-C1B-NB	4.65	115.15	110.33
24	a	409	CLA	C2B-C1B-NB	4.65	115.15	110.33
24	C	503	CLA	C2B-C1B-NB	4.65	115.15	110.33
24	c	507	CLA	C2B-C1B-NB	4.65	115.15	110.33
24	c	508	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
24	c	518	CLA	C2C-C1C-NC	4.65	114.87	109.98
24	B	615	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
24	B	608	CLA	C2C-C1C-NC	4.64	114.86	109.98
24	B	606	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
24	C	511	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
24	C	507	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
24	b	625	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
24	c	508	CLA	C3D-C4D-ND	4.63	117.51	109.99
24	A	410	CLA	C2B-C1B-NB	4.63	115.13	110.33
24	A	406	CLA	C1C-C2C-C3C	-4.63	102.11	106.98
24	C	506	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
24	b	610	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
24	A	410	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
24	B	606	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
24	B	602	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
24	C	512	CLA	C2B-C1B-NB	4.62	115.11	110.33
24	B	613	CLA	C3B-C2B-C1B	-4.62	101.73	107.17
24	B	602	CLA	C3D-C4D-ND	4.62	117.49	109.99
26	B	620	BCR	C15-C14-C13	-4.62	120.80	127.28
24	C	506	CLA	C4A-NA-C1A	-4.61	104.58	106.68
24	b	614	CLA	CHD-C1D-ND	-4.60	118.32	124.80
24	C	509	CLA	C4A-NA-C1A	-4.60	104.58	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	C3D-C4D-ND	4.60	117.46	109.99
24	B	602	CLA	C2B-C1B-NB	4.60	115.09	110.33
24	b	611	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
24	b	618	CLA	C3D-C4D-ND	4.59	117.46	109.99
24	b	620	CLA	C4A-NA-C1A	-4.59	104.58	106.68
24	C	506	CLA	O2D-CGD-CBD	4.59	119.26	111.23
33	c	524	LMG	O7-C10-C11	4.59	121.41	111.48
24	B	604	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
24	b	619	CLA	C3D-C4D-ND	4.59	117.44	109.99
24	B	603	CLA	C2C-C1C-NC	4.58	114.79	109.98
24	C	501	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
24	b	618	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
24	c	509	CLA	C4A-NA-C1A	-4.58	104.59	106.68
33	A	421	LMG	O7-C10-C11	4.58	121.38	111.48
24	a	410	CLA	C3D-C2D-C1D	-4.58	99.59	105.83
24	B	604	CLA	O2D-CGD-O1D	-4.57	114.95	123.85
24	C	509	CLA	O2D-CGD-CBD	4.57	119.22	111.23
24	A	405	CLA	CHD-C4C-C3C	-4.57	118.11	124.77
24	b	619	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
35	B	625	HTG	O5-C1-C2	4.57	116.61	110.32
24	B	617	CLA	C3B-C2B-C1B	-4.57	101.79	107.17
24	b	623	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
24	c	510	CLA	C3C-C4C-NC	4.56	116.28	110.43
24	c	508	CLA	C2B-C1B-NB	4.56	115.06	110.33
24	b	623	CLA	C3B-C2B-C1B	-4.56	101.80	107.17
24	b	620	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
24	b	618	CLA	O2D-CGD-CBD	4.55	119.19	111.23
24	b	615	CLA	C2B-C1B-NB	4.55	115.05	110.33
24	d	402	CLA	O2D-CGD-CBD	4.55	119.18	111.23
24	a	412	CLA	C3D-C4D-ND	4.55	117.38	109.99
24	b	621	CLA	C3C-C4C-NC	4.54	116.25	110.43
24	A	407	CLA	CHD-C1D-ND	-4.54	118.41	124.80
24	A	406	CLA	CBC-CAC-C3C	-4.54	100.11	112.42
24	d	403	CLA	C3D-C4D-ND	4.54	117.37	109.99
24	d	403	CLA	C2B-C1B-NB	4.53	115.03	110.33
24	C	513	CLA	C3D-C4D-ND	4.53	117.35	109.99
24	c	515	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
24	c	506	CLA	C4A-NA-C1A	-4.53	104.61	106.68
24	b	620	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
24	B	611	CLA	C3D-C4D-ND	4.52	117.33	109.99
24	B	615	CLA	C2C-C1C-NC	4.51	114.72	109.98
24	C	508	CLA	C4A-NA-C1A	-4.51	104.62	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	C2C-C1C-NC	4.50	114.71	109.98
24	D	402	CLA	C3D-C4D-ND	4.50	117.30	109.99
24	a	412	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
24	B	603	CLA	C3D-C4D-ND	4.50	117.30	109.99
24	b	616	CLA	CHD-C1D-ND	-4.49	118.48	124.80
36	e	101	DGD	O2G-C1B-C2B	4.49	121.19	111.48
24	c	514	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
24	B	610	CLA	C3D-C4D-ND	4.49	117.28	109.99
24	C	513	CLA	C2C-C1C-NC	4.48	114.69	109.98
24	A	410	CLA	O2D-CGD-CBD	4.48	119.07	111.23
24	c	517	CLA	C3D-C4D-ND	4.48	117.27	109.99
35	B	624	HTG	C1'-S1-C1	4.48	110.13	100.45
24	b	616	CLA	C1C-C2C-C3C	-4.48	102.27	106.98
24	C	502	CLA	C2C-C1C-NC	4.48	114.68	109.98
33	C	520	LMG	O7-C10-C11	4.48	121.16	111.48
24	B	616	CLA	C3D-C2D-C1D	-4.47	99.72	105.83
24	B	602	CLA	C2C-C1C-NC	4.47	114.68	109.98
24	C	513	CLA	C3D-C2D-C1D	-4.47	99.72	105.83
24	C	507	CLA	C4A-NA-C1A	-4.47	104.64	106.68
24	c	509	CLA	C3B-C2B-C1B	-4.47	101.90	107.17
24	C	503	CLA	C2C-C1C-NC	4.47	114.68	109.98
24	C	512	CLA	C2C-C1C-NC	4.47	114.68	109.98
24	C	505	CLA	C2B-C1B-NB	4.47	114.96	110.33
24	b	617	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
24	C	505	CLA	C3C-C4C-NC	4.46	116.15	110.43
24	b	619	CLA	C2B-C1B-NB	4.46	114.95	110.33
24	c	516	CLA	C2C-C1C-NC	4.46	114.67	109.98
24	b	625	CLA	C3D-C4D-ND	4.46	117.24	109.99
24	c	513	CLA	C3D-C4D-ND	4.46	117.23	109.99
24	c	510	CLA	C3B-C2B-C1B	-4.46	101.92	107.17
24	b	621	CLA	C4A-NA-C1A	-4.46	104.65	106.68
24	a	412	CLA	C1C-C2C-C3C	-4.45	102.30	106.98
24	b	623	CLA	C3D-C4D-ND	4.45	117.22	109.99
24	a	410	CLA	C2C-C1C-NC	4.45	114.66	109.98
24	c	506	CLA	C2B-C1B-NB	4.45	114.94	110.33
24	c	511	CLA	O2D-CGD-CBD	4.45	119.00	111.23
24	B	611	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
24	B	612	CLA	C4A-NA-C1A	-4.45	104.65	106.68
24	b	621	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
24	c	514	CLA	C3B-C4B-NB	4.44	114.49	110.53
24	b	611	CLA	C3D-C4D-ND	4.44	117.20	109.99
24	C	503	CLA	C3B-C2B-C1B	-4.44	101.94	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
24	c	515	CLA	C1-C2-C3	-4.44	118.93	126.20
24	c	513	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
24	C	510	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
35	c	526	HTG	C1'-S1-C1	4.43	110.02	100.45
24	b	617	CLA	C2B-C1B-NB	4.43	114.92	110.33
35	b	632	HTG	C1'-S1-C1	4.43	110.02	100.45
24	C	502	CLA	C3B-C2B-C1B	-4.43	101.95	107.17
24	C	502	CLA	O2D-CGD-CBD	4.43	118.97	111.23
24	b	610	CLA	C3D-C4D-ND	4.43	117.18	109.99
24	b	620	CLA	C3D-C4D-ND	4.43	117.18	109.99
24	C	507	CLA	C2B-C1B-NB	4.42	114.91	110.33
24	c	511	CLA	C4A-NA-C1A	-4.42	104.66	106.68
24	b	611	CLA	CHD-C1D-ND	-4.42	118.58	124.80
24	B	608	CLA	C3B-C2B-C1B	-4.42	101.96	107.17
24	b	624	CLA	C3D-C4D-ND	4.42	117.17	109.99
24	a	410	CLA	C3B-C2B-C1B	-4.42	101.96	107.17
24	B	617	CLA	C1D-CHD-C4C	-4.41	116.64	126.02
24	b	610	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
26	B	618	BCR	C33-C5-C6	-4.41	119.67	124.48
24	B	611	CLA	O2D-CGD-CBD	4.41	118.94	111.23
24	c	518	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
24	b	618	CLA	CMB-C2B-C1B	4.41	132.13	125.42
38	e	103	HEM	CHC-C4B-NB	4.41	129.17	124.42
24	d	402	CLA	CHD-C1D-ND	-4.41	118.60	124.80
24	C	509	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
24	c	517	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
24	a	412	CLA	C4A-NA-C1A	-4.40	104.67	106.68
24	B	612	CLA	C3B-C2B-C1B	-4.40	101.98	107.17
24	C	511	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
24	b	611	CLA	C2C-C1C-NC	4.40	114.60	109.98
24	C	511	CLA	C3D-C4D-ND	4.40	117.14	109.99
24	B	616	CLA	C2B-C1B-NB	4.40	114.89	110.33
35	b	631	HTG	C1'-S1-C1	4.40	109.95	100.45
24	B	604	CLA	C3D-C4D-ND	4.40	117.14	109.99
24	a	412	CLA	C2B-C1B-NB	4.39	114.88	110.33
24	C	513	CLA	CHD-C1D-ND	-4.39	118.62	124.80
24	C	502	CLA	C3D-C4D-ND	4.39	117.13	109.99
24	B	610	CLA	CMB-C2B-C1B	4.39	132.10	125.42
24	D	402	CLA	C3C-C4C-NC	4.39	116.05	110.43
24	C	513	CLA	O2D-CGD-CBD	4.38	118.89	111.23
24	b	616	CLA	C3B-C2B-C1B	-4.38	102.00	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	623	CLA	C2B-C1B-NB	4.38	114.87	110.33
27	A	412	SQD	O6-C1-C2	4.38	114.92	108.27
24	D	402	CLA	C3B-C2B-C1B	-4.38	102.01	107.17
24	d	403	CLA	CHD-C1D-ND	-4.37	118.65	124.80
24	b	620	CLA	O2D-CGD-CBD	4.37	118.88	111.23
24	B	612	CLA	C3D-C4D-ND	4.37	117.09	109.99
24	C	504	CLA	C3B-C2B-C1B	-4.37	102.02	107.17
24	c	509	CLA	C3D-C4D-ND	4.37	117.09	109.99
24	B	615	CLA	C2B-C1B-NB	4.37	114.86	110.33
24	b	612	CLA	C3B-C2B-C1B	-4.37	102.02	107.17
24	d	401	CLA	C3D-C4D-ND	4.37	117.09	109.99
24	C	503	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
24	B	609	CLA	C3D-C4D-ND	4.37	117.09	109.99
24	A	410	CLA	C3D-C4D-ND	4.37	117.08	109.99
24	c	508	CLA	O2D-CGD-CBD	4.36	118.86	111.23
24	b	612	CLA	C3D-C4D-ND	4.36	117.08	109.99
24	B	616	CLA	C2C-C1C-NC	4.36	114.56	109.98
24	C	504	CLA	C4A-NA-C1A	-4.36	104.69	106.68
24	a	410	CLA	C2B-C1B-NB	4.36	114.84	110.33
24	c	515	CLA	C3B-C4B-NB	4.35	114.42	110.53
24	d	403	CLA	C2C-C1C-NC	4.35	114.55	109.98
24	b	613	CLA	C3B-C4B-NB	4.35	114.41	110.53
24	B	616	CLA	CMB-C2B-C1B	4.35	132.04	125.42
24	C	504	CLA	CHD-C1D-ND	-4.35	118.69	124.80
24	a	409	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
24	c	517	CLA	C2C-C1C-NC	4.35	114.55	109.98
24	d	401	CLA	C1D-CHD-C4C	-4.34	116.79	126.02
24	c	509	CLA	CHD-C1D-ND	-4.34	118.70	124.80
24	b	610	CLA	C2C-C1C-NC	4.34	114.54	109.98
24	A	406	CLA	C3D-C4D-ND	4.34	117.04	109.99
26	d	404	BCR	C24-C23-C22	-4.33	119.82	126.23
24	B	614	CLA	C3B-C2B-C1B	-4.33	102.06	107.17
24	c	516	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
24	c	507	CLA	C3D-C4D-ND	4.33	117.02	109.99
24	A	407	CLA	C3D-C2D-C1D	-4.33	99.93	105.83
24	b	624	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
24	c	514	CLA	C1D-CHD-C4C	-4.32	116.83	126.02
24	C	501	CLA	CHD-C1D-ND	-4.32	118.72	124.80
24	c	514	CLA	C4A-NA-C1A	-4.32	104.71	106.68
24	b	625	CLA	C3B-C4B-NB	4.32	114.39	110.53
24	C	512	CLA	C3D-C4D-ND	4.32	117.01	109.99
24	b	612	CLA	CAA-C2A-C3A	-4.32	101.33	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	401	CLA	C1C-C2C-C3C	-4.32	102.44	106.98
24	D	402	CLA	CHD-C1D-ND	-4.31	118.74	124.80
24	C	508	CLA	C3D-C4D-ND	4.31	116.99	109.99
24	B	616	CLA	CHD-C1D-ND	-4.31	118.74	124.80
24	b	615	CLA	C3D-C4D-ND	4.30	116.98	109.99
40	V	205	HEC	CBB-CAB-C3B	-4.30	118.83	127.43
24	b	625	CLA	C1D-CHD-C4C	-4.30	116.87	126.02
24	c	510	CLA	C3D-C4D-ND	4.30	116.98	109.99
33	c	501	LMG	O7-C10-C11	4.30	120.78	111.48
24	a	410	CLA	CHD-C1D-ND	-4.30	118.75	124.80
24	B	603	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
24	C	511	CLA	O2D-CGD-CBD	4.29	118.72	111.23
24	a	409	CLA	CHD-C1D-ND	-4.28	118.77	124.80
24	C	510	CLA	C3D-C4D-ND	4.28	116.95	109.99
24	c	511	CLA	C3B-C4B-NB	4.28	114.35	110.53
36	e	101	DGD	O6E-C5E-C4E	4.28	117.41	109.70
24	c	507	CLA	O2D-CGD-CBD	4.28	118.71	111.23
24	c	512	CLA	C3C-C4C-NC	4.28	115.91	110.43
24	B	615	CLA	O2D-CGD-O1D	-4.28	115.52	123.85
24	B	606	CLA	C1D-CHD-C4C	-4.27	116.94	126.02
24	C	502	CLA	C4A-NA-C1A	-4.27	104.73	106.68
24	b	613	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
24	B	606	CLA	C3C-C4C-NC	4.27	115.90	110.43
24	c	514	CLA	C1-C2-C3	-4.27	119.21	126.20
24	c	515	CLA	C3D-C4D-ND	4.26	116.92	109.99
24	c	511	CLA	C3D-C4D-ND	4.26	116.91	109.99
40	v	205	HEC	CBB-CAB-C3B	-4.26	118.93	127.43
24	b	621	CLA	C2B-C1B-NB	4.25	114.73	110.33
24	b	624	CLA	C2B-C1B-NB	4.25	114.73	110.33
24	c	508	CLA	C1D-CHD-C4C	-4.25	116.99	126.02
38	e	103	HEM	CHD-C1D-ND	4.25	128.99	124.42
24	B	609	CLA	C1C-C2C-C3C	-4.25	102.51	106.98
36	c	522	DGD	O2G-C1B-C2B	4.25	120.67	111.48
26	C	514	BCR	C7-C8-C9	-4.25	119.95	126.23
35	C	523	HTG	C1'-S1-C1	4.24	109.62	100.45
24	B	608	CLA	CHD-C1D-ND	-4.24	118.83	124.80
24	C	503	CLA	CHD-C1D-ND	-4.24	118.83	124.80
24	c	518	CLA	CHD-C1D-ND	-4.24	118.83	124.80
24	C	510	CLA	C1-C2-C3	-4.24	119.25	126.20
24	b	613	CLA	C3C-C4C-NC	4.24	115.86	110.43
24	D	402	CLA	O2D-CGD-CBD	4.24	118.64	111.23
24	b	624	CLA	C3B-C2B-C1B	-4.23	102.18	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	409	CLA	C3D-C4D-ND	4.23	116.87	109.99
26	c	519	BCR	C7-C8-C9	-4.23	119.97	126.23
27	a	414	SQD	O47-C7-C8	4.23	120.64	111.48
24	b	622	CLA	C3B-C4B-NB	4.23	114.31	110.53
24	b	623	CLA	C1-C2-C3	-4.23	119.27	126.20
24	C	510	CLA	C4A-NA-C1A	-4.23	104.75	106.68
24	c	515	CLA	C4A-NA-C1A	-4.23	104.75	106.68
24	b	625	CLA	C2C-C1C-NC	4.23	114.42	109.98
25	a	418[A]	PHO	O2D-CGD-O1D	-4.23	115.62	123.85
26	y	101	BCR	C33-C5-C6	-4.23	119.87	124.48
29	C	521	LMT	O1B-C4'-C3'	4.23	117.97	107.23
24	b	622	CLA	C2B-C1B-NB	4.22	114.71	110.33
24	c	511	CLA	C3B-C2B-C1B	-4.22	102.19	107.17
24	c	511	CLA	C1C-C2C-C3C	-4.22	102.54	106.98
24	a	409	CLA	C1C-C2C-C3C	-4.22	102.54	106.98
24	B	602	CLA	CHD-C1D-ND	-4.22	118.87	124.80
24	b	616	CLA	C2B-C1B-NB	4.21	114.69	110.33
24	B	606	CLA	C2C-C1C-NC	4.21	114.41	109.98
24	d	401	CLA	O2D-CGD-CBD	4.21	118.59	111.23
24	D	403	CLA	C3D-C4D-ND	4.21	116.83	109.99
26	d	404	BCR	C38-C26-C25	-4.21	119.89	124.48
24	c	508	CLA	C3C-C4C-NC	4.21	115.82	110.43
24	b	620	CLA	C2B-C1B-NB	4.21	114.69	110.33
24	b	615	CLA	C3C-C4C-NC	4.21	115.82	110.43
24	B	615	CLA	C3D-C4D-ND	4.21	116.82	109.99
24	b	615	CLA	C3B-C4B-NB	4.21	114.28	110.53
24	D	402	CLA	C2B-C1B-NB	4.20	114.69	110.33
24	B	603	CLA	CHD-C1D-ND	-4.20	118.89	124.80
24	b	612	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
24	B	614	CLA	C3C-C4C-NC	4.20	115.81	110.43
24	b	616	CLA	C3D-C4D-ND	4.20	116.81	109.99
24	b	613	CLA	C3B-C2B-C1B	-4.20	102.22	107.17
24	c	512	CLA	C1C-C2C-C3C	-4.19	102.57	106.98
24	B	611	CLA	CAA-C2A-C3A	-4.19	101.67	113.00
24	B	612	CLA	CMC-C2C-C1C	4.19	131.58	125.03
24	c	507	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
24	b	612	CLA	C1D-CHD-C4C	-4.18	117.13	126.02
24	B	612	CLA	C1D-CHD-C4C	-4.18	117.13	126.02
24	C	509	CLA	C3D-C4D-ND	4.18	116.78	109.99
24	c	514	CLA	C3D-C4D-ND	4.17	116.77	109.99
40	v	205	HEC	CHC-C4B-NB	4.16	128.99	124.45
24	B	605	CLA	C3C-C4C-NC	4.16	115.76	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	C2B-C1B-NB	4.16	114.64	110.33
24	b	614	CLA	C2B-C1B-NB	4.16	114.64	110.33
24	B	608	CLA	C3D-C4D-ND	4.16	116.74	109.99
24	b	625	CLA	CAC-C3C-C4C	4.15	130.19	124.79
24	c	511	CLA	CHD-C1D-ND	-4.15	118.96	124.80
24	B	606	CLA	C2B-C1B-NB	4.15	114.63	110.33
24	b	617	CLA	C3D-C4D-ND	4.15	116.74	109.99
24	A	405	CLA	C3D-C4D-ND	4.15	116.73	109.99
24	B	607	CLA	C1C-C2C-C3C	-4.15	102.62	106.98
24	c	513	CLA	C3B-C4B-NB	4.14	114.23	110.53
24	C	504	CLA	C3D-C4D-ND	4.14	116.72	109.99
24	c	514	CLA	C2B-C1B-NB	4.14	114.62	110.33
24	B	610	CLA	C2B-C1B-NB	4.14	114.62	110.33
38	e	103	HEM	CHD-C4C-NC	4.14	128.96	124.45
24	B	607	CLA	CHD-C1D-ND	-4.14	118.98	124.80
24	b	621	CLA	C3D-C4D-ND	4.14	116.71	109.99
24	B	606	CLA	CMB-C2B-C1B	4.14	131.72	125.42
29	D	401	LMT	O1B-C4'-C3'	4.13	117.74	107.23
24	A	405	CLA	C3B-C4B-NB	4.13	114.22	110.53
24	A	405	CLA	C1D-CHD-C4C	-4.13	117.23	126.02
24	b	612	CLA	C3C-C4C-NC	4.13	115.72	110.43
26	b	626	BCR	C7-C8-C9	-4.13	120.12	126.23
24	c	509	CLA	C1C-C2C-C3C	-4.13	102.64	106.98
24	c	518	CLA	O2D-CGD-CBD	4.13	118.45	111.23
24	c	509	CLA	C3C-C4C-NC	4.13	115.72	110.43
24	b	610	CLA	C1D-CHD-C4C	-4.12	117.25	126.02
31	a	415[A]	PL9	C22-C23-C24	-4.12	118.19	127.62
26	k	101	BCR	C24-C23-C22	-4.12	120.14	126.23
24	C	503	CLA	C1D-CHD-C4C	-4.11	117.27	126.02
24	A	410	CLA	C3C-C4C-NC	4.11	115.70	110.43
24	C	507	CLA	C3D-C4D-ND	4.11	116.67	109.99
24	b	621	CLA	CMD-C2D-C1D	4.11	131.97	124.73
24	c	516	CLA	C4A-NA-C1A	-4.11	104.80	106.68
36	D	406	DGD	O2G-C1B-C2B	4.11	120.37	111.48
24	c	511	CLA	C2B-C1B-NB	4.11	114.59	110.33
24	B	604	CLA	C3C-C4C-NC	4.11	115.69	110.43
29	A	417	LMT	O5'-C5'-C4'	4.11	118.22	109.72
24	d	402	CLA	C3D-C2D-C1D	-4.11	100.23	105.83
24	b	614	CLA	C3B-C2B-C1B	-4.11	102.33	107.17
24	c	509	CLA	C1D-CHD-C4C	-4.10	117.30	126.02
24	C	511	CLA	C1D-CHD-C4C	-4.10	117.31	126.02
24	B	604	CLA	C1D-CHD-C4C	-4.10	117.31	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H	101	BCR	C38-C26-C25	-4.10	120.01	124.48
24	B	604	CLA	C3D-C2D-C1D	-4.09	100.24	105.83
24	C	511	CLA	C2B-C1B-NB	4.09	114.57	110.33
24	c	510	CLA	C2B-C1B-NB	4.09	114.57	110.33
24	C	512	CLA	C1-C2-C3	-4.09	119.49	126.20
24	C	505	CLA	C3D-C4D-ND	4.09	116.63	109.99
24	B	611	CLA	CHD-C1D-ND	-4.09	119.05	124.80
24	c	510	CLA	C1D-CHD-C4C	-4.09	117.33	126.02
24	c	518	CLA	C1D-CHD-C4C	-4.09	117.33	126.02
24	b	621	CLA	C1D-CHD-C4C	-4.08	117.34	126.02
24	B	612	CLA	C3C-C4C-NC	4.08	115.66	110.43
24	B	604	CLA	CAA-C2A-C3A	-4.08	101.96	113.00
24	b	620	CLA	C1-C2-C3	-4.08	119.51	126.20
26	D	404	BCR	C33-C5-C6	-4.08	120.03	124.48
24	b	625	CLA	C2B-C1B-NB	4.08	114.56	110.33
24	C	510	CLA	C3B-C2B-C1B	-4.08	102.36	107.17
24	B	615	CLA	C3C-C4C-NC	4.07	115.65	110.43
24	C	507	CLA	C2C-C1C-NC	4.07	114.26	109.98
24	c	512	CLA	O2D-CGD-O1D	-4.07	115.92	123.85
24	c	515	CLA	C2B-C1B-NB	4.07	114.55	110.33
24	B	613	CLA	C2C-C1C-NC	4.07	114.25	109.98
24	b	615	CLA	C1D-CHD-C4C	-4.06	117.38	126.02
24	C	508	CLA	CHD-C1D-ND	-4.06	119.08	124.80
24	B	606	CLA	CMC-C2C-C1C	4.06	131.38	125.03
24	D	402	CLA	C3B-C4B-NB	4.06	114.16	110.53
31	a	415[A]	PL9	C32-C33-C34	-4.06	118.33	127.62
24	C	504	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
24	D	402	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
24	c	516	CLA	CHD-C1D-ND	-4.06	119.09	124.80
24	c	512	CLA	C1D-CHD-C4C	-4.06	117.40	126.02
24	c	506	CLA	O2D-CGD-O1D	-4.05	115.96	123.85
24	B	602	CLA	C1D-CHD-C4C	-4.05	117.41	126.02
24	a	409	CLA	C1-C2-C3	-4.05	119.56	126.20
24	c	506	CLA	C3D-C4D-ND	4.05	116.57	109.99
24	D	402	CLA	C1-C2-C3	-4.05	119.56	126.20
24	c	506	CLA	CHD-C1D-ND	-4.05	119.11	124.80
24	a	412	CLA	C1-C2-C3	-4.05	119.57	126.20
24	c	515	CLA	C3D-C2D-C1D	-4.04	100.31	105.83
24	d	402	CLA	C3B-C4B-NB	4.04	114.14	110.53
24	B	608	CLA	C2B-C1B-NB	4.04	114.52	110.33
24	B	607	CLA	C1D-CHD-C4C	-4.04	117.43	126.02
24	b	624	CLA	C1D-CHD-C4C	-4.04	117.44	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	615	CLA	CHD-C1D-ND	-4.04	119.12	124.80
24	C	501	CLA	C4A-NA-C1A	-4.04	104.84	106.68
24	C	503	CLA	C3C-C4C-NC	4.04	115.60	110.43
33	Z	101	LMG	O7-C10-C11	4.04	120.21	111.48
24	B	609	CLA	CHD-C1D-ND	-4.04	119.12	124.80
24	c	513	CLA	C3C-C4C-NC	4.04	115.60	110.43
24	b	616	CLA	C3C-C4C-NC	4.03	115.60	110.43
31	a	415[B]	PL9	C22-C23-C24	-4.03	118.39	127.62
24	C	506	CLA	C3D-C4D-ND	4.03	116.54	109.99
24	b	623	CLA	CHD-C1D-ND	-4.03	119.14	124.80
24	B	617	CLA	C3D-C4D-ND	4.03	116.53	109.99
24	C	505	CLA	C1D-CHD-C4C	-4.02	117.47	126.02
24	C	512	CLA	C3C-C4C-NC	4.02	115.58	110.43
24	c	507	CLA	C1D-CHD-C4C	-4.02	117.47	126.02
24	b	624	CLA	CHD-C1D-ND	-4.02	119.14	124.80
24	b	622	CLA	C4A-NA-C1A	-4.02	104.84	106.68
24	C	501	CLA	C3B-C2B-C1B	-4.01	102.44	107.17
24	C	502	CLA	CHD-C1D-ND	-4.01	119.15	124.80
24	b	622	CLA	C3C-C4C-NC	4.01	115.57	110.43
24	B	612	CLA	C3B-C4B-NB	4.01	114.11	110.53
24	B	607	CLA	C3D-C4D-ND	4.01	116.51	109.99
35	b	632	HTG	O5-C1-C2	4.01	115.85	110.32
26	y	101	BCR	C15-C14-C13	-4.01	121.65	127.28
24	d	401	CLA	CBC-CAC-C3C	-4.01	101.55	112.42
31	a	415[B]	PL9	C32-C33-C34	-4.01	118.45	127.62
24	C	505	CLA	CMB-C2B-C1B	4.01	131.52	125.42
24	b	618	CLA	C3B-C2B-C1B	-4.00	102.45	107.17
24	B	605	CLA	C3B-C4B-NB	4.00	114.10	110.53
24	A	407	CLA	C2C-C1C-NC	4.00	114.18	109.98
24	b	614	CLA	C1D-CHD-C4C	-4.00	117.53	126.02
24	d	402	CLA	C1C-C2C-C3C	-4.00	102.78	106.98
24	b	610	CLA	O2D-CGD-O1D	-3.99	116.07	123.85
24	c	512	CLA	C3D-C4D-ND	3.99	116.48	109.99
24	B	613	CLA	C2B-C1B-NB	3.99	114.47	110.33
24	b	614	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
24	B	615	CLA	CAC-C3C-C4C	3.99	129.98	124.79
24	b	615	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
24	C	501	CLA	C2B-C1B-NB	3.99	114.46	110.33
24	B	616	CLA	C3C-C4C-NC	3.98	115.53	110.43
24	B	615	CLA	CHD-C1D-ND	-3.98	119.20	124.80
24	A	406	CLA	CHD-C1D-ND	-3.98	119.20	124.80
24	b	614	CLA	C3C-C4C-NC	3.98	115.52	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	C4A-NA-C1A	-3.98	104.86	106.68
26	D	404	BCR	C24-C23-C22	-3.97	120.36	126.23
24	B	610	CLA	C3B-C2B-C1B	-3.97	102.49	107.17
26	H	101	BCR	C16-C17-C18	-3.97	121.71	127.28
24	b	619	CLA	C1-C2-C3	-3.97	119.70	126.20
27	a	405	SQD	O47-C7-C8	3.97	120.06	111.48
24	C	502	CLA	C2B-C1B-NB	3.97	114.44	110.33
24	B	609	CLA	C4A-NA-C1A	-3.97	104.87	106.68
24	b	623	CLA	O2D-CGD-O1D	-3.96	116.13	123.85
24	D	403	CLA	CHD-C1D-ND	-3.96	119.23	124.80
24	b	610	CLA	CHD-C1D-ND	-3.96	119.23	124.80
24	C	504	CLA	C3B-C4B-NB	3.96	114.06	110.53
24	b	623	CLA	C1C-C2C-C3C	-3.96	102.82	106.98
24	c	506	CLA	C3B-C4B-NB	3.96	114.06	110.53
24	b	612	CLA	C2B-C1B-NB	3.95	114.42	110.33
24	C	506	CLA	C3B-C2B-C1B	-3.95	102.51	107.17
24	b	611	CLA	CAA-C2A-C3A	-3.95	102.33	113.00
24	B	612	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
24	c	515	CLA	C1C-C2C-C3C	-3.94	102.83	106.98
24	b	612	CLA	CHD-C1D-ND	-3.94	119.25	124.80
24	b	618	CLA	C3C-C4C-NC	3.94	115.48	110.43
37	D	409	LHG	O7-C7-C8	3.94	120.00	111.48
24	C	501	CLA	C1C-C2C-C3C	-3.94	102.84	106.98
24	B	610	CLA	CHD-C1D-ND	-3.94	119.26	124.80
24	c	508	CLA	CHD-C1D-ND	-3.93	119.27	124.80
24	d	402	CLA	C1-C2-C3	-3.93	119.75	126.20
24	b	618	CLA	CHD-C1D-ND	-3.93	119.27	124.80
24	d	401	CLA	C2B-C1B-NB	3.93	114.40	110.33
24	b	624	CLA	O2D-CGD-CBD	3.92	118.08	111.23
24	c	507	CLA	C3C-C4C-NC	3.92	115.45	110.43
24	d	402	CLA	C2B-C1B-NB	3.92	114.39	110.33
33	b	629	LMG	O7-C10-C11	3.91	119.95	111.48
24	a	409	CLA	C1D-CHD-C4C	-3.91	117.70	126.02
24	C	507	CLA	CHD-C1D-ND	-3.91	119.30	124.80
24	B	614	CLA	C4A-NA-C1A	-3.91	104.89	106.68
24	B	604	CLA	C1C-C2C-C3C	-3.91	102.86	106.98
24	B	617	CLA	C2B-C1B-NB	3.91	114.38	110.33
38	F	102	HEM	CHD-C4C-NC	3.91	128.71	124.45
38	F	102	HEM	CAD-CBD-CGD	3.91	124.03	113.67
24	A	405	CLA	C3D-C2D-C1D	-3.91	100.50	105.83
24	B	607	CLA	C3C-C4C-NC	3.91	115.43	110.43
24	c	508	CLA	C2C-C1C-NC	3.90	114.08	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	619	CLA	CHD-C1D-ND	-3.90	119.31	124.80
24	A	405	CLA	CAA-C2A-C3A	-3.90	102.45	113.00
24	C	509	CLA	CHD-C1D-ND	-3.90	119.31	124.80
24	B	616	CLA	C1D-CHD-C4C	-3.90	117.74	126.02
27	A	412	SQD	C45-O47-C7	-3.90	108.47	117.80
24	B	604	CLA	C2B-C1B-NB	3.89	114.36	110.33
24	B	605	CLA	C1C-C2C-C3C	-3.89	102.89	106.98
27	L	102	SQD	C3-C4-C5	3.89	117.29	110.23
24	B	613	CLA	CHD-C1D-ND	-3.89	119.32	124.80
24	b	620	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
24	B	610	CLA	O2D-CGD-CBD	3.89	118.03	111.23
24	C	506	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
24	a	410	CLA	C3C-C4C-NC	3.88	115.40	110.43
37	D	407	LHG	O7-C7-C8	3.87	119.85	111.48
24	C	506	CLA	CHD-C1D-ND	-3.86	119.36	124.80
24	b	613	CLA	C2B-C1B-NB	3.86	114.33	110.33
24	b	620	CLA	CHD-C1D-ND	-3.86	119.37	124.80
24	b	618	CLA	C1D-CHD-C4C	-3.86	117.82	126.02
24	b	620	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
24	C	510	CLA	CHD-C1D-ND	-3.86	119.37	124.80
24	b	624	CLA	C3C-C4C-NC	3.86	115.37	110.43
24	C	504	CLA	CBC-CAC-C3C	-3.86	101.96	112.42
24	b	621	CLA	C4C-C3C-C2C	-3.86	101.28	106.89
24	b	621	CLA	C3B-C4B-NB	3.85	113.97	110.53
24	B	610	CLA	C1D-CHD-C4C	-3.85	117.83	126.02
24	C	512	CLA	C1D-CHD-C4C	-3.85	117.84	126.02
36	c	520	DGD	O2G-C1B-C2B	3.84	119.80	111.48
27	A	416	SQD	O47-C7-C8	3.84	119.80	111.48
24	d	402	CLA	C3B-C2B-C1B	-3.84	102.64	107.17
33	C	519	LMG	O7-C10-C11	3.84	119.78	111.48
31	d	405[A]	PL9	C42-C43-C44	-3.84	118.84	127.62
24	B	606	CLA	CHD-C1D-ND	-3.84	119.40	124.80
24	C	507	CLA	C1D-CHD-C4C	-3.83	117.87	126.02
24	b	625	CLA	CHD-C1D-ND	-3.83	119.41	124.80
24	B	612	CLA	C2B-C1B-NB	3.83	114.30	110.33
24	c	517	CLA	C1D-CHD-C4C	-3.83	117.88	126.02
27	A	416	SQD	O48-C23-C24	3.83	123.51	111.83
24	C	512	CLA	CHD-C1D-ND	-3.83	119.42	124.80
24	c	506	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
24	C	510	CLA	C3B-C4B-NB	3.82	113.94	110.53
24	B	605	CLA	C3B-C2B-C1B	-3.82	102.66	107.17
24	c	506	CLA	CAC-C3C-C4C	3.82	129.76	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	415[A]	PL9	C15-C14-C16	3.82	121.86	115.23
24	b	622	CLA	C1C-C2C-C3C	-3.82	102.97	106.98
36	c	521	DGD	O2G-C1B-C2B	3.82	119.74	111.48
40	V	205	HEC	CHC-C4B-NB	3.81	128.61	124.45
26	h	101	BCR	C16-C17-C18	-3.81	121.93	127.28
24	c	511	CLA	C1D-CHD-C4C	-3.81	117.93	126.02
24	A	406	CLA	C1D-CHD-C4C	-3.81	117.93	126.02
24	c	515	CLA	C4-C3-C5	3.81	121.83	115.23
24	b	617	CLA	C3C-C4C-NC	3.80	115.30	110.43
24	B	608	CLA	C3C-C4C-NC	3.80	115.30	110.43
24	C	507	CLA	C3C-C4C-NC	3.80	115.30	110.43
36	D	406	DGD	C1D-C2D-C3D	3.80	118.00	110.01
24	c	515	CLA	CHD-C1D-ND	-3.80	119.45	124.80
24	B	614	CLA	CHD-C1D-ND	-3.80	119.46	124.80
27	a	405	SQD	O48-C23-C24	3.79	123.40	111.83
24	B	602	CLA	O2D-CGD-O1D	-3.79	116.47	123.85
24	c	512	CLA	CHD-C1D-ND	-3.79	119.47	124.80
24	c	517	CLA	CHD-C1D-ND	-3.79	119.47	124.80
24	c	516	CLA	C1D-CHD-C4C	-3.79	117.97	126.02
36	C	517	DGD	O2G-C1B-C2B	3.79	119.67	111.48
24	C	510	CLA	C1D-CHD-C4C	-3.79	117.97	126.02
24	c	513	CLA	C1D-CHD-C4C	-3.78	117.98	126.02
24	D	403	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
24	B	617	CLA	C3C-C4C-NC	3.78	115.27	110.43
24	c	517	CLA	C1C-C2C-C3C	-3.78	103.01	106.98
24	B	609	CLA	C3B-C4B-NB	3.78	113.90	110.53
24	b	624	CLA	CMB-C2B-C1B	3.77	131.16	125.42
24	C	513	CLA	C1D-CHD-C4C	-3.77	118.00	126.02
24	B	612	CLA	CAC-C3C-C4C	3.77	129.70	124.79
24	A	410	CLA	C1D-CHD-C4C	-3.77	118.01	126.02
24	B	603	CLA	C1D-CHD-C4C	-3.76	118.02	126.02
24	A	405	CLA	O2D-CGD-CBD	3.76	117.80	111.23
24	C	506	CLA	C2B-C1B-NB	3.76	114.22	110.33
26	T	103	BCR	C33-C5-C6	-3.75	120.39	124.48
26	t	101	BCR	C15-C16-C17	-3.75	115.84	123.52
24	a	412	CLA	C1D-CHD-C4C	-3.75	118.05	126.02
24	B	614	CLA	C3D-C4D-ND	3.75	116.08	109.99
24	C	511	CLA	C1C-C2C-C3C	-3.75	103.04	106.98
24	b	617	CLA	C1D-CHD-C4C	-3.75	118.05	126.02
24	B	605	CLA	CHD-C1D-ND	-3.75	119.53	124.80
24	c	518	CLA	C1C-C2C-C3C	-3.75	103.04	106.98
24	C	510	CLA	C3C-C4C-NC	3.74	115.23	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	415[A]	PL9	C7-C3-C4	3.74	119.99	116.91
37	E	101	LHG	O7-C7-C8	3.74	119.57	111.48
24	A	410	CLA	CAC-C3C-C4C	3.74	129.66	124.79
33	c	524	LMG	O6-C5-C4	3.74	116.44	109.70
24	b	611	CLA	C1D-CHD-C4C	-3.74	118.07	126.02
24	C	502	CLA	C3C-C4C-NC	3.74	115.22	110.43
24	b	617	CLA	O2D-CGD-CBD	3.74	117.77	111.23
24	C	509	CLA	C3C-C4C-NC	3.74	115.22	110.43
24	d	403	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
24	b	622	CLA	C3D-C4D-ND	3.73	116.05	109.99
24	b	625	CLA	C3C-C4C-NC	3.73	115.21	110.43
24	c	514	CLA	C3C-C4C-NC	3.73	115.20	110.43
24	D	403	CLA	C1D-CHD-C4C	-3.73	118.10	126.02
24	C	511	CLA	CHD-C1D-ND	-3.73	119.56	124.80
36	e	101	DGD	C3E-C4E-C5E	3.72	116.98	110.23
24	a	412	CLA	CMB-C2B-C1B	3.72	131.09	125.42
24	a	412	CLA	CHD-C1D-ND	-3.72	119.56	124.80
24	b	618	CLA	C2B-C1B-NB	3.72	114.19	110.33
24	b	619	CLA	C3C-C4C-NC	3.72	115.19	110.43
24	C	509	CLA	C1C-C2C-C3C	-3.72	103.07	106.98
24	c	512	CLA	CMB-C2B-C1B	3.72	131.08	125.42
24	B	604	CLA	CMC-C2C-C1C	3.72	130.84	125.03
24	C	504	CLA	O2D-CGD-O1D	-3.71	116.62	123.85
24	a	412	CLA	O2D-CGD-O1D	-3.71	116.62	123.85
24	b	617	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
24	B	610	CLA	C3B-C4B-NB	3.71	113.84	110.53
24	c	509	CLA	C2B-C1B-NB	3.71	114.17	110.33
24	b	622	CLA	C1-C2-C3	-3.70	120.13	126.20
24	b	619	CLA	C1D-CHD-C4C	-3.70	118.15	126.02
24	C	504	CLA	C1D-CHD-C4C	-3.70	118.16	126.02
24	b	612	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
24	B	610	CLA	C3C-C4C-NC	3.69	115.16	110.43
24	B	605	CLA	C1D-CHD-C4C	-3.69	118.17	126.02
31	D	405[A]	PL9	C42-C43-C44	-3.69	119.18	127.62
35	B	632	HTG	C1'-S1-C1	3.68	108.41	100.45
24	C	505	CLA	C3D-C2D-C1D	-3.68	100.81	105.83
24	b	616	CLA	C4A-NA-C1A	-3.68	105.00	106.68
24	d	401	CLA	CHD-C1D-ND	-3.68	119.62	124.80
24	B	614	CLA	C2B-C1B-NB	3.68	114.14	110.33
24	C	506	CLA	CAC-C3C-C4C	3.68	129.58	124.79
29	a	404	LMT	C1'-O5'-C5'	3.68	120.90	113.72
24	B	612	CLA	CHD-C1D-ND	-3.68	119.63	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
24	b	623	CLA	C3C-C4C-NC	3.67	115.14	110.43
26	C	514	BCR	C33-C5-C6	-3.67	120.48	124.48
24	c	510	CLA	O2D-CGD-O1D	-3.67	116.70	123.85
24	C	508	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
24	c	506	CLA	C3C-C4C-NC	3.66	115.12	110.43
24	d	403	CLA	C1D-CHD-C4C	-3.66	118.23	126.02
24	D	403	CLA	C3C-C4C-NC	3.66	115.12	110.43
24	a	410	CLA	C1D-CHD-C4C	-3.66	118.24	126.02
24	B	603	CLA	C3C-C4C-NC	3.66	115.11	110.43
31	a	415[B]	PL9	C7-C3-C4	3.66	119.92	116.91
26	b	627	BCR	C29-C30-C25	3.65	115.75	110.44
24	C	506	CLA	C3B-C4B-NB	3.65	113.79	110.53
24	A	405	CLA	O2A-CGA-CBA	3.64	122.94	111.83
24	b	621	CLA	O2A-CGA-CBA	3.64	122.94	111.83
29	a	404	LMT	O5'-C5'-C4'	3.64	117.25	109.72
24	B	614	CLA	C3B-C4B-NB	3.64	113.78	110.53
24	C	511	CLA	CAC-C3C-C4C	3.64	129.53	124.79
24	b	613	CLA	C1D-CHD-C4C	-3.64	118.28	126.02
24	c	507	CLA	CHD-C1D-ND	-3.64	119.68	124.80
24	c	514	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
24	B	611	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
24	c	515	CLA	C3C-C4C-NC	3.63	115.08	110.43
24	B	608	CLA	C1D-CHD-C4C	-3.63	118.30	126.02
24	C	513	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
24	C	506	CLA	C1D-CHD-C4C	-3.63	118.30	126.02
24	C	501	CLA	CMB-C2B-C1B	3.63	130.95	125.42
24	B	616	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
24	C	509	CLA	C3B-C4B-NB	3.63	113.77	110.53
24	C	511	CLA	C3C-C4C-NC	3.63	115.08	110.43
31	A	419[B]	PL9	C7-C3-C4	3.63	119.90	116.91
24	C	504	CLA	C3C-C4C-NC	3.63	115.08	110.43
38	e	103	HEM	C1B-NB-C4B	3.63	109.50	105.21
24	B	610	CLA	C1C-C2C-C3C	-3.63	103.17	106.98
24	b	610	CLA	C3C-C4C-NC	3.62	115.07	110.43
24	B	605	CLA	C3D-C4D-ND	3.62	115.88	109.99
24	C	501	CLA	C1D-CHD-C4C	-3.62	118.32	126.02
24	B	605	CLA	C1-C2-C3	-3.62	120.26	126.20
24	D	403	CLA	C3B-C4B-NB	3.62	113.76	110.53
24	b	618	CLA	C1C-C2C-C3C	-3.62	103.17	106.98
24	D	403	CLA	CAC-C3C-C4C	3.62	129.50	124.79
24	C	503	CLA	O2D-CGD-CBD	3.62	117.56	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	516	CLA	O2D-CGD-CBD	3.62	117.55	111.23
24	B	602	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
24	C	508	CLA	C3B-C4B-NB	3.61	113.75	110.53
37	L	101	LHG	O7-C7-C8	3.61	119.29	111.48
24	c	511	CLA	C4B-C3B-C2B	-3.61	102.82	107.30
24	C	501	CLA	O2D-CGD-O1D	-3.61	116.83	123.85
24	b	623	CLA	C1D-CHD-C4C	-3.60	118.37	126.02
24	B	607	CLA	C3B-C4B-NB	3.60	113.74	110.53
24	C	502	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
24	c	511	CLA	CBC-CAC-C3C	-3.60	102.67	112.42
24	b	622	CLA	C1D-CHD-C4C	-3.60	118.37	126.02
24	c	515	CLA	C1D-CHD-C4C	-3.60	118.37	126.02
24	C	509	CLA	C1D-CHD-C4C	-3.60	118.38	126.02
26	c	519	BCR	C33-C5-C6	-3.60	120.56	124.48
24	B	611	CLA	C3C-C4C-NC	3.59	115.03	110.43
24	B	606	CLA	CHD-C4C-NC	3.59	129.80	124.23
24	A	405	CLA	C3C-C4C-NC	3.59	115.03	110.43
33	z	101	LMG	O7-C10-C11	3.59	119.24	111.48
26	D	404	BCR	C38-C26-C25	-3.59	120.57	124.48
24	C	501	CLA	C1-C2-C3	-3.59	120.32	126.20
24	B	609	CLA	C3C-C4C-NC	3.59	115.03	110.43
24	B	603	CLA	C1C-C2C-C3C	-3.59	103.21	106.98
24	B	607	CLA	CMC-C2C-C1C	3.58	130.64	125.03
27	F	103	SQD	O6-C1-C2	3.58	113.72	108.27
24	d	402	CLA	C4B-C3B-C2B	-3.58	102.85	107.30
24	C	508	CLA	C3C-C4C-NC	3.58	115.02	110.43
33	c	523	LMG	O8-C28-C29	3.58	122.76	111.83
24	b	612	CLA	C3B-C4B-NB	3.58	113.73	110.53
24	a	412	CLA	C3C-C4C-NC	3.58	115.01	110.43
24	d	401	CLA	C3C-C4C-NC	3.58	115.01	110.43
27	a	414	SQD	C1-C2-C3	-3.58	102.48	110.01
24	B	615	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
24	B	613	CLA	C3B-C4B-NB	3.57	113.72	110.53
31	A	419[A]	PL9	C37-C38-C39	-3.57	119.44	127.62
24	C	502	CLA	C1D-CHD-C4C	-3.57	118.43	126.02
24	B	604	CLA	CHD-C1D-ND	-3.57	119.78	124.80
35	b	607	HTG	C1'-S1-C1	3.57	108.15	100.45
24	c	509	CLA	C4-C3-C5	3.57	121.42	115.23
24	b	617	CLA	CHD-C1D-ND	-3.57	119.78	124.80
31	A	419[B]	PL9	C32-C33-C34	-3.57	119.46	127.62
24	B	603	CLA	O2D-CGD-O1D	-3.57	116.91	123.85
24	b	614	CLA	CHD-C4C-NC	3.56	129.76	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	C4A-NA-C1A	-3.56	105.05	106.68
24	b	611	CLA	C3C-C4C-NC	3.56	114.99	110.43
24	B	608	CLA	C3B-C4B-NB	3.56	113.71	110.53
24	b	612	CLA	CMC-C2C-C1C	3.55	130.59	125.03
24	B	608	CLA	C1C-C2C-C3C	-3.55	103.24	106.98
24	B	613	CLA	C4A-NA-C1A	-3.55	105.06	106.68
26	k	101	BCR	C7-C8-C9	-3.55	120.98	126.23
24	B	603	CLA	CAA-C2A-C3A	-3.55	103.41	113.00
31	a	415[B]	PL9	C15-C14-C16	3.55	121.39	115.23
24	c	510	CLA	C1C-C2C-C3C	-3.54	103.25	106.98
38	F	102	HEM	C1B-NB-C4B	3.54	109.40	105.21
24	A	410	CLA	CHD-C1D-ND	-3.54	119.83	124.80
24	B	617	CLA	C3B-C4B-NB	3.53	113.69	110.53
24	C	510	CLA	C2B-C1B-NB	3.53	113.99	110.33
26	b	626	BCR	C15-C14-C13	-3.53	122.32	127.28
26	d	404	BCR	C7-C8-C9	-3.53	121.01	126.23
24	c	509	CLA	C1-C2-C3	-3.53	120.41	126.20
33	c	523	LMG	O7-C10-C11	3.53	119.12	111.48
31	a	415[B]	PL9	C7-C8-C9	-3.53	120.75	126.83
33	c	524	LMG	C3-C4-C5	3.53	116.63	110.23
24	B	605	CLA	C4B-C3B-C2B	-3.53	102.92	107.30
24	B	602	CLA	C3C-C4C-NC	3.53	114.95	110.43
24	D	403	CLA	O2D-CGD-O1D	-3.52	116.99	123.85
24	A	405	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
24	a	410	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
24	b	624	CLA	C3B-C4B-NB	3.52	113.67	110.53
24	A	407	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
29	C	521	LMT	C1'-O5'-C5'	3.52	120.59	113.72
26	H	101	BCR	C24-C23-C22	-3.52	121.03	126.23
24	a	410	CLA	CMC-C2C-C1C	3.52	130.53	125.03
24	b	611	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
24	B	607	CLA	O2D-CGD-O1D	-3.52	117.01	123.85
24	C	512	CLA	CMB-C2B-C1B	3.51	130.76	125.42
35	B	624	HTG	C1-O5-C5	3.51	118.86	112.56
24	B	614	CLA	C1C-C2C-C3C	-3.51	103.29	106.98
25	A	409[B]	PHO	C1A-C2A-C3A	-3.51	99.50	102.84
31	a	415[B]	PL9	C7-C3-C2	-3.51	119.26	123.39
24	b	623	CLA	C3B-C4B-NB	3.50	113.66	110.53
31	A	419[B]	PL9	C7-C3-C2	-3.50	119.26	123.39
26	T	103	BCR	C11-C10-C9	-3.50	122.37	127.28
24	a	409	CLA	CAA-C2A-C3A	-3.49	103.56	113.00
24	c	510	CLA	C4C-C3C-C2C	-3.49	101.81	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	d	405[B]	PL9	C42-C43-C44	-3.49	119.63	127.62
25	a	418[A]	PHO	C1A-C2A-C3A	-3.49	99.52	102.84
24	b	611	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
24	d	403	CLA	C3C-C4C-NC	3.49	114.90	110.43
24	B	616	CLA	CMC-C2C-C1C	3.49	130.48	125.03
24	B	609	CLA	C1D-CHD-C4C	-3.49	118.61	126.02
24	b	613	CLA	C4B-C3B-C2B	-3.48	102.97	107.30
24	c	518	CLA	C3C-C4C-NC	3.48	114.89	110.43
24	c	517	CLA	C3C-C4C-NC	3.48	114.89	110.43
24	b	625	CLA	C4C-C3C-C2C	-3.48	101.83	106.89
25	a	418[B]	PHO	C1A-C2A-C3A	-3.48	99.53	102.84
24	c	508	CLA	C4C-C3C-C2C	-3.48	101.83	106.89
24	c	516	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
24	A	407	CLA	C1D-CHD-C4C	-3.47	118.64	126.02
25	a	418[B]	PHO	O2D-CGD-O1D	-3.47	117.09	123.85
31	a	415[B]	PL9	C17-C18-C19	-3.46	119.69	127.62
24	B	614	CLA	C1-C2-C3	-3.46	120.52	126.20
24	c	513	CLA	C1-C2-C3	-3.46	120.52	126.20
24	C	504	CLA	C4B-C3B-C2B	-3.46	103.00	107.30
24	C	512	CLA	C1C-C2C-C3C	-3.46	103.34	106.98
24	c	510	CLA	C3D-C2D-C1D	-3.46	101.11	105.83
24	b	620	CLA	C3C-C4C-NC	3.46	114.86	110.43
31	D	405[A]	PL9	C40-C39-C41	3.46	121.23	115.23
24	C	508	CLA	C1D-CHD-C4C	-3.46	118.67	126.02
26	C	515	BCR	C7-C8-C9	-3.46	121.12	126.23
37	d	407	LHG	O7-C7-C8	3.45	118.95	111.48
24	C	506	CLA	C3C-C4C-NC	3.45	114.85	110.43
26	C	515	BCR	C33-C5-C6	-3.45	120.72	124.48
24	c	511	CLA	C3C-C4C-NC	3.45	114.85	110.43
24	b	614	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
24	c	512	CLA	C2B-C1B-NB	3.44	113.90	110.33
27	a	414	SQD	O9-S-C6	3.44	111.90	106.76
31	A	419[A]	PL9	C32-C33-C34	-3.44	119.75	127.62
26	c	528	BCR	C15-C14-C13	-3.44	122.46	127.28
24	c	506	CLA	C1D-CHD-C4C	-3.44	118.71	126.02
24	C	505	CLA	C4C-C3C-C2C	-3.44	101.89	106.89
36	h	102	DGD	O2G-C1B-C2B	3.44	118.91	111.48
24	B	615	CLA	C3B-C4B-NB	3.43	113.60	110.53
24	B	606	CLA	C4-C3-C5	3.43	121.19	115.23
24	a	409	CLA	C3C-C4C-NC	3.43	114.83	110.43
31	a	415[A]	PL9	C17-C18-C19	-3.43	119.76	127.62
24	C	513	CLA	C3C-C4C-NC	3.43	114.82	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	619	BCR	C29-C30-C25	3.43	115.42	110.44
24	D	402	CLA	C4B-C3B-C2B	-3.43	103.04	107.30
24	B	615	CLA	C1D-CHD-C4C	-3.42	118.75	126.02
25	a	418[A]	PHO	C4-C3-C5	3.42	121.17	115.23
26	B	619	BCR	C28-C27-C26	-3.42	107.96	114.06
25	a	418[A]	PHO	C4D-CHA-CBD	3.42	110.09	108.45
24	c	516	CLA	C3C-C4C-NC	3.42	114.81	110.43
24	b	620	CLA	C3B-C4B-NB	3.42	113.58	110.53
24	c	508	CLA	CMB-C2B-C1B	3.41	130.62	125.42
24	C	502	CLA	C3B-C4B-NB	3.41	113.58	110.53
24	B	613	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
24	c	511	CLA	C1-C2-C3	-3.41	120.61	126.20
24	A	407	CLA	C3C-C4C-NC	3.41	114.80	110.43
24	b	610	CLA	C1C-C2C-C3C	-3.41	103.40	106.98
27	f	101	SQD	C1-O5-C5	3.41	120.37	113.72
24	A	407	CLA	C4-C3-C5	3.40	121.13	115.23
26	A	411	BCR	C33-C5-C6	-3.40	120.77	124.48
24	b	614	CLA	C2A-C1A-CHA	-3.40	117.97	123.87
24	C	510	CLA	C1C-C2C-C3C	-3.40	103.41	106.98
24	B	604	CLA	O2A-CGA-O1A	-3.40	115.13	123.63
24	c	514	CLA	CHD-C1D-ND	-3.39	120.03	124.80
24	B	602	CLA	O2A-CGA-CBA	3.39	122.17	111.83
24	A	405	CLA	CHD-C1D-ND	-3.39	120.03	124.80
24	B	613	CLA	C4C-C3C-C2C	-3.39	101.96	106.89
24	B	614	CLA	C4C-C3C-C2C	-3.38	101.97	106.89
29	T	104	LMT	C1'-O5'-C5'	3.38	120.33	113.72
24	d	401	CLA	CAA-C2A-C3A	-3.38	103.86	113.00
24	b	624	CLA	C1C-C2C-C3C	-3.38	103.43	106.98
31	a	415[A]	PL9	C7-C8-C9	-3.38	121.01	126.83
24	A	410	CLA	C1C-C2C-C3C	-3.38	103.43	106.98
26	C	514	BCR	C15-C14-C13	-3.37	122.55	127.28
24	d	403	CLA	CMC-C2C-C1C	3.37	130.30	125.03
24	b	614	CLA	C4-C3-C5	3.37	121.07	115.23
24	B	608	CLA	C1-C2-C3	-3.36	120.69	126.20
24	A	406	CLA	C4A-NA-C1A	-3.36	105.15	106.68
24	B	611	CLA	C1D-CHD-C4C	-3.36	118.89	126.02
24	c	507	CLA	C4C-C3C-C2C	-3.36	102.01	106.89
24	c	507	CLA	C3B-C4B-NB	3.36	113.53	110.53
31	D	405[B]	PL9	C42-C43-C44	-3.36	119.94	127.62
24	A	406	CLA	C4B-C3B-C2B	-3.36	103.13	107.30
24	c	516	CLA	C3B-C4B-NB	3.36	113.53	110.53
24	B	605	CLA	C2B-C1B-NB	3.35	113.81	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	501	CLA	CMC-C2C-C1C	3.35	130.28	125.03
24	B	615	CLA	O2A-CGA-O1A	-3.35	115.24	123.63
24	b	619	CLA	C1C-C2C-C3C	-3.35	103.45	106.98
24	d	402	CLA	C3C-C4C-NC	3.35	114.72	110.43
31	a	415[A]	PL9	C42-C43-C44	-3.35	119.95	127.62
24	B	613	CLA	CMC-C2C-C1C	3.35	130.27	125.03
40	v	205	HEC	CHA-C1A-NA	3.35	128.10	124.45
24	C	501	CLA	CBC-CAC-C3C	-3.34	103.36	112.42
24	B	609	CLA	C1-C2-C3	-3.34	120.72	126.20
24	A	410	CLA	C4A-NA-C1A	-3.34	105.16	106.68
31	a	415[B]	PL9	C37-C38-C39	-3.34	119.98	127.62
24	B	613	CLA	C1D-CHD-C4C	-3.34	118.93	126.02
24	C	506	CLA	C4B-C3B-C2B	-3.33	103.16	107.30
24	c	507	CLA	C1C-C2C-C3C	-3.33	103.47	106.98
31	A	419[A]	PL9	C7-C3-C4	3.33	119.65	116.91
24	B	608	CLA	CAA-C2A-C3A	-3.33	104.01	113.00
24	b	616	CLA	CMB-C2B-C1B	3.33	130.49	125.42
24	c	510	CLA	CMB-C2B-C1B	3.33	130.48	125.42
24	A	407	CLA	CBC-CAC-C3C	-3.32	103.41	112.42
24	c	513	CLA	CHD-C1D-ND	-3.32	120.13	124.80
24	d	402	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
33	B	622	LMG	O8-C28-C29	3.32	121.95	111.83
24	C	503	CLA	C1C-C2C-C3C	-3.32	103.49	106.98
33	c	501	LMG	C8-O7-C10	-3.32	109.86	117.80
31	a	415[B]	PL9	C27-C28-C29	-3.32	120.03	127.62
24	b	621	CLA	O2A-CGA-O1A	-3.31	115.34	123.63
24	A	406	CLA	C3C-C4C-NC	3.31	114.67	110.43
31	d	405[B]	PL9	C37-C38-C39	-3.31	120.04	127.62
24	A	410	CLA	C3B-C4B-NB	3.31	113.49	110.53
24	b	619	CLA	C4C-C3C-C2C	-3.31	102.07	106.89
24	c	508	CLA	CAC-C3C-C4C	3.31	129.10	124.79
24	C	513	CLA	C1-C2-C3	-3.31	120.77	126.20
24	b	625	CLA	O2A-CGA-CBA	3.31	121.92	111.83
31	A	419[A]	PL9	C20-C19-C21	3.30	120.96	115.23
31	A	419[B]	PL9	C37-C38-C39	-3.30	120.06	127.62
24	b	616	CLA	C1D-CHD-C4C	-3.30	119.00	126.02
24	A	410	CLA	C4C-C3C-C2C	-3.30	102.09	106.89
24	b	613	CLA	CHD-C1D-ND	-3.30	120.16	124.80
24	C	501	CLA	C3C-C4C-NC	3.29	114.65	110.43
24	b	615	CLA	C4-C3-C5	3.29	120.94	115.23
24	C	507	CLA	CMC-C2C-C1C	3.29	130.18	125.03
31	D	405[B]	PL9	C37-C38-C39	-3.29	120.10	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	508	CLA	C1-C2-C3	-3.29	120.81	126.20
24	B	617	CLA	CAC-C3C-C4C	3.28	129.06	124.79
24	c	518	CLA	CMC-C2C-C1C	3.28	130.16	125.03
24	B	606	CLA	C1C-C2C-C3C	-3.28	103.53	106.98
24	C	512	CLA	C3B-C4B-NB	3.28	113.46	110.53
24	d	403	CLA	CHD-C4C-NC	3.28	129.31	124.23
24	C	510	CLA	C4B-C3B-C2B	-3.28	103.22	107.30
24	c	508	CLA	CMC-C2C-C1C	3.27	130.15	125.03
24	B	607	CLA	CBC-CAC-C3C	-3.27	103.55	112.42
24	B	617	CLA	CHD-C1D-ND	-3.27	120.20	124.80
26	D	404	BCR	C29-C30-C25	3.27	115.19	110.44
24	D	403	CLA	CMB-C2B-C1B	3.27	130.40	125.42
24	b	624	CLA	CAC-C3C-C4C	3.27	129.04	124.79
24	B	617	CLA	C4C-C3C-C2C	-3.26	102.14	106.89
24	b	616	CLA	C3B-C4B-NB	3.26	113.44	110.53
24	c	513	CLA	CAC-C3C-C4C	3.26	129.03	124.79
24	C	505	CLA	CHD-C1D-ND	-3.26	120.22	124.80
24	C	507	CLA	C1C-C2C-C3C	-3.26	103.56	106.98
24	c	514	CLA	CAC-C3C-C4C	3.25	129.02	124.79
31	D	405[A]	PL9	C7-C8-C9	-3.25	121.23	126.83
27	B	621	SQD	O7-S-C6	3.25	111.61	106.76
24	c	507	CLA	CMB-C2B-C1B	3.25	130.37	125.42
24	c	513	CLA	C4C-C3C-C2C	-3.25	102.16	106.89
24	C	505	CLA	C1C-C2C-C3C	-3.25	103.56	106.98
24	C	509	CLA	CAC-C3C-C4C	3.25	129.01	124.79
26	B	618	BCR	C7-C8-C9	-3.25	121.43	126.23
24	a	412	CLA	C3B-C4B-NB	3.24	113.42	110.53
24	B	611	CLA	C4C-C3C-C2C	-3.24	102.17	106.89
24	C	506	CLA	C1-C2-C3	-3.24	120.88	126.20
24	c	515	CLA	C4B-C3B-C2B	-3.24	103.27	107.30
24	b	610	CLA	C3B-C4B-NB	3.24	113.42	110.53
24	C	511	CLA	C4A-NA-C1A	-3.24	105.20	106.68
24	B	617	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
40	v	205	HEC	CHD-C4C-NC	3.24	127.98	124.45
26	c	528	BCR	C11-C10-C9	-3.24	122.74	127.28
24	B	604	CLA	O2A-CGA-CBA	3.23	121.70	111.83
24	B	615	CLA	O2A-CGA-CBA	3.23	121.69	111.83
24	B	605	CLA	CAC-C3C-C4C	3.23	129.00	124.79
24	A	407	CLA	CMB-C2B-C1B	3.23	130.34	125.42
24	d	402	CLA	CAC-C3C-C4C	3.23	128.99	124.79
24	C	512	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
24	b	619	CLA	CAC-C3C-C4C	3.23	128.99	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	CHC-C1C-C2C	-3.23	117.78	126.95
24	B	606	CLA	C2A-C1A-CHA	-3.22	118.27	123.87
24	A	406	CLA	CHD-C4C-NC	3.22	129.23	124.23
31	a	415[A]	PL9	C27-C28-C29	-3.22	120.25	127.62
25	A	408	PHO	C1A-C2A-C3A	-3.22	99.77	102.84
37	d	408	LHG	O7-C7-C8	3.22	118.44	111.48
24	B	611	CLA	O2A-CGA-CBA	3.22	121.64	111.83
31	a	415[B]	PL9	C42-C43-C44	-3.22	120.26	127.62
26	K	101	BCR	C24-C23-C22	-3.21	121.48	126.23
24	B	613	CLA	C1-C2-C3	-3.21	120.93	126.20
24	C	506	CLA	CBC-CAC-C3C	-3.21	103.71	112.42
24	C	506	CLA	CHC-C1C-C2C	-3.21	117.82	126.95
33	C	519	LMG	O8-C28-C29	3.21	121.63	111.83
24	A	410	CLA	C1-C2-C3	-3.21	120.94	126.20
33	D	413	LMG	O7-C10-C11	3.21	118.42	111.48
24	c	510	CLA	CAC-C3C-C4C	3.21	128.96	124.79
24	c	517	CLA	C1-C2-C3	-3.21	120.94	126.20
24	B	613	CLA	C1C-C2C-C3C	-3.21	103.61	106.98
24	a	409	CLA	C3B-C4B-NB	3.20	113.39	110.53
31	d	405[B]	PL9	C27-C28-C29	-3.20	120.29	127.62
24	b	622	CLA	C4C-C3C-C2C	-3.20	102.23	106.89
36	H	102	DGD	O1G-C1A-C2A	3.20	121.60	111.83
24	A	406	CLA	CHC-C1C-C2C	-3.20	117.85	126.95
24	c	509	CLA	CMC-C2C-C1C	3.20	130.03	125.03
24	C	501	CLA	C3B-C4B-NB	3.20	113.38	110.53
24	C	511	CLA	CHC-C1C-C2C	-3.20	117.87	126.95
24	D	402	CLA	C4C-C3C-C2C	-3.19	102.24	106.89
24	B	606	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
24	B	607	CLA	CAC-C3C-C4C	3.19	128.94	124.79
37	D	407	LHG	O8-C23-C24	3.19	121.56	111.83
31	A	419[A]	PL9	C8-C7-C3	3.19	120.27	112.03
24	b	624	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
24	d	402	CLA	C1D-CHD-C4C	-3.19	119.24	126.02
24	b	619	CLA	C3B-C4B-NB	3.19	113.38	110.53
24	A	407	CLA	CHD-C4C-NC	3.19	129.17	124.23
31	D	405[A]	PL9	C10-C9-C11	3.19	120.76	115.23
24	b	621	CLA	C4B-C3B-C2B	-3.19	103.34	107.30
25	A	409[A]	PHO	C4-C3-C5	3.19	120.76	115.23
24	b	613	CLA	CAC-C3C-C4C	3.18	128.93	124.79
31	A	419[A]	PL9	C22-C23-C24	-3.18	120.34	127.62
24	B	614	CLA	C1D-CHD-C4C	-3.18	119.26	126.02
35	C	523	HTG	O5-C5-C4	3.18	115.43	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	612	CLA	CHD-C4C-NC	3.18	129.16	124.23
40	v	205	HEC	CBC-CAC-C3C	-3.18	121.08	127.43
24	c	518	CLA	C1-C2-C3	-3.18	120.99	126.20
24	b	622	CLA	CAC-C3C-C4C	3.18	128.92	124.79
37	b	634	LHG	O8-C23-C24	3.18	121.52	111.83
24	D	402	CLA	C1D-CHD-C4C	-3.17	119.27	126.02
24	B	614	CLA	O2D-CGD-CBD	3.17	116.78	111.23
24	C	503	CLA	CMB-C2B-C1B	3.17	130.25	125.42
37	b	634	LHG	O7-C7-C8	3.17	118.34	111.48
40	V	205	HEC	CBC-CAC-C3C	-3.17	121.10	127.43
24	C	505	CLA	O2D-CGD-O1D	-3.17	117.69	123.85
25	A	409[B]	PHO	C4-C3-C5	3.16	120.72	115.23
24	b	610	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
24	b	615	CLA	CMC-C2C-C1C	3.16	129.97	125.03
24	B	613	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
24	C	502	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
24	c	516	CLA	C1-C2-C3	-3.16	121.02	126.20
24	c	511	CLA	CAA-C2A-C3A	-3.16	104.47	113.00
27	a	414	SQD	O8-S-C6	3.15	112.06	105.97
24	B	610	CLA	C4B-C3B-C2B	-3.15	103.38	107.30
26	d	404	BCR	C33-C5-C6	-3.15	121.05	124.48
24	C	509	CLA	C1-O2A-CGA	3.15	124.27	116.65
24	C	510	CLA	C4C-C3C-C2C	-3.15	102.31	106.89
24	A	410	CLA	C4-C3-C5	3.14	120.69	115.23
24	b	622	CLA	CHC-C1C-C2C	-3.14	118.01	126.95
24	d	402	CLA	C2A-C1A-CHA	-3.14	118.41	123.87
24	b	620	CLA	CMB-C2B-C1B	3.14	130.20	125.42
24	C	504	CLA	CAC-C3C-C4C	3.14	128.88	124.79
24	c	509	CLA	C3B-C4B-NB	3.14	113.33	110.53
24	B	616	CLA	O2D-CGD-CBD	3.14	116.72	111.23
26	T	103	BCR	C15-C16-C17	-3.14	117.10	123.52
24	b	615	CLA	C4B-C3B-C2B	-3.14	103.40	107.30
33	Z	101	LMG	O6-C5-C4	3.14	115.35	109.70
24	B	617	CLA	CBC-CAC-C3C	-3.14	103.92	112.42
26	c	528	BCR	C33-C5-C6	-3.13	121.06	124.48
31	a	415[A]	PL9	C20-C19-C21	3.13	120.67	115.23
24	c	514	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
24	a	409	CLA	CHC-C1C-C2C	-3.13	118.04	126.95
24	b	610	CLA	C4C-C3C-C2C	-3.13	102.33	106.89
24	c	507	CLA	C1-C2-C3	-3.13	121.07	126.20
35	B	623	HTG	C1'-S1-C1	3.13	107.21	100.45
24	c	518	CLA	CMB-C2B-C1B	3.13	130.19	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	418[B]	PHO	C4-C3-C5	3.13	120.66	115.23
24	c	513	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
24	b	621	CLA	CAC-C3C-C4C	3.13	128.86	124.79
24	C	512	CLA	C4C-C3C-C2C	-3.13	102.34	106.89
31	A	419[B]	PL9	C20-C19-C21	3.13	120.66	115.23
24	B	608	CLA	CAC-C3C-C4C	3.13	128.86	124.79
24	B	615	CLA	C4C-C3C-C2C	-3.13	102.34	106.89
25	A	408	PHO	CBC-CAC-C3C	-3.12	108.40	112.87
24	C	508	CLA	C4C-C3C-C2C	-3.12	102.34	106.89
31	a	415[A]	PL9	C10-C9-C11	3.12	120.65	115.23
24	B	616	CLA	CHD-C4C-NC	3.12	129.07	124.23
24	b	621	CLA	C1-C2-C3	-3.12	121.08	126.20
24	b	617	CLA	C3B-C4B-NB	3.12	113.31	110.53
24	C	503	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
37	D	407	LHG	O8-C23-O10	-3.12	115.83	123.63
24	b	616	CLA	CAA-C2A-C3A	-3.12	104.58	113.00
37	D	409	LHG	O8-C23-C24	3.12	121.34	111.83
24	b	612	CLA	C4B-C3B-C2B	-3.12	103.43	107.30
37	E	101	LHG	O8-C23-C24	3.11	121.33	111.83
24	B	611	CLA	C3B-C4B-NB	3.11	113.31	110.53
24	B	611	CLA	CAC-C3C-C4C	3.11	128.84	124.79
24	b	613	CLA	CHC-C1C-C2C	-3.11	118.10	126.95
26	C	514	BCR	C16-C17-C18	-3.11	122.91	127.28
31	D	405[B]	PL9	C7-C8-C9	-3.11	121.47	126.83
24	d	401	CLA	C4B-C3B-C2B	-3.11	103.43	107.30
24	C	508	CLA	CHC-C1C-C2C	-3.11	118.11	126.95
24	b	610	CLA	CHD-C4C-NC	3.11	129.05	124.23
25	A	409[B]	PHO	CMB-C2B-C3B	3.11	130.89	124.68
24	C	510	CLA	C4-C3-C5	3.11	120.62	115.23
40	V	205	HEC	CHD-C4C-NC	3.11	127.84	124.45
24	C	508	CLA	C4B-C3B-C2B	-3.11	103.44	107.30
24	B	602	CLA	CHD-C4C-NC	3.11	129.05	124.23
31	a	415[B]	PL9	C10-C9-C11	3.11	120.62	115.23
24	c	510	CLA	CHD-C1D-ND	-3.11	120.43	124.80
24	b	615	CLA	O2A-CGA-O1A	-3.11	115.86	123.63
24	b	625	CLA	C1-C2-C3	-3.10	121.11	126.20
24	c	511	CLA	CHC-C1C-C2C	-3.10	118.13	126.95
24	B	607	CLA	C1-C2-C3	-3.10	121.12	126.20
36	C	518	DGD	O2G-C1B-C2B	3.10	118.18	111.48
24	b	620	CLA	CHC-C1C-C2C	-3.10	118.15	126.95
31	A	419[B]	PL9	C22-C23-C24	-3.10	120.53	127.62
27	F	103	SQD	O5-C5-C4	3.10	115.28	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	C3D-C4D-ND	3.10	115.02	109.99
24	B	617	CLA	C1C-C2C-C3C	-3.09	103.73	106.98
26	K	101	BCR	C15-C14-C13	-3.09	122.94	127.28
24	c	516	CLA	CAC-C3C-C4C	3.09	128.81	124.79
26	b	627	BCR	C38-C26-C25	-3.09	121.11	124.48
38	F	102	HEM	CBD-CAD-C3D	-3.09	103.99	112.53
24	C	511	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
31	a	415[B]	PL9	C20-C19-C21	3.08	120.58	115.23
24	b	611	CLA	C3B-C4B-NB	3.08	113.28	110.53
26	h	101	BCR	C38-C26-C25	-3.08	121.12	124.48
24	b	611	CLA	C4C-C3C-C2C	-3.07	102.42	106.89
24	a	412	CLA	CAA-C2A-C3A	-3.07	104.69	113.00
26	D	404	BCR	C28-C27-C26	-3.07	108.58	114.06
24	B	617	CLA	CHC-C1C-C2C	-3.07	118.22	126.95
26	d	404	BCR	C29-C30-C25	3.07	114.90	110.44
36	H	102	DGD	O2G-C1B-C2B	3.07	118.12	111.48
24	d	401	CLA	C2A-C1A-CHA	-3.07	118.54	123.87
24	B	615	CLA	CMC-C2C-C1C	3.07	129.83	125.03
24	a	410	CLA	O2A-CGA-O1A	-3.07	115.96	123.63
24	c	512	CLA	CMC-C2C-C1C	3.06	129.82	125.03
24	C	501	CLA	C4B-C3B-C2B	-3.06	103.49	107.30
24	c	506	CLA	CHC-C1C-C2C	-3.06	118.24	126.95
27	a	414	SQD	C44-O6-C1	-3.06	107.23	113.80
24	c	515	CLA	CHC-C1C-C2C	-3.06	118.25	126.95
25	a	411	PHO	C1-O2A-CGA	3.06	124.05	116.65
24	c	513	CLA	CHC-C1C-C2C	-3.06	118.26	126.95
31	A	419[B]	PL9	C7-C8-C9	-3.05	121.57	126.83
24	A	407	CLA	C2A-C1A-CHA	-3.05	118.57	123.87
24	A	406	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
26	Y	101	BCR	C10-C11-C12	-3.05	114.36	123.20
31	d	405[A]	PL9	C37-C38-C39	-3.05	120.64	127.62
24	a	409	CLA	CAA-C2A-C1A	-3.05	101.97	111.97
26	C	515	BCR	C24-C23-C22	-3.05	121.72	126.23
24	a	409	CLA	O2A-CGA-CBA	3.05	121.14	111.83
31	A	419[B]	PL9	C27-C28-C29	-3.05	120.64	127.62
27	F	103	SQD	O48-C23-C24	3.05	121.13	111.83
31	d	405[A]	PL9	C40-C39-C41	3.05	120.52	115.23
24	b	625	CLA	CHC-C1C-C2C	-3.05	118.29	126.95
26	b	628	BCR	C38-C26-C25	-3.05	121.16	124.48
31	D	405[B]	PL9	C10-C9-C11	3.05	120.52	115.23
24	A	405	CLA	CHC-C1C-C2C	-3.05	118.29	126.95
24	b	625	CLA	C4B-C3B-C2B	-3.04	103.52	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	511	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
24	c	517	CLA	CMC-C2C-C1C	3.04	129.78	125.03
24	C	505	CLA	CAC-C3C-C4C	3.04	128.74	124.79
24	d	401	CLA	CHC-C1C-C2C	-3.04	118.32	126.95
24	b	615	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
24	C	501	CLA	C1-O2A-CGA	3.04	124.00	116.65
24	b	620	CLA	CAC-C3C-C4C	3.03	128.74	124.79
24	C	506	CLA	C4-C3-C5	3.03	120.49	115.23
26	B	620	BCR	C38-C26-C25	-3.03	121.18	124.48
38	e	103	HEM	CHB-C1B-NB	3.03	128.12	124.37
24	A	405	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
24	b	624	CLA	C4B-C3B-C2B	-3.03	103.54	107.30
24	B	609	CLA	CHC-C1C-C2C	-3.03	118.34	126.95
24	C	509	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
24	b	616	CLA	CMC-C2C-C1C	3.03	129.76	125.03
24	C	504	CLA	C4-C3-C5	3.03	120.48	115.23
24	b	621	CLA	CHD-C1D-ND	-3.02	120.55	124.80
31	A	419[B]	PL9	C42-C43-C44	-3.02	120.70	127.62
24	d	401	CLA	CHD-C4C-NC	3.02	128.91	124.23
24	c	510	CLA	C1-C2-C3	-3.02	121.25	126.20
24	C	507	CLA	CMB-C2B-C1B	3.02	130.02	125.42
24	B	613	CLA	C2A-C1A-CHA	-3.02	118.63	123.87
24	B	603	CLA	C1-C2-C3	-3.02	121.25	126.20
24	b	624	CLA	CHC-C1C-C2C	-3.02	118.37	126.95
24	c	518	CLA	CAC-C3C-C4C	3.02	128.71	124.79
24	a	410	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
24	D	402	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
27	f	101	SQD	O5-C5-C4	3.01	115.13	109.70
35	b	608	HTG	C1-O5-C5	3.01	117.97	112.56
37	D	408	LHG	O7-C7-C8	3.01	118.00	111.48
26	K	101	BCR	C7-C8-C9	-3.01	121.78	126.23
24	d	403	CLA	C3B-C4B-NB	3.01	113.22	110.53
24	b	616	CLA	CHC-C1C-C2C	-3.01	118.40	126.95
24	c	512	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
24	C	512	CLA	CHD-C4C-NC	3.01	128.90	124.23
31	a	415[A]	PL9	C37-C38-C39	-3.01	120.74	127.62
24	c	517	CLA	C4-C3-C5	3.01	120.45	115.23
24	C	502	CLA	CMB-C2B-C1B	3.01	130.00	125.42
24	b	621	CLA	C1C-C2C-C3C	-3.01	103.82	106.98
24	b	622	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
24	b	613	CLA	CMC-C2C-C1C	3.00	129.73	125.03
24	D	403	CLA	C4C-C3C-C2C	-3.00	102.52	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	B	622	LMG	O7-C10-C11	3.00	117.98	111.48
36	D	406	DGD	O1G-C1A-C2A	3.00	120.99	111.83
24	b	611	CLA	CMB-C2B-C1B	3.00	129.99	125.42
24	c	506	CLA	C4C-C3C-C2C	-3.00	102.52	106.89
24	B	611	CLA	CHC-C1C-C2C	-3.00	118.42	126.95
24	c	515	CLA	CBC-CAC-C3C	-3.00	104.29	112.42
24	B	608	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
36	c	520	DGD	C2G-O2G-C1B	-3.00	110.62	117.80
24	C	508	CLA	C1-C2-C3	-3.00	121.29	126.20
36	C	517	DGD	O1G-C1A-C2A	3.00	120.97	111.83
24	A	410	CLA	CAA-C2A-C3A	-2.99	104.91	113.00
24	c	507	CLA	CHC-C1C-C2C	-2.99	118.44	126.95
24	A	405	CLA	O2A-CGA-O1A	-2.99	116.14	123.63
24	b	614	CLA	O2A-CGA-O1A	-2.99	116.14	123.63
24	B	604	CLA	C3B-C4B-NB	2.99	113.20	110.53
24	B	610	CLA	CAC-C3C-C4C	2.99	128.68	124.79
25	a	418[B]	PHO	CMB-C2B-C3B	2.99	130.66	124.68
26	d	404	BCR	C15-C14-C13	-2.99	123.08	127.28
24	B	613	CLA	CAC-C3C-C4C	2.99	128.68	124.79
26	Y	101	BCR	C37-C22-C23	2.99	122.65	118.09
24	B	605	CLA	CHC-C1C-C2C	-2.99	118.45	126.95
24	c	514	CLA	CHC-C1C-C2C	-2.99	118.45	126.95
24	b	618	CLA	C4C-C3C-C2C	-2.99	102.55	106.89
24	C	509	CLA	C4B-C3B-C2B	-2.99	103.59	107.30
24	b	612	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
31	A	419[A]	PL9	C12-C13-C14	-2.98	120.80	127.62
24	B	603	CLA	C3B-C4B-NB	2.98	113.19	110.53
24	B	603	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
24	a	410	CLA	C2A-C1A-CHA	-2.98	118.69	123.87
24	b	625	CLA	CHD-C4C-NC	2.98	128.85	124.23
24	C	508	CLA	CAC-C3C-C4C	2.98	128.67	124.79
25	a	411	PHO	C1A-C2A-C3A	-2.98	100.00	102.84
36	C	517	DGD	C2G-O2G-C1B	-2.98	110.67	117.80
24	C	507	CLA	CHD-C4C-NC	2.98	128.85	124.23
24	C	506	CLA	CAA-C2A-C3A	-2.98	104.95	113.00
31	A	419[A]	PL9	C45-C44-C46	2.98	120.39	115.23
24	C	509	CLA	C4C-C3C-C2C	-2.98	102.56	106.89
24	C	503	CLA	CHD-C4C-NC	2.97	128.84	124.23
24	B	608	CLA	CMC-C2C-C1C	2.97	129.68	125.03
36	h	102	DGD	O1G-C1A-C2A	2.97	120.90	111.83
24	A	406	CLA	CAA-C2A-C3A	-2.97	104.97	113.00
24	B	613	CLA	C4-C3-C5	2.97	120.38	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	CHC-C1C-C2C	-2.97	118.51	126.95
37	d	406	LHG	O8-C23-C24	2.97	120.88	111.83
24	a	412	CLA	CBC-CAC-C3C	-2.97	104.38	112.42
24	b	617	CLA	CMC-C2C-C1C	2.97	129.67	125.03
24	C	501	CLA	CAC-C3C-C4C	2.96	128.65	124.79
24	c	517	CLA	CHD-C4C-NC	2.96	128.83	124.23
24	d	402	CLA	CMB-C2B-C1B	2.96	129.93	125.42
24	b	622	CLA	CED-O2D-CGD	2.96	122.64	115.92
31	A	419[A]	PL9	C27-C28-C29	-2.96	120.84	127.62
24	B	605	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
24	C	504	CLA	CMC-C2C-C1C	2.96	129.66	125.03
24	b	622	CLA	CMB-C2B-C1B	2.96	129.93	125.42
38	F	102	HEM	CHD-C1D-ND	2.96	127.61	124.42
24	b	614	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
31	A	419[A]	PL9	C53-C6-C1	2.96	121.33	115.28
24	B	602	CLA	CMB-C2B-C1B	2.96	129.92	125.42
24	C	507	CLA	C4C-C3C-C2C	-2.96	102.59	106.89
24	C	504	CLA	CHC-C1C-C2C	-2.96	118.55	126.95
24	B	616	CLA	C3B-C4B-NB	2.96	113.17	110.53
24	C	502	CLA	C4B-C3B-C2B	-2.95	103.63	107.30
31	D	405[A]	PL9	C15-C14-C16	2.95	120.36	115.23
26	B	619	BCR	C33-C5-C6	-2.95	121.26	124.48
24	B	604	CLA	CHD-C4C-NC	2.95	128.81	124.23
37	e	102	LHG	O7-C7-C8	2.95	117.86	111.48
26	c	528	BCR	C16-C17-C18	-2.95	123.14	127.28
24	d	402	CLA	CHC-C1C-C2C	-2.95	118.57	126.95
24	C	508	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
24	c	508	CLA	CHD-C4C-NC	2.95	128.80	124.23
24	a	410	CLA	CAA-C2A-C3A	-2.95	105.04	113.00
26	y	101	BCR	C16-C17-C18	-2.95	123.15	127.28
24	b	616	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
27	a	405	SQD	O8-S-C6	2.94	111.66	105.97
24	B	616	CLA	CBC-CAC-C3C	-2.94	104.44	112.42
24	d	403	CLA	C2A-C1A-CHA	-2.94	118.76	123.87
24	b	620	CLA	CBC-CAC-C3C	-2.94	104.44	112.42
24	c	514	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
26	h	101	BCR	C11-C10-C9	-2.94	123.15	127.28
24	C	503	CLA	O2A-CGA-CBA	2.94	120.80	111.83
24	a	412	CLA	C4-C3-C5	2.94	120.33	115.23
24	c	513	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
24	B	604	CLA	C4C-C3C-C2C	-2.94	102.62	106.89
24	B	614	CLA	C4B-C3B-C2B	-2.93	103.65	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	C4-C3-C5	2.93	120.32	115.23
24	d	401	CLA	CMA-C3A-C2A	-2.93	102.64	113.98
24	C	511	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
24	B	610	CLA	C4C-C3C-C2C	-2.93	102.62	106.89
24	B	612	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
24	a	410	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
26	B	619	BCR	C2-C1-C6	2.93	114.69	110.44
24	b	625	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
24	c	516	CLA	CHD-C4C-NC	2.93	128.77	124.23
24	d	402	CLA	O2A-CGA-CBA	2.93	120.76	111.83
36	c	522	DGD	O1G-C1A-C2A	2.93	120.76	111.83
24	b	613	CLA	CMB-C2B-C1B	2.93	129.87	125.42
24	A	405	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
26	C	515	BCR	C11-C10-C9	-2.92	123.18	127.28
31	a	415[A]	PL9	C35-C34-C36	2.92	120.30	115.23
24	b	623	CLA	CHC-C1C-C2C	-2.92	118.64	126.95
24	b	624	CLA	CHD-C4C-NC	2.92	128.76	124.23
24	B	602	CLA	C3B-C4B-NB	2.92	113.14	110.53
24	b	612	CLA	O2A-CGA-CBA	2.92	120.74	111.83
31	D	405[B]	PL9	C22-C23-C24	-2.92	120.94	127.62
24	b	622	CLA	O2D-CGD-CBD	2.92	116.33	111.23
24	b	611	CLA	CHD-C4C-NC	2.92	128.76	124.23
26	b	628	BCR	C2-C1-C6	2.92	114.67	110.44
31	d	405[A]	PL9	C10-C9-C11	2.92	120.29	115.23
24	a	412	CLA	CMA-C3A-C2A	-2.91	102.72	113.98
24	D	403	CLA	CHC-C1C-C2C	-2.91	118.67	126.95
37	d	406	LHG	O8-C23-O10	-2.91	116.35	123.63
31	D	405[B]	PL9	C27-C28-C29	-2.91	120.96	127.62
24	b	620	CLA	C4B-C3B-C2B	-2.91	103.68	107.30
24	b	622	CLA	CHD-C1D-ND	-2.91	120.71	124.80
24	A	407	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
37	D	409	LHG	O8-C23-O10	-2.91	116.36	123.63
26	B	620	BCR	C10-C11-C12	-2.90	114.78	123.20
24	C	502	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
24	b	618	CLA	CHD-C4C-NC	2.90	128.73	124.23
24	a	410	CLA	CHD-C4C-NC	2.90	128.73	124.23
26	c	519	BCR	C38-C26-C25	-2.90	121.32	124.48
24	D	403	CLA	C4-C3-C5	2.90	120.26	115.23
24	B	617	CLA	C4B-C3B-C2B	-2.90	103.69	107.30
24	b	624	CLA	C4-C3-C5	2.90	120.26	115.23
24	b	612	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
24	c	515	CLA	O2A-CGA-CBA	2.90	120.67	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	409[A]	PHO	CMB-C2B-C3B	2.90	130.47	124.68
24	D	402	CLA	O2A-CGA-CBA	2.90	120.67	111.83
24	b	614	CLA	C4C-C3C-C2C	-2.90	102.68	106.89
24	B	617	CLA	CHD-C4C-NC	2.89	128.71	124.23
24	a	410	CLA	CMB-C2B-C1B	2.89	129.82	125.42
24	c	514	CLA	CHD-C4C-NC	2.89	128.71	124.23
24	c	510	CLA	CHC-C1C-C2C	-2.89	118.74	126.95
35	b	608	HTG	C1'-S1-C1	2.89	106.69	100.45
24	B	614	CLA	CAC-C3C-C4C	2.89	128.54	124.79
24	b	621	CLA	C4-C3-C5	2.88	120.23	115.23
24	A	410	CLA	CMB-C2B-C1B	2.88	129.81	125.42
24	b	616	CLA	C4-C3-C5	2.88	120.23	115.23
24	b	612	CLA	CMA-C3A-C2A	-2.88	102.84	113.98
24	C	510	CLA	CHD-C4C-NC	2.88	128.70	124.23
24	c	517	CLA	O2A-CGA-CBA	2.88	120.62	111.83
24	D	402	CLA	CMC-C2C-C1C	2.88	129.53	125.03
24	B	609	CLA	O2A-CGA-CBA	2.88	120.61	111.83
24	b	610	CLA	CHC-C1C-C2C	-2.88	118.77	126.95
25	a	411	PHO	CMA-C3A-C4A	-2.88	108.41	114.61
24	b	616	CLA	CHD-C4C-NC	2.88	128.69	124.23
31	d	405[A]	PL9	C27-C28-C29	-2.88	121.04	127.62
24	c	518	CLA	CHD-C4C-NC	2.87	128.69	124.23
24	b	615	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
24	B	610	CLA	CHD-C4C-NC	2.87	128.69	124.23
24	C	502	CLA	O2A-CGA-O1A	-2.87	116.44	123.63
24	b	620	CLA	CHD-C4C-NC	2.87	128.69	124.23
24	a	409	CLA	O2A-CGA-O1A	-2.87	116.46	123.63
24	B	607	CLA	CHC-C1C-C2C	-2.87	118.80	126.95
24	b	612	CLA	CAC-C3C-C4C	2.87	128.52	124.79
24	C	507	CLA	O2A-CGA-CBA	2.86	120.57	111.83
24	B	605	CLA	CMC-C2C-C1C	2.86	129.51	125.03
24	C	511	CLA	C4-C3-C5	2.86	120.20	115.23
24	C	513	CLA	C4C-C3C-C2C	-2.86	102.72	106.89
31	a	415[A]	PL9	C7-C3-C2	-2.86	120.01	123.39
24	A	406	CLA	C4-C3-C5	2.86	120.19	115.23
31	A	419[A]	PL9	C7-C8-C9	-2.86	121.90	126.83
24	a	409	CLA	O2D-CGD-CBD	2.86	116.23	111.23
31	d	405[B]	PL9	C40-C39-C41	2.86	120.19	115.23
24	c	512	CLA	CHD-C4C-NC	2.86	128.66	124.23
24	B	617	CLA	CMB-C2B-C1B	2.86	129.77	125.42
24	b	623	CLA	C2A-C1A-CHA	-2.86	118.91	123.87
24	c	506	CLA	C4B-C3B-C2B	-2.86	103.75	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	509	CLA	CMC-C2C-C1C	2.86	129.50	125.03
24	b	613	CLA	C1-C2-C3	-2.86	121.52	126.20
24	a	410	CLA	O2A-CGA-CBA	2.86	120.55	111.83
24	C	502	CLA	CHD-C4C-NC	2.86	128.66	124.23
24	b	611	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
24	b	613	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
24	c	516	CLA	O2A-CGA-CBA	2.85	120.54	111.83
26	k	101	BCR	C20-C21-C22	-2.85	123.28	127.28
24	B	607	CLA	C4B-C3B-C2B	-2.85	103.75	107.30
31	a	415[A]	PL9	C40-C39-C41	2.85	120.18	115.23
24	c	512	CLA	C1-C2-C3	-2.85	121.52	126.20
24	b	619	CLA	O2A-CGA-CBA	2.85	120.53	111.83
24	B	612	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
24	B	602	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
24	b	619	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
24	c	507	CLA	O2A-CGA-CBA	2.85	120.52	111.83
24	c	518	CLA	C4C-C3C-C2C	-2.85	102.75	106.89
24	C	513	CLA	O2A-CGA-CBA	2.85	120.51	111.83
24	c	507	CLA	CAC-C3C-C4C	2.85	128.49	124.79
24	B	608	CLA	C4B-C3B-C2B	-2.84	103.77	107.30
27	A	412	SQD	O9-S-C6	2.84	111.00	106.76
24	c	514	CLA	CMB-C2B-C1B	2.84	129.74	125.42
24	c	518	CLA	O2A-CGA-CBA	2.84	120.50	111.83
24	c	518	CLA	CAA-C2A-C3A	-2.84	105.32	113.00
24	B	615	CLA	C4-C3-C5	2.84	120.16	115.23
24	c	514	CLA	O2A-CGA-CBA	2.84	120.49	111.83
33	z	101	LMG	O8-C28-C29	2.84	120.49	111.83
24	b	622	CLA	C4-C3-C5	2.84	120.15	115.23
24	B	606	CLA	C1-C2-C3	-2.84	121.55	126.20
24	a	410	CLA	CAC-C3C-C4C	2.83	128.48	124.79
24	C	512	CLA	CHC-C1C-C2C	-2.83	118.90	126.95
24	B	603	CLA	CAC-C3C-C4C	2.83	128.47	124.79
24	C	509	CLA	O2A-CGA-CBA	2.83	120.46	111.83
24	c	506	CLA	CMC-C2C-C1C	2.83	129.45	125.03
24	b	617	CLA	C4C-C3C-C2C	-2.83	102.78	106.89
24	a	412	CLA	CHD-C4C-NC	2.83	128.61	124.23
24	D	402	CLA	CAA-C2A-C3A	-2.83	105.36	113.00
24	B	609	CLA	CMB-C2B-C1B	2.83	129.72	125.42
24	c	511	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
24	c	515	CLA	C4C-C3C-C2C	-2.82	102.78	106.89
25	a	418[B]	PHO	CMA-C3A-C4A	-2.82	108.53	114.61
26	t	101	BCR	C1-C6-C7	2.82	123.31	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	617	CLA	CBC-CAC-C3C	-2.82	104.77	112.42
40	V	205	HEC	CHA-C1A-NA	2.82	127.53	124.45
24	B	609	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
26	B	620	BCR	C2-C1-C6	2.82	114.54	110.44
24	D	402	CLA	CHC-C1C-C2C	-2.82	118.93	126.95
24	a	412	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
35	B	625	HTG	C1-O5-C5	2.82	117.62	112.56
35	V	206	HTG	C1-C2-C3	-2.82	105.04	110.55
33	b	629	LMG	O8-C28-C29	2.82	120.42	111.83
24	B	608	CLA	CBC-CAC-C3C	-2.82	104.78	112.42
24	B	615	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
24	C	510	CLA	CHC-C1C-C2C	-2.81	118.95	126.95
24	c	509	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
24	B	606	CLA	O2A-CGA-CBA	2.81	120.40	111.83
24	b	623	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
24	B	616	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
33	d	413	LMG	O7-C10-C11	2.81	117.56	111.48
24	b	618	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
24	B	611	CLA	CMB-C2B-C1B	2.81	129.69	125.42
24	B	615	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
24	d	403	CLA	CAA-C2A-C3A	-2.80	105.42	113.00
24	c	511	CLA	CHD-C4C-NC	2.80	128.58	124.23
26	Y	101	BCR	C15-C14-C13	-2.80	123.35	127.28
24	B	612	CLA	CMB-C2B-C1B	2.80	129.69	125.42
24	b	612	CLA	CHD-C4C-NC	2.80	128.57	124.23
24	c	518	CLA	C2A-C1A-CHA	-2.80	119.01	123.87
27	L	102	SQD	O48-C23-C24	2.80	120.37	111.83
24	c	509	CLA	C4B-C3B-C2B	-2.80	103.82	107.30
31	a	415[A]	PL9	C53-C6-C1	2.80	121.01	115.28
24	b	623	CLA	CMC-C2C-C1C	2.80	129.41	125.03
26	c	519	BCR	C15-C14-C13	-2.80	123.35	127.28
24	B	613	CLA	CBC-CAC-C3C	-2.80	104.83	112.42
24	B	607	CLA	CHD-C4C-NC	2.80	128.57	124.23
26	y	101	BCR	C10-C11-C12	-2.80	115.09	123.20
31	a	415[B]	PL9	C35-C34-C36	2.80	120.08	115.23
24	b	618	CLA	CHC-C1C-C2C	-2.80	119.00	126.95
35	b	632	HTG	C1-O5-C5	2.80	117.58	112.56
24	d	403	CLA	C4-C3-C5	2.79	120.08	115.23
24	c	516	CLA	CMC-C2C-C1C	2.79	129.39	125.03
24	b	616	CLA	CBC-CAC-C3C	-2.79	104.86	112.42
24	c	516	CLA	C4C-C3C-C2C	-2.79	102.83	106.89
24	b	620	CLA	C4C-C3C-C2C	-2.79	102.83	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	618	CLA	C4B-C3B-C2B	-2.79	103.84	107.30
26	t	101	BCR	C11-C10-C9	-2.79	123.37	127.28
24	D	402	CLA	C2A-C1A-CHA	-2.78	119.03	123.87
24	C	506	CLA	C4C-C3C-C2C	-2.78	102.84	106.89
27	a	414	SQD	C45-O47-C7	-2.78	111.14	117.80
27	A	412	SQD	O48-C23-C24	2.78	120.32	111.83
24	b	619	CLA	CHC-C1C-C2C	-2.78	119.05	126.95
31	a	415[B]	PL9	C25-C24-C26	2.78	120.05	115.23
24	C	504	CLA	C1-O2A-CGA	2.78	123.38	116.65
24	B	604	CLA	C2A-C1A-CHA	-2.78	119.05	123.87
24	b	617	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
24	b	615	CLA	CHC-C1C-C2C	-2.78	119.05	126.95
24	A	407	CLA	C4C-C3C-C2C	-2.78	102.85	106.89
24	B	604	CLA	CMB-C2B-C1B	2.77	129.64	125.42
24	B	608	CLA	CHC-C1C-C2C	-2.77	119.07	126.95
24	b	617	CLA	CHC-C1C-C2C	-2.77	119.07	126.95
31	D	405[B]	PL9	C40-C39-C41	2.77	120.04	115.23
24	B	607	CLA	O2A-CGA-CBA	2.77	120.29	111.83
24	b	613	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
24	c	511	CLA	C4-C3-C5	2.77	120.04	115.23
24	d	403	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
24	C	509	CLA	CHC-C1C-C2C	-2.77	119.08	126.95
24	b	615	CLA	O2A-CGA-CBA	2.77	120.28	111.83
24	a	412	CLA	C2A-C1A-CHA	-2.77	119.06	123.87
24	d	403	CLA	CAC-C3C-C4C	2.77	128.39	124.79
36	C	516	DGD	C3G-C2G-C1G	-2.77	105.34	111.78
26	b	628	BCR	C24-C23-C22	-2.76	122.15	126.23
33	c	501	LMG	O8-C28-C29	2.76	120.26	111.83
26	K	101	BCR	C3-C4-C5	-2.76	109.13	114.06
24	B	609	CLA	C4C-C3C-C2C	-2.76	102.87	106.89
26	H	101	BCR	C10-C11-C12	-2.76	115.20	123.20
24	C	507	CLA	CAC-C3C-C4C	2.76	128.38	124.79
24	b	611	CLA	O2A-CGA-CBA	2.76	120.25	111.83
27	A	412	SQD	O8-S-C6	2.76	111.30	105.97
35	c	526	HTG	C1-O5-C5	2.76	117.51	112.56
24	A	410	CLA	CHC-C1C-C2C	-2.76	119.11	126.95
24	b	615	CLA	CHD-C4C-NC	2.76	128.51	124.23
24	c	516	CLA	CHC-C1C-C2C	-2.76	119.11	126.95
24	B	606	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
24	b	623	CLA	C4B-C3B-C2B	-2.76	103.88	107.30
24	B	602	CLA	CHC-C1C-C2C	-2.76	119.12	126.95
24	c	509	CLA	CHC-C1C-C2C	-2.76	119.12	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	e	102	LHG	O8-C23-C24	2.76	120.24	111.83
24	B	603	CLA	C4B-C3B-C2B	-2.75	103.88	107.30
26	h	101	BCR	C10-C11-C12	-2.75	115.22	123.20
24	C	513	CLA	CHC-C1C-C2C	-2.75	119.13	126.95
24	b	623	CLA	CBC-CAC-C3C	-2.75	104.96	112.42
24	B	606	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
31	a	415[A]	PL9	C25-C24-C26	2.75	120.00	115.23
27	F	103	SQD	O7-S-C6	2.75	110.86	106.76
24	A	410	CLA	CMA-C3A-C4A	-2.75	104.39	111.77
24	B	615	CLA	C2A-C1A-CHA	-2.75	119.10	123.87
24	B	603	CLA	CHD-C4C-NC	2.75	128.49	124.23
24	C	513	CLA	CMB-C2B-C1B	2.75	129.60	125.42
24	c	512	CLA	C3B-C4B-NB	2.74	112.98	110.53
24	D	403	CLA	C2A-C1A-CHA	-2.74	119.11	123.87
26	h	101	BCR	C7-C8-C9	-2.74	122.19	126.23
24	B	612	CLA	C4C-C3C-C2C	-2.74	102.91	106.89
25	A	409[A]	PHO	O2D-CGD-O1D	-2.74	118.52	123.85
24	c	517	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
31	D	405[A]	PL9	C37-C38-C39	-2.73	121.37	127.62
24	B	613	CLA	CHD-C4C-NC	2.73	128.47	124.23
24	b	619	CLA	CHD-C4C-NC	2.73	128.47	124.23
24	b	611	CLA	C4-C3-C5	2.73	119.97	115.23
24	a	410	CLA	C4B-C3B-C2B	-2.73	103.91	107.30
36	C	518	DGD	O1G-C1A-C2A	2.73	120.16	111.83
38	F	102	HEM	CHB-C1B-NB	2.73	127.75	124.37
24	d	402	CLA	C4-C3-C5	2.73	119.97	115.23
31	D	405[A]	PL9	C22-C23-C24	-2.73	121.37	127.62
24	b	613	CLA	O2A-CGA-CBA	2.73	120.16	111.83
24	b	625	CLA	CMB-C2B-C1B	2.73	129.57	125.42
27	B	621	SQD	O48-C23-C24	2.73	120.15	111.83
31	d	405[B]	PL9	C12-C13-C14	-2.73	121.38	127.62
24	c	512	CLA	CHC-C1C-C2C	-2.72	119.20	126.95
24	b	618	CLA	C4-C3-C5	2.72	119.96	115.23
24	D	403	CLA	CAA-C2A-C3A	-2.72	105.64	113.00
24	b	614	CLA	C3B-C4B-NB	2.72	112.96	110.53
24	C	505	CLA	CMC-C2C-C1C	2.72	129.29	125.03
24	B	607	CLA	C4-C3-C5	2.72	119.95	115.23
24	b	618	CLA	O2A-CGA-O1A	-2.72	116.82	123.63
24	C	501	CLA	CHD-C4C-NC	2.72	128.45	124.23
24	C	502	CLA	CHC-C1C-C2C	-2.72	119.22	126.95
24	B	609	CLA	CBC-CAC-C3C	-2.72	105.05	112.42
24	b	616	CLA	C4C-C3C-C2C	-2.72	102.94	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	409	CLA	C2A-C1A-CHA	-2.72	119.15	123.87
25	A	409[A]	PHO	C4A-C3A-C2A	-2.71	100.26	102.84
24	C	506	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
24	C	505	CLA	C3B-C4B-NB	2.71	112.95	110.53
24	a	410	CLA	C3B-C4B-NB	2.71	112.95	110.53
31	D	405[A]	PL9	C53-C6-C1	2.71	120.83	115.28
24	C	511	CLA	C1-C2-C3	-2.71	121.76	126.20
24	b	623	CLA	O2A-CGA-CBA	2.71	120.09	111.83
24	c	517	CLA	C3B-C4B-NB	2.71	112.95	110.53
31	A	419[B]	PL9	C12-C13-C14	-2.71	121.43	127.62
36	C	516	DGD	O1G-C1A-O1A	-2.71	116.86	123.63
24	c	512	CLA	C4-C3-C5	2.70	119.92	115.23
36	h	102	DGD	O1G-C1A-O1A	-2.70	116.86	123.63
24	B	602	CLA	C2A-C1A-CHA	-2.70	119.17	123.87
24	A	407	CLA	CAA-C2A-C3A	-2.70	105.70	113.00
31	a	415[B]	PL9	C53-C6-C1	2.70	120.81	115.28
24	C	511	CLA	CHD-C4C-NC	2.70	128.42	124.23
24	b	618	CLA	C3B-C4B-NB	2.70	112.94	110.53
31	D	405[B]	PL9	C25-C24-C26	2.70	119.91	115.23
29	f	102	LMT	C1B-O5B-C5B	2.70	118.99	113.72
26	C	514	BCR	C20-C21-C22	-2.70	123.49	127.28
26	t	101	BCR	C15-C14-C13	2.70	131.06	127.28
24	c	507	CLA	CHD-C4C-NC	2.70	128.42	124.23
24	b	611	CLA	CAC-C3C-C4C	2.70	128.30	124.79
24	c	510	CLA	C3B-C4B-NB	2.70	112.94	110.53
24	b	617	CLA	CHD-C4C-NC	2.70	128.41	124.23
31	A	419[B]	PL9	C53-C6-C1	2.70	120.80	115.28
24	c	510	CLA	C4B-C3B-C2B	-2.69	103.95	107.30
37	d	408	LHG	O8-C23-C24	2.69	120.05	111.83
24	c	509	CLA	CBC-CAC-C3C	-2.69	105.12	112.42
31	d	405[B]	PL9	C15-C14-C16	2.69	119.90	115.23
24	B	604	CLA	C4B-C3B-C2B	-2.69	103.95	107.30
24	C	513	CLA	CHD-C4C-NC	2.69	128.41	124.23
24	b	621	CLA	CHC-C1C-C2C	-2.69	119.30	126.95
35	b	608	HTG	O5-C1-C2	2.69	114.03	110.32
24	b	617	CLA	O2A-CGA-CBA	2.69	120.04	111.83
26	T	103	BCR	C35-C13-C12	2.69	122.20	118.09
31	a	415[B]	PL9	C40-C39-C41	2.69	119.89	115.23
24	C	504	CLA	C2A-C1A-CHA	-2.69	119.20	123.87
24	c	508	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
26	Y	101	BCR	C16-C17-C18	-2.69	123.51	127.28
24	c	509	CLA	CMB-C2B-C1B	2.69	129.51	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	402	CLA	C4C-C3C-C2C	-2.69	102.98	106.89
25	A	409[A]	PHO	C1A-C2A-C3A	-2.69	100.28	102.84
27	B	621	SQD	C3-C4-C5	2.68	115.10	110.23
35	V	206	HTG	C1'-S1-C1	2.68	106.25	100.45
31	D	405[A]	PL9	C2-C1-C6	2.68	122.19	119.00
24	A	410	CLA	CHB-C4A-NA	2.68	128.27	124.40
24	b	618	CLA	O2A-CGA-CBA	2.68	120.01	111.83
25	a	418[B]	PHO	C4D-CHA-CBD	2.68	109.74	108.45
24	d	401	CLA	C4C-C3C-C2C	-2.68	102.99	106.89
24	a	409	CLA	C4C-C3C-C2C	-2.68	102.99	106.89
24	C	511	CLA	O2A-CGA-CBA	2.68	120.01	111.83
24	C	505	CLA	CHC-C1C-C2C	-2.68	119.33	126.95
24	d	403	CLA	C4C-C3C-C2C	-2.68	102.99	106.89
24	a	412	CLA	C4C-C3C-C2C	-2.68	102.99	106.89
24	B	609	CLA	C4B-C3B-C2B	-2.68	103.97	107.30
31	D	405[A]	PL9	C7-C3-C4	2.68	119.11	116.91
26	K	101	BCR	C2-C1-C6	2.67	114.32	110.44
24	B	607	CLA	O2A-CGA-O1A	-2.67	116.94	123.63
26	B	619	BCR	C31-C1-C6	-2.67	106.05	110.24
25	A	409[B]	PHO	O2D-CGD-O1D	-2.67	118.65	123.85
24	B	614	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
24	c	516	CLA	C4-C3-C5	2.67	119.86	115.23
27	A	412	SQD	O48-C23-O10	-2.67	116.95	123.63
37	D	407	LHG	C5-O7-C7	-2.67	111.41	117.80
24	B	606	CLA	CAC-C3C-C4C	2.67	128.26	124.79
26	t	101	BCR	C7-C6-C5	-2.67	115.41	121.56
24	b	616	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
24	c	517	CLA	CBC-CAC-C3C	-2.67	105.19	112.42
31	D	405[A]	PL9	C27-C28-C29	-2.67	121.52	127.62
24	c	509	CLA	CHD-C4C-NC	2.67	128.36	124.23
27	A	416	SQD	O48-C23-O10	-2.66	116.96	123.63
24	b	611	CLA	C1-C2-C3	-2.66	121.83	126.20
25	A	408	PHO	CMA-C3A-C4A	-2.66	108.87	114.61
24	C	511	CLA	CMB-C2B-C1B	2.66	129.48	125.42
24	A	405	CLA	CAA-C2A-C1A	-2.66	103.25	111.97
36	H	102	DGD	O1G-C1A-O1A	-2.66	116.97	123.63
26	C	515	BCR	C21-C20-C19	-2.66	115.48	123.20
26	T	103	BCR	C21-C20-C19	-2.66	115.48	123.20
33	C	520	LMG	O8-C28-C29	2.66	119.95	111.83
31	d	405[A]	PL9	C20-C19-C21	2.66	119.85	115.23
24	C	501	CLA	CHC-C1C-C2C	-2.66	119.38	126.95
24	B	614	CLA	CMB-C2B-C1B	2.66	129.47	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	617	CLA	C1-O2A-CGA	2.66	123.09	116.65
24	c	517	CLA	C4C-C3C-C2C	-2.66	103.02	106.89
36	c	520	DGD	O2G-C1B-O1B	-2.66	117.49	123.70
24	b	614	CLA	O2A-CGA-CBA	2.66	119.94	111.83
24	B	611	CLA	CMA-C3A-C4A	-2.66	104.63	111.77
24	b	619	CLA	CAA-C2A-C3A	-2.66	105.82	113.00
27	a	414	SQD	O48-C23-C24	2.66	119.93	111.83
27	L	102	SQD	O47-C7-O49	-2.65	117.50	123.70
24	B	605	CLA	O2A-CGA-O1A	-2.65	116.99	123.63
31	A	419[B]	PL9	C45-C44-C46	2.65	119.83	115.23
36	e	101	DGD	O1G-C1A-C2A	2.65	119.92	111.83
33	c	523	LMG	C8-O7-C10	-2.65	111.45	117.80
24	B	609	CLA	CMA-C3A-C4A	-2.65	104.65	111.77
31	A	419[B]	PL9	C17-C18-C19	-2.65	121.56	127.62
27	f	101	SQD	O47-C7-O49	-2.65	117.51	123.70
24	d	403	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
24	d	401	CLA	CMB-C2B-C1B	2.65	129.45	125.42
31	A	419[B]	PL9	C15-C14-C16	2.65	119.82	115.23
24	b	614	CLA	CHC-C1C-C2C	-2.65	119.43	126.95
31	d	405[B]	PL9	C20-C19-C21	2.64	119.82	115.23
37	L	101	LHG	O8-C23-C24	2.64	119.90	111.83
24	b	620	CLA	O2A-CGA-CBA	2.64	119.89	111.83
24	B	616	CLA	CAC-C3C-C4C	2.64	128.23	124.79
24	C	507	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
38	e	103	HEM	CHA-C4D-ND	2.64	127.63	124.37
24	b	620	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
31	a	415[B]	PL9	C30-C29-C31	2.64	119.81	115.23
26	c	519	BCR	C3-C4-C5	-2.64	109.35	114.06
24	B	617	CLA	C2A-C1A-CHA	-2.64	119.29	123.87
31	A	419[B]	PL9	C25-C24-C26	2.64	119.81	115.23
24	c	510	CLA	C4-C3-C5	2.64	119.80	115.23
24	c	515	CLA	CHD-C4C-NC	2.64	128.32	124.23
24	c	509	CLA	C2A-C1A-CHA	-2.64	119.29	123.87
24	C	503	CLA	CMC-C2C-C1C	2.63	129.15	125.03
24	C	513	CLA	C3B-C4B-NB	2.63	112.88	110.53
24	C	511	CLA	CBC-CAC-C3C	-2.63	105.29	112.42
26	T	103	BCR	C2-C1-C6	2.63	114.26	110.44
38	e	103	HEM	CHA-C1A-NA	2.63	128.63	123.86
33	Z	101	LMG	C1-O6-C5	2.63	118.85	113.72
27	f	101	SQD	O48-C23-C24	2.63	119.85	111.83
26	t	101	BCR	C20-C21-C22	-2.63	123.59	127.28
24	B	609	CLA	CAC-C3C-C4C	2.63	128.21	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	v	205	HEC	CHA-C4D-ND	2.63	128.62	123.86
24	c	511	CLA	C4C-C3C-C2C	-2.63	103.07	106.89
24	B	610	CLA	CBC-CAC-C3C	-2.63	105.30	112.42
24	B	611	CLA	C4B-C3B-C2B	-2.62	104.04	107.30
24	c	506	CLA	CBC-CAC-C3C	-2.62	105.31	112.42
26	h	101	BCR	C16-C15-C14	-2.62	118.16	123.52
24	c	518	CLA	CHC-C1C-C2C	-2.62	119.50	126.95
26	y	101	BCR	C21-C20-C19	-2.62	115.61	123.20
31	d	405[B]	PL9	C53-C6-C1	2.62	120.64	115.28
24	c	517	CLA	CMB-C2B-C1B	2.61	129.40	125.42
27	L	102	SQD	C44-O6-C1	-2.61	108.19	113.80
24	b	617	CLA	C4B-C3B-C2B	-2.61	104.05	107.30
36	e	101	DGD	C1E-O6E-C5E	2.61	118.82	113.72
31	d	405[B]	PL9	C10-C9-C11	2.61	119.76	115.23
24	B	607	CLA	C4C-C3C-C2C	-2.61	103.09	106.89
24	B	612	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
27	F	103	SQD	C3-C4-C5	2.61	114.96	110.23
24	c	509	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
24	c	514	CLA	CMC-C2C-C1C	2.61	129.11	125.03
31	A	419[A]	PL9	C42-C43-C44	-2.61	121.65	127.62
26	t	101	BCR	C21-C20-C19	-2.61	115.64	123.20
26	H	101	BCR	C29-C30-C25	2.61	114.23	110.44
24	c	513	CLA	CAA-C2A-C3A	-2.61	105.95	113.00
36	C	517	DGD	O1G-C1A-O1A	-2.61	117.11	123.63
38	e	103	HEM	C3B-C4B-NB	-2.61	107.60	109.47
24	b	615	CLA	CAC-C3C-C4C	2.61	128.18	124.79
24	A	407	CLA	CMC-C2C-C1C	2.61	129.10	125.03
24	B	608	CLA	C2A-C1A-CHA	-2.60	119.35	123.87
31	A	419[A]	PL9	C25-C24-C26	2.60	119.74	115.23
24	C	504	CLA	CHD-C4C-NC	2.60	128.26	124.23
24	c	508	CLA	C2A-C1A-CHA	-2.60	119.35	123.87
33	c	524	LMG	O8-C28-C29	2.60	119.77	111.83
24	b	617	CLA	C1-C2-C3	-2.60	121.94	126.20
31	D	405[A]	PL9	C25-C24-C26	2.60	119.74	115.23
24	a	409	CLA	CAC-C3C-C4C	2.60	128.17	124.79
24	c	517	CLA	CHC-C1C-C2C	-2.60	119.56	126.95
24	B	612	CLA	C1-C2-C3	-2.60	121.94	126.20
24	c	512	CLA	O2A-CGA-CBA	2.60	119.76	111.83
24	C	505	CLA	CHD-C4C-NC	2.60	128.26	124.23
24	C	506	CLA	CMC-C2C-C1C	2.60	129.09	125.03
26	y	101	BCR	C24-C23-C22	-2.60	122.39	126.23
26	d	404	BCR	C2-C1-C6	2.60	114.21	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
36	C	516	DGD	C2G-O2G-C1B	-2.60	111.58	117.80
24	C	503	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
24	b	624	CLA	CBC-CAC-C3C	-2.59	105.39	112.42
24	B	617	CLA	O2A-CGA-CBA	2.59	119.73	111.83
24	b	612	CLA	O2A-CGA-O1A	-2.59	117.15	123.63
26	t	101	BCR	C3-C4-C5	-2.59	109.44	114.06
24	C	512	CLA	C4B-C3B-C2B	-2.59	104.08	107.30
24	a	409	CLA	C4B-C3B-C2B	-2.59	104.08	107.30
24	B	609	CLA	CAA-C2A-C3A	-2.59	106.01	113.00
26	d	404	BCR	C28-C27-C26	-2.59	109.44	114.06
29	M	103	LMT	O1B-C1B-C2B	2.59	114.45	108.09
24	b	615	CLA	CAA-C2A-C3A	-2.59	106.01	113.00
35	b	601	HTG	C1'-S1-C1	2.58	106.03	100.45
24	B	609	CLA	CHB-C4A-NA	2.58	128.13	124.40
24	b	618	CLA	C2A-C1A-CHA	-2.58	119.38	123.87
31	A	419[A]	PL9	C30-C29-C31	2.58	119.71	115.23
24	b	623	CLA	CAC-C3C-C4C	2.58	128.15	124.79
24	C	509	CLA	CHD-C4C-NC	2.58	128.23	124.23
24	b	623	CLA	CHD-C4C-NC	2.58	128.23	124.23
26	B	618	BCR	C15-C14-C13	-2.58	123.67	127.28
24	c	517	CLA	O1D-CGD-CBD	-2.58	119.44	124.52
24	B	602	CLA	C4B-C3B-C2B	-2.58	104.10	107.30
24	d	403	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
24	C	510	CLA	CAC-C3C-C4C	2.57	128.14	124.79
24	c	509	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
24	b	618	CLA	CMC-C2C-C1C	2.57	129.06	125.03
24	b	612	CLA	CHC-C1C-C2C	-2.57	119.64	126.95
24	C	501	CLA	C4-C3-C5	2.57	119.69	115.23
26	H	101	BCR	C7-C8-C9	-2.57	122.44	126.23
24	c	516	CLA	C4B-C3B-C2B	-2.57	104.11	107.30
24	b	619	CLA	C4-C3-C5	2.57	119.68	115.23
24	A	410	CLA	C4B-C3B-C2B	-2.57	104.11	107.30
24	b	617	CLA	CAC-C3C-C4C	2.56	128.13	124.79
24	c	513	CLA	O2A-CGA-CBA	2.56	119.65	111.83
24	b	612	CLA	C2A-C1A-CHA	-2.56	119.42	123.87
24	a	412	CLA	CMC-C2C-C1C	2.56	129.04	125.03
24	B	614	CLA	O2A-CGA-CBA	2.56	119.64	111.83
24	C	504	CLA	C4C-C3C-C2C	-2.56	103.17	106.89
24	B	611	CLA	CBC-CAC-C3C	-2.56	105.48	112.42
24	C	513	CLA	CAA-C2A-C3A	-2.56	106.09	113.00
29	m	103	LMT	O5'-C5'-C4'	2.56	115.01	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	619	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
24	b	625	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
24	C	508	CLA	C4-C3-C5	2.56	119.66	115.23
31	A	419[B]	PL9	C30-C29-C31	2.55	119.66	115.23
24	A	407	CLA	CHC-C1C-C2C	-2.55	119.69	126.95
24	b	611	CLA	C4B-C3B-C2B	-2.55	104.13	107.30
24	B	608	CLA	CHD-C4C-NC	2.55	128.19	124.23
31	A	419[A]	PL9	C7-C3-C2	-2.55	120.38	123.39
24	A	410	CLA	CMC-C2C-C1C	2.55	129.02	125.03
24	b	613	CLA	O1D-CGD-CBD	-2.55	119.48	124.52
35	B	624	HTG	C1-C2-C3	2.55	115.54	110.55
24	B	613	CLA	O2A-CGA-CBA	2.55	119.61	111.83
26	K	101	BCR	C20-C21-C22	-2.55	123.70	127.28
24	c	509	CLA	CAC-C3C-C4C	2.55	128.11	124.79
24	A	407	CLA	C1-C2-C3	-2.55	122.02	126.20
24	b	622	CLA	O2A-CGA-CBA	2.55	119.61	111.83
24	d	402	CLA	CAA-C2A-C3A	-2.55	106.11	113.00
24	C	513	CLA	C4-C3-C5	2.55	119.65	115.23
24	B	614	CLA	CMC-C2C-C1C	2.55	129.01	125.03
31	D	405[A]	PL9	C12-C13-C14	-2.55	121.80	127.62
31	A	419[A]	PL9	C15-C14-C16	2.55	119.65	115.23
24	c	518	CLA	C4-C3-C5	2.54	119.64	115.23
24	D	403	CLA	C4B-C3B-C2B	-2.54	104.14	107.30
24	B	611	CLA	CHD-C4C-NC	2.54	128.17	124.23
31	a	415[A]	PL9	C30-C29-C31	2.54	119.64	115.23
24	D	402	CLA	C4-C3-C5	2.54	119.64	115.23
24	A	406	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
26	k	101	BCR	C10-C11-C12	-2.54	115.84	123.20
24	C	502	CLA	CBC-CAC-C3C	-2.54	105.53	112.42
24	C	513	CLA	CAC-C3C-C4C	2.54	128.09	124.79
24	B	603	CLA	C2A-C1A-CHA	-2.54	119.46	123.87
24	a	410	CLA	C4-C3-C5	2.54	119.63	115.23
24	B	609	CLA	CHD-C4C-NC	2.54	128.16	124.23
24	A	407	CLA	C4B-C3B-C2B	-2.54	104.15	107.30
24	b	625	CLA	C4-C3-C5	2.54	119.63	115.23
36	C	516	DGD	O3G-C3G-C2G	-2.54	104.65	110.82
24	B	615	CLA	CHD-C4C-NC	2.54	128.16	124.23
24	C	507	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
38	F	102	HEM	CHA-C1A-NA	2.53	128.45	123.86
24	C	513	CLA	C4B-C3B-C2B	-2.53	104.15	107.30
24	C	502	CLA	CAC-C3C-C4C	2.53	128.08	124.79
24	b	619	CLA	CMB-C2B-C1B	2.53	129.27	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	CMC-C2C-C1C	2.53	128.98	125.03
26	h	101	BCR	C20-C21-C22	-2.52	123.74	127.28
24	C	503	CLA	C4B-C3B-C2B	-2.52	104.16	107.30
24	b	620	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
24	c	508	CLA	O2A-CGA-CBA	2.52	119.53	111.83
24	C	501	CLA	C4C-C3C-C2C	-2.52	103.22	106.89
31	D	405[B]	PL9	C12-C13-C14	-2.52	121.85	127.62
26	k	101	BCR	C11-C10-C9	-2.52	123.74	127.28
24	b	614	CLA	CMB-C2B-C1B	2.52	129.26	125.42
31	D	405[A]	PL9	C42-C41-C39	-2.52	104.83	113.19
24	B	614	CLA	C4-C3-C5	2.52	119.60	115.23
25	a	418[A]	PHO	CMB-C2B-C3B	2.52	129.72	124.68
24	d	401	CLA	C1-C2-C3	-2.52	122.07	126.20
24	a	412	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
24	B	609	CLA	CMC-C2C-C1C	2.52	128.97	125.03
24	c	507	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
24	b	623	CLA	CMB-C2B-C1B	2.51	129.25	125.42
24	a	410	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
24	B	603	CLA	C1-O2A-CGA	2.51	122.73	116.65
24	c	513	CLA	C4-C3-C5	2.51	119.59	115.23
24	B	608	CLA	CMB-C2B-C1B	2.51	129.24	125.42
24	A	405	CLA	C2A-C1A-CHA	-2.51	119.51	123.87
24	c	506	CLA	CMB-C2B-C1B	2.51	129.24	125.42
24	b	623	CLA	CAA-C2A-C3A	-2.50	106.23	113.00
24	c	515	CLA	O2A-CGA-O1A	-2.50	117.36	123.63
24	B	605	CLA	CMB-C2B-C1B	2.50	129.23	125.42
25	A	409[B]	PHO	C4D-CHA-CBD	2.50	109.66	108.45
24	C	505	CLA	C1-O2A-CGA	2.50	122.71	116.65
24	C	512	CLA	CBC-CAC-C3C	-2.50	105.64	112.42
24	c	507	CLA	O2A-CGA-O1A	-2.50	117.37	123.63
26	K	101	BCR	C33-C5-C6	-2.50	121.76	124.48
33	C	520	LMG	C8-O7-C10	-2.50	111.81	117.80
24	C	506	CLA	CHD-C4C-NC	2.50	128.11	124.23
24	B	608	CLA	C4-C3-C5	2.50	119.57	115.23
26	a	413	BCR	C33-C5-C6	-2.49	121.76	124.48
24	A	405	CLA	CMA-C3A-C4A	-2.49	105.07	111.77
24	C	502	CLA	C4-C3-C5	2.49	119.56	115.23
38	e	103	HEM	CHD-C1D-C2D	-2.49	121.09	125.03
24	C	509	CLA	C4-C3-C5	2.49	119.55	115.23
24	B	610	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
24	d	402	CLA	CMA-C3A-C2A	-2.49	104.37	113.98
27	a	414	SQD	O47-C7-O49	-2.48	117.90	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	CMC-C2C-C1C	2.48	128.91	125.03
24	B	604	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
31	d	405[A]	PL9	C53-C6-C1	2.48	120.36	115.28
24	b	625	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
27	A	412	SQD	C1-C2-C3	-2.48	104.79	110.01
24	C	502	CLA	O2A-CGA-CBA	2.48	119.40	111.83
31	D	405[B]	PL9	C17-C18-C19	-2.48	121.95	127.62
24	C	508	CLA	O2A-CGA-CBA	2.48	119.39	111.83
24	d	403	CLA	O2A-CGA-CBA	2.48	119.39	111.83
24	c	514	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
24	c	517	CLA	CBA-CAA-C2A	-2.48	106.42	113.79
24	B	616	CLA	CHC-C1C-C2C	-2.48	119.91	126.95
31	D	405[B]	PL9	C20-C19-C21	2.48	119.53	115.23
24	b	617	CLA	OBD-CAD-C3D	-2.48	122.63	128.42
33	c	524	LMG	C8-O7-C10	-2.48	111.87	117.80
24	c	506	CLA	O2A-CGA-CBA	2.48	119.38	111.83
24	B	611	CLA	C4-C3-C5	2.48	119.53	115.23
24	b	624	CLA	C1-C2-C3	-2.47	122.14	126.20
24	c	511	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
24	a	410	CLA	CBC-CAC-C3C	-2.47	105.72	112.42
24	B	605	CLA	O2A-CGA-CBA	2.47	119.38	111.83
37	D	407	LHG	O7-C7-O9	-2.47	117.93	123.70
24	B	614	CLA	CHD-C4C-NC	2.47	128.06	124.23
24	A	410	CLA	O2A-CGA-CBA	2.47	119.37	111.83
24	C	512	CLA	C1-O2A-CGA	2.47	122.62	116.65
26	C	514	BCR	C37-C22-C23	2.47	121.85	118.09
24	B	607	CLA	C1-O2A-CGA	2.47	122.62	116.65
24	C	502	CLA	C2A-C1A-CHA	-2.47	119.59	123.87
24	c	515	CLA	CMB-C2B-C1B	2.46	129.17	125.42
25	A	408	PHO	C4-C3-C5	2.46	119.50	115.23
24	B	602	CLA	CBC-CAC-C3C	-2.46	105.74	112.42
37	d	406	LHG	O7-C7-C8	2.46	116.81	111.48
24	c	516	CLA	C1-O2A-CGA	2.46	122.61	116.65
24	A	410	CLA	CED-O2D-CGD	2.46	121.50	115.92
24	C	510	CLA	C2A-C1A-CHA	-2.46	119.59	123.87
24	C	511	CLA	CMC-C2C-C1C	2.46	128.88	125.03
24	b	616	CLA	C2A-C1A-CHA	-2.46	119.59	123.87
40	V	205	HEC	O2D-CGD-CBD	2.46	121.78	114.00
24	A	407	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
37	L	101	LHG	C5-O7-C7	-2.46	111.91	117.80
24	C	512	CLA	CMC-C2C-C1C	2.46	128.88	125.03
36	c	521	DGD	O1G-C1A-C2A	2.46	119.33	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	621	CLA	CHD-C4C-NC	2.46	128.04	124.23
31	a	415[A]	PL9	C51-C49-C50	2.46	120.25	114.59
24	C	513	CLA	CBC-CAC-C3C	-2.46	105.76	112.42
24	c	511	CLA	O2A-CGA-CBA	2.46	119.33	111.83
31	d	405[A]	PL9	C12-C13-C14	-2.46	122.00	127.62
24	A	405	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
24	B	616	CLA	C1-C2-C3	-2.45	122.18	126.20
24	b	617	CLA	C2A-C1A-CHA	-2.45	119.61	123.87
26	D	404	BCR	C10-C11-C12	-2.45	116.09	123.20
24	A	410	CLA	CHD-C4C-NC	2.45	128.03	124.23
31	a	415[B]	PL9	C51-C49-C50	2.45	120.23	114.59
24	C	510	CLA	O2A-CGA-CBA	2.45	119.31	111.83
24	C	507	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
27	A	412	SQD	O47-C7-O49	-2.45	117.97	123.70
26	Y	101	BCR	C34-C9-C8	2.45	121.83	118.09
31	D	405[A]	PL9	C32-C33-C34	-2.45	122.02	127.62
26	T	103	BCR	C29-C28-C27	-2.45	105.89	111.28
40	v	205	HEC	CHB-C1B-NB	2.45	128.30	123.86
36	e	101	DGD	O5D-C1E-C2E	2.45	111.99	108.27
24	c	514	CLA	C4-C3-C5	2.45	119.47	115.23
26	B	619	BCR	C37-C22-C21	-2.44	118.86	122.82
24	b	620	CLA	CMC-C2C-C1C	2.44	128.85	125.03
24	B	603	CLA	CMB-C2B-C1B	2.44	129.14	125.42
27	F	103	SQD	C44-O6-C1	-2.44	108.56	113.80
24	c	518	CLA	C3B-C4B-NB	2.44	112.71	110.53
24	D	403	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
26	b	627	BCR	C28-C27-C26	-2.44	109.70	114.06
24	B	607	CLA	CAA-C2A-C3A	-2.44	106.41	113.00
24	c	509	CLA	O2A-CGA-CBA	2.44	119.27	111.83
26	d	404	BCR	C3-C4-C5	-2.44	109.71	114.06
24	B	604	CLA	CAC-C3C-C4C	2.44	127.96	124.79
24	b	621	CLA	CED-O2D-CGD	2.44	121.44	115.92
24	C	513	CLA	CMC-C2C-C1C	2.44	128.84	125.03
24	b	622	CLA	CMA-C3A-C4A	-2.43	105.23	111.77
24	B	614	CLA	CHB-C4A-NA	2.43	127.91	124.40
24	b	621	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
24	b	624	CLA	CMC-C2C-C1C	2.43	128.83	125.03
24	C	512	CLA	O2A-CGA-CBA	2.43	119.24	111.83
31	A	419[B]	PL9	C8-C7-C3	2.43	118.31	112.03
24	d	402	CLA	CMC-C2C-C1C	2.43	128.83	125.03
24	b	618	CLA	CAC-C3C-C4C	2.43	127.95	124.79
24	a	412	CLA	O2A-CGA-CBA	2.42	119.22	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	528	BCR	C29-C30-C25	2.42	113.96	110.44
24	c	507	CLA	C4B-C3B-C2B	-2.42	104.29	107.30
24	C	512	CLA	CAC-C3C-C4C	2.42	127.94	124.79
27	a	405	SQD	O48-C23-O10	-2.42	117.57	123.63
35	V	206	HTG	O5-C1-C2	-2.42	106.98	110.32
33	Z	101	LMG	C9-O8-C28	2.42	123.05	117.08
40	V	205	HEC	C4B-NB-C1B	2.42	109.76	105.82
36	C	517	DGD	O2G-C1B-O1B	-2.42	118.05	123.70
31	A	419[A]	PL9	C10-C9-C11	2.42	119.42	115.23
24	C	503	CLA	O2D-CGD-O1D	-2.42	119.15	123.85
24	c	515	CLA	CAC-C3C-C4C	2.41	127.93	124.79
31	D	405[B]	PL9	C53-C6-C1	2.41	120.22	115.28
24	A	406	CLA	C4C-C3C-C2C	-2.41	103.38	106.89
24	b	621	CLA	CAA-C2A-C3A	-2.41	106.48	113.00
26	C	515	BCR	C15-C16-C17	-2.41	118.58	123.52
24	a	410	CLA	C1-C2-C3	-2.41	122.25	126.20
26	k	101	BCR	C2-C1-C6	2.41	113.94	110.44
24	d	403	CLA	C1-C2-C3	-2.41	122.25	126.20
33	c	523	LMG	O8-C28-O10	-2.41	117.61	123.63
24	B	612	CLA	O2A-CGA-CBA	2.41	119.17	111.83
33	c	501	LMG	C7-O1-C1	-2.40	108.64	113.80
24	b	612	CLA	CBC-CAC-C3C	-2.40	105.91	112.42
29	M	103	LMT	O5'-C5'-C4'	2.40	114.69	109.72
24	b	615	CLA	CBC-CAC-C3C	-2.40	105.91	112.42
24	b	616	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
24	a	412	CLA	CHB-C4A-NA	2.40	127.86	124.40
31	D	405[B]	PL9	C32-C33-C34	-2.40	122.14	127.62
27	F	103	SQD	O47-C7-O49	-2.40	118.11	123.70
25	A	408	PHO	O2D-CGD-O1D	-2.40	119.19	123.85
31	A	419[A]	PL9	C17-C18-C19	-2.39	122.14	127.62
24	B	614	CLA	CMA-C3A-C2A	-2.39	104.73	113.98
26	B	620	BCR	C32-C1-C6	-2.39	106.49	110.24
24	c	517	CLA	CAC-C3C-C4C	2.39	127.90	124.79
24	B	610	CLA	C1-O2A-CGA	2.39	122.44	116.65
24	c	513	CLA	C2A-C1A-CHA	-2.39	119.72	123.87
24	b	610	CLA	C2A-C1A-CHA	-2.39	119.72	123.87
24	d	401	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
24	c	516	CLA	CED-O2D-CGD	2.39	121.33	115.92
24	c	506	CLA	OBD-CAD-C3D	-2.39	122.84	128.42
24	B	611	CLA	CAA-CBA-CGA	-2.39	106.43	113.21
24	b	623	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
24	C	503	CLA	C2A-C1A-CHA	-2.38	119.73	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	103	BCR	C1-C6-C7	2.38	122.12	115.65
24	C	508	CLA	CHD-C4C-NC	2.38	127.93	124.23
24	D	402	CLA	CHD-C4C-NC	2.38	127.93	124.23
24	b	617	CLA	CMB-C2B-C1B	2.38	129.04	125.42
27	a	414	SQD	O48-C23-O10	-2.38	117.68	123.63
37	d	407	LHG	O8-C23-C24	2.38	119.09	111.83
24	b	623	CLA	CHB-C4A-NA	2.38	127.83	124.40
31	A	419[B]	PL9	C10-C9-C11	2.38	119.35	115.23
24	D	403	CLA	CHD-C4C-NC	2.38	127.92	124.23
29	C	521	LMT	O5'-C5'-C4'	2.38	114.63	109.72
24	C	504	CLA	CAA-C2A-C3A	-2.37	106.59	113.00
26	C	515	BCR	C15-C14-C13	-2.37	123.95	127.28
24	B	605	CLA	CHD-C4C-NC	2.37	127.91	124.23
24	B	614	CLA	OBD-CAD-C3D	-2.37	122.88	128.42
40	v	205	HEC	C4C-NC-C1C	2.37	109.68	105.82
36	C	516	DGD	O1G-C1A-C2A	2.37	119.06	111.83
33	D	413	LMG	O8-C28-O10	-2.37	117.70	123.63
24	c	516	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
24	c	510	CLA	CHD-C4C-NC	2.37	127.90	124.23
24	b	625	CLA	C2A-C1A-CHA	-2.37	119.76	123.87
33	A	421	LMG	C8-O7-C10	-2.36	112.14	117.80
24	C	507	CLA	C1-C2-C3	-2.36	122.33	126.20
25	A	408	PHO	C1-C2-C3	-2.36	122.33	126.20
24	b	615	CLA	C2A-C1A-CHA	-2.36	119.77	123.87
24	c	517	CLA	C4B-C3B-C2B	-2.36	104.36	107.30
31	D	405[B]	PL9	C2-C1-C6	2.36	121.81	119.00
24	c	506	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
24	b	611	CLA	C1-O2A-CGA	2.36	122.37	116.65
38	e	103	HEM	C4D-ND-C1D	2.36	108.00	105.21
36	D	406	DGD	C4D-C3D-C2D	2.36	114.97	110.83
24	b	618	CLA	C1-O2A-CGA	2.36	122.36	116.65
37	D	408	LHG	O8-C23-C24	2.36	119.03	111.83
27	L	102	SQD	C1-C2-C3	-2.36	105.05	110.01
27	B	621	SQD	O47-C7-O49	-2.36	118.19	123.70
24	D	403	CLA	CMC-C2C-C1C	2.36	128.72	125.03
24	c	516	CLA	CBC-CAC-C3C	-2.36	106.03	112.42
33	D	413	LMG	C7-O1-C1	-2.36	108.74	113.80
33	A	421	LMG	O8-C28-C29	2.36	119.02	111.83
27	L	102	SQD	O7-S-C6	2.36	110.27	106.76
24	C	509	CLA	C2A-C1A-CHA	-2.35	119.78	123.87
37	D	408	LHG	O8-C23-O10	-2.35	117.75	123.63
24	C	505	CLA	C4B-C3B-C2B	-2.35	104.38	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	405[B]	PL9	C15-C14-C16	2.35	119.31	115.23
33	B	622	LMG	O6-C5-C4	2.35	113.93	109.70
26	d	404	BCR	C10-C11-C12	-2.35	116.39	123.20
25	A	409[B]	PHO	O2A-CGA-CBA	2.35	119.00	111.83
24	c	515	CLA	C2A-C1A-CHA	-2.35	119.79	123.87
24	A	406	CLA	CMA-C3A-C4A	-2.35	105.46	111.77
24	B	616	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
24	D	402	CLA	CAC-C3C-C4C	2.35	127.84	124.79
33	Z	101	LMG	C1-C2-C3	2.35	114.94	110.01
24	B	604	CLA	CMA-C3A-C2A	-2.35	104.91	113.98
35	C	523	HTG	O5-C1-C2	2.34	113.55	110.32
24	A	410	CLA	C2A-C1A-CHA	-2.34	119.80	123.87
31	D	405[A]	PL9	C51-C49-C50	2.34	119.98	114.59
27	L	102	SQD	O8-S-C6	2.34	110.50	105.97
40	V	205	HEC	CHB-C1B-NB	2.34	128.11	123.86
26	t	101	BCR	C16-C15-C14	2.34	128.31	123.52
24	B	614	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
24	B	605	CLA	C4-C3-C5	2.34	119.29	115.23
24	c	513	CLA	CHD-C4C-NC	2.34	127.86	124.23
24	a	409	CLA	CHD-C4C-NC	2.34	127.86	124.23
26	Y	101	BCR	C21-C20-C19	-2.34	116.43	123.20
24	B	612	CLA	CBC-CAC-C3C	-2.34	106.09	112.42
24	B	611	CLA	CHB-C4A-NA	2.34	127.77	124.40
24	c	506	CLA	CHD-C4C-NC	2.34	127.85	124.23
26	k	101	BCR	C39-C30-C25	-2.33	106.58	110.24
24	c	510	CLA	CBC-CAC-C3C	-2.33	106.09	112.42
27	A	412	SQD	C1-O5-C5	-2.33	109.17	113.72
24	b	614	CLA	CAC-C3C-C2C	2.33	131.84	127.56
40	V	205	HEC	CHA-C4D-ND	2.33	128.09	123.86
31	a	415[A]	PL9	C8-C7-C3	2.33	118.05	112.03
24	b	624	CLA	C11-C10-C8	-2.33	108.23	115.97
31	D	405[B]	PL9	C45-C44-C46	2.33	119.26	115.23
33	d	413	LMG	O6-C5-C4	2.32	113.89	109.70
27	a	414	SQD	C1-O5-C5	-2.32	109.18	113.72
24	D	402	CLA	CED-O2D-CGD	2.32	121.19	115.92
24	B	612	CLA	C2A-C1A-CHA	-2.32	119.83	123.87
24	C	501	CLA	C2A-C1A-CHA	-2.32	119.84	123.87
24	A	410	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
40	v	205	HEC	C4B-NB-C1B	2.32	109.61	105.82
31	D	405[A]	PL9	C40-C39-C38	-2.32	117.67	123.63
26	b	628	BCR	C15-C14-C13	-2.32	124.02	127.28
35	B	625	HTG	C1-C2-C3	2.32	115.09	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	405	CLA	CMA-C3A-C2A	-2.32	105.01	113.98
33	b	629	LMG	O7-C10-O9	-2.32	118.28	123.70
24	d	403	CLA	CMB-C2B-C1B	2.32	128.95	125.42
24	b	625	CLA	O1D-CGD-CBD	-2.32	119.95	124.52
26	K	101	BCR	C16-C17-C18	-2.32	124.03	127.28
24	B	615	CLA	CMB-C2B-C1B	2.32	128.95	125.42
24	B	610	CLA	O2A-CGA-CBA	2.32	118.90	111.83
24	C	503	CLA	C3B-C4B-NB	2.31	112.60	110.53
24	B	611	CLA	C1-C2-C3	-2.31	122.41	126.20
31	D	405[B]	PL9	C7-C3-C2	-2.31	120.66	123.39
24	b	616	CLA	CED-O2D-CGD	2.31	121.16	115.92
24	b	625	CLA	CBC-CAC-C3C	-2.31	106.15	112.42
24	c	518	CLA	C4B-C3B-C2B	-2.31	104.43	107.30
24	D	402	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
24	c	508	CLA	C4B-C3B-C2B	-2.31	104.43	107.30
24	B	606	CLA	CHC-C1C-C2C	-2.31	120.39	126.95
24	b	624	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
24	b	622	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
24	A	410	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
24	A	407	CLA	C3B-C4B-NB	2.31	112.59	110.53
27	F	103	SQD	O9-S-C6	2.31	110.20	106.76
31	d	405[B]	PL9	C22-C23-C24	-2.31	122.35	127.62
24	C	506	CLA	CMB-C2B-C1B	2.30	128.93	125.42
29	B	635	LMT	C1'-O5'-C5'	2.30	118.22	113.72
24	c	513	CLA	CMB-C2B-C1B	2.30	128.92	125.42
24	B	612	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
25	a	418[B]	PHO	O2A-CGA-CBA	2.30	118.84	111.83
24	B	617	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
24	B	616	CLA	C4B-C3B-C2B	-2.30	104.44	107.30
25	a	411	PHO	CAA-CBA-CGA	-2.30	106.68	113.21
24	C	503	CLA	CAC-C3C-C4C	2.30	127.78	124.79
26	T	103	BCR	C16-C17-C18	-2.30	124.06	127.28
40	v	205	HEC	C2A-C1A-NA	-2.30	108.11	110.32
24	B	604	CLA	C4-C3-C5	2.30	119.21	115.23
24	c	511	CLA	C2A-C1A-CHA	-2.30	119.88	123.87
36	c	522	DGD	C2G-O2G-C1B	-2.29	112.30	117.80
24	B	616	CLA	C2A-C1A-CHA	-2.29	119.89	123.87
37	L	101	LHG	O7-C7-O9	-2.29	118.34	123.70
24	A	406	CLA	CED-O2D-CGD	2.29	121.12	115.92
24	B	603	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
24	C	503	CLA	C4-C3-C5	2.29	119.21	115.23
24	b	624	CLA	O2A-CGA-CBA	2.29	118.82	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	511	CLA	CGD-CBD-CAD	-2.29	103.43	110.85
24	a	409	CLA	CMC-C2C-C1C	2.29	128.61	125.03
36	C	516	DGD	O2G-C1B-O1B	-2.29	118.35	123.70
26	B	619	BCR	C30-C25-C26	-2.29	119.51	122.64
24	b	619	CLA	CMA-C3A-C2A	-2.29	105.14	113.98
31	a	415[B]	PL9	C45-C44-C46	2.29	119.20	115.23
26	t	101	BCR	C29-C28-C27	-2.29	106.25	111.28
25	a	418[A]	PHO	C4A-C3A-C2A	-2.29	100.66	102.84
26	c	519	BCR	C21-C20-C19	-2.29	116.58	123.20
24	c	511	CLA	CMC-C2C-C1C	2.29	128.60	125.03
37	d	407	LHG	C6-C5-C4	-2.28	106.46	111.78
25	a	411	PHO	CBA-CAA-C2A	-2.28	107.05	113.78
36	c	521	DGD	C2G-O2G-C1B	-2.28	112.33	117.80
24	C	513	CLA	C2A-C1A-CHA	-2.28	119.90	123.87
24	b	617	CLA	CMA-C3A-C2A	-2.28	105.15	113.98
33	Z	101	LMG	C8-O7-C10	-2.28	112.33	117.80
33	D	413	LMG	O8-C28-C29	2.28	118.79	111.83
31	A	419[B]	PL9	C40-C39-C41	2.28	119.19	115.23
31	D	405[B]	PL9	C35-C34-C36	2.28	119.19	115.23
36	C	518	DGD	C3G-C2G-C1G	-2.28	106.47	111.78
24	b	612	CLA	C4-C3-C5	2.28	119.19	115.23
24	A	406	CLA	CAC-C3C-C4C	2.28	127.76	124.79
24	A	406	CLA	CAA-CBA-CGA	2.28	119.68	113.21
27	F	103	SQD	C1-C2-C3	-2.28	105.22	110.01
26	C	515	BCR	C28-C27-C26	-2.28	110.00	114.06
24	b	610	CLA	O2A-CGA-CBA	2.28	118.78	111.83
24	A	407	CLA	CMA-C3A-C2A	-2.28	105.18	113.98
24	B	613	CLA	CMB-C2B-C1B	2.28	128.88	125.42
36	c	521	DGD	C3B-C2B-C1B	-2.27	105.36	113.69
24	b	620	CLA	CMA-C3A-C4A	-2.27	105.66	111.77
31	d	405[A]	PL9	C25-C24-C26	2.27	119.17	115.23
24	d	401	CLA	CAC-C3C-C4C	2.27	127.75	124.79
24	C	507	CLA	C4B-C3B-C2B	-2.27	104.48	107.30
24	b	613	CLA	CHA-C1A-NA	-2.27	121.25	126.39
24	B	613	CLA	CMA-C3A-C2A	-2.27	105.20	113.98
31	d	405[A]	PL9	C15-C14-C16	2.27	119.17	115.23
24	C	510	CLA	CMC-C2C-C1C	2.27	128.58	125.03
24	d	401	CLA	O2A-CGA-CBA	2.27	118.75	111.83
24	C	511	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
26	B	618	BCR	C11-C10-C9	-2.27	124.10	127.28
24	B	603	CLA	C4-C3-C5	2.27	119.16	115.23
24	c	508	CLA	C4-C3-C5	2.27	119.16	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	413	BCR	C7-C8-C9	-2.27	122.88	126.23
36	H	102	DGD	C2G-O2G-C1B	-2.26	112.38	117.80
24	C	508	CLA	C2A-C1A-CHA	-2.26	119.94	123.87
24	b	619	CLA	CMC-C2C-C1C	2.26	128.57	125.03
24	c	518	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
31	d	405[B]	PL9	C45-C44-C46	2.26	119.16	115.23
24	C	513	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
26	B	619	BCR	C37-C22-C23	2.26	121.54	118.09
24	C	507	CLA	CBC-CAC-C3C	-2.26	106.30	112.42
35	d	411	HTG	C1-O5-C5	2.26	116.61	112.56
29	a	404	LMT	C1B-O1B-C4'	-2.26	112.63	117.98
24	d	401	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
24	b	612	CLA	C7-C6-C5	-2.25	107.25	113.26
24	B	603	CLA	CMC-C2C-C1C	2.25	128.56	125.03
24	b	618	CLA	CMA-C3A-C4A	-2.25	105.72	111.77
24	d	402	CLA	CBC-CAC-C3C	-2.25	106.32	112.42
24	d	401	CLA	C4-C3-C5	2.25	119.14	115.23
26	B	620	BCR	C28-C27-C26	-2.25	110.04	114.06
25	a	411	PHO	O2A-CGA-CBA	2.25	118.69	111.83
24	B	611	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
24	B	616	CLA	O2A-CGA-CBA	2.25	118.69	111.83
24	c	510	CLA	C2A-C1A-CHA	-2.25	119.97	123.87
24	c	508	CLA	C1-O2A-CGA	2.25	122.09	116.65
24	A	406	CLA	CMA-C3A-C2A	-2.24	105.30	113.98
24	B	614	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
24	b	610	CLA	CAC-C3C-C4C	2.24	127.71	124.79
24	c	516	CLA	CMB-C2B-C1B	2.24	128.83	125.42
26	t	101	BCR	C37-C22-C23	2.24	121.51	118.09
24	C	510	CLA	CMB-C2B-C1B	2.24	128.83	125.42
24	b	611	CLA	CMC-C2C-C1C	2.24	128.53	125.03
24	c	514	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
24	b	622	CLA	C2A-C1A-CHA	-2.24	119.98	123.87
36	h	102	DGD	C2G-O2G-C1B	-2.23	112.45	117.80
27	a	414	SQD	O9-S-O7	-2.23	106.56	113.82
24	c	517	CLA	CHB-C1B-C2B	-2.23	120.94	127.43
24	d	403	CLA	CBC-CAC-C3C	-2.23	106.37	112.42
24	c	515	CLA	CMC-C2C-C1C	2.23	128.52	125.03
24	B	608	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
24	b	619	CLA	C2A-C1A-CHA	-2.23	120.00	123.87
38	e	103	HEM	C2A-C1A-NA	-2.23	107.68	110.15
24	c	508	CLA	CHC-C1C-C2C	-2.23	120.62	126.95
24	b	621	CLA	C2A-C1A-CHA	-2.23	120.00	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	CAA-C2A-C3A	-2.23	106.98	113.00
37	d	407	LHG	O8-C23-O10	-2.22	118.06	123.63
24	B	608	CLA	C1-O2A-CGA	2.22	122.03	116.65
24	B	615	CLA	CAA-C2A-C3A	-2.22	106.99	113.00
24	A	406	CLA	C2A-C1A-CHA	-2.22	120.01	123.87
26	b	626	BCR	C29-C30-C25	2.22	113.67	110.44
29	m	103	LMT	C1'-O5'-C5'	2.22	118.06	113.72
24	B	602	CLA	CHB-C4A-NA	2.22	127.61	124.40
24	C	511	CLA	C1-O2A-CGA	2.22	122.03	116.65
24	c	511	CLA	CAC-C3C-C4C	2.22	127.68	124.79
35	B	632	HTG	C3-C4-C5	2.22	114.26	110.23
24	B	610	CLA	C7-C6-C5	-2.22	107.35	113.26
36	D	406	DGD	O6D-C5D-C6D	2.22	111.09	106.69
29	m	103	LMT	C1B-O1B-C4'	-2.21	112.73	117.98
24	D	402	CLA	CMA-C3A-C4A	-2.21	105.82	111.77
26	b	628	BCR	C21-C20-C19	-2.21	116.79	123.20
24	A	407	CLA	CAA-CBA-CGA	2.21	119.49	113.21
38	e	103	HEM	CAD-CBD-CGD	2.21	119.53	113.67
24	b	617	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
24	c	513	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
25	A	409[A]	PHO	O2A-CGA-CBA	2.21	118.58	111.83
38	F	102	HEM	O2A-CGA-CBA	2.21	120.99	114.00
26	t	101	BCR	C2-C1-C6	2.21	113.65	110.44
24	B	616	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
26	C	515	BCR	C38-C26-C25	-2.21	122.08	124.48
24	b	613	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
35	b	601	HTG	C1-O5-C5	2.20	116.52	112.56
24	C	510	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
24	B	606	CLA	C3B-C4B-NB	2.20	112.50	110.53
40	v	205	HEC	O2D-CGD-CBD	2.20	120.95	114.00
37	L	101	LHG	O8-C23-O10	-2.20	118.12	123.63
36	C	518	DGD	O3G-C3G-C2G	-2.20	105.47	110.82
24	B	614	CLA	C2A-C1A-CHA	-2.20	120.05	123.87
33	z	101	LMG	C8-O7-C10	-2.20	112.53	117.80
26	b	626	BCR	C10-C11-C12	-2.20	116.83	123.20
29	A	417	LMT	C4B-C3B-C2B	-2.20	106.97	110.83
37	E	101	LHG	C5-O7-C7	-2.20	112.53	117.80
24	c	510	CLA	CED-O2D-CGD	2.20	120.90	115.92
36	c	520	DGD	O1G-C1A-C2A	2.20	118.53	111.83
31	a	415[B]	PL9	C12-C13-C14	-2.20	122.59	127.62
24	B	609	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
24	A	410	CLA	CBC-CAC-C3C	-2.20	106.47	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	101	BCR	C38-C26-C25	-2.19	122.09	124.48
24	B	610	CLA	C2A-C1A-CHA	-2.19	120.06	123.87
26	T	103	BCR	C12-C13-C14	-2.19	115.56	119.01
26	b	627	BCR	C37-C22-C21	-2.19	119.26	122.82
24	d	403	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
24	C	507	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
26	d	404	BCR	C21-C20-C19	-2.19	116.86	123.20
36	e	101	DGD	O2G-C1B-O1B	-2.19	118.59	123.70
24	b	622	CLA	CHD-C4C-NC	2.19	127.62	124.23
24	B	605	CLA	C11-C10-C8	-2.19	108.69	115.97
35	B	632	HTG	C6-C5-C4	-2.19	107.65	113.02
24	B	617	CLA	C4-C3-C5	2.19	119.02	115.23
24	a	409	CLA	CHB-C1B-C2B	-2.19	121.08	127.43
24	C	506	CLA	CED-O2D-CGD	2.19	120.87	115.92
24	b	624	CLA	CHA-C1A-NA	-2.18	121.44	126.39
36	H	102	DGD	C3G-O3G-C1D	-2.18	109.11	113.80
24	C	512	CLA	C4-C3-C5	2.18	119.02	115.23
24	a	409	CLA	C4-C3-C5	2.18	119.02	115.23
26	T	103	BCR	C34-C9-C10	-2.18	119.28	122.82
24	B	604	CLA	CBC-CAC-C3C	-2.18	106.50	112.42
24	b	610	CLA	C1-O2A-CGA	2.18	121.93	116.65
24	C	510	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
35	b	631	HTG	C1-C2-C3	2.18	114.81	110.55
24	a	410	CLA	CAA-CBA-CGA	2.18	119.40	113.21
24	c	518	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
24	a	410	CLA	CMA-C3A-C2A	-2.18	105.57	113.98
24	B	607	CLA	OBD-CAD-C3D	-2.18	123.33	128.42
24	c	517	CLA	C1-O2A-CGA	2.18	121.92	116.65
40	v	205	HEC	O2A-CGA-CBA	2.17	120.87	114.00
26	Y	101	BCR	C15-C16-C17	-2.17	119.07	123.52
33	C	519	LMG	O7-C10-O9	-2.17	118.63	123.70
25	a	418[B]	PHO	C4A-C3A-C2A	-2.17	100.77	102.84
24	d	402	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
26	H	101	BCR	C39-C30-C25	-2.17	106.84	110.24
31	D	405[B]	PL9	C51-C49-C50	2.17	119.58	114.59
38	e	103	HEM	C4C-NC-C1C	2.17	109.36	105.82
37	b	634	LHG	O8-C23-O10	-2.17	118.20	123.63
24	C	507	CLA	C4-C3-C5	2.17	118.99	115.23
24	C	505	CLA	C4-C3-C5	2.17	118.99	115.23
24	A	406	CLA	O2A-CGA-CBA	2.17	118.44	111.83
24	b	618	CLA	CBC-CAC-C3C	-2.17	106.55	112.42
24	B	613	CLA	CHC-C1C-C2C	-2.17	120.79	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	f	101	SQD	O48-C23-O10	-2.17	118.21	123.63
27	f	101	SQD	O7-S-C6	2.17	109.99	106.76
24	c	509	CLA	C11-C10-C8	-2.16	108.77	115.97
31	A	419[B]	PL9	C35-C34-C36	2.16	118.98	115.23
24	d	401	CLA	C1-O2A-CGA	2.16	121.88	116.65
24	B	602	CLA	C1-C2-C3	-2.16	122.66	126.20
36	C	516	DGD	O6D-C5D-C6D	2.16	110.97	106.69
24	b	619	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
31	d	405[A]	PL9	C22-C23-C24	-2.16	122.69	127.62
25	A	409[B]	PHO	C4A-C3A-C2A	-2.16	100.79	102.84
26	B	618	BCR	C29-C30-C25	2.15	113.57	110.44
40	V	205	HEC	CHD-C1D-ND	2.15	127.77	123.86
24	B	602	CLA	CMC-C2C-C1C	2.15	128.40	125.03
26	t	101	BCR	C12-C13-C14	-2.15	115.62	119.01
24	C	504	CLA	OBD-CAD-C3D	-2.15	123.39	128.42
24	c	515	CLA	C4-C3-C2	-2.15	118.10	123.63
26	d	404	BCR	C39-C30-C25	-2.15	106.87	110.24
29	A	417	LMT	C6'-C5'-C4'	-2.15	107.33	113.38
24	D	403	CLA	CHB-C4A-NA	2.15	127.50	124.40
26	H	101	BCR	C15-C14-C13	-2.15	124.26	127.28
24	c	512	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
31	A	419[A]	PL9	C47-C46-C44	-2.15	106.06	113.19
24	C	505	CLA	C2A-C1A-CHA	-2.15	120.14	123.87
24	D	403	CLA	O2A-CGA-CBA	2.15	118.38	111.83
36	c	521	DGD	O1G-C1A-O1A	-2.15	118.26	123.63
24	B	614	CLA	CAA-C2A-C3A	-2.15	107.20	113.00
24	b	620	CLA	CHB-C4A-NA	2.15	127.50	124.40
26	C	514	BCR	C23-C24-C25	-2.14	121.27	127.00
24	a	409	CLA	O2D-CGD-O1D	-2.14	119.67	123.85
26	b	628	BCR	C16-C17-C18	-2.14	124.27	127.28
24	B	611	CLA	CGD-CBD-CAD	-2.14	103.91	110.85
24	b	614	CLA	CMC-C2C-C1C	2.14	128.38	125.03
24	A	407	CLA	O2A-CGA-CBA	2.14	118.36	111.83
26	C	514	BCR	C38-C26-C25	-2.14	122.15	124.48
33	B	622	LMG	O8-C28-O10	-2.14	118.28	123.63
24	B	615	CLA	OBD-CAD-C3D	-2.14	123.42	128.42
24	d	401	CLA	CED-O2D-CGD	2.13	120.76	115.92
26	D	404	BCR	C3-C4-C5	-2.13	110.25	114.06
24	B	603	CLA	O2A-CGA-CBA	2.13	118.34	111.83
33	b	629	LMG	O8-C28-O10	-2.13	118.30	123.63
24	b	625	CLA	CAA-C2A-C3A	-2.13	107.24	113.00
24	c	507	CLA	C2A-C1A-CHA	-2.13	120.17	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	CMC-C2C-C1C	2.13	128.36	125.03
24	C	505	CLA	CHA-C1A-NA	-2.13	121.57	126.39
38	e	103	HEM	C4C-CHD-C1D	-2.13	121.49	126.02
40	V	205	HEC	CAA-C2A-C3A	-2.13	123.88	127.87
26	B	618	BCR	C21-C20-C19	-2.13	117.03	123.20
24	B	604	CLA	CBA-CAA-C2A	2.13	120.12	113.79
33	c	524	LMG	O7-C10-O9	-2.13	118.73	123.70
24	d	401	CLA	CMC-C2C-C1C	2.13	128.36	125.03
31	d	405[A]	PL9	C40-C39-C38	-2.13	118.17	123.63
25	a	411	PHO	CMC-C2C-C1C	2.12	128.56	124.73
25	a	411	PHO	CAC-C3C-C4C	2.12	129.49	124.03
38	F	102	HEM	C2A-C1A-NA	-2.12	107.80	110.15
26	a	413	BCR	C38-C26-C25	-2.12	122.17	124.48
24	B	614	CLA	CMA-C3A-C4A	-2.12	106.07	111.77
31	d	405[A]	PL9	O1-C4-C3	-2.12	118.49	120.73
31	d	405[B]	PL9	C25-C24-C26	2.12	118.91	115.23
24	b	621	CLA	CHB-C4A-NA	2.12	127.46	124.40
24	c	506	CLA	C4-C3-C5	2.12	118.91	115.23
26	a	413	BCR	C8-C7-C6	-2.12	121.33	127.00
24	C	506	CLA	O2A-CGA-CBA	2.12	118.30	111.83
27	A	412	SQD	C44-O6-C1	-2.12	109.25	113.80
24	B	605	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
35	C	522	HTG	C1-O5-C5	2.12	116.36	112.56
24	A	405	CLA	CMC-C2C-C1C	2.12	128.34	125.03
24	A	406	CLA	CMB-C2B-C1B	2.12	128.64	125.42
31	D	405[A]	PL9	C47-C48-C49	-2.12	120.59	127.64
36	c	522	DGD	O1G-C1A-O1A	-2.12	118.34	123.63
31	D	405[A]	PL9	C7-C3-C2	-2.11	120.89	123.39
33	D	413	LMG	O7-C10-O9	-2.11	118.76	123.70
26	Y	101	BCR	C40-C30-C25	-2.11	106.93	110.24
26	b	626	BCR	C21-C20-C19	-2.11	117.08	123.20
36	c	520	DGD	O6D-C5D-C6D	2.11	110.88	106.69
24	B	611	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
24	b	614	CLA	C1-C2-C3	-2.11	122.74	126.20
24	B	608	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
26	B	619	BCR	C8-C7-C6	-2.11	121.37	127.00
24	B	610	CLA	CED-O2D-CGD	2.11	120.69	115.92
24	b	620	CLA	C2A-C1A-CHA	-2.11	120.21	123.87
25	A	409[B]	PHO	CMA-C3A-C4A	-2.11	110.07	114.61
26	K	101	BCR	C36-C18-C19	2.11	121.30	118.09
24	c	514	CLA	CHB-C1B-NB	-2.11	120.89	124.05
37	d	406	LHG	O7-C7-O9	-2.10	118.79	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	M	103	LMT	O5B-C5B-C4B	2.10	113.49	109.70
26	A	411	BCR	C8-C7-C6	-2.10	121.38	127.00
24	B	607	CLA	C2A-C1A-CHA	-2.10	120.22	123.87
24	b	610	CLA	CHB-C1B-C2B	-2.10	121.33	127.43
24	B	612	CLA	CED-O2D-CGD	2.10	120.68	115.92
31	D	405[A]	PL9	C35-C34-C36	2.10	118.87	115.23
26	A	411	BCR	C3-C4-C5	-2.10	110.32	114.06
31	a	415[B]	PL9	C8-C7-C3	2.10	117.45	112.03
26	T	103	BCR	C28-C27-C26	-2.09	110.32	114.06
37	b	634	LHG	O4-P-O5	2.09	122.19	112.44
24	C	503	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
26	A	411	BCR	C24-C23-C22	-2.09	123.14	126.23
24	B	615	CLA	C1-C2-C3	-2.09	122.77	126.20
24	b	621	CLA	CMC-C2C-C1C	2.09	128.31	125.03
31	a	415[A]	PL9	C45-C44-C46	2.09	118.86	115.23
24	A	405	CLA	CHB-C4A-NA	2.09	127.42	124.40
25	a	418[A]	PHO	CMA-C3A-C4A	-2.09	110.11	114.61
24	C	511	CLA	C2A-C1A-CHA	-2.09	120.24	123.87
31	A	419[A]	PL9	C2-C1-C6	2.09	121.48	119.00
27	F	103	SQD	O48-C23-O10	-2.09	118.41	123.63
24	c	514	CLA	CBC-CAC-C3C	-2.08	106.77	112.42
24	B	610	CLA	C1-C2-C3	-2.08	122.79	126.20
31	D	405[A]	PL9	C20-C19-C21	2.08	118.84	115.23
24	b	611	CLA	CMA-C3A-C2A	-2.08	105.95	113.98
36	H	102	DGD	C3B-C2B-C1B	-2.08	106.08	113.69
24	b	611	CLA	C2A-C1A-CHA	-2.08	120.26	123.87
24	B	612	CLA	C1-O2A-CGA	2.08	121.68	116.65
24	b	615	CLA	C1-C2-C3	-2.08	122.79	126.20
24	b	623	CLA	C4-C3-C5	2.08	118.83	115.23
31	D	405[A]	PL9	C36-C37-C38	-2.08	101.75	112.02
27	L	102	SQD	O5-C5-C4	2.07	113.44	109.70
26	D	404	BCR	C1-C6-C7	2.07	121.28	115.65
33	d	413	LMG	C1-O6-C5	2.07	117.77	113.72
24	B	602	CLA	CAC-C3C-C4C	2.07	127.49	124.79
24	c	509	CLA	CAA-C2A-C3A	-2.07	107.40	113.00
26	c	519	BCR	C16-C17-C18	-2.07	124.37	127.28
27	a	405	SQD	C3-C4-C5	2.07	113.99	110.23
24	b	613	CLA	CHD-C4C-NC	2.07	127.44	124.23
33	b	629	LMG	C9-C8-C7	-2.07	106.96	111.78
24	A	410	CLA	CMA-C3A-C2A	-2.07	105.97	113.98
24	c	517	CLA	CMA-C3A-C4A	-2.07	106.21	111.77
29	a	419	LMT	C1B-O1B-C4'	-2.07	113.07	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	CMA-C3A-C2A	-2.07	105.98	113.98
37	E	101	LHG	O8-C23-O10	-2.07	118.45	123.63
26	A	411	BCR	C38-C26-C25	-2.07	122.23	124.48
24	B	609	CLA	CMA-C3A-C2A	-2.07	105.98	113.98
33	B	622	LMG	C9-C8-C7	-2.07	106.96	111.78
24	B	609	CLA	C2A-C1A-CHA	-2.07	120.28	123.87
26	b	626	BCR	C16-C17-C18	-2.07	124.38	127.28
24	B	608	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
25	a	411	PHO	CMB-C2B-C3B	2.07	128.81	124.68
24	c	512	CLA	C4B-C3B-C2B	-2.07	104.73	107.30
24	c	509	CLA	CMA-C3A-C2A	-2.07	105.99	113.98
24	B	606	CLA	CAA-C2A-C3A	-2.07	107.42	113.00
24	c	512	CLA	OBD-CAD-C3D	-2.07	123.59	128.42
31	d	405[A]	PL9	C8-C7-C3	2.06	117.37	112.03
24	b	617	CLA	CAA-C2A-C3A	-2.06	107.42	113.00
24	c	516	CLA	C2A-C1A-CHA	-2.06	120.29	123.87
33	c	524	LMG	O8-C28-O10	-2.06	118.48	123.63
26	D	404	BCR	C7-C6-C5	-2.06	116.81	121.56
24	B	605	CLA	OBD-CAD-C3D	-2.06	123.60	128.42
26	K	101	BCR	C10-C11-C12	-2.06	117.23	123.20
24	B	605	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
26	C	515	BCR	C2-C1-C6	2.06	113.43	110.44
24	A	406	CLA	CMC-C2C-C1C	2.06	128.25	125.03
26	Y	101	BCR	C28-C27-C26	-2.06	110.39	114.06
26	A	411	BCR	C7-C8-C9	-2.05	123.19	126.23
26	T	103	BCR	C36-C18-C19	2.05	121.22	118.09
24	B	613	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
24	c	509	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
25	a	418[A]	PHO	O2A-CGA-CBA	2.05	118.09	111.83
24	b	614	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
33	C	519	LMG	O8-C28-O10	-2.05	118.50	123.63
27	f	101	SQD	C4-C3-C2	-2.05	107.23	110.83
25	a	411	PHO	C4A-C3A-C2A	-2.05	100.89	102.84
24	C	507	CLA	CHB-C1B-C2B	-2.05	121.48	127.43
24	B	606	CLA	C4B-C3B-C2B	-2.05	104.76	107.30
25	A	408	PHO	O2A-CGA-CBA	2.05	118.08	111.83
36	H	102	DGD	O6E-C5E-C6E	2.05	111.51	106.44
38	e	103	HEM	CBD-CAD-C3D	-2.05	106.88	112.53
31	A	419[A]	PL9	C40-C39-C41	2.05	118.78	115.23
24	c	515	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
24	C	501	CLA	O2A-CGA-CBA	2.05	118.07	111.83
31	A	419[B]	PL9	C51-C49-C50	2.04	119.29	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	507	CLA	C3B-C4B-NB	2.04	112.35	110.53
26	a	413	BCR	C3-C4-C5	-2.04	110.42	114.06
24	b	614	CLA	OBD-CAD-C3D	-2.04	123.65	128.42
26	C	515	BCR	C40-C30-C25	-2.04	107.05	110.24
24	B	605	CLA	CHA-C1A-NA	-2.04	121.78	126.39
38	F	102	HEM	CHA-C4D-ND	2.04	126.89	124.37
24	c	508	CLA	CHB-C1B-C2B	-2.04	121.52	127.43
24	b	623	CLA	C4-C3-C2	-2.04	118.40	123.63
24	D	403	CLA	C1-O2A-CGA	2.04	121.58	116.65
24	B	608	CLA	CED-O2D-CGD	2.03	120.53	115.92
36	c	521	DGD	O2G-C1B-O1B	-2.03	118.95	123.70
26	k	101	BCR	C38-C26-C25	-2.03	122.26	124.48
24	d	403	CLA	CGD-CBD-CAD	-2.03	104.26	110.85
24	C	510	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
26	B	618	BCR	C24-C23-C22	-2.03	123.23	126.23
24	A	407	CLA	CAC-C3C-C4C	2.03	127.44	124.79
38	F	102	HEM	C4B-C3B-C2B	-2.03	105.41	107.28
24	C	506	CLA	C2A-C1A-CHA	-2.03	120.34	123.87
26	a	413	BCR	C15-C14-C13	-2.03	124.43	127.28
24	d	402	CLA	CHD-C4C-NC	2.03	127.38	124.23
24	c	518	CLA	CBC-CAC-C3C	-2.03	106.92	112.42
26	y	101	BCR	C40-C30-C25	-2.03	107.07	110.24
36	c	522	DGD	O2G-C1B-O1B	-2.02	118.97	123.70
26	k	101	BCR	C29-C30-C25	2.02	113.38	110.44
33	c	501	LMG	O7-C10-O9	-2.02	118.97	123.70
24	a	412	CLA	OBD-CAD-C3D	-2.02	123.69	128.42
26	K	101	BCR	C29-C30-C25	2.02	113.38	110.44
24	b	614	CLA	CAA-C2A-C3A	-2.02	107.54	113.00
24	c	511	CLA	CHB-C4A-NA	2.02	127.32	124.40
31	d	405[B]	PL9	C35-C34-C36	2.02	118.73	115.23
26	C	514	BCR	C11-C10-C9	-2.02	124.45	127.28
24	C	507	CLA	CED-O2D-CGD	2.02	120.49	115.92
26	T	103	BCR	C7-C6-C5	-2.02	116.91	121.56
24	B	603	CLA	CHB-C1B-C2B	-2.02	121.57	127.43
24	B	607	CLA	CMB-C2B-C1B	2.02	128.49	125.42
24	C	512	CLA	CHB-C4A-NA	2.02	127.31	124.40
24	c	518	CLA	CHB-C1B-C2B	-2.02	121.58	127.43
24	b	616	CLA	OBD-CAD-C3D	-2.01	123.71	128.42
24	c	509	CLA	C6-C7-C8	-2.01	109.28	115.97
24	C	509	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
31	d	405[A]	PL9	C35-C34-C36	2.01	118.72	115.23
27	B	621	SQD	C44-O6-C1	-2.01	109.48	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	528	BCR	C34-C9-C8	2.01	121.16	118.09
24	b	610	CLA	CMB-C2B-C1B	2.01	128.48	125.42
29	m	102	LMT	O1B-C1B-C2B	2.01	113.03	108.09
24	b	621	CLA	OBD-CAD-C3D	-2.01	123.72	128.42
31	A	419[A]	PL9	C51-C49-C50	2.01	119.21	114.59
26	t	101	BCR	C35-C13-C12	2.01	121.15	118.09
24	b	625	CLA	CMA-C3A-C2A	-2.01	106.22	113.98
33	A	421	LMG	O7-C10-O9	-2.01	119.02	123.70
24	c	512	CLA	CHB-C4A-NA	2.01	127.29	124.40
24	B	612	CLA	CAA-C2A-C3A	-2.00	107.59	113.00
24	B	608	CLA	CHB-C4A-NA	2.00	127.29	124.40
29	F	101	LMT	C1B-O5B-C5B	2.00	117.63	113.72
24	b	612	CLA	O1D-CGD-CBD	-2.00	120.57	124.52

