



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 13, 2026 – 02:58 PM JST

PDB ID : 9LP8 / pdb_00009lp8
Title : Extrinsic-protein reconstituted PSII of Thermosynechococcus vulcanus NIES-2134
Authors : Nakajima, Y.; Kato, K.; Shen, J.R.; Nagao, R.
Deposited on : 2025-01-24
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

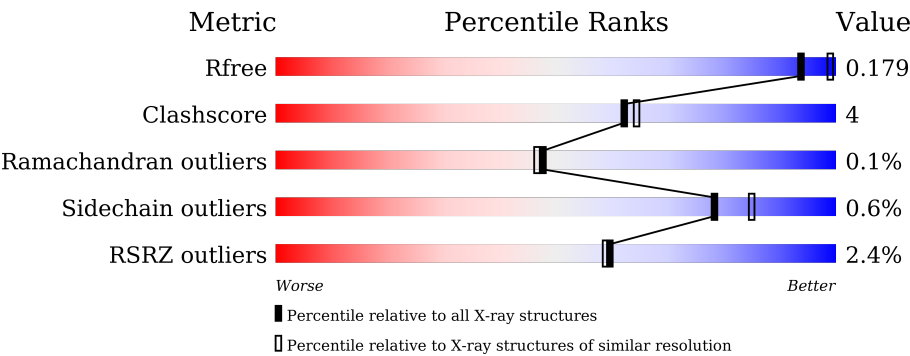
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.00 Å.

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



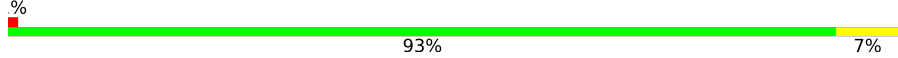
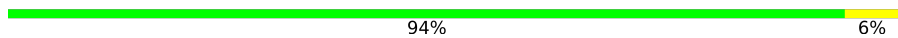
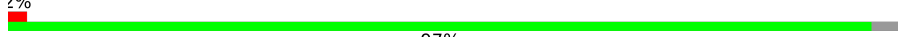
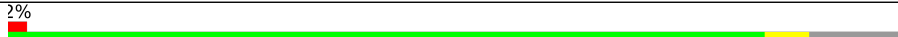
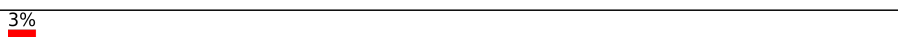
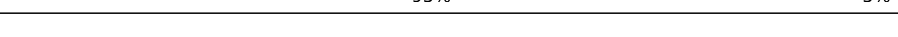
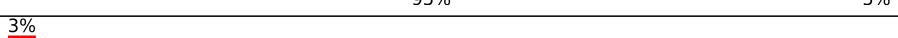
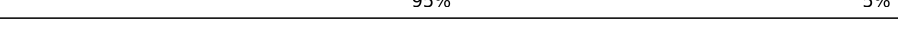
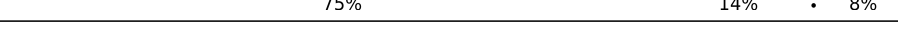
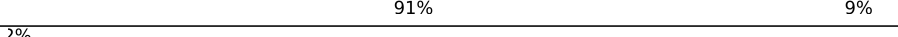
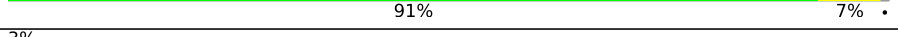
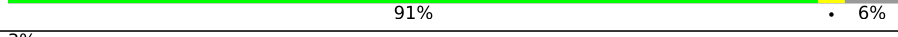
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	360	2% 86% 6% 7%
1	a	360	3% 88% 5% 7%
2	B	505	2% 94% 5%
2	b	505	3% 94% 5%
3	C	473	% 88% 7% 5%
3	c	473	% 90% 7%

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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	163	

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Mol	Chain	Length	Quality of chain
16	v	163	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	34	

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 54054 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2620	1719	429	457	15			
1	a	334	Total	C	N	O	S	0	3	0
			2615	1716	428	456	15			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	8	0
			3991	2621	664	693	13			
2	b	501	Total	C	N	O	S	0	11	0
			3959	2603	656	687	13			

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	2	0
			3488	2284	583	608	13			
3	c	455	Total	C	N	O	S	0	4	0
			3536	2315	593	615	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2726	1809	443	462	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	341	Total	C	N	O	S	0	3	0
			2733	1812	446	463	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O		0	0	0
			657	429	106	122				
5	e	79	Total	C	N	O		0	0	0
			627	413	97	117				

- 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
			274	187	45	41	1			
6	f	32	Total	C	N	O	S	0	0	0
			255	173	43	38	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			291	198	45	47	1			
8	i	38	Total	C	N	O	S	0	0	0
			311	210	48	52	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	39	Total	C	N	O	S	0	0	0
			267	180	40	46	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	1	0
			287	201	42	44			
10	k	37	Total	C	N	O	0	0	0
			283	197	42	44			

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	1	0
			296	200	45	51			
11	l	37	Total	C	N	O	0	2	0
			300	204	45	51			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			261	176	37	47	1			
12	m	34	Total	C	N	O	S	0	2	0
			275	187	39	48	1			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 13 is a protein called Photosystem II extrinsic protein O.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	5	0
			1865	1170	310	380	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	o	241	Total	C	N	O	S	0	5	0
			1837	1154	302	375	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	1	0
			265	185	37	41	2			

- Molecule 15 is a protein called Photosystem II extrinsic protein U.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	S	0	0	0
			766	486	128	152				
15	u	97	Total	C	N	O	S	0	1	0
			769	489	129	151				

- Molecule 16 is a protein called Photosystem II extrinsic protein V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1057	672	178	203	4			
16	v	137	Total	C	N	O	S	0	1	0
			1050	667	176	203	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			193	127	32	31	3			
17	y	28	Total	C	N	O	S	0	0	0
			196	128	33	32	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	S	0	1	0
			280	190	44	46				
18	x	38	Total	C	N	O	S	0	1	0
			280	190	44	46				

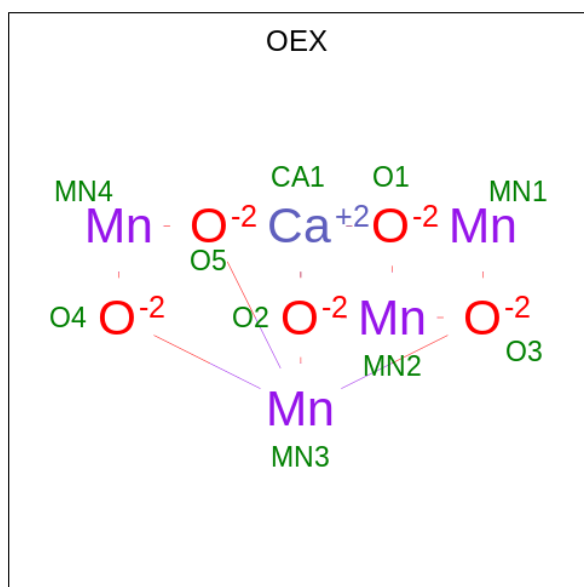
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			452	313	66	72	1			
19	z	60	Total	C	N	O	S	0	0	0
			432	301	64	66	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	30	Total	C	N	O	0	0	0
			162	99	33	30			

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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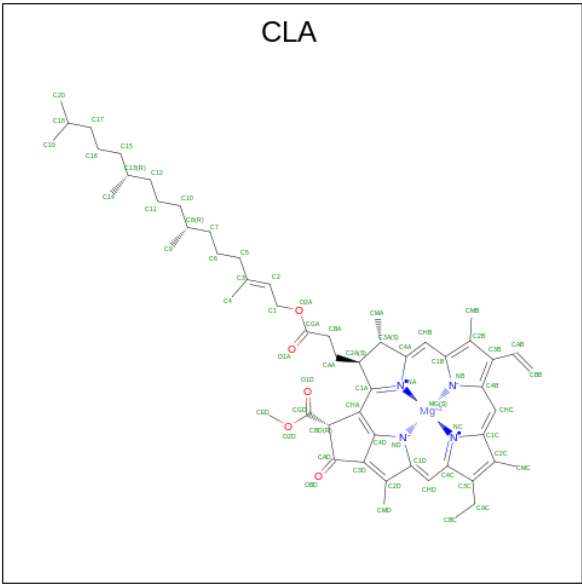
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	1	Total	Fe	0	0
			1	1		

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

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

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



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

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

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

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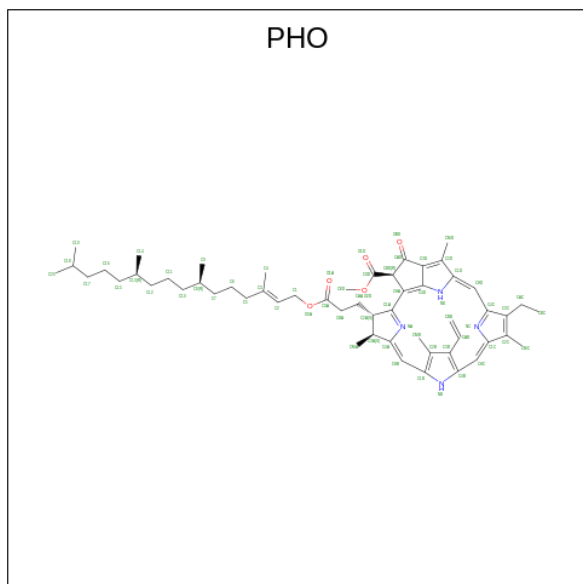
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N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

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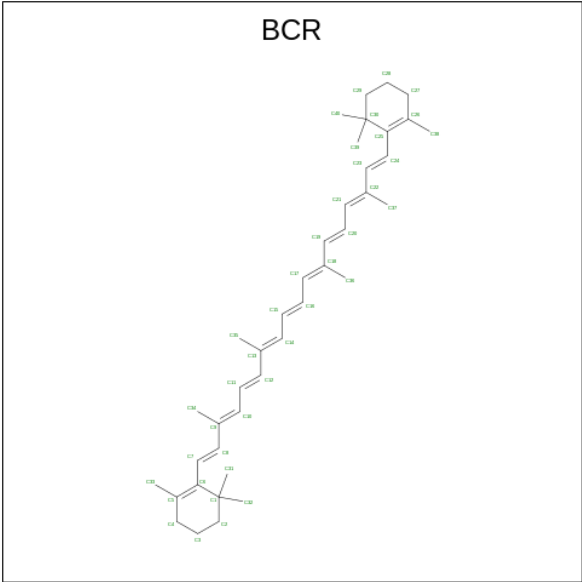
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



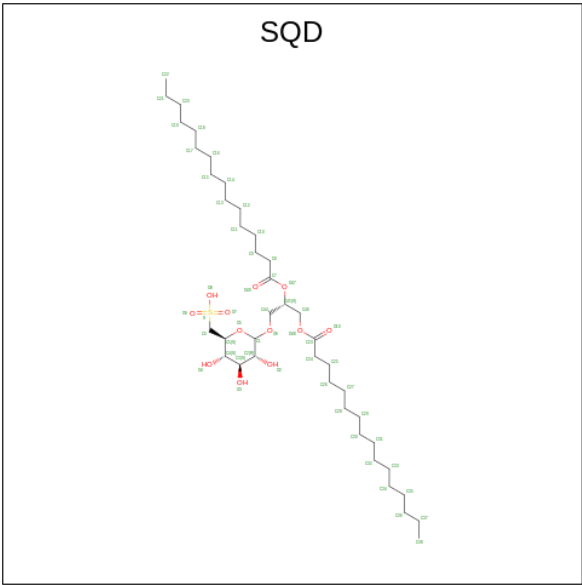
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total C 40 40	0	0
26	a	1	Total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

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

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



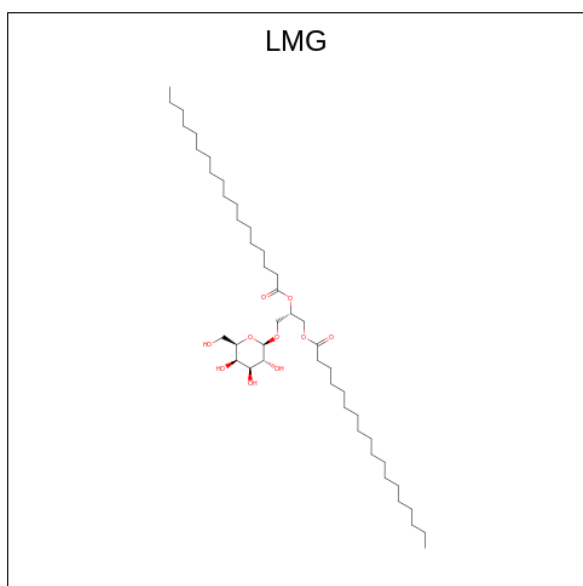
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O S 52 39 12 1	0	0
27	A	1	Total C O S 54 41 12 1	0	0
27	B	1	Total C O S 54 41 12 1	0	0
27	F	1	Total C O S 37 25 11 1	0	0
27	a	1	Total C O S 54 41 12 1	0	0

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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	f	1	Total	C	O	S	0	0
			33	23	9	1		

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



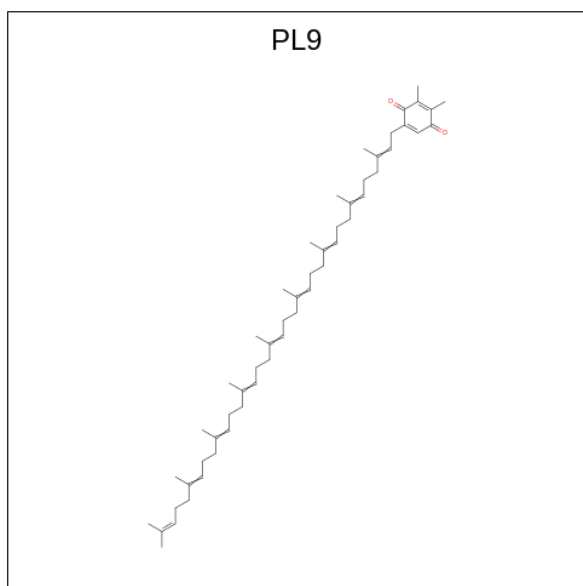
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O		0	0
			51	41	10			
28	B	1	Total	C	O		0	0
			51	41	10			
28	C	1	Total	C	O		0	0
			49	39	10			
28	C	1	Total	C	O		0	0
			51	41	10			
28	D	1	Total	C	O		0	0
			48	38	10			
28	a	1	Total	C	O		0	0
			51	41	10			
28	b	1	Total	C	O		0	0
			51	41	10	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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	c	1	Total	C	O	0	0
			51	41	10		
28	d	1	Total	C	O	0	0
			48	38	10		

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



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

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	3	Total	C	O	0	0
			54	49	5		
30	B	6	Total	C	O	0	0
			78	75	3		

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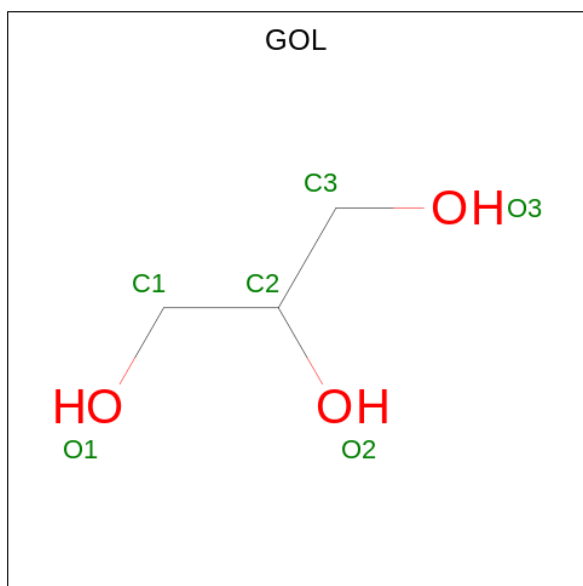
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	C	4	Total C O 66 59 7	0	0
30	D	2	Total C O 53 48 5	0	0
30	E	2	Total C 29 29	0	0
30	H	1	Total C 7 7	0	0
30	I	3	Total C 38 38	0	0
30	J	2	Total C 29 29	0	0
30	M	1	Total C 16 16	0	0
30	T	1	Total C 15 15	0	0
30	Y	1	Total C 10 10	0	0
30	X	1	Total C 16 16	0	0
30	a	3	Total C O 56 51 5	0	0
30	b	5	Total C O 63 59 4	0	0
30	c	5	Total C O 74 65 9	0	0
30	d	3	Total C O 72 63 9	0	0
30	e	1	Total C 15 15	0	0
30	h	1	Total C 7 7	0	0
30	i	4	Total C O 55 53 2	0	0
30	j	2	Total C O 32 30 2	0	0
30	m	1	Total C 13 13	0	0
30	t	1	Total C 12 12	0	0
30	v	1	Total C 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	y	1	Total C 10 10	0	0

- Molecule 31 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	H	1	Total 6	C 3	O 3	0	0
31	L	1	Total 6	C 3	O 3	0	0
31	O	1	Total 6	C 3	O 3	0	0
31	O	1	Total 6	C 3	O 3	0	0
31	O	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	Z	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0

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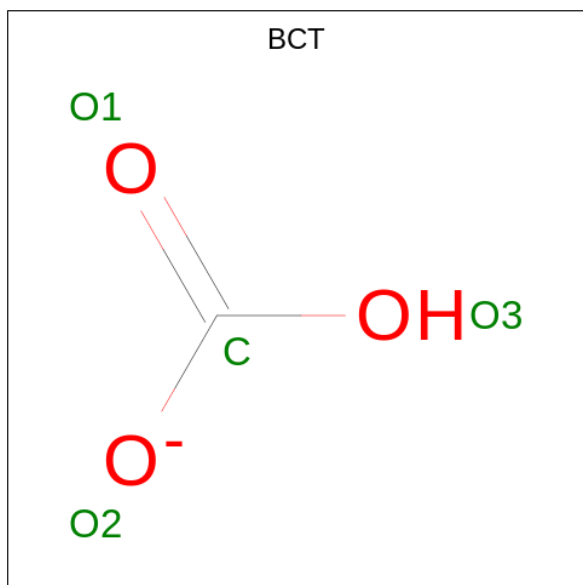
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	f	1	Total	C	O	0	0
			6	3	3		
31	h	1	Total	C	O	0	0
			6	3	3		
31	o	1	Total	C	O	0	0
			6	3	3		
31	o	1	Total	C	O	0	0
			6	3	3		
31	t	1	Total	C	O	0	0
			6	3	3		
31	u	1	Total	C	O	0	0
			6	3	3		
31	u	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	v	1	Total	C	O	0	0
			6	3	3		
31	v	1	Total	C	O	0	0
			6	3	3		
31	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



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

- Molecule 33 is CALCIUM ION (CCD ID: CA) (formula: Ca).

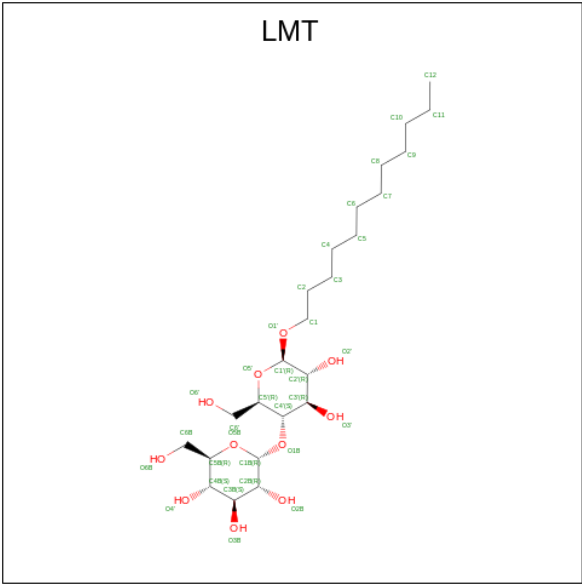
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	1	Total	Ca	0	0
			1	1		
33	F	1	Total	Ca	0	0
			1	1		
33	O	1	Total	Ca	0	0
			1	1		
33	b	1	Total	Ca	0	0
			1	1		

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

- Molecule 34 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



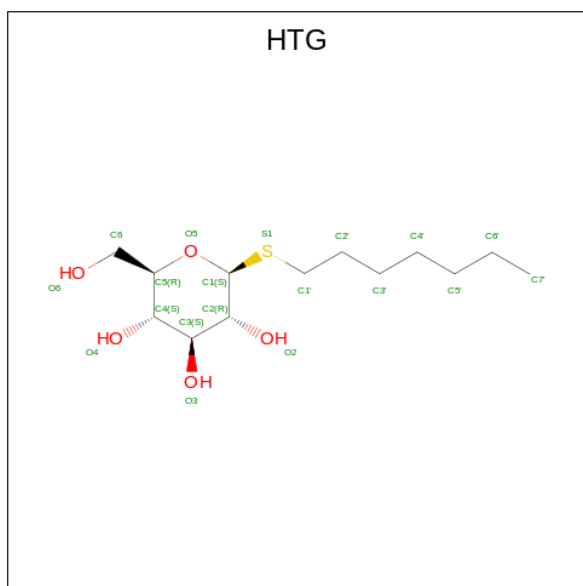
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			35	24	11		
34	C	1	Total	C	O	0	0
			35	24	11		
34	D	1	Total	C	O	0	0
			35	24	11		
34	F	1	Total	C	O	0	0
			26	15	11		
34	J	1	Total	C	O	0	0
			23	18	5		
34	M	1	Total	C	O	0	0
			35	24	11		
34	M	1	Total	C	O	0	0
			35	24	11		
34	T	1	Total	C	O	0	0
			24	18	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	Z	1	Total	C	O	0	0
			35	24	11		
34	a	1	Total	C	O	0	0
			35	24	11		
34	b	1	Total	C	O	0	0
			25	19	6		
34	c	1	Total	C	O	0	0
			35	24	11		
34	m	1	Total	C	O	0	0
			35	24	11		
34	m	1	Total	C	O	0	0
			35	24	11		
34	t	1	Total	C	O	0	0
			24	18	6		
34	z	1	Total	C	O	0	0
			32	21	11		

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



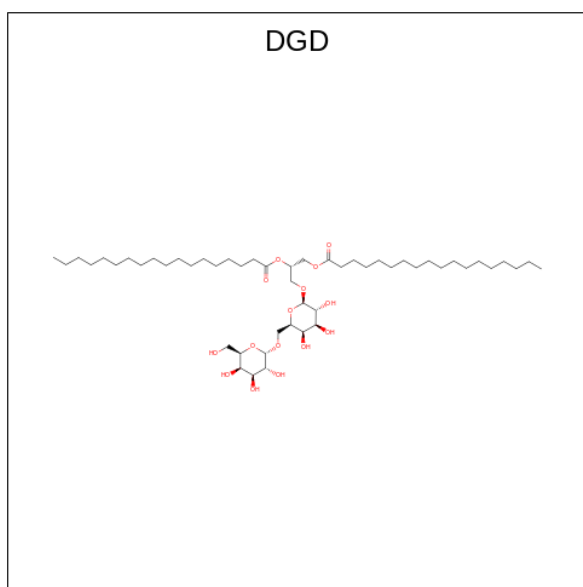
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		

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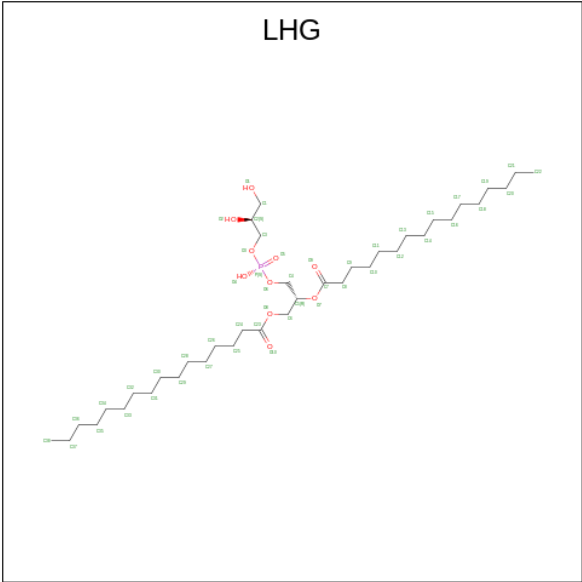
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	H	1	Total	C	O	S	0	0
			16	13	2	1		
35	O	1	Total	C	O	S	0	0
			19	13	5	1		
35	U	1	Total	C	S		0	0
			9	8	1			
35	V	1	Total	C	O	S	0	0
			13	7	5	1		
35	X	1	Total	C	O	S	0	0
			12	7	4	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	d	1	Total	C	O	S	0	0
			19	13	5	1		
35	o	1	Total	C	O	S	0	0
			19	13	5	1		
35	u	1	Total	C	O	S	0	0
			14	10	3	1		
35	v	1	Total	C	O	S	0	0
			13	7	5	1		

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



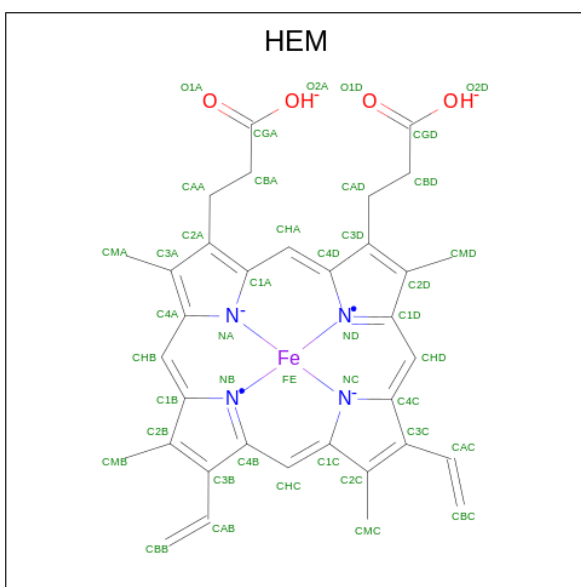
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			56	41	15		
36	C	1	Total	C	O	0	0
			58	43	15		
36	D	1	Total	C	O	0	0
			53	42	11		
36	H	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			55	40	15		
36	c	1	Total	C	O	0	0
			60	45	15		
36	e	1	Total	C	O	0	0
			39	30	9		
36	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



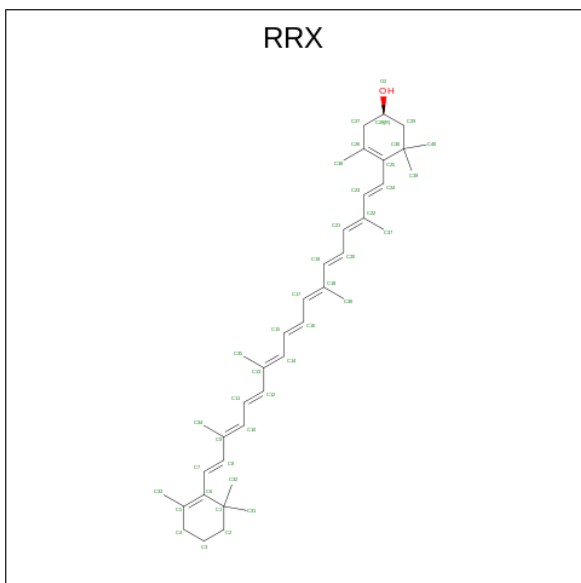
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			46	35	10	1		
37	E	1	Total	C	O	P	0	0
			49	38	10	1		
37	L	1	Total	C	O	P	0	0
			49	38	10	1		
37	b	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			40	29	10	1		
37	e	1	Total	C	O	P	0	0
			27	17	9	1		

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



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

- Molecule 39 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).

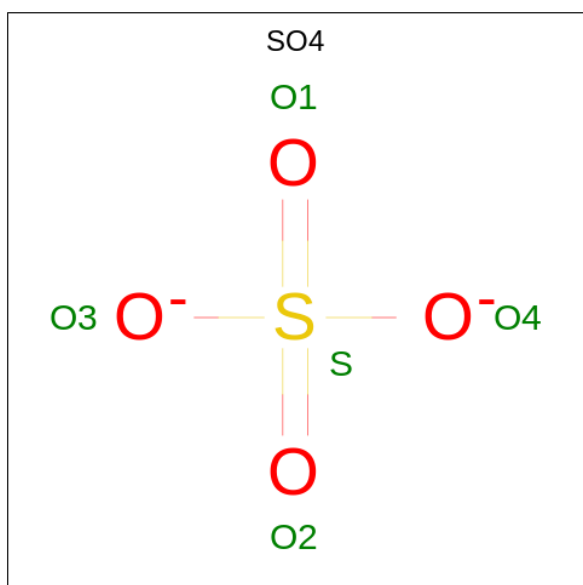


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
39	H	1	Total	C	O	0	0
			41	40	1		
39	h	1	Total	C	O	0	0
			41	40	1		

- Molecule 40 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 41 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
41	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	A	151	Total	O	0	2
			153	153		
42	B	303	Total	O	0	7
			310	310		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	C	233	Total 237	O 237	0	4
42	D	151	Total 154	O 154	0	3
42	E	35	Total 36	O 36	0	1
42	F	17	Total 17	O 17	0	0
42	H	50	Total 51	O 51	0	1
42	I	11	Total 11	O 11	0	0
42	J	10	Total 10	O 10	0	0
42	K	7	Total 7	O 7	0	0
42	L	16	Total 16	O 16	0	0
42	M	17	Total 17	O 17	0	0
42	O	170	Total 176	O 176	0	6
42	T	16	Total 16	O 16	0	0
42	U	89	Total 90	O 90	0	1
42	V	134	Total 136	O 136	0	2
42	Y	7	Total 7	O 7	0	0
42	X	12	Total 12	O 12	0	0
42	a	156	Total 156	O 156	0	0
42	b	287	Total 291	O 291	0	4
42	c	225	Total 229	O 229	0	4
42	d	152	Total 157	O 157	0	5
42	e	24	Total 25	O 25	0	1

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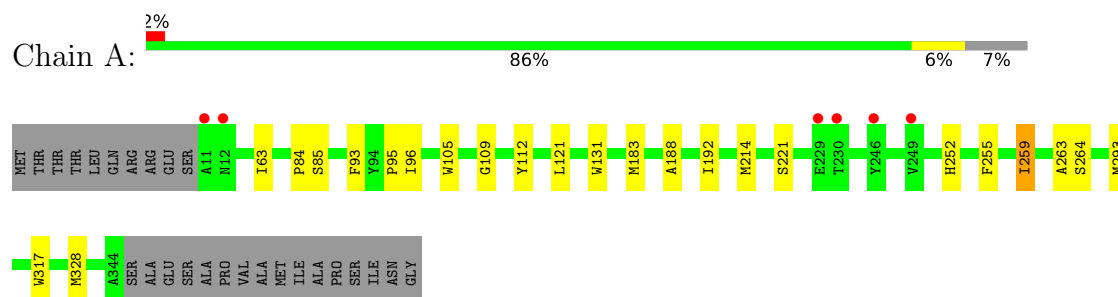
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	f	12	Total 12	O 12	0	0
42	h	37	Total 40	O 40	0	3
42	i	13	Total 13	O 13	0	0
42	j	8	Total 8	O 8	0	0
42	k	7	Total 7	O 7	0	0
42	l	13	Total 14	O 14	0	1
42	m	16	Total 16	O 16	0	0
42	o	152	Total 154	O 154	0	2
42	t	17	Total 19	O 19	0	2
42	u	94	Total 97	O 97	0	3
42	v	93	Total 97	O 97	0	4
42	y	4	Total 4	O 4	0	0
42	x	8	Total 8	O 8	0	0
42	z	3	Total 3	O 3	0	0

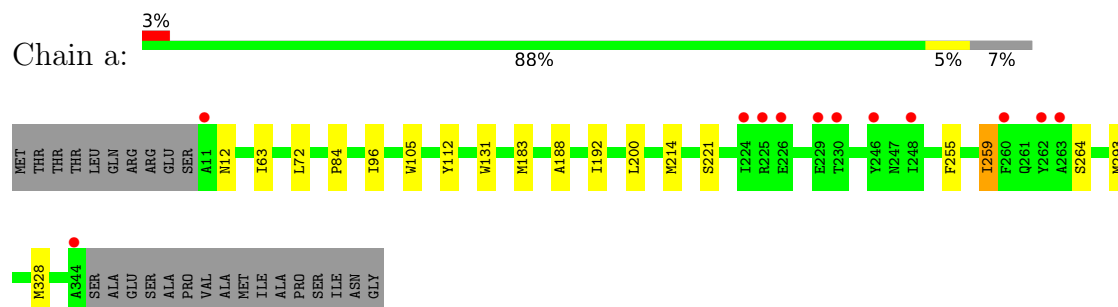
3 Residue-property plots [i](#)

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

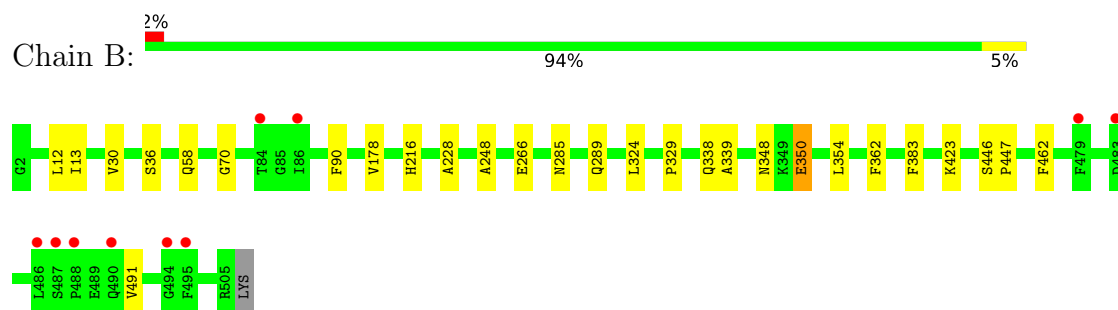
- Molecule 1: Photosystem II protein D1



- Molecule 1: Photosystem II protein D1

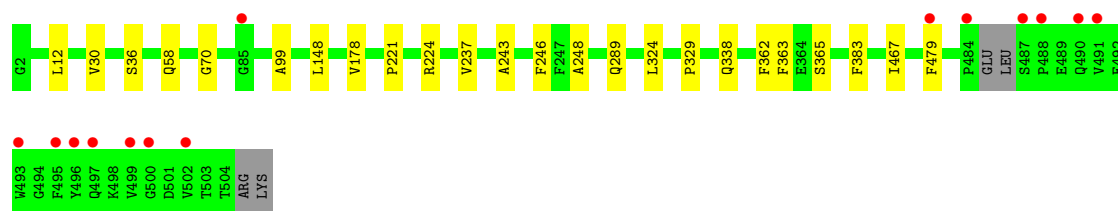


- Molecule 2: Photosystem II CP47 reaction center protein

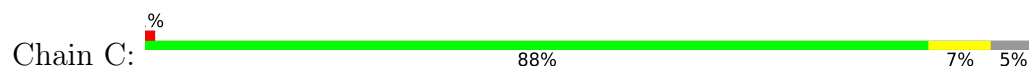


- Molecule 2: Photosystem II CP47 reaction center protein

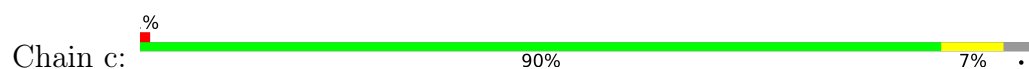




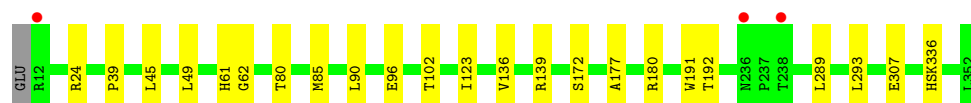
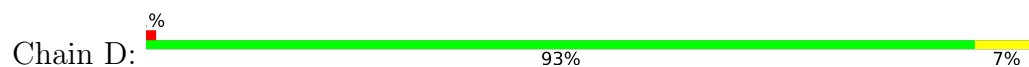
• Molecule 3: Photosystem II 44 kDa reaction center protein



• Molecule 3: Photosystem II 44 kDa reaction center protein



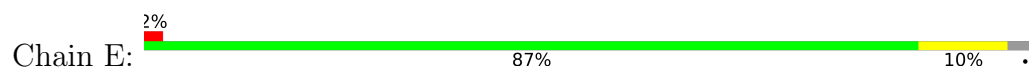
• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein

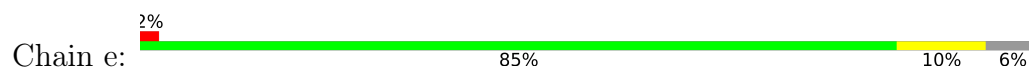


• Molecule 5: Cytochrome b559 subunit alpha





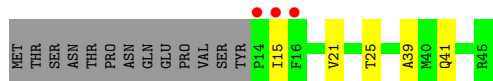
- Molecule 5: Cytochrome b559 subunit alpha



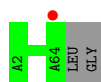
- Molecule 6: Cytochrome b559 subunit beta



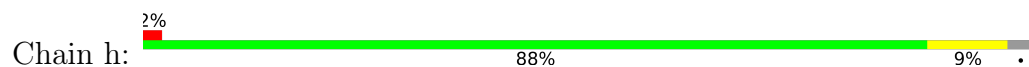
- Molecule 6: Cytochrome b559 subunit beta



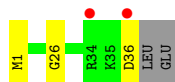
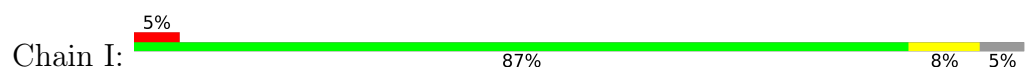
- Molecule 7: Photosystem II reaction center protein H



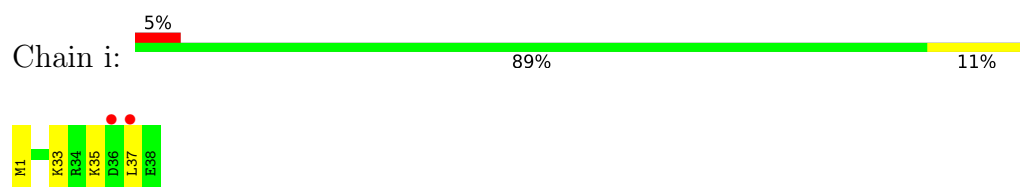
- Molecule 7: Photosystem II reaction center protein H



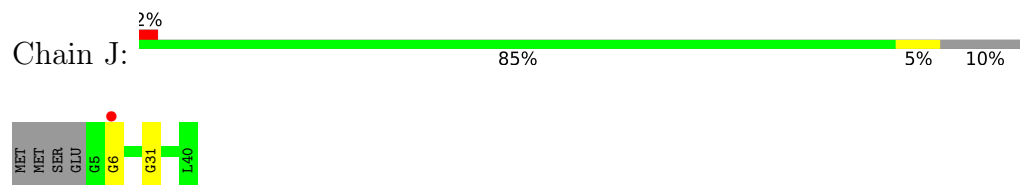
- Molecule 8: Photosystem II reaction center protein I



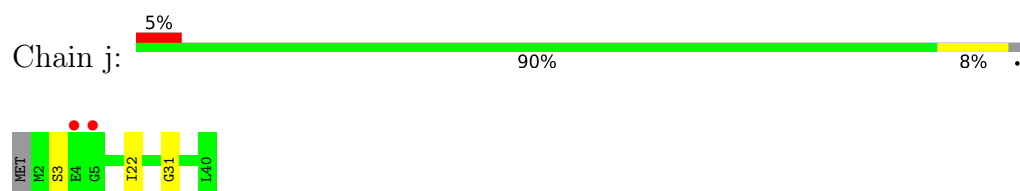
- Molecule 8: Photosystem II reaction center protein I



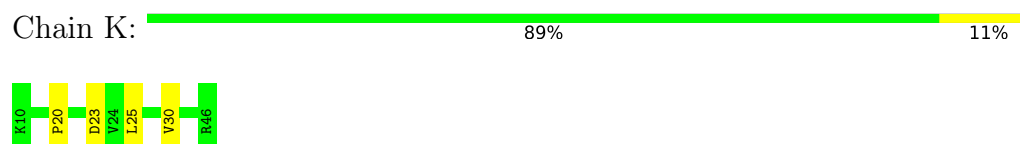
- Molecule 9: Photosystem II reaction center protein J



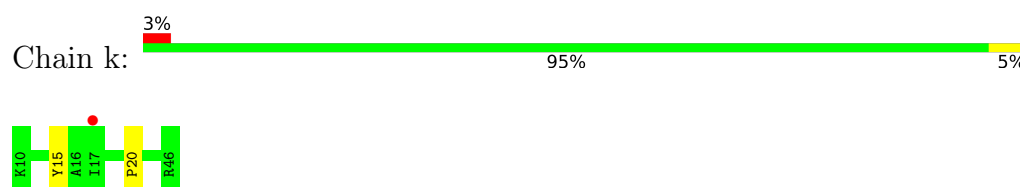
- Molecule 9: Photosystem II reaction center protein J



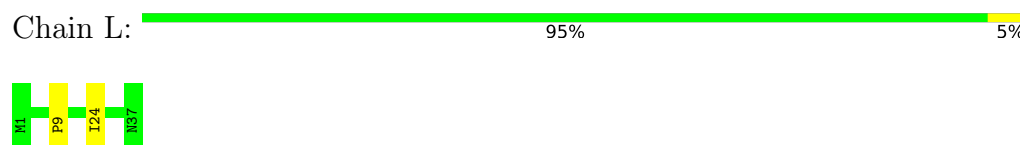
- Molecule 10: Photosystem II reaction center protein K



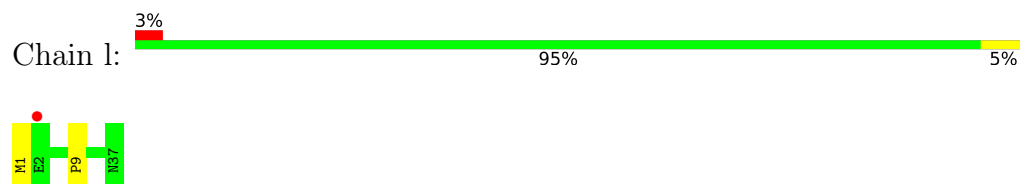
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

Chain M:  75% 14% • 8%



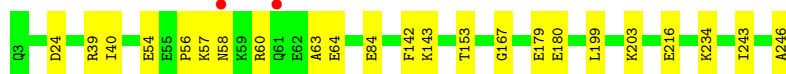
- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 17% • 6%



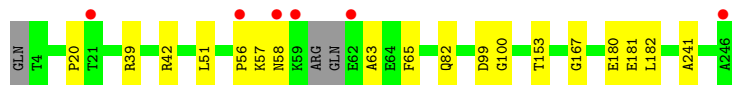
- Molecule 13: Photosystem II extrinsic protein O

Chain O:  91% 9%



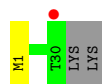
- Molecule 13: Photosystem II extrinsic protein O

Chain o:  91% 7% • 2%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  91% 6% • 3%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  81% 12% 6%



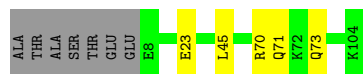
- Molecule 15: Photosystem II extrinsic protein U

Chain U:  89% 7%



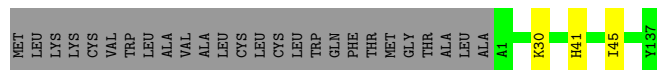
- Molecule 15: Photosystem II extrinsic protein U

Chain u:  88% 5% 7%



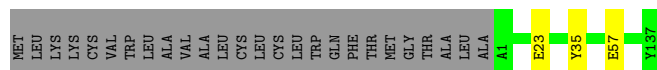
- Molecule 16: Photosystem II extrinsic protein V

Chain V:  82% 16%



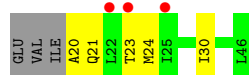
- Molecule 16: Photosystem II extrinsic protein V

Chain v:  82% 16%



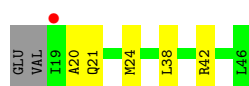
- Molecule 17: Photosystem II reaction center protein Psb30

Chain Y:  10% 73% 17% 10%



- Molecule 17: Photosystem II reaction center protein Psb30

Chain y:  3% 77% 17% 7%

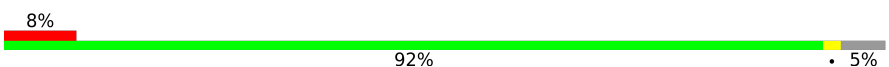


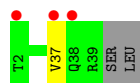
- Molecule 18: Photosystem II reaction center protein X

Chain X:  88% 8% 5%

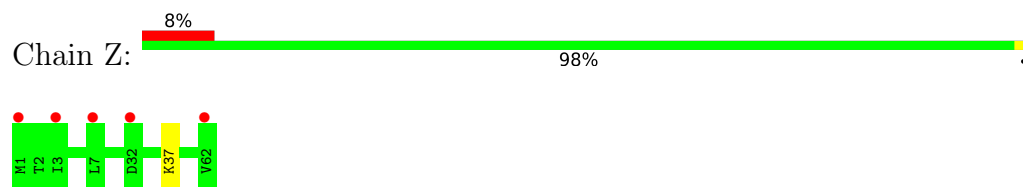


- Molecule 18: Photosystem II reaction center protein X

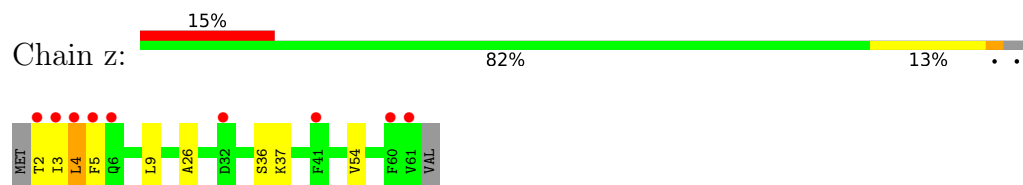
Chain x:  8% 92% 5%



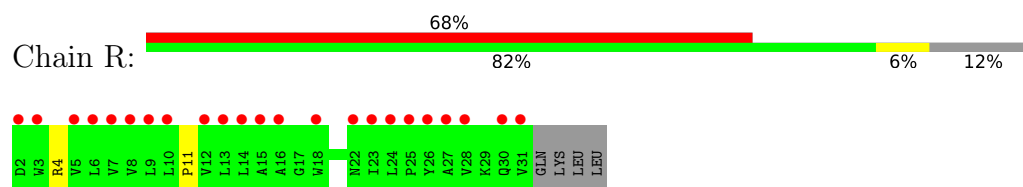
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	123.34Å 228.88Å 286.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.10 – 2.00 49.10 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.10-2.00) 99.9 (49.10-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0103, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.152 , 0.178 0.154 , 0.179	Depositor DCC
R_{free} test set	27141 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	54054	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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: GOL, FME, PL9, BCR, FE2, LMG, CLA, HEM, MG, OEX, SQD, HTG, RRX, CA, PHO, LMT, CL, HSK, BCT, DGD, LHG, SO4, UNL

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	0.34	0/2714	0.50	0/3703
1	a	0.33	0/2708	0.50	0/3695
2	B	0.31	0/4152	0.47	0/5659
2	b	0.29	1/4129 (0.0%)	0.46	0/5627
3	C	0.27	0/3607	0.43	0/4911
3	c	0.25	0/3662	0.42	0/4986
4	D	0.34	0/2804	0.48	0/3820
4	d	0.31	0/2814	0.45	0/3833
5	E	0.25	0/676	0.41	0/924
5	e	0.22	0/646	0.40	0/885
6	F	0.26	0/283	0.41	0/386
6	f	0.32	0/262	0.39	0/356
7	H	0.25	0/511	0.41	0/697
7	h	0.23	0/511	0.42	0/697
8	I	0.20	0/288	0.33	0/390
8	i	0.23	0/308	0.37	0/415
9	J	0.22	0/257	0.37	0/349
9	j	0.21	0/273	0.34	0/371
10	K	0.24	0/300	0.38	0/414
10	k	0.22	0/293	0.36	0/404
11	L	0.36	0/306	0.44	0/418
11	l	0.33	0/313	0.41	0/428
12	M	0.35	0/257	0.52	0/352
12	m	0.30	0/274	0.48	0/374
13	O	0.29	0/1911	0.48	0/2595
13	o	0.26	0/1882	0.45	0/2555
14	T	0.32	0/255	0.42	0/346
14	t	0.32	0/264	0.41	0/359
15	U	0.28	0/777	0.47	0/1055
15	u	0.30	0/783	0.47	0/1063
16	V	0.31	0/1081	0.47	0/1469

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.25	0/1074	0.42	0/1462
17	Y	0.19	0/194	0.32	0/259
17	y	0.18	0/197	0.35	0/264
18	X	0.17	0/286	0.28	0/387
18	x	0.15	0/286	0.30	0/387
19	Z	0.17	0/463	0.36	0/636
19	z	0.17	0/443	0.36	0/609
20	R	0.18	0/162	0.30	0/224
All	All	0.29	1/42406 (0.0%)	0.45	0/57764

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	221	PRO	CA-C	5.85	1.55	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2620	0	2520	17	0
1	a	2615	0	2520	13	0
2	B	3991	0	3844	22	0
2	b	3959	0	3806	19	0
3	C	3488	0	3410	29	0
3	c	3536	0	3460	22	0
4	D	2726	0	2629	18	0
4	d	2733	0	2641	17	0
5	E	657	0	637	7	0
5	e	627	0	595	6	0
6	F	274	0	279	4	0
6	f	255	0	263	3	0
7	H	498	0	518	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	h	498	0	518	8	0
8	I	291	0	302	2	0
8	i	311	0	326	2	0
9	J	251	0	257	1	0
9	j	267	0	266	3	0
10	K	287	0	292	4	0
10	k	283	0	283	2	0
11	L	296	0	305	2	0
11	l	300	0	314	2	0
12	M	261	0	280	4	0
12	m	275	0	304	6	0
13	O	1865	0	1829	17	0
13	o	1837	0	1800	11	0
14	T	256	0	256	0	0
14	t	265	0	262	4	0
15	U	766	0	758	3	0
15	u	769	0	764	3	0
16	V	1057	0	1063	2	0
16	v	1050	0	1043	3	0
17	Y	193	0	210	4	0
17	y	196	0	208	3	0
18	X	280	0	312	3	0
18	x	280	0	312	2	0
19	Z	452	0	469	1	0
19	z	432	0	441	6	0
20	R	162	0	103	1	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	260	0	288	8	0
24	B	1040	0	1152	31	0
24	C	845	0	936	36	0
24	D	130	0	144	2	0
24	a	195	0	216	5	0
24	b	1040	0	1152	29	0
24	c	845	0	936	28	0
24	d	195	0	216	7	0
25	A	128	0	148	3	0
25	a	128	0	148	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	40	0	56	0	0
26	B	120	0	168	8	0
26	C	80	0	112	4	0
26	D	40	0	56	2	0
26	K	40	0	56	1	0
26	T	40	0	56	5	0
26	Y	40	0	56	1	0
26	a	40	0	56	2	0
26	b	120	0	168	7	0
26	c	80	0	112	5	0
26	d	40	0	56	1	0
26	k	40	0	56	2	0
26	t	40	0	56	6	0
26	y	40	0	56	2	0
27	A	106	0	149	3	0
27	B	54	0	78	1	0
27	F	37	0	46	1	0
27	a	108	0	156	7	0
27	b	54	0	78	1	0
27	f	33	0	39	1	0
28	A	51	0	72	2	0
28	B	51	0	72	4	0
28	C	100	0	140	2	0
28	D	48	0	66	3	0
28	a	51	0	72	2	0
28	b	51	0	72	1	0
28	c	102	0	144	1	0
28	d	48	0	66	0	0
29	A	55	0	80	5	0
29	D	55	0	80	0	0
29	a	55	0	80	5	0
29	d	55	0	80	0	0
30	A	54	0	0	0	0
30	B	78	0	0	0	0
30	C	66	0	0	0	0
30	D	53	0	0	0	0
30	E	29	0	0	0	0
30	H	7	0	0	0	0
30	I	38	0	0	0	0
30	J	29	0	0	0	0
30	M	16	0	0	0	0
30	T	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	X	16	0	0	0	0
30	Y	10	0	0	0	0
30	a	56	0	0	0	0
30	b	63	0	0	0	0
30	c	74	0	0	0	0
30	d	72	0	0	0	0
30	e	15	0	0	0	0
30	h	7	0	0	0	0
30	i	55	0	0	0	0
30	j	32	0	0	0	0
30	m	13	0	0	0	0
30	t	12	0	0	0	0
30	v	7	0	0	0	0
30	y	10	0	0	0	0
31	A	18	0	24	2	0
31	B	36	0	48	1	0
31	C	36	0	48	4	0
31	H	6	0	8	1	0
31	L	6	0	8	0	0
31	O	18	0	24	1	0
31	V	24	0	30	0	0
31	Z	6	0	8	0	0
31	a	18	0	24	1	0
31	b	42	0	56	0	0
31	c	60	0	80	9	0
31	f	6	0	7	0	0
31	h	6	0	8	1	0
31	o	12	0	16	0	0
31	t	6	0	8	0	0
31	u	12	0	15	0	0
31	v	18	0	24	0	0
32	A	4	0	0	0	0
32	a	4	0	0	0	0
33	B	1	0	0	0	0
33	F	1	0	0	0	0
33	O	1	0	0	0	0
33	b	1	0	0	0	0
33	c	1	0	0	0	0
33	f	1	0	0	0	0
33	o	1	0	0	0	0
34	B	35	0	46	1	0
34	C	35	0	46	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	D	35	0	46	0	0
34	F	26	0	25	0	0
34	J	23	0	32	0	0
34	M	70	0	92	2	0
34	T	24	0	35	0	0
34	Z	35	0	46	1	0
34	a	35	0	46	1	0
34	b	25	0	35	1	0
34	c	35	0	46	0	0
34	m	70	0	92	1	0
34	t	24	0	35	0	0
34	z	32	0	33	4	0
35	B	76	0	104	0	0
35	C	57	0	78	4	0
35	H	16	0	20	1	0
35	O	19	0	26	0	0
35	U	9	0	15	1	0
35	V	13	0	11	0	0
35	X	12	0	8	0	0
35	b	76	0	104	3	0
35	c	38	0	52	1	0
35	d	19	0	26	1	0
35	o	19	0	26	0	0
35	u	14	0	19	0	0
35	v	13	0	11	0	0
36	C	176	0	226	5	0
36	D	53	0	71	4	0
36	H	62	0	82	1	0
36	c	177	0	228	1	0
36	e	39	0	47	1	0
36	h	62	0	82	1	0
37	D	144	0	213	4	0
37	E	49	0	74	6	0
37	L	49	0	74	1	0
37	b	49	0	74	2	0
37	d	138	0	198	7	0
37	e	27	0	30	2	0
38	F	43	0	30	2	0
38	V	43	0	30	1	0
38	f	43	0	30	2	0
38	v	43	0	30	0	0
39	H	41	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	h	41	0	56	3	0
40	J	1	0	0	0	0
40	j	1	0	0	0	0
41	O	5	0	0	0	0
42	A	153	0	0	0	0
42	B	310	0	0	1	0
42	C	237	0	0	5	0
42	D	154	0	0	2	0
42	E	36	0	0	0	0
42	F	17	0	0	0	0
42	H	51	0	0	1	0
42	I	11	0	0	1	0
42	J	10	0	0	0	0
42	K	7	0	0	1	0
42	L	16	0	0	0	0
42	M	17	0	0	0	0
42	O	176	0	0	3	0
42	T	16	0	0	0	0
42	U	90	0	0	3	0
42	V	136	0	0	1	0
42	X	12	0	0	0	0
42	Y	7	0	0	1	0
42	a	156	0	0	0	0
42	b	291	0	0	0	0
42	c	229	0	0	4	0
42	d	157	0	0	0	0
42	e	25	0	0	0	0
42	f	12	0	0	0	0
42	h	40	0	0	0	0
42	i	13	0	0	1	0
42	j	8	0	0	0	0
42	k	7	0	0	0	0
42	l	14	0	0	1	0
42	m	16	0	0	1	0
42	o	154	0	0	0	0
42	t	19	0	0	1	0
42	u	97	0	0	1	0
42	v	97	0	0	1	0
42	x	8	0	0	0	0
42	y	4	0	0	0	0
42	z	3	0	0	0	0
All	All	54054	0	51647	422	0

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

All (422) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:609:CLA:HHC	24:b:609:CLA:HBB1	1.58	0.85
36:D:406:DGD:HD4	5:E:45:ASP:HB3	1.59	0.83
3:c:320:ARG:HG3	31:c:927:GOL:H2	1.65	0.78
3:c:378:ASN:ND2	42:c:1001:HOH:O	2.18	0.77
24:B:611:CLA:HHC	24:B:611:CLA:HBB1	1.67	0.76
8:i:37:LEU:O	42:i:901:HOH:O	2.05	0.74
24:B:615:CLA:H18	28:B:622:LMG:H422	1.69	0.74
1:a:72:LEU:HD11	34:a:402:LMT:H52	1.71	0.73
3:c:19:ASN:ND2	42:c:1002:HOH:O	2.24	0.71
4:d:192:THR:HG23	24:d:404:CLA:HBC2	1.72	0.70
24:a:413:CLA:H152	24:c:907:CLA:H142	1.71	0.70
15:u:23:GLU:OE2	42:u:301[A]:HOH:O	2.09	0.70
12:M:16[A]:LEU:HD23	12:m:16[A]:LEU:HD23	1.74	0.69
4:D:102:THR:OG1	36:D:406:DGD:HG31	1.94	0.68
5:e:9:PRO:HA	37:e:101:LHG:HC2	1.77	0.67
31:H:101:GOL:O1	42:H:201:HOH:O	2.12	0.67
13:o:39:ARG:NH2	13:o:82:GLN:OE1	2.27	0.66
36:C:518:DGD:HAF1	28:D:410:LMG:H201	1.77	0.66
24:b:615:CLA:H142	37:b:639:LHG:H361	1.77	0.65
15:U:23:GLU:OE1	42:U:301:HOH:O	2.15	0.65
24:A:407:CLA:H142	28:D:410:LMG:H241	1.80	0.64
24:c:902:CLA:C4D	24:c:904:CLA:H2	2.28	0.64
24:c:909:CLA:H92	37:d:410:LHG:H141	1.81	0.63
31:A:420:GOL:H32	5:E:63:ILE:HD11	1.81	0.62
26:Y:101:BCR:H321	26:Y:101:BCR:HC8	1.81	0.62
4:d:24:ARG:HE	18:x:37:VAL:HG22	1.65	0.62
2:b:99:ALA:HA	24:b:610:CLA:H121	1.82	0.61
24:B:614:CLA:H122	28:B:622:LMG:H232	1.81	0.61
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.36	0.60
24:b:618:CLA:H8	26:b:621:BCR:H362	1.82	0.60
24:B:616:CLA:H2	24:B:617:CLA:HBB2	1.83	0.60
24:B:615:CLA:H151	14:t:8:PHE:HE1	1.67	0.60
24:C:506:CLA:HMC2	24:C:507:CLA:H102	1.83	0.60
38:F:102:HEM:HMB1	38:F:102:HEM:HBB2	1.84	0.60
24:B:617:CLA:HED2	24:B:617:CLA:H43	1.83	0.59
29:a:417:PL9:H512	27:f:102:SQD:H321	1.83	0.59
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:70:ARG:NH1	15:u:73[A]:GLN:OE1	2.36	0.59
29:A:414:PL9:H403	6:F:22:ALA:HB2	1.85	0.59
1:A:183:MET:HA	24:A:405:CLA:HMD1	1.85	0.59
24:C:502:CLA:H61	24:C:512:CLA:H42	1.84	0.58
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.86	0.57
24:D:403:CLA:H171	18:X:15[A]:LEU:HG	1.86	0.57
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.39	0.57
24:b:619:CLA:H2	24:b:620:CLA:HBB2	1.86	0.57
13:O:84:GLU:OE2	42:O:401:HOH:O	2.17	0.57
31:a:420:GOL:H11	12:m:1:FME:HG2	1.85	0.57
35:d:403:HTG:H1	7:h:25:TRP:CD1	2.40	0.57
31:c:927:GOL:H31	42:c:1121:HOH:O	2.04	0.57
36:C:517:DGD:HB52	28:C:519:LMG:H372	1.87	0.56
1:a:183:MET:HA	24:a:409:CLA:HMD1	1.86	0.56
24:B:616:CLA:H122	24:B:617:CLA:H93	1.87	0.56
3:C:378[A]:ASN:ND2	42:C:602:HOH:O	2.33	0.56
24:C:506:CLA:H61	34:C:520:LMT:H92	1.87	0.56
13:O:57:LYS:HE3	2:b:338:GLN:HA	1.87	0.56
24:A:407:CLA:H171	29:A:414:PL9:H271	1.87	0.56
24:b:619:CLA:HHC	24:b:619:CLA:HBB1	1.86	0.56
24:c:902:CLA:H202	24:c:908:CLA:HBB1	1.86	0.56
24:c:907:CLA:HMC2	24:c:908:CLA:H102	1.86	0.56
26:T:702:BCR:H321	26:T:702:BCR:HC8	1.88	0.56
5:e:68:ASP:OD2	5:e:71:GLU:HB2	2.06	0.56
4:D:192:THR:HG23	24:D:402:CLA:HBC2	1.88	0.55
37:E:101:LHG:O2	6:F:19:ARG:NH1	2.39	0.55
16:V:30:LYS:NZ	42:V:302:HOH:O	2.39	0.55
24:B:605:CLA:H43	24:B:606:CLA:H2	1.87	0.55
11:l:1:MET:N	42:l:101:HOH:O	2.38	0.55
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.42	0.55
24:c:902:CLA:C3D	24:c:904:CLA:H2	2.36	0.55
24:C:501:CLA:C4D	24:C:503:CLA:H2	2.36	0.55
24:B:615:CLA:H43	27:B:621:SQD:H122	1.89	0.54
24:c:914:CLA:HAB	26:c:915:BCR:H24C	1.90	0.54
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.90	0.54
3:C:286:ALA:HB2	24:C:502:CLA:HMD2	1.90	0.54
3:C:320:ARG:HB2	31:C:531:GOL:H11	1.90	0.54
26:T:702:BCR:H19C	26:b:622:BCR:H363	1.89	0.54
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.07	0.54
4:D:61:HIS:HD2	42:D:637:HOH:O	1.90	0.54
1:a:200:LEU:HG	36:c:919:DGD:HAT2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:94:THR:HG22	24:C:501:CLA:HED1	1.89	0.53
38:f:101:HEM:HBB2	38:f:101:HEM:HMB2	1.88	0.53
26:y:101:BCR:H321	26:y:101:BCR:HC8	1.90	0.53
2:B:248:ALA:HA	24:B:604:CLA:H42	1.91	0.53
24:B:612:CLA:H142	37:L:101:LHG:H372	1.90	0.53
2:b:248:ALA:HA	24:b:607:CLA:H42	1.90	0.53
12:m:5:GLN:O	42:m:1601:HOH:O	2.18	0.53
27:A:417:SQD:H141	26:T:702:BCR:HC41	1.91	0.53
3:C:242:LEU:HD12	35:C:528:HTG:H7'1	1.90	0.53
1:A:121[B]:LEU:HG	28:A:413:LMG:H181	1.90	0.53
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.91	0.52
1:A:259:ILE:HD12	29:A:414:PL9:H252	1.91	0.52
2:b:36:SER:OG	26:b:622:BCR:H362	2.09	0.52
24:b:605:CLA:HAA2	35:b:627:HTG:H62	1.89	0.52
27:F:101:SQD:H321	18:X:24:THR:HA	1.90	0.52
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.45	0.52
27:a:415:SQD:H141	37:d:410:LHG:H182	1.90	0.52
24:b:610:CLA:H72	26:b:623:BCR:H311	1.92	0.52
3:c:60:ILE:HG22	24:c:904:CLA:HHD	1.92	0.52
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.92	0.52
2:b:148[B]:LEU:HD23	24:b:608:CLA:H191	1.92	0.51
24:b:605:CLA:C3B	24:b:605:CLA:H152	2.41	0.51
13:O:39:ARG:HG2	13:O:246:ALA:HB2	1.93	0.51
34:M:303:LMT:H6D	11:l:9:PRO:HA	1.92	0.51
19:z:37:LYS:HE3	34:z:101:LMT:H4'	1.93	0.51
24:C:501:CLA:C3D	24:C:503:CLA:H2	2.40	0.51
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.91	0.51
34:C:520:LMT:H6'1	8:I:26:GLY:HA3	1.93	0.51
1:a:259:ILE:HD12	29:a:417:PL9:H222	1.94	0.50
24:b:614:CLA:H151	24:b:614:CLA:H203	1.92	0.50
24:d:405:CLA:H142	7:h:36:GLY:HA3	1.92	0.50
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.93	0.50
24:b:617:CLA:HBB1	24:b:617:CLA:HMB1	1.94	0.50
37:d:409:LHG:H322	14:t:21:ILE:HD11	1.94	0.50
1:A:63:ILE:HB	3:C:335:THR:HG21	1.94	0.50
24:B:606:CLA:C14	24:B:611:CLA:HED2	2.41	0.50
4:D:62:GLY:HA3	5:E:63:ILE:HD13	1.93	0.50
2:B:266:GLU:HB3	31:B:630:GOL:H31	1.93	0.50
26:B:619:BCR:H292	27:a:401:SQD:H351	1.92	0.50
8:i:33:LYS:O	8:i:35:LYS:HG3	2.12	0.50
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:58:ASN:C	13:O:60:ARG:H	2.19	0.50
3:c:436:PHE:CE2	24:c:905:CLA:H162	2.47	0.50
6:f:21:VAL:O	6:f:25:THR:HG23	2.12	0.50
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.94	0.49
35:C:521:HTG:H6'2	28:C:534:LMG:H331	1.93	0.49
5:E:27:ILE:HG12	38:F:102:HEM:HMC3	1.93	0.49
3:C:377:LEU:HG	3:C:381:LYS:HE2	1.94	0.49
13:O:56:PRO:HD3	13:O:63:ALA:HB2	1.93	0.49
13:O:143:LYS:HG3	31:O:306:GOL:H11	1.93	0.49
26:B:619:BCR:H363	26:t:903:BCR:H19C	1.95	0.49
35:b:603:HTG:H7'2	24:b:610:CLA:H141	1.93	0.49
24:b:617:CLA:H18	37:d:408:LHG:H202	1.93	0.49
31:c:926:GOL:H12	16:v:35:TYR:HA	1.95	0.49
2:B:36[A]:SER:OG	26:B:619:BCR:H362	2.13	0.49
29:a:417:PL9:H502	4:d:39:PRO:HG3	1.94	0.49
3:c:417:VAL:HG13	31:c:926:GOL:H31	1.94	0.49
1:a:84:PRO:HA	1:a:112:TYR:CG	2.48	0.48
27:a:415:SQD:H302	24:c:909:CLA:H71	1.94	0.48
3:C:42:LEU:HD21	24:C:511:CLA:H2A	1.95	0.48
36:D:406:DGD:O1B	36:D:406:DGD:O2D	2.23	0.48
13:O:180:GLU:OE2	42:O:402:HOH:O	2.19	0.48
3:c:377:LEU:HG	3:c:381:LYS:HE3	1.94	0.48
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.96	0.48
24:d:401:CLA:HMB1	24:d:401:CLA:HBB1	1.95	0.48
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.95	0.48
13:O:179:GLU:OE2	42:O:403:HOH:O	2.20	0.48
13:O:180:GLU:CD	13:O:180:GLU:H	2.22	0.48
27:a:415:SQD:H381	9:j:22:ILE:HD11	1.94	0.48
5:e:27:ILE:HG12	38:f:101:HEM:HMC3	1.95	0.48
36:e:102:DGD:HD2	36:e:102:DGD:HG31	1.65	0.48
24:a:409:CLA:HBB1	24:a:409:CLA:HMB3	1.96	0.47
13:o:99:ASP:OD1	13:o:100:GLY:N	2.46	0.47
29:A:414:PL9:H251	37:E:101:LHG:H201	1.95	0.47
3:C:391:ARG:HD2	42:C:804:HOH:O	2.14	0.47
12:M:28:GLN:O	12:M:32:GLN:HG3	2.14	0.47
1:A:84:PRO:HA	1:A:112:TYR:CG	2.49	0.47
6:F:21:VAL:O	6:F:25:THR:HG23	2.13	0.47
24:b:614:CLA:HHC	24:b:614:CLA:HBB1	1.97	0.47
24:c:906:CLA:HAA1	24:c:906:CLA:HBD	1.95	0.47
2:B:339:ALA:HB2	13:o:58:ASN:HB3	1.97	0.47
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:266:TRP:CD1	37:d:409:LHG:HC31	2.50	0.47
26:k:101:BCR:H24C	26:k:101:BCR:H371	1.71	0.47
3:C:182:PHE:HA	35:C:521:HTG:H61	1.97	0.47
11:L:9:PRO:HA	34:m:1502:LMT:H6D	1.96	0.47
13:O:40:ILE:HG12	13:O:243:ILE:HD13	1.97	0.47
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.95	0.47
2:b:30:VAL:HG12	24:b:609:CLA:HHD	1.96	0.47
2:B:216:HIS:HE1	24:B:610:CLA:C1A	2.27	0.47
2:B:462:PHE:CE2	24:B:614:CLA:HMB2	2.49	0.47
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.15	0.47
13:O:54:GLU:HG2	13:O:64:GLU:O	2.15	0.47
3:C:443:TRP:CE2	24:C:508:CLA:HMD2	2.50	0.47
13:O:24:ASP:HA	13:O:203:LYS:HE2	1.97	0.47
17:Y:23:THR:HB	17:Y:24:MET:HE2	1.97	0.47
1:A:263:ALA:HA	37:E:101:LHG:H291	1.97	0.46
3:C:38:GLY:HA3	24:C:511:CLA:HMD2	1.96	0.46
3:C:429:SER:HB3	36:C:517:DGD:HBT2	1.96	0.46
26:T:702:BCR:H331	26:T:702:BCR:HC7	1.56	0.46
24:b:605:CLA:HBD	24:b:605:CLA:H42	1.97	0.46
3:c:41:ARG:NH1	24:c:912:CLA:HMD1	2.30	0.46
1:a:221[A]:SER:HB2	4:d:139:ARG:O	2.15	0.46
24:b:608:CLA:H43	24:b:609:CLA:H2	1.98	0.46
26:b:622:BCR:H331	26:b:622:BCR:C8	2.45	0.46
24:b:619:CLA:H2	24:b:620:CLA:CBB	2.46	0.46
24:A:405:CLA:CBD	24:A:406:CLA:HAC2	2.45	0.46
28:A:413:LMG:H292	3:C:214:LEU:O	2.15	0.46
24:B:615:CLA:H72	26:B:618:BCR:H362	1.96	0.46
3:c:213:LEU:HD11	26:c:916:BCR:C20	2.46	0.46
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.51	0.46
24:C:512:CLA:H143	24:C:513:CLA:H142	1.98	0.46
24:b:619:CLA:H161	7:h:7:LEU:HD21	1.96	0.46
37:d:410:LHG:H242	37:d:410:LHG:H272	1.75	0.46
5:e:8:ARG:NH2	9:j:3:SER:O	2.47	0.46
25:A:409:PHO:ND	25:A:409:PHO:NC	2.64	0.46
1:a:264:SER:OG	29:a:417:PL9:O2	2.34	0.46
3:C:279:LEU:HD22	24:C:509:CLA:HED2	1.97	0.46
4:D:45:LEU:HD21	28:D:410:LMG:H372	1.98	0.46
26:t:903:BCR:HC7	26:t:903:BCR:H331	1.48	0.46
1:A:221[A]:SER:HB2	4:D:139:ARG:O	2.16	0.46
29:A:414:PL9:H502	4:D:39:PRO:HG3	1.98	0.46
5:E:68:ASP:OD2	5:E:71:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:201[B]:ASN:HD22	35:c:924:HTG:H4	1.82	0.46
2:B:338:GLN:HA	13:o:57:LYS:HE3	1.97	0.45
26:t:903:BCR:H321	26:t:903:BCR:HC8	1.97	0.45
25:A:409:PHO:HBC2	25:A:409:PHO:HHD	1.98	0.45
2:B:12:LEU:HB2	24:B:613:CLA:HMC2	1.97	0.45
3:C:52:ALA:HB2	24:C:511:CLA:HMA2	1.98	0.45
24:C:508:CLA:H203	10:K:30:VAL:HG13	1.98	0.45
37:D:409:LHG:H152	37:D:409:LHG:H341	1.98	0.45
3:C:259:TRP:CD2	34:C:520:LMT:H42	2.51	0.45
24:B:616:CLA:H111	24:B:616:CLA:H152	1.79	0.45
3:c:286:ALA:HB2	24:c:903:CLA:HMD2	1.98	0.45
2:B:350:GLU:H	2:B:350:GLU:HG2	1.55	0.45
28:B:622:LMG:HC5	34:M:302:LMT:H12	1.97	0.45
24:c:913:CLA:O2D	24:c:914:CLA:HBB2	2.17	0.45
10:k:15:TYR:CE2	19:z:5:PHE:HZ	2.35	0.45
24:A:405:CLA:H192	24:A:405:CLA:H161	1.77	0.45
24:B:615:CLA:H151	14:t:8:PHE:CE1	2.49	0.45
3:C:223:TRP:CG	3:C:224:ILE:H	2.35	0.45
25:a:412:PHO:ND	25:a:412:PHO:NC	2.65	0.45
24:b:620:CLA:HBB1	24:b:620:CLA:HMB3	1.99	0.45
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.98	0.45
3:C:288:CYS:SG	36:C:516:DGD:HB32	2.57	0.45
1:a:63:ILE:HB	3:c:335:THR:HG21	1.99	0.45
12:m:28:GLN:O	12:m:32:GLN:HG3	2.17	0.45
2:b:224:ARG:HH21	34:b:625:LMT:H2'	1.82	0.44
24:b:617:CLA:H111	24:b:617:CLA:H72	1.76	0.44
15:u:45:LEU:HD21	15:u:71:GLN:HB3	1.99	0.44
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.52	0.44
3:C:406:SER:HA	3:C:420:VAL:HG23	1.99	0.44
3:c:79:LYS:HB3	3:c:84:GLN:NE2	2.32	0.44
13:o:180:GLU:CD	13:o:180:GLU:H	2.26	0.44
2:b:12:LEU:HB2	24:b:616:CLA:HMC2	1.99	0.44
24:C:510:CLA:H152	24:C:510:CLA:H112	1.77	0.44
26:c:915:BCR:H15C	26:c:915:BCR:H351	1.76	0.44
24:A:410:CLA:H111	24:A:410:CLA:H151	1.84	0.44
26:B:620:BCR:H331	26:B:620:BCR:C8	2.47	0.44
24:c:906:CLA:HBC2	26:c:916:BCR:H341	2.00	0.44
7:h:38:PHE:HB2	39:h:101:RRX:C10	2.46	0.44
2:B:228:ALA:HB2	34:B:623:LMT:H21	1.98	0.44
2:B:285:ASN:O	2:B:289:GLN:HG2	2.17	0.44
24:c:913:CLA:H121	24:c:914:CLA:H142	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:20:PRO:HB3	17:y:21:GLN:HG3	1.99	0.44
13:o:51:LEU:HB3	13:o:65:PHE:HB3	2.00	0.44
2:b:237:VAL:HG11	24:b:614:CLA:H201	2.00	0.44
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.53	0.44
17:y:38:LEU:O	17:y:42:ARG:HG2	2.18	0.44
35:H:105:HTG:H5'1	35:H:105:HTG:H2'1	1.65	0.44
26:b:623:BCR:H20C	26:b:623:BCR:H361	1.91	0.44
24:d:405:CLA:H162	7:h:33:VAL:HG13	1.98	0.44
24:a:409:CLA:CBD	24:d:401:CLA:HAC2	2.48	0.43
24:b:606:CLA:H101	24:b:613:CLA:H193	2.00	0.43
3:c:362:ARG:HB3	31:c:932:GOL:H32	2.00	0.43
24:C:512:CLA:H93	24:C:513:CLA:H161	2.00	0.43
12:m:34:LYS:HE3	12:m:34:LYS:HB2	1.90	0.43
2:B:30:VAL:HG12	24:B:606:CLA:HHD	1.99	0.43
16:V:41:HIS:HA	16:V:45:ILE:O	2.18	0.43
37:b:639:LHG:H312	12:m:18:PRO:HB3	1.99	0.43
24:C:513:CLA:H171	26:C:514:BCR:H373	1.99	0.43
26:T:702:BCR:HC8	26:T:702:BCR:H311	2.01	0.43
3:c:50:LEU:HD11	24:c:914:CLA:HBB1	1.99	0.43
3:C:425:TRP:CD1	24:C:504:CLA:HMA3	2.53	0.43
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.52	0.43
26:K:101:BCR:H371	26:K:101:BCR:H24C	1.80	0.43
13:O:142:PHE:HB2	13:O:199:LEU:HD12	2.00	0.43
24:c:914:CLA:HMD3	34:z:101:LMT:H5'	2.00	0.43
13:o:56:PRO:HD3	13:o:63:ALA:HB2	2.01	0.43
24:B:608:CLA:H2	28:B:622:LMG:H152	2.01	0.43
4:D:85:MET:CE	4:D:96:GLU:HG2	2.48	0.43
4:D:307:GLU:HG3	42:D:607:HOH:O	2.17	0.43
4:d:160:TYR:HA	4:d:290:ALA:HB2	1.99	0.43
26:t:903:BCR:HC8	26:t:903:BCR:H311	2.01	0.43
24:B:614:CLA:H121	24:B:614:CLA:H162	1.90	0.43
3:c:334:PRO:HA	13:o:153:THR:OG1	2.18	0.43
16:v:57:GLU:H	16:v:57:GLU:CD	2.27	0.43
1:A:252:HIS:CE1	1:A:264:SER:HB3	2.54	0.43
29:a:417:PL9:HC8	29:a:417:PL9:HC2	1.72	0.43
3:c:387:TRP:CE3	31:c:937:GOL:H2	2.53	0.43
24:c:910:CLA:HMB1	24:c:910:CLA:HBB1	1.99	0.43
28:c:921:LMG:H232	28:c:921:LMG:H382	2.01	0.43
25:A:408:PHO:NC	25:A:408:PHO:ND	2.67	0.42
2:b:324:LEU:HA	4:d:293[A]:LEU:HG	2.00	0.42
31:A:422:GOL:H11	12:M:1:FME:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:501:CLA:H42	24:C:502:CLA:HMD3	2.01	0.42
37:E:101:LHG:H212	37:E:101:LHG:H181	1.79	0.42
11:L:24[A]:ILE:CD1	12:M:18:PRO:HB2	2.49	0.42
3:c:406:SER:HA	3:c:420:VAL:HG23	2.00	0.42
4:d:85:MET:CE	4:d:96:GLU:HG2	2.49	0.42
42:B:805:HOH:O	13:O:179:GLU:HG3	2.18	0.42
1:a:131:TRP:CH2	24:c:906:CLA:HAA2	2.53	0.42
24:c:912:CLA:HAA1	24:c:912:CLA:HBD	2.01	0.42
26:k:101:BCR:H15C	26:k:101:BCR:H351	1.91	0.42
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.83	0.42
24:C:502:CLA:H193	35:C:521:HTG:H3'2	2.02	0.42
39:H:102:RRX:H47	39:H:102:RRX:H43	1.83	0.42
8:I:36:ASP:HB2	42:I:206:HOH:O	2.20	0.42
15:U:86:GLU:HG2	42:U:339:HOH:O	2.18	0.42
3:c:223:TRP:CG	3:c:224:ILE:H	2.38	0.42
24:c:904:CLA:H101	24:c:904:CLA:H62	1.71	0.42
24:B:607:CLA:H13	24:B:607:CLA:H102	1.70	0.42
24:B:611:CLA:H51	24:B:611:CLA:H8	1.94	0.42
4:D:123:ILE:HD11	36:H:103:DGD:HAE1	2.00	0.42
24:b:613:CLA:NC	39:h:101:RRX:H56	2.34	0.42
19:z:26:ALA:HB1	19:z:36:SER:HB3	2.01	0.42
3:C:50:LEU:HD11	24:C:513:CLA:HBB1	2.01	0.42
4:D:49:LEU:HD13	26:D:404:BCR:C15	2.50	0.42
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.54	0.42
24:b:607:CLA:CGA	24:b:607:CLA:H3A	2.50	0.42
24:c:906:CLA:H111	24:c:906:CLA:H93	1.83	0.42
24:d:401:CLA:H162	24:d:401:CLA:H203	1.83	0.42
16:v:35:TYR:OH	42:v:301:HOH:O	2.22	0.42
24:c:906:CLA:H112	24:c:906:CLA:H72	1.86	0.42
24:c:909:CLA:H142	24:c:909:CLA:H112	1.86	0.42
39:h:101:RRX:H28	39:h:101:RRX:H32	1.82	0.42
13:o:42:ARG:O	13:o:241:ALA:HA	2.19	0.42
27:A:412:SQD:H121	27:A:412:SQD:H91	1.78	0.42
24:C:501:CLA:HHC	24:C:501:CLA:HBB1	2.02	0.42
35:U:201:HTG:H7'3	42:U:339:HOH:O	2.19	0.42
27:a:415:SQD:H122	27:a:415:SQD:H151	1.70	0.42
28:a:416:LMG:HC71	3:c:216:SER:HB2	2.02	0.42
37:e:101:LHG:H132	37:e:101:LHG:H161	1.86	0.42
3:C:23:ALA:N	42:C:612:HOH:O	2.52	0.42
24:C:507:CLA:H142	26:C:515:BCR:H16C	2.01	0.42
4:d:126:MET:HE3	4:d:143:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:y:20:ALA:O	17:y:24:MET:HG2	2.19	0.42
24:A:406:CLA:HBB1	24:A:406:CLA:HMB1	2.02	0.42
27:A:412:SQD:H271	37:D:409:LHG:H142	2.01	0.42
24:B:602:CLA:H12	24:B:602:CLA:H52	1.83	0.42
24:B:615:CLA:H161	24:B:615:CLA:H122	1.59	0.42
24:C:503:CLA:HMC3	24:C:513:CLA:H191	2.02	0.42
24:C:510:CLA:H91	24:C:510:CLA:H111	1.89	0.42
37:d:410:LHG:H152	37:d:410:LHG:H121	1.89	0.42
19:z:2:THR:C	19:z:4:LEU:H	2.27	0.42
24:C:513:CLA:H3A	24:C:513:CLA:HBA1	1.66	0.41
36:C:517:DGD:HBE2	36:C:517:DGD:HBFB	1.69	0.41
27:b:601:SQD:H341	27:b:601:SQD:H311	1.77	0.41
4:d:272:LEU:C	4:d:272:LEU:HD23	2.44	0.41
1:A:131:TRP:CD2	1:A:131:TRP:C	2.97	0.41
24:B:615:CLA:H93	24:B:615:CLA:H111	1.73	0.41
26:B:619:BCR:H11C	26:B:619:BCR:H341	1.94	0.41
24:b:609:CLA:HBB1	24:b:609:CLA:CHC	2.41	0.41
24:A:410:CLA:H3A	24:A:410:CLA:HBA1	1.89	0.41
24:B:615:CLA:HAA1	24:B:615:CLA:HBD	2.01	0.41
3:C:334:PRO:HA	13:O:153:THR:OG1	2.20	0.41
26:C:515:BCR:H15C	26:C:515:BCR:H351	1.89	0.41
19:Z:37:LYS:HE3	34:Z:101:LMT:H4'	2.02	0.41
28:a:416:LMG:H161	28:a:416:LMG:H192	1.78	0.41
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.50	0.41
19:z:37:LYS:NZ	34:z:101:LMT:H4B	2.36	0.41
37:D:409:LHG:H111	37:D:409:LHG:H141	1.78	0.41
2:b:58:GLN:C	2:b:329:PRO:HB3	2.46	0.41
28:b:624:LMG:H301	28:b:624:LMG:H331	1.85	0.41
14:t:25[B]:GLU:OE1	42:t:1001:HOH:O	2.22	0.41
26:t:903:BCR:H20C	26:t:903:BCR:H361	1.92	0.41
37:D:409:LHG:H331	37:D:409:LHG:H302	1.67	0.41
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	2.01	0.41
35:b:626:HTG:H7'3	35:b:626:HTG:H4'1	1.80	0.41
2:B:58:GLN:C	2:B:329:PRO:HB3	2.46	0.41
2:B:348:ASN:HB3	2:B:354:LEU:HD11	2.03	0.41
3:C:147:PHE:CE2	24:C:513:CLA:HBA1	2.55	0.41
31:C:531:GOL:O3	38:V:202:HEM:O2D	2.39	0.41
24:a:409:CLA:H203	24:a:409:CLA:H161	1.76	0.41
26:B:619:BCR:C8	26:B:619:BCR:H331	2.50	0.41
31:C:531:GOL:H2	42:C:603:HOH:O	2.20	0.41
26:D:404:BCR:H312	36:D:406:DGD:HB81	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:E:101:LHG:H272	37:E:101:LHG:H242	1.81	0.41
17:Y:20:ALA:N	42:Y:202:HOH:O	2.53	0.41
24:C:512:CLA:C1B	26:C:514:BCR:H401	2.51	0.41
37:E:101:LHG:H351	37:E:101:LHG:H383	1.80	0.41
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.56	0.41
1:A:85:SER:HA	1:A:109:GLY:HA3	2.02	0.41
24:B:604:CLA:H3A	24:B:604:CLA:CGA	2.50	0.41
24:B:611:CLA:H122	24:B:616:CLA:HAA1	2.02	0.41
24:C:506:CLA:H52	34:C:520:LMT:H72	2.03	0.41
24:C:508:CLA:H162	24:C:508:CLA:H122	1.81	0.41
2:b:363:PHE:HB3	2:b:365:SER:O	2.21	0.41
3:c:52:ALA:HB2	24:c:912:CLA:HMA2	2.03	0.41
26:c:915:BCR:H24C	26:c:915:BCR:H371	1.96	0.41
26:d:406:BCR:H11C	26:d:406:BCR:H341	1.95	0.41
3:C:443:TRP:CD2	24:C:508:CLA:HMD2	2.57	0.41
24:C:505:CLA:HAA1	24:C:505:CLA:HBD	2.03	0.41
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.56	0.41
13:O:216:GLU:CD	13:O:234:LYS:HD2	2.45	0.41
15:U:45:LEU:HD23	15:U:45:LEU:HA	1.94	0.41
31:c:929:GOL:H12	13:o:20:PRO:HG3	2.02	0.41
5:e:35:TRP:CD2	6:f:39:ALA:HB2	2.55	0.41
26:t:903:BCR:H23C	26:t:903:BCR:H382	2.02	0.41
24:C:509:CLA:H141	24:C:512:CLA:HMD3	2.03	0.40
2:b:467:ILE:HG13	4:d:126:MET:HE1	2.02	0.40
3:c:390:ARG:HB3	31:c:936:GOL:H12	2.02	0.40
24:c:907:CLA:HBA2	24:c:908:CLA:H202	2.03	0.40
24:c:910:CLA:H141	24:c:913:CLA:HMD3	2.02	0.40
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.56	0.40
1:A:131:TRP:CH2	24:C:505:CLA:HAA2	2.56	0.40
2:B:423:LYS:HA	2:B:423:LYS:HD3	1.89	0.40
26:B:618:BCR:H11C	26:B:618:BCR:H341	1.91	0.40
4:D:61:HIS:HE1	4:D:80:THR:O	2.04	0.40
26:a:414:BCR:H20C	26:a:414:BCR:H361	1.93	0.40
4:d:123:ILE:HD11	36:h:102:DGD:HAE1	2.03	0.40
2:B:13:ILE:HG12	24:B:613:CLA:HAC2	2.03	0.40
3:C:189:TRP:CH2	31:C:530:GOL:H32	2.57	0.40
24:C:512:CLA:HBB1	24:C:512:CLA:HMB1	2.02	0.40
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.03	0.40
10:K:25:LEU:HB2	42:K:205:HOH:O	2.21	0.40
26:a:414:BCR:H15C	26:a:414:BCR:H351	1.96	0.40
31:c:927:GOL:H11	42:c:1121:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:401:CLA:C4A	24:d:401:CLA:HBA1	2.50	0.40
26:y:101:BCR:HC7	26:y:101:BCR:H331	1.93	0.40
34:z:101:LMT:H2B	34:z:101:LMT:O3'	2.21	0.40
3:C:215:LYS:NZ	42:C:613:HOH:O	2.53	0.40
5:E:33:ALA:HB2	20:R:11:PRO:HB2	2.02	0.40
39:H:102:RRX:H32	39:H:102:RRX:H28	1.84	0.40
4:d:24:ARG:NE	18:x:37:VAL:HG22	2.33	0.40
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.56	0.40
2:B:90:PHE:CE2	24:B:607:CLA:H151	2.56	0.40
2:B:324:LEU:HA	4:D:293[A]:LEU:HG	2.03	0.40
2:B:446:SER:HB2	2:B:447:PRO:HD2	2.04	0.40
27:a:415:SQD:H181	27:a:415:SQD:H152	1.91	0.40
27:a:415:SQD:H301	27:a:415:SQD:H331	1.89	0.40
26:b:621:BCR:H24C	26:b:621:BCR:H371	1.89	0.40
7:h:6:TRP:CD1	31:h:103:GOL:H12	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/360 (93%)	331 (99%)	3 (1%)	1 (0%)	36	35
1	a	335/360 (93%)	330 (98%)	4 (1%)	1 (0%)	36	35
2	B	510/505 (101%)	505 (99%)	5 (1%)	0	100	100
2	b	508/505 (101%)	501 (99%)	7 (1%)	0	100	100
3	C	451/473 (95%)	443 (98%)	7 (2%)	1 (0%)	43	42
3	c	457/473 (97%)	446 (98%)	9 (2%)	2 (0%)	30	27
4	D	339/342 (99%)	333 (98%)	6 (2%)	0	100	100
4	d	340/342 (99%)	333 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	79/84 (94%)	79 (100%)	0	0	100	100
5	e	77/84 (92%)	77 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	30/45 (67%)	30 (100%)	0	0	100	100
7	H	61/65 (94%)	60 (98%)	1 (2%)	0	100	100
7	h	61/65 (94%)	59 (97%)	2 (3%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
9	J	34/40 (85%)	32 (94%)	1 (3%)	1 (3%)	3	1
9	j	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
10	K	36/37 (97%)	36 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	37/37 (100%)	37 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	247/244 (101%)	241 (98%)	6 (2%)	0	100	100
13	o	242/244 (99%)	237 (98%)	5 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
16	V	136/163 (83%)	134 (98%)	2 (2%)	0	100	100
16	v	136/163 (83%)	133 (98%)	3 (2%)	0	100	100
17	Y	25/30 (83%)	25 (100%)	0	0	100	100
17	y	26/30 (87%)	26 (100%)	0	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	58/62 (94%)	56 (97%)	1 (2%)	1 (2%)	7	3
20	R	28/34 (82%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5246/5508 (95%)	5153 (98%)	86 (2%)	7 (0%)	48	46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
3	c	416[A]	SER
3	c	416[B]	SER
9	J	6	GLY
1	A	259	ILE
19	z	3	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	269/290 (93%)	269 (100%)	0	100	100
1	a	269/290 (93%)	268 (100%)	1 (0%)	84	89
2	B	403/403 (100%)	401 (100%)	2 (0%)	81	87
2	b	397/403 (98%)	395 (100%)	2 (0%)	81	87
3	C	353/374 (94%)	349 (99%)	4 (1%)	65	73
3	c	358/374 (96%)	353 (99%)	5 (1%)	59	66
4	D	275/276 (100%)	274 (100%)	1 (0%)	84	89
4	d	277/276 (100%)	275 (99%)	2 (1%)	76	82
5	E	71/73 (97%)	70 (99%)	1 (1%)	59	66
5	e	66/73 (90%)	65 (98%)	1 (2%)	57	64
6	F	27/39 (69%)	27 (100%)	0	100	100
6	f	25/39 (64%)	24 (96%)	1 (4%)	28	27
7	H	53/54 (98%)	53 (100%)	0	100	100
7	h	53/54 (98%)	53 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	30/34 (88%)	30 (100%)	0	100	100
8	i	33/34 (97%)	33 (100%)	0	100	100
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	28/30 (93%)	28 (100%)	0	100	100
10	k	27/30 (90%)	27 (100%)	0	100	100
11	L	33/35 (94%)	33 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/32 (91%)	28 (97%)	1 (3%)	32	33
12	m	31/32 (97%)	31 (100%)	0	100	100
13	O	204/207 (99%)	204 (100%)	0	100	100
13	o	202/207 (98%)	200 (99%)	2 (1%)	68	75
14	T	25/28 (89%)	25 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	82/89 (92%)	81 (99%)	1 (1%)	63	70
15	u	82/89 (92%)	82 (100%)	0	100	100
16	V	114/138 (83%)	114 (100%)	0	100	100
16	v	112/138 (81%)	111 (99%)	1 (1%)	70	78
17	Y	18/23 (78%)	17 (94%)	1 (6%)	19	16
17	y	18/23 (78%)	18 (100%)	0	100	100
18	X	30/33 (91%)	30 (100%)	0	100	100
18	x	30/33 (91%)	30 (100%)	0	100	100
19	Z	45/52 (86%)	45 (100%)	0	100	100
19	z	41/52 (79%)	40 (98%)	1 (2%)	43	47
20	R	4/29 (14%)	3 (75%)	1 (25%)	0	0
All	All	4221/4505 (94%)	4193 (99%)	28 (1%)	78	82

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	350	GLU
2	B	362	PHE
3	C	289	PHE

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Mol	Chain	Res	Type
3	C	315	MET
3	C	391	ARG
3	C	462	GLU
4	D	90	LEU
5	E	4	THR
12	M	5	GLN
15	U	70	ARG
17	Y	30	ILE
1	a	12	ASN
2	b	362	PHE
2	b	479	PHE
3	c	21	ILE
3	c	289	PHE
3	c	315	MET
3	c	391[A]	ARG
3	c	391[B]	ARG
4	d	24	ARG
4	d	90	LEU
5	e	7	GLU
6	f	15	ILE
13	o	181	GLU
13	o	182	LEU
16	v	23	GLU
19	z	4	LEU
20	R	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
4	D	61	HIS
4	D	186	GLN
4	D	255	GLN
5	E	74	GLN
13	O	88	ASN
15	U	78	ASN
15	U	81	HIS
1	a	165	GLN
1	a	296	ASN
2	b	289	GLN
2	b	331	ASN
3	c	44	ASN

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Mol	Chain	Res	Type
4	d	186	GLN
4	d	301	GLN
6	f	44	GLN
15	u	78	ASN
15	u	81	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
14	FME	t	1	14	8,9,10	0.69	0	7,9,11	1.38	1 (14%)
12	FME	M	1	12	8,9,10	0.60	0	7,9,11	1.89	3 (42%)
8	FME	I	1	8	8,9,10	0.63	0	7,9,11	1.64	2 (28%)
12	FME	m	1	12	8,9,10	0.70	0	7,9,11	1.81	3 (42%)
4	HSK	D	336[A]	-	9,10,12	5.24	1 (11%)	6,12,16	1.74	2 (33%)
4	HSK	D	336[B]	-	9,11,12	1.92	2 (22%)	6,14,16	3.76	4 (66%)
8	FME	i	1	8	8,9,10	0.58	0	7,9,11	1.48	1 (14%)
4	HSK	d	336[A]	-	9,10,12	13.67	1 (11%)	6,12,16	1.60	2 (33%)
4	HSK	d	336[B]	-	9,11,12	1.69	2 (22%)	6,14,16	4.07	4 (66%)
14	FME	T	1	14	8,9,10	0.68	0	7,9,11	1.54	1 (14%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336[A]	HSK	OM-ND1	40.87	1.92	1.38
4	D	336[A]	HSK	OM-ND1	-15.34	1.18	1.38
4	D	336[B]	HSK	OM-ND1	4.37	1.44	1.38
4	d	336[B]	HSK	OM-ND1	3.33	1.43	1.38
4	d	336[B]	HSK	CE1-ND1	-2.60	1.32	1.37
4	D	336[B]	HSK	CE1-ND1	-2.33	1.33	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	336[B]	HSK	ND1-CE1-NE2	-6.24	103.94	111.75
4	D	336[B]	HSK	ND1-CE1-NE2	-5.79	104.50	111.75
4	d	336[B]	HSK	CE1-ND1-CG	5.77	114.76	107.37
4	D	336[B]	HSK	CE1-ND1-CG	5.55	114.47	107.37
4	d	336[B]	HSK	CD2-NE2-CE1	3.78	109.83	105.22
4	d	336[B]	HSK	CB-CG-ND1	3.35	128.53	122.89
12	m	1	FME	CE-SD-CG	3.28	111.68	100.40
4	D	336[B]	HSK	CD2-NE2-CE1	3.27	109.20	105.22
12	M	1	FME	CE-SD-CG	3.17	111.29	100.40
4	D	336[B]	HSK	CB-CG-ND1	2.74	127.51	122.89
14	t	1	FME	O-C-CA	-2.72	117.66	124.78
8	I	1	FME	CA-N-CN	-2.70	118.66	122.82
12	M	1	FME	CA-N-CN	-2.57	118.87	122.82
14	T	1	FME	O-C-CA	-2.57	118.06	124.78
4	D	336[A]	HSK	ND1-CE1-NE2	-2.47	108.66	111.75
4	D	336[A]	HSK	CD2-NE2-CE1	2.38	108.11	105.22
8	i	1	FME	CE-SD-CG	2.35	108.46	100.40
12	m	1	FME	O-C-CA	-2.32	118.71	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1	FME	O1-CN-N	-2.16	119.58	125.27
8	I	1	FME	O-C-CA	-2.13	119.21	124.78
4	d	336[A]	HSK	ND1-CE1-NE2	-2.11	109.11	111.75
4	d	336[A]	HSK	CD2-NE2-CE1	2.10	107.78	105.22
12	M	1	FME	O1-CN-N	-2.01	119.97	125.27

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 310 ligands modelled in this entry, 15 are monoatomic and 55 are unknown - leaving 240 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$
34	LMT	b	625	-	25,25,36	0.53	1 (4%)	30,30,47	1.11	2 (6%)
31	GOL	f	104	33	5,5,5	0.99	0	5,5,5	0.93	0
24	CLA	c	903	3	69,73,73	2.39	24 (34%)	83,113,113	2.44	29 (34%)
31	GOL	Z	102	-	5,5,5	0.88	0	5,5,5	1.01	0
31	GOL	c	936	-	5,5,5	0.93	0	5,5,5	0.96	0
37	LHG	d	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.02	5 (9%)
21	OEX	A	401	1,42,3	0,14,14	-	-	-	-	-
28	LMG	C	534	-	51,51,55	1.00	3 (5%)	59,59,63	1.31	6 (10%)
31	GOL	B	631	-	5,5,5	0.86	0	5,5,5	0.93	0
26	BCR	c	916	-	41,41,41	0.81	0	56,56,56	1.33	7 (12%)
24	CLA	B	603	2	69,73,73	2.42	23 (33%)	83,113,113	2.50	29 (34%)
24	CLA	b	619	2	69,73,73	2.35	22 (31%)	83,113,113	2.38	25 (30%)
31	GOL	c	934	-	5,5,5	0.82	0	5,5,5	1.12	0
37	LHG	d	408	-	48,48,48	0.90	2 (4%)	51,54,54	1.12	4 (7%)
24	CLA	B	608	42	69,73,73	2.30	22 (31%)	83,113,113	2.47	26 (31%)
26	BCR	T	702	-	41,41,41	0.73	0	56,56,56	1.55	11 (19%)
35	HTG	b	603	-	19,19,19	1.04	2 (10%)	23,24,24	1.08	1 (4%)
25	PHO	A	408	-	58,69,69	2.53	13 (22%)	56,99,99	2.81	14 (25%)
35	HTG	H	105	-	14,16,19	1.05	1 (7%)	15,18,24	1.43	1 (6%)
31	GOL	O	304	-	5,5,5	0.88	0	5,5,5	1.00	0
31	GOL	V	206	-	5,5,5	0.84	0	5,5,5	1.01	0
24	CLA	B	606	2	69,73,73	2.32	21 (30%)	83,113,113	2.46	24 (28%)
35	HTG	c	923	-	19,19,19	1.04	2 (10%)	23,24,24	1.20	1 (4%)
38	HEM	V	202	16	50,50,50	1.90	8 (16%)	66,82,82	1.47	7 (10%)
31	GOL	c	929	-	5,5,5	0.92	0	5,5,5	1.01	0
24	CLA	d	405	4	69,73,73	2.38	25 (36%)	83,113,113	2.54	30 (36%)
34	LMT	J	102	-	23,23,36	0.61	1 (4%)	28,28,47	0.92	1 (3%)
35	HTG	X	902	-	11,12,19	0.63	0	14,17,24	0.93	1 (7%)
24	CLA	b	607	2	69,73,73	2.42	24 (34%)	83,113,113	2.42	29 (34%)
36	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	1.00	4 (5%)
34	LMT	c	922	-	36,36,36	0.48	1 (2%)	47,47,47	0.82	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	b	623	-	41,41,41	0.70	0	56,56,56	1.36	8 (14%)
31	GOL	b	631	-	5,5,5	0.73	0	5,5,5	1.03	0
24	CLA	D	403	4	69,73,73	2.45	24 (34%)	83,113,113	2.54	31 (37%)
34	LMT	C	520	-	36,36,36	0.47	0	47,47,47	1.23	4 (8%)
24	CLA	b	609	2	69,73,73	2.27	24 (34%)	83,113,113	2.59	28 (33%)
35	HTG	o	301	-	19,19,19	1.11	1 (5%)	23,24,24	1.09	1 (4%)
27	SQD	B	621	-	53,54,54	1.06	4 (7%)	62,65,65	1.53	10 (16%)
35	HTG	C	522	-	19,19,19	0.99	1 (5%)	23,24,24	1.74	4 (17%)
24	CLA	C	501	3	69,73,73	2.36	22 (31%)	83,113,113	2.49	25 (30%)
24	CLA	C	512	3	69,73,73	2.66	23 (33%)	83,113,113	2.54	28 (33%)
24	CLA	b	617	2	69,73,73	2.38	24 (34%)	83,113,113	2.56	28 (33%)
24	CLA	C	513	3	69,73,73	2.53	25 (36%)	83,113,113	2.38	25 (30%)
24	CLA	b	616	2	69,73,73	2.41	22 (31%)	83,113,113	2.50	24 (28%)
24	CLA	c	904	3	69,73,73	2.71	24 (34%)	83,113,113	2.29	26 (31%)
29	PL9	a	417	-	55,55,55	0.64	2 (3%)	68,69,69	1.92	20 (29%)
31	GOL	A	422	-	5,5,5	1.18	1 (20%)	5,5,5	0.94	0
37	LHG	e	101	-	26,26,48	0.95	1 (3%)	28,31,54	1.01	2 (7%)
24	CLA	B	615	2	69,73,73	2.27	21 (30%)	83,113,113	2.72	29 (34%)
31	GOL	C	525	-	5,5,5	1.16	0	5,5,5	0.80	0
31	GOL	a	421	-	5,5,5	1.11	0	5,5,5	0.95	0
27	SQD	A	412	-	51,52,54	0.99	3 (5%)	60,63,65	1.74	12 (20%)
26	BCR	b	621	-	41,41,41	0.82	1 (2%)	56,56,56	1.40	7 (12%)
35	HTG	U	201	-	8,8,19	0.37	0	7,7,24	1.17	1 (14%)
27	SQD	a	415	-	53,54,54	0.96	3 (5%)	62,65,65	1.74	11 (17%)
24	CLA	C	510	3	69,73,73	2.52	25 (36%)	83,113,113	2.50	30 (36%)
27	SQD	f	102	-	31,32,54	1.97	4 (12%)	34,36,65	1.62	5 (14%)
26	BCR	B	619	-	41,41,41	0.88	0	56,56,56	1.21	9 (16%)
35	HTG	b	602	-	19,19,19	1.09	2 (10%)	23,24,24	1.54	3 (13%)
31	GOL	C	533	-	5,5,5	0.83	0	5,5,5	1.08	0
36	DGD	e	102	-	39,39,67	1.12	2 (5%)	47,47,81	1.70	9 (19%)
26	BCR	k	101	-	41,41,41	0.70	0	56,56,56	1.44	8 (14%)
24	CLA	b	606	2	69,73,73	2.44	23 (33%)	83,113,113	2.41	28 (33%)
24	CLA	b	613	2	69,73,73	2.64	24 (34%)	83,113,113	2.48	31 (37%)
27	SQD	b	601	-	53,54,54	1.05	3 (5%)	62,65,65	1.74	11 (17%)
26	BCR	C	514	-	41,41,41	0.73	0	56,56,56	1.44	8 (14%)
31	GOL	c	937	-	5,5,5	0.94	0	5,5,5	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SQD	a	401	-	53,54,54	1.02	3 (5%)	62,65,65	1.24	4 (6%)
28	LMG	c	921	-	51,51,55	0.94	2 (3%)	59,59,63	1.25	7 (11%)
36	DGD	c	919	-	61,61,67	0.85	3 (4%)	75,75,81	0.99	4 (5%)
34	LMT	t	904	-	24,24,36	0.57	1 (4%)	29,29,47	0.89	1 (3%)
35	HTG	u	201	-	10,13,19	1.11	1 (10%)	13,14,24	1.60	1 (7%)
24	CLA	a	410	42	69,73,73	2.34	21 (30%)	83,113,113	2.62	30 (36%)
24	CLA	c	914	3	69,73,73	2.47	24 (34%)	83,113,113	2.35	24 (28%)
26	BCR	A	411	-	41,41,41	0.72	0	56,56,56	1.35	6 (10%)
26	BCR	K	101	-	41,41,41	0.74	0	56,56,56	1.44	7 (12%)
28	LMG	A	413	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	5 (8%)
34	LMT	Z	101	-	36,36,36	0.43	0	47,47,47	0.87	0
24	CLA	C	507	42	69,73,73	2.55	25 (36%)	83,113,113	2.51	29 (34%)
35	HTG	C	521	-	19,19,19	0.96	2 (10%)	23,24,24	1.19	1 (4%)
24	CLA	B	604	2	69,73,73	2.38	23 (33%)	83,113,113	2.58	27 (32%)
35	HTG	V	203	-	12,13,19	0.53	0	16,18,24	2.40	4 (25%)
34	LMT	B	623	-	36,36,36	0.43	0	47,47,47	1.29	7 (14%)
24	CLA	c	912	3	69,73,73	2.46	20 (28%)	83,113,113	2.51	32 (38%)
24	CLA	c	908	42	69,73,73	2.48	24 (34%)	83,113,113	2.50	28 (33%)
24	CLA	B	614	2	69,73,73	2.33	22 (31%)	83,113,113	2.56	29 (34%)
24	CLA	D	402	4	69,73,73	2.11	23 (33%)	83,113,113	2.66	30 (36%)
31	GOL	b	640	-	5,5,5	0.90	0	5,5,5	1.07	0
31	GOL	C	530	-	5,5,5	1.00	0	5,5,5	1.05	0
31	GOL	c	938	-	5,5,5	0.96	0	5,5,5	1.05	0
24	CLA	c	905	42	69,73,73	2.34	25 (36%)	83,113,113	2.69	29 (34%)
24	CLA	c	907	3	69,73,73	2.66	25 (36%)	83,113,113	2.37	28 (33%)
26	BCR	b	622	-	41,41,41	0.79	0	56,56,56	1.17	7 (12%)
34	LMT	T	703	-	24,24,36	0.44	0	29,29,47	1.35	2 (6%)
24	CLA	C	503	3	69,73,73	2.55	24 (34%)	83,113,113	2.39	26 (31%)
31	GOL	c	926	-	5,5,5	1.03	0	5,5,5	0.83	0
31	GOL	V	201	33	5,5,5	0.78	0	5,5,5	1.04	0
34	LMT	a	402	-	36,36,36	0.50	1 (2%)	47,47,47	0.95	2 (4%)
26	BCR	B	620	-	41,41,41	0.74	0	56,56,56	1.25	3 (5%)
24	CLA	b	614	42	69,73,73	2.30	22 (31%)	83,113,113	2.49	27 (32%)
28	LMG	B	622	-	51,51,55	0.95	2 (3%)	59,59,63	1.14	4 (6%)
29	PL9	D	405	-	55,55,55	0.75	2 (3%)	68,69,69	1.53	15 (22%)
34	LMT	M	303	-	36,36,36	0.42	0	47,47,47	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GOL	o	303	-	5,5,5	0.85	0	5,5,5	0.90	0
31	GOL	u	203	-	5,5,5	1.04	0	5,5,5	0.91	0
26	BCR	c	915	-	41,41,41	0.75	0	56,56,56	1.43	8 (14%)
31	GOL	L	102	-	5,5,5	1.12	0	5,5,5	1.01	0
24	CLA	C	502	3	69,73,73	2.58	24 (34%)	83,113,113	2.37	26 (31%)
35	HTG	B	627	-	19,19,19	0.99	1 (5%)	23,24,24	1.45	2 (8%)
37	LHG	d	410	-	39,39,48	1.04	2 (5%)	42,45,54	0.97	3 (7%)
25	PHO	A	409	-	58,69,69	2.66	13 (22%)	56,99,99	2.91	14 (25%)
24	CLA	C	504	42	69,73,73	2.42	24 (34%)	83,113,113	2.48	25 (30%)
31	GOL	O	305	-	5,5,5	0.84	0	5,5,5	1.04	0
37	LHG	L	101	-	48,48,48	0.91	3 (6%)	51,54,54	0.95	2 (3%)
24	CLA	b	611	42	69,73,73	2.39	24 (34%)	83,113,113	2.47	30 (36%)
24	CLA	b	620	2	69,73,73	2.39	22 (31%)	83,113,113	2.49	26 (31%)
24	CLA	B	613	2	69,73,73	2.22	22 (31%)	83,113,113	2.58	24 (28%)
24	CLA	B	607	2	69,73,73	2.40	22 (31%)	83,113,113	2.54	31 (37%)
24	CLA	B	616	2	69,73,73	2.50	22 (31%)	83,113,113	2.49	26 (31%)
35	HTG	b	627	-	19,19,19	1.03	1 (5%)	23,24,24	1.74	2 (8%)
36	DGD	H	103	-	63,63,67	0.90	3 (4%)	77,77,81	0.89	2 (2%)
31	GOL	o	304	-	5,5,5	0.90	0	5,5,5	1.00	0
31	GOL	t	902	-	5,5,5	1.06	0	5,5,5	1.07	0
34	LMT	D	401	-	36,36,36	0.43	0	47,47,47	0.95	0
28	LMG	D	410	40	48,48,55	0.84	2 (4%)	56,56,63	0.99	3 (5%)
28	LMG	a	416	-	51,51,55	0.90	2 (3%)	59,59,63	1.23	4 (6%)
35	HTG	B	625	-	19,19,19	0.98	1 (5%)	23,24,24	1.82	3 (13%)
35	HTG	b	626	-	19,19,19	0.83	1 (5%)	23,24,24	1.42	1 (4%)
21	OEX	a	404	1,42,3	0,14,14	-	-	-	-	-
31	GOL	B	633	-	5,5,5	1.42	1 (20%)	5,5,5	0.95	0
31	GOL	a	419	-	5,5,5	1.01	0	5,5,5	1.02	0
24	CLA	b	605	42	69,73,73	2.50	24 (34%)	83,113,113	2.37	25 (30%)
24	CLA	A	405	1	69,73,73	2.39	23 (33%)	83,113,113	2.46	27 (32%)
25	PHO	a	411	-	58,69,69	2.52	12 (20%)	56,99,99	2.77	14 (25%)
27	SQD	F	101	-	36,37,54	1.00	2 (5%)	44,47,65	1.46	6 (13%)
31	GOL	B	629	-	5,5,5	1.02	0	5,5,5	0.93	0
31	GOL	V	204	-	5,5,5	1.40	2 (40%)	5,5,5	0.92	0
34	LMT	F	103	-	27,27,36	0.54	1 (3%)	37,38,47	0.89	0
28	LMG	C	519	-	49,49,55	0.96	2 (4%)	57,57,63	1.17	6 (10%)
31	GOL	b	630	-	5,5,5	0.92	0	5,5,5	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LHG	E	101	-	48,48,48	0.96	2 (4%)	51,54,54	1.00	2 (3%)
31	GOL	b	632	-	5,5,5	1.02	0	5,5,5	1.18	1 (20%)
31	GOL	B	632	-	5,5,5	0.49	0	5,5,5	1.13	0
26	BCR	y	101	-	41,41,41	0.74	1 (2%)	56,56,56	1.59	10 (17%)
32	BCT	A	421	22	2,3,3	0.65	0	2,3,3	0.66	0
24	CLA	c	909	3	69,73,73	2.52	25 (36%)	83,113,113	2.49	27 (32%)
36	DGD	C	518	-	59,59,67	0.90	2 (3%)	73,73,81	1.08	4 (5%)
24	CLA	b	612	2	69,73,73	2.60	24 (34%)	83,113,113	2.42	28 (33%)
28	LMG	d	411	40	48,48,55	0.95	2 (4%)	56,56,63	0.91	3 (5%)
31	GOL	O	306	-	5,5,5	0.90	0	5,5,5	0.98	0
31	GOL	c	939	-	5,5,5	0.90	0	5,5,5	1.19	1 (20%)
31	GOL	a	420	-	5,5,5	0.85	0	5,5,5	1.09	1 (20%)
31	GOL	b	629	-	5,5,5	0.91	0	5,5,5	0.98	0
34	LMT	m	1502	-	36,36,36	0.49	0	47,47,47	0.90	1 (2%)
31	GOL	b	638	-	5,5,5	0.83	0	5,5,5	1.07	0
36	DGD	C	517	-	57,57,67	0.88	2 (3%)	71,71,81	0.97	4 (5%)
26	BCR	t	903	-	41,41,41	0.73	0	56,56,56	1.62	15 (26%)
37	LHG	D	407	-	48,48,48	0.84	2 (4%)	51,54,54	1.16	3 (5%)
35	HTG	d	403	-	19,19,19	1.10	2 (10%)	23,24,24	1.39	2 (8%)
37	LHG	b	639	-	48,48,48	0.91	3 (6%)	51,54,54	0.90	3 (5%)
35	HTG	O	303	-	19,19,19	1.06	1 (5%)	23,24,24	1.03	2 (8%)
24	CLA	d	404	4	69,73,73	2.40	24 (34%)	83,113,113	2.54	28 (33%)
26	BCR	Y	101	-	41,41,41	0.79	0	56,56,56	1.57	8 (14%)
31	GOL	V	205	-	5,5,5	0.94	0	5,5,5	0.94	0
27	SQD	A	417	-	53,54,54	1.05	3 (5%)	62,65,65	1.24	8 (12%)
31	GOL	c	928	-	5,5,5	0.83	0	5,5,5	1.05	1 (20%)
26	BCR	C	515	-	41,41,41	0.71	0	56,56,56	1.38	5 (8%)
41	SO4	O	302	-	4,4,4	0.19	0	6,6,6	0.08	0
32	BCT	a	408	22	2,3,3	0.61	0	2,3,3	0.64	0
24	CLA	c	906	3	69,73,73	2.47	24 (34%)	83,113,113	2.45	26 (31%)
34	LMT	M	302	-	36,36,36	0.56	1 (2%)	47,47,47	0.93	2 (4%)
39	RRX	h	101	-	42,42,42	0.72	0	57,58,58	1.33	7 (12%)
31	GOL	A	420	-	5,5,5	1.09	0	5,5,5	0.94	0
37	LHG	D	408	-	48,48,48	0.88	2 (4%)	51,54,54	1.04	4 (7%)
31	GOL	b	628	-	5,5,5	0.72	0	5,5,5	1.17	1 (20%)
31	GOL	B	628	-	5,5,5	0.79	0	5,5,5	0.88	0
38	HEM	F	102	6,5	50,50,50	1.88	10 (20%)	66,82,82	1.53	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GOL	h	103	-	5,5,5	0.90	0	5,5,5	0.97	0
31	GOL	c	932	-	5,5,5	0.75	0	5,5,5	1.14	1 (20%)
28	LMG	b	624	-	51,51,55	0.90	2 (3%)	59,59,63	1.19	4 (6%)
24	CLA	a	413	1	69,73,73	2.27	22 (31%)	83,113,113	2.55	29 (34%)
36	DGD	c	918	-	56,56,67	0.93	2 (3%)	70,70,81	0.98	1 (1%)
24	CLA	d	401	42	69,73,73	2.28	23 (33%)	83,113,113	2.79	35 (42%)
24	CLA	a	409	1	69,73,73	2.32	23 (33%)	83,113,113	2.57	27 (32%)
39	RRX	H	102	-	42,42,42	0.72	0	57,58,58	1.35	6 (10%)
29	PL9	d	407	-	55,55,55	0.71	1 (1%)	68,69,69	1.47	13 (19%)
24	CLA	B	610	2	69,73,73	2.44	21 (30%)	83,113,113	2.44	29 (34%)
24	CLA	C	509	3	69,73,73	2.46	24 (34%)	83,113,113	2.42	27 (32%)
24	CLA	b	615	2	69,73,73	2.48	23 (33%)	83,113,113	2.53	30 (36%)
26	BCR	d	406	-	41,41,41	0.77	0	56,56,56	1.82	13 (23%)
24	CLA	A	406	42	69,73,73	2.26	22 (31%)	83,113,113	2.60	28 (33%)
25	PHO	a	412	-	58,69,69	2.65	12 (20%)	56,99,99	2.77	13 (23%)
35	HTG	B	624	-	19,19,19	0.81	1 (5%)	23,24,24	1.36	1 (4%)
31	GOL	H	101	-	5,5,5	0.98	0	5,5,5	1.08	0
24	CLA	C	508	3	69,73,73	2.47	24 (34%)	83,113,113	2.42	24 (28%)
35	HTG	B	626	-	19,19,19	1.05	2 (10%)	23,24,24	1.51	4 (17%)
36	DGD	c	917	-	63,63,67	0.79	2 (3%)	77,77,81	1.11	6 (7%)
24	CLA	c	913	3	69,73,73	2.55	24 (34%)	83,113,113	2.60	29 (34%)
28	LMG	c	920	-	51,51,55	0.95	2 (3%)	59,59,63	1.04	2 (3%)
24	CLA	B	605	2	69,73,73	2.63	23 (33%)	83,113,113	2.55	26 (31%)
36	DGD	C	516	-	63,63,67	0.83	2 (3%)	77,77,81	1.05	6 (7%)
24	CLA	c	902	3	69,73,73	2.40	23 (33%)	83,113,113	2.62	27 (32%)
31	GOL	v	201	-	5,5,5	0.82	0	5,5,5	1.06	0
31	GOL	B	630	-	5,5,5	1.21	1 (20%)	5,5,5	0.45	0
38	HEM	v	202	16	50,50,50	1.84	9 (18%)	66,82,82	1.44	7 (10%)
31	GOL	v	203	-	5,5,5	1.19	0	5,5,5	0.79	0
24	CLA	B	612	2	69,73,73	2.28	22 (31%)	83,113,113	2.53	27 (32%)
31	GOL	C	531	-	5,5,5	0.89	0	5,5,5	1.19	0
24	CLA	B	617	2	69,73,73	2.30	23 (33%)	83,113,113	2.60	27 (32%)
31	GOL	C	524	-	5,5,5	0.89	0	5,5,5	1.03	0
34	LMT	m	1503	-	36,36,36	0.60	1 (2%)	47,47,47	1.09	4 (8%)
24	CLA	B	611	42	69,73,73	2.44	24 (34%)	83,113,113	2.51	30 (36%)
24	CLA	b	610	2	69,73,73	2.36	22 (31%)	83,113,113	2.44	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	a	414	-	41,41,41	0.76	0	56,56,56	1.19	3 (5%)
38	HEM	f	101	6,5	50,50,50	1.89	9 (18%)	66,82,82	1.45	7 (10%)
31	GOL	c	927	-	5,5,5	1.12	0	5,5,5	1.11	1 (20%)
24	CLA	b	618	2	69,73,73	2.31	21 (30%)	83,113,113	2.67	31 (37%)
26	BCR	D	404	-	41,41,41	0.80	0	56,56,56	1.70	9 (16%)
31	GOL	A	419	-	5,5,5	0.83	0	5,5,5	1.26	1 (20%)
26	BCR	B	618	-	41,41,41	0.73	0	56,56,56	1.33	4 (7%)
31	GOL	u	202	-	5,5,5	0.92	0	5,5,5	0.89	0
24	CLA	c	911	3	69,73,73	2.39	23 (33%)	83,113,113	2.46	31 (37%)
31	GOL	v	204	-	5,5,5	0.77	0	5,5,5	1.07	0
29	PL9	A	414	-	55,55,55	0.62	2 (3%)	68,69,69	1.91	20 (29%)
24	CLA	B	609	2	69,73,73	2.38	24 (34%)	83,113,113	2.46	27 (32%)
35	HTG	C	528	-	19,19,19	1.11	2 (10%)	23,24,24	1.59	4 (17%)
35	HTG	c	924	-	19,19,19	0.99	2 (10%)	23,24,24	1.69	3 (13%)
37	LHG	D	409	-	45,45,48	0.93	2 (4%)	48,51,54	1.03	4 (8%)
24	CLA	A	407	42	69,73,73	2.20	22 (31%)	83,113,113	2.61	29 (34%)
24	CLA	A	410	1	69,73,73	2.24	24 (34%)	83,113,113	2.63	29 (34%)
24	CLA	b	608	2	69,73,73	2.69	24 (34%)	83,113,113	2.51	30 (36%)
24	CLA	C	511	3	69,73,73	2.48	23 (33%)	83,113,113	2.41	27 (32%)
24	CLA	C	505	3	69,73,73	2.61	25 (36%)	83,113,113	2.31	24 (28%)
24	CLA	C	506	3	69,73,73	2.54	25 (36%)	83,113,113	2.41	29 (34%)
24	CLA	B	602	42	69,73,73	2.61	26 (37%)	83,113,113	2.38	25 (30%)
35	HTG	v	205	-	12,13,19	0.75	0	16,18,24	1.64	5 (31%)
36	DGD	D	406	-	53,53,67	0.98	2 (3%)	60,61,81	1.32	7 (11%)
24	CLA	c	910	3	69,73,73	2.58	26 (37%)	83,113,113	2.34	27 (32%)
34	LMT	z	101	-	32,32,36	0.49	0	42,42,47	0.92	1 (2%)
31	GOL	C	527	-	5,5,5	0.82	0	5,5,5	1.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMT	b	625	-	-	4/17/37/61	0/1/1/2
31	GOL	f	104	33	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	903	3	-	3/39/115/115	-
31	GOL	Z	102	-	-	0/4/4/4	-
31	GOL	c	936	-	-	2/4/4/4	-
37	LHG	d	409	-	-	11/53/53/53	-
28	LMG	C	534	-	-	9/46/66/70	0/1/1/1
31	GOL	B	631	-	-	2/4/4/4	-
26	BCR	c	916	-	-	2/29/63/63	0/2/2/2
24	CLA	B	603	2	-	5/39/115/115	-
24	CLA	b	619	2	-	9/39/115/115	-
31	GOL	c	934	-	-	4/4/4/4	-
37	LHG	d	408	-	-	6/53/53/53	-
24	CLA	B	608	42	-	1/39/115/115	-
26	BCR	T	702	-	-	1/29/63/63	0/2/2/2
35	HTG	b	603	-	-	1/10/30/30	0/1/1/1
25	PHO	A	408	-	-	4/37/103/103	0/5/6/6
35	HTG	H	105	-	-	3/10/20/30	0/1/1/1
31	GOL	O	304	-	-	0/4/4/4	-
31	GOL	V	206	-	-	0/4/4/4	-
24	CLA	B	606	2	-	4/39/115/115	-
35	HTG	c	923	-	-	1/10/30/30	0/1/1/1
38	HEM	V	202	16	-	4/14/54/54	-
31	GOL	c	929	-	-	2/4/4/4	-
24	CLA	d	405	4	-	8/39/115/115	-
34	LMT	J	102	-	-	3/13/33/61	0/1/1/2
35	HTG	X	902	-	-	2/2/22/30	0/1/1/1
24	CLA	b	607	2	-	5/39/115/115	-
36	DGD	h	102	-	-	5/51/91/95	0/2/2/2
34	LMT	c	922	-	-	2/21/61/61	0/2/2/2
26	BCR	b	623	-	-	2/29/63/63	0/2/2/2
31	GOL	b	631	-	-	2/4/4/4	-
24	CLA	D	403	4	-	8/39/115/115	-
34	LMT	C	520	-	-	8/21/61/61	0/2/2/2
24	CLA	b	609	2	-	3/39/115/115	-
35	HTG	o	301	-	-	1/10/30/30	0/1/1/1
27	SQD	B	621	-	-	25/49/69/69	0/1/1/1
35	HTG	C	522	-	-	2/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	501	3	-	4/39/115/115	-
24	CLA	C	512	3	-	8/39/115/115	-
24	CLA	b	617	2	-	3/39/115/115	-
24	CLA	C	513	3	-	5/39/115/115	-
24	CLA	b	616	2	-	3/39/115/115	-
24	CLA	c	904	3	-	5/39/115/115	-
29	PL9	a	417	-	-	10/53/73/73	0/1/1/1
31	GOL	A	422	-	-	2/4/4/4	-
37	LHG	e	101	-	-	3/30/30/53	-
24	CLA	B	615	2	-	5/39/115/115	-
31	GOL	C	525	-	-	0/4/4/4	-
31	GOL	a	421	-	-	4/4/4/4	-
27	SQD	A	412	-	-	10/47/67/69	0/1/1/1
26	BCR	b	621	-	-	2/29/63/63	0/2/2/2
35	HTG	U	201	-	-	1/6/6/30	-
27	SQD	a	415	-	-	10/49/69/69	0/1/1/1
24	CLA	C	510	3	-	6/39/115/115	-
27	SQD	f	102	-	-	11/33/33/69	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
35	HTG	b	602	-	-	2/10/30/30	0/1/1/1
31	GOL	C	533	-	-	2/4/4/4	-
36	DGD	e	102	-	-	4/33/53/95	0/1/1/2
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2
24	CLA	b	606	2	-	3/39/115/115	-
24	CLA	b	613	2	-	4/39/115/115	-
27	SQD	b	601	-	-	28/49/69/69	0/1/1/1
26	BCR	C	514	-	-	3/29/63/63	0/2/2/2
31	GOL	c	937	-	-	2/4/4/4	-
27	SQD	a	401	-	-	14/49/69/69	0/1/1/1
28	LMG	c	921	-	-	4/46/66/70	0/1/1/1
36	DGD	c	919	-	-	6/49/89/95	0/2/2/2
34	LMT	t	904	-	-	9/15/35/61	0/1/1/2
35	HTG	u	201	-	-	6/12/14/30	-
24	CLA	a	410	42	-	6/39/115/115	-
24	CLA	c	914	3	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	A	411	-	-	0/29/63/63	0/2/2/2
26	BCR	K	101	-	-	1/29/63/63	0/2/2/2
28	LMG	A	413	-	-	17/46/66/70	0/1/1/1
34	LMT	Z	101	-	-	10/21/61/61	0/2/2/2
24	CLA	C	507	42	-	5/39/115/115	-
35	HTG	C	521	-	-	1/10/30/30	0/1/1/1
24	CLA	B	604	2	-	4/39/115/115	-
35	HTG	V	203	-	-	1/4/24/30	0/1/1/1
34	LMT	B	623	-	-	10/21/61/61	0/2/2/2
24	CLA	c	912	3	-	1/39/115/115	-
24	CLA	c	908	42	-	8/39/115/115	-
24	CLA	B	614	2	-	6/39/115/115	-
24	CLA	D	402	4	-	3/39/115/115	-
31	GOL	b	640	-	-	0/4/4/4	-
31	GOL	C	530	-	-	0/4/4/4	-
31	GOL	c	938	-	-	2/4/4/4	-
24	CLA	c	905	42	-	7/39/115/115	-
24	CLA	c	907	3	-	6/39/115/115	-
26	BCR	b	622	-	-	0/29/63/63	0/2/2/2
34	LMT	T	703	-	-	12/15/35/61	0/1/1/2
24	CLA	C	503	3	-	4/39/115/115	-
31	GOL	c	926	-	-	2/4/4/4	-
31	GOL	V	201	33	-	3/4/4/4	-
34	LMT	a	402	-	-	6/21/61/61	0/2/2/2
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
24	CLA	b	614	42	-	8/39/115/115	-
28	LMG	B	622	-	-	10/46/66/70	0/1/1/1
29	PL9	D	405	-	-	3/53/73/73	0/1/1/1
34	LMT	M	303	-	-	1/21/61/61	0/2/2/2
31	GOL	o	303	-	-	2/4/4/4	-
31	GOL	u	203	-	-	0/4/4/4	-
26	BCR	c	915	-	-	1/29/63/63	0/2/2/2
31	GOL	L	102	-	-	0/4/4/4	-
24	CLA	C	502	3	-	7/39/115/115	-
35	HTG	B	627	-	-	1/10/30/30	0/1/1/1
37	LHG	d	410	-	-	10/44/44/53	-
25	PHO	A	409	-	-	3/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	504	42	-	7/39/115/115	-
31	GOL	O	305	-	-	2/4/4/4	-
37	LHG	L	101	-	-	8/53/53/53	-
24	CLA	b	611	42	-	1/39/115/115	-
24	CLA	b	620	2	-	7/39/115/115	-
24	CLA	B	613	2	-	4/39/115/115	-
24	CLA	B	607	2	-	5/39/115/115	-
24	CLA	B	616	2	-	10/39/115/115	-
35	HTG	b	627	-	-	3/10/30/30	0/1/1/1
36	DGD	H	103	-	-	4/51/91/95	0/2/2/2
31	GOL	o	304	-	-	2/4/4/4	-
31	GOL	t	902	-	-	1/4/4/4	-
34	LMT	D	401	-	-	5/21/61/61	0/2/2/2
28	LMG	D	410	40	-	7/43/63/70	0/1/1/1
28	LMG	a	416	-	-	13/46/66/70	0/1/1/1
35	HTG	B	625	-	-	3/10/30/30	0/1/1/1
35	HTG	b	626	-	-	2/10/30/30	0/1/1/1
31	GOL	a	419	-	-	1/4/4/4	-
31	GOL	B	633	-	-	0/4/4/4	-
24	CLA	b	605	42	-	8/39/115/115	-
24	CLA	A	405	1	-	4/39/115/115	-
25	PHO	a	411	-	-	5/37/103/103	0/5/6/6
27	SQD	F	101	-	-	9/30/50/69	0/1/1/1
31	GOL	B	629	-	-	0/4/4/4	-
31	GOL	V	204	-	-	1/4/4/4	-
34	LMT	F	103	-	-	2/12/52/61	0/2/2/2
28	LMG	C	519	-	-	9/44/64/70	0/1/1/1
31	GOL	b	630	-	-	0/4/4/4	-
37	LHG	E	101	-	-	16/53/53/53	-
31	GOL	b	632	-	-	2/4/4/4	-
31	GOL	B	632	-	-	0/4/4/4	-
26	BCR	y	101	-	-	5/29/63/63	0/2/2/2
36	DGD	C	518	-	-	4/47/87/95	0/2/2/2
24	CLA	c	909	3	-	3/39/115/115	-
24	CLA	b	612	2	-	2/39/115/115	-
28	LMG	d	411	40	-	11/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GOL	O	306	-	-	2/4/4/4	-
31	GOL	c	939	-	-	0/4/4/4	-
31	GOL	a	420	-	-	2/4/4/4	-
31	GOL	b	629	-	-	2/4/4/4	-
34	LMT	m	1502	-	-	1/21/61/61	0/2/2/2
31	GOL	b	638	-	-	2/4/4/4	-
36	DGD	C	517	-	-	13/45/85/95	0/2/2/2
26	BCR	t	903	-	-	1/29/63/63	0/2/2/2
37	LHG	D	407	-	-	6/53/53/53	-
35	HTG	d	403	-	-	2/10/30/30	0/1/1/1
37	LHG	b	639	-	-	9/53/53/53	-
35	HTG	O	303	-	-	1/10/30/30	0/1/1/1
24	CLA	d	404	4	-	3/39/115/115	-
26	BCR	Y	101	-	-	5/29/63/63	0/2/2/2
31	GOL	V	205	-	-	0/4/4/4	-
27	SQD	A	417	-	-	12/49/69/69	0/1/1/1
31	GOL	c	928	-	-	0/4/4/4	-
26	BCR	C	515	-	-	1/29/63/63	0/2/2/2
24	CLA	c	906	3	-	5/39/115/115	-
34	LMT	M	302	-	-	7/21/61/61	0/2/2/2
39	RRX	h	101	-	-	2/29/65/65	0/2/2/2
31	GOL	A	420	-	-	2/4/4/4	-
37	LHG	D	408	-	-	8/53/53/53	-
31	GOL	b	628	-	-	2/4/4/4	-
31	GOL	B	628	-	-	2/4/4/4	-
38	HEM	F	102	6,5	-	1/14/54/54	-
31	GOL	h	103	-	-	0/4/4/4	-
31	GOL	c	932	-	-	2/4/4/4	-
28	LMG	b	624	-	-	14/46/66/70	0/1/1/1
24	CLA	a	413	1	-	8/39/115/115	-
36	DGD	c	918	-	-	7/44/84/95	0/2/2/2
24	CLA	d	401	42	-	6/39/115/115	-
24	CLA	a	409	1	-	5/39/115/115	-
39	RRX	H	102	-	-	2/29/65/65	0/2/2/2
29	PL9	d	407	-	-	3/53/73/73	0/1/1/1
24	CLA	B	610	2	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	509	3	-	5/39/115/115	-
24	CLA	b	615	2	-	6/39/115/115	-
26	BCR	d	406	-	-	8/29/63/63	0/2/2/2
24	CLA	A	406	42	-	4/39/115/115	-
25	PHO	a	412	-	-	3/37/103/103	0/5/6/6
35	HTG	B	624	-	-	4/10/30/30	0/1/1/1
31	GOL	H	101	-	-	0/4/4/4	-
24	CLA	C	508	3	-	5/39/115/115	-
35	HTG	B	626	-	-	3/10/30/30	0/1/1/1
36	DGD	c	917	-	-	15/51/91/95	0/2/2/2
24	CLA	c	913	3	-	7/39/115/115	-
28	LMG	c	920	-	-	5/46/66/70	0/1/1/1
24	CLA	B	605	2	-	5/39/115/115	-
36	DGD	C	516	-	-	11/51/91/95	0/2/2/2
24	CLA	c	902	3	-	4/39/115/115	-
31	GOL	v	201	-	-	2/4/4/4	-
31	GOL	B	630	-	-	4/4/4/4	-
38	HEM	v	202	16	-	4/14/54/54	-
31	GOL	v	203	-	-	1/4/4/4	-
24	CLA	B	612	2	-	1/39/115/115	-
31	GOL	C	531	-	-	0/4/4/4	-
24	CLA	B	617	2	-	8/39/115/115	-
31	GOL	C	524	-	-	0/4/4/4	-
34	LMT	m	1503	-	-	2/21/61/61	0/2/2/2
24	CLA	B	611	42	-	2/39/115/115	-
24	CLA	b	610	2	-	6/39/115/115	-
26	BCR	a	414	-	-	1/29/63/63	0/2/2/2
38	HEM	f	101	6,5	-	1/14/54/54	-
31	GOL	c	927	-	-	0/4/4/4	-
24	CLA	b	618	2	-	11/39/115/115	-
26	BCR	D	404	-	-	8/29/63/63	0/2/2/2
31	GOL	A	419	-	-	1/4/4/4	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
31	GOL	u	202	-	-	3/4/4/4	-
24	CLA	c	911	3	-	4/39/115/115	-
31	GOL	v	204	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PL9	A	414	-	-	9/53/73/73	0/1/1/1
24	CLA	B	609	2	-	1/39/115/115	-
35	HTG	C	528	-	-	0/10/30/30	0/1/1/1
35	HTG	c	924	-	-	3/10/30/30	0/1/1/1
37	LHG	D	409	-	-	8/50/50/53	-
24	CLA	A	407	42	-	2/39/115/115	-
24	CLA	A	410	1	-	4/39/115/115	-
24	CLA	b	608	2	-	2/39/115/115	-
24	CLA	C	511	3	-	1/39/115/115	-
24	CLA	C	505	3	-	3/39/115/115	-
24	CLA	C	506	3	-	9/39/115/115	-
24	CLA	B	602	42	-	14/39/115/115	-
35	HTG	v	205	-	-	1/4/24/30	0/1/1/1
36	DGD	D	406	-	-	14/47/68/95	0/1/1/2
24	CLA	c	910	3	-	8/39/115/115	-
34	LMT	z	101	-	-	5/15/55/61	0/2/2/2
31	GOL	C	527	-	-	2/4/4/4	-

