



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2022 – 12:54 pm GMT

PDB ID : 5E7C
Title : Macromolecular diffractive imaging using imperfect crystals - Bragg data
Authors : Ayer, K.; Yefanov, O.; Oberthuer, D.; Roy-Chowdhury, S.; Galli, L.; Mariani, V.; Basu, S.; Coe, J.; Conrad, C.E.; Fromme, R.; Schaffner, A.; Doerner, K.; James, D.; Kupitz, C.; Metz, M.; Nelson, G.; Xavier, P.L.; Beyerlein, K.R.; Schmidt, M.; Sarrou, I.; Spence, J.C.H.; Weierstall, U.; White, T.A.; Yang, J.-H.; Zhao, Y.; Liang, M.; Aquila, A.; Hunter, M.S.; Robinson, J.S.; Koglin, J.E.; Boutet, S.; Fromme, P.; Barty, A.; Chapman, H.N.
Deposited on : 2015-10-12
Resolution : 4.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

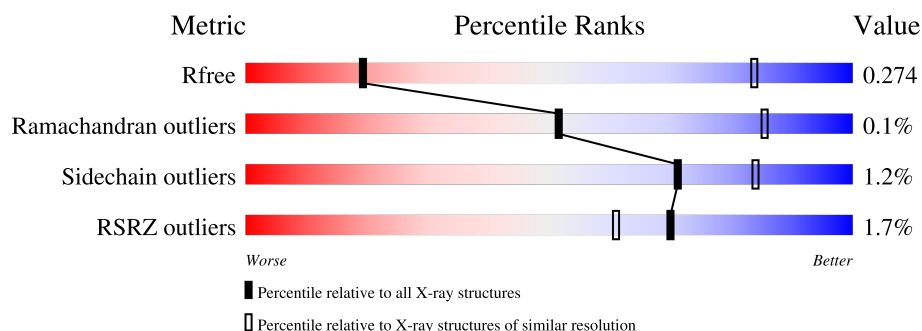
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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.



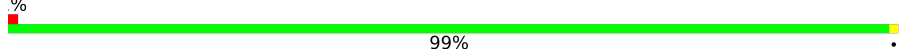

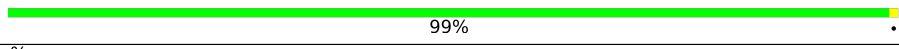
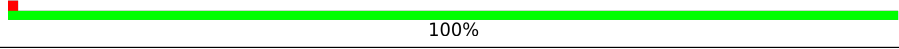
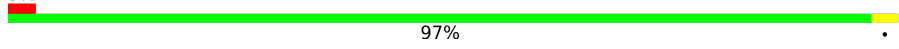
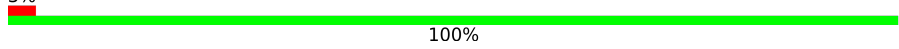
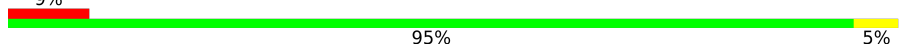
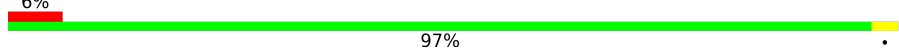
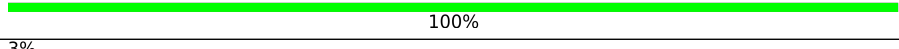
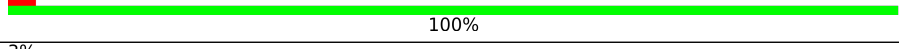
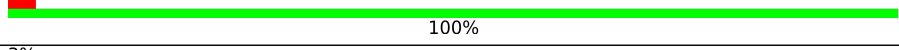
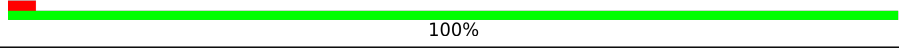
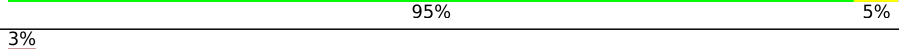
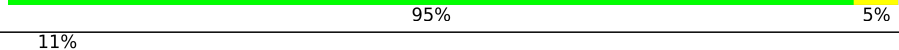
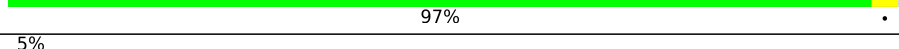
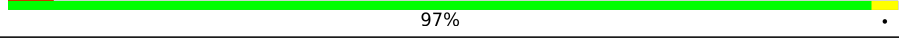
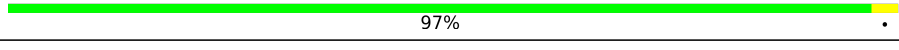
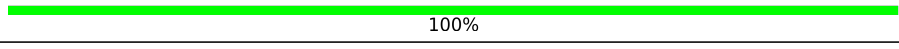
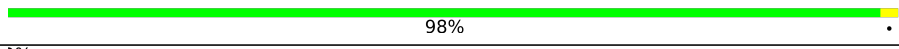
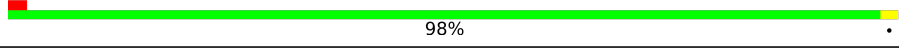
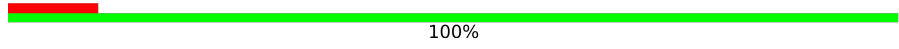

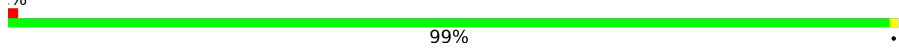
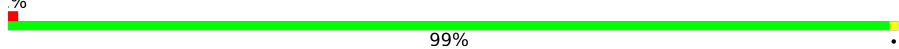
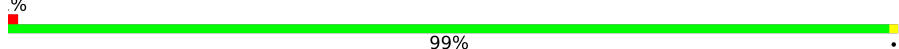
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1055 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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	334	<div> <div style="width: 100%;"></div> <div>100%</div> </div>
1	a	334	<div> <div style="width: 99%;"></div> <div>99%</div> </div>
2	B	504	<div> <div style="width: 100%;"></div> <div>100%</div> </div>
2	b	504	<div> <div style="width: 99%;"></div> <div>99%</div> </div>
3	C	451	<div> <div style="width: 99%;"></div> <div>99%</div> </div>
3	c	451	<div> <div style="width: 99%;"></div> <div>99%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	342	%  99% .
4	d	342	%  100%
5	E	81	 99% .
5	e	81	%  100%
6	F	34	3%  97% .
6	f	34	3%  100%
7	H	65	9%  95% 5%
7	h	65	6%  97% .
8	I	38	 100%
8	i	38	3%  100%
9	J	38	3%  100%
9	j	38	3%  100%
10	K	37	 95% 5%
10	k	37	3%  95% 5%
11	L	37	11%  97% .
11	l	37	5%  97% .
12	M	34	 97% .
12	m	34	 100%
13	O	243	 98% .
13	o	243	2%  98% .
14	T	30	10%  100%
14	t	30	 100%
15	U	97	%  99% .
15	u	97	%  99% .
16	V	137	%  99% .

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Mol	Chain	Length	Quality of chain
16	v	137	 2% 99%
17	Y	29	 3% 97%
17	y	29	 100%
18	X	39	 18% 100%
18	x	39	 8% 97%
19	Z	62	 2% 97%
19	z	62	 3% 95%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	605	X	-	-	-
23	CLA	A	606	X	-	-	-
23	CLA	A	608	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607[A]	X	-	-	-
23	CLA	B	607[B]	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	X
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	X
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	X
23	CLA	C	513	X	-	-	X
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	604	X	-	-	-
23	CLA	a	605	X	-	-	-
23	CLA	a	607	X	-	-	-
23	CLA	a	613	X	-	-	-
23	CLA	b	604	X	-	-	X
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609[A]	X	-	-	X
23	CLA	b	609[B]	X	-	-	X
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	X
23	CLA	c	514	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
25	BCR	A	609	-	X	-	X
25	BCR	B	618	-	X	-	-
25	BCR	B	619	-	X	-	-
25	BCR	B	620	-	X	-	-
25	BCR	C	514	-	X	-	-
25	BCR	C	515	-	X	-	-
25	BCR	C	521	-	X	-	-
25	BCR	F	101	-	X	-	-
25	BCR	H	101	-	X	-	X
25	BCR	K	101	-	X	-	-
25	BCR	T	101	-	X	-	X
25	BCR	a	608	-	X	-	X
25	BCR	b	620	-	X	-	X
25	BCR	b	621	-	X	-	-
25	BCR	b	622	-	X	-	X
25	BCR	c	515	-	X	-	X
25	BCR	c	516	-	X	-	-
25	BCR	c	522	-	X	-	-
25	BCR	f	101	-	X	-	-
25	BCR	h	101	-	X	-	X
25	BCR	k	101	-	X	-	-
25	BCR	t	101	-	X	-	-
26	PL9	A	610	-	X	-	-
26	PL9	a	609	-	X	-	X
26	PL9	d	404	-	X	-	-
27	SQD	A	611	-	-	-	X
27	SQD	a	610	-	-	-	X
27	SQD	b	602	-	-	-	X
27	SQD	x	101	-	-	-	X
28	LMG	C	519	-	-	-	X
28	LMG	C	520	-	-	-	X
28	LMG	c	521	-	-	-	X
28	LMG	z	101	-	-	-	X
30	CA	B	601	-	-	-	X
30	CA	b	603	-	-	-	X
32	DGD	D	406	-	-	-	X
32	DGD	d	405	-	-	-	X

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 49966 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	4	0
			2637	1730	432	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2637	1730	432	460	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ALA	THR	conflict	UNP P0A444
a	286	ALA	THR	conflict	UNP P0A444

- 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
			4024	2641	668	702	13			
2	b	504	Total	C	N	O	S	6	10	0
			4024	2641	668	702	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	5	0
			3506	2296	584	613	13			
3	c	451	Total	C	N	O	S	0	5	0
			3506	2296	584	613	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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

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

- 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	34	Total	C	N	O	S	0	0	0
			275	187	45	42	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	2	0
			525	351	86	86	2			
7	h	65	Total	C	N	O	S	0	2	0
			525	351	86	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	1	0
			320	215	49	54	2			
8	i	38	Total	C	N	O	S	0	1	0
			320	215	49	54	2			

- 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	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			

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

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

- 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
			272	183	40	48	1			
12	m	34	Total	C	N	O	S	0	1	0
			272	183	40	48	1			

- 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	4	0
			1883	1178	315	385	5			
13	o	243	Total	C	N	O	S	0	4	0
			1883	1178	315	385	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	2	0
			270	189	37	41	3			
14	t	30	Total	C	N	O	S	0	2	0
			270	189	37	41	3			

- 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	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	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			

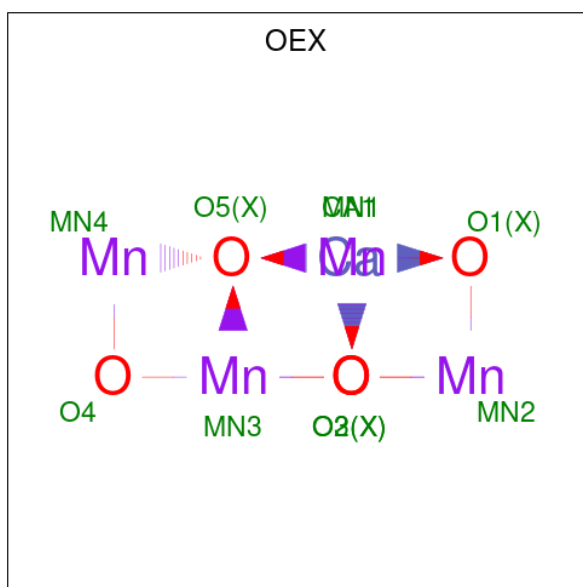
- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	0	1	0
			292	196	46	50			
18	x	39	Total	C	N	O	0	1	0
			292	196	46	50			

- 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 CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).

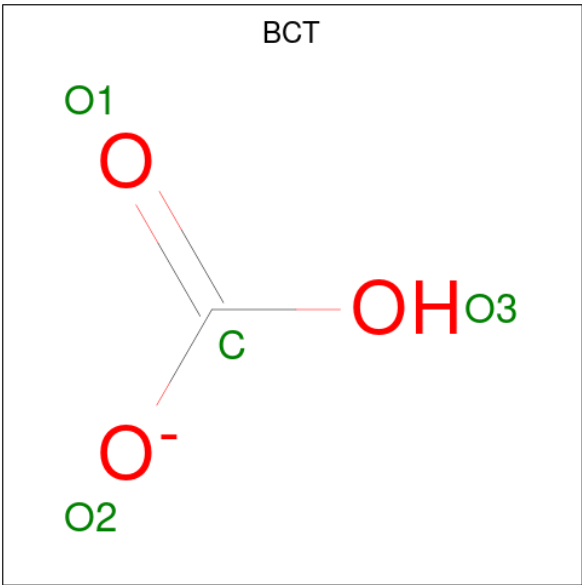


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 21 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

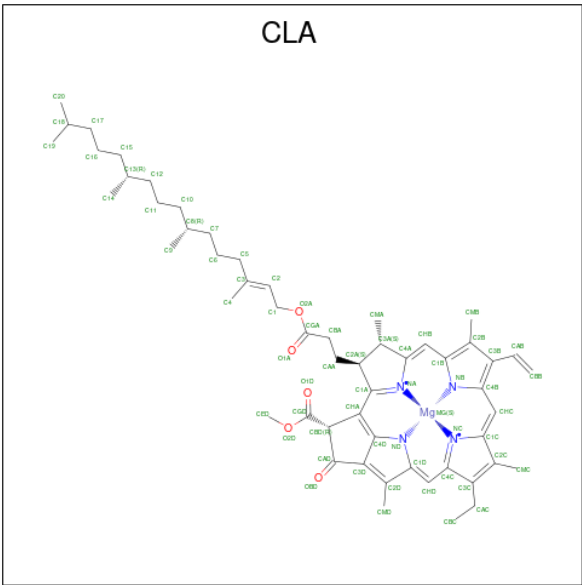
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	2	Total	Cl	0	0
			2	2		
21	V	1	Total	Cl	0	0
			1	1		
21	a	1	Total	Cl	0	0
			1	1		
21	c	1	Total	Cl	0	0
			1	1		
21	u	1	Total	Cl	0	0
			1	1		

- Molecule 22 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



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

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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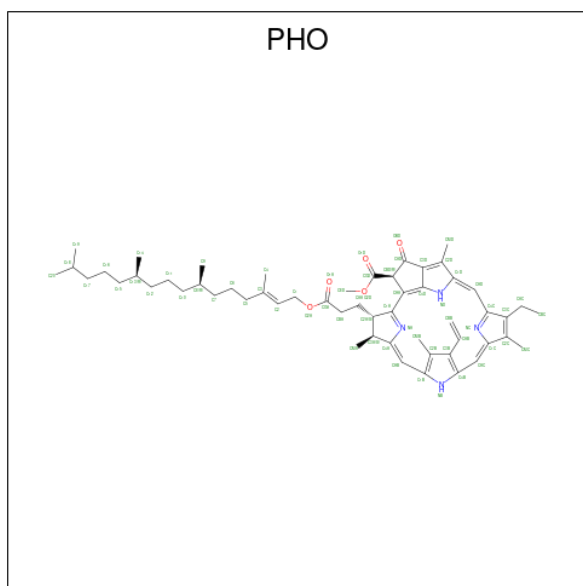
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1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

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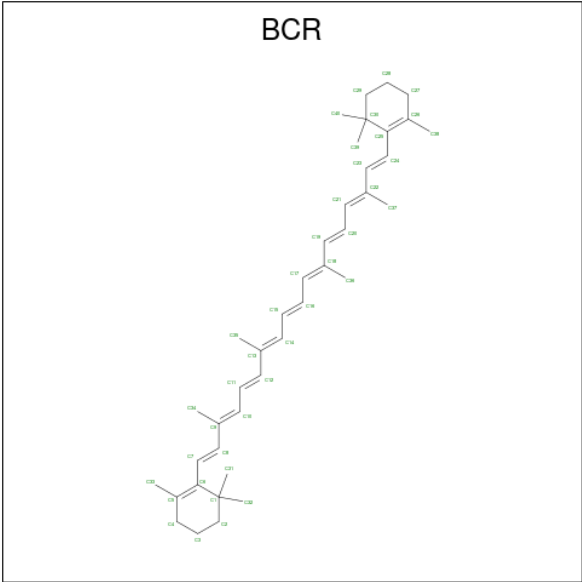
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



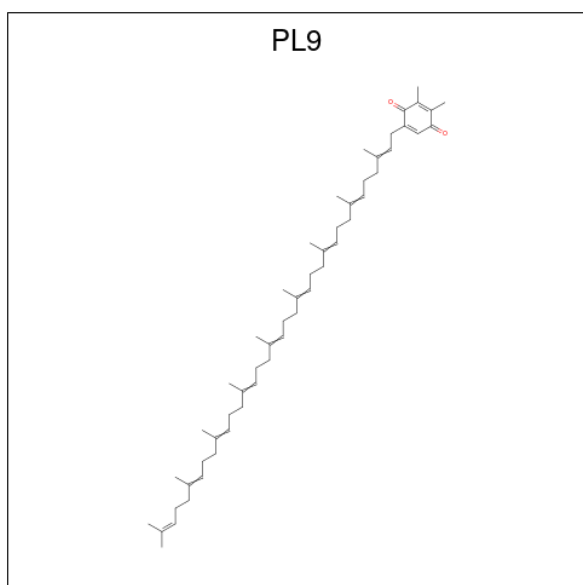
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	F	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	a	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	f	1	Total C 40 40	0	0
25	h	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0

- Molecule 26 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 (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



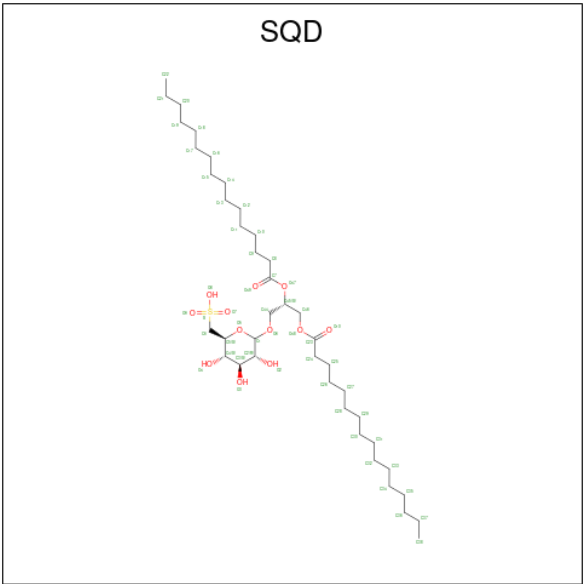
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O 55 53 2	0	0
26	D	1	Total C O 55 53 2	0	0

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

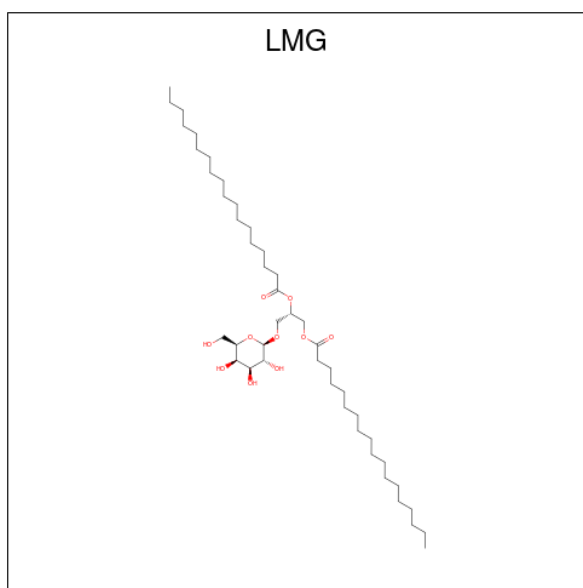
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	X	1	Total	C	O	S	0	0
			43	30	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	b	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	x	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter

code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			51	41	10		
28	B	1	Total	C	O	0	0
			51	41	10		
28	C	1	Total	C	O	0	0
			51	41	10		
28	C	1	Total	C	O	0	0
			51	41	10		
28	J	1	Total	C	O	0	0
			51	41	10		
28	Z	1	Total	C	O	0	0
			37	27	10		
28	a	1	Total	C	O	0	0
			51	41	10		
28	b	1	Total	C	O	0	0
			51	41	10		
28	c	1	Total	C	O	0	0
			51	41	10		
28	c	1	Total	C	O	0	0
			51	41	10		
28	j	1	Total	C	O	0	0
			51	41	10		
28	z	1	Total	C	O	0	0
			37	27	10		

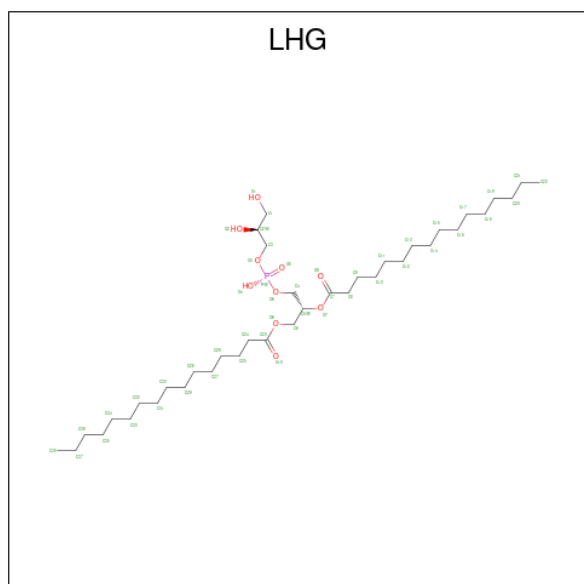
- Molecule 29 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 30 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	B	1	Total Ca 1 1	0	0
30	F	1	Total Ca 1 1	0	0
30	O	1	Total Ca 1 1	0	0
30	b	1	Total Ca 1 1	0	0
30	f	1	Total Ca 1 1	0	0
30	o	1	Total Ca 1 1	0	0

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



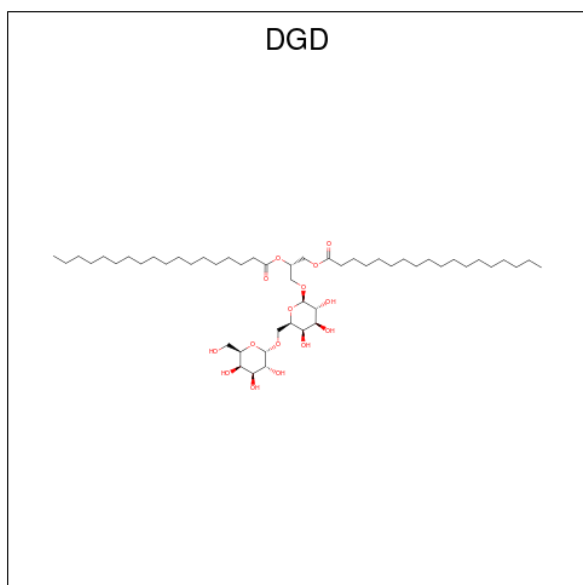
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C O P 49 38 10 1	0	0

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

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



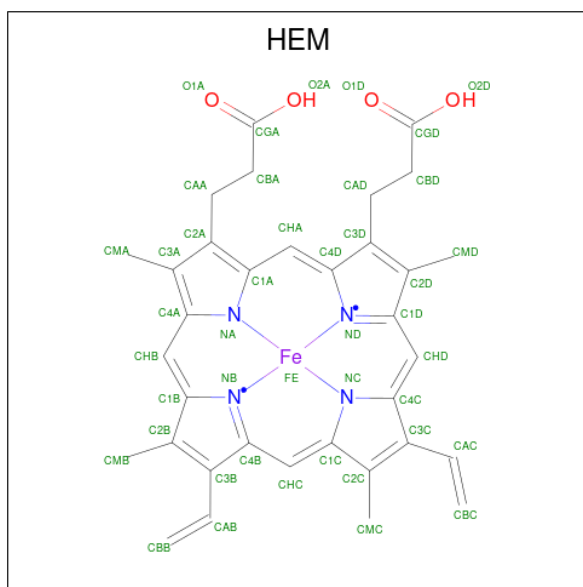
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		

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

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

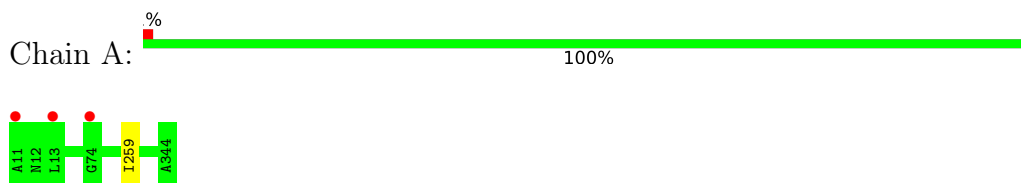
- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

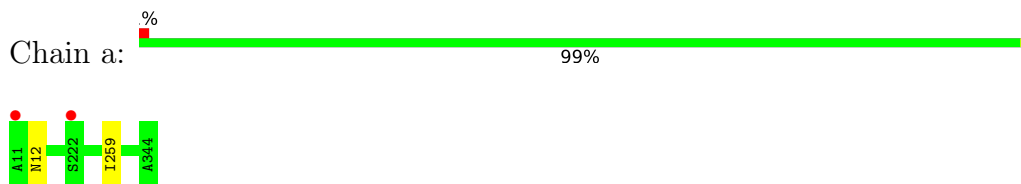
3 Residue-property plots

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

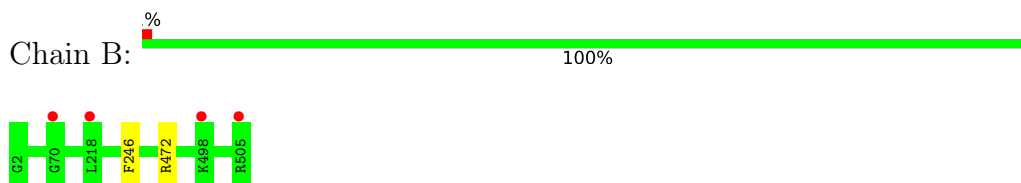
- Molecule 1: Photosystem II protein D1 1



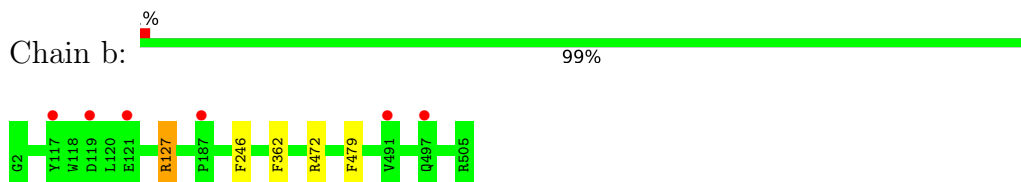
- Molecule 1: Photosystem II protein D1 1



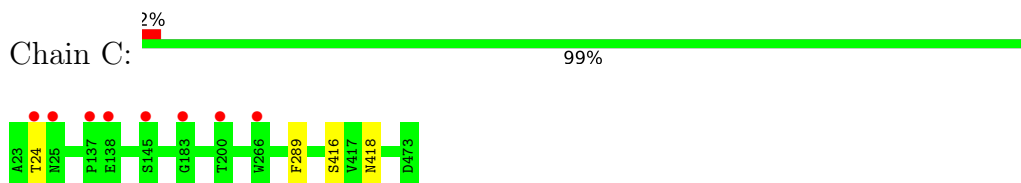
- Molecule 2: Photosystem II CP47 reaction center protein



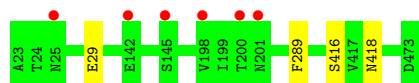
- Molecule 2: Photosystem II CP47 reaction center protein



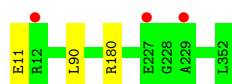
- Molecule 3: Photosystem II CP43 reaction center protein



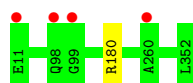
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



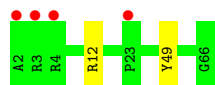
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



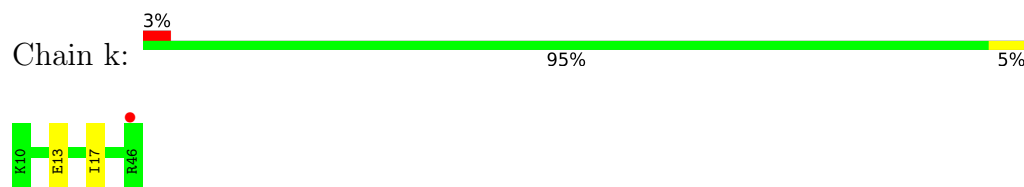
- Molecule 9: Photosystem II reaction center protein J



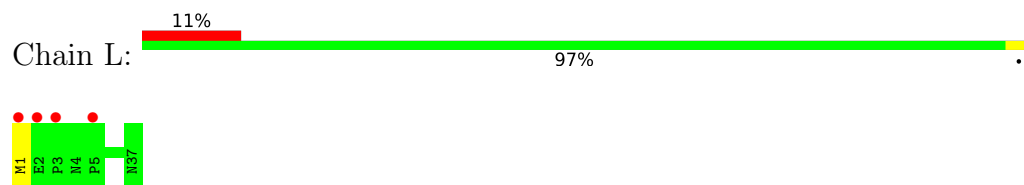
- Molecule 10: Photosystem II reaction center protein K



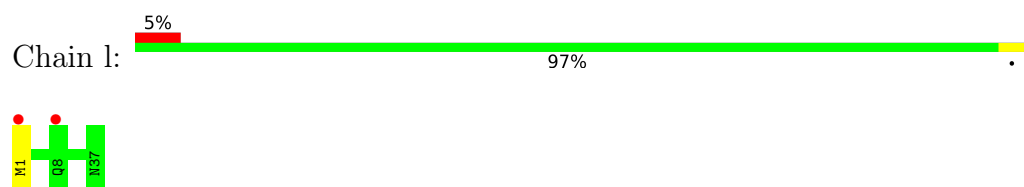
- Molecule 10: Photosystem II reaction center protein K



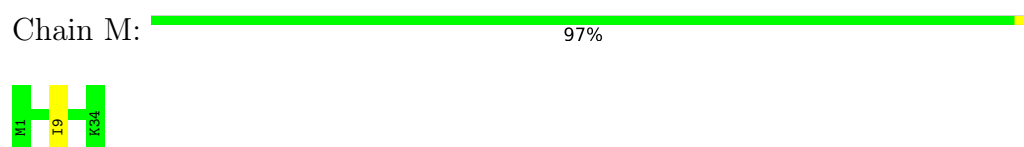
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

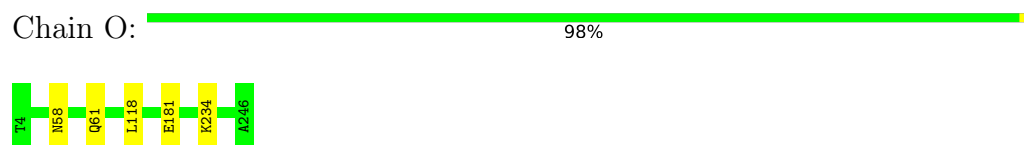


- Molecule 12: Photosystem II reaction center protein M

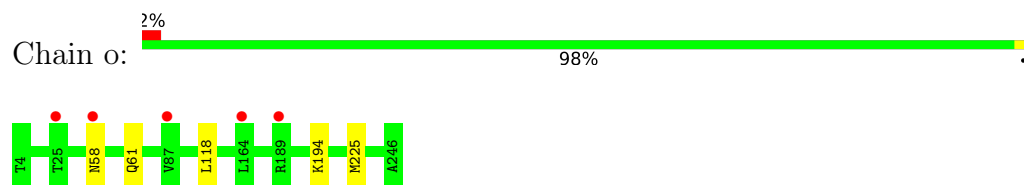


There are no outlier residues recorded for this chain.

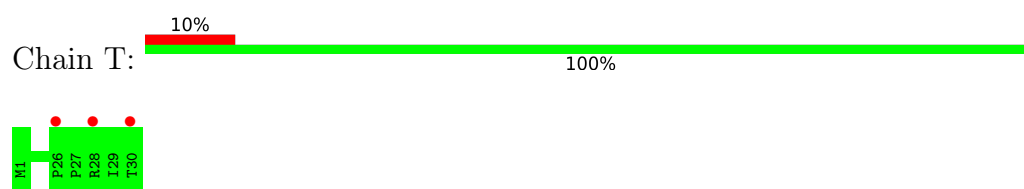
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II reaction center protein T

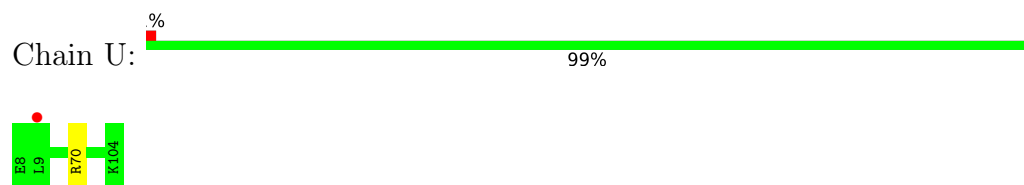


- Molecule 14: Photosystem II reaction center protein T

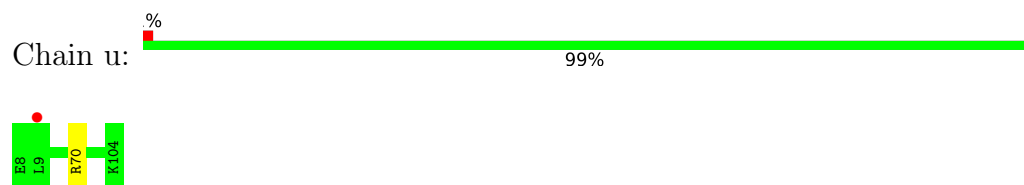


There are no outlier residues recorded for this chain.

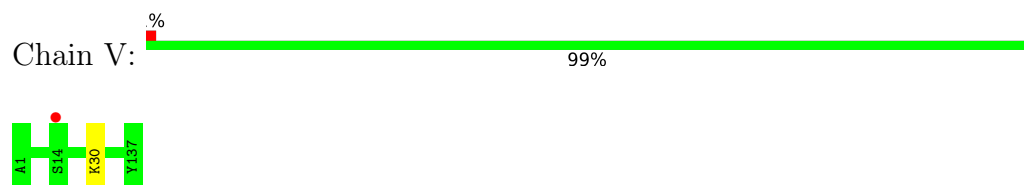
- Molecule 15: Photosystem II 12 kDa extrinsic protein



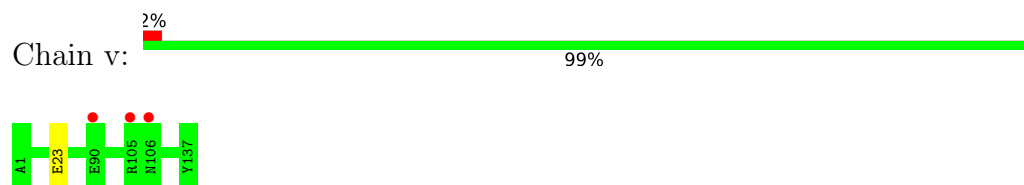
- Molecule 15: Photosystem II 12 kDa extrinsic protein



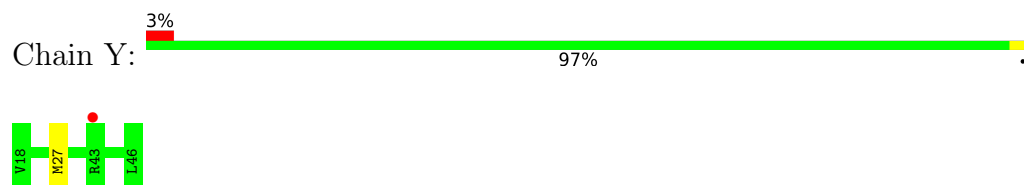
- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550



- Molecule 17: Photosystem II reaction center protein Ycf12



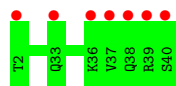
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: Photosystem II reaction center X protein

Chain X:  18% 100%



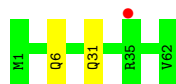
- Molecule 18: Photosystem II reaction center X protein

Chain x:  8% 97%



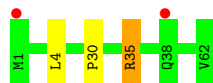
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  2% 97%



- Molecule 19: Photosystem II reaction center protein Z

Chain z:  3% 95%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.25Å 226.26Å 307.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 4.50 36.50 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.93-4.50) 99.9 (36.50-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 4.44Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.246 , 0.275 0.250 , 0.274	Depositor DCC
R_{free} test set	2721 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	211.4	Xtrriage
Anisotropy	0.314	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	49966	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.33	0/2734	0.53	0/3727
1	a	0.33	0/2734	0.53	0/3727
2	B	0.30	0/4194	0.51	0/5713
2	b	0.31	0/4194	0.52	1/5713 (0.0%)
3	C	0.31	0/3634	0.49	0/4947
3	c	0.32	0/3634	0.52	0/4947
4	D	0.31	0/2821	0.50	0/3844
4	d	0.30	0/2821	0.50	0/3844
5	E	0.30	0/693	0.49	0/944
5	e	0.31	0/693	0.55	0/944
6	F	0.34	0/284	0.49	0/387
6	f	0.40	0/284	0.74	0/387
7	H	0.29	0/544	0.52	0/739
7	h	0.28	0/544	0.52	0/739
8	I	0.31	0/327	0.54	0/439
8	i	0.31	0/327	0.60	0/439
9	J	0.27	0/278	0.44	0/376
9	j	0.31	0/278	0.50	0/376
10	K	0.31	0/303	0.57	0/416
10	k	0.34	0/303	0.55	0/416
11	L	0.28	0/319	0.44	0/433
11	l	0.28	0/319	0.45	0/433
12	M	0.33	0/278	0.56	0/378
12	m	0.34	0/278	0.57	0/378
13	O	0.29	0/1926	0.53	0/2611
13	o	0.32	0/1926	0.58	0/2611
14	T	0.34	0/282	0.52	0/382
14	t	0.34	0/282	0.51	0/382
15	U	0.28	0/785	0.51	0/1064
15	u	0.31	0/785	0.56	0/1064
16	V	0.29	0/1096	0.50	0/1487
16	v	0.29	0/1096	0.56	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.33	0/216	0.49	0/289
17	y	0.36	0/216	0.59	0/289
18	X	0.29	0/298	0.42	0/403
18	x	0.32	0/298	0.54	0/403
19	Z	0.32	0/490	0.46	0/669
19	z	0.41	0/490	0.68	1/669 (0.1%)
All	All	0.31	0/43004	0.52	2/58496 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	z	35	ARG	CB-CG-CD	6.51	128.53	111.60
2	b	127	ARG	CG-CD-NE	5.53	123.42	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	336/334 (101%)	332 (99%)	3 (1%)	1 (0%)	41	76
1	a	336/334 (101%)	330 (98%)	5 (2%)	1 (0%)	41	76
2	B	512/504 (102%)	507 (99%)	5 (1%)	0	100	100
2	b	512/504 (102%)	503 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	454/451 (101%)	443 (98%)	9 (2%)	2 (0%)	34	72
3	c	454/451 (101%)	441 (97%)	11 (2%)	2 (0%)	34	72
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	333 (98%)	7 (2%)	0	100	100
5	E	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
5	e	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
7	h	65/65 (100%)	57 (88%)	8 (12%)	0	100	100
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	J	36/38 (95%)	36 (100%)	0	0	100	100
9	j	36/38 (95%)	36 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/34 (97%)	33 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	34	72
13	o	245/243 (101%)	235 (96%)	9 (4%)	1 (0%)	34	72
14	T	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
14	t	29/30 (97%)	29 (100%)	0	0	100	100
15	U	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
15	u	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
17	Y	27/29 (93%)	27 (100%)	0	0	100	100
17	y	27/29 (93%)	27 (100%)	0	0	100	100
18	X	38/39 (97%)	37 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	x	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5252/5264 (100%)	5134 (98%)	110 (2%)	8 (0%)	51	81

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/269 (102%)	273 (100%)	0	100	100
1	a	273/269 (102%)	272 (100%)	1 (0%)	91	94
2	B	412/402 (102%)	410 (100%)	2 (0%)	88	93
2	b	412/402 (102%)	407 (99%)	5 (1%)	71	84
3	C	357/352 (101%)	354 (99%)	3 (1%)	81	89
3	c	357/352 (101%)	354 (99%)	3 (1%)	81	89
4	D	277/277 (100%)	274 (99%)	3 (1%)	73	85
4	d	277/277 (100%)	276 (100%)	1 (0%)	91	94
5	E	74/72 (103%)	73 (99%)	1 (1%)	67	81
5	e	74/72 (103%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	28/28 (100%)	27 (96%)	1 (4%)	35	60
6	f	28/28 (100%)	28 (100%)	0	100	100
7	H	56/54 (104%)	52 (93%)	4 (7%)	14	41
7	h	56/54 (104%)	53 (95%)	3 (5%)	22	49
8	I	36/35 (103%)	36 (100%)	0	100	100
8	i	36/35 (103%)	36 (100%)	0	100	100
9	J	26/26 (100%)	26 (100%)	0	100	100
9	j	26/26 (100%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	16	43
10	k	30/30 (100%)	28 (93%)	2 (7%)	16	43
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	65
11	l	36/35 (103%)	35 (97%)	1 (3%)	43	65
12	M	32/31 (103%)	31 (97%)	1 (3%)	40	63
12	m	32/31 (103%)	32 (100%)	0	100	100
13	O	210/206 (102%)	206 (98%)	4 (2%)	57	75
13	o	210/206 (102%)	206 (98%)	4 (2%)	57	75
14	T	29/27 (107%)	29 (100%)	0	100	100
14	t	29/27 (107%)	29 (100%)	0	100	100
15	U	84/84 (100%)	83 (99%)	1 (1%)	71	84
15	u	84/84 (100%)	83 (99%)	1 (1%)	71	84
16	V	118/117 (101%)	117 (99%)	1 (1%)	81	89
16	v	118/117 (101%)	117 (99%)	1 (1%)	81	89
17	Y	22/22 (100%)	21 (96%)	1 (4%)	27	54
17	y	22/22 (100%)	22 (100%)	0	100	100
18	X	33/32 (103%)	33 (100%)	0	100	100
18	x	33/32 (103%)	32 (97%)	1 (3%)	41	63
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	58
19	z	52/52 (100%)	49 (94%)	3 (6%)	20	47
All	All	4370/4302 (102%)	4317 (99%)	53 (1%)	71	84

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	246	PHE
2	B	472	ARG
3	C	24	THR
3	C	289	PHE
3	C	418	ASN
4	D	11	GLU
4	D	90	LEU
4	D	180	ARG
5	E	71	GLU
6	F	44	GLN
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	49	TYR
7	H	65	LEU
10	K	13	GLU
10	K	17	ILE
11	L	1	MET
12	M	9	ILE
13	O	61	GLN
13	O	118	LEU
13	O	181	GLU
13	O	234	LYS
15	U	70	ARG
16	V	30	LYS
17	Y	27	MET
19	Z	6	GLN
19	Z	31	GLN
1	a	12	ASN
2	b	127	ARG
2	b	246	PHE
2	b	362	PHE
2	b	472	ARG
2	b	479	PHE
3	c	29	GLU
3	c	289	PHE
3	c	418	ASN
4	d	180	ARG
7	h	12[A]	ARG
7	h	12[B]	ARG
7	h	49	TYR
10	k	13	GLU
10	k	17	ILE
11	l	1	MET

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Mol	Chain	Res	Type
13	o	61	GLN
13	o	118	LEU
13	o	194	LYS
13	o	225	MET
15	u	70	ARG
16	v	23	GLU
18	x	2	THR
19	z	4	LEU
19	z	30	PRO
19	z	35	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
12	M	33	GLN
1	a	198	HIS
3	c	25	ASN
12	m	33	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 166 ligands modelled in this entry, 16 are monoatomic - leaving 150 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	508	-	56,73,73	3.86	21 (37%)	55,113,113	2.13	13 (23%)
23	CLA	b	604	-	56,73,73	3.88	21 (37%)	55,113,113	2.00	12 (21%)
23	CLA	B	606	-	56,73,73	3.83	21 (37%)	55,113,113	2.00	11 (20%)
23	CLA	b	615	-	56,73,73	3.84	21 (37%)	55,113,113	2.06	13 (23%)
25	BCR	F	101	-	41,41,41	9.25	29 (70%)	56,56,56	6.08	28 (50%)
23	CLA	b	610	-	56,73,73	3.83	21 (37%)	55,113,113	2.02	16 (29%)
23	CLA	C	510	-	56,73,73	3.84	21 (37%)	55,113,113	2.00	12 (21%)
32	DGD	c	519	-	63,63,67	1.67	16 (25%)	77,77,81	1.06	4 (5%)
28	LMG	Z	101	-	37,37,55	1.42	4 (10%)	45,45,63	1.25	3 (6%)
24	PHO	d	401	-	67,69,69	1.28	7 (10%)	85,99,99	1.04	4 (4%)
27	SQD	X	101	-	42,43,54	1.21	3 (7%)	51,54,65	1.45	7 (13%)
27	SQD	a	612	-	53,54,54	1.05	3 (5%)	62,65,65	1.22	6 (9%)
27	SQD	A	611	-	53,54,54	0.98	3 (5%)	62,65,65	1.53	11 (17%)
23	CLA	B	605	-	56,73,73	3.86	21 (37%)	55,113,113	2.10	14 (25%)
25	BCR	c	515	-	41,41,41	9.14	30 (73%)	56,56,56	6.26	33 (58%)
23	CLA	c	512	3	56,73,73	3.82	21 (37%)	55,113,113	2.05	12 (21%)
31	LHG	a	614	-	48,48,48	1.09	2 (4%)	51,54,54	1.02	3 (5%)
23	CLA	C	503	-	56,73,73	3.85	21 (37%)	55,113,113	2.01	11 (20%)
33	HEM	E	102	6,5	27,50,50	2.11	6 (22%)	17,82,82	1.77	3 (17%)
25	BCR	k	101	-	41,41,41	9.29	30 (73%)	56,56,56	5.70	26 (46%)
23	CLA	a	613	-	56,73,73	3.83	21 (37%)	55,113,113	2.08	14 (25%)
23	CLA	b	606	-	56,73,73	3.85	21 (37%)	55,113,113	2.06	14 (25%)
25	BCR	C	514	-	41,41,41	9.14	31 (75%)	56,56,56	6.17	31 (55%)
23	CLA	d	402	-	56,73,73	3.82	21 (37%)	55,113,113	1.94	11 (20%)
32	DGD	C	517	-	63,63,67	1.65	17 (26%)	77,77,81	1.02	5 (6%)
28	LMG	B	621	-	51,51,55	1.27	4 (7%)	59,59,63	0.90	2 (3%)
23	CLA	B	609	-	56,73,73	3.88	21 (37%)	55,113,113	2.10	16 (29%)
23	CLA	B	603	-	56,73,73	3.85	21 (37%)	55,113,113	2.12	16 (29%)
32	DGD	c	518	-	63,63,67	1.66	17 (26%)	77,77,81	1.00	5 (6%)
25	BCR	A	609	-	41,41,41	9.39	30 (73%)	56,56,56	5.67	28 (50%)
28	LMG	c	520	-	51,51,55	1.32	4 (7%)	59,59,63	1.02	2 (3%)
23	CLA	c	506	-	56,73,73	3.86	21 (37%)	55,113,113	2.04	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	f	101	-	41,41,41	9.23	30 (73%)	56,56,56	5.80	28 (50%)
24	PHO	A	607	-	67,69,69	1.27	10 (14%)	85,99,99	1.03	4 (4%)
23	CLA	C	513	-	56,73,73	3.79	21 (37%)	55,113,113	2.06	15 (27%)
23	CLA	b	614	-	56,73,73	3.85	21 (37%)	55,113,113	2.13	13 (23%)
32	DGD	C	518	-	63,63,67	1.68	16 (25%)	77,77,81	1.03	5 (6%)
23	CLA	C	506	-	56,73,73	3.81	21 (37%)	55,113,113	2.11	13 (23%)
32	DGD	c	517	-	63,63,67	1.71	16 (25%)	77,77,81	0.92	3 (3%)
23	CLA	B	602	-	56,73,73	3.94	21 (37%)	55,113,113	1.98	11 (20%)
23	CLA	B	613	-	56,73,73	3.86	21 (37%)	55,113,113	2.05	14 (25%)
25	BCR	b	621	-	41,41,41	9.18	30 (73%)	56,56,56	5.68	31 (55%)
26	PL9	d	404	-	55,55,55	4.26	19 (34%)	68,69,69	3.70	35 (51%)
25	BCR	B	618	-	41,41,41	9.17	30 (73%)	56,56,56	6.07	30 (53%)
23	CLA	c	513	-	56,73,73	3.84	21 (37%)	55,113,113	2.05	16 (29%)
25	BCR	H	101	-	41,41,41	9.23	30 (73%)	56,56,56	5.84	36 (64%)
31	LHG	e	101	-	41,41,48	1.20	3 (7%)	44,47,54	0.95	2 (4%)
24	PHO	a	606	-	67,69,69	1.26	10 (14%)	85,99,99	1.02	4 (4%)
23	CLA	c	505	-	56,73,73	3.85	21 (37%)	55,113,113	2.09	13 (23%)
25	BCR	C	515	-	41,41,41	9.29	30 (73%)	56,56,56	5.97	30 (53%)
23	CLA	b	618	-	56,73,73	3.85	21 (37%)	55,113,113	2.02	13 (23%)
22	BCT	A	604	29	0,3,3	-	-	0,3,3	-	-
23	CLA	a	605	-	56,73,73	3.84	21 (37%)	55,113,113	2.06	13 (23%)
23	CLA	C	512	-	56,73,73	3.85	21 (37%)	55,113,113	2.13	16 (29%)
23	CLA	c	504	-	56,73,73	3.86	21 (37%)	55,113,113	1.96	13 (23%)
23	CLA	B	612	-	56,73,73	3.86	21 (37%)	55,113,113	2.16	13 (23%)
31	LHG	E	101	-	41,41,48	1.20	3 (7%)	44,47,54	0.91	3 (6%)
23	CLA	b	608	-	56,73,73	3.82	21 (37%)	55,113,113	2.01	12 (21%)
23	CLA	A	605	-	56,73,73	3.86	21 (37%)	55,113,113	2.08	12 (21%)
23	CLA	B	607[B]	-	56,73,73	3.84	21 (37%)	55,113,113	2.16	15 (27%)
23	CLA	c	503	-	56,73,73	3.84	21 (37%)	55,113,113	2.10	13 (23%)
28	LMG	z	101	-	37,37,55	1.43	4 (10%)	45,45,63	1.21	4 (8%)
28	LMG	a	611	-	51,51,55	1.30	4 (7%)	59,59,63	1.00	2 (3%)
32	DGD	C	516	-	63,63,67	1.71	16 (25%)	77,77,81	0.92	2 (2%)
31	LHG	D	407	-	48,48,48	1.11	3 (6%)	51,54,54	0.90	3 (5%)
25	BCR	t	101	-	41,41,41	9.30	29 (70%)	56,56,56	5.77	28 (50%)
23	CLA	a	604	-	56,73,73	3.84	21 (37%)	55,113,113	2.09	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SQD	b	602	-	53,54,54	1.08	4 (7%)	62,65,65	1.44	9 (14%)
23	CLA	D	404	-	56,73,73	3.85	21 (37%)	55,113,113	2.14	15 (27%)
22	BCT	a	603	29	0,3,3	-	-	0,3,3	-	-
23	CLA	b	609[A]	-	56,73,73	3.84	21 (37%)	55,113,113	2.17	15 (27%)
23	CLA	C	502	-	56,73,73	3.83	21 (37%)	55,113,113	2.10	11 (20%)
25	BCR	B	620	-	41,41,41	9.20	30 (73%)	56,56,56	6.08	32 (57%)
28	LMG	C	520	-	51,51,55	1.30	5 (9%)	59,59,63	1.01	4 (6%)
23	CLA	b	607	-	56,73,73	3.88	21 (37%)	55,113,113	2.15	14 (25%)
28	LMG	C	519	-	51,51,55	1.32	4 (7%)	59,59,63	1.06	2 (3%)
23	CLA	B	614	-	56,73,73	3.86	21 (37%)	55,113,113	2.01	13 (23%)
26	PL9	A	610	-	55,55,55	4.25	22 (40%)	68,69,69	3.74	39 (57%)
23	CLA	B	611	-	56,73,73	3.90	21 (37%)	55,113,113	2.05	11 (20%)
23	CLA	b	605	-	56,73,73	3.84	21 (37%)	55,113,113	2.12	14 (25%)
26	PL9	D	405	-	55,55,55	4.25	19 (34%)	68,69,69	3.72	35 (51%)
25	BCR	T	101	-	41,41,41	9.24	29 (70%)	56,56,56	6.00	30 (53%)
25	BCR	h	101	-	41,41,41	9.22	30 (73%)	56,56,56	5.85	37 (66%)
23	CLA	d	403	-	56,73,73	3.84	21 (37%)	55,113,113	2.11	13 (23%)
23	CLA	A	608	-	56,73,73	3.79	21 (37%)	55,113,113	2.05	14 (25%)
23	CLA	b	617	-	56,73,73	3.82	21 (37%)	55,113,113	2.06	13 (23%)
33	HEM	V	202	16	27,50,50	2.07	5 (18%)	17,82,82	1.83	6 (35%)
23	CLA	a	607	-	56,73,73	3.83	21 (37%)	55,113,113	2.03	14 (25%)
25	BCR	c	516	-	41,41,41	9.34	30 (73%)	56,56,56	5.82	27 (48%)
28	LMG	b	623	-	51,51,55	1.29	4 (7%)	59,59,63	0.94	2 (3%)
23	CLA	b	616	-	56,73,73	3.85	21 (37%)	55,113,113	2.07	14 (25%)
23	CLA	B	604	-	56,73,73	3.81	21 (37%)	55,113,113	2.08	14 (25%)
23	CLA	A	606	-	56,73,73	3.83	21 (37%)	55,113,113	2.08	13 (23%)
23	CLA	C	505	-	56,73,73	3.89	21 (37%)	55,113,113	2.08	12 (21%)
23	CLA	C	507	-	56,73,73	3.77	20 (35%)	55,113,113	2.19	14 (25%)
31	LHG	l	101	-	48,48,48	1.12	2 (4%)	51,54,54	0.89	2 (3%)
27	SQD	b	601	-	53,54,54	1.05	3 (5%)	62,65,65	1.22	6 (9%)
23	CLA	c	514	-	56,73,73	3.79	21 (37%)	55,113,113	2.05	11 (20%)
20	OEX	a	601	1,3	0,15,15	-	-	-	-	-
23	CLA	b	613	-	56,73,73	3.91	21 (37%)	55,113,113	2.07	11 (20%)
25	BCR	C	521	-	41,41,41	9.29	30 (73%)	56,56,56	5.89	26 (46%)
25	BCR	c	522	-	41,41,41	9.22	30 (73%)	56,56,56	5.86	28 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	504	-	56,73,73	3.83	21 (37%)	55,113,113	2.09	13 (23%)
25	BCR	a	608	-	41,41,41	9.29	30 (73%)	56,56,56	5.68	26 (46%)
24	PHO	D	401	-	67,69,69	1.27	7 (10%)	85,99,99	1.06	4 (4%)
25	BCR	B	619	-	41,41,41	9.63	30 (73%)	56,56,56	5.36	29 (51%)
31	LHG	B	622	-	48,48,48	1.14	3 (6%)	51,54,54	0.96	4 (7%)
23	CLA	c	510	-	56,73,73	3.84	21 (37%)	55,113,113	2.10	14 (25%)
23	CLA	D	403	-	56,73,73	3.85	21 (37%)	55,113,113	1.99	13 (23%)
23	CLA	b	611	-	56,73,73	3.87	21 (37%)	55,113,113	2.17	16 (29%)
28	LMG	j	101	34	51,51,55	1.30	4 (7%)	59,59,63	0.92	4 (6%)
23	CLA	b	619	-	56,73,73	3.85	21 (37%)	55,113,113	2.04	12 (21%)
31	LHG	d	406	-	48,48,48	1.11	3 (6%)	51,54,54	0.90	3 (5%)
23	CLA	B	615	-	56,73,73	3.83	21 (37%)	55,113,113	2.06	14 (25%)
23	CLA	b	609[B]	-	56,73,73	3.84	21 (37%)	55,113,113	2.14	15 (27%)
31	LHG	b	624	-	48,48,48	1.10	3 (6%)	51,54,54	0.96	3 (5%)
32	DGD	H	102	-	63,63,67	1.70	15 (23%)	77,77,81	0.92	3 (3%)
28	LMG	A	612	-	51,51,55	1.30	4 (7%)	59,59,63	0.97	3 (5%)
33	HEM	e	102	6,5	27,50,50	2.07	6 (22%)	17,82,82	1.81	4 (23%)
26	PL9	a	609	-	55,55,55	4.23	21 (38%)	68,69,69	3.79	35 (51%)
23	CLA	c	509	-	56,73,73	3.84	21 (37%)	55,113,113	2.19	12 (21%)
32	DGD	d	405	-	63,63,67	1.71	15 (23%)	77,77,81	1.03	6 (7%)
25	BCR	b	622	-	41,41,41	9.32	31 (75%)	56,56,56	5.84	32 (57%)
23	CLA	D	402	-	56,73,73	3.83	21 (37%)	55,113,113	2.08	14 (25%)
33	HEM	v	201	16	27,50,50	2.13	5 (18%)	17,82,82	1.83	4 (23%)
32	DGD	h	102	-	63,63,67	1.69	15 (23%)	77,77,81	0.97	4 (5%)
32	DGD	D	406	-	63,63,67	1.73	14 (22%)	77,77,81	1.13	7 (9%)
23	CLA	B	607[A]	-	56,73,73	3.81	21 (37%)	55,113,113	2.16	15 (27%)
23	CLA	c	502	-	56,73,73	3.81	21 (37%)	55,113,113	2.12	13 (23%)
23	CLA	C	509	-	56,73,73	3.80	20 (35%)	55,113,113	2.08	14 (25%)
28	LMG	c	521	-	51,51,55	1.31	4 (7%)	59,59,63	1.01	3 (5%)
27	SQD	a	610	-	53,54,54	0.99	3 (5%)	62,65,65	1.53	11 (17%)
23	CLA	B	616	-	56,73,73	3.84	21 (37%)	55,113,113	2.01	13 (23%)
23	CLA	B	610	-	56,73,73	3.84	21 (37%)	55,113,113	2.08	12 (21%)
23	CLA	c	511	-	56,73,73	3.86	21 (37%)	55,113,113	1.96	12 (21%)
31	LHG	D	408	-	48,48,48	1.11	3 (6%)	51,54,54	0.97	3 (5%)
31	LHG	L	101	-	48,48,48	1.10	3 (6%)	51,54,54	0.87	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LMG	J	101	34	51,51,55	1.31	4 (7%)	59,59,63	0.99	4 (6%)
23	CLA	B	617	-	56,73,73	3.86	21 (37%)	55,113,113	2.03	11 (20%)
25	BCR	b	620	-	41,41,41	9.09	30 (73%)	56,56,56	5.87	29 (51%)
20	OEX	A	601	1,3	0,15,15	-	-	-	-	-
23	CLA	c	508	-	56,73,73	3.80	20 (35%)	55,113,113	2.21	14 (25%)
23	CLA	C	501	-	56,73,73	3.79	21 (37%)	55,113,113	2.16	15 (27%)
23	CLA	B	608	-	56,73,73	3.84	21 (37%)	55,113,113	2.07	15 (27%)
23	CLA	c	507	-	56,73,73	3.85	21 (37%)	55,113,113	2.15	15 (27%)
27	SQD	x	101	-	42,43,54	1.21	3 (7%)	51,54,65	1.46	7 (13%)
23	CLA	b	612	-	56,73,73	3.81	21 (37%)	55,113,113	2.04	13 (23%)
23	CLA	C	511	3	56,73,73	3.85	21 (37%)	55,113,113	2.05	12 (21%)
25	BCR	K	101	-	41,41,41	9.19	30 (73%)	56,56,56	5.89	26 (46%)
27	SQD	B	623	-	53,54,54	1.07	4 (7%)	62,65,65	1.44	9 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	508	-	1/1/15/20	5/37/115/115	-
23	CLA	b	604	-	1/1/15/20	19/37/115/115	-
23	CLA	B	606	-	1/1/15/20	6/37/115/115	-
23	CLA	b	615	-	1/1/15/20	5/37/115/115	-
25	BCR	F	101	-	-	23/29/63/63	0/2/2/2
23	CLA	b	610	-	1/1/15/20	3/37/115/115	-
23	CLA	C	510	-	1/1/15/20	10/37/115/115	-
32	DGD	c	519	-	-	18/51/91/95	0/2/2/2
28	LMG	Z	101	-	-	15/31/51/70	0/1/1/1
24	PHO	d	401	-	-	1/53/103/103	0/5/6/6
27	SQD	X	101	-	-	16/38/58/69	0/1/1/1
27	SQD	a	612	-	-	23/49/69/69	0/1/1/1
27	SQD	A	611	-	-	16/49/69/69	0/1/1/1
23	CLA	B	605	-	1/1/15/20	8/37/115/115	-
25	BCR	c	515	-	-	25/29/63/63	0/2/2/2
23	CLA	c	512	3	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	a	614	-	-	16/53/53/53	-
23	CLA	C	503	-	1/1/15/20	3/37/115/115	-
33	HEM	E	102	6,5	-	0/6/54/54	-
25	BCR	k	101	-	-	19/29/63/63	0/2/2/2
23	CLA	a	613	-	1/1/15/20	5/37/115/115	-
23	CLA	b	606	-	1/1/15/20	7/37/115/115	-
25	BCR	C	514	-	-	23/29/63/63	0/2/2/2
23	CLA	d	402	-	1/1/15/20	2/37/115/115	-
32	DGD	C	517	-	-	29/51/91/95	0/2/2/2
28	LMG	B	621	-	-	22/46/66/70	0/1/1/1
23	CLA	B	609	-	1/1/15/20	4/37/115/115	-
23	CLA	B	603	-	1/1/15/20	3/37/115/115	-
32	DGD	c	518	-	-	30/51/91/95	0/2/2/2
25	BCR	A	609	-	-	21/29/63/63	0/2/2/2
28	LMG	c	520	-	-	22/46/66/70	0/1/1/1
23	CLA	c	506	-	1/1/15/20	7/37/115/115	-
25	BCR	f	101	-	-	24/29/63/63	0/2/2/2
24	PHO	A	607	-	-	4/53/103/103	0/5/6/6
23	CLA	C	513	-	1/1/15/20	11/37/115/115	-
23	CLA	b	614	-	1/1/15/20	5/37/115/115	-
32	DGD	C	518	-	-	16/51/91/95	0/2/2/2
23	CLA	C	506	-	1/1/15/20	16/37/115/115	-
32	DGD	c	517	-	-	25/51/91/95	0/2/2/2
23	CLA	B	602	-	1/1/15/20	17/37/115/115	-
23	CLA	B	613	-	1/1/15/20	5/37/115/115	-
25	BCR	b	621	-	-	21/29/63/63	0/2/2/2
26	PL9	d	404	-	-	27/53/73/73	0/1/1/1
25	BCR	B	618	-	-	24/29/63/63	0/2/2/2
23	CLA	c	513	-	1/1/15/20	7/37/115/115	-
25	BCR	H	101	-	-	23/29/63/63	0/2/2/2
31	LHG	e	101	-	-	23/46/46/53	-
24	PHO	a	606	-	-	3/53/103/103	0/5/6/6
23	CLA	c	505	-	1/1/15/20	11/37/115/115	-
25	BCR	C	515	-	-	21/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	618	-	1/1/15/20	11/37/115/115	-
23	CLA	a	605	-	1/1/15/20	8/37/115/115	-
23	CLA	C	512	-	1/1/15/20	9/37/115/115	-
23	CLA	c	504	-	1/1/15/20	3/37/115/115	-
23	CLA	B	612	-	1/1/15/20	5/37/115/115	-
31	LHG	E	101	-	-	24/46/46/53	-
23	CLA	b	608	-	1/1/15/20	6/37/115/115	-
23	CLA	A	605	-	1/1/15/20	0/37/115/115	-
23	CLA	B	607[B]	-	1/1/15/20	10/37/115/115	-
23	CLA	c	503	-	1/1/15/20	8/37/115/115	-
28	LMG	z	101	-	-	18/31/51/70	0/1/1/1
28	LMG	a	611	-	-	31/46/66/70	0/1/1/1
32	DGD	C	516	-	-	25/51/91/95	0/2/2/2
31	LHG	D	407	-	-	14/53/53/53	-
25	BCR	t	101	-	-	23/29/63/63	0/2/2/2
23	CLA	a	604	-	1/1/15/20	1/37/115/115	-
27	SQD	b	602	-	-	29/49/69/69	0/1/1/1
23	CLA	D	404	-	1/1/15/20	14/37/115/115	-
25	BCR	B	620	-	-	17/29/63/63	0/2/2/2
23	CLA	b	609[A]	-	1/1/15/20	8/37/115/115	-
23	CLA	C	502	-	1/1/15/20	8/37/115/115	-
28	LMG	C	520	-	-	19/46/66/70	0/1/1/1
23	CLA	b	607	-	1/1/15/20	9/37/115/115	-
28	LMG	C	519	-	-	21/46/66/70	0/1/1/1
23	CLA	B	614	-	1/1/15/20	5/37/115/115	-
26	PL9	A	610	-	-	25/53/73/73	0/1/1/1
23	CLA	B	611	-	1/1/15/20	9/37/115/115	-
23	CLA	b	605	-	1/1/15/20	5/37/115/115	-
26	PL9	D	405	-	-	25/53/73/73	0/1/1/1
25	BCR	T	101	-	-	24/29/63/63	0/2/2/2
25	BCR	h	101	-	-	25/29/63/63	0/2/2/2
23	CLA	d	403	-	1/1/15/20	13/37/115/115	-
23	CLA	A	608	-	1/1/15/20	13/37/115/115	-
23	CLA	b	617	-	1/1/15/20	13/37/115/115	-
33	HEM	V	202	16	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	607	-	1/1/15/20	14/37/115/115	-
25	BCR	c	516	-	-	21/29/63/63	0/2/2/2
28	LMG	b	623	-	-	21/46/66/70	0/1/1/1
23	CLA	b	616	-	1/1/15/20	4/37/115/115	-
23	CLA	B	604	-	1/1/15/20	8/37/115/115	-
23	CLA	A	606	-	1/1/15/20	9/37/115/115	-
23	CLA	C	505	-	1/1/15/20	7/37/115/115	-
23	CLA	C	507	-	1/1/15/20	8/37/115/115	-
31	LHG	l	101	-	-	22/53/53/53	-
27	SQD	b	601	-	-	23/49/69/69	0/1/1/1
23	CLA	c	514	-	1/1/15/20	11/37/115/115	-
23	CLA	b	613	-	1/1/15/20	8/37/115/115	-
25	BCR	C	521	-	-	17/29/63/63	0/2/2/2
25	BCR	c	522	-	-	20/29/63/63	0/2/2/2
23	CLA	C	504	-	1/1/15/20	8/37/115/115	-
25	BCR	a	608	-	-	19/29/63/63	0/2/2/2
24	PHO	D	401	-	-	2/53/103/103	0/5/6/6
25	BCR	B	619	-	-	24/29/63/63	0/2/2/2
31	LHG	B	622	-	-	13/53/53/53	-
23	CLA	c	510	-	1/1/15/20	8/37/115/115	-
23	CLA	D	403	-	1/1/15/20	2/37/115/115	-
23	CLA	b	611	-	1/1/15/20	3/37/115/115	-
28	LMG	j	101	34	-	18/46/66/70	0/1/1/1
23	CLA	b	619	-	1/1/15/20	14/37/115/115	-
31	LHG	d	406	-	-	14/53/53/53	-
23	CLA	B	615	-	1/1/15/20	14/37/115/115	-
23	CLA	b	609[B]	-	1/1/15/20	10/37/115/115	-
31	LHG	b	624	-	-	13/53/53/53	-
32	DGD	H	102	-	-	23/51/91/95	0/2/2/2
28	LMG	A	612	-	-	31/46/66/70	0/1/1/1
33	HEM	e	102	6,5	-	0/6/54/54	-
26	PL9	a	609	-	-	26/53/73/73	0/1/1/1
23	CLA	c	509	-	1/1/15/20	5/37/115/115	-
32	DGD	d	405	-	-	33/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	b	622	-	-	21/29/63/63	0/2/2/2
23	CLA	D	402	-	1/1/15/20	3/37/115/115	-
33	HEM	v	201	16	-	2/6/54/54	-
32	DGD	h	102	-	-	19/51/91/95	0/2/2/2
32	DGD	D	406	-	-	34/51/91/95	0/2/2/2
23	CLA	B	607[A]	-	1/1/15/20	9/37/115/115	-
23	CLA	c	502	-	1/1/15/20	11/37/115/115	-
23	CLA	C	509	-	1/1/15/20	7/37/115/115	-
28	LMG	c	521	-	-	19/46/66/70	0/1/1/1
27	SQD	a	610	-	-	16/49/69/69	0/1/1/1
23	CLA	B	616	-	1/1/15/20	11/37/115/115	-
23	CLA	B	610	-	1/1/15/20	6/37/115/115	-
23	CLA	c	511	-	1/1/15/20	11/37/115/115	-
31	LHG	D	408	-	-	17/53/53/53	-
31	LHG	L	101	-	-	18/53/53/53	-
28	LMG	J	101	34	-	19/46/66/70	0/1/1/1
23	CLA	B	617	-	1/1/15/20	14/37/115/115	-
25	BCR	b	620	-	-	18/29/63/63	0/2/2/2
23	CLA	c	508	-	1/1/15/20	9/37/115/115	-
23	CLA	C	501	-	1/1/15/20	11/37/115/115	-
23	CLA	B	608	-	1/1/15/20	3/37/115/115	-
23	CLA	c	507	-	1/1/15/20	14/37/115/115	-
27	SQD	x	101	-	-	16/38/58/69	0/1/1/1
23	CLA	b	612	-	1/1/15/20	6/37/115/115	-
23	CLA	C	511	3	1/1/15/20	6/37/115/115	-
25	BCR	K	101	-	-	21/29/63/63	0/2/2/2
27	SQD	B	623	-	-	29/49/69/69	0/1/1/1