All (63) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	406	CLA	ND
24	A	410	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
24	B	616	CLA	ND
24	B	617	CLA	ND
24	C	501	CLA	ND
24	C	503	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

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Mol	Chain	Res	Type	Atom
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	D	402	CLA	ND
24	D	403	CLA	ND
24	a	409	CLA	ND
24	a	412	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
24	b	616	CLA	ND
24	b	618	CLA	ND
24	b	619	CLA	ND
24	b	620	CLA	ND
24	b	621	CLA	ND
24	b	622	CLA	ND
24	b	623	CLA	ND
24	b	624	CLA	ND
24	b	625	CLA	ND
24	c	506	CLA	ND
24	c	507	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	c	515	CLA	ND
24	c	516	CLA	ND
24	c	517	CLA	ND
24	d	401	CLA	ND
24	d	402	CLA	ND
24	d	403	CLA	ND

All (1262) torsion outliers are listed below:

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Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CAD-CBD-CGD-O1D
24	B	602	CLA	CAD-CBD-CGD-O2D
24	B	603	CLA	C14-C13-C15-C16
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	C2-C3-C5-C6
24	B	615	CLA	C4-C3-C5-C6
24	C	507	CLA	C2B-C3B-CAB-CBB
24	C	507	CLA	C4B-C3B-CAB-CBB
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	C2-C1-O2A-CGA
24	b	614	CLA	C4-C3-C5-C6
24	b	623	CLA	CAD-CBD-CGD-O1D
24	b	623	CLA	CAD-CBD-CGD-O2D
24	c	512	CLA	CHA-CBD-CGD-O1D
24	c	512	CLA	CHA-CBD-CGD-O2D
24	c	517	CLA	C2B-C3B-CAB-CBB
24	c	517	CLA	C4B-C3B-CAB-CBB
26	D	404	BCR	C21-C22-C23-C24
26	Y	101	BCR	C1-C6-C7-C8
26	Y	101	BCR	C5-C6-C7-C8
26	d	404	BCR	C21-C22-C23-C24
26	d	404	BCR	C37-C22-C23-C24
26	y	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
27	A	416	SQD	O6-C44-C45-O47
27	B	621	SQD	O49-C7-O47-C45
27	B	621	SQD	C5-C6-S-O7
27	B	621	SQD	C5-C6-S-O9
27	F	103	SQD	O49-C7-O47-C45
27	F	103	SQD	C5-C6-S-O7
27	L	102	SQD	O5-C1-O6-C44
27	L	102	SQD	O49-C7-O47-C45
27	a	405	SQD	O6-C44-C45-O47
27	a	405	SQD	O5-C5-C6-S
27	f	101	SQD	O49-C7-O47-C45
27	f	101	SQD	C8-C7-O47-C45
27	f	101	SQD	C5-C6-S-O7
27	f	101	SQD	C5-C6-S-O8
27	f	101	SQD	C5-C6-S-O9

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Mol	Chain	Res	Type	Atoms
28	A	414	GOL	C1-C2-C3-O3
28	A	415	GOL	C1-C2-C3-O3
28	A	422	GOL	O1-C1-C2-C3
28	B	627	GOL	O1-C1-C2-C3
28	B	628	GOL	O1-C1-C2-C3
28	B	630	GOL	O1-C1-C2-C3
28	B	630	GOL	C1-C2-C3-O3
28	C	524	GOL	O1-C1-C2-C3
28	T	102	GOL	O1-C1-C2-O2
28	T	102	GOL	O1-C1-C2-C3
28	V	201	GOL	C1-C2-C3-O3
28	a	402	GOL	O1-C1-C2-C3
28	a	420	GOL	O1-C1-C2-C3
28	b	604	GOL	O1-C1-C2-C3
29	F	101	LMT	O5'-C1'-O1'-C1
29	M	103	LMT	O5'-C1'-O1'-C1
29	a	404	LMT	C2'-C1'-O1'-C1
29	a	404	LMT	O5'-C1'-O1'-C1
29	b	630	LMT	C2'-C1'-O1'-C1
31	a	415[B]	PL9	C12-C11-C9-C10
33	C	520	LMG	C11-C10-O7-C8
33	Z	101	LMG	O6-C1-O1-C7
33	Z	101	LMG	O9-C10-O7-C8
33	Z	101	LMG	C11-C10-O7-C8
33	z	101	LMG	O6-C1-O1-C7
33	z	101	LMG	O9-C10-O7-C8
35	B	624	HTG	C2'-C1'-S1-C1
35	B	625	HTG	O5-C1-S1-C1'
35	b	632	HTG	O5-C1-S1-C1'
36	D	406	DGD	C2B-C1B-O2G-C2G
36	e	101	DGD	C2B-C1B-O2G-C2G
36	e	101	DGD	O1B-C1B-O2G-C2G
36	e	101	DGD	O6E-C1E-O5D-C6D
37	D	408	LHG	C4-O6-P-O3
37	D	408	LHG	C4-O6-P-O4
37	E	101	LHG	C3-O3-P-O4
37	E	101	LHG	C3-O3-P-O5
37	E	101	LHG	C3-O3-P-O6
37	E	101	LHG	C4-O6-P-O5
37	L	101	LHG	C4-O6-P-O3
37	L	101	LHG	C4-O6-P-O4
37	L	101	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
37	b	634	LHG	C4-O6-P-O3
37	b	634	LHG	C4-O6-P-O4
37	d	407	LHG	C3-O3-P-O4
37	d	407	LHG	C3-O3-P-O6
37	e	102	LHG	C3-O3-P-O5
37	e	102	LHG	C3-O3-P-O6
38	F	102	HEM	C2B-C3B-CAB-CBB
38	F	102	HEM	C2C-C3C-CAC-CBC
40	V	205	HEC	C2B-C3B-CAB-CBB
40	V	205	HEC	C4B-C3B-CAB-CBB
40	V	205	HEC	C2C-C3C-CAC-CBC
40	V	205	HEC	C4C-C3C-CAC-CBC
40	v	205	HEC	C2B-C3B-CAB-CBB
40	v	205	HEC	C4B-C3B-CAB-CBB
40	v	205	HEC	C2C-C3C-CAC-CBC
40	v	205	HEC	C4C-C3C-CAC-CBC
29	C	521	LMT	C3'-C4'-O1B-C1B
29	D	401	LMT	C3'-C4'-O1B-C1B
37	e	102	LHG	O10-C23-O8-C6
37	E	101	LHG	O10-C23-O8-C6
33	C	520	LMG	O9-C10-O7-C8
36	D	406	DGD	O1B-C1B-O2G-C2G
24	A	410	CLA	C3-C5-C6-C7
24	B	617	CLA	C3-C5-C6-C7
24	b	623	CLA	C3-C5-C6-C7
37	E	101	LHG	C24-C23-O8-C6
37	e	102	LHG	C24-C23-O8-C6
27	B	621	SQD	C8-C7-O47-C45
27	F	103	SQD	C8-C7-O47-C45
27	L	102	SQD	C8-C7-O47-C45
33	z	101	LMG	C11-C10-O7-C8
24	B	606	CLA	C4-C3-C5-C6
24	b	623	CLA	C4-C3-C5-C6
31	a	415[A]	PL9	C12-C11-C9-C10
31	a	415[B]	PL9	C20-C19-C21-C22
24	B	606	CLA	C2-C3-C5-C6
24	b	614	CLA	C2-C3-C5-C6
24	b	623	CLA	C2-C3-C5-C6
31	a	415[B]	PL9	C18-C19-C21-C22
24	B	615	CLA	C3-C5-C6-C7
24	c	511	CLA	C3-C5-C6-C7
24	c	516	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	C	516	DGD	C2A-C3A-C4A-C5A
37	E	101	LHG	O2-C2-C3-O3
37	d	407	LHG	O2-C2-C3-O3
33	z	101	LMG	O6-C5-C6-O5
29	M	103	LMT	O5'-C5'-C6'-O6'
29	f	102	LMT	C4'-C5'-C6'-O6'
33	A	421	LMG	C11-C10-O7-C8
24	B	602	CLA	C3-C5-C6-C7
29	f	102	LMT	O5'-C5'-C6'-O6'
35	b	632	HTG	S1-C1'-C2'-C3'
31	A	419[A]	PL9	C25-C24-C26-C27
31	A	419[B]	PL9	C25-C24-C26-C27
31	a	415[A]	PL9	C15-C14-C16-C17
31	a	415[A]	PL9	C20-C19-C21-C22
31	a	415[B]	PL9	C15-C14-C16-C17
31	a	415[B]	PL9	C25-C24-C26-C27
31	A	419[A]	PL9	C23-C24-C26-C27
31	A	419[B]	PL9	C23-C24-C26-C27
31	a	415[A]	PL9	C13-C14-C16-C17
31	a	415[A]	PL9	C23-C24-C26-C27
31	a	415[B]	PL9	C13-C14-C16-C17
31	a	415[B]	PL9	C23-C24-C26-C27
33	C	520	LMG	O6-C5-C6-O5
31	D	405[A]	PL9	C39-C41-C42-C43
31	d	405[A]	PL9	C39-C41-C42-C43
31	d	405[B]	PL9	C39-C41-C42-C43
29	M	103	LMT	O5B-C5B-C6B-O6B
38	e	103	HEM	C3D-CAD-CBD-CGD
24	C	509	CLA	C3-C5-C6-C7
27	B	621	SQD	O5-C1-O6-C44
29	A	417	LMT	O5'-C1'-O1'-C1
29	B	635	LMT	O5'-C1'-O1'-C1
29	C	521	LMT	O5'-C1'-O1'-C1
29	T	104	LMT	O5'-C1'-O1'-C1
29	a	419	LMT	O5'-C1'-O1'-C1
29	b	630	LMT	O5'-C1'-O1'-C1
29	f	102	LMT	O5'-C1'-O1'-C1
36	D	406	DGD	O6D-C1D-O3G-C3G
33	z	101	LMG	C4-C5-C6-O5
29	M	101	LMT	O5B-C5B-C6B-O6B
24	C	509	CLA	O1A-CGA-O2A-C1
33	A	421	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
24	C	509	CLA	CBA-CGA-O2A-C1
29	M	103	LMT	C4'-C5'-C6'-O6'
31	a	415[A]	PL9	C25-C24-C26-C27
31	a	415[A]	PL9	C12-C11-C9-C8
24	B	602	CLA	C11-C10-C8-C9
24	B	617	CLA	C6-C7-C8-C9
24	C	501	CLA	C11-C12-C13-C14
24	b	619	CLA	C11-C12-C13-C14
24	c	511	CLA	C6-C7-C8-C9
24	c	514	CLA	C11-C10-C8-C9
29	A	417	LMT	C2'-C1'-O1'-C1
29	B	635	LMT	C2'-C1'-O1'-C1
29	C	521	LMT	C2'-C1'-O1'-C1
29	F	101	LMT	C2'-C1'-O1'-C1
29	T	104	LMT	C2'-C1'-O1'-C1
29	a	419	LMT	C2'-C1'-O1'-C1
29	f	102	LMT	C2'-C1'-O1'-C1
36	D	406	DGD	C2D-C1D-O3G-C3G
36	e	101	DGD	C2E-C1E-O5D-C6D
29	m	103	LMT	O5'-C5'-C6'-O6'
26	D	404	BCR	C37-C22-C23-C24
35	V	206	HTG	S1-C1'-C2'-C3'
33	Z	101	LMG	C10-C11-C12-C13
29	D	401	LMT	O5B-C5B-C6B-O6B
24	B	615	CLA	C5-C6-C7-C8
24	b	610	CLA	C2-C1-O2A-CGA
24	B	602	CLA	C10-C11-C12-C13
24	B	615	CLA	C8-C10-C11-C12
28	B	627	GOL	O1-C1-C2-O2
28	V	202	GOL	O1-C1-C2-O2
28	a	402	GOL	O1-C1-C2-O2
28	a	420	GOL	O1-C1-C2-O2
28	b	605	GOL	O1-C1-C2-O2
28	v	203	GOL	O1-C1-C2-O2
29	M	101	LMT	C4B-C5B-C6B-O6B
24	b	615	CLA	C12-C13-C15-C16
35	B	625	HTG	O5-C5-C6-O6
24	B	616	CLA	C8-C10-C11-C12
33	c	501	LMG	C17-C18-C19-C20
27	A	416	SQD	C23-C24-C25-C26
27	B	621	SQD	C7-C8-C9-C10
33	C	520	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
33	c	523	LMG	C10-C11-C12-C13
36	c	522	DGD	C1A-C2A-C3A-C4A
24	C	501	CLA	C15-C16-C17-C18
24	b	624	CLA	C10-C11-C12-C13
29	A	417	LMT	O5B-C5B-C6B-O6B
24	C	508	CLA	C10-C11-C12-C13
33	B	622	LMG	C15-C16-C17-C18
36	e	101	DGD	O6D-C1D-O3G-C3G
24	A	410	CLA	C13-C15-C16-C17
24	B	615	CLA	C10-C11-C12-C13
24	c	513	CLA	C15-C16-C17-C18
33	c	501	LMG	C10-C11-C12-C13
29	T	104	LMT	O1'-C1-C2-C3
24	c	516	CLA	O1D-CGD-O2D-CED
33	C	520	LMG	C4-C5-C6-O5
24	b	623	CLA	C5-C6-C7-C8
24	C	508	CLA	C5-C6-C7-C8
24	a	412	CLA	C8-C10-C11-C12
37	E	101	LHG	C1-C2-C3-O3
24	B	607	CLA	C2A-CAA-CBA-CGA
24	b	615	CLA	C2A-CAA-CBA-CGA
35	c	525	HTG	C1'-C2'-C3'-C4'
24	C	506	CLA	C5-C6-C7-C8
24	C	506	CLA	C13-C15-C16-C17
24	c	514	CLA	C13-C15-C16-C17
35	b	632	HTG	O5-C5-C6-O6
35	c	525	HTG	S1-C1'-C2'-C3'
24	B	617	CLA	C10-C11-C12-C13
24	C	504	CLA	C15-C16-C17-C18
24	b	615	CLA	C13-C15-C16-C17
31	a	415[A]	PL9	C30-C29-C31-C32
24	b	623	CLA	C13-C15-C16-C17
24	D	403	CLA	C3-C5-C6-C7
33	c	523	LMG	C11-C10-O7-C8
35	C	523	HTG	O5-C5-C6-O6
29	M	103	LMT	C4B-C5B-C6B-O6B
27	A	416	SQD	C2-C1-O6-C44
29	D	401	LMT	C2'-C1'-O1'-C1
29	m	102	LMT	C2'-C1'-O1'-C1
36	C	517	DGD	C2E-C1E-O5D-C6D
36	c	521	DGD	C2E-C1E-O5D-C6D
36	e	101	DGD	C2D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
24	b	610	CLA	C8-C10-C11-C12
31	a	415[A]	PL9	C9-C11-C12-C13
31	a	415[B]	PL9	C9-C11-C12-C13
35	b	601	HTG	C1'-C2'-C3'-C4'
35	b	632	HTG	C1'-C2'-C3'-C4'
27	A	416	SQD	C26-C27-C28-C29
37	e	102	LHG	C11-C12-C13-C14
37	D	407	LHG	C23-C24-C25-C26
26	D	404	BCR	C7-C8-C9-C34
36	c	520	DGD	O6D-C5D-C6D-O5D
24	c	514	CLA	C15-C16-C17-C18
28	B	626	GOL	C1-C2-C3-O3
28	B	629	GOL	O1-C1-C2-C3
28	V	202	GOL	O1-C1-C2-C3
28	b	605	GOL	O1-C1-C2-C3
28	o	301	GOL	O1-C1-C2-C3
28	o	301	GOL	C1-C2-C3-O3
28	v	201	GOL	O1-C1-C2-C3
28	v	203	GOL	O1-C1-C2-C3
37	D	407	LHG	O1-C1-C2-C3
27	F	103	SQD	C26-C27-C28-C29
24	a	412	CLA	C16-C17-C18-C19
24	b	623	CLA	C16-C17-C18-C19
29	m	102	LMT	O5'-C5'-C6'-O6'
33	c	523	LMG	O9-C10-O7-C8
29	m	102	LMT	O5'-C1'-O1'-C1
24	c	509	CLA	C15-C16-C17-C18
31	a	415[A]	PL9	C18-C19-C21-C22
37	D	408	LHG	C32-C33-C34-C35
33	d	413	LMG	O6-C5-C6-O5
27	L	102	SQD	C24-C23-O48-C46
29	a	404	LMT	C4B-C5B-C6B-O6B
24	B	617	CLA	C2-C1-O2A-CGA
24	c	514	CLA	C2-C1-O2A-CGA
24	a	412	CLA	C10-C11-C12-C13
24	c	518	CLA	C10-C11-C12-C13
27	A	416	SQD	C30-C31-C32-C33
29	T	104	LMT	C11-C10-C9-C8
27	A	412	SQD	C9-C10-C11-C12
29	M	103	LMT	C2-C3-C4-C5
33	A	421	LMG	C14-C15-C16-C17
35	B	624	HTG	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
36	C	516	DGD	C4B-C5B-C6B-C7B
36	C	517	DGD	C9A-CAA-CBA-CCA
36	D	406	DGD	C6A-C7A-C8A-C9A
29	T	104	LMT	C1-C2-C3-C4
27	B	621	SQD	C30-C31-C32-C33
36	H	102	DGD	CBB-CCB-CDB-CEB
37	e	102	LHG	C24-C25-C26-C27
28	A	414	GOL	O2-C2-C3-O3
28	B	628	GOL	O1-C1-C2-O2
28	B	630	GOL	O1-C1-C2-O2
28	B	630	GOL	O2-C2-C3-O3
28	v	201	GOL	O1-C1-C2-O2
24	c	514	CLA	C3-C5-C6-C7
24	C	502	CLA	C4B-C3B-CAB-CBB
24	C	512	CLA	C4B-C3B-CAB-CBB
24	b	616	CLA	C4B-C3B-CAB-CBB
24	b	618	CLA	C4B-C3B-CAB-CBB
24	c	507	CLA	C4B-C3B-CAB-CBB
24	d	402	CLA	C4B-C3B-CAB-CBB
29	T	104	LMT	C4-C5-C6-C7
33	B	622	LMG	C29-C30-C31-C32
33	d	413	LMG	C17-C18-C19-C20
24	b	620	CLA	C16-C17-C18-C19
29	B	635	LMT	C3-C4-C5-C6
36	C	518	DGD	CAA-CBA-CCA-CDA
36	c	521	DGD	C9A-CAA-CBA-CCA
24	B	614	CLA	C13-C15-C16-C17
24	B	616	CLA	C11-C12-C13-C15
33	c	501	LMG	C21-C22-C23-C24
33	c	523	LMG	C34-C35-C36-C37
36	c	521	DGD	C4A-C5A-C6A-C7A
27	L	102	SQD	C27-C28-C29-C30
36	c	522	DGD	C6A-C7A-C8A-C9A
26	t	101	BCR	C13-C14-C15-C16
24	a	412	CLA	C16-C17-C18-C20
29	C	521	LMT	O5B-C5B-C6B-O6B
36	C	516	DGD	C3B-C4B-C5B-C6B
36	c	520	DGD	C5A-C6A-C7A-C8A
35	B	632	HTG	C4-C5-C6-O6
33	C	519	LMG	C11-C12-C13-C14
36	e	101	DGD	CCA-CDA-CEA-CFA
37	e	102	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	L	102	SQD	C12-C13-C14-C15
36	C	516	DGD	C5B-C6B-C7B-C8B
36	c	522	DGD	C7B-C8B-C9B-CAB
37	L	101	LHG	C14-C15-C16-C17
36	h	102	DGD	C4E-C5E-C6E-O5E
27	a	414	SQD	C11-C12-C13-C14
33	b	629	LMG	C32-C33-C34-C35
36	c	520	DGD	C9A-CAA-CBA-CCA
35	C	523	HTG	S1-C1'-C2'-C3'
36	c	522	DGD	CBA-CCA-CDA-CEA
24	b	623	CLA	C16-C17-C18-C20
24	b	624	CLA	C16-C17-C18-C19
24	b	618	CLA	C2B-C3B-CAB-CBB
26	B	618	BCR	C1-C6-C7-C8
35	b	631	HTG	C2'-C3'-C4'-C5'
24	C	511	CLA	CBA-CGA-O2A-C1
24	c	511	CLA	C15-C16-C17-C18
33	z	101	LMG	C15-C16-C17-C18
36	D	406	DGD	C2A-C3A-C4A-C5A
36	e	101	DGD	C8B-C9B-CAB-CBB
36	e	101	DGD	O6D-C5D-C6D-O5D
38	e	103	HEM	C2A-CAA-CBA-CGA
37	D	409	LHG	C29-C30-C31-C32
37	d	406	LHG	C32-C33-C34-C35
24	C	511	CLA	O1A-CGA-O2A-C1
27	L	102	SQD	O10-C23-O48-C46
36	h	102	DGD	CAA-CBA-CCA-CDA
24	c	515	CLA	C4-C3-C5-C6
33	c	501	LMG	C14-C15-C16-C17
33	d	413	LMG	C36-C37-C38-C39
33	z	101	LMG	C12-C13-C14-C15
31	a	415[B]	PL9	C12-C11-C9-C8
27	a	414	SQD	C29-C30-C31-C32
37	D	407	LHG	C34-C35-C36-C37
37	D	409	LHG	C24-C25-C26-C27
36	e	101	DGD	C2A-C1A-O1G-C1G
24	b	610	CLA	C11-C10-C8-C9
29	T	104	LMT	C7-C8-C9-C10
33	D	413	LMG	C19-C20-C21-C22
33	Z	101	LMG	C19-C20-C21-C22
27	A	416	SQD	O5-C1-O6-C44
29	D	401	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
36	C	517	DGD	O6E-C1E-O5D-C6D
36	c	521	DGD	O6E-C1E-O5D-C6D
36	c	520	DGD	C4D-C5D-C6D-O5D
33	A	421	LMG	C11-C12-C13-C14
27	F	103	SQD	C2-C1-O6-C44
33	Z	101	LMG	C2-C1-O1-C7
29	C	521	LMT	O5'-C5'-C6'-O6'
33	b	629	LMG	C38-C39-C40-C41
36	c	522	DGD	C7A-C8A-C9A-CAA
36	c	522	DGD	C6B-C7B-C8B-C9B
27	B	621	SQD	C24-C23-O48-C46
24	c	515	CLA	C8-C10-C11-C12
37	D	407	LHG	C24-C25-C26-C27
33	d	413	LMG	C19-C20-C21-C22
24	b	624	CLA	C16-C17-C18-C20
37	E	101	LHG	C24-C25-C26-C27
31	d	405[B]	PL9	C13-C14-C16-C17
38	e	103	HEM	C2C-C3C-CAC-CBC
29	A	417	LMT	C6-C7-C8-C9
24	a	412	CLA	C15-C16-C17-C18
36	c	520	DGD	C8B-C9B-CAB-CBB
36	e	101	DGD	C2A-C3A-C4A-C5A
27	a	414	SQD	C9-C10-C11-C12
37	d	408	LHG	C29-C30-C31-C32
24	B	602	CLA	C8-C10-C11-C12
24	B	616	CLA	C5-C6-C7-C8
27	A	412	SQD	C13-C14-C15-C16
24	c	517	CLA	CBA-CGA-O2A-C1
33	B	622	LMG	C36-C37-C38-C39
37	d	406	LHG	C29-C30-C31-C32
38	F	102	HEM	C4B-C3B-CAB-CBB
38	F	102	HEM	C4C-C3C-CAC-CBC
24	b	620	CLA	C16-C17-C18-C20
27	A	412	SQD	C14-C15-C16-C17
36	c	520	DGD	O6E-C5E-C6E-O5E
36	C	517	DGD	C4B-C5B-C6B-C7B
24	c	517	CLA	C15-C16-C17-C18
24	C	512	CLA	CBA-CGA-O2A-C1
27	B	621	SQD	C31-C32-C33-C34
27	L	102	SQD	C31-C32-C33-C34
29	a	404	LMT	C2-C3-C4-C5
27	a	405	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
33	A	421	LMG	C30-C31-C32-C33
31	d	405[B]	PL9	C43-C44-C46-C47
33	B	622	LMG	C31-C32-C33-C34
27	L	102	SQD	C29-C30-C31-C32
29	B	635	LMT	C7-C8-C9-C10
29	a	419	LMT	C6-C7-C8-C9
36	H	102	DGD	C7A-C8A-C9A-CAA
36	c	520	DGD	CAB-CBB-CCB-CDB
27	a	405	SQD	C31-C32-C33-C34
24	b	619	CLA	C16-C17-C18-C20
28	A	415	GOL	O2-C2-C3-O3
28	A	422	GOL	O1-C1-C2-O2
28	C	524	GOL	O1-C1-C2-O2
28	V	201	GOL	O2-C2-C3-O3
35	B	632	HTG	C2'-C3'-C4'-C5'
24	C	506	CLA	C1A-C2A-CAA-CBA
24	b	613	CLA	C13-C15-C16-C17
33	d	413	LMG	C35-C36-C37-C38
36	C	516	DGD	O6E-C5E-C6E-O5E
36	e	101	DGD	C5A-C6A-C7A-C8A
37	b	634	LHG	C27-C28-C29-C30
33	Z	101	LMG	O6-C5-C6-O5
24	B	602	CLA	C11-C10-C8-C7
24	B	615	CLA	C12-C13-C15-C16
24	C	512	CLA	C11-C10-C8-C7
24	b	610	CLA	C6-C7-C8-C10
24	b	623	CLA	C11-C12-C13-C15
24	c	511	CLA	C6-C7-C8-C10
24	C	512	CLA	O1A-CGA-O2A-C1
24	c	517	CLA	O1A-CGA-O2A-C1
36	e	101	DGD	O1A-C1A-O1G-C1G
36	C	517	DGD	C8A-C9A-CAA-CBA
27	B	621	SQD	C35-C36-C37-C38
31	D	405[A]	PL9	C15-C14-C16-C17
31	D	405[B]	PL9	C15-C14-C16-C17
24	c	515	CLA	C2-C3-C5-C6
37	b	634	LHG	C33-C34-C35-C36
24	B	616	CLA	C14-C13-C15-C16
24	a	410	CLA	C14-C13-C15-C16
24	b	610	CLA	C6-C7-C8-C9
24	b	623	CLA	C11-C12-C13-C14
24	c	511	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	c	514	CLA	C6-C7-C8-C9
35	b	631	HTG	C3'-C4'-C5'-C6'
29	a	404	LMT	O5B-C5B-C6B-O6B
29	B	635	LMT	C11-C10-C9-C8
24	B	602	CLA	CBA-CGA-O2A-C1
27	L	102	SQD	C24-C25-C26-C27
27	A	416	SQD	O6-C44-C45-C46
27	B	621	SQD	C44-C45-C46-O48
27	F	103	SQD	C44-C45-C46-O48
27	a	405	SQD	O6-C44-C45-C46
33	c	501	LMG	C7-C8-C9-O8
36	D	406	DGD	O1G-C1G-C2G-C3G
36	e	101	DGD	O1G-C1G-C2G-C3G
37	E	101	LHG	C4-C5-C6-O8
24	b	623	CLA	CBD-CGD-O2D-CED
29	B	635	LMT	C2-C3-C4-C5
29	f	102	LMT	C5-C6-C7-C8
33	b	629	LMG	C33-C34-C35-C36
33	c	501	LMG	C29-C30-C31-C32
29	b	630	LMT	C3'-C4'-O1B-C1B
36	C	516	DGD	O6D-C5D-C6D-O5D
27	B	621	SQD	O10-C23-O48-C46
24	c	509	CLA	C4-C3-C5-C6
31	D	405[A]	PL9	C13-C14-C16-C17
31	a	415[A]	PL9	C28-C29-C31-C32
36	D	406	DGD	C8B-C9B-CAB-CBB
33	D	413	LMG	O6-C5-C6-O5
26	D	404	BCR	C7-C8-C9-C10
24	B	604	CLA	C5-C6-C7-C8
24	c	512	CLA	C5-C6-C7-C8
27	L	102	SQD	C35-C36-C37-C38
24	b	612	CLA	C5-C6-C7-C8
33	A	421	LMG	C10-C11-C12-C13
24	B	602	CLA	O1A-CGA-O2A-C1
27	L	102	SQD	C30-C31-C32-C33
33	c	501	LMG	C33-C34-C35-C36
24	b	610	CLA	CBA-CGA-O2A-C1
37	d	408	LHG	C31-C32-C33-C34
29	A	417	LMT	O1'-C1-C2-C3
27	F	103	SQD	C31-C32-C33-C34
27	a	414	SQD	C15-C16-C17-C18
36	h	102	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
37	D	407	LHG	C25-C26-C27-C28
27	A	412	SQD	C18-C19-C20-C21
37	d	407	LHG	C1-C2-C3-O3
24	a	412	CLA	CBA-CGA-O2A-C1
24	c	516	CLA	CBA-CGA-O2A-C1
29	a	404	LMT	C3-C4-C5-C6
36	c	520	DGD	C7B-C8B-C9B-CAB
36	h	102	DGD	C5B-C6B-C7B-C8B
27	L	102	SQD	C32-C33-C34-C35
31	d	405[B]	PL9	C15-C14-C16-C17
24	C	510	CLA	C2-C3-C5-C6
27	A	416	SQD	C11-C12-C13-C14
33	d	413	LMG	C38-C39-C40-C41
24	B	611	CLA	C16-C17-C18-C20
24	b	619	CLA	C16-C17-C18-C19
35	b	601	HTG	C2'-C3'-C4'-C5'
36	D	406	DGD	C1B-C2B-C3B-C4B
29	m	102	LMT	C1-C2-C3-C4
27	f	101	SQD	O6-C44-C45-O47
33	Z	101	LMG	O1-C7-C8-O7
27	a	405	SQD	C28-C29-C30-C31
37	d	406	LHG	C25-C26-C27-C28
36	c	522	DGD	C2A-C1A-O1G-C1G
29	C	521	LMT	C9-C10-C11-C12
36	c	521	DGD	C2B-C3B-C4B-C5B
37	E	101	LHG	C10-C11-C12-C13
24	C	512	CLA	C3-C5-C6-C7
33	A	421	LMG	C13-C14-C15-C16
33	A	421	LMG	C36-C37-C38-C39
36	H	102	DGD	CDB-CEB-CFB-CGB
37	E	101	LHG	C19-C20-C21-C22
36	H	102	DGD	CDA-CEA-CFA-CGA
29	a	404	LMT	C7-C8-C9-C10
33	C	520	LMG	C11-C12-C13-C14
33	b	629	LMG	C40-C41-C42-C43
27	L	102	SQD	C28-C29-C30-C31
27	A	416	SQD	C24-C23-O48-C46
37	D	409	LHG	C24-C23-O8-C6
27	B	621	SQD	C11-C10-C9-C8
33	C	519	LMG	C14-C15-C16-C17
36	C	517	DGD	CAB-CBB-CCB-CDB
37	L	101	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
28	b	604	GOL	O1-C1-C2-O2
28	c	503	GOL	O1-C1-C2-O2
28	o	301	GOL	O1-C1-C2-O2
24	B	615	CLA	C14-C13-C15-C16
24	C	512	CLA	C11-C10-C8-C9
24	b	615	CLA	C14-C13-C15-C16
37	D	409	LHG	C12-C13-C14-C15
24	a	410	CLA	C10-C11-C12-C13
24	b	623	CLA	C10-C11-C12-C13
36	e	101	DGD	C4D-C5D-C6D-O5D
24	A	410	CLA	C4B-C3B-CAB-CBB
24	B	608	CLA	C4B-C3B-CAB-CBB
24	b	611	CLA	C4B-C3B-CAB-CBB
24	c	506	CLA	C4B-C3B-CAB-CBB
24	c	512	CLA	C4B-C3B-CAB-CBB
24	d	403	CLA	C4B-C3B-CAB-CBB
36	D	406	DGD	C7A-C8A-C9A-CAA
37	D	408	LHG	C26-C27-C28-C29
24	B	612	CLA	C15-C16-C17-C18
27	F	103	SQD	C30-C31-C32-C33
37	e	102	LHG	O6-C4-C5-C6
33	z	101	LMG	C13-C14-C15-C16
24	B	616	CLA	C12-C13-C15-C16
24	c	511	CLA	C11-C10-C8-C7
24	c	514	CLA	C6-C7-C8-C10
24	c	517	CLA	C11-C10-C8-C7
36	h	102	DGD	O6E-C5E-C6E-O5E
33	c	501	LMG	C35-C36-C37-C38
35	B	625	HTG	C3'-C4'-C5'-C6'
24	C	513	CLA	C3A-C2A-CAA-CBA
31	a	415[A]	PL9	C45-C44-C46-C47
33	d	413	LMG	C13-C14-C15-C16
24	a	412	CLA	O1A-CGA-O2A-C1
24	c	516	CLA	O1A-CGA-O2A-C1
37	D	409	LHG	C28-C29-C30-C31
33	C	519	LMG	C29-C28-O8-C9
36	C	518	DGD	C2A-C1A-O1G-C1G
26	T	103	BCR	C13-C14-C15-C16
29	F	101	LMT	O1'-C1-C2-C3
33	b	629	LMG	C39-C40-C41-C42
36	C	517	DGD	C5A-C6A-C7A-C8A
33	C	519	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
27	L	102	SQD	C44-C45-C46-O48
33	A	421	LMG	C7-C8-C9-O8
33	Z	101	LMG	C7-C8-C9-O8
33	c	523	LMG	O1-C7-C8-C9
33	c	523	LMG	C7-C8-C9-O8
37	e	102	LHG	C4-C5-C6-O8
24	B	611	CLA	C16-C17-C18-C19
33	C	519	LMG	C30-C31-C32-C33
33	d	413	LMG	C29-C30-C31-C32
31	d	405[B]	PL9	C45-C44-C46-C47
24	A	410	CLA	CBA-CGA-O2A-C1
24	b	610	CLA	O1A-CGA-O2A-C1
29	B	635	LMT	C4-C5-C6-C7
27	a	405	SQD	C23-C24-C25-C26
37	e	102	LHG	O6-C4-C5-O7
26	B	618	BCR	C5-C6-C7-C8
26	b	626	BCR	C1-C6-C7-C8
26	d	404	BCR	C23-C24-C25-C30
27	F	103	SQD	C34-C35-C36-C37
36	C	516	DGD	C4D-C5D-C6D-O5D
24	c	514	CLA	C10-C11-C12-C13
27	A	416	SQD	C24-C25-C26-C27
36	e	101	DGD	CAA-CBA-CCA-CDA
36	h	102	DGD	O2G-C1B-C2B-C3B
27	a	414	SQD	O6-C44-C45-O47
33	Z	101	LMG	O7-C8-C9-O8
36	D	406	DGD	O2G-C2G-C3G-O3G
31	A	419[A]	PL9	C4-C3-C7-C8
31	A	419[B]	PL9	C4-C3-C7-C8
31	a	415[A]	PL9	C4-C3-C7-C8
31	a	415[B]	PL9	C4-C3-C7-C8
36	c	521	DGD	C3B-C4B-C5B-C6B
24	C	510	CLA	C4-C3-C5-C6
25	A	408	PHO	C4-C3-C5-C6
31	d	405[A]	PL9	C45-C44-C46-C47
24	B	614	CLA	C15-C16-C17-C18
24	c	509	CLA	C2-C3-C5-C6
25	A	408	PHO	C2-C3-C5-C6
31	D	405[B]	PL9	C13-C14-C16-C17
27	a	414	SQD	C34-C35-C36-C37
33	d	413	LMG	C14-C15-C16-C17
31	A	419[A]	PL9	C2-C3-C7-C8

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Mol	Chain	Res	Type	Atoms
33	b	629	LMG	C37-C38-C39-C40
36	e	101	DGD	C4A-C5A-C6A-C7A
24	b	613	CLA	CBD-CGD-O2D-CED
24	B	612	CLA	C14-C13-C15-C16
24	c	514	CLA	C11-C12-C13-C14
24	c	517	CLA	C11-C10-C8-C9
35	B	625	HTG	C4-C5-C6-O6
36	C	517	DGD	C4A-C5A-C6A-C7A
25	a	411	PHO	C2C-C3C-CAC-CBC
27	A	412	SQD	C15-C16-C17-C18
27	f	101	SQD	C24-C25-C26-C27
33	c	501	LMG	C12-C13-C14-C15
37	d	406	LHG	C11-C10-C9-C8
24	C	513	CLA	C3-C5-C6-C7
29	a	404	LMT	C6-C7-C8-C9
37	d	407	LHG	C34-C35-C36-C37
24	b	625	CLA	C10-C11-C12-C13
31	D	405[B]	PL9	C9-C11-C12-C13
27	L	102	SQD	C11-C12-C13-C14
36	C	518	DGD	CDA-CEA-CFA-CGA
35	b	601	HTG	C3'-C4'-C5'-C6'
28	a	401	GOL	O2-C2-C3-O3
28	v	202	GOL	O1-C1-C2-O2
37	D	407	LHG	O1-C1-C2-O2
24	C	510	CLA	CBA-CGA-O2A-C1
24	b	625	CLA	C4-C3-C5-C6
31	A	419[A]	PL9	C15-C14-C16-C17
35	b	607	HTG	C4'-C5'-C6'-C7'
31	D	405[B]	PL9	C28-C29-C31-C32
31	d	405[A]	PL9	C43-C44-C46-C47
36	h	102	DGD	CDB-CEB-CFB-CGB
24	A	405	CLA	C13-C15-C16-C17
37	D	409	LHG	O10-C23-O8-C6
36	e	101	DGD	C2B-C3B-C4B-C5B
26	d	404	BCR	C7-C8-C9-C34
27	F	103	SQD	C32-C33-C34-C35
36	c	520	DGD	CBA-CCA-CDA-CEA
29	C	521	LMT	O1'-C1-C2-C3
24	B	612	CLA	C12-C13-C15-C16
24	B	617	CLA	C6-C7-C8-C10
36	c	521	DGD	C6A-C7A-C8A-C9A
33	c	523	LMG	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
33	b	629	LMG	C30-C31-C32-C33
26	d	404	BCR	C7-C8-C9-C10
33	C	519	LMG	C29-C30-C31-C32
33	C	519	LMG	O10-C28-O8-C9
36	c	522	DGD	O1A-C1A-O1G-C1G
27	B	621	SQD	C5-C6-S-O8
27	F	103	SQD	C5-C6-S-O8
33	C	520	LMG	C8-C7-O1-C1
36	c	521	DGD	C2G-C3G-O3G-C1D
36	c	521	DGD	C5D-C6D-O5D-C1E
24	D	403	CLA	C8-C10-C11-C12
24	b	623	CLA	C15-C16-C17-C18
37	E	101	LHG	C8-C7-O7-C5
36	H	102	DGD	O2G-C1B-C2B-C3B
24	A	410	CLA	O1A-CGA-O2A-C1
24	C	510	CLA	O1A-CGA-O2A-C1
31	a	415[A]	PL9	C43-C44-C46-C47
38	e	103	HEM	C2B-C3B-CAB-CBB
28	v	202	GOL	O1-C1-C2-C3
35	d	411	HTG	C4-C5-C6-O6
27	A	416	SQD	O10-C23-O48-C46
33	A	421	LMG	C12-C13-C14-C15
36	C	518	DGD	C8A-C9A-CAA-CBA
36	c	522	DGD	C5B-C6B-C7B-C8B
27	a	414	SQD	C27-C28-C29-C30
36	C	518	DGD	O1A-C1A-O1G-C1G
24	C	503	CLA	C8-C10-C11-C12
24	c	508	CLA	C8-C10-C11-C12
24	b	610	CLA	CAA-CBA-CGA-O2A
27	F	103	SQD	O5-C1-O6-C44
27	a	414	SQD	O6-C44-C45-C46
31	D	405[B]	PL9	C39-C41-C42-C43
31	a	415[A]	PL9	C39-C41-C42-C43
33	A	421	LMG	O1-C7-C8-C9
33	z	101	LMG	O1-C7-C8-C9
37	L	101	LHG	C7-C8-C9-C10
24	b	610	CLA	C10-C11-C12-C13
24	C	509	CLA	C16-C17-C18-C19
24	c	507	CLA	C16-C17-C18-C19
29	m	103	LMT	C1-C2-C3-C4
37	D	409	LHG	C25-C26-C27-C28
31	A	419[B]	PL9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
31	D	405[A]	PL9	C45-C44-C46-C47
31	D	405[B]	PL9	C45-C44-C46-C47
24	b	625	CLA	C2-C3-C5-C6
37	e	102	LHG	C14-C15-C16-C17
29	D	401	LMT	O5B-C1B-O1B-C4'
29	f	102	LMT	C4-C5-C6-C7
27	L	102	SQD	O47-C45-C46-O48
33	c	501	LMG	O7-C8-C9-O8
33	c	523	LMG	O1-C7-C8-O7
33	c	523	LMG	O7-C8-C9-O8
36	D	406	DGD	O1G-C1G-C2G-O2G
37	E	101	LHG	O7-C5-C6-O8
37	e	102	LHG	O7-C5-C6-O8
24	d	403	CLA	C15-C16-C17-C18
24	b	623	CLA	C11-C10-C8-C9
24	B	616	CLA	C16-C17-C18-C20
27	f	101	SQD	C31-C32-C33-C34
33	A	421	LMG	C32-C33-C34-C35
33	d	413	LMG	C16-C17-C18-C19
27	F	103	SQD	C7-C8-C9-C10
33	C	520	LMG	C16-C17-C18-C19
35	B	632	HTG	O5-C5-C6-O6
36	h	102	DGD	C9B-CAB-CBB-CCB
27	a	405	SQD	C19-C20-C21-C22
27	a	414	SQD	C35-C36-C37-C38
33	c	524	LMG	O6-C5-C6-O5
24	c	512	CLA	C4-C3-C5-C6
33	c	524	LMG	C10-C11-C12-C13
31	A	419[A]	PL9	C13-C14-C16-C17
24	b	614	CLA	C8-C10-C11-C12
24	b	617	CLA	C13-C15-C16-C17
36	c	520	DGD	C3A-C4A-C5A-C6A
37	E	101	LHG	C15-C16-C17-C18
37	d	406	LHG	C33-C34-C35-C36
27	a	414	SQD	C19-C20-C21-C22
24	C	509	CLA	CBD-CGD-O2D-CED
33	B	622	LMG	C16-C17-C18-C19
28	O	301	GOL	O1-C1-C2-O2
29	M	103	LMT	C2-C1-O1'-C1'
31	D	405[A]	PL9	C9-C11-C12-C13
24	B	616	CLA	C4B-C3B-CAB-CBB
24	C	505	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	c	513	CLA	C1A-C2A-CAA-CBA
33	c	523	LMG	C39-C40-C41-C42
36	c	522	DGD	C2A-C3A-C4A-C5A
36	C	516	DGD	C1B-C2B-C3B-C4B
36	H	102	DGD	C3B-C4B-C5B-C6B
29	C	521	LMT	C1-C2-C3-C4
24	A	407	CLA	C11-C10-C8-C7
24	a	410	CLA	C11-C10-C8-C7
24	d	402	CLA	C11-C12-C13-C15
24	B	616	CLA	C16-C17-C18-C19
37	D	408	LHG	O2-C2-C3-O3
27	B	621	SQD	C17-C18-C19-C20
27	a	405	SQD	C29-C30-C31-C32
29	m	103	LMT	C11-C10-C9-C8
37	E	101	LHG	C25-C26-C27-C28
37	d	406	LHG	C30-C31-C32-C33
29	D	401	LMT	C4B-C5B-C6B-O6B
36	e	101	DGD	C6A-C7A-C8A-C9A
33	D	413	LMG	C13-C14-C15-C16
37	D	409	LHG	C2-C3-O3-P
37	d	408	LHG	C2-C3-O3-P
36	C	517	DGD	CBB-CCB-CDB-CEB
37	E	101	LHG	O9-C7-O7-C5
24	c	515	CLA	CBA-CGA-O2A-C1
33	c	523	LMG	C36-C37-C38-C39
24	B	613	CLA	C8-C10-C11-C12
24	b	621	CLA	C8-C10-C11-C12
36	C	518	DGD	C9A-CAA-CBA-CCA
27	A	416	SQD	O5-C5-C6-S
27	F	103	SQD	O47-C45-C46-O48
33	A	421	LMG	O1-C7-C8-O7
33	z	101	LMG	O1-C7-C8-O7
36	e	101	DGD	O1G-C1G-C2G-O2G
37	E	101	LHG	C23-C24-C25-C26
37	b	634	LHG	C10-C11-C12-C13
27	f	101	SQD	O6-C44-C45-C46
33	Z	101	LMG	O1-C7-C8-C9
24	B	606	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
24	b	610	CLA	CAD-CBD-CGD-O2D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	c	507	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	c	509	CLA	CAD-CBD-CGD-O2D
24	c	511	CLA	CAD-CBD-CGD-O2D
24	a	409	CLA	C2C-C3C-CAC-CBC
29	m	102	LMT	C5-C6-C7-C8
33	c	501	LMG	C31-C32-C33-C34
24	c	515	CLA	O1A-CGA-O2A-C1
27	B	621	SQD	C12-C13-C14-C15
37	d	408	LHG	C30-C31-C32-C33
27	a	414	SQD	C30-C31-C32-C33
27	L	102	SQD	C11-C10-C9-C8
35	V	206	HTG	C2'-C3'-C4'-C5'
36	e	101	DGD	C7B-C8B-C9B-CAB
24	B	606	CLA	CAD-CBD-CGD-O1D
24	B	610	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	b	610	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O1D
24	c	507	CLA	CAD-CBD-CGD-O1D
24	c	511	CLA	CAD-CBD-CGD-O1D
24	c	514	CLA	CHA-CBD-CGD-O1D
24	c	514	CLA	CHA-CBD-CGD-O2D
26	h	101	BCR	C9-C10-C11-C12
37	D	408	LHG	C4-O6-P-O5
37	b	634	LHG	C4-O6-P-O5
24	C	502	CLA	C3-C5-C6-C7
29	m	103	LMT	C4'-C5'-C6'-O6'
27	A	412	SQD	C16-C17-C18-C19
31	a	415[B]	PL9	C45-C44-C46-C47
24	C	502	CLA	C2B-C3B-CAB-CBB
24	C	505	CLA	C2B-C3B-CAB-CBB
24	C	512	CLA	C2B-C3B-CAB-CBB
24	b	616	CLA	C2B-C3B-CAB-CBB
24	c	507	CLA	C2B-C3B-CAB-CBB
24	d	402	CLA	C2B-C3B-CAB-CBB
27	a	405	SQD	C27-C28-C29-C30
29	m	103	LMT	C2-C3-C4-C5
36	D	406	DGD	C3B-C4B-C5B-C6B
37	d	407	LHG	O10-C23-O8-C6
36	H	102	DGD	CCA-CDA-CEA-CFA
28	B	626	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
28	B	629	GOL	O1-C1-C2-O2
28	a	420	GOL	O2-C2-C3-O3
28	o	301	GOL	O2-C2-C3-O3
24	C	509	CLA	C10-C11-C12-C13
37	b	634	LHG	C17-C18-C19-C20
27	a	405	SQD	C24-C25-C26-C27
24	C	509	CLA	C8-C10-C11-C12
27	B	621	SQD	C46-C45-O47-C7
27	L	102	SQD	C46-C45-O47-C7
24	d	401	CLA	C2C-C3C-CAC-CBC
33	C	520	LMG	C15-C16-C17-C18
31	a	415[A]	PL9	C14-C16-C17-C18
24	C	509	CLA	C13-C15-C16-C17
37	D	407	LHG	C17-C18-C19-C20
24	b	610	CLA	C16-C17-C18-C20
27	a	405	SQD	C35-C36-C37-C38
24	B	616	CLA	C11-C12-C13-C14
24	c	514	CLA	C11-C10-C8-C7
37	d	408	LHG	C33-C34-C35-C36
33	A	421	LMG	C17-C18-C19-C20
24	A	405	CLA	C15-C16-C17-C18
24	B	607	CLA	C10-C11-C12-C13
24	a	412	CLA	C4-C3-C5-C6
24	A	405	CLA	C16-C17-C18-C19
24	c	507	CLA	C16-C17-C18-C20
27	B	621	SQD	O47-C45-C46-O48
36	c	521	DGD	C1A-C2A-C3A-C4A
37	E	101	LHG	C7-C8-C9-C10
36	c	522	DGD	C4A-C5A-C6A-C7A
36	e	101	DGD	C9B-CAB-CBB-CCB
27	L	102	SQD	C33-C34-C35-C36
36	C	518	DGD	C2A-C3A-C4A-C5A
24	B	616	CLA	C4-C3-C5-C6
29	D	401	LMT	C2B-C1B-O1B-C4'
31	A	419[B]	PL9	C13-C14-C16-C17
31	a	415[B]	PL9	C14-C16-C17-C18
36	D	406	DGD	C1G-C2G-C3G-O3G
36	D	406	DGD	C4B-C5B-C6B-C7B
33	c	501	LMG	C22-C23-C24-C25
33	Z	101	LMG	C8-C7-O1-C1
36	D	406	DGD	C2G-C3G-O3G-C1D
24	b	619	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	A	419[A]	PL9	C45-C44-C46-C47
35	B	624	HTG	C1'-C2'-C3'-C4'
24	a	412	CLA	C2-C3-C5-C6
31	a	415[B]	PL9	C43-C44-C46-C47
37	d	407	LHG	C24-C23-O8-C6
36	c	522	DGD	O6D-C5D-C6D-O5D
24	a	409	CLA	C4C-C3C-CAC-CBC
28	b	606	GOL	O1-C1-C2-O2
24	A	407	CLA	C11-C10-C8-C9
24	a	410	CLA	C11-C10-C8-C9
24	b	625	CLA	C11-C12-C13-C14
33	A	421	LMG	C18-C19-C20-C21
37	e	102	LHG	C13-C14-C15-C16
35	B	623	HTG	C4-C5-C6-O6
24	B	602	CLA	C4B-C3B-CAB-CBB
29	f	102	LMT	C2B-C1B-O1B-C4'
29	m	102	LMT	C4'-C5'-C6'-O6'
37	b	634	LHG	C12-C13-C14-C15
36	D	406	DGD	C2B-C3B-C4B-C5B
27	A	412	SQD	C7-C8-C9-C10
24	c	518	CLA	C4-C3-C5-C6
24	B	610	CLA	C2-C3-C5-C6
24	B	616	CLA	C2-C3-C5-C6
31	A	419[A]	PL9	C43-C44-C46-C47
33	b	629	LMG	C20-C21-C22-C23
24	B	616	CLA	C13-C15-C16-C17
29	a	419	LMT	C7-C8-C9-C10
38	e	103	HEM	C4C-C3C-CAC-CBC
33	D	413	LMG	C34-C35-C36-C37
24	C	506	CLA	C6-C7-C8-C10
24	b	623	CLA	C12-C13-C15-C16
24	c	515	CLA	C12-C13-C15-C16
24	C	513	CLA	O1A-CGA-O2A-C1
24	b	618	CLA	C3A-C2A-CAA-CBA
31	A	419[B]	PL9	C43-C44-C46-C47
37	D	407	LHG	C33-C34-C35-C36
29	M	101	LMT	C3-C4-C5-C6
33	c	501	LMG	C30-C31-C32-C33
24	b	615	CLA	C8-C10-C11-C12
36	c	520	DGD	O6E-C1E-O5D-C6D
24	A	406	CLA	C2C-C3C-CAC-CBC
24	c	516	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
27	a	414	SQD	C17-C18-C19-C20
31	d	405[B]	PL9	C28-C29-C31-C32
36	C	518	DGD	C6B-C7B-C8B-C9B
40	V	205	HEC	CAD-CBD-CGD-O2D
31	A	419[A]	PL9	C19-C21-C22-C23
24	B	608	CLA	C6-C7-C8-C9
24	B	615	CLA	C6-C7-C8-C9
24	C	506	CLA	C6-C7-C8-C9
24	c	514	CLA	C14-C13-C15-C16
28	O	301	GOL	O1-C1-C2-C3
37	b	634	LHG	C34-C35-C36-C37
33	D	413	LMG	C20-C21-C22-C23
36	c	520	DGD	C2A-C3A-C4A-C5A
36	C	517	DGD	C3A-C4A-C5A-C6A
37	E	101	LHG	C14-C15-C16-C17
36	C	517	DGD	C1A-C2A-C3A-C4A
24	b	610	CLA	C16-C17-C18-C19
27	a	414	SQD	C12-C13-C14-C15
24	B	605	CLA	CBD-CGD-O2D-CED
31	D	405[A]	PL9	C43-C44-C46-C47
36	e	101	DGD	CAB-CBB-CCB-CDB
24	b	621	CLA	C1A-C2A-CAA-CBA
24	c	511	CLA	C1A-C2A-CAA-CBA
27	L	102	SQD	C7-C8-C9-C10
24	C	504	CLA	C13-C15-C16-C17
24	B	602	CLA	C2B-C3B-CAB-CBB
24	B	616	CLA	C2B-C3B-CAB-CBB
24	c	512	CLA	C2B-C3B-CAB-CBB
26	C	514	BCR	C1-C6-C7-C8
26	C	515	BCR	C1-C6-C7-C8
26	D	404	BCR	C1-C6-C7-C8
26	D	404	BCR	C23-C24-C25-C30
26	b	626	BCR	C5-C6-C7-C8
26	d	404	BCR	C23-C24-C25-C26
38	F	102	HEM	CAD-CBD-CGD-O1D
36	H	102	DGD	C4E-C5E-C6E-O5E
24	B	609	CLA	C13-C15-C16-C17
24	c	511	CLA	C10-C11-C12-C13
33	C	519	LMG	C16-C17-C18-C19
37	D	407	LHG	C11-C10-C9-C8
24	B	605	CLA	C4-C3-C5-C6
24	A	406	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	C	504	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C10-C8-C7
24	b	625	CLA	C11-C12-C13-C15
24	c	514	CLA	C12-C13-C15-C16
33	d	413	LMG	C18-C19-C20-C21
36	H	102	DGD	C5B-C6B-C7B-C8B
36	D	406	DGD	C1A-C2A-C3A-C4A
24	b	610	CLA	C4-C3-C5-C6
24	d	403	CLA	C4-C3-C5-C6
31	A	419[A]	PL9	C20-C19-C21-C22
31	A	419[A]	PL9	C40-C39-C41-C42
31	A	419[B]	PL9	C30-C29-C31-C32
24	C	513	CLA	CBA-CGA-O2A-C1
24	b	615	CLA	C10-C11-C12-C13
24	c	518	CLA	C2-C3-C5-C6
24	C	513	CLA	C2-C1-O2A-CGA
24	b	611	CLA	C16-C17-C18-C19
33	D	413	LMG	C16-C17-C18-C19
24	C	505	CLA	C11-C12-C13-C14
36	c	521	DGD	C2A-C3A-C4A-C5A
27	A	416	SQD	C17-C18-C19-C20
37	d	408	LHG	C28-C29-C30-C31
31	A	419[A]	PL9	C30-C29-C31-C32
31	A	419[B]	PL9	C45-C44-C46-C47
31	D	405[B]	PL9	C35-C34-C36-C37
38	F	102	HEM	CAD-CBD-CGD-O2D
24	c	512	CLA	C2-C3-C5-C6
29	D	401	LMT	C5-C6-C7-C8
33	C	519	LMG	C12-C13-C14-C15
36	c	521	DGD	C3A-C4A-C5A-C6A
37	D	409	LHG	C9-C10-C11-C12
24	C	501	CLA	C13-C15-C16-C17
24	b	610	CLA	C13-C15-C16-C17
24	b	620	CLA	C8-C10-C11-C12
40	V	205	HEC	CAD-CBD-CGD-O1D
33	c	523	LMG	C20-C21-C22-C23
35	B	623	HTG	C3'-C4'-C5'-C6'
31	A	419[B]	PL9	C19-C21-C22-C23
36	h	102	DGD	O1G-C1G-C2G-C3G
36	D	406	DGD	CBA-CCA-CDA-CEA
24	B	602	CLA	CAA-CBA-CGA-O2A
33	c	523	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
27	A	412	SQD	O49-C7-O47-C45
28	V	203	GOL	O2-C2-C3-O3
31	A	419[B]	PL9	C20-C19-C21-C22
31	D	405[A]	PL9	C35-C34-C36-C37
36	c	521	DGD	C7A-C8A-C9A-CAA
37	d	408	LHG	C9-C10-C11-C12
25	a	411	PHO	C2-C3-C5-C6
27	A	412	SQD	C12-C13-C14-C15
27	A	412	SQD	C8-C7-O47-C45
29	b	630	LMT	C6-C7-C8-C9
37	D	408	LHG	C13-C14-C15-C16
24	a	412	CLA	C4B-C3B-CAB-CBB
40	v	205	HEC	CAD-CBD-CGD-O2D
33	B	622	LMG	O8-C28-C29-C30
29	f	102	LMT	C9-C10-C11-C12
24	d	401	CLA	C15-C16-C17-C18
29	D	401	LMT	O1'-C1-C2-C3
37	L	101	LHG	C26-C27-C28-C29
37	L	101	LHG	O6-C4-C5-C6
37	b	634	LHG	O6-C4-C5-C6
33	A	421	LMG	O7-C8-C9-O8
33	c	524	LMG	O7-C8-C9-O8
36	C	516	DGD	O2G-C1B-C2B-C3B
31	A	419[A]	PL9	C28-C29-C31-C32
29	m	103	LMT	O5'-C1'-O1'-C1
24	b	625	CLA	C12-C13-C15-C16
27	A	416	SQD	C25-C26-C27-C28
24	b	623	CLA	O1D-CGD-O2D-CED
24	b	610	CLA	C3-C5-C6-C7
36	h	102	DGD	CDA-CEA-CFA-CGA
24	a	410	CLA	C11-C12-C13-C14
24	b	612	CLA	C6-C7-C8-C9
24	d	402	CLA	C11-C12-C13-C14
27	A	412	SQD	C45-C44-O6-C1
36	C	516	DGD	C5D-C6D-O5D-C1E
36	c	520	DGD	C5D-C6D-O5D-C1E
24	B	611	CLA	C2A-CAA-CBA-CGA
24	B	602	CLA	C2-C1-O2A-CGA
24	C	511	CLA	C2-C1-O2A-CGA
24	B	608	CLA	C3A-C2A-CAA-CBA
24	B	610	CLA	C3A-C2A-CAA-CBA
24	b	618	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	c	517	CLA	C3-C5-C6-C7
36	C	516	DGD	CAA-CBA-CCA-CDA
40	v	205	HEC	CAD-CBD-CGD-O1D
36	c	520	DGD	C2E-C1E-O5D-C6D
27	A	416	SQD	C12-C13-C14-C15
37	b	634	LHG	C13-C14-C15-C16
37	L	101	LHG	C33-C34-C35-C36
37	d	406	LHG	C34-C35-C36-C37
33	z	101	LMG	C11-C12-C13-C14
25	a	411	PHO	C4-C3-C5-C6
24	C	509	CLA	C16-C17-C18-C20
33	C	519	LMG	C21-C22-C23-C24
36	e	101	DGD	C3A-C4A-C5A-C6A
37	d	406	LHG	C26-C27-C28-C29
31	a	415[B]	PL9	C39-C41-C42-C43
38	e	103	HEM	C4B-C3B-CAB-CBB
24	B	615	CLA	C16-C17-C18-C19
29	m	102	LMT	C9-C10-C11-C12
27	A	416	SQD	C29-C30-C31-C32
33	A	421	LMG	C37-C38-C39-C40
24	C	506	CLA	C4-C3-C5-C6
26	k	101	BCR	C9-C10-C11-C12
33	D	413	LMG	C30-C31-C32-C33
33	c	524	LMG	C32-C33-C34-C35
27	B	621	SQD	C19-C20-C21-C22
33	c	501	LMG	C18-C19-C20-C21
37	L	101	LHG	C30-C31-C32-C33
27	a	405	SQD	O10-C23-O48-C46
37	e	102	LHG	O8-C23-C24-C25
35	B	624	HTG	C3'-C4'-C5'-C6'
24	B	610	CLA	C4-C3-C5-C6
36	C	517	DGD	C6B-C7B-C8B-C9B
33	z	101	LMG	O7-C10-C11-C12
37	b	634	LHG	C7-C8-C9-C10
27	a	405	SQD	C24-C23-O48-C46
24	A	407	CLA	C12-C13-C15-C16
24	A	410	CLA	C12-C13-C15-C16
24	B	603	CLA	C12-C13-C15-C16
24	C	505	CLA	C11-C12-C13-C15
24	b	612	CLA	C6-C7-C8-C10
29	a	404	LMT	C1-C2-C3-C4
24	b	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	A	410	CLA	C2B-C3B-CAB-CBB
24	B	608	CLA	C2B-C3B-CAB-CBB
24	a	412	CLA	C2B-C3B-CAB-CBB
24	b	611	CLA	C2B-C3B-CAB-CBB
24	c	506	CLA	C2B-C3B-CAB-CBB
24	c	514	CLA	C2B-C3B-CAB-CBB
24	d	403	CLA	C2B-C3B-CAB-CBB
26	C	514	BCR	C5-C6-C7-C8
26	C	515	BCR	C5-C6-C7-C8
26	D	404	BCR	C5-C6-C7-C8
26	D	404	BCR	C23-C24-C25-C26
26	c	519	BCR	C1-C6-C7-C8
37	d	408	LHG	C11-C12-C13-C14
24	C	510	CLA	CAA-CBA-CGA-O2A
24	C	512	CLA	CAA-CBA-CGA-O2A
27	f	101	SQD	O47-C7-C8-C9
24	b	622	CLA	C2-C1-O2A-CGA
24	c	517	CLA	C2-C1-O2A-CGA
35	b	632	HTG	C4-C5-C6-O6
31	A	419[A]	PL9	C9-C11-C12-C13
37	d	406	LHG	O8-C23-C24-C25
24	b	618	CLA	C4-C3-C5-C6
31	d	405[A]	PL9	C30-C29-C31-C32
33	Z	101	LMG	O7-C10-C11-C12
31	d	405[A]	PL9	C28-C29-C31-C32
29	f	102	LMT	C1-C2-C3-C4
35	b	632	HTG	C2'-C1'-S1-C1
35	c	525	HTG	C2'-C1'-S1-C1
37	D	409	LHG	C33-C34-C35-C36
37	L	101	LHG	C18-C19-C20-C21
24	C	513	CLA	C5-C6-C7-C8
29	F	101	LMT	C1-C2-C3-C4
35	B	624	HTG	C4'-C5'-C6'-C7'
33	c	501	LMG	C13-C14-C15-C16
24	c	517	CLA	CAA-CBA-CGA-O2A
31	d	405[B]	PL9	C18-C19-C21-C22
38	e	103	HEM	CAD-CBD-CGD-O1D
37	d	408	LHG	C25-C26-C27-C28
31	a	415[A]	PL9	C2-C3-C7-C8
36	h	102	DGD	O1B-C1B-C2B-C3B
37	e	102	LHG	C28-C29-C30-C31
33	z	101	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	B	605	CLA	C13-C15-C16-C17
24	a	409	CLA	C15-C16-C17-C18
36	C	518	DGD	C8B-C9B-CAB-CBB
37	b	634	LHG	C14-C15-C16-C17
35	B	623	HTG	C4'-C5'-C6'-C7'
24	C	505	CLA	C11-C10-C8-C9
24	C	507	CLA	C11-C10-C8-C9
24	b	625	CLA	C14-C13-C15-C16
24	c	513	CLA	C6-C7-C8-C9
24	c	515	CLA	C11-C12-C13-C14
26	K	101	BCR	C7-C8-C9-C34
37	L	101	LHG	O7-C7-C8-C9
24	b	615	CLA	C15-C16-C17-C18
38	F	102	HEM	CAA-CBA-CGA-O2A
27	a	405	SQD	C12-C13-C14-C15
37	L	101	LHG	C16-C17-C18-C19
24	d	401	CLA	C4C-C3C-CAC-CBC
24	c	515	CLA	CAA-CBA-CGA-O2A
36	D	406	DGD	O1G-C1A-C2A-C3A
36	c	522	DGD	O1G-C1A-C2A-C3A
27	A	412	SQD	O6-C44-C45-O47
38	F	102	HEM	CAA-CBA-CGA-O1A
38	e	103	HEM	CAA-CBA-CGA-O1A
26	K	101	BCR	C7-C8-C9-C10
26	Y	101	BCR	C21-C22-C23-C24
29	m	103	LMT	C5-C6-C7-C8
36	e	101	DGD	O2G-C1B-C2B-C3B
37	E	101	LHG	O8-C23-C24-C25
24	a	409	CLA	C2A-CAA-CBA-CGA
29	C	521	LMT	C3-C4-C5-C6
29	M	103	LMT	C2'-C1'-O1'-C1
37	D	407	LHG	C26-C27-C28-C29
24	b	611	CLA	C16-C17-C18-C20
27	F	103	SQD	C5-C6-S-O9
24	C	510	CLA	C8-C10-C11-C12
31	d	405[B]	PL9	C30-C29-C31-C32
24	b	623	CLA	C2-C1-O2A-CGA
24	c	518	CLA	C2-C1-O2A-CGA
24	B	613	CLA	CAA-CBA-CGA-O2A
24	B	614	CLA	CAA-CBA-CGA-O2A
27	B	621	SQD	C14-C15-C16-C17
24	A	410	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	C	501	CLA	C11-C12-C13-C15
24	a	410	CLA	C11-C12-C13-C15
24	b	619	CLA	C11-C12-C13-C15
33	b	629	LMG	C29-C28-O8-C9
24	C	502	CLA	C13-C15-C16-C17
27	a	414	SQD	C7-C8-C9-C10
38	e	103	HEM	CAD-CBD-CGD-O2D
25	a	418[B]	PHO	C2C-C3C-CAC-CBC
36	C	518	DGD	CBB-CCB-CDB-CEB
33	A	421	LMG	O6-C5-C6-O5
24	b	611	CLA	C2A-CAA-CBA-CGA
24	b	623	CLA	C2A-CAA-CBA-CGA
24	c	506	CLA	C2A-CAA-CBA-CGA
36	H	102	DGD	C8A-C9A-CAA-CBA
24	C	507	CLA	C5-C6-C7-C8
27	F	103	SQD	C33-C34-C35-C36
38	e	103	HEM	CAA-CBA-CGA-O2A
37	b	634	LHG	O7-C7-C8-C9
33	C	520	LMG	C13-C14-C15-C16
36	D	406	DGD	C5B-C6B-C7B-C8B
24	c	511	CLA	C13-C15-C16-C17
27	f	101	SQD	C30-C31-C32-C33
24	b	610	CLA	CAA-CBA-CGA-O1A
37	d	406	LHG	O10-C23-C24-C25
33	z	101	LMG	O9-C10-C11-C12
24	A	405	CLA	C2A-CAA-CBA-CGA
24	D	403	CLA	C11-C10-C8-C9
36	H	102	DGD	O1B-C1B-C2B-C3B
27	a	414	SQD	C10-C11-C12-C13
29	F	101	LMT	C2-C3-C4-C5
36	h	102	DGD	CBB-CCB-CDB-CEB
24	A	410	CLA	C8-C10-C11-C12
24	d	401	CLA	C13-C15-C16-C17
24	B	605	CLA	C2-C3-C5-C6
24	d	403	CLA	C2-C3-C5-C6
27	L	102	SQD	O5-C5-C6-S
24	C	509	CLA	O1D-CGD-O2D-CED
36	c	521	DGD	CCB-CDB-CEB-CFB
36	c	522	DGD	O1A-C1A-C2A-C3A
37	b	634	LHG	O1-C1-C2-O2
36	C	516	DGD	C6A-C7A-C8A-C9A
24	b	622	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	c	510	CLA	CBD-CGD-O2D-CED
29	m	102	LMT	O1'-C1-C2-C3
27	f	101	SQD	O49-C7-C8-C9
36	D	406	DGD	O1A-C1A-C2A-C3A
37	e	102	LHG	O10-C23-C24-C25
33	z	101	LMG	C8-C7-O1-C1
36	H	102	DGD	O1G-C1G-C2G-O2G
24	C	510	CLA	CAA-CBA-CGA-O1A
24	C	512	CLA	CAA-CBA-CGA-O1A
24	C	507	CLA	C2A-CAA-CBA-CGA
33	Z	101	LMG	O9-C10-C11-C12
29	f	102	LMT	O5B-C1B-O1B-C4'
24	A	410	CLA	C15-C16-C17-C18
24	b	623	CLA	C8-C10-C11-C12
33	b	629	LMG	O8-C28-C29-C30
27	f	101	SQD	C34-C35-C36-C37
36	C	516	DGD	C4A-C5A-C6A-C7A
24	B	608	CLA	CAD-CBD-CGD-O2D
24	B	617	CLA	CAD-CBD-CGD-O2D
24	D	403	CLA	CAD-CBD-CGD-O2D
24	b	625	CLA	CAD-CBD-CGD-O2D
24	c	518	CLA	CAD-CBD-CGD-O2D
33	D	413	LMG	C12-C13-C14-C15
24	c	517	CLA	CAA-CBA-CGA-O1A
33	b	629	LMG	O10-C28-O8-C9
36	C	517	DGD	O6D-C5D-C6D-O5D
36	D	406	DGD	O6D-C5D-C6D-O5D
29	M	103	LMT	C2B-C1B-O1B-C4'
29	M	101	LMT	O5'-C1'-O1'-C1
36	e	101	DGD	O1B-C1B-C2B-C3B
36	c	521	DGD	O2G-C1B-C2B-C3B
36	C	517	DGD	CAA-CBA-CCA-CDA
36	e	101	DGD	C6B-C7B-C8B-C9B
37	E	101	LHG	O10-C23-C24-C25
37	L	101	LHG	O9-C7-C8-C9
27	L	102	SQD	C23-C24-C25-C26
37	d	406	LHG	C7-C8-C9-C10
33	A	421	LMG	O8-C28-C29-C30
25	A	408	PHO	C10-C11-C12-C13
37	D	407	LHG	C28-C29-C30-C31
24	C	505	CLA	CAA-CBA-CGA-O2A
33	c	501	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
37	E	101	LHG	O7-C7-C8-C9
37	d	408	LHG	O8-C23-C24-C25
24	B	613	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