All (1854) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	MG-ND	-10.48	1.85	2.05
24	C	503	CLA	MG-NA	9.73	2.29	2.06
24	C	507	CLA	MG-NA	9.35	2.28	2.06
25	a	412	PHO	C1D-C2D	9.32	1.49	1.39
24	c	904	CLA	MG-NA	9.27	2.28	2.06
24	c	910	CLA	MG-NA	9.18	2.28	2.06
24	C	511	CLA	MG-NA	9.17	2.28	2.06
24	c	907	CLA	MG-ND	-9.17	1.87	2.05
25	A	408	PHO	C1D-C2D	9.17	1.49	1.39
25	A	409	PHO	C1B-C2B	8.98	1.49	1.39
24	C	512	CLA	MG-ND	-8.97	1.88	2.05
24	C	505	CLA	MG-ND	-8.94	1.88	2.05
24	c	912	CLA	MG-NA	8.93	2.27	2.06
25	a	412	PHO	C1B-C2B	8.93	1.49	1.39
24	b	608	CLA	MG-NA	8.92	2.27	2.06
24	c	904	CLA	MG-NC	8.92	2.27	2.06
24	B	616	CLA	MG-NA	8.89	2.27	2.06
24	B	607	CLA	MG-NA	8.75	2.27	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	906	CLA	MG-NA	8.57	2.26	2.06
25	A	409	PHO	C1D-C2D	8.50	1.49	1.39
24	b	613	CLA	MG-NC	8.40	2.26	2.06
25	a	411	PHO	C1B-C2B	8.36	1.48	1.39
24	c	908	CLA	MG-NA	8.35	2.26	2.06
25	A	408	PHO	C1B-C2B	8.34	1.48	1.39
24	C	505	CLA	MG-NA	8.18	2.25	2.06
24	b	615	CLA	MG-NA	8.18	2.25	2.06
24	c	902	CLA	MG-NA	8.12	2.25	2.06
24	b	613	CLA	MG-NA	8.11	2.25	2.06
24	c	913	CLA	MG-ND	-8.07	1.89	2.05
25	a	411	PHO	C1D-C2D	8.02	1.48	1.39
24	b	606	CLA	MG-NC	7.88	2.25	2.06
24	c	913	CLA	MG-NA	7.86	2.24	2.06
38	f	101	HEM	C3D-C2D	7.83	1.53	1.36
24	B	608	CLA	MG-NA	7.81	2.24	2.06
24	C	512	CLA	MG-NA	7.79	2.24	2.06
24	c	914	CLA	MG-NC	7.77	2.24	2.06
24	C	506	CLA	MG-NA	7.74	2.24	2.06
38	F	102	HEM	C3D-C2D	7.73	1.53	1.36
24	b	605	CLA	MG-NA	7.71	2.24	2.06
24	b	608	CLA	MG-ND	-7.70	1.90	2.05
24	b	612	CLA	MG-NC	7.70	2.24	2.06
38	V	202	HEM	C3D-C2D	7.65	1.53	1.36
38	v	202	HEM	C3D-C2D	7.59	1.52	1.36
24	B	602	CLA	MG-NA	7.52	2.24	2.06
24	B	605	CLA	MG-NA	7.51	2.24	2.06
24	B	604	CLA	MG-ND	-7.40	1.91	2.05
24	b	619	CLA	MG-NA	7.40	2.23	2.06
24	b	616	CLA	MG-NA	7.30	2.23	2.06
24	B	614	CLA	MG-NA	7.28	2.23	2.06
24	B	603	CLA	MG-NA	7.28	2.23	2.06
27	f	102	SQD	C6-S	-7.26	1.67	1.77
24	d	401	CLA	MG-ND	-7.25	1.91	2.05
24	C	509	CLA	MG-NA	7.24	2.23	2.06
24	C	510	CLA	MG-NA	7.22	2.23	2.06
24	b	608	CLA	MG-NC	7.22	2.23	2.06
24	B	610	CLA	MG-NA	7.15	2.23	2.06
24	b	617	CLA	MG-ND	-7.12	1.91	2.05
24	c	909	CLA	MG-ND	-7.11	1.91	2.05
24	d	404	CLA	MG-ND	-7.05	1.91	2.05
24	c	907	CLA	MG-NC	7.02	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	MG-NC	6.91	2.22	2.06
24	b	612	CLA	MG-ND	-6.88	1.92	2.05
24	b	610	CLA	MG-NA	6.83	2.22	2.06
24	C	510	CLA	MG-ND	-6.83	1.92	2.05
24	b	607	CLA	MG-NA	6.81	2.22	2.06
24	b	620	CLA	MG-NA	6.80	2.22	2.06
24	b	615	CLA	MG-ND	-6.76	1.92	2.05
24	a	410	CLA	MG-NA	6.75	2.22	2.06
24	B	615	CLA	MG-NA	6.74	2.22	2.06
24	B	606	CLA	MG-NA	6.74	2.22	2.06
24	D	403	CLA	MG-NC	6.73	2.22	2.06
24	C	502	CLA	MG-ND	-6.70	1.92	2.05
24	c	903	CLA	MG-NA	6.69	2.22	2.06
25	A	409	PHO	C3B-C4B	6.68	1.49	1.41
24	B	617	CLA	MG-NA	6.62	2.22	2.06
24	c	911	CLA	MG-NA	6.58	2.21	2.06
24	B	616	CLA	MG-ND	-6.56	1.92	2.05
24	b	611	CLA	MG-NA	6.54	2.21	2.06
24	C	513	CLA	MG-NC	6.52	2.21	2.06
24	B	602	CLA	MG-ND	-6.49	1.92	2.05
24	d	404	CLA	MG-NA	6.45	2.21	2.06
24	B	611	CLA	MG-ND	-6.43	1.93	2.05
24	c	909	CLA	MG-NC	6.42	2.21	2.06
24	A	405	CLA	MG-NA	6.40	2.21	2.06
24	B	612	CLA	MG-NA	6.40	2.21	2.06
24	c	905	CLA	MG-NA	6.38	2.21	2.06
24	c	907	CLA	C1D-ND	6.37	1.45	1.37
24	C	502	CLA	MG-NA	6.37	2.21	2.06
24	B	605	CLA	C1D-ND	6.37	1.45	1.37
24	C	508	CLA	MG-ND	-6.36	1.93	2.05
24	b	608	CLA	C1D-ND	6.36	1.45	1.37
24	C	501	CLA	MG-NA	6.32	2.21	2.06
25	a	412	PHO	C3B-C4B	6.32	1.48	1.41
24	B	603	CLA	MG-ND	-6.27	1.93	2.05
24	c	904	CLA	C1D-ND	6.26	1.45	1.37
24	C	506	CLA	MG-ND	-6.25	1.93	2.05
24	C	506	CLA	C1D-ND	6.21	1.45	1.37
24	d	405	CLA	MG-NC	6.20	2.21	2.06
24	c	902	CLA	MG-ND	-6.18	1.93	2.05
24	B	613	CLA	MG-NA	6.06	2.20	2.06
24	B	617	CLA	MG-ND	-6.04	1.93	2.05
24	b	611	CLA	MG-ND	-6.03	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	605	CLA	C3C-C2C	6.03	1.49	1.36
24	C	503	CLA	MG-NC	6.02	2.20	2.06
24	B	611	CLA	MG-NC	6.02	2.20	2.06
24	b	612	CLA	C1D-ND	6.01	1.45	1.37
24	B	605	CLA	MG-NC	6.00	2.20	2.06
24	b	613	CLA	C1D-ND	5.98	1.45	1.37
24	A	405	CLA	MG-ND	-5.98	1.93	2.05
24	c	909	CLA	C3C-C2C	5.95	1.49	1.36
24	C	508	CLA	C3C-C2C	5.94	1.49	1.36
24	D	403	CLA	C1D-ND	5.92	1.45	1.37
24	B	610	CLA	MG-ND	-5.92	1.94	2.05
24	C	513	CLA	MG-NA	5.90	2.20	2.06
24	c	911	CLA	C3C-C2C	5.89	1.49	1.36
24	C	512	CLA	C3C-C2C	5.88	1.49	1.36
24	c	908	CLA	MG-NC	5.86	2.20	2.06
24	b	605	CLA	C1D-ND	5.85	1.45	1.37
24	c	910	CLA	C1D-ND	5.85	1.45	1.37
24	b	606	CLA	C3C-C2C	5.84	1.49	1.36
24	c	904	CLA	C3C-C2C	5.84	1.49	1.36
24	C	503	CLA	C1D-ND	5.82	1.44	1.37
24	B	609	CLA	MG-ND	-5.81	1.94	2.05
24	B	611	CLA	C1D-ND	5.81	1.44	1.37
27	f	102	SQD	O47-C7	5.80	1.46	1.33
24	C	508	CLA	MG-NC	5.80	2.20	2.06
24	c	914	CLA	C1D-ND	5.79	1.44	1.37
24	B	609	CLA	MG-NA	5.79	2.20	2.06
24	b	612	CLA	C3C-C2C	5.77	1.49	1.36
24	B	603	CLA	C3C-C2C	5.76	1.49	1.36
24	B	602	CLA	C3C-C2C	5.76	1.49	1.36
24	D	403	CLA	C3C-C2C	5.76	1.49	1.36
24	b	609	CLA	MG-NA	5.76	2.19	2.06
24	d	404	CLA	C3C-C2C	5.75	1.49	1.36
24	B	602	CLA	C1D-ND	5.75	1.44	1.37
24	C	507	CLA	C1D-ND	5.75	1.44	1.37
24	b	618	CLA	MG-ND	-5.75	1.94	2.05
24	B	611	CLA	C3C-C2C	5.74	1.48	1.36
24	C	503	CLA	C3C-C2C	5.72	1.48	1.36
24	c	909	CLA	C1D-ND	5.72	1.44	1.37
25	a	411	PHO	C3B-C4B	5.72	1.48	1.41
25	a	411	PHO	C3B-C2B	5.72	1.48	1.40
24	c	910	CLA	C3C-C2C	5.72	1.48	1.36
24	C	504	CLA	C1D-ND	5.72	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	C1D-ND	5.72	1.44	1.37
24	C	502	CLA	C1D-ND	5.72	1.44	1.37
24	b	607	CLA	MG-ND	-5.72	1.94	2.05
24	C	509	CLA	C1D-ND	5.71	1.44	1.37
24	b	612	CLA	MG-NA	5.71	2.19	2.06
24	B	610	CLA	MG-NC	5.69	2.19	2.06
24	d	401	CLA	C3C-C2C	5.69	1.48	1.36
24	a	413	CLA	C3C-C2C	5.67	1.48	1.36
24	b	617	CLA	MG-NA	5.67	2.19	2.06
24	C	510	CLA	C1D-ND	5.67	1.44	1.37
24	B	606	CLA	C1D-ND	5.67	1.44	1.37
24	c	913	CLA	C1D-ND	5.67	1.44	1.37
24	C	502	CLA	C3C-C2C	5.66	1.48	1.36
24	C	506	CLA	C3C-C2C	5.66	1.48	1.36
24	b	614	CLA	C3C-C2C	5.66	1.48	1.36
24	C	512	CLA	C1D-ND	5.66	1.44	1.37
24	B	609	CLA	C3C-C2C	5.65	1.48	1.36
24	C	513	CLA	C1D-ND	5.65	1.44	1.37
24	c	913	CLA	C3C-C2C	5.64	1.48	1.36
24	d	405	CLA	C1D-ND	5.64	1.44	1.37
24	A	405	CLA	C3C-C2C	5.63	1.48	1.36
24	b	610	CLA	C3C-C2C	5.63	1.48	1.36
24	B	609	CLA	C1D-ND	5.63	1.44	1.37
24	b	614	CLA	C1D-ND	5.62	1.44	1.37
24	c	911	CLA	C1D-ND	5.61	1.44	1.37
24	b	613	CLA	MG-ND	-5.60	1.94	2.05
24	C	509	CLA	C3C-C2C	5.59	1.48	1.36
24	c	906	CLA	C1D-ND	5.58	1.44	1.37
24	C	501	CLA	C1D-ND	5.58	1.44	1.37
24	c	914	CLA	C3C-C2C	5.58	1.48	1.36
24	b	609	CLA	C3C-C2C	5.57	1.48	1.36
24	A	410	CLA	C3C-C2C	5.57	1.48	1.36
24	c	908	CLA	C3C-C2C	5.57	1.48	1.36
24	C	502	CLA	MG-NC	5.57	2.19	2.06
24	B	603	CLA	C1D-ND	5.56	1.44	1.37
24	b	616	CLA	C3C-C2C	5.56	1.48	1.36
24	B	604	CLA	C1D-ND	5.55	1.44	1.37
24	B	607	CLA	C1D-ND	5.53	1.44	1.37
24	c	903	CLA	C3C-C2C	5.53	1.48	1.36
24	C	507	CLA	C3C-C2C	5.53	1.48	1.36
24	d	405	CLA	C3C-C2C	5.52	1.48	1.36
24	C	504	CLA	C3C-C2C	5.51	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	C3C-C2C	5.51	1.48	1.36
24	b	618	CLA	MG-NC	5.50	2.19	2.06
24	C	505	CLA	C3C-C2C	5.50	1.48	1.36
24	C	505	CLA	MG-NC	5.50	2.19	2.06
24	C	507	CLA	MG-NC	5.49	2.19	2.06
24	c	906	CLA	C3C-C2C	5.49	1.48	1.36
24	B	615	CLA	C3C-C2C	5.49	1.48	1.36
24	C	510	CLA	C3C-C2C	5.49	1.48	1.36
24	b	606	CLA	C1D-ND	5.48	1.44	1.37
24	c	906	CLA	MG-ND	-5.48	1.94	2.05
24	c	907	CLA	C3C-C2C	5.47	1.48	1.36
24	b	614	CLA	MG-NC	5.46	2.19	2.06
24	B	607	CLA	C3C-C2C	5.46	1.48	1.36
24	b	617	CLA	C3C-C2C	5.46	1.48	1.36
24	C	513	CLA	MG-ND	-5.46	1.95	2.05
24	C	513	CLA	C3C-C2C	5.46	1.48	1.36
24	a	409	CLA	MG-ND	-5.45	1.95	2.05
24	c	905	CLA	C3C-C2C	5.44	1.48	1.36
24	b	620	CLA	C1D-ND	5.44	1.44	1.37
24	c	907	CLA	MG-NA	5.42	2.19	2.06
24	C	502	CLA	CHC-C1C	5.41	1.49	1.38
24	b	611	CLA	MG-NC	5.41	2.19	2.06
24	b	619	CLA	C3C-C2C	5.41	1.48	1.36
25	A	408	PHO	C3B-C2B	5.40	1.47	1.40
24	a	409	CLA	C3C-C2C	5.40	1.48	1.36
24	B	604	CLA	MG-NC	5.39	2.19	2.06
24	b	616	CLA	MG-ND	-5.39	1.95	2.05
24	b	607	CLA	C3C-C2C	5.39	1.48	1.36
24	a	413	CLA	MG-ND	-5.38	1.95	2.05
24	B	604	CLA	C3C-C2C	5.38	1.48	1.36
24	B	602	CLA	MG-NB	5.38	2.16	2.05
24	B	616	CLA	C1D-ND	5.37	1.44	1.37
24	a	409	CLA	C1D-ND	5.37	1.44	1.37
24	b	613	CLA	C3C-C2C	5.37	1.48	1.36
24	b	619	CLA	C1D-ND	5.37	1.44	1.37
24	D	402	CLA	C3C-C2C	5.37	1.48	1.36
24	A	406	CLA	C1D-ND	5.36	1.44	1.37
24	A	410	CLA	MG-NC	5.35	2.19	2.06
24	A	406	CLA	MG-NA	5.35	2.19	2.06
24	c	912	CLA	C1D-ND	5.35	1.44	1.37
24	b	613	CLA	O2D-CGD	5.34	1.46	1.33
25	A	408	PHO	C4D-CHA	5.34	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	C1D-ND	5.34	1.44	1.37
24	b	610	CLA	MG-NC	5.33	2.18	2.06
24	B	614	CLA	C3C-C2C	5.33	1.48	1.36
24	c	903	CLA	MG-ND	-5.33	1.95	2.05
24	B	610	CLA	C1D-ND	5.32	1.44	1.37
24	C	511	CLA	C3C-C2C	5.32	1.48	1.36
24	b	618	CLA	C1D-ND	5.31	1.44	1.37
24	a	409	CLA	MG-NA	5.31	2.18	2.06
24	C	513	CLA	CHC-C1C	5.31	1.49	1.38
24	b	610	CLA	C1D-ND	5.31	1.44	1.37
24	a	410	CLA	C3C-C2C	5.30	1.48	1.36
24	B	605	CLA	C3C-C2C	5.29	1.48	1.36
24	B	606	CLA	C3C-C2C	5.29	1.48	1.36
24	B	614	CLA	MG-ND	-5.29	1.95	2.05
24	b	605	CLA	MG-NC	5.29	2.18	2.06
24	c	902	CLA	C3C-C2C	5.29	1.48	1.36
24	c	905	CLA	O2D-CGD	5.28	1.46	1.33
24	A	406	CLA	C3C-C2C	5.28	1.47	1.36
24	B	610	CLA	C3C-C2C	5.28	1.47	1.36
24	B	606	CLA	MG-NC	5.26	2.18	2.06
24	a	410	CLA	MG-ND	-5.26	1.95	2.05
24	b	620	CLA	C3C-C2C	5.26	1.47	1.36
24	B	612	CLA	C1D-ND	5.26	1.44	1.37
24	b	607	CLA	C1D-ND	5.26	1.44	1.37
24	C	507	CLA	MG-ND	-5.25	1.95	2.05
24	b	620	CLA	MG-ND	-5.25	1.95	2.05
24	A	407	CLA	C3C-C2C	5.24	1.47	1.36
24	c	912	CLA	C3C-C2C	5.24	1.47	1.36
24	C	508	CLA	C1D-ND	5.24	1.44	1.37
24	B	602	CLA	CHC-C1C	5.23	1.49	1.38
25	A	409	PHO	C4D-CHA	5.23	1.47	1.39
24	c	911	CLA	MG-NC	5.23	2.18	2.06
24	A	405	CLA	MG-NC	5.22	2.18	2.06
24	B	615	CLA	C1D-ND	5.21	1.44	1.37
25	A	409	PHO	C3C-C2C	5.20	1.47	1.36
24	c	908	CLA	C1D-ND	5.20	1.44	1.37
24	c	903	CLA	C1D-ND	5.19	1.44	1.37
24	B	616	CLA	C3C-C2C	5.19	1.47	1.36
24	c	914	CLA	MG-NA	5.19	2.18	2.06
24	B	616	CLA	CHC-C1C	5.18	1.49	1.38
25	a	411	PHO	C4D-CHA	5.18	1.47	1.39
24	C	501	CLA	C3C-C2C	5.18	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	611	CLA	C3C-C2C	5.18	1.47	1.36
25	a	411	PHO	C3C-C2C	5.18	1.47	1.36
24	C	504	CLA	MG-NA	5.18	2.18	2.06
25	a	412	PHO	C3B-C2B	5.18	1.47	1.40
24	C	506	CLA	O2D-CGD	5.16	1.45	1.33
25	A	409	PHO	C3B-C2B	5.16	1.47	1.40
24	C	504	CLA	MG-ND	-5.15	1.95	2.05
24	c	902	CLA	C1D-ND	5.15	1.44	1.37
24	B	613	CLA	C3C-C2C	5.15	1.47	1.36
24	b	615	CLA	C1D-ND	5.14	1.44	1.37
24	b	617	CLA	MG-NC	5.13	2.18	2.06
24	B	612	CLA	C3C-C2C	5.13	1.47	1.36
24	a	413	CLA	C1D-ND	5.12	1.44	1.37
24	c	906	CLA	MG-NC	5.12	2.18	2.06
24	b	615	CLA	C3C-C2C	5.12	1.47	1.36
24	B	617	CLA	C3C-C2C	5.11	1.47	1.36
24	B	604	CLA	CHC-C1C	5.10	1.48	1.38
24	C	512	CLA	CHC-C1C	5.10	1.48	1.38
24	C	508	CLA	MG-NB	5.09	2.15	2.05
24	D	403	CLA	CHC-C1C	5.08	1.48	1.38
24	b	616	CLA	CHC-C1C	5.08	1.48	1.38
24	c	905	CLA	MG-ND	-5.08	1.95	2.05
24	B	608	CLA	C3C-C2C	5.07	1.47	1.36
24	b	607	CLA	MG-NC	5.07	2.18	2.06
24	b	608	CLA	C3C-C2C	5.07	1.47	1.36
24	c	905	CLA	C1D-ND	5.07	1.44	1.37
24	b	617	CLA	O2D-CGD	5.06	1.45	1.33
24	C	506	CLA	MG-NC	5.05	2.18	2.06
24	c	914	CLA	CHD-C1D	5.05	1.48	1.38
25	A	408	PHO	C3C-C2C	5.05	1.47	1.36
38	V	202	HEM	FE-ND	5.04	2.10	1.94
24	D	403	CLA	O2D-CGD	5.04	1.45	1.33
25	a	412	PHO	C4D-CHA	5.04	1.47	1.39
24	A	410	CLA	C1D-ND	5.04	1.44	1.37
24	B	602	CLA	O2D-CGD	5.03	1.45	1.33
24	c	914	CLA	CHC-C1C	5.03	1.48	1.38
24	B	603	CLA	CHC-C1C	5.03	1.48	1.38
24	c	909	CLA	MG-NA	5.03	2.18	2.06
24	b	615	CLA	O2D-CGD	5.03	1.45	1.33
24	b	612	CLA	CHC-C1C	5.02	1.48	1.38
24	b	618	CLA	O2D-CGD	5.01	1.45	1.33
24	C	509	CLA	MG-NC	5.00	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	904	CLA	CHD-C1D	5.00	1.48	1.38
24	c	909	CLA	CHC-C1C	4.99	1.48	1.38
24	A	405	CLA	C1D-ND	4.99	1.43	1.37
24	C	511	CLA	C1D-ND	4.98	1.43	1.37
24	c	913	CLA	CHC-C1C	4.98	1.48	1.38
24	B	617	CLA	O2D-CGD	4.97	1.45	1.33
25	a	412	PHO	C3C-C2C	4.97	1.47	1.36
24	a	413	CLA	O2D-CGD	4.97	1.45	1.33
25	A	409	PHO	O2D-CGD	4.96	1.45	1.33
24	b	611	CLA	O2D-CGD	4.96	1.45	1.33
24	b	607	CLA	O2D-CGD	4.96	1.45	1.33
24	B	610	CLA	O2D-CGD	4.96	1.45	1.33
24	b	609	CLA	C1D-ND	4.95	1.43	1.37
24	a	410	CLA	CHC-C1C	4.95	1.48	1.38
24	C	509	CLA	O2D-CGD	4.95	1.45	1.33
24	b	605	CLA	O2D-CGD	4.94	1.45	1.33
24	b	608	CLA	O2D-CGD	4.94	1.45	1.33
24	B	611	CLA	CHC-C1C	4.94	1.48	1.38
24	d	404	CLA	MG-NC	4.94	2.18	2.06
24	c	912	CLA	CHC-C1C	4.93	1.48	1.38
24	c	910	CLA	O2D-CGD	4.93	1.45	1.33
24	A	407	CLA	O2D-CGD	4.92	1.45	1.33
24	C	503	CLA	CHC-C1C	4.92	1.48	1.38
24	C	511	CLA	CHC-C1C	4.92	1.48	1.38
24	a	409	CLA	MG-NC	4.92	2.18	2.06
24	C	504	CLA	CHC-C1C	4.92	1.48	1.38
24	B	617	CLA	C1D-ND	4.91	1.43	1.37
24	b	606	CLA	MG-NA	4.91	2.17	2.06
24	C	508	CLA	CHC-C1C	4.90	1.48	1.38
24	b	605	CLA	CHC-C1C	4.90	1.48	1.38
24	b	619	CLA	CHC-C1C	4.89	1.48	1.38
24	b	610	CLA	CHC-C1C	4.89	1.48	1.38
24	c	910	CLA	CHC-C1C	4.89	1.48	1.38
24	C	502	CLA	O2D-CGD	4.88	1.45	1.33
24	C	502	CLA	MG-NB	4.88	2.15	2.05
24	b	620	CLA	O2D-CGD	4.88	1.45	1.33
24	B	606	CLA	O2D-CGD	4.88	1.45	1.33
24	b	614	CLA	MG-NA	4.88	2.17	2.06
24	D	403	CLA	MG-NB	4.87	2.15	2.05
24	c	904	CLA	CHC-C1C	4.87	1.48	1.38
24	b	619	CLA	MG-NC	4.87	2.17	2.06
24	B	614	CLA	O2D-CGD	4.87	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C1D-ND	4.86	1.43	1.37
24	d	401	CLA	C1D-ND	4.86	1.43	1.37
24	C	509	CLA	CHC-C1C	4.86	1.48	1.38
24	c	912	CLA	MG-NB	4.86	2.15	2.05
24	d	405	CLA	MG-ND	-4.86	1.96	2.05
24	b	606	CLA	O2D-CGD	4.86	1.45	1.33
24	d	405	CLA	CHC-C1C	4.85	1.48	1.38
25	a	411	PHO	O2D-CGD	4.85	1.45	1.33
24	a	413	CLA	CHC-C1C	4.85	1.48	1.38
24	B	609	CLA	CHC-C1C	4.85	1.48	1.38
24	b	609	CLA	CHC-C1C	4.84	1.48	1.38
24	c	908	CLA	O2D-CGD	4.83	1.45	1.33
24	C	509	CLA	CHD-C1D	4.83	1.47	1.38
24	b	613	CLA	CHD-C1D	4.83	1.47	1.38
24	B	612	CLA	CHC-C1C	4.83	1.48	1.38
24	c	910	CLA	MG-NC	4.83	2.17	2.06
24	c	905	CLA	CHC-C1C	4.83	1.48	1.38
25	a	412	PHO	O2D-CGD	4.82	1.45	1.33
24	B	606	CLA	CHC-C1C	4.82	1.48	1.38
24	C	513	CLA	CHD-C1D	4.82	1.47	1.38
24	b	611	CLA	CHC-C1C	4.81	1.48	1.38
24	c	907	CLA	O2D-CGD	4.81	1.44	1.33
24	B	613	CLA	MG-ND	-4.81	1.96	2.05
24	C	511	CLA	O2D-CGD	4.81	1.44	1.33
24	c	907	CLA	CHD-C1D	4.80	1.47	1.38
24	b	616	CLA	C1D-ND	4.80	1.43	1.37
24	C	501	CLA	CHC-C1C	4.80	1.48	1.38
24	A	405	CLA	CHC-C1C	4.80	1.48	1.38
24	C	513	CLA	O2D-CGD	4.79	1.44	1.33
38	f	101	HEM	FE-ND	4.79	2.09	1.94
24	b	616	CLA	O2D-CGD	4.79	1.44	1.33
24	B	611	CLA	MG-NA	4.78	2.17	2.06
24	d	405	CLA	O2D-CGD	4.78	1.44	1.33
24	C	512	CLA	MG-NC	4.78	2.17	2.06
24	C	508	CLA	O2D-CGD	4.78	1.44	1.33
24	C	501	CLA	MG-NC	4.78	2.17	2.06
24	b	606	CLA	CHD-C1D	4.77	1.47	1.38
24	c	907	CLA	CHC-C1C	4.77	1.48	1.38
24	C	507	CLA	CHD-C1D	4.77	1.47	1.38
24	B	602	CLA	CHD-C1D	4.77	1.47	1.38
24	b	615	CLA	CHC-C1C	4.77	1.48	1.38
24	b	620	CLA	CHC-C1C	4.77	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	620	CLA	CHD-C1D	4.76	1.47	1.38
24	C	502	CLA	CHD-C1D	4.76	1.47	1.38
24	C	505	CLA	O2D-CGD	4.75	1.44	1.33
24	C	511	CLA	MG-ND	-4.75	1.96	2.05
24	B	607	CLA	O2D-CGD	4.75	1.44	1.33
24	B	610	CLA	CHC-C1C	4.74	1.48	1.38
24	b	606	CLA	CHC-C1C	4.74	1.48	1.38
24	B	613	CLA	CHC-C1C	4.74	1.48	1.38
24	b	612	CLA	CHD-C1D	4.74	1.47	1.38
24	c	903	CLA	CHC-C1C	4.73	1.48	1.38
24	A	410	CLA	O2D-CGD	4.72	1.44	1.33
24	B	614	CLA	CHC-C1C	4.72	1.48	1.38
24	c	906	CLA	CHD-C1D	4.71	1.47	1.38
24	B	604	CLA	O2D-CGD	4.71	1.44	1.33
24	C	501	CLA	MG-ND	-4.71	1.96	2.05
24	C	507	CLA	O2D-CGD	4.71	1.44	1.33
24	c	908	CLA	CHC-C1C	4.70	1.48	1.38
24	c	904	CLA	O2D-CGD	4.70	1.44	1.33
24	a	413	CLA	MG-NA	4.70	2.17	2.06
24	c	911	CLA	CHC-C1C	4.70	1.48	1.38
24	b	605	CLA	CHD-C1D	4.70	1.47	1.38
24	c	911	CLA	CHB-C1B	4.70	1.49	1.39
24	b	607	CLA	CHC-C1C	4.70	1.48	1.38
24	c	914	CLA	O2D-CGD	4.69	1.44	1.33
24	b	608	CLA	CHC-C1C	4.69	1.48	1.38
24	b	617	CLA	CHC-C1C	4.69	1.48	1.38
24	b	611	CLA	C1D-ND	4.69	1.43	1.37
24	c	902	CLA	O2D-CGD	4.69	1.44	1.33
24	A	407	CLA	C1D-ND	4.69	1.43	1.37
24	C	505	CLA	CHD-C1D	4.68	1.47	1.38
24	b	607	CLA	CHD-C1D	4.67	1.47	1.38
24	c	903	CLA	O2D-CGD	4.67	1.44	1.33
24	B	613	CLA	CHB-C1B	4.67	1.49	1.39
24	C	506	CLA	CHD-C1D	4.67	1.47	1.38
25	A	408	PHO	C3B-C4B	4.66	1.46	1.41
24	b	618	CLA	CHC-C1C	4.66	1.48	1.38
24	b	614	CLA	CHC-C1C	4.66	1.48	1.38
24	A	407	CLA	CHD-C1D	4.66	1.47	1.38
24	C	506	CLA	CHC-C1C	4.66	1.48	1.38
24	b	608	CLA	CHD-C1D	4.65	1.47	1.38
24	B	612	CLA	O2D-CGD	4.65	1.44	1.33
24	d	404	CLA	O2A-CGA	4.65	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	CHB-C1B	4.65	1.49	1.39
24	B	609	CLA	MG-NC	4.65	2.17	2.06
25	A	409	PHO	OBD-CAD	4.65	1.28	1.22
24	c	904	CLA	MG-ND	-4.64	1.96	2.05
24	c	909	CLA	CHD-C1D	4.64	1.47	1.38
24	b	616	CLA	CHB-C1B	4.64	1.49	1.39
24	A	405	CLA	CHB-C1B	4.63	1.49	1.39
24	b	612	CLA	O2D-CGD	4.63	1.44	1.33
27	A	417	SQD	O48-C23	4.63	1.46	1.33
38	f	101	HEM	FE-NB	4.63	2.09	1.94
24	B	606	CLA	CHD-C1D	4.62	1.47	1.38
24	B	607	CLA	CHC-C1C	4.62	1.47	1.38
38	F	102	HEM	FE-ND	4.62	2.09	1.94
24	c	910	CLA	CHB-C1B	4.62	1.49	1.39
24	B	610	CLA	CHD-C1D	4.61	1.47	1.38
24	c	902	CLA	CHB-C1B	4.61	1.49	1.39
24	B	608	CLA	O2D-CGD	4.61	1.44	1.33
24	B	602	CLA	O2A-CGA	4.60	1.46	1.33
24	d	404	CLA	O2D-CGD	4.60	1.44	1.33
24	C	510	CLA	CHC-C1C	4.60	1.47	1.38
24	c	913	CLA	O2D-CGD	4.60	1.44	1.33
24	b	619	CLA	O2D-CGD	4.60	1.44	1.33
24	C	510	CLA	O2D-CGD	4.60	1.44	1.33
24	b	605	CLA	O2A-CGA	4.60	1.46	1.33
24	D	403	CLA	MG-ND	-4.60	1.96	2.05
24	B	615	CLA	CHC-C1C	4.59	1.47	1.38
24	B	608	CLA	CHC-C1C	4.59	1.47	1.38
24	b	614	CLA	O2D-CGD	4.59	1.44	1.33
24	B	603	CLA	O2D-CGD	4.59	1.44	1.33
24	a	409	CLA	CHC-C1C	4.58	1.47	1.38
24	c	906	CLA	CHC-C1C	4.58	1.47	1.38
24	B	613	CLA	O2D-CGD	4.58	1.44	1.33
24	C	504	CLA	CHD-C1D	4.58	1.47	1.38
24	B	609	CLA	CHD-C1D	4.58	1.47	1.38
24	c	910	CLA	CHD-C1D	4.58	1.47	1.38
25	A	408	PHO	O2D-CGD	4.58	1.44	1.33
24	c	912	CLA	O2D-CGD	4.57	1.44	1.33
24	a	409	CLA	O2D-CGD	4.57	1.44	1.33
27	b	601	SQD	O47-C7	4.57	1.47	1.34
24	C	504	CLA	O2D-CGD	4.57	1.44	1.33
24	B	609	CLA	O2D-CGD	4.57	1.44	1.33
24	C	512	CLA	O2D-CGD	4.56	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	MG-NC	4.56	2.17	2.06
24	b	609	CLA	O2D-CGD	4.56	1.44	1.33
24	B	615	CLA	O2D-CGD	4.56	1.44	1.33
24	B	607	CLA	MG-NC	4.56	2.17	2.06
24	A	405	CLA	O2D-CGD	4.55	1.44	1.33
24	D	402	CLA	MG-NA	4.55	2.17	2.06
24	B	616	CLA	O2D-CGD	4.54	1.44	1.33
24	A	406	CLA	O2D-CGD	4.54	1.44	1.33
24	c	911	CLA	CHD-C1D	4.54	1.47	1.38
24	c	911	CLA	O2D-CGD	4.53	1.44	1.33
24	B	603	CLA	CHD-C1D	4.53	1.47	1.38
24	c	906	CLA	O2D-CGD	4.53	1.44	1.33
27	F	101	SQD	O48-C23	4.53	1.46	1.33
24	C	513	CLA	CHB-C1B	4.53	1.49	1.39
24	C	507	CLA	CHC-C1C	4.53	1.47	1.38
24	b	610	CLA	CHD-C1D	4.52	1.47	1.38
24	d	401	CLA	O2D-CGD	4.52	1.44	1.33
24	c	909	CLA	O2D-CGD	4.52	1.44	1.33
28	B	622	LMG	O8-C28	4.52	1.46	1.33
24	B	611	CLA	CHD-C1D	4.52	1.47	1.38
24	c	913	CLA	MG-NC	4.51	2.17	2.06
25	A	408	PHO	OBD-CAD	4.51	1.28	1.22
24	A	407	CLA	CHC-C1C	4.50	1.47	1.38
25	a	412	PHO	C3D-C2D	4.50	1.47	1.39
24	b	609	CLA	MG-NC	4.49	2.16	2.06
24	c	903	CLA	CHB-C1B	4.49	1.49	1.39
24	A	410	CLA	CHD-C1D	4.49	1.47	1.38
27	B	621	SQD	O47-C7	4.49	1.47	1.34
24	c	908	CLA	CHD-C1D	4.49	1.47	1.38
24	A	406	CLA	CHC-C1C	4.48	1.47	1.38
24	C	501	CLA	CHD-C1D	4.48	1.47	1.38
24	b	612	CLA	O2A-CGA	4.48	1.46	1.33
24	C	511	CLA	CHB-C1B	4.48	1.49	1.39
24	b	616	CLA	OBD-CAD	4.48	1.30	1.22
24	d	401	CLA	CHC-C1C	4.47	1.47	1.38
25	a	412	PHO	OBD-CAD	4.47	1.28	1.22
28	C	534	LMG	O8-C28	4.47	1.46	1.33
24	d	405	CLA	CHD-C1D	4.47	1.47	1.38
24	C	510	CLA	CHB-C1B	4.46	1.49	1.39
24	c	903	CLA	MG-NC	4.45	2.16	2.06
24	b	612	CLA	CHC-C4B	4.45	1.49	1.39
24	B	608	CLA	C1D-ND	4.45	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	O2D-CGD	4.45	1.44	1.33
24	C	503	CLA	CHC-C4B	4.45	1.49	1.39
24	C	505	CLA	CHC-C1C	4.44	1.47	1.38
24	D	402	CLA	O2A-CGA	4.44	1.46	1.33
24	C	504	CLA	CHB-C1B	4.43	1.49	1.39
24	a	410	CLA	C1D-ND	4.43	1.43	1.37
24	D	403	CLA	CHD-C1D	4.43	1.47	1.38
28	C	519	LMG	O8-C28	4.43	1.46	1.33
24	B	616	CLA	CHC-C4B	4.42	1.49	1.39
24	B	604	CLA	O2A-CGA	4.42	1.46	1.33
24	B	605	CLA	CHC-C1C	4.42	1.47	1.38
24	C	506	CLA	O2A-CGA	4.41	1.46	1.33
24	C	503	CLA	CHD-C1D	4.41	1.47	1.38
24	b	613	CLA	CHC-C1C	4.41	1.47	1.38
24	c	910	CLA	MG-ND	-4.41	1.97	2.05
24	b	614	CLA	CHD-C1D	4.40	1.46	1.38
24	C	509	CLA	CHB-C1B	4.40	1.49	1.39
24	C	512	CLA	CHD-C1D	4.40	1.46	1.38
24	C	511	CLA	CHD-C1D	4.39	1.46	1.38
24	c	912	CLA	CHB-C1B	4.39	1.49	1.39
24	C	508	CLA	CHD-C1D	4.39	1.46	1.38
24	B	607	CLA	CHD-C1D	4.38	1.46	1.38
28	C	534	LMG	O7-C10	4.38	1.46	1.34
28	b	624	LMG	O8-C28	4.38	1.46	1.33
24	a	410	CLA	CHB-C1B	4.38	1.49	1.39
24	a	413	CLA	CHD-C1D	4.38	1.46	1.38
24	c	902	CLA	CHC-C1C	4.38	1.47	1.38
25	a	411	PHO	OBD-CAD	4.38	1.28	1.22
24	b	605	CLA	MG-ND	-4.38	1.97	2.05
24	C	502	CLA	CHB-C1B	4.37	1.49	1.39
24	d	404	CLA	CHC-C1C	4.37	1.47	1.38
24	A	410	CLA	CHC-C1C	4.37	1.47	1.38
24	d	401	CLA	CHD-C1D	4.37	1.46	1.38
24	b	613	CLA	CHB-C1B	4.36	1.49	1.39
24	B	608	CLA	CHB-C1B	4.36	1.49	1.39
24	b	608	CLA	CHB-C1B	4.36	1.49	1.39
24	C	510	CLA	CHD-C1D	4.36	1.46	1.38
28	c	920	LMG	O8-C28	4.36	1.46	1.33
28	A	413	LMG	O7-C10	4.36	1.46	1.34
24	B	605	CLA	CHB-C1B	4.35	1.49	1.39
25	A	409	PHO	C3D-C4D	-4.35	1.35	1.41
24	c	912	CLA	O2A-CGA	4.34	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	CHB-C1B	4.34	1.49	1.39
24	c	904	CLA	CHB-C1B	4.34	1.49	1.39
27	a	401	SQD	O47-C7	4.34	1.46	1.34
24	B	615	CLA	CHD-C1D	4.34	1.46	1.38
24	d	404	CLA	CHB-C1B	4.34	1.49	1.39
24	B	615	CLA	MG-ND	-4.34	1.97	2.05
24	b	615	CLA	CHB-C1B	4.33	1.49	1.39
24	B	611	CLA	CHC-C4B	4.33	1.49	1.39
24	c	913	CLA	CHD-C1D	4.33	1.46	1.38
36	e	102	DGD	O2G-C1B	4.32	1.46	1.34
36	D	406	DGD	O2G-C1B	4.32	1.46	1.34
24	b	611	CLA	CHD-C1D	4.32	1.46	1.38
24	C	509	CLA	MG-ND	-4.32	1.97	2.05
24	B	602	CLA	CHC-C4B	4.31	1.49	1.39
36	D	406	DGD	O1G-C1A	4.31	1.45	1.33
37	E	101	LHG	O8-C23	4.31	1.45	1.33
24	B	612	CLA	CHC-C4B	4.31	1.49	1.39
24	a	410	CLA	O2D-CGD	4.31	1.43	1.33
24	c	903	CLA	CHD-C1D	4.31	1.46	1.38
24	B	605	CLA	CHD-C1D	4.30	1.46	1.38
24	c	906	CLA	CHB-C1B	4.30	1.49	1.39
24	B	607	CLA	MG-ND	-4.30	1.97	2.05
24	d	401	CLA	MG-NA	4.29	2.16	2.06
27	A	417	SQD	O47-C7	4.29	1.46	1.34
24	b	611	CLA	CHB-C1B	4.29	1.49	1.39
24	B	610	CLA	OBD-CAD	4.29	1.29	1.22
27	a	401	SQD	O48-C23	4.29	1.45	1.33
24	D	402	CLA	CHC-C1C	4.28	1.47	1.38
37	E	101	LHG	O7-C7	4.28	1.46	1.34
24	D	402	CLA	MG-ND	-4.28	1.97	2.05
24	C	501	CLA	O2D-CGD	4.27	1.43	1.33
24	b	620	CLA	CHB-C1B	4.27	1.49	1.39
24	c	914	CLA	O2A-CGA	4.27	1.45	1.33
24	C	501	CLA	CHC-C4B	4.27	1.49	1.39
24	b	612	CLA	CHB-C1B	4.27	1.49	1.39
27	f	102	SQD	O48-C23	4.27	1.45	1.33
24	b	620	CLA	MG-NC	4.27	2.16	2.06
24	C	506	CLA	CHB-C1B	4.27	1.49	1.39
24	b	615	CLA	CHD-C1D	4.26	1.46	1.38
25	A	409	PHO	C3D-C2D	4.26	1.47	1.39
24	b	610	CLA	O2D-CGD	4.26	1.43	1.33
24	b	605	CLA	CHB-C1B	4.26	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	MG-NB	4.26	2.14	2.05
24	d	404	CLA	C1D-ND	4.26	1.43	1.37
36	c	918	DGD	O1G-C1A	4.26	1.45	1.33
24	c	911	CLA	MG-ND	-4.25	1.97	2.05
24	B	617	CLA	CHB-C1B	4.25	1.49	1.39
24	b	610	CLA	CHB-C1B	4.25	1.49	1.39
24	b	616	CLA	CHD-C1D	4.25	1.46	1.38
24	c	904	CLA	CHC-C4B	4.25	1.48	1.39
24	b	618	CLA	CHD-C1D	4.25	1.46	1.38
38	F	102	HEM	FE-NA	4.25	2.09	1.95
24	D	403	CLA	CHB-C1B	4.25	1.48	1.39
24	b	615	CLA	MG-NB	4.24	2.14	2.05
24	B	605	CLA	O2D-CGD	4.24	1.43	1.33
24	b	605	CLA	CHC-C4B	4.24	1.48	1.39
24	b	620	CLA	O2A-CGA	4.24	1.45	1.33
24	c	908	CLA	O2A-CGA	4.24	1.45	1.33
24	B	617	CLA	CHC-C1C	4.24	1.47	1.38
24	C	512	CLA	O2A-CGA	4.24	1.45	1.33
37	d	410	LHG	O7-C7	4.24	1.46	1.34
24	c	908	CLA	CHB-C1B	4.24	1.48	1.39
24	C	501	CLA	CHB-C1B	4.24	1.48	1.39
24	a	410	CLA	MG-NB	4.23	2.14	2.05
24	d	405	CLA	O2A-CGA	4.23	1.45	1.33
24	B	611	CLA	CHB-C1B	4.23	1.48	1.39
24	B	606	CLA	CHB-C1B	4.23	1.48	1.39
24	C	511	CLA	O2A-CGA	4.22	1.45	1.33
24	c	902	CLA	CHD-C1D	4.22	1.46	1.38
24	B	612	CLA	CHD-C1D	4.22	1.46	1.38
24	c	912	CLA	CHD-C1D	4.22	1.46	1.38
24	A	406	CLA	CHD-C1D	4.21	1.46	1.38
24	C	507	CLA	O2A-CGA	4.21	1.45	1.33
24	b	609	CLA	CHC-C4B	4.21	1.48	1.39
28	c	921	LMG	O7-C10	4.21	1.46	1.34
28	A	413	LMG	O8-C28	4.21	1.45	1.33
24	b	619	CLA	O2A-CGA	4.21	1.45	1.33
24	c	905	CLA	CHD-C1D	4.21	1.46	1.38
27	b	601	SQD	O48-C23	4.21	1.45	1.33
24	A	407	CLA	MG-ND	-4.20	1.97	2.05
24	A	406	CLA	O2A-CGA	4.20	1.45	1.33
28	c	921	LMG	O8-C28	4.20	1.45	1.33
24	B	603	CLA	MG-NC	4.20	2.16	2.06
24	c	907	CLA	CHB-C1B	4.20	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	617	CLA	O2A-CGA	4.19	1.45	1.33
24	b	606	CLA	O2A-CGA	4.19	1.45	1.33
24	C	503	CLA	CHB-C1B	4.19	1.48	1.39
24	c	914	CLA	CHC-C4B	4.18	1.48	1.39
25	A	408	PHO	C3D-C2D	4.18	1.46	1.39
24	d	401	CLA	O2A-CGA	4.18	1.45	1.33
24	c	902	CLA	O2A-CGA	4.18	1.45	1.33
24	c	910	CLA	O2A-CGA	4.18	1.45	1.33
24	C	508	CLA	O2A-CGA	4.17	1.45	1.33
24	A	406	CLA	MG-ND	-4.17	1.97	2.05
24	C	513	CLA	MG-NB	4.17	2.14	2.05
38	v	202	HEM	FE-NB	4.17	2.07	1.94
24	c	910	CLA	CHD-C4C	4.17	1.48	1.39
28	c	920	LMG	O7-C10	4.17	1.46	1.34
37	e	101	LHG	O7-C7	4.17	1.46	1.34
25	a	411	PHO	C3D-C2D	4.17	1.46	1.39
24	b	618	CLA	MG-NA	4.16	2.16	2.06
36	e	102	DGD	O1G-C1A	4.16	1.45	1.33
36	C	518	DGD	O1G-C1A	4.16	1.45	1.33
24	C	510	CLA	CHC-C4B	4.16	1.48	1.39
24	b	616	CLA	CHC-C4B	4.16	1.48	1.39
24	A	410	CLA	MG-NA	4.16	2.16	2.06
24	c	909	CLA	O2A-CGA	4.16	1.45	1.33
24	c	913	CLA	O2A-CGA	4.16	1.45	1.33
24	B	608	CLA	CHD-C1D	4.15	1.46	1.38
24	C	513	CLA	CHC-C4B	4.15	1.48	1.39
24	b	614	CLA	CHC-C4B	4.15	1.48	1.39
25	a	412	PHO	C3D-C4D	-4.15	1.35	1.41
24	a	413	CLA	O2A-CGA	4.14	1.45	1.33
24	C	512	CLA	CHB-C1B	4.14	1.48	1.39
24	C	508	CLA	MG-NA	4.14	2.16	2.06
25	a	411	PHO	C3D-C4D	-4.14	1.35	1.41
24	B	606	CLA	CHC-C4B	4.14	1.48	1.39
24	C	512	CLA	CHC-C4B	4.14	1.48	1.39
27	B	621	SQD	O48-C23	4.13	1.45	1.33
24	B	611	CLA	MG-NB	4.13	2.14	2.05
24	D	402	CLA	CHB-C1B	4.13	1.48	1.39
24	B	614	CLA	CHD-C1D	4.13	1.46	1.38
24	B	608	CLA	CHC-C4B	4.13	1.48	1.39
24	d	404	CLA	CHD-C1D	4.12	1.46	1.38
24	b	608	CLA	CHC-C4B	4.12	1.48	1.39
24	C	509	CLA	CHC-C4B	4.12	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	O2A-CGA	4.12	1.45	1.33
24	C	502	CLA	O2A-CGA	4.11	1.45	1.33
24	B	611	CLA	O2D-CGD	4.11	1.43	1.33
24	b	617	CLA	CHB-C1B	4.11	1.48	1.39
24	B	616	CLA	MG-NB	4.11	2.13	2.05
24	B	613	CLA	CHD-C1D	4.11	1.46	1.38
35	o	301	HTG	C1'-S1	-4.11	1.76	1.81
28	a	416	LMG	O8-C28	4.11	1.45	1.33
24	C	501	CLA	O2A-CGA	4.10	1.45	1.33
24	C	509	CLA	O2A-CGA	4.10	1.45	1.33
24	a	410	CLA	O2A-CGA	4.10	1.45	1.33
24	a	409	CLA	CHB-C1B	4.10	1.48	1.39
24	d	405	CLA	CHC-C4B	4.10	1.48	1.39
24	b	607	CLA	CHB-C1B	4.10	1.48	1.39
24	b	605	CLA	C3D-C2D	4.10	1.50	1.39
24	c	909	CLA	CHC-C4B	4.10	1.48	1.39
24	D	402	CLA	O2D-CGD	4.09	1.43	1.33
24	A	407	CLA	CHB-C1B	4.09	1.48	1.39
24	c	905	CLA	CHB-C1B	4.09	1.48	1.39
24	B	607	CLA	CHB-C1B	4.09	1.48	1.39
24	A	406	CLA	CHC-C4B	4.09	1.48	1.39
24	B	608	CLA	CHD-C4C	4.09	1.48	1.39
24	b	619	CLA	CHC-C4B	4.09	1.48	1.39
24	b	607	CLA	O2A-CGA	4.09	1.45	1.33
24	C	504	CLA	CHD-C4C	4.09	1.48	1.39
27	A	412	SQD	O47-C7	4.09	1.45	1.34
24	b	615	CLA	CHC-C4B	4.09	1.48	1.39
24	B	602	CLA	CHB-C1B	4.08	1.48	1.39
24	b	613	CLA	O2A-CGA	4.08	1.45	1.33
24	B	604	CLA	MG-NA	4.08	2.16	2.06
24	B	603	CLA	CHC-C4B	4.08	1.48	1.39
27	A	412	SQD	O48-C23	4.08	1.45	1.33
24	C	502	CLA	CHC-C4B	4.08	1.48	1.39
24	C	508	CLA	CHB-C1B	4.08	1.48	1.39
24	C	505	CLA	CHB-C1B	4.07	1.48	1.39
24	b	619	CLA	CHD-C1D	4.07	1.46	1.38
28	d	411	LMG	O8-C28	4.07	1.45	1.33
37	d	409	LHG	O8-C23	4.07	1.45	1.33
24	C	504	CLA	O2A-CGA	4.06	1.45	1.33
24	b	618	CLA	CHD-C4C	4.06	1.48	1.39
24	B	609	CLA	O2A-CGA	4.06	1.45	1.33
24	A	410	CLA	MG-ND	-4.06	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	907	CLA	O2A-CGA	4.06	1.45	1.33
24	A	406	CLA	MG-NC	4.06	2.15	2.06
24	C	513	CLA	O2A-CGA	4.06	1.45	1.33
24	B	602	CLA	CHD-C4C	4.05	1.48	1.39
24	B	614	CLA	CHC-C4B	4.05	1.48	1.39
37	b	639	LHG	O8-C23	4.05	1.45	1.33
28	d	411	LMG	O7-C10	4.05	1.45	1.34
24	B	616	CLA	CHD-C1D	4.05	1.46	1.38
24	c	912	CLA	OBD-CAD	4.05	1.29	1.22
25	A	409	PHO	O2A-CGA	4.04	1.45	1.33
24	B	616	CLA	OBD-CAD	4.04	1.29	1.22
24	b	616	CLA	O2A-CGA	4.04	1.45	1.33
24	B	608	CLA	OBD-CAD	4.04	1.29	1.22
24	c	912	CLA	MG-ND	-4.04	1.97	2.05
24	c	913	CLA	CHB-C1B	4.04	1.48	1.39
24	b	606	CLA	CHC-C4B	4.04	1.48	1.39
27	a	415	SQD	O48-C23	4.03	1.45	1.33
36	H	103	DGD	O1G-C1A	4.03	1.45	1.33
24	c	913	CLA	CHC-C4B	4.03	1.48	1.39
24	a	409	CLA	CHD-C1D	4.03	1.46	1.38
24	c	911	CLA	CHC-C4B	4.03	1.48	1.39
28	B	622	LMG	O7-C10	4.02	1.45	1.34
24	b	610	CLA	CHC-C4B	4.02	1.48	1.39
24	A	410	CLA	CHB-C1B	4.02	1.48	1.39
35	O	303	HTG	C1'-S1	-4.02	1.76	1.81
24	b	615	CLA	MG-NC	4.02	2.15	2.06
28	a	416	LMG	O7-C10	4.01	1.45	1.34
24	c	914	CLA	CHB-C1B	4.01	1.48	1.39
24	B	614	CLA	CHB-C1B	4.01	1.48	1.39
28	C	519	LMG	O7-C10	4.01	1.45	1.34
24	c	906	CLA	CHC-C4B	4.01	1.48	1.39
24	B	615	CLA	CHB-C1B	4.01	1.48	1.39
24	B	617	CLA	CHD-C1D	4.01	1.46	1.38
24	b	618	CLA	CHC-C4B	4.00	1.48	1.39
24	c	905	CLA	C3D-C2D	4.00	1.50	1.39
36	h	102	DGD	O2G-C1B	4.00	1.45	1.34
24	C	508	CLA	CHC-C4B	4.00	1.48	1.39
24	b	618	CLA	CHB-C1B	4.00	1.48	1.39
24	c	912	CLA	C3D-C2D	4.00	1.50	1.39
24	C	511	CLA	C3D-C2D	3.99	1.50	1.39
24	b	609	CLA	CHD-C1D	3.99	1.46	1.38
24	B	616	CLA	O2A-CGA	3.99	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	OBD-CAD	3.99	1.29	1.22
24	b	610	CLA	O2A-CGA	3.98	1.45	1.33
24	c	907	CLA	CHD-C4C	3.98	1.48	1.39
24	B	615	CLA	C4B-NB	-3.98	1.32	1.37
24	c	903	CLA	O2A-CGA	3.98	1.45	1.33
24	b	606	CLA	C3D-C2D	3.98	1.50	1.39
24	b	614	CLA	CHB-C1B	3.98	1.48	1.39
24	C	511	CLA	CHD-C4C	3.97	1.48	1.39
24	b	611	CLA	CHC-C4B	3.97	1.48	1.39
36	C	516	DGD	O2G-C1B	3.97	1.45	1.34
24	B	603	CLA	CHB-C1B	3.97	1.48	1.39
24	C	506	CLA	CHD-C4C	3.97	1.48	1.39
24	B	603	CLA	O2A-CGA	3.97	1.44	1.33
37	D	409	LHG	O7-C7	3.96	1.45	1.34
24	b	607	CLA	CHC-C4B	3.96	1.48	1.39
24	B	606	CLA	C3D-C2D	3.96	1.49	1.39
24	b	613	CLA	OBD-CAD	3.96	1.29	1.22
24	c	911	CLA	CHD-C4C	3.96	1.48	1.39
24	B	609	CLA	C3D-C2D	3.96	1.49	1.39
24	D	402	CLA	C1D-ND	3.96	1.42	1.37
24	c	903	CLA	C3D-C2D	3.95	1.49	1.39
24	a	410	CLA	CHD-C1D	3.95	1.46	1.38
24	c	908	CLA	CHC-C4B	3.95	1.48	1.39
36	c	918	DGD	O2G-C1B	3.95	1.45	1.34
24	c	912	CLA	CHD-C4C	3.95	1.48	1.39
36	c	919	DGD	O1G-C1A	3.94	1.44	1.33
24	C	501	CLA	CHD-C4C	3.94	1.48	1.39
24	A	410	CLA	CHC-C4B	3.94	1.48	1.39
24	c	914	CLA	MG-ND	-3.94	1.98	2.05
24	C	508	CLA	C3D-C2D	3.94	1.49	1.39
24	c	909	CLA	CHB-C1B	3.94	1.48	1.39
38	F	102	HEM	FE-NB	3.94	2.07	1.94
24	b	619	CLA	CHB-C1B	3.94	1.48	1.39
24	B	606	CLA	O2A-CGA	3.94	1.44	1.33
24	a	413	CLA	CHB-C1B	3.93	1.48	1.39
24	B	610	CLA	CHC-C4B	3.93	1.48	1.39
24	C	507	CLA	CHB-C1B	3.92	1.48	1.39
24	b	614	CLA	C3D-C2D	3.92	1.49	1.39
24	c	910	CLA	CHC-C4B	3.92	1.48	1.39
24	C	509	CLA	CHD-C4C	3.92	1.48	1.39
38	V	202	HEM	FE-NC	3.92	2.08	1.95
24	C	502	CLA	C3D-C2D	3.92	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	CHC-C4B	3.92	1.48	1.39
24	C	510	CLA	CHD-C4C	3.92	1.48	1.39
24	d	405	CLA	CHB-C1B	3.91	1.48	1.39
25	A	408	PHO	C3D-C4D	-3.91	1.35	1.41
24	a	410	CLA	OBD-CAD	3.91	1.29	1.22
24	c	903	CLA	CHC-C4B	3.91	1.48	1.39
24	b	614	CLA	OBD-CAD	3.91	1.29	1.22
24	A	407	CLA	OBD-CAD	3.90	1.29	1.22
24	C	513	CLA	CHD-C4C	3.90	1.48	1.39
24	c	914	CLA	C3D-C2D	3.90	1.49	1.39
24	C	509	CLA	C3D-C2D	3.90	1.49	1.39
24	B	610	CLA	O2A-CGA	3.90	1.44	1.33
24	B	613	CLA	C1B-NB	-3.90	1.33	1.37
24	b	605	CLA	CHD-C4C	3.89	1.48	1.39
24	c	908	CLA	OBD-CAD	3.89	1.29	1.22
37	L	101	LHG	O8-C23	3.89	1.44	1.33
24	b	620	CLA	OBD-CAD	3.89	1.29	1.22
24	D	403	CLA	CHC-C4B	3.89	1.48	1.39
24	A	405	CLA	OBD-CAD	3.89	1.29	1.22
24	B	615	CLA	O2A-CGA	3.88	1.44	1.33
36	C	517	DGD	O1G-C1A	3.88	1.44	1.33
24	c	903	CLA	CHD-C4C	3.88	1.48	1.39
24	b	613	CLA	CHC-C4B	3.88	1.48	1.39
38	V	202	HEM	FE-NB	3.88	2.06	1.94
24	C	504	CLA	C3D-C2D	3.87	1.49	1.39
24	B	604	CLA	CHD-C1D	3.87	1.45	1.38
24	B	609	CLA	CHC-C4B	3.87	1.48	1.39
24	b	608	CLA	O2A-CGA	3.87	1.44	1.33
24	b	617	CLA	O2A-CGA	3.87	1.44	1.33
24	C	503	CLA	CHD-C4C	3.87	1.48	1.39
24	c	909	CLA	OBD-CAD	3.86	1.29	1.22
24	C	507	CLA	CHC-C4B	3.86	1.48	1.39
24	d	401	CLA	CHB-C1B	3.86	1.48	1.39
24	b	610	CLA	CHD-C4C	3.86	1.48	1.39
37	d	408	LHG	O8-C23	3.86	1.44	1.33
24	c	910	CLA	OBD-CAD	3.86	1.29	1.22
24	b	619	CLA	C3D-C2D	3.86	1.49	1.39
24	c	914	CLA	CHD-C4C	3.86	1.48	1.39
25	A	408	PHO	O2A-CGA	3.85	1.44	1.33
24	c	906	CLA	O2A-CGA	3.85	1.44	1.33
24	c	904	CLA	C3D-C2D	3.85	1.49	1.39
24	b	619	CLA	OBD-CAD	3.85	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	h	102	DGD	O1G-C1A	3.84	1.44	1.33
24	c	907	CLA	CHC-C4B	3.84	1.48	1.39
24	C	501	CLA	OBD-CAD	3.84	1.29	1.22
24	d	405	CLA	CHD-C4C	3.84	1.48	1.39
24	B	610	CLA	C3D-C2D	3.84	1.49	1.39
24	B	612	CLA	MG-ND	-3.84	1.98	2.05
24	C	506	CLA	CHC-C4B	3.84	1.48	1.39
24	C	502	CLA	CHD-C4C	3.83	1.48	1.39
24	b	616	CLA	C3D-C2D	3.83	1.49	1.39
24	c	904	CLA	O2A-CGA	3.83	1.44	1.33
24	C	501	CLA	C3D-C2D	3.83	1.49	1.39
24	b	609	CLA	CHB-C1B	3.83	1.48	1.39
24	b	607	CLA	CHD-C4C	3.83	1.48	1.39
24	c	908	CLA	CHD-C4C	3.83	1.48	1.39
24	b	617	CLA	CHC-C4B	3.83	1.48	1.39
24	c	905	CLA	O2A-CGA	3.82	1.44	1.33
24	A	407	CLA	C3D-C2D	3.82	1.49	1.39
24	A	410	CLA	C3D-C2D	3.82	1.49	1.39
24	b	614	CLA	MG-ND	-3.82	1.98	2.05
24	A	410	CLA	O2A-CGA	3.82	1.44	1.33
24	C	503	CLA	O2A-CGA	3.82	1.44	1.33
24	b	608	CLA	OBD-CAD	3.82	1.29	1.22
24	B	616	CLA	C3D-C2D	3.82	1.49	1.39
24	D	402	CLA	CHD-C4C	3.82	1.47	1.39
24	B	607	CLA	CHC-C4B	3.82	1.48	1.39
24	B	602	CLA	OBD-CAD	3.82	1.29	1.22
24	A	406	CLA	CHB-C1B	3.81	1.48	1.39
24	b	612	CLA	OBD-CAD	3.81	1.29	1.22
24	B	602	CLA	MG-NC	3.81	2.15	2.06
24	b	619	CLA	CHD-C4C	3.81	1.47	1.39
24	B	609	CLA	CHB-C1B	3.81	1.48	1.39
27	a	415	SQD	O47-C7	3.81	1.45	1.34
24	C	509	CLA	OBD-CAD	3.81	1.29	1.22
25	a	412	PHO	O2A-CGA	3.81	1.44	1.33
24	b	615	CLA	O2A-CGA	3.80	1.44	1.33
24	B	613	CLA	C1D-ND	3.80	1.42	1.37
24	C	507	CLA	OBD-CAD	3.80	1.29	1.22
24	B	612	CLA	CHB-C1B	3.79	1.47	1.39
24	B	613	CLA	OBD-CAD	3.79	1.29	1.22
24	C	512	CLA	C3D-C2D	3.79	1.49	1.39
24	b	610	CLA	C3D-C2D	3.79	1.49	1.39
24	B	613	CLA	O2A-CGA	3.79	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	CHD-C4C	3.79	1.47	1.39
24	B	614	CLA	OBD-CAD	3.79	1.29	1.22
24	B	612	CLA	MG-NC	3.78	2.15	2.06
24	C	506	CLA	C3D-C2D	3.78	1.49	1.39
24	b	609	CLA	O2A-CGA	3.78	1.44	1.33
24	a	410	CLA	C1B-NB	-3.78	1.33	1.37
35	C	528	HTG	C1'-S1	-3.78	1.76	1.81
24	c	912	CLA	CHC-C4B	3.78	1.47	1.39
24	b	611	CLA	O2A-CGA	3.78	1.44	1.33
24	D	402	CLA	CHD-C1D	3.78	1.45	1.38
24	A	410	CLA	CHD-C4C	3.78	1.47	1.39
24	C	505	CLA	CHC-C4B	3.78	1.47	1.39
35	d	403	HTG	C1'-S1	-3.77	1.76	1.81
24	C	510	CLA	OBD-CAD	3.77	1.29	1.22
24	b	617	CLA	CHD-C1D	3.77	1.45	1.38
24	A	407	CLA	O2A-CGA	3.77	1.44	1.33
24	A	406	CLA	OBD-CAD	3.77	1.29	1.22
28	b	624	LMG	O7-C10	3.77	1.44	1.34
24	c	905	CLA	CHD-C4C	3.76	1.47	1.39
24	A	405	CLA	CHD-C1D	3.76	1.45	1.38
24	B	608	CLA	MG-ND	-3.76	1.98	2.05
24	C	503	CLA	C3D-C2D	3.76	1.49	1.39
24	D	403	CLA	OBD-CAD	3.76	1.29	1.22
24	c	909	CLA	CHD-C4C	3.75	1.47	1.39
36	C	516	DGD	O1G-C1A	3.75	1.44	1.33
24	b	609	CLA	CHD-C4C	3.75	1.47	1.39
24	a	410	CLA	C3D-C2D	3.75	1.49	1.39
24	C	511	CLA	OBD-CAD	3.75	1.28	1.22
24	A	407	CLA	CHC-C4B	3.75	1.47	1.39
37	D	409	LHG	O8-C23	3.75	1.44	1.33
36	c	917	DGD	O2G-C1B	3.75	1.44	1.34
24	C	508	CLA	OBD-CAD	3.75	1.28	1.22
37	D	408	LHG	O8-C23	3.75	1.44	1.33
24	D	403	CLA	CHD-C4C	3.74	1.47	1.39
24	C	508	CLA	CHD-C4C	3.74	1.47	1.39
24	C	510	CLA	C3D-C2D	3.74	1.49	1.39
24	a	409	CLA	CHD-C4C	3.73	1.47	1.39
24	c	910	CLA	C3D-C2D	3.73	1.49	1.39
24	a	413	CLA	MG-NC	3.73	2.15	2.06
37	d	410	LHG	O8-C23	3.73	1.44	1.33
24	B	616	CLA	CHB-C1B	3.73	1.47	1.39
24	c	904	CLA	CHD-C4C	3.73	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	409	CLA	OBD-CAD	3.72	1.28	1.22
24	d	404	CLA	CHC-C4B	3.72	1.47	1.39
24	B	603	CLA	CHD-C4C	3.72	1.47	1.39
24	c	909	CLA	MG-NB	3.72	2.13	2.05
24	B	611	CLA	C3D-C2D	3.72	1.49	1.39
24	C	511	CLA	CHC-C4B	3.72	1.47	1.39
24	C	513	CLA	C3D-C2D	3.71	1.49	1.39
24	A	406	CLA	C3D-C2D	3.71	1.49	1.39
35	b	627	HTG	C1'-S1	-3.71	1.76	1.81
24	A	406	CLA	CHD-C4C	3.71	1.47	1.39
24	C	504	CLA	CHC-C4B	3.71	1.47	1.39
24	B	617	CLA	C3D-C2D	3.71	1.49	1.39
35	B	626	HTG	C1'-S1	-3.71	1.76	1.81
24	A	405	CLA	C1B-NB	-3.70	1.33	1.37
24	b	605	CLA	OBD-CAD	3.70	1.28	1.22
24	c	913	CLA	CHD-C4C	3.70	1.47	1.39
24	c	908	CLA	C3D-C2D	3.70	1.49	1.39
24	c	903	CLA	OBD-CAD	3.70	1.28	1.22
24	B	614	CLA	MG-NC	3.70	2.15	2.06
24	B	605	CLA	CHC-C4B	3.69	1.47	1.39
24	c	905	CLA	CHC-C4B	3.69	1.47	1.39
24	c	907	CLA	C3D-C2D	3.69	1.49	1.39
24	B	615	CLA	CHD-C4C	3.69	1.47	1.39
24	C	510	CLA	O2A-CGA	3.69	1.44	1.33
24	A	407	CLA	MG-NA	3.68	2.15	2.06
24	B	612	CLA	CHD-C4C	3.68	1.47	1.39
24	D	403	CLA	O2A-CGA	3.68	1.44	1.33
36	C	517	DGD	O2G-C1B	3.68	1.44	1.34
24	a	413	CLA	CHC-C4B	3.68	1.47	1.39
24	d	405	CLA	C1B-NB	-3.68	1.33	1.37
24	B	615	CLA	C3D-C2D	3.68	1.49	1.39
24	A	407	CLA	CHD-C4C	3.68	1.47	1.39
24	C	506	CLA	OBD-CAD	3.67	1.28	1.22
24	d	401	CLA	C3D-C2D	3.67	1.49	1.39
24	A	407	CLA	C1B-NB	-3.67	1.33	1.37
24	c	902	CLA	MG-NC	3.67	2.15	2.06
24	b	618	CLA	O2A-CGA	3.67	1.44	1.33
36	c	919	DGD	O2G-C1B	3.67	1.44	1.34
24	B	604	CLA	CHB-C1B	3.67	1.47	1.39
24	b	606	CLA	OBD-CAD	3.67	1.28	1.22
35	c	923	HTG	C1'-S1	-3.67	1.76	1.81
24	b	610	CLA	OBD-CAD	3.67	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	611	CLA	C3D-C2D	3.67	1.49	1.39
24	C	512	CLA	CHD-C4C	3.66	1.47	1.39
24	a	409	CLA	CHC-C4B	3.66	1.47	1.39
24	B	602	CLA	C3D-C2D	3.66	1.49	1.39
24	B	608	CLA	O2A-CGA	3.66	1.44	1.33
24	D	403	CLA	C3D-C2D	3.64	1.49	1.39
37	d	409	LHG	O7-C7	3.64	1.44	1.34
24	C	505	CLA	O2A-CGA	3.64	1.44	1.33
24	b	620	CLA	C3D-C2D	3.64	1.49	1.39
24	B	614	CLA	C3D-C2D	3.64	1.49	1.39
24	b	615	CLA	C3D-C2D	3.64	1.49	1.39
24	c	909	CLA	C3D-C2D	3.64	1.49	1.39
24	c	906	CLA	CHD-C4C	3.64	1.47	1.39
24	B	612	CLA	MG-NB	3.63	2.13	2.05
24	B	604	CLA	C3D-C2D	3.63	1.49	1.39
24	a	410	CLA	CHD-C4C	3.63	1.47	1.39
24	b	608	CLA	C3D-C2D	3.63	1.49	1.39
24	B	615	CLA	CHC-C4B	3.63	1.47	1.39
24	b	608	CLA	CHD-C4C	3.62	1.47	1.39
24	c	902	CLA	CHC-C4B	3.62	1.47	1.39
24	A	407	CLA	MG-NC	3.62	2.14	2.06
24	d	405	CLA	MG-NA	3.62	2.14	2.06
24	c	902	CLA	CHD-C4C	3.62	1.47	1.39
24	B	614	CLA	O2A-CGA	3.62	1.43	1.33
24	D	402	CLA	CHC-C4B	3.62	1.47	1.39
28	D	410	LMG	O7-C10	3.62	1.44	1.34
24	b	606	CLA	MG-ND	-3.62	1.98	2.05
24	a	410	CLA	CHC-C4B	3.62	1.47	1.39
24	b	612	CLA	C3D-C2D	3.61	1.49	1.39
35	b	603	HTG	C1'-S1	-3.61	1.76	1.81
24	c	913	CLA	C3D-C2D	3.61	1.49	1.39
25	a	411	PHO	O2A-CGA	3.61	1.43	1.33
24	a	413	CLA	CHD-C4C	3.60	1.47	1.39
24	B	617	CLA	MG-NC	3.60	2.14	2.06
24	B	611	CLA	CHD-C4C	3.60	1.47	1.39
24	B	617	CLA	OBD-CAD	3.60	1.28	1.22
24	C	507	CLA	CHD-C4C	3.59	1.47	1.39
37	L	101	LHG	O7-C7	3.59	1.44	1.34
24	D	402	CLA	MG-NC	3.59	2.14	2.06
24	B	608	CLA	C1B-NB	-3.59	1.33	1.37
35	B	627	HTG	C1'-S1	-3.59	1.76	1.81
24	A	405	CLA	CHD-C4C	3.59	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	CHD-C4C	3.59	1.47	1.39
24	b	614	CLA	CHD-C4C	3.59	1.47	1.39
37	d	408	LHG	O7-C7	3.58	1.44	1.34
24	d	405	CLA	C3D-C2D	3.58	1.48	1.39
24	b	614	CLA	O2A-CGA	3.58	1.43	1.33
36	c	917	DGD	O1G-C1A	3.57	1.43	1.33
37	D	408	LHG	O7-C7	3.57	1.44	1.34
24	b	618	CLA	C3D-C2D	3.57	1.48	1.39
37	b	639	LHG	O7-C7	3.57	1.44	1.34
24	B	606	CLA	OBD-CAD	3.57	1.28	1.22
36	C	518	DGD	O2G-C1B	3.57	1.44	1.34
24	b	609	CLA	C3D-C2D	3.57	1.48	1.39
24	b	620	CLA	CHC-C4B	3.56	1.47	1.39
24	A	405	CLA	CHC-C4B	3.56	1.47	1.39
24	b	609	CLA	OBD-CAD	3.56	1.28	1.22
24	b	618	CLA	C1B-NB	-3.56	1.33	1.37
24	B	609	CLA	CHD-C4C	3.55	1.47	1.39
24	B	603	CLA	OBD-CAD	3.55	1.28	1.22
24	C	507	CLA	C3D-C2D	3.55	1.48	1.39
24	C	505	CLA	C3D-C2D	3.55	1.48	1.39
24	b	612	CLA	CHD-C4C	3.55	1.47	1.39
35	b	602	HTG	C1'-S1	-3.55	1.76	1.81
35	H	105	HTG	C1'-S1	-3.55	1.76	1.81
24	D	402	CLA	OBD-CAD	3.54	1.28	1.22
24	b	607	CLA	OBD-CAD	3.54	1.28	1.22
24	c	902	CLA	C3D-C2D	3.54	1.48	1.39
24	B	607	CLA	CHD-C4C	3.54	1.47	1.39
28	D	410	LMG	O8-C28	3.54	1.43	1.33
24	c	906	CLA	OBD-CAD	3.53	1.28	1.22
24	b	620	CLA	CHD-C4C	3.53	1.47	1.39
24	b	615	CLA	CHD-C4C	3.53	1.47	1.39
24	b	619	CLA	MG-ND	-3.52	1.98	2.05
24	B	603	CLA	C3D-C2D	3.52	1.48	1.39
24	c	911	CLA	O2A-CGA	3.52	1.43	1.33
24	B	616	CLA	CHD-C4C	3.51	1.47	1.39
24	B	607	CLA	C3D-C2D	3.51	1.48	1.39
24	a	413	CLA	OBD-CAD	3.51	1.28	1.22
24	b	616	CLA	MG-NC	3.51	2.14	2.06
24	B	609	CLA	OBD-CAD	3.51	1.28	1.22
24	c	913	CLA	OBD-CAD	3.51	1.28	1.22
24	A	405	CLA	O2A-CGA	3.51	1.43	1.33
24	c	908	CLA	MG-ND	-3.50	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	911	CLA	OBD-CAD	3.50	1.28	1.22
24	B	612	CLA	C3D-C2D	3.49	1.48	1.39
24	C	513	CLA	OBD-CAD	3.49	1.28	1.22
24	c	905	CLA	OBD-CAD	3.49	1.28	1.22
24	c	914	CLA	OBD-CAD	3.49	1.28	1.22
24	a	413	CLA	C3D-C2D	3.49	1.48	1.39
24	c	907	CLA	MG-NB	3.49	2.12	2.05
24	b	613	CLA	C3D-C2D	3.48	1.48	1.39
24	A	405	CLA	C3D-C2D	3.48	1.48	1.39
24	B	614	CLA	C1B-NB	-3.47	1.33	1.37
24	B	610	CLA	CHD-C4C	3.47	1.47	1.39
24	B	608	CLA	C3D-C2D	3.47	1.48	1.39
24	A	410	CLA	OBD-CAD	3.47	1.28	1.22
24	C	503	CLA	OBD-CAD	3.47	1.28	1.22
24	c	906	CLA	C3D-C2D	3.46	1.48	1.39
24	B	613	CLA	C3D-C2D	3.46	1.48	1.39
36	H	103	DGD	O2G-C1B	3.46	1.44	1.34
24	b	609	CLA	MG-ND	-3.46	1.98	2.05
24	B	611	CLA	O2A-CGA	3.45	1.43	1.33
24	b	608	CLA	C4D-CHA	3.45	1.50	1.38
24	B	613	CLA	CHC-C4B	3.45	1.47	1.39
24	b	617	CLA	CHD-C4C	3.45	1.47	1.39
24	a	409	CLA	C3D-C2D	3.45	1.48	1.39
24	C	504	CLA	OBD-CAD	3.45	1.28	1.22
24	c	911	CLA	C3D-C2D	3.44	1.48	1.39
24	c	907	CLA	OBD-CAD	3.44	1.28	1.22
24	b	613	CLA	CHD-C4C	3.44	1.47	1.39
24	B	614	CLA	CHD-C4C	3.44	1.47	1.39
24	a	409	CLA	O2A-CGA	3.43	1.43	1.33
24	b	617	CLA	C3D-C2D	3.43	1.48	1.39
24	C	505	CLA	OBD-CAD	3.42	1.28	1.22
24	c	907	CLA	C1B-NB	-3.42	1.33	1.37
35	c	924	HTG	C1'-S1	-3.42	1.77	1.81
24	c	905	CLA	C4B-NB	-3.42	1.33	1.37
35	B	625	HTG	C1'-S1	-3.42	1.77	1.81
24	B	605	CLA	O2A-CGA	3.42	1.43	1.33
24	B	605	CLA	OBD-CAD	3.42	1.28	1.22
35	u	201	HTG	C1'-S1	-3.41	1.77	1.81
37	D	407	LHG	O8-C23	3.41	1.43	1.33
24	B	612	CLA	O2A-CGA	3.41	1.43	1.33
24	d	404	CLA	CHD-C4C	3.40	1.47	1.39
24	b	611	CLA	C1B-C2B	3.40	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	401	CLA	OBD-CAD	3.40	1.28	1.22
24	C	505	CLA	CHD-C4C	3.40	1.47	1.39
24	C	510	CLA	C1B-NB	-3.40	1.33	1.37
24	d	405	CLA	OBD-CAD	3.39	1.28	1.22
24	B	606	CLA	CHD-C4C	3.38	1.47	1.39
24	B	613	CLA	CHD-C4C	3.38	1.46	1.39
24	B	617	CLA	CHC-C4B	3.38	1.47	1.39
24	d	404	CLA	C3D-C2D	3.38	1.48	1.39
24	B	615	CLA	OBD-CAD	3.37	1.28	1.22
35	C	522	HTG	C1'-S1	-3.37	1.77	1.81
24	c	904	CLA	OBD-CAD	3.37	1.28	1.22
24	C	510	CLA	MG-NB	3.37	2.12	2.05
24	B	617	CLA	CHD-C4C	3.35	1.46	1.39
24	b	617	CLA	OBD-CAD	3.35	1.28	1.22
24	C	503	CLA	MG-ND	-3.34	1.99	2.05
38	v	202	HEM	FE-ND	3.34	2.05	1.94
24	c	912	CLA	C4B-NB	-3.33	1.33	1.37
24	D	403	CLA	C1B-NB	-3.32	1.33	1.37
24	b	607	CLA	C3D-C2D	3.32	1.48	1.39
24	b	611	CLA	CHD-C4C	3.32	1.46	1.39
24	B	612	CLA	OBD-CAD	3.32	1.28	1.22
24	C	511	CLA	MG-NC	3.31	2.14	2.06
24	c	908	CLA	MG-NB	-3.30	1.99	2.05
24	C	512	CLA	OBD-CAD	3.30	1.28	1.22
24	C	509	CLA	C4B-NB	-3.30	1.33	1.37
24	B	607	CLA	OBD-CAD	3.29	1.28	1.22
24	B	604	CLA	CHD-C4C	3.29	1.46	1.39
24	B	616	CLA	C4B-NB	-3.28	1.33	1.37
24	C	507	CLA	C4D-CHA	3.27	1.50	1.38
24	c	902	CLA	OBD-CAD	3.27	1.28	1.22
35	C	521	HTG	C1'-S1	-3.26	1.77	1.81
24	d	405	CLA	MG-NB	3.26	2.12	2.05
24	B	615	CLA	C1B-NB	-3.25	1.33	1.37
37	D	407	LHG	O7-C7	3.25	1.43	1.34
25	A	409	PHO	C3A-C2A	-3.25	1.51	1.54
24	d	401	CLA	CHD-C4C	3.25	1.46	1.39
24	c	909	CLA	C1B-NB	-3.24	1.33	1.37
24	A	405	CLA	C4B-NB	-3.24	1.33	1.37
24	d	401	CLA	C1B-NB	-3.24	1.33	1.37
24	c	910	CLA	C4D-CHA	3.23	1.49	1.38
24	b	616	CLA	CHD-C4C	3.22	1.46	1.39
24	d	401	CLA	CHC-C4B	3.22	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	620	CLA	C4B-NB	-3.21	1.33	1.37
24	c	908	CLA	C4D-CHA	3.21	1.49	1.38
24	b	618	CLA	OBD-CAD	3.19	1.28	1.22
24	D	403	CLA	C1B-C2B	3.19	1.50	1.43
24	d	405	CLA	C4B-NB	-3.19	1.33	1.37
24	d	404	CLA	OBD-CAD	3.18	1.28	1.22
24	a	409	CLA	C4B-NB	-3.18	1.33	1.37
24	B	602	CLA	C3B-C4B	3.18	1.50	1.42
24	B	605	CLA	C3D-C2D	3.16	1.47	1.39
24	c	904	CLA	C4D-CHA	3.16	1.49	1.38
24	b	609	CLA	C1B-NB	-3.16	1.33	1.37
24	d	404	CLA	C1B-NB	-3.15	1.33	1.37
24	B	609	CLA	C1B-NB	-3.15	1.33	1.37
24	B	611	CLA	C1B-NB	-3.15	1.33	1.37
38	v	202	HEM	CAB-C3B	3.14	1.56	1.47
24	D	403	CLA	MG-NA	3.14	2.13	2.06
24	C	508	CLA	C1B-NB	-3.13	1.33	1.37
24	D	402	CLA	C1B-C2B	3.12	1.50	1.43
24	b	609	CLA	C3B-C4B	3.12	1.50	1.42
24	b	614	CLA	C1B-NB	-3.12	1.33	1.37
24	D	403	CLA	C4B-NB	-3.12	1.33	1.37
24	b	619	CLA	C3B-C4B	3.12	1.50	1.42
24	c	905	CLA	C1B-NB	-3.11	1.34	1.37
24	B	604	CLA	OBD-CAD	3.11	1.27	1.22
25	a	412	PHO	C3A-C2A	-3.11	1.51	1.54
24	C	511	CLA	C4D-CHA	3.10	1.49	1.38
38	f	101	HEM	CAB-C3B	3.10	1.55	1.47
38	v	202	HEM	FE-NA	3.10	2.05	1.95
24	D	402	CLA	C3D-C2D	3.09	1.47	1.39
24	c	911	CLA	C1B-C2B	3.09	1.50	1.43
24	b	616	CLA	C1B-C2B	3.09	1.50	1.43
24	B	613	CLA	MG-NC	3.08	2.13	2.06
24	c	906	CLA	C1B-C2B	3.07	1.50	1.43
24	B	604	CLA	C1B-NB	-3.06	1.34	1.37
24	b	611	CLA	C1B-NB	-3.06	1.34	1.37
24	a	413	CLA	C1B-NB	-3.06	1.34	1.37
38	V	202	HEM	CAC-C3C	3.05	1.55	1.47
24	B	607	CLA	C4D-CHA	3.05	1.49	1.38
24	c	911	CLA	C1B-NB	-3.05	1.34	1.37
24	c	910	CLA	C1B-C2B	3.04	1.50	1.43
24	C	511	CLA	C4B-NB	-3.04	1.34	1.37
38	F	102	HEM	CAB-C3B	3.04	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	C1B-NB	-3.04	1.34	1.37
24	b	616	CLA	C1B-NB	-3.04	1.34	1.37
24	B	607	CLA	C1B-C2B	3.04	1.50	1.43
38	v	202	HEM	CAC-C3C	3.04	1.55	1.47
24	a	413	CLA	C1B-C2B	3.04	1.50	1.43
24	b	620	CLA	C4D-CHA	3.04	1.49	1.38
24	C	507	CLA	C1B-C2B	3.04	1.50	1.43
24	B	604	CLA	C3B-C4B	3.03	1.49	1.42
24	B	612	CLA	C1B-NB	-3.02	1.34	1.37
24	b	613	CLA	C1C-NC	-3.02	1.33	1.37
24	A	406	CLA	C4B-NB	-3.02	1.34	1.37
24	a	409	CLA	C1B-NB	-3.02	1.34	1.37
24	c	903	CLA	C4B-NB	-3.02	1.34	1.37
24	B	606	CLA	C3B-C4B	3.02	1.49	1.42
35	B	624	HTG	C1'-S1	-3.02	1.77	1.81
38	f	101	HEM	FE-NA	3.01	2.05	1.95
24	C	505	CLA	C1B-NB	-3.01	1.34	1.37
24	B	611	CLA	C3B-C4B	3.01	1.49	1.42
24	C	510	CLA	C4B-NB	-3.01	1.34	1.37
24	b	611	CLA	OBD-CAD	3.00	1.27	1.22
24	C	502	CLA	C1B-NB	-3.00	1.34	1.37
24	b	605	CLA	C4D-CHA	2.99	1.49	1.38
24	B	616	CLA	C1B-NB	-2.99	1.34	1.37
24	c	912	CLA	C1B-C2B	2.99	1.50	1.43
24	C	511	CLA	C1B-C2B	2.99	1.50	1.43
24	C	504	CLA	C1B-NB	-2.99	1.34	1.37
24	b	615	CLA	C1B-C2B	2.99	1.50	1.43
35	b	626	HTG	C1'-S1	-2.99	1.77	1.81
24	B	614	CLA	C4D-CHA	2.98	1.49	1.38
24	C	509	CLA	C4D-CHA	2.98	1.49	1.38
24	c	914	CLA	C3B-C4B	2.98	1.49	1.42
24	c	906	CLA	C4D-CHA	2.98	1.49	1.38
24	c	908	CLA	C1B-C2B	2.98	1.50	1.43
24	A	407	CLA	C4B-NB	-2.97	1.34	1.37
24	B	617	CLA	C4B-NB	-2.97	1.34	1.37
24	c	902	CLA	C4D-CHA	2.97	1.48	1.38
24	C	505	CLA	C1B-C2B	2.97	1.50	1.43
24	B	608	CLA	C4D-CHA	2.97	1.48	1.38
24	b	619	CLA	C4D-CHA	2.97	1.48	1.38
24	C	505	CLA	C4D-CHA	2.96	1.48	1.38
24	A	407	CLA	C1B-C2B	2.96	1.50	1.43
24	C	513	CLA	C1B-C2B	2.96	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	C4D-CHA	2.96	1.48	1.38
24	b	610	CLA	C4B-NB	-2.96	1.34	1.37
24	a	413	CLA	C4B-NB	-2.95	1.34	1.37
24	d	401	CLA	C1B-C2B	2.95	1.50	1.43
24	C	501	CLA	C3B-C4B	2.95	1.49	1.42
24	c	912	CLA	C1B-NB	-2.95	1.34	1.37
24	a	410	CLA	C4D-CHA	2.95	1.48	1.38
24	b	613	CLA	MG-NB	-2.95	1.99	2.05
24	b	613	CLA	C4D-CHA	2.95	1.48	1.38
38	v	202	HEM	FE-NC	2.95	2.05	1.95
24	b	620	CLA	C1C-NC	-2.95	1.33	1.37
24	D	402	CLA	C1B-NB	-2.95	1.34	1.37
24	c	913	CLA	C4D-CHA	2.95	1.48	1.38
24	b	607	CLA	C4D-CHA	2.94	1.48	1.38
24	C	512	CLA	C1B-NB	-2.94	1.34	1.37
24	b	612	CLA	C4B-NB	-2.93	1.34	1.37
24	B	605	CLA	C4D-CHA	2.93	1.48	1.38
24	B	617	CLA	C4D-CHA	2.93	1.48	1.38
24	c	903	CLA	C1B-C2B	2.92	1.50	1.43
24	B	616	CLA	C1B-C2B	2.92	1.50	1.43
24	B	611	CLA	OBD-CAD	2.92	1.27	1.22
38	f	101	HEM	CAC-C3C	2.92	1.55	1.47
24	b	615	CLA	C4D-CHA	2.92	1.48	1.38
24	c	911	CLA	C4D-CHA	2.92	1.48	1.38
24	C	503	CLA	C4D-CHA	2.91	1.48	1.38
24	C	513	CLA	C1B-NB	-2.91	1.34	1.37
24	C	512	CLA	C4D-CHA	2.90	1.48	1.38
24	B	616	CLA	C3B-C4B	2.90	1.49	1.42
24	B	608	CLA	C1B-C2B	2.90	1.50	1.43
24	B	606	CLA	MG-ND	-2.89	2.00	2.05
24	D	403	CLA	C3B-C4B	2.89	1.49	1.42
24	C	506	CLA	C4B-NB	-2.89	1.34	1.37
24	c	910	CLA	C1B-NB	-2.89	1.34	1.37
24	C	503	CLA	C1C-C2C	2.89	1.50	1.44
24	B	605	CLA	C1B-C2B	2.89	1.50	1.43
24	b	614	CLA	C3B-C4B	2.88	1.49	1.42
24	C	512	CLA	C3B-C4B	2.88	1.49	1.42
24	c	912	CLA	C4D-CHA	2.88	1.48	1.38
24	b	605	CLA	C3B-C4B	2.88	1.49	1.42
24	B	617	CLA	C1C-NC	-2.88	1.33	1.37
24	B	604	CLA	C1B-C2B	2.88	1.50	1.43
24	B	609	CLA	C3B-C4B	2.87	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	C4D-CHA	2.87	1.48	1.38
27	f	102	SQD	O47-C45	-2.87	1.43	1.46
24	B	616	CLA	C4D-CHA	2.87	1.48	1.38
24	d	401	CLA	C4B-NB	-2.87	1.34	1.37
24	C	506	CLA	C1B-NB	-2.87	1.34	1.37
24	C	501	CLA	C4D-CHA	2.87	1.48	1.38
24	b	615	CLA	OBD-CAD	2.87	1.27	1.22
24	B	612	CLA	C4B-NB	-2.87	1.34	1.37
24	c	913	CLA	C1B-C2B	2.87	1.50	1.43
24	B	608	CLA	MG-NC	2.87	2.13	2.06
24	c	905	CLA	MG-NC	2.86	2.13	2.06
24	b	611	CLA	C4D-CHA	2.86	1.48	1.38
24	B	613	CLA	C4B-NB	-2.85	1.34	1.37
24	B	613	CLA	C1B-C2B	2.85	1.50	1.43
24	b	620	CLA	C1B-C2B	2.85	1.50	1.43
24	C	502	CLA	C1C-C2C	2.84	1.50	1.44
24	b	617	CLA	C1B-NB	-2.84	1.34	1.37
24	C	513	CLA	C3B-C4B	2.84	1.49	1.42
24	C	509	CLA	C1B-NB	-2.84	1.34	1.37
24	B	611	CLA	C1B-C2B	2.83	1.49	1.43
24	B	602	CLA	C4D-CHA	2.83	1.48	1.38
24	B	614	CLA	C1B-C2B	2.83	1.49	1.43
24	b	620	CLA	C3B-C4B	2.83	1.49	1.42
24	c	908	CLA	C1C-C2C	2.83	1.50	1.44
24	B	609	CLA	C4B-NB	-2.82	1.34	1.37
24	C	510	CLA	C4D-CHA	2.82	1.48	1.38
24	B	611	CLA	C4D-CHA	2.82	1.48	1.38
24	B	609	CLA	C4D-CHA	2.82	1.48	1.38
24	c	903	CLA	C4D-CHA	2.82	1.48	1.38
24	C	513	CLA	C4D-CHA	2.82	1.48	1.38
24	C	509	CLA	C1B-C2B	2.82	1.49	1.43
24	b	610	CLA	MG-ND	-2.82	2.00	2.05
24	B	606	CLA	C1B-C2B	2.82	1.49	1.43
24	c	904	CLA	C1C-NC	-2.81	1.33	1.37
24	C	507	CLA	C4B-NB	-2.81	1.34	1.37
24	B	603	CLA	C1B-NB	-2.81	1.34	1.37
24	c	910	CLA	C4B-NB	-2.81	1.34	1.37
27	A	417	SQD	C6-S	-2.81	1.67	1.77
24	B	603	CLA	C1B-C2B	2.81	1.49	1.43
24	c	904	CLA	C1B-C2B	2.81	1.49	1.43
24	b	607	CLA	C3B-C4B	2.80	1.49	1.42
24	A	406	CLA	C4D-CHA	2.80	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	907	CLA	C3B-C4B	2.80	1.49	1.42
24	B	602	CLA	C4B-NB	-2.80	1.34	1.37
24	b	610	CLA	C4D-CHA	2.80	1.48	1.38
24	A	406	CLA	C1B-NB	-2.80	1.34	1.37
24	b	618	CLA	C1B-C2B	2.80	1.49	1.43
24	C	504	CLA	C4D-CHA	2.80	1.48	1.38
24	A	410	CLA	C4B-NB	-2.80	1.34	1.37
24	b	610	CLA	C3B-C4B	2.80	1.49	1.42
24	c	914	CLA	C4D-CHA	2.79	1.48	1.38
24	C	512	CLA	C1C-C2C	2.79	1.50	1.44
24	b	619	CLA	C1B-C2B	2.79	1.49	1.43
24	C	506	CLA	C4D-CHA	2.79	1.48	1.38
35	b	602	HTG	C1-S1	-2.78	1.76	1.80
24	c	903	CLA	MG-NB	2.78	2.11	2.05
24	B	610	CLA	C1B-C2B	2.78	1.49	1.43
24	b	609	CLA	C1C-C2C	2.77	1.49	1.44
24	B	615	CLA	MG-NB	2.77	2.11	2.05
24	b	616	CLA	C4D-CHA	2.77	1.48	1.38
24	A	406	CLA	C3B-C4B	2.77	1.49	1.42
24	C	501	CLA	C1C-C2C	2.77	1.49	1.44
24	B	607	CLA	C1B-NB	-2.77	1.34	1.37
24	c	902	CLA	C1B-C2B	2.77	1.49	1.43
24	a	409	CLA	C1B-C2B	2.77	1.49	1.43
27	a	415	SQD	C6-S	-2.76	1.67	1.77
24	c	914	CLA	C1B-NB	-2.76	1.34	1.37
24	c	914	CLA	C1B-C2B	2.76	1.49	1.43
24	b	614	CLA	C4B-NB	-2.76	1.34	1.37
24	b	610	CLA	C1B-NB	-2.75	1.34	1.37
24	C	502	CLA	C3B-C4B	2.75	1.49	1.42
38	V	202	HEM	CAB-C3B	2.75	1.54	1.47
24	C	508	CLA	C4B-NB	-2.75	1.34	1.37
24	b	607	CLA	C1B-C2B	2.75	1.49	1.43
24	A	410	CLA	C4D-CHA	2.75	1.48	1.38
24	c	911	CLA	C4B-NB	-2.75	1.34	1.37
24	b	610	CLA	C1B-C2B	2.75	1.49	1.43
24	b	612	CLA	C3B-C4B	2.74	1.49	1.42
24	b	609	CLA	C4D-CHA	2.74	1.48	1.38
24	A	407	CLA	C4D-CHA	2.74	1.48	1.38
24	b	614	CLA	C1B-C2B	2.74	1.49	1.43
24	C	502	CLA	C4D-CHA	2.74	1.48	1.38
24	C	504	CLA	C3B-C4B	2.74	1.49	1.42
27	A	412	SQD	C6-S	-2.73	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	F	102	HEM	CAC-C3C	2.73	1.54	1.47
24	B	603	CLA	C4D-CHA	2.73	1.48	1.38
24	c	907	CLA	C4D-CHA	2.73	1.48	1.38
24	b	606	CLA	C3B-C4B	2.73	1.49	1.42
24	a	413	CLA	C4D-CHA	2.73	1.48	1.38
24	c	913	CLA	C1B-NB	-2.73	1.34	1.37
24	b	608	CLA	C1B-C2B	2.73	1.49	1.43
24	C	503	CLA	C3B-C4B	2.73	1.49	1.42
24	C	509	CLA	C4C-C3C	2.72	1.49	1.45
24	a	410	CLA	C3B-C4B	2.72	1.49	1.42
24	B	615	CLA	C4D-CHA	2.72	1.48	1.38
24	b	617	CLA	C1B-C2B	2.72	1.49	1.43
24	b	615	CLA	C3B-C4B	2.72	1.49	1.42
24	d	404	CLA	C1C-NC	-2.71	1.33	1.37
24	A	405	CLA	C1B-C2B	2.71	1.49	1.43
24	b	613	CLA	C1B-C2B	2.71	1.49	1.43
24	c	908	CLA	C4B-NB	-2.71	1.34	1.37
24	b	610	CLA	C1C-C2C	2.71	1.49	1.44
24	b	614	CLA	C4D-CHA	2.71	1.48	1.38
24	C	502	CLA	C1B-C2B	2.71	1.49	1.43
24	B	606	CLA	C4D-CHA	2.71	1.48	1.38
24	d	405	CLA	C1B-C2B	2.71	1.49	1.43
24	A	405	CLA	C4D-CHA	2.70	1.48	1.38
24	C	508	CLA	C3B-C4B	2.70	1.49	1.42
24	B	614	CLA	C4B-NB	-2.70	1.34	1.37
24	B	613	CLA	C4D-CHA	2.70	1.48	1.38
29	a	417	PL9	C6-C5	2.70	1.49	1.35
24	C	510	CLA	C1C-C2C	2.70	1.49	1.44
24	B	603	CLA	C3B-C4B	2.69	1.49	1.42
24	B	602	CLA	C1B-NB	-2.69	1.34	1.37
24	D	402	CLA	C4D-CHA	2.69	1.48	1.38
24	D	403	CLA	C4D-CHA	2.69	1.48	1.38
24	c	905	CLA	C4D-CHA	2.69	1.48	1.38
24	c	910	CLA	MG-NB	2.69	2.11	2.05
24	c	904	CLA	C4B-NB	-2.68	1.34	1.37
24	c	909	CLA	C4D-CHA	2.68	1.47	1.38
24	b	612	CLA	C4D-CHA	2.68	1.47	1.38
24	b	617	CLA	C4D-CHA	2.68	1.47	1.38
24	A	406	CLA	C1B-C2B	2.68	1.49	1.43
24	b	606	CLA	C1B-C2B	2.68	1.49	1.43
24	c	903	CLA	C3B-C4B	2.68	1.49	1.42
24	a	410	CLA	C1B-C2B	2.67	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	914	CLA	C4C-C3C	2.67	1.49	1.45
24	C	505	CLA	C1C-NC	-2.66	1.33	1.37
24	B	612	CLA	C3B-C4B	2.66	1.49	1.42
24	d	401	CLA	MG-NB	2.66	2.11	2.05
24	c	913	CLA	C3B-C4B	2.66	1.49	1.42
38	V	202	HEM	CMC-C2C	2.66	1.56	1.50
24	b	605	CLA	C1B-C2B	2.65	1.49	1.43
24	C	512	CLA	C1B-C2B	2.65	1.49	1.43
24	d	404	CLA	C4D-CHA	2.65	1.47	1.38
24	a	410	CLA	C4B-NB	-2.65	1.34	1.37
24	d	405	CLA	C3B-C4B	2.64	1.48	1.42
24	b	607	CLA	C4B-NB	-2.64	1.34	1.37
24	A	410	CLA	C1B-C2B	2.64	1.49	1.43
24	B	609	CLA	C1B-C2B	2.64	1.49	1.43
24	c	905	CLA	C1C-C2C	2.64	1.49	1.44
24	c	909	CLA	C3B-C4B	2.64	1.48	1.42
24	C	510	CLA	C1B-C2B	2.64	1.49	1.43
24	b	612	CLA	C1B-C2B	2.64	1.49	1.43
24	C	501	CLA	C1B-C2B	2.63	1.49	1.43
24	B	615	CLA	C1B-C2B	2.63	1.49	1.43
24	C	512	CLA	C4B-NB	-2.63	1.34	1.37
24	B	617	CLA	C1B-C2B	2.63	1.49	1.43
24	B	604	CLA	C1C-C2C	2.63	1.49	1.44
24	b	620	CLA	C1B-NB	-2.62	1.34	1.37
24	b	611	CLA	MG-NB	2.62	2.11	2.05
24	c	904	CLA	C1C-C2C	2.62	1.49	1.44
24	C	513	CLA	C1C-C2C	2.62	1.49	1.44
24	A	410	CLA	C1B-NB	-2.62	1.34	1.37
24	C	510	CLA	C4C-C3C	2.62	1.49	1.45
24	a	409	CLA	C4D-CHA	2.62	1.47	1.38
24	b	609	CLA	C4B-NB	-2.62	1.34	1.37
24	b	616	CLA	C3B-C4B	2.62	1.48	1.42
24	b	606	CLA	C4B-NB	-2.62	1.34	1.37
35	d	403	HTG	C1-S1	-2.62	1.76	1.80
24	b	607	CLA	C1C-C2C	2.62	1.49	1.44
24	b	607	CLA	C1B-NB	-2.62	1.34	1.37
24	b	608	CLA	C1C-C2C	2.61	1.49	1.44
27	b	601	SQD	C6-S	-2.61	1.67	1.77
24	C	505	CLA	C4B-NB	-2.61	1.34	1.37
24	C	507	CLA	C1C-NC	-2.61	1.33	1.37
24	a	410	CLA	C1C-C2C	2.61	1.49	1.44
24	b	605	CLA	C1B-NB	-2.60	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	905	CLA	MG-NB	2.60	2.10	2.05
24	C	509	CLA	C3B-C4B	2.59	1.48	1.42
24	d	404	CLA	C1B-C2B	2.59	1.49	1.43
24	B	610	CLA	C1B-NB	-2.59	1.34	1.37
24	c	910	CLA	C3B-C2B	2.59	1.50	1.41
24	c	914	CLA	C1C-C2C	2.58	1.49	1.44
24	b	606	CLA	C1B-NB	-2.58	1.34	1.37
24	c	904	CLA	C3B-C4B	2.58	1.48	1.42
24	C	511	CLA	C1B-NB	-2.58	1.34	1.37
24	b	609	CLA	C1B-C2B	2.58	1.49	1.43
24	b	612	CLA	C1C-NC	-2.58	1.34	1.37
24	A	407	CLA	C3D-C4D	-2.57	1.38	1.44
29	d	407	PL9	C6-C5	2.57	1.48	1.35
24	C	502	CLA	C4B-NB	-2.57	1.34	1.37
24	B	606	CLA	C1B-NB	-2.57	1.34	1.37
29	A	414	PL9	C6-C5	2.57	1.48	1.35
24	B	610	CLA	C4D-CHA	2.57	1.47	1.38
24	d	405	CLA	C4D-CHA	2.57	1.47	1.38
24	B	602	CLA	C1B-C2B	2.57	1.49	1.43
24	c	910	CLA	C4C-C3C	2.57	1.49	1.45
27	a	401	SQD	C6-S	-2.57	1.67	1.77
24	B	612	CLA	C1B-C2B	2.56	1.49	1.43
24	C	506	CLA	C3B-C4B	2.56	1.48	1.42
24	c	907	CLA	C1C-NC	-2.56	1.34	1.37
24	c	907	CLA	C3D-C4D	-2.56	1.38	1.44
24	b	616	CLA	C4B-NB	-2.56	1.34	1.37
24	c	911	CLA	C3B-C4B	2.56	1.48	1.42
24	c	912	CLA	C3B-C4B	2.56	1.48	1.42
24	C	508	CLA	C1B-C2B	2.55	1.49	1.43
24	B	615	CLA	C3B-C4B	2.55	1.48	1.42
24	c	902	CLA	C1C-NC	-2.55	1.34	1.37
24	c	902	CLA	C1B-NB	-2.55	1.34	1.37
24	C	503	CLA	C4B-NB	-2.55	1.34	1.37
24	C	511	CLA	C1C-C2C	2.55	1.49	1.44
24	C	504	CLA	C1B-C2B	2.55	1.49	1.43
24	c	905	CLA	C1B-C2B	2.55	1.49	1.43
24	c	902	CLA	C4B-NB	-2.54	1.34	1.37
24	C	505	CLA	C4C-C3C	2.54	1.49	1.45
24	B	607	CLA	C3B-C4B	2.54	1.48	1.42
27	B	621	SQD	C6-S	-2.54	1.68	1.77
24	C	513	CLA	C4B-NB	-2.54	1.34	1.37
24	b	612	CLA	C1C-C2C	2.53	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	406	CLA	C1C-C2C	2.53	1.49	1.44
24	C	511	CLA	C3B-C4B	2.53	1.48	1.42
24	B	611	CLA	C4B-NB	-2.53	1.34	1.37
36	H	103	DGD	O5D-C1E	2.53	1.44	1.40
24	B	604	CLA	C4D-CHA	2.52	1.47	1.38
24	c	909	CLA	C3B-C2B	2.52	1.49	1.41
24	D	402	CLA	C3B-C4B	2.52	1.48	1.42
24	c	913	CLA	C1C-C2C	2.52	1.49	1.44
24	b	618	CLA	C4B-NB	-2.52	1.34	1.37
24	b	605	CLA	C1C-C2C	2.52	1.49	1.44
24	C	505	CLA	C3B-C4B	2.51	1.48	1.42
24	a	413	CLA	C3B-C4B	2.51	1.48	1.42
24	c	911	CLA	C1C-C2C	2.51	1.49	1.44
24	b	606	CLA	C1C-C2C	2.51	1.49	1.44
24	B	609	CLA	C1C-C2C	2.51	1.49	1.44
24	c	908	CLA	C1C-NC	-2.51	1.34	1.37
24	b	608	CLA	C3B-C4B	2.51	1.48	1.42
29	D	405	PL9	C6-C5	2.51	1.48	1.35
24	c	909	CLA	C1B-C2B	2.50	1.49	1.43
24	c	910	CLA	C1C-C2C	2.50	1.49	1.44
24	d	404	CLA	C3B-C4B	2.50	1.48	1.42
35	C	528	HTG	C1-S1	-2.50	1.76	1.80
24	b	608	CLA	C4B-NB	-2.50	1.34	1.37
24	C	509	CLA	C1C-C2C	2.49	1.49	1.44
24	c	905	CLA	C4C-C3C	2.49	1.49	1.45
24	b	610	CLA	C3B-C2B	2.49	1.49	1.41
24	c	902	CLA	C1C-C2C	2.49	1.49	1.44
24	d	401	CLA	C4D-CHA	2.49	1.47	1.38
27	F	101	SQD	C6-S	-2.49	1.68	1.77
24	b	611	CLA	C3B-C4B	2.49	1.48	1.42
24	b	618	CLA	C4D-CHA	2.48	1.47	1.38
24	c	907	CLA	C4B-NB	-2.48	1.34	1.37
24	C	507	CLA	C1C-C2C	2.48	1.49	1.44
24	c	905	CLA	C3B-C4B	2.48	1.48	1.42
24	a	409	CLA	C3B-C4B	2.47	1.48	1.42
24	b	620	CLA	C3B-C2B	2.47	1.49	1.41
24	d	404	CLA	C3D-C4D	-2.47	1.38	1.44
24	C	510	CLA	C3B-C4B	2.47	1.48	1.42
24	B	607	CLA	C1C-C2C	2.46	1.49	1.44
24	b	615	CLA	C1B-NB	-2.46	1.34	1.37
24	b	617	CLA	MG-NB	2.46	2.10	2.05
24	b	617	CLA	C1C-NC	-2.46	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	405	CLA	C1C-C2C	2.46	1.49	1.44
24	C	506	CLA	C1C-NC	-2.46	1.34	1.37
24	c	910	CLA	C3B-C4B	2.46	1.48	1.42
24	c	906	CLA	C1C-C2C	2.46	1.49	1.44
29	D	405	PL9	C2-C3	2.46	1.41	1.34
38	f	101	HEM	FE-NC	2.45	2.03	1.95
24	C	501	CLA	C1B-NB	-2.45	1.34	1.37
24	c	907	CLA	C1B-C2B	2.45	1.49	1.43
24	d	404	CLA	C1C-C2C	2.45	1.49	1.44
24	A	410	CLA	C3B-C2B	2.45	1.49	1.41
24	B	613	CLA	C1C-C2C	2.45	1.49	1.44
38	F	102	HEM	FE-NC	2.44	2.03	1.95
24	B	615	CLA	C3D-C4D	-2.44	1.38	1.44
24	b	614	CLA	C4C-C3C	2.44	1.49	1.45
24	b	619	CLA	C1B-NB	-2.44	1.34	1.37
24	b	617	CLA	C3B-C4B	2.44	1.48	1.42
24	C	508	CLA	C3B-C2B	2.43	1.49	1.41
24	b	616	CLA	C1C-NC	-2.42	1.34	1.37
24	c	906	CLA	C4B-NB	-2.42	1.34	1.37
24	C	513	CLA	C1C-NC	-2.42	1.34	1.37
24	b	615	CLA	C3B-C2B	2.42	1.49	1.41
24	a	409	CLA	C4C-C3C	2.42	1.49	1.45
24	D	403	CLA	C1C-C2C	2.41	1.49	1.44
24	B	610	CLA	C1C-NC	-2.41	1.34	1.37
24	c	913	CLA	C4B-NB	-2.41	1.34	1.37
24	b	617	CLA	C4B-NB	-2.41	1.34	1.37
35	B	626	HTG	C1-S1	-2.41	1.77	1.80
24	C	503	CLA	C1B-C2B	2.41	1.48	1.43
24	C	504	CLA	C4B-NB	-2.40	1.34	1.37
24	b	606	CLA	C1C-NC	-2.40	1.34	1.37
24	C	508	CLA	C4C-C3C	2.40	1.49	1.45
24	c	909	CLA	C4C-C3C	2.40	1.49	1.45
24	B	609	CLA	C4C-C3C	2.40	1.49	1.45
24	B	603	CLA	C4C-C3C	2.40	1.49	1.45
36	h	102	DGD	O5D-C1E	2.40	1.44	1.40
24	C	511	CLA	C4C-C3C	2.40	1.49	1.45
24	B	604	CLA	C4B-NB	-2.40	1.34	1.37
24	C	503	CLA	C1B-NB	-2.39	1.34	1.37
24	a	409	CLA	MG-NB	2.39	2.10	2.05
24	C	508	CLA	C4D-CHA	2.39	1.46	1.38
24	B	602	CLA	C1C-C2C	2.39	1.49	1.44
24	B	608	CLA	C4C-C3C	2.39	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	C1C-C2C	2.39	1.49	1.44
24	a	410	CLA	C3D-C4D	-2.39	1.38	1.44
24	b	617	CLA	C1C-C2C	2.39	1.49	1.44
24	b	613	CLA	C1C-C2C	2.38	1.49	1.44
24	b	618	CLA	C3B-C4B	2.38	1.48	1.42
25	a	411	PHO	C3A-C2A	-2.38	1.52	1.54
24	B	617	CLA	C3B-C2B	2.38	1.49	1.41
24	C	507	CLA	C4C-C3C	2.37	1.49	1.45
24	C	506	CLA	C1B-C2B	2.37	1.48	1.43
24	b	617	CLA	C3D-C4D	-2.37	1.38	1.44
24	C	512	CLA	C3B-C2B	2.37	1.49	1.41
27	B	621	SQD	O6-C1	2.37	1.44	1.40
24	C	510	CLA	C3B-C2B	2.37	1.49	1.41
24	B	605	CLA	C3B-C4B	2.37	1.48	1.42
24	b	607	CLA	C4C-C3C	2.36	1.49	1.45
24	C	513	CLA	C3B-C2B	2.36	1.49	1.41
24	b	611	CLA	C1C-C2C	2.36	1.49	1.44
24	c	903	CLA	C1B-NB	-2.36	1.34	1.37
24	B	609	CLA	C1C-NC	-2.36	1.34	1.37
24	a	409	CLA	C1C-NC	-2.35	1.34	1.37
24	B	611	CLA	C4C-C3C	2.35	1.49	1.45
25	A	408	PHO	C3A-C2A	-2.35	1.52	1.54
24	b	609	CLA	MG-NB	2.35	2.10	2.05
24	c	903	CLA	C3D-C4D	-2.35	1.38	1.44
24	c	903	CLA	C1C-C2C	2.35	1.49	1.44
24	C	505	CLA	C1C-C2C	2.34	1.49	1.44
24	A	405	CLA	C1C-NC	-2.34	1.34	1.37
24	B	608	CLA	C3B-C4B	2.34	1.48	1.42
24	C	511	CLA	C1C-NC	-2.34	1.34	1.37
24	a	409	CLA	C3B-C2B	2.33	1.49	1.41
24	A	406	CLA	C3B-C2B	2.33	1.49	1.41
24	A	410	CLA	C3B-C4B	2.33	1.48	1.42
24	c	904	CLA	C4C-C3C	2.33	1.49	1.45
24	b	607	CLA	C3B-C2B	2.33	1.49	1.41
24	b	612	CLA	C4C-C3C	2.33	1.49	1.45
24	c	908	CLA	C4C-C3C	2.33	1.49	1.45
24	d	401	CLA	C1C-C2C	2.32	1.49	1.44
34	m	1503	LMT	O1'-C1'	2.32	1.44	1.40
24	b	606	CLA	C3B-C2B	2.32	1.49	1.41
24	b	615	CLA	C4B-NB	-2.32	1.34	1.37
24	c	909	CLA	C1C-C2C	2.32	1.49	1.44
24	b	615	CLA	C3D-C4D	-2.32	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	906	CLA	C3B-C4B	2.32	1.48	1.42
24	B	602	CLA	C3B-C2B	2.32	1.49	1.41
24	c	906	CLA	C1B-NB	-2.32	1.34	1.37
24	B	603	CLA	C4B-NB	-2.32	1.34	1.37
24	c	906	CLA	C4C-C3C	2.31	1.49	1.45
24	C	504	CLA	C4C-C3C	2.31	1.49	1.45
24	d	401	CLA	MG-NC	2.31	2.11	2.06
24	C	502	CLA	C4C-C3C	2.31	1.49	1.45
24	b	608	CLA	C3B-C2B	2.31	1.49	1.41
24	b	613	CLA	C1B-NB	-2.31	1.34	1.37
24	b	616	CLA	C1C-C2C	2.31	1.49	1.44
24	c	903	CLA	C3B-C2B	2.31	1.49	1.41
24	B	608	CLA	C3B-C2B	2.31	1.49	1.41
24	C	504	CLA	C1C-C2C	2.30	1.49	1.44
24	C	510	CLA	C3D-C4D	-2.30	1.39	1.44
24	C	509	CLA	C3B-C2B	2.30	1.49	1.41
24	B	605	CLA	C4B-NB	-2.29	1.35	1.37
24	c	912	CLA	C3B-C2B	2.29	1.48	1.41
24	d	405	CLA	C4C-C3C	2.29	1.49	1.45
24	c	909	CLA	C4B-NB	-2.29	1.35	1.37
24	A	410	CLA	C1C-NC	-2.28	1.34	1.37
35	c	923	HTG	C1-S1	-2.28	1.77	1.80
24	B	614	CLA	C1C-C2C	2.28	1.49	1.44
24	b	616	CLA	C3B-C2B	2.28	1.48	1.41
24	A	405	CLA	C3B-C4B	2.28	1.48	1.42
24	c	906	CLA	C1C-NC	-2.27	1.34	1.37
24	b	606	CLA	C4C-C3C	2.27	1.49	1.45
24	a	413	CLA	C1C-C2C	2.27	1.49	1.44
24	B	609	CLA	C3D-C4D	-2.27	1.39	1.44
24	B	604	CLA	C1C-NC	-2.27	1.34	1.37
34	J	102	LMT	O1'-C1'	2.27	1.44	1.40
24	b	605	CLA	C1C-NC	-2.27	1.34	1.37
24	A	407	CLA	C3B-C4B	2.27	1.48	1.42
24	b	611	CLA	C4B-NB	-2.27	1.35	1.37
24	c	904	CLA	C1B-NB	-2.27	1.35	1.37
24	C	503	CLA	C3B-C2B	2.27	1.48	1.41
24	c	910	CLA	C1C-NC	-2.26	1.34	1.37
24	B	617	CLA	C1B-NB	-2.26	1.35	1.37
24	B	607	CLA	C4C-C3C	2.26	1.48	1.45
24	b	608	CLA	C1C-NC	-2.26	1.34	1.37
24	b	613	CLA	C3B-C4B	2.26	1.48	1.42
24	C	506	CLA	C1C-C2C	2.26	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	913	CLA	C3B-C2B	2.26	1.48	1.41
24	b	619	CLA	C1C-C2C	2.26	1.48	1.44
24	b	608	CLA	C4C-C3C	2.26	1.48	1.45
24	d	404	CLA	C4B-NB	-2.25	1.35	1.37
24	B	607	CLA	C3B-C2B	2.25	1.48	1.41
38	v	202	HEM	CMD-C2D	2.25	1.55	1.50
24	b	620	CLA	C3D-C4D	-2.25	1.39	1.44
24	c	902	CLA	C4C-C3C	2.25	1.48	1.45
24	b	608	CLA	C1B-NB	-2.25	1.35	1.37
38	F	102	HEM	CMA-C3A	2.25	1.55	1.50
24	c	914	CLA	C4B-NB	-2.25	1.35	1.37
24	A	405	CLA	C1C-C2C	2.25	1.48	1.44
24	C	502	CLA	C3B-C2B	2.25	1.48	1.41
24	c	914	CLA	C3B-C2B	2.25	1.48	1.41
24	B	612	CLA	C3B-C2B	2.25	1.48	1.41
24	c	911	CLA	C3B-C2B	2.25	1.48	1.41
24	b	617	CLA	C3B-C2B	2.24	1.48	1.41
24	b	618	CLA	C3D-C4D	-2.24	1.39	1.44
24	B	609	CLA	C3B-C2B	2.24	1.48	1.41
24	C	512	CLA	C3D-C4D	-2.24	1.39	1.44
24	B	605	CLA	C1C-C2C	2.24	1.48	1.44
24	c	906	CLA	C3B-C2B	2.24	1.48	1.41
24	b	608	CLA	C4D-ND	2.23	1.40	1.37
24	b	613	CLA	C4B-NB	-2.23	1.35	1.37
24	D	402	CLA	C3B-C2B	2.23	1.48	1.41
24	c	914	CLA	C1C-NC	-2.23	1.34	1.37
24	B	611	CLA	C3D-C4D	-2.23	1.39	1.44
24	b	607	CLA	C3D-C4D	-2.23	1.39	1.44
34	M	302	LMT	O1'-C1'	2.22	1.44	1.40
24	C	504	CLA	C3B-C2B	2.22	1.48	1.41
24	C	505	CLA	C3B-C2B	2.22	1.48	1.41
24	C	503	CLA	C4C-C3C	2.22	1.48	1.45
24	a	413	CLA	C1C-NC	-2.22	1.34	1.37
24	B	610	CLA	C1C-C2C	2.22	1.48	1.44
24	C	506	CLA	C4C-C3C	2.22	1.48	1.45
24	B	603	CLA	C3D-C4D	-2.22	1.39	1.44
24	C	511	CLA	C3B-C2B	2.22	1.48	1.41
24	c	913	CLA	C3D-C4D	-2.22	1.39	1.44
36	c	919	DGD	O2G-C2G	-2.22	1.41	1.46
24	d	404	CLA	C4C-C3C	2.21	1.48	1.45
24	C	501	CLA	C1C-NC	-2.21	1.34	1.37
24	C	507	CLA	MG-NB	-2.21	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	902	CLA	C3B-C2B	2.21	1.48	1.41
24	c	905	CLA	C3D-C4D	-2.21	1.39	1.44
24	d	405	CLA	C3B-C2B	2.21	1.48	1.41
24	C	501	CLA	C4B-NB	-2.20	1.35	1.37
24	b	612	CLA	C3B-C2B	2.20	1.48	1.41
24	c	910	CLA	C4D-ND	2.20	1.40	1.37
24	B	610	CLA	C4B-NB	-2.20	1.35	1.37
24	B	605	CLA	C3B-C2B	2.20	1.48	1.41
24	B	603	CLA	C3B-C2B	2.19	1.48	1.41
24	A	406	CLA	C1C-NC	-2.19	1.34	1.37
24	C	509	CLA	C3D-C4D	-2.19	1.39	1.44
24	B	613	CLA	C1C-NC	-2.19	1.34	1.37
24	d	401	CLA	C1C-NC	-2.19	1.34	1.37
24	c	913	CLA	MG-NB	2.19	2.10	2.05
38	f	101	HEM	CMC-C2C	2.19	1.55	1.50
24	B	602	CLA	C3D-C4D	-2.19	1.39	1.44
24	B	606	CLA	C1C-C2C	2.19	1.48	1.44
24	C	507	CLA	C3B-C2B	2.19	1.48	1.41
24	D	403	CLA	C1C-NC	-2.18	1.34	1.37
24	B	617	CLA	C3D-C4D	-2.18	1.39	1.44
24	c	905	CLA	C3B-C2B	2.18	1.48	1.41
24	C	508	CLA	C1C-C2C	2.18	1.48	1.44
24	b	605	CLA	C3B-C2B	2.18	1.48	1.41
35	b	603	HTG	C1-S1	-2.18	1.77	1.80
24	C	503	CLA	C1C-NC	-2.18	1.34	1.37
24	B	605	CLA	C3D-C4D	-2.18	1.39	1.44
24	d	405	CLA	C3D-C4D	-2.18	1.39	1.44
24	c	907	CLA	C3B-C2B	2.18	1.48	1.41
24	c	902	CLA	C3D-C4D	-2.17	1.39	1.44
24	B	605	CLA	C1C-NC	-2.17	1.34	1.37
24	B	614	CLA	C4C-C3C	2.17	1.48	1.45
24	A	407	CLA	C3B-C2B	2.17	1.48	1.41
34	t	904	LMT	O1'-C1'	2.17	1.43	1.40
35	c	924	HTG	C1-S1	-2.17	1.77	1.80
24	b	615	CLA	C1C-NC	-2.17	1.34	1.37
24	b	614	CLA	C1C-NC	-2.16	1.34	1.37
24	B	617	CLA	C1C-C2C	2.16	1.48	1.44
31	V	204	GOL	C1-C2	2.16	1.60	1.51
24	C	505	CLA	C4D-ND	2.16	1.40	1.37
24	c	904	CLA	C3B-C2B	2.16	1.48	1.41
24	c	908	CLA	C1B-NB	-2.16	1.35	1.37
37	L	101	LHG	O7-C5	-2.16	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	C3B-C2B	2.16	1.48	1.41
24	D	403	CLA	C3B-C2B	2.16	1.48	1.41
24	b	613	CLA	C3B-C2B	2.16	1.48	1.41
24	b	607	CLA	C1C-NC	-2.15	1.34	1.37
24	c	911	CLA	C1C-NC	-2.15	1.34	1.37
24	b	605	CLA	C4B-NB	-2.15	1.35	1.37
24	b	610	CLA	C3D-C4D	-2.15	1.39	1.44
24	B	616	CLA	MG-NC	2.15	2.11	2.06
24	A	410	CLA	C1C-C2C	2.15	1.48	1.44
24	A	410	CLA	C4C-C3C	2.15	1.48	1.45
24	b	611	CLA	C3D-C4D	-2.15	1.39	1.44
34	a	402	LMT	O1'-C1'	2.15	1.43	1.40
24	A	410	CLA	C3D-C4D	-2.15	1.39	1.44
24	B	608	CLA	C3D-C4D	-2.15	1.39	1.44
24	C	504	CLA	C3D-C4D	-2.15	1.39	1.44
24	d	401	CLA	C3B-C4B	2.15	1.47	1.42
24	b	613	CLA	C4C-C3C	2.15	1.48	1.45
24	B	604	CLA	C3D-C4D	-2.14	1.39	1.44
24	b	619	CLA	C3B-C2B	2.14	1.48	1.41
24	d	401	CLA	C3B-C2B	2.14	1.48	1.41
35	C	521	HTG	C1-S1	-2.14	1.77	1.80
24	b	609	CLA	C3B-C2B	2.13	1.48	1.41
24	B	605	CLA	C1B-NB	-2.13	1.35	1.37
24	C	505	CLA	C3D-C4D	-2.13	1.39	1.44
24	B	614	CLA	C3B-C2B	2.13	1.48	1.41
24	b	612	CLA	C3D-C4D	-2.13	1.39	1.44
24	c	908	CLA	C3B-C2B	2.13	1.48	1.41
24	c	914	CLA	C3D-C4D	-2.13	1.39	1.44
24	B	610	CLA	C3B-C2B	2.13	1.48	1.41
24	C	509	CLA	C1C-NC	-2.13	1.34	1.37
24	c	913	CLA	C4C-C3C	2.13	1.48	1.45
38	v	202	HEM	CMC-C2C	2.12	1.55	1.50
24	C	507	CLA	C3B-C4B	2.12	1.47	1.42
24	c	911	CLA	C3D-C4D	-2.12	1.39	1.44
38	f	101	HEM	CMB-C2B	2.12	1.55	1.50
24	C	506	CLA	C3D-C4D	-2.12	1.39	1.44
25	A	409	PHO	C4B-NB	-2.11	1.34	1.38
24	B	611	CLA	C1C-C2C	2.11	1.48	1.44
24	b	618	CLA	C1C-C2C	2.11	1.48	1.44
24	B	616	CLA	C1C-C2C	2.11	1.48	1.44
31	B	633	GOL	C3-C2	2.11	1.60	1.51
24	C	507	CLA	C4D-ND	2.10	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	602	CLA	C1D-C2D	2.10	1.49	1.45
24	D	402	CLA	C1C-NC	-2.10	1.34	1.37
38	V	202	HEM	CMB-C2B	2.10	1.55	1.50
24	A	407	CLA	C1C-NC	-2.10	1.34	1.37
24	b	619	CLA	C4B-NB	-2.10	1.35	1.37
24	B	613	CLA	C3B-C2B	2.10	1.48	1.41
24	B	606	CLA	C4B-NB	-2.10	1.35	1.37
24	d	404	CLA	C3B-C2B	2.09	1.48	1.41
24	B	602	CLA	C1C-NC	-2.09	1.34	1.37
24	B	607	CLA	C3D-C4D	-2.09	1.39	1.44
24	B	615	CLA	C3B-C2B	2.09	1.48	1.41
24	D	402	CLA	C3D-C4D	-2.09	1.39	1.44
24	C	508	CLA	C3D-C4D	-2.09	1.39	1.44
24	c	908	CLA	C3B-C4B	2.09	1.47	1.42
24	b	609	CLA	C3D-C4D	-2.08	1.39	1.44
24	a	413	CLA	C4C-C3C	2.08	1.48	1.45
31	V	204	GOL	C3-C2	2.08	1.60	1.51
24	C	507	CLA	C3D-C4D	-2.08	1.39	1.44
24	c	905	CLA	C1C-NC	-2.08	1.34	1.37
24	B	604	CLA	C3B-C2B	2.08	1.48	1.41
24	c	907	CLA	C1C-C2C	2.08	1.48	1.44
24	B	612	CLA	C1C-C2C	2.08	1.48	1.44
28	C	534	LMG	O1-C1	2.07	1.43	1.40
24	C	502	CLA	C3D-C4D	-2.07	1.39	1.44
24	C	506	CLA	C3B-C2B	2.07	1.48	1.41
24	A	405	CLA	C3B-C2B	2.07	1.48	1.41
24	c	910	CLA	C3D-C4D	-2.07	1.39	1.44
31	A	422	GOL	C3-C2	2.07	1.60	1.51
24	B	606	CLA	C3B-C2B	2.07	1.48	1.41
24	d	405	CLA	C1D-C2D	2.06	1.49	1.45
24	B	613	CLA	C3B-C4B	2.06	1.47	1.42
34	b	625	LMT	O1'-C1'	2.06	1.43	1.40
24	A	405	CLA	C4C-C3C	2.06	1.48	1.45
24	C	506	CLA	C1D-C2D	2.06	1.49	1.45
24	c	906	CLA	C3D-C4D	-2.05	1.39	1.44
24	c	909	CLA	C3D-C4D	-2.05	1.39	1.44
24	c	903	CLA	C1C-NC	-2.05	1.34	1.37
24	C	510	CLA	C1C-NC	-2.05	1.34	1.37
24	B	614	CLA	C3B-C4B	2.05	1.47	1.42
26	b	621	BCR	C1-C6	-2.05	1.51	1.53
29	a	417	PL9	C2-C3	2.05	1.40	1.34
25	A	408	PHO	CBD-CGD	-2.05	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	b	639	LHG	O7-C5	-2.04	1.41	1.46
24	C	513	CLA	C3D-C4D	-2.04	1.39	1.44
24	b	619	CLA	C3D-C4D	-2.04	1.39	1.44
24	C	504	CLA	C1C-NC	-2.04	1.34	1.37
38	F	102	HEM	CMC-C2C	2.04	1.55	1.50
24	c	907	CLA	C4C-C3C	2.03	1.48	1.45
24	b	605	CLA	C3D-C4D	-2.03	1.39	1.44
24	c	909	CLA	C1C-NC	-2.03	1.34	1.37
24	C	501	CLA	C3B-C2B	2.02	1.48	1.41
29	A	414	PL9	C2-C3	2.02	1.40	1.34
24	b	611	CLA	C3B-C2B	2.02	1.48	1.41
24	c	904	CLA	C1A-CHA	2.02	1.51	1.43
24	D	403	CLA	C4C-C3C	2.02	1.48	1.45
24	B	608	CLA	C4B-NB	-2.02	1.35	1.37
31	B	630	GOL	O2-C2	-2.01	1.37	1.43
24	b	611	CLA	C4C-C3C	2.01	1.48	1.45
24	b	614	CLA	C3B-C2B	2.01	1.48	1.41
34	c	922	LMT	O1'-C1'	2.01	1.43	1.40
24	B	602	CLA	C4C-C3C	2.01	1.48	1.45
24	B	617	CLA	C3B-C4B	2.01	1.47	1.42
24	B	616	CLA	C3D-C4D	-2.01	1.39	1.44
34	F	103	LMT	O1'-C1'	2.01	1.43	1.40
24	C	513	CLA	C1D-C2D	2.01	1.49	1.45
24	C	503	CLA	C3D-C4D	-2.00	1.39	1.44
24	D	402	CLA	C1C-C2C	2.00	1.48	1.44
24	D	402	CLA	C4B-NB	-2.00	1.35	1.37
38	F	102	HEM	CMB-C2B	2.00	1.55	1.50
24	b	605	CLA	C4D-ND	2.00	1.40	1.37
26	y	101	BCR	C30-C25	-2.00	1.51	1.53
24	b	609	CLA	C1C-NC	-2.00	1.34	1.37