All (2565) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	609	BCR	C14-C13	27.78	1.72	1.35
25	a	608	BCR	C14-C13	27.64	1.72	1.35
25	C	521	BCR	C14-C13	27.51	1.72	1.35
25	t	101	BCR	C14-C13	27.47	1.72	1.35
25	C	515	BCR	C14-C13	27.41	1.72	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	101	BCR	C14-C13	27.32	1.72	1.35
25	c	522	BCR	C14-C13	27.28	1.71	1.35
25	F	101	BCR	C14-C13	27.27	1.71	1.35
25	c	516	BCR	C14-C13	27.24	1.71	1.35
25	b	622	BCR	C14-C13	26.87	1.71	1.35
25	K	101	BCR	C14-C13	26.69	1.71	1.35
25	k	101	BCR	C14-C13	26.65	1.71	1.35
25	H	101	BCR	C14-C13	26.65	1.71	1.35
25	B	620	BCR	C14-C13	26.55	1.71	1.35
25	b	621	BCR	C14-C13	26.52	1.70	1.35
25	b	620	BCR	C14-C13	26.51	1.70	1.35
25	h	101	BCR	C14-C13	26.49	1.70	1.35
25	f	101	BCR	C14-C13	26.45	1.70	1.35
25	B	619	BCR	C21-C22	-26.31	1.00	1.35
25	B	618	BCR	C14-C13	26.17	1.70	1.35
25	B	619	BCR	C14-C13	26.07	1.70	1.35
25	C	514	BCR	C14-C13	25.68	1.69	1.35
25	c	515	BCR	C14-C13	25.64	1.69	1.35
25	H	101	BCR	C21-C22	-23.87	1.04	1.35
25	F	101	BCR	C21-C22	-23.08	1.05	1.35
25	C	514	BCR	C21-C22	-23.08	1.05	1.35
25	c	516	BCR	C21-C22	-23.01	1.05	1.35
25	c	515	BCR	C21-C22	-22.95	1.05	1.35
25	C	515	BCR	C21-C22	-22.94	1.05	1.35
25	C	521	BCR	C21-C22	-22.88	1.05	1.35
25	B	620	BCR	C21-C22	-22.45	1.06	1.35
25	k	101	BCR	C21-C22	-22.32	1.06	1.35
25	B	618	BCR	C21-C22	-22.29	1.06	1.35
25	h	101	BCR	C21-C22	-22.12	1.06	1.35
25	b	622	BCR	C21-C22	-22.09	1.06	1.35
25	A	609	BCR	C21-C22	-22.05	1.06	1.35
25	b	620	BCR	C21-C22	-21.93	1.06	1.35
25	f	101	BCR	C21-C22	-21.73	1.07	1.35
25	t	101	BCR	C21-C22	-21.67	1.07	1.35
25	c	522	BCR	C21-C22	-21.29	1.07	1.35
25	A	609	BCR	C10-C9	21.24	1.63	1.35
25	b	622	BCR	C10-C9	21.23	1.63	1.35
25	t	101	BCR	C10-C9	21.20	1.63	1.35
25	T	101	BCR	C10-C9	21.12	1.63	1.35
25	c	522	BCR	C10-C9	21.10	1.63	1.35
25	b	621	BCR	C21-C22	-21.10	1.07	1.35
25	a	608	BCR	C10-C9	21.04	1.63	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	K	101	BCR	C21-C22	-21.03	1.07	1.35
25	c	516	BCR	C10-C9	21.00	1.63	1.35
25	h	101	BCR	C10-C9	20.98	1.63	1.35
25	k	101	BCR	C10-C9	20.98	1.63	1.35
25	B	620	BCR	C10-C9	20.68	1.63	1.35
25	a	608	BCR	C21-C22	-20.66	1.08	1.35
25	C	521	BCR	C10-C9	20.66	1.63	1.35
25	T	101	BCR	C21-C22	-20.63	1.08	1.35
25	C	515	BCR	C10-C9	20.61	1.63	1.35
25	c	515	BCR	C10-C9	20.54	1.63	1.35
25	f	101	BCR	C10-C9	20.49	1.62	1.35
25	K	101	BCR	C10-C9	20.47	1.62	1.35
25	H	101	BCR	C10-C9	20.47	1.62	1.35
25	F	101	BCR	C10-C9	20.44	1.62	1.35
25	C	514	BCR	C10-C9	20.21	1.62	1.35
25	b	621	BCR	C10-C9	20.08	1.62	1.35
25	B	619	BCR	C10-C9	20.01	1.62	1.35
25	B	618	BCR	C10-C9	19.86	1.62	1.35
25	b	620	BCR	C10-C9	19.75	1.62	1.35
23	B	611	CLA	C4B-NB	18.50	1.51	1.35
23	B	602	CLA	C4B-NB	18.48	1.51	1.35
23	b	613	CLA	C4B-NB	18.42	1.51	1.35
23	b	616	CLA	C4B-NB	18.29	1.51	1.35
23	b	604	CLA	C4B-NB	18.28	1.51	1.35
23	D	404	CLA	C4B-NB	18.20	1.51	1.35
23	d	403	CLA	C4B-NB	18.11	1.51	1.35
23	B	610	CLA	C4B-NB	18.09	1.51	1.35
23	B	607[B]	CLA	C4B-NB	18.07	1.51	1.35
23	B	612	CLA	C4B-NB	18.02	1.51	1.35
23	C	504	CLA	C4B-NB	18.01	1.51	1.35
23	b	611	CLA	C4B-NB	18.01	1.51	1.35
23	b	607	CLA	C4B-NB	18.00	1.51	1.35
23	c	505	CLA	C4B-NB	17.98	1.51	1.35
23	C	505	CLA	C4B-NB	17.97	1.51	1.35
23	B	614	CLA	C4B-NB	17.95	1.51	1.35
23	B	609	CLA	C4B-NB	17.95	1.51	1.35
23	c	503	CLA	C4B-NB	17.93	1.51	1.35
23	C	511	CLA	C4B-NB	17.93	1.51	1.35
23	c	508	CLA	C4B-NB	17.92	1.51	1.35
23	A	608	CLA	C4B-NB	17.90	1.51	1.35
23	c	511	CLA	C4B-NB	17.88	1.51	1.35
23	B	608	CLA	C4B-NB	17.87	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	C4B-NB	17.87	1.51	1.35
23	c	504	CLA	C4B-NB	17.86	1.51	1.35
23	b	609[A]	CLA	C4B-NB	17.86	1.51	1.35
23	b	619	CLA	C4B-NB	17.84	1.51	1.35
23	a	607	CLA	C4B-NB	17.83	1.51	1.35
23	B	617	CLA	C4B-NB	17.83	1.51	1.35
23	B	605	CLA	C4B-NB	17.82	1.51	1.35
23	c	502	CLA	C4B-NB	17.82	1.51	1.35
23	b	609[B]	CLA	C4B-NB	17.81	1.51	1.35
23	B	616	CLA	C4B-NB	17.78	1.51	1.35
23	B	615	CLA	C4B-NB	17.77	1.51	1.35
23	C	502	CLA	C4B-NB	17.76	1.51	1.35
23	B	613	CLA	C4B-NB	17.76	1.51	1.35
23	B	607[A]	CLA	C4B-NB	17.75	1.51	1.35
23	b	614	CLA	C4B-NB	17.75	1.51	1.35
23	b	618	CLA	C4B-NB	17.72	1.51	1.35
23	b	617	CLA	C4B-NB	17.72	1.51	1.35
23	C	506	CLA	C4B-NB	17.71	1.51	1.35
23	c	509	CLA	C4B-NB	17.68	1.51	1.35
23	c	513	CLA	C4B-NB	17.67	1.51	1.35
23	c	507	CLA	C4B-NB	17.66	1.51	1.35
23	C	507	CLA	C4B-NB	17.65	1.51	1.35
23	b	606	CLA	C4B-NB	17.64	1.50	1.35
23	A	605	CLA	C4B-NB	17.64	1.50	1.35
23	a	605	CLA	C4B-NB	17.64	1.50	1.35
23	C	510	CLA	C4B-NB	17.62	1.50	1.35
23	C	503	CLA	C4B-NB	17.61	1.50	1.35
23	b	615	CLA	C4B-NB	17.59	1.50	1.35
23	C	512	CLA	C4B-NB	17.59	1.50	1.35
23	c	510	CLA	C4B-NB	17.58	1.50	1.35
23	B	603	CLA	C4B-NB	17.57	1.50	1.35
23	a	613	CLA	C4B-NB	17.57	1.50	1.35
23	A	606	CLA	C4B-NB	17.56	1.50	1.35
23	c	506	CLA	C4B-NB	17.56	1.50	1.35
23	C	508	CLA	C4B-NB	17.54	1.50	1.35
23	b	605	CLA	C4B-NB	17.53	1.50	1.35
23	b	608	CLA	C4B-NB	17.53	1.50	1.35
23	C	513	CLA	C4B-NB	17.50	1.50	1.35
23	c	512	CLA	C4B-NB	17.49	1.50	1.35
23	C	501	CLA	C4B-NB	17.48	1.50	1.35
23	D	402	CLA	C4B-NB	17.48	1.50	1.35
23	B	606	CLA	C4B-NB	17.47	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	C4B-NB	17.44	1.50	1.35
23	b	610	CLA	C4B-NB	17.38	1.50	1.35
23	d	402	CLA	C4B-NB	17.35	1.50	1.35
23	a	604	CLA	C4B-NB	17.34	1.50	1.35
23	D	403	CLA	C4B-NB	17.33	1.50	1.35
23	B	604	CLA	C4B-NB	17.32	1.50	1.35
23	c	514	CLA	C4B-NB	17.26	1.50	1.35
25	B	618	BCR	C20-C19	16.15	1.76	1.34
25	K	101	BCR	C20-C19	15.97	1.75	1.34
25	C	514	BCR	C20-C19	15.96	1.75	1.34
25	b	622	BCR	C20-C19	15.93	1.75	1.34
25	T	101	BCR	C20-C19	15.79	1.75	1.34
25	t	101	BCR	C20-C19	15.72	1.75	1.34
25	k	101	BCR	C20-C19	15.69	1.75	1.34
25	b	621	BCR	C20-C19	15.66	1.74	1.34
25	a	608	BCR	C20-C19	15.64	1.74	1.34
25	B	620	BCR	C20-C19	15.59	1.74	1.34
25	f	101	BCR	C20-C19	15.59	1.74	1.34
25	A	609	BCR	C20-C19	15.57	1.74	1.34
25	c	516	BCR	C20-C19	15.56	1.74	1.34
25	b	620	BCR	C20-C19	15.56	1.74	1.34
25	B	619	BCR	C19-C18	-15.42	1.12	1.45
25	c	522	BCR	C20-C19	15.35	1.74	1.34
25	C	515	BCR	C20-C19	15.31	1.74	1.34
25	c	515	BCR	C20-C19	15.31	1.74	1.34
25	B	619	BCR	C20-C19	15.27	1.73	1.34
25	F	101	BCR	C20-C19	15.17	1.73	1.34
25	h	101	BCR	C20-C19	15.16	1.73	1.34
25	C	521	BCR	C20-C19	15.06	1.73	1.34
25	H	101	BCR	C20-C19	15.05	1.73	1.34
25	B	619	BCR	C36-C18	15.01	1.81	1.50
25	B	619	BCR	C5-C6	14.78	1.60	1.34
25	b	621	BCR	C5-C6	14.76	1.60	1.34
25	C	514	BCR	C5-C6	14.60	1.59	1.34
23	B	602	CLA	C4C-NC	14.59	1.48	1.35
25	t	101	BCR	C5-C6	14.51	1.59	1.34
25	c	515	BCR	C5-C6	14.50	1.59	1.34
25	b	622	BCR	C5-C6	14.36	1.59	1.34
23	B	603	CLA	C4C-NC	14.31	1.48	1.35
23	B	609	CLA	C4C-NC	14.31	1.48	1.35
23	b	618	CLA	C4C-NC	14.20	1.47	1.35
25	k	101	BCR	C5-C6	14.17	1.59	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C4C-NC	14.16	1.47	1.35
23	b	611	CLA	C4C-NC	14.16	1.47	1.35
25	H	101	BCR	C36-C18	14.14	1.80	1.50
23	c	504	CLA	C4C-NC	14.14	1.47	1.35
25	C	514	BCR	C36-C18	14.11	1.80	1.50
23	B	617	CLA	C4C-NC	14.11	1.47	1.35
25	K	101	BCR	C5-C6	14.09	1.58	1.34
23	C	505	CLA	C4C-NC	14.08	1.47	1.35
25	B	620	BCR	C5-C6	14.07	1.58	1.34
23	C	512	CLA	C4C-NC	14.05	1.47	1.35
25	b	622	BCR	C36-C18	14.05	1.79	1.50
23	C	503	CLA	C4C-NC	14.04	1.47	1.35
23	C	508	CLA	C4C-NC	14.03	1.47	1.35
25	T	101	BCR	C16-C15	13.99	1.72	1.36
23	c	506	CLA	C4C-NC	13.98	1.47	1.35
23	c	514	CLA	C4C-NC	13.96	1.47	1.35
23	B	611	CLA	C4C-NC	13.95	1.47	1.35
23	c	513	CLA	C4C-NC	13.95	1.47	1.35
23	b	609[A]	CLA	C4C-NC	13.94	1.47	1.35
23	B	606	CLA	C4C-NC	13.93	1.47	1.35
23	b	604	CLA	C4C-NC	13.93	1.47	1.35
23	c	507	CLA	C4C-NC	13.93	1.47	1.35
23	c	509	CLA	C4C-NC	13.91	1.47	1.35
23	c	510	CLA	C4C-NC	13.87	1.47	1.35
23	b	613	CLA	C4C-NC	13.86	1.47	1.35
25	F	101	BCR	C19-C18	-13.86	1.16	1.45
25	C	515	BCR	C5-C6	13.85	1.58	1.34
25	k	101	BCR	C36-C18	13.85	1.79	1.50
23	D	403	CLA	C4C-NC	13.85	1.47	1.35
23	b	605	CLA	C4C-NC	13.85	1.47	1.35
23	b	619	CLA	C4C-NC	13.84	1.47	1.35
23	a	604	CLA	C4C-NC	13.84	1.47	1.35
25	c	516	BCR	C5-C6	13.83	1.58	1.34
23	c	511	CLA	C4C-NC	13.82	1.47	1.35
23	b	607	CLA	C4C-NC	13.81	1.47	1.35
25	a	608	BCR	C36-C18	13.80	1.79	1.50
25	K	101	BCR	C19-C18	-13.80	1.16	1.45
25	c	522	BCR	C36-C18	13.80	1.79	1.50
23	A	605	CLA	C4C-NC	13.79	1.47	1.35
23	a	605	CLA	C4C-NC	13.78	1.47	1.35
25	C	521	BCR	C36-C18	13.78	1.79	1.50
23	D	402	CLA	C4C-NC	13.77	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	C4C-NC	13.77	1.47	1.35
25	T	101	BCR	C5-C6	13.75	1.58	1.34
23	c	512	CLA	C4C-NC	13.75	1.47	1.35
25	C	515	BCR	C36-C18	13.73	1.79	1.50
25	c	522	BCR	C5-C6	13.72	1.58	1.34
25	C	521	BCR	C5-C6	13.72	1.58	1.34
23	c	505	CLA	C4C-NC	13.71	1.47	1.35
25	A	609	BCR	C5-C6	13.70	1.58	1.34
23	c	503	CLA	C4C-NC	13.69	1.47	1.35
23	C	511	CLA	C4C-NC	13.69	1.47	1.35
23	B	615	CLA	C4C-NC	13.68	1.47	1.35
23	B	608	CLA	C4C-NC	13.68	1.47	1.35
23	C	502	CLA	C4C-NC	13.68	1.47	1.35
25	a	608	BCR	C5-C6	13.67	1.58	1.34
23	a	613	CLA	C4C-NC	13.67	1.47	1.35
23	b	609[B]	CLA	C4C-NC	13.67	1.47	1.35
23	B	613	CLA	C4C-NC	13.66	1.47	1.35
23	b	615	CLA	C4C-NC	13.65	1.47	1.35
23	C	510	CLA	C4C-NC	13.64	1.47	1.35
23	C	513	CLA	C4C-NC	13.64	1.47	1.35
25	f	101	BCR	C36-C18	13.63	1.79	1.50
23	D	404	CLA	C4C-NC	13.62	1.47	1.35
25	C	521	BCR	C16-C15	13.62	1.71	1.36
25	c	516	BCR	C36-C18	13.61	1.79	1.50
23	d	403	CLA	C4C-NC	13.61	1.47	1.35
23	B	610	CLA	C4C-NC	13.60	1.47	1.35
23	b	610	CLA	C4C-NC	13.59	1.47	1.35
25	A	609	BCR	C36-C18	13.59	1.79	1.50
25	t	101	BCR	C36-C18	13.58	1.79	1.50
25	h	101	BCR	C19-C18	-13.58	1.16	1.45
23	C	506	CLA	C4C-NC	13.58	1.47	1.35
23	B	612	CLA	C4C-NC	13.57	1.47	1.35
25	c	515	BCR	C36-C18	13.56	1.78	1.50
23	C	507	CLA	C4C-NC	13.55	1.47	1.35
23	B	607[A]	CLA	C4C-NC	13.54	1.47	1.35
25	b	620	BCR	C36-C18	13.54	1.78	1.50
23	b	608	CLA	C4C-NC	13.54	1.47	1.35
23	B	614	CLA	C4C-NC	13.53	1.47	1.35
25	f	101	BCR	C5-C6	13.52	1.57	1.34
23	A	606	CLA	C4C-NC	13.51	1.47	1.35
25	C	521	BCR	C19-C18	-13.50	1.16	1.45
25	b	621	BCR	C19-C18	-13.50	1.16	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607[B]	CLA	C4C-NC	13.49	1.47	1.35
25	K	101	BCR	C16-C15	13.48	1.71	1.36
23	c	508	CLA	C4C-NC	13.48	1.47	1.35
25	F	101	BCR	C5-C6	13.48	1.57	1.34
23	b	614	CLA	C4C-NC	13.48	1.47	1.35
23	d	402	CLA	C4C-NC	13.48	1.47	1.35
23	b	617	CLA	C4C-NC	13.47	1.47	1.35
25	t	101	BCR	C16-C15	13.47	1.71	1.36
23	C	501	CLA	C4C-NC	13.46	1.47	1.35
23	B	604	CLA	C4C-NC	13.46	1.47	1.35
23	c	502	CLA	C4C-NC	13.45	1.47	1.35
25	B	618	BCR	C16-C15	13.42	1.70	1.36
25	T	101	BCR	C19-C18	-13.41	1.17	1.45
23	b	616	CLA	C4C-NC	13.41	1.47	1.35
23	b	612	CLA	C4C-NC	13.40	1.47	1.35
23	C	509	CLA	C4C-NC	13.39	1.47	1.35
25	c	515	BCR	C19-C18	-13.39	1.17	1.45
25	H	101	BCR	C5-C6	13.39	1.57	1.34
25	k	101	BCR	C19-C18	-13.38	1.17	1.45
25	h	101	BCR	C16-C15	13.37	1.70	1.36
23	C	504	CLA	C4C-NC	13.37	1.47	1.35
25	A	609	BCR	C16-C15	13.36	1.70	1.36
25	B	620	BCR	C36-C18	13.36	1.78	1.50
23	a	607	CLA	C4C-NC	13.31	1.47	1.35
25	B	618	BCR	C5-C6	13.29	1.57	1.34
25	h	101	BCR	C5-C6	13.28	1.57	1.34
25	B	618	BCR	C36-C18	13.25	1.78	1.50
25	b	620	BCR	C16-C15	13.25	1.70	1.36
25	c	522	BCR	C19-C18	-13.24	1.17	1.45
25	a	608	BCR	C16-C15	13.20	1.70	1.36
25	b	620	BCR	C5-C6	13.18	1.57	1.34
23	b	606	CLA	C4C-NC	13.14	1.46	1.35
25	f	101	BCR	C19-C18	-13.11	1.17	1.45
25	f	101	BCR	C16-C15	13.08	1.70	1.36
25	b	622	BCR	C16-C15	13.08	1.70	1.36
25	c	516	BCR	C16-C15	13.03	1.69	1.36
25	H	101	BCR	C16-C15	13.01	1.69	1.36
25	h	101	BCR	C36-C18	12.98	1.77	1.50
25	B	618	BCR	C37-C22	12.96	1.77	1.50
25	c	522	BCR	C16-C15	12.95	1.69	1.36
25	k	101	BCR	C16-C15	12.93	1.69	1.36
25	C	515	BCR	C16-C15	12.92	1.69	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	515	BCR	C16-C15	12.90	1.69	1.36
25	F	101	BCR	C16-C15	12.85	1.69	1.36
25	b	621	BCR	C36-C18	12.84	1.77	1.50
25	B	620	BCR	C16-C15	12.83	1.69	1.36
23	A	608	CLA	C4C-NC	12.82	1.46	1.35
25	b	620	BCR	C19-C18	-12.77	1.18	1.45
25	B	619	BCR	C16-C15	12.77	1.69	1.36
25	t	101	BCR	C19-C18	-12.76	1.18	1.45
25	K	101	BCR	C36-C18	12.75	1.77	1.50
25	F	101	BCR	C36-C18	12.75	1.77	1.50
25	B	620	BCR	C19-C18	-12.73	1.18	1.45
25	C	514	BCR	C19-C18	-12.72	1.18	1.45
25	A	609	BCR	C19-C18	-12.72	1.18	1.45
25	T	101	BCR	C36-C18	12.66	1.77	1.50
25	C	514	BCR	C16-C15	12.66	1.68	1.36
25	a	608	BCR	C19-C18	-12.64	1.18	1.45
25	b	621	BCR	C16-C15	12.64	1.68	1.36
25	B	619	BCR	C37-C22	12.54	1.76	1.50
25	b	622	BCR	C19-C18	-12.53	1.19	1.45
25	c	516	BCR	C19-C18	-12.49	1.19	1.45
25	C	515	BCR	C19-C18	-12.47	1.19	1.45
25	H	101	BCR	C19-C18	-12.46	1.19	1.45
25	B	618	BCR	C19-C18	-12.39	1.19	1.45
25	b	622	BCR	C37-C22	12.34	1.76	1.50
25	T	101	BCR	C37-C22	12.24	1.76	1.50
25	b	621	BCR	C37-C22	12.13	1.76	1.50
25	h	101	BCR	C37-C22	12.04	1.75	1.50
25	B	620	BCR	C37-C22	12.03	1.75	1.50
25	T	101	BCR	C20-C21	12.01	1.80	1.43
25	c	516	BCR	C37-C22	11.96	1.75	1.50
25	K	101	BCR	C37-C22	11.93	1.75	1.50
25	K	101	BCR	C20-C21	11.92	1.80	1.43
25	B	618	BCR	C20-C21	11.78	1.79	1.43
25	a	608	BCR	C20-C21	11.77	1.79	1.43
25	k	101	BCR	C37-C22	11.76	1.75	1.50
25	t	101	BCR	C20-C21	11.74	1.79	1.43
25	b	622	BCR	C20-C21	11.73	1.79	1.43
25	c	515	BCR	C37-C22	11.72	1.75	1.50
25	A	609	BCR	C37-C22	11.68	1.75	1.50
25	b	620	BCR	C37-C22	11.62	1.74	1.50
25	b	621	BCR	C20-C21	11.61	1.79	1.43
25	f	101	BCR	C20-C21	11.60	1.79	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	515	BCR	C37-C22	11.56	1.74	1.50
25	a	608	BCR	C37-C22	11.55	1.74	1.50
25	A	609	BCR	C20-C21	11.55	1.79	1.43
25	k	101	BCR	C20-C21	11.54	1.79	1.43
25	t	101	BCR	C37-C22	11.53	1.74	1.50
25	B	620	BCR	C20-C21	11.49	1.79	1.43
25	f	101	BCR	C37-C22	11.46	1.74	1.50
25	h	101	BCR	C20-C21	11.45	1.78	1.43
25	c	516	BCR	C8-C7	11.45	1.67	1.33
25	A	609	BCR	C8-C7	11.40	1.67	1.33
25	C	514	BCR	C20-C21	11.37	1.78	1.43
25	f	101	BCR	C8-C7	11.34	1.67	1.33
25	c	522	BCR	C20-C21	11.32	1.78	1.43
25	b	620	BCR	C20-C21	11.32	1.78	1.43
25	a	608	BCR	C8-C7	11.30	1.67	1.33
25	F	101	BCR	C8-C7	11.27	1.67	1.33
25	t	101	BCR	C8-C7	11.20	1.66	1.33
25	C	515	BCR	C8-C7	11.19	1.66	1.33
25	c	516	BCR	C20-C21	11.18	1.78	1.43
25	c	515	BCR	C20-C21	11.16	1.78	1.43
25	K	101	BCR	C8-C7	11.14	1.66	1.33
25	k	101	BCR	C8-C7	11.13	1.66	1.33
25	C	515	BCR	C20-C21	11.13	1.77	1.43
25	B	618	BCR	C8-C7	11.11	1.66	1.33
25	b	620	BCR	C8-C7	11.09	1.66	1.33
25	c	522	BCR	C37-C22	11.08	1.73	1.50
25	C	514	BCR	C37-C22	11.07	1.73	1.50
25	C	521	BCR	C20-C21	11.05	1.77	1.43
25	c	522	BCR	C8-C7	11.03	1.66	1.33
25	B	619	BCR	C20-C21	11.01	1.77	1.43
25	b	621	BCR	C8-C7	11.00	1.66	1.33
25	C	521	BCR	C37-C22	11.00	1.73	1.50
25	B	619	BCR	C8-C7	10.98	1.66	1.33
25	T	101	BCR	C8-C7	10.89	1.66	1.33
25	F	101	BCR	C20-C21	10.89	1.77	1.43
25	H	101	BCR	C8-C7	10.88	1.66	1.33
25	H	101	BCR	C20-C21	10.86	1.77	1.43
25	F	101	BCR	C37-C22	10.85	1.73	1.50
25	C	521	BCR	C8-C7	10.84	1.65	1.33
25	h	101	BCR	C8-C7	10.79	1.65	1.33
25	H	101	BCR	C37-C22	10.77	1.73	1.50
25	b	622	BCR	C8-C7	10.77	1.65	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	514	BCR	C8-C7	10.73	1.65	1.33
25	c	515	BCR	C8-C7	10.72	1.65	1.33
26	a	609	PL9	C18-C19	10.69	1.58	1.33
26	A	610	PL9	C18-C19	10.63	1.58	1.33
26	D	405	PL9	C18-C19	10.63	1.58	1.33
26	d	404	PL9	C18-C19	10.62	1.58	1.33
25	B	620	BCR	C8-C7	10.56	1.65	1.33
25	T	101	BCR	C16-C17	10.25	1.75	1.43
25	B	619	BCR	C26-C25	10.14	1.52	1.34
26	D	405	PL9	C38-C39	9.95	1.56	1.33
26	d	404	PL9	C23-C24	9.89	1.56	1.33
25	C	521	BCR	C16-C17	9.86	1.74	1.43
25	b	621	BCR	C26-C25	9.84	1.51	1.34
26	A	610	PL9	C38-C39	9.83	1.56	1.33
26	D	405	PL9	C23-C24	9.83	1.56	1.33
26	d	404	PL9	C38-C39	9.81	1.56	1.33
25	b	620	BCR	C16-C17	9.76	1.73	1.43
26	A	610	PL9	C23-C24	9.75	1.56	1.33
26	a	609	PL9	C38-C39	9.74	1.56	1.33
25	f	101	BCR	C16-C17	9.73	1.73	1.43
25	t	101	BCR	C16-C17	9.68	1.73	1.43
25	h	101	BCR	C16-C17	9.65	1.73	1.43
25	B	618	BCR	C16-C17	9.64	1.73	1.43
25	a	608	BCR	C16-C17	9.59	1.73	1.43
26	a	609	PL9	C23-C24	9.59	1.56	1.33
25	c	522	BCR	C16-C17	9.58	1.73	1.43
25	b	622	BCR	C16-C17	9.46	1.72	1.43
25	A	609	BCR	C16-C17	9.42	1.72	1.43
25	c	516	BCR	C16-C17	9.38	1.72	1.43
25	H	101	BCR	C16-C17	9.38	1.72	1.43
25	C	515	BCR	C16-C17	9.35	1.72	1.43
25	F	101	BCR	C26-C25	9.33	1.50	1.34
25	c	515	BCR	C16-C17	9.30	1.72	1.43
25	A	609	BCR	C26-C25	9.26	1.50	1.34
25	K	101	BCR	C16-C17	9.24	1.72	1.43
25	B	619	BCR	C16-C17	9.22	1.72	1.43
25	a	608	BCR	C26-C25	9.21	1.50	1.34
25	f	101	BCR	C26-C25	9.12	1.50	1.34
25	k	101	BCR	C16-C17	9.11	1.71	1.43
25	B	620	BCR	C16-C17	9.08	1.71	1.43
25	F	101	BCR	C16-C17	9.03	1.71	1.43
25	C	514	BCR	C16-C17	9.01	1.71	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	405	PL9	C13-C14	8.97	1.54	1.33
26	d	404	PL9	C13-C14	8.94	1.54	1.33
26	a	609	PL9	C48-C49	8.82	1.57	1.32
25	b	621	BCR	C16-C17	8.81	1.70	1.43
26	A	610	PL9	C13-C14	8.81	1.54	1.33
26	D	405	PL9	C48-C49	8.76	1.57	1.32
26	D	405	PL9	C43-C44	8.71	1.53	1.33
26	d	404	PL9	C43-C44	8.71	1.53	1.33
26	a	609	PL9	C28-C29	8.70	1.53	1.33
26	d	404	PL9	C28-C29	8.69	1.53	1.33
26	d	404	PL9	C48-C49	8.68	1.57	1.32
25	H	101	BCR	C26-C25	8.67	1.49	1.34
25	h	101	BCR	C26-C25	8.62	1.49	1.34
26	a	609	PL9	C13-C14	8.62	1.53	1.33
26	A	610	PL9	C43-C44	8.61	1.53	1.33
26	A	610	PL9	C28-C29	8.57	1.53	1.33
26	D	405	PL9	C8-C9	8.52	1.53	1.33
26	A	610	PL9	C48-C49	8.52	1.56	1.32
26	d	404	PL9	C8-C9	8.51	1.53	1.33
26	a	609	PL9	C8-C9	8.50	1.53	1.33
26	A	610	PL9	C8-C9	8.43	1.53	1.33
26	D	405	PL9	C28-C29	8.41	1.53	1.33
26	a	609	PL9	C43-C44	8.40	1.53	1.33
26	A	610	PL9	C33-C34	8.28	1.52	1.33
25	b	620	BCR	C26-C25	8.20	1.48	1.34
26	a	609	PL9	C33-C34	8.16	1.52	1.33
26	d	404	PL9	C33-C34	8.09	1.52	1.33
26	D	405	PL9	C33-C34	8.05	1.52	1.33
25	A	609	BCR	C8-C9	8.05	1.63	1.45
25	c	516	BCR	C26-C25	8.02	1.48	1.34
25	a	608	BCR	C8-C9	7.97	1.63	1.45
26	D	405	PL9	O1-C4	7.93	1.40	1.23
25	k	101	BCR	C26-C25	7.91	1.48	1.34
26	d	404	PL9	O1-C4	7.90	1.40	1.23
25	C	515	BCR	C26-C25	7.88	1.48	1.34
25	c	522	BCR	C26-C25	7.83	1.48	1.34
25	b	622	BCR	C26-C25	7.82	1.48	1.34
25	c	516	BCR	C8-C9	7.82	1.62	1.45
25	C	521	BCR	C26-C25	7.77	1.47	1.34
25	B	620	BCR	C26-C25	7.74	1.47	1.34
25	c	522	BCR	C8-C9	7.71	1.62	1.45
25	K	101	BCR	C26-C25	7.71	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	f	101	BCR	C8-C9	7.70	1.62	1.45
25	C	515	BCR	C8-C9	7.67	1.62	1.45
25	t	101	BCR	C8-C9	7.67	1.62	1.45
23	A	605	CLA	C3A-C2A	-7.67	1.33	1.54
25	B	618	BCR	C26-C25	7.62	1.47	1.34
23	a	604	CLA	C3A-C2A	-7.62	1.33	1.54
25	T	101	BCR	C8-C9	7.60	1.62	1.45
25	C	514	BCR	C26-C25	7.60	1.47	1.34
23	a	607	CLA	C3A-C2A	-7.59	1.33	1.54
23	b	611	CLA	C3A-C2A	-7.59	1.33	1.54
23	B	609	CLA	C3A-C2A	-7.55	1.33	1.54
25	K	101	BCR	C8-C9	7.55	1.62	1.45
26	A	610	PL9	O1-C4	7.54	1.39	1.23
23	b	610	CLA	C3A-C2A	-7.53	1.33	1.54
23	B	607[A]	CLA	C3A-C2A	-7.52	1.33	1.54
23	C	510	CLA	C3A-C2A	-7.52	1.33	1.54
23	B	607[B]	CLA	C3A-C2A	-7.51	1.33	1.54
25	h	101	BCR	C8-C9	7.51	1.62	1.45
23	b	613	CLA	C3A-C2A	-7.50	1.33	1.54
26	a	609	PL9	O1-C4	7.50	1.39	1.23
23	b	615	CLA	C3A-C2A	-7.50	1.33	1.54
25	k	101	BCR	C8-C9	7.49	1.62	1.45
23	C	505	CLA	C3A-C2A	-7.49	1.33	1.54
23	D	404	CLA	C3A-C2A	-7.49	1.33	1.54
23	b	607	CLA	C3A-C2A	-7.49	1.33	1.54
23	b	605	CLA	C3A-C2A	-7.49	1.33	1.54
23	c	511	CLA	C3A-C2A	-7.48	1.33	1.54
23	d	403	CLA	C3A-C2A	-7.48	1.33	1.54
23	c	507	CLA	C3A-C2A	-7.48	1.33	1.54
23	B	613	CLA	C3A-C2A	-7.47	1.33	1.54
23	B	611	CLA	C3A-C2A	-7.46	1.33	1.54
23	A	608	CLA	C3A-C2A	-7.46	1.33	1.54
23	b	609[B]	CLA	C3A-C2A	-7.45	1.33	1.54
23	D	403	CLA	C3A-C2A	-7.45	1.33	1.54
25	F	101	BCR	C8-C9	7.44	1.61	1.45
23	B	615	CLA	C3A-C2A	-7.44	1.33	1.54
23	b	617	CLA	C3A-C2A	-7.44	1.33	1.54
25	H	101	BCR	C8-C9	7.44	1.61	1.45
23	D	402	CLA	C3A-C2A	-7.44	1.33	1.54
23	B	614	CLA	C3A-C2A	-7.43	1.33	1.54
23	C	508	CLA	C3A-C2A	-7.42	1.33	1.54
23	b	606	CLA	C3A-C2A	-7.41	1.33	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	C3A-C2A	-7.41	1.33	1.54
23	C	512	CLA	C3A-C2A	-7.40	1.33	1.54
23	b	604	CLA	C3A-C2A	-7.40	1.33	1.54
23	C	501	CLA	C3A-C2A	-7.40	1.33	1.54
23	c	513	CLA	C3A-C2A	-7.40	1.33	1.54
23	B	605	CLA	C3A-C2A	-7.39	1.33	1.54
23	b	616	CLA	C3A-C2A	-7.39	1.33	1.54
25	c	515	BCR	C26-C25	7.39	1.47	1.34
23	d	402	CLA	C3A-C2A	-7.39	1.33	1.54
23	b	619	CLA	C3A-C2A	-7.39	1.33	1.54
23	C	502	CLA	C3A-C2A	-7.39	1.33	1.54
23	B	603	CLA	C3A-C2A	-7.38	1.33	1.54
23	c	512	CLA	C3A-C2A	-7.38	1.33	1.54
23	c	506	CLA	C3A-C2A	-7.38	1.33	1.54
23	a	613	CLA	C3A-C2A	-7.38	1.33	1.54
23	b	609[A]	CLA	C3A-C2A	-7.38	1.33	1.54
23	b	614	CLA	C3A-C2A	-7.37	1.33	1.54
23	c	503	CLA	C3A-C2A	-7.36	1.33	1.54
25	C	521	BCR	C8-C9	7.36	1.61	1.45
23	B	606	CLA	C3A-C2A	-7.36	1.33	1.54
23	b	608	CLA	C3A-C2A	-7.36	1.33	1.54
23	a	605	CLA	C3A-C2A	-7.35	1.33	1.54
23	C	503	CLA	C3A-C2A	-7.35	1.33	1.54
23	C	511	CLA	C3A-C2A	-7.35	1.33	1.54
23	B	612	CLA	C3A-C2A	-7.34	1.34	1.54
23	c	514	CLA	C3A-C2A	-7.34	1.34	1.54
23	B	608	CLA	C3A-C2A	-7.34	1.34	1.54
23	B	604	CLA	C3A-C2A	-7.33	1.34	1.54
23	c	502	CLA	C3A-C2A	-7.33	1.34	1.54
23	b	618	CLA	C3A-C2A	-7.33	1.34	1.54
23	c	509	CLA	C3A-C2A	-7.32	1.34	1.54
25	B	619	BCR	C8-C9	7.32	1.61	1.45
23	c	510	CLA	C3A-C2A	-7.31	1.34	1.54
23	C	504	CLA	C3A-C2A	-7.30	1.34	1.54
23	C	506	CLA	C3A-C2A	-7.30	1.34	1.54
23	A	606	CLA	C3A-C2A	-7.30	1.34	1.54
23	B	617	CLA	C3A-C2A	-7.30	1.34	1.54
23	c	505	CLA	C3A-C2A	-7.29	1.34	1.54
23	B	610	CLA	C3A-C2A	-7.29	1.34	1.54
23	B	602	CLA	C3A-C2A	-7.29	1.34	1.54
25	c	515	BCR	C34-C9	-7.28	1.35	1.50
23	C	509	CLA	C3A-C2A	-7.27	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	C3A-C2A	-7.26	1.34	1.54
25	t	101	BCR	C26-C25	7.24	1.47	1.34
25	b	622	BCR	C8-C9	7.22	1.61	1.45
25	B	618	BCR	C34-C9	-7.21	1.36	1.50
23	C	513	CLA	C3A-C2A	-7.20	1.34	1.54
25	B	619	BCR	C34-C9	-7.19	1.36	1.50
25	b	621	BCR	C8-C9	7.19	1.61	1.45
25	K	101	BCR	C34-C9	-7.18	1.36	1.50
25	b	621	BCR	C34-C9	-7.18	1.36	1.50
23	B	616	CLA	C3A-C2A	-7.17	1.34	1.54
23	c	508	CLA	C3A-C2A	-7.17	1.34	1.54
25	T	101	BCR	C26-C25	7.17	1.46	1.34
25	c	515	BCR	C8-C9	7.14	1.61	1.45
25	b	620	BCR	C8-C9	7.11	1.61	1.45
23	C	507	CLA	C3A-C2A	-7.10	1.34	1.54
25	k	101	BCR	C34-C9	-7.09	1.36	1.50
25	B	618	BCR	C8-C9	7.08	1.61	1.45
25	c	516	BCR	C34-C9	-7.03	1.36	1.50
25	C	514	BCR	C8-C9	7.03	1.61	1.45
25	B	620	BCR	C8-C9	7.00	1.61	1.45
25	B	620	BCR	C34-C9	-6.96	1.36	1.50
25	H	101	BCR	C34-C9	-6.93	1.36	1.50
25	b	620	BCR	C34-C9	-6.93	1.36	1.50
25	f	101	BCR	C38-C26	6.92	1.62	1.50
25	C	515	BCR	C34-C9	-6.92	1.36	1.50
25	f	101	BCR	C34-C9	-6.90	1.36	1.50
25	T	101	BCR	C34-C9	-6.89	1.36	1.50
25	t	101	BCR	C34-C9	-6.89	1.36	1.50
25	C	514	BCR	C34-C9	-6.88	1.36	1.50
25	a	608	BCR	C34-C9	-6.87	1.36	1.50
25	F	101	BCR	C34-C9	-6.85	1.36	1.50
25	A	609	BCR	C34-C9	-6.83	1.36	1.50
25	h	101	BCR	C34-C9	-6.82	1.36	1.50
25	C	521	BCR	C34-C9	-6.81	1.36	1.50
25	F	101	BCR	C38-C26	6.79	1.62	1.50
25	b	622	BCR	C34-C9	-6.79	1.36	1.50
25	c	522	BCR	C34-C9	-6.76	1.36	1.50
25	A	609	BCR	C38-C26	6.62	1.61	1.50
23	b	607	CLA	C1B-NB	-6.60	1.29	1.35
26	a	609	PL9	O2-C1	6.58	1.42	1.24
23	b	606	CLA	C1B-NB	-6.57	1.29	1.35
23	b	610	CLA	C1B-NB	-6.56	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	CLA	C1B-NB	-6.54	1.29	1.35
25	h	101	BCR	C38-C26	6.54	1.61	1.50
23	B	612	CLA	C1B-NB	-6.54	1.29	1.35
23	D	403	CLA	C1B-NB	-6.53	1.29	1.35
23	C	508	CLA	C1B-NB	-6.53	1.29	1.35
23	c	507	CLA	C1B-NB	-6.52	1.29	1.35
23	b	614	CLA	C1B-NB	-6.51	1.29	1.35
25	H	101	BCR	C38-C26	6.51	1.61	1.50
26	A	610	PL9	O2-C1	6.51	1.41	1.24
23	B	604	CLA	C1B-NB	-6.49	1.29	1.35
25	a	608	BCR	C38-C26	6.49	1.61	1.50
25	B	619	BCR	C38-C26	6.48	1.61	1.50
23	B	605	CLA	C1B-NB	-6.43	1.29	1.35
23	C	509	CLA	C1B-NB	-6.43	1.29	1.35
23	B	613	CLA	C1B-NB	-6.40	1.29	1.35
23	b	615	CLA	C1B-NB	-6.39	1.29	1.35
26	D	405	PL9	O2-C1	6.38	1.41	1.24
23	b	605	CLA	C1B-NB	-6.38	1.29	1.35
25	b	621	BCR	C38-C26	6.38	1.61	1.50
23	C	502	CLA	C1B-NB	-6.27	1.29	1.35
23	c	509	CLA	C1B-NB	-6.24	1.29	1.35
23	c	502	CLA	C1B-NB	-6.23	1.29	1.35
26	d	404	PL9	O2-C1	6.23	1.41	1.24
23	A	606	CLA	C1B-NB	-6.20	1.29	1.35
25	B	618	BCR	C23-C22	6.19	1.59	1.45
25	c	522	BCR	C38-C26	6.18	1.61	1.50
23	C	510	CLA	C1B-NB	-6.17	1.29	1.35
25	C	515	BCR	C38-C26	6.15	1.61	1.50
23	C	512	CLA	C1B-NB	-6.15	1.29	1.35
25	b	622	BCR	C23-C22	6.14	1.59	1.45
23	b	606	CLA	C3D-C2D	-6.14	1.28	1.39
23	B	614	CLA	C1B-NB	-6.14	1.29	1.35
23	b	609[B]	CLA	C1B-NB	-6.14	1.29	1.35
23	c	510	CLA	C1B-NB	-6.13	1.29	1.35
23	a	604	CLA	C1B-NB	-6.13	1.29	1.35
23	C	503	CLA	C1B-NB	-6.13	1.29	1.35
23	B	603	CLA	C1B-NB	-6.12	1.29	1.35
25	c	516	BCR	C38-C26	6.12	1.61	1.50
23	a	605	CLA	C1B-NB	-6.11	1.29	1.35
23	b	610	CLA	C3D-C2D	-6.10	1.28	1.39
23	B	606	CLA	C3D-C2D	-6.10	1.28	1.39
23	b	608	CLA	C3D-C2D	-6.10	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	C1B-NB	-6.08	1.29	1.35
23	C	501	CLA	C1B-NB	-6.06	1.29	1.35
25	C	521	BCR	C38-C26	6.05	1.60	1.50
23	C	503	CLA	C3D-C2D	-6.04	1.28	1.39
25	k	101	BCR	C38-C26	6.02	1.60	1.50
25	B	620	BCR	C38-C26	6.02	1.60	1.50
23	a	613	CLA	C1B-NB	-6.02	1.29	1.35
25	B	620	BCR	C23-C22	6.00	1.58	1.45
25	b	622	BCR	C38-C26	6.00	1.60	1.50
23	A	605	CLA	C1B-NB	-5.97	1.29	1.35
23	b	617	CLA	C1B-NB	-5.96	1.29	1.35
23	c	506	CLA	C1B-NB	-5.96	1.29	1.35
23	D	402	CLA	C1B-NB	-5.96	1.29	1.35
23	a	605	CLA	C3D-C2D	-5.95	1.28	1.39
23	c	512	CLA	C1B-NB	-5.95	1.29	1.35
23	A	606	CLA	C3D-C2D	-5.94	1.28	1.39
23	b	608	CLA	C1B-NB	-5.94	1.29	1.35
23	B	607[A]	CLA	C1B-NB	-5.93	1.29	1.35
23	c	511	CLA	C1B-NB	-5.92	1.29	1.35
23	C	509	CLA	C3D-C2D	-5.92	1.28	1.39
23	b	617	CLA	C3D-C2D	-5.91	1.28	1.39
25	K	101	BCR	C38-C26	5.91	1.60	1.50
23	b	615	CLA	C3D-C2D	-5.90	1.28	1.39
23	b	609[B]	CLA	C3D-C2D	-5.89	1.28	1.39
23	c	506	CLA	C3D-C2D	-5.89	1.28	1.39
23	C	505	CLA	C1B-NB	-5.89	1.30	1.35
23	B	616	CLA	C3D-C2D	-5.89	1.28	1.39
23	C	506	CLA	C1B-NB	-5.89	1.30	1.35
23	c	514	CLA	C1B-NB	-5.89	1.30	1.35
23	B	614	CLA	C3D-C2D	-5.89	1.28	1.39
23	C	504	CLA	C1B-NB	-5.88	1.30	1.35
23	b	618	CLA	C3D-C2D	-5.87	1.28	1.39
23	C	510	CLA	C3D-C2D	-5.87	1.28	1.39
23	B	607[B]	CLA	C1B-NB	-5.86	1.30	1.35
23	C	511	CLA	C1B-NB	-5.86	1.30	1.35
25	b	620	BCR	C38-C26	5.85	1.60	1.50
23	b	616	CLA	C1B-NB	-5.85	1.30	1.35
23	c	504	CLA	C3D-C2D	-5.84	1.28	1.39
25	C	514	BCR	C38-C26	5.83	1.60	1.50
23	c	505	CLA	C3D-C2D	-5.83	1.29	1.39
23	c	511	CLA	C3D-C2D	-5.83	1.29	1.39
23	d	402	CLA	C3D-C2D	-5.83	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	C3D-C2D	-5.83	1.29	1.39
23	b	609[A]	CLA	C1B-NB	-5.82	1.30	1.35
23	B	615	CLA	C1B-NB	-5.82	1.30	1.35
23	c	510	CLA	C3D-C2D	-5.82	1.29	1.39
23	c	503	CLA	C1B-NB	-5.82	1.30	1.35
23	A	605	CLA	C3D-C2D	-5.82	1.29	1.39
23	b	607	CLA	C3D-C2D	-5.82	1.29	1.39
23	D	403	CLA	C3D-C2D	-5.80	1.29	1.39
23	a	607	CLA	C3D-C2D	-5.80	1.29	1.39
23	C	506	CLA	C3D-C2D	-5.80	1.29	1.39
23	B	606	CLA	C1B-NB	-5.80	1.30	1.35
23	a	613	CLA	C3D-C2D	-5.79	1.29	1.39
23	C	513	CLA	C1B-NB	-5.79	1.30	1.35
23	A	608	CLA	C1B-NB	-5.78	1.30	1.35
23	B	617	CLA	C1B-NB	-5.78	1.30	1.35
23	b	619	CLA	C1B-NB	-5.77	1.30	1.35
23	B	615	CLA	C3D-C2D	-5.77	1.29	1.39
25	T	101	BCR	C38-C26	5.77	1.60	1.50
23	c	505	CLA	C1B-NB	-5.77	1.30	1.35
23	b	616	CLA	C3D-C2D	-5.76	1.29	1.39
23	C	511	CLA	C3D-C2D	-5.76	1.29	1.39
23	a	607	CLA	C1B-NB	-5.76	1.30	1.35
23	d	403	CLA	C1B-NB	-5.75	1.30	1.35
25	c	515	BCR	C38-C26	5.75	1.60	1.50
23	B	607[B]	CLA	C3D-C2D	-5.74	1.29	1.39
23	C	505	CLA	C3D-C2D	-5.74	1.29	1.39
23	D	402	CLA	C3D-C2D	-5.74	1.29	1.39
23	B	613	CLA	C3D-C2D	-5.74	1.29	1.39
23	a	604	CLA	C3D-C2D	-5.73	1.29	1.39
23	B	609	CLA	C3D-C2D	-5.73	1.29	1.39
25	B	618	BCR	C38-C26	5.73	1.60	1.50
23	B	605	CLA	C3D-C2D	-5.72	1.29	1.39
25	t	101	BCR	C38-C26	5.72	1.60	1.50
23	b	618	CLA	C1B-NB	-5.71	1.30	1.35
23	b	613	CLA	C1B-NB	-5.71	1.30	1.35
23	b	605	CLA	C3D-C2D	-5.70	1.29	1.39
23	c	507	CLA	C3D-C2D	-5.70	1.29	1.39
23	C	508	CLA	C3D-C2D	-5.70	1.29	1.39
23	D	404	CLA	C1B-NB	-5.69	1.30	1.35
23	c	504	CLA	C1B-NB	-5.69	1.30	1.35
23	c	512	CLA	C3D-C2D	-5.69	1.29	1.39
23	c	513	CLA	C3D-C2D	-5.69	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	101	BCR	C23-C22	5.68	1.58	1.45
23	B	602	CLA	C3D-C2D	-5.68	1.29	1.39
23	B	603	CLA	C3D-C2D	-5.68	1.29	1.39
23	b	614	CLA	C3D-C2D	-5.67	1.29	1.39
23	B	617	CLA	C3D-C2D	-5.67	1.29	1.39
23	B	608	CLA	C3D-C2D	-5.66	1.29	1.39
23	D	404	CLA	C3D-C2D	-5.65	1.29	1.39
23	b	604	CLA	C3D-C2D	-5.65	1.29	1.39
23	C	513	CLA	C3D-C2D	-5.65	1.29	1.39
23	b	619	CLA	C3D-C2D	-5.64	1.29	1.39
23	B	616	CLA	C1B-NB	-5.64	1.30	1.35
23	B	607[A]	CLA	C3D-C2D	-5.63	1.29	1.39
23	c	508	CLA	C1B-NB	-5.63	1.30	1.35
23	c	509	CLA	C3D-C2D	-5.63	1.29	1.39
23	C	504	CLA	C3D-C2D	-5.63	1.29	1.39
25	K	101	BCR	C23-C22	5.62	1.58	1.45
23	B	611	CLA	C1B-NB	-5.62	1.30	1.35
25	t	101	BCR	C23-C22	5.61	1.58	1.45
23	b	611	CLA	C3D-C2D	-5.60	1.29	1.39
23	C	507	CLA	C3D-C2D	-5.60	1.29	1.39
23	b	613	CLA	C3D-C2D	-5.57	1.29	1.39
23	B	608	CLA	C1B-NB	-5.56	1.30	1.35
23	b	609[A]	CLA	C3D-C2D	-5.56	1.29	1.39
23	c	514	CLA	C3D-C2D	-5.55	1.29	1.39
23	c	503	CLA	C3D-C2D	-5.55	1.29	1.39
23	A	608	CLA	C3D-C2D	-5.54	1.29	1.39
23	B	612	CLA	C3D-C2D	-5.54	1.29	1.39
23	c	508	CLA	C3D-C2D	-5.53	1.29	1.39
23	c	502	CLA	C3D-C2D	-5.52	1.29	1.39
23	B	602	CLA	C1B-NB	-5.51	1.30	1.35
25	b	621	BCR	C24-C23	5.51	1.49	1.33
25	C	514	BCR	C23-C22	5.50	1.57	1.45
25	h	101	BCR	C23-C22	5.49	1.57	1.45
25	k	101	BCR	C23-C22	5.49	1.57	1.45
25	c	516	BCR	C11-C12	5.49	1.48	1.34
23	C	512	CLA	C3D-C2D	-5.49	1.29	1.39
25	c	516	BCR	C23-C22	5.49	1.57	1.45
33	v	201	HEM	C3D-C2D	5.47	1.53	1.37
23	b	604	CLA	C1B-NB	-5.47	1.30	1.35
23	B	609	CLA	C1B-NB	-5.47	1.30	1.35
25	C	521	BCR	C24-C23	5.47	1.49	1.33
23	B	610	CLA	C3D-C2D	-5.46	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	621	BCR	C23-C22	5.46	1.57	1.45
23	B	610	CLA	C1B-NB	-5.46	1.30	1.35
25	c	522	BCR	C24-C23	5.45	1.49	1.33
23	b	611	CLA	C1B-NB	-5.45	1.30	1.35
23	C	507	CLA	C1B-NB	-5.44	1.30	1.35
23	C	501	CLA	C3D-C2D	-5.44	1.29	1.39
25	t	101	BCR	C11-C12	5.43	1.48	1.34
23	B	611	CLA	C3D-C2D	-5.43	1.29	1.39
23	C	502	CLA	C3D-C2D	-5.43	1.29	1.39
25	T	101	BCR	C11-C12	5.42	1.48	1.34
25	B	618	BCR	C24-C23	5.41	1.49	1.33
23	d	403	CLA	C3D-C2D	-5.40	1.29	1.39
25	F	101	BCR	C24-C23	5.39	1.49	1.33
23	b	612	CLA	C3D-C2D	-5.39	1.29	1.39
25	h	101	BCR	C11-C12	5.36	1.48	1.34
26	d	404	PL9	C3-C4	-5.36	1.40	1.49
25	a	608	BCR	C11-C12	5.36	1.48	1.34
25	B	619	BCR	C24-C23	5.35	1.49	1.33
25	A	609	BCR	C11-C12	5.35	1.48	1.34
25	C	515	BCR	C23-C22	5.35	1.57	1.45
25	B	620	BCR	C24-C23	5.34	1.49	1.33
25	c	522	BCR	C11-C12	5.32	1.48	1.34
33	V	202	HEM	C3D-C2D	5.31	1.53	1.37
33	e	102	HEM	C3D-C2D	5.30	1.53	1.37
25	C	521	BCR	C23-C22	5.29	1.57	1.45
25	c	522	BCR	C23-C22	5.29	1.57	1.45
25	a	608	BCR	C24-C23	5.28	1.49	1.33
25	f	101	BCR	C24-C23	5.28	1.49	1.33
25	b	622	BCR	C24-C23	5.28	1.49	1.33
25	k	101	BCR	C11-C12	5.27	1.48	1.34
25	t	101	BCR	C24-C23	5.25	1.48	1.33
25	C	515	BCR	C11-C12	5.25	1.48	1.34
25	C	515	BCR	C17-C18	5.25	1.42	1.35
33	E	102	HEM	C3D-C2D	5.25	1.53	1.37
25	f	101	BCR	C23-C22	5.24	1.57	1.45
25	H	101	BCR	C11-C12	5.22	1.48	1.34
25	b	622	BCR	C11-C12	5.21	1.48	1.34
25	c	515	BCR	C23-C22	5.21	1.57	1.45
25	k	101	BCR	C24-C23	5.18	1.48	1.33
25	c	516	BCR	C24-C23	5.17	1.48	1.33
25	A	609	BCR	C24-C23	5.17	1.48	1.33
25	K	101	BCR	C24-C23	5.16	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	609	BCR	C23-C22	5.15	1.57	1.45
25	C	521	BCR	C11-C12	5.13	1.47	1.34
25	B	619	BCR	C17-C18	5.13	1.42	1.35
25	C	515	BCR	C24-C23	5.12	1.48	1.33
25	B	620	BCR	C11-C12	5.11	1.47	1.34
25	C	514	BCR	C24-C23	5.10	1.48	1.33
23	b	612	CLA	C1B-NB	-5.08	1.30	1.35
26	A	610	PL9	C3-C4	-5.06	1.41	1.49
26	D	405	PL9	C3-C4	-5.05	1.41	1.49
25	a	608	BCR	C23-C22	5.03	1.56	1.45
25	K	101	BCR	C11-C12	5.00	1.47	1.34
25	F	101	BCR	C23-C22	4.99	1.56	1.45
26	a	609	PL9	C3-C4	-4.98	1.41	1.49
25	B	618	BCR	C11-C12	4.96	1.47	1.34
25	c	515	BCR	C11-C12	4.96	1.47	1.34
25	B	619	BCR	C24-C25	4.96	1.62	1.45
25	c	515	BCR	C24-C23	4.88	1.47	1.33
25	f	101	BCR	C11-C12	4.87	1.47	1.34
25	F	101	BCR	C24-C25	4.86	1.62	1.45
25	H	101	BCR	C24-C23	4.86	1.47	1.33
23	a	613	CLA	C4B-CHC	-4.86	1.27	1.41
25	b	620	BCR	C23-C22	4.86	1.56	1.45
25	T	101	BCR	C24-C23	4.85	1.47	1.33
25	F	101	BCR	C11-C12	4.85	1.47	1.34
23	B	605	CLA	C4B-CHC	-4.85	1.27	1.41
25	b	620	BCR	C24-C23	4.85	1.47	1.33
25	b	621	BCR	C24-C25	4.84	1.62	1.45
23	b	610	CLA	C4B-CHC	-4.82	1.27	1.41
25	C	514	BCR	C11-C12	4.81	1.47	1.34
23	b	614	CLA	C4B-CHC	-4.80	1.27	1.41
25	a	608	BCR	C24-C25	4.77	1.62	1.45
23	B	617	CLA	C4B-CHC	-4.76	1.27	1.41
25	b	620	BCR	C17-C18	4.76	1.42	1.35
25	H	101	BCR	C23-C22	4.76	1.56	1.45
25	b	620	BCR	C11-C12	4.76	1.46	1.34
25	a	608	BCR	C17-C18	4.74	1.42	1.35
25	B	619	BCR	C11-C12	4.72	1.46	1.34
25	h	101	BCR	C24-C23	4.72	1.47	1.33
23	b	607	CLA	C4B-CHC	-4.72	1.27	1.41
23	c	510	CLA	C4B-CHC	-4.71	1.27	1.41
23	B	608	CLA	C4B-CHC	-4.71	1.27	1.41
23	b	606	CLA	C4B-CHC	-4.70	1.27	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	H	101	BCR	C17-C18	4.70	1.42	1.35
23	c	513	CLA	C4B-CHC	-4.69	1.27	1.41
23	B	614	CLA	C4B-CHC	-4.69	1.27	1.41
25	f	101	BCR	C24-C25	4.69	1.61	1.45
23	B	612	CLA	C4B-CHC	-4.68	1.28	1.41
23	C	512	CLA	C4B-CHC	-4.68	1.28	1.41
23	C	510	CLA	C4B-CHC	-4.67	1.28	1.41
23	b	619	CLA	C4B-CHC	-4.66	1.28	1.41
23	B	604	CLA	C4B-CHC	-4.66	1.28	1.41
25	A	609	BCR	C24-C25	4.66	1.61	1.45
23	C	504	CLA	C4B-CHC	-4.66	1.28	1.41
23	b	615	CLA	C4B-CHC	-4.66	1.28	1.41
23	C	508	CLA	C4B-CHC	-4.65	1.28	1.41
23	B	613	CLA	C4B-CHC	-4.65	1.28	1.41
25	B	619	BCR	C23-C22	4.65	1.55	1.45
23	C	509	CLA	C4B-CHC	-4.63	1.28	1.41
23	c	511	CLA	C4B-CHC	-4.62	1.28	1.41
23	D	402	CLA	C4B-CHC	-4.62	1.28	1.41
23	a	607	CLA	C4C-CHD	-4.62	1.28	1.41
23	C	506	CLA	C4B-CHC	-4.62	1.28	1.41
23	C	507	CLA	C4B-CHC	-4.62	1.28	1.41
31	B	622	LHG	O8-C23	4.61	1.46	1.33
23	d	402	CLA	C4B-CHC	-4.61	1.28	1.41
23	b	616	CLA	C4B-CHC	-4.61	1.28	1.41
23	B	606	CLA	C4B-CHC	-4.61	1.28	1.41
25	b	621	BCR	C11-C12	4.61	1.46	1.34
23	c	506	CLA	C4B-CHC	-4.61	1.28	1.41
23	a	605	CLA	C4B-CHC	-4.61	1.28	1.41
23	c	503	CLA	C4B-CHC	-4.60	1.28	1.41
23	B	602	CLA	C4B-CHC	-4.60	1.28	1.41
23	c	508	CLA	C4B-CHC	-4.60	1.28	1.41
26	d	404	PL9	C6-C1	-4.60	1.40	1.48
23	b	604	CLA	C4B-CHC	-4.60	1.28	1.41
23	B	610	CLA	C4B-CHC	-4.59	1.28	1.41
23	c	512	CLA	C4B-CHC	-4.59	1.28	1.41
23	b	617	CLA	C4B-CHC	-4.58	1.28	1.41
26	D	405	PL9	C6-C1	-4.58	1.40	1.48
23	A	606	CLA	C4B-CHC	-4.58	1.28	1.41
28	c	521	LMG	O7-C10	4.58	1.47	1.34
23	a	604	CLA	C4B-CHC	-4.57	1.28	1.41
23	D	403	CLA	C4B-CHC	-4.57	1.28	1.41
23	c	505	CLA	C4B-CHC	-4.57	1.28	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	501	CLA	C4B-CHC	-4.57	1.28	1.41
23	B	616	CLA	C4B-CHC	-4.57	1.28	1.41
28	C	520	LMG	O7-C10	4.56	1.47	1.34
23	c	507	CLA	C4B-CHC	-4.55	1.28	1.41
23	C	503	CLA	C4B-CHC	-4.55	1.28	1.41
23	d	403	CLA	C4B-CHC	-4.54	1.28	1.41
27	X	101	SQD	O48-C23	4.54	1.46	1.33
23	c	504	CLA	C4B-CHC	-4.54	1.28	1.41
23	B	607[A]	CLA	C4B-CHC	-4.54	1.28	1.41
23	C	502	CLA	C4B-CHC	-4.54	1.28	1.41
27	x	101	SQD	O48-C23	4.53	1.46	1.33
23	D	404	CLA	C4B-CHC	-4.53	1.28	1.41
23	B	609	CLA	C4B-CHC	-4.53	1.28	1.41
23	b	608	CLA	C4B-CHC	-4.53	1.28	1.41
31	l	101	LHG	O8-C23	4.53	1.46	1.33
23	b	618	CLA	C4B-CHC	-4.52	1.28	1.41
23	C	511	CLA	C4B-CHC	-4.52	1.28	1.41
23	c	502	CLA	C4B-CHC	-4.52	1.28	1.41
28	c	520	LMG	O7-C10	4.52	1.47	1.34
23	C	507	CLA	C4C-CHD	-4.51	1.28	1.41
23	c	509	CLA	C4B-CHC	-4.51	1.28	1.41
23	B	615	CLA	C4B-CHC	-4.50	1.28	1.41
23	b	609[B]	CLA	C4B-CHC	-4.49	1.28	1.41
23	b	612	CLA	C4B-CHC	-4.49	1.28	1.41
28	a	611	LMG	O7-C10	4.49	1.47	1.34
31	d	406	LHG	O8-C23	4.49	1.46	1.33
23	B	603	CLA	C4B-CHC	-4.49	1.28	1.41
23	c	508	CLA	C4C-CHD	-4.49	1.28	1.41
27	b	601	SQD	O48-C23	4.48	1.46	1.33
27	a	612	SQD	O48-C23	4.48	1.46	1.33
23	b	605	CLA	C4B-CHC	-4.48	1.28	1.41
27	X	101	SQD	O47-C7	4.47	1.46	1.34
25	C	514	BCR	C17-C18	4.47	1.41	1.35
27	x	101	SQD	O47-C7	4.47	1.46	1.34
23	B	614	CLA	C4C-CHD	-4.47	1.28	1.41
23	B	616	CLA	C4C-CHD	-4.47	1.28	1.41
23	b	613	CLA	C4B-CHC	-4.47	1.28	1.41
23	c	514	CLA	C4B-CHC	-4.46	1.28	1.41
23	A	608	CLA	C4C-CHD	-4.46	1.28	1.41
23	c	506	CLA	C4C-CHD	-4.46	1.28	1.41
23	b	609[A]	CLA	C4B-CHC	-4.46	1.28	1.41
23	A	605	CLA	C4B-CHC	-4.46	1.28	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	C4C-CHD	-4.45	1.28	1.41
23	C	505	CLA	C4B-CHC	-4.45	1.28	1.41
23	A	608	CLA	C4B-CHC	-4.45	1.28	1.41
23	b	608	CLA	C4C-CHD	-4.45	1.28	1.41
23	b	614	CLA	C4C-CHD	-4.45	1.28	1.41
28	z	101	LMG	O7-C10	4.45	1.46	1.34
28	C	519	LMG	O7-C10	4.45	1.46	1.34
31	e	101	LHG	O8-C23	4.45	1.46	1.33
31	D	407	LHG	O8-C23	4.45	1.46	1.33
23	B	607[B]	CLA	C4B-CHC	-4.45	1.28	1.41
23	b	618	CLA	C4C-CHD	-4.44	1.28	1.41
25	c	516	BCR	C17-C18	4.44	1.41	1.35
23	b	606	CLA	C4C-CHD	-4.44	1.28	1.41
23	C	509	CLA	C4C-CHD	-4.43	1.28	1.41
23	B	611	CLA	C4B-CHC	-4.43	1.28	1.41
25	c	522	BCR	C17-C18	4.42	1.41	1.35
23	c	510	CLA	C4C-CHD	-4.42	1.28	1.41
28	A	612	LMG	O7-C10	4.42	1.46	1.34
23	C	513	CLA	C4B-CHC	-4.42	1.28	1.41
23	b	611	CLA	C4B-CHC	-4.41	1.28	1.41
27	B	623	SQD	O48-C23	4.41	1.46	1.33
23	B	613	CLA	C4C-CHD	-4.41	1.28	1.41
25	c	522	BCR	C24-C25	4.41	1.60	1.45
27	b	602	SQD	O48-C23	4.41	1.46	1.33
23	b	612	CLA	C4C-CHD	-4.41	1.28	1.41
25	f	101	BCR	C17-C18	4.41	1.41	1.35
23	D	404	CLA	C4C-CHD	-4.41	1.28	1.41
23	b	615	CLA	C4C-CHD	-4.41	1.28	1.41
23	C	508	CLA	C4C-CHD	-4.41	1.28	1.41
23	C	505	CLA	C4C-CHD	-4.40	1.28	1.41
23	b	604	CLA	C4C-CHD	-4.40	1.28	1.41
23	B	606	CLA	C4C-CHD	-4.40	1.28	1.41
32	D	406	DGD	O2G-C1B	4.40	1.46	1.34
27	b	602	SQD	O47-C7	4.40	1.46	1.34
23	b	610	CLA	C4C-CHD	-4.40	1.28	1.41
23	b	613	CLA	C4C-CHD	-4.40	1.28	1.41
23	C	503	CLA	C4C-CHD	-4.40	1.28	1.41
23	b	619	CLA	C4C-CHD	-4.40	1.28	1.41
23	B	607[B]	CLA	C4C-CHD	-4.40	1.28	1.41
23	B	607[A]	CLA	C4C-CHD	-4.39	1.28	1.41
27	B	623	SQD	O47-C7	4.39	1.46	1.34
23	C	512	CLA	C4C-CHD	-4.39	1.28	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	H	101	BCR	C24-C25	4.38	1.60	1.45
23	C	502	CLA	C4C-CHD	-4.38	1.28	1.41
23	c	511	CLA	C4C-CHD	-4.38	1.28	1.41
31	E	101	LHG	O8-C23	4.38	1.46	1.33
23	C	506	CLA	C4C-CHD	-4.38	1.28	1.41
23	a	607	CLA	C4B-CHC	-4.38	1.28	1.41
28	Z	101	LMG	O7-C10	4.38	1.46	1.34
23	b	609[B]	CLA	C4C-CHD	-4.38	1.28	1.41
23	b	617	CLA	C4C-CHD	-4.38	1.28	1.41
31	L	101	LHG	O8-C23	4.37	1.46	1.33
23	B	611	CLA	C4C-CHD	-4.37	1.28	1.41
23	c	503	CLA	C4C-CHD	-4.37	1.28	1.41
23	d	403	CLA	C4C-CHD	-4.37	1.28	1.41
23	A	606	CLA	C4C-CHD	-4.37	1.28	1.41
31	b	624	LHG	O8-C23	4.36	1.46	1.33
23	B	605	CLA	C4C-CHD	-4.36	1.28	1.41
31	a	614	LHG	O8-C23	4.36	1.46	1.33
23	B	610	CLA	C4C-CHD	-4.35	1.28	1.41
25	k	101	BCR	C24-C25	4.35	1.60	1.45
23	c	512	CLA	C4C-CHD	-4.35	1.28	1.41
23	c	504	CLA	C4C-CHD	-4.34	1.28	1.41
23	C	501	CLA	C4C-CHD	-4.34	1.28	1.41
23	D	403	CLA	C4C-CHD	-4.33	1.29	1.41
23	C	511	CLA	C4C-CHD	-4.32	1.29	1.41
32	d	405	DGD	O2G-C1B	4.32	1.46	1.34
23	c	513	CLA	C4C-CHD	-4.32	1.29	1.41
31	D	408	LHG	O8-C23	4.31	1.45	1.33
25	K	101	BCR	C24-C25	4.31	1.60	1.45
25	B	620	BCR	C24-C25	4.31	1.60	1.45
23	B	615	CLA	C4C-CHD	-4.31	1.29	1.41
26	A	610	PL9	C6-C1	-4.31	1.40	1.48
28	b	623	LMG	O7-C10	4.31	1.46	1.34
23	B	608	CLA	C4C-CHD	-4.30	1.29	1.41
23	B	602	CLA	C4C-CHD	-4.30	1.29	1.41
23	b	609[A]	CLA	C4C-CHD	-4.30	1.29	1.41
23	b	605	CLA	C4C-CHD	-4.30	1.29	1.41
23	B	612	CLA	C4C-CHD	-4.30	1.29	1.41
23	B	617	CLA	C4C-CHD	-4.30	1.29	1.41
23	b	607	CLA	C4C-CHD	-4.30	1.29	1.41
23	c	509	CLA	C4C-CHD	-4.30	1.29	1.41
23	C	510	CLA	C4C-CHD	-4.29	1.29	1.41
23	C	513	CLA	C4C-CHD	-4.29	1.29	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	601	SQD	O47-C7	4.28	1.46	1.34
23	d	402	CLA	C4C-CHD	-4.28	1.29	1.41
27	a	612	SQD	O47-C7	4.28	1.46	1.34
23	c	505	CLA	C4C-CHD	-4.27	1.29	1.41
23	c	507	CLA	C4C-CHD	-4.27	1.29	1.41
25	b	622	BCR	C24-C25	4.26	1.60	1.45
23	C	504	CLA	C4C-CHD	-4.26	1.29	1.41
23	a	605	CLA	C4C-CHD	-4.26	1.29	1.41
23	c	502	CLA	C4C-CHD	-4.25	1.29	1.41
25	c	515	BCR	C17-C18	4.25	1.41	1.35
23	a	604	CLA	C4C-CHD	-4.25	1.29	1.41
23	B	604	CLA	C4C-CHD	-4.25	1.29	1.41
23	B	603	CLA	C4C-CHD	-4.25	1.29	1.41
26	a	609	PL9	C6-C1	-4.24	1.41	1.48
23	A	605	CLA	C4C-CHD	-4.24	1.29	1.41
28	B	621	LMG	O7-C10	4.23	1.46	1.34
25	h	101	BCR	C24-C25	4.23	1.60	1.45
32	D	406	DGD	O1G-C1A	4.23	1.45	1.33
31	l	101	LHG	O7-C7	4.23	1.46	1.34
28	j	101	LMG	O7-C10	4.23	1.46	1.34
25	C	521	BCR	C24-C25	4.22	1.60	1.45
25	c	516	BCR	C24-C25	4.21	1.60	1.45
28	J	101	LMG	O7-C10	4.21	1.46	1.34
23	B	609	CLA	C4C-CHD	-4.21	1.29	1.41
32	C	516	DGD	O2G-C1B	4.20	1.46	1.34
31	E	101	LHG	O7-C7	4.20	1.46	1.34
31	e	101	LHG	O7-C7	4.20	1.46	1.34
23	c	514	CLA	C4C-CHD	-4.19	1.29	1.41
23	D	402	CLA	C4C-CHD	-4.18	1.29	1.41
23	b	611	CLA	C4C-CHD	-4.18	1.29	1.41
23	a	613	CLA	CMA-C3A	-4.17	1.44	1.53
32	h	102	DGD	O2G-C1B	4.17	1.46	1.34
25	C	515	BCR	C24-C25	4.16	1.59	1.45
33	v	201	HEM	C3C-C2C	-4.16	1.34	1.40
32	c	517	DGD	O2G-C1B	4.16	1.46	1.34
32	C	517	DGD	O2G-C1B	4.16	1.46	1.34
25	b	622	BCR	C17-C18	4.16	1.41	1.35
23	B	605	CLA	CMA-C3A	-4.16	1.44	1.53
23	a	613	CLA	C4C-CHD	-4.15	1.29	1.41
31	D	408	LHG	O7-C7	4.15	1.46	1.34
23	c	506	CLA	C1D-C2D	-4.14	1.33	1.42
23	B	607[B]	CLA	CMA-C3A	-4.14	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	CMA-C3A	-4.13	1.44	1.53
32	C	518	DGD	O2G-C2G	-4.13	1.36	1.46
23	A	608	CLA	CMA-C3A	-4.13	1.44	1.53
23	c	512	CLA	CMA-C3A	-4.12	1.44	1.53
32	c	517	DGD	O1G-C1A	4.12	1.45	1.33
23	C	511	CLA	CMA-C3A	-4.12	1.44	1.53
27	A	611	SQD	O47-C7	4.12	1.45	1.34
25	A	609	BCR	C17-C18	4.12	1.41	1.35
32	H	102	DGD	O1G-C1A	4.11	1.45	1.33
31	d	406	LHG	O7-C7	4.11	1.45	1.34
27	a	610	SQD	O47-C7	4.11	1.45	1.34
23	D	402	CLA	CMA-C3A	-4.11	1.44	1.53
32	d	405	DGD	O1G-C1A	4.10	1.45	1.33
23	c	510	CLA	CMA-C3A	-4.10	1.44	1.53
31	L	101	LHG	O7-C7	4.09	1.45	1.34
23	B	607[A]	CLA	CMA-C3A	-4.09	1.44	1.53
32	c	519	DGD	O2G-C2G	-4.08	1.36	1.46
26	a	609	PL9	C7-C3	4.08	1.55	1.51
25	B	618	BCR	C24-C25	4.08	1.59	1.45
32	C	516	DGD	O1G-C1A	4.08	1.45	1.33
23	b	608	CLA	CMA-C3A	-4.08	1.44	1.53
23	b	606	CLA	C1D-C2D	-4.07	1.33	1.42
32	c	518	DGD	O1G-C1A	4.07	1.45	1.33
31	B	622	LHG	O7-C7	4.07	1.45	1.34
32	c	518	DGD	O2G-C1B	4.07	1.45	1.34
32	c	519	DGD	O2G-C1B	4.07	1.45	1.34
23	C	504	CLA	CMA-C3A	-4.07	1.44	1.53
23	C	510	CLA	CMA-C3A	-4.07	1.44	1.53
23	b	612	CLA	CMA-C3A	-4.06	1.44	1.53
23	b	606	CLA	CMA-C3A	-4.06	1.44	1.53
23	b	609[B]	CLA	CMA-C3A	-4.06	1.44	1.53
31	D	407	LHG	O7-C7	4.05	1.45	1.34
25	h	101	BCR	C17-C18	4.05	1.41	1.35
23	b	615	CLA	CMA-C3A	-4.05	1.44	1.53
23	B	608	CLA	CMA-C3A	-4.05	1.44	1.53
26	A	610	PL9	C7-C3	4.05	1.55	1.51
25	B	620	BCR	C17-C18	4.05	1.41	1.35
23	B	612	CLA	CMA-C3A	-4.04	1.44	1.53
23	c	505	CLA	CMA-C3A	-4.04	1.44	1.53
23	C	505	CLA	CMA-C3A	-4.04	1.44	1.53
23	a	605	CLA	CMA-C3A	-4.04	1.44	1.53
32	C	518	DGD	O2G-C1B	4.03	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	CMA-C3A	-4.03	1.44	1.53
23	b	611	CLA	CMA-C3A	-4.03	1.44	1.53
23	c	506	CLA	CMA-C3A	-4.03	1.44	1.53
23	B	609	CLA	CMA-C3A	-4.03	1.44	1.53
31	a	614	LHG	O7-C7	4.02	1.45	1.34
27	a	610	SQD	O48-C23	4.02	1.45	1.33
23	c	507	CLA	CMA-C3A	-4.02	1.44	1.53
23	a	607	CLA	CMA-C3A	-4.02	1.44	1.53
23	b	604	CLA	CMA-C3A	-4.02	1.44	1.53
32	c	518	DGD	O2G-C2G	-4.01	1.36	1.46
32	c	517	DGD	O2G-C2G	-4.01	1.36	1.46
23	D	403	CLA	CMA-C3A	-4.01	1.44	1.53
23	B	606	CLA	CMA-C3A	-4.01	1.44	1.53
23	c	509	CLA	CMA-C3A	-4.00	1.44	1.53
25	T	101	BCR	C17-C18	4.00	1.41	1.35
23	a	604	CLA	CMA-C3A	-4.00	1.44	1.53
23	b	617	CLA	CMA-C3A	-4.00	1.44	1.53
23	b	609[A]	CLA	CMA-C3A	-4.00	1.44	1.53
23	A	606	CLA	CMA-C3A	-3.99	1.44	1.53
23	B	615	CLA	CMA-C3A	-3.99	1.44	1.53
32	H	102	DGD	O2G-C1B	3.99	1.45	1.34
23	d	403	CLA	CMA-C3A	-3.99	1.44	1.53
25	t	101	BCR	C24-C25	3.99	1.59	1.45
31	b	624	LHG	O7-C7	3.99	1.45	1.34
27	A	611	SQD	O48-C23	3.99	1.45	1.33
23	B	610	CLA	CMA-C3A	-3.98	1.44	1.53
23	d	402	CLA	CMA-C3A	-3.98	1.44	1.53
23	C	501	CLA	CMA-C3A	-3.98	1.44	1.53
23	C	509	CLA	CMA-C3A	-3.98	1.44	1.53
25	k	101	BCR	C17-C18	3.98	1.41	1.35
23	c	514	CLA	CMA-C3A	-3.98	1.44	1.53
32	C	516	DGD	O2G-C2G	-3.97	1.36	1.46
23	A	605	CLA	CMA-C3A	-3.97	1.44	1.53
23	c	503	CLA	CMA-C3A	-3.96	1.44	1.53
33	v	201	HEM	C3B-CAB	3.96	1.56	1.47
32	h	102	DGD	O1G-C1A	3.96	1.44	1.33
23	b	605	CLA	CMA-C3A	-3.96	1.44	1.53
33	E	102	HEM	C3C-CAC	3.96	1.55	1.47
23	B	614	CLA	CMA-C3A	-3.96	1.44	1.53
23	C	506	CLA	CMA-C3A	-3.96	1.44	1.53
23	C	508	CLA	CMA-C3A	-3.95	1.44	1.53
23	c	511	CLA	CMA-C3A	-3.95	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	C1D-C2D	-3.95	1.33	1.42
23	B	611	CLA	CMA-C3A	-3.95	1.44	1.53
23	b	618	CLA	CMA-C3A	-3.95	1.44	1.53
23	c	513	CLA	CMA-C3A	-3.95	1.44	1.53
23	D	404	CLA	CMA-C3A	-3.95	1.44	1.53
23	c	504	CLA	CMA-C3A	-3.95	1.44	1.53
25	C	514	BCR	C24-C25	3.95	1.59	1.45
32	H	102	DGD	O2G-C2G	-3.94	1.36	1.46
25	c	522	BCR	C40-C30	3.94	1.61	1.53
23	b	614	CLA	CMA-C3A	-3.94	1.44	1.53
23	C	512	CLA	CMA-C3A	-3.94	1.44	1.53
25	c	516	BCR	C40-C30	3.94	1.61	1.53
32	C	517	DGD	O1G-C1A	3.93	1.44	1.33
23	b	607	CLA	CMA-C3A	-3.92	1.44	1.53
25	b	620	BCR	C24-C25	3.92	1.59	1.45
23	C	502	CLA	CMA-C3A	-3.92	1.44	1.53
32	H	102	DGD	O6E-C5E	3.91	1.53	1.44
25	C	521	BCR	C40-C30	3.90	1.61	1.53
23	b	613	CLA	CMA-C3A	-3.89	1.44	1.53
25	B	620	BCR	C40-C30	3.89	1.61	1.53
23	C	513	CLA	CMA-C3A	-3.89	1.44	1.53
23	c	502	CLA	CMA-C3A	-3.89	1.44	1.53
23	B	602	CLA	CMA-C3A	-3.89	1.44	1.53
23	B	603	CLA	CMA-C3A	-3.89	1.44	1.53
23	B	604	CLA	C1D-C2D	-3.89	1.33	1.42
32	C	517	DGD	O2G-C2G	-3.89	1.36	1.46
32	C	518	DGD	O1G-C1A	3.88	1.44	1.33
26	A	610	PL9	C36-C34	3.87	1.59	1.51
25	k	101	BCR	C40-C30	3.87	1.61	1.53
23	c	508	CLA	CMA-C3A	-3.86	1.44	1.53
33	V	202	HEM	C3C-C2C	-3.86	1.35	1.40
25	C	515	BCR	C40-C30	3.86	1.61	1.53
25	F	101	BCR	C2-C3	3.85	1.62	1.52
25	c	515	BCR	C24-C25	3.85	1.58	1.45
23	b	619	CLA	CMA-C3A	-3.85	1.44	1.53
25	B	618	BCR	C2-C3	3.85	1.62	1.52
23	b	616	CLA	CMA-C3A	-3.84	1.44	1.53
32	h	102	DGD	O6E-C5E	3.84	1.53	1.44
32	D	406	DGD	O2G-C2G	-3.84	1.37	1.46
28	C	519	LMG	O8-C28	3.84	1.44	1.33
23	C	507	CLA	CMA-C3A	-3.84	1.44	1.53
23	B	604	CLA	CMA-C3A	-3.84	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	E	102	HEM	C3B-CAB	3.83	1.55	1.47
23	B	617	CLA	CMA-C3A	-3.83	1.44	1.53
33	E	102	HEM	C3B-C2B	-3.83	1.35	1.40
33	V	202	HEM	C3B-CAB	3.82	1.55	1.47
32	c	519	DGD	O1G-C1A	3.82	1.44	1.33
23	C	503	CLA	CMA-C3A	-3.82	1.45	1.53
32	h	102	DGD	O2G-C2G	-3.82	1.37	1.46
23	D	404	CLA	O2A-CGA	3.81	1.44	1.33
28	z	101	LMG	O6-C1	3.81	1.51	1.41
23	a	604	CLA	C1A-CHA	-3.81	1.27	1.43
28	j	101	LMG	O6-C1	3.80	1.51	1.41
33	e	102	HEM	C3B-CAB	3.80	1.55	1.47
32	d	405	DGD	O2G-C2G	-3.79	1.37	1.46
28	Z	101	LMG	O6-C1	3.79	1.51	1.41
23	c	511	CLA	CAA-C2A	-3.78	1.47	1.54
33	v	201	HEM	C3C-CAC	3.78	1.55	1.47
28	C	519	LMG	O6-C1	3.78	1.51	1.41
25	H	101	BCR	C40-C30	3.78	1.61	1.53
25	f	101	BCR	C2-C3	3.78	1.61	1.52
25	T	101	BCR	C24-C25	3.77	1.58	1.45
23	B	613	CLA	C1A-CHA	-3.77	1.27	1.43
23	b	617	CLA	C1A-CHA	-3.77	1.27	1.43
23	C	508	CLA	C1D-C2D	-3.77	1.34	1.42
28	A	612	LMG	O8-C28	3.77	1.44	1.33
23	B	616	CLA	CMA-C3A	-3.76	1.45	1.53
23	C	505	CLA	CAA-C2A	-3.76	1.47	1.54
23	B	612	CLA	C1A-CHA	-3.76	1.27	1.43
28	J	101	LMG	O6-C1	3.75	1.51	1.41
32	D	406	DGD	O6E-C5E	3.75	1.53	1.44
23	d	403	CLA	O2A-CGA	3.74	1.44	1.33
32	d	405	DGD	O6E-C5E	3.74	1.53	1.44
23	C	501	CLA	C1A-CHA	-3.74	1.27	1.43
25	t	101	BCR	C17-C18	3.74	1.40	1.35
23	A	605	CLA	C1A-CHA	-3.73	1.27	1.43
33	e	102	HEM	C3B-C2B	-3.73	1.35	1.40
33	e	102	HEM	C3C-CAC	3.73	1.55	1.47
25	b	620	BCR	C2-C3	3.73	1.61	1.52
25	b	622	BCR	C40-C30	3.73	1.61	1.53
23	C	504	CLA	C1A-CHA	-3.73	1.27	1.43
23	a	607	CLA	C1D-C2D	-3.72	1.34	1.42
33	V	202	HEM	C3C-CAC	3.72	1.55	1.47
23	B	609	CLA	C1A-CHA	-3.72	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	C1A-CHA	-3.72	1.27	1.43
23	c	503	CLA	C1A-CHA	-3.72	1.27	1.43
28	c	521	LMG	O8-C28	3.72	1.44	1.33
23	b	611	CLA	C1A-CHA	-3.72	1.27	1.43
28	c	520	LMG	O8-C28	3.72	1.44	1.33
23	B	608	CLA	CAA-C2A	-3.71	1.47	1.54
23	C	510	CLA	C1A-CHA	-3.71	1.27	1.43
23	d	402	CLA	C1D-C2D	-3.71	1.34	1.42
23	a	604	CLA	CAA-C2A	-3.71	1.47	1.54
25	K	101	BCR	C40-C30	3.71	1.61	1.53
23	A	605	CLA	CAA-C2A	-3.71	1.47	1.54
23	C	507	CLA	O2A-CGA	3.71	1.44	1.33
32	C	516	DGD	O6E-C5E	3.70	1.53	1.44
23	A	608	CLA	C1A-CHA	-3.70	1.27	1.43
28	c	520	LMG	O6-C1	3.70	1.51	1.41
23	B	605	CLA	C1D-C2D	-3.70	1.34	1.42
23	b	619	CLA	C1D-C2D	-3.70	1.34	1.42
23	B	604	CLA	C1A-CHA	-3.70	1.27	1.43
28	a	611	LMG	O8-C28	3.70	1.44	1.33
23	B	615	CLA	C1A-CHA	-3.70	1.27	1.43
23	B	608	CLA	C1A-CHA	-3.69	1.27	1.43
23	B	613	CLA	C1D-C2D	-3.69	1.34	1.42
23	b	614	CLA	C1D-C2D	-3.69	1.34	1.42
25	a	608	BCR	C2-C3	3.69	1.61	1.52
23	b	609[B]	CLA	C1D-C2D	-3.69	1.34	1.42
32	c	519	DGD	O6E-C5E	3.69	1.53	1.44
33	e	102	HEM	C3C-C2C	-3.68	1.35	1.40
23	b	612	CLA	CAA-C2A	-3.68	1.47	1.54
23	B	606	CLA	C1D-C2D	-3.68	1.34	1.42
28	b	623	LMG	O6-C1	3.68	1.51	1.41
23	b	605	CLA	C1A-CHA	-3.68	1.27	1.43
23	b	608	CLA	C1D-C2D	-3.68	1.34	1.42
23	a	607	CLA	O2A-CGA	3.67	1.44	1.33
23	d	402	CLA	C1A-CHA	-3.67	1.27	1.43
23	c	506	CLA	CAA-C2A	-3.67	1.47	1.54
23	c	505	CLA	C1A-CHA	-3.66	1.27	1.43
23	b	607	CLA	O2A-CGA	3.66	1.44	1.33
23	D	402	CLA	C1A-CHA	-3.66	1.27	1.43
23	b	615	CLA	C1D-C2D	-3.66	1.34	1.42
23	b	615	CLA	C1A-CHA	-3.66	1.27	1.43
23	C	508	CLA	C1A-CHA	-3.66	1.27	1.43
23	A	606	CLA	C1A-CHA	-3.66	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	623	LMG	O8-C28	3.66	1.44	1.33
23	C	510	CLA	CAA-C2A	-3.66	1.47	1.54
23	C	513	CLA	C1A-CHA	-3.65	1.28	1.43
23	C	511	CLA	C1D-C2D	-3.65	1.34	1.42
24	d	401	PHO	C3B-C4B	3.65	1.50	1.43
23	b	612	CLA	C1D-C2D	-3.65	1.34	1.42
25	c	522	BCR	C2-C3	3.65	1.61	1.52
23	b	609[B]	CLA	C1A-CHA	-3.64	1.28	1.43
23	c	510	CLA	O2A-CGA	3.64	1.44	1.33
23	b	608	CLA	C1A-CHA	-3.64	1.28	1.43
23	a	607	CLA	C1A-CHA	-3.64	1.28	1.43
33	E	102	HEM	C3C-C2C	-3.64	1.35	1.40
23	C	506	CLA	C1D-C2D	-3.64	1.34	1.42
23	b	613	CLA	CAA-C2A	-3.64	1.47	1.54
32	c	517	DGD	O6E-C5E	3.64	1.53	1.44
23	c	507	CLA	CAA-C2A	-3.63	1.47	1.54
23	b	619	CLA	C1A-CHA	-3.63	1.28	1.43
23	D	403	CLA	C1D-C2D	-3.63	1.34	1.42
25	C	521	BCR	C2-C3	3.63	1.61	1.52
26	d	404	PL9	C36-C34	3.63	1.58	1.51
23	c	507	CLA	C1D-C2D	-3.63	1.34	1.42
23	b	605	CLA	CAA-C2A	-3.62	1.47	1.54
32	C	518	DGD	O6E-C5E	3.62	1.53	1.44
23	a	613	CLA	C1A-CHA	-3.62	1.28	1.43
28	B	621	LMG	O8-C28	3.62	1.43	1.33
25	h	101	BCR	C40-C30	3.62	1.60	1.53
23	B	614	CLA	C1A-CHA	-3.62	1.28	1.43
23	C	509	CLA	C1D-C2D	-3.62	1.34	1.42
23	C	512	CLA	C1D-C2D	-3.62	1.34	1.42
23	B	602	CLA	C1A-CHA	-3.62	1.28	1.43
23	c	511	CLA	C1D-C2D	-3.62	1.34	1.42
23	B	607[B]	CLA	C1D-C2D	-3.62	1.34	1.42
23	B	603	CLA	C1A-CHA	-3.62	1.28	1.43
28	c	521	LMG	O6-C1	3.61	1.51	1.41
28	C	520	LMG	O8-C28	3.61	1.43	1.33
23	B	602	CLA	O2A-CGA	3.61	1.43	1.33
23	b	606	CLA	O2A-CGA	3.61	1.43	1.33
23	c	505	CLA	C1D-C2D	-3.61	1.34	1.42
23	B	613	CLA	CAA-C2A	-3.61	1.47	1.54
23	c	503	CLA	O2A-CGA	3.61	1.43	1.33
23	c	511	CLA	C1A-CHA	-3.61	1.28	1.43
23	c	508	CLA	O2A-CGA	3.61	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	O2A-CGA	3.60	1.43	1.33
23	b	613	CLA	C1A-CHA	-3.60	1.28	1.43
23	B	617	CLA	O2A-CGA	3.60	1.43	1.33
25	h	101	BCR	C2-C3	3.60	1.61	1.52
23	B	614	CLA	CBD-CGD	-3.60	1.41	1.52
23	b	607	CLA	C1A-CHA	-3.60	1.28	1.43
23	b	614	CLA	C1A-CHA	-3.60	1.28	1.43
24	D	401	PHO	C3B-C4B	3.60	1.50	1.43
23	B	607[A]	CLA	C1A-CHA	-3.59	1.28	1.43
23	b	607	CLA	C1D-C2D	-3.59	1.34	1.42
23	b	610	CLA	C1A-CHA	-3.59	1.28	1.43
25	A	609	BCR	C2-C3	3.59	1.61	1.52
23	B	616	CLA	C1D-C2D	-3.59	1.34	1.42
23	b	615	CLA	CAA-C2A	-3.59	1.47	1.54
23	C	511	CLA	C1A-CHA	-3.59	1.28	1.43
23	A	606	CLA	O2A-CGA	3.59	1.43	1.33
23	A	608	CLA	O2A-CGA	3.59	1.43	1.33
23	B	616	CLA	C1A-CHA	-3.58	1.28	1.43
23	c	506	CLA	C1A-CHA	-3.58	1.28	1.43
32	c	518	DGD	O6E-C5E	3.58	1.53	1.44
28	B	621	LMG	O6-C1	3.58	1.51	1.41
23	b	609[A]	CLA	C1A-CHA	-3.58	1.28	1.43
23	c	502	CLA	C1A-CHA	-3.58	1.28	1.43
23	B	616	CLA	O2A-CGA	3.58	1.43	1.33
25	c	515	BCR	C40-C30	3.58	1.60	1.53
23	b	616	CLA	CAA-C2A	-3.58	1.47	1.54
23	b	605	CLA	C1D-C2D	-3.58	1.34	1.42
23	c	513	CLA	O2A-CGA	3.58	1.43	1.33
33	V	202	HEM	C3B-C2B	-3.58	1.35	1.40
23	C	509	CLA	O2A-CGA	3.57	1.43	1.33
23	B	617	CLA	C1A-CHA	-3.57	1.28	1.43
23	B	603	CLA	C1D-C2D	-3.57	1.34	1.42
23	C	502	CLA	C1A-CHA	-3.57	1.28	1.43
23	b	617	CLA	C1D-C2D	-3.57	1.34	1.42
23	B	610	CLA	C1A-CHA	-3.57	1.28	1.43
23	b	616	CLA	C1D-C2D	-3.57	1.34	1.42
23	b	610	CLA	C1D-C2D	-3.57	1.34	1.42
23	b	604	CLA	O2A-CGA	3.56	1.43	1.33
23	B	607[B]	CLA	C1A-CHA	-3.56	1.28	1.43
23	D	404	CLA	C1A-CHA	-3.56	1.28	1.43
23	B	610	CLA	CAA-C2A	-3.56	1.47	1.54
23	c	509	CLA	C1D-C2D	-3.56	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	618	CLA	C1D-C2D	-3.56	1.34	1.42
23	b	613	CLA	C1D-C2D	-3.56	1.34	1.42
23	C	505	CLA	C1A-CHA	-3.56	1.28	1.43
23	B	614	CLA	CAA-C2A	-3.56	1.47	1.54
23	b	609[A]	CLA	C1D-C2D	-3.55	1.34	1.42
23	c	509	CLA	C1A-CHA	-3.55	1.28	1.43
23	C	507	CLA	C1D-C2D	-3.55	1.34	1.42
23	a	605	CLA	C1A-CHA	-3.55	1.28	1.43
23	b	618	CLA	O2A-CGA	3.55	1.43	1.33
23	C	512	CLA	CAA-C2A	-3.55	1.47	1.54
23	c	513	CLA	C1A-CHA	-3.55	1.28	1.43
23	c	512	CLA	O2A-CGA	3.55	1.43	1.33
23	b	612	CLA	C1A-CHA	-3.55	1.28	1.43
23	B	607[A]	CLA	C1D-C2D	-3.55	1.34	1.42
23	C	512	CLA	C1A-CHA	-3.55	1.28	1.43
23	B	612	CLA	C1D-C2D	-3.54	1.34	1.42
23	d	403	CLA	C1A-CHA	-3.54	1.28	1.43
23	C	502	CLA	O2A-CGA	3.54	1.43	1.33
28	C	520	LMG	O6-C1	3.54	1.50	1.41
23	b	614	CLA	CBD-CGD	-3.54	1.41	1.52
23	B	611	CLA	C1D-C2D	-3.54	1.34	1.42
25	A	609	BCR	C40-C30	3.54	1.60	1.53
23	D	403	CLA	CAA-C2A	-3.54	1.47	1.54
23	c	513	CLA	C1D-C2D	-3.54	1.34	1.42
25	b	621	BCR	C27-C26	3.54	1.58	1.51
23	c	504	CLA	CBD-CGD	-3.54	1.41	1.52
28	j	101	LMG	O8-C28	3.54	1.43	1.33
23	A	606	CLA	C1D-C2D	-3.54	1.34	1.42
23	c	507	CLA	C1A-CHA	-3.54	1.28	1.43
23	B	606	CLA	C1A-CHA	-3.54	1.28	1.43
25	F	101	BCR	C40-C30	3.53	1.60	1.53
23	c	509	CLA	CAA-C2A	-3.53	1.47	1.54
23	C	503	CLA	C1D-C2D	-3.53	1.34	1.42
23	c	510	CLA	C1D-C2D	-3.53	1.34	1.42
33	v	201	HEM	C3B-C2B	-3.53	1.35	1.40
23	c	514	CLA	C1D-C2D	-3.52	1.34	1.42
28	J	101	LMG	O8-C28	3.52	1.43	1.33
23	c	508	CLA	C1D-C2D	-3.52	1.34	1.42
25	b	620	BCR	C40-C30	3.52	1.60	1.53
23	b	604	CLA	C1A-CHA	-3.52	1.28	1.43
23	c	504	CLA	C1A-CHA	-3.52	1.28	1.43
23	C	513	CLA	C1D-C2D	-3.52	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	CBD-CGD	-3.51	1.41	1.52
23	C	511	CLA	O2A-CGA	3.51	1.43	1.33
28	A	612	LMG	O6-C1	3.51	1.50	1.41
23	c	508	CLA	C1A-CHA	-3.51	1.28	1.43
23	a	605	CLA	C1D-C2D	-3.51	1.34	1.42
23	B	607[B]	CLA	CAA-C2A	-3.51	1.47	1.54
32	C	518	DGD	C3D-C2D	-3.51	1.43	1.52
23	a	613	CLA	CBD-CGD	-3.51	1.41	1.52
23	b	619	CLA	O2A-CGA	3.51	1.43	1.33
23	B	608	CLA	CBD-CGD	-3.50	1.41	1.52
23	b	613	CLA	O2A-CGA	3.50	1.43	1.33
23	b	614	CLA	O2A-CGA	3.50	1.43	1.33
23	C	506	CLA	C1A-CHA	-3.50	1.28	1.43
23	C	508	CLA	CAA-C2A	-3.50	1.47	1.54
25	C	514	BCR	C40-C30	3.50	1.60	1.53
23	c	510	CLA	C1A-CHA	-3.50	1.28	1.43
23	c	512	CLA	C1A-CHA	-3.50	1.28	1.43
23	B	617	CLA	C1D-C2D	-3.50	1.34	1.42
25	B	619	BCR	C27-C26	3.50	1.57	1.51
25	B	618	BCR	C40-C30	3.49	1.60	1.53
23	B	605	CLA	O2A-CGA	3.49	1.43	1.33
23	c	503	CLA	C1D-C2D	-3.49	1.34	1.42
23	B	612	CLA	O2A-CGA	3.49	1.43	1.33
28	a	611	LMG	O6-C1	3.49	1.50	1.41
25	A	609	BCR	C27-C26	3.49	1.57	1.51
23	b	609[B]	CLA	O2A-CGA	3.49	1.43	1.33
32	c	519	DGD	C3D-C2D	-3.49	1.43	1.52
23	B	605	CLA	C1A-CHA	-3.49	1.28	1.43
23	B	608	CLA	C1D-C2D	-3.49	1.34	1.42
23	C	509	CLA	C1A-CHA	-3.48	1.28	1.43
25	T	101	BCR	C2-C3	3.48	1.61	1.52
23	c	514	CLA	C1A-CHA	-3.48	1.28	1.43
32	C	517	DGD	O6E-C5E	3.48	1.52	1.44
23	B	614	CLA	C1D-C2D	-3.48	1.34	1.42
23	b	609[A]	CLA	O2A-CGA	3.48	1.43	1.33
23	B	617	CLA	CAA-C2A	-3.48	1.47	1.54
23	c	511	CLA	CBD-CGD	-3.48	1.41	1.52
25	f	101	BCR	C27-C26	3.48	1.57	1.51
23	A	605	CLA	C1D-C2D	-3.48	1.34	1.42
25	c	516	BCR	C2-C3	3.48	1.61	1.52
23	b	609[B]	CLA	CAA-C2A	-3.48	1.47	1.54
23	D	402	CLA	C1D-C2D	-3.48	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	O2A-CGA	3.47	1.43	1.33
23	b	618	CLA	C1A-CHA	-3.47	1.28	1.43
23	b	606	CLA	C1A-CHA	-3.47	1.28	1.43
23	b	613	CLA	CBD-CGD	-3.47	1.41	1.52
23	b	604	CLA	C1D-C2D	-3.47	1.34	1.42
23	B	611	CLA	C1A-CHA	-3.47	1.28	1.43
23	B	611	CLA	CBD-CGD	-3.47	1.41	1.52
23	C	501	CLA	C1D-C2D	-3.47	1.34	1.42
23	c	502	CLA	C1D-C2D	-3.47	1.34	1.42
23	c	504	CLA	C1D-C2D	-3.47	1.34	1.42
23	a	604	CLA	C1D-C2D	-3.47	1.34	1.42
23	D	402	CLA	CBD-CGD	-3.46	1.41	1.52
23	C	503	CLA	CAA-C2A	-3.46	1.47	1.54
23	A	608	CLA	C1D-C2D	-3.46	1.34	1.42
23	C	501	CLA	CBD-CGD	-3.46	1.41	1.52
23	d	402	CLA	CBD-CGD	-3.46	1.41	1.52
23	C	504	CLA	CBD-CGD	-3.46	1.41	1.52
23	c	502	CLA	O2A-CGA	3.46	1.43	1.33
23	d	402	CLA	O2A-CGA	3.45	1.43	1.33
25	B	619	BCR	C2-C3	3.45	1.61	1.52
23	B	610	CLA	C1D-C2D	-3.45	1.34	1.42
23	C	504	CLA	O2A-CGA	3.45	1.43	1.33
25	f	101	BCR	C40-C30	3.45	1.60	1.53
25	H	101	BCR	C2-C3	3.45	1.61	1.52
23	b	616	CLA	C1A-CHA	-3.45	1.28	1.43
23	B	611	CLA	O2A-CGA	3.45	1.43	1.33
23	B	615	CLA	O2A-CGA	3.45	1.43	1.33
23	C	504	CLA	C1D-C2D	-3.44	1.34	1.42
25	C	515	BCR	C2-C3	3.44	1.61	1.52
23	B	602	CLA	CBD-CGD	-3.44	1.41	1.52
23	d	403	CLA	C1D-C2D	-3.44	1.34	1.42
23	c	502	CLA	CAA-C2A	-3.44	1.47	1.54
23	C	501	CLA	O2A-CGA	3.44	1.43	1.33
23	b	619	CLA	CAA-C2A	-3.44	1.47	1.54
23	b	608	CLA	O2A-CGA	3.43	1.43	1.33
23	B	607[A]	CLA	O2A-CGA	3.43	1.43	1.33
23	C	506	CLA	CAA-C2A	-3.43	1.47	1.54
23	C	512	CLA	O2A-CGA	3.43	1.43	1.33
23	C	512	CLA	CBD-CGD	-3.43	1.41	1.52
23	C	503	CLA	C1A-CHA	-3.42	1.28	1.43
23	D	404	CLA	C1D-C2D	-3.42	1.34	1.42
23	C	508	CLA	O2A-CGA	3.42	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	CAA-C2A	-3.42	1.47	1.54
23	B	609	CLA	C1D-C2D	-3.42	1.34	1.42
23	A	606	CLA	CBD-CGD	-3.42	1.41	1.52
26	D	405	PL9	C36-C34	3.42	1.58	1.51
23	B	615	CLA	C1D-C2D	-3.42	1.34	1.42
23	C	510	CLA	CBD-CGD	-3.42	1.41	1.52
23	b	610	CLA	CBD-CGD	-3.42	1.41	1.52
23	C	511	CLA	CAA-C2A	-3.42	1.47	1.54
23	B	611	CLA	CAA-C2A	-3.41	1.47	1.54
23	c	505	CLA	O2A-CGA	3.41	1.43	1.33
23	d	402	CLA	CAA-C2A	-3.41	1.47	1.54
25	c	516	BCR	C12-C13	3.41	1.53	1.45
23	a	605	CLA	O2A-CGA	3.41	1.43	1.33
23	c	504	CLA	O2A-CGA	3.41	1.43	1.33
23	A	608	CLA	CBD-CGD	-3.41	1.41	1.52
23	c	512	CLA	C1D-C2D	-3.41	1.34	1.42
23	C	507	CLA	C1A-CHA	-3.41	1.29	1.43
32	D	406	DGD	O6D-C5D	3.41	1.52	1.44
23	a	604	CLA	CBD-CGD	-3.41	1.41	1.52
24	A	607	PHO	C3B-C4B	3.41	1.50	1.43
25	B	620	BCR	C2-C3	3.40	1.61	1.52
25	a	608	BCR	C40-C30	3.40	1.60	1.53
23	B	606	CLA	O2A-CGA	3.40	1.43	1.33
23	b	615	CLA	O2A-CGA	3.40	1.43	1.33
23	C	502	CLA	C1D-C2D	-3.40	1.34	1.42
23	a	613	CLA	O2A-CGA	3.39	1.43	1.33
23	b	608	CLA	CAA-C2A	-3.39	1.47	1.54
23	C	510	CLA	C1D-C2D	-3.39	1.34	1.42
23	c	512	CLA	CBD-CGD	-3.39	1.41	1.52
23	B	607[B]	CLA	O2A-CGA	3.39	1.43	1.33
23	B	616	CLA	CBD-CGD	-3.39	1.41	1.52
26	a	609	PL9	C36-C34	3.39	1.58	1.51
23	c	505	CLA	CBD-CGD	-3.39	1.41	1.52
23	B	603	CLA	CAA-C2A	-3.39	1.47	1.54
23	A	605	CLA	O2A-CGA	3.39	1.43	1.33
23	b	606	CLA	CAA-C2A	-3.39	1.47	1.54
32	C	518	DGD	O6D-C5D	3.38	1.52	1.44
23	c	512	CLA	CAA-C2A	-3.38	1.47	1.54
25	F	101	BCR	C27-C26	3.38	1.57	1.51
23	c	513	CLA	CBD-CGD	-3.38	1.41	1.52
23	b	605	CLA	O2A-CGA	3.37	1.43	1.33
25	T	101	BCR	C40-C30	3.37	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	CAA-C2A	-3.37	1.47	1.54
23	B	602	CLA	C1D-C2D	-3.37	1.34	1.42
23	c	507	CLA	O2A-CGA	3.37	1.43	1.33
23	B	607[A]	CLA	CAA-C2A	-3.37	1.47	1.54
23	b	614	CLA	CAA-C2A	-3.37	1.47	1.54
23	a	605	CLA	CBD-CGD	-3.37	1.41	1.52
23	C	501	CLA	CAA-C2A	-3.36	1.47	1.54
23	C	503	CLA	CBD-CGD	-3.36	1.41	1.52
23	a	613	CLA	C1D-C2D	-3.36	1.35	1.42
23	c	505	CLA	CAA-C2A	-3.36	1.47	1.54
23	b	609[A]	CLA	CBD-CGD	-3.36	1.41	1.52
23	C	506	CLA	O2A-CGA	3.36	1.43	1.33
23	B	615	CLA	CBD-CGD	-3.36	1.41	1.52
23	B	613	CLA	O2A-CGA	3.36	1.43	1.33
23	c	514	CLA	O2A-CGA	3.35	1.43	1.33
23	D	404	CLA	CBD-CGD	-3.35	1.41	1.52
23	b	609[A]	CLA	CAA-C2A	-3.35	1.47	1.54
25	f	101	BCR	C4-C5	3.35	1.57	1.51
25	b	622	BCR	C2-C3	3.35	1.60	1.52
23	D	403	CLA	O2A-CGA	3.35	1.43	1.33
25	b	621	BCR	C2-C3	3.35	1.60	1.52
32	C	516	DGD	O6D-C5D	3.35	1.52	1.44
23	C	511	CLA	C1B-CHB	3.35	1.50	1.41
23	B	604	CLA	CBD-CGD	-3.35	1.41	1.52
23	B	615	CLA	CAA-C2A	-3.35	1.47	1.54
23	B	603	CLA	O2A-CGA	3.34	1.43	1.33
23	B	612	CLA	CBD-CGD	-3.34	1.42	1.52
23	b	618	CLA	CBD-CGD	-3.34	1.42	1.52
32	d	405	DGD	O6D-C5D	3.34	1.52	1.44
23	c	512	CLA	C1B-CHB	3.33	1.50	1.41
25	b	621	BCR	C4-C5	3.33	1.57	1.51
23	b	611	CLA	O2A-CGA	3.33	1.43	1.33
25	K	101	BCR	C31-C1	-3.33	1.47	1.53
23	c	504	CLA	CAA-C2A	-3.33	1.47	1.54
25	K	101	BCR	C1-C6	-3.33	1.49	1.53
23	c	514	CLA	CAA-C2A	-3.32	1.47	1.54
25	c	522	BCR	C12-C13	3.32	1.53	1.45
23	c	506	CLA	C1B-CHB	3.32	1.50	1.41
23	B	607[A]	CLA	CBD-CGD	-3.32	1.42	1.52
23	b	612	CLA	O2A-CGA	3.32	1.43	1.33
23	b	609[B]	CLA	CBD-CGD	-3.32	1.42	1.52
23	a	605	CLA	CAA-C2A	-3.32	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	O2A-CGA	3.31	1.43	1.33
23	C	511	CLA	CBD-CGD	-3.31	1.42	1.52
25	B	619	BCR	C4-C5	3.31	1.57	1.51
23	D	402	CLA	O2A-CGA	3.31	1.43	1.33
23	D	402	CLA	CAA-C2A	-3.31	1.48	1.54
24	a	606	PHO	C3B-C4B	3.31	1.50	1.43
23	B	617	CLA	C1B-CHB	3.30	1.50	1.41
23	B	617	CLA	CBD-CGD	-3.30	1.42	1.52
25	k	101	BCR	C4-C5	3.30	1.57	1.51
23	b	612	CLA	C3D-CAD	3.30	1.54	1.46
32	c	517	DGD	C3D-C2D	-3.30	1.43	1.52
23	A	606	CLA	CAA-C2A	-3.30	1.48	1.54
23	c	503	CLA	CBD-CGD	-3.30	1.42	1.52
23	A	605	CLA	CBD-CGD	-3.30	1.42	1.52
23	C	503	CLA	O2A-CGA	3.30	1.43	1.33
23	a	604	CLA	O2A-CGA	3.30	1.43	1.33
23	C	508	CLA	CBD-CGD	-3.30	1.42	1.52
23	b	606	CLA	CBD-CGD	-3.29	1.42	1.52
23	a	613	CLA	CAA-C2A	-3.29	1.48	1.54
25	t	101	BCR	C40-C30	3.29	1.60	1.53
23	c	510	CLA	C1B-CHB	3.29	1.50	1.41
23	b	608	CLA	CBD-CGD	-3.29	1.42	1.52
23	d	403	CLA	C3D-CAD	3.29	1.54	1.46
23	b	605	CLA	CBD-CGD	-3.29	1.42	1.52
23	B	613	CLA	CBD-CGD	-3.29	1.42	1.52
23	C	502	CLA	CBD-CGD	-3.28	1.42	1.52
32	H	102	DGD	C3D-C2D	-3.28	1.44	1.52
23	C	505	CLA	O2A-CGA	3.28	1.42	1.33
23	B	609	CLA	CAA-C2A	-3.27	1.48	1.54
23	B	604	CLA	CAA-C2A	-3.27	1.48	1.54
23	c	510	CLA	CAA-C2A	-3.27	1.48	1.54
32	h	102	DGD	O6D-C5D	3.27	1.52	1.44
23	B	610	CLA	O2A-CGA	3.27	1.42	1.33
23	b	610	CLA	O2A-CGA	3.27	1.42	1.33
25	b	620	BCR	C1-C6	-3.26	1.49	1.53
23	b	616	CLA	CBD-CGD	-3.26	1.42	1.52
23	c	511	CLA	O2A-CGA	3.26	1.42	1.33
23	B	606	CLA	CBD-CGD	-3.26	1.42	1.52
23	b	617	CLA	CAA-C2A	-3.26	1.48	1.54
23	B	608	CLA	O2A-CGA	3.25	1.42	1.33
23	b	611	CLA	C1D-C2D	-3.25	1.35	1.42
25	C	514	BCR	C2-C3	3.25	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	403	CLA	CBD-CGD	-3.25	1.42	1.52
23	B	605	CLA	CBD-CGD	-3.25	1.42	1.52
23	D	404	CLA	C1B-CHB	3.25	1.50	1.41
23	b	604	CLA	C1B-CHB	3.25	1.50	1.41
23	a	607	CLA	C1B-CHB	3.24	1.50	1.41
23	d	403	CLA	C1B-CHB	3.24	1.50	1.41
23	b	618	CLA	CAA-C2A	-3.24	1.48	1.54
23	b	611	CLA	CAA-C2A	-3.24	1.48	1.54
23	B	607[B]	CLA	CBD-CGD	-3.23	1.42	1.52
23	b	604	CLA	CBD-CGD	-3.23	1.42	1.52
23	b	612	CLA	O2D-CGD	3.23	1.41	1.33
23	b	617	CLA	O2A-CGA	3.23	1.42	1.33
23	c	508	CLA	CBD-CGD	-3.23	1.42	1.52
23	B	609	CLA	O2A-CGA	3.23	1.42	1.33
25	a	608	BCR	C27-C26	3.23	1.57	1.51
23	C	509	CLA	CBD-CGD	-3.23	1.42	1.52
23	c	502	CLA	CBD-CGD	-3.22	1.42	1.52
23	C	502	CLA	C3D-CAD	3.22	1.54	1.46
23	b	617	CLA	CBD-CGD	-3.22	1.42	1.52
23	B	609	CLA	CBD-CGD	-3.22	1.42	1.52
32	D	406	DGD	C3D-C2D	-3.22	1.44	1.52
23	C	513	CLA	CAA-C2A	-3.22	1.48	1.54
23	C	513	CLA	C1B-CHB	3.21	1.49	1.41
23	c	509	CLA	O2A-CGA	3.21	1.42	1.33
23	C	510	CLA	O2A-CGA	3.21	1.42	1.33
23	b	610	CLA	CAA-C2A	-3.21	1.48	1.54
23	B	602	CLA	CAA-C2A	-3.21	1.48	1.54
23	c	503	CLA	C3D-CAD	3.20	1.54	1.46
23	C	513	CLA	O2D-CGD	3.20	1.41	1.33
32	c	517	DGD	O6D-C5D	3.20	1.52	1.44
23	b	614	CLA	C1B-CHB	3.20	1.49	1.41
23	c	503	CLA	CAA-C2A	-3.20	1.48	1.54
23	c	509	CLA	C3D-CAD	3.20	1.54	1.46
23	B	604	CLA	OBD-CAD	-3.20	1.17	1.22
23	B	605	CLA	CAA-C2A	-3.20	1.48	1.54
23	a	604	CLA	C3D-CAD	3.20	1.54	1.46
23	b	607	CLA	CBD-CGD	-3.20	1.42	1.52
23	C	504	CLA	CAA-C2A	-3.20	1.48	1.54
25	B	618	BCR	C17-C18	3.20	1.40	1.35
23	B	609	CLA	C1B-CHB	3.19	1.49	1.41
23	A	608	CLA	C1B-CHB	3.19	1.49	1.41
23	C	505	CLA	C1B-CHB	3.19	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	521	BCR	C17-C18	3.19	1.40	1.35
23	b	611	CLA	C3D-CAD	3.19	1.54	1.46
23	B	605	CLA	C1B-CHB	3.19	1.49	1.41
25	K	101	BCR	C2-C3	3.19	1.60	1.52
23	B	612	CLA	CAA-C2A	-3.18	1.48	1.54
23	b	606	CLA	C1B-CHB	3.18	1.49	1.41
23	b	619	CLA	C1B-CHB	3.18	1.49	1.41
23	B	602	CLA	C1B-CHB	3.18	1.49	1.41
23	B	608	CLA	C1B-CHB	3.18	1.49	1.41
23	c	514	CLA	C1B-CHB	3.18	1.49	1.41
32	H	102	DGD	O6D-C5D	3.18	1.52	1.44
23	C	509	CLA	O2D-CGD	3.18	1.41	1.33
23	c	507	CLA	CBD-CGD	-3.17	1.42	1.52
25	k	101	BCR	C27-C26	3.17	1.57	1.51
32	h	102	DGD	C3D-C2D	-3.17	1.44	1.52
23	b	611	CLA	C1B-CHB	3.17	1.49	1.41
25	b	621	BCR	C17-C18	3.17	1.40	1.35
32	C	516	DGD	C3D-C2D	-3.17	1.44	1.52
28	J	101	LMG	O7-C8	-3.17	1.38	1.46
23	C	501	CLA	C3D-CAD	3.17	1.54	1.46
23	b	616	CLA	O2A-CGA	3.17	1.42	1.33
32	c	519	DGD	O6D-C5D	3.17	1.52	1.44
23	C	506	CLA	O2D-CGD	3.17	1.40	1.33
23	B	609	CLA	C3D-CAD	3.17	1.54	1.46
23	B	610	CLA	C3D-CAD	3.17	1.54	1.46
23	A	608	CLA	C3D-CAD	3.16	1.54	1.46
23	C	508	CLA	C3D-CAD	3.16	1.54	1.46
23	C	505	CLA	CBD-CGD	-3.16	1.42	1.52
23	C	509	CLA	CAA-C2A	-3.16	1.48	1.54
25	K	101	BCR	C4-C5	3.16	1.57	1.51
23	B	603	CLA	C3D-CAD	3.16	1.54	1.46
23	b	613	CLA	C1B-CHB	3.16	1.49	1.41
23	C	512	CLA	C3D-CAD	3.16	1.54	1.46
25	k	101	BCR	C31-C1	-3.16	1.47	1.53
23	C	502	CLA	C1B-CHB	3.16	1.49	1.41
23	C	503	CLA	C1B-CHB	3.16	1.49	1.41
23	b	616	CLA	C1B-CHB	3.16	1.49	1.41
23	c	504	CLA	C1B-CHB	3.16	1.49	1.41
23	c	508	CLA	C1B-CHB	3.15	1.49	1.41
23	a	607	CLA	CBD-CGD	-3.15	1.42	1.52
23	b	607	CLA	CAA-C2A	-3.15	1.48	1.54
23	A	606	CLA	C1B-CHB	3.15	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	515	BCR	C2-C3	3.15	1.60	1.52
25	t	101	BCR	C27-C26	3.15	1.57	1.51
23	c	511	CLA	C1B-CHB	3.15	1.49	1.41
23	B	611	CLA	C3D-CAD	3.15	1.54	1.46
24	a	606	PHO	CHC-C1C	3.15	1.44	1.38
25	T	101	BCR	C27-C26	3.14	1.57	1.51
25	F	101	BCR	C4-C5	3.14	1.57	1.51
23	D	404	CLA	C3D-CAD	3.14	1.54	1.46
23	c	514	CLA	CBD-CGD	-3.14	1.42	1.52
25	b	621	BCR	C40-C30	3.14	1.59	1.53
23	B	614	CLA	C1B-CHB	3.14	1.49	1.41
25	A	609	BCR	C4-C5	3.14	1.57	1.51
26	A	610	PL9	C21-C19	3.14	1.57	1.51
25	T	101	BCR	C12-C13	3.14	1.52	1.45
25	h	101	BCR	C12-C13	3.14	1.52	1.45
28	b	623	LMG	O7-C8	-3.14	1.38	1.46
25	b	622	BCR	C27-C26	3.13	1.57	1.51
23	B	616	CLA	C1B-CHB	3.13	1.49	1.41
25	B	618	BCR	C1-C6	-3.13	1.49	1.53
23	c	513	CLA	C1B-CHB	3.13	1.49	1.41
32	d	405	DGD	C3D-C2D	-3.13	1.44	1.52
23	B	612	CLA	C3D-CAD	3.13	1.54	1.46
23	b	611	CLA	CBD-CGD	-3.13	1.42	1.52
23	b	604	CLA	CAA-C2A	-3.13	1.48	1.54
23	b	619	CLA	CBD-CGD	-3.13	1.42	1.52
26	a	609	PL9	C21-C19	3.12	1.57	1.51
23	c	510	CLA	O2D-CGD	3.12	1.40	1.33
25	k	101	BCR	C1-C6	-3.12	1.49	1.53
23	c	513	CLA	CAA-C2A	-3.12	1.48	1.54
23	B	610	CLA	C1B-CHB	3.12	1.49	1.41
23	B	602	CLA	C3D-CAD	3.12	1.54	1.46
23	C	510	CLA	C1B-CHB	3.12	1.49	1.41
23	C	507	CLA	CBD-CGD	-3.12	1.42	1.52
23	C	506	CLA	C3D-CAD	3.11	1.54	1.46
23	b	604	CLA	C3D-CAD	3.11	1.54	1.46
23	c	510	CLA	CBD-CGD	-3.11	1.42	1.52
25	C	515	BCR	C1-C6	-3.11	1.49	1.53
23	C	509	CLA	C1B-CHB	3.10	1.49	1.41
23	c	505	CLA	C3D-CAD	3.10	1.53	1.46
23	C	507	CLA	C3D-CAD	3.10	1.53	1.46
23	B	606	CLA	C1B-CHB	3.10	1.49	1.41
23	B	603	CLA	CBD-CGD	-3.10	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	h	101	BCR	C35-C13	-3.09	1.44	1.50
25	k	101	BCR	C2-C3	3.09	1.60	1.52
25	k	101	BCR	C35-C13	-3.09	1.44	1.50
26	D	405	PL9	C7-C3	3.09	1.54	1.51
23	c	514	CLA	O2D-CGD	3.09	1.40	1.33
23	b	612	CLA	CBD-CGD	-3.09	1.42	1.52
23	B	613	CLA	C3D-CAD	3.09	1.53	1.46
25	a	608	BCR	C4-C5	3.09	1.57	1.51
23	B	615	CLA	C1B-CHB	3.08	1.49	1.41
23	C	507	CLA	CAA-C2A	-3.08	1.48	1.54
23	c	503	CLA	C1B-CHB	3.08	1.49	1.41
23	b	608	CLA	C1B-CHB	3.08	1.49	1.41
25	C	514	BCR	C27-C26	3.08	1.57	1.51
23	c	508	CLA	CAA-C2A	-3.08	1.48	1.54
23	B	614	CLA	OBD-CAD	-3.08	1.18	1.22
25	c	516	BCR	C4-C5	3.07	1.57	1.51
24	D	401	PHO	CHC-C1C	3.07	1.44	1.38
25	B	620	BCR	C27-C26	3.07	1.57	1.51
23	C	506	CLA	CBD-CGD	-3.07	1.42	1.52
23	b	617	CLA	C1B-CHB	3.07	1.49	1.41
23	B	610	CLA	CBD-CGD	-3.07	1.42	1.52
23	b	612	CLA	C1B-CHB	3.07	1.49	1.41
23	c	506	CLA	O2A-CGA	3.07	1.42	1.33
23	C	513	CLA	CBD-CGD	-3.07	1.42	1.52
25	c	515	BCR	C27-C26	3.07	1.57	1.51
23	C	504	CLA	C3D-CAD	3.07	1.53	1.46
23	B	607[B]	CLA	C3D-CAD	3.06	1.53	1.46
23	C	508	CLA	C1B-CHB	3.06	1.49	1.41
23	A	605	CLA	C1B-CHB	3.06	1.49	1.41
23	b	615	CLA	CBD-CGD	-3.06	1.42	1.52
23	A	605	CLA	C3D-CAD	3.06	1.53	1.46
32	c	518	DGD	C3D-C2D	-3.06	1.44	1.52
23	C	507	CLA	C1B-CHB	3.06	1.49	1.41
23	C	512	CLA	C1B-CHB	3.06	1.49	1.41
23	B	616	CLA	CAA-C2A	-3.05	1.48	1.54
23	B	610	CLA	O2D-CGD	3.05	1.40	1.33
23	b	607	CLA	C1B-CHB	3.05	1.49	1.41
23	a	604	CLA	C1B-CHB	3.05	1.49	1.41
23	D	402	CLA	C3D-CAD	3.05	1.53	1.46
23	b	613	CLA	C3D-CAD	3.05	1.53	1.46
25	B	618	BCR	C35-C13	-3.05	1.44	1.50
25	t	101	BCR	C12-C13	3.05	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C1B-CHB	3.05	1.49	1.41
23	a	607	CLA	CAA-C2A	-3.05	1.48	1.54
23	B	608	CLA	C3D-CAD	3.04	1.53	1.46
23	B	611	CLA	C1B-CHB	3.04	1.49	1.41
26	d	404	PL9	C21-C19	3.04	1.57	1.51
23	b	619	CLA	O2D-CGD	3.04	1.40	1.33
23	b	615	CLA	C3D-CAD	3.04	1.53	1.46
25	B	619	BCR	C40-C30	3.04	1.59	1.53
23	C	504	CLA	C1B-CHB	3.04	1.49	1.41
23	c	509	CLA	CBD-CGD	-3.04	1.42	1.52
24	A	607	PHO	CHC-C1C	3.04	1.44	1.38
23	C	505	CLA	C3D-CAD	3.04	1.53	1.46
25	C	514	BCR	C4-C5	3.04	1.57	1.51
23	B	604	CLA	C1B-CHB	3.03	1.49	1.41
23	c	502	CLA	C3D-CAD	3.03	1.53	1.46
26	D	405	PL9	C21-C19	3.03	1.57	1.51
23	C	513	CLA	C3D-CAD	3.03	1.53	1.46
25	h	101	BCR	C27-C26	3.03	1.57	1.51
23	C	509	CLA	C3D-CAD	3.03	1.53	1.46
23	a	607	CLA	O2D-CGD	3.03	1.40	1.33
23	c	514	CLA	C3D-CAD	3.03	1.53	1.46
23	D	403	CLA	OBD-CAD	-3.03	1.18	1.22
25	b	622	BCR	C4-C5	3.03	1.57	1.51
25	K	101	BCR	C27-C26	3.03	1.57	1.51
23	c	507	CLA	C3D-CAD	3.03	1.53	1.46
25	A	609	BCR	C12-C13	3.03	1.52	1.45
23	b	614	CLA	C3B-CAB	3.03	1.54	1.47
23	B	613	CLA	C1B-CHB	3.02	1.49	1.41
23	b	610	CLA	C1B-CHB	3.02	1.49	1.41
23	b	615	CLA	C1B-CHB	3.02	1.49	1.41
23	c	506	CLA	C3D-CAD	3.02	1.53	1.46
23	b	606	CLA	OBD-CAD	-3.02	1.18	1.22
23	B	607[A]	CLA	C3D-CAD	3.02	1.53	1.46
26	d	404	PL9	C7-C3	3.02	1.54	1.51
23	c	502	CLA	C1B-CHB	3.02	1.49	1.41
25	C	515	BCR	C12-C13	3.02	1.52	1.45
23	b	605	CLA	O2D-CGD	3.02	1.40	1.33
23	a	605	CLA	C3D-CAD	3.02	1.53	1.46
23	b	609[A]	CLA	C1B-CHB	3.02	1.49	1.41
23	c	506	CLA	CBD-CGD	-3.02	1.43	1.52
23	b	618	CLA	C1B-CHB	3.02	1.49	1.41
23	c	506	CLA	O2D-CGD	3.01	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	f	101	BCR	C1-C6	-3.01	1.49	1.53
25	B	619	BCR	C31-C1	-3.01	1.47	1.53
25	H	101	BCR	C27-C26	3.01	1.56	1.51
23	c	505	CLA	C1B-CHB	3.01	1.49	1.41
25	B	620	BCR	C4-C5	3.01	1.56	1.51
25	C	521	BCR	C4-C5	3.01	1.56	1.51
23	b	609[A]	CLA	C3D-CAD	3.00	1.53	1.46
23	c	511	CLA	C3D-CAD	3.00	1.53	1.46
23	A	608	CLA	O2D-CGD	3.00	1.40	1.33
23	B	605	CLA	O2D-CGD	3.00	1.40	1.33
23	c	510	CLA	MG-NA	-3.00	1.99	2.06
23	a	607	CLA	C3D-CAD	3.00	1.53	1.46
28	j	101	LMG	O7-C8	-3.00	1.39	1.46
23	b	609[B]	CLA	C3D-CAD	3.00	1.53	1.46
23	C	506	CLA	C1B-CHB	2.99	1.49	1.41
23	B	606	CLA	O2D-CGD	2.99	1.40	1.33
23	b	609[B]	CLA	C1B-CHB	2.99	1.49	1.41
23	c	508	CLA	C3D-CAD	2.99	1.53	1.46
25	B	620	BCR	C1-C6	-2.99	1.49	1.53
23	B	615	CLA	C3D-CAD	2.99	1.53	1.46
23	B	612	CLA	O2D-CGD	2.99	1.40	1.33
23	C	511	CLA	O2D-CGD	2.99	1.40	1.33
23	A	605	CLA	MG-NA	-2.99	1.99	2.06
23	a	604	CLA	MG-NA	-2.99	1.99	2.06
23	C	511	CLA	C3D-CAD	2.98	1.53	1.46
23	b	619	CLA	C3D-CAD	2.98	1.53	1.46
23	B	613	CLA	MG-NA	-2.98	1.99	2.06
25	b	621	BCR	C31-C1	-2.98	1.47	1.53
28	B	621	LMG	O7-C8	-2.98	1.39	1.46
24	d	401	PHO	CHC-C1C	2.98	1.44	1.38
23	a	605	CLA	C1B-CHB	2.98	1.49	1.41
23	a	613	CLA	C1B-CHB	2.98	1.49	1.41
23	C	510	CLA	OBD-CAD	-2.98	1.18	1.22
23	b	605	CLA	C3D-CAD	2.98	1.53	1.46
23	d	402	CLA	C3D-CAD	2.98	1.53	1.46
23	B	617	CLA	C3D-CAD	2.98	1.53	1.46
23	D	402	CLA	MG-NA	-2.97	1.99	2.06
25	b	622	BCR	C35-C13	-2.97	1.44	1.50
25	K	101	BCR	C17-C18	2.97	1.39	1.35
23	D	402	CLA	C1B-CHB	2.97	1.49	1.41
23	B	609	CLA	O2D-CGD	2.97	1.40	1.33
23	D	403	CLA	C1B-CHB	2.97	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	515	BCR	C35-C13	-2.97	1.44	1.50
25	f	101	BCR	C35-C13	-2.97	1.44	1.50
23	b	606	CLA	O2D-CGD	2.96	1.40	1.33
25	B	619	BCR	C35-C13	-2.96	1.44	1.50
24	D	401	PHO	C4C-NC	2.96	1.43	1.36
23	b	614	CLA	C3D-CAD	2.95	1.53	1.46
23	D	403	CLA	C3D-CAD	2.95	1.53	1.46
23	c	513	CLA	C3D-CAD	2.95	1.53	1.46
23	c	504	CLA	C3D-CAD	2.95	1.53	1.46
23	c	507	CLA	O2D-CGD	2.95	1.40	1.33
32	C	517	DGD	O6D-C5D	2.95	1.51	1.44
23	b	606	CLA	C3B-CAB	2.95	1.53	1.47
23	B	607[B]	CLA	C1B-CHB	2.95	1.49	1.41
23	C	501	CLA	C1B-CHB	2.95	1.49	1.41
28	C	519	LMG	O7-C8	-2.94	1.39	1.46
25	a	608	BCR	C35-C13	-2.94	1.44	1.50
23	b	607	CLA	C3D-CAD	2.94	1.53	1.46
23	b	607	CLA	O2D-CGD	2.94	1.40	1.33
23	C	510	CLA	C3B-CAB	2.94	1.53	1.47
23	b	614	CLA	MG-NA	-2.94	1.99	2.06
23	b	619	CLA	OBD-CAD	-2.94	1.18	1.22
23	d	402	CLA	C1B-CHB	2.93	1.49	1.41
25	C	521	BCR	C27-C26	2.93	1.56	1.51
28	c	520	LMG	O7-C8	-2.93	1.39	1.46
23	b	615	CLA	O2D-CGD	2.93	1.40	1.33
23	a	605	CLA	O2D-CGD	2.93	1.40	1.33
23	A	606	CLA	C3D-CAD	2.93	1.53	1.46
23	A	606	CLA	C3B-CAB	2.93	1.53	1.47
23	b	619	CLA	MG-NA	-2.93	1.99	2.06
23	b	608	CLA	O2D-CGD	2.92	1.40	1.33
23	c	502	CLA	O2D-CGD	2.92	1.40	1.33
23	b	612	CLA	MG-NA	-2.92	1.99	2.06
25	t	101	BCR	C31-C1	-2.92	1.48	1.53
23	b	617	CLA	C3D-CAD	2.92	1.53	1.46
23	a	613	CLA	MG-NA	-2.92	1.99	2.06
25	c	522	BCR	C4-C5	2.92	1.56	1.51
23	b	616	CLA	C3D-CAD	2.92	1.53	1.46
32	C	517	DGD	C3D-C2D	-2.92	1.44	1.52
23	B	603	CLA	O2D-CGD	2.91	1.40	1.33
23	B	613	CLA	O2D-CGD	2.91	1.40	1.33
23	a	613	CLA	C3D-CAD	2.91	1.53	1.46
23	d	402	CLA	MG-NA	-2.91	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Z	101	LMG	O7-C8	-2.91	1.39	1.46
23	B	604	CLA	C3B-CAB	2.91	1.53	1.47
25	C	515	BCR	C4-C5	2.91	1.56	1.51
23	B	607[A]	CLA	C1B-CHB	2.91	1.49	1.41
23	c	509	CLA	C1B-CHB	2.91	1.49	1.41
23	c	510	CLA	C3D-CAD	2.91	1.53	1.46
23	B	607[B]	CLA	O2D-CGD	2.91	1.40	1.33
23	C	510	CLA	C3D-CAD	2.91	1.53	1.46
23	A	606	CLA	MG-NA	-2.90	1.99	2.06
28	z	101	LMG	O7-C8	-2.90	1.39	1.46
23	c	508	CLA	O2D-CGD	2.90	1.40	1.33
23	C	505	CLA	O2D-CGD	2.90	1.40	1.33
23	d	402	CLA	OBD-CAD	-2.90	1.18	1.22
23	b	613	CLA	OBD-CAD	-2.90	1.18	1.22
23	D	403	CLA	MG-NA	-2.90	1.99	2.06
25	c	515	BCR	C4-C5	2.89	1.56	1.51
23	b	606	CLA	MG-NA	-2.89	1.99	2.06
23	D	404	CLA	O2D-CGD	2.89	1.40	1.33
23	b	611	CLA	O2D-CGD	2.89	1.40	1.33
23	c	512	CLA	C3D-CAD	2.89	1.53	1.46
23	B	616	CLA	C3D-CAD	2.89	1.53	1.46
23	a	607	CLA	MG-NA	-2.89	1.99	2.06
25	b	620	BCR	C4-C5	2.89	1.56	1.51
23	b	604	CLA	O2D-CGD	2.89	1.40	1.33
25	c	516	BCR	C27-C26	2.89	1.56	1.51
25	C	515	BCR	C27-C26	2.89	1.56	1.51
25	T	101	BCR	C35-C13	-2.88	1.44	1.50
28	A	612	LMG	O7-C8	-2.88	1.39	1.46
23	b	617	CLA	O2D-CGD	2.88	1.40	1.33
23	B	602	CLA	O2D-CGD	2.88	1.40	1.33
25	a	608	BCR	C12-C13	2.88	1.52	1.45
25	b	621	BCR	C35-C13	-2.88	1.44	1.50
23	c	505	CLA	MG-NA	-2.88	1.99	2.06
23	b	611	CLA	C3B-CAB	2.88	1.53	1.47
23	B	615	CLA	O2D-CGD	2.88	1.40	1.33
23	A	608	CLA	CAA-C2A	-2.88	1.48	1.54
23	c	507	CLA	OBD-CAD	-2.88	1.18	1.22
25	h	101	BCR	C4-C5	2.88	1.56	1.51
23	B	617	CLA	O2D-CGD	2.88	1.40	1.33
23	b	618	CLA	C3D-CAD	2.88	1.53	1.46
23	b	605	CLA	MG-NA	-2.87	1.99	2.06
23	B	617	CLA	MG-NA	-2.87	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	401	PHO	C4C-NC	2.87	1.43	1.36
23	B	605	CLA	C3D-CAD	2.87	1.53	1.46
23	C	504	CLA	MG-NA	-2.87	1.99	2.06
23	B	607[A]	CLA	O2D-CGD	2.86	1.40	1.33
23	D	402	CLA	C3B-CAB	2.86	1.53	1.47
23	b	615	CLA	MG-NA	-2.86	1.99	2.06
23	C	507	CLA	O2D-CGD	2.86	1.40	1.33
23	c	509	CLA	O2D-CGD	2.86	1.40	1.33
25	B	620	BCR	C35-C13	-2.86	1.45	1.50
23	A	605	CLA	O2D-CED	-2.85	1.38	1.45
23	C	513	CLA	MG-NA	-2.85	1.99	2.06
23	a	604	CLA	O2D-CED	-2.85	1.38	1.45
23	d	403	CLA	O2D-CGD	2.85	1.40	1.33
28	c	521	LMG	O7-C8	-2.85	1.39	1.46
25	B	618	BCR	C27-C26	2.85	1.56	1.51
32	C	517	DGD	C6E-C5E	-2.85	1.42	1.51
23	b	617	CLA	MG-NA	-2.85	1.99	2.06
23	c	507	CLA	C1B-CHB	2.85	1.48	1.41
23	c	514	CLA	MG-NA	-2.85	1.99	2.06
23	B	617	CLA	OBD-CAD	-2.85	1.18	1.22
23	b	616	CLA	O2D-CGD	2.85	1.40	1.33
32	c	518	DGD	O6D-C5D	2.84	1.51	1.44
23	b	610	CLA	O2D-CGD	2.84	1.40	1.33
23	B	606	CLA	OBD-CAD	-2.84	1.18	1.22
28	a	611	LMG	O7-C8	-2.84	1.39	1.46
23	b	609[A]	CLA	O2D-CGD	2.84	1.40	1.33
23	b	609[B]	CLA	O2D-CGD	2.84	1.40	1.33
23	a	605	CLA	C3B-CAB	2.84	1.53	1.47
25	t	101	BCR	C4-C5	2.84	1.56	1.51
23	C	512	CLA	O2D-CGD	2.84	1.40	1.33
23	b	608	CLA	C3D-CAD	2.84	1.53	1.46
25	t	101	BCR	C2-C3	2.84	1.59	1.52
25	T	101	BCR	C4-C5	2.84	1.56	1.51
23	B	604	CLA	C3D-CAD	2.83	1.53	1.46
23	a	613	CLA	OBD-CAD	-2.83	1.18	1.22
23	c	503	CLA	O2D-CGD	2.83	1.40	1.33
23	B	603	CLA	MG-NA	-2.83	1.99	2.06
25	c	516	BCR	C35-C13	-2.83	1.45	1.50
23	A	605	CLA	OBD-CAD	-2.83	1.18	1.22
32	C	518	DGD	C6E-C5E	-2.83	1.42	1.51
23	B	612	CLA	C3B-CAB	2.83	1.53	1.47
23	c	506	CLA	MG-NA	-2.83	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	514	BCR	C35-C13	-2.82	1.45	1.50
23	a	607	CLA	C3B-CAB	2.82	1.53	1.47
25	C	521	BCR	C12-C13	2.82	1.52	1.45
23	C	511	CLA	MG-NA	-2.82	1.99	2.06
23	c	509	CLA	MG-NA	-2.82	1.99	2.06
23	d	403	CLA	CAA-C2A	-2.82	1.48	1.54
23	B	603	CLA	C1B-CHB	2.82	1.48	1.41
23	a	605	CLA	MG-NA	-2.82	1.99	2.06
32	c	519	DGD	C6E-C5E	-2.82	1.42	1.51
32	c	517	DGD	C6E-C5E	-2.81	1.42	1.51
32	H	102	DGD	C6E-C5E	-2.81	1.42	1.51
23	B	614	CLA	C3D-CAD	2.81	1.53	1.46
23	C	509	CLA	MG-NA	-2.81	1.99	2.06
23	B	611	CLA	O2D-CED	-2.81	1.38	1.45
23	B	605	CLA	MG-NA	-2.81	1.99	2.06
32	c	518	DGD	C6E-C5E	-2.81	1.42	1.51
23	C	503	CLA	MG-NA	-2.81	1.99	2.06
23	B	604	CLA	O2D-CGD	2.81	1.40	1.33
25	B	618	BCR	C4-C5	2.81	1.56	1.51
24	A	607	PHO	C4C-NC	2.81	1.43	1.36
25	k	101	BCR	C12-C13	2.81	1.52	1.45
25	c	522	BCR	C27-C26	2.80	1.56	1.51
23	B	604	CLA	MG-NA	-2.80	1.99	2.06
25	A	609	BCR	C35-C13	-2.80	1.45	1.50
23	B	611	CLA	O2D-CGD	2.80	1.40	1.33
23	C	503	CLA	C3B-CAB	2.80	1.53	1.47
23	c	504	CLA	O2D-CED	-2.80	1.38	1.45
23	C	505	CLA	C3B-CAB	2.80	1.53	1.47
32	h	102	DGD	C6E-C5E	-2.80	1.42	1.51
23	B	611	CLA	OBD-CAD	-2.80	1.18	1.22
23	D	402	CLA	OBD-CAD	-2.80	1.18	1.22
25	c	522	BCR	C35-C13	-2.79	1.45	1.50
32	C	516	DGD	C6E-C5E	-2.79	1.42	1.51
28	C	520	LMG	O7-C8	-2.79	1.39	1.46
23	b	618	CLA	O2D-CGD	2.79	1.40	1.33
23	C	504	CLA	OBD-CAD	-2.79	1.18	1.22
23	A	605	CLA	C3B-CAB	2.79	1.53	1.47
23	b	616	CLA	OBD-CAD	-2.79	1.18	1.22
23	b	614	CLA	O2D-CGD	2.79	1.40	1.33
27	A	611	SQD	C6-S	-2.78	1.67	1.77
23	c	505	CLA	O2D-CGD	2.78	1.40	1.33
23	a	605	CLA	OBD-CAD	-2.78	1.18	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	515	BCR	C31-C1	-2.78	1.48	1.53
23	B	610	CLA	MG-NA	-2.78	1.99	2.06
23	b	610	CLA	OBD-CAD	-2.78	1.18	1.22
23	D	404	CLA	CAA-C2A	-2.78	1.48	1.54
23	C	505	CLA	MG-NA	-2.78	1.99	2.06
23	C	509	CLA	C3B-CAB	2.78	1.53	1.47
23	b	614	CLA	OBD-CAD	-2.78	1.18	1.22
23	b	613	CLA	O2D-CGD	2.78	1.40	1.33
23	C	508	CLA	O2D-CGD	2.78	1.40	1.33
25	H	101	BCR	C4-C5	2.78	1.56	1.51
23	C	503	CLA	C3D-CAD	2.78	1.53	1.46
23	B	608	CLA	O2D-CGD	2.78	1.40	1.33
32	C	517	DGD	O2D-C2D	2.77	1.49	1.43
27	a	610	SQD	C6-S	-2.77	1.67	1.77
25	B	619	BCR	C1-C6	-2.77	1.50	1.53
32	d	405	DGD	C6E-C5E	-2.77	1.42	1.51
23	B	606	CLA	C3D-CAD	2.77	1.53	1.46
25	c	515	BCR	C35-C13	-2.77	1.45	1.50
25	H	101	BCR	C12-C13	2.77	1.51	1.45
25	f	101	BCR	C12-C13	2.76	1.51	1.45
23	c	504	CLA	C3B-CAB	2.76	1.53	1.47
23	B	602	CLA	C3B-CAB	2.76	1.53	1.47
25	B	620	BCR	C31-C1	-2.76	1.48	1.53
23	c	513	CLA	C3B-CAB	2.76	1.53	1.47
23	b	613	CLA	O2D-CED	-2.76	1.38	1.45
23	C	502	CLA	O2D-CGD	2.76	1.39	1.33
32	H	102	DGD	O6E-C1E	2.76	1.48	1.41
23	c	509	CLA	C3B-CAB	2.76	1.53	1.47
23	C	512	CLA	C3B-CAB	2.75	1.53	1.47
25	F	101	BCR	C1-C6	-2.75	1.50	1.53
23	A	606	CLA	O2D-CGD	2.75	1.39	1.33
23	c	512	CLA	O2D-CED	-2.75	1.38	1.45
23	b	607	CLA	C3B-CAB	2.75	1.53	1.47
23	c	504	CLA	OBD-CAD	-2.75	1.18	1.22
25	b	620	BCR	C35-C13	-2.75	1.45	1.50
23	b	618	CLA	OBD-CAD	-2.75	1.18	1.22
23	B	609	CLA	C3B-CAB	2.75	1.53	1.47
23	c	511	CLA	OBD-CAD	-2.74	1.18	1.22
32	D	406	DGD	O6E-C1E	2.74	1.48	1.41
32	D	406	DGD	O5D-C1E	2.74	1.44	1.40
23	C	501	CLA	C3B-CAB	2.74	1.53	1.47
23	c	512	CLA	O2D-CGD	2.74	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	OBD-CAD	-2.74	1.18	1.22
23	b	610	CLA	C3D-CAD	2.74	1.53	1.46
23	c	513	CLA	O2D-CGD	2.74	1.39	1.33
23	A	605	CLA	O2D-CGD	2.74	1.39	1.33
23	D	403	CLA	C3B-CAB	2.74	1.53	1.47
25	t	101	BCR	C35-C13	-2.73	1.45	1.50
25	c	516	BCR	C1-C6	-2.73	1.50	1.53
23	C	503	CLA	O2D-CGD	2.73	1.39	1.33
24	D	401	PHO	C4C-C3C	2.73	1.50	1.45
23	C	501	CLA	OBD-CAD	-2.73	1.18	1.22
23	A	608	CLA	MG-NA	-2.73	1.99	2.06
23	A	606	CLA	OBD-CAD	-2.73	1.18	1.22
32	D	406	DGD	C6E-C5E	-2.73	1.42	1.51
23	C	506	CLA	MG-NA	-2.72	1.99	2.06
23	C	508	CLA	C3B-CAB	2.72	1.53	1.47
24	A	607	PHO	C1A-NA	2.72	1.42	1.37
23	c	512	CLA	C3B-CAB	2.72	1.53	1.47
25	b	620	BCR	C31-C1	-2.72	1.48	1.53
23	B	612	CLA	MG-NA	-2.72	1.99	2.06
23	b	605	CLA	OBD-CAD	-2.72	1.18	1.22
23	B	615	CLA	OBD-CAD	-2.71	1.18	1.22
23	C	501	CLA	O2D-CGD	2.71	1.39	1.33
23	c	511	CLA	O2D-CED	-2.71	1.38	1.45
25	F	101	BCR	C35-C13	-2.71	1.45	1.50
25	b	622	BCR	C31-C1	-2.71	1.48	1.53
23	c	502	CLA	MG-NA	-2.71	1.99	2.06
23	b	605	CLA	C1B-CHB	2.71	1.48	1.41
32	c	518	DGD	O2D-C2D	2.71	1.49	1.43
23	b	606	CLA	C3D-CAD	2.71	1.52	1.46
23	d	402	CLA	C3B-CAB	2.71	1.53	1.47
23	b	608	CLA	MG-NA	-2.70	1.99	2.06
23	C	503	CLA	OBD-CAD	-2.70	1.18	1.22
23	C	504	CLA	O2D-CGD	2.70	1.39	1.33
27	b	601	SQD	C6-S	-2.70	1.67	1.77
23	B	615	CLA	MG-NA	-2.70	1.99	2.06
23	B	613	CLA	C3B-CAB	2.70	1.53	1.47
23	b	609[B]	CLA	MG-NA	-2.70	1.99	2.06
23	b	607	CLA	OBD-CAD	-2.69	1.18	1.22
23	B	608	CLA	O2D-CED	-2.69	1.39	1.45
23	b	617	CLA	OBD-CAD	-2.69	1.18	1.22
32	C	516	DGD	O2D-C2D	2.69	1.49	1.43
23	B	606	CLA	MG-NA	-2.69	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	MG-NA	-2.69	1.99	2.06
23	C	505	CLA	OBD-CAD	-2.69	1.18	1.22
23	c	502	CLA	C3B-CAB	2.69	1.53	1.47
24	a	606	PHO	C4C-NC	2.69	1.42	1.36
23	D	403	CLA	O2D-CED	-2.69	1.39	1.45
23	B	610	CLA	C3B-CAB	2.69	1.53	1.47
23	c	503	CLA	MG-NA	-2.68	1.99	2.06
23	B	616	CLA	O2D-CGD	2.68	1.39	1.33
23	C	508	CLA	OBD-CAD	-2.68	1.18	1.22
23	C	502	CLA	MG-NA	-2.68	1.99	2.06
23	C	503	CLA	O2D-CED	-2.68	1.39	1.45
23	d	402	CLA	O2D-CED	-2.68	1.39	1.45
27	a	612	SQD	C6-S	-2.68	1.67	1.77
25	b	622	BCR	C12-C13	2.68	1.51	1.45
23	d	403	CLA	C3B-CAB	2.68	1.53	1.47
23	c	502	CLA	OBD-CAD	-2.67	1.18	1.22
23	c	506	CLA	C3B-CAB	2.67	1.53	1.47
23	c	512	CLA	OBD-CAD	-2.67	1.18	1.22
23	B	614	CLA	C3B-CAB	2.67	1.53	1.47
23	b	616	CLA	C3B-CAB	2.67	1.53	1.47
23	c	512	CLA	MG-NA	-2.67	1.99	2.06
25	h	101	BCR	C1-C6	-2.67	1.50	1.53
25	K	101	BCR	C12-C13	2.67	1.51	1.45
23	a	613	CLA	C3B-CAB	2.67	1.53	1.47
23	c	514	CLA	OBD-CAD	-2.66	1.18	1.22
23	a	604	CLA	C3B-CAB	2.66	1.53	1.47
23	C	511	CLA	OBD-CAD	-2.66	1.18	1.22
25	C	514	BCR	C31-C1	-2.66	1.48	1.53
32	C	518	DGD	O2D-C2D	2.66	1.49	1.43
23	a	613	CLA	O2D-CED	-2.65	1.39	1.45
32	c	519	DGD	O2D-C2D	2.65	1.49	1.43
23	B	603	CLA	OBD-CAD	-2.65	1.18	1.22
24	a	606	PHO	C1A-NA	2.65	1.42	1.37
23	C	510	CLA	MG-NA	-2.65	2.00	2.06
32	C	516	DGD	C3E-C2E	-2.65	1.45	1.52
23	d	403	CLA	MG-NA	-2.65	2.00	2.06
23	c	506	CLA	OBD-CAD	-2.65	1.18	1.22
23	C	501	CLA	MG-NA	-2.65	2.00	2.06
23	b	611	CLA	OBD-CAD	-2.65	1.18	1.22
23	b	611	CLA	MG-NA	-2.65	2.00	2.06
23	b	610	CLA	MG-NA	-2.65	2.00	2.06
23	c	514	CLA	C3B-CAB	2.65	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404	CLA	C3B-CAB	2.64	1.53	1.47
32	d	405	DGD	O2D-C2D	2.64	1.49	1.43
23	B	616	CLA	OBD-CAD	-2.64	1.18	1.22
23	b	604	CLA	C3B-CAB	2.64	1.53	1.47
23	B	607[A]	CLA	MG-NA	-2.64	2.00	2.06
23	C	513	CLA	OBD-CAD	-2.64	1.18	1.22
32	c	517	DGD	O2D-C2D	2.64	1.49	1.43
23	D	402	CLA	O2D-CGD	2.64	1.39	1.33
23	c	513	CLA	OBD-CAD	-2.64	1.18	1.22
27	X	101	SQD	C6-S	-2.64	1.67	1.77
25	b	620	BCR	C27-C26	2.64	1.56	1.51
25	C	521	BCR	C31-C1	-2.63	1.48	1.53
32	c	517	DGD	C3E-C2E	-2.63	1.45	1.52
23	C	512	CLA	MG-NA	-2.63	2.00	2.06
23	C	504	CLA	O2D-CED	-2.63	1.39	1.45
23	B	614	CLA	MG-NA	-2.63	2.00	2.06
32	H	102	DGD	O2D-C2D	2.63	1.49	1.43
25	A	609	BCR	C1-C6	-2.62	1.50	1.53
24	d	401	PHO	C4C-C3C	2.62	1.49	1.45
23	B	614	CLA	O2D-CED	-2.62	1.39	1.45
23	c	509	CLA	OBD-CAD	-2.62	1.18	1.22
27	x	101	SQD	C6-S	-2.62	1.67	1.77
32	h	102	DGD	O2D-C2D	2.62	1.49	1.43
23	B	612	CLA	OBD-CAD	-2.62	1.18	1.22
23	c	505	CLA	OBD-CAD	-2.62	1.18	1.22
23	b	604	CLA	MG-NA	-2.61	2.00	2.06
23	C	504	CLA	C3B-CAB	2.61	1.53	1.47
23	D	403	CLA	O2D-CGD	2.61	1.39	1.33
23	a	604	CLA	C2A-C1A	-2.61	1.46	1.52
23	c	504	CLA	MG-NA	-2.61	2.00	2.06
23	B	614	CLA	O2D-CGD	2.61	1.39	1.33
25	H	101	BCR	C35-C13	-2.61	1.45	1.50
23	B	608	CLA	MG-NA	-2.61	2.00	2.06
32	d	405	DGD	O6E-C1E	2.61	1.48	1.41
23	C	511	CLA	C3B-CAB	2.61	1.53	1.47
32	H	102	DGD	O5D-C1E	2.61	1.44	1.40
23	B	610	CLA	OBD-CAD	-2.61	1.18	1.22
23	b	616	CLA	MG-NA	-2.61	2.00	2.06
23	c	511	CLA	C3B-CAB	2.60	1.53	1.47
23	b	615	CLA	C3B-CAB	2.60	1.53	1.47
23	B	605	CLA	OBD-CAD	-2.60	1.18	1.22
23	B	616	CLA	MG-NA	-2.60	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	607	PHO	C4C-C3C	2.60	1.49	1.45
23	A	608	CLA	OBD-CAD	-2.60	1.18	1.22
23	B	608	CLA	C3B-CAB	2.60	1.53	1.47
25	C	521	BCR	C35-C13	-2.60	1.45	1.50
23	b	613	CLA	MG-NA	-2.60	2.00	2.06
23	b	609[A]	CLA	MG-NA	-2.60	2.00	2.06
23	c	511	CLA	MG-NA	-2.60	2.00	2.06
23	c	505	CLA	O2D-CED	-2.60	1.39	1.45
23	c	513	CLA	MG-NA	-2.59	2.00	2.06
23	b	613	CLA	C3B-CAB	2.59	1.53	1.47
23	C	510	CLA	O2D-CGD	2.59	1.39	1.33
23	d	402	CLA	O2D-CGD	2.59	1.39	1.33
23	b	608	CLA	OBD-CAD	-2.59	1.18	1.22
23	C	513	CLA	C3B-CAB	2.59	1.53	1.47
23	B	607[B]	CLA	MG-NA	-2.59	2.00	2.06
23	B	611	CLA	MG-NA	-2.59	2.00	2.06
23	C	510	CLA	O2D-CED	-2.59	1.39	1.45
23	B	605	CLA	C3B-CAB	2.59	1.53	1.47
32	D	406	DGD	O2D-C2D	2.59	1.49	1.43
23	a	613	CLA	O2D-CGD	2.59	1.39	1.33
23	D	404	CLA	O2D-CED	-2.59	1.39	1.45
23	B	613	CLA	OBD-CAD	-2.58	1.18	1.22
23	c	507	CLA	MG-NA	-2.58	2.00	2.06
32	h	102	DGD	O6E-C1E	2.58	1.48	1.41
23	b	618	CLA	MG-NA	-2.58	2.00	2.06
23	b	615	CLA	OBD-CAD	-2.58	1.18	1.22
23	a	607	CLA	OBD-CAD	-2.58	1.18	1.22
23	B	615	CLA	C3B-CAB	2.58	1.53	1.47
23	b	610	CLA	C3B-CAB	2.58	1.53	1.47
23	b	607	CLA	MG-NA	-2.57	2.00	2.06
23	B	616	CLA	O2D-CED	-2.57	1.39	1.45
23	a	604	CLA	O2D-CGD	2.57	1.39	1.33
23	c	511	CLA	O2D-CGD	2.57	1.39	1.33
23	D	402	CLA	O2D-CED	-2.57	1.39	1.45
23	B	610	CLA	O2D-CED	-2.57	1.39	1.45
25	B	618	BCR	C31-C1	-2.57	1.48	1.53
23	C	502	CLA	OBD-CAD	-2.57	1.18	1.22
23	c	504	CLA	O2D-CGD	2.57	1.39	1.33
23	C	507	CLA	MG-NA	-2.57	2.00	2.06
23	b	609[A]	CLA	OBD-CAD	-2.57	1.18	1.22
32	d	405	DGD	O5D-C1E	2.56	1.44	1.40
23	c	503	CLA	OBD-CAD	-2.56	1.18	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	h	102	DGD	O5D-C1E	2.56	1.44	1.40
25	F	101	BCR	C12-C13	2.56	1.51	1.45
23	A	605	CLA	C2A-C1A	-2.56	1.46	1.52
23	b	610	CLA	O2D-CED	-2.56	1.39	1.45
25	b	622	BCR	C1-C6	-2.56	1.50	1.53
23	b	604	CLA	O2D-CED	-2.56	1.39	1.45
27	b	602	SQD	C6-S	-2.55	1.68	1.77
26	d	404	PL9	C41-C39	2.55	1.56	1.51
25	c	516	BCR	C31-C1	-2.55	1.48	1.53
23	C	506	CLA	OBD-CAD	-2.55	1.18	1.22
23	c	510	CLA	C3B-CAB	2.55	1.53	1.47
25	b	621	BCR	C7-C6	2.55	1.54	1.45
23	C	512	CLA	OBD-CAD	-2.55	1.18	1.22
23	B	608	CLA	C2A-C1A	-2.55	1.46	1.52
23	C	502	CLA	O2D-CED	-2.55	1.39	1.45
26	D	405	PL9	C41-C39	2.55	1.56	1.51
23	b	617	CLA	C3B-CAB	2.55	1.53	1.47
23	A	606	CLA	O2D-CED	-2.55	1.39	1.45
25	c	522	BCR	C31-C1	-2.55	1.48	1.53
23	b	617	CLA	O2D-CED	-2.54	1.39	1.45
23	b	616	CLA	O2D-CED	-2.54	1.39	1.45
23	B	607[A]	CLA	OBD-CAD	-2.54	1.18	1.22
23	b	618	CLA	O2D-CED	-2.54	1.39	1.45
23	d	403	CLA	O2D-CED	-2.54	1.39	1.45
23	b	615	CLA	O2D-CED	-2.54	1.39	1.45
23	b	612	CLA	OBD-CAD	-2.54	1.18	1.22
23	B	602	CLA	MG-NA	-2.54	2.00	2.06
23	C	501	CLA	O2D-CED	-2.54	1.39	1.45
23	B	606	CLA	O2D-CED	-2.53	1.39	1.45
23	B	611	CLA	C3B-CAB	2.53	1.53	1.47
25	f	101	BCR	C31-C1	-2.53	1.48	1.53
23	c	505	CLA	C3B-CAB	2.52	1.53	1.47
23	c	513	CLA	O2D-CED	-2.52	1.39	1.45
23	B	609	CLA	OBD-CAD	-2.52	1.18	1.22
23	D	404	CLA	MG-NA	-2.52	2.00	2.06
25	h	101	BCR	C31-C1	-2.52	1.48	1.53
25	C	521	BCR	C1-C6	-2.52	1.50	1.53
23	B	604	CLA	O2D-CED	-2.52	1.39	1.45
23	B	613	CLA	O2D-CED	-2.52	1.39	1.45
23	B	608	CLA	OBD-CAD	-2.52	1.18	1.22
27	B	623	SQD	C6-S	-2.52	1.68	1.77
25	B	618	BCR	C12-C13	2.51	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	OBD-CAD	-2.51	1.18	1.22
23	a	604	CLA	OBD-CAD	-2.51	1.18	1.22
23	C	509	CLA	OBD-CAD	-2.51	1.18	1.22
23	B	607[A]	CLA	O2D-CED	-2.51	1.39	1.45
23	A	608	CLA	C3B-CAB	2.51	1.53	1.47
23	B	607[B]	CLA	O2D-CED	-2.51	1.39	1.45
23	C	512	CLA	O2D-CED	-2.51	1.39	1.45
23	C	511	CLA	O2D-CED	-2.51	1.39	1.45
25	c	515	BCR	C12-C13	2.51	1.51	1.45
25	A	609	BCR	C31-C1	-2.50	1.48	1.53
23	c	503	CLA	O2D-CED	-2.50	1.39	1.45
23	b	612	CLA	O2D-CED	-2.50	1.39	1.45
23	b	609[B]	CLA	O2D-CED	-2.50	1.39	1.45
23	c	502	CLA	O2D-CED	-2.50	1.39	1.45
25	K	101	BCR	C35-C13	-2.50	1.45	1.50
23	B	615	CLA	O2D-CED	-2.49	1.39	1.45
23	b	604	CLA	OBD-CAD	-2.49	1.18	1.22
23	b	606	CLA	O2D-CED	-2.49	1.39	1.45
23	C	505	CLA	O2D-CED	-2.49	1.39	1.45
23	B	602	CLA	O2D-CED	-2.48	1.39	1.45
25	B	620	BCR	C12-C13	2.48	1.51	1.45
23	B	617	CLA	O2D-CED	-2.48	1.39	1.45
25	C	515	BCR	C31-C1	-2.48	1.48	1.53
23	b	608	CLA	C2A-C1A	-2.48	1.46	1.52
32	h	102	DGD	C3E-C2E	-2.48	1.46	1.52
32	C	518	DGD	C3E-C2E	-2.48	1.46	1.52
32	C	516	DGD	O6E-C1E	2.48	1.48	1.41
23	c	507	CLA	O2D-CED	-2.48	1.39	1.45
23	b	617	CLA	C2A-C1A	-2.47	1.46	1.52
23	C	505	CLA	C2A-C1A	-2.47	1.46	1.52
23	B	602	CLA	OBD-CAD	-2.47	1.18	1.22
25	b	621	BCR	C1-C6	-2.47	1.50	1.53
23	b	609[A]	CLA	O2D-CED	-2.47	1.39	1.45
24	a	606	PHO	C4C-C3C	2.47	1.49	1.45
23	c	507	CLA	C3B-CAB	2.47	1.53	1.47
32	d	405	DGD	O6D-C1D	2.47	1.48	1.41
23	a	607	CLA	O2D-CED	-2.46	1.39	1.45
23	b	618	CLA	C3B-CAB	2.46	1.53	1.47
23	C	506	CLA	C3B-CAB	2.46	1.53	1.47
23	D	403	CLA	C2A-C1A	-2.46	1.46	1.52
23	c	510	CLA	OBD-CAD	-2.46	1.18	1.22
32	C	517	DGD	O3D-C3D	2.46	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	509	CLA	O2D-CED	-2.46	1.39	1.45
23	b	611	CLA	O2D-CED	-2.46	1.39	1.45
23	B	609	CLA	MG-NA	-2.45	2.00	2.06
23	C	502	CLA	C3B-CAB	2.45	1.52	1.47
23	c	506	CLA	C2A-C1A	-2.45	1.46	1.52
25	a	608	BCR	C31-C1	-2.45	1.48	1.53
23	b	614	CLA	O2D-CED	-2.45	1.39	1.45
23	B	609	CLA	O2D-CED	-2.45	1.39	1.45
23	b	605	CLA	C3B-CAB	2.45	1.52	1.47
23	c	503	CLA	C3B-CAB	2.44	1.52	1.47
25	t	101	BCR	C7-C6	2.44	1.53	1.45
23	b	608	CLA	O2D-CED	-2.44	1.39	1.45
23	c	508	CLA	MG-NA	-2.44	2.00	2.06
23	b	612	CLA	C3B-CAB	2.44	1.52	1.47
32	D	406	DGD	O3D-C3D	2.44	1.48	1.43
23	b	609[B]	CLA	OBD-CAD	-2.43	1.18	1.22
32	C	516	DGD	O3D-C3D	2.43	1.48	1.43
32	c	517	DGD	O6D-C1D	2.43	1.48	1.41
23	a	605	CLA	O2D-CED	-2.43	1.39	1.45
32	C	518	DGD	O6E-C1E	2.43	1.48	1.41
25	B	619	BCR	C7-C6	2.43	1.53	1.45
23	c	506	CLA	O2D-CED	-2.43	1.39	1.45
23	b	605	CLA	C2A-C1A	-2.43	1.46	1.52
25	k	101	BCR	C7-C6	2.43	1.53	1.45
23	B	606	CLA	C3B-CAB	2.43	1.52	1.47
23	C	506	CLA	O2D-CED	-2.43	1.39	1.45
32	D	406	DGD	O6D-C1D	2.43	1.48	1.41
23	A	608	CLA	O2D-CED	-2.43	1.39	1.45
23	C	508	CLA	C2A-C1A	-2.43	1.46	1.52
23	B	603	CLA	C3B-CAB	2.42	1.52	1.47
25	C	514	BCR	C7-C6	2.42	1.53	1.45
23	b	608	CLA	C3B-CAB	2.42	1.52	1.47
32	H	102	DGD	C3E-C2E	-2.42	1.46	1.52
23	B	616	CLA	C3B-CAB	2.42	1.52	1.47
23	B	617	CLA	C3B-CAB	2.42	1.52	1.47
32	d	405	DGD	O3D-C3D	2.41	1.48	1.43
23	B	603	CLA	O2D-CED	-2.41	1.39	1.45
25	b	622	BCR	C7-C6	2.41	1.53	1.45
23	B	606	CLA	C2A-C1A	-2.41	1.46	1.52
23	d	402	CLA	C2A-C1A	-2.41	1.46	1.52
23	C	508	CLA	O2D-CED	-2.41	1.39	1.45
23	B	612	CLA	O2D-CED	-2.41	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	516	DGD	O6D-C1D	2.40	1.48	1.41
32	c	518	DGD	O3D-C3D	2.40	1.48	1.43
23	b	619	CLA	O2D-CED	-2.40	1.39	1.45
23	B	609	CLA	C2A-C1A	-2.40	1.46	1.52
25	A	609	BCR	C7-C6	2.40	1.53	1.45
32	H	102	DGD	O3D-C3D	2.40	1.48	1.43
25	H	101	BCR	C31-C1	-2.40	1.49	1.53
23	C	504	CLA	C2A-C1A	-2.40	1.46	1.52
23	c	510	CLA	O2D-CED	-2.39	1.39	1.45
32	d	405	DGD	O3G-C1D	2.39	1.44	1.40
23	b	607	CLA	O2D-CED	-2.39	1.39	1.45
23	B	607[B]	CLA	OBD-CAD	-2.39	1.18	1.22
23	b	611	CLA	C2A-C1A	-2.39	1.46	1.52
32	c	517	DGD	O3D-C3D	2.39	1.48	1.43
25	H	101	BCR	C1-C6	-2.39	1.50	1.53
23	B	605	CLA	O2D-CED	-2.38	1.39	1.45
32	c	519	DGD	C3E-C2E	-2.38	1.46	1.52
32	h	102	DGD	O6D-C1D	2.38	1.47	1.41
23	c	514	CLA	O2D-CED	-2.38	1.39	1.45
32	D	406	DGD	O3G-C1D	2.38	1.44	1.40
32	c	518	DGD	C3E-C2E	-2.38	1.46	1.52
23	c	514	CLA	C2A-C1A	-2.37	1.46	1.52
24	d	401	PHO	C1A-NA	2.37	1.42	1.37
32	c	517	DGD	O6E-C1E	2.37	1.47	1.41
23	C	513	CLA	O2D-CED	-2.37	1.39	1.45
24	d	401	PHO	C1C-NC	-2.36	1.33	1.38
23	C	507	CLA	O2D-CED	-2.36	1.39	1.45
23	C	510	CLA	C2A-C1A	-2.36	1.46	1.52
23	c	508	CLA	O2D-CED	-2.36	1.39	1.45
23	B	615	CLA	C2A-C1A	-2.36	1.46	1.52
32	C	518	DGD	O3D-C3D	2.36	1.48	1.43
25	F	101	BCR	C31-C1	-2.36	1.49	1.53
23	C	509	CLA	O2D-CED	-2.35	1.39	1.45
32	c	519	DGD	O3D-C3D	2.35	1.48	1.43
25	c	516	BCR	C7-C6	2.35	1.53	1.45
32	C	517	DGD	C3E-C2E	-2.34	1.46	1.52
23	C	513	CLA	C2A-C1A	-2.34	1.47	1.52
32	c	519	DGD	O6E-C1E	2.33	1.47	1.41
25	B	620	BCR	C7-C6	2.33	1.53	1.45
23	B	617	CLA	C2A-C1A	-2.33	1.47	1.52
25	a	608	BCR	C7-C6	2.33	1.53	1.45
23	B	604	CLA	C2A-C1A	-2.33	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	C2A-C1A	-2.33	1.47	1.52
23	B	603	CLA	C2A-C1A	-2.33	1.47	1.52
23	B	613	CLA	C2A-C1A	-2.33	1.47	1.52
32	C	518	DGD	C1D-C2D	-2.32	1.45	1.52
25	a	608	BCR	C1-C6	-2.32	1.50	1.53
23	b	615	CLA	C2A-C1A	-2.32	1.47	1.52
23	b	612	CLA	C2A-C1A	-2.32	1.47	1.52
25	b	620	BCR	C12-C13	2.31	1.50	1.45
23	b	610	CLA	C2A-C1A	-2.31	1.47	1.52
23	b	605	CLA	O2D-CED	-2.31	1.39	1.45
23	b	609[A]	CLA	C3B-CAB	2.31	1.52	1.47
23	c	511	CLA	C2A-C1A	-2.31	1.47	1.52
32	H	102	DGD	O6D-C1D	2.30	1.47	1.41
23	d	403	CLA	OBD-CAD	-2.30	1.19	1.22
24	d	401	PHO	CHD-C1D	2.30	1.43	1.38
32	c	517	DGD	C6D-C5D	-2.30	1.44	1.51
23	c	505	CLA	C2A-C1A	-2.30	1.47	1.52
23	c	507	CLA	C2A-C1A	-2.30	1.47	1.52
32	c	519	DGD	C1D-C2D	-2.29	1.45	1.52
32	c	519	DGD	C6D-C5D	-2.29	1.44	1.51
23	D	402	CLA	C2A-C1A	-2.29	1.47	1.52
23	D	404	CLA	OBD-CAD	-2.29	1.19	1.22
32	C	516	DGD	C1D-C2D	-2.29	1.45	1.52
32	C	517	DGD	O6E-C1E	2.28	1.47	1.41
23	b	609[B]	CLA	C3B-CAB	2.28	1.52	1.47
32	c	519	DGD	O5D-C1E	2.27	1.44	1.40
25	f	101	BCR	C7-C6	2.27	1.53	1.45
32	C	518	DGD	C6D-C5D	-2.27	1.44	1.51
32	c	518	DGD	C6D-C5D	-2.27	1.44	1.51
23	b	619	CLA	C3B-CAB	2.27	1.52	1.47
28	z	101	LMG	O8-C28	2.27	1.44	1.33
25	T	101	BCR	C31-C1	-2.27	1.49	1.53
23	B	614	CLA	C2A-C1A	-2.26	1.47	1.52
28	Z	101	LMG	O8-C28	2.26	1.44	1.33
32	C	516	DGD	O5D-C1E	2.26	1.44	1.40
23	b	609[B]	CLA	C2A-C1A	-2.25	1.47	1.52
23	c	509	CLA	C2A-C1A	-2.25	1.47	1.52
24	D	401	PHO	C1C-NC	-2.25	1.33	1.38
24	D	401	PHO	CHD-C1D	2.25	1.43	1.38
32	h	102	DGD	O3D-C3D	2.25	1.48	1.43
23	C	511	CLA	C2A-C1A	-2.24	1.47	1.52
23	A	608	CLA	C2A-C1A	-2.23	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	PHO	C1A-NA	2.23	1.41	1.37
32	c	518	DGD	C1E-C2E	-2.23	1.46	1.52
23	B	602	CLA	C2A-C1A	-2.23	1.47	1.52
23	b	619	CLA	C2A-C1A	-2.23	1.47	1.52
23	A	606	CLA	C2A-C1A	-2.23	1.47	1.52
25	c	515	BCR	C7-C6	2.23	1.53	1.45
23	B	607[A]	CLA	C3B-CAB	2.23	1.52	1.47
32	C	516	DGD	C6D-C5D	-2.22	1.44	1.51
23	B	607[B]	CLA	C3B-CAB	2.22	1.52	1.47
25	h	101	BCR	C7-C6	2.22	1.53	1.45
32	C	517	DGD	O5D-C1E	2.22	1.44	1.40
24	A	607	PHO	C1C-NC	-2.21	1.33	1.38
32	c	518	DGD	O6E-C1E	2.21	1.47	1.41
23	c	502	CLA	C2A-C1A	-2.21	1.47	1.52
23	C	502	CLA	C2A-C1A	-2.21	1.47	1.52
23	a	613	CLA	C2A-C1A	-2.21	1.47	1.52
25	F	101	BCR	C7-C6	2.20	1.52	1.45
25	K	101	BCR	C7-C6	2.20	1.52	1.45
32	H	102	DGD	C6D-C5D	-2.20	1.44	1.51
32	h	102	DGD	C1D-C2D	-2.20	1.46	1.52
23	b	618	CLA	C2A-C1A	-2.20	1.47	1.52
32	c	519	DGD	O6D-C1D	2.20	1.47	1.41
23	b	613	CLA	C2A-C1A	-2.19	1.47	1.52
32	C	517	DGD	O6D-C1D	2.19	1.47	1.41
24	a	606	PHO	C1C-NC	-2.19	1.33	1.38
23	b	606	CLA	C2A-C1A	-2.19	1.47	1.52
25	c	522	BCR	C7-C6	2.19	1.52	1.45
23	a	605	CLA	C2A-C1A	-2.19	1.47	1.52
32	c	517	DGD	O5D-C1E	2.19	1.43	1.40
32	C	516	DGD	C1E-C2E	-2.19	1.46	1.52
26	A	610	PL9	C41-C39	2.19	1.55	1.51
32	d	405	DGD	C6D-C5D	-2.19	1.44	1.51
23	B	612	CLA	C2A-C1A	-2.19	1.47	1.52
23	c	503	CLA	C2A-C1A	-2.19	1.47	1.52
23	c	504	CLA	C2A-C1A	-2.18	1.47	1.52
32	C	518	DGD	O6D-C1D	2.18	1.47	1.41
25	T	101	BCR	C7-C6	2.17	1.52	1.45
32	c	518	DGD	O6D-C1D	2.17	1.47	1.41
32	c	517	DGD	C1E-C2E	-2.17	1.46	1.52
24	A	607	PHO	CHD-C1D	2.17	1.42	1.38
31	e	101	LHG	C8-C7	2.16	1.57	1.50
23	b	609[A]	CLA	C2A-C1A	-2.16	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	518	DGD	O5D-C1E	2.16	1.43	1.40
23	B	607[B]	CLA	C2A-C1A	-2.16	1.47	1.52
32	H	102	DGD	C1D-C2D	-2.16	1.46	1.52
32	C	518	DGD	C1E-C2E	-2.16	1.46	1.52
31	D	408	LHG	C8-C7	2.15	1.57	1.50
25	b	620	BCR	C7-C6	2.15	1.52	1.45
32	d	405	DGD	C3E-C2E	-2.15	1.46	1.52
23	c	508	CLA	C3B-CAB	2.15	1.52	1.47
25	H	101	BCR	C7-C6	2.14	1.52	1.45
32	D	406	DGD	C6D-C5D	-2.14	1.44	1.51
26	a	609	PL9	C41-C39	2.14	1.55	1.51
31	E	101	LHG	C8-C7	2.14	1.57	1.50
25	B	619	BCR	C12-C13	2.14	1.50	1.45
32	C	517	DGD	C1E-C2E	-2.14	1.46	1.52
23	C	512	CLA	C2A-C1A	-2.13	1.47	1.52
24	A	607	PHO	C1B-C2B	2.13	1.50	1.45
25	C	514	BCR	C12-C13	2.13	1.50	1.45
33	E	102	HEM	CAA-C2A	2.13	1.55	1.52
27	b	602	SQD	O6-C1	2.13	1.43	1.40
23	c	512	CLA	C2A-C1A	-2.13	1.47	1.52
23	b	614	CLA	C2A-C1A	-2.13	1.47	1.52
26	A	610	PL9	C37-C38	2.13	1.57	1.50
32	c	517	DGD	C1D-C2D	-2.13	1.46	1.52
23	B	616	CLA	C2A-C1A	-2.12	1.47	1.52
31	B	622	LHG	C8-C7	2.12	1.56	1.50
23	c	510	CLA	C2A-C1A	-2.12	1.47	1.52
33	e	102	HEM	CAA-C2A	2.12	1.55	1.52
26	d	404	PL9	C22-C23	2.12	1.57	1.50
23	C	501	CLA	C2A-C1A	-2.11	1.47	1.52
32	c	519	DGD	C1E-C2E	-2.11	1.46	1.52
32	C	517	DGD	C6D-C5D	-2.11	1.45	1.51
25	C	515	BCR	C7-C6	2.11	1.52	1.45
23	B	607[A]	CLA	C2A-C1A	-2.11	1.47	1.52
26	d	404	PL9	C37-C38	2.11	1.57	1.50
25	c	522	BCR	C1-C6	-2.10	1.50	1.53
32	h	102	DGD	C6D-C5D	-2.10	1.45	1.51
32	C	517	DGD	O3G-C1D	2.10	1.43	1.40
27	B	623	SQD	O6-C1	2.10	1.43	1.40
25	C	514	BCR	C33-C5	2.10	1.54	1.50
26	A	610	PL9	C5-C4	-2.10	1.39	1.47
24	a	606	PHO	C1B-C2B	2.09	1.50	1.45
26	D	405	PL9	C37-C38	2.09	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	521	BCR	C7-C6	2.09	1.52	1.45
23	C	506	CLA	C2A-C1A	-2.09	1.47	1.52
24	a	606	PHO	CHD-C1D	2.08	1.42	1.38
23	b	604	CLA	C2A-C1A	-2.08	1.47	1.52
23	a	607	CLA	C2A-C1A	-2.08	1.47	1.52
26	A	610	PL9	C22-C23	2.07	1.57	1.50
23	b	607	CLA	C2A-C1A	-2.07	1.47	1.52
26	a	609	PL9	C17-C18	2.07	1.57	1.50
32	C	517	DGD	C1D-C2D	-2.07	1.46	1.52
32	c	518	DGD	O3G-C1D	2.06	1.43	1.40
23	b	616	CLA	C2A-C1A	-2.06	1.47	1.52
25	C	514	BCR	C1-C6	-2.06	1.50	1.53
24	a	606	PHO	C4B-NB	2.06	1.41	1.36
23	B	605	CLA	C2A-C1A	-2.06	1.47	1.52
26	a	609	PL9	C2-C3	2.05	1.40	1.34
23	c	513	CLA	C2A-C1A	-2.05	1.47	1.52
26	D	405	PL9	C22-C23	2.05	1.57	1.50
23	C	503	CLA	C2A-C1A	-2.05	1.47	1.52
23	d	403	CLA	C2A-C1A	-2.05	1.47	1.52
26	a	609	PL9	C5-C4	-2.04	1.39	1.47
25	b	622	BCR	C33-C5	2.04	1.54	1.50
23	D	404	CLA	CBA-CGA	2.04	1.56	1.50
23	B	611	CLA	C2A-C1A	-2.04	1.47	1.52
25	B	618	BCR	C7-C6	2.04	1.52	1.45
32	C	518	DGD	O5D-C1E	2.03	1.43	1.40
25	c	515	BCR	C33-C5	2.03	1.54	1.50
31	D	407	LHG	C8-C7	2.03	1.56	1.50
31	d	406	LHG	C8-C7	2.03	1.56	1.50
31	b	624	LHG	C8-C7	2.03	1.56	1.50
24	A	607	PHO	C4B-NB	2.02	1.41	1.36
26	A	610	PL9	C2-C3	2.02	1.40	1.34
28	C	520	LMG	C7-C8	2.02	1.56	1.50
32	c	518	DGD	C1D-C2D	-2.02	1.46	1.52
26	A	610	PL9	C17-C18	2.02	1.57	1.50
26	a	609	PL9	C22-C23	2.01	1.57	1.50
24	A	607	PHO	C1C-C2C	2.01	1.50	1.45
23	C	507	CLA	C3B-CAB	2.01	1.52	1.47
31	L	101	LHG	C8-C7	2.00	1.56	1.50
25	b	621	BCR	C12-C13	2.00	1.50	1.45
24	a	606	PHO	C1C-C2C	2.00	1.50	1.45