159 monomers are involved in 345 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	608	CLA	1	0
36	C	516	DGD	1	0
24	b	618	CLA	1	0
28	a	402	GOL	1	0
27	L	102	SQD	3	0
24	b	623	CLA	1	0
35	c	525	HTG	1	0
36	C	517	DGD	2	0
24	b	624	CLA	5	0
24	A	410	CLA	4	0
27	A	412	SQD	6	0
24	C	509	CLA	3	0
28	a	420	GOL	1	0
33	C	519	LMG	4	0
24	b	620	CLA	3	0
27	f	101	SQD	1	1
24	b	619	CLA	4	0
24	C	513	CLA	6	0
24	b	614	CLA	6	0
24	b	621	CLA	2	0
24	A	407	CLA	1	0
24	c	512	CLA	3	0
24	C	502	CLA	3	0
25	A	408	PHO	1	0
24	b	613	CLA	2	0
27	a	405	SQD	1	0
26	T	103	BCR	5	0
26	Y	101	BCR	4	0
25	A	409[B]	PHO	2	0
26	B	618	BCR	3	0
26	b	628	BCR	3	0
36	e	101	DGD	7	0
24	C	507	CLA	3	0
36	c	521	DGD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	511	CLA	2	0
31	A	419[B]	PL9	4	0
26	h	101	BCR	4	0
28	c	503	GOL	2	0
24	c	513	CLA	6	0
24	c	516	CLA	2	0
29	M	103	LMT	1	0
37	d	406	LHG	2	0
24	B	613	CLA	1	0
24	B	615	CLA	4	0
37	D	407	LHG	1	0
29	a	419	LMT	1	0
33	b	629	LMG	3	0
26	B	619	BCR	3	0
24	B	610	CLA	3	0
26	C	514	BCR	6	0
37	D	408	LHG	1	0
24	c	518	CLA	5	0
29	b	630	LMT	3	0
38	F	102	HEM	2	0
27	a	414	SQD	2	0
35	B	623	HTG	1	0
37	d	408	LHG	6	0
25	a	418[B]	PHO	1	0
36	C	518	DGD	1	0
24	C	503	CLA	3	0
26	H	101	BCR	3	0
35	D	412	HTG	2	0
29	C	521	LMT	1	0
33	c	524	LMG	2	0
24	C	501	CLA	1	0
24	B	611	CLA	1	0
28	A	414	GOL	1	0
24	c	517	CLA	2	0
29	A	417	LMT	2	0
31	a	415[B]	PL9	7	0
24	c	510	CLA	7	0
28	T	102	GOL	2	0
24	B	607	CLA	4	0
24	b	612	CLA	2	0
24	B	614	CLA	3	0
26	A	411	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	409[A]	PHO	3	0
26	b	626	BCR	4	0
24	d	402	CLA	3	0
24	a	409	CLA	4	0
26	b	627	BCR	3	0
37	E	101	LHG	2	0
26	t	101	BCR	5	0
26	C	515	BCR	5	0
24	c	514	CLA	3	0
24	d	401	CLA	4	0
24	B	609	CLA	1	0
24	c	509	CLA	1	0
27	B	621	SQD	3	0
35	d	411	HTG	3	0
33	B	622	LMG	1	0
24	C	512	CLA	4	0
24	A	406	CLA	3	0
38	e	103	HEM	5	0
24	D	402	CLA	3	0
36	c	520	DGD	1	0
24	B	612	CLA	1	0
24	C	510	CLA	3	0
24	a	410	CLA	3	0
33	c	523	LMG	3	0
37	e	102	LHG	4	0
28	v	201	GOL	1	0
37	D	409	LHG	9	0
24	D	403	CLA	1	0
29	D	401	LMT	1	0
36	D	406	DGD	2	0
24	B	604	CLA	2	0
25	a	418[A]	PHO	2	0
28	T	101	GOL	1	0
29	M	101	LMT	3	0
29	f	102	LMT	1	0
29	a	404	LMT	1	0
29	m	103	LMT	2	0
24	B	606	CLA	2	0
27	A	416	SQD	1	0
33	C	520	LMG	3	0
26	D	404	BCR	1	0
33	D	413	LMG	1	0

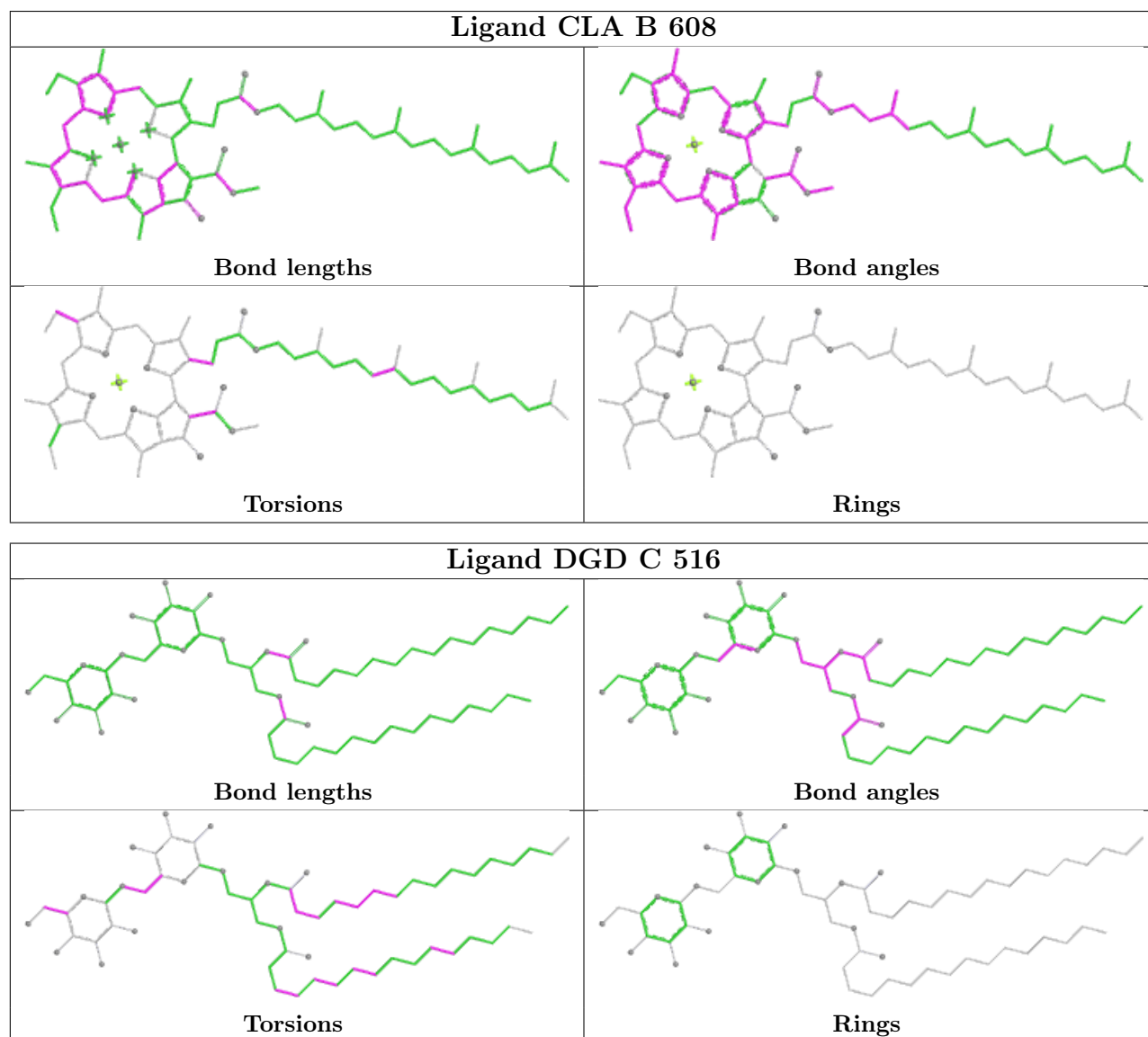
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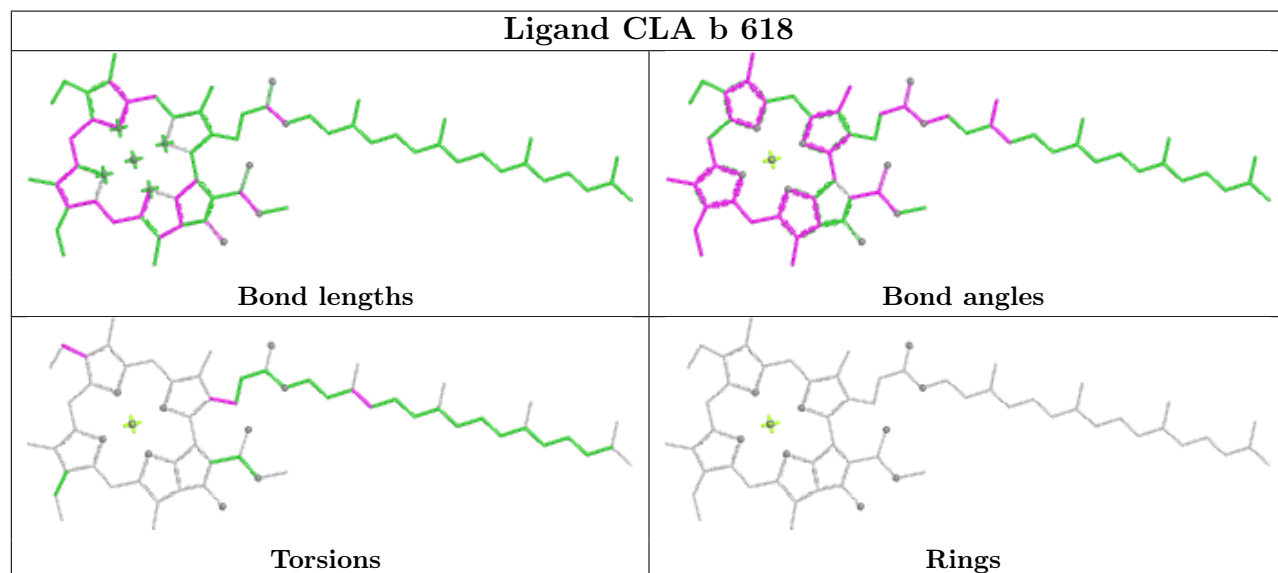
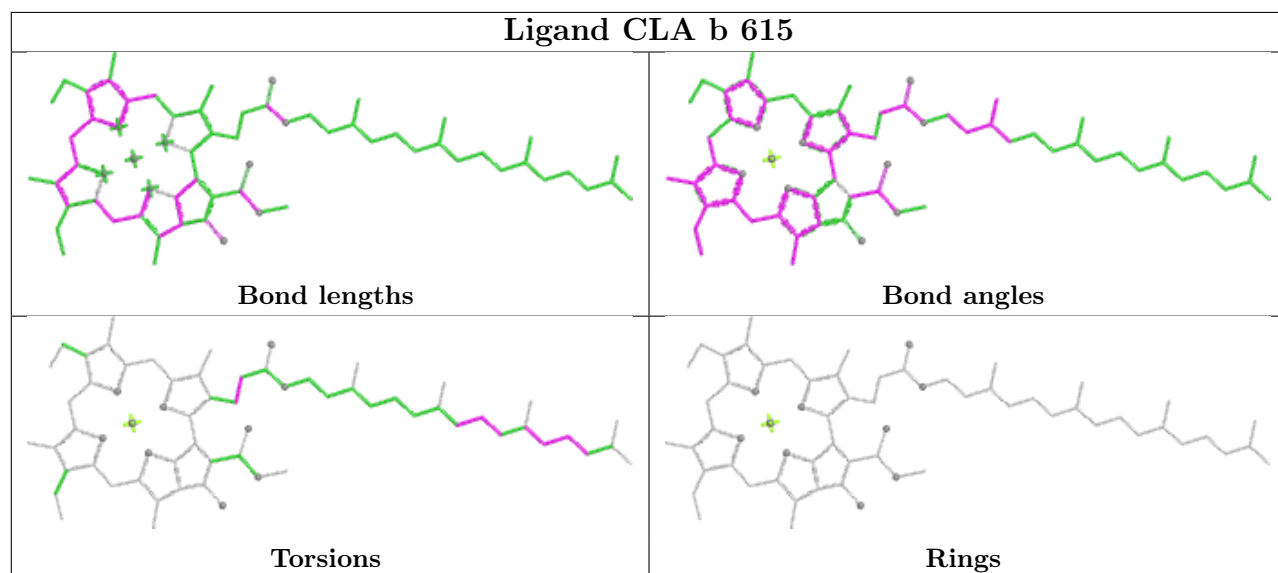
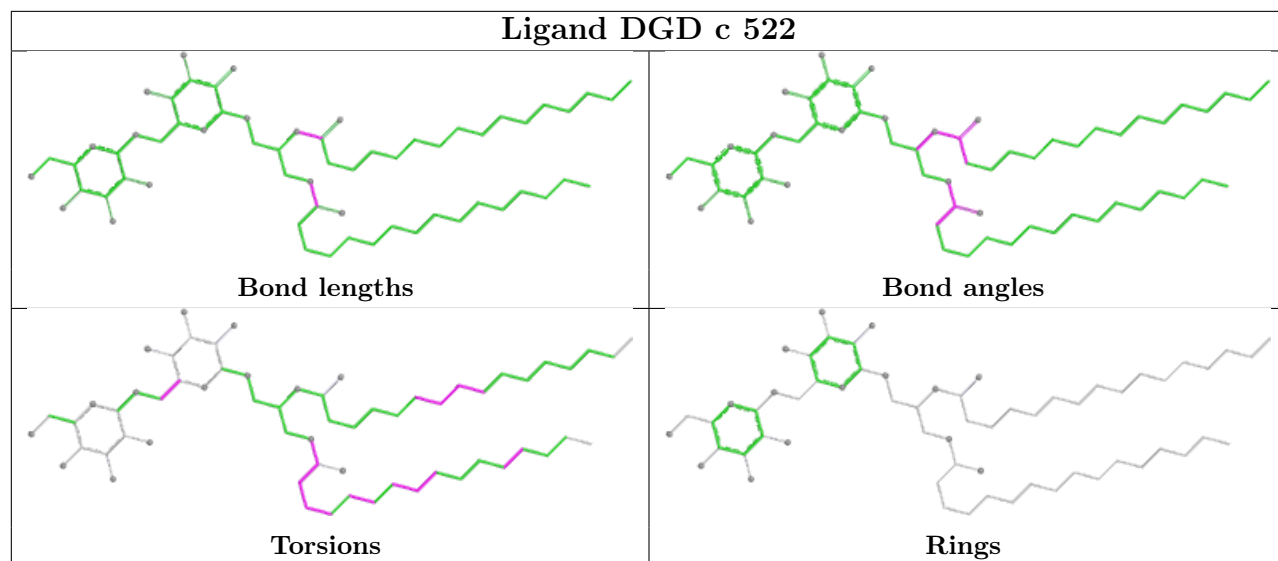
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	519	BCR	3	0
26	B	620	BCR	5	0
24	b	625	CLA	2	0
37	d	407	LHG	1	0
24	C	506	CLA	2	0
24	B	602	CLA	2	0
26	c	528	BCR	2	0
33	Z	101	LMG	1	0
24	c	507	CLA	4	0
31	a	415[A]	PL9	7	0
31	A	419[A]	PL9	5	0
24	c	515	CLA	2	0
31	D	405[B]	PL9	1	0
24	C	505	CLA	5	0
24	b	622	CLA	3	0
24	B	616	CLA	6	0
33	z	101	LMG	5	0
27	F	103	SQD	2	0
24	B	603	CLA	2	0
24	a	412	CLA	2	0
24	c	508	CLA	2	0
33	A	421	LMG	4	0
37	b	634	LHG	3	0
24	A	405	CLA	4	0
26	y	101	BCR	2	0
35	V	206	HTG	1	0
24	B	617	CLA	6	0
33	c	501	LMG	2	0
26	a	413	BCR	1	0
28	t	102	GOL	1	0
33	d	413	LMG	2	0
26	d	404	BCR	3	0
35	b	601	HTG	1	0
24	b	610	CLA	2	0
24	C	508	CLA	3	0
24	c	506	CLA	3	0
29	m	102	LMT	1	0
24	c	511	CLA	2	0
28	B	630	GOL	1	0
24	d	403	CLA	2	0
26	k	101	BCR	1	0

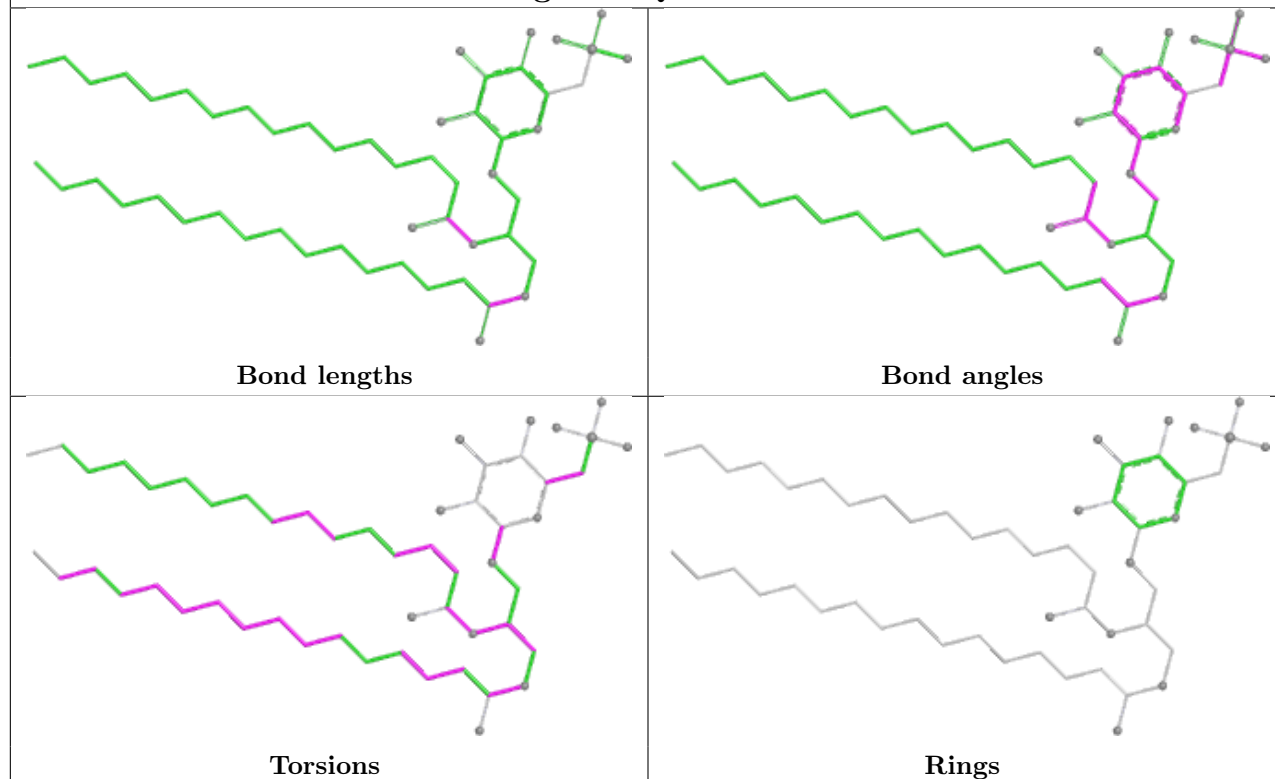
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

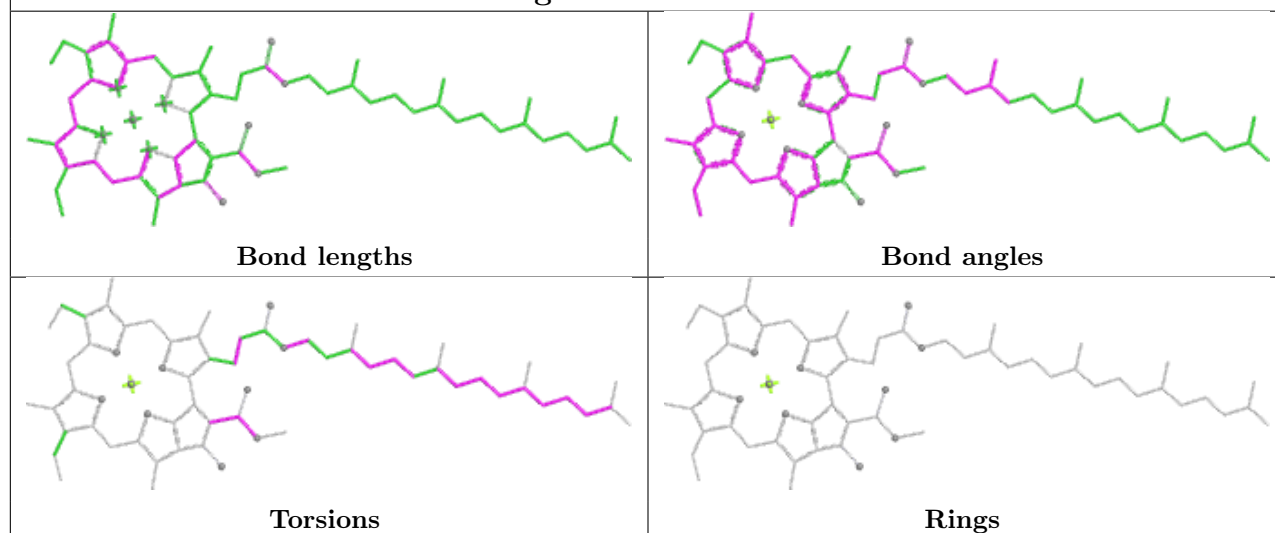




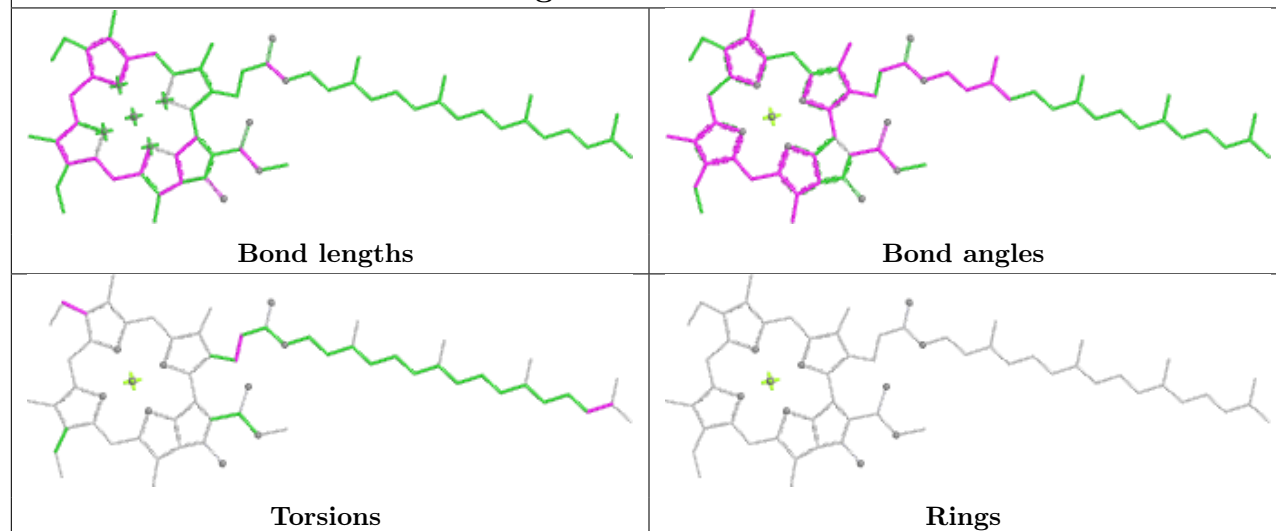
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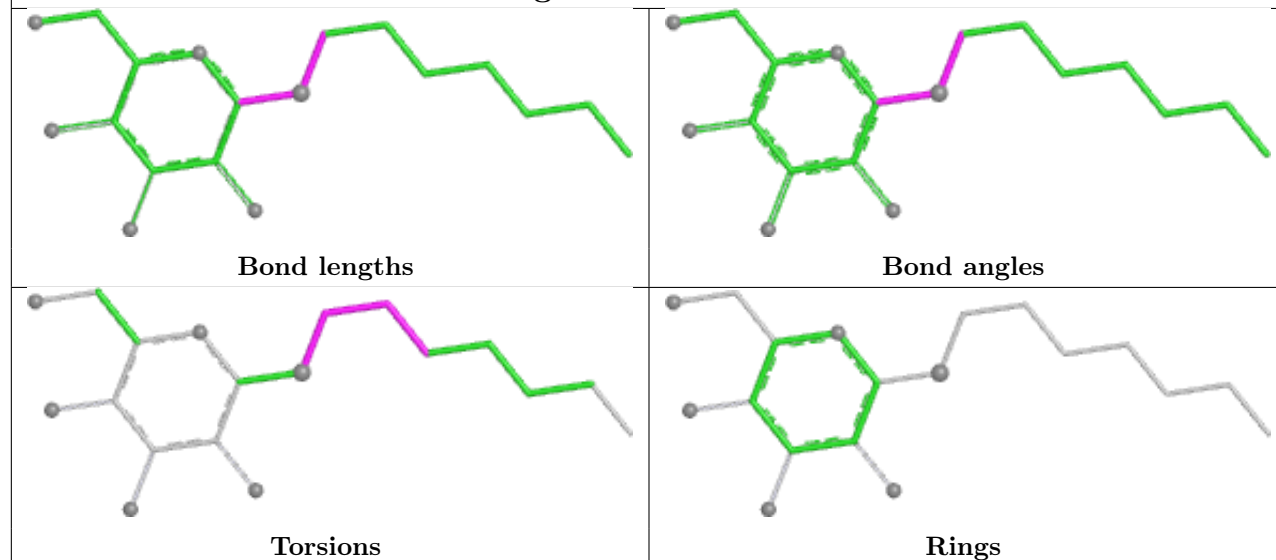
Ligand CLA b 623



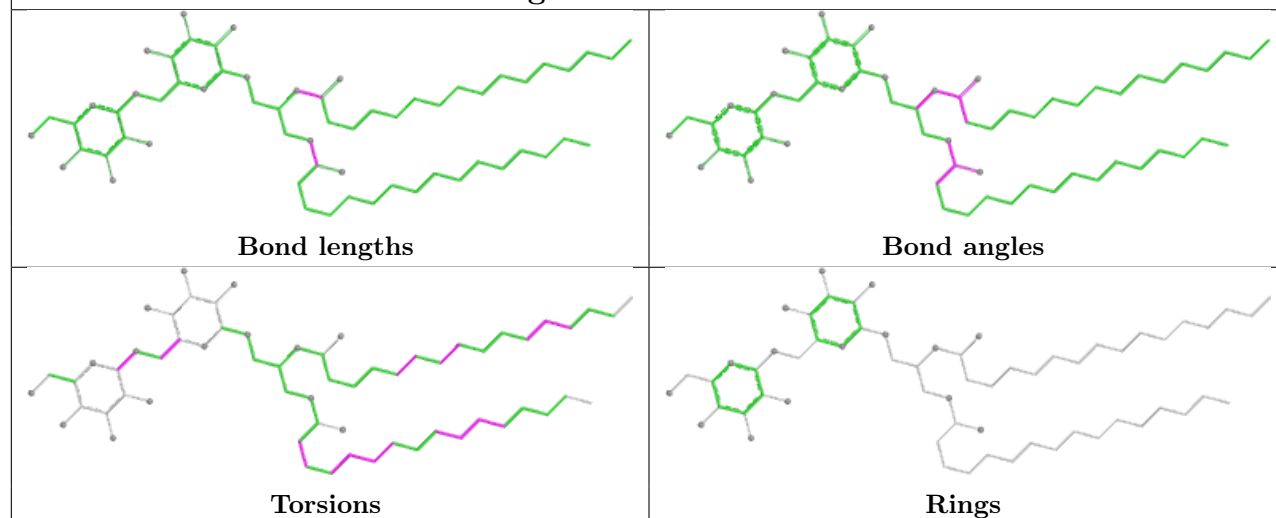
Ligand CLA b 611



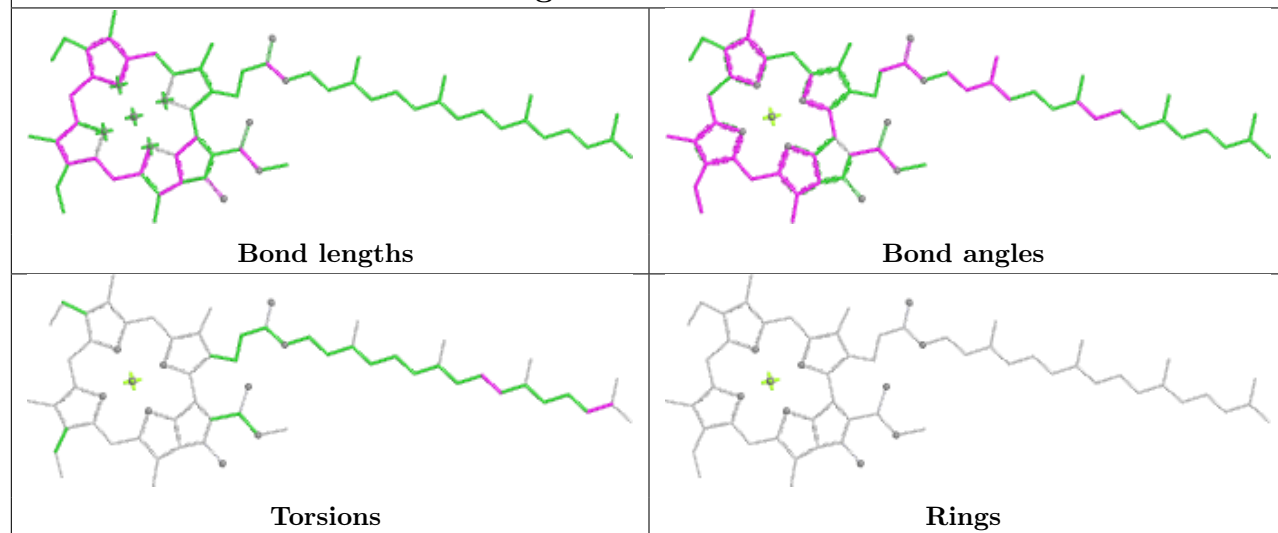
Ligand HTG c 525



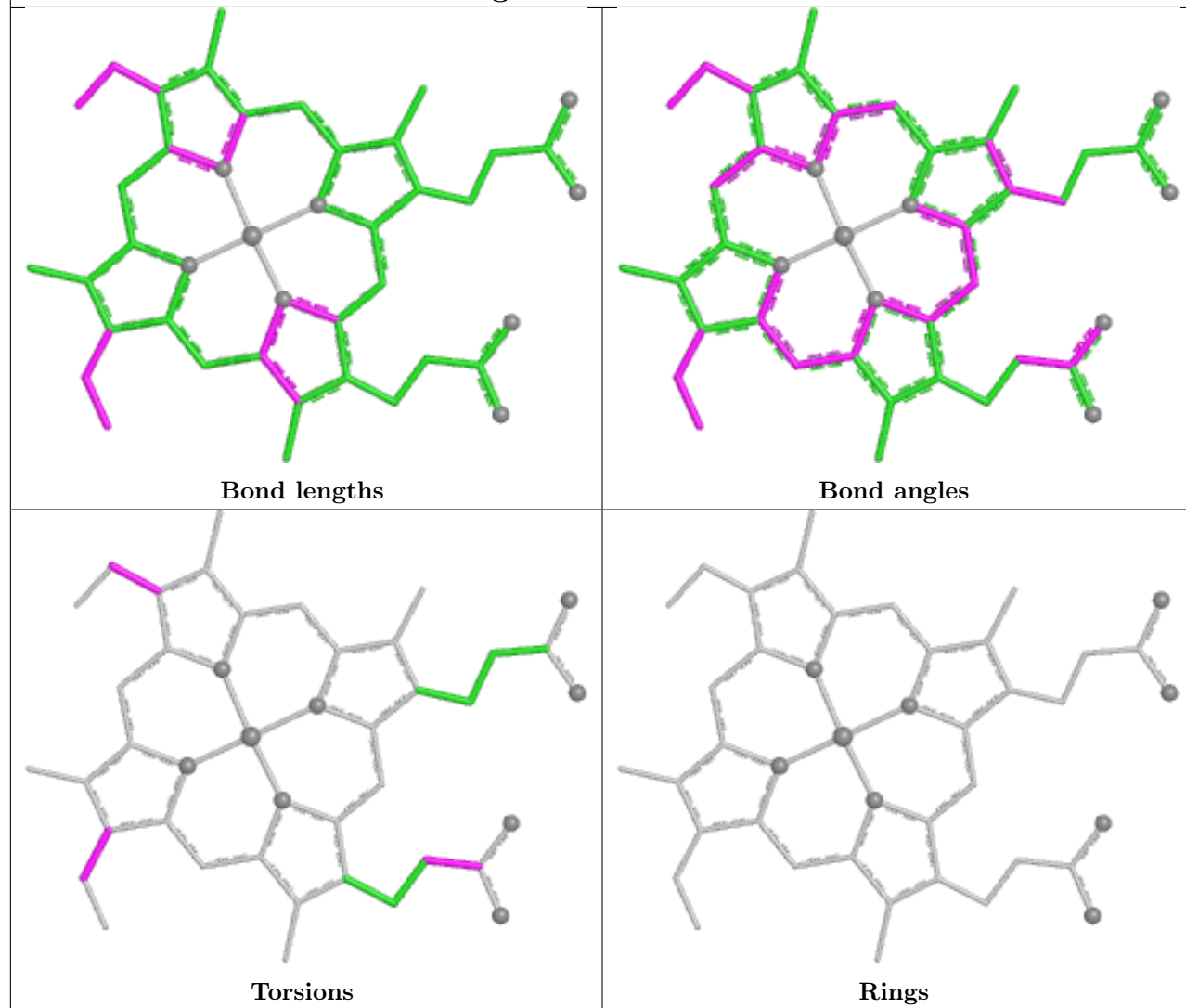
Ligand DGD C 517



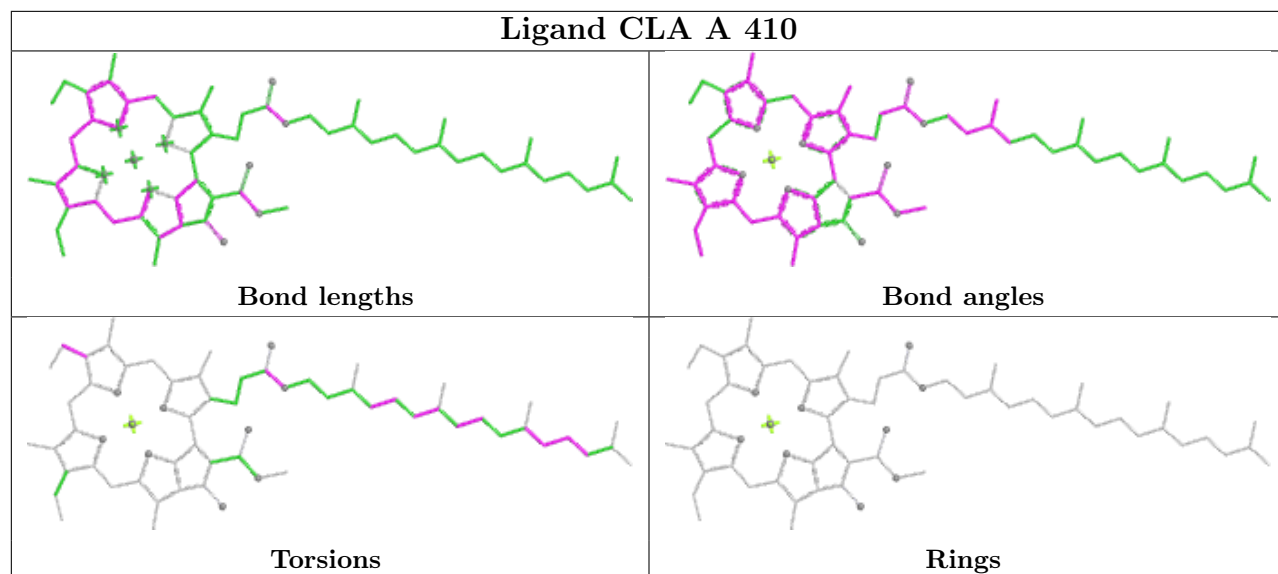
Ligand CLA b 624



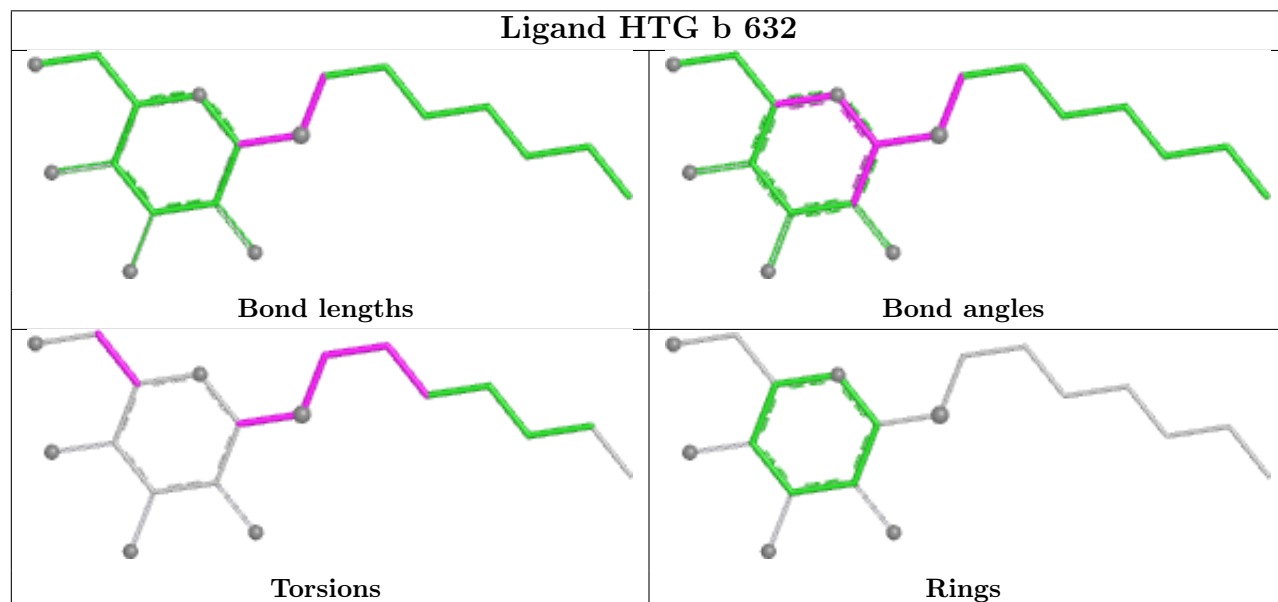
Ligand HEC V 205

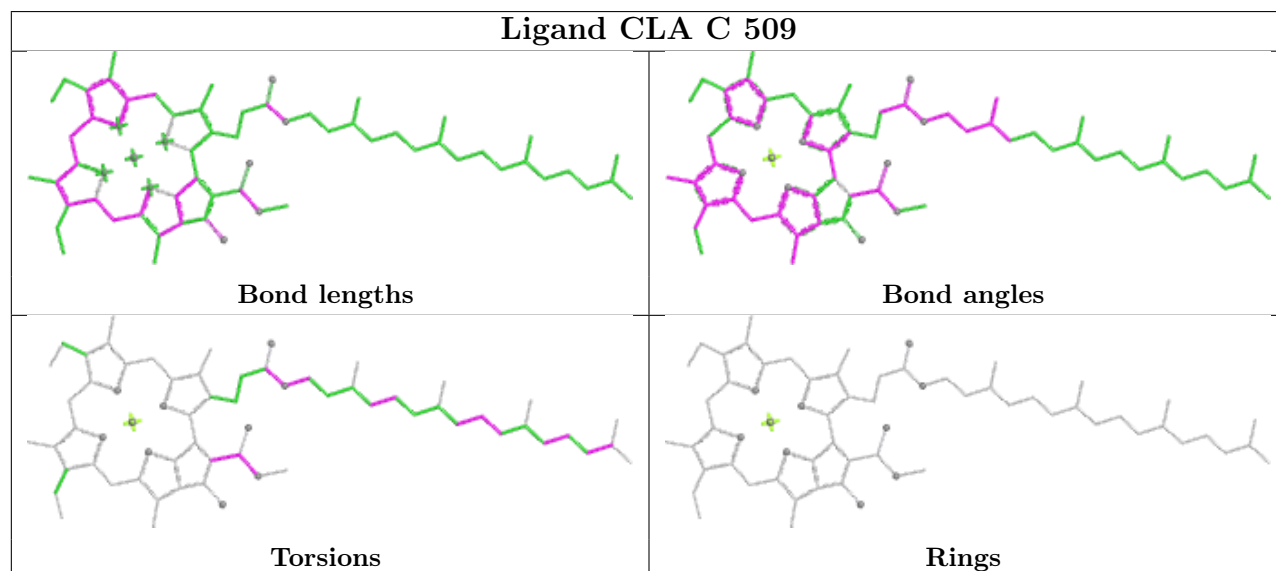
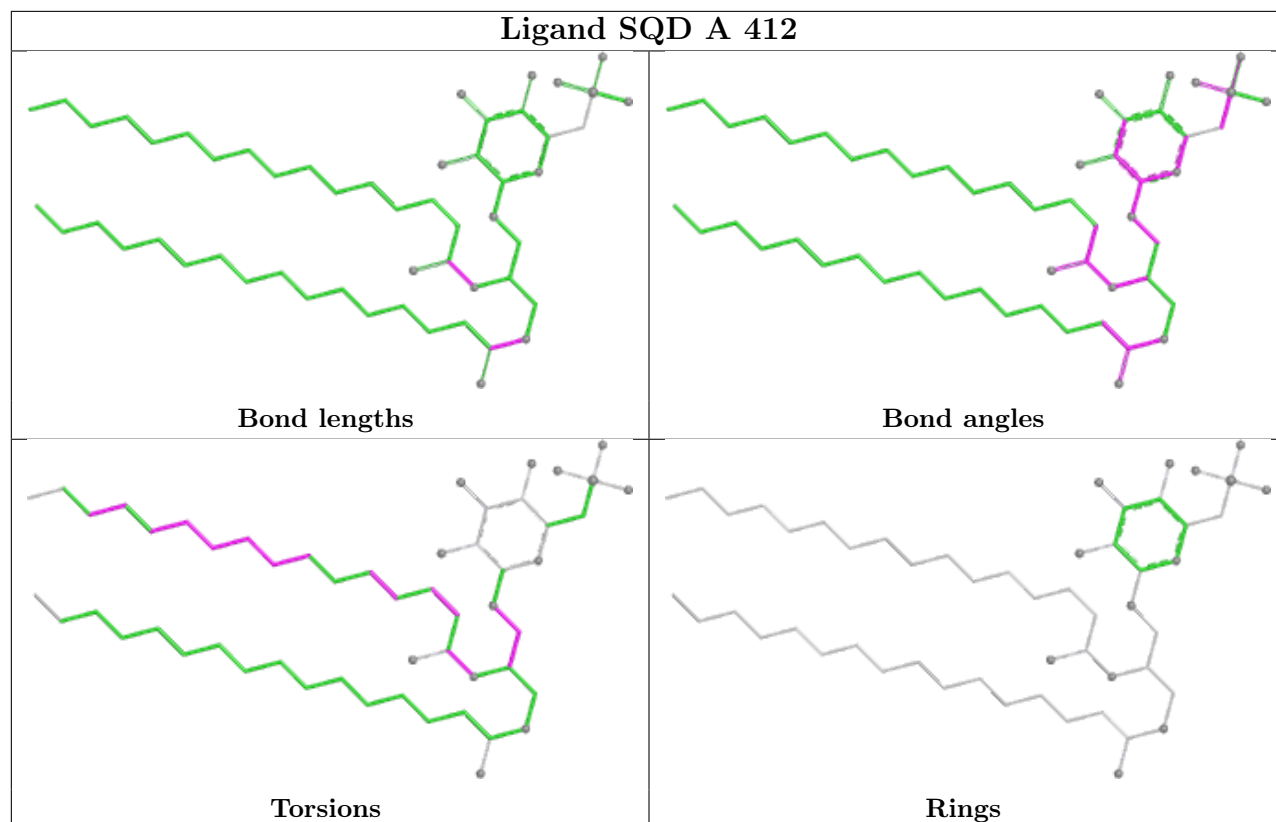


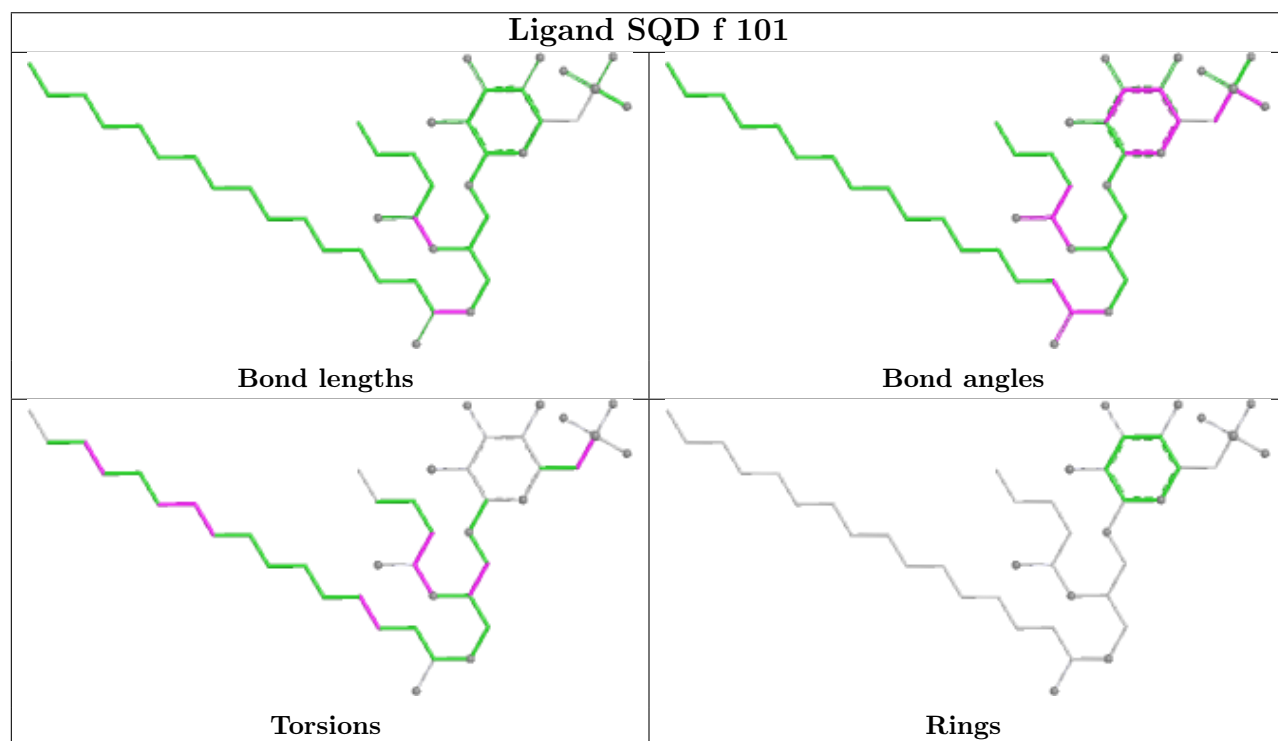
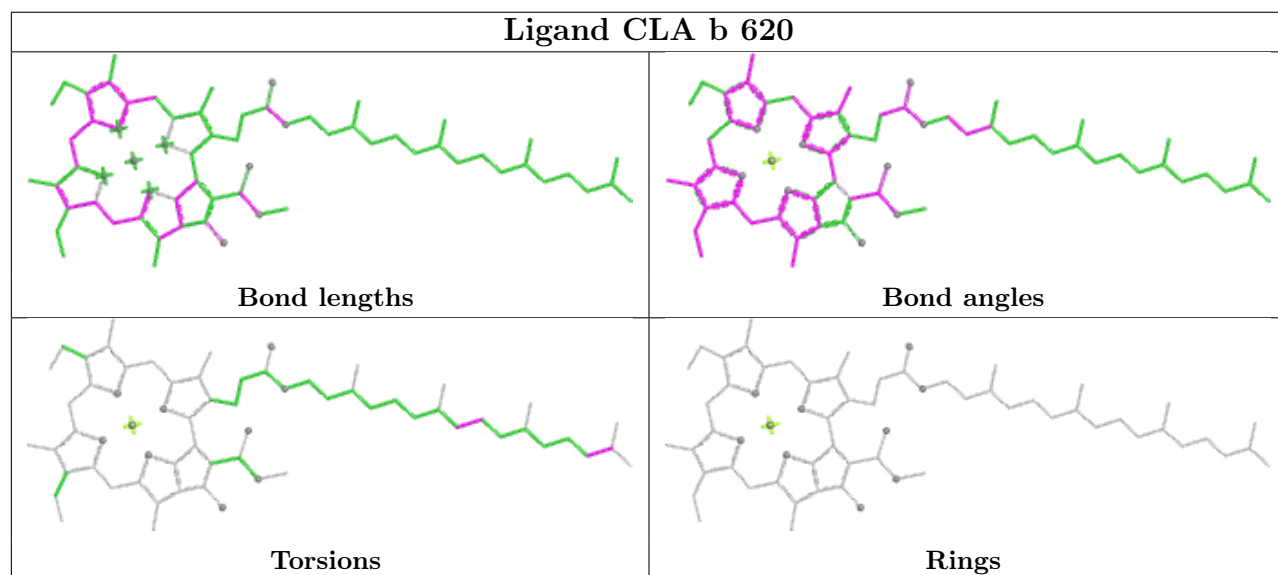
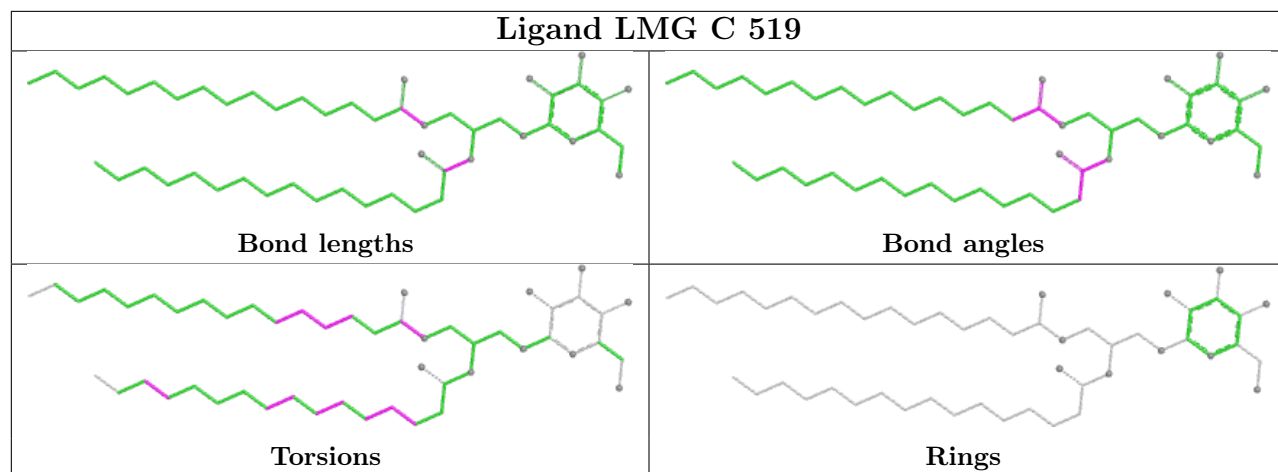
Ligand CLA A 410



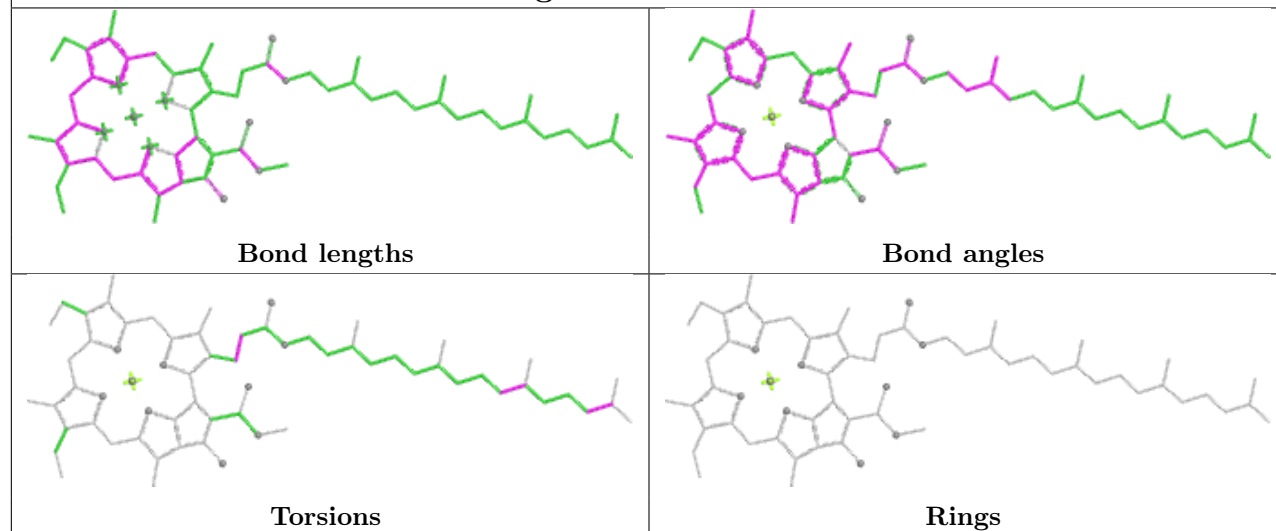
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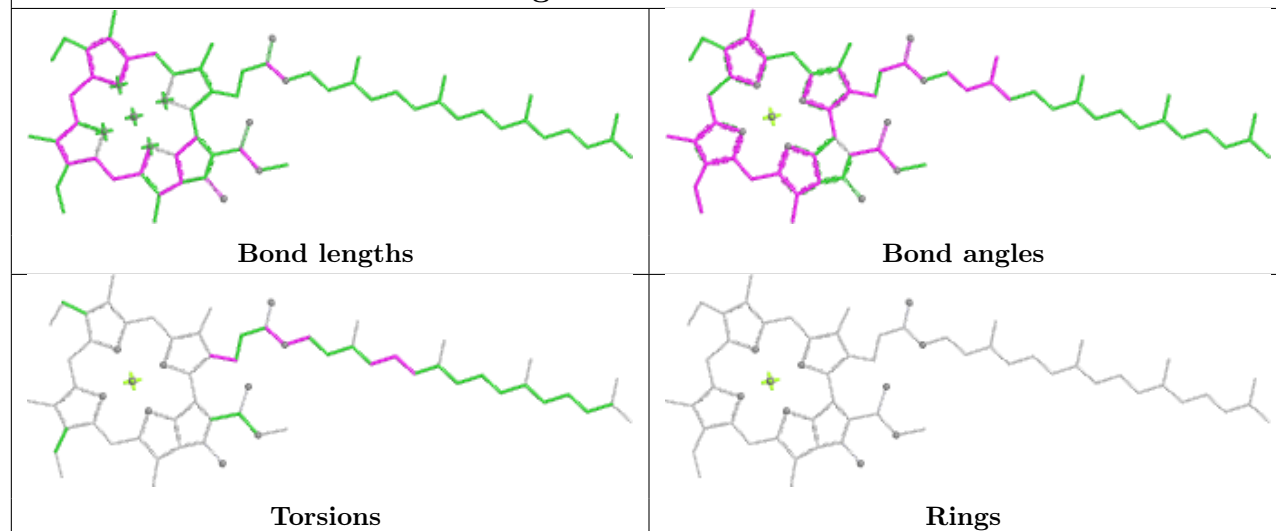




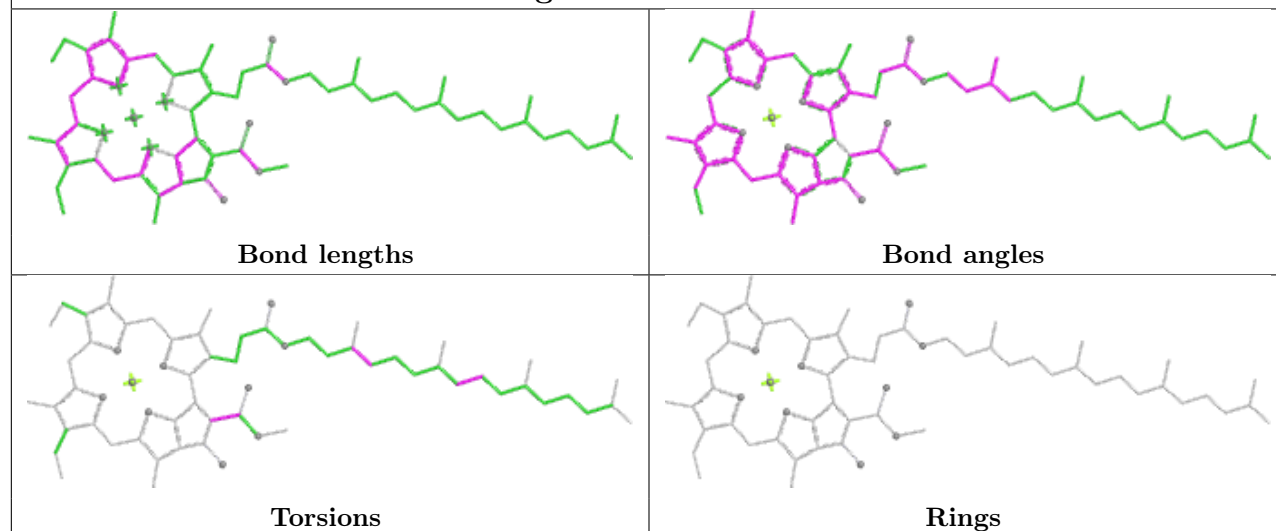
Ligand CLA b 619



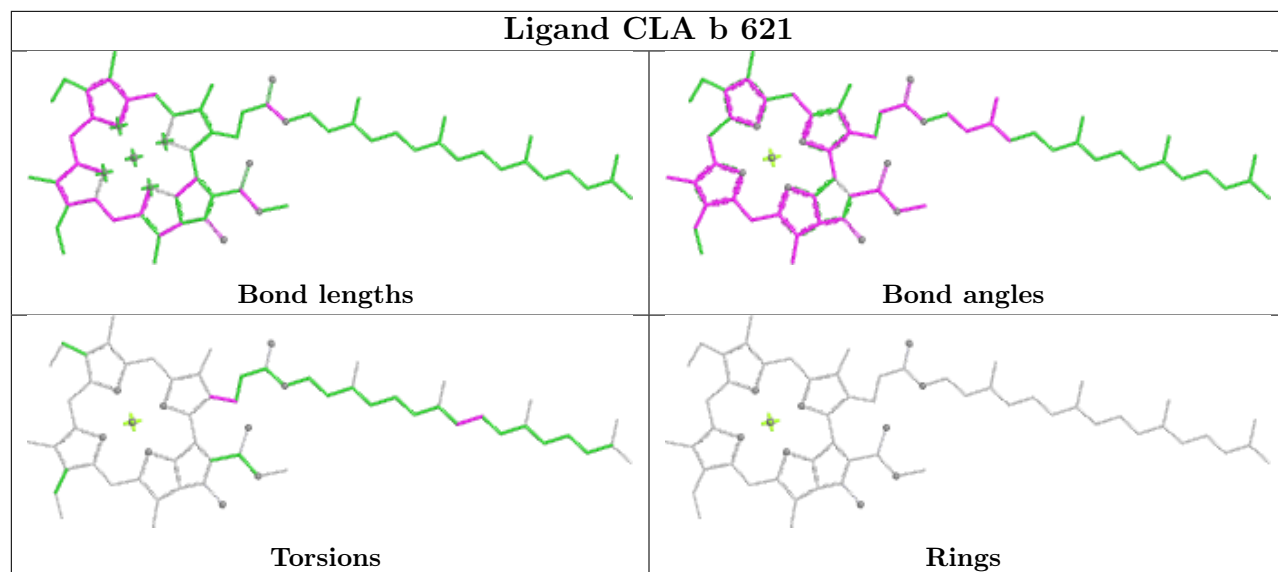
Ligand CLA C 513



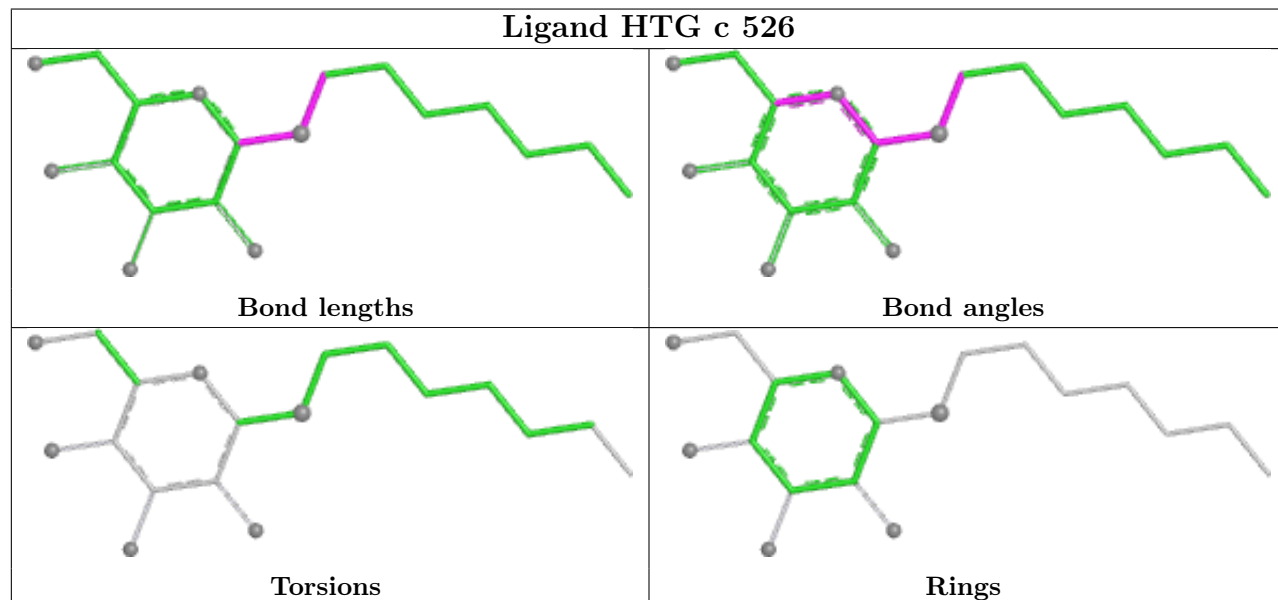
Ligand CLA b 614



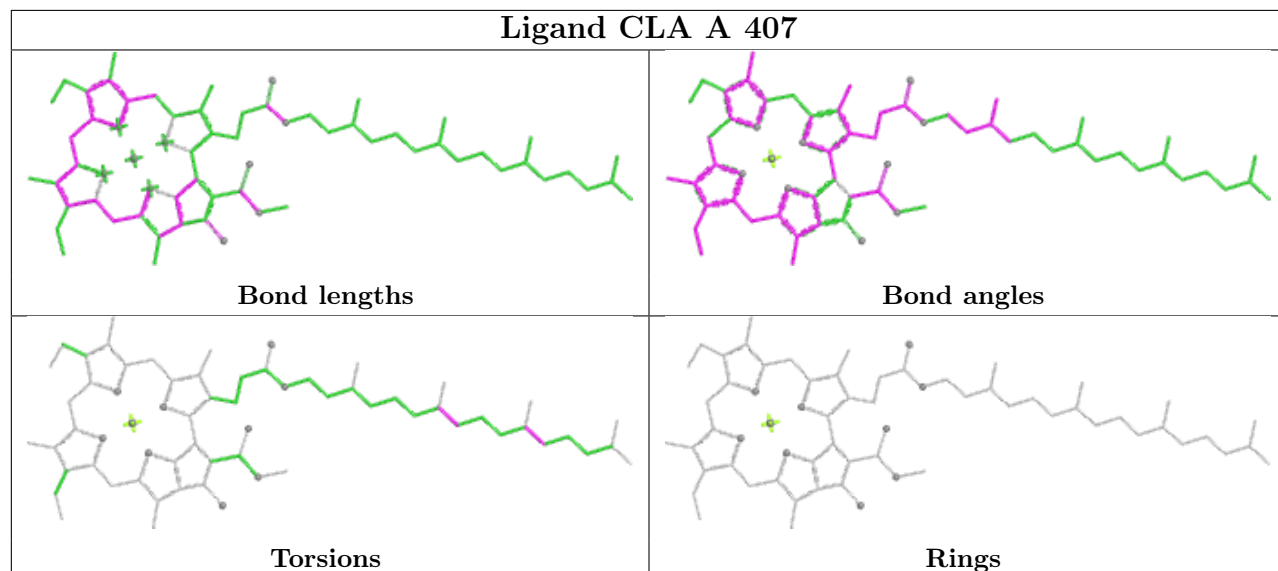
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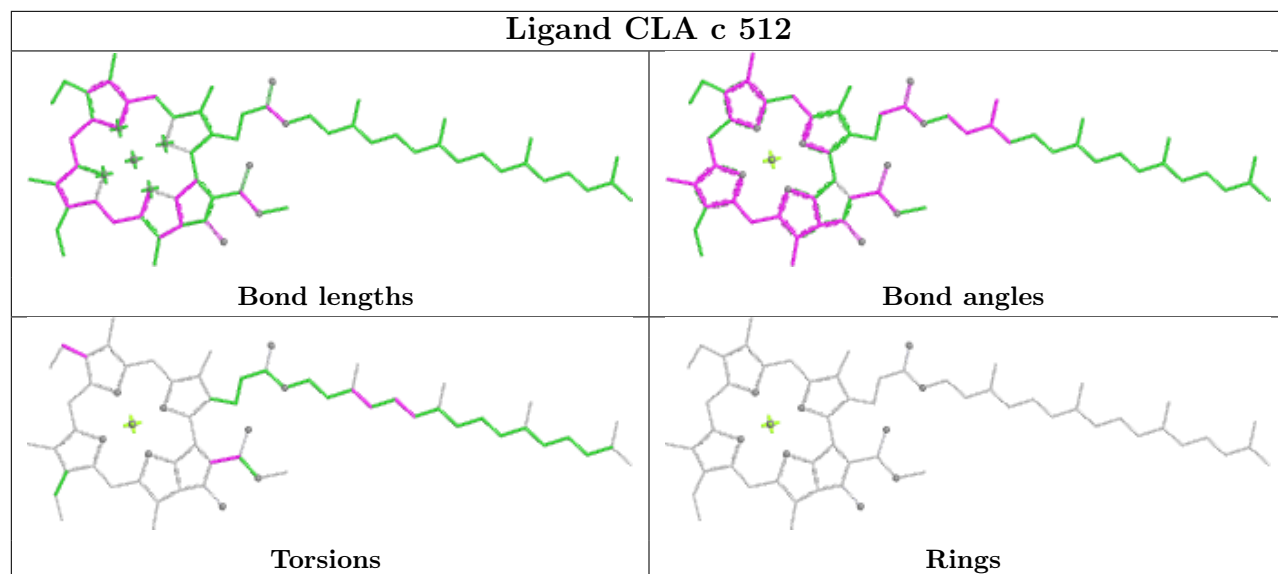
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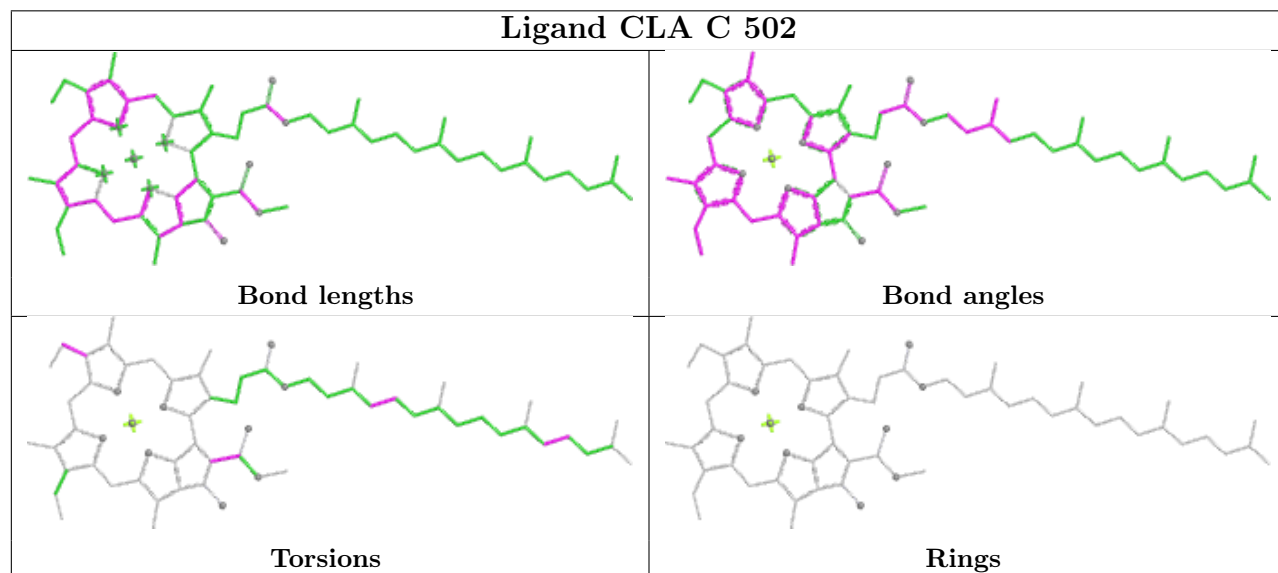
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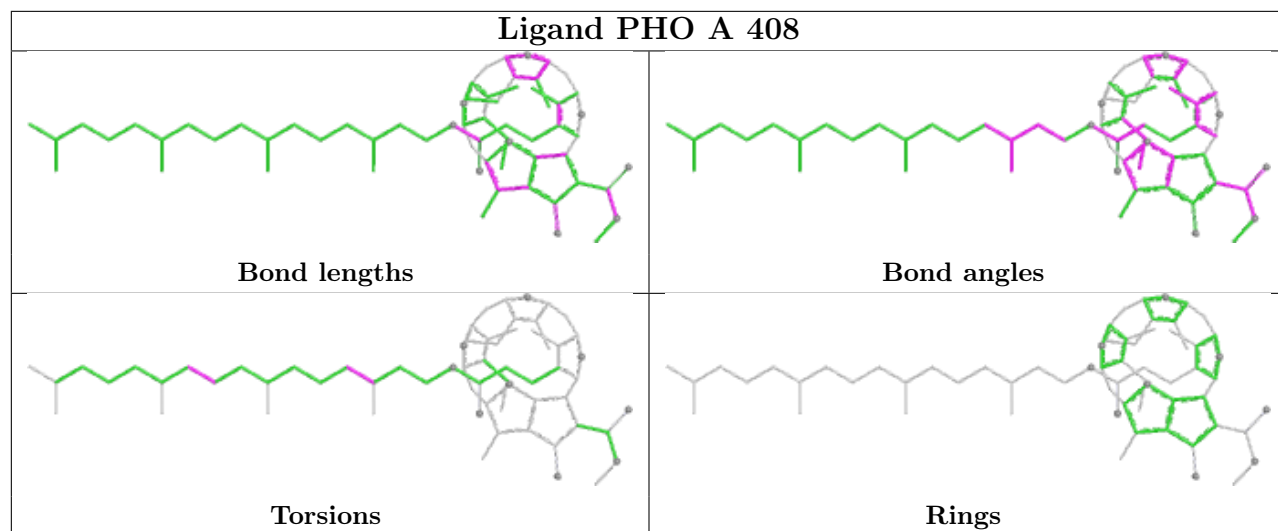
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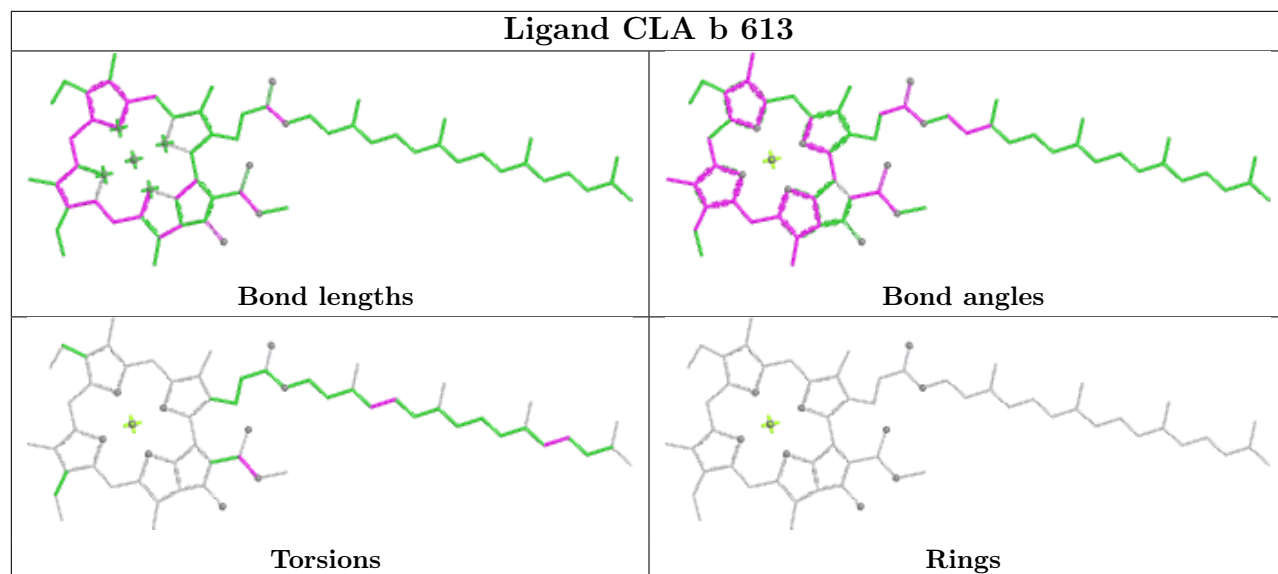
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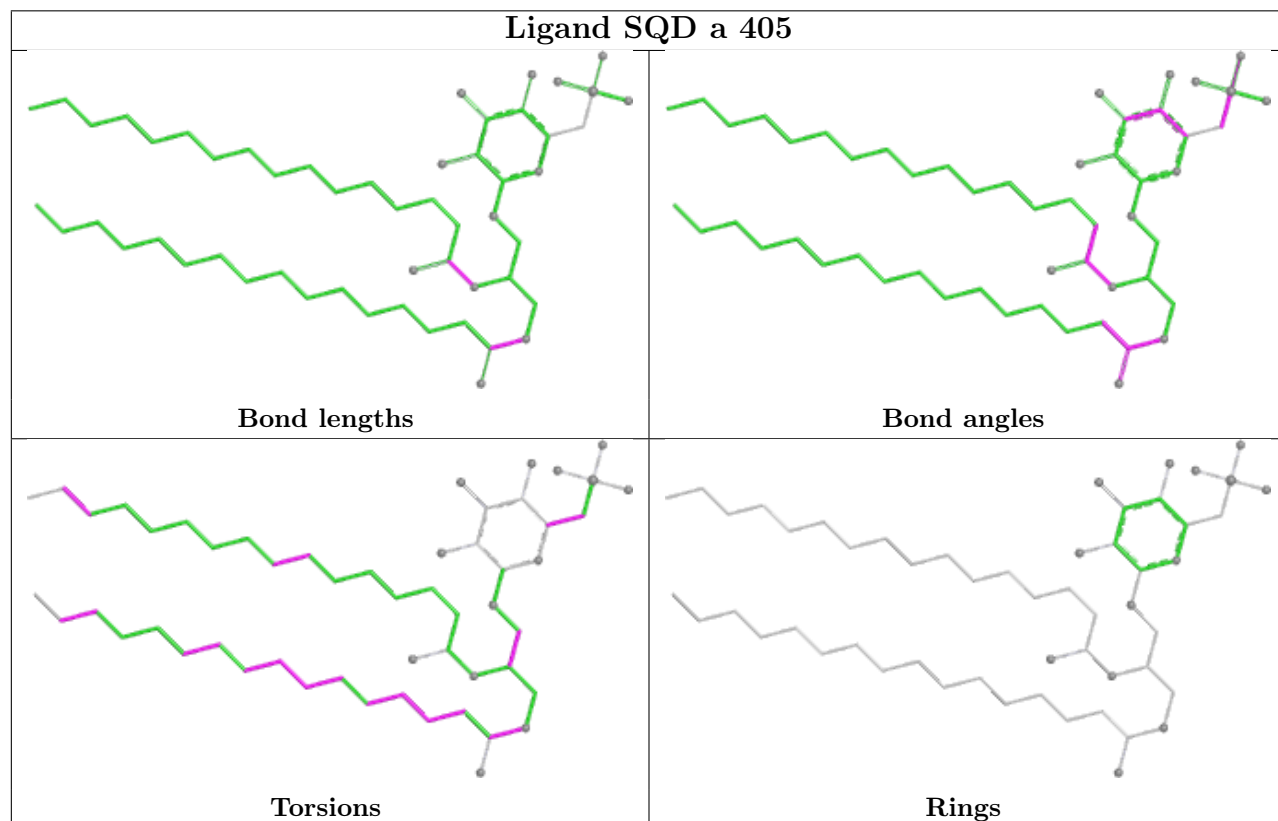
Ligand PHO A 408



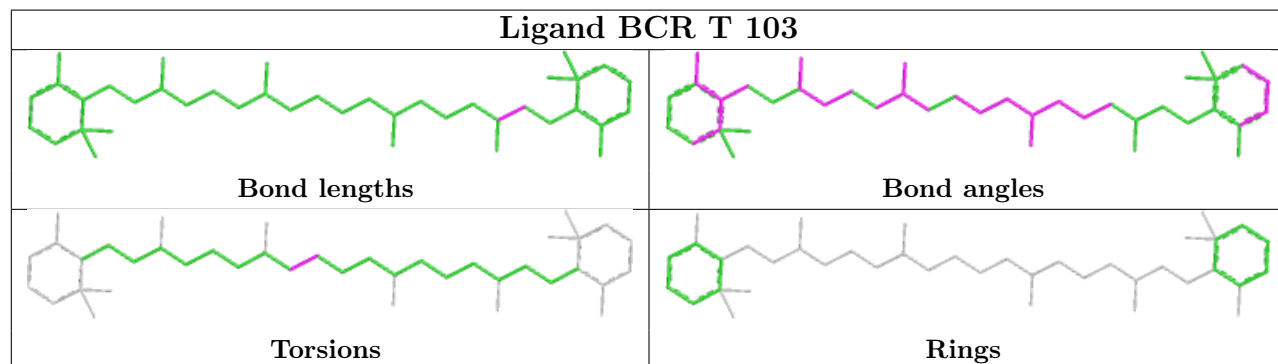
Ligand CLA b 613

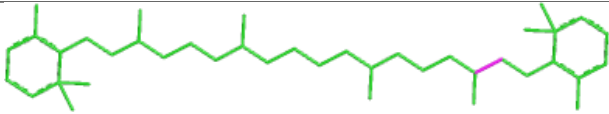
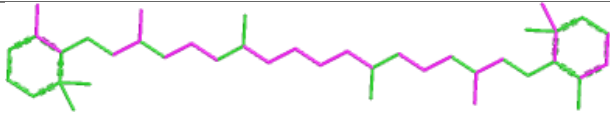
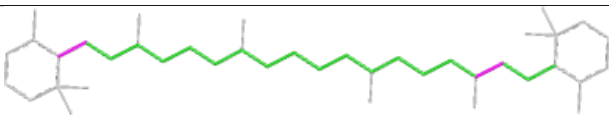
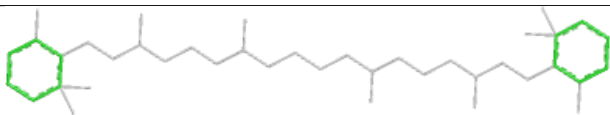


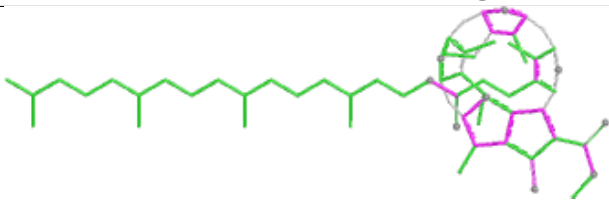
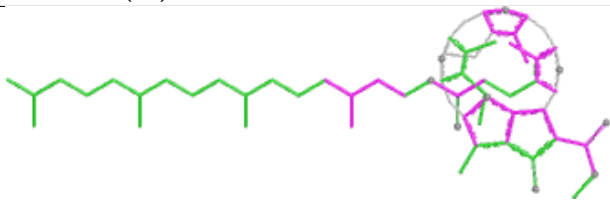
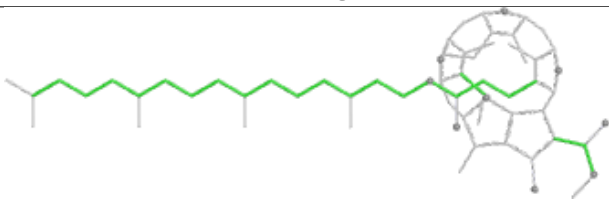
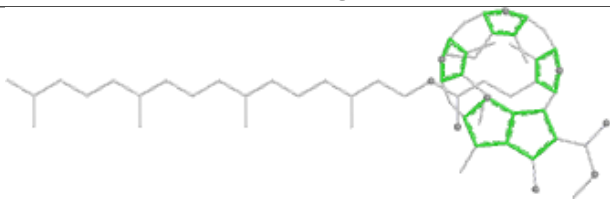
Ligand SQD a 405

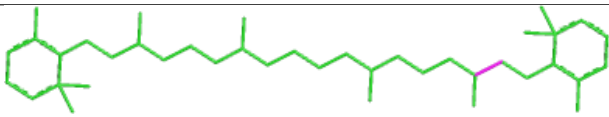
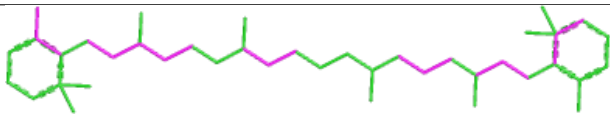
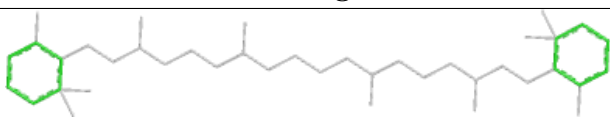


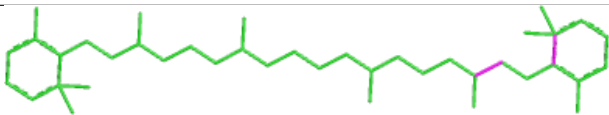
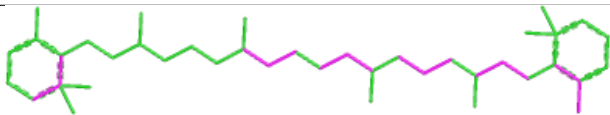
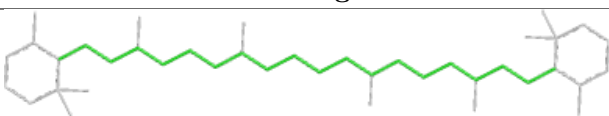
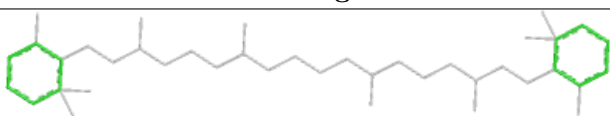
Ligand BCR T 103



Ligand BCR Y 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PHO A 409 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

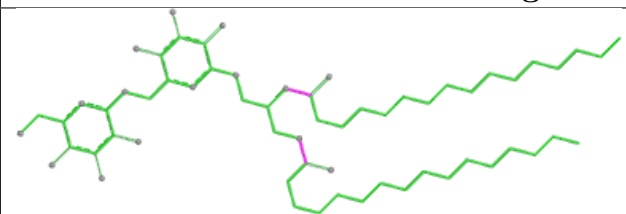
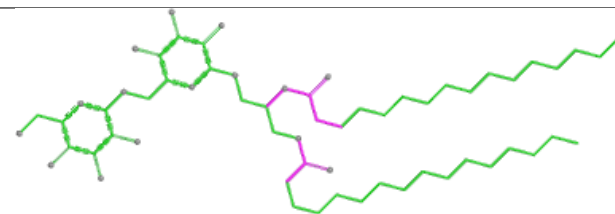
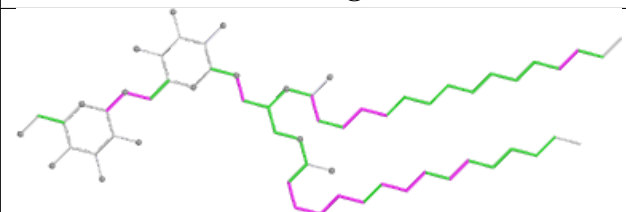
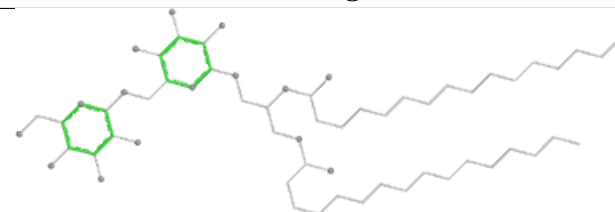
Ligand BCR b 628	
 Bond lengths	 Bond angles
 Torsions	 Rings

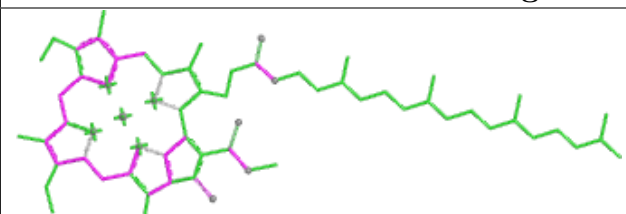
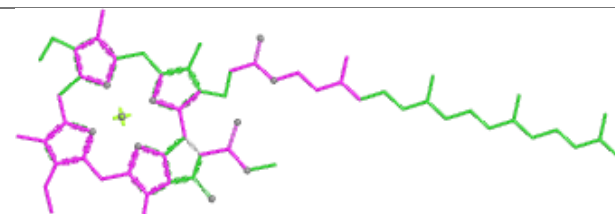
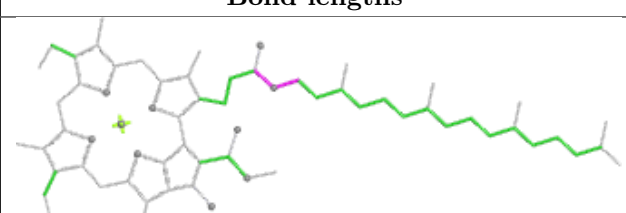
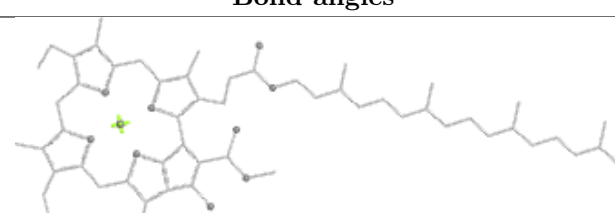
Ligand PL9 d 405 (B)	
Bond lengths	Bond angles
Torsions	Rings

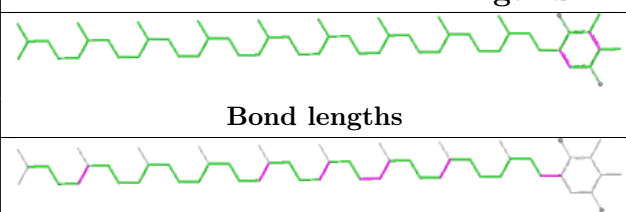
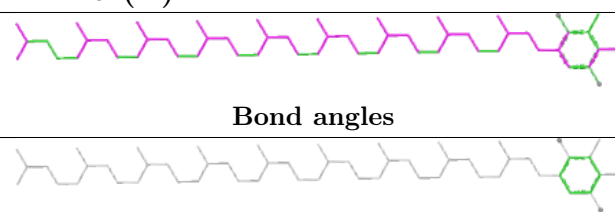
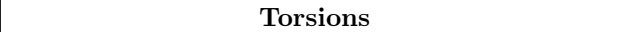
Ligand PL9 D 405 (A)	
Bond lengths	Bond angles
Torsions	Rings

Ligand DGD e 101	
Bond lengths	Bond angles
Torsions	Rings

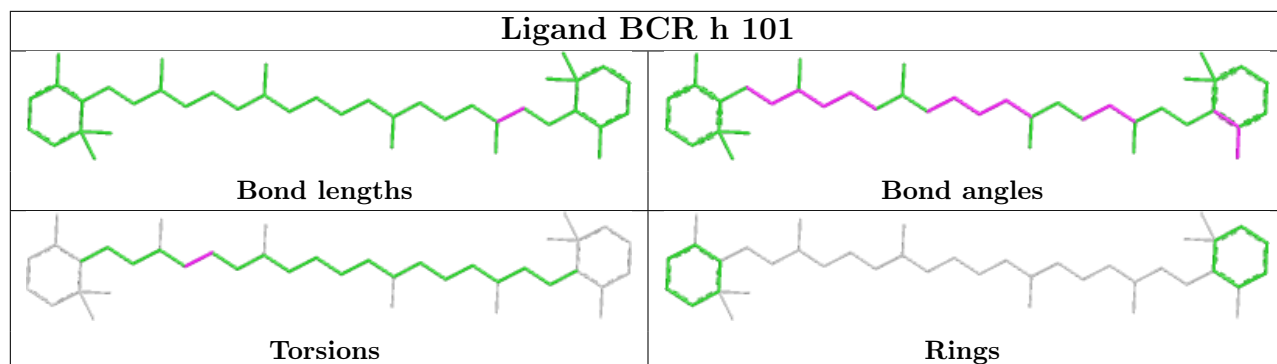
Ligand CLA C 507	
Bond lengths	Bond angles
Torsions	Rings

Ligand DGD c 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

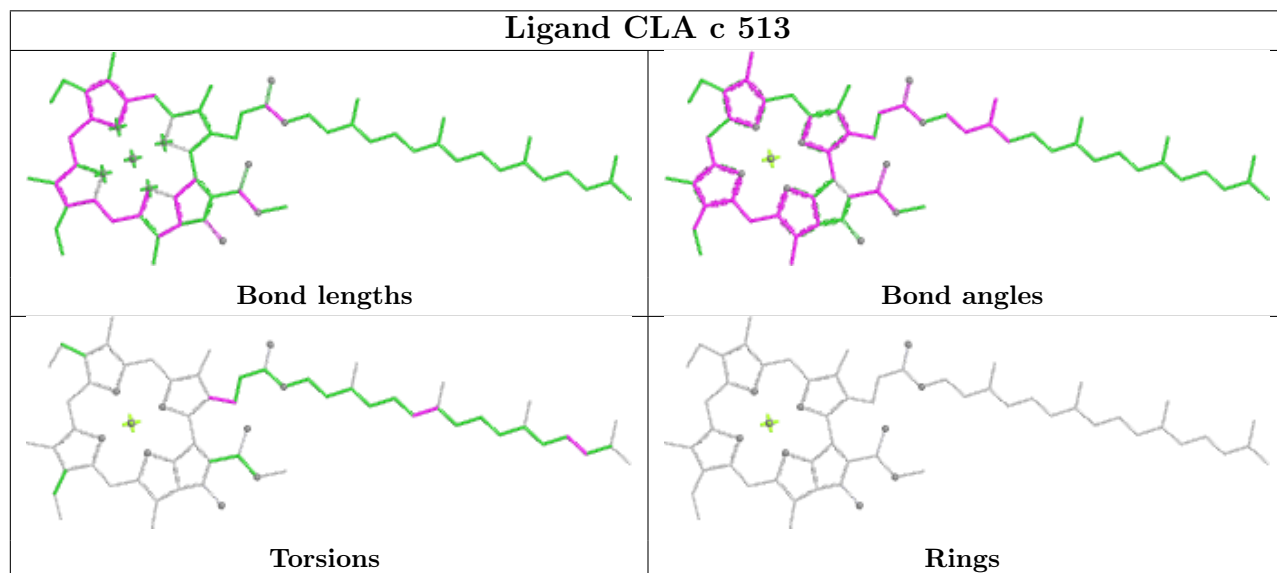
Ligand CLA C 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 A 419 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