All (2540) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	402	CLA	C1D-ND-C4D	-10.22	99.07	106.33
24	d	401	CLA	C1D-ND-C4D	-10.22	99.08	106.33
24	c	902	CLA	C1D-ND-C4D	-10.01	99.22	106.33
24	B	613	CLA	C1D-ND-C4D	-10.00	99.23	106.33
24	B	605	CLA	C1D-ND-C4D	-9.96	99.26	106.33
24	b	617	CLA	C1D-ND-C4D	-9.93	99.28	106.33
25	A	409	PHO	C2D-C1D-ND	9.91	116.37	109.53
24	B	610	CLA	C1D-ND-C4D	-9.78	99.39	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	PHO	C2D-C1D-ND	9.76	116.27	109.53
24	a	410	CLA	C1D-ND-C4D	-9.76	99.40	106.33
24	B	617	CLA	C1D-ND-C4D	-9.72	99.43	106.33
24	a	409	CLA	C1D-ND-C4D	-9.67	99.47	106.33
24	c	909	CLA	C1D-ND-C4D	-9.66	99.48	106.33
24	C	508	CLA	C1D-ND-C4D	-9.61	99.51	106.33
24	c	905	CLA	C1D-ND-C4D	-9.59	99.52	106.33
24	C	504	CLA	C1D-ND-C4D	-9.56	99.54	106.33
24	b	609	CLA	C1D-ND-C4D	-9.55	99.55	106.33
24	B	604	CLA	C1D-ND-C4D	-9.52	99.57	106.33
24	D	403	CLA	C1D-ND-C4D	-9.48	99.60	106.33
24	B	614	CLA	C1D-ND-C4D	-9.45	99.63	106.33
24	b	616	CLA	C1D-ND-C4D	-9.41	99.65	106.33
24	A	407	CLA	C1D-ND-C4D	-9.41	99.65	106.33
24	b	618	CLA	C1D-ND-C4D	-9.38	99.67	106.33
24	a	413	CLA	C1D-ND-C4D	-9.38	99.67	106.33
24	d	404	CLA	C1D-ND-C4D	-9.30	99.73	106.33
24	b	615	CLA	C1D-ND-C4D	-9.29	99.74	106.33
24	A	405	CLA	C1D-ND-C4D	-9.27	99.75	106.33
24	B	614	CLA	C2D-C1D-ND	9.25	116.92	110.10
24	c	913	CLA	C1D-ND-C4D	-9.25	99.76	106.33
24	C	512	CLA	C1D-ND-C4D	-9.25	99.77	106.33
24	A	410	CLA	C1D-ND-C4D	-9.24	99.77	106.33
24	C	510	CLA	C1D-ND-C4D	-9.24	99.77	106.33
24	b	612	CLA	C1D-ND-C4D	-9.22	99.79	106.33
24	B	609	CLA	C1D-ND-C4D	-9.19	99.80	106.33
24	c	903	CLA	C1D-ND-C4D	-9.18	99.82	106.33
24	d	405	CLA	C1D-ND-C4D	-9.11	99.87	106.33
24	D	402	CLA	C2D-C1D-ND	9.10	116.81	110.10
24	A	406	CLA	C1D-ND-C4D	-9.09	99.88	106.33
24	B	603	CLA	C1D-ND-C4D	-9.05	99.91	106.33
24	B	612	CLA	C1D-ND-C4D	-9.05	99.91	106.33
24	b	614	CLA	C1D-ND-C4D	-9.01	99.93	106.33
24	c	911	CLA	C1D-ND-C4D	-9.01	99.93	106.33
24	B	608	CLA	C1D-ND-C4D	-9.01	99.94	106.33
24	B	615	CLA	C1D-ND-C4D	-8.98	99.95	106.33
24	B	606	CLA	C1D-ND-C4D	-8.96	99.97	106.33
24	b	611	CLA	C1D-ND-C4D	-8.96	99.97	106.33
24	B	616	CLA	C1D-ND-C4D	-8.93	99.99	106.33
24	B	613	CLA	C2D-C1D-ND	8.93	116.69	110.10
24	C	513	CLA	C1D-ND-C4D	-8.93	99.99	106.33
24	b	613	CLA	C1D-ND-C4D	-8.92	100.00	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	905	CLA	C2D-C1D-ND	8.92	116.68	110.10
24	C	501	CLA	C1D-ND-C4D	-8.91	100.01	106.33
24	B	616	CLA	C2D-C1D-ND	8.88	116.65	110.10
25	a	411	PHO	C2D-C1D-ND	8.88	115.66	109.53
24	b	615	CLA	C2D-C1D-ND	8.81	116.60	110.10
24	B	608	CLA	C2D-C1D-ND	8.78	116.57	110.10
24	b	617	CLA	C2D-C1D-ND	8.75	116.55	110.10
24	B	607	CLA	C1D-ND-C4D	-8.74	100.12	106.33
24	c	902	CLA	C2D-C1D-ND	8.74	116.54	110.10
24	b	619	CLA	C1D-ND-C4D	-8.72	100.14	106.33
24	B	617	CLA	C2D-C1D-ND	8.72	116.53	110.10
24	b	607	CLA	C1D-ND-C4D	-8.69	100.16	106.33
24	c	912	CLA	C1D-ND-C4D	-8.69	100.16	106.33
24	c	907	CLA	C1D-ND-C4D	-8.68	100.17	106.33
24	C	506	CLA	C1D-ND-C4D	-8.66	100.18	106.33
24	a	410	CLA	C2D-C1D-ND	8.66	116.48	110.10
24	b	611	CLA	C2D-C1D-ND	8.62	116.46	110.10
24	C	502	CLA	C1D-ND-C4D	-8.60	100.23	106.33
24	d	401	CLA	C2D-C1D-ND	8.58	116.42	110.10
24	c	906	CLA	C1D-ND-C4D	-8.56	100.25	106.33
24	b	620	CLA	C1D-ND-C4D	-8.55	100.26	106.33
24	B	611	CLA	C1D-ND-C4D	-8.55	100.26	106.33
24	b	608	CLA	C1D-ND-C4D	-8.54	100.27	106.33
24	b	610	CLA	C1D-ND-C4D	-8.52	100.28	106.33
24	A	410	CLA	C2D-C1D-ND	8.51	116.38	110.10
24	B	612	CLA	C2D-C1D-ND	8.50	116.37	110.10
24	b	609	CLA	C2D-C1D-ND	8.48	116.35	110.10
24	a	409	CLA	C2D-C1D-ND	8.46	116.34	110.10
24	B	602	CLA	C1D-ND-C4D	-8.46	100.33	106.33
25	A	409	PHO	C2B-C1B-NB	8.43	115.35	109.53
24	B	607	CLA	C2D-C1D-ND	8.43	116.32	110.10
24	c	914	CLA	C1D-ND-C4D	-8.39	100.38	106.33
25	a	412	PHO	C2D-C1D-ND	8.39	115.32	109.53
24	C	503	CLA	C1D-ND-C4D	-8.39	100.38	106.33
24	c	909	CLA	C2D-C1D-ND	8.34	116.25	110.10
24	A	406	CLA	C2D-C1D-ND	8.33	116.25	110.10
24	b	616	CLA	C2D-C1D-ND	8.32	116.23	110.10
24	C	509	CLA	C1D-ND-C4D	-8.32	100.43	106.33
24	A	405	CLA	C2D-C1D-ND	8.30	116.22	110.10
24	A	407	CLA	C2D-C1D-ND	8.25	116.18	110.10
24	b	605	CLA	C1D-ND-C4D	-8.25	100.48	106.33
24	C	511	CLA	C1D-ND-C4D	-8.23	100.49	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	C1D-ND-C4D	-8.21	100.50	106.33
24	c	912	CLA	C2D-C1D-ND	8.19	116.14	110.10
24	b	614	CLA	C2D-C1D-ND	8.18	116.13	110.10
24	c	908	CLA	C1D-ND-C4D	-8.18	100.53	106.33
24	c	913	CLA	C2D-C1D-ND	8.17	116.13	110.10
24	B	615	CLA	C2D-C1D-ND	8.17	116.12	110.10
25	A	408	PHO	C4D-ND-C1D	-8.16	100.52	108.83
24	C	512	CLA	C2D-C1D-ND	8.15	116.11	110.10
24	B	606	CLA	C2D-C1D-ND	8.14	116.10	110.10
24	C	511	CLA	C2D-C1D-ND	8.13	116.09	110.10
24	C	504	CLA	C2D-C1D-ND	8.12	116.09	110.10
25	a	411	PHO	O2D-CGD-CBD	8.12	121.28	111.00
25	A	409	PHO	C4D-ND-C1D	-8.10	100.59	108.83
24	b	606	CLA	C1D-ND-C4D	-8.09	100.58	106.33
24	B	611	CLA	C2D-C1D-ND	8.05	116.03	110.10
24	B	605	CLA	C2D-C1D-ND	8.04	116.03	110.10
24	b	618	CLA	C2D-C1D-ND	8.04	116.03	110.10
24	b	619	CLA	C2D-C1D-ND	8.00	116.00	110.10
24	B	604	CLA	C2D-C1D-ND	7.95	115.96	110.10
24	b	608	CLA	C2D-C1D-ND	7.94	115.95	110.10
24	c	903	CLA	C2D-C1D-ND	7.93	115.95	110.10
24	C	508	CLA	C2D-C1D-ND	7.86	115.90	110.10
24	D	403	CLA	C2D-C1D-ND	7.85	115.89	110.10
24	c	910	CLA	C1D-ND-C4D	-7.85	100.76	106.33
24	B	609	CLA	C2D-C1D-ND	7.81	115.86	110.10
25	A	408	PHO	C2B-C1B-NB	7.79	114.91	109.53
24	C	507	CLA	C1D-ND-C4D	-7.78	100.81	106.33
24	d	405	CLA	C2D-C1D-ND	7.78	115.84	110.10
25	a	411	PHO	C2B-C1B-NB	7.78	114.90	109.53
24	a	413	CLA	C2D-C1D-ND	7.76	115.82	110.10
24	C	503	CLA	C2D-C1D-ND	7.75	115.82	110.10
24	B	610	CLA	C2D-C1D-ND	7.73	115.80	110.10
24	b	620	CLA	C2D-C1D-ND	7.71	115.79	110.10
24	d	404	CLA	C2D-C1D-ND	7.69	115.77	110.10
24	C	501	CLA	C2D-C1D-ND	7.68	115.77	110.10
24	C	510	CLA	C2D-C1D-ND	7.66	115.75	110.10
25	a	411	PHO	C4D-ND-C1D	-7.60	101.10	108.83
24	c	908	CLA	C2D-C1D-ND	7.59	115.70	110.10
24	c	904	CLA	C1D-ND-C4D	-7.56	100.97	106.33
24	c	904	CLA	C2D-C1D-ND	7.52	115.65	110.10
25	a	412	PHO	C2B-C1B-NB	7.48	114.69	109.53
24	B	603	CLA	C2D-C1D-ND	7.48	115.61	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	C2D-C1D-ND	7.45	115.59	110.10
24	c	911	CLA	C2D-C1D-ND	7.40	115.56	110.10
25	a	412	PHO	C4D-ND-C1D	-7.40	101.30	108.83
24	b	610	CLA	C2D-C1D-ND	7.39	115.55	110.10
25	a	412	PHO	O2D-CGD-CBD	7.32	120.28	111.00
24	C	507	CLA	C2D-C1D-ND	7.32	115.50	110.10
24	C	502	CLA	C2D-C1D-ND	7.26	115.45	110.10
24	C	513	CLA	C2D-C1D-ND	7.22	115.43	110.10
24	b	605	CLA	C2D-C1D-ND	7.13	115.36	110.10
24	b	612	CLA	C2D-C1D-ND	7.12	115.35	110.10
24	C	509	CLA	C2D-C1D-ND	7.10	115.33	110.10
24	c	908	CLA	O2D-CGD-CBD	7.05	123.80	111.27
24	c	906	CLA	C2D-C1D-ND	7.02	115.28	110.10
35	b	627	HTG	C1'-S1-C1	6.99	113.17	100.09
24	c	910	CLA	C2D-C1D-ND	6.97	115.24	110.10
24	B	609	CLA	C2B-C1B-NB	6.96	114.90	110.23
25	A	408	PHO	C1C-C2C-C3C	-6.93	102.85	108.61
25	A	408	PHO	O2D-CGD-CBD	6.91	119.75	111.00
25	a	411	PHO	C1C-C2C-C3C	-6.89	102.88	108.61
24	C	507	CLA	CMD-C2D-C1D	6.86	136.81	124.71
24	C	506	CLA	C2D-C1D-ND	6.85	115.15	110.10
24	B	605	CLA	CMD-C2D-C1D	6.83	136.75	124.71
38	V	202	HEM	C4D-ND-C1D	6.73	112.03	105.07
24	B	602	CLA	CMD-C2D-C1D	6.73	136.57	124.71
24	b	606	CLA	C2D-C1D-ND	6.72	115.06	110.10
24	b	607	CLA	C2D-C1D-ND	6.71	115.05	110.10
24	B	602	CLA	C2D-C1D-ND	6.68	115.03	110.10
24	B	607	CLA	CMD-C2D-C1D	6.68	136.49	124.71
24	c	907	CLA	C2D-C1D-ND	6.67	115.02	110.10
24	b	617	CLA	CMD-C2D-C1D	6.67	136.47	124.71
24	c	914	CLA	C2D-C1D-ND	6.62	114.98	110.10
24	b	613	CLA	CMD-C2D-C1D	6.57	136.29	124.71
24	a	409	CLA	CMD-C2D-C1D	6.57	136.29	124.71
24	C	505	CLA	C2D-C1D-ND	6.57	114.94	110.10
24	B	615	CLA	O2D-CGD-CBD	6.54	122.89	111.27
24	A	410	CLA	C2B-C1B-NB	6.52	114.60	110.23
24	d	405	CLA	C2B-C1B-NB	6.48	114.58	110.23
24	c	907	CLA	CMD-C2D-C1D	6.48	136.13	124.71
25	A	409	PHO	C3D-C4D-ND	6.43	116.49	107.72
38	F	102	HEM	C4D-ND-C1D	6.37	111.65	105.07
24	b	608	CLA	O2D-CGD-CBD	6.36	122.57	111.27
24	C	501	CLA	O2D-CGD-CBD	6.33	122.51	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	CMD-C2D-C1D	6.32	135.85	124.71
24	d	405	CLA	CMD-C2D-C1D	6.31	135.84	124.71
24	c	911	CLA	CMD-C2D-C1D	6.30	135.81	124.71
24	d	404	CLA	CMD-C2D-C1D	6.30	135.81	124.71
24	b	610	CLA	CMD-C2D-C1D	6.29	135.80	124.71
25	A	409	PHO	O2D-CGD-CBD	6.29	118.96	111.00
24	b	618	CLA	C2B-C1B-NB	6.27	114.44	110.23
24	b	612	CLA	CMD-C2D-C1D	6.27	135.76	124.71
27	a	415	SQD	O6-C1-C2	6.27	118.09	108.30
25	A	408	PHO	C3D-C4D-ND	6.26	116.25	107.72
35	B	625	HTG	C1'-S1-C1	6.25	111.78	100.09
24	C	503	CLA	CMD-C2D-C1D	6.25	135.72	124.71
24	d	401	CLA	C2B-C1B-NB	6.20	114.39	110.23
24	c	902	CLA	CMD-C2D-C1D	6.19	135.61	124.71
24	D	403	CLA	CMD-C2D-C1D	6.18	135.61	124.71
24	c	913	CLA	O2D-CGD-CBD	6.18	122.24	111.27
24	B	603	CLA	CMD-C2D-C1D	6.17	135.59	124.71
27	A	412	SQD	O6-C1-C2	6.17	117.93	108.30
24	B	604	CLA	C2B-C1B-NB	6.16	114.36	110.23
24	B	615	CLA	C2B-C1B-NB	6.14	114.35	110.23
24	C	510	CLA	CMD-C2D-C1D	6.12	135.49	124.71
24	C	507	CLA	O2D-CGD-CBD	6.09	122.09	111.27
25	a	412	PHO	C1C-C2C-C3C	-6.08	103.56	108.61
25	a	412	PHO	C3D-C4D-ND	6.08	116.00	107.72
24	C	513	CLA	CMD-C2D-C1D	6.07	135.41	124.71
29	a	417	PL9	C7-C8-C9	-6.07	116.69	126.79
24	B	611	CLA	CMD-C2D-C1D	6.07	135.40	124.71
24	b	609	CLA	C2B-C1B-NB	6.06	114.29	110.23
24	C	509	CLA	CMD-C2D-C1D	6.06	135.39	124.71
24	B	615	CLA	CMD-C2D-C1D	6.04	135.35	124.71
24	C	505	CLA	CMD-C2D-C1D	6.02	135.32	124.71
24	D	402	CLA	CMD-C2D-C1D	6.02	135.31	124.71
25	a	411	PHO	C3D-C4D-ND	6.00	115.90	107.72
24	C	501	CLA	CMD-C2D-C1D	5.99	135.28	124.71
24	c	905	CLA	CMD-C2D-C1D	5.99	135.27	124.71
24	b	618	CLA	O2D-CGD-CBD	5.99	121.91	111.27
24	c	909	CLA	C2B-C1B-NB	5.96	114.23	110.23
24	C	512	CLA	C2B-C1B-NB	5.94	114.22	110.23
24	c	913	CLA	C2B-C1B-NB	5.94	114.21	110.23
38	f	101	HEM	C4D-ND-C1D	5.93	111.20	105.07
24	b	620	CLA	C2B-C1B-NB	5.93	114.21	110.23
35	c	924	HTG	C1'-S1-C1	5.92	111.16	100.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	CMD-C2D-C1D	5.89	135.09	124.71
24	c	914	CLA	CMD-C2D-C1D	5.89	135.09	124.71
24	c	910	CLA	CMD-C2D-C1D	5.88	135.08	124.71
24	A	406	CLA	CMD-C2D-C1D	5.88	135.07	124.71
24	b	620	CLA	O2D-CGD-CBD	5.87	121.69	111.27
24	b	609	CLA	CMD-C2D-C1D	5.85	135.03	124.71
35	V	203	HTG	O5-C1-C2	-5.85	102.95	110.31
24	a	413	CLA	C2B-C1B-NB	5.84	114.14	110.23
24	B	617	CLA	O2D-CGD-CBD	5.83	121.63	111.27
25	A	409	PHO	C1C-C2C-C3C	-5.82	103.77	108.61
24	b	618	CLA	CMD-C2D-C1D	5.81	134.96	124.71
24	c	905	CLA	O2D-CGD-CBD	5.80	121.58	111.27
24	B	604	CLA	CMD-C2D-C1D	5.80	134.94	124.71
24	a	410	CLA	CHD-C1D-ND	-5.79	119.13	124.45
24	B	612	CLA	CMD-C2D-C1D	5.79	134.92	124.71
24	b	614	CLA	C2B-C1B-NB	5.79	114.11	110.23
24	A	407	CLA	C2B-C1B-NB	5.79	114.11	110.23
24	b	605	CLA	CMD-C2D-C1D	5.77	134.88	124.71
24	b	608	CLA	CMD-C2D-C1D	5.76	134.87	124.71
24	b	620	CLA	CMD-C2D-C1D	5.76	134.87	124.71
24	C	509	CLA	C2B-C1B-NB	5.74	114.08	110.23
24	b	614	CLA	CMD-C2D-C1D	5.73	134.81	124.71
24	B	613	CLA	C2B-C1B-NB	5.73	114.07	110.23
24	D	403	CLA	C2B-C1B-NB	5.73	114.07	110.23
38	v	202	HEM	C4D-ND-C1D	5.72	110.99	105.07
24	b	619	CLA	CMD-C2D-C1D	5.72	134.80	124.71
24	b	607	CLA	CMD-C2D-C1D	5.72	134.79	124.71
24	b	611	CLA	CMD-C2D-C1D	5.72	134.79	124.71
24	c	906	CLA	O2D-CGD-CBD	5.71	121.42	111.27
35	C	522	HTG	C1'-S1-C1	5.70	110.76	100.09
24	b	607	CLA	C2B-C1B-NB	5.70	114.05	110.23
24	c	913	CLA	CMD-C2D-C1D	5.70	134.75	124.71
24	b	616	CLA	O2D-CGD-CBD	5.68	121.36	111.27
24	C	510	CLA	O2D-CGD-CBD	5.65	121.31	111.27
24	B	613	CLA	O2D-CGD-CBD	5.65	121.30	111.27
24	b	606	CLA	C2B-C1B-NB	5.65	114.02	110.23
24	B	608	CLA	CMD-C2D-C1D	5.64	134.66	124.71
24	B	603	CLA	C2B-C1B-NB	5.63	114.01	110.23
27	f	102	SQD	O47-C7-O49	-5.63	118.41	125.57
24	b	606	CLA	CMD-C2D-C1D	5.62	134.62	124.71
24	b	605	CLA	O2D-CGD-CBD	5.62	121.25	111.27
24	C	503	CLA	C2B-C1B-NB	5.61	113.99	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	906	CLA	CMD-C2D-C1D	5.60	134.59	124.71
24	B	610	CLA	CMD-C2D-C1D	5.60	134.58	124.71
24	c	914	CLA	C2B-C1B-NB	5.59	113.98	110.23
24	C	512	CLA	CMD-C2D-C1D	5.54	134.48	124.71
24	C	508	CLA	O2D-CGD-CBD	5.54	121.11	111.27
24	b	619	CLA	C2B-C1B-NB	5.54	113.95	110.23
24	B	602	CLA	O2D-CGD-CBD	5.53	121.10	111.27
24	A	410	CLA	CMD-C2D-C1D	5.52	134.45	124.71
24	A	406	CLA	C2B-C1B-NB	5.52	113.93	110.23
24	A	405	CLA	CMD-C2D-C1D	5.52	134.44	124.71
24	C	507	CLA	C2B-C1B-NB	5.51	113.92	110.23
24	a	410	CLA	CMD-C2D-C1D	5.49	134.40	124.71
24	B	614	CLA	C2B-C1B-NB	5.49	113.92	110.23
24	A	407	CLA	CMD-C2D-C1D	5.49	134.39	124.71
24	c	905	CLA	C2B-C1B-NB	5.49	113.91	110.23
24	b	618	CLA	C1-C2-C3	-5.48	116.56	126.04
24	B	602	CLA	C2B-C1B-NB	5.48	113.91	110.23
24	b	615	CLA	CMD-C2D-C1D	5.48	134.37	124.71
24	B	606	CLA	C2B-C1B-NB	5.47	113.90	110.23
24	C	511	CLA	CMD-C2D-C1D	5.47	134.35	124.71
24	c	912	CLA	CMD-C2D-C1D	5.46	134.33	124.71
35	u	201	HTG	C1'-S1-C1	5.45	110.29	100.09
24	B	604	CLA	O2D-CGD-CBD	5.45	120.95	111.27
24	a	409	CLA	C2B-C1B-NB	5.44	113.88	110.23
24	B	614	CLA	CMD-C2D-C1D	5.44	134.31	124.71
24	c	904	CLA	CMD-C2D-C1D	5.44	134.29	124.71
24	C	512	CLA	O2D-CGD-CBD	5.38	120.83	111.27
24	b	608	CLA	C2B-C1B-NB	5.37	113.83	110.23
24	b	605	CLA	C2B-C1B-NB	5.36	113.83	110.23
24	B	616	CLA	C2B-C1B-NB	5.35	113.82	110.23
24	B	612	CLA	C2B-C1B-NB	5.33	113.81	110.23
24	b	613	CLA	C2B-C1B-NB	5.33	113.81	110.23
35	V	203	HTG	C1-C2-C3	-5.33	100.07	110.59
24	b	612	CLA	C2B-C1B-NB	5.32	113.80	110.23
24	a	413	CLA	CMD-C2D-C1D	5.28	134.02	124.71
24	d	401	CLA	CMD-C2D-C1D	5.28	134.02	124.71
24	C	502	CLA	CMD-C2D-C1D	5.28	134.01	124.71
24	C	508	CLA	C2B-C1B-NB	5.27	113.77	110.23
35	b	602	HTG	C1'-S1-C1	5.26	109.93	100.09
24	B	616	CLA	CMD-C2D-C1D	5.26	133.98	124.71
24	c	908	CLA	CMD-C2D-C1D	5.25	133.97	124.71
24	c	903	CLA	CMD-C2D-C1D	5.24	133.94	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	C2B-C1B-NB	5.23	113.74	110.23
24	B	607	CLA	O2D-CGD-CBD	5.22	120.55	111.27
24	B	606	CLA	CMD-C2D-C1D	5.22	133.91	124.71
24	c	907	CLA	C2B-C1B-NB	5.22	113.73	110.23
24	D	402	CLA	CHD-C1D-ND	-5.22	119.66	124.45
24	B	611	CLA	O2D-CGD-CBD	5.21	120.52	111.27
24	c	902	CLA	O2D-CGD-CBD	5.20	120.51	111.27
24	c	906	CLA	C2B-C1B-NB	5.19	113.71	110.23
24	B	617	CLA	CMD-C2D-C1D	5.18	133.85	124.71
24	C	502	CLA	C1-C2-C3	-5.18	117.09	126.04
24	B	605	CLA	C2B-C1B-NB	5.17	113.70	110.23
24	d	401	CLA	CHD-C4C-C3C	-5.17	117.24	124.84
24	b	606	CLA	O2D-CGD-CBD	5.16	120.43	111.27
24	B	617	CLA	C2B-C1B-NB	5.14	113.68	110.23
26	C	515	BCR	C7-C8-C9	-5.14	118.47	126.23
27	B	621	SQD	C1-O5-C5	5.13	123.76	113.69
24	d	404	CLA	C2B-C1B-NB	5.12	113.66	110.23
36	e	102	DGD	C3D-C4D-C5D	5.11	117.73	109.77
24	a	410	CLA	CHD-C4C-C3C	-5.09	117.36	124.84
27	B	621	SQD	O47-C7-C8	5.08	122.45	111.50
27	a	401	SQD	O8-S-C6	5.08	113.83	105.74
24	d	401	CLA	C2C-C1C-NC	5.08	114.73	109.97
24	b	610	CLA	C2B-C1B-NB	5.07	113.63	110.23
24	B	608	CLA	C3D-C2D-C1D	-5.07	98.92	105.83
24	B	611	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
24	B	615	CLA	C2C-C1C-NC	5.05	114.71	109.97
35	B	627	HTG	C1'-S1-C1	5.05	109.54	100.09
24	B	607	CLA	C3D-C2D-C1D	-5.05	98.95	105.83
24	B	612	CLA	O2D-CGD-CBD	5.04	120.23	111.27
35	B	624	HTG	C1'-S1-C1	5.04	109.52	100.09
24	a	413	CLA	O2D-CGD-CBD	5.04	120.23	111.27
35	b	626	HTG	C1'-S1-C1	5.04	109.51	100.09
24	C	507	CLA	C3B-C2B-C1B	-5.04	101.08	107.16
26	D	404	BCR	C7-C8-C9	-5.03	118.63	126.23
24	A	407	CLA	O2D-CGD-CBD	5.03	120.21	111.27
24	B	607	CLA	C2B-C1B-NB	5.02	113.60	110.23
24	C	511	CLA	C2B-C1B-NB	5.02	113.60	110.23
24	b	615	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
26	D	404	BCR	C24-C23-C22	-5.01	118.66	126.23
24	B	616	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
24	C	510	CLA	C2B-C1B-NB	5.00	113.58	110.23
24	b	611	CLA	C3D-C2D-C1D	-4.99	99.02	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	905	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
24	d	401	CLA	C1C-C2C-C3C	-4.99	101.71	106.96
24	c	910	CLA	O2D-CGD-CBD	4.97	120.09	111.27
24	c	908	CLA	C2B-C1B-NB	4.96	113.56	110.23
24	C	506	CLA	C2B-C1B-NB	4.96	113.56	110.23
27	b	601	SQD	O47-C7-C8	4.95	122.17	111.50
24	C	504	CLA	C2B-C1B-NB	4.94	113.55	110.23
24	c	912	CLA	CHD-C4C-C3C	-4.93	117.59	124.84
24	c	905	CLA	CHD-C1D-ND	-4.93	119.92	124.45
24	C	509	CLA	O2D-CGD-CBD	4.92	120.01	111.27
24	B	603	CLA	O2D-CGD-CBD	4.91	120.00	111.27
24	c	912	CLA	C2B-C1B-NB	4.91	113.52	110.23
24	b	617	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
27	b	601	SQD	O7-S-C6	4.91	112.77	106.94
24	B	615	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
24	C	503	CLA	C1-C2-C3	-4.87	117.62	126.04
24	D	403	CLA	O2D-CGD-CBD	4.87	119.92	111.27
24	d	405	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
24	b	617	CLA	C2B-C1B-NB	4.86	113.49	110.23
24	b	609	CLA	CHD-C4C-C3C	-4.86	117.69	124.84
24	b	616	CLA	C2B-C1B-NB	4.85	113.49	110.23
24	c	904	CLA	C2B-C1B-NB	4.85	113.48	110.23
24	A	410	CLA	C3B-C2B-C1B	-4.85	101.31	107.16
24	a	410	CLA	O2D-CGD-CBD	4.85	119.88	111.27
36	D	406	DGD	O2G-C1B-C2B	4.84	121.94	111.50
24	c	909	CLA	O2D-CGD-CBD	4.84	119.87	111.27
24	c	902	CLA	C2B-C1B-NB	4.84	113.47	110.23
24	B	612	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
24	B	605	CLA	C2C-C1C-NC	4.83	114.50	109.97
24	B	614	CLA	C1-C2-C3	-4.83	117.69	126.04
24	A	406	CLA	C1C-C2C-C3C	-4.83	101.88	106.96
24	B	614	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
24	d	405	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
24	b	609	CLA	CHD-C1D-ND	-4.81	120.03	124.45
24	A	406	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
24	b	612	CLA	O2D-CGD-CBD	4.80	119.80	111.27
24	D	402	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
24	C	513	CLA	C2B-C1B-NB	4.79	113.44	110.23
24	C	508	CLA	CMD-C2D-C1D	4.79	133.15	124.71
28	B	622	LMG	O7-C10-C11	4.78	121.81	111.50
24	A	410	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
24	B	615	CLA	C3B-C2B-C1B	-4.78	101.40	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	909	CLA	CMD-C2D-C1D	4.77	133.12	124.71
24	a	409	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
24	d	401	CLA	CHD-C1D-ND	-4.76	120.08	124.45
24	b	610	CLA	O2D-CGD-CBD	4.76	119.73	111.27
24	b	615	CLA	C2B-C1B-NB	4.76	113.42	110.23
24	c	903	CLA	O2D-CGD-CBD	4.75	119.70	111.27
24	c	904	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
24	c	912	CLA	CHD-C1D-ND	-4.74	120.10	124.45
24	A	406	CLA	C2C-C1C-NC	4.73	114.40	109.97
35	d	403	HTG	C1'-S1-C1	4.73	108.94	100.09
24	A	407	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
24	D	403	CLA	C3B-C2B-C1B	-4.73	101.46	107.16
24	A	405	CLA	C2B-C1B-NB	4.72	113.40	110.23
24	c	914	CLA	O2D-CGD-CBD	4.72	119.66	111.27
24	A	406	CLA	CHD-C1D-ND	-4.72	120.11	124.45
24	b	609	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
24	A	406	CLA	O2D-CGD-CBD	4.71	119.64	111.27
24	B	609	CLA	C3B-C2B-C1B	-4.70	101.49	107.16
36	e	102	DGD	O2G-C1B-C2B	4.69	121.62	111.50
35	B	626	HTG	C1'-S1-C1	4.69	108.87	100.09
24	d	404	CLA	C2C-C1C-NC	4.69	114.37	109.97
24	a	410	CLA	C2B-C1B-NB	4.68	113.37	110.23
24	B	606	CLA	CHD-C4C-C3C	-4.68	117.97	124.84
24	C	503	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
24	a	410	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
26	t	903	BCR	C33-C5-C6	-4.67	119.29	124.53
24	c	903	CLA	C2B-C1B-NB	4.66	113.36	110.23
24	C	508	CLA	C3D-C4D-ND	4.66	117.78	110.24
24	B	606	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
24	B	610	CLA	C3D-C4D-ND	4.65	117.76	110.24
24	d	401	CLA	C3D-C4D-ND	4.65	117.76	110.24
28	C	534	LMG	O7-C10-C11	4.64	121.50	111.50
27	A	412	SQD	O47-C7-C8	4.64	121.50	111.50
24	c	913	CLA	C3B-C2B-C1B	-4.63	101.57	107.16
24	b	620	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	c	902	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	b	615	CLA	O2D-CGD-CBD	4.62	119.48	111.27
24	B	616	CLA	CHD-C4C-C3C	-4.62	118.05	124.84
24	b	608	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
24	b	618	CLA	C3D-C2D-C1D	-4.61	99.53	105.83
24	B	617	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
24	C	509	CLA	C3B-C2B-C1B	-4.61	101.60	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	CMD-C2D-C1D	4.60	132.82	124.71
24	C	507	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
24	b	619	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
24	C	502	CLA	C2B-C1B-NB	4.59	113.31	110.23
35	C	521	HTG	C1'-S1-C1	4.59	108.68	100.09
24	C	504	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
24	b	618	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
27	b	601	SQD	C3-C4-C5	4.59	118.43	110.24
26	D	404	BCR	C38-C26-C25	-4.59	119.38	124.53
24	c	908	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
24	C	511	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
24	b	616	CLA	CHD-C4C-C3C	-4.58	118.10	124.84
26	b	621	BCR	C33-C5-C6	-4.58	119.38	124.53
24	B	617	CLA	CHD-C4C-C3C	-4.58	118.11	124.84
24	c	913	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
24	C	512	CLA	C3D-C2D-C1D	-4.58	99.59	105.83
35	c	923	HTG	C1'-S1-C1	4.57	108.65	100.09
24	c	909	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
24	b	615	CLA	CHD-C4C-C3C	-4.57	118.13	124.84
24	C	504	CLA	O2D-CGD-CBD	4.57	119.38	111.27
24	b	614	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
24	C	513	CLA	O2D-CGD-CBD	4.56	119.36	111.27
26	d	406	BCR	C38-C26-C25	-4.55	119.41	124.53
24	c	906	CLA	C3B-C2B-C1B	-4.54	101.68	107.16
24	B	613	CLA	CMD-C2D-C1D	4.53	132.70	124.71
24	C	502	CLA	O2D-CGD-CBD	4.53	119.31	111.27
24	B	606	CLA	O2D-CGD-CBD	4.52	119.31	111.27
24	d	401	CLA	C3B-C2B-C1B	-4.52	101.70	107.16
24	B	613	CLA	CHD-C4C-C3C	-4.52	118.19	124.84
24	d	404	CLA	O2D-CGD-CBD	4.52	119.29	111.27
24	b	610	CLA	CHD-C4C-C3C	-4.51	118.22	124.84
24	D	402	CLA	C2B-C1B-NB	4.50	113.25	110.23
24	B	616	CLA	C3B-C2B-C1B	-4.50	101.73	107.16
24	B	608	CLA	C2C-C1C-NC	4.50	114.18	109.97
24	C	501	CLA	O2D-CGD-O1D	-4.48	115.08	123.84
24	D	403	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
25	A	409	PHO	C1-C2-C3	-4.47	118.31	126.04
24	B	604	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
24	b	609	CLA	C3B-C2B-C1B	-4.46	101.77	107.16
24	C	507	CLA	C2C-C1C-NC	4.46	114.15	109.97
24	C	503	CLA	C3B-C2B-C1B	-4.45	101.78	107.16
24	a	413	CLA	C2C-C1C-NC	4.45	114.14	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	401	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
24	C	501	CLA	C2B-C1B-NB	4.45	113.22	110.23
24	B	612	CLA	CHD-C4C-C3C	-4.45	118.30	124.84
24	B	615	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
24	B	605	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
24	b	610	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
24	B	605	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
24	c	912	CLA	C3B-C2B-C1B	-4.43	101.82	107.16
24	c	905	CLA	C2C-C1C-NC	4.42	114.12	109.97
24	B	615	CLA	CHD-C4C-C3C	-4.42	118.34	124.84
24	B	605	CLA	O2D-CGD-CBD	4.42	119.12	111.27
24	c	911	CLA	C2B-C1B-NB	4.42	113.19	110.23
37	D	407	LHG	O8-C23-O10	-4.41	112.46	123.59
24	A	406	CLA	CBC-CAC-C3C	-4.41	100.27	112.43
24	b	619	CLA	CHD-C4C-C3C	-4.41	118.36	124.84
24	b	606	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
24	B	608	CLA	C2B-C1B-NB	4.40	113.18	110.23
24	a	409	CLA	CHD-C1D-ND	-4.40	120.41	124.45
24	c	911	CLA	CHD-C4C-C3C	-4.40	118.37	124.84
24	A	407	CLA	C3D-C4D-ND	4.40	117.35	110.24
24	c	903	CLA	CHD-C4C-C3C	-4.39	118.38	124.84
24	b	617	CLA	C1-C2-C3	-4.39	118.45	126.04
24	c	912	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
24	c	911	CLA	O2D-CGD-CBD	4.38	119.06	111.27
24	B	614	CLA	CHD-C4C-C3C	-4.38	118.39	124.84
24	C	512	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
24	A	410	CLA	C2C-C1C-NC	4.38	114.08	109.97
24	A	407	CLA	C3B-C2B-C1B	-4.38	101.88	107.16
24	D	402	CLA	C3D-C4D-ND	4.38	117.32	110.24
24	c	904	CLA	C3B-C2B-C1B	-4.38	101.88	107.16
28	A	413	LMG	O7-C10-C11	4.37	120.92	111.50
24	c	906	CLA	C2C-C1C-NC	4.37	114.06	109.97
24	C	503	CLA	CHD-C4C-C3C	-4.37	118.42	124.84
24	c	909	CLA	C3B-C2B-C1B	-4.37	101.89	107.16
24	C	505	CLA	C2C-C1C-NC	4.36	114.06	109.97
35	b	603	HTG	C1'-S1-C1	4.36	108.25	100.09
24	a	413	CLA	C3B-C2B-C1B	-4.36	101.89	107.16
24	A	405	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
24	c	902	CLA	C2C-C1C-NC	4.36	114.05	109.97
24	C	505	CLA	O2D-CGD-CBD	4.36	119.01	111.27
24	c	907	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
24	C	501	CLA	C3D-C2D-C1D	-4.35	99.89	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	903	CLA	C3B-C2B-C1B	-4.35	101.91	107.16
24	c	903	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
24	b	620	CLA	C3B-C2B-C1B	-4.35	101.92	107.16
24	c	902	CLA	C1C-C2C-C3C	-4.35	102.39	106.96
28	a	416	LMG	O7-C10-C11	4.34	120.85	111.50
36	D	406	DGD	C3D-C4D-C5D	4.34	117.97	110.24
24	C	505	CLA	C3B-C2B-C1B	-4.33	101.93	107.16
36	c	917	DGD	O2G-C1B-C2B	4.33	120.84	111.50
24	B	613	CLA	C3B-C2B-C1B	-4.33	101.93	107.16
24	B	617	CLA	C3B-C2B-C1B	-4.33	101.93	107.16
25	a	412	PHO	C1-C2-C3	-4.33	118.56	126.04
26	d	406	BCR	C24-C23-C22	-4.33	119.69	126.23
24	a	409	CLA	C2C-C1C-NC	4.33	114.03	109.97
35	H	105	HTG	C1'-S1-C1	4.32	108.37	100.16
24	b	611	CLA	O2D-CGD-CBD	4.32	118.95	111.27
27	b	601	SQD	O6-C1-C2	4.32	115.05	108.30
24	a	410	CLA	C3D-C4D-ND	4.32	117.22	110.24
29	A	414	PL9	C7-C8-C9	-4.32	119.61	126.79
24	B	614	CLA	C3B-C2B-C1B	-4.32	101.95	107.16
24	c	910	CLA	C2B-C1B-NB	4.32	113.12	110.23
24	c	902	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
24	A	407	CLA	C2C-C1C-NC	4.30	114.00	109.97
24	b	613	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
24	b	614	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
24	C	510	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
35	C	522	HTG	C1-O5-C5	4.30	120.51	112.58
24	B	604	CLA	CHD-C4C-C3C	-4.30	118.52	124.84
24	a	409	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
24	B	603	CLA	C3D-C2D-C1D	-4.29	99.97	105.83
24	B	607	CLA	C2C-C1C-NC	4.29	113.99	109.97
24	C	511	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
24	B	607	CLA	CHD-C4C-C3C	-4.28	118.55	124.84
24	B	615	CLA	CHD-C1D-ND	-4.28	120.52	124.45
24	B	609	CLA	O2D-CGD-CBD	4.27	118.86	111.27
28	C	519	LMG	O7-C10-C11	4.27	120.71	111.50
24	C	511	CLA	CHD-C4C-C3C	-4.27	118.56	124.84
24	c	902	CLA	CHD-C1D-ND	-4.27	120.53	124.45
24	B	612	CLA	C3B-C2B-C1B	-4.27	102.01	107.16
24	A	406	CLA	CHD-C4C-C3C	-4.27	118.57	124.84
28	c	921	LMG	O7-C10-C11	4.26	120.68	111.50
24	c	911	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
24	D	402	CLA	CHD-C4C-C3C	-4.26	118.58	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	CHD-C1D-ND	-4.26	120.54	124.45
24	c	908	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
24	c	905	CLA	CHD-C4C-C3C	-4.25	118.59	124.84
24	b	610	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
24	B	611	CLA	C2B-C1B-NB	4.25	113.08	110.23
24	c	905	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
24	C	513	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
24	B	612	CLA	CAC-C3C-C4C	4.25	130.32	124.81
24	C	509	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
24	B	602	CLA	CHD-C1D-ND	-4.24	120.55	124.45
34	C	520	LMT	O1B-C4'-C3'	4.24	118.57	107.28
24	C	504	CLA	C3D-C4D-ND	4.24	117.10	110.24
26	k	101	BCR	C24-C23-C22	-4.24	119.83	126.23
24	B	613	CLA	C3D-C4D-ND	4.24	117.10	110.24
24	B	608	CLA	O2D-CGD-CBD	4.24	118.80	111.27
24	b	612	CLA	C3D-C4D-ND	4.23	117.08	110.24
24	D	403	CLA	C3D-C4D-ND	4.23	117.08	110.24
24	c	902	CLA	CHD-C4C-C3C	-4.23	118.63	124.84
29	A	414	PL9	C32-C33-C34	-4.23	117.48	127.66
24	A	407	CLA	CHD-C1D-ND	-4.23	120.57	124.45
24	B	604	CLA	C3B-C2B-C1B	-4.22	102.07	107.16
24	C	506	CLA	C2C-C1C-NC	4.22	113.92	109.97
24	b	605	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
24	C	506	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
24	b	607	CLA	C3B-C2B-C1B	-4.22	102.07	107.16
27	F	101	SQD	O6-C1-C2	4.21	114.88	108.30
24	b	616	CLA	CMD-C2D-C1D	4.21	132.14	124.71
24	B	604	CLA	C3D-C4D-ND	4.21	117.05	110.24
24	B	610	CLA	C2B-C1B-NB	4.21	113.06	110.23
24	C	513	CLA	C3D-C2D-C1D	-4.21	100.09	105.83
24	c	908	CLA	C3D-C2D-C1D	-4.21	100.09	105.83
24	C	507	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
24	B	602	CLA	C3B-C2B-C1B	-4.19	102.10	107.16
24	c	903	CLA	C3D-C4D-ND	4.19	117.02	110.24
24	A	405	CLA	C2C-C1C-NC	4.19	113.90	109.97
24	b	607	CLA	C2C-C1C-NC	4.19	113.89	109.97
24	B	615	CLA	O2D-CGD-O1D	-4.19	115.65	123.84
24	C	504	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
24	C	508	CLA	C3B-C2B-C1B	-4.18	102.11	107.16
24	C	508	CLA	C3D-C2D-C1D	-4.18	100.12	105.83
24	b	616	CLA	C3C-C4C-NC	4.18	115.26	110.57
38	F	102	HEM	CBD-CAD-C3D	-4.18	101.01	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	910	CLA	C3D-C2D-C1D	-4.18	100.13	105.83
24	c	908	CLA	C2C-C1C-NC	4.17	113.88	109.97
26	d	406	BCR	C33-C5-C6	-4.17	119.84	124.53
24	B	603	CLA	C3B-C2B-C1B	-4.17	102.12	107.16
24	a	413	CLA	C3D-C4D-ND	4.17	116.99	110.24
28	b	624	LMG	O7-C10-C11	4.17	120.49	111.50
24	A	407	CLA	CHD-C4C-C3C	-4.17	118.71	124.84
24	C	512	CLA	C1-C2-C3	-4.17	118.83	126.04
24	b	619	CLA	CHD-C1D-ND	-4.17	120.62	124.45
24	D	402	CLA	C2C-C1C-NC	4.17	113.88	109.97
24	d	401	CLA	CBC-CAC-C3C	-4.17	100.94	112.43
24	A	410	CLA	CHD-C1D-ND	-4.17	120.62	124.45
24	B	608	CLA	C1C-C2C-C3C	-4.17	102.58	106.96
24	c	905	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
34	T	703	LMT	C1-O1'-C1'	-4.16	106.94	113.84
26	d	406	BCR	C7-C8-C9	-4.16	119.95	126.23
24	B	613	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
24	B	608	CLA	CHD-C1D-ND	-4.15	120.64	124.45
24	A	410	CLA	O2D-CGD-CBD	4.15	118.64	111.27
27	a	415	SQD	C1-O5-C5	-4.15	105.55	113.69
24	b	606	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
24	A	410	CLA	C1C-C2C-C3C	-4.15	102.60	106.96
26	c	915	BCR	C15-C14-C13	-4.15	121.39	127.31
24	C	502	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
24	d	404	CLA	C3C-C4C-NC	4.14	115.21	110.57
24	c	909	CLA	C3D-C4D-ND	4.14	116.93	110.24
24	b	614	CLA	C2C-C1C-NC	4.14	113.85	109.97
24	B	602	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
24	C	504	CLA	CHD-C1D-ND	-4.13	120.66	124.45
26	K	101	BCR	C33-C5-C6	-4.13	119.89	124.53
24	b	613	CLA	C3B-C2B-C1B	-4.13	102.18	107.16
24	c	905	CLA	C3D-C4D-ND	4.13	116.91	110.24
36	c	918	DGD	O2G-C1B-C2B	4.13	120.39	111.50
24	C	513	CLA	C3D-C4D-ND	4.13	116.91	110.24
24	b	605	CLA	CHD-C4C-C3C	-4.12	118.78	124.84
24	b	616	CLA	C3D-C4D-ND	4.12	116.91	110.24
24	b	607	CLA	O2D-CGD-CBD	4.12	118.60	111.27
24	b	607	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
28	C	534	LMG	O6-C5-C4	4.12	117.18	109.69
24	d	404	CLA	C3D-C4D-ND	4.12	116.90	110.24
24	B	613	CLA	C3C-C4C-NC	4.12	115.19	110.57
24	B	606	CLA	C3B-C2B-C1B	-4.12	102.19	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	621	SQD	O7-S-C6	4.11	111.83	106.94
24	B	609	CLA	C3D-C4D-ND	4.11	116.89	110.24
24	d	404	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
24	b	619	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
24	B	609	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
24	b	608	CLA	C1-C2-C3	-4.11	118.94	126.04
24	A	406	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
24	C	511	CLA	C2C-C1C-NC	4.10	113.82	109.97
24	a	409	CLA	C3D-C4D-ND	4.10	116.87	110.24
24	b	618	CLA	C3D-C4D-ND	4.10	116.87	110.24
26	T	702	BCR	C15-C16-C17	-4.10	115.08	123.47
26	c	915	BCR	C33-C5-C6	-4.10	119.93	124.53
29	D	405	PL9	C40-C39-C41	4.09	122.16	115.27
24	B	617	CLA	C3D-C4D-ND	4.09	116.86	110.24
24	c	902	CLA	O2D-CGD-O1D	-4.09	115.84	123.84
26	Y	101	BCR	C33-C5-C6	-4.09	119.94	124.53
27	a	415	SQD	O47-C7-C8	4.09	120.31	111.50
24	D	402	CLA	O2D-CGD-CBD	4.09	118.53	111.27
24	c	904	CLA	O2D-CGD-CBD	4.08	118.52	111.27
24	b	620	CLA	CHD-C4C-C3C	-4.08	118.84	124.84
24	b	613	CLA	C2C-C1C-NC	4.08	113.79	109.97
35	C	528	HTG	C1'-S1-C1	4.08	107.71	100.09
24	b	608	CLA	C3B-C2B-C1B	-4.08	102.24	107.16
24	b	612	CLA	C3D-C2D-C1D	-4.07	100.28	105.83
24	b	609	CLA	C3D-C4D-ND	4.07	116.82	110.24
24	b	615	CLA	C3B-C2B-C1B	-4.07	102.25	107.16
26	y	101	BCR	C33-C5-C6	-4.06	119.96	124.53
24	B	612	CLA	CHD-C1D-ND	-4.06	120.72	124.45
34	B	623	LMT	C1-O1'-C1'	-4.06	107.10	113.84
24	c	914	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
24	b	616	CLA	C1-C2-C3	-4.06	119.02	126.04
24	C	502	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
24	C	510	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
24	c	902	CLA	C3D-C4D-ND	4.06	116.80	110.24
24	B	614	CLA	C2C-C1C-NC	4.06	113.77	109.97
24	b	617	CLA	C3D-C4D-ND	4.06	116.80	110.24
36	C	517	DGD	O2G-C1B-C2B	4.05	120.24	111.50
24	b	617	CLA	CHD-C4C-C3C	-4.05	118.88	124.84
24	b	606	CLA	C4-C3-C5	4.05	122.09	115.27
24	b	606	CLA	C3D-C4D-ND	4.05	116.78	110.24
24	C	509	CLA	C2C-C1C-NC	4.05	113.76	109.97
24	b	612	CLA	C3B-C2B-C1B	-4.05	102.28	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	514	BCR	C33-C5-C6	-4.04	119.99	124.53
24	B	603	CLA	C2C-C1C-NC	4.04	113.75	109.97
35	C	528	HTG	C3-C4-C5	4.04	117.44	110.24
24	B	607	CLA	C3B-C2B-C1B	-4.03	102.30	107.16
24	b	616	CLA	C3D-C2D-C1D	-4.03	100.34	105.83
24	b	614	CLA	C3D-C4D-ND	4.02	116.74	110.24
24	C	510	CLA	C3D-C4D-ND	4.01	116.73	110.24
24	B	607	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
35	B	625	HTG	O5-C1-C2	4.00	115.35	110.31
24	C	501	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
27	a	401	SQD	O47-C7-C8	4.00	120.12	111.50
24	c	914	CLA	C3D-C4D-ND	4.00	116.71	110.24
24	d	405	CLA	CHD-C1D-ND	-3.99	120.78	124.45
24	d	405	CLA	O2D-CGD-CBD	3.99	118.36	111.27
24	B	611	CLA	C2C-C1C-NC	3.99	113.71	109.97
29	a	417	PL9	C32-C33-C34	-3.99	118.06	127.66
24	d	405	CLA	C3D-C4D-ND	3.99	116.69	110.24
29	A	414	PL9	C17-C18-C19	-3.98	118.07	127.66
24	b	605	CLA	C3B-C2B-C1B	-3.98	102.35	107.16
24	B	613	CLA	CHD-C1D-ND	-3.98	120.79	124.45
24	D	403	CLA	CHD-C1D-ND	-3.98	120.80	124.45
24	B	606	CLA	C3D-C4D-ND	3.98	116.68	110.24
24	c	907	CLA	C3D-C4D-ND	3.98	116.67	110.24
24	C	502	CLA	C3D-C4D-ND	3.98	116.67	110.24
29	a	417	PL9	C25-C24-C26	3.98	121.96	115.27
37	E	101	LHG	O7-C7-C8	3.97	120.06	111.50
29	A	414	PL9	C37-C38-C39	-3.97	118.10	127.66
24	C	503	CLA	O2D-CGD-CBD	3.97	118.32	111.27
26	T	702	BCR	C33-C5-C6	-3.97	120.07	124.53
24	C	501	CLA	C3D-C4D-ND	3.96	116.64	110.24
24	c	911	CLA	CHD-C1D-ND	-3.96	120.82	124.45
26	B	618	BCR	C33-C5-C6	-3.96	120.08	124.53
24	c	910	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
24	a	413	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
24	b	608	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
24	B	617	CLA	C2C-C1C-NC	3.95	113.68	109.97
24	c	914	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
24	b	607	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
24	C	512	CLA	CHD-C4C-C3C	-3.95	119.04	124.84
26	B	618	BCR	C7-C8-C9	-3.95	120.27	126.23
24	C	506	CLA	C3D-C4D-ND	3.95	116.62	110.24
24	A	410	CLA	C3D-C4D-ND	3.95	116.62	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	410	CLA	C1-C2-C3	-3.94	119.22	126.04
24	B	609	CLA	C2C-C1C-NC	3.94	113.67	109.97
27	a	415	SQD	C1-C2-C3	-3.94	101.79	110.00
24	C	501	CLA	CHD-C1D-ND	-3.94	120.83	124.45
27	f	102	SQD	O9-S-C6	3.93	111.65	106.92
24	c	911	CLA	C3D-C4D-ND	3.93	116.60	110.24
24	A	406	CLA	C3D-C4D-ND	3.93	116.60	110.24
24	b	618	CLA	O2D-CGD-O1D	-3.93	116.15	123.84
24	b	611	CLA	C2C-C1C-NC	3.93	113.65	109.97
24	C	504	CLA	C2C-C1C-NC	3.93	113.65	109.97
24	a	413	CLA	C3D-C2D-C1D	-3.93	100.47	105.83
24	B	610	CLA	C3D-C2D-C1D	-3.92	100.48	105.83
24	B	605	CLA	C3B-C2B-C1B	-3.91	102.44	107.16
24	b	618	CLA	CHD-C4C-C3C	-3.91	119.09	124.84
24	b	608	CLA	C2C-C1C-NC	3.91	113.63	109.97
24	c	911	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
26	c	916	BCR	C7-C8-C9	-3.91	120.33	126.23
25	a	412	PHO	O2D-CGD-O1D	-3.91	116.20	123.84
24	b	610	CLA	C3D-C4D-ND	3.90	116.55	110.24
24	B	611	CLA	CHD-C4C-C3C	-3.90	119.11	124.84
24	B	610	CLA	C3B-C2B-C1B	-3.90	102.46	107.16
24	a	413	CLA	CHD-C4C-C3C	-3.90	119.11	124.84
37	d	408	LHG	O8-C23-O10	-3.89	113.77	123.59
24	B	610	CLA	C2C-C1C-NC	3.88	113.61	109.97
24	c	913	CLA	CHD-C4C-C3C	-3.88	119.13	124.84
24	B	614	CLA	CHD-C1D-ND	-3.88	120.89	124.45
24	B	603	CLA	C3D-C4D-ND	3.88	116.52	110.24
24	B	611	CLA	C3C-C4C-NC	3.88	114.93	110.57
24	b	616	CLA	C3B-C2B-C1B	-3.88	102.48	107.16
24	B	611	CLA	CAC-C3C-C4C	3.88	129.84	124.81
24	B	617	CLA	C3C-C4C-NC	3.88	114.92	110.57
24	c	909	CLA	CHD-C4C-C3C	-3.88	119.14	124.84
24	C	506	CLA	O2D-CGD-CBD	3.88	118.16	111.27
24	d	401	CLA	C3B-C4B-NB	3.87	114.11	110.52
24	B	615	CLA	C3D-C4D-ND	3.87	116.50	110.24
24	c	913	CLA	CBC-CAC-C3C	-3.87	101.76	112.43
24	c	913	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
24	b	609	CLA	O2D-CGD-CBD	3.87	118.14	111.27
36	C	516	DGD	O2G-C1B-C2B	3.87	119.84	111.50
34	T	703	LMT	O1'-C1'-C2'	3.87	114.34	108.30
24	B	604	CLA	C3C-C4C-NC	3.87	114.91	110.57
24	d	405	CLA	C1C-C2C-C3C	-3.86	102.89	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	617	CLA	C3C-C4C-NC	3.86	114.90	110.57
28	c	921	LMG	C3-C4-C5	3.86	117.13	110.24
24	A	405	CLA	C3B-C2B-C1B	-3.86	102.50	107.16
36	e	102	DGD	C4D-C3D-C2D	3.86	117.56	110.82
24	c	903	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
24	b	611	CLA	CHD-C4C-C3C	-3.86	119.17	124.84
24	A	405	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
24	C	505	CLA	C3C-C4C-NC	3.85	114.89	110.57
24	B	602	CLA	C3D-C4D-ND	3.85	116.47	110.24
24	d	404	CLA	C1-C2-C3	-3.85	119.38	126.04
24	C	501	CLA	CHD-C4C-C3C	-3.85	119.18	124.84
24	b	617	CLA	C2C-C1C-NC	3.85	113.58	109.97
24	b	610	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
24	B	610	CLA	CHD-C4C-C3C	-3.84	119.19	124.84
24	B	616	CLA	CMB-C2B-C1B	3.84	131.22	125.37
24	c	911	CLA	C3B-C2B-C1B	-3.84	102.53	107.16
24	C	506	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
24	A	405	CLA	CAA-C2A-C1A	-3.84	99.40	111.97
24	c	908	CLA	CHD-C4C-C3C	-3.84	119.20	124.84
24	D	403	CLA	CHD-C4C-C3C	-3.83	119.21	124.84
24	c	906	CLA	CHD-C4C-C3C	-3.83	119.21	124.84
24	b	607	CLA	C3D-C4D-ND	3.83	116.43	110.24
24	d	404	CLA	CHD-C4C-C3C	-3.83	119.22	124.84
24	C	512	CLA	C3D-C4D-ND	3.82	116.42	110.24
28	c	920	LMG	O7-C10-C11	3.82	119.72	111.50
24	A	407	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
24	d	401	CLA	C3C-C4C-NC	3.82	114.85	110.57
24	A	410	CLA	CHD-C4C-C3C	-3.81	119.24	124.84
24	C	501	CLA	CMB-C2B-C1B	3.81	131.18	125.37
24	C	512	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
24	A	405	CLA	C3D-C4D-ND	3.81	116.40	110.24
24	b	620	CLA	C1D-CHD-C4C	-3.81	117.85	126.06
27	A	417	SQD	O48-C23-C24	3.80	123.85	111.91
24	b	607	CLA	CHD-C4C-C3C	-3.80	119.25	124.84
24	b	611	CLA	C3D-C4D-ND	3.80	116.38	110.24
24	C	501	CLA	C2C-C1C-NC	3.80	113.53	109.97
24	c	913	CLA	CBA-CAA-C2A	-3.80	102.66	113.86
24	b	618	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
24	b	605	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
27	A	412	SQD	C1-C2-C3	-3.79	102.11	110.00
24	c	906	CLA	C3D-C2D-C1D	-3.79	100.66	105.83
24	b	611	CLA	C1C-C2C-C3C	-3.79	102.97	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	605	CLA	CHD-C1D-ND	-3.79	120.97	124.45
24	d	404	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
24	C	509	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
24	B	605	CLA	C3D-C4D-ND	3.77	116.34	110.24
24	c	910	CLA	O2D-CGD-O1D	-3.77	116.47	123.84
24	A	405	CLA	CAA-C2A-C3A	-3.77	102.46	112.78
28	C	519	LMG	O8-C28-C29	3.77	123.73	111.91
24	c	905	CLA	C4-C3-C5	3.76	121.60	115.27
24	c	912	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
24	C	507	CLA	CHD-C4C-C3C	-3.76	119.31	124.84
29	d	407	PL9	C7-C8-C9	-3.76	120.53	126.79
24	B	611	CLA	C3B-C2B-C1B	-3.76	102.62	107.16
24	b	606	CLA	C2C-C1C-NC	3.76	113.49	109.97
24	B	605	CLA	C1D-CHD-C4C	-3.76	117.96	126.06
24	B	614	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
24	b	605	CLA	C3D-C4D-ND	3.75	116.31	110.24
24	a	409	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
24	C	510	CLA	C2C-C1C-NC	3.75	113.48	109.97
24	B	607	CLA	CHD-C1D-ND	-3.75	121.01	124.45
26	b	623	BCR	C24-C23-C22	-3.75	120.57	126.23
24	C	506	CLA	C3B-C2B-C1B	-3.74	102.64	107.16
24	B	616	CLA	C3C-C4C-NC	3.74	114.77	110.57
24	b	615	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
24	b	609	CLA	C4-C3-C5	3.74	121.56	115.27
24	a	410	CLA	C3C-C4C-NC	3.74	114.76	110.57
24	c	911	CLA	C2C-C1C-NC	3.73	113.47	109.97
24	B	610	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
24	C	502	CLA	CHD-C4C-C3C	-3.73	119.35	124.84
29	a	417	PL9	C42-C43-C44	-3.73	118.69	127.66
24	B	615	CLA	C4-C3-C5	3.73	121.54	115.27
24	c	913	CLA	C3D-C4D-ND	3.72	116.26	110.24
24	c	902	CLA	CBC-CAC-C3C	-3.72	102.17	112.43
24	b	613	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
26	Y	101	BCR	C38-C26-C25	-3.72	120.35	124.53
24	A	405	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
24	c	907	CLA	C2C-C1C-NC	3.72	113.46	109.97
24	B	604	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
24	B	602	CLA	CHD-C4C-C3C	-3.72	119.38	124.84
24	C	509	CLA	C3D-C4D-ND	3.71	116.25	110.24
24	c	906	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
24	c	912	CLA	C2C-C1C-NC	3.71	113.45	109.97
24	b	619	CLA	C3D-C4D-ND	3.71	116.23	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	609	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
24	c	912	CLA	C3D-C4D-ND	3.70	116.23	110.24
29	A	414	PL9	C15-C14-C16	3.70	121.49	115.27
24	d	405	CLA	C2C-C1C-NC	3.70	113.44	109.97
24	B	603	CLA	CAA-C2A-C3A	-3.70	102.66	112.78
24	C	505	CLA	C3D-C2D-C1D	-3.70	100.79	105.83
24	b	606	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
24	B	604	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
24	d	404	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
24	b	613	CLA	C3D-C4D-ND	3.69	116.20	110.24
24	b	605	CLA	C2C-C1C-NC	3.68	113.42	109.97
24	b	618	CLA	C2C-C1C-NC	3.68	113.42	109.97
35	c	924	HTG	C1-O5-C5	3.68	119.36	112.58
26	t	903	BCR	C15-C16-C17	-3.68	115.94	123.47
24	B	609	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
24	C	507	CLA	C4A-NA-C1A	3.67	108.36	106.71
24	b	611	CLA	C2B-C1B-NB	3.67	112.69	110.23
27	a	415	SQD	C44-O6-C1	-3.67	106.57	113.74
24	A	407	CLA	C4-C3-C5	3.67	121.44	115.27
24	B	614	CLA	C3D-C4D-ND	3.67	116.17	110.24
24	D	402	CLA	C3B-C2B-C1B	-3.66	102.74	107.16
24	C	501	CLA	CBC-CAC-C3C	-3.66	102.34	112.43
24	b	620	CLA	C4C-C3C-C2C	-3.66	101.56	106.90
24	C	509	CLA	CHD-C1D-ND	-3.66	121.09	124.45
24	c	913	CLA	C2C-C1C-NC	3.66	113.40	109.97
24	d	401	CLA	CAA-C2A-C3A	-3.65	102.77	112.78
24	c	906	CLA	C1-O2A-CGA	3.65	126.03	116.44
24	B	616	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
24	b	614	CLA	CMA-C3A-C4A	-3.65	101.97	111.77
24	b	607	CLA	C3D-C2D-C1D	-3.64	100.86	105.83
24	D	402	CLA	C3C-C4C-NC	3.64	114.65	110.57
24	C	510	CLA	CHD-C1D-ND	-3.64	121.11	124.45
24	B	608	CLA	CBC-CAC-C3C	-3.64	102.40	112.43
24	b	609	CLA	O2D-CGD-O1D	-3.64	116.73	123.84
24	b	617	CLA	CHD-C1D-ND	-3.64	121.11	124.45
24	c	907	CLA	CBC-CAC-C3C	-3.63	102.41	112.43
24	b	610	CLA	C4-C3-C5	3.63	121.38	115.27
29	A	414	PL9	C27-C28-C29	-3.63	118.92	127.66
24	c	906	CLA	C3C-C4C-NC	3.63	114.64	110.57
37	d	408	LHG	O8-C23-C24	3.63	123.30	111.91
24	C	508	CLA	CHD-C1D-ND	-3.63	121.12	124.45
24	B	603	CLA	CHD-C4C-C3C	-3.62	119.51	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	F	101	SQD	O7-S-C6	3.62	111.25	106.94
24	c	912	CLA	O2D-CGD-CBD	3.62	117.71	111.27
24	B	605	CLA	C3C-C4C-NC	3.62	114.63	110.57
24	b	615	CLA	C3D-C4D-ND	3.62	116.10	110.24
24	C	513	CLA	CHD-C1D-ND	-3.62	121.13	124.45
24	B	612	CLA	C3D-C4D-ND	3.62	116.09	110.24
24	A	405	CLA	CHD-C4C-C3C	-3.61	119.53	124.84
24	B	608	CLA	C3D-C4D-ND	3.61	116.08	110.24
24	a	410	CLA	C3B-C2B-C1B	-3.61	102.80	107.16
24	D	402	CLA	CMC-C2C-C1C	3.61	130.54	125.04
24	C	504	CLA	C3B-C2B-C1B	-3.61	102.81	107.16
24	d	405	CLA	CHD-C4C-C3C	-3.60	119.55	124.84
24	C	501	CLA	C3B-C2B-C1B	-3.60	102.81	107.16
24	d	401	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
24	b	614	CLA	CHD-C4C-C3C	-3.60	119.55	124.84
24	c	910	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
26	b	621	BCR	C7-C8-C9	-3.59	120.81	126.23
24	c	907	CLA	C3B-C2B-C1B	-3.59	102.83	107.16
24	B	615	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
24	c	913	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
24	B	604	CLA	C2C-C1C-NC	3.58	113.33	109.97
24	b	620	CLA	C3D-C4D-ND	3.58	116.03	110.24
24	b	617	CLA	C3B-C2B-C1B	-3.58	102.84	107.16
34	b	625	LMT	C1'-O5'-C5'	3.58	120.71	113.69
24	c	904	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
24	c	909	CLA	C2C-C1C-NC	3.57	113.32	109.97
24	c	906	CLA	C3D-C4D-ND	3.57	116.02	110.24
24	a	409	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
24	b	611	CLA	CBC-CAC-C3C	-3.57	102.58	112.43
24	c	905	CLA	CBC-CAC-C3C	-3.57	102.58	112.43
24	B	613	CLA	C2C-C1C-NC	3.57	113.32	109.97
24	C	510	CLA	CHD-C4C-C3C	-3.57	119.59	124.84
24	B	608	CLA	C3B-C2B-C1B	-3.57	102.86	107.16
27	F	101	SQD	O9-S-C6	3.57	111.18	106.94
24	b	611	CLA	CHD-C1D-ND	-3.56	121.18	124.45
24	B	606	CLA	C1D-CHD-C4C	-3.56	118.39	126.06
24	b	609	CLA	CMB-C2B-C1B	3.56	130.78	125.37
24	d	401	CLA	CMA-C3A-C2A	-3.56	99.49	113.83
24	c	913	CLA	C1-O2A-CGA	3.55	125.77	116.44
24	b	614	CLA	O2D-CGD-CBD	3.55	117.58	111.27
24	c	903	CLA	CHD-C1D-ND	-3.55	121.19	124.45
24	b	616	CLA	C4C-C3C-C2C	-3.54	101.73	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	d	410	LHG	O7-C7-C8	3.54	119.13	111.50
24	c	903	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
25	a	412	PHO	CMB-C2B-C3B	3.54	131.30	124.68
24	c	910	CLA	C2C-C1C-NC	3.54	113.29	109.97
34	m	1503	LMT	C1'-O5'-C5'	3.54	120.63	113.69
24	B	609	CLA	CHD-C4C-C3C	-3.54	119.64	124.84
24	d	404	CLA	C3B-C2B-C1B	-3.54	102.89	107.16
28	a	416	LMG	C7-O1-C1	-3.53	106.84	113.74
24	C	503	CLA	CHD-C1D-ND	-3.53	121.21	124.45
24	b	606	CLA	CAA-C2A-C3A	-3.53	103.11	112.78
24	C	506	CLA	C1-C2-C3	-3.53	119.94	126.04
24	B	603	CLA	C3C-C4C-NC	3.53	114.53	110.57
24	b	620	CLA	C3C-C4C-NC	3.53	114.53	110.57
24	C	511	CLA	C1D-CHD-C4C	-3.53	118.45	126.06
24	b	618	CLA	O2A-CGA-O1A	-3.53	114.69	123.59
24	C	511	CLA	C3D-C4D-ND	3.52	115.94	110.24
24	a	409	CLA	CAC-C3C-C4C	3.52	129.38	124.81
29	D	405	PL9	C7-C8-C9	-3.52	120.93	126.79
24	B	614	CLA	C3C-C4C-NC	3.52	114.52	110.57
35	O	303	HTG	C1'-S1-C1	3.52	106.67	100.09
24	a	410	CLA	CMC-C2C-C1C	3.52	130.40	125.04
24	B	605	CLA	C3B-C4B-NB	3.51	113.78	110.52
24	c	914	CLA	C2C-C1C-NC	3.51	113.26	109.97
26	K	101	BCR	C20-C21-C22	-3.51	122.30	127.31
24	C	503	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
24	C	513	CLA	CHD-C4C-C3C	-3.51	119.68	124.84
24	B	613	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
24	B	609	CLA	CMA-C3A-C4A	-3.51	102.34	111.77
24	b	610	CLA	C2C-C1C-NC	3.51	113.26	109.97
24	D	402	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
24	a	410	CLA	C2C-C1C-NC	3.51	113.26	109.97
24	b	620	CLA	C2C-C1C-NC	3.51	113.26	109.97
24	A	407	CLA	C3B-C4B-NB	3.51	113.77	110.52
24	b	615	CLA	C3C-C4C-NC	3.50	114.50	110.57
24	C	511	CLA	O2D-CGD-CBD	3.50	117.49	111.27
35	o	301	HTG	C1'-S1-C1	3.50	106.64	100.09
24	c	912	CLA	C1-O2A-CGA	3.50	125.62	116.44
24	A	410	CLA	CMA-C3A-C4A	-3.50	102.38	111.77
24	c	908	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
24	B	616	CLA	CHD-C1D-ND	-3.49	121.25	124.45
24	C	502	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
24	c	912	CLA	C4-C3-C5	3.49	121.14	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	508	CLA	C2C-C1C-NC	3.49	113.24	109.97
24	C	505	CLA	C4C-C3C-C2C	-3.49	101.82	106.90
24	b	609	CLA	C2C-C1C-NC	3.48	113.24	109.97
24	C	505	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
24	C	509	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
24	B	611	CLA	C4C-C3C-C2C	-3.48	101.83	106.90
24	C	505	CLA	C3D-C4D-ND	3.48	115.86	110.24
24	B	606	CLA	CHD-C1D-ND	-3.48	121.26	124.45
24	b	608	CLA	C4A-NA-C1A	3.48	108.27	106.71
27	B	621	SQD	O5-C1-C2	3.47	117.70	110.35
25	A	409	PHO	O2D-CGD-O1D	-3.47	117.05	123.84
24	B	617	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
24	c	907	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
24	b	615	CLA	C2C-C1C-NC	3.47	113.22	109.97
24	c	909	CLA	C1D-CHD-C4C	-3.47	118.58	126.06
24	C	506	CLA	CHD-C1D-ND	-3.47	121.27	124.45
24	B	607	CLA	C1D-CHD-C4C	-3.47	118.58	126.06
27	A	412	SQD	C45-O47-C7	-3.47	109.26	117.79
24	B	617	CLA	CHD-C1D-ND	-3.46	121.27	124.45
24	B	612	CLA	C1D-CHD-C4C	-3.46	118.59	126.06
24	A	407	CLA	C1D-CHD-C4C	-3.46	118.59	126.06
36	C	518	DGD	O2G-C1B-C2B	3.46	118.96	111.50
24	C	512	CLA	C1D-CHD-C4C	-3.46	118.60	126.06
24	B	606	CLA	C2C-C1C-NC	3.46	113.21	109.97
24	b	606	CLA	CHD-C4C-C3C	-3.46	119.76	124.84
24	C	510	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
24	c	907	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
26	C	514	BCR	C7-C8-C9	-3.45	121.02	126.23
24	c	907	CLA	O2D-CGD-CBD	3.45	117.39	111.27
24	b	618	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
24	b	617	CLA	C3B-C4B-NB	3.45	113.71	110.52
24	B	617	CLA	C4C-C3C-C2C	-3.45	101.88	106.90
24	c	907	CLA	CAA-C2A-C3A	-3.44	103.35	112.78
24	C	502	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
24	b	613	CLA	C1-C2-C3	-3.44	120.09	126.04
24	c	904	CLA	C2C-C1C-NC	3.44	113.19	109.97
24	c	908	CLA	CMB-C2B-C1B	3.43	130.60	125.37
24	B	616	CLA	C2C-C1C-NC	3.43	113.19	109.97
24	B	613	CLA	CMC-C2C-C1C	3.43	130.26	125.04
27	A	417	SQD	O47-C7-C8	3.43	118.89	111.50
24	C	511	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
39	H	102	RRX	C16-C17-C18	-3.43	122.42	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	CLA	C4C-C3C-C2C	-3.43	101.90	106.90
24	B	611	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
24	b	620	CLA	CAC-C3C-C4C	3.43	129.25	124.81
24	B	603	CLA	C1D-CHD-C4C	-3.42	118.67	126.06
27	b	601	SQD	O48-C23-C24	3.42	122.64	111.91
27	a	415	SQD	C45-O47-C7	-3.42	109.38	117.79
24	c	905	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
24	B	610	CLA	CHD-C1D-ND	-3.42	121.31	124.45
24	B	613	CLA	C3B-C4B-NB	3.41	113.68	110.52
24	C	511	CLA	C4A-NA-C1A	3.41	108.24	106.71
24	B	612	CLA	CMC-C2C-C1C	3.41	130.24	125.04
24	C	501	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
24	b	616	CLA	C2C-C1C-NC	3.41	113.17	109.97
24	B	617	CLA	C1-O2A-CGA	3.41	125.39	116.44
24	B	605	CLA	CHD-C4C-C3C	-3.41	119.83	124.84
24	c	903	CLA	C2C-C1C-NC	3.41	113.17	109.97
24	b	619	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
26	y	101	BCR	C15-C14-C13	-3.41	122.45	127.31
24	C	506	CLA	CHD-C4C-C3C	-3.41	119.83	124.84
24	A	405	CLA	C3C-C4C-NC	3.40	114.39	110.57
24	b	611	CLA	C3B-C4B-NB	3.40	113.67	110.52
24	a	413	CLA	CBC-CAC-C3C	-3.40	103.05	112.43
24	b	619	CLA	C2C-C1C-NC	3.40	113.16	109.97
24	c	903	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
24	c	908	CLA	C3D-C4D-ND	3.40	115.74	110.24
24	a	413	CLA	CHD-C1D-ND	-3.40	121.33	124.45
36	e	102	DGD	O3G-C3G-C2G	-3.39	102.72	110.90
24	b	620	CLA	C3B-C4B-NB	3.39	113.66	110.52
24	C	505	CLA	CHD-C4C-C3C	-3.39	119.86	124.84
24	B	604	CLA	CAA-C2A-C3A	-3.39	103.50	112.78
29	a	417	PL9	C15-C14-C16	3.39	120.97	115.27
24	B	613	CLA	C4C-C3C-C2C	-3.39	101.96	106.90
24	c	909	CLA	C3C-C4C-NC	3.39	114.37	110.57
24	b	617	CLA	C1C-C2C-C3C	-3.39	103.40	106.96
24	B	611	CLA	C3D-C4D-ND	3.39	115.71	110.24
24	B	607	CLA	C3C-C4C-NC	3.38	114.36	110.57
24	b	616	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
24	c	910	CLA	C1-C2-C3	-3.38	120.20	126.04
35	v	205	HTG	C4-C3-C2	-3.38	104.93	110.82
39	H	102	RRX	C24-C23-C22	-3.37	121.14	126.23
37	e	101	LHG	O7-C7-C8	3.37	118.77	111.50
29	A	414	PL9	C22-C23-C24	-3.37	119.54	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	413	CLA	C3B-C4B-NB	3.37	113.64	110.52
24	C	512	CLA	C3C-C4C-NC	3.37	114.35	110.57
24	b	609	CLA	C3C-C4C-NC	3.37	114.35	110.57
24	b	616	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
24	C	512	CLA	C2C-C1C-NC	3.37	113.13	109.97
24	B	603	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
24	B	616	CLA	C3D-C4D-ND	3.36	115.68	110.24
24	b	613	CLA	CBC-CAC-C3C	-3.36	103.16	112.43
24	b	611	CLA	C4-C3-C5	3.36	120.93	115.27
24	d	401	CLA	O2D-CGD-CBD	3.36	117.24	111.27
24	b	614	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
24	B	610	CLA	C3C-C4C-NC	3.36	114.34	110.57
24	b	614	CLA	CAC-C3C-C4C	3.36	129.17	124.81
24	b	611	CLA	C3B-C2B-C1B	-3.36	103.11	107.16
28	b	624	LMG	O8-C28-C29	3.36	122.45	111.91
24	C	511	CLA	CHD-C1D-ND	-3.36	121.37	124.45
24	a	409	CLA	CAA-C2A-C3A	-3.36	103.59	112.78
24	c	909	CLA	C1C-C2C-C3C	-3.36	103.43	106.96
24	C	505	CLA	C1D-CHD-C4C	-3.35	118.82	126.06
24	B	608	CLA	CHD-C4C-C3C	-3.35	119.91	124.84
24	C	511	CLA	C3C-C4C-NC	3.35	114.33	110.57
24	C	506	CLA	C1D-CHD-C4C	-3.35	118.84	126.06
24	C	508	CLA	CHD-C4C-C3C	-3.35	119.92	124.84
26	B	620	BCR	C38-C26-C25	-3.34	120.78	124.53
24	b	619	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
24	c	914	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
24	B	606	CLA	C3C-C4C-NC	3.34	114.31	110.57
24	a	413	CLA	C3C-C4C-NC	3.33	114.31	110.57
24	b	608	CLA	CAC-C3C-C4C	3.33	129.13	124.81
24	B	604	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
24	B	616	CLA	CAC-C3C-C4C	3.33	129.13	124.81
24	a	410	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
26	B	620	BCR	C24-C23-C22	-3.33	121.20	126.23
24	B	612	CLA	C3C-C4C-NC	3.33	114.30	110.57
27	A	412	SQD	C1-O5-C5	-3.32	107.16	113.69
24	C	508	CLA	C1C-C2C-C3C	-3.32	103.46	106.96
24	C	503	CLA	C3D-C4D-ND	3.32	115.61	110.24
25	A	409	PHO	CMA-C3A-C4A	-3.32	107.10	114.38
24	B	612	CLA	C2C-C1C-NC	3.32	113.08	109.97
24	B	615	CLA	O2A-CGA-O1A	-3.32	115.21	123.59
24	c	904	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
24	c	904	CLA	CMB-C2B-C1B	3.32	130.42	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	C3C-C4C-NC	3.32	114.29	110.57
24	c	910	CLA	C4A-NA-C1A	3.32	108.20	106.71
26	A	411	BCR	C20-C21-C22	-3.31	122.58	127.31
24	b	605	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
24	c	914	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
24	A	407	CLA	CBC-CAC-C3C	-3.31	103.31	112.43
29	a	417	PL9	C10-C9-C11	3.31	120.84	115.27
24	B	608	CLA	CAA-C2A-C3A	-3.31	103.72	112.78
25	A	409	PHO	C4D-CHA-CBD	3.31	110.01	108.52
36	D	406	DGD	C4D-C3D-C2D	3.30	116.59	110.82
24	b	611	CLA	C3C-C4C-NC	3.30	114.28	110.57
24	c	910	CLA	CHD-C1D-ND	-3.30	121.42	124.45
24	b	620	CLA	O2A-CGA-CBA	3.30	122.26	111.91
24	b	606	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
24	c	906	CLA	C1D-CHD-C4C	-3.30	118.94	126.06
24	d	405	CLA	C4-C3-C5	3.30	120.82	115.27
24	b	610	CLA	C3C-C4C-NC	3.30	114.27	110.57
24	C	507	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
34	B	623	LMT	O1'-C1'-C2'	3.29	113.44	108.30
24	a	413	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
24	b	614	CLA	C1D-CHD-C4C	-3.29	118.96	126.06
24	D	403	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
24	c	904	CLA	C4A-NA-C1A	3.29	108.19	106.71
24	c	910	CLA	C1D-CHD-C4C	-3.29	118.97	126.06
24	B	602	CLA	C1D-CHD-C4C	-3.28	118.97	126.06
24	b	606	CLA	C1D-CHD-C4C	-3.28	118.98	126.06
24	C	504	CLA	C1D-CHD-C4C	-3.28	118.98	126.06
36	h	102	DGD	O2G-C1B-C2B	3.28	118.56	111.50
24	b	613	CLA	CHD-C4C-C3C	-3.28	120.02	124.84
24	b	612	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
24	c	911	CLA	CMA-C3A-C4A	-3.27	102.97	111.77
24	c	912	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
24	c	914	CLA	C1-C2-C3	-3.27	120.39	126.04
24	C	509	CLA	CHD-C4C-C3C	-3.27	120.03	124.84
24	b	605	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
24	C	508	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
24	b	614	CLA	O2A-CGA-CBA	3.27	122.16	111.91
25	a	412	PHO	C4D-CHA-CBD	3.27	109.99	108.52
24	b	615	CLA	CBC-CAC-C3C	-3.26	103.43	112.43
24	C	504	CLA	C4-C3-C5	3.26	120.76	115.27
24	c	914	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
24	C	509	CLA	C1-C2-C3	-3.26	120.41	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	O2D-CGD-O1D	-3.25	117.47	123.84
35	C	528	HTG	O5-C5-C4	3.25	115.60	109.69
24	c	909	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
25	a	412	PHO	C4-C3-C5	3.25	120.73	115.27
24	b	616	CLA	C4-C3-C5	3.25	120.73	115.27
24	B	609	CLA	C1D-CHD-C4C	-3.24	119.06	126.06
24	B	603	CLA	CHD-C1D-ND	-3.24	121.47	124.45
24	c	914	CLA	CAC-C3C-C4C	3.24	129.02	124.81
24	B	606	CLA	CMB-C2B-C1B	3.24	130.31	125.37
34	C	520	LMT	C2'-C3'-C4'	-3.24	102.28	109.68
24	b	610	CLA	C1D-CHD-C4C	-3.24	119.07	126.06
26	c	916	BCR	C38-C26-C25	-3.24	120.89	124.53
24	D	402	CLA	O2A-CGA-CBA	3.23	122.06	111.91
24	B	606	CLA	C4-C3-C5	3.23	120.71	115.27
24	B	607	CLA	C3D-C4D-ND	3.23	115.47	110.24
24	b	620	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
24	C	503	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
24	C	512	CLA	CBC-CAC-C3C	-3.23	103.53	112.43
28	C	534	LMG	C3-C4-C5	3.23	116.00	110.24
24	C	502	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
24	c	903	CLA	O2A-CGA-CBA	3.23	122.03	111.91
28	c	920	LMG	O8-C28-C29	3.22	122.03	111.91
24	B	617	CLA	C3B-C4B-NB	3.22	113.51	110.52
24	D	402	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
24	B	611	CLA	O2A-CGA-CBA	3.22	122.02	111.91
24	c	906	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
24	b	617	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
24	C	506	CLA	CBC-CAC-C3C	-3.22	103.55	112.43
24	A	407	CLA	C1-C2-C3	-3.22	120.47	126.04
24	C	507	CLA	CMB-C2B-C1B	3.22	130.27	125.37
24	b	607	CLA	O2A-CGA-O1A	-3.22	115.47	123.59
24	a	410	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
26	C	514	BCR	C15-C14-C13	-3.22	122.72	127.31
24	C	504	CLA	CBC-CAC-C3C	-3.22	103.56	112.43
26	D	404	BCR	C33-C5-C6	-3.22	120.92	124.53
24	B	611	CLA	CMB-C2B-C1B	3.22	130.27	125.37
24	b	610	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
24	a	409	CLA	CAA-C2A-C1A	-3.21	101.44	111.97
24	b	612	CLA	C4C-C3C-C2C	-3.21	102.21	106.90
24	d	404	CLA	C1D-CHD-C4C	-3.21	119.12	126.06
24	C	501	CLA	CMC-C2C-C1C	3.21	129.93	125.04
27	a	401	SQD	O48-C23-C24	3.21	121.99	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	615	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
24	B	614	CLA	C3B-C4B-NB	3.21	113.49	110.52
24	B	603	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
24	C	513	CLA	C1-C2-C3	-3.21	120.49	126.04
24	a	409	CLA	CHD-C4C-C3C	-3.21	120.12	124.84
24	C	511	CLA	C4-C3-C5	3.21	120.67	115.27
38	V	202	HEM	C1B-NB-C4B	3.21	108.39	105.07
24	c	904	CLA	C4-C3-C5	3.21	120.66	115.27
24	A	407	CLA	CAA-C2A-C3A	-3.21	104.00	112.78
24	c	910	CLA	CHD-C4C-C3C	-3.20	120.14	124.84
24	b	616	CLA	C3B-C4B-NB	3.20	113.48	110.52
24	c	904	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
24	B	610	CLA	C1D-CHD-C4C	-3.19	119.17	126.06
24	C	510	CLA	C3C-C4C-NC	3.19	114.15	110.57
24	B	609	CLA	C3C-C4C-NC	3.19	114.15	110.57
24	b	605	CLA	C4-C3-C5	3.19	120.63	115.27
24	C	507	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
24	a	410	CLA	CMB-C2B-C1B	3.18	130.22	125.37
24	b	612	CLA	O2A-CGA-CBA	3.18	121.89	111.91
26	C	515	BCR	C38-C26-C25	-3.18	120.95	124.53
24	B	611	CLA	C1D-CHD-C4C	-3.18	119.19	126.06
24	b	619	CLA	C3C-C4C-NC	3.18	114.14	110.57
24	c	914	CLA	CHD-C1D-ND	-3.18	121.53	124.45
24	B	605	CLA	O2A-CGA-O1A	-3.18	115.57	123.59
24	c	908	CLA	C4A-NA-C1A	3.17	108.13	106.71
24	c	910	CLA	C3D-C4D-ND	3.17	115.37	110.24
24	c	902	CLA	CMB-C2B-C1B	3.17	130.19	125.37
24	b	613	CLA	CHC-C4B-NB	3.17	127.61	124.26
24	B	617	CLA	CBC-CAC-C3C	-3.16	103.71	112.43
24	b	617	CLA	O2D-CGD-CBD	3.16	116.89	111.27
29	d	407	PL9	C40-C39-C41	3.16	120.59	115.27
24	b	618	CLA	CHD-C1D-ND	-3.16	121.55	124.45
27	a	415	SQD	O9-S-C6	3.16	110.69	106.94
29	a	417	PL9	C37-C38-C39	-3.16	120.06	127.66
39	h	101	RRX	C11-C10-C9	-3.15	122.81	127.31
24	b	608	CLA	C3C-C4C-NC	3.15	114.10	110.57
24	c	908	CLA	C3C-C4C-NC	3.15	114.10	110.57
26	C	514	BCR	C38-C26-C25	-3.15	120.99	124.53
29	a	417	PL9	C20-C19-C21	3.15	120.57	115.27
24	b	614	CLA	C3C-C4C-NC	3.14	114.09	110.57
27	A	412	SQD	O9-S-C6	3.14	110.67	106.94
26	A	411	BCR	C15-C14-C13	-3.14	122.83	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	CLA	C3B-C4B-NB	3.14	113.43	110.52
28	c	921	LMG	O6-C5-C4	3.14	115.39	109.69
26	b	623	BCR	C38-C26-C25	-3.14	121.00	124.53
26	k	101	BCR	C33-C5-C6	-3.14	121.01	124.53
29	A	414	PL9	C42-C43-C44	-3.14	120.11	127.66
24	B	610	CLA	CMB-C2B-C1B	3.14	130.15	125.37
28	a	416	LMG	C8-O7-C10	-3.13	110.07	117.79
24	C	513	CLA	CAC-C3C-C4C	3.13	128.88	124.81
39	H	102	RRX	C10-C11-C12	-3.13	113.44	123.22
24	a	413	CLA	CMB-C2B-C1B	3.13	130.14	125.37
24	b	614	CLA	CAA-C2A-C3A	-3.13	104.20	112.78
24	A	410	CLA	CBC-CAC-C3C	-3.13	103.80	112.43
24	B	616	CLA	CHA-C1A-NA	-3.13	119.24	126.40
24	C	507	CLA	C3C-C4C-NC	3.13	114.08	110.57
24	b	612	CLA	C3C-C4C-NC	3.13	114.08	110.57
36	h	102	DGD	O1G-C1A-O1A	-3.13	115.70	123.59
24	a	413	CLA	C1D-CHD-C4C	-3.13	119.31	126.06
24	b	608	CLA	CMC-C2C-C1C	3.12	129.79	125.04
24	c	911	CLA	C1D-CHD-C4C	-3.12	119.33	126.06
24	A	405	CLA	C3B-C4B-NB	3.12	113.41	110.52
24	D	402	CLA	C1-C2-C3	-3.12	120.65	126.04
24	c	905	CLA	C3B-C4B-NB	3.12	113.41	110.52
24	B	604	CLA	CMC-C2C-C1C	3.12	129.79	125.04
24	B	603	CLA	CMA-C3A-C4A	-3.12	103.39	111.77
24	b	607	CLA	CBC-CAC-C3C	-3.12	103.84	112.43
24	c	912	CLA	CBC-CAC-C3C	-3.11	103.84	112.43
27	a	415	SQD	O8-S-C6	3.11	110.70	105.74
29	D	405	PL9	C25-C24-C26	3.11	120.51	115.27
36	C	518	DGD	O1G-C1A-C2A	3.11	121.68	111.91
24	B	603	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
39	H	102	RRX	C7-C8-C9	-3.11	121.53	126.23
24	c	902	CLA	C1D-CHD-C4C	-3.11	119.35	126.06
39	H	102	RRX	C38-C26-C25	-3.11	121.03	124.53
24	c	913	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
36	C	516	DGD	O3G-C3G-C2G	-3.11	103.40	110.90
26	y	101	BCR	C24-C23-C22	-3.11	121.54	126.23
24	B	613	CLA	CAC-C3C-C4C	3.11	128.84	124.81
24	c	908	CLA	C1D-CHD-C4C	-3.11	119.36	126.06
24	b	614	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
24	b	612	CLA	C2C-C1C-NC	3.11	112.88	109.97
29	d	407	PL9	C42-C43-C44	-3.10	120.19	127.66
24	B	607	CLA	CMC-C2C-C1C	3.10	129.76	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	905	CLA	CMC-C2C-C1C	3.10	129.76	125.04
24	B	605	CLA	CMB-C2B-C1B	3.10	130.09	125.37
24	D	403	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
24	B	616	CLA	CMC-C2C-C1C	3.10	129.75	125.04
24	C	505	CLA	CHA-C1A-NA	-3.10	119.31	126.40
24	c	913	CLA	CMB-C2B-C1B	3.10	130.08	125.37
24	c	904	CLA	C3C-C4C-NC	3.09	114.04	110.57
24	a	409	CLA	C3B-C4B-NB	3.09	113.39	110.52
29	A	414	PL9	C53-C6-C1	3.09	121.31	114.99
24	B	617	CLA	CMB-C2B-C1B	3.09	130.07	125.37
24	b	607	CLA	C4-C3-C5	3.09	120.47	115.27
24	B	610	CLA	CBC-CAC-C3C	-3.09	103.92	112.43
24	D	402	CLA	C4A-NA-C1A	-3.09	105.32	106.71
24	D	403	CLA	C4-C3-C5	3.09	120.46	115.27
24	b	614	CLA	CAA-CBA-CGA	-3.08	104.25	113.25
28	B	622	LMG	O8-C28-C29	3.08	121.58	111.91
24	c	906	CLA	CMB-C2B-C1B	3.08	130.06	125.37
24	C	506	CLA	O2A-CGA-CBA	3.08	121.57	111.91
24	c	909	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
24	B	607	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
24	C	508	CLA	C3C-C4C-NC	3.08	114.02	110.57
24	C	503	CLA	C2C-C1C-NC	3.07	112.85	109.97
24	d	404	CLA	O2A-CGA-CBA	3.07	121.55	111.91
24	c	914	CLA	CMC-C2C-C1C	3.07	129.72	125.04
24	A	405	CLA	CMA-C3A-C4A	-3.07	103.52	111.77
24	C	513	CLA	C4-C3-C5	3.07	120.44	115.27
24	b	619	CLA	O2D-CGD-CBD	3.07	116.73	111.27
24	C	508	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
24	D	403	CLA	C3C-C4C-NC	3.07	114.01	110.57
24	B	616	CLA	C4-C3-C5	3.07	120.44	115.27
24	b	613	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
24	c	911	CLA	C4-C3-C5	3.07	120.43	115.27
27	B	621	SQD	O48-C23-C24	3.06	121.52	111.91
24	a	410	CLA	CAA-C2A-C3A	-3.06	104.39	112.78
24	c	903	CLA	C3C-C4C-NC	3.06	114.01	110.57
24	b	608	CLA	C3D-C4D-ND	3.06	115.19	110.24
24	D	402	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
24	A	406	CLA	C1D-CHD-C4C	-3.06	119.46	126.06
24	b	612	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
24	D	402	CLA	C3B-C4B-NB	3.06	113.35	110.52
24	b	608	CLA	C3B-C4B-NB	3.06	113.35	110.52
24	b	608	CLA	C1D-CHD-C4C	-3.05	119.47	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
27	F	101	SQD	O48-C23-C24	3.05	121.48	111.91
24	A	406	CLA	CMA-C3A-C4A	-3.05	103.58	111.77
24	B	613	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
24	c	906	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
24	c	911	CLA	C3C-C4C-NC	3.05	113.99	110.57
24	D	403	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
37	D	409	LHG	O8-C23-O10	-3.04	115.91	123.59
24	B	612	CLA	C1-C2-C3	-3.04	120.78	126.04
24	b	615	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
39	h	101	RRX	C16-C17-C18	-3.04	122.97	127.31
24	b	605	CLA	C3C-C4C-NC	3.04	113.98	110.57
24	c	909	CLA	C1-C2-C3	-3.04	120.78	126.04
24	c	910	CLA	C3B-C4B-NB	3.04	113.34	110.52
24	c	902	CLA	C3C-C4C-NC	3.04	113.98	110.57
34	C	520	LMT	C1'-O5'-C5'	3.04	119.66	113.69
24	B	611	CLA	CMA-C3A-C4A	-3.04	103.61	111.77
24	C	510	CLA	C4-C3-C5	3.04	120.38	115.27
24	B	611	CLA	CAA-CBA-CGA	-3.04	104.38	113.25
24	b	606	CLA	CHD-C1D-ND	-3.03	121.67	124.45
24	b	610	CLA	CBC-CAC-C3C	-3.03	104.07	112.43
24	b	618	CLA	C3C-C4C-NC	3.03	113.97	110.57
29	A	414	PL9	C10-C9-C11	3.03	120.37	115.27
24	B	604	CLA	CHD-C1D-ND	-3.03	121.67	124.45
24	C	510	CLA	C1-C2-C3	-3.03	120.81	126.04
28	C	519	LMG	C8-O7-C10	-3.03	110.34	117.79
26	t	903	BCR	C11-C10-C9	-3.02	122.99	127.31
24	B	614	CLA	C1D-CHD-C4C	-3.02	119.53	126.06
24	a	413	CLA	C1-C2-C3	-3.02	120.82	126.04
24	d	405	CLA	C1D-CHD-C4C	-3.02	119.54	126.06
24	C	513	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
24	B	612	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
38	F	102	HEM	C4A-NA-C1A	3.02	108.30	105.35
24	b	612	CLA	CHD-C4C-C3C	-3.02	120.41	124.84
24	B	606	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
24	c	913	CLA	C3C-C4C-NC	3.02	113.95	110.57
38	V	202	HEM	CBD-CAD-C3D	-3.01	104.26	112.63
24	c	911	CLA	C3B-C4B-NB	3.01	113.31	110.52
24	B	608	CLA	C3B-C4B-NB	3.00	113.30	110.52
24	b	619	CLA	CMC-C2C-C1C	3.00	129.61	125.04
24	a	410	CLA	CBC-CAC-C3C	-3.00	104.15	112.43
24	d	404	CLA	CHD-C1D-ND	-3.00	121.69	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	CMB-C2B-C1B	3.00	129.94	125.37
24	B	602	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
24	b	613	CLA	O2D-CGD-CBD	3.00	116.60	111.27
37	D	409	LHG	O7-C7-C8	3.00	117.96	111.50
24	a	409	CLA	CMA-C3A-C4A	-3.00	103.72	111.77
26	y	101	BCR	C38-C26-C25	-2.99	121.17	124.53
39	h	101	RRX	C7-C8-C9	-2.99	121.71	126.23
24	C	511	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
24	b	616	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
24	C	501	CLA	C3C-C4C-NC	2.99	113.93	110.57
24	B	610	CLA	O2D-CGD-CBD	2.99	116.58	111.27
24	b	610	CLA	O2A-CGA-O1A	-2.98	116.06	123.59
25	a	411	PHO	CMB-C2B-C3B	2.98	130.26	124.68
24	d	405	CLA	CMC-C2C-C1C	2.98	129.58	125.04
25	A	409	PHO	C4-C3-C5	2.98	120.29	115.27
24	A	406	CLA	C3B-C4B-NB	2.98	113.28	110.52
27	A	412	SQD	C44-O6-C1	-2.98	107.92	113.74
24	b	607	CLA	CAA-C2A-C3A	-2.98	104.62	112.78
24	B	604	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
24	c	904	CLA	C3D-C4D-ND	2.98	115.06	110.24
35	B	627	HTG	C1-O5-C5	2.98	118.07	112.58
24	C	506	CLA	C3C-C4C-NC	2.97	113.91	110.57
24	b	616	CLA	CHD-C1D-ND	-2.97	121.72	124.45
24	B	605	CLA	C1-C2-C3	-2.97	120.91	126.04
24	C	504	CLA	CHD-C4C-C3C	-2.97	120.47	124.84
26	Y	101	BCR	C15-C14-C13	-2.97	123.07	127.31
35	v	205	HTG	C1-O5-C5	2.97	118.06	112.58
24	B	609	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
24	C	502	CLA	CHD-C1D-ND	-2.97	121.73	124.45
24	c	904	CLA	CHA-C1A-NA	-2.97	119.60	126.40
24	c	908	CLA	CBC-CAC-C3C	-2.97	104.25	112.43
24	B	617	CLA	C1C-C2C-C3C	-2.97	103.84	106.96
24	B	614	CLA	CED-O2D-CGD	2.97	122.64	115.94
24	A	410	CLA	C4-C3-C5	2.97	120.26	115.27
24	B	602	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
24	B	615	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
24	B	611	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
24	A	410	CLA	C3B-C4B-NB	2.96	113.26	110.52
24	b	608	CLA	CHD-C4C-C3C	-2.96	120.49	124.84
29	d	407	PL9	C53-C6-C1	2.96	121.04	114.99
24	b	606	CLA	C3C-C4C-NC	2.96	113.89	110.57
24	a	410	CLA	C4C-C3C-C2C	-2.95	102.59	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	609	CLA	C1D-CHD-C4C	-2.95	119.69	126.06
24	C	504	CLA	CMC-C2C-C1C	2.95	129.53	125.04
24	B	606	CLA	C1C-C2C-C3C	-2.95	103.85	106.96
24	b	615	CLA	CHD-C1D-ND	-2.95	121.75	124.45
38	v	202	HEM	C4C-NC-C1C	2.95	108.23	105.35
29	a	417	PL9	C30-C29-C31	2.94	120.22	115.27
24	b	616	CLA	O2A-CGA-CBA	2.94	121.15	111.91
24	C	504	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
26	K	101	BCR	C24-C23-C22	-2.94	121.79	126.23
24	b	613	CLA	C1D-CHD-C4C	-2.94	119.71	126.06
24	b	620	CLA	CBC-CAC-C3C	-2.94	104.32	112.43
24	b	617	CLA	C1D-CHD-C4C	-2.94	119.71	126.06
24	C	511	CLA	C1-O2A-CGA	2.94	124.16	116.44
37	d	408	LHG	O7-C7-C8	2.94	117.84	111.50
24	C	502	CLA	CMC-C2C-C1C	2.94	129.51	125.04
24	B	612	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
26	Y	101	BCR	C16-C17-C18	-2.94	123.12	127.31
24	A	406	CLA	CAA-C2A-C3A	-2.94	104.73	112.78
24	c	914	CLA	CHD-C4C-C3C	-2.94	120.52	124.84
24	A	405	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
24	b	619	CLA	CMB-C2B-C1B	2.93	129.84	125.37
27	f	102	SQD	O48-C23-C24	2.93	121.12	111.91
24	C	510	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
24	c	907	CLA	C3C-C4C-NC	2.93	113.86	110.57
24	b	618	CLA	O2A-CGA-CBA	2.93	121.10	111.91
24	B	602	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
26	k	101	BCR	C20-C21-C22	-2.93	123.13	127.31
24	C	513	CLA	CBC-CAC-C3C	-2.93	104.36	112.43
24	B	615	CLA	CBC-CAC-C3C	-2.93	104.37	112.43
38	f	101	HEM	CBD-CAD-C3D	-2.92	104.50	112.63
24	b	613	CLA	C4-C3-C5	2.92	120.19	115.27
24	A	405	CLA	CHD-C1D-ND	-2.92	121.77	124.45
24	B	613	CLA	C4-C3-C5	2.92	120.17	115.27
24	B	610	CLA	C3B-C4B-NB	2.91	113.22	110.52
24	c	904	CLA	C1-C2-C3	-2.91	121.00	126.04
24	c	907	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
24	B	608	CLA	C1D-CHD-C4C	-2.91	119.78	126.06
38	v	202	HEM	CBD-CAD-C3D	-2.91	104.54	112.63
24	C	512	CLA	C4-C3-C5	2.91	120.16	115.27
24	c	912	CLA	C4A-NA-C1A	2.91	108.01	106.71
24	B	602	CLA	C3C-C4C-NC	2.91	113.83	110.57
24	C	513	CLA	C4C-C3C-C2C	-2.91	102.66	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	617	CLA	CAC-C3C-C4C	2.90	128.58	124.81
24	c	910	CLA	CAC-C3C-C4C	2.90	128.58	124.81
24	d	404	CLA	C4-C3-C5	2.90	120.16	115.27
24	c	905	CLA	C3C-C4C-NC	2.90	113.83	110.57
24	C	512	CLA	CHD-C1D-ND	-2.90	121.79	124.45
24	b	618	CLA	CBC-CAC-C3C	-2.90	104.43	112.43
24	d	405	CLA	CBC-CAC-C3C	-2.90	104.43	112.43
24	c	909	CLA	CAA-C2A-C3A	-2.90	104.83	112.78
24	C	512	CLA	CBA-CAA-C2A	-2.90	105.30	113.86
24	C	511	CLA	CBC-CAC-C3C	-2.90	104.43	112.43
27	A	412	SQD	O48-C23-C24	2.90	121.01	111.91
38	f	101	HEM	C4C-NC-C1C	2.90	108.19	105.35
37	D	409	LHG	O8-C23-C24	2.90	121.01	111.91
24	B	615	CLA	O2A-CGA-CBA	2.90	121.00	111.91
24	C	513	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	a	411	PHO	O2D-CGD-O1D	-2.90	118.17	123.84
24	C	507	CLA	CHD-C1D-ND	-2.89	121.79	124.45
37	D	408	LHG	O8-C23-O10	-2.89	116.29	123.59
24	c	911	CLA	CBC-CAC-C3C	-2.89	104.45	112.43
24	b	615	CLA	C1-C2-C3	-2.89	121.04	126.04
24	B	611	CLA	CAA-C2A-C3A	-2.89	104.86	112.78
24	b	613	CLA	C3B-C4B-NB	2.89	113.20	110.52
24	c	903	CLA	O2A-CGA-O1A	-2.89	116.30	123.59
27	b	601	SQD	O5-C5-C4	2.89	114.94	109.69
24	b	615	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
24	B	615	CLA	C3C-C4C-NC	2.89	113.81	110.57
24	c	907	CLA	CHD-C4C-C3C	-2.89	120.59	124.84
24	A	406	CLA	C3C-C4C-NC	2.89	113.81	110.57
24	C	502	CLA	C2C-C1C-NC	2.89	112.67	109.97
24	C	509	CLA	CBC-CAC-C3C	-2.88	104.48	112.43
25	A	409	PHO	CMB-C2B-C3B	2.88	130.07	124.68
24	B	607	CLA	CBC-CAC-C3C	-2.88	104.48	112.43
24	c	908	CLA	C4-C3-C5	2.88	120.12	115.27
24	c	914	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
24	b	618	CLA	CMC-C2C-C1C	2.88	129.43	125.04
24	b	612	CLA	C1D-CHD-C4C	-2.88	119.84	126.06
24	A	407	CLA	O2A-CGA-O1A	-2.88	116.33	123.59
24	C	512	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
35	B	626	HTG	O5-C5-C4	2.87	114.92	109.69
24	A	405	CLA	O2D-CGD-CBD	2.87	116.38	111.27
24	C	510	CLA	C1D-CHD-C4C	-2.87	119.86	126.06
24	b	606	CLA	C4C-C3C-C2C	-2.87	102.71	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	CHD-C1D-ND	-2.87	121.82	124.45
24	C	509	CLA	C1D-CHD-C4C	-2.87	119.87	126.06
24	b	614	CLA	O2A-CGA-O1A	-2.87	116.35	123.59
36	h	102	DGD	O1G-C1A-C2A	2.87	120.91	111.91
24	b	612	CLA	C1-C2-C3	-2.86	121.09	126.04
24	C	507	CLA	CHC-C4B-NB	2.86	127.29	124.26
24	A	410	CLA	C1D-CHD-C4C	-2.86	119.89	126.06
24	A	407	CLA	C3C-C4C-NC	2.86	113.78	110.57
24	C	511	CLA	C3B-C4B-NB	2.86	113.17	110.52
24	C	502	CLA	C3C-C4C-NC	2.86	113.78	110.57
24	B	610	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
24	C	510	CLA	C1-O2A-CGA	2.86	123.94	116.44
24	C	507	CLA	C3D-C4D-ND	2.85	114.85	110.24
24	D	403	CLA	C1D-CHD-C4C	-2.85	119.90	126.06
24	b	611	CLA	CAA-C2A-C3A	-2.85	104.97	112.78
24	b	613	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
24	C	513	CLA	C1D-CHD-C4C	-2.85	119.91	126.06
24	b	610	CLA	CMC-C2C-C1C	2.85	129.38	125.04
24	b	609	CLA	CBC-CAC-C3C	-2.85	104.58	112.43
24	c	906	CLA	CHA-C1A-NA	-2.85	119.88	126.40
24	C	502	CLA	CMB-C2B-C1B	2.85	129.70	125.37
24	b	612	CLA	O2A-CGA-O1A	-2.84	116.41	123.59
24	B	604	CLA	C4-C3-C5	2.84	120.06	115.27
24	B	604	CLA	O2A-CGA-CBA	2.84	120.83	111.91
25	a	411	PHO	CMA-C3A-C4A	-2.84	108.15	114.38
24	C	512	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
24	C	513	CLA	CMC-C2C-C1C	2.84	129.37	125.04
24	D	403	CLA	CHB-C1B-NB	-2.84	121.25	124.26
24	c	908	CLA	CHC-C4B-NB	2.84	127.26	124.26
24	C	503	CLA	C3C-C4C-NC	2.84	113.75	110.57
24	a	409	CLA	C3C-C4C-NC	2.84	113.75	110.57
24	C	506	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
24	d	405	CLA	C3C-C4C-NC	2.83	113.75	110.57
24	c	907	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
26	A	411	BCR	C33-C5-C6	-2.83	121.35	124.53
24	a	413	CLA	C4-C3-C5	2.83	120.04	115.27
24	B	602	CLA	C2C-C1C-NC	2.83	112.62	109.97
24	c	912	CLA	C3C-C4C-NC	2.83	113.75	110.57
39	h	101	RRX	C10-C11-C12	-2.83	114.39	123.22
24	B	610	CLA	CED-O2D-CGD	2.83	122.34	115.94
24	B	617	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	b	615	CLA	CAC-C3C-C4C	2.83	128.48	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	912	CLA	CHC-C1C-C2C	-2.83	118.88	126.73
24	d	405	CLA	CAC-C3C-C4C	2.83	128.48	124.81
24	C	509	CLA	C3C-C4C-NC	2.82	113.74	110.57
27	a	415	SQD	O48-C23-C24	2.82	120.77	111.91
24	c	902	CLA	CMC-C2C-C1C	2.82	129.34	125.04
24	c	906	CLA	CAA-CBA-CGA	-2.82	105.00	113.25
24	B	606	CLA	O2A-CGA-O1A	-2.82	116.47	123.59
24	b	605	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
24	B	616	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
27	A	412	SQD	O8-S-C6	2.82	110.23	105.74
24	c	908	CLA	CMC-C2C-C1C	2.82	129.33	125.04
26	t	903	BCR	C1-C6-C7	2.82	123.75	115.78
27	b	601	SQD	C44-O6-C1	-2.82	108.23	113.74
24	D	403	CLA	C2C-C1C-NC	2.82	112.61	109.97
24	a	413	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
24	c	903	CLA	CMB-C2B-C1B	2.81	129.66	125.37
24	b	619	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
24	a	410	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
26	d	406	BCR	C15-C14-C13	-2.81	123.30	127.31
26	d	406	BCR	C16-C17-C18	-2.81	123.30	127.31
24	d	405	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
24	b	605	CLA	CBC-CAC-C3C	-2.81	104.69	112.43
24	d	405	CLA	O2A-CGA-CBA	2.81	120.72	111.91
24	C	506	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
37	D	407	LHG	O8-C23-C24	2.81	120.71	111.91
24	C	507	CLA	C1-C2-C3	-2.80	121.19	126.04
24	b	612	CLA	CAC-C3C-C4C	2.80	128.45	124.81
24	C	512	CLA	O2A-CGA-CBA	2.80	120.70	111.91
24	b	613	CLA	CHA-C1A-NA	-2.80	119.98	126.40
27	A	417	SQD	O8-S-C6	2.80	110.20	105.74
24	C	505	CLA	CAC-C3C-C4C	2.80	128.44	124.81
34	m	1503	LMT	O1'-C1'-C2'	2.80	112.67	108.30
24	B	613	CLA	C1D-CHD-C4C	-2.80	120.02	126.06
24	c	912	CLA	CHD-C4C-NC	2.79	128.61	124.20
24	b	607	CLA	C3C-C4C-NC	2.79	113.70	110.57
27	A	417	SQD	O9-S-C6	2.79	110.26	106.94
24	b	608	CLA	O2A-CGA-CBA	2.79	120.67	111.91
24	d	405	CLA	C1-C2-C3	-2.79	121.22	126.04
24	B	615	CLA	C3B-C4B-NB	2.79	113.10	110.52
24	A	406	CLA	CMA-C3A-C2A	-2.79	102.57	113.83
26	T	702	BCR	C16-C17-C18	-2.79	123.33	127.31
24	a	413	CLA	CAA-C2A-C3A	-2.79	105.15	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	907	CLA	O2A-CGA-O1A	-2.78	116.56	123.59
24	B	616	CLA	O2D-CGD-CBD	2.78	116.21	111.27
35	V	203	HTG	C1-O5-C5	-2.78	107.45	112.58
35	U	201	HTG	C1-S1-C1'	2.78	109.95	100.40
24	c	910	CLA	O2A-CGA-CBA	2.78	120.63	111.91
24	A	410	CLA	CMA-C3A-C2A	-2.78	102.61	113.83
26	K	101	BCR	C11-C10-C9	-2.78	123.34	127.31
24	b	608	CLA	O1D-CGD-CBD	-2.78	118.80	124.48
28	C	534	LMG	O8-C28-C29	2.78	120.63	111.91
37	L	101	LHG	O8-C23-O10	-2.78	116.58	123.59
36	e	102	DGD	C2G-O2G-C1B	-2.78	110.95	117.79
24	D	402	CLA	O2A-CGA-O1A	-2.78	116.58	123.59
36	H	103	DGD	O1G-C1A-O1A	-2.78	116.58	123.59
24	C	503	CLA	CMC-C2C-C1C	2.77	129.26	125.04
24	B	608	CLA	O2A-CGA-O1A	-2.77	116.59	123.59
24	b	608	CLA	CHA-C1A-NA	-2.77	120.05	126.40
24	a	409	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
24	C	503	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
24	b	609	CLA	CMC-C2C-C1C	2.77	129.26	125.04
24	a	413	CLA	CMA-C3A-C2A	-2.77	102.66	113.83
24	d	401	CLA	CHC-C1C-C2C	-2.77	119.05	126.73
24	a	409	CLA	O2A-CGA-CBA	2.77	120.59	111.91
24	b	609	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
24	B	602	CLA	O2A-CGA-CBA	2.76	120.58	111.91
26	D	404	BCR	C28-C27-C26	-2.76	109.14	114.08
35	B	625	HTG	C1-C2-C3	2.76	116.05	110.59
24	C	507	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
24	B	606	CLA	CMC-C2C-C1C	2.76	129.25	125.04
24	d	401	CLA	C1-C2-C3	-2.76	121.27	126.04
38	f	101	HEM	C4A-NA-C1A	2.76	108.05	105.35
24	c	911	CLA	C1-C2-C3	-2.76	121.28	126.04
24	b	607	CLA	C3B-C4B-NB	2.76	113.07	110.52
24	C	505	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
24	B	609	CLA	O2A-CGA-CBA	2.75	120.55	111.91
24	c	914	CLA	C3C-C4C-NC	2.75	113.66	110.57
36	C	517	DGD	O2G-C1B-O1B	-2.75	117.05	123.70
24	B	614	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
24	c	904	CLA	CHD-C4C-C3C	-2.75	120.80	124.84
24	C	509	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
36	e	102	DGD	O6D-C5D-C4D	2.75	114.45	109.52
29	a	417	PL9	C53-C6-C1	2.75	120.61	114.99
25	A	408	PHO	C4B-NB-C1B	-2.75	104.58	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	914	CLA	C4-C3-C5	2.75	119.89	115.27
24	b	616	CLA	O2A-CGA-O1A	-2.75	116.66	123.59
24	B	616	CLA	C1-O2A-CGA	2.74	123.64	116.44
24	B	612	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
24	c	912	CLA	C1-C2-C3	-2.74	121.30	126.04
26	C	515	BCR	C33-C5-C6	-2.74	121.45	124.53
24	C	502	CLA	O2A-C1-C2	2.74	115.84	108.64
29	D	405	PL9	C53-C6-C1	2.74	120.59	114.99
24	C	510	CLA	CBC-CAC-C3C	-2.74	104.88	112.43
24	a	410	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
24	C	513	CLA	C3C-C4C-NC	2.74	113.64	110.57
24	a	413	CLA	CMA-C3A-C4A	-2.74	104.41	111.77
24	c	903	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
24	D	403	CLA	CMB-C2B-C1B	2.74	129.54	125.37
24	B	614	CLA	CMC-C2C-C1C	2.74	129.21	125.04
26	d	406	BCR	C28-C27-C26	-2.74	109.19	114.08
39	h	101	RRX	C38-C26-C25	-2.74	121.46	124.53
37	d	410	LHG	O8-C23-O10	-2.73	116.70	123.59
24	b	611	CLA	CMC-C2C-C1C	2.73	129.20	125.04
26	c	916	BCR	C33-C5-C6	-2.73	121.46	124.53
24	C	504	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
36	c	919	DGD	O3G-C3G-C2G	-2.72	104.33	110.90
24	B	612	CLA	C4-C3-C5	2.72	119.85	115.27
24	c	907	CLA	CHA-C1A-NA	-2.72	120.17	126.40
24	c	902	CLA	C3B-C4B-NB	2.71	113.03	110.52
26	K	101	BCR	C38-C26-C25	-2.71	121.48	124.53
24	c	903	CLA	CMC-C2C-C1C	2.71	129.17	125.04
35	v	205	HTG	O2-C2-C1	2.71	115.25	110.27
24	D	403	CLA	C1-C2-C3	-2.71	121.36	126.04
37	D	408	LHG	O8-C23-C24	2.71	120.41	111.91
24	b	614	CLA	CMB-C2B-C1B	2.71	129.50	125.37
24	C	509	CLA	C3B-C4B-NB	2.71	113.03	110.52
24	A	410	CLA	C3C-C4C-NC	2.71	113.61	110.57
26	b	623	BCR	C15-C14-C13	-2.71	123.45	127.31
24	c	905	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
29	a	417	PL9	C40-C39-C41	2.71	119.82	115.27
24	d	404	CLA	C4A-NA-C1A	-2.70	105.49	106.71
24	b	619	CLA	C1-C2-C3	-2.70	121.37	126.04
29	A	414	PL9	C37-C36-C34	-2.70	104.08	112.98
29	A	414	PL9	C20-C19-C21	2.70	119.82	115.27
24	b	612	CLA	CMA-C3A-C2A	-2.70	102.94	113.83
25	A	408	PHO	CMB-C2B-C3B	2.70	129.72	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	612	CLA	CMA-C3A-C4A	-2.70	104.53	111.77
24	D	402	CLA	CED-O2D-CGD	2.70	122.03	115.94
24	C	512	CLA	CMA-C3A-C4A	-2.69	104.53	111.77
24	B	607	CLA	C1-C2-C3	-2.69	121.38	126.04
24	c	914	CLA	CAA-C2A-C3A	-2.69	105.40	112.78
24	C	505	CLA	C1-C2-C3	-2.69	121.39	126.04
24	A	406	CLA	O2A-CGA-O1A	-2.69	116.80	123.59
24	C	502	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
24	C	513	CLA	CMB-C2B-C1B	2.69	129.47	125.37
24	b	620	CLA	CHD-C1D-ND	-2.69	121.98	124.45
24	C	510	CLA	C3B-C4B-NB	2.69	113.01	110.52
24	B	611	CLA	CHD-C1D-ND	-2.69	121.98	124.45
24	b	611	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
24	b	606	CLA	CMA-C3A-C4A	-2.68	104.57	111.77
24	C	507	CLA	CHA-C1A-NA	-2.68	120.26	126.40
24	C	508	CLA	C1D-CHD-C4C	-2.68	120.28	126.06
24	d	401	CLA	CHB-C1B-NB	-2.68	121.42	124.26
24	c	911	CLA	C4C-C3C-C2C	-2.68	103.00	106.90
24	B	617	CLA	O2A-C1-C2	2.68	115.67	108.64
24	C	503	CLA	CHA-C1A-NA	-2.67	120.27	126.40
24	B	611	CLA	C1-C2-C3	-2.67	121.42	126.04
24	b	610	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
24	D	402	CLA	C4-C3-C5	2.67	119.77	115.27
24	b	618	CLA	C4-C3-C5	2.67	119.77	115.27
24	B	607	CLA	C3B-C4B-NB	2.67	112.99	110.52
24	b	608	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
24	b	616	CLA	CMC-C2C-C1C	2.67	129.10	125.04
24	b	611	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
24	C	507	CLA	CBC-CAC-C3C	-2.67	105.08	112.43
24	c	908	CLA	C4C-C3C-C2C	-2.66	103.01	106.90
24	B	616	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
24	C	508	CLA	O2A-CGA-O1A	-2.66	116.87	123.59
24	C	509	CLA	CMB-C2B-C1B	2.66	129.42	125.37
24	b	613	CLA	CHD-C1D-ND	-2.66	122.01	124.45
24	B	604	CLA	C3B-C4B-NB	2.66	112.98	110.52
26	t	903	BCR	C7-C6-C5	-2.66	115.03	121.46
29	A	414	PL9	C45-C44-C46	2.66	119.74	115.27
29	a	417	PL9	C27-C28-C29	-2.66	121.26	127.66
24	B	609	CLA	C3B-C4B-NB	2.65	112.98	110.52
24	a	410	CLA	O2A-CGA-CBA	2.65	120.22	111.91
24	C	510	CLA	C6-C7-C8	-2.65	107.35	115.92
24	C	509	CLA	O2A-CGA-O1A	-2.65	116.91	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	609	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
36	c	919	DGD	O1G-C1A-C2A	2.65	120.22	111.91
24	B	603	CLA	CHA-C1A-NA	-2.65	120.34	126.40
29	d	407	PL9	C36-C37-C38	-2.64	103.19	111.88
24	C	509	CLA	O2A-CGA-CBA	2.64	120.20	111.91
24	c	910	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
24	d	404	CLA	CAA-C2A-C3A	-2.64	105.55	112.78
24	b	607	CLA	O2A-CGA-CBA	2.64	120.19	111.91
24	B	607	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
24	c	903	CLA	C4A-NA-C1A	2.64	107.89	106.71
24	c	904	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
24	c	909	CLA	C4-C3-C5	2.64	119.70	115.27
26	C	514	BCR	C16-C17-C18	-2.63	123.55	127.31
34	a	402	LMT	C1'-O5'-C5'	2.63	118.86	113.69
24	C	512	CLA	CHA-C1A-NA	-2.63	120.37	126.40
29	a	417	PL9	C17-C18-C19	-2.63	121.33	127.66
24	C	502	CLA	CBC-CAC-C3C	-2.63	105.18	112.43
24	b	608	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
27	A	412	SQD	O48-C23-O10	-2.63	116.95	123.59
24	B	605	CLA	CHC-C4B-NB	2.63	127.04	124.26
36	c	919	DGD	O2G-C1B-C2B	2.63	117.17	111.50
37	L	101	LHG	O8-C23-C24	2.63	120.16	111.91
27	b	601	SQD	C45-O47-C7	-2.63	111.32	117.79
24	B	603	CLA	C4-C3-C5	2.63	119.69	115.27
27	A	417	SQD	O48-C23-O10	-2.62	116.97	123.59
24	A	410	CLA	CHC-C4B-NB	2.62	127.03	124.26
24	c	913	CLA	C4C-C3C-C2C	-2.62	103.07	106.90
27	B	621	SQD	O9-S-C6	2.62	110.06	106.94
29	A	414	PL9	C30-C29-C31	2.62	119.68	115.27
24	c	913	CLA	CHA-C1A-NA	-2.62	120.40	126.40
24	c	908	CLA	O2A-CGA-CBA	2.62	120.13	111.91
27	F	101	SQD	C1-C2-C3	-2.62	104.55	110.00
24	C	504	CLA	C3B-C4B-NB	2.62	112.94	110.52
24	B	605	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
26	B	619	BCR	C11-C10-C9	-2.61	123.58	127.31
24	a	409	CLA	O2D-CGD-CBD	2.61	115.91	111.27
38	v	202	HEM	C1B-NB-C4B	2.61	107.77	105.07
36	D	406	DGD	O1G-C1A-C2A	2.61	120.11	111.91
24	C	511	CLA	CAC-C3C-C4C	2.61	128.20	124.81
24	c	906	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
24	B	610	CLA	C1-C2-C3	-2.61	121.53	126.04
24	A	405	CLA	CMC-C2C-C1C	2.61	129.01	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D	407	LHG	O7-C7-C8	2.61	117.12	111.50
24	B	605	CLA	CHA-C1A-NA	-2.60	120.44	126.40
24	a	409	CLA	O2A-CGA-O1A	-2.60	117.02	123.59
37	D	408	LHG	C6-C5-C4	-2.60	105.63	111.79
37	b	639	LHG	O8-C23-C24	2.60	120.07	111.91
24	c	913	CLA	C4-C3-C5	2.60	119.64	115.27
24	b	615	CLA	CMB-C2B-C1B	2.59	129.31	125.37
24	B	603	CLA	C3B-C4B-NB	2.59	112.92	110.52
24	B	605	CLA	CMC-C2C-C1C	2.59	128.98	125.04
24	c	912	CLA	O2A-CGA-CBA	2.59	120.03	111.91
25	a	411	PHO	O1D-CGD-CBD	-2.59	120.43	124.74
24	c	908	CLA	O1D-CGD-CBD	-2.58	119.19	124.48
24	B	608	CLA	CHC-C1C-C2C	-2.58	119.55	126.73
29	D	405	PL9	C51-C49-C50	2.58	120.31	114.60
24	c	912	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
29	D	405	PL9	C22-C23-C24	-2.58	121.45	127.66
24	c	911	CLA	CMB-C2B-C1B	2.58	129.29	125.37
38	v	202	HEM	C4A-NA-C1A	2.58	107.87	105.35
29	d	407	PL9	C10-C9-C11	2.58	119.61	115.27
24	c	907	CLA	C3B-C4B-NB	2.58	112.90	110.52
24	c	902	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
24	A	406	CLA	CAA-CBA-CGA	2.57	120.77	113.25
24	b	618	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
24	A	405	CLA	O2A-CGA-CBA	2.57	119.97	111.91
24	b	618	CLA	C3B-C4B-NB	2.57	112.90	110.52
24	B	609	CLA	CHD-C1D-ND	-2.57	122.09	124.45
38	v	202	HEM	C3B-C2B-C1B	2.57	108.39	106.49
24	B	614	CLA	C1-O2A-CGA	2.57	123.18	116.44
28	a	416	LMG	O8-C28-C29	2.57	119.96	111.91
24	d	401	CLA	CMB-C2B-C1B	2.56	129.27	125.37
34	B	623	LMT	O5B-C5B-C4B	2.56	114.35	109.69
24	b	610	CLA	O2A-CGA-CBA	2.56	119.95	111.91
24	A	410	CLA	CMC-C2C-C1C	2.56	128.94	125.04
24	b	607	CLA	CMC-C2C-C1C	2.56	128.94	125.04
24	C	505	CLA	CMB-C2B-C1B	2.56	129.27	125.37
24	A	407	CLA	C4C-C3C-C2C	-2.56	103.17	106.90
24	b	607	CLA	CHD-C1D-ND	-2.56	122.10	124.45
24	c	908	CLA	CHD-C1D-ND	-2.56	122.10	124.45
24	C	506	CLA	C3B-C4B-NB	2.55	112.89	110.52
24	B	611	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
24	b	612	CLA	C3B-C4B-NB	2.55	112.88	110.52
24	B	609	CLA	O2D-CGD-O1D	-2.55	118.85	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	402	CLA	CAA-C2A-C3A	-2.55	105.79	112.78
24	C	508	CLA	O2A-CGA-CBA	2.55	119.91	111.91
24	d	405	CLA	CMB-C2B-C1B	2.55	129.25	125.37
24	b	615	CLA	CHC-C1C-C2C	-2.55	119.65	126.73
24	B	614	CLA	O2D-CGD-CBD	2.55	115.79	111.27
24	B	605	CLA	O2A-CGA-CBA	2.54	119.89	111.91
24	d	401	CLA	C6-C5-C3	-2.54	106.79	113.45
24	b	605	CLA	CMB-C2B-C1B	2.54	129.24	125.37
24	c	906	CLA	C3B-C4B-NB	2.54	112.87	110.52
29	D	405	PL9	C36-C37-C38	-2.54	103.54	111.88
24	d	405	CLA	C4C-C3C-C2C	-2.54	103.20	106.90
24	D	403	CLA	C11-C10-C8	-2.54	107.72	115.92
24	B	610	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
24	c	912	CLA	C4C-C3C-C2C	-2.54	103.20	106.90
24	C	507	CLA	O2A-CGA-O1A	-2.53	117.19	123.59
24	c	908	CLA	C3B-C4B-NB	2.53	112.87	110.52
24	c	913	CLA	CHD-C1D-ND	-2.53	122.13	124.45
29	D	405	PL9	C10-C9-C11	2.53	119.53	115.27
26	b	623	BCR	C3-C4-C5	-2.53	109.56	114.08
24	c	912	CLA	C3B-C4B-NB	2.53	112.86	110.52
36	H	103	DGD	O1G-C1A-C2A	2.53	119.83	111.91
24	c	904	CLA	CBC-CAC-C3C	-2.52	105.47	112.43
24	A	410	CLA	CAA-C2A-C3A	-2.52	105.87	112.78
24	c	907	CLA	O2A-CGA-CBA	2.52	119.82	111.91
26	c	916	BCR	C21-C20-C19	-2.52	115.35	123.22
26	c	915	BCR	C20-C21-C22	-2.52	123.72	127.31
24	b	616	CLA	CMB-C2B-C1B	2.52	129.21	125.37
24	B	610	CLA	CMA-C3A-C4A	-2.52	105.00	111.77
24	b	606	CLA	CBC-CAC-C3C	-2.52	105.49	112.43
24	B	610	CLA	CHC-C4B-NB	2.52	126.92	124.26
28	C	519	LMG	O7-C10-O9	-2.52	117.62	123.70
24	A	407	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
38	f	101	HEM	C1B-NB-C4B	2.52	107.67	105.07
28	c	921	LMG	O8-C28-C29	2.52	119.80	111.91
26	t	903	BCR	C29-C28-C27	-2.51	105.76	111.38
35	B	626	HTG	C3-C4-C5	2.51	114.72	110.24
24	B	611	CLA	CHA-C1A-NA	-2.51	120.64	126.40
24	C	505	CLA	C3B-C4B-NB	2.51	112.85	110.52
24	B	607	CLA	CAC-C3C-C4C	2.51	128.07	124.81
24	a	409	CLA	CMA-C3A-C2A	-2.51	103.69	113.83
24	B	607	CLA	C4-C3-C5	2.51	119.50	115.27
24	b	613	CLA	CMC-C2C-C1C	2.51	128.86	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	617	CLA	CMA-C3A-C4A	-2.51	105.02	111.77
24	C	510	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
29	d	407	PL9	C37-C38-C39	-2.51	121.62	127.66
29	a	417	PL9	C45-C44-C46	2.51	119.49	115.27
24	d	405	CLA	CAA-C2A-C3A	-2.51	105.91	112.78
24	c	905	CLA	CAC-C3C-C4C	2.51	128.06	124.81
24	C	511	CLA	CMC-C2C-C1C	2.51	128.86	125.04
28	d	411	LMG	O7-C10-C11	2.51	116.91	111.50
24	C	510	CLA	CAC-C3C-C4C	2.51	128.06	124.81
28	D	410	LMG	O8-C28-O10	-2.50	117.27	123.59
24	c	905	CLA	C1-O2A-CGA	2.50	123.02	116.44
35	C	522	HTG	O5-C5-C4	2.50	114.24	109.69
24	c	911	CLA	C4A-NA-C1A	2.50	107.83	106.71
26	B	619	BCR	C28-C27-C26	-2.50	109.61	114.08
24	B	615	CLA	OBD-CAD-C3D	-2.50	122.50	128.52
24	b	617	CLA	C4-C3-C5	2.50	119.48	115.27
24	B	609	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
27	f	102	SQD	O7-S-C6	2.50	109.92	106.92
29	a	417	PL9	C22-C23-C24	-2.50	121.64	127.66
24	c	903	CLA	CBC-CAC-C3C	-2.50	105.55	112.43
26	d	406	BCR	C3-C4-C5	-2.50	109.62	114.08
26	T	702	BCR	C23-C24-C25	-2.50	120.19	127.20
24	d	401	CLA	CAA-CBA-CGA	2.50	120.54	113.25
24	c	910	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
26	c	915	BCR	C38-C26-C25	-2.49	121.73	124.53
26	c	916	BCR	C3-C4-C5	-2.49	109.63	114.08
24	C	513	CLA	C2C-C1C-NC	2.49	112.30	109.97
24	C	501	CLA	C1-C2-C3	-2.49	121.74	126.04
24	C	501	CLA	CAC-C3C-C4C	2.49	128.04	124.81
24	C	511	CLA	CHA-C1A-NA	-2.49	120.70	126.40
24	C	502	CLA	CAC-C3C-C4C	2.48	128.03	124.81
24	b	619	CLA	CHA-C1A-NA	-2.48	120.71	126.40
24	b	620	CLA	C1-C2-C3	-2.48	121.75	126.04
27	B	621	SQD	O47-C7-O49	-2.48	117.71	123.70
24	A	410	CLA	C4C-C3C-C2C	-2.48	103.28	106.90
24	b	617	CLA	O2A-CGA-CBA	2.48	119.69	111.91
36	C	516	DGD	C3G-C2G-C1G	-2.48	105.93	111.79
24	A	405	CLA	CAC-C3C-C4C	2.48	128.02	124.81
24	B	611	CLA	C4-C3-C5	2.48	119.44	115.27
24	C	501	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
35	b	602	HTG	C3-C4-C5	2.48	114.66	110.24
27	B	621	SQD	O48-C23-O10	-2.47	117.35	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	406	BCR	C38-C26-C27	2.47	118.36	113.62
39	h	101	RRX	C24-C23-C22	-2.47	122.50	126.23
24	C	506	CLA	CAC-C3C-C4C	2.47	128.02	124.81
36	C	516	DGD	O1G-C1A-O1A	-2.47	117.36	123.59
24	c	902	CLA	C4A-NA-C1A	2.47	107.82	106.71
24	b	611	CLA	C1D-CHD-C4C	-2.47	120.73	126.06
24	c	905	CLA	C4C-C3C-C2C	-2.47	103.30	106.90
24	d	401	CLA	O2A-CGA-CBA	2.47	119.65	111.91
27	a	401	SQD	O48-C23-O10	-2.47	117.36	123.59
24	c	908	CLA	O2A-CGA-O1A	-2.47	117.37	123.59
26	B	619	BCR	C38-C26-C25	-2.46	121.76	124.53
24	d	401	CLA	CAC-C3C-C2C	2.46	131.74	127.53
24	B	608	CLA	C3C-C4C-NC	2.46	113.33	110.57
26	D	404	BCR	C3-C4-C5	-2.46	109.68	114.08
24	b	619	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
26	c	915	BCR	C11-C10-C9	-2.46	123.80	127.31
24	A	407	CLA	CMC-C2C-C1C	2.46	128.79	125.04
26	B	618	BCR	C24-C23-C22	-2.46	122.52	126.23
24	C	513	CLA	C4A-NA-C1A	2.46	107.81	106.71
24	a	410	CLA	C4-C3-C5	2.46	119.41	115.27
24	B	604	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
24	c	912	CLA	CAC-C3C-C4C	2.46	128.00	124.81
24	C	508	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
26	b	622	BCR	C8-C7-C6	-2.46	120.30	127.20
24	b	618	CLA	CMB-C2B-C1B	2.46	129.11	125.37
31	b	628	GOL	C3-C2-C1	-2.45	102.16	111.70
24	D	402	CLA	C1D-CHD-C4C	-2.45	120.76	126.06
24	b	615	CLA	CMA-C3A-C4A	-2.45	105.18	111.77
24	b	615	CLA	C7-C6-C5	-2.45	106.70	113.36
24	C	510	CLA	CMC-C2C-C1C	2.45	128.77	125.04
24	B	614	CLA	CMA-C3A-C4A	-2.45	105.19	111.77
36	c	917	DGD	O4D-C4D-C3D	-2.45	104.69	110.35
24	C	502	CLA	C4-C3-C5	2.45	119.39	115.27
24	C	503	CLA	CMB-C2B-C1B	2.45	129.10	125.37
26	t	903	BCR	C3-C4-C5	-2.45	109.71	114.08
24	b	619	CLA	CBC-CAC-C3C	-2.45	105.69	112.43
24	a	413	CLA	CHC-C1C-C2C	-2.45	119.94	126.73
26	D	404	BCR	C29-C28-C27	-2.44	105.92	111.38
24	A	407	CLA	O2A-CGA-CBA	2.44	119.57	111.91
24	b	608	CLA	C6-C5-C3	-2.44	107.05	113.45
27	a	415	SQD	O48-C23-O10	-2.44	117.43	123.59
26	t	903	BCR	C35-C13-C12	2.44	121.92	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	607	CLA	C4C-C3C-C2C	-2.44	103.34	106.90
27	A	417	SQD	C1-C2-C3	-2.44	104.92	110.00
24	a	409	CLA	CHC-C1C-C2C	-2.43	119.97	126.73
24	C	509	CLA	CAC-C3C-C4C	2.43	127.97	124.81
24	c	914	CLA	O2A-CGA-CBA	2.43	119.54	111.91
24	C	501	CLA	C4-C3-C5	2.43	119.36	115.27
24	B	611	CLA	CMC-C2C-C1C	2.43	128.74	125.04
24	b	611	CLA	C4A-NA-C1A	2.43	107.80	106.71
24	D	403	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
24	D	402	CLA	CMB-C2B-C1B	2.43	129.06	125.37
24	c	909	CLA	C6-C7-C8	-2.43	108.08	115.92
26	b	622	BCR	C38-C26-C25	-2.43	121.80	124.53
24	c	912	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
26	t	903	BCR	C28-C27-C26	-2.42	109.75	114.08
39	H	102	RRX	C11-C10-C9	-2.42	123.85	127.31
24	B	615	CLA	CMC-C2C-C1C	2.42	128.73	125.04
24	c	907	CLA	CHD-C1D-ND	-2.42	122.23	124.45
28	d	411	LMG	O8-C28-O10	-2.42	117.48	123.59
24	B	608	CLA	C1-O2A-CGA	2.42	122.80	116.44
24	C	504	CLA	C3C-C4C-NC	2.42	113.28	110.57
24	C	503	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
36	c	917	DGD	O2G-C1B-O1B	-2.42	117.86	123.70
24	C	504	CLA	C1-O2A-CGA	2.42	122.78	116.44
24	C	506	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
38	F	102	HEM	C4C-NC-C1C	2.41	107.71	105.35
24	B	617	CLA	CHC-C1C-C2C	-2.41	120.03	126.73
34	J	102	LMT	C1'-O5'-C5'	2.41	117.82	113.67
34	m	1503	LMT	C1B-O1B-C4'	-2.41	112.00	117.96
24	c	913	CLA	CMA-C3A-C4A	-2.41	105.30	111.77
24	b	609	CLA	CAA-C2A-C3A	-2.41	106.18	112.78
25	A	409	PHO	C4B-NB-C1B	-2.41	105.10	108.83
24	b	613	CLA	O2A-CGA-O1A	-2.40	117.52	123.59
36	e	102	DGD	C3A-C2A-C1A	-2.40	104.88	113.62
24	b	615	CLA	C3B-C4B-NB	2.40	112.75	110.52
24	d	404	CLA	CHA-C1A-NA	-2.40	120.89	126.40
38	f	101	HEM	CBA-CAA-C2A	-2.40	105.95	112.63
24	C	501	CLA	C4C-C3C-C2C	-2.40	103.40	106.90
24	B	616	CLA	C11-C10-C8	-2.40	108.16	115.92
24	b	615	CLA	CHA-C1A-NA	-2.40	120.90	126.40
36	C	518	DGD	C2G-O2G-C1B	-2.40	111.88	117.79
37	E	101	LHG	O8-C23-C24	2.40	119.44	111.91
24	B	612	CLA	CMB-C2B-C1B	2.40	129.02	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	401	CLA	C4C-C3C-C2C	-2.40	103.41	106.90
35	V	203	HTG	O5-C1-S1	2.39	115.98	110.14
34	m	1503	LMT	O1B-C1B-C2B	2.39	114.30	108.10
26	y	101	BCR	C10-C11-C12	-2.39	115.75	123.22
24	C	503	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
26	C	515	BCR	C15-C14-C13	-2.39	123.89	127.31
26	a	414	BCR	C33-C5-C6	-2.39	121.84	124.53
26	c	915	BCR	C8-C7-C6	-2.39	120.48	127.20
26	B	619	BCR	C29-C28-C27	-2.39	106.03	111.38
24	B	605	CLA	C4A-NA-C1A	2.39	107.78	106.71
26	T	702	BCR	C16-C15-C14	2.39	128.37	123.47
36	D	406	DGD	C1D-C2D-C3D	2.39	114.97	110.00
24	c	906	CLA	CHD-C1D-ND	-2.39	122.26	124.45
24	d	405	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
36	c	917	DGD	C2G-O2G-C1B	-2.39	111.91	117.79
24	c	912	CLA	CMC-C2C-C1C	2.39	128.68	125.04
26	K	101	BCR	C10-C11-C12	-2.39	115.77	123.22
24	a	410	CLA	CMA-C3A-C2A	-2.39	104.21	113.83
35	C	528	HTG	C4-C3-C2	2.38	114.98	110.82
24	d	404	CLA	CMA-C3A-C2A	-2.38	104.21	113.83
24	B	610	CLA	O2A-CGA-CBA	2.38	119.39	111.91
24	D	402	CLA	CHC-C4B-NB	2.38	126.78	124.26
24	d	401	CLA	CHC-C4B-NB	2.38	126.78	124.26
24	A	406	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
29	d	407	PL9	C15-C14-C16	2.38	119.28	115.27
36	C	517	DGD	O1G-C1A-O1A	-2.38	117.59	123.59
26	t	903	BCR	C2-C3-C4	-2.38	106.06	111.38
24	c	903	CLA	O2A-C1-C2	2.38	114.88	108.64
35	c	924	HTG	O5-C5-C4	2.38	114.01	109.69
24	B	614	CLA	CHA-C1A-NA	-2.38	120.96	126.40
24	b	607	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
37	D	408	LHG	O7-C7-C8	2.37	116.62	111.50
24	c	910	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
28	b	624	LMG	O7-C10-O9	-2.37	117.97	123.70
24	b	618	CLA	C4-C3-C2	-2.37	117.59	123.68
24	B	604	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
24	B	617	CLA	CHA-C1A-NA	-2.37	120.97	126.40
24	C	508	CLA	C1-C2-C3	-2.37	121.94	126.04
26	b	621	BCR	C15-C14-C13	-2.37	123.93	127.31
29	D	405	PL9	C42-C43-C44	-2.37	121.96	127.66
37	d	409	LHG	O7-C7-C8	2.37	116.60	111.50
24	A	410	CLA	O2D-CGD-O1D	-2.37	119.21	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	623	BCR	C21-C20-C19	-2.37	115.83	123.22
24	B	605	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
26	a	414	BCR	C34-C9-C10	-2.37	119.61	122.92
28	C	534	LMG	C8-O7-C10	-2.37	111.97	117.79
26	Y	101	BCR	C24-C23-C22	-2.37	122.66	126.23
24	c	913	CLA	CMC-C2C-C1C	2.37	128.64	125.04
24	A	405	CLA	CMA-C3A-C2A	-2.37	104.29	113.83
37	b	639	LHG	O8-C23-O10	-2.36	117.62	123.59
24	C	507	CLA	O2A-CGA-CBA	2.36	119.33	111.91
24	C	506	CLA	CMB-C2B-C1B	2.36	128.97	125.37
24	b	605	CLA	CHA-C1A-NA	-2.36	120.99	126.40
24	c	910	CLA	C3C-C4C-NC	2.36	113.22	110.57
26	b	622	BCR	C29-C30-C25	2.36	114.11	110.48
24	B	603	CLA	C1-C2-C3	-2.36	121.96	126.04
24	b	617	CLA	CHA-C1A-NA	-2.36	120.99	126.40
24	b	609	CLA	OBD-CAD-C3D	-2.36	122.84	128.52
24	C	507	CLA	C3B-C4B-NB	2.36	112.70	110.52
35	d	403	HTG	C4-C3-C2	-2.36	106.71	110.82
31	A	419	GOL	C3-C2-C1	-2.36	102.54	111.70
24	B	603	CLA	CAC-C3C-C4C	2.36	127.87	124.81
24	D	403	CLA	CAC-C3C-C4C	2.36	127.87	124.81
24	C	505	CLA	C4-C3-C5	2.36	119.23	115.27
24	c	910	CLA	CMC-C2C-C1C	2.36	128.63	125.04
26	T	702	BCR	C35-C13-C12	2.35	121.79	118.08
24	c	911	CLA	O2A-CGA-CBA	2.35	119.29	111.91
24	b	619	CLA	C4-C3-C5	2.35	119.23	115.27
24	d	401	CLA	C4-C3-C5	2.35	119.23	115.27
24	d	401	CLA	CHD-C4C-NC	2.35	127.91	124.20
24	A	405	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
24	b	620	CLA	CHA-C1A-NA	-2.35	121.01	126.40
25	A	408	PHO	O1D-CGD-CBD	-2.35	120.83	124.74
24	C	511	CLA	CMB-C2B-C1B	2.35	128.94	125.37
24	c	905	CLA	CMB-C2B-C1B	2.35	128.94	125.37
24	C	510	CLA	CMA-C3A-C4A	-2.35	105.46	111.77
26	C	514	BCR	C23-C24-C25	-2.35	120.61	127.20
24	b	611	CLA	CHC-C4B-NB	2.35	126.74	124.26
24	c	904	CLA	O2A-CGA-CBA	2.35	119.27	111.91
24	b	605	CLA	O2A-CGA-CBA	2.35	119.27	111.91
24	B	617	CLA	CHC-C4B-NB	2.34	126.74	124.26
24	A	406	CLA	O2A-CGA-CBA	2.34	119.26	111.91
24	b	606	CLA	CHA-C1A-NA	-2.34	121.03	126.40
26	b	621	BCR	C16-C17-C18	-2.34	123.97	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	O2A-CGA-CBA	2.34	119.25	111.91
29	D	405	PL9	C40-C39-C38	-2.34	117.68	123.68
24	B	607	CLA	CHA-C1A-NA	-2.34	121.04	126.40
26	Y	101	BCR	C10-C11-C12	-2.34	115.92	123.22
24	C	508	CLA	CHC-C1C-C2C	-2.34	120.24	126.73
24	B	607	CLA	CMB-C2B-C1B	2.34	128.93	125.37
24	D	402	CLA	CAC-C3C-C4C	2.34	127.84	124.81
26	B	619	BCR	C8-C7-C6	-2.34	120.64	127.20
24	a	410	CLA	CHD-C4C-NC	2.33	127.88	124.20
24	C	511	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
24	C	510	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
24	b	607	CLA	CHB-C1B-C2B	-2.33	120.65	127.24
24	b	620	CLA	C4-C3-C5	2.33	119.19	115.27
39	h	101	RRX	C16-C15-C14	-2.33	118.70	123.47
24	b	615	CLA	C4A-NA-C1A	2.33	107.75	106.71
24	B	603	CLA	CAA-CBA-CGA	-2.33	106.45	113.25
24	B	609	CLA	CMC-C2C-C1C	2.33	128.58	125.04
27	a	415	SQD	O47-C7-O49	-2.33	118.08	123.70
24	b	608	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
24	c	905	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
24	D	403	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
38	f	101	HEM	CHC-C1C-NC	2.33	126.95	124.44
24	c	910	CLA	CHA-C1A-NA	-2.33	121.07	126.40
27	A	412	SQD	O47-C7-O49	-2.32	118.09	123.70
26	b	621	BCR	C40-C30-C25	-2.32	106.53	110.30
24	B	607	CLA	CAA-C2A-C3A	-2.32	106.42	112.78
24	a	410	CLA	CAC-C3C-C4C	2.32	127.82	124.81
35	b	627	HTG	O5-C1-C2	2.32	113.23	110.31
24	c	904	CLA	CAC-C3C-C4C	2.32	127.82	124.81
24	c	907	CLA	CAC-C3C-C4C	2.32	127.82	124.81
24	d	404	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
24	B	612	CLA	CBC-CAC-C3C	-2.32	106.04	112.43
24	B	612	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
24	b	608	CLA	CMB-C2B-C1B	2.32	128.90	125.37
24	d	401	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
38	F	102	HEM	C1B-NB-C4B	2.32	107.47	105.07
34	B	623	LMT	O1B-C4'-C5'	-2.32	103.10	109.45
24	B	615	CLA	CHD-C4C-NC	2.32	127.85	124.20
24	C	506	CLA	CGD-CBD-CAD	-2.32	103.23	110.73
26	A	411	BCR	C23-C24-C25	-2.32	120.70	127.20
29	d	407	PL9	C27-C28-C29	-2.31	122.09	127.66
24	c	909	CLA	CAC-C3C-C2C	2.31	131.49	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	602	CLA	C1-C2-C3	-2.31	122.04	126.04
24	A	407	CLA	CAC-C3C-C4C	2.31	127.81	124.81
24	b	613	CLA	CAC-C3C-C4C	2.31	127.81	124.81
29	d	407	PL9	C20-C19-C21	2.31	119.15	115.27
26	b	622	BCR	C28-C27-C26	-2.30	109.96	114.08
34	a	402	LMT	O5'-C5'-C4'	2.30	114.61	109.75
26	y	101	BCR	C35-C13-C14	-2.30	119.70	122.92
24	B	614	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
24	C	513	CLA	O2A-CGA-CBA	2.30	119.13	111.91
24	b	620	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
24	c	914	CLA	CMB-C2B-C1B	2.30	128.88	125.37
24	C	504	CLA	C4C-C3C-C2C	-2.30	103.54	106.90
24	a	413	CLA	CHB-C4A-NA	2.30	127.69	124.51
24	c	905	CLA	CHC-C1C-C2C	-2.30	120.34	126.73
24	c	904	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
24	B	602	CLA	CMB-C2B-C1B	2.29	128.86	125.37
34	C	520	LMT	C1B-O5B-C5B	2.29	118.19	113.69
26	D	404	BCR	C38-C26-C27	2.29	118.02	113.62
24	c	909	CLA	CHD-C1D-ND	-2.29	122.35	124.45
26	C	515	BCR	C23-C24-C25	-2.29	120.77	127.20
24	b	612	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
24	A	406	CLA	CHC-C1C-C2C	-2.29	120.37	126.73
29	d	407	PL9	C12-C13-C14	-2.29	122.15	127.66
37	d	410	LHG	O8-C23-C24	2.29	119.09	111.91
24	b	612	CLA	CHD-C1D-ND	-2.29	122.35	124.45
24	B	610	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
24	B	612	CLA	CHA-C1A-NA	-2.29	121.16	126.40
25	A	408	PHO	O2D-CGD-O1D	-2.29	119.37	123.84
24	c	912	CLA	CHC-C1C-NC	2.29	127.67	124.20
24	c	911	CLA	C11-C10-C8	-2.28	108.53	115.92
24	B	615	CLA	C7-C6-C5	-2.28	107.15	113.36
25	A	408	PHO	CMA-C3A-C4A	-2.28	109.38	114.38
24	C	503	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
24	c	906	CLA	CAC-C3C-C4C	2.28	127.77	124.81
24	B	612	CLA	CHC-C1C-C2C	-2.28	120.39	126.73
24	c	902	CLA	CHC-C4B-NB	2.28	126.67	124.26
24	c	905	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
26	T	702	BCR	C21-C20-C19	-2.28	116.11	123.22
26	t	903	BCR	C23-C24-C25	-2.28	120.81	127.20
24	b	610	CLA	CAA-C2A-C3A	-2.28	106.55	112.78
24	D	402	CLA	CMA-C3A-C4A	-2.28	105.66	111.77
28	B	622	LMG	O7-C10-O9	-2.27	118.21	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Y	101	BCR	C37-C22-C23	2.27	121.66	118.08
26	k	101	BCR	C10-C11-C12	-2.27	116.13	123.22
26	y	101	BCR	C21-C20-C19	-2.27	116.13	123.22
28	c	921	LMG	C8-O7-C10	-2.27	112.20	117.79
24	A	406	CLA	CMC-C2C-C1C	2.27	128.50	125.04
24	c	914	CLA	C3B-C4B-NB	2.27	112.62	110.52
24	b	608	CLA	C6-C7-C8	-2.27	108.59	115.92
24	a	413	CLA	O2A-CGA-CBA	2.27	119.02	111.91
24	B	614	CLA	C4-C3-C5	2.27	119.08	115.27
24	B	603	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
38	V	202	HEM	CHD-C1D-ND	2.27	126.88	124.42
24	B	613	CLA	O2A-C1-C2	-2.27	102.68	108.64
24	b	612	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
24	b	611	CLA	CAA-CBA-CGA	2.26	119.87	113.25
24	d	405	CLA	C3B-C4B-NB	2.26	112.61	110.52
24	C	503	CLA	O2A-CGA-CBA	2.26	119.01	111.91
24	b	606	CLA	CMA-C3A-C2A	-2.26	104.70	113.83
28	C	519	LMG	C30-C29-C28	-2.26	105.40	113.62
24	b	620	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
24	D	403	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
24	A	410	CLA	O2A-CGA-CBA	2.26	119.00	111.91
24	b	617	CLA	CMB-C2B-C1B	2.26	128.81	125.37
24	A	405	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
24	c	907	CLA	CHC-C1C-C2C	-2.26	120.46	126.73
24	c	911	CLA	C1-O2A-CGA	2.26	122.37	116.44
24	B	611	CLA	CHC-C1C-C2C	-2.26	120.46	126.73
24	C	506	CLA	CHB-C1B-C2B	-2.26	120.86	127.24
24	b	618	CLA	CAC-C3C-C4C	2.26	127.74	124.81
29	A	414	PL9	C51-C49-C50	2.26	119.59	114.60
26	T	702	BCR	C1-C6-C7	2.26	122.16	115.78
26	t	903	BCR	C33-C5-C4	2.26	117.95	113.62
26	d	406	BCR	C16-C15-C14	-2.26	118.85	123.47
24	C	511	CLA	CHC-C1C-C2C	-2.25	120.47	126.73
27	A	417	SQD	O6-C1-C2	2.25	111.82	108.30
26	c	915	BCR	C35-C13-C14	-2.25	119.77	122.92
24	b	609	CLA	CHD-C4C-NC	2.25	127.75	124.20
24	c	905	CLA	C6-C5-C3	2.25	119.36	113.45
28	D	410	LMG	O8-C28-C29	2.25	118.98	111.91
24	C	504	CLA	CAC-C3C-C4C	2.25	127.73	124.81
24	B	608	CLA	O2A-CGA-CBA	2.25	118.97	111.91
25	A	408	PHO	C4-C3-C5	2.25	119.06	115.27
24	b	618	CLA	CMA-C3A-C2A	-2.25	104.75	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	908	CLA	CHA-C1A-NA	-2.25	121.25	126.40
24	B	602	CLA	CAC-C3C-C4C	2.25	127.73	124.81
24	c	913	CLA	CHC-C1C-C2C	-2.25	120.48	126.73
24	C	507	CLA	CMC-C2C-C1C	2.25	128.46	125.04
28	A	413	LMG	C7-O1-C1	-2.25	109.35	113.74
27	B	621	SQD	C4-C3-C2	-2.25	106.90	110.82
34	z	101	LMT	C1B-O1B-C4'	-2.25	112.40	117.96
34	B	623	LMT	C1B-O5B-C5B	2.25	118.10	113.69
24	C	509	CLA	CHC-C1C-C2C	-2.24	120.50	126.73
24	B	610	CLA	C1-O2A-CGA	2.24	122.33	116.44
24	C	508	CLA	CAC-C3C-C4C	2.24	127.72	124.81
24	D	403	CLA	C3B-C4B-NB	2.24	112.59	110.52
24	c	907	CLA	C4-C3-C5	2.24	119.04	115.27
24	A	405	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
34	c	922	LMT	C1B-O1B-C4'	-2.24	112.42	117.96
24	C	510	CLA	CHA-C1A-NA	-2.24	121.27	126.40
37	b	639	LHG	C6-C5-C4	-2.24	106.49	111.79
24	B	608	CLA	C1-C2-C3	-2.24	122.17	126.04
37	d	409	LHG	O8-C23-C24	2.24	118.93	111.91
24	b	608	CLA	CHC-C4B-NB	2.24	126.63	124.26
24	B	608	CLA	CAC-C3C-C4C	2.24	127.71	124.81
24	B	607	CLA	C1-O2A-CGA	2.24	122.31	116.44
36	D	406	DGD	O6D-C5D-C4D	2.24	113.76	109.69
24	b	613	CLA	C1-O2A-CGA	2.24	122.31	116.44
24	c	906	CLA	CMA-C3A-C4A	-2.23	105.77	111.77
24	c	911	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
24	B	604	CLA	CAC-C3C-C4C	2.23	127.71	124.81
24	b	611	CLA	CAC-C3C-C4C	2.23	127.71	124.81
37	d	409	LHG	C6-C5-C4	-2.23	106.50	111.79
28	D	410	LMG	O7-C10-C11	2.23	116.31	111.50
24	B	608	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
24	B	609	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
24	B	606	CLA	CHD-C4C-NC	2.23	127.72	124.20
36	C	517	DGD	O6E-C5E-C6E	2.23	111.98	106.44
24	b	610	CLA	C3B-C4B-NB	2.23	112.58	110.52
24	a	409	CLA	CMC-C2C-C1C	2.23	128.43	125.04
24	C	502	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
26	t	903	BCR	C21-C20-C19	-2.23	116.27	123.22
26	A	411	BCR	C8-C7-C6	-2.22	120.95	127.20
24	b	618	CLA	CED-O2D-CGD	2.22	120.97	115.94
24	b	612	CLA	CMC-C2C-C1C	2.22	128.43	125.04
24	C	504	CLA	C1-C2-C3	-2.22	122.20	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	CMA-C3A-C2A	-2.22	104.86	113.83
24	A	407	CLA	CMA-C3A-C2A	-2.22	104.86	113.83
24	C	512	CLA	C3B-C4B-NB	2.22	112.58	110.52
24	C	509	CLA	C4-C3-C5	2.22	119.01	115.27
24	b	620	CLA	CHC-C1C-C2C	-2.22	120.56	126.73
24	b	620	CLA	OBD-CAD-C3D	-2.22	123.18	128.52
29	a	417	PL9	C51-C49-C50	2.22	119.51	114.60
34	M	302	LMT	O1'-C1'-C2'	2.22	111.77	108.30
24	b	613	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
28	b	624	LMG	O8-C28-O10	-2.22	118.00	123.59
26	D	404	BCR	C10-C11-C12	-2.22	116.30	123.22
24	c	911	CLA	CMC-C2C-C1C	2.22	128.41	125.04
24	B	603	CLA	CMA-C3A-C2A	-2.21	104.90	113.83
29	a	417	PL9	C7-C3-C2	-2.21	120.39	123.30
24	B	603	CLA	CHC-C1C-C2C	-2.21	120.58	126.73
34	M	302	LMT	O1B-C1B-C2B	2.21	113.83	108.10
24	C	512	CLA	CAC-C3C-C2C	2.21	131.31	127.53
24	B	606	CLA	CAC-C3C-C4C	2.21	127.68	124.81
24	B	604	CLA	CMA-C3A-C2A	-2.21	104.92	113.83
24	B	612	CLA	C1-O2A-CGA	2.21	122.24	116.44
24	d	405	CLA	CHA-C1A-NA	-2.21	121.35	126.40
26	c	916	BCR	C23-C24-C25	-2.21	121.01	127.20
29	A	414	PL9	C47-C48-C49	-2.21	120.21	127.75
24	B	609	CLA	CHB-C1B-C2B	-2.21	121.01	127.24
36	c	917	DGD	O3G-C3G-C2G	-2.21	105.58	110.90
29	a	417	PL9	C35-C34-C36	2.20	118.98	115.27
24	b	606	CLA	C5-C3-C2	-2.20	116.66	121.12
24	B	605	CLA	CHC-C1C-C2C	-2.20	120.61	126.73
27	b	601	SQD	C25-C24-C23	-2.20	105.61	113.62
24	B	609	CLA	C11-C12-C13	-2.20	108.80	115.92
24	A	407	CLA	CHC-C1C-C2C	-2.20	120.62	126.73
24	A	410	CLA	C6-C7-C8	-2.20	108.81	115.92
24	B	604	CLA	CAA-C2A-C1A	-2.20	104.77	111.97
24	c	908	CLA	CAC-C3C-C4C	2.20	127.66	124.81
24	B	614	CLA	CHC-C1C-C2C	-2.20	120.62	126.73
34	t	904	LMT	C1'-O5'-C5'	2.20	118.00	113.69
24	a	413	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
31	c	932	GOL	C3-C2-C1	-2.20	103.17	111.70
24	c	913	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
24	D	403	CLA	CMC-C2C-C1C	2.20	128.38	125.04
24	b	605	CLA	CAA-C2A-C3A	-2.20	106.77	112.78
24	C	503	CLA	CHB-C1B-C2B	-2.19	121.04	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	606	CLA	C3B-C4B-NB	2.19	112.55	110.52
26	k	101	BCR	C11-C10-C9	-2.19	124.18	127.31
24	c	906	CLA	C11-C10-C8	-2.19	108.83	115.92
24	a	409	CLA	CAA-CBA-CGA	-2.19	106.85	113.25
24	C	507	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
24	B	607	CLA	CHC-C4B-NB	2.19	126.58	124.26
26	d	406	BCR	C21-C20-C19	-2.19	116.38	123.22
24	b	618	CLA	CHC-C1C-C2C	-2.19	120.65	126.73
24	C	502	CLA	CHA-C1A-NA	-2.19	121.38	126.40
28	d	411	LMG	O8-C28-C29	2.19	118.78	111.91
35	B	626	HTG	C6-C5-C4	-2.19	107.88	113.00
24	B	602	CLA	CHA-C1A-NA	-2.19	121.39	126.40
24	b	614	CLA	CHC-C1C-C2C	-2.19	120.65	126.73
29	d	407	PL9	C25-C24-C26	2.19	118.95	115.27
24	B	617	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
24	d	401	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
29	a	417	PL9	C12-C13-C14	-2.18	122.40	127.66
29	D	405	PL9	C20-C19-C21	2.18	118.94	115.27
24	A	407	CLA	CMB-C2B-C1B	2.18	128.69	125.37
24	D	403	CLA	C7-C6-C5	-2.18	107.43	113.36
24	B	602	CLA	C4-C3-C5	2.18	118.94	115.27
38	V	202	HEM	C4A-NA-C1A	2.18	107.48	105.35
24	B	613	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
24	b	617	CLA	C16-C15-C13	-2.18	108.87	115.92
24	A	410	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
24	c	912	CLA	C6-C5-C3	-2.18	107.74	113.45
24	b	611	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
24	C	512	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
24	c	913	CLA	C3B-C4B-NB	2.18	112.54	110.52
24	b	614	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
24	C	507	CLA	OBD-CAD-C3D	-2.18	123.28	128.52
24	C	503	CLA	C4-C3-C5	2.18	118.93	115.27
24	c	902	CLA	CHC-C1C-C2C	-2.17	120.69	126.73
25	a	412	PHO	CMA-C3A-C4A	-2.17	109.62	114.38
38	V	202	HEM	CBB-CAB-C3B	-2.17	116.82	127.62
24	B	602	CLA	CHC-C1C-C2C	-2.17	120.70	126.73
24	B	615	CLA	C4C-C3C-C2C	-2.17	103.73	106.90
26	C	514	BCR	C20-C21-C22	-2.17	124.21	127.31
31	c	939	GOL	C3-C2-C1	-2.17	103.27	111.70
24	b	609	CLA	CMA-C3A-C4A	-2.17	105.94	111.77
24	C	506	CLA	CHC-C1C-C2C	-2.17	120.71	126.73
34	c	922	LMT	O1'-C1'-C2'	2.17	111.69	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	d	408	LHG	O7-C7-O9	-2.17	118.46	123.70
27	A	412	SQD	O9-S-O7	-2.17	106.45	113.95
27	B	621	SQD	O5-C5-C4	2.17	113.63	109.69
26	t	903	BCR	C12-C13-C14	-2.17	115.62	118.94
24	a	410	CLA	C3B-C4B-NB	2.17	112.53	110.52
24	C	503	CLA	CHD-C4C-NC	2.17	127.62	124.20
24	b	613	CLA	CMA-C3A-C4A	-2.17	105.95	111.77
26	b	622	BCR	C20-C21-C22	-2.17	124.22	127.31
24	c	903	CLA	CAC-C3C-C4C	2.16	127.62	124.81
24	A	406	CLA	CHD-C4C-NC	2.16	127.61	124.20
25	a	411	PHO	CBC-CAC-C3C	-2.16	109.71	112.88
26	B	619	BCR	C37-C22-C23	2.16	121.49	118.08
24	b	614	CLA	C4-C3-C5	2.16	118.91	115.27
24	B	605	CLA	CHD-C1D-ND	-2.16	122.47	124.45
34	b	625	LMT	O5'-C1'-C2'	2.16	114.92	110.35
24	b	607	CLA	CMA-C3A-C2A	-2.16	105.12	113.83
26	y	101	BCR	C1-C6-C7	2.16	121.88	115.78
24	d	405	CLA	CHC-C1C-C2C	-2.16	120.74	126.73
28	c	921	LMG	C4-C3-C2	2.15	114.58	110.82
24	c	909	CLA	C3B-C4B-NB	2.15	112.51	110.52
26	B	619	BCR	C33-C5-C6	-2.15	122.11	124.53
26	K	101	BCR	C33-C5-C4	2.15	117.75	113.62
35	X	902	HTG	C6-C5-C4	-2.15	109.10	113.07
24	b	606	CLA	CMC-C2C-C1C	2.15	128.31	125.04
27	F	101	SQD	C3-C4-C5	2.15	114.08	110.24
24	a	409	CLA	C4-C3-C5	2.15	118.89	115.27
36	c	919	DGD	C6B-C5B-C4B	-2.15	103.51	114.42
24	b	614	CLA	C3B-C4B-NB	2.15	112.51	110.52
35	b	602	HTG	O5-C5-C4	2.15	113.59	109.69
25	A	408	PHO	CBA-CAA-C2A	-2.15	107.54	113.81
24	C	510	CLA	C4A-NA-C1A	2.15	107.67	106.71
24	A	410	CLA	CHC-C1C-C2C	-2.15	120.77	126.73
24	c	912	CLA	CHA-C1A-NA	-2.15	121.48	126.40
24	B	602	CLA	CBC-CAC-C3C	-2.15	106.52	112.43
24	b	607	CLA	CAC-C3C-C4C	2.14	127.59	124.81
25	a	411	PHO	C4B-NB-C1B	-2.14	105.51	108.83
34	m	1502	LMT	C3'-C4'-C5'	-2.14	106.01	110.93
24	B	613	CLA	CAA-CBA-CGA	-2.14	106.99	113.25
28	B	622	LMG	O8-C28-O10	-2.14	118.18	123.59
26	T	702	BCR	C7-C6-C5	-2.14	116.27	121.46
24	B	615	CLA	CMB-C2B-C1B	2.14	128.63	125.37
24	B	610	CLA	CMC-C2C-C1C	2.14	128.30	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	D	406	DGD	O2G-C1B-O1B	-2.14	118.53	123.70
26	k	101	BCR	C38-C26-C25	-2.14	122.12	124.53
24	B	608	CLA	C4C-C3C-C2C	-2.14	103.78	106.90
24	B	617	CLA	CMA-C3A-C4A	-2.14	106.02	111.77
24	d	404	CLA	CAC-C3C-C4C	2.14	127.59	124.81
24	c	905	CLA	C11-C10-C8	-2.14	109.00	115.92
24	B	616	CLA	CHC-C1C-C2C	-2.14	120.79	126.73
28	A	413	LMG	C9-C8-C7	-2.14	106.73	111.79
36	C	516	DGD	O1G-C1A-C2A	2.14	118.62	111.91
38	F	102	HEM	CBA-CAA-C2A	-2.14	106.69	112.63
24	b	611	CLA	CHC-C1C-C2C	-2.14	120.79	126.73
24	C	506	CLA	CMC-C2C-C1C	2.14	128.29	125.04
36	h	102	DGD	C6D-C5D-C4D	2.14	116.55	112.09
24	b	615	CLA	CMC-C2C-C1C	2.14	128.29	125.04
29	D	405	PL9	C27-C28-C29	-2.14	122.52	127.66
24	C	502	CLA	O2A-CGA-CBA	2.13	118.60	111.91
25	a	412	PHO	C4B-NB-C1B	-2.13	105.53	108.83
24	b	617	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
26	b	623	BCR	C16-C17-C18	-2.13	124.27	127.31
24	b	611	CLA	O2A-CGA-CBA	2.13	118.59	111.91
27	b	601	SQD	C4-C3-C2	2.13	114.54	110.82
24	a	410	CLA	CHC-C1C-C2C	-2.13	120.82	126.73
24	C	506	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
24	b	612	CLA	C11-C10-C8	-2.13	109.05	115.92
24	b	609	CLA	C1-C2-C3	-2.13	122.37	126.04
24	C	509	CLA	C16-C15-C13	-2.13	109.05	115.92
24	b	617	CLA	CAC-C3C-C4C	2.13	127.57	124.81
38	F	102	HEM	C2A-C1A-NA	-2.13	107.77	110.15
24	C	505	CLA	CMA-C3A-C4A	-2.13	106.06	111.77
24	c	911	CLA	CHD-C4C-NC	2.12	127.55	124.20
38	F	102	HEM	CMD-C2D-C1D	2.12	128.27	125.04
24	b	615	CLA	OBD-CAD-C3D	-2.12	123.41	128.52
26	b	623	BCR	C8-C7-C6	-2.12	121.24	127.20
27	f	102	SQD	O48-C23-O10	-2.12	118.23	123.59
24	c	909	CLA	O2A-CGA-CBA	2.12	118.57	111.91
24	C	508	CLA	CMB-C2B-C1B	2.12	128.60	125.37
24	C	512	CLA	CHC-C1C-C2C	-2.12	120.83	126.73
24	b	617	CLA	CED-O2D-CGD	2.12	120.74	115.94
24	c	902	CLA	O2A-CGA-CBA	2.12	118.56	111.91
26	d	406	BCR	C29-C30-C25	2.12	113.74	110.48
24	C	509	CLA	CHA-C1A-NA	-2.12	121.55	126.40
28	A	413	LMG	O1-C1-C2	2.12	111.61	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	c	917	DGD	O1G-C1A-O1A	-2.12	118.25	123.59
24	c	907	CLA	C7-C6-C5	-2.12	107.61	113.36
24	d	401	CLA	CHB-C4A-NA	2.12	127.44	124.51
24	c	909	CLA	CHC-C1C-C2C	-2.12	120.85	126.73
24	B	616	CLA	CBC-CAC-C3C	-2.12	106.60	112.43
26	y	101	BCR	C35-C13-C12	2.12	121.41	118.08
24	B	606	CLA	O2A-CGA-CBA	2.12	118.55	111.91
24	C	508	CLA	C3B-C4B-NB	2.11	112.48	110.52
37	e	101	LHG	C5-O7-C7	-2.11	112.58	117.79
24	c	910	CLA	CHC-C1C-C2C	-2.11	120.86	126.73
26	a	414	BCR	C11-C10-C9	-2.11	124.29	127.31
24	c	912	CLA	CMA-C3A-C4A	2.11	117.45	111.77
24	B	607	CLA	O2A-CGA-CBA	2.11	118.54	111.91
24	b	611	CLA	CMA-C3A-C2A	-2.11	105.31	113.83
31	c	928	GOL	C3-C2-C1	-2.11	103.50	111.70
29	D	405	PL9	C37-C38-C39	-2.11	122.58	127.66
37	d	409	LHG	O8-C23-O10	-2.11	118.27	123.59
24	B	611	CLA	OBD-CAD-C3D	-2.11	123.44	128.52
24	B	611	CLA	C6-C7-C8	-2.11	109.10	115.92
24	c	907	CLA	CED-O2D-CGD	2.11	120.70	115.94
35	v	205	HTG	O5-C5-C4	2.11	113.52	109.69
24	D	403	CLA	O2A-CGA-CBA	2.10	118.51	111.91
24	b	612	CLA	CHA-C1A-NA	-2.10	121.58	126.40
24	c	902	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
24	A	407	CLA	CHD-C4C-NC	2.10	127.52	124.20
24	b	617	CLA	CMC-C2C-C1C	2.10	128.24	125.04
24	C	510	CLA	CHC-C1C-C2C	-2.10	120.89	126.73
29	d	407	PL9	C22-C23-C24	-2.10	122.61	127.66
26	t	903	BCR	C20-C21-C22	-2.10	124.32	127.31
25	A	409	PHO	O2A-CGA-CBA	2.10	118.49	111.91
24	b	611	CLA	CAA-C2A-C1A	-2.10	105.11	111.97
24	b	609	CLA	CHA-C1A-NA	-2.10	121.60	126.40
24	d	405	CLA	CHB-C1B-NB	-2.09	122.04	124.26
27	A	417	SQD	O6-C44-C45	-2.09	105.85	110.90
24	b	619	CLA	CHD-C4C-NC	2.09	127.50	124.20
24	b	619	CLA	CAC-C3C-C4C	2.09	127.52	124.81
24	B	603	CLA	CMB-C2B-C1B	2.09	128.55	125.37
31	c	927	GOL	C3-C2-C1	-2.09	103.58	111.70
35	C	522	HTG	O5-C1-C2	2.09	112.94	110.31
28	c	921	LMG	O7-C10-O9	-2.09	118.66	123.70
26	T	702	BCR	C12-C13-C14	-2.09	115.74	118.94
26	b	621	BCR	C33-C5-C4	2.09	117.62	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	F	102	HEM	CHA-C4D-ND	2.09	126.95	124.37
24	A	406	CLA	C4C-C3C-C2C	-2.09	103.86	106.90
26	d	406	BCR	C29-C28-C27	-2.09	106.72	111.38
26	B	619	BCR	C37-C22-C21	-2.08	120.00	122.92
24	c	911	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
24	c	907	CLA	CGD-CBD-CAD	-2.08	103.99	110.73
26	b	622	BCR	C37-C22-C21	-2.08	120.01	122.92
26	k	101	BCR	C34-C9-C8	2.08	121.36	118.08
24	C	511	CLA	O2A-CGA-CBA	2.08	118.44	111.91
24	B	609	CLA	CMA-C3A-C2A	-2.08	105.44	113.83
24	B	608	CLA	OBD-CAD-C3D	-2.08	123.52	128.52
24	b	608	CLA	CAA-CBA-CGA	-2.08	107.18	113.25
24	b	606	CLA	CMB-C2B-C1B	2.08	128.53	125.37
24	C	505	CLA	C1-O2A-CGA	2.08	121.90	116.44
24	b	617	CLA	CHC-C1C-C2C	-2.08	120.96	126.73
24	B	602	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
27	b	601	SQD	O6-C44-C45	2.08	115.91	110.90
24	B	609	CLA	C4-C3-C5	2.08	118.76	115.27
24	B	607	CLA	OBD-CAD-C3D	-2.07	123.53	128.52
24	A	405	CLA	CHC-C4B-NB	2.07	126.45	124.26
26	b	622	BCR	C11-C10-C9	-2.07	124.35	127.31
24	b	618	CLA	OBD-CAD-C3D	-2.07	123.53	128.52
26	B	619	BCR	C15-C16-C17	-2.07	119.23	123.47
29	D	405	PL9	C30-C29-C31	2.07	118.76	115.27
24	b	613	CLA	CED-O2D-CGD	2.07	120.62	115.94
26	y	101	BCR	C32-C1-C6	-2.07	106.94	110.30
26	c	916	BCR	C15-C16-C17	-2.07	119.23	123.47
24	c	909	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
24	B	614	CLA	CMB-C2B-C1B	2.07	128.52	125.37
24	b	605	CLA	C3B-C4B-NB	2.07	112.44	110.52
24	B	614	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
26	A	411	BCR	C15-C16-C17	-2.07	119.24	123.47
28	A	413	LMG	O8-C28-C29	2.07	118.40	111.91
26	B	618	BCR	C21-C20-C19	-2.07	116.77	123.22
24	C	506	CLA	CHA-C1A-NA	-2.07	121.67	126.40
24	D	402	CLA	CBC-CAC-C3C	-2.06	106.74	112.43
24	b	610	CLA	CHD-C4C-NC	2.06	127.46	124.20
24	c	911	CLA	CHA-C1A-NA	-2.06	121.67	126.40
36	e	102	DGD	O2G-C1B-O1B	-2.06	118.72	123.70
24	d	404	CLA	CMB-C2B-C1B	2.06	128.51	125.37
24	B	614	CLA	O2A-CGA-CBA	2.06	118.38	111.91
34	B	623	LMT	O1B-C4'-C3'	2.06	112.76	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	519	LMG	O8-C28-O10	-2.06	118.39	123.59
24	b	614	CLA	CMC-C2C-C1C	2.06	128.18	125.04
29	A	414	PL9	C17-C16-C14	-2.06	106.20	112.98
24	b	605	CLA	CAC-C3C-C2C	2.06	131.05	127.53
24	D	403	CLA	CHB-C4A-NA	2.06	127.36	124.51
24	c	903	CLA	CHD-C4C-NC	2.06	127.45	124.20
24	a	410	CLA	C1-C2-C3	-2.06	122.48	126.04
24	b	606	CLA	CED-O2D-CGD	2.06	120.59	115.94
25	a	411	PHO	C1-O2A-CGA	2.06	121.84	116.44
26	Y	101	BCR	C21-C20-C19	-2.06	116.80	123.22
26	C	514	BCR	C11-C10-C9	-2.06	124.38	127.31
24	c	902	CLA	CAC-C3C-C4C	2.06	127.48	124.81
24	c	903	CLA	CHA-C1A-NA	-2.05	121.69	126.40
24	B	616	CLA	CHB-C4A-NA	2.05	127.35	124.51
24	c	902	CLA	C4-C3-C5	2.05	118.73	115.27
37	d	409	LHG	C32-C31-C30	-2.05	104.01	114.42
24	c	903	CLA	C3B-C4B-NB	2.05	112.42	110.52
24	C	512	CLA	CHB-C1B-C2B	-2.05	121.44	127.24
26	b	623	BCR	C10-C11-C12	-2.05	116.82	123.22
24	c	905	CLA	CHD-C4C-NC	2.05	127.43	124.20
24	c	903	CLA	CHC-C1C-C2C	-2.05	121.05	126.73
24	d	405	CLA	CMA-C3A-C2A	-2.05	105.57	113.83
24	B	607	CLA	CHB-C1B-C2B	-2.05	121.46	127.24
24	a	410	CLA	CHA-C1A-NA	-2.05	121.71	126.40
24	b	618	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
24	c	913	CLA	C1-C2-C3	-2.04	122.51	126.04
28	C	534	LMG	O7-C10-O9	-2.04	118.77	123.70
35	O	303	HTG	C1-O5-C5	2.04	116.35	112.58
24	d	404	CLA	CHC-C4B-NB	2.04	126.42	124.26
24	C	513	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
24	C	501	CLA	O2A-CGA-CBA	2.04	118.31	111.91
26	k	101	BCR	C15-C14-C13	-2.04	124.40	127.31
24	C	504	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
38	F	102	HEM	O1D-CGD-CBD	-2.03	116.55	123.08
36	C	516	DGD	O1G-C1G-C2G	-2.03	102.52	108.43
24	c	910	CLA	C6-C5-C3	-2.03	108.12	113.45
24	B	610	CLA	CHC-C1C-C2C	-2.03	121.08	126.73
26	T	702	BCR	C29-C28-C27	-2.03	106.83	111.38
24	b	607	CLA	CAA-CBA-CGA	2.03	119.19	113.25
24	C	505	CLA	CHC-C1C-C2C	-2.03	121.09	126.73
29	A	414	PL9	O1-C4-C3	-2.03	118.48	120.72
25	a	411	PHO	CBA-CAA-C2A	-2.03	107.88	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	911	CLA	CHC-C1C-C2C	-2.03	121.09	126.73
24	c	913	CLA	C11-C12-C13	-2.03	109.36	115.92
24	d	401	CLA	CHA-C1A-NA	-2.03	121.75	126.40
24	B	603	CLA	CHB-C1B-C2B	-2.03	121.50	127.24
24	c	904	CLA	CHC-C4B-NB	2.03	126.41	124.26
24	C	510	CLA	CMB-C2B-C1B	2.03	128.46	125.37
31	b	632	GOL	C3-C2-C1	-2.03	103.82	111.70
24	b	609	CLA	CAC-C3C-C2C	2.03	131.00	127.53
24	B	606	CLA	CHA-C1A-NA	-2.03	121.76	126.40
24	B	613	CLA	C1-C2-C3	-2.03	122.54	126.04
24	b	619	CLA	CHB-C1B-C2B	-2.03	121.52	127.24
24	B	610	CLA	C4-C3-C5	2.03	118.68	115.27
25	A	408	PHO	CBC-CAC-C3C	-2.02	109.92	112.88
31	a	420	GOL	C3-C2-C1	-2.02	103.83	111.70
24	a	413	CLA	CAC-C3C-C4C	2.02	127.44	124.81
24	b	610	CLA	CHA-C1A-NA	-2.02	121.76	126.40
24	B	607	CLA	CHC-C1C-C2C	-2.02	121.11	126.73
24	B	612	CLA	C3B-C4B-NB	2.02	112.39	110.52
24	b	607	CLA	CHA-C1A-NA	-2.02	121.77	126.40
24	b	616	CLA	CAC-C3C-C4C	2.02	127.43	124.81
29	a	417	PL9	C2-C3-C4	2.02	121.58	118.80
24	c	904	CLA	CMC-C2C-C1C	2.02	128.12	125.04
24	B	614	CLA	CAC-C3C-C4C	2.02	127.43	124.81
24	c	909	CLA	CHB-C4A-NA	2.02	127.31	124.51
29	A	414	PL9	C11-C12-C13	-2.02	105.25	111.88
38	v	202	HEM	CAD-C3D-C4D	2.02	128.18	124.66
38	V	202	HEM	C4C-NC-C1C	2.02	107.32	105.35
24	b	615	CLA	C4-C3-C5	2.01	118.66	115.27
24	B	604	CLA	CHB-C1B-C2B	-2.01	121.55	127.24
29	D	405	PL9	C12-C13-C14	-2.01	122.81	127.66
24	A	406	CLA	OBD-CAD-C3D	-2.01	123.67	128.52
37	D	409	LHG	O4-P-O5	2.01	122.19	112.24
24	D	403	CLA	CHC-C1C-C2C	-2.01	121.14	126.73
24	c	906	CLA	CMC-C2C-C1C	2.01	128.10	125.04
24	d	401	CLA	CMC-C2C-C1C	2.01	128.10	125.04
24	c	903	CLA	C4-C3-C5	2.01	118.65	115.27
35	v	205	HTG	C1-C2-C3	-2.01	106.62	110.59
36	e	102	DGD	C3G-O3G-C1D	2.01	117.66	113.74
24	b	606	CLA	CAC-C3C-C4C	2.01	127.42	124.81
36	C	518	DGD	O1G-C1A-O1A	-2.01	118.53	123.59
26	B	620	BCR	C2-C3-C4	-2.01	106.89	111.38
24	b	607	CLA	CHC-C1C-C2C	-2.01	121.16	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	605	CLA	C1-O2A-CGA	2.01	121.71	116.44
24	b	608	CLA	CHD-C1D-C2D	-2.01	121.27	125.48
29	A	414	PL9	C40-C39-C41	2.01	118.64	115.27
26	b	621	BCR	C2-C3-C4	-2.00	106.90	111.38
24	C	501	CLA	CHC-C1C-C2C	-2.00	121.16	126.73
24	C	507	CLA	C1-O2A-CGA	2.00	121.70	116.44
24	B	615	CLA	CAC-C3C-C4C	2.00	127.41	124.81
24	c	909	CLA	C11-C12-C13	-2.00	109.45	115.92
34	B	623	LMT	C3B-C4B-C5B	2.00	113.81	110.24
26	c	915	BCR	C16-C17-C18	-2.00	124.45	127.31
24	b	615	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
24	B	609	CLA	CHA-C1A-NA	-2.00	121.82	126.40