All (1959) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	621	BCR	C15-C16-C17	26.27	177.29	123.47
25	c	515	BCR	C15-C16-C17	25.42	175.54	123.47
25	T	101	BCR	C15-C16-C17	25.32	175.34	123.47
25	A	609	BCR	C15-C16-C17	25.24	175.18	123.47
25	a	608	BCR	C15-C16-C17	25.24	175.17	123.47
25	C	515	BCR	C15-C16-C17	25.12	174.94	123.47
25	F	101	BCR	C15-C16-C17	24.93	174.55	123.47
25	K	101	BCR	C15-C16-C17	24.92	174.52	123.47
25	t	101	BCR	C15-C16-C17	24.92	174.52	123.47
25	c	516	BCR	C15-C16-C17	24.66	173.98	123.47
25	B	619	BCR	C15-C16-C17	24.59	173.84	123.47
25	c	522	BCR	C15-C16-C17	24.54	173.74	123.47
25	b	622	BCR	C15-C16-C17	24.52	173.69	123.47
25	C	514	BCR	C15-C16-C17	24.48	173.62	123.47
25	B	620	BCR	C15-C16-C17	24.47	173.61	123.47
25	f	101	BCR	C15-C16-C17	24.47	173.60	123.47
25	k	101	BCR	C15-C16-C17	24.29	173.24	123.47
25	B	618	BCR	C15-C16-C17	23.95	172.54	123.47
25	C	521	BCR	C15-C16-C17	23.95	172.53	123.47
25	h	101	BCR	C15-C16-C17	23.60	171.81	123.47
25	H	101	BCR	C15-C16-C17	23.39	171.38	123.47
25	b	620	BCR	C15-C16-C17	22.00	168.55	123.47
25	c	516	BCR	C21-C20-C19	18.08	179.63	123.22
25	c	515	BCR	C21-C20-C19	17.82	178.82	123.22
25	C	514	BCR	C21-C20-C19	17.79	178.74	123.22
25	B	620	BCR	C21-C20-C19	17.75	178.62	123.22
25	b	620	BCR	C21-C20-C19	17.69	178.41	123.22
25	C	521	BCR	C21-C20-C19	17.64	178.26	123.22
25	h	101	BCR	C21-C20-C19	17.57	178.05	123.22
25	C	515	BCR	C21-C20-C19	17.52	177.89	123.22
25	b	621	BCR	C21-C20-C19	17.49	177.78	123.22
25	a	608	BCR	C21-C20-C19	17.34	177.34	123.22
25	t	101	BCR	C21-C20-C19	17.33	177.28	123.22
25	A	609	BCR	C21-C20-C19	17.16	176.77	123.22
25	H	101	BCR	C21-C20-C19	17.05	176.44	123.22
25	c	522	BCR	C21-C20-C19	17.05	176.43	123.22
25	f	101	BCR	C21-C20-C19	16.95	176.11	123.22
25	b	622	BCR	C21-C20-C19	16.90	175.94	123.22
25	K	101	BCR	C21-C20-C19	16.65	175.16	123.22
25	F	101	BCR	C21-C20-C19	16.41	174.43	123.22
25	B	618	BCR	C21-C20-C19	16.18	173.72	123.22
25	T	101	BCR	C21-C20-C19	16.02	173.22	123.22
25	k	101	BCR	C21-C20-C19	15.99	173.12	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	622	BCR	C38-C26-C25	-14.75	107.96	124.53
25	T	101	BCR	C33-C5-C6	-14.64	108.08	124.53
25	B	620	BCR	C38-C26-C25	-14.48	108.27	124.53
25	c	515	BCR	C38-C26-C25	-14.13	108.66	124.53
25	C	514	BCR	C38-C26-C25	-13.75	109.09	124.53
25	F	101	BCR	C33-C5-C6	-13.68	109.17	124.53
25	T	101	BCR	C38-C26-C25	-13.60	109.26	124.53
25	t	101	BCR	C38-C26-C25	-13.59	109.27	124.53
25	b	620	BCR	C33-C5-C6	-13.50	109.36	124.53
25	B	619	BCR	C21-C20-C19	13.48	165.28	123.22
25	B	618	BCR	C38-C26-C25	-13.40	109.48	124.53
25	K	101	BCR	C38-C26-C25	-13.34	109.55	124.53
25	B	618	BCR	C33-C5-C6	-13.33	109.56	124.53
25	C	521	BCR	C33-C5-C6	-13.31	109.58	124.53
25	k	101	BCR	C38-C26-C25	-13.28	109.62	124.53
25	b	620	BCR	C15-C14-C13	-13.21	108.45	127.31
25	f	101	BCR	C33-C5-C6	-13.13	109.79	124.53
25	h	101	BCR	C33-C5-C6	-13.12	109.79	124.53
25	A	609	BCR	C33-C5-C6	-13.06	109.86	124.53
25	c	522	BCR	C33-C5-C6	-12.92	110.02	124.53
25	k	101	BCR	C33-C5-C6	-12.87	110.07	124.53
25	C	514	BCR	C16-C17-C18	-12.79	109.06	127.31
25	a	608	BCR	C33-C5-C6	-12.75	110.21	124.53
25	C	521	BCR	C38-C26-C25	-12.74	110.22	124.53
25	K	101	BCR	C33-C5-C6	-12.66	110.31	124.53
25	H	101	BCR	C33-C5-C6	-12.36	110.64	124.53
25	c	515	BCR	C16-C17-C18	-12.33	109.71	127.31
25	c	516	BCR	C33-C5-C6	-12.32	110.69	124.53
25	F	101	BCR	C16-C17-C18	-12.29	109.77	127.31
25	T	101	BCR	C24-C23-C22	-12.25	107.72	126.23
25	H	101	BCR	C16-C17-C18	-12.16	109.95	127.31
25	c	522	BCR	C38-C26-C25	-12.16	110.87	124.53
25	c	516	BCR	C38-C26-C25	-11.96	111.09	124.53
25	C	515	BCR	C38-C26-C25	-11.81	111.27	124.53
25	C	514	BCR	C24-C23-C22	-11.62	108.68	126.23
25	B	618	BCR	C11-C10-C9	-11.47	110.94	127.31
25	b	620	BCR	C11-C10-C9	-11.41	111.03	127.31
25	B	620	BCR	C16-C17-C18	-11.30	111.18	127.31
25	h	101	BCR	C16-C17-C18	-10.95	111.69	127.31
25	h	101	BCR	C38-C26-C25	-10.92	112.26	124.53
25	B	619	BCR	C16-C17-C18	-10.91	111.74	127.31
25	B	620	BCR	C33-C5-C6	-10.74	112.47	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	515	BCR	C24-C23-C22	-10.72	110.03	126.23
25	c	515	BCR	C33-C5-C6	-10.71	112.50	124.53
25	t	101	BCR	C33-C5-C6	-10.71	112.50	124.53
25	B	618	BCR	C15-C14-C13	-10.70	112.04	127.31
25	C	515	BCR	C33-C5-C6	-10.66	112.56	124.53
25	b	620	BCR	C38-C26-C25	-10.54	112.69	124.53
25	C	515	BCR	C24-C23-C22	-10.53	110.33	126.23
25	H	101	BCR	C38-C26-C25	-10.52	112.72	124.53
25	b	622	BCR	C33-C5-C6	-10.47	112.77	124.53
25	F	101	BCR	C24-C23-C22	-10.44	110.46	126.23
25	C	514	BCR	C33-C5-C6	-10.43	112.82	124.53
25	b	621	BCR	C33-C5-C6	-10.39	112.86	124.53
25	A	609	BCR	C38-C26-C25	-10.35	112.90	124.53
25	B	619	BCR	C11-C10-C9	-10.30	112.61	127.31
25	a	608	BCR	C38-C26-C25	-10.21	113.06	124.53
25	k	101	BCR	C16-C17-C18	-10.13	112.86	127.31
25	B	620	BCR	C15-C14-C13	-9.99	113.06	127.31
25	t	101	BCR	C24-C23-C22	-9.96	111.18	126.23
25	C	521	BCR	C16-C17-C18	-9.93	113.14	127.31
26	d	404	PL9	C7-C8-C9	-9.85	110.39	126.79
26	D	405	PL9	C7-C8-C9	-9.73	110.59	126.79
25	c	516	BCR	C24-C23-C22	-9.73	111.53	126.23
25	A	609	BCR	C16-C17-C18	-9.64	113.55	127.31
25	f	101	BCR	C30-C25-C26	-9.58	109.12	122.61
25	b	622	BCR	C24-C23-C22	-9.57	111.78	126.23
25	b	622	BCR	C15-C14-C13	-9.52	113.72	127.31
25	B	619	BCR	C33-C5-C6	-9.51	113.85	124.53
25	b	621	BCR	C24-C23-C22	-9.30	112.19	126.23
25	B	619	BCR	C24-C23-C22	-9.26	112.24	126.23
25	C	515	BCR	C7-C8-C9	-9.23	112.29	126.23
25	f	101	BCR	C11-C10-C9	-9.20	114.18	127.31
25	b	621	BCR	C16-C17-C18	-9.14	114.26	127.31
25	B	620	BCR	C8-C7-C6	-9.14	101.53	127.20
25	c	522	BCR	C24-C23-C22	-9.08	112.51	126.23
25	K	101	BCR	C11-C10-C9	-9.08	114.36	127.31
25	F	101	BCR	C7-C8-C9	-9.06	112.54	126.23
25	C	515	BCR	C4-C5-C6	-9.06	109.58	122.73
25	c	522	BCR	C16-C17-C18	-9.03	114.42	127.31
25	F	101	BCR	C30-C25-C26	-9.01	109.92	122.61
25	H	101	BCR	C15-C14-C13	-8.99	114.48	127.31
25	K	101	BCR	C16-C17-C18	-8.89	114.62	127.31
25	C	515	BCR	C11-C10-C9	-8.84	114.69	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	521	BCR	C24-C23-C22	-8.83	112.89	126.23
25	b	621	BCR	C15-C14-C13	-8.74	114.83	127.31
25	c	516	BCR	C16-C17-C18	-8.74	114.84	127.31
25	C	514	BCR	C8-C7-C6	-8.59	103.07	127.20
25	b	621	BCR	C11-C10-C9	-8.54	115.13	127.31
25	h	101	BCR	C24-C23-C22	-8.51	113.37	126.23
25	c	522	BCR	C20-C21-C22	-8.50	115.18	127.31
25	a	608	BCR	C16-C17-C18	-8.48	115.21	127.31
25	f	101	BCR	C16-C17-C18	-8.43	115.28	127.31
25	b	621	BCR	C38-C26-C25	-8.36	115.14	124.53
25	f	101	BCR	C24-C23-C22	-8.28	113.72	126.23
25	C	515	BCR	C27-C26-C25	-8.27	110.73	122.73
25	f	101	BCR	C7-C8-C9	-8.25	113.76	126.23
25	B	618	BCR	C7-C8-C9	-8.22	113.82	126.23
25	c	515	BCR	C15-C14-C13	-8.22	115.58	127.31
25	K	101	BCR	C30-C25-C26	-8.19	111.07	122.61
25	F	101	BCR	C38-C26-C25	-8.14	115.39	124.53
25	b	620	BCR	C7-C8-C9	-8.10	114.00	126.23
25	B	618	BCR	C20-C21-C22	-8.09	115.77	127.31
25	C	514	BCR	C15-C14-C13	-8.08	115.78	127.31
25	t	101	BCR	C30-C25-C26	-8.06	111.25	122.61
25	b	622	BCR	C8-C7-C6	-8.06	104.55	127.20
25	B	620	BCR	C24-C23-C22	-8.03	114.09	126.23
25	c	516	BCR	C4-C5-C6	-8.00	111.12	122.73
25	c	516	BCR	C27-C26-C25	-7.98	111.14	122.73
25	b	620	BCR	C4-C5-C6	-7.96	111.17	122.73
25	h	101	BCR	C15-C14-C13	-7.93	115.99	127.31
25	B	620	BCR	C8-C9-C10	-7.92	106.79	118.94
25	a	608	BCR	C11-C10-C9	-7.92	116.01	127.31
25	F	101	BCR	C11-C10-C9	-7.92	116.01	127.31
25	T	101	BCR	C7-C6-C5	-7.85	102.44	121.46
25	B	619	BCR	C15-C14-C13	-7.80	116.18	127.31
25	T	101	BCR	C30-C25-C26	-7.80	111.63	122.61
25	K	101	BCR	C27-C26-C25	-7.78	111.43	122.73
25	f	101	BCR	C15-C14-C13	-7.77	116.23	127.31
25	T	101	BCR	C27-C26-C25	-7.75	111.49	122.73
25	a	608	BCR	C24-C23-C22	-7.74	114.54	126.23
25	t	101	BCR	C11-C10-C9	-7.73	116.28	127.31
25	B	619	BCR	C7-C8-C9	-7.70	114.59	126.23
25	a	608	BCR	C4-C5-C6	-7.68	111.58	122.73
25	B	618	BCR	C4-C5-C6	-7.66	111.61	122.73
25	a	608	BCR	C1-C6-C5	-7.66	111.83	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	f	101	BCR	C38-C26-C25	-7.63	115.96	124.53
25	k	101	BCR	C30-C25-C26	-7.59	111.92	122.61
26	A	610	PL9	C37-C38-C39	-7.57	109.42	127.66
25	F	101	BCR	C20-C21-C22	-7.54	116.55	127.31
25	h	101	BCR	C4-C5-C6	-7.51	111.83	122.73
25	b	620	BCR	C1-C6-C5	-7.47	112.09	122.61
25	C	515	BCR	C1-C6-C5	-7.42	112.16	122.61
25	c	515	BCR	C11-C10-C9	-7.39	116.76	127.31
26	a	609	PL9	C37-C38-C39	-7.37	109.91	127.66
25	c	515	BCR	C30-C25-C26	-7.37	112.23	122.61
25	H	101	BCR	C4-C5-C6	-7.36	112.04	122.73
26	a	609	PL9	C7-C8-C9	-7.31	114.63	126.79
25	t	101	BCR	C27-C26-C25	-7.29	112.15	122.73
25	B	620	BCR	C30-C25-C26	-7.28	112.36	122.61
25	A	609	BCR	C4-C5-C6	-7.25	112.21	122.73
23	B	610	CLA	CAD-C3D-C4D	-7.21	104.45	108.47
25	A	609	BCR	C1-C6-C5	-7.17	112.51	122.61
25	C	515	BCR	C16-C17-C18	-7.15	117.10	127.31
25	F	101	BCR	C36-C18-C17	-7.12	112.95	122.92
25	c	516	BCR	C1-C6-C5	-7.11	112.59	122.61
25	A	609	BCR	C11-C10-C9	-7.11	117.17	127.31
25	A	609	BCR	C24-C23-C22	-7.10	115.51	126.23
26	d	404	PL9	C32-C33-C34	-7.09	110.58	127.66
25	B	618	BCR	C1-C6-C5	-7.08	112.64	122.61
23	c	509	CLA	CAD-C3D-C4D	-7.07	104.53	108.47
25	f	101	BCR	C27-C26-C25	-7.05	112.49	122.73
25	H	101	BCR	C24-C23-C22	-7.04	115.60	126.23
26	d	404	PL9	C12-C13-C14	-6.99	110.84	127.66
25	K	101	BCR	C15-C14-C13	-6.98	117.34	127.31
25	c	522	BCR	C30-C25-C26	-6.97	112.80	122.61
25	C	521	BCR	C30-C25-C26	-6.95	112.83	122.61
23	A	605	CLA	C4A-NA-C1A	-6.95	103.58	106.71
26	A	610	PL9	C27-C28-C29	-6.94	110.95	127.66
25	c	515	BCR	C27-C26-C25	-6.91	112.69	122.73
23	b	612	CLA	CAD-C3D-C4D	-6.90	104.62	108.47
25	k	101	BCR	C27-C26-C25	-6.89	112.72	122.73
25	C	514	BCR	C8-C9-C10	-6.88	108.38	118.94
26	d	404	PL9	C27-C28-C29	-6.87	111.11	127.66
23	c	507	CLA	CAD-C3D-C4D	-6.87	104.64	108.47
26	A	610	PL9	C7-C8-C9	-6.86	115.37	126.79
23	C	502	CLA	CAD-C3D-C4D	-6.84	104.65	108.47
23	C	501	CLA	CAD-C3D-C4D	-6.83	104.66	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	t	101	BCR	C15-C14-C13	-6.82	117.58	127.31
25	A	609	BCR	C15-C14-C13	-6.80	117.60	127.31
26	D	405	PL9	C27-C28-C29	-6.79	111.30	127.66
25	F	101	BCR	C4-C5-C6	-6.79	112.87	122.73
25	f	101	BCR	C1-C6-C5	-6.79	113.05	122.61
25	C	521	BCR	C20-C21-C22	-6.78	117.63	127.31
23	B	617	CLA	CAD-C3D-C4D	-6.77	104.69	108.47
25	c	515	BCR	C8-C7-C6	-6.76	108.20	127.20
23	a	604	CLA	C4A-NA-C1A	-6.76	103.67	106.71
26	A	610	PL9	C42-C43-C44	-6.73	111.46	127.66
26	A	610	PL9	C16-C14-C13	-6.72	107.51	121.12
26	a	609	PL9	C27-C28-C29	-6.71	111.49	127.66
26	a	609	PL9	C42-C43-C44	-6.71	111.51	127.66
25	k	101	BCR	C15-C14-C13	-6.68	117.77	127.31
26	a	609	PL9	C16-C14-C13	-6.68	107.60	121.12
23	b	605	CLA	CAD-C3D-C4D	-6.65	104.76	108.47
23	b	619	CLA	CAD-C3D-C4D	-6.63	104.77	108.47
23	C	508	CLA	CAD-C3D-C4D	-6.62	104.78	108.47
23	B	611	CLA	CAD-C3D-C4D	-6.62	104.78	108.47
25	c	515	BCR	C7-C8-C9	-6.61	116.24	126.23
25	f	101	BCR	C4-C5-C6	-6.61	113.13	122.73
23	d	403	CLA	CAD-C3D-C4D	-6.61	104.78	108.47
26	a	609	PL9	C22-C23-C24	-6.59	111.79	127.66
25	C	514	BCR	C30-C25-C26	-6.59	113.33	122.61
25	F	101	BCR	C1-C6-C5	-6.58	113.34	122.61
23	C	505	CLA	C3A-C2A-C1A	6.58	111.19	101.34
23	B	603	CLA	CAD-C3D-C4D	-6.56	104.81	108.47
26	D	405	PL9	C32-C33-C34	-6.55	111.88	127.66
26	D	405	PL9	C16-C14-C13	-6.55	107.86	121.12
26	A	610	PL9	C17-C18-C19	-6.53	111.93	127.66
25	B	618	BCR	C30-C25-C26	-6.52	113.43	122.61
26	a	609	PL9	C17-C18-C19	-6.51	111.98	127.66
26	D	405	PL9	C12-C13-C14	-6.51	111.99	127.66
25	C	521	BCR	C15-C14-C13	-6.49	118.04	127.31
25	B	620	BCR	C4-C5-C6	-6.47	113.33	122.73
23	B	605	CLA	CAD-C3D-C4D	-6.47	104.86	108.47
25	c	522	BCR	C27-C26-C25	-6.47	113.34	122.73
23	C	504	CLA	CAD-C3D-C4D	-6.46	104.87	108.47
23	b	613	CLA	CAD-C3D-C4D	-6.44	104.88	108.47
23	b	607	CLA	CAD-C3D-C4D	-6.43	104.89	108.47
25	F	101	BCR	C27-C26-C25	-6.42	113.42	122.73
25	b	622	BCR	C30-C25-C26	-6.41	113.58	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	610	PL9	C22-C23-C24	-6.41	112.22	127.66
25	b	622	BCR	C8-C9-C10	-6.41	109.11	118.94
25	b	620	BCR	C23-C24-C25	-6.40	109.22	127.20
23	B	614	CLA	CAD-C3D-C4D	-6.40	104.90	108.47
23	C	506	CLA	CAD-C3D-C4D	-6.40	104.90	108.47
25	C	521	BCR	C11-C10-C9	-6.39	118.18	127.31
23	C	512	CLA	CAD-C3D-C4D	-6.38	104.91	108.47
23	B	612	CLA	CAD-C3D-C4D	-6.38	104.91	108.47
25	K	101	BCR	C34-C9-C10	-6.37	113.99	122.92
25	c	516	BCR	C11-C10-C9	-6.37	118.21	127.31
23	c	502	CLA	CAD-C3D-C4D	-6.37	104.92	108.47
23	c	506	CLA	C3A-C2A-C1A	6.37	110.88	101.34
23	B	604	CLA	CAD-C3D-C4D	-6.37	104.92	108.47
25	T	101	BCR	C11-C10-C9	-6.36	118.23	127.31
25	C	521	BCR	C8-C7-C6	-6.36	109.34	127.20
23	D	403	CLA	CAD-C3D-C4D	-6.36	104.93	108.47
25	k	101	BCR	C34-C9-C10	-6.35	114.02	122.92
25	H	101	BCR	C1-C6-C5	-6.35	113.67	122.61
23	B	608	CLA	CAD-C3D-C4D	-6.33	104.94	108.47
25	K	101	BCR	C24-C23-C22	-6.33	116.67	126.23
25	a	608	BCR	C20-C21-C22	-6.32	118.29	127.31
26	d	404	PL9	C16-C14-C13	-6.31	108.34	121.12
23	b	614	CLA	CAD-C3D-C4D	-6.31	104.95	108.47
23	c	505	CLA	CAD-C3D-C4D	-6.29	104.96	108.47
23	c	508	CLA	CAD-C3D-C4D	-6.28	104.97	108.47
25	C	521	BCR	C4-C5-C6	-6.27	113.63	122.73
23	c	508	CLA	O2D-CGD-CBD	6.25	122.37	111.27
23	a	604	CLA	CAD-C3D-C4D	-6.25	104.99	108.47
23	c	503	CLA	CAD-C3D-C4D	-6.24	104.99	108.47
25	c	522	BCR	C4-C5-C6	-6.23	113.68	122.73
25	b	622	BCR	C16-C17-C18	-6.23	118.42	127.31
25	c	516	BCR	C30-C25-C26	-6.23	113.84	122.61
23	c	506	CLA	CAD-C3D-C4D	-6.22	105.00	108.47
23	A	605	CLA	CAD-C3D-C4D	-6.21	105.01	108.47
23	b	618	CLA	CAD-C3D-C4D	-6.21	105.01	108.47
25	C	521	BCR	C27-C26-C25	-6.20	113.72	122.73
25	h	101	BCR	C1-C6-C5	-6.18	113.90	122.61
25	c	516	BCR	C7-C8-C9	-6.18	116.89	126.23
26	d	404	PL9	C17-C18-C19	-6.18	112.78	127.66
25	B	618	BCR	C27-C26-C25	-6.18	113.76	122.73
23	C	505	CLA	CAD-C3D-C4D	-6.18	105.03	108.47
25	b	620	BCR	C38-C26-C27	-6.18	101.75	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	515	BCR	C30-C25-C26	-6.17	113.92	122.61
23	b	616	CLA	CAD-C3D-C4D	-6.16	105.03	108.47
23	A	608	CLA	CAD-C3D-C4D	-6.15	105.04	108.47
25	C	514	BCR	C27-C26-C25	-6.14	113.81	122.73
25	c	522	BCR	C8-C7-C6	-6.13	109.98	127.20
25	B	618	BCR	C24-C23-C22	-6.12	116.99	126.23
23	b	609[A]	CLA	CAD-C3D-C4D	-6.12	105.06	108.47
26	D	405	PL9	C17-C18-C19	-6.11	112.95	127.66
23	C	507	CLA	CAD-C3D-C4D	-6.11	105.06	108.47
23	C	507	CLA	O2D-CGD-CBD	6.11	122.12	111.27
25	H	101	BCR	C7-C8-C9	-6.09	117.04	126.23
26	a	609	PL9	C45-C44-C43	-6.07	108.10	123.68
26	a	609	PL9	C11-C9-C8	-6.07	108.83	121.12
25	k	101	BCR	C1-C6-C5	-6.07	114.06	122.61
23	c	512	CLA	CAD-C3D-C4D	-6.07	105.09	108.47
25	t	101	BCR	C16-C17-C18	-6.06	118.66	127.31
25	B	620	BCR	C27-C26-C25	-6.05	113.95	122.73
26	A	610	PL9	C45-C44-C43	-6.05	108.17	123.68
26	D	405	PL9	C11-C9-C8	-6.04	108.89	121.12
23	b	604	CLA	CAD-C3D-C4D	-6.03	105.11	108.47
26	d	404	PL9	C22-C23-C24	-6.03	113.14	127.66
25	T	101	BCR	C20-C21-C22	-6.02	118.72	127.31
25	c	515	BCR	C20-C21-C22	-6.02	118.72	127.31
25	c	522	BCR	C11-C10-C9	-6.01	118.73	127.31
26	a	609	PL9	C12-C13-C14	-6.01	113.18	127.66
23	b	612	CLA	C3A-C2A-C1A	6.01	110.34	101.34
23	c	512	CLA	C3A-C2A-C1A	6.01	110.34	101.34
23	C	511	CLA	C3A-C2A-C1A	6.00	110.33	101.34
23	D	402	CLA	CAD-C3D-C4D	-5.99	105.13	108.47
23	C	510	CLA	CAD-C3D-C4D	-5.98	105.13	108.47
23	a	613	CLA	CAD-C3D-C4D	-5.98	105.14	108.47
26	D	405	PL9	C22-C23-C24	-5.97	113.28	127.66
25	B	619	BCR	C38-C26-C27	-5.97	102.15	113.62
23	B	607[B]	CLA	CAD-C3D-C4D	-5.96	105.14	108.47
26	A	610	PL9	C11-C9-C8	-5.96	109.06	121.12
25	K	101	BCR	C8-C7-C6	-5.94	110.53	127.20
25	f	101	BCR	C36-C18-C17	-5.94	114.61	122.92
25	k	101	BCR	C8-C7-C6	-5.93	110.53	127.20
23	B	616	CLA	CAD-C3D-C4D	-5.93	105.16	108.47
25	t	101	BCR	C8-C7-C6	-5.93	110.54	127.20
23	c	504	CLA	C3A-C2A-C1A	5.92	110.21	101.34
23	b	606	CLA	CAD-C3D-C4D	-5.92	105.17	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	CAD-C3D-C4D	-5.92	105.17	108.47
26	a	609	PL9	C40-C39-C38	-5.91	108.52	123.68
23	c	514	CLA	CAD-C3D-C4D	-5.91	105.17	108.47
23	a	607	CLA	CAD-C3D-C4D	-5.91	105.18	108.47
23	C	513	CLA	CAD-C3D-C4D	-5.90	105.18	108.47
26	a	609	PL9	C32-C33-C34	-5.90	113.46	127.66
25	C	514	BCR	C16-C15-C14	-5.90	111.40	123.47
23	C	511	CLA	CAD-C3D-C4D	-5.89	105.18	108.47
23	c	502	CLA	C3A-C2A-C1A	5.89	110.17	101.34
25	b	622	BCR	C4-C5-C6	-5.89	114.18	122.73
26	D	405	PL9	C37-C38-C39	-5.89	113.48	127.66
23	C	509	CLA	CAD-C3D-C4D	-5.89	105.19	108.47
25	T	101	BCR	C7-C8-C9	-5.88	117.35	126.23
23	B	605	CLA	C3A-C2A-C1A	5.88	110.14	101.34
23	B	607[A]	CLA	CAD-C3D-C4D	-5.87	105.19	108.47
23	b	611	CLA	CAD-C3D-C4D	-5.87	105.19	108.47
23	D	404	CLA	CAD-C3D-C4D	-5.87	105.20	108.47
23	B	607[B]	CLA	C3A-C2A-C1A	5.85	110.09	101.34
26	d	404	PL9	C46-C44-C43	-5.84	109.30	121.12
25	k	101	BCR	C11-C10-C9	-5.84	118.97	127.31
26	A	610	PL9	C10-C9-C8	-5.84	108.71	123.68
25	c	522	BCR	C36-C18-C17	-5.84	114.75	122.92
23	B	613	CLA	CAD-C3D-C4D	-5.83	105.22	108.47
23	c	510	CLA	CAD-C3D-C4D	-5.82	105.22	108.47
26	d	404	PL9	C42-C43-C44	-5.82	113.64	127.66
26	D	405	PL9	C30-C29-C28	-5.82	108.75	123.68
23	B	614	CLA	C3A-C2A-C1A	5.81	110.05	101.34
25	B	619	BCR	C38-C26-C25	-5.81	118.01	124.53
26	d	404	PL9	C11-C9-C8	-5.81	109.37	121.12
23	c	513	CLA	CAD-C3D-C4D	-5.80	105.23	108.47
23	b	617	CLA	CAD-C3D-C4D	-5.79	105.24	108.47
23	C	512	CLA	C3A-C2A-C1A	5.78	110.00	101.34
23	B	610	CLA	C3A-C2A-C1A	5.78	110.00	101.34
26	d	404	PL9	C37-C38-C39	-5.78	113.75	127.66
23	b	615	CLA	CAD-C3D-C4D	-5.77	105.25	108.47
26	a	609	PL9	C26-C24-C23	-5.75	109.48	121.12
26	A	610	PL9	C12-C13-C14	-5.75	113.82	127.66
23	c	509	CLA	C3A-C2A-C1A	5.75	109.94	101.34
23	B	615	CLA	CAD-C3D-C4D	-5.75	105.27	108.47
23	C	503	CLA	C3A-C2A-C1A	5.74	109.94	101.34
25	c	522	BCR	C1-C6-C5	-5.74	114.53	122.61
23	a	605	CLA	CAD-C3D-C4D	-5.74	105.27	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	C3A-C2A-C1A	5.74	109.93	101.34
25	k	101	BCR	C24-C23-C22	-5.74	117.57	126.23
26	d	404	PL9	C21-C19-C18	-5.74	109.51	121.12
23	C	506	CLA	C3A-C2A-C1A	5.73	109.92	101.34
23	b	609[B]	CLA	CAD-C3D-C4D	-5.72	105.28	108.47
23	c	507	CLA	C3A-C2A-C1A	5.71	109.90	101.34
26	a	609	PL9	C25-C24-C23	-5.71	109.04	123.68
23	b	610	CLA	CAD-C3D-C4D	-5.71	105.29	108.47
25	H	101	BCR	C11-C10-C9	-5.70	119.17	127.31
23	B	607[A]	CLA	C3A-C2A-C1A	5.70	109.87	101.34
25	c	522	BCR	C7-C6-C5	-5.68	107.70	121.46
23	B	608	CLA	C2A-C3A-C4A	5.68	111.04	101.87
23	b	614	CLA	C3A-C2A-C1A	5.67	109.83	101.34
23	C	501	CLA	C3A-C2A-C1A	5.67	109.83	101.34
23	A	606	CLA	CAD-C3D-C4D	-5.67	105.31	108.47
23	B	616	CLA	C2A-C3A-C4A	5.66	111.02	101.87
25	c	515	BCR	C4-C5-C6	-5.66	114.52	122.73
25	A	609	BCR	C30-C25-C26	-5.66	114.65	122.61
26	D	405	PL9	C21-C19-C18	-5.65	109.67	121.12
23	b	618	CLA	C2A-C3A-C4A	5.65	111.00	101.87
23	C	503	CLA	CAD-C3D-C4D	-5.65	105.32	108.47
26	a	609	PL9	C10-C9-C8	-5.65	109.18	123.68
23	C	507	CLA	C2A-C3A-C4A	5.65	110.99	101.87
25	C	521	BCR	C7-C6-C5	-5.63	107.82	121.46
23	B	602	CLA	C3A-C2A-C1A	5.63	109.77	101.34
23	b	609[B]	CLA	C3A-C2A-C1A	5.62	109.76	101.34
23	c	504	CLA	CAD-C3D-C4D	-5.62	105.34	108.47
23	B	602	CLA	CAD-C3D-C4D	-5.61	105.34	108.47
23	c	511	CLA	CAD-C3D-C4D	-5.61	105.34	108.47
23	B	609	CLA	CAD-C3D-C4D	-5.61	105.34	108.47
25	b	620	BCR	C27-C26-C25	-5.60	114.60	122.73
26	a	609	PL9	C46-C44-C43	-5.60	109.79	121.12
26	A	610	PL9	C40-C39-C38	-5.60	109.32	123.68
23	B	615	CLA	C3A-C2A-C1A	5.59	109.72	101.34
23	B	606	CLA	C2A-C3A-C4A	5.59	110.89	101.87
23	C	508	CLA	C3A-C2A-C1A	5.58	109.70	101.34
26	D	405	PL9	C42-C43-C44	-5.58	114.22	127.66
23	C	513	CLA	C3A-C2A-C1A	5.58	109.70	101.34
23	b	608	CLA	C2A-C3A-C4A	5.58	110.88	101.87
23	b	609[A]	CLA	C3A-C2A-C1A	5.58	109.69	101.34
23	b	605	CLA	O2D-CGD-CBD	5.58	121.17	111.27
26	A	610	PL9	C26-C24-C23	-5.57	109.84	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	609	PL9	C15-C14-C13	-5.57	109.38	123.68
23	b	617	CLA	C3A-C2A-C1A	5.56	109.67	101.34
23	B	606	CLA	CAD-C3D-C4D	-5.56	105.37	108.47
23	C	502	CLA	C3A-C2A-C1A	5.56	109.67	101.34
26	d	404	PL9	C10-C9-C8	-5.56	109.41	123.68
23	b	619	CLA	C3A-C2A-C1A	5.56	109.67	101.34
25	b	622	BCR	C20-C21-C22	-5.56	119.38	127.31
25	b	622	BCR	C27-C26-C25	-5.56	114.66	122.73
26	d	404	PL9	C30-C29-C28	-5.56	109.42	123.68
23	c	511	CLA	C3A-C2A-C1A	5.55	109.65	101.34
25	H	101	BCR	C27-C26-C25	-5.55	114.68	122.73
23	b	611	CLA	C3A-C2A-C1A	5.54	109.64	101.34
23	c	508	CLA	C2A-C3A-C4A	5.54	110.82	101.87
25	c	515	BCR	C24-C25-C26	-5.54	108.05	121.46
23	b	618	CLA	C3A-C2A-C1A	5.53	109.62	101.34
23	c	513	CLA	C3A-C2A-C1A	5.53	109.62	101.34
23	B	617	CLA	C3A-C2A-C1A	5.52	109.61	101.34
23	C	505	CLA	O2D-CGD-CBD	5.51	121.06	111.27
23	b	610	CLA	C2A-C3A-C4A	5.51	110.77	101.87
25	K	101	BCR	C7-C8-C9	-5.51	117.91	126.23
25	F	101	BCR	C15-C14-C13	-5.50	119.45	127.31
25	a	608	BCR	C30-C25-C26	-5.50	114.86	122.61
23	c	507	CLA	C2A-C3A-C4A	5.50	110.76	101.87
25	C	514	BCR	C11-C10-C9	-5.50	119.46	127.31
23	b	609[B]	CLA	C2A-C3A-C4A	5.50	110.76	101.87
25	h	101	BCR	C8-C7-C6	-5.50	111.76	127.20
23	C	509	CLA	C3A-C2A-C1A	5.49	109.56	101.34
23	c	514	CLA	C3A-C2A-C1A	5.48	109.54	101.34
23	b	604	CLA	C3A-C2A-C1A	5.47	109.53	101.34
25	b	621	BCR	C12-C13-C14	-5.47	110.55	118.94
25	C	515	BCR	C20-C21-C22	-5.46	119.52	127.31
25	h	101	BCR	C23-C24-C25	-5.46	111.87	127.20
23	b	606	CLA	C3A-C2A-C1A	5.46	109.51	101.34
23	b	611	CLA	C4A-NA-C1A	-5.45	104.25	106.71
23	b	615	CLA	C3A-C2A-C1A	5.45	109.51	101.34
23	B	603	CLA	O2D-CGD-CBD	5.45	120.95	111.27
23	c	510	CLA	C3A-C2A-C1A	5.45	109.50	101.34
25	C	521	BCR	C36-C18-C17	-5.44	115.30	122.92
23	B	606	CLA	C3A-C2A-C1A	5.44	109.48	101.34
23	b	613	CLA	C3A-C2A-C1A	5.44	109.48	101.34
25	T	101	BCR	C4-C5-C6	-5.43	114.84	122.73
23	b	615	CLA	O2D-CGD-CBD	5.43	120.92	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	522	BCR	C15-C14-C13	-5.43	119.56	127.31
25	c	515	BCR	C7-C6-C5	-5.43	108.31	121.46
23	a	607	CLA	C3A-C2A-C1A	5.42	109.46	101.34
25	C	521	BCR	C1-C6-C5	-5.42	114.98	122.61
26	d	404	PL9	C15-C14-C13	-5.42	109.78	123.68
23	B	612	CLA	C3A-C2A-C1A	5.41	109.45	101.34
23	C	504	CLA	C2A-C3A-C4A	5.39	110.58	101.87
23	A	608	CLA	C3A-C2A-C1A	5.39	109.41	101.34
23	c	503	CLA	C3A-C2A-C1A	5.38	109.39	101.34
23	c	506	CLA	O2D-CGD-CBD	5.38	120.82	111.27
25	H	101	BCR	C7-C6-C5	-5.37	108.46	121.46
23	b	610	CLA	C3A-C2A-C1A	5.37	109.38	101.34
23	b	608	CLA	CAD-C3D-C4D	-5.37	105.48	108.47
23	c	514	CLA	C4A-NA-C1A	-5.36	104.30	106.71
25	c	516	BCR	C15-C14-C13	-5.36	119.66	127.31
26	D	405	PL9	C45-C44-C43	-5.36	109.93	123.68
23	B	609	CLA	C3A-C2A-C1A	5.36	109.36	101.34
23	b	608	CLA	C3A-C2A-C1A	5.35	109.35	101.34
25	C	521	BCR	C7-C8-C9	-5.34	118.16	126.23
23	a	613	CLA	C3A-C2A-C1A	5.34	109.34	101.34
25	H	101	BCR	C23-C24-C25	-5.34	112.20	127.20
25	B	618	BCR	C37-C22-C21	-5.34	115.44	122.92
23	b	607	CLA	C3A-C2A-C1A	5.33	109.33	101.34
23	B	607[B]	CLA	C2A-C3A-C4A	5.33	110.47	101.87
23	b	605	CLA	C3A-C2A-C1A	5.33	109.32	101.34
23	C	508	CLA	C2A-C3A-C4A	5.33	110.47	101.87
23	B	610	CLA	C2A-C3A-C4A	5.32	110.47	101.87
23	b	618	CLA	O2D-CGD-CBD	5.32	120.73	111.27
25	h	101	BCR	C27-C26-C25	-5.31	115.02	122.73
26	D	405	PL9	C46-C44-C43	-5.31	110.36	121.12
25	T	101	BCR	C15-C14-C13	-5.31	119.73	127.31
23	A	606	CLA	C2A-C3A-C4A	5.31	110.45	101.87
25	a	608	BCR	C15-C14-C13	-5.31	119.73	127.31
23	B	604	CLA	C2A-C3A-C4A	5.31	110.44	101.87
23	B	613	CLA	C2A-C3A-C4A	5.31	110.44	101.87
23	c	505	CLA	C2A-C3A-C4A	5.29	110.42	101.87
23	C	510	CLA	C3A-C2A-C1A	5.29	109.26	101.34
23	B	616	CLA	C3A-C2A-C1A	5.29	109.26	101.34
23	D	404	CLA	C4A-NA-C1A	-5.29	104.33	106.71
26	A	610	PL9	C25-C24-C23	-5.28	110.13	123.68
25	C	514	BCR	C20-C21-C22	-5.27	119.79	127.31
23	b	606	CLA	C2A-C3A-C4A	5.27	110.38	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607[A]	CLA	C2A-C3A-C4A	5.27	110.38	101.87
23	b	612	CLA	C2A-C3A-C4A	5.27	110.38	101.87
23	C	509	CLA	C2A-C3A-C4A	5.26	110.37	101.87
25	H	101	BCR	C29-C30-C25	5.26	118.58	110.48
25	t	101	BCR	C4-C5-C6	-5.26	115.09	122.73
23	B	612	CLA	C2A-C3A-C4A	5.26	110.36	101.87
23	b	609[A]	CLA	C2A-C3A-C4A	5.25	110.36	101.87
26	A	610	PL9	C30-C29-C28	-5.25	110.22	123.68
23	c	503	CLA	C2A-C3A-C4A	5.24	110.34	101.87
26	A	610	PL9	C15-C14-C13	-5.24	110.23	123.68
23	D	404	CLA	C3A-C2A-C1A	5.24	109.19	101.34
25	t	101	BCR	C7-C6-C5	-5.24	108.78	121.46
25	b	620	BCR	C11-C12-C13	-5.23	111.71	126.42
23	C	501	CLA	C2A-C3A-C4A	5.23	110.31	101.87
23	B	611	CLA	C3A-C2A-C1A	5.23	109.17	101.34
23	D	403	CLA	C3A-C2A-C1A	5.23	109.17	101.34
23	B	605	CLA	C2A-C3A-C4A	5.22	110.30	101.87
26	D	405	PL9	C15-C14-C13	-5.22	110.28	123.68
23	b	604	CLA	C2A-C3A-C4A	5.22	110.30	101.87
23	a	605	CLA	C3A-C2A-C1A	5.22	109.16	101.34
23	B	616	CLA	O2D-CGD-CBD	5.21	120.53	111.27
23	B	602	CLA	C2A-C3A-C4A	5.21	110.28	101.87
25	K	101	BCR	C1-C6-C5	-5.21	115.28	122.61
26	D	405	PL9	C10-C9-C8	-5.20	110.33	123.68
23	C	502	CLA	C4A-NA-C1A	-5.20	104.37	106.71
23	b	606	CLA	C2A-C1A-CHA	5.20	132.95	123.86
23	B	613	CLA	C3A-C2A-C1A	5.20	109.12	101.34
25	b	621	BCR	C1-C6-C5	-5.19	115.30	122.61
23	c	508	CLA	C3A-C2A-C1A	5.17	109.08	101.34
25	B	619	BCR	C1-C6-C5	-5.17	115.34	122.61
25	b	621	BCR	C38-C26-C27	-5.16	103.69	113.62
23	b	615	CLA	C2A-C3A-C4A	5.16	110.20	101.87
25	T	101	BCR	C23-C24-C25	-5.16	112.71	127.20
25	C	515	BCR	C15-C14-C13	-5.15	119.97	127.31
23	C	501	CLA	O2D-CGD-CBD	5.14	120.41	111.27
26	a	609	PL9	C35-C34-C33	-5.14	110.49	123.68
25	C	514	BCR	C24-C25-C26	-5.14	109.01	121.46
23	b	614	CLA	O2D-CGD-CBD	5.13	120.39	111.27
23	D	404	CLA	C2A-C3A-C4A	5.13	110.15	101.87
26	d	404	PL9	C45-C44-C43	-5.13	110.53	123.68
23	C	507	CLA	C3A-C2A-C1A	5.12	109.02	101.34
23	b	607	CLA	C4A-NA-C1A	-5.12	104.40	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	C2A-C3A-C4A	5.12	110.14	101.87
23	B	608	CLA	C3A-C2A-C1A	5.11	109.00	101.34
23	a	605	CLA	C2A-C3A-C4A	5.11	110.12	101.87
25	b	621	BCR	C7-C8-C9	-5.11	118.51	126.23
23	c	510	CLA	C2A-C3A-C4A	5.10	110.11	101.87
23	D	402	CLA	C2A-C3A-C4A	5.10	110.11	101.87
23	c	505	CLA	C3A-C2A-C1A	5.10	108.98	101.34
23	c	513	CLA	O2D-CGD-CBD	5.10	120.33	111.27
23	b	607	CLA	C2A-C3A-C4A	5.09	110.09	101.87
25	K	101	BCR	C23-C22-C21	-5.09	111.14	118.94
25	B	618	BCR	C8-C7-C6	-5.08	112.95	127.20
23	d	402	CLA	C3A-C2A-C1A	5.08	108.94	101.34
23	c	504	CLA	C2A-C3A-C4A	5.07	110.06	101.87
23	a	607	CLA	O2D-CGD-CBD	5.06	120.26	111.27
26	A	610	PL9	C32-C33-C34	-5.06	115.48	127.66
23	b	613	CLA	C4A-NA-C1A	-5.05	104.44	106.71
23	C	513	CLA	C2A-C3A-C4A	5.04	110.01	101.87
26	D	405	PL9	C25-C24-C23	-5.03	110.76	123.68
25	h	101	BCR	C7-C6-C5	-5.03	109.27	121.46
23	b	619	CLA	O2D-CGD-CBD	5.03	120.21	111.27
23	C	502	CLA	C2A-C3A-C4A	5.03	109.99	101.87
23	d	403	CLA	C3A-C2A-C1A	5.02	108.86	101.34
25	K	101	BCR	C4-C5-C6	-5.01	115.46	122.73
23	b	614	CLA	C2A-C3A-C4A	5.00	109.94	101.87
23	A	606	CLA	C3A-C2A-C1A	5.00	108.82	101.34
23	B	617	CLA	O2D-CGD-CBD	4.99	120.14	111.27
23	A	606	CLA	C2A-C1A-CHA	4.99	132.58	123.86
23	a	613	CLA	C2A-C1A-CHA	4.99	132.58	123.86
26	D	405	PL9	C31-C29-C28	-4.99	111.03	121.12
23	D	402	CLA	C3A-C2A-C1A	4.98	108.81	101.34
23	A	606	CLA	O2D-CGD-CBD	4.97	120.10	111.27
25	b	622	BCR	C7-C6-C5	-4.97	109.42	121.46
23	c	509	CLA	O2D-CGD-CBD	4.97	120.09	111.27
23	B	614	CLA	C2A-C3A-C4A	4.96	109.88	101.87
23	c	512	CLA	C4A-NA-C1A	-4.96	104.48	106.71
26	a	609	PL9	C20-C19-C18	-4.96	110.96	123.68
23	b	619	CLA	C2A-C3A-C4A	4.96	109.88	101.87
26	d	404	PL9	C40-C39-C38	-4.95	110.97	123.68
23	b	617	CLA	C2A-C3A-C4A	4.95	109.87	101.87
23	c	506	CLA	C2A-C3A-C4A	4.95	109.87	101.87
25	c	515	BCR	C34-C9-C10	-4.95	116.00	122.92
23	D	404	CLA	C2A-C1A-CHA	4.94	132.50	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	404	PL9	C41-C39-C38	-4.94	111.11	121.12
25	C	514	BCR	C23-C24-C25	-4.94	113.33	127.20
23	B	615	CLA	C2A-C3A-C4A	4.94	109.85	101.87
23	c	502	CLA	C2A-C3A-C4A	4.93	109.83	101.87
23	B	604	CLA	C3A-C2A-C1A	4.92	108.72	101.34
25	a	608	BCR	C7-C8-C9	-4.92	118.80	126.23
23	B	617	CLA	C2A-C3A-C4A	4.92	109.81	101.87
25	C	514	BCR	C7-C6-C5	-4.91	109.56	121.46
25	K	101	BCR	C7-C6-C5	-4.91	109.57	121.46
25	h	101	BCR	C29-C30-C25	4.91	118.03	110.48
26	D	405	PL9	C20-C19-C18	-4.90	111.10	123.68
23	A	608	CLA	C2A-C3A-C4A	4.90	109.79	101.87
25	C	514	BCR	C4-C5-C6	-4.90	115.61	122.73
23	c	513	CLA	C2A-C3A-C4A	4.90	109.78	101.87
23	B	612	CLA	O2D-CGD-CBD	4.89	119.96	111.27
26	A	610	PL9	C21-C19-C18	-4.89	111.22	121.12
26	A	610	PL9	C46-C44-C43	-4.89	111.22	121.12
23	C	511	CLA	C4A-NA-C1A	-4.89	104.51	106.71
25	B	618	BCR	C23-C24-C25	-4.88	113.50	127.20
26	A	610	PL9	C20-C19-C18	-4.87	111.18	123.68
23	B	609	CLA	O2D-CGD-CBD	4.87	119.92	111.27
23	D	402	CLA	C2A-C1A-CHA	4.87	132.37	123.86
23	C	506	CLA	C2A-C1A-CHA	4.86	132.36	123.86
26	A	610	PL9	C35-C34-C33	-4.86	111.22	123.68
26	a	609	PL9	C30-C29-C28	-4.85	111.23	123.68
25	T	101	BCR	C37-C22-C21	-4.85	116.13	122.92
25	T	101	BCR	C8-C7-C6	-4.85	113.58	127.20
23	a	613	CLA	C2A-C3A-C4A	4.85	109.70	101.87
23	C	505	CLA	C2A-C3A-C4A	4.85	109.70	101.87
25	B	620	BCR	C7-C6-C5	-4.84	109.73	121.46
23	C	506	CLA	C2A-C3A-C4A	4.84	109.69	101.87
23	a	605	CLA	O2D-CGD-CBD	4.84	119.87	111.27
26	D	405	PL9	C35-C34-C33	-4.83	111.28	123.68
23	D	403	CLA	C2A-C3A-C4A	4.83	109.67	101.87
23	C	504	CLA	C3A-C2A-C1A	4.83	108.57	101.34
25	F	101	BCR	C12-C13-C14	-4.83	111.53	118.94
23	C	503	CLA	C4A-NA-C1A	-4.82	104.54	106.71
23	c	510	CLA	O2D-CGD-CBD	4.82	119.83	111.27
23	B	603	CLA	C2A-C1A-CHA	4.82	132.28	123.86
23	b	616	CLA	C2A-C3A-C4A	4.82	109.65	101.87
26	a	609	PL9	C41-C39-C38	-4.81	111.39	121.12
33	e	102	HEM	CBD-CAD-C3D	-4.80	103.62	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	404	PL9	C25-C24-C23	-4.80	111.36	123.68
23	A	608	CLA	O2D-CGD-CBD	4.80	119.80	111.27
23	B	604	CLA	C2A-C1A-CHA	4.80	132.25	123.86
23	c	503	CLA	C4A-NA-C1A	-4.79	104.55	106.71
23	d	403	CLA	C4A-NA-C1A	-4.79	104.55	106.71
25	k	101	BCR	C7-C6-C5	-4.78	109.88	121.46
23	A	605	CLA	C2A-C1A-CHA	4.78	132.22	123.86
26	a	609	PL9	C21-C19-C18	-4.78	111.45	121.12
25	b	620	BCR	C30-C25-C26	-4.77	115.89	122.61
23	B	611	CLA	C2A-C1A-CHA	4.77	132.20	123.86
25	t	101	BCR	C24-C25-C26	-4.77	109.91	121.46
23	C	512	CLA	C2A-C3A-C4A	4.77	109.57	101.87
23	C	510	CLA	C2A-C3A-C4A	4.77	109.57	101.87
25	B	618	BCR	C38-C26-C27	-4.77	104.46	113.62
23	c	512	CLA	C2A-C3A-C4A	4.77	109.57	101.87
23	d	403	CLA	C2A-C3A-C4A	4.77	109.57	101.87
23	B	611	CLA	C2A-C3A-C4A	4.76	109.56	101.87
23	c	502	CLA	O2D-CGD-CBD	4.76	119.72	111.27
23	B	603	CLA	C3A-C2A-C1A	4.76	108.46	101.34
23	c	514	CLA	C2A-C3A-C4A	4.76	109.55	101.87
25	c	516	BCR	C38-C26-C27	-4.75	104.48	113.62
23	c	503	CLA	O2D-CGD-CBD	4.75	119.71	111.27
23	B	603	CLA	C2A-C3A-C4A	4.75	109.55	101.87
23	c	510	CLA	C4A-NA-C1A	-4.75	104.57	106.71
23	c	505	CLA	C4A-NA-C1A	-4.74	104.58	106.71
25	b	621	BCR	C34-C9-C10	-4.74	116.29	122.92
25	B	618	BCR	C7-C6-C5	-4.73	109.99	121.46
23	b	611	CLA	O2D-CGD-CBD	4.73	119.67	111.27
23	B	607[B]	CLA	O2D-CGD-CBD	4.73	119.67	111.27
23	B	609	CLA	C2A-C3A-C4A	4.72	109.50	101.87
23	b	616	CLA	O2D-CGD-CBD	4.71	119.65	111.27
23	C	512	CLA	O2D-CGD-CBD	4.71	119.64	111.27
23	B	607[A]	CLA	C2A-C1A-CHA	4.71	132.09	123.86
25	c	515	BCR	C23-C24-C25	-4.71	113.98	127.20
23	C	503	CLA	C2A-C3A-C4A	4.70	109.46	101.87
23	C	507	CLA	C2A-C1A-CHA	4.70	132.08	123.86
23	c	507	CLA	C2A-C1A-CHA	4.70	132.07	123.86
23	a	607	CLA	C2A-C3A-C4A	4.69	109.45	101.87
23	C	506	CLA	O2D-CGD-CBD	4.68	119.59	111.27
23	d	402	CLA	C2A-C3A-C4A	4.68	109.43	101.87
27	a	610	SQD	O6-C1-C2	4.68	115.61	108.30
23	B	613	CLA	O2D-CGD-CBD	4.68	119.58	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	O2D-CGD-CBD	4.67	119.58	111.27
23	c	508	CLA	C2A-C1A-CHA	4.67	132.03	123.86
23	C	504	CLA	C2A-C1A-CHA	4.67	132.02	123.86
27	A	611	SQD	O6-C1-C2	4.66	115.58	108.30
23	c	514	CLA	O2D-CGD-CBD	4.65	119.54	111.27
23	B	614	CLA	C2A-C1A-CHA	4.65	131.99	123.86
25	k	101	BCR	C4-C5-C6	-4.64	115.99	122.73
23	b	609[A]	CLA	C2A-C1A-CHA	4.64	131.96	123.86
23	B	604	CLA	O2D-CGD-CBD	4.63	119.50	111.27
23	a	613	CLA	O2D-CGD-CBD	4.63	119.50	111.27
23	a	605	CLA	C2A-C1A-CHA	4.63	131.96	123.86
23	B	611	CLA	C4A-NA-C1A	-4.63	104.62	106.71
23	C	501	CLA	C2A-C1A-CHA	4.63	131.95	123.86
23	b	613	CLA	C2A-C1A-CHA	4.63	131.95	123.86
23	b	609[B]	CLA	C2A-C1A-CHA	4.62	131.94	123.86
23	B	607[A]	CLA	O2D-CGD-CBD	4.61	119.47	111.27
33	E	102	HEM	CBD-CAD-C3D	-4.61	103.98	112.48
25	t	101	BCR	C23-C24-C25	-4.61	114.25	127.20
26	d	404	PL9	C26-C24-C23	-4.61	111.79	121.12
23	c	505	CLA	C2A-C1A-CHA	4.60	131.89	123.86
25	a	608	BCR	C8-C7-C6	-4.59	114.30	127.20
23	C	508	CLA	O2D-CGD-CBD	4.59	119.43	111.27
23	b	613	CLA	C2A-C3A-C4A	4.59	109.29	101.87
23	C	511	CLA	C2A-C3A-C4A	4.59	109.28	101.87
23	C	509	CLA	O2D-CGD-CBD	4.59	119.42	111.27
26	d	404	PL9	C47-C48-C49	-4.59	112.07	127.75
23	b	605	CLA	C2A-C3A-C4A	4.59	109.28	101.87
26	A	610	PL9	C50-C49-C48	-4.58	109.40	122.65
23	C	513	CLA	O2D-CGD-CBD	4.58	119.41	111.27
26	D	405	PL9	C26-C24-C23	-4.58	111.85	121.12
23	b	609[A]	CLA	O2D-CGD-CBD	4.57	119.39	111.27
25	B	620	BCR	C31-C1-C6	-4.57	102.89	110.30
23	c	507	CLA	O2D-CGD-CBD	4.57	119.38	111.27
23	B	607[B]	CLA	C2A-C1A-CHA	4.56	131.84	123.86
23	c	511	CLA	C2A-C3A-C4A	4.56	109.23	101.87
26	d	404	PL9	C20-C19-C18	-4.56	111.98	123.68
23	C	504	CLA	O2D-CGD-CBD	4.56	119.37	111.27
23	B	608	CLA	C2A-C1A-CHA	4.55	131.82	123.86
26	D	405	PL9	C40-C39-C38	-4.55	112.01	123.68
25	b	620	BCR	C8-C7-C6	-4.55	114.43	127.20
23	b	607	CLA	C2A-C1A-CHA	4.54	131.80	123.86
23	d	403	CLA	C2A-C1A-CHA	4.54	131.79	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	C2A-C3A-C4A	4.53	109.19	101.87
23	b	609[B]	CLA	O2D-CGD-CBD	4.53	119.32	111.27
23	c	509	CLA	C2A-C1A-CHA	4.53	131.78	123.86
23	B	605	CLA	C2A-C1A-CHA	4.52	131.77	123.86
25	H	101	BCR	C20-C21-C22	-4.52	120.86	127.31
23	b	616	CLA	C4A-NA-C1A	-4.52	104.67	106.71
25	c	522	BCR	C38-C26-C27	-4.52	104.93	113.62
25	b	622	BCR	C38-C26-C27	-4.52	104.94	113.62
23	d	403	CLA	O2D-CGD-CBD	4.52	119.29	111.27
25	h	101	BCR	C35-C13-C14	-4.51	116.60	122.92
23	b	604	CLA	C2A-C1A-CHA	4.51	131.74	123.86
23	B	614	CLA	O2D-CGD-CBD	4.51	119.28	111.27
26	D	405	PL9	C47-C48-C49	-4.50	112.37	127.75
23	c	502	CLA	C4A-NA-C1A	-4.50	104.68	106.71
25	B	619	BCR	C30-C25-C26	-4.50	116.28	122.61
23	C	510	CLA	C4A-NA-C1A	-4.50	104.69	106.71
26	D	405	PL9	C41-C39-C38	-4.47	112.07	121.12
25	c	515	BCR	C2-C1-C6	4.47	117.36	110.48
23	C	511	CLA	O2D-CGD-CBD	4.46	119.19	111.27
23	c	510	CLA	C2A-C1A-CHA	4.46	131.65	123.86
23	c	514	CLA	C2A-C1A-CHA	4.46	131.65	123.86
23	B	606	CLA	C2A-C1A-CHA	4.46	131.65	123.86
23	b	605	CLA	C1B-CHB-C4A	-4.45	121.30	130.12
23	B	615	CLA	O2D-CGD-CBD	4.45	119.18	111.27
23	a	604	CLA	O2D-CGD-CBD	4.45	119.18	111.27
23	C	503	CLA	C2A-C1A-CHA	4.45	131.64	123.86
23	c	504	CLA	C2A-C1A-CHA	4.45	131.64	123.86
23	C	502	CLA	O2D-CGD-CBD	4.45	119.17	111.27
23	C	503	CLA	O2D-CGD-CBD	4.45	119.17	111.27
25	b	620	BCR	C7-C6-C5	-4.45	110.69	121.46
26	A	610	PL9	C7-C3-C4	4.44	120.49	116.88
31	a	614	LHG	O7-C7-C8	4.43	121.06	111.50
25	k	101	BCR	C38-C26-C27	-4.43	105.10	113.62
25	B	618	BCR	C11-C12-C13	-4.43	113.97	126.42
23	C	512	CLA	C4A-NA-C1A	-4.42	104.72	106.71
25	A	609	BCR	C36-C18-C17	-4.41	116.74	122.92
25	A	609	BCR	C7-C6-C5	-4.41	110.78	121.46
25	B	620	BCR	C38-C26-C27	-4.40	105.16	113.62
25	F	101	BCR	C7-C6-C5	-4.40	110.80	121.46
26	a	609	PL9	C36-C34-C33	-4.40	112.22	121.12
23	b	609[A]	CLA	C4A-NA-C1A	-4.39	104.73	106.71
23	B	609	CLA	C2A-C1A-CHA	4.39	131.53	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	C2A-C1A-CHA	4.39	131.53	123.86
25	C	515	BCR	C38-C26-C27	-4.38	105.19	113.62
25	h	101	BCR	C8-C9-C10	-4.38	112.22	118.94
23	b	616	CLA	C2A-C1A-CHA	4.38	131.52	123.86
23	B	603	CLA	C1B-CHB-C4A	-4.37	121.46	130.12
25	B	620	BCR	C23-C24-C25	-4.37	114.92	127.20
23	C	509	CLA	C2A-C1A-CHA	4.37	131.50	123.86
25	t	101	BCR	C2-C1-C6	4.37	117.21	110.48
25	T	101	BCR	C24-C25-C26	-4.37	110.87	121.46
25	k	101	BCR	C23-C24-C25	-4.37	114.94	127.20
23	B	609	CLA	C4A-NA-C1A	-4.37	104.74	106.71
23	C	504	CLA	C4A-NA-C1A	-4.36	104.74	106.71
23	B	602	CLA	C4A-NA-C1A	-4.36	104.75	106.71
25	B	619	BCR	C4-C5-C6	-4.36	116.40	122.73
25	H	101	BCR	C38-C26-C27	-4.35	105.26	113.62
23	B	615	CLA	C4A-NA-C1A	-4.34	104.75	106.71
23	c	511	CLA	C2A-C1A-CHA	4.33	131.44	123.86
23	D	404	CLA	O2D-CGD-CBD	4.33	118.97	111.27
27	A	611	SQD	O47-C7-C8	4.33	120.84	111.50
23	B	612	CLA	C2A-C1A-CHA	4.33	131.43	123.86
23	b	611	CLA	C2A-C1A-CHA	4.33	131.43	123.86
27	a	610	SQD	O9-S-C6	4.33	112.08	106.94
25	a	608	BCR	C7-C6-C5	-4.33	110.97	121.46
23	B	607[A]	CLA	C4A-NA-C1A	-4.32	104.76	106.71
27	a	610	SQD	O47-C7-C8	4.32	120.82	111.50
23	A	608	CLA	C2A-C1A-CHA	4.32	131.42	123.86
25	h	101	BCR	C24-C25-C26	-4.32	110.99	121.46
23	c	508	CLA	C4A-NA-C1A	-4.32	104.76	106.71
23	c	506	CLA	C2A-C1A-CHA	4.32	131.41	123.86
27	A	611	SQD	O9-S-C6	4.31	112.07	106.94
23	c	503	CLA	C2A-C1A-CHA	4.31	131.40	123.86
25	h	101	BCR	C20-C21-C22	-4.30	121.17	127.31
25	A	609	BCR	C7-C8-C9	-4.29	119.75	126.23
23	b	607	CLA	O2D-CGD-CBD	4.28	118.88	111.27
25	B	620	BCR	C37-C22-C21	-4.28	116.92	122.92
25	t	101	BCR	C20-C21-C22	-4.28	121.20	127.31
23	D	403	CLA	O2D-CGD-CBD	4.28	118.87	111.27
32	c	519	DGD	O2G-C1B-C2B	4.28	120.72	111.50
23	d	402	CLA	O2D-CGD-CBD	4.28	118.86	111.27
25	f	101	BCR	C7-C6-C5	-4.27	111.11	121.46
25	H	101	BCR	C34-C9-C10	-4.27	116.95	122.92
23	C	510	CLA	O2D-CGD-CBD	4.26	118.84	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	C2A-C1A-CHA	4.26	131.31	123.86
25	H	101	BCR	C24-C25-C26	-4.26	111.15	121.46
25	C	514	BCR	C2-C1-C6	4.26	117.04	110.48
25	b	622	BCR	C31-C1-C6	-4.25	103.40	110.30
27	B	623	SQD	O6-C1-C2	4.25	114.94	108.30
23	B	602	CLA	C2A-C1A-CHA	4.25	131.29	123.86
27	b	602	SQD	O6-C1-C2	4.24	114.93	108.30
25	b	622	BCR	C35-C13-C14	-4.24	116.98	122.92
26	d	404	PL9	C31-C29-C28	-4.24	112.54	121.12
25	k	101	BCR	C35-C13-C14	-4.23	116.99	122.92
25	A	609	BCR	C8-C7-C6	-4.23	115.31	127.20
23	c	504	CLA	O2D-CGD-CBD	4.23	118.78	111.27
23	a	604	CLA	C2A-C1A-CHA	4.22	131.24	123.86
23	c	512	CLA	C2A-C1A-CHA	4.22	131.24	123.86
23	C	511	CLA	C2A-C1A-CHA	4.22	131.23	123.86
23	B	606	CLA	O2D-CGD-CBD	4.22	118.76	111.27
25	c	515	BCR	C31-C1-C6	-4.21	103.47	110.30
25	K	101	BCR	C38-C26-C27	-4.21	105.53	113.62
25	h	101	BCR	C38-C26-C27	-4.20	105.54	113.62
23	C	508	CLA	C2A-C1A-CHA	4.20	131.21	123.86
25	b	620	BCR	C24-C23-C22	-4.20	119.88	126.23
32	h	102	DGD	O2G-C1B-C2B	4.20	120.55	111.50
23	b	605	CLA	C2A-C1A-CHA	4.19	131.19	123.86
26	A	610	PL9	C51-C49-C48	-4.19	110.55	122.65
23	b	612	CLA	C2A-C1A-CHA	4.18	131.17	123.86
25	C	521	BCR	C24-C25-C26	-4.18	111.34	121.46
25	T	101	BCR	C1-C6-C5	-4.18	116.73	122.61
23	b	617	CLA	C2A-C1A-CHA	4.17	131.16	123.86
23	C	505	CLA	C2A-C1A-CHA	4.17	131.15	123.86
23	B	615	CLA	C2A-C1A-CHA	4.17	131.15	123.86
25	C	515	BCR	C37-C22-C21	-4.17	117.08	122.92
26	a	609	PL9	C31-C29-C28	-4.16	112.69	121.12
23	D	402	CLA	O2D-CGD-CBD	4.16	118.67	111.27
23	b	604	CLA	O2D-CGD-CBD	4.16	118.66	111.27
23	b	612	CLA	C1B-CHB-C4A	-4.16	121.88	130.12
23	B	602	CLA	O2D-CGD-CBD	4.15	118.65	111.27
23	c	505	CLA	O2D-CGD-CBD	4.15	118.64	111.27
23	C	507	CLA	C4A-NA-C1A	-4.14	104.84	106.71
23	b	617	CLA	O2D-CGD-CBD	4.14	118.62	111.27
23	a	604	CLA	C2A-C3A-C4A	4.14	108.55	101.87
26	a	609	PL9	C7-C3-C4	4.13	120.23	116.88
25	b	622	BCR	C2-C1-C6	4.13	116.84	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	101	SQD	O6-C1-C2	4.13	114.75	108.30
27	x	101	SQD	O6-C1-C2	4.13	114.75	108.30
23	C	502	CLA	C2A-C1A-CHA	4.13	131.08	123.86
23	B	613	CLA	C2A-C1A-CHA	4.12	131.06	123.86
25	c	522	BCR	C7-C8-C9	-4.12	120.01	126.23
25	C	521	BCR	C38-C26-C27	-4.12	105.71	113.62
25	c	515	BCR	C16-C15-C14	-4.12	115.04	123.47
25	b	621	BCR	C32-C1-C6	4.10	116.96	110.30
23	b	604	CLA	C4A-NA-C1A	-4.10	104.86	106.71
23	C	506	CLA	C1B-CHB-C4A	-4.09	122.02	130.12
25	H	101	BCR	C2-C1-C6	4.08	116.76	110.48
26	A	610	PL9	C41-C39-C38	-4.07	112.88	121.12
26	a	609	PL9	C47-C48-C49	-4.07	113.84	127.75
23	B	612	CLA	C4A-NA-C1A	-4.07	104.88	106.71
23	C	508	CLA	C4A-NA-C1A	-4.06	104.88	106.71
23	b	612	CLA	O2D-CGD-CBD	4.06	118.49	111.27
28	a	611	LMG	O7-C10-C11	4.06	120.25	111.50
28	C	519	LMG	O7-C10-C11	4.06	120.25	111.50
23	c	502	CLA	C2A-C1A-CHA	4.06	130.96	123.86
23	D	403	CLA	C1B-CHB-C4A	-4.06	122.08	130.12
23	B	617	CLA	C2A-C1A-CHA	4.05	130.94	123.86
31	b	624	LHG	O7-C7-C8	4.04	120.21	111.50
23	b	614	CLA	C4A-NA-C1A	-4.04	104.89	106.71
25	c	516	BCR	C34-C9-C10	-4.04	117.27	122.92
23	c	511	CLA	C4A-NA-C1A	-4.04	104.89	106.71
25	H	101	BCR	C8-C7-C6	-4.03	115.87	127.20
25	b	621	BCR	C30-C25-C26	-4.03	116.94	122.61
23	b	606	CLA	O2D-CGD-CBD	4.03	118.43	111.27
25	A	609	BCR	C39-C30-C25	4.03	116.83	110.30
23	c	511	CLA	O2D-CGD-CBD	4.02	118.42	111.27
25	C	514	BCR	C31-C1-C6	-4.02	103.78	110.30
28	Z	101	LMG	O7-C10-C11	4.02	120.16	111.50
23	a	604	CLA	C3A-C2A-C1A	4.00	107.34	101.34
23	b	615	CLA	C2A-C1A-CHA	3.99	130.83	123.86
25	B	618	BCR	C24-C25-C26	-3.98	111.81	121.46
25	c	516	BCR	C7-C6-C5	-3.98	111.81	121.46
23	b	608	CLA	O2D-CGD-CBD	3.98	118.33	111.27
26	A	610	PL9	C47-C48-C49	-3.98	114.16	127.75
27	B	623	SQD	O47-C7-C8	3.97	120.05	111.50
23	C	510	CLA	C2A-C1A-CHA	3.96	130.79	123.86
25	c	522	BCR	C24-C25-C26	-3.96	111.86	121.46
27	b	602	SQD	O47-C7-C8	3.96	120.04	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	C2A-C1A-CHA	3.96	130.78	123.86
31	e	101	LHG	O7-C7-C8	3.96	120.03	111.50
23	B	605	CLA	O2D-CGD-CBD	3.94	118.28	111.27
23	B	608	CLA	C4A-NA-C1A	-3.94	104.93	106.71
31	B	622	LHG	O7-C7-C8	3.94	120.00	111.50
26	A	610	PL9	C36-C34-C33	-3.94	113.14	121.12
23	a	607	CLA	C2A-C1A-CHA	3.94	130.75	123.86
25	h	101	BCR	C2-C1-C6	3.94	116.54	110.48
23	b	608	CLA	C2A-C1A-CHA	3.93	130.73	123.86
23	B	606	CLA	C4-C3-C5	3.93	121.88	115.27
31	D	408	LHG	O7-C7-C8	3.93	119.97	111.50
33	v	201	HEM	CBA-CAA-C2A	-3.93	105.24	112.49
26	D	405	PL9	C36-C34-C33	-3.93	113.17	121.12
28	c	520	LMG	O7-C10-C11	3.92	119.96	111.50
31	l	101	LHG	O7-C7-C8	3.92	119.96	111.50
23	b	617	CLA	C4A-NA-C1A	-3.91	104.95	106.71
23	a	613	CLA	C1B-CHB-C4A	-3.91	122.37	130.12
23	B	610	CLA	C2A-C1A-CHA	3.91	130.69	123.86
23	b	608	CLA	C4-C3-C5	3.91	121.85	115.27
23	b	610	CLA	C4A-NA-C1A	-3.90	104.95	106.71
23	d	402	CLA	C1B-CHB-C4A	-3.90	122.39	130.12
28	c	521	LMG	O7-C10-C11	3.90	119.91	111.50
32	c	517	DGD	O2G-C1B-C2B	3.90	119.90	111.50
23	b	614	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
23	B	613	CLA	C4A-NA-C1A	-3.89	104.96	106.71
27	b	602	SQD	O7-S-C6	3.88	111.56	106.94
25	B	620	BCR	C20-C21-C22	-3.88	121.77	127.31
23	A	605	CLA	O2D-CGD-CBD	3.88	118.16	111.27
23	B	611	CLA	C1B-CHB-C4A	-3.88	122.44	130.12
25	B	620	BCR	C2-C1-C6	3.86	116.43	110.48
23	c	509	CLA	C4A-NA-C1A	-3.86	104.97	106.71
25	F	101	BCR	C8-C7-C6	-3.86	116.37	127.20
25	C	515	BCR	C33-C5-C4	-3.86	106.21	113.62
25	a	608	BCR	C39-C30-C25	3.86	116.55	110.30
23	A	605	CLA	C2A-C3A-C4A	3.85	108.09	101.87
25	B	619	BCR	C36-C18-C17	-3.85	117.53	122.92
23	b	610	CLA	O2D-CGD-CBD	3.85	118.11	111.27
23	B	610	CLA	C1B-CHB-C4A	-3.85	122.50	130.12
26	d	404	PL9	C50-C49-C48	-3.84	111.53	122.65
27	B	623	SQD	O7-S-C6	3.84	111.50	106.94
25	B	620	BCR	C24-C25-C26	-3.84	112.16	121.46
23	b	613	CLA	O2D-CGD-CBD	3.84	118.09	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	101	BCR	C23-C24-C25	-3.84	116.43	127.20
25	h	101	BCR	C31-C1-C6	-3.83	104.09	110.30
25	B	619	BCR	C29-C30-C25	3.83	116.37	110.48
23	B	616	CLA	C2A-C1A-CHA	3.82	130.54	123.86
27	b	602	SQD	C3-C4-C5	3.82	117.06	110.24
25	b	621	BCR	C20-C21-C22	-3.82	121.86	127.31
23	b	619	CLA	C2A-C1A-CHA	3.81	130.52	123.86
23	C	505	CLA	C1B-CHB-C4A	-3.81	122.58	130.12
25	b	621	BCR	C4-C5-C6	-3.81	117.21	122.73
27	B	623	SQD	C3-C4-C5	3.81	117.03	110.24
25	h	101	BCR	C7-C8-C9	-3.81	120.48	126.23
25	F	101	BCR	C33-C5-C4	-3.80	106.31	113.62
25	b	622	BCR	C23-C24-C25	-3.80	116.52	127.20
26	a	609	PL9	C40-C39-C41	-3.80	108.88	115.27
26	A	610	PL9	C40-C39-C41	-3.80	108.89	115.27
26	A	610	PL9	C15-C14-C16	-3.80	108.89	115.27
28	A	612	LMG	O7-C10-C11	3.78	119.66	111.50
25	B	620	BCR	C11-C10-C9	-3.78	121.91	127.31
23	B	609	CLA	C1B-CHB-C4A	-3.78	122.63	130.12
25	C	521	BCR	C23-C24-C25	-3.78	116.59	127.20
26	d	404	PL9	C45-C44-C46	-3.78	108.92	115.27
23	b	613	CLA	C1B-CHB-C4A	-3.78	122.64	130.12
23	B	612	CLA	CMB-C2B-C1B	-3.77	122.66	128.46
25	C	515	BCR	C16-C15-C14	-3.77	115.75	123.47
23	c	509	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
26	a	609	PL9	C50-C49-C48	-3.77	111.77	122.65
23	A	605	CLA	C1B-CHB-C4A	-3.76	122.67	130.12
27	x	101	SQD	O47-C7-C8	3.76	119.61	111.50
25	k	101	BCR	C23-C22-C21	-3.76	113.17	118.94
23	C	504	CLA	C1B-CHB-C4A	-3.76	122.67	130.12
23	c	507	CLA	C1B-CHB-C4A	-3.76	122.67	130.12
27	X	101	SQD	O47-C7-C8	3.76	119.60	111.50
23	c	506	CLA	C1B-CHB-C4A	-3.76	122.68	130.12
23	a	607	CLA	C1B-CHB-C4A	-3.74	122.70	130.12
23	c	504	CLA	C1B-CHB-C4A	-3.74	122.71	130.12
31	d	406	LHG	O7-C7-C8	3.73	119.55	111.50
25	b	620	BCR	C20-C21-C22	-3.73	121.99	127.31
23	b	615	CLA	C4A-NA-C1A	-3.72	105.03	106.71
23	c	512	CLA	O2D-CGD-CBD	3.72	117.88	111.27
25	H	101	BCR	C30-C25-C26	-3.72	117.38	122.61
25	B	618	BCR	C34-C9-C10	-3.72	117.72	122.92
23	b	611	CLA	C1B-CHB-C4A	-3.71	122.76	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	516	BCR	C8-C7-C6	-3.71	116.78	127.20
26	a	609	PL9	C15-C14-C16	-3.71	109.03	115.27
25	b	622	BCR	C24-C25-C26	-3.71	112.48	121.46
25	k	101	BCR	C24-C25-C26	-3.70	112.49	121.46
25	f	101	BCR	C8-C7-C6	-3.70	116.81	127.20
25	K	101	BCR	C12-C13-C14	-3.70	113.27	118.94
23	B	607[B]	CLA	C4A-NA-C1A	-3.69	105.05	106.71
23	C	501	CLA	C4A-NA-C1A	-3.69	105.05	106.71
28	z	101	LMG	O7-C10-C11	3.69	119.45	111.50
26	a	609	PL9	C45-C44-C46	-3.69	109.07	115.27
23	c	505	CLA	C1B-CHB-C4A	-3.69	122.82	130.12
25	A	609	BCR	C23-C22-C21	-3.69	113.29	118.94
25	H	101	BCR	C33-C5-C4	-3.68	106.54	113.62
31	D	407	LHG	O7-C7-C8	3.68	119.44	111.50
23	C	513	CLA	C1B-CHB-C4A	-3.68	122.82	130.12
25	B	619	BCR	C34-C9-C10	-3.68	117.77	122.92
26	D	405	PL9	C45-C44-C46	-3.68	109.08	115.27
25	B	619	BCR	C20-C19-C18	-3.68	116.08	126.42
25	c	515	BCR	C3-C4-C5	-3.68	107.51	114.08
32	C	517	DGD	O2G-C1B-C2B	3.66	119.40	111.50
23	c	509	CLA	C1B-CHB-C4A	-3.65	122.89	130.12
32	C	518	DGD	O2G-C1B-C2B	3.65	119.37	111.50
26	D	405	PL9	C51-C49-C48	-3.65	112.10	122.65
26	D	405	PL9	C50-C49-C48	-3.65	112.11	122.65
26	d	404	PL9	C51-C49-C48	-3.65	112.11	122.65
23	D	402	CLA	C1B-CHB-C4A	-3.64	122.90	130.12
23	c	513	CLA	C4A-NA-C1A	-3.64	105.07	106.71
31	L	101	LHG	O7-C7-C8	3.64	119.35	111.50
23	B	607[B]	CLA	C1B-CHB-C4A	-3.63	122.94	130.12
32	C	516	DGD	O2G-C1B-C2B	3.63	119.31	111.50
23	B	613	CLA	C1B-CHB-C4A	-3.62	122.94	130.12
23	B	606	CLA	C1B-CHB-C4A	-3.62	122.95	130.12
23	c	507	CLA	CMB-C2B-C1B	-3.62	122.91	128.46
28	C	520	LMG	O7-C10-C11	3.61	119.28	111.50
23	A	605	CLA	C3A-C2A-C1A	3.60	106.74	101.34
25	h	101	BCR	C33-C5-C4	-3.60	106.71	113.62
25	h	101	BCR	C11-C10-C9	-3.59	122.18	127.31
23	c	502	CLA	C1B-CHB-C4A	-3.59	123.01	130.12
23	C	509	CLA	C4A-NA-C1A	-3.59	105.09	106.71
23	b	609[B]	CLA	C4A-NA-C1A	-3.59	105.09	106.71
23	b	610	CLA	C2A-C1A-CHA	3.59	130.13	123.86
23	a	607	CLA	C4-C3-C5	3.59	121.30	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
23	B	607[A]	CLA	C1B-CHB-C4A	-3.57	123.04	130.12
23	B	612	CLA	C1B-CHB-C4A	-3.57	123.04	130.12
23	c	512	CLA	C1B-CHB-C4A	-3.57	123.04	130.12
23	C	512	CLA	C2A-C1A-CHA	3.57	130.10	123.86
23	a	605	CLA	C1B-CHB-C4A	-3.57	123.05	130.12
23	A	608	CLA	C4-C3-C5	3.56	121.27	115.27
23	C	506	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
23	b	609[A]	CLA	C1B-CHB-C4A	-3.55	123.08	130.12
25	C	514	BCR	C37-C22-C21	-3.55	117.95	122.92
23	C	507	CLA	C1B-CHB-C4A	-3.55	123.08	130.12
26	D	405	PL9	C7-C3-C4	3.55	119.76	116.88
25	C	515	BCR	C8-C7-C6	-3.54	117.26	127.20
26	D	405	PL9	C10-C9-C11	-3.53	109.33	115.27
32	D	406	DGD	O2G-C1B-C2B	3.53	119.12	111.50
23	a	607	CLA	CHA-C1A-NA	-3.53	118.32	126.40
28	b	623	LMG	O7-C10-C11	3.53	119.10	111.50
25	C	514	BCR	C38-C26-C27	-3.51	106.87	113.62
25	C	514	BCR	C10-C11-C12	-3.51	112.25	123.22
23	b	618	CLA	C2A-C1A-CHA	3.51	129.99	123.86
25	B	620	BCR	C11-C12-C13	-3.50	116.58	126.42
23	C	509	CLA	C1B-CHB-C4A	-3.49	123.20	130.12
23	b	608	CLA	C4A-NA-C1A	-3.49	105.14	106.71
31	E	101	LHG	O7-C7-C8	3.49	119.02	111.50
33	V	202	HEM	C1D-C2D-C3D	-3.49	104.57	107.00
28	Z	101	LMG	O1-C1-C2	3.49	113.75	108.30
23	C	503	CLA	C1B-CHB-C4A	-3.49	123.22	130.12
25	b	620	BCR	C34-C9-C10	-3.48	118.04	122.92
25	C	514	BCR	C34-C9-C10	-3.48	118.05	122.92
23	a	604	CLA	C1B-CHB-C4A	-3.48	123.23	130.12
23	A	606	CLA	C1B-CHB-C4A	-3.48	123.23	130.12
25	c	516	BCR	C16-C15-C14	-3.47	116.36	123.47
25	a	608	BCR	C11-C12-C13	-3.47	116.66	126.42
23	b	606	CLA	C1B-CHB-C4A	-3.47	123.25	130.12
25	B	620	BCR	C35-C13-C14	-3.47	118.07	122.92
23	b	608	CLA	C1B-CHB-C4A	-3.46	123.26	130.12
26	D	405	PL9	C30-C29-C31	-3.46	109.45	115.27
23	b	617	CLA	C1B-CHB-C4A	-3.46	123.27	130.12
23	c	503	CLA	C1B-CHB-C4A	-3.45	123.28	130.12
23	B	604	CLA	C1B-CHB-C4A	-3.45	123.28	130.12
28	J	101	LMG	O7-C10-C11	3.45	118.94	111.50
25	B	619	BCR	C11-C12-C13	-3.45	116.73	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	601	SQD	O9-S-C6	3.44	111.03	106.94
23	b	617	CLA	C4-C3-C5	3.44	121.06	115.27
23	B	615	CLA	C4-C3-C5	3.44	121.06	115.27
28	j	101	LMG	O7-C10-C11	3.44	118.91	111.50
25	a	608	BCR	C36-C18-C17	-3.43	118.11	122.92
25	H	101	BCR	C31-C1-C6	-3.43	104.73	110.30
32	H	102	DGD	O2G-C1B-C2B	3.43	118.89	111.50
23	B	611	CLA	O2D-CGD-CBD	3.42	117.35	111.27
28	B	621	LMG	O7-C10-C11	3.42	118.87	111.50
23	B	602	CLA	C1B-CHB-C4A	-3.41	123.35	130.12
23	A	608	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
25	B	618	BCR	C33-C5-C4	-3.41	107.06	113.62
26	d	404	PL9	C35-C34-C33	-3.41	114.94	123.68
26	a	609	PL9	C51-C49-C48	-3.41	112.80	122.65
23	b	609[B]	CLA	C1B-CHB-C4A	-3.40	123.38	130.12
23	b	611	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
23	B	608	CLA	C1B-CHB-C4A	-3.40	123.39	130.12
25	F	101	BCR	C34-C9-C10	-3.40	118.16	122.92
23	c	514	CLA	C1B-CHB-C4A	-3.40	123.39	130.12
25	b	620	BCR	C2-C3-C4	3.40	118.97	111.38
27	a	612	SQD	O9-S-C6	3.40	110.97	106.94
23	B	605	CLA	O1D-CGD-CBD	-3.39	117.55	124.48
23	D	404	CLA	C1-O2A-CGA	3.39	125.34	116.44
25	a	608	BCR	C27-C26-C25	-3.38	117.82	122.73
32	D	406	DGD	C4E-C3E-C2E	3.38	116.73	110.82
26	A	610	PL9	C31-C29-C28	-3.38	114.28	121.12
23	A	605	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
27	a	612	SQD	O47-C7-C8	3.37	118.77	111.50
23	b	619	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
25	b	620	BCR	C30-C25-C24	-3.36	106.26	115.78
32	d	405	DGD	O2G-C1B-C2B	3.36	118.75	111.50
27	b	601	SQD	O47-C7-C8	3.36	118.74	111.50
25	T	101	BCR	C34-C9-C10	-3.36	118.22	122.92
27	A	611	SQD	O8-S-C6	3.35	111.07	105.74
25	b	622	BCR	C11-C10-C9	-3.35	122.53	127.31
27	a	610	SQD	O8-S-C6	3.34	111.07	105.74
23	C	511	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
26	A	610	PL9	C45-C44-C46	-3.33	109.67	115.27
23	C	501	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
27	A	611	SQD	C1-C2-C3	-3.33	103.06	110.00
23	C	508	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
27	a	610	SQD	C1-C2-C3	-3.32	103.08	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	403	CLA	C1B-CHB-C4A	-3.32	123.55	130.12
23	c	508	CLA	C1B-CHB-C4A	-3.31	123.56	130.12
23	C	512	CLA	C1B-CHB-C4A	-3.31	123.56	130.12
33	v	201	HEM	C1D-C2D-C3D	-3.31	104.69	107.00
23	C	512	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
23	C	512	CLA	C4-C3-C5	3.31	120.84	115.27
23	A	608	CLA	C1-O2A-CGA	3.31	125.12	116.44
25	h	101	BCR	C20-C19-C18	-3.31	117.13	126.42
25	t	101	BCR	C7-C8-C9	-3.30	121.24	126.23
25	B	619	BCR	C32-C1-C6	3.30	115.65	110.30
25	H	101	BCR	C8-C9-C10	-3.30	113.88	118.94
23	c	513	CLA	C4-C3-C5	3.30	120.82	115.27
24	D	401	PHO	O2D-CGD-O1D	-3.30	117.39	123.84
23	c	511	CLA	C1B-CHB-C4A	-3.29	123.60	130.12
23	C	513	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
23	c	504	CLA	C4A-NA-C1A	-3.29	105.23	106.71
23	B	615	CLA	C1B-CHB-C4A	-3.29	123.61	130.12
23	b	616	CLA	C1B-CHB-C4A	-3.28	123.62	130.12
23	C	502	CLA	C1B-CHB-C4A	-3.28	123.62	130.12
25	C	514	BCR	C12-C13-C14	-3.27	113.92	118.94
23	c	513	CLA	C2A-C1A-CHA	3.27	129.57	123.86
25	T	101	BCR	C20-C19-C18	-3.27	117.24	126.42
25	C	515	BCR	C7-C6-C5	-3.27	113.55	121.46
23	A	606	CLA	C4A-NA-C1A	-3.26	105.24	106.71
23	B	616	CLA	C4A-NA-C1A	-3.26	105.24	106.71
23	B	613	CLA	C4-C3-C5	3.25	120.74	115.27
32	c	518	DGD	O2G-C1B-C2B	3.25	118.50	111.50
23	B	609	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
23	b	615	CLA	C4-C3-C5	3.25	120.73	115.27
23	c	502	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
23	b	604	CLA	C1B-CHB-C4A	-3.24	123.69	130.12
25	K	101	BCR	C24-C25-C26	-3.24	113.62	121.46
25	f	101	BCR	C34-C9-C10	-3.24	118.39	122.92
25	b	620	BCR	C24-C25-C26	-3.23	113.63	121.46
23	D	404	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
23	b	614	CLA	C1B-CHB-C4A	-3.23	123.73	130.12
23	a	604	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
25	T	101	BCR	C2-C1-C6	3.22	115.44	110.48
25	F	101	BCR	C16-C15-C14	-3.22	116.88	123.47
25	t	101	BCR	C35-C13-C14	-3.22	118.42	122.92
23	B	617	CLA	C1B-CHB-C4A	-3.21	123.77	130.12
25	h	101	BCR	C11-C12-C13	-3.21	117.41	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	403	CLA	C4A-NA-C1A	-3.20	105.27	106.71
23	b	618	CLA	C1B-CHB-C4A	-3.20	123.77	130.12
25	a	608	BCR	C38-C26-C27	-3.20	107.47	113.62
25	t	101	BCR	C34-C9-C10	-3.20	118.44	122.92
23	d	403	CLA	C1-O2A-CGA	3.19	124.82	116.44
23	C	510	CLA	C1B-CHB-C4A	-3.19	123.79	130.12
23	A	606	CLA	CMB-C2B-C1B	-3.19	123.57	128.46
25	h	101	BCR	C30-C25-C26	-3.18	118.13	122.61
23	B	603	CLA	C4-C3-C5	3.18	120.62	115.27
23	D	402	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
23	c	510	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
27	x	101	SQD	O7-S-C6	3.18	110.71	106.94
26	d	404	PL9	C15-C14-C16	-3.17	109.94	115.27
27	X	101	SQD	O7-S-C6	3.17	110.71	106.94
25	K	101	BCR	C11-C12-C13	-3.17	117.51	126.42
23	b	615	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
33	V	202	HEM	CBA-CAA-C2A	-3.16	106.66	112.49
23	a	605	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
25	B	618	BCR	C36-C18-C19	3.15	123.03	118.08
23	B	605	CLA	C1B-CHB-C4A	-3.15	123.89	130.12
25	C	515	BCR	C1-C6-C7	-3.15	106.88	115.78
25	F	101	BCR	C2-C3-C4	3.14	118.40	111.38
25	c	522	BCR	C33-C5-C4	-3.14	107.58	113.62
25	H	101	BCR	C36-C18-C17	-3.14	118.53	122.92
23	b	605	CLA	C4-C3-C5	3.13	120.54	115.27
23	a	605	CLA	C4-C3-C5	3.13	120.54	115.27
25	C	521	BCR	C33-C5-C4	-3.13	107.60	113.62
23	C	506	CLA	C4-C3-C5	3.13	120.54	115.27
25	h	101	BCR	C16-C15-C14	-3.13	117.06	123.47
25	b	622	BCR	C11-C12-C13	-3.13	117.63	126.42
23	A	606	CLA	C4-C3-C5	3.13	120.53	115.27
23	c	513	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
25	A	609	BCR	C27-C26-C25	-3.11	118.21	122.73
25	H	101	BCR	C11-C12-C13	-3.11	117.68	126.42
25	t	101	BCR	C11-C12-C13	-3.11	117.68	126.42
25	c	516	BCR	C33-C5-C4	-3.11	107.64	113.62
23	D	404	CLA	CHA-C1A-NA	-3.11	119.28	126.40
32	C	518	DGD	O3G-C3G-C2G	-3.11	103.40	110.90
25	A	609	BCR	C33-C5-C4	-3.11	107.65	113.62
23	c	508	CLA	C4-C3-C5	3.10	120.49	115.27
25	b	620	BCR	C23-C22-C21	-3.10	114.18	118.94
26	D	405	PL9	C15-C14-C16	-3.10	110.06	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	C4-C3-C5	3.10	120.49	115.27
23	B	602	CLA	O2A-CGA-CBA	3.10	121.63	111.91
25	H	101	BCR	C20-C19-C18	-3.10	117.71	126.42
23	D	403	CLA	C2A-C1A-CHA	3.09	129.27	123.86
23	A	608	CLA	CHA-C1A-NA	-3.09	119.32	126.40
27	a	612	SQD	O6-C1-C2	3.09	113.13	108.30
23	C	501	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
27	X	101	SQD	O9-S-C6	3.09	110.61	106.94
23	B	616	CLA	C1B-CHB-C4A	-3.09	124.01	130.12
25	c	516	BCR	C35-C13-C14	-3.08	118.61	122.92
27	x	101	SQD	O9-S-C6	3.08	110.60	106.94
27	b	601	SQD	O6-C1-C2	3.07	113.10	108.30
26	d	404	PL9	C10-C9-C11	-3.07	110.10	115.27
23	D	402	CLA	C4A-NA-C1A	-3.07	105.33	106.71
23	a	605	CLA	C4A-NA-C1A	-3.07	105.33	106.71
23	b	608	CLA	C1-O2A-CGA	3.07	124.50	116.44
25	h	101	BCR	C40-C30-C25	-3.07	105.32	110.30
23	C	507	CLA	C4-C3-C5	3.07	120.43	115.27
23	C	509	CLA	CMB-C2B-C1B	-3.06	123.75	128.46
25	f	101	BCR	C37-C22-C23	-3.06	113.25	118.08
25	C	515	BCR	C24-C25-C26	-3.06	114.04	121.46
25	k	101	BCR	C8-C9-C10	-3.05	114.26	118.94
25	f	101	BCR	C35-C13-C14	-3.05	118.65	122.92
23	b	607	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
23	B	604	CLA	C4-C3-C5	3.05	120.39	115.27
23	b	611	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	C	504	CLA	C4-C3-C5	3.04	120.38	115.27
23	A	608	CLA	C4A-NA-C1A	-3.03	105.34	106.71
33	E	102	HEM	C1D-C2D-C3D	-3.03	104.89	107.00
23	d	403	CLA	CHA-C1A-NA	-3.03	119.45	126.40
25	c	516	BCR	C20-C21-C22	-3.03	122.98	127.31
23	B	605	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
23	b	606	CLA	C4-C3-C5	3.02	120.36	115.27
23	a	607	CLA	C4A-NA-C1A	-3.02	105.35	106.71
25	B	620	BCR	C16-C15-C14	-3.02	117.29	123.47
25	B	619	BCR	C27-C26-C25	-3.02	118.35	122.73
23	D	402	CLA	O1D-CGD-CBD	-3.02	118.31	124.48
23	c	505	CLA	C4-C3-C5	3.01	120.34	115.27
23	A	606	CLA	CHA-C1A-NA	-3.01	119.51	126.40
25	b	621	BCR	C23-C22-C21	-3.01	114.33	118.94
23	D	402	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
25	a	608	BCR	C33-C5-C4	-2.99	107.87	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
23	C	510	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
25	b	620	BCR	C33-C5-C4	-2.98	107.89	113.62
23	a	605	CLA	O1D-CGD-CBD	-2.96	118.42	124.48
23	B	614	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
25	k	101	BCR	C37-C22-C21	-2.96	118.78	122.92
25	c	522	BCR	C23-C24-C25	-2.96	118.89	127.20
23	B	610	CLA	C4A-NA-C1A	-2.96	105.38	106.71
23	b	604	CLA	O2A-CGA-CBA	2.96	121.19	111.91
32	D	406	DGD	C1E-C2E-C3E	2.95	116.14	110.00
23	c	510	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
25	c	516	BCR	C23-C24-C25	-2.95	118.92	127.20
23	C	506	CLA	C4A-NA-C1A	-2.95	105.38	106.71
27	X	101	SQD	O48-C23-C24	2.95	121.16	111.91
25	T	101	BCR	C38-C26-C27	-2.95	107.96	113.62
27	a	612	SQD	O48-C23-C24	2.94	121.14	111.91
23	b	609[B]	CLA	C4-C3-C5	2.94	120.22	115.27
23	B	607[B]	CLA	C4-C3-C5	2.94	120.22	115.27
23	c	513	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
27	x	101	SQD	O48-C23-C24	2.93	121.12	111.91
25	b	621	BCR	C37-C22-C21	-2.93	118.82	122.92
25	B	618	BCR	C2-C3-C4	2.93	117.92	111.38
24	A	607	PHO	O2D-CGD-O1D	-2.93	118.12	123.84
27	b	601	SQD	O48-C23-C24	2.93	121.09	111.91
23	B	607[A]	CLA	C4-C3-C5	2.92	120.19	115.27
25	c	515	BCR	C20-C19-C18	-2.92	118.20	126.42
23	C	505	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
25	t	101	BCR	C38-C26-C27	-2.92	108.00	113.62
25	C	514	BCR	C11-C12-C13	-2.92	118.21	126.42
25	b	621	BCR	C8-C7-C6	-2.92	119.01	127.20
23	B	608	CLA	C1-C2-C3	-2.92	121.00	126.04
23	b	617	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
23	b	610	CLA	C1-C2-C3	-2.91	121.00	126.04
25	k	101	BCR	C33-C5-C4	-2.91	108.02	113.62
25	K	101	BCR	C33-C5-C4	-2.91	108.03	113.62
28	z	101	LMG	O1-C1-C2	2.91	112.84	108.30
23	c	506	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
23	a	613	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
25	C	515	BCR	C23-C24-C25	-2.90	119.05	127.20
23	C	513	CLA	C4A-NA-C1A	-2.90	105.40	106.71
25	H	101	BCR	C40-C30-C25	-2.90	105.60	110.30
25	c	522	BCR	C34-C9-C10	-2.90	118.86	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	621	BCR	C16-C15-C14	-2.89	117.55	123.47
23	b	609[A]	CLA	C4-C3-C5	2.89	120.13	115.27
23	C	513	CLA	O2A-CGA-CBA	2.89	120.97	111.91
25	b	621	BCR	C7-C6-C5	-2.89	114.47	121.46
23	C	507	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
23	B	608	CLA	O2D-CGD-CBD	2.88	116.39	111.27
25	f	101	BCR	C2-C3-C4	2.88	117.82	111.38
23	B	612	CLA	C1-C2-C3	-2.88	121.06	126.04
23	b	614	CLA	C1-C2-C3	-2.88	121.06	126.04
25	F	101	BCR	C23-C22-C21	2.88	123.36	118.94
25	c	515	BCR	C12-C13-C14	-2.88	114.53	118.94
32	c	519	DGD	O3G-C3G-C2G	-2.88	103.96	110.90
23	c	511	CLA	CMB-C2B-C1B	-2.88	124.05	128.46
23	D	402	CLA	C4-C3-C5	2.87	120.10	115.27
23	b	606	CLA	CMB-C2B-C1B	-2.87	124.06	128.46
23	b	617	CLA	CMB-C2B-C1B	-2.87	124.06	128.46
23	a	613	CLA	C4-C3-C5	2.87	120.09	115.27
23	b	618	CLA	C4A-NA-C1A	-2.86	105.42	106.71
33	e	102	HEM	C1D-C2D-C3D	-2.86	105.01	107.00
25	A	609	BCR	C16-C15-C14	-2.86	117.62	123.47
25	b	621	BCR	C10-C11-C12	-2.85	114.31	123.22
23	B	608	CLA	C4-C3-C5	2.85	120.07	115.27
27	a	610	SQD	C45-O47-C7	-2.85	110.77	117.79
25	A	609	BCR	C38-C26-C27	-2.85	108.14	113.62
27	A	611	SQD	C45-O47-C7	-2.85	110.78	117.79
23	b	607	CLA	CMB-C2B-C1B	-2.84	124.09	128.46
25	f	101	BCR	C33-C5-C4	-2.84	108.15	113.62
25	A	609	BCR	C34-C9-C10	-2.84	118.95	122.92
25	A	609	BCR	C11-C12-C13	-2.83	118.46	126.42
23	b	610	CLA	C4-C3-C5	2.82	120.02	115.27
25	B	620	BCR	C10-C11-C12	-2.82	114.41	123.22
23	a	613	CLA	CHA-C1A-NA	-2.82	119.95	126.40
25	C	515	BCR	C20-C19-C18	-2.82	118.50	126.42
23	B	603	CLA	C4A-NA-C1A	-2.81	105.44	106.71
25	c	522	BCR	C29-C28-C27	2.81	117.66	111.38
23	b	615	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	c	508	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	B	614	CLA	C4A-NA-C1A	-2.81	105.44	106.71
23	c	509	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
25	C	521	BCR	C37-C22-C21	-2.81	118.99	122.92
25	b	622	BCR	C33-C5-C4	-2.80	108.23	113.62
28	J	101	LMG	O6-C5-C4	2.80	114.78	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	611	SQD	C44-O6-C1	-2.80	108.28	113.74
26	d	404	PL9	C30-C29-C31	-2.79	110.58	115.27
23	D	402	CLA	CHA-C1A-NA	-2.79	120.02	126.40
23	C	513	CLA	CHA-C1A-NA	-2.78	120.02	126.40
23	a	605	CLA	CHA-C1A-NA	-2.78	120.02	126.40
23	B	612	CLA	CHA-C1A-NA	-2.78	120.02	126.40
26	a	609	PL9	C53-C6-C1	2.78	120.68	114.99
27	a	610	SQD	C44-O6-C1	-2.78	108.32	113.74
23	b	607	CLA	C4-C3-C5	2.77	119.93	115.27
26	A	610	PL9	C53-C6-C1	2.77	120.65	114.99
25	f	101	BCR	C16-C15-C14	-2.76	117.82	123.47
23	b	611	CLA	O1D-CGD-CBD	-2.76	118.84	124.48
23	c	509	CLA	C4-C3-C5	2.75	119.90	115.27
23	b	607	CLA	O2A-CGA-CBA	2.75	120.55	111.91
25	t	101	BCR	C33-C5-C4	-2.75	108.33	113.62
23	C	508	CLA	C4-C3-C5	2.75	119.90	115.27
23	C	501	CLA	CHA-C1A-NA	-2.75	120.10	126.40
31	b	624	LHG	C5-O7-C7	-2.75	111.03	117.79
32	C	517	DGD	O1G-C1A-C2A	2.75	120.53	111.91
25	t	101	BCR	C36-C18-C17	-2.74	119.08	122.92
23	B	605	CLA	C4-C3-C5	2.74	119.89	115.27
33	V	202	HEM	CBD-CAD-C3D	-2.74	107.42	112.48
24	d	401	PHO	CMB-C2B-C1B	-2.74	120.84	125.06
31	a	614	LHG	O8-C23-C24	2.74	120.50	111.91
32	c	518	DGD	O1G-C1A-C2A	2.74	120.50	111.91
23	b	617	CLA	C1-O2A-CGA	2.74	123.62	116.44
32	D	406	DGD	C3E-C4E-C5E	2.73	115.11	110.24
23	B	616	CLA	O2A-CGA-CBA	2.73	120.48	111.91
28	C	519	LMG	O8-C28-C29	2.73	120.48	111.91
23	b	606	CLA	O1D-CGD-CBD	-2.73	118.90	124.48
23	c	508	CLA	O2A-CGA-CBA	2.73	120.47	111.91
24	d	401	PHO	O2D-CGD-O1D	-2.73	118.51	123.84
27	B	623	SQD	O48-C23-C24	2.73	120.47	111.91
23	b	610	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
27	b	602	SQD	O48-C23-C24	2.72	120.44	111.91
23	D	404	CLA	CMB-C2B-C1B	-2.71	124.29	128.46
23	a	613	CLA	O2A-CGA-CBA	2.71	120.42	111.91
23	b	609[B]	CLA	CMB-C2B-C1B	-2.71	124.29	128.46
23	B	612	CLA	C1-O2A-CGA	2.71	123.56	116.44
25	c	515	BCR	C38-C26-C27	-2.71	108.41	113.62
23	B	607[B]	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
23	B	615	CLA	O1D-CGD-CBD	-2.71	118.94	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	h	101	BCR	C34-C9-C10	-2.71	119.13	122.92
24	d	401	PHO	C1-C2-C3	-2.71	121.36	126.04
25	b	622	BCR	C36-C18-C19	2.70	122.34	118.08
23	d	402	CLA	C4A-NA-C1A	-2.70	105.49	106.71
23	A	606	CLA	O2A-CGA-CBA	2.70	120.38	111.91
27	b	602	SQD	O9-S-C6	2.70	110.15	106.94
26	d	404	PL9	C7-C3-C4	2.70	119.07	116.88
28	c	520	LMG	O8-C28-C29	2.70	120.38	111.91
23	c	513	CLA	O2A-CGA-CBA	2.70	120.38	111.91
23	b	609[A]	CLA	CMB-C2B-C1B	-2.70	124.32	128.46
23	c	504	CLA	C4-C3-C5	2.70	119.81	115.27
26	A	610	PL9	C25-C24-C26	-2.70	110.73	115.27
23	B	617	CLA	C4A-NA-C1A	-2.70	105.49	106.71
25	c	516	BCR	C24-C25-C26	-2.69	114.93	121.46
23	b	607	CLA	O1D-CGD-CBD	-2.69	118.97	124.48
23	b	609[A]	CLA	O1D-CGD-CBD	-2.69	118.97	124.48
25	B	619	BCR	C16-C15-C14	-2.69	117.97	123.47
25	B	620	BCR	C20-C19-C18	-2.69	118.86	126.42
23	C	503	CLA	C4-C3-C5	2.69	119.79	115.27
23	B	604	CLA	CHB-C4A-NA	-2.68	120.80	124.51
24	D	401	PHO	CMB-C2B-C1B	-2.68	120.93	125.06
31	B	622	LHG	O8-C23-C24	2.68	120.32	111.91
27	B	623	SQD	O9-S-C6	2.68	110.12	106.94
25	F	101	BCR	C10-C11-C12	-2.68	114.85	123.22
23	B	604	CLA	C4A-NA-C1A	-2.68	105.50	106.71
23	b	613	CLA	O2A-CGA-CBA	2.68	120.30	111.91
27	B	623	SQD	C4-C3-C2	2.68	115.49	110.82
23	b	605	CLA	O1D-CGD-CBD	-2.67	119.01	124.48
23	B	611	CLA	O2A-CGA-CBA	2.67	120.29	111.91
23	D	403	CLA	C4-C3-C5	2.67	119.77	115.27
31	B	622	LHG	C5-O7-C7	-2.67	111.22	117.79
23	c	502	CLA	O2A-CGA-CBA	2.67	120.28	111.91
23	c	512	CLA	O1D-CGD-CBD	-2.67	119.03	124.48
23	b	619	CLA	CHA-C1A-NA	-2.67	120.29	126.40
27	b	602	SQD	C4-C3-C2	2.66	115.47	110.82
23	d	402	CLA	C4-C3-C5	2.66	119.75	115.27
31	D	407	LHG	O8-C23-C24	2.66	120.27	111.91
31	b	624	LHG	O8-C23-C24	2.66	120.26	111.91
23	b	610	CLA	CMB-C2B-C1B	-2.66	124.38	128.46
23	a	607	CLA	O2A-CGA-CBA	2.66	120.25	111.91
23	a	613	CLA	C4A-NA-C1A	-2.66	105.51	106.71
23	B	607[A]	CLA	CMB-C2B-C1B	-2.66	124.38	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	O2A-CGA-CBA	2.66	120.25	111.91
23	c	506	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
25	b	620	BCR	C36-C18-C17	-2.65	119.21	122.92
23	b	616	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
23	B	607[B]	CLA	C1-C2-C3	-2.65	121.46	126.04
25	h	101	BCR	C10-C11-C12	-2.65	114.95	123.22
25	b	620	BCR	C37-C22-C21	-2.65	119.21	122.92
23	b	609[B]	CLA	C1-C2-C3	-2.65	121.47	126.04
32	c	519	DGD	C2G-O2G-C1B	-2.65	111.28	117.79
25	h	101	BCR	C37-C22-C21	-2.64	119.22	122.92
25	f	101	BCR	C11-C12-C13	-2.64	118.99	126.42
25	A	609	BCR	C24-C25-C26	-2.64	115.06	121.46
23	C	507	CLA	O2A-CGA-CBA	2.64	120.19	111.91
25	b	621	BCR	C27-C26-C25	-2.64	118.90	122.73
23	C	512	CLA	O2A-CGA-CBA	2.63	120.17	111.91
31	D	408	LHG	O8-C23-C24	2.63	120.17	111.91
23	C	511	CLA	C1-O2A-CGA	2.63	123.34	116.44
23	b	615	CLA	O2A-CGA-CBA	2.63	120.16	111.91
23	B	603	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
23	B	605	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
25	K	101	BCR	C35-C13-C14	-2.63	119.24	122.92
23	c	503	CLA	CHA-C1A-NA	-2.63	120.38	126.40
26	D	405	PL9	C7-C3-C2	-2.63	119.85	123.30
23	b	610	CLA	O1D-CGD-CBD	-2.63	119.11	124.48
24	a	606	PHO	O2D-CGD-O1D	-2.62	118.71	123.84
23	C	501	CLA	O2A-CGA-CBA	2.62	120.14	111.91
23	c	504	CLA	CMB-C2B-C1B	-2.62	124.43	128.46
23	B	617	CLA	O2A-CGA-CBA	2.62	120.14	111.91
23	D	403	CLA	O2A-CGA-CBA	2.62	120.13	111.91
23	B	608	CLA	CHB-C4A-NA	-2.62	120.89	124.51
24	D	401	PHO	O1D-CGD-CBD	2.62	129.84	124.48
25	f	101	BCR	C1-C6-C7	-2.61	108.38	115.78
32	H	102	DGD	O1G-C1A-C2A	2.61	120.11	111.91
25	C	521	BCR	C40-C30-C25	2.61	114.54	110.30
25	C	514	BCR	C34-C9-C8	2.61	122.19	118.08
25	K	101	BCR	C37-C22-C23	-2.61	113.97	118.08
23	c	503	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
23	c	503	CLA	C4-C3-C5	2.60	119.65	115.27
23	C	511	CLA	C4-C3-C5	2.60	119.65	115.27
25	T	101	BCR	C16-C17-C18	-2.60	123.59	127.31
23	b	618	CLA	C4-C3-C5	2.60	119.65	115.27
23	c	512	CLA	C4-C3-C5	2.60	119.64	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	620	BCR	C1-C6-C5	-2.60	118.96	122.61
23	b	609[B]	CLA	O1D-CGD-CBD	-2.59	119.18	124.48
23	B	605	CLA	O2A-CGA-CBA	2.59	120.05	111.91
23	C	509	CLA	O2A-CGA-CBA	2.59	120.04	111.91
23	b	606	CLA	CHB-C4A-NA	-2.59	120.93	124.51
23	B	616	CLA	C4-C3-C5	2.59	119.62	115.27
23	B	612	CLA	O1D-CGD-CBD	-2.59	119.19	124.48
23	c	508	CLA	O1D-CGD-CBD	-2.58	119.20	124.48
25	B	618	BCR	C35-C13-C14	-2.58	119.31	122.92
23	C	502	CLA	C4-C3-C5	2.58	119.61	115.27
23	b	616	CLA	C4-C3-C5	2.58	119.61	115.27
25	F	101	BCR	C37-C22-C21	-2.58	119.31	122.92
25	H	101	BCR	C1-C6-C7	-2.58	108.49	115.78
23	b	609[A]	CLA	C1-O2A-CGA	2.57	123.20	116.44
23	B	614	CLA	C4-C3-C5	2.57	119.60	115.27
25	F	101	BCR	C36-C18-C19	2.57	122.13	118.08
25	c	515	BCR	C11-C12-C13	-2.57	119.20	126.42
23	B	605	CLA	C4A-NA-C1A	-2.56	105.55	106.71
23	c	513	CLA	C1-C2-C3	-2.56	121.61	126.04
32	h	102	DGD	O1G-C1A-C2A	2.56	119.95	111.91
23	B	613	CLA	CMB-C2B-C1B	-2.56	124.53	128.46
23	B	609	CLA	O1D-CGD-CBD	-2.56	119.24	124.48
26	d	404	PL9	C53-C6-C1	2.56	120.23	114.99
25	a	608	BCR	C16-C15-C14	-2.56	118.23	123.47
23	B	613	CLA	O2A-CGA-CBA	2.56	119.94	111.91
23	b	607	CLA	CHA-C1A-NA	-2.56	120.53	126.40
23	B	607[A]	CLA	C1-O2A-CGA	2.56	123.16	116.44
26	a	609	PL9	C35-C34-C36	-2.56	110.96	115.27
23	B	615	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
27	b	601	SQD	O8-S-C6	2.56	109.81	105.74
23	C	512	CLA	C1-C2-C3	-2.56	121.62	126.04
23	C	511	CLA	O1D-CGD-CBD	-2.55	119.26	124.48
23	D	402	CLA	O2A-CGA-CBA	2.55	119.92	111.91
23	A	608	CLA	O1D-CGD-CBD	-2.55	119.27	124.48
23	B	611	CLA	C4-C3-C5	2.55	119.55	115.27
23	d	403	CLA	CMB-C2B-C1B	-2.55	124.55	128.46
25	B	619	BCR	C20-C21-C22	-2.54	123.69	127.31
23	B	607[A]	CLA	O1D-CGD-CBD	-2.54	119.29	124.48
25	T	101	BCR	C11-C12-C13	-2.54	119.29	126.42
27	a	612	SQD	O8-S-C6	2.53	109.78	105.74
23	b	619	CLA	O2A-CGA-CBA	2.53	119.85	111.91
25	A	609	BCR	C20-C21-C22	-2.53	123.70	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609[B]	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
23	b	607	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
27	A	611	SQD	C1-O5-C5	-2.53	108.72	113.69
23	C	509	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
25	B	618	BCR	C30-C25-C24	-2.53	108.62	115.78
24	A	607	PHO	CMB-C2B-C1B	-2.52	121.18	125.06
24	D	401	PHO	C1-C2-C3	-2.52	121.69	126.04
23	c	512	CLA	O2A-CGA-CBA	2.52	119.81	111.91
23	b	613	CLA	C4-C3-C5	2.51	119.50	115.27
23	D	404	CLA	C4-C3-C5	2.51	119.50	115.27
25	T	101	BCR	C8-C9-C10	-2.51	115.08	118.94
25	H	101	BCR	C36-C18-C19	2.51	122.03	118.08
23	C	510	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
23	B	604	CLA	CHA-C1A-NA	-2.51	120.66	126.40
23	d	403	CLA	C4-C3-C5	2.51	119.49	115.27
25	F	101	BCR	C1-C6-C7	-2.51	108.69	115.78
28	C	520	LMG	C3-C4-C5	2.51	114.71	110.24
23	B	609	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
33	v	201	HEM	CMB-C2B-C3B	2.50	129.36	124.68
25	C	521	BCR	C10-C11-C12	-2.50	115.41	123.22
23	a	604	CLA	O2A-CGA-CBA	2.50	119.76	111.91
23	c	513	CLA	CHA-C1A-NA	-2.50	120.67	126.40
23	c	514	CLA	O2A-CGA-CBA	2.50	119.76	111.91
27	a	610	SQD	C1-O5-C5	-2.50	108.78	113.69
32	d	405	DGD	O1G-C1A-C2A	2.50	119.75	111.91
23	c	506	CLA	O1D-CGD-CBD	-2.50	119.38	124.48
23	b	606	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
23	B	609	CLA	O2A-CGA-CBA	2.50	119.74	111.91
23	a	613	CLA	O1D-CGD-CBD	-2.49	119.39	124.48
28	c	521	LMG	O8-C28-C29	2.49	119.71	111.91
23	B	607[B]	CLA	C1-O2A-CGA	2.49	122.97	116.44
28	J	101	LMG	C6-C5-C4	-2.49	107.18	113.00
26	a	609	PL9	C25-C24-C26	-2.48	111.09	115.27
25	c	522	BCR	C8-C9-C10	-2.48	115.13	118.94
25	C	521	BCR	C8-C9-C10	-2.48	115.13	118.94
25	B	618	BCR	C37-C22-C23	-2.48	114.17	118.08
23	b	618	CLA	O2A-CGA-CBA	2.48	119.69	111.91
23	b	615	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
23	b	617	CLA	O1D-CGD-CBD	-2.48	119.41	124.48
23	b	618	CLA	O1D-CGD-CBD	-2.48	119.41	124.48
32	D	406	DGD	O2G-C1B-O1B	-2.48	117.71	123.70
23	c	507	CLA	C4A-NA-C1A	-2.48	105.59	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	d	405	DGD	O2G-C1B-O1B	-2.48	117.72	123.70
23	b	614	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
32	C	518	DGD	C2G-O2G-C1B	-2.47	111.71	117.79
23	C	505	CLA	O1D-CGD-CBD	-2.47	119.44	124.48
33	V	202	HEM	C4A-C3A-C2A	2.47	108.71	107.00
23	C	502	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
23	C	504	CLA	C1-O2A-CGA	2.46	122.91	116.44
23	b	609[B]	CLA	C1-O2A-CGA	2.46	122.91	116.44
32	D	406	DGD	O1G-C1A-C2A	2.46	119.64	111.91
23	b	612	CLA	C1-C2-C3	-2.46	121.78	126.04
26	a	609	PL9	C20-C19-C21	-2.46	111.13	115.27
24	d	401	PHO	O1D-CGD-CBD	2.46	129.52	124.48
23	D	403	CLA	CHA-C1A-NA	-2.46	120.76	126.40
25	c	515	BCR	C10-C11-C12	-2.46	115.54	123.22
24	a	606	PHO	CBD-CHA-C4D	-2.46	105.77	108.54
25	b	622	BCR	C10-C11-C12	-2.45	115.56	123.22
25	c	515	BCR	C35-C13-C14	-2.45	119.49	122.92
23	b	609[A]	CLA	C1-C2-C3	-2.45	121.81	126.04
23	d	402	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
23	c	512	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
25	h	101	BCR	C36-C18-C17	-2.45	119.50	122.92
23	c	514	CLA	C4-C3-C5	2.45	119.39	115.27
25	B	618	BCR	C16-C17-C18	-2.45	123.82	127.31
23	C	513	CLA	C4-C3-C5	2.44	119.38	115.27
25	C	521	BCR	C34-C9-C10	-2.44	119.50	122.92
23	b	606	CLA	CHA-C1A-NA	-2.44	120.80	126.40
23	c	503	CLA	O1D-CGD-CBD	-2.44	119.49	124.48
24	a	606	PHO	O1D-CGD-CBD	2.44	129.48	124.48
23	B	610	CLA	C1-C2-C3	-2.43	121.83	126.04
23	C	509	CLA	CHA-C1A-NA	-2.43	120.83	126.40
26	D	405	PL9	C20-C19-C21	-2.43	111.18	115.27
23	B	607[A]	CLA	C1-C2-C3	-2.43	121.84	126.04
23	b	604	CLA	CHA-C1A-NA	-2.43	120.84	126.40
24	A	607	PHO	CBD-CHA-C4D	-2.42	105.81	108.54
31	d	406	LHG	O8-C23-C24	2.42	119.51	111.91
28	b	623	LMG	O8-C28-C29	2.42	119.50	111.91
25	b	622	BCR	C1-C6-C5	-2.42	119.21	122.61
23	b	609[A]	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
23	c	509	CLA	CMB-C2B-C3B	2.42	129.20	124.68
23	b	616	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
23	B	608	CLA	CED-O2D-CGD	2.42	121.40	115.94
23	C	505	CLA	O2D-CGD-O1D	-2.41	119.12	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	606	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
25	c	516	BCR	C20-C19-C18	-2.41	119.64	126.42
24	A	607	PHO	O1D-CGD-CBD	2.41	129.42	124.48
26	A	610	PL9	C51-C49-C50	-2.41	109.28	114.60
25	C	515	BCR	C34-C9-C10	-2.41	119.55	122.92
23	d	403	CLA	O2A-CGA-CBA	2.41	119.47	111.91
31	e	101	LHG	O8-C23-C24	2.41	119.47	111.91
23	b	618	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
23	C	510	CLA	CHA-C1A-NA	-2.41	120.89	126.40
25	C	514	BCR	C33-C5-C4	-2.40	109.00	113.62
26	D	405	PL9	C53-C6-C1	2.40	119.90	114.99
23	b	605	CLA	O2A-CGA-CBA	2.40	119.44	111.91
32	c	518	DGD	O6D-C5D-C4D	-2.40	105.34	109.69
23	B	614	CLA	O1D-CGD-CBD	-2.40	119.58	124.48
23	c	505	CLA	CMB-C2B-C1B	-2.39	124.78	128.46
28	Z	101	LMG	O2-C2-C3	-2.39	104.82	110.35
33	E	102	HEM	CMB-C2B-C3B	2.39	129.15	124.68
25	B	620	BCR	C1-C6-C7	-2.39	109.01	115.78
25	C	514	BCR	C30-C25-C24	-2.39	109.01	115.78
23	C	507	CLA	O1D-CGD-CBD	-2.39	119.60	124.48
25	b	621	BCR	C29-C30-C25	2.39	114.16	110.48
25	b	622	BCR	C36-C18-C17	-2.38	119.58	122.92
26	A	610	PL9	C30-C29-C31	-2.38	111.26	115.27
23	c	511	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
23	c	510	CLA	O2A-CGA-CBA	2.38	119.38	111.91
23	B	603	CLA	C1-C2-C3	-2.37	121.94	126.04
23	B	616	CLA	CHA-C1A-NA	-2.37	120.97	126.40
25	b	620	BCR	C35-C13-C14	-2.37	119.60	122.92
23	b	605	CLA	CHB-C4A-NA	-2.37	121.24	124.51
23	b	611	CLA	CHA-C1A-NA	-2.36	121.00	126.40
23	b	605	CLA	C1-C2-C3	-2.36	121.96	126.04
26	d	404	PL9	C20-C19-C21	-2.36	111.31	115.27
25	a	608	BCR	C24-C25-C26	-2.36	115.76	121.46
32	c	519	DGD	C3G-C2G-C1G	-2.36	106.22	111.79
23	C	506	CLA	CED-O2D-CGD	2.36	121.26	115.94
32	d	405	DGD	C4E-C3E-C2E	2.35	114.93	110.82
23	D	403	CLA	CMB-C2B-C1B	-2.35	124.85	128.46
23	b	614	CLA	C1-O2A-CGA	2.35	122.61	116.44
23	b	605	CLA	CHA-C1A-NA	-2.35	121.02	126.40
23	c	514	CLA	CMB-C2B-C1B	-2.35	124.85	128.46
32	c	518	DGD	C1E-O6E-C5E	-2.35	109.08	113.69
33	v	201	HEM	CMD-C2D-C3D	2.35	129.37	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	O1D-CGD-CBD	-2.35	119.69	124.48
31	E	101	LHG	O8-C23-C24	2.34	119.26	111.91
25	B	619	BCR	C7-C6-C5	-2.34	115.80	121.46
23	b	606	CLA	O2A-CGA-CBA	2.34	119.24	111.91
23	C	509	CLA	C1-O2A-CGA	2.34	122.58	116.44
32	D	406	DGD	O6D-C5D-C6D	2.34	111.38	106.67
23	C	507	CLA	CHA-C1A-NA	-2.34	121.05	126.40
25	t	101	BCR	C37-C22-C21	-2.33	119.66	122.92
23	B	615	CLA	O2A-CGA-CBA	2.33	119.22	111.91
25	T	101	BCR	C30-C25-C24	-2.33	109.19	115.78
23	C	512	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
23	B	617	CLA	CHA-C1A-NA	-2.33	121.07	126.40
23	C	503	CLA	O2A-CGA-CBA	2.33	119.21	111.91
25	c	522	BCR	C10-C11-C12	-2.33	115.96	123.22
23	B	611	CLA	CHA-C1A-NA	-2.32	121.08	126.40
25	C	515	BCR	C35-C13-C14	-2.32	119.67	122.92
25	H	101	BCR	C10-C11-C12	-2.32	115.97	123.22
23	A	605	CLA	O2A-CGA-CBA	2.32	119.19	111.91
23	c	511	CLA	O2A-CGA-CBA	2.32	119.19	111.91
25	t	101	BCR	C1-C6-C5	-2.32	119.34	122.61
28	B	621	LMG	O8-C28-C29	2.32	119.19	111.91
23	B	603	CLA	CMB-C2B-C1B	-2.32	124.90	128.46
23	C	506	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
23	c	510	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
25	b	620	BCR	C10-C11-C12	-2.32	115.98	123.22
33	V	202	HEM	CMB-C2B-C3B	2.32	129.01	124.68
23	B	613	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
23	b	610	CLA	C1-O2A-CGA	2.32	122.52	116.44
23	b	610	CLA	O2A-CGA-CBA	2.32	119.18	111.91
23	b	614	CLA	CHA-C1A-NA	-2.31	121.10	126.40
23	B	607[A]	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
23	C	503	CLA	CMB-C2B-C1B	-2.31	124.91	128.46
23	c	503	CLA	C1-O2A-CGA	2.31	122.51	116.44
25	B	620	BCR	C33-C5-C4	-2.31	109.17	113.62
25	B	619	BCR	C8-C7-C6	-2.31	120.71	127.20
26	d	404	PL9	C7-C3-C2	-2.31	120.26	123.30
23	C	506	CLA	CMB-C2B-C3B	2.31	129.00	124.68
25	f	101	BCR	C30-C25-C24	-2.31	109.25	115.78
25	h	101	BCR	C34-C9-C8	2.31	121.71	118.08
23	c	510	CLA	C1-O2A-CGA	2.31	122.50	116.44
23	b	615	CLA	CHA-C1A-NA	-2.31	121.11	126.40
23	b	613	CLA	CHA-C1A-NA	-2.30	121.12	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	515	BCR	C8-C9-C10	-2.30	115.41	118.94
23	B	615	CLA	C1-O2A-CGA	2.30	122.49	116.44
23	B	605	CLA	CHA-C1A-NA	-2.30	121.12	126.40
23	b	609[B]	CLA	CHA-C1A-NA	-2.30	121.12	126.40
23	c	508	CLA	CHA-C1A-NA	-2.30	121.12	126.40
23	B	603	CLA	C1-O2A-CGA	2.30	122.48	116.44
25	B	619	BCR	C12-C13-C14	-2.30	115.41	118.94
23	C	512	CLA	CED-O2D-CGD	2.30	121.14	115.94
23	b	611	CLA	C4-C3-C5	2.29	119.13	115.27
23	C	511	CLA	O2A-CGA-CBA	2.29	119.10	111.91
32	C	516	DGD	O1G-C1A-C2A	2.29	119.10	111.91
23	A	605	CLA	C4-C3-C5	2.29	119.12	115.27
28	C	520	LMG	O8-C28-C29	2.29	119.09	111.91
33	e	102	HEM	CMB-C2B-C3B	2.29	128.96	124.68
27	a	612	SQD	C3-C4-C5	2.29	114.32	110.24
23	B	607[A]	CLA	O2A-CGA-CBA	2.29	119.09	111.91
25	b	621	BCR	C40-C30-C25	2.29	114.01	110.30
23	B	609	CLA	C4-C3-C5	2.29	119.11	115.27
23	B	606	CLA	C1-O2A-CGA	2.28	122.44	116.44
32	h	102	DGD	O6D-C5D-C6D	2.28	111.27	106.67
25	f	101	BCR	C37-C22-C21	-2.28	119.73	122.92
23	B	607[A]	CLA	CHA-C1A-NA	-2.28	121.17	126.40
23	c	507	CLA	CHB-C4A-NA	-2.28	121.36	124.51
28	j	101	LMG	O6-C5-C4	2.28	113.83	109.69
23	B	604	CLA	O2A-CGA-CBA	2.28	119.05	111.91
26	A	610	PL9	C7-C3-C2	-2.28	120.31	123.30
28	c	521	LMG	C3-C4-C5	2.28	114.30	110.24
25	B	619	BCR	C2-C3-C4	2.28	116.46	111.38
23	b	605	CLA	CMB-C2B-C1B	-2.28	124.97	128.46
23	C	508	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
23	b	616	CLA	C1-O2A-CGA	2.27	122.41	116.44
23	C	501	CLA	O1D-CGD-CBD	-2.27	119.83	124.48
26	A	610	PL9	C10-C9-C11	-2.27	111.45	115.27
25	h	101	BCR	C2-C3-C4	2.27	116.45	111.38
27	b	601	SQD	C3-C4-C5	2.27	114.29	110.24
23	b	611	CLA	C11-C12-C13	-2.27	108.58	115.92
23	c	513	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
23	C	503	CLA	CHA-C1A-NA	-2.27	121.21	126.40
23	C	513	CLA	CMB-C2B-C3B	2.27	128.92	124.68
23	B	617	CLA	O1D-CGD-CBD	-2.26	119.85	124.48
23	B	609	CLA	CMB-C2B-C3B	2.26	128.91	124.68
25	f	101	BCR	C20-C19-C18	-2.26	120.06	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	z	101	LMG	O2-C2-C3	-2.26	105.12	110.35
32	d	405	DGD	C1E-C2E-C3E	2.26	114.70	110.00
23	B	609	CLA	C11-C12-C13	-2.26	108.62	115.92
23	A	605	CLA	CMB-C2B-C3B	2.26	128.90	124.68
28	J	101	LMG	O8-C28-C29	2.26	118.99	111.91
23	a	604	CLA	C4-C3-C5	2.26	119.07	115.27
23	D	404	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
23	c	503	CLA	O2A-CGA-CBA	2.25	118.98	111.91
25	H	101	BCR	C35-C13-C12	2.25	121.63	118.08
25	h	101	BCR	C1-C6-C7	-2.25	109.41	115.78
23	B	602	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
25	H	101	BCR	C16-C15-C14	-2.25	118.86	123.47
25	b	622	BCR	C1-C6-C7	-2.25	109.41	115.78
23	c	507	CLA	CMB-C2B-C3B	2.25	128.89	124.68
24	a	606	PHO	CMB-C2B-C1B	-2.25	121.60	125.06
23	A	605	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
23	D	403	CLA	CHB-C4A-NA	-2.25	121.40	124.51
23	c	512	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
23	A	608	CLA	O2A-CGA-CBA	2.25	118.96	111.91
23	B	610	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
25	c	522	BCR	C40-C30-C25	2.24	113.94	110.30
23	a	607	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
23	C	509	CLA	CED-O2D-CGD	2.24	121.01	115.94
23	B	613	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
23	B	607[B]	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
23	b	618	CLA	CHA-C1A-NA	-2.24	121.27	126.40
23	C	512	CLA	CHA-C1A-NA	-2.24	121.28	126.40
23	B	607[B]	CLA	O1D-CGD-CBD	-2.24	119.91	124.48
23	a	605	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
23	c	505	CLA	C1-O2A-CGA	2.23	122.31	116.44
32	C	518	DGD	O1G-C1A-O1A	-2.23	117.95	123.59
23	B	603	CLA	O2A-CGA-CBA	2.23	118.92	111.91
23	b	607	CLA	C1-O2A-CGA	2.23	122.30	116.44
23	b	609[A]	CLA	CHA-C1A-NA	-2.23	121.29	126.40
23	C	504	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
23	C	505	CLA	CHA-C1A-NA	-2.22	121.30	126.40
25	b	621	BCR	C8-C9-C10	-2.22	115.53	118.94
23	c	513	CLA	C1-O2A-CGA	2.22	122.28	116.44
25	c	522	BCR	C37-C22-C21	-2.22	119.81	122.92
25	C	515	BCR	C23-C22-C21	-2.22	115.53	118.94
31	B	622	LHG	O7-C7-O9	-2.22	118.33	123.70
27	A	611	SQD	O48-C23-C24	2.22	118.88	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	619	BCR	C31-C1-C6	-2.22	106.70	110.30
28	j	101	LMG	O8-C28-C29	2.22	118.87	111.91
23	B	616	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
23	b	608	CLA	O2D-CGD-O1D	-2.22	119.51	123.84
23	b	608	CLA	O1D-CGD-CBD	-2.21	119.95	124.48
23	C	511	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
27	X	101	SQD	O48-C23-O10	-2.21	118.01	123.59
23	B	607[B]	CLA	CHA-C1A-NA	-2.21	121.33	126.40
27	a	610	SQD	O48-C23-C24	2.21	118.84	111.91
25	T	101	BCR	C33-C5-C4	-2.21	109.37	113.62
23	b	609[A]	CLA	O2A-CGA-CBA	2.21	118.84	111.91
23	B	614	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
23	B	616	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
23	b	612	CLA	O2A-CGA-CBA	2.21	118.83	111.91
27	x	101	SQD	O48-C23-O10	-2.21	118.03	123.59
23	D	402	CLA	CMB-C2B-C3B	2.20	128.80	124.68
25	C	515	BCR	C11-C12-C13	-2.20	120.22	126.42
25	c	515	BCR	C1-C6-C7	-2.20	109.54	115.78
25	A	609	BCR	C20-C19-C18	-2.20	120.23	126.42
23	B	606	CLA	C4A-NA-C1A	-2.20	105.72	106.71
25	B	618	BCR	C36-C18-C17	-2.20	119.84	122.92
23	C	508	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
25	B	619	BCR	C10-C11-C12	-2.20	116.35	123.22
25	B	620	BCR	C23-C22-C21	-2.20	115.57	118.94
31	D	407	LHG	C5-O7-C7	-2.20	112.38	117.79
23	b	604	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
23	b	615	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
23	A	608	CLA	CED-O2D-CGD	2.20	120.90	115.94
23	B	614	CLA	C1-C2-C3	-2.20	122.25	126.04
23	c	507	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
23	c	510	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
31	a	614	LHG	C5-O7-C7	-2.19	112.39	117.79
33	e	102	HEM	CMC-C2C-C3C	2.19	128.78	124.68
23	D	404	CLA	O2A-CGA-CBA	2.19	118.79	111.91
23	C	508	CLA	CHA-C1A-NA	-2.19	121.38	126.40
31	d	406	LHG	C5-O7-C7	-2.19	112.40	117.79
25	H	101	BCR	C37-C22-C21	-2.19	119.86	122.92
25	T	101	BCR	C35-C13-C14	-2.19	119.86	122.92
25	A	609	BCR	C37-C22-C21	-2.19	119.86	122.92
23	d	402	CLA	CHA-C1A-NA	-2.19	121.39	126.40
23	b	611	CLA	CMB-C2B-C3B	2.18	128.77	124.68
27	A	611	SQD	O48-C23-O10	-2.18	118.08	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	610	SQD	O48-C23-O10	-2.18	118.08	123.59
23	C	502	CLA	CHA-C1A-NA	-2.18	121.39	126.40
23	b	616	CLA	C1-C2-C3	-2.18	122.27	126.04
23	B	615	CLA	CHA-C1A-NA	-2.18	121.40	126.40
23	b	619	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
23	C	507	CLA	C1-O2A-CGA	2.18	122.16	116.44
25	b	621	BCR	C11-C12-C13	-2.18	120.29	126.42
23	C	502	CLA	O2A-CGA-CBA	2.18	118.75	111.91
23	C	512	CLA	CMB-C2B-C3B	2.18	128.75	124.68
25	c	516	BCR	C30-C25-C24	-2.18	109.62	115.78
23	a	604	CLA	CMB-C2B-C3B	2.18	128.75	124.68
23	B	613	CLA	CHA-C1A-NA	-2.18	121.42	126.40
23	c	511	CLA	CHA-C1A-NA	-2.18	121.42	126.40
23	C	507	CLA	CHB-C4A-NA	-2.17	121.51	124.51
23	b	616	CLA	CHA-C1A-NA	-2.17	121.42	126.40
25	A	609	BCR	C35-C13-C14	-2.17	119.88	122.92
23	a	607	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
25	c	515	BCR	C30-C25-C24	-2.17	109.64	115.78
25	b	622	BCR	C20-C19-C18	-2.17	120.33	126.42
25	b	621	BCR	C2-C3-C4	2.17	116.22	111.38
25	B	620	BCR	C34-C9-C10	-2.17	119.89	122.92
32	c	517	DGD	O6D-C5D-C6D	2.16	111.03	106.67
23	c	509	CLA	CHA-C1A-NA	-2.16	121.44	126.40
23	B	604	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
23	C	501	CLA	C4-C3-C5	2.16	118.91	115.27
23	c	502	CLA	C4-C3-C5	2.16	118.91	115.27
23	b	611	CLA	O2A-CGA-CBA	2.16	118.68	111.91
23	a	607	CLA	C1-O2A-CGA	2.16	122.11	116.44
25	k	101	BCR	C7-C8-C9	-2.16	122.98	126.23
25	a	608	BCR	C34-C9-C10	-2.16	119.90	122.92
23	c	505	CLA	CHA-C1A-NA	-2.16	121.46	126.40
25	c	516	BCR	C1-C6-C7	-2.16	109.68	115.78
26	A	610	PL9	C20-C19-C21	-2.15	111.65	115.27
23	c	506	CLA	CMD-C2D-C3D	2.15	128.70	124.68
23	b	619	CLA	C4A-NA-C1A	-2.15	105.74	106.71
25	b	622	BCR	C19-C18-C17	-2.15	115.64	118.94
25	K	101	BCR	C31-C1-C6	-2.15	106.81	110.30
23	B	612	CLA	O2A-CGA-CBA	2.15	118.65	111.91
25	f	101	BCR	C28-C27-C26	-2.14	110.25	114.08
25	T	101	BCR	C31-C1-C6	-2.14	106.82	110.30
23	B	607[B]	CLA	O2A-CGA-CBA	2.14	118.63	111.91
31	L	101	LHG	O8-C23-C24	2.14	118.63	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	C1-O2A-CGA	2.14	122.06	116.44
23	B	614	CLA	O2A-CGA-CBA	2.14	118.63	111.91
23	B	602	CLA	CHA-C1A-NA	-2.14	121.50	126.40
23	c	513	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
23	b	612	CLA	C4A-NA-C1A	-2.14	105.75	106.71
23	B	615	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
23	C	510	CLA	O2A-CGA-CBA	2.14	118.61	111.91
25	h	101	BCR	C30-C25-C24	-2.14	109.73	115.78
23	B	603	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
25	k	101	BCR	C11-C12-C13	-2.14	120.42	126.42
23	b	613	CLA	CED-O2D-CGD	2.14	120.77	115.94
23	b	616	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
25	C	515	BCR	C19-C18-C17	2.13	122.22	118.94
23	c	508	CLA	CHB-C4A-NA	-2.13	121.56	124.51
23	c	514	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
23	b	610	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
25	B	620	BCR	C34-C9-C8	2.13	121.43	118.08
23	B	603	CLA	CHA-C1A-NA	-2.13	121.52	126.40
23	c	504	CLA	O2A-CGA-CBA	2.13	118.59	111.91
23	b	609[B]	CLA	O2A-CGA-CBA	2.13	118.58	111.91
23	c	507	CLA	CED-O2D-CGD	2.13	120.75	115.94
23	a	605	CLA	CMB-C2B-C3B	2.13	128.66	124.68
23	B	608	CLA	CMB-C2B-C1B	-2.13	125.20	128.46
27	b	602	SQD	O47-C7-O49	-2.13	118.57	123.70
25	a	608	BCR	C35-C13-C14	-2.12	119.95	122.92
25	c	522	BCR	C11-C12-C13	-2.12	120.45	126.42
23	C	505	CLA	CMD-C2D-C3D	2.12	128.65	124.68
23	b	608	CLA	CED-O2D-CGD	2.12	120.74	115.94
23	c	508	CLA	C1-O2A-CGA	2.12	122.01	116.44
28	a	611	LMG	O8-C28-C29	2.12	118.56	111.91
23	c	505	CLA	C7-C6-C5	-2.12	107.60	113.36
32	d	405	DGD	C3E-C4E-C5E	2.12	114.02	110.24
27	B	623	SQD	O47-C7-O49	-2.12	118.58	123.70
25	b	620	BCR	C37-C22-C23	-2.12	114.74	118.08
25	c	515	BCR	C36-C18-C17	-2.11	119.96	122.92
32	C	517	DGD	C1E-O6E-C5E	-2.11	109.54	113.69
27	B	623	SQD	O5-C1-C2	-2.11	105.88	110.35
23	b	619	CLA	C4-C3-C5	2.11	118.82	115.27
32	h	102	DGD	O6E-C5E-C6E	2.11	111.69	106.44
32	C	517	DGD	C4E-C3E-C2E	2.11	114.51	110.82
23	C	504	CLA	C7-C6-C5	-2.11	107.63	113.36
25	F	101	BCR	C30-C25-C24	-2.11	109.81	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	608	BCR	C34-C9-C8	2.11	121.40	118.08
27	b	602	SQD	O5-C1-C2	-2.11	105.89	110.35
28	j	101	LMG	C6-C5-C4	-2.11	108.07	113.00
23	B	610	CLA	CMB-C2B-C1B	-2.10	125.23	128.46
23	C	504	CLA	CHA-C1A-NA	-2.10	121.58	126.40
23	C	501	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
23	C	513	CLA	CED-O2D-CGD	2.10	120.69	115.94
23	b	612	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
23	c	502	CLA	C1-C2-C3	-2.10	122.41	126.04
23	B	610	CLA	CHA-C1A-NA	-2.10	121.59	126.40
23	B	603	CLA	CHB-C4A-NA	-2.10	121.61	124.51
23	B	617	CLA	C4-C3-C5	2.10	118.80	115.27
23	b	619	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
32	C	517	DGD	C3E-C4E-C5E	2.10	113.98	110.24
23	b	612	CLA	CHB-C4A-NA	-2.10	121.61	124.51
23	c	507	CLA	CHA-C1A-NA	-2.10	121.60	126.40
23	C	505	CLA	CHB-C4A-NA	-2.10	121.61	124.51
31	l	101	LHG	O8-C23-C24	2.10	118.49	111.91
23	b	611	CLA	C11-C10-C8	-2.10	109.14	115.92
33	V	202	HEM	CAD-CBD-CGD	-2.10	109.16	112.67
23	C	508	CLA	CMB-C2B-C3B	2.09	128.60	124.68
23	C	509	CLA	C4-C3-C5	2.09	118.79	115.27
26	d	404	PL9	C25-C24-C26	-2.09	111.75	115.27
28	C	520	LMG	O6-C5-C4	2.09	113.49	109.69
25	b	622	BCR	C30-C25-C24	-2.09	109.86	115.78
23	C	501	CLA	C1-C2-C3	-2.09	122.44	126.04
23	B	604	CLA	O2D-CGD-O1D	-2.08	119.76	123.84
25	C	514	BCR	C20-C19-C18	-2.08	120.56	126.42
23	a	604	CLA	CHA-C1A-NA	-2.08	121.63	126.40
25	b	622	BCR	C34-C9-C8	2.08	121.36	118.08
23	c	505	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
23	B	606	CLA	CED-O2D-CGD	2.08	120.64	115.94
23	c	510	CLA	C4-C3-C5	2.08	118.77	115.27
23	B	609	CLA	CHA-C1A-NA	-2.08	121.64	126.40
23	B	611	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
23	a	604	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
23	b	618	CLA	C11-C10-C8	-2.08	109.20	115.92
23	D	403	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
23	C	510	CLA	C4-C3-C5	2.08	118.77	115.27
23	b	610	CLA	CED-O2D-CGD	2.08	120.63	115.94
23	b	605	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
23	B	609	CLA	C11-C10-C8	-2.07	109.21	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	501	CLA	CMB-C2B-C3B	2.07	128.56	124.68
27	X	101	SQD	C3-C4-C5	2.07	113.94	110.24
23	B	610	CLA	C1-O2A-CGA	2.07	121.88	116.44
23	b	614	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
28	A	612	LMG	O8-C28-C29	2.07	118.41	111.91
23	A	608	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
23	B	616	CLA	C11-C10-C8	-2.07	109.23	115.92
23	c	506	CLA	CHA-C1A-NA	-2.07	121.66	126.40
32	c	517	DGD	C2G-O2G-C1B	-2.06	112.71	117.79
23	c	513	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
27	x	101	SQD	C3-C4-C5	2.06	113.92	110.24
25	t	101	BCR	C16-C15-C14	-2.06	119.25	123.47
23	C	513	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
25	C	514	BCR	C3-C4-C5	-2.06	110.39	114.08
23	C	512	CLA	C1-O2A-CGA	2.06	121.85	116.44
31	E	101	LHG	O7-C7-O9	-2.06	118.72	123.70
23	a	607	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
32	c	518	DGD	O6E-C5E-C6E	2.06	111.55	106.44
23	c	504	CLA	O2D-CGD-O1D	-2.06	119.82	123.84
25	C	515	BCR	C12-C13-C14	-2.06	115.79	118.94
23	c	507	CLA	CBA-CAA-C2A	-2.05	107.80	113.86
25	B	618	BCR	C29-C28-C27	2.05	115.97	111.38
28	z	101	LMG	C4-C3-C2	2.05	114.41	110.82
25	k	101	BCR	C10-C11-C12	-2.05	116.82	123.22
23	b	612	CLA	CED-O2D-CGD	2.05	120.57	115.94
23	C	504	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
23	b	617	CLA	CHA-C1A-NA	-2.05	121.71	126.40
23	c	511	CLA	C4-C3-C5	2.05	118.71	115.27
23	a	613	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
23	b	610	CLA	CHA-C1A-NA	-2.04	121.72	126.40
23	b	606	CLA	C1-O2A-CGA	2.04	121.81	116.44
27	A	611	SQD	O5-C1-C2	-2.04	106.02	110.35
23	C	506	CLA	CHA-C1A-NA	-2.04	121.72	126.40
23	c	504	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
23	b	612	CLA	CHA-C1A-NA	-2.04	121.72	126.40
23	B	608	CLA	C1-O2A-CGA	2.04	121.80	116.44
25	b	621	BCR	C20-C19-C18	-2.04	120.69	126.42
23	c	502	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
23	b	604	CLA	C1-O2A-CGA	2.04	121.78	116.44
25	T	101	BCR	C16-C15-C14	-2.04	119.31	123.47
25	H	101	BCR	C30-C25-C24	-2.03	110.03	115.78
23	d	403	CLA	C6-C7-C8	-2.03	109.35	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	518	DGD	C3G-C2G-C1G	-2.03	106.98	111.79
32	H	102	DGD	O6E-C5E-C6E	2.03	111.49	106.44
23	B	602	CLA	CED-O2D-CGD	2.03	120.53	115.94
23	B	608	CLA	CHA-C1A-NA	-2.03	121.75	126.40
23	B	614	CLA	CHA-C1A-NA	-2.02	121.77	126.40
23	c	510	CLA	CHA-C1A-NA	-2.02	121.77	126.40
23	D	404	CLA	C6-C7-C8	-2.02	109.38	115.92
23	c	504	CLA	CHA-C1A-NA	-2.02	121.77	126.40
25	c	515	BCR	C35-C13-C12	2.02	121.26	118.08
23	D	404	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
23	A	606	CLA	CMB-C2B-C3B	2.02	128.45	124.68
23	C	513	CLA	C1-O2A-CGA	2.01	121.73	116.44
26	A	610	PL9	C35-C34-C36	-2.01	111.88	115.27
23	a	613	CLA	CMC-C2C-C3C	2.01	128.74	124.94
31	D	408	LHG	O8-C23-O10	-2.01	118.51	123.59
27	a	610	SQD	O5-C1-C2	-2.01	106.09	110.35
23	B	608	CLA	O2A-CGA-CBA	2.01	118.22	111.91
23	b	604	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
25	t	101	BCR	C3-C4-C5	-2.01	110.49	114.08
23	c	506	CLA	C4A-NA-C1A	-2.01	105.80	106.71
23	c	502	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
23	B	613	CLA	CHB-C4A-NA	-2.00	121.74	124.51
25	c	516	BCR	C31-C1-C6	-2.00	107.05	110.30
28	A	612	LMG	O1-C1-C2	2.00	111.43	108.30
25	B	619	BCR	C23-C22-C21	-2.00	115.87	118.94
25	b	621	BCR	C33-C5-C4	-2.00	109.77	113.62

All (72) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	605	CLA	ND
23	A	606	CLA	ND
23	A	608	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607[A]	CLA	ND
23	B	607[B]	CLA	ND
23	B	608	CLA	ND
23	B	609	CLA	ND

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Mol	Chain	Res	Type	Atom
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	B	617	CLA	ND
23	C	501	CLA	ND
23	C	502	CLA	ND
23	C	503	CLA	ND
23	C	504	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	D	402	CLA	ND
23	D	403	CLA	ND
23	D	404	CLA	ND
23	a	604	CLA	ND
23	a	605	CLA	ND
23	a	607	CLA	ND
23	a	613	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	608	CLA	ND
23	b	609[A]	CLA	ND
23	b	609[B]	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND

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Mol	Chain	Res	Type	Atom
23	b	617	CLA	ND
23	b	618	CLA	ND
23	b	619	CLA	ND
23	c	502	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	c	514	CLA	ND
23	d	402	CLA	ND
23	d	403	CLA	ND