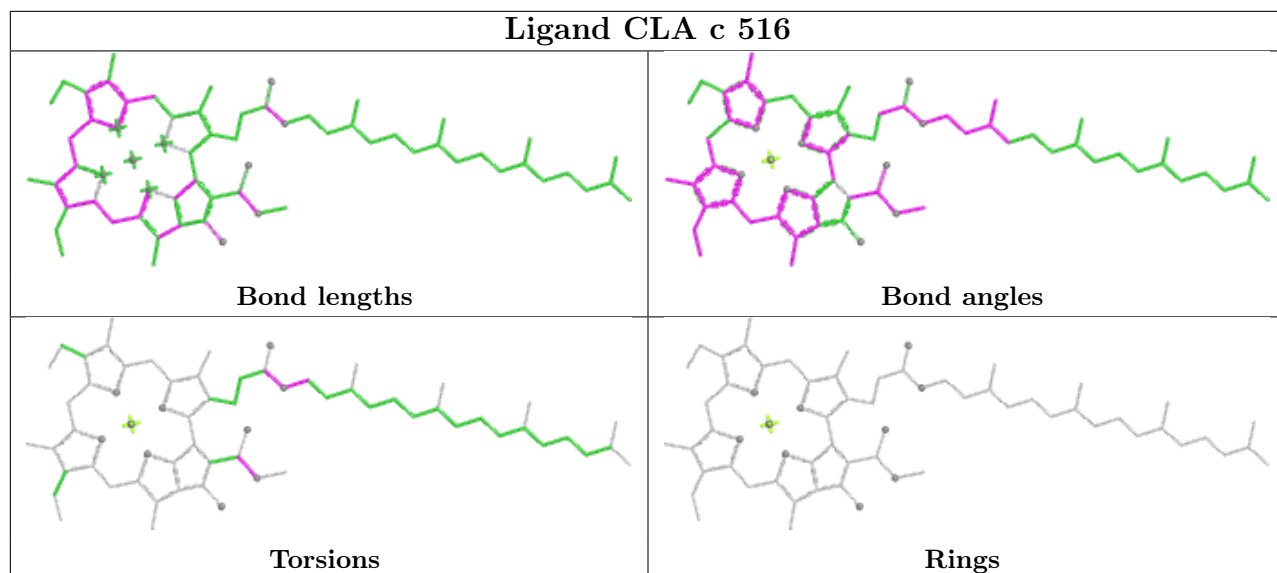
Ligand BCR h 101

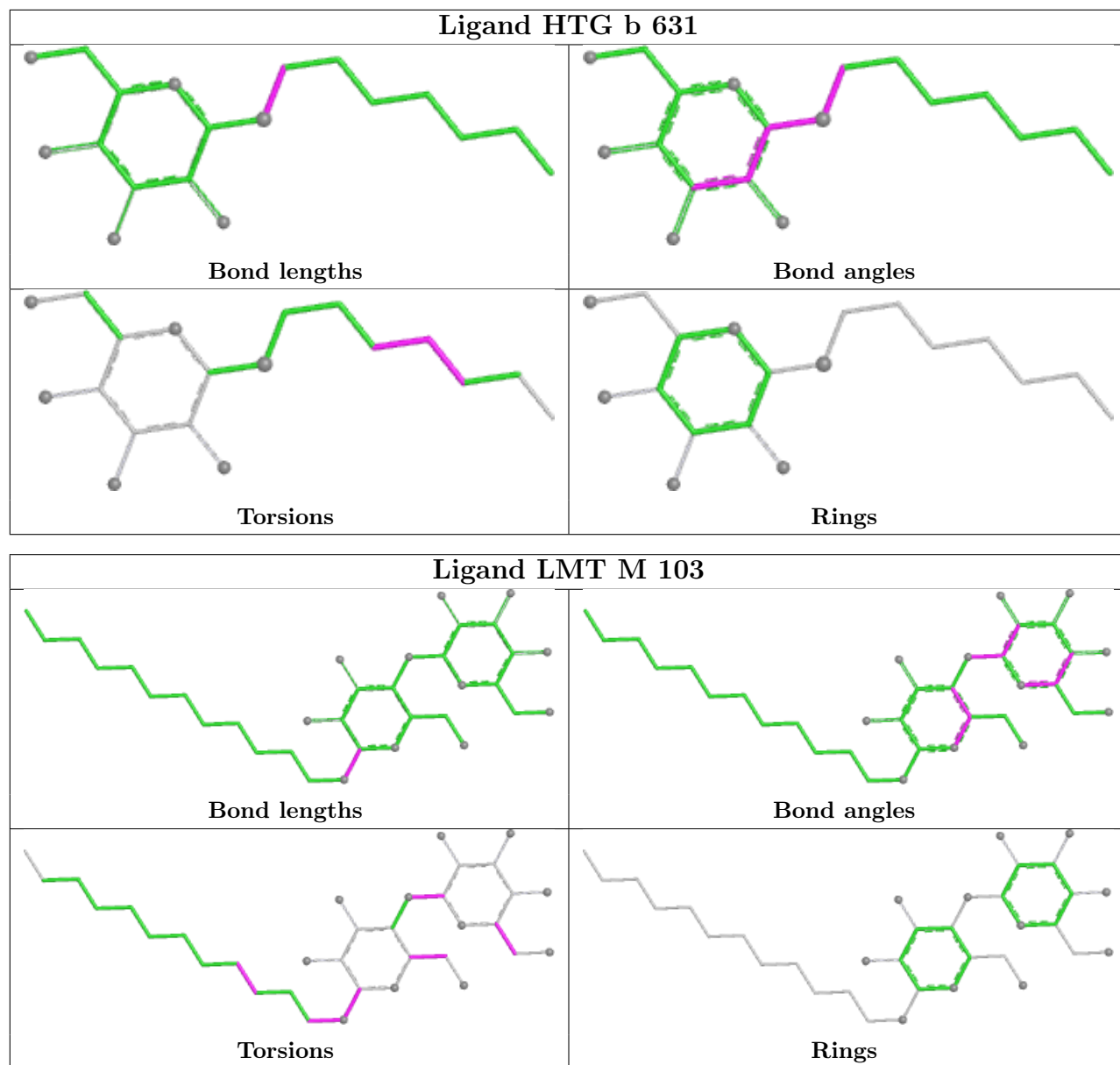


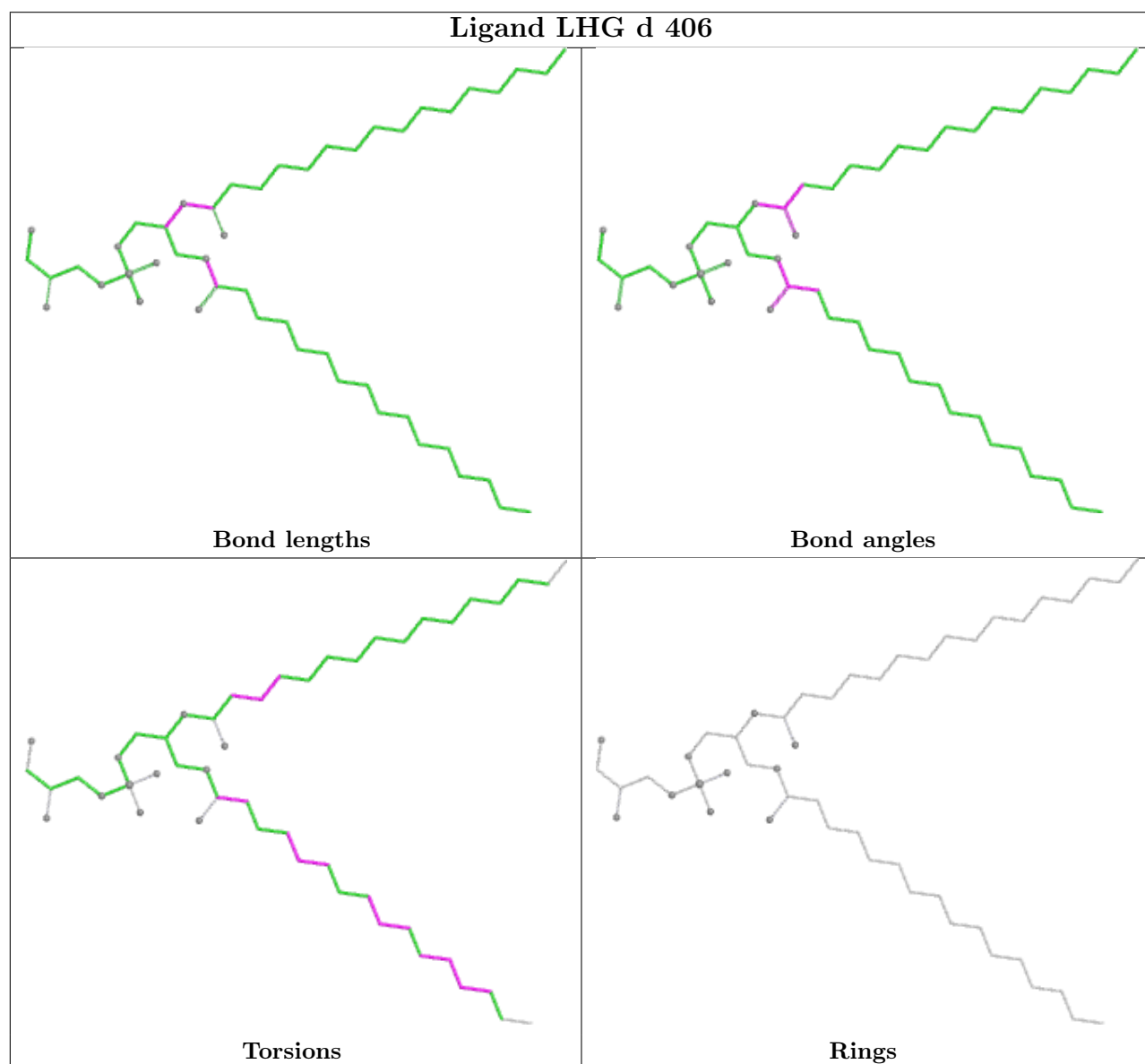
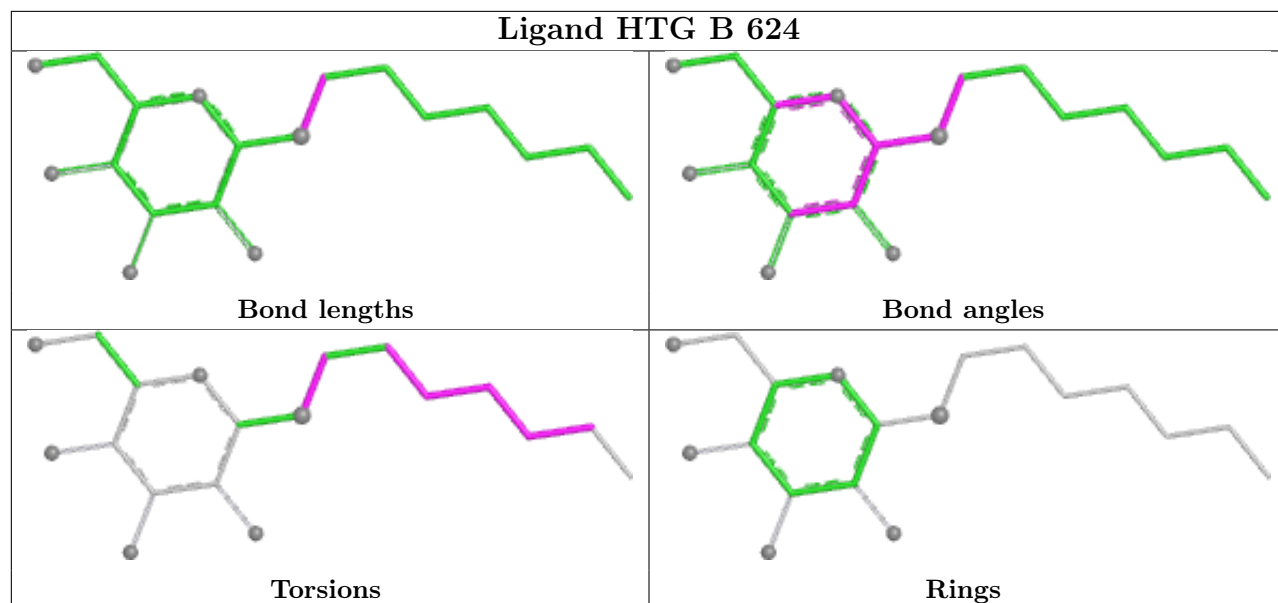
Ligand CLA c 513

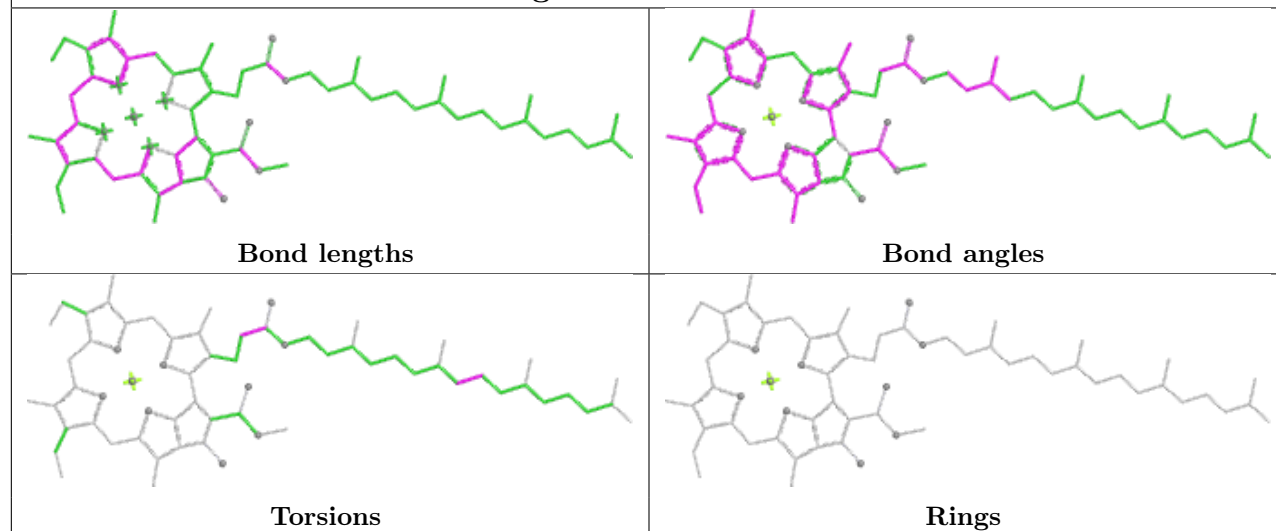
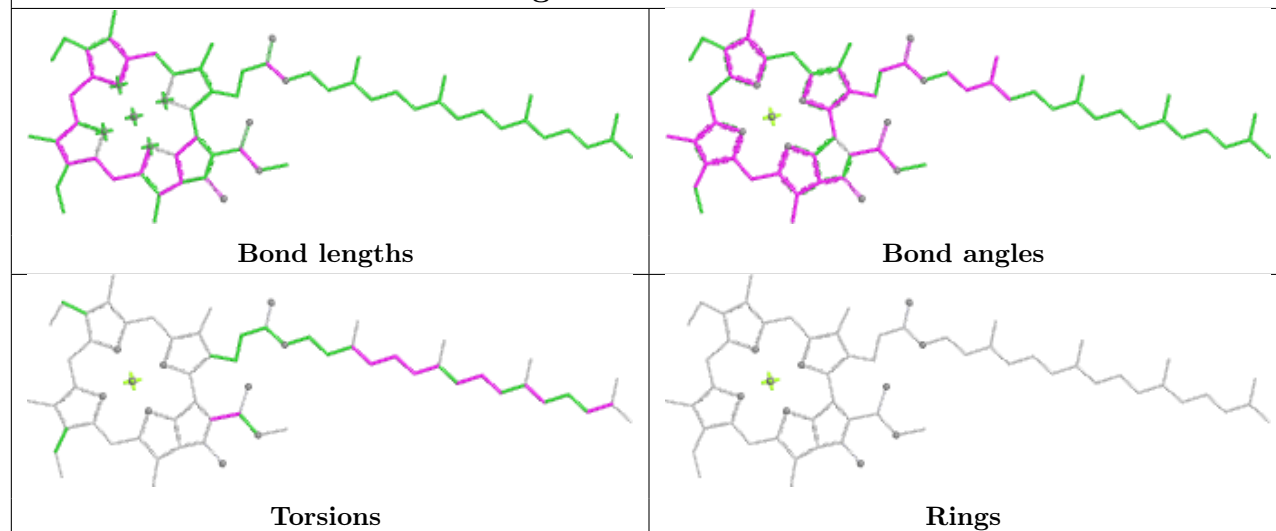


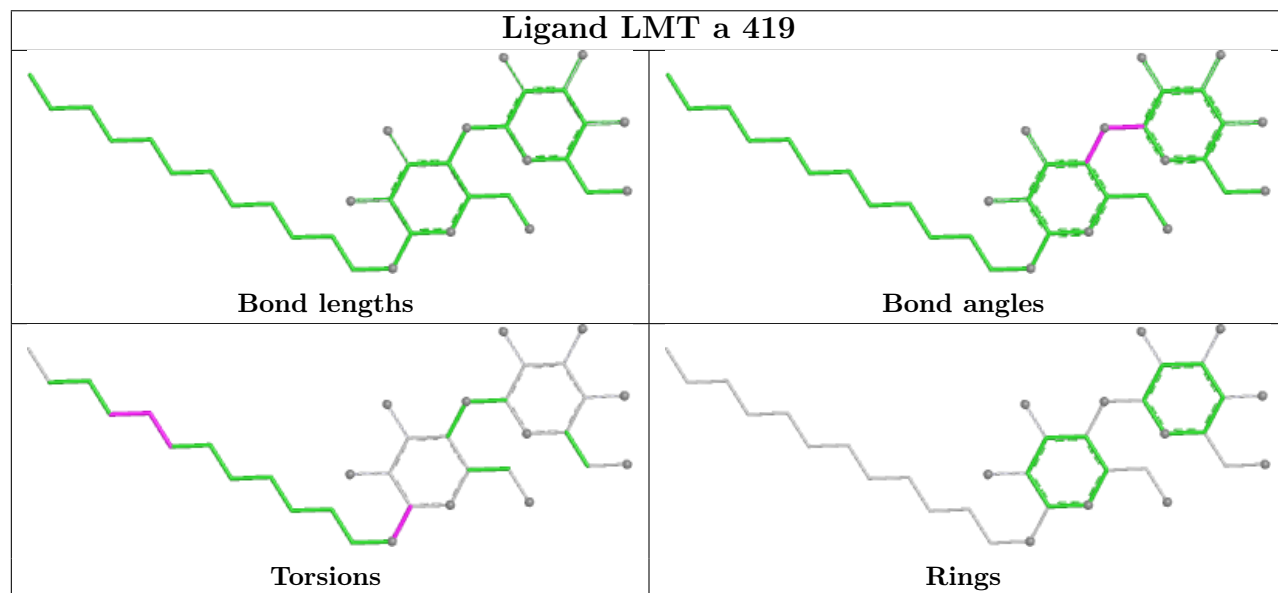
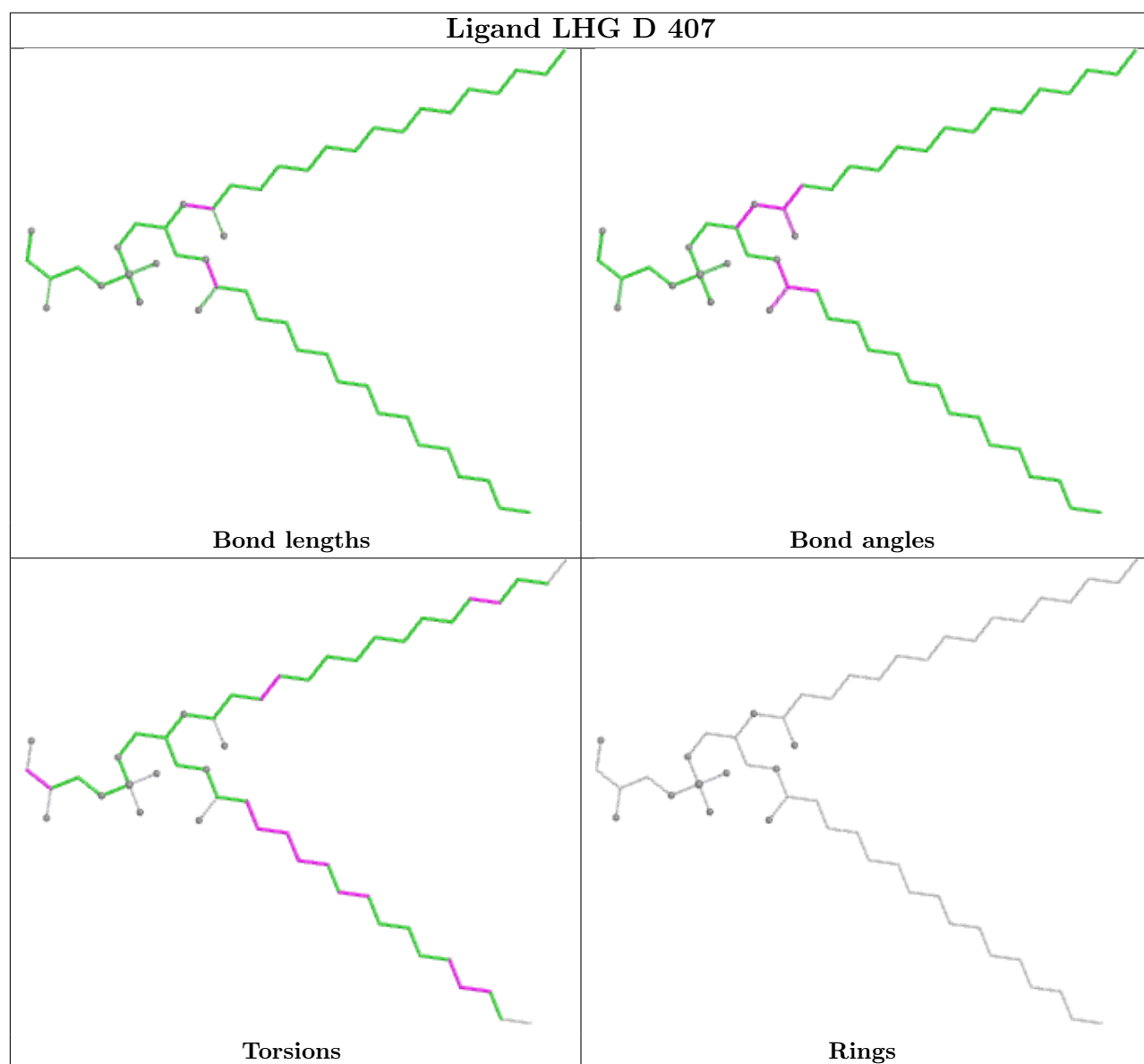
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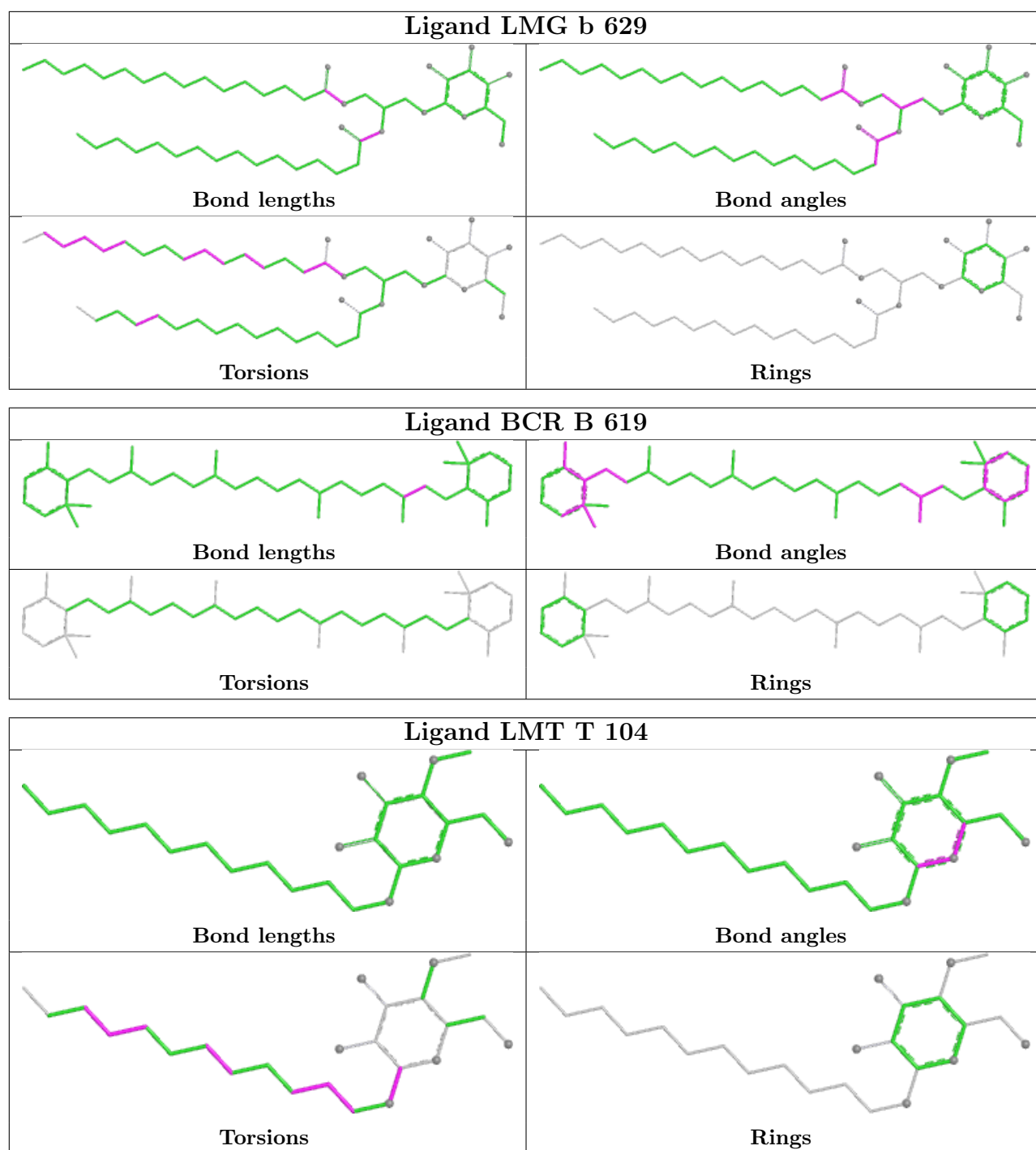




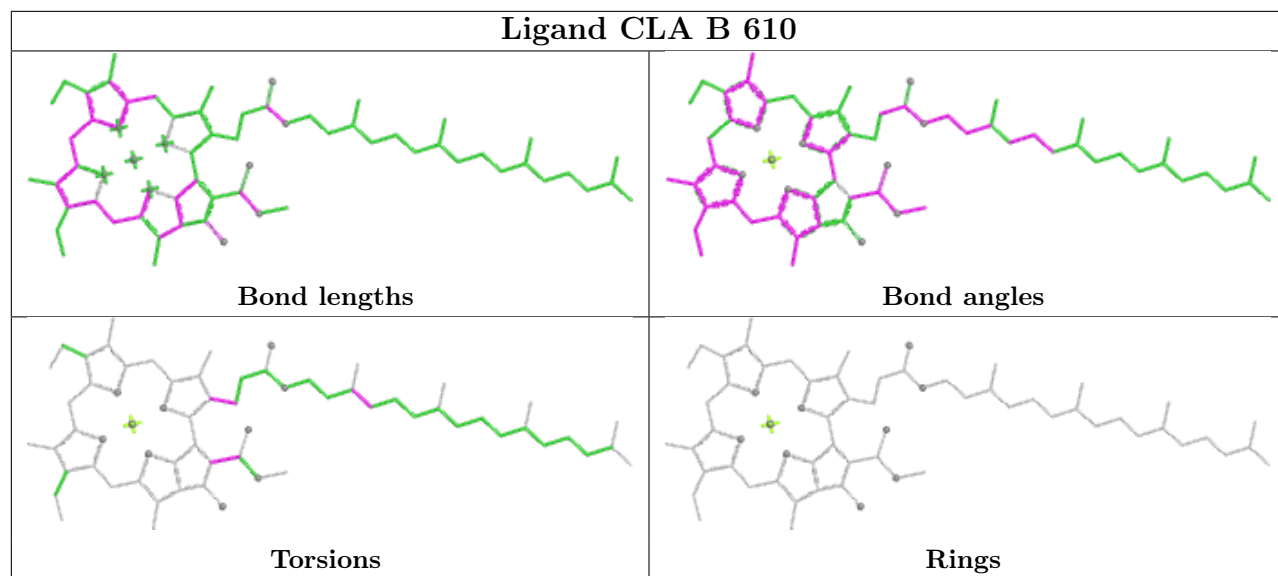


Ligand CLA B 613**Ligand CLA B 615**

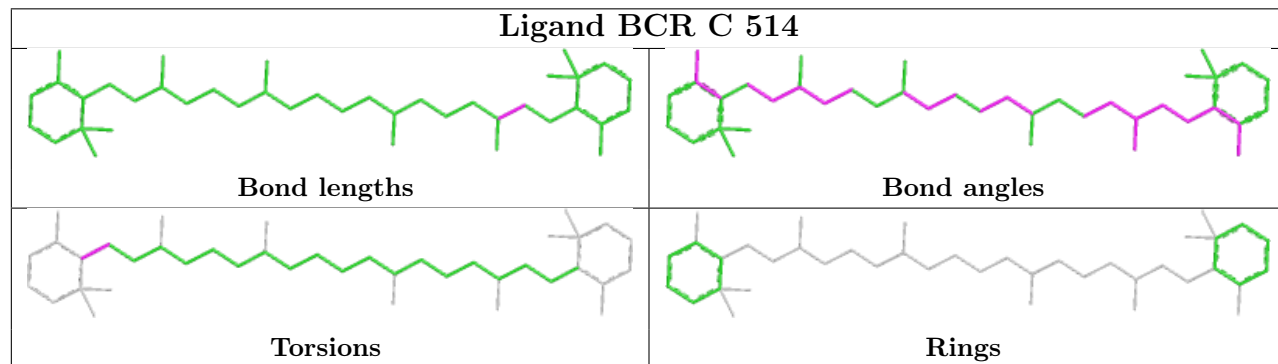


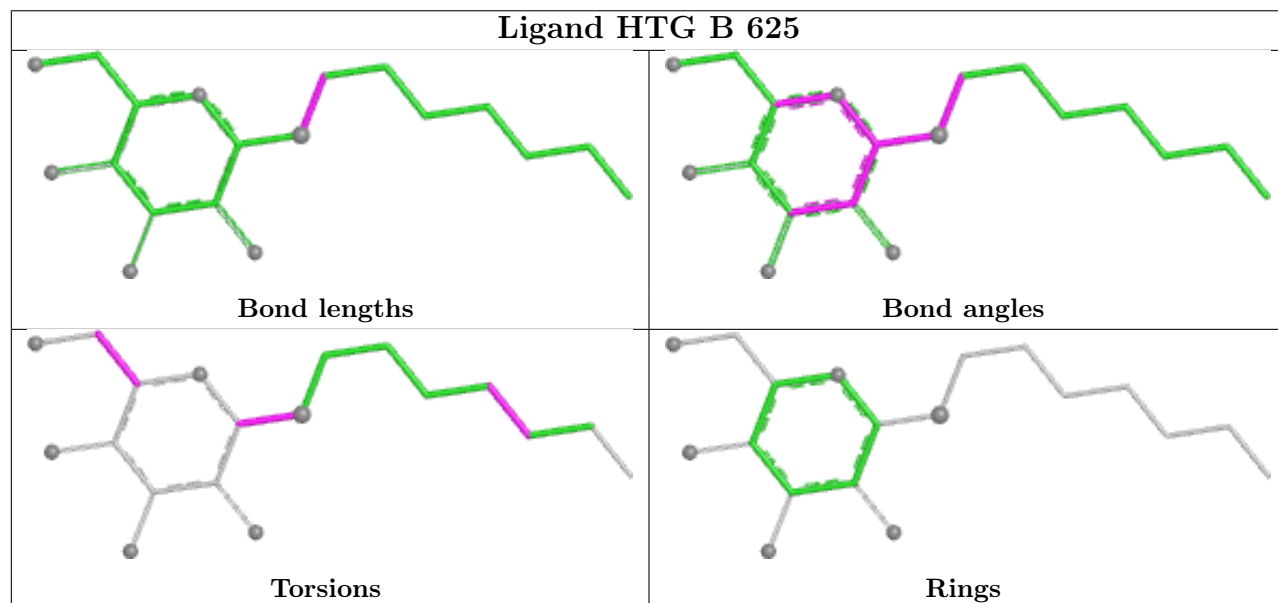
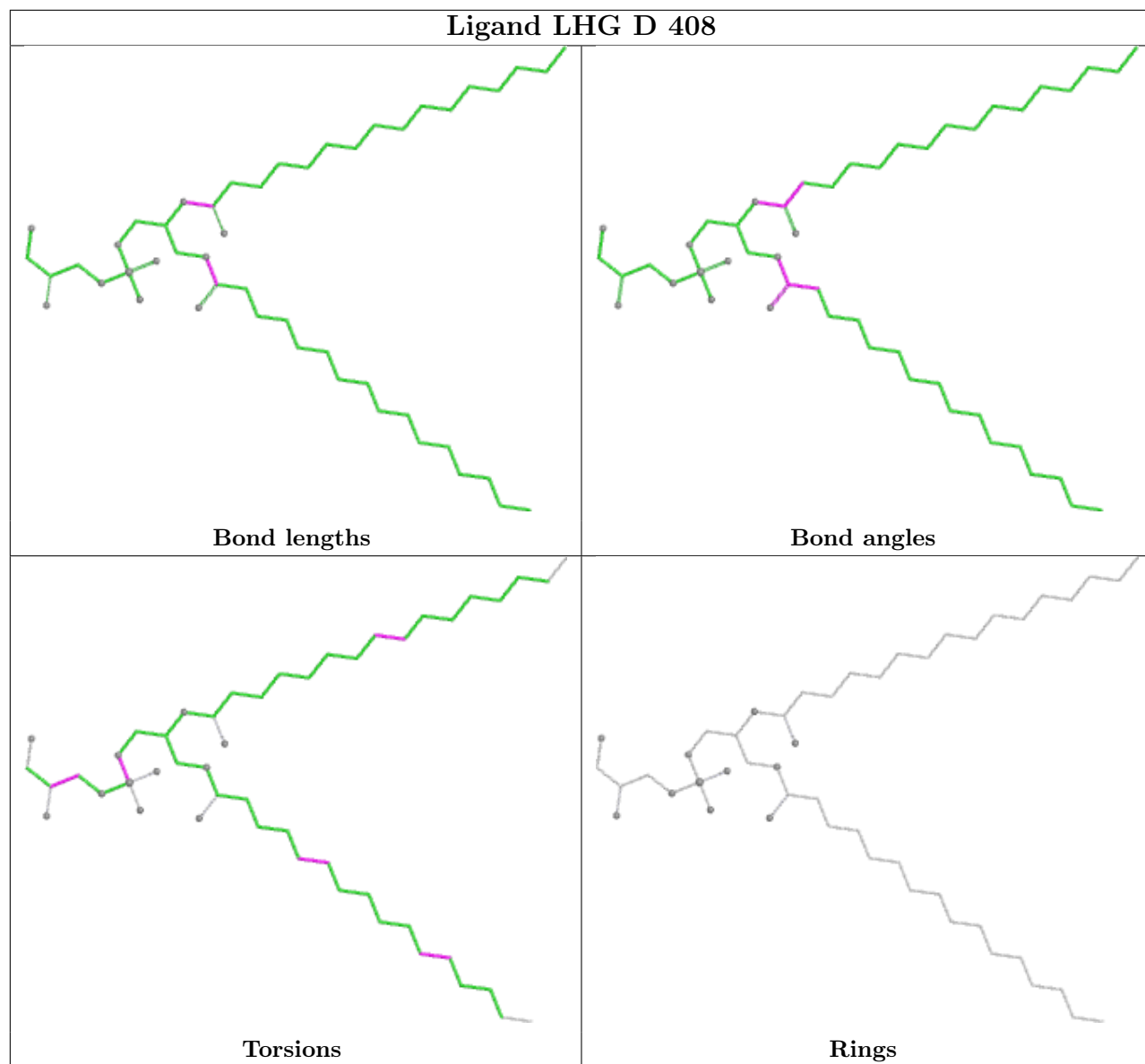


Ligand CLA B 610

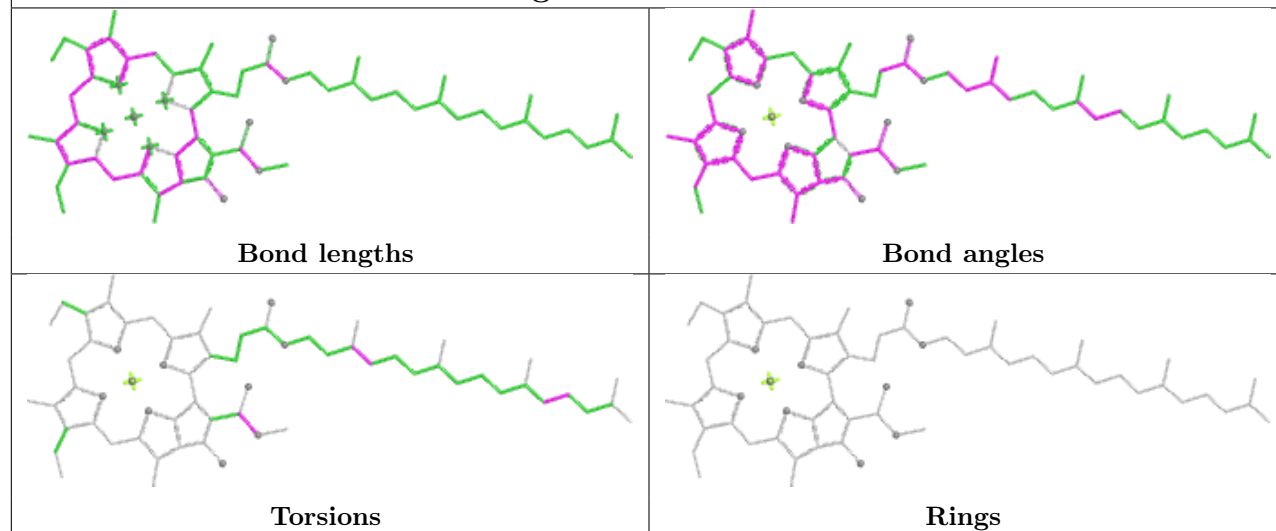


Ligand BCR C 514

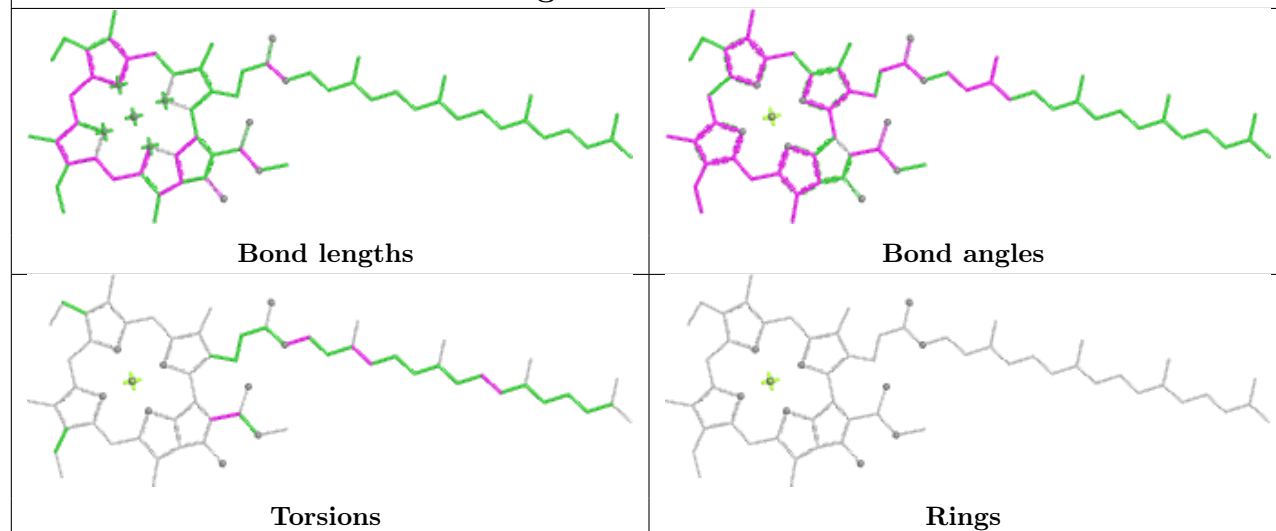




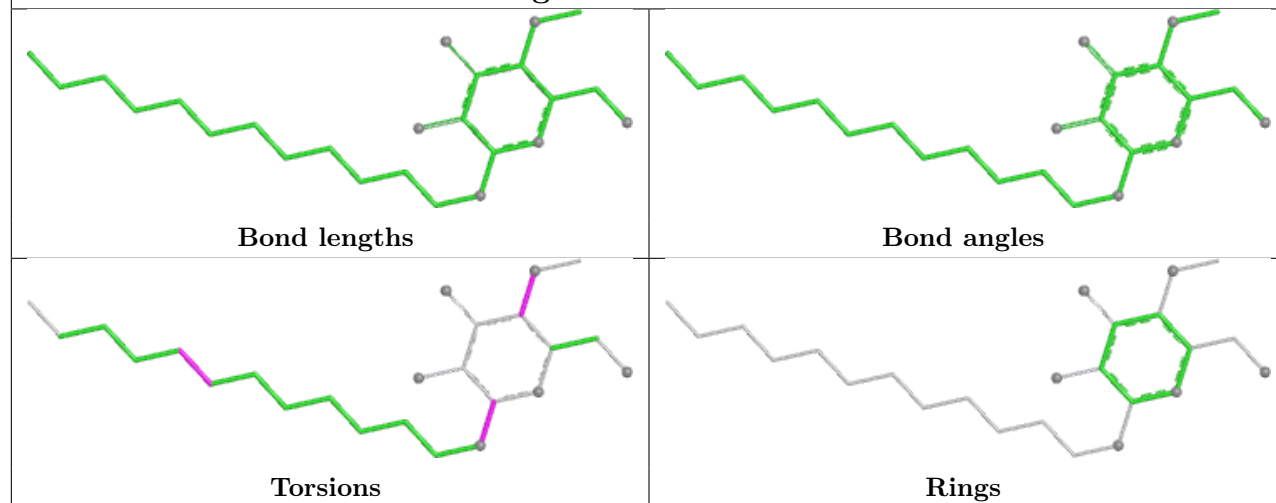
Ligand CLA B 605

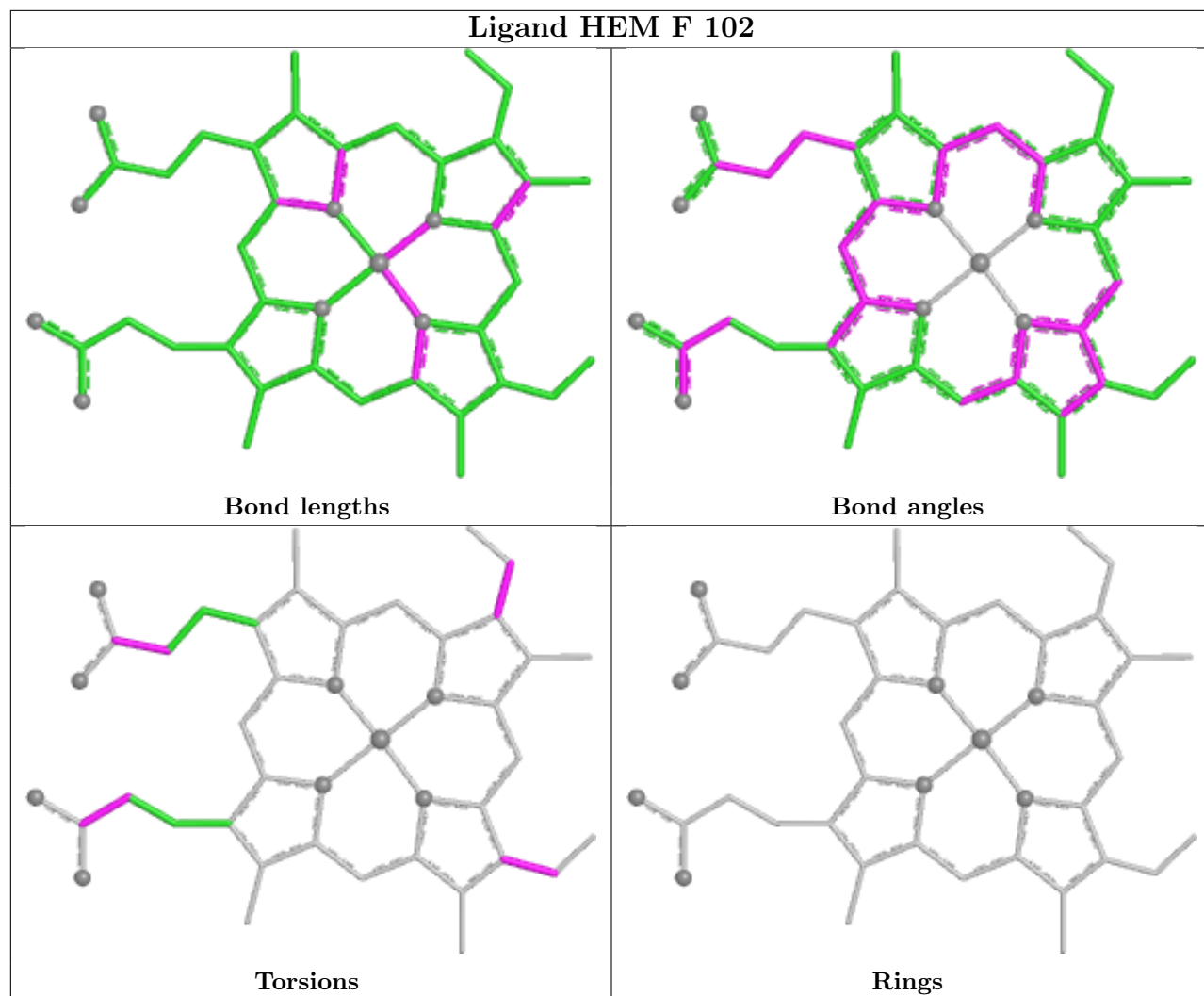


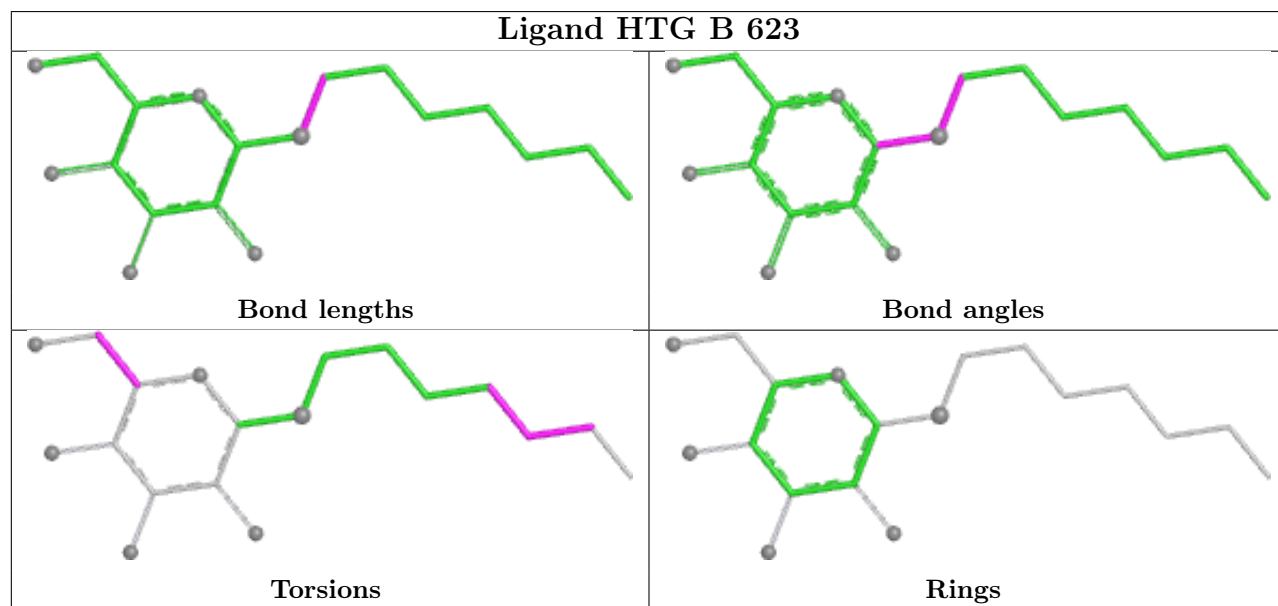
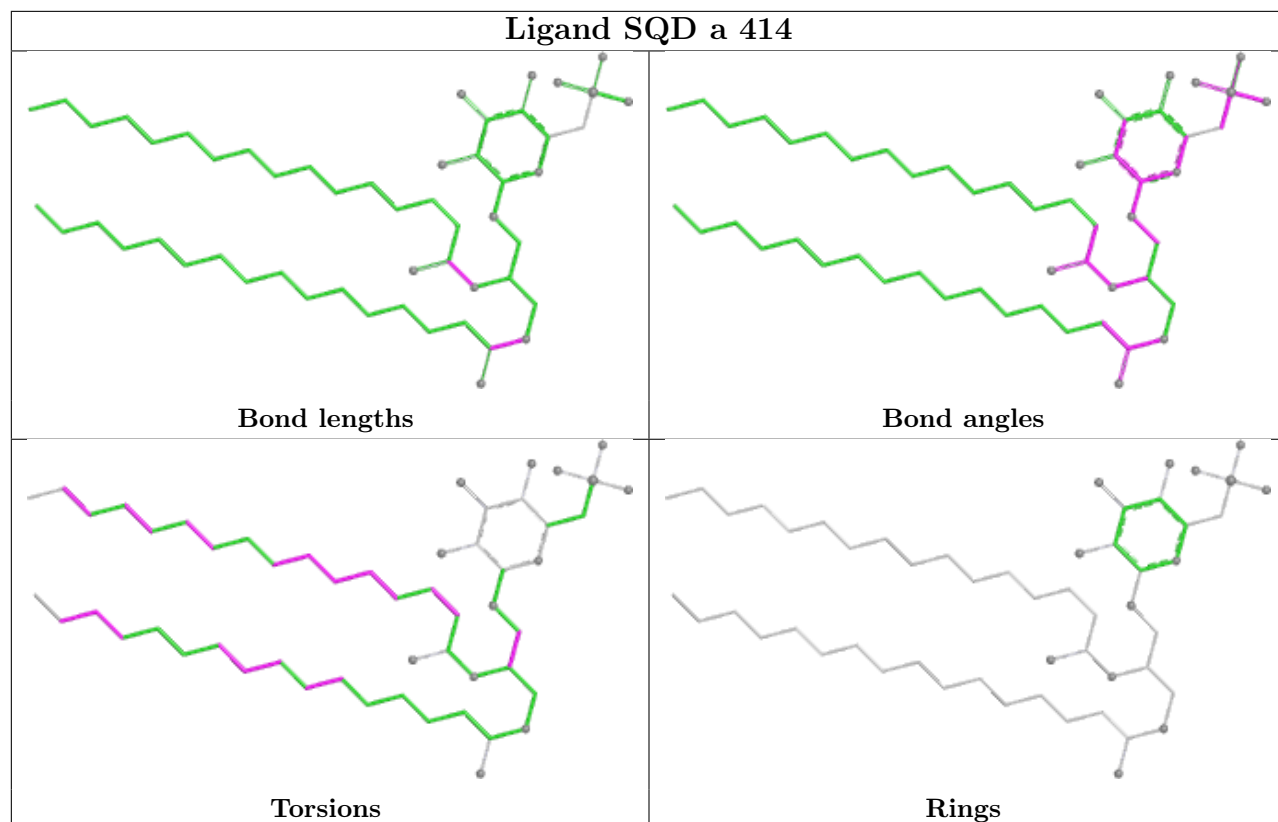
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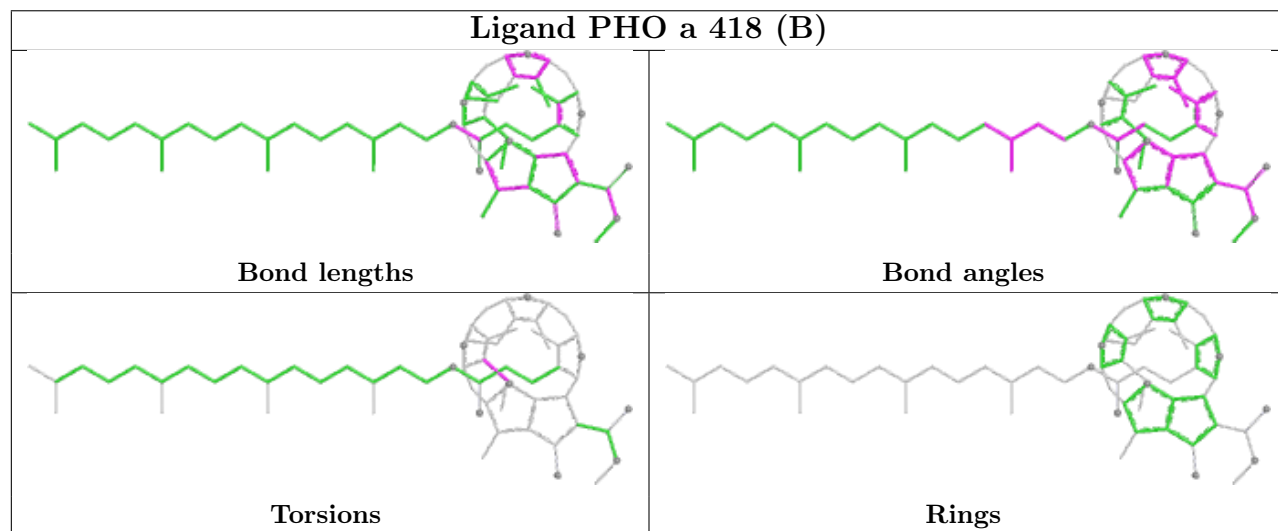
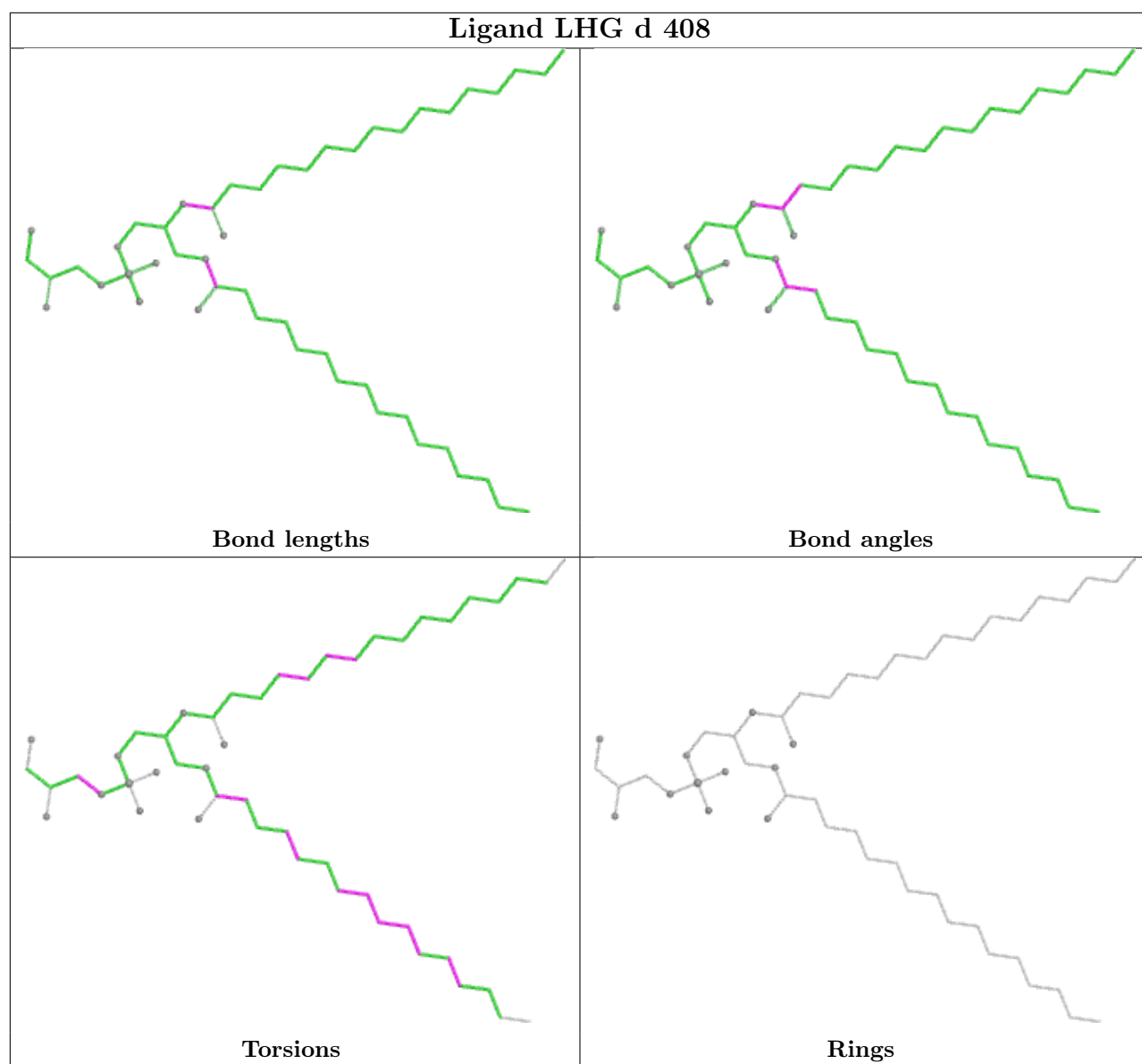


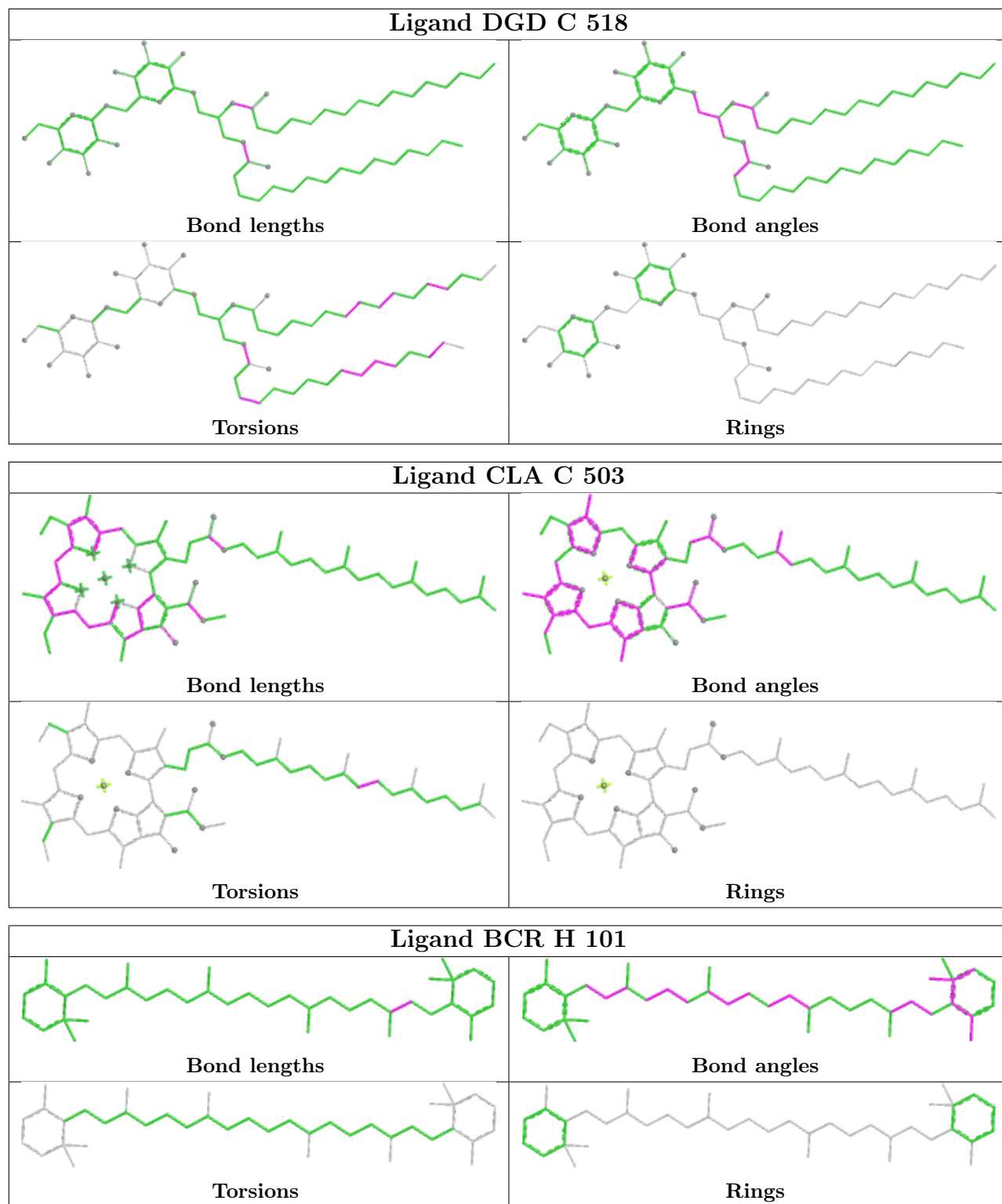
Ligand LMT b 630

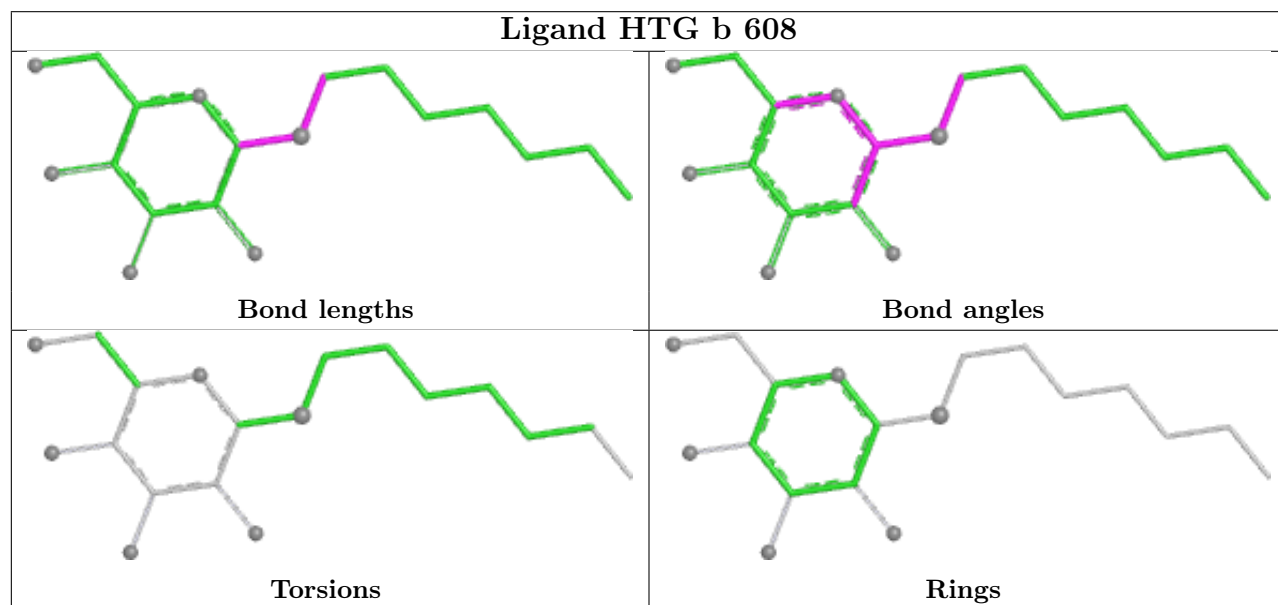
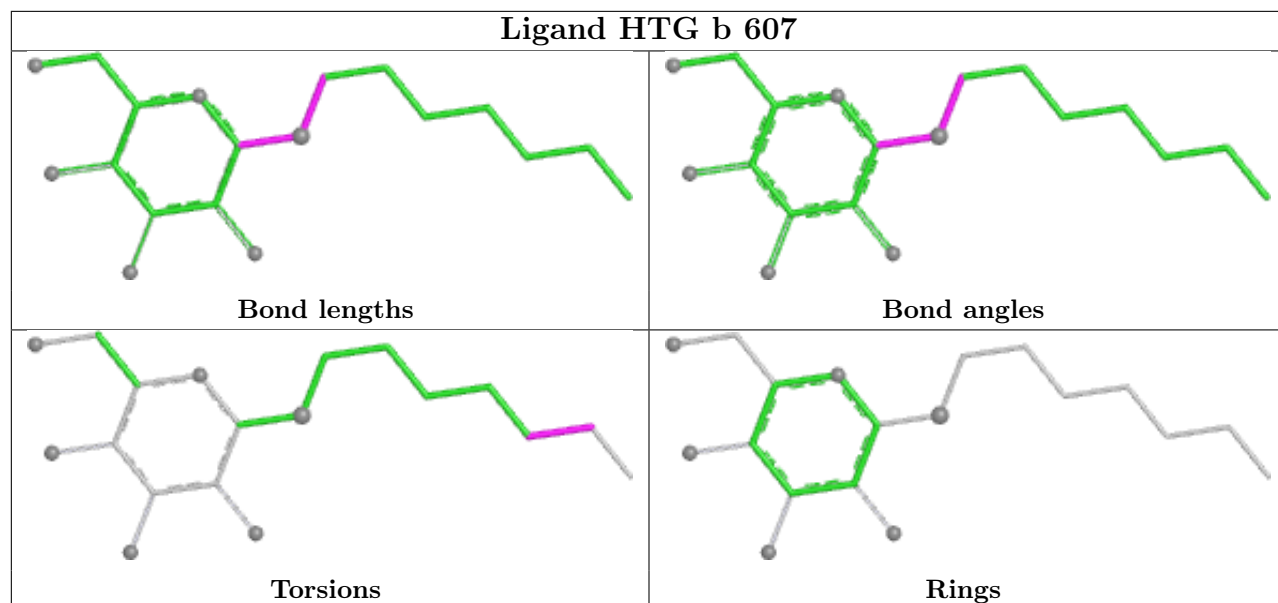


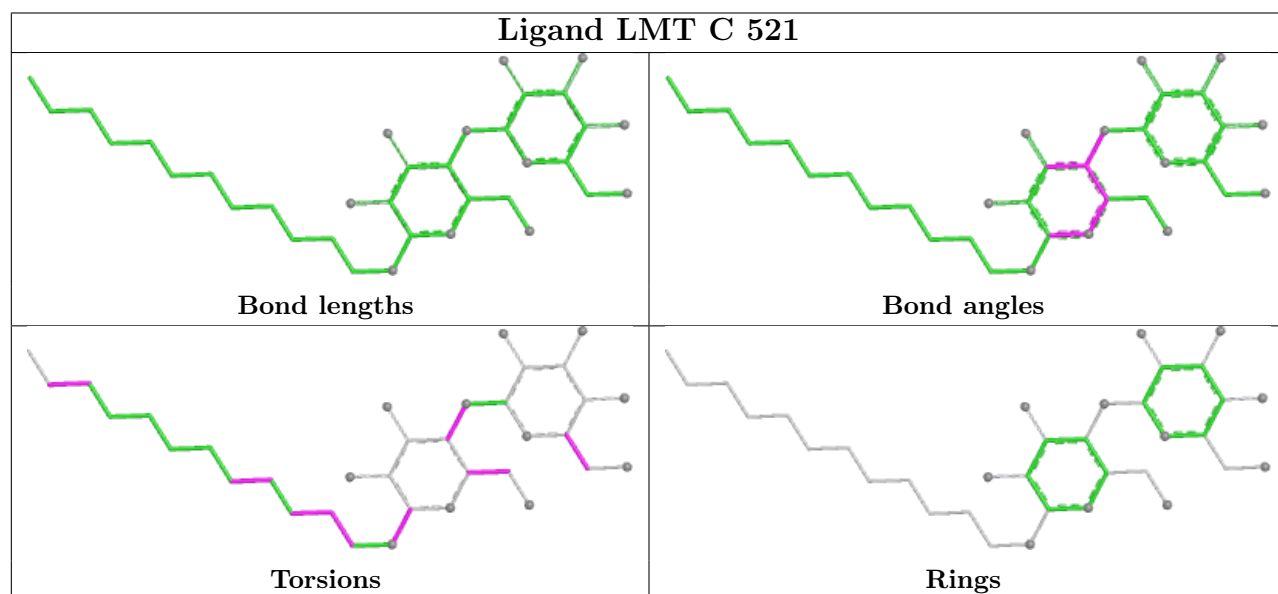
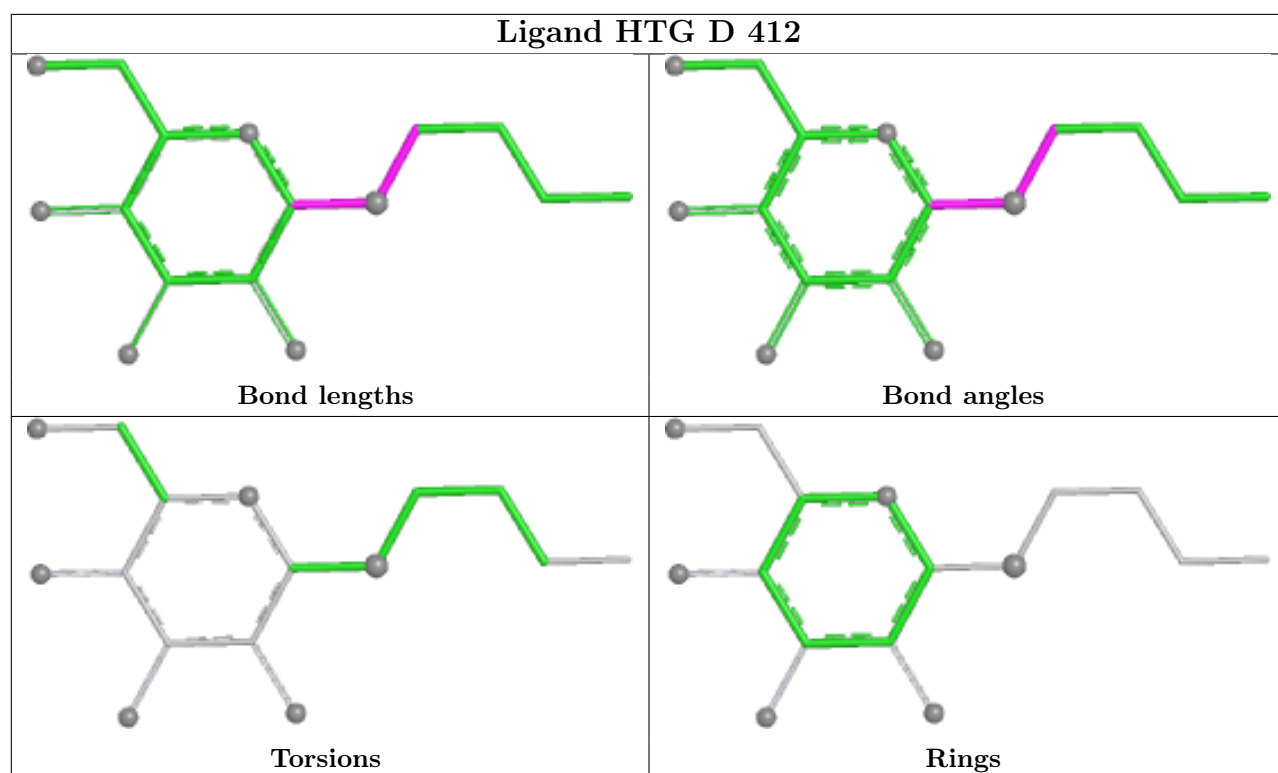




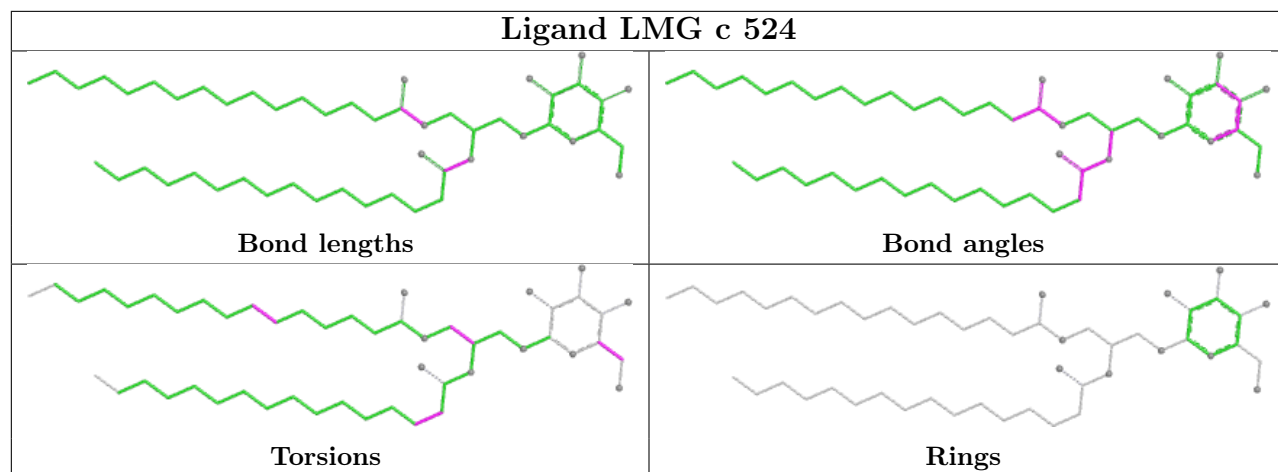




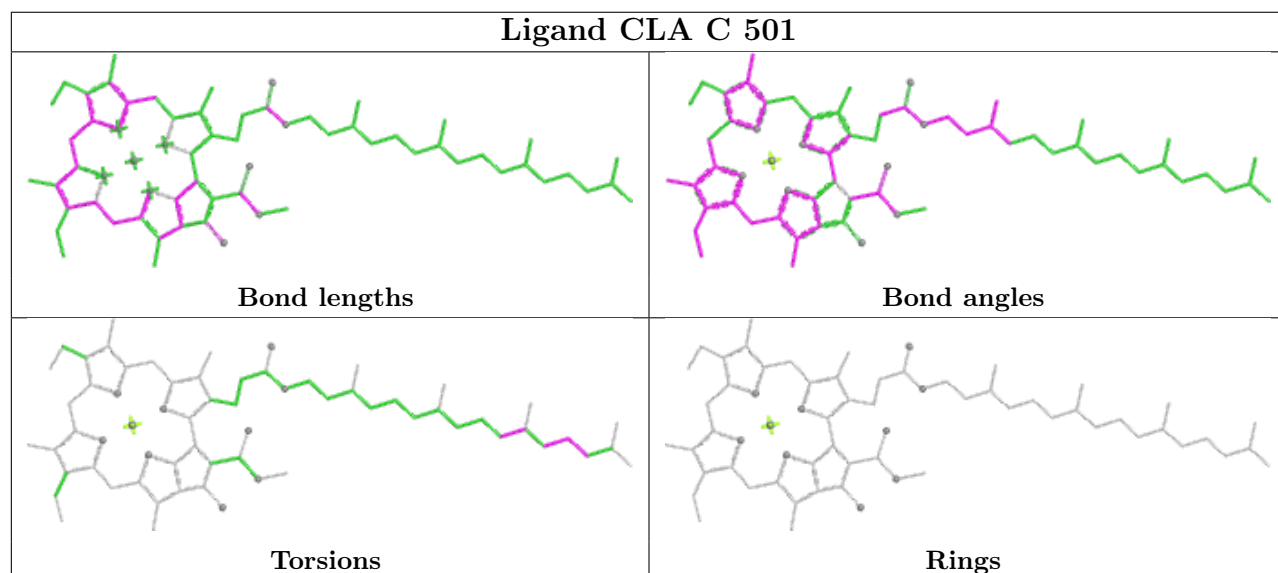




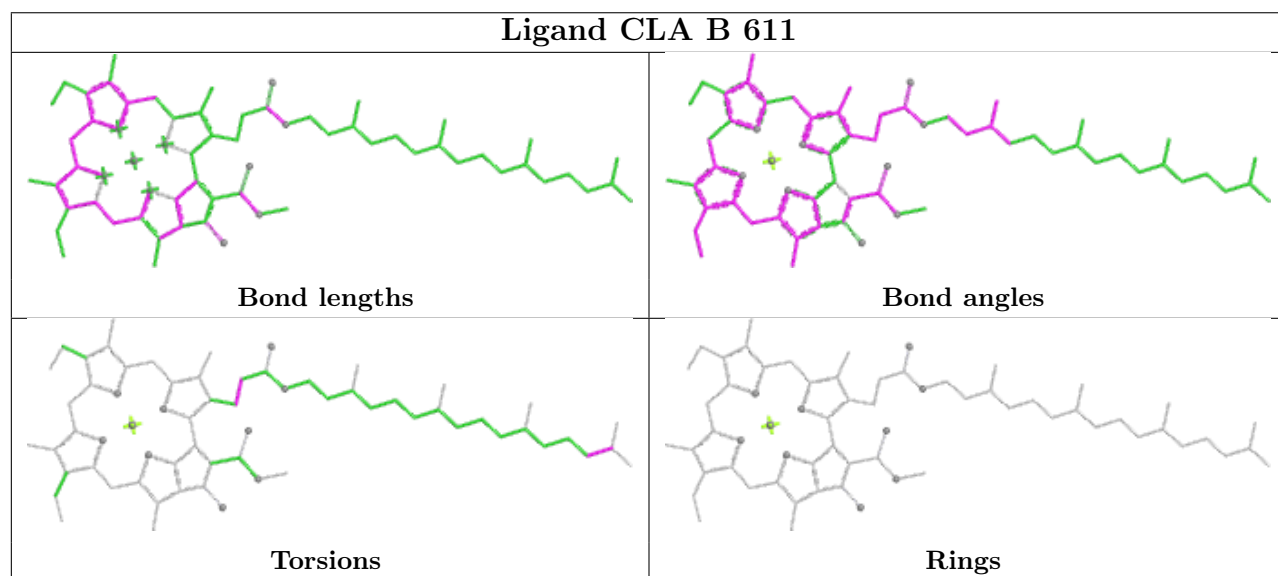
Ligand LMG c 524

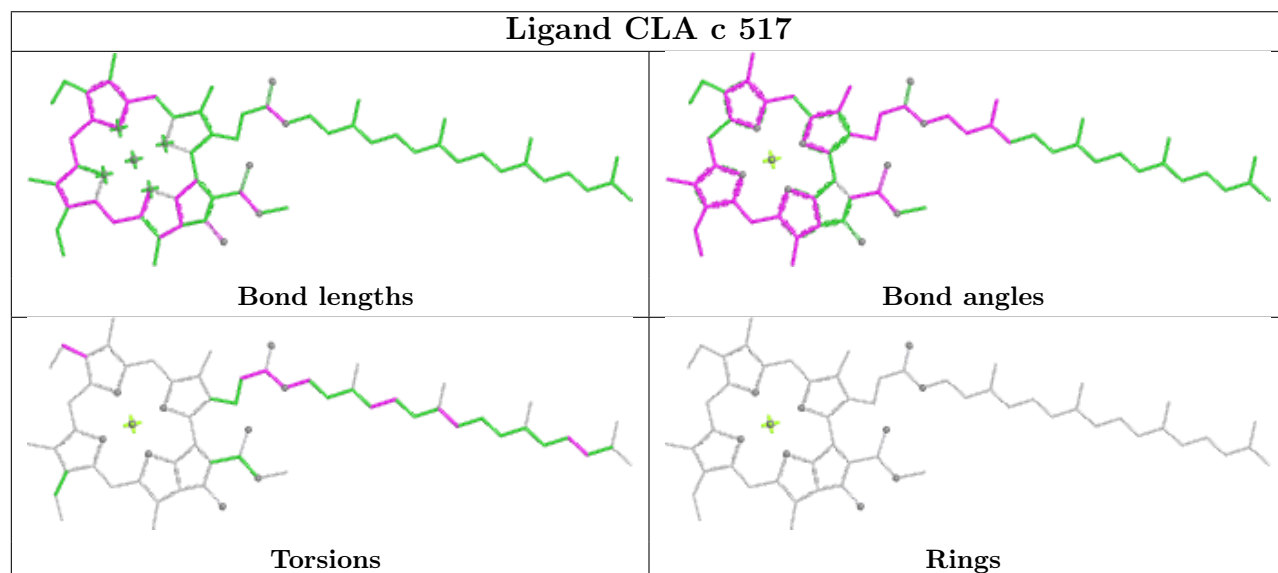
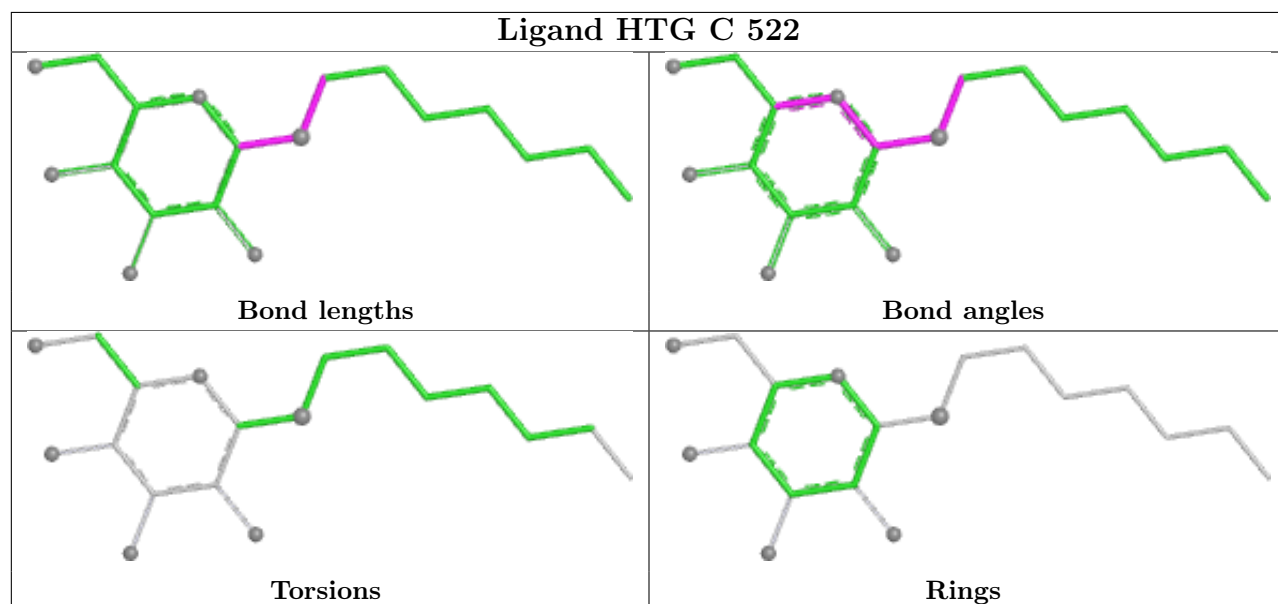
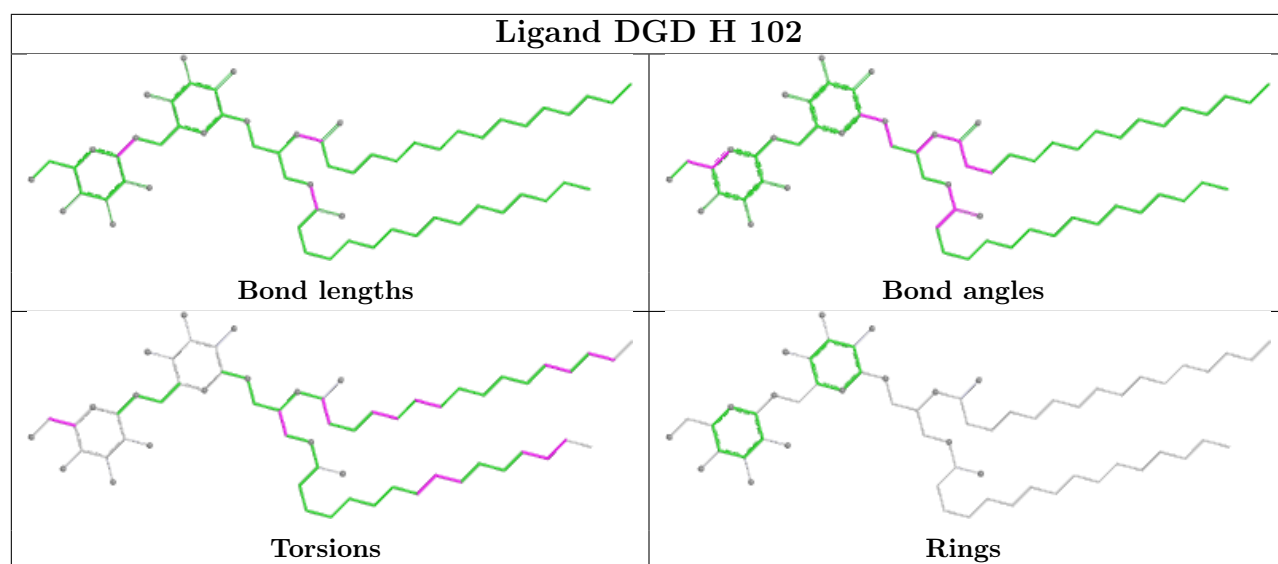


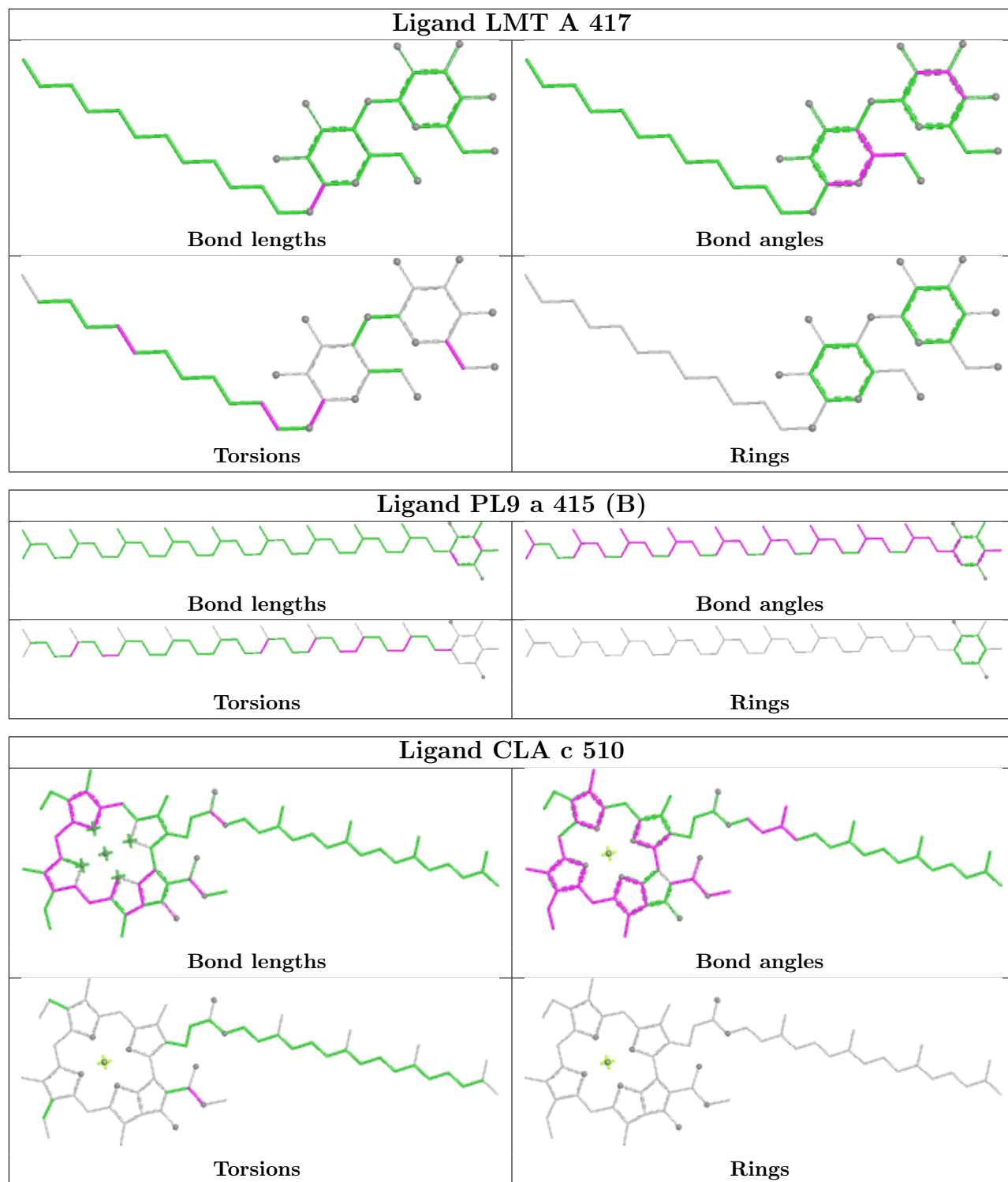
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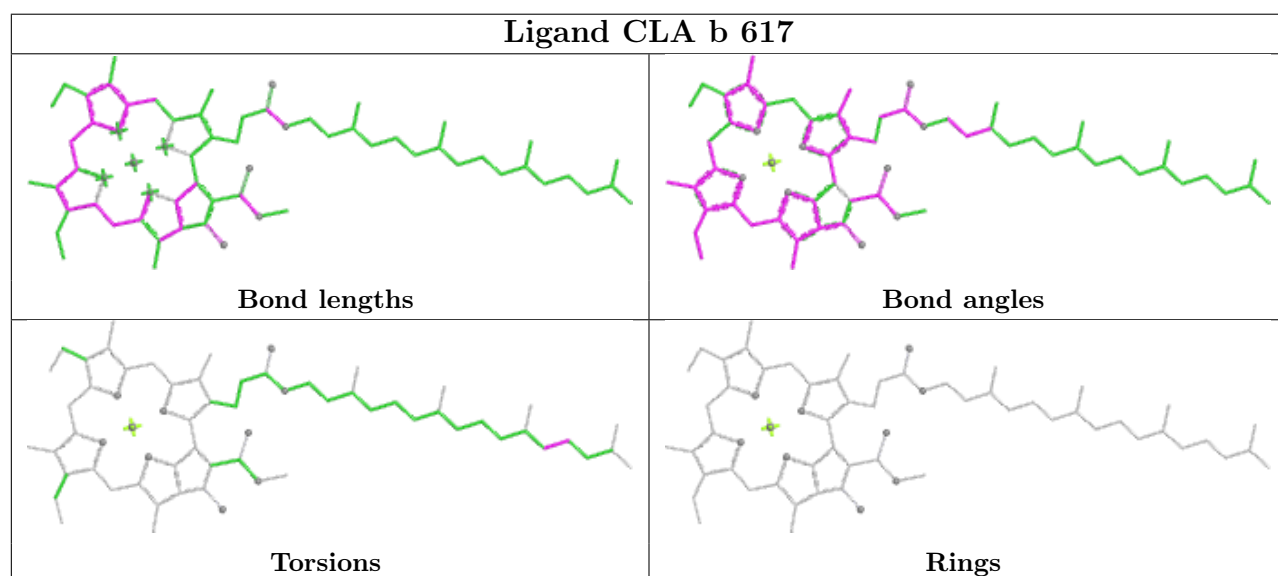
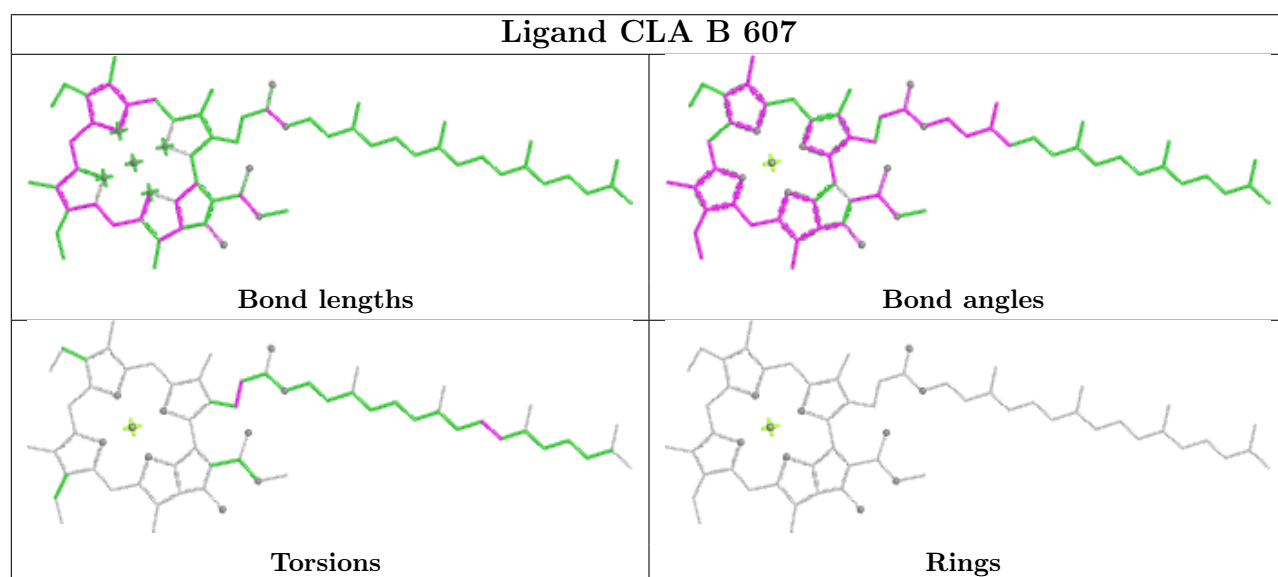
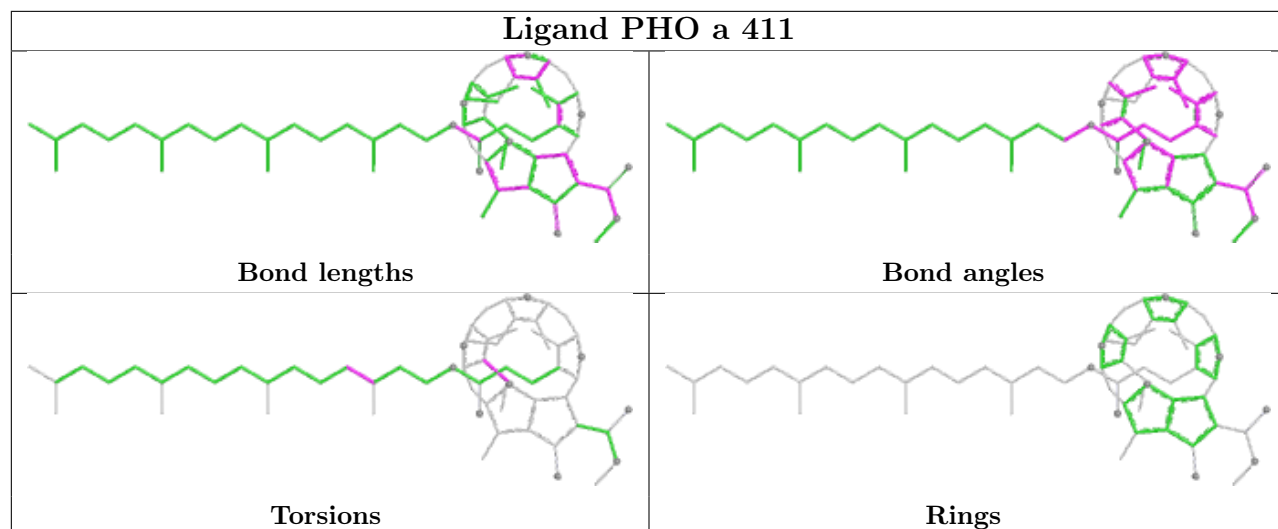


Ligand CLA B 611

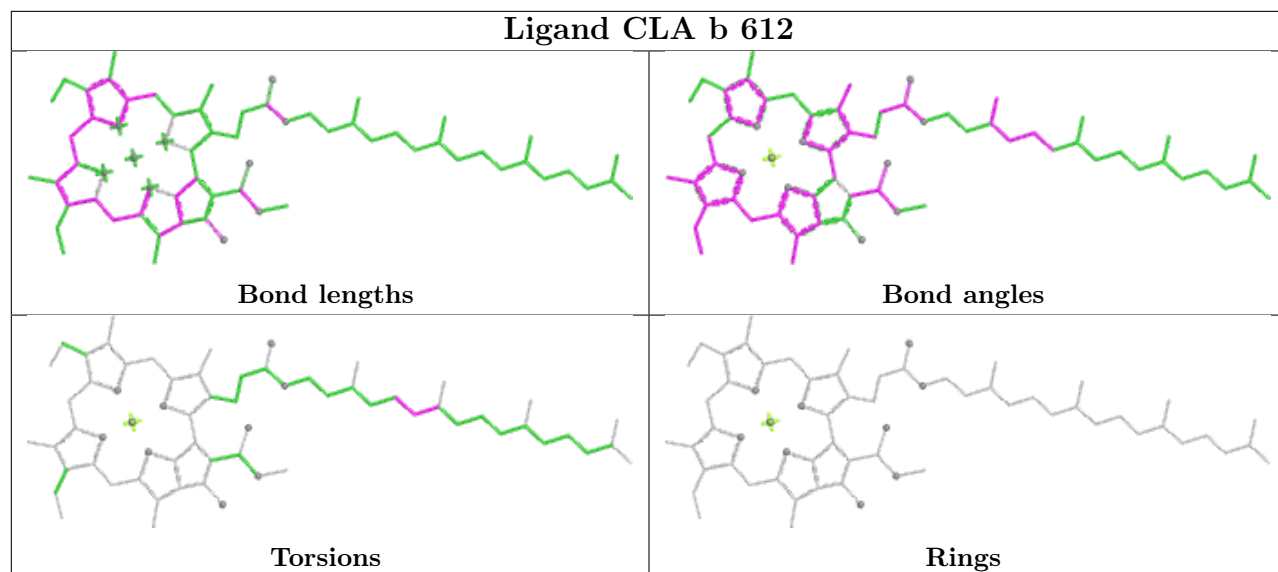




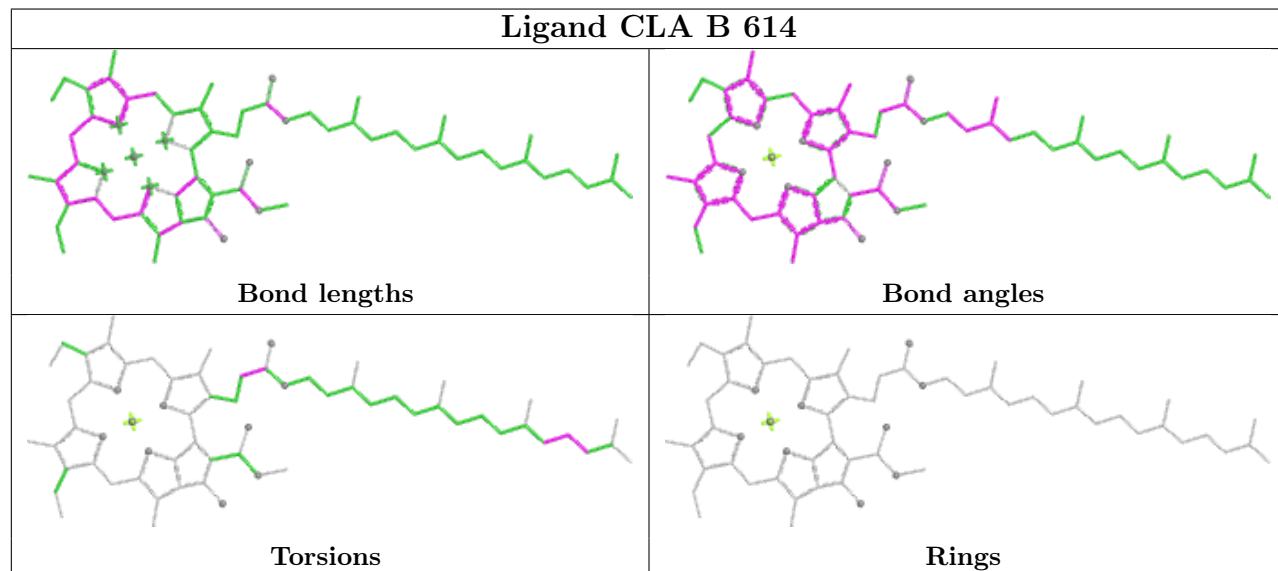




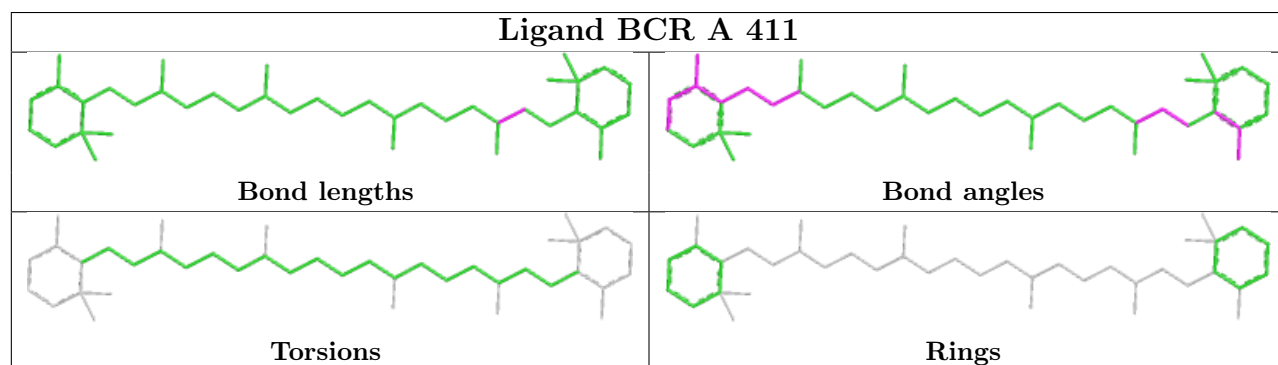
Ligand CLA b 612

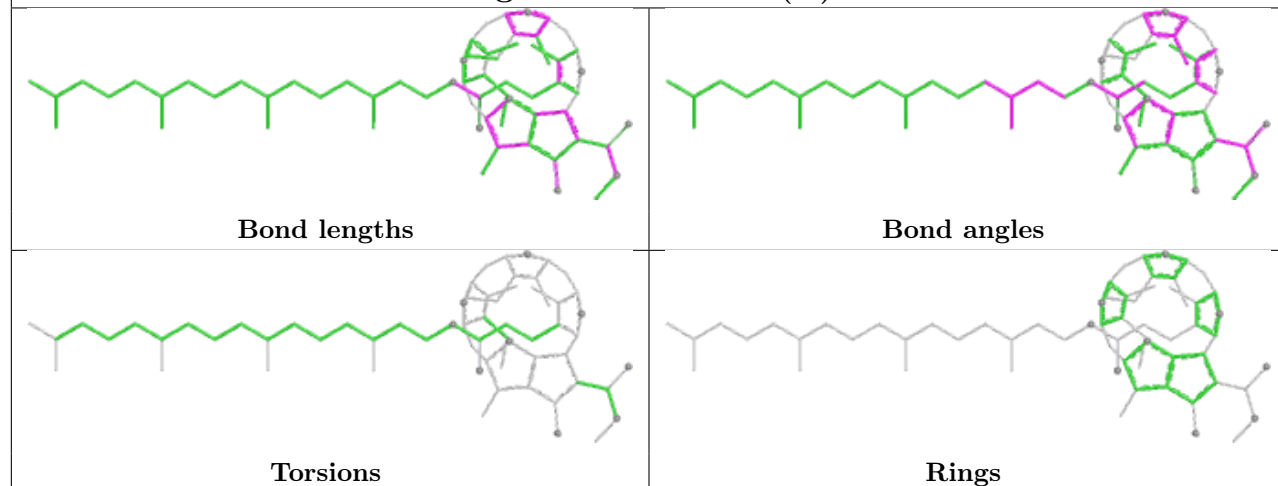
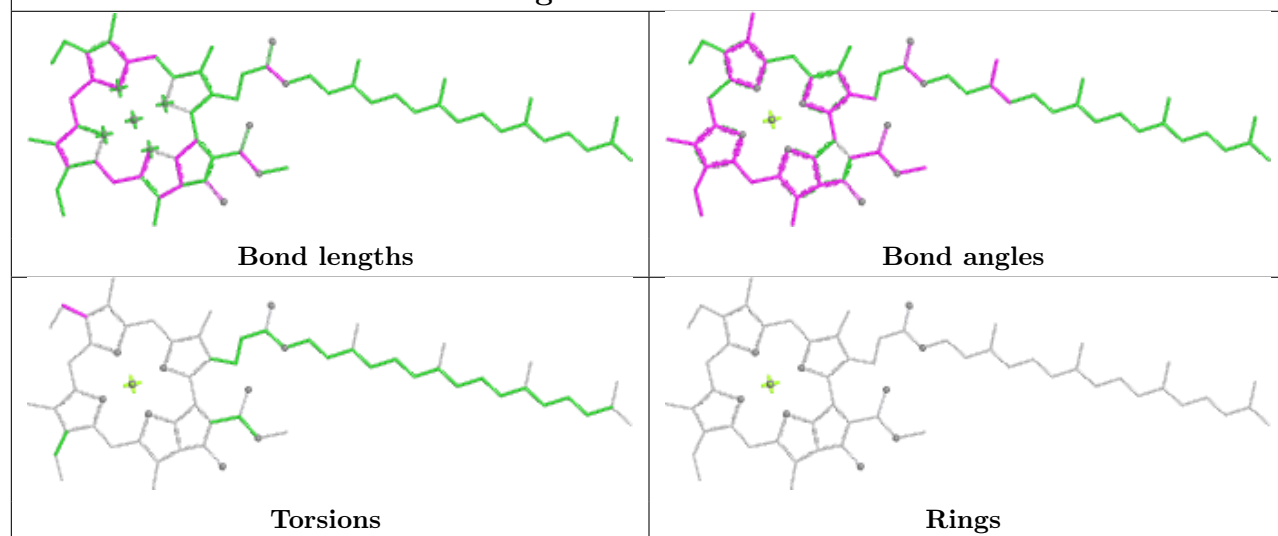
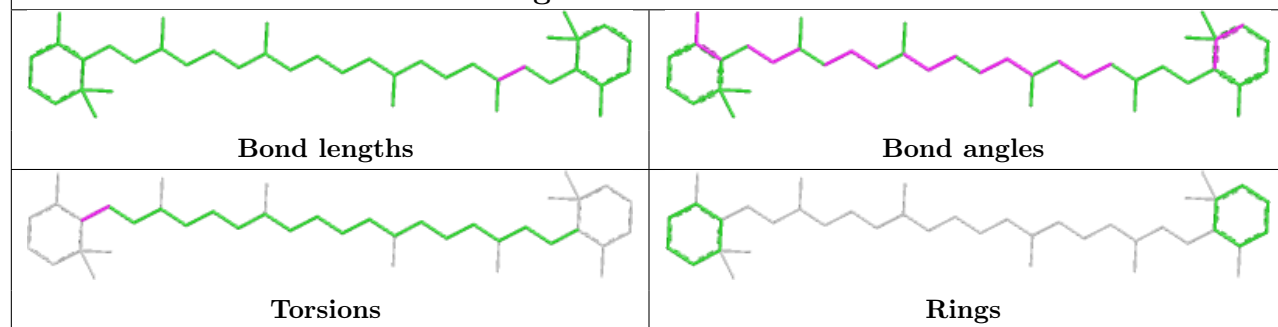


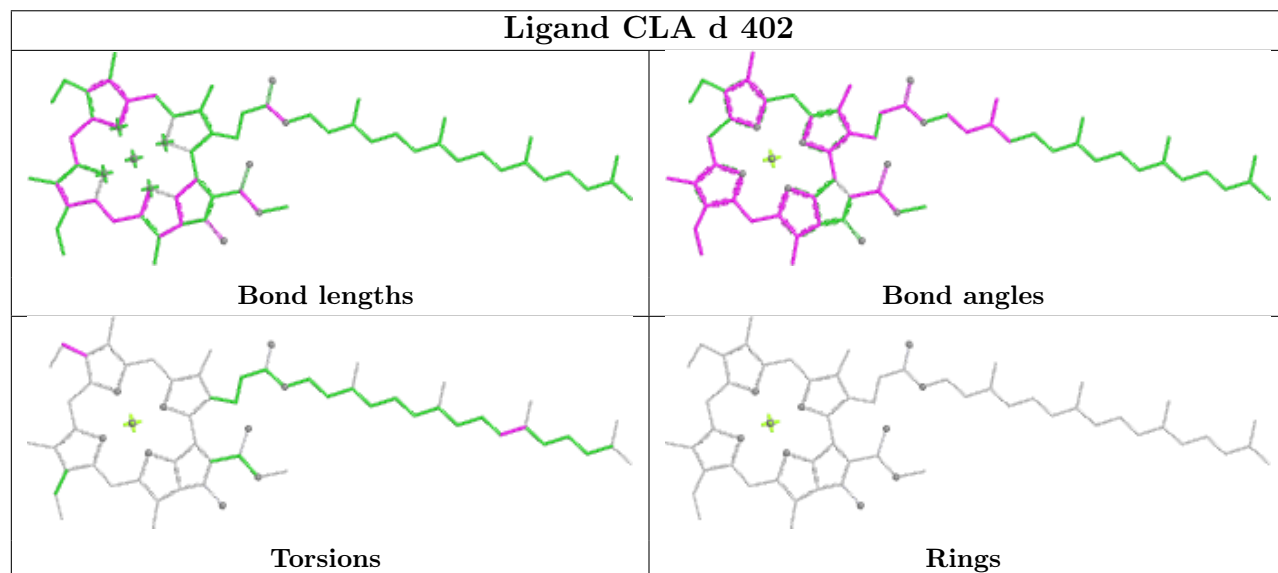
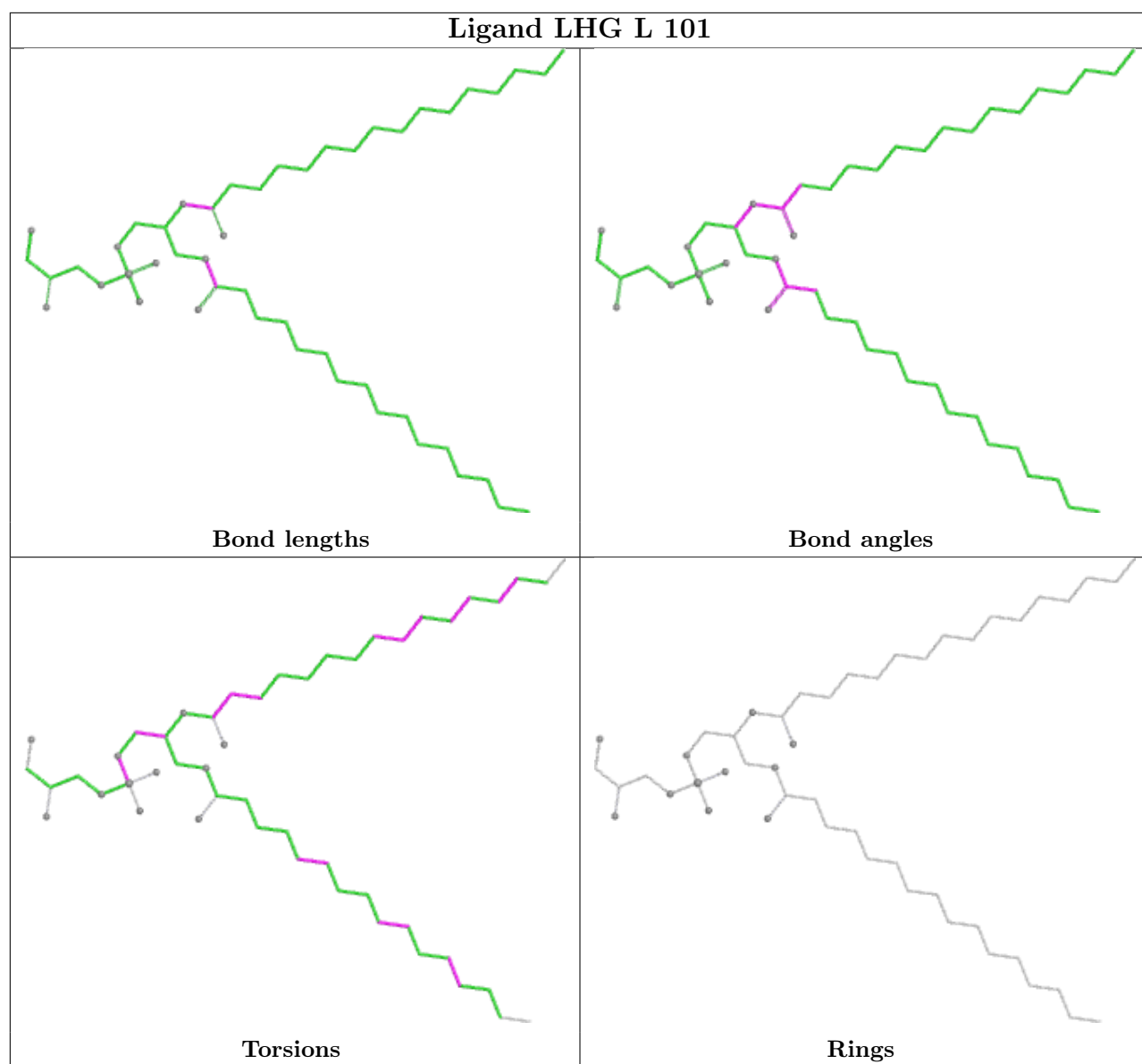
Ligand CLA B 614

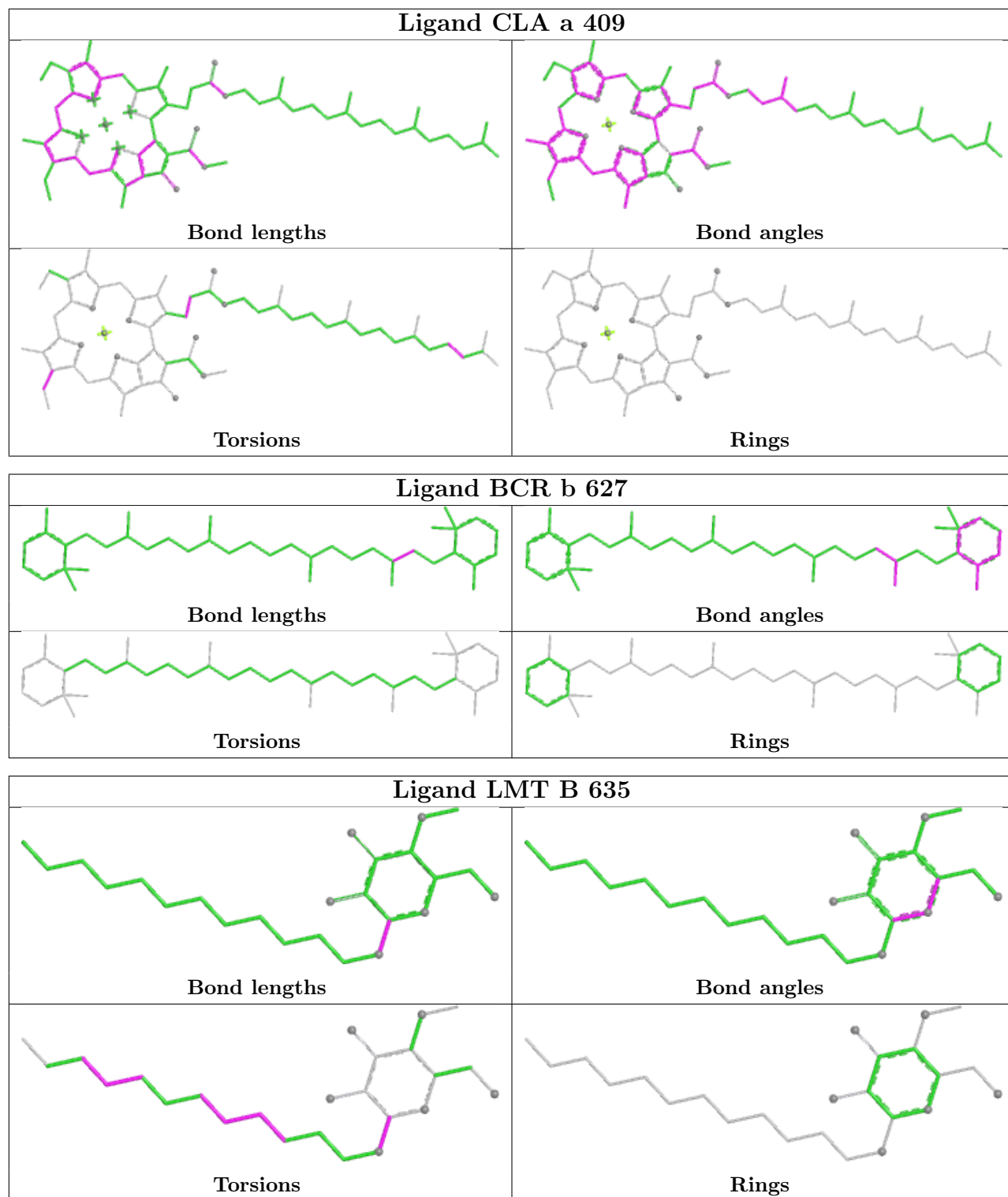


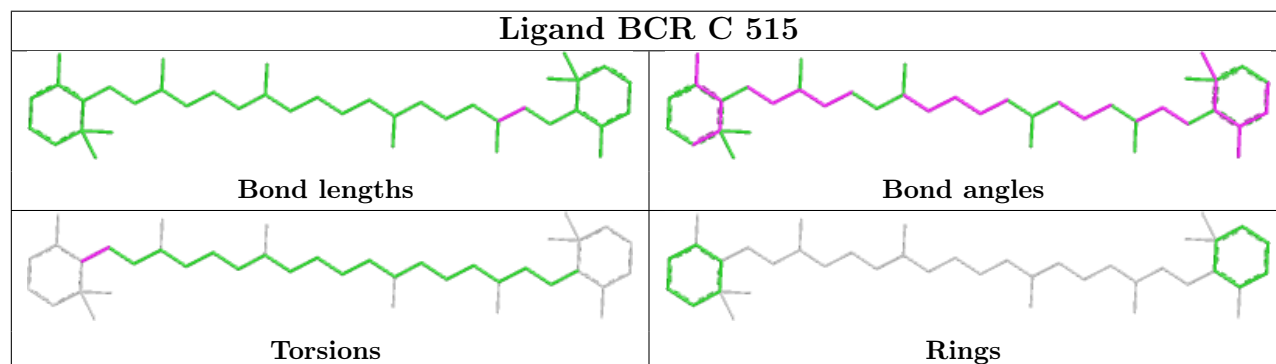
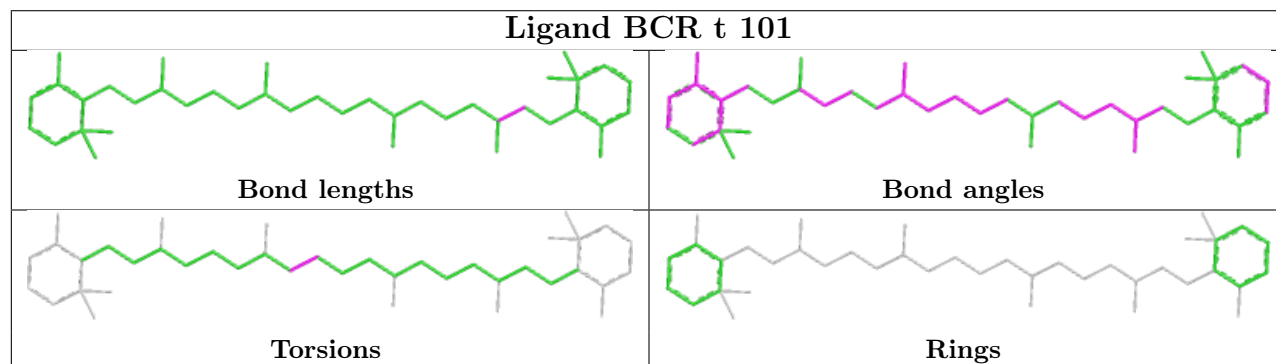
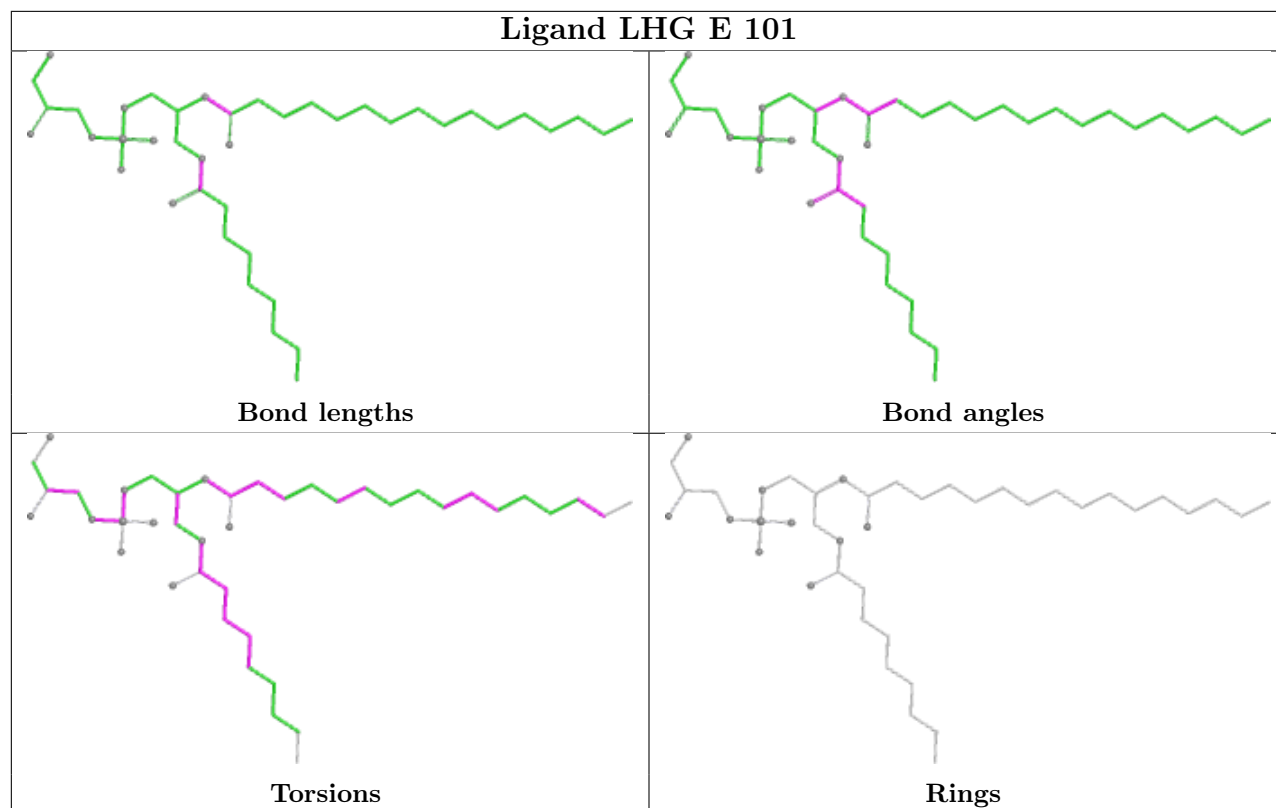
Ligand BCR A 411