There are no chirality outliers.

All (1039) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	406	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	C11-C10-C8-C9
24	B	606	CLA	C2-C3-C5-C6
24	B	606	CLA	C4-C3-C5-C6
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	C2B-C3B-CAB-CBB
24	C	503	CLA	C4B-C3B-CAB-CBB
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	C	513	CLA	C1A-C2A-CAA-CBA
24	C	513	CLA	C3A-C2A-CAA-CBA
24	b	610	CLA	CHA-CBD-CGD-O1D
24	b	610	CLA	CHA-CBD-CGD-O2D
24	b	618	CLA	CHA-CBD-CGD-O1D
24	b	618	CLA	CHA-CBD-CGD-O2D
24	b	618	CLA	CAD-CBD-CGD-O1D
24	b	618	CLA	CAD-CBD-CGD-O2D
24	c	908	CLA	CHA-CBD-CGD-O2D
24	c	908	CLA	C2-C3-C5-C6
24	c	908	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	c	909	CLA	CHA-CBD-CGD-O1D
24	c	909	CLA	CHA-CBD-CGD-O2D
24	d	405	CLA	C2-C3-C5-C6
24	d	405	CLA	C4-C3-C5-C6
26	D	404	BCR	C7-C8-C9-C10
26	D	404	BCR	C7-C8-C9-C34
26	Y	101	BCR	C21-C22-C23-C24
26	Y	101	BCR	C37-C22-C23-C24
26	d	406	BCR	C7-C8-C9-C10
26	d	406	BCR	C7-C8-C9-C34
26	y	101	BCR	C21-C22-C23-C24
26	y	101	BCR	C37-C22-C23-C24
27	A	417	SQD	O6-C44-C45-O47
27	B	621	SQD	O5-C1-O6-C44
27	B	621	SQD	O49-C7-O47-C45
27	B	621	SQD	C5-C6-S-O7
27	B	621	SQD	C5-C6-S-O8
27	B	621	SQD	C5-C6-S-O9
27	a	401	SQD	O6-C44-C45-O47
27	a	401	SQD	O5-C5-C6-S
27	a	401	SQD	C5-C6-S-O8
27	b	601	SQD	C2-C1-O6-C44
27	b	601	SQD	O5-C1-O6-C44
27	b	601	SQD	O49-C7-O47-C45
27	b	601	SQD	C5-C6-S-O7
27	b	601	SQD	C5-C6-S-O8
27	b	601	SQD	C5-C6-S-O9
27	f	102	SQD	O6-C44-C45-O47
27	f	102	SQD	O49-C7-O47-C45
29	a	417	PL9	C19-C21-C22-C23
31	A	420	GOL	C1-C2-C3-O3
31	A	420	GOL	O2-C2-C3-O3
31	B	628	GOL	C1-C2-C3-O3
31	B	630	GOL	O1-C1-C2-C3
31	B	631	GOL	C1-C2-C3-O3
31	C	533	GOL	C1-C2-C3-O3
31	O	305	GOL	O1-C1-C2-C3
31	O	306	GOL	C1-C2-C3-O3
31	V	201	GOL	O1-C1-C2-C3
31	a	420	GOL	C1-C2-C3-O3
31	a	421	GOL	O1-C1-C2-C3
31	b	628	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
31	b	629	GOL	O1-C1-C2-O2
31	b	629	GOL	O1-C1-C2-C3
31	b	631	GOL	O1-C1-C2-C3
31	b	638	GOL	O1-C1-C2-O2
31	c	926	GOL	C1-C2-C3-O3
31	c	929	GOL	O1-C1-C2-C3
31	c	932	GOL	C1-C2-C3-O3
31	c	932	GOL	O2-C2-C3-O3
31	c	934	GOL	O1-C1-C2-C3
31	c	934	GOL	C1-C2-C3-O3
31	c	936	GOL	C1-C2-C3-O3
31	c	937	GOL	C1-C2-C3-O3
31	c	937	GOL	O2-C2-C3-O3
31	o	303	GOL	O1-C1-C2-C3
31	o	304	GOL	O1-C1-C2-C3
34	F	103	LMT	C2'-C1'-O1'-C1
34	F	103	LMT	O5'-C1'-O1'-C1
34	J	102	LMT	C2'-C1'-O1'-C1
34	M	302	LMT	O5'-C1'-O1'-C1
34	Z	101	LMT	C2'-C1'-O1'-C1
34	Z	101	LMT	O5'-C1'-O1'-C1
34	Z	101	LMT	C2-C1-O1'-C1'
34	b	625	LMT	C2'-C1'-O1'-C1
34	b	625	LMT	O5'-C1'-O1'-C1
34	t	904	LMT	C2'-C1'-O1'-C1
35	B	625	HTG	O5-C1-S1-C1'
35	C	521	HTG	C2'-C1'-S1-C1
35	H	105	HTG	C2'-C1'-S1-C1
35	V	203	HTG	O5-C1-S1-C1'
35	X	902	HTG	C2-C1-S1-C1'
35	X	902	HTG	O5-C1-S1-C1'
35	b	603	HTG	O5-C1-S1-C1'
35	b	627	HTG	O5-C1-S1-C1'
35	c	923	HTG	C2'-C1'-S1-C1
35	u	201	HTG	O5-C1-C2-O2
35	u	201	HTG	O2-C2-C3-O3
35	v	205	HTG	O5-C1-S1-C1'
36	D	406	DGD	C2B-C1B-O2G-C2G
36	D	406	DGD	O2G-C2G-C3G-O3G
36	e	102	DGD	C2D-C1D-O3G-C3G
37	D	408	LHG	C3-O3-P-O4
37	E	101	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
37	L	101	LHG	C4-O6-P-O4
37	b	639	LHG	C4-O6-P-O4
37	d	409	LHG	O2-C2-C3-O3
37	d	409	LHG	C3-O3-P-O4
37	d	409	LHG	C3-O3-P-O5
37	d	409	LHG	C3-O3-P-O6
37	d	409	LHG	C4-O6-P-O4
24	C	501	CLA	CBD-CGD-O2D-CED
34	C	520	LMT	C3'-C4'-O1B-C1B
24	b	614	CLA	C15-C16-C17-C18
28	A	413	LMG	O9-C10-O7-C8
36	D	406	DGD	O1B-C1B-O2G-C2G
24	B	605	CLA	C3-C5-C6-C7
27	B	621	SQD	C8-C7-O47-C45
27	b	601	SQD	C8-C7-O47-C45
34	z	101	LMT	O5'-C1'-O1'-C1
34	B	623	LMT	O5B-C5B-C6B-O6B
24	B	607	CLA	C2A-CAA-CBA-CGA
24	b	610	CLA	C2A-CAA-CBA-CGA
24	a	413	CLA	C3-C5-C6-C7
27	F	101	SQD	C24-C23-O48-C46
35	C	522	HTG	S1-C1'-C2'-C3'
27	F	101	SQD	O10-C23-O48-C46
34	z	101	LMT	C2'-C1'-O1'-C1
26	T	702	BCR	C13-C14-C15-C16
34	M	302	LMT	O5'-C5'-C6'-O6'
35	u	201	HTG	C1-C2-C3-O3
27	b	601	SQD	C24-C23-O48-C46
28	A	413	LMG	C11-C10-O7-C8
34	C	520	LMT	O5B-C5B-C6B-O6B
34	t	904	LMT	O5'-C5'-C6'-O6'
34	M	302	LMT	C4'-C5'-C6'-O6'
27	b	601	SQD	O10-C23-O48-C46
34	T	703	LMT	O5'-C5'-C6'-O6'
24	B	617	CLA	C4-C3-C5-C6
24	b	618	CLA	C4-C3-C5-C6
29	a	417	PL9	C30-C29-C31-C32
34	B	623	LMT	C4B-C5B-C6B-O6B
24	B	617	CLA	C2-C3-C5-C6
24	b	618	CLA	C2-C3-C5-C6
29	a	417	PL9	C28-C29-C31-C32
37	d	410	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
35	u	201	HTG	O5-C1-C2-C3
28	C	534	LMG	O6-C5-C6-O5
34	t	904	LMT	O5'-C1'-O1'-C1
29	A	414	PL9	C24-C26-C27-C28
35	B	626	HTG	C4-C5-C6-O6
37	d	409	LHG	C1-C2-C3-O3
34	t	904	LMT	C4'-C5'-C6'-O6'
36	C	516	DGD	C2A-C3A-C4A-C5A
36	C	517	DGD	CBB-CCB-CDB-CEB
24	c	907	CLA	C13-C15-C16-C17
27	F	101	SQD	C44-C45-C46-O48
34	T	703	LMT	C4'-C5'-C6'-O6'
27	b	601	SQD	O6-C44-C45-O47
27	A	412	SQD	C9-C10-C11-C12
37	d	410	LHG	C12-C13-C14-C15
29	a	417	PL9	C23-C24-C26-C27
24	A	410	CLA	C14-C13-C15-C16
24	C	504	CLA	C11-C12-C13-C14
24	C	506	CLA	C6-C7-C8-C9
24	C	509	CLA	C11-C10-C8-C9
24	b	605	CLA	C14-C13-C15-C16
24	c	905	CLA	C11-C12-C13-C14
28	a	416	LMG	C16-C17-C18-C19
26	D	404	BCR	C37-C22-C23-C24
26	d	406	BCR	C37-C22-C23-C24
26	D	404	BCR	C21-C22-C23-C24
26	d	406	BCR	C21-C22-C23-C24
35	B	625	HTG	C4-C5-C6-O6
27	A	412	SQD	C7-C8-C9-C10
36	C	517	DGD	C1B-C2B-C3B-C4B
24	C	507	CLA	C15-C16-C17-C18
37	d	408	LHG	C23-C24-C25-C26
35	b	627	HTG	C1'-C2'-C3'-C4'
24	A	410	CLA	C15-C16-C17-C18
24	a	409	CLA	C15-C16-C17-C18
24	b	620	CLA	C15-C16-C17-C18
27	f	102	SQD	O5-C1-O6-C44
31	B	630	GOL	O2-C2-C3-O3
31	C	533	GOL	O2-C2-C3-O3
31	O	305	GOL	O1-C1-C2-O2
31	a	420	GOL	O2-C2-C3-O3
31	c	936	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
31	o	304	GOL	O1-C1-C2-O2
27	A	417	SQD	C23-C24-C25-C26
24	B	602	CLA	C3-C5-C6-C7
27	A	417	SQD	C26-C27-C28-C29
34	m	1503	LMT	O5'-C5'-C6'-O6'
24	a	413	CLA	C10-C11-C12-C13
24	c	907	CLA	C15-C16-C17-C18
37	E	101	LHG	C7-C8-C9-C10
37	L	101	LHG	C7-C8-C9-C10
27	a	415	SQD	C17-C18-C19-C20
29	a	417	PL9	C25-C24-C26-C27
24	B	616	CLA	C11-C12-C13-C15
24	B	617	CLA	C12-C13-C15-C16
24	b	610	CLA	C11-C12-C13-C15
24	b	615	CLA	C12-C13-C15-C16
24	c	906	CLA	C11-C12-C13-C15
37	b	639	LHG	C7-C8-C9-C10
24	C	507	CLA	C2A-CAA-CBA-CGA
24	C	501	CLA	O1D-CGD-O2D-CED
34	J	102	LMT	O5'-C1'-O1'-C1
29	A	414	PL9	C9-C11-C12-C13
29	A	414	PL9	C19-C21-C22-C23
29	a	417	PL9	C9-C11-C12-C13
27	B	621	SQD	C31-C32-C33-C34
34	z	101	LMT	O5B-C1B-O1B-C4'
35	B	626	HTG	O5-C5-C6-O6
28	C	534	LMG	C4-C5-C6-O5
34	t	904	LMT	O1'-C1-C2-C3
28	b	624	LMG	C30-C31-C32-C33
27	F	101	SQD	O47-C45-C46-O48
24	b	620	CLA	C10-C11-C12-C13
37	D	408	LHG	C3-O3-P-O6
37	E	101	LHG	C4-O6-P-O3
37	L	101	LHG	C4-O6-P-O3
37	b	639	LHG	C4-O6-P-O3
37	d	409	LHG	C4-O6-P-O3
24	D	403	CLA	C3-C5-C6-C7
24	d	405	CLA	C3-C5-C6-C7
35	B	624	HTG	C1'-C2'-C3'-C4'
34	Z	101	LMT	O5'-C5'-C6'-O6'
24	D	403	CLA	C4-C3-C5-C6
24	D	403	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	B	617	CLA	C13-C15-C16-C17
34	z	101	LMT	C2B-C1B-O1B-C4'
34	t	904	LMT	C7-C8-C9-C10
36	C	518	DGD	CAA-CBA-CCA-CDA
27	A	412	SQD	C16-C17-C18-C19
27	B	621	SQD	C10-C11-C12-C13
27	b	601	SQD	C26-C27-C28-C29
27	b	601	SQD	C30-C31-C32-C33
35	B	626	HTG	C2'-C3'-C4'-C5'
36	D	406	DGD	C9B-CAB-CBB-CCB
27	a	415	SQD	C34-C35-C36-C37
27	b	601	SQD	C10-C11-C12-C13
28	C	534	LMG	C18-C19-C20-C21
36	D	406	DGD	CBB-CCB-CDB-CEB
37	D	409	LHG	C28-C29-C30-C31
37	E	101	LHG	C25-C26-C27-C28
37	d	408	LHG	C30-C31-C32-C33
28	a	416	LMG	O9-C10-O7-C8
34	T	703	LMT	C4-C5-C6-C7
34	t	904	LMT	C4-C5-C6-C7
36	C	517	DGD	C6B-C7B-C8B-C9B
28	C	534	LMG	C17-C18-C19-C20
34	M	302	LMT	C2-C3-C4-C5
37	D	408	LHG	C14-C15-C16-C17
27	B	621	SQD	C2-C1-O6-C44
34	C	520	LMT	C2'-C1'-O1'-C1
34	M	302	LMT	C2'-C1'-O1'-C1
36	C	518	DGD	C8B-C9B-CAB-CBB
35	B	625	HTG	O5-C5-C6-O6
35	B	624	HTG	C2'-C3'-C4'-C5'
36	C	516	DGD	C4B-C5B-C6B-C7B
24	b	615	CLA	C14-C13-C15-C16
24	c	908	CLA	C11-C10-C8-C9
28	A	413	LMG	C17-C18-C19-C20
28	A	413	LMG	C18-C19-C20-C21
34	T	703	LMT	O1'-C1-C2-C3
36	e	102	DGD	C2A-C3A-C4A-C5A
28	A	413	LMG	C12-C13-C14-C15
28	C	519	LMG	C31-C32-C33-C34
36	c	918	DGD	C8B-C9B-CAB-CBB
31	A	422	GOL	C1-C2-C3-O3
31	B	630	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
31	V	201	GOL	C1-C2-C3-O3
31	a	419	GOL	C1-C2-C3-O3
31	a	421	GOL	C1-C2-C3-O3
31	b	632	GOL	O1-C1-C2-C3
31	b	638	GOL	O1-C1-C2-C3
31	c	938	GOL	O1-C1-C2-C3
31	f	104	GOL	C1-C2-C3-O3
31	u	202	GOL	C1-C2-C3-O3
31	v	203	GOL	O1-C1-C2-C3
28	a	416	LMG	C11-C10-O7-C8
27	B	621	SQD	C13-C14-C15-C16
27	a	415	SQD	C32-C33-C34-C35
36	C	516	DGD	C5B-C6B-C7B-C8B
27	A	412	SQD	C15-C16-C17-C18
27	B	621	SQD	C28-C29-C30-C31
28	a	416	LMG	C17-C18-C19-C20
28	a	416	LMG	C20-C21-C22-C23
36	C	518	DGD	CBA-CCA-CDA-CEA
36	D	406	DGD	C2A-C3A-C4A-C5A
24	c	913	CLA	C4B-C3B-CAB-CBB
24	c	914	CLA	C4B-C3B-CAB-CBB
29	D	405	PL9	C39-C41-C42-C43
28	A	413	LMG	C13-C14-C15-C16
37	d	408	LHG	C29-C30-C31-C32
34	a	402	LMT	C1-C2-C3-C4
27	B	621	SQD	C30-C31-C32-C33
28	B	622	LMG	C32-C33-C34-C35
28	D	410	LMG	C35-C36-C37-C38
28	b	624	LMG	C20-C21-C22-C23
28	d	411	LMG	C35-C36-C37-C38
27	A	417	SQD	C15-C16-C17-C18
24	C	506	CLA	C3A-C2A-CAA-CBA
26	t	903	BCR	C13-C14-C15-C16
34	B	623	LMT	C2-C1-O1'-C1'
34	M	302	LMT	C2-C1-O1'-C1'
28	d	411	LMG	C16-C17-C18-C19
37	d	408	LHG	C27-C28-C29-C30
28	a	416	LMG	C7-C8-C9-O8
34	C	520	LMT	C3-C4-C5-C6
34	B	623	LMT	C2-C3-C4-C5
24	b	613	CLA	C4-C3-C5-C6
24	C	505	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	b	613	CLA	C2-C3-C5-C6
31	B	628	GOL	O2-C2-C3-O3
31	B	630	GOL	O1-C1-C2-O2
31	O	306	GOL	O2-C2-C3-O3
31	b	628	GOL	O2-C2-C3-O3
31	c	929	GOL	O1-C1-C2-O2
31	c	934	GOL	O1-C1-C2-O2
31	c	938	GOL	O1-C1-C2-O2
31	o	303	GOL	O1-C1-C2-O2
27	A	412	SQD	C11-C12-C13-C14
28	C	519	LMG	C30-C31-C32-C33
28	C	519	LMG	C38-C39-C40-C41
34	t	904	LMT	C11-C10-C9-C8
28	d	411	LMG	C17-C18-C19-C20
24	c	913	CLA	C2B-C3B-CAB-CBB
24	c	914	CLA	C2B-C3B-CAB-CBB
24	c	914	CLA	C10-C11-C12-C13
27	a	401	SQD	C25-C26-C27-C28
28	a	416	LMG	C36-C37-C38-C39
28	a	416	LMG	C32-C33-C34-C35
34	Z	101	LMT	C4-C5-C6-C7
34	Z	101	LMT	C1-C2-C3-C4
24	B	617	CLA	C2-C1-O2A-CGA
24	b	605	CLA	C2-C1-O2A-CGA
28	b	624	LMG	C38-C39-C40-C41
24	a	410	CLA	C13-C15-C16-C17
37	d	410	LHG	C11-C12-C13-C14
26	B	618	BCR	C1-C6-C7-C8
26	B	618	BCR	C5-C6-C7-C8
26	D	404	BCR	C23-C24-C25-C26
26	D	404	BCR	C23-C24-C25-C30
26	Y	101	BCR	C1-C6-C7-C8
26	Y	101	BCR	C5-C6-C7-C8
26	b	621	BCR	C1-C6-C7-C8
26	b	621	BCR	C5-C6-C7-C8
26	d	406	BCR	C23-C24-C25-C26
26	d	406	BCR	C23-C24-C25-C30
26	y	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
28	d	411	LMG	C19-C20-C21-C22
34	B	623	LMT	C3'-C4'-O1B-C1B
34	B	623	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
36	c	917	DGD	C7A-C8A-C9A-CAA
37	D	407	LHG	C23-C24-C25-C26
34	C	520	LMT	C1-C2-C3-C4
24	b	618	CLA	C10-C11-C12-C13
34	a	402	LMT	C2-C3-C4-C5
37	d	410	LHG	C24-C25-C26-C27
24	A	410	CLA	C12-C13-C15-C16
24	B	602	CLA	C11-C10-C8-C7
24	C	506	CLA	C11-C12-C13-C15
24	b	610	CLA	C6-C7-C8-C10
35	U	201	HTG	S1-C1'-C2'-C3'
35	u	201	HTG	S1-C1'-C2'-C3'
24	c	910	CLA	C15-C16-C17-C18
24	b	618	CLA	C16-C17-C18-C20
28	B	622	LMG	C10-C11-C12-C13
28	c	920	LMG	C28-C29-C30-C31
28	B	622	LMG	C37-C38-C39-C40
36	D	406	DGD	CBA-CCA-CDA-CEA
37	d	410	LHG	C28-C29-C30-C31
34	B	623	LMT	C1-C2-C3-C4
24	C	509	CLA	C13-C15-C16-C17
36	C	516	DGD	C3B-C4B-C5B-C6B
36	C	517	DGD	C5B-C6B-C7B-C8B
37	L	101	LHG	C11-C10-C9-C8
36	c	918	DGD	C3B-C4B-C5B-C6B
36	c	919	DGD	CBA-CCA-CDA-CEA
37	d	410	LHG	C14-C15-C16-C17
34	T	703	LMT	C1-C2-C3-C4
28	c	920	LMG	C29-C30-C31-C32
28	c	921	LMG	O6-C5-C6-O5
24	c	910	CLA	C16-C17-C18-C19
34	C	520	LMT	O5'-C1'-O1'-C1
24	B	603	CLA	C15-C16-C17-C18
36	c	917	DGD	C5B-C6B-C7B-C8B
37	b	639	LHG	C11-C10-C9-C8
28	d	411	LMG	O6-C5-C6-O5
28	C	534	LMG	C38-C39-C40-C41
27	a	415	SQD	C31-C32-C33-C34
28	b	624	LMG	C17-C18-C19-C20
34	D	401	LMT	C7-C8-C9-C10
37	d	410	LHG	C11-C10-C9-C8
24	a	413	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
37	E	101	LHG	O7-C5-C6-O8
24	B	602	CLA	CBA-CGA-O2A-C1
28	d	411	LMG	C36-C37-C38-C39
34	Z	101	LMT	O5B-C1B-O1B-C4'
36	c	917	DGD	O6E-C5E-C6E-O5E
24	C	505	CLA	C4-C3-C5-C6
25	a	411	PHO	C2-C3-C5-C6
24	B	616	CLA	C11-C12-C13-C14
24	B	617	CLA	C14-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C14
24	b	620	CLA	C14-C13-C15-C16
24	c	906	CLA	C11-C12-C13-C14
37	D	408	LHG	C11-C12-C13-C14
35	C	522	HTG	O5-C5-C6-O6
35	d	403	HTG	C3'-C4'-C5'-C6'
24	C	506	CLA	C1A-C2A-CAA-CBA
24	c	907	CLA	C1A-C2A-CAA-CBA
24	c	909	CLA	C1A-C2A-CAA-CBA
24	C	502	CLA	C16-C17-C18-C20
24	c	910	CLA	C16-C17-C18-C20
37	d	409	LHG	C32-C33-C34-C35
24	c	911	CLA	C8-C10-C11-C12
27	f	102	SQD	C23-C24-C25-C26
36	C	517	DGD	C4B-C5B-C6B-C7B
35	b	627	HTG	O5-C5-C6-O6
25	A	409	PHO	C2C-C3C-CAC-CBC
34	J	102	LMT	C7-C8-C9-C10
37	b	639	LHG	C27-C28-C29-C30
28	C	519	LMG	C16-C17-C18-C19
34	a	402	LMT	C11-C10-C9-C8
36	c	917	DGD	C4B-C5B-C6B-C7B
24	b	607	CLA	C5-C6-C7-C8
37	e	101	LHG	C7-C8-C9-C10
28	c	920	LMG	C13-C14-C15-C16
36	h	102	DGD	C5B-C6B-C7B-C8B
25	a	411	PHO	C4-C3-C5-C6
27	b	601	SQD	C9-C10-C11-C12
36	C	517	DGD	CAB-CBB-CCB-CDB
36	D	406	DGD	C5A-C6A-C7A-C8A
35	d	403	HTG	O5-C5-C6-O6
27	A	417	SQD	O6-C44-C45-C46
27	B	621	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
27	b	601	SQD	O6-C44-C45-C46
28	A	413	LMG	C14-C15-C16-C17
34	b	625	LMT	C9-C10-C11-C12
24	B	602	CLA	O1A-CGA-O2A-C1
27	b	601	SQD	C45-C44-O6-C1
36	C	517	DGD	C5D-C6D-O5D-C1E
36	c	918	DGD	C2G-C3G-O3G-C1D
36	c	918	DGD	C5D-C6D-O5D-C1E
35	O	303	HTG	C3'-C4'-C5'-C6'
35	b	602	HTG	C4'-C5'-C6'-C7'
37	b	639	LHG	C28-C29-C30-C31
28	A	413	LMG	C22-C23-C24-C25
34	T	703	LMT	C2-C3-C4-C5
37	D	409	LHG	C29-C30-C31-C32
24	C	506	CLA	C16-C17-C18-C20
29	d	407	PL9	C39-C41-C42-C43
28	B	622	LMG	C40-C41-C42-C43
27	f	102	SQD	O6-C1-O5-C5
31	V	201	GOL	O1-C1-C2-O2
31	a	421	GOL	O1-C1-C2-O2
31	b	631	GOL	O1-C1-C2-O2
31	c	926	GOL	O2-C2-C3-O3
34	t	904	LMT	C1-C2-C3-C4
36	H	103	DGD	C5B-C6B-C7B-C8B
34	D	401	LMT	O1'-C1-C2-C3
36	C	517	DGD	C6A-C7A-C8A-C9A
34	z	101	LMT	C3-C4-C5-C6
37	D	407	LHG	C26-C27-C28-C29
28	D	410	LMG	O6-C5-C6-O5
29	A	414	PL9	C20-C19-C21-C22
29	a	417	PL9	C12-C11-C9-C10
29	A	414	PL9	C13-C14-C16-C17
35	B	624	HTG	C4'-C5'-C6'-C7'
34	D	401	LMT	O5B-C5B-C6B-O6B
36	C	516	DGD	O6E-C5E-C6E-O5E
27	a	415	SQD	C13-C14-C15-C16
36	c	917	DGD	C9A-CAA-CBA-CCA
35	B	627	HTG	O5-C5-C6-O6
28	b	624	LMG	C21-C22-C23-C24
27	A	417	SQD	C16-C17-C18-C19
24	B	602	CLA	C10-C11-C12-C13
36	C	516	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
36	c	917	DGD	C6A-C7A-C8A-C9A
29	A	414	PL9	C15-C14-C16-C17
34	D	401	LMT	C6-C7-C8-C9
24	C	504	CLA	C11-C12-C13-C15
24	D	403	CLA	C11-C10-C8-C7
24	a	410	CLA	C11-C10-C8-C7
24	a	413	CLA	C11-C10-C8-C7
24	b	614	CLA	C12-C13-C15-C16
24	c	905	CLA	C11-C10-C8-C7
24	c	907	CLA	C12-C13-C15-C16
24	d	405	CLA	C11-C10-C8-C7
29	A	414	PL9	C18-C19-C21-C22
29	a	417	PL9	C12-C11-C9-C8
24	B	616	CLA	C11-C10-C8-C9
24	D	403	CLA	C11-C10-C8-C9
24	a	410	CLA	C6-C7-C8-C9
24	b	619	CLA	C11-C10-C8-C9
24	c	907	CLA	C14-C13-C15-C16
27	F	101	SQD	C23-C24-C25-C26
28	d	411	LMG	C39-C40-C41-C42
34	T	703	LMT	C3-C4-C5-C6
34	b	625	LMT	C6-C7-C8-C9
28	a	416	LMG	C30-C31-C32-C33
36	c	917	DGD	CDA-CEA-CFA-CGA
36	c	917	DGD	CAB-CBB-CCB-CDB
28	d	411	LMG	C34-C35-C36-C37
24	C	510	CLA	C8-C10-C11-C12
27	F	101	SQD	C33-C34-C35-C36
24	C	502	CLA	C4B-C3B-CAB-CBB
24	C	513	CLA	C4B-C3B-CAB-CBB
24	c	902	CLA	C4B-C3B-CAB-CBB
24	b	612	CLA	C13-C15-C16-C17
28	b	624	LMG	C19-C20-C21-C22
34	Z	101	LMT	O1'-C1-C2-C3
27	F	101	SQD	C34-C35-C36-C37
24	b	609	CLA	C4-C3-C5-C6
24	b	609	CLA	C2-C3-C5-C6
28	b	624	LMG	C37-C38-C39-C40
34	T	703	LMT	C6-C7-C8-C9
24	B	602	CLA	C8-C10-C11-C12
28	A	413	LMG	C38-C39-C40-C41
36	c	919	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
24	C	510	CLA	C16-C17-C18-C19
27	f	102	SQD	C24-C23-O48-C46
36	h	102	DGD	O2G-C1B-C2B-C3B
36	C	517	DGD	C7A-C8A-C9A-CAA
37	D	407	LHG	C31-C32-C33-C34
24	C	512	CLA	CBA-CGA-O2A-C1
27	B	621	SQD	C27-C28-C29-C30
37	D	409	LHG	C24-C25-C26-C27
24	b	615	CLA	C13-C15-C16-C17
24	b	618	CLA	C8-C10-C11-C12
27	a	401	SQD	O6-C44-C45-C46
36	D	406	DGD	C1G-C2G-C3G-O3G
37	E	101	LHG	C4-C5-C6-O8
28	B	622	LMG	C17-C18-C19-C20
36	D	406	DGD	CCB-CDB-CEB-CFB
24	b	618	CLA	C16-C17-C18-C19
34	a	402	LMT	C7-C8-C9-C10
34	T	703	LMT	C7-C8-C9-C10
37	e	101	LHG	C4-O6-P-O3
31	a	421	GOL	O2-C2-C3-O3
37	L	101	LHG	C31-C32-C33-C34
24	C	512	CLA	O1A-CGA-O2A-C1
37	D	409	LHG	C16-C17-C18-C19
24	C	513	CLA	C2B-C3B-CAB-CBB
37	d	409	LHG	C31-C32-C33-C34
24	B	614	CLA	C15-C16-C17-C18
37	D	408	LHG	C32-C33-C34-C35
34	C	520	LMT	C4B-C5B-C6B-O6B
35	c	924	HTG	C4-C5-C6-O6
27	a	415	SQD	O6-C44-C45-O47
28	A	413	LMG	O1-C7-C8-O7
24	B	614	CLA	C13-C15-C16-C17
27	b	601	SQD	C24-C25-C26-C27
28	d	411	LMG	C29-C30-C31-C32
24	c	908	CLA	C5-C6-C7-C8
24	B	602	CLA	C14-C13-C15-C16
24	B	605	CLA	C6-C7-C8-C9
24	b	614	CLA	C14-C13-C15-C16
24	d	405	CLA	C11-C10-C8-C9
24	B	616	CLA	C13-C15-C16-C17
24	a	413	CLA	C8-C10-C11-C12
37	D	409	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
24	A	406	CLA	C2C-C3C-CAC-CBC
28	D	410	LMG	C19-C20-C21-C22
34	Z	101	LMT	C2B-C1B-O1B-C4'
26	C	514	BCR	C1-C6-C7-C8
26	C	514	BCR	C5-C6-C7-C8
26	d	406	BCR	C5-C6-C7-C8
24	b	605	CLA	CAA-CBA-CGA-O2A
26	b	623	BCR	C37-C22-C23-C24
26	b	623	BCR	C21-C22-C23-C24
28	c	921	LMG	C40-C41-C42-C43
27	B	621	SQD	C19-C20-C21-C22
24	B	605	CLA	C6-C7-C8-C10
24	B	616	CLA	C12-C13-C15-C16
24	C	507	CLA	C12-C13-C15-C16
24	b	619	CLA	C11-C10-C8-C7
24	b	620	CLA	C12-C13-C15-C16
39	H	102	RRX	C9-C10-C11-C12
39	h	101	RRX	C9-C10-C11-C12
24	b	615	CLA	C16-C17-C18-C20
36	c	919	DGD	C8B-C9B-CAB-CBB
24	b	619	CLA	C8-C10-C11-C12
36	H	103	DGD	O2G-C1B-C2B-C3B
28	D	410	LMG	C20-C21-C22-C23
28	b	624	LMG	C18-C19-C20-C21
35	B	624	HTG	C2'-C1'-S1-C1
27	a	401	SQD	C28-C29-C30-C31
36	c	919	DGD	C2A-C1A-O1G-C1G
27	B	621	SQD	C16-C17-C18-C19
27	B	621	SQD	C17-C18-C19-C20
24	C	508	CLA	C5-C6-C7-C8
27	f	102	SQD	O10-C23-O48-C46
24	B	617	CLA	CAD-CBD-CGD-O2D
24	C	512	CLA	CAD-CBD-CGD-O2D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	b	620	CLA	CAD-CBD-CGD-O2D
24	c	913	CLA	CAD-CBD-CGD-O2D
25	A	408	PHO	CAD-CBD-CGD-O2D
25	A	409	PHO	CAD-CBD-CGD-O2D
24	b	620	CLA	C13-C15-C16-C17
37	L	101	LHG	C28-C29-C30-C31
24	C	502	CLA	C16-C17-C18-C19
27	a	415	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
27	f	102	SQD	O6-C44-C45-C46
37	d	410	LHG	C2-C3-O3-P
36	c	919	DGD	O1A-C1A-O1G-C1G
24	d	405	CLA	C10-C11-C12-C13
24	A	406	CLA	CHA-CBD-CGD-O2D
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O2D
24	C	502	CLA	CHA-CBD-CGD-O1D
24	C	502	CLA	CHA-CBD-CGD-O2D
24	b	613	CLA	CHA-CBD-CGD-O1D
24	c	908	CLA	CHA-CBD-CGD-O1D
24	c	913	CLA	CHA-CBD-CGD-O1D
34	B	623	LMT	C3-C4-C5-C6
24	B	612	CLA	C15-C16-C17-C18
31	c	934	GOL	O2-C2-C3-O3
31	f	104	GOL	O2-C2-C3-O3
31	v	201	GOL	O1-C1-C2-O2
36	C	516	DGD	C5A-C6A-C7A-C8A
24	c	911	CLA	C4-C3-C5-C6
24	A	407	CLA	C13-C15-C16-C17
24	B	616	CLA	C14-C13-C15-C16
24	C	507	CLA	C14-C13-C15-C16
24	b	610	CLA	C11-C12-C13-C14
36	C	516	DGD	C4D-C5D-C6D-O5D
27	f	102	SQD	C27-C28-C29-C30
37	D	409	LHG	C13-C14-C15-C16
37	d	408	LHG	O1-C1-C2-C3
24	B	603	CLA	C13-C15-C16-C17
27	A	412	SQD	C10-C11-C12-C13
28	B	622	LMG	C16-C17-C18-C19
27	F	101	SQD	C26-C27-C28-C29
27	a	401	SQD	C31-C32-C33-C34
24	b	619	CLA	C4-C3-C5-C6
28	C	519	LMG	C12-C13-C14-C15
37	D	407	LHG	C4-O6-P-O5
37	L	101	LHG	C4-O6-P-O5
37	b	639	LHG	C4-O6-P-O5
37	d	409	LHG	C4-O6-P-O5
24	d	401	CLA	C2C-C3C-CAC-CBC
34	B	623	LMT	O1'-C1-C2-C3
24	a	409	CLA	C2C-C3C-CAC-CBC
27	f	102	SQD	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
24	b	619	CLA	C10-C11-C12-C13
27	b	601	SQD	C7-C8-C9-C10
34	B	623	LMT	C5-C6-C7-C8
28	a	416	LMG	C40-C41-C42-C43
24	B	602	CLA	CAD-CBD-CGD-O1D
24	B	606	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	b	605	CLA	CAD-CBD-CGD-O1D
24	b	613	CLA	CAD-CBD-CGD-O1D
24	c	903	CLA	CAD-CBD-CGD-O1D
27	a	401	SQD	C5-C6-S-O7
27	a	401	SQD	C23-C24-C25-C26
37	E	101	LHG	C24-C23-O8-C6
24	C	506	CLA	C16-C17-C18-C19
24	c	905	CLA	C11-C12-C13-C15
24	c	911	CLA	C2-C3-C5-C6
27	B	621	SQD	C11-C10-C9-C8
28	a	416	LMG	C12-C13-C14-C15
36	c	917	DGD	CAA-CBA-CCA-CDA
36	c	918	DGD	CBB-CCB-CDB-CEB
37	d	408	LHG	C7-C8-C9-C10
37	E	101	LHG	O10-C23-O8-C6
27	A	417	SQD	C24-C25-C26-C27
24	B	602	CLA	C13-C15-C16-C17
27	A	417	SQD	C31-C32-C33-C34
28	C	519	LMG	C10-C11-C12-C13
36	c	917	DGD	O6D-C5D-C6D-O5D
28	D	410	LMG	C32-C33-C34-C35
27	B	621	SQD	O47-C45-C46-O48
28	a	416	LMG	O7-C8-C9-O8
28	C	534	LMG	C29-C30-C31-C32
36	C	517	DGD	C2G-C3G-O3G-C1D
24	a	409	CLA	C16-C17-C18-C20
27	A	412	SQD	C28-C29-C30-C31
27	f	102	SQD	C24-C25-C26-C27
24	B	604	CLA	C6-C7-C8-C9
24	a	413	CLA	C11-C10-C8-C9
24	b	614	CLA	C11-C12-C13-C14
36	C	517	DGD	O6E-C1E-O5D-C6D
36	e	102	DGD	C2B-C3B-C4B-C5B
24	C	502	CLA	C2B-C3B-CAB-CBB
24	D	402	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	c	902	CLA	C2B-C3B-CAB-CBB
24	d	404	CLA	C2B-C3B-CAB-CBB
27	A	412	SQD	C18-C19-C20-C21
36	c	917	DGD	C4D-C5D-C6D-O5D
24	B	609	CLA	C13-C15-C16-C17
24	B	607	CLA	C10-C11-C12-C13
27	B	621	SQD	C46-C45-O47-C7
24	b	618	CLA	C2-C1-O2A-CGA
24	c	903	CLA	C2-C1-O2A-CGA
24	d	404	CLA	C2-C1-O2A-CGA
28	b	624	LMG	C40-C41-C42-C43
27	a	401	SQD	O10-C23-O48-C46
27	a	415	SQD	C14-C15-C16-C17
34	a	402	LMT	O1'-C1-C2-C3
28	C	534	LMG	C16-C17-C18-C19
34	M	302	LMT	O1'-C1-C2-C3
24	C	506	CLA	O1A-CGA-O2A-C1
28	b	624	LMG	C10-C11-C12-C13
24	c	905	CLA	C4-C3-C5-C6
26	D	404	BCR	C5-C6-C7-C8
37	L	101	LHG	C16-C17-C18-C19
27	a	401	SQD	C24-C23-O48-C46
24	C	510	CLA	C16-C17-C18-C20
34	M	303	LMT	O5'-C1'-O1'-C1
28	A	413	LMG	C2-C1-O1-C7
29	a	417	PL9	C24-C26-C27-C28
34	T	703	LMT	C2'-C1'-O1'-C1
34	c	922	LMT	C2'-C1'-O1'-C1
36	C	517	DGD	C2E-C1E-O5D-C6D
37	d	410	LHG	C25-C26-C27-C28
25	A	409	PHO	CHA-CBD-CGD-O1D
37	D	408	LHG	C10-C11-C12-C13
28	A	413	LMG	O1-C7-C8-C9
27	b	601	SQD	C27-C28-C29-C30
24	B	607	CLA	C12-C13-C15-C16
24	B	610	CLA	C2-C3-C5-C6
24	a	410	CLA	C6-C7-C8-C10
24	c	908	CLA	C11-C10-C8-C7
25	A	408	PHO	C2-C3-C5-C6
28	d	411	LMG	C12-C13-C14-C15
24	a	410	CLA	C11-C10-C8-C9
24	c	905	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
35	H	105	HTG	C3'-C4'-C5'-C6'
31	C	527	GOL	O1-C1-C2-C3
31	V	204	GOL	O1-C1-C2-C3
31	u	202	GOL	O1-C1-C2-C3
37	D	409	LHG	O1-C1-C2-C3
28	c	921	LMG	C35-C36-C37-C38
28	B	622	LMG	C30-C31-C32-C33
24	D	403	CLA	C8-C10-C11-C12
31	A	422	GOL	O2-C2-C3-O3
31	u	202	GOL	O2-C2-C3-O3
28	B	622	LMG	C15-C16-C17-C18
37	E	101	LHG	C24-C25-C26-C27
24	B	616	CLA	C16-C17-C18-C19
24	C	513	CLA	C10-C11-C12-C13
27	A	412	SQD	C30-C31-C32-C33
28	c	921	LMG	C33-C34-C35-C36
24	C	504	CLA	C4B-C3B-CAB-CBB
24	D	402	CLA	C4B-C3B-CAB-CBB
24	d	404	CLA	C4B-C3B-CAB-CBB
28	A	413	LMG	O6-C1-O1-C7
34	T	703	LMT	O5'-C1'-O1'-C1
34	c	922	LMT	O5'-C1'-O1'-C1
24	C	511	CLA	O1A-CGA-O2A-C1
37	b	639	LHG	C31-C32-C33-C34
24	d	405	CLA	O1A-CGA-O2A-C1
38	V	202	HEM	C4C-C3C-CAC-CBC
38	v	202	HEM	C4B-C3B-CAB-CBB
36	H	103	DGD	C7A-C8A-C9A-CAA
36	c	917	DGD	C2B-C3B-C4B-C5B
36	h	102	DGD	C7A-C8A-C9A-CAA
24	B	610	CLA	C4-C3-C5-C6
25	A	408	PHO	C4-C3-C5-C6
24	a	413	CLA	C2-C3-C5-C6
24	b	615	CLA	C2-C3-C5-C6
29	D	405	PL9	C13-C14-C16-C17
24	B	614	CLA	C2-C1-O2A-CGA
24	D	402	CLA	C2-C1-O2A-CGA
37	E	101	LHG	C33-C34-C35-C36
24	A	405	CLA	C2C-C3C-CAC-CBC
24	B	611	CLA	C2A-CAA-CBA-CGA
35	u	201	HTG	S1-C1-C2-O2
36	C	516	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
24	c	906	CLA	C3A-C2A-CAA-CBA
24	a	413	CLA	C4-C3-C5-C6
29	D	405	PL9	C15-C14-C16-C17
29	a	417	PL9	C4-C3-C7-C8
24	A	407	CLA	C11-C12-C13-C14
24	B	615	CLA	C11-C10-C8-C9
24	C	512	CLA	C11-C12-C13-C14
24	b	620	CLA	C6-C7-C8-C9
38	V	202	HEM	CAD-CBD-CGD-O1D
38	V	202	HEM	CAD-CBD-CGD-O2D
27	b	601	SQD	C25-C26-C27-C28
27	b	601	SQD	C31-C32-C33-C34
37	b	639	LHG	C16-C17-C18-C19
24	B	616	CLA	C16-C17-C18-C20
24	b	614	CLA	C16-C17-C18-C20
24	c	906	CLA	C16-C17-C18-C19
27	A	417	SQD	C24-C23-O48-C46
34	a	402	LMT	O5'-C1'-O1'-C1
36	c	917	DGD	O6E-C1E-O5D-C6D
29	A	414	PL9	C39-C41-C42-C43
28	B	622	LMG	C36-C37-C38-C39
38	v	202	HEM	CAD-CBD-CGD-O2D
27	b	601	SQD	C44-C45-O47-C7
27	b	601	SQD	C46-C45-O47-C7
24	C	504	CLA	C6-C7-C8-C10
24	b	605	CLA	C12-C13-C15-C16
24	c	904	CLA	C6-C7-C8-C10
24	c	913	CLA	C12-C13-C15-C16
38	v	202	HEM	CAD-CBD-CGD-O1D
37	e	101	LHG	C2-C3-O3-P
24	c	913	CLA	C10-C11-C12-C13
37	D	409	LHG	C10-C11-C12-C13
28	A	413	LMG	O8-C28-C29-C30
24	D	403	CLA	C10-C11-C12-C13
28	C	519	LMG	C39-C40-C41-C42
27	F	101	SQD	C28-C29-C30-C31
35	b	626	HTG	C2'-C3'-C4'-C5'
27	B	621	SQD	C7-C8-C9-C10
29	d	407	PL9	C13-C14-C16-C17
24	C	504	CLA	C2B-C3B-CAB-CBB
28	c	920	LMG	C31-C32-C33-C34
27	a	415	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	A	412	SQD	O6-C44-C45-O47
27	b	601	SQD	C19-C20-C21-C22
37	E	101	LHG	C35-C36-C37-C38
27	a	401	SQD	C13-C14-C15-C16
36	C	516	DGD	O6E-C1E-O5D-C6D
28	A	413	LMG	C36-C37-C38-C39
24	b	619	CLA	C2-C3-C5-C6
24	d	401	CLA	C4C-C3C-CAC-CBC
24	b	614	CLA	C16-C17-C18-C19
24	b	607	CLA	C6-C7-C8-C9
27	A	417	SQD	O10-C23-O48-C46
36	D	406	DGD	C8A-C9A-CAA-CBA
28	b	624	LMG	C28-C29-C30-C31
24	B	602	CLA	CAA-CBA-CGA-O2A
37	D	407	LHG	C29-C30-C31-C32
26	C	514	BCR	C23-C24-C25-C30
26	C	515	BCR	C23-C24-C25-C30
26	D	404	BCR	C1-C6-C7-C8
26	K	101	BCR	C1-C6-C7-C8
26	Y	101	BCR	C23-C24-C25-C30
26	c	915	BCR	C1-C6-C7-C8
26	c	916	BCR	C1-C6-C7-C8
26	d	406	BCR	C1-C6-C7-C8
26	k	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C23-C24-C25-C30
39	H	102	RRX	C23-C24-C25-C30
39	h	101	RRX	C23-C24-C25-C30
36	D	406	DGD	O1G-C1A-C2A-C3A
36	e	102	DGD	O1G-C1A-C2A-C3A
35	H	105	HTG	C2'-C3'-C4'-C5'
31	v	201	GOL	O1-C1-C2-C3
34	C	520	LMT	O1'-C1-C2-C3
24	B	604	CLA	C5-C6-C7-C8
24	B	613	CLA	C13-C15-C16-C17
27	B	621	SQD	C45-C44-O6-C1
36	C	516	DGD	C5D-C6D-O5D-C1E
36	c	917	DGD	C5D-C6D-O5D-C1E
24	c	904	CLA	C5-C6-C7-C8
37	E	101	LHG	C11-C12-C13-C14
24	d	405	CLA	CBA-CGA-O2A-C1
35	b	626	HTG	C4'-C5'-C6'-C7'
24	c	904	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	c	906	CLA	C16-C17-C18-C20
24	B	613	CLA	C8-C10-C11-C12
24	A	405	CLA	C4C-C3C-CAC-CBC
24	B	604	CLA	C6-C7-C8-C10
24	B	614	CLA	C11-C10-C8-C7
24	b	607	CLA	C6-C7-C8-C10
31	B	631	GOL	O2-C2-C3-O3
27	b	601	SQD	C35-C36-C37-C38
27	A	417	SQD	C25-C26-C27-C28
35	c	924	HTG	O5-C5-C6-O6
27	b	601	SQD	C11-C10-C9-C8
24	C	506	CLA	CBA-CGA-O2A-C1
24	B	606	CLA	C8-C10-C11-C12
24	a	409	CLA	C4C-C3C-CAC-CBC
24	b	605	CLA	C11-C10-C8-C9
24	b	606	CLA	C14-C13-C15-C16
24	c	910	CLA	C6-C7-C8-C9
36	D	406	DGD	O6D-C5D-C6D-O5D
24	B	604	CLA	CAD-CBD-CGD-O2D
24	B	605	CLA	CAD-CBD-CGD-O2D
24	B	611	CLA	CAD-CBD-CGD-O2D
24	B	613	CLA	CAD-CBD-CGD-O2D
24	C	510	CLA	CAD-CBD-CGD-O2D
24	b	607	CLA	CAD-CBD-CGD-O2D
24	b	608	CLA	CAD-CBD-CGD-O2D
24	b	609	CLA	CAD-CBD-CGD-O2D
24	b	616	CLA	CAD-CBD-CGD-O2D
24	c	902	CLA	CAD-CBD-CGD-O2D
24	c	910	CLA	CAD-CBD-CGD-O2D
24	b	619	CLA	C5-C6-C7-C8
24	C	510	CLA	C2-C3-C5-C6
28	a	416	LMG	O8-C28-C29-C30
34	m	1502	LMT	O5'-C5'-C6'-O6'
25	a	412	PHO	C2C-C3C-CAC-CBC
24	B	616	CLA	C5-C6-C7-C8
24	C	503	CLA	C10-C11-C12-C13
24	C	503	CLA	C15-C16-C17-C18
28	C	534	LMG	C11-C12-C13-C14
24	b	607	CLA	C13-C15-C16-C17
24	B	617	CLA	O2A-C1-C2-C3
24	C	509	CLA	O2A-C1-C2-C3
24	c	910	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
24	c	913	CLA	O2A-C1-C2-C3
25	A	408	PHO	O2A-C1-C2-C3
25	a	411	PHO	O2A-C1-C2-C3
34	D	401	LMT	C11-C10-C9-C8
38	V	202	HEM	C4B-C3B-CAB-CBB
38	v	202	HEM	C4C-C3C-CAC-CBC
24	b	608	CLA	C13-C15-C16-C17
27	B	621	SQD	C29-C30-C31-C32
27	b	601	SQD	C23-C24-C25-C26
27	b	601	SQD	C45-C46-O48-C23
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	C	512	CLA	CHA-CBD-CGD-O2D
24	b	605	CLA	CHA-CBD-CGD-O1D
24	b	606	CLA	CHA-CBD-CGD-O1D
24	b	606	CLA	CHA-CBD-CGD-O2D
24	c	903	CLA	CHA-CBD-CGD-O2D
24	d	401	CLA	CHA-CBD-CGD-O2D
24	b	619	CLA	C16-C17-C18-C19
28	C	534	LMG	C19-C20-C21-C22
25	a	411	PHO	C8-C10-C11-C12
28	B	622	LMG	O9-C10-O7-C8
24	C	501	CLA	C2A-CAA-CBA-CGA
34	m	1503	LMT	C1-C2-C3-C4
25	a	411	PHO	CHA-CBD-CGD-O1D
25	a	412	PHO	CHA-CBD-CGD-O1D
25	a	412	PHO	CHA-CBD-CGD-O2D
31	b	632	GOL	O1-C1-C2-O2
36	C	518	DGD	O6E-C5E-C6E-O5E
27	A	417	SQD	C11-C12-C13-C14
24	A	405	CLA	C13-C15-C16-C17
24	c	905	CLA	C2-C3-C5-C6
29	A	414	PL9	C4-C3-C7-C8
28	b	624	LMG	O9-C10-O7-C8
37	d	409	LHG	C26-C27-C28-C29
24	C	504	CLA	C6-C7-C8-C9
24	b	617	CLA	C2B-C3B-CAB-CBB
24	c	904	CLA	C2B-C3B-CAB-CBB
24	d	401	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	B	614	CLA	CAA-CBA-CGA-O2A
24	c	904	CLA	C15-C16-C17-C18
24	B	605	CLA	C13-C15-C16-C17
24	c	907	CLA	C5-C6-C7-C8
24	b	619	CLA	C16-C17-C18-C20
24	A	406	CLA	C4C-C3C-CAC-CBC
24	b	615	CLA	C4-C3-C5-C6
31	A	419	GOL	C1-C2-C3-O3
37	d	410	LHG	C16-C17-C18-C19
24	b	616	CLA	CBA-CGA-O2A-C1
28	C	519	LMG	C35-C36-C37-C38
24	C	512	CLA	C1A-C2A-CAA-CBA
24	D	403	CLA	O1A-CGA-O2A-C1
24	B	602	CLA	C2-C1-O2A-CGA
24	b	612	CLA	C2-C1-O2A-CGA
24	b	617	CLA	C2-C1-O2A-CGA
27	B	621	SQD	C26-C27-C28-C29
24	c	908	CLA	C2A-CAA-CBA-CGA
24	b	605	CLA	CAA-CBA-CGA-O1A
38	F	102	HEM	CAD-CBD-CGD-O1D
27	a	415	SQD	C19-C20-C21-C22
34	T	703	LMT	C11-C10-C9-C8
29	d	407	PL9	C15-C14-C16-C17
36	c	917	DGD	C2E-C1E-O5D-C6D
36	c	918	DGD	C2E-C1E-O5D-C6D
24	a	409	CLA	C13-C15-C16-C17
24	c	910	CLA	C10-C11-C12-C13
28	b	624	LMG	C29-C30-C31-C32
34	Z	101	LMT	C5-C6-C7-C8
24	B	616	CLA	C4B-C3B-CAB-CBB
24	a	410	CLA	C4B-C3B-CAB-CBB
37	D	408	LHG	C4-O6-P-O5
28	A	413	LMG	C30-C31-C32-C33
24	A	410	CLA	C8-C10-C11-C12
26	c	916	BCR	C23-C24-C25-C30
24	C	501	CLA	C13-C15-C16-C17
24	c	911	CLA	CAA-CBA-CGA-O2A
24	b	616	CLA	C8-C10-C11-C12
36	H	103	DGD	C9A-CAA-CBA-CCA
35	o	301	HTG	S1-C1'-C2'-C3'
36	h	102	DGD	O1B-C1B-C2B-C3B
24	B	608	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	B	610	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	b	611	CLA	CAD-CBD-CGD-O1D
24	c	905	CLA	CAD-CBD-CGD-O1D
24	d	401	CLA	CAD-CBD-CGD-O1D
27	a	401	SQD	C5-C6-S-O9
24	c	912	CLA	O1A-CGA-O2A-C1
24	C	510	CLA	CAA-CBA-CGA-O2A
37	D	408	LHG	O2-C2-C3-O3
24	C	508	CLA	C11-C10-C8-C9
24	c	910	CLA	C14-C13-C15-C16
27	a	401	SQD	C17-C18-C19-C20
31	C	527	GOL	O1-C1-C2-O2
31	t	902	GOL	O2-C2-C3-O3
36	h	102	DGD	C9A-CAA-CBA-CCA
35	b	602	HTG	C3'-C4'-C5'-C6'
24	C	512	CLA	CAA-CBA-CGA-O2A
37	E	101	LHG	C13-C14-C15-C16
35	c	924	HTG	S1-C1'-C2'-C3'
28	c	920	LMG	C22-C23-C24-C25
24	d	401	CLA	C15-C16-C17-C18
24	B	613	CLA	CAA-CBA-CGA-O2A
28	C	519	LMG	O7-C10-C11-C12
37	E	101	LHG	O8-C23-C24-C25
28	d	411	LMG	C32-C33-C34-C35
38	f	101	HEM	CAA-CBA-CGA-O2A
28	A	413	LMG	C20-C21-C22-C23
24	C	505	CLA	CAA-CBA-CGA-O2A
24	b	617	CLA	CAA-CBA-CGA-O2A
24	A	405	CLA	C15-C16-C17-C18
37	E	101	LHG	O10-C23-C24-C25
26	a	414	BCR	C19-C20-C21-C22
28	b	624	LMG	C15-C16-C17-C18
36	D	406	DGD	CCA-CDA-CEA-CFA
36	c	919	DGD	O1G-C1A-C2A-C3A
36	c	918	DGD	O6E-C1E-O5D-C6D
24	B	614	CLA	CAA-CBA-CGA-O1A
37	E	101	LHG	C31-C32-C33-C34
28	D	410	LMG	O7-C10-C11-C12
36	C	517	DGD	O2G-C1B-C2B-C3B
37	D	407	LHG	O8-C23-C24-C25
24	C	512	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
27	B	621	SQD	C25-C26-C27-C28
24	B	603	CLA	C8-C10-C11-C12
24	C	508	CLA	C13-C15-C16-C17
24	b	614	CLA	C5-C6-C7-C8
28	D	410	LMG	O9-C10-C11-C12
24	c	902	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

158 monomers are involved in 284 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	b	625	LMT	1	0
24	c	903	CLA	1	0
31	c	936	GOL	1	0
37	d	409	LHG	2	0
28	C	534	LMG	1	0
26	c	916	BCR	2	0
24	b	619	CLA	4	0
37	d	408	LHG	1	0
24	B	608	CLA	1	0
26	T	702	BCR	5	0
35	b	603	HTG	1	0
25	A	408	PHO	1	0
35	H	105	HTG	1	0
24	B	606	CLA	3	0
38	V	202	HEM	1	0
31	c	929	GOL	1	0
24	d	405	CLA	2	0
24	b	607	CLA	2	0
36	h	102	DGD	1	0
26	b	623	BCR	2	0
24	D	403	CLA	1	0
34	C	520	LMT	4	0
24	b	609	CLA	4	0
27	B	621	SQD	1	0
24	C	501	CLA	5	0
24	C	512	CLA	6	0
24	b	617	CLA	3	0
24	C	513	CLA	7	0
24	b	616	CLA	1	0
24	c	904	CLA	4	0
29	a	417	PL9	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	422	GOL	1	0
37	e	101	LHG	2	0
24	B	615	CLA	8	0
27	A	412	SQD	2	0
26	b	621	BCR	2	0
35	U	201	HTG	1	0
27	a	415	SQD	6	0
24	C	510	CLA	2	0
27	f	102	SQD	1	0
26	B	619	BCR	5	0
36	e	102	DGD	1	0
26	k	101	BCR	2	0
24	b	606	CLA	1	0
24	b	613	CLA	2	0
27	b	601	SQD	1	0
26	C	514	BCR	2	0
31	c	937	GOL	1	0
27	a	401	SQD	1	0
28	c	921	LMG	1	0
36	c	919	DGD	1	0
24	c	914	CLA	5	0
26	K	101	BCR	1	0
28	A	413	LMG	2	0
34	Z	101	LMT	1	0
24	C	507	CLA	2	0
35	C	521	HTG	3	0
24	B	604	CLA	2	0
34	B	623	LMT	1	0
24	c	912	CLA	3	0
24	c	908	CLA	3	0
24	B	614	CLA	3	0
24	D	402	CLA	1	0
31	C	530	GOL	1	0
24	c	905	CLA	1	0
24	c	907	CLA	3	0
26	b	622	BCR	3	0
24	C	503	CLA	3	0
31	c	926	GOL	2	0
34	a	402	LMT	1	0
26	B	620	BCR	1	0
24	b	614	CLA	3	0
28	B	622	LMG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	M	303	LMT	1	0
26	c	915	BCR	3	0
24	C	502	CLA	4	0
37	d	410	LHG	4	0
25	A	409	PHO	2	0
24	C	504	CLA	1	0
37	L	101	LHG	1	0
24	b	620	CLA	3	0
24	B	613	CLA	2	0
24	B	607	CLA	2	0
24	B	616	CLA	4	0
35	b	627	HTG	1	0
36	H	103	DGD	1	0
28	D	410	LMG	3	0
28	a	416	LMG	2	0
35	b	626	HTG	1	0
24	b	605	CLA	3	0
24	A	405	CLA	3	0
27	F	101	SQD	1	0
28	C	519	LMG	1	0
37	E	101	LHG	6	0
26	y	101	BCR	2	0
24	c	909	CLA	3	0
36	C	518	DGD	1	0
31	O	306	GOL	1	0
31	a	420	GOL	1	0
34	m	1502	LMT	1	0
36	C	517	DGD	3	0
26	t	903	BCR	6	0
35	d	403	HTG	1	0
37	b	639	LHG	2	0
24	d	404	CLA	1	0
26	Y	101	BCR	1	0
27	A	417	SQD	1	0
26	C	515	BCR	2	0
24	c	906	CLA	5	0
34	M	302	LMT	1	0
39	h	101	RRX	3	0
31	A	420	GOL	1	0
38	F	102	HEM	2	0
31	h	103	GOL	1	0
31	c	932	GOL	1	0