All (2015) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	606	CLA	CHA-CBD-CGD-O1D
23	A	606	CLA	CHA-CBD-CGD-O2D
23	B	602	CLA	CHA-CBD-CGD-O1D
23	B	602	CLA	CHA-CBD-CGD-O2D
23	B	603	CLA	CHA-CBD-CGD-O1D
23	B	603	CLA	CHA-CBD-CGD-O2D
23	B	605	CLA	C2C-C3C-CAC-CBC
23	B	606	CLA	C2-C3-C5-C6
23	B	606	CLA	C4-C3-C5-C6
23	B	607[A]	CLA	CHA-CBD-CGD-O2D
23	B	607[B]	CLA	CHA-CBD-CGD-O2D
23	B	608	CLA	C1A-C2A-CAA-CBA
23	B	615	CLA	CHA-CBD-CGD-O1D
23	B	615	CLA	CAD-CBD-CGD-O1D
23	B	615	CLA	CAD-CBD-CGD-O2D
23	C	502	CLA	CHA-CBD-CGD-O1D
23	D	402	CLA	CHA-CBD-CGD-O2D
23	a	613	CLA	C2C-C3C-CAC-CBC
23	a	613	CLA	CHA-CBD-CGD-O1D
23	a	613	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	b	604	CLA	CHA-CBD-CGD-O1D
23	b	604	CLA	CHA-CBD-CGD-O2D
23	b	605	CLA	CHA-CBD-CGD-O1D
23	b	605	CLA	CHA-CBD-CGD-O2D
23	b	607	CLA	C2C-C3C-CAC-CBC
23	b	608	CLA	C2-C3-C5-C6
23	b	608	CLA	C4-C3-C5-C6
23	b	609[A]	CLA	CHA-CBD-CGD-O2D
23	b	609[B]	CLA	CHA-CBD-CGD-O2D
23	b	610	CLA	C1A-C2A-CAA-CBA
23	b	610	CLA	C3A-C2A-CAA-CBA
23	b	617	CLA	CHA-CBD-CGD-O1D
23	b	617	CLA	CAD-CBD-CGD-O1D
23	b	617	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O1D
25	A	609	BCR	C1-C6-C7-C8
25	A	609	BCR	C11-C10-C9-C8
25	A	609	BCR	C11-C12-C13-C14
25	A	609	BCR	C12-C13-C14-C15
25	A	609	BCR	C13-C14-C15-C16
25	A	609	BCR	C14-C15-C16-C17
25	A	609	BCR	C16-C17-C18-C36
25	A	609	BCR	C36-C18-C19-C20
25	A	609	BCR	C18-C19-C20-C21
25	A	609	BCR	C20-C21-C22-C37
25	A	609	BCR	C37-C22-C23-C24
25	A	609	BCR	C23-C24-C25-C30
25	B	618	BCR	C10-C11-C12-C13
25	B	618	BCR	C11-C12-C13-C14
25	B	618	BCR	C11-C12-C13-C35
25	B	618	BCR	C12-C13-C14-C15
25	B	618	BCR	C35-C13-C14-C15
25	B	618	BCR	C16-C17-C18-C19
25	B	618	BCR	C16-C17-C18-C36
25	B	618	BCR	C17-C18-C19-C20
25	B	618	BCR	C36-C18-C19-C20
25	B	618	BCR	C18-C19-C20-C21
25	B	618	BCR	C20-C21-C22-C23
25	B	618	BCR	C21-C22-C23-C24
25	B	618	BCR	C22-C23-C24-C25
25	B	619	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
25	B	619	BCR	C11-C10-C9-C34
25	B	619	BCR	C10-C11-C12-C13
25	B	619	BCR	C11-C12-C13-C35
25	B	619	BCR	C12-C13-C14-C15
25	B	619	BCR	C14-C15-C16-C17
25	B	619	BCR	C16-C17-C18-C19
25	B	619	BCR	C16-C17-C18-C36
25	B	619	BCR	C36-C18-C19-C20
25	B	619	BCR	C20-C21-C22-C23
25	B	619	BCR	C20-C21-C22-C37
25	B	620	BCR	C7-C8-C9-C10
25	B	620	BCR	C11-C10-C9-C34
25	B	620	BCR	C14-C15-C16-C17
25	B	620	BCR	C16-C17-C18-C19
25	B	620	BCR	C16-C17-C18-C36
25	B	620	BCR	C17-C18-C19-C20
25	B	620	BCR	C36-C18-C19-C20
25	B	620	BCR	C18-C19-C20-C21
25	B	620	BCR	C20-C21-C22-C23
25	B	620	BCR	C20-C21-C22-C37
25	C	514	BCR	C6-C7-C8-C9
25	C	514	BCR	C11-C10-C9-C34
25	C	514	BCR	C10-C11-C12-C13
25	C	514	BCR	C12-C13-C14-C15
25	C	514	BCR	C16-C17-C18-C19
25	C	514	BCR	C16-C17-C18-C36
25	C	514	BCR	C17-C18-C19-C20
25	C	514	BCR	C18-C19-C20-C21
25	C	514	BCR	C19-C20-C21-C22
25	C	514	BCR	C20-C21-C22-C23
25	C	514	BCR	C20-C21-C22-C37
25	C	514	BCR	C22-C23-C24-C25
25	C	514	BCR	C23-C24-C25-C26
25	C	515	BCR	C6-C7-C8-C9
25	C	515	BCR	C7-C8-C9-C34
25	C	515	BCR	C11-C12-C13-C35
25	C	515	BCR	C12-C13-C14-C15
25	C	515	BCR	C35-C13-C14-C15
25	C	515	BCR	C14-C15-C16-C17
25	C	515	BCR	C17-C18-C19-C20
25	C	515	BCR	C18-C19-C20-C21
25	C	515	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
25	C	515	BCR	C22-C23-C24-C25
25	C	521	BCR	C5-C6-C7-C8
25	C	521	BCR	C10-C11-C12-C13
25	C	521	BCR	C11-C12-C13-C14
25	C	521	BCR	C11-C12-C13-C35
25	C	521	BCR	C14-C15-C16-C17
25	C	521	BCR	C17-C18-C19-C20
25	C	521	BCR	C20-C21-C22-C37
25	C	521	BCR	C21-C22-C23-C24
25	F	101	BCR	C6-C7-C8-C9
25	F	101	BCR	C10-C11-C12-C13
25	F	101	BCR	C11-C12-C13-C35
25	F	101	BCR	C12-C13-C14-C15
25	F	101	BCR	C35-C13-C14-C15
25	F	101	BCR	C14-C15-C16-C17
25	F	101	BCR	C16-C17-C18-C36
25	F	101	BCR	C17-C18-C19-C20
25	F	101	BCR	C36-C18-C19-C20
25	F	101	BCR	C18-C19-C20-C21
25	F	101	BCR	C20-C21-C22-C23
25	F	101	BCR	C20-C21-C22-C37
25	F	101	BCR	C21-C22-C23-C24
25	F	101	BCR	C37-C22-C23-C24
25	F	101	BCR	C22-C23-C24-C25
25	F	101	BCR	C23-C24-C25-C26
25	H	101	BCR	C6-C7-C8-C9
25	H	101	BCR	C7-C8-C9-C10
25	H	101	BCR	C11-C10-C9-C8
25	H	101	BCR	C10-C11-C12-C13
25	H	101	BCR	C14-C15-C16-C17
25	H	101	BCR	C16-C17-C18-C19
25	H	101	BCR	C16-C17-C18-C36
25	H	101	BCR	C17-C18-C19-C20
25	H	101	BCR	C36-C18-C19-C20
25	H	101	BCR	C18-C19-C20-C21
25	H	101	BCR	C20-C21-C22-C23
25	H	101	BCR	C20-C21-C22-C37
25	H	101	BCR	C21-C22-C23-C24
25	H	101	BCR	C37-C22-C23-C24
25	H	101	BCR	C22-C23-C24-C25
25	K	101	BCR	C1-C6-C7-C8
25	K	101	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	K	101	BCR	C7-C8-C9-C34
25	K	101	BCR	C11-C10-C9-C8
25	K	101	BCR	C10-C11-C12-C13
25	K	101	BCR	C11-C12-C13-C35
25	K	101	BCR	C12-C13-C14-C15
25	K	101	BCR	C14-C15-C16-C17
25	K	101	BCR	C16-C17-C18-C19
25	K	101	BCR	C16-C17-C18-C36
25	K	101	BCR	C20-C21-C22-C37
25	K	101	BCR	C37-C22-C23-C24
25	K	101	BCR	C22-C23-C24-C25
25	T	101	BCR	C6-C7-C8-C9
25	T	101	BCR	C7-C8-C9-C10
25	T	101	BCR	C11-C10-C9-C8
25	T	101	BCR	C11-C10-C9-C34
25	T	101	BCR	C10-C11-C12-C13
25	T	101	BCR	C12-C13-C14-C15
25	T	101	BCR	C14-C15-C16-C17
25	T	101	BCR	C15-C16-C17-C18
25	T	101	BCR	C18-C19-C20-C21
25	T	101	BCR	C19-C20-C21-C22
25	T	101	BCR	C20-C21-C22-C23
25	T	101	BCR	C37-C22-C23-C24
25	T	101	BCR	C22-C23-C24-C25
25	T	101	BCR	C23-C24-C25-C26
25	a	608	BCR	C9-C10-C11-C12
25	a	608	BCR	C10-C11-C12-C13
25	a	608	BCR	C11-C12-C13-C35
25	a	608	BCR	C14-C15-C16-C17
25	a	608	BCR	C36-C18-C19-C20
25	a	608	BCR	C18-C19-C20-C21
25	a	608	BCR	C20-C21-C22-C37
25	a	608	BCR	C23-C24-C25-C30
25	b	620	BCR	C9-C10-C11-C12
25	b	620	BCR	C10-C11-C12-C13
25	b	620	BCR	C11-C12-C13-C14
25	b	620	BCR	C12-C13-C14-C15
25	b	620	BCR	C35-C13-C14-C15
25	b	620	BCR	C17-C18-C19-C20
25	b	620	BCR	C18-C19-C20-C21
25	b	620	BCR	C22-C23-C24-C25
25	b	621	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	b	621	BCR	C11-C12-C13-C35
25	b	621	BCR	C12-C13-C14-C15
25	b	621	BCR	C14-C15-C16-C17
25	b	621	BCR	C16-C17-C18-C19
25	b	621	BCR	C16-C17-C18-C36
25	b	621	BCR	C17-C18-C19-C20
25	b	621	BCR	C36-C18-C19-C20
25	b	621	BCR	C18-C19-C20-C21
25	b	621	BCR	C20-C21-C22-C23
25	b	621	BCR	C20-C21-C22-C37
25	b	621	BCR	C21-C22-C23-C24
25	b	622	BCR	C6-C7-C8-C9
25	b	622	BCR	C11-C10-C9-C34
25	b	622	BCR	C12-C13-C14-C15
25	b	622	BCR	C35-C13-C14-C15
25	b	622	BCR	C14-C15-C16-C17
25	b	622	BCR	C16-C17-C18-C19
25	b	622	BCR	C16-C17-C18-C36
25	b	622	BCR	C17-C18-C19-C20
25	b	622	BCR	C36-C18-C19-C20
25	b	622	BCR	C18-C19-C20-C21
25	b	622	BCR	C20-C21-C22-C23
25	b	622	BCR	C20-C21-C22-C37
25	b	622	BCR	C37-C22-C23-C24
25	c	515	BCR	C5-C6-C7-C8
25	c	515	BCR	C7-C8-C9-C10
25	c	515	BCR	C7-C8-C9-C34
25	c	515	BCR	C11-C10-C9-C8
25	c	515	BCR	C10-C11-C12-C13
25	c	515	BCR	C12-C13-C14-C15
25	c	515	BCR	C14-C15-C16-C17
25	c	515	BCR	C15-C16-C17-C18
25	c	515	BCR	C16-C17-C18-C19
25	c	515	BCR	C16-C17-C18-C36
25	c	515	BCR	C17-C18-C19-C20
25	c	515	BCR	C36-C18-C19-C20
25	c	515	BCR	C18-C19-C20-C21
25	c	515	BCR	C19-C20-C21-C22
25	c	515	BCR	C20-C21-C22-C23
25	c	515	BCR	C20-C21-C22-C37
25	c	515	BCR	C23-C24-C25-C26
25	c	516	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	c	516	BCR	C7-C8-C9-C10
25	c	516	BCR	C10-C11-C12-C13
25	c	516	BCR	C11-C12-C13-C35
25	c	516	BCR	C12-C13-C14-C15
25	c	516	BCR	C35-C13-C14-C15
25	c	516	BCR	C13-C14-C15-C16
25	c	516	BCR	C14-C15-C16-C17
25	c	516	BCR	C36-C18-C19-C20
25	c	516	BCR	C18-C19-C20-C21
25	c	516	BCR	C20-C21-C22-C23
25	c	516	BCR	C21-C22-C23-C24
25	c	516	BCR	C22-C23-C24-C25
25	c	522	BCR	C5-C6-C7-C8
25	c	522	BCR	C6-C7-C8-C9
25	c	522	BCR	C7-C8-C9-C34
25	c	522	BCR	C11-C10-C9-C8
25	c	522	BCR	C10-C11-C12-C13
25	c	522	BCR	C13-C14-C15-C16
25	c	522	BCR	C14-C15-C16-C17
25	c	522	BCR	C17-C18-C19-C20
25	c	522	BCR	C18-C19-C20-C21
25	c	522	BCR	C20-C21-C22-C37
25	c	522	BCR	C21-C22-C23-C24
25	c	522	BCR	C23-C24-C25-C30
25	f	101	BCR	C6-C7-C8-C9
25	f	101	BCR	C7-C8-C9-C34
25	f	101	BCR	C10-C11-C12-C13
25	f	101	BCR	C11-C12-C13-C14
25	f	101	BCR	C12-C13-C14-C15
25	f	101	BCR	C35-C13-C14-C15
25	f	101	BCR	C13-C14-C15-C16
25	f	101	BCR	C14-C15-C16-C17
25	f	101	BCR	C16-C17-C18-C19
25	f	101	BCR	C16-C17-C18-C36
25	f	101	BCR	C17-C18-C19-C20
25	f	101	BCR	C20-C21-C22-C37
25	f	101	BCR	C21-C22-C23-C24
25	f	101	BCR	C22-C23-C24-C25
25	f	101	BCR	C23-C24-C25-C26
25	h	101	BCR	C6-C7-C8-C9
25	h	101	BCR	C7-C8-C9-C34
25	h	101	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
25	h	101	BCR	C10-C11-C12-C13
25	h	101	BCR	C12-C13-C14-C15
25	h	101	BCR	C14-C15-C16-C17
25	h	101	BCR	C16-C17-C18-C19
25	h	101	BCR	C16-C17-C18-C36
25	h	101	BCR	C36-C18-C19-C20
25	h	101	BCR	C19-C20-C21-C22
25	h	101	BCR	C20-C21-C22-C23
25	h	101	BCR	C20-C21-C22-C37
25	h	101	BCR	C21-C22-C23-C24
25	h	101	BCR	C37-C22-C23-C24
25	h	101	BCR	C22-C23-C24-C25
25	k	101	BCR	C7-C8-C9-C34
25	k	101	BCR	C11-C10-C9-C8
25	k	101	BCR	C10-C11-C12-C13
25	k	101	BCR	C11-C12-C13-C35
25	k	101	BCR	C12-C13-C14-C15
25	k	101	BCR	C15-C16-C17-C18
25	k	101	BCR	C16-C17-C18-C19
25	k	101	BCR	C16-C17-C18-C36
25	k	101	BCR	C20-C21-C22-C37
25	k	101	BCR	C23-C24-C25-C30
25	t	101	BCR	C6-C7-C8-C9
25	t	101	BCR	C11-C10-C9-C8
25	t	101	BCR	C10-C11-C12-C13
25	t	101	BCR	C11-C12-C13-C14
25	t	101	BCR	C12-C13-C14-C15
25	t	101	BCR	C14-C15-C16-C17
25	t	101	BCR	C15-C16-C17-C18
25	t	101	BCR	C16-C17-C18-C36
25	t	101	BCR	C36-C18-C19-C20
25	t	101	BCR	C18-C19-C20-C21
25	t	101	BCR	C37-C22-C23-C24
25	t	101	BCR	C22-C23-C24-C25
26	A	610	PL9	C7-C8-C9-C10
26	A	610	PL9	C12-C11-C9-C10
26	A	610	PL9	C9-C11-C12-C13
26	A	610	PL9	C12-C13-C14-C15
26	A	610	PL9	C17-C18-C19-C20
26	A	610	PL9	C19-C21-C22-C23
26	A	610	PL9	C22-C23-C24-C25
26	A	610	PL9	C25-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
26	A	610	PL9	C32-C33-C34-C35
26	D	405	PL9	C7-C8-C9-C10
26	D	405	PL9	C17-C18-C19-C20
26	D	405	PL9	C22-C23-C24-C25
26	D	405	PL9	C27-C28-C29-C30
26	a	609	PL9	C7-C8-C9-C10
26	a	609	PL9	C12-C11-C9-C10
26	a	609	PL9	C14-C16-C17-C18
26	a	609	PL9	C18-C19-C21-C22
26	a	609	PL9	C19-C21-C22-C23
26	a	609	PL9	C25-C24-C26-C27
26	a	609	PL9	C24-C26-C27-C28
26	a	609	PL9	C32-C33-C34-C35
26	d	404	PL9	C17-C18-C19-C20
26	d	404	PL9	C22-C23-C24-C25
26	d	404	PL9	C27-C28-C29-C30
27	B	623	SQD	O5-C1-O6-C44
27	B	623	SQD	C8-C7-O47-C45
27	B	623	SQD	O5-C5-C6-S
27	X	101	SQD	C2-C1-O6-C44
27	X	101	SQD	O5-C1-O6-C44
27	a	612	SQD	O6-C44-C45-O47
27	b	601	SQD	O6-C44-C45-O47
27	b	602	SQD	O5-C1-O6-C44
27	b	602	SQD	C8-C7-O47-C45
27	b	602	SQD	O5-C5-C6-S
27	x	101	SQD	C2-C1-O6-C44
27	x	101	SQD	O5-C1-O6-C44
28	Z	101	LMG	O6-C1-O1-C7
28	Z	101	LMG	O9-C10-O7-C8
28	z	101	LMG	O6-C1-O1-C7
28	z	101	LMG	O1-C7-C8-O7
28	z	101	LMG	O9-C10-O7-C8
31	D	407	LHG	O1-C1-C2-C3
31	D	407	LHG	O2-C2-C3-O3
31	D	407	LHG	C3-O3-P-O5
31	E	101	LHG	C8-C7-O7-C5
31	L	101	LHG	C4-O6-P-O3
31	L	101	LHG	C4-O6-P-O4
31	L	101	LHG	C4-O6-P-O5
31	d	406	LHG	O1-C1-C2-C3
31	d	406	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
31	d	406	LHG	O2-C2-C3-O3
31	d	406	LHG	C3-O3-P-O4
31	d	406	LHG	C3-O3-P-O5
31	e	101	LHG	C8-C7-O7-C5
31	e	101	LHG	O10-C23-O8-C6
31	l	101	LHG	C4-O6-P-O3
31	l	101	LHG	C4-O6-P-O4
31	l	101	LHG	C4-O6-P-O5
32	D	406	DGD	C2B-C1B-O2G-C2G
32	D	406	DGD	C2E-C1E-O5D-C6D
32	D	406	DGD	O6E-C1E-O5D-C6D
32	d	405	DGD	C2B-C1B-O2G-C2G
32	d	405	DGD	C2E-C1E-O5D-C6D
32	d	405	DGD	O6E-C1E-O5D-C6D
33	v	201	HEM	C2D-C3D-CAD-CBD
33	v	201	HEM	C4D-C3D-CAD-CBD
28	Z	101	LMG	C29-C28-O8-C9
28	z	101	LMG	C29-C28-O8-C9
27	X	101	SQD	O10-C23-O48-C46
27	x	101	SQD	O10-C23-O48-C46
31	E	101	LHG	O10-C23-O8-C6
27	X	101	SQD	C24-C23-O48-C46
27	x	101	SQD	C24-C23-O48-C46
31	e	101	LHG	C24-C23-O8-C6
23	B	617	CLA	O1A-CGA-O2A-C1
23	b	619	CLA	O1A-CGA-O2A-C1
23	B	605	CLA	CBD-CGD-O2D-CED
23	B	615	CLA	CBD-CGD-O2D-CED
27	B	623	SQD	O49-C7-O47-C45
27	b	602	SQD	O49-C7-O47-C45
31	E	101	LHG	O9-C7-O7-C5
32	D	406	DGD	O1B-C1B-O2G-C2G
32	d	405	DGD	O1B-C1B-O2G-C2G
23	B	615	CLA	C3-C5-C6-C7
23	b	617	CLA	C3-C5-C6-C7
23	b	619	CLA	CBA-CGA-O2A-C1
31	E	101	LHG	C24-C23-O8-C6
28	Z	101	LMG	O10-C28-O8-C9
28	z	101	LMG	O10-C28-O8-C9
28	Z	101	LMG	C11-C10-O7-C8
28	z	101	LMG	C11-C10-O7-C8
23	b	607	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	A	610	PL9	C18-C19-C21-C22
26	D	405	PL9	C18-C19-C21-C22
26	a	609	PL9	C38-C39-C41-C42
23	B	607[A]	CLA	C2A-CAA-CBA-CGA
23	B	607[B]	CLA	C2A-CAA-CBA-CGA
23	b	609[A]	CLA	C2A-CAA-CBA-CGA
23	b	609[B]	CLA	C2A-CAA-CBA-CGA
23	B	602	CLA	C3-C5-C6-C7
23	b	604	CLA	C3-C5-C6-C7
23	B	617	CLA	CBA-CGA-O2A-C1
26	A	610	PL9	C27-C28-C29-C30
26	A	610	PL9	C37-C38-C39-C40
26	A	610	PL9	C42-C43-C44-C45
26	D	405	PL9	C12-C13-C14-C15
26	D	405	PL9	C32-C33-C34-C35
26	D	405	PL9	C37-C38-C39-C40
26	a	609	PL9	C12-C13-C14-C15
26	a	609	PL9	C22-C23-C24-C25
26	a	609	PL9	C27-C28-C29-C30
26	a	609	PL9	C37-C38-C39-C40
26	a	609	PL9	C42-C43-C44-C45
26	d	404	PL9	C7-C8-C9-C10
26	d	404	PL9	C12-C13-C14-C15
26	d	404	PL9	C32-C33-C34-C35
26	d	404	PL9	C37-C38-C39-C40
26	d	404	PL9	C42-C43-C44-C45
31	e	101	LHG	O9-C7-O7-C5
25	A	609	BCR	C19-C20-C21-C22
25	B	618	BCR	C19-C20-C21-C22
25	B	619	BCR	C13-C14-C15-C16
25	B	620	BCR	C19-C20-C21-C22
25	C	515	BCR	C13-C14-C15-C16
25	C	515	BCR	C15-C16-C17-C18
25	C	515	BCR	C19-C20-C21-C22
25	C	521	BCR	C13-C14-C15-C16
25	F	101	BCR	C13-C14-C15-C16
25	H	101	BCR	C15-C16-C17-C18
25	K	101	BCR	C15-C16-C17-C18
25	T	101	BCR	C13-C14-C15-C16
25	a	608	BCR	C15-C16-C17-C18
25	a	608	BCR	C19-C20-C21-C22
25	b	621	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
25	b	621	BCR	C15-C16-C17-C18
25	b	622	BCR	C15-C16-C17-C18
25	t	101	BCR	C19-C20-C21-C22
23	C	511	CLA	CBD-CGD-O2D-CED
28	j	101	LMG	O6-C5-C6-O5
23	c	514	CLA	CBD-CGD-O2D-CED
25	C	514	BCR	C14-C15-C16-C17
25	k	101	BCR	C14-C15-C16-C17
23	b	608	CLA	O1D-CGD-O2D-CED
28	C	520	LMG	O6-C5-C6-O5
28	J	101	LMG	O6-C5-C6-O5
26	A	610	PL9	C47-C48-C49-C50
26	D	405	PL9	C47-C48-C49-C51
26	a	609	PL9	C47-C48-C49-C50
26	d	404	PL9	C47-C48-C49-C51
28	c	521	LMG	O6-C5-C6-O5
32	c	519	DGD	O1A-C1A-O1G-C1G
32	C	516	DGD	O6D-C1D-O3G-C3G
26	A	610	PL9	C24-C26-C27-C28
26	D	405	PL9	C29-C31-C32-C33
26	D	405	PL9	C39-C41-C42-C43
26	D	405	PL9	C44-C46-C47-C48
26	d	404	PL9	C39-C41-C42-C43
26	d	404	PL9	C44-C46-C47-C48
26	A	610	PL9	C47-C48-C49-C51
26	a	609	PL9	C17-C18-C19-C20
31	D	407	LHG	C1-C2-C3-O3
28	c	521	LMG	C4-C5-C6-O5
23	C	505	CLA	O1A-CGA-O2A-C1
32	C	516	DGD	C2A-C3A-C4A-C5A
25	C	521	BCR	C19-C20-C21-C22
25	F	101	BCR	C19-C20-C21-C22
25	a	608	BCR	C13-C14-C15-C16
32	d	405	DGD	C1B-C2B-C3B-C4B
28	J	101	LMG	C4-C5-C6-O5
32	d	405	DGD	O6E-C5E-C6E-O5E
28	A	612	LMG	C28-C29-C30-C31
28	Z	101	LMG	O1-C7-C8-O7
28	C	520	LMG	C4-C5-C6-O5
23	B	602	CLA	C11-C10-C8-C9
23	C	501	CLA	C11-C12-C13-C14
23	C	502	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	C	504	CLA	C11-C12-C13-C14
23	C	509	CLA	C6-C7-C8-C9
23	b	604	CLA	C11-C10-C8-C9
23	c	502	CLA	C11-C12-C13-C14
23	c	503	CLA	C14-C13-C15-C16
23	c	505	CLA	C11-C12-C13-C14
23	c	510	CLA	C6-C7-C8-C9
25	A	609	BCR	C7-C8-C9-C34
25	B	619	BCR	C37-C22-C23-C24
25	C	514	BCR	C36-C18-C19-C20
25	C	514	BCR	C37-C22-C23-C24
25	H	101	BCR	C11-C12-C13-C35
25	K	101	BCR	C36-C18-C19-C20
25	T	101	BCR	C7-C8-C9-C34
25	c	515	BCR	C37-C22-C23-C24
25	c	516	BCR	C37-C22-C23-C24
25	h	101	BCR	C11-C12-C13-C35
25	k	101	BCR	C36-C18-C19-C20
25	B	619	BCR	C7-C8-C9-C10
25	B	619	BCR	C21-C22-C23-C24
25	C	514	BCR	C21-C22-C23-C24
25	T	101	BCR	C21-C22-C23-C24
25	a	608	BCR	C11-C12-C13-C14
25	b	621	BCR	C7-C8-C9-C10
25	c	515	BCR	C21-C22-C23-C24
25	h	101	BCR	C17-C18-C19-C20
25	k	101	BCR	C17-C18-C19-C20
25	t	101	BCR	C21-C22-C23-C24
28	C	520	LMG	C28-C29-C30-C31
23	A	608	CLA	C10-C11-C12-C13
23	B	616	CLA	C5-C6-C7-C8
23	a	607	CLA	C10-C11-C12-C13
23	b	618	CLA	C5-C6-C7-C8
32	C	517	DGD	O6E-C5E-C6E-O5E
23	A	608	CLA	C13-C15-C16-C17
23	B	602	CLA	C10-C11-C12-C13
23	a	607	CLA	C13-C15-C16-C17
23	b	604	CLA	C10-C11-C12-C13
28	C	519	LMG	C28-C29-C30-C31
31	b	624	LHG	C23-C24-C25-C26
23	B	615	CLA	C5-C6-C7-C8
23	B	615	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	C	509	CLA	C8-C10-C11-C12
23	b	617	CLA	C5-C6-C7-C8
23	b	617	CLA	C10-C11-C12-C13
23	c	510	CLA	C8-C10-C11-C12
31	d	406	LHG	O1-C1-C2-O2
27	B	623	SQD	C7-C8-C9-C10
27	b	602	SQD	C7-C8-C9-C10
28	c	521	LMG	C28-C29-C30-C31
31	B	622	LHG	C23-C24-C25-C26
32	C	517	DGD	C1B-C2B-C3B-C4B
32	D	406	DGD	C1B-C2B-C3B-C4B
32	c	518	DGD	C1B-C2B-C3B-C4B
32	d	405	DGD	C1A-C2A-C3A-C4A
23	B	607[A]	CLA	C13-C15-C16-C17
23	b	609[A]	CLA	C13-C15-C16-C17
28	A	612	LMG	O9-C10-O7-C8
23	C	506	CLA	C5-C6-C7-C8
23	D	404	CLA	C8-C10-C11-C12
23	d	403	CLA	C8-C10-C11-C12
27	a	612	SQD	C23-C24-C25-C26
27	b	601	SQD	C23-C24-C25-C26
28	a	611	LMG	C28-C29-C30-C31
32	D	406	DGD	C1A-C2A-C3A-C4A
23	b	608	CLA	CBD-CGD-O2D-CED
32	d	405	DGD	C4E-C5E-C6E-O5E
23	c	507	CLA	C5-C6-C7-C8
28	A	612	LMG	O10-C28-O8-C9
25	B	618	BCR	C9-C10-C11-C12
25	B	618	BCR	C13-C14-C15-C16
25	C	514	BCR	C13-C14-C15-C16
25	b	621	BCR	C9-C10-C11-C12
25	b	622	BCR	C19-C20-C21-C22
25	c	515	BCR	C13-C14-C15-C16
25	c	516	BCR	C19-C20-C21-C22
23	B	606	CLA	O1D-CGD-O2D-CED
23	B	611	CLA	O1D-CGD-O2D-CED
23	c	504	CLA	O1D-CGD-O2D-CED
23	B	607[A]	CLA	C15-C16-C17-C18
23	D	404	CLA	C10-C11-C12-C13
23	b	609[A]	CLA	C15-C16-C17-C18
23	d	403	CLA	C10-C11-C12-C13
25	c	515	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
32	C	518	DGD	O1A-C1A-O1G-C1G
23	A	606	CLA	C13-C15-C16-C17
23	a	605	CLA	C13-C15-C16-C17
23	B	612	CLA	O1D-CGD-O2D-CED
26	A	610	PL9	C14-C16-C17-C18
26	D	405	PL9	C9-C11-C12-C13
26	a	609	PL9	C9-C11-C12-C13
26	d	404	PL9	C9-C11-C12-C13
26	d	404	PL9	C29-C31-C32-C33
28	Z	101	LMG	C10-C11-C12-C13
28	z	101	LMG	C10-C11-C12-C13
25	A	609	BCR	C10-C11-C12-C13
25	B	619	BCR	C18-C19-C20-C21
25	K	101	BCR	C18-C19-C20-C21
25	b	621	BCR	C10-C11-C12-C13
25	b	622	BCR	C10-C11-C12-C13
25	f	101	BCR	C18-C19-C20-C21
25	h	101	BCR	C18-C19-C20-C21
32	D	406	DGD	O6E-C5E-C6E-O5E
23	C	509	CLA	C13-C15-C16-C17
23	c	510	CLA	C13-C15-C16-C17
28	a	611	LMG	O10-C28-O8-C9
23	A	608	CLA	C15-C16-C17-C18
23	B	612	CLA	C15-C16-C17-C18
23	a	607	CLA	C15-C16-C17-C18
23	b	614	CLA	C15-C16-C17-C18
31	D	407	LHG	C14-C15-C16-C17
28	j	101	LMG	C4-C5-C6-O5
32	C	517	DGD	C4E-C5E-C6E-O5E
23	B	607[B]	CLA	C10-C11-C12-C13
23	B	617	CLA	C10-C11-C12-C13
23	C	501	CLA	C15-C16-C17-C18
23	C	506	CLA	C10-C11-C12-C13
23	b	609[B]	CLA	C10-C11-C12-C13
23	b	619	CLA	C10-C11-C12-C13
23	c	502	CLA	C15-C16-C17-C18
23	c	507	CLA	C10-C11-C12-C13
31	D	407	LHG	C3-O3-P-O6
31	d	406	LHG	C3-O3-P-O6
32	c	517	DGD	O6D-C5D-C6D-O5D
28	c	520	LMG	C28-C29-C30-C31
32	c	517	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
23	A	606	CLA	C16-C17-C18-C20
23	a	605	CLA	C16-C17-C18-C20
32	c	519	DGD	C2A-C1A-O1G-C1G
32	H	102	DGD	C6B-C7B-C8B-C9B
25	B	619	BCR	C15-C16-C17-C18
25	C	521	BCR	C15-C16-C17-C18
25	H	101	BCR	C19-C20-C21-C22
25	b	620	BCR	C19-C20-C21-C22
28	j	101	LMG	C16-C17-C18-C19
31	b	624	LHG	C32-C33-C34-C35
32	C	517	DGD	C3A-C4A-C5A-C6A
28	a	611	LMG	C11-C10-O7-C8
25	A	609	BCR	C35-C13-C14-C15
25	B	618	BCR	C20-C21-C22-C37
25	C	514	BCR	C35-C13-C14-C15
25	H	101	BCR	C11-C10-C9-C34
25	T	101	BCR	C35-C13-C14-C15
25	a	608	BCR	C11-C10-C9-C34
25	a	608	BCR	C16-C17-C18-C36
25	b	620	BCR	C20-C21-C22-C37
25	b	621	BCR	C11-C10-C9-C34
25	c	515	BCR	C11-C10-C9-C34
25	c	515	BCR	C35-C13-C14-C15
25	c	516	BCR	C20-C21-C22-C37
25	h	101	BCR	C11-C10-C9-C34
25	h	101	BCR	C35-C13-C14-C15
25	t	101	BCR	C11-C10-C9-C34
27	A	611	SQD	C11-C12-C13-C14
27	X	101	SQD	C26-C27-C28-C29
27	X	101	SQD	C29-C30-C31-C32
27	X	101	SQD	C34-C35-C36-C37
27	a	610	SQD	C11-C12-C13-C14
27	a	612	SQD	C15-C16-C17-C18
27	b	601	SQD	C15-C16-C17-C18
27	x	101	SQD	C26-C27-C28-C29
27	x	101	SQD	C29-C30-C31-C32
27	x	101	SQD	C34-C35-C36-C37
28	B	621	LMG	C37-C38-C39-C40
28	C	520	LMG	C29-C30-C31-C32
28	a	611	LMG	C34-C35-C36-C37
28	b	623	LMG	C14-C15-C16-C17
28	b	623	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
28	c	520	LMG	C15-C16-C17-C18
28	j	101	LMG	C12-C13-C14-C15
28	j	101	LMG	C14-C15-C16-C17
31	B	622	LHG	C25-C26-C27-C28
31	b	624	LHG	C29-C30-C31-C32
31	l	101	LHG	C12-C13-C14-C15
32	C	517	DGD	CAA-CBA-CCA-CDA
32	c	517	DGD	C8B-C9B-CAB-CBB
32	c	518	DGD	C9A-CAA-CBA-CCA
32	c	518	DGD	CAB-CBB-CCB-CDB
32	c	519	DGD	C9B-CAB-CBB-CCB
23	C	506	CLA	C16-C17-C18-C19
23	c	507	CLA	C16-C17-C18-C19
27	A	611	SQD	C28-C29-C30-C31
27	a	610	SQD	C28-C29-C30-C31
28	A	612	LMG	C12-C13-C14-C15
28	B	621	LMG	C14-C15-C16-C17
28	C	519	LMG	C15-C16-C17-C18
28	J	101	LMG	C14-C15-C16-C17
28	J	101	LMG	C16-C17-C18-C19
28	c	521	LMG	C29-C30-C31-C32
28	c	521	LMG	C31-C32-C33-C34
28	j	101	LMG	C39-C40-C41-C42
31	E	101	LHG	C13-C14-C15-C16
31	E	101	LHG	C15-C16-C17-C18
32	D	406	DGD	C7B-C8B-C9B-CAB
32	c	519	DGD	C2A-C3A-C4A-C5A
32	d	405	DGD	C2A-C3A-C4A-C5A
32	d	405	DGD	CCB-CDB-CEB-CFB
32	h	102	DGD	CBA-CCA-CDA-CEA
28	a	611	LMG	O9-C10-O7-C8
28	B	621	LMG	C32-C33-C34-C35
28	J	101	LMG	C12-C13-C14-C15
32	c	517	DGD	C5B-C6B-C7B-C8B
23	c	506	CLA	O1A-CGA-O2A-C1
27	A	611	SQD	C12-C13-C14-C15
27	A	611	SQD	C15-C16-C17-C18
27	a	610	SQD	C12-C13-C14-C15
27	a	610	SQD	C15-C16-C17-C18
28	A	612	LMG	C15-C16-C17-C18
28	A	612	LMG	C34-C35-C36-C37
28	J	101	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
28	b	623	LMG	C17-C18-C19-C20
31	B	622	LHG	C29-C30-C31-C32
31	e	101	LHG	C14-C15-C16-C17
31	e	101	LHG	C24-C25-C26-C27
32	C	516	DGD	C8B-C9B-CAB-CBB
32	H	102	DGD	C7A-C8A-C9A-CAA
32	c	517	DGD	C4B-C5B-C6B-C7B
31	E	101	LHG	C14-C15-C16-C17
32	C	517	DGD	C9A-CAA-CBA-CCA
31	D	408	LHG	C7-C8-C9-C10
32	C	517	DGD	C1A-C2A-C3A-C4A
25	A	609	BCR	C16-C17-C18-C19
25	C	514	BCR	C11-C10-C9-C8
25	C	515	BCR	C11-C10-C9-C8
25	F	101	BCR	C16-C17-C18-C19
25	a	608	BCR	C11-C10-C9-C8
25	a	608	BCR	C12-C13-C14-C15
25	a	608	BCR	C20-C21-C22-C23
25	b	620	BCR	C16-C17-C18-C19
25	c	516	BCR	C11-C10-C9-C8
25	c	522	BCR	C16-C17-C18-C19
25	f	101	BCR	C11-C10-C9-C8
25	k	101	BCR	C20-C21-C22-C23
32	D	406	DGD	C2D-C1D-O3G-C3G
32	d	405	DGD	C2D-C1D-O3G-C3G
28	C	520	LMG	C31-C32-C33-C34
28	a	611	LMG	C15-C16-C17-C18
28	j	101	LMG	C13-C14-C15-C16
31	L	101	LHG	C25-C26-C27-C28
31	b	624	LHG	C25-C26-C27-C28
31	e	101	LHG	C13-C14-C15-C16
31	e	101	LHG	C25-C26-C27-C28
32	H	102	DGD	CBA-CCA-CDA-CEA
32	c	518	DGD	C3A-C4A-C5A-C6A
23	B	614	CLA	C15-C16-C17-C18
23	b	616	CLA	C15-C16-C17-C18
23	c	512	CLA	O1A-CGA-O2A-C1
23	D	404	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C19
23	c	511	CLA	O1D-CGD-O2D-CED
26	D	405	PL9	C42-C43-C44-C45
28	J	101	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
28	a	611	LMG	C12-C13-C14-C15
31	E	101	LHG	C24-C25-C26-C27
31	L	101	LHG	C33-C34-C35-C36
32	C	517	DGD	CAB-CBB-CCB-CDB
23	B	604	CLA	C6-C7-C8-C9
23	b	606	CLA	C6-C7-C8-C9
32	C	516	DGD	O6D-C5D-C6D-O5D
28	B	621	LMG	C10-C11-C12-C13
27	B	623	SQD	C34-C35-C36-C37
27	X	101	SQD	C24-C25-C26-C27
27	b	602	SQD	C34-C35-C36-C37
27	x	101	SQD	C24-C25-C26-C27
28	B	621	LMG	C12-C13-C14-C15
28	Z	101	LMG	C16-C17-C18-C19
28	j	101	LMG	C15-C16-C17-C18
28	z	101	LMG	C12-C13-C14-C15
28	z	101	LMG	C16-C17-C18-C19
31	B	622	LHG	C32-C33-C34-C35
31	E	101	LHG	C25-C26-C27-C28
31	E	101	LHG	C27-C28-C29-C30
32	C	516	DGD	CAB-CBB-CCB-CDB
32	D	406	DGD	C2A-C3A-C4A-C5A
32	d	405	DGD	CCA-CDA-CEA-CFA
32	h	102	DGD	C7A-C8A-C9A-CAA
23	B	617	CLA	C8-C10-C11-C12
23	b	619	CLA	C8-C10-C11-C12
32	c	517	DGD	O6E-C5E-C6E-O5E
25	B	618	BCR	C37-C22-C23-C24
25	C	515	BCR	C37-C22-C23-C24
25	H	101	BCR	C7-C8-C9-C34
25	b	620	BCR	C11-C12-C13-C35
25	b	620	BCR	C37-C22-C23-C24
25	f	101	BCR	C11-C12-C13-C35
27	A	611	SQD	C16-C17-C18-C19
27	B	623	SQD	C31-C32-C33-C34
27	a	610	SQD	C16-C17-C18-C19
28	b	623	LMG	C16-C17-C18-C19
31	L	101	LHG	C13-C14-C15-C16
31	a	614	LHG	C15-C16-C17-C18
31	l	101	LHG	C11-C12-C13-C14
32	D	406	DGD	C8B-C9B-CAB-CBB
32	c	518	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
32	d	405	DGD	C9A-CAA-CBA-CCA
31	B	622	LHG	O1-C1-C2-C3
25	A	609	BCR	C17-C18-C19-C20
25	B	619	BCR	C17-C18-C19-C20
25	K	101	BCR	C17-C18-C19-C20
25	a	608	BCR	C17-C18-C19-C20
25	k	101	BCR	C7-C8-C9-C10
28	A	612	LMG	C11-C10-O7-C8
27	B	623	SQD	C11-C12-C13-C14
27	b	602	SQD	C31-C32-C33-C34
28	A	612	LMG	C18-C19-C20-C21
28	C	520	LMG	C30-C31-C32-C33
28	c	520	LMG	C32-C33-C34-C35
31	E	101	LHG	C18-C19-C20-C21
31	l	101	LHG	C33-C34-C35-C36
32	D	406	DGD	CCB-CDB-CEB-CFB
32	d	405	DGD	C7B-C8B-C9B-CAB
28	b	623	LMG	C10-C11-C12-C13
31	e	101	LHG	C7-C8-C9-C10
32	c	518	DGD	C1A-C2A-C3A-C4A
27	B	623	SQD	C11-C10-C9-C8
27	a	612	SQD	C16-C17-C18-C19
27	b	601	SQD	C16-C17-C18-C19
27	b	602	SQD	C11-C10-C9-C8
27	b	602	SQD	C11-C12-C13-C14
28	A	612	LMG	C14-C15-C16-C17
28	B	621	LMG	C16-C17-C18-C19
28	a	611	LMG	C14-C15-C16-C17
28	b	623	LMG	C37-C38-C39-C40
31	e	101	LHG	C18-C19-C20-C21
31	l	101	LHG	C13-C14-C15-C16
31	l	101	LHG	C34-C35-C36-C37
32	c	517	DGD	CAB-CBB-CCB-CDB
32	c	518	DGD	C4A-C5A-C6A-C7A
32	d	405	DGD	C9B-CAB-CBB-CCB
27	A	611	SQD	C9-C10-C11-C12
27	B	623	SQD	C24-C25-C26-C27
27	a	610	SQD	C9-C10-C11-C12
27	a	612	SQD	C26-C27-C28-C29
27	b	601	SQD	C26-C27-C28-C29
27	b	602	SQD	C24-C25-C26-C27
28	a	611	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
28	b	623	LMG	C12-C13-C14-C15
28	c	521	LMG	C17-C18-C19-C20
31	D	408	LHG	C15-C16-C17-C18
32	C	516	DGD	C6A-C7A-C8A-C9A
32	C	517	DGD	C4A-C5A-C6A-C7A
32	c	518	DGD	CBB-CCB-CDB-CEB
32	d	405	DGD	CBA-CCA-CDA-CEA
32	C	516	DGD	C4D-C5D-C6D-O5D
27	b	601	SQD	C28-C29-C30-C31
28	J	101	LMG	C13-C14-C15-C16
28	c	521	LMG	C30-C31-C32-C33
28	j	101	LMG	C36-C37-C38-C39
31	B	622	LHG	C24-C25-C26-C27
32	C	516	DGD	C4B-C5B-C6B-C7B
32	C	516	DGD	C7B-C8B-C9B-CAB
32	D	406	DGD	C5B-C6B-C7B-C8B
32	D	406	DGD	C9B-CAB-CBB-CCB
32	c	517	DGD	C4A-C5A-C6A-C7A
31	E	101	LHG	C7-C8-C9-C10
31	d	406	LHG	O10-C23-O8-C6
27	a	612	SQD	C28-C29-C30-C31
28	A	612	LMG	C13-C14-C15-C16
32	C	516	DGD	C6B-C7B-C8B-C9B
32	C	518	DGD	C6A-C7A-C8A-C9A
32	H	102	DGD	CCB-CDB-CEB-CFB
32	c	517	DGD	C6A-C7A-C8A-C9A
23	a	613	CLA	O1D-CGD-O2D-CED
23	b	612	CLA	O1D-CGD-O2D-CED
28	a	611	LMG	C38-C39-C40-C41
28	j	101	LMG	C30-C31-C32-C33
31	a	614	LHG	C10-C11-C12-C13
32	D	406	DGD	CCA-CDA-CEA-CFA
25	B	619	BCR	C9-C10-C11-C12
25	h	101	BCR	C13-C14-C15-C16
27	X	101	SQD	C31-C32-C33-C34
27	x	101	SQD	C31-C32-C33-C34
28	B	621	LMG	C31-C32-C33-C34
28	c	520	LMG	C34-C35-C36-C37
31	L	101	LHG	C12-C13-C14-C15
32	C	518	DGD	C2A-C3A-C4A-C5A
32	D	406	DGD	C9A-CAA-CBA-CCA
23	b	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	B	623	SQD	C10-C11-C12-C13
27	b	602	SQD	C10-C11-C12-C13
32	C	517	DGD	C6B-C7B-C8B-C9B
32	C	517	DGD	CBB-CCB-CDB-CEB
32	h	102	DGD	CCB-CDB-CEB-CFB
28	c	520	LMG	C38-C39-C40-C41
31	e	101	LHG	C15-C16-C17-C18
31	e	101	LHG	C27-C28-C29-C30
32	c	518	DGD	C6B-C7B-C8B-C9B
23	C	509	CLA	O1D-CGD-O2D-CED
28	J	101	LMG	C38-C39-C40-C41
28	z	101	LMG	C19-C20-C21-C22
32	c	519	DGD	C6A-C7A-C8A-C9A
26	d	404	PL9	C30-C29-C31-C32
27	X	101	SQD	C30-C31-C32-C33
27	x	101	SQD	C30-C31-C32-C33
28	c	520	LMG	C29-C30-C31-C32
26	a	609	PL9	C47-C48-C49-C51
31	D	407	LHG	O1-C1-C2-O2
28	C	520	LMG	C17-C18-C19-C20
28	Z	101	LMG	C12-C13-C14-C15
28	Z	101	LMG	C19-C20-C21-C22
28	z	101	LMG	C15-C16-C17-C18
31	D	408	LHG	C10-C11-C12-C13
31	b	624	LHG	C24-C25-C26-C27
32	D	406	DGD	CAA-CBA-CCA-CDA
32	D	406	DGD	CBA-CCA-CDA-CEA
23	C	507	CLA	C16-C17-C18-C19
23	c	508	CLA	C16-C17-C18-C19
23	B	605	CLA	C13-C15-C16-C17
28	C	520	LMG	C18-C19-C20-C21
28	B	621	LMG	C15-C16-C17-C18
28	B	621	LMG	C17-C18-C19-C20
28	c	521	LMG	C18-C19-C20-C21
31	l	101	LHG	C31-C32-C33-C34
32	c	518	DGD	C9B-CAB-CBB-CCB
23	b	607	CLA	C13-C15-C16-C17
27	A	611	SQD	C32-C33-C34-C35
27	a	610	SQD	C32-C33-C34-C35
28	C	519	LMG	C16-C17-C18-C19
31	a	614	LHG	C27-C28-C29-C30
31	b	624	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
32	c	517	DGD	C6B-C7B-C8B-C9B
28	c	520	LMG	C16-C17-C18-C19
32	C	516	DGD	C5B-C6B-C7B-C8B
28	C	519	LMG	C38-C39-C40-C41
31	a	614	LHG	C29-C30-C31-C32
28	C	519	LMG	C10-C11-C12-C13
25	B	618	BCR	C1-C6-C7-C8
25	B	618	BCR	C23-C24-C25-C26
25	B	619	BCR	C1-C6-C7-C8
25	B	620	BCR	C5-C6-C7-C8
25	C	514	BCR	C5-C6-C7-C8
25	C	515	BCR	C5-C6-C7-C8
25	C	515	BCR	C23-C24-C25-C26
25	C	521	BCR	C23-C24-C25-C30
25	F	101	BCR	C5-C6-C7-C8
25	H	101	BCR	C5-C6-C7-C8
25	H	101	BCR	C23-C24-C25-C26
25	K	101	BCR	C5-C6-C7-C8
25	K	101	BCR	C23-C24-C25-C30
25	T	101	BCR	C1-C6-C7-C8
25	a	608	BCR	C1-C6-C7-C8
25	b	620	BCR	C1-C6-C7-C8
25	b	621	BCR	C23-C24-C25-C30
25	b	622	BCR	C5-C6-C7-C8
25	b	622	BCR	C23-C24-C25-C26
25	c	516	BCR	C23-C24-C25-C26
25	f	101	BCR	C5-C6-C7-C8
25	h	101	BCR	C5-C6-C7-C8
25	h	101	BCR	C23-C24-C25-C26
25	k	101	BCR	C1-C6-C7-C8
25	t	101	BCR	C1-C6-C7-C8
25	t	101	BCR	C5-C6-C7-C8
25	t	101	BCR	C23-C24-C25-C30
28	a	611	LMG	C32-C33-C34-C35
32	c	518	DGD	C8B-C9B-CAB-CBB
23	c	512	CLA	CBA-CGA-O2A-C1
27	a	612	SQD	C24-C23-O48-C46
27	b	601	SQD	C24-C23-O48-C46
23	C	506	CLA	C13-C15-C16-C17
23	c	507	CLA	C13-C15-C16-C17
27	X	101	SQD	C8-C7-O47-C45
27	x	101	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
28	b	623	LMG	C11-C10-O7-C8
28	C	519	LMG	C32-C33-C34-C35
28	c	521	LMG	C33-C34-C35-C36
31	l	101	LHG	C32-C33-C34-C35
28	c	520	LMG	C10-C11-C12-C13
27	b	602	SQD	C32-C33-C34-C35
27	B	623	SQD	C32-C33-C34-C35
31	L	101	LHG	C31-C32-C33-C34
32	C	516	DGD	C4A-C5A-C6A-C7A
24	A	607	PHO	C4-C3-C5-C6
26	D	405	PL9	C45-C44-C46-C47
23	A	606	CLA	C6-C7-C8-C10
23	B	604	CLA	C6-C7-C8-C10
23	B	611	CLA	C12-C13-C15-C16
23	B	617	CLA	C6-C7-C8-C10
23	C	504	CLA	C11-C12-C13-C15
23	C	510	CLA	C2-C3-C5-C6
23	a	605	CLA	C6-C7-C8-C10
23	b	606	CLA	C6-C7-C8-C10
23	b	613	CLA	C12-C13-C15-C16
23	b	619	CLA	C6-C7-C8-C10
23	c	505	CLA	C11-C12-C13-C15
23	c	511	CLA	C2-C3-C5-C6
26	D	405	PL9	C43-C44-C46-C47
26	d	404	PL9	C28-C29-C31-C32
32	d	405	DGD	O1A-C1A-O1G-C1G
27	B	623	SQD	C29-C30-C31-C32
27	b	602	SQD	C29-C30-C31-C32
28	a	611	LMG	C18-C19-C20-C21
23	C	504	CLA	C13-C15-C16-C17
23	c	505	CLA	C13-C15-C16-C17
25	B	618	BCR	C15-C16-C17-C18
28	B	621	LMG	O9-C10-O7-C8
28	C	520	LMG	O9-C10-O7-C8
28	c	521	LMG	O9-C10-O7-C8
23	c	506	CLA	CBA-CGA-O2A-C1
28	A	612	LMG	C36-C37-C38-C39
28	C	520	LMG	C15-C16-C17-C18
31	D	407	LHG	C32-C33-C34-C35
31	L	101	LHG	C27-C28-C29-C30
32	C	518	DGD	C9B-CAB-CBB-CCB
27	B	623	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
27	b	602	SQD	C18-C19-C20-C21
32	D	406	DGD	C3A-C4A-C5A-C6A
32	d	405	DGD	C5B-C6B-C7B-C8B
28	B	621	LMG	C38-C39-C40-C41
28	C	519	LMG	C34-C35-C36-C37
28	b	623	LMG	C15-C16-C17-C18
28	b	623	LMG	C38-C39-C40-C41
27	a	610	SQD	C30-C31-C32-C33
32	C	518	DGD	C3B-C4B-C5B-C6B
25	B	620	BCR	C6-C7-C8-C9
25	C	521	BCR	C22-C23-C24-C25
25	c	515	BCR	C6-C7-C8-C9
25	k	101	BCR	C6-C7-C8-C9
23	C	505	CLA	CBA-CGA-O2A-C1
32	C	517	DGD	O6E-C1E-O5D-C6D
32	D	406	DGD	O6D-C1D-O3G-C3G
32	H	102	DGD	O6E-C1E-O5D-C6D
32	c	518	DGD	O6E-C1E-O5D-C6D
32	d	405	DGD	O6D-C1D-O3G-C3G
23	C	501	CLA	C13-C15-C16-C17
23	c	502	CLA	C13-C15-C16-C17
27	A	611	SQD	C30-C31-C32-C33
28	C	519	LMG	C17-C18-C19-C20
32	h	102	DGD	CBB-CCB-CDB-CEB
28	b	623	LMG	C28-C29-C30-C31
31	D	408	LHG	C29-C30-C31-C32
23	B	607[A]	CLA	CBD-CGD-O2D-CED
23	B	612	CLA	CBD-CGD-O2D-CED
31	L	101	LHG	C11-C12-C13-C14
32	C	517	DGD	C9B-CAB-CBB-CCB
27	X	101	SQD	O49-C7-O47-C45
27	x	101	SQD	O49-C7-O47-C45
28	C	520	LMG	C38-C39-C40-C41
32	C	517	DGD	C8B-C9B-CAB-CBB
32	d	405	DGD	CAA-CBA-CCA-CDA
28	z	101	LMG	C2-C1-O1-C7
32	C	517	DGD	C2E-C1E-O5D-C6D
32	c	518	DGD	C2E-C1E-O5D-C6D
28	b	623	LMG	C31-C32-C33-C34
32	H	102	DGD	CBB-CCB-CDB-CEB
23	C	510	CLA	C4-C3-C5-C6
23	c	511	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	d	404	PL9	C45-C44-C46-C47
32	c	517	DGD	C1B-C2B-C3B-C4B
26	A	610	PL9	C38-C39-C41-C42
26	d	404	PL9	C18-C19-C21-C22
26	A	610	PL9	C4-C3-C7-C8
26	a	609	PL9	C4-C3-C7-C8
23	A	606	CLA	C6-C7-C8-C9
23	B	611	CLA	C14-C13-C15-C16
23	B	616	CLA	C14-C13-C15-C16
23	B	617	CLA	C6-C7-C8-C9
23	D	404	CLA	C11-C10-C8-C9
23	a	605	CLA	C6-C7-C8-C9
23	b	613	CLA	C14-C13-C15-C16
23	b	618	CLA	C14-C13-C15-C16
23	b	619	CLA	C6-C7-C8-C9
23	d	403	CLA	C11-C10-C8-C9
27	a	612	SQD	C18-C19-C20-C21
28	B	621	LMG	C18-C19-C20-C21
28	b	623	LMG	C34-C35-C36-C37
28	j	101	LMG	C19-C20-C21-C22
25	C	515	BCR	C36-C18-C19-C20
25	C	521	BCR	C36-C18-C19-C20
25	c	522	BCR	C36-C18-C19-C20
27	A	611	SQD	C34-C35-C36-C37
27	b	601	SQD	C18-C19-C20-C21
28	c	520	LMG	C17-C18-C19-C20
25	c	516	BCR	C17-C18-C19-C20
23	b	615	CLA	O1A-CGA-O2A-C1
27	a	612	SQD	O10-C23-O48-C46
27	b	601	SQD	O10-C23-O48-C46
23	b	616	CLA	O1D-CGD-O2D-CED
23	C	505	CLA	C1A-C2A-CAA-CBA
32	C	516	DGD	O6E-C5E-C6E-O5E
23	B	605	CLA	C16-C17-C18-C20
23	C	506	CLA	C16-C17-C18-C20
23	D	404	CLA	C16-C17-C18-C20
23	b	607	CLA	C16-C17-C18-C20
23	d	403	CLA	C16-C17-C18-C20
27	a	610	SQD	C34-C35-C36-C37
31	a	614	LHG	C12-C13-C14-C15
23	B	607[B]	CLA	C15-C16-C17-C18
23	C	507	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	b	609[B]	CLA	C15-C16-C17-C18
23	c	508	CLA	C5-C6-C7-C8
32	d	405	DGD	CBB-CCB-CDB-CEB
27	X	101	SQD	C23-C24-C25-C26
27	x	101	SQD	C23-C24-C25-C26
32	c	519	DGD	C4A-C5A-C6A-C7A
23	D	404	CLA	C13-C15-C16-C17
23	d	403	CLA	C13-C15-C16-C17
28	a	611	LMG	C31-C32-C33-C34
28	c	520	LMG	C11-C12-C13-C14
31	L	101	LHG	C32-C33-C34-C35
27	b	602	SQD	C27-C28-C29-C30
31	D	408	LHG	C27-C28-C29-C30
23	A	608	CLA	C16-C17-C18-C19
23	C	507	CLA	C16-C17-C18-C20
23	a	607	CLA	C16-C17-C18-C19
23	c	507	CLA	C16-C17-C18-C20
23	c	508	CLA	C16-C17-C18-C20
27	B	623	SQD	C27-C28-C29-C30
28	J	101	LMG	C35-C36-C37-C38
28	c	520	LMG	C19-C20-C21-C22
28	Z	101	LMG	C15-C16-C17-C18
26	d	404	PL9	C47-C48-C49-C50
27	B	623	SQD	C28-C29-C30-C31
27	b	602	SQD	C28-C29-C30-C31
28	c	520	LMG	C39-C40-C41-C42
31	l	101	LHG	C1-C2-C3-O3
26	D	405	PL9	C25-C24-C26-C27
26	A	610	PL9	C28-C29-C31-C32
28	C	519	LMG	C19-C20-C21-C22
28	j	101	LMG	C38-C39-C40-C41
31	D	408	LHG	C12-C13-C14-C15
31	L	101	LHG	C24-C25-C26-C27
32	c	518	DGD	C7B-C8B-C9B-CAB
32	c	519	DGD	C8B-C9B-CAB-CBB
27	a	610	SQD	C27-C28-C29-C30
31	e	101	LHG	C11-C10-C9-C8
28	c	521	LMG	C11-C10-O7-C8
27	A	611	SQD	C27-C28-C29-C30
28	b	623	LMG	C18-C19-C20-C21
32	D	406	DGD	C4B-C5B-C6B-C7B
32	D	406	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
32	d	405	DGD	C8B-C9B-CAB-CBB
23	A	606	CLA	C16-C17-C18-C19
23	a	605	CLA	C16-C17-C18-C19
27	a	612	SQD	O6-C44-C45-C46
27	b	601	SQD	O6-C44-C45-C46
28	A	612	LMG	C7-C8-C9-O8
28	a	611	LMG	C7-C8-C9-O8
28	c	520	LMG	C21-C22-C23-C24
28	z	101	LMG	O1-C7-C8-C9
32	D	406	DGD	O1G-C1G-C2G-C3G
32	H	102	DGD	O1G-C1G-C2G-C3G
32	h	102	DGD	O1G-C1G-C2G-C3G
23	C	509	CLA	C10-C11-C12-C13
23	c	510	CLA	C10-C11-C12-C13
27	X	101	SQD	C35-C36-C37-C38
27	x	101	SQD	C35-C36-C37-C38
28	z	101	LMG	C4-C5-C6-O5
27	B	623	SQD	C35-C36-C37-C38
27	b	602	SQD	C35-C36-C37-C38
28	A	612	LMG	C30-C31-C32-C33
31	B	622	LHG	C13-C14-C15-C16
31	B	622	LHG	C33-C34-C35-C36
27	B	623	SQD	C13-C14-C15-C16
27	b	602	SQD	C13-C14-C15-C16
28	z	101	LMG	C13-C14-C15-C16
32	d	405	DGD	C3A-C4A-C5A-C6A
32	h	102	DGD	C6B-C7B-C8B-C9B
31	B	622	LHG	C15-C16-C17-C18
32	d	405	DGD	C5A-C6A-C7A-C8A
32	h	102	DGD	CDB-CEB-CFB-CGB
27	b	601	SQD	C19-C20-C21-C22
28	Z	101	LMG	C13-C14-C15-C16
32	C	517	DGD	C3B-C4B-C5B-C6B
28	C	520	LMG	C29-C28-O8-C9
27	a	612	SQD	C19-C20-C21-C22
28	a	611	LMG	C36-C37-C38-C39
32	C	518	DGD	C9A-CAA-CBA-CCA
32	H	102	DGD	CDB-CEB-CFB-CGB
28	C	520	LMG	C33-C34-C35-C36
32	h	102	DGD	C9A-CAA-CBA-CCA
27	A	611	SQD	C35-C36-C37-C38
27	a	610	SQD	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
31	E	101	LHG	C9-C10-C11-C12
23	B	613	CLA	C13-C15-C16-C17
23	b	615	CLA	C13-C15-C16-C17
25	A	609	BCR	C11-C10-C9-C34
25	B	620	BCR	C35-C13-C14-C15
25	K	101	BCR	C11-C10-C9-C34
25	t	101	BCR	C35-C13-C14-C15
31	a	614	LHG	C30-C31-C32-C33
32	C	517	DGD	C5A-C6A-C7A-C8A
32	c	517	DGD	C7B-C8B-C9B-CAB
26	d	404	PL9	C43-C44-C46-C47
23	A	608	CLA	C5-C6-C7-C8
23	a	607	CLA	C5-C6-C7-C8
23	c	510	CLA	C2-C1-O2A-CGA
26	D	405	PL9	C42-C43-C44-C46
31	D	408	LHG	C17-C18-C19-C20
32	c	519	DGD	C2B-C3B-C4B-C5B
28	C	519	LMG	C20-C21-C22-C23
31	L	101	LHG	C34-C35-C36-C37
32	H	102	DGD	CAA-CBA-CCA-CDA
32	c	519	DGD	C9A-CAA-CBA-CCA
28	C	519	LMG	C13-C14-C15-C16
31	l	101	LHG	O2-C2-C3-O3
31	D	407	LHG	O10-C23-O8-C6
28	A	612	LMG	C31-C32-C33-C34
31	l	101	LHG	C24-C25-C26-C27
32	C	516	DGD	CAA-CBA-CCA-CDA
32	C	517	DGD	C7B-C8B-C9B-CAB
28	a	611	LMG	C10-C11-C12-C13
25	T	101	BCR	C16-C17-C18-C19
25	c	522	BCR	C12-C13-C14-C15
25	f	101	BCR	C20-C21-C22-C23
28	Z	101	LMG	C2-C1-O1-C7
32	c	517	DGD	C2A-C3A-C4A-C5A
23	b	604	CLA	CAA-CBA-CGA-O2A
32	H	102	DGD	O2G-C1B-C2B-C3B
28	J	101	LMG	C19-C20-C21-C22
28	c	520	LMG	C13-C14-C15-C16
28	b	623	LMG	O9-C10-O7-C8
32	D	406	DGD	O1A-C1A-O1G-C1G
28	c	521	LMG	C38-C39-C40-C41
32	c	519	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
26	a	609	PL9	C45-C44-C46-C47
32	D	406	DGD	CAB-CBB-CCB-CDB
32	c	518	DGD	C3B-C4B-C5B-C6B
23	A	608	CLA	C11-C10-C8-C7
23	B	602	CLA	C6-C7-C8-C10
23	B	602	CLA	C11-C10-C8-C7
23	B	616	CLA	C12-C13-C15-C16
23	B	617	CLA	C11-C12-C13-C15
23	C	501	CLA	C11-C12-C13-C15
23	C	506	CLA	C11-C12-C13-C15
23	C	508	CLA	C11-C10-C8-C7
23	C	512	CLA	C11-C10-C8-C7
23	C	513	CLA	C6-C7-C8-C10
23	D	404	CLA	C11-C10-C8-C7
23	a	607	CLA	C11-C10-C8-C7
23	b	604	CLA	C6-C7-C8-C10
23	b	604	CLA	C11-C10-C8-C7
23	b	618	CLA	C12-C13-C15-C16
23	b	619	CLA	C11-C12-C13-C15
23	c	502	CLA	C11-C12-C13-C15
23	c	507	CLA	C11-C12-C13-C15
23	c	509	CLA	C11-C10-C8-C7
23	c	513	CLA	C11-C10-C8-C7
23	c	514	CLA	C6-C7-C8-C10
23	d	403	CLA	C11-C10-C8-C7
26	D	405	PL9	C28-C29-C31-C32
23	C	512	CLA	O1A-CGA-O2A-C1
23	B	617	CLA	C11-C12-C13-C14
23	C	501	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	C	508	CLA	C11-C10-C8-C9
23	C	513	CLA	C11-C12-C13-C14
23	b	619	CLA	C11-C12-C13-C14
23	c	502	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C12-C13-C14
23	c	509	CLA	C11-C10-C8-C9
23	c	514	CLA	C11-C12-C13-C14
25	C	514	BCR	C15-C16-C17-C18
25	h	101	BCR	C15-C16-C17-C18
27	A	611	SQD	C14-C15-C16-C17
27	a	610	SQD	C14-C15-C16-C17
31	b	624	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
32	H	102	DGD	C9B-CAB-CBB-CCB
32	c	519	DGD	CBA-CCA-CDA-CEA
25	b	620	BCR	C36-C18-C19-C20
25	f	101	BCR	C36-C18-C19-C20
23	A	608	CLA	C16-C17-C18-C20
23	B	605	CLA	C16-C17-C18-C19
23	B	617	CLA	C16-C17-C18-C20
23	a	607	CLA	C16-C17-C18-C20
23	b	607	CLA	C16-C17-C18-C19
23	b	619	CLA	C16-C17-C18-C20
27	a	612	SQD	C25-C26-C27-C28
27	b	601	SQD	C25-C26-C27-C28
28	a	611	LMG	C22-C23-C24-C25
32	D	406	DGD	C4E-C5E-C6E-O5E
25	C	515	BCR	C21-C22-C23-C24
25	T	101	BCR	C11-C12-C13-C14
25	T	101	BCR	C17-C18-C19-C20
25	h	101	BCR	C11-C12-C13-C14
25	t	101	BCR	C17-C18-C19-C20
31	l	101	LHG	C26-C27-C28-C29
31	e	101	LHG	C12-C13-C14-C15
23	C	512	CLA	CBA-CGA-O2A-C1
27	B	623	SQD	C24-C23-O48-C46
27	b	602	SQD	C24-C23-O48-C46
28	A	612	LMG	C29-C28-O8-C9
28	a	611	LMG	C29-C28-O8-C9
27	A	611	SQD	C19-C20-C21-C22
27	a	610	SQD	C19-C20-C21-C22
25	c	522	BCR	C22-C23-C24-C25
32	H	102	DGD	CCA-CDA-CEA-CFA
27	a	612	SQD	O5-C1-O6-C44
27	b	601	SQD	O5-C1-O6-C44
27	a	612	SQD	C31-C32-C33-C34
27	b	601	SQD	C31-C32-C33-C34
28	j	101	LMG	C20-C21-C22-C23
31	d	406	LHG	C34-C35-C36-C37
31	D	408	LHG	C18-C19-C20-C21
32	C	518	DGD	C6B-C7B-C8B-C9B
32	H	102	DGD	O6E-C5E-C6E-O5E
32	D	406	DGD	C5A-C6A-C7A-C8A
24	A	607	PHO	C2-C3-C5-C6
26	D	405	PL9	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
26	d	404	PL9	C13-C14-C16-C17
32	C	517	DGD	CDB-CEB-CFB-CGB
23	b	611	CLA	C13-C15-C16-C17
23	B	604	CLA	C16-C17-C18-C20
23	b	606	CLA	C16-C17-C18-C20
28	C	520	LMG	C40-C41-C42-C43
32	C	517	DGD	C6A-C7A-C8A-C9A
32	d	405	DGD	C4B-C5B-C6B-C7B
23	B	609	CLA	C13-C15-C16-C17
31	B	622	LHG	C24-C23-O8-C6
31	E	101	LHG	C26-C27-C28-C29
23	B	608	CLA	C3A-C2A-CAA-CBA
28	b	623	LMG	C33-C34-C35-C36
25	A	609	BCR	C9-C10-C11-C12
25	F	101	BCR	C15-C16-C17-C18
25	f	101	BCR	C19-C20-C21-C22
28	A	612	LMG	C22-C23-C24-C25
28	B	621	LMG	C33-C34-C35-C36
31	e	101	LHG	C9-C10-C11-C12
23	B	616	CLA	C13-C15-C16-C17
23	b	618	CLA	C13-C15-C16-C17
23	c	509	CLA	C5-C6-C7-C8
32	C	518	DGD	C5B-C6B-C7B-C8B
27	a	612	SQD	C32-C33-C34-C35
27	b	601	SQD	C32-C33-C34-C35
31	e	101	LHG	C17-C18-C19-C20
23	C	508	CLA	C5-C6-C7-C8
27	B	623	SQD	C44-C45-C46-O48
27	b	602	SQD	C44-C45-C46-O48
32	d	405	DGD	O1G-C1G-C2G-C3G
28	A	612	LMG	C32-C33-C34-C35
28	C	519	LMG	C29-C30-C31-C32
31	B	622	LHG	C11-C10-C9-C8
32	C	517	DGD	C8A-C9A-CAA-CBA
31	E	101	LHG	C11-C10-C9-C8
28	B	621	LMG	C11-C10-O7-C8
28	c	521	LMG	C40-C41-C42-C43
23	C	513	CLA	O1D-CGD-O2D-CED
32	H	102	DGD	C9A-CAA-CBA-CCA
28	c	520	LMG	C29-C28-O8-C9
28	c	521	LMG	C15-C16-C17-C18
27	a	612	SQD	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
27	b	601	SQD	C35-C36-C37-C38
23	B	616	CLA	C10-C11-C12-C13
23	b	618	CLA	C10-C11-C12-C13
23	C	510	CLA	O1A-CGA-O2A-C1
28	J	101	LMG	C30-C31-C32-C33
28	j	101	LMG	C35-C36-C37-C38
27	B	623	SQD	O47-C45-C46-O48
27	b	602	SQD	O47-C45-C46-O48
28	A	612	LMG	O1-C7-C8-O7
28	A	612	LMG	O7-C8-C9-O8
32	d	405	DGD	O1G-C1G-C2G-O2G
31	d	406	LHG	C24-C23-O8-C6
28	c	520	LMG	C20-C21-C22-C23
31	B	622	LHG	C31-C32-C33-C34
25	A	609	BCR	C15-C16-C17-C18
25	B	620	BCR	C15-C16-C17-C18
25	c	516	BCR	C15-C16-C17-C18
23	B	602	CLA	C16-C17-C18-C20
23	b	604	CLA	C16-C17-C18-C20
31	l	101	LHG	C27-C28-C29-C30
32	H	102	DGD	C4E-C5E-C6E-O5E
28	C	519	LMG	C39-C40-C41-C42
32	C	517	DGD	CDA-CEA-CFA-CGA
32	c	517	DGD	CBB-CCB-CDB-CEB
32	c	519	DGD	C3B-C4B-C5B-C6B
23	b	604	CLA	C2-C1-O2A-CGA
32	C	518	DGD	C8B-C9B-CAB-CBB
23	B	615	CLA	C11-C12-C13-C14
23	B	615	CLA	C14-C13-C15-C16
23	C	507	CLA	C11-C10-C8-C9
23	b	617	CLA	C11-C12-C13-C14
23	b	617	CLA	C14-C13-C15-C16
23	c	508	CLA	C11-C10-C8-C9
23	B	602	CLA	C15-C16-C17-C18
23	B	607[A]	CLA	C8-C10-C11-C12
23	b	604	CLA	C15-C16-C17-C18
23	b	609[A]	CLA	C8-C10-C11-C12
28	a	611	LMG	C30-C31-C32-C33
28	a	611	LMG	C33-C34-C35-C36
25	B	619	BCR	C23-C24-C25-C30
25	B	620	BCR	C23-C24-C25-C30
25	b	620	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	t	101	BCR	C23-C24-C25-C26
27	B	623	SQD	C16-C17-C18-C19
23	C	511	CLA	O1A-CGA-O2A-C1
25	b	620	BCR	C21-C22-C23-C24
25	c	522	BCR	C11-C12-C13-C14
23	C	502	CLA	C15-C16-C17-C18
23	c	503	CLA	C15-C16-C17-C18
27	b	602	SQD	C16-C17-C18-C19
25	B	618	BCR	C14-C15-C16-C17
28	C	519	LMG	C14-C15-C16-C17
31	d	406	LHG	C32-C33-C34-C35
23	B	607[B]	CLA	C16-C17-C18-C19
23	C	501	CLA	C16-C17-C18-C19
23	C	502	CLA	C16-C17-C18-C20
23	b	609[B]	CLA	C16-C17-C18-C19
23	c	502	CLA	C16-C17-C18-C19
23	c	503	CLA	C16-C17-C18-C20
31	E	101	LHG	C19-C20-C21-C22
31	b	624	LHG	C13-C14-C15-C16
32	c	517	DGD	C9A-CAA-CBA-CCA
31	L	101	LHG	O6-C4-C5-C6
31	l	101	LHG	O6-C4-C5-C6
28	C	519	LMG	C31-C32-C33-C34
23	B	612	CLA	C12-C13-C15-C16
23	B	615	CLA	C11-C12-C13-C15
23	B	616	CLA	C11-C10-C8-C7
23	B	617	CLA	C12-C13-C15-C16
23	C	501	CLA	C12-C13-C15-C16
23	C	507	CLA	C11-C10-C8-C7
23	C	513	CLA	C11-C12-C13-C15
23	D	404	CLA	C6-C7-C8-C10
23	b	614	CLA	C12-C13-C15-C16
23	b	617	CLA	C11-C12-C13-C15
23	b	618	CLA	C11-C10-C8-C7
23	b	619	CLA	C12-C13-C15-C16
23	c	502	CLA	C12-C13-C15-C16
23	c	514	CLA	C11-C12-C13-C15
23	d	403	CLA	C6-C7-C8-C10
27	B	623	SQD	O10-C23-O48-C46
27	b	602	SQD	O10-C23-O48-C46
28	C	519	LMG	C11-C12-C13-C14
25	F	101	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	b	621	BCR	C19-C20-C21-C22
25	c	522	BCR	C15-C16-C17-C18
25	f	101	BCR	C15-C16-C17-C18
25	t	101	BCR	C13-C14-C15-C16
32	c	518	DGD	C5A-C6A-C7A-C8A
31	a	614	LHG	C17-C18-C19-C20
31	l	101	LHG	C25-C26-C27-C28
25	B	619	BCR	C35-C13-C14-C15
25	C	521	BCR	C11-C10-C9-C34
25	c	516	BCR	C16-C17-C18-C36
25	c	522	BCR	C11-C10-C9-C34
32	H	102	DGD	C5B-C6B-C7B-C8B
28	B	621	LMG	C28-C29-C30-C31
28	B	621	LMG	C30-C31-C32-C33
32	c	519	DGD	C7A-C8A-C9A-CAA
23	B	617	CLA	C16-C17-C18-C19
23	b	619	CLA	C16-C17-C18-C19
23	C	510	CLA	CBA-CGA-O2A-C1
23	C	511	CLA	CBA-CGA-O2A-C1
31	D	407	LHG	C24-C23-O8-C6
31	a	614	LHG	C24-C23-O8-C6
28	A	612	LMG	C38-C39-C40-C41
32	d	405	DGD	C6A-C7A-C8A-C9A
23	C	503	CLA	C8-C10-C11-C12
23	c	504	CLA	C8-C10-C11-C12
23	c	504	CLA	CBD-CGD-O2D-CED
27	x	101	SQD	C11-C10-C9-C8
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	509	CLA	CAD-CBD-CGD-O2D
23	D	404	CLA	CAD-CBD-CGD-O2D
23	a	604	CLA	CAD-CBD-CGD-O2D
23	b	607	CLA	CAD-CBD-CGD-O2D
23	c	510	CLA	CAD-CBD-CGD-O2D
23	c	514	CLA	CAD-CBD-CGD-O2D
27	X	101	SQD	C11-C10-C9-C8
28	J	101	LMG	C36-C37-C38-C39
23	C	506	CLA	CBA-CGA-O2A-C1
28	Z	101	LMG	O1-C7-C8-C9
31	D	408	LHG	C2-C3-O3-P
32	C	516	DGD	O1A-C1A-O1G-C1G
28	C	520	LMG	C11-C10-O7-C8
31	L	101	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
31	l	101	LHG	O6-C4-C5-O7
32	c	518	DGD	O6E-C5E-C6E-O5E
27	a	612	SQD	C24-C25-C26-C27
27	b	601	SQD	C24-C25-C26-C27
28	J	101	LMG	C20-C21-C22-C23
32	c	517	DGD	CAA-CBA-CCA-CDA
32	c	517	DGD	CCA-CDA-CEA-CFA
28	A	612	LMG	C10-C11-C12-C13
23	b	614	CLA	O1A-CGA-O2A-C1
23	B	604	CLA	C16-C17-C18-C19
23	b	606	CLA	C16-C17-C18-C19
32	h	102	DGD	C3B-C4B-C5B-C6B
23	B	604	CLA	CHA-CBD-CGD-O2D
23	B	607[A]	CLA	CHA-CBD-CGD-O1D
23	B	607[B]	CLA	CHA-CBD-CGD-O1D
23	B	608	CLA	CHA-CBD-CGD-O2D
23	B	610	CLA	CHA-CBD-CGD-O2D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O1D
23	a	605	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	b	608	CLA	CHA-CBD-CGD-O2D
23	b	609[A]	CLA	CHA-CBD-CGD-O1D
23	b	609[B]	CLA	CHA-CBD-CGD-O1D
23	b	610	CLA	CHA-CBD-CGD-O2D
23	b	612	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O2D
23	c	505	CLA	CHA-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	511	CLA	CHA-CBD-CGD-O2D
25	H	101	BCR	C13-C14-C15-C16
28	J	101	LMG	C34-C35-C36-C37
32	H	102	DGD	O6D-C5D-C6D-O5D
25	B	619	BCR	C11-C10-C9-C8
25	c	522	BCR	C20-C21-C22-C23
27	a	612	SQD	C2-C1-O6-C44
27	b	601	SQD	C2-C1-O6-C44
28	A	612	LMG	C2-C1-O1-C7
28	a	611	LMG	O7-C8-C9-O8
32	D	406	DGD	O1G-C1G-C2G-O2G
32	H	102	DGD	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
27	a	612	SQD	C29-C30-C31-C32
27	b	601	SQD	C29-C30-C31-C32
23	B	602	CLA	C16-C17-C18-C19
23	C	501	CLA	C16-C17-C18-C20
23	b	604	CLA	C16-C17-C18-C19
23	c	502	CLA	C16-C17-C18-C20
23	C	503	CLA	O1D-CGD-O2D-CED
31	D	408	LHG	C24-C25-C26-C27
31	e	101	LHG	C26-C27-C28-C29
26	d	404	PL9	C4-C3-C7-C8
27	a	612	SQD	C27-C28-C29-C30
27	b	601	SQD	C27-C28-C29-C30
23	A	608	CLA	C11-C12-C13-C14
23	B	612	CLA	C14-C13-C15-C16
23	D	404	CLA	C6-C7-C8-C9
23	a	607	CLA	C11-C12-C13-C14
23	b	614	CLA	C14-C13-C15-C16
23	d	403	CLA	C6-C7-C8-C9
31	D	408	LHG	C9-C10-C11-C12
23	B	613	CLA	O1A-CGA-O2A-C1
32	c	517	DGD	O1A-C1A-O1G-C1G
31	D	408	LHG	C30-C31-C32-C33
23	C	513	CLA	CBD-CGD-O2D-CED
25	B	618	BCR	C7-C8-C9-C34
25	T	101	BCR	C36-C18-C19-C20
25	b	621	BCR	C7-C8-C9-C34
28	A	612	LMG	C29-C30-C31-C32
32	H	102	DGD	CDA-CEA-CFA-CGA
32	h	102	DGD	CCA-CDA-CEA-CFA
25	b	622	BCR	C7-C8-C9-C10
23	C	506	CLA	C1A-C2A-CAA-CBA
23	C	512	CLA	C1A-C2A-CAA-CBA
23	c	506	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	C1A-C2A-CAA-CBA
23	b	613	CLA	C8-C10-C11-C12
28	a	611	LMG	C29-C30-C31-C32
23	B	617	CLA	C2-C1-O2A-CGA
28	C	519	LMG	C21-C22-C23-C24
31	e	101	LHG	C4-O6-P-O3
28	C	519	LMG	C12-C13-C14-C15
32	D	406	DGD	C6A-C7A-C8A-C9A
28	z	101	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
31	a	614	LHG	C2-C3-O3-P
31	D	407	LHG	C3-O3-P-O4
31	D	407	LHG	C4-O6-P-O5
23	B	611	CLA	C16-C17-C18-C19
23	b	613	CLA	C16-C17-C18-C19
32	C	516	DGD	O6E-C1E-O5D-C6D
23	B	611	CLA	C8-C10-C11-C12
23	B	614	CLA	C13-C15-C16-C17
23	b	616	CLA	C13-C15-C16-C17
27	a	612	SQD	C9-C10-C11-C12
23	B	615	CLA	C2A-CAA-CBA-CGA
23	B	605	CLA	C3-C5-C6-C7
27	b	601	SQD	C9-C10-C11-C12
32	c	518	DGD	CDA-CEA-CFA-CGA
23	B	602	CLA	CAD-CBD-CGD-O1D
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	510	CLA	CAD-CBD-CGD-O1D
23	b	604	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
27	a	610	SQD	C23-C24-C25-C26
32	c	517	DGD	C5A-C6A-C7A-C8A
27	B	623	SQD	C19-C20-C21-C22
23	b	607	CLA	C3-C5-C6-C7
27	b	602	SQD	C19-C20-C21-C22
27	A	611	SQD	C23-C24-C25-C26
27	X	101	SQD	C28-C29-C30-C31
27	x	101	SQD	C28-C29-C30-C31
28	c	520	LMG	C12-C13-C14-C15
23	b	618	CLA	C16-C17-C18-C20
26	d	404	PL9	C25-C24-C26-C27
23	A	606	CLA	C11-C10-C8-C7
23	B	615	CLA	C12-C13-C15-C16
23	C	504	CLA	C12-C13-C15-C16
23	C	506	CLA	C6-C7-C8-C10
23	C	509	CLA	C6-C7-C8-C10
23	D	404	CLA	C11-C12-C13-C15
23	D	404	CLA	C12-C13-C15-C16
23	a	605	CLA	C11-C10-C8-C7
23	b	617	CLA	C12-C13-C15-C16
23	c	505	CLA	C12-C13-C15-C16
23	c	507	CLA	C6-C7-C8-C10
23	c	508	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	c	510	CLA	C6-C7-C8-C10
23	d	403	CLA	C12-C13-C15-C16
28	Z	101	LMG	C18-C19-C20-C21
31	B	622	LHG	C34-C35-C36-C37
28	A	612	LMG	C21-C22-C23-C24
32	h	102	DGD	C9B-CAB-CBB-CCB
23	B	616	CLA	C16-C17-C18-C20
32	D	406	DGD	CDB-CEB-CFB-CGB
28	A	612	LMG	O1-C7-C8-C9
28	a	611	LMG	O1-C7-C8-C9
28	c	520	LMG	C30-C31-C32-C33
31	d	406	LHG	C12-C13-C14-C15
28	a	611	LMG	O1-C7-C8-O7
31	E	101	LHG	O7-C5-C6-O8
32	h	102	DGD	O1G-C1G-C2G-O2G
32	C	516	DGD	C5A-C6A-C7A-C8A
28	b	623	LMG	C39-C40-C41-C42
31	E	101	LHG	C10-C11-C12-C13
32	h	102	DGD	C5B-C6B-C7B-C8B
28	C	520	LMG	C8-C7-O1-C1
28	c	521	LMG	C8-C7-O1-C1
32	C	517	DGD	C2G-C3G-O3G-C1D
32	C	517	DGD	C5D-C6D-O5D-C1E
32	c	518	DGD	C2G-C3G-O3G-C1D
32	c	518	DGD	C5D-C6D-O5D-C1E
32	h	102	DGD	O2G-C1B-C2B-C3B
23	c	514	CLA	C3-C5-C6-C7
26	A	610	PL9	C15-C14-C16-C17
26	a	609	PL9	C15-C14-C16-C17
31	e	101	LHG	C19-C20-C21-C22
23	A	606	CLA	C11-C10-C8-C9
23	B	617	CLA	C14-C13-C15-C16
23	C	504	CLA	C14-C13-C15-C16
23	C	512	CLA	C11-C10-C8-C9
23	a	605	CLA	C11-C10-C8-C9
23	b	619	CLA	C14-C13-C15-C16
23	c	505	CLA	C14-C13-C15-C16
23	c	513	CLA	C11-C10-C8-C9
28	z	101	LMG	C17-C18-C19-C20
23	C	513	CLA	C3-C5-C6-C7
28	j	101	LMG	C17-C18-C19-C20
32	C	516	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
32	c	518	DGD	CBA-CCA-CDA-CEA
32	d	405	DGD	CDB-CEB-CFB-CGB
31	D	407	LHG	C33-C34-C35-C36
32	c	517	DGD	CDA-CEA-CFA-CGA
25	k	101	BCR	C37-C22-C23-C24
32	c	519	DGD	CAB-CBB-CCB-CDB
26	a	609	PL9	C28-C29-C31-C32
23	c	505	CLA	O1D-CGD-O2D-CED
27	B	623	SQD	C14-C15-C16-C17
27	b	602	SQD	C14-C15-C16-C17
31	d	406	LHG	C10-C11-C12-C13
32	c	519	DGD	C3A-C4A-C5A-C6A
27	B	623	SQD	C46-C45-O47-C7
27	b	602	SQD	C46-C45-O47-C7
23	C	505	CLA	C2A-CAA-CBA-CGA
23	B	602	CLA	C2-C1-O2A-CGA
23	C	506	CLA	C2-C1-O2A-CGA
23	b	619	CLA	C2-C1-O2A-CGA
31	a	614	LHG	C13-C14-C15-C16
31	l	101	LHG	C11-C10-C9-C8
32	C	518	DGD	C7A-C8A-C9A-CAA
32	h	102	DGD	CDA-CEA-CFA-CGA
28	A	612	LMG	C11-C12-C13-C14
32	c	517	DGD	CBA-CCA-CDA-CEA
26	A	610	PL9	C35-C34-C36-C37
26	D	405	PL9	C30-C29-C31-C32
23	c	507	CLA	O1D-CGD-O2D-CED
32	d	405	DGD	C2A-C1A-O1G-C1G
23	C	512	CLA	C16-C17-C18-C19
23	c	513	CLA	C16-C17-C18-C19
28	A	612	LMG	O6-C1-O1-C7
32	C	516	DGD	C2E-C1E-O5D-C6D
28	a	611	LMG	C39-C40-C41-C42
32	C	516	DGD	CBA-CCA-CDA-CEA
31	E	101	LHG	C3-O3-P-O6
31	E	101	LHG	C4-O6-P-O3
31	e	101	LHG	C3-O3-P-O6
23	B	611	CLA	C16-C17-C18-C20
32	c	518	DGD	C7A-C8A-C9A-CAA
31	E	101	LHG	C4-C5-C6-O8
26	A	610	PL9	C45-C44-C46-C47
23	C	506	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	c	507	CLA	C12-C13-C15-C16
23	d	403	CLA	C11-C12-C13-C15
32	C	517	DGD	C7A-C8A-C9A-CAA
23	A	608	CLA	C11-C10-C8-C9
23	B	602	CLA	C6-C7-C8-C9
23	B	616	CLA	C11-C10-C8-C9
23	C	506	CLA	C6-C7-C8-C9
23	C	513	CLA	C6-C7-C8-C9
23	a	607	CLA	C11-C10-C8-C9
23	b	604	CLA	C6-C7-C8-C9
23	b	618	CLA	C11-C10-C8-C9
23	c	507	CLA	C6-C7-C8-C9
23	c	514	CLA	C6-C7-C8-C9
25	B	619	BCR	C19-C20-C21-C22
23	b	613	CLA	C16-C17-C18-C20
32	C	518	DGD	C2A-C1A-O1G-C1G
28	c	520	LMG	C14-C15-C16-C17
32	h	102	DGD	CAB-CBB-CCB-CDB
23	C	502	CLA	C16-C17-C18-C19
23	c	503	CLA	C16-C17-C18-C19
23	b	614	CLA	CBA-CGA-O2A-C1
31	b	624	LHG	O1-C1-C2-C3
31	a	614	LHG	C16-C17-C18-C19
23	B	606	CLA	O1A-CGA-O2A-C1
32	c	518	DGD	C4E-C5E-C6E-O5E
23	B	616	CLA	C16-C17-C18-C19
23	b	618	CLA	C16-C17-C18-C19
28	c	521	LMG	C29-C28-O8-C9
26	a	609	PL9	C2-C3-C7-C8
23	c	511	CLA	O1A-CGA-O2A-C1
32	C	516	DGD	C8A-C9A-CAA-CBA
28	a	611	LMG	C17-C18-C19-C20
31	b	624	LHG	C11-C10-C9-C8
23	a	607	CLA	O1A-CGA-O2A-C1
23	c	513	CLA	CBA-CGA-O2A-C1
28	B	621	LMG	C36-C37-C38-C39
32	C	516	DGD	CBB-CCB-CDB-CEB
23	B	602	CLA	C2A-CAA-CBA-CGA
25	K	101	BCR	C19-C20-C21-C22
25	b	620	BCR	C13-C14-C15-C16
25	b	622	BCR	C9-C10-C11-C12
25	t	101	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	A	612	LMG	C19-C20-C21-C22
31	E	101	LHG	O6-C4-C5-O7
23	B	611	CLA	C13-C15-C16-C17
23	b	613	CLA	C13-C15-C16-C17
27	b	601	SQD	C10-C11-C12-C13
28	c	521	LMG	C36-C37-C38-C39
27	a	612	SQD	C10-C11-C12-C13
23	b	605	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
23	c	502	CLA	C2A-CAA-CBA-CGA
23	c	514	CLA	O1D-CGD-O2D-CED
23	B	616	CLA	C3A-C2A-CAA-CBA
23	b	618	CLA	C3A-C2A-CAA-CBA
28	b	623	LMG	C35-C36-C37-C38
28	c	520	LMG	C22-C23-C24-C25
23	b	604	CLA	CBA-CGA-O2A-C1
32	c	517	DGD	C4E-C5E-C6E-O5E
28	A	612	LMG	C16-C17-C18-C19
26	d	404	PL9	C12-C11-C9-C10
28	z	101	LMG	C18-C19-C20-C21
32	C	517	DGD	CBA-CCA-CDA-CEA
32	D	406	DGD	C3B-C4B-C5B-C6B
28	a	611	LMG	O6-C5-C6-O5
28	b	623	LMG	C30-C31-C32-C33
32	C	517	DGD	C5B-C6B-C7B-C8B
32	C	518	DGD	C4B-C5B-C6B-C7B
28	b	623	LMG	C36-C37-C38-C39
32	c	519	DGD	C5B-C6B-C7B-C8B
25	B	618	BCR	C11-C10-C9-C34
23	C	510	CLA	C8-C10-C11-C12
28	j	101	LMG	C32-C33-C34-C35
23	C	512	CLA	C16-C17-C18-C20
23	c	513	CLA	C16-C17-C18-C20
23	D	403	CLA	O2A-C1-C2-C3
23	d	402	CLA	O2A-C1-C2-C3
32	H	102	DGD	O1B-C1B-C2B-C3B
23	B	617	CLA	C13-C15-C16-C17
23	c	511	CLA	C8-C10-C11-C12
23	b	619	CLA	C13-C15-C16-C17
23	B	611	CLA	C1A-C2A-CAA-CBA
23	A	608	CLA	C12-C13-C15-C16
23	B	607[B]	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	C	502	CLA	C12-C13-C15-C16
23	C	504	CLA	C11-C10-C8-C7
23	a	607	CLA	C12-C13-C15-C16
23	b	609[B]	CLA	C11-C10-C8-C7
23	c	503	CLA	C12-C13-C15-C16
23	c	505	CLA	C11-C10-C8-C7
28	B	621	LMG	C35-C36-C37-C38
23	b	604	CLA	O1A-CGA-O2A-C1
23	b	612	CLA	O1A-CGA-O2A-C1
23	C	501	CLA	C2A-CAA-CBA-CGA
23	b	613	CLA	C2A-CAA-CBA-CGA
23	b	617	CLA	C2A-CAA-CBA-CGA
28	C	519	LMG	C22-C23-C24-C25
32	C	518	DGD	CBA-CCA-CDA-CEA
32	c	518	DGD	C8A-C9A-CAA-CBA
28	c	521	LMG	C39-C40-C41-C42
28	j	101	LMG	C11-C12-C13-C14
32	c	518	DGD	C5B-C6B-C7B-C8B
32	c	518	DGD	CDB-CEB-CFB-CGB
23	C	513	CLA	C16-C17-C18-C19
23	c	514	CLA	C16-C17-C18-C19
28	C	519	LMG	C33-C34-C35-C36
27	A	611	SQD	O6-C44-C45-O47
27	a	610	SQD	O6-C44-C45-O47
25	B	620	BCR	C9-C10-C11-C12
28	a	611	LMG	C16-C17-C18-C19
31	a	614	LHG	C11-C10-C9-C8
23	B	602	CLA	O1A-CGA-O2A-C1
26	D	405	PL9	C34-C36-C37-C38
23	b	604	CLA	CAA-CBA-CGA-O1A
23	c	507	CLA	C2-C1-O2A-CGA
31	b	624	LHG	C17-C18-C19-C20
28	c	521	LMG	C16-C17-C18-C19
26	A	610	PL9	C2-C3-C7-C8
23	B	602	CLA	CAA-CBA-CGA-O2A
32	h	102	DGD	CAA-CBA-CCA-CDA
23	B	604	CLA	C2A-CAA-CBA-CGA
23	C	504	CLA	O1A-CGA-O2A-C1
31	a	614	LHG	O10-C23-O8-C6
25	C	515	BCR	C1-C6-C7-C8
25	C	515	BCR	C23-C24-C25-C30
25	F	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	c	515	BCR	C1-C6-C7-C8
25	f	101	BCR	C1-C6-C7-C8
28	J	101	LMG	C7-C8-C9-O8
25	b	622	BCR	C13-C14-C15-C16
23	C	513	CLA	C4-C3-C5-C6
23	c	514	CLA	C4-C3-C5-C6
23	B	610	CLA	C2-C3-C5-C6
23	b	612	CLA	C2-C3-C5-C6
32	C	516	DGD	C5D-C6D-O5D-C1E
28	A	612	LMG	C39-C40-C41-C42
28	c	520	LMG	C31-C32-C33-C34
32	C	516	DGD	CDA-CEA-CFA-CGA
32	c	517	DGD	C8A-C9A-CAA-CBA
32	c	517	DGD	O6E-C1E-O5D-C6D
23	C	507	CLA	C4-C3-C5-C6
23	c	508	CLA	C4-C3-C5-C6
32	c	518	DGD	C4B-C5B-C6B-C7B
23	b	615	CLA	CBA-CGA-O2A-C1
23	B	604	CLA	CBD-CGD-O2D-CED
28	C	520	LMG	C11-C12-C13-C14
23	c	511	CLA	CAA-CBA-CGA-O2A
32	D	406	DGD	O2G-C2G-C3G-O3G
28	J	101	LMG	C11-C12-C13-C14
23	B	609	CLA	C4C-C3C-CAC-CBC
25	C	521	BCR	C16-C17-C18-C36
32	c	519	DGD	O6D-C5D-C6D-O5D
26	a	609	PL9	C35-C34-C36-C37
23	c	511	CLA	CBA-CGA-O2A-C1
31	D	408	LHG	C24-C23-O8-C6
27	b	602	SQD	C33-C34-C35-C36
23	B	607[A]	CLA	C11-C12-C13-C14
23	B	607[B]	CLA	C11-C10-C8-C9
23	C	510	CLA	C6-C7-C8-C9
23	D	404	CLA	C11-C12-C13-C14
23	b	609[A]	CLA	C11-C12-C13-C14
23	b	609[B]	CLA	C11-C10-C8-C9
23	c	511	CLA	C6-C7-C8-C9
23	d	403	CLA	C11-C12-C13-C14
27	B	623	SQD	C33-C34-C35-C36
23	B	604	CLA	C13-C15-C16-C17
23	b	606	CLA	C13-C15-C16-C17
23	B	611	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	C	501	CLA	CAD-CBD-CGD-O2D
23	C	506	CLA	CAD-CBD-CGD-O2D
23	C	508	CLA	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	615	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
24	A	607	PHO	CAD-CBD-CGD-O2D
31	l	101	LHG	O10-C23-O8-C6
27	B	623	SQD	C17-C18-C19-C20
32	H	102	DGD	C4D-C5D-C6D-O5D
23	A	608	CLA	C4-C3-C5-C6
23	a	607	CLA	C4-C3-C5-C6
26	d	404	PL9	C15-C14-C16-C17
28	B	621	LMG	C39-C40-C41-C42
31	L	101	LHG	O7-C7-C8-C9
31	e	101	LHG	O7-C7-C8-C9
32	C	518	DGD	O1G-C1A-C2A-C3A
32	c	519	DGD	O1G-C1A-C2A-C3A
27	b	602	SQD	C17-C18-C19-C20
28	c	520	LMG	O10-C28-O8-C9
26	D	405	PL9	C14-C16-C17-C18
23	B	609	CLA	C2C-C3C-CAC-CBC
23	D	402	CLA	C2C-C3C-CAC-CBC
31	E	101	LHG	O7-C7-C8-C9
31	l	101	LHG	O7-C7-C8-C9
23	B	605	CLA	O2A-C1-C2-C3
23	B	614	CLA	O2A-C1-C2-C3
23	b	605	CLA	O2A-C1-C2-C3
23	b	607	CLA	O2A-C1-C2-C3
24	A	607	PHO	O2A-C1-C2-C3
24	a	606	PHO	O2A-C1-C2-C3
23	C	503	CLA	CBD-CGD-O2D-CED
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	610	CLA	CHA-CBD-CGD-O1D
23	B	613	CLA	CHA-CBD-CGD-O2D
23	C	502	CLA	CHA-CBD-CGD-O2D
23	C	507	CLA	CHA-CBD-CGD-O2D
23	C	511	CLA	CHA-CBD-CGD-O1D
23	c	505	CLA	CHA-CBD-CGD-O1D
23	c	506	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	512	CLA	CHA-CBD-CGD-O1D
24	D	401	PHO	CHA-CBD-CGD-O2D
24	d	401	PHO	CHA-CBD-CGD-O2D
26	D	405	PL9	C12-C11-C9-C8
32	H	102	DGD	C7B-C8B-C9B-CAB
23	B	607[A]	CLA	C16-C17-C18-C20
23	b	609[A]	CLA	C16-C17-C18-C20
32	c	518	DGD	C6A-C7A-C8A-C9A
32	d	405	DGD	O2G-C2G-C3G-O3G
28	b	623	LMG	C13-C14-C15-C16
23	c	513	CLA	CAA-CBA-CGA-O2A
28	J	101	LMG	O7-C10-C11-C12
32	H	102	DGD	CAB-CBB-CCB-CDB
23	A	608	CLA	C11-C12-C13-C15
23	a	607	CLA	C11-C12-C13-C15
31	b	624	LHG	C15-C16-C17-C18
23	B	605	CLA	C6-C7-C8-C9
23	C	504	CLA	C11-C10-C8-C9
23	C	505	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	D	404	CLA	C14-C13-C15-C16
23	b	607	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C10-C8-C9
23	c	506	CLA	C14-C13-C15-C16
23	c	507	CLA	C14-C13-C15-C16
23	d	403	CLA	C14-C13-C15-C16
26	d	404	PL9	C24-C26-C27-C28
26	d	404	PL9	C34-C36-C37-C38
23	C	510	CLA	CAA-CBA-CGA-O2A
27	A	611	SQD	C18-C19-C20-C21
27	a	610	SQD	C18-C19-C20-C21
26	A	610	PL9	C21-C22-C23-C24
26	d	404	PL9	C36-C37-C38-C39
31	D	408	LHG	O10-C23-C24-C25
23	C	512	CLA	CAA-CBA-CGA-O2A
32	C	518	DGD	CDB-CEB-CFB-CGB
23	C	513	CLA	C16-C17-C18-C20
23	c	514	CLA	C16-C17-C18-C20
23	B	610	CLA	C4-C3-C5-C6
23	b	612	CLA	C4-C3-C5-C6
23	B	614	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	B	621	LMG	C13-C14-C15-C16
31	a	614	LHG	C18-C19-C20-C21
23	B	602	CLA	C1A-C2A-CAA-CBA
23	B	603	CLA	C1A-C2A-CAA-CBA
23	B	609	CLA	C1A-C2A-CAA-CBA
23	B	610	CLA	C1A-C2A-CAA-CBA
23	b	605	CLA	C1A-C2A-CAA-CBA
23	b	611	CLA	C1A-C2A-CAA-CBA
23	b	612	CLA	C1A-C2A-CAA-CBA
23	b	613	CLA	C1A-C2A-CAA-CBA
23	C	512	CLA	CAA-CBA-CGA-O1A
26	a	609	PL9	C31-C32-C33-C34
32	c	518	DGD	O1B-C1B-C2B-C3B
27	a	612	SQD	C11-C12-C13-C14
27	b	601	SQD	C11-C12-C13-C14
28	B	621	LMG	C34-C35-C36-C37
28	a	611	LMG	C11-C12-C13-C14
31	D	408	LHG	O8-C23-C24-C25
23	b	611	CLA	C2A-CAA-CBA-CGA
31	b	624	LHG	C34-C35-C36-C37
28	A	612	LMG	O10-C28-C29-C30
23	B	606	CLA	C13-C15-C16-C17
23	b	608	CLA	C13-C15-C16-C17
32	c	517	DGD	C2E-C1E-O5D-C6D
31	D	408	LHG	C4-O6-P-O5
31	d	406	LHG	C4-O6-P-O5
23	c	511	CLA	CAA-CBA-CGA-O1A
32	C	517	DGD	O1B-C1B-C2B-C3B
32	d	405	DGD	O1A-C1A-C2A-C3A
25	T	101	BCR	C5-C6-C7-C8
25	k	101	BCR	C5-C6-C7-C8
23	c	510	CLA	O1D-CGD-O2D-CED
32	C	518	DGD	C4A-C5A-C6A-C7A
31	E	101	LHG	C12-C13-C14-C15
32	h	102	DGD	C7B-C8B-C9B-CAB
25	C	521	BCR	C18-C19-C20-C21
23	c	506	CLA	C2A-CAA-CBA-CGA
31	L	101	LHG	O10-C23-O8-C6
24	D	401	PHO	C8-C10-C11-C12
23	b	617	CLA	CBD-CGD-O2D-CED
26	a	609	PL9	C21-C22-C23-C24
23	B	610	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	c	505	CLA	CAD-CBD-CGD-O1D
31	a	614	LHG	O10-C23-C24-C25
32	C	516	DGD	CCA-CDA-CEA-CFA
32	D	406	DGD	O6D-C5D-C6D-O5D
23	A	608	CLA	C14-C13-C15-C16
23	B	607[B]	CLA	C14-C13-C15-C16
23	C	511	CLA	C6-C7-C8-C9
23	D	402	CLA	C11-C12-C13-C14
23	a	607	CLA	C14-C13-C15-C16
23	a	613	CLA	C11-C12-C13-C14
23	b	609[B]	CLA	C14-C13-C15-C16
23	c	512	CLA	C6-C7-C8-C9
31	a	614	LHG	O8-C23-C24-C25
27	B	623	SQD	C45-C46-O48-C23
27	b	602	SQD	C45-C46-O48-C23
28	a	611	LMG	O10-C28-C29-C30
28	C	520	LMG	C16-C17-C18-C19
23	B	613	CLA	CAA-CBA-CGA-O2A
23	C	501	CLA	CAA-CBA-CGA-O2A
23	B	616	CLA	C15-C16-C17-C18
31	D	408	LHG	C13-C14-C15-C16
23	C	505	CLA	CAA-CBA-CGA-O1A
32	D	406	DGD	O1A-C1A-C2A-C3A
23	b	618	CLA	C15-C16-C17-C18
28	C	520	LMG	C36-C37-C38-C39
23	B	615	CLA	O1A-CGA-O2A-C1
23	B	607[B]	CLA	C12-C13-C15-C16
23	B	615	CLA	C11-C10-C8-C7
23	C	505	CLA	C12-C13-C15-C16
23	C	507	CLA	C11-C12-C13-C15
23	C	510	CLA	C6-C7-C8-C10
23	C	511	CLA	C6-C7-C8-C10
23	D	403	CLA	C12-C13-C15-C16
23	b	609[B]	CLA	C12-C13-C15-C16
23	b	617	CLA	C11-C10-C8-C7
23	c	506	CLA	C12-C13-C15-C16
23	c	508	CLA	C11-C12-C13-C15
23	c	511	CLA	C6-C7-C8-C10
23	c	512	CLA	C6-C7-C8-C10
23	d	402	CLA	C12-C13-C15-C16
24	a	606	PHO	C2-C3-C5-C6
31	l	101	LHG	O9-C7-C8-C9

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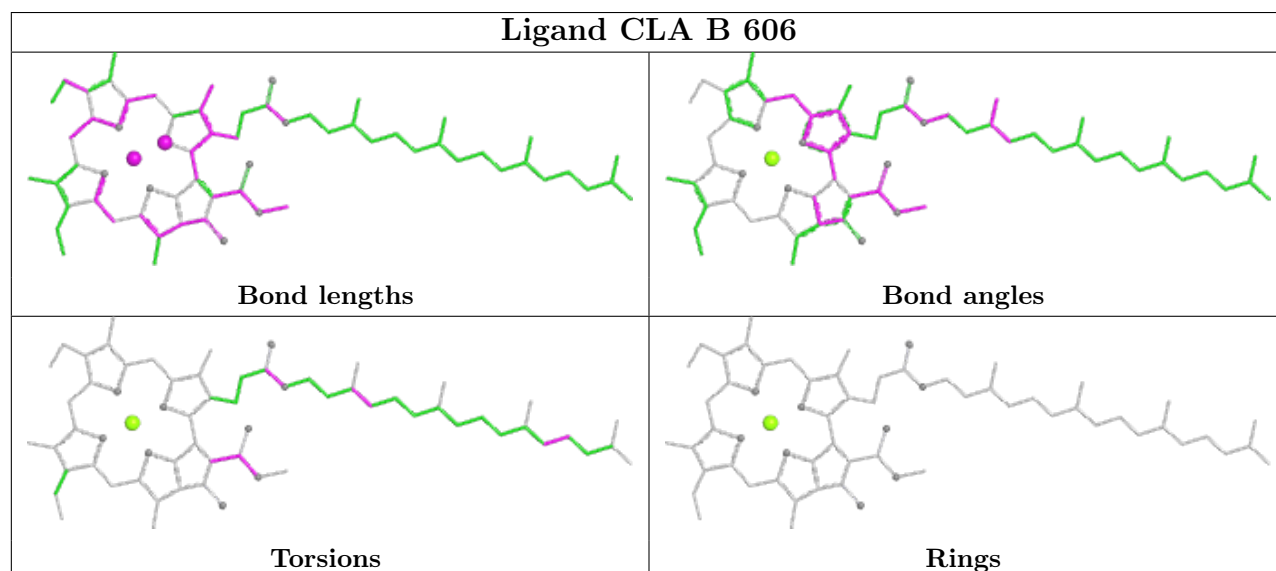
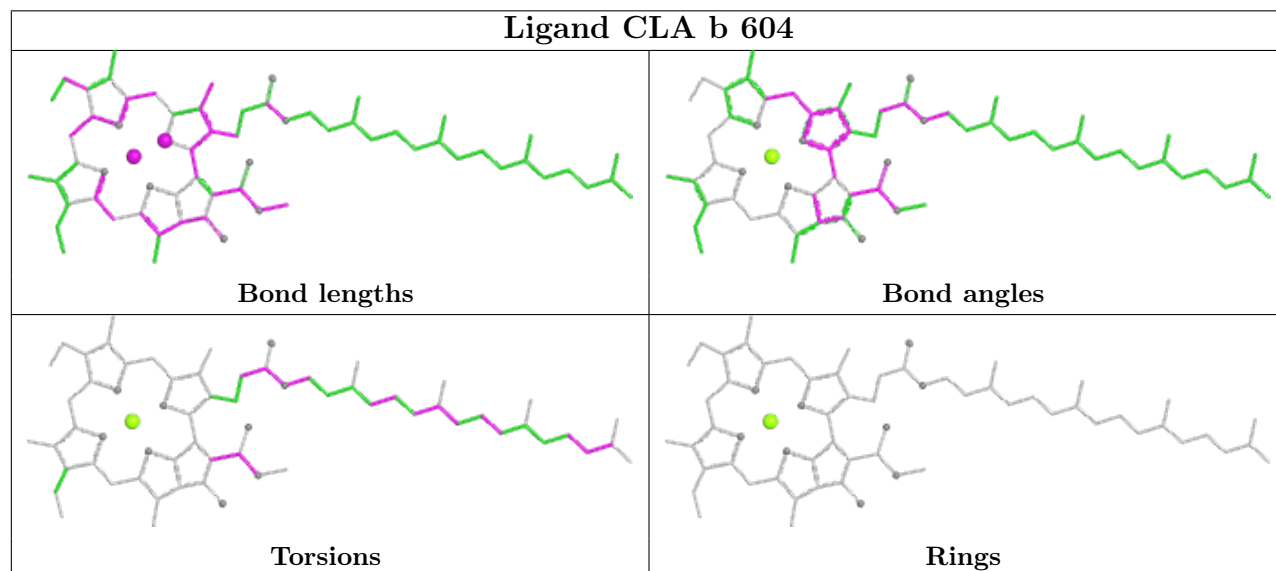
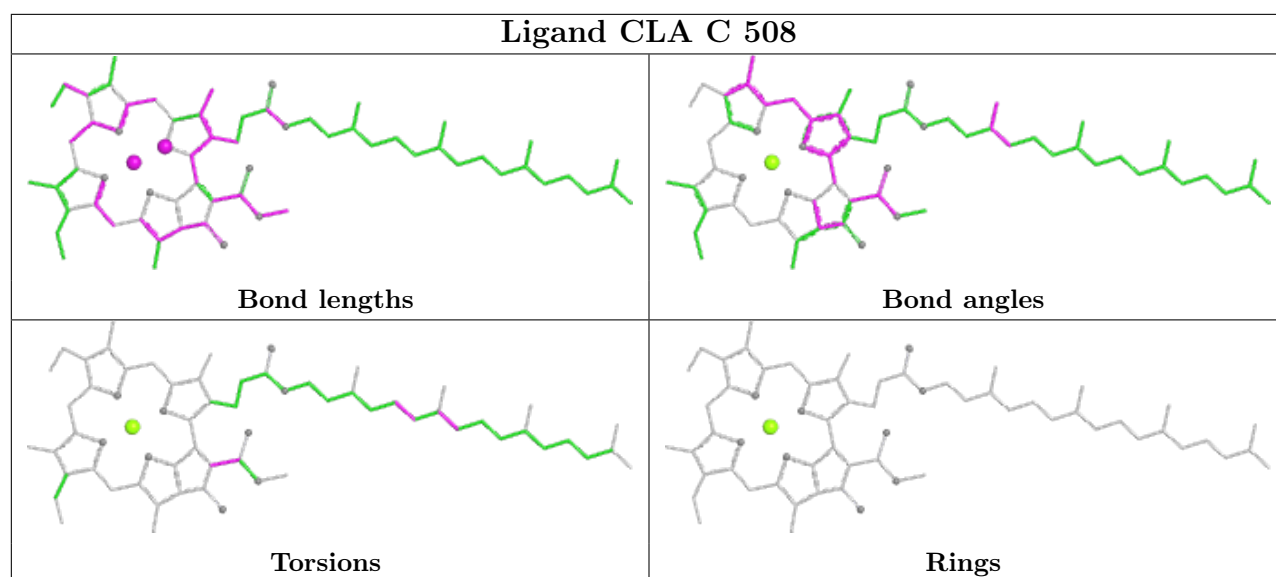
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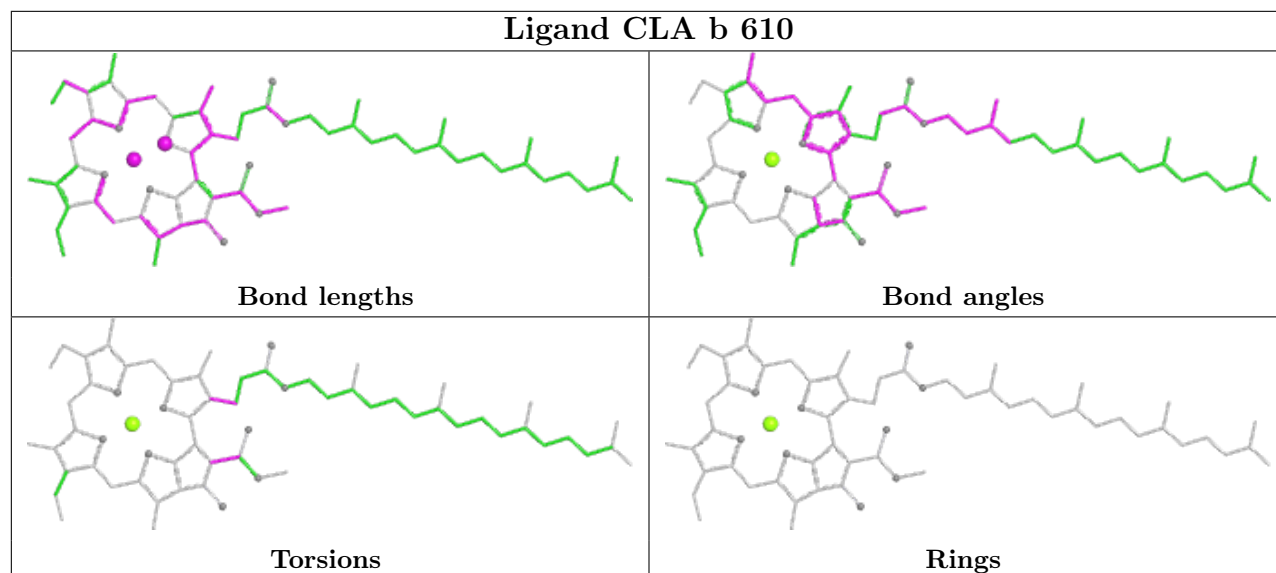
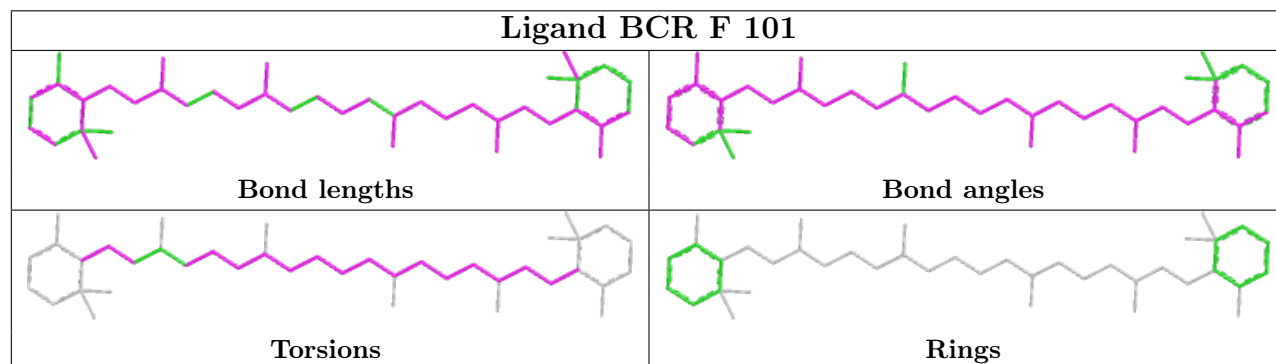
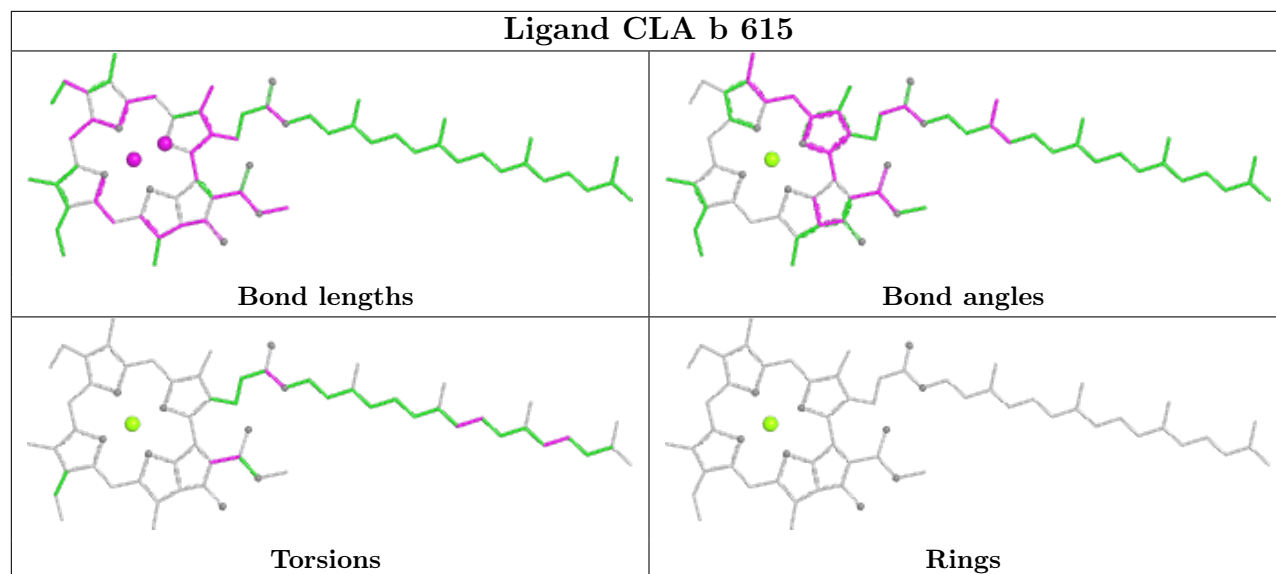
Mol	Chain	Res	Type	Atoms
23	c	502	CLA	CAA-CBA-CGA-O2A
28	j	101	LMG	O7-C10-C11-C12
31	D	407	LHG	O8-C23-C24-C25
32	c	518	DGD	O2G-C1B-C2B-C3B
25	C	514	BCR	C7-C8-C9-C10
31	e	101	LHG	O10-C23-C24-C25
32	d	405	DGD	O1G-C1A-C2A-C3A
23	b	615	CLA	C8-C10-C11-C12
28	J	101	LMG	C29-C28-O8-C9
26	D	405	PL9	C19-C21-C22-C23
23	B	613	CLA	C8-C10-C11-C12
28	a	611	LMG	C21-C22-C23-C24
32	C	517	DGD	O2G-C1B-C2B-C3B
31	L	101	LHG	O9-C7-C8-C9
31	e	101	LHG	O9-C7-C8-C9
23	C	506	CLA	C15-C16-C17-C18
23	c	507	CLA	C15-C16-C17-C18
32	h	102	DGD	O1B-C1B-C2B-C3B
24	a	606	PHO	C4-C3-C5-C6
28	B	621	LMG	O8-C28-C29-C30
28	C	519	LMG	O7-C10-C11-C12

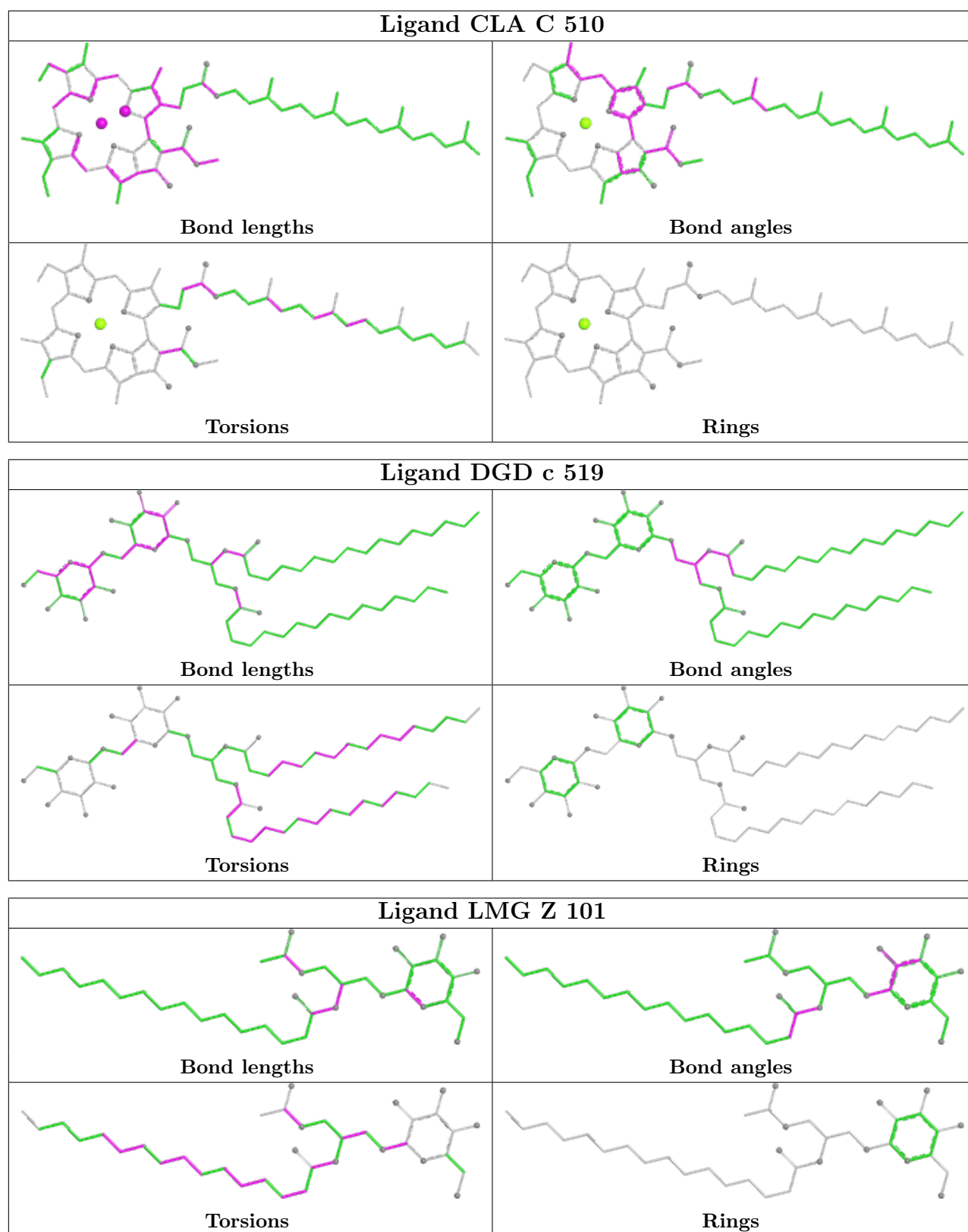
There are no ring outliers.

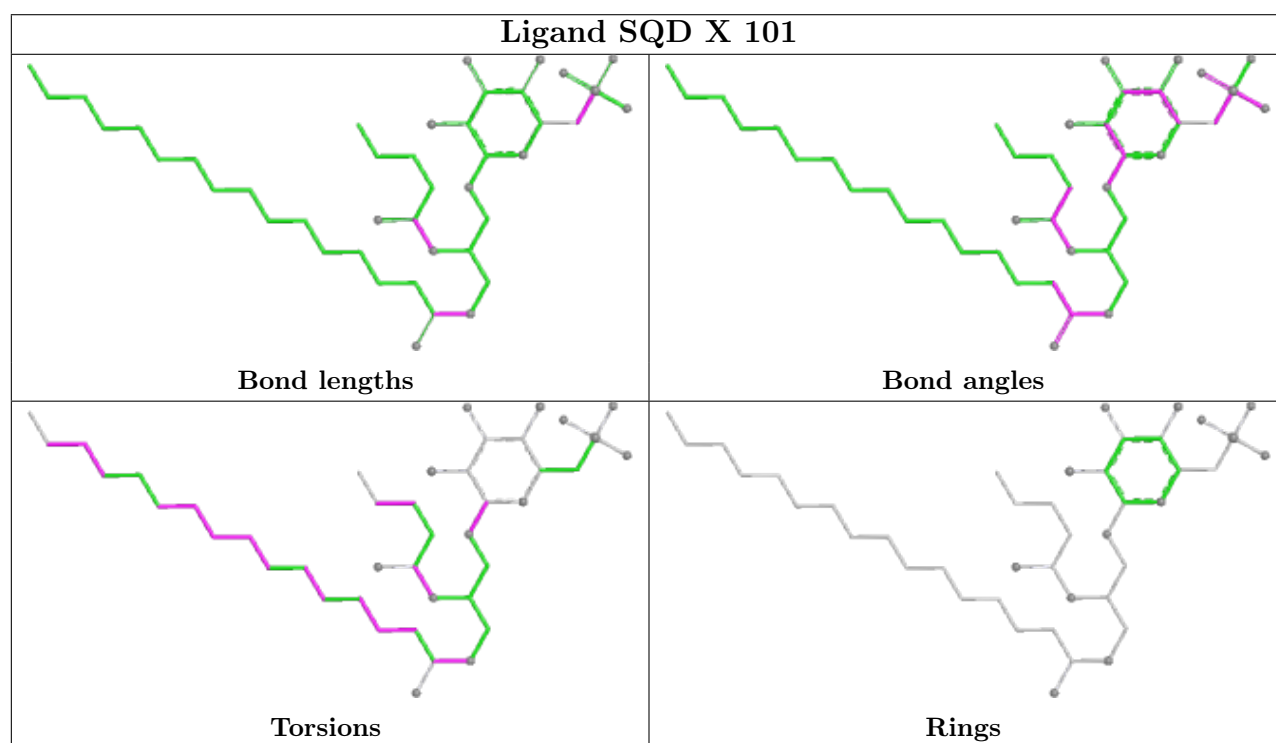
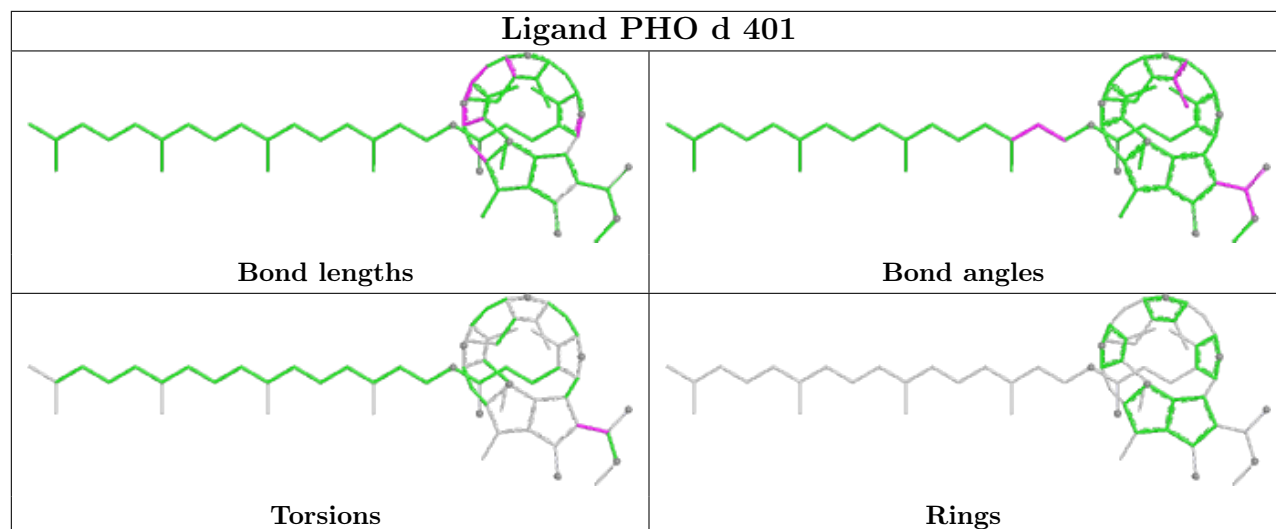
No monomer is involved in short contacts.