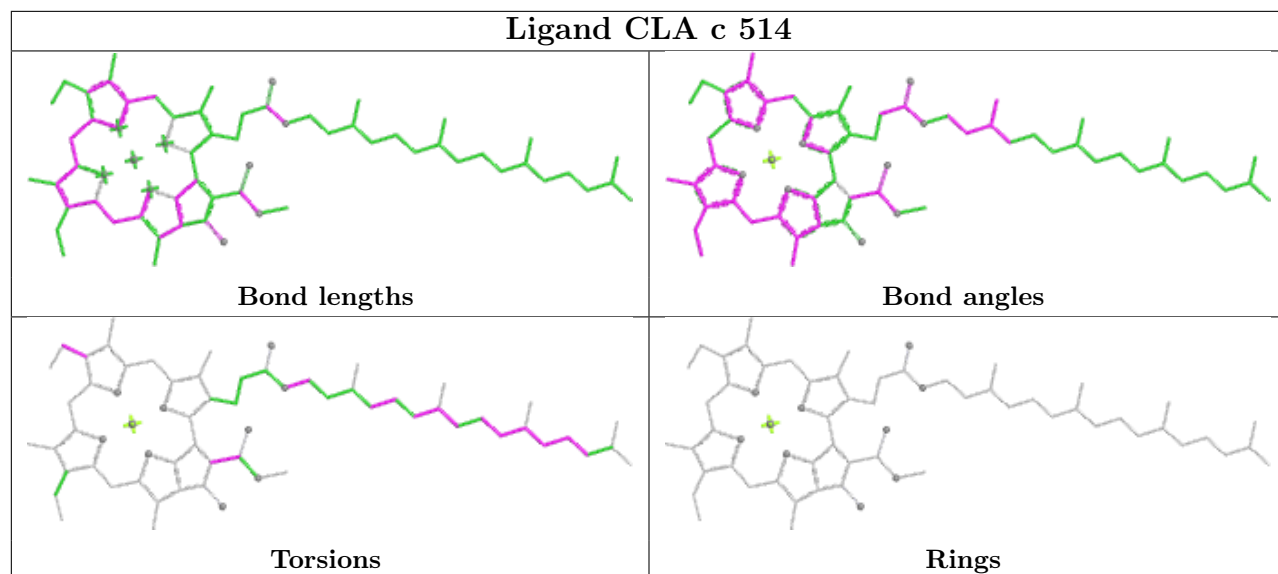
Ligand PHO A 409 (A)**Ligand CLA b 616****Ligand BCR b 626**



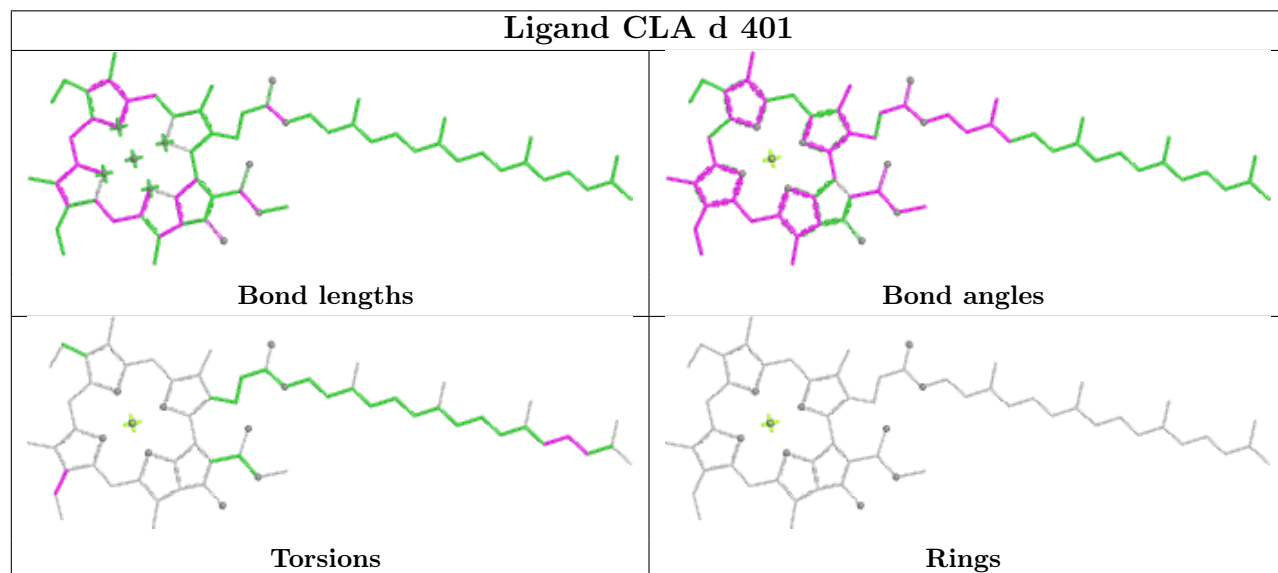




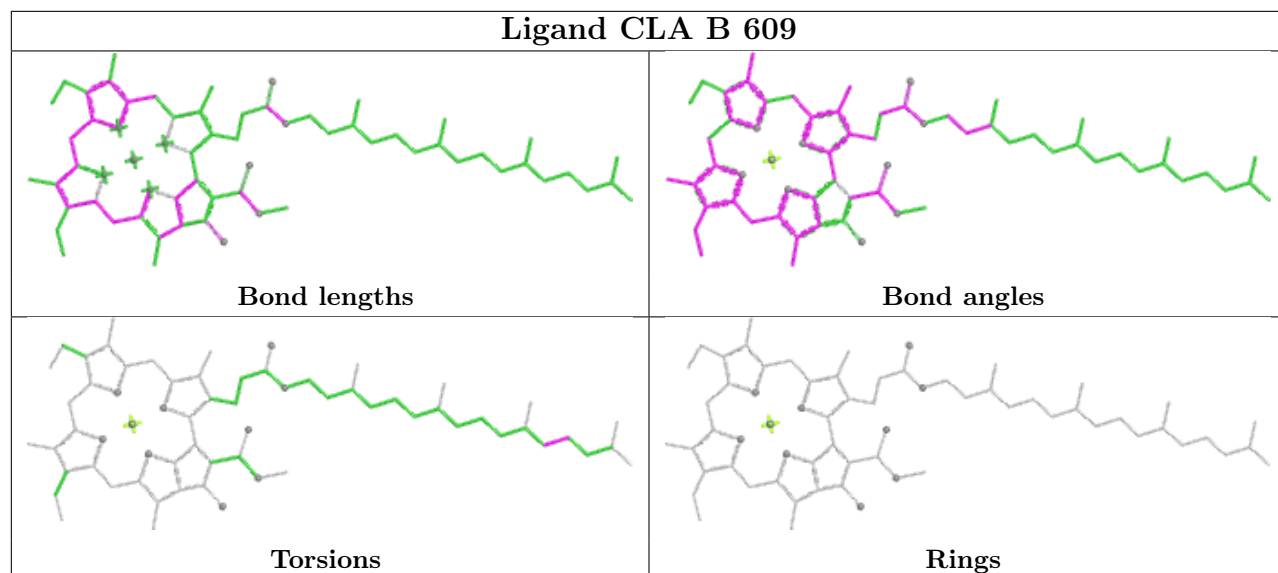
Ligand CLA c 514



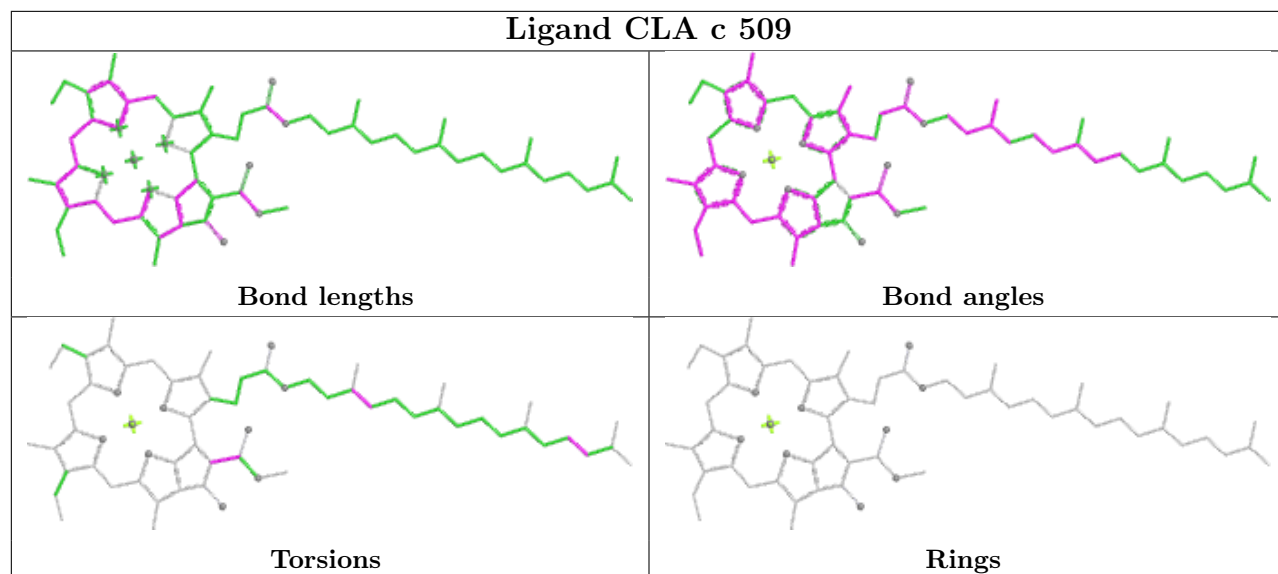
Ligand CLA d 401



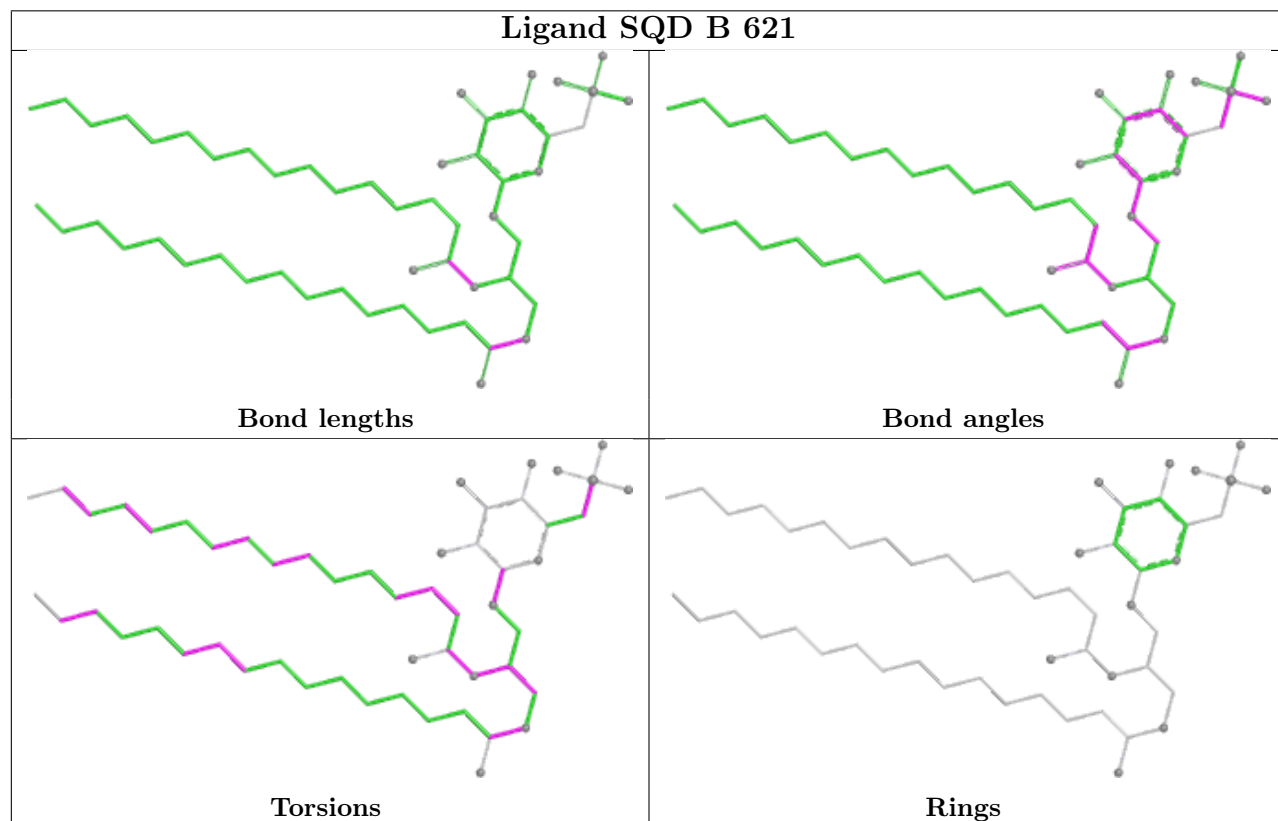
Ligand CLA B 609

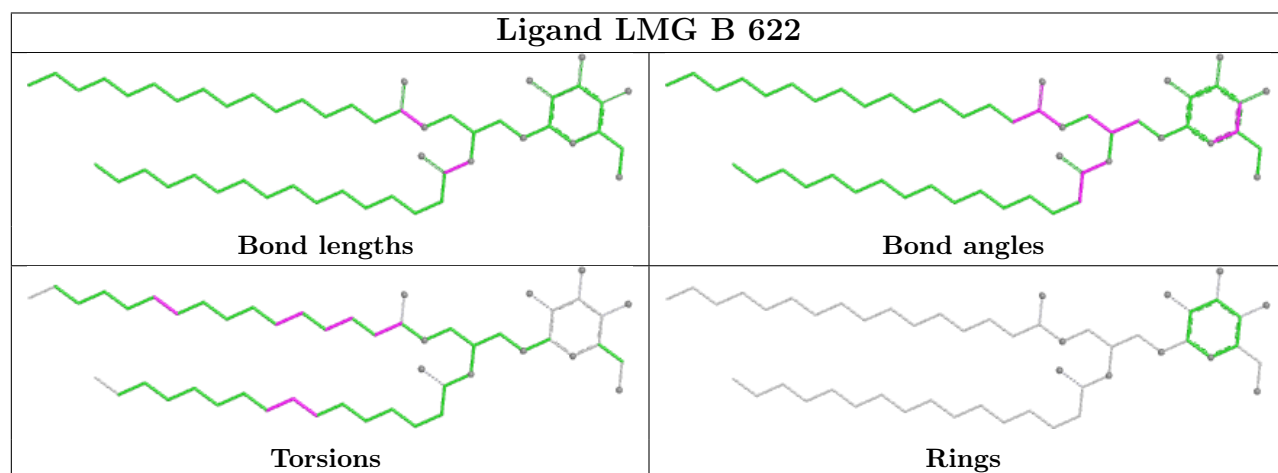
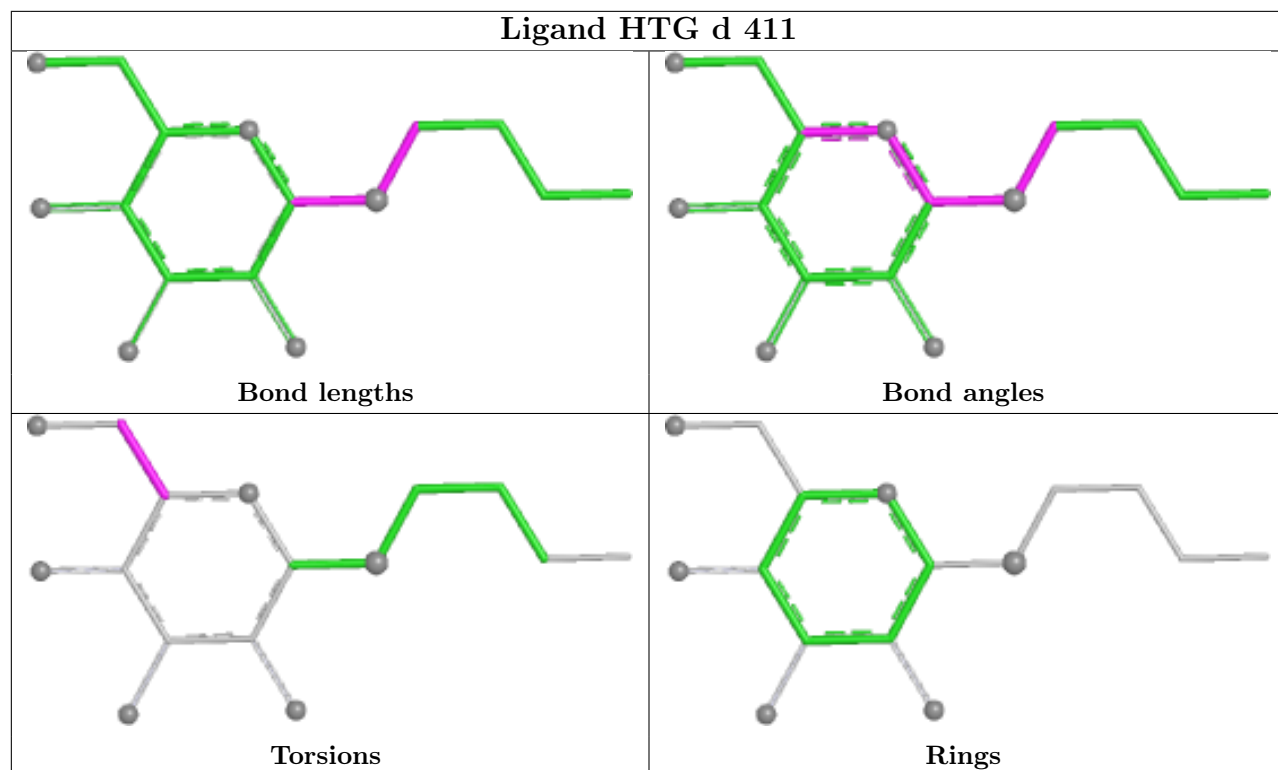


Ligand CLA c 509

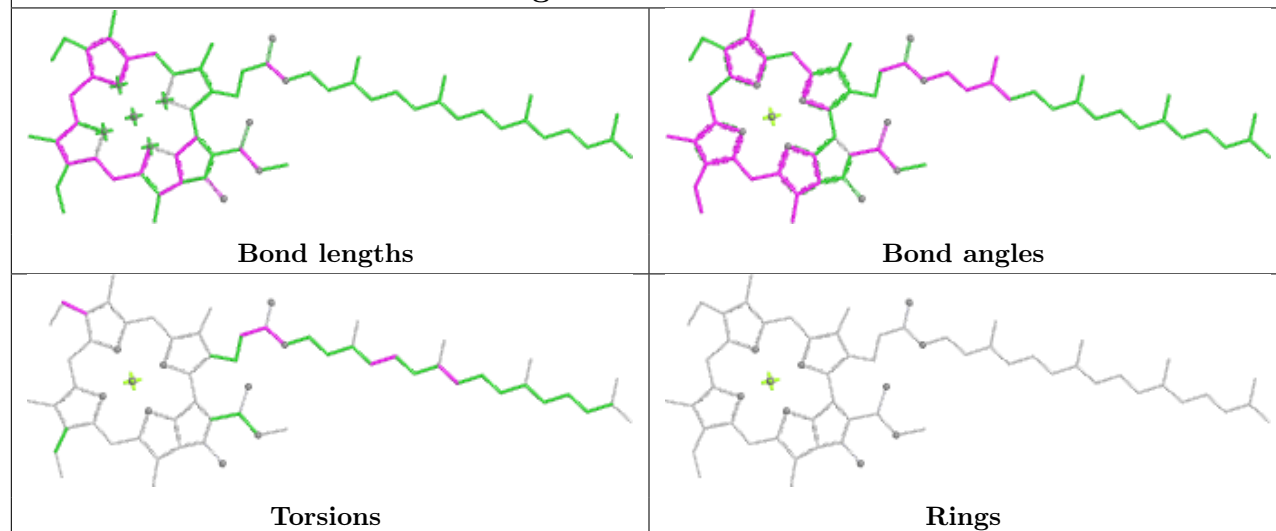


Ligand SQD B 621

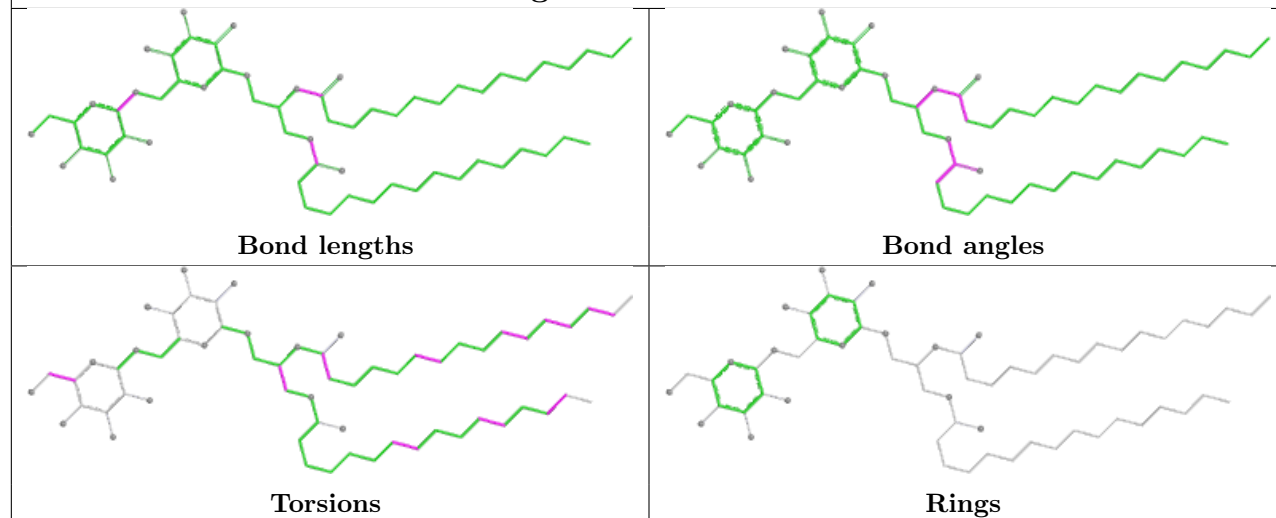




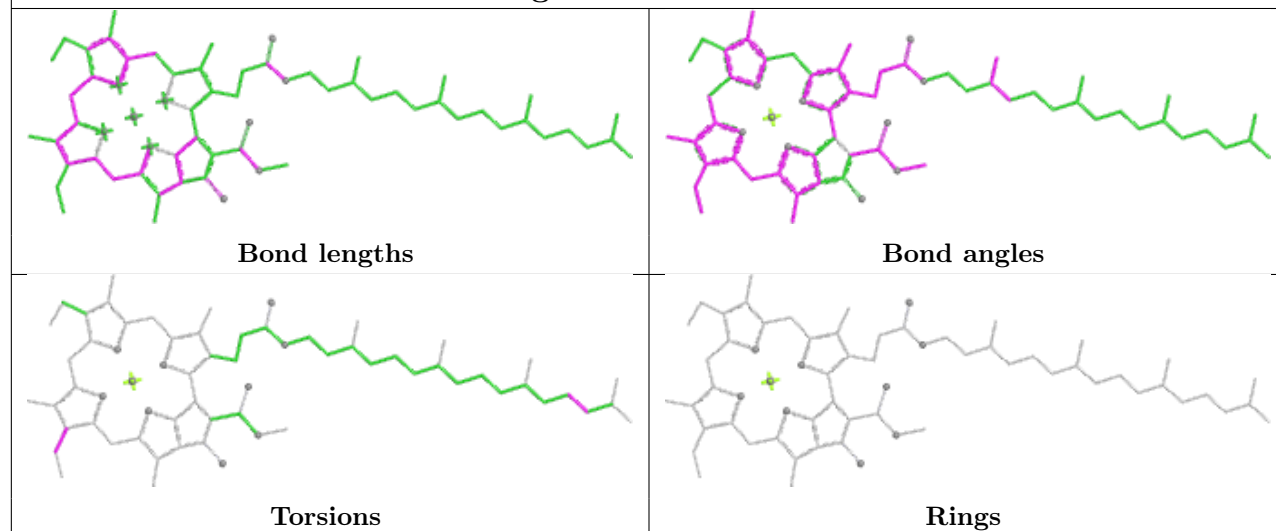
Ligand CLA C 512



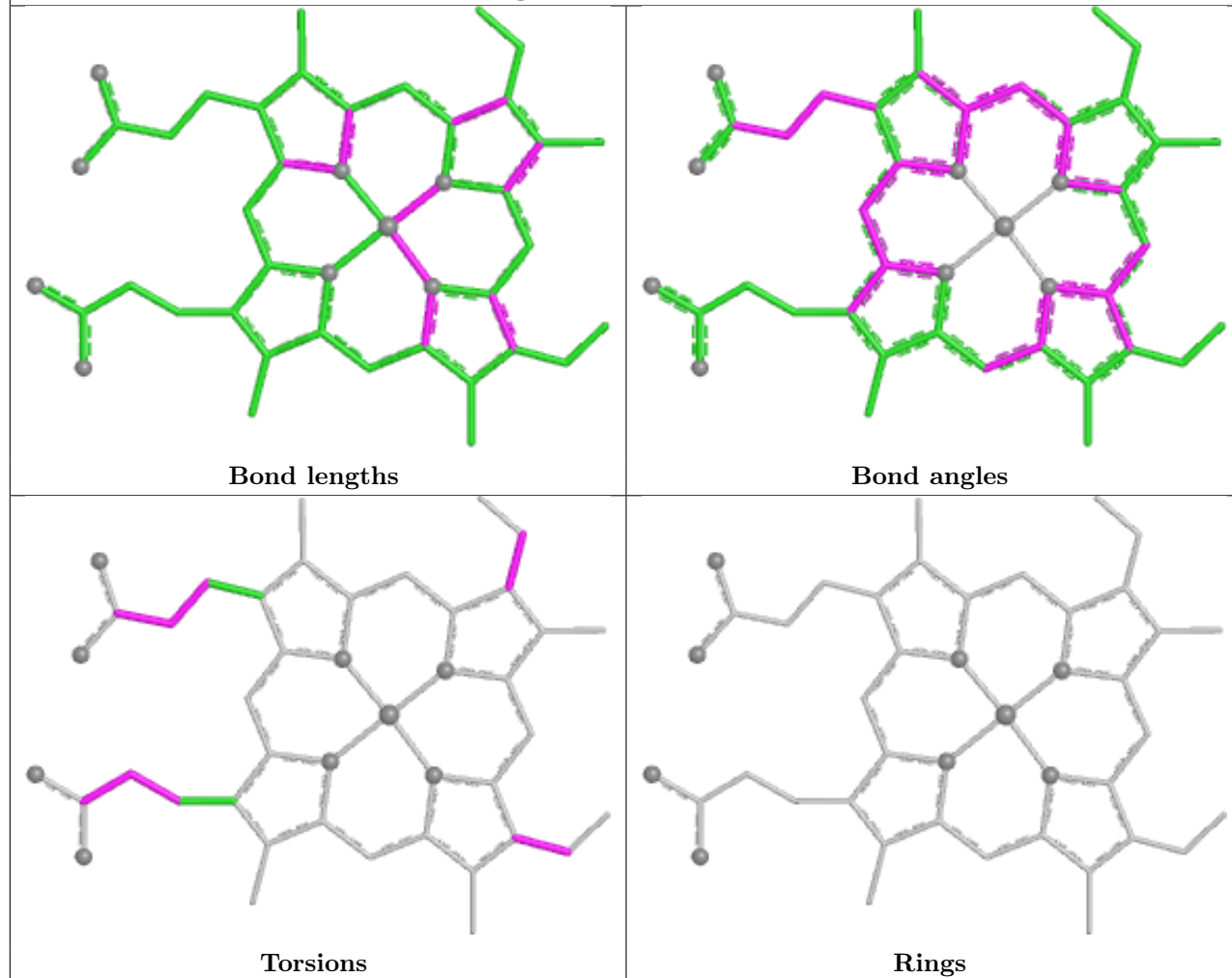
Ligand DGD h 102



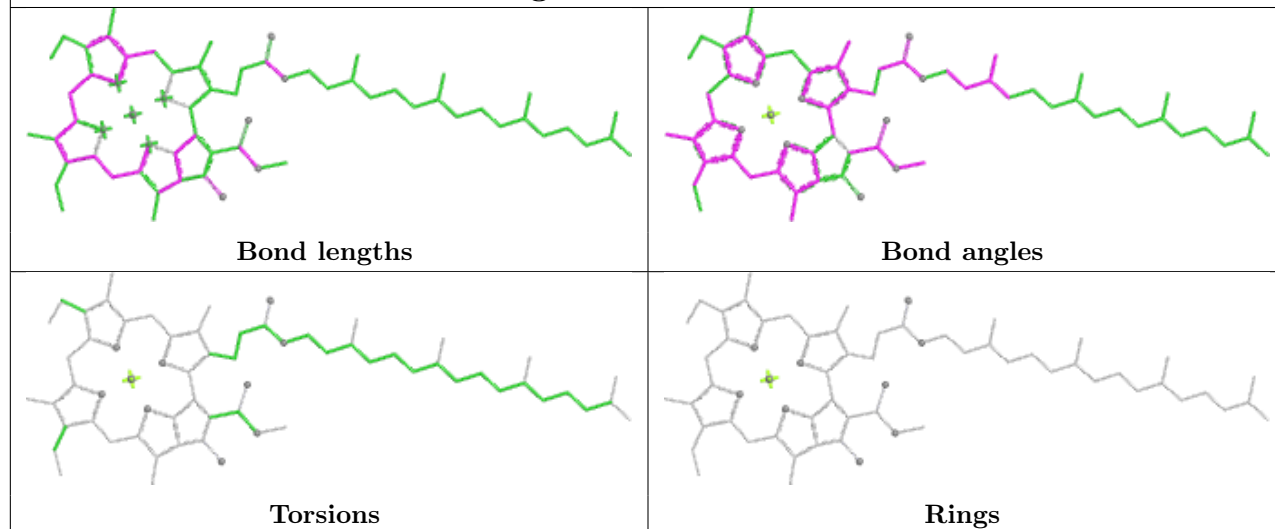
Ligand CLA A 406



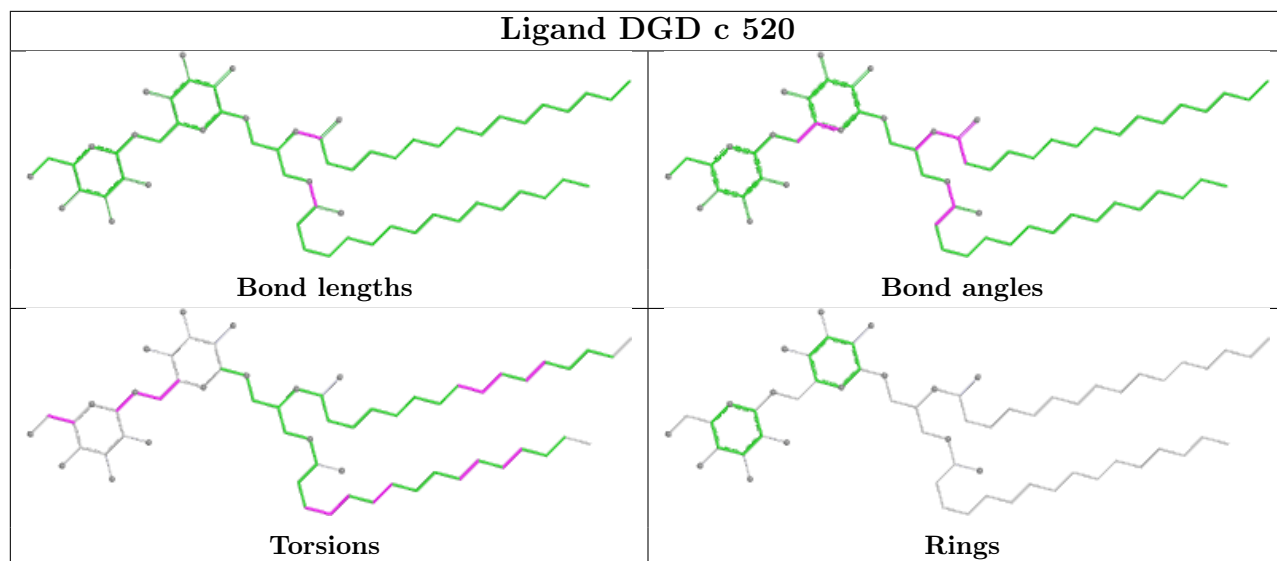
Ligand HEM e 103



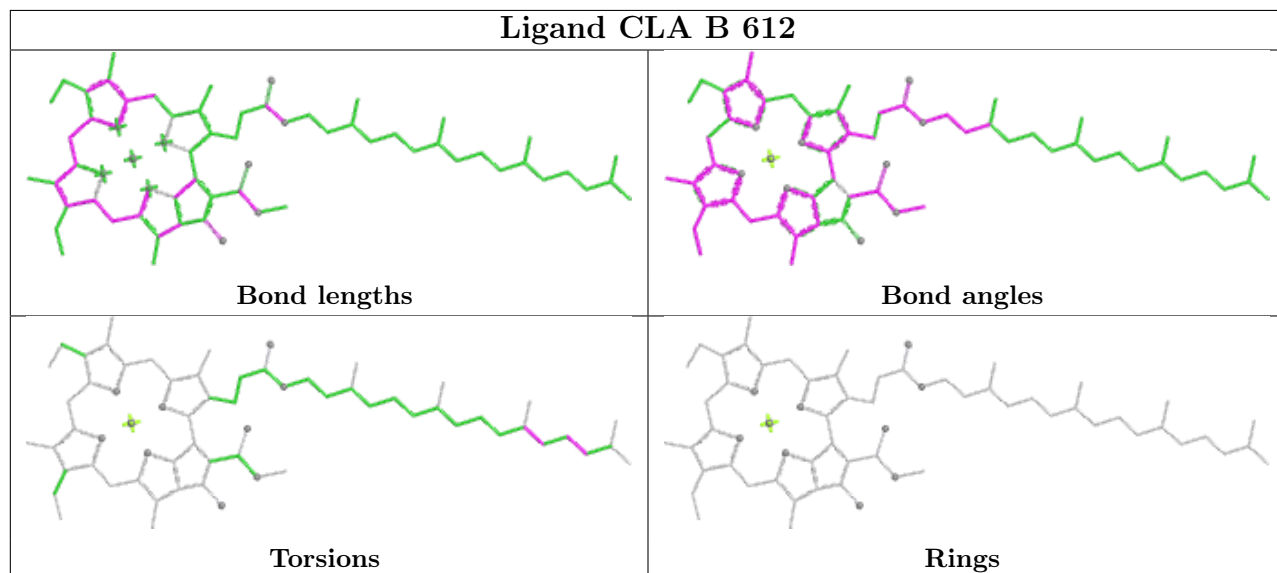
Ligand CLA D 402



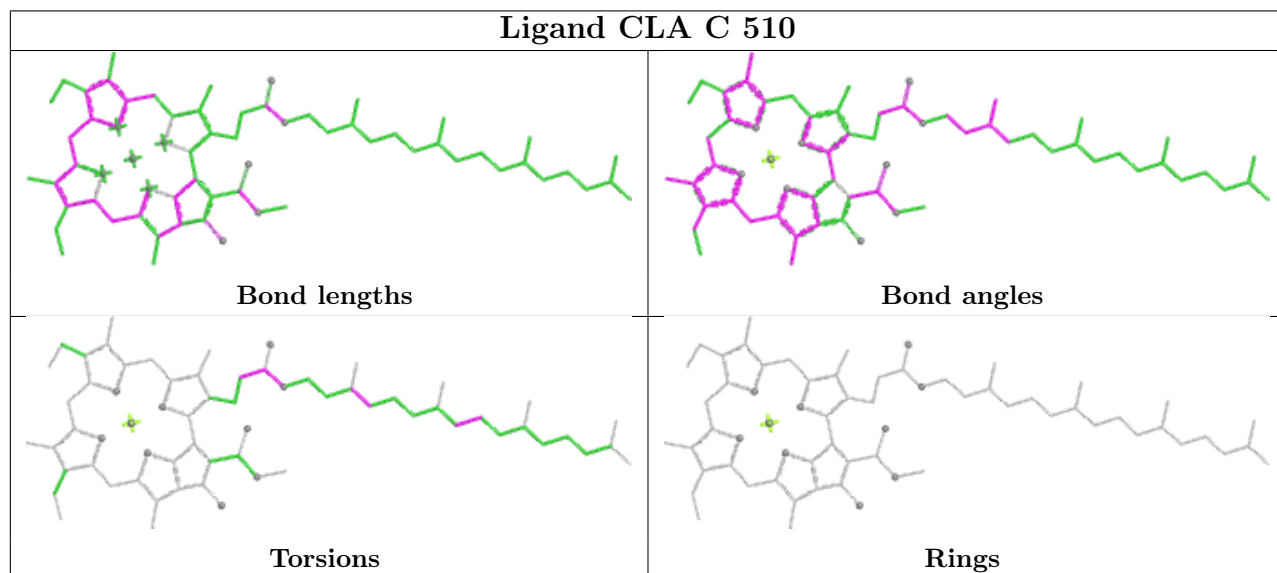
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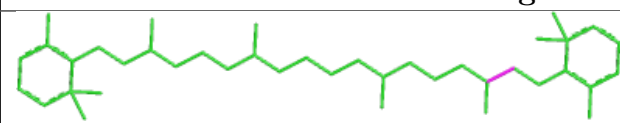
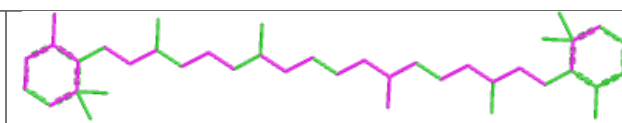
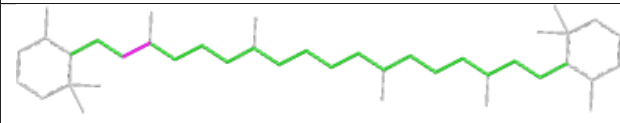
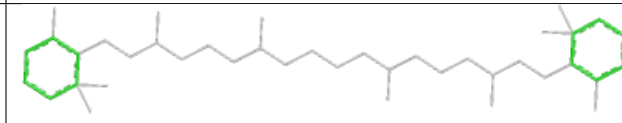


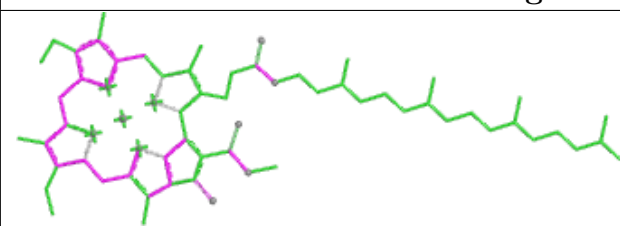
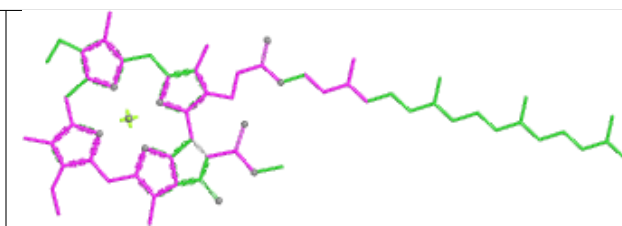
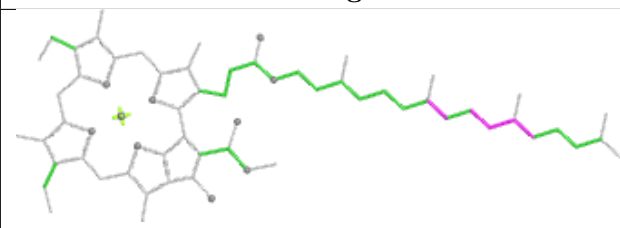
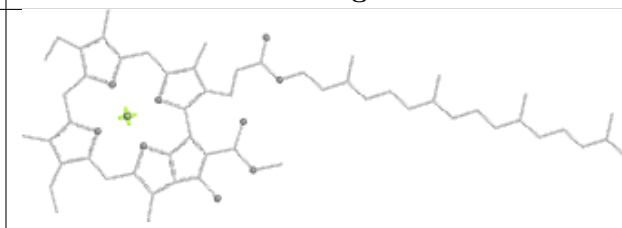
Ligand CLA B 612

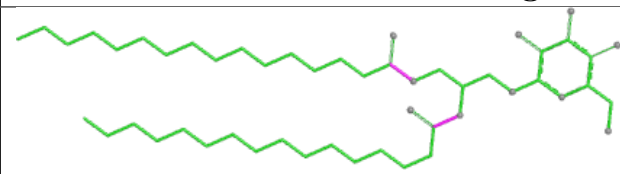
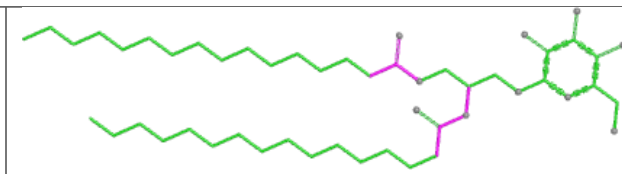
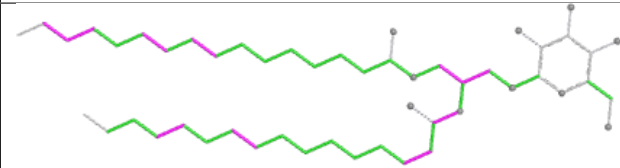
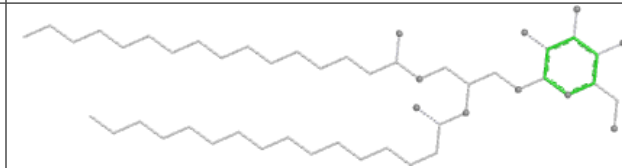


Ligand CLA C 510

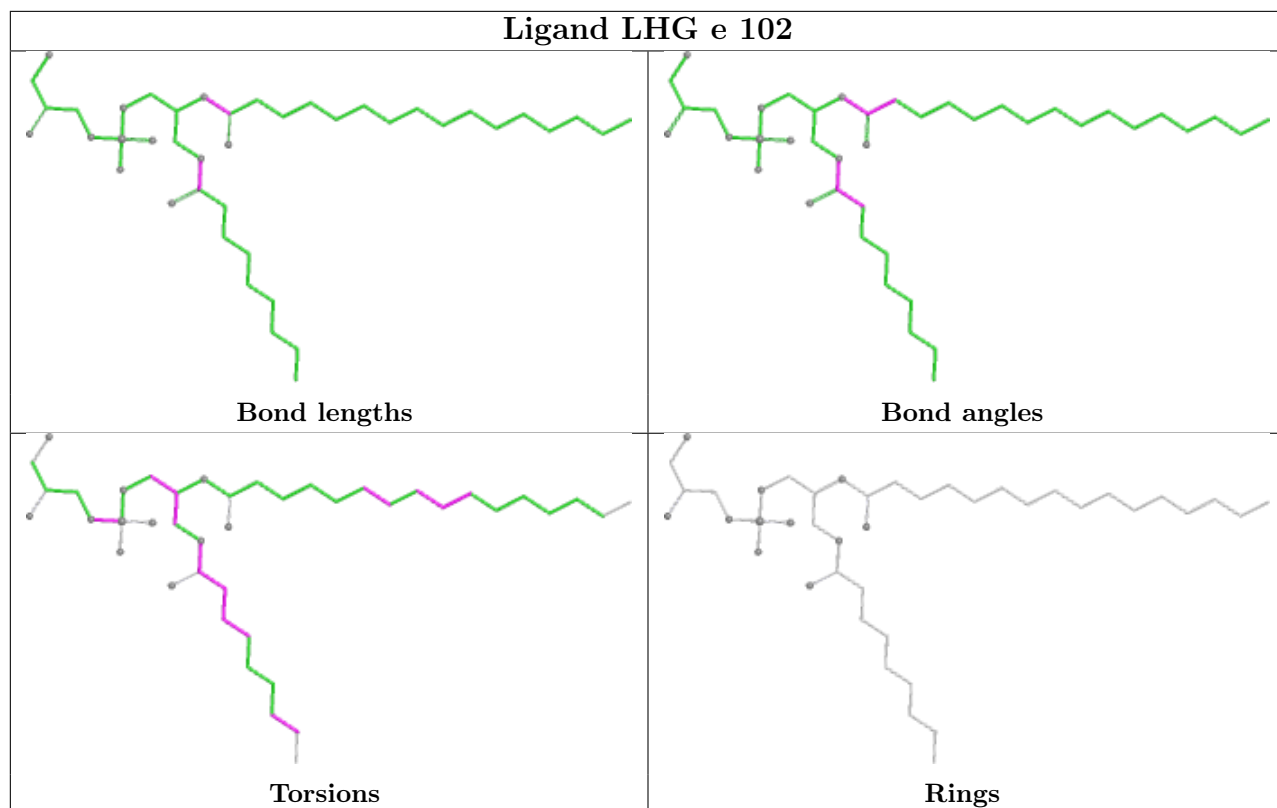


Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

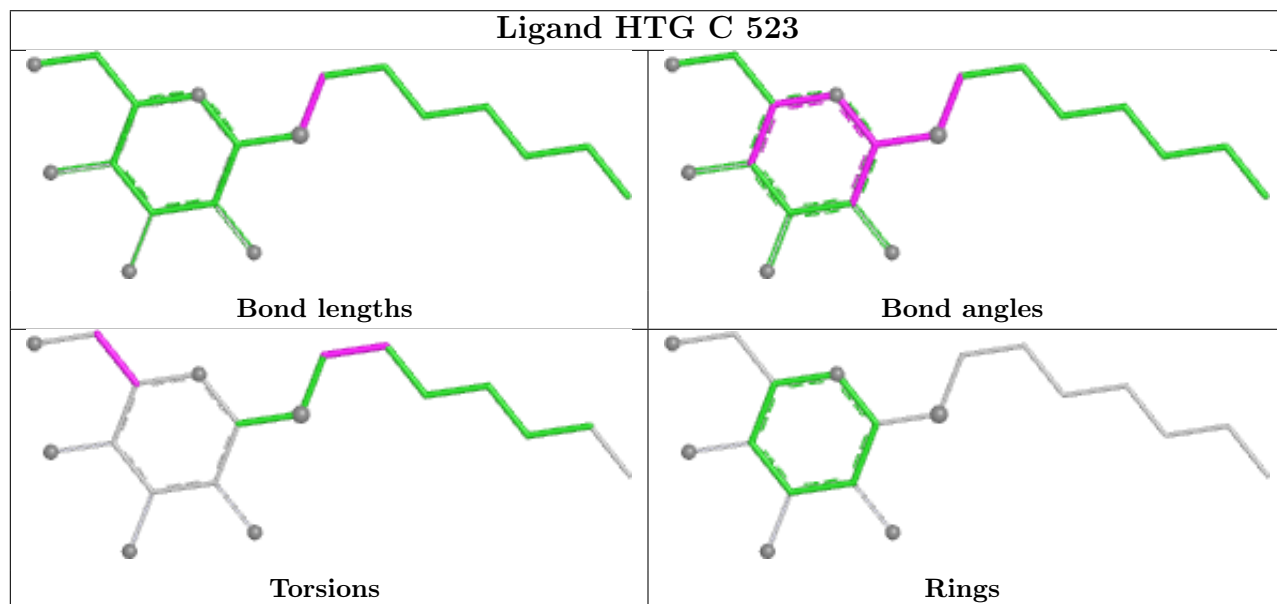
Ligand CLA a 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

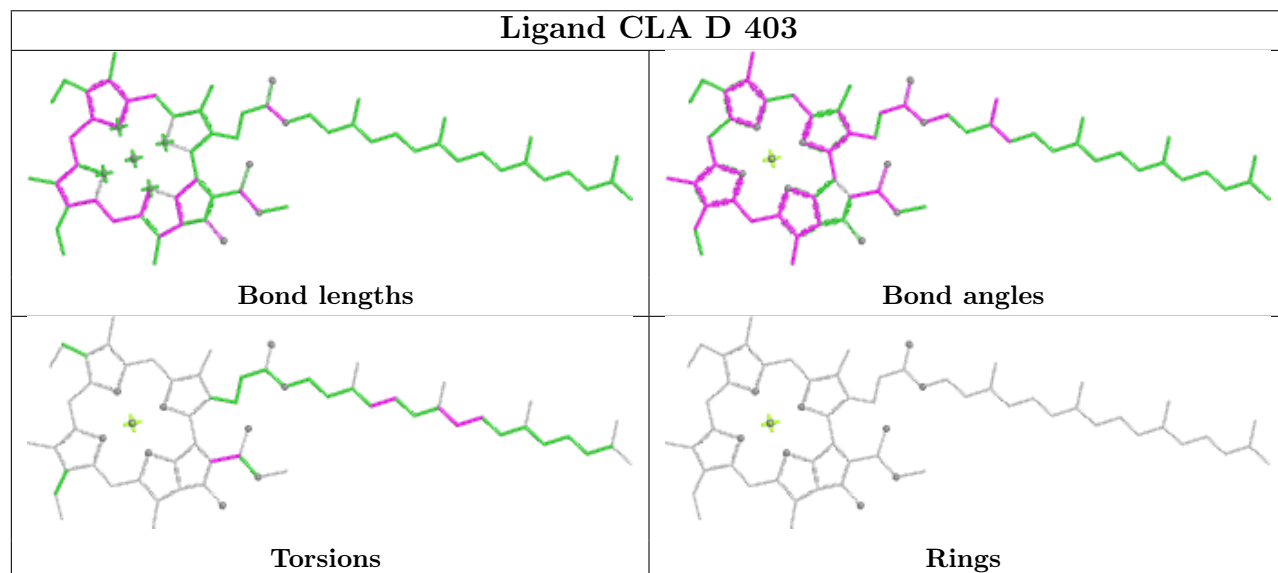
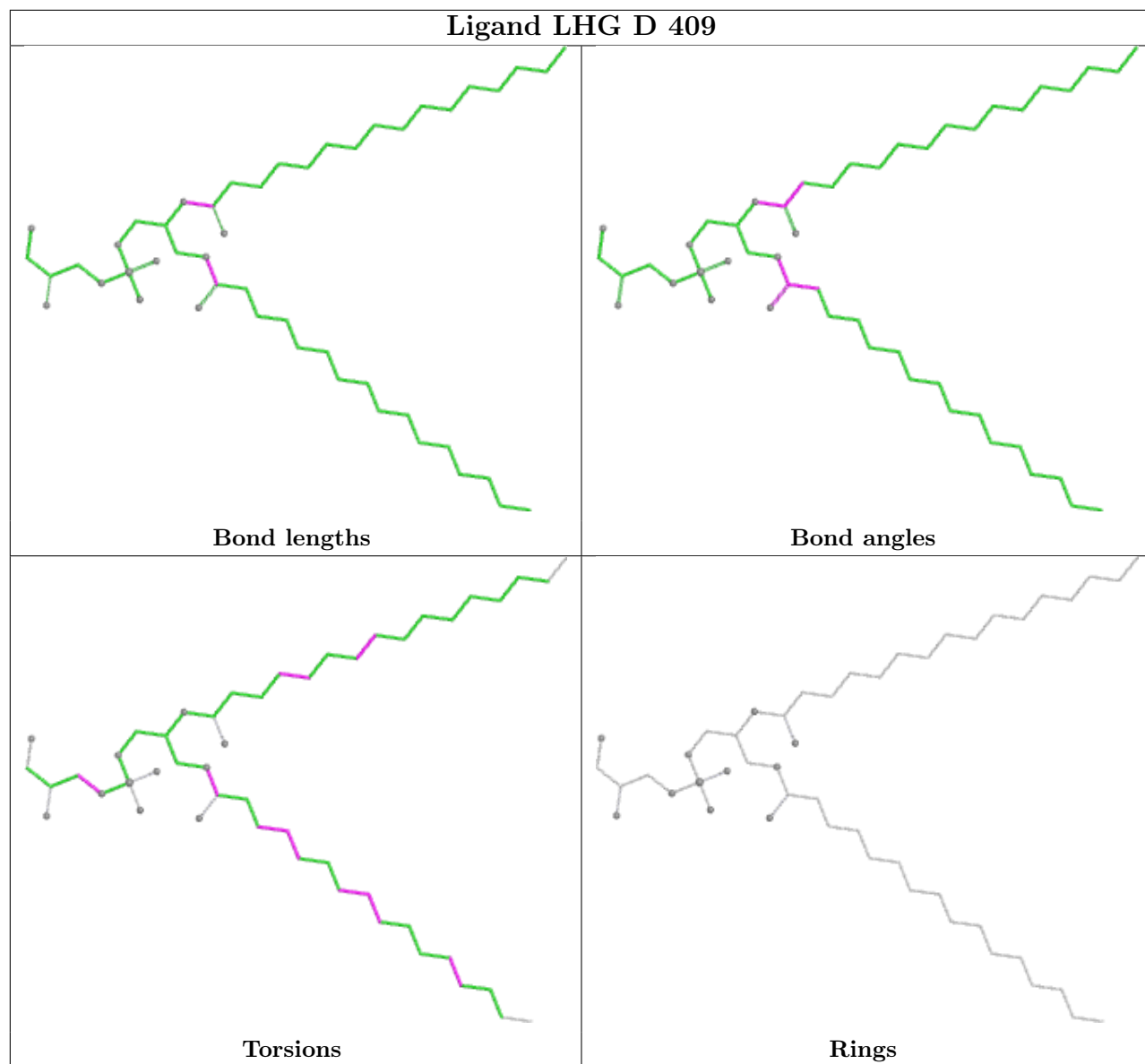
Ligand LMG c 523	
	
Bond lengths	Bond angles
	
Torsions	Rings

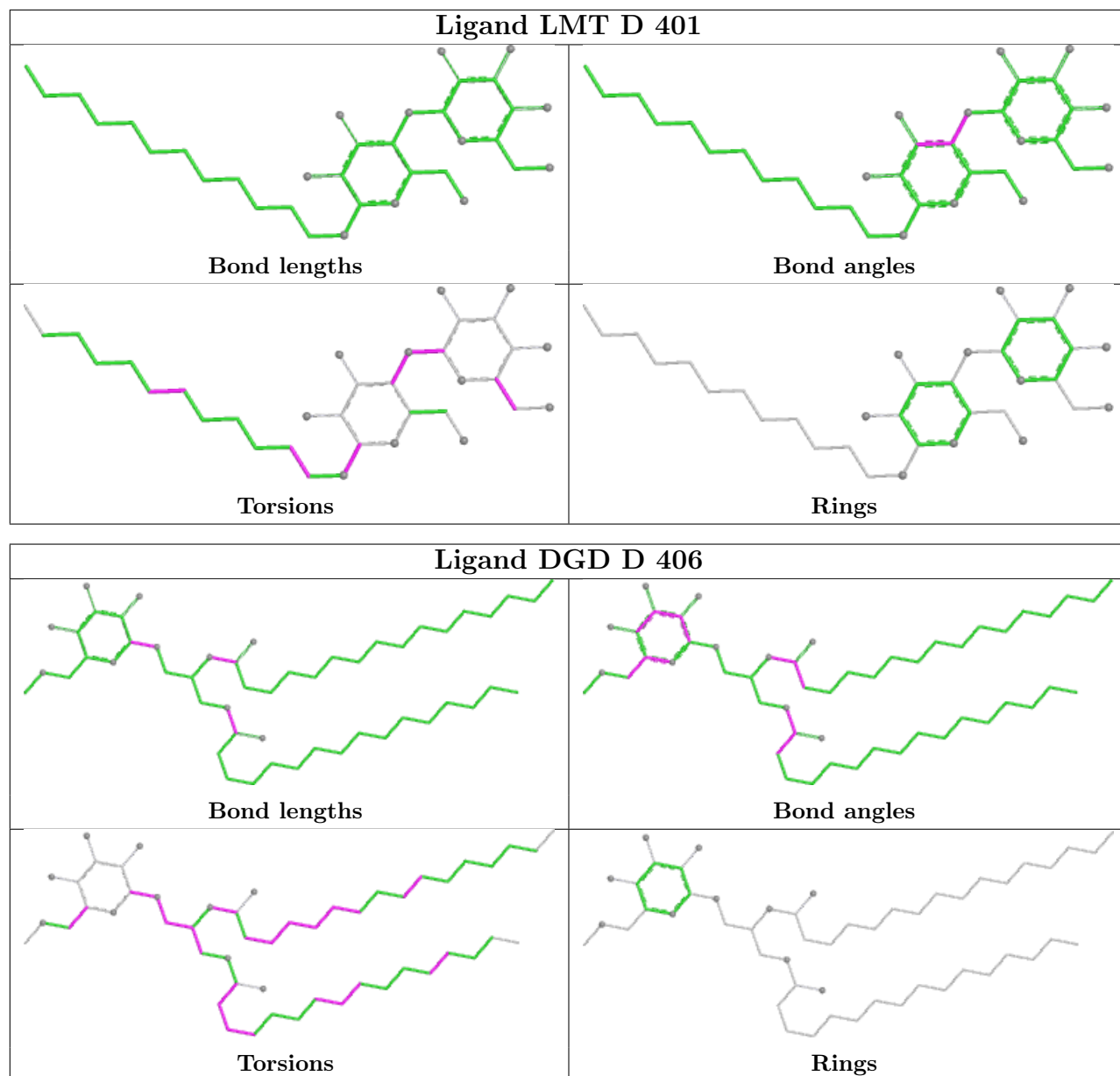
Ligand LHG e 102

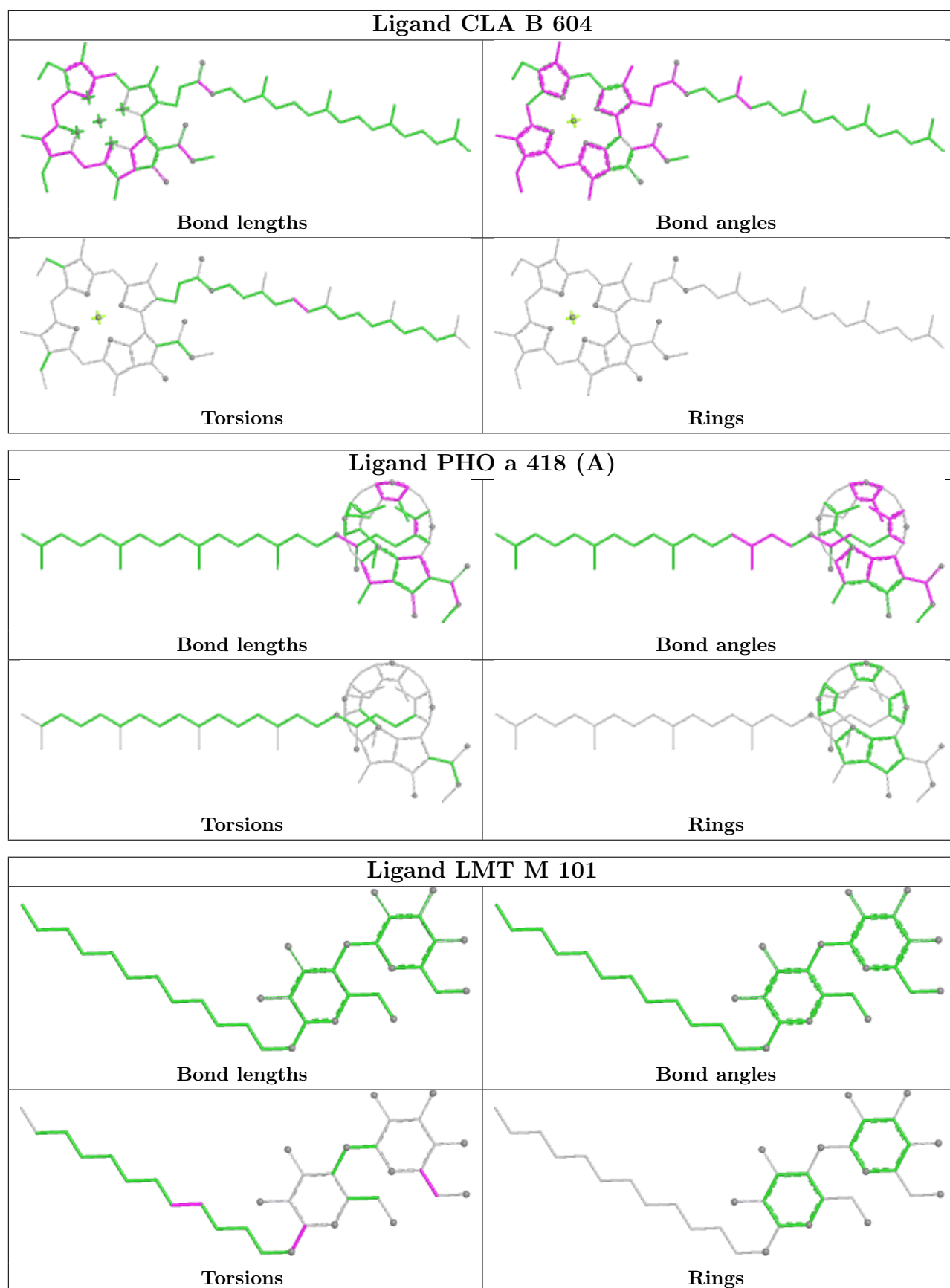


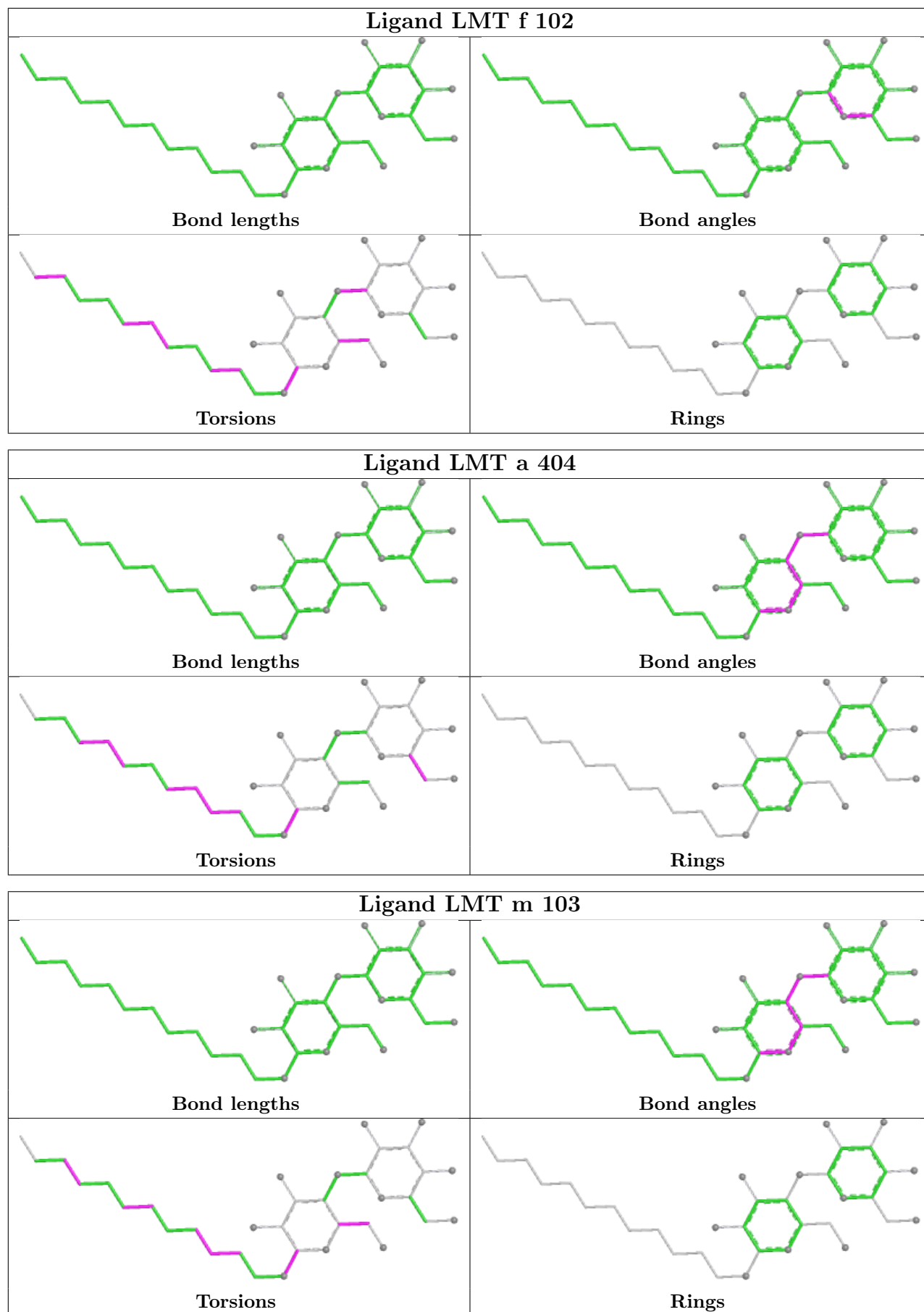
Ligand HTG C 523



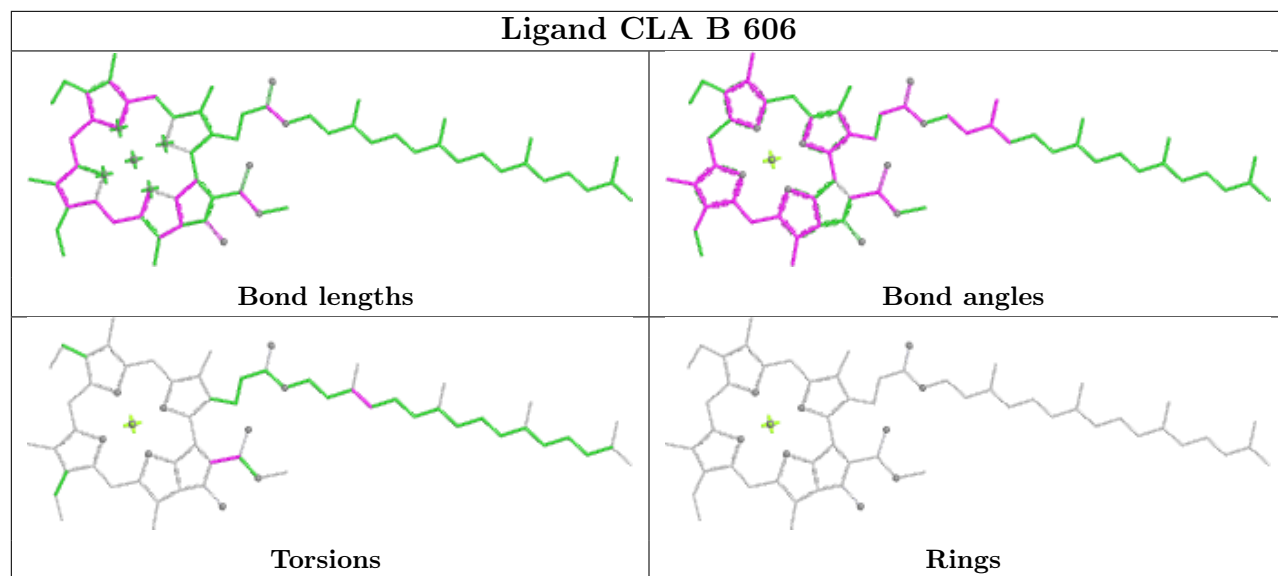




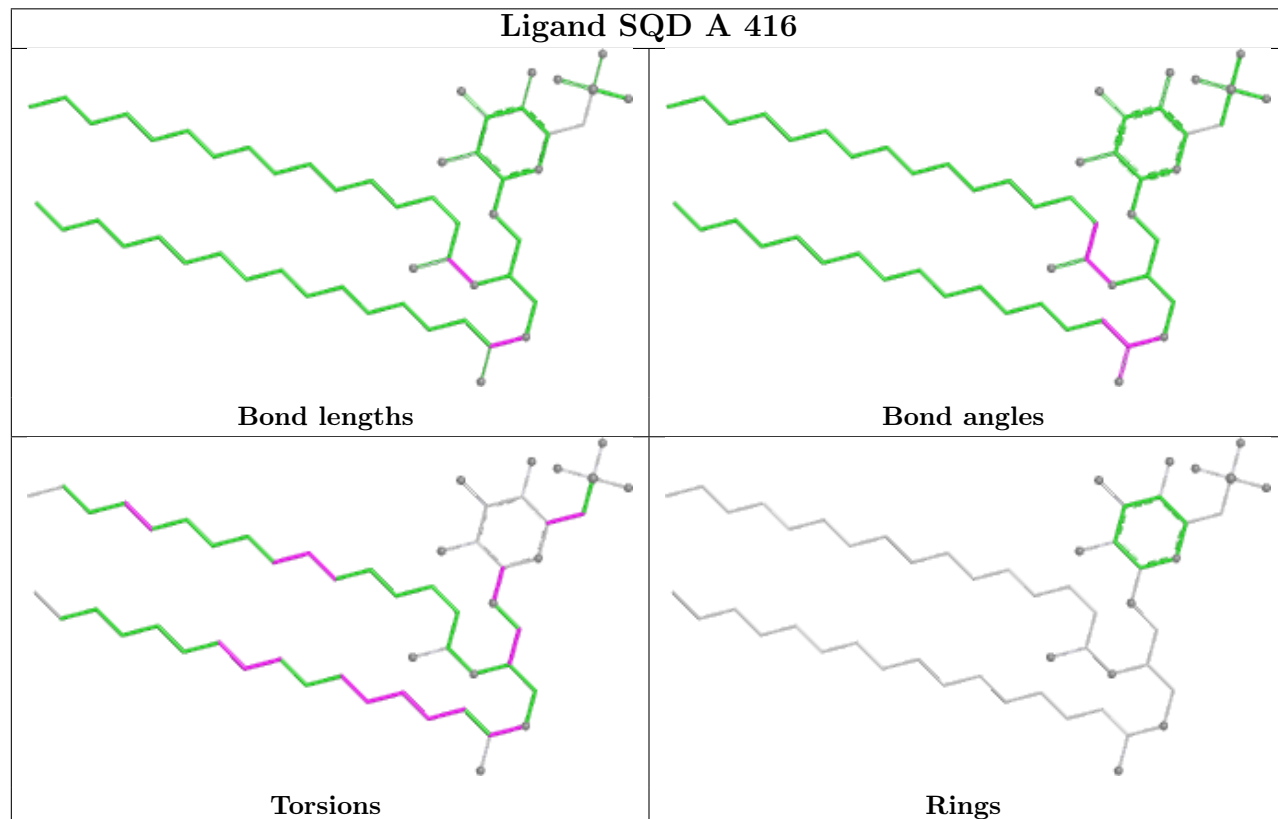


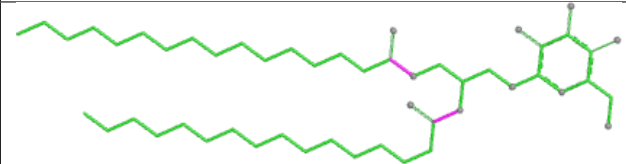
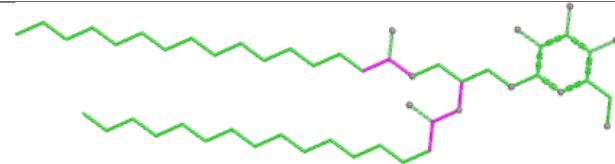
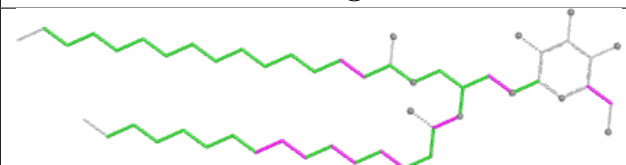
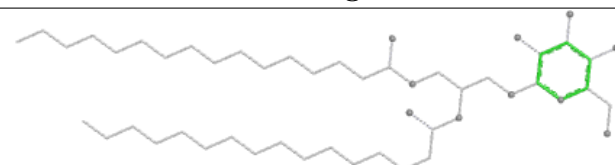


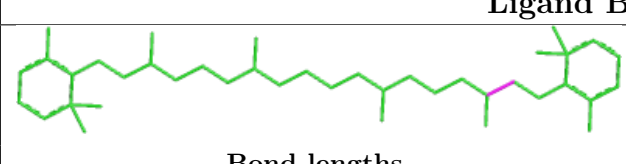
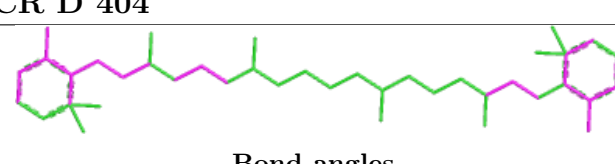
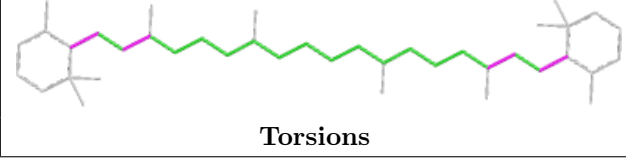
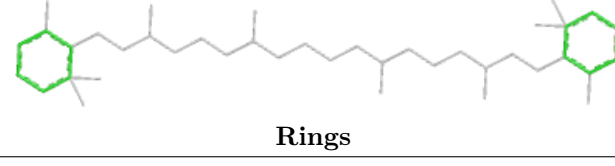
Ligand CLA B 606

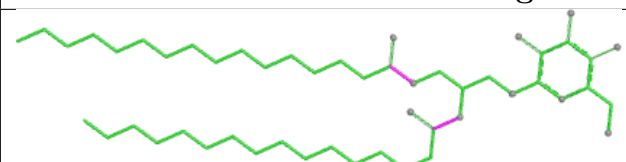
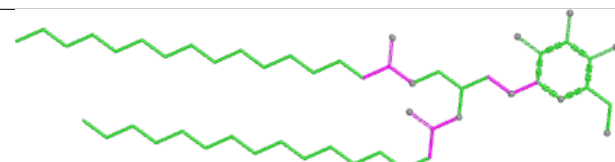
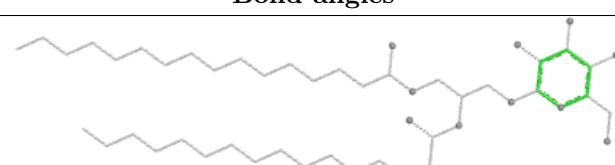


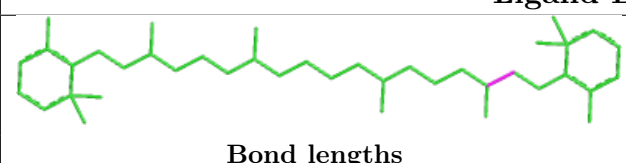
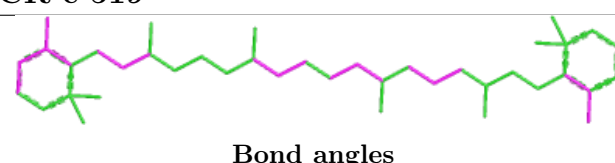
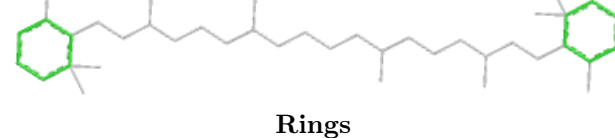
Ligand SQD A 416

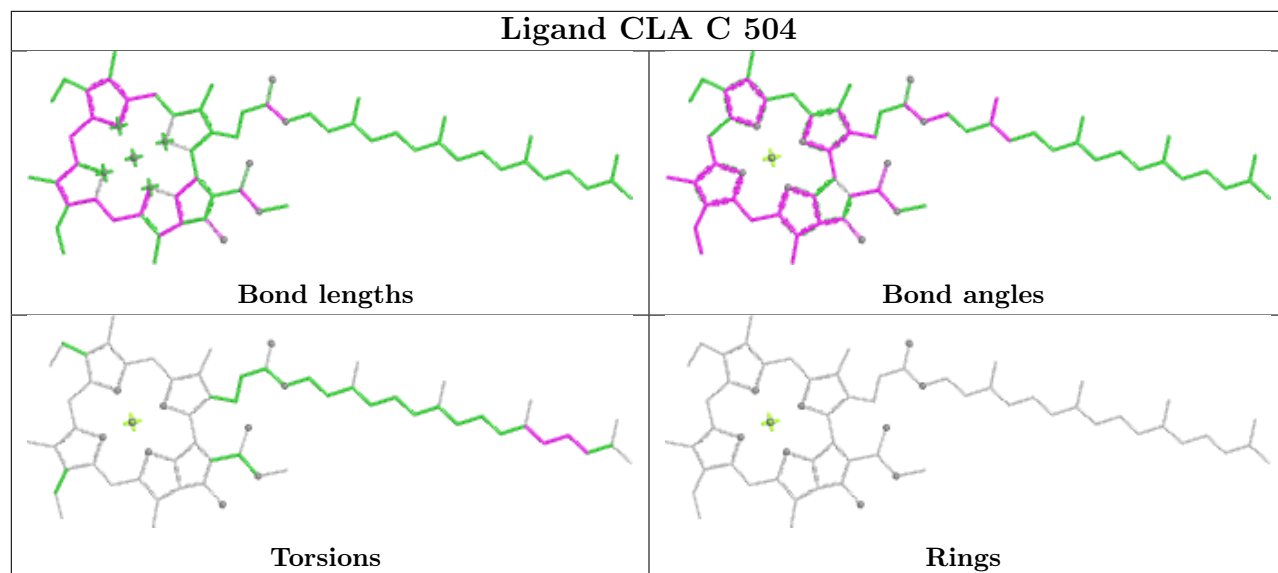
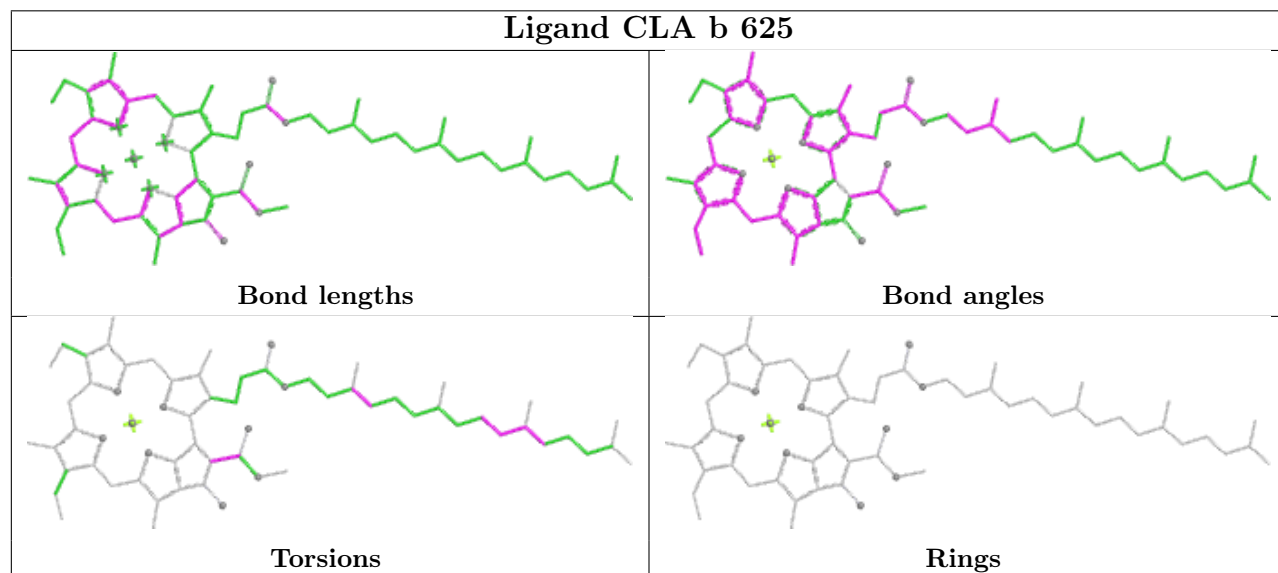
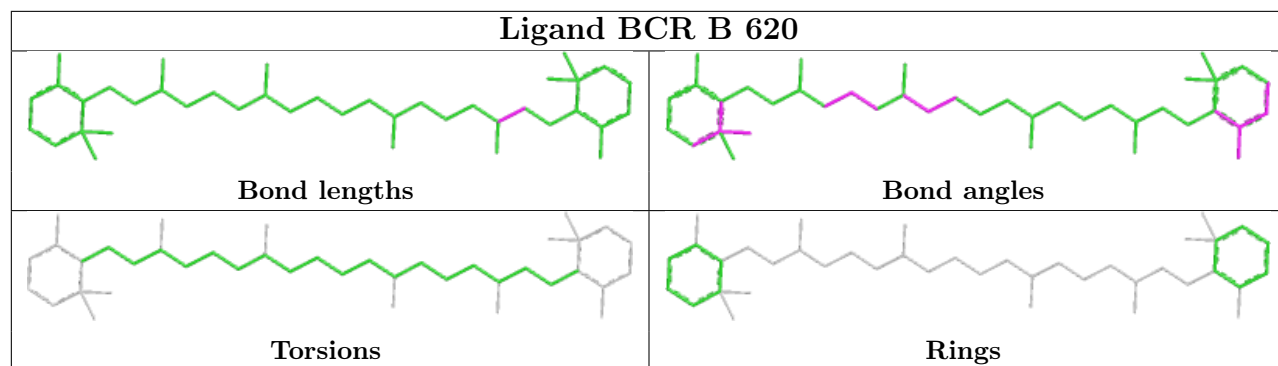


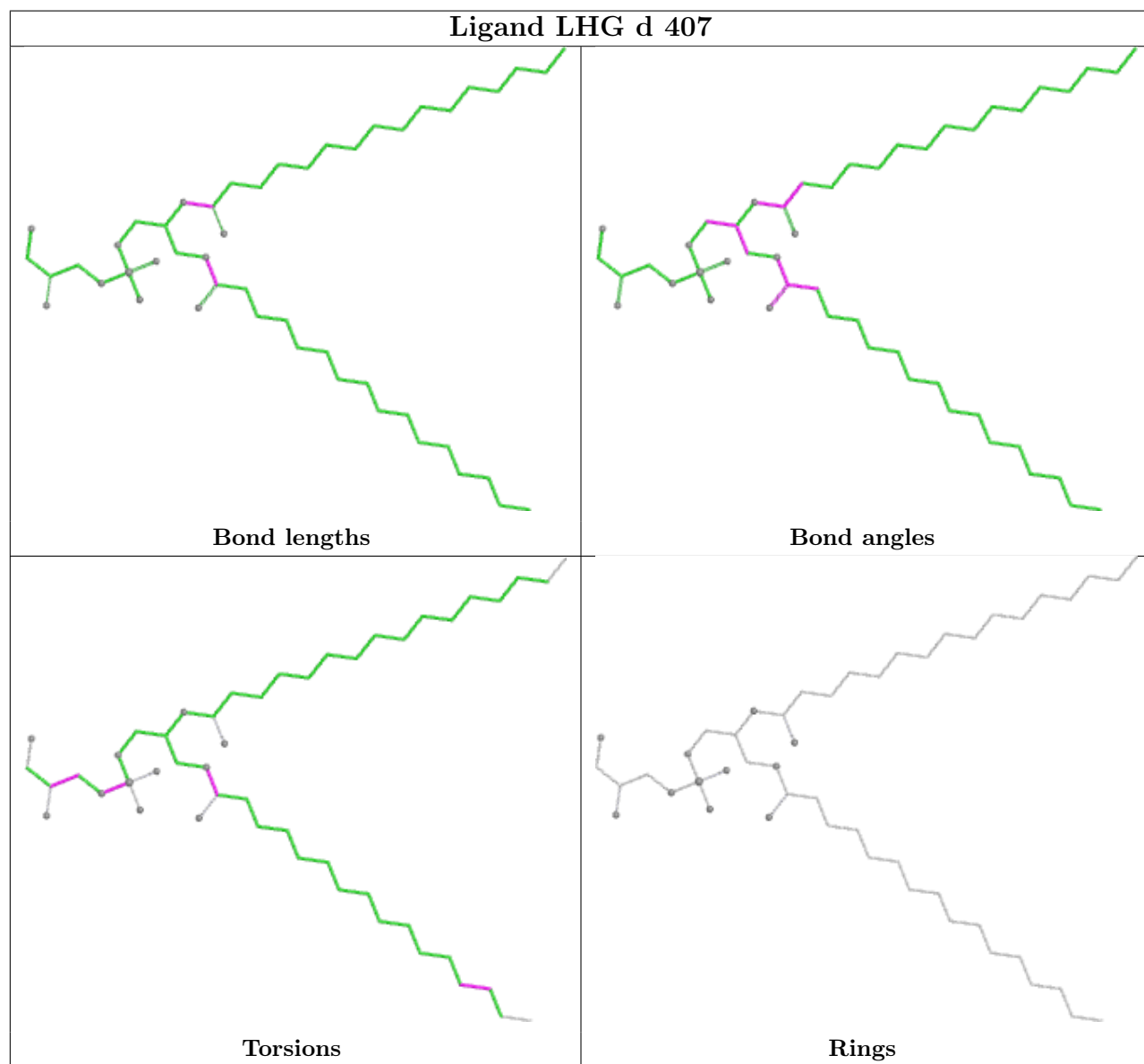
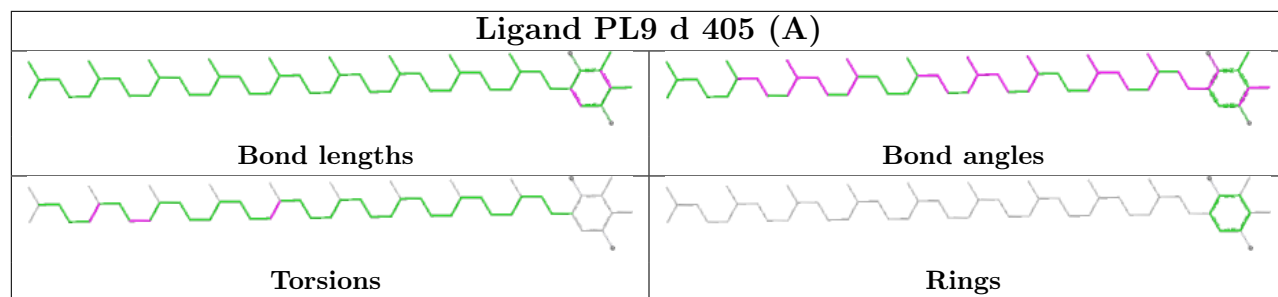
Ligand LMG C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

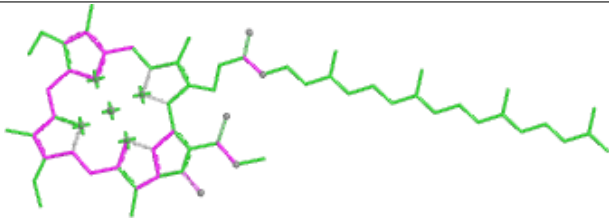
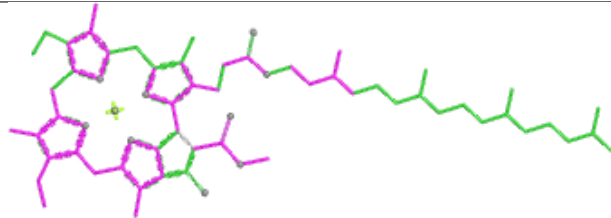
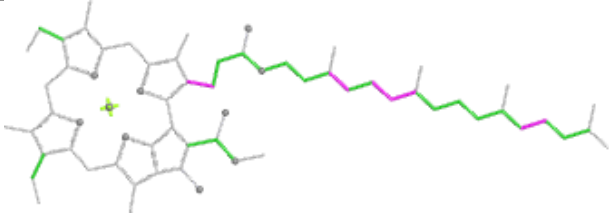
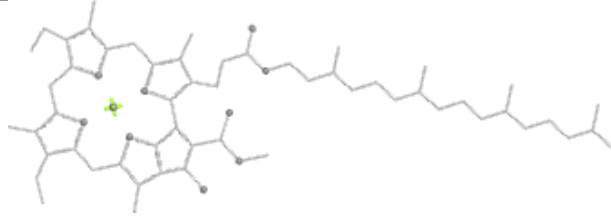
Ligand BCR D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

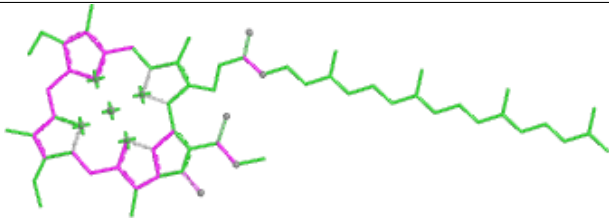
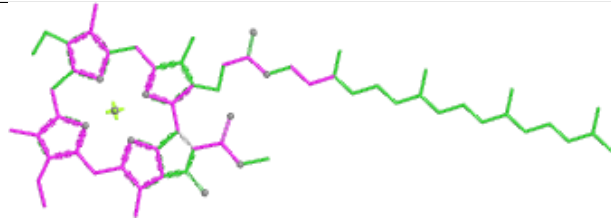
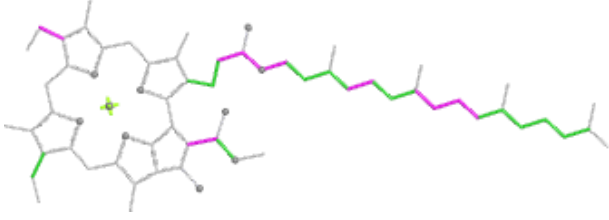
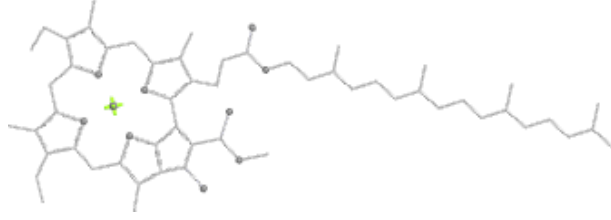
Ligand LMG D 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

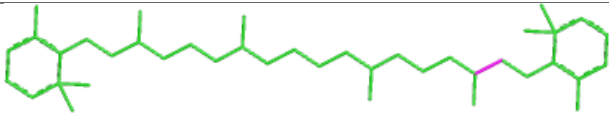
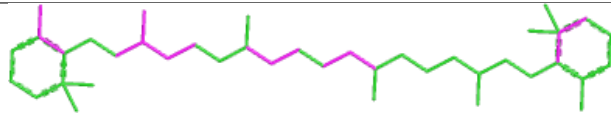
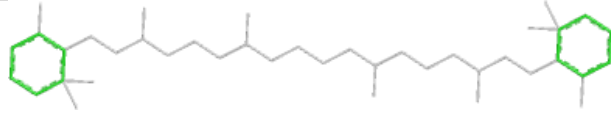
Ligand BCR c 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

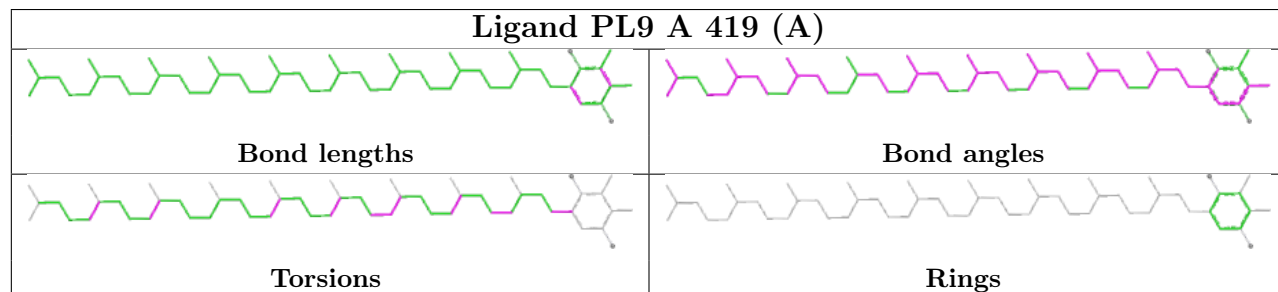
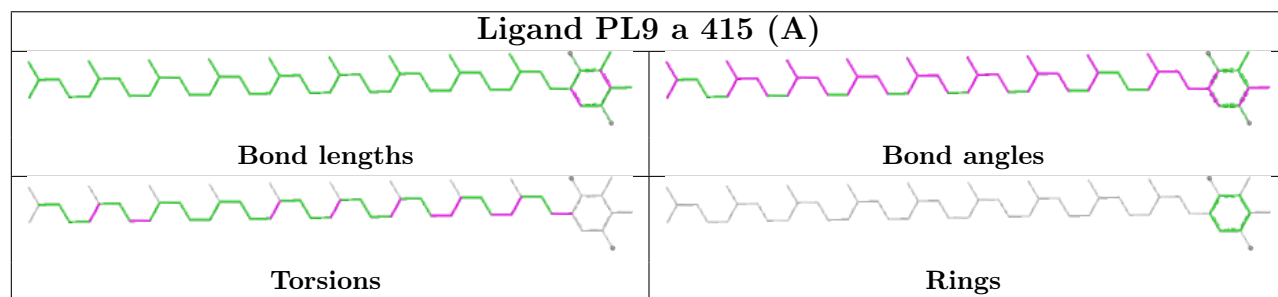
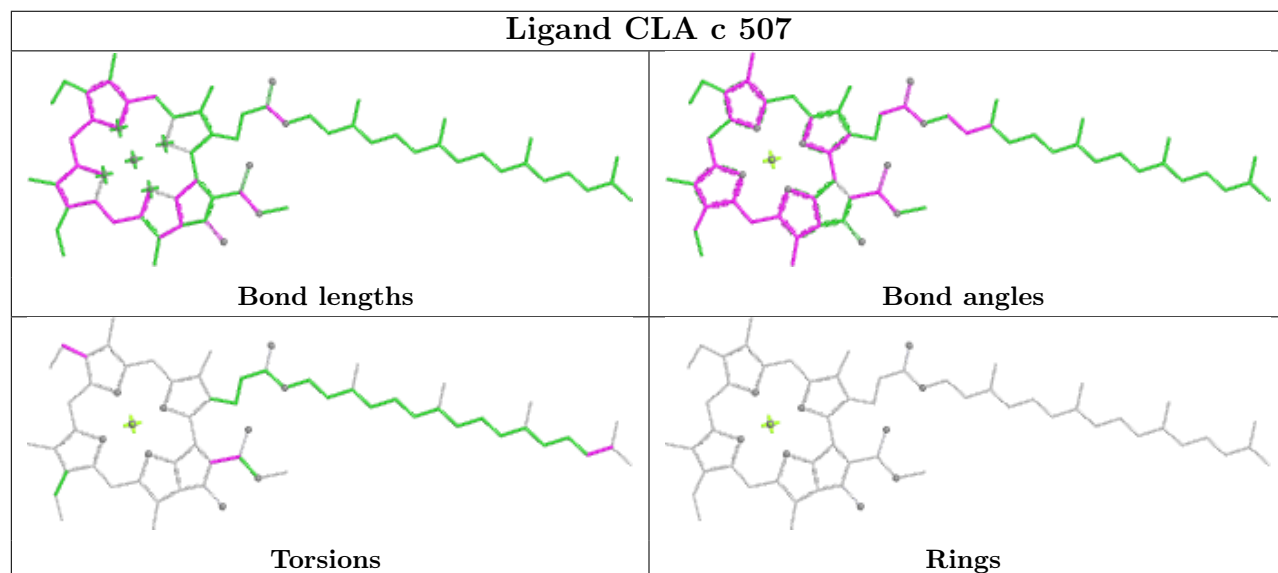
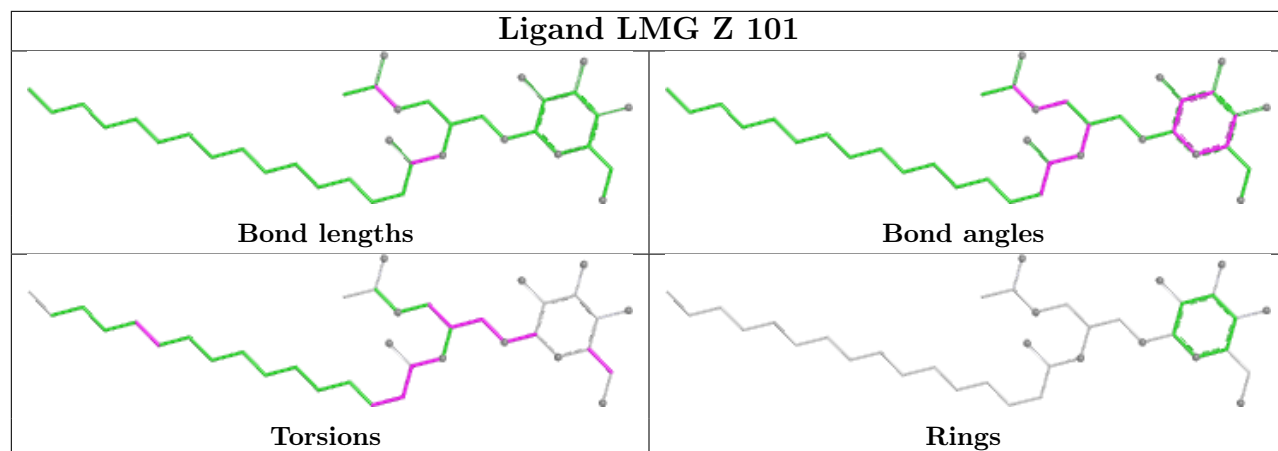


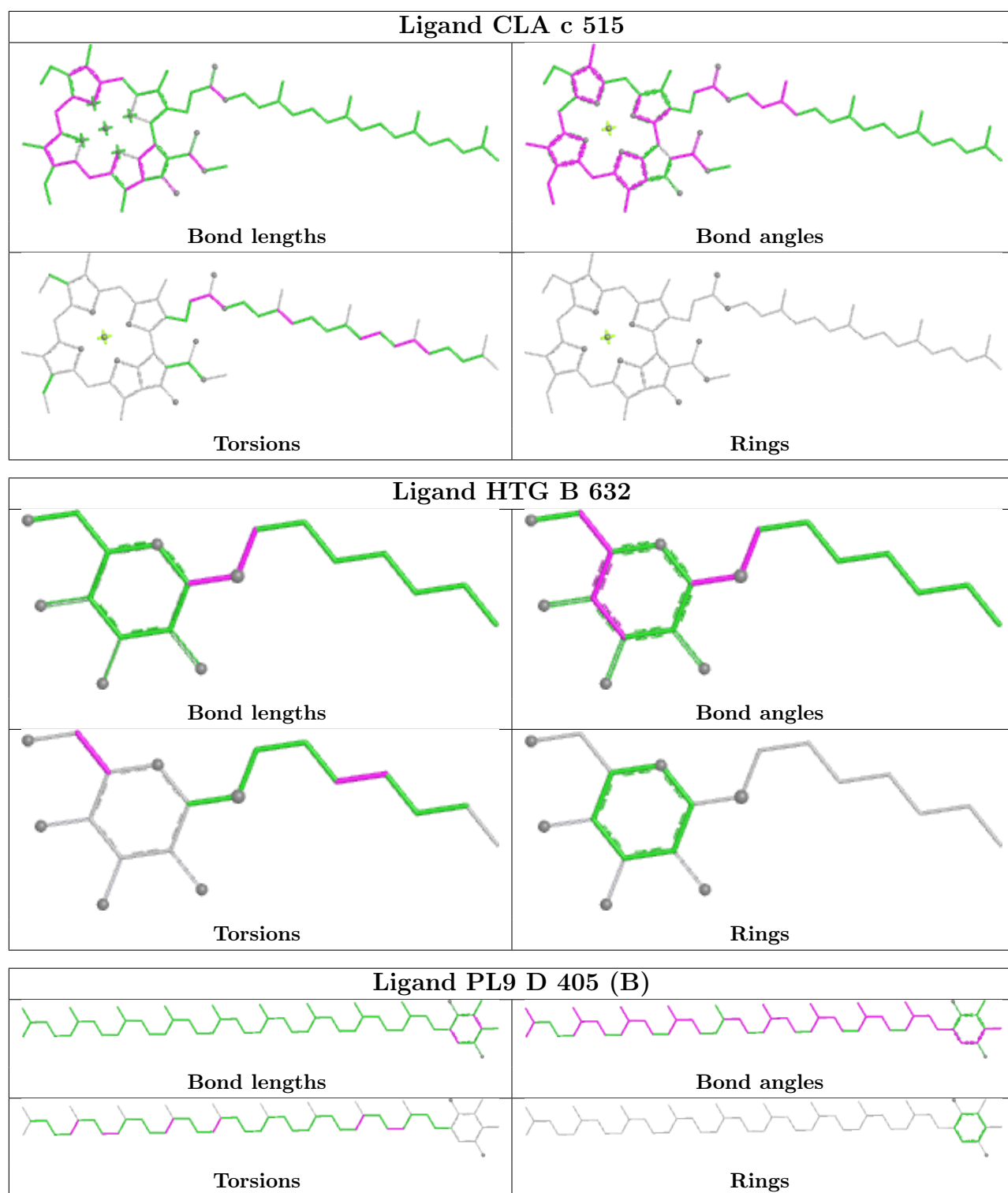


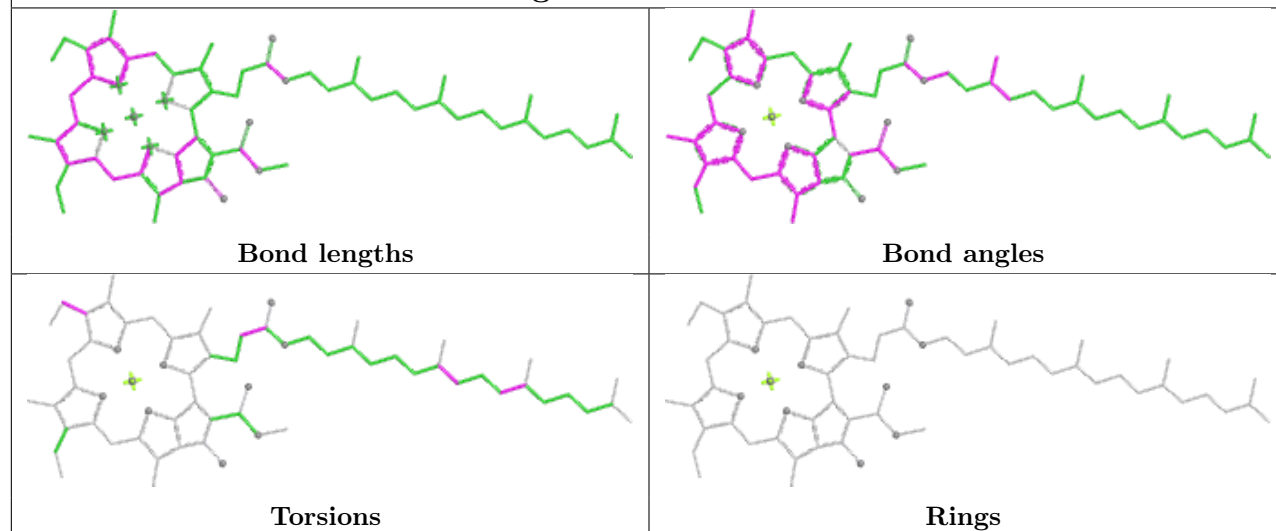
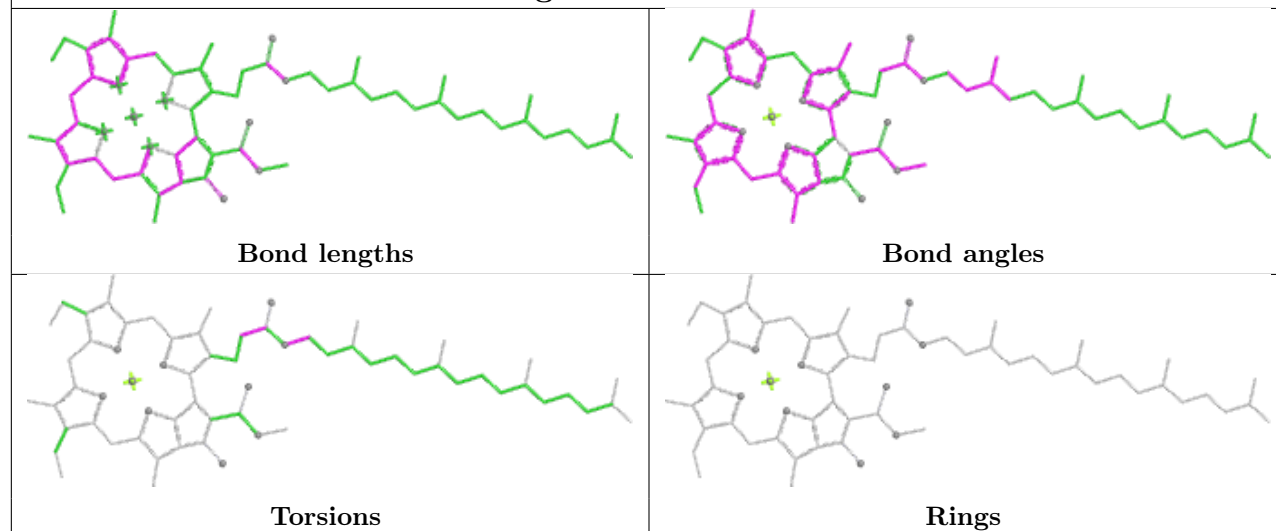
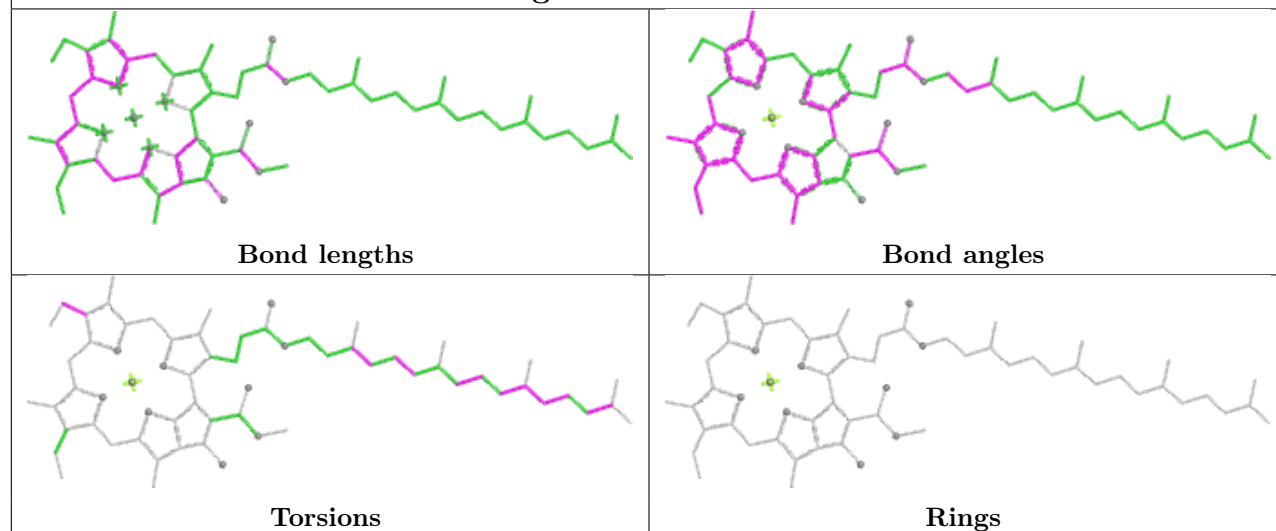
Ligand CLA C 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