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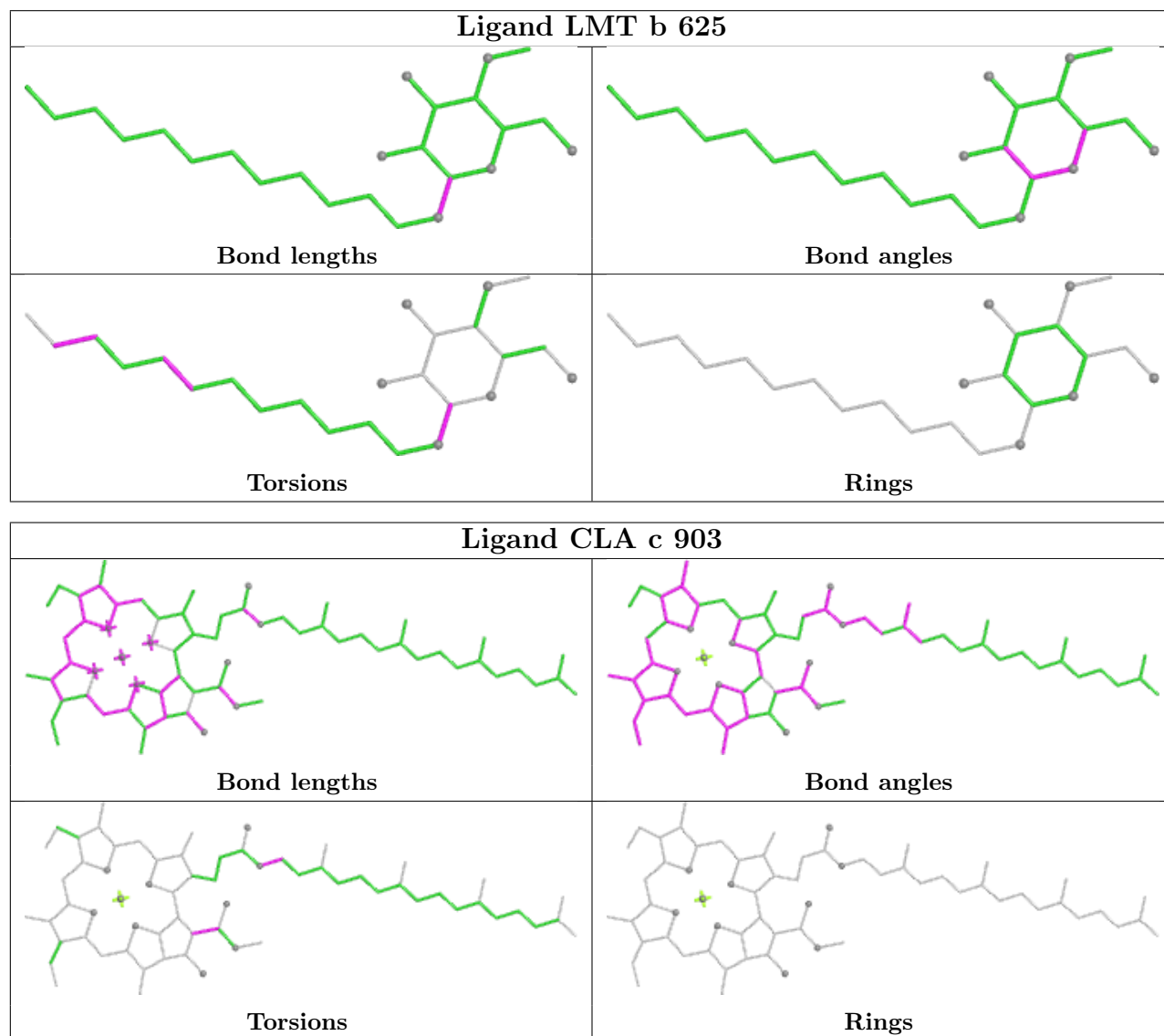
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	b	624	LMG	1	0
24	a	413	CLA	1	0
24	d	401	CLA	4	0
24	a	409	CLA	4	0
39	H	102	RRX	2	0
24	B	610	CLA	1	0
24	C	509	CLA	3	0
24	b	615	CLA	1	0
26	d	406	BCR	1	0
24	A	406	CLA	2	0
25	a	412	PHO	1	0
31	H	101	GOL	1	0
24	C	508	CLA	4	0
24	c	913	CLA	3	0
24	B	605	CLA	1	0
36	C	516	DGD	1	0
24	c	902	CLA	3	0
31	B	630	GOL	1	0
24	B	612	CLA	1	0
31	C	531	GOL	3	0
24	B	617	CLA	3	0
24	B	611	CLA	4	0
24	b	610	CLA	3	0
26	a	414	BCR	2	0
38	f	101	HEM	2	0
31	c	927	GOL	3	0
24	b	618	CLA	1	0
26	D	404	BCR	2	0
26	B	618	BCR	2	0
29	A	414	PL9	5	0
35	C	528	HTG	1	0
35	c	924	HTG	1	0
37	D	409	LHG	4	0
24	A	407	CLA	2	0
24	A	410	CLA	2	0
24	b	608	CLA	2	0
24	C	511	CLA	3	0
24	C	505	CLA	2	0
24	C	506	CLA	3	0
24	B	602	CLA	1	0
36	D	406	DGD	4	0
24	c	910	CLA	2	0

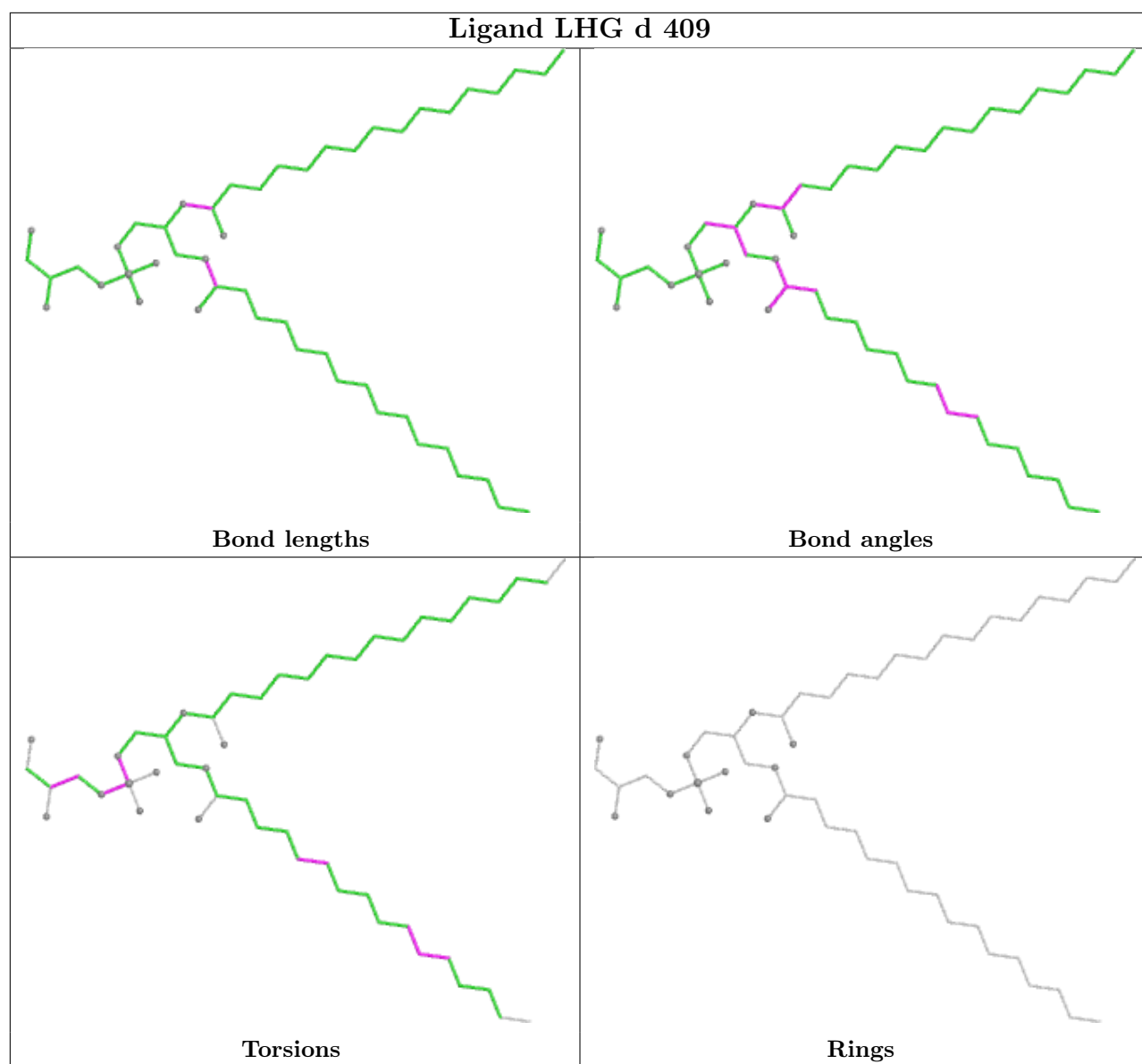
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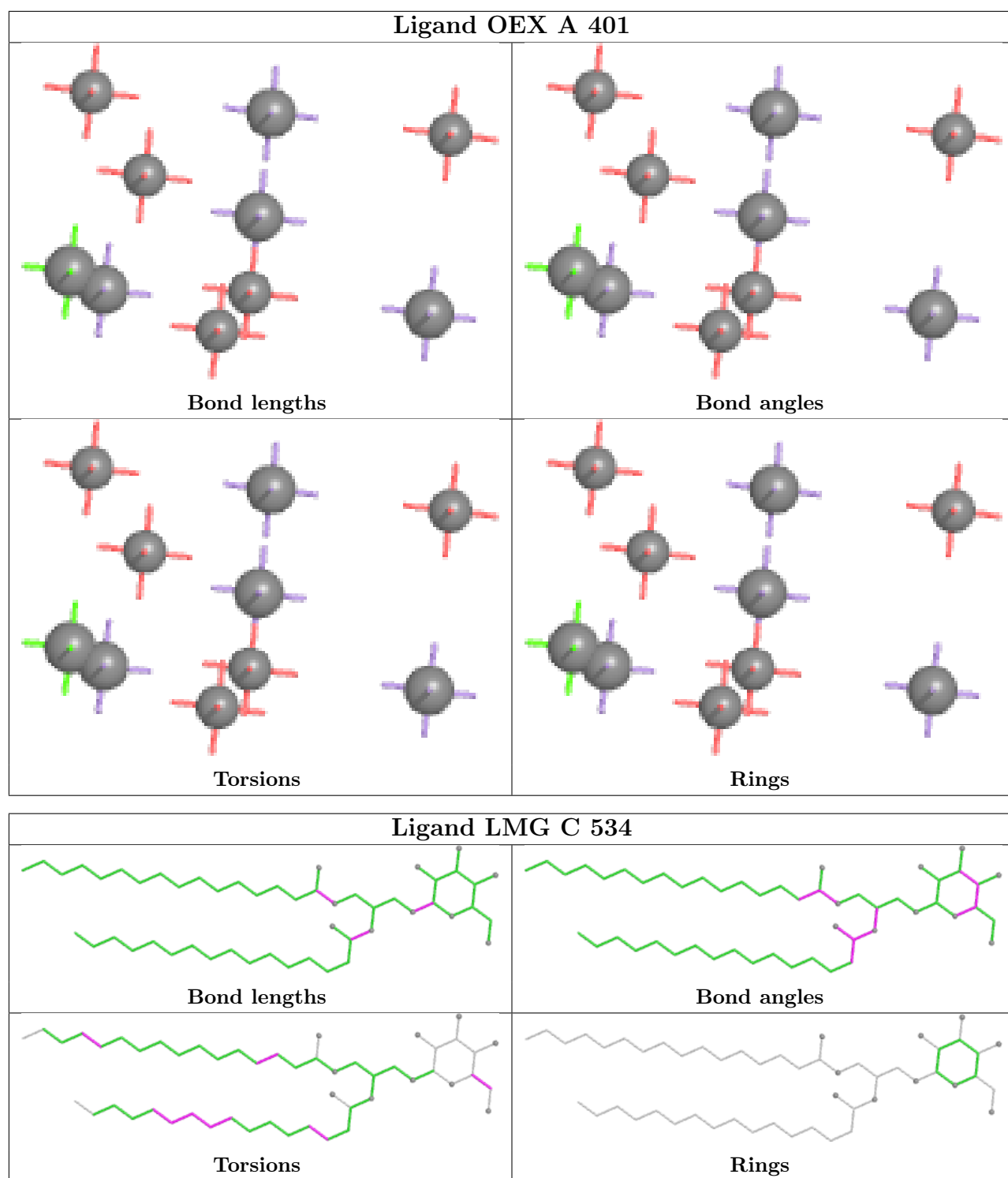
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	z	101	LMT	4	0

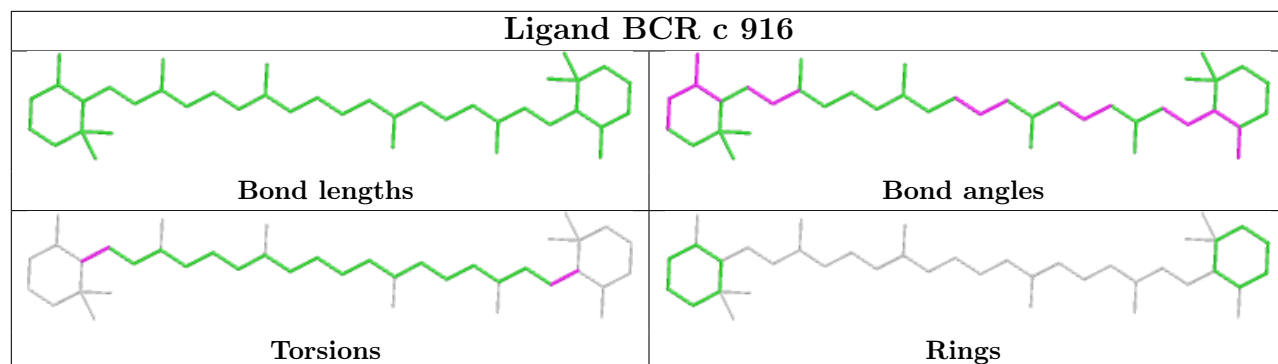
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



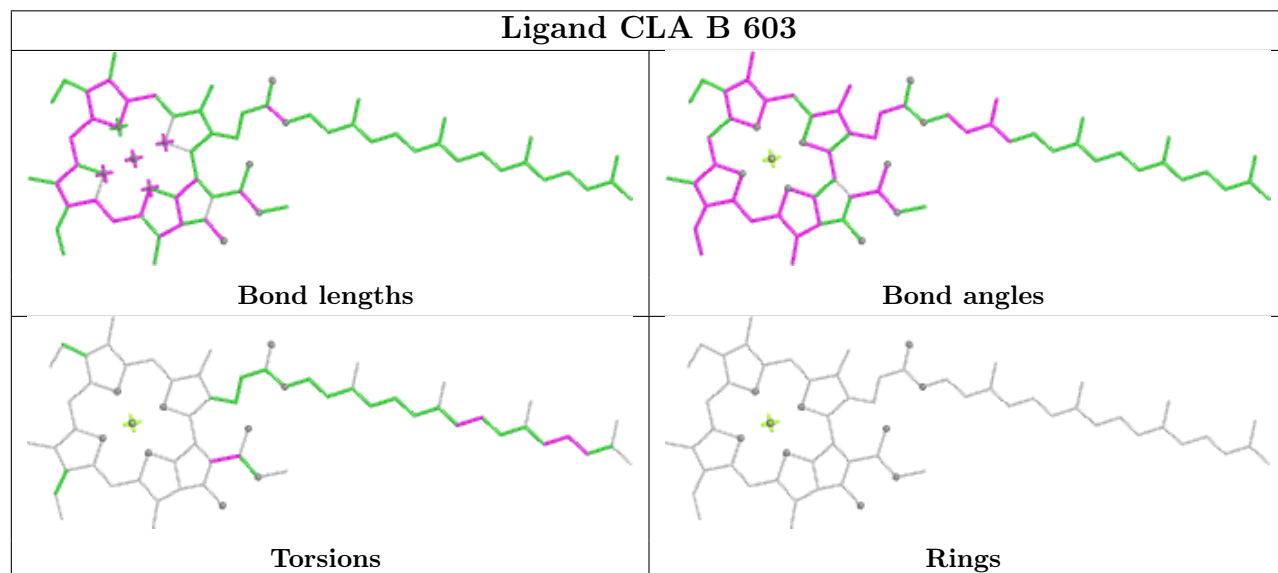




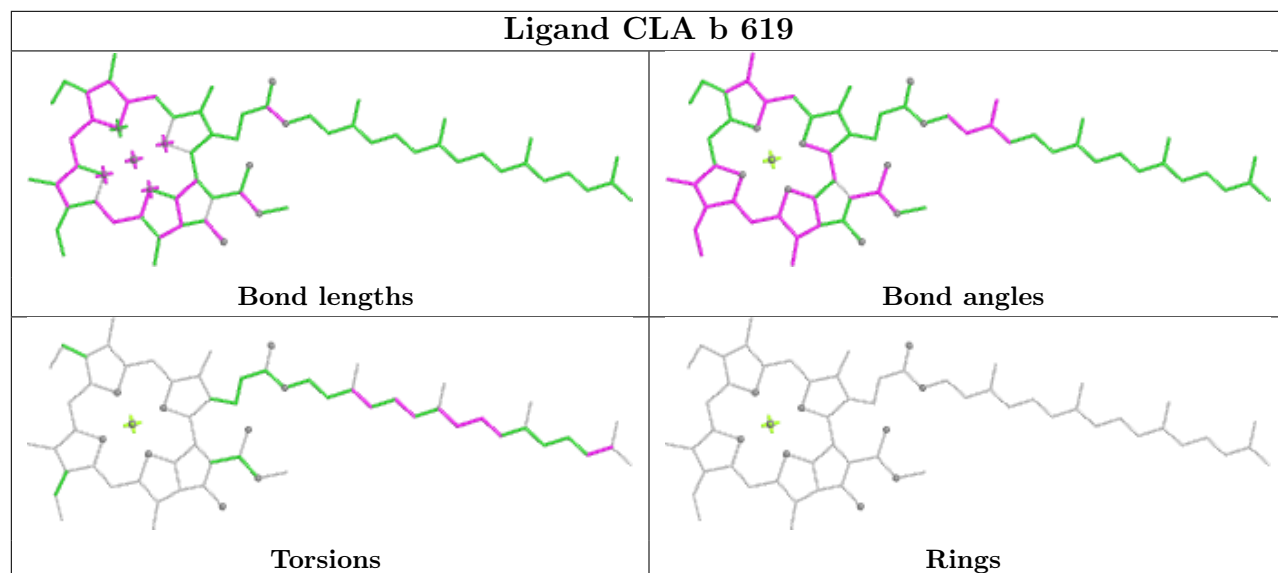
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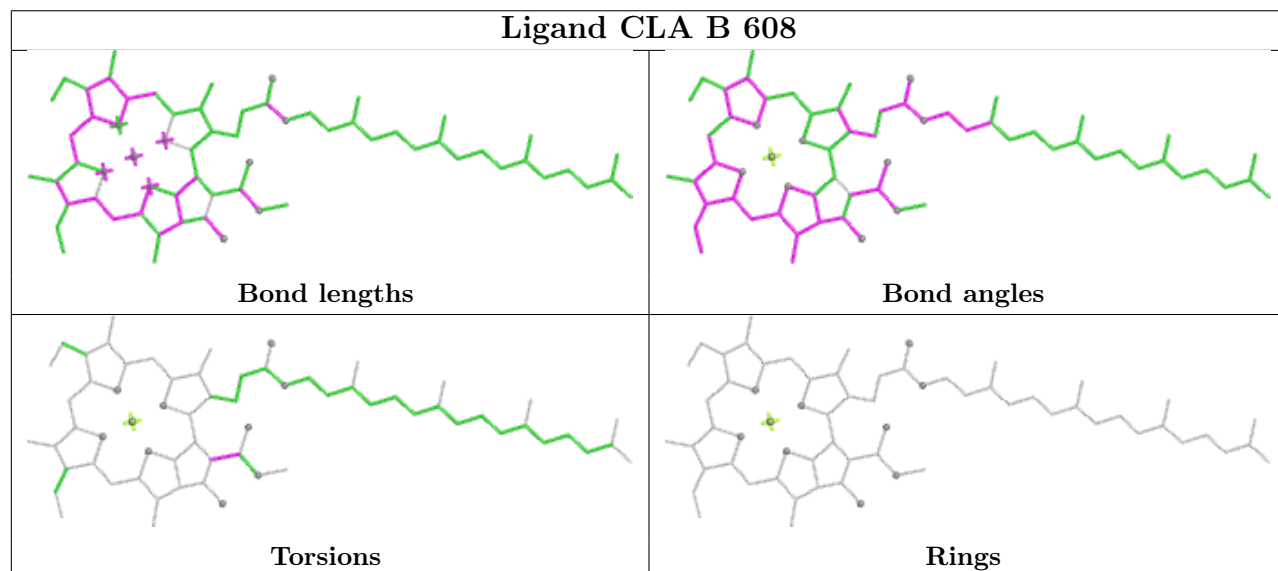
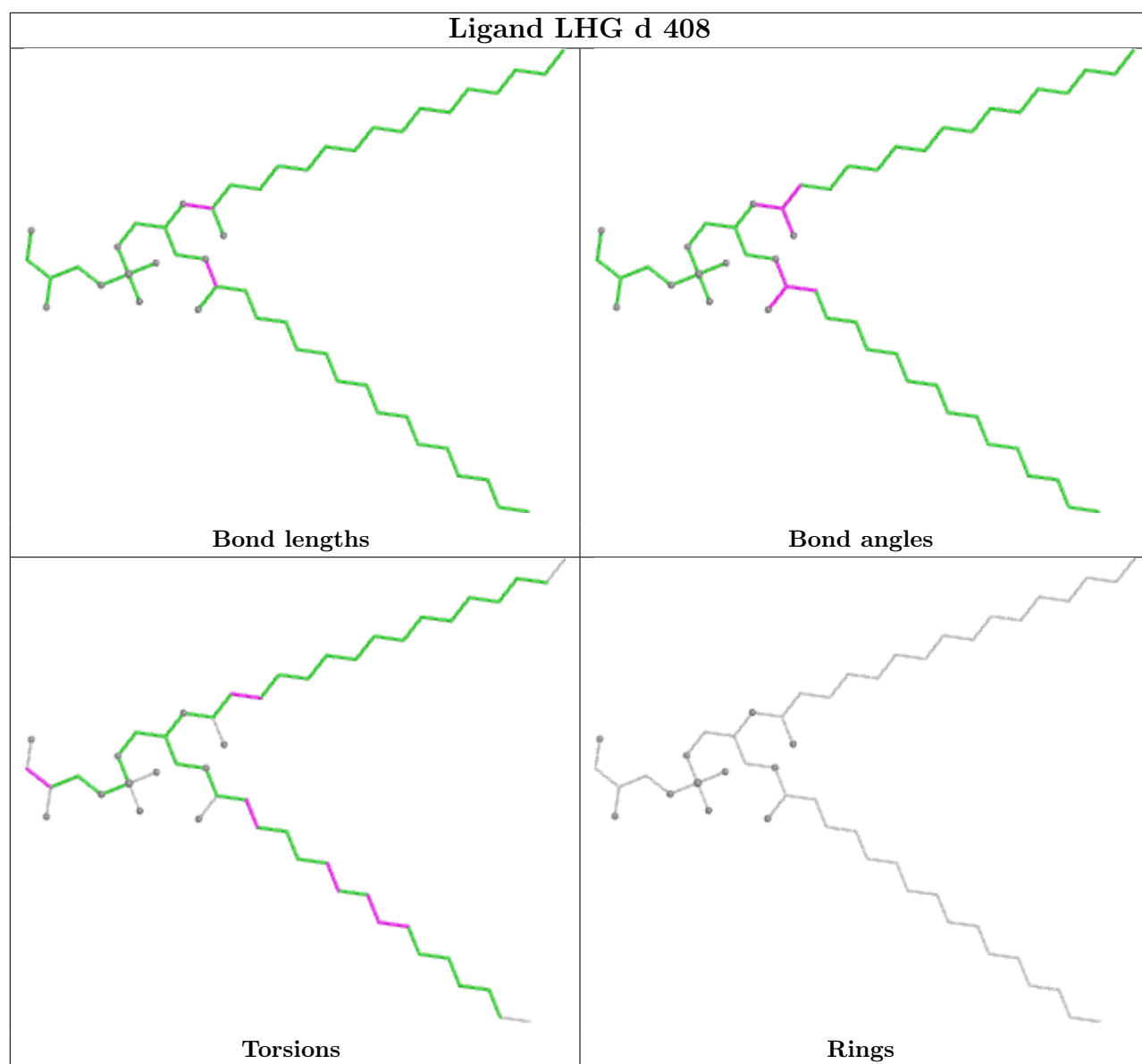


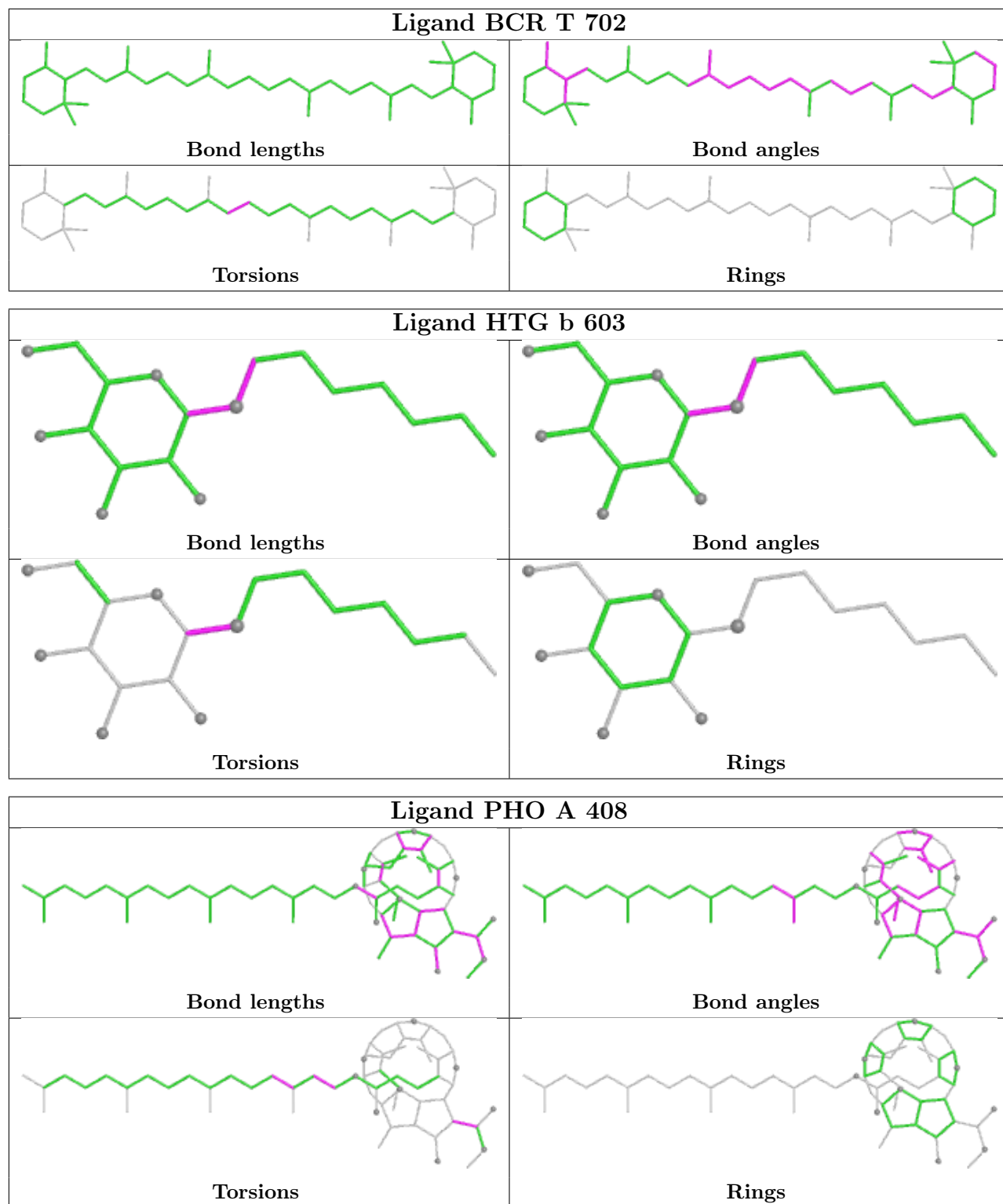
Ligand CLA B 603

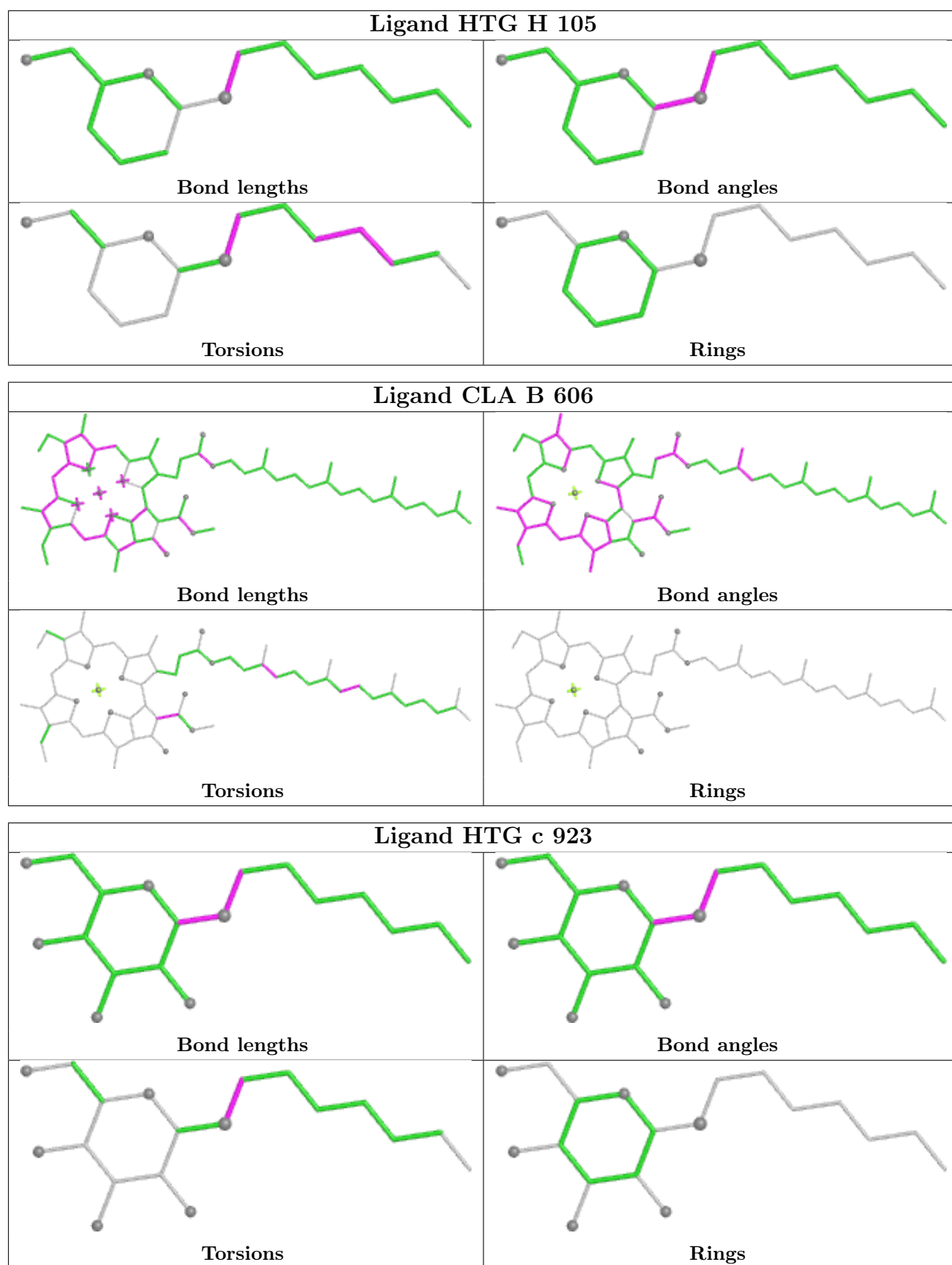


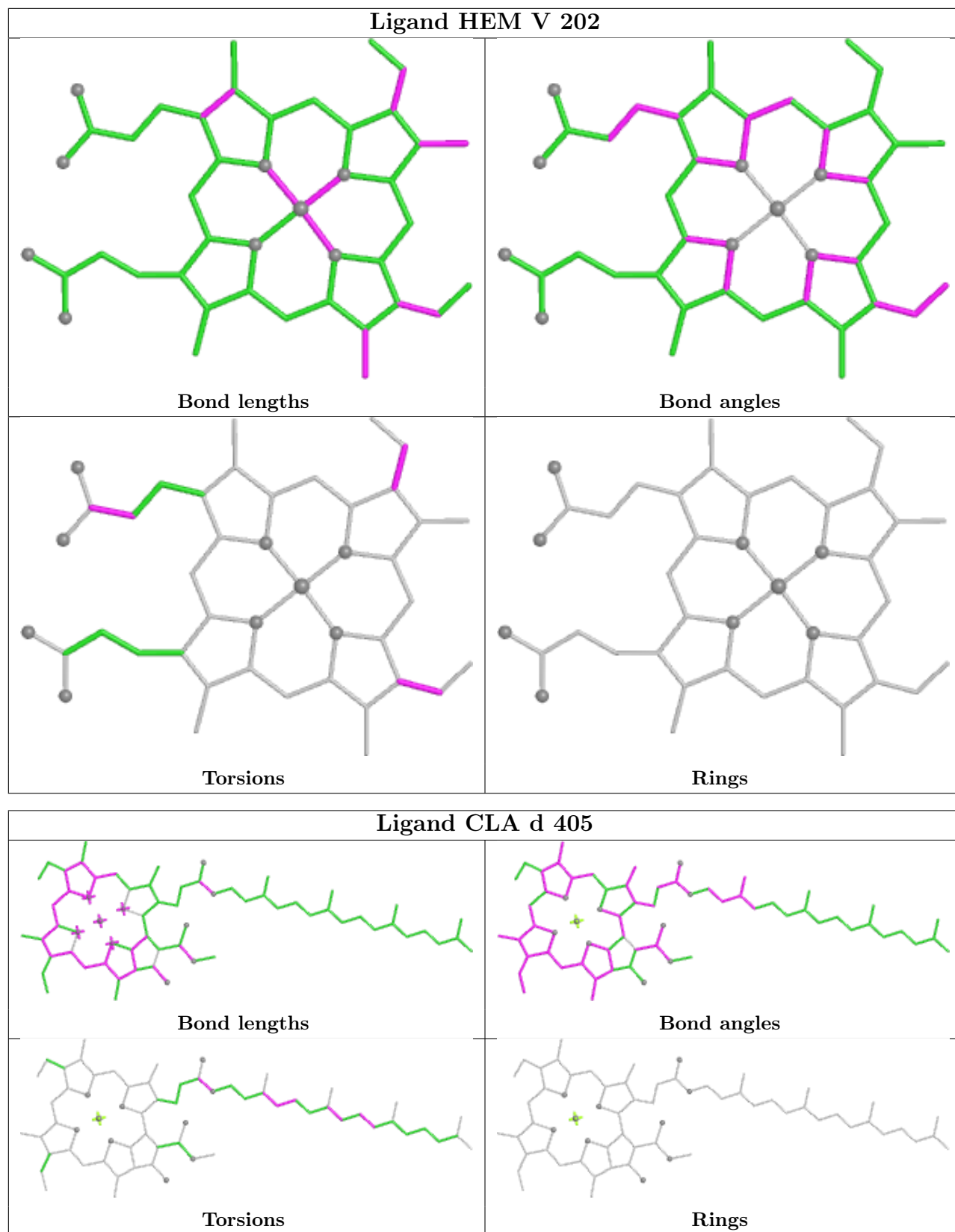
Ligand CLA b 619

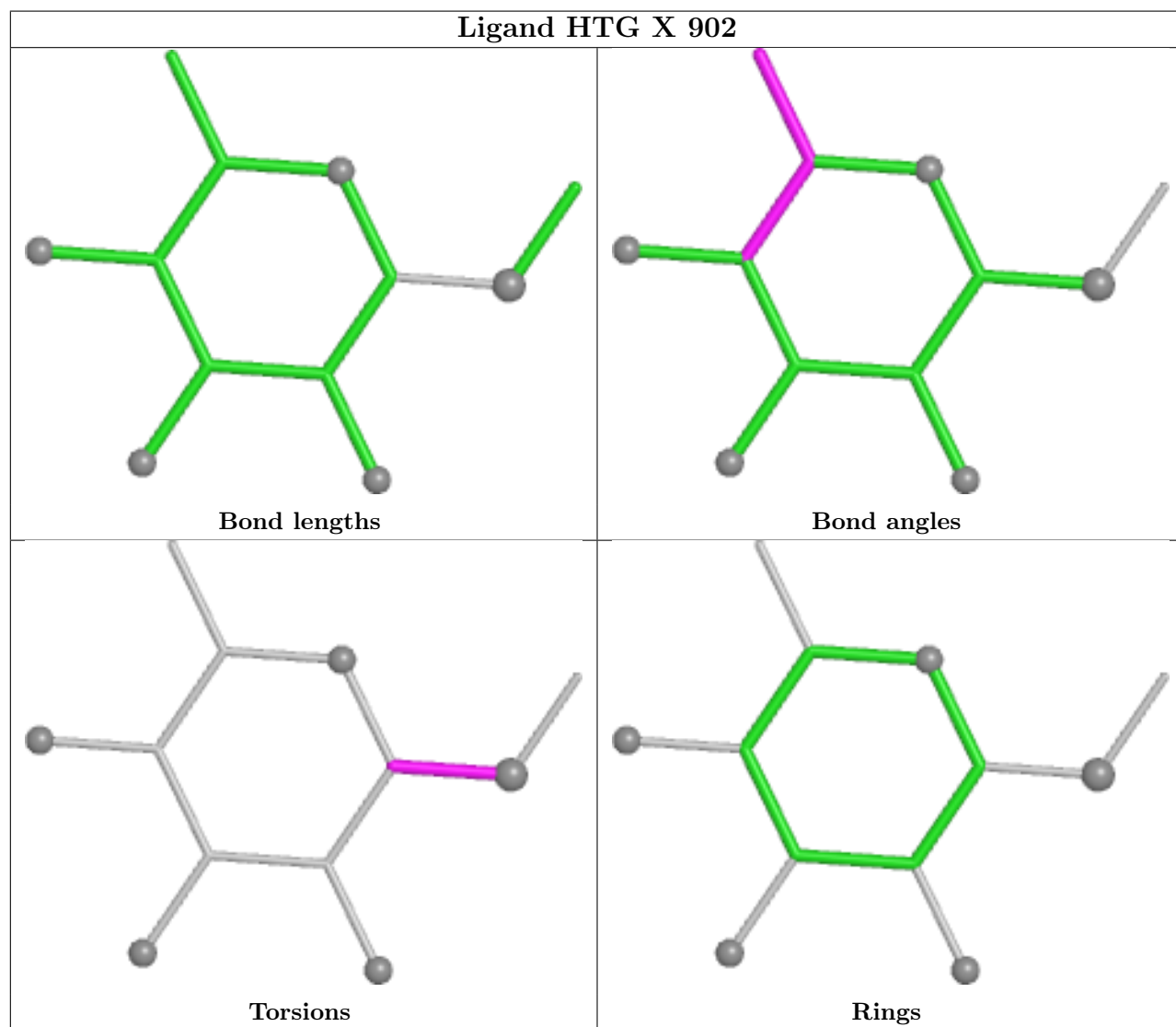
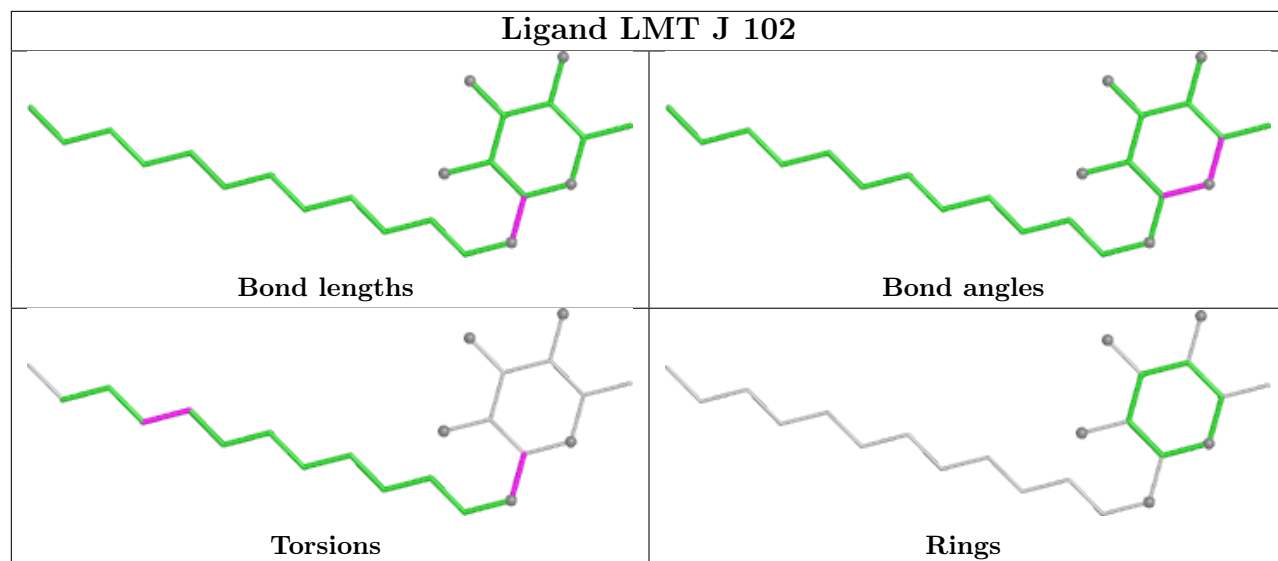


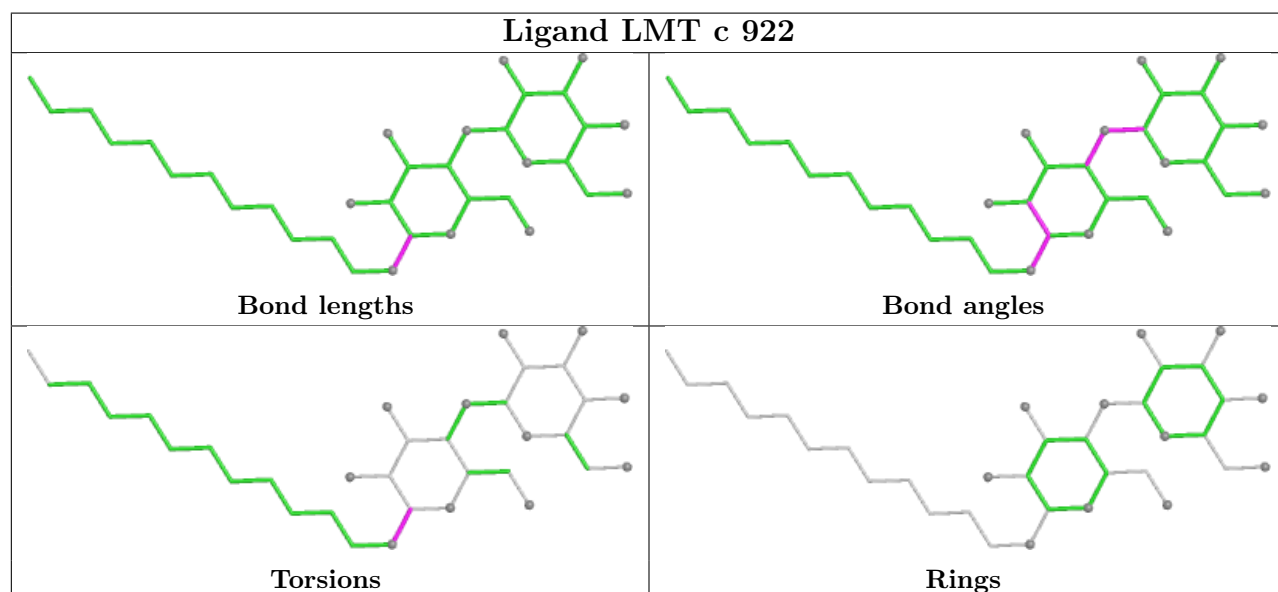
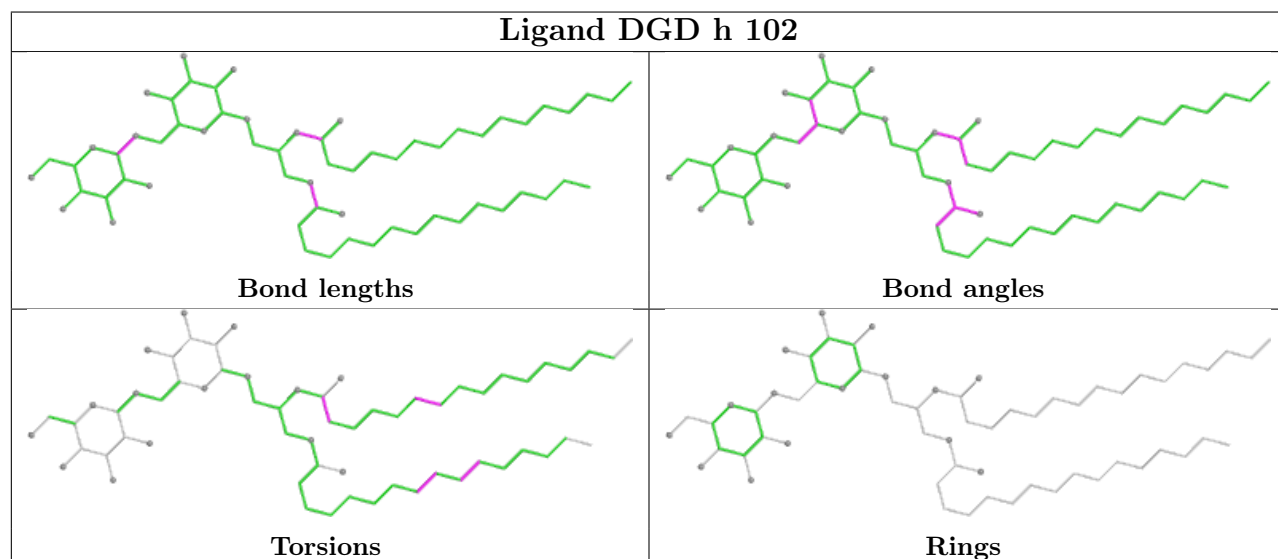
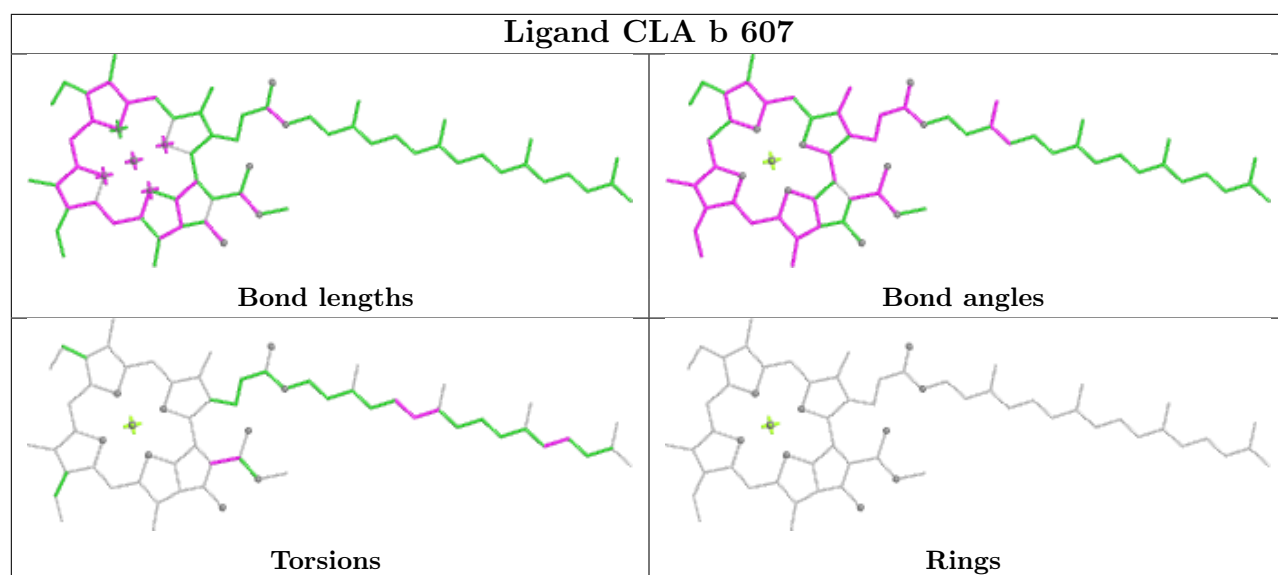


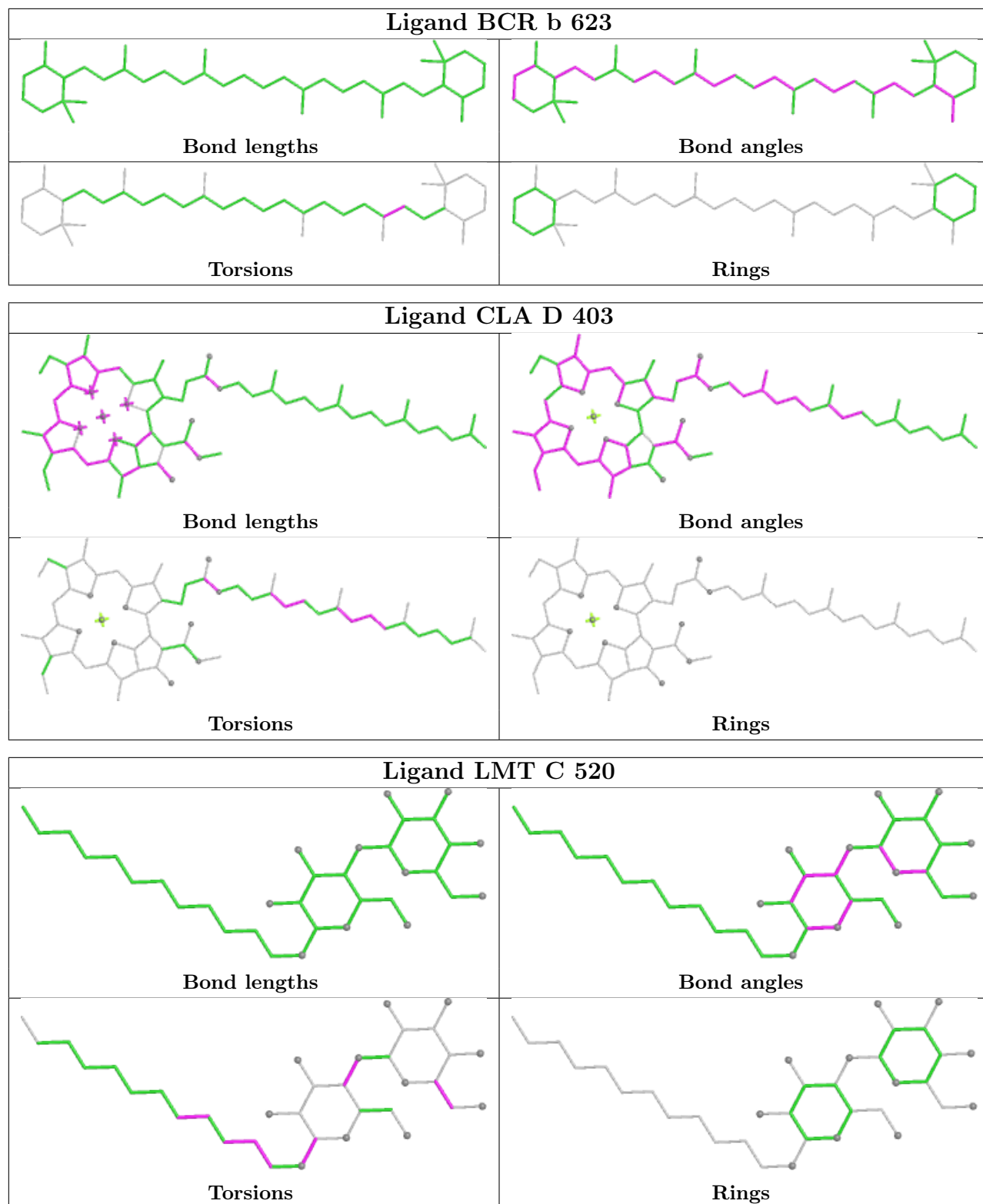




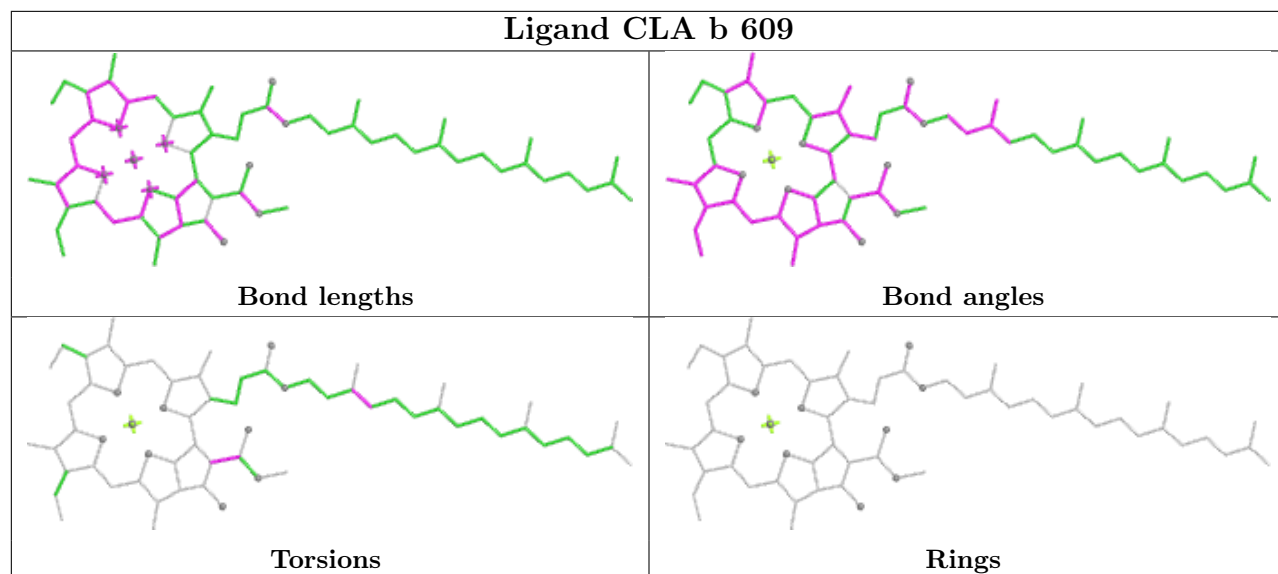




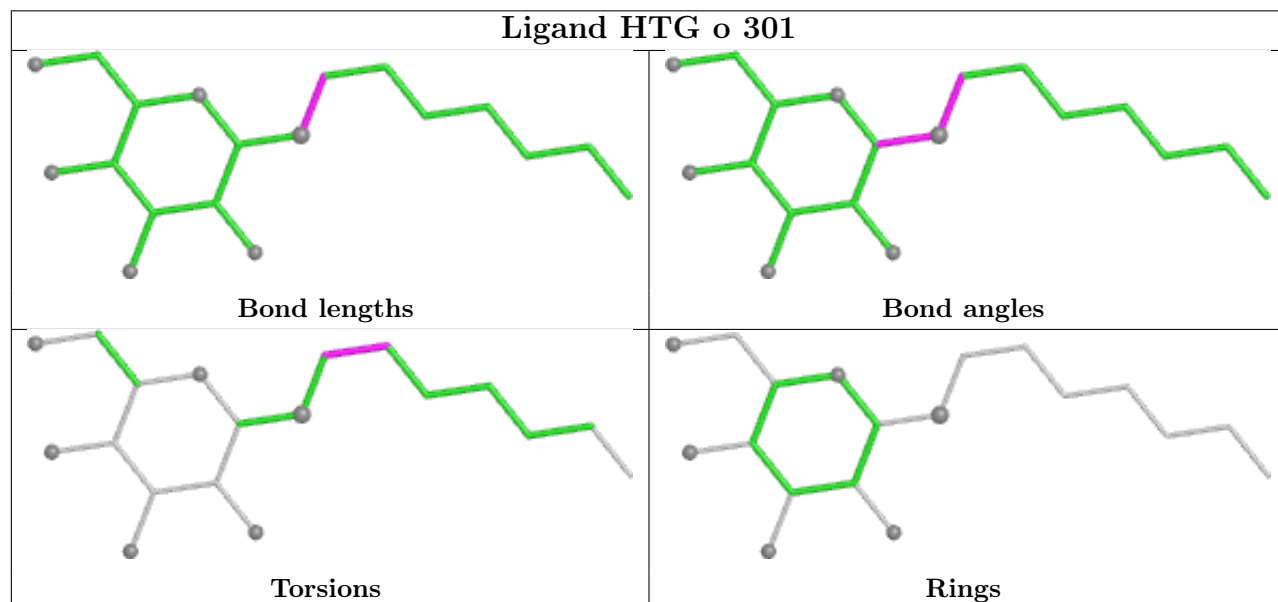


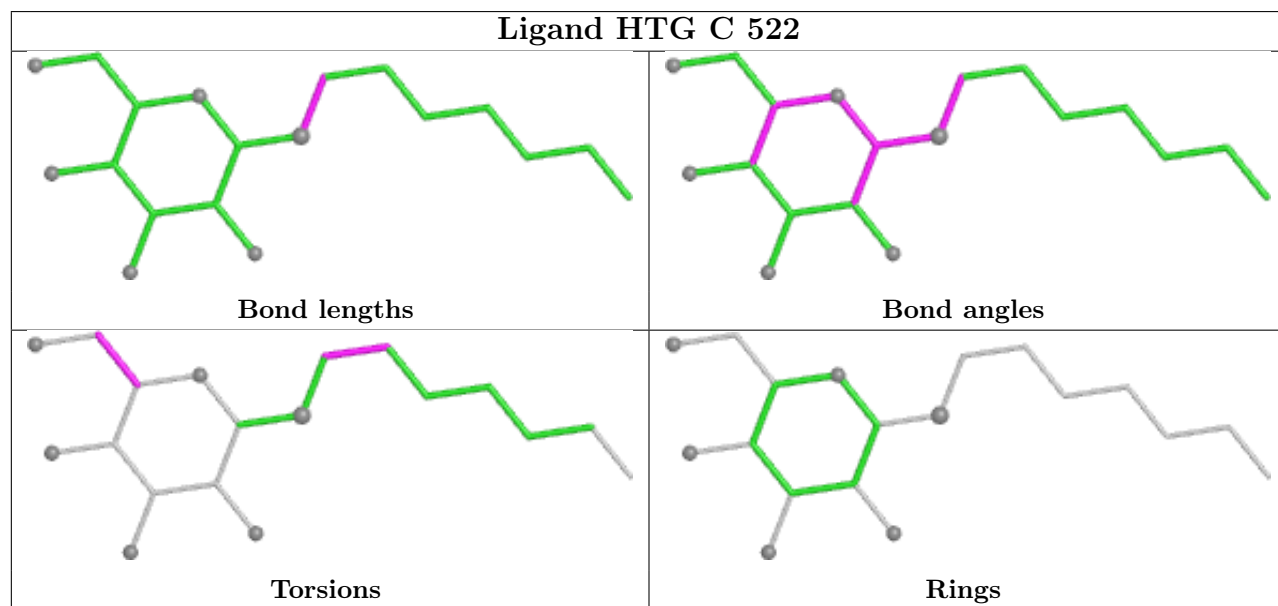
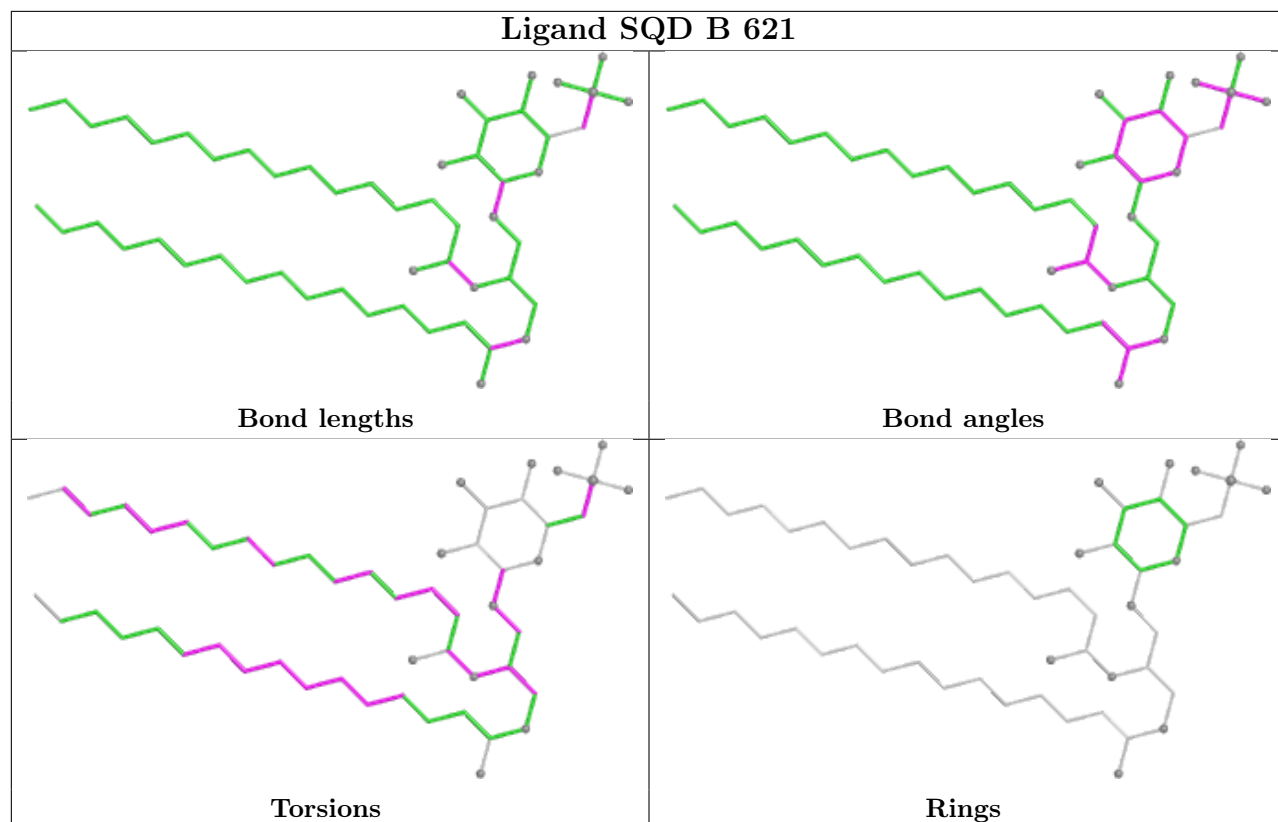


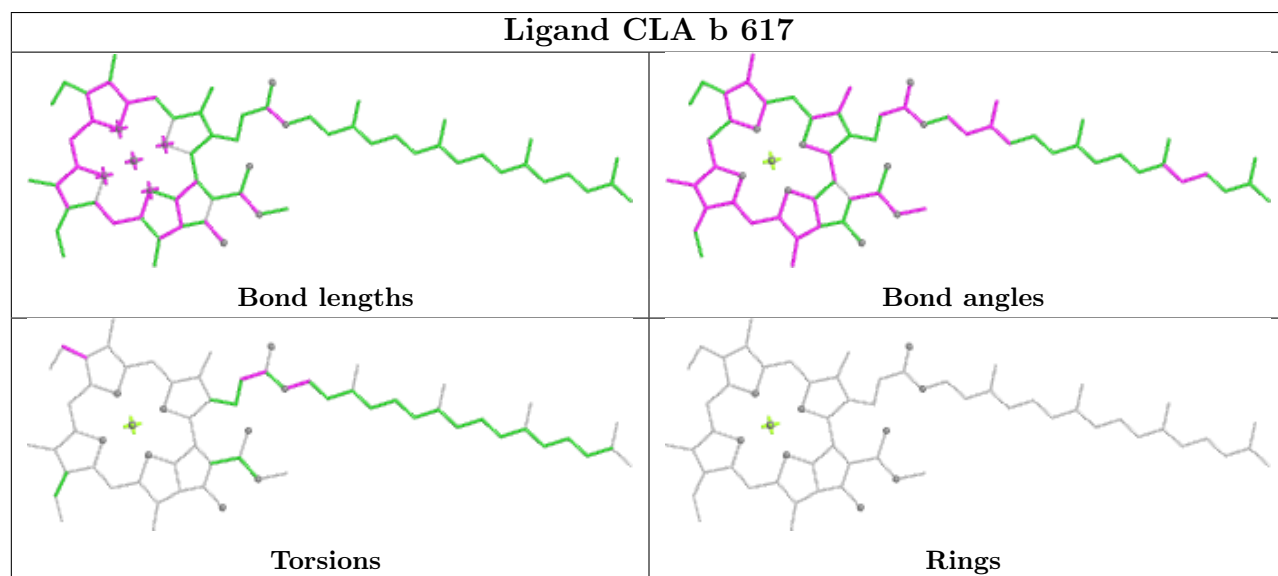
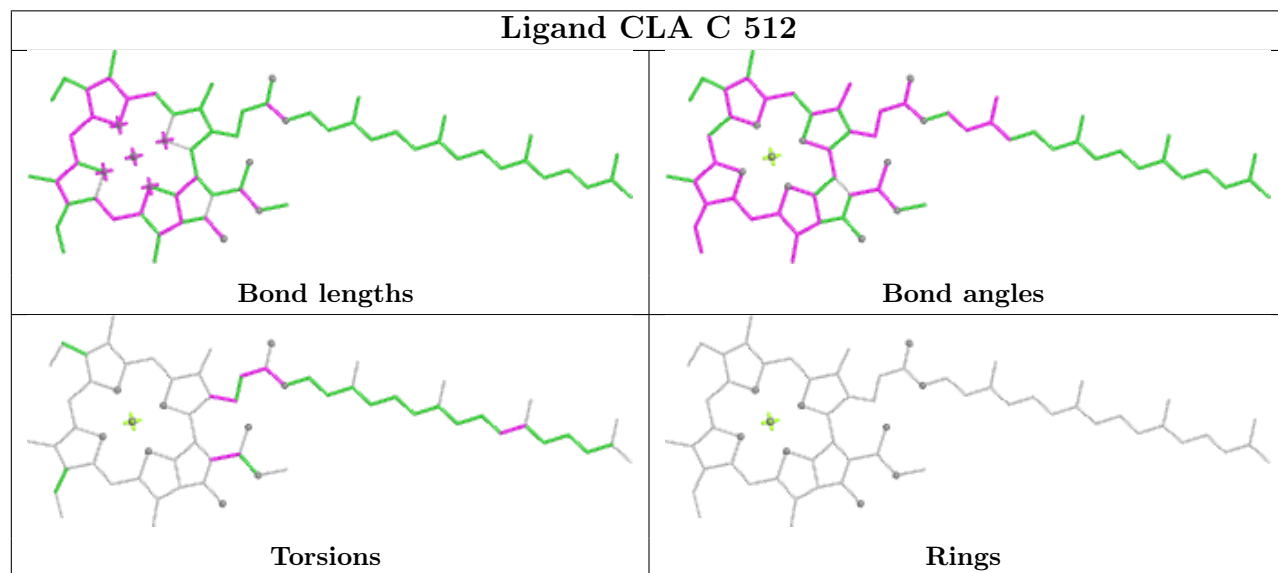
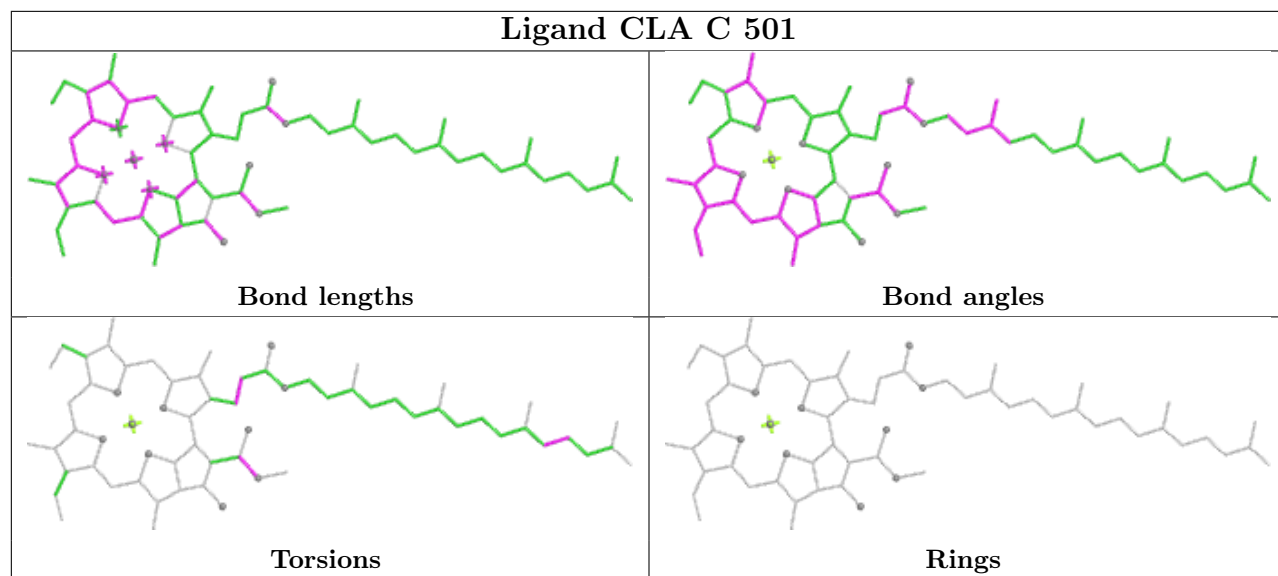
Ligand CLA b 609



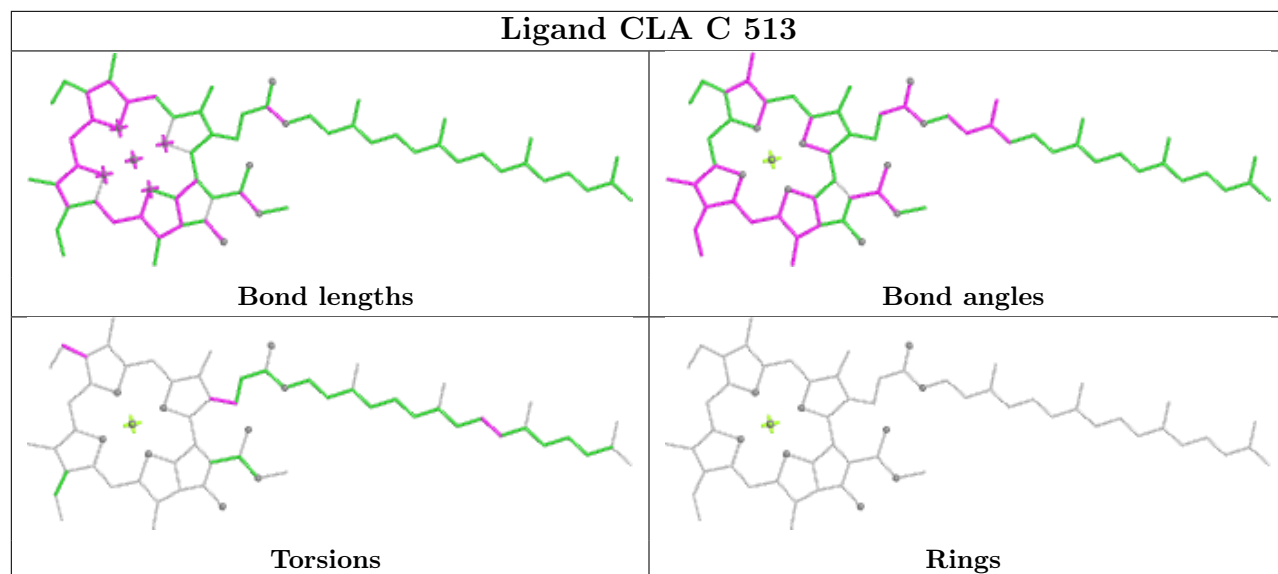
Ligand HTG o 301



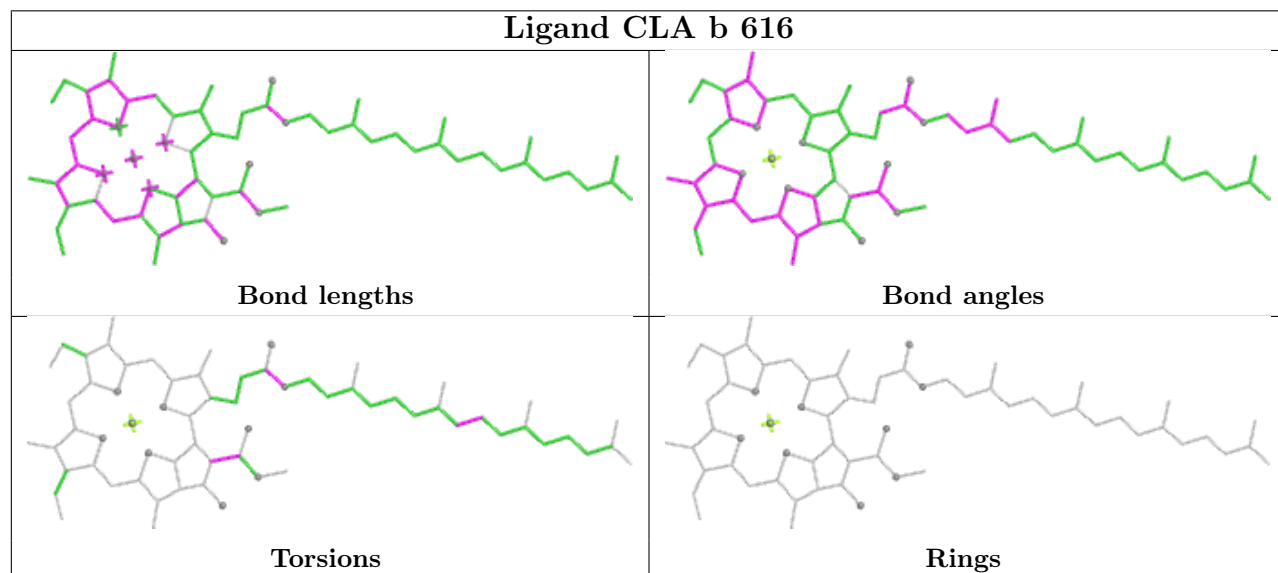




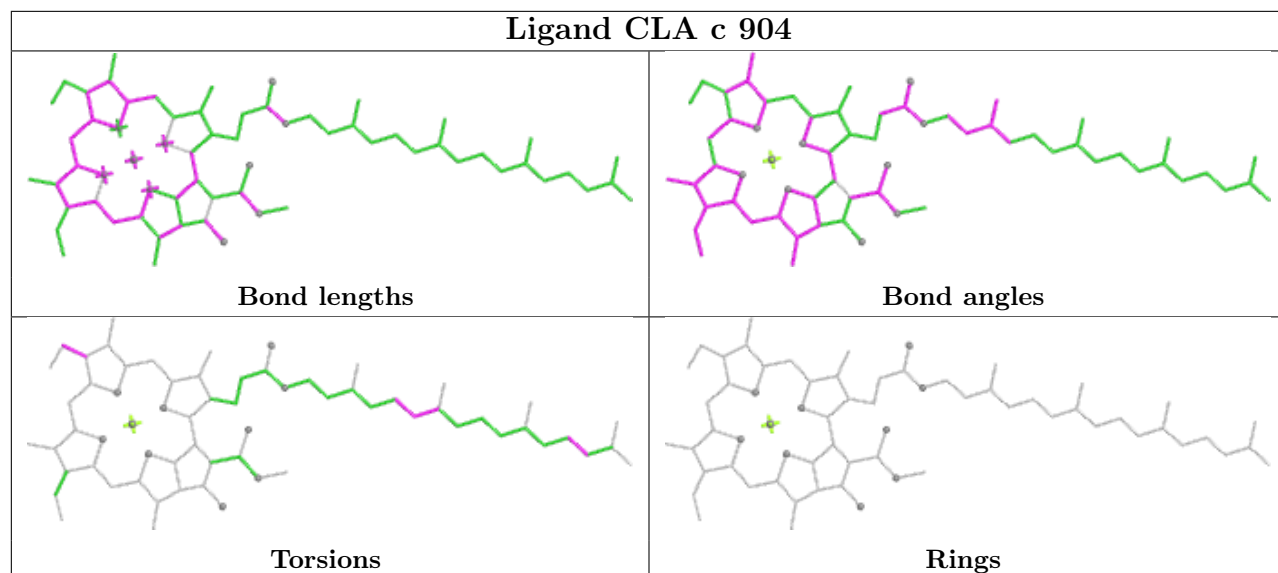
Ligand CLA C 513

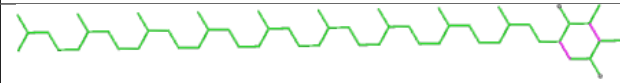
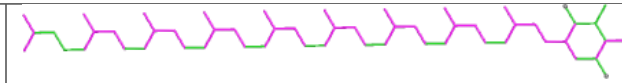
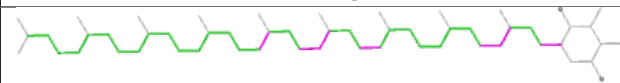
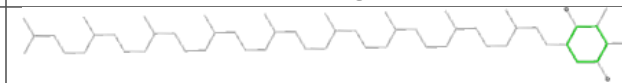


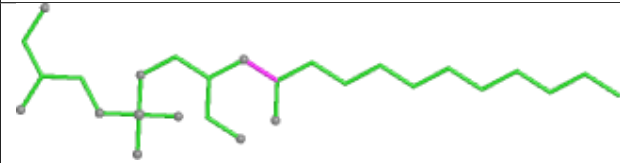
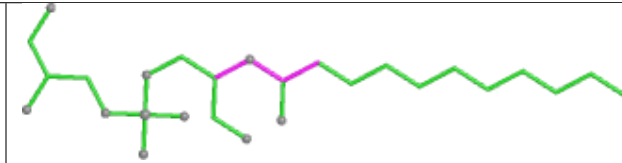
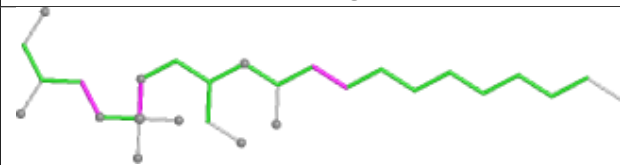
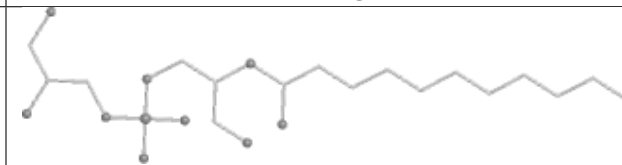
Ligand CLA b 616

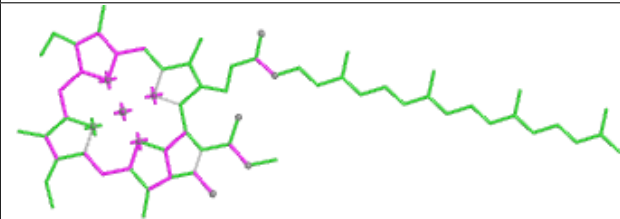
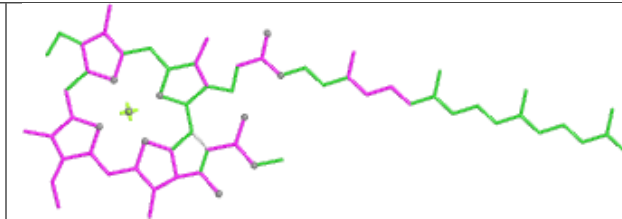
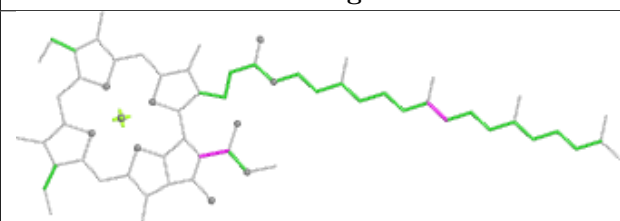
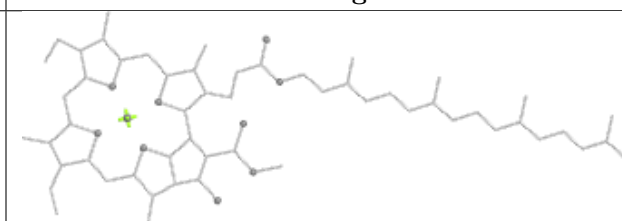


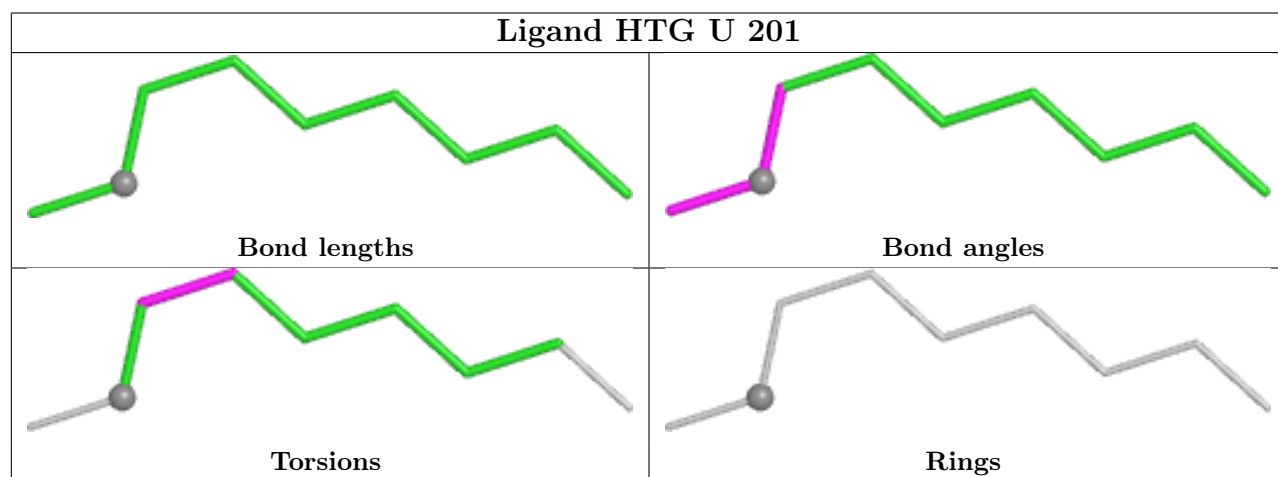
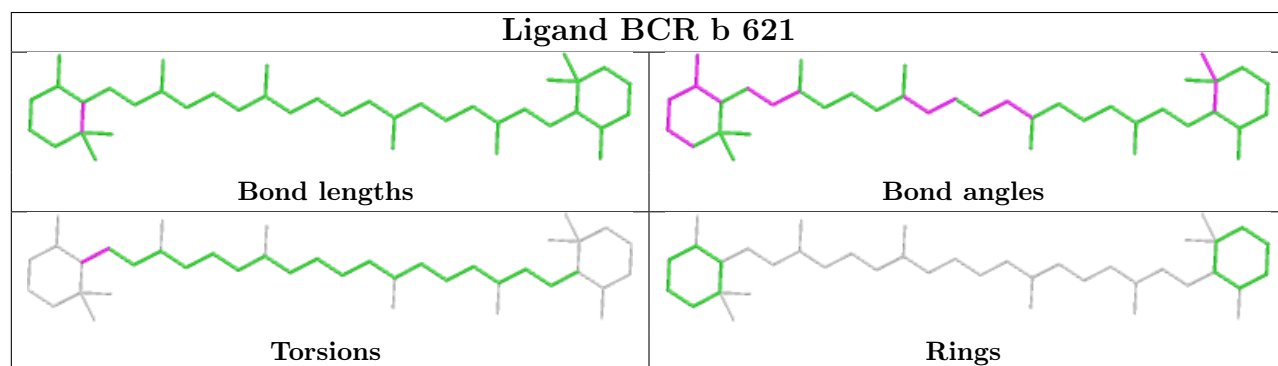
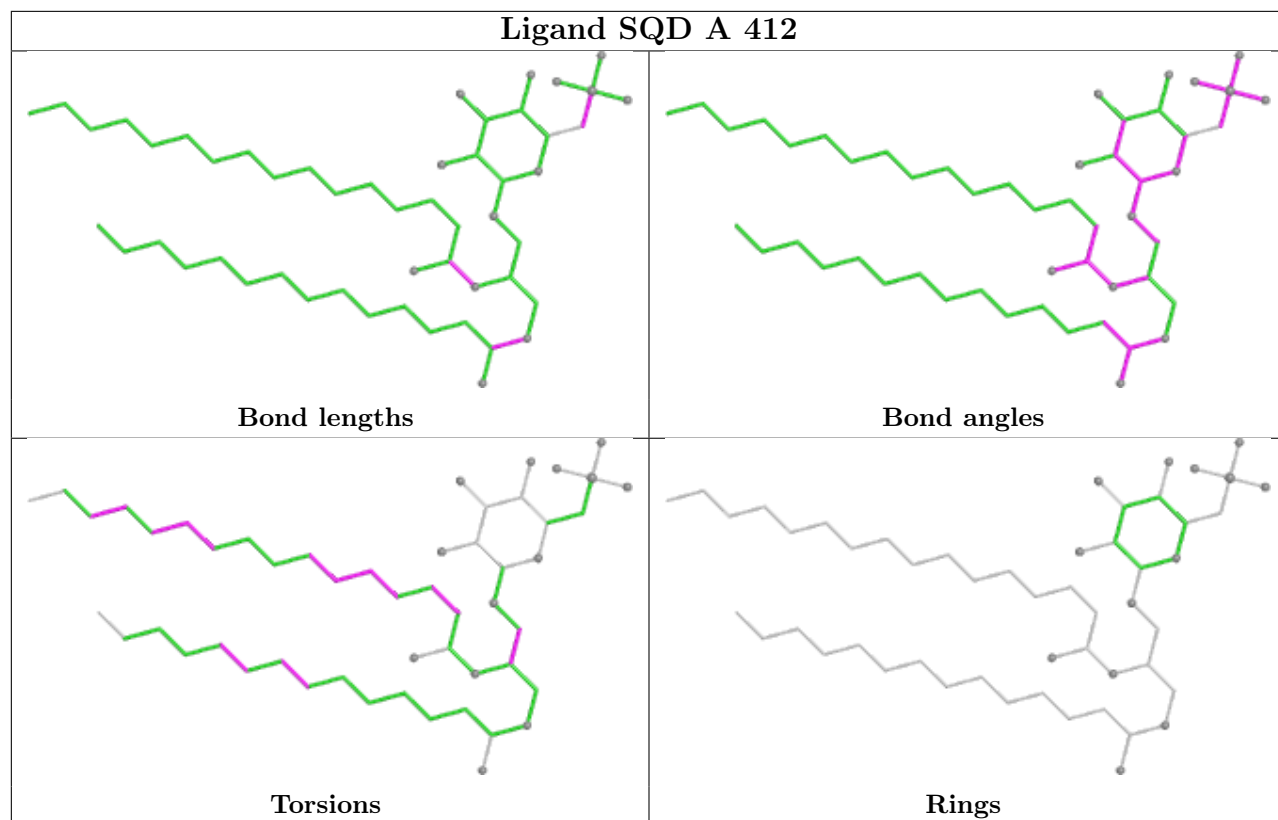
Ligand CLA c 904

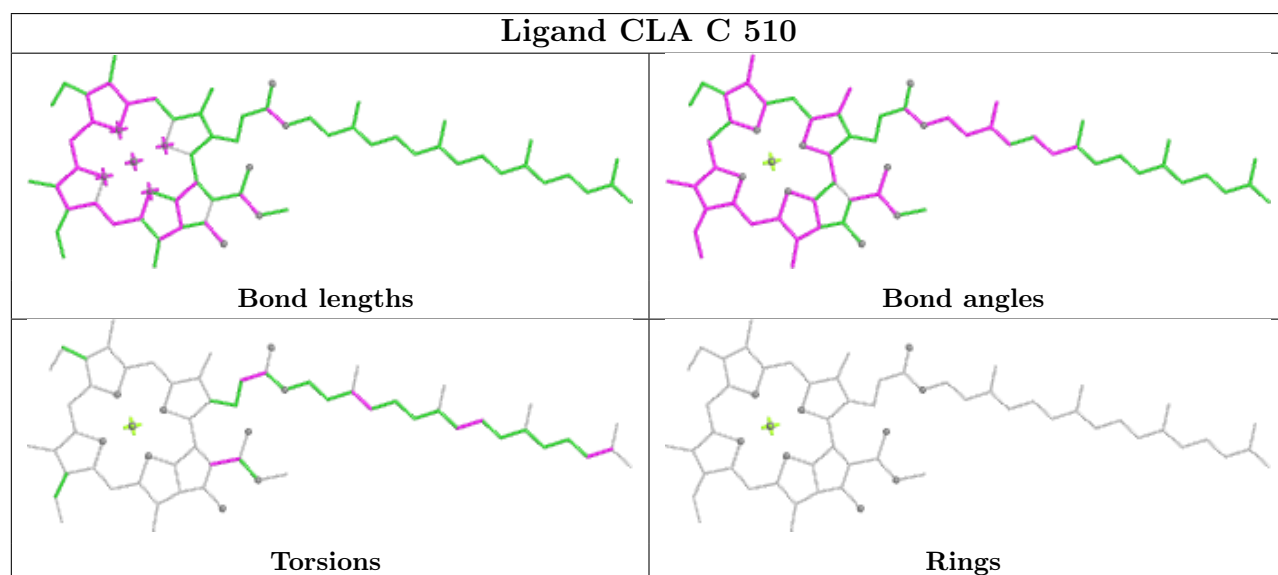
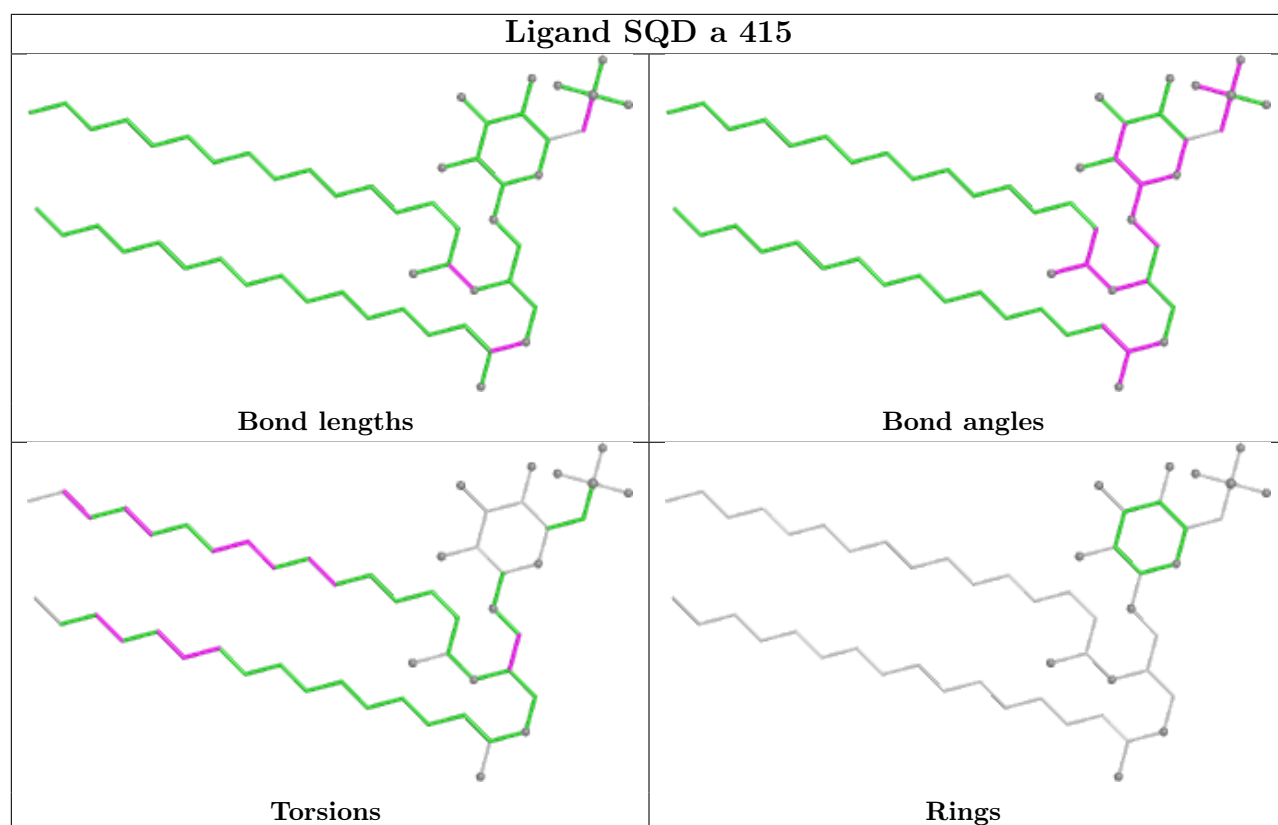


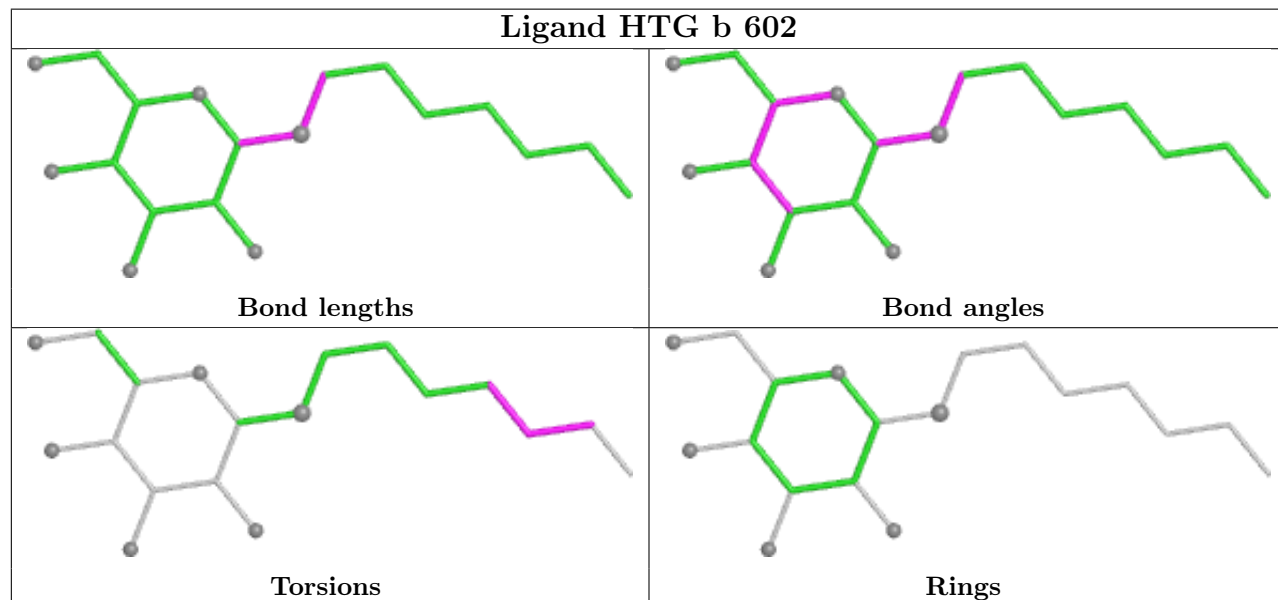
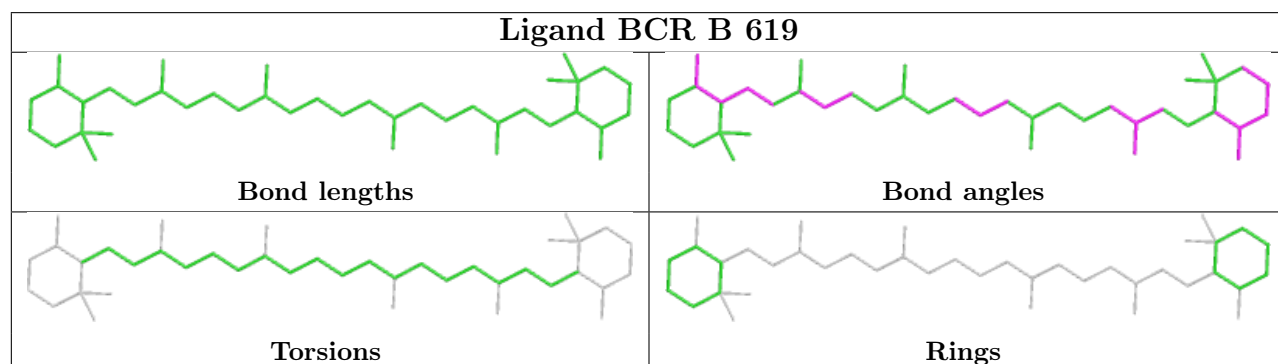
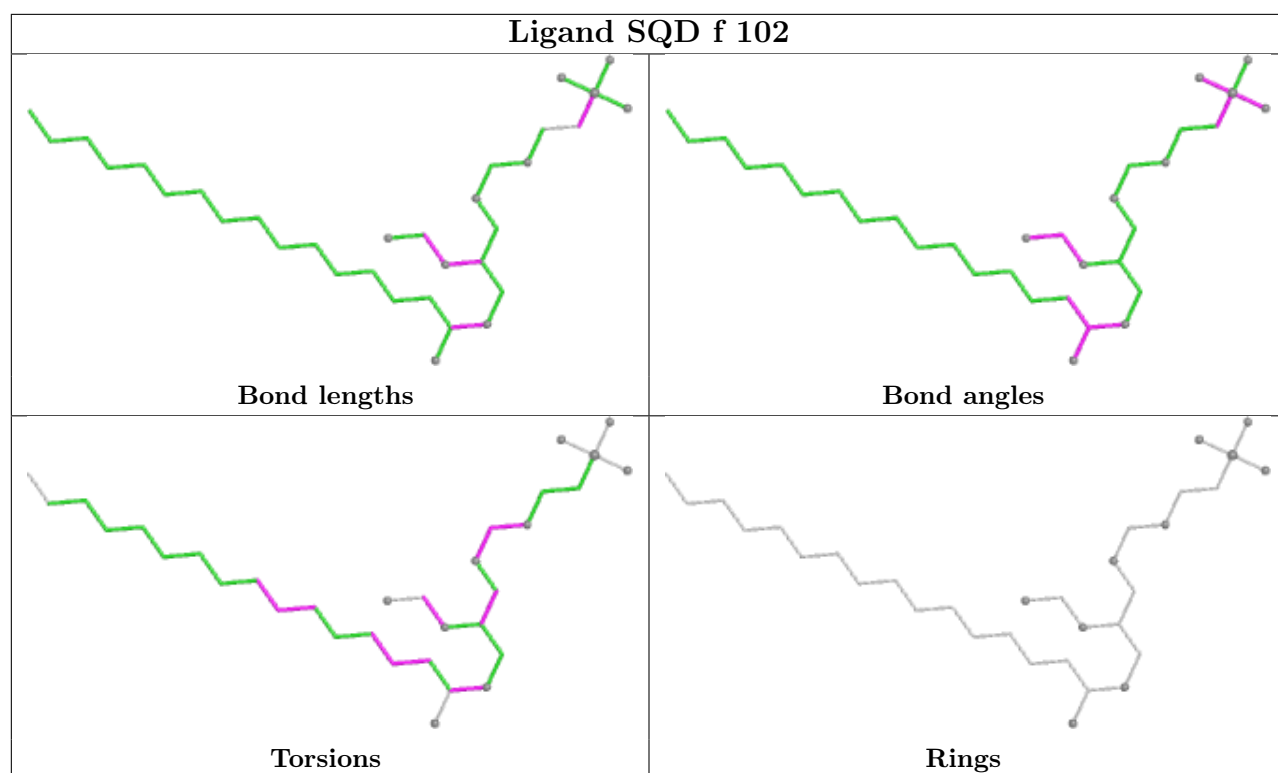
Ligand PL9 a 417	
 Bond lengths	 Bond angles
 Torsions	 Rings

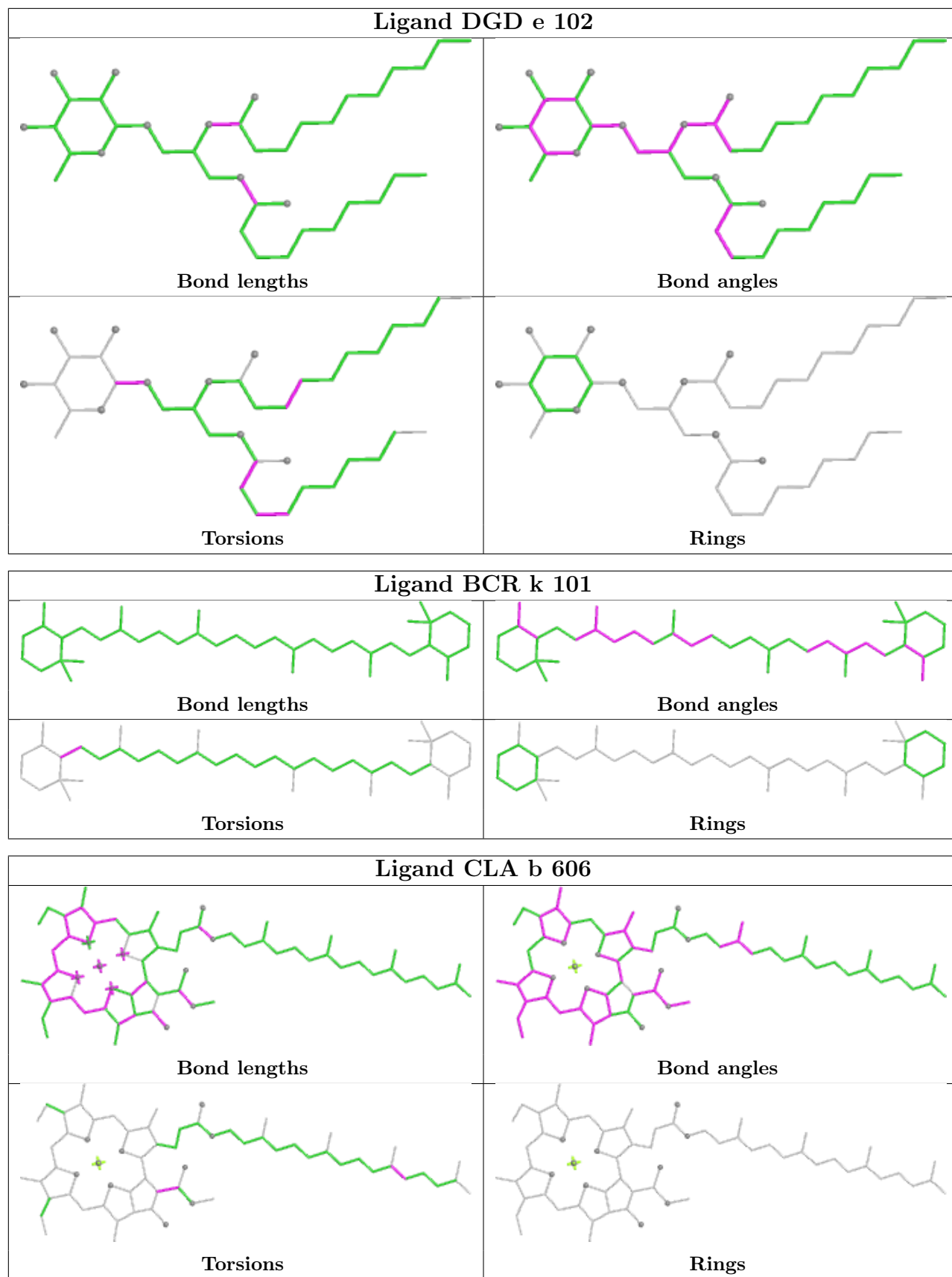
Ligand LHG e 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

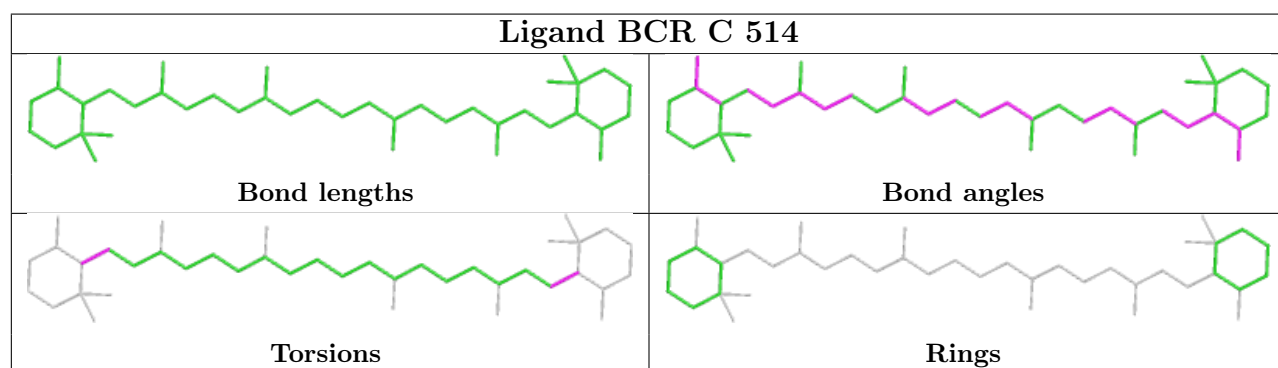
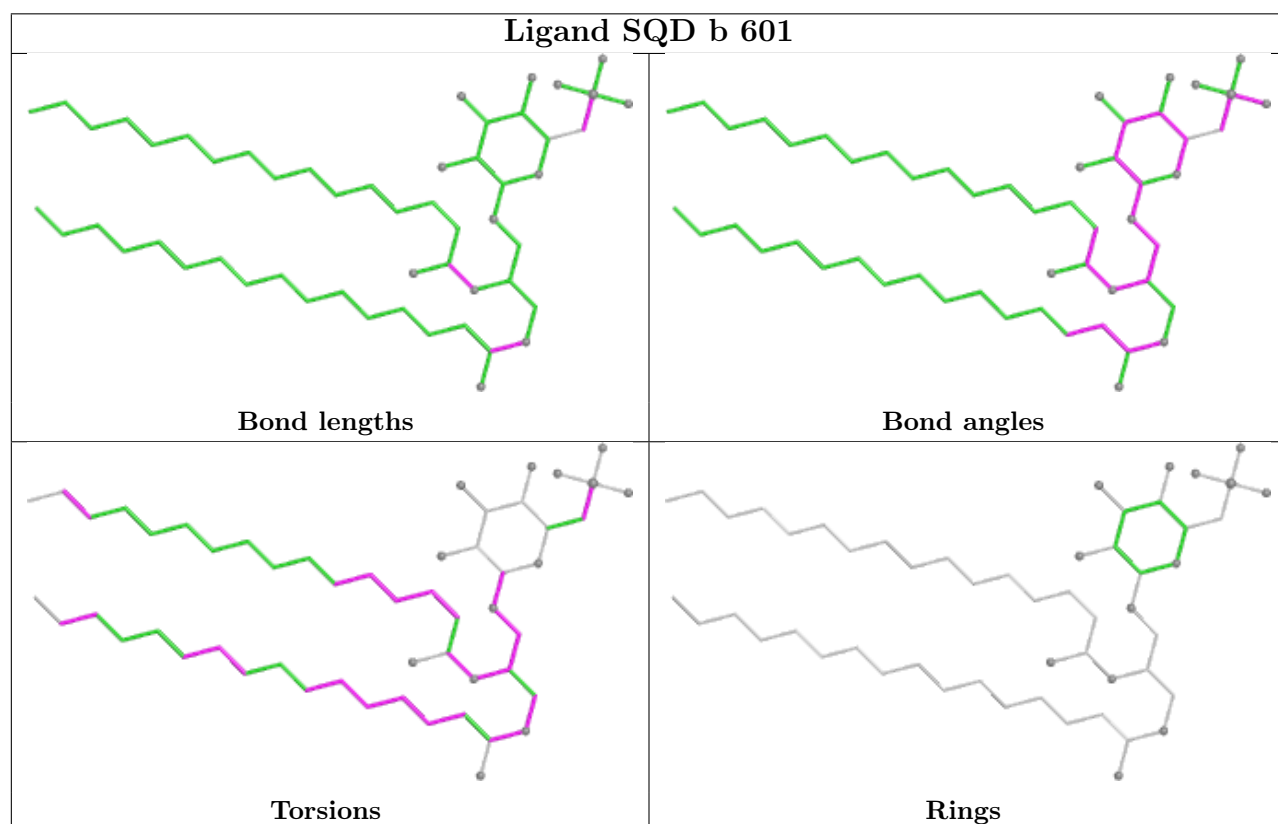
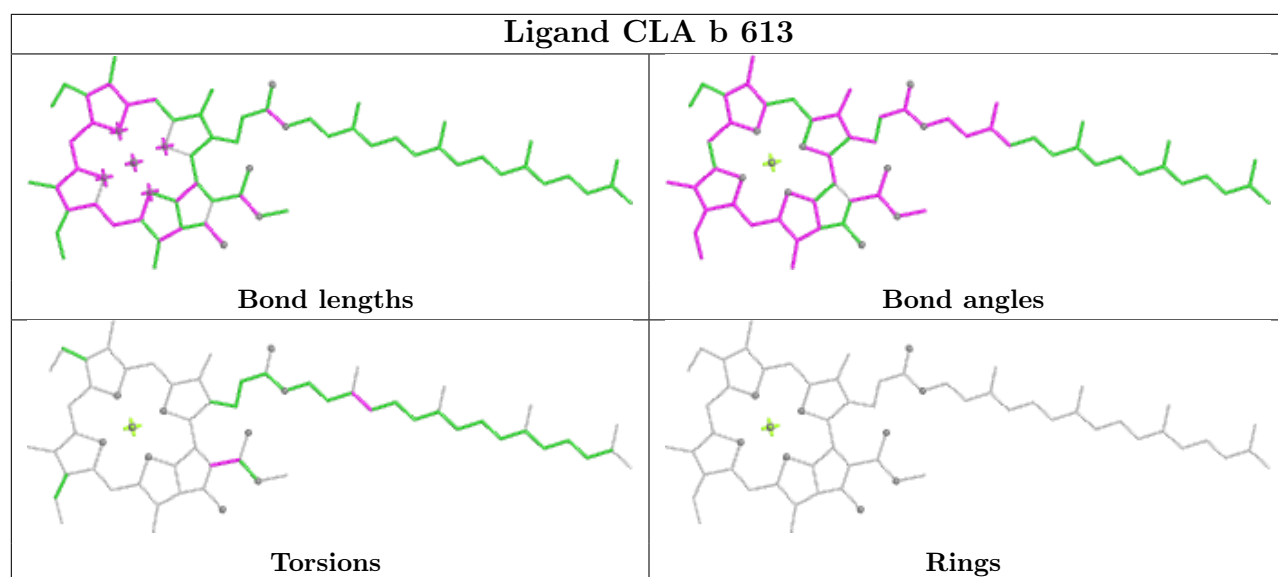
Ligand CLA B 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

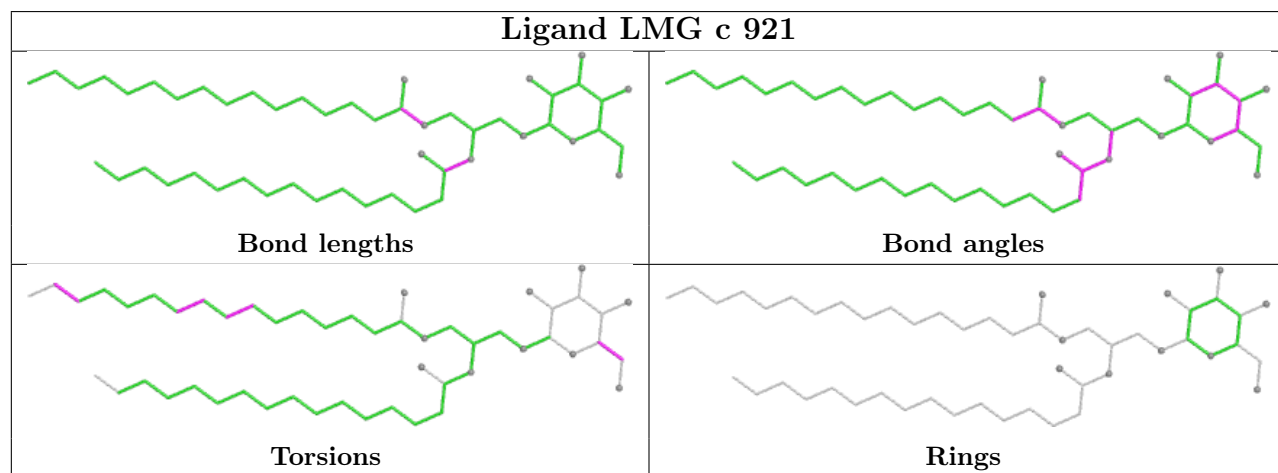
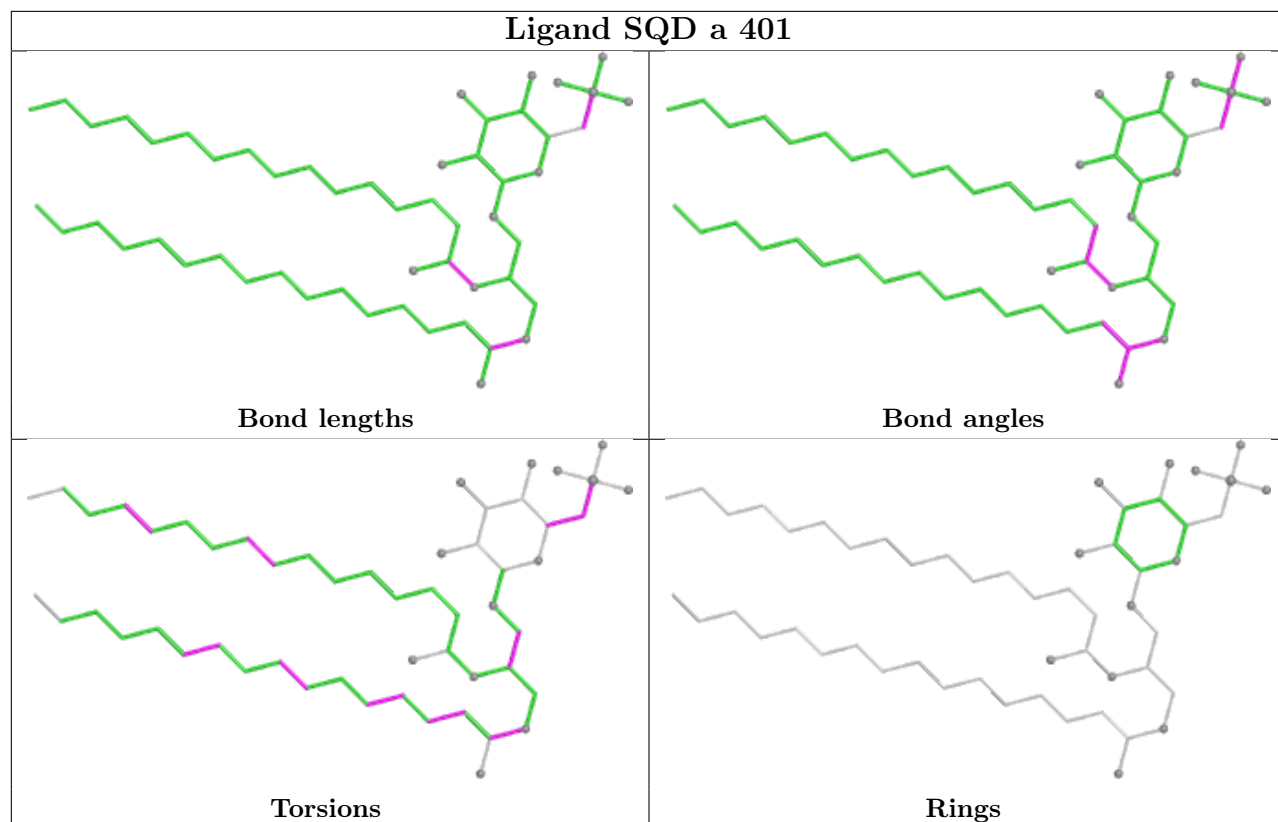