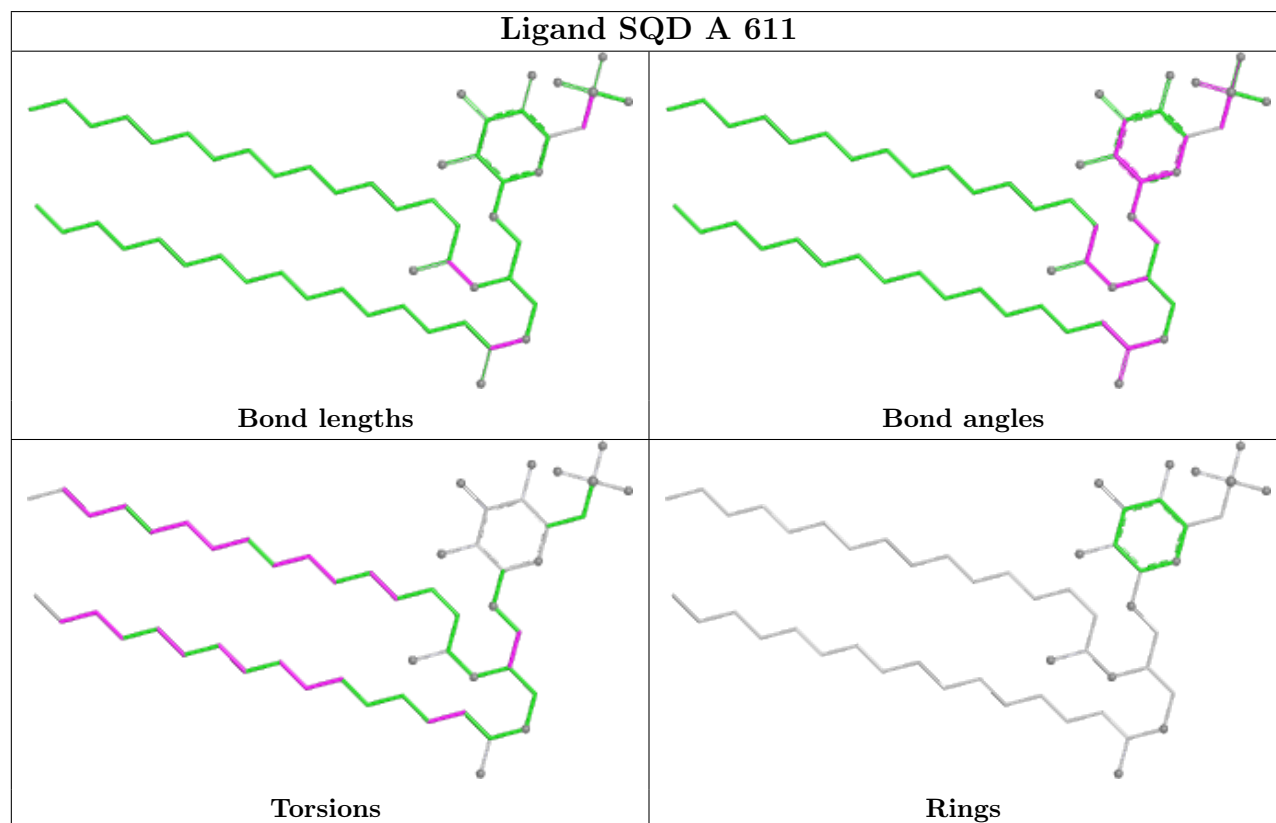
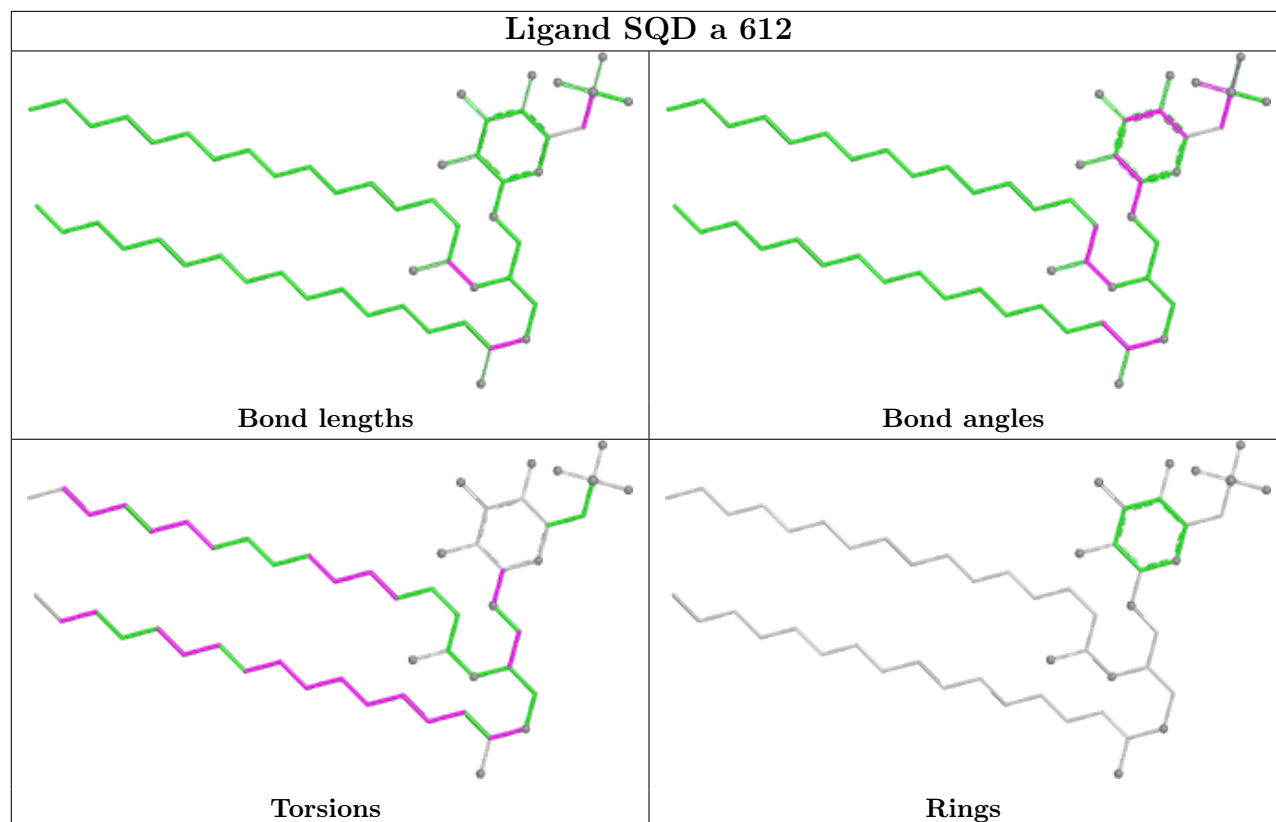
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

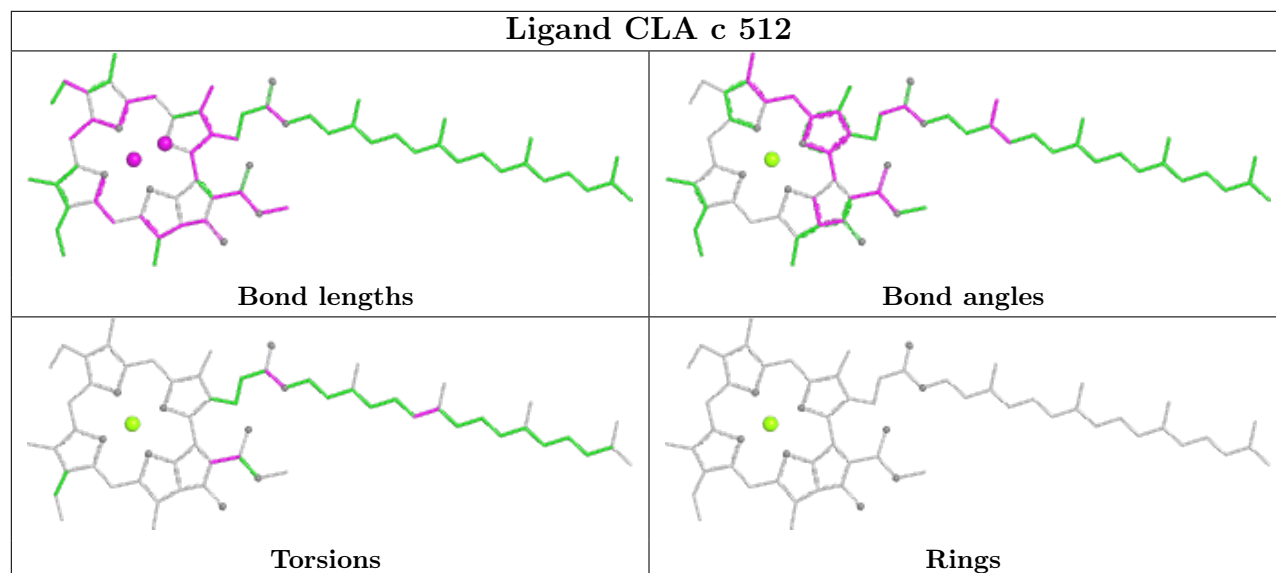
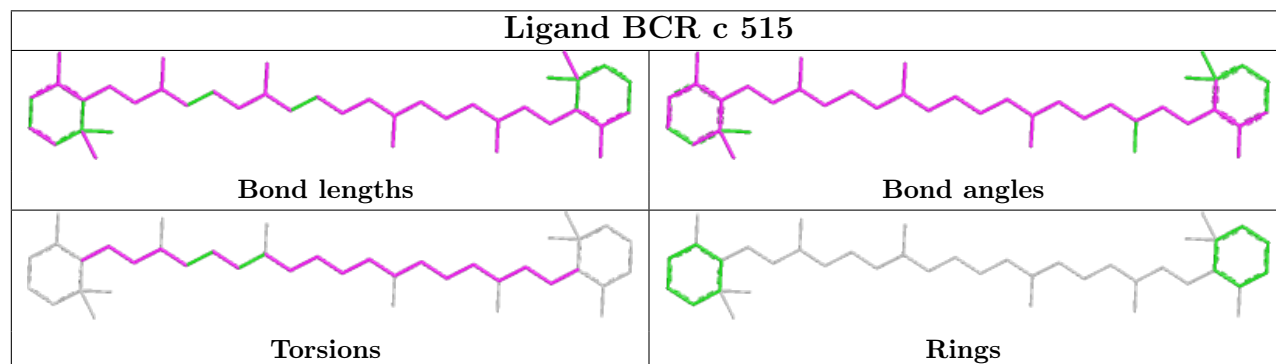
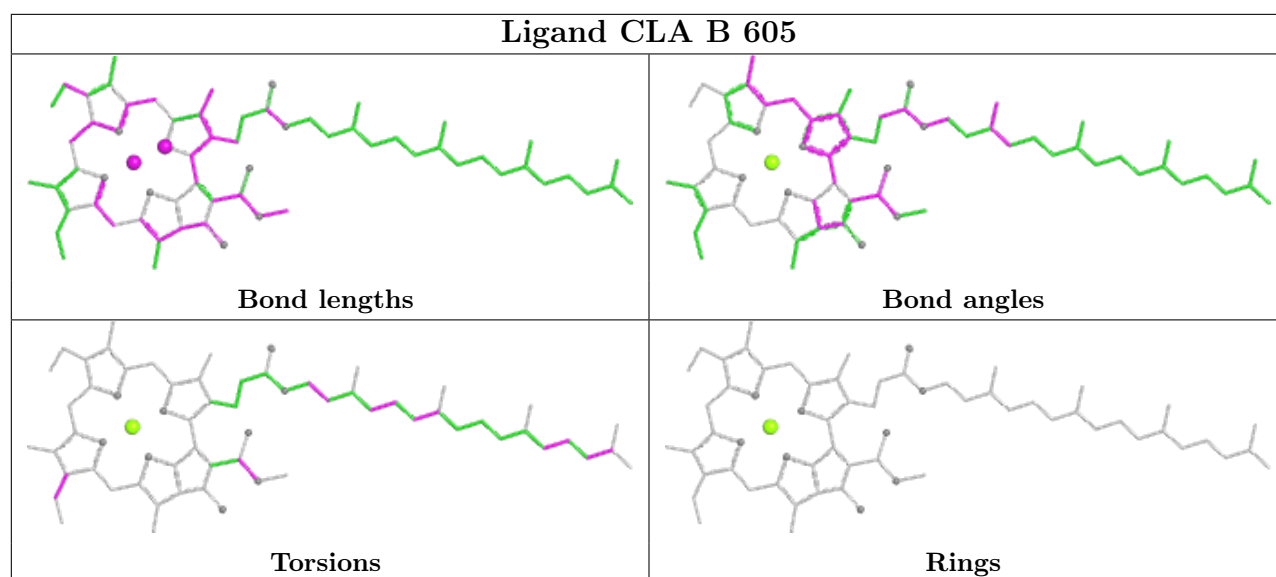


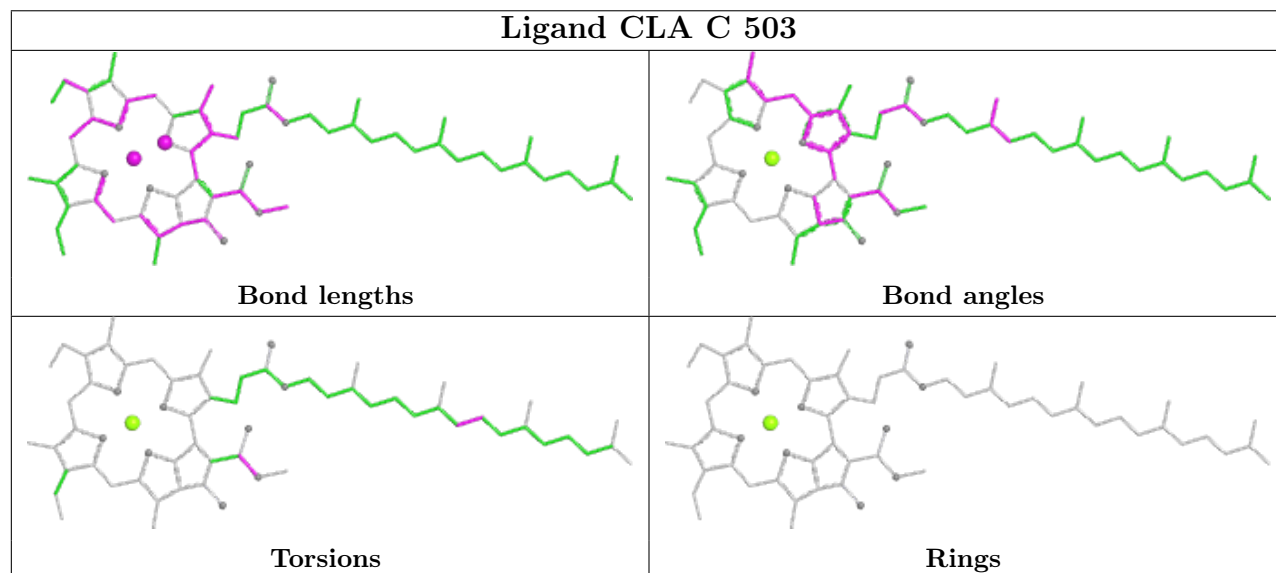
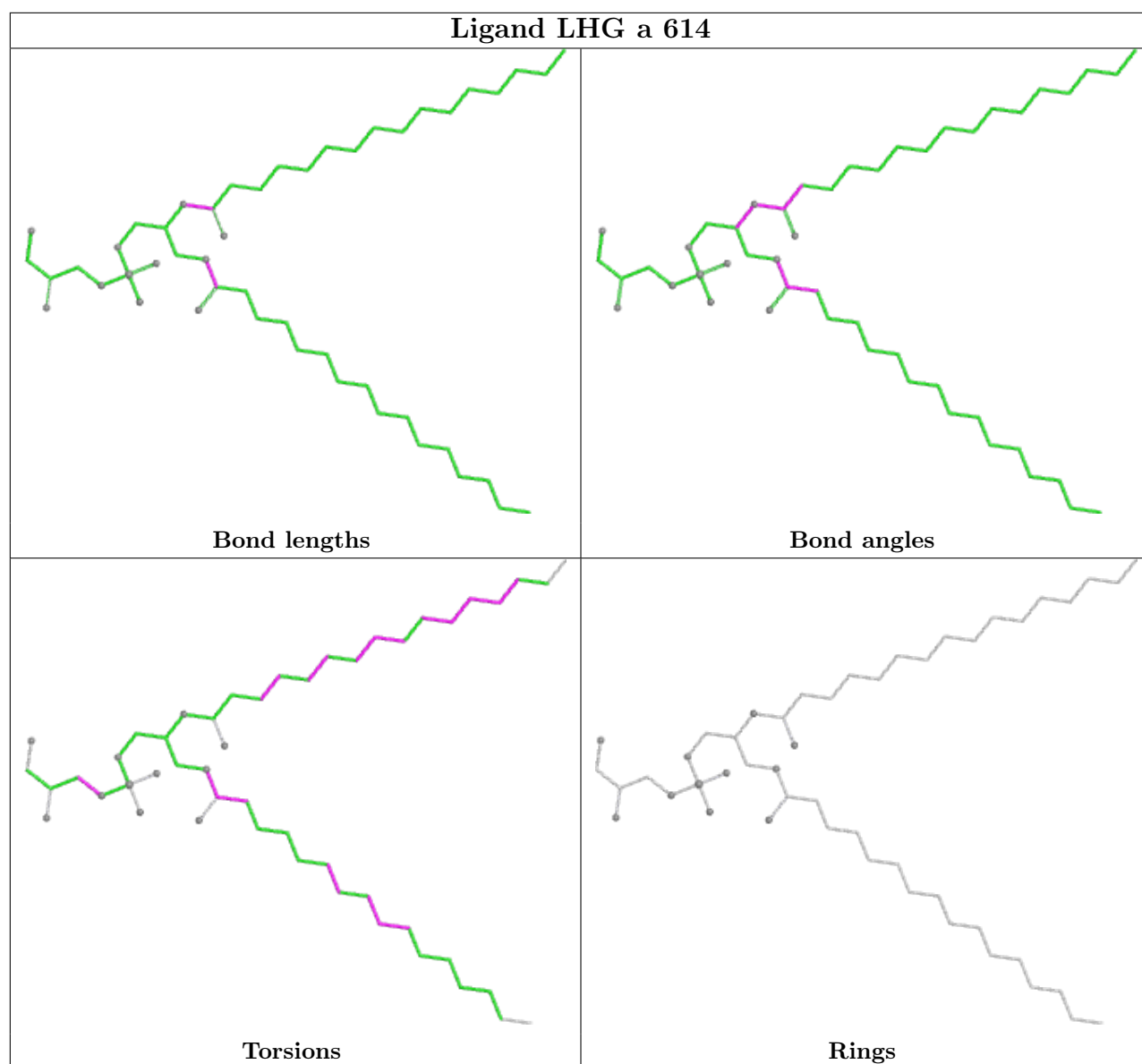


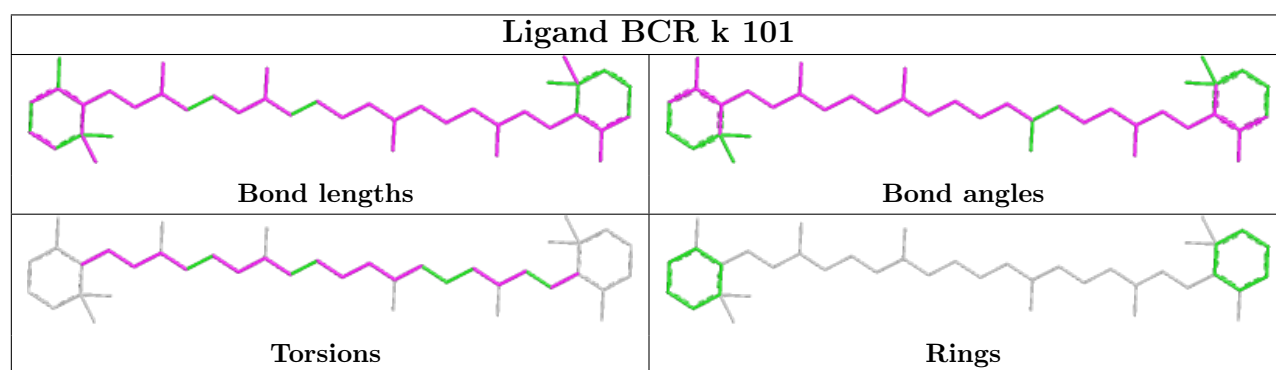
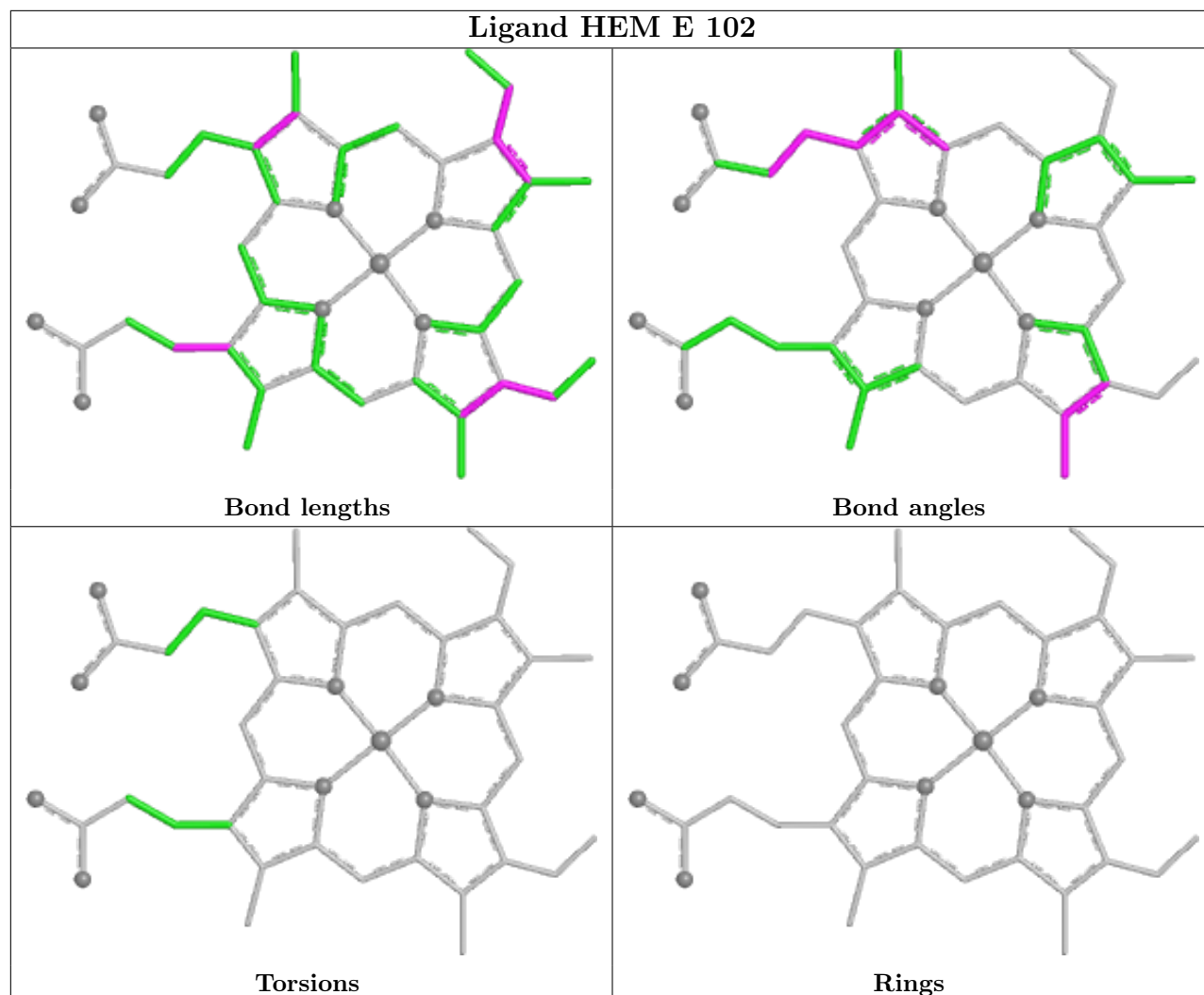


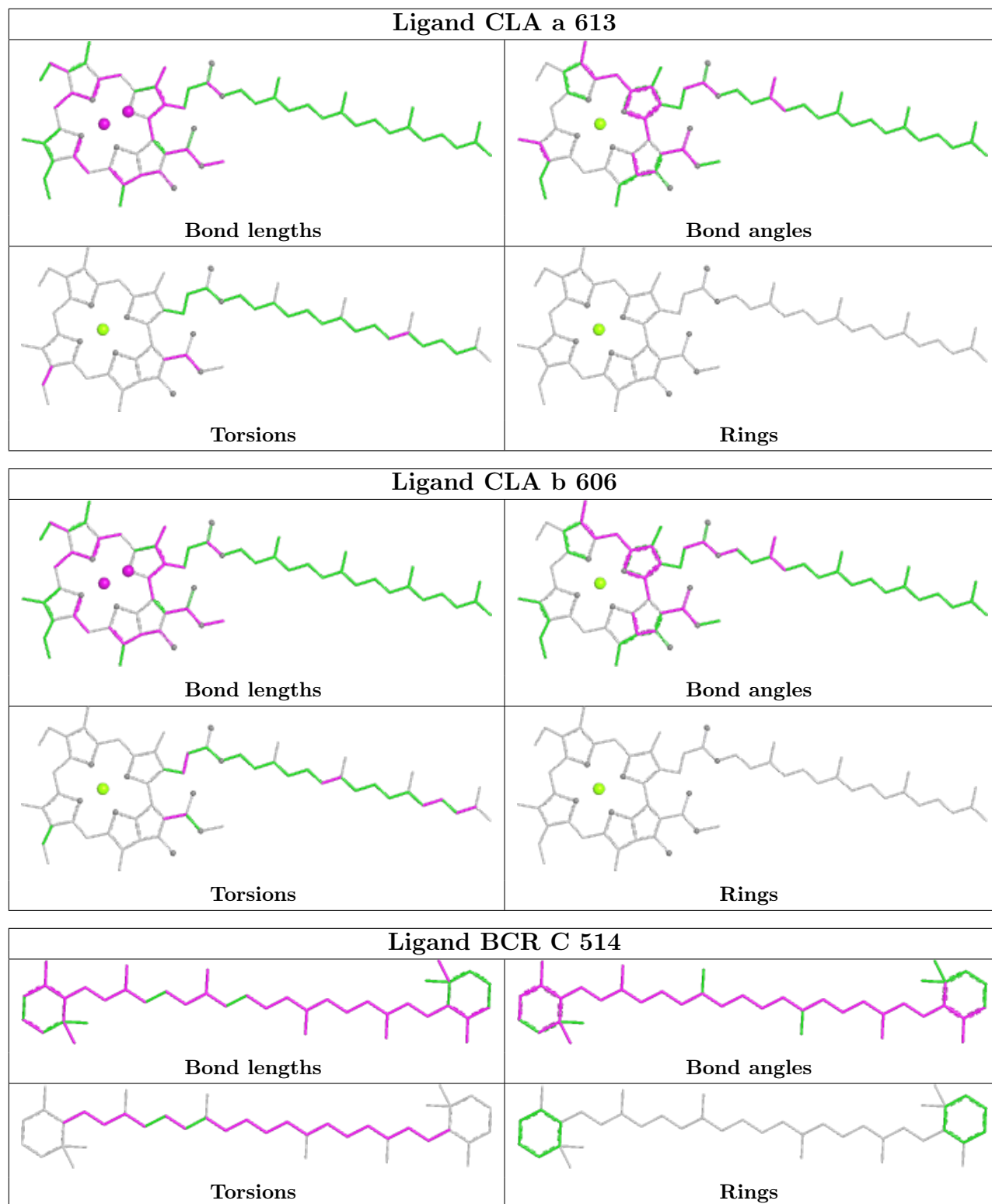




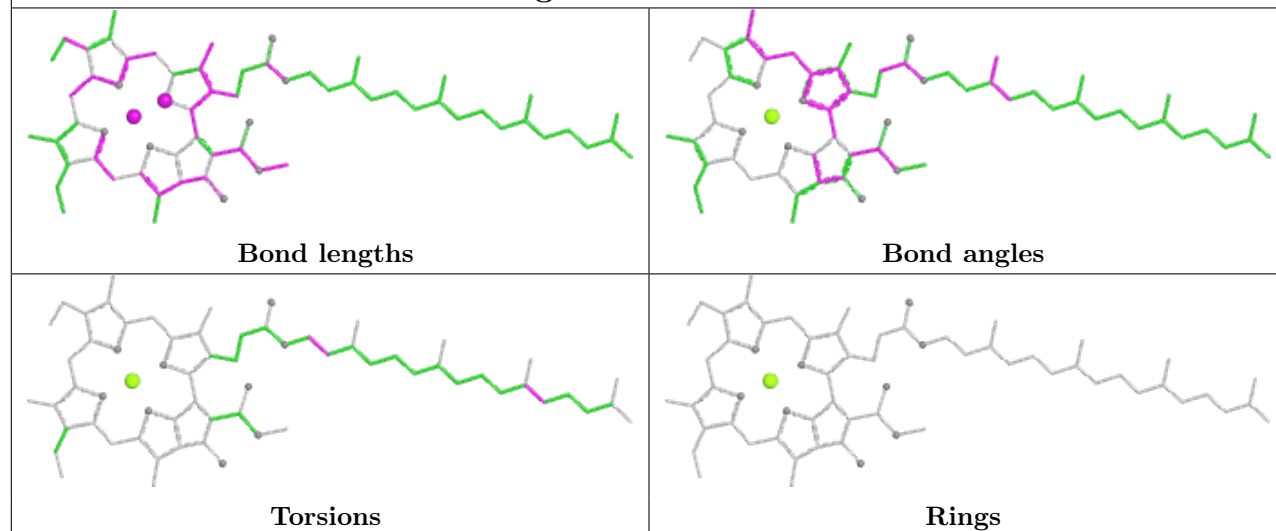




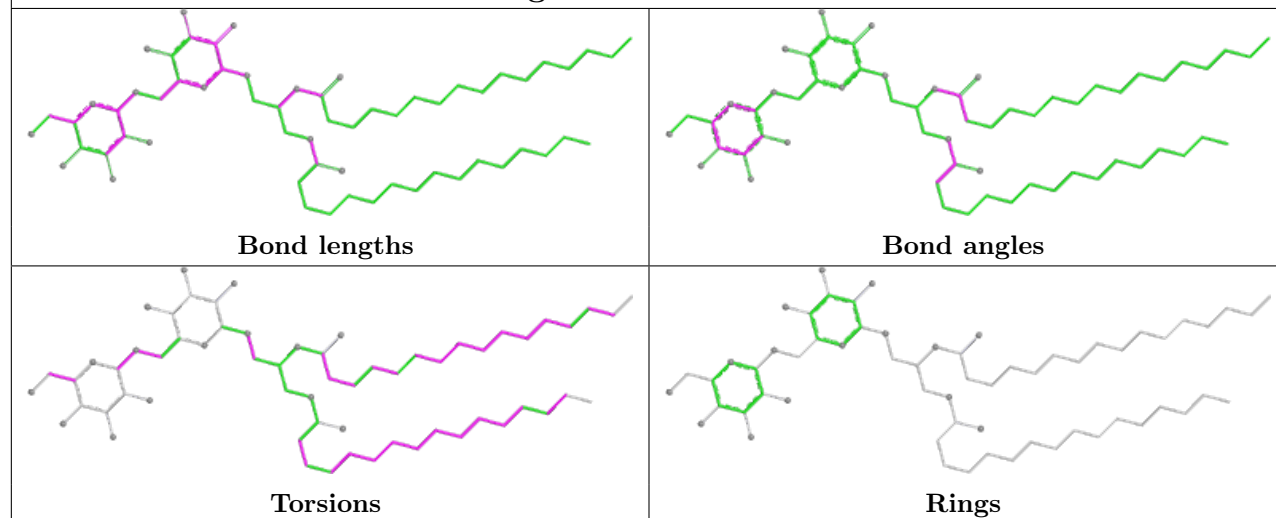




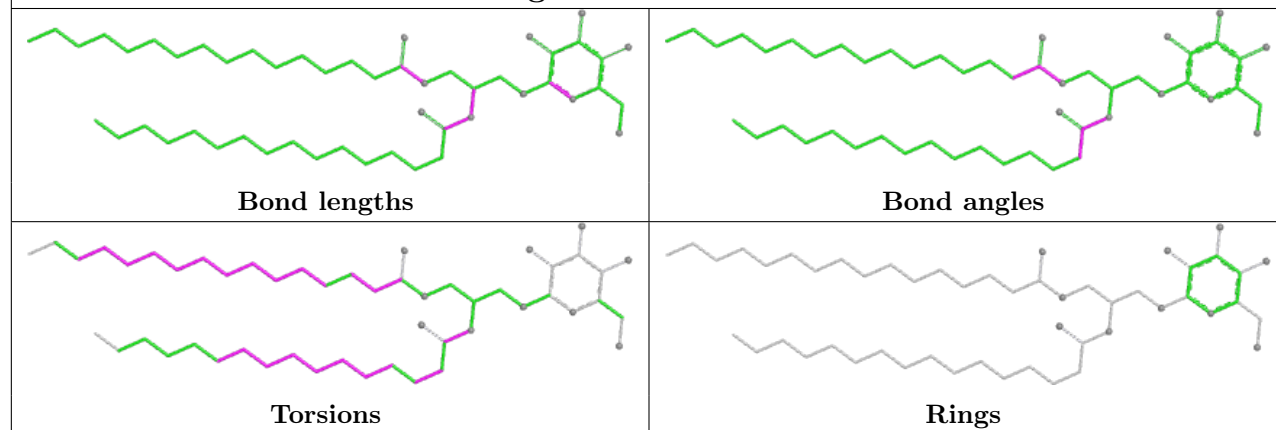
Ligand CLA d 402

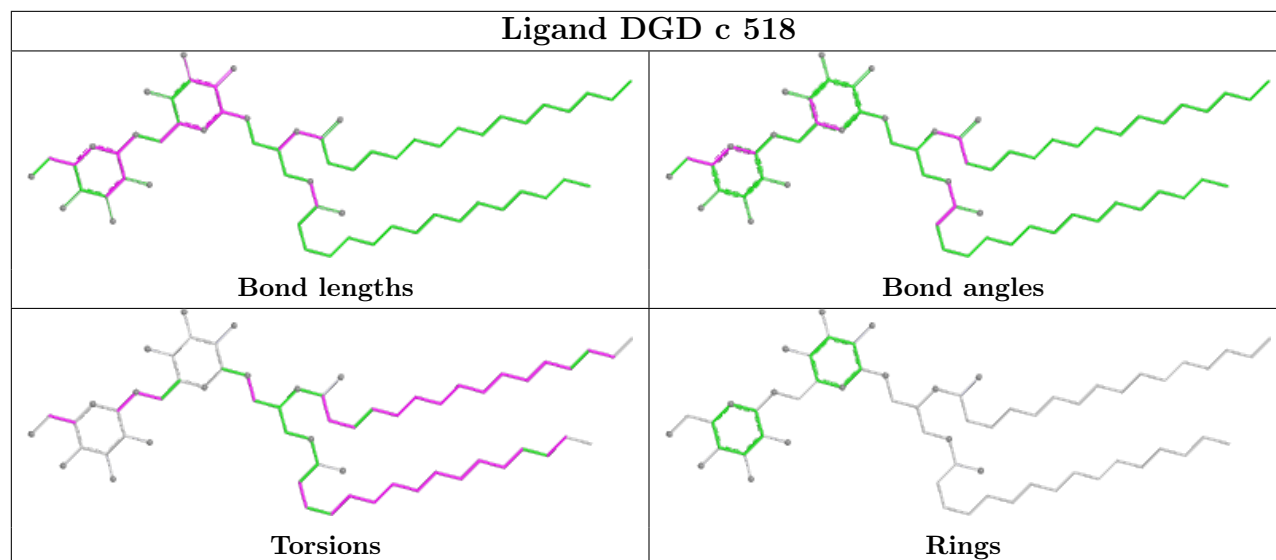
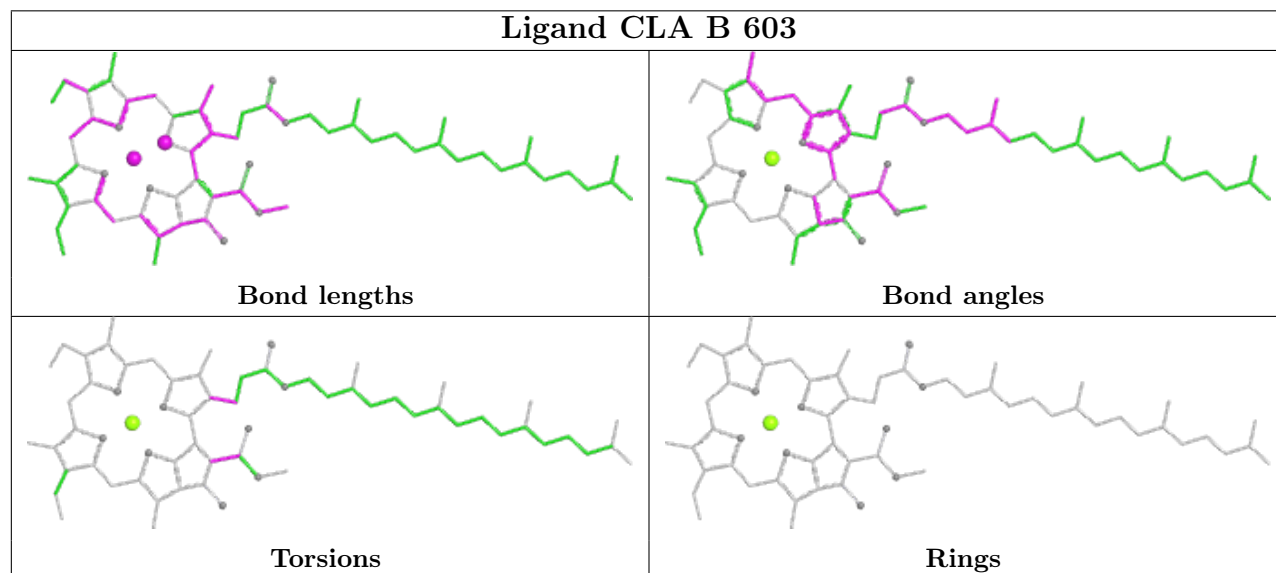
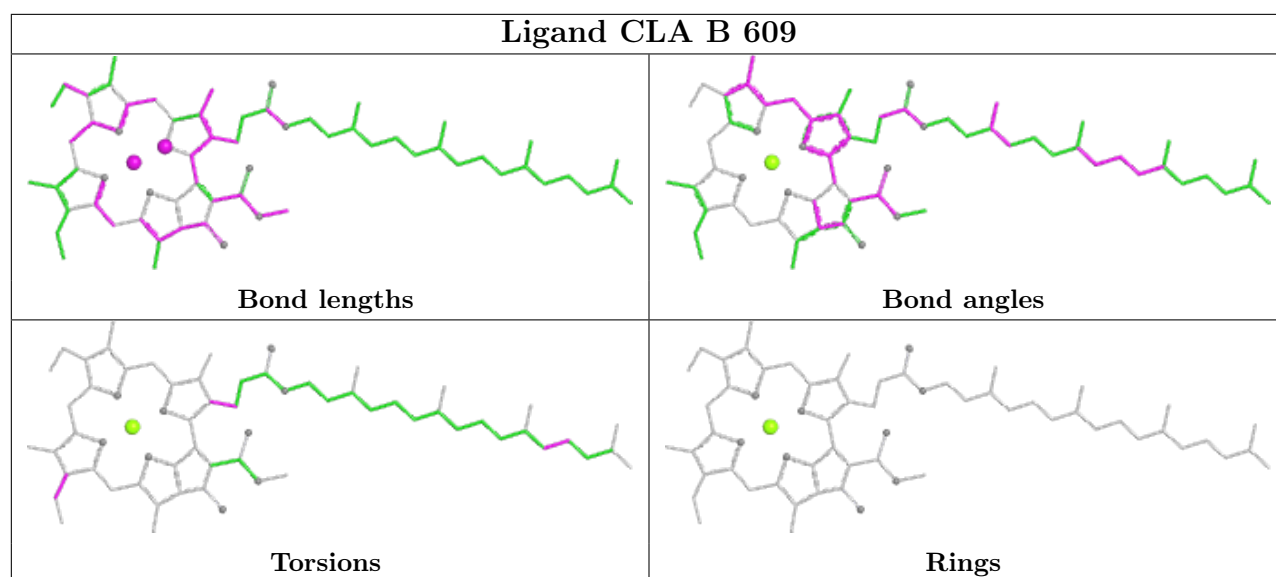


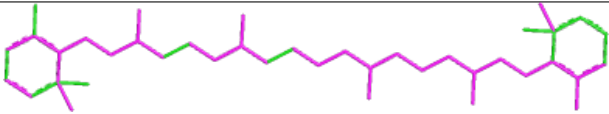
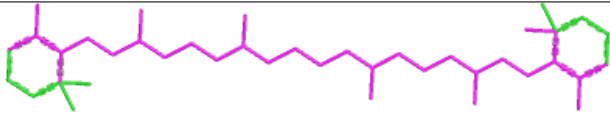
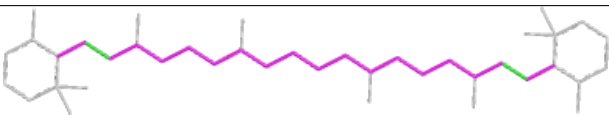
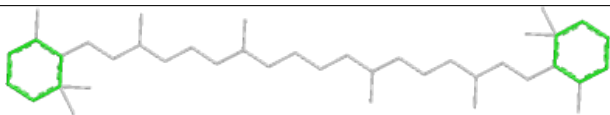
Ligand DGD C 517

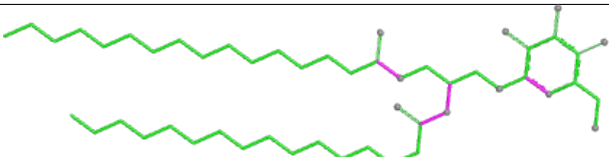
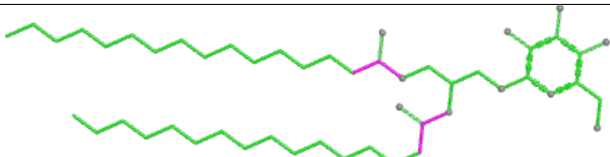
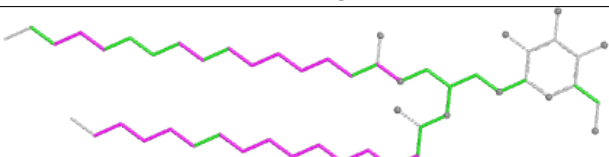
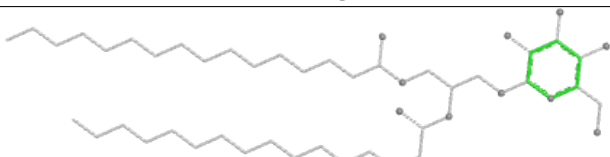


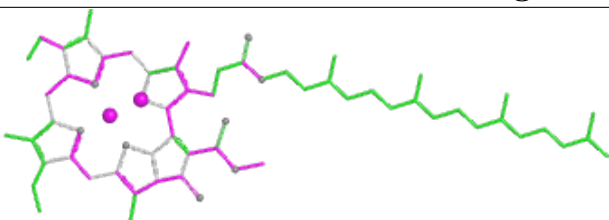
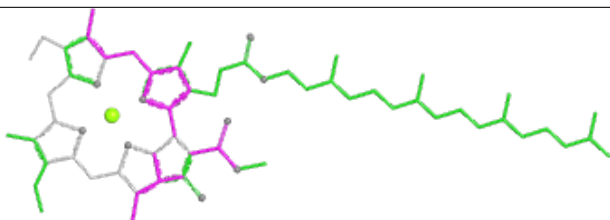
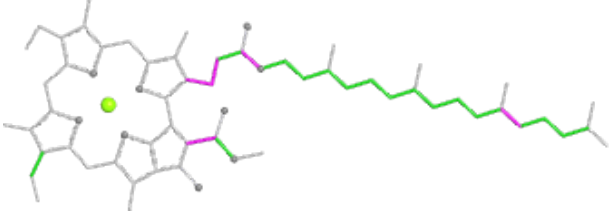
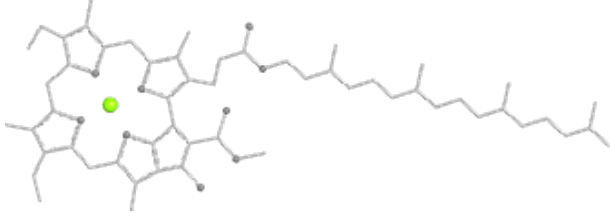
Ligand LMG B 621

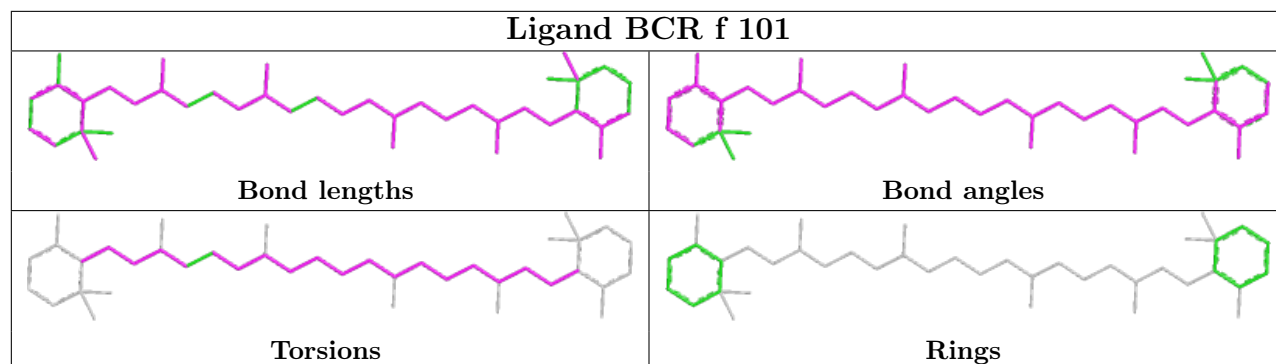
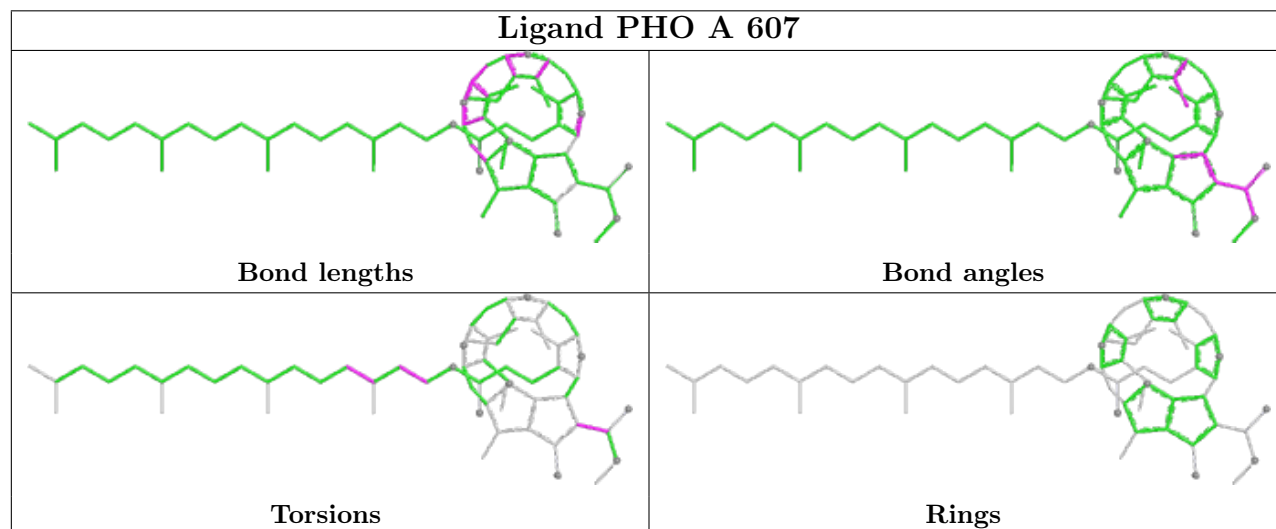
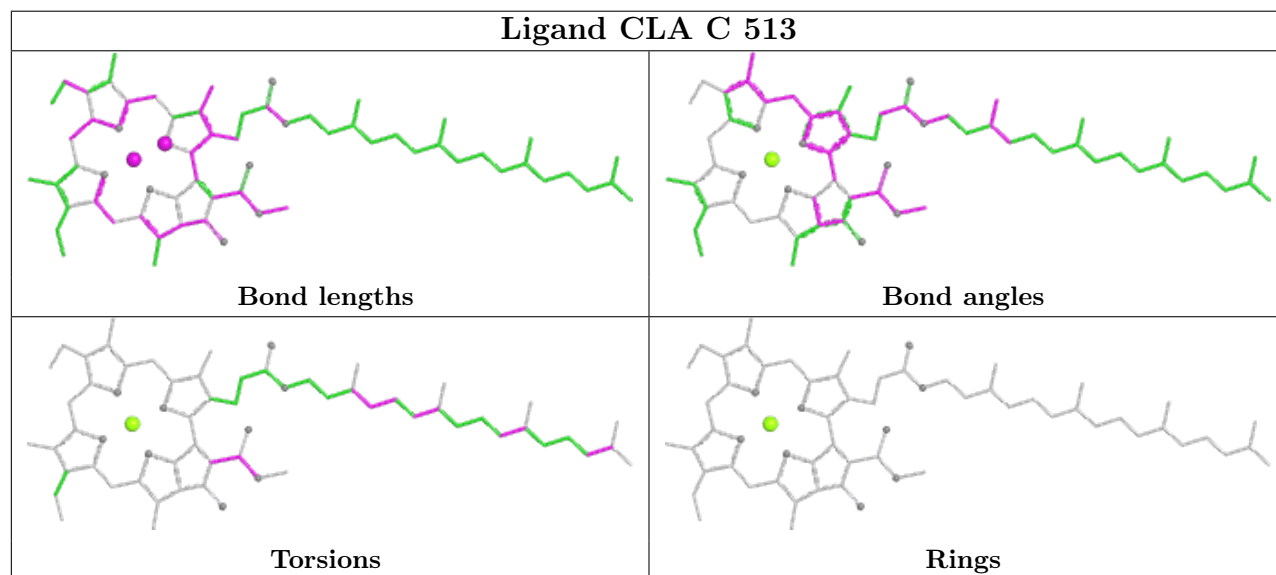




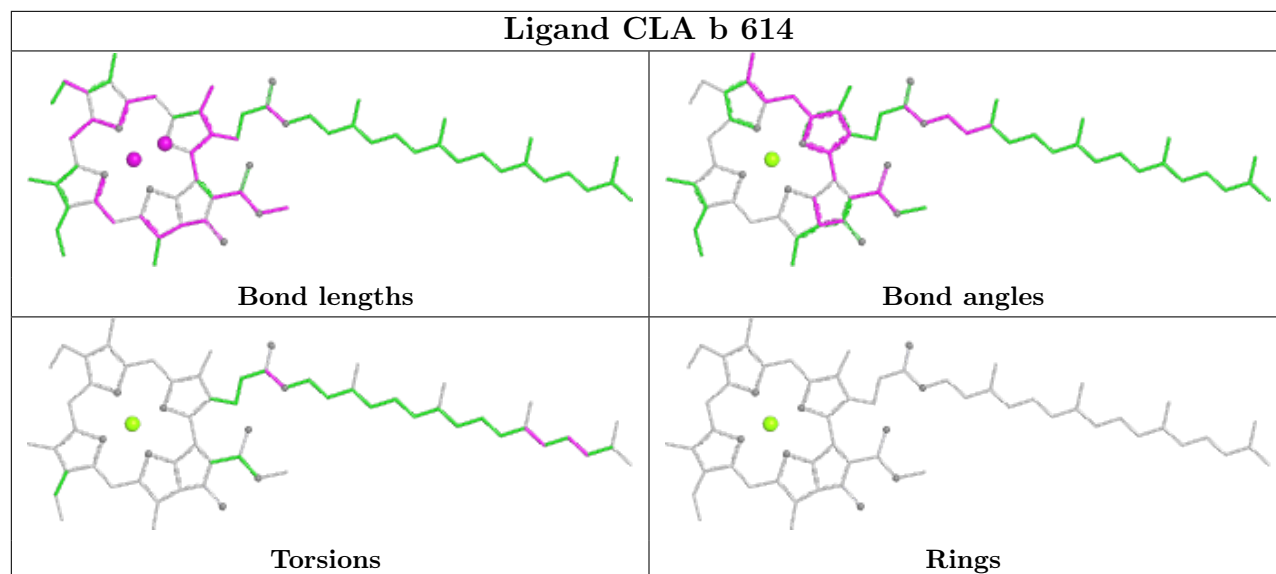
Ligand BCR A 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG c 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

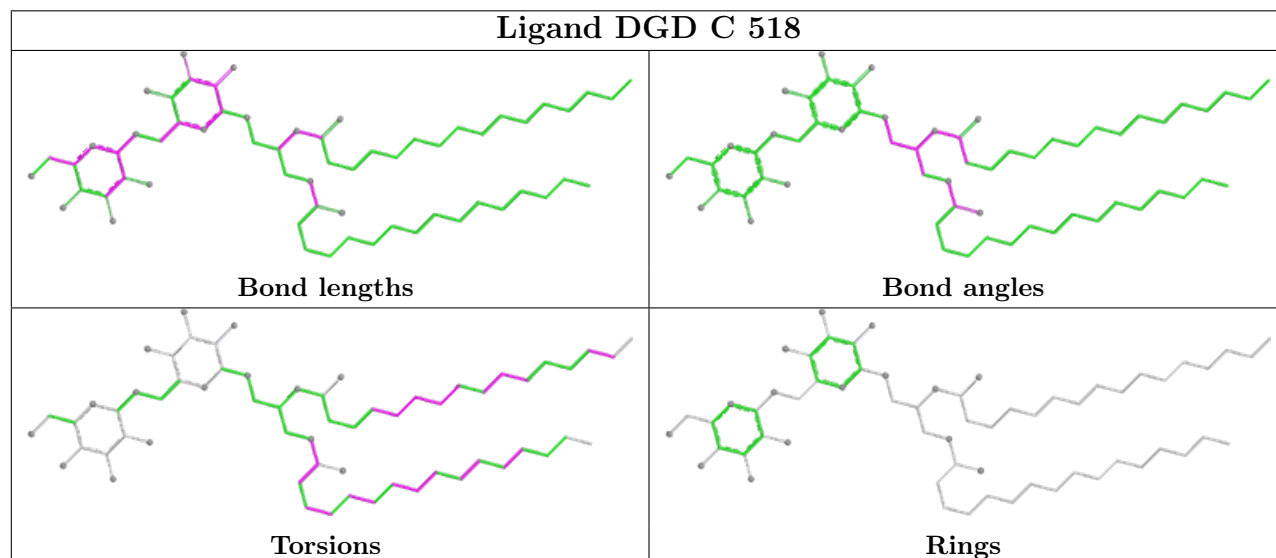
Ligand CLA c 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR f 101**Ligand PHO A 607****Ligand CLA C 513**

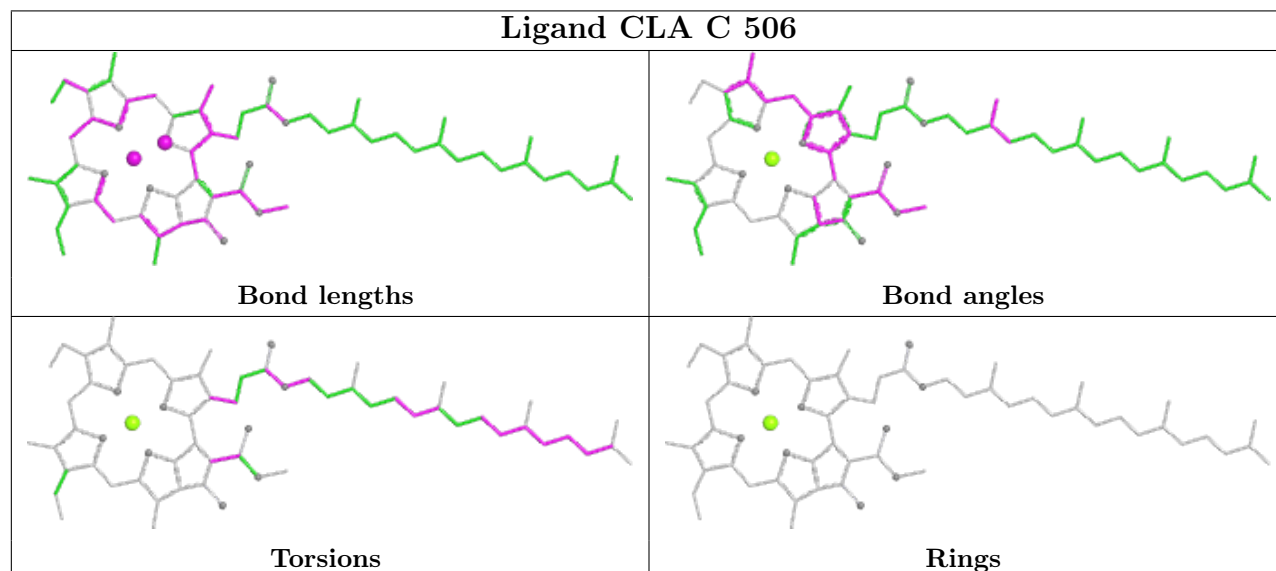
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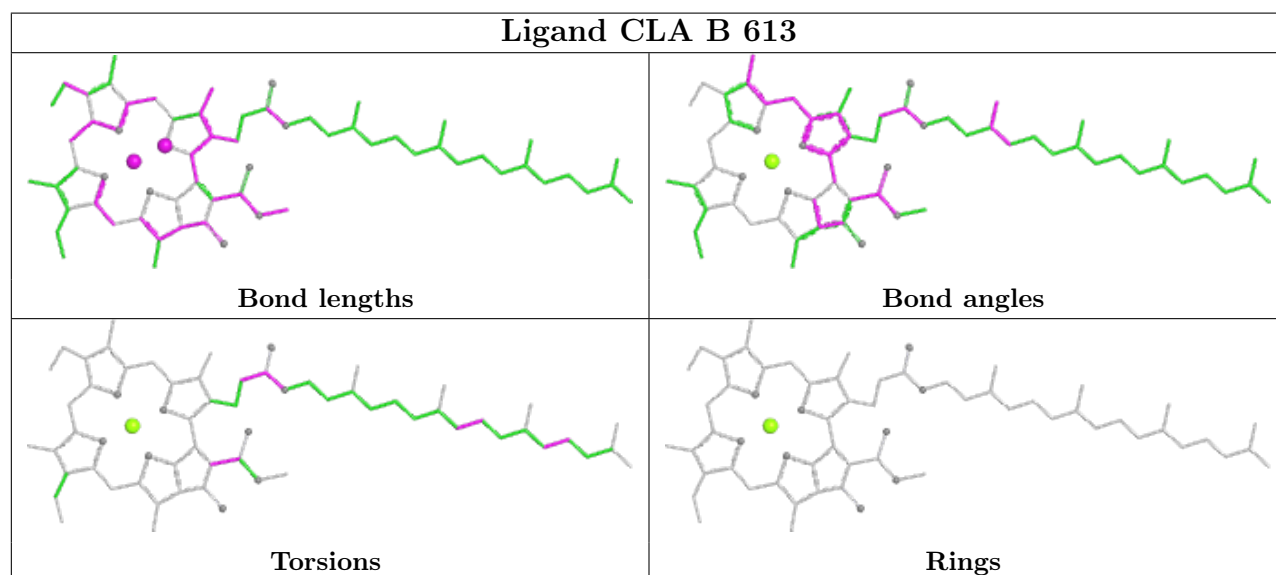
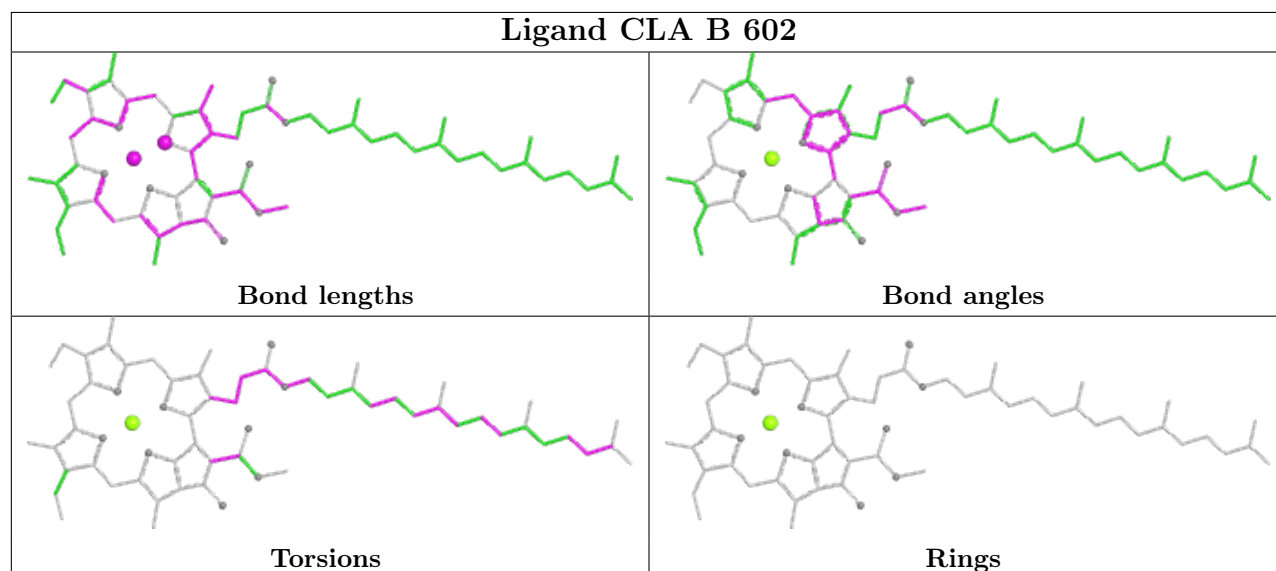
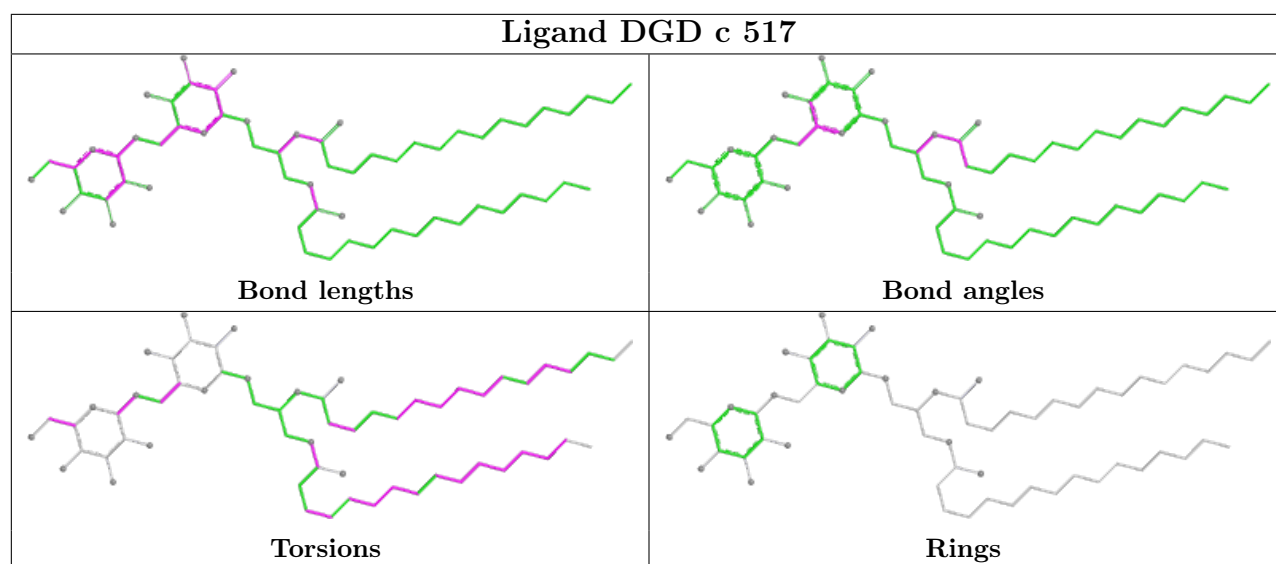


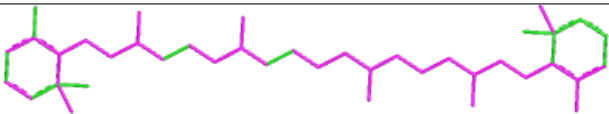
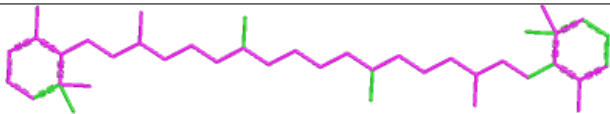
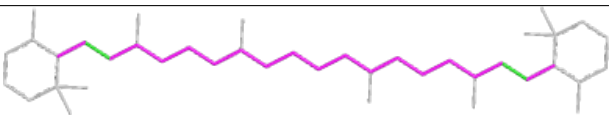
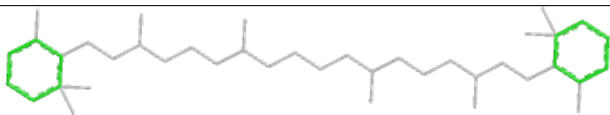
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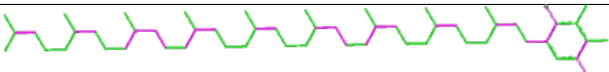
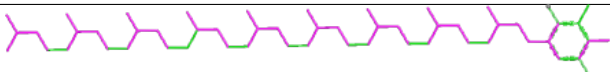
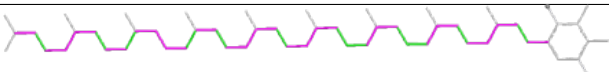
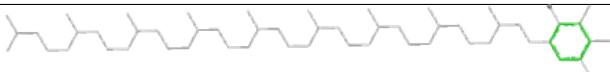


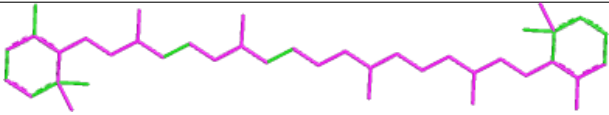
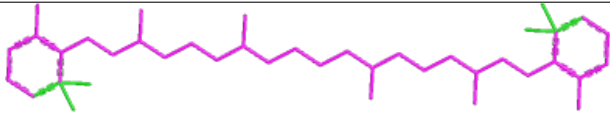
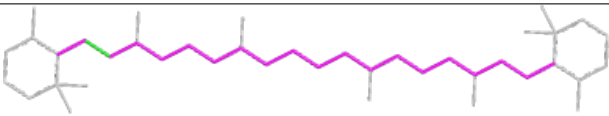
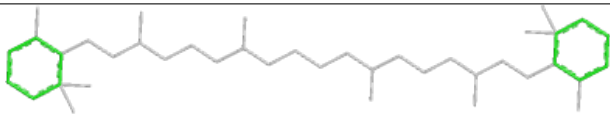
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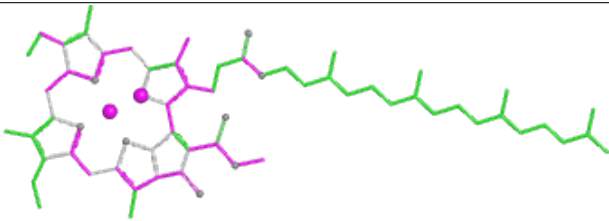
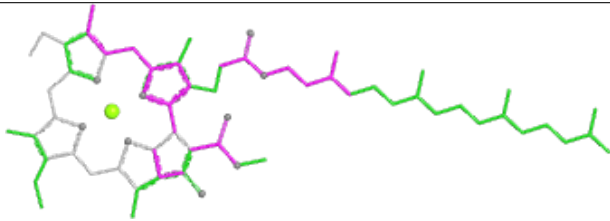
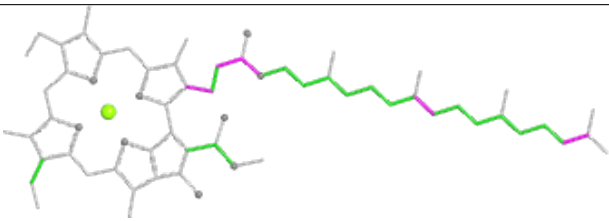
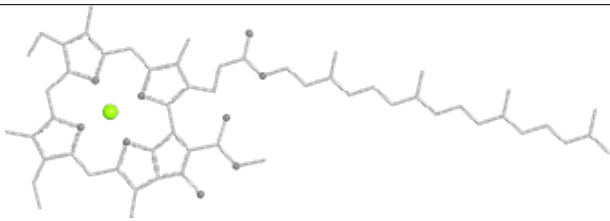


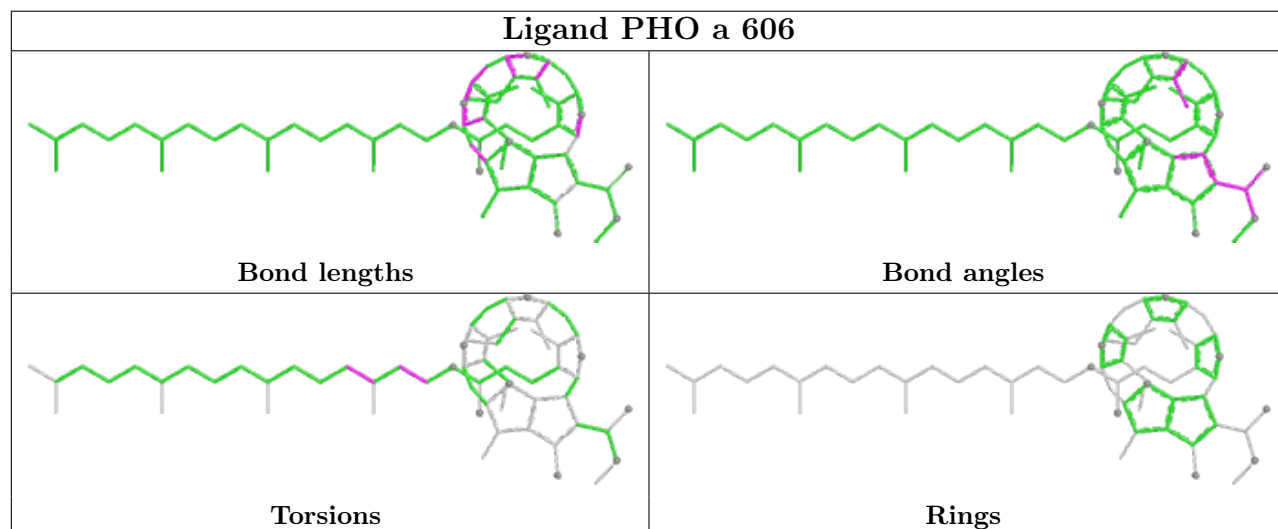
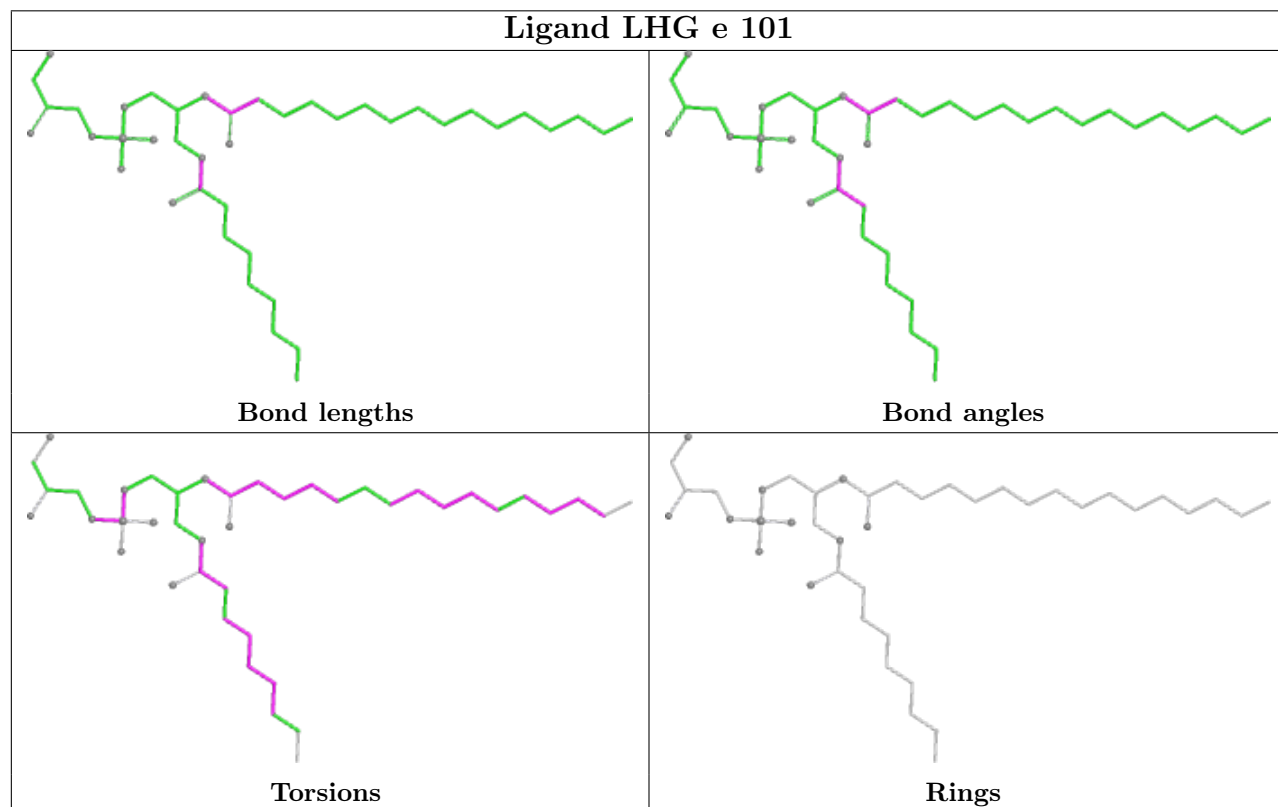
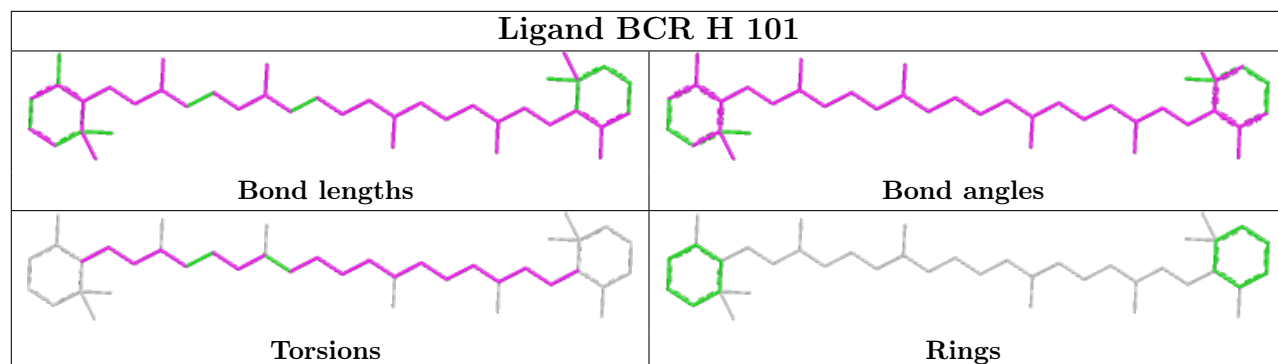


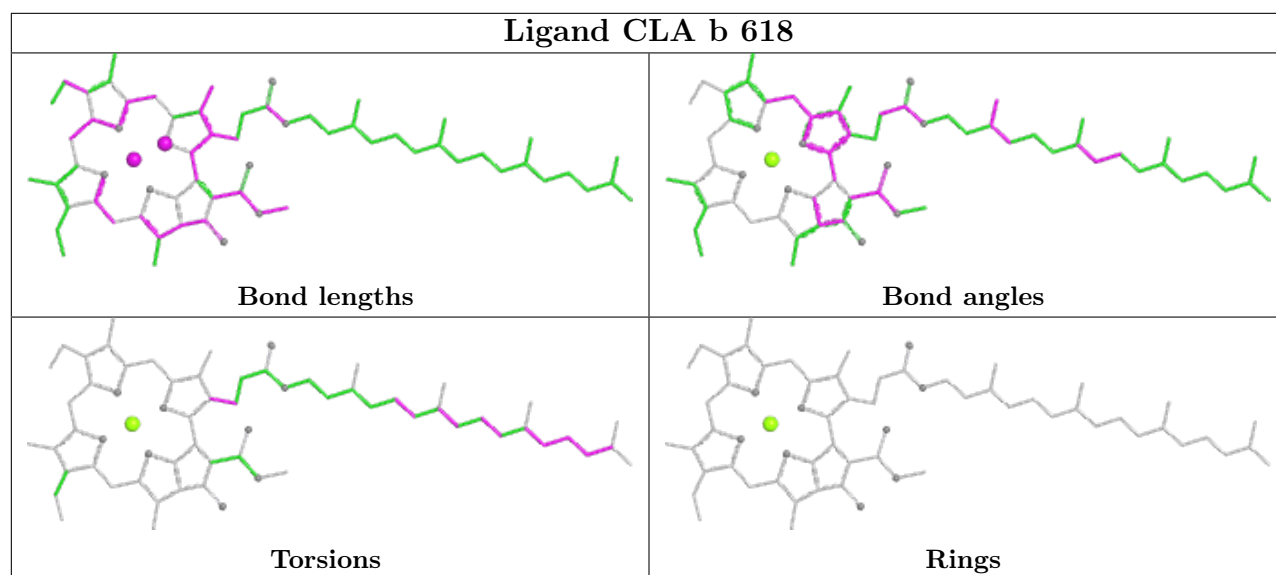
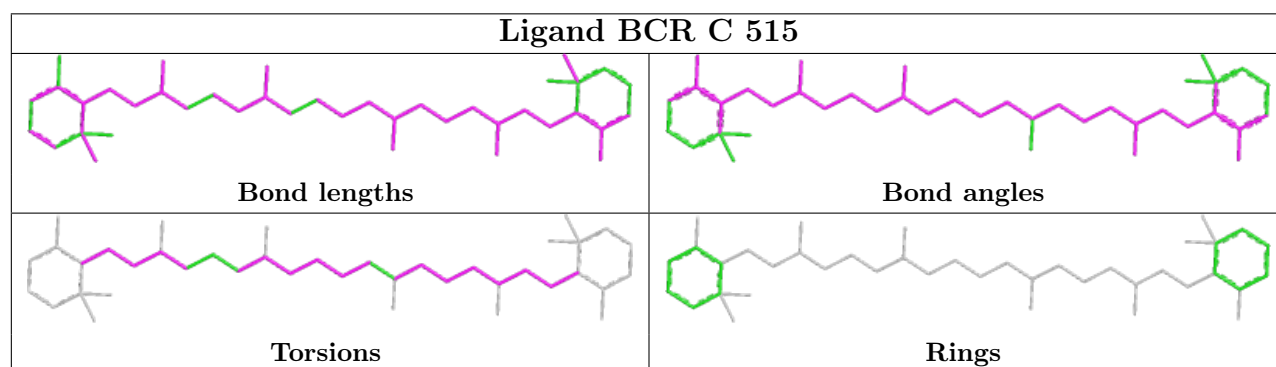
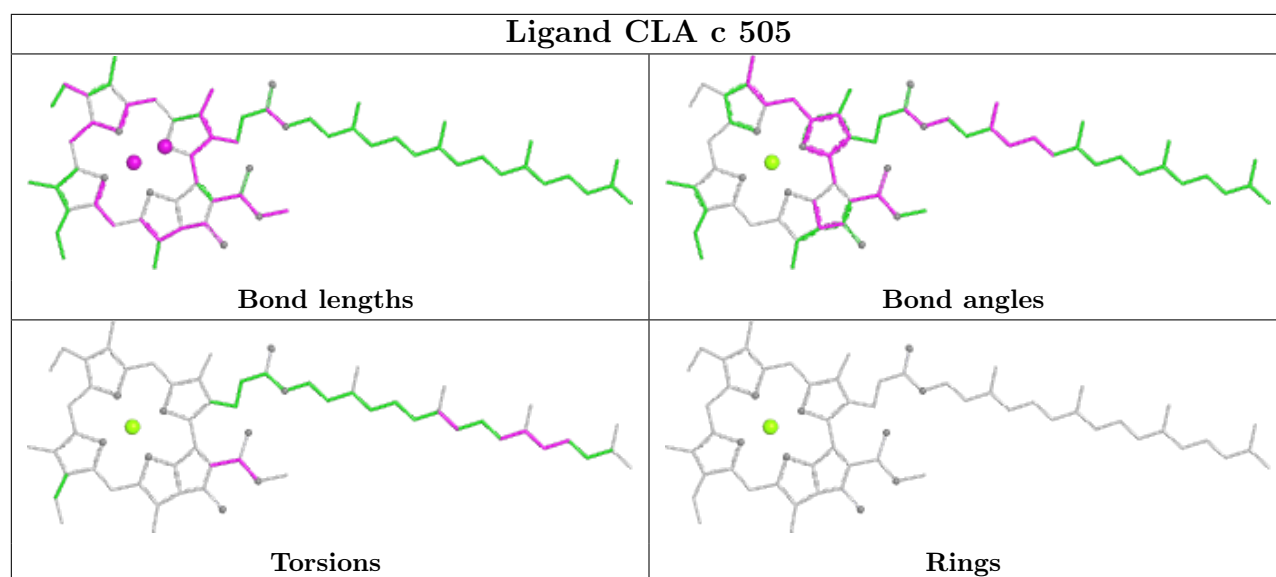
Ligand BCR b 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

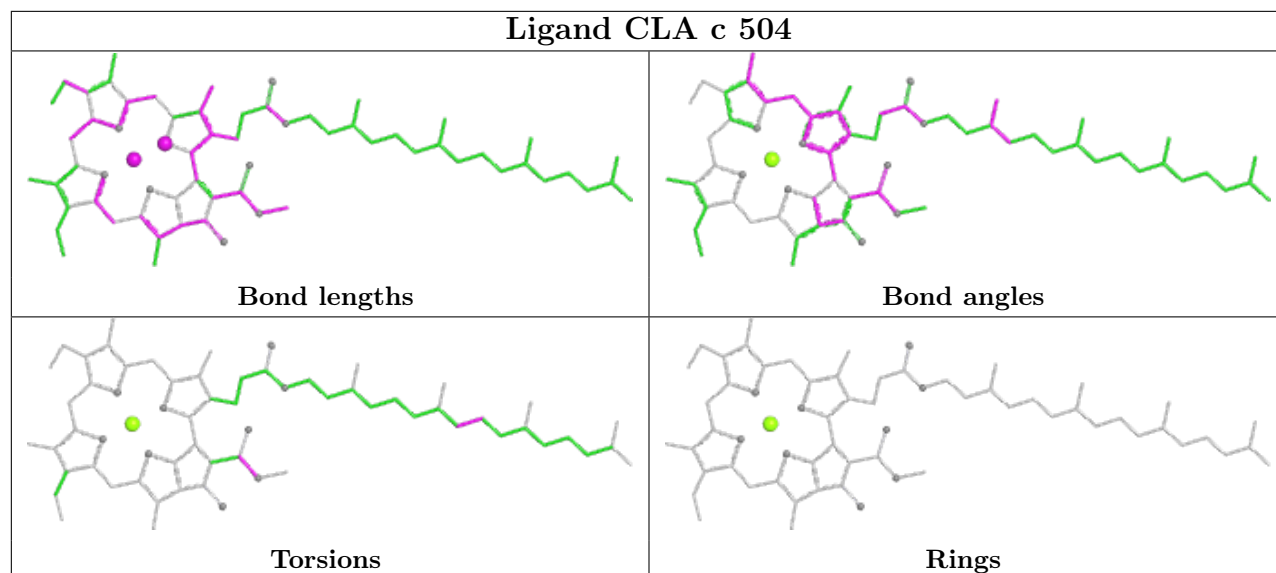
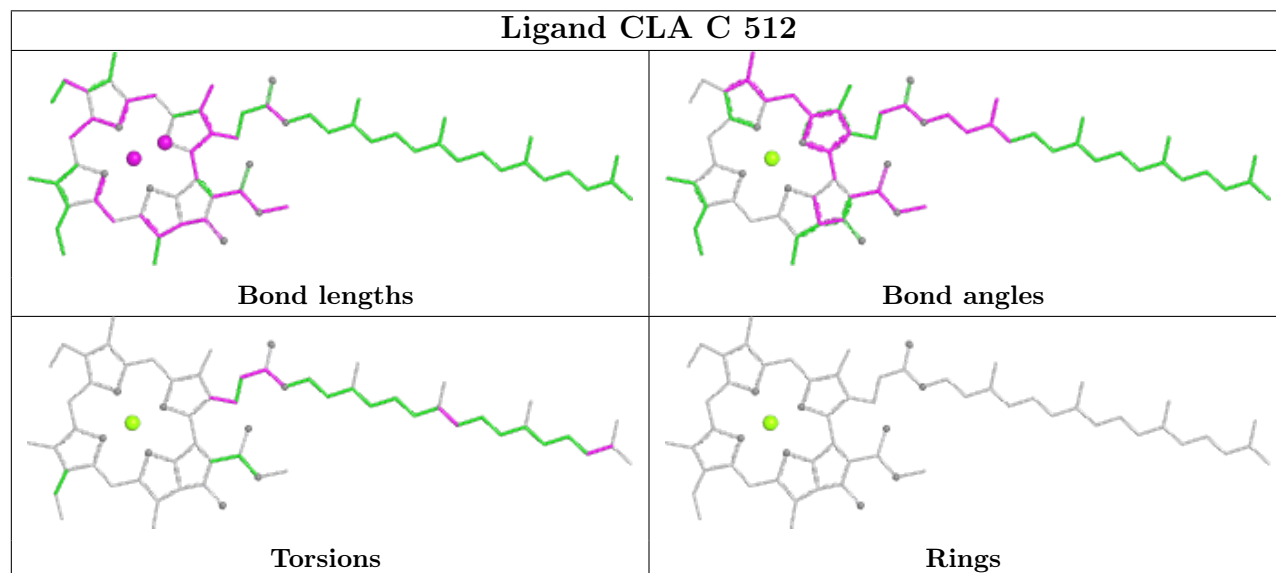
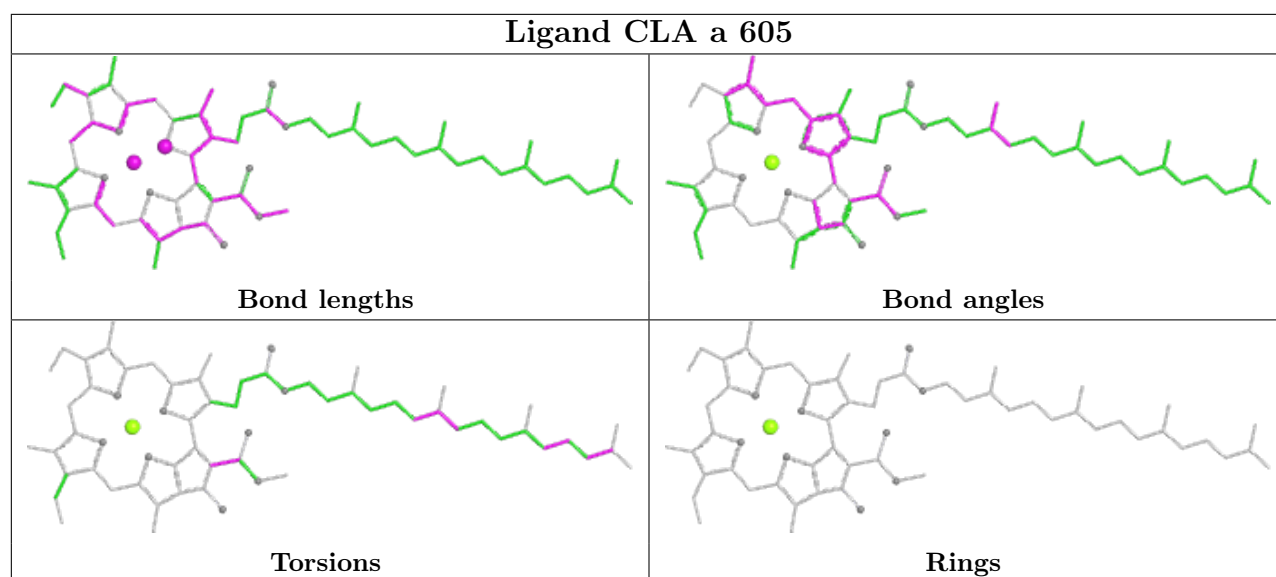
Ligand PL9 d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

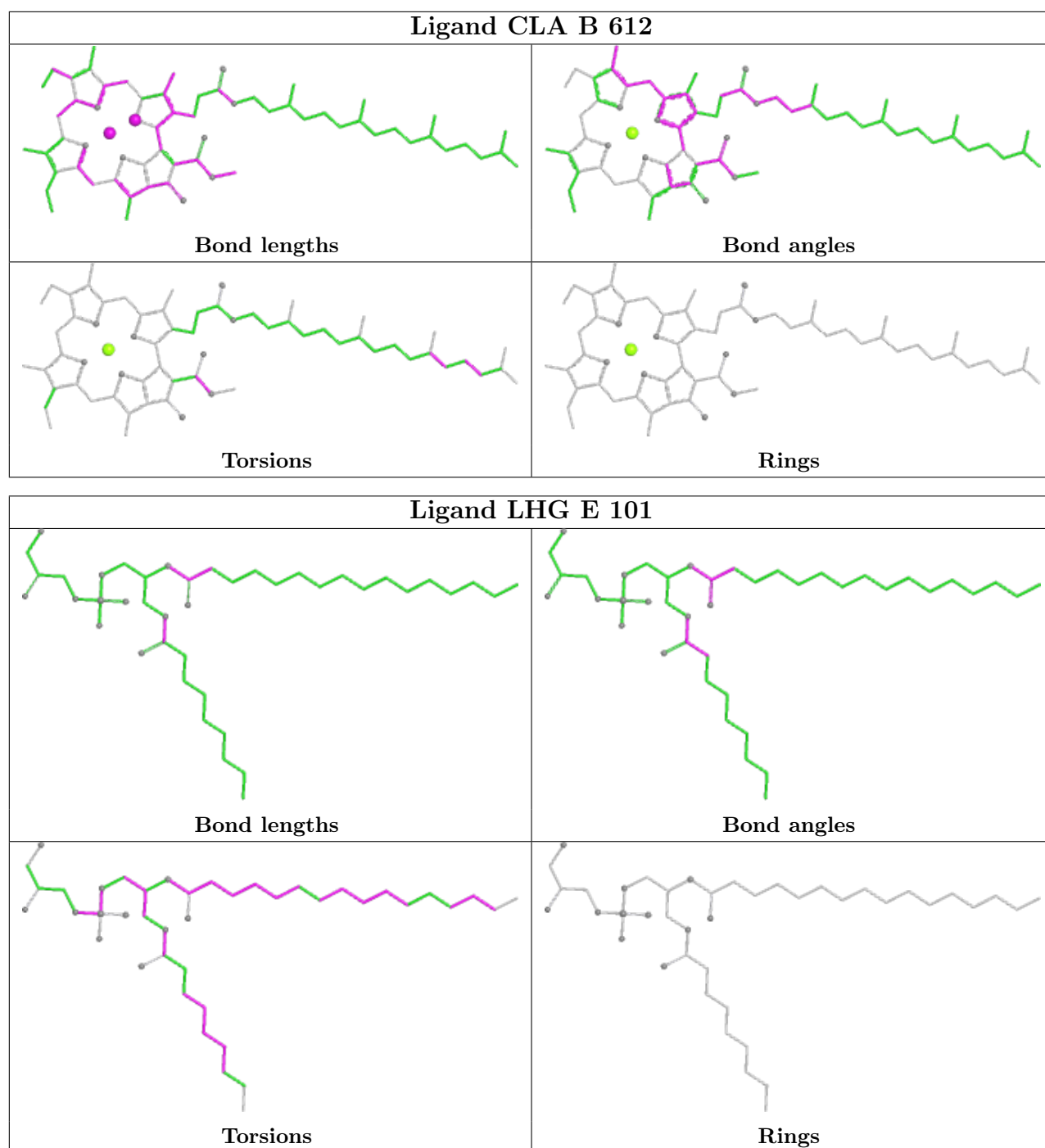
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

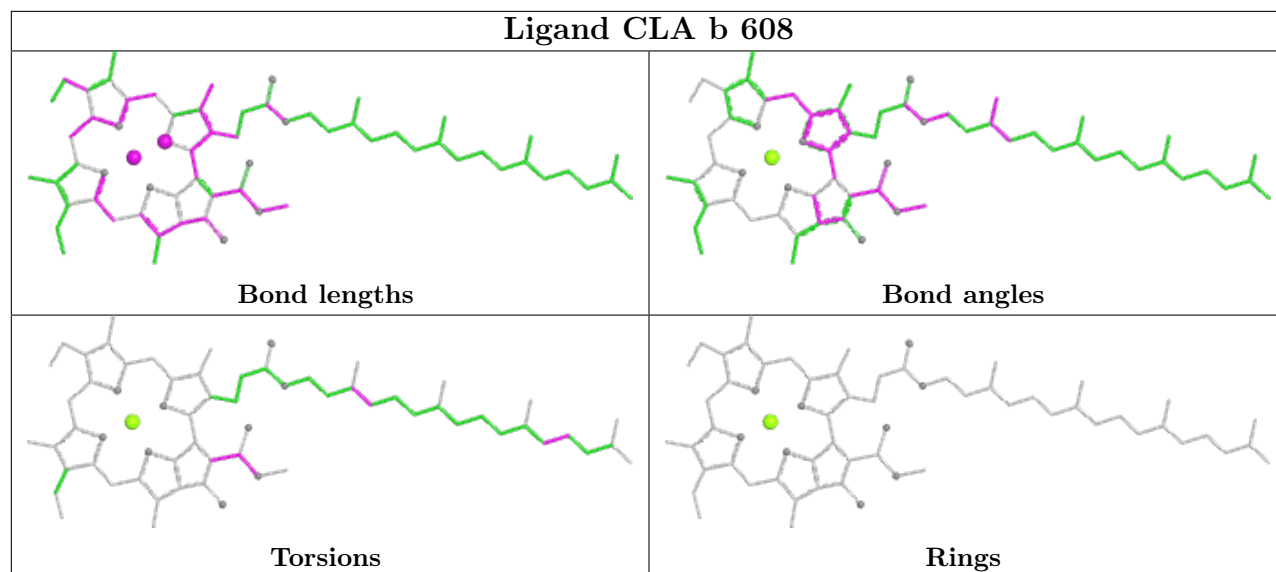




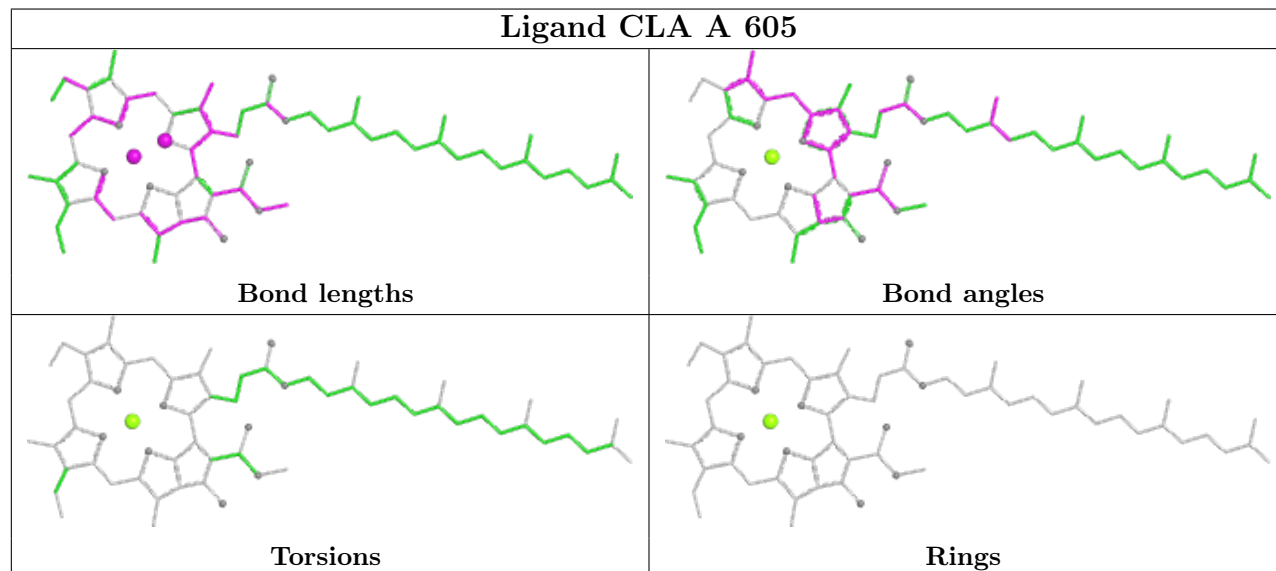




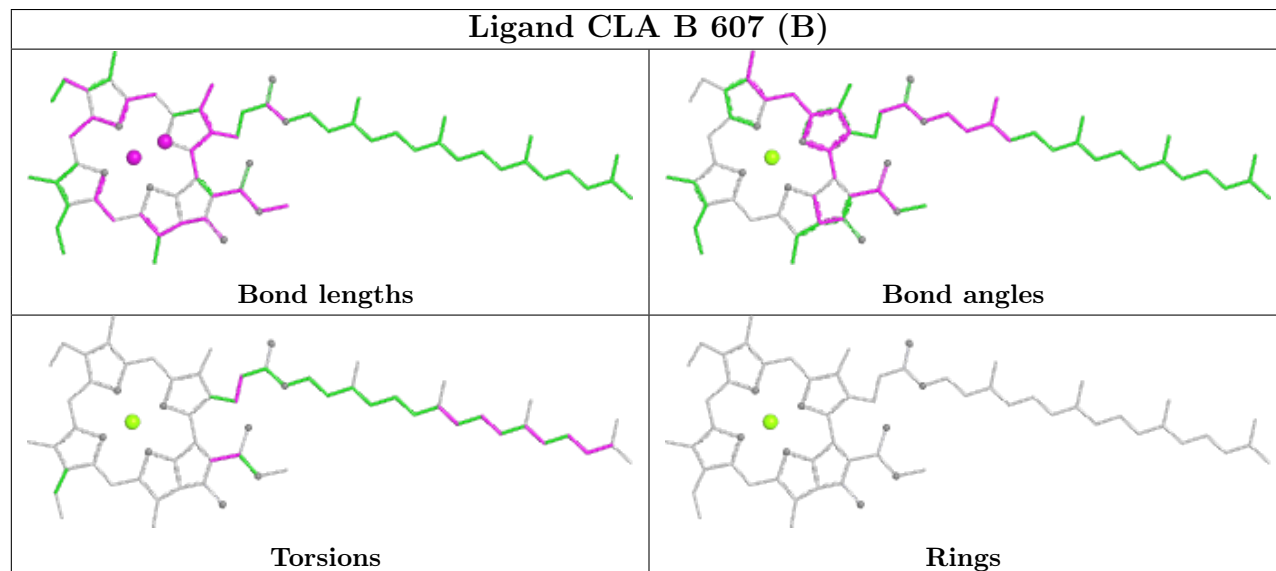
Ligand CLA b 608

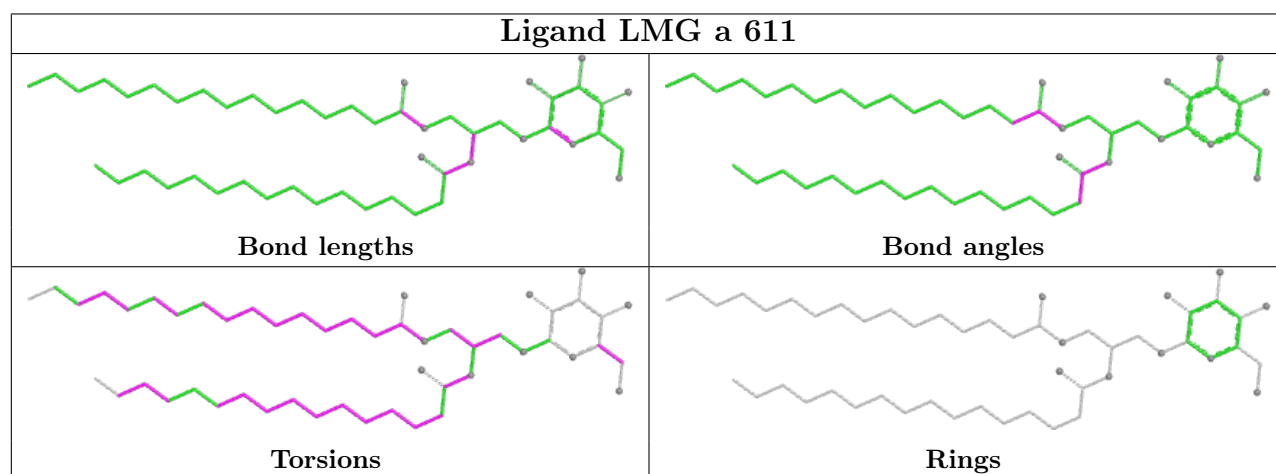
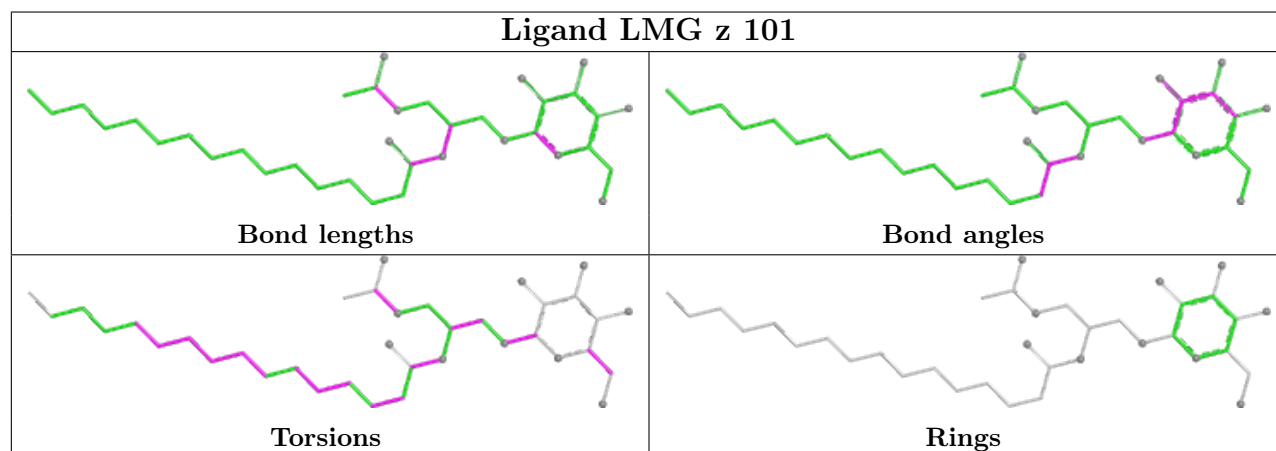
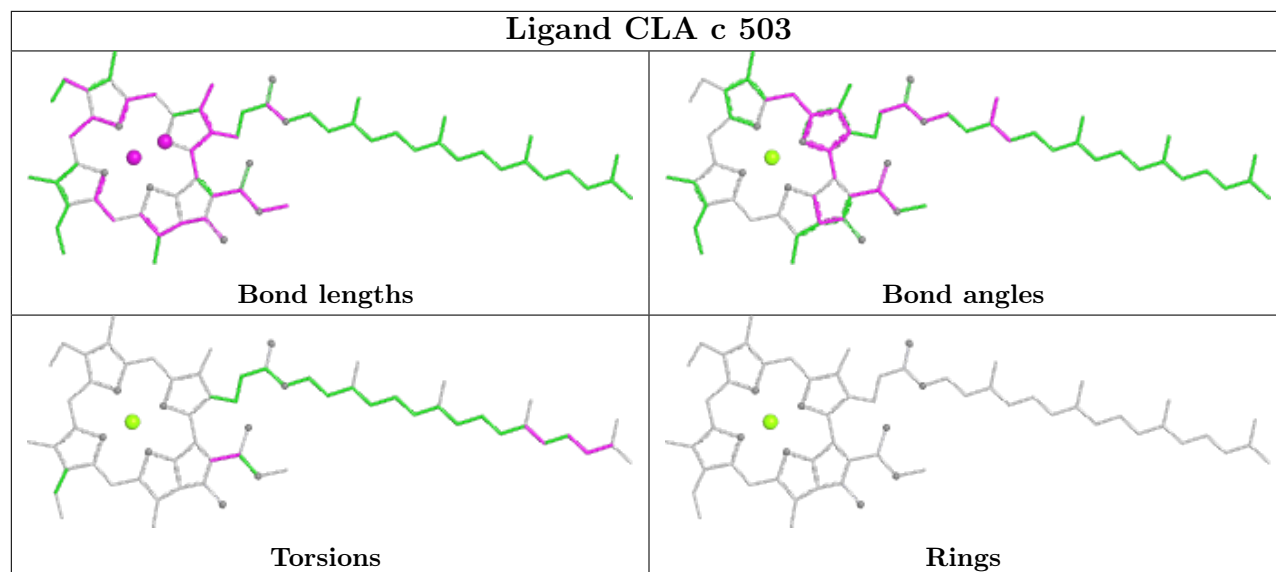


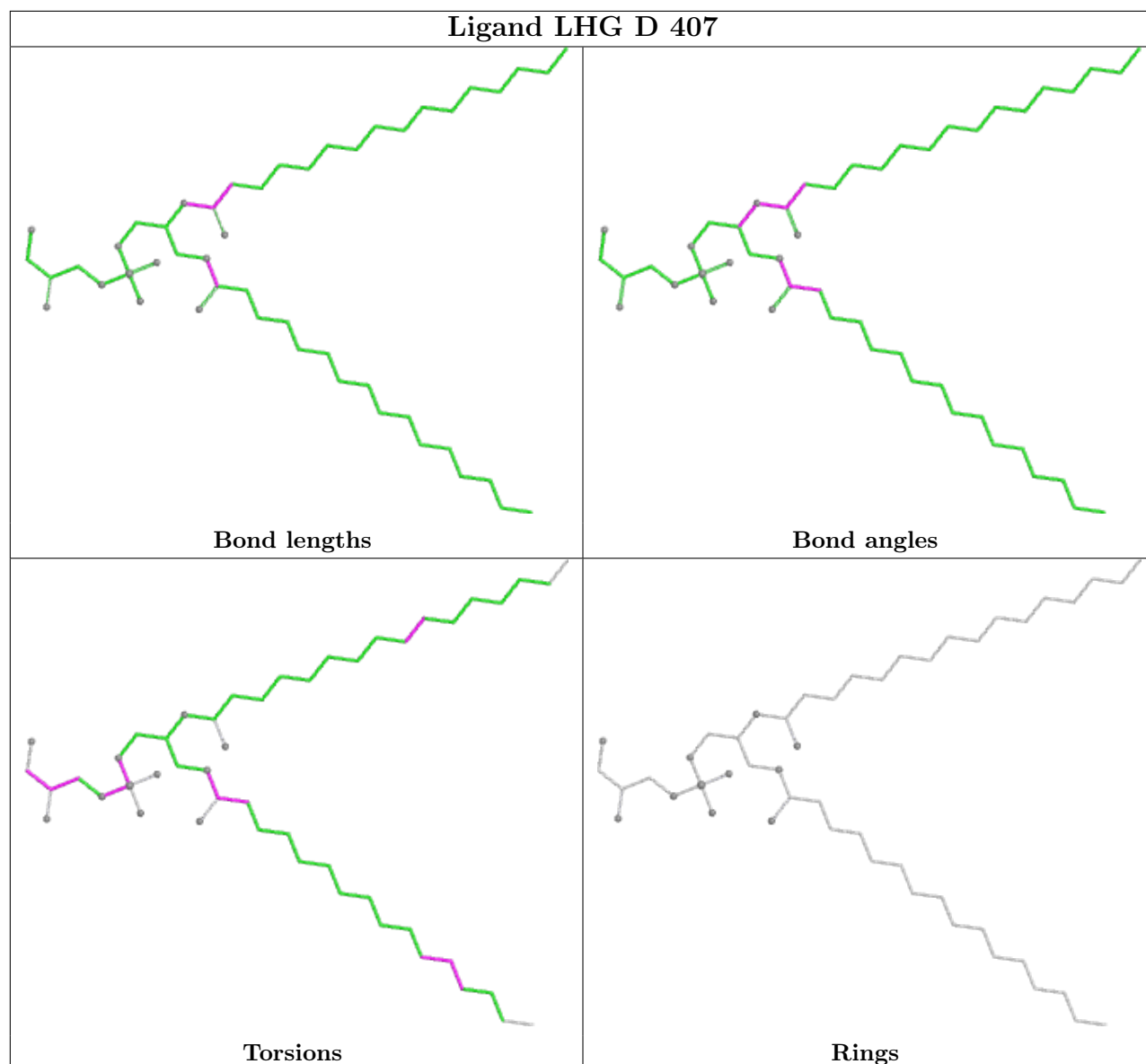
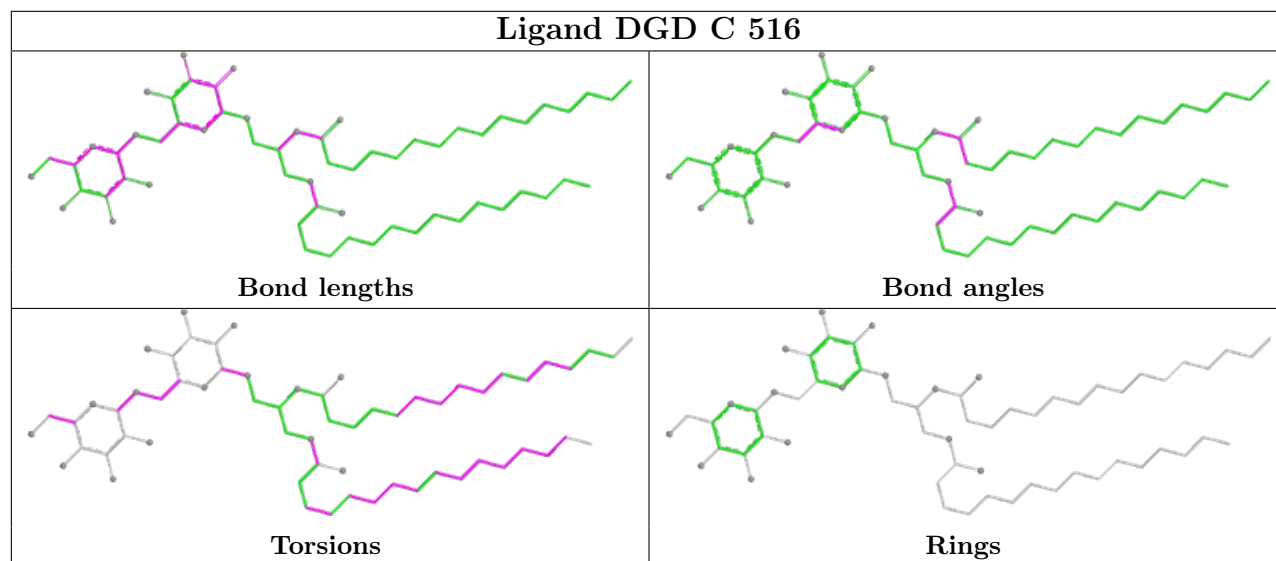
Ligand CLA A 605

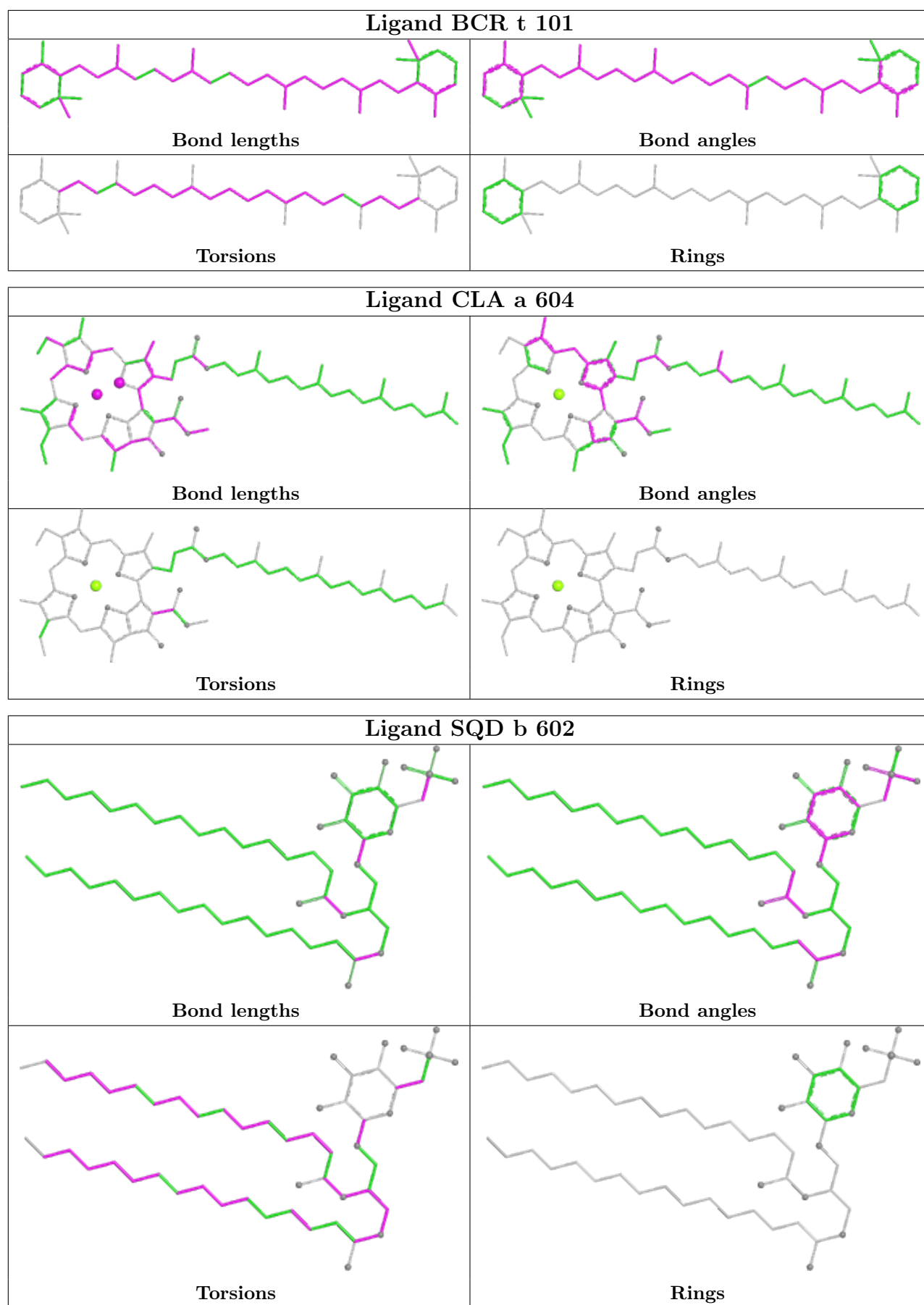


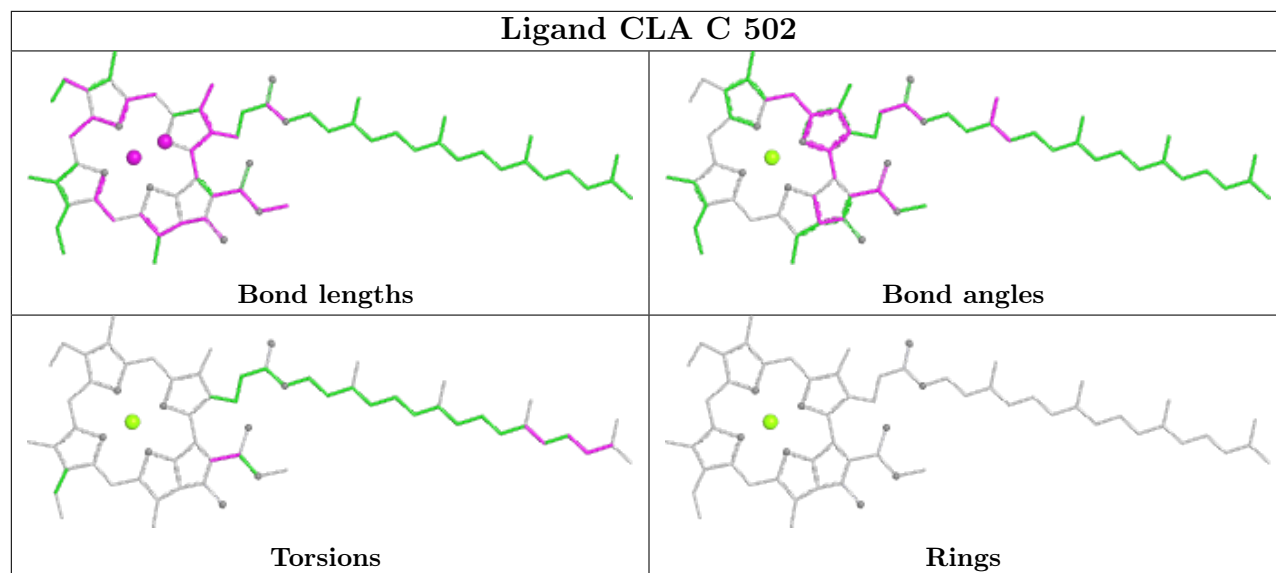
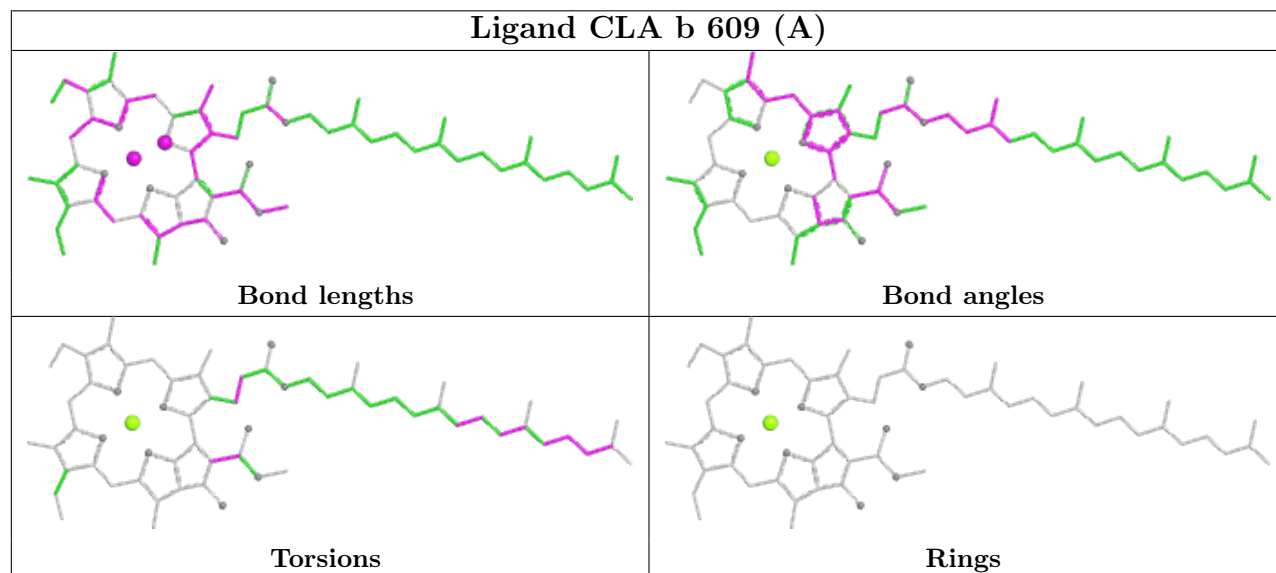
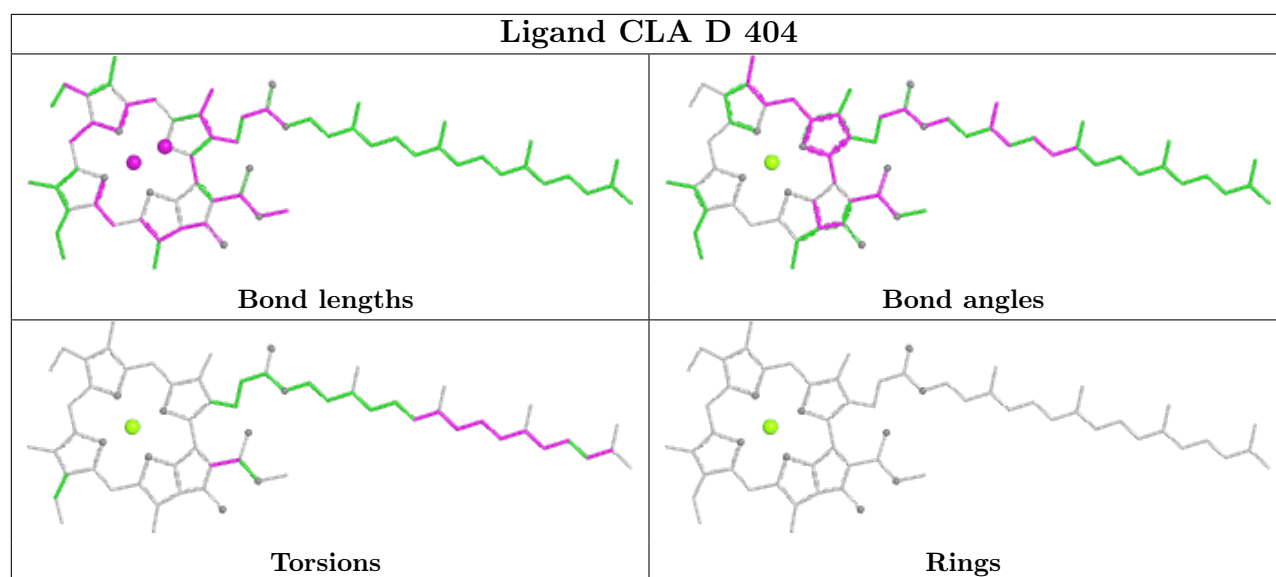
Ligand CLA B 607 (B)

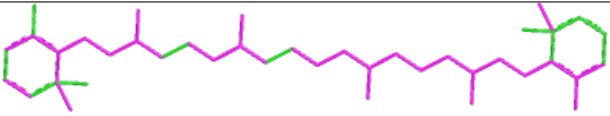
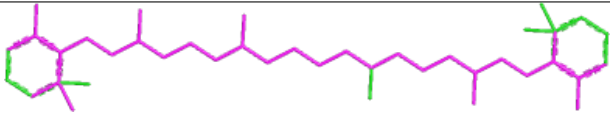
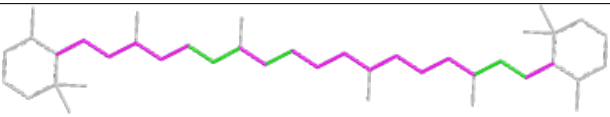
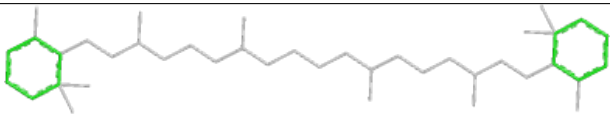
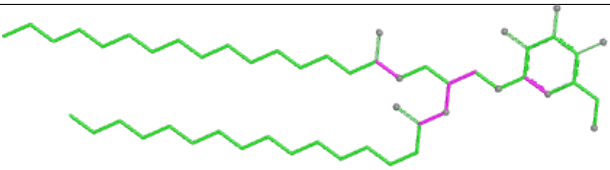
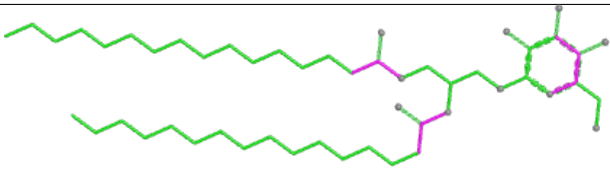
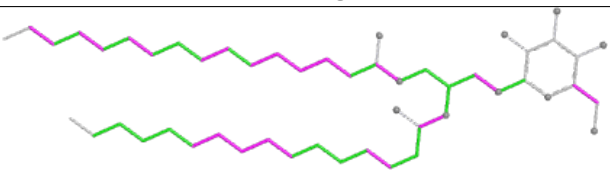
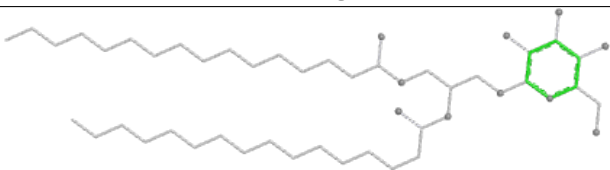
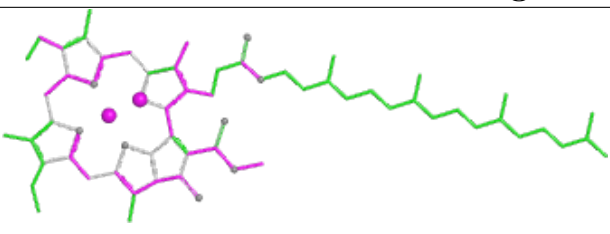
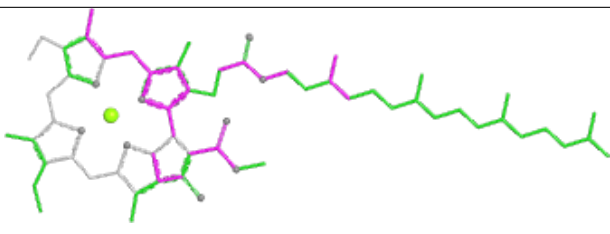
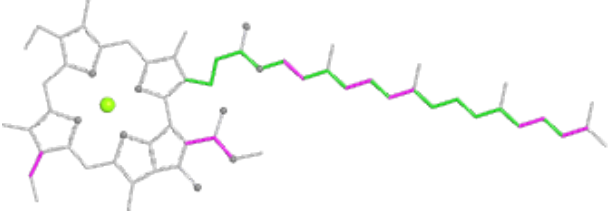
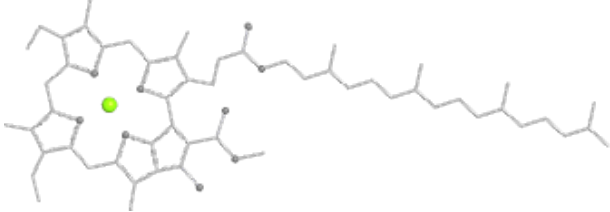


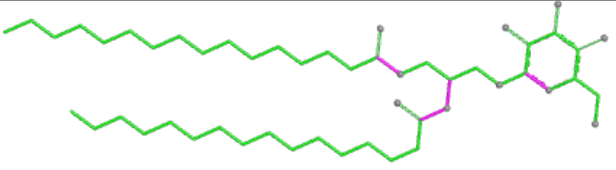
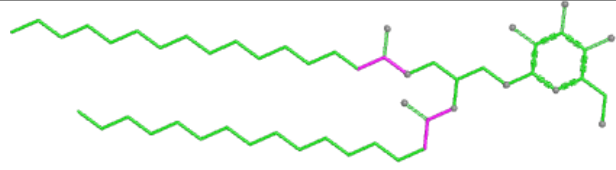
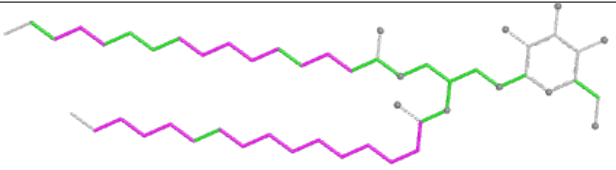
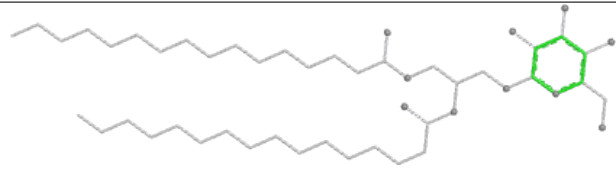


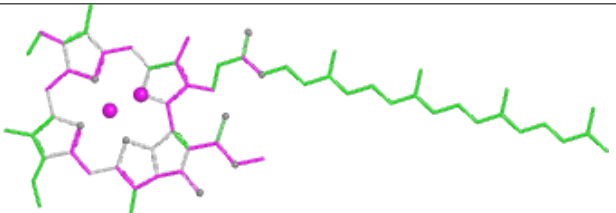
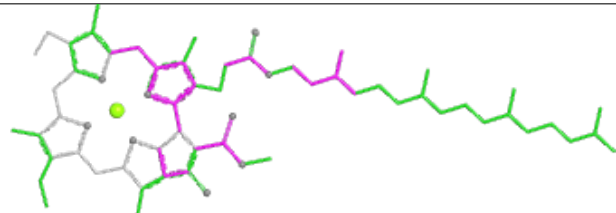
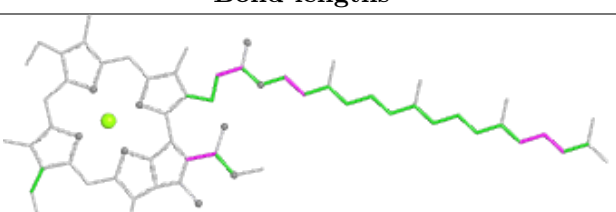
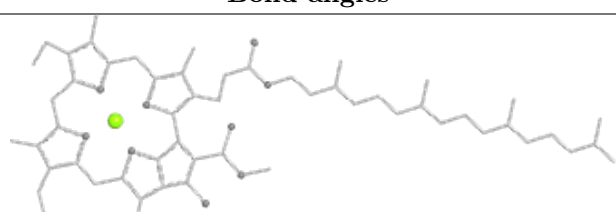


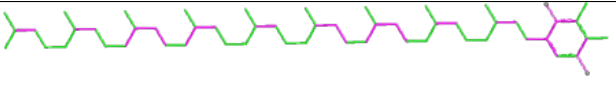
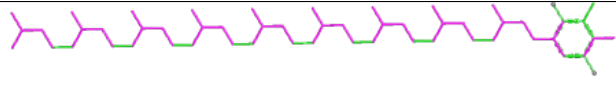
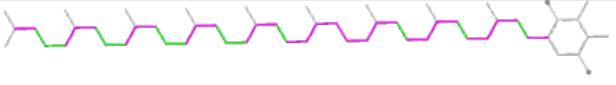



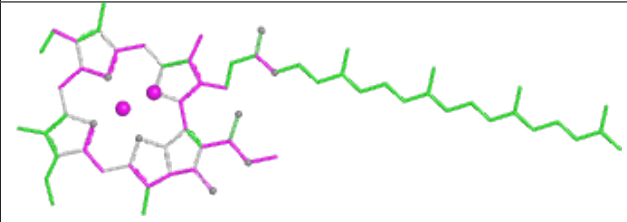
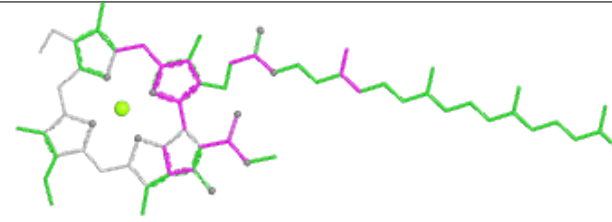
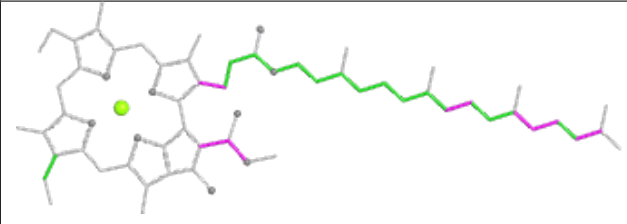
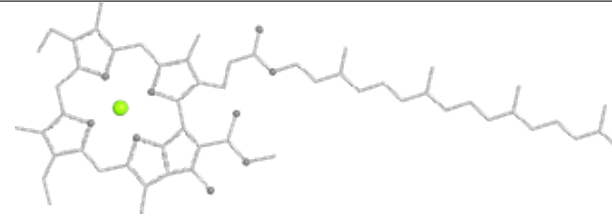


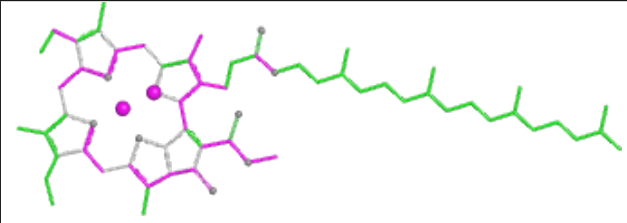
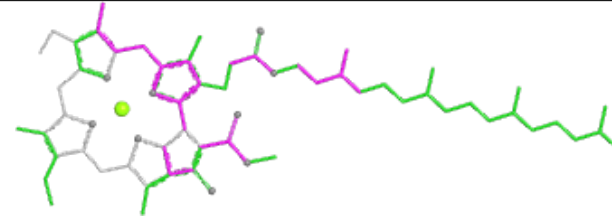
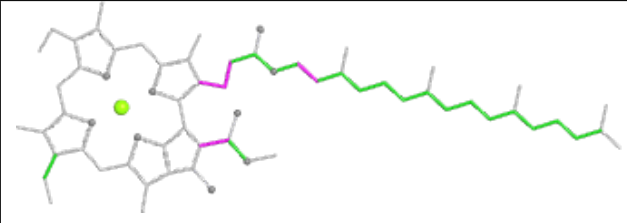
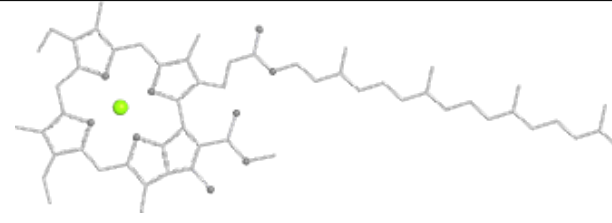
Ligand BCR B 620	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG C 520	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA b 607	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

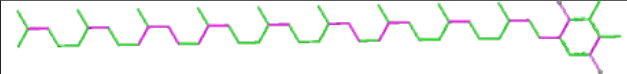
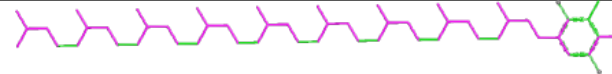
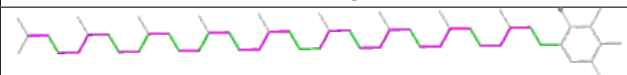

Ligand LMG C 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

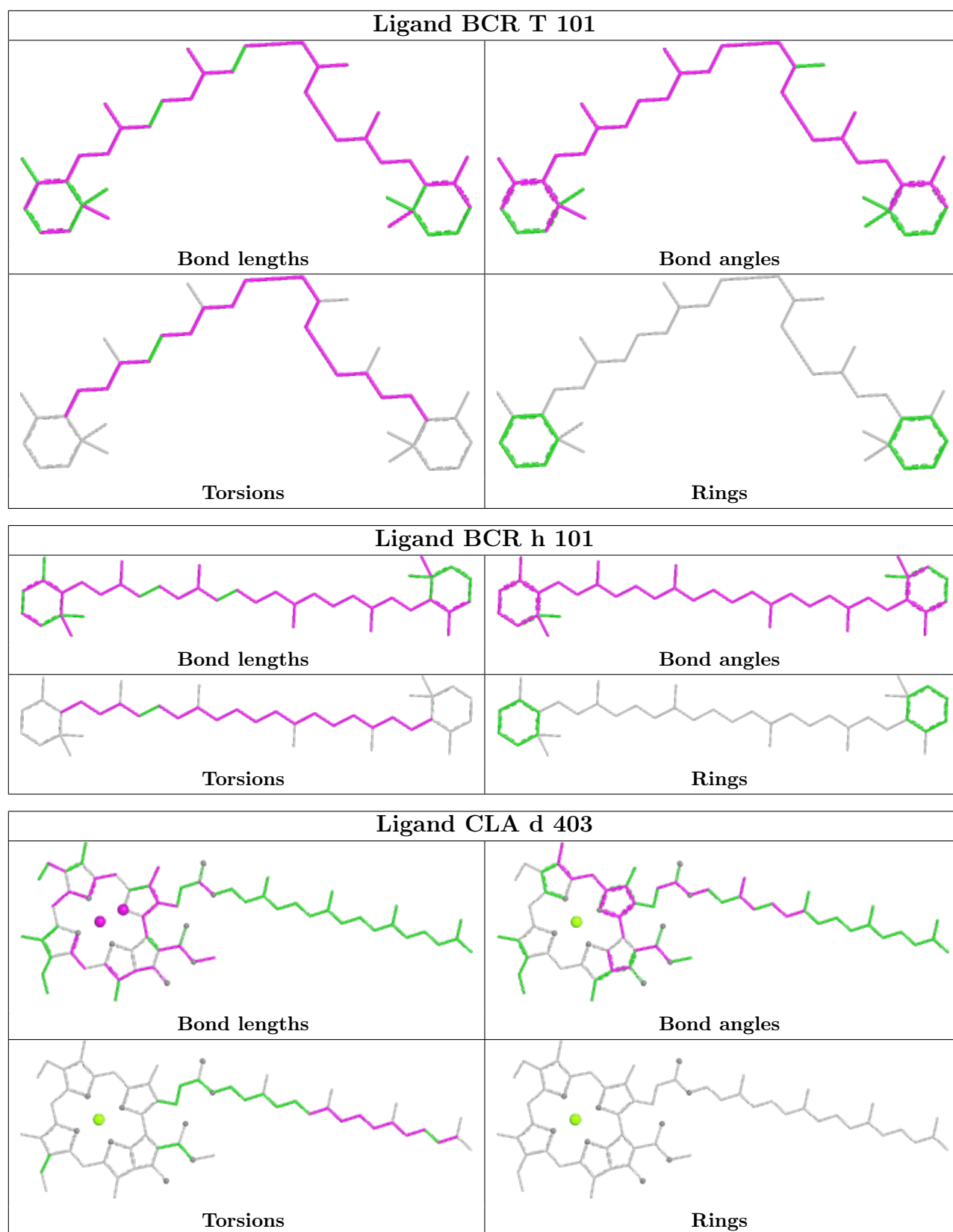
Ligand CLA B 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 A 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

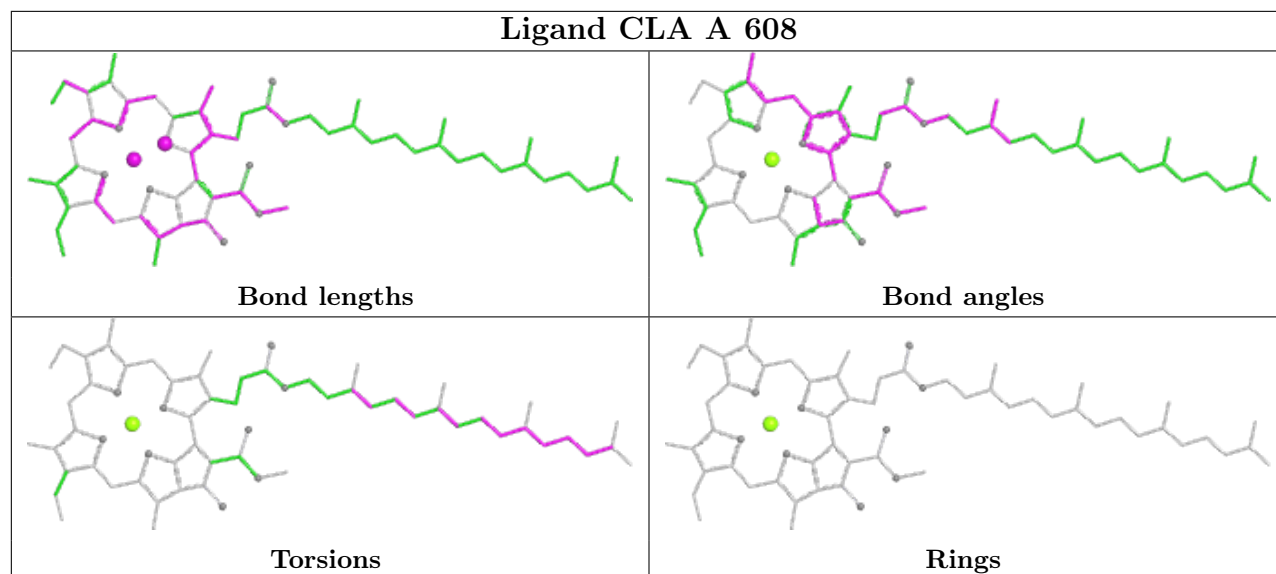
Ligand CLA B 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

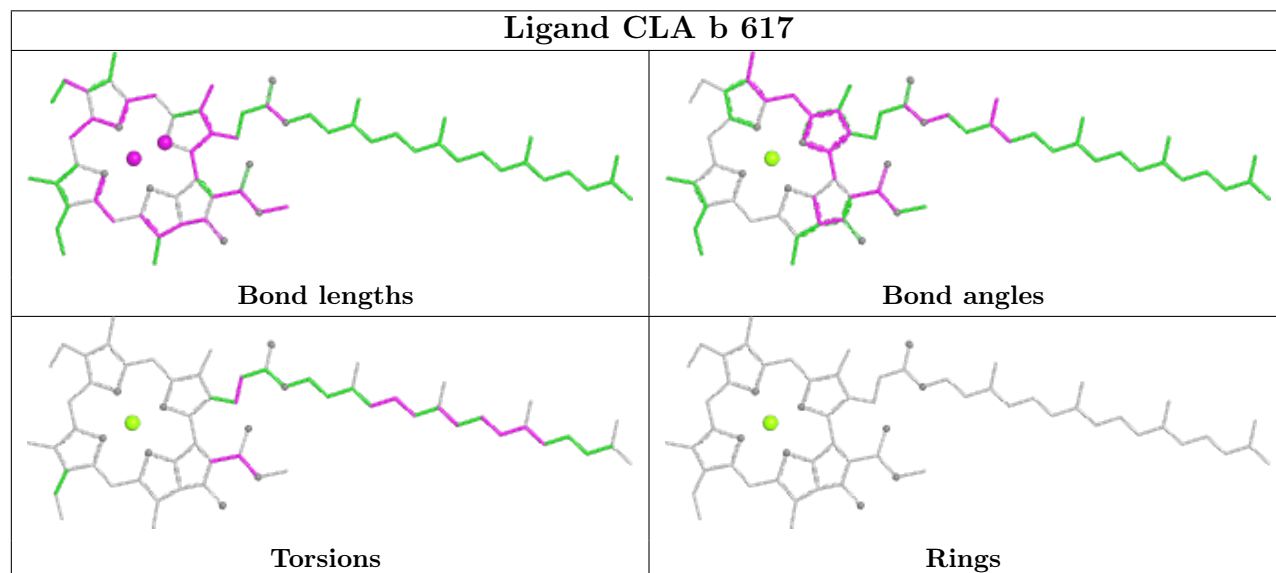
Ligand PL9 D 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