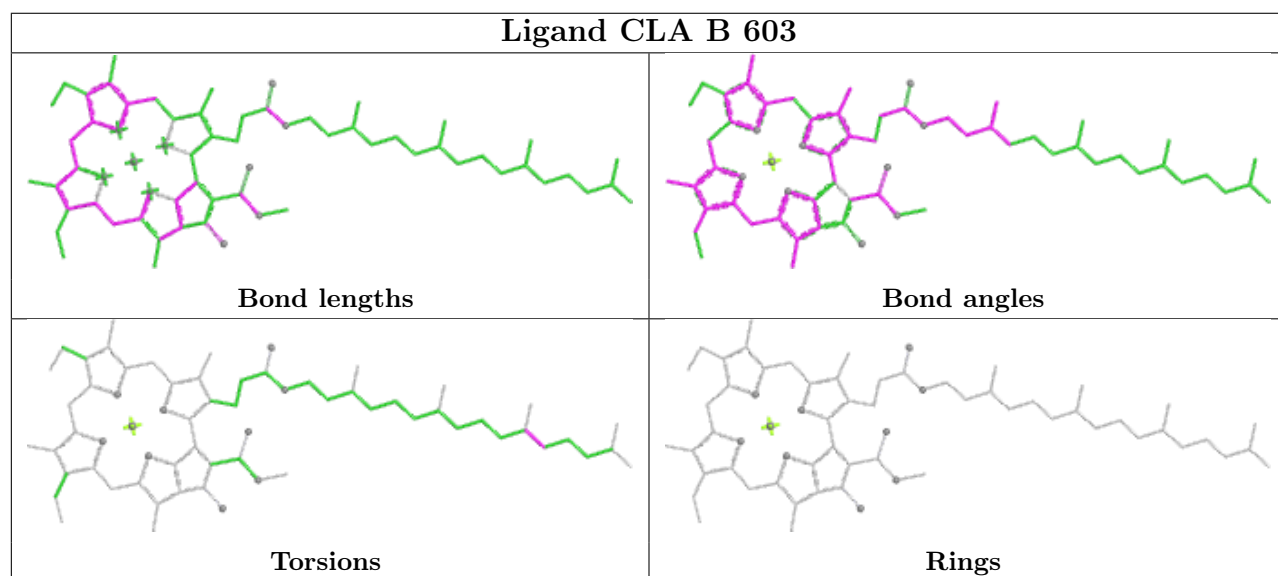
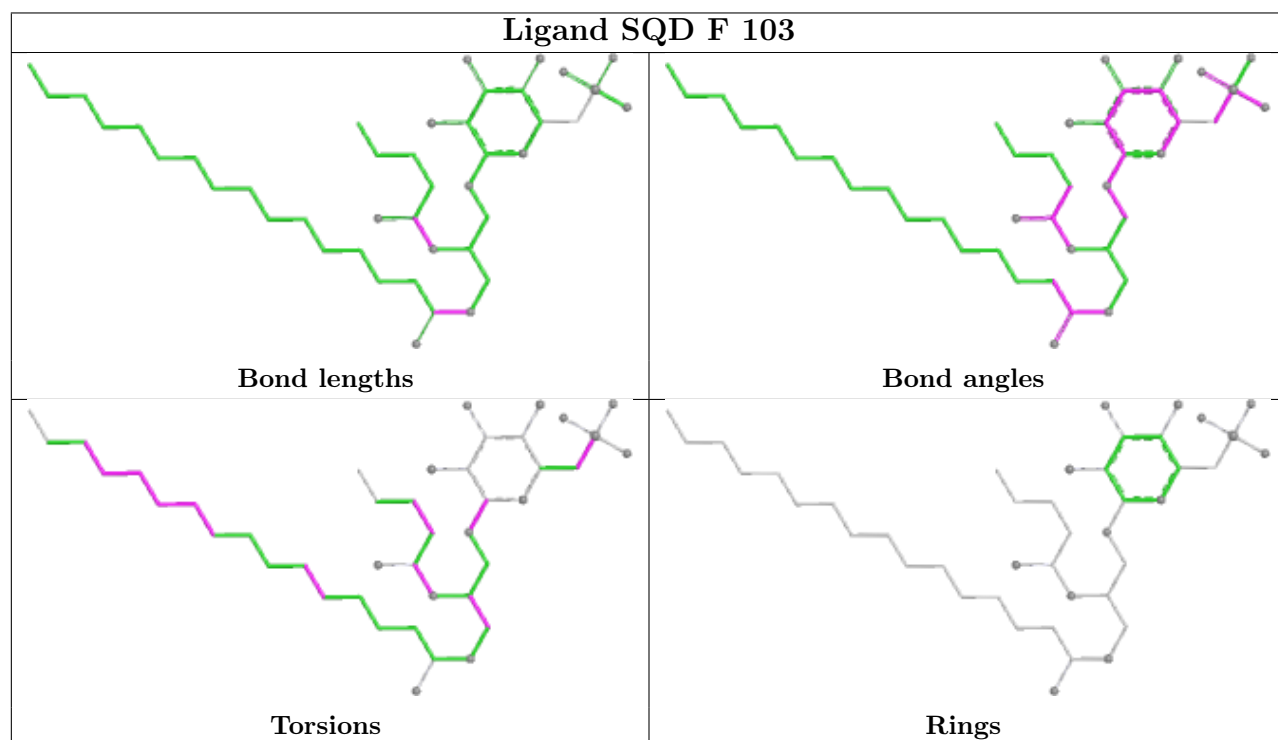
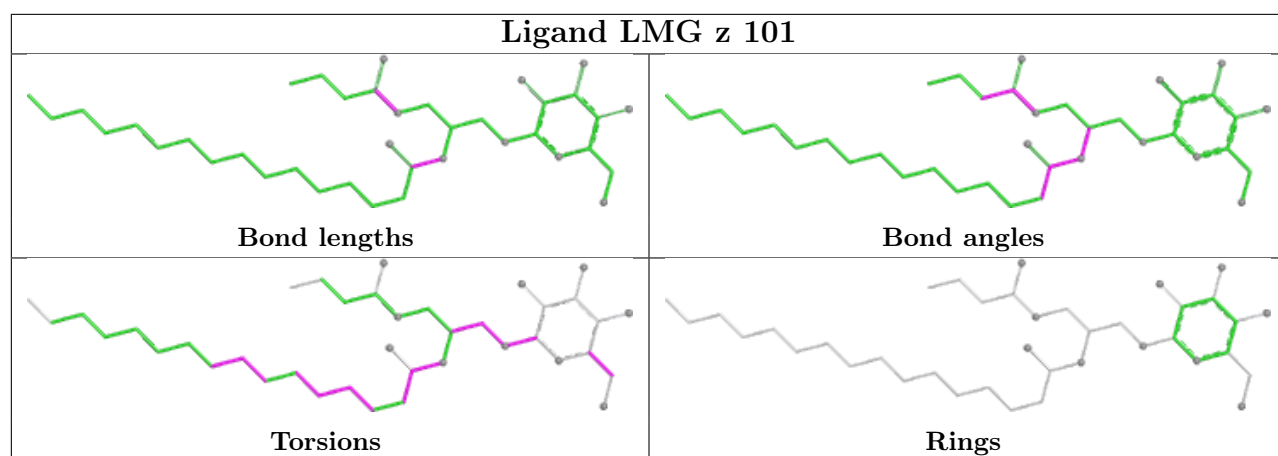
Ligand CLA B 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR c 528	
	
Bond lengths	Bond angles
	
Torsions	Rings

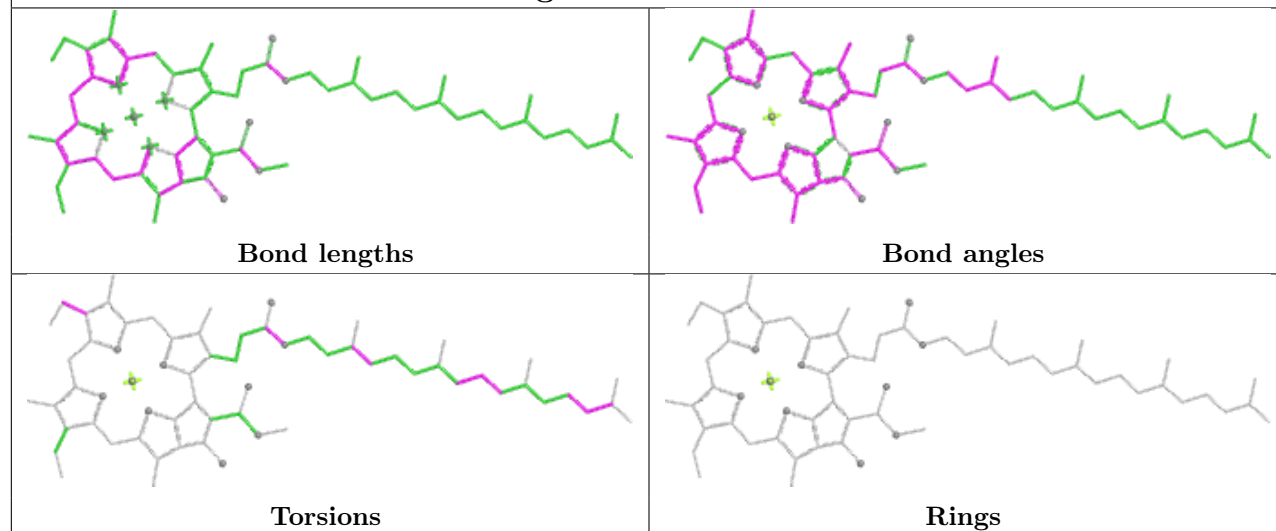




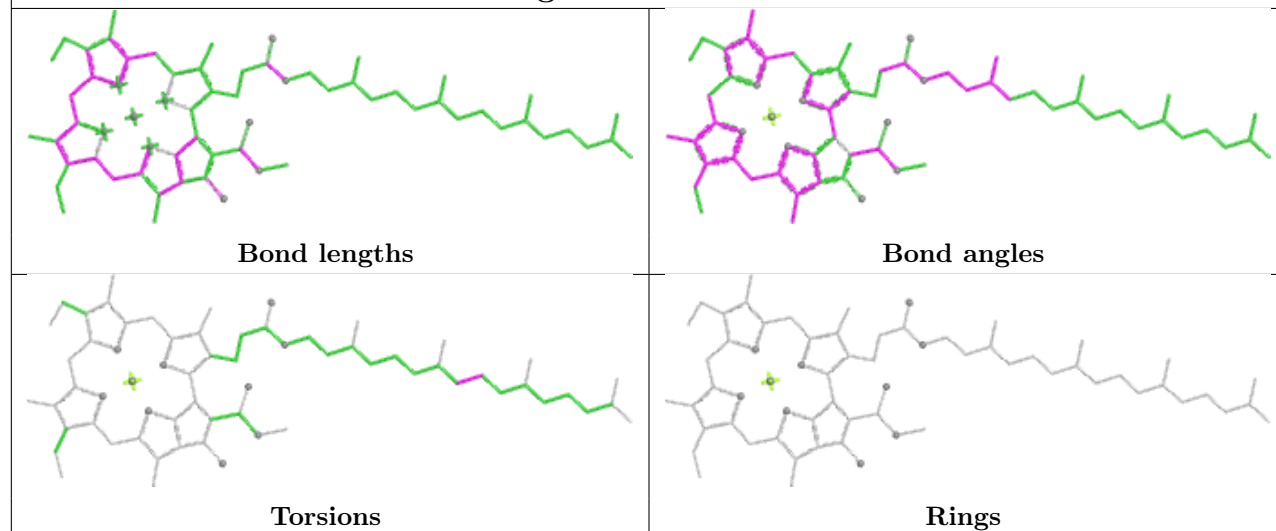
Ligand CLA C 505**Ligand CLA b 622****Ligand CLA B 616**



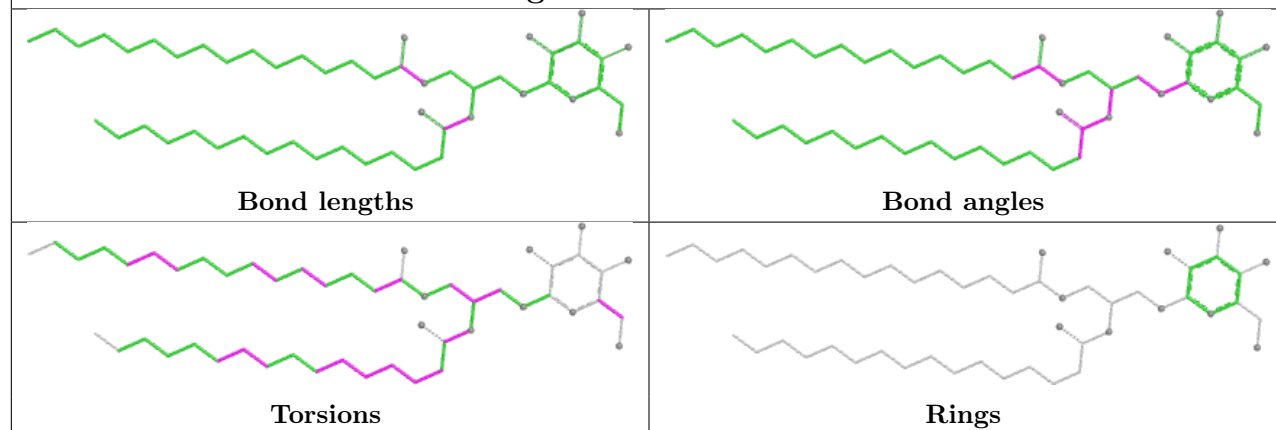
Ligand CLA a 412

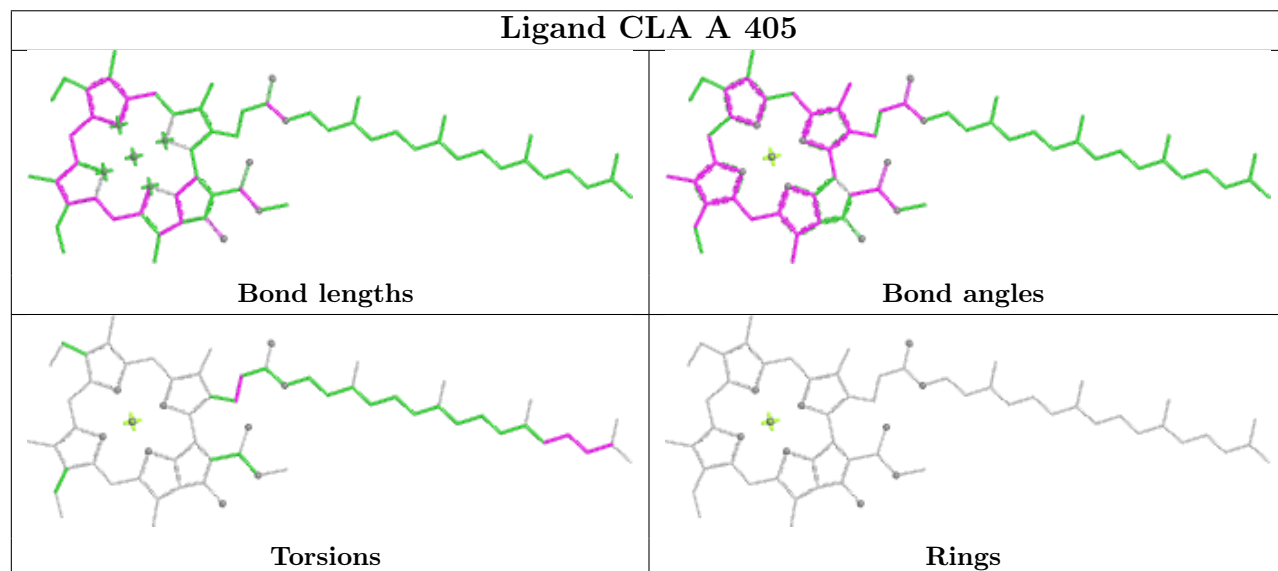
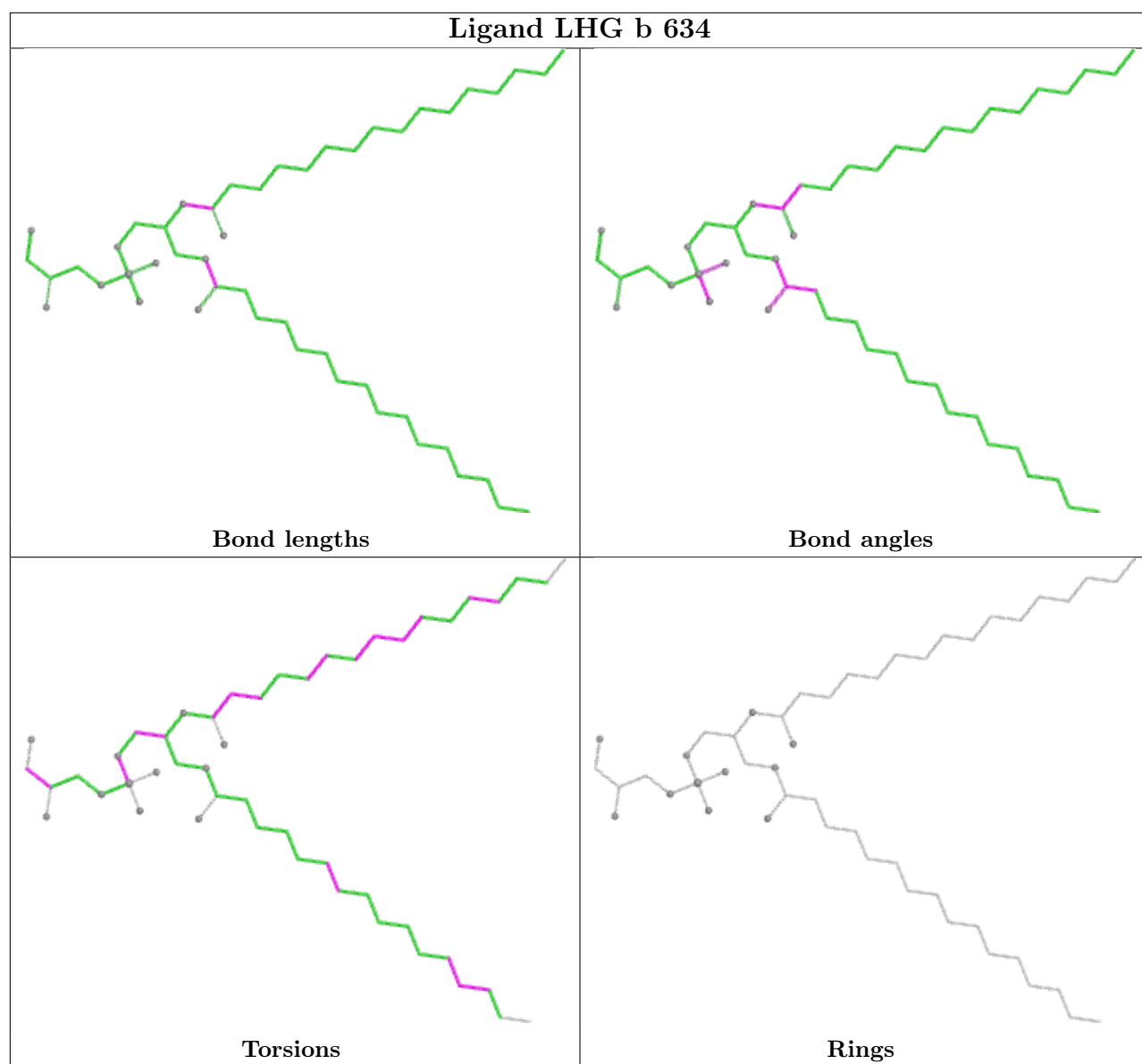


Ligand CLA c 508

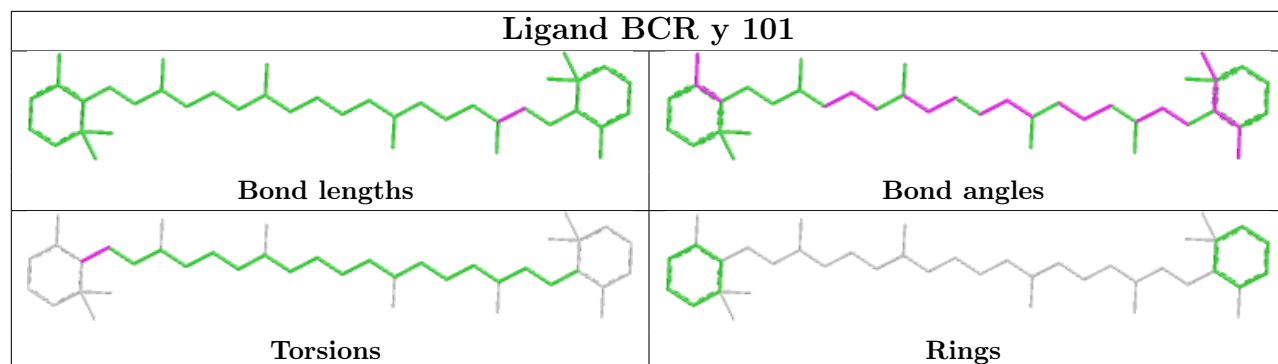


Ligand LMG A 421

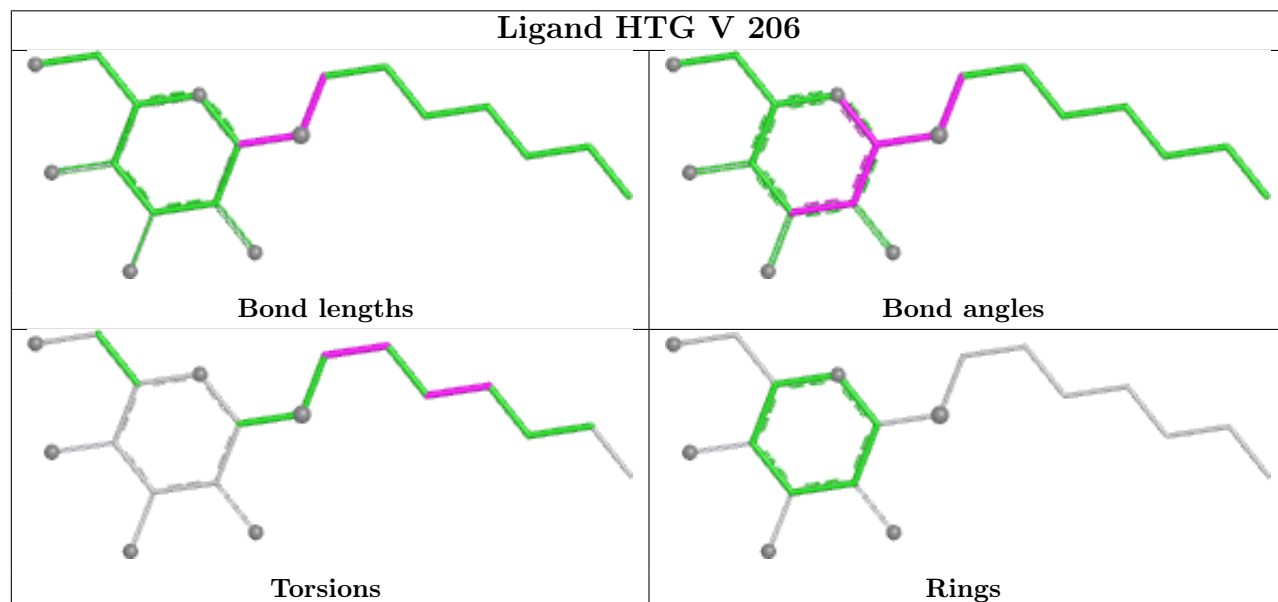




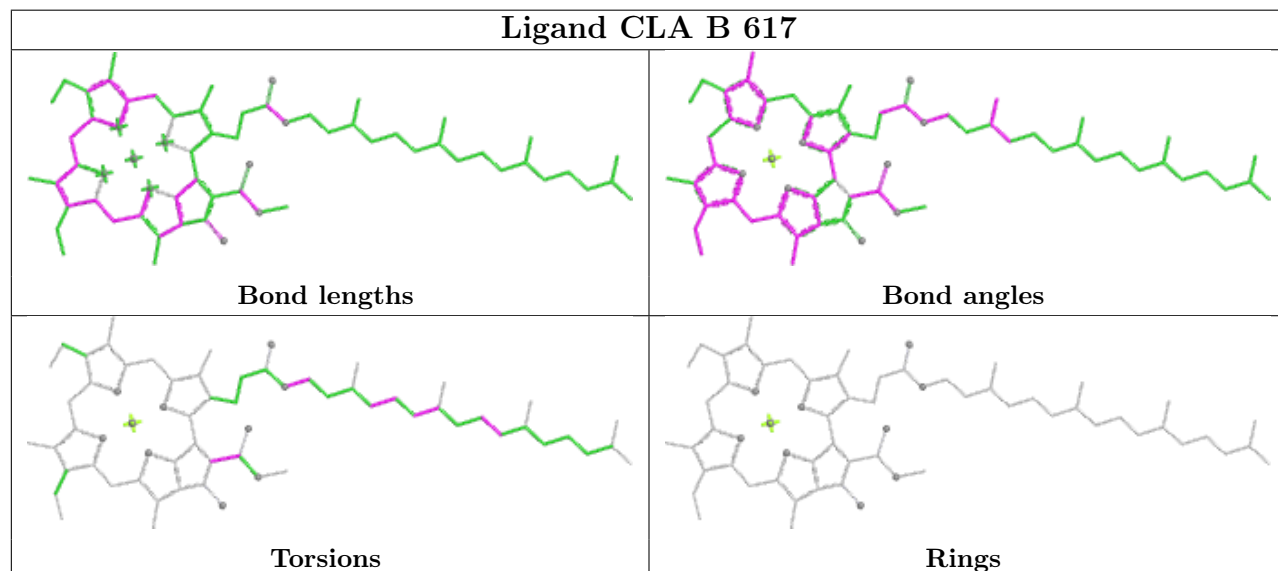
Ligand BCR y 101

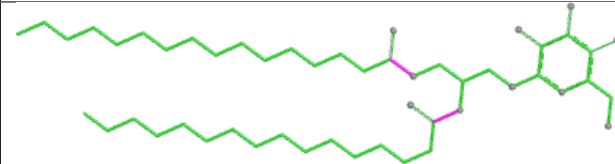
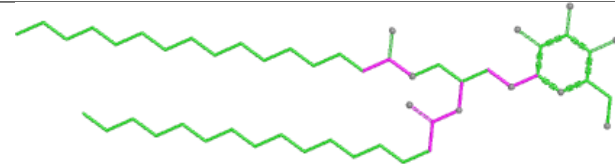
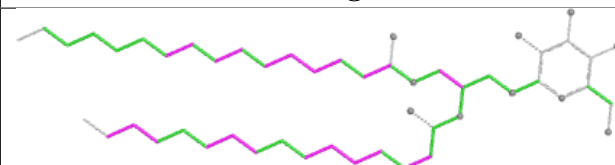
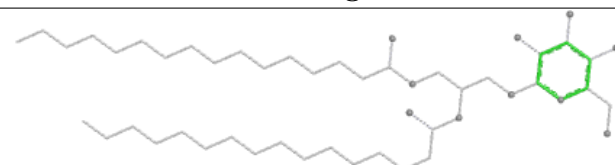


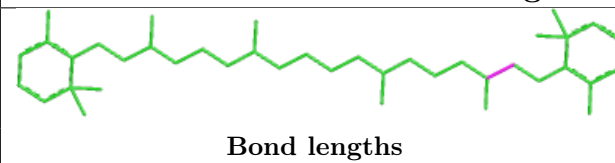
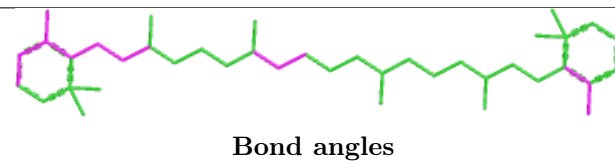
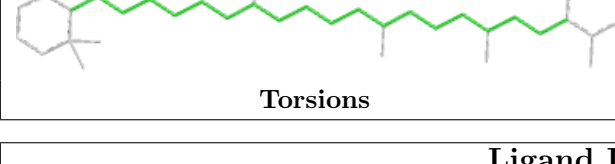
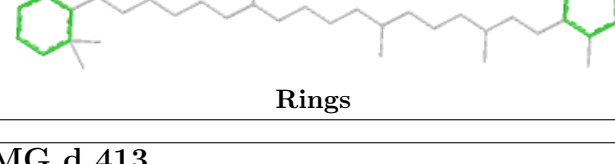
Ligand HTG V 206

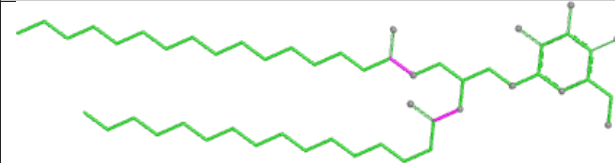
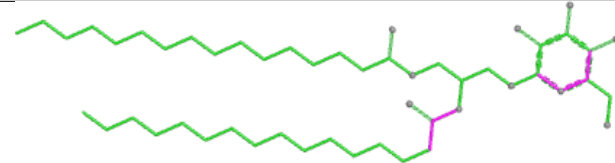
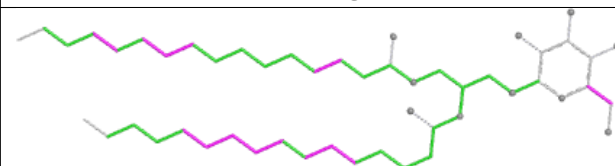
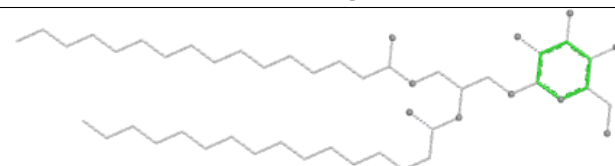


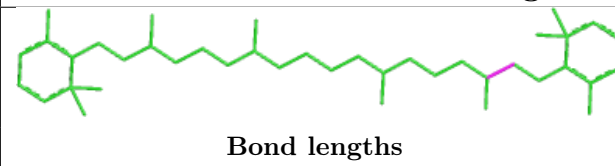
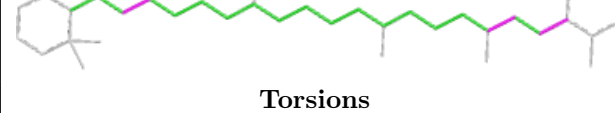
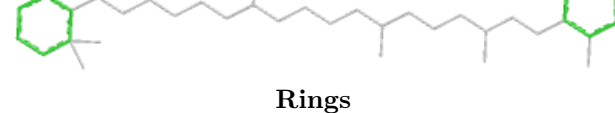
Ligand CLA B 617

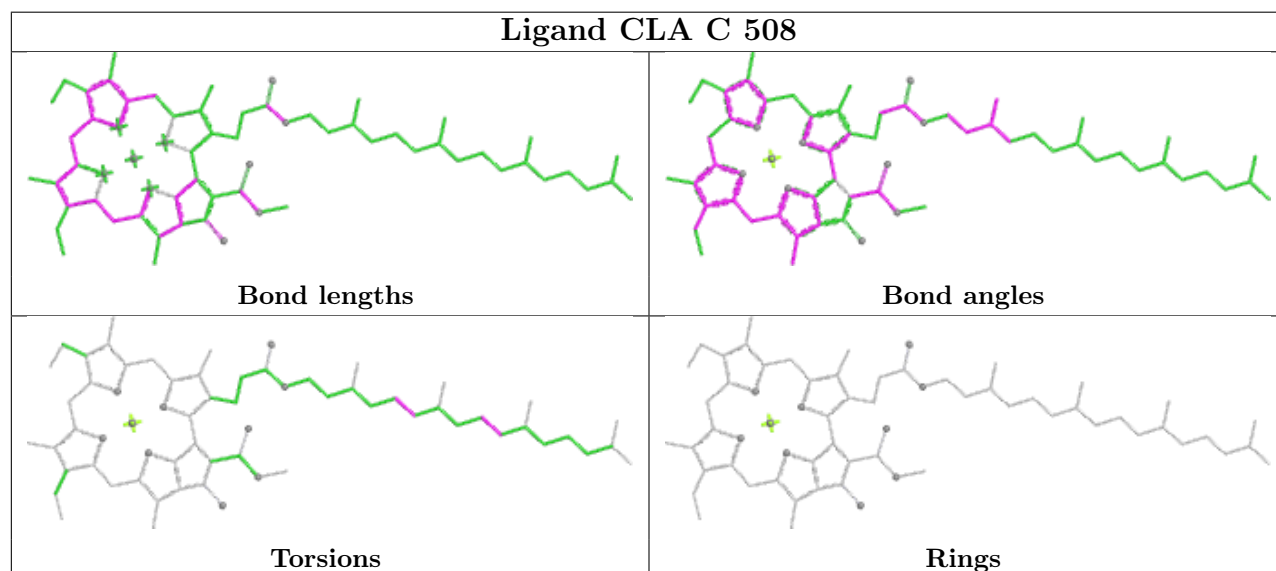
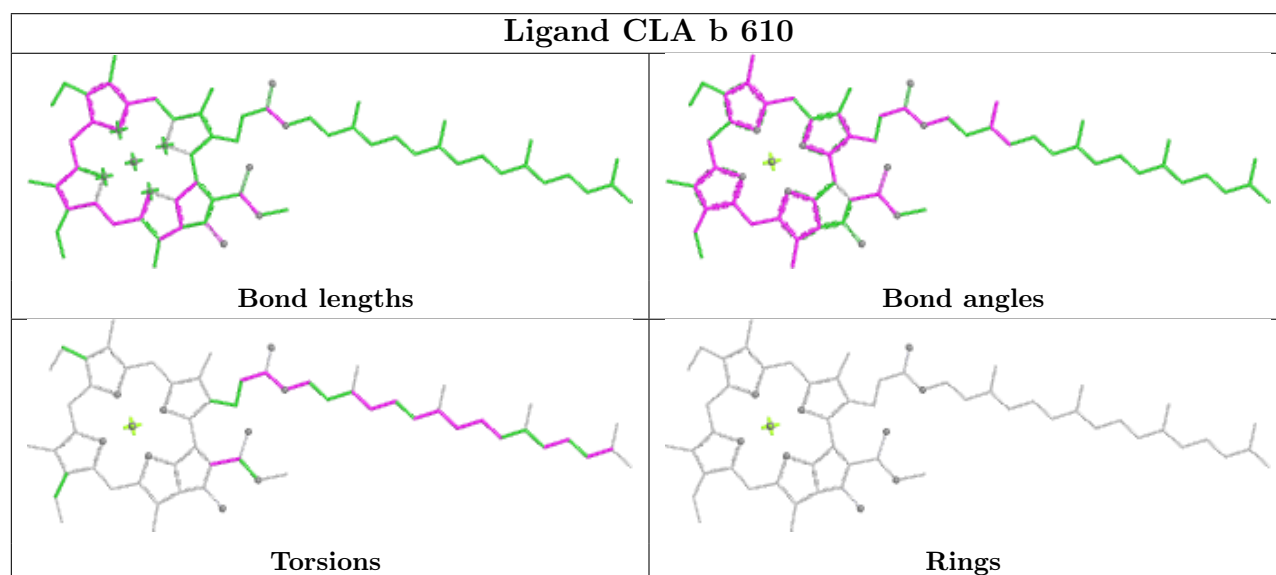
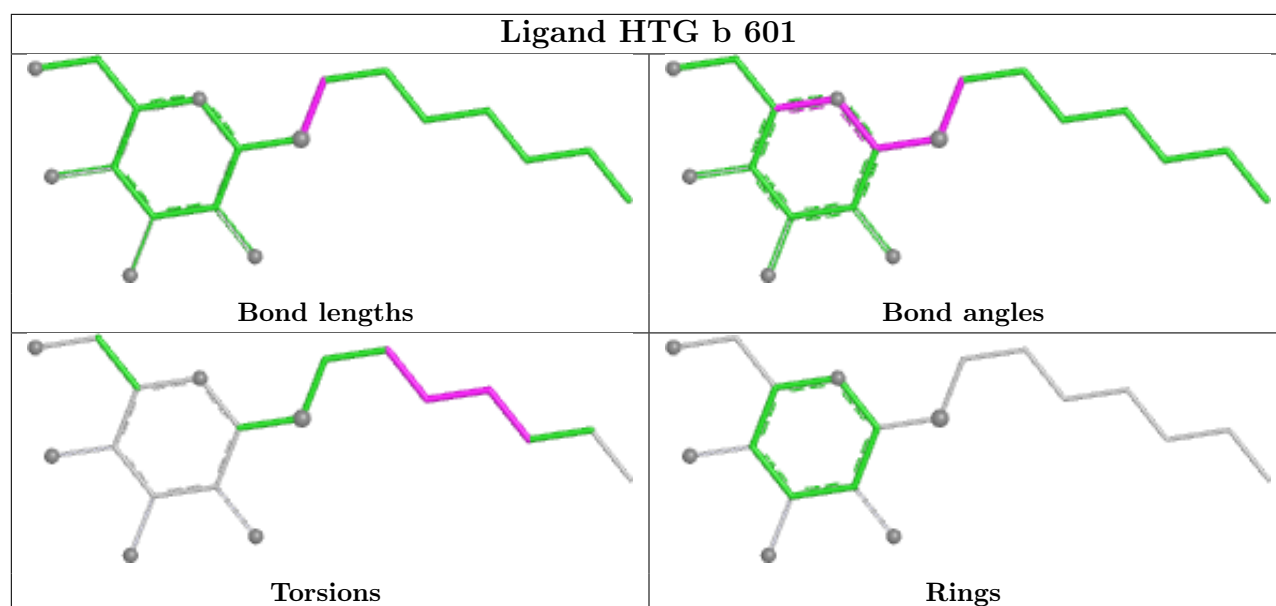


Ligand LMG c 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

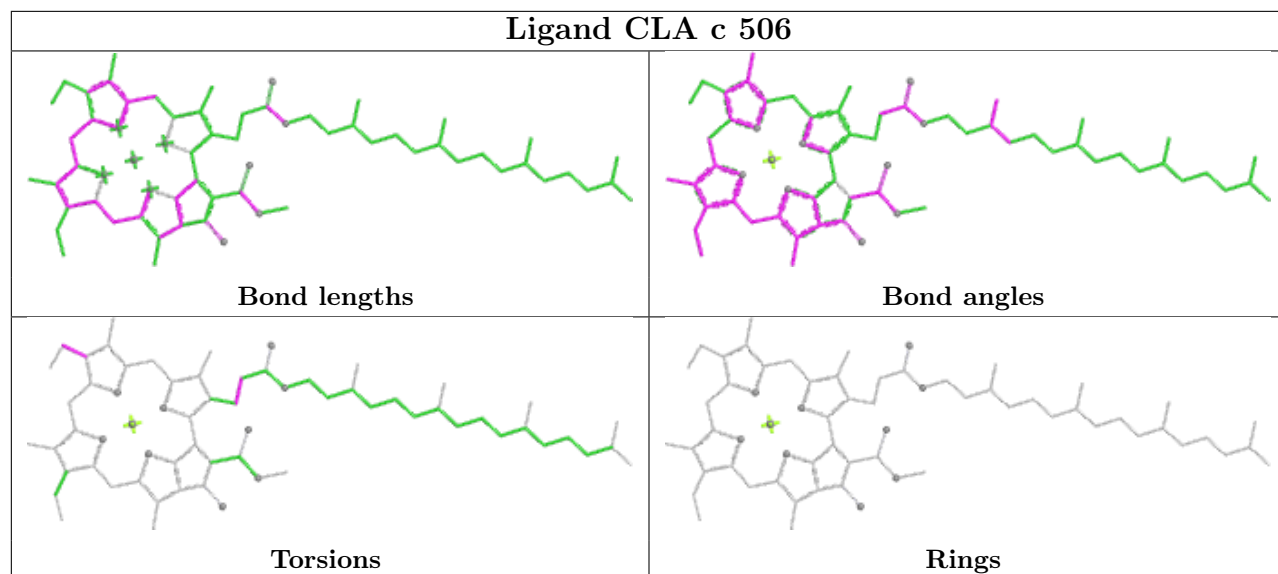
Ligand BCR a 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG d 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

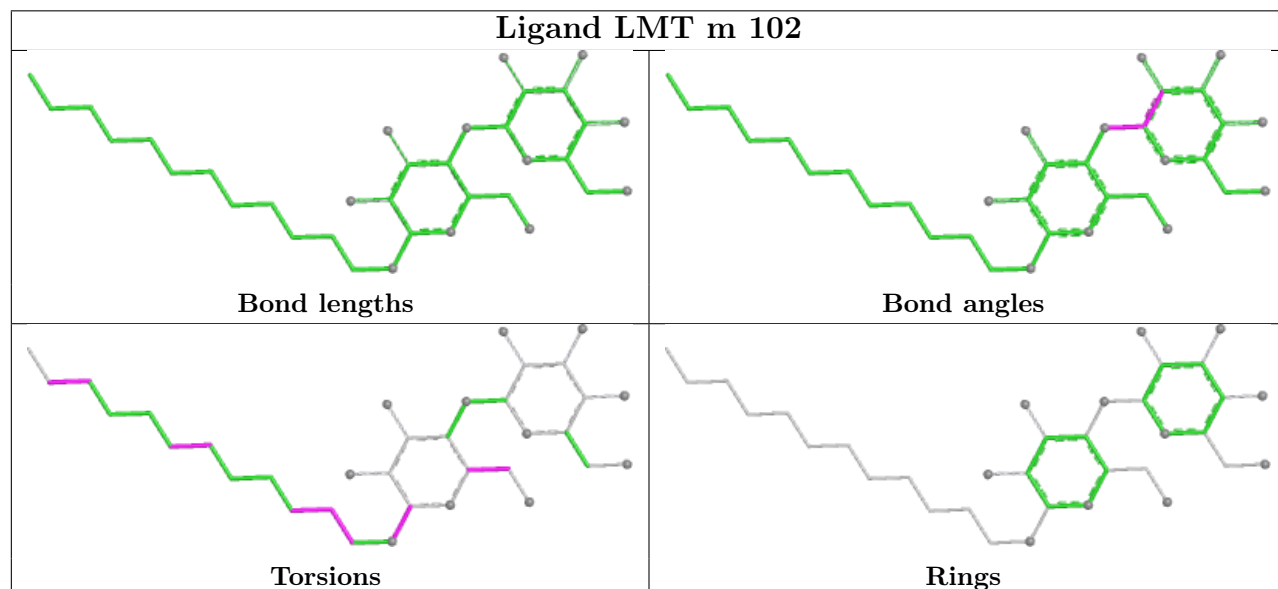
Ligand BCR d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings



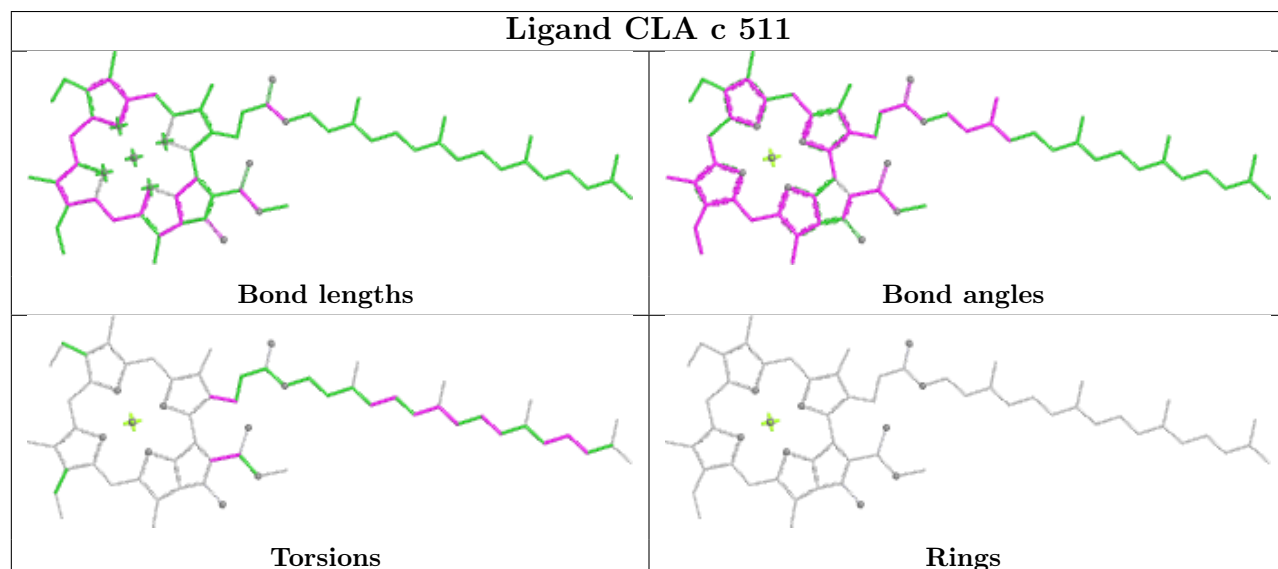
Ligand CLA c 506

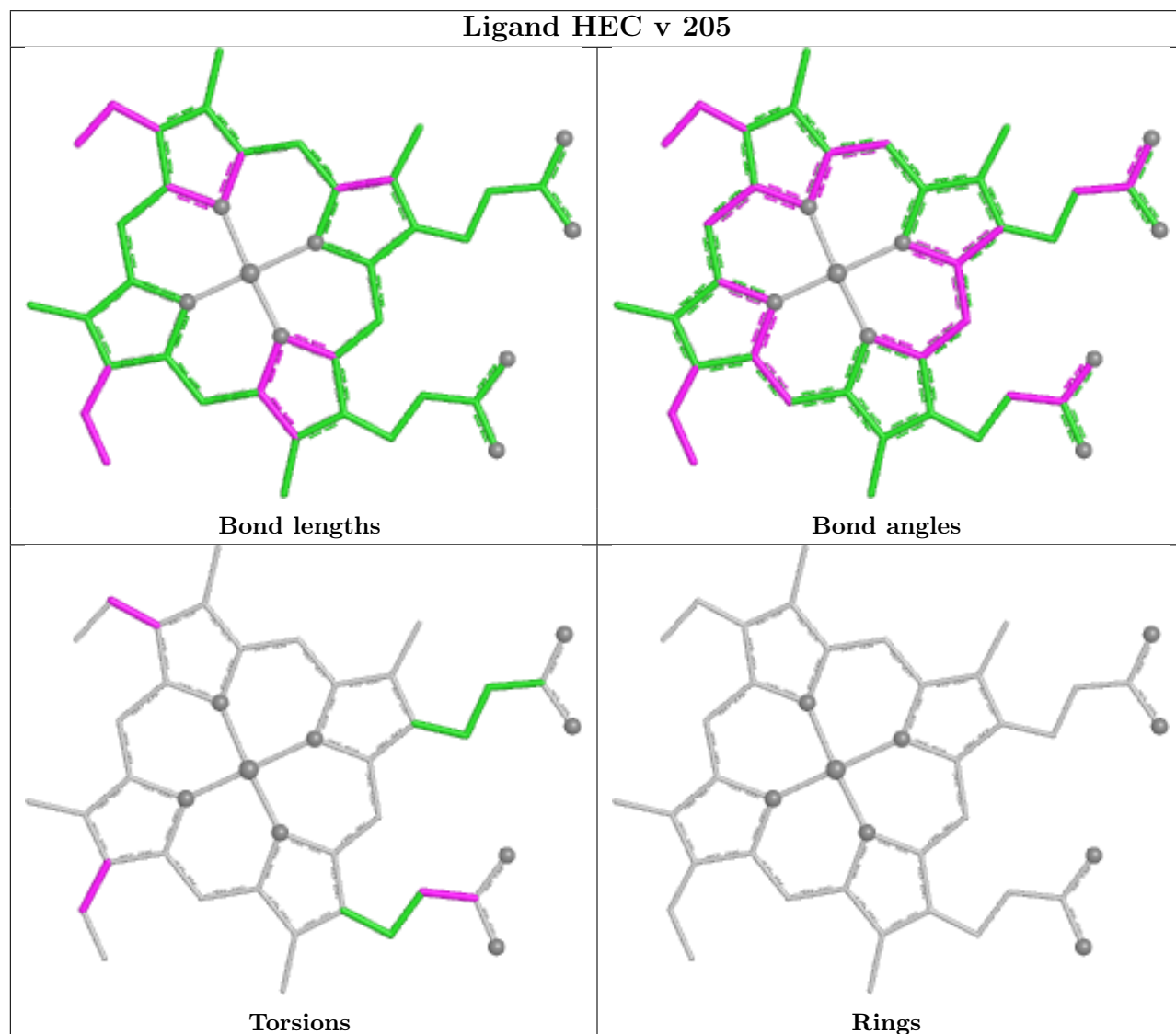
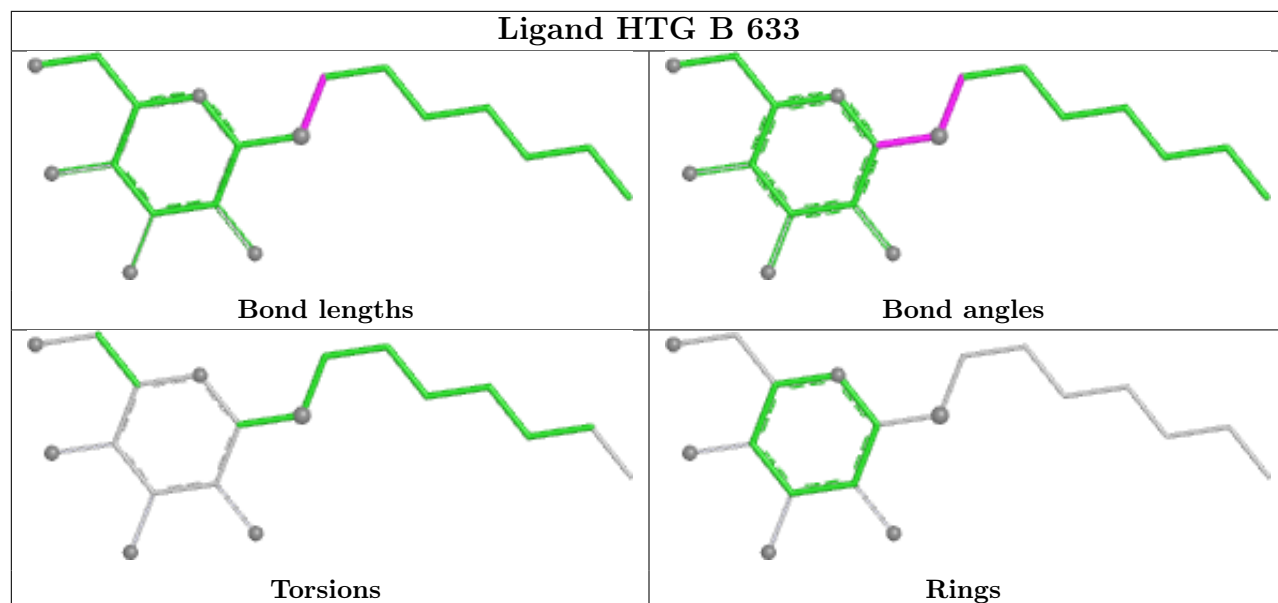


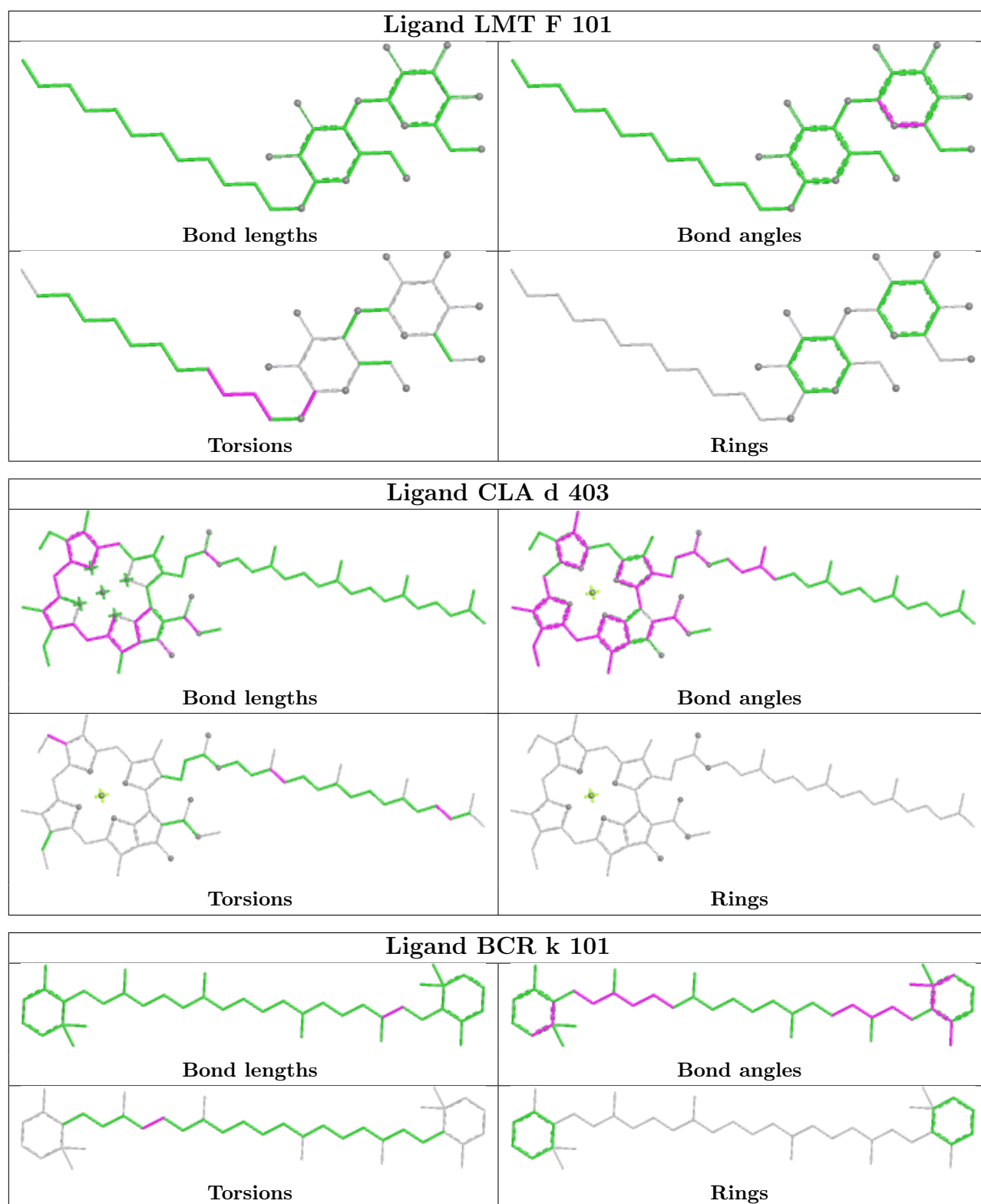
Ligand LMT m 102



Ligand CLA c 511







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.70	0 100 100	16, 37, 62, 117	53 (15%)
1	a	334/344 (97%)	-0.66	4 (1%) 76 79	17, 38, 70, 152	55 (16%)
2	B	504/505 (99%)	-0.63	2 (0%) 88 90	23, 43, 77, 123	10 (1%)
2	b	503/505 (99%)	-0.54	6 (1%) 76 79	26, 43, 78, 180	12 (2%)
3	C	451/455 (99%)	-0.52	0 100 100	17, 51, 70, 116	7 (1%)
3	c	455/455 (100%)	-0.52	0 100 100	19, 53, 70, 115	13 (2%)
4	D	341/342 (99%)	-0.74	0 100 100	18, 39, 61, 131	16 (4%)
4	d	341/342 (99%)	-0.72	1 (0%) 90 91	19, 41, 60, 122	16 (4%)
5	E	81/84 (96%)	-0.09	1 (1%) 76 79	32, 63, 94, 130	2 (2%)
5	e	81/84 (96%)	-0.00	2 (2%) 58 62	36, 64, 115, 176	2 (2%)
6	F	34/44 (77%)	-0.18	0 100 100	46, 56, 90, 105	0
6	f	32/44 (72%)	-0.15	1 (3%) 51 55	47, 57, 116, 141	0
7	H	65/65 (100%)	-0.31	2 (3%) 51 55	35, 52, 72, 150	1 (1%)
7	h	65/65 (100%)	-0.39	2 (3%) 51 55	42, 55, 75, 163	0
8	I	37/38 (97%)	-0.26	0 100 100	43, 54, 108, 151	0
8	i	37/38 (97%)	-0.23	1 (2%) 56 60	42, 52, 98, 131	0
9	J	38/39 (97%)	0.09	2 (5%) 32 36	46, 61, 135, 169	0
9	j	39/39 (100%)	-0.05	1 (2%) 57 61	47, 61, 131, 171	0
10	K	37/37 (100%)	-0.29	0 100 100	51, 61, 77, 101	0
10	k	37/37 (100%)	-0.32	0 100 100	52, 61, 77, 102	0
11	L	37/37 (100%)	-0.72	0 100 100	18, 35, 100, 120	1 (2%)
11	l	37/37 (100%)	-0.65	0 100 100	22, 35, 99, 120	1 (2%)
12	M	33/36 (91%)	-0.72	0 100 100	22, 37, 63, 113	1 (3%)
12	m	33/36 (91%)	-0.67	0 100 100	32, 38, 68, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.57	2 (0%) 82 84	24, 48, 91, 137	8 (3%)
13	o	243/244 (99%)	-0.48	2 (0%) 82 84	27, 50, 104, 170	5 (2%)
14	T	29/32 (90%)	-0.74	1 (3%) 48 52	31, 37, 64, 133	1 (3%)
14	t	29/32 (90%)	-0.67	1 (3%) 48 52	29, 37, 64, 133	1 (3%)
15	U	97/104 (93%)	-0.65	0 100 100	37, 48, 77, 116	0
15	u	97/104 (93%)	-0.64	0 100 100	39, 49, 71, 116	0
16	V	137/137 (100%)	-0.54	0 100 100	20, 49, 78, 116	2 (1%)
16	v	137/137 (100%)	-0.54	1 (0%) 84 85	21, 55, 84, 118	1 (0%)
17	Y	29/30 (96%)	0.76	3 (10%) 12 13	66, 80, 141, 149	0
17	y	29/30 (96%)	0.42	3 (10%) 12 13	66, 81, 142, 149	0
18	X	39/40 (97%)	0.09	1 (2%) 57 61	51, 61, 115, 136	0
18	x	38/40 (95%)	0.19	2 (5%) 32 36	53, 62, 116, 137	0
19	Z	62/62 (100%)	0.28	4 (6%) 25 28	66, 78, 125, 165	0
19	z	62/62 (100%)	0.44	3 (4%) 35 40	68, 80, 126, 166	0
20	R	18/34 (52%)	2.74	12 (66%) 0 0	106, 137, 176, 178	0
All	All	5275/5384 (97%)	-0.50	60 (1%) 78 80	16, 47, 90, 180	208 (3%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	15	ALA	5.2
20	R	3	TRP	4.3
19	z	3	ILE	4.0
2	b	499	VAL	3.9
20	R	13	LEU	3.9
7	h	65	LEU	3.8
18	x	2	THR	3.8
20	R	9	LEU	3.7
20	R	5	VAL	3.5
5	e	5	THR	3.5
7	H	66	GLY	3.4
2	b	495	PHE	3.4
20	R	12	VAL	3.4
2	B	479	PHE	3.3
17	Y	18	VAL	3.2
2	b	486	LEU	3.2
7	H	65	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
20	R	10	LEU	3.2
20	R	14	LEU	3.1
20	R	6	LEU	3.1
2	B	495	PHE	3.0
5	e	4	THR	3.0
14	t	30	THR	3.0
17	y	18	VAL	2.9
13	o	58	ASN	2.8
17	Y	20	ALA	2.8
20	R	16	ALA	2.8
2	b	502	VAL	2.8
20	R	18	TRP	2.8
19	Z	3	ILE	2.8
19	Z	61	VAL	2.7
5	E	4	THR	2.7
18	x	37	VAL	2.7
9	j	1	MET	2.6
20	R	7	VAL	2.6
17	y	20	ALA	2.6
1	a	11	ALA	2.6
17	y	19	ILE	2.6
7	h	66	GLY	2.6
19	Z	33	TRP	2.5
9	J	2	SER	2.5
17	Y	19	ILE	2.5
6	f	14	PRO	2.4
2	b	493	TRP	2.4
1	a	263	ALA	2.4
8	i	37	LEU	2.4
18	X	37	VAL	2.4
19	Z	62	VAL	2.4
13	o	4	THR	2.4
1	a	260	PHE	2.3
19	z	62	VAL	2.3
13	O	4	THR	2.2
19	z	5	PHE	2.2
16	v	106	ASN	2.1
14	T	30	THR	2.1
1	a	248[A]	ILE	2.1
4	d	12	ARG	2.1
9	J	5	GLY	2.0
2	b	479	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
13	O	56	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.96	0.06	35,38,64,74	0
12	FME	m	1	10/11	0.96	0.08	34,43,98,115	0
8	FME	I	1	10/11	0.97	0.07	37,45,52,53	0
8	FME	i	1	10/11	0.97	0.06	41,51,56,58	0
12	FME	M	1	10/11	0.97	0.07	31,47,81,85	0
14	FME	t	1	10/11	0.97	0.05	28,38,44,87	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
36	DGD	e	101	62/66	0.69	0.16	70,118,175,181	0
36	DGD	D	406	52/66	0.70	0.15	65,108,147,157	0
37	LHG	e	102	42/49	0.70	0.13	69,134,167,172	0
29	LMT	F	101	35/35	0.73	0.15	86,125,152,156	0
34	CA	b	609	1/1	0.75	0.12	134,134,134,134	0
29	LMT	b	630	25/35	0.75	0.14	72,92,147,149	0
29	LMT	C	521	35/35	0.76	0.14	90,123,152,162	0
32	UNL	M	102	10/-	0.76	0.12	47,64,75,75	0
29	LMT	a	419	35/35	0.77	0.14	87,111,130,134	0
32	UNL	a	403	30/-	0.77	0.14	69,91,126,131	0
27	SQD	f	101	43/54	0.77	0.14	86,120,144,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	UNL	m	101	10/-	0.78	0.15	49,60,85,88	0
35	HTG	D	412	16/19	0.79	0.14	75,142,157,157	0
32	UNL	j	101	10/-	0.79	0.14	70,82,96,99	0
28	GOL	V	201	6/6	0.79	0.14	64,77,86,93	0
29	LMT	f	102	35/35	0.79	0.13	72,121,149,154	0
29	LMT	M	103	35/35	0.80	0.14	41,102,141,150	0
32	UNL	A	420	28/-	0.80	0.14	61,86,104,106	0
35	HTG	c	526	19/19	0.80	0.12	66,105,123,137	0
32	UNL	C	527	34/-	0.81	0.13	73,108,129,134	0
32	UNL	I	101	40/-	0.81	0.14	41,84,142,153	0
29	LMT	A	417	35/35	0.82	0.12	40,80,108,129	0
35	HTG	V	206	19/19	0.82	0.12	66,94,116,209	0
32	UNL	J	101	10/-	0.82	0.13	47,72,89,101	0
33	LMG	C	520	51/55	0.82	0.12	56,109,125,129	0
32	UNL	i	101	40/-	0.82	0.13	48,78,138,141	0
37	LHG	E	101	42/49	0.82	0.12	67,101,123,128	0
35	HTG	B	625	19/19	0.82	0.11	70,112,141,147	0
35	HTG	b	608	19/19	0.83	0.12	56,108,148,148	0
29	LMT	D	401	35/35	0.83	0.12	67,118,146,155	0
32	UNL	D	411	40/-	0.83	0.12	52,79,130,139	0
35	HTG	d	411	16/19	0.84	0.11	65,109,124,127	0
28	GOL	c	503	6/6	0.84	0.17	76,80,97,101	0
32	UNL	b	633	33/-	0.84	0.14	50,94,155,158	0
32	UNL	c	527	32/-	0.84	0.13	67,100,136,144	0
35	HTG	B	633	19/19	0.84	0.11	56,109,139,175	0
33	LMG	z	101	39/55	0.85	0.13	67,115,138,158	0
34	CA	B	601	1/1	0.85	0.08	130,130,130,130	0
31	PL9	A	419[A]	55/55	0.85	0.14	68,94,108,110	55
31	PL9	A	419[B]	55/55	0.85	0.14	69,94,108,111	55
31	PL9	a	415[A]	55/55	0.85	0.15	75,104,117,119	55
31	PL9	a	415[B]	55/55	0.85	0.15	73,103,117,120	55
29	LMT	a	404	35/35	0.85	0.12	47,82,112,131	0
32	UNL	d	410	36/-	0.85	0.11	51,76,129,142	0
32	UNL	B	634	33/-	0.85	0.14	56,87,134,138	0
27	SQD	B	621	54/54	0.85	0.12	51,88,147,155	0
28	GOL	O	301	6/6	0.85	0.10	64,79,82,85	0
27	SQD	F	103	43/54	0.85	0.11	76,102,119,129	0
33	LMG	Z	101	37/55	0.85	0.14	54,111,132,135	0
33	LMG	c	524	51/55	0.85	0.11	49,106,129,132	0
35	HTG	C	523	19/19	0.86	0.10	79,91,124,126	0
27	SQD	a	405	54/54	0.86	0.10	47,77,116,122	0
35	HTG	b	632	19/19	0.86	0.11	66,118,148,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	GOL	C	524	6/6	0.87	0.12	59,63,76,80	0
27	SQD	A	416	54/54	0.87	0.11	52,73,111,128	0
35	HTG	B	624	19/19	0.87	0.12	48,64,89,93	0
29	LMT	B	635	25/35	0.87	0.12	40,80,134,138	0
28	GOL	T	102	6/6	0.87	0.13	94,108,113,115	0
27	SQD	L	102	54/54	0.87	0.10	50,77,123,141	0
29	LMT	m	103	35/35	0.87	0.11	40,96,125,132	0
28	GOL	a	402	6/6	0.87	0.12	70,93,94,94	0
34	CA	f	103	1/1	0.88	0.07	106,106,106,106	0
28	GOL	v	201	6/6	0.89	0.12	68,88,90,92	0
29	LMT	T	104	25/35	0.89	0.12	37,79,133,138	0
35	HTG	C	522	19/19	0.89	0.09	72,85,101,107	0
35	HTG	b	631	19/19	0.89	0.12	56,71,84,96	0
28	GOL	T	101	6/6	0.89	0.14	58,74,93,97	0
35	HTG	c	525	19/19	0.89	0.09	87,92,102,120	0
28	GOL	A	415	6/6	0.90	0.11	52,75,79,82	0
33	LMG	c	523	51/55	0.90	0.10	48,86,111,115	0
28	GOL	B	630	6/6	0.90	0.12	48,59,72,76	0
22	CL	U	201	1/1	0.90	0.11	92,92,92,92	0
28	GOL	t	102	6/6	0.90	0.14	51,80,90,96	0
33	LMG	A	421	51/55	0.90	0.09	57,82,106,115	0
33	LMG	C	519	51/55	0.90	0.10	49,83,108,117	0
29	LMT	m	102	35/35	0.90	0.09	42,81,100,107	0
33	LMG	c	501	51/55	0.91	0.10	57,79,98,99	0
28	GOL	B	626	6/6	0.91	0.10	44,54,59,80	0
28	GOL	b	606	6/6	0.91	0.10	64,79,86,86	0
29	LMT	M	101	35/35	0.91	0.09	41,80,99,100	0
38	HEM	F	102	43/43	0.91	0.09	44,66,89,137	0
28	GOL	v	202	6/6	0.92	0.10	70,79,96,112	0
23	BCT	a	417[A]	4/4	0.92	0.08	59,60,62,70	4
32	UNL	X	101	18/-	0.92	0.10	54,73,97,100	0
28	GOL	B	636	6/6	0.92	0.08	48,56,62,62	0
28	GOL	b	605	6/6	0.92	0.14	70,80,101,103	0
23	BCT	a	417[B]	4/4	0.92	0.08	50,59,61,66	4
24	CLA	c	518	65/65	0.92	0.09	56,80,99,108	0
32	UNL	d	412	18/-	0.92	0.10	60,72,112,113	0
27	SQD	A	412	54/54	0.92	0.09	45,78,95,98	0
28	GOL	B	628	6/6	0.92	0.10	54,73,79,84	0
24	CLA	C	506	65/65	0.93	0.08	46,62,105,114	0
28	GOL	A	414	6/6	0.93	0.12	49,59,62,64	0
24	CLA	C	513	65/65	0.93	0.08	52,66,102,109	0
28	GOL	A	422	6/6	0.93	0.07	68,73,74,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	b	610	65/65	0.93	0.09	44,68,104,134	0
35	HTG	B	632	19/19	0.93	0.08	45,72,101,109	0
24	CLA	B	602	65/65	0.93	0.09	41,62,95,124	0
32	UNL	d	409	17/-	0.93	0.10	47,69,97,101	0
37	LHG	D	409	49/49	0.93	0.10	39,55,116,129	0
28	GOL	a	420	6/6	0.93	0.09	78,80,91,92	0
26	BCR	C	514	40/40	0.93	0.08	49,67,81,84	0
26	BCR	y	101	40/40	0.93	0.08	43,63,72,80	0
33	LMG	B	622	51/55	0.94	0.07	33,50,74,90	0
26	BCR	t	101	40/40	0.94	0.06	34,47,64,65	0
28	GOL	A	413	6/6	0.94	0.09	45,49,54,58	0
33	LMG	D	413	51/55	0.94	0.09	38,60,105,128	0
24	CLA	C	504	65/65	0.94	0.07	34,47,81,94	0
33	LMG	b	629	51/55	0.94	0.08	42,51,72,94	0
24	CLA	b	615	65/65	0.94	0.07	32,44,88,106	0
23	BCT	A	404[B]	4/4	0.94	0.08	47,48,62,72	4
23	BCT	A	404[A]	4/4	0.94	0.08	47,55,60,72	4
33	LMG	d	413	51/55	0.94	0.08	45,58,100,110	0
28	GOL	B	627	6/6	0.94	0.11	52,62,79,94	0
36	DGD	C	517	62/66	0.94	0.07	42,54,96,112	0
26	BCR	D	404	40/40	0.94	0.07	41,50,92,105	0
26	BCR	c	528	40/40	0.94	0.08	60,73,83,85	0
37	LHG	D	407	49/49	0.94	0.08	31,49,62,73	0
28	GOL	o	301	6/6	0.94	0.09	65,78,89,107	0
32	UNL	D	410	17/-	0.94	0.08	40,70,83,89	0
26	BCR	d	404	40/40	0.94	0.07	40,52,79,83	0
27	SQD	a	414	54/54	0.94	0.09	57,80,103,109	0
34	CA	F	104	1/1	0.95	0.04	84,84,84,84	0
26	BCR	h	101	40/40	0.95	0.06	38,55,66,68	0
28	GOL	B	631	6/6	0.95	0.10	43,76,84,87	0
26	BCR	k	101	40/40	0.95	0.07	44,59,73,75	0
24	CLA	b	623	65/65	0.95	0.07	26,40,88,115	0
24	CLA	b	625	65/65	0.95	0.08	35,52,101,109	0
24	CLA	c	508	65/65	0.95	0.07	41,52,62,86	0
24	CLA	c	511	65/65	0.95	0.07	43,63,91,107	0
24	CLA	c	512	65/65	0.95	0.07	42,54,67,72	0
24	CLA	c	517	65/65	0.95	0.06	49,63,82,86	0
24	CLA	C	512	65/65	0.95	0.07	48,64,81,92	0
28	GOL	b	602	6/6	0.95	0.09	56,58,65,89	0
26	BCR	A	411	40/40	0.95	0.06	28,39,46,48	0
24	CLA	B	615	65/65	0.95	0.07	26,40,90,99	0
24	CLA	C	505	65/65	0.95	0.07	38,47,68,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	BCR	H	101	40/40	0.95	0.06	35,51,65,67	0
31	PL9	d	405[A]	55/55	0.95	0.06	27,37,46,57	55
36	DGD	C	516	62/66	0.95	0.07	33,47,88,96	0
31	PL9	d	405[B]	55/55	0.95	0.06	24,38,46,57	55
26	BCR	K	101	40/40	0.95	0.07	43,57,65,68	0
36	DGD	H	102	62/66	0.95	0.07	35,48,66,78	0
36	DGD	c	521	62/66	0.95	0.07	41,52,105,128	0
36	DGD	c	522	62/66	0.95	0.07	38,52,87,96	0
26	BCR	T	103	40/40	0.95	0.06	31,46,61,62	0
26	BCR	Y	101	40/40	0.95	0.06	47,60,71,80	0
28	GOL	v	203	6/6	0.95	0.10	48,49,57,59	0
26	BCR	b	627	40/40	0.95	0.06	31,42,60,67	0
37	LHG	d	408	49/49	0.95	0.09	34,53,104,109	0
24	CLA	B	617	65/65	0.95	0.09	36,49,116,118	0
24	CLA	b	618	65/65	0.95	0.06	37,49,58,71	0
24	CLA	c	510	65/65	0.96	0.06	36,48,67,78	0
24	CLA	C	508	65/65	0.96	0.06	36,48,114,125	0
24	CLA	C	509	65/65	0.96	0.07	43,55,74,81	0
24	CLA	c	513	65/65	0.96	0.07	35,48,113,129	0
24	CLA	c	515	65/65	0.96	0.06	39,52,65,71	0
24	CLA	c	516	65/65	0.96	0.07	43,55,75,88	0
24	CLA	C	510	65/65	0.96	0.06	39,51,62,71	0
24	CLA	C	511	65/65	0.96	0.07	41,58,69,83	0
24	CLA	d	403	65/65	0.96	0.07	41,51,103,111	0
25	PHO	a	418[A]	64/64	0.96	0.05	28,41,47,50	64
25	PHO	a	418[B]	64/64	0.96	0.05	28,41,48,51	64
28	GOL	B	629	6/6	0.96	0.09	50,52,55,60	0
24	CLA	A	410	65/65	0.96	0.07	30,45,122,130	0
31	PL9	D	405[A]	55/55	0.96	0.05	26,37,44,57	55
31	PL9	D	405[B]	55/55	0.96	0.05	28,36,45,62	55
26	BCR	B	619	40/40	0.96	0.05	27,40,56,63	0
26	BCR	B	620	40/40	0.96	0.06	35,46,58,60	0
24	CLA	A	407	65/65	0.96	0.06	28,39,101,116	0
26	BCR	C	515	40/40	0.96	0.06	39,54,63,65	0
24	CLA	D	403	65/65	0.96	0.07	38,51,101,119	0
24	CLA	a	412	65/65	0.96	0.08	31,46,114,124	0
35	HTG	b	601	19/19	0.96	0.07	40,47,70,71	0
35	HTG	b	607	19/19	0.96	0.06	47,71,80,81	0
24	CLA	C	501	65/65	0.96	0.06	38,50,73,81	0
28	GOL	V	202	6/6	0.96	0.07	39,47,52,62	0
28	GOL	V	203	6/6	0.96	0.08	54,59,59,63	0
28	GOL	V	204	6/6	0.96	0.08	72,78,80,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	C	503	65/65	0.96	0.06	40,50,61,64	0
24	CLA	b	616	65/65	0.96	0.05	24,35,44,54	0
24	CLA	B	607	65/65	0.96	0.07	32,44,93,103	0
28	GOL	b	604	6/6	0.96	0.07	58,63,68,86	0
36	DGD	C	518	62/66	0.96	0.06	35,51,74,87	0
26	BCR	c	519	40/40	0.96	0.06	39,54,66,70	0
24	CLA	b	619	65/65	0.96	0.06	36,45,53,62	0
36	DGD	c	520	62/66	0.96	0.07	36,48,94,107	0
24	CLA	b	620	65/65	0.96	0.06	29,39,49,55	0
24	CLA	b	622	65/65	0.96	0.06	27,39,56,62	0
24	CLA	B	611	65/65	0.96	0.06	36,46,54,69	0
36	DGD	h	102	62/66	0.96	0.06	39,50,67,79	0
24	CLA	b	624	65/65	0.96	0.05	33,46,62,70	0
24	CLA	B	614	65/65	0.96	0.06	27,36,66,74	0
24	CLA	c	506	65/65	0.96	0.06	41,55,65,70	0
37	LHG	d	406	49/49	0.96	0.07	37,51,59,74	0
24	CLA	c	507	65/65	0.96	0.06	40,51,66,73	0
24	CLA	C	507	65/65	0.96	0.07	41,56,68,70	0
24	CLA	c	509	65/65	0.96	0.06	38,53,74,79	0
25	PHO	a	411	64/64	0.97	0.04	28,36,41,47	0
24	CLA	B	613	65/65	0.97	0.05	27,37,46,54	0
24	CLA	A	406	65/65	0.97	0.04	25,32,42,51	0
24	CLA	b	621	65/65	0.97	0.05	28,40,49,52	0
24	CLA	B	603	65/65	0.97	0.05	35,43,50,53	0
24	CLA	B	616	65/65	0.97	0.06	34,45,65,77	0
24	CLA	B	604	65/65	0.97	0.05	34,43,49,63	0
22	CL	v	204	1/1	0.97	0.07	95,95,95,95	0
24	CLA	C	502	65/65	0.97	0.05	36,46,61,78	0
24	CLA	a	409	65/65	0.97	0.05	27,35,49,58	0
24	CLA	a	410	65/65	0.97	0.06	31,41,105,114	0
24	CLA	B	608	65/65	0.97	0.05	24,35,47,52	0
24	CLA	B	609	65/65	0.97	0.05	35,43,56,60	0
26	BCR	a	413	40/40	0.97	0.04	28,39,48,56	0
26	BCR	b	626	40/40	0.97	0.04	32,41,47,49	0
24	CLA	b	611	65/65	0.97	0.06	32,46,52,57	0
26	BCR	b	628	40/40	0.97	0.05	35,50,62,66	0
24	CLA	b	612	65/65	0.97	0.05	33,44,54,59	0
24	CLA	b	613	65/65	0.97	0.05	27,38,73,79	0
24	CLA	c	514	65/65	0.97	0.07	43,54,74,85	0
24	CLA	b	614	65/65	0.97	0.06	28,39,52,55	0
24	CLA	B	610	65/65	0.97	0.05	34,46,55,64	0
28	GOL	a	401	6/6	0.97	0.08	49,63,68,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	A	405	65/65	0.97	0.05	25,33,45,67	0
24	CLA	b	617	65/65	0.97	0.05	32,45,53,60	0
24	CLA	d	401	65/65	0.97	0.04	26,33,43,52	0
37	LHG	D	408	49/49	0.97	0.06	33,43,61,89	0
28	GOL	b	603	6/6	0.97	0.06	45,63,75,80	0
24	CLA	B	612	65/65	0.97	0.05	26,38,50,57	0
37	LHG	L	101	49/49	0.97	0.06	33,45,56,59	0
37	LHG	b	634	49/49	0.97	0.06	36,45,58,64	0
25	PHO	A	408	64/64	0.97	0.05	28,34,40,40	0
25	PHO	A	409[A]	64/64	0.97	0.05	33,40,47,49	64
35	HTG	B	623	19/19	0.97	0.07	40,56,72,76	0
25	PHO	A	409[B]	64/64	0.97	0.05	27,40,48,49	64
38	HEM	e	103	43/43	0.97	0.10	55,81,121,150	0
22	CL	A	403[B]	1/1	0.98	0.08	35,35,35,35	1
26	BCR	B	618	40/40	0.98	0.04	27,39,46,48	0
22	CL	A	403[A]	1/1	0.98	0.08	33,33,33,33	1
24	CLA	B	605	65/65	0.98	0.05	27,36,71,75	0
24	CLA	B	606	65/65	0.98	0.05	29,39,54,58	0
37	LHG	d	407	49/49	0.98	0.06	32,42,57,88	0
24	CLA	d	402	65/65	0.98	0.05	26,36,60,71	0
24	CLA	D	402	65/65	0.98	0.05	24,34,55,61	0
28	GOL	c	502	6/6	0.98	0.05	38,44,46,48	0
28	GOL	C	525	6/6	0.98	0.04	32,42,44,45	0
39	MG	j	102	1/1	0.98	0.09	57,57,57,57	0
30	OEX	A	418[A]	10/10	0.99	0.03	30,36,43,56	10
34	CA	C	526	1/1	0.99	0.07	70,70,70,70	0
30	OEX	A	418[B]	10/10	0.99	0.03	33,37,39,39	10
22	CL	a	407[A]	1/1	0.99	0.05	36,36,36,36	1
34	CA	c	504	1/1	0.99	0.07	67,67,67,67	0
34	CA	c	505	1/1	0.99	0.03	75,75,75,75	0
22	CL	a	407[B]	1/1	0.99	0.05	37,37,37,37	1
39	MG	J	102	1/1	0.99	0.03	52,52,52,52	0
34	CA	o	302	1/1	0.99	0.03	90,90,90,90	0
40	HEC	V	205	43/43	0.99	0.05	34,40,51,56	0
40	HEC	v	205	43/43	0.99	0.05	41,52,56,60	0
22	CL	a	408[B]	1/1	1.00	0.01	40,40,40,40	1
22	CL	A	402[B]	1/1	1.00	0.01	32,32,32,32	1
21	FE2	A	401[A]	1/1	1.00	0.01	47,47,47,47	1
30	OEX	a	416[A]	10/10	1.00	0.02	34,37,40,52	10
30	OEX	a	416[B]	10/10	1.00	0.02	32,38,43,46	10
21	FE2	A	401[B]	1/1	1.00	0.01	50,50,50,50	1
34	CA	O	302	1/1	1.00	0.03	81,81,81,81	0

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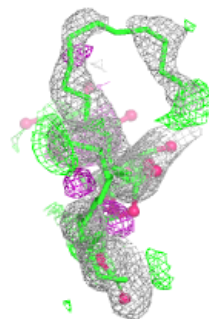
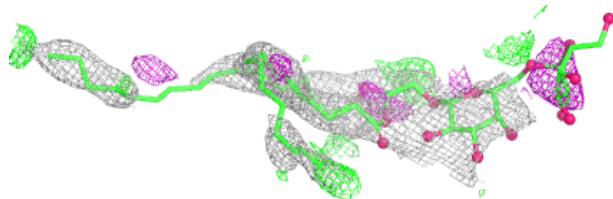
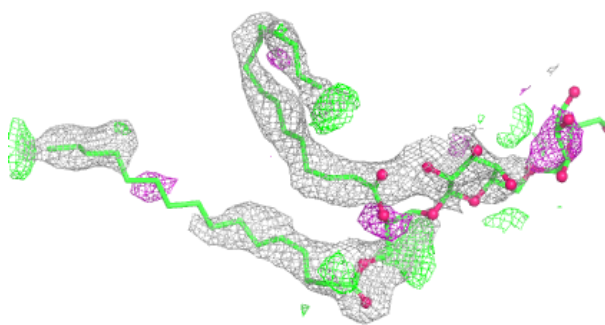
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	FE2	a	406[A]	1/1	1.00	0.02	48,48,48,48	1
21	FE2	a	406[B]	1/1	1.00	0.02	48,48,48,48	1
22	CL	A	402[A]	1/1	1.00	0.01	32,32,32,32	1
22	CL	a	408[A]	1/1	1.00	0.01	40,40,40,40	1

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.

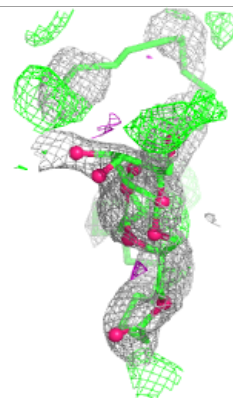
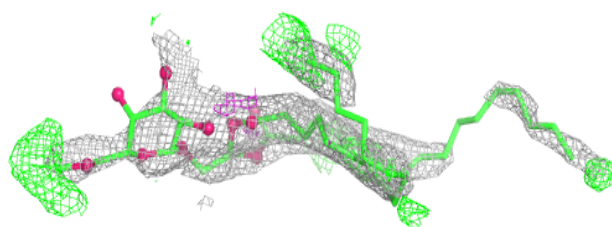
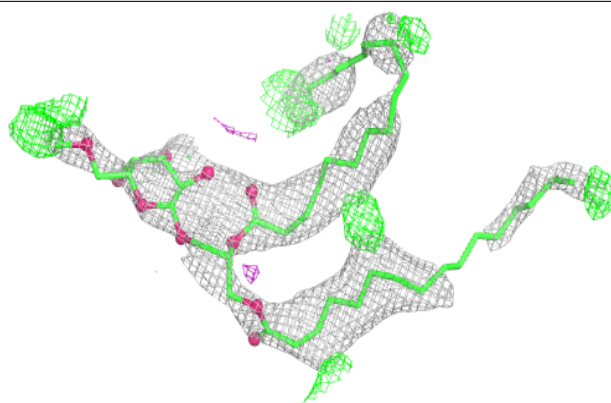
Electron density around DGD e 101:

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

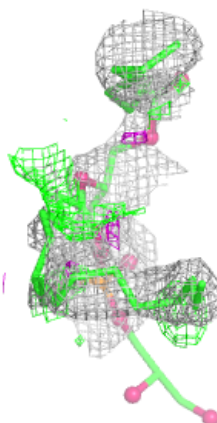
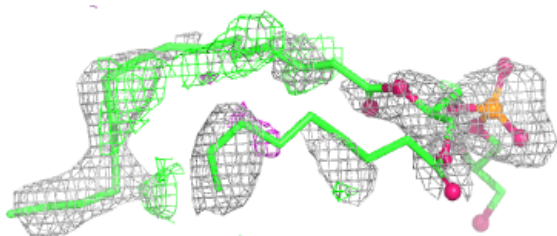
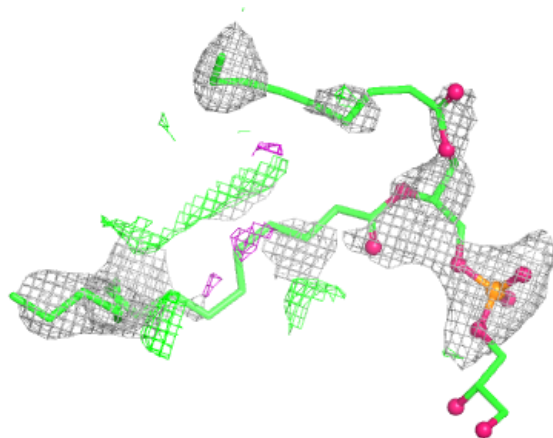


Electron density around DGD D 406:

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

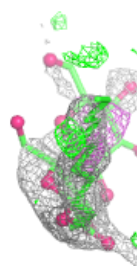
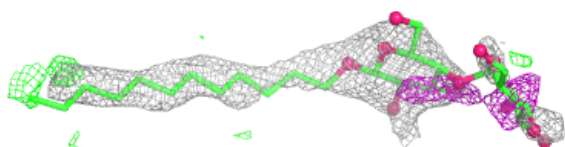
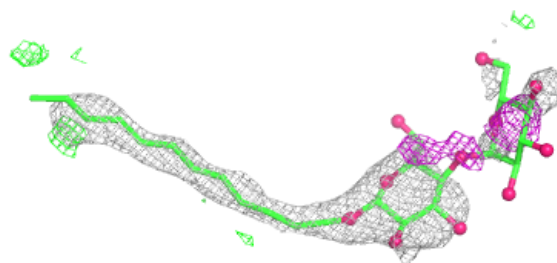
**Electron density around LHG e 102:**

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

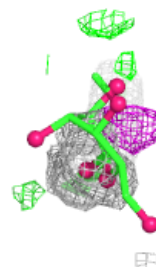
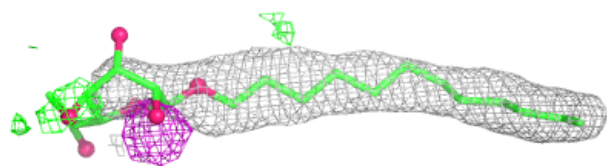
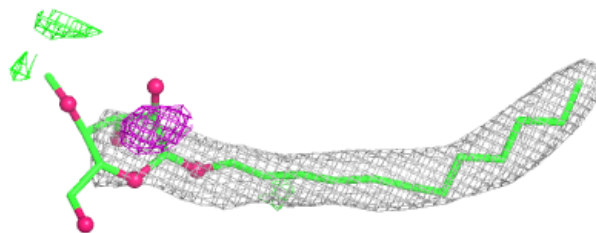


Electron density around LMT F 101:

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

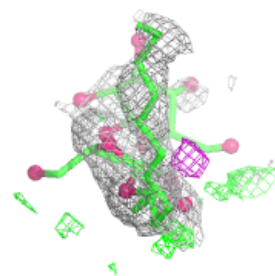
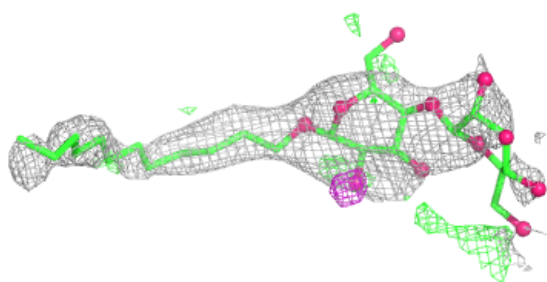
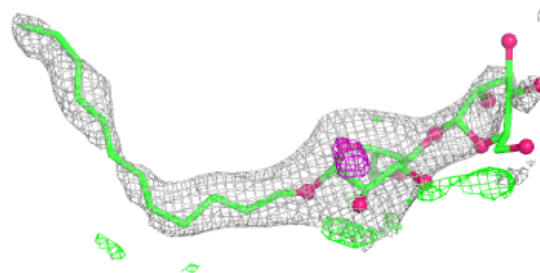
**Electron density around LMT b 630:**

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

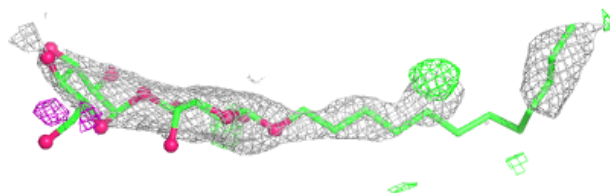
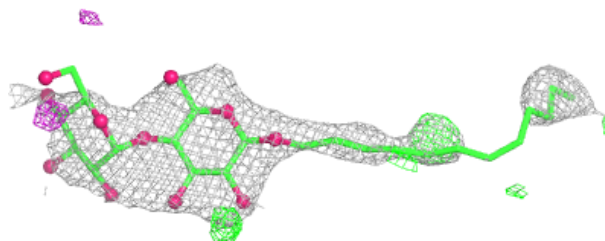


Electron density around LMT C 521:

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

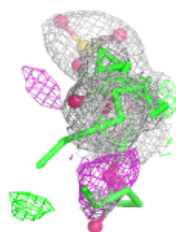
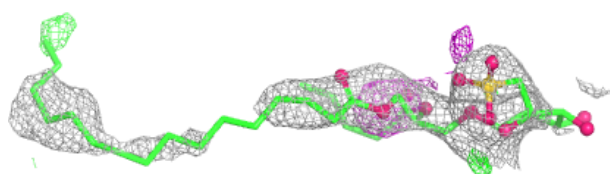
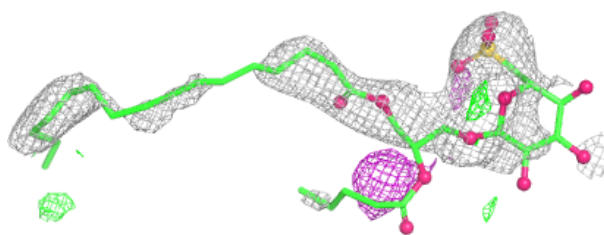
**Electron density around LMT a 419:**

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

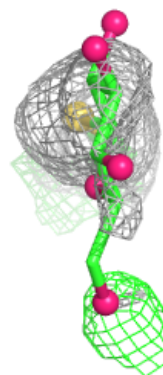
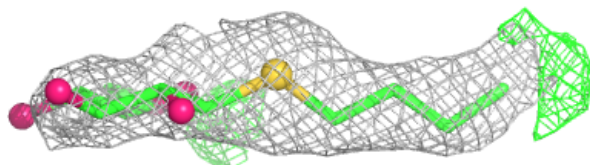
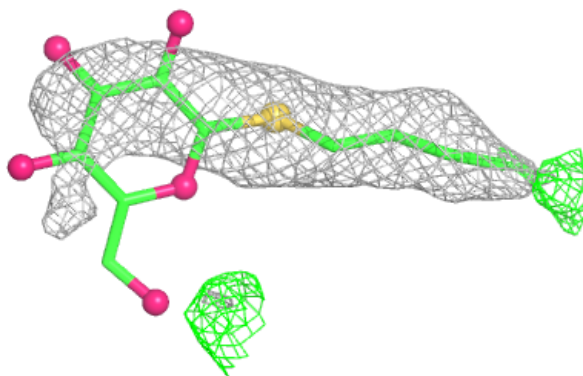


Electron density around SQD f 101:

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

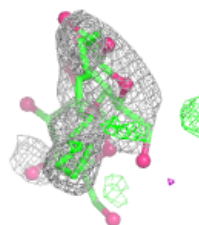
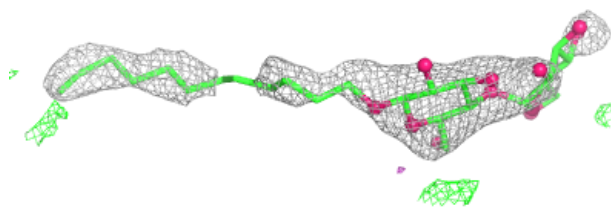
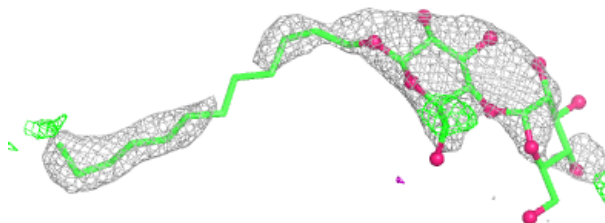
**Electron density around HTG D 412:**

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

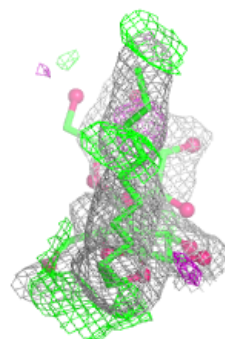
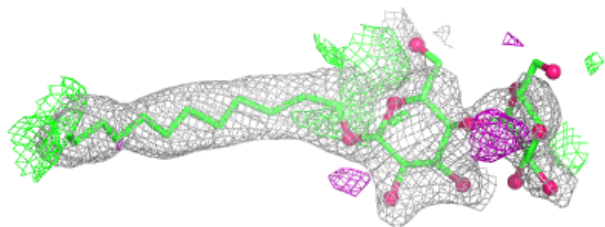
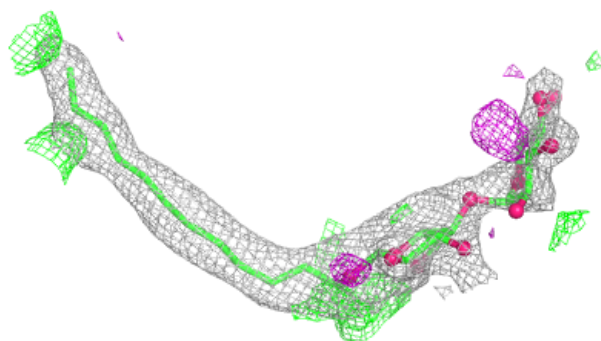


Electron density around LMT f 102:

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

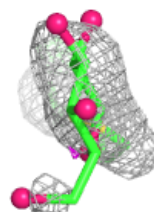
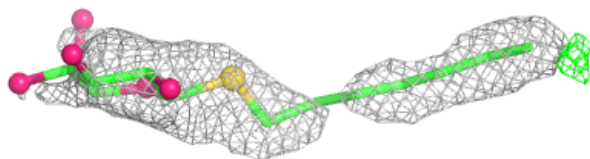
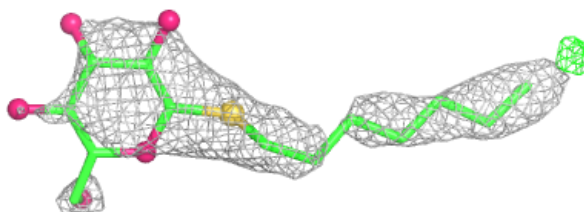
**Electron density around LMT M 103:**

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

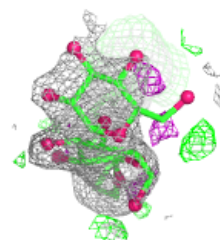
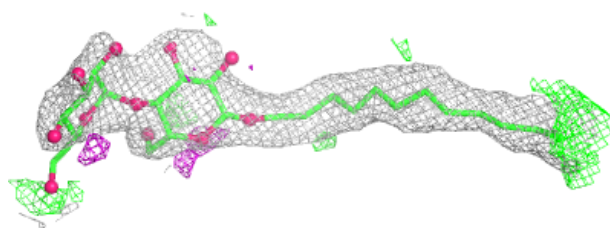
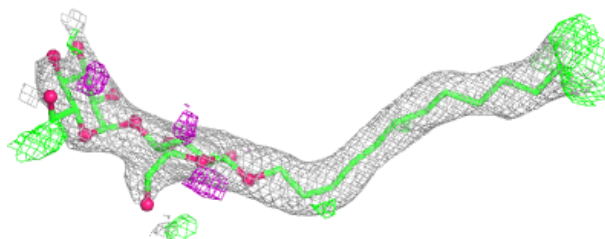


Electron density around HTG c 526:

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

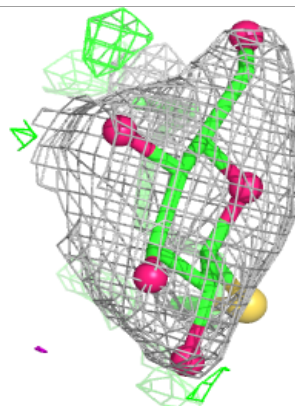
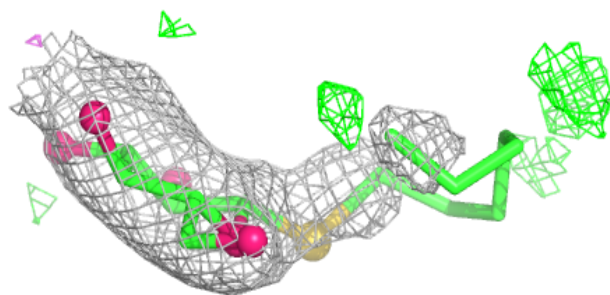
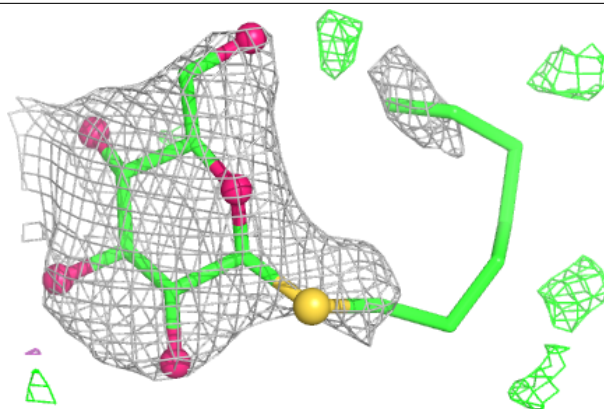
**Electron density around LMT A 417:**

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

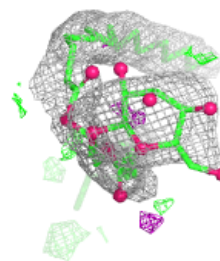
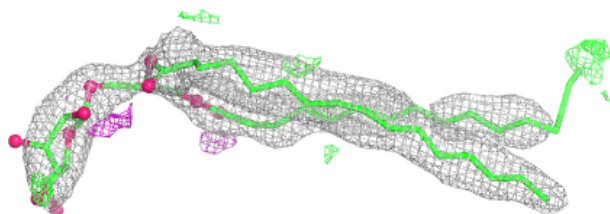
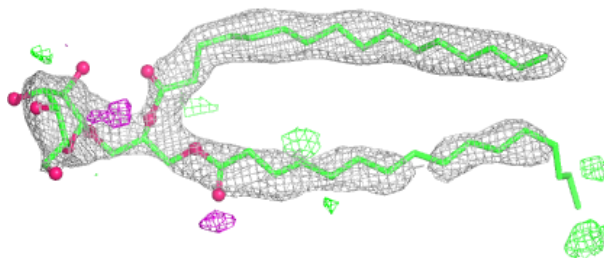


Electron density around HTG V 206:

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

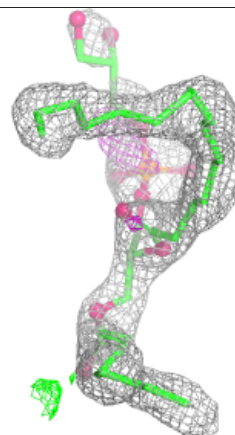
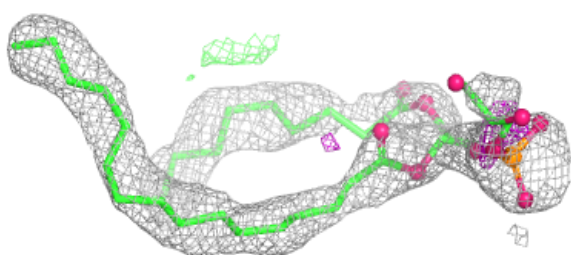
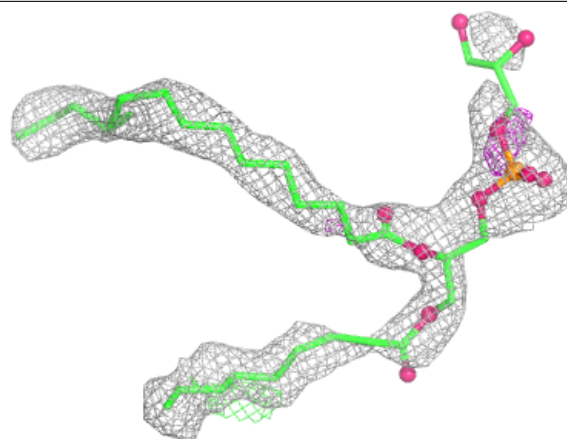
**Electron density around LMG C 520:**

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



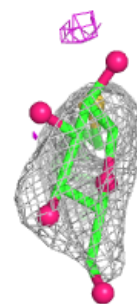
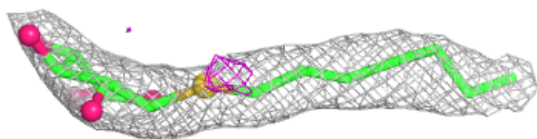
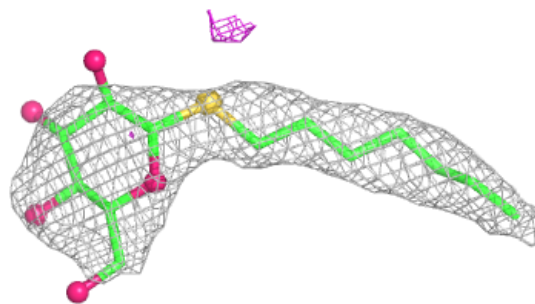
Electron density around LHG E 101:

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

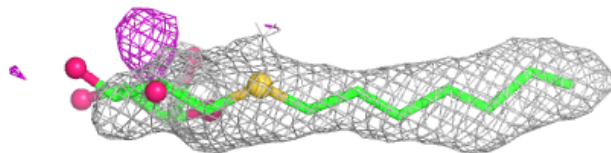
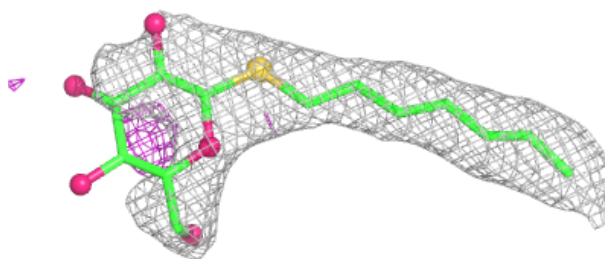


Electron density around HTG B 625:

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

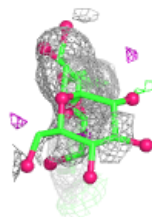
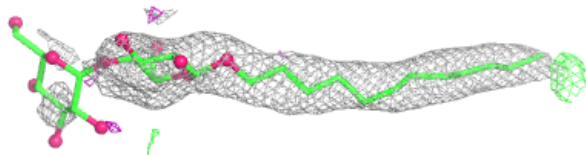
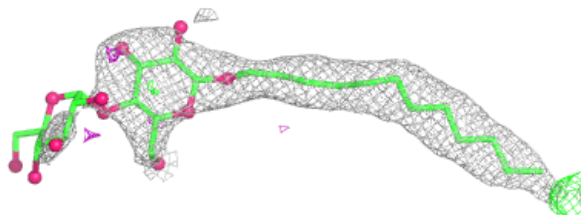
**Electron density around HTG b 608:**

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

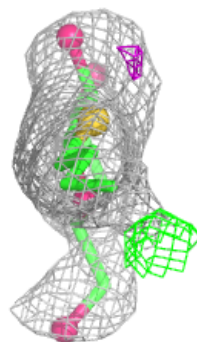
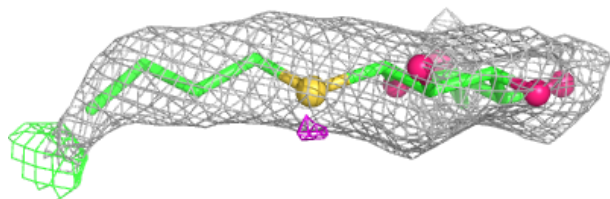
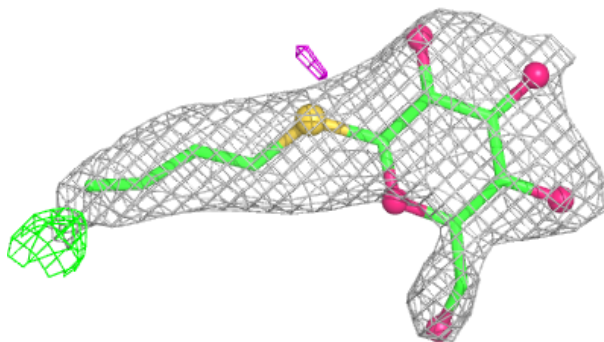


Electron density around LMT D 401:

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

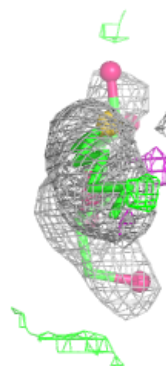
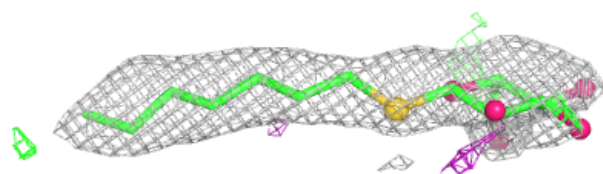
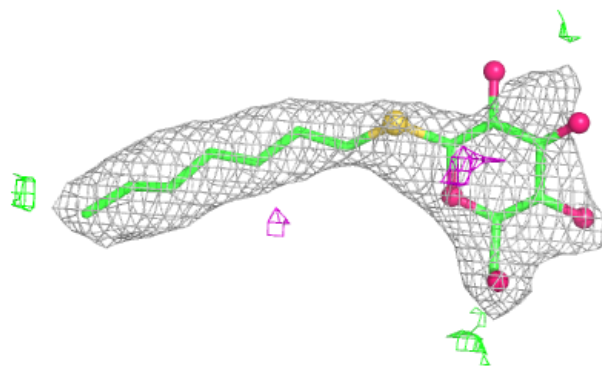
**Electron density around HTG d 411:**

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

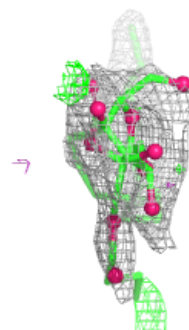
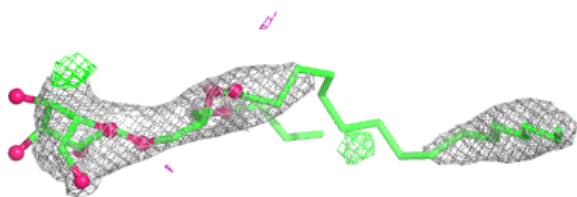


Electron density around HTG B 633:

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

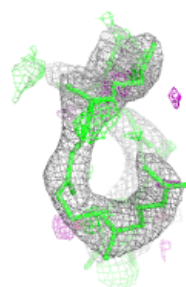
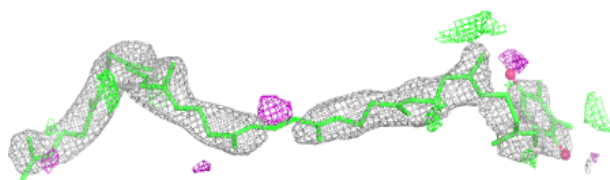
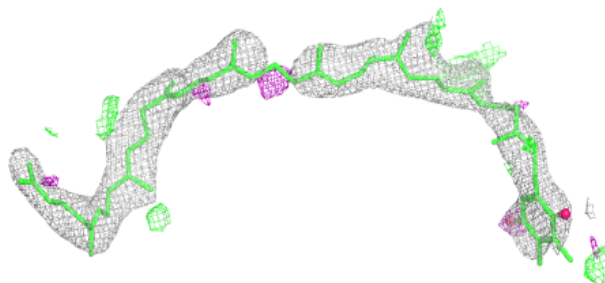
**Electron density around LMG z 101:**

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

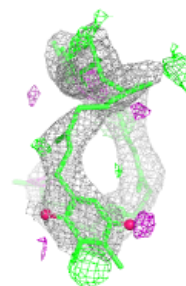
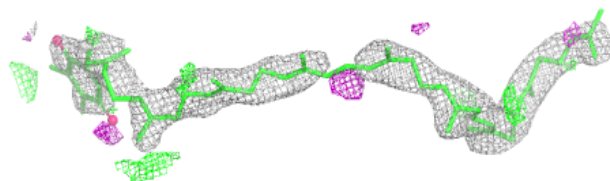
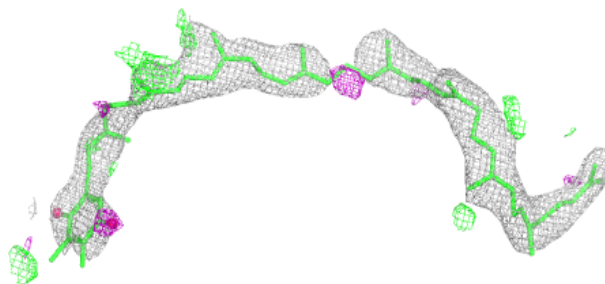


Electron density around PL9 A 419 (A):

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

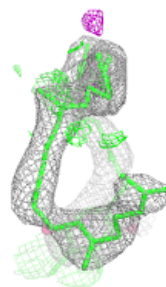
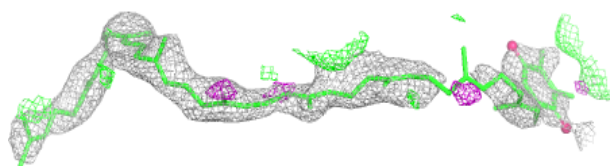
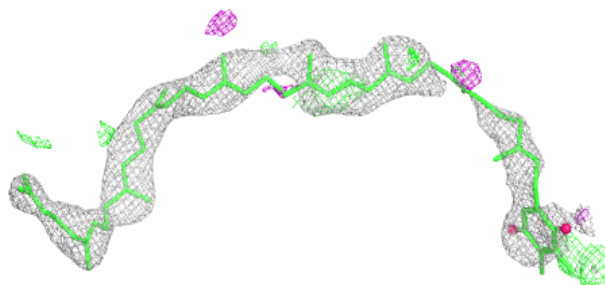
**Electron density around PL9 A 419 (B):**

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

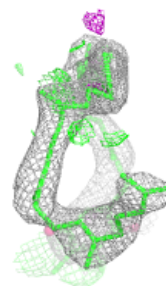
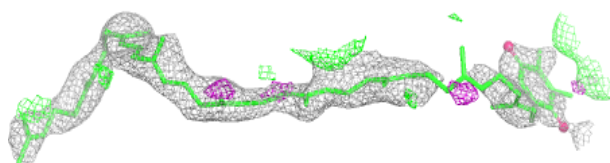
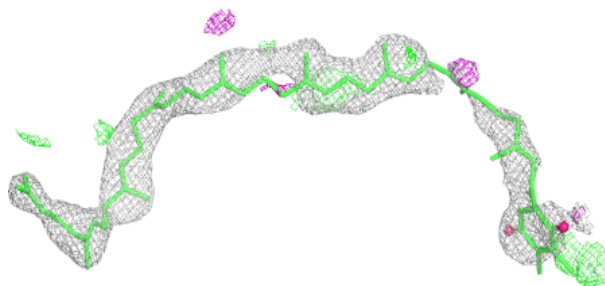


Electron density around PL9 a 415 (A):

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

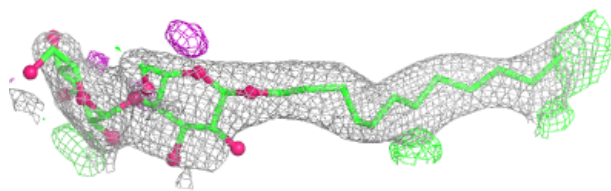
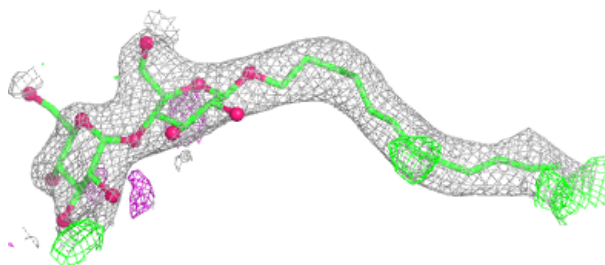
**Electron density around PL9 a 415 (B):**

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

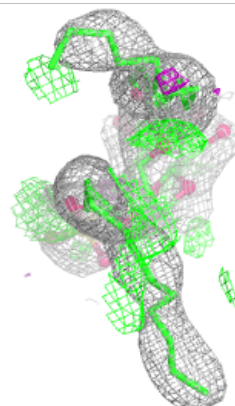
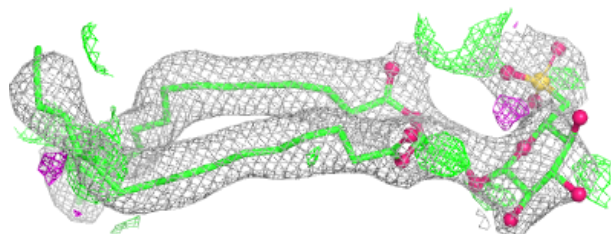
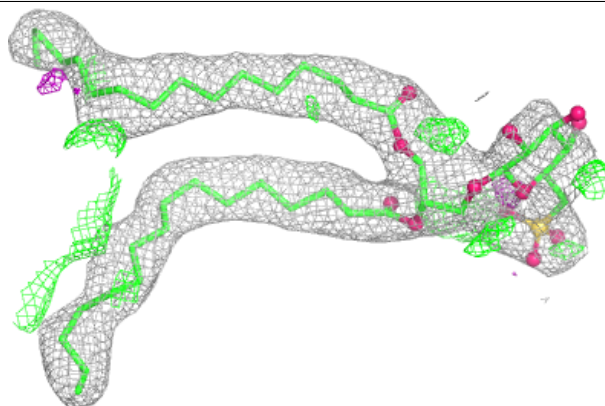


Electron density around LMT a 404:

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

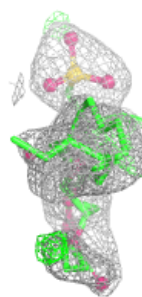
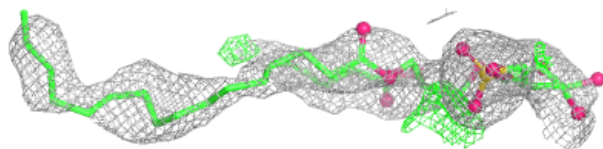
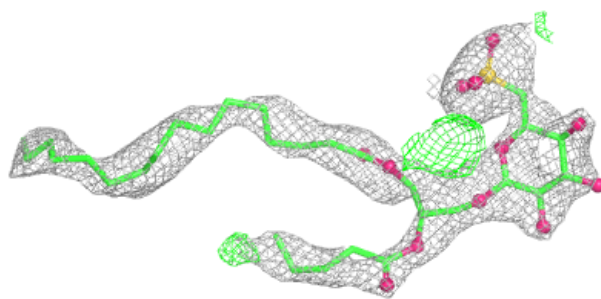
**Electron density around SQD B 621:**