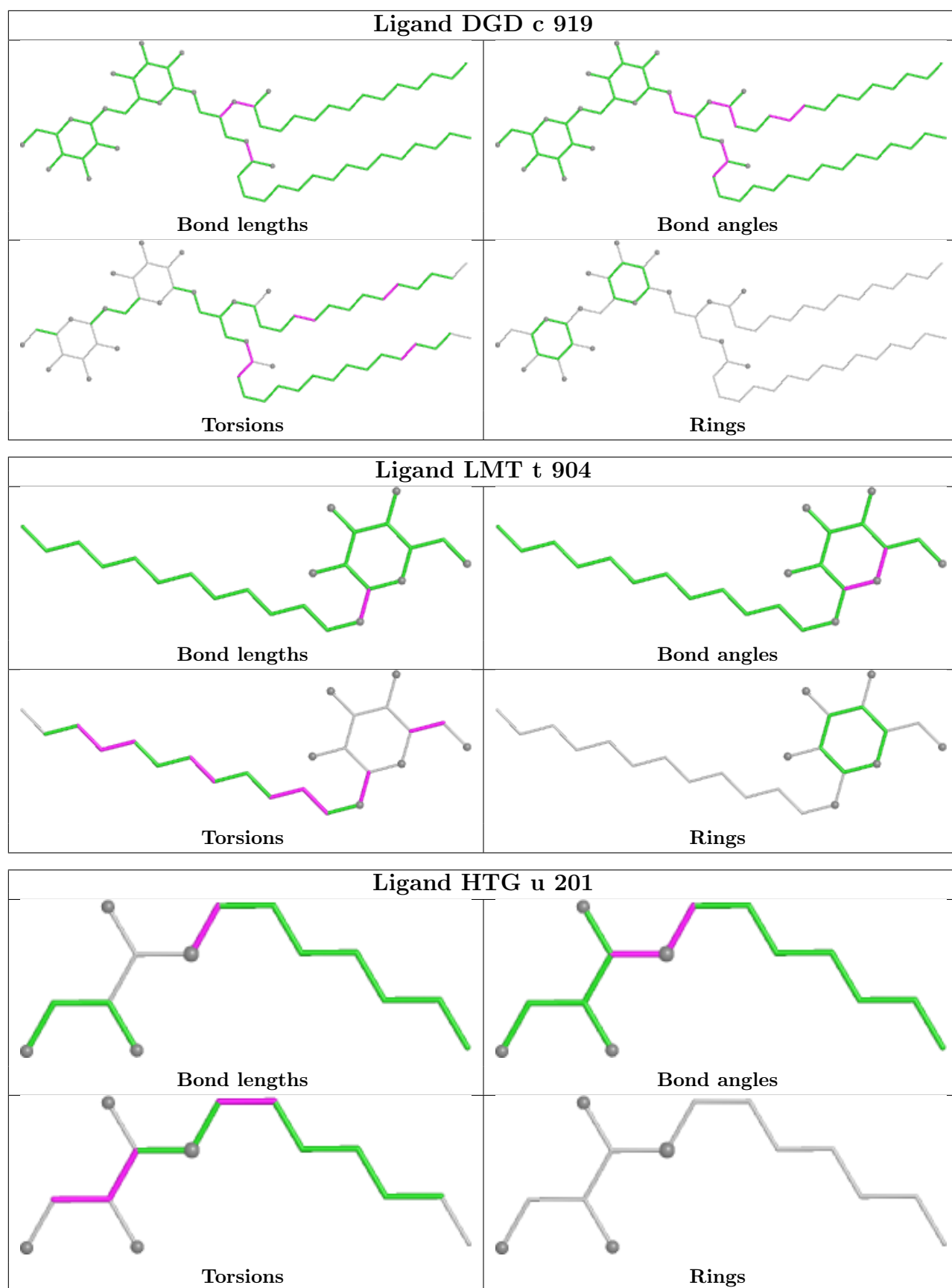




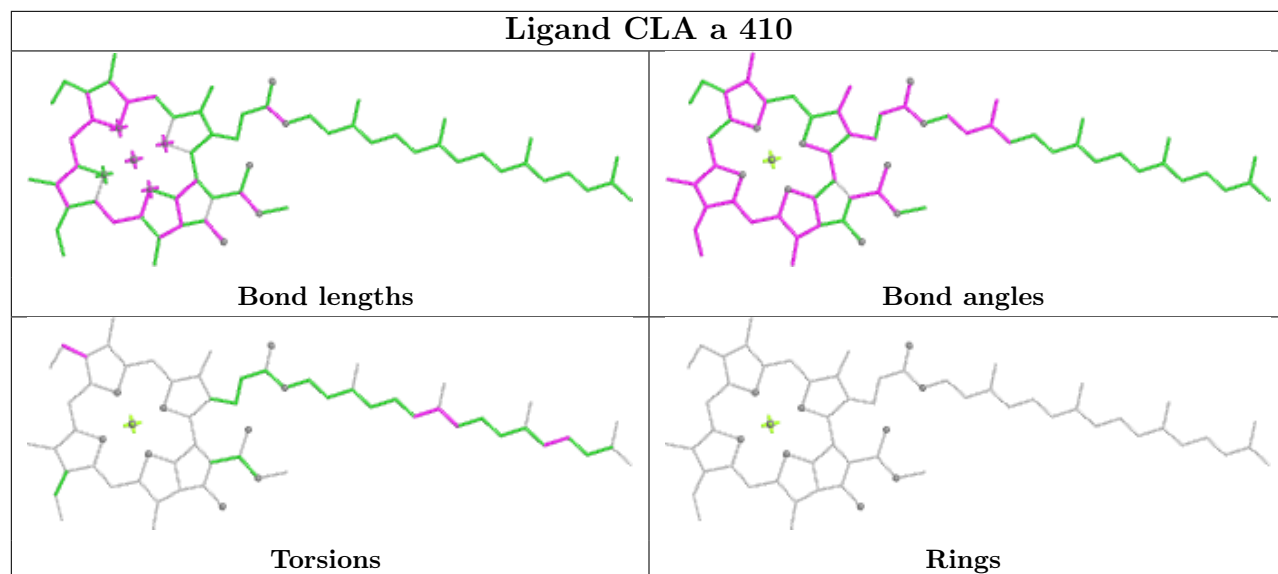




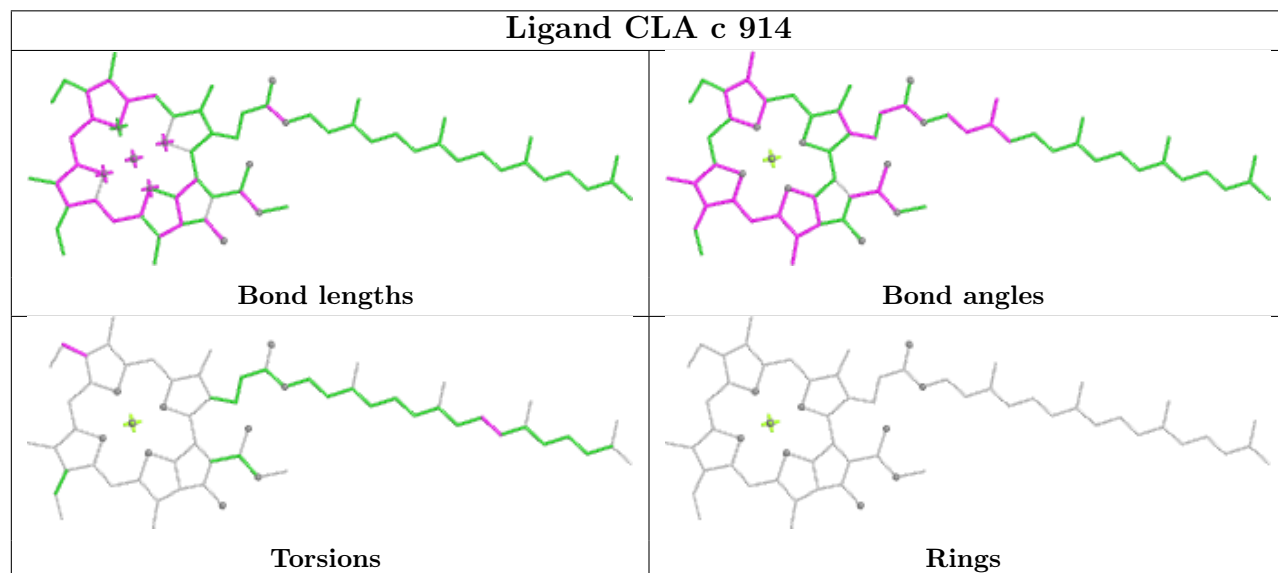




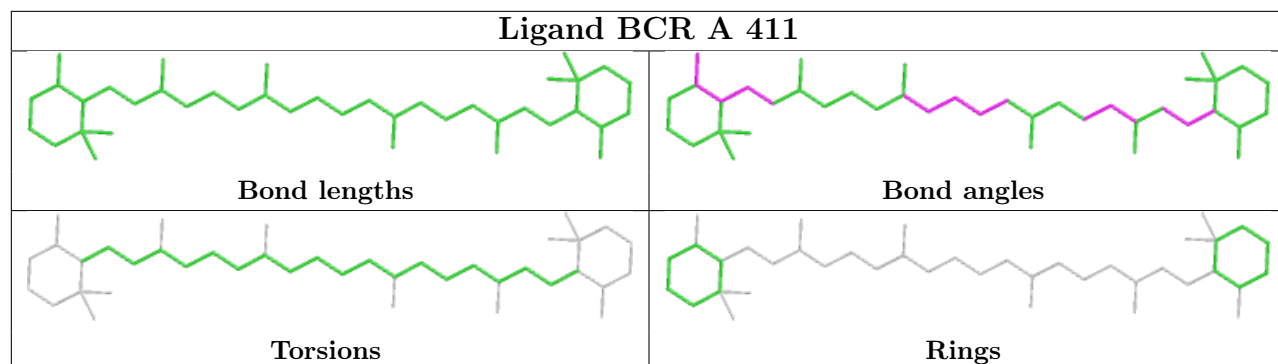
Ligand CLA a 410

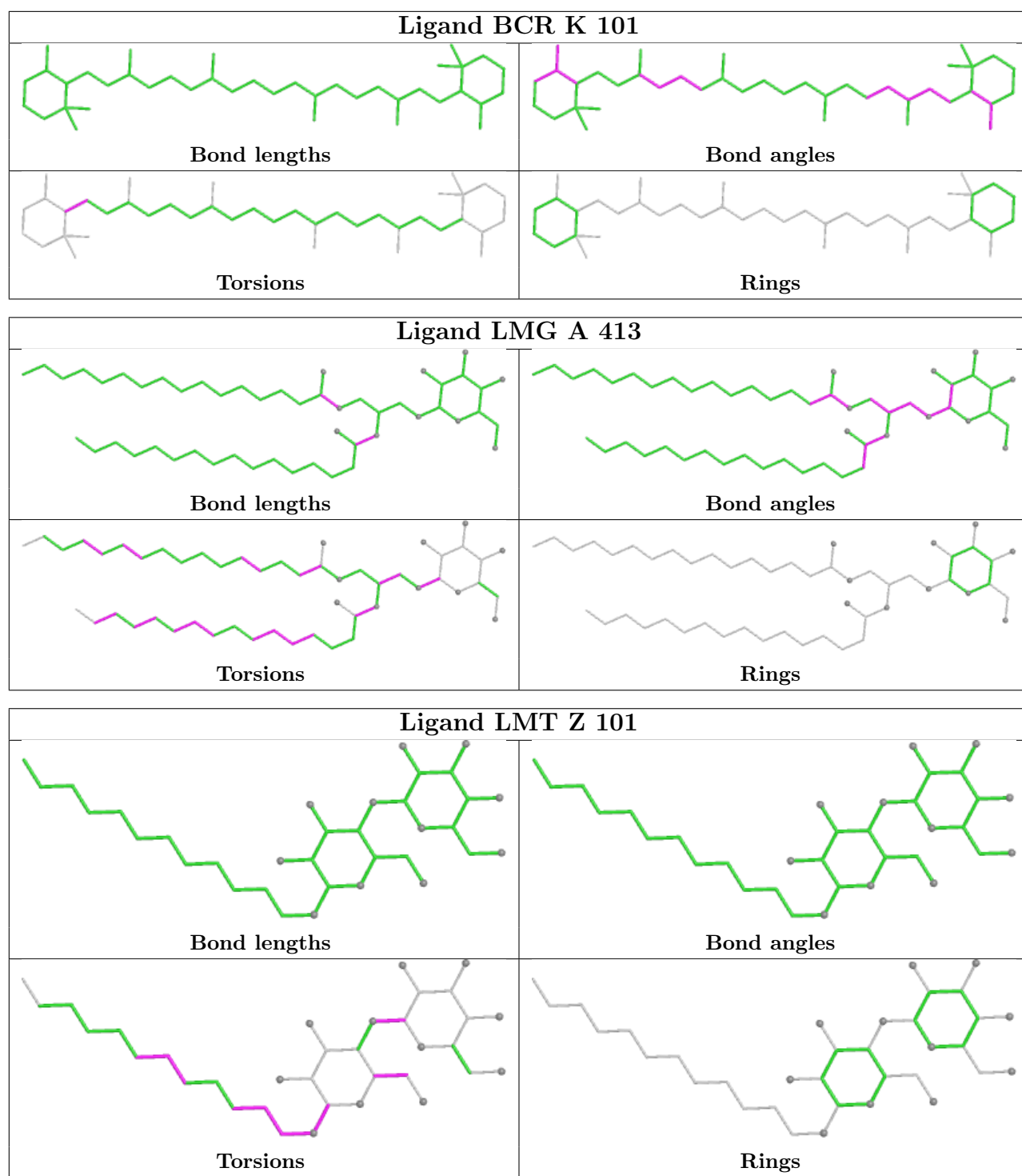


Ligand CLA c 914

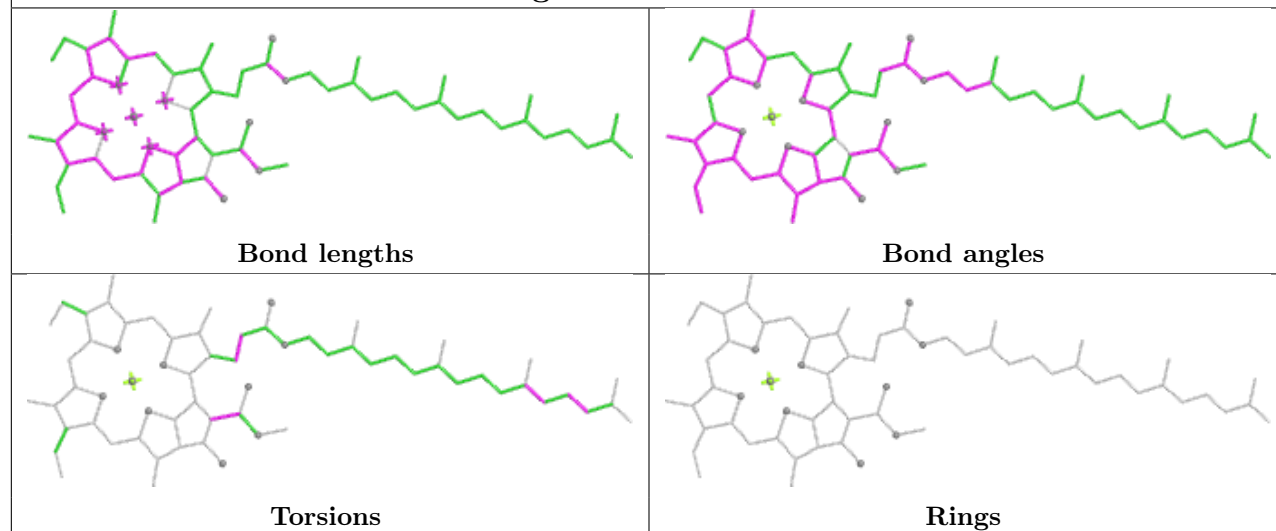


Ligand BCR A 411

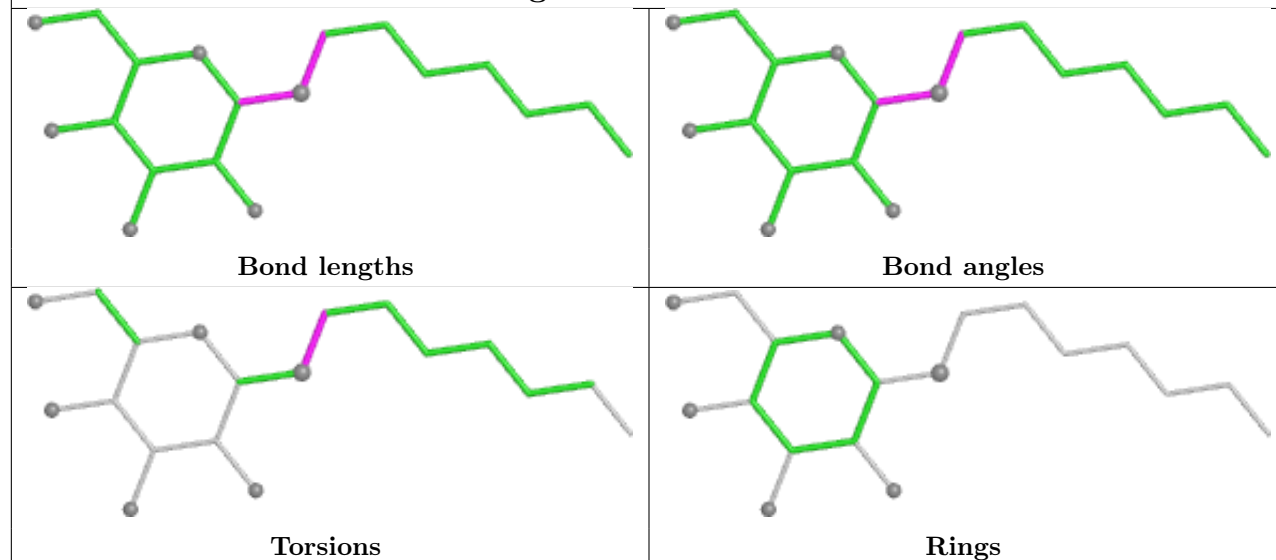




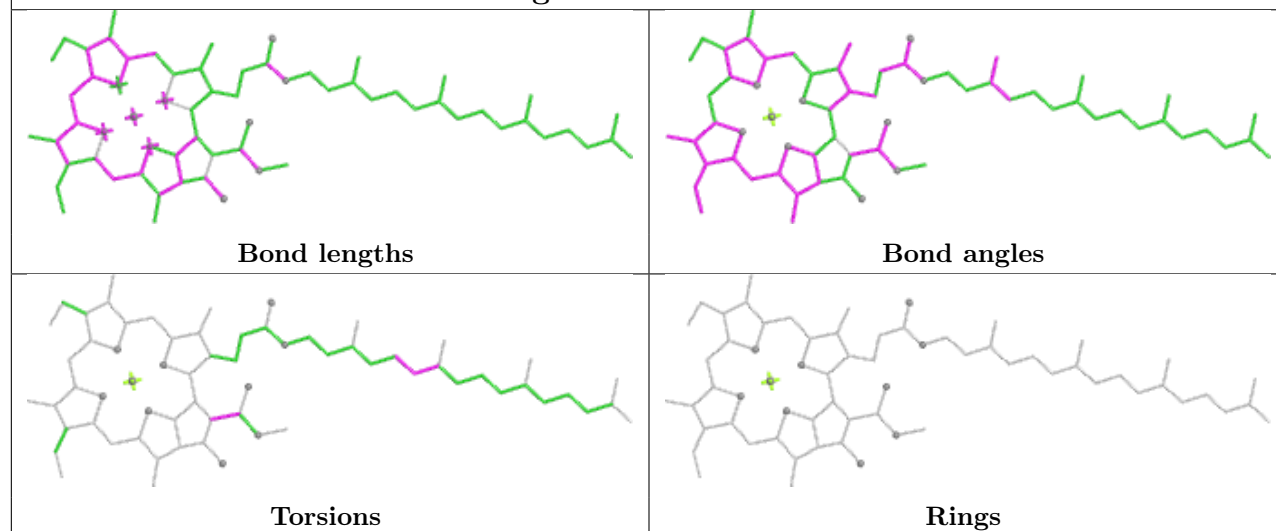
Ligand CLA C 507

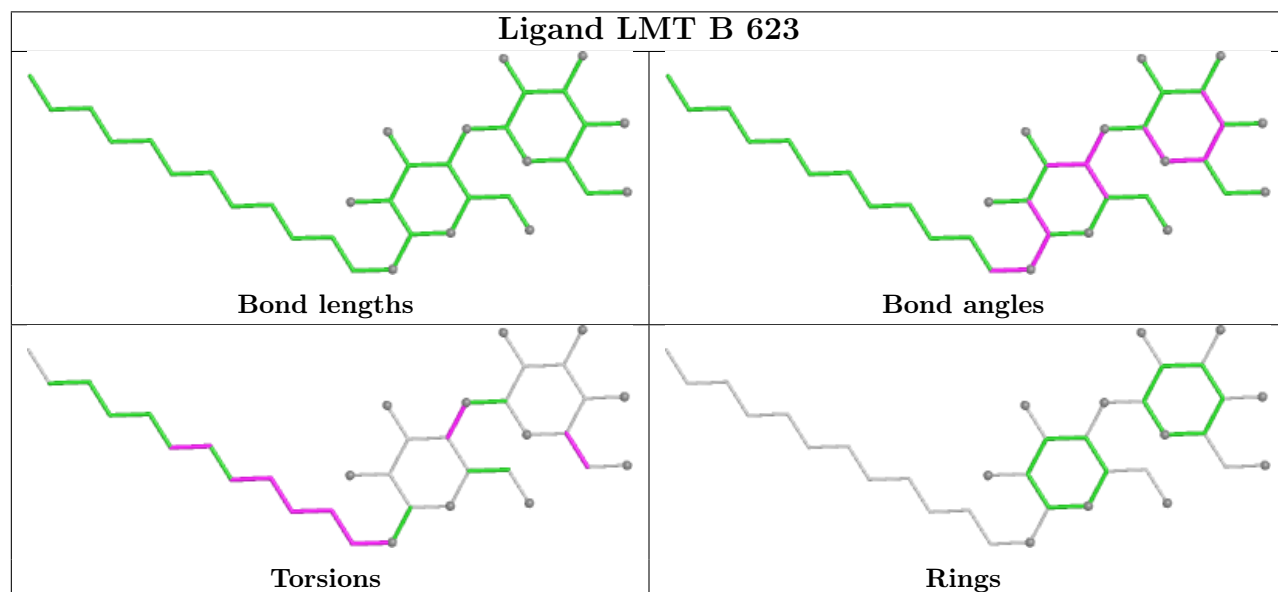
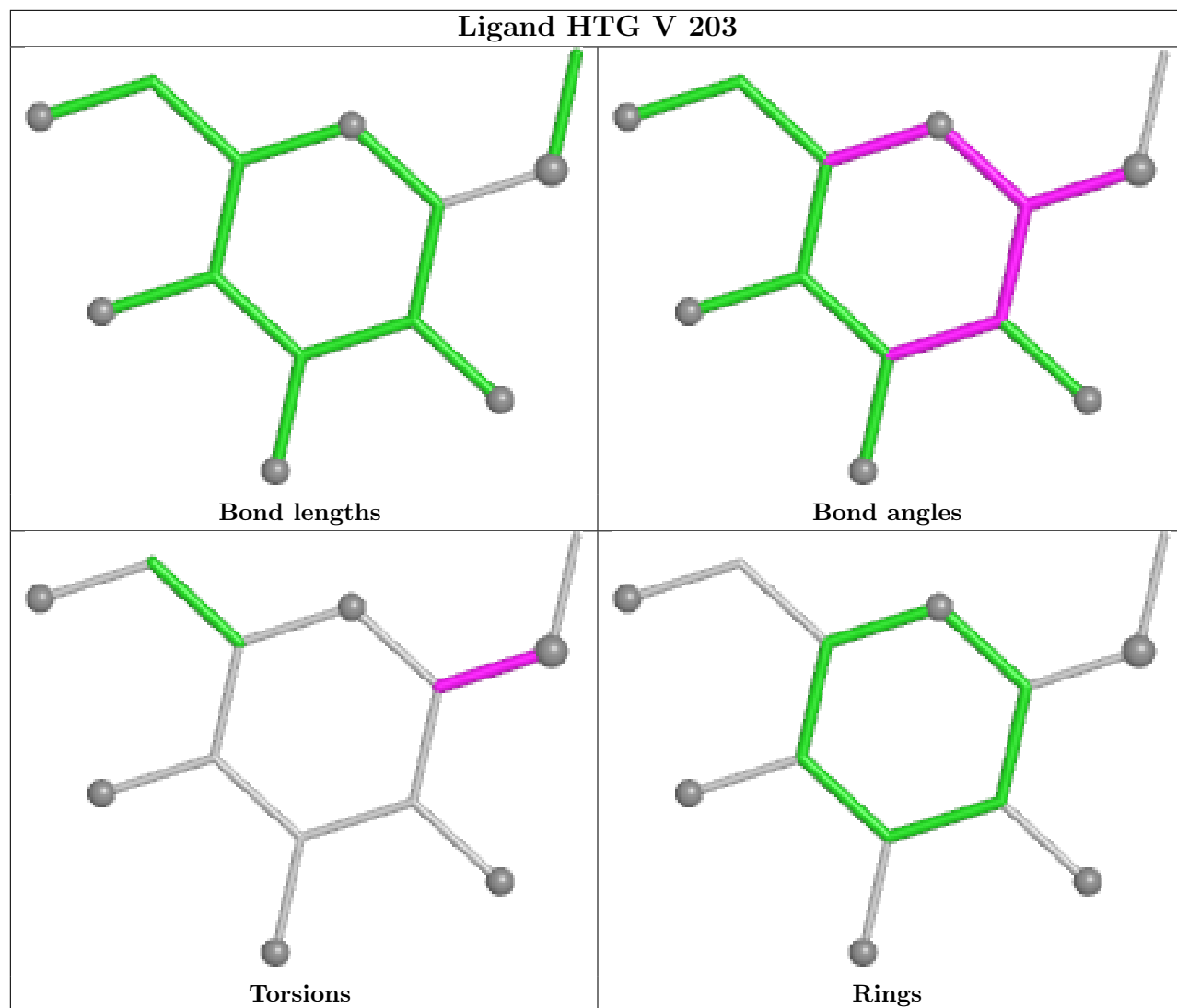


Ligand HTG C 521

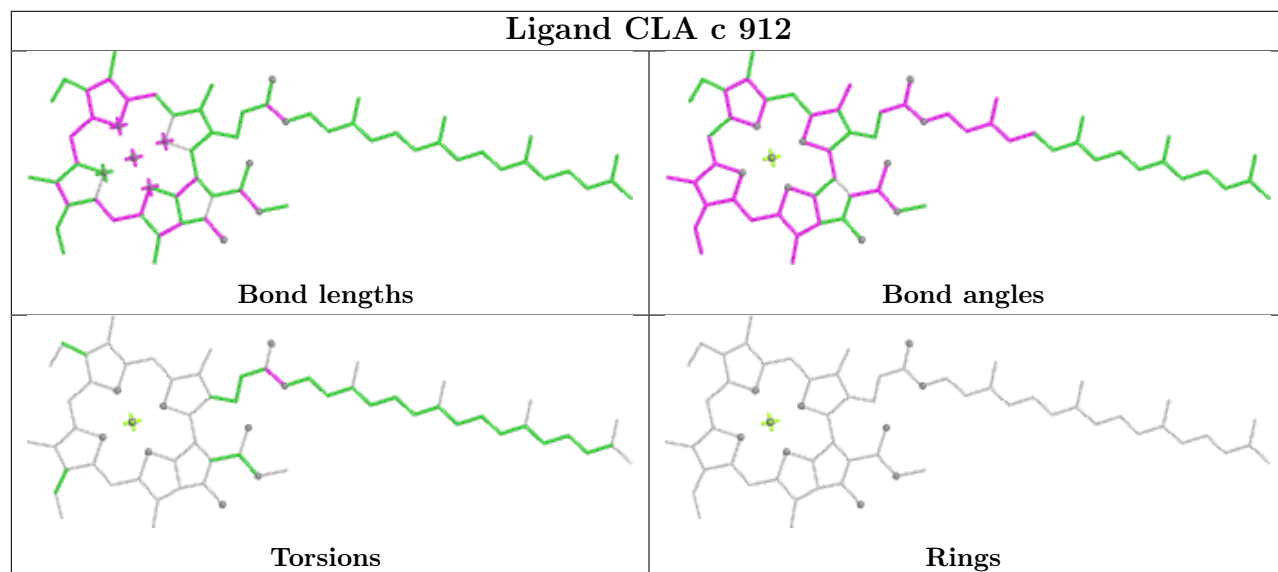


Ligand CLA B 604

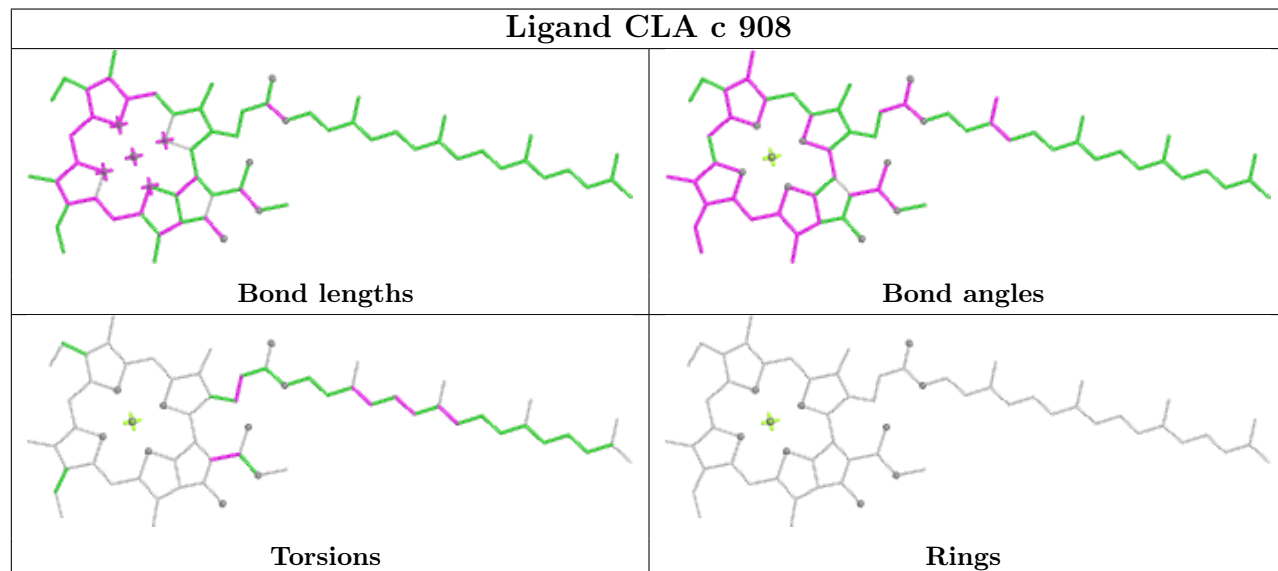




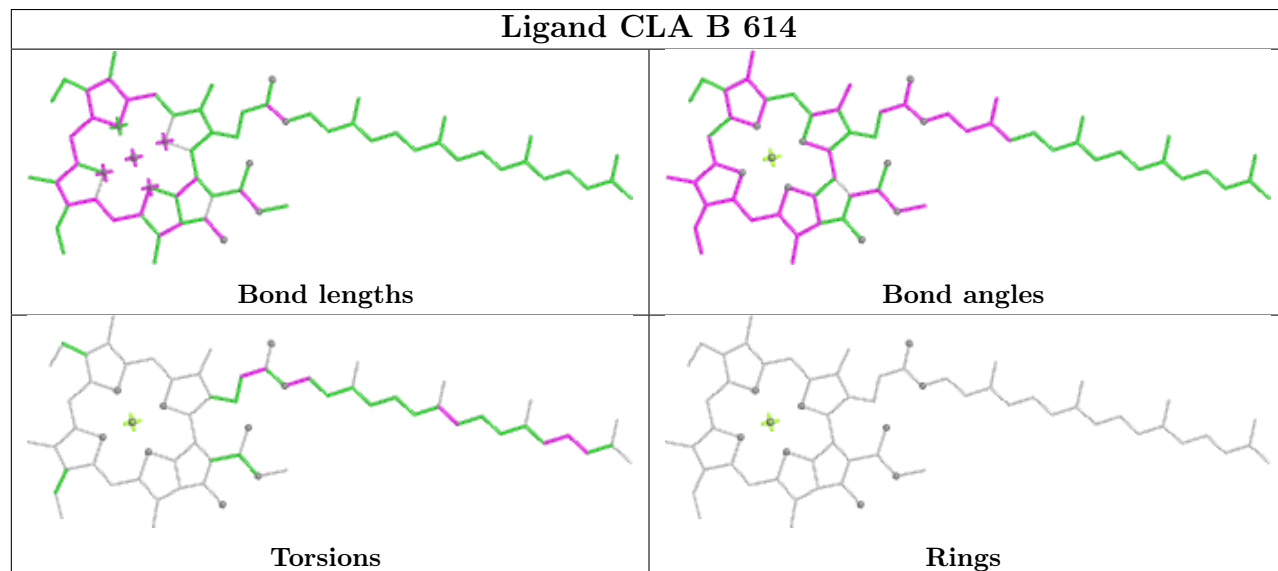
Ligand CLA c 912



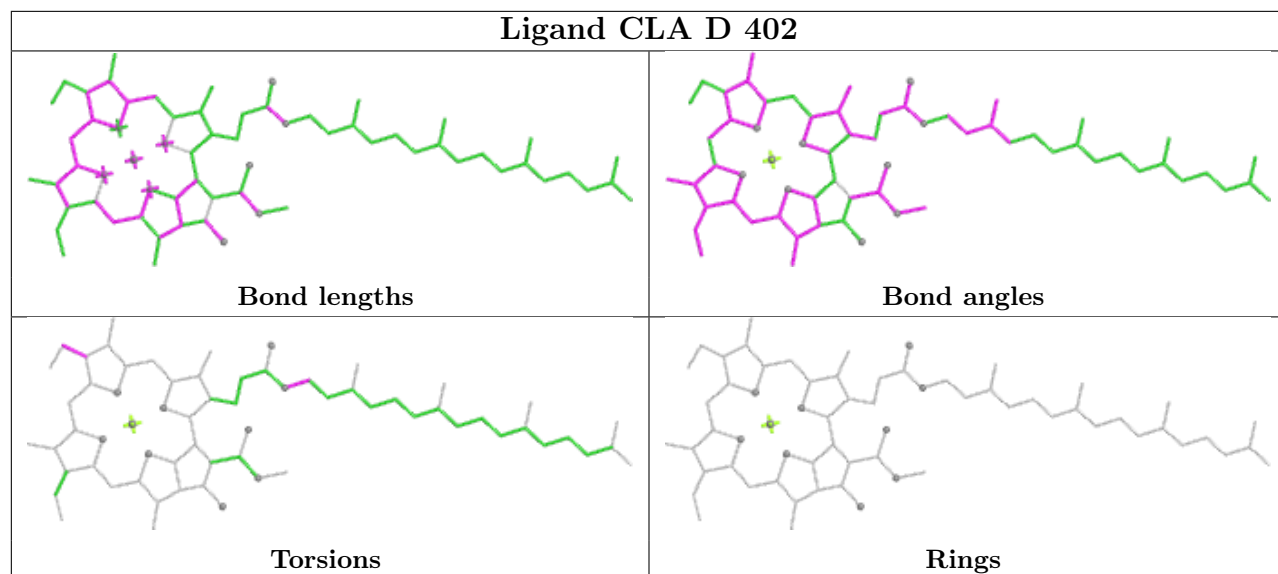
Ligand CLA c 908



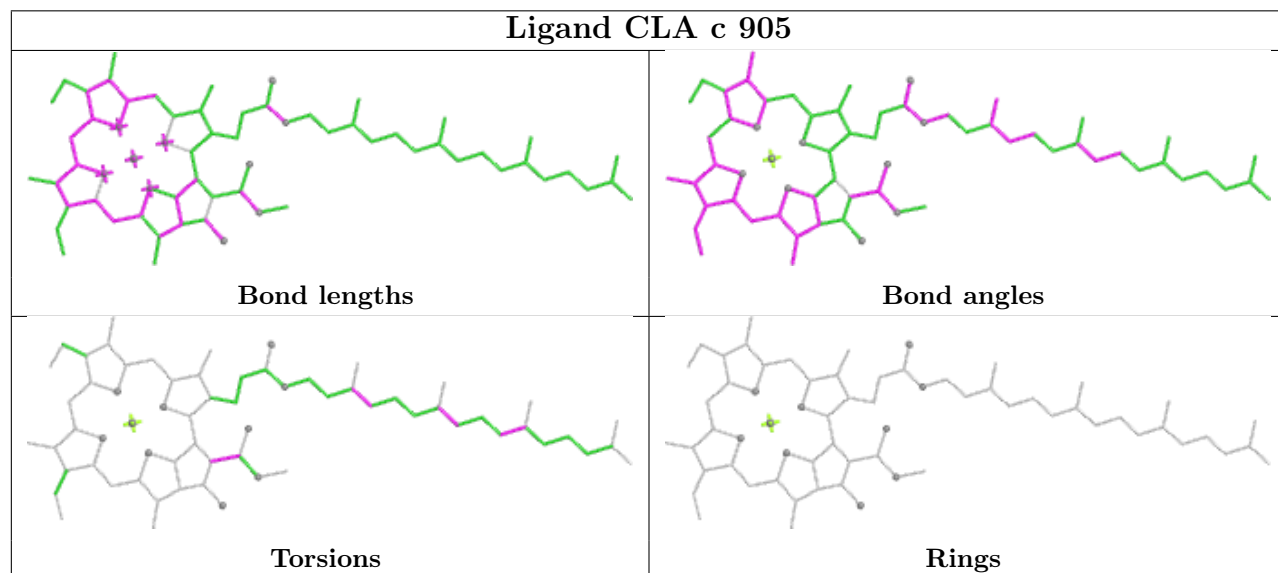
Ligand CLA B 614



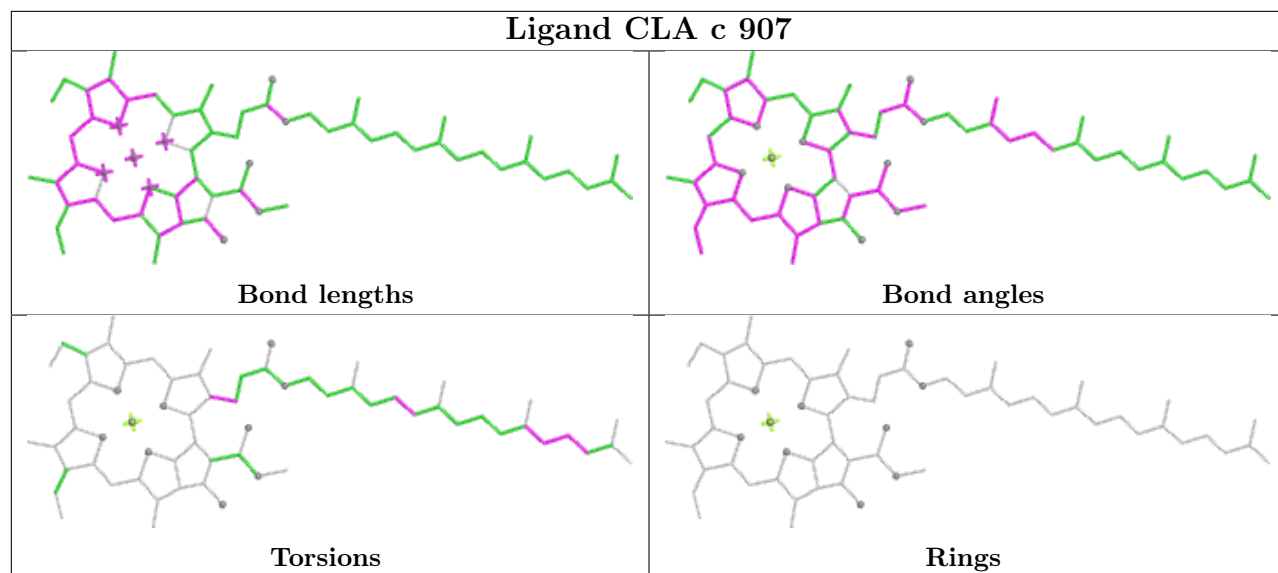
Ligand CLA D 402

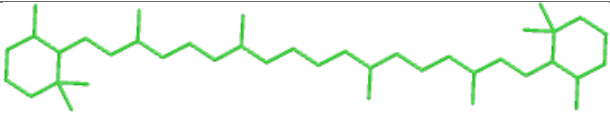
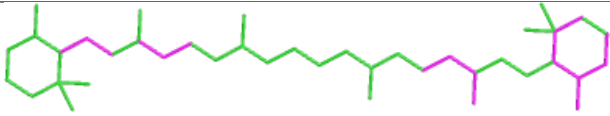
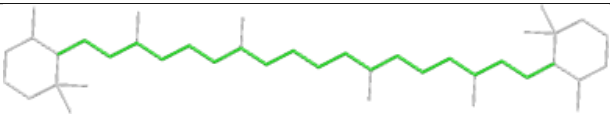
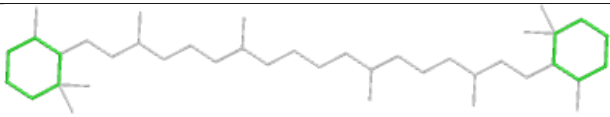
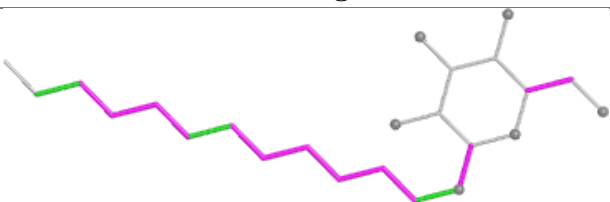
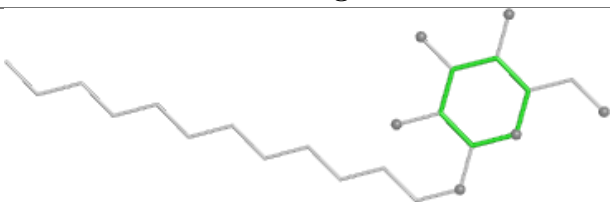
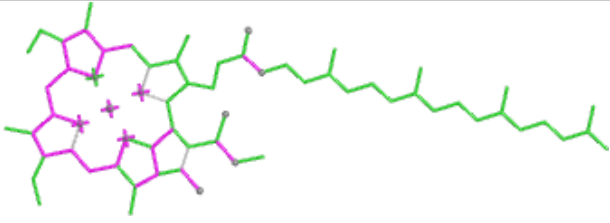
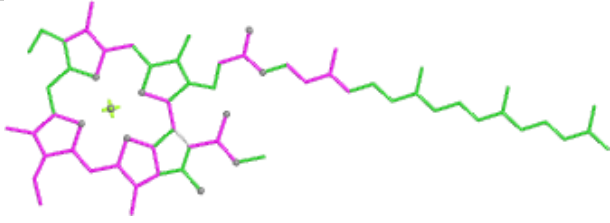
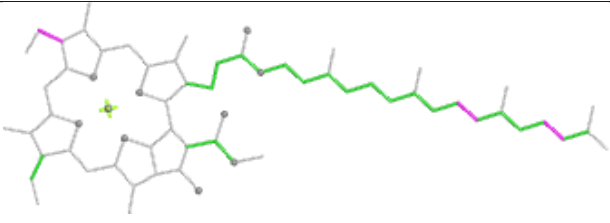
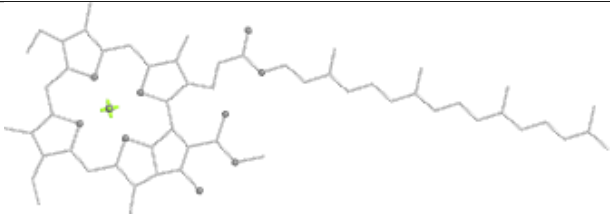


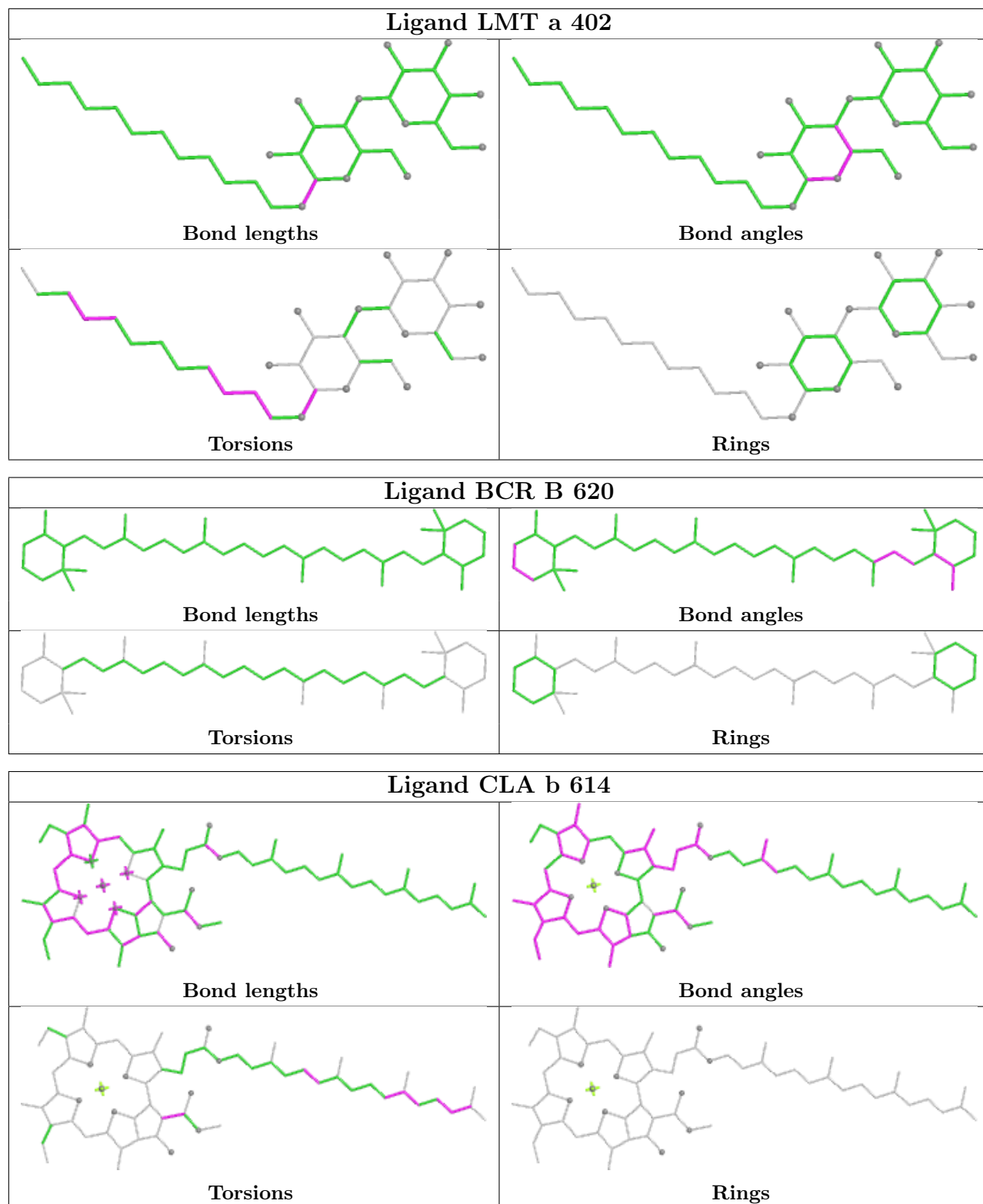
Ligand CLA c 905

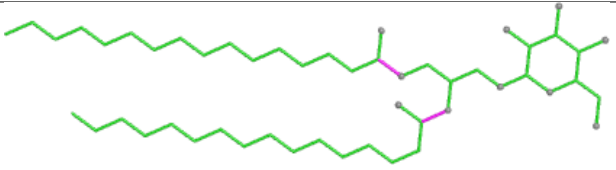
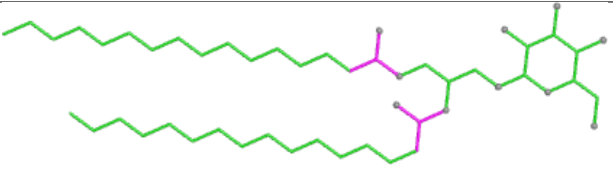
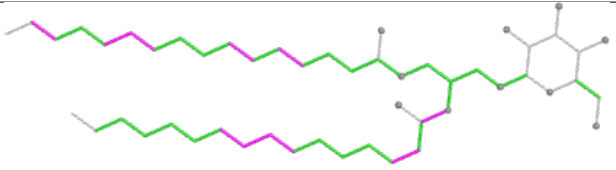
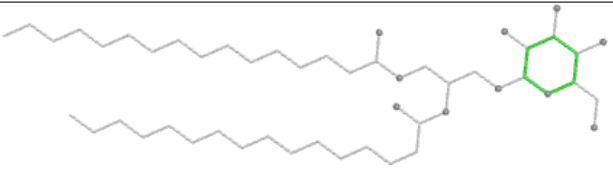
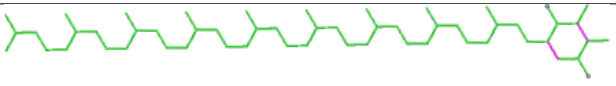
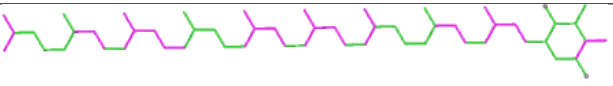
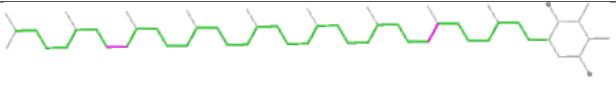
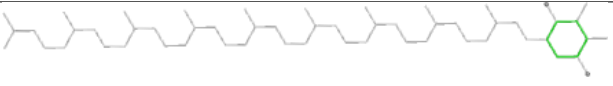
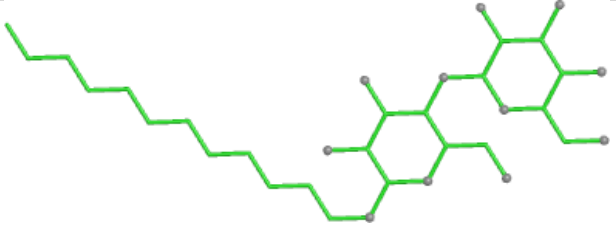
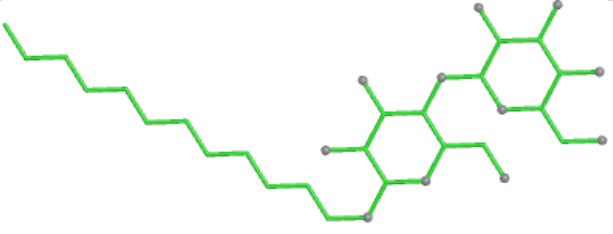
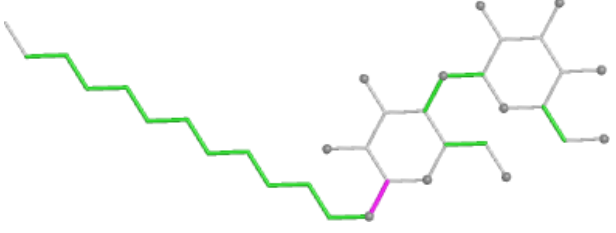
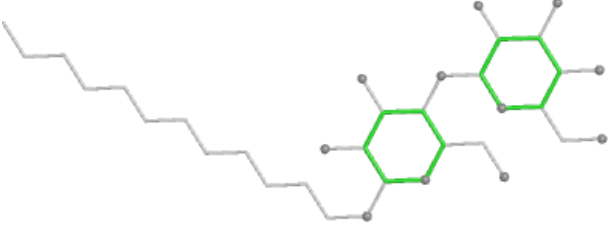
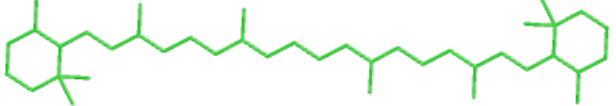
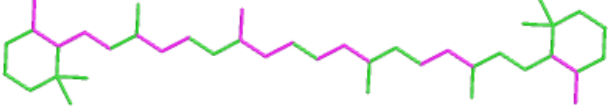
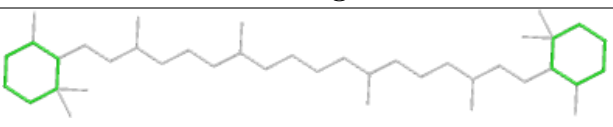


Ligand CLA c 907

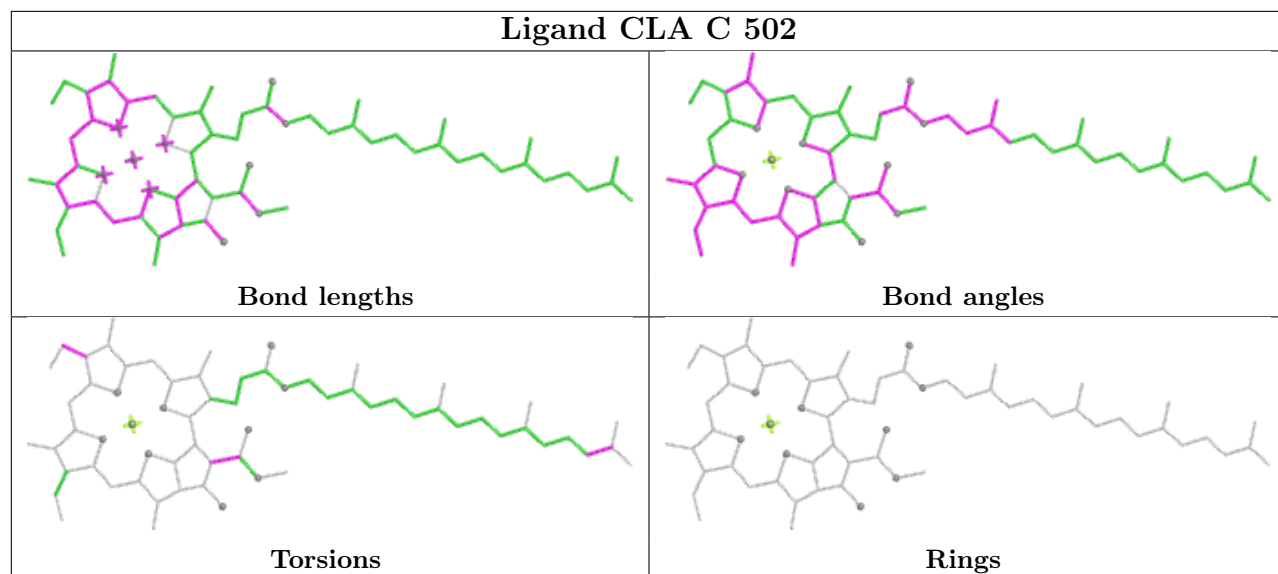


Ligand BCR b 622	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT T 703	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

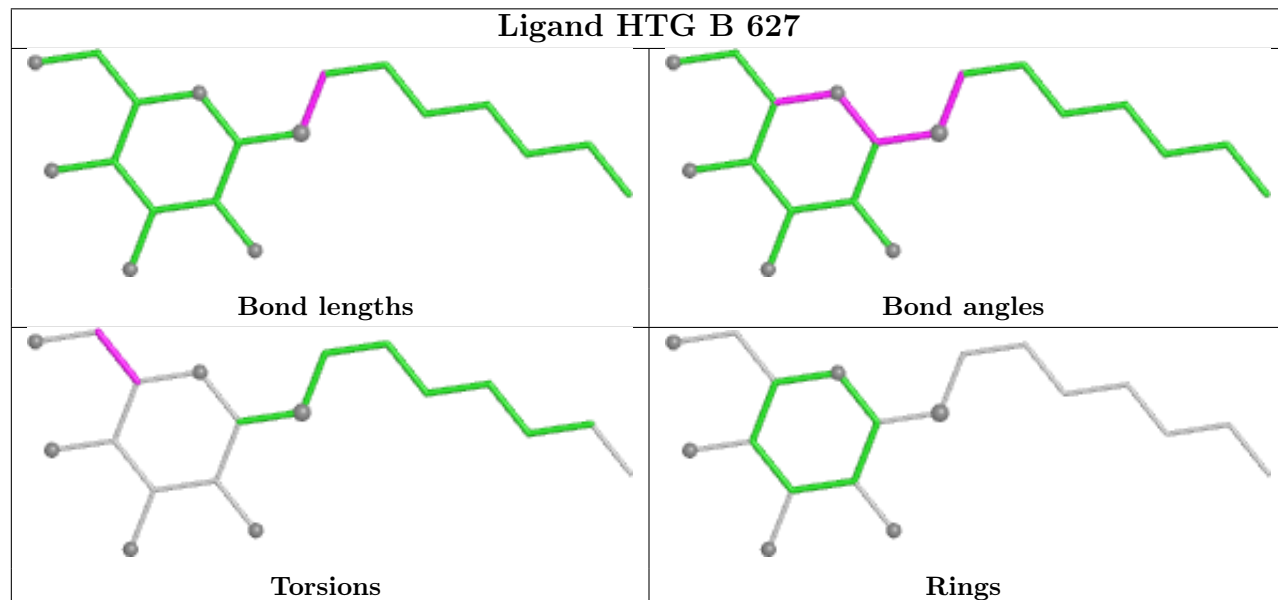


Ligand LMG B 622	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 D 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT M 303	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR c 915	
 Bond lengths	 Bond angles
 Torsions	 Rings

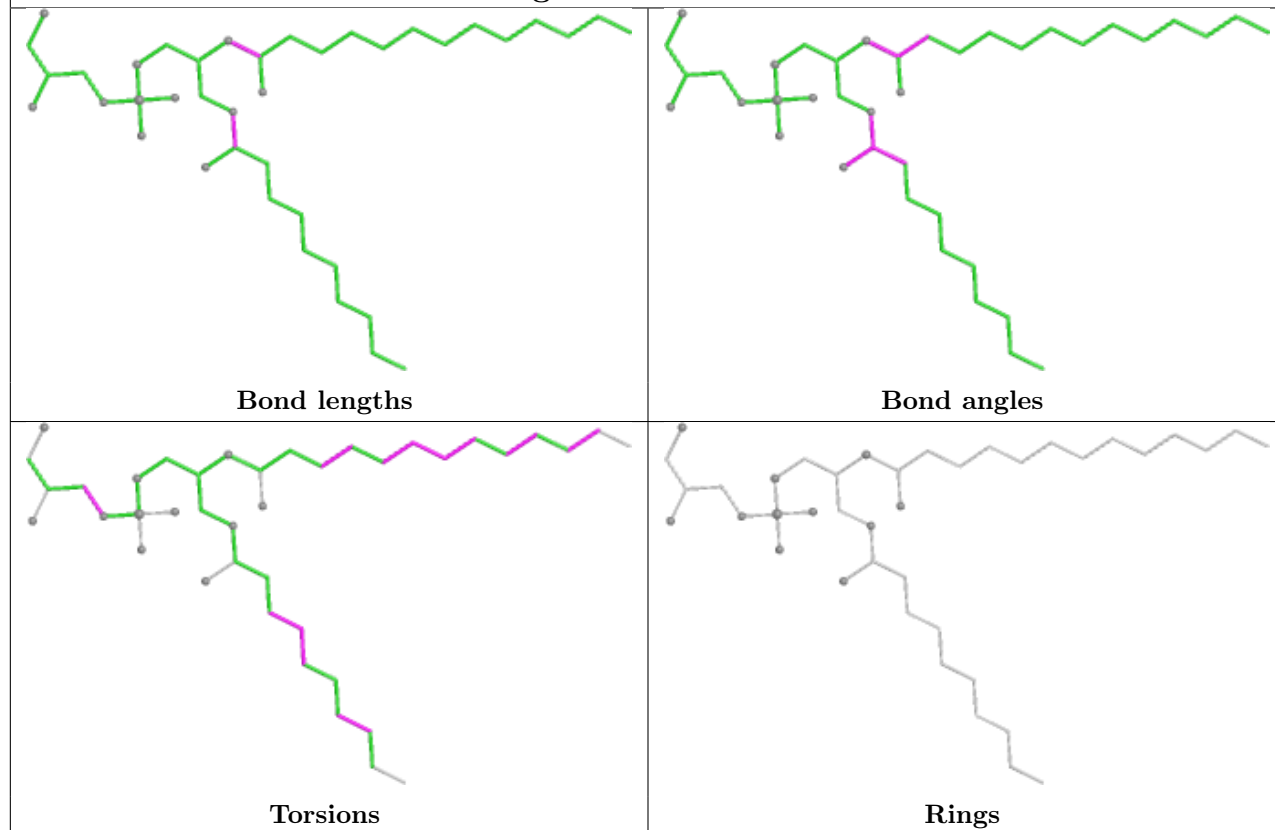
Ligand CLA C 502



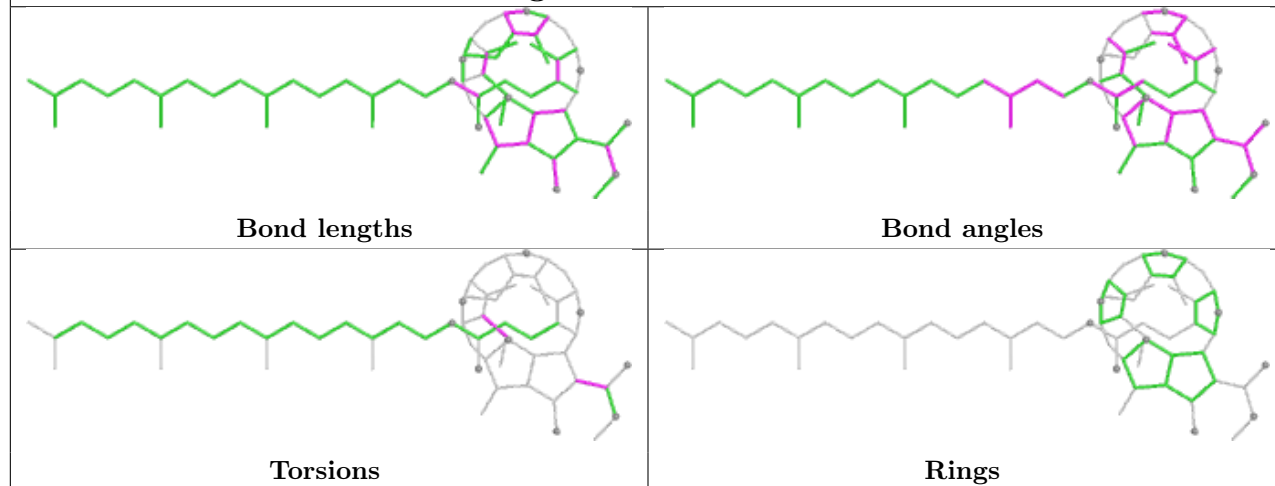
Ligand HTG B 627

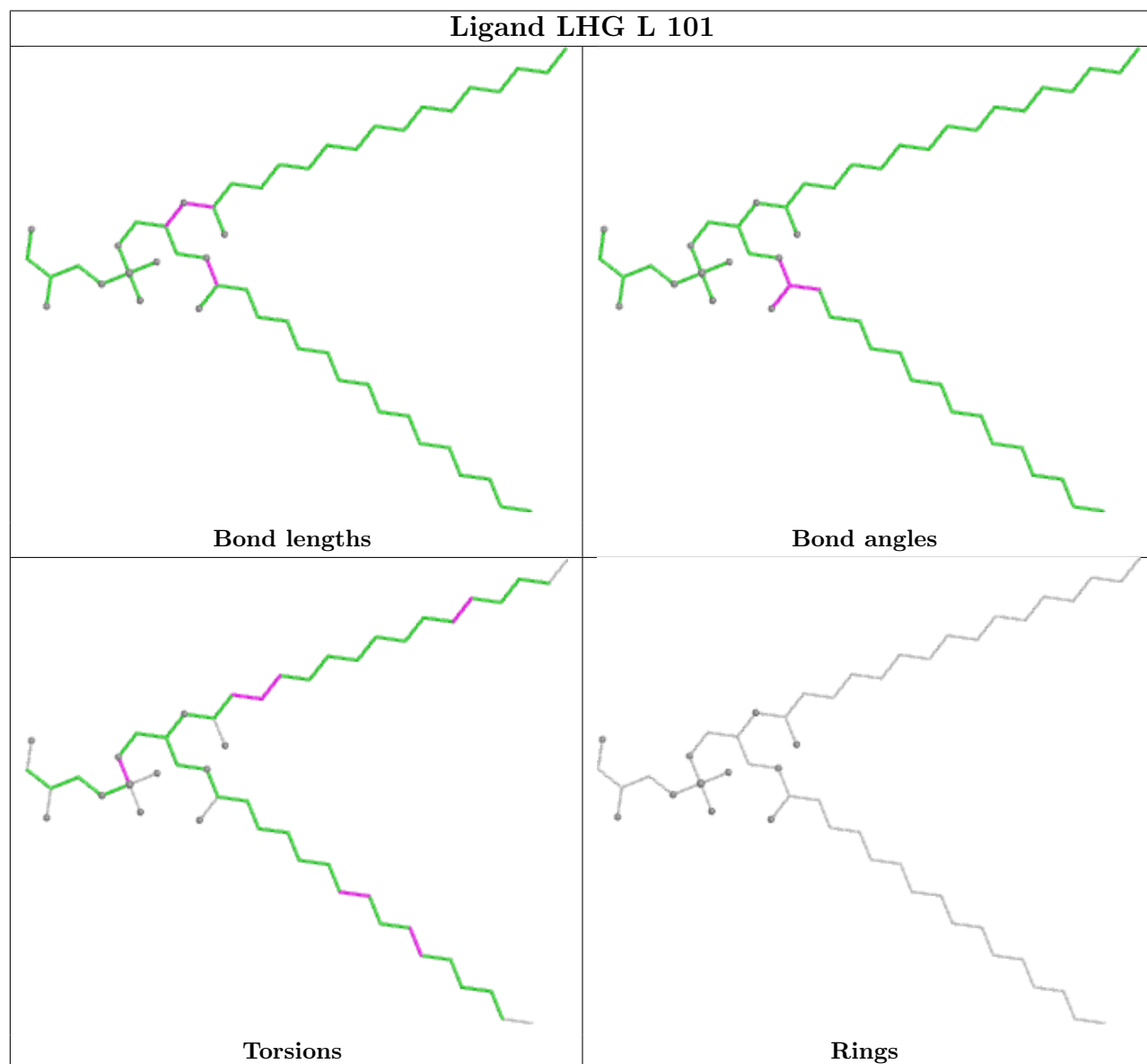
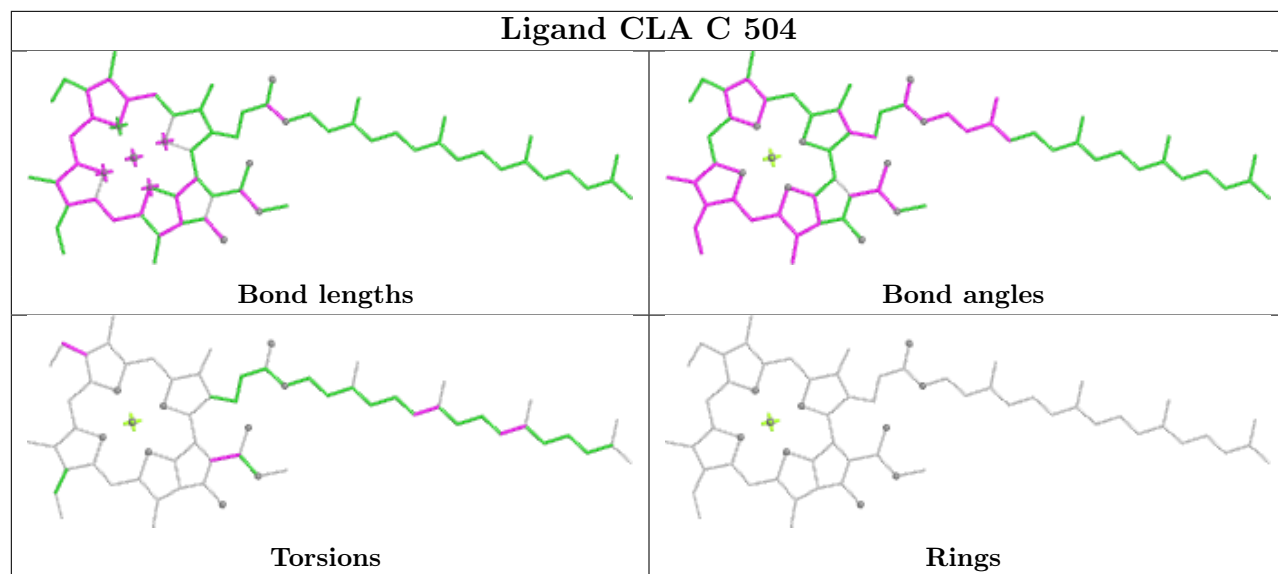


Ligand LHG d 410

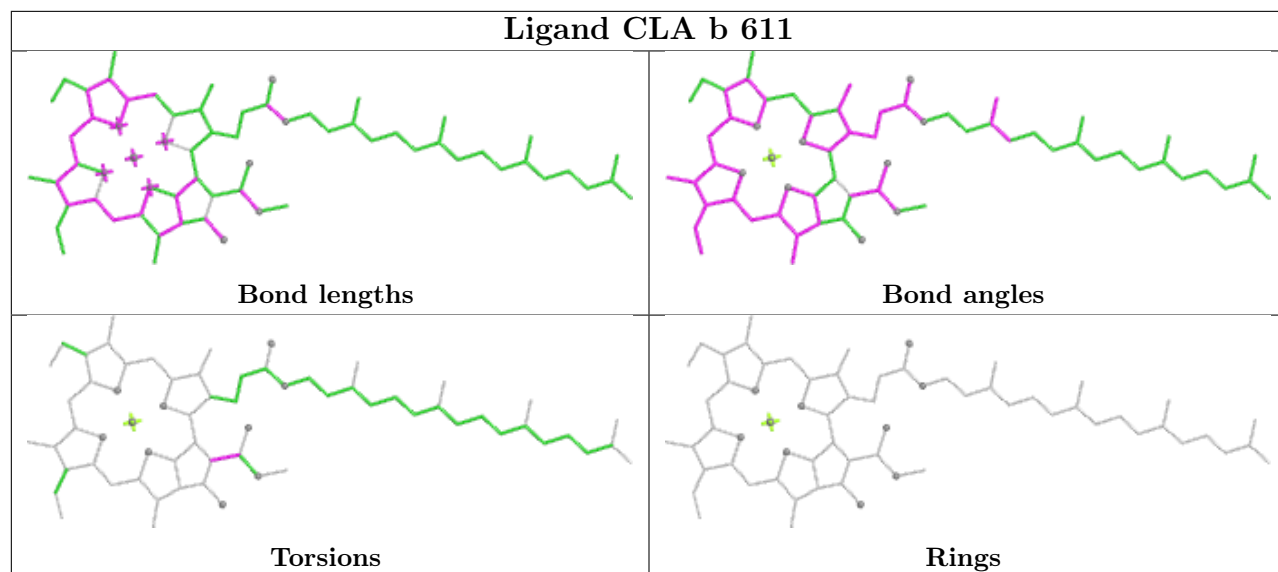


Ligand PHO A 409

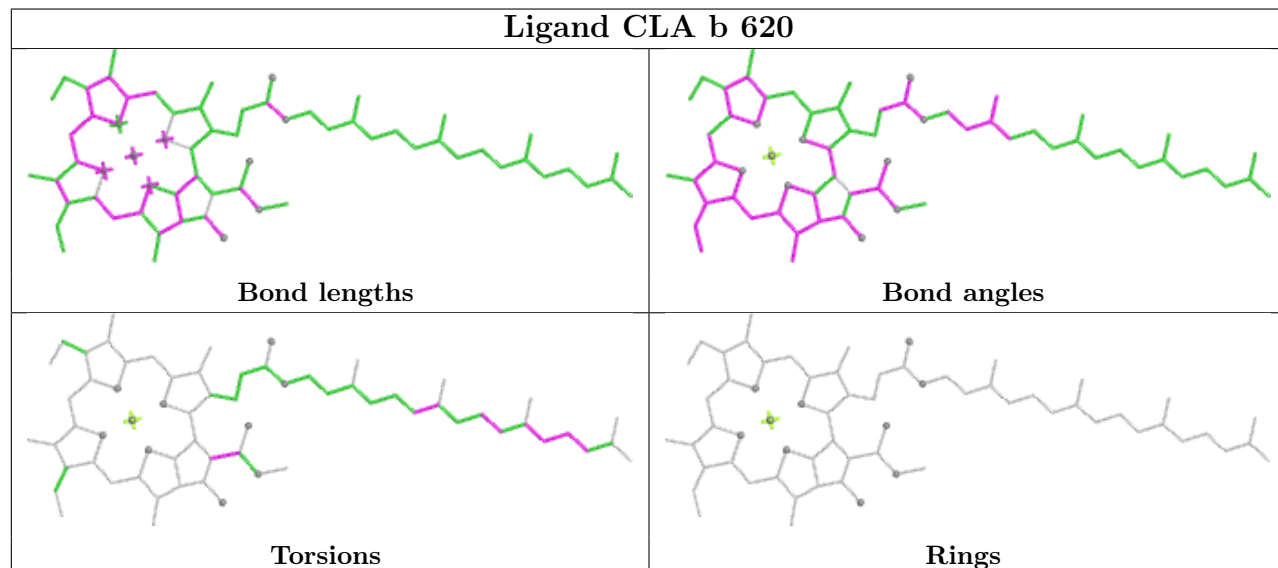




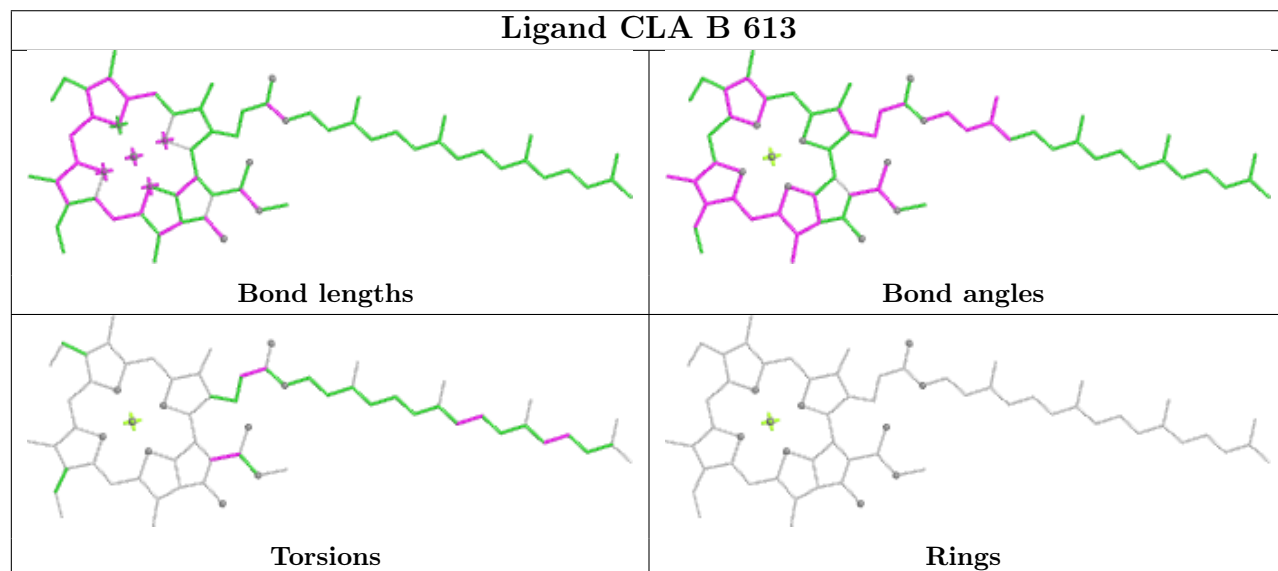
Ligand CLA b 611



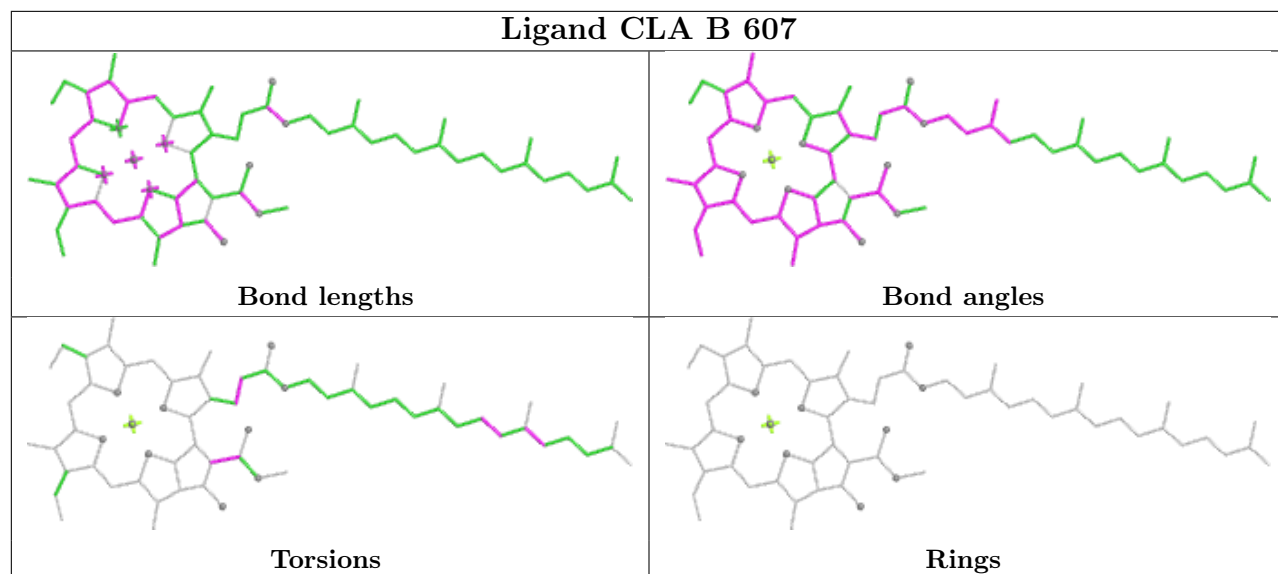
Ligand CLA b 620



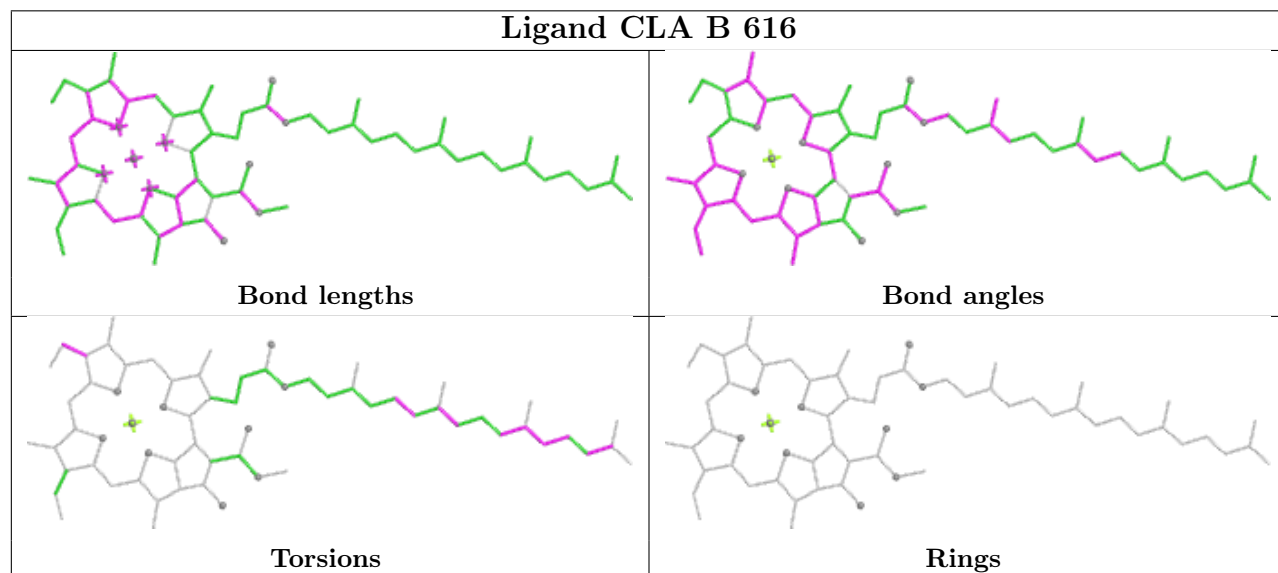
Ligand CLA B 613



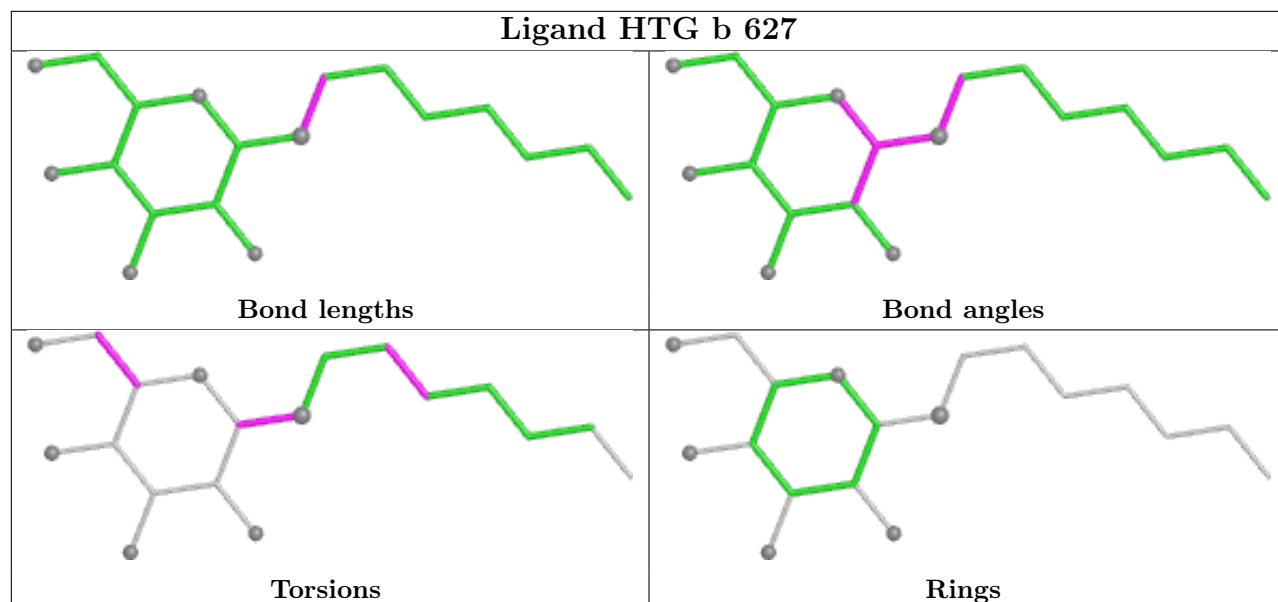
Ligand CLA B 607

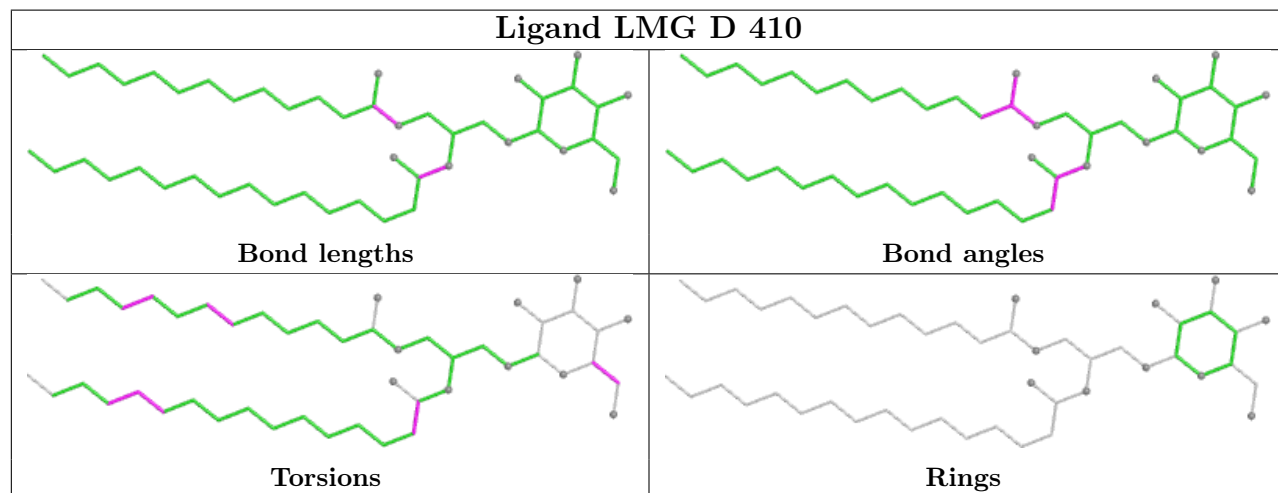
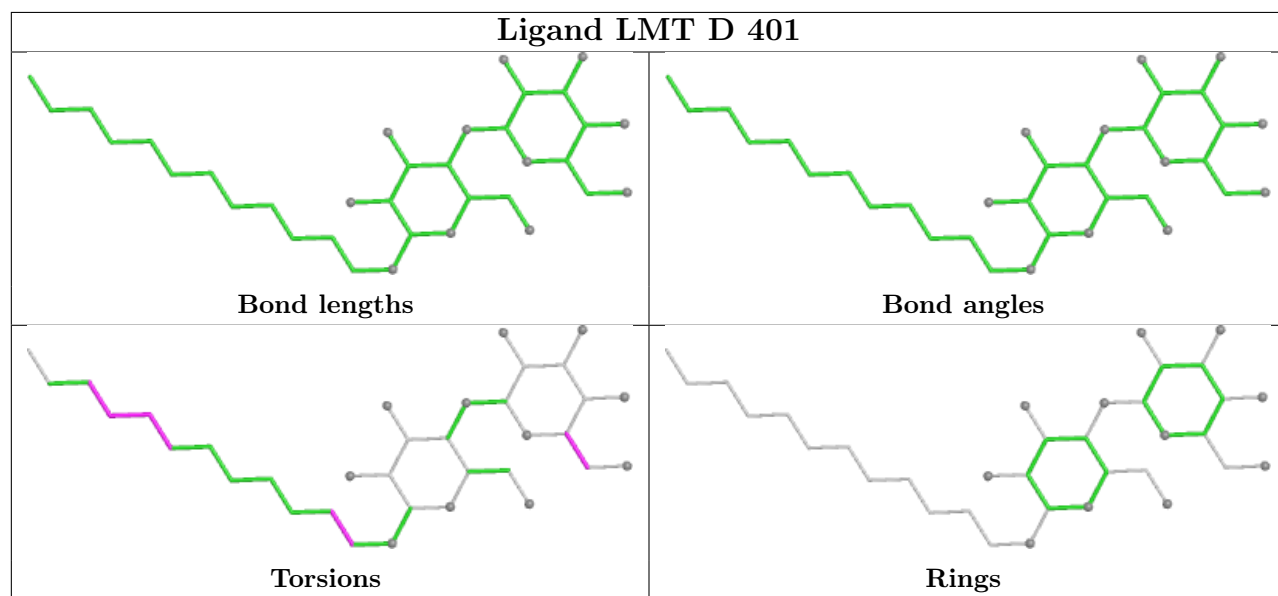
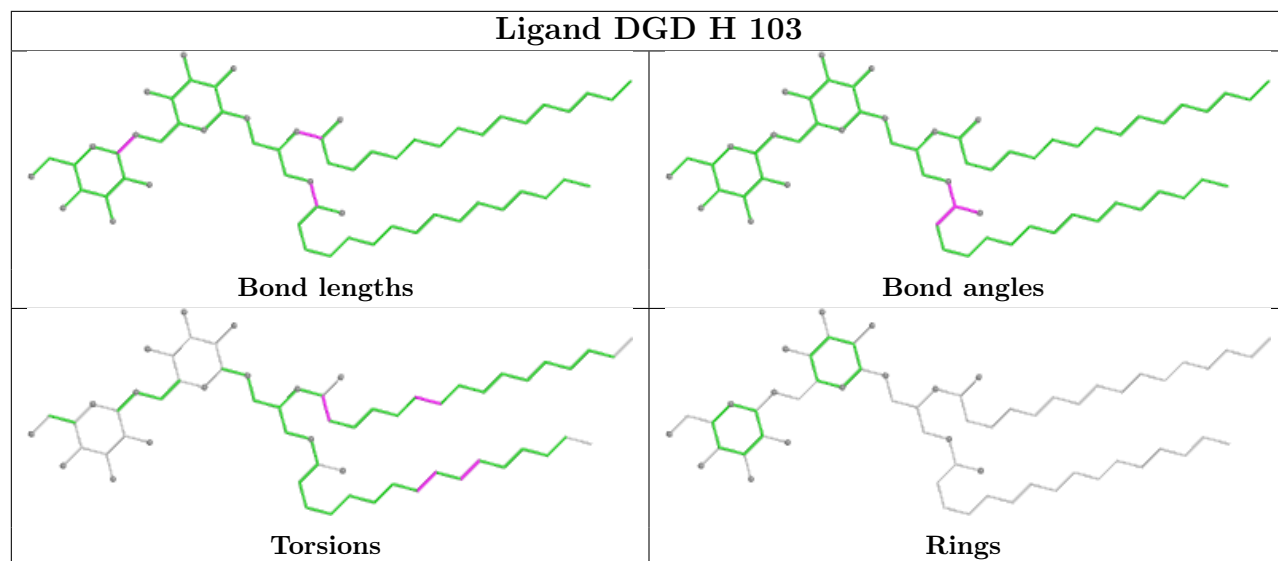


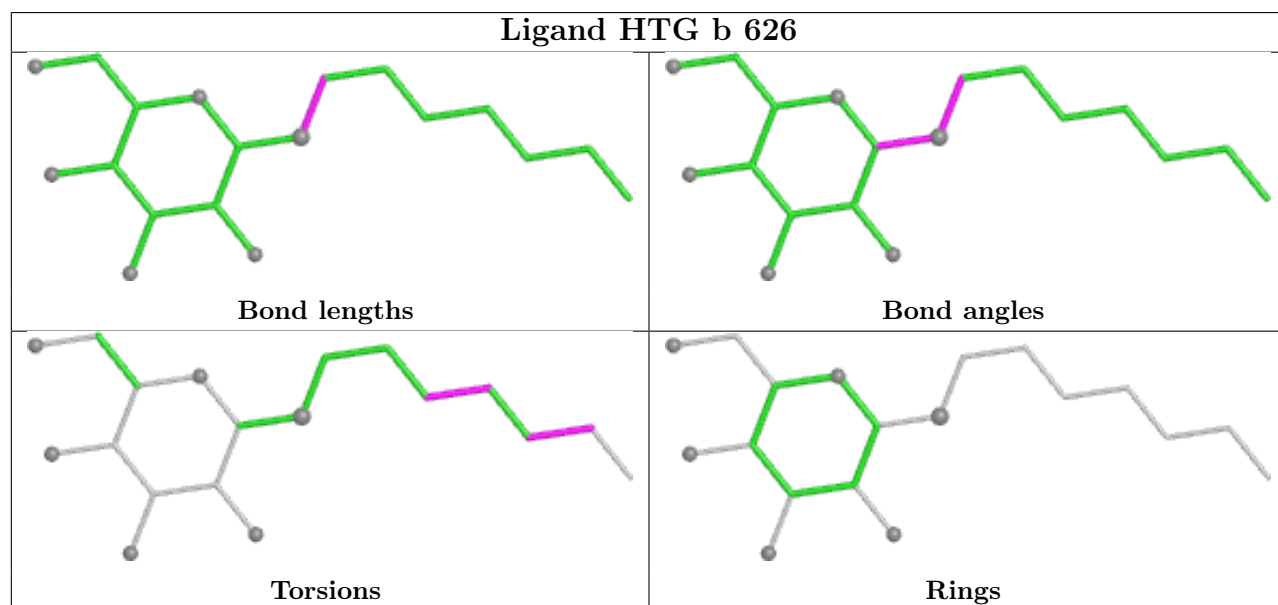
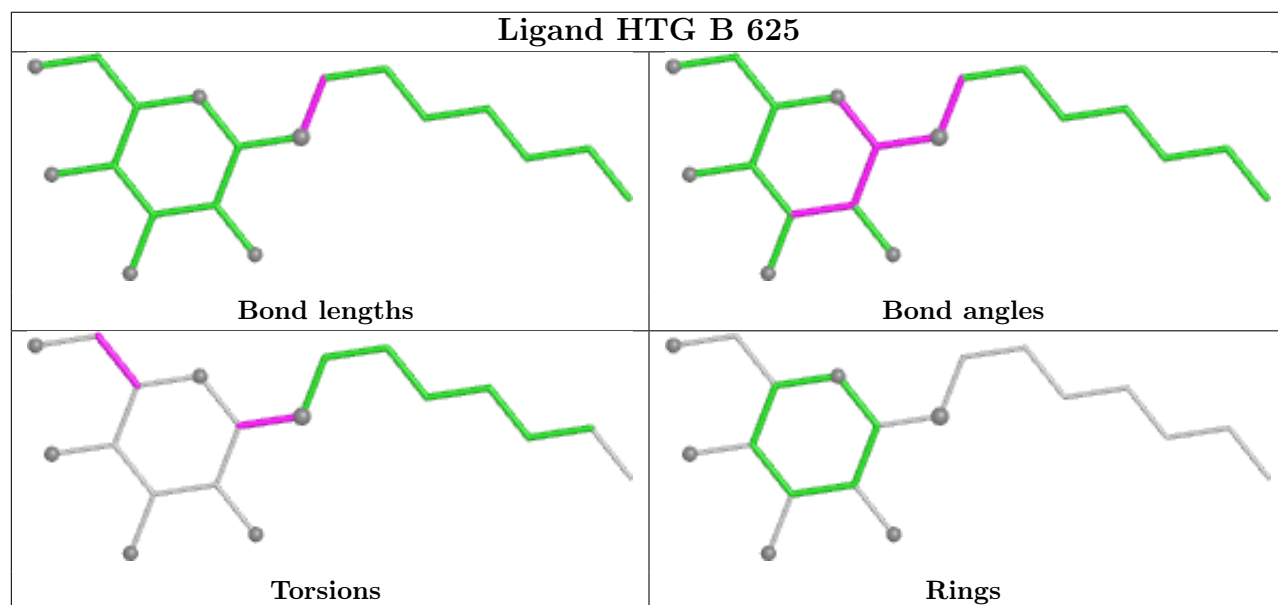
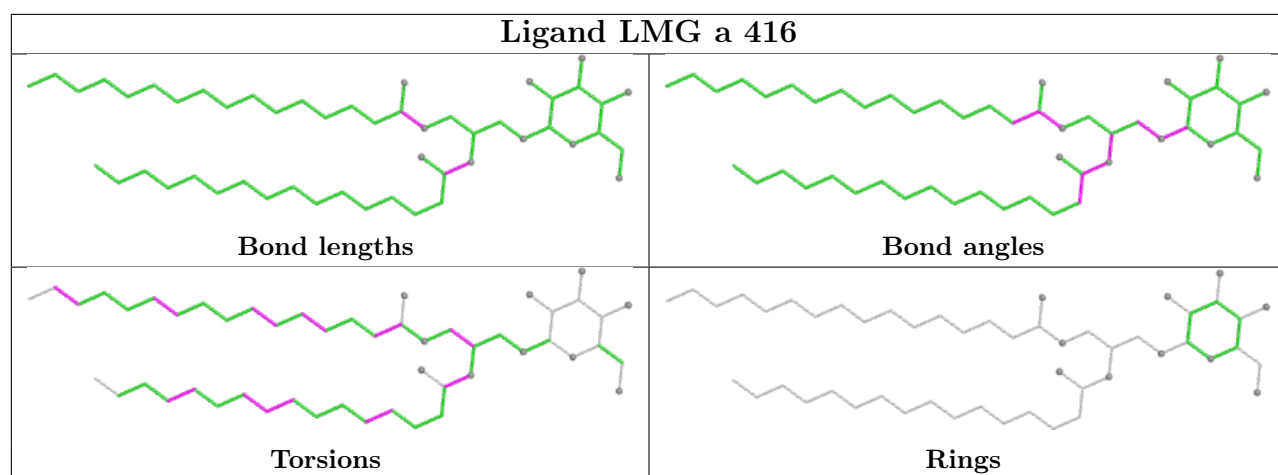
Ligand CLA B 616

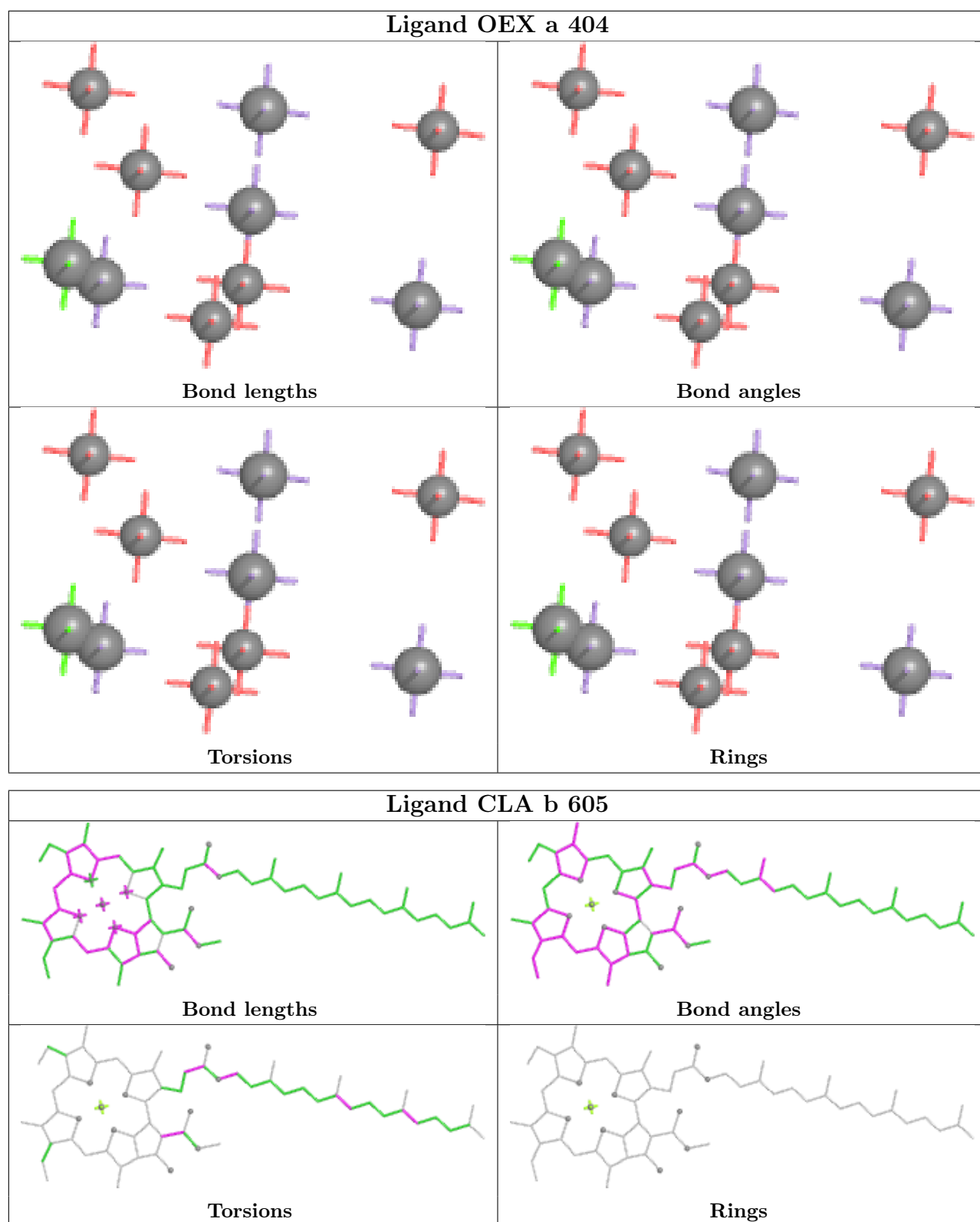


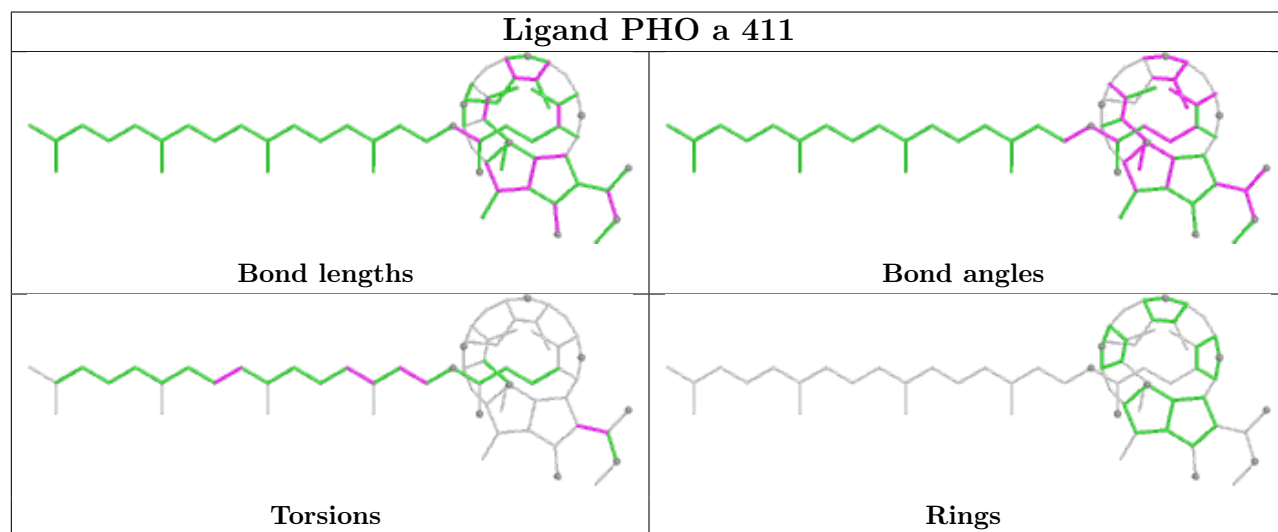
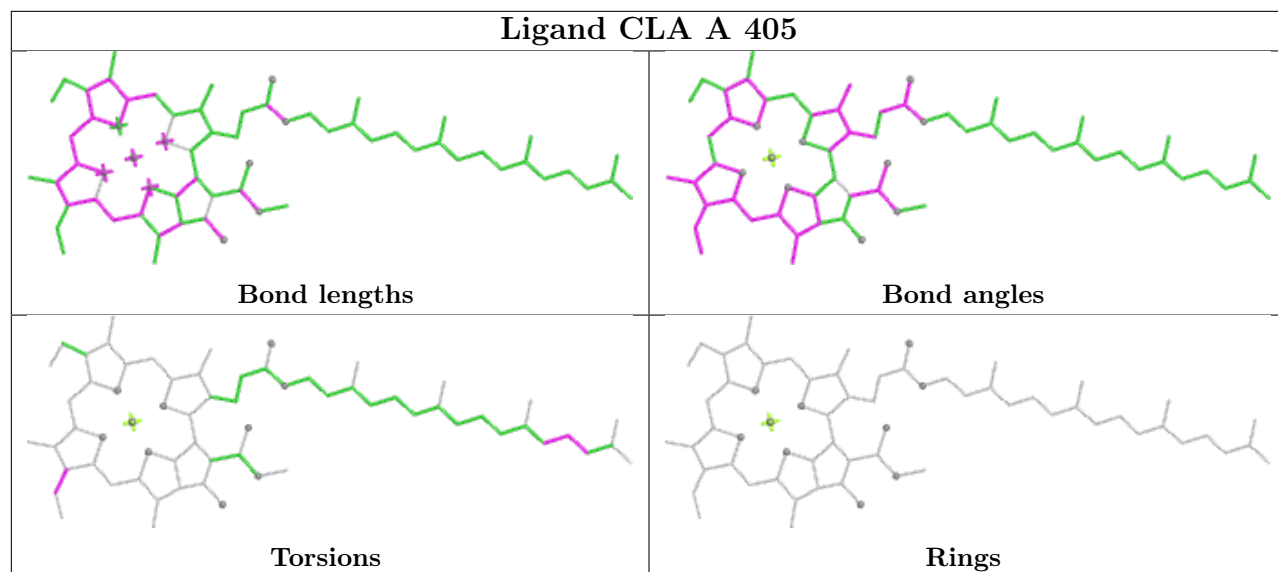
Ligand HTG b 627

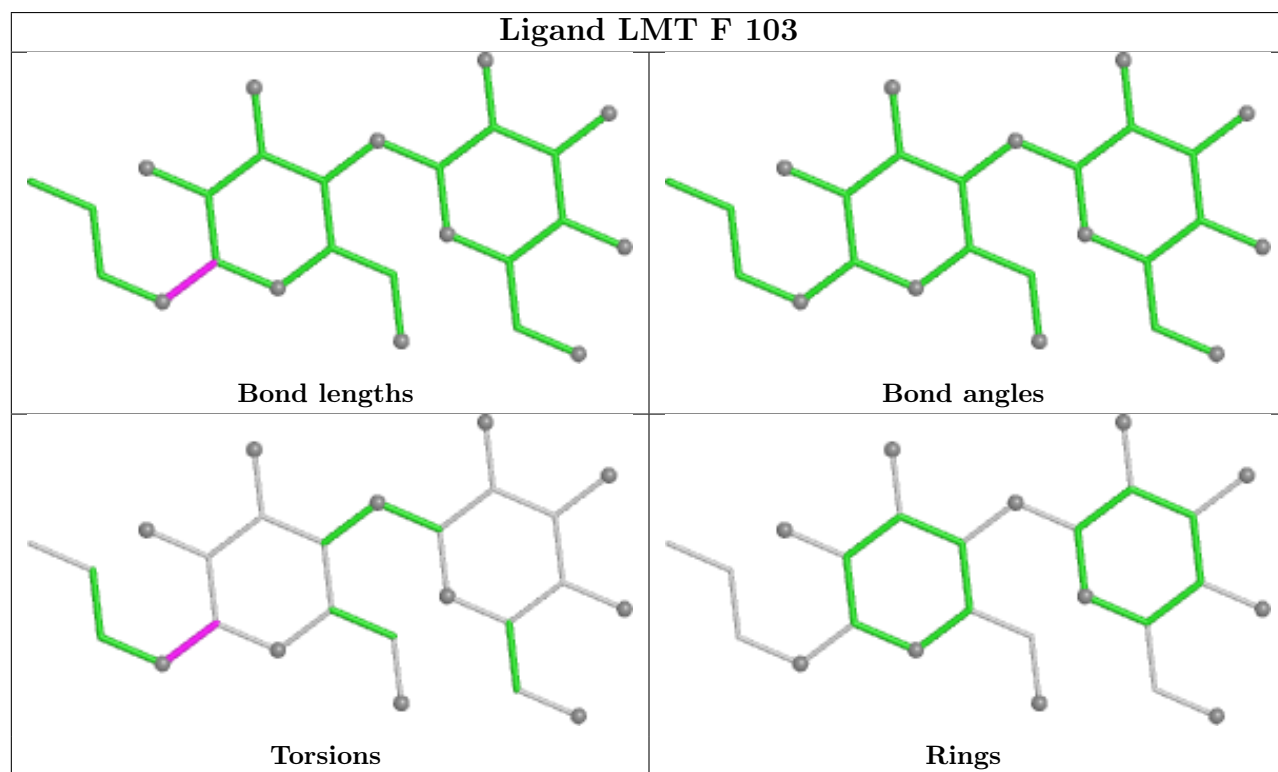
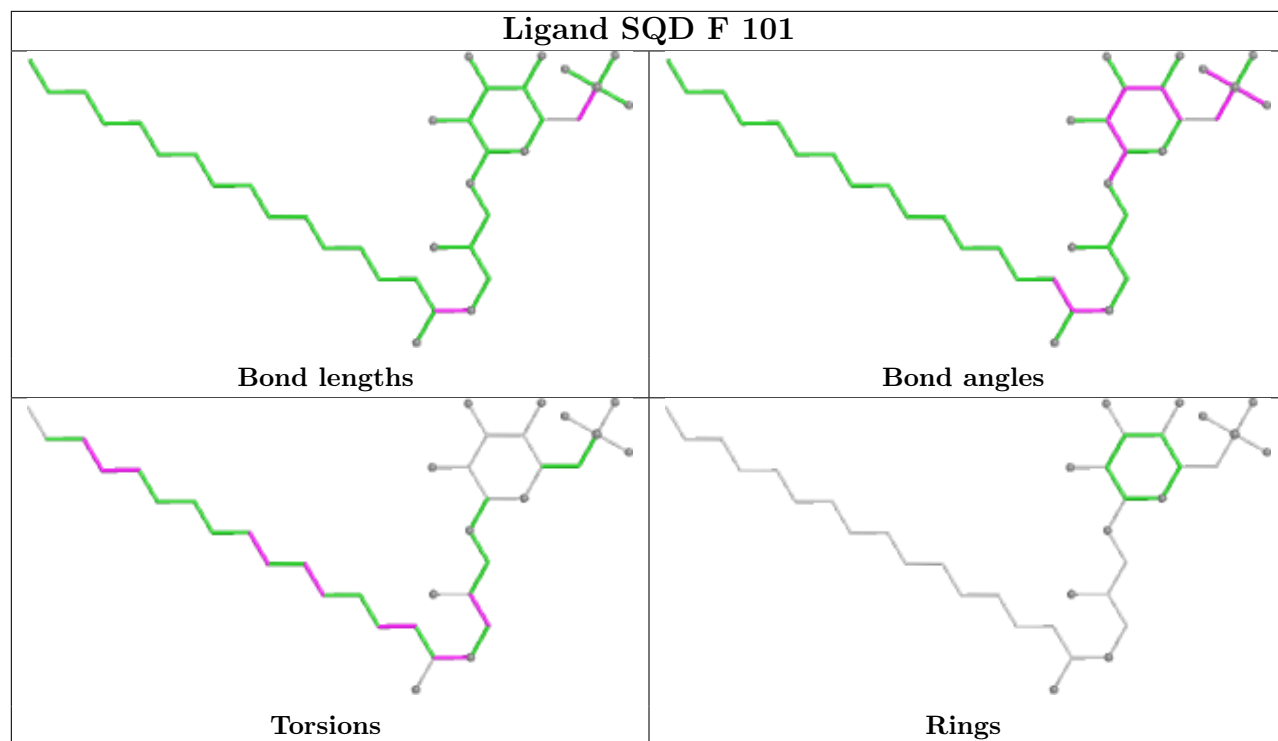


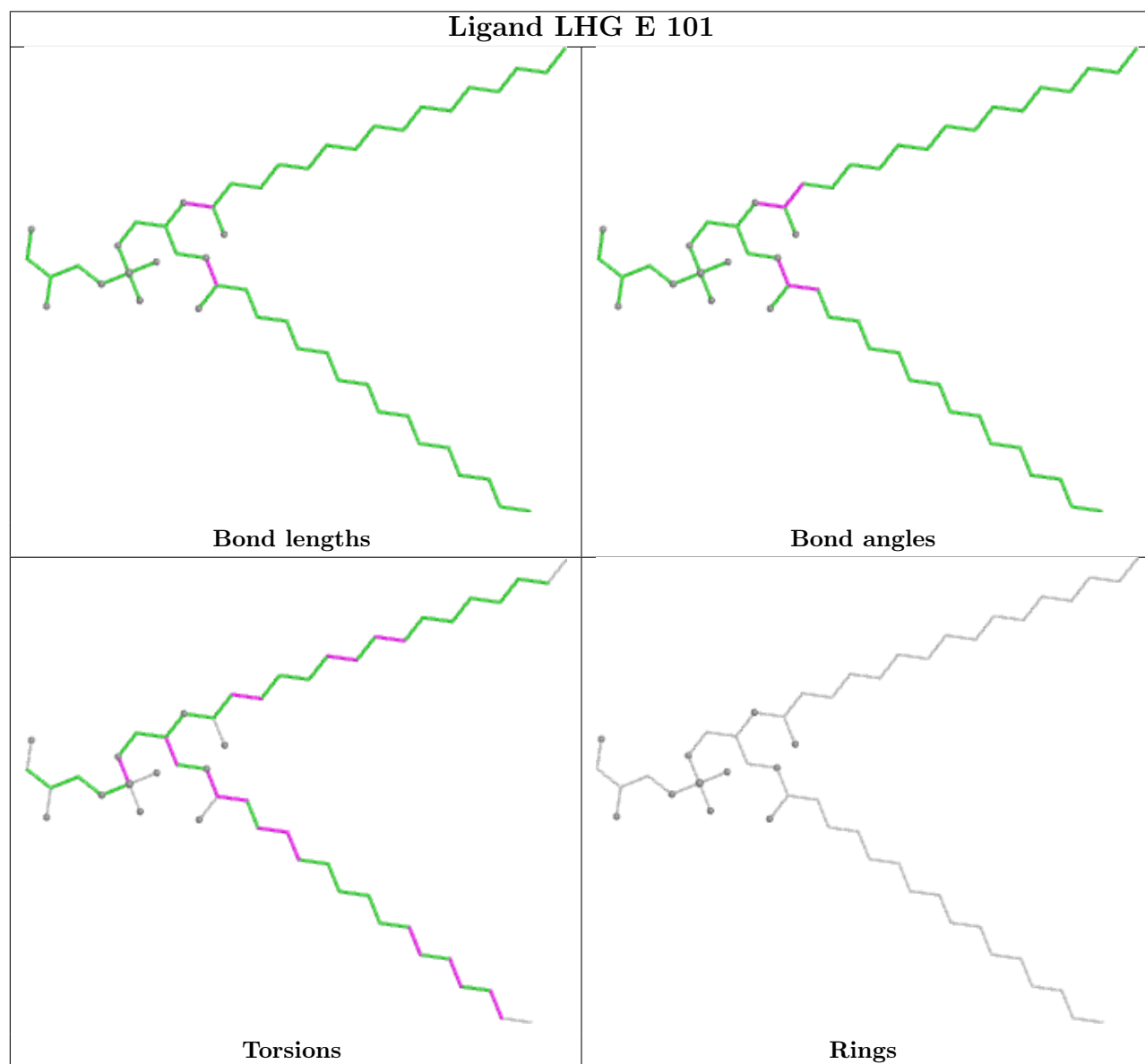
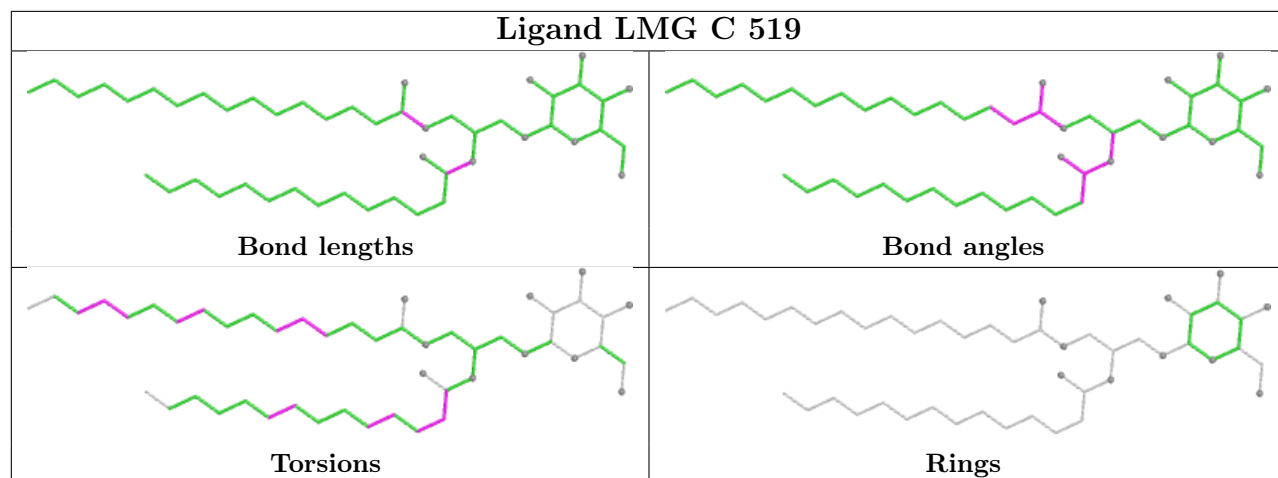




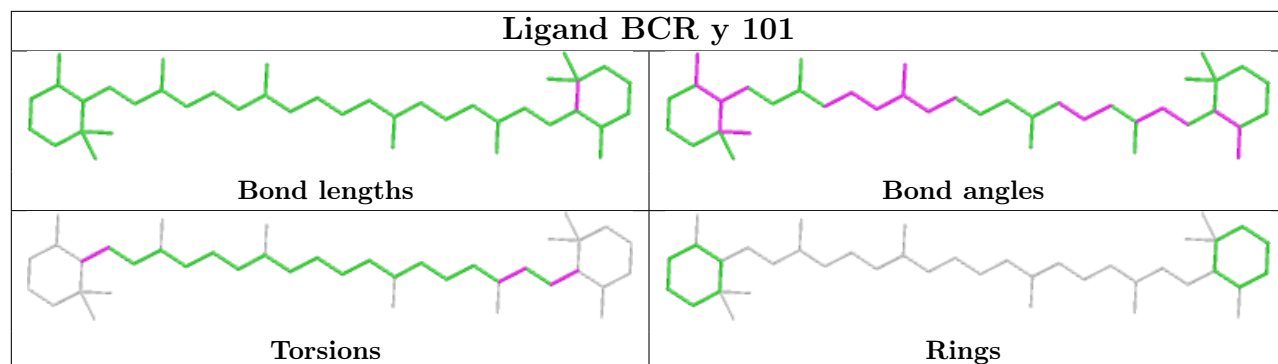




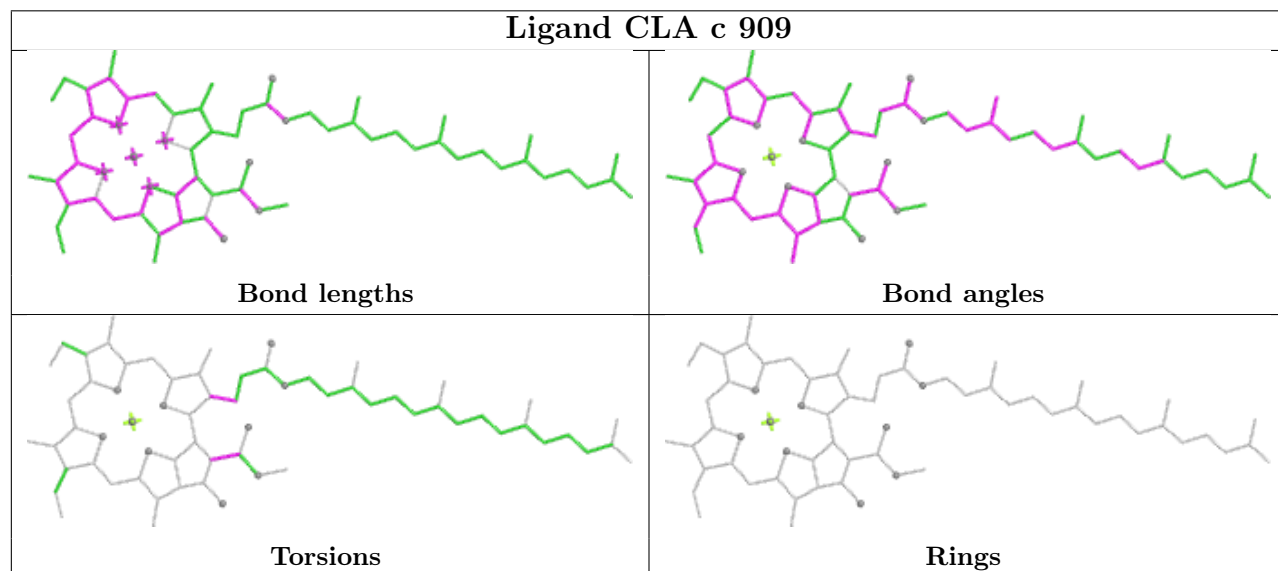




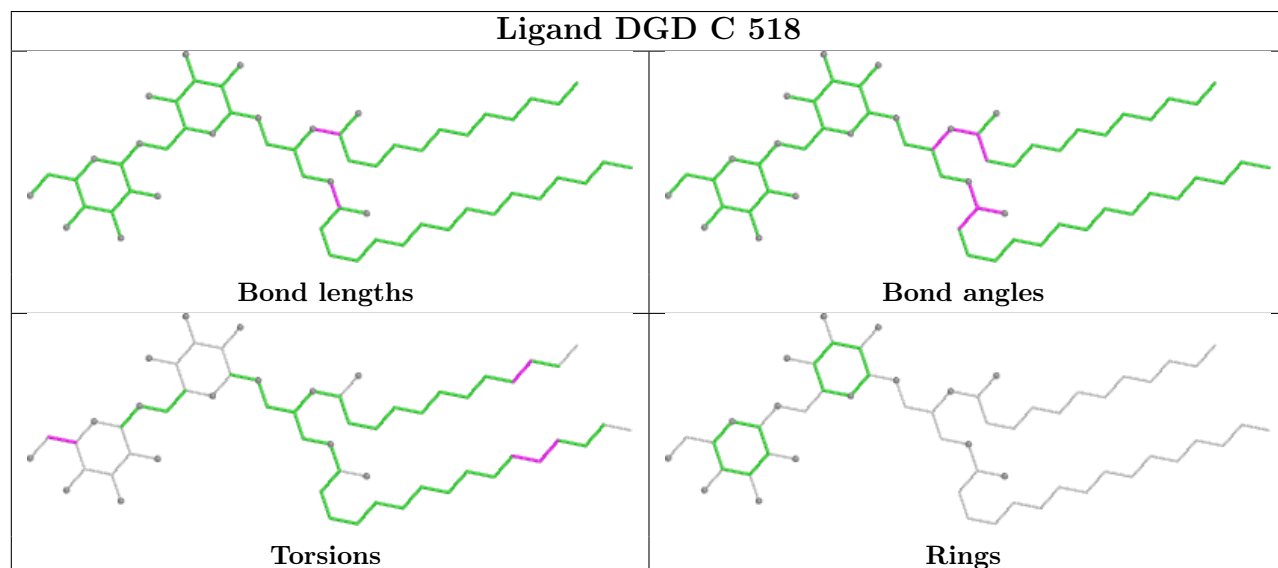
Ligand BCR y 101

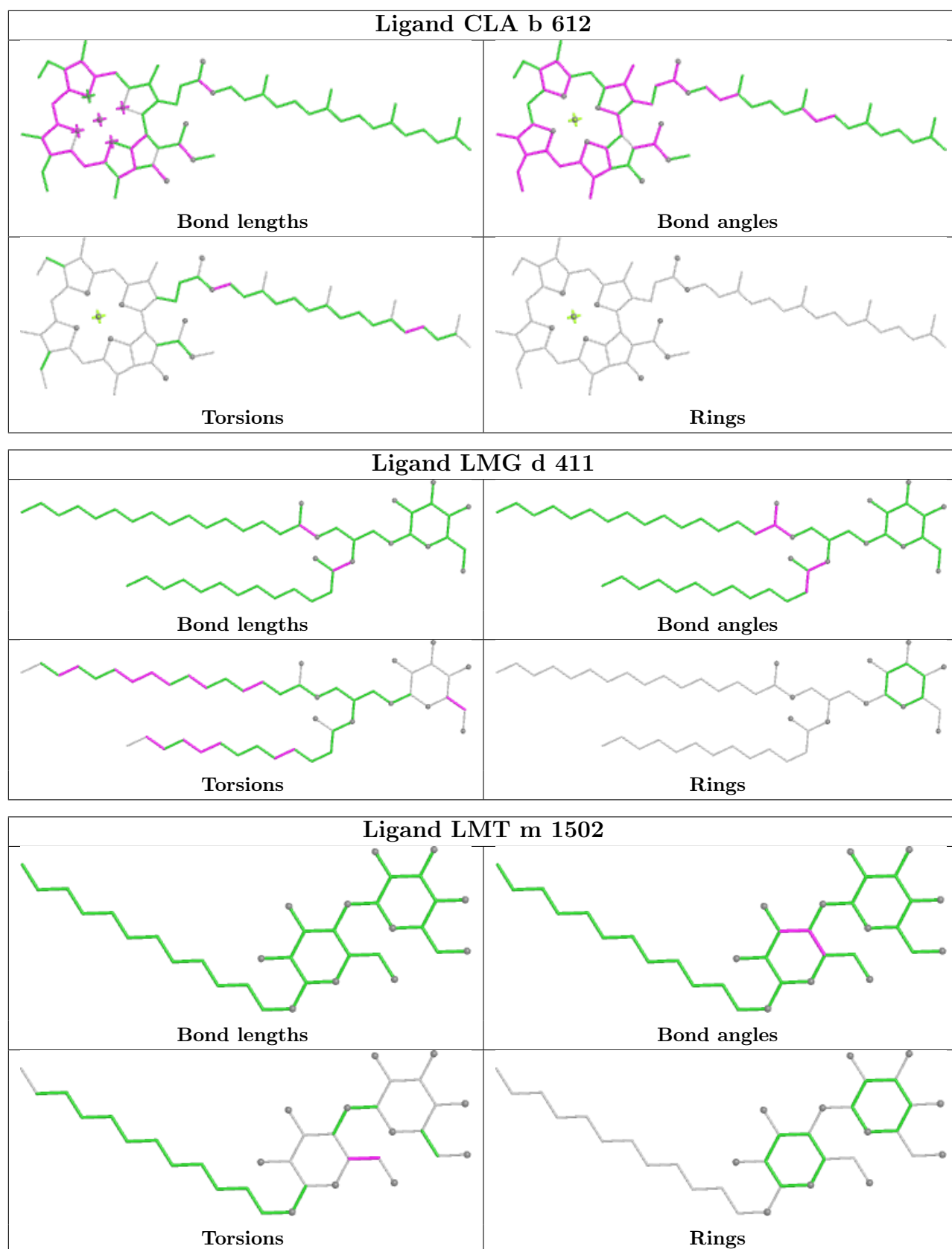


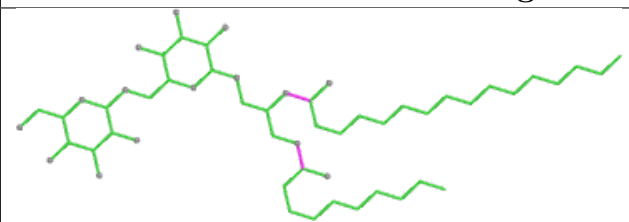
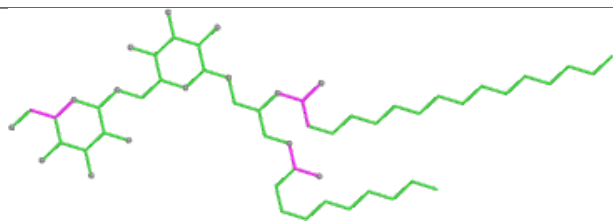
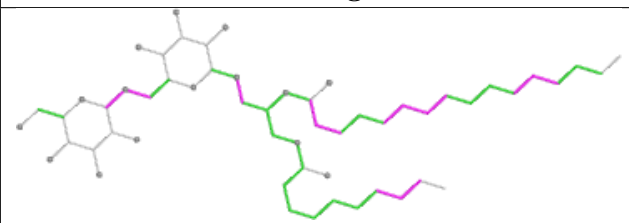
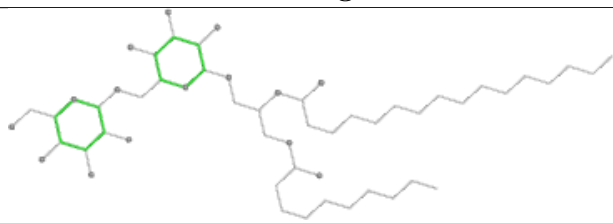
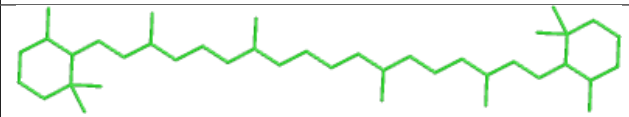
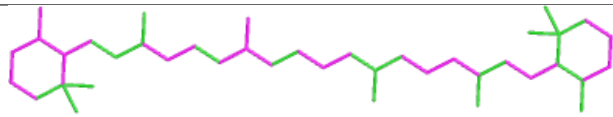
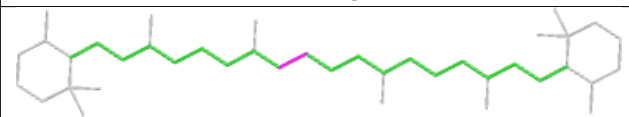
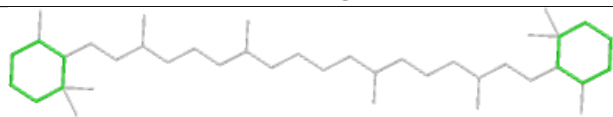
Ligand CLA c 909

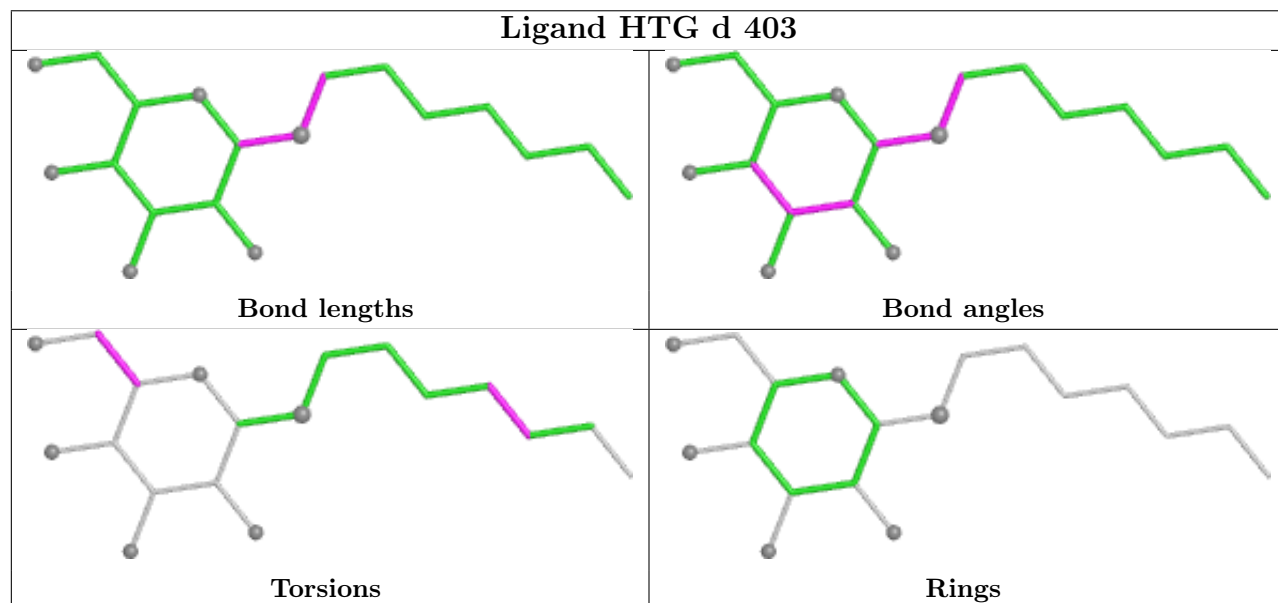
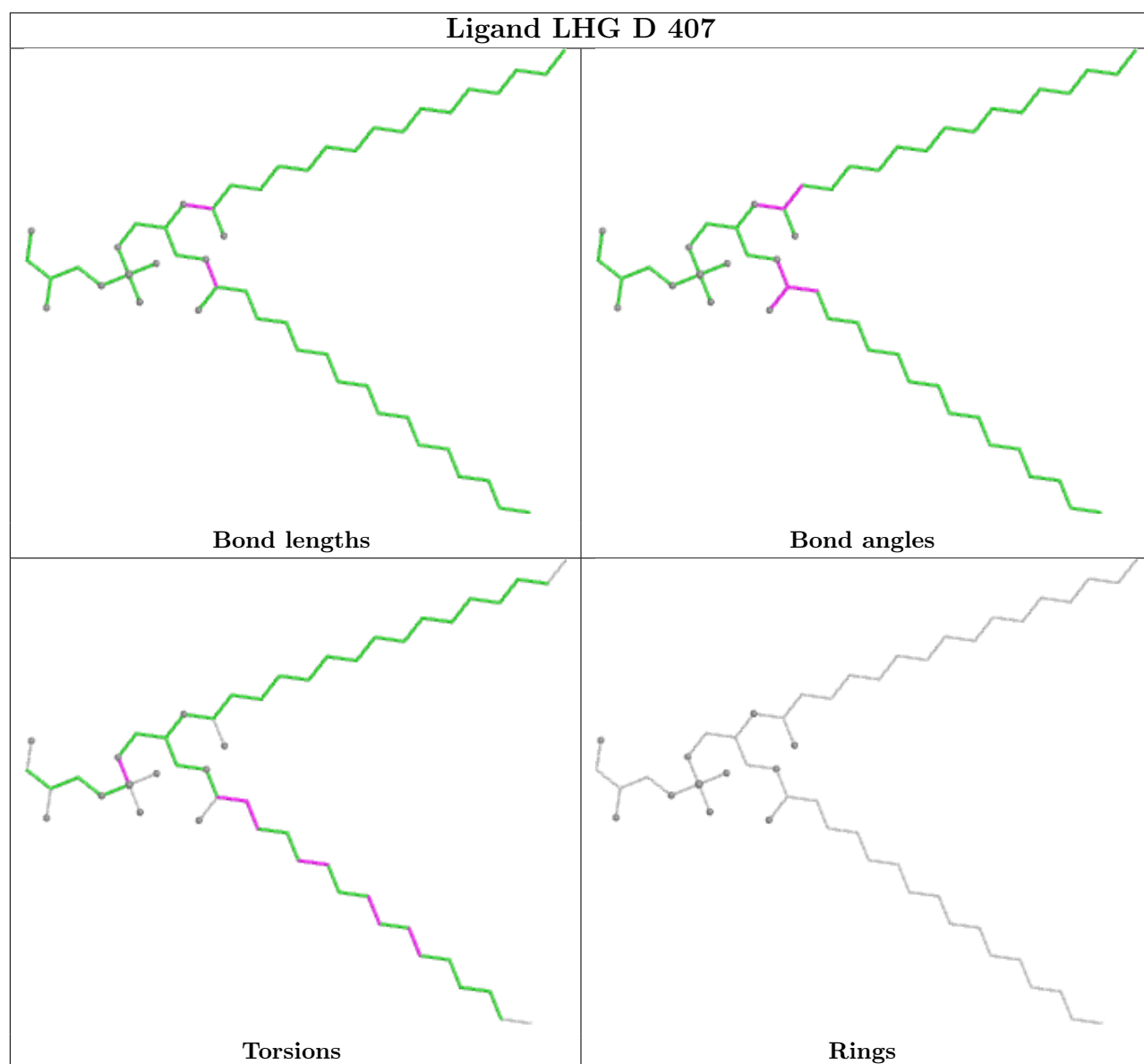