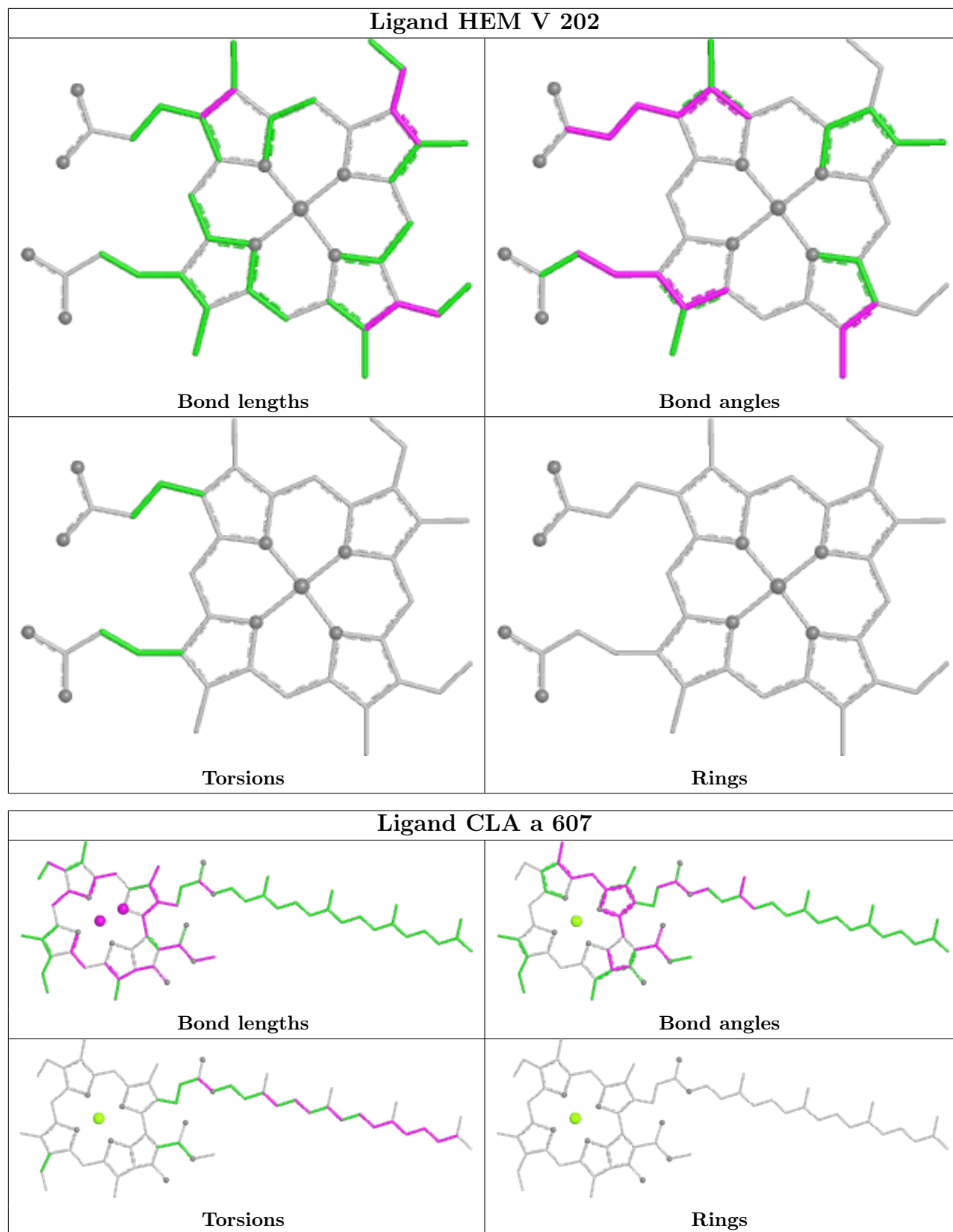


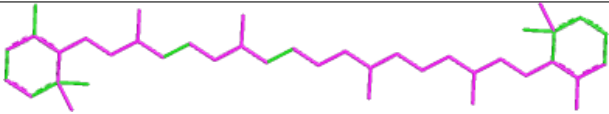
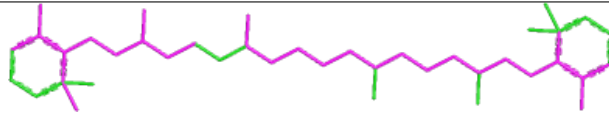
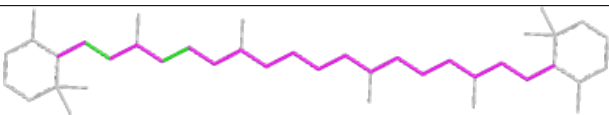
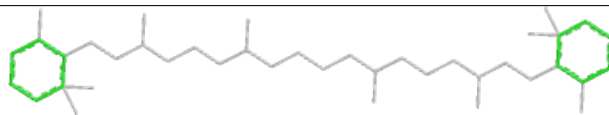
Ligand CLA A 608

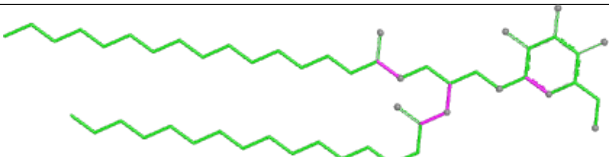
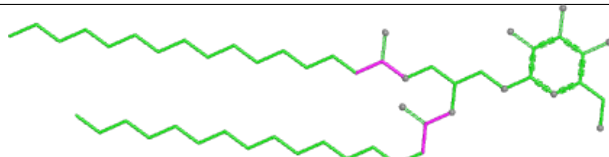
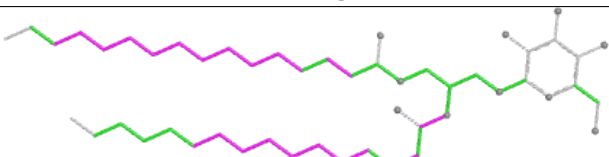



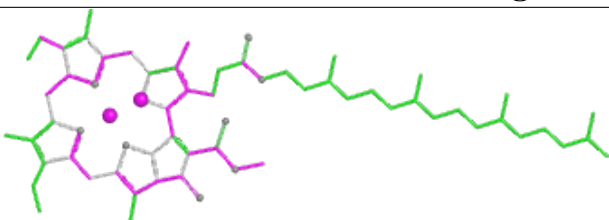
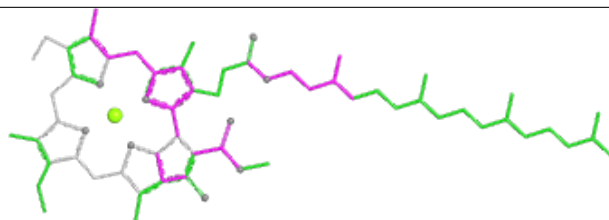
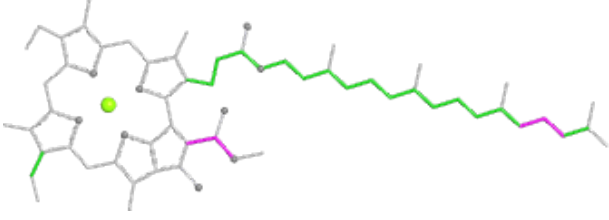
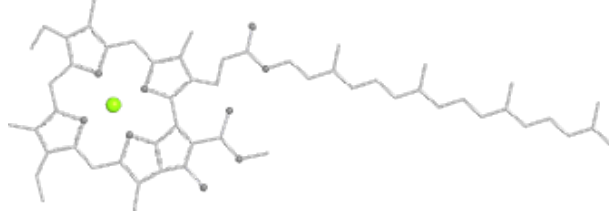
Ligand CLA b 617



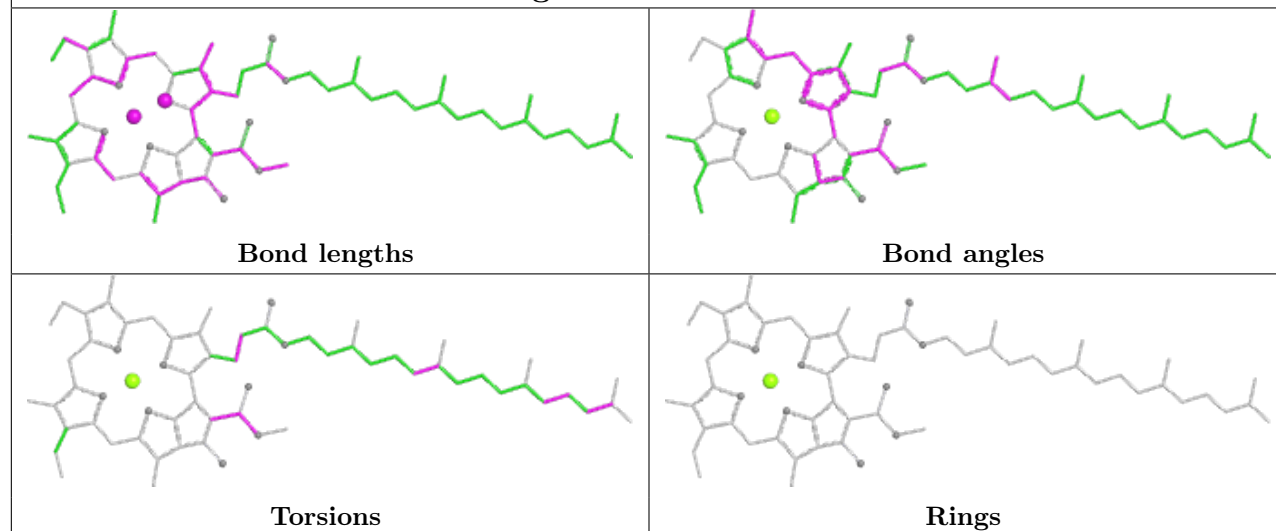


Ligand BCR c 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

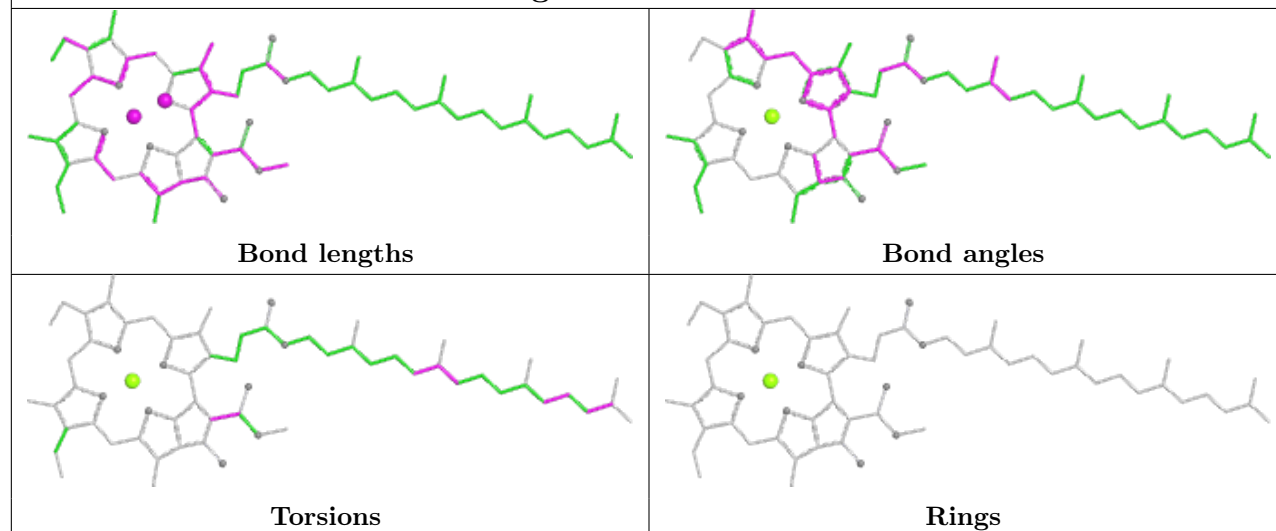
Ligand LMG b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

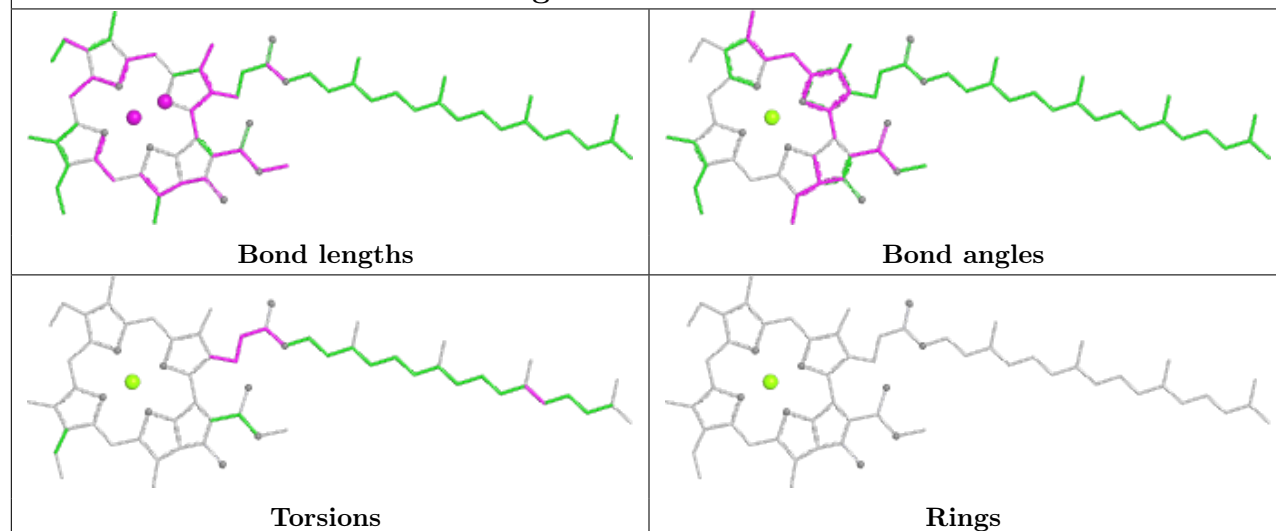
Ligand CLA B 604

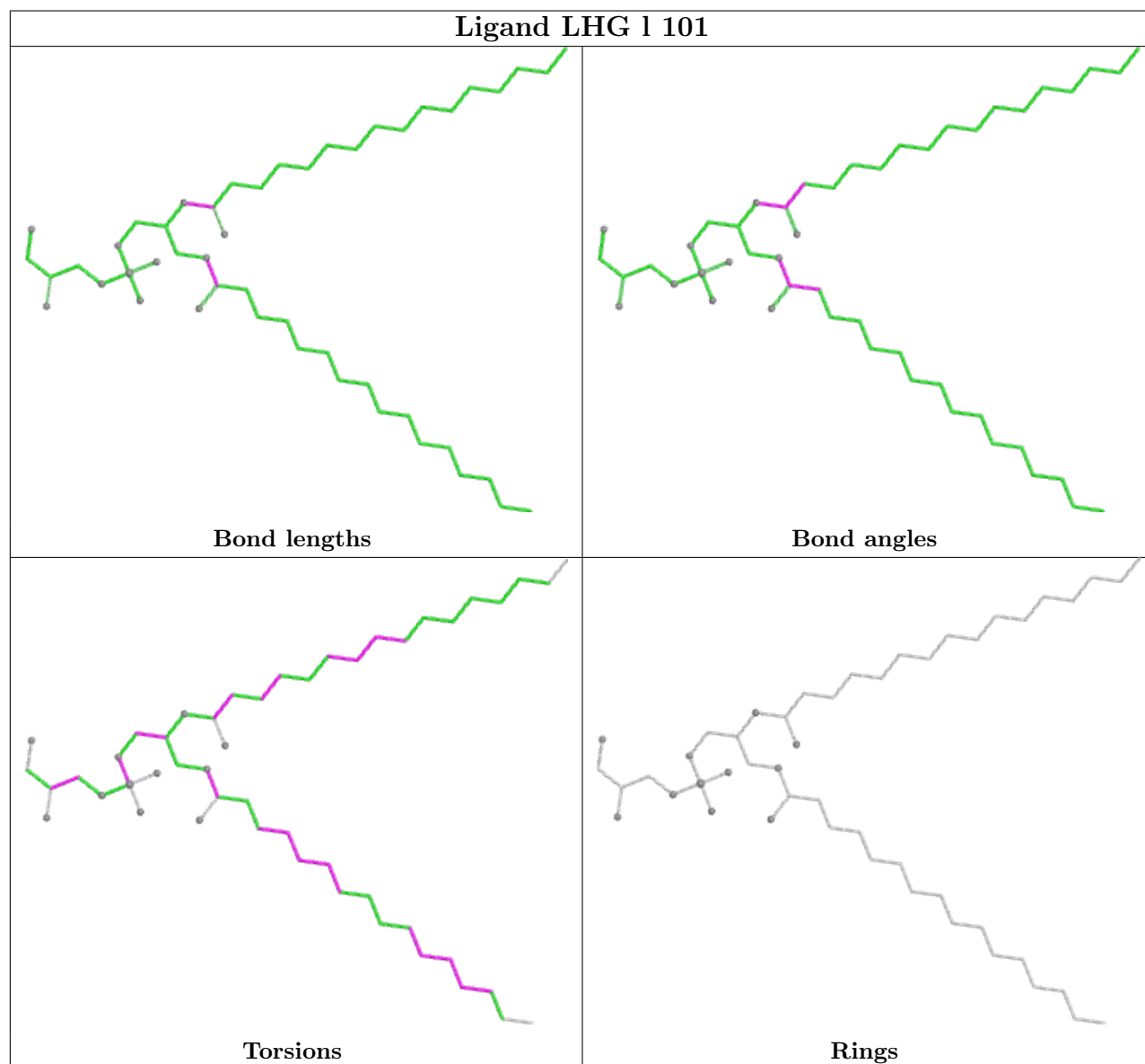
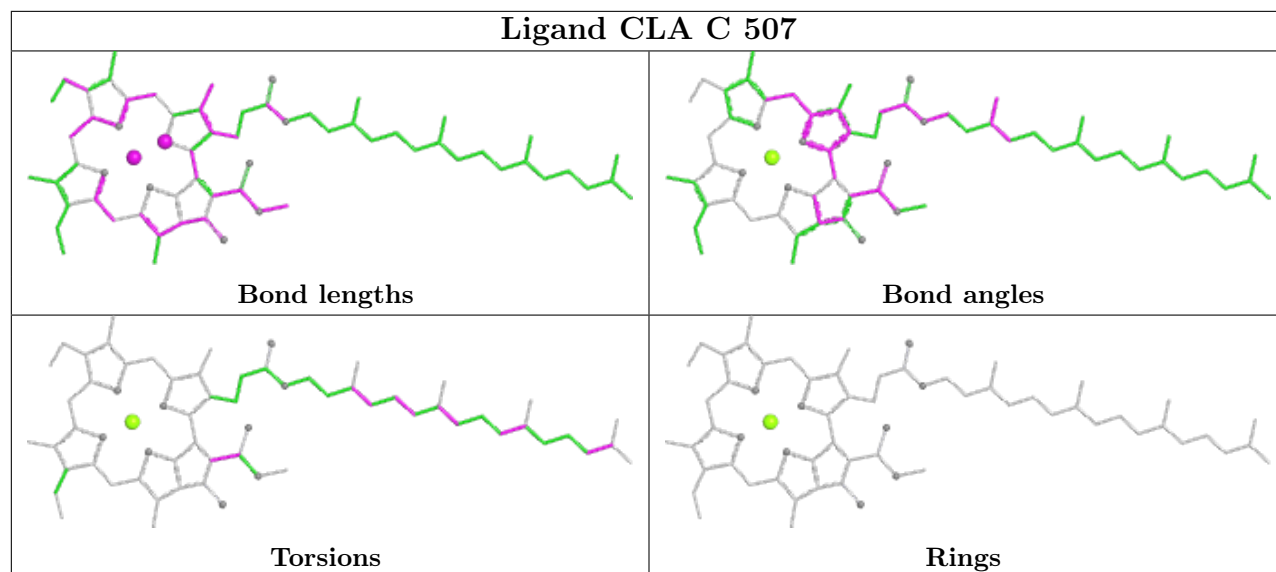


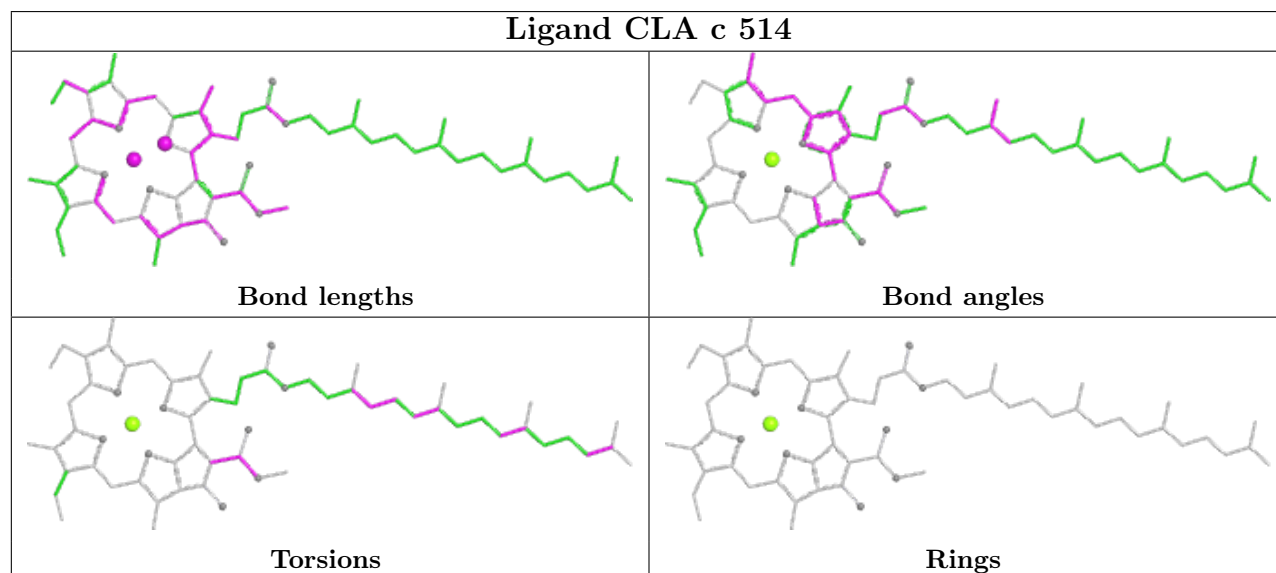
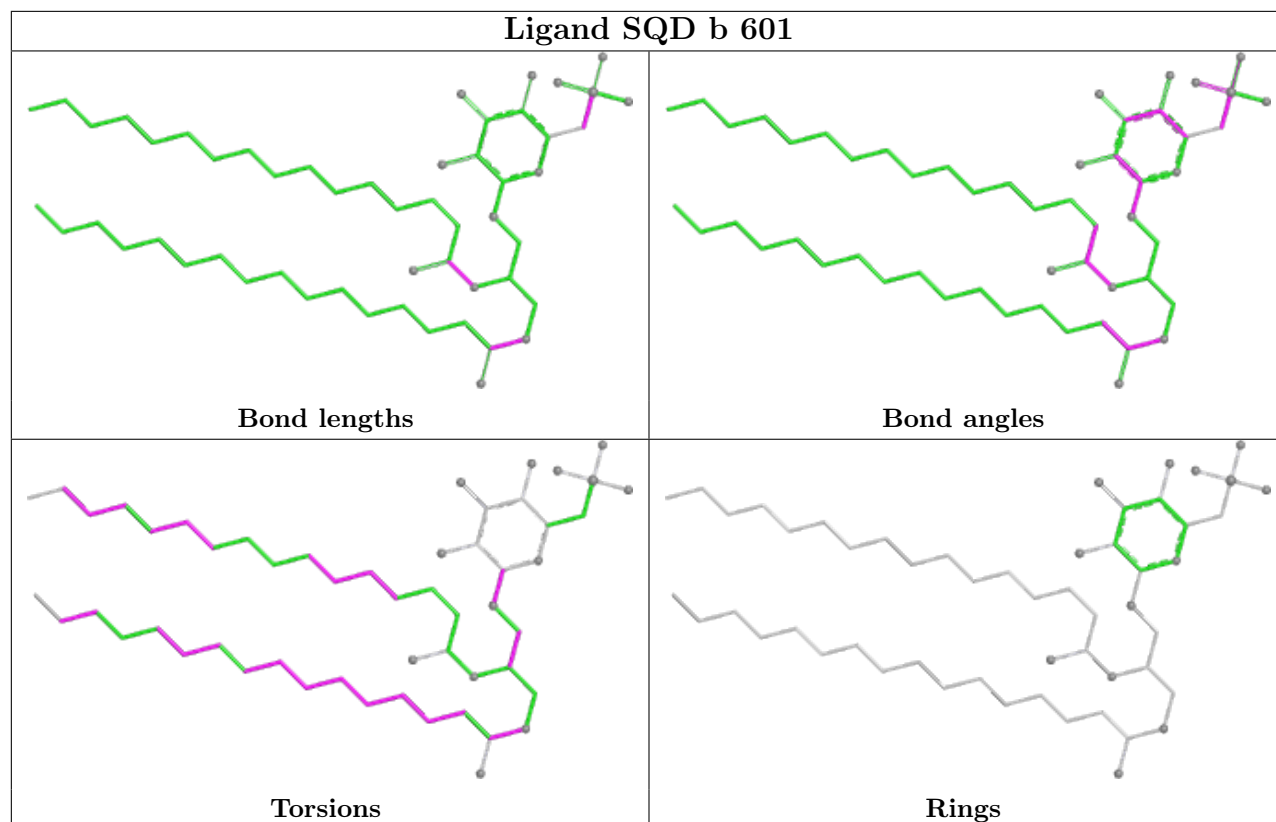
Ligand CLA A 606

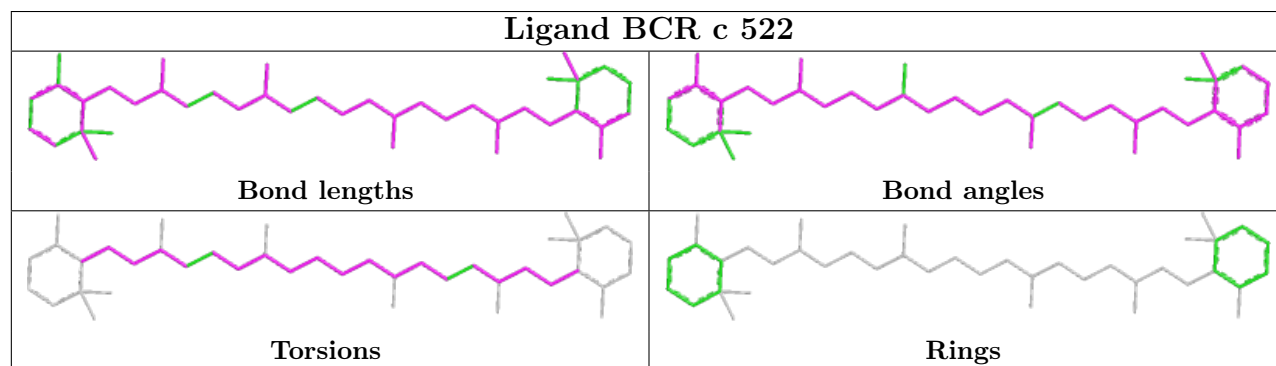
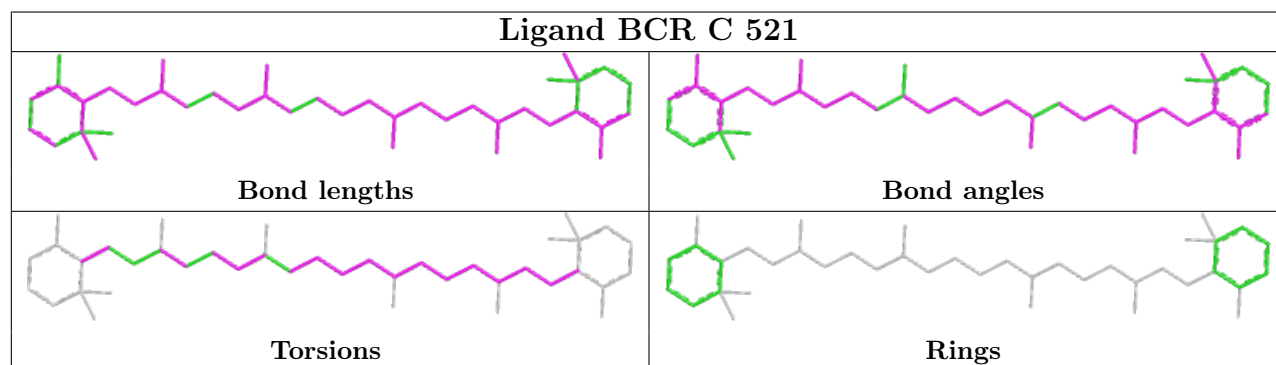
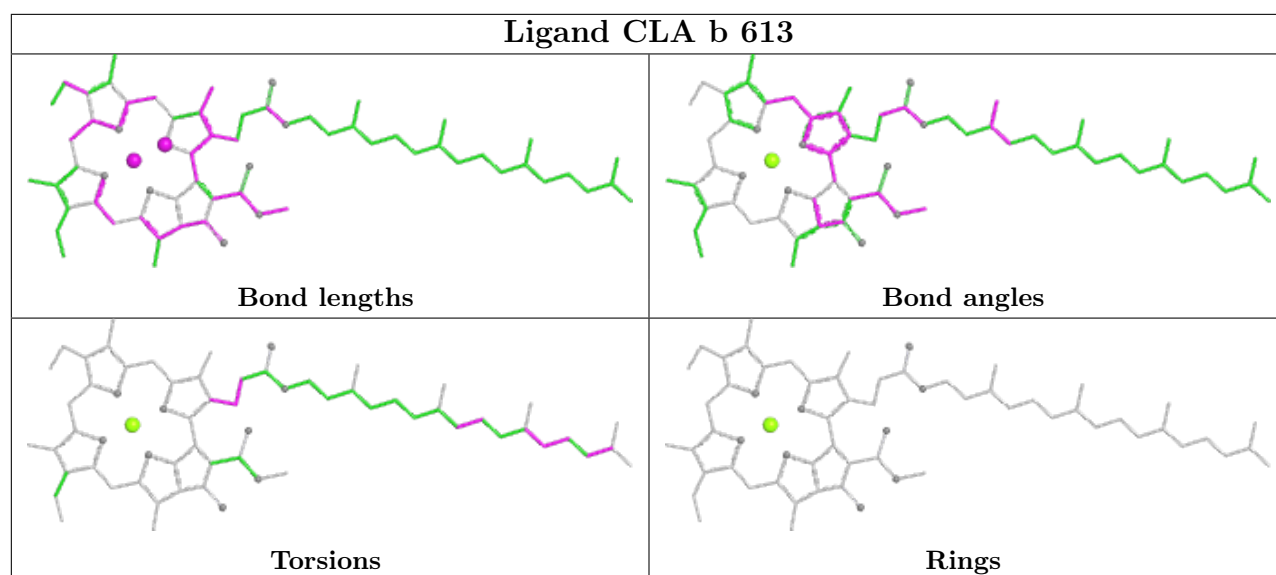


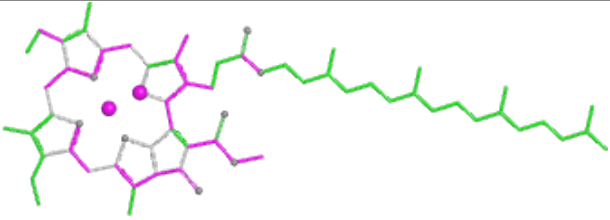
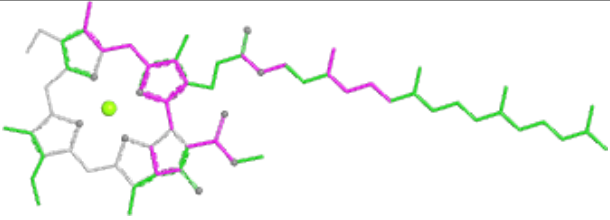
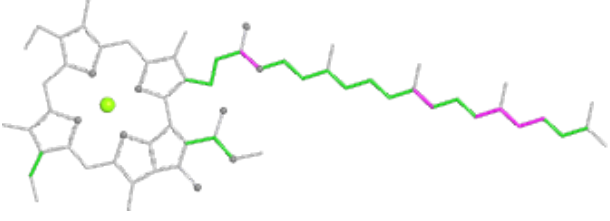
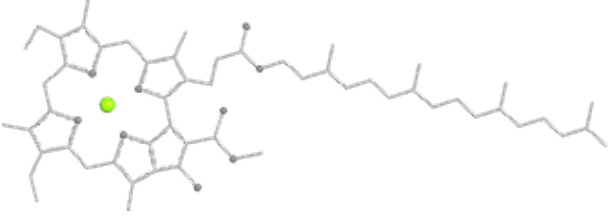
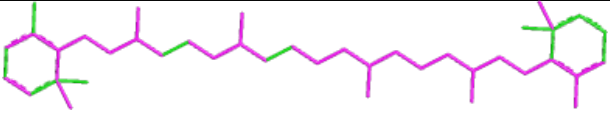
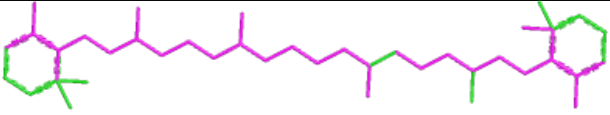

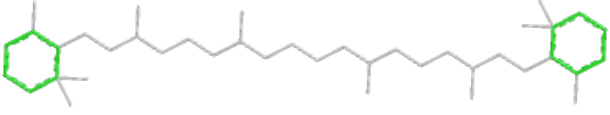
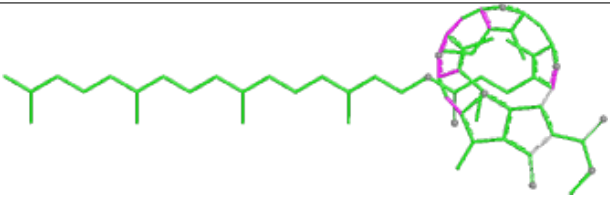
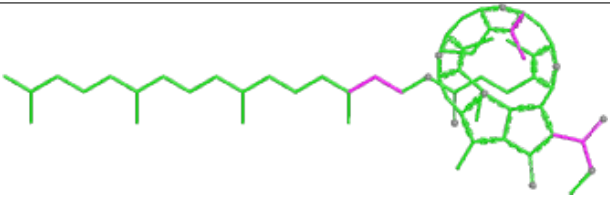
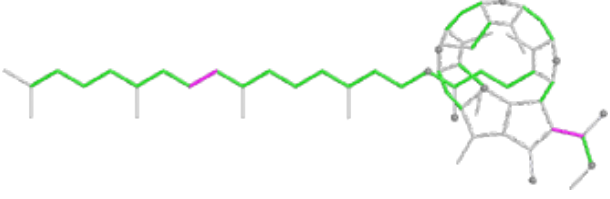
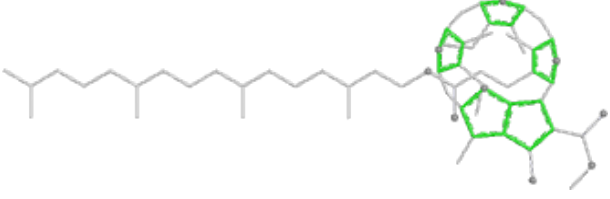
Ligand CLA C 505

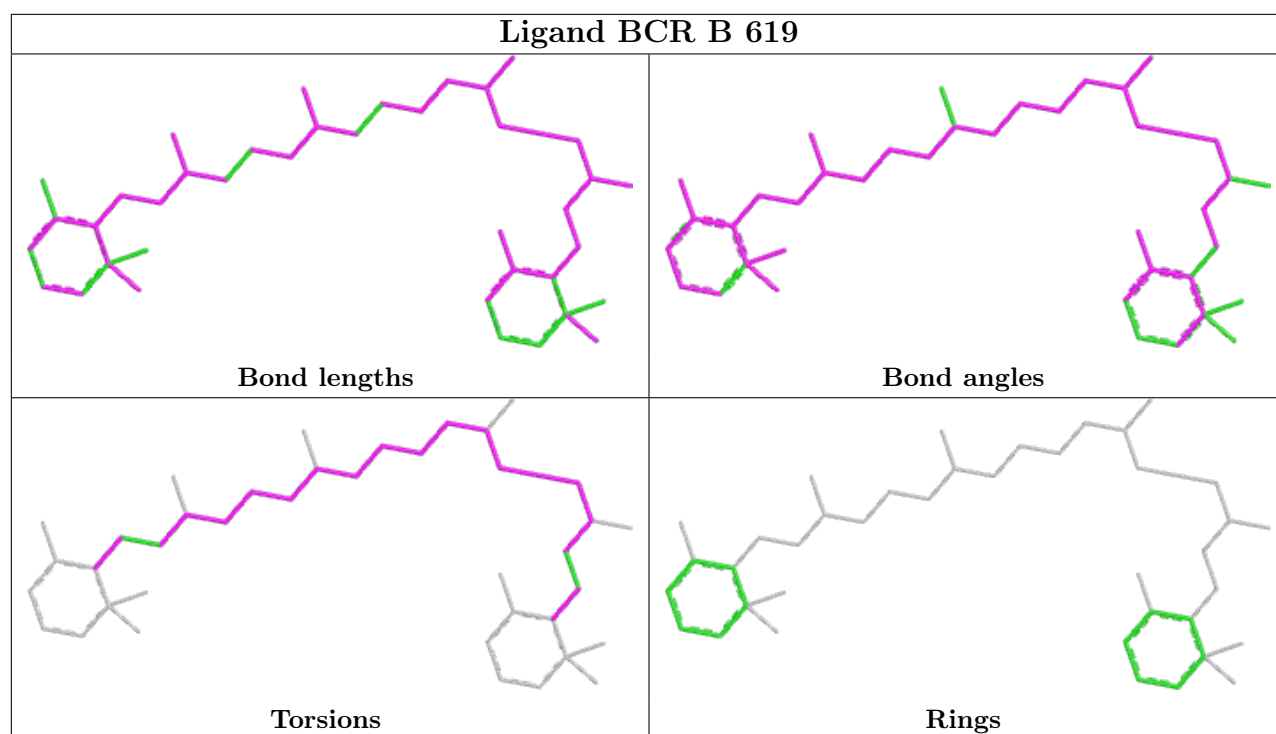


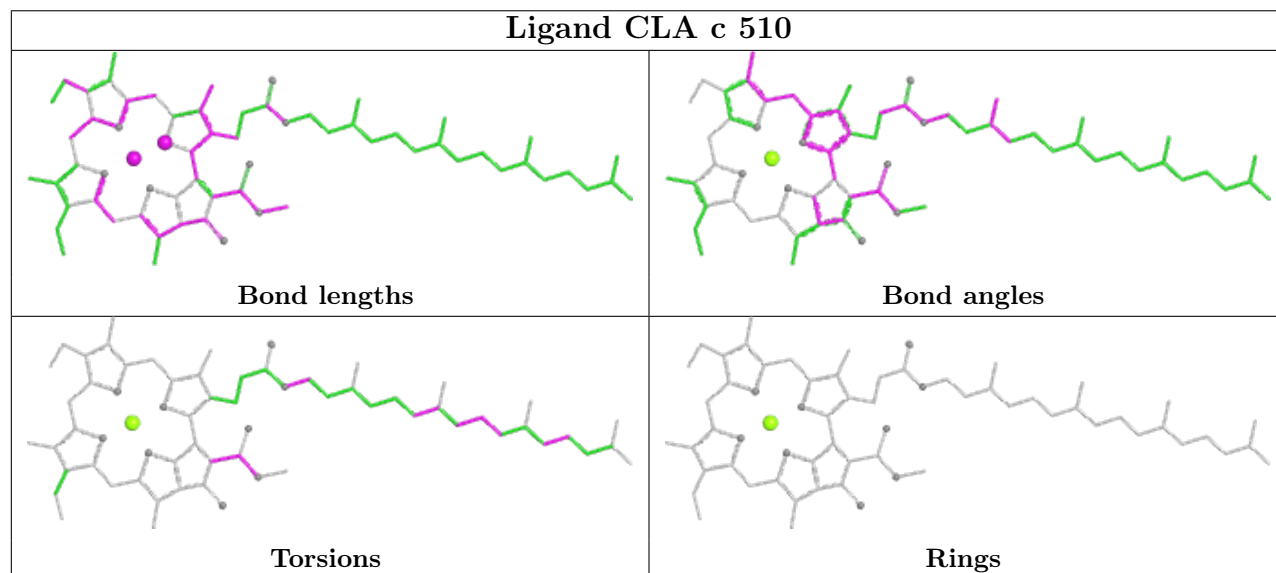
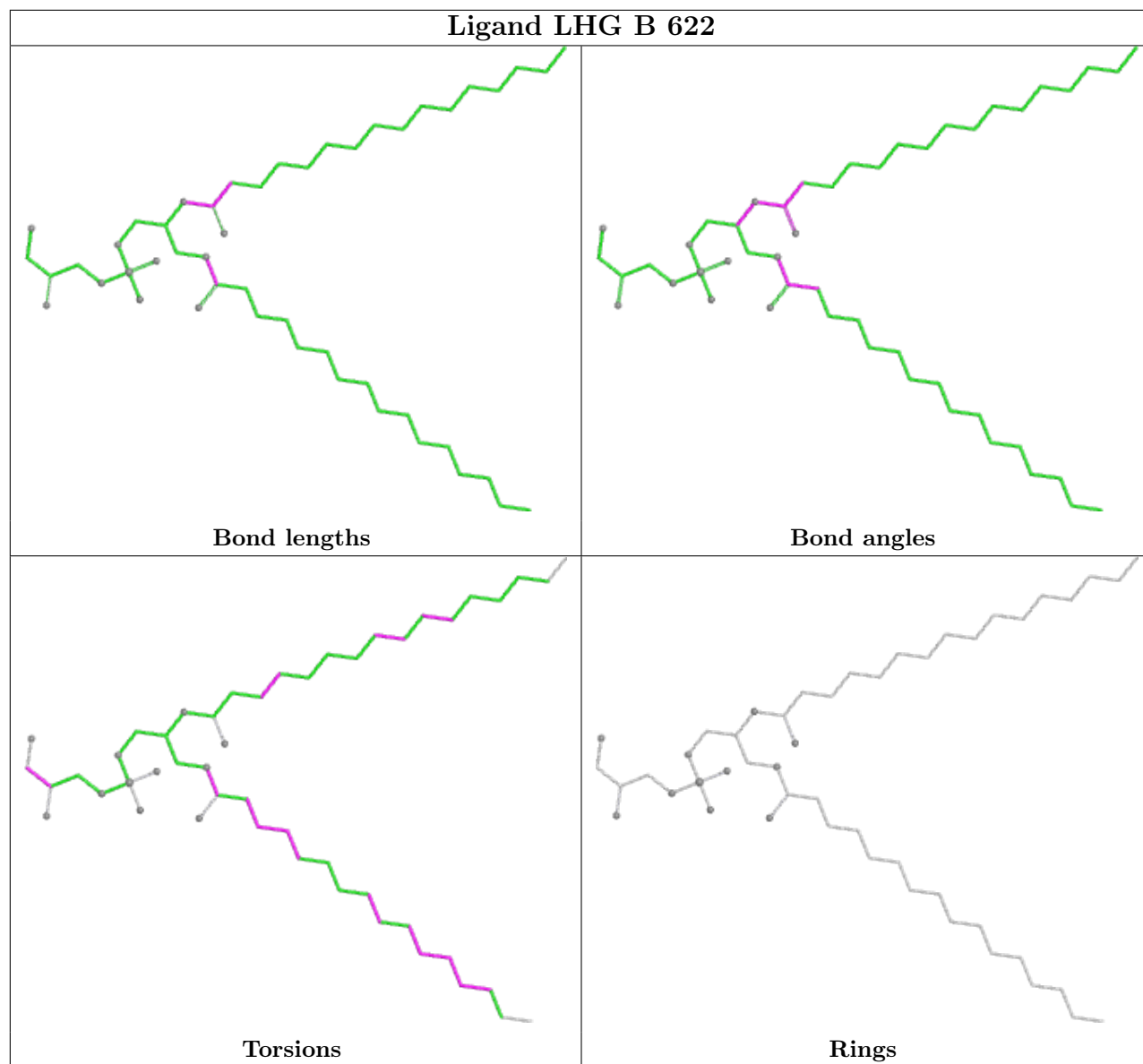


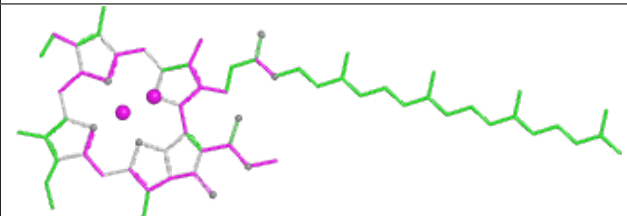
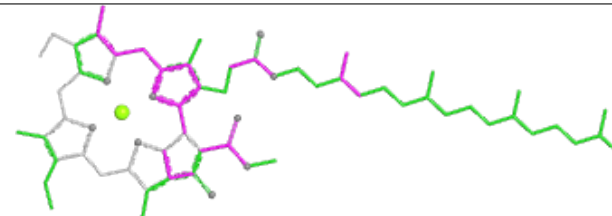
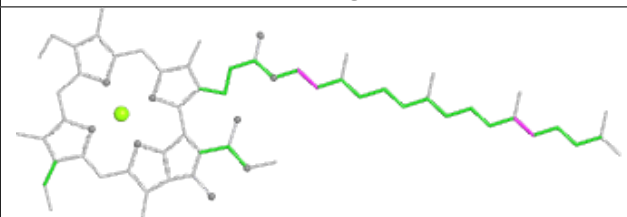
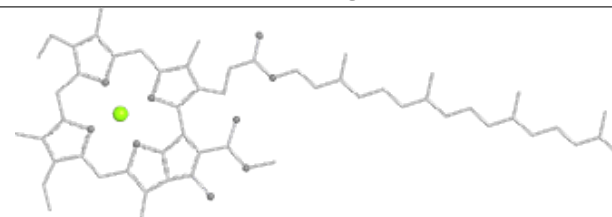


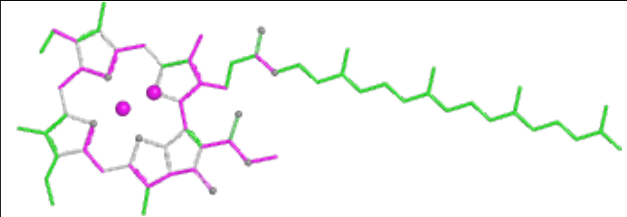
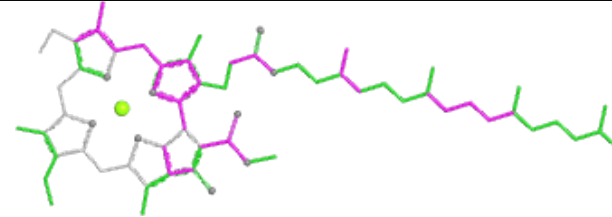
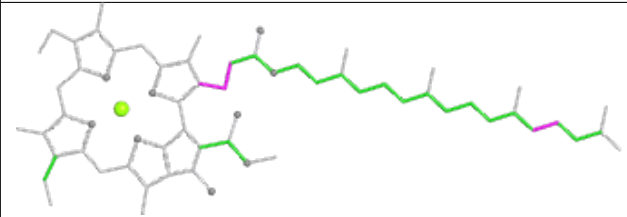
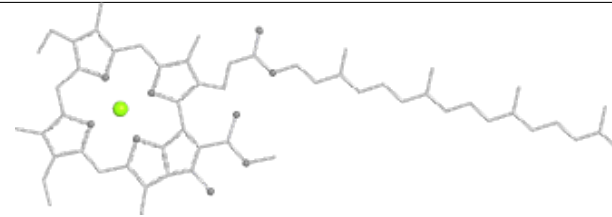


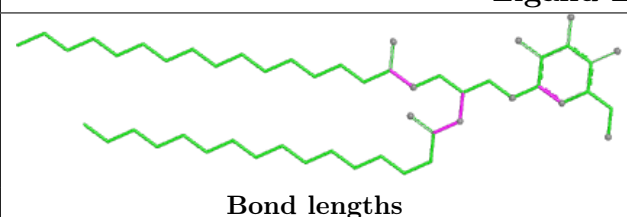
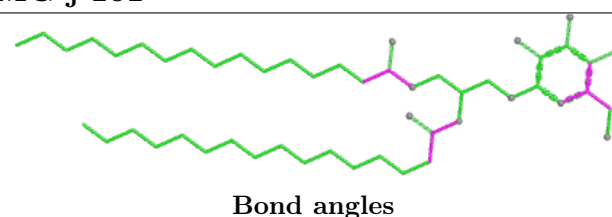
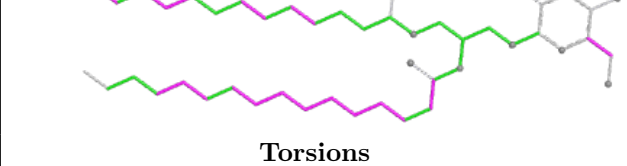

Ligand CLA C 504	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR a 608	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PHO D 401	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

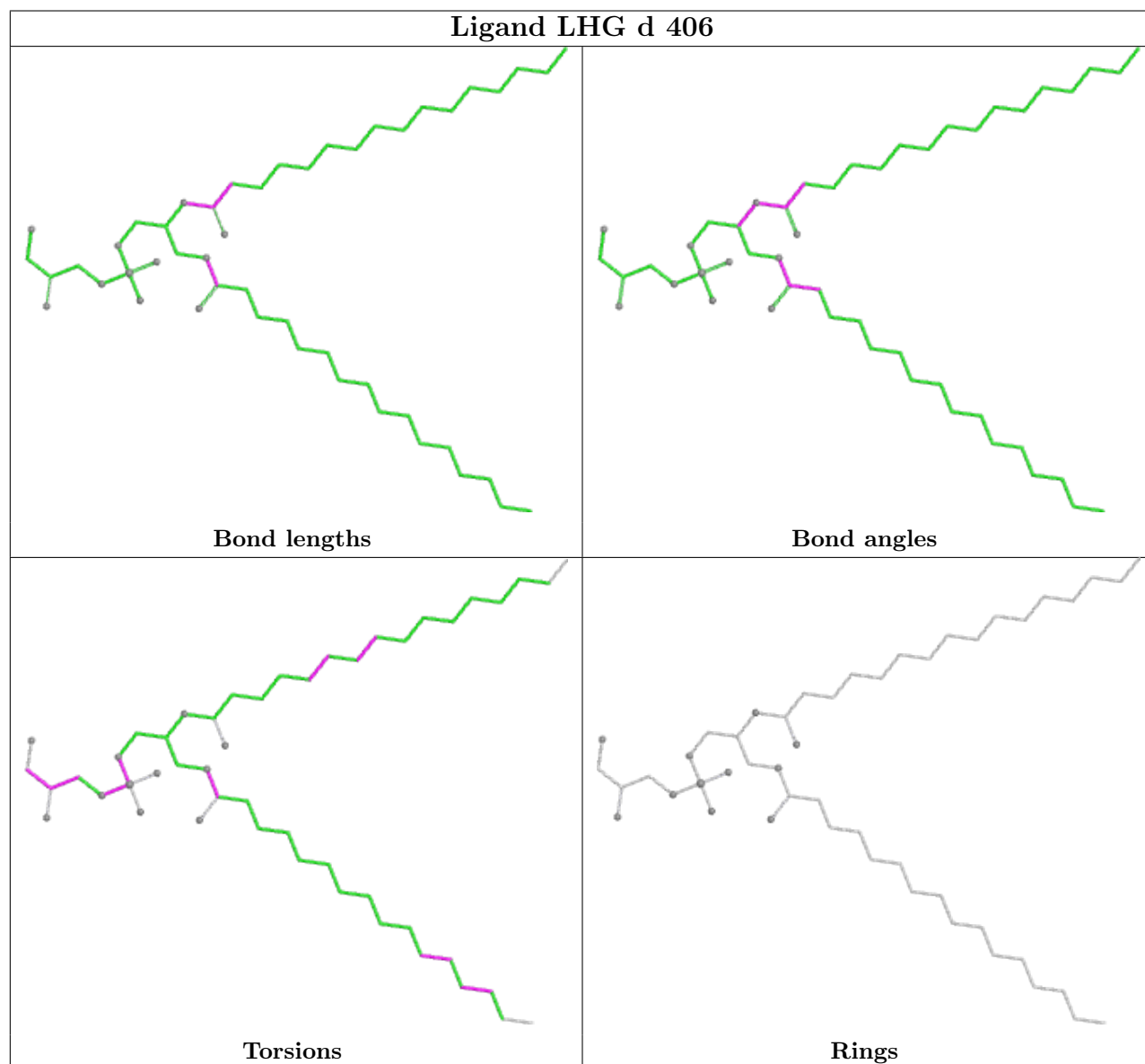
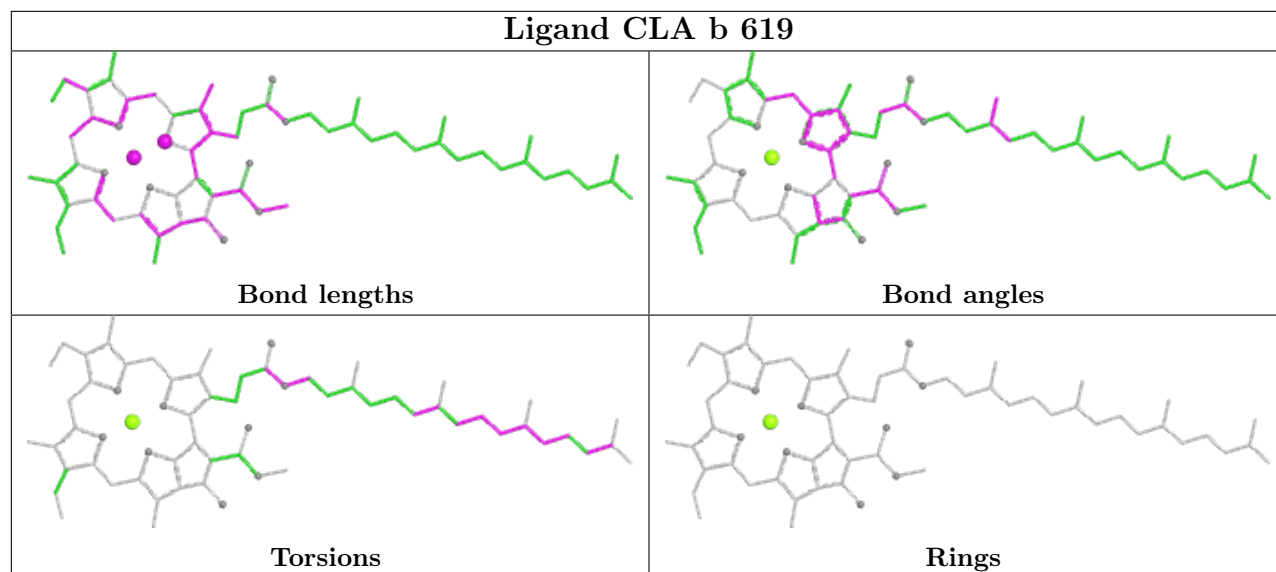




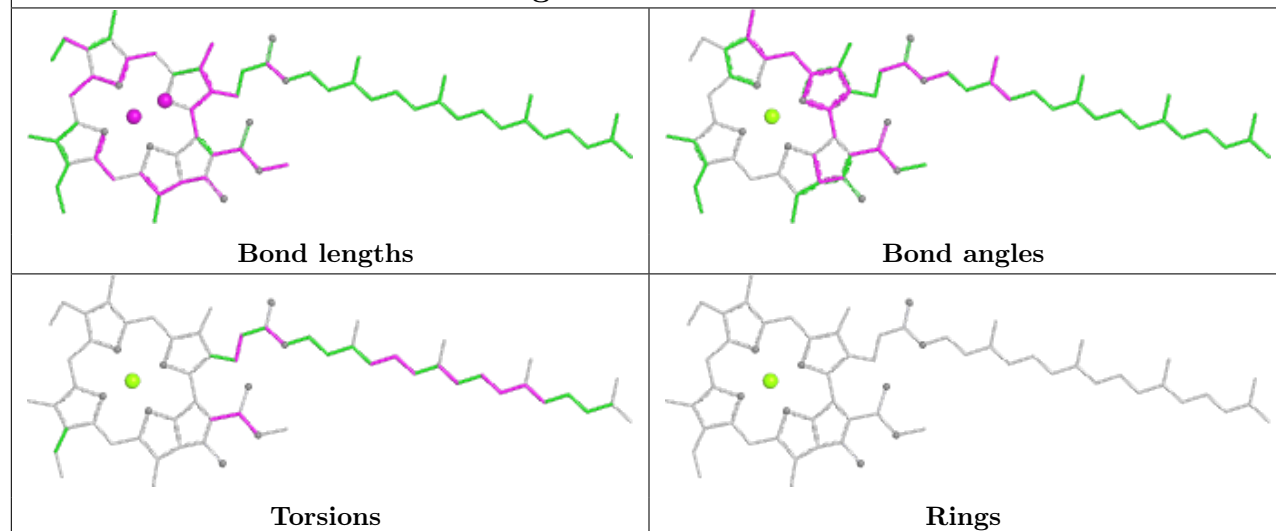
Ligand CLA D 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

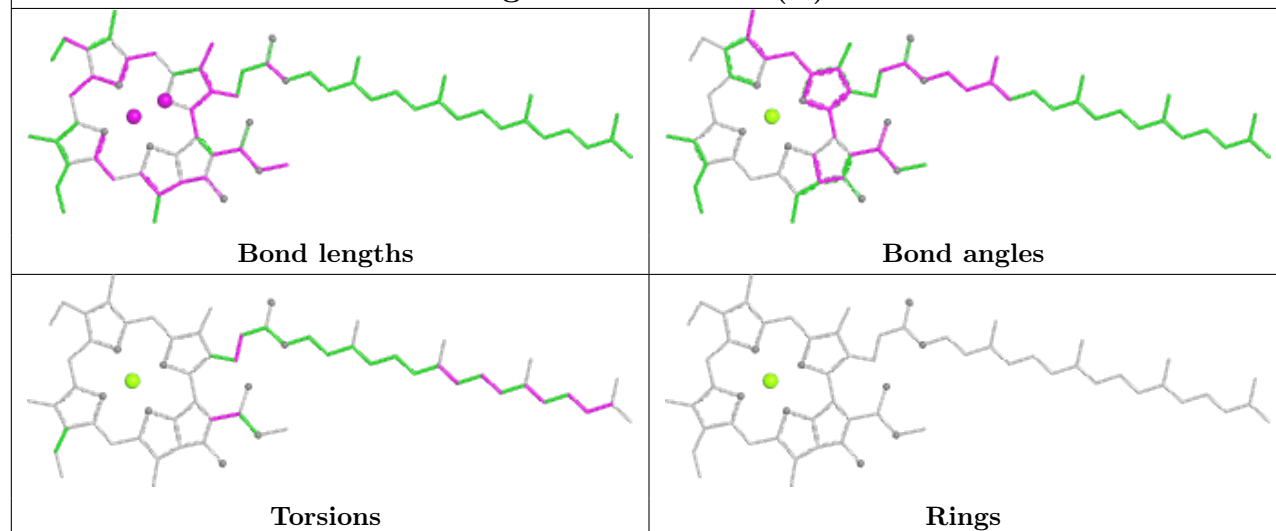
Ligand LMG j 101	
	
Bond lengths	Bond angles
	
Torsions	Rings



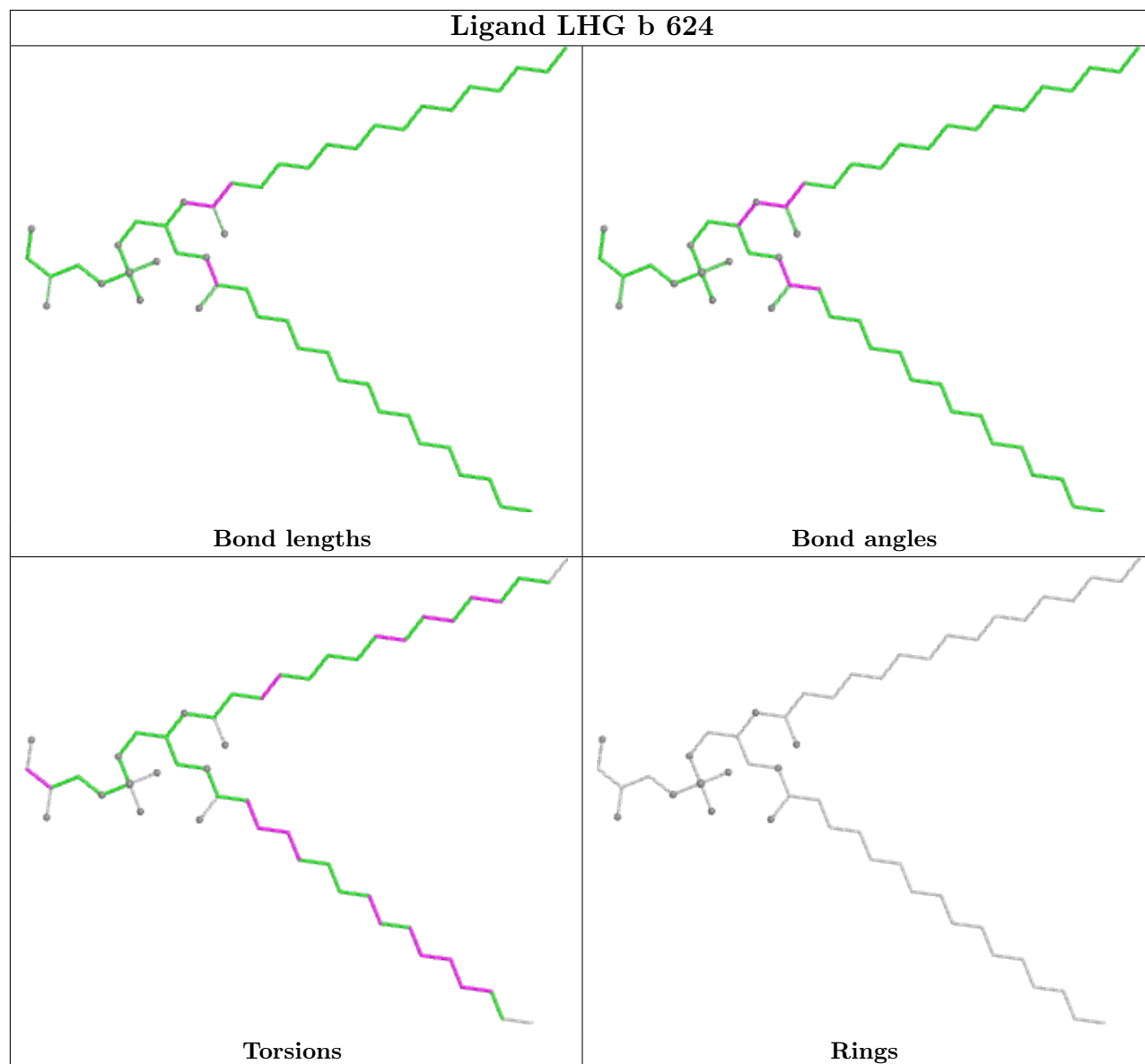
Ligand CLA B 615



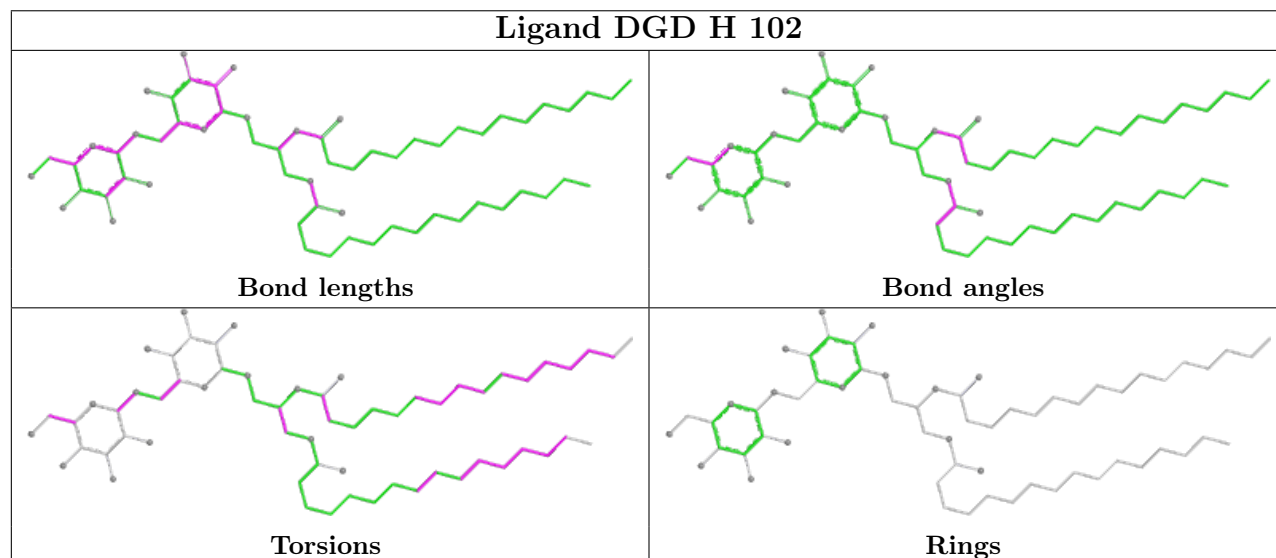
Ligand CLA b 609 (B)

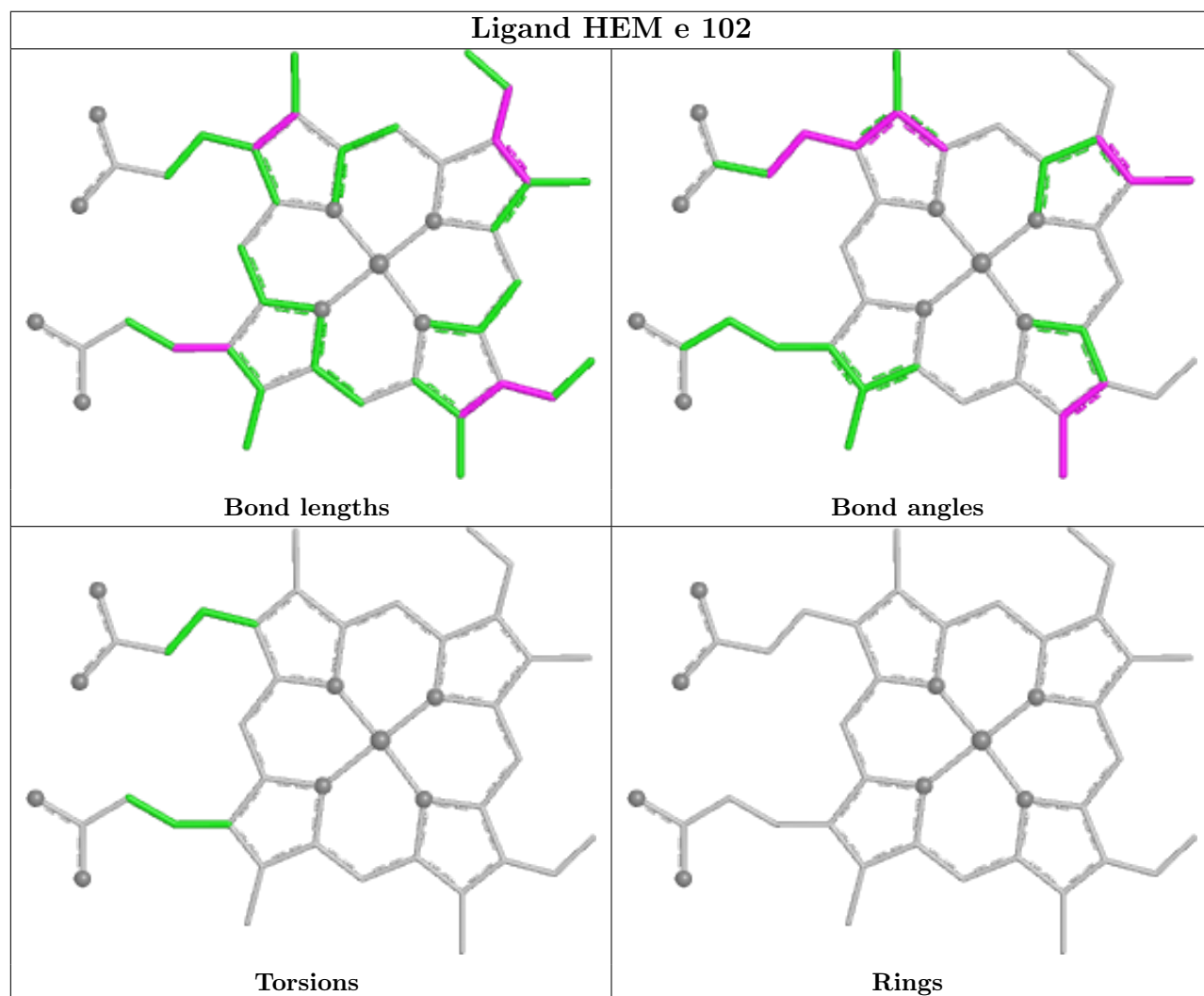
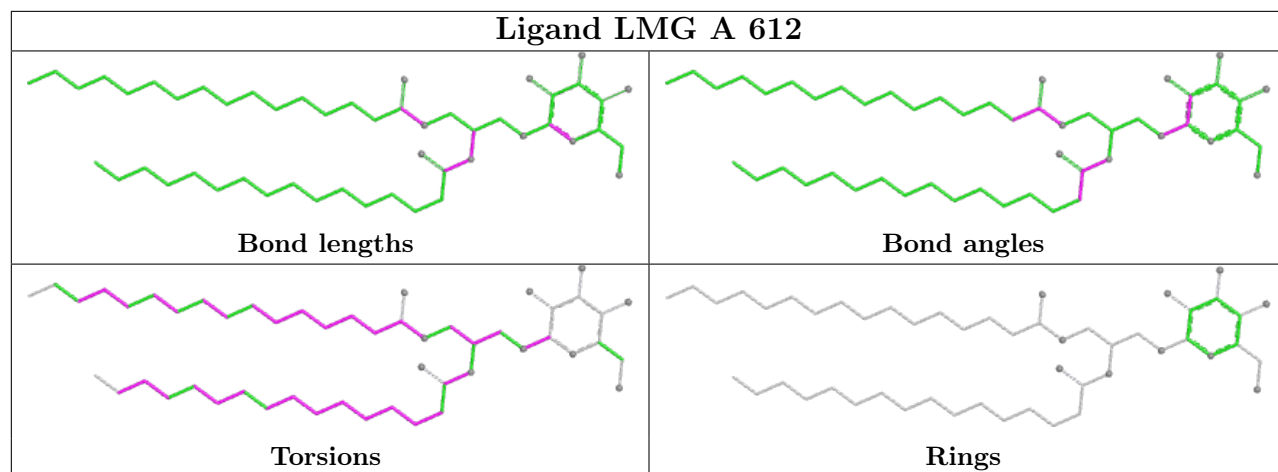


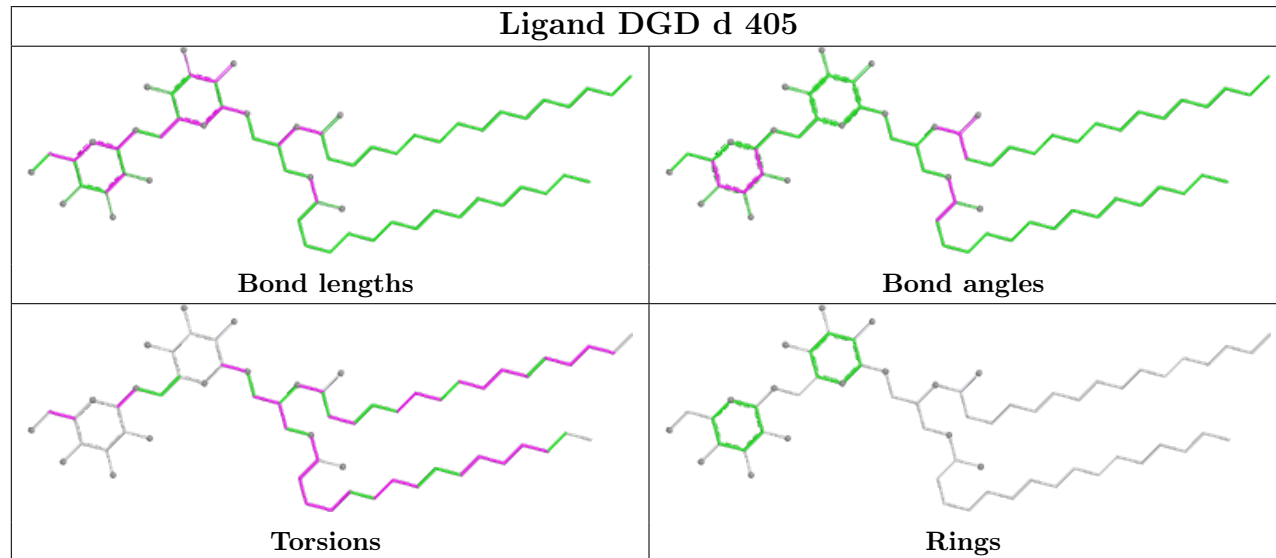
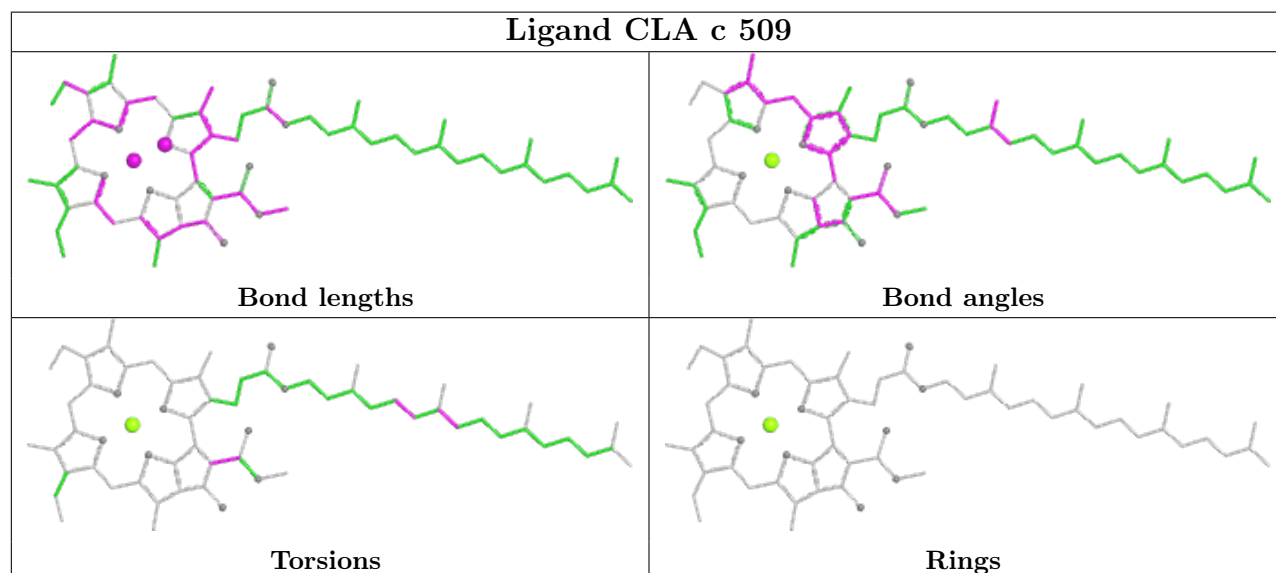
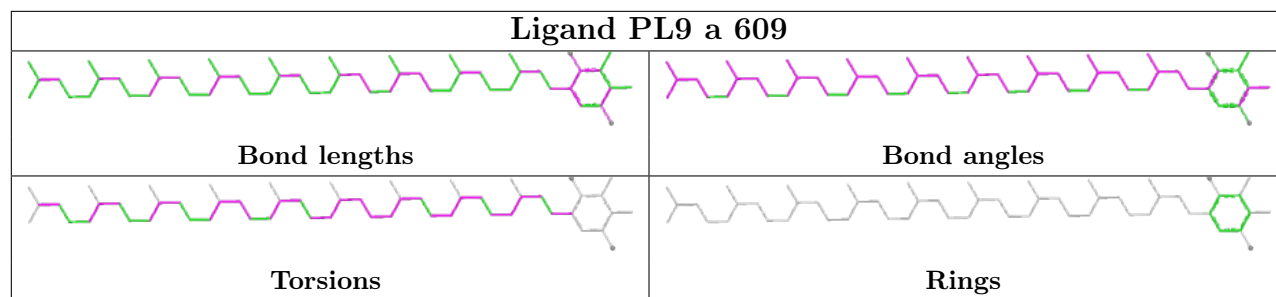
Ligand LHG b 624

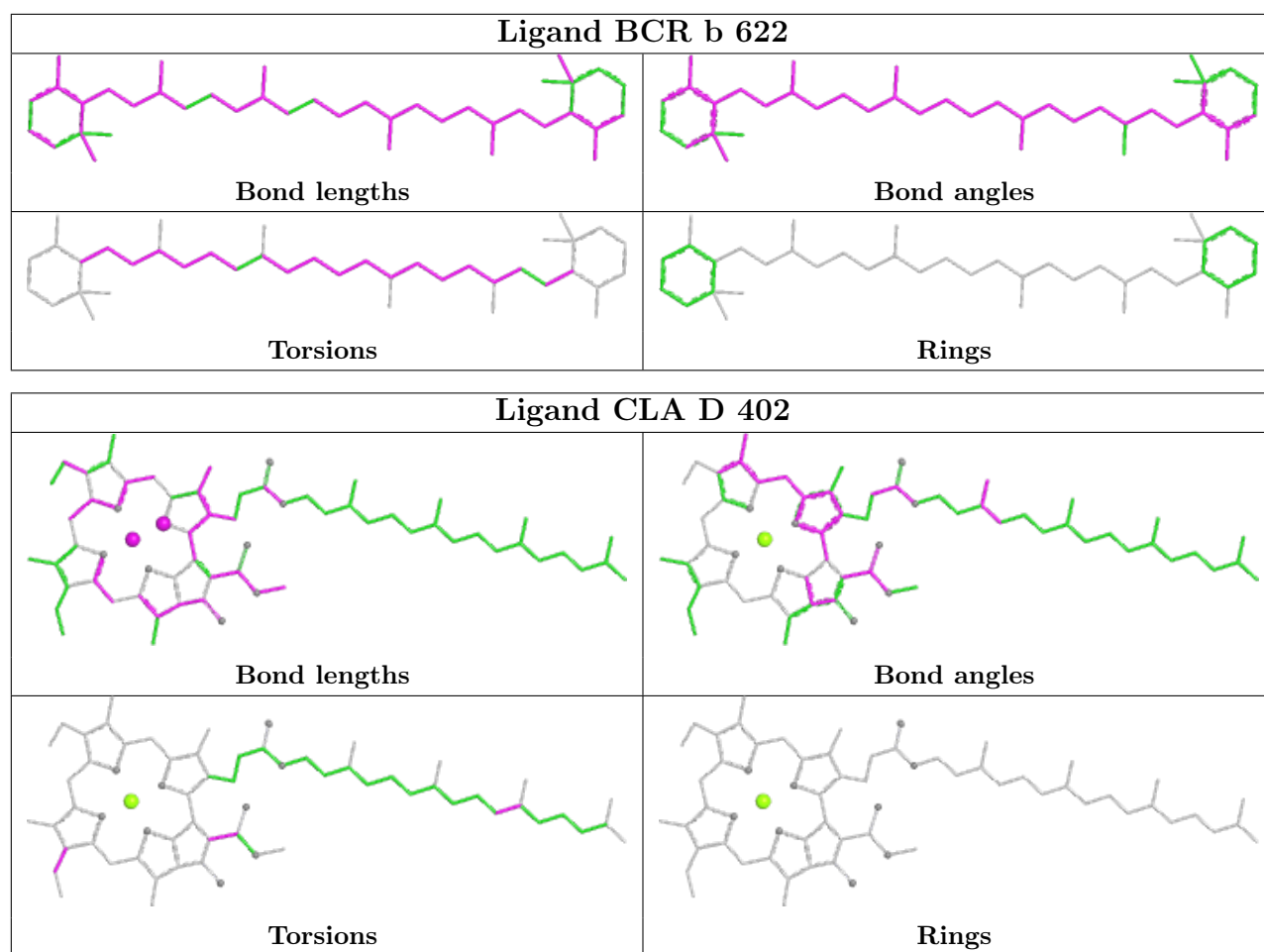


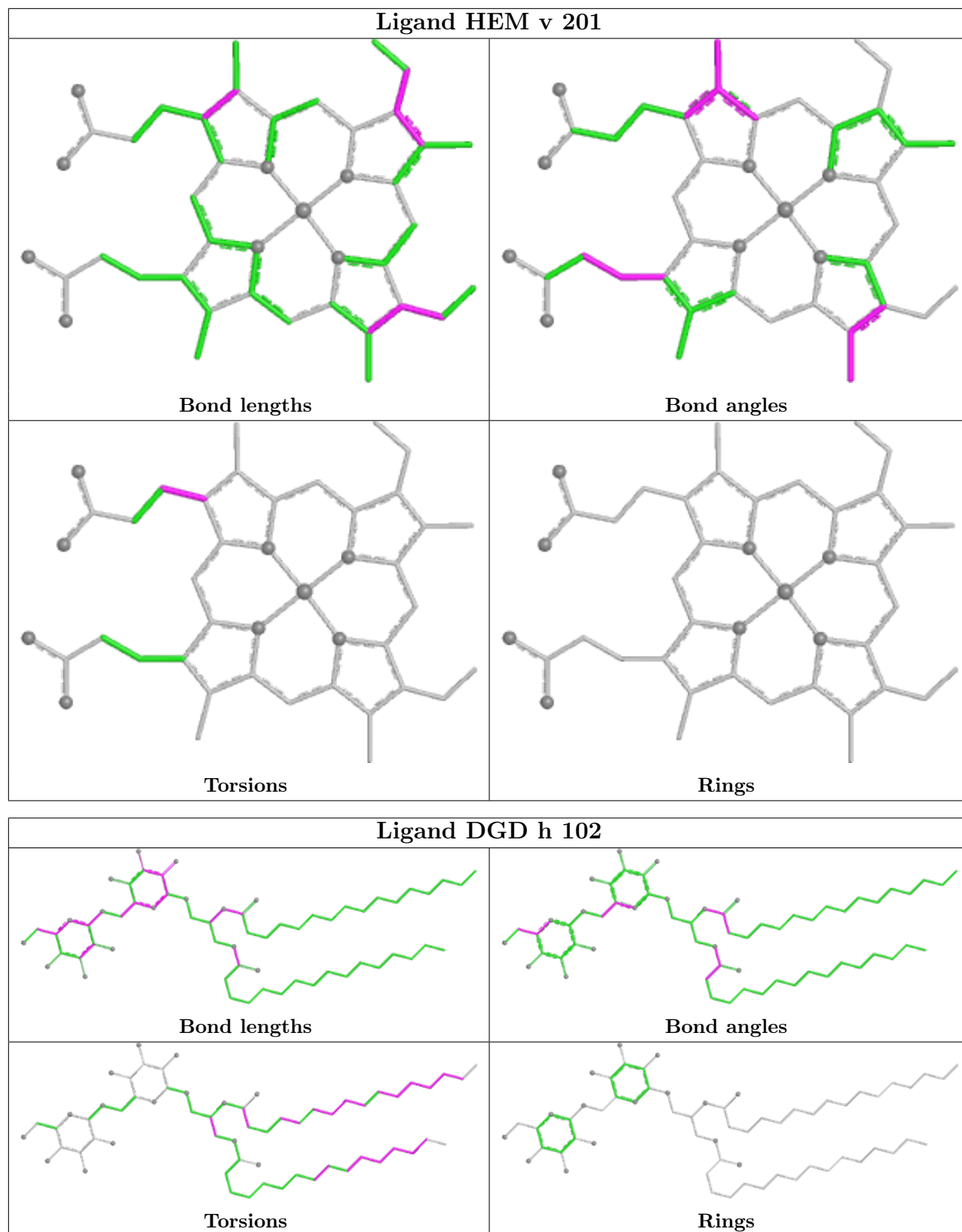
Ligand DGD H 102

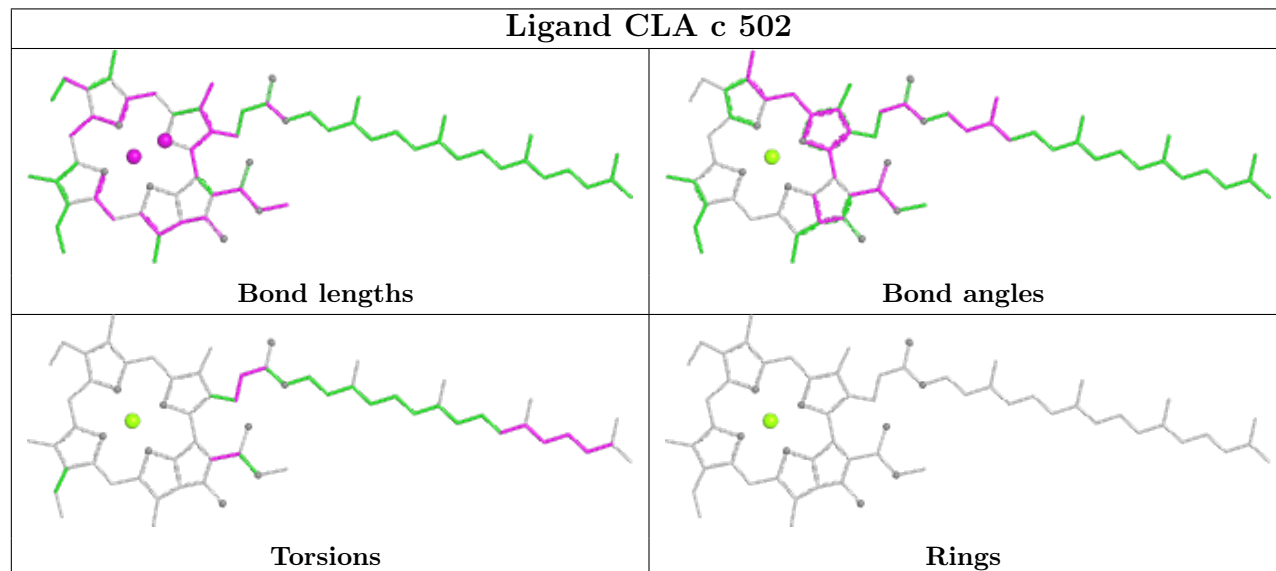
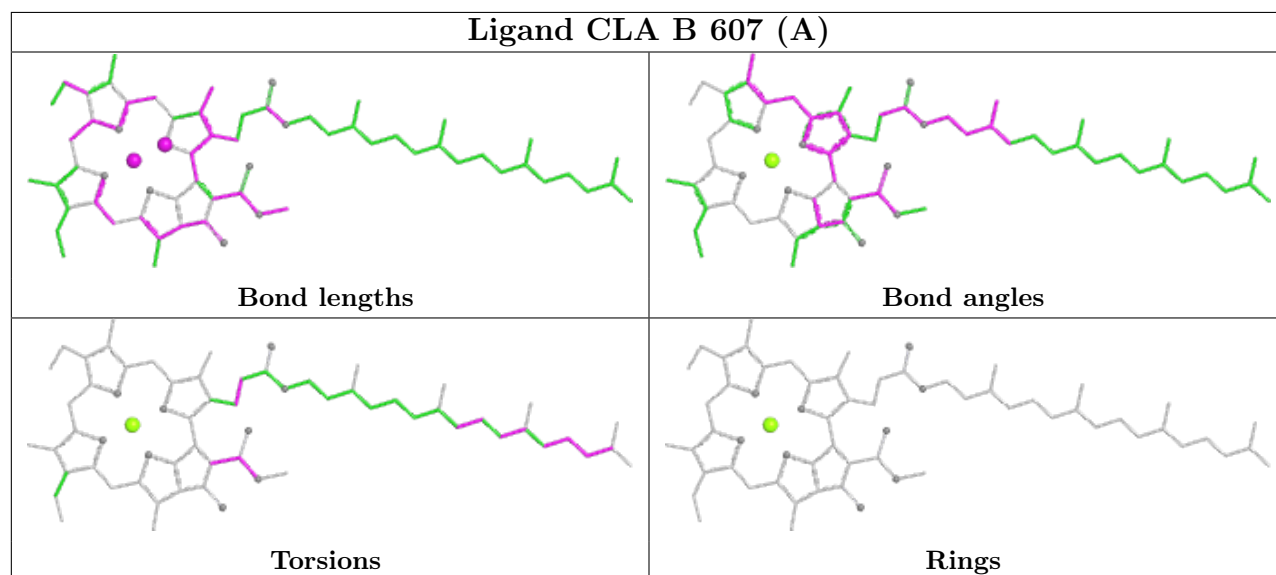
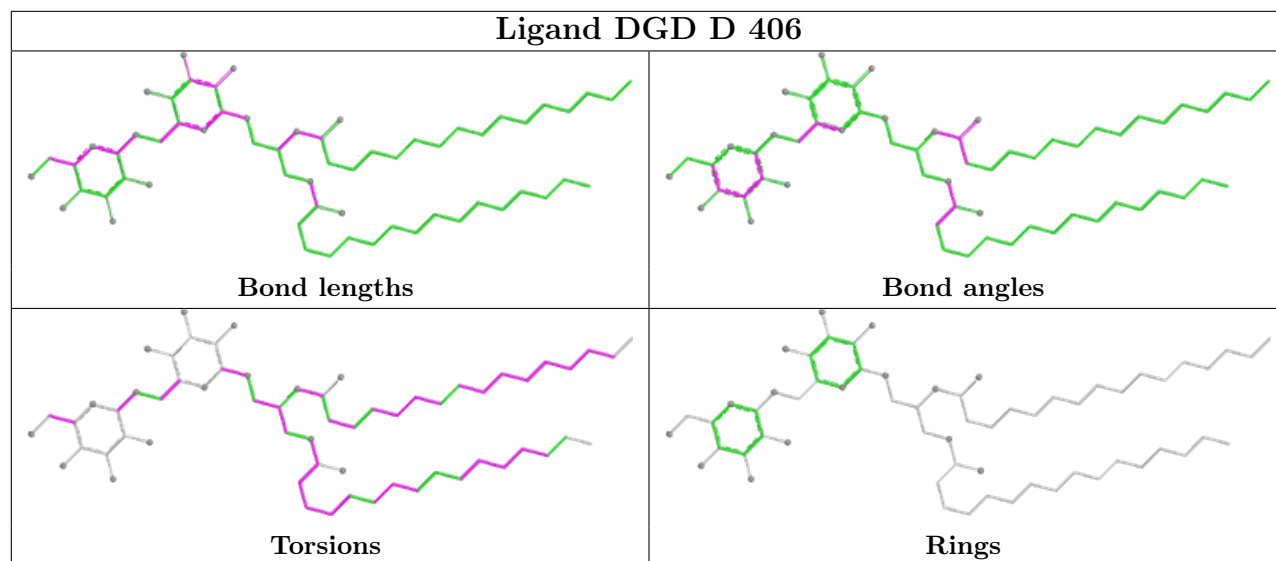


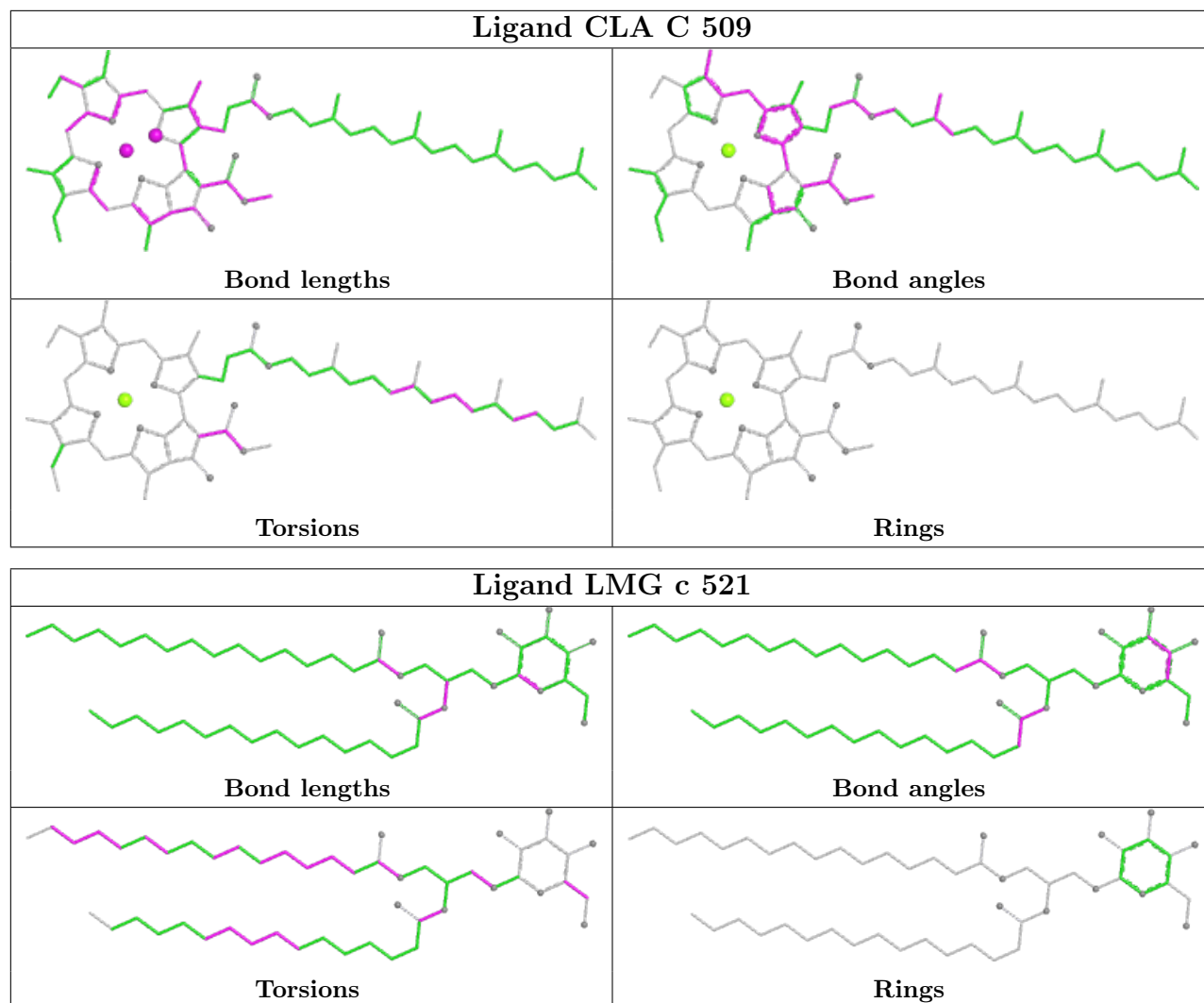


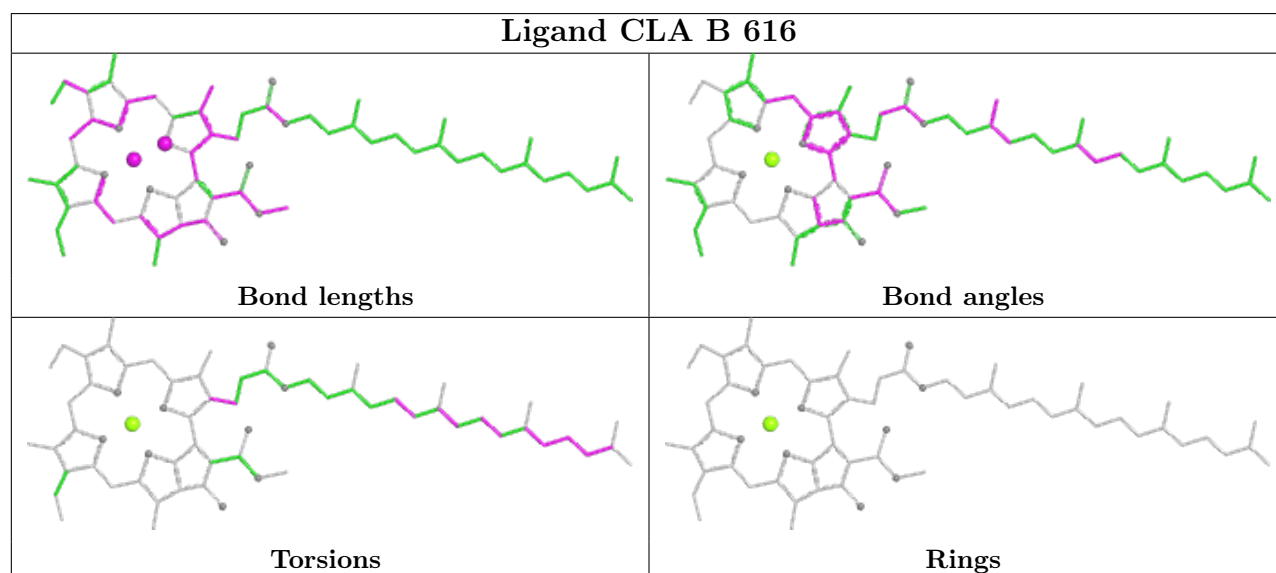
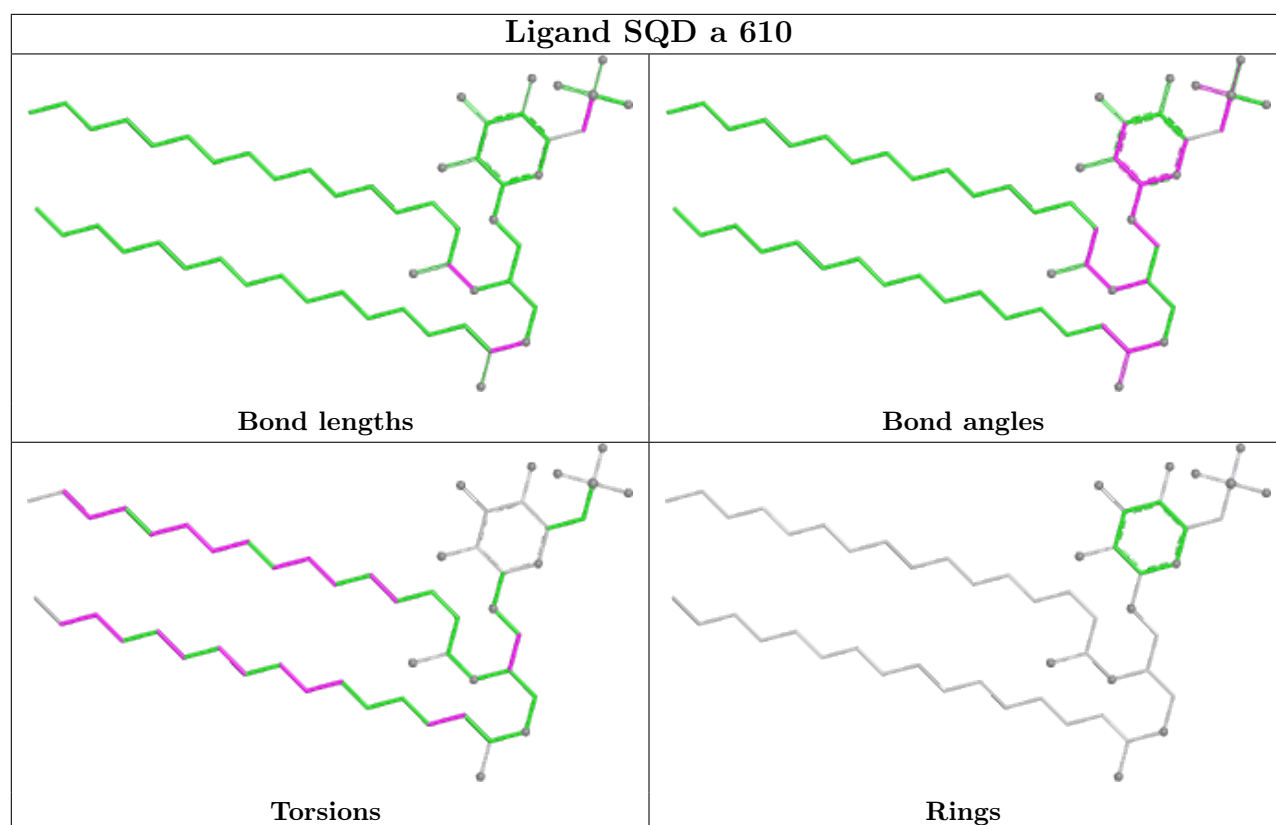




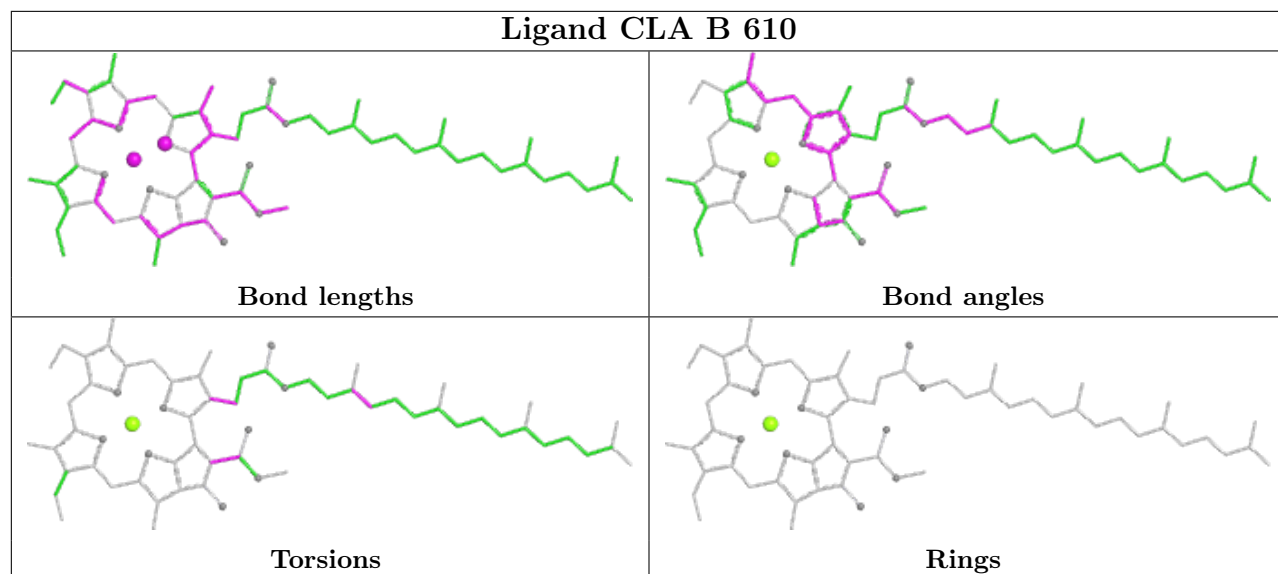




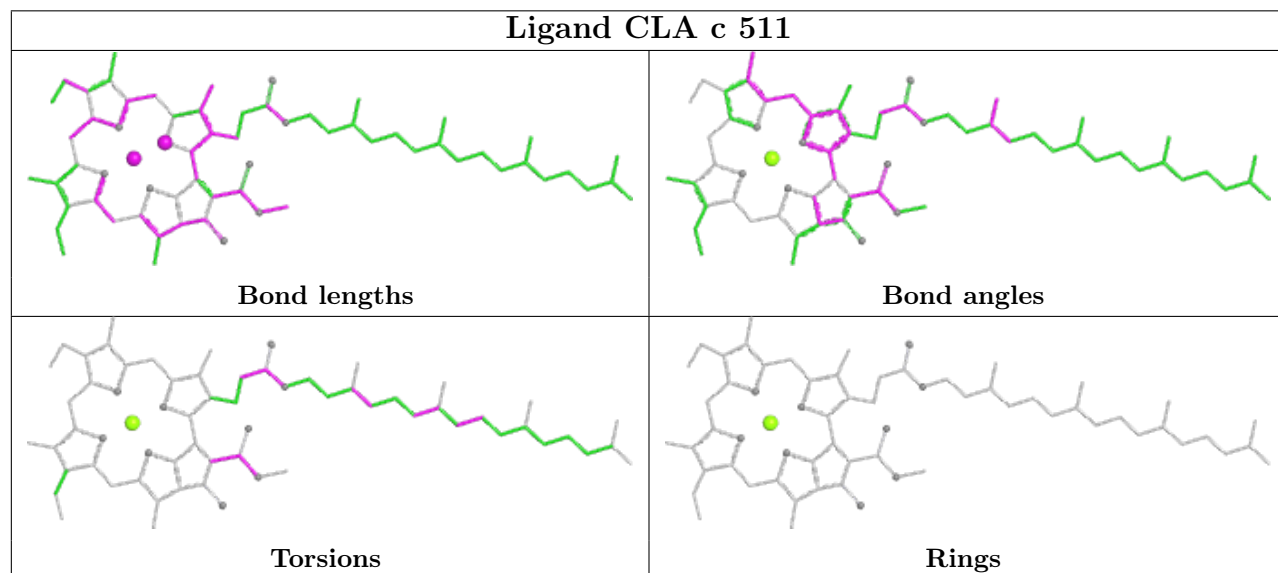


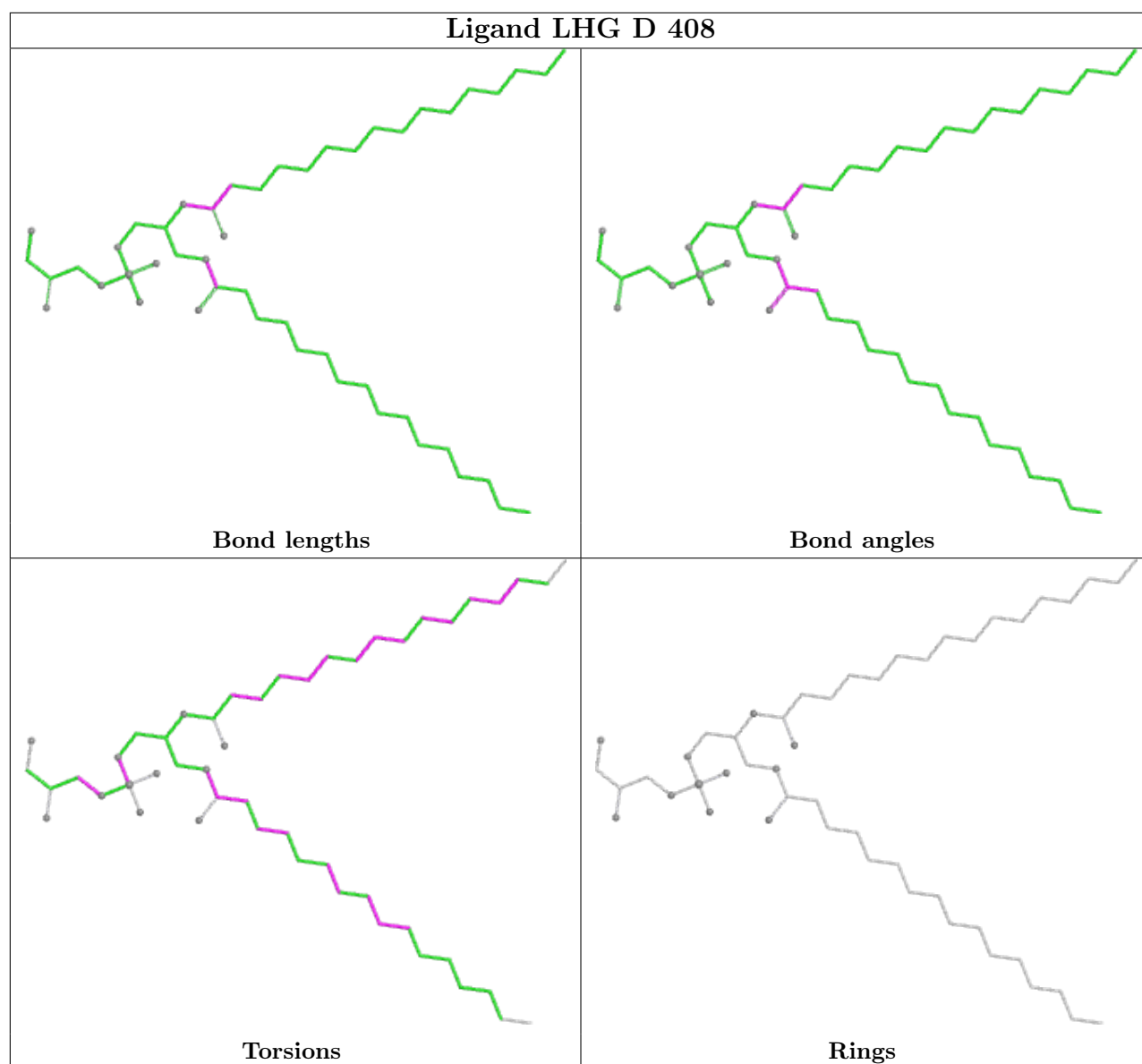


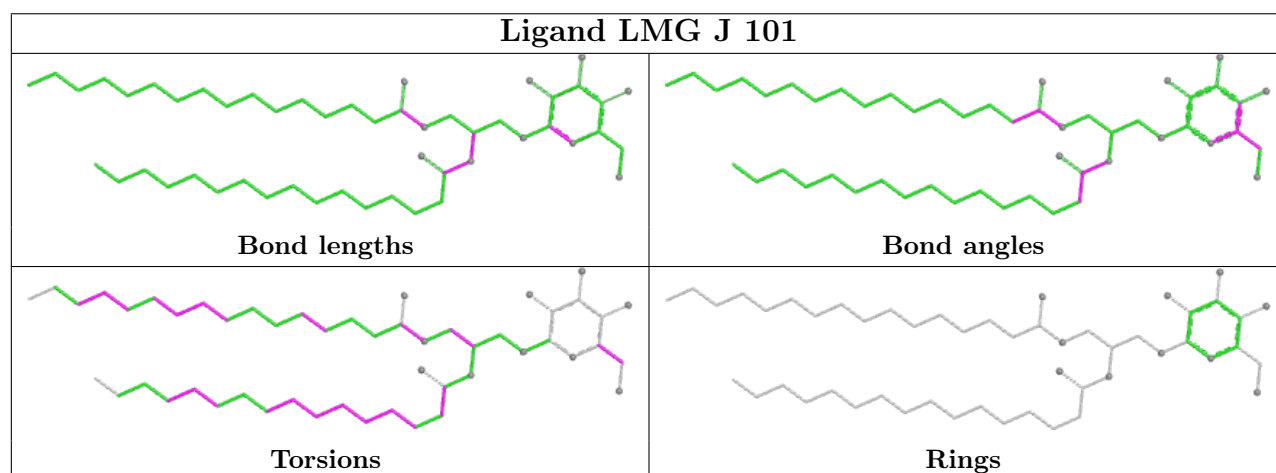
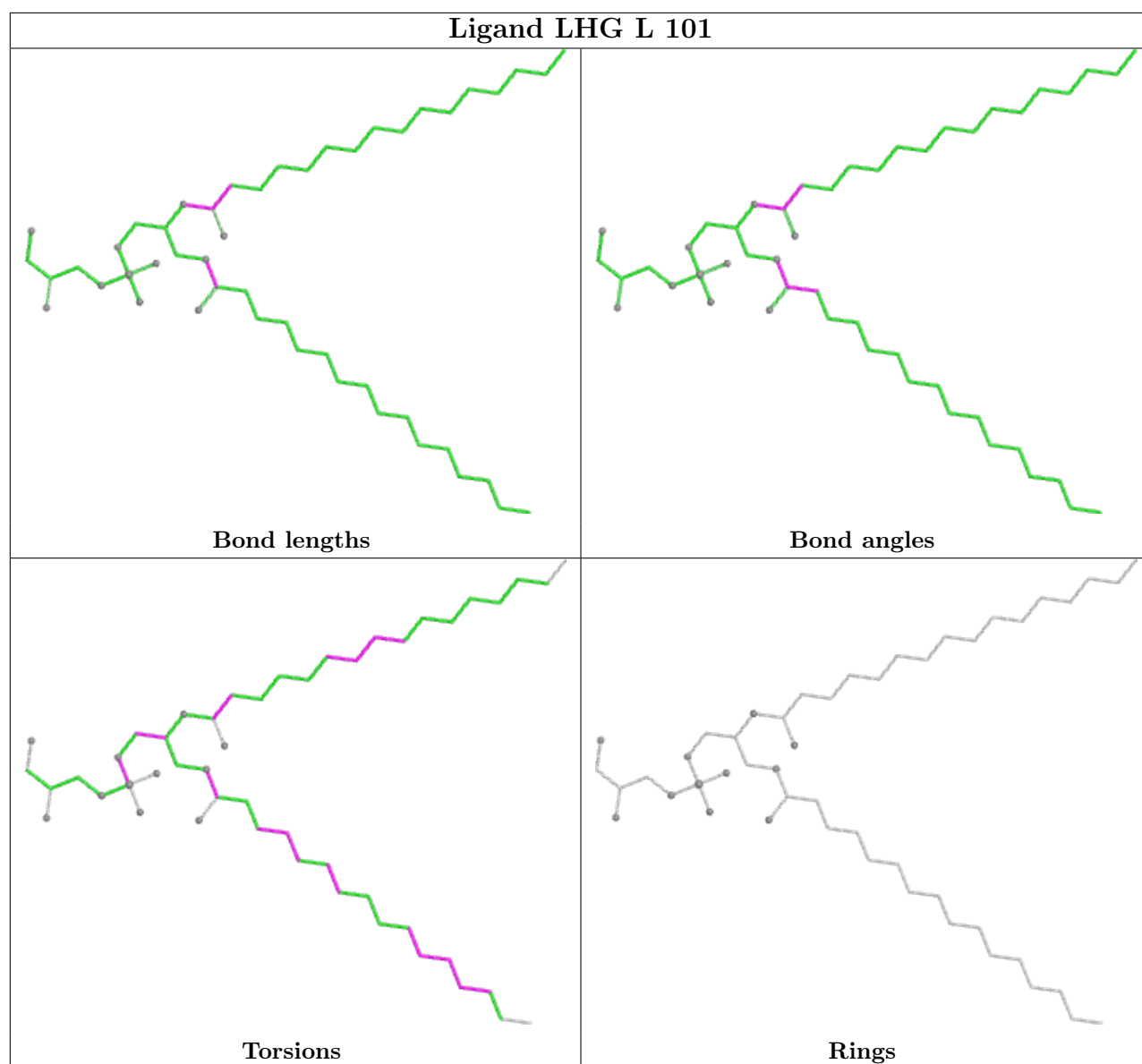
Ligand CLA B 610

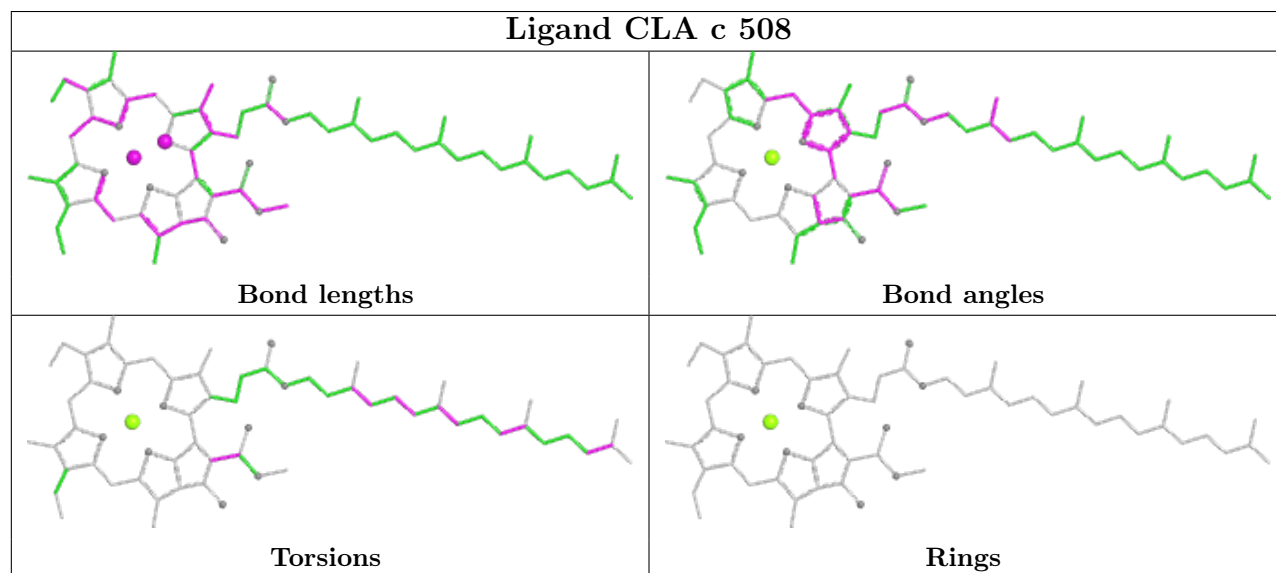
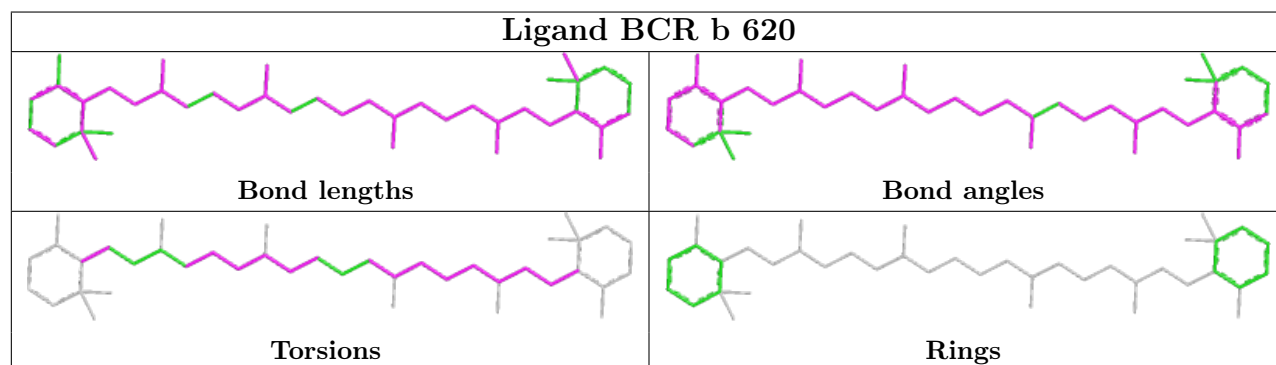
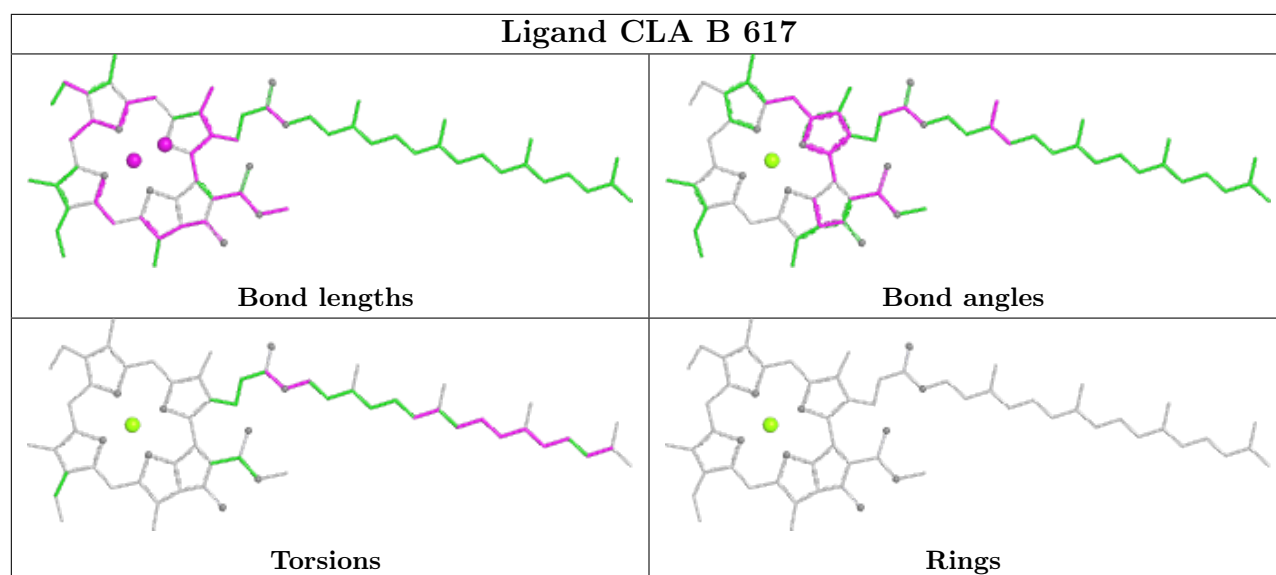


Ligand CLA c 511

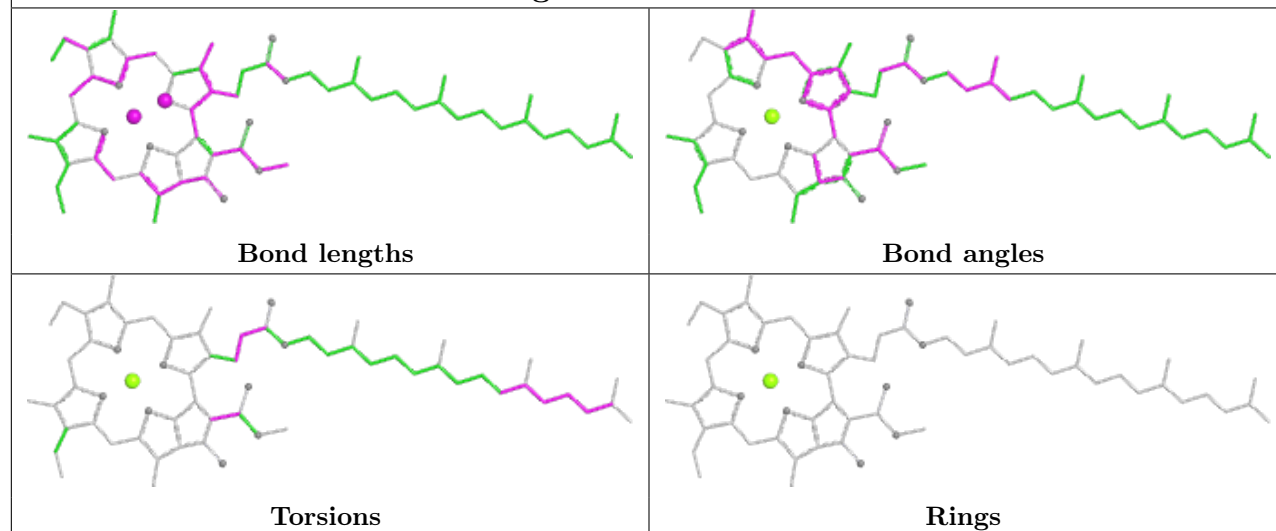




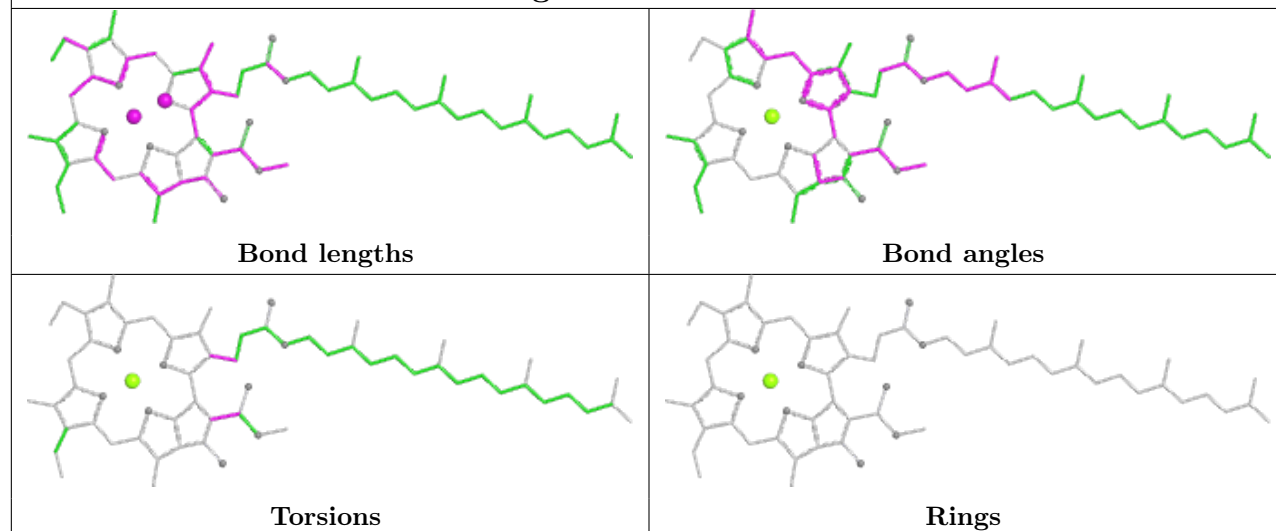




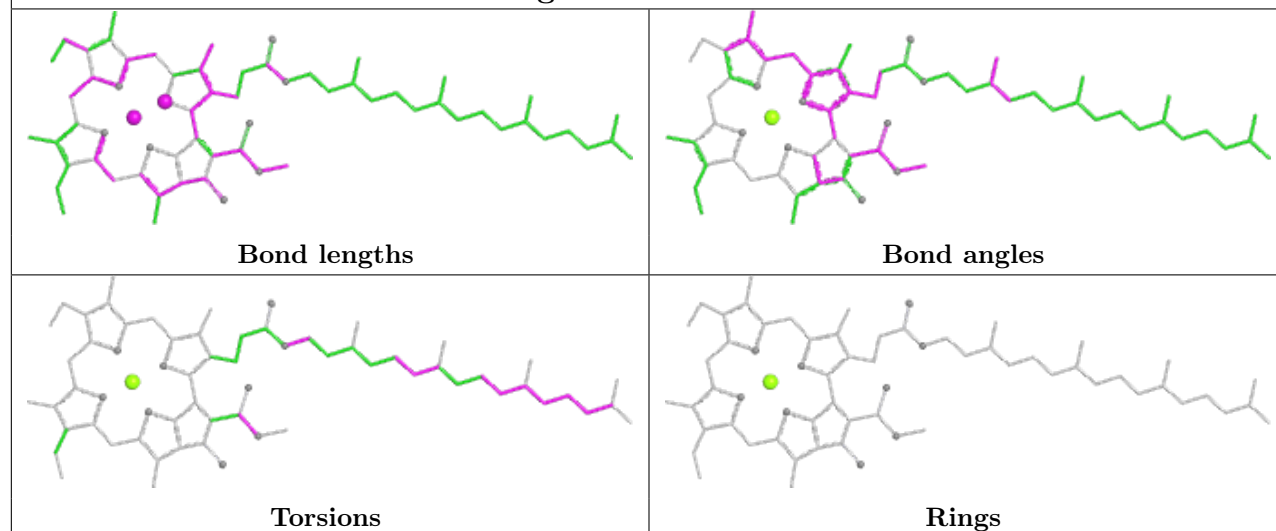
Ligand CLA C 501

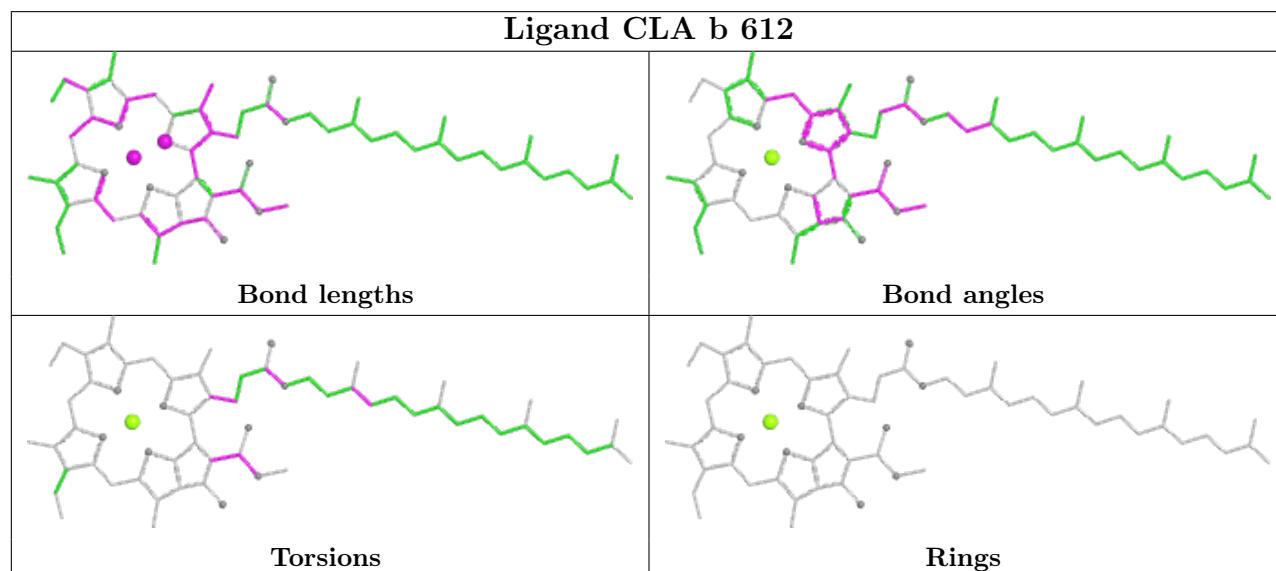
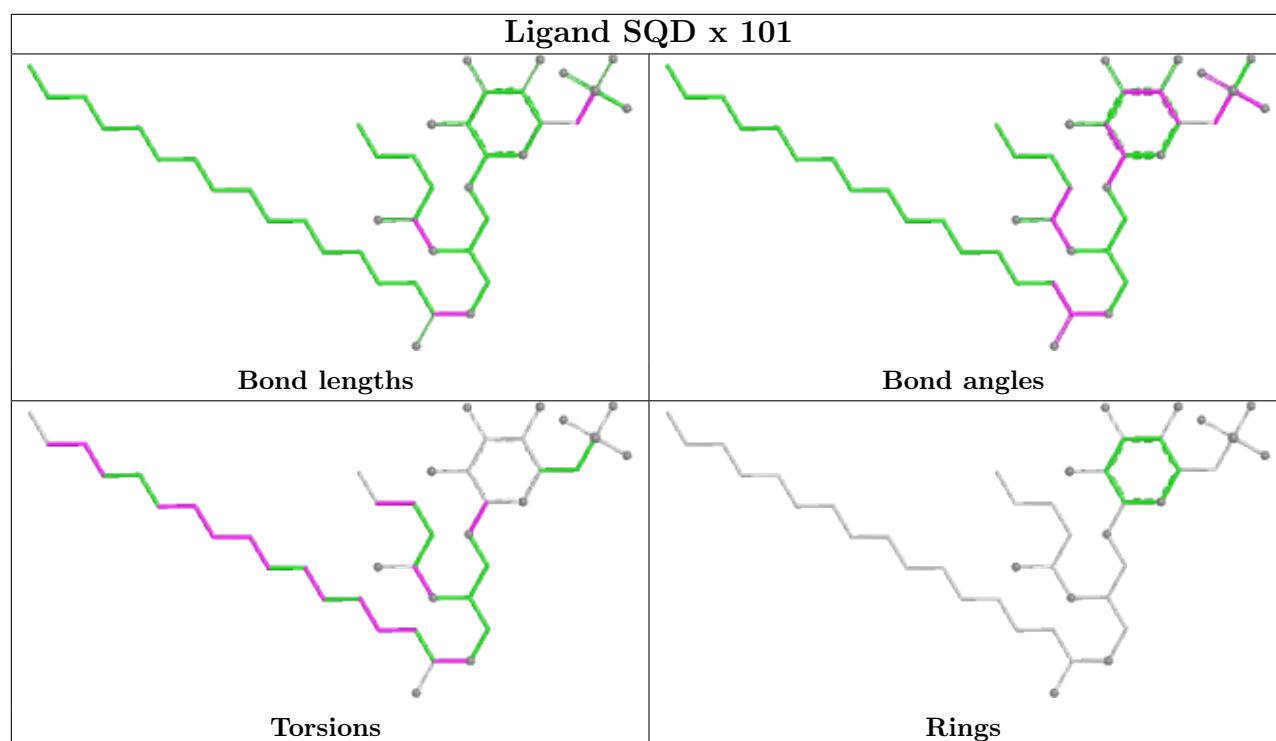