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

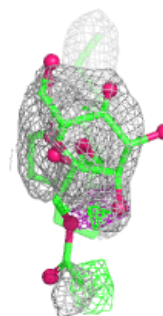
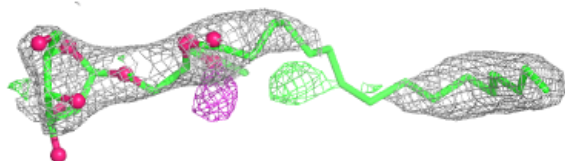
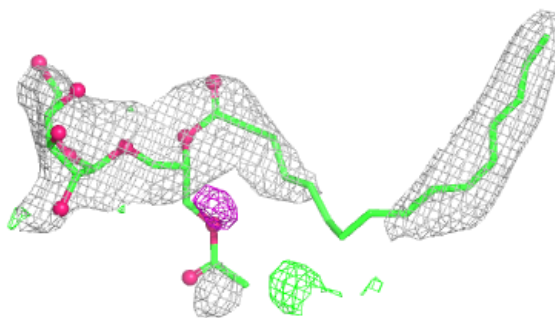


Electron density around SQD F 103:

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

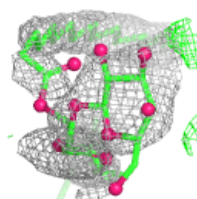
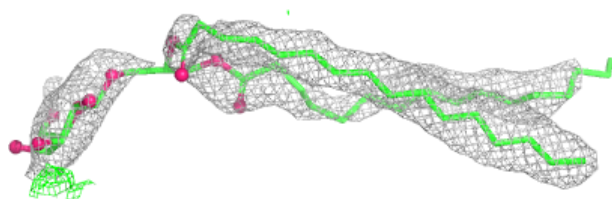
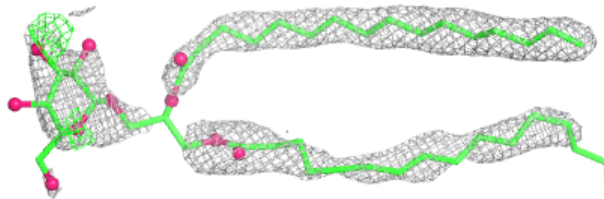
**Electron density around LMG Z 101:**

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

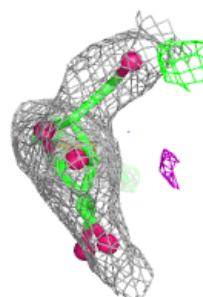
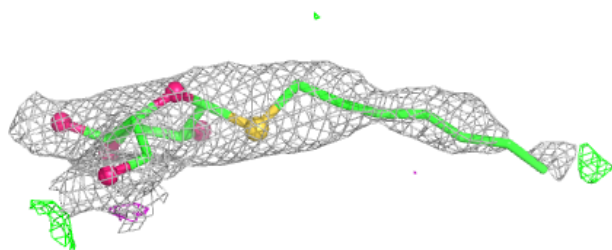
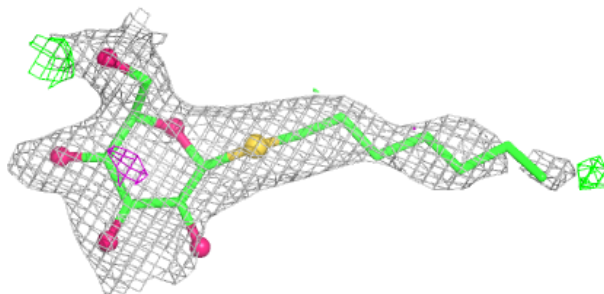


Electron density around LMG c 524:

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

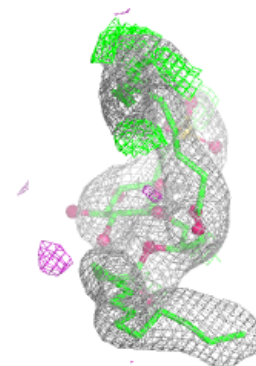
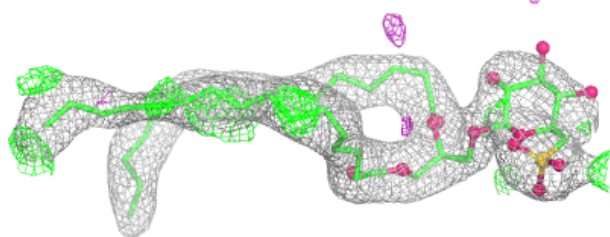
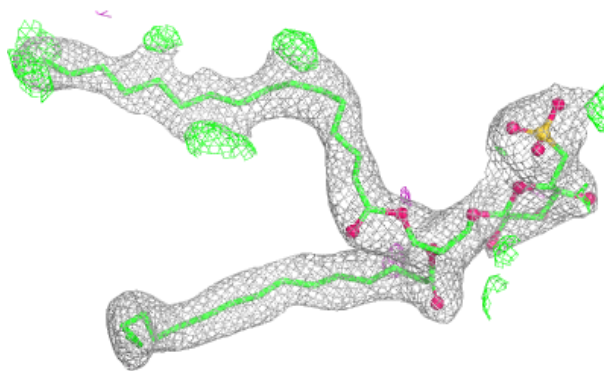
**Electron density around HTG C 523:**

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

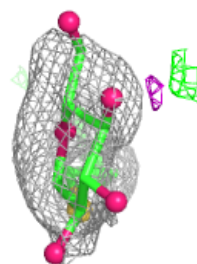
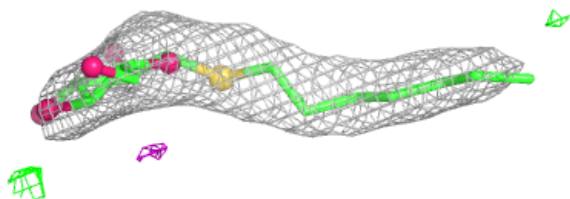
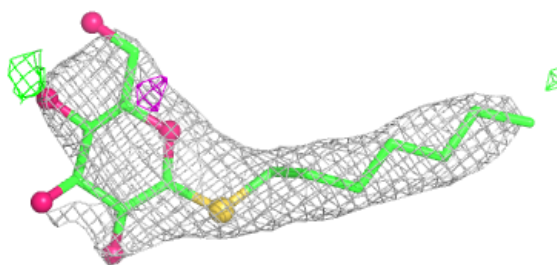


Electron density around SQD a 405:

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

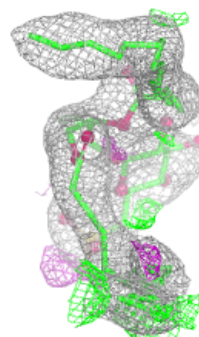
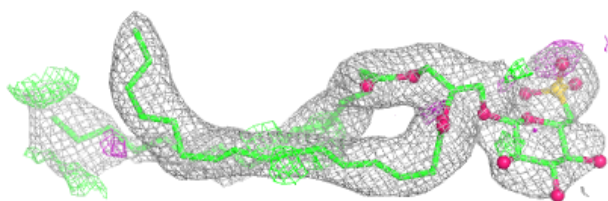
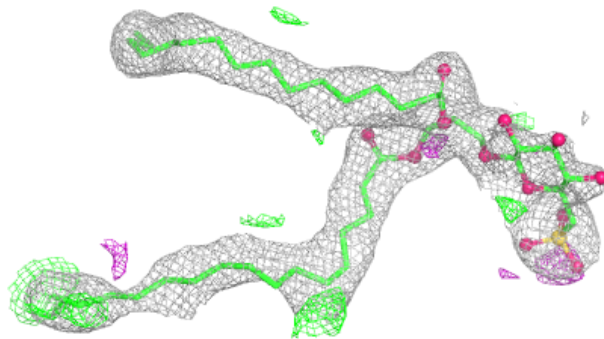
**Electron density around HTG b 632:**

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

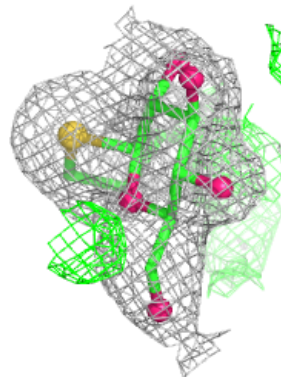
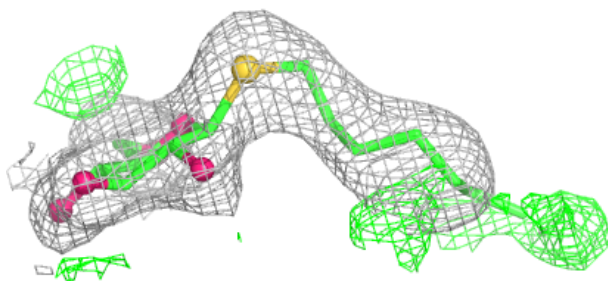
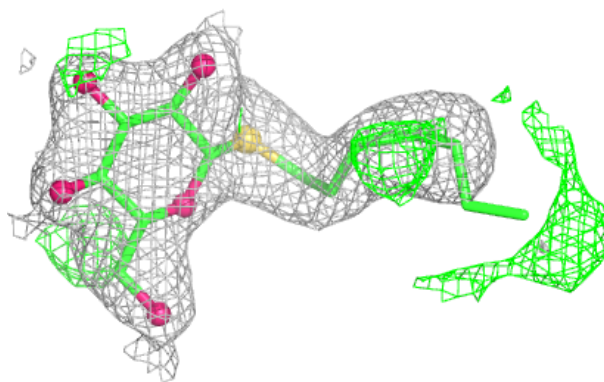


Electron density around SQD A 416:

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

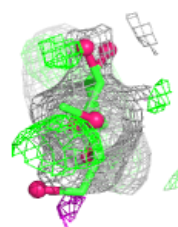
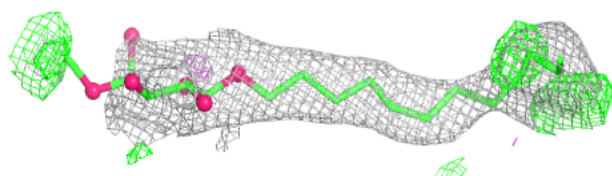
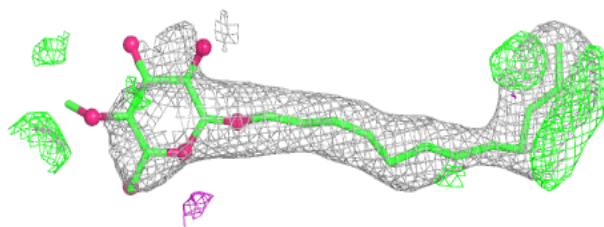
**Electron density around HTG B 624:**

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

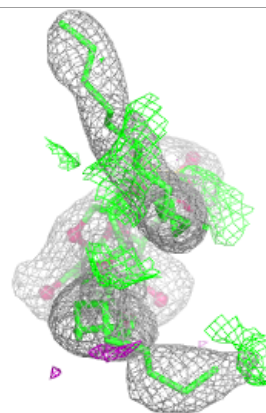
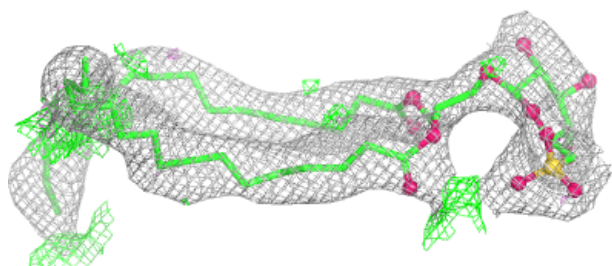
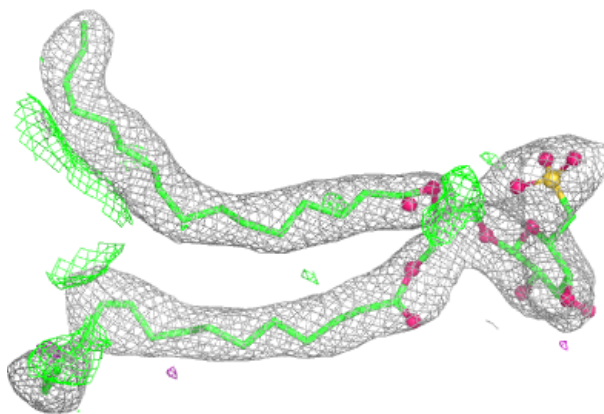


Electron density around LMT B 635:

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

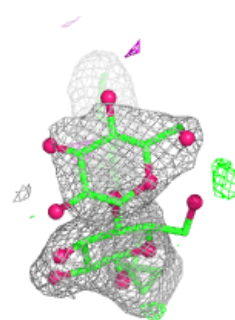
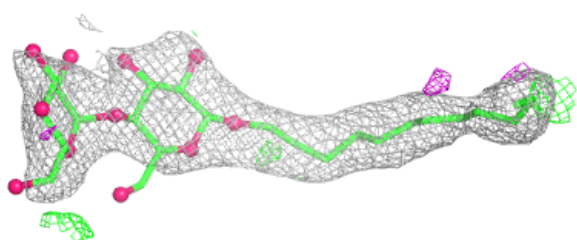
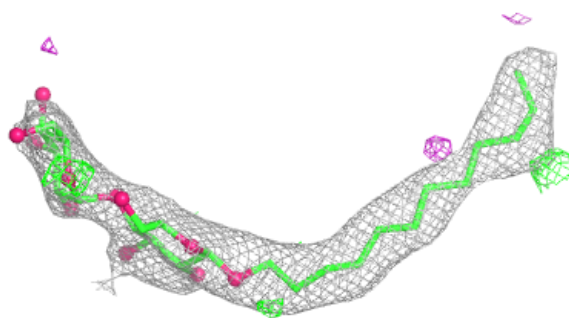
**Electron density around SQD L 102:**

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

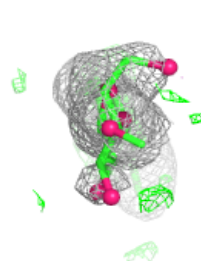
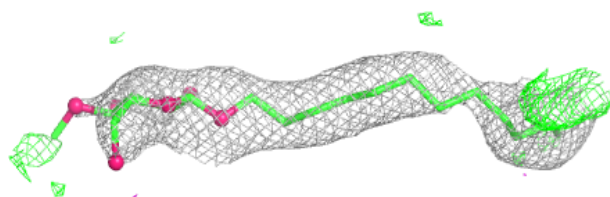
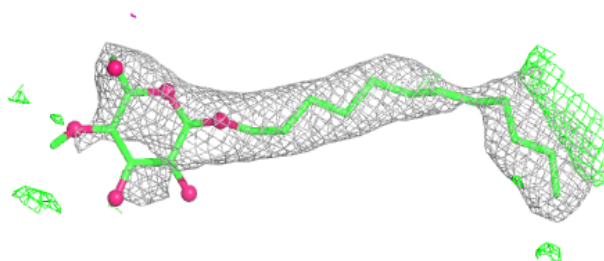


Electron density around LMT m 103:

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

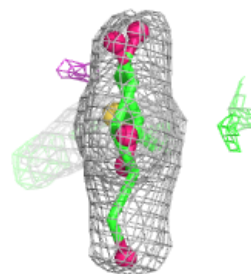
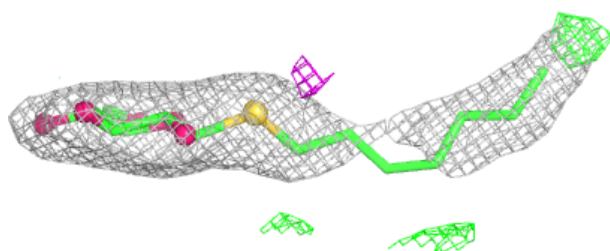
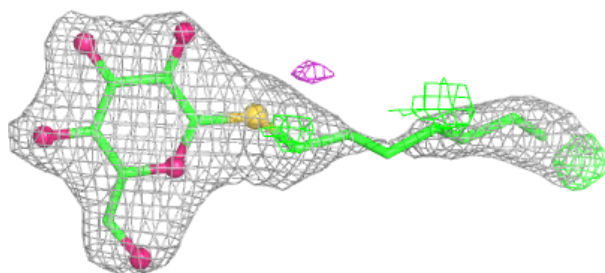
**Electron density around LMT T 104:**

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

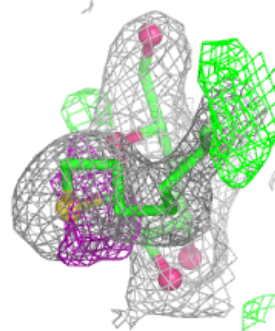
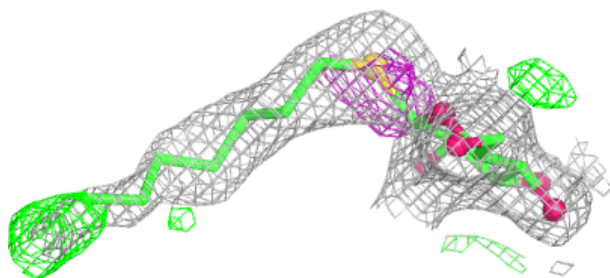
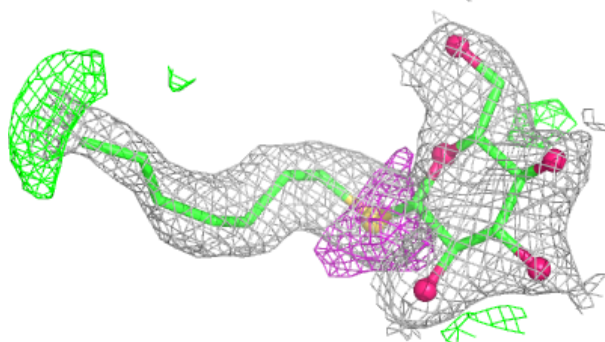


Electron density around HTG C 522:

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

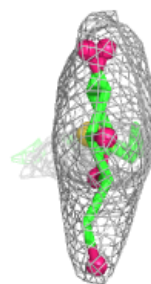
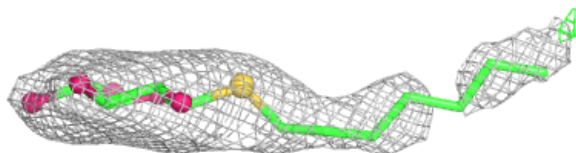
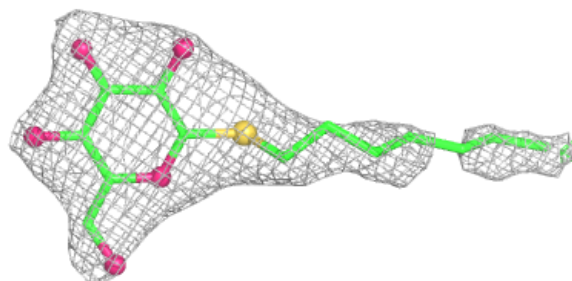
**Electron density around HTG b 631:**

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



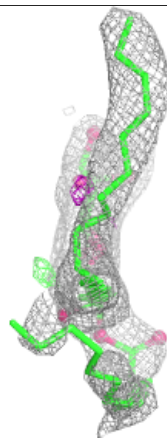
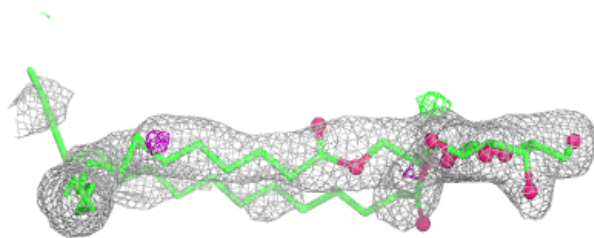
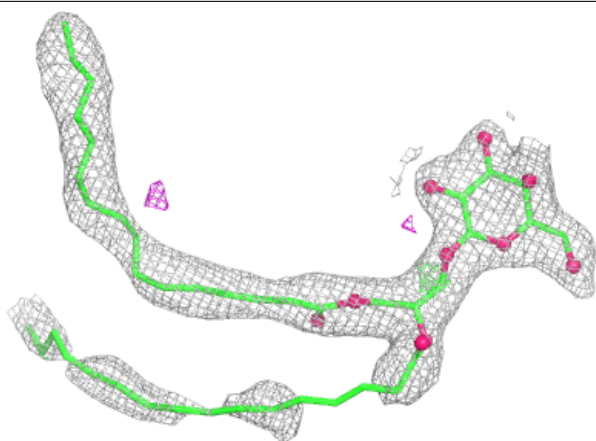
Electron density around HTG c 525:

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

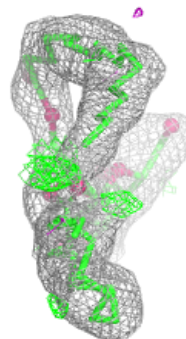
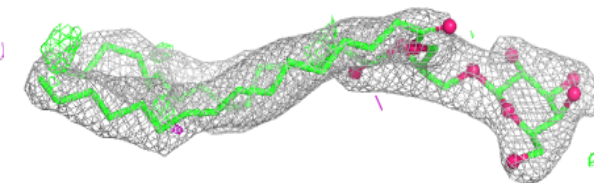
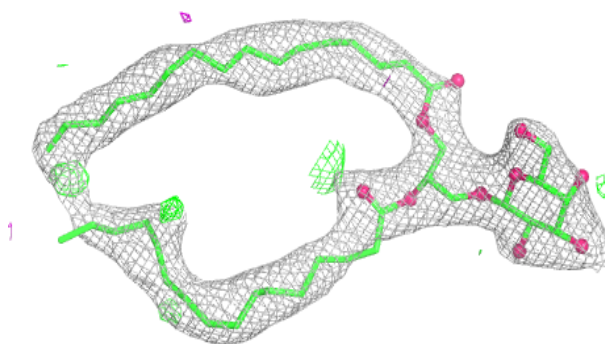


Electron density around LMG c 523:

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

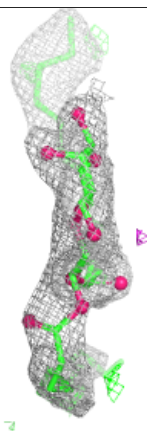
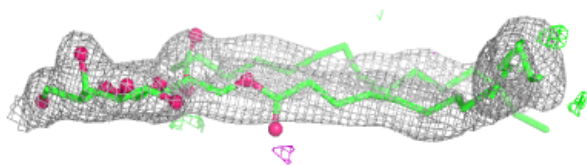
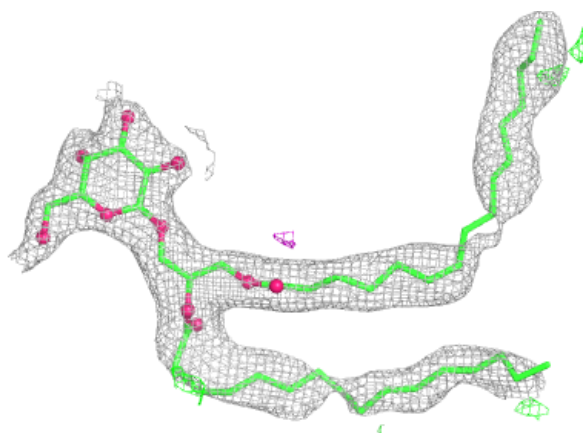
**Electron density around LMG A 421:**

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

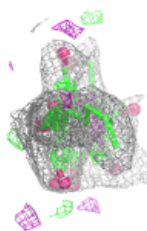
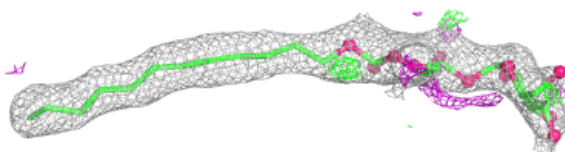
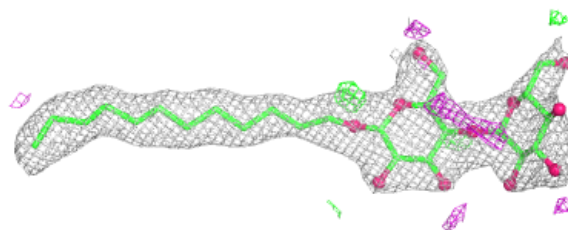


Electron density around LMG C 519:

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

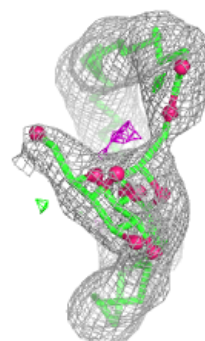
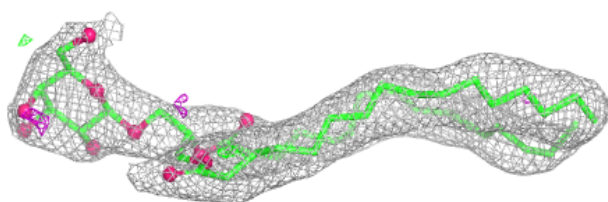
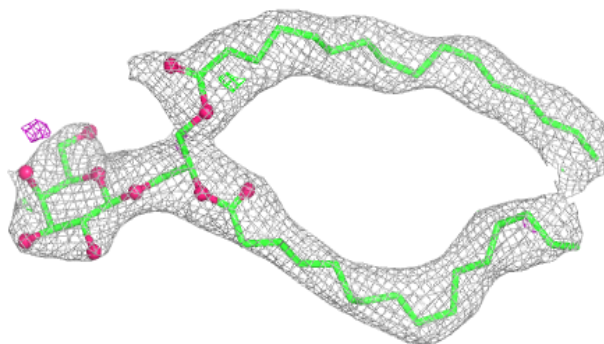
**Electron density around LMT m 102:**

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

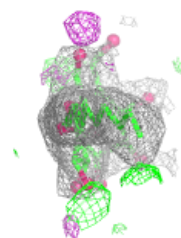
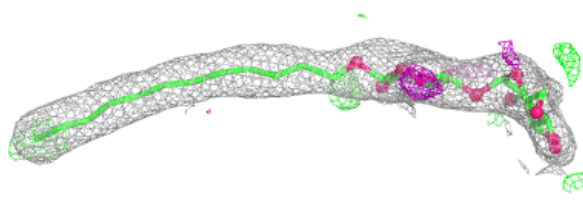
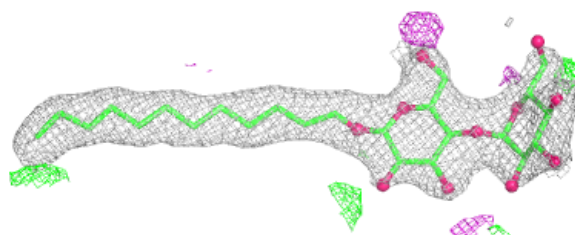


Electron density around LMG c 501:

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

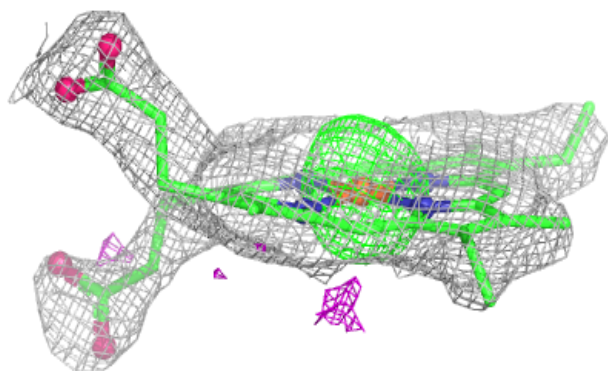
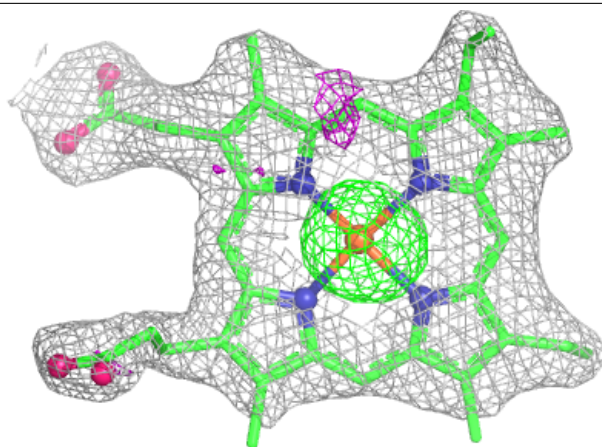
**Electron density around LMT M 101:**

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

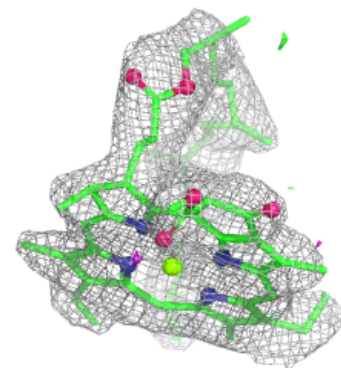
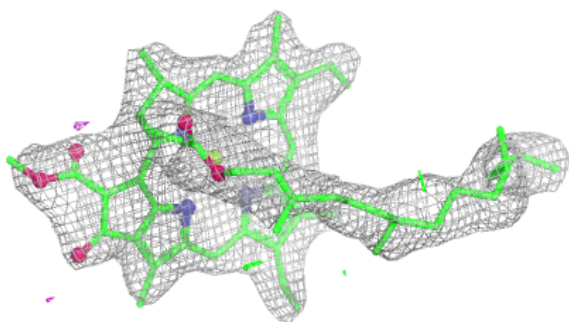
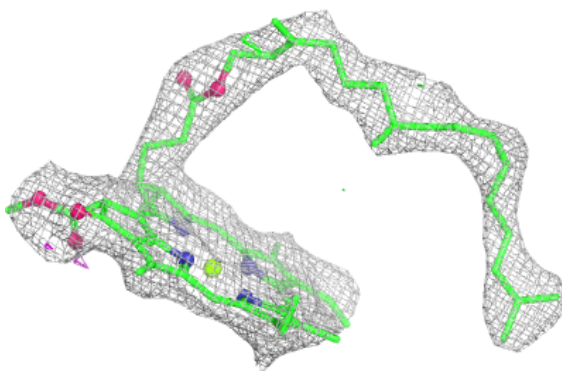


Electron density around HEM F 102:

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

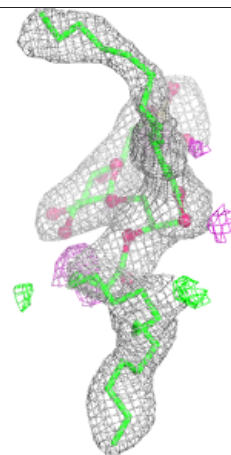
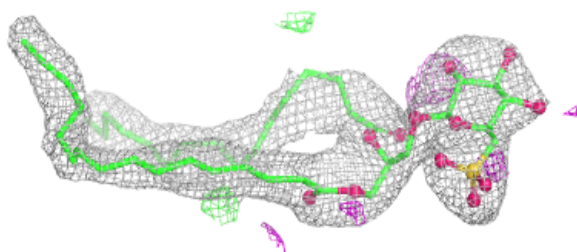
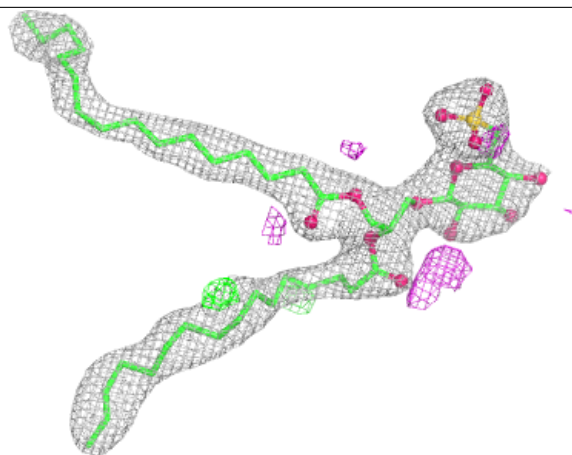
**Electron density around CLA c 518:**

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



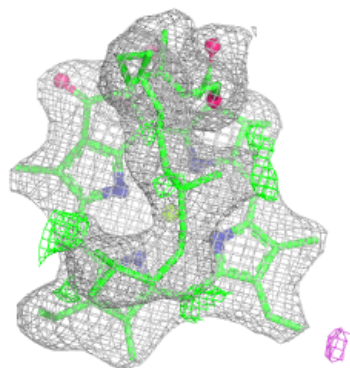
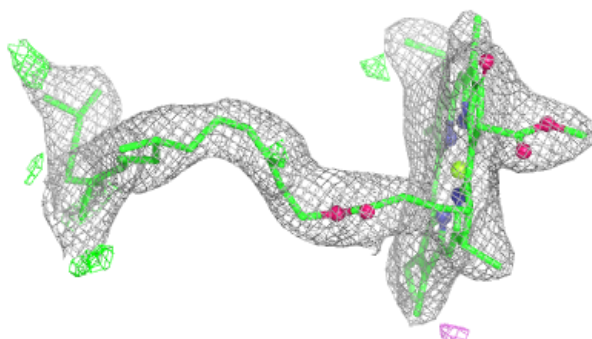
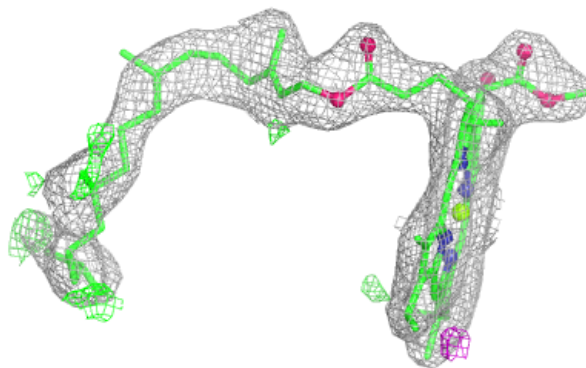
Electron density around SQD A 412:

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

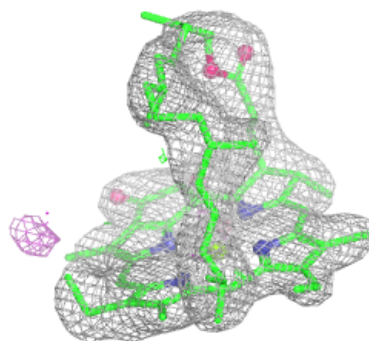
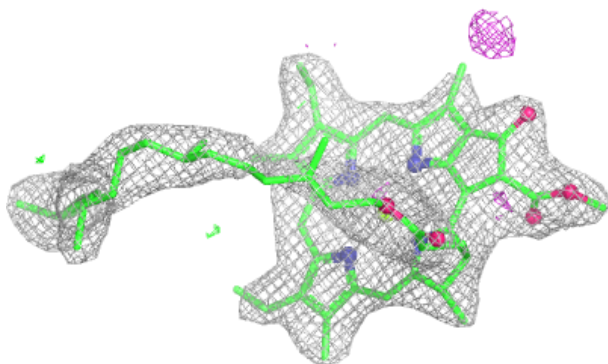
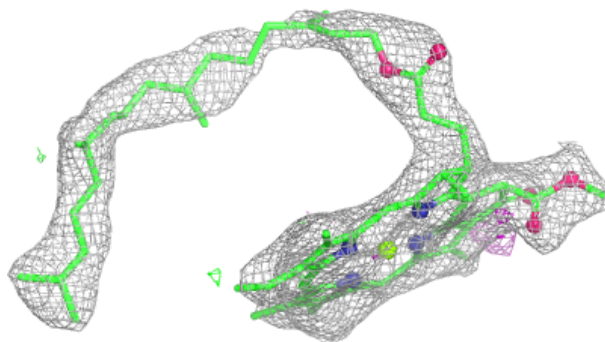


Electron density around CLA C 506:

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

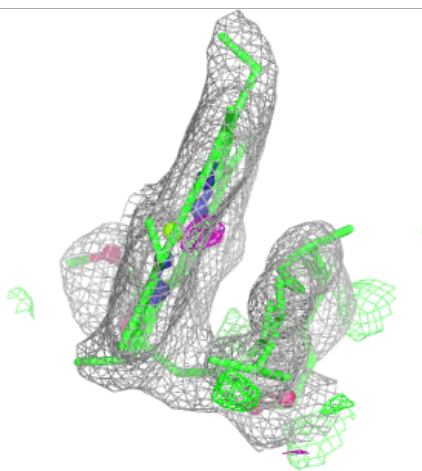
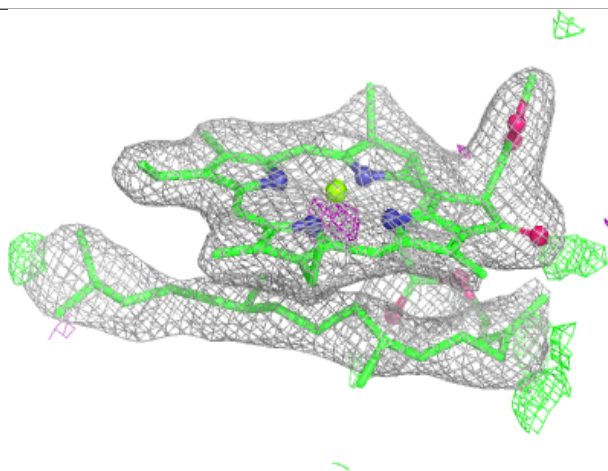
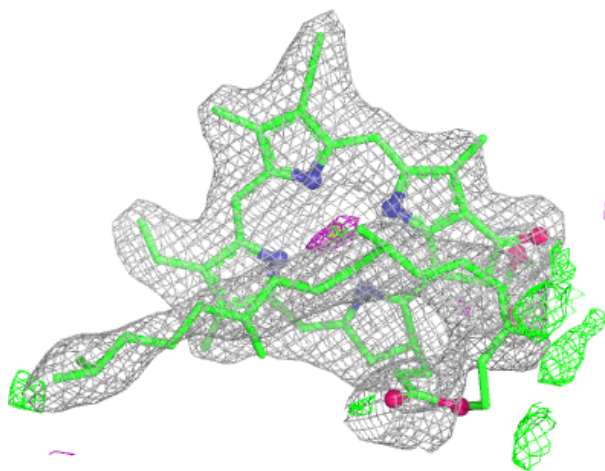
**Electron density around CLA C 513:**

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



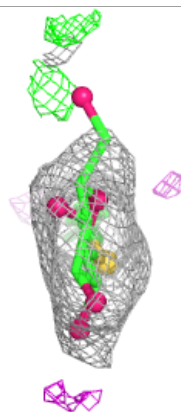
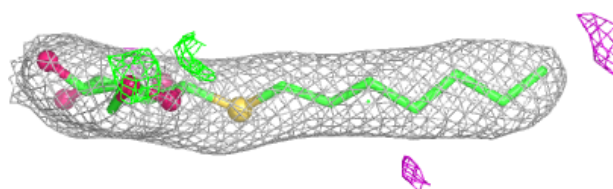
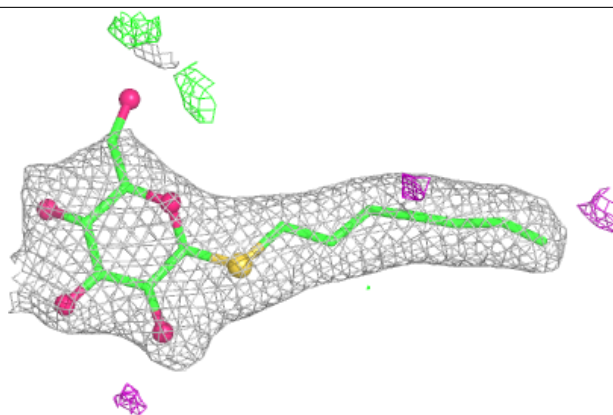
Electron density around CLA b 610:

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

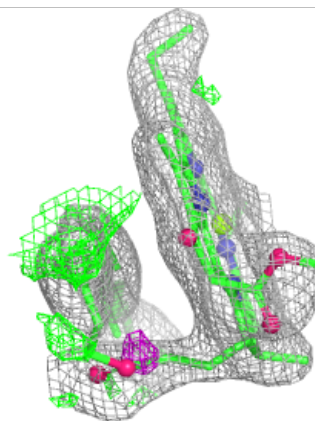
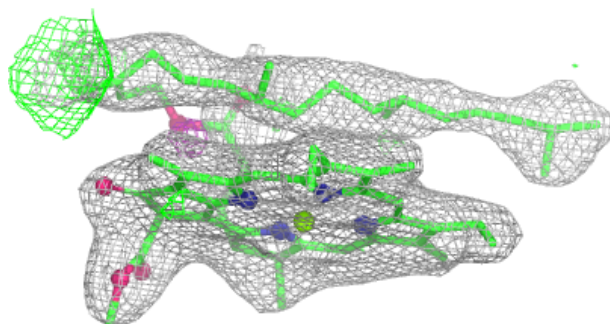
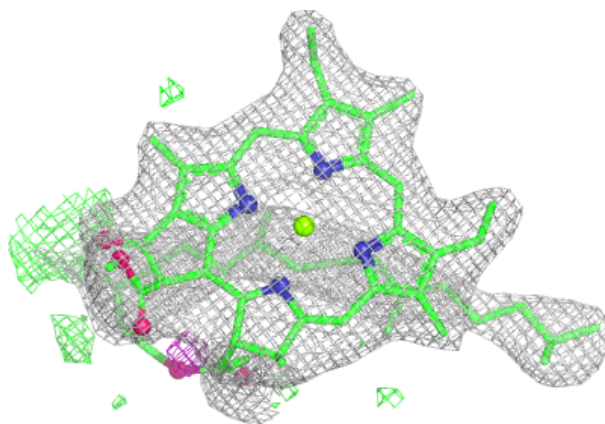


Electron density around HTG B 632:

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

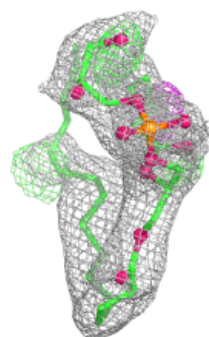
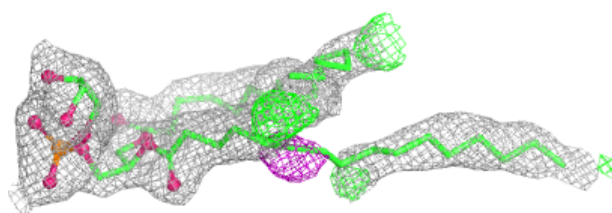
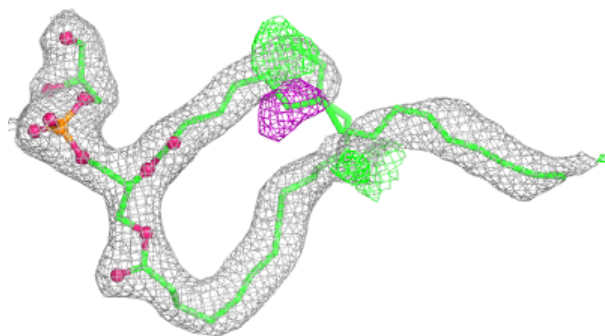
**Electron density around CLA B 602:**

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

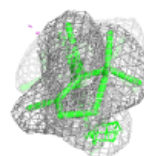
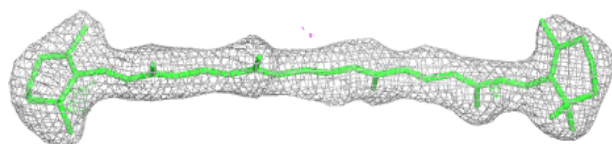
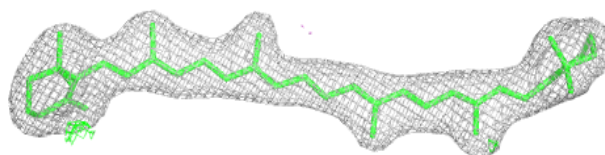


Electron density around LHG D 409:

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

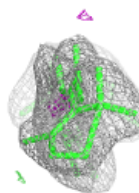
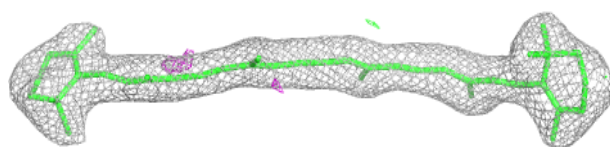
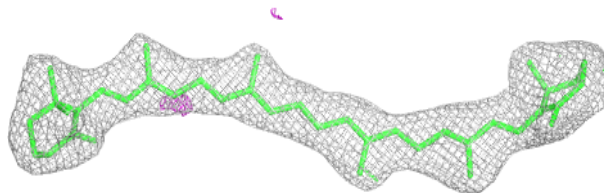
**Electron density around BCR C 514:**

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

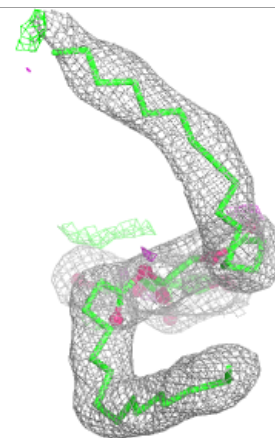
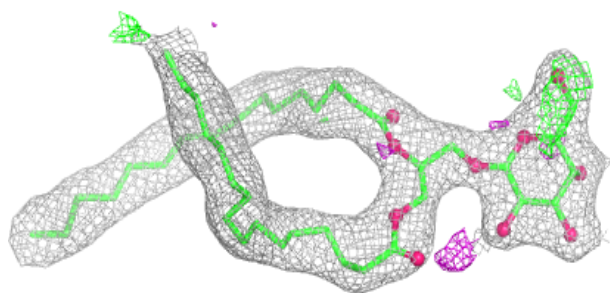
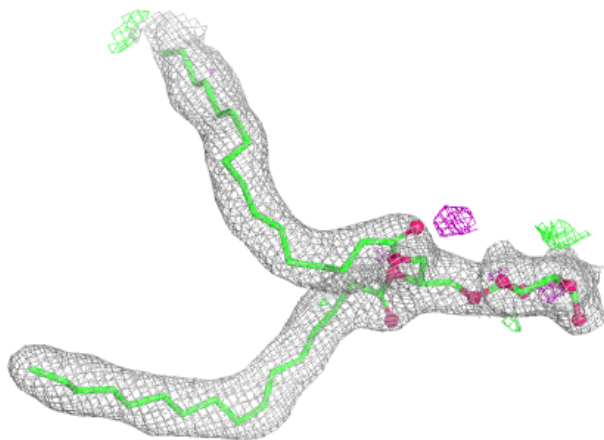


Electron density around BCR y 101:

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

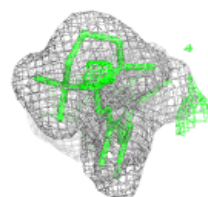
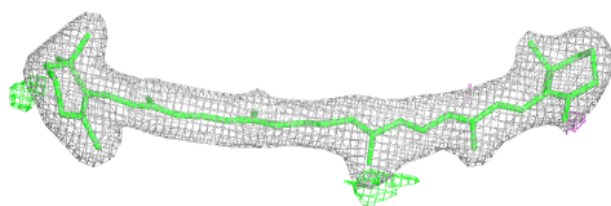
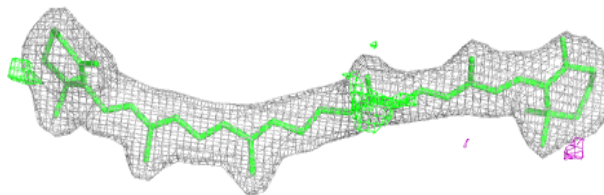
**Electron density around LMG B 622:**

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

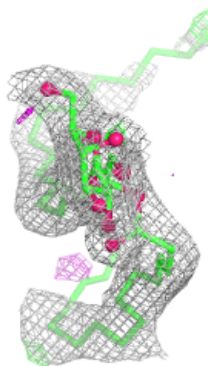
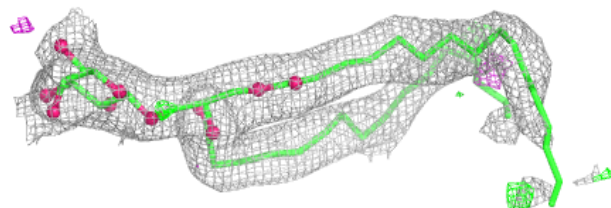
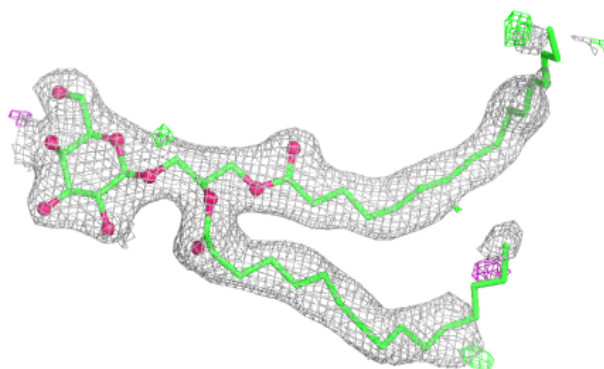


Electron density around BCR t 101:

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

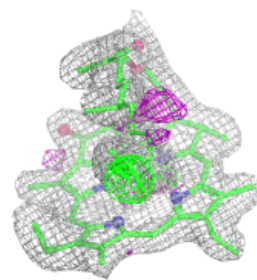
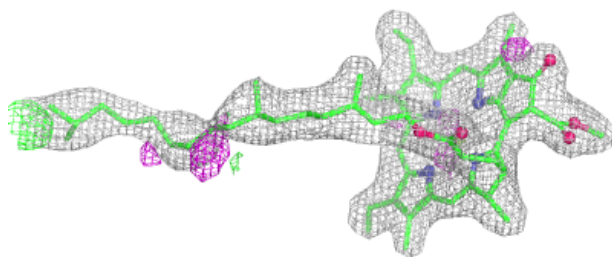
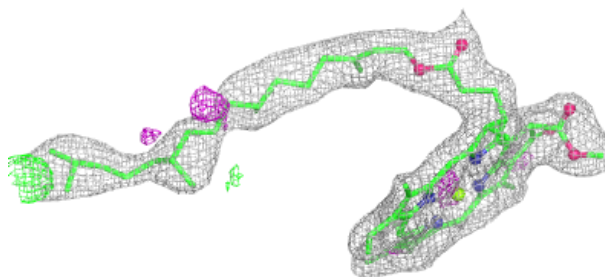
**Electron density around LMG D 413:**

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

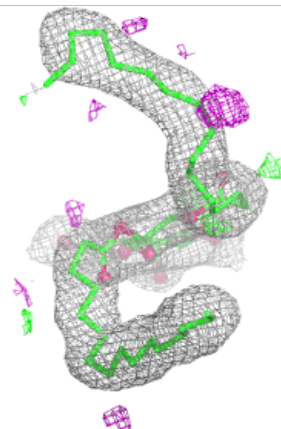
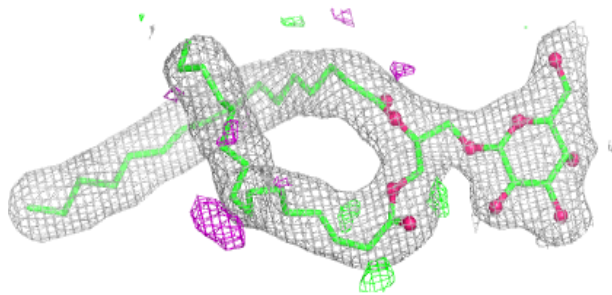
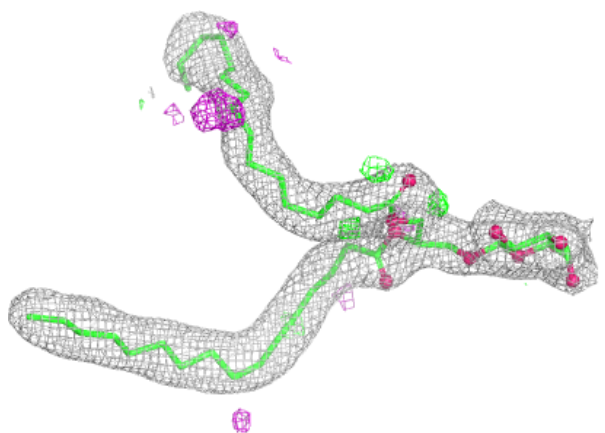


Electron density around CLA C 504:

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

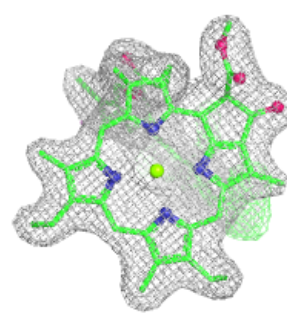
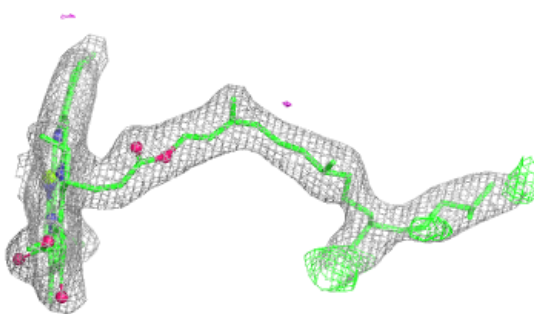
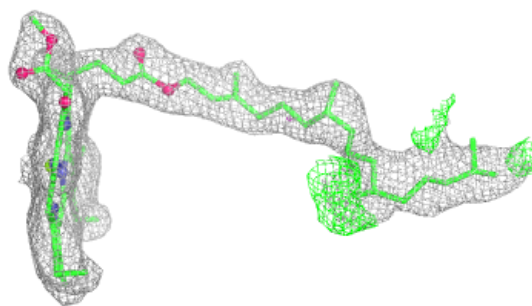
**Electron density around LMG b 629:**

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

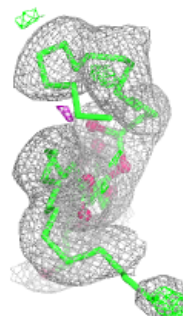
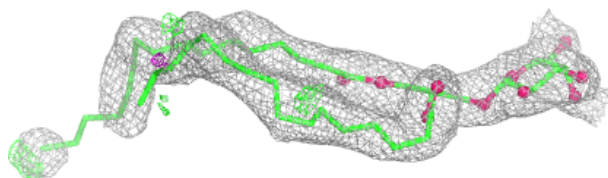
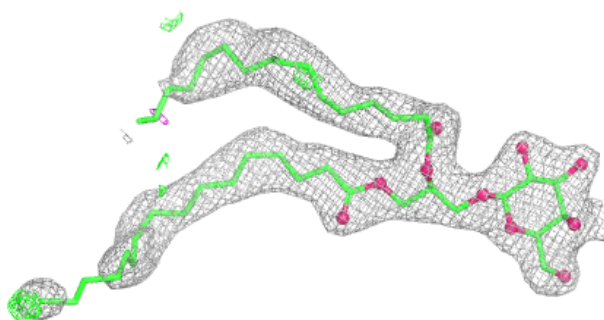


Electron density around CLA b 615:

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

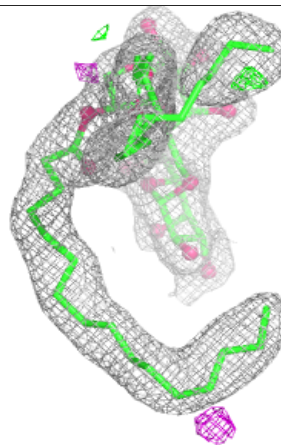
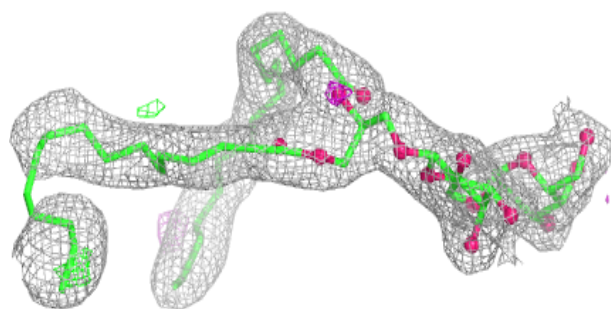
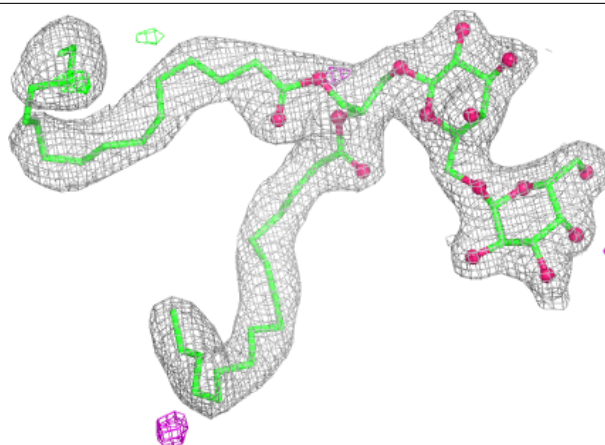
**Electron density around LMG d 413:**

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

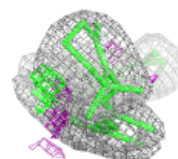
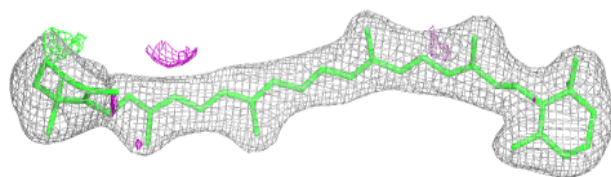
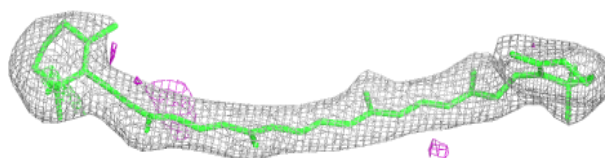


Electron density around DGD C 517:

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

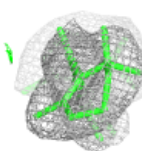
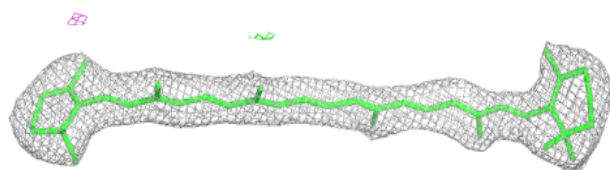
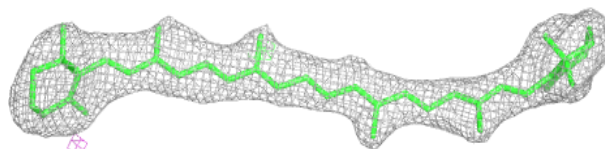
**Electron density around BCR D 404:**

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

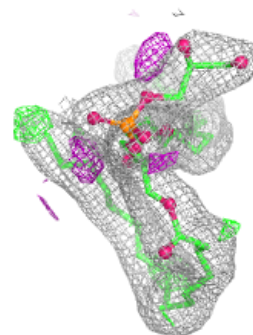
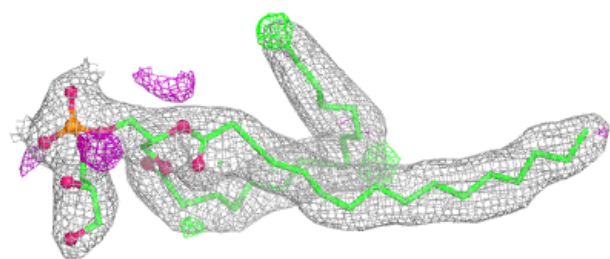
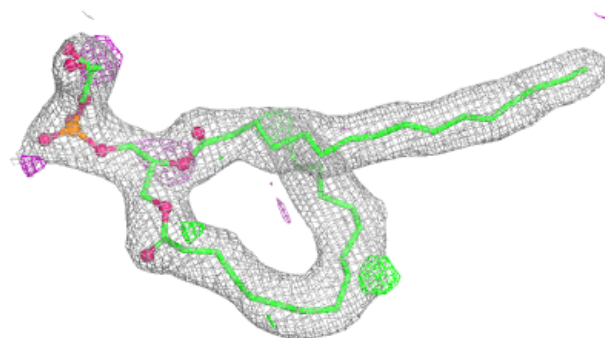


Electron density around BCR c 528:

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

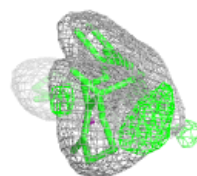
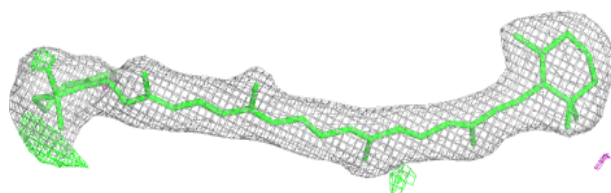
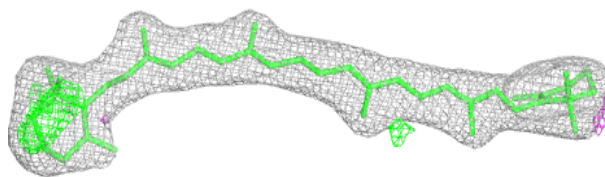
**Electron density around LHG D 407:**

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



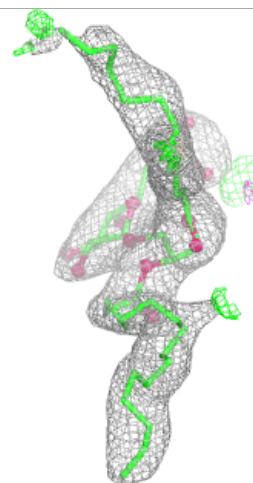
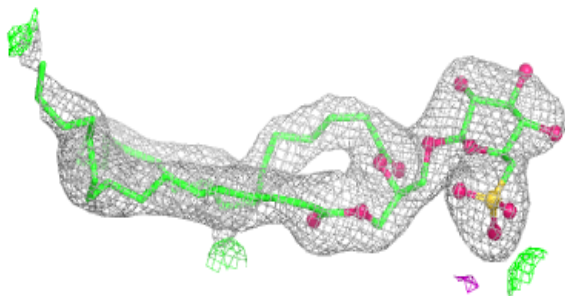
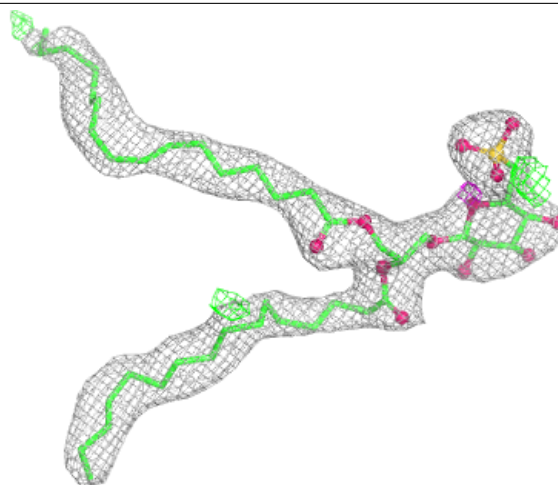
Electron density around BCR d 404:

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



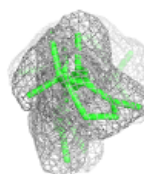
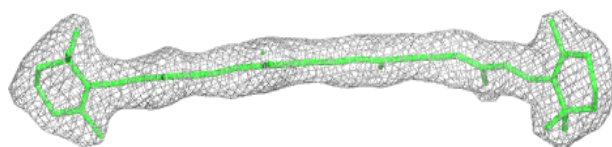
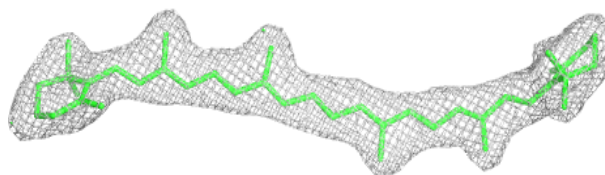
Electron density around SQD a 414:

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

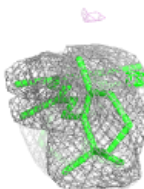
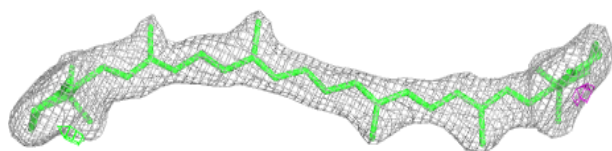
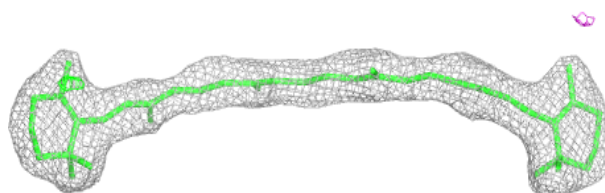


Electron density around BCR h 101:

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

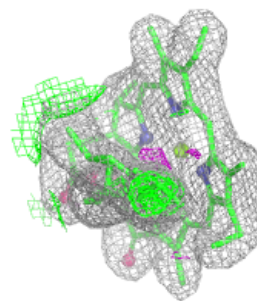
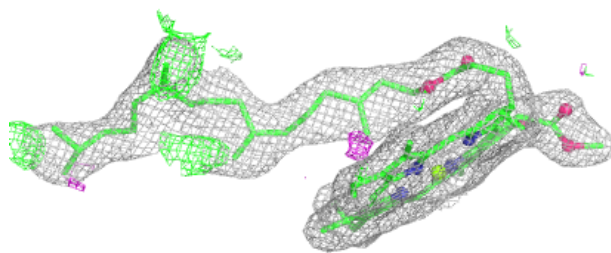
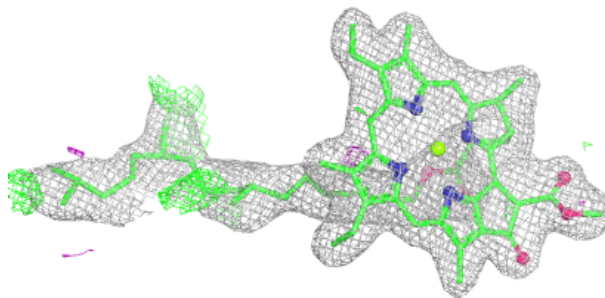
**Electron density around BCR k 101:**

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



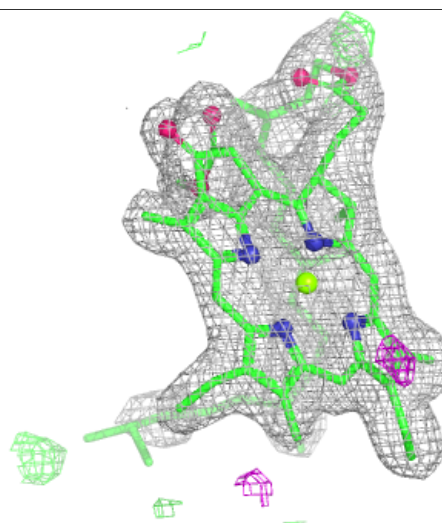
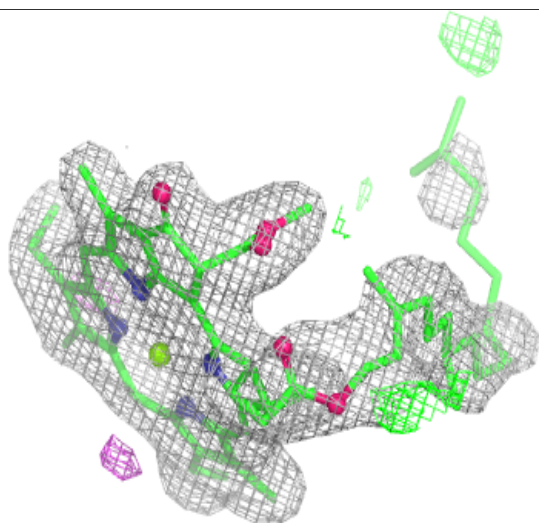
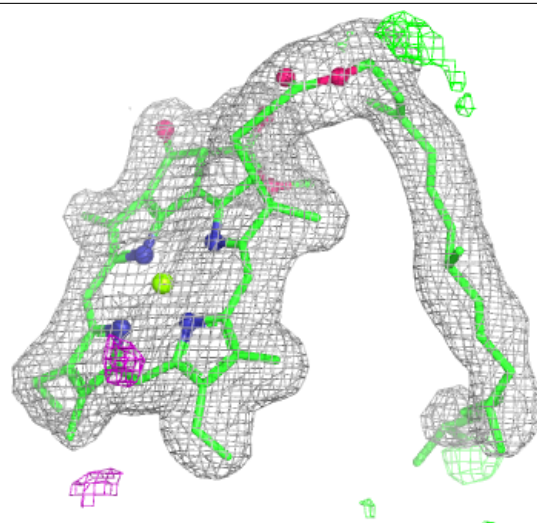
Electron density around CLA b 623:

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



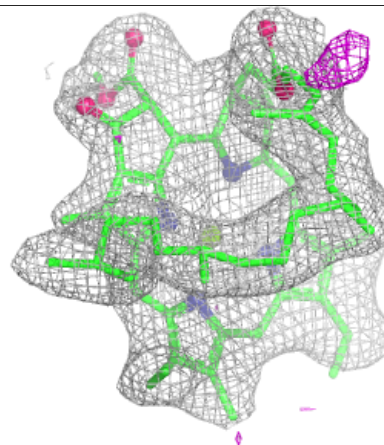
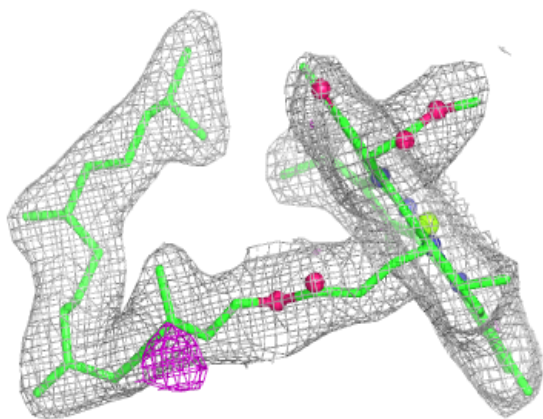
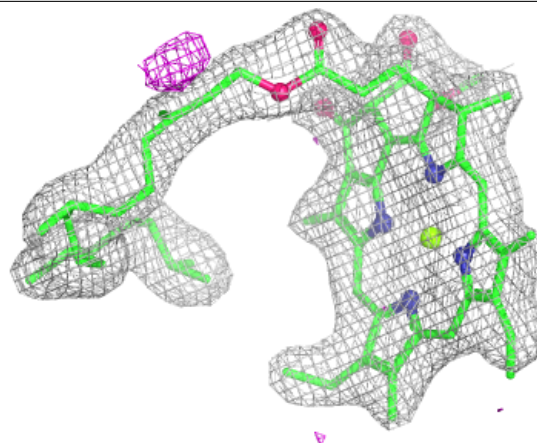
Electron density around CLA b 625:

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



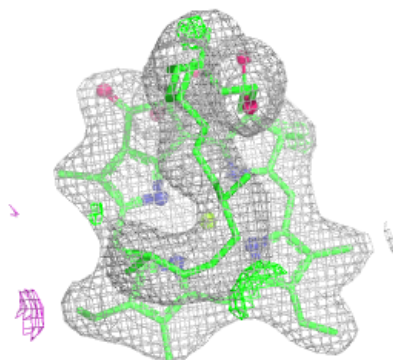
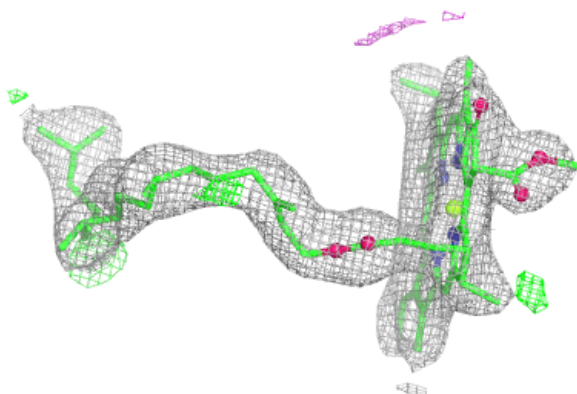
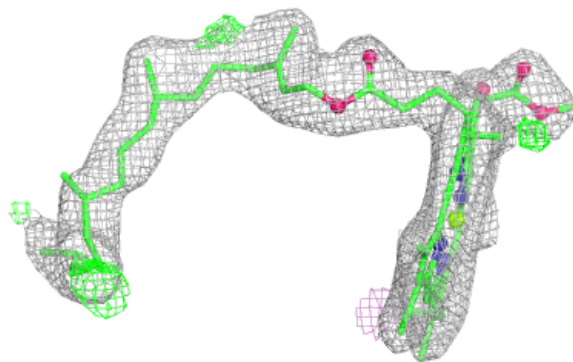
Electron density around CLA c 508:

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



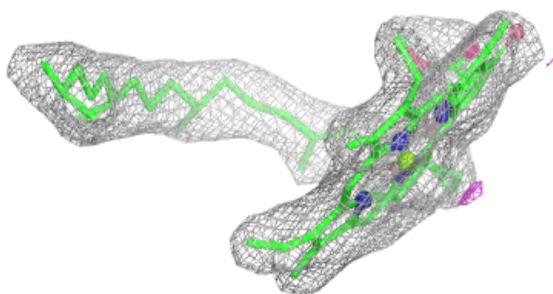
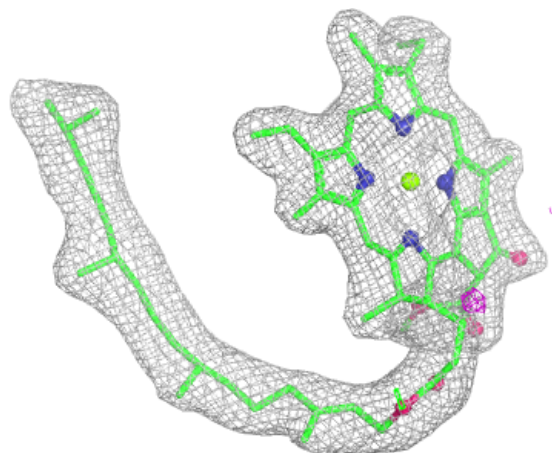
Electron density around CLA c 511:

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



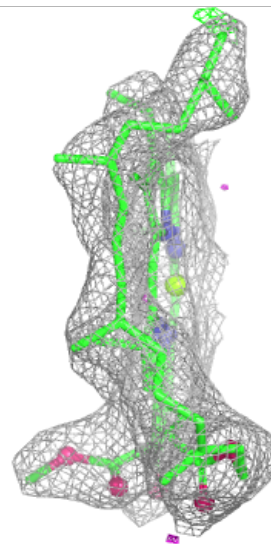
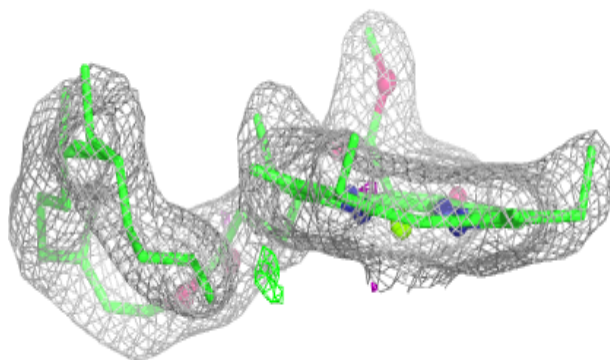
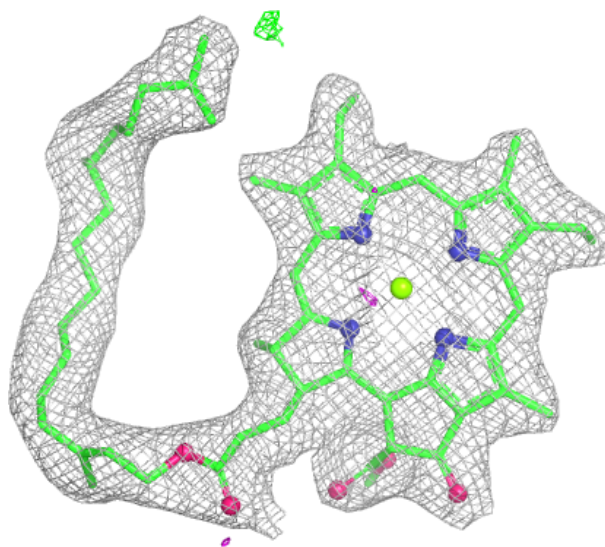
Electron density around CLA c 512:

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



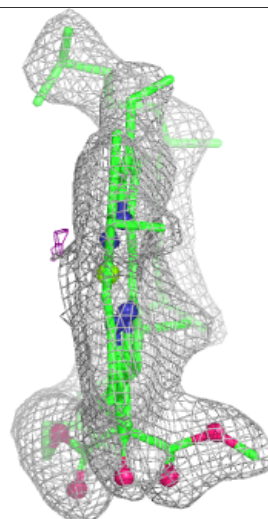
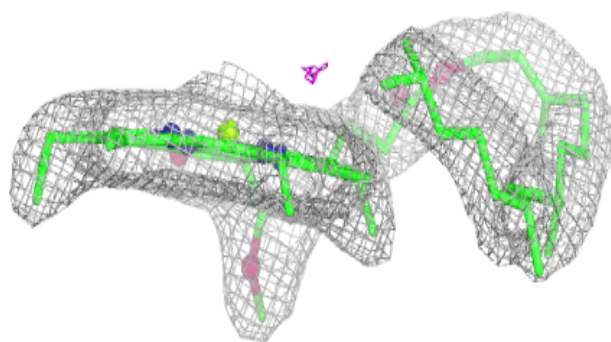
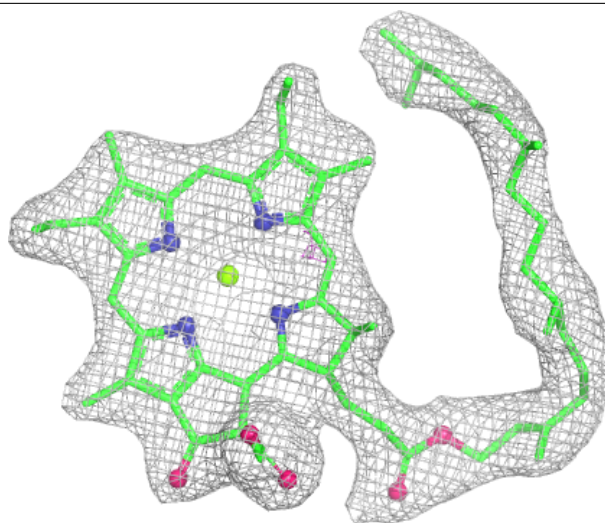
Electron density around CLA c 517:

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



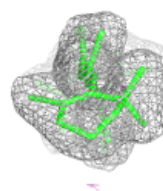
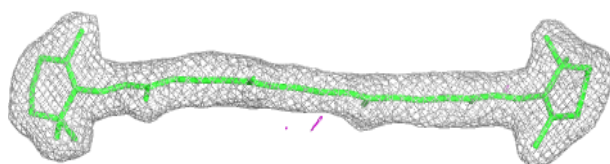
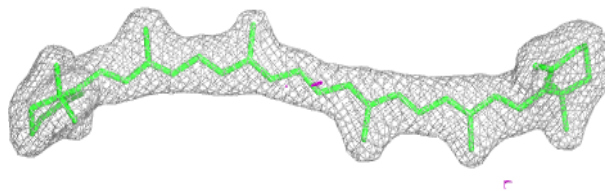
Electron density around CLA C 512:

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

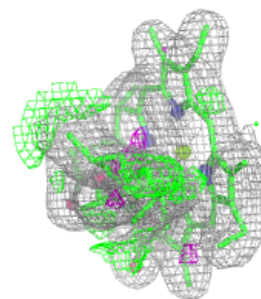
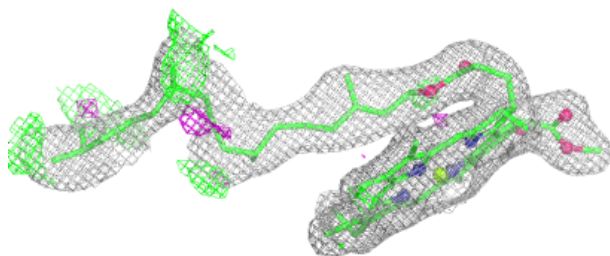
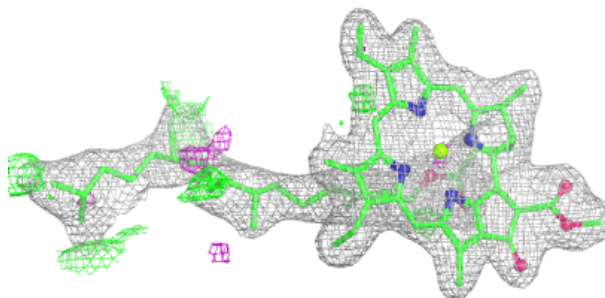


Electron density around BCR A 411:

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

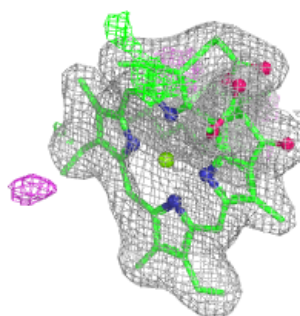
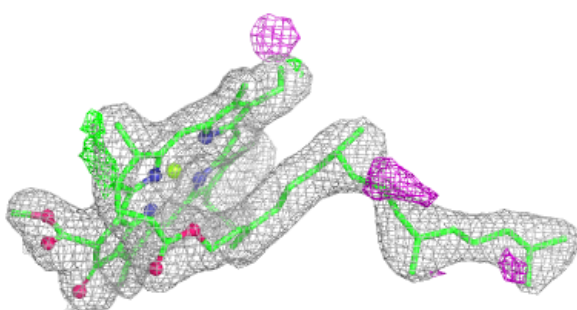
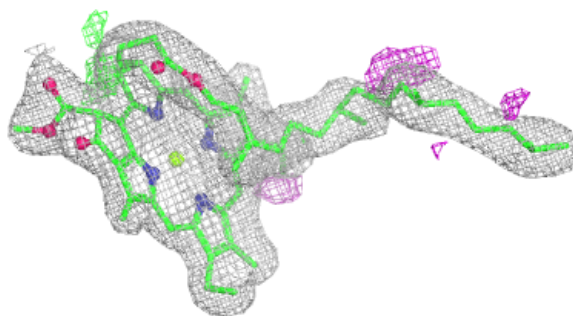
**Electron density around CLA B 615:**

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

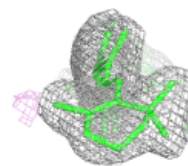
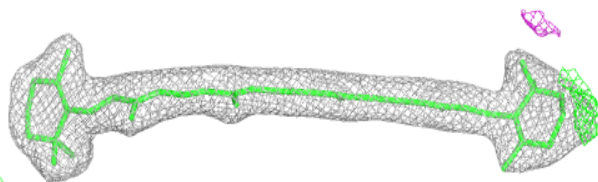
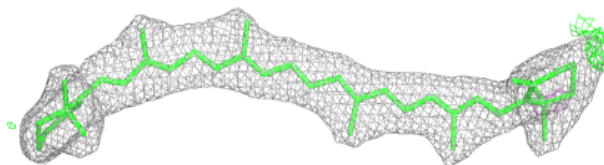


Electron density around CLA C 505:

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

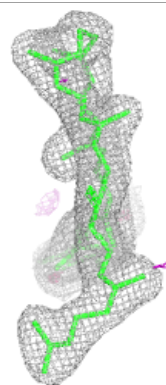
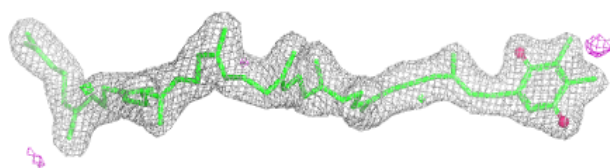
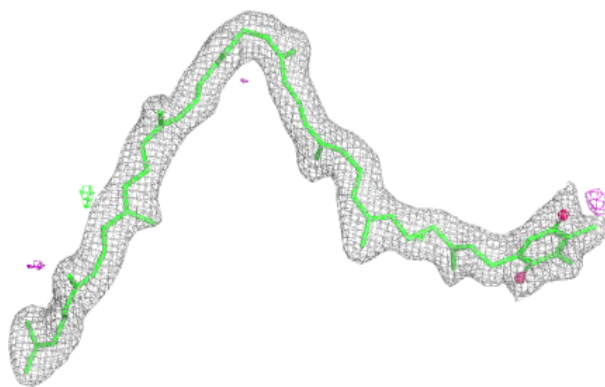
**Electron density around BCR H 101:**

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

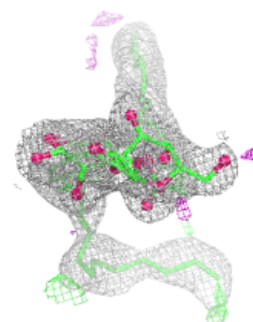
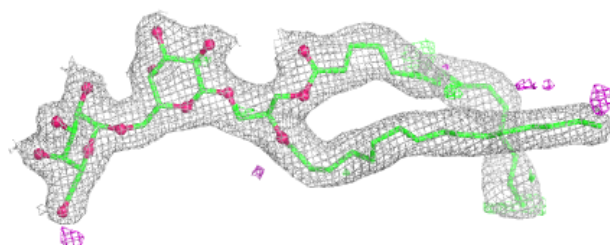
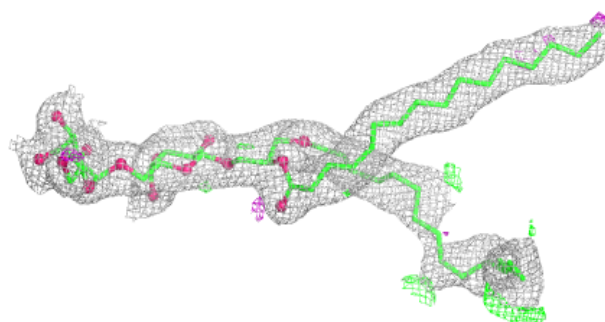


Electron density around PL9 d 405 (A):

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

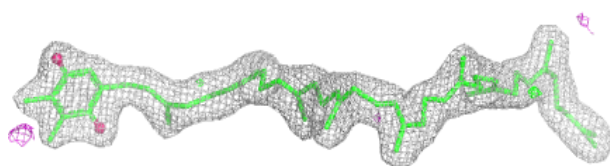
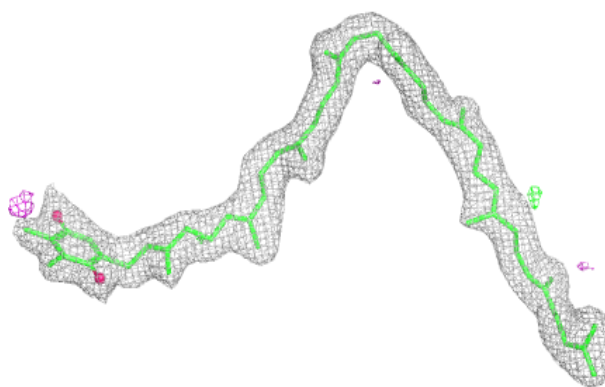
**Electron density around DGD C 516:**

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

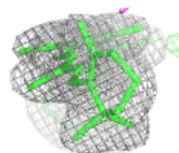
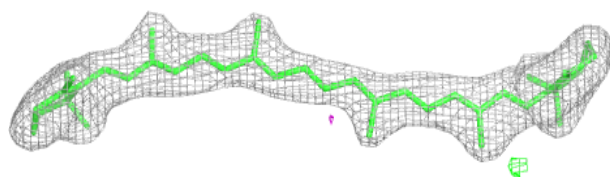
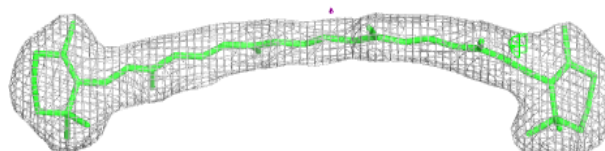


Electron density around PL9 d 405 (B):

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

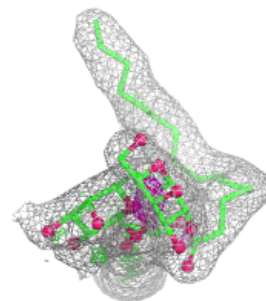
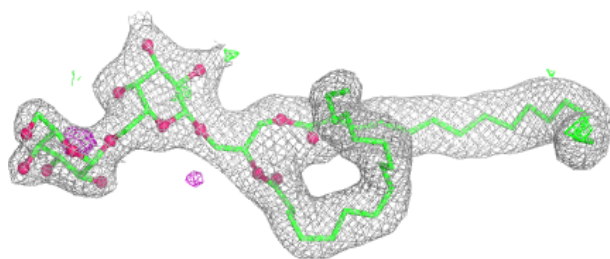
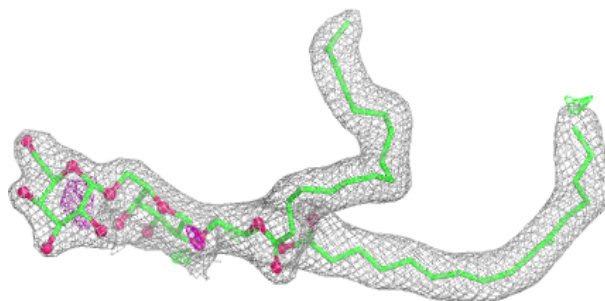
**Electron density around BCR K 101:**

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

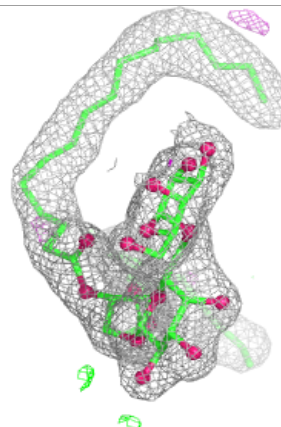
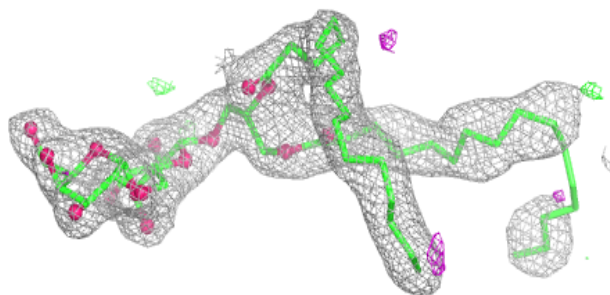
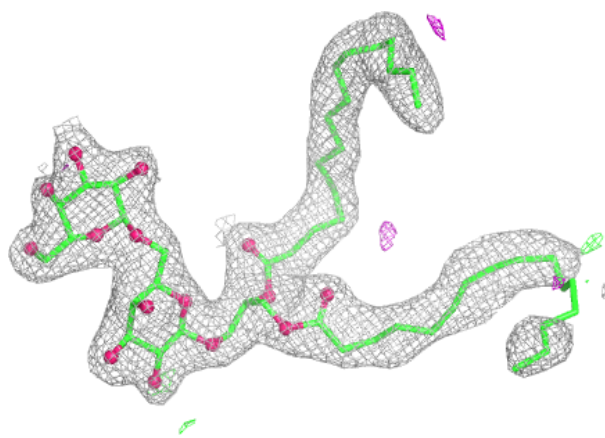


Electron density around DGD H 102:

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

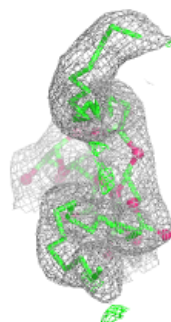
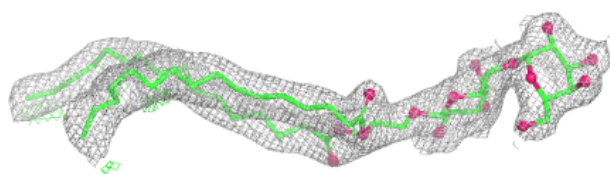
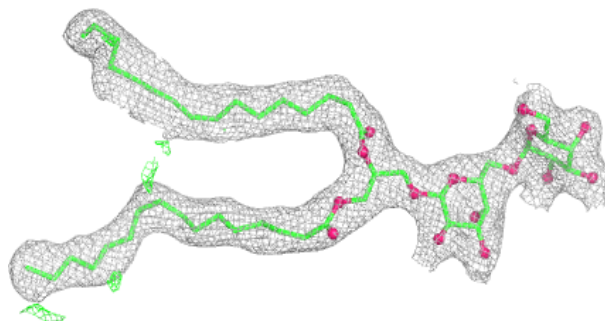
**Electron density around DGD c 521:**

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

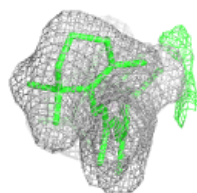
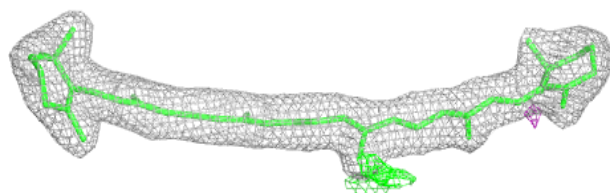
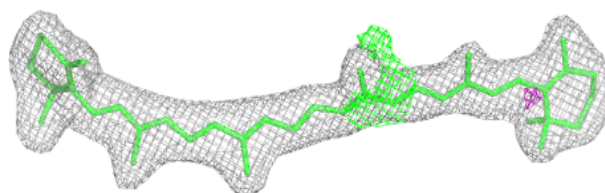


Electron density around DGD c 522:

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

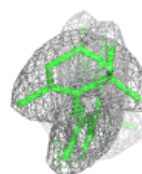
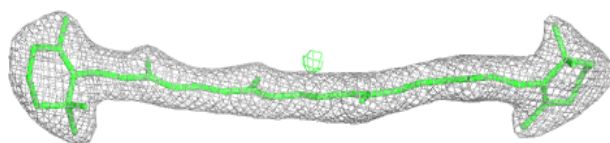
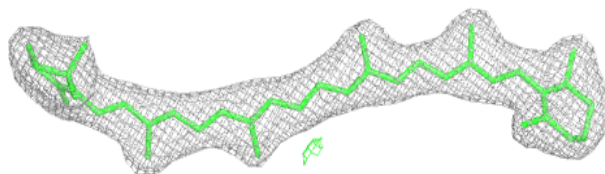
**Electron density around BCR T 103:**

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

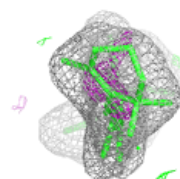
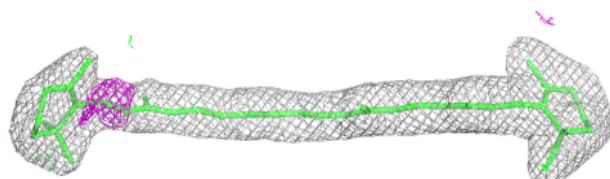
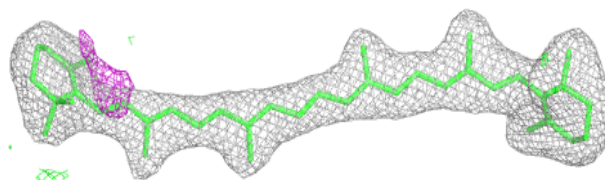


Electron density around BCR Y 101:

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

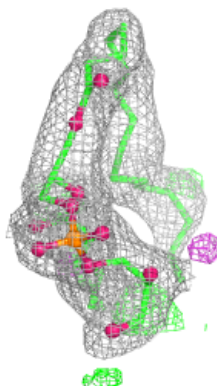
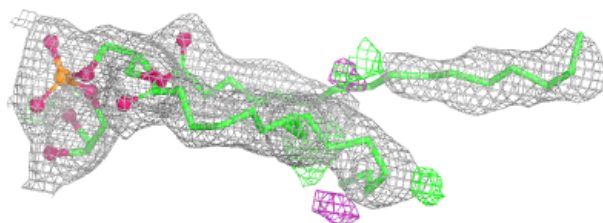
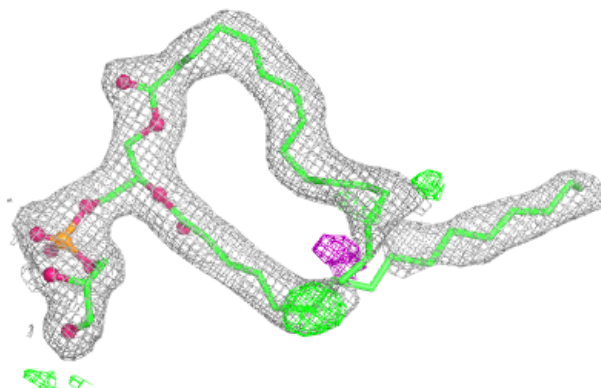
**Electron density around BCR b 627:**

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



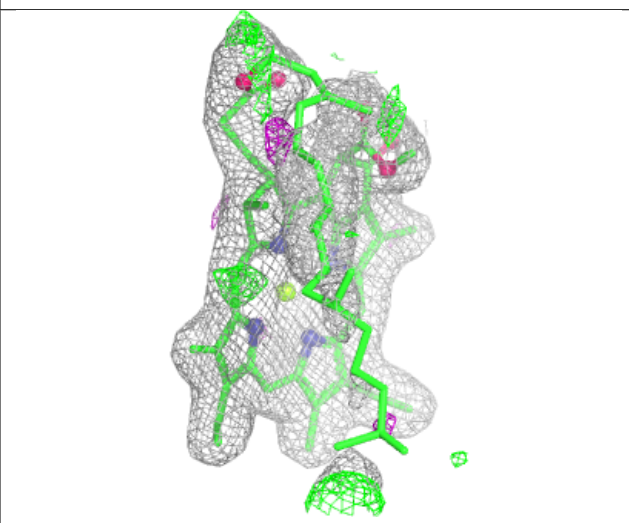
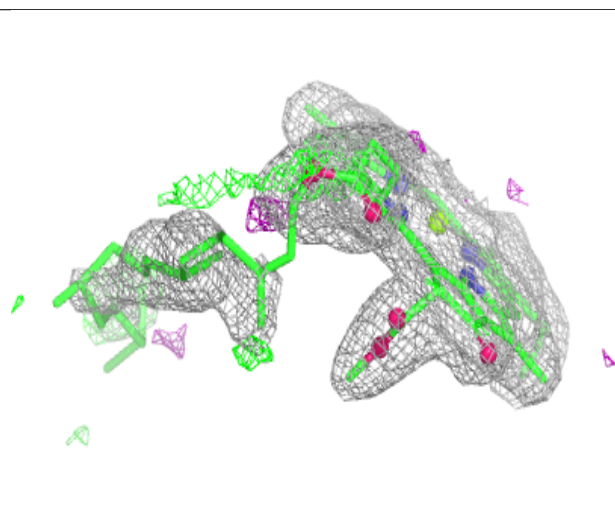
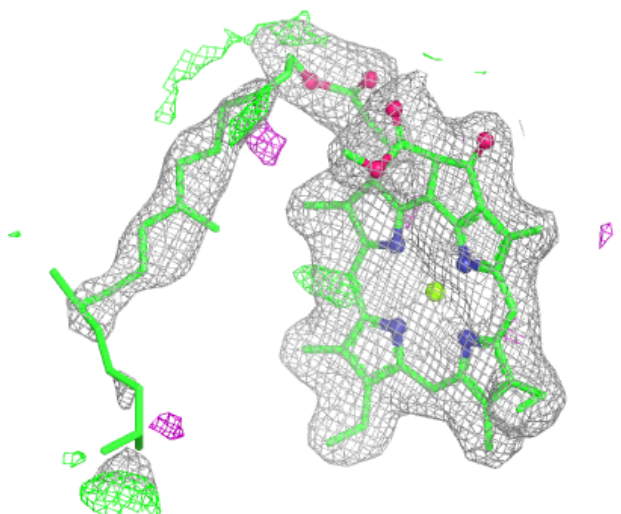
Electron density around LHG d 408:

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



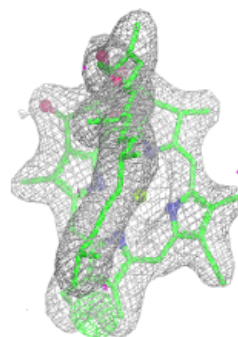
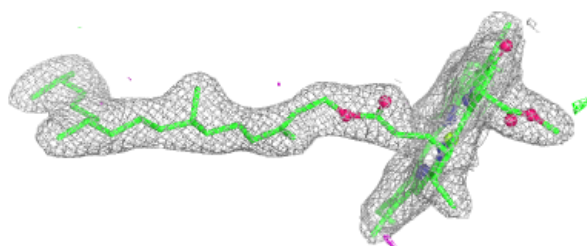
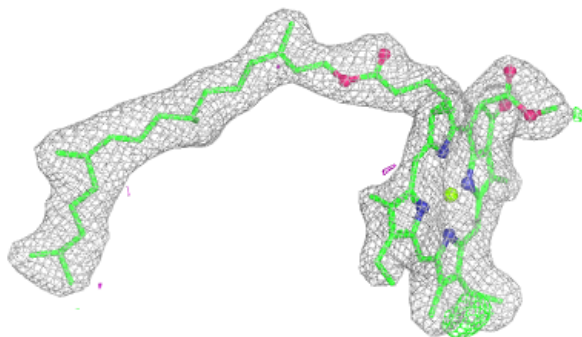
Electron density around CLA B 617:

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

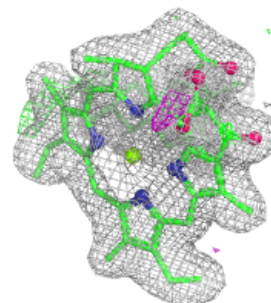
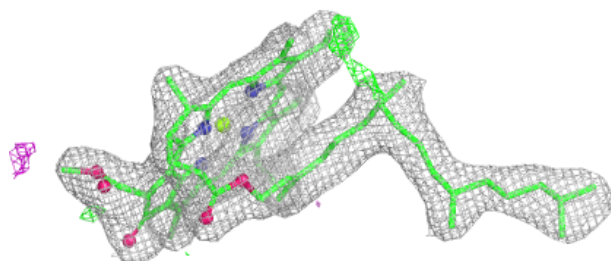
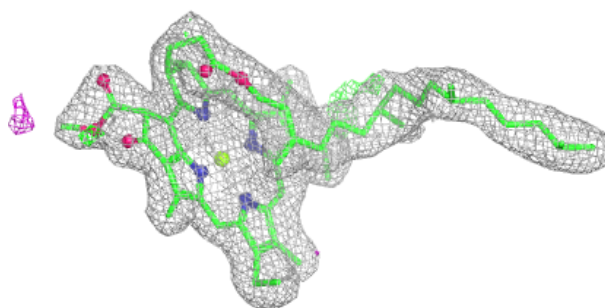


Electron density around CLA b 618:

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

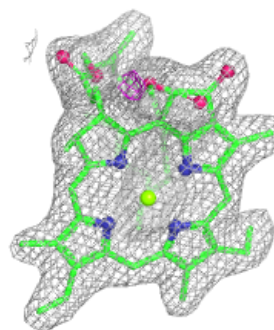
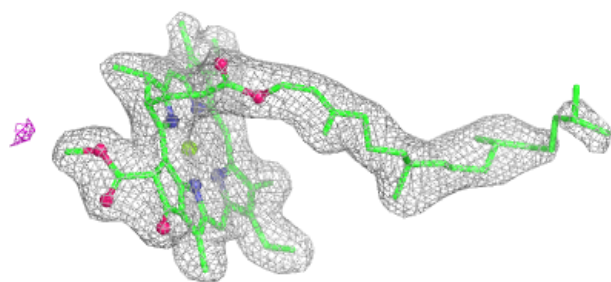
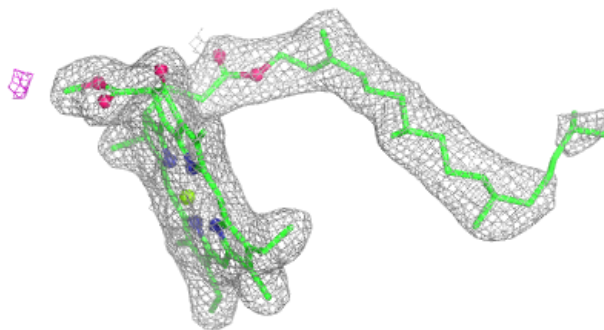
**Electron density around CLA c 510:**

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



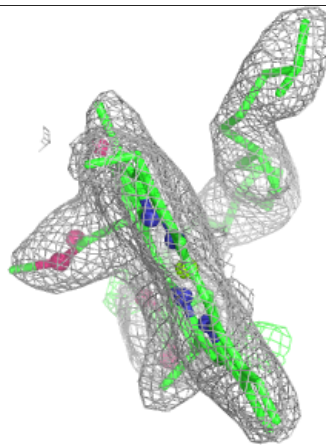
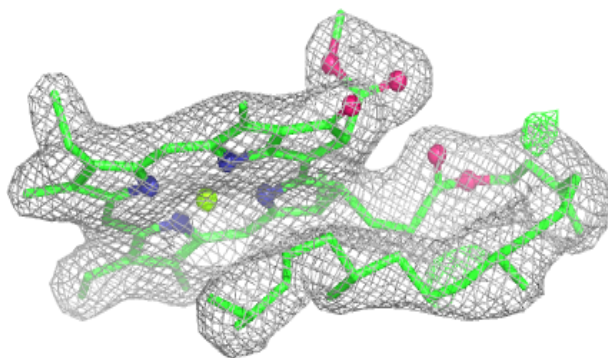
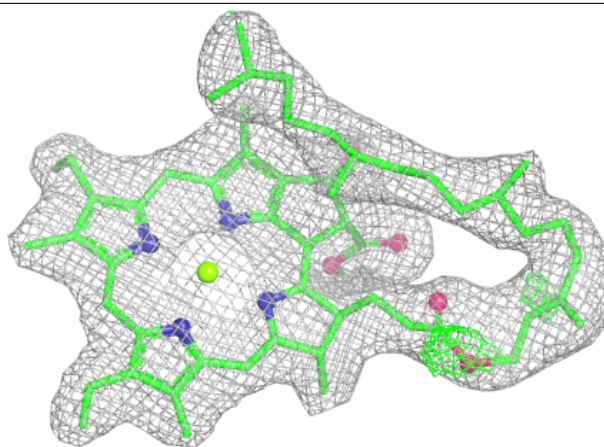
Electron density around CLA C 508:

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



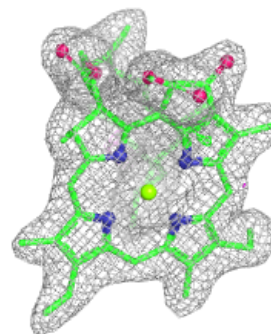
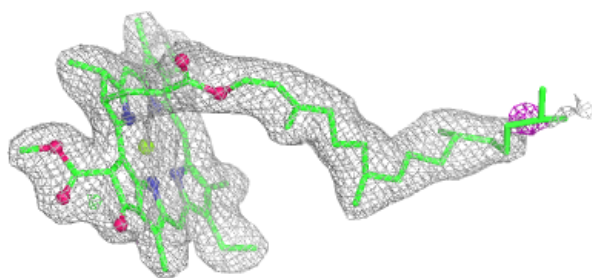
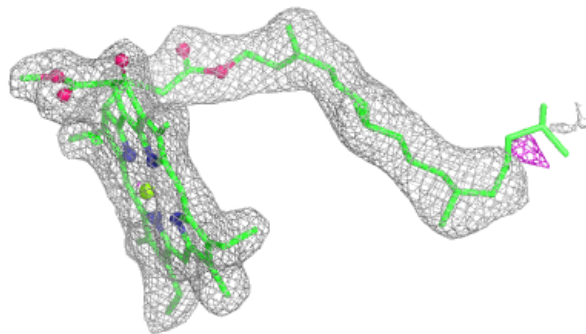
Electron density around CLA C 509:

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



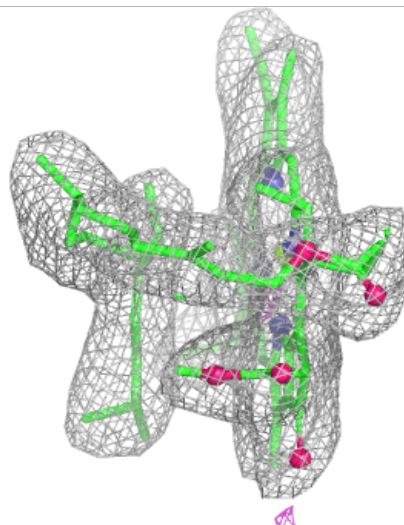
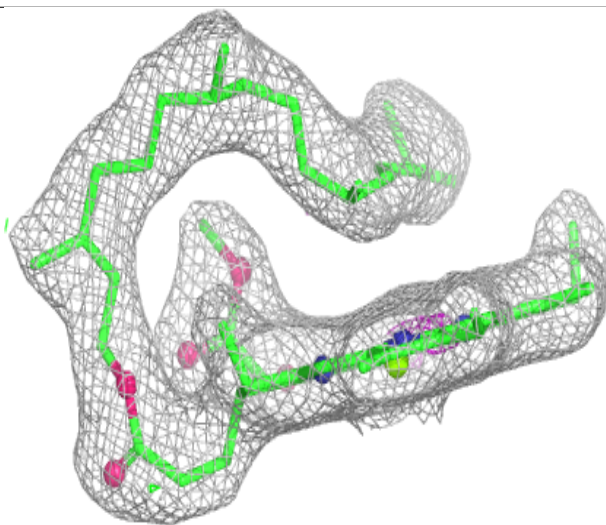
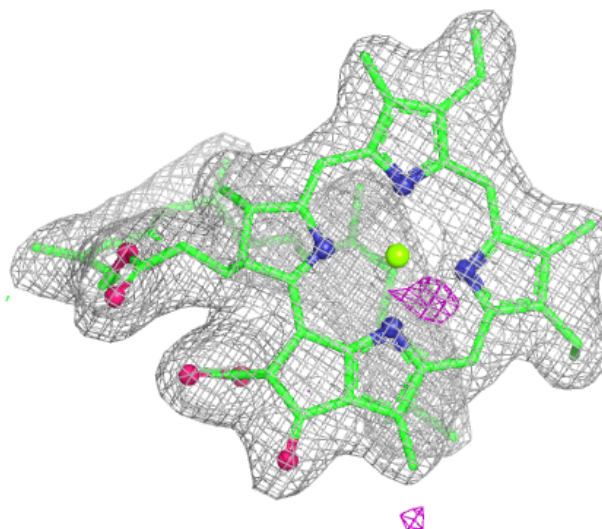
Electron density around CLA c 513:

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



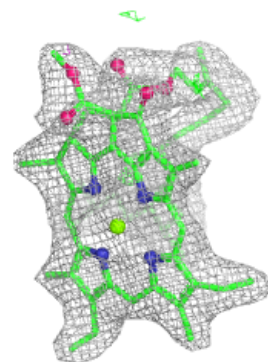
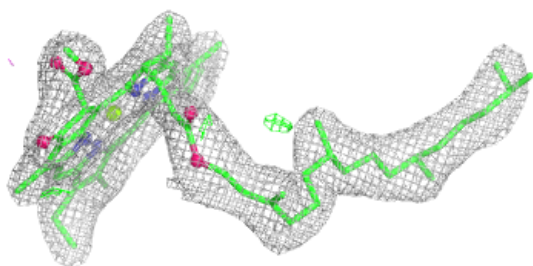
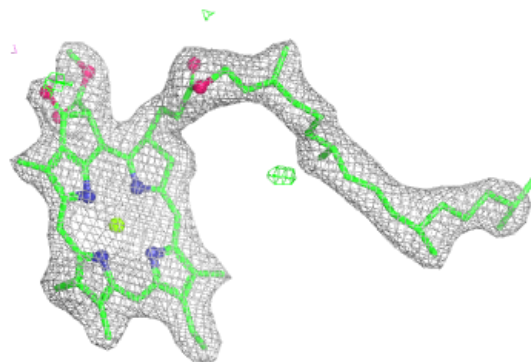
Electron density around CLA c 515:

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



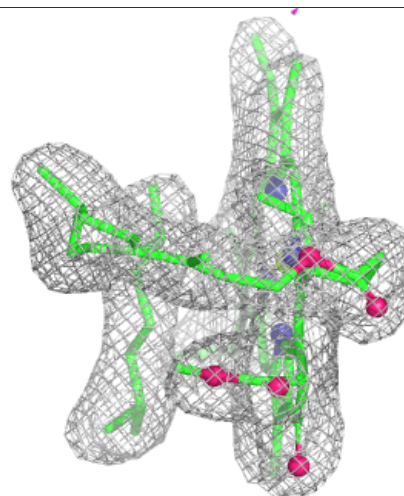
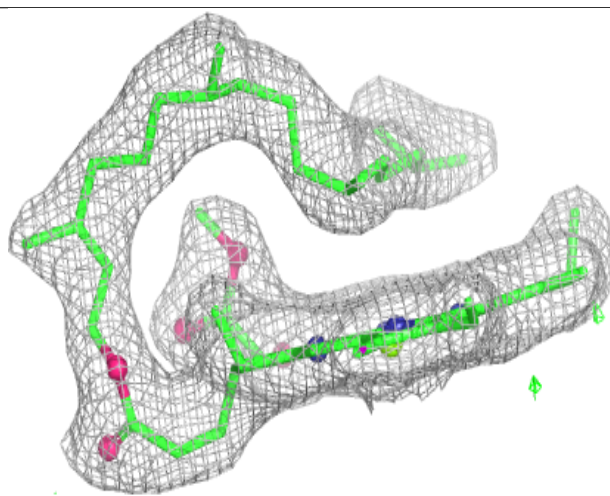
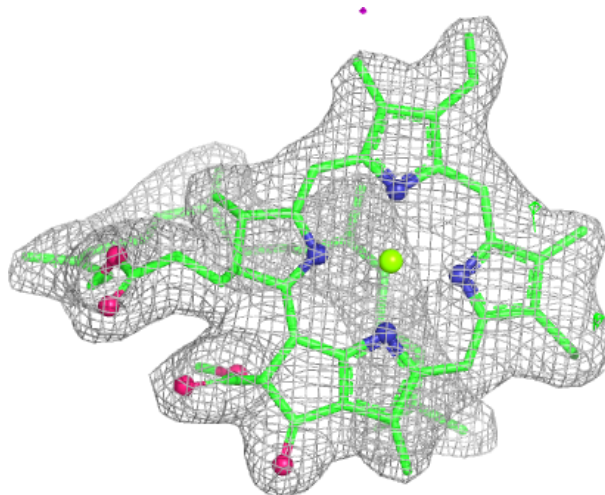
Electron density around CLA c 516:

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



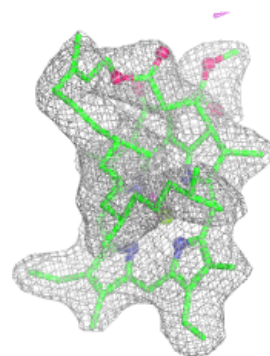
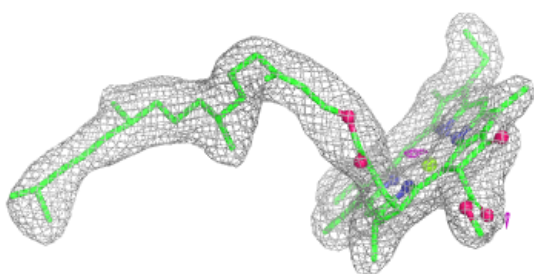
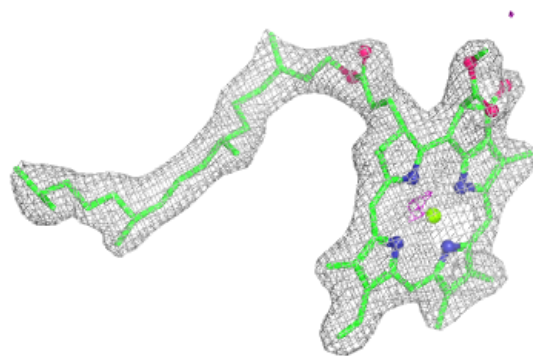
Electron density around CLA C 510:

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

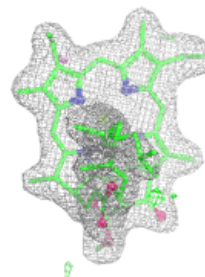
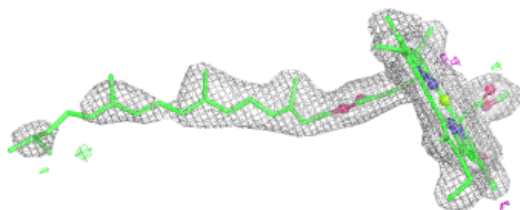
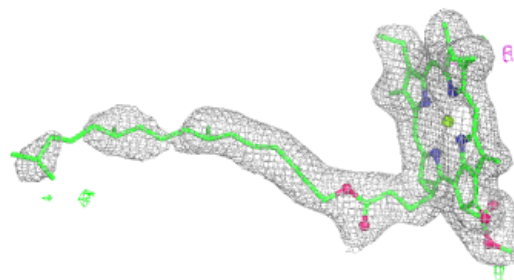


Electron density around CLA C 511:

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

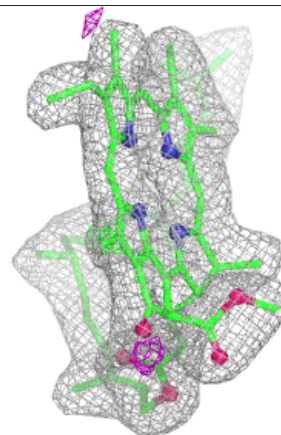
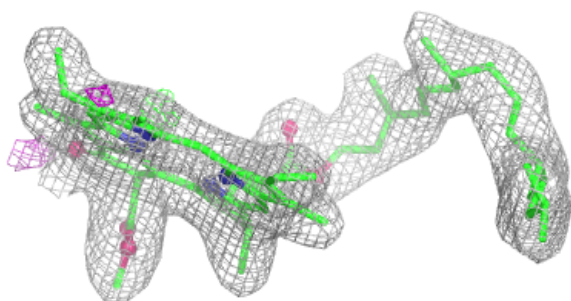
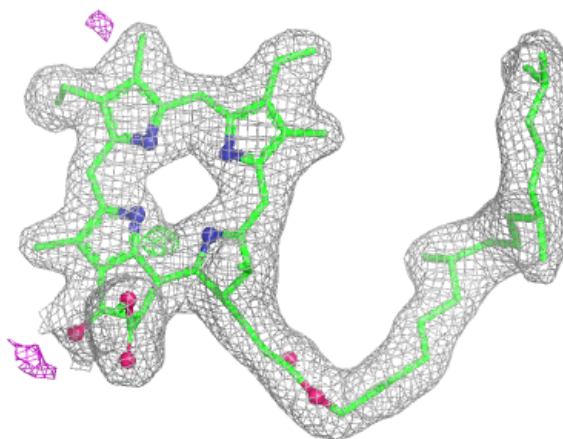
**Electron density around CLA d 403:**

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



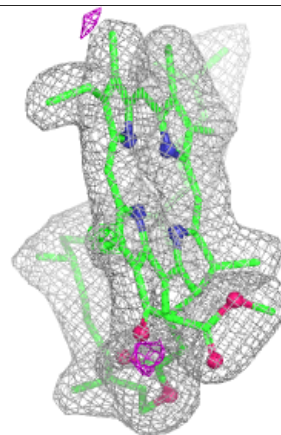
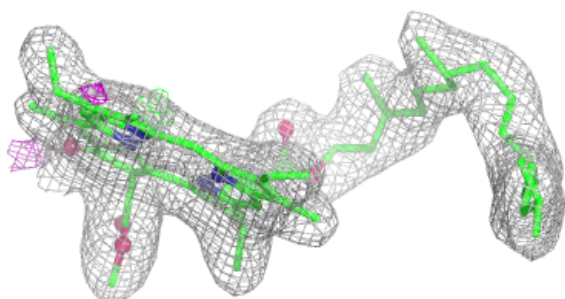
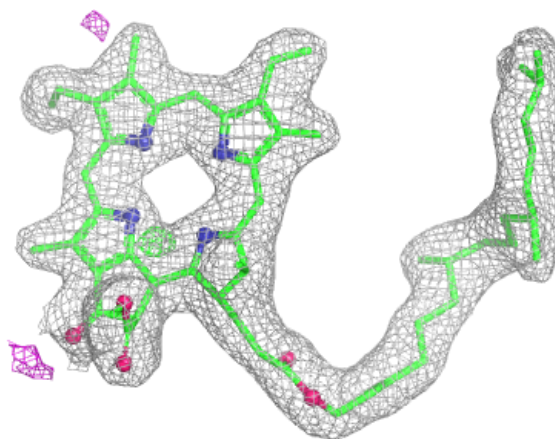
Electron density around PHO a 418 (A):

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



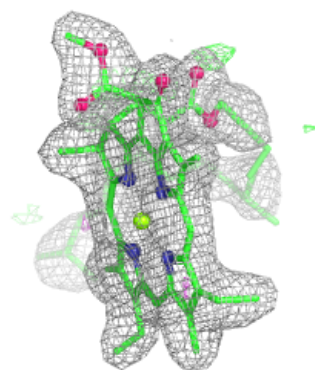
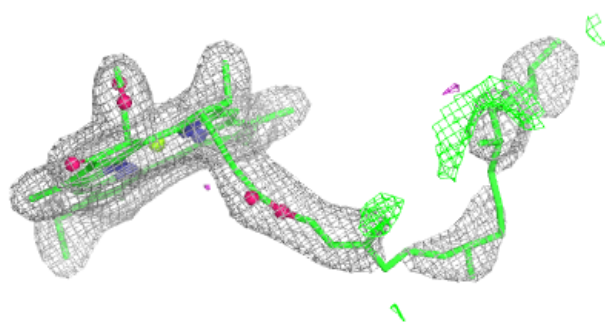
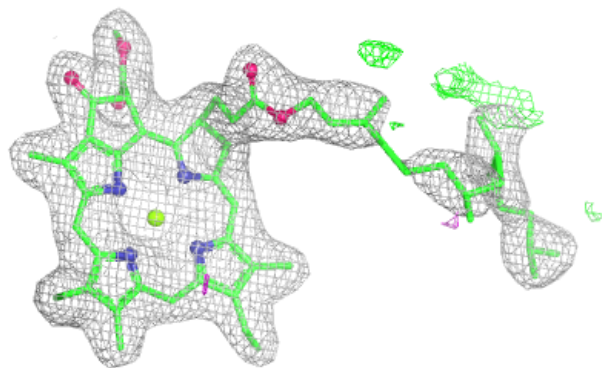
Electron density around PHO a 418 (B):

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

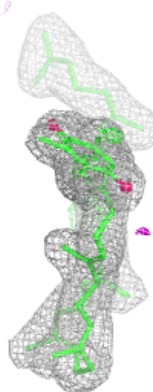
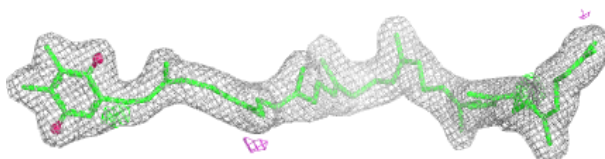
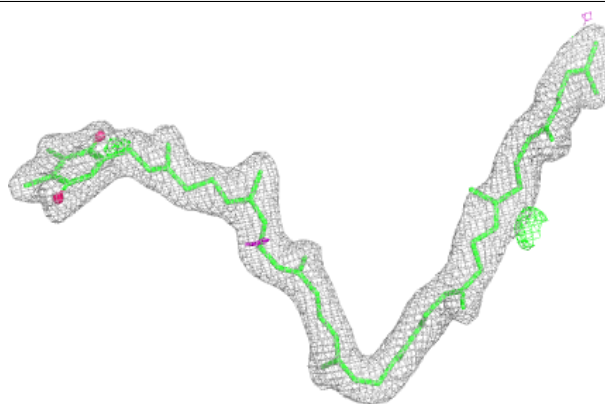


Electron density around CLA A 410:

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

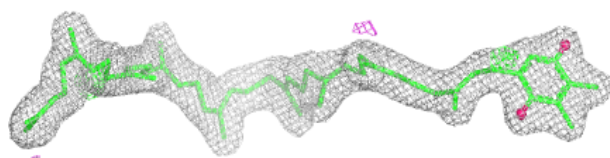
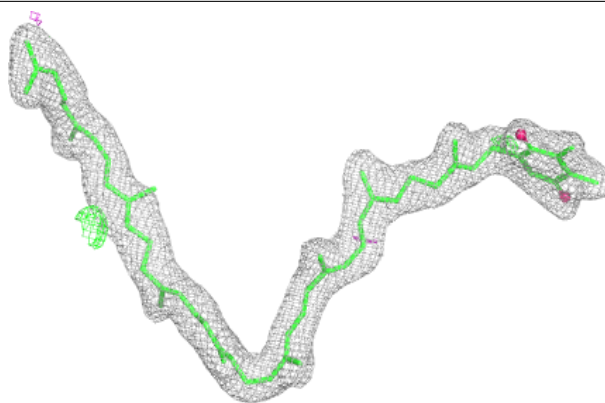
**Electron density around PL9 D 405 (A):**

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

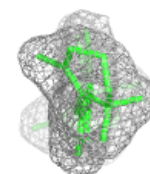
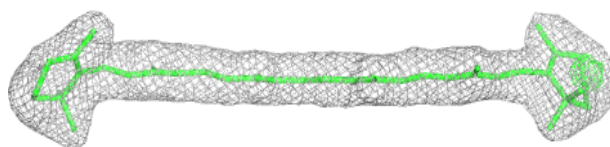
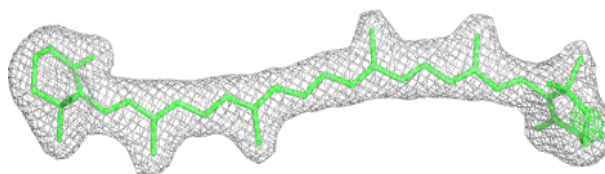


Electron density around PL9 D 405 (B):

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

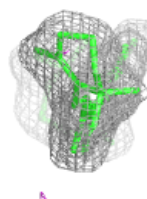
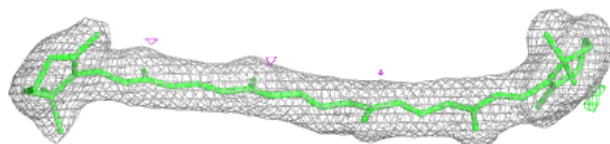
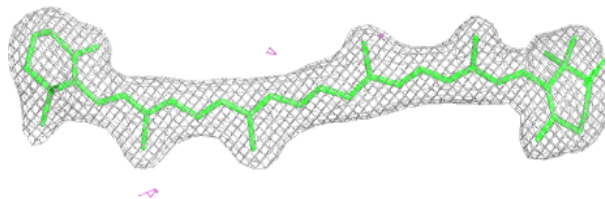
**Electron density around BCR B 619:**

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

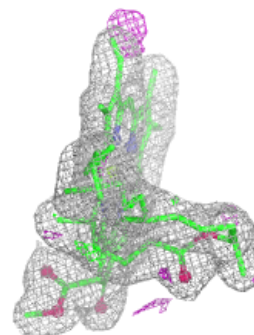
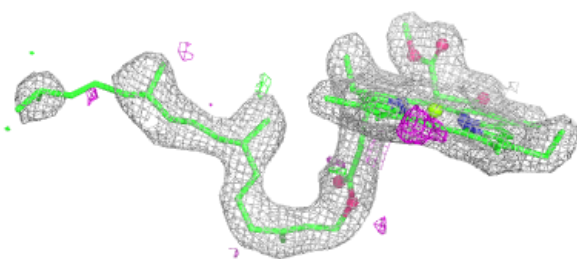
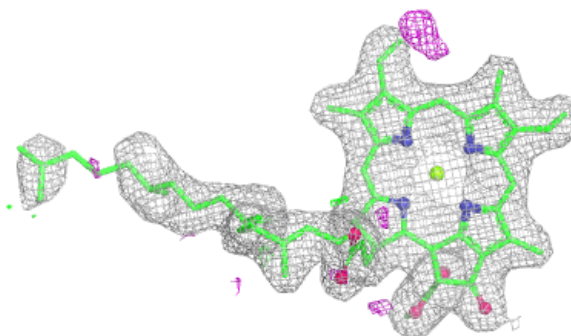


Electron density around BCR B 620:

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

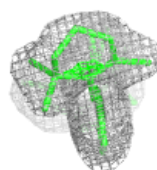
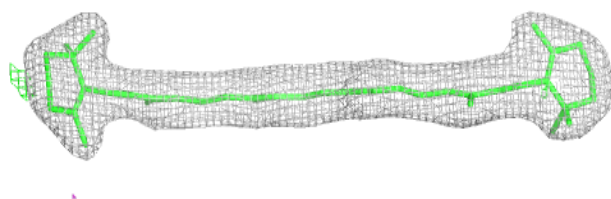
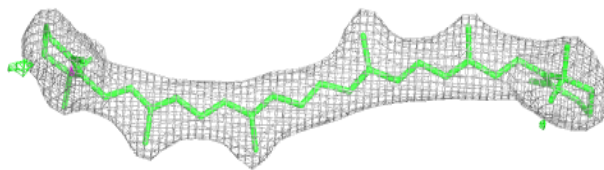
**Electron density around CLA A 407:**

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

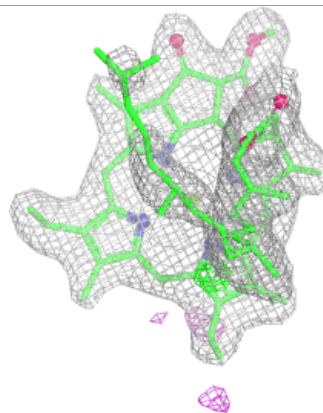
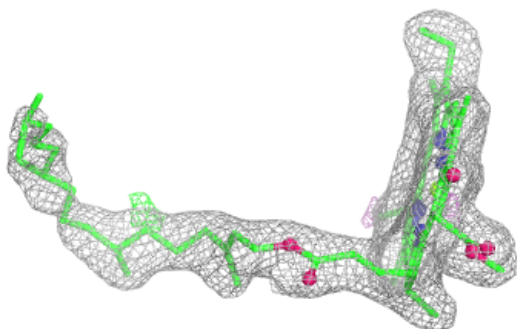
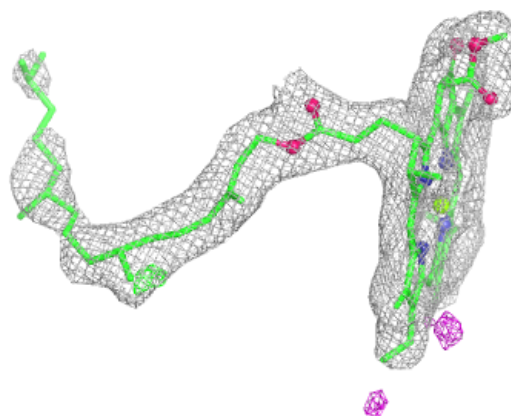


Electron density around BCR C 515:

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

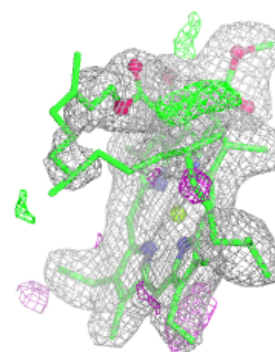
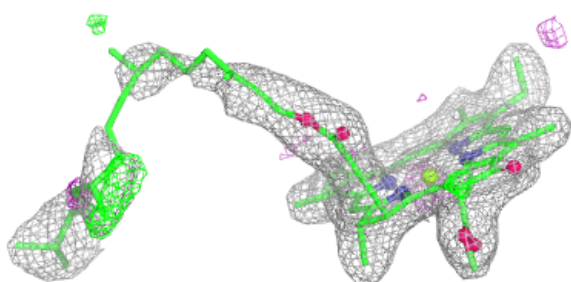
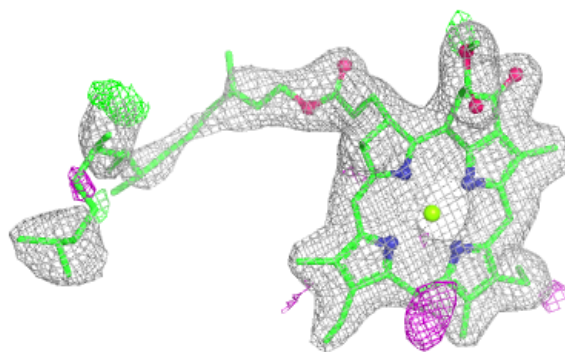
**Electron density around CLA D 403:**

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

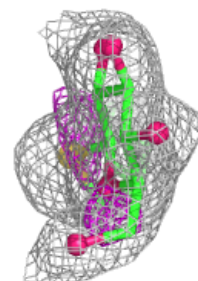
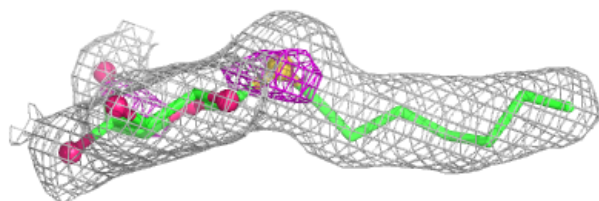
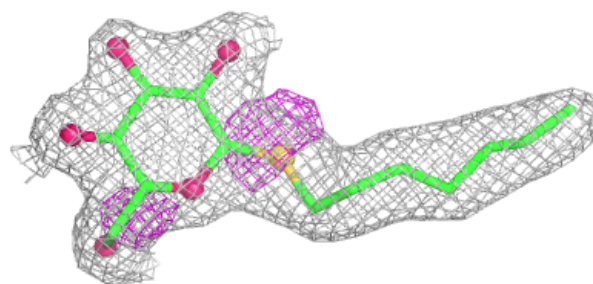


Electron density around CLA a 412:

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

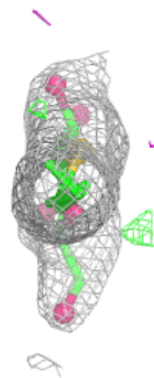
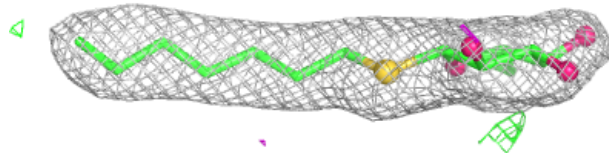
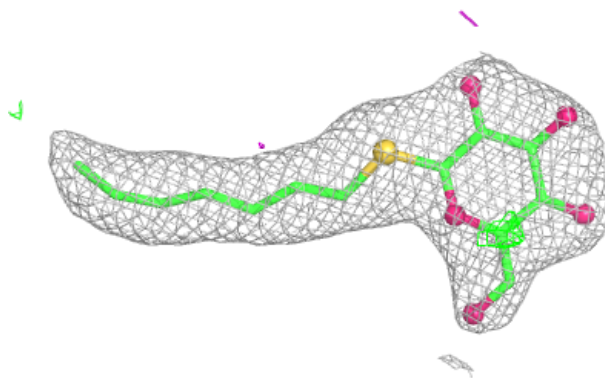
**Electron density around HTG b 601:**

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

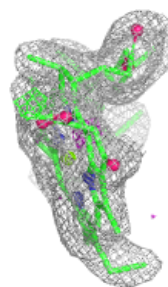
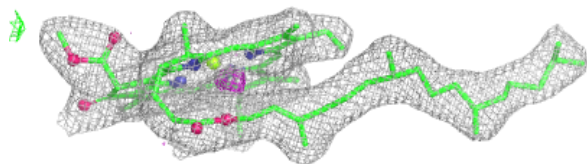
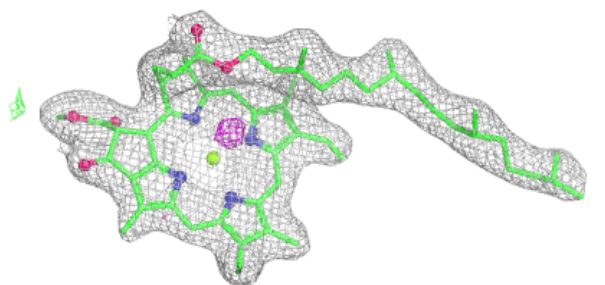


Electron density around HTG b 607:

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

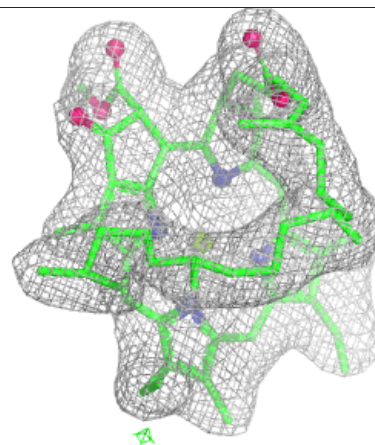
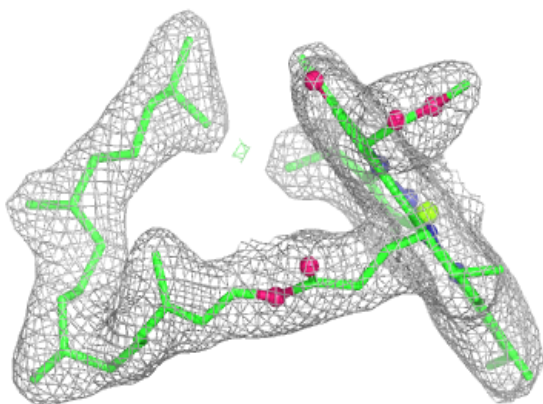
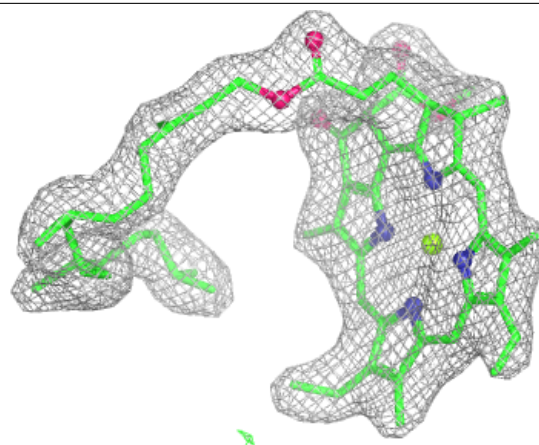
**Electron density around CLA C 501:**

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



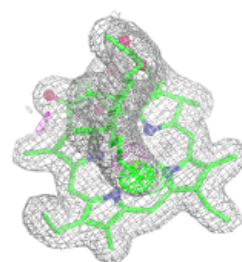
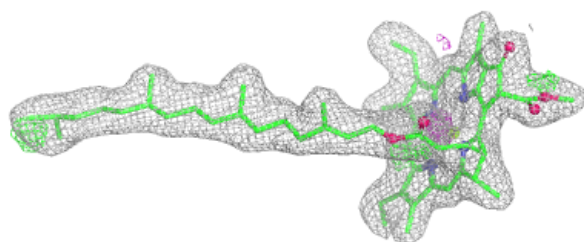
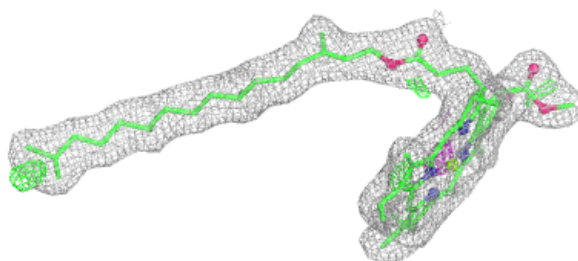
Electron density around CLA C 503:

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

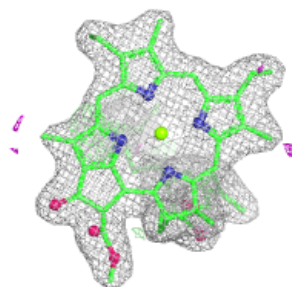
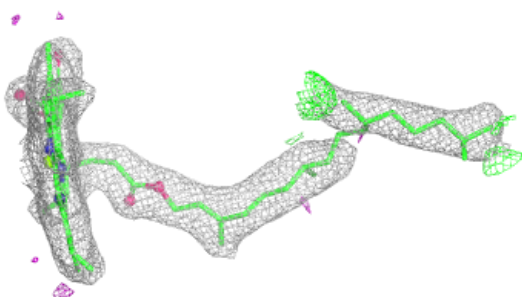
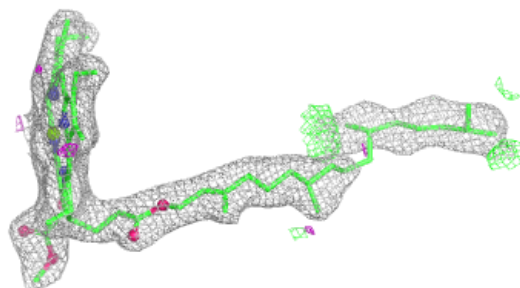


Electron density around CLA b 616:

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

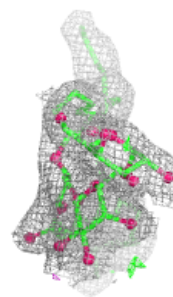
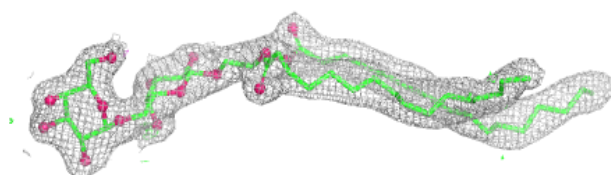
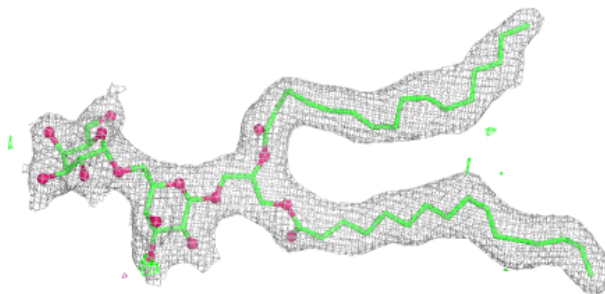
**Electron density around CLA B 607:**

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

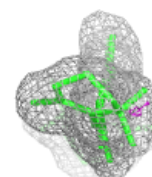
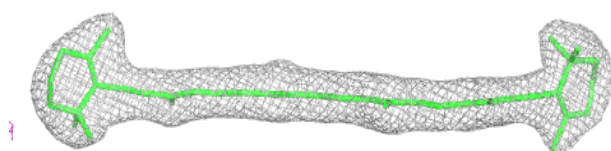
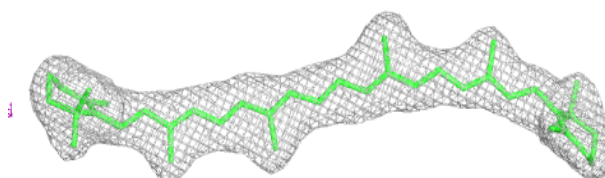


Electron density around DGD C 518:

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

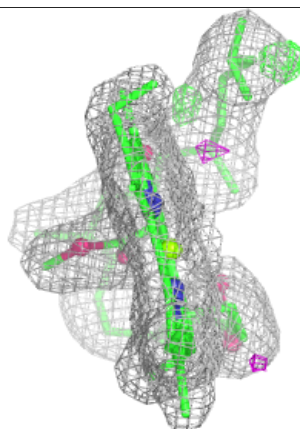
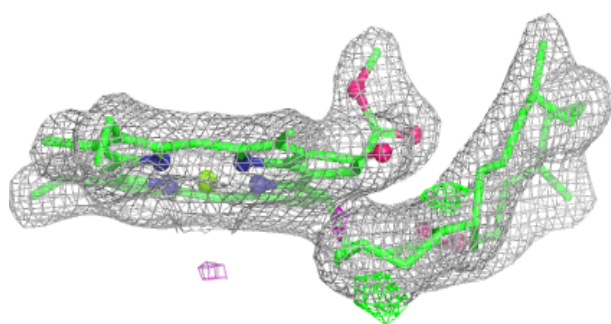
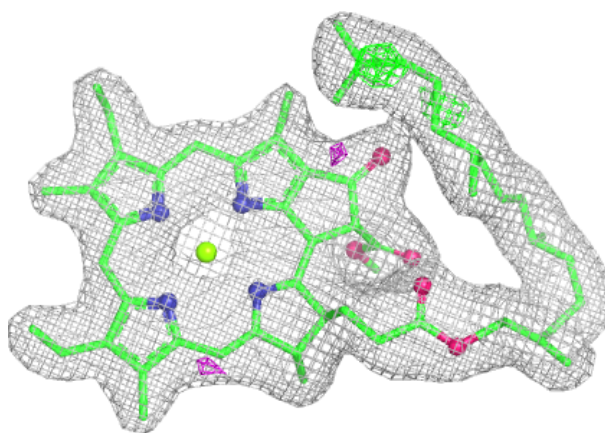
**Electron density around BCR c 519:**

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

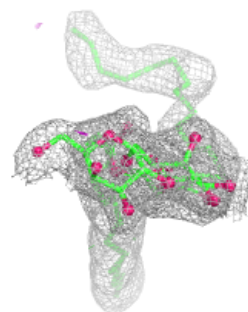
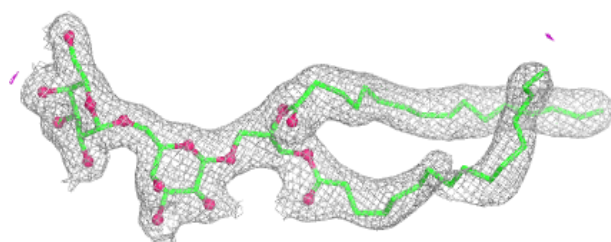
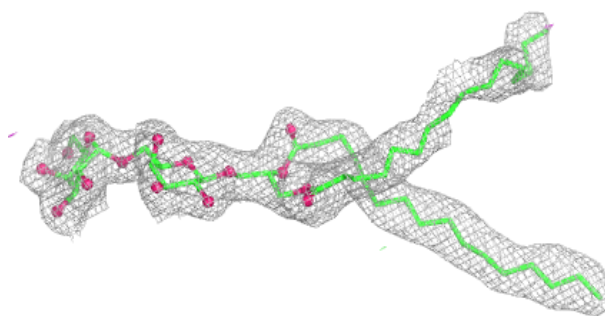


Electron density around CLA b 619:

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

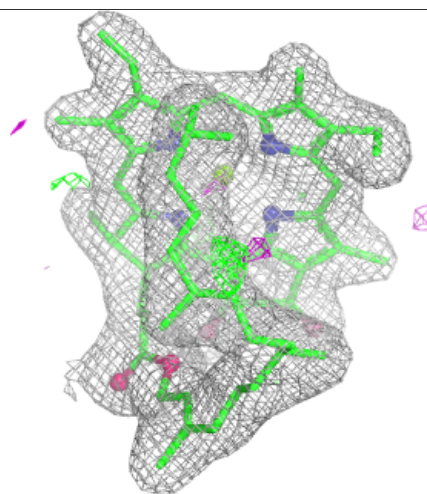
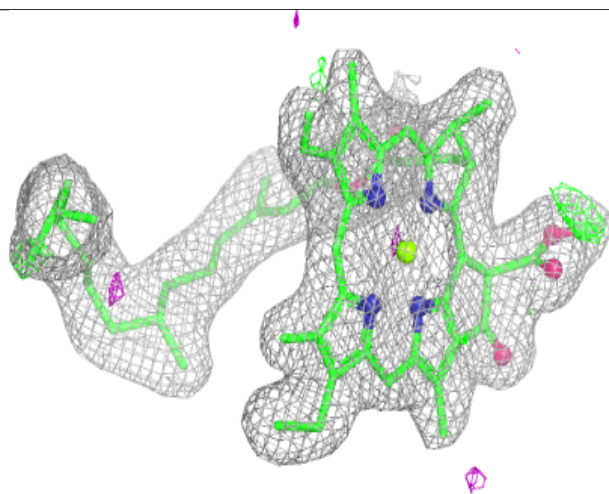
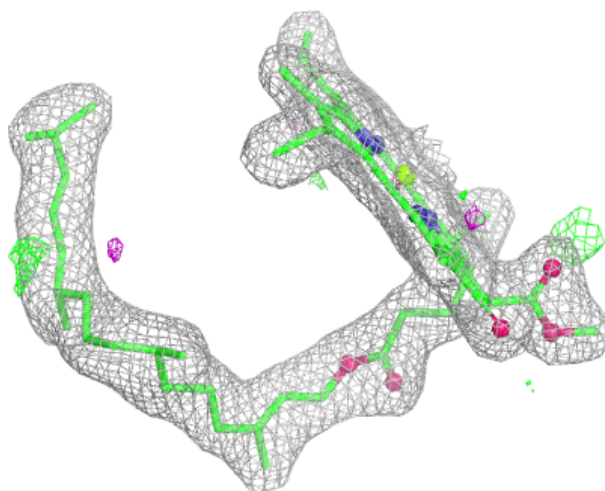
**Electron density around DGD c 520:**

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



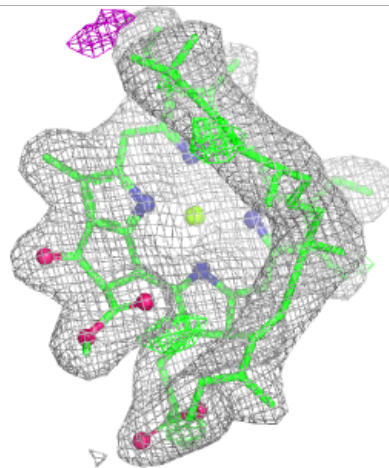
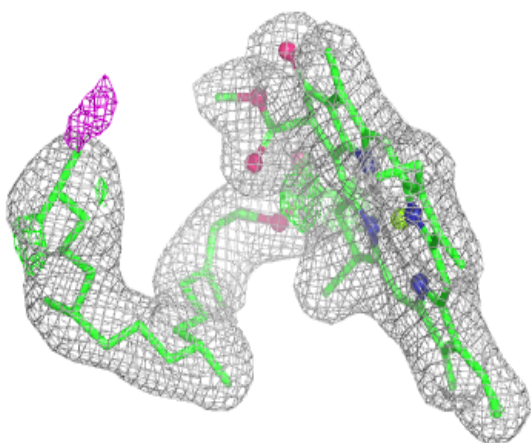
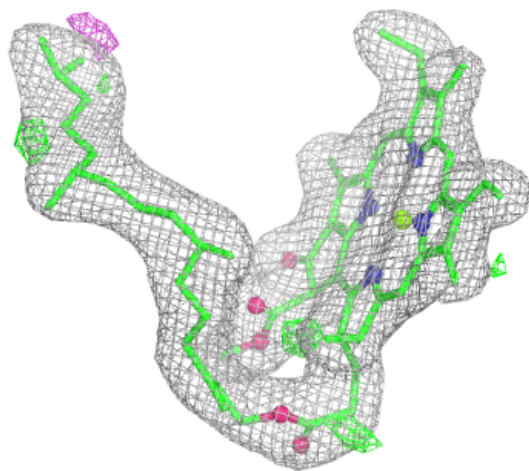
Electron density around CLA b 620:

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



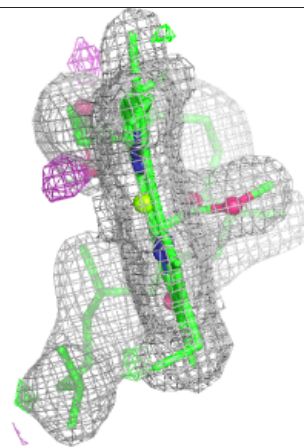
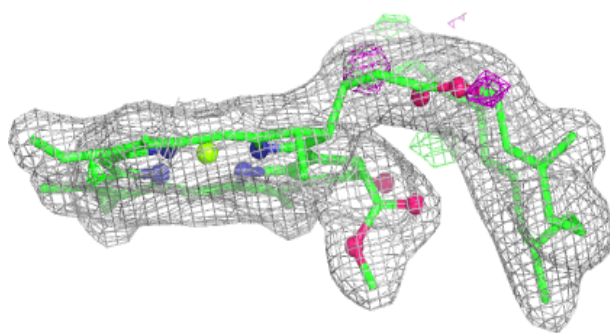
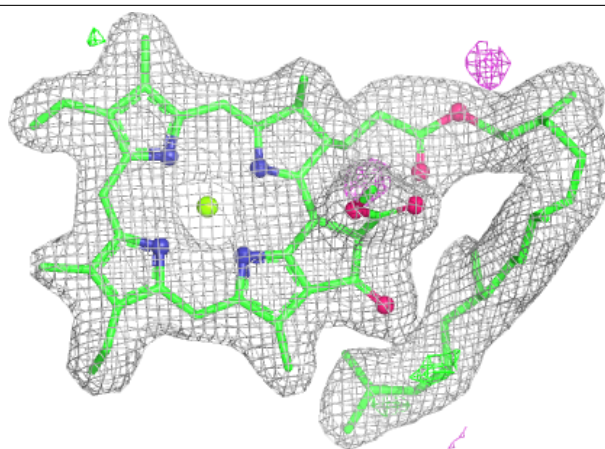
Electron density around CLA b 622:

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

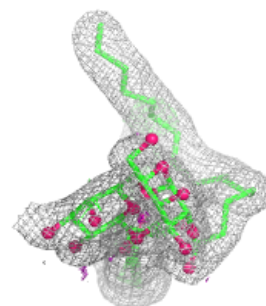
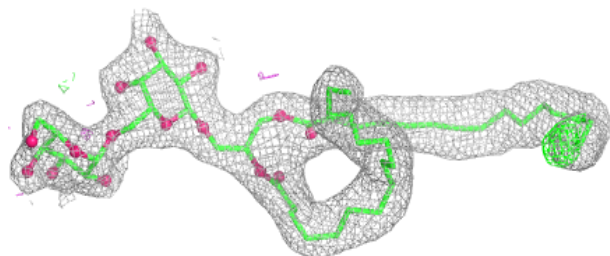
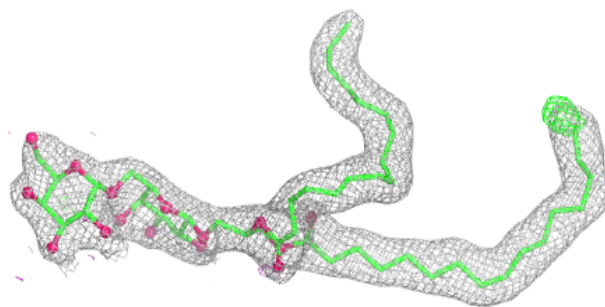


Electron density around CLA B 611:

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

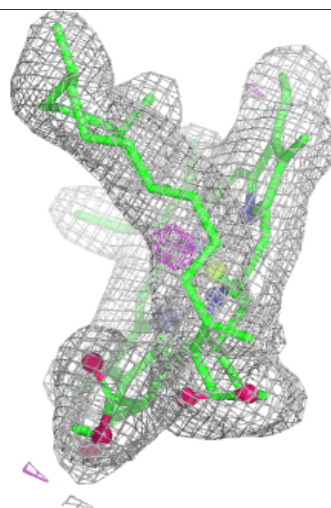
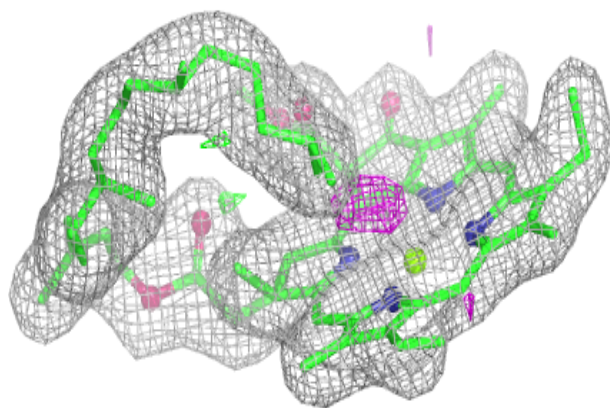
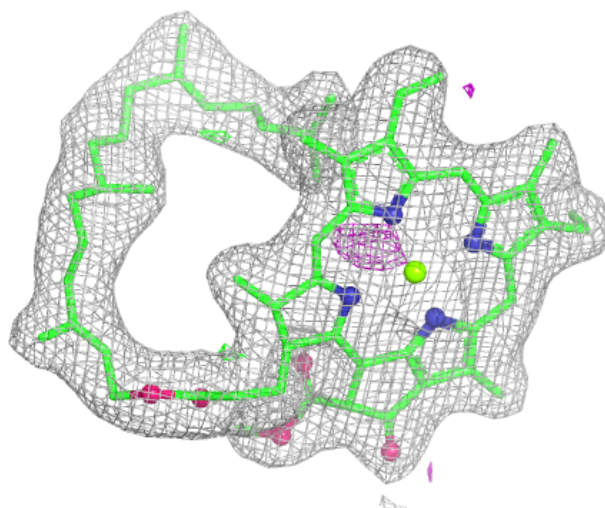
**Electron density around DGD h 102:**

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



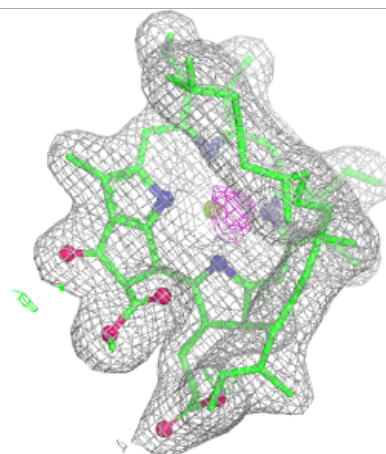
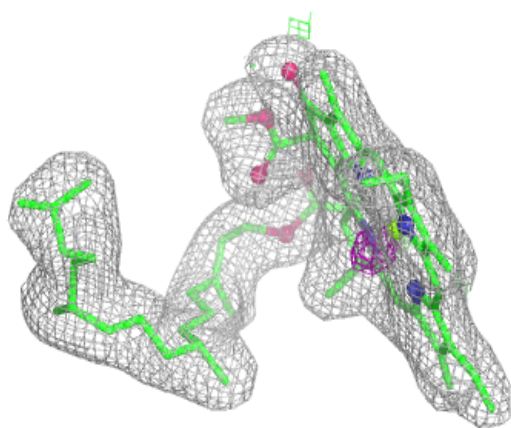
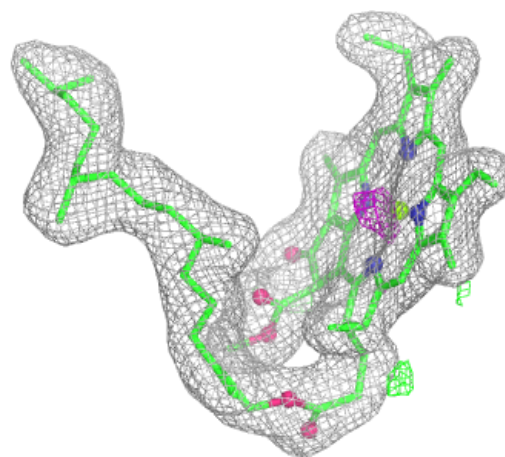
Electron density around CLA b 624:

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



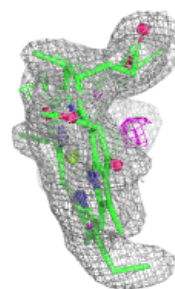
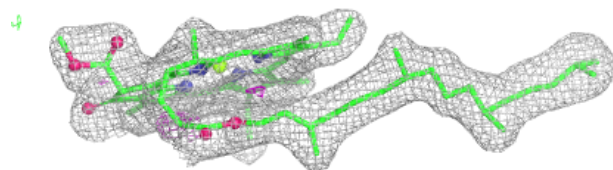
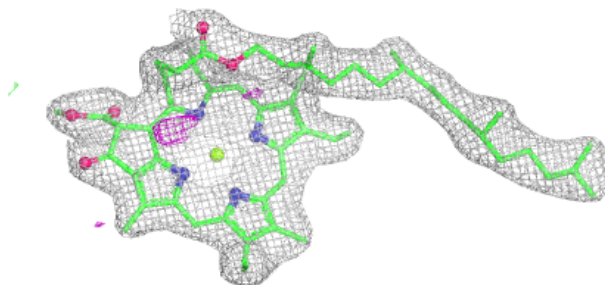
Electron density around CLA B 614:

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

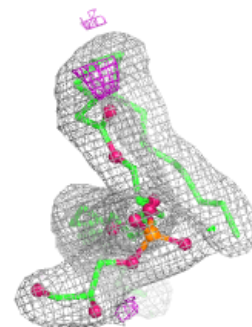
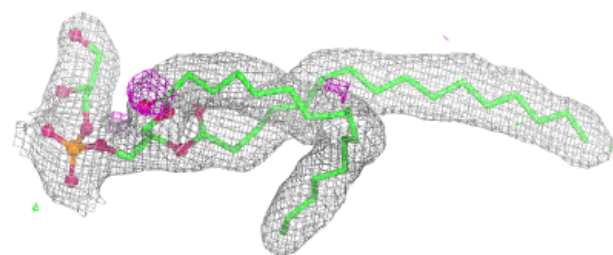
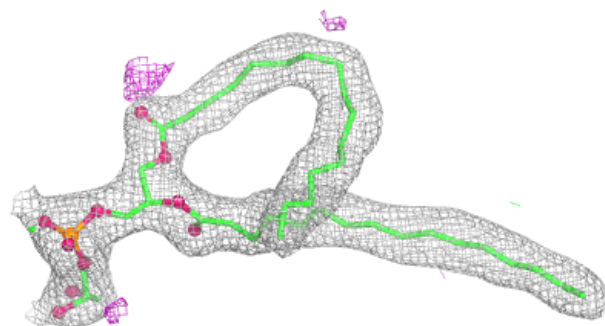


Electron density around CLA c 506:

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

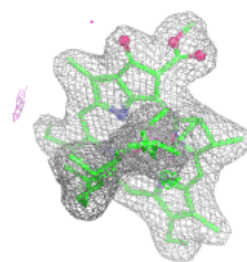
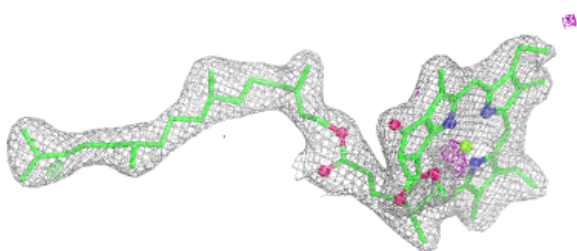
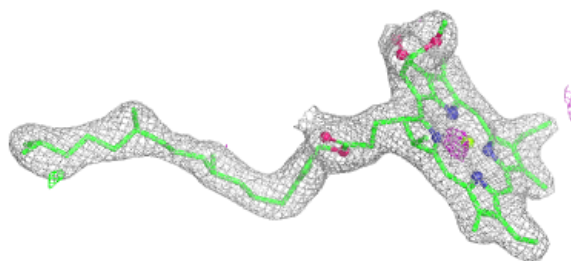
**Electron density around LHG d 406:**

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



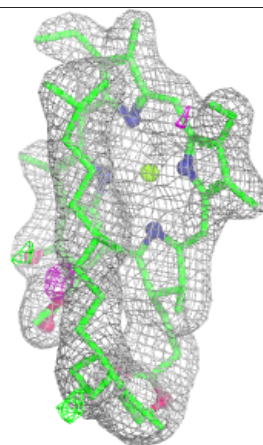
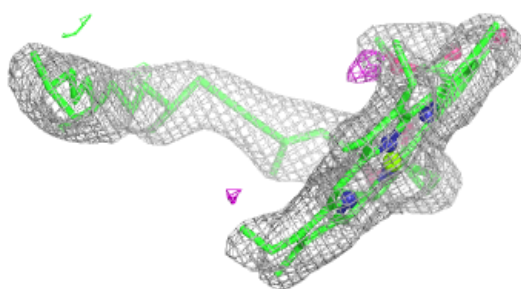
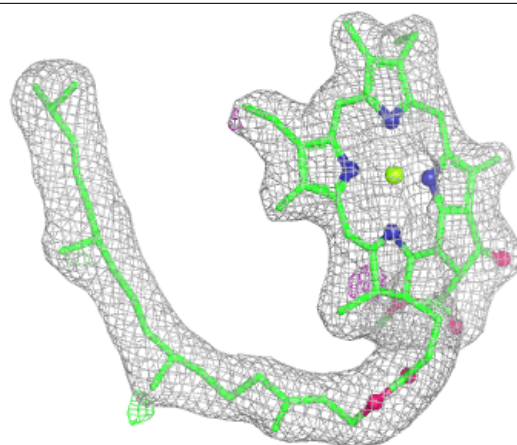
Electron density around CLA c 507:

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

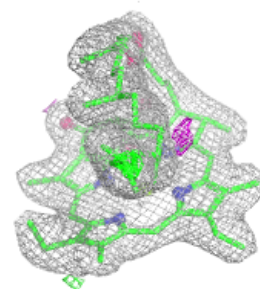
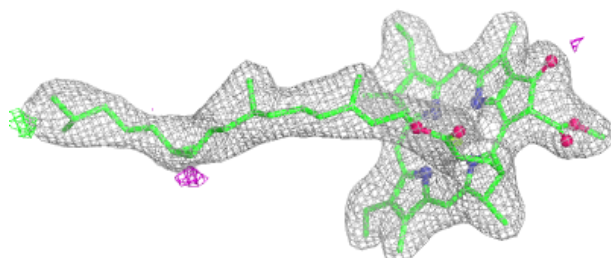
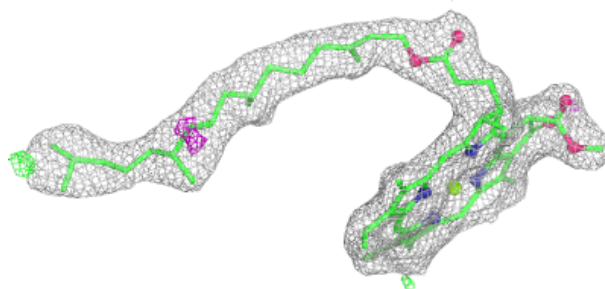


Electron density around CLA C 507:

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

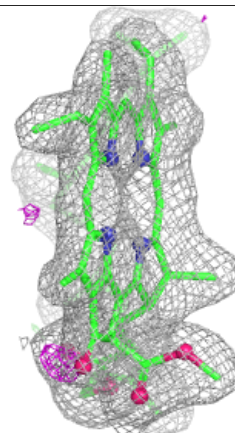
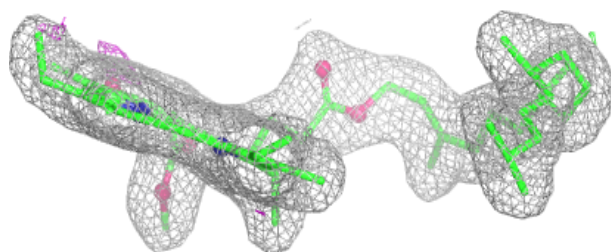
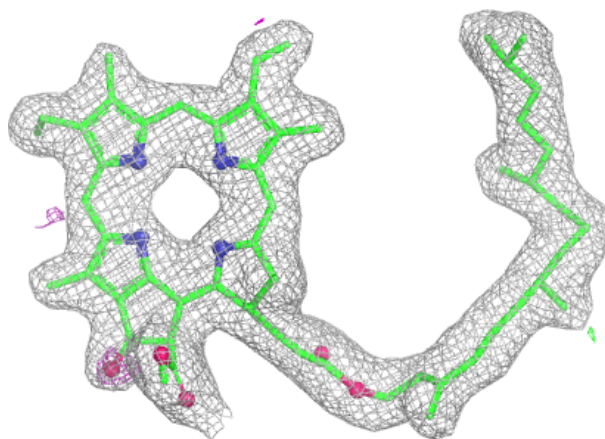
**Electron density around CLA c 509:**

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

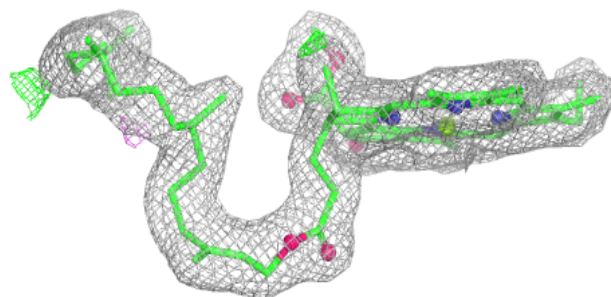
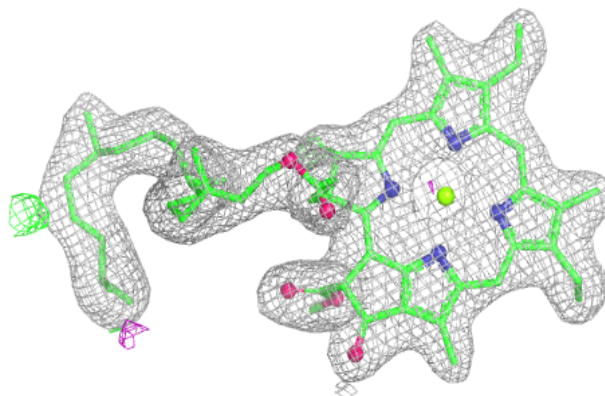


Electron density around PHO a 411:

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

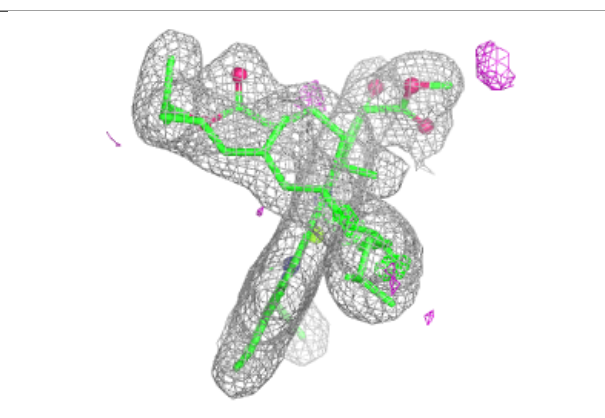
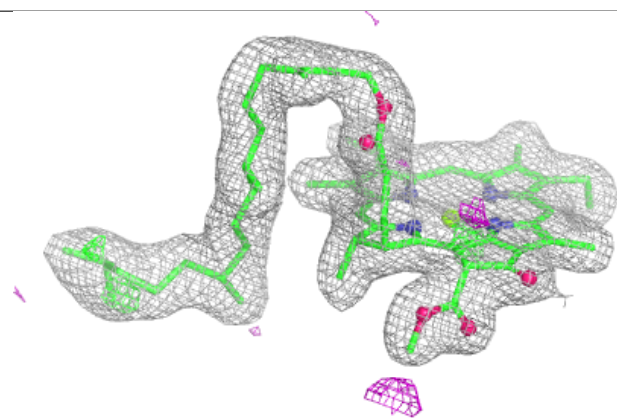
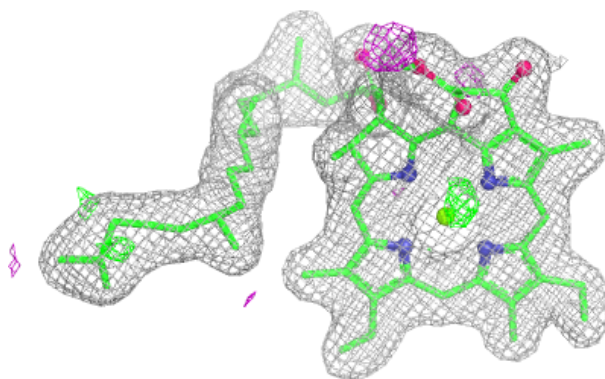
**Electron density around CLA B 613:**

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

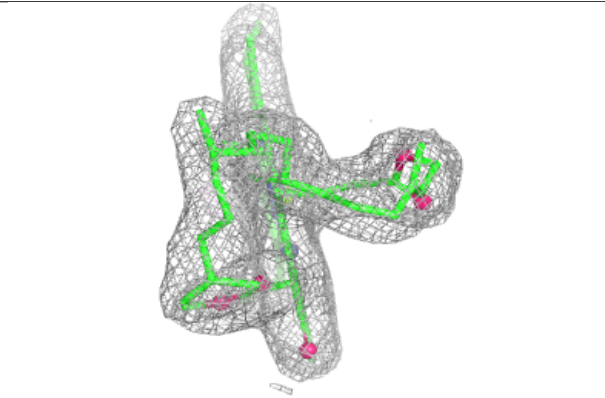
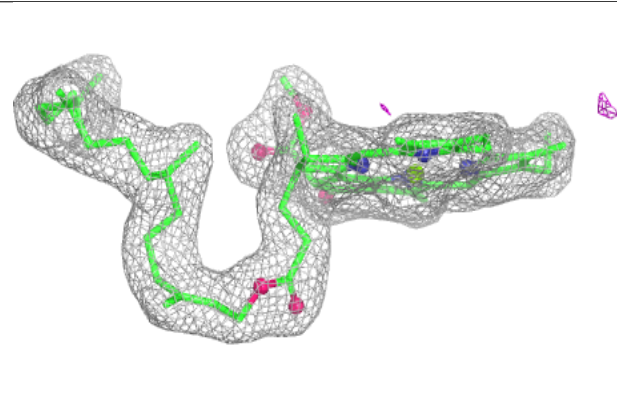
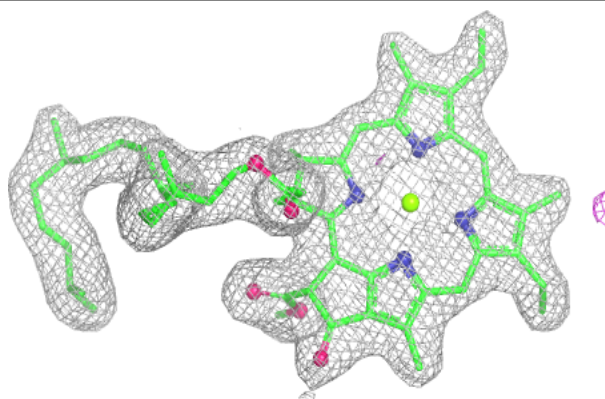


Electron density around CLA A 406:

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

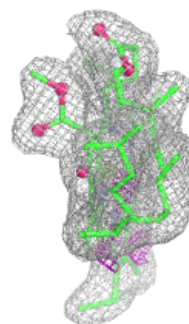
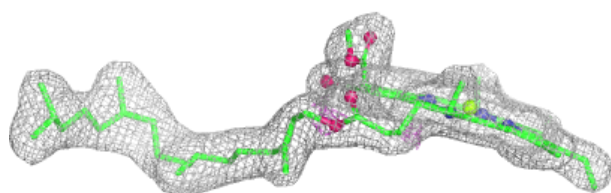
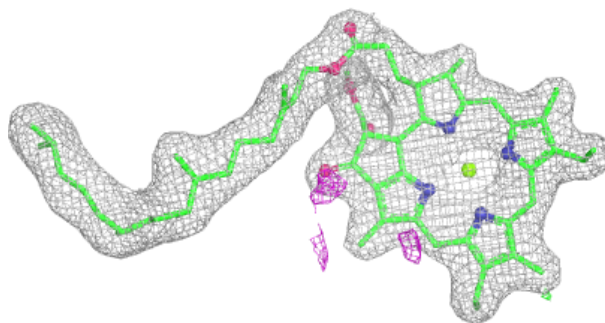
**Electron density around CLA b 621:**

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



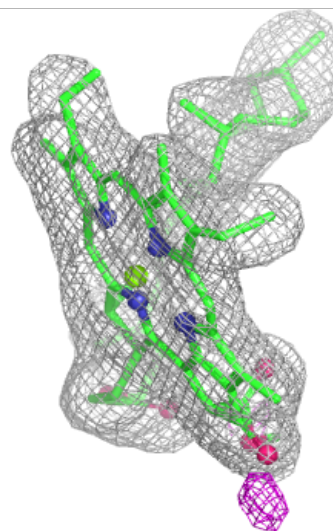
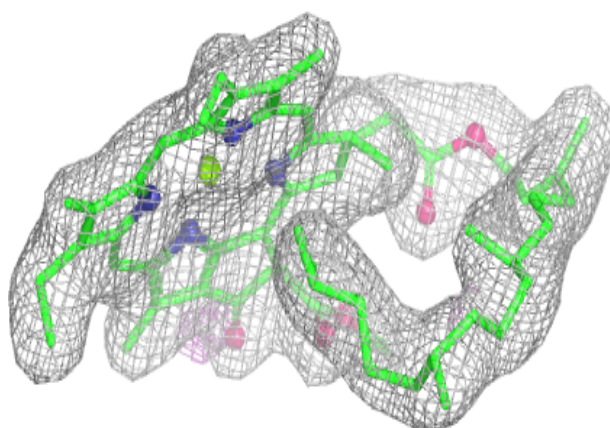
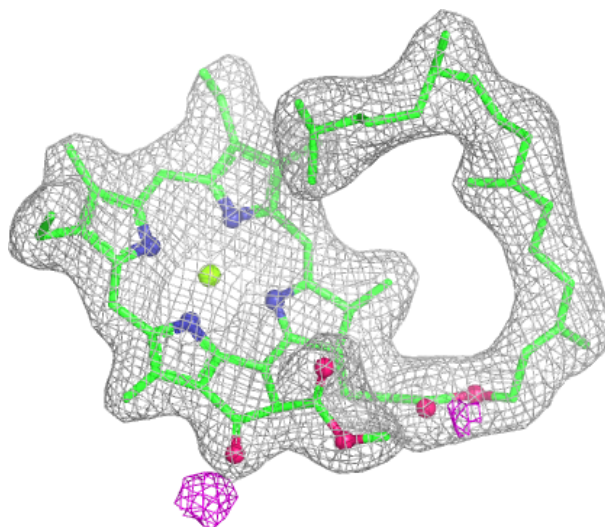
Electron density around CLA B 603:

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



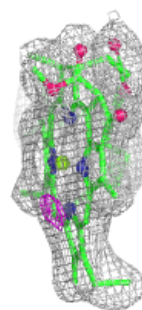
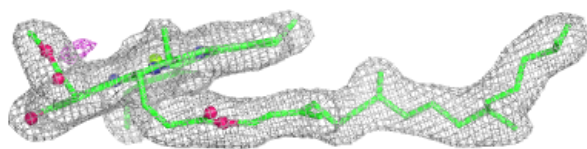
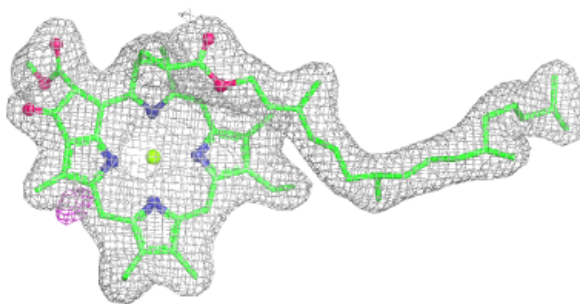
Electron density around CLA B 616:

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

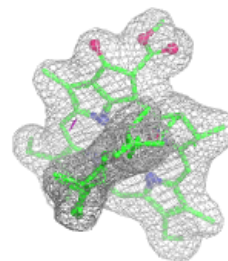
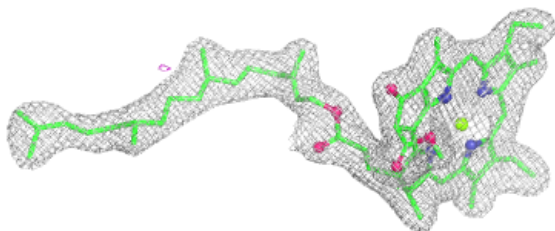
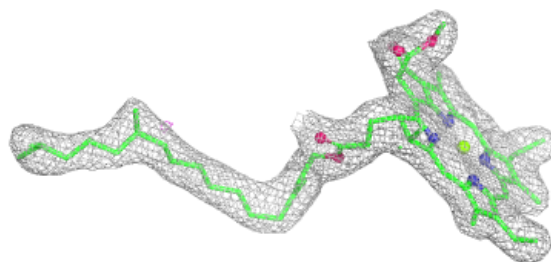


Electron density around CLA B 604:

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

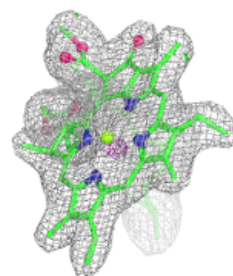
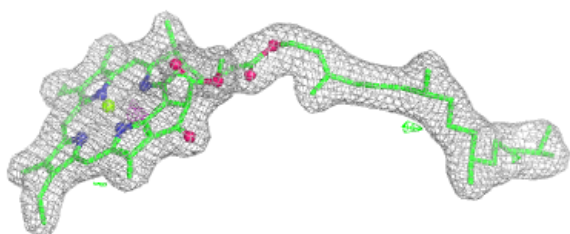
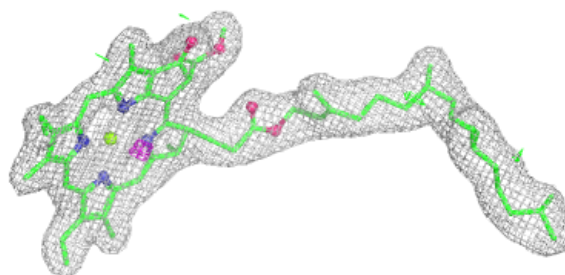
**Electron density around CLA C 502:**

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

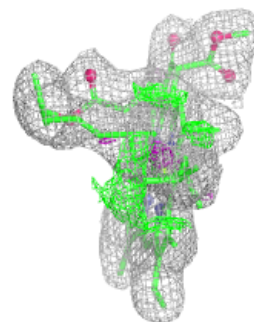
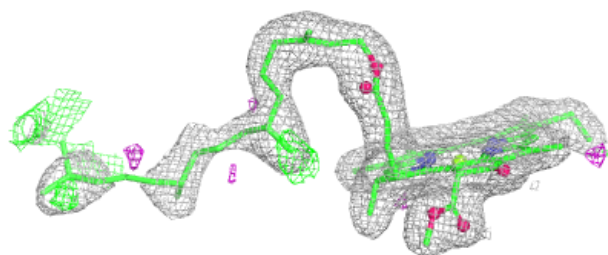
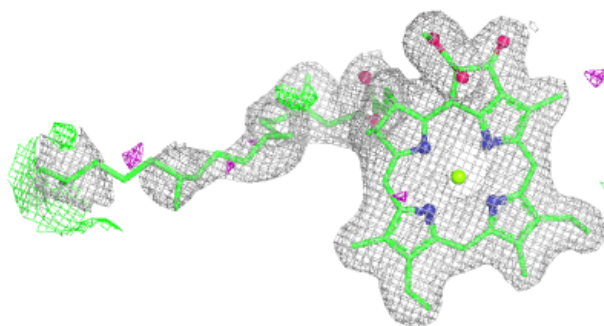


Electron density around CLA a 409:

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

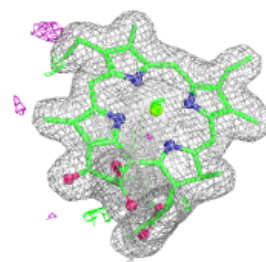
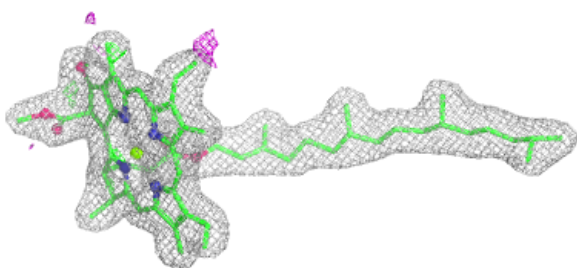
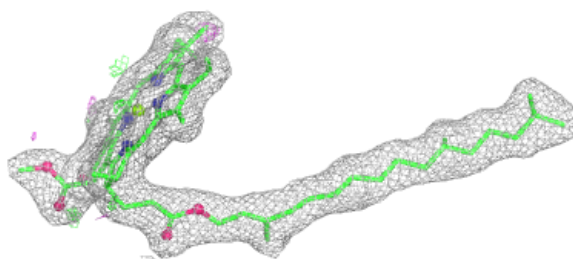
**Electron density around CLA a 410:**

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

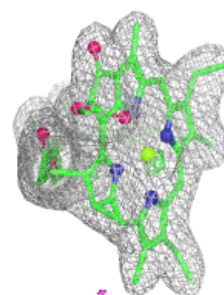
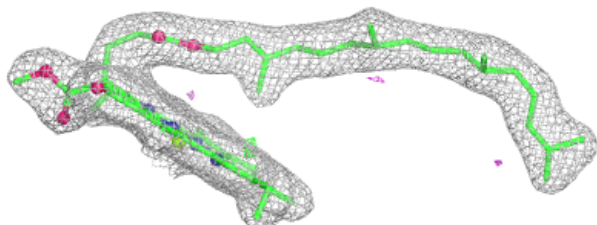
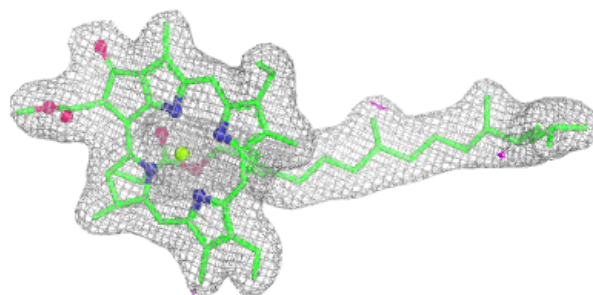


Electron density around CLA B 608:

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

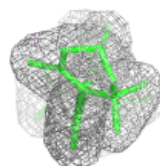
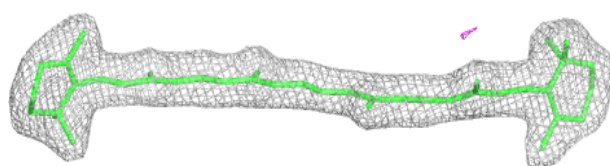
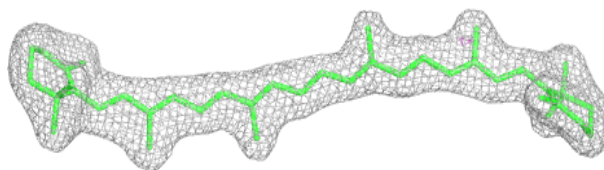
**Electron density around CLA B 609:**

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

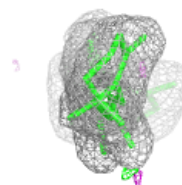
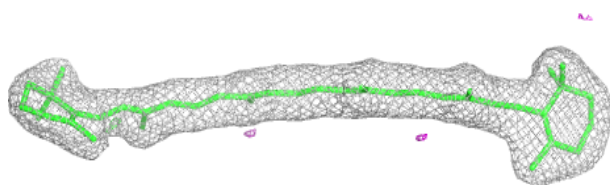
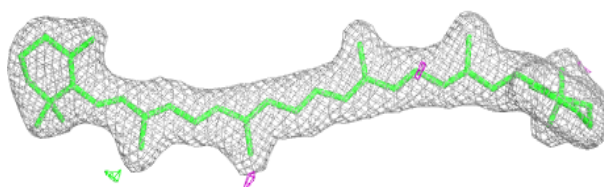


Electron density around BCR a 413:

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

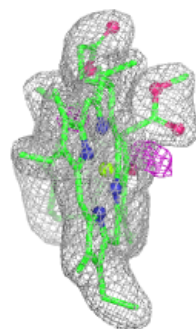
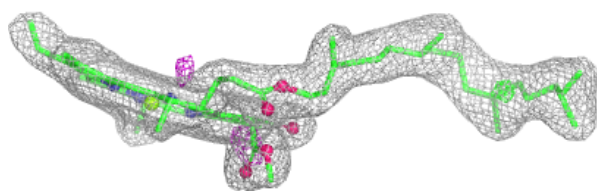
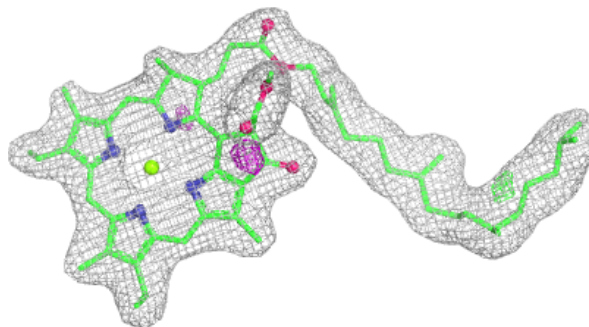
**Electron density around BCR b 626:**

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

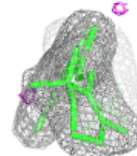
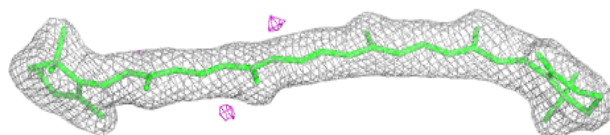
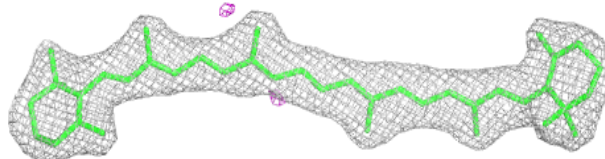


Electron density around CLA b 611:

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

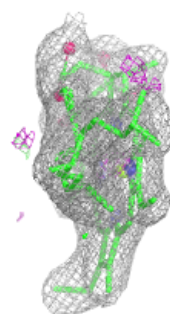
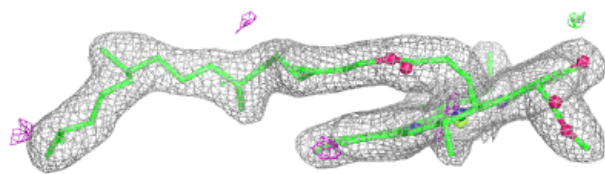
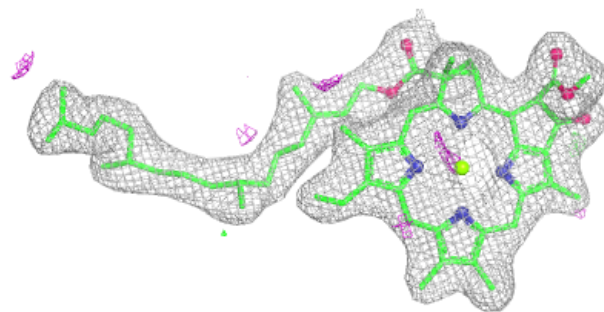
**Electron density around BCR b 628:**

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

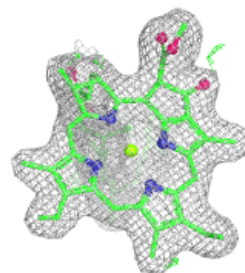
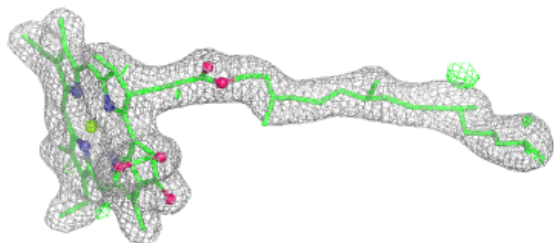
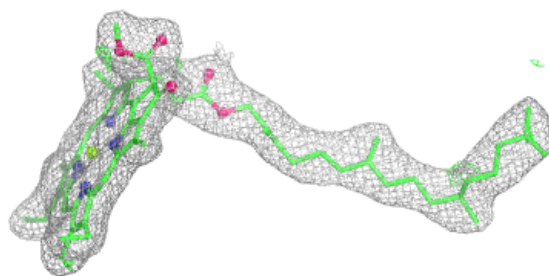


Electron density around CLA b 612:

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

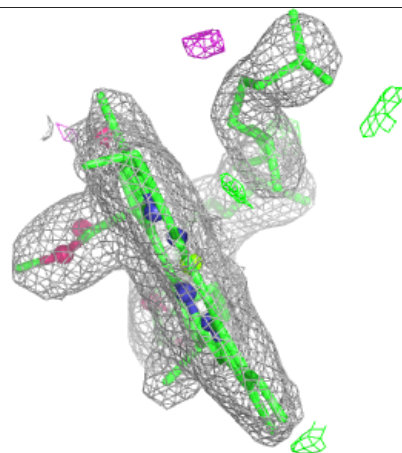
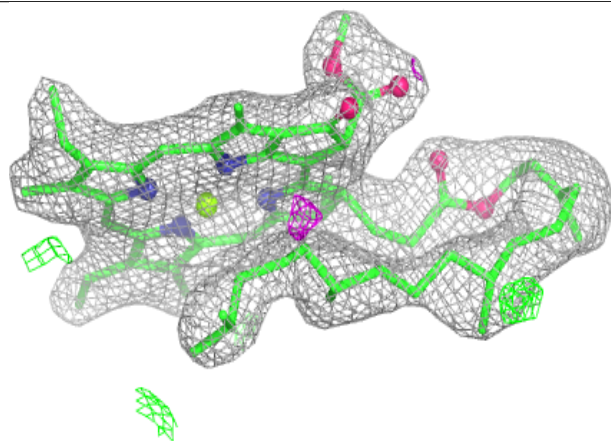
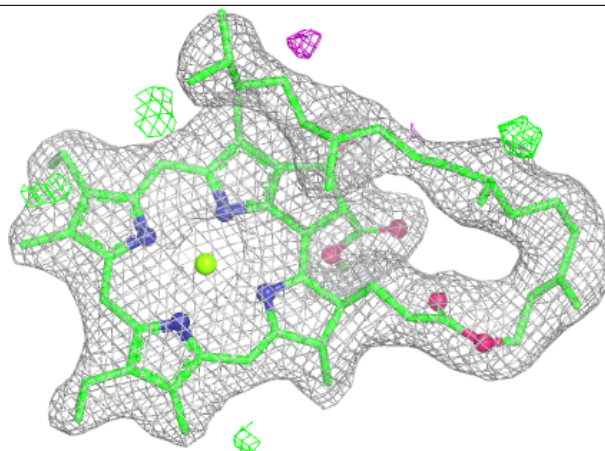
**Electron density around CLA b 613:**

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



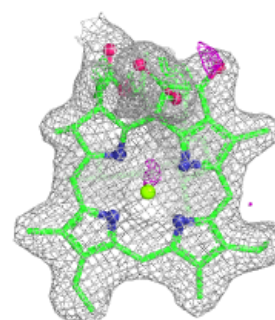
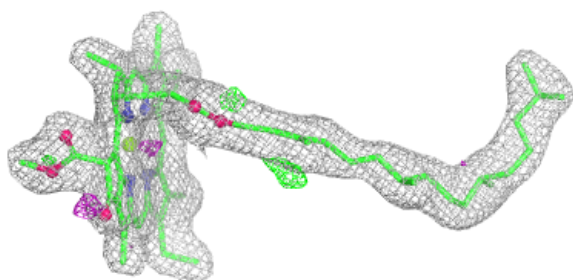
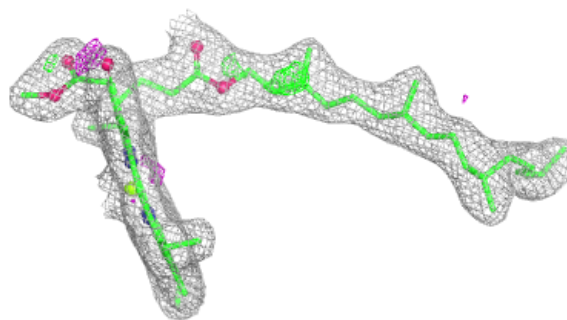
Electron density around CLA c 514:

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

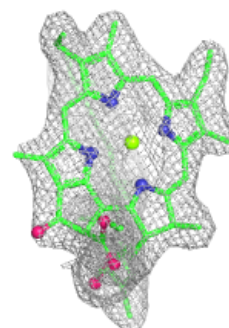
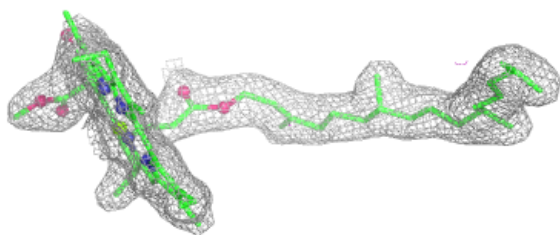
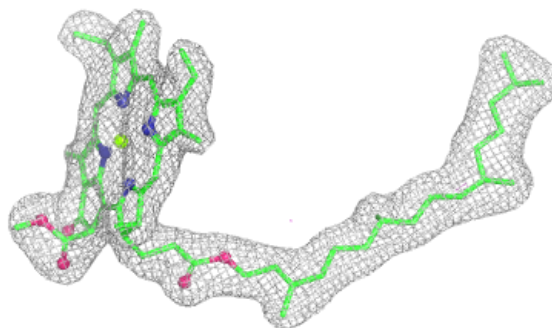


Electron density around CLA b 614:

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

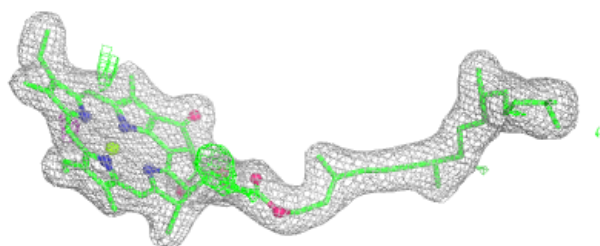
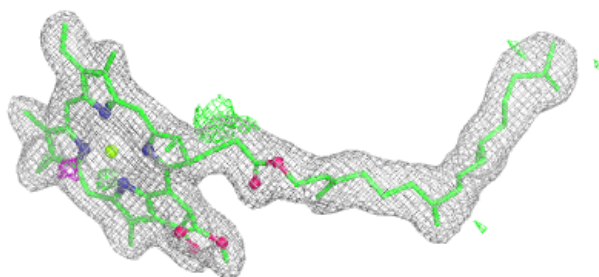
**Electron density around CLA B 610:**

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

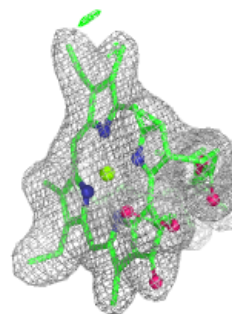
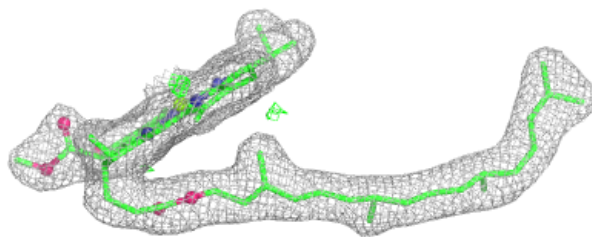
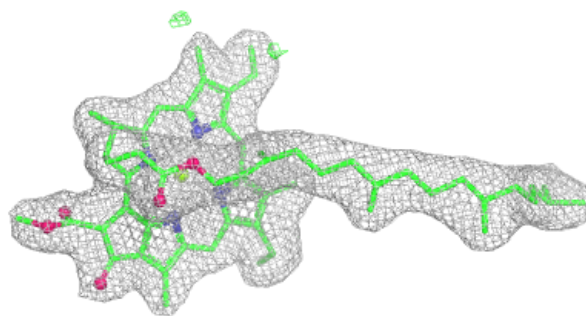


Electron density around CLA A 405:

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

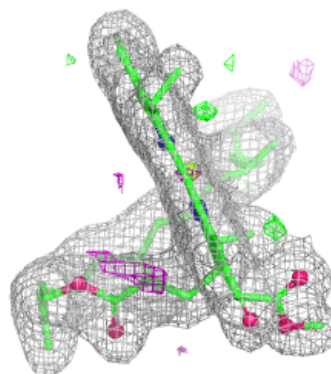
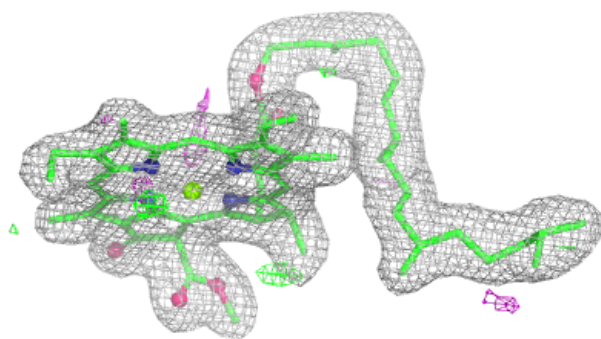
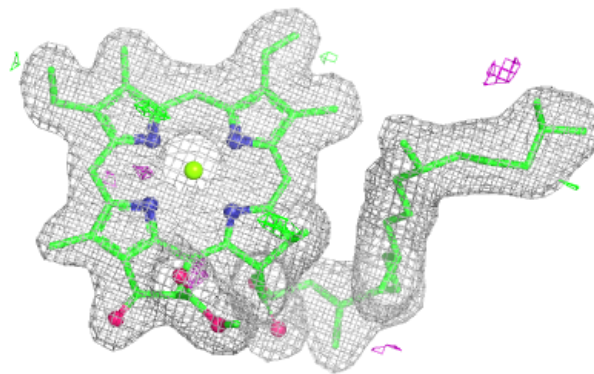
**Electron density around CLA b 617:**

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



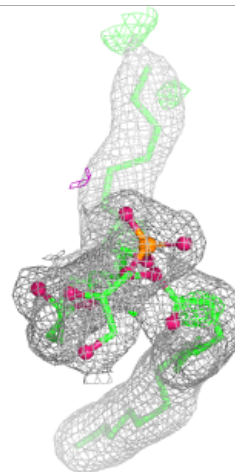
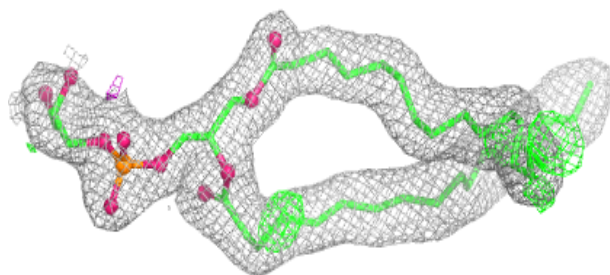
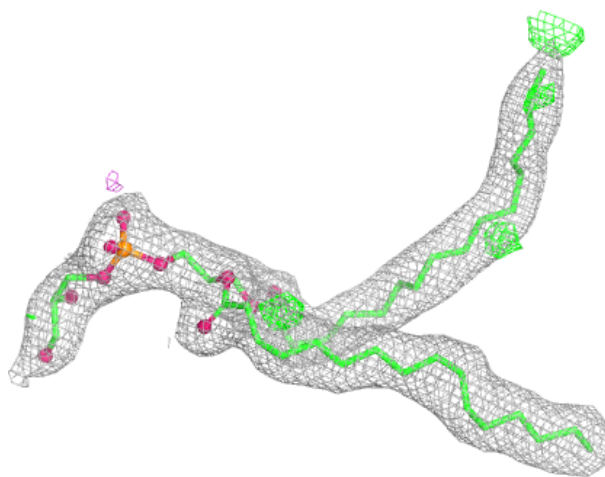
Electron density around CLA d 401:

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



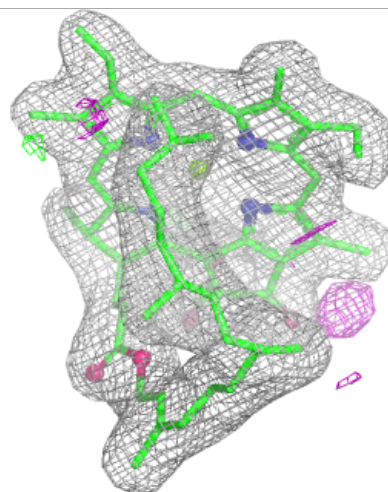
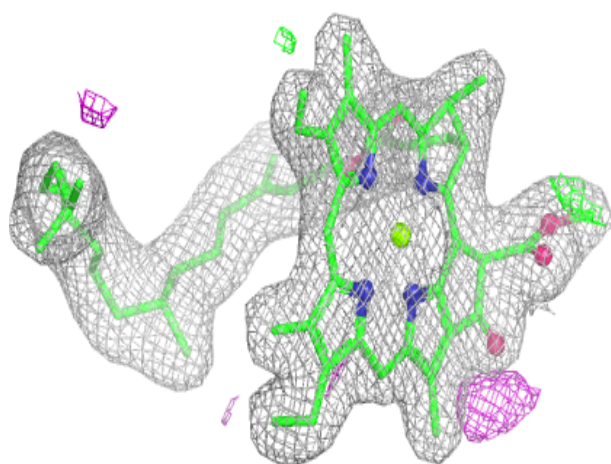
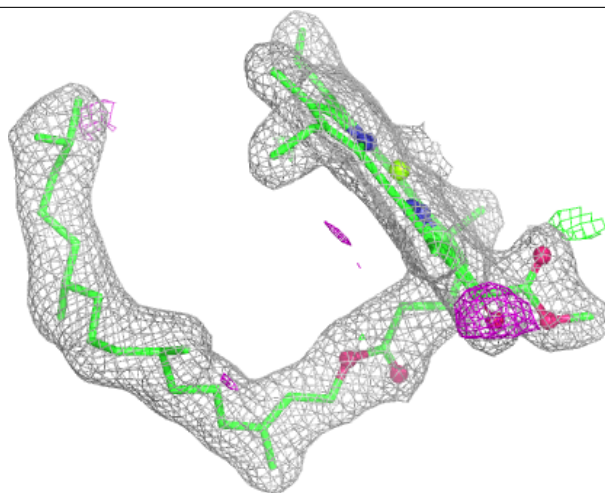
Electron density around LHG D 408:

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



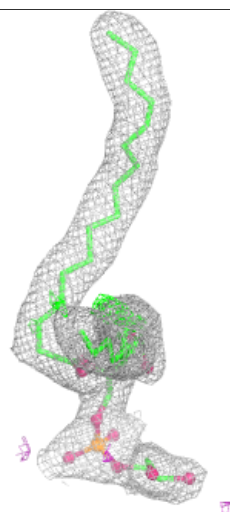
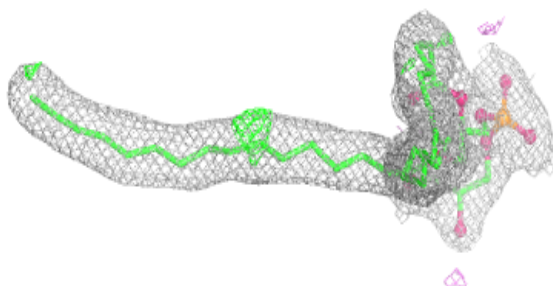
Electron density around CLA B 612:

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



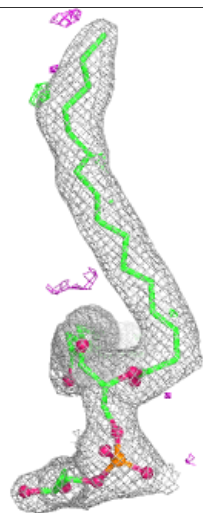
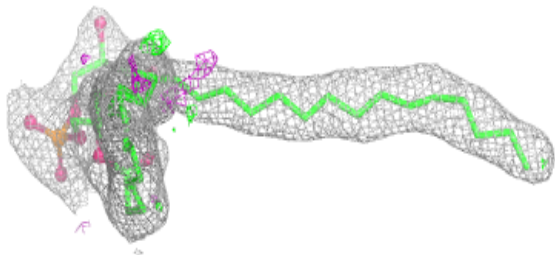
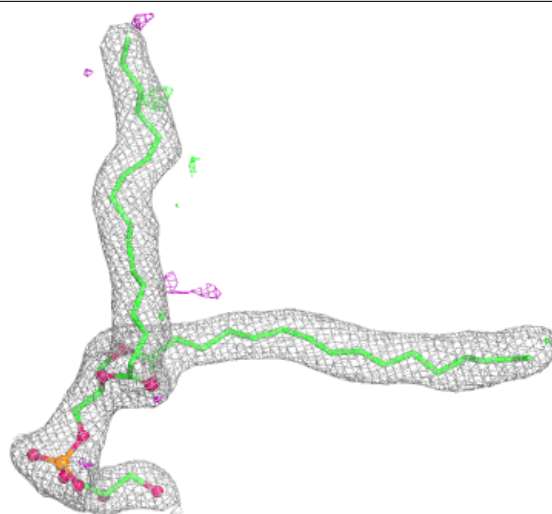
Electron density around LHG L 101:

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



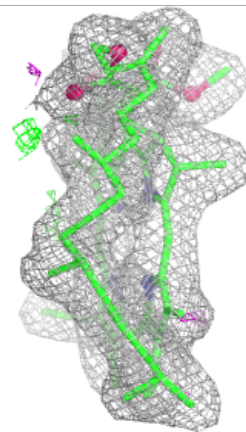
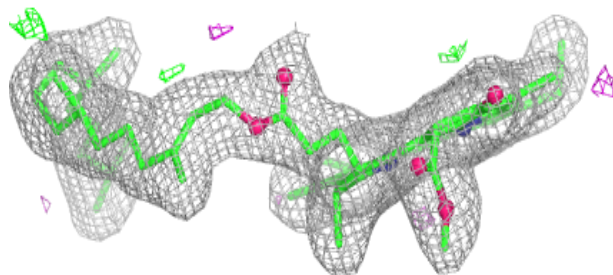
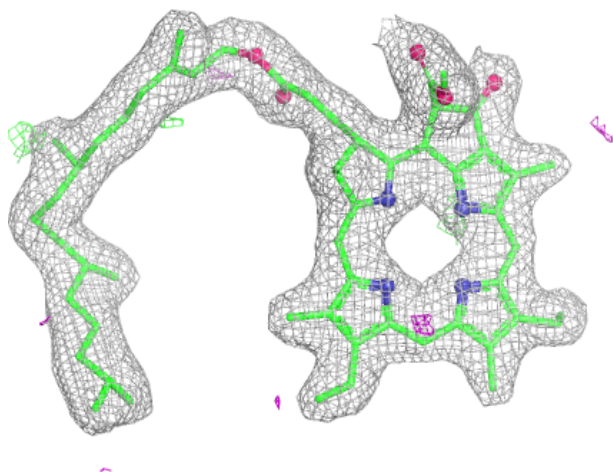
Electron density around LHG b 634:

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



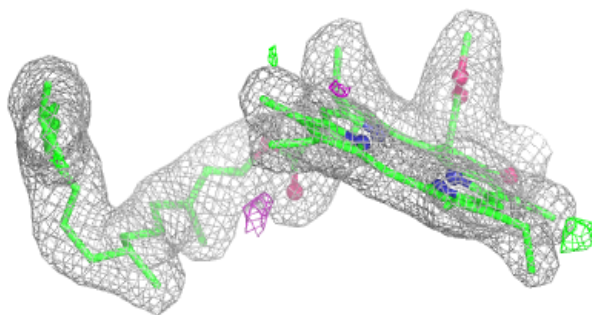
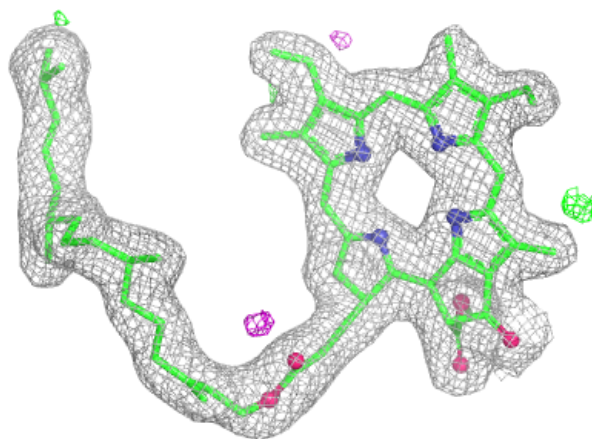
Electron density around PHO A 408:

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

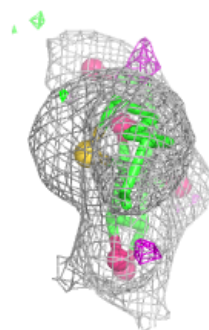
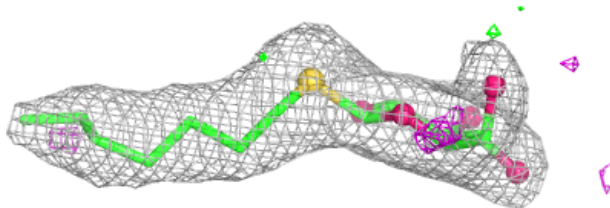
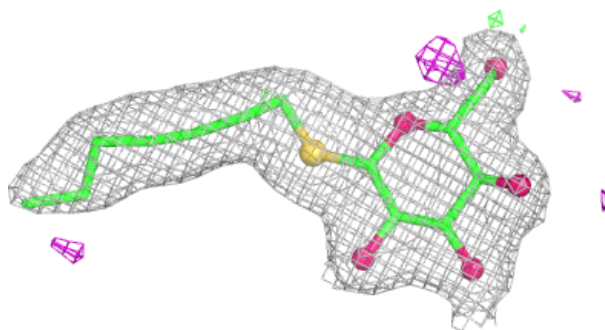


Electron density around PHO A 409 (A):

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

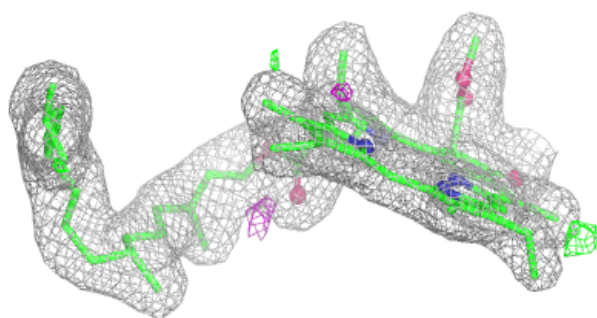
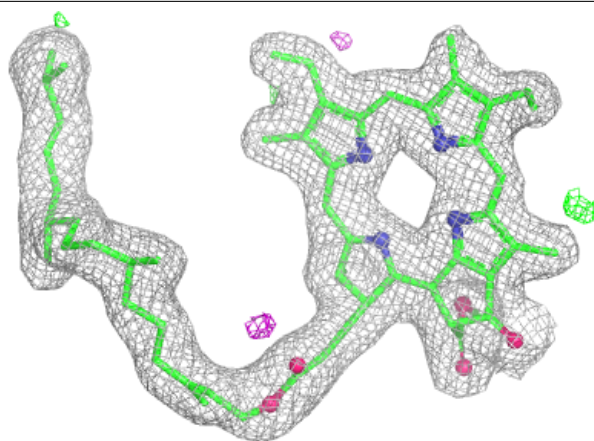
**Electron density around HTG B 623:**

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



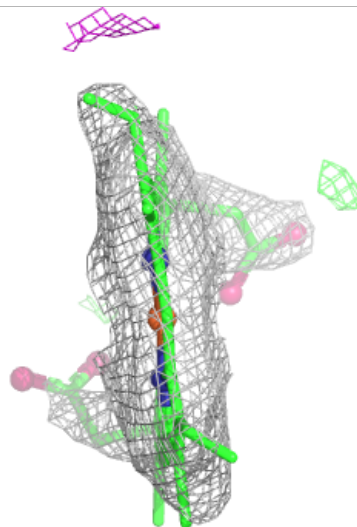
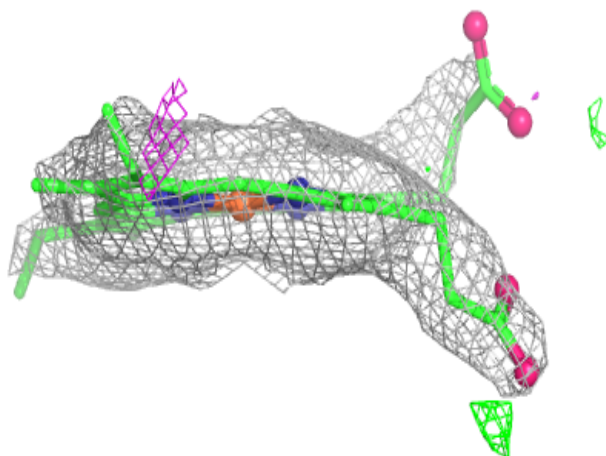
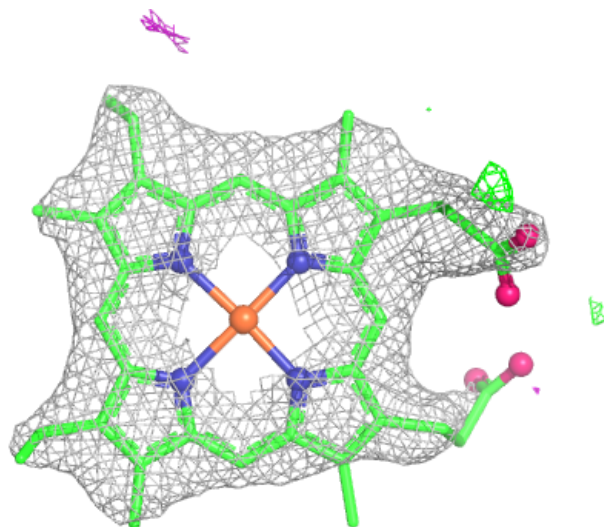
Electron density around PHO A 409 (B):

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



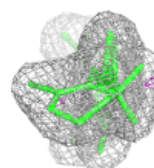
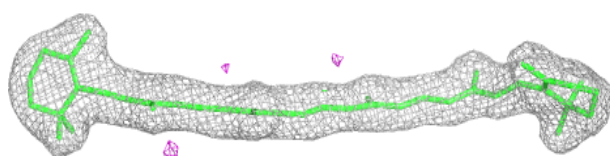
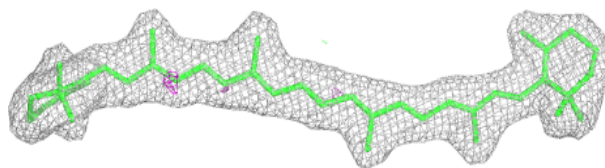
Electron density around HEM e 103:

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

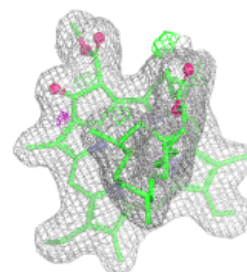
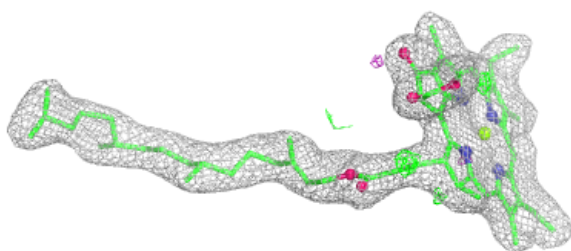
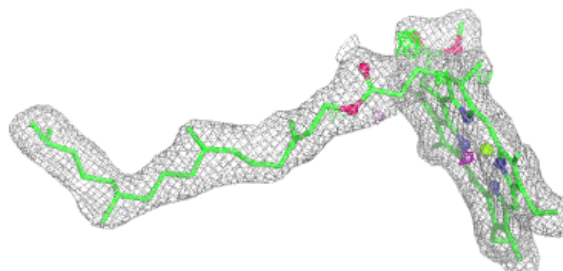


Electron density around BCR B 618:

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

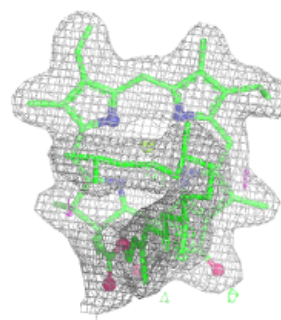
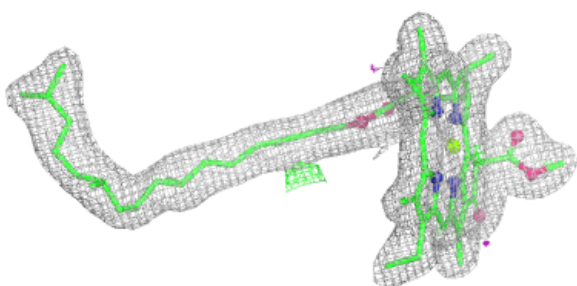
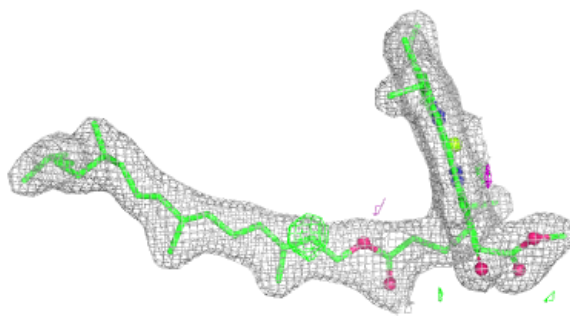
**Electron density around CLA B 605:**

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



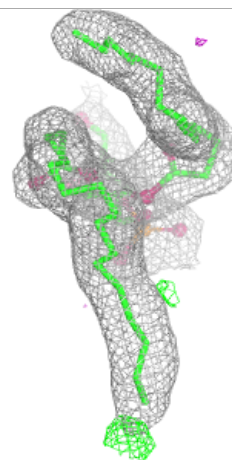
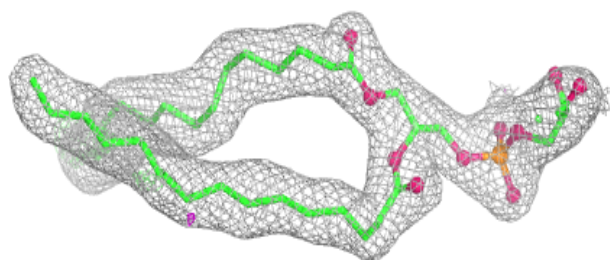
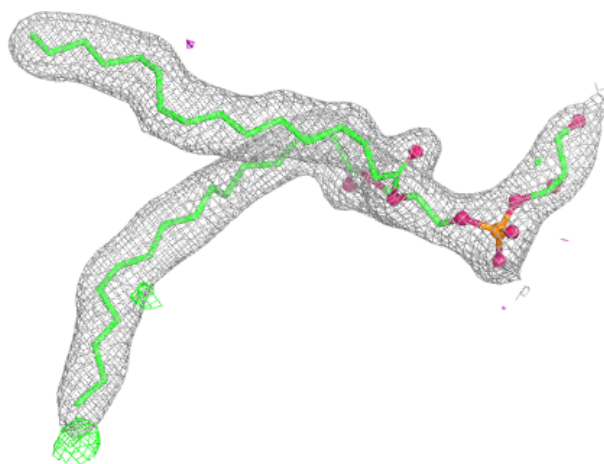
Electron density around CLA B 606:

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



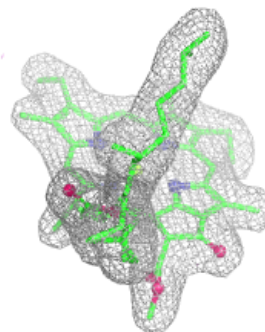
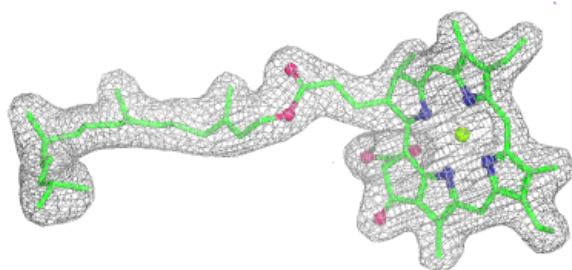
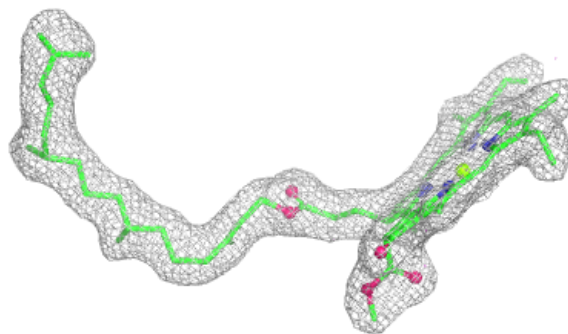
Electron density around LHG d 407:

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

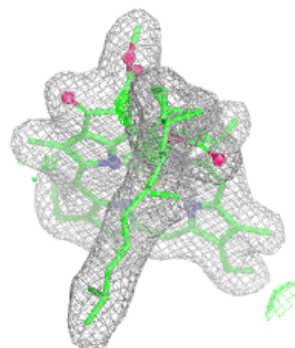
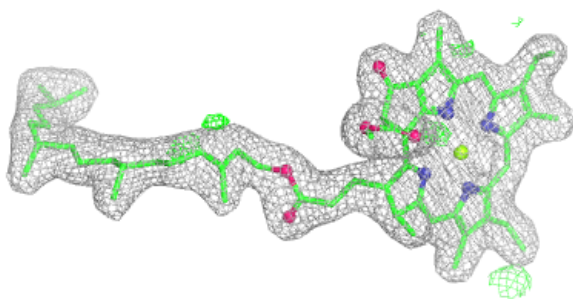
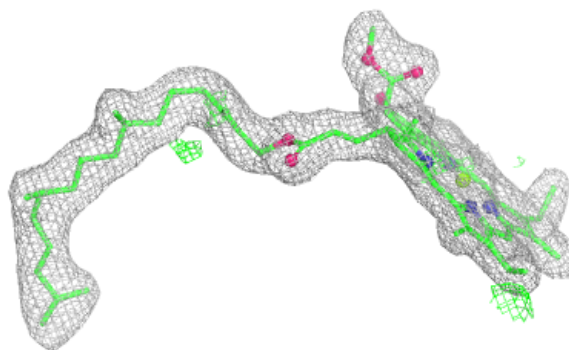


Electron density around CLA d 402:

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

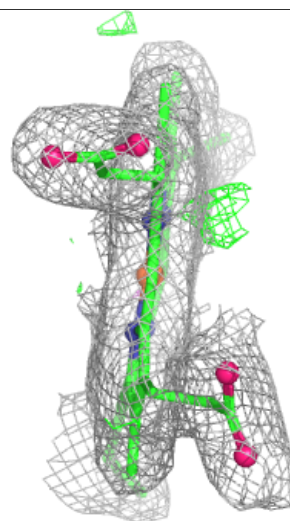
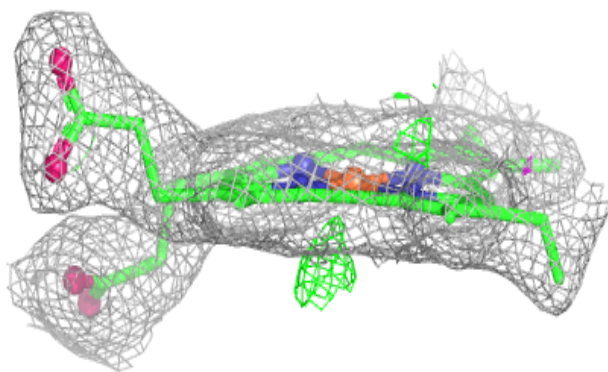
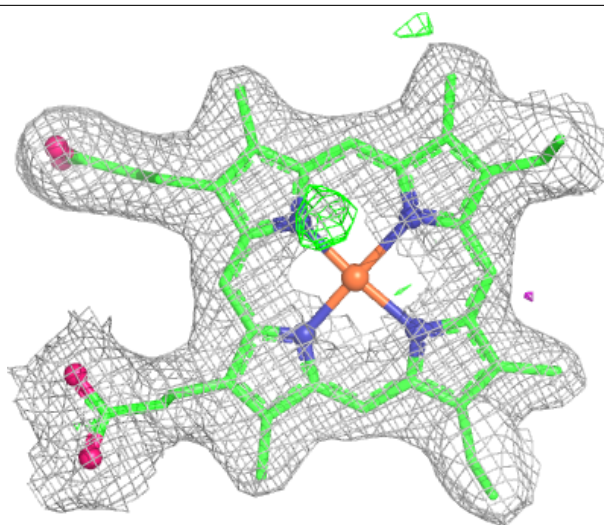
**Electron density around CLA D 402:**

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



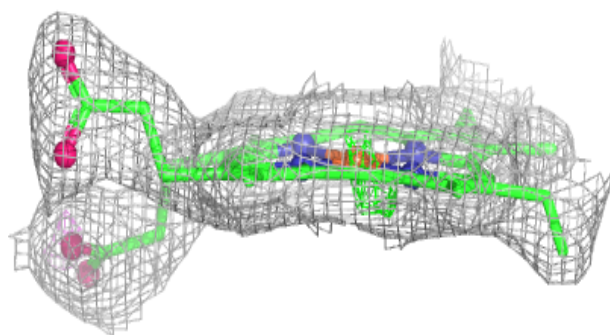
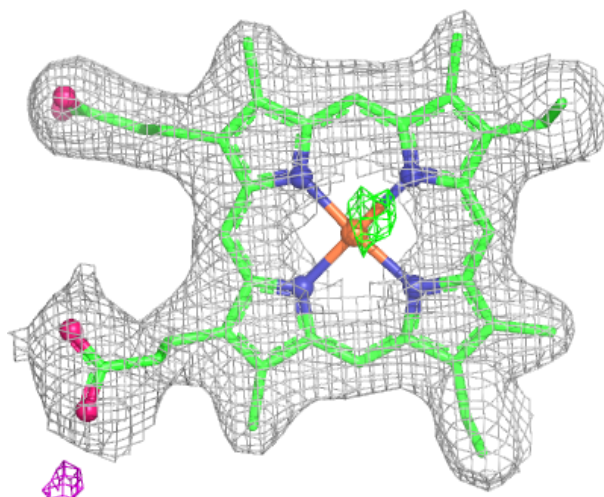
Electron density around HEC V 205:

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



Electron density around HEC v 205:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.