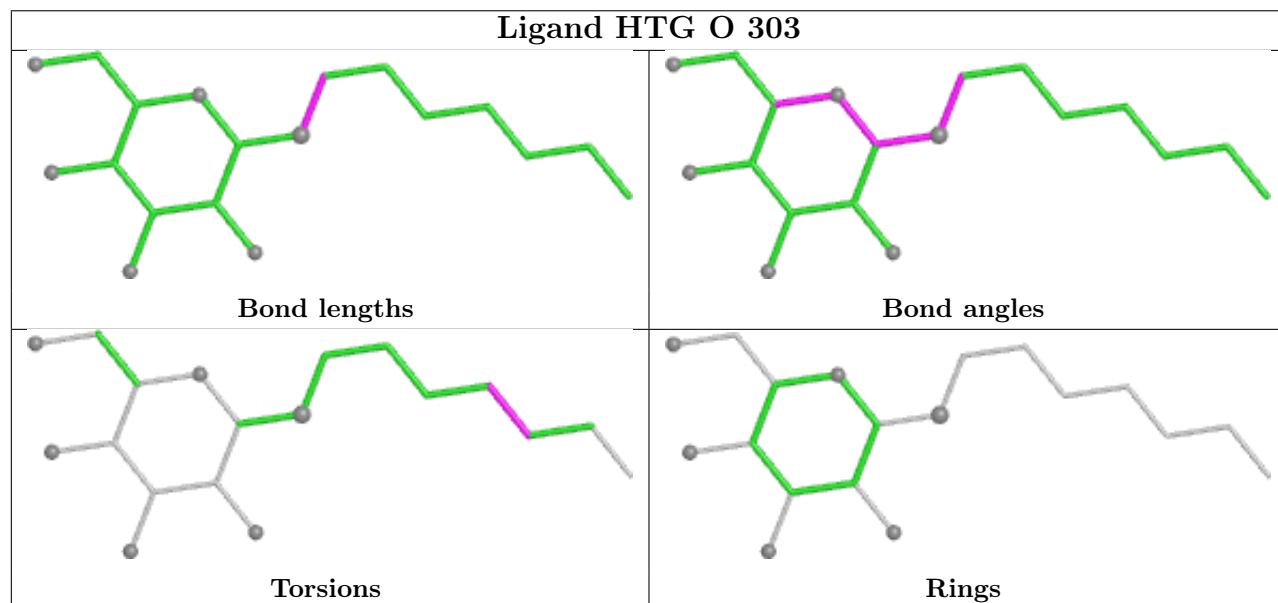
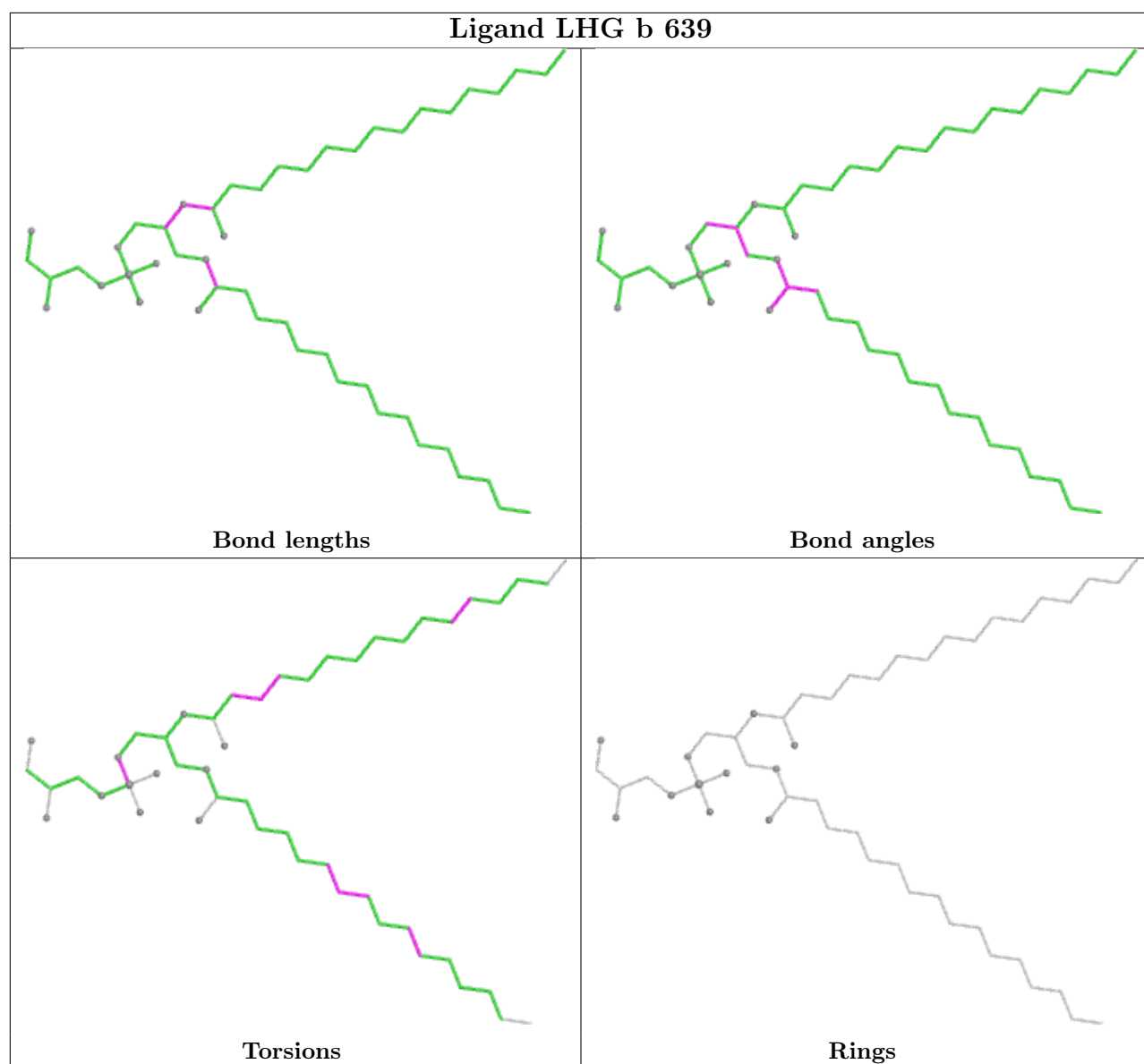
Ligand DGD C 518

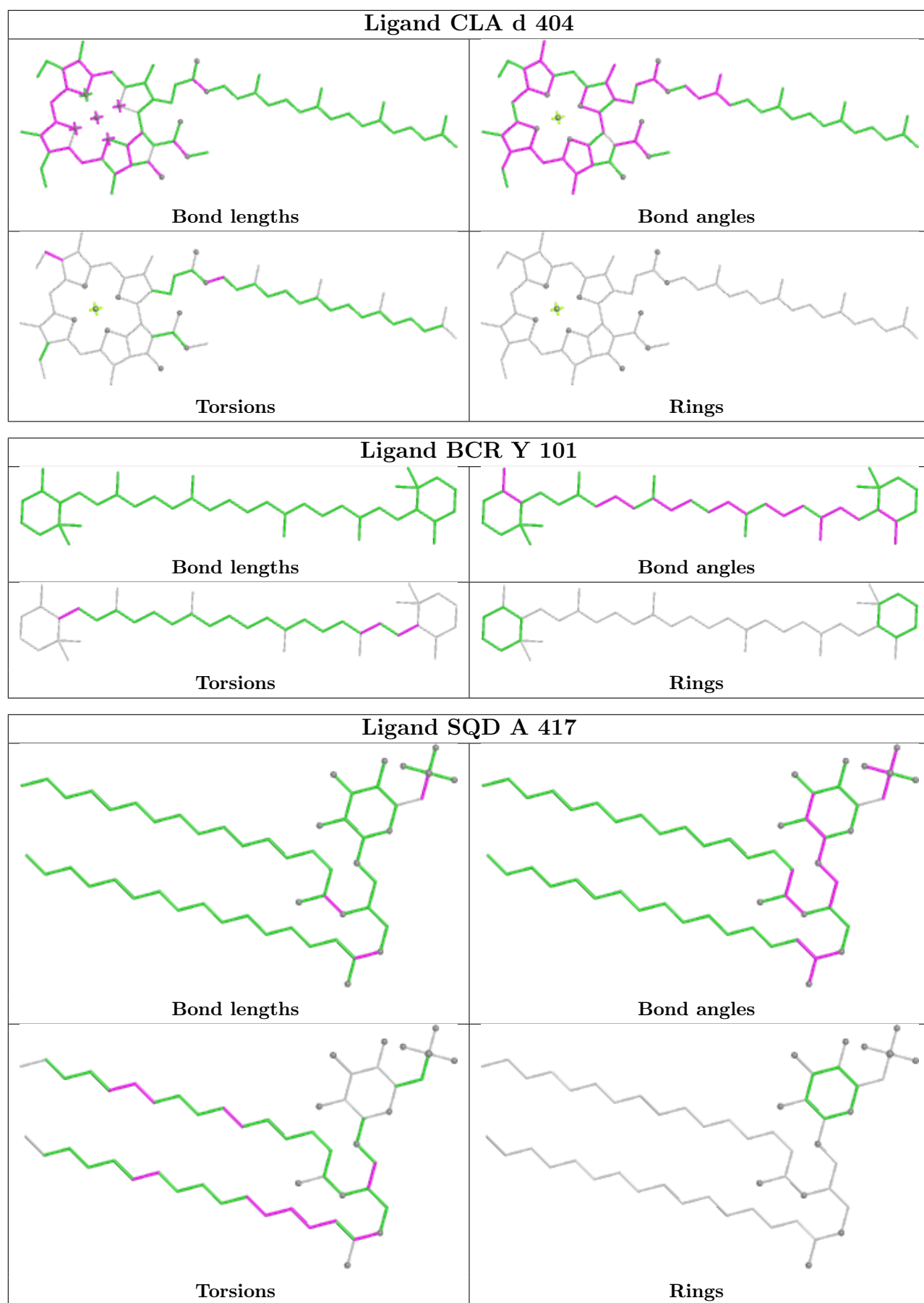


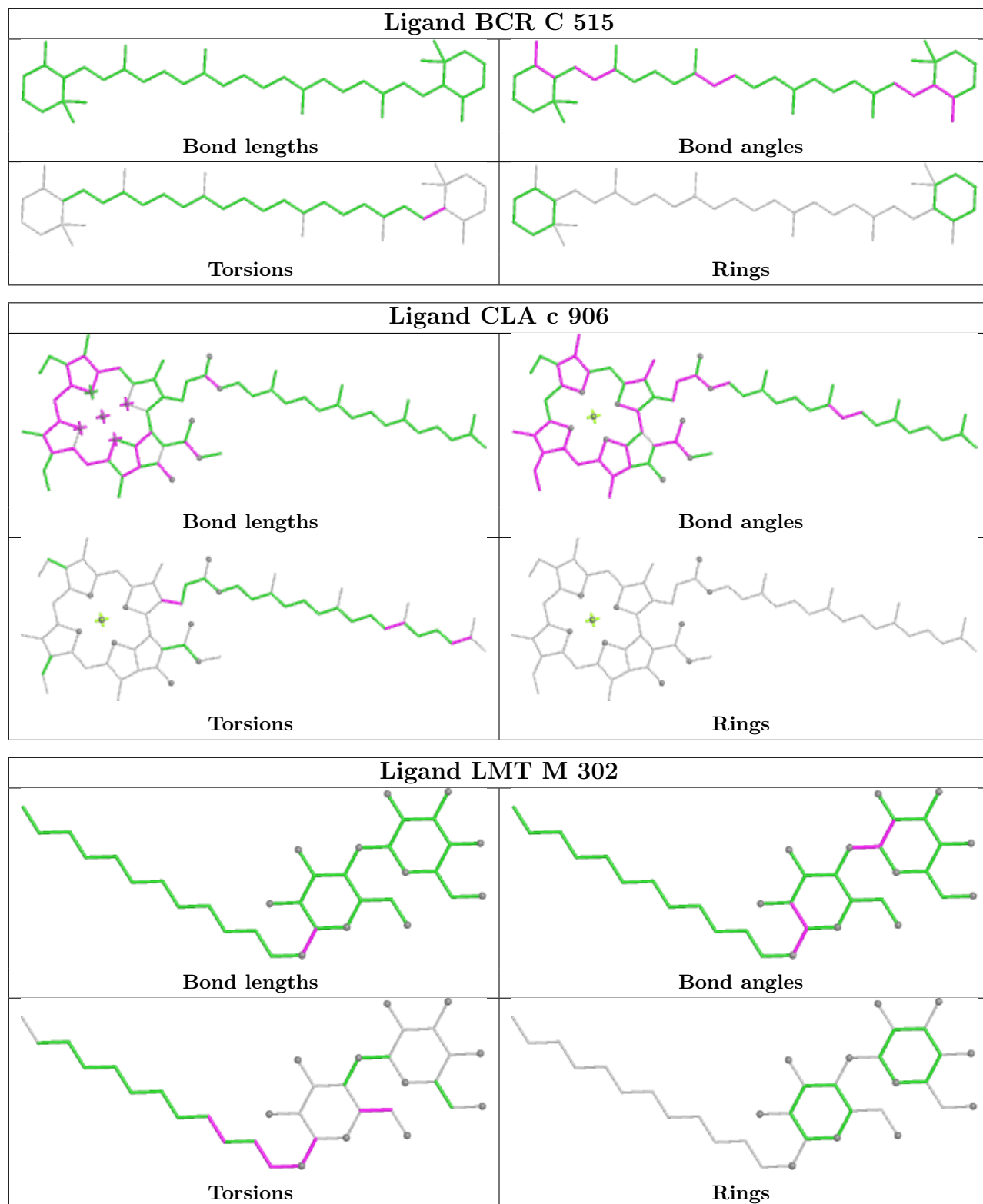


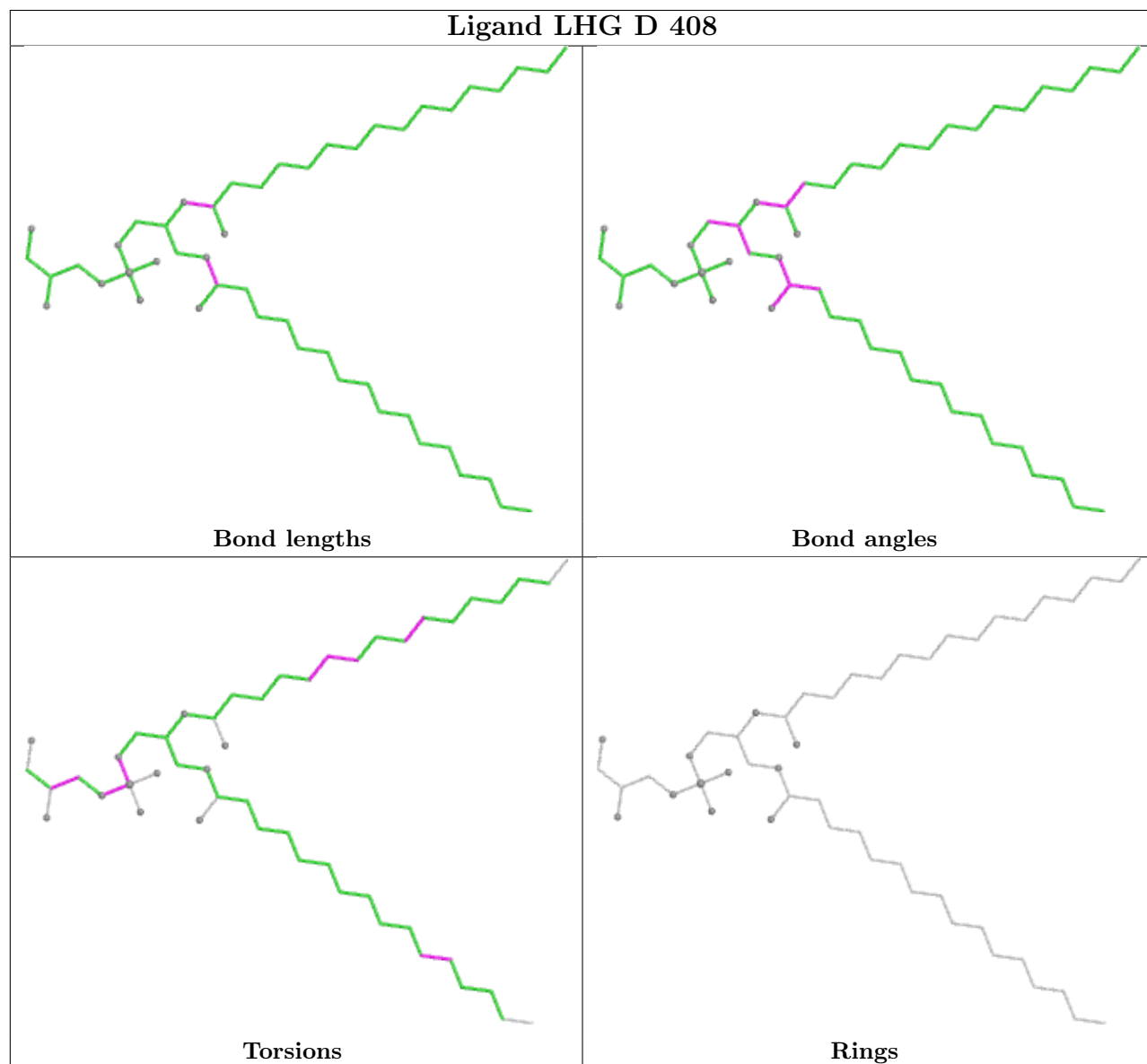
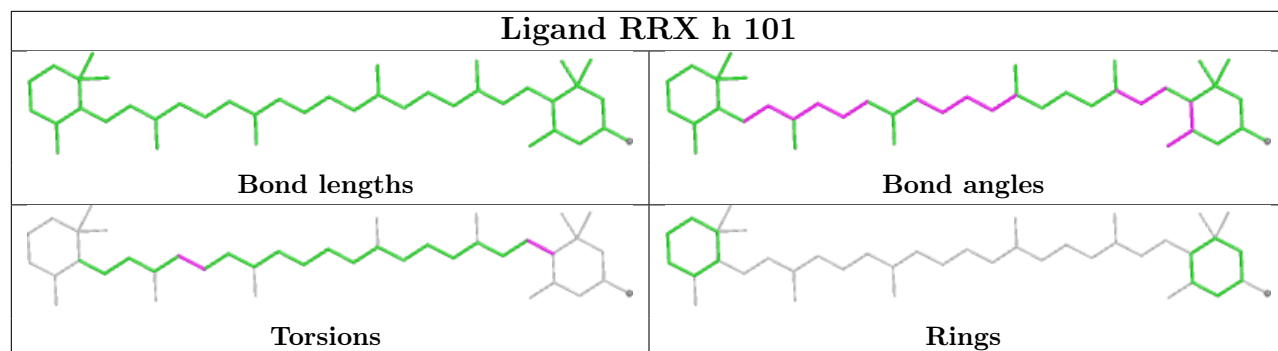
Ligand DGD C 517	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR t 903	
 Bond lengths	 Bond angles
 Torsions	 Rings

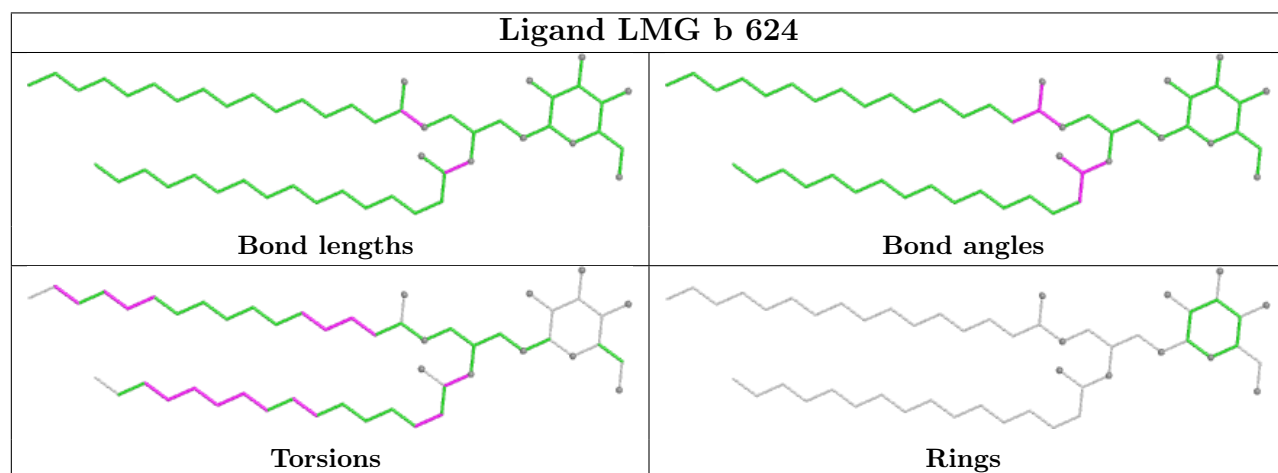
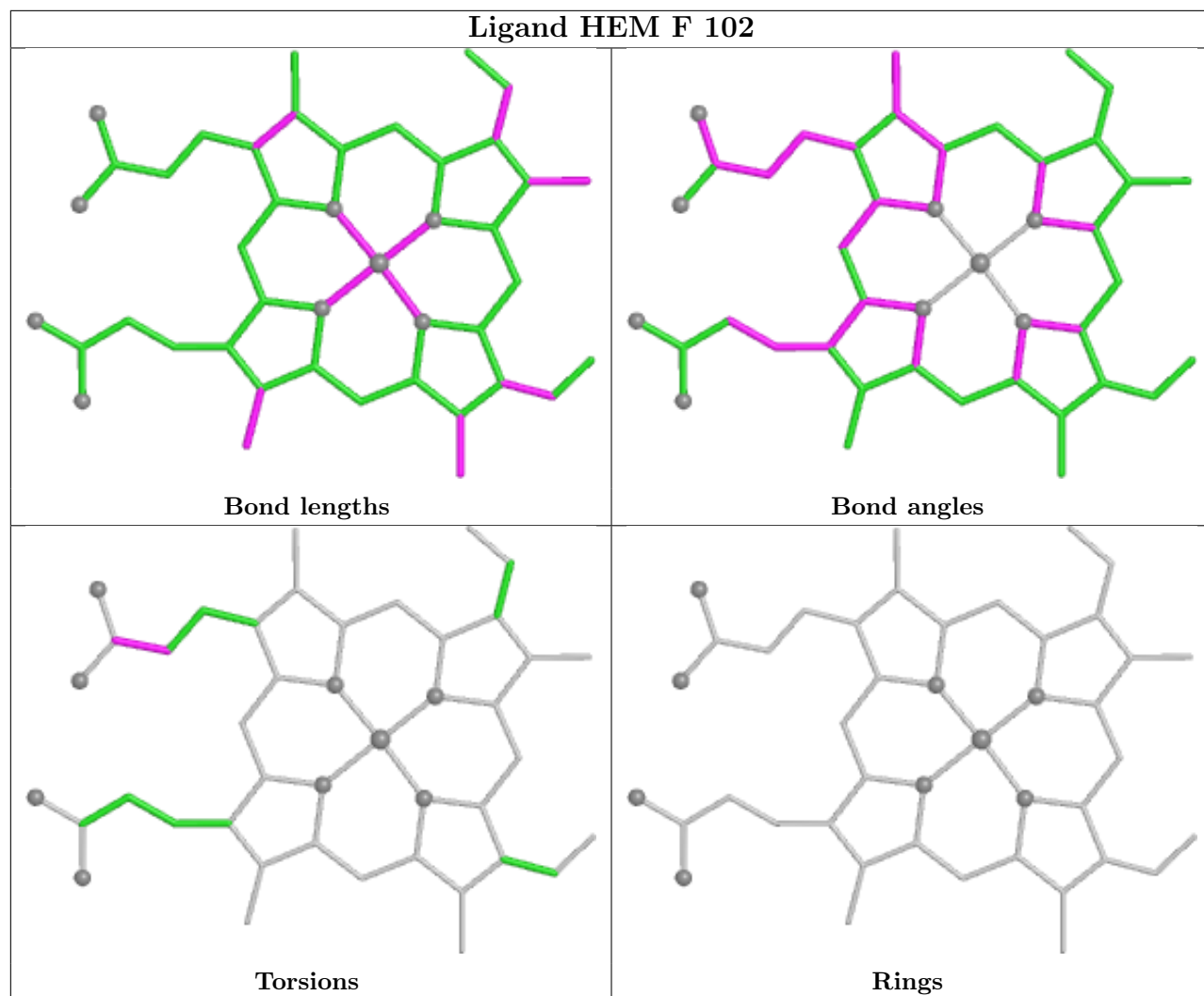




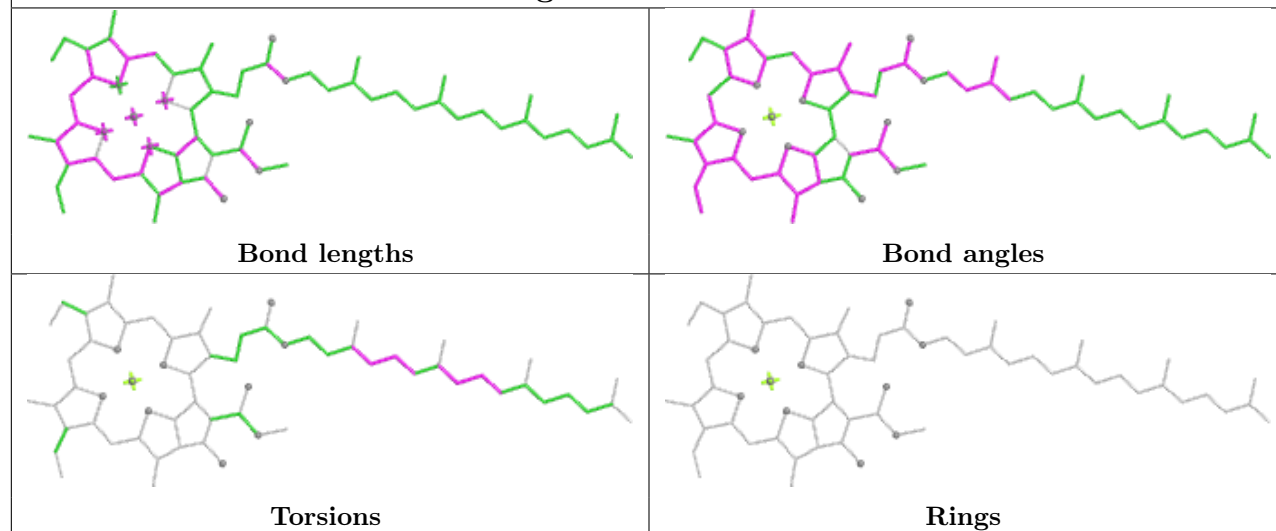




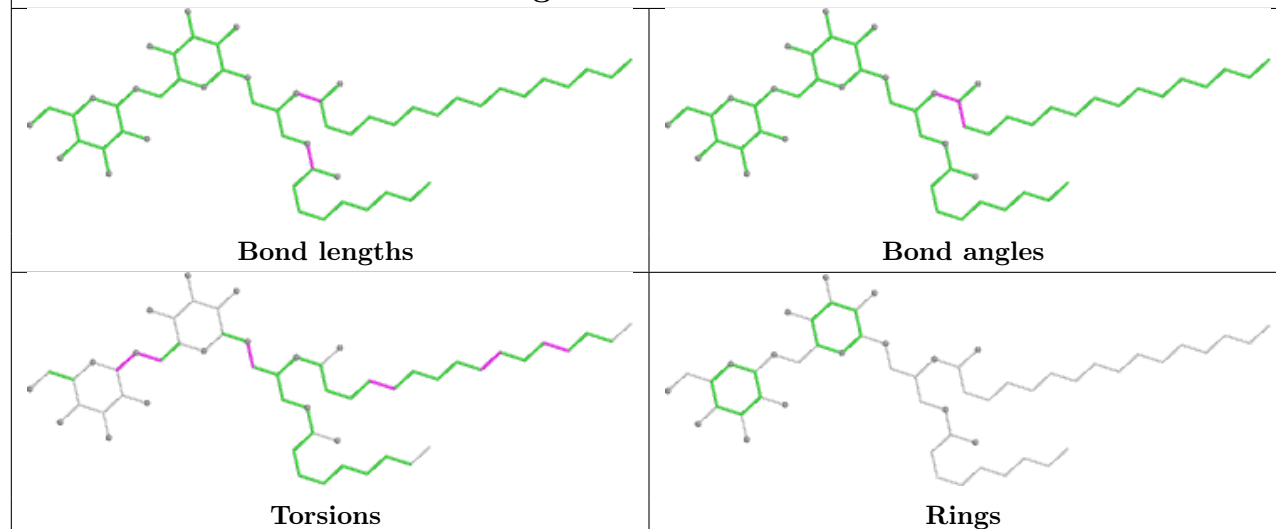




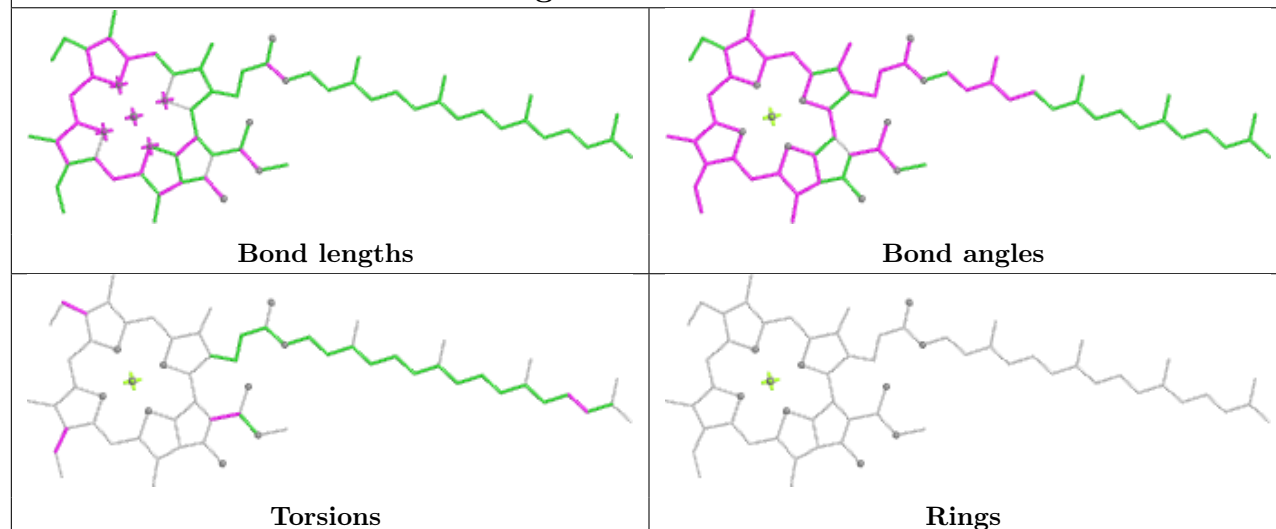
Ligand CLA a 413

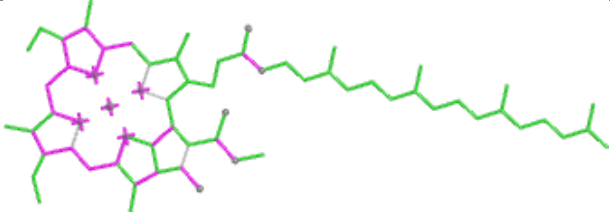
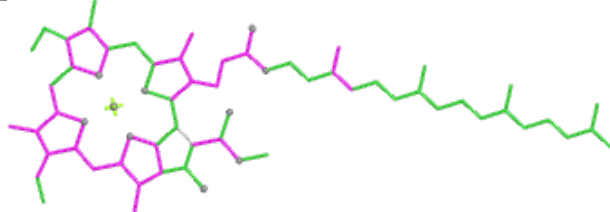
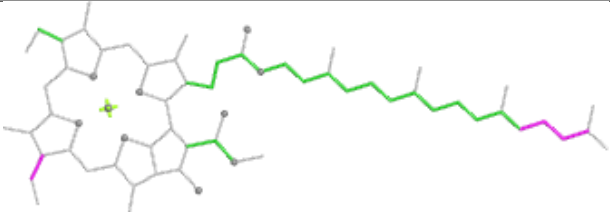
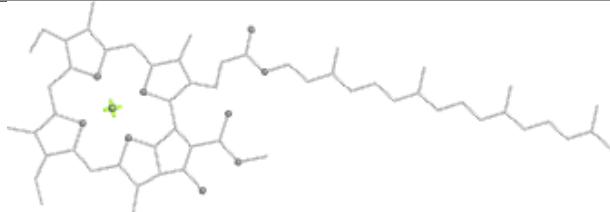
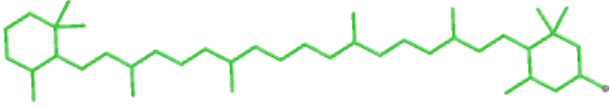
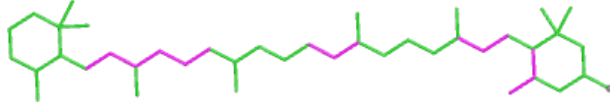
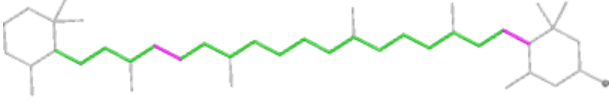
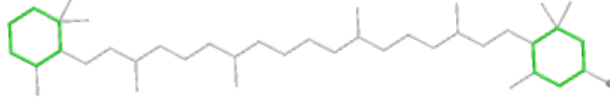
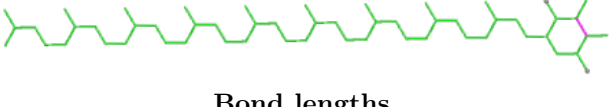
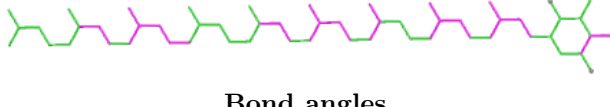
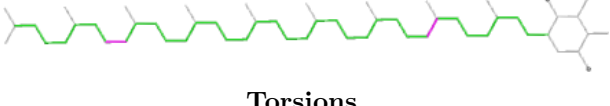


Ligand DGD c 918

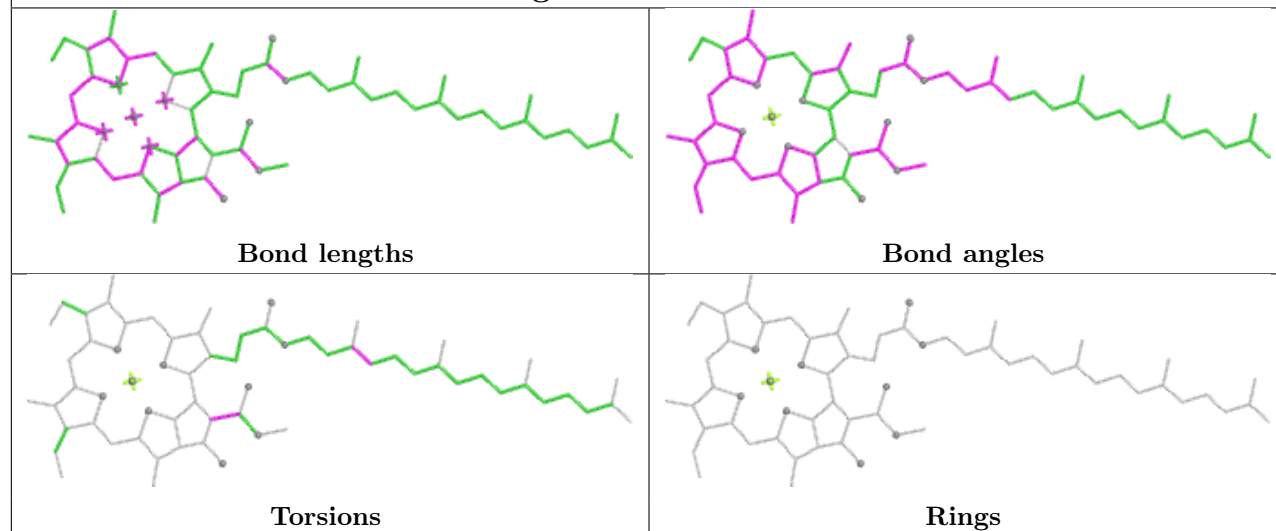


Ligand CLA d 401

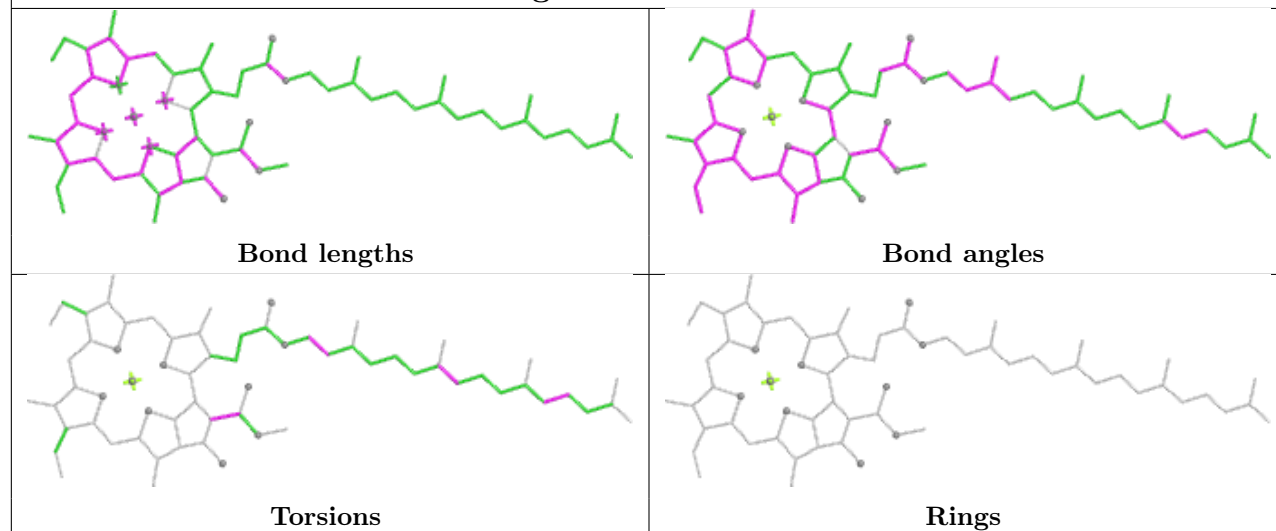


Ligand CLA a 409	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand RRX H 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 d 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

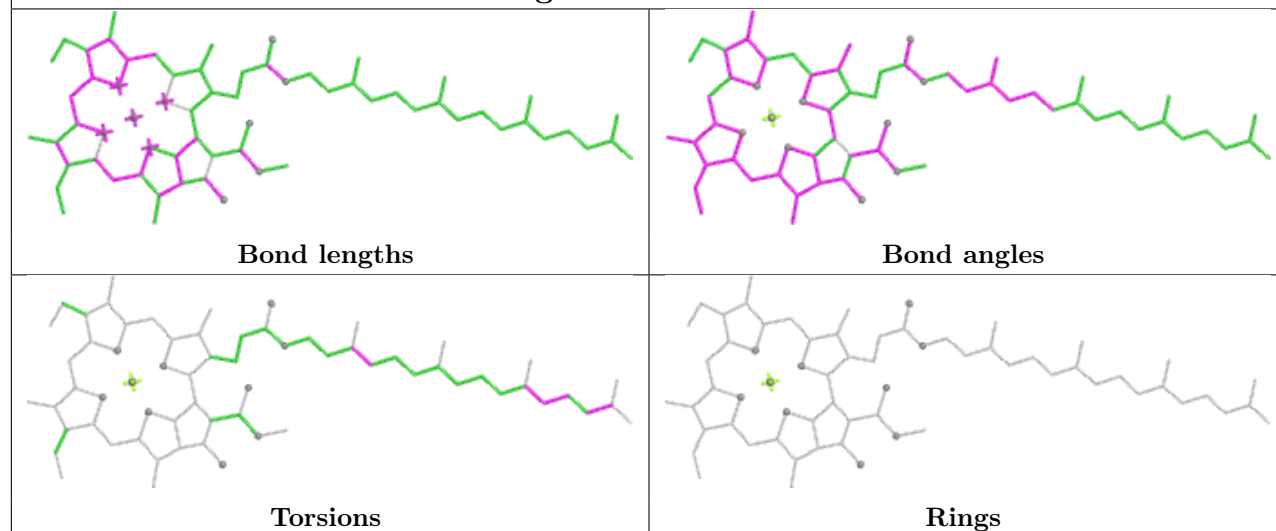
Ligand CLA B 610

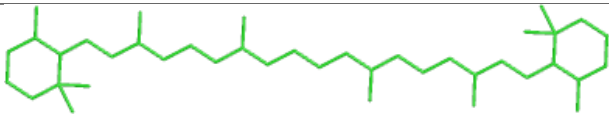
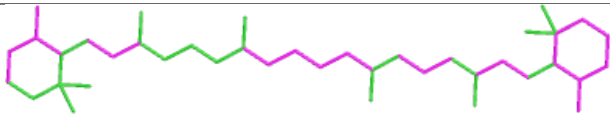
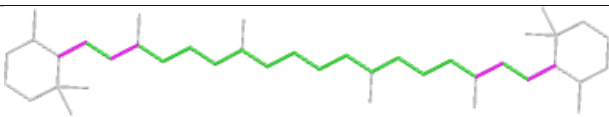
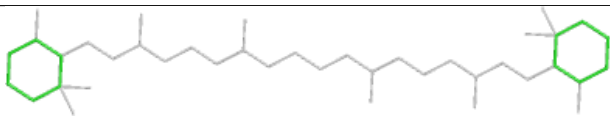


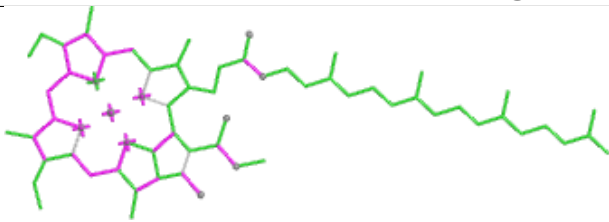
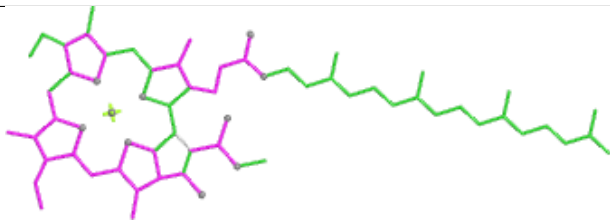
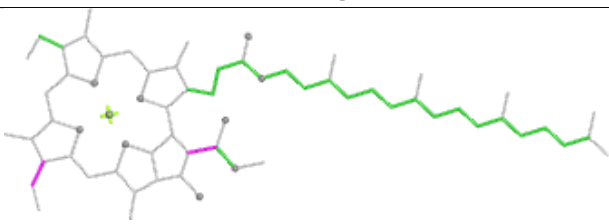
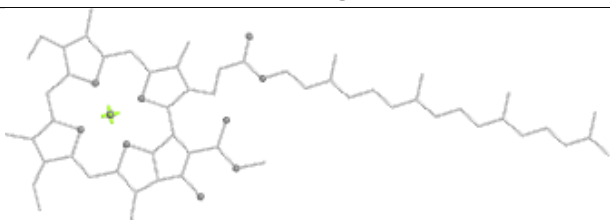
Ligand CLA C 509

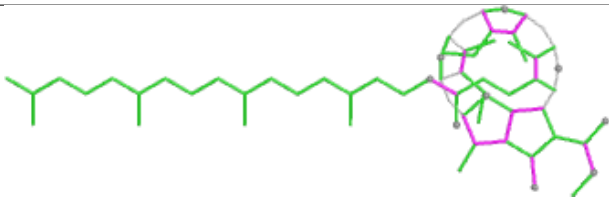
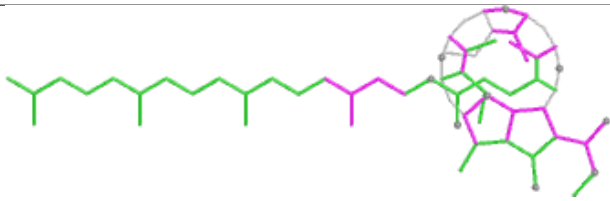
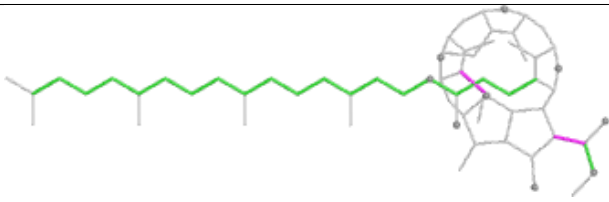
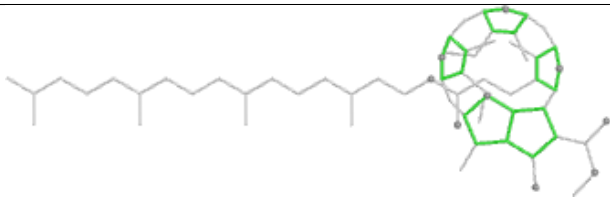


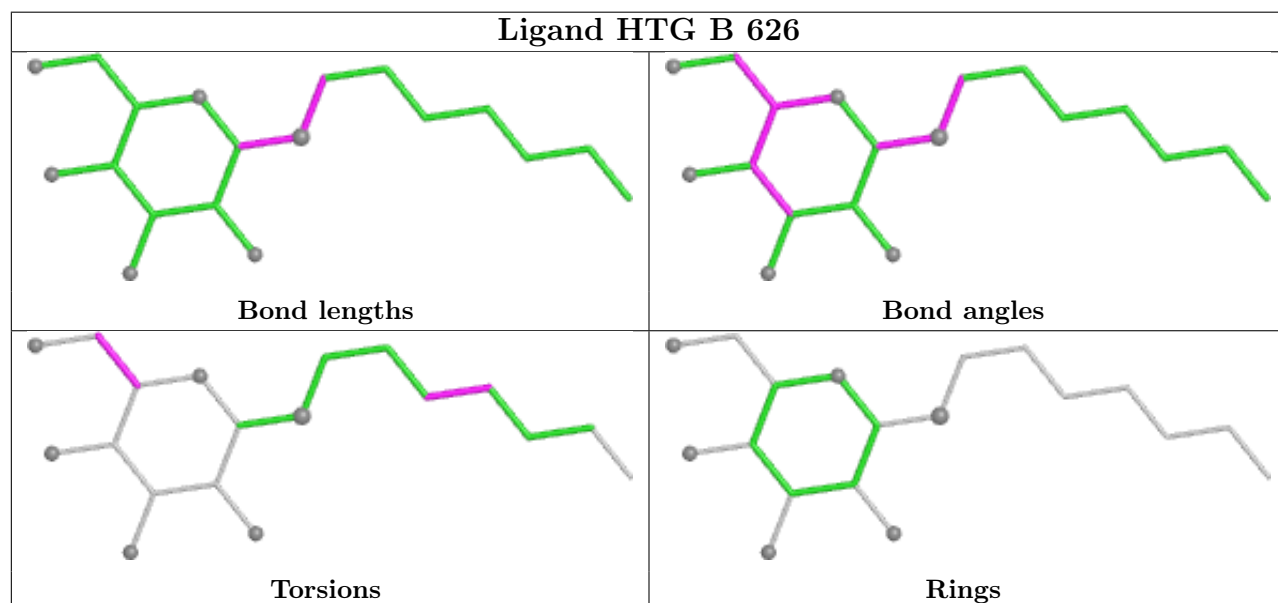
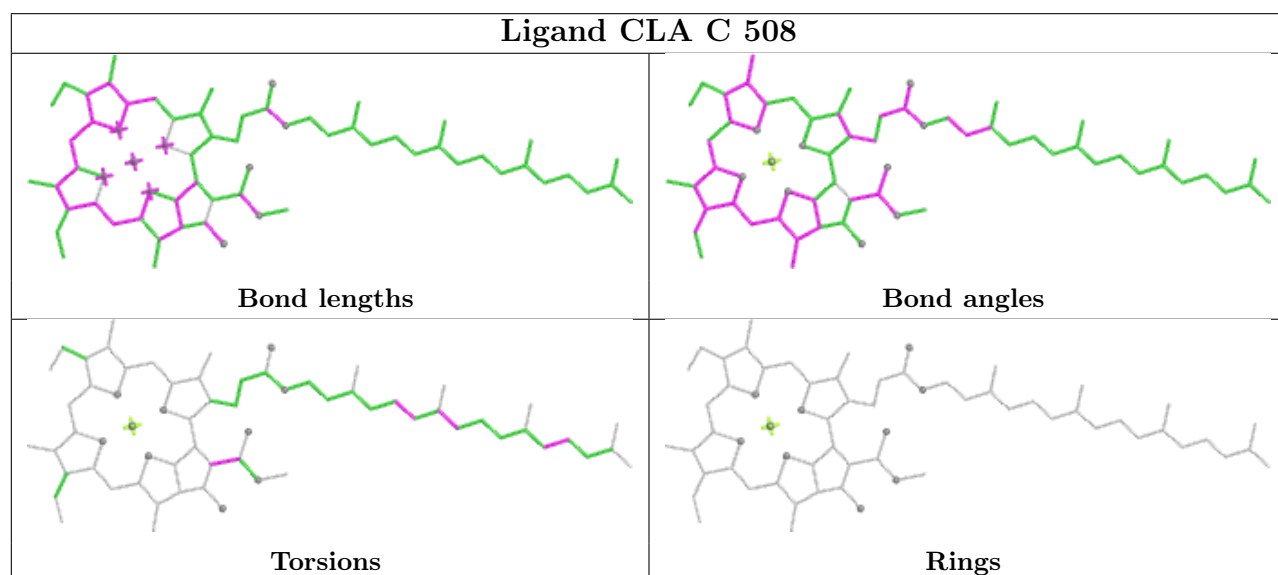
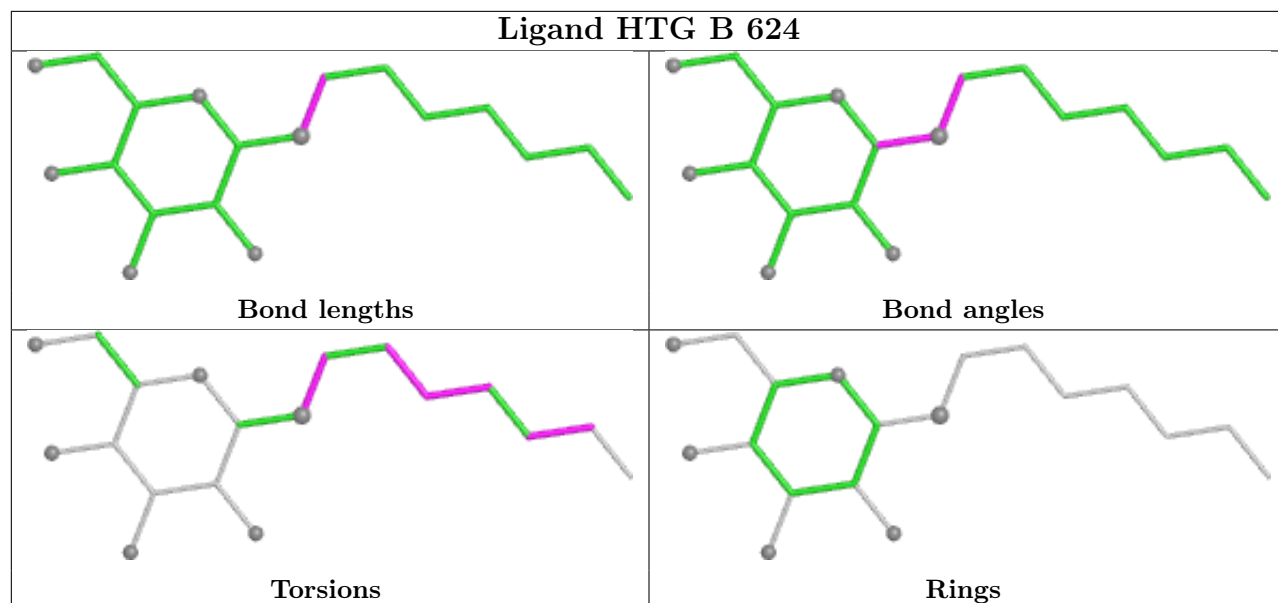
Ligand CLA b 615

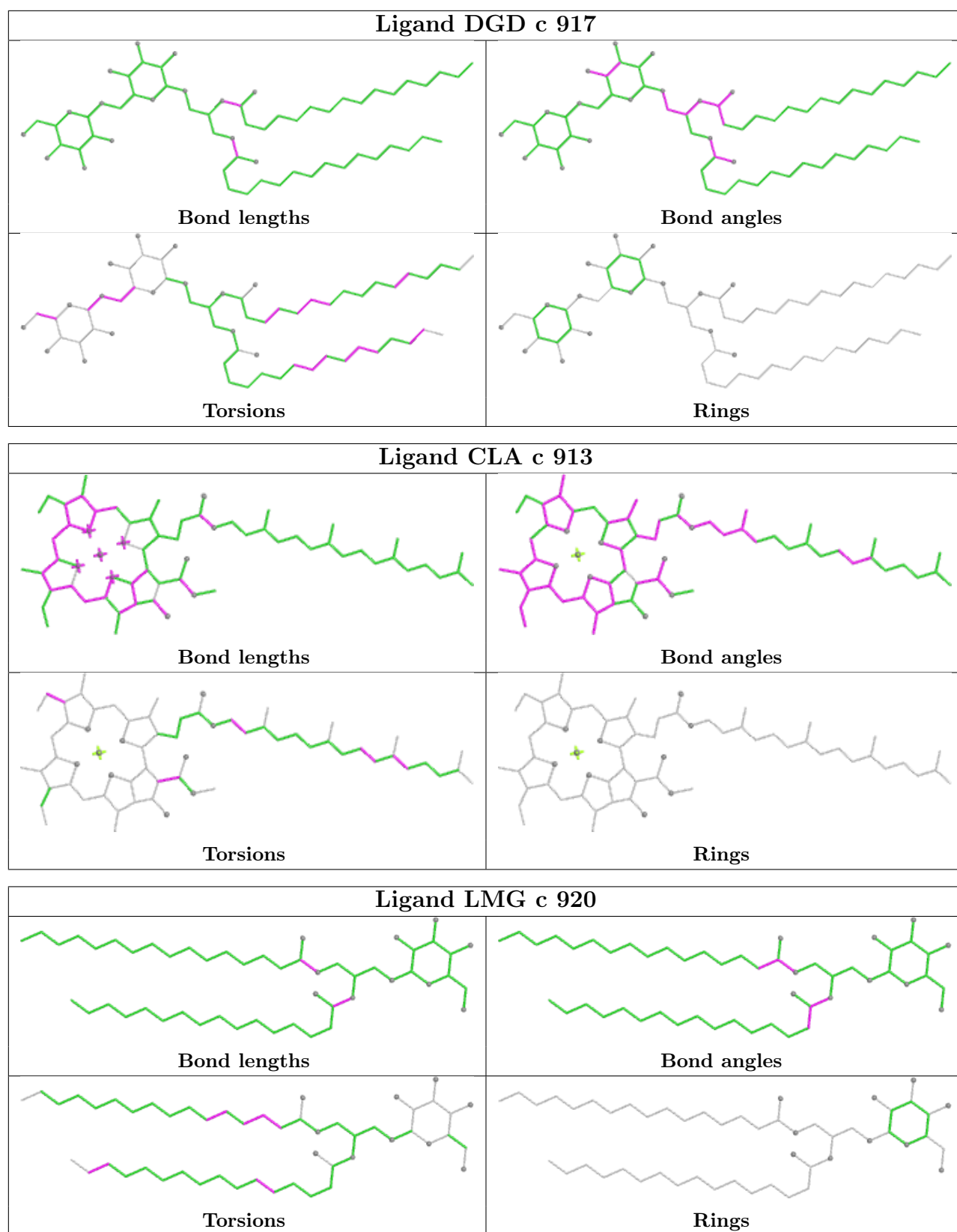


Ligand BCR d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

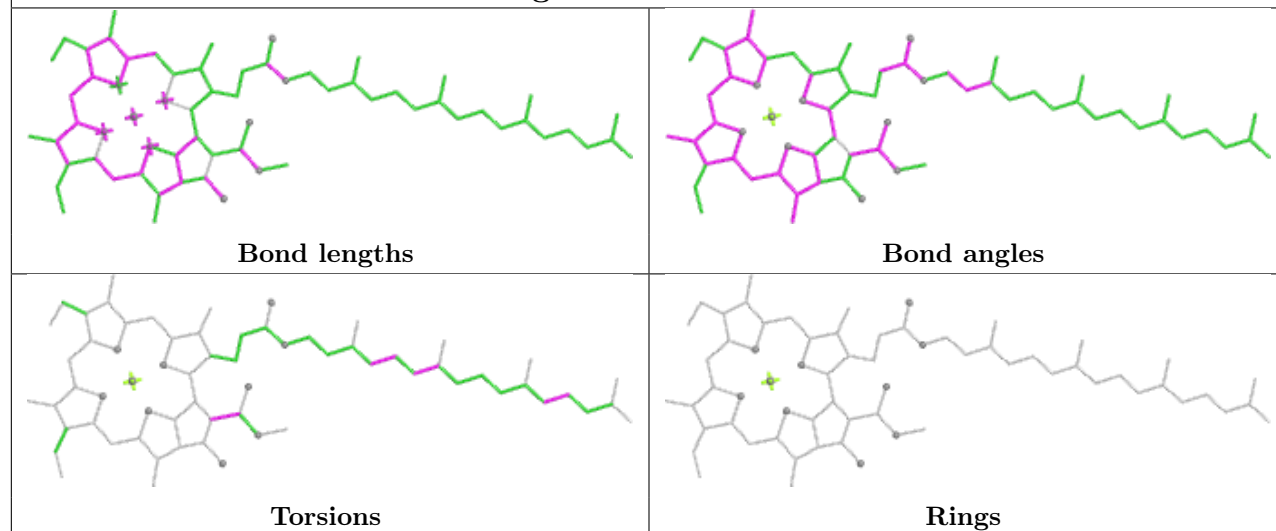
Ligand CLA A 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO a 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

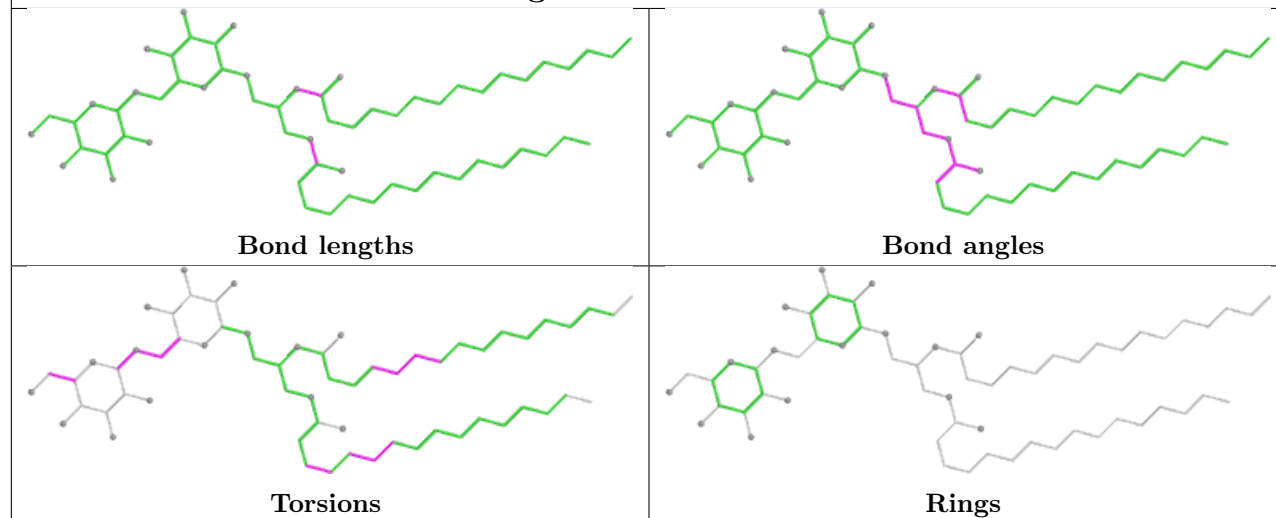




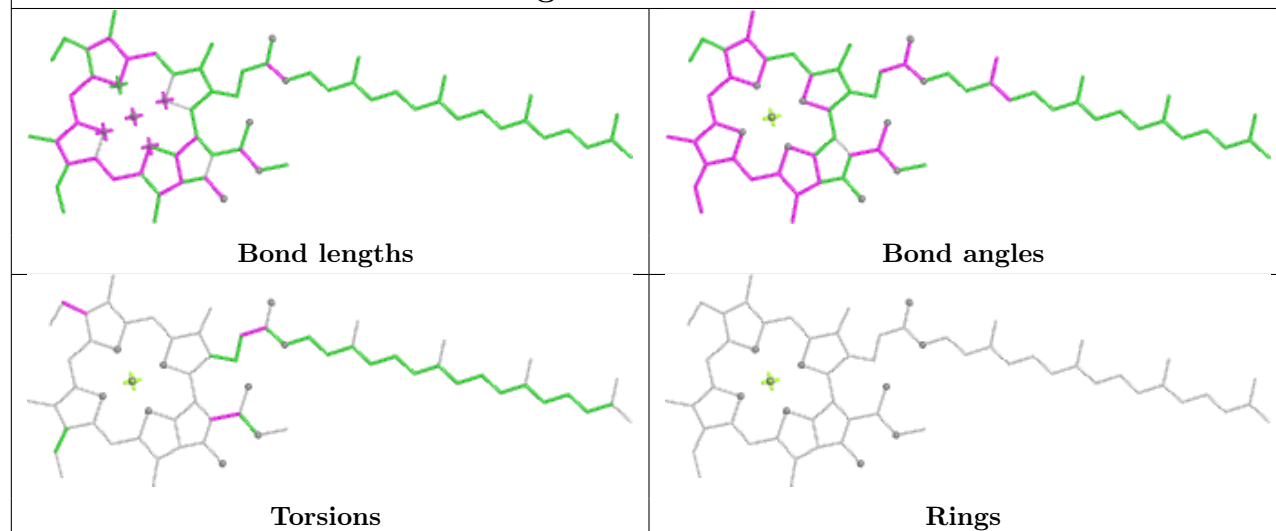
Ligand CLA B 605



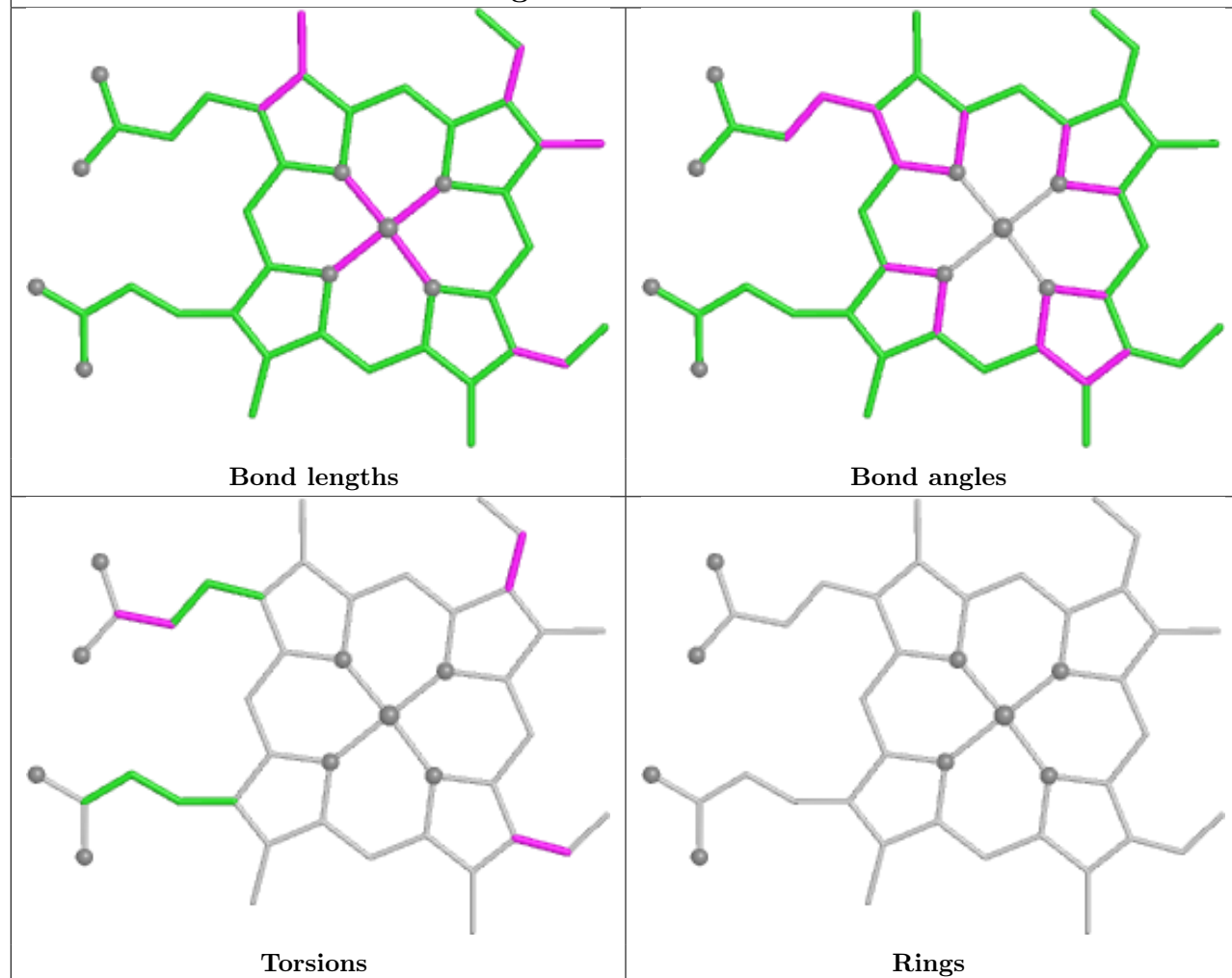
Ligand DGD C 516



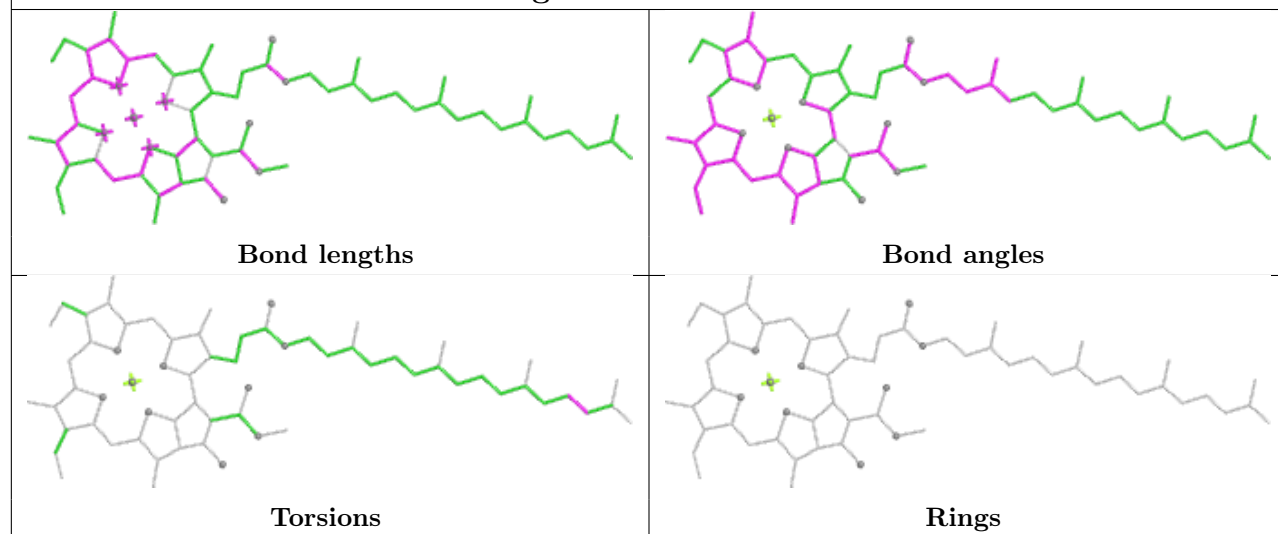
Ligand CLA c 902



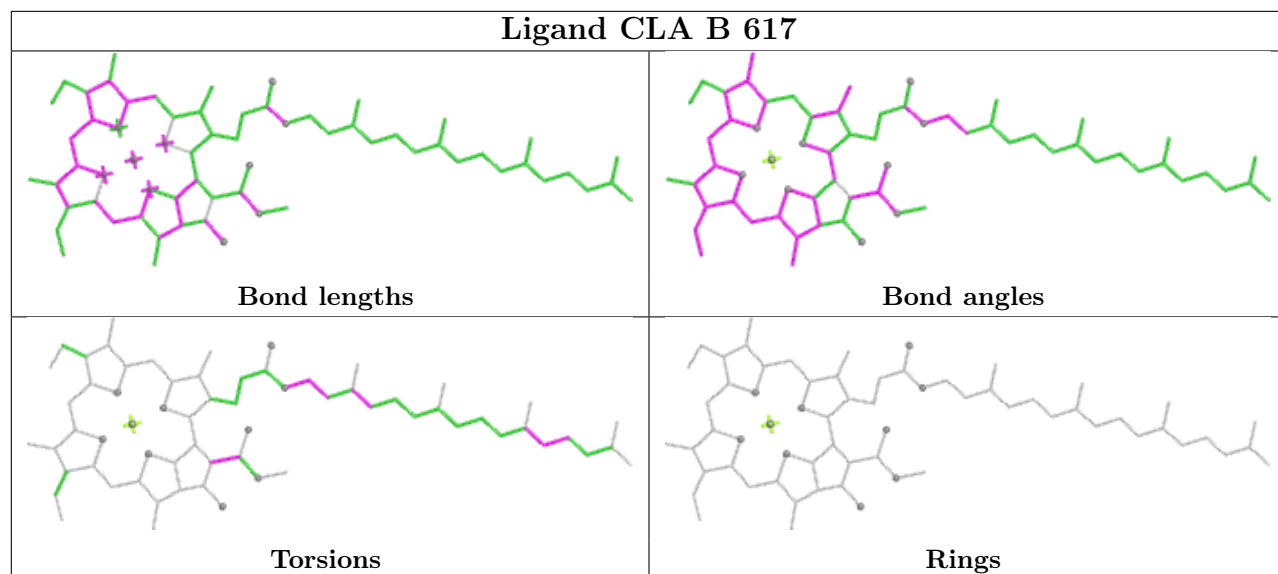
Ligand HEM v 202



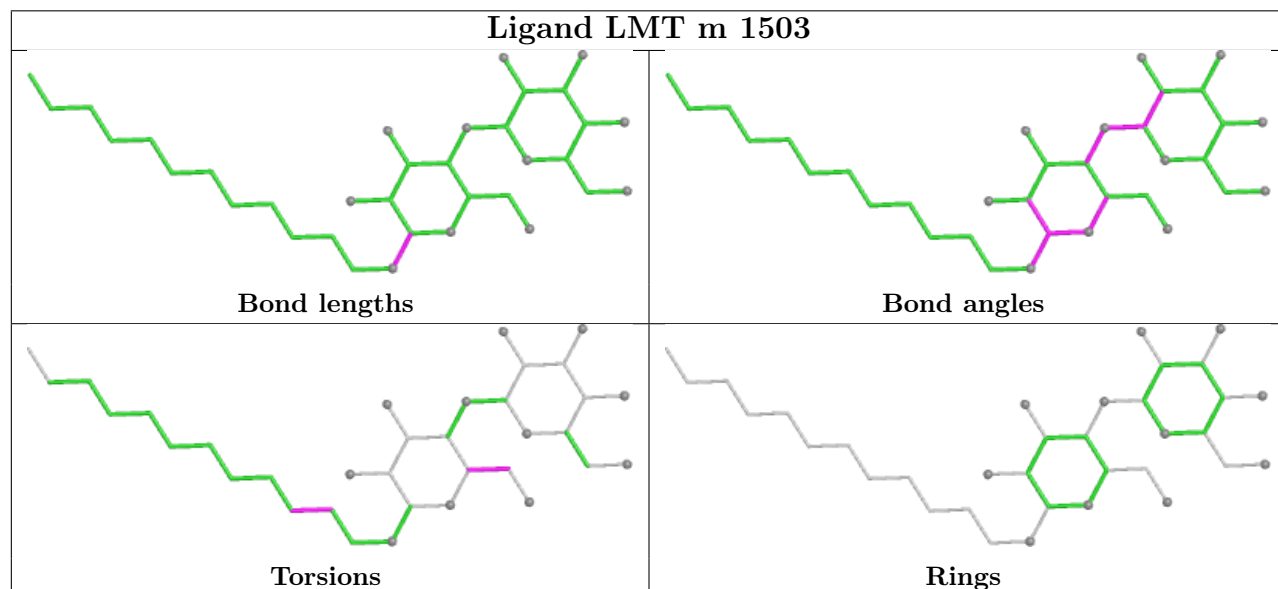
Ligand CLA B 612



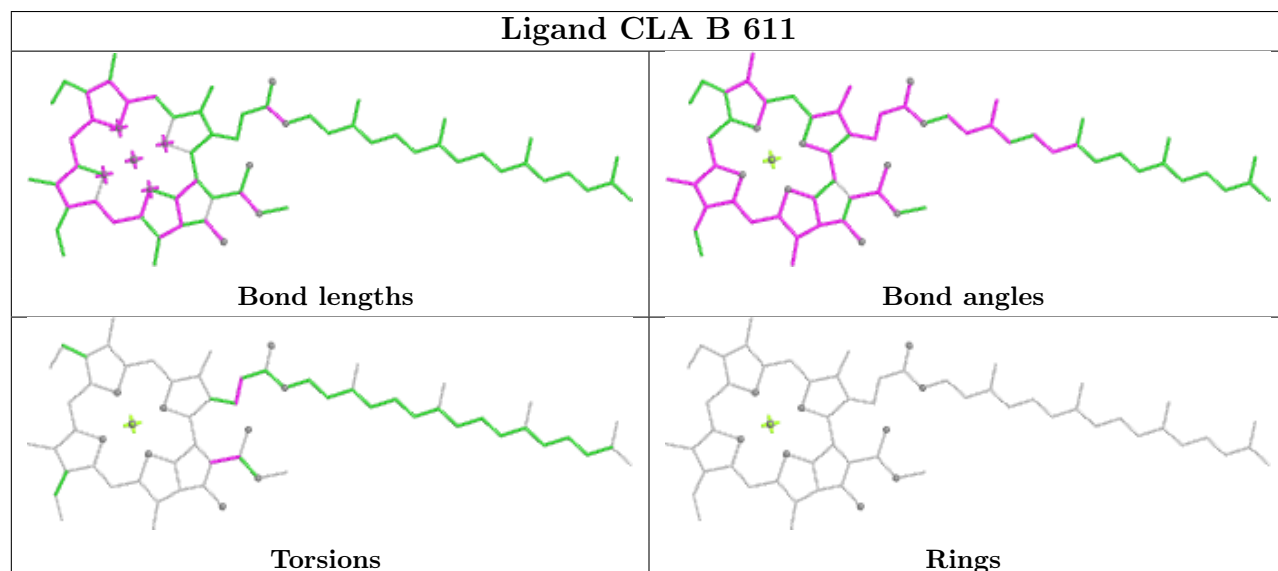
Ligand CLA B 617

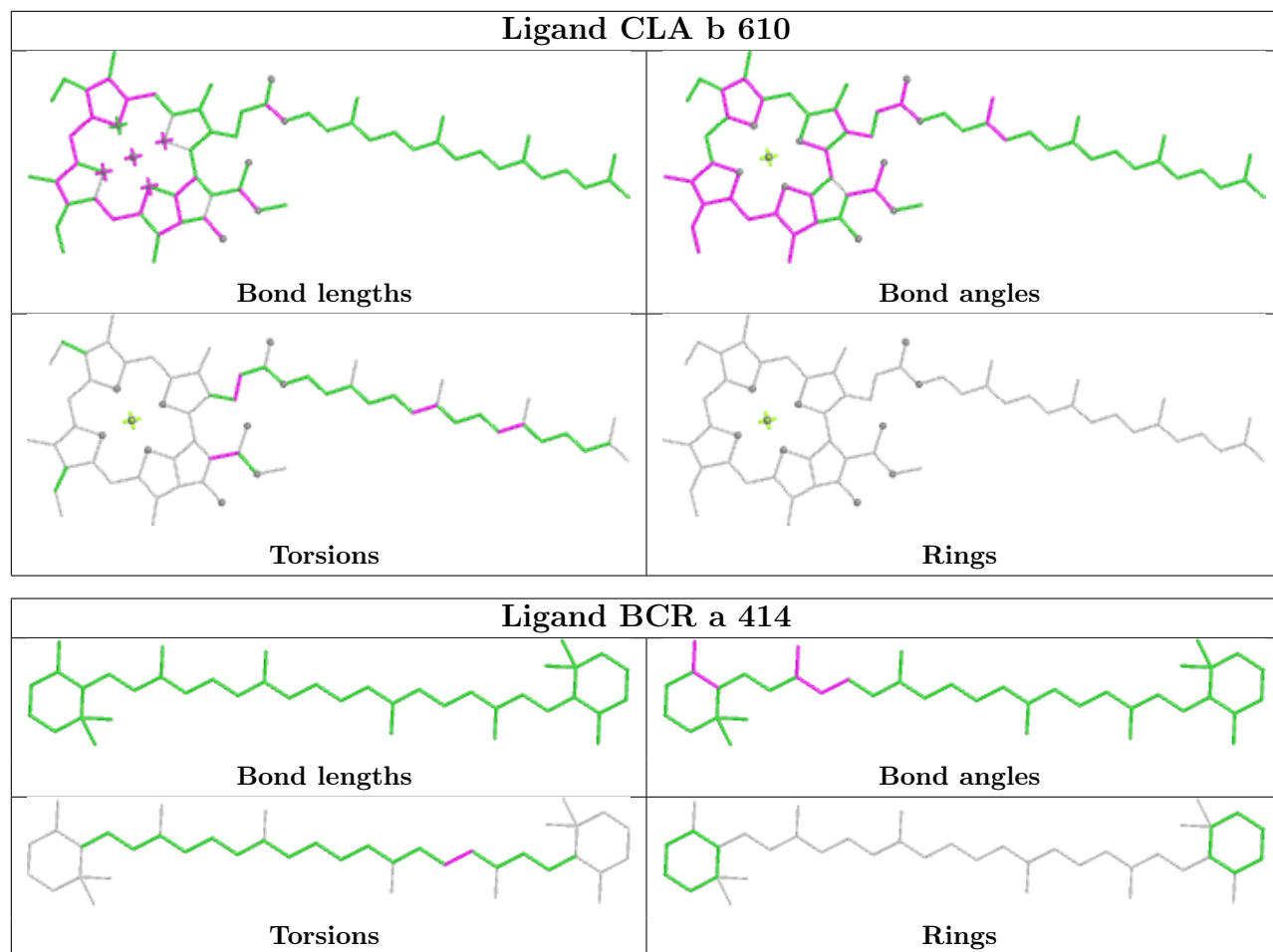


Ligand LMT m 1503

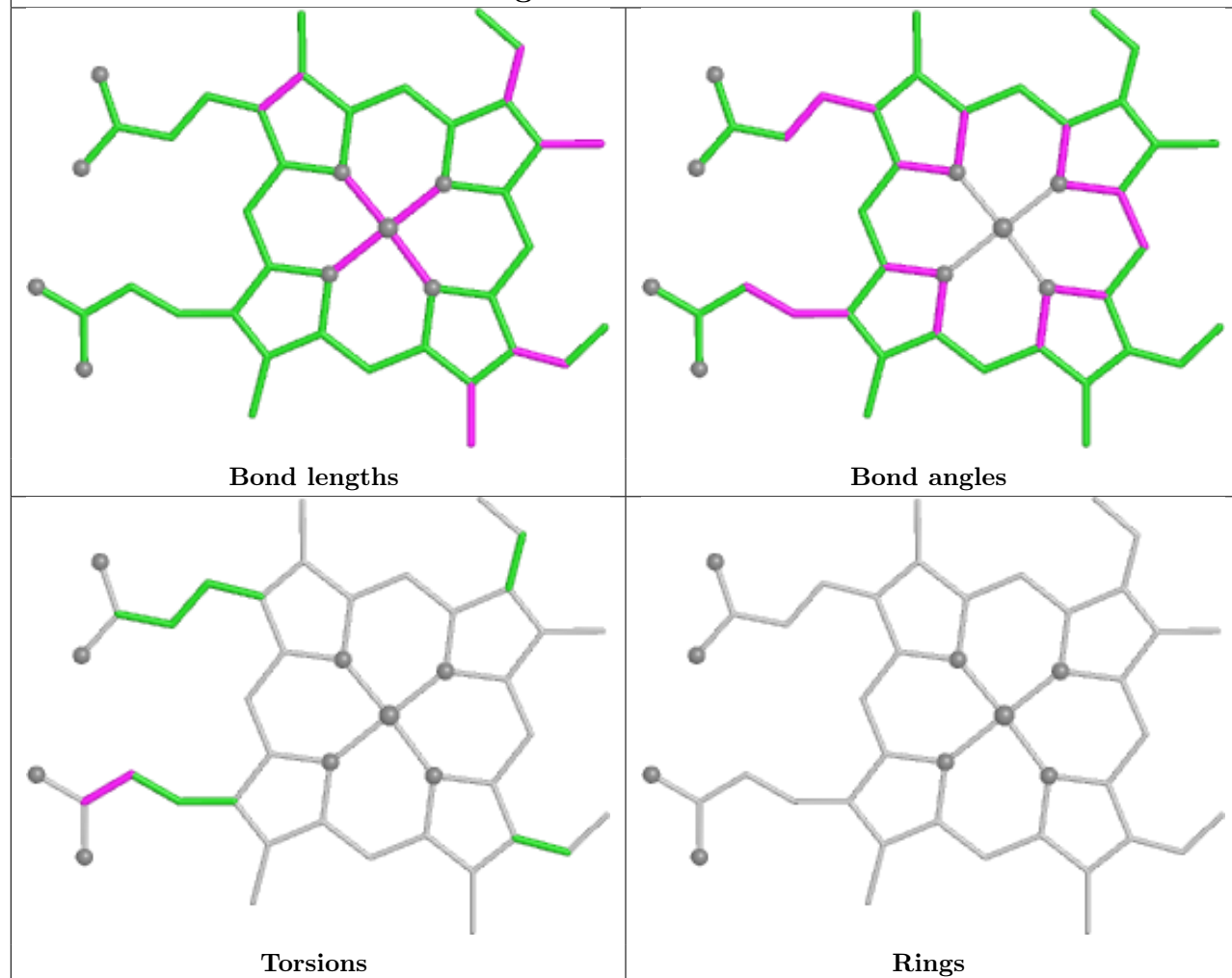


Ligand CLA B 611

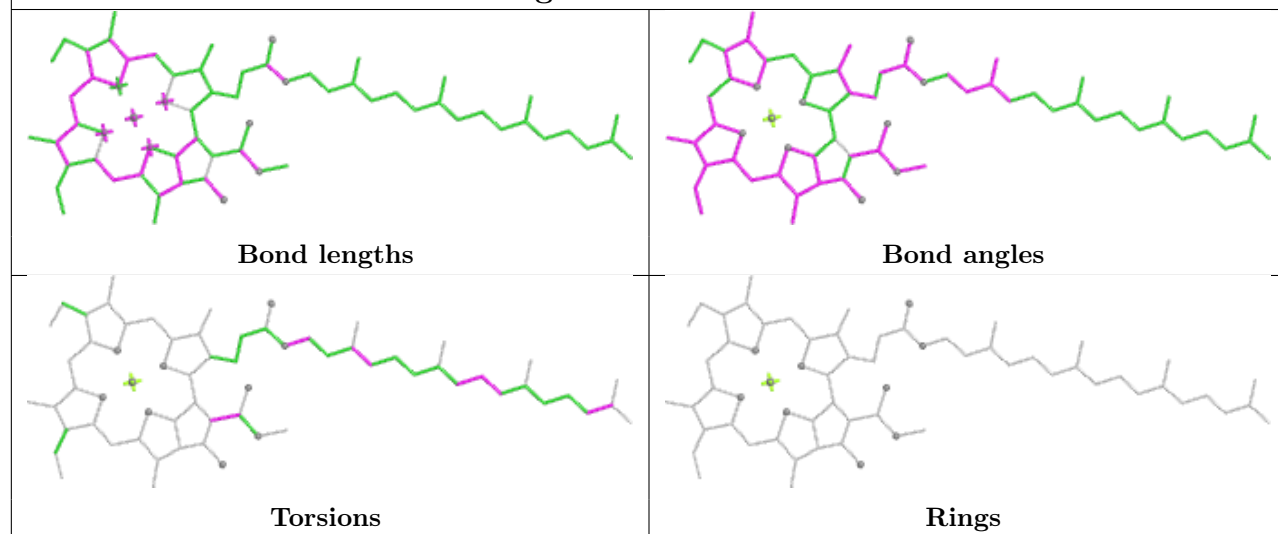


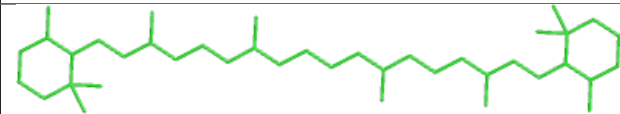
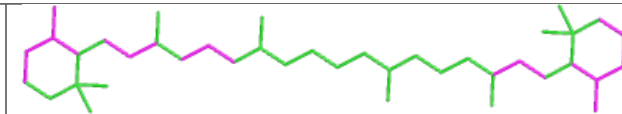
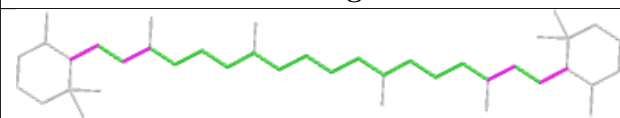
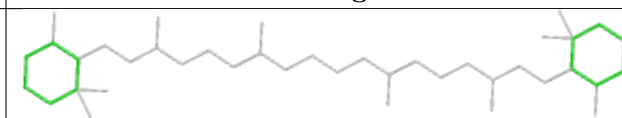
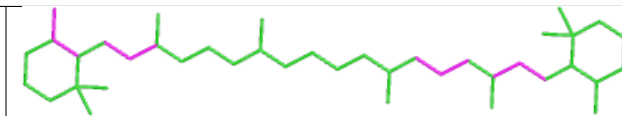
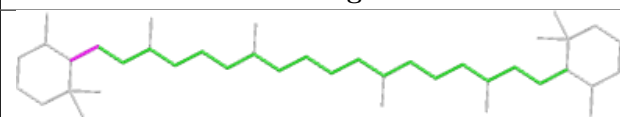
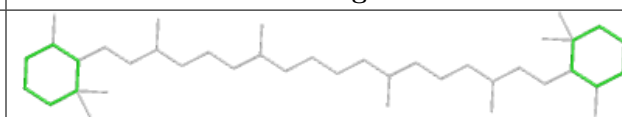
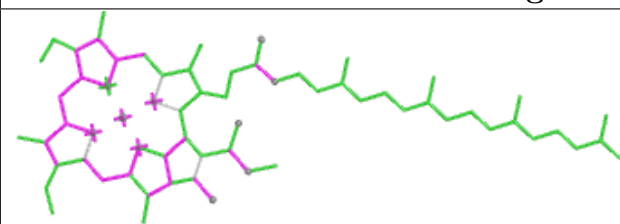
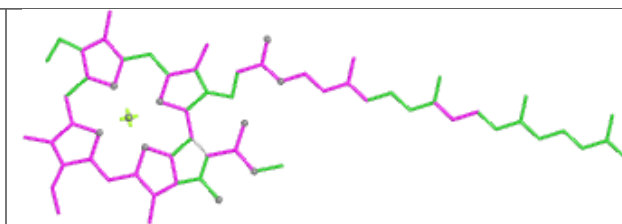
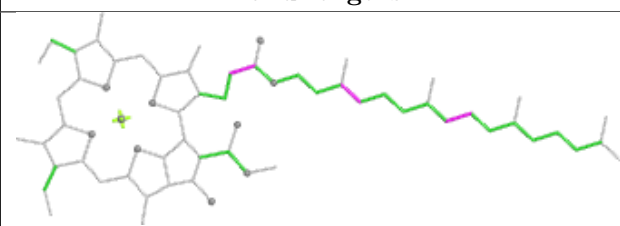
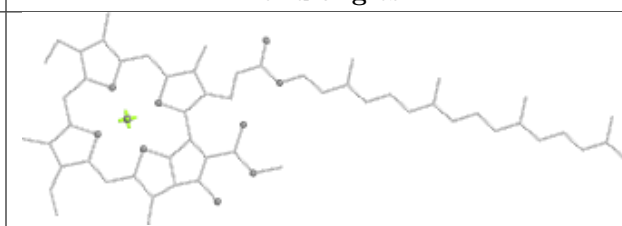
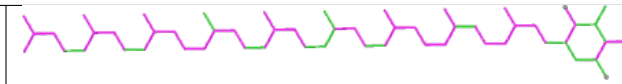
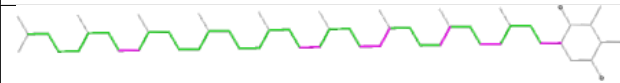
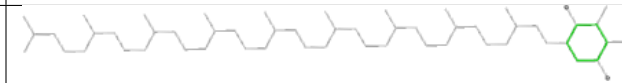


Ligand HEM f 101

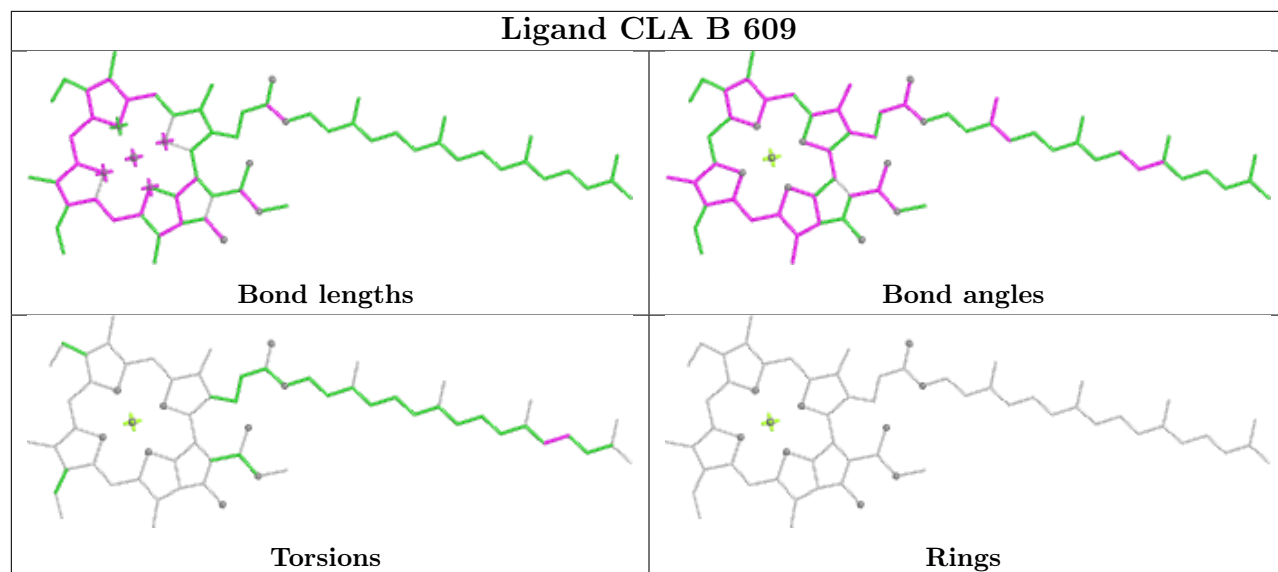


Ligand CLA b 618

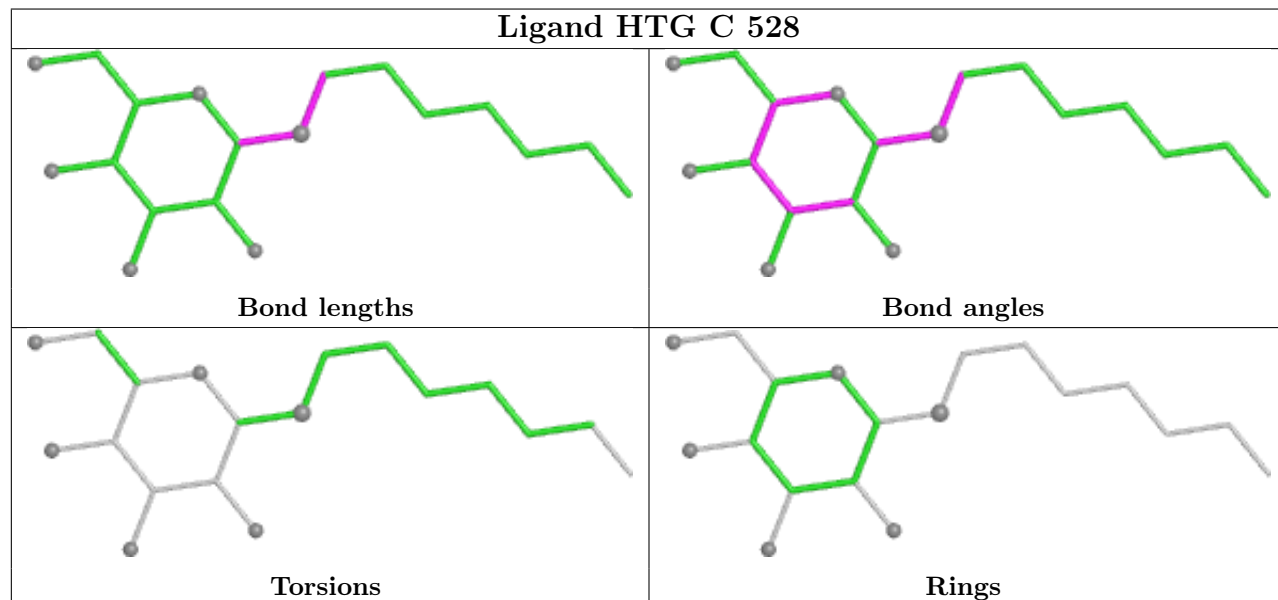


Ligand BCR D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA c 911	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand PL9 A 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

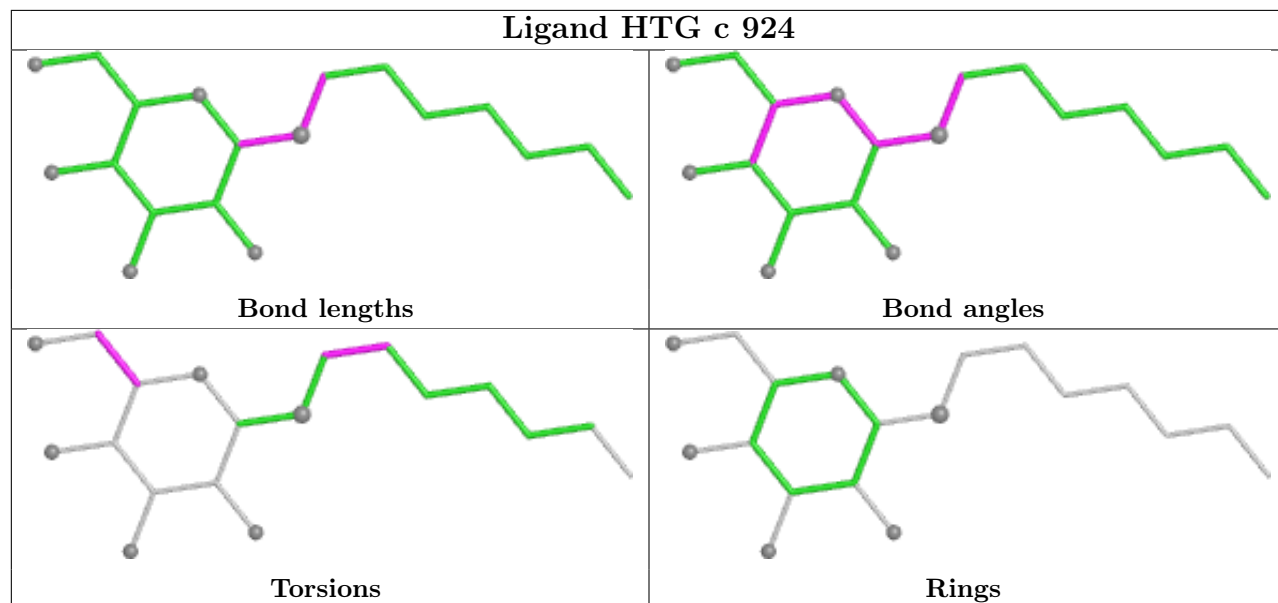
Ligand CLA B 609

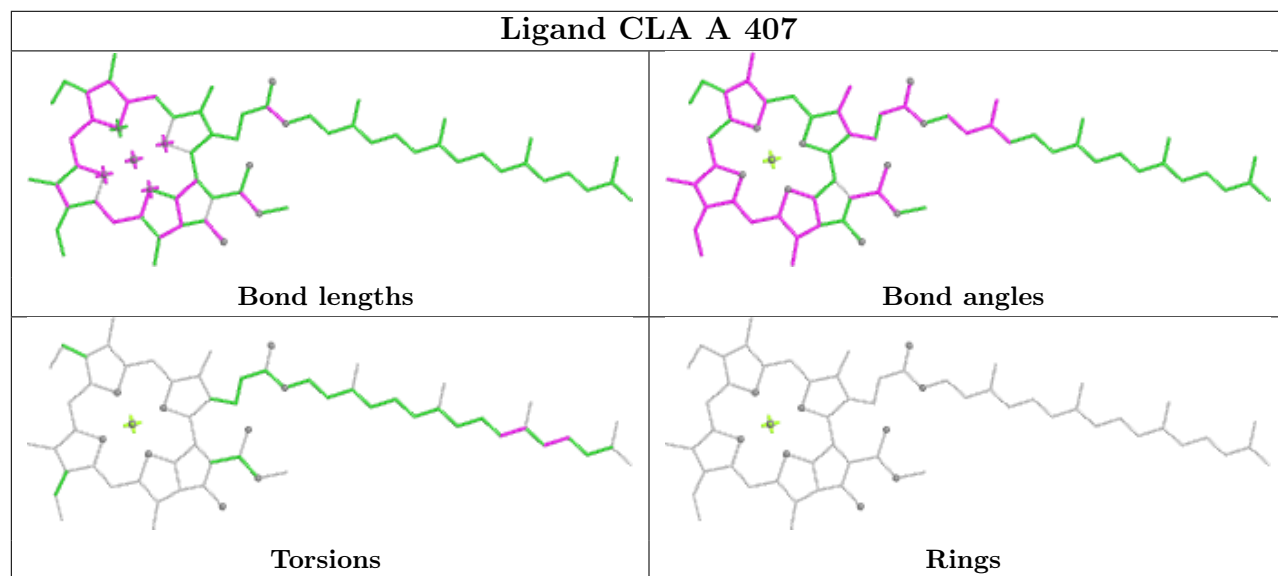
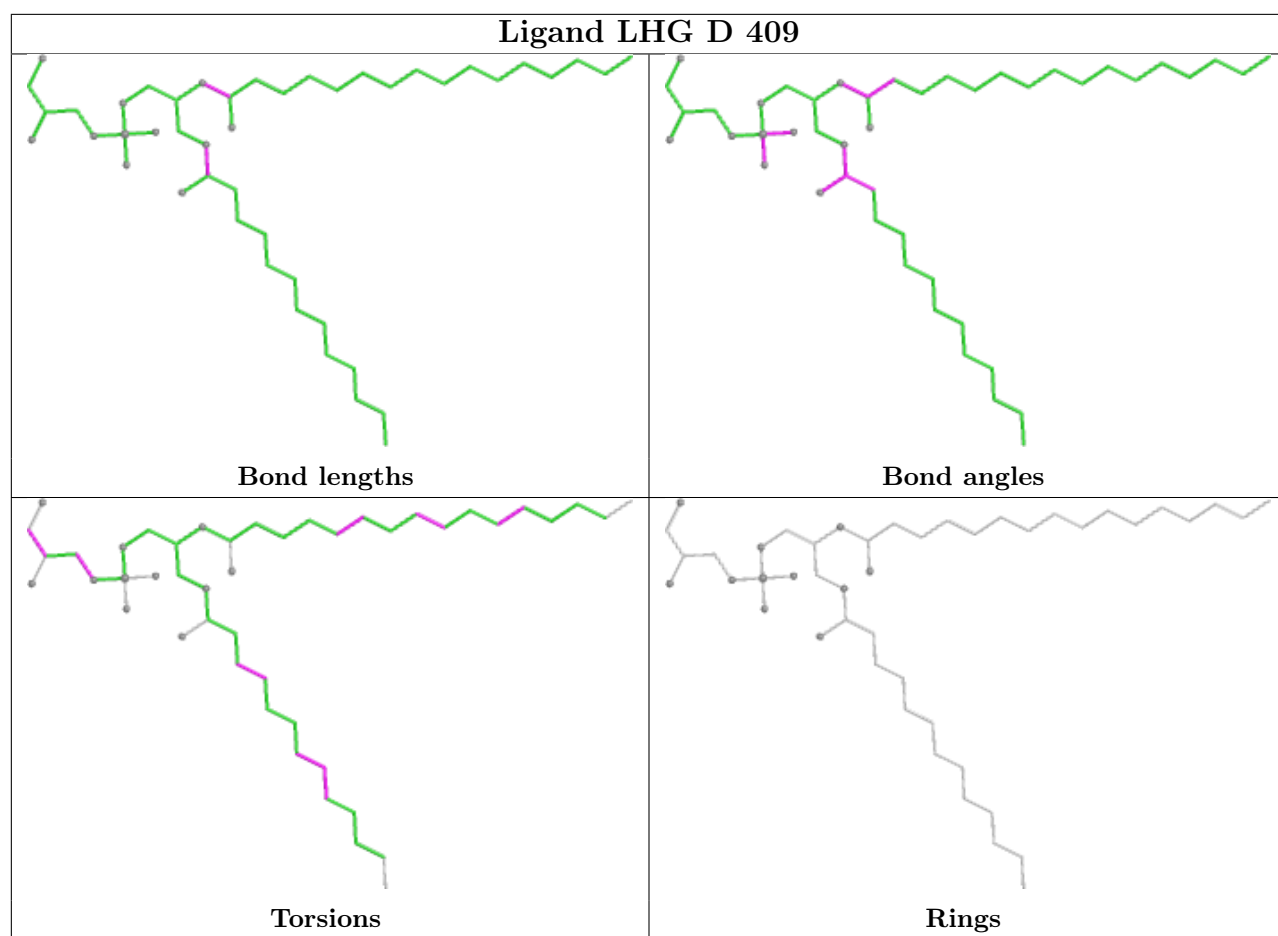


Ligand HTG C 528

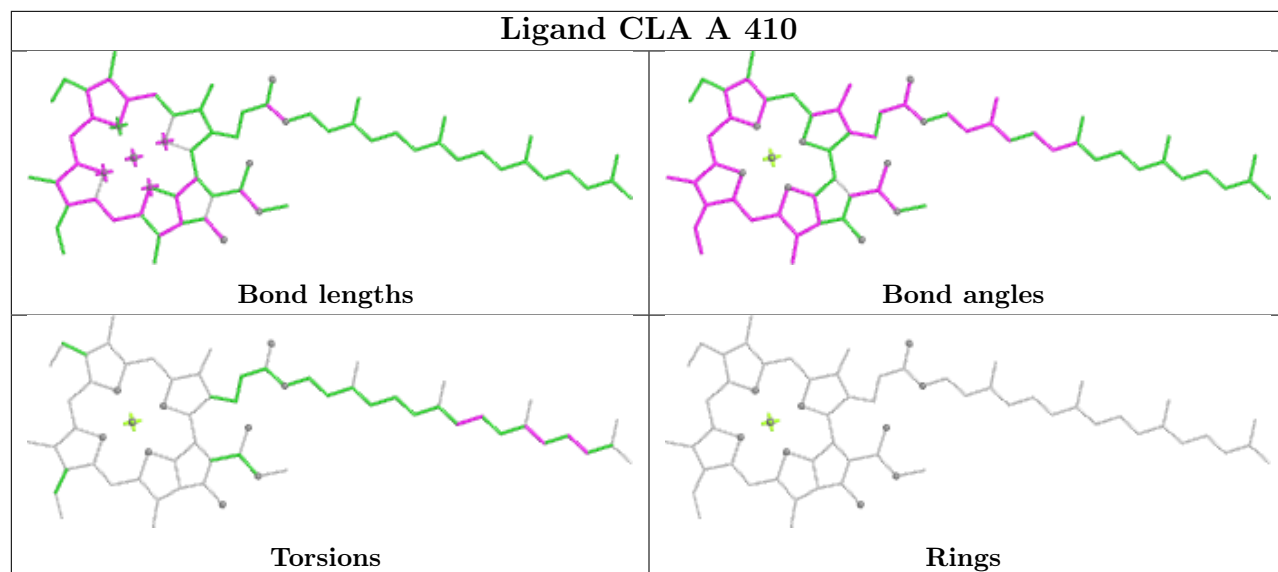


Ligand HTG c 924

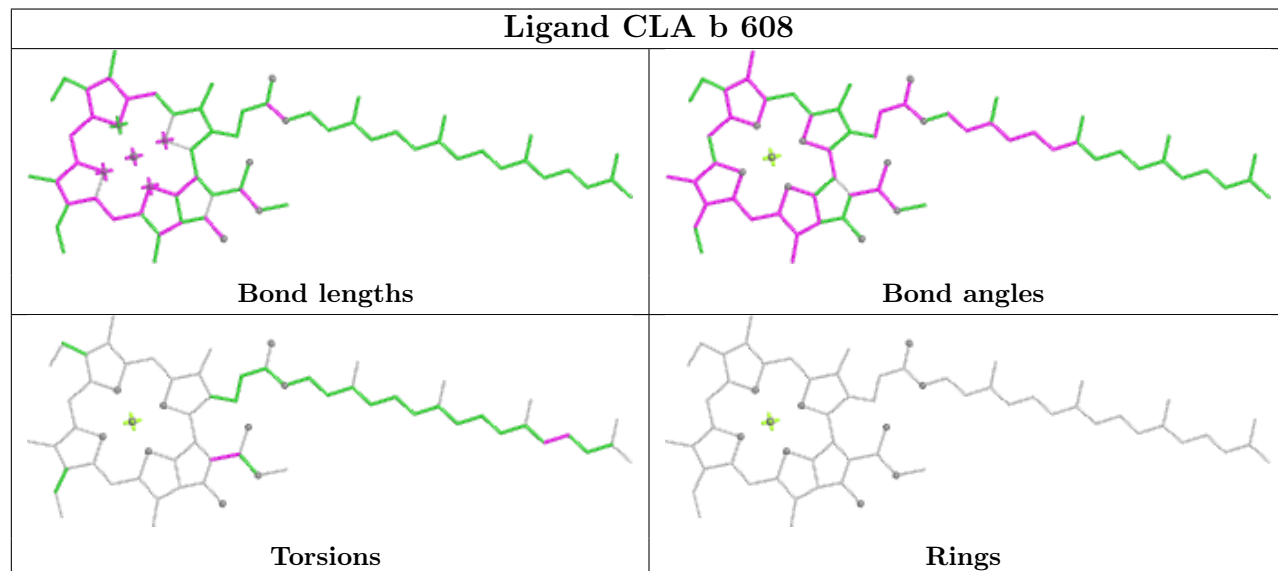




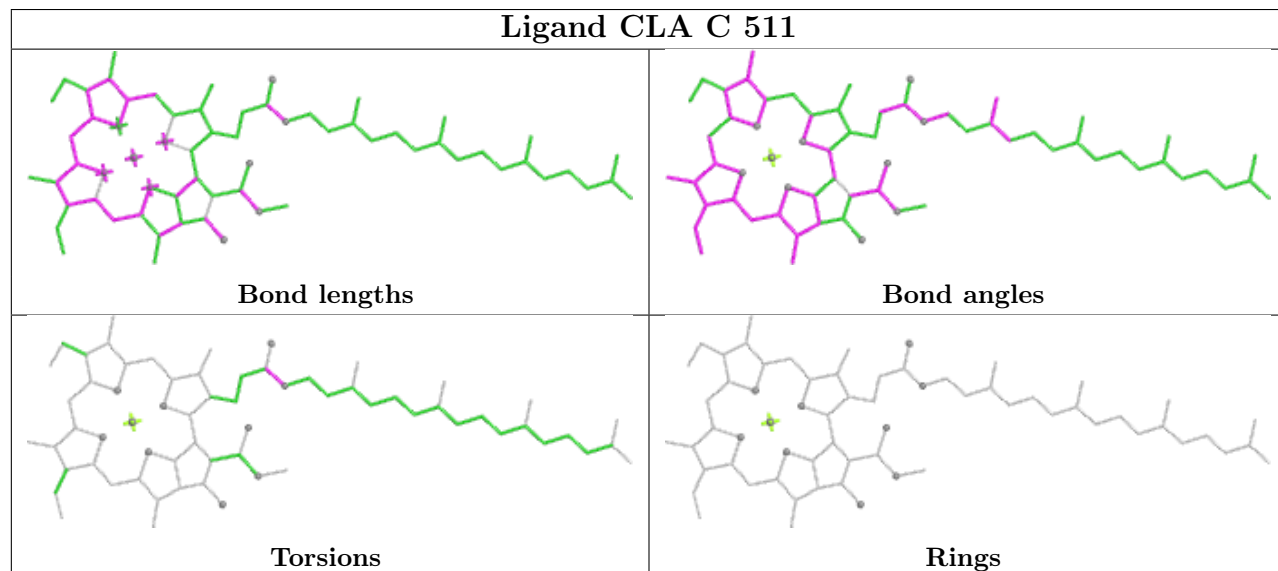
Ligand CLA A 410

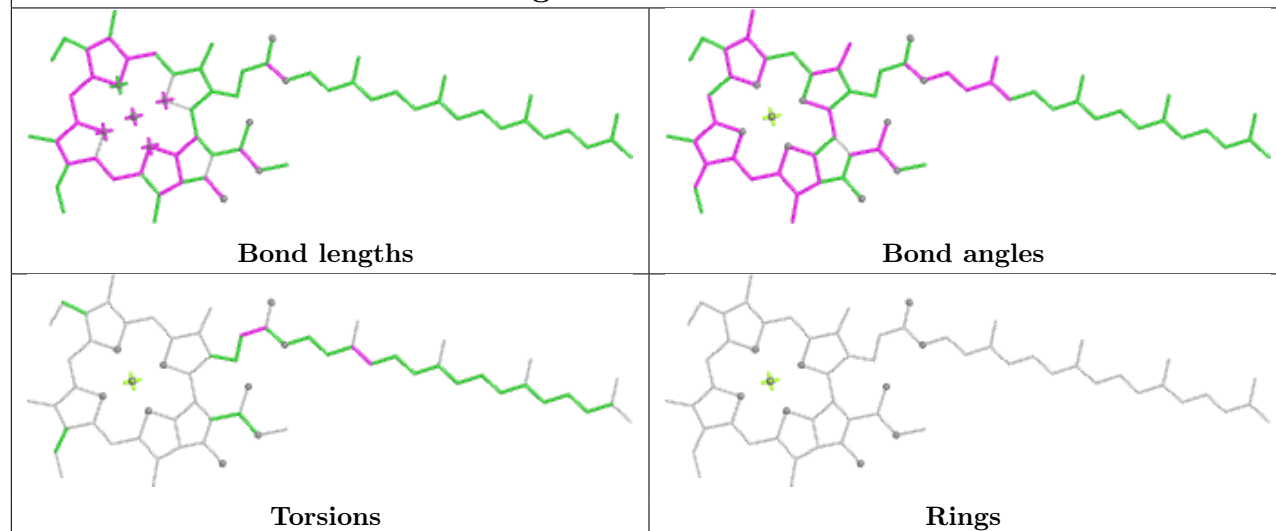
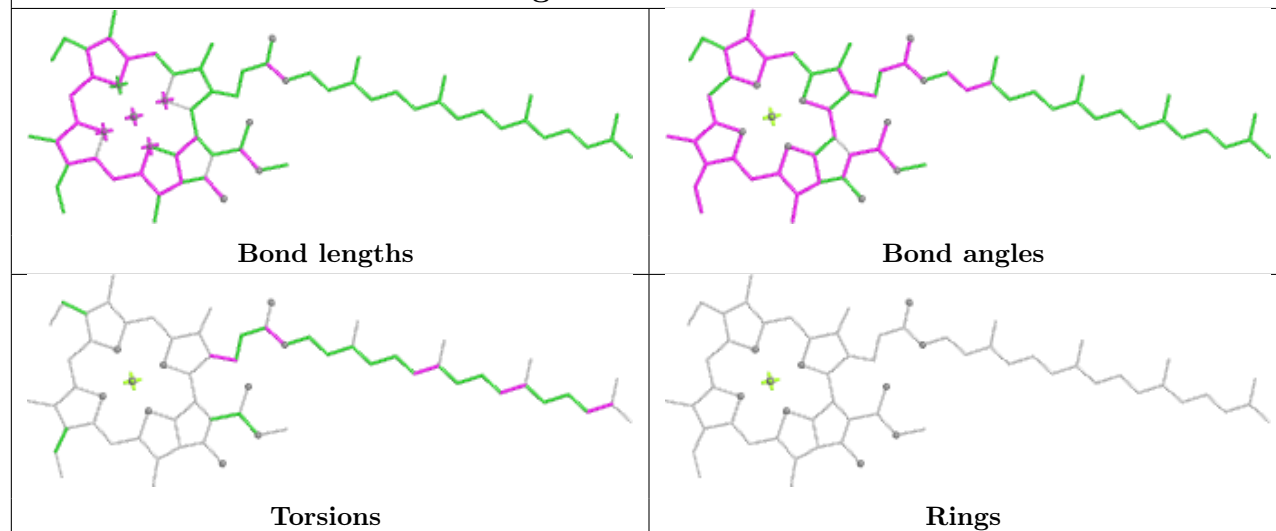
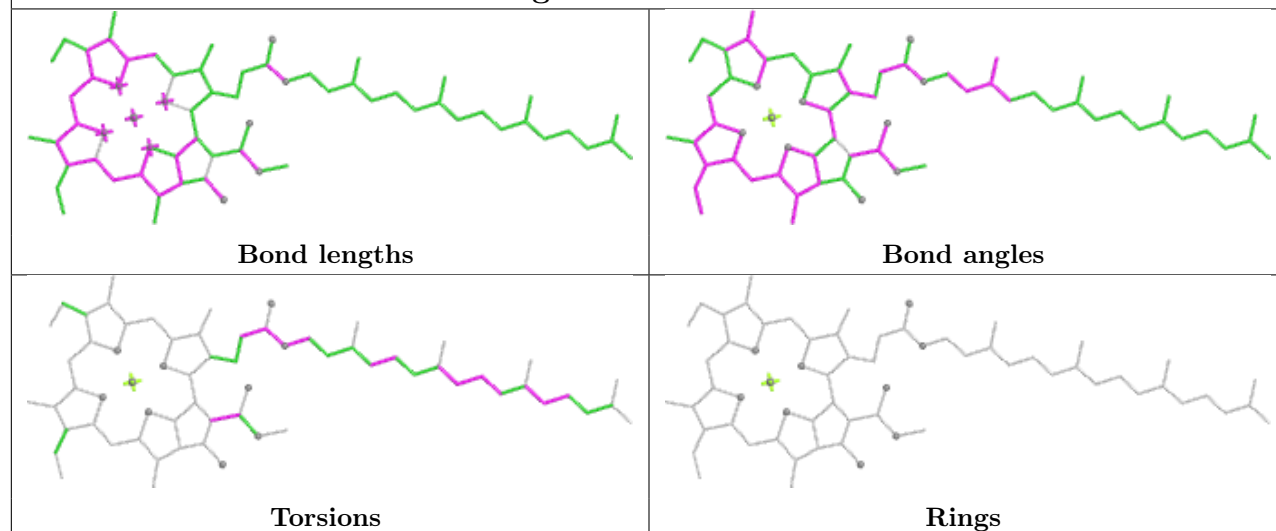


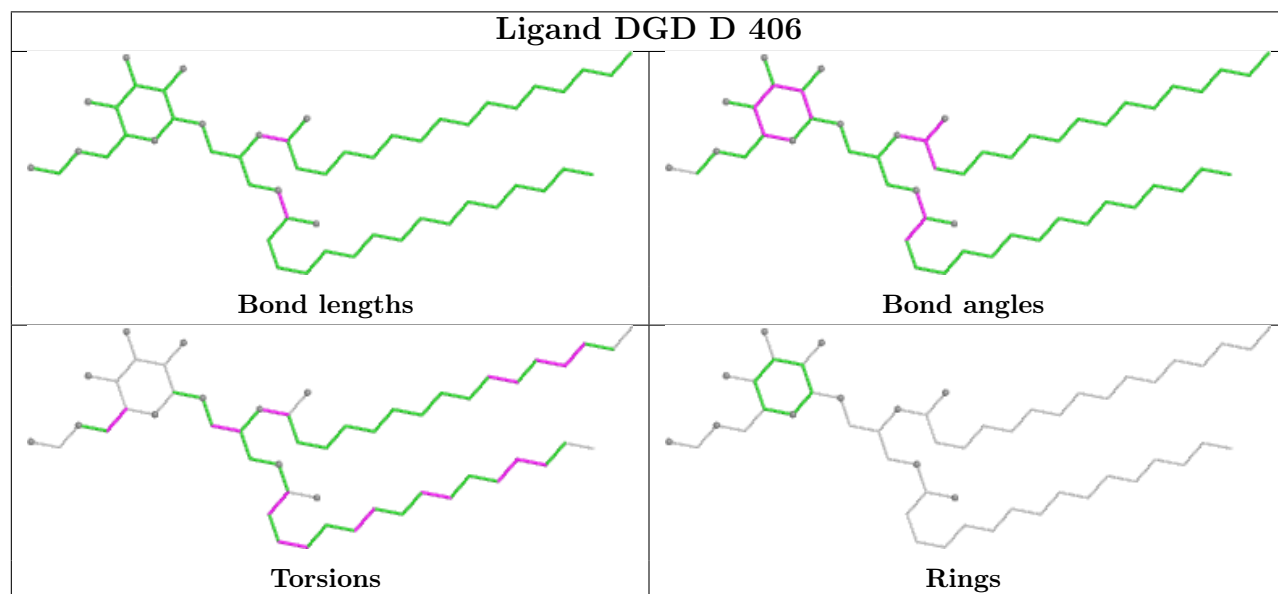
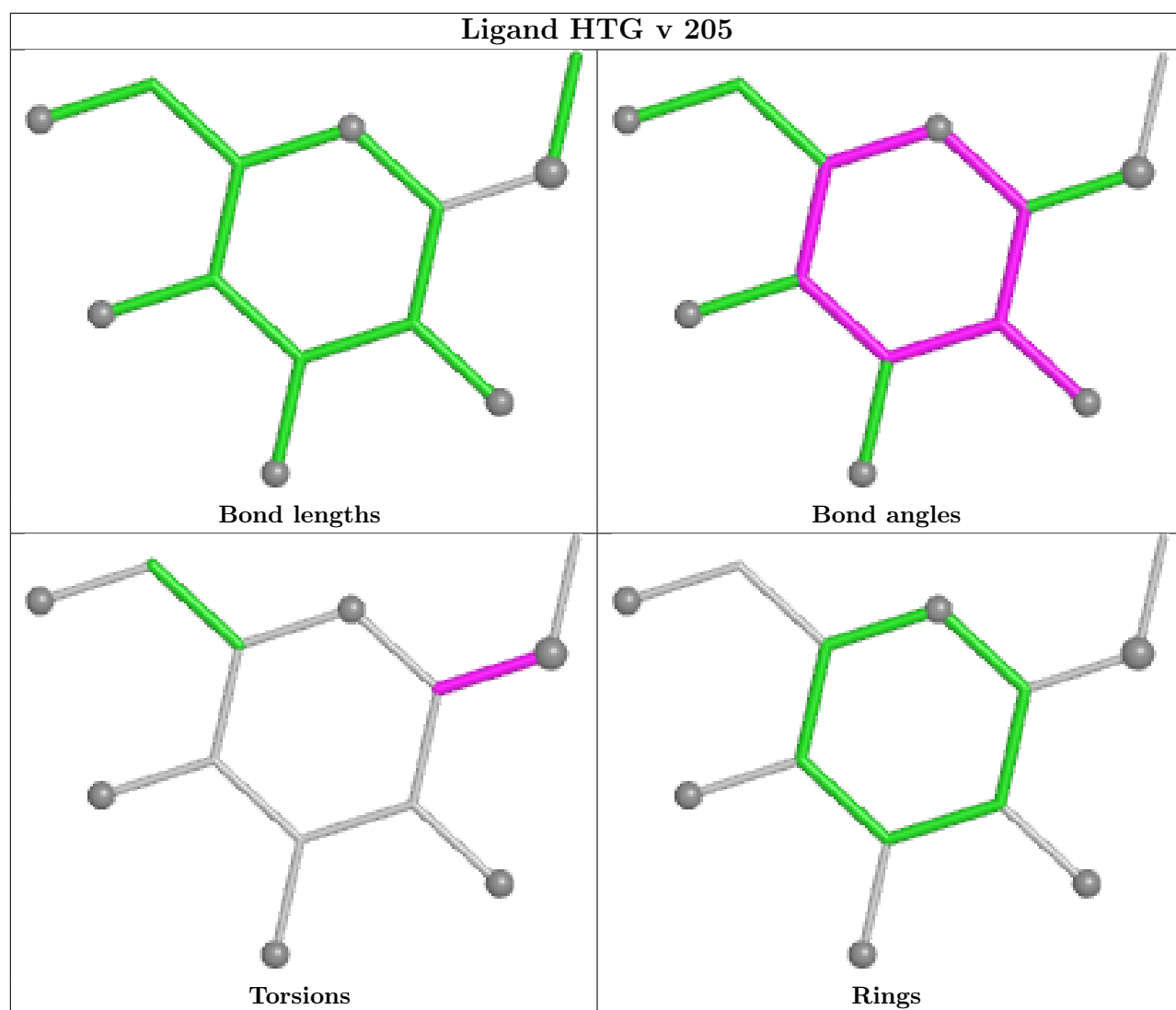
Ligand CLA b 608

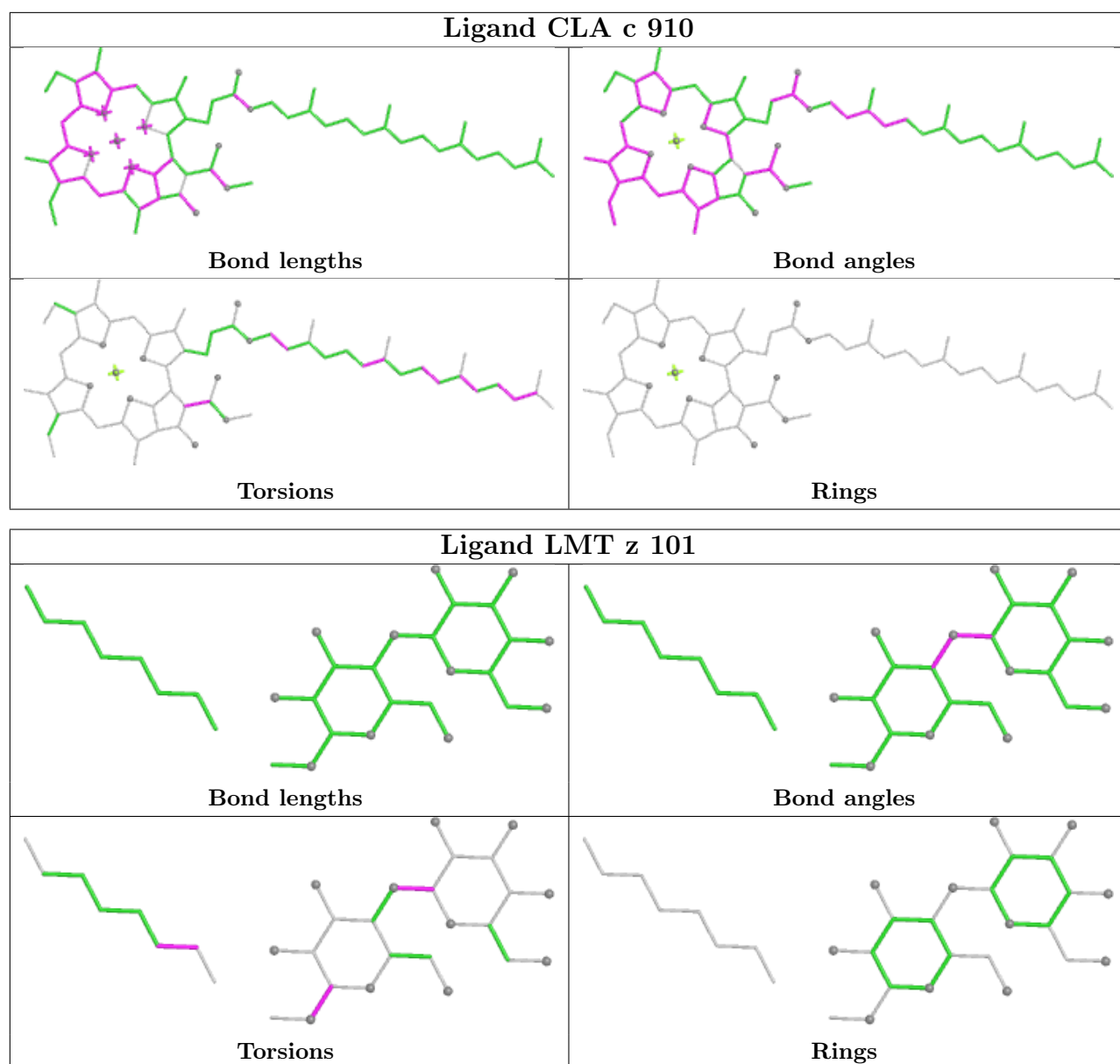


Ligand CLA C 511



Ligand CLA C 505**Ligand CLA C 506****Ligand CLA B 602**





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	334/360 (92%)	-0.43	6 (1%) 67 67	24, 36, 63, 91	3 (0%)
1	a	334/360 (92%)	-0.32	12 (3%) 46 45	25, 39, 68, 104	5 (1%)
2	B	504/505 (99%)	-0.34	10 (1%) 65 64	23, 42, 67, 94	11 (2%)
2	b	501/505 (99%)	-0.24	14 (2%) 55 54	27, 45, 71, 110	12 (2%)
3	C	451/473 (95%)	-0.27	5 (1%) 78 77	33, 47, 64, 117	2 (0%)
3	c	455/473 (96%)	-0.15	4 (0%) 81 80	32, 52, 66, 101	5 (1%)
4	D	340/342 (99%)	-0.53	3 (0%) 81 80	20, 37, 57, 101	1 (0%)
4	d	340/342 (99%)	-0.43	1 (0%) 90 89	22, 42, 63, 95	2 (0%)
5	E	81/84 (96%)	0.20	2 (2%) 58 58	41, 58, 77, 105	0
5	e	79/84 (94%)	0.27	2 (2%) 58 58	49, 62, 87, 105	1 (1%)
6	F	34/45 (75%)	-0.11	0 100 100	43, 49, 76, 87	1 (2%)
6	f	32/45 (71%)	0.14	3 (9%) 14 13	47, 56, 104, 120	0
7	H	63/65 (96%)	-0.16	1 (1%) 70 70	39, 49, 58, 80	0
7	h	63/65 (96%)	0.17	1 (1%) 70 70	44, 55, 65, 104	0
8	I	35/38 (92%)	0.17	2 (5%) 29 28	44, 51, 79, 106	0
8	i	37/38 (97%)	-0.04	2 (5%) 31 30	43, 50, 85, 93	0
9	J	36/40 (90%)	-0.04	1 (2%) 55 54	40, 55, 84, 97	0
9	j	39/40 (97%)	0.38	2 (5%) 33 32	48, 60, 84, 89	0
10	K	37/37 (100%)	-0.17	0 100 100	36, 54, 64, 66	1 (2%)
10	k	37/37 (100%)	0.24	1 (2%) 56 55	53, 61, 73, 75	0
11	L	37/37 (100%)	-0.55	0 100 100	20, 34, 67, 97	1 (2%)
11	l	37/37 (100%)	-0.44	1 (2%) 56 55	21, 36, 80, 110	2 (5%)
12	M	32/36 (88%)	-0.46	0 100 100	21, 36, 48, 70	2 (6%)
12	m	33/36 (91%)	-0.36	0 100 100	21, 36, 57, 84	3 (9%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	-0.19	2 (0%) 82 82	26, 49, 83, 125	7 (2%)
13	o	241/244 (98%)	0.02	6 (2%) 58 58	26, 50, 84, 120	7 (2%)
14	T	29/32 (90%)	-0.39	1 (3%) 48 47	31, 37, 62, 93	0
14	t	29/32 (90%)	-0.28	1 (3%) 48 47	25, 37, 62, 99	1 (3%)
15	U	97/104 (93%)	-0.27	0 100 100	38, 47, 68, 78	4 (4%)
15	u	97/104 (93%)	-0.26	0 100 100	34, 50, 62, 95	1 (1%)
16	V	137/163 (84%)	-0.44	0 100 100	25, 45, 57, 74	2 (1%)
16	v	137/163 (84%)	-0.22	0 100 100	30, 57, 71, 94	1 (0%)
17	Y	27/30 (90%)	0.56	3 (11%) 10 9	59, 66, 95, 101	0
17	y	28/30 (93%)	0.90	1 (3%) 46 45	66, 75, 99, 112	0
18	X	38/40 (95%)	0.14	0 100 100	33, 57, 75, 81	1 (2%)
18	x	38/40 (95%)	0.38	3 (7%) 18 17	35, 63, 94, 108	1 (2%)
19	Z	62/62 (100%)	0.45	5 (8%) 18 17	58, 68, 99, 104	0
19	z	60/62 (96%)	0.94	9 (15%) 5 5	68, 76, 105, 123	0
20	R	30/34 (88%)	2.45	23 (76%) 0 0	85, 107, 118, 123	0
All	All	5265/5508 (95%)	-0.20	127 (2%) 59 59	20, 46, 77, 125	77 (1%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	h	64	ALA	6.0
13	O	58	ASN	4.9
19	z	3	ILE	4.8
2	b	495	PHE	4.7
14	T	30	THR	4.6
8	i	36	ASP	4.5
13	o	59	LYS	4.3
2	B	487	SER	4.3
20	R	26	TYR	4.2
1	A	230	THR	4.1
20	R	7	VAL	3.8
20	R	28	VAL	3.7
7	H	64	ALA	3.5
20	R	15	ALA	3.5
20	R	10	LEU	3.5
14	t	30	THR	3.5
2	B	479	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	486	LEU	3.4
6	f	15	ILE	3.4
18	x	2	THR	3.3
13	O	61	GLN	3.3
18	x	38	GLN	3.3
9	j	5	GLY	3.3
4	D	12	ARG	3.2
2	b	479	PHE	3.2
20	R	5	VAL	3.2
2	b	491	VAL	3.1
5	E	4	THR	3.1
20	R	25	PRO	3.1
8	i	37	LEU	3.1
19	Z	1	MET	3.1
3	C	257	PHE	3.0
13	o	62	GLU	3.0
18	x	37	VAL	3.0
20	R	24	LEU	3.0
2	b	484	PRO	3.0
1	a	11	ALA	3.0
20	R	12	VAL	3.0
1	a	260	PHE	3.0
8	I	34	ARG	2.9
2	B	494	GLY	2.9
20	R	18	TRP	2.9
4	D	238	THR	2.9
19	z	2	THR	2.9
1	a	246	TYR	2.9
19	z	61	VAL	2.8
9	j	4	GLU	2.8
2	b	499	VAL	2.8
3	C	255	THR	2.8
1	A	246	TYR	2.8
6	f	16	PHE	2.8
2	B	86	ILE	2.8
3	c	21	ILE	2.8
2	B	490	GLN	2.7
1	a	344	ALA	2.7
1	a	230	THR	2.7
20	R	6	LEU	2.7
20	R	9	LEU	2.7
2	b	487	SER	2.7

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Mol	Chain	Res	Type	RSRZ
20	R	14	LEU	2.6
2	B	488	PRO	2.6
2	B	483	ASP	2.6
2	b	502	VAL	2.6
5	e	84	LYS	2.6
13	o	21	THR	2.6
2	b	85	GLY	2.5
2	b	490	GLN	2.5
20	R	3	TRP	2.5
1	A	11	ALA	2.5
4	d	237	PRO	2.5
20	R	30	GLN	2.5
3	C	471	SER	2.5
4	D	236	ASN	2.5
17	Y	23	THR	2.4
5	e	61	ARG	2.4
2	B	495	PHE	2.4
19	z	5	PHE	2.4
17	Y	25	ILE	2.4
13	o	56	PRO	2.4
20	R	22	ASN	2.4
1	A	229	GLU	2.4
19	z	6	GLN	2.4
19	z	32	ASP	2.4
2	b	488	PRO	2.4
2	b	496	TYR	2.4
1	a	263	ALA	2.4
2	b	497	GLN	2.4
1	a	224	ILE	2.4
19	Z	3	ILE	2.4
1	a	225	ARG	2.4
20	R	8	VAL	2.4
1	A	12	ASN	2.3
19	Z	62	VAL	2.3
3	c	200	THR	2.3
2	b	500	GLY	2.3
17	y	19	ILE	2.3
20	R	31	VAL	2.3
20	R	16	ALA	2.3
17	Y	22	LEU	2.3
19	Z	7	LEU	2.3
1	a	248	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
19	z	4	LEU	2.3
1	a	262	TYR	2.3
1	a	229	GLU	2.2
11	l	2	GLU	2.2
2	B	84	THR	2.2
3	C	23	ALA	2.2
19	z	41	PHE	2.2
3	C	24	THR	2.2
13	o	58	ASN	2.2
19	Z	32	ASP	2.2
19	z	60	PHE	2.2
8	I	36	ASP	2.2
13	o	246	ALA	2.2
20	R	13	LEU	2.2
1	a	226	GLU	2.1
20	R	23	ILE	2.1
9	J	6	GLY	2.1
20	R	27	ALA	2.1
3	c	45	LEU	2.1
20	R	2	ASP	2.1
2	b	493	TRP	2.1
10	k	17	ILE	2.0
1	A	249	VAL	2.0
3	c	20	SER	2.0
5	E	29	ALA	2.0
6	f	14	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.92	0.10	35,39,52,64	0
12	FME	m	1	10/11	0.93	0.13	40,47,63,69	0
4	HSK	d	336[A]	10/12	0.94	0.09	44,46,47,47	7
4	HSK	d	336[B]	11/12	0.94	0.09	44,46,46,47	8
12	FME	M	1	10/11	0.95	0.11	39,47,68,68	0
14	FME	T	1	10/11	0.95	0.08	37,42,55,60	0
4	HSK	D	336[A]	10/12	0.97	0.07	40,41,42,43	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	HSK	D	336[B]	11/12	0.97	0.07	40,41,42,42	8
8	FME	I	1	10/11	0.98	0.06	42,49,55,57	0
8	FME	i	1	10/11	0.98	0.07	44,51,57,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	HTG	X	902	12/19	0.46	0.16	107,121,127,127	0
34	LMT	M	302	35/35	0.70	0.18	53,76,89,91	0
31	GOL	h	103	6/6	0.73	0.13	83,88,89,91	0
30	UNL	j	1401	18/-	0.73	0.23	65,78,86,91	0
31	GOL	Z	102	6/6	0.73	0.15	108,110,112,118	0
30	UNL	E	103	13/-	0.74	0.25	81,89,92,92	0
31	GOL	O	305	6/6	0.74	0.15	98,101,103,104	0
30	UNL	M	301	16/-	0.75	0.24	59,67,81,82	0
36	DGD	D	406	53/66	0.75	0.19	82,93,104,108	0
35	HTG	u	201	14/19	0.76	0.19	73,87,103,108	0
30	UNL	y	102	10/-	0.76	0.28	93,99,101,103	0
36	DGD	e	102	39/66	0.76	0.18	83,100,111,113	0
30	UNL	a	418	40/-	0.77	0.19	76,86,97,103	0
31	GOL	C	533	6/6	0.77	0.17	86,88,90,96	0
35	HTG	V	203	13/19	0.78	0.13	60,67,81,99	0
30	UNL	B	635	10/-	0.78	0.24	68,77,86,91	0
31	GOL	o	303	6/6	0.78	0.14	69,76,83,88	0
34	LMT	F	103	26/35	0.78	0.19	59,71,79,82	26
30	UNL	E	102	16/-	0.78	0.25	76,80,88,88	0
41	SO4	O	302	5/5	0.78	0.12	93,106,108,126	0
30	UNL	c	933	9/-	0.79	0.23	74,83,93,97	0
31	GOL	c	934	6/6	0.79	0.17	67,77,78,80	0
34	LMT	m	1503	35/35	0.79	0.15	52,76,88,88	0
35	HTG	B	625	19/19	0.79	0.13	66,96,101,101	0
34	LMT	C	520	35/35	0.79	0.16	82,89,94,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	UNL	c	931	18/-	0.80	0.20	87,93,101,104	0
30	UNL	C	523	34/-	0.80	0.18	79,87,96,101	0
30	UNL	e	103	15/-	0.80	0.19	66,75,83,83	0
30	UNL	C	526	19/-	0.80	0.17	70,82,93,94	0
30	UNL	m	1501	13/-	0.80	0.23	63,67,77,81	0
30	UNL	A	415	36/-	0.80	0.18	68,78,90,91	0
35	HTG	B	627	19/19	0.80	0.17	75,92,105,106	0
28	LMG	C	534	51/55	0.80	0.16	67,87,95,105	0
30	UNL	J	104	13/-	0.80	0.23	78,84,93,94	0
35	HTG	c	924	19/19	0.80	0.13	75,96,105,109	0
30	UNL	B	636	15/-	0.80	0.24	69,82,91,92	0
30	UNL	B	638	22/-	0.80	0.14	71,79,97,100	0
31	GOL	c	937	6/6	0.80	0.15	99,99,99,100	0
30	UNL	a	422	10/-	0.80	0.21	69,72,84,90	0
30	UNL	i	804	9/-	0.81	0.18	80,82,84,84	0
34	LMT	t	904	24/35	0.81	0.17	56,65,87,95	0
31	GOL	a	421	6/6	0.81	0.16	69,77,77,80	0
30	UNL	A	418	4/-	0.81	0.24	78,79,82,84	0
30	UNL	j	1403	14/-	0.81	0.19	70,76,79,87	0
31	GOL	c	939	6/6	0.81	0.16	78,79,83,84	0
30	UNL	Y	102	10/-	0.81	0.23	82,87,93,98	0
30	UNL	c	935	6/-	0.81	0.19	75,82,87,87	0
31	GOL	C	531	6/6	0.81	0.15	52,55,58,59	0
30	UNL	b	636	8/-	0.81	0.18	61,68,73,78	0
30	UNL	i	803	16/-	0.81	0.18	71,79,88,91	0
30	UNL	t	901	12/-	0.82	0.18	70,77,83,85	0
35	HTG	d	403	19/19	0.82	0.14	83,97,112,112	0
30	UNL	b	633	18/-	0.82	0.19	59,64,79,79	0
30	UNL	b	635	9/-	0.82	0.23	71,78,82,83	0
34	LMT	T	703	24/35	0.82	0.17	53,67,81,92	0
34	LMT	B	623	35/35	0.82	0.14	63,79,93,96	0
30	UNL	i	801	18/-	0.83	0.19	53,64,80,89	0
35	HTG	b	627	19/19	0.83	0.14	89,109,113,114	0
34	LMT	c	922	35/35	0.83	0.14	77,85,101,103	0
31	GOL	t	902	6/6	0.83	0.15	54,59,60,60	0
30	UNL	A	416	14/-	0.83	0.18	66,76,88,89	0
31	GOL	O	304	6/6	0.83	0.10	69,76,77,85	0
27	SQD	B	621	54/54	0.83	0.15	62,75,100,111	0
37	LHG	E	101	49/49	0.83	0.18	72,94,100,105	0
27	SQD	b	601	54/54	0.83	0.15	55,71,92,98	0
35	HTG	C	522	19/19	0.84	0.12	76,93,101,104	0
34	LMT	J	102	23/35	0.84	0.17	65,77,93,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	UNL	B	637	11/-	0.84	0.20	72,78,85,91	0
35	HTG	b	603	19/19	0.84	0.14	78,91,101,106	0
30	UNL	h	104	7/-	0.84	0.17	65,68,75,77	0
34	LMT	Z	101	35/35	0.84	0.15	71,96,106,112	0
34	LMT	b	625	25/35	0.84	0.15	72,87,99,101	0
31	GOL	v	201	6/6	0.84	0.17	102,103,103,105	0
33	CA	B	601	1/1	0.84	0.11	86,86,86,86	0
27	SQD	a	401	54/54	0.84	0.14	53,70,88,95	0
30	UNL	T	701	15/-	0.84	0.20	73,80,88,89	0
27	SQD	f	102	33/54	0.84	0.15	83,92,110,112	0
30	UNL	c	925	30/-	0.85	0.17	83,94,106,108	0
31	GOL	u	202	6/6	0.85	0.11	76,80,89,95	0
30	UNL	B	634	15/-	0.85	0.18	54,60,76,81	0
31	GOL	L	102	6/6	0.85	0.14	55,56,59,60	0
35	HTG	v	205	13/19	0.85	0.12	69,80,89,92	0
35	HTG	U	201	9/19	0.85	0.20	79,83,102,116	0
30	UNL	B	639	5/-	0.85	0.16	72,72,75,76	0
30	UNL	H	104	7/-	0.85	0.18	61,66,76,79	0
30	UNL	d	402	36/-	0.85	0.18	63,74,89,92	0
27	SQD	A	417	54/54	0.86	0.13	52,68,83,87	0
29	PL9	a	417	55/55	0.86	0.18	68,79,90,94	0
30	UNL	b	634	18/-	0.86	0.20	83,94,109,115	0
30	UNL	I	102	12/-	0.86	0.17	63,68,74,74	0
30	UNL	I	103	12/-	0.86	0.16	67,71,84,88	0
30	UNL	X	901	16/-	0.86	0.15	50,53,69,72	0
31	GOL	b	631	6/6	0.86	0.16	60,64,65,72	0
34	LMT	z	101	32/35	0.86	0.14	66,98,106,107	0
31	GOL	c	927	6/6	0.86	0.13	58,61,62,64	0
31	GOL	c	932	6/6	0.86	0.14	67,68,74,75	0
31	GOL	C	530	6/6	0.86	0.21	84,85,85,87	0
37	LHG	e	101	27/49	0.86	0.13	102,117,131,137	0
30	UNL	J	103	16/-	0.86	0.21	82,88,104,107	0
35	HTG	H	105	16/19	0.87	0.16	82,95,106,108	0
31	GOL	u	203	6/6	0.87	0.12	71,72,77,78	0
31	GOL	b	632	6/6	0.87	0.16	57,60,65,66	0
30	UNL	C	532	4/-	0.87	0.20	76,78,80,80	0
29	PL9	A	414	55/55	0.87	0.18	65,74,87,90	0
31	GOL	B	630	6/6	0.87	0.14	47,51,55,57	0
35	HTG	c	923	19/19	0.87	0.11	88,93,99,102	0
30	UNL	I	101	14/-	0.87	0.17	54,59,72,77	0
30	UNL	c	930	11/-	0.88	0.13	82,91,105,109	0
28	LMG	c	921	51/55	0.88	0.13	60,87,94,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	GOL	c	938	6/6	0.88	0.12	60,64,70,77	0
30	UNL	i	802	12/-	0.88	0.19	66,71,81,81	0
30	UNL	D	411	37/-	0.88	0.16	54,67,82,84	0
31	GOL	B	632	6/6	0.88	0.14	52,55,61,71	0
34	LMT	M	303	35/35	0.88	0.11	46,58,66,66	0
30	UNL	a	403	6/-	0.88	0.17	73,79,79,80	0
27	SQD	F	101	37/54	0.88	0.12	60,74,80,84	0
30	UNL	C	529	9/-	0.88	0.16	80,81,83,84	0
31	GOL	H	101	6/6	0.88	0.15	95,95,98,100	0
34	LMT	a	402	35/35	0.89	0.11	47,60,70,77	0
30	UNL	v	206	7/-	0.89	0.17	69,72,76,78	0
30	UNL	b	637	10/-	0.89	0.16	63,83,91,91	0
34	LMT	m	1502	35/35	0.89	0.10	44,56,63,66	0
35	HTG	C	528	19/19	0.89	0.12	89,101,108,114	0
31	GOL	C	525	6/6	0.89	0.13	48,51,56,60	0
33	CA	b	604	1/1	0.89	0.08	107,107,107,107	0
30	UNL	d	412	18/-	0.90	0.14	54,66,76,78	0
30	UNL	D	412	16/-	0.90	0.15	45,54,68,70	0
31	GOL	o	304	6/6	0.90	0.13	87,89,89,89	0
28	LMG	b	624	51/55	0.90	0.12	42,54,60,64	0
31	GOL	b	638	6/6	0.90	0.18	91,91,92,95	0
34	LMT	D	401	35/35	0.90	0.11	50,61,74,75	0
35	HTG	b	602	19/19	0.90	0.11	52,62,69,76	0
28	LMG	a	416	51/55	0.90	0.12	56,69,76,79	0
35	HTG	b	626	19/19	0.90	0.14	47,54,76,79	0
35	HTG	C	521	19/19	0.90	0.11	77,83,92,94	0
28	LMG	C	519	49/55	0.91	0.13	43,67,78,81	0
35	HTG	B	626	19/19	0.91	0.11	50,64,70,73	0
31	GOL	B	631	6/6	0.91	0.11	43,51,54,61	0
31	GOL	c	936	6/6	0.91	0.16	87,87,87,87	0
31	GOL	v	204	6/6	0.91	0.10	65,71,77,79	0
31	GOL	b	630	6/6	0.91	0.11	44,49,55,56	0
28	LMG	B	622	51/55	0.91	0.11	39,50,59,63	0
28	LMG	c	920	51/55	0.91	0.13	47,71,83,85	0
31	GOL	C	527	6/6	0.91	0.17	74,75,75,76	0
31	GOL	c	926	6/6	0.91	0.11	56,63,69,74	0
31	GOL	B	628	6/6	0.91	0.11	47,52,55,58	0
31	GOL	c	929	6/6	0.91	0.11	62,63,72,72	0
31	GOL	A	422	6/6	0.92	0.10	41,43,45,47	0
26	BCR	t	903	40/40	0.92	0.09	34,47,56,59	0
28	LMG	A	413	51/55	0.92	0.11	54,66,75,79	0
31	GOL	V	204	6/6	0.92	0.12	38,47,48,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	SQD	A	412	52/54	0.92	0.12	41,66,75,79	0
35	HTG	B	624	19/19	0.92	0.14	43,51,69,69	0
31	GOL	a	419	6/6	0.92	0.11	40,45,50,52	0
24	CLA	B	602	65/65	0.92	0.10	44,58,78,81	0
31	GOL	b	628	6/6	0.92	0.11	56,60,64,66	0
24	CLA	C	506	65/65	0.92	0.11	48,59,75,78	0
30	UNL	d	413	18/-	0.92	0.14	58,65,82,84	0
24	CLA	b	605	65/65	0.92	0.10	49,65,82,88	0
37	LHG	D	407	49/49	0.92	0.10	37,44,52,56	0
24	CLA	c	914	65/65	0.92	0.10	55,68,83,86	0
26	BCR	T	702	40/40	0.92	0.09	36,48,57,58	0
31	GOL	A	420	6/6	0.92	0.11	47,53,60,60	0
31	GOL	b	629	6/6	0.93	0.11	52,57,57,61	0
24	CLA	C	513	65/65	0.93	0.10	55,66,80,81	0
27	SQD	a	415	54/54	0.93	0.12	42,71,82,83	0
26	BCR	d	406	40/40	0.93	0.10	45,52,67,71	0
31	GOL	B	633	6/6	0.93	0.10	47,50,52,54	0
31	GOL	O	306	6/6	0.93	0.09	73,77,81,86	0
24	CLA	B	617	65/65	0.93	0.10	37,44,71,73	0
24	CLA	b	618	65/65	0.93	0.10	33,40,65,71	0
24	CLA	b	620	65/65	0.93	0.10	40,47,77,79	0
24	CLA	c	907	65/65	0.93	0.12	49,58,71,75	0
39	RRX	h	101	41/41	0.93	0.10	44,54,63,71	0
24	CLA	B	615	65/65	0.93	0.10	32,38,63,67	0
24	CLA	b	610	65/65	0.94	0.09	37,46,58,64	0
26	BCR	C	514	40/40	0.94	0.09	52,62,67,70	0
26	BCR	D	404	40/40	0.94	0.10	41,47,68,69	0
26	BCR	K	101	40/40	0.94	0.09	47,51,56,58	0
32	BCT	a	408	4/4	0.94	0.09	45,46,52,59	0
31	GOL	A	419	6/6	0.94	0.08	41,45,46,50	0
37	LHG	D	409	46/49	0.94	0.10	37,45,76,78	0
24	CLA	C	512	65/65	0.94	0.09	52,58,73,76	0
37	LHG	d	408	49/49	0.94	0.09	40,47,54,58	0
26	BCR	c	915	40/40	0.94	0.10	61,69,75,75	0
28	LMG	D	410	48/55	0.94	0.10	39,45,69,75	0
24	CLA	c	913	65/65	0.94	0.09	53,60,74,78	0
24	CLA	C	508	65/65	0.95	0.08	38,44,70,73	0
31	GOL	V	205	6/6	0.95	0.07	59,66,69,75	0
24	CLA	d	405	65/65	0.95	0.09	43,51,79,82	0
26	BCR	B	618	40/40	0.95	0.07	37,42,47,49	0
31	GOL	a	420	6/6	0.95	0.07	42,44,45,49	0
28	LMG	d	411	48/55	0.95	0.09	44,50,70,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	BCR	B	619	40/40	0.95	0.07	34,43,54,59	0
24	CLA	B	607	65/65	0.95	0.08	34,42,60,65	0
29	PL9	d	407	55/55	0.95	0.07	31,37,42,45	0
24	CLA	C	504	65/65	0.95	0.08	37,43,63,69	0
31	GOL	v	203	6/6	0.95	0.09	43,51,53,54	0
24	CLA	c	905	65/65	0.95	0.08	42,48,65,68	0
36	DGD	H	103	62/66	0.95	0.09	37,43,51,54	0
36	DGD	c	917	62/66	0.95	0.09	38,47,74,79	0
24	CLA	a	413	65/65	0.95	0.09	35,40,77,79	0
36	DGD	h	102	62/66	0.95	0.08	42,48,55,59	0
31	GOL	b	640	6/6	0.95	0.08	44,52,54,54	0
26	BCR	Y	101	40/40	0.95	0.08	49,54,61,62	0
26	BCR	b	623	40/40	0.95	0.08	43,48,59,60	0
37	LHG	b	639	49/49	0.95	0.09	36,45,54,65	0
24	CLA	c	908	65/65	0.95	0.09	43,50,64,67	0
24	CLA	c	909	65/65	0.95	0.09	40,46,77,81	0
24	CLA	A	410	65/65	0.95	0.10	35,39,77,82	0
26	BCR	y	101	40/40	0.95	0.09	51,60,66,67	0
24	CLA	a	410	65/65	0.96	0.09	35,39,75,85	0
24	CLA	c	911	65/65	0.96	0.07	42,49,54,64	0
31	GOL	V	206	6/6	0.96	0.06	50,53,55,58	0
24	CLA	C	507	65/65	0.96	0.08	44,49,64,66	0
24	CLA	C	503	65/65	0.96	0.07	42,47,55,63	0
32	BCT	A	421	4/4	0.96	0.07	41,42,49,57	0
24	CLA	b	606	65/65	0.96	0.07	40,44,50,55	0
24	CLA	C	509	65/65	0.96	0.07	43,47,59,62	0
24	CLA	b	613	65/65	0.96	0.07	44,48,53,56	0
26	BCR	B	620	40/40	0.96	0.07	40,46,59,60	0
24	CLA	b	614	65/65	0.96	0.07	38,44,47,49	0
26	BCR	C	515	40/40	0.96	0.08	44,52,56,58	0
31	GOL	B	629	6/6	0.96	0.08	42,44,46,47	0
24	CLA	C	510	65/65	0.96	0.07	40,45,53,59	0
35	HTG	o	301	19/19	0.96	0.08	41,45,54,54	0
24	CLA	b	619	65/65	0.96	0.07	38,46,59,63	0
24	CLA	C	511	65/65	0.96	0.07	42,52,58,59	0
36	DGD	C	516	62/66	0.96	0.09	35,43,72,77	0
36	DGD	C	517	56/66	0.96	0.07	38,46,67,71	0
36	DGD	C	518	58/66	0.96	0.08	36,43,61,69	0
24	CLA	c	902	65/65	0.96	0.08	42,51,58,61	0
26	BCR	a	414	40/40	0.96	0.07	33,40,47,48	0
26	BCR	b	621	40/40	0.96	0.07	38,44,48,52	0
36	DGD	c	918	55/66	0.96	0.08	41,52,65,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	DGD	c	919	60/66	0.96	0.08	42,48,60,68	0
26	BCR	b	622	40/40	0.96	0.07	36,44,56,59	0
24	CLA	c	904	65/65	0.96	0.07	44,52,58,70	0
24	CLA	B	611	65/65	0.96	0.07	37,40,44,47	0
37	LHG	D	408	49/49	0.96	0.08	32,40,52,57	0
26	BCR	c	916	40/40	0.96	0.08	48,53,58,59	0
29	PL9	D	405	55/55	0.96	0.06	30,35,39,42	0
31	GOL	f	104	6/6	0.96	0.07	61,63,66,68	0
24	CLA	C	501	65/65	0.96	0.08	40,47,55,60	0
37	LHG	d	409	49/49	0.96	0.08	35,41,52,57	0
37	LHG	d	410	40/49	0.96	0.09	42,48,76,78	0
26	BCR	k	101	40/40	0.96	0.08	51,58,66,67	0
39	RRX	H	102	41/41	0.96	0.07	41,48,58,70	0
24	CLA	D	403	65/65	0.96	0.07	38,44,72,74	0
31	GOL	V	201	6/6	0.96	0.07	53,58,62,62	0
24	CLA	B	608	65/65	0.97	0.06	30,35,46,49	0
24	CLA	b	607	65/65	0.97	0.06	38,42,49,54	0
24	CLA	b	608	65/65	0.97	0.06	33,37,63,68	0
25	PHO	A	408	64/64	0.97	0.05	28,33,38,40	0
25	PHO	A	409	64/64	0.97	0.06	31,37,45,51	0
25	PHO	a	411	64/64	0.97	0.06	31,35,39,44	0
25	PHO	a	412	64/64	0.97	0.06	34,41,48,57	0
26	BCR	A	411	40/40	0.97	0.07	34,40,47,48	0
24	CLA	b	609	65/65	0.97	0.06	34,38,49,51	0
24	CLA	C	505	65/65	0.97	0.07	38,44,57,60	0
24	CLA	b	611	65/65	0.97	0.06	32,37,47,48	0
24	CLA	b	612	65/65	0.97	0.06	39,44,52,56	0
24	CLA	B	609	65/65	0.97	0.06	34,39,47,50	0
24	CLA	B	610	65/65	0.97	0.06	39,42,47,54	0
24	CLA	b	615	65/65	0.97	0.06	33,38,48,52	0
24	CLA	b	616	65/65	0.97	0.06	33,39,44,48	0
31	GOL	c	928	6/6	0.97	0.07	42,44,45,46	0
24	CLA	b	617	65/65	0.97	0.06	32,37,58,63	0
24	CLA	B	603	65/65	0.97	0.07	36,40,47,48	0
24	CLA	B	612	65/65	0.97	0.06	30,35,45,48	0
24	CLA	B	613	65/65	0.97	0.06	30,36,42,44	0
24	CLA	B	614	65/65	0.97	0.06	30,35,56,60	0
24	CLA	c	903	65/65	0.97	0.07	40,47,60,71	0
24	CLA	B	604	65/65	0.97	0.06	34,38,46,48	0
24	CLA	B	616	65/65	0.97	0.07	37,41,56,59	0
37	LHG	L	101	49/49	0.97	0.07	35,43,53,61	0
24	CLA	c	906	65/65	0.97	0.06	41,45,56,64	0

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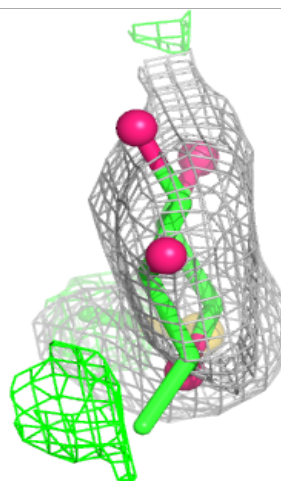
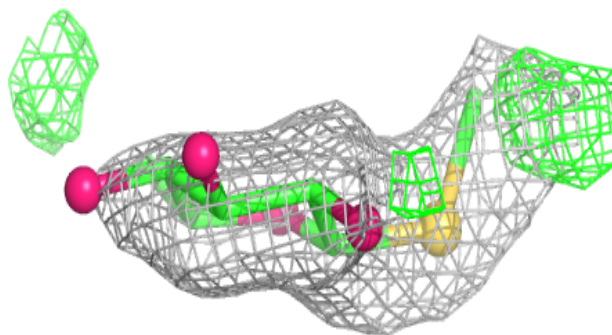
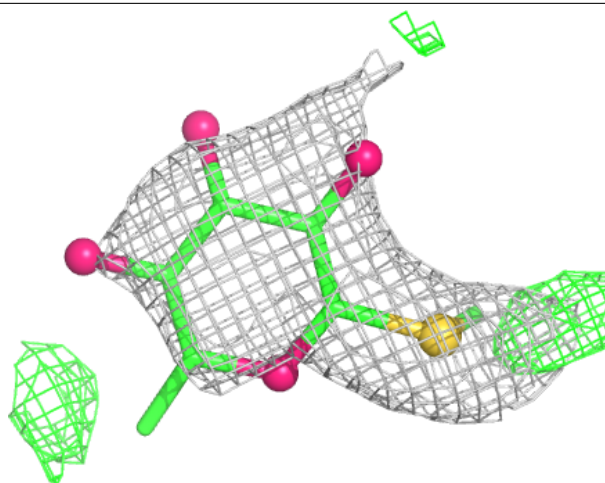
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	B	605	65/65	0.97	0.07	30,34,57,68	0
24	CLA	B	606	65/65	0.97	0.06	32,35,45,49	0
24	CLA	C	502	65/65	0.97	0.06	39,42,54,60	0
24	CLA	c	910	65/65	0.97	0.07	44,50,61,66	0
38	HEM	F	102	43/43	0.97	0.08	53,58,70,74	0
38	HEM	f	101	43/43	0.97	0.08	59,65,75,91	0
35	HTG	O	303	19/19	0.97	0.08	41,45,57,58	0
24	CLA	A	407	65/65	0.97	0.07	29,34,73,77	0
40	MG	j	1402	1/1	0.97	0.14	51,51,51,51	0
24	CLA	c	912	65/65	0.97	0.07	45,54,63,65	0
24	CLA	A	406	65/65	0.98	0.05	27,31,40,43	0
24	CLA	d	401	65/65	0.98	0.05	30,33,41,48	0
24	CLA	d	404	65/65	0.98	0.06	30,35,55,59	0
24	CLA	a	409	65/65	0.98	0.05	31,35,40,51	0
38	HEM	v	202	43/43	0.98	0.06	44,49,51,54	0
24	CLA	A	405	65/65	0.98	0.05	27,31,38,49	0
24	CLA	D	402	65/65	0.98	0.05	25,31,49,54	0
31	GOL	C	524	6/6	0.98	0.06	37,38,40,40	0
33	CA	f	103	1/1	0.98	0.08	70,70,70,70	0
33	CA	O	301	1/1	0.99	0.06	68,68,68,68	0
38	HEM	V	202	43/43	0.99	0.06	37,40,43,45	0
21	OEX	a	404	10/10	0.99	0.03	38,39,41,44	0
33	CA	c	901	1/1	0.99	0.05	61,61,61,61	0
23	CL	A	403	1/1	0.99	0.06	36,36,36,36	0
33	CA	o	302	1/1	0.99	0.04	69,69,69,69	0
40	MG	J	101	1/1	0.99	0.08	43,43,43,43	0
21	OEX	A	401	10/10	0.99	0.04	34,37,40,41	0
33	CA	F	104	1/1	0.99	0.06	63,63,63,63	0
23	CL	A	404	1/1	1.00	0.03	35,35,35,35	0
23	CL	a	406	1/1	1.00	0.07	43,43,43,43	0
23	CL	a	407	1/1	1.00	0.02	41,41,41,41	0
22	FE2	a	405	1/1	1.00	0.02	41,41,41,41	0
22	FE2	A	402	1/1	1.00	0.01	37,37,37,37	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.

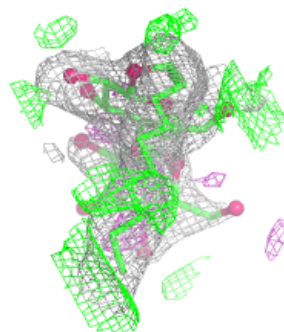
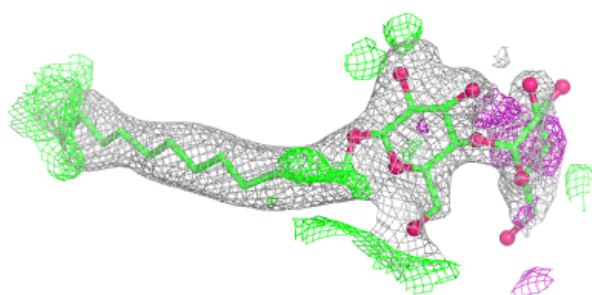
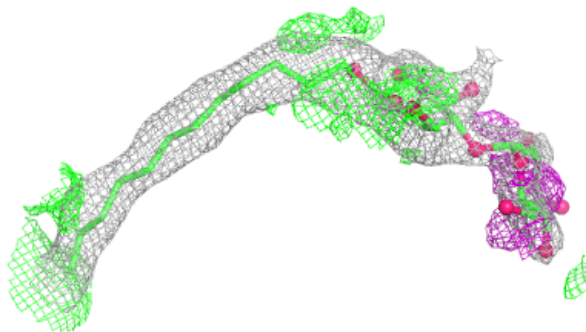
Electron density around HTG X 902:

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

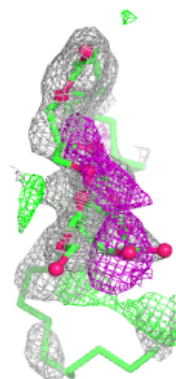
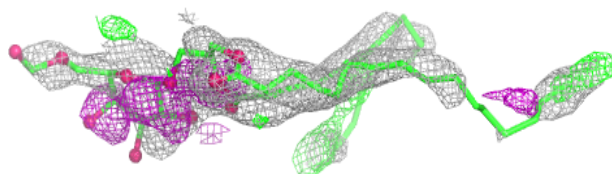
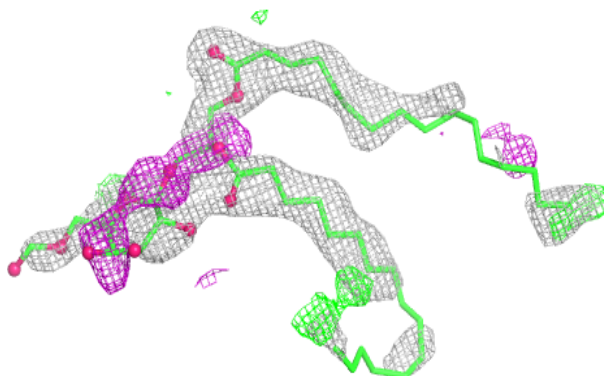


Electron density around LMT M 302:

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

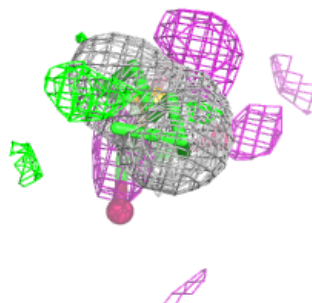
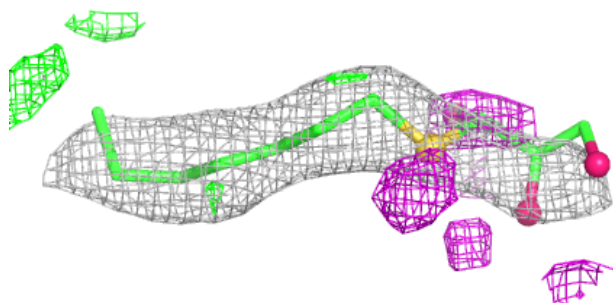
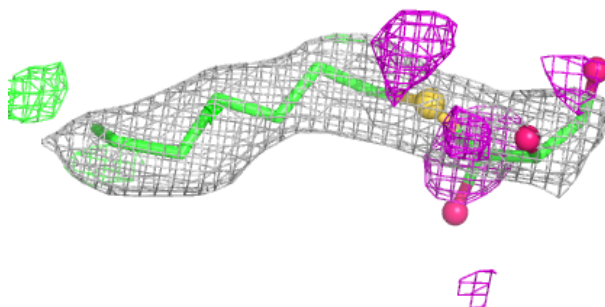
**Electron density around DGD D 406:**

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

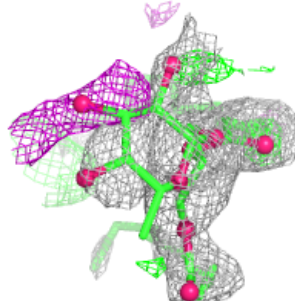
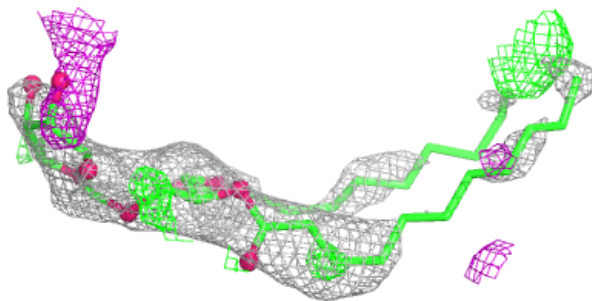
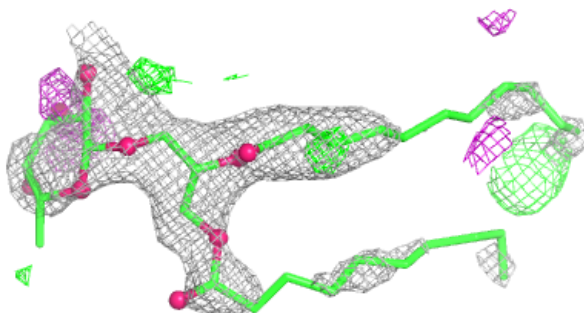


Electron density around HTG u 201:

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

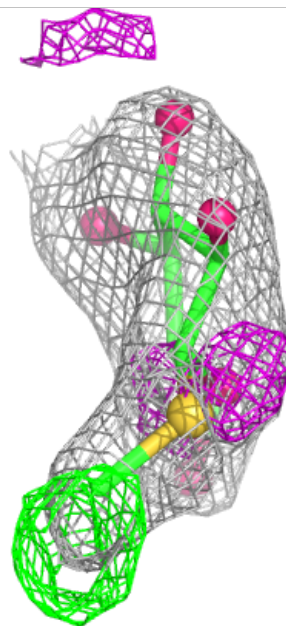
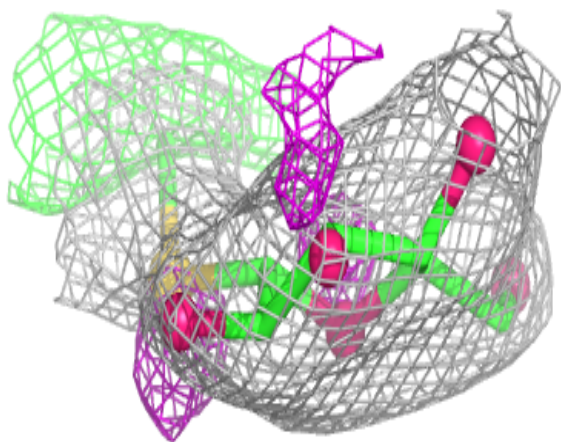
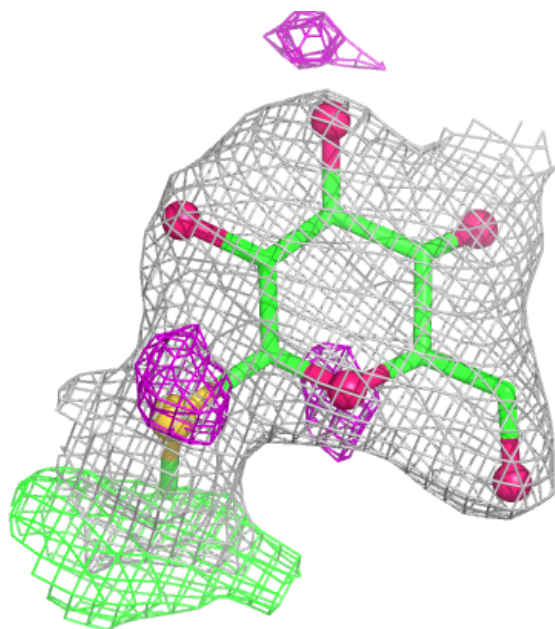
**Electron density around DGD e 102:**

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



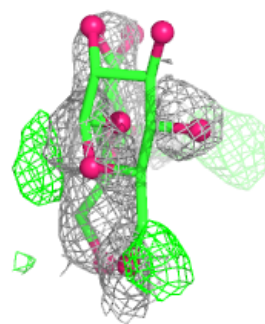
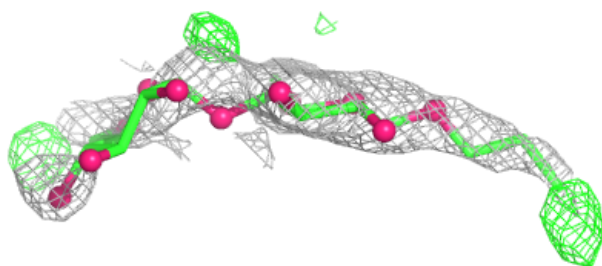
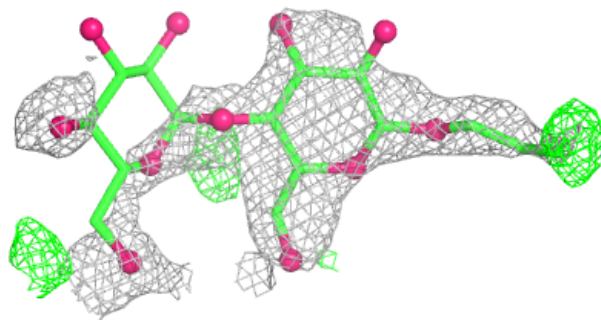
Electron density around HTG V 203:

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

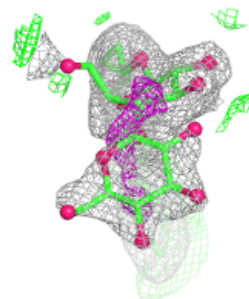
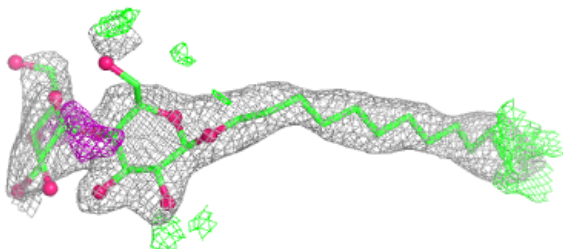
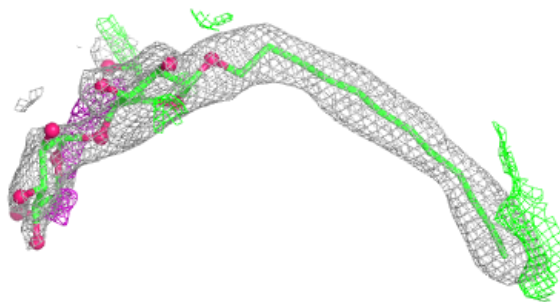


Electron density around LMT F 103:

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

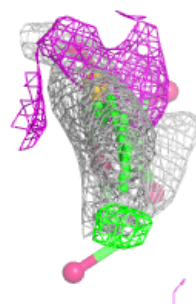
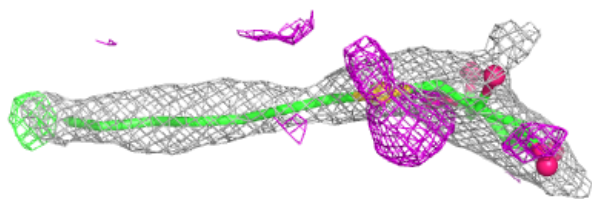
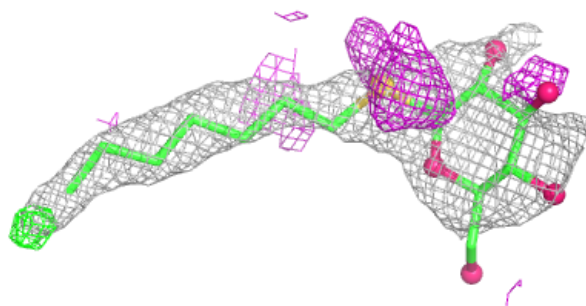
**Electron density around LMT m 1503:**

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

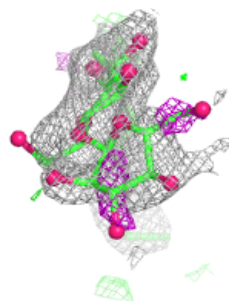
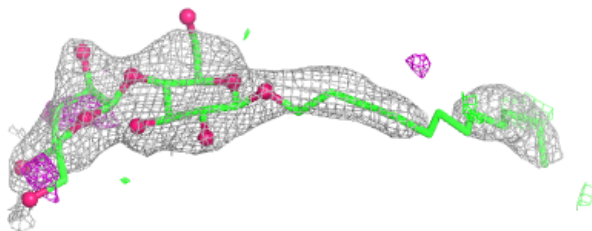
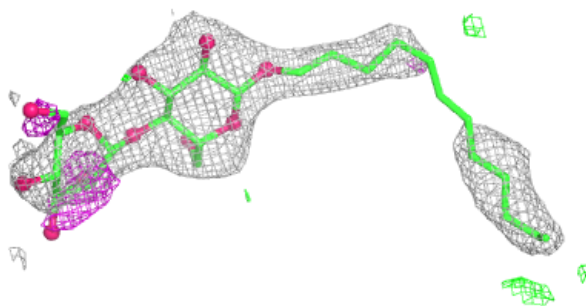


Electron density around HTG B 625:

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

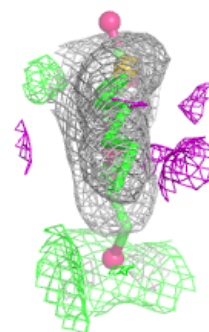
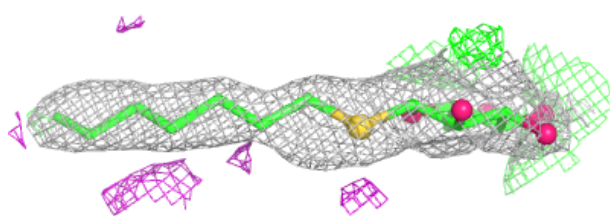
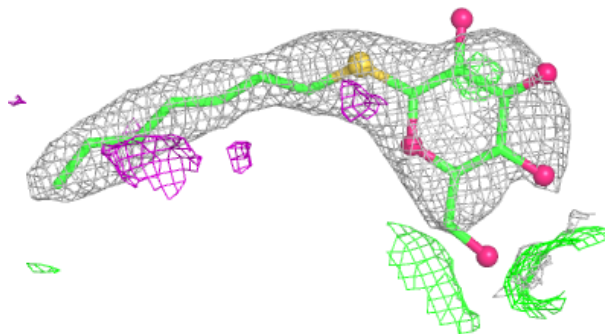
**Electron density around LMT C 520:**

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

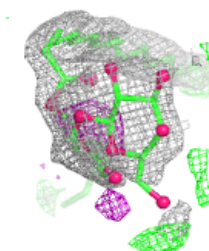
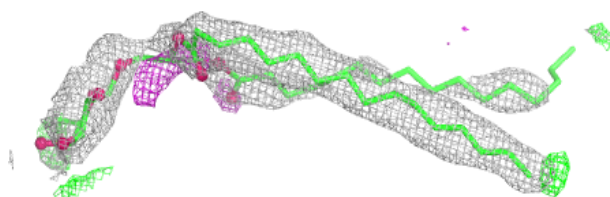
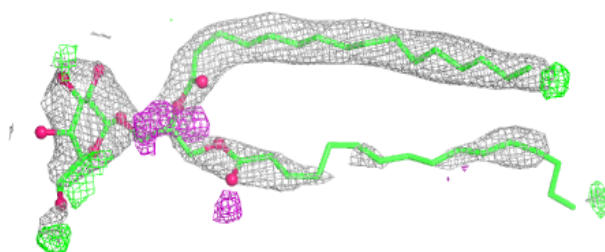


Electron density around HTG B 627:

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

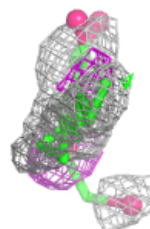
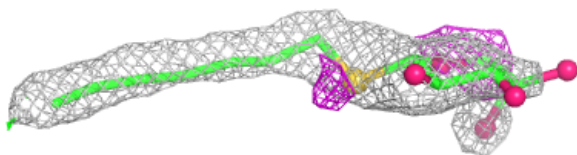
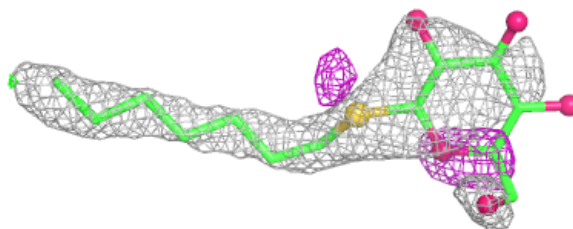
**Electron density around LMG C 534:**

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

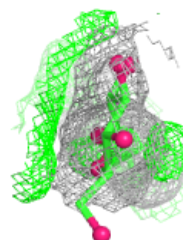
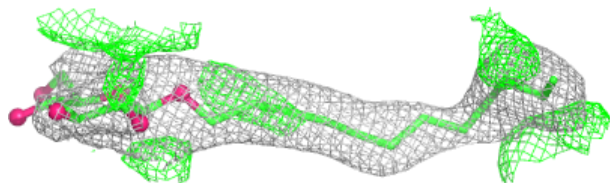
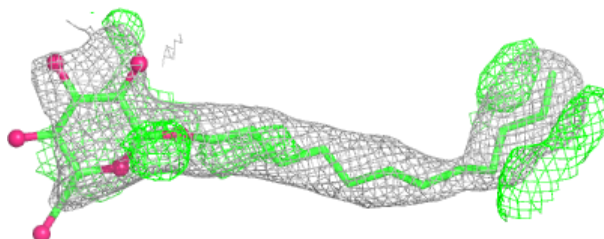


Electron density around HTG c 924:

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

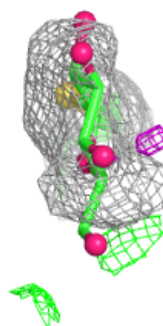
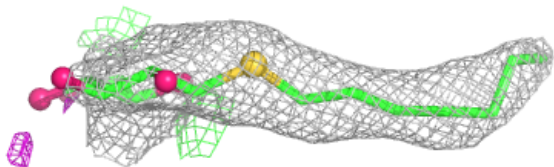
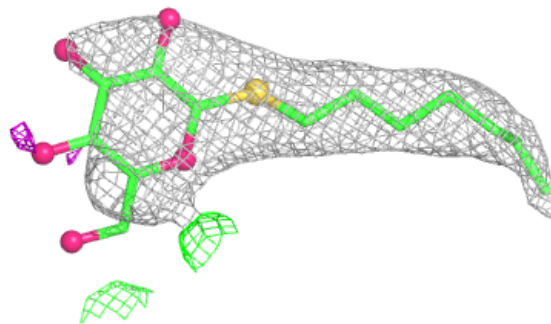
**Electron density around LMT t 904:**

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

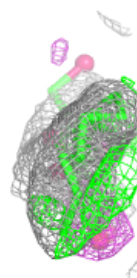
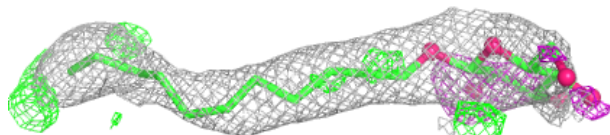
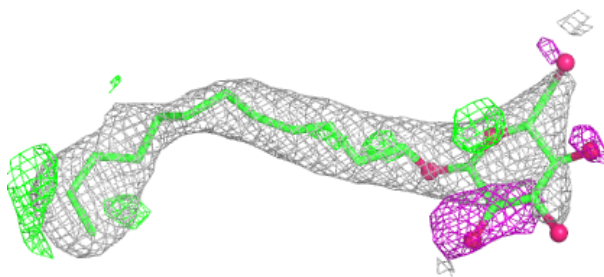


Electron density around HTG d 403:

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

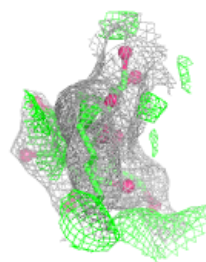
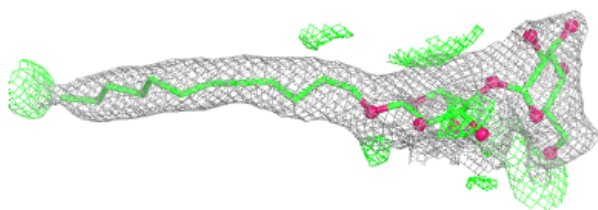
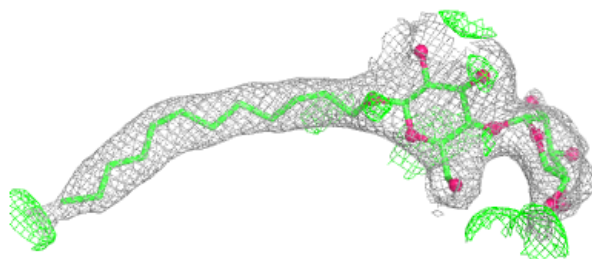
**Electron density around LMT T 703:**

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

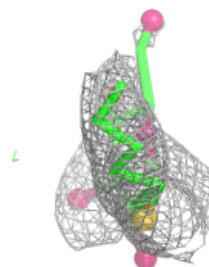
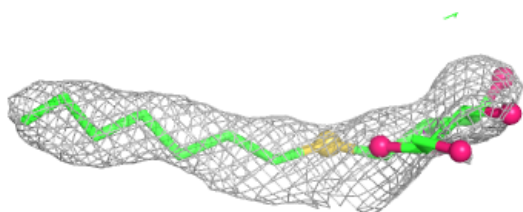
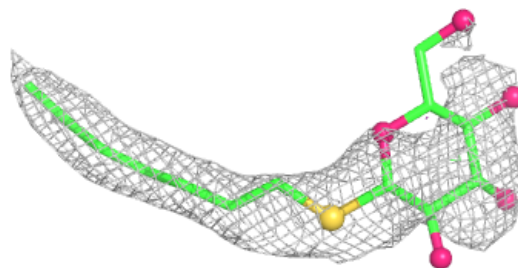


Electron density around LMT B 623:

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

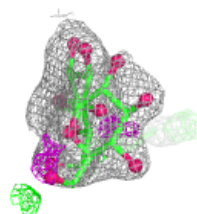
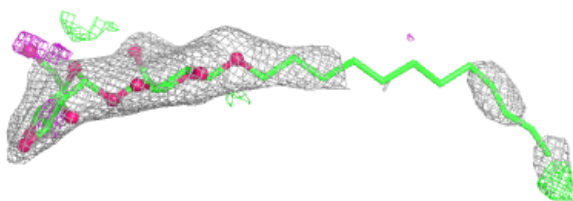
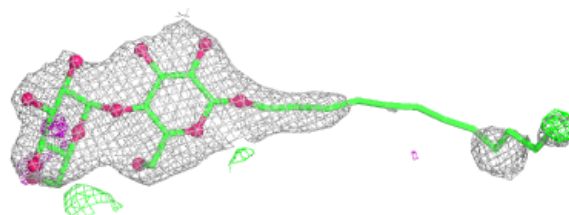
**Electron density around HTG b 627:**

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

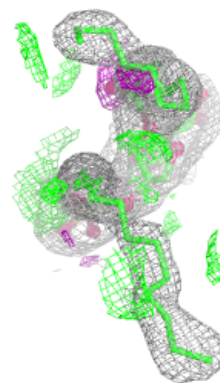
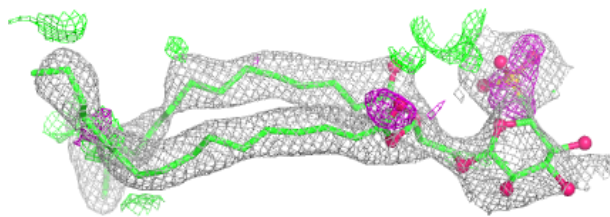
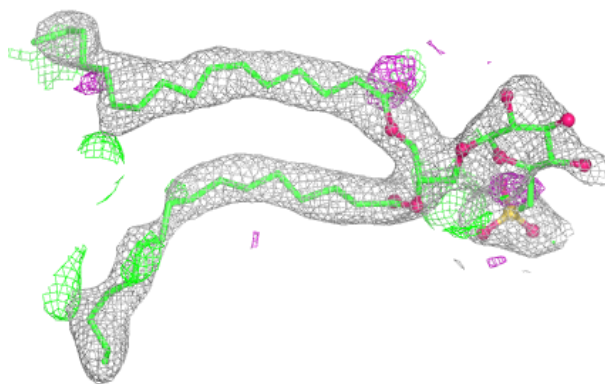


Electron density around LMT c 922:

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

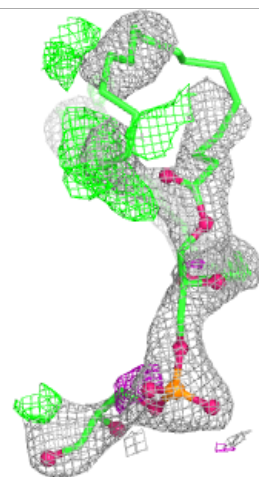
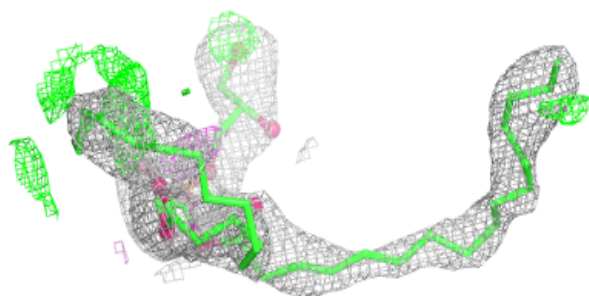
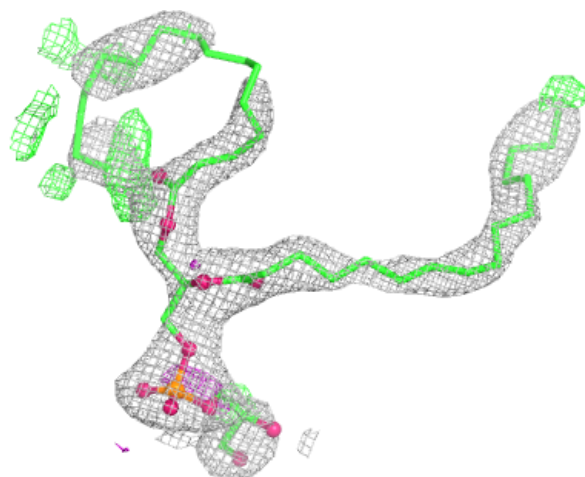
**Electron density around SQD B 621:**

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



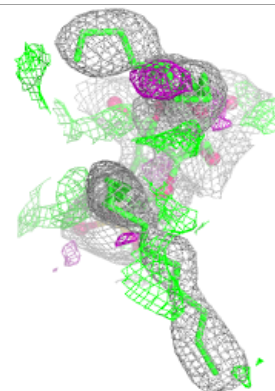
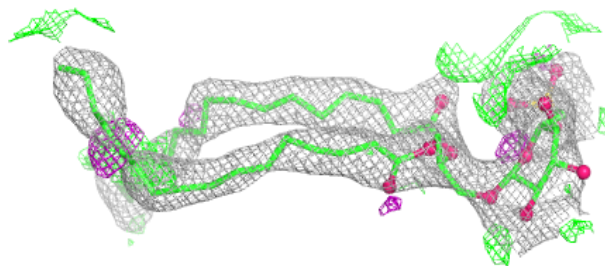
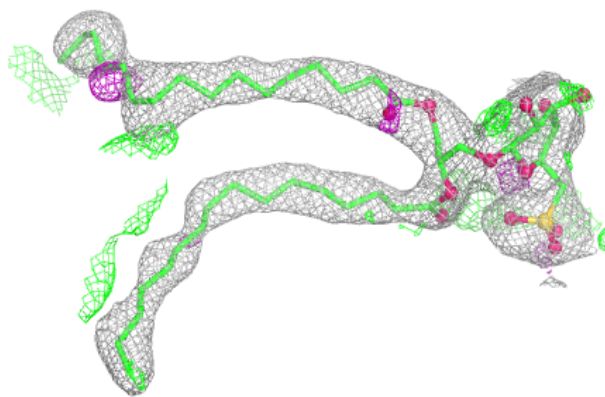
Electron density around LHG E 101:

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

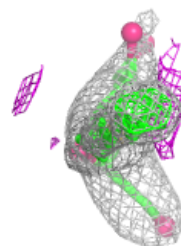
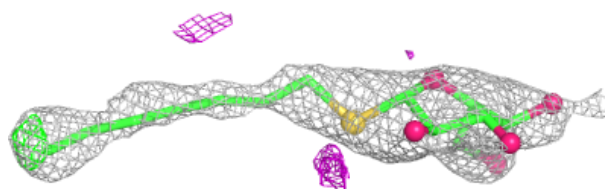
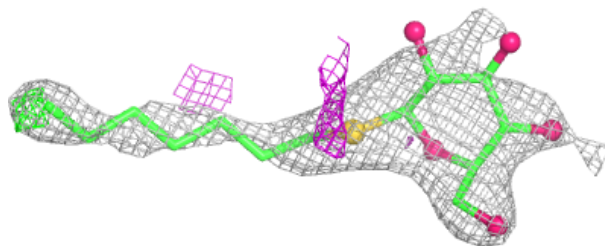


Electron density around SQD b 601:

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

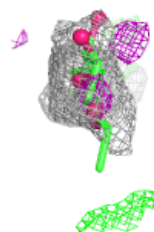
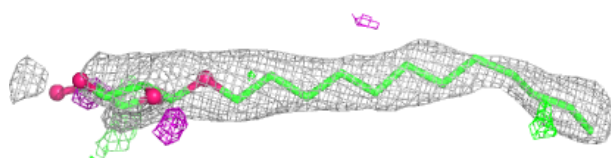
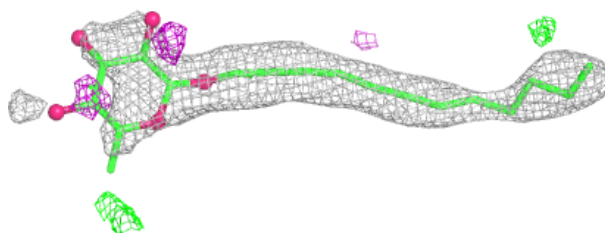
**Electron density around HTG C 522:**

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

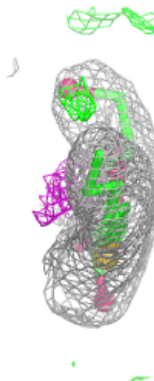
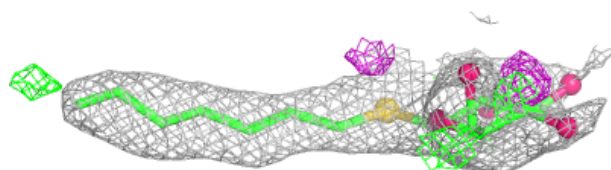
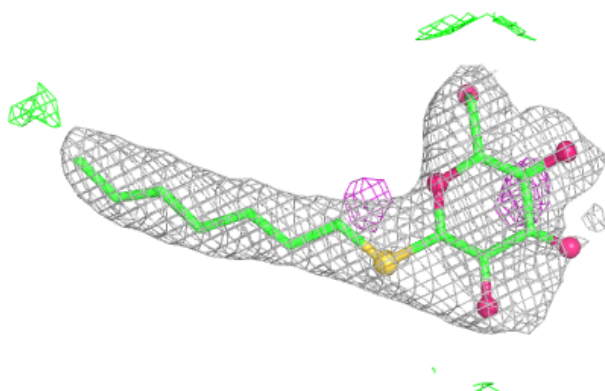


Electron density around LMT J 102:

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

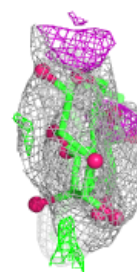
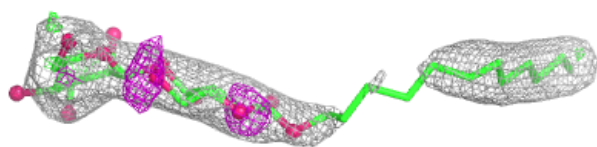
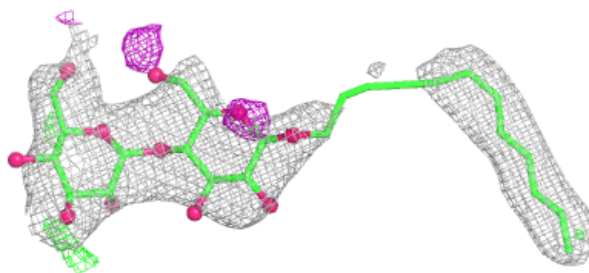
**Electron density around HTG b 603:**

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

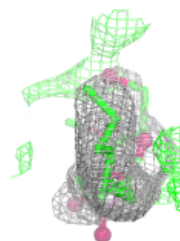
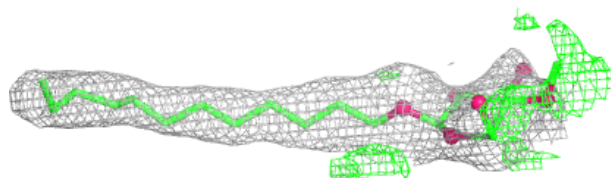
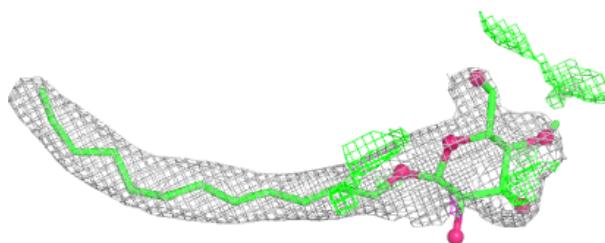


Electron density around LMT Z 101:

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

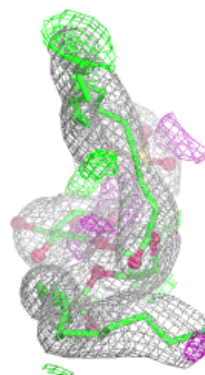
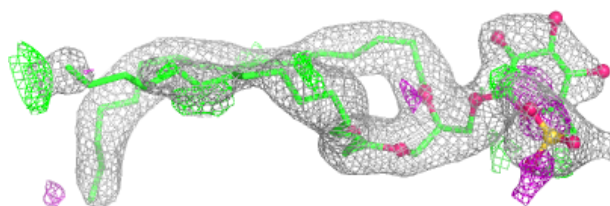
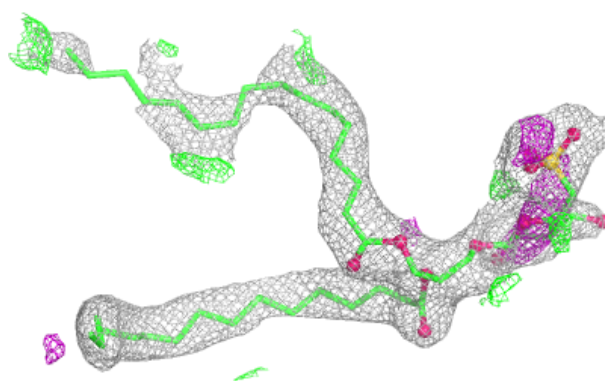
**Electron density around LMT b 625:**

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

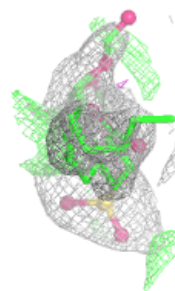
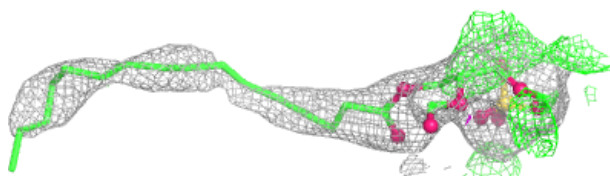
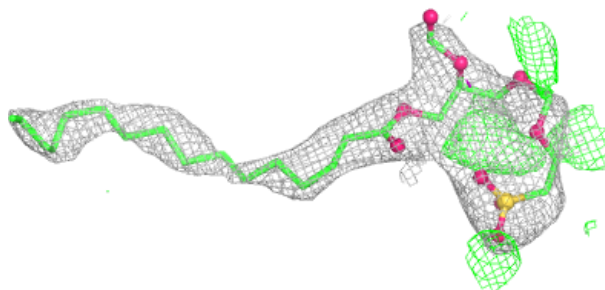


Electron density around SQD a 401:

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

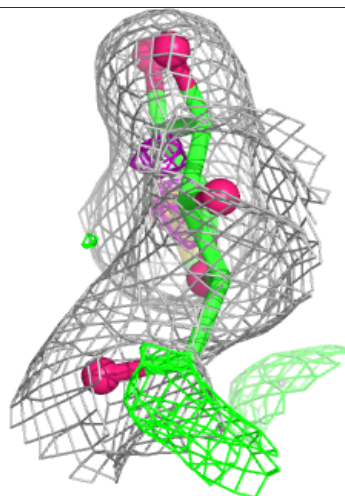
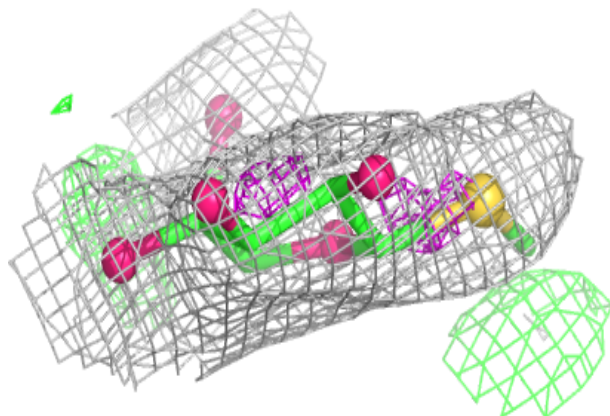
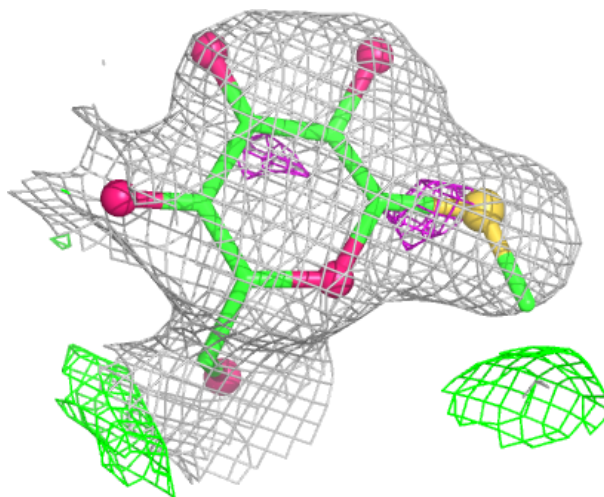
**Electron density around SQD f 102:**

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



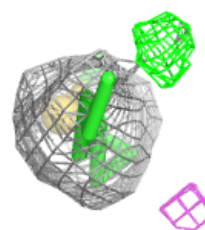
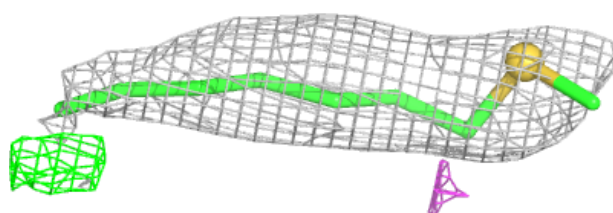
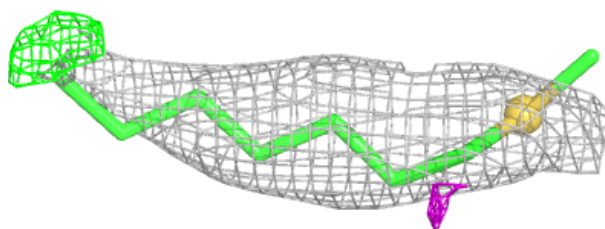
Electron density around HTG v 205:

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

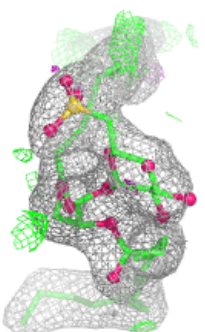
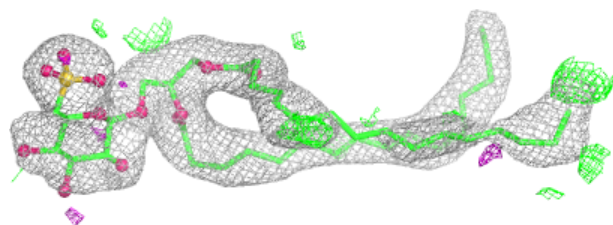
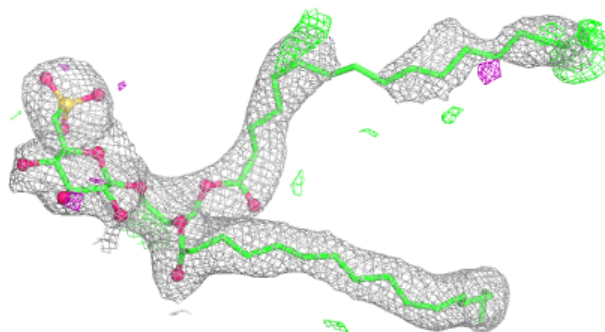


Electron density around HTG U 201:

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

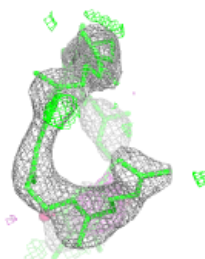
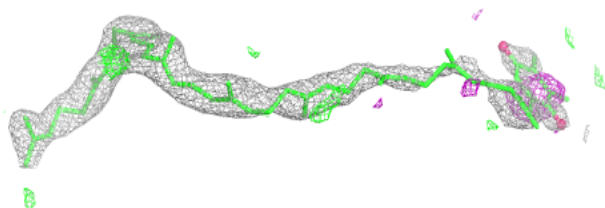
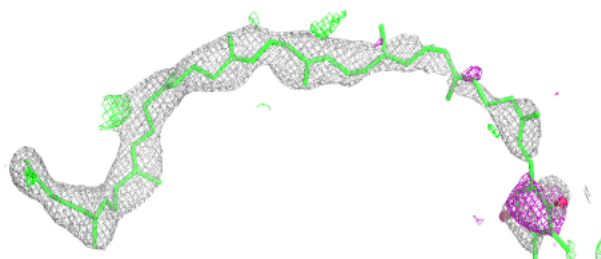
**Electron density around SQD A 417:**

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

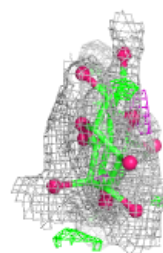
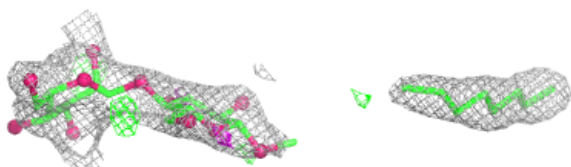
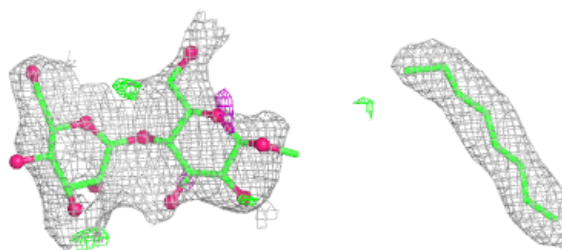


Electron density around PL9 a 417:

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

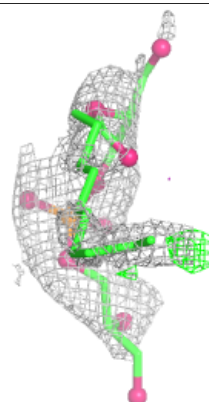
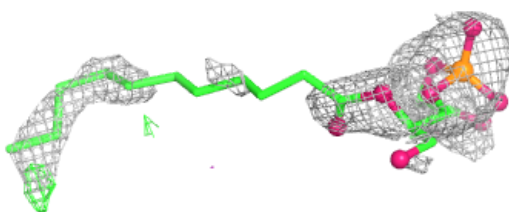
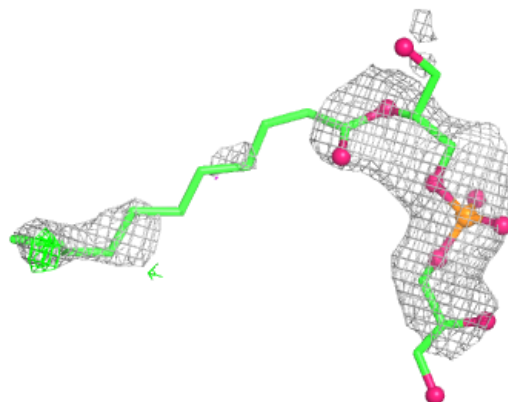
**Electron density around LMT z 101:**

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

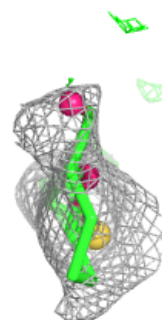
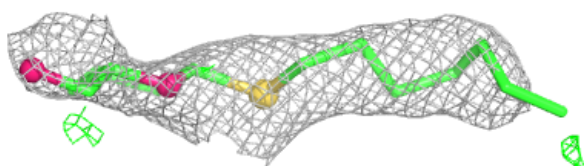
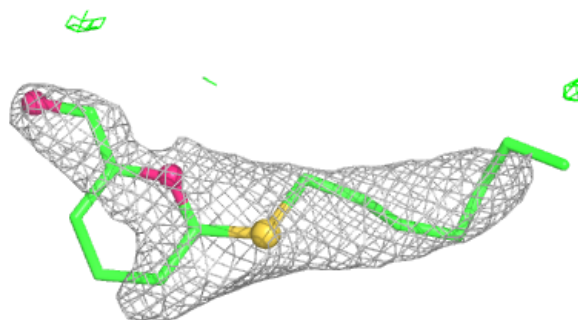


Electron density around LHG e 101:

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

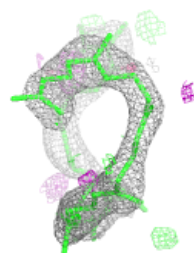
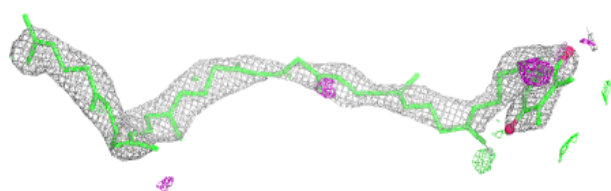
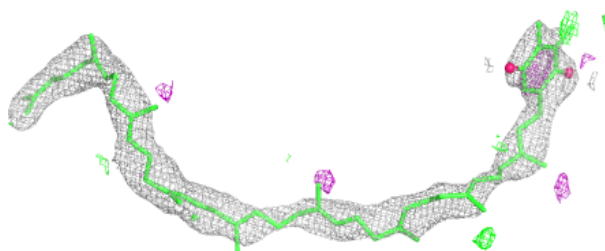
**Electron density around HTG H 105:**

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

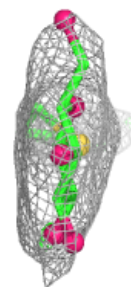
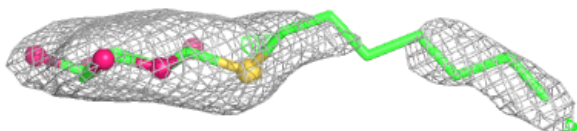
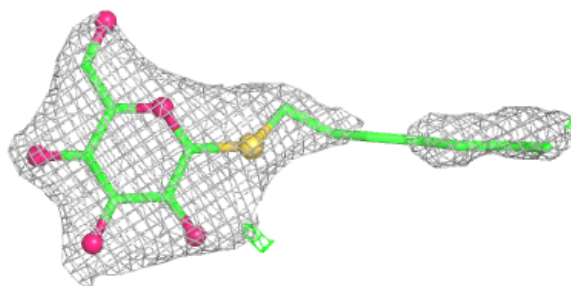


Electron density around PL9 A 414:

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

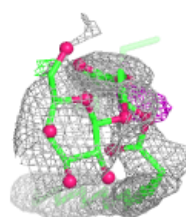
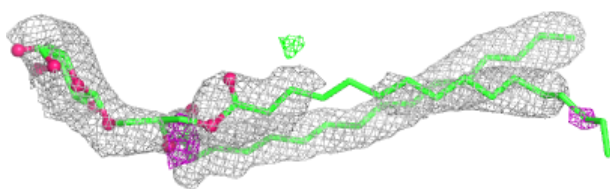
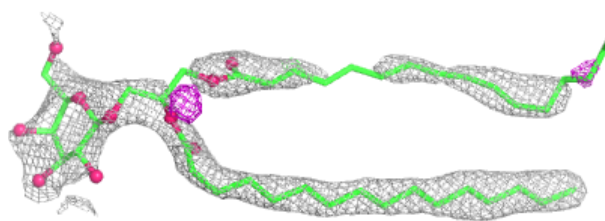
**Electron density around HTG c 923:**

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

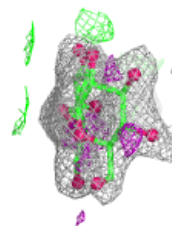
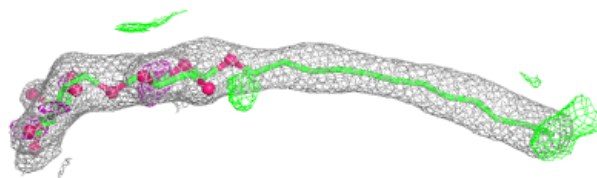
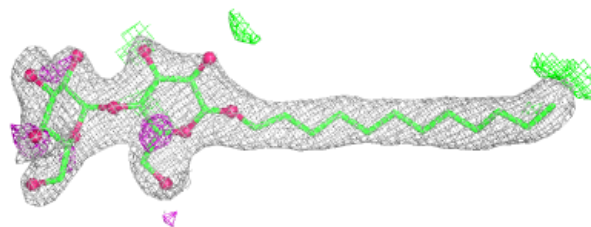


Electron density around LMG c 921:

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

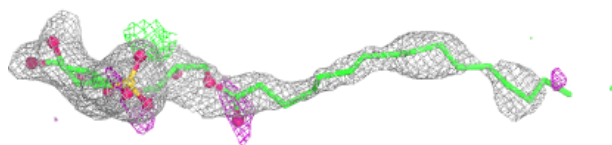
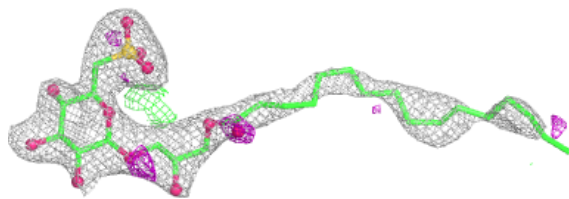
**Electron density around LMT M 303:**

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

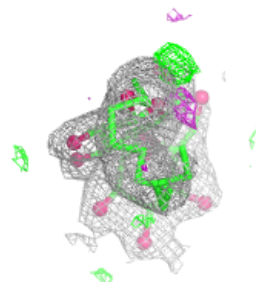
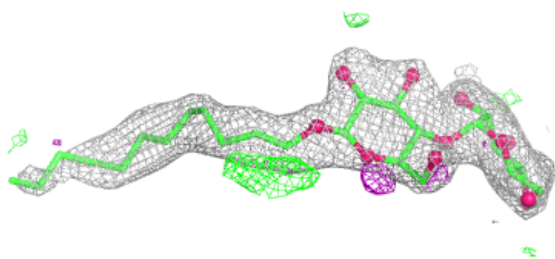
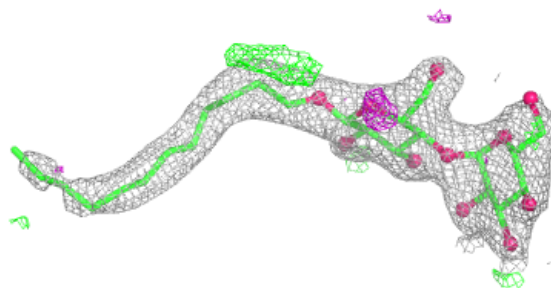


Electron density around SQD F 101:

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

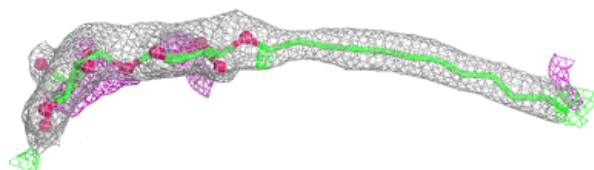
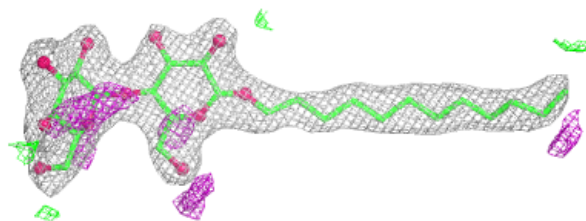
**Electron density around LMT a 402:**

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

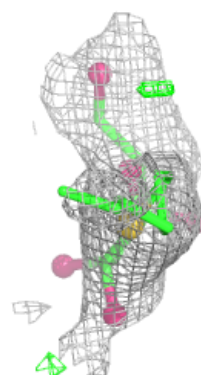
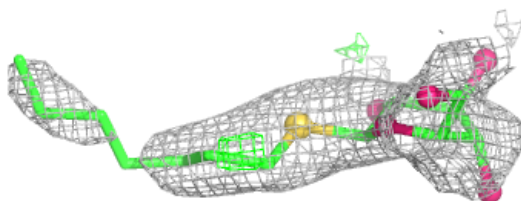


Electron density around LMT m 1502:

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

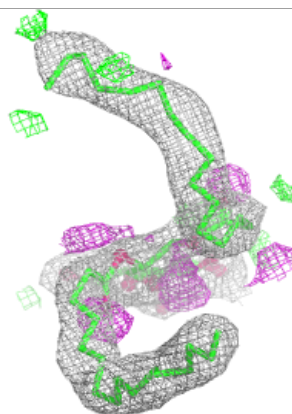
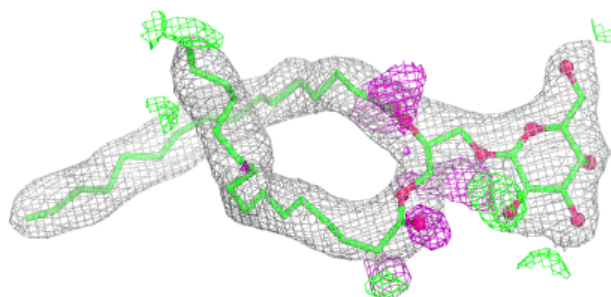
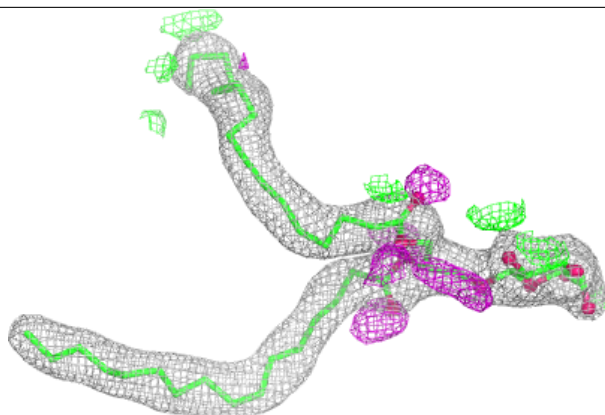
**Electron density around HTG C 528:**

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

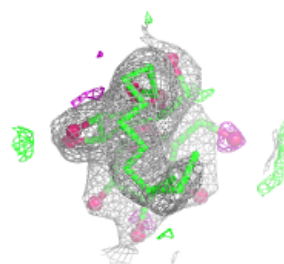
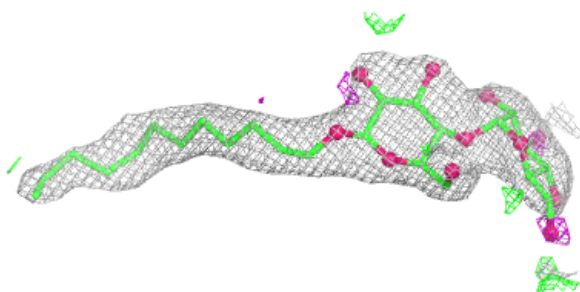
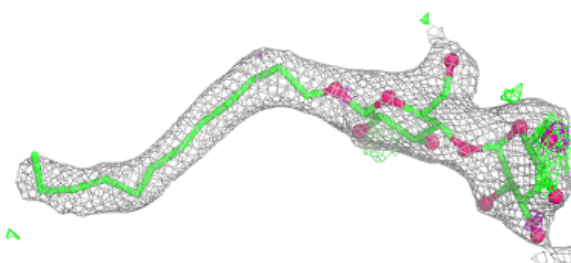


Electron density around LMG b 624:

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

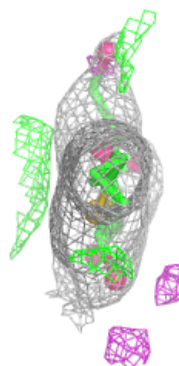
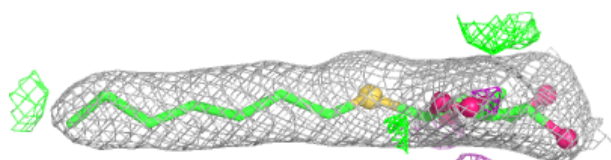
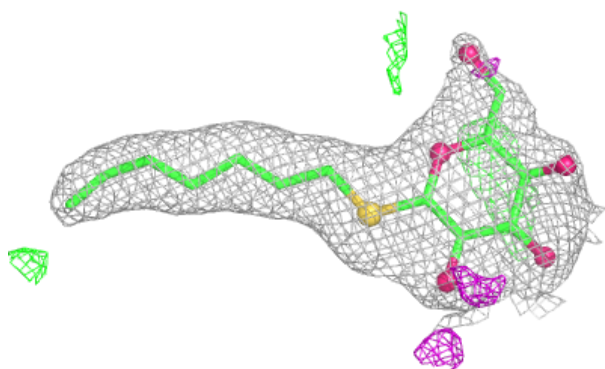
**Electron density around LMT D 401:**

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

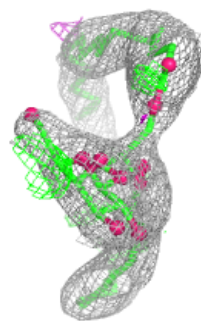
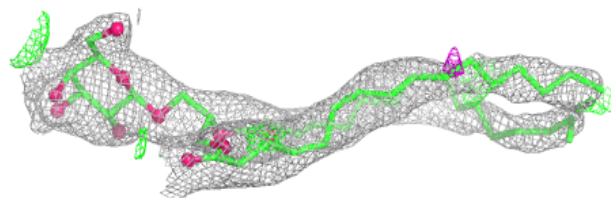
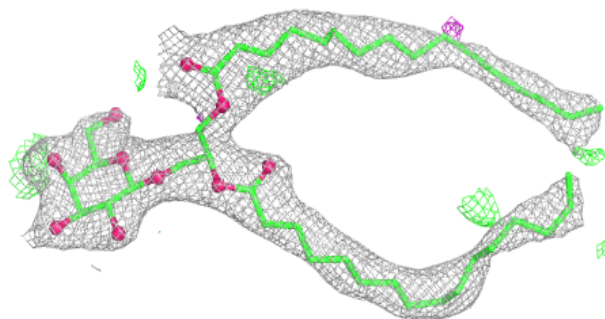


Electron density around HTG b 602:

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

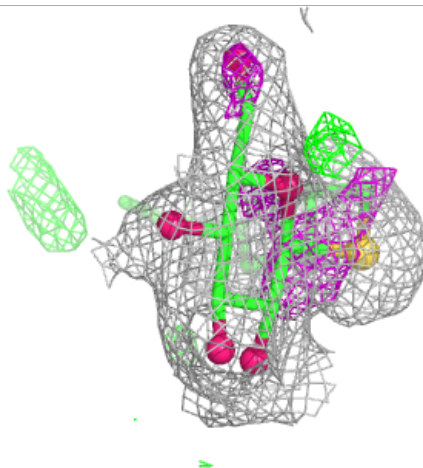
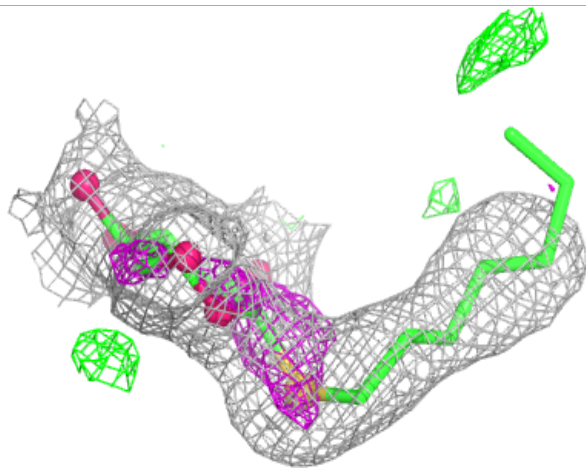
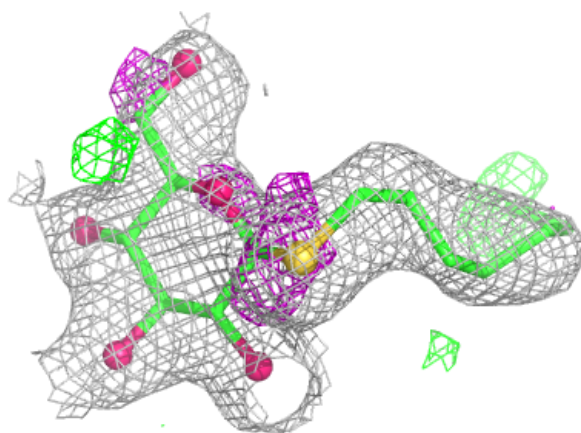
**Electron density around LMG a 416:**

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



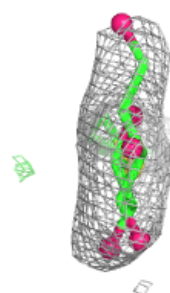
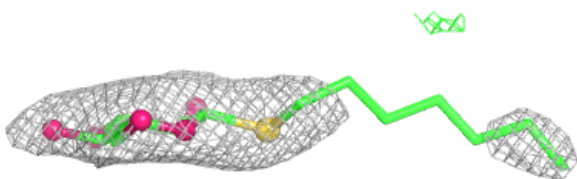
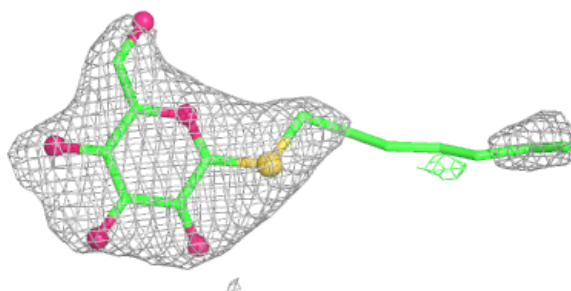
Electron density around HTG b 626:

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



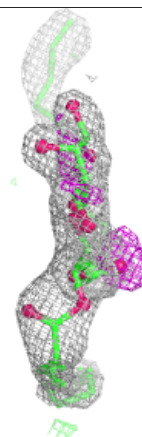
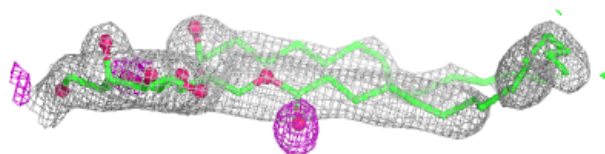
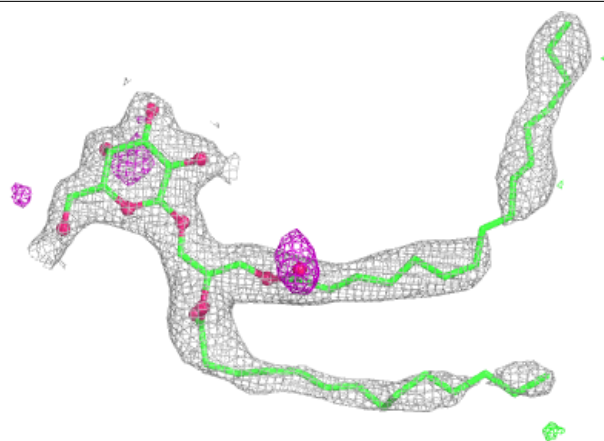
Electron density around HTG C 521:

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

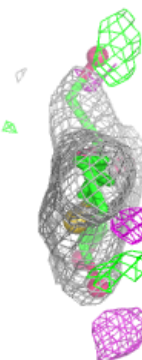
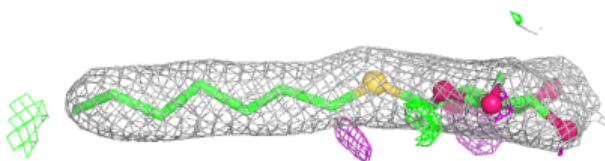
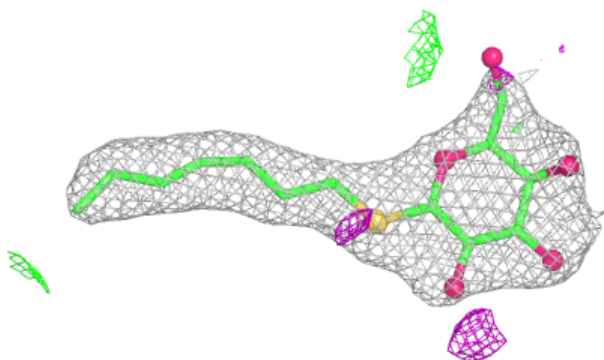


Electron density around LMG C 519:

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

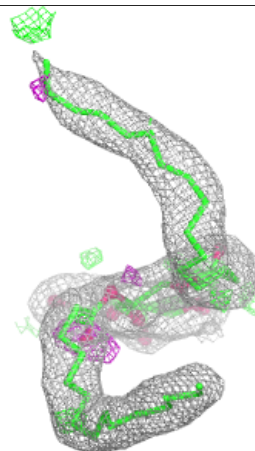
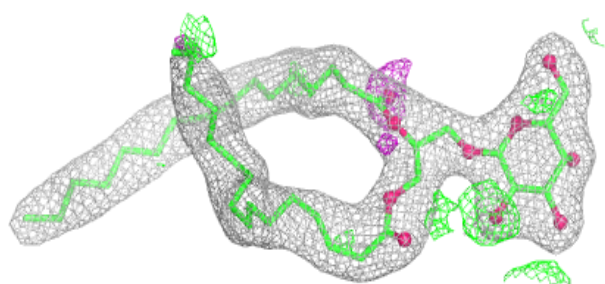
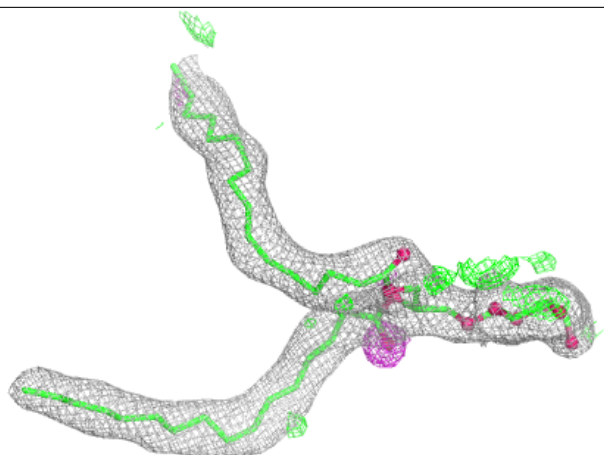
**Electron density around HTG B 626:**

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



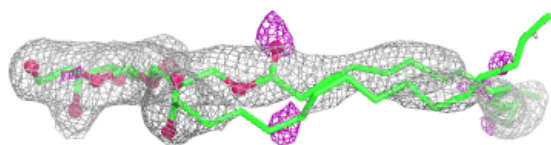
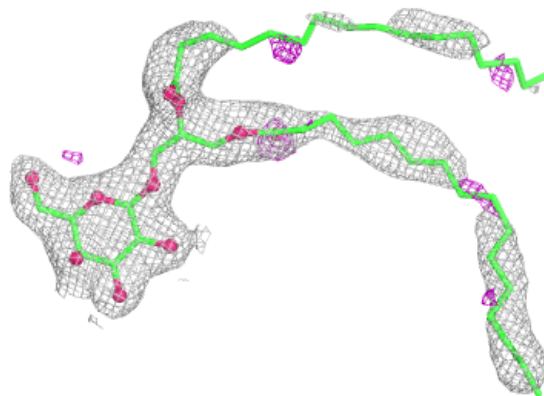
Electron density around LMG B 622:

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

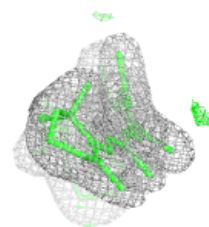
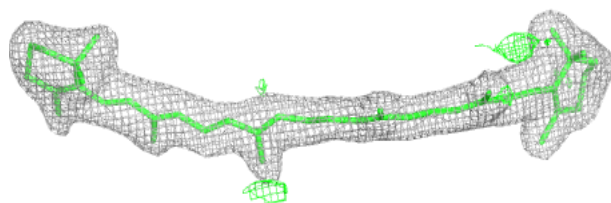
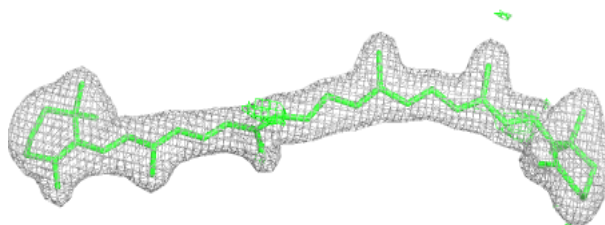


Electron density around LMG c 920:

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

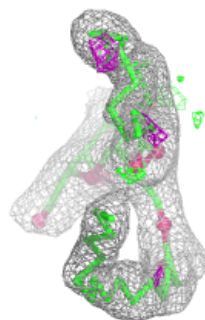
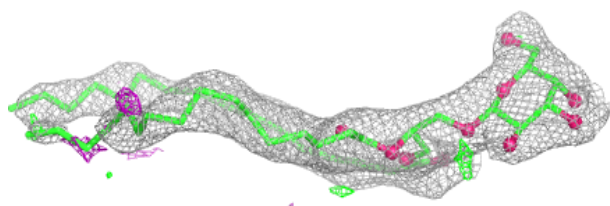
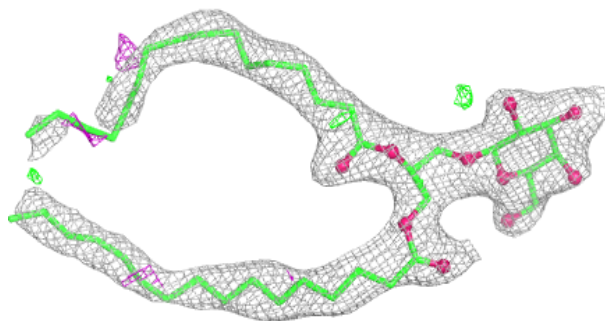
**Electron density around BCR t 903:**

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



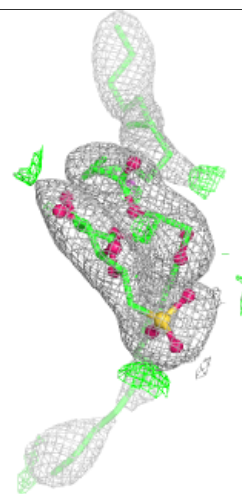
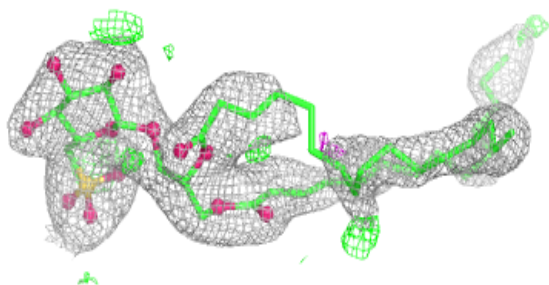
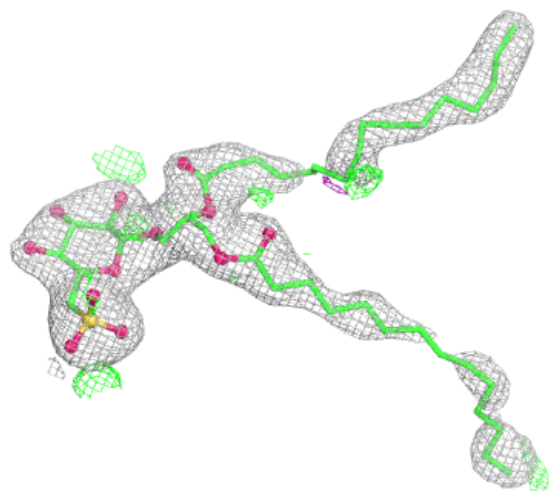
Electron density around LMG A 413:

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



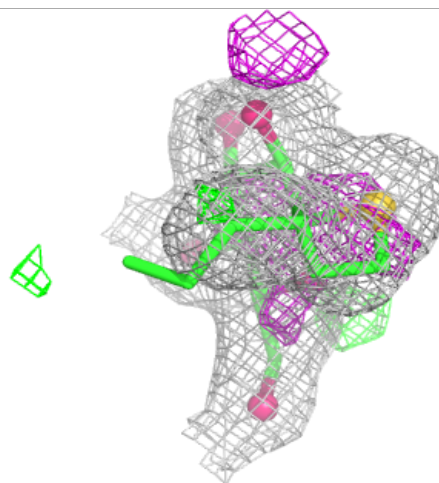
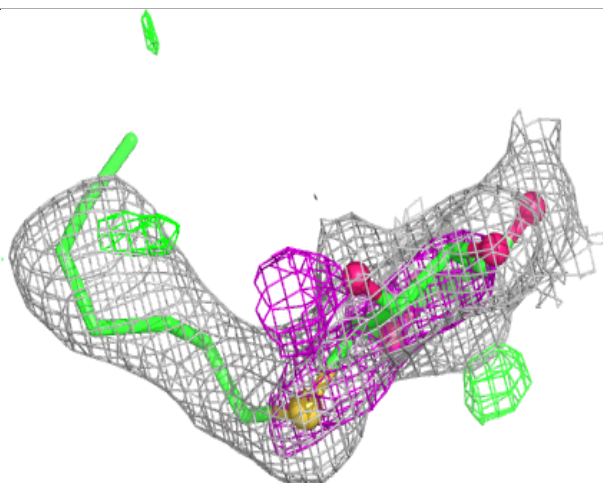
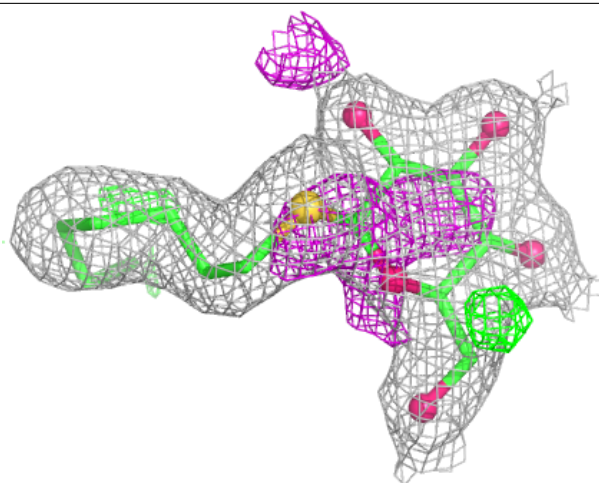
Electron density around SQD A 412:

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



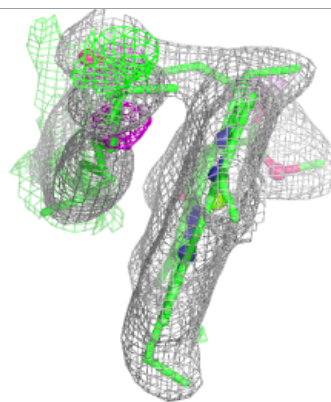
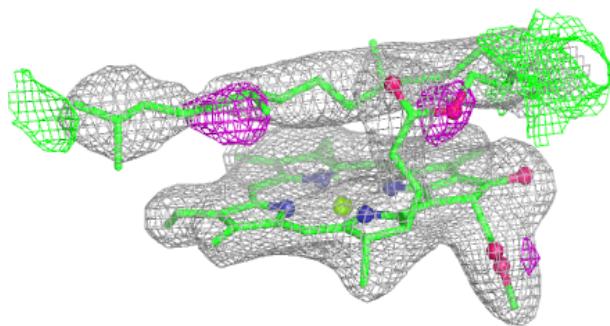
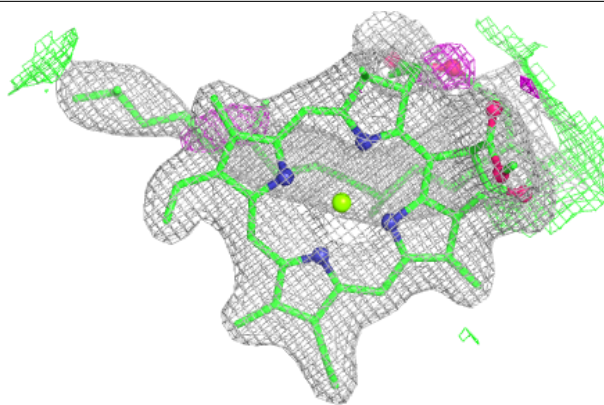
Electron density around HTG B 624:

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

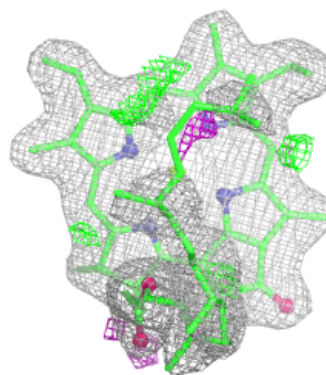
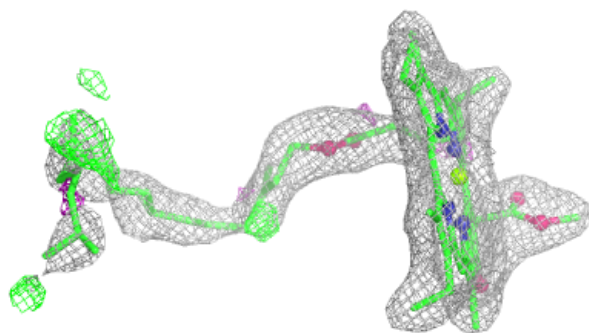
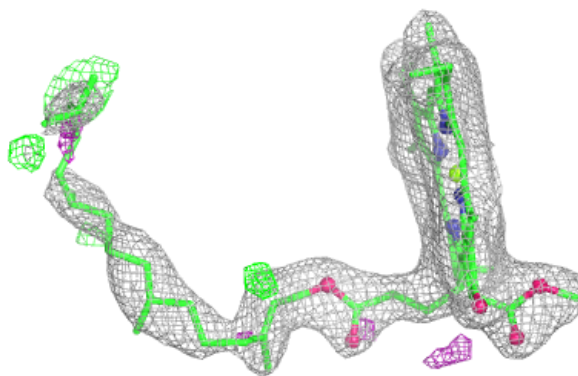


Electron density around CLA B 602:

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

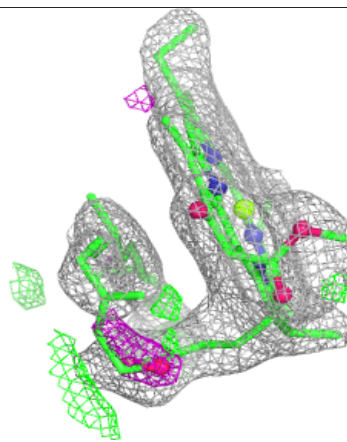
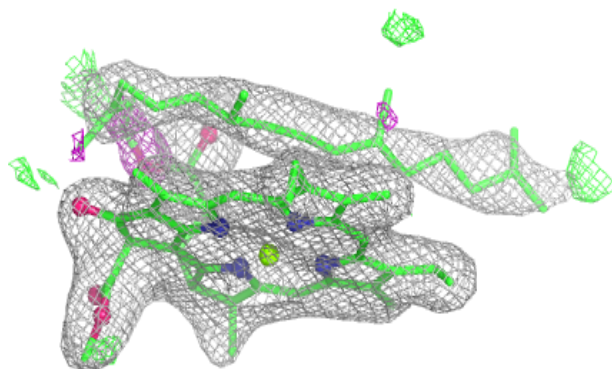
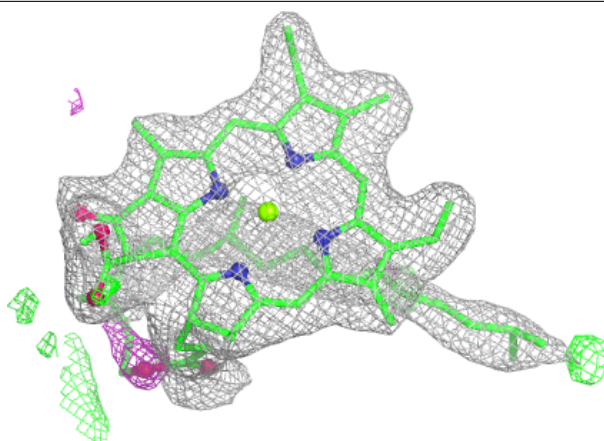
**Electron density around CLA C 506:**

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

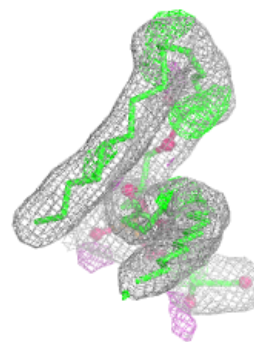
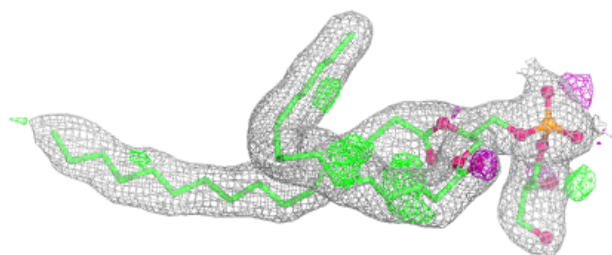
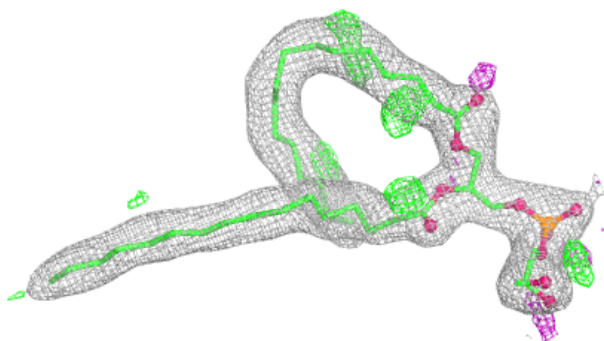


Electron density around CLA b 605:

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

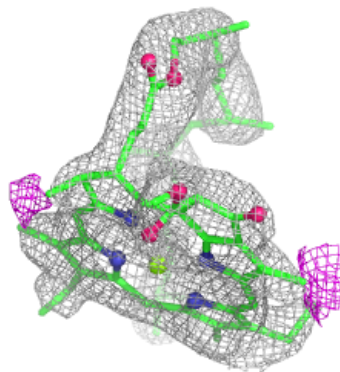
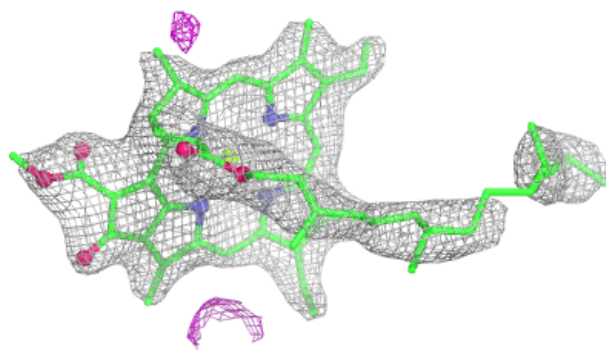
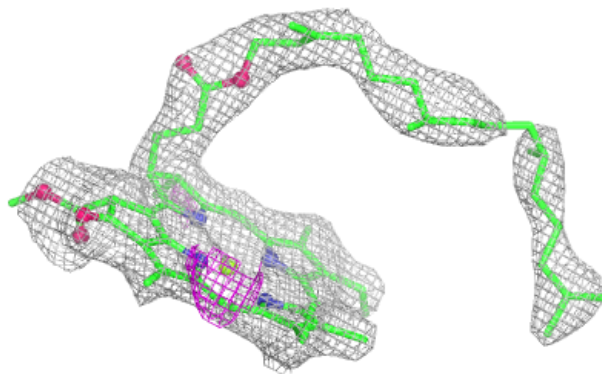
**Electron density around LHG D 407:**

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

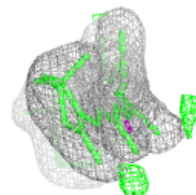
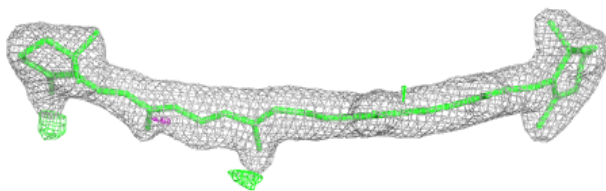
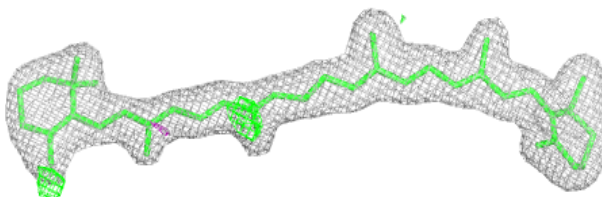


Electron density around CLA c 914:

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

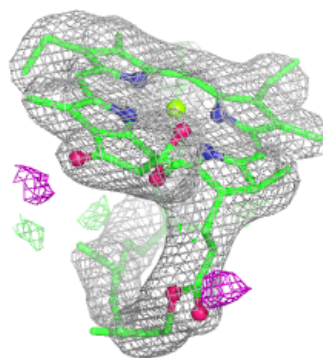
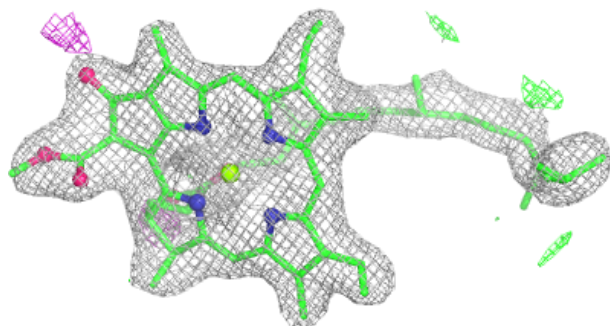
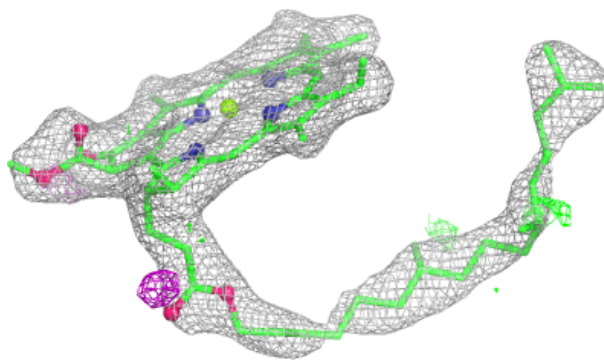
**Electron density around BCR T 702:**

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



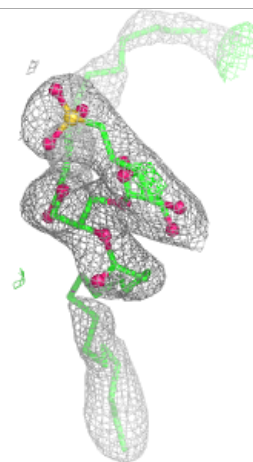
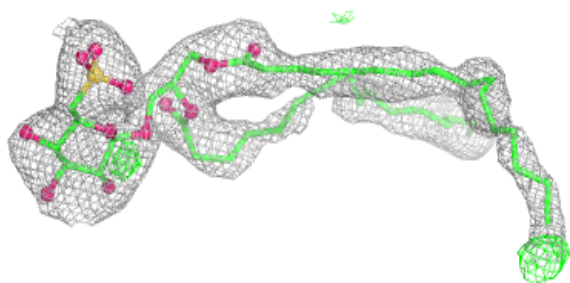
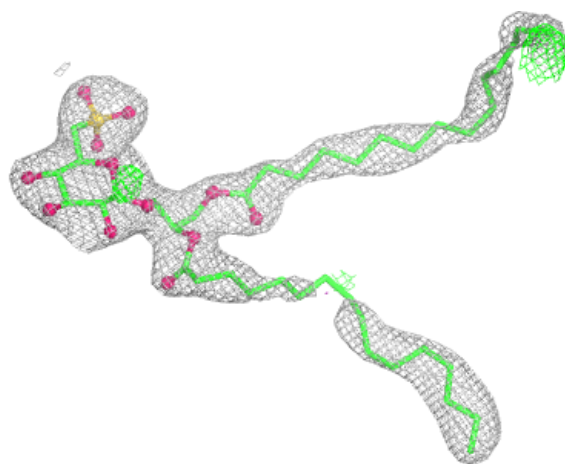
Electron density around CLA C 513:

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



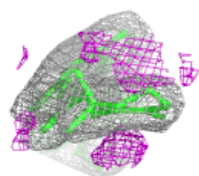
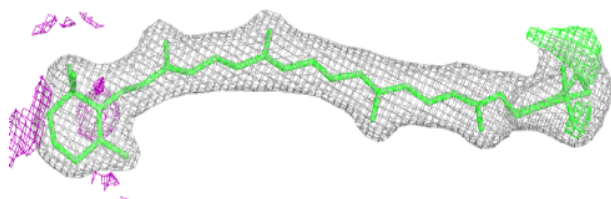
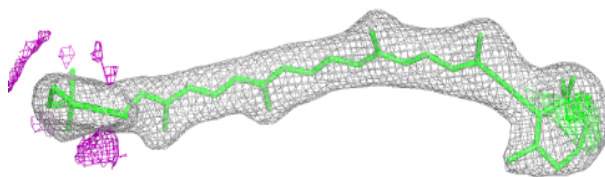
Electron density around SQD a 415:

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



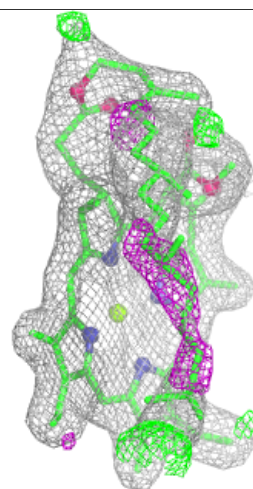
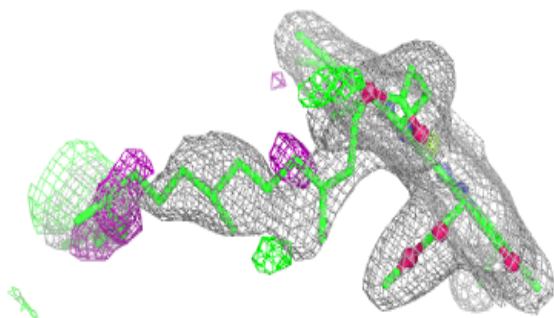