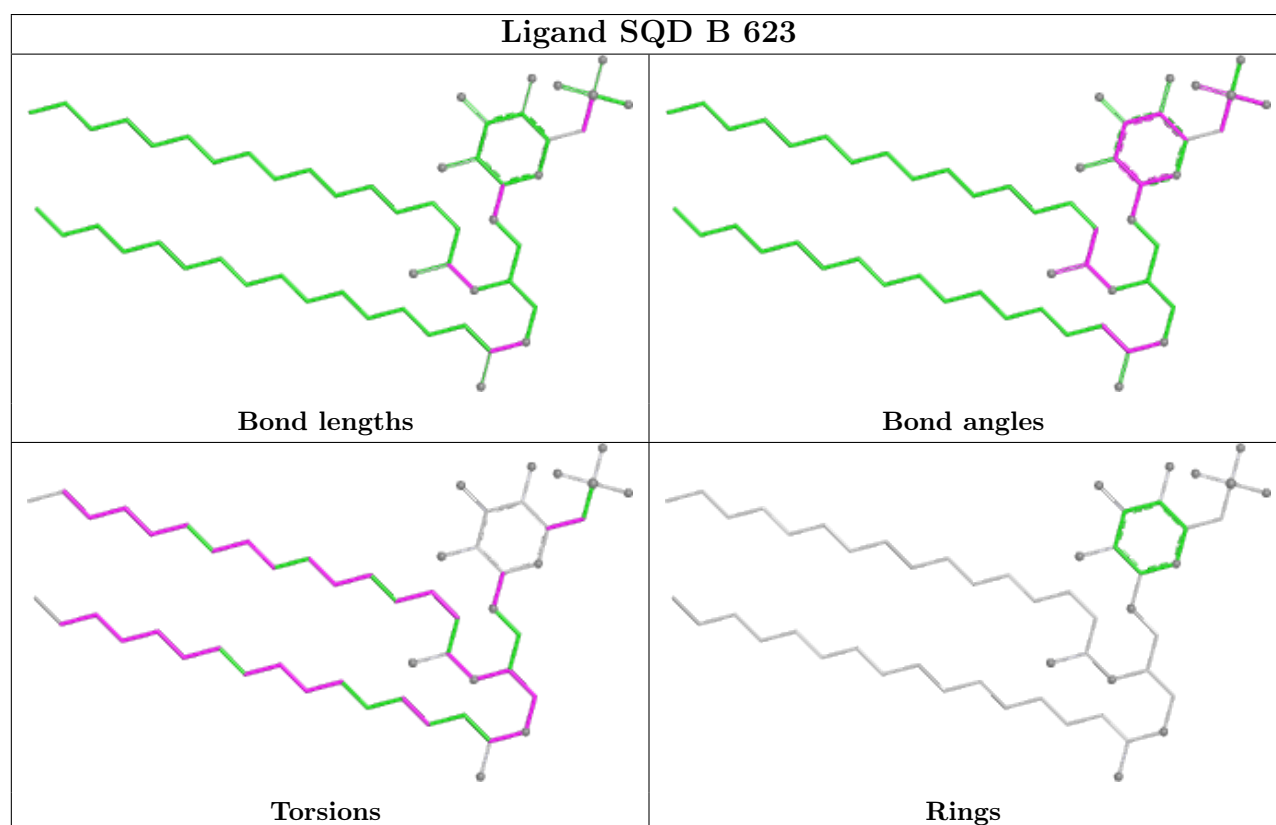
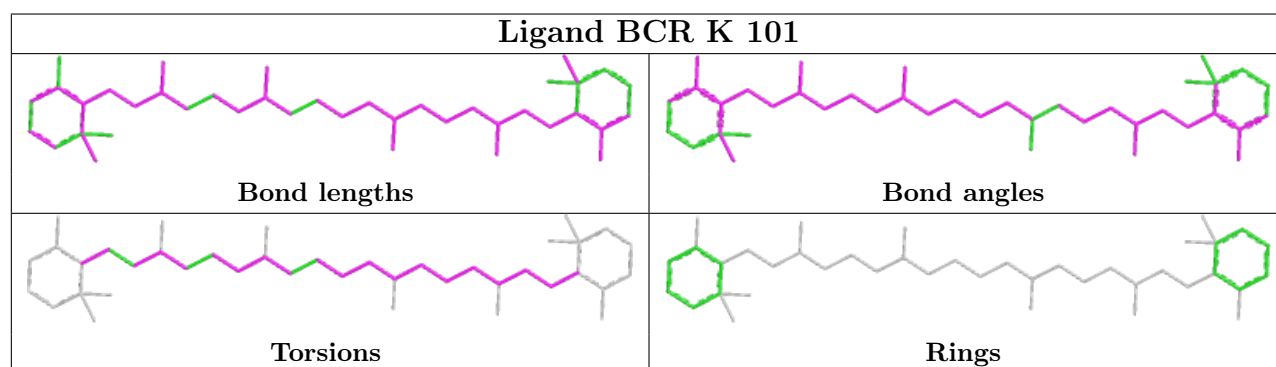
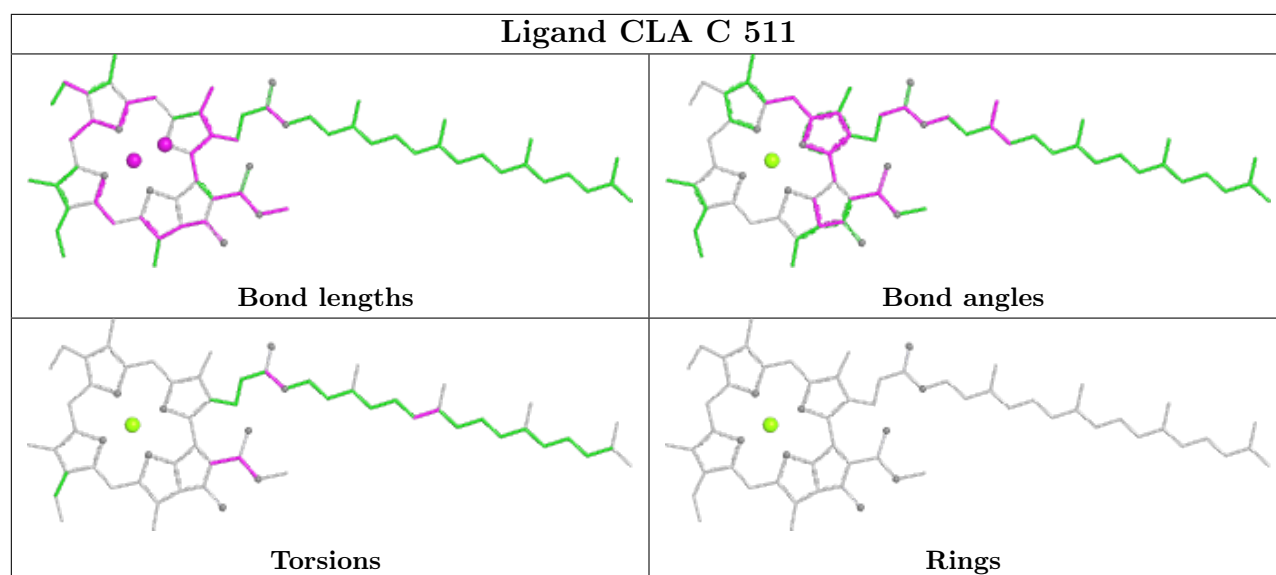
Ligand CLA B 608



Ligand CLA c 507







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.32	3 (0%) 84 77	57, 63, 84, 93	0
1	a	334/334 (100%)	-0.22	2 (0%) 89 84	78, 84, 104, 114	0
2	B	504/504 (100%)	-0.20	4 (0%) 86 79	59, 68, 89, 111	0
2	b	504/504 (100%)	-0.12	6 (1%) 79 70	80, 88, 110, 131	0
3	C	451/451 (100%)	-0.06	8 (1%) 68 59	61, 72, 85, 97	0
3	c	451/451 (100%)	-0.19	6 (1%) 77 68	82, 93, 105, 118	0
4	D	342/342 (100%)	-0.29	3 (0%) 84 77	57, 64, 80, 102	0
4	d	342/342 (100%)	-0.22	4 (1%) 79 70	78, 85, 101, 123	0
5	E	81/81 (100%)	-0.12	0 100 100	68, 81, 98, 104	0
5	e	81/81 (100%)	0.09	1 (1%) 79 70	89, 102, 119, 125	0
6	F	34/34 (100%)	-0.29	1 (2%) 51 41	68, 74, 99, 102	0
6	f	34/34 (100%)	-0.22	1 (2%) 51 41	89, 95, 120, 122	0
7	H	65/65 (100%)	0.25	6 (9%) 9 8	64, 74, 81, 99	0
7	h	65/65 (100%)	0.37	4 (6%) 20 17	85, 95, 102, 120	0
8	I	38/38 (100%)	-0.24	0 100 100	70, 74, 105, 109	0
8	i	38/38 (100%)	-0.10	1 (2%) 56 46	90, 95, 126, 130	0
9	J	38/38 (100%)	-0.17	1 (2%) 56 46	66, 78, 109, 112	0
9	j	38/38 (100%)	-0.18	1 (2%) 56 46	87, 99, 129, 133	0
10	K	37/37 (100%)	-0.55	0 100 100	74, 79, 86, 88	0
10	k	37/37 (100%)	-0.02	1 (2%) 54 45	94, 100, 107, 108	0
11	L	37/37 (100%)	0.01	4 (10%) 5 6	58, 62, 90, 99	0
11	l	37/37 (100%)	-0.04	2 (5%) 25 22	79, 83, 111, 120	0
12	M	34/34 (100%)	-0.63	0 100 100	62, 64, 77, 93	0
12	m	34/34 (100%)	-0.46	0 100 100	83, 84, 98, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/243 (100%)	-0.25	0 100 100	59, 73, 95, 111	0
13	o	243/243 (100%)	0.03	5 (2%) 63 54	79, 94, 116, 132	0
14	T	30/30 (100%)	-0.12	3 (10%) 7 7	60, 64, 85, 93	0
14	t	30/30 (100%)	-0.43	0 100 100	80, 85, 105, 114	0
15	U	97/97 (100%)	-0.10	1 (1%) 82 74	64, 71, 89, 90	0
15	u	97/97 (100%)	-0.20	1 (1%) 82 74	84, 92, 110, 111	0
16	V	137/137 (100%)	-0.30	1 (0%) 87 82	64, 69, 80, 88	0
16	v	137/137 (100%)	-0.24	3 (2%) 62 52	84, 89, 101, 109	0
17	Y	29/29 (100%)	-0.15	1 (3%) 45 36	82, 89, 115, 118	0
17	y	29/29 (100%)	-0.31	0 100 100	103, 110, 136, 138	0
18	X	39/39 (100%)	0.06	7 (17%) 1 2	74, 80, 107, 108	0
18	x	39/39 (100%)	-0.11	3 (7%) 13 12	95, 101, 127, 129	0
19	Z	62/62 (100%)	-0.31	1 (1%) 72 62	80, 89, 109, 112	0
19	z	62/62 (100%)	-0.14	2 (3%) 47 38	101, 110, 129, 133	0
All	All	5264/5264 (100%)	-0.17	87 (1%) 70 61	57, 83, 107, 138	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	L	2	GLU	4.5
7	H	2	ALA	4.2
11	L	3	PRO	4.2
7	h	2	ALA	4.1
18	X	2	THR	4.0
5	e	84	LYS	3.7
9	J	3	SER	3.6
9	j	3	SER	3.6
3	C	138	GLU	3.5
6	F	12	SER	3.5
13	o	189	ARG	3.4
18	X	38	GLN	3.4
4	D	12	ARG	3.3
18	X	37	VAL	3.2
11	l	1	MET	3.2
11	L	1	MET	3.2
7	h	3	ARG	3.2
15	U	9	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
13	o	25	THR	3.2
3	C	137	PRO	3.2
17	Y	43	ARG	3.1
18	X	33	GLN	3.0
6	f	12	SER	3.0
2	b	117	TYR	3.0
2	B	505	ARG	2.9
4	d	260	ALA	2.8
4	d	98	GLN	2.8
3	C	145[A]	SER	2.7
16	v	105	ARG	2.7
18	x	2	THR	2.7
1	a	11	ALA	2.7
8	i	38	GLU	2.7
7	H	64	ALA	2.7
3	c	200	THR	2.6
3	c	142	GLU	2.6
7	H	3	ARG	2.6
18	X	39	ARG	2.6
11	L	5	PRO	2.6
7	h	4	ARG	2.5
4	d	11	GLU	2.5
18	X	36	LYS	2.5
2	b	497	GLN	2.5
3	C	25	ASN	2.5
2	b	119	ASP	2.5
18	x	3	ILE	2.5
2	b	187	PRO	2.5
3	c	198	VAL	2.4
16	v	106	ASN	2.4
14	T	28	ARG	2.4
4	d	99	GLY	2.4
11	l	8	GLN	2.4
1	A	11	ALA	2.4
2	b	491	VAL	2.4
7	H	56	ASP	2.4
7	h	23	PRO	2.4
19	Z	35	ARG	2.4
18	x	40	SER	2.4
10	k	46	ARG	2.4
3	C	200	THR	2.4
2	b	121	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	218	LEU	2.3
3	C	183	GLY	2.3
3	c	145[A]	SER	2.3
1	A	13	LEU	2.2
1	A	74	GLY	2.2
16	V	14	SER	2.2
7	H	27	THR	2.2
3	c	201	ASN	2.2
3	C	266	TRP	2.2
14	T	30	THR	2.2
2	B	70	GLY	2.2
7	H	16	SER	2.1
13	o	58	ASN	2.1
1	a	222	SER	2.1
19	z	1	MET	2.1
13	o	164	LEU	2.1
15	u	9	LEU	2.1
2	B	498	LYS	2.1
19	z	38	GLN	2.1
14	T	26	PRO	2.1
16	v	90	GLU	2.1
13	o	87	VAL	2.0
3	c	25	ASN	2.0
18	X	40	SER	2.0
3	C	24	THR	2.0
4	D	229	ALA	2.0
4	D	227	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides 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
21	CL	u	201	1/1	0.09	0.16	112,112,112,112	0
21	CL	V	201	1/1	0.20	0.34	91,91,91,91	0
30	CA	B	601	1/1	0.21	1.14	117,117,117,117	0
30	CA	b	603	1/1	0.22	0.57	137,137,137,137	0
26	PL9	A	610	55/55	0.48	0.36	93,109,118,119	0
25	BCR	h	101	40/40	0.51	0.62	87,94,103,104	0
25	BCR	c	522	40/40	0.58	0.39	91,95,98,99	0
32	DGD	d	405	62/66	0.58	0.48	138,151,164,165	0
26	PL9	a	609	55/55	0.59	0.45	113,130,139,140	0
25	BCR	H	101	40/40	0.62	0.56	67,74,83,83	0
25	BCR	a	608	40/40	0.63	0.64	83,89,93,94	0
21	CL	a	602	1/1	0.63	0.17	86,86,86,86	0
28	LMG	C	520	51/55	0.64	0.54	83,117,122,123	0
26	PL9	d	404	55/55	0.67	0.31	80,84,91,93	0
25	BCR	C	521	40/40	0.69	0.30	70,74,78,78	0
32	DGD	D	406	62/66	0.69	0.45	118,130,143,144	0
27	SQD	a	610	54/54	0.69	0.51	110,119,128,128	0
25	BCR	T	101	40/40	0.70	0.40	65,78,85,86	0
25	BCR	b	622	40/40	0.71	0.54	89,94,100,101	0
31	LHG	E	101	42/49	0.72	0.39	110,124,127,127	0
27	SQD	x	101	43/54	0.72	0.50	128,136,140,140	0
23	CLA	C	513	65/65	0.72	0.47	80,85,105,105	0
28	LMG	c	521	51/55	0.73	0.51	104,137,142,143	0
31	LHG	e	101	42/49	0.74	0.40	131,145,147,148	0
27	SQD	A	611	54/54	0.75	0.41	90,98,107,108	0
23	CLA	C	512	65/65	0.75	0.41	78,82,103,104	0
27	SQD	b	602	54/54	0.75	0.42	99,107,121,121	0
23	CLA	B	617	65/65	0.75	0.44	63,69,118,119	0
25	BCR	C	515	40/40	0.75	0.34	71,78,81,82	0
25	BCR	f	101	40/40	0.75	0.35	87,91,109,110	0
25	BCR	F	101	40/40	0.76	0.33	66,71,88,90	0
23	CLA	b	609[B]	65/65	0.76	0.45	83,87,93,95	65
25	BCR	C	514	40/40	0.76	0.39	78,84,87,88	0
23	CLA	C	507	65/65	0.76	0.41	70,74,92,94	0
25	BCR	b	621	40/40	0.76	0.39	83,89,101,101	0
23	CLA	b	609[A]	65/65	0.76	0.45	85,90,102,103	65
25	BCR	b	620	40/40	0.77	0.61	84,88,90,90	0
25	BCR	A	609	40/40	0.77	0.56	63,68,73,73	0
23	CLA	b	604	65/65	0.77	0.72	94,102,127,128	0
23	CLA	c	502	65/65	0.77	0.35	90,93,106,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	c	513	65/65	0.77	0.41	99,102,124,124	0
28	LMG	z	101	37/55	0.77	0.52	117,145,149,150	0
25	BCR	t	101	40/40	0.78	0.36	86,99,106,106	0
27	SQD	B	623	54/54	0.78	0.30	119,127,141,142	0
23	CLA	b	618	65/65	0.78	0.39	86,89,107,108	0
28	LMG	c	520	51/55	0.78	0.38	92,118,134,135	0
21	CL	A	602	1/1	0.79	0.23	65,65,65,65	0
28	LMG	b	623	51/55	0.80	0.39	91,100,112,116	0
23	CLA	B	607[A]	65/65	0.80	0.40	65,69,81,82	65
27	SQD	X	101	43/54	0.80	0.39	108,115,119,119	0
25	BCR	c	515	40/40	0.80	0.44	99,105,108,108	0
23	CLA	c	504	65/65	0.80	0.29	89,93,96,97	0
30	CA	F	102	1/1	0.80	0.59	97,97,97,97	0
23	CLA	B	607[B]	65/65	0.80	0.40	63,67,72,75	65
30	CA	f	102	1/1	0.80	0.37	118,118,118,118	0
28	LMG	C	519	51/55	0.80	0.41	72,98,113,114	0
25	BCR	K	101	40/40	0.80	0.37	75,78,79,80	0
28	LMG	J	101	51/55	0.80	0.34	66,76,106,108	0
28	LMG	Z	101	37/55	0.80	0.41	96,124,129,129	0
27	SQD	b	601	54/54	0.81	0.33	91,103,109,109	0
23	CLA	c	503	65/65	0.81	0.36	85,87,101,103	0
25	BCR	B	620	40/40	0.81	0.39	68,74,80,80	0
23	CLA	C	511	65/65	0.81	0.33	70,75,78,79	0
23	CLA	c	508	65/65	0.81	0.32	91,94,113,115	0
29	FE2	a	615	1/1	0.81	0.16	88,88,88,88	0
23	CLA	B	602	65/65	0.81	0.40	73,82,107,107	0
25	BCR	c	516	40/40	0.82	0.27	92,98,102,102	0
23	CLA	b	619	65/65	0.82	0.43	83,90,139,139	0
31	LHG	l	101	49/49	0.82	0.29	84,92,104,106	0
25	BCR	B	618	40/40	0.82	0.37	63,68,69,70	0
32	DGD	c	519	62/66	0.82	0.47	83,93,113,117	0
23	CLA	b	617	65/65	0.82	0.37	82,86,121,122	0
23	CLA	B	616	65/65	0.83	0.35	65,68,86,87	0
23	CLA	C	506	65/65	0.83	0.30	72,79,115,115	0
23	CLA	a	605	65/65	0.83	0.33	80,83,124,126	0
23	CLA	d	403	65/65	0.84	0.33	86,89,126,128	0
23	CLA	a	607	65/65	0.84	0.42	83,85,133,133	0
28	LMG	A	612	51/55	0.85	0.30	94,100,105,105	0
28	LMG	B	621	51/55	0.85	0.34	70,80,92,95	0
23	CLA	B	608	65/65	0.85	0.35	58,61,73,74	0
27	SQD	a	612	54/54	0.85	0.31	111,124,129,130	0
24	PHO	D	401	64/64	0.85	0.31	59,63,69,73	0

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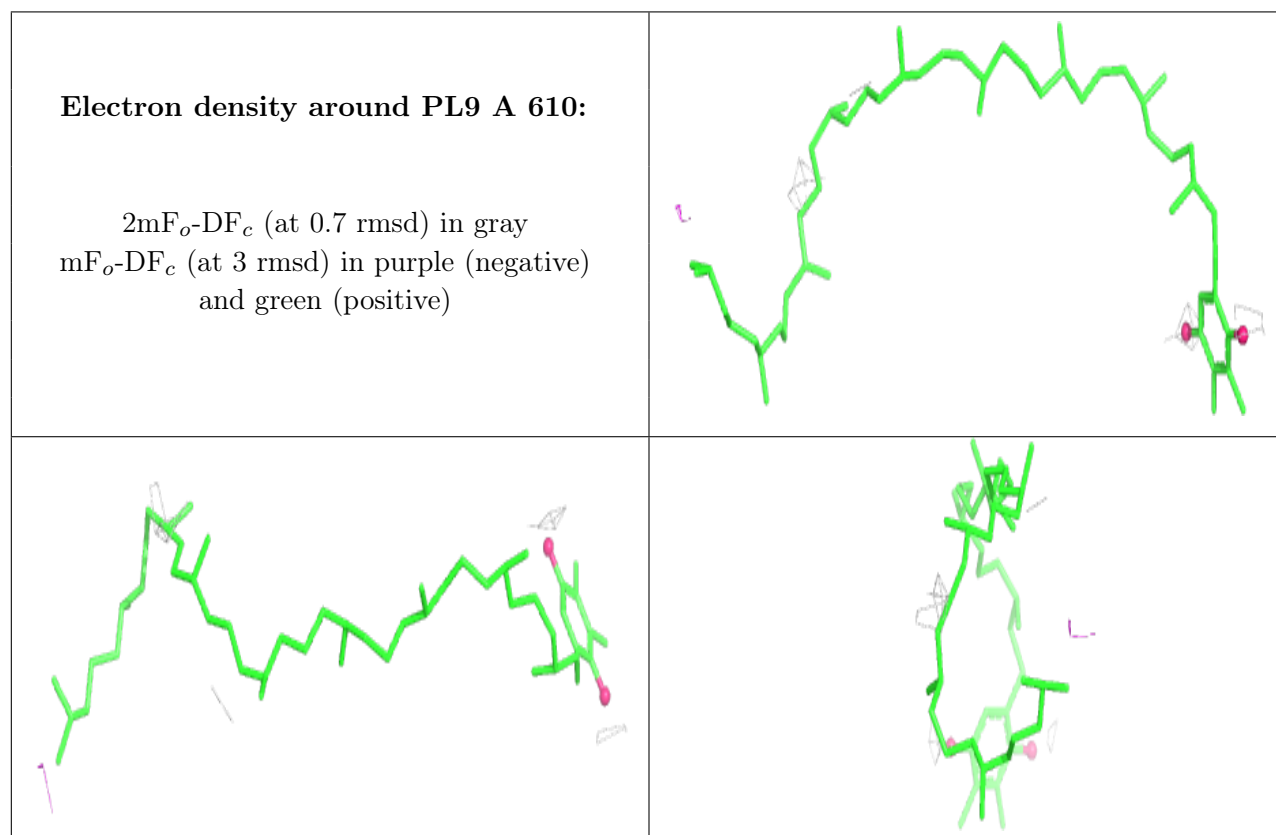
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	a	604	65/65	0.85	0.30	77,80,87,95	0
23	CLA	C	505	65/65	0.85	0.30	69,71,85,85	0
31	LHG	D	408	49/49	0.86	0.36	67,74,103,104	0
26	PL9	D	405	55/55	0.86	0.21	60,64,70,72	0
31	LHG	a	614	49/49	0.86	0.35	87,94,124,125	0
23	CLA	c	514	65/65	0.86	0.30	101,106,125,126	0
28	LMG	a	611	51/55	0.86	0.26	114,121,126,126	0
32	DGD	C	518	62/66	0.86	0.35	62,72,93,97	0
25	BCR	k	101	40/40	0.86	0.32	95,99,100,100	0
32	DGD	c	517	62/66	0.86	0.26	84,94,122,124	0
23	CLA	b	613	65/65	0.86	0.43	82,86,94,98	0
23	CLA	c	507	65/65	0.86	0.30	93,100,136,136	0
34	MG	j	102	1/1	0.86	0.18	89,89,89,89	0
23	CLA	b	615	65/65	0.87	0.35	81,85,91,92	0
24	PHO	d	401	64/64	0.87	0.28	80,84,90,94	0
23	CLA	c	510	65/65	0.87	0.26	91,93,108,108	0
23	CLA	D	404	65/65	0.87	0.34	65,68,106,107	0
29	FE2	A	613	1/1	0.87	0.28	67,67,67,67	0
23	CLA	b	612	65/65	0.87	0.27	85,90,92,93	0
23	CLA	C	508	65/65	0.87	0.30	66,70,95,99	0
23	CLA	C	501	65/65	0.88	0.35	69,73,85,87	0
31	LHG	b	624	49/49	0.88	0.25	91,96,102,102	0
31	LHG	d	406	49/49	0.88	0.35	85,89,98,102	0
23	CLA	b	606	65/65	0.88	0.28	79,84,92,96	0
24	PHO	a	606	64/64	0.88	0.32	78,83,86,87	0
32	DGD	C	517	62/66	0.88	0.31	63,75,103,104	0
23	CLA	C	509	65/65	0.88	0.24	70,72,87,88	0
23	CLA	c	512	65/65	0.88	0.25	90,95,99,99	0
23	CLA	b	616	65/65	0.88	0.32	80,84,106,108	0
32	DGD	c	518	62/66	0.88	0.30	84,96,124,124	0
25	BCR	B	619	40/40	0.88	0.30	62,69,81,81	0
23	CLA	B	615	65/65	0.88	0.27	61,65,101,102	0
28	LMG	j	101	51/55	0.88	0.24	87,96,126,129	0
23	CLA	A	608	65/65	0.89	0.35	62,65,112,113	0
32	DGD	C	516	62/66	0.89	0.22	64,73,102,103	0
22	BCT	a	603	4/4	0.89	0.48	100,101,101,103	0
31	LHG	B	622	49/49	0.89	0.25	70,75,81,82	0
23	CLA	B	610	65/65	0.89	0.30	64,69,72,73	0
32	DGD	H	102	62/66	0.89	0.23	66,72,79,81	0
23	CLA	C	504	65/65	0.89	0.29	66,68,95,95	0
23	CLA	B	611	65/65	0.89	0.27	62,65,73,77	0
23	CLA	b	605	65/65	0.89	0.24	85,88,93,94	0

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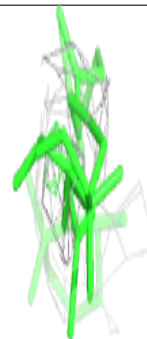
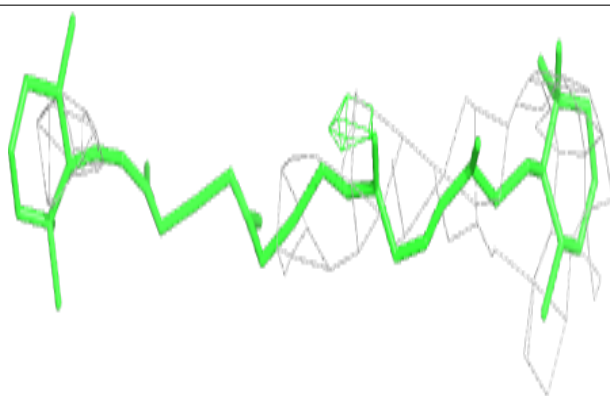
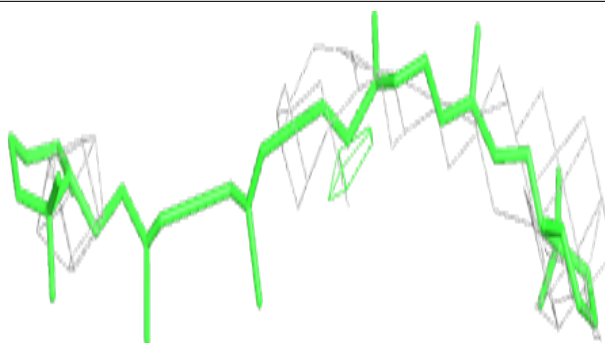
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	CLA	A	606	65/65	0.89	0.31	60,62,104,106	0
32	DGD	h	102	62/66	0.89	0.25	87,93,99,101	0
33	HEM	e	102	43/43	0.89	0.45	101,103,107,108	0
23	CLA	b	608	65/65	0.89	0.27	80,84,95,97	0
23	CLA	B	606	65/65	0.90	0.23	59,64,75,76	0
23	CLA	c	506	65/65	0.90	0.22	89,92,106,106	0
33	HEM	E	102	43/43	0.90	0.28	80,82,86,87	0
23	CLA	b	610	65/65	0.90	0.31	79,82,94,95	0
23	CLA	b	611	65/65	0.90	0.26	82,86,92,93	0
23	CLA	C	502	65/65	0.91	0.33	65,67,80,83	0
23	CLA	c	509	65/65	0.91	0.27	87,90,115,119	0
23	CLA	C	503	65/65	0.91	0.33	68,72,76,77	0
23	CLA	B	604	65/65	0.91	0.25	58,63,72,76	0
23	CLA	a	613	65/65	0.91	0.34	75,79,91,96	0
23	CLA	B	605	65/65	0.91	0.25	60,63,91,91	0
23	CLA	B	613	65/65	0.91	0.29	61,64,71,72	0
23	CLA	D	403	65/65	0.91	0.28	54,59,75,76	0
23	CLA	B	614	65/65	0.91	0.26	60,63,85,87	0
33	HEM	v	201	43/43	0.91	0.30	84,86,88,90	0
34	MG	J	102	1/1	0.91	0.48	68,68,68,68	0
31	LHG	D	407	49/49	0.91	0.21	64,69,78,81	0
23	CLA	B	609	65/65	0.92	0.24	61,65,71,72	0
23	CLA	A	605	65/65	0.92	0.26	56,59,66,75	0
23	CLA	B	603	65/65	0.92	0.23	64,67,72,73	0
23	CLA	b	614	65/65	0.92	0.29	80,83,94,96	0
31	LHG	L	101	49/49	0.92	0.23	63,72,83,85	0
23	CLA	D	402	65/65	0.93	0.28	54,59,70,76	0
23	CLA	c	505	65/65	0.93	0.26	86,89,115,116	0
21	CL	A	603	1/1	0.93	0.20	62,62,62,62	0
24	PHO	A	607	64/64	0.93	0.26	57,62,65,67	0
23	CLA	c	511	65/65	0.93	0.24	86,90,96,99	0
23	CLA	b	607	65/65	0.93	0.24	81,84,111,112	0
20	OEX	A	601	10/10	0.94	0.31	63,64,67,67	0
23	CLA	B	612	65/65	0.94	0.24	60,62,73,75	0
23	CLA	d	402	65/65	0.94	0.25	75,80,95,96	0
33	HEM	V	202	43/43	0.94	0.26	63,65,68,69	0
21	CL	c	501	1/1	0.95	0.18	83,83,83,83	0
23	CLA	C	510	65/65	0.95	0.23	65,69,76,78	0
20	OEX	a	601	10/10	0.96	0.32	83,84,87,88	0
30	CA	o	301	1/1	0.96	0.24	110,110,110,110	0
30	CA	O	301	1/1	0.97	0.17	90,90,90,90	0
22	BCT	A	604	4/4	0.97	0.21	79,80,81,82	0

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

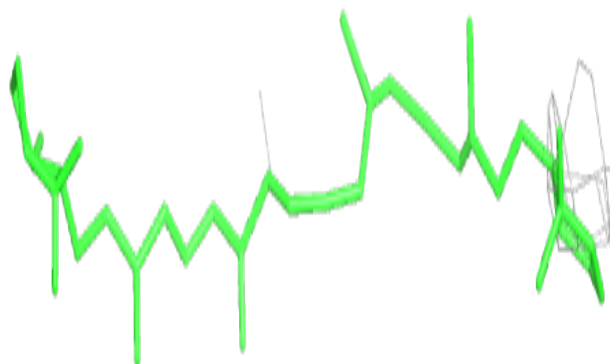
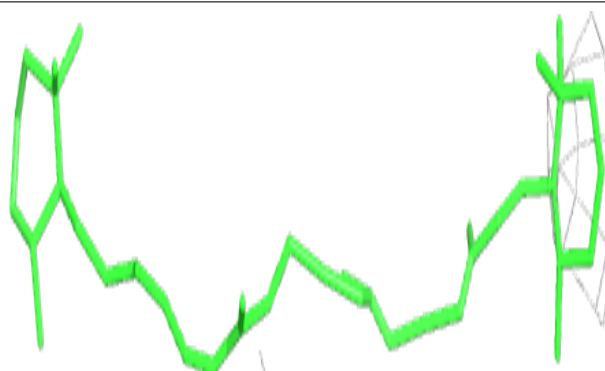


Electron density around BCR h 101:

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

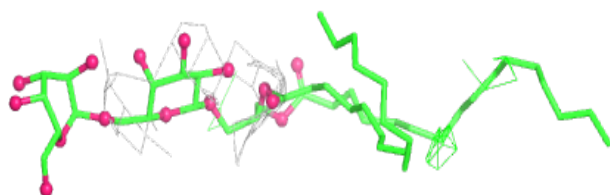
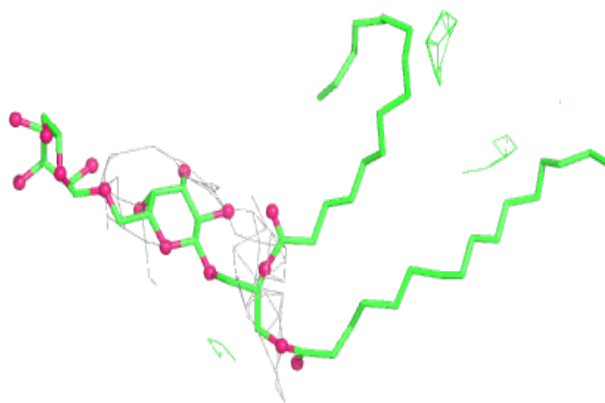
**Electron density around BCR c 522:**

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

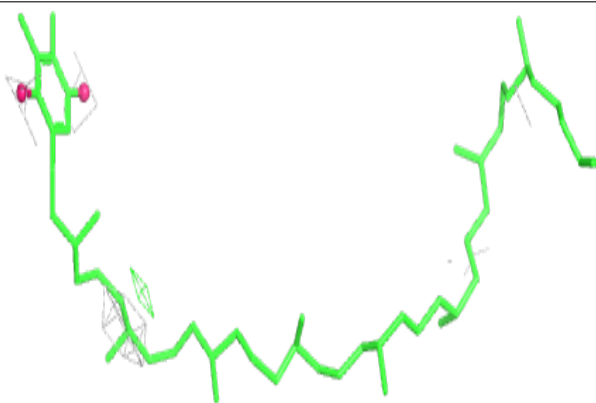


Electron density around DGD d 405:

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

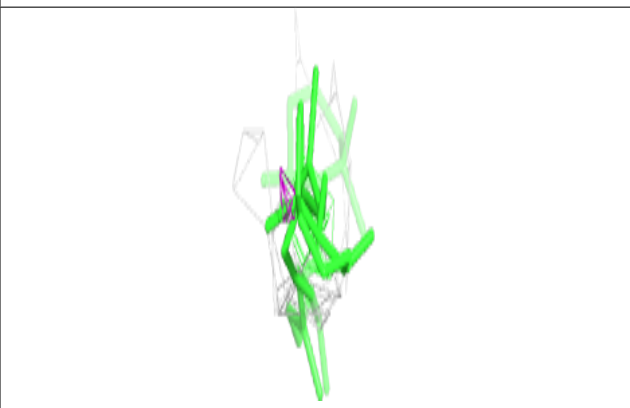
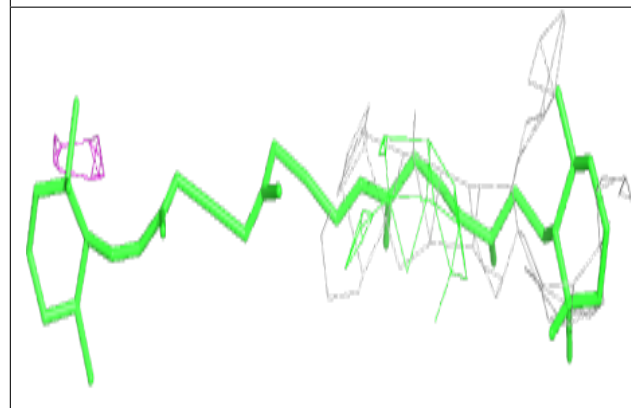
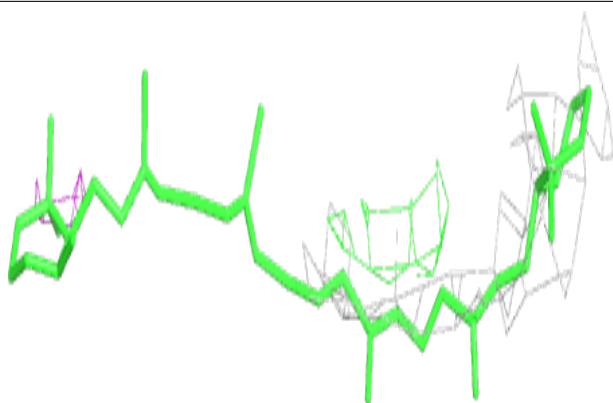
**Electron density around PL9 a 609:**

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

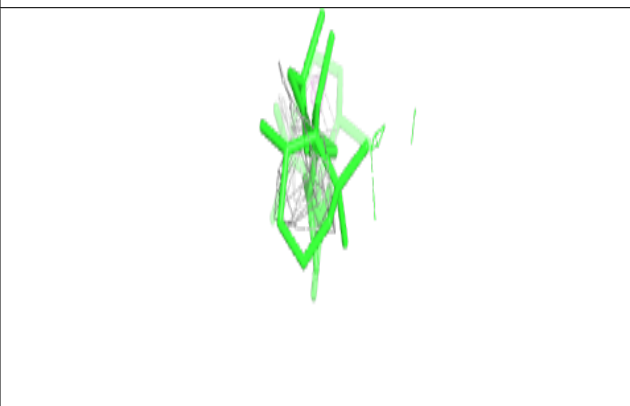
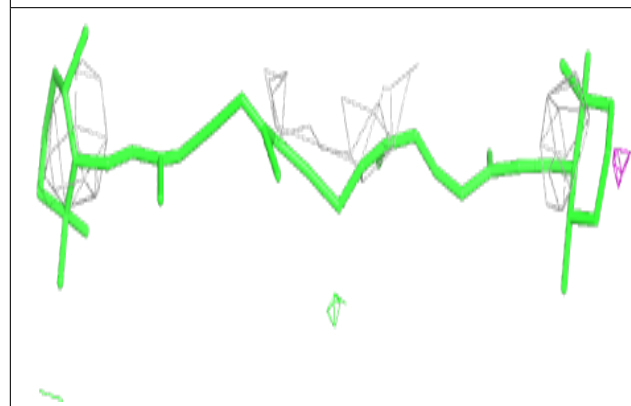
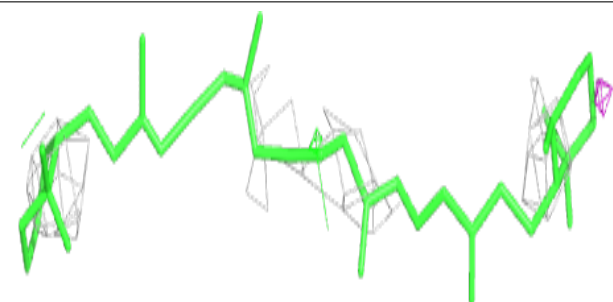


Electron density around BCR H 101:

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

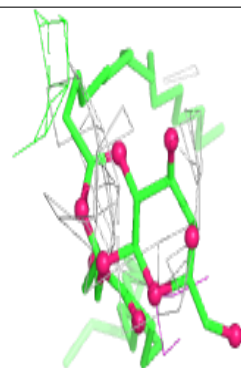
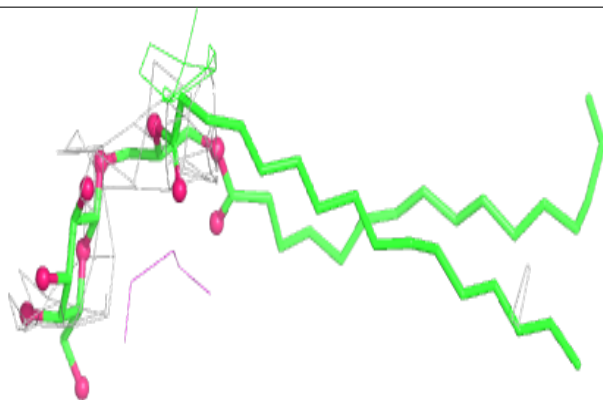
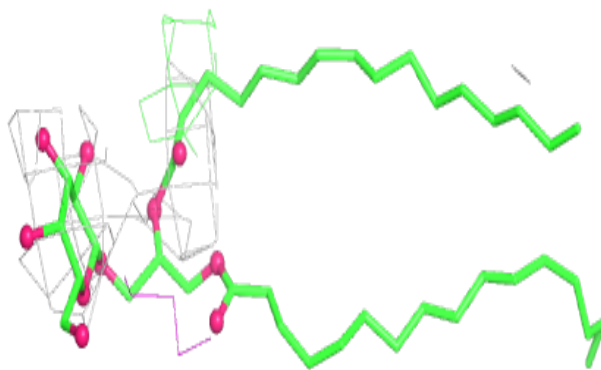
**Electron density around BCR a 608:**

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

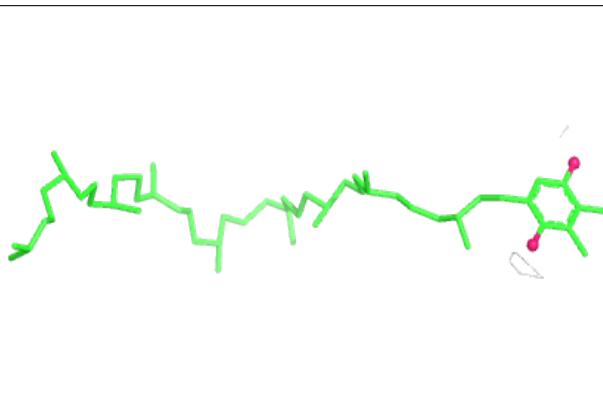
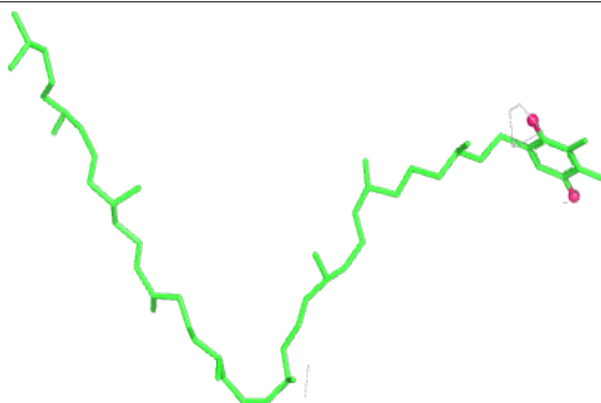


Electron density around LMG C 520:

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

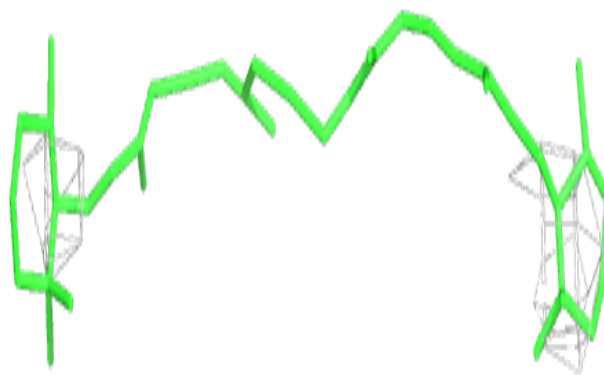
**Electron density around PL9 d 404:**

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

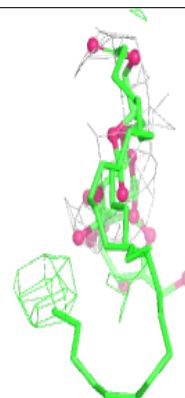
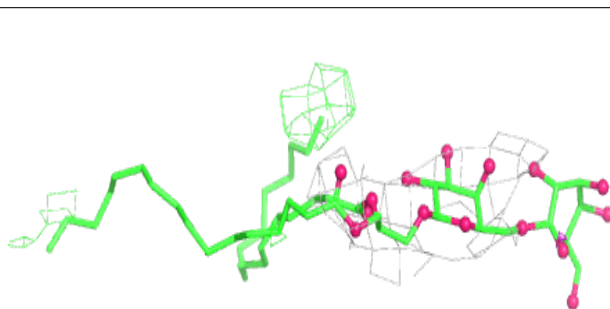


Electron density around BCR C 521:

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

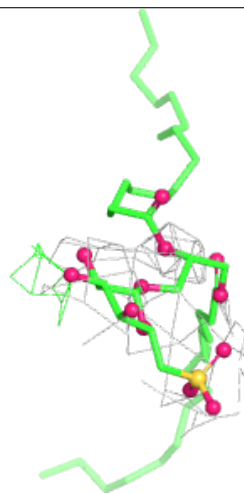
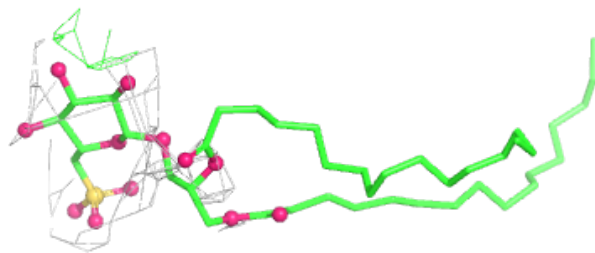
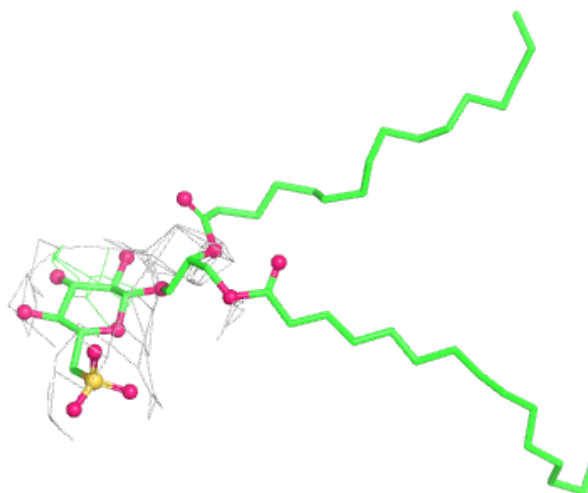
**Electron density around DGD D 406:**

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



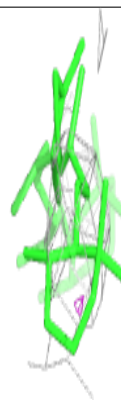
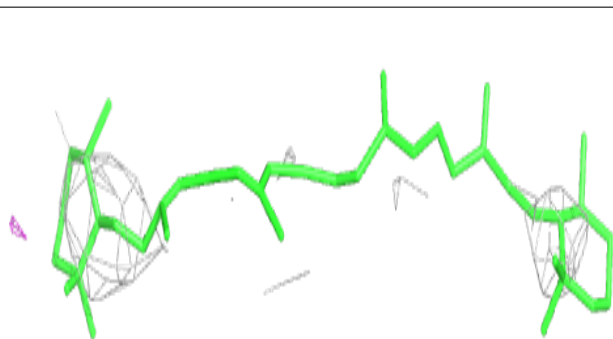
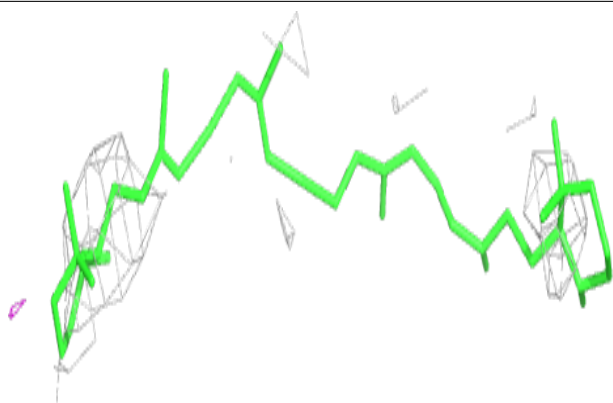
Electron density around SQD a 610:

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

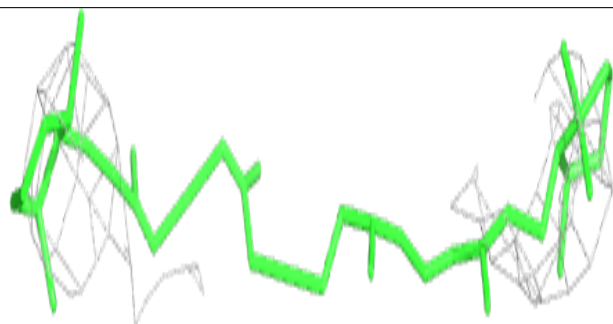
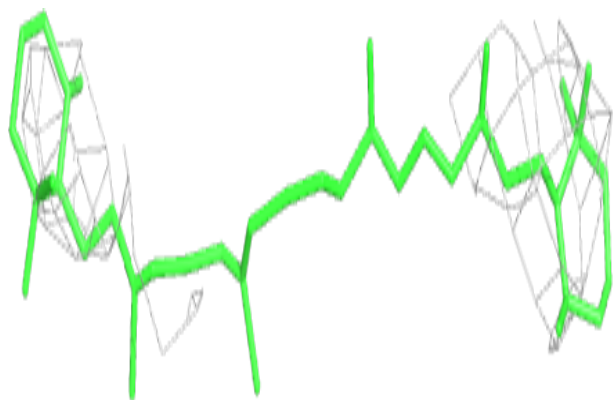


Electron density around BCR T 101:

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

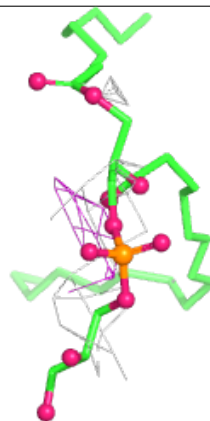
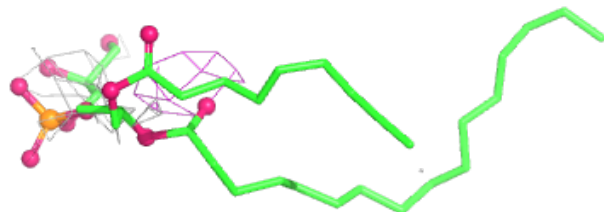
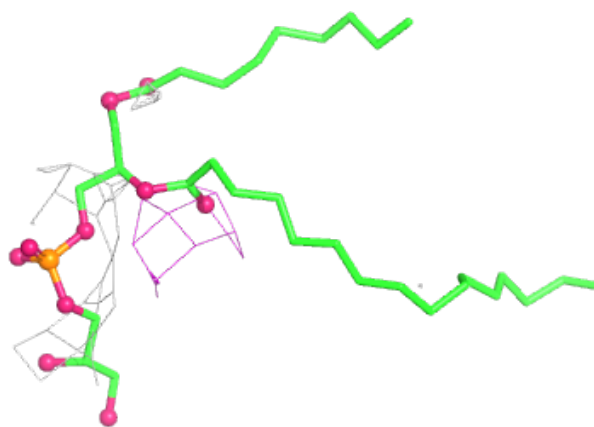
**Electron density around BCR b 622:**

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



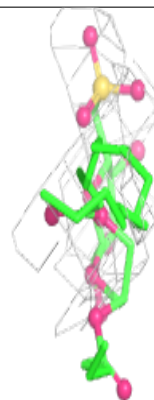
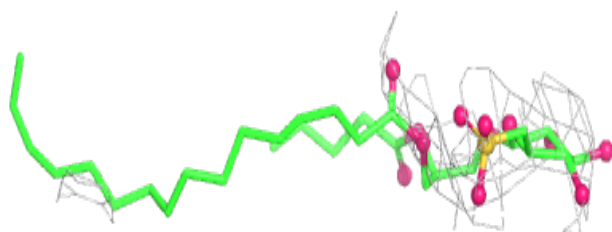
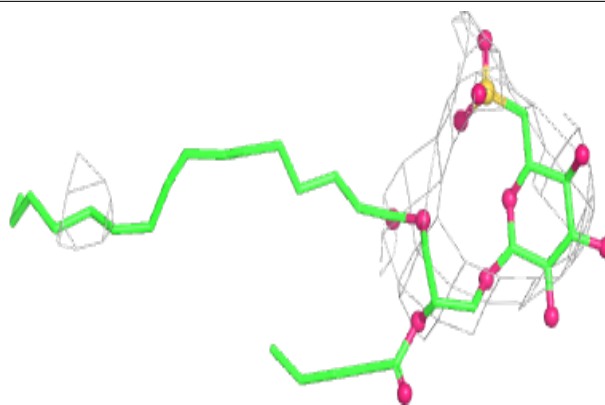
Electron density around LHG E 101:

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

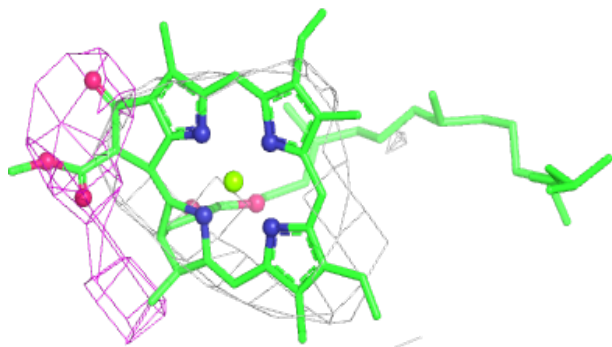
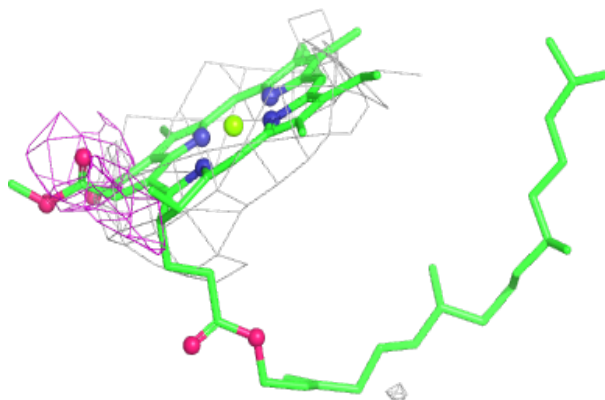


Electron density around SQD x 101:

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

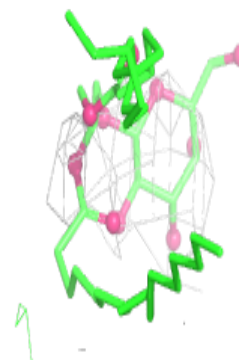
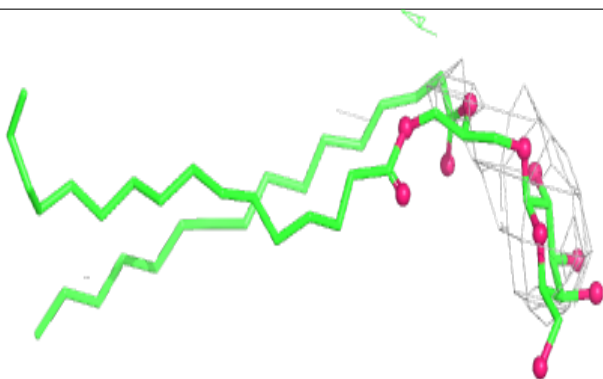
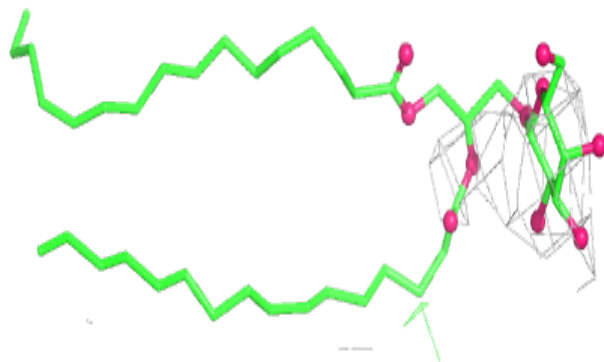
**Electron density around CLA C 513:**

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

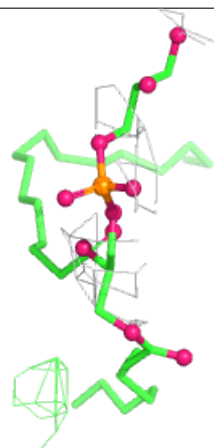
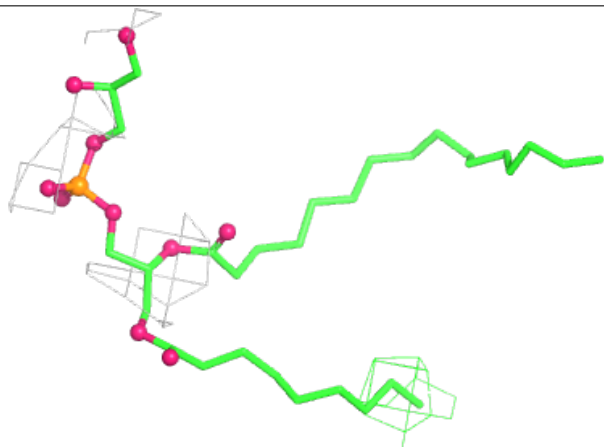


Electron density around LMG c 521:

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

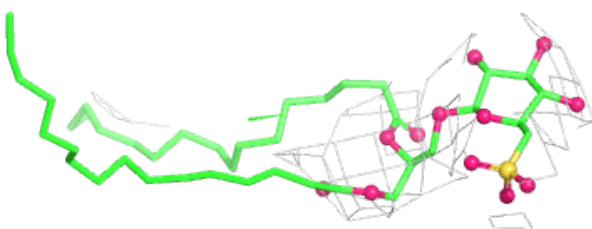
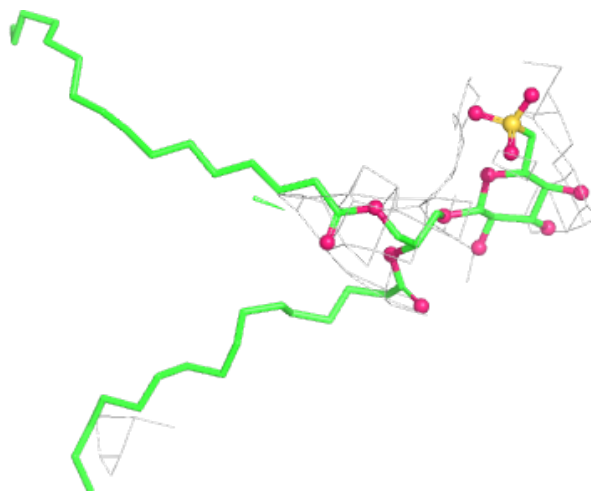
**Electron density around LHG e 101:**

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



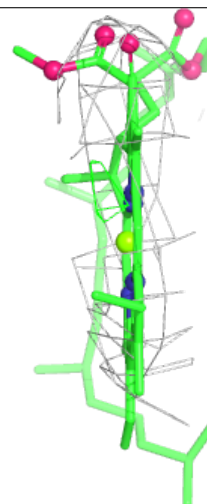
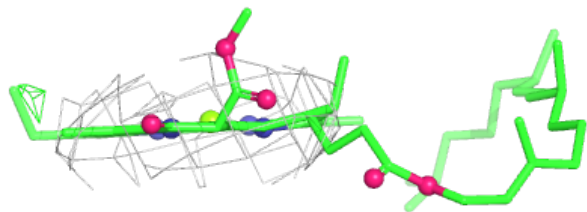
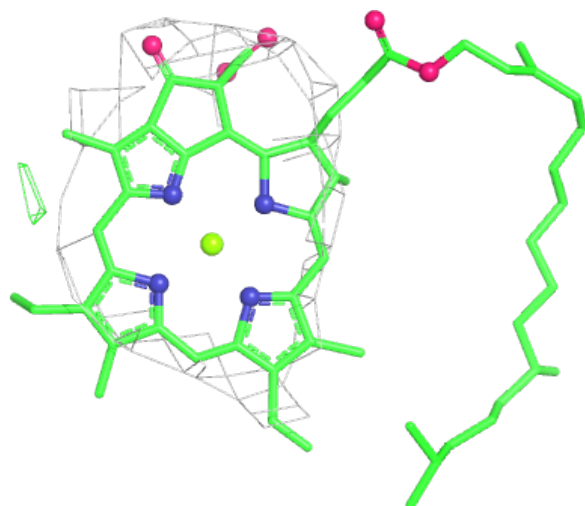
Electron density around SQD A 611:

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



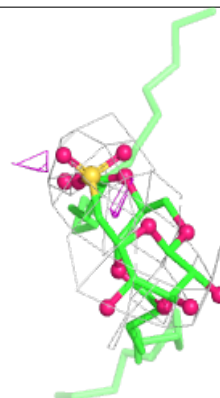
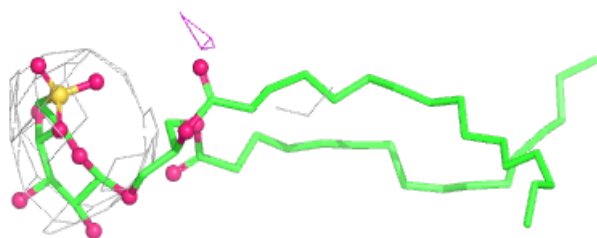
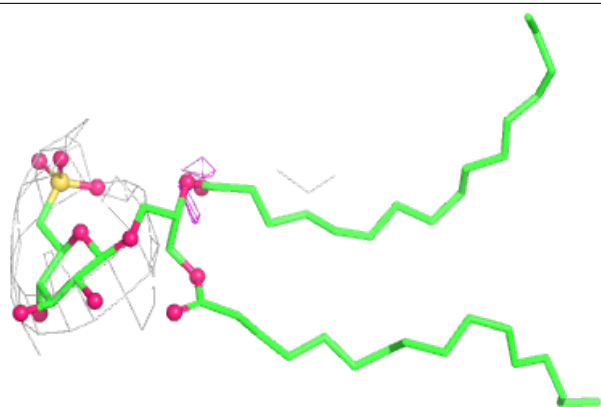
Electron density around CLA C 512:

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



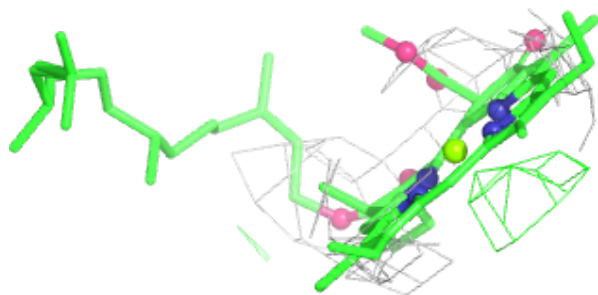
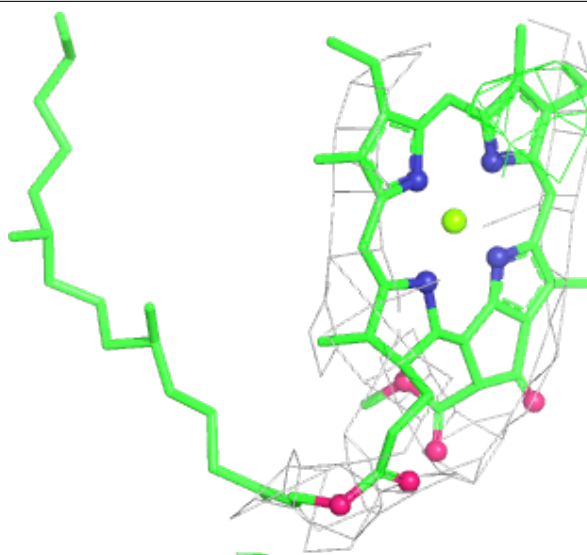
Electron density around SQD b 602:

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



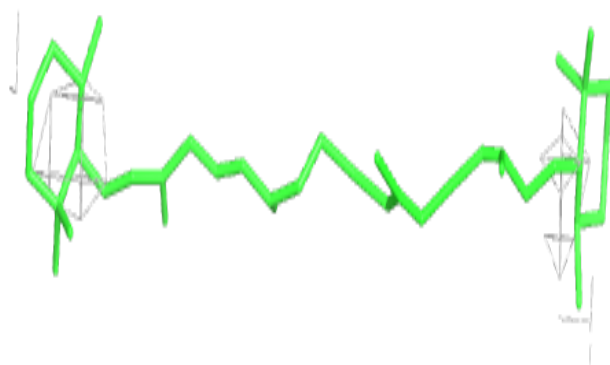
Electron density around CLA B 617:

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

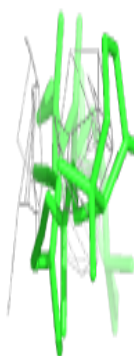
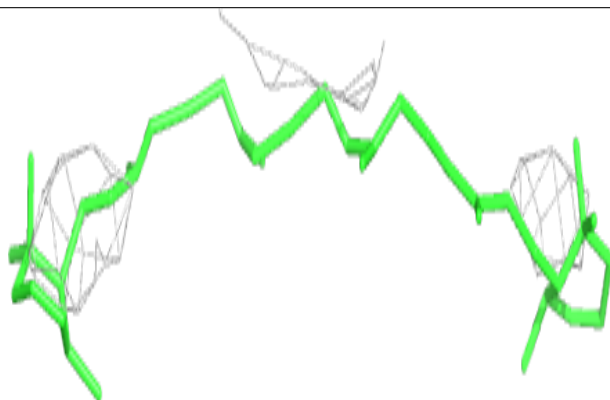
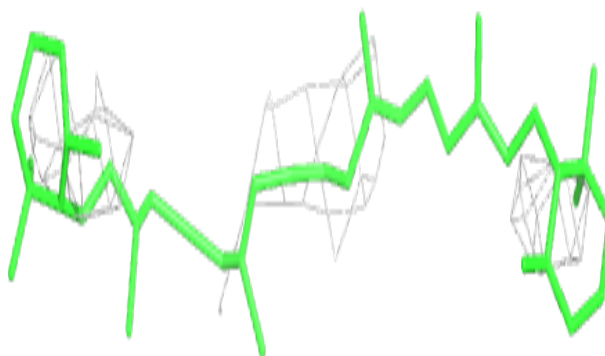


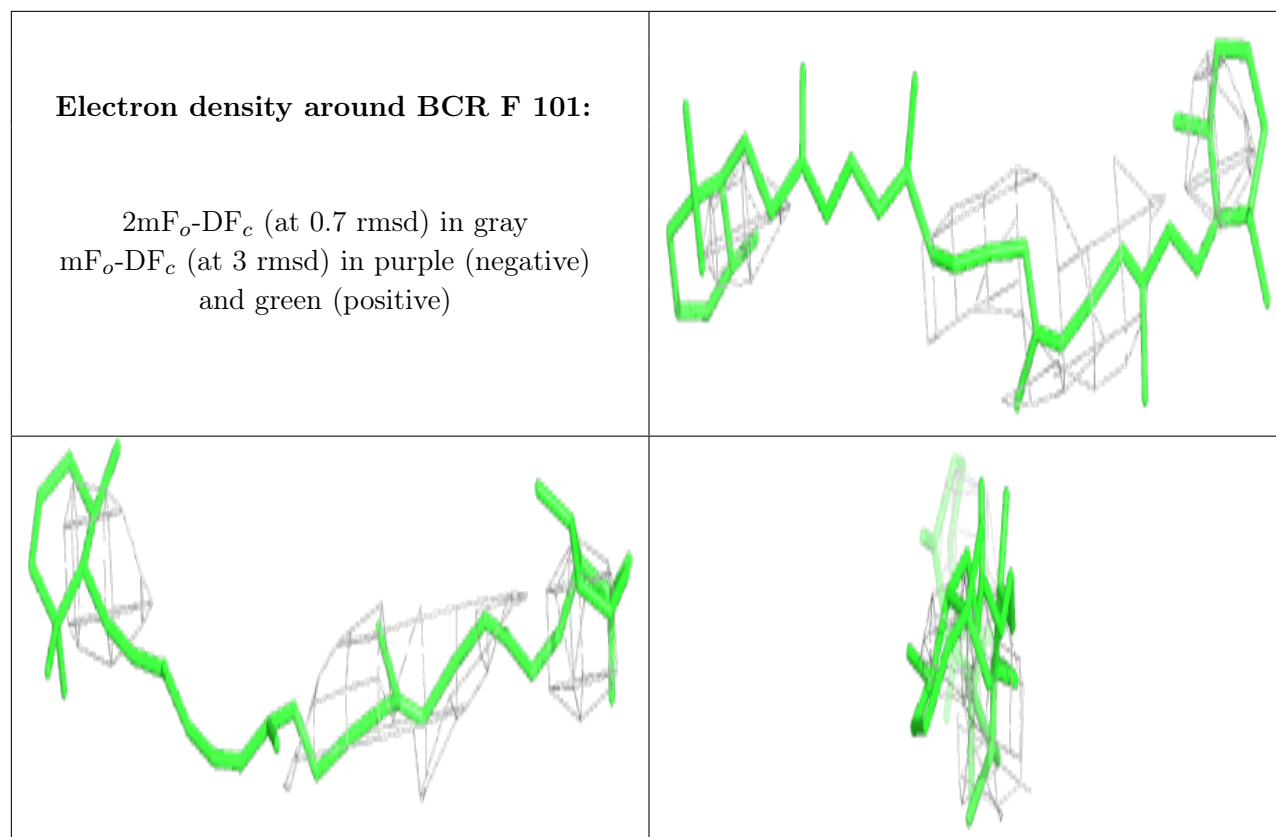
Electron density around BCR C 515:

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

**Electron density around BCR f 101:**

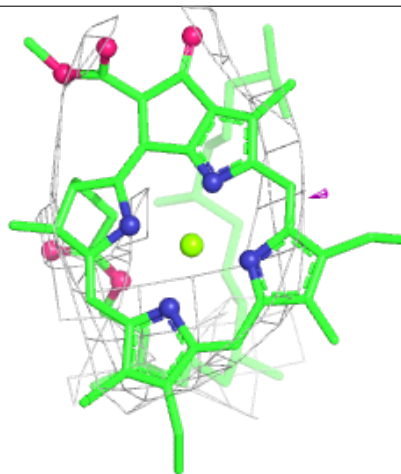
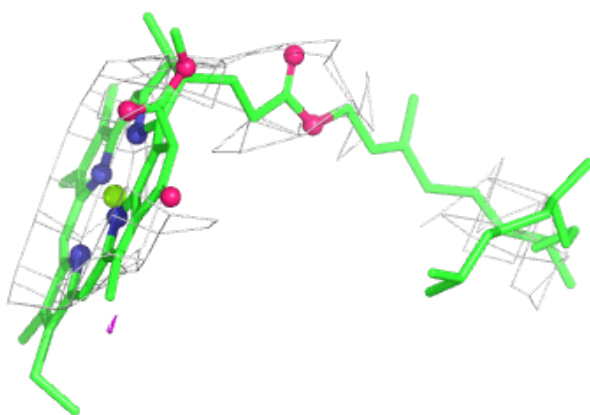
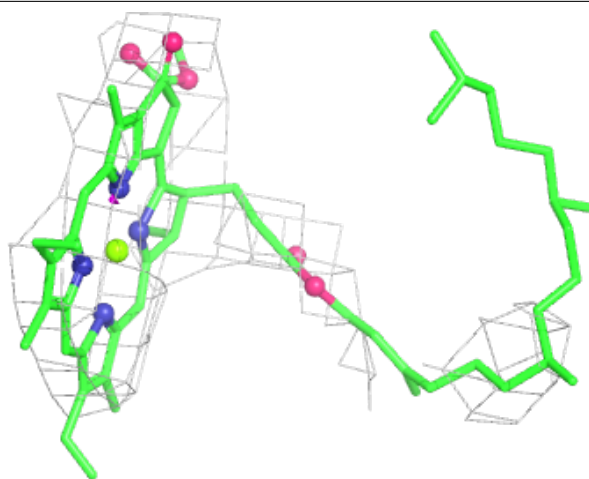
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





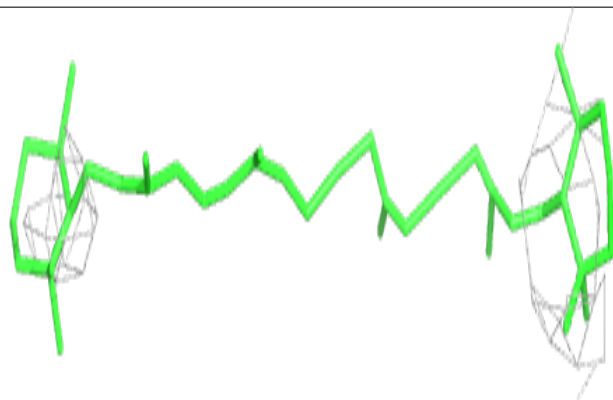
Electron density around CLA b 609 (B):

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



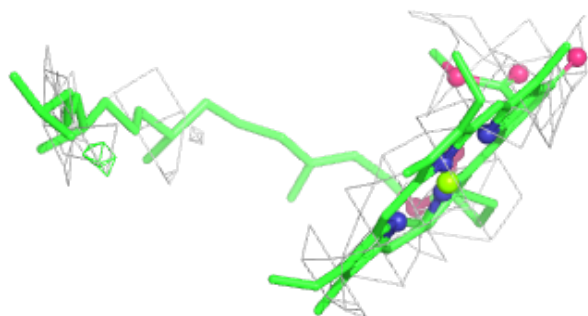
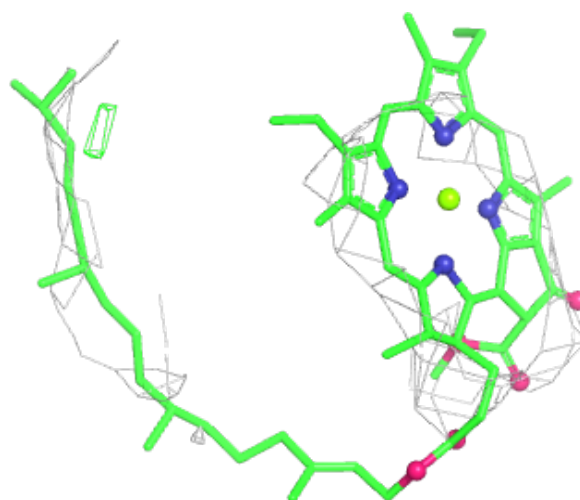
Electron density around BCR C 514:

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



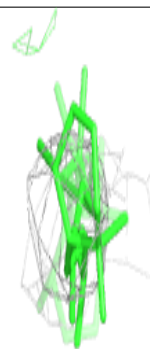
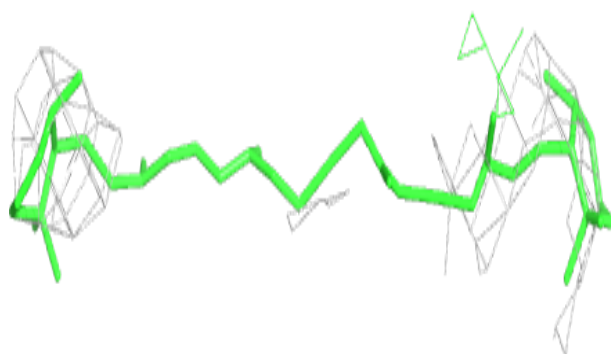
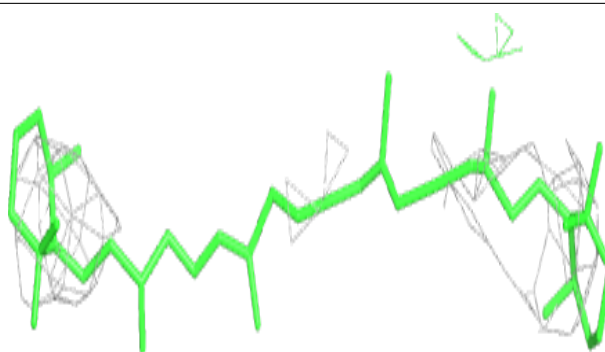
Electron density around CLA C 507:

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

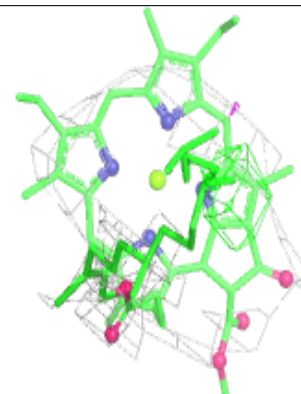
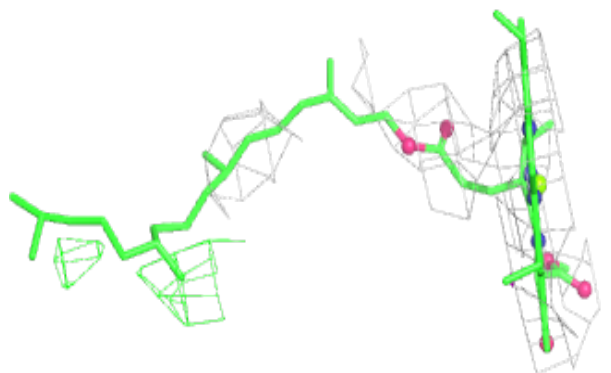
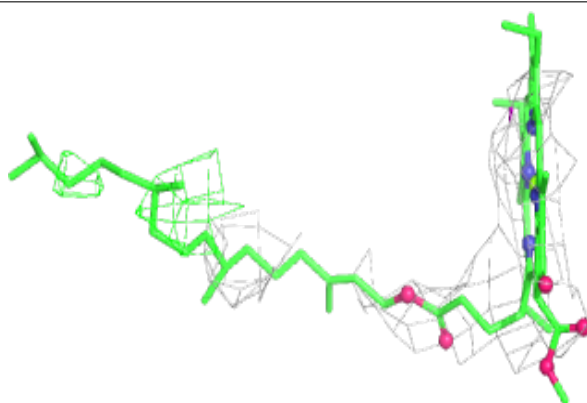


Electron density around BCR b 621:

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

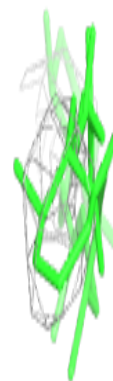
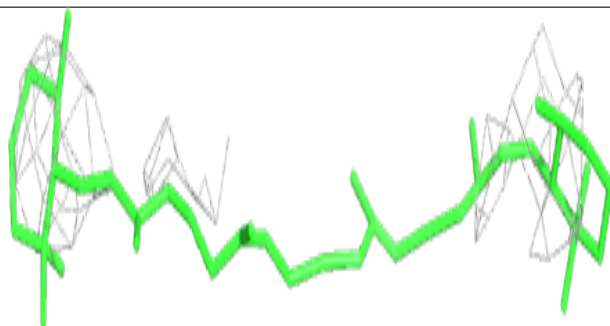
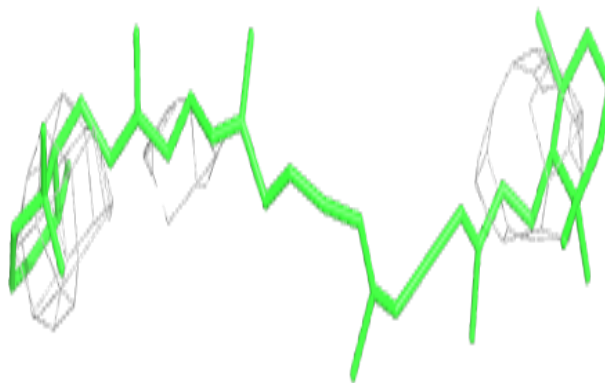
**Electron density around CLA b 609 (A):**

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

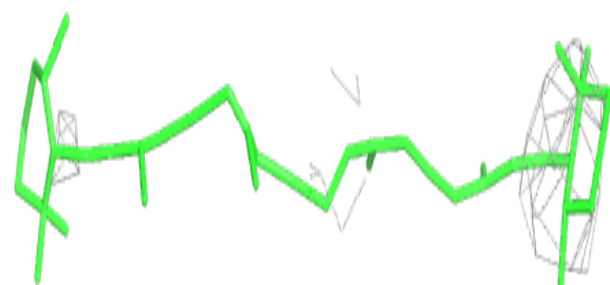


Electron density around BCR b 620:

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

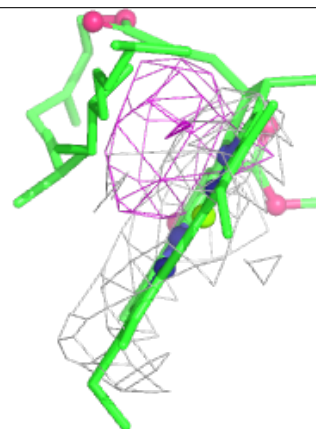
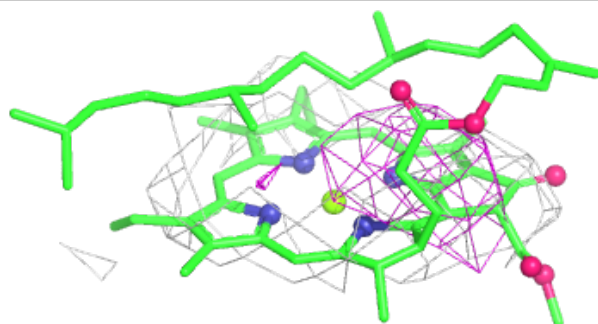
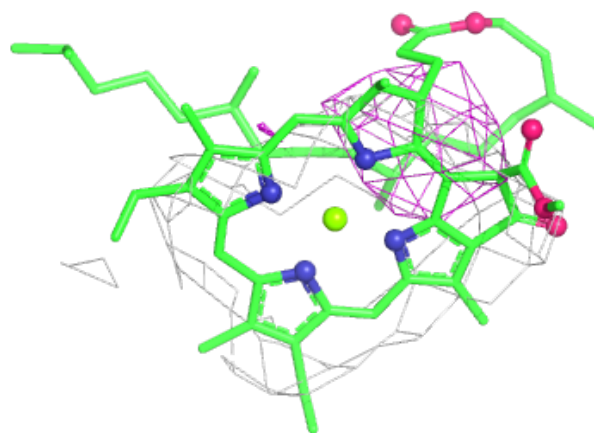
**Electron density around BCR A 609:**

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

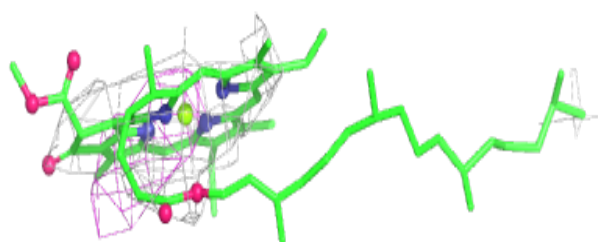
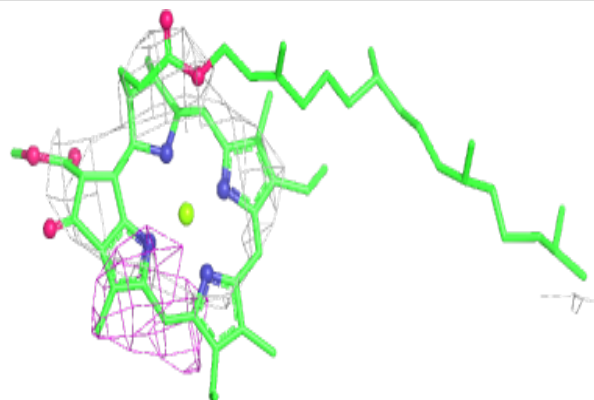


Electron density around CLA b 604:

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

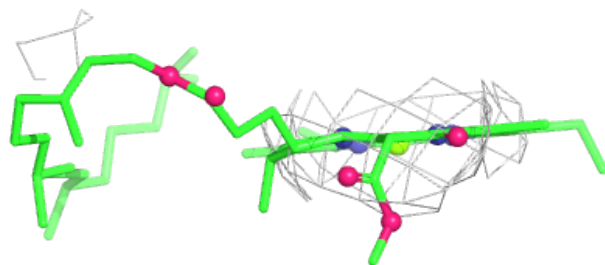
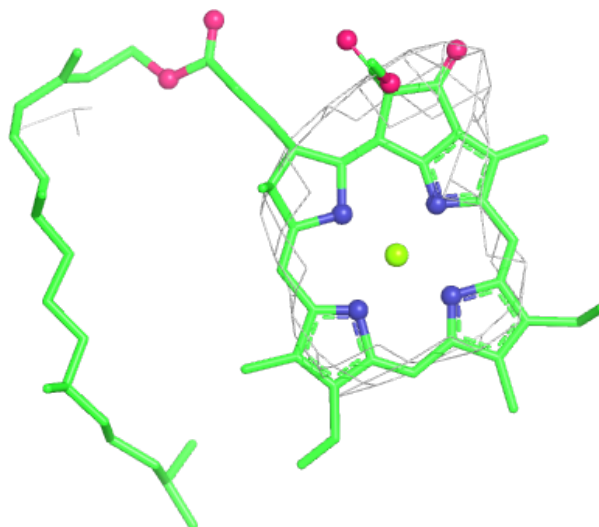
**Electron density around CLA c 502:**

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



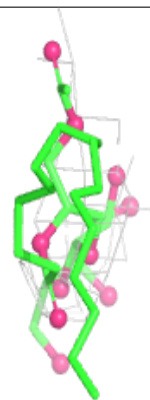
Electron density around CLA c 513:

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

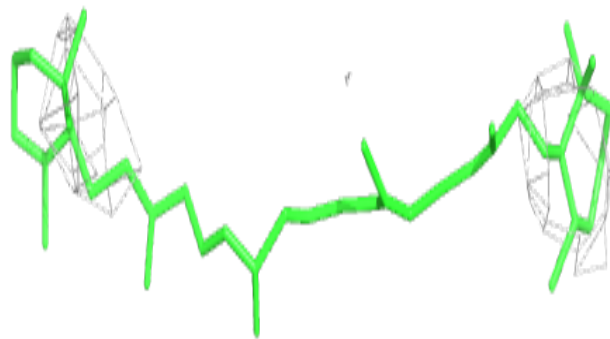
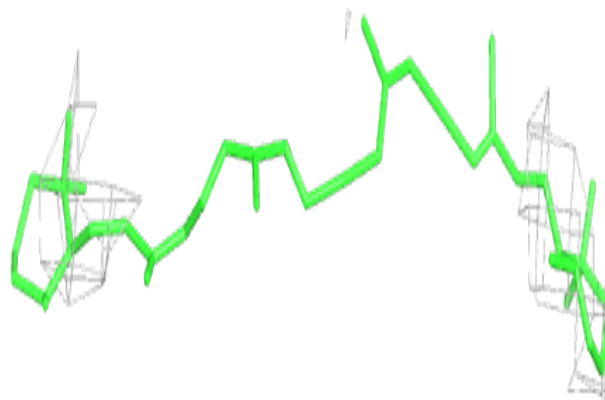


Electron density around LMG z 101:

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

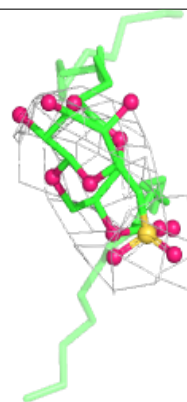
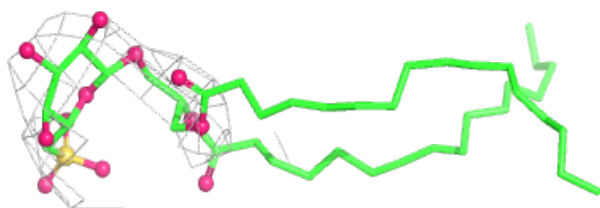
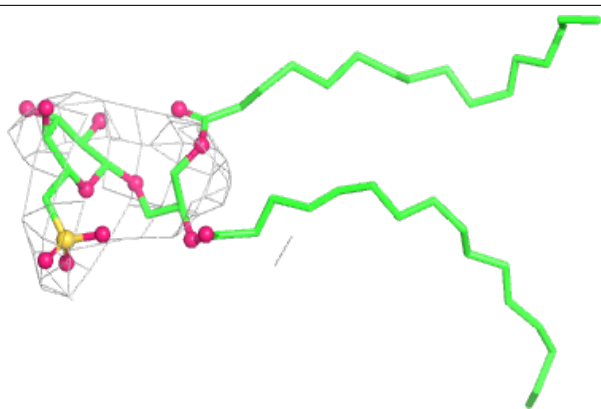
**Electron density around BCR t 101:**

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



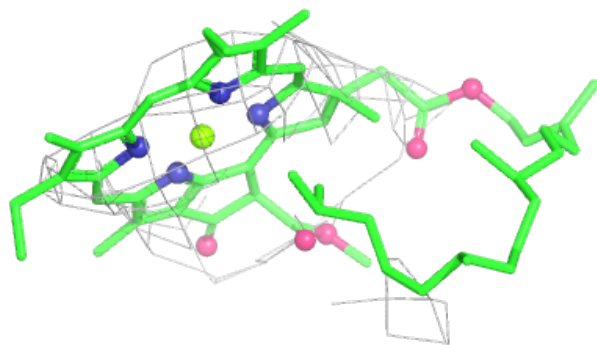
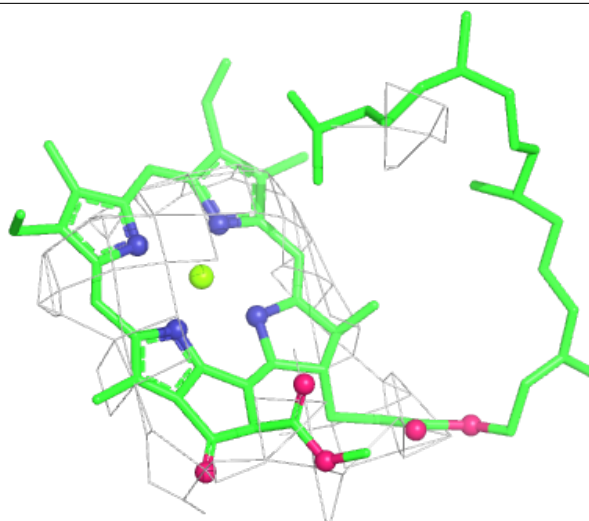
Electron density around SQD B 623:

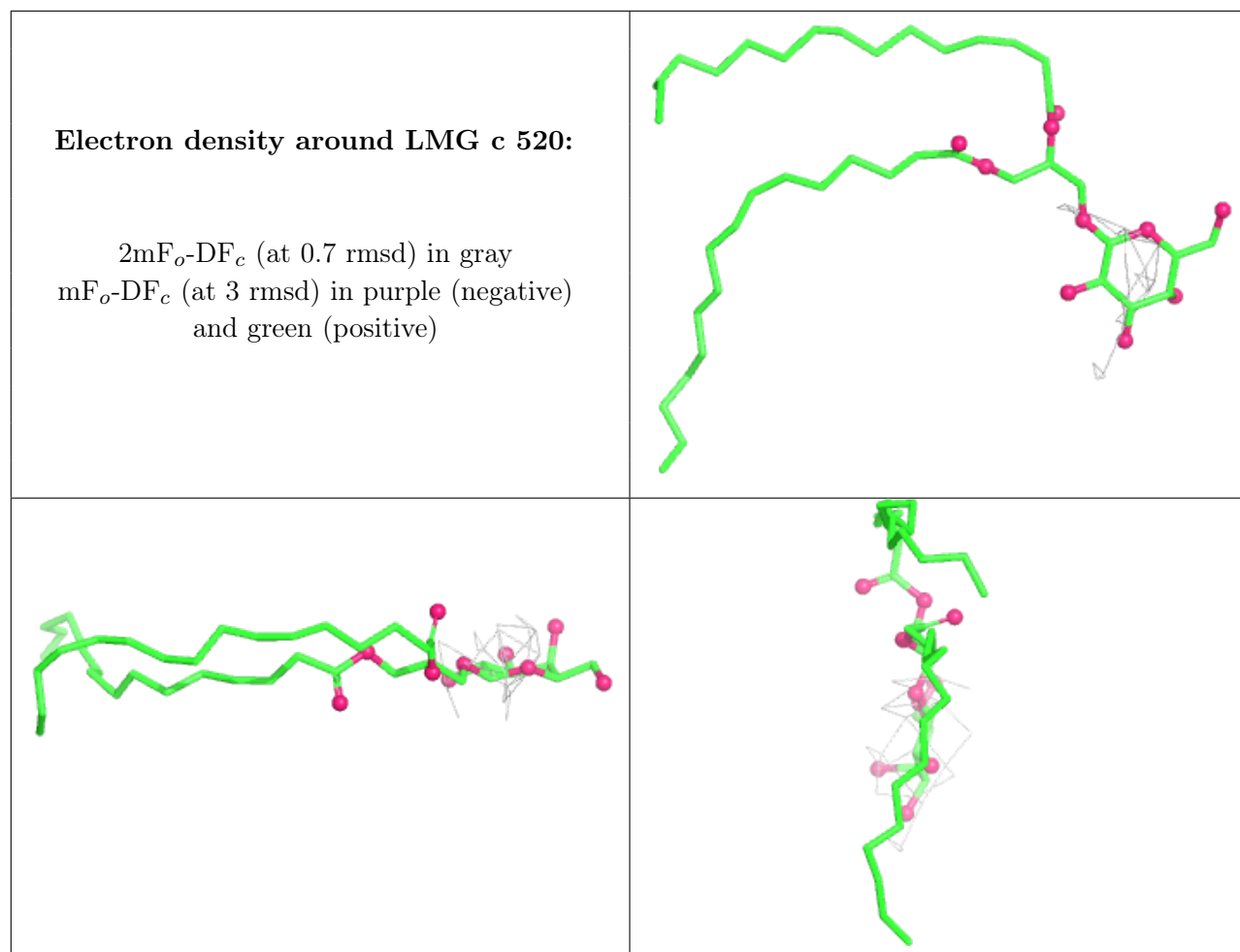
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 618:

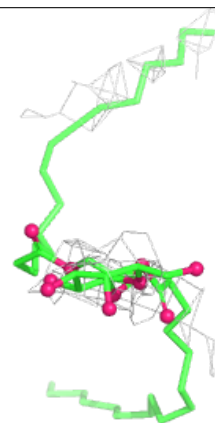
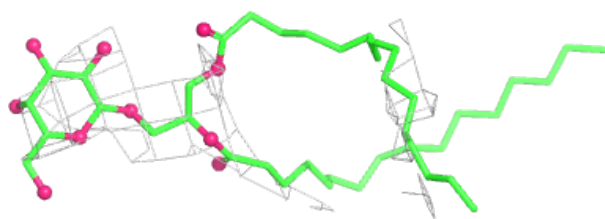
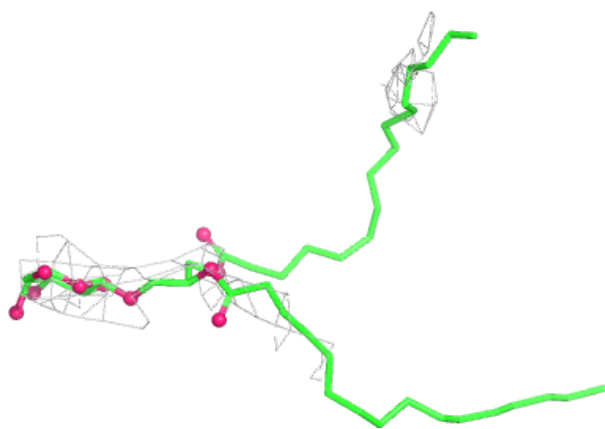
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



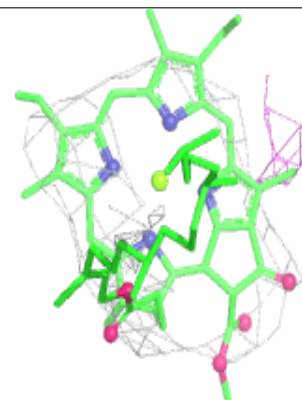
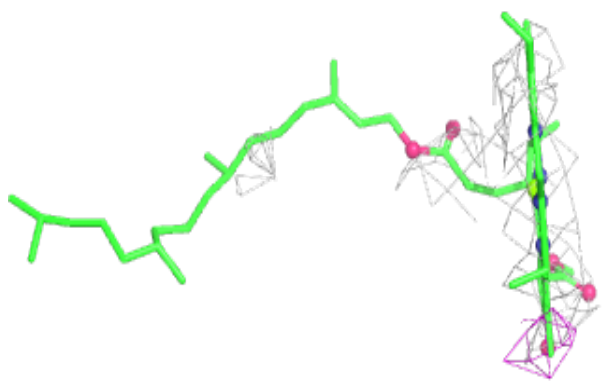
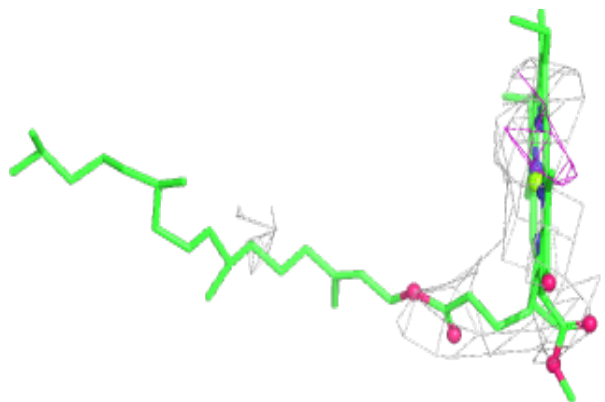


Electron density around LMG b 623:

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

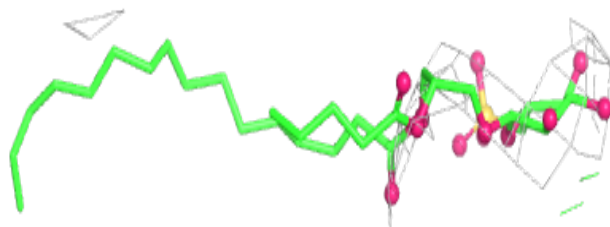
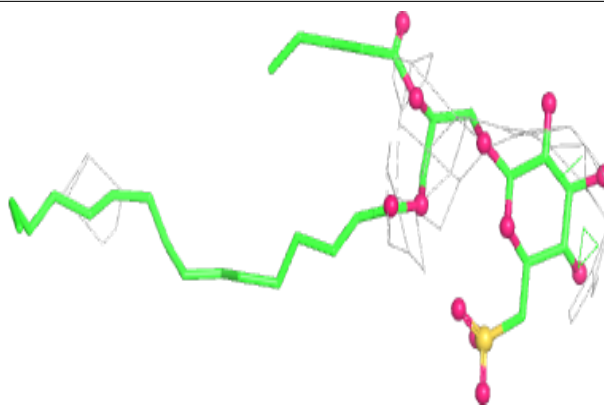
**Electron density around CLA B 607 (A):**

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

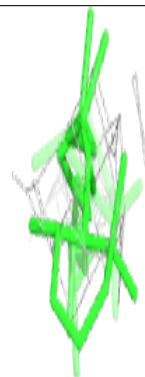
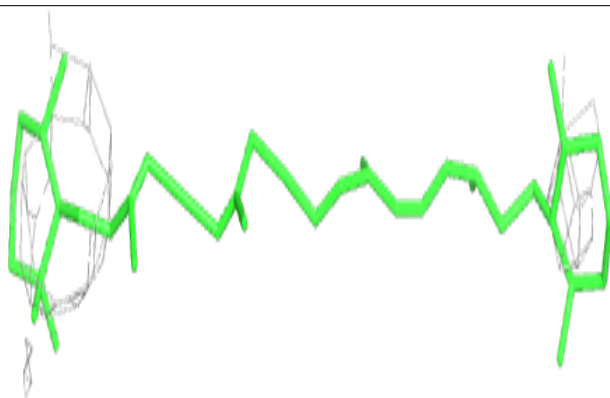


Electron density around SQD X 101:

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

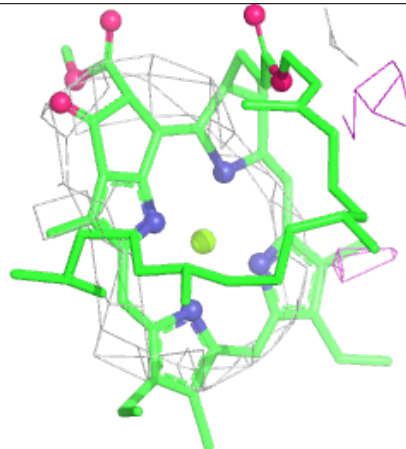
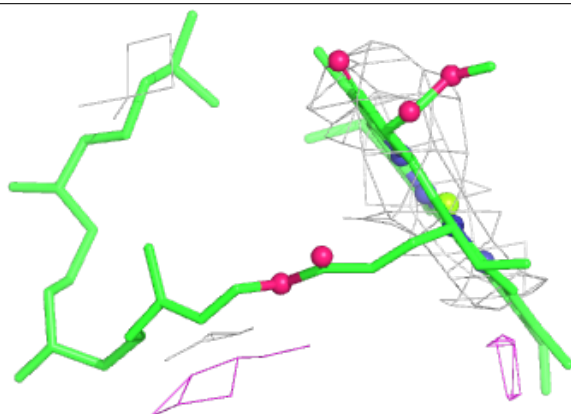
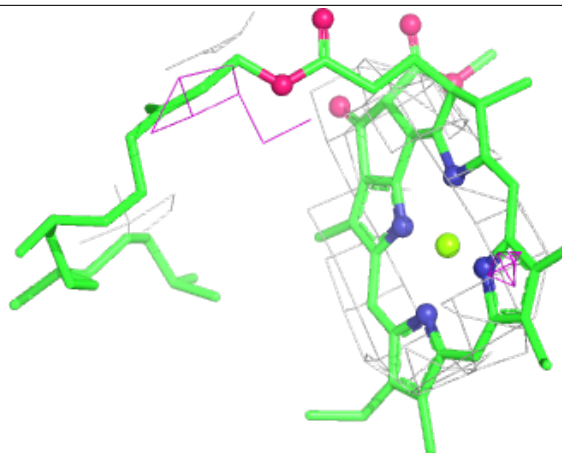
**Electron density around BCR c 515:**

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



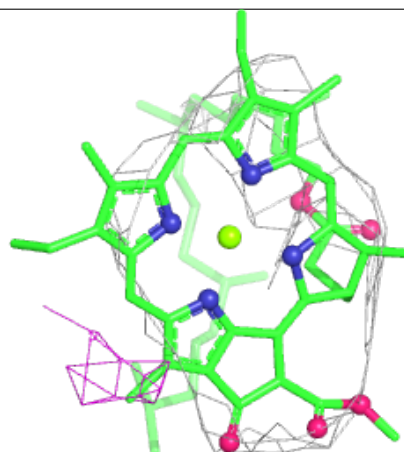
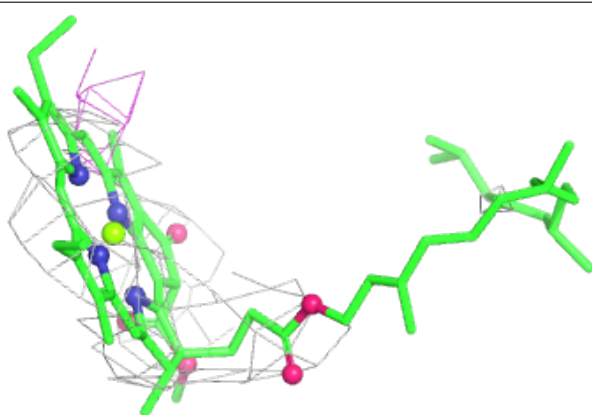
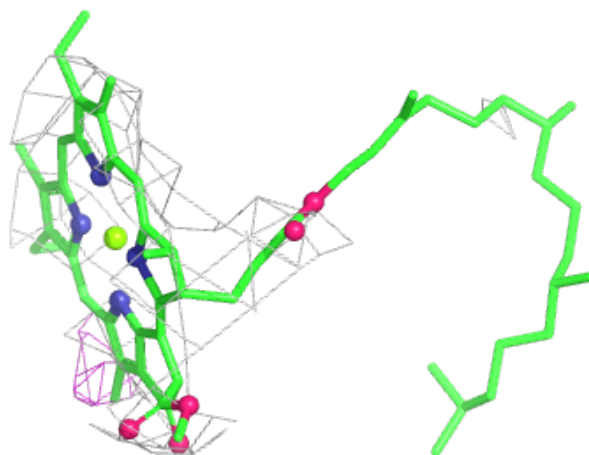
Electron density around CLA c 504:

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



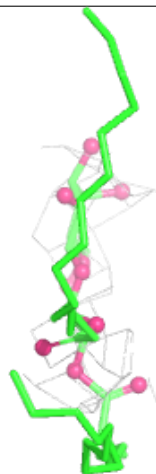
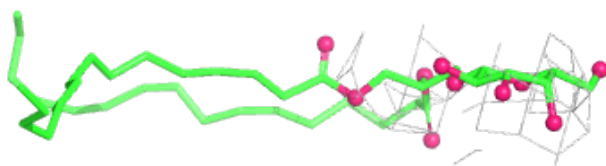
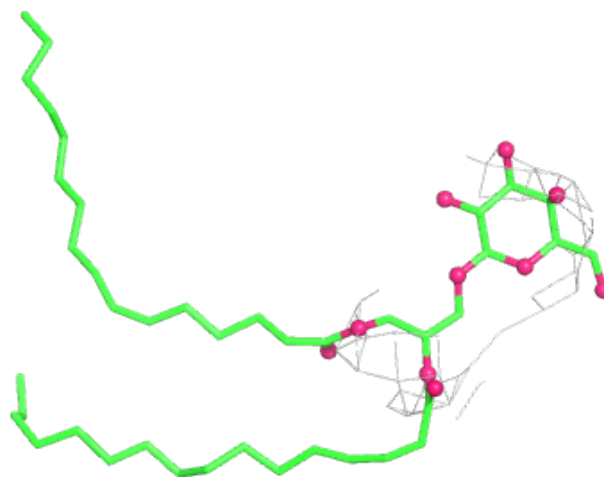
Electron density around CLA B 607 (B):

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



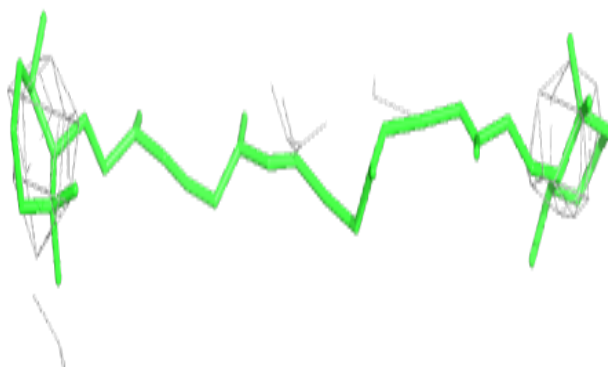
Electron density around LMG C 519:

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

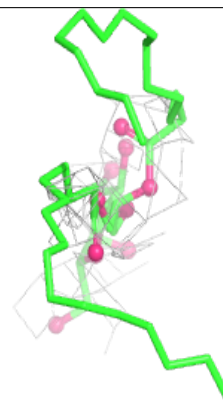
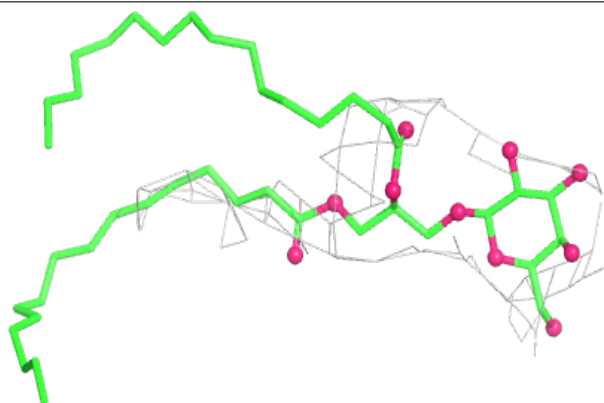


Electron density around BCR K 101:

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

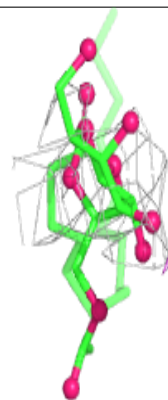
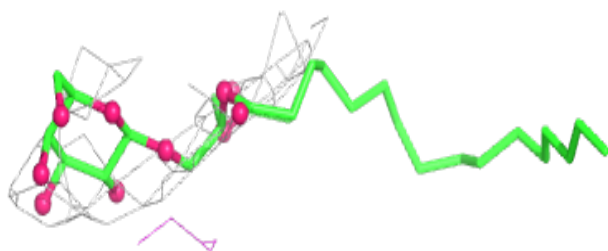
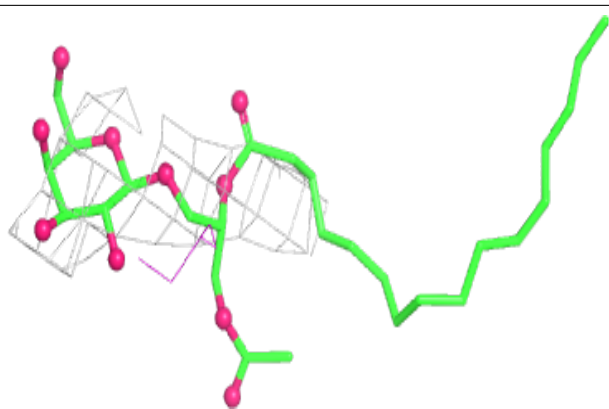
**Electron density around LMG J 101:**

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

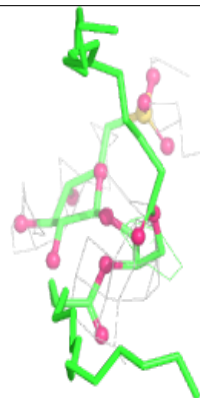
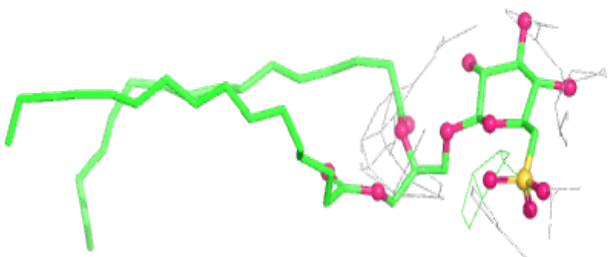
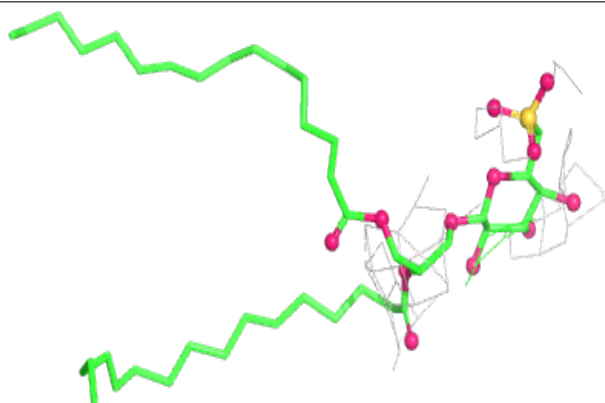


Electron density around LMG Z 101:

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

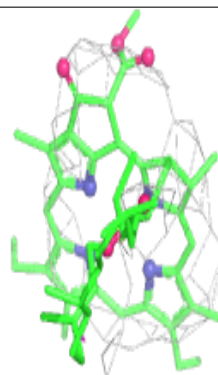
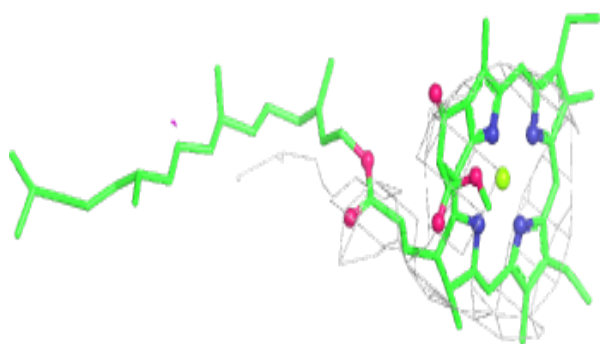
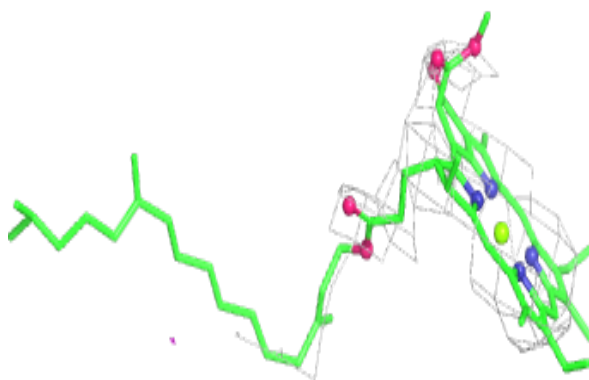
**Electron density around SQD b 601:**

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

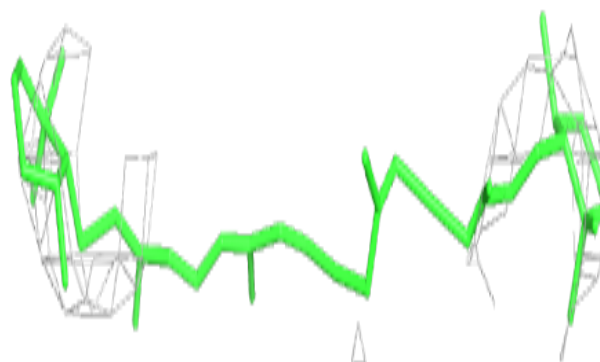
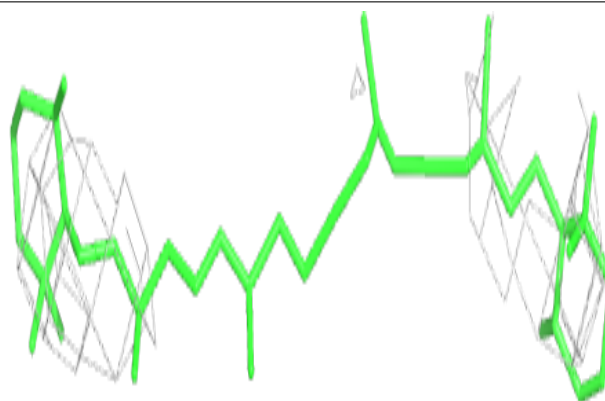


Electron density around CLA c 503:

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

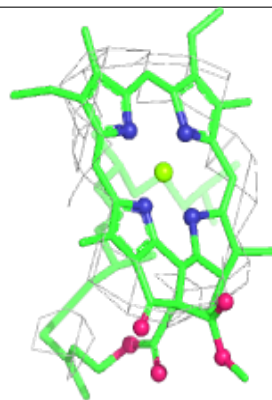
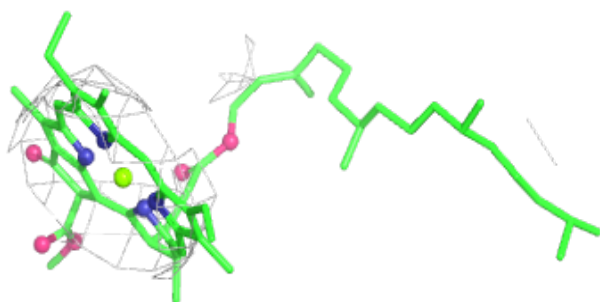
**Electron density around BCR B 620:**

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



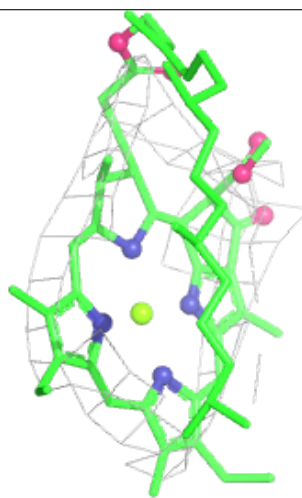
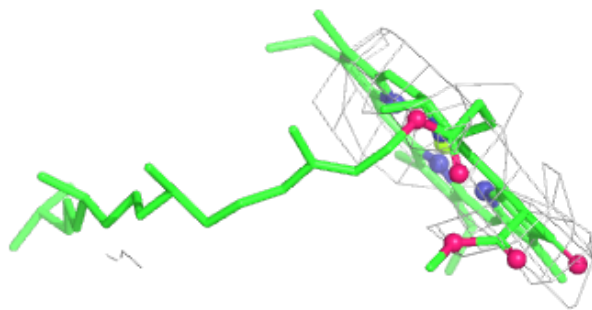
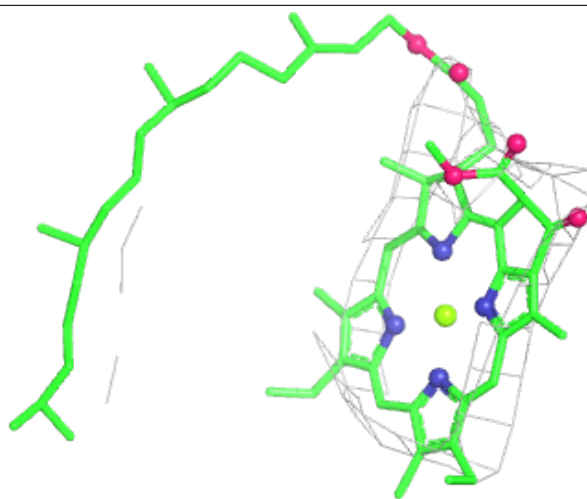
Electron density around CLA C 511:

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



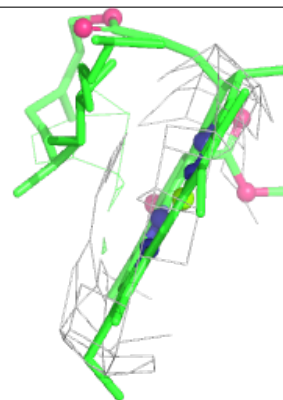
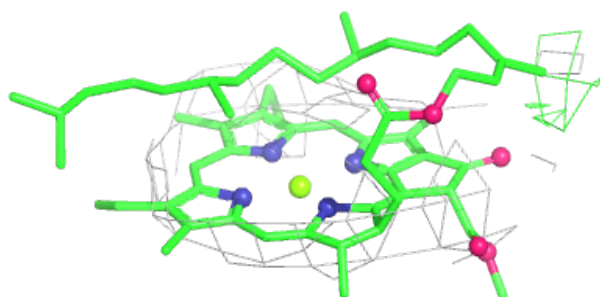
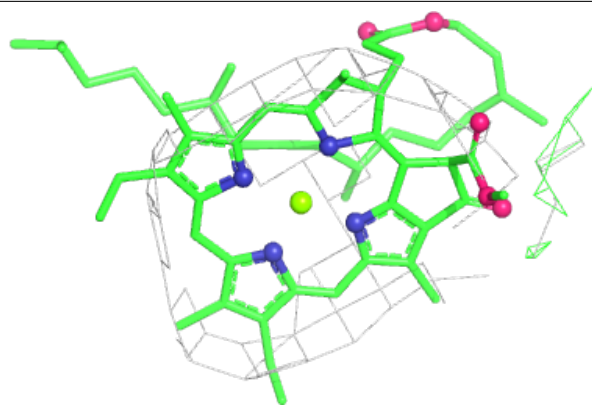
Electron density around CLA c 508:

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

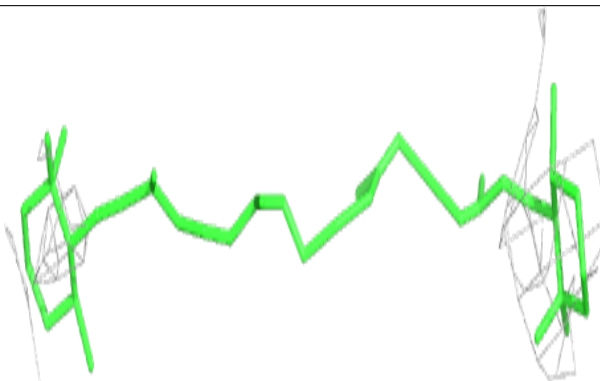


Electron density around CLA B 602:

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

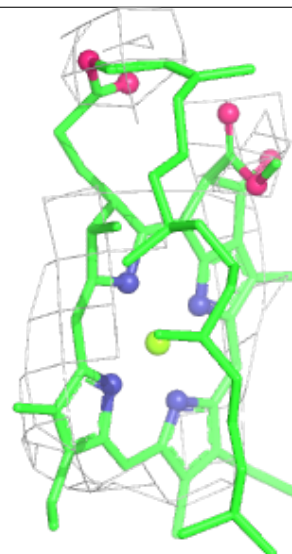
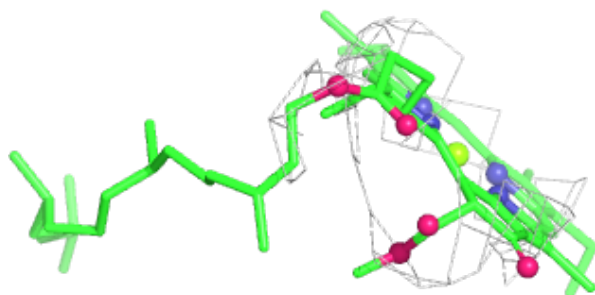
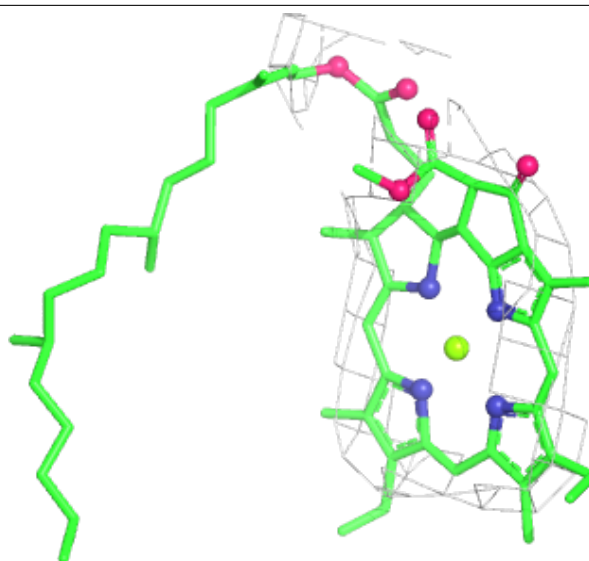
**Electron density around BCR c 516:**

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



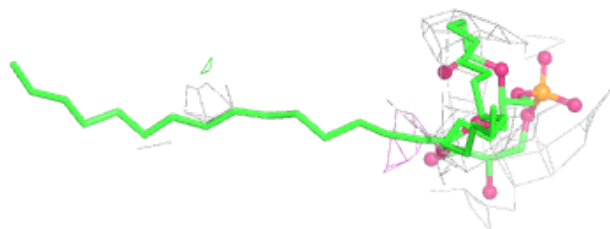
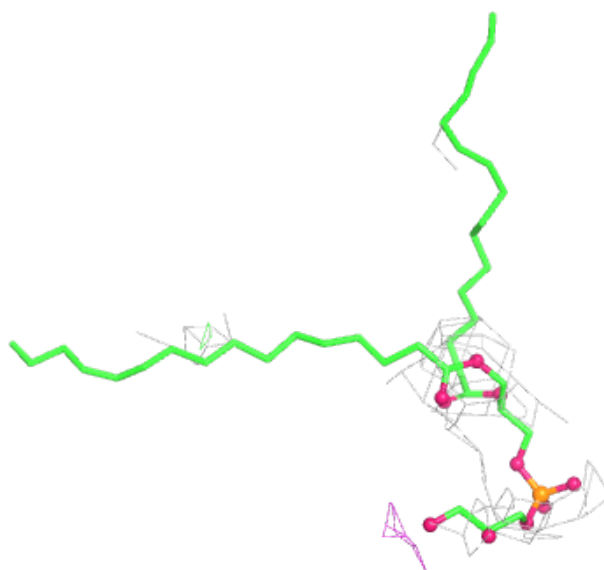
Electron density around CLA b 619:

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



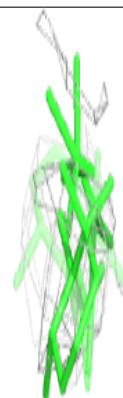
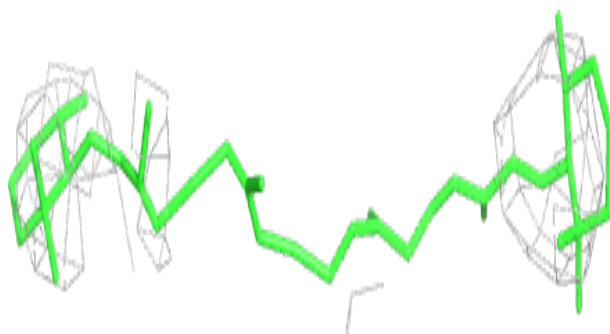
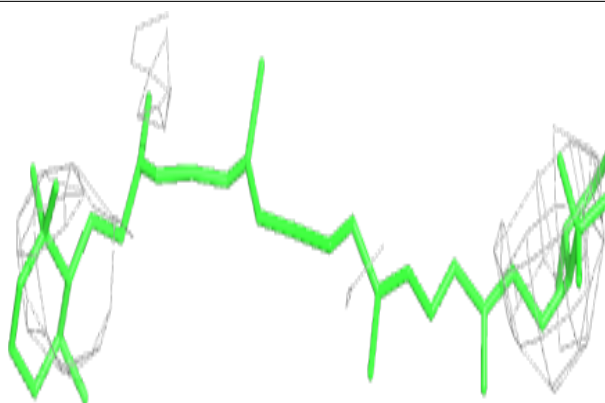
Electron density around LHG 1 101:

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

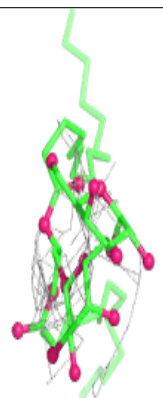
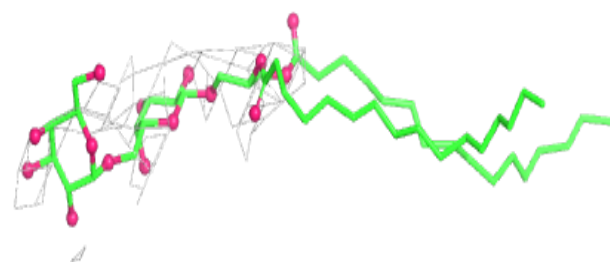
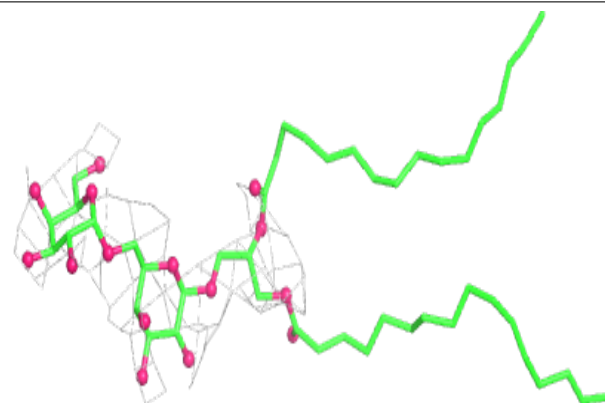


Electron density around BCR B 618:

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

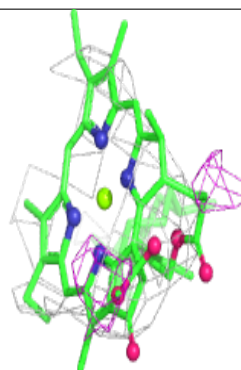
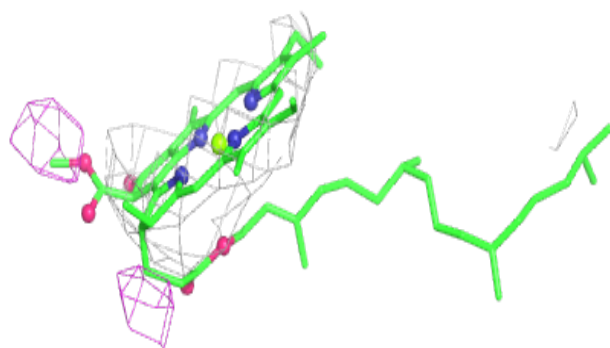
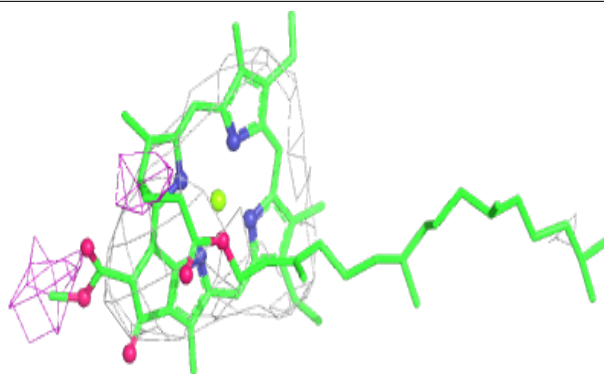
**Electron density around DGD c 519:**

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



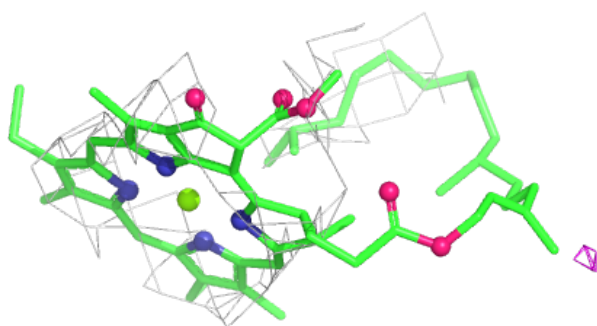
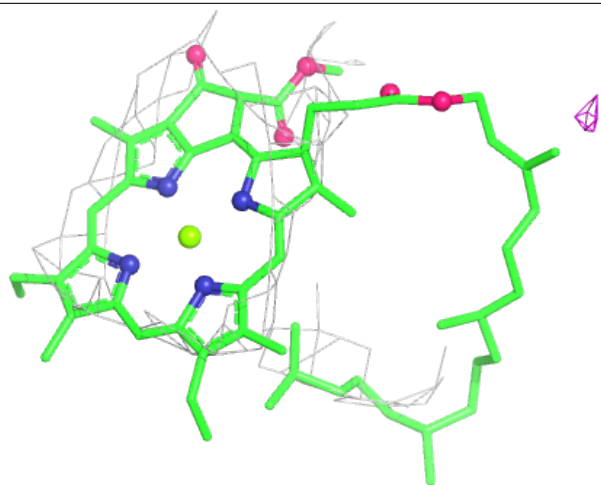
Electron density around CLA b 617:

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



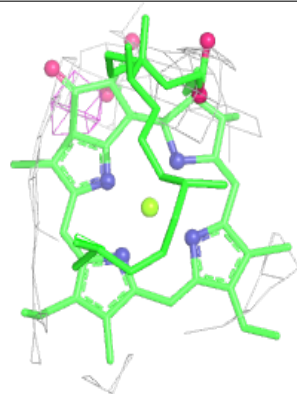
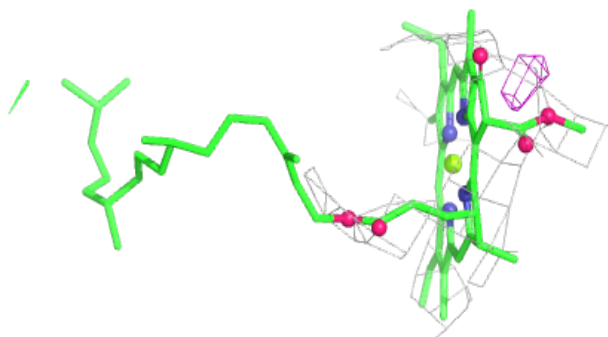
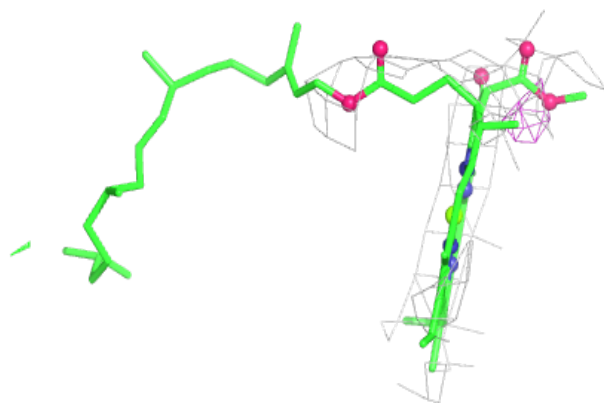
Electron density around CLA B 616:

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

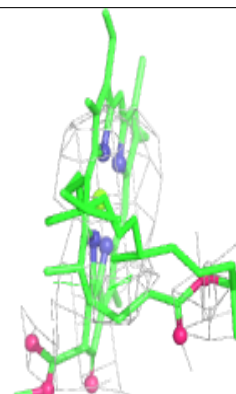
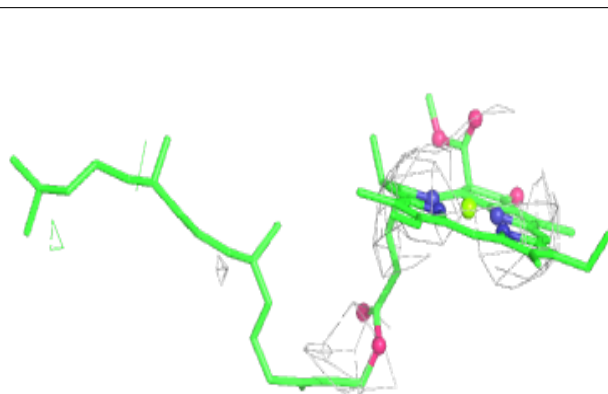
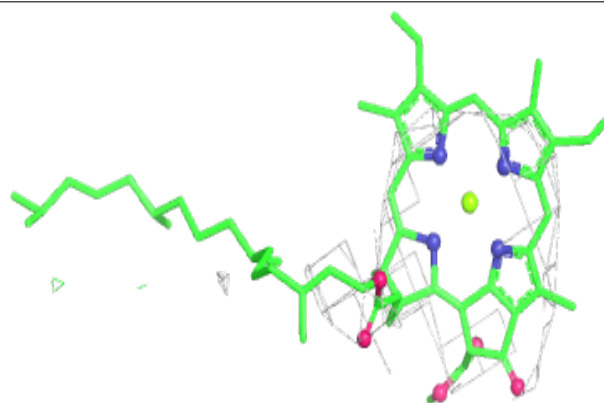


Electron density around CLA C 506:

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

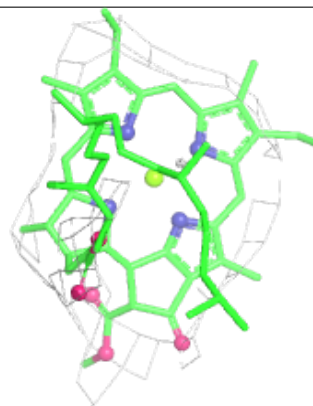
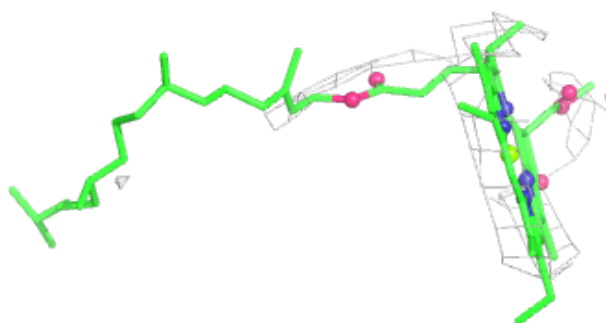
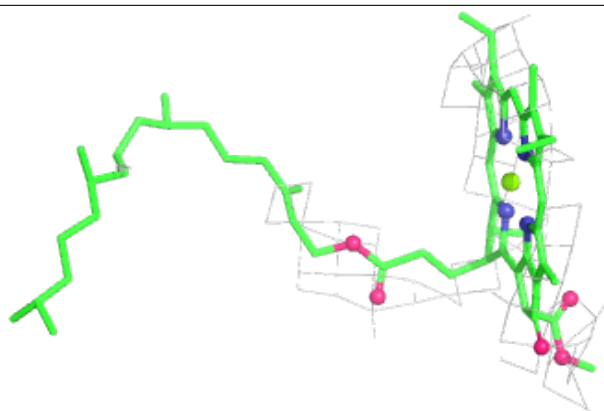
**Electron density around CLA a 605:**

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

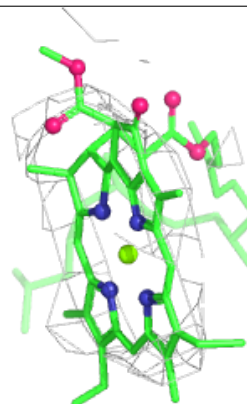
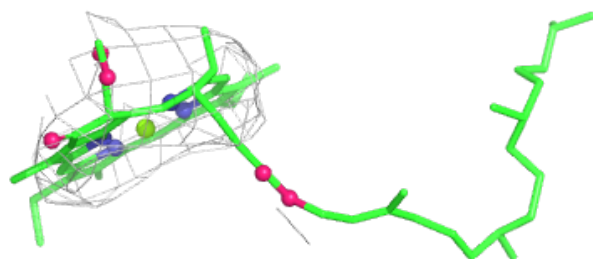
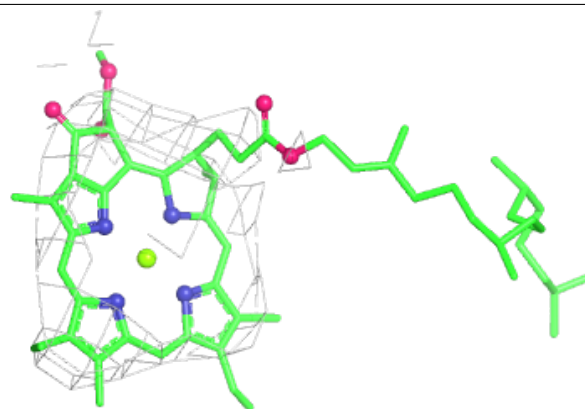


Electron density around CLA d 403:

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

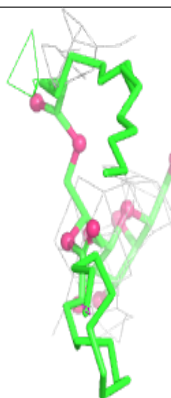
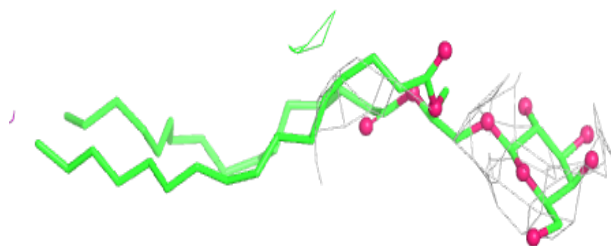
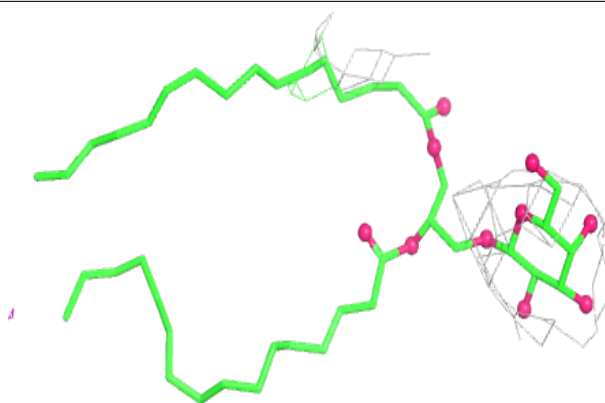
**Electron density around CLA a 607:**

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

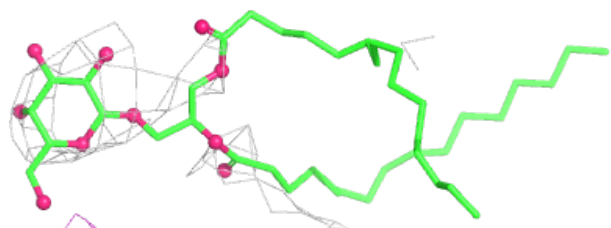
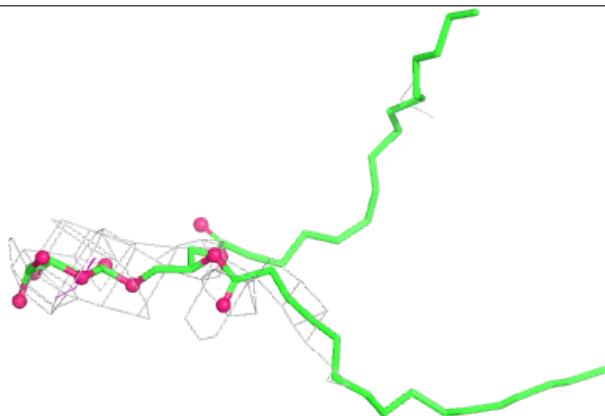


Electron density around LMG A 612:

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

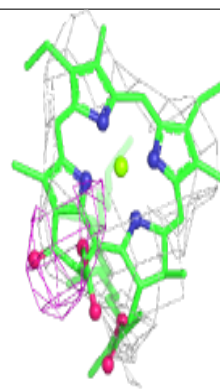
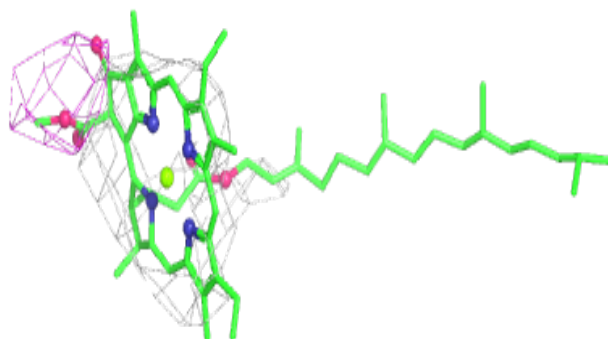
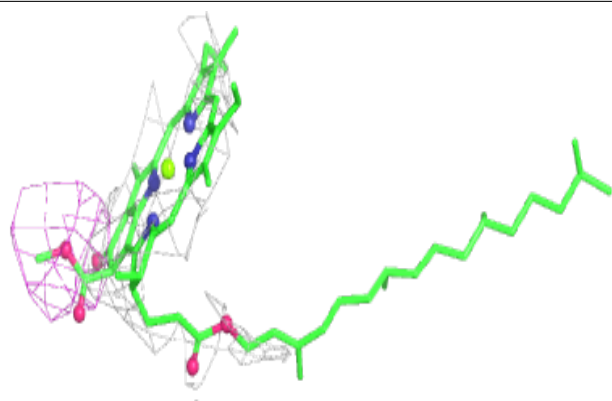
**Electron density around LMG B 621:**

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

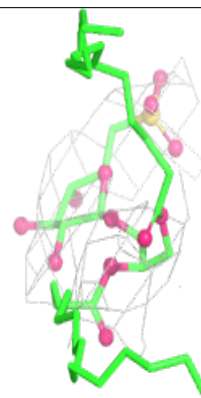
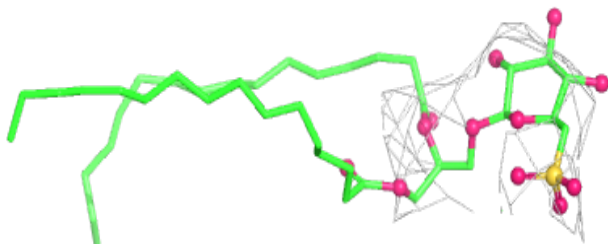
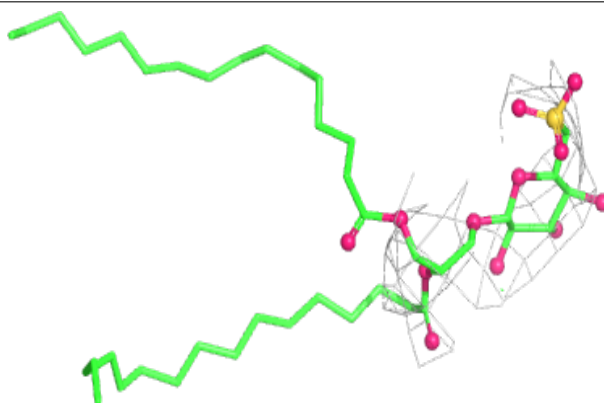


Electron density around CLA B 608:

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

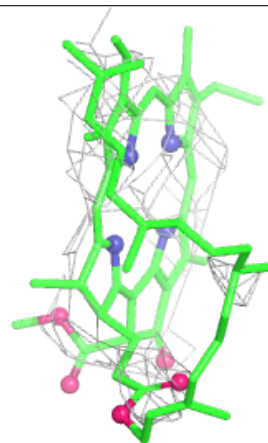
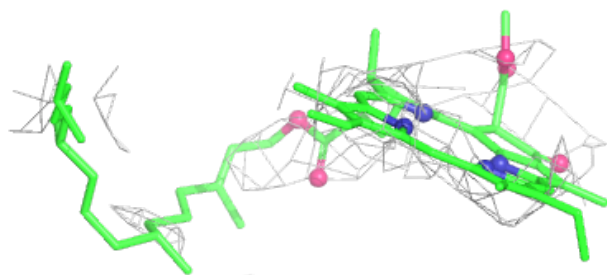
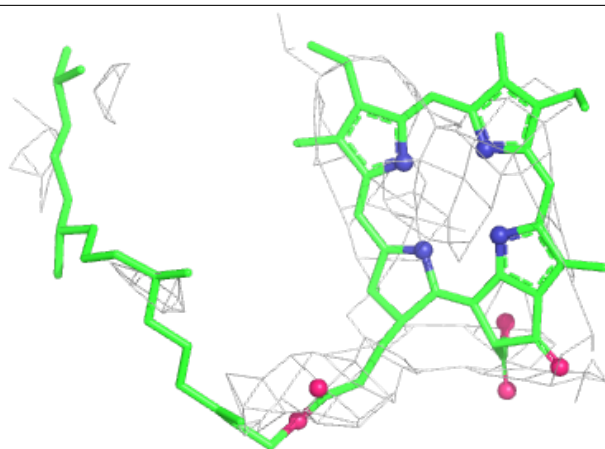
**Electron density around SQD a 612:**

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

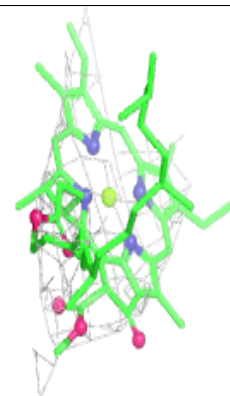
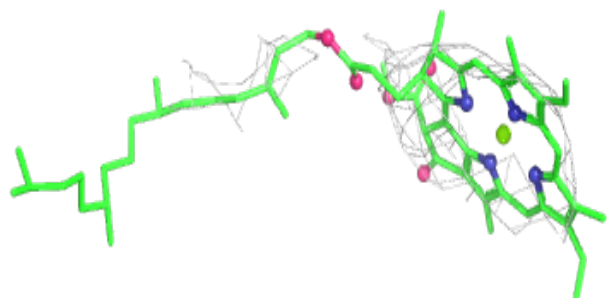
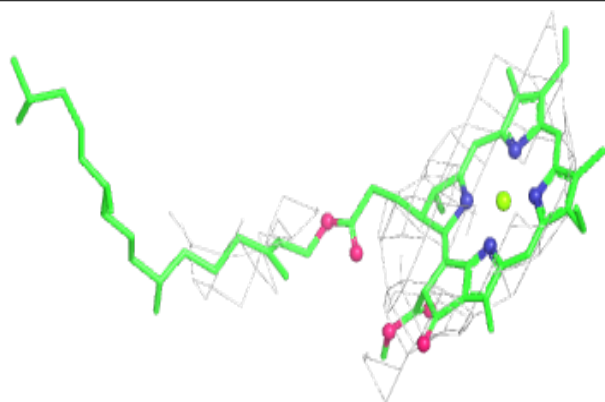


Electron density around PHO D 401:

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

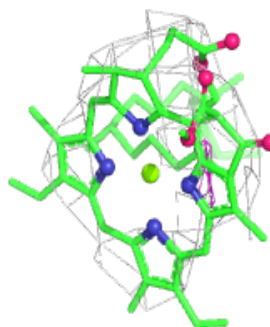
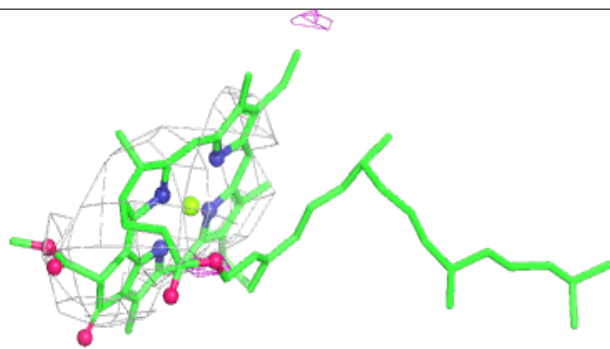
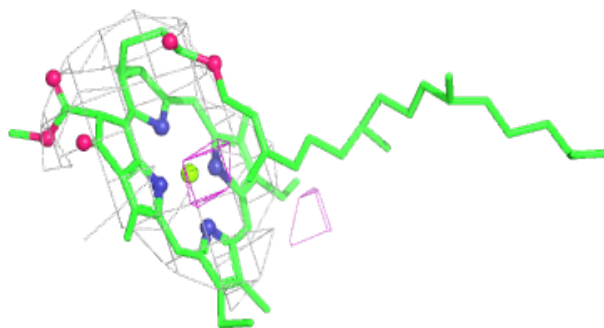
**Electron density around CLA a 604:**

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

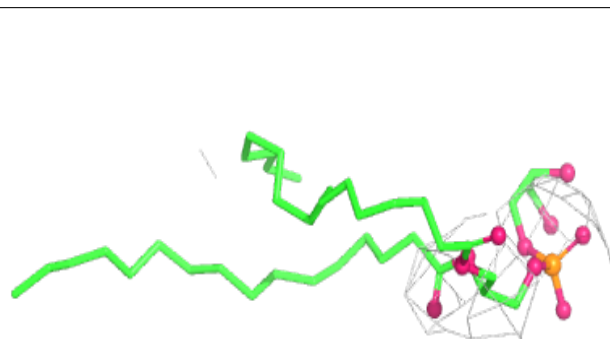


Electron density around CLA C 505:

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

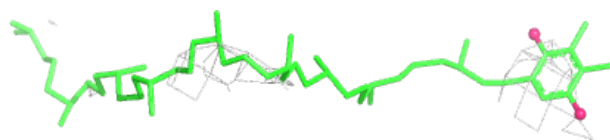
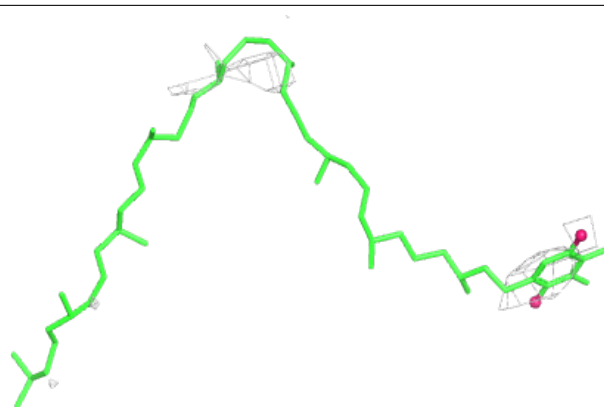
**Electron density around LHG D 408:**

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

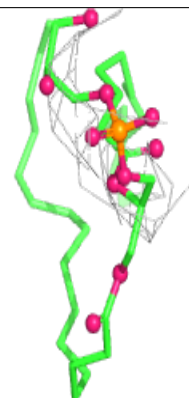


Electron density around PL9 D 405:

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

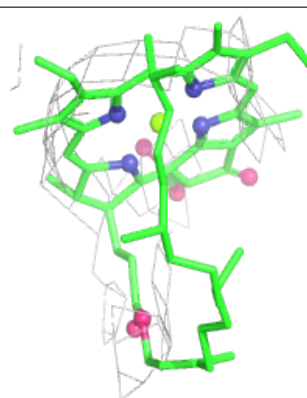
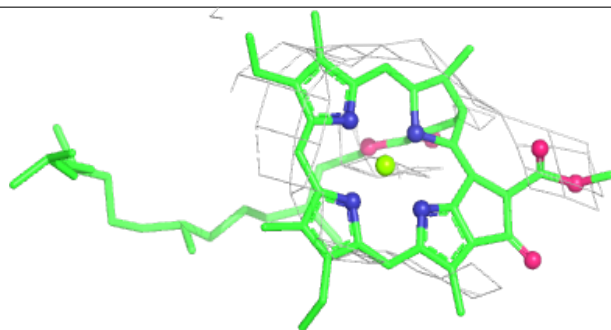
**Electron density around LHG a 614:**

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

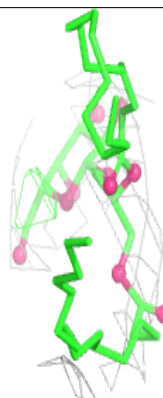
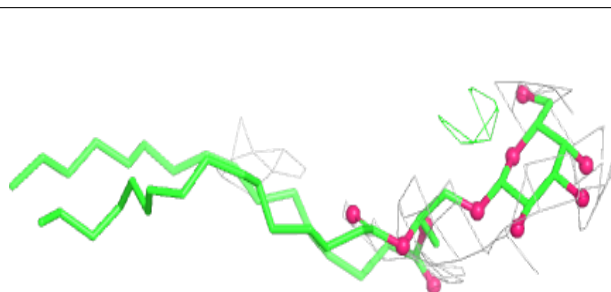
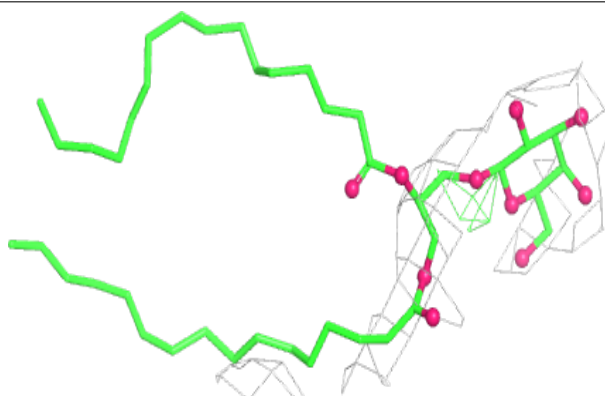


Electron density around CLA c 514:

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

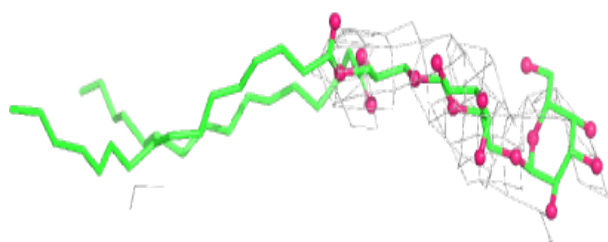
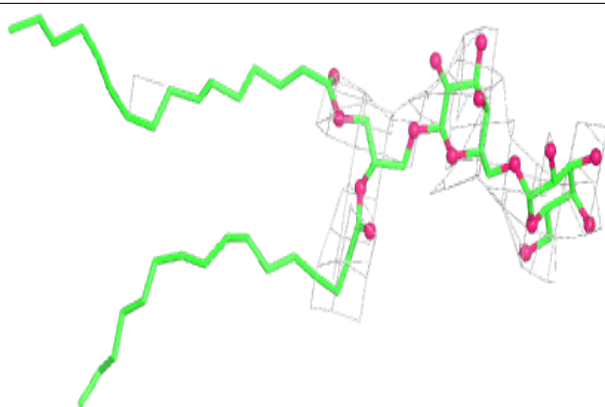
**Electron density around LMG a 611:**

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

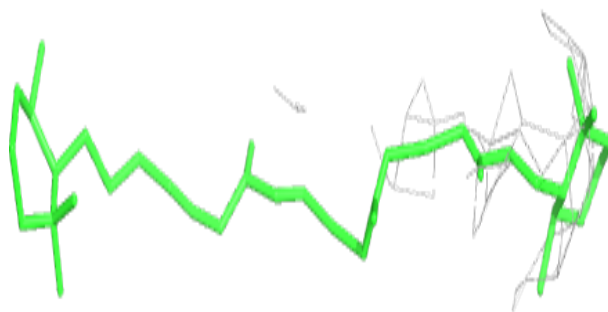
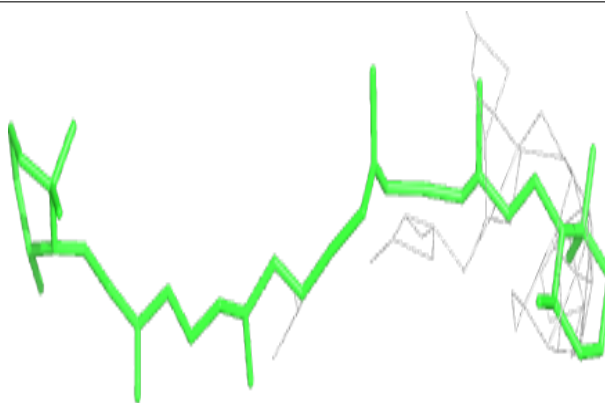


Electron density around DGD C 518:

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

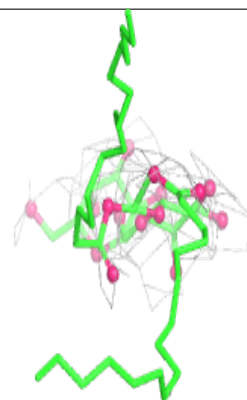
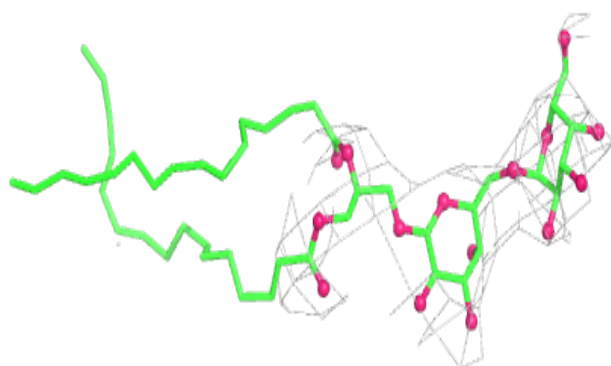
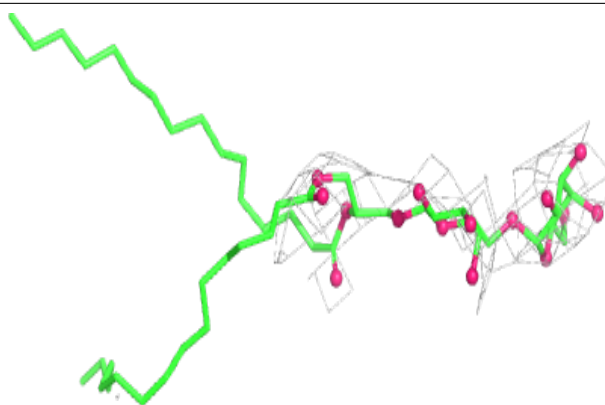
**Electron density around BCR k 101:**

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

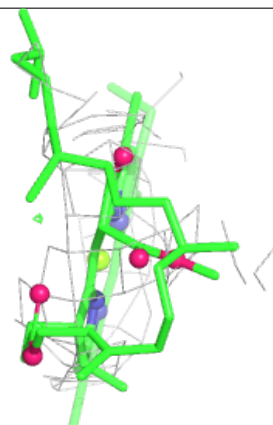
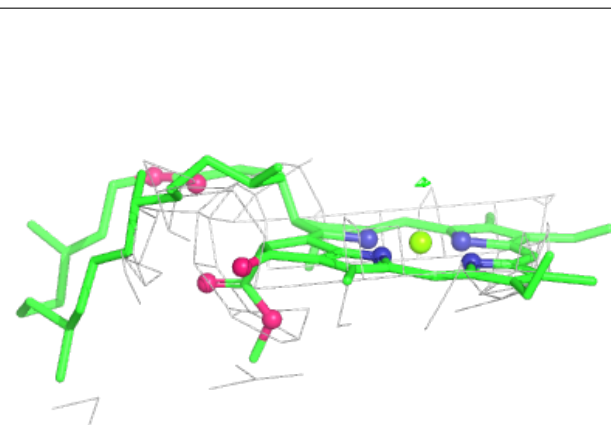
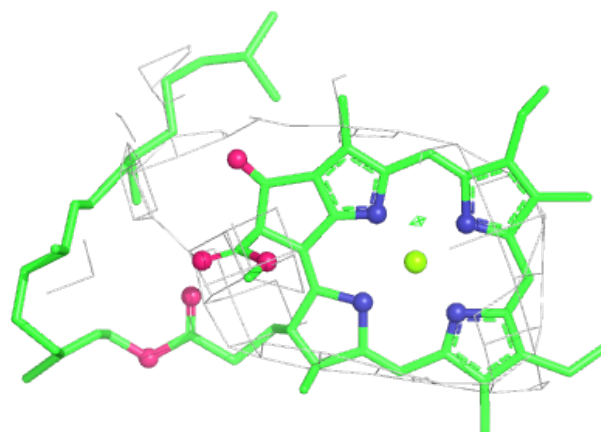


Electron density around DGD c 517:

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

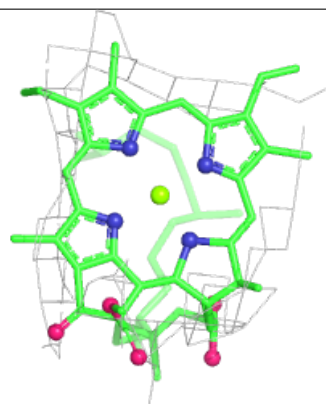
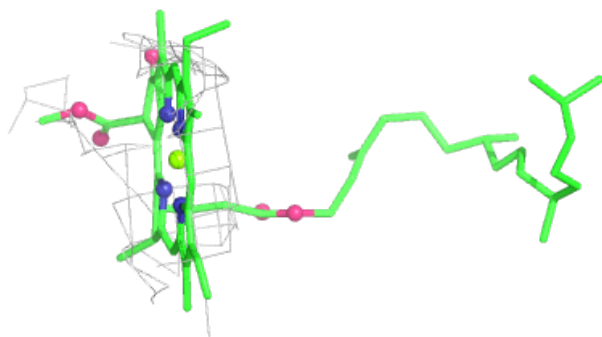
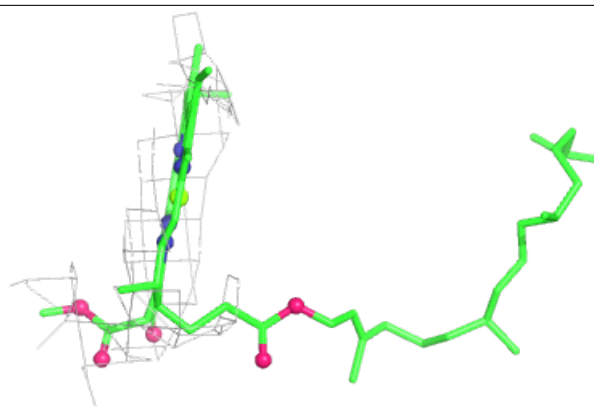
**Electron density around CLA b 613:**

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

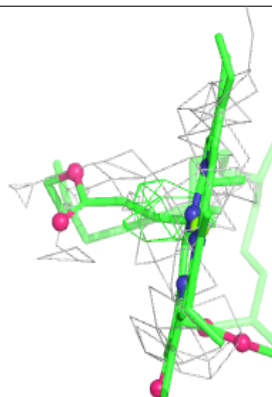
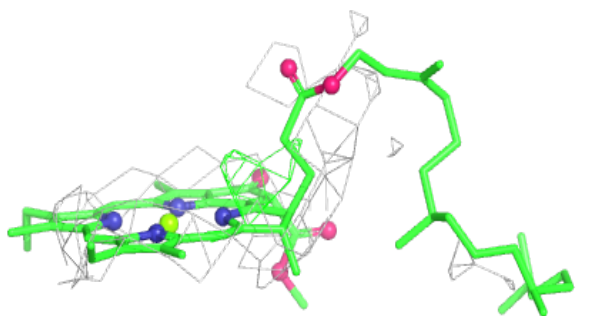
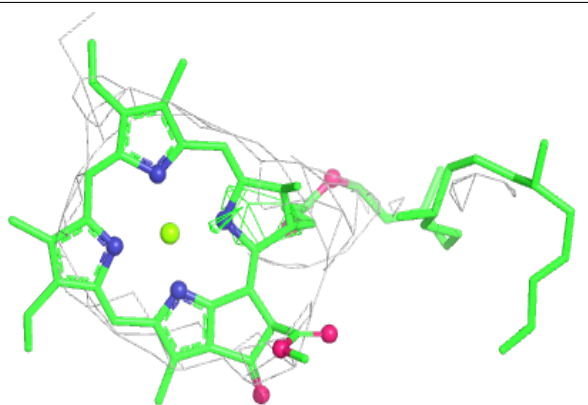


Electron density around CLA c 507:

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

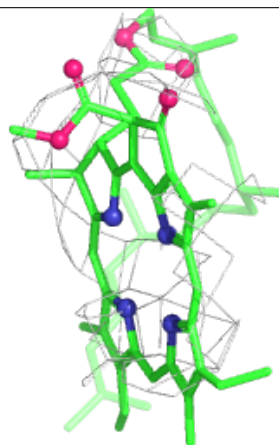
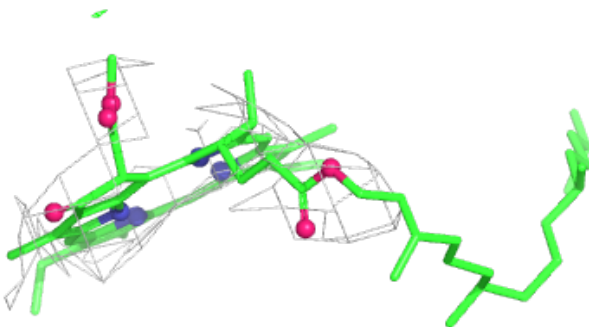
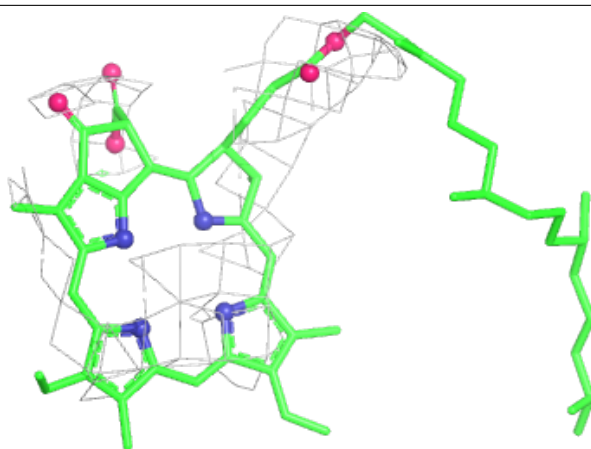
**Electron density around CLA b 615:**

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



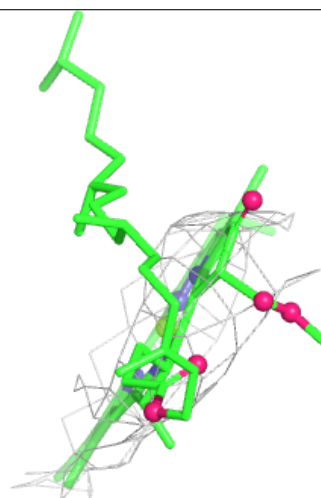
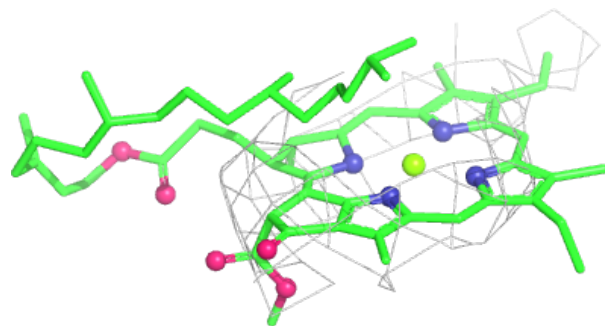
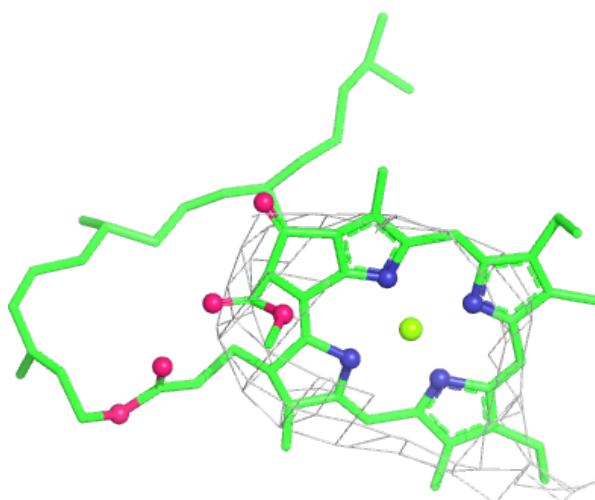
Electron density around PHO d 401:

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



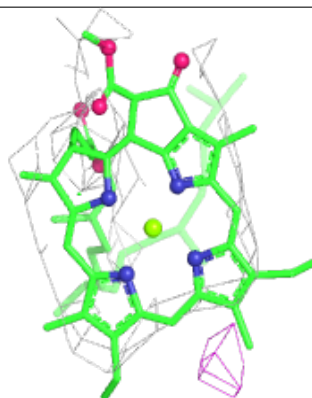
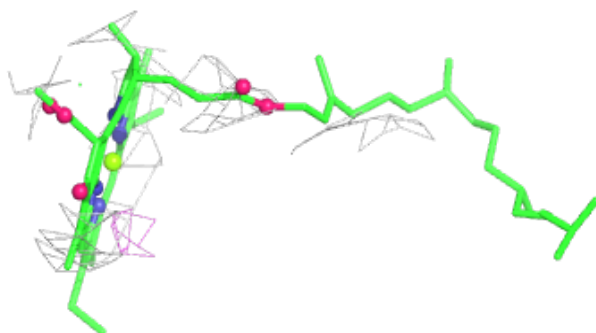
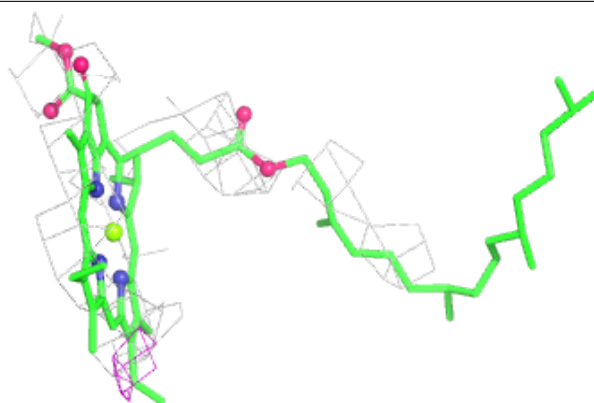
Electron density around CLA c 510:

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

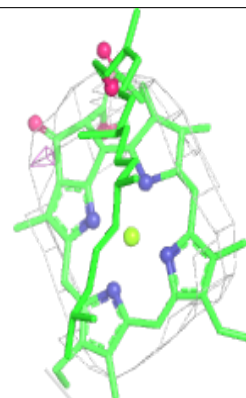
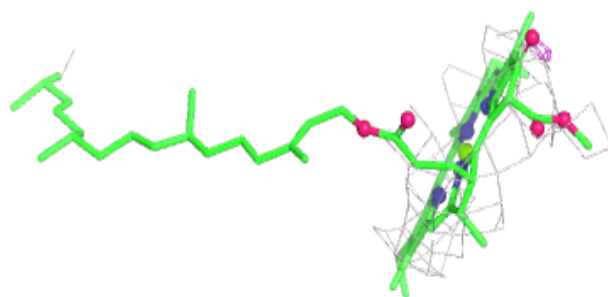
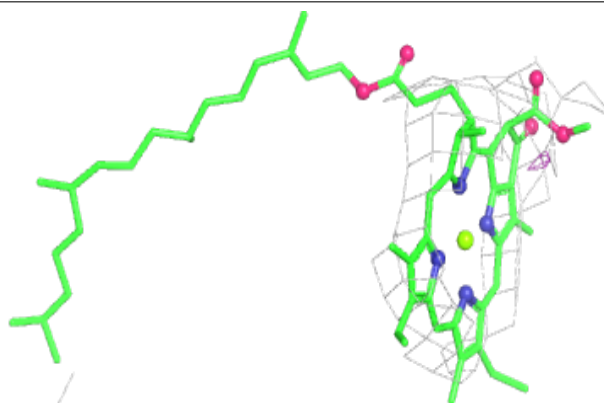


Electron density around CLA D 404:

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

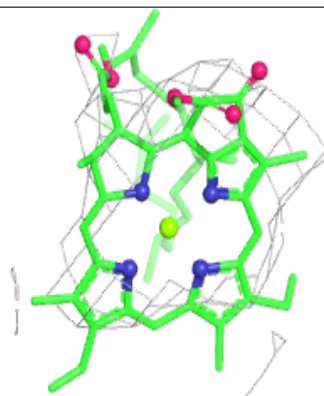
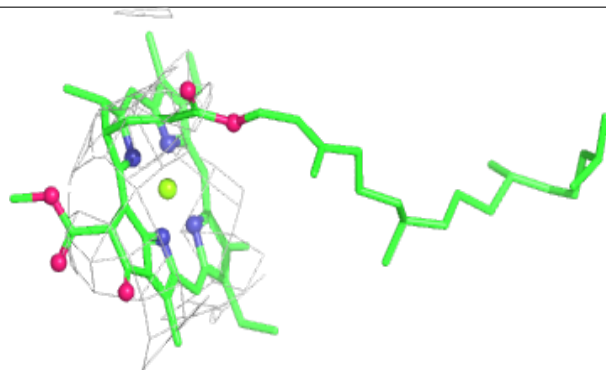
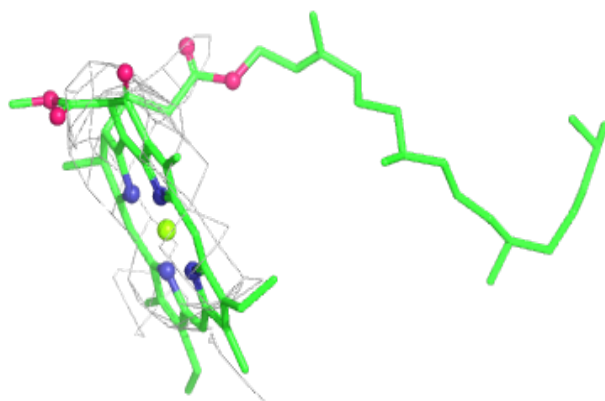
**Electron density around CLA b 612:**

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

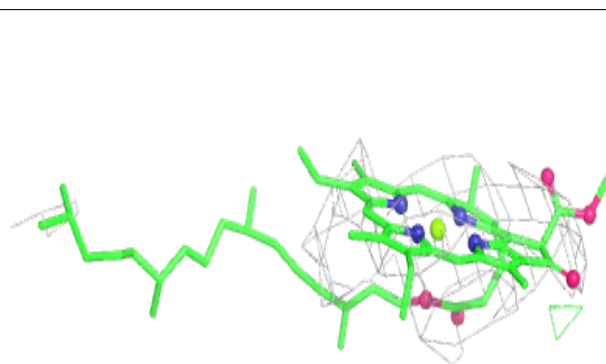
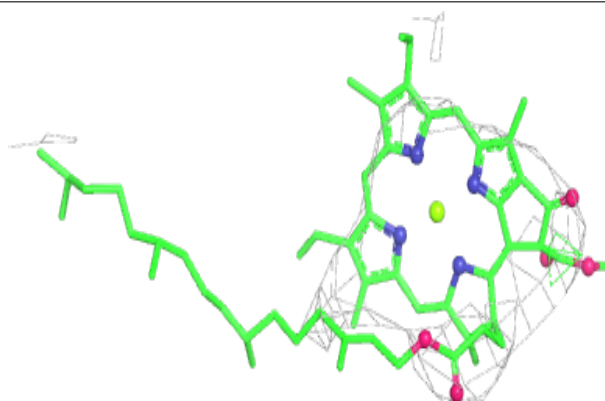


Electron density around CLA C 508:

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

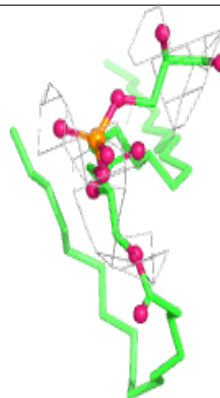
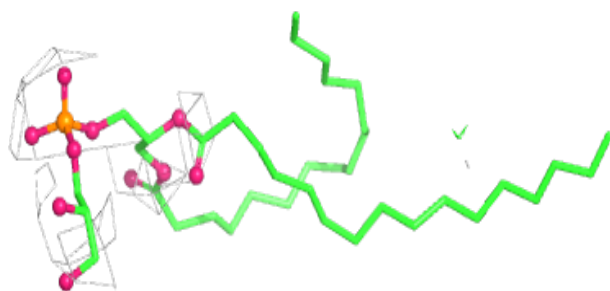
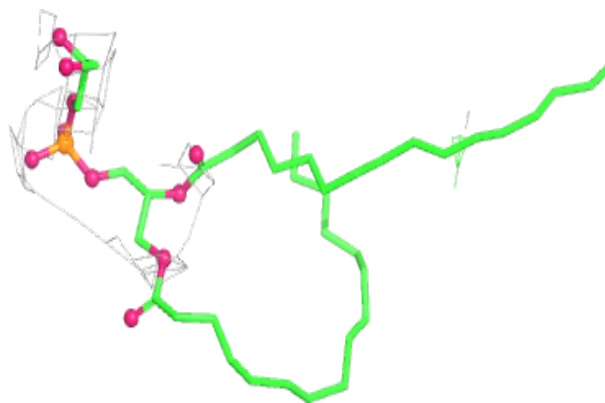
**Electron density around CLA C 501:**

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

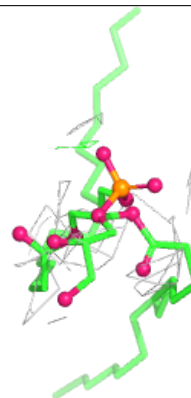
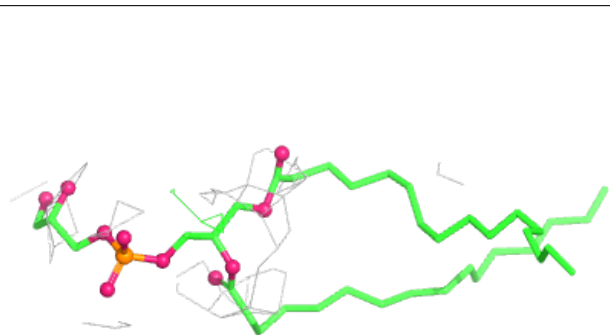
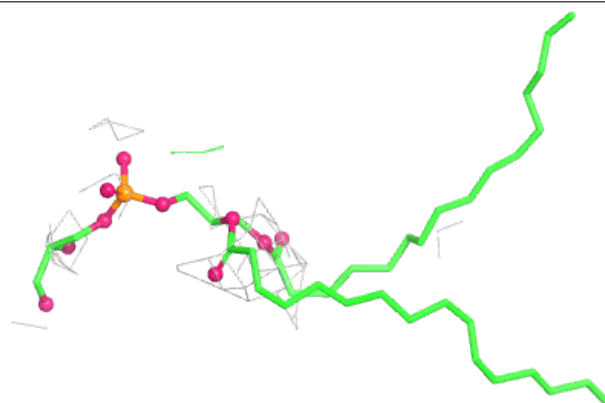


Electron density around LHG b 624:

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

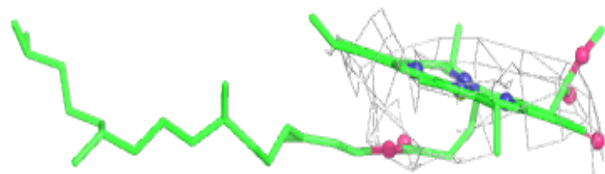
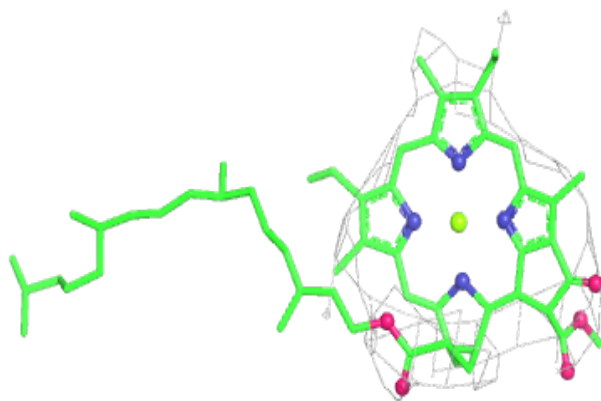
**Electron density around LHG d 406:**

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

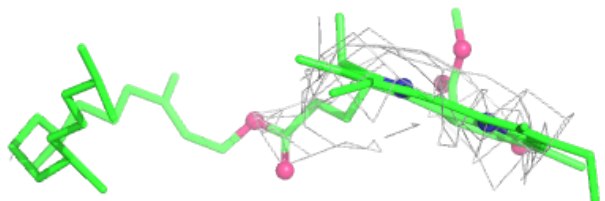
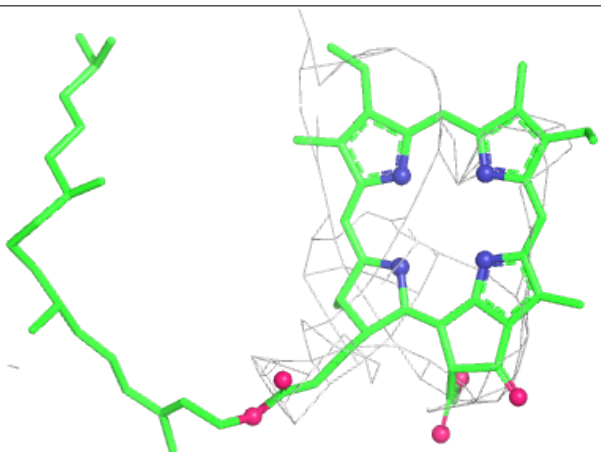


Electron density around CLA b 606:

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

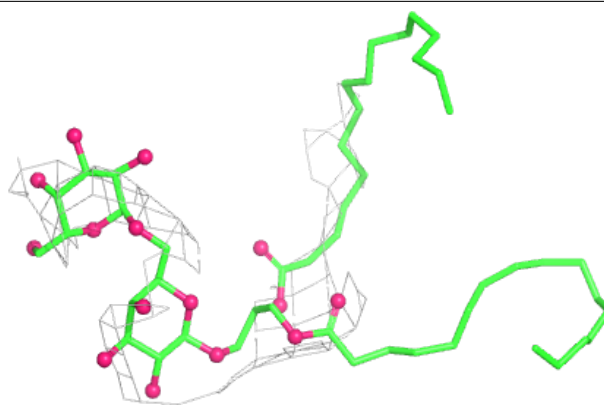
**Electron density around PHO a 606:**

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



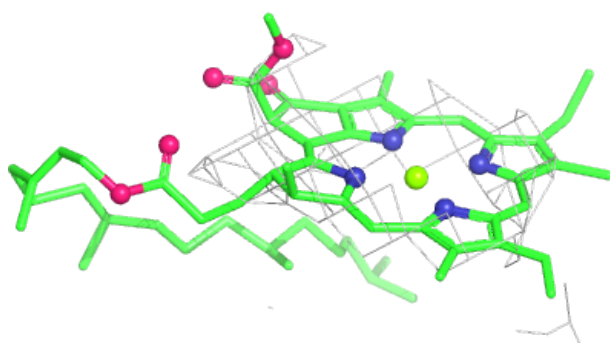
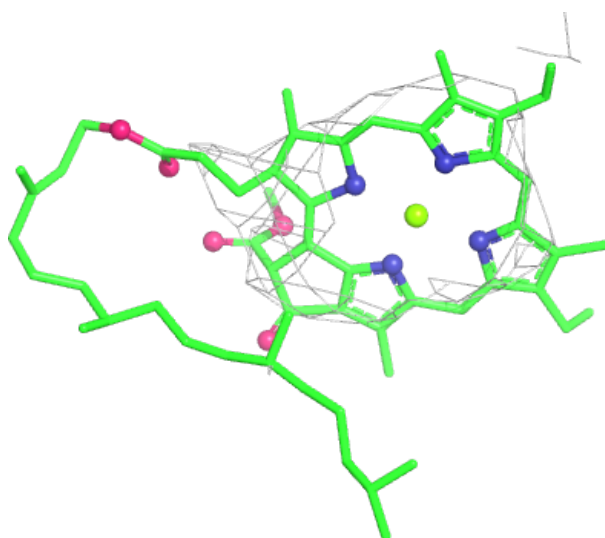
Electron density around DGD C 517:

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



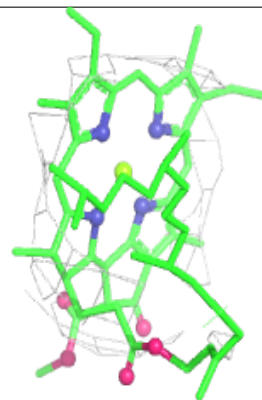
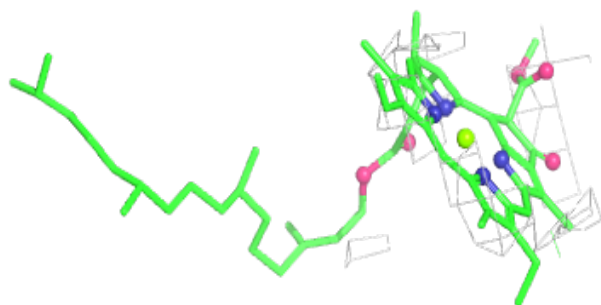
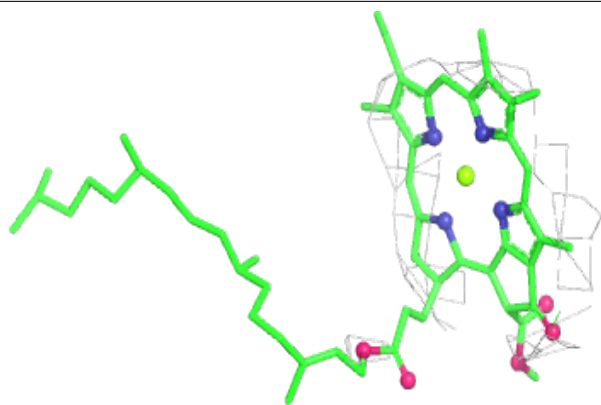
Electron density around CLA C 509:

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



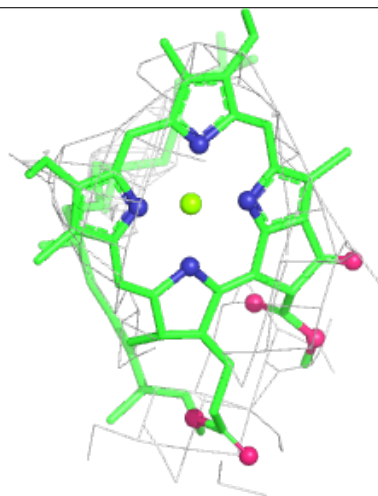
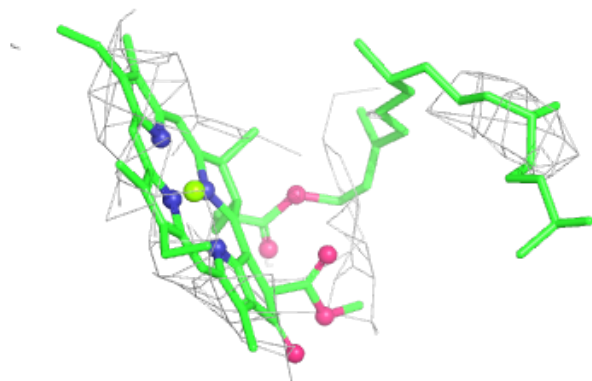
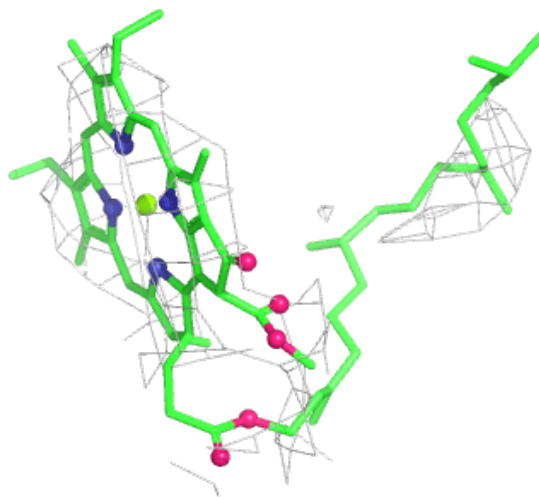
Electron density around CLA c 512:

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



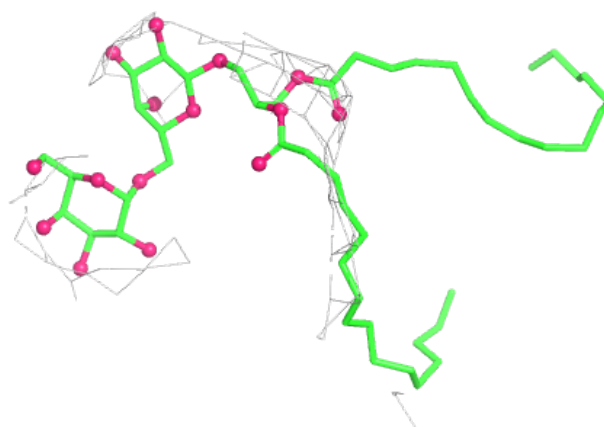
Electron density around CLA b 616:

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

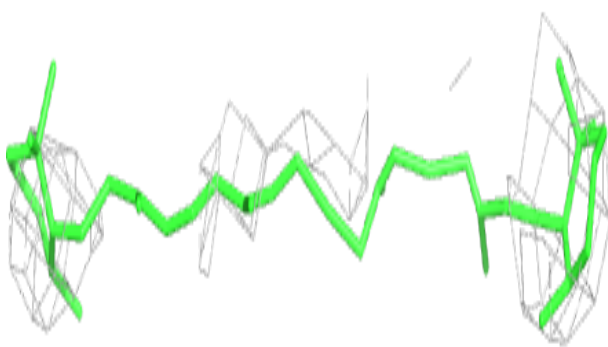
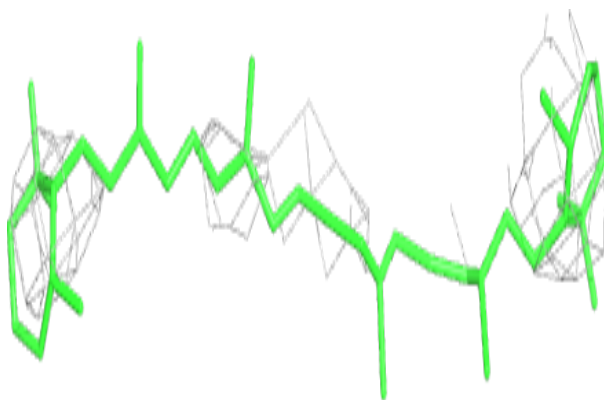


Electron density around DGD c 518:

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

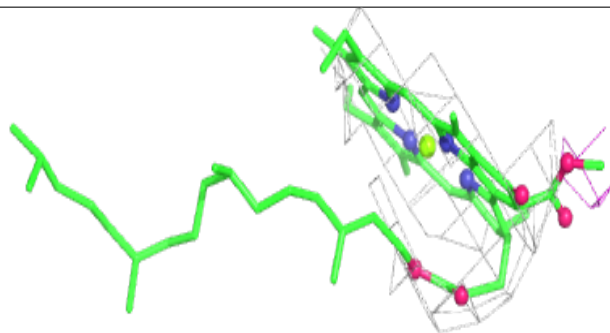
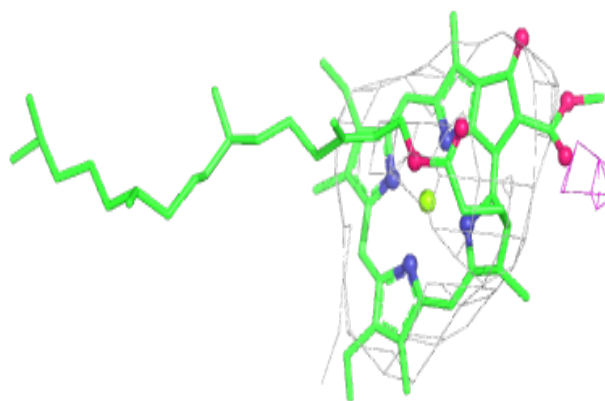
**Electron density around BCR B 619:**

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

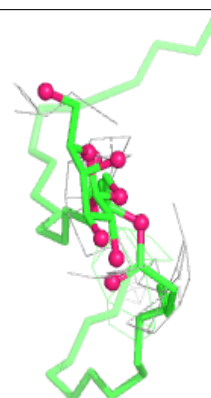
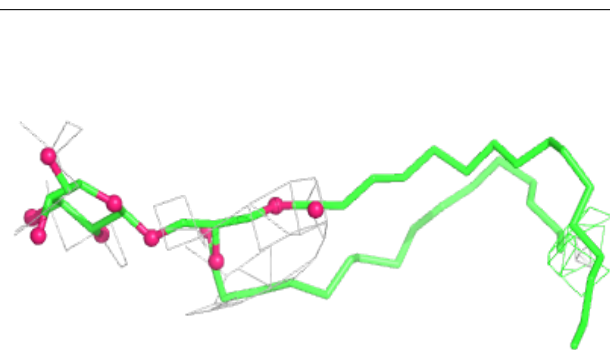
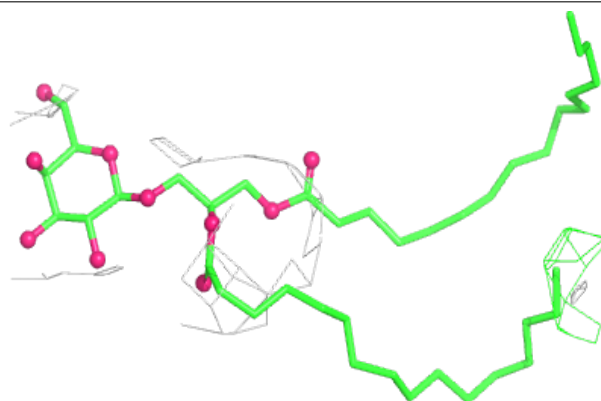


Electron density around CLA B 615:

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

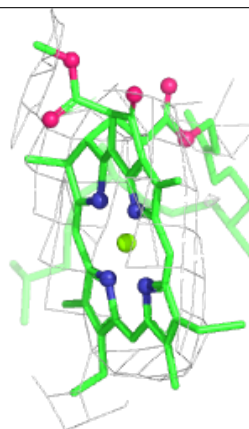
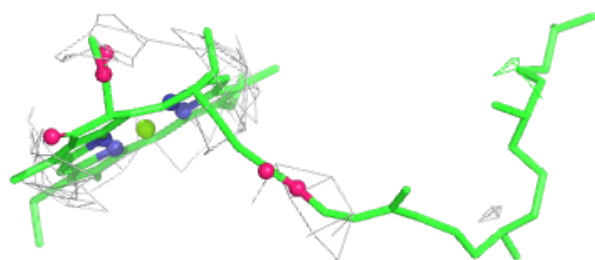
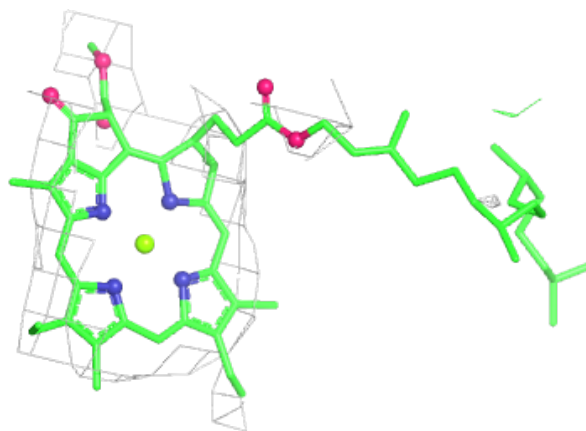
**Electron density around LMG j 101:**

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

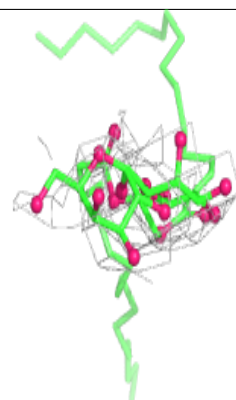
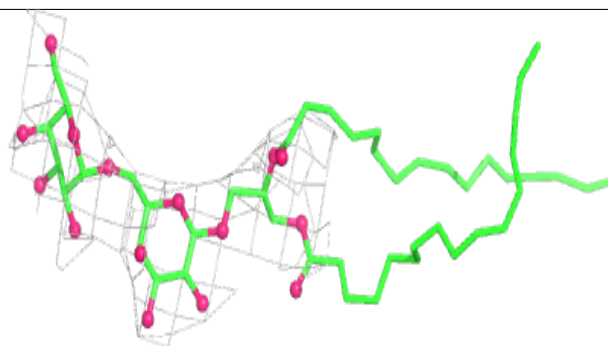
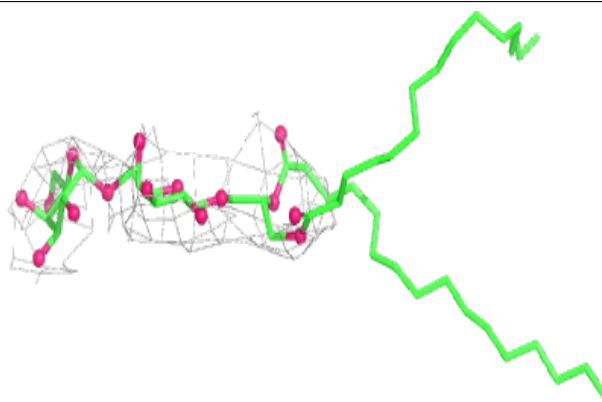


Electron density around CLA A 608:

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

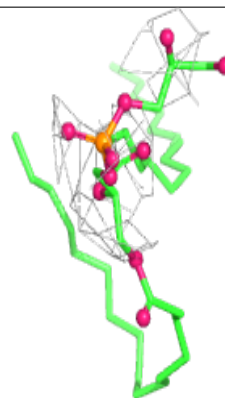
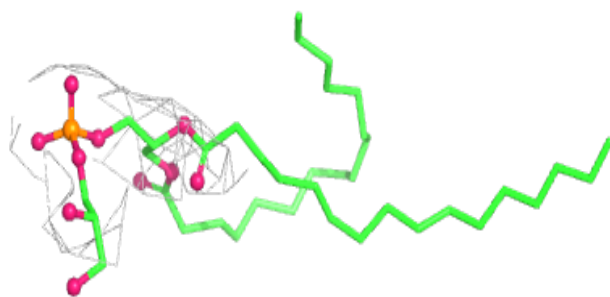
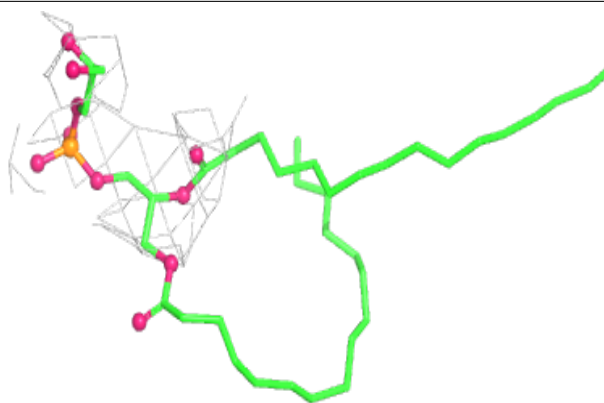
**Electron density around DGD C 516:**

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

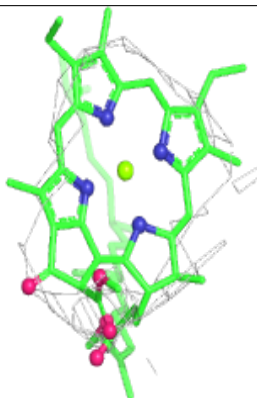
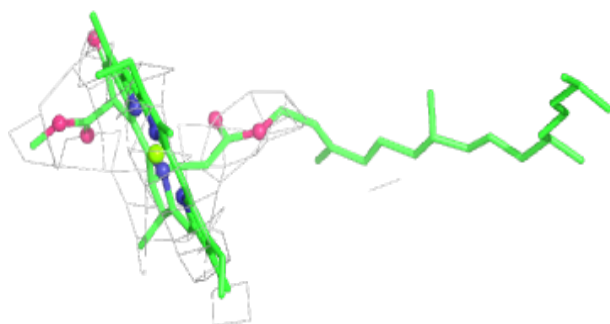


Electron density around LHG B 622:

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

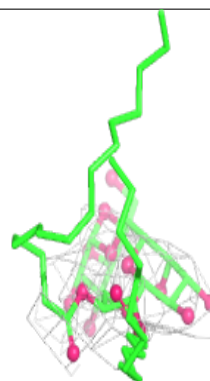
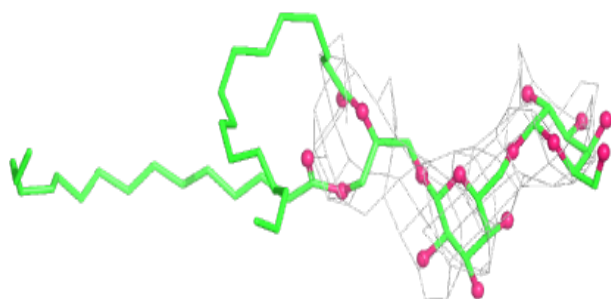
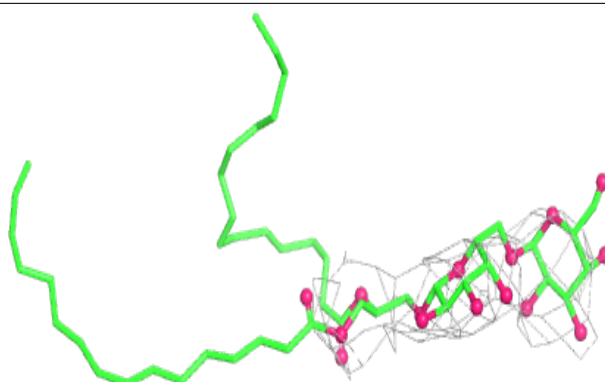
**Electron density around CLA B 610:**

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

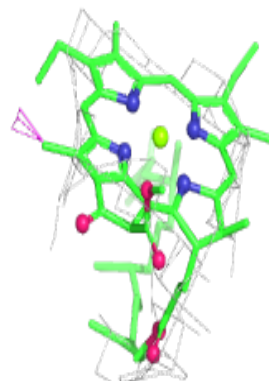
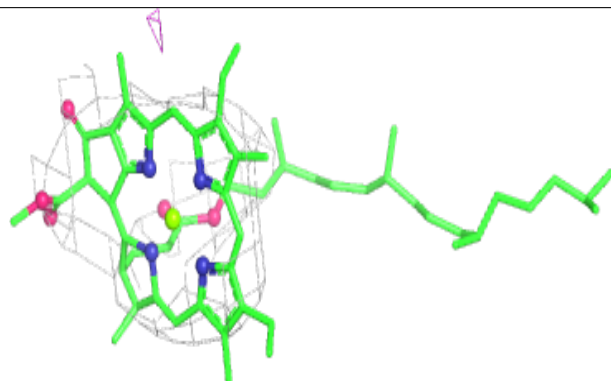
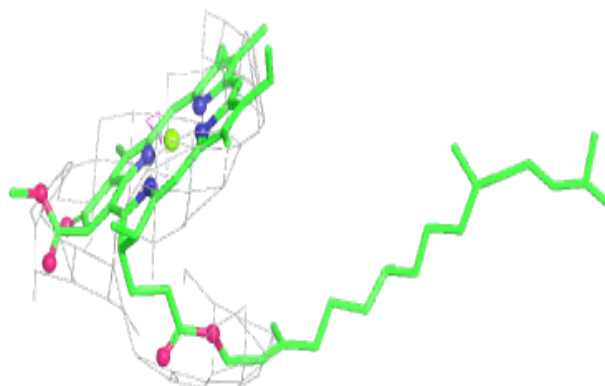


Electron density around DGD H 102:

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

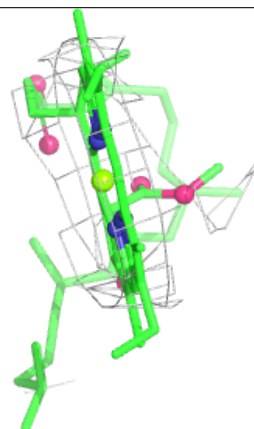
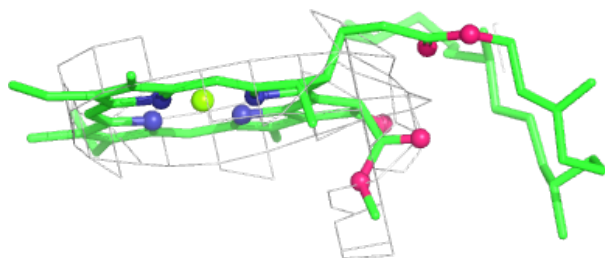
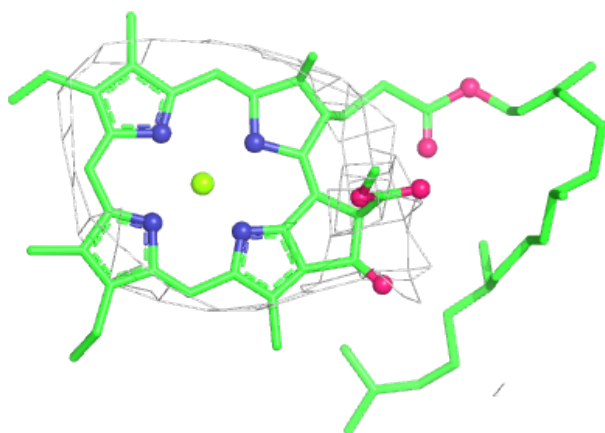
**Electron density around CLA C 504:**

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

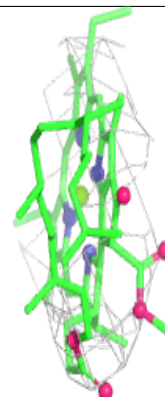
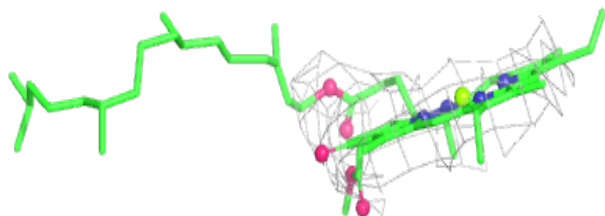
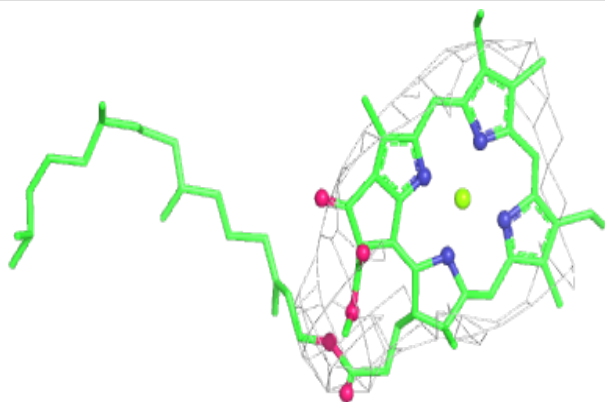


Electron density around CLA B 611:

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

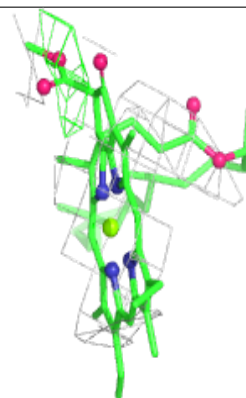
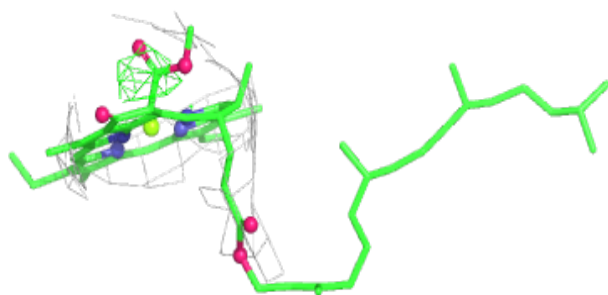
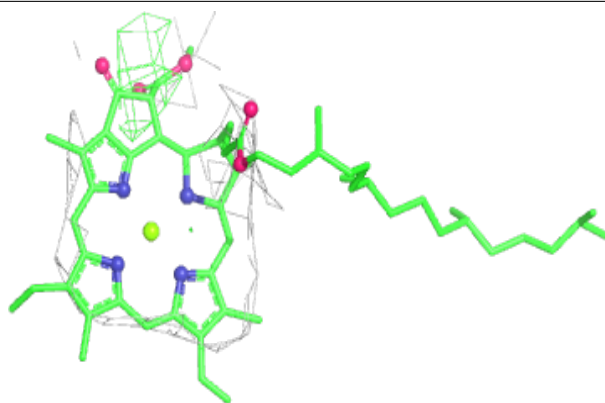
**Electron density around CLA b 605:**

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

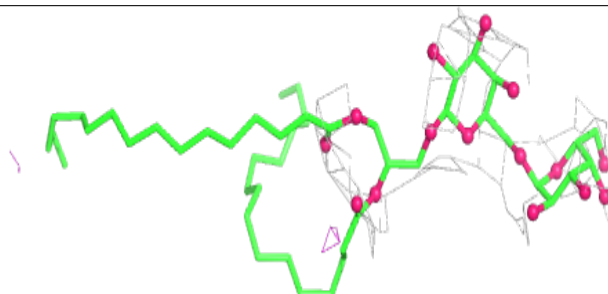
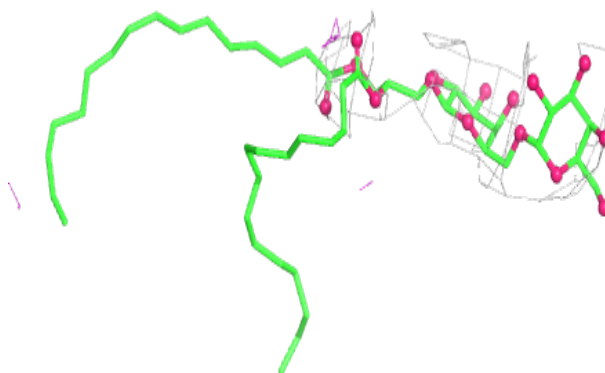


Electron density around CLA A 606:

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

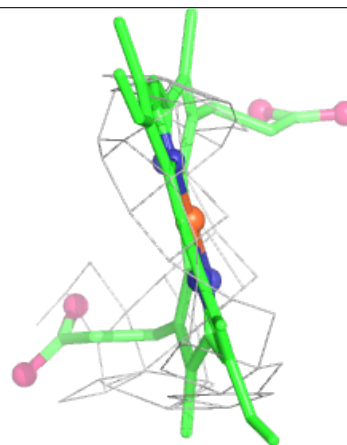
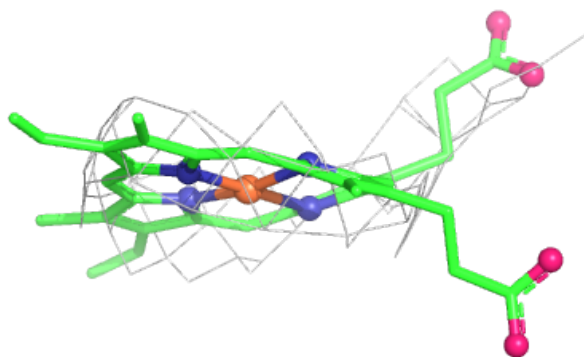
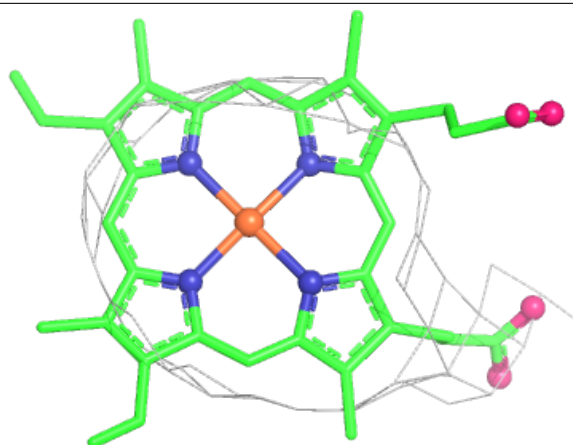
**Electron density around DGD h 102:**

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

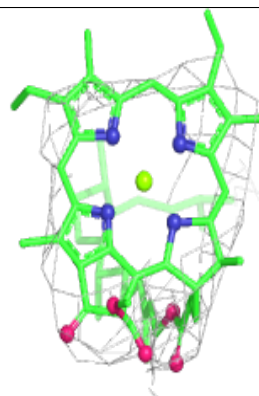
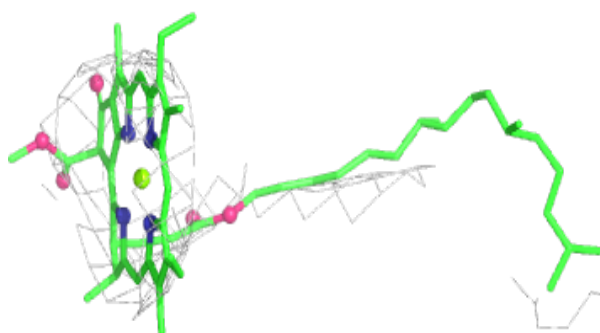
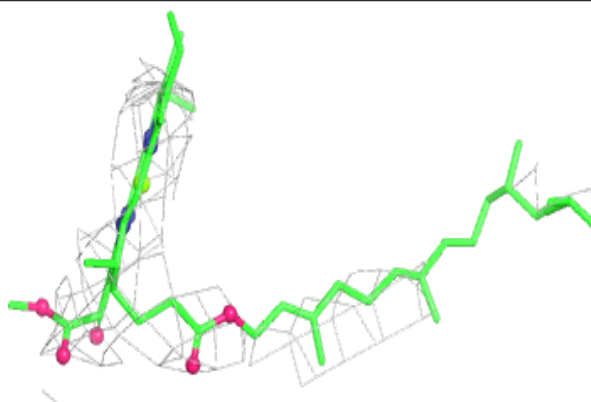


Electron density around HEM e 102:

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

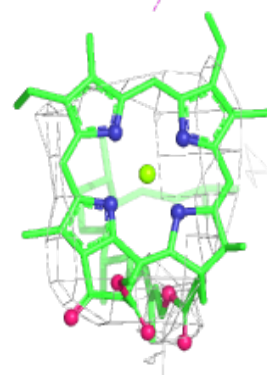
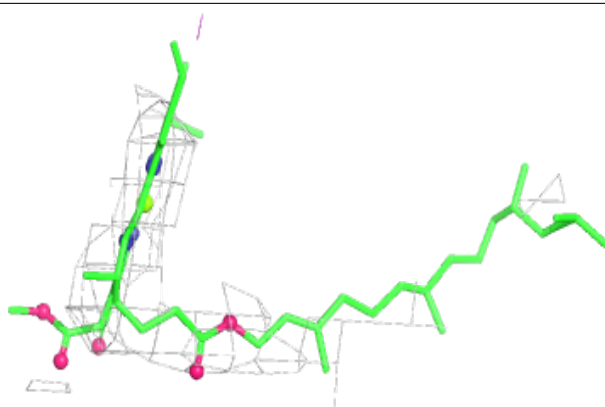
**Electron density around CLA b 608:**

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

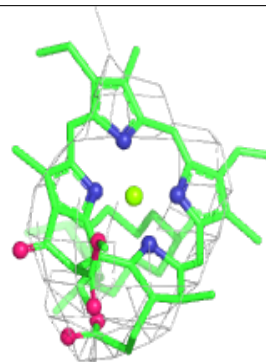
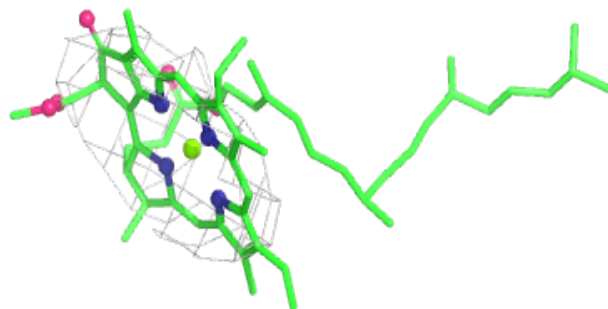
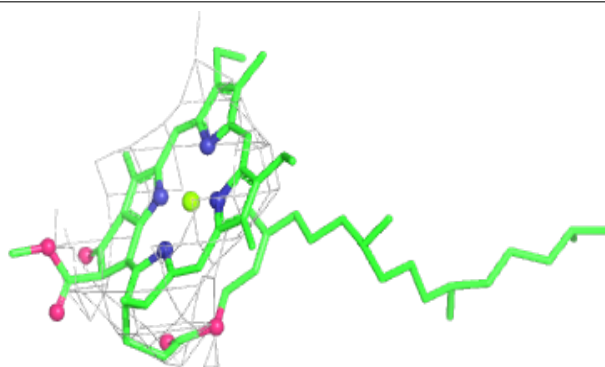


Electron density around CLA B 606:

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

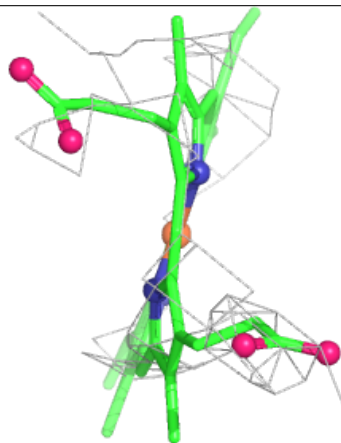
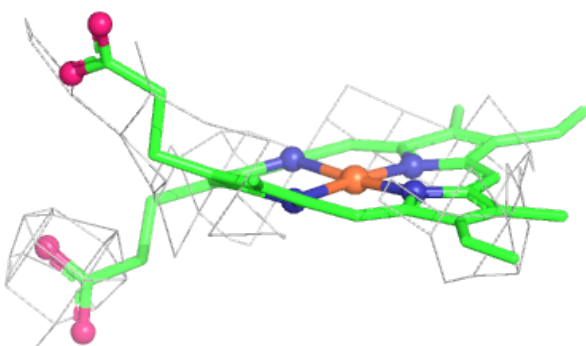
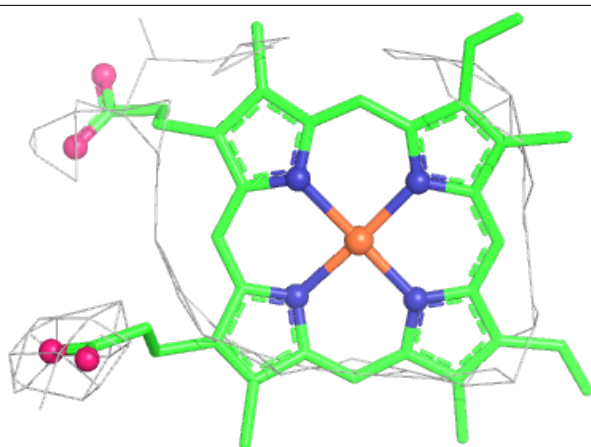
**Electron density around CLA c 506:**

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

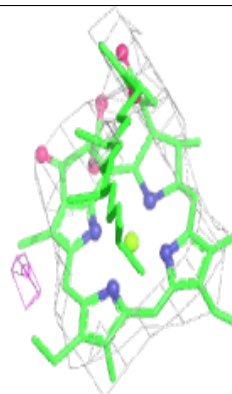
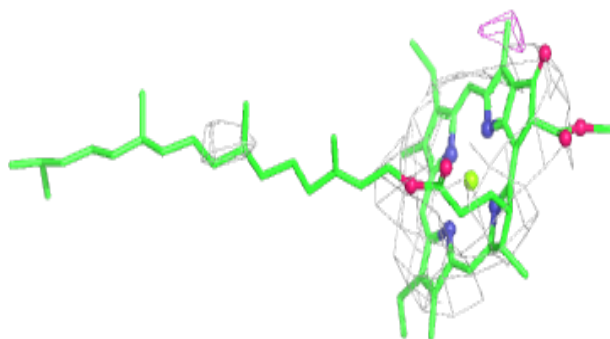
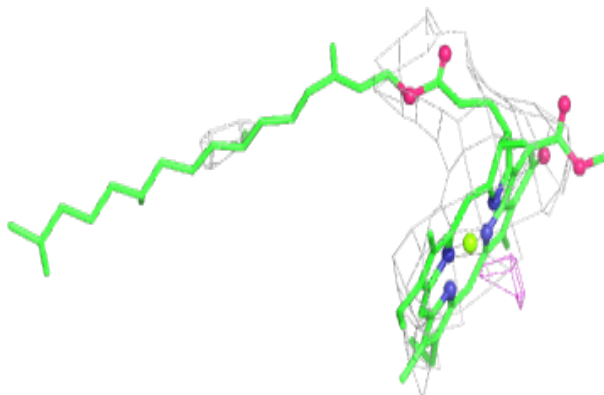


Electron density around HEM E 102:

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

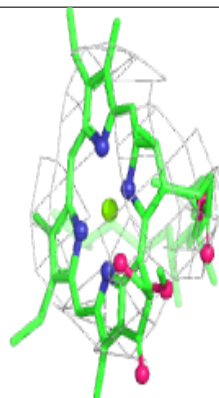
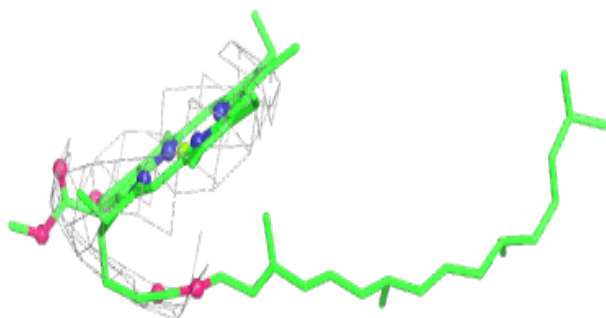
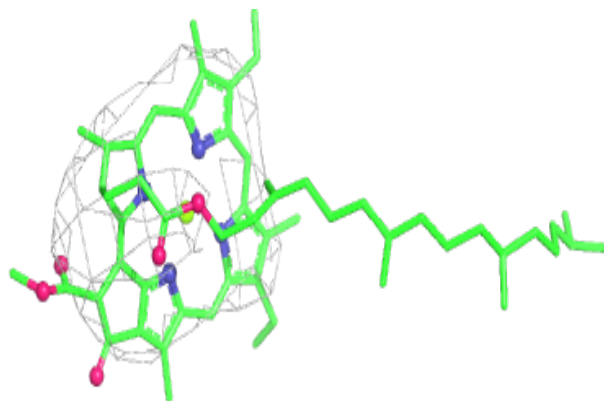
**Electron density around CLA b 610:**

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

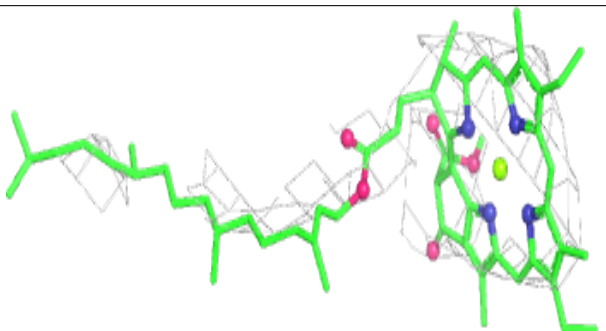
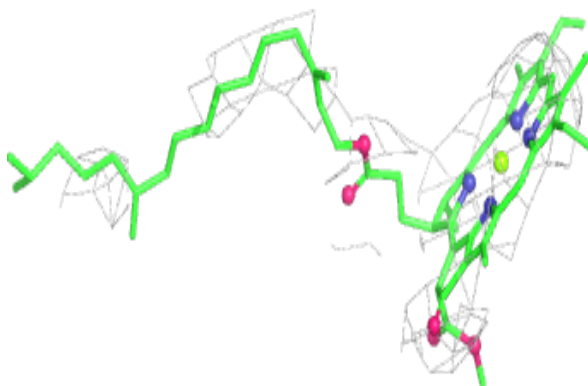


Electron density around CLA b 611:

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

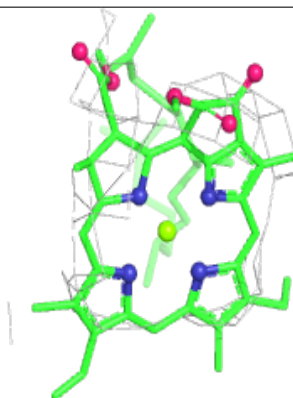
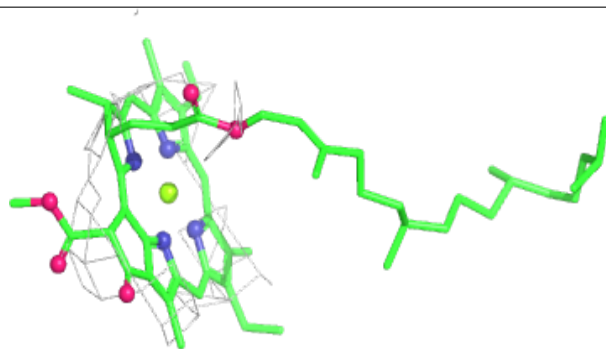
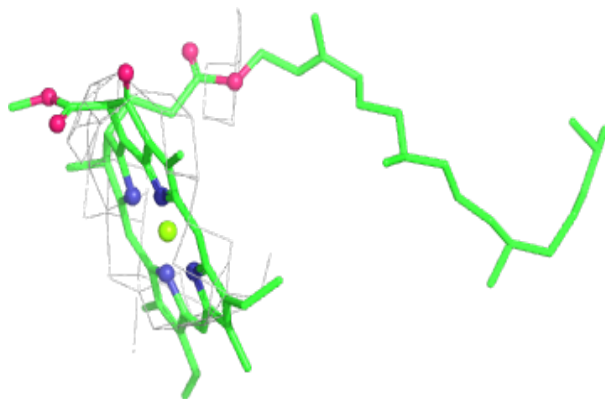
**Electron density around CLA C 502:**

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



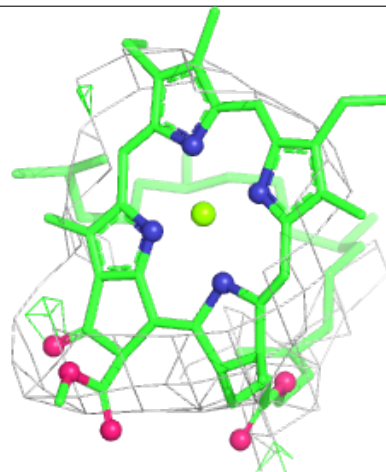
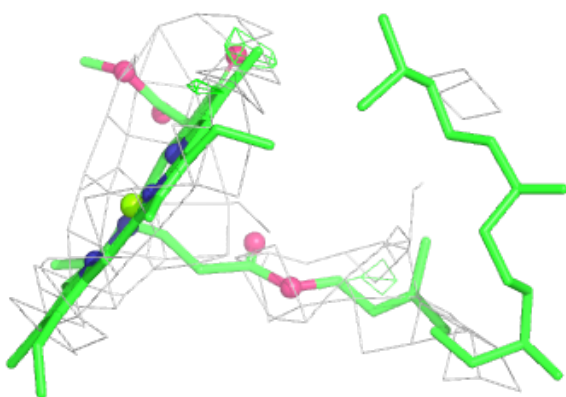
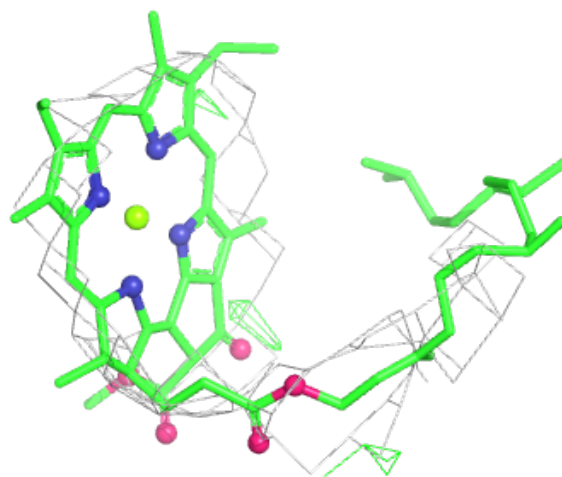
Electron density around CLA c 509:

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



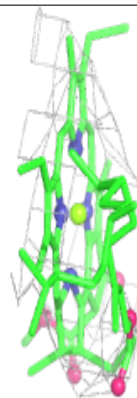
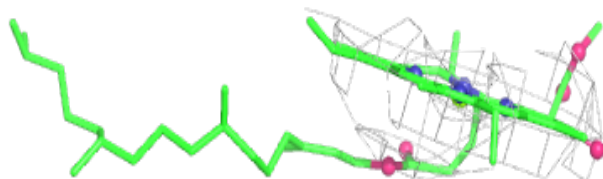
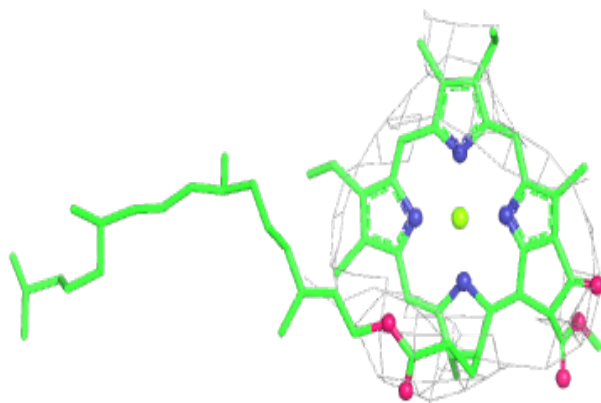
Electron density around CLA C 503:

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

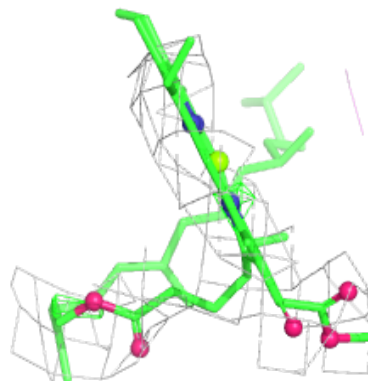
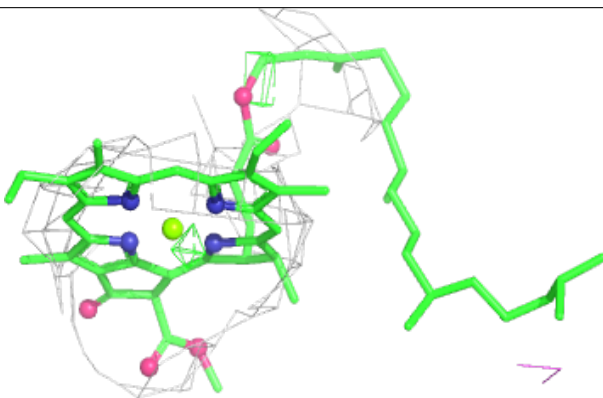
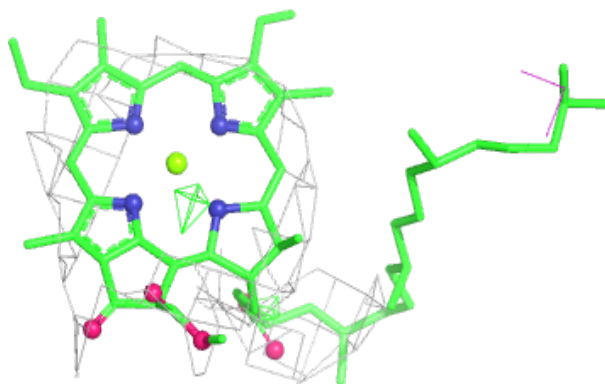


Electron density around CLA B 604:

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

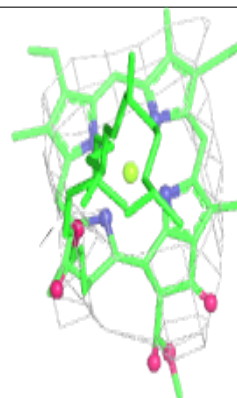
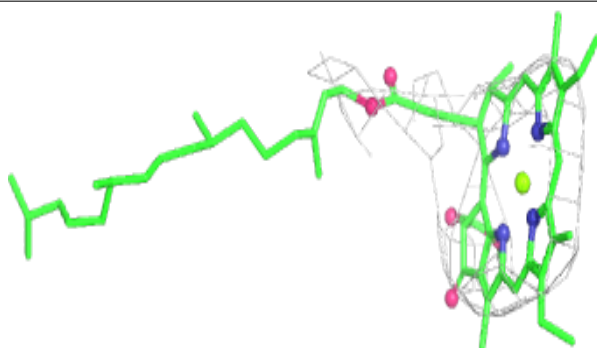
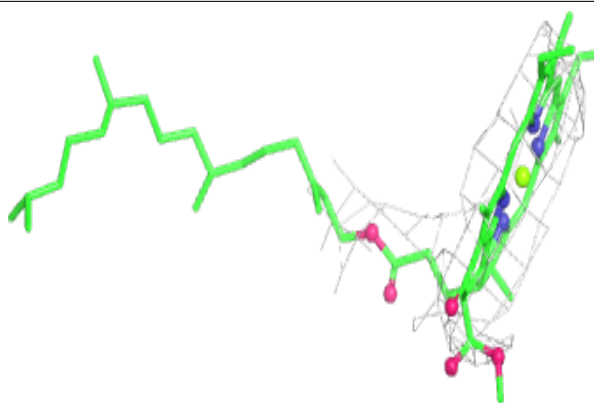
**Electron density around CLA a 613:**

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

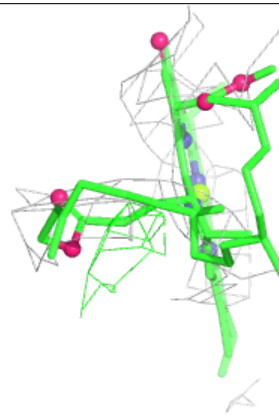
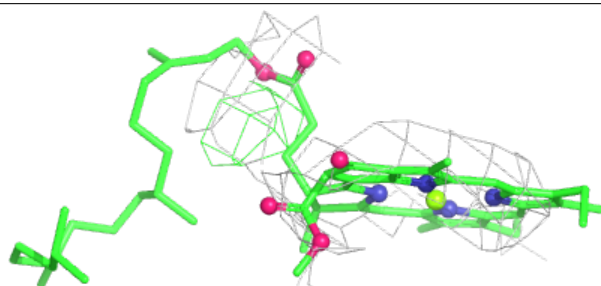
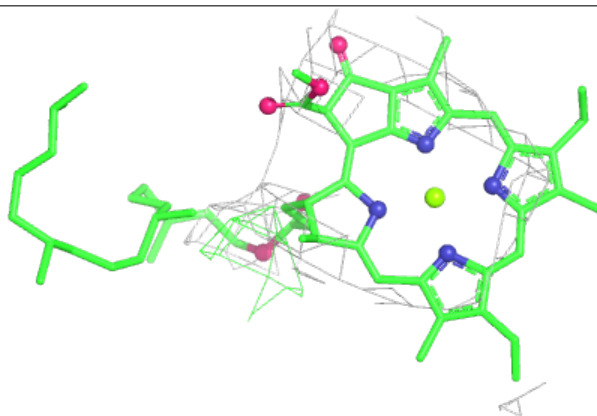


Electron density around CLA B 605:

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

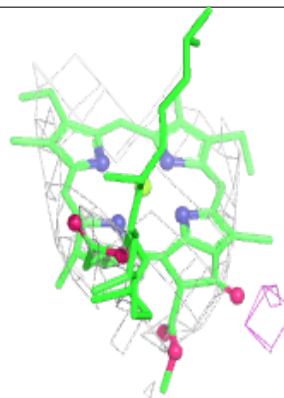
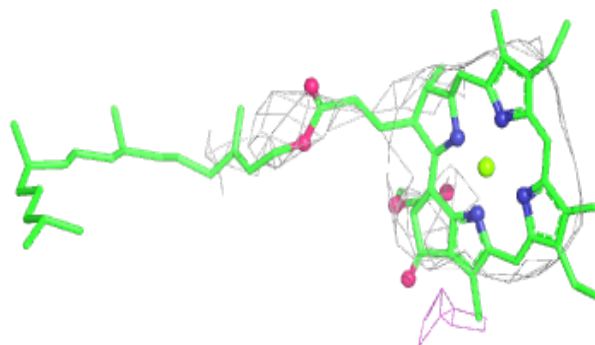
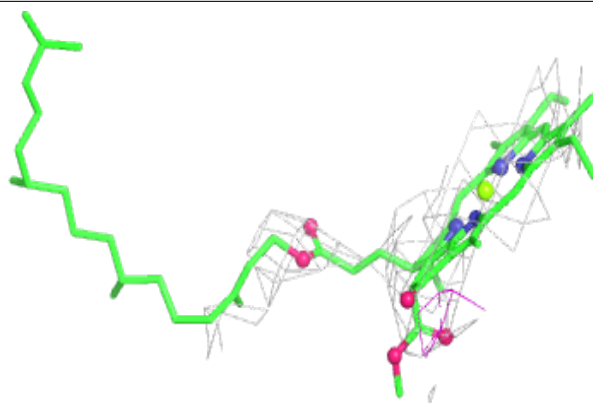
**Electron density around CLA B 613:**

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



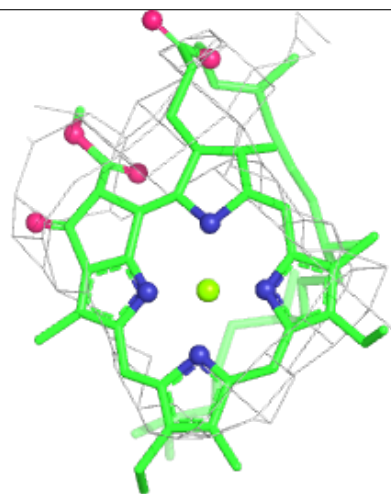
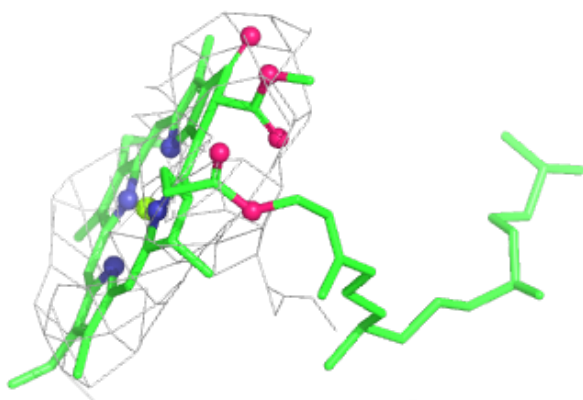
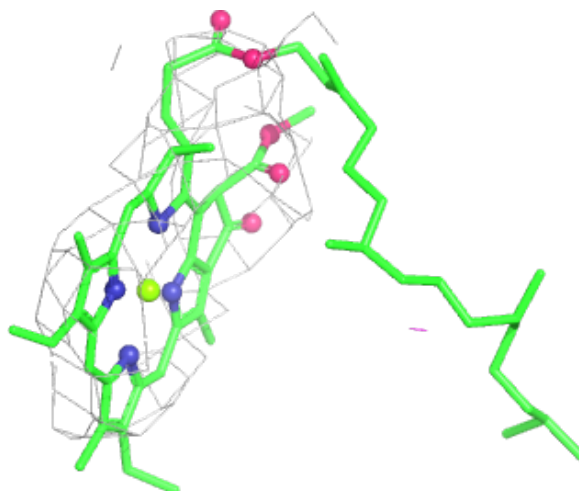
Electron density around CLA D 403:

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



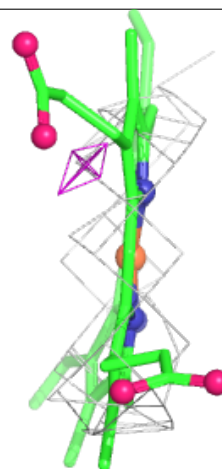
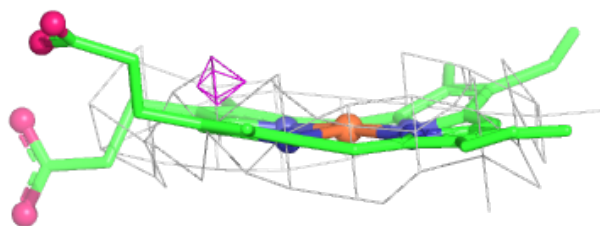
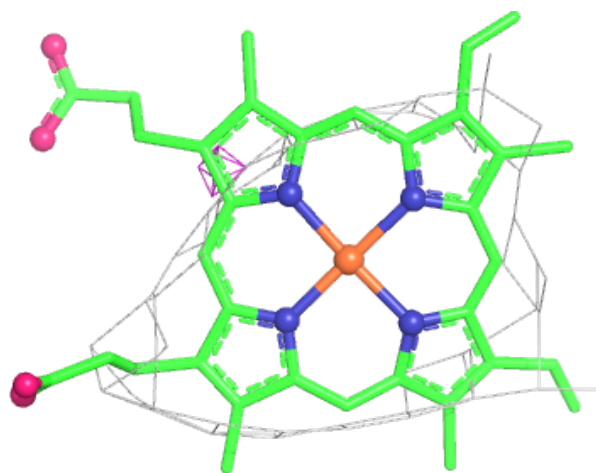
Electron density around CLA B 614:

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



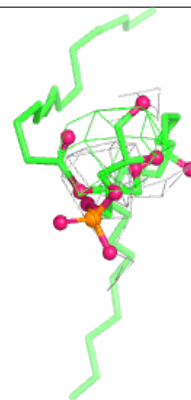
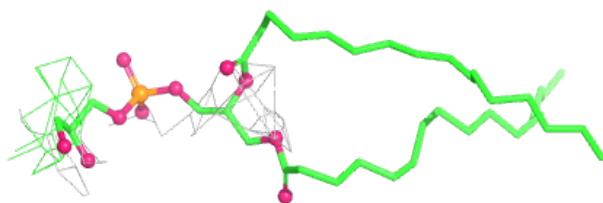
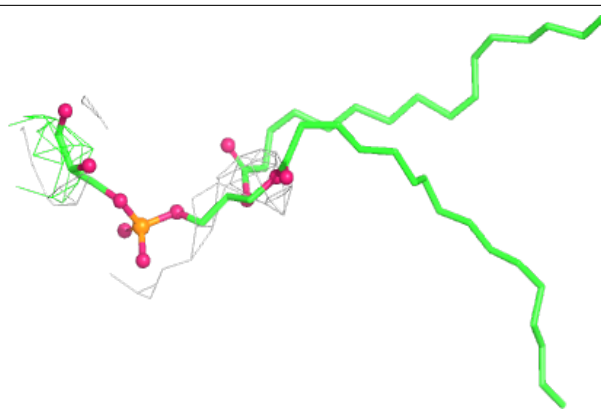
Electron density around HEM v 201:

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

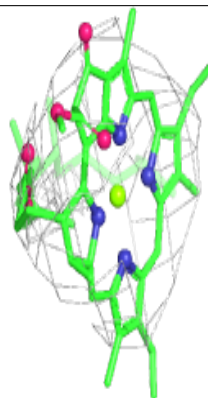
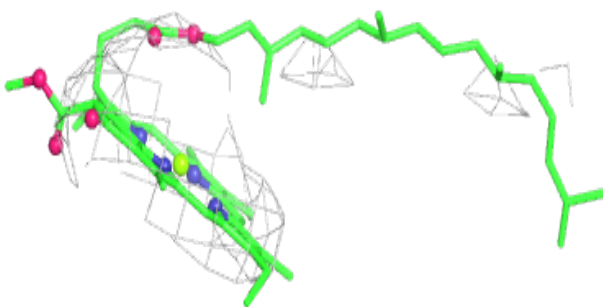
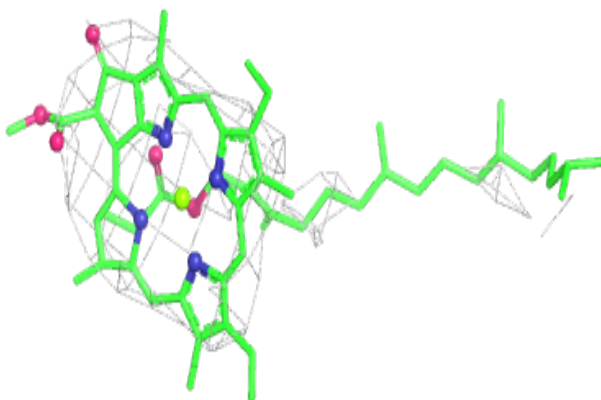


Electron density around LHG D 407:

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

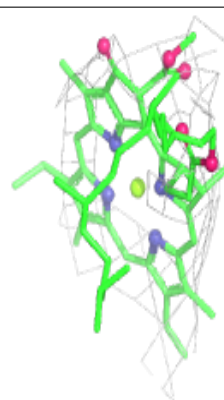
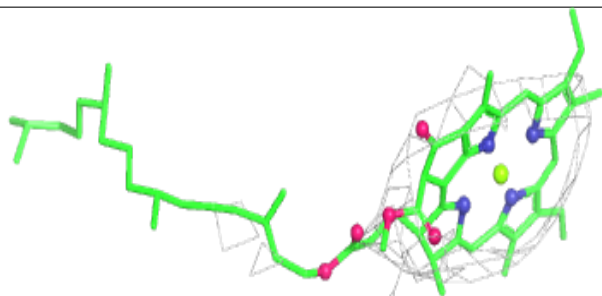
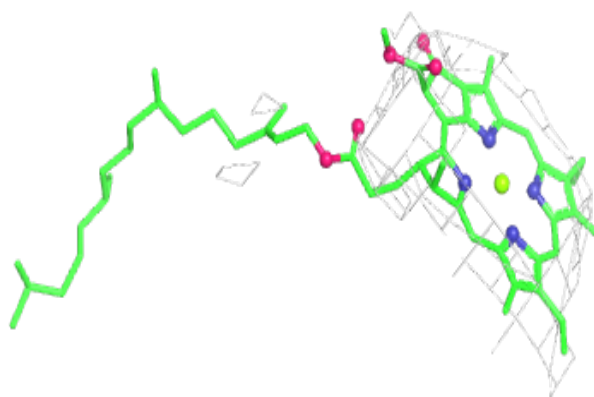
**Electron density around CLA B 609:**

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

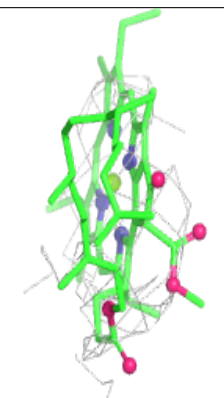
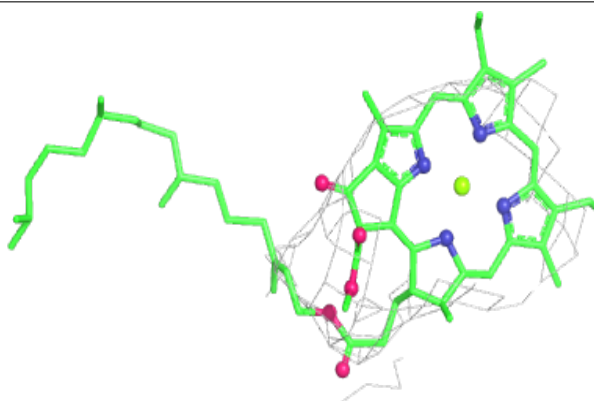


Electron density around CLA A 605:

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

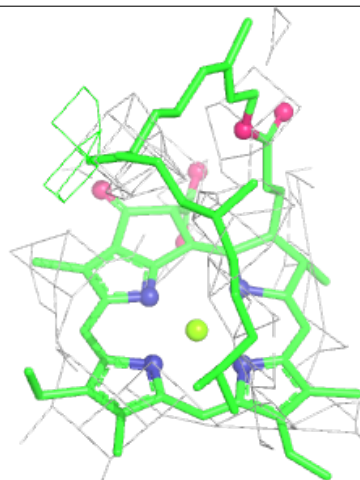
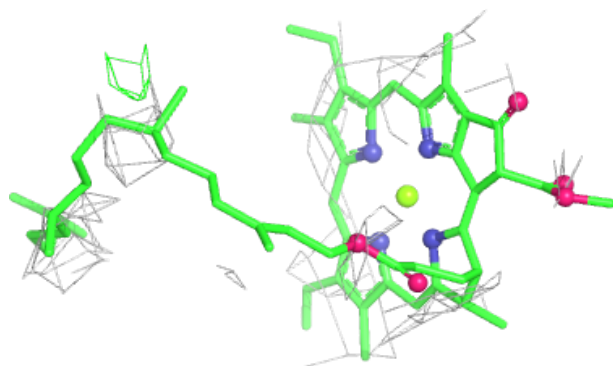
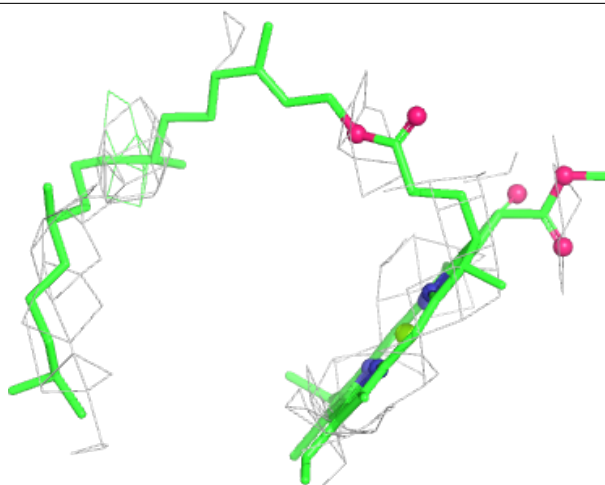
**Electron density around CLA B 603:**

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



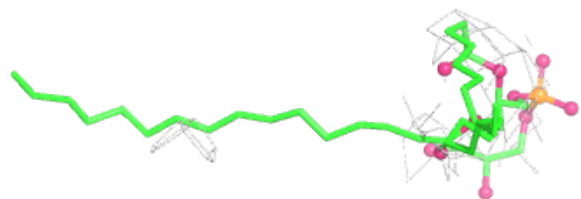
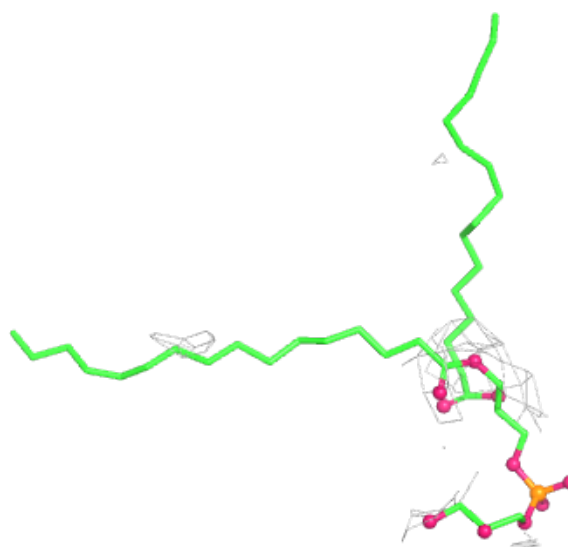
Electron density around CLA b 614:

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



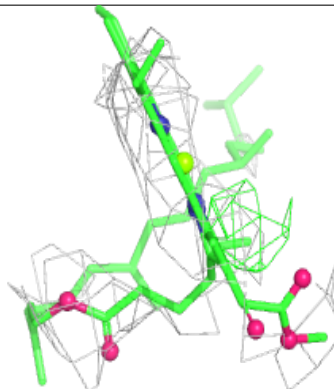
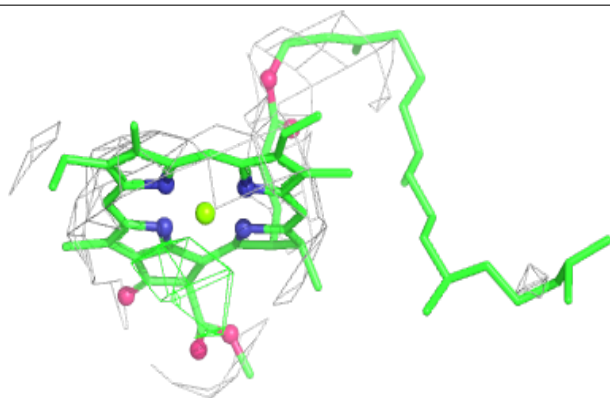
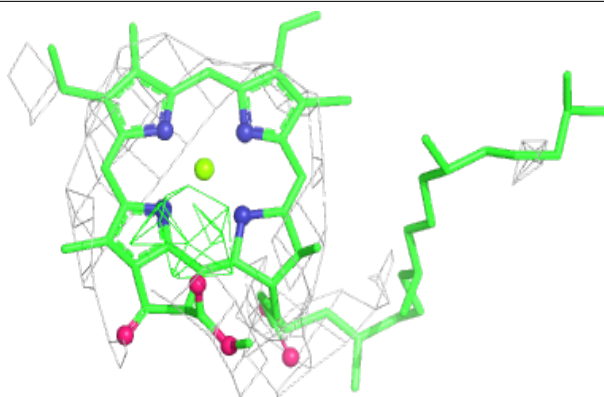
Electron density around LHG L 101:

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

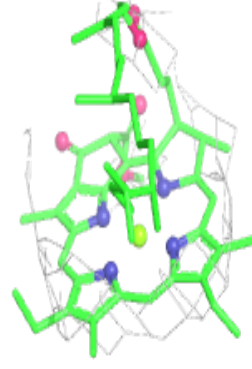
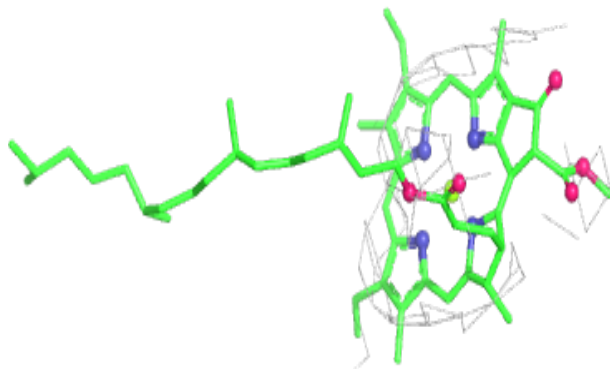
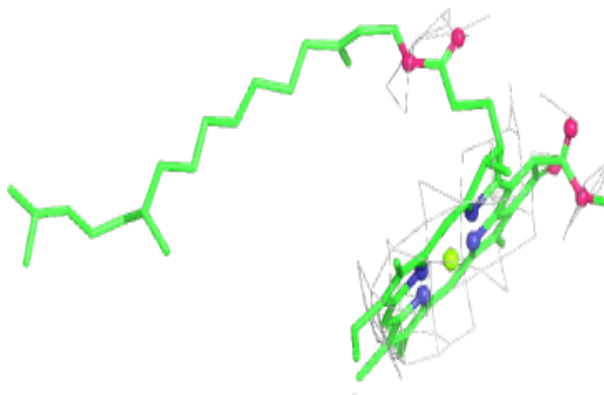


Electron density around CLA D 402:

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

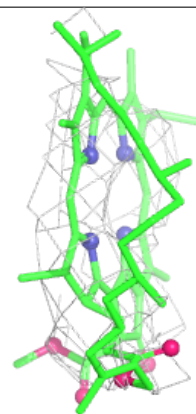
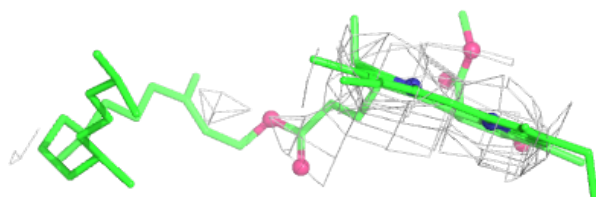
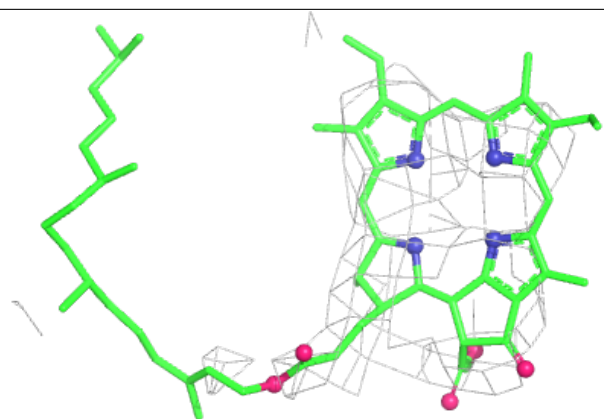
**Electron density around CLA c 505:**

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



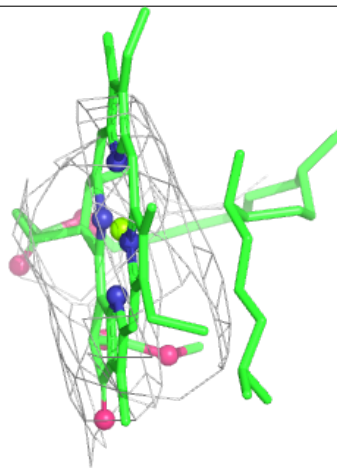
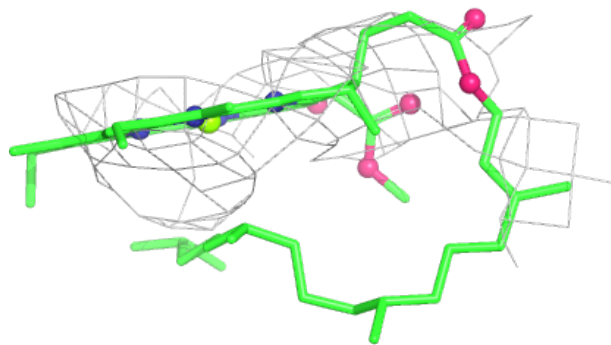
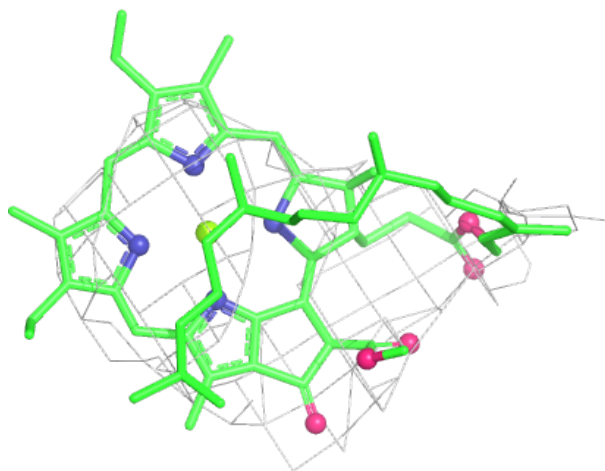
Electron density around PHO A 607:

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



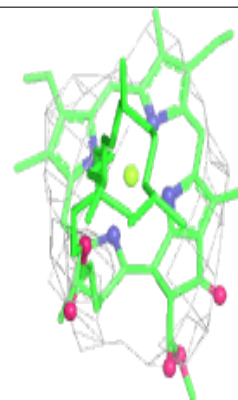
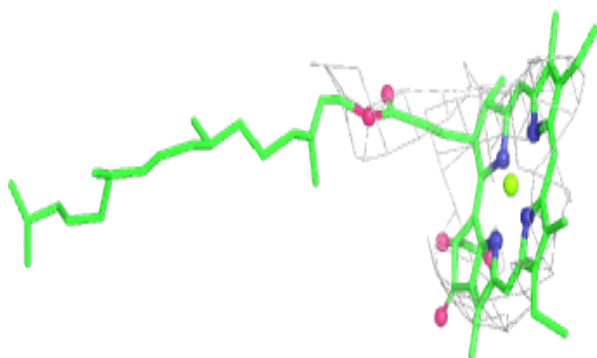
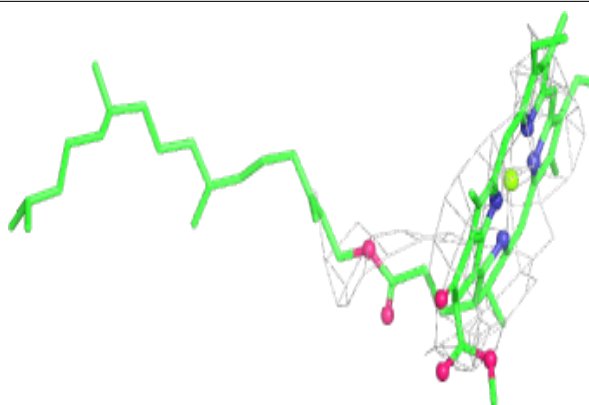
Electron density around CLA c 511:

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



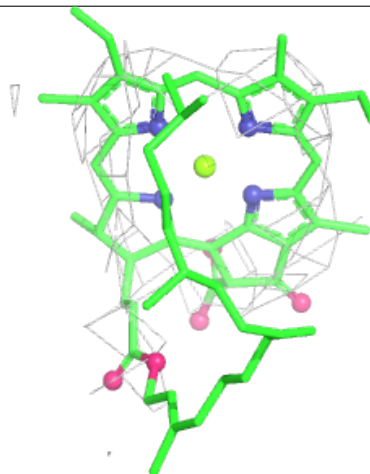
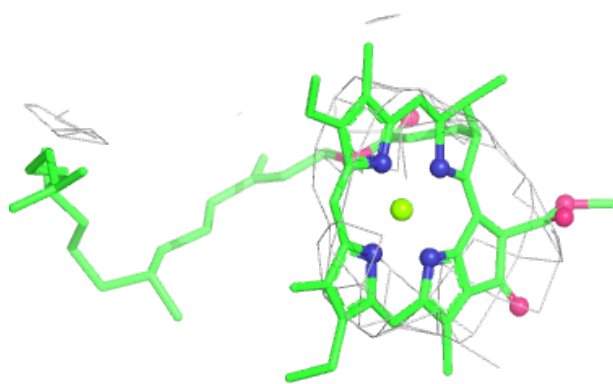
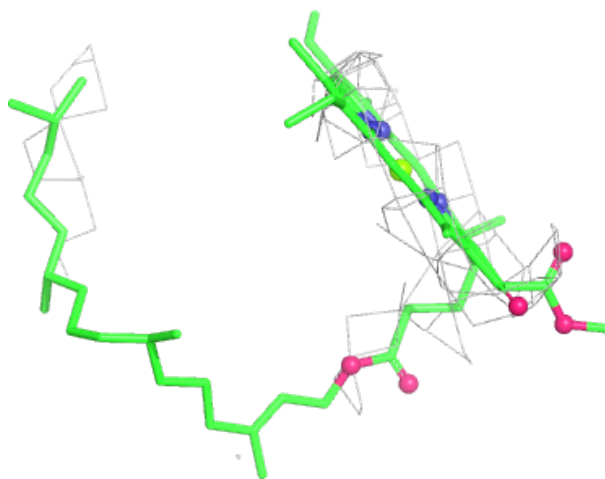
Electron density around CLA b 607:

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



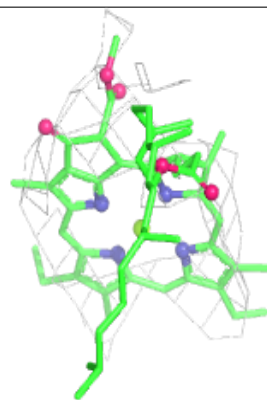
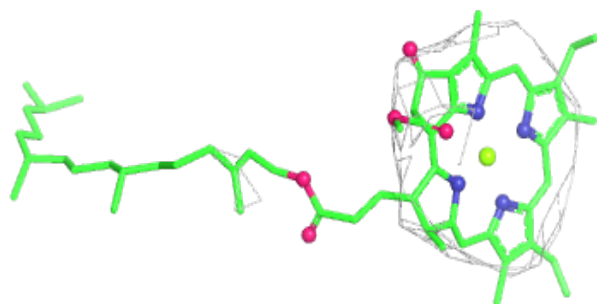
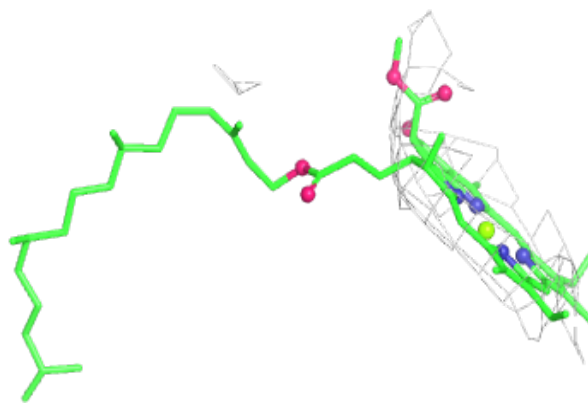
Electron density around CLA B 612:

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



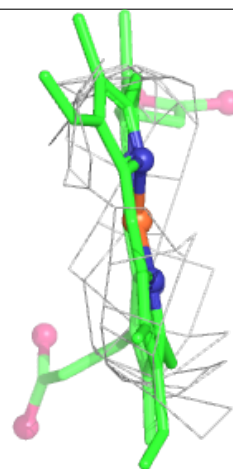
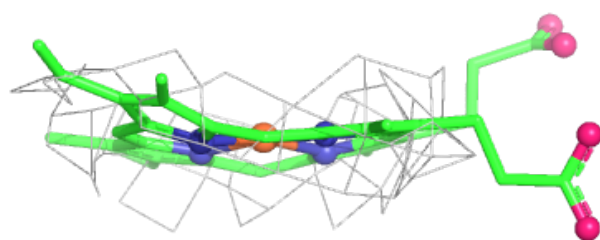
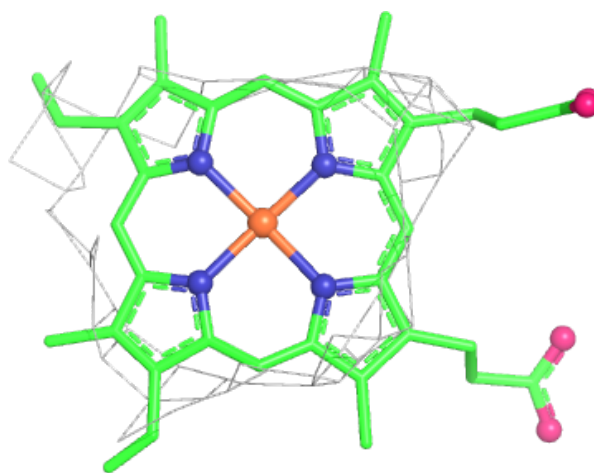
Electron density around CLA d 402:

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



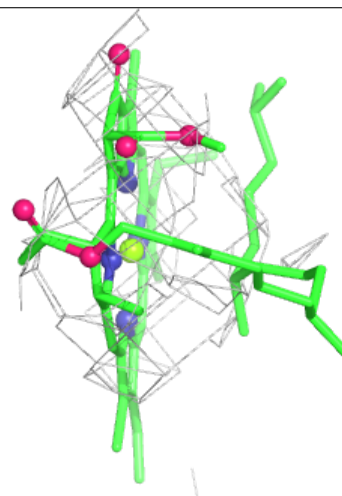
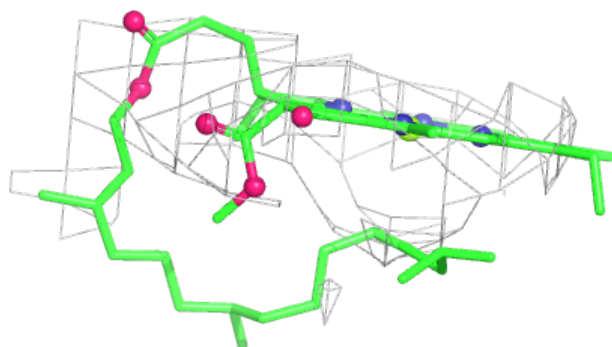
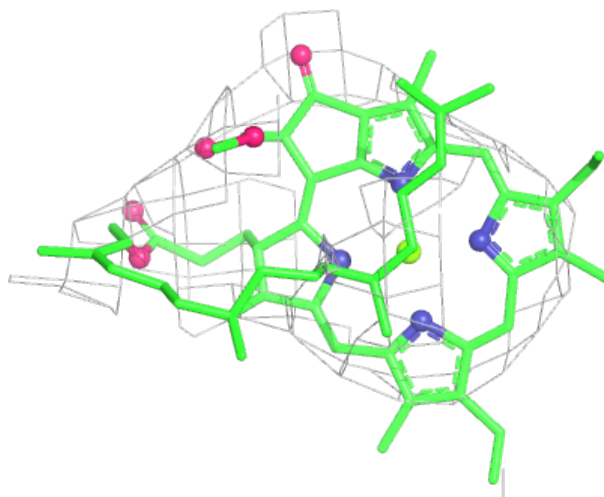
Electron density around HEM V 202:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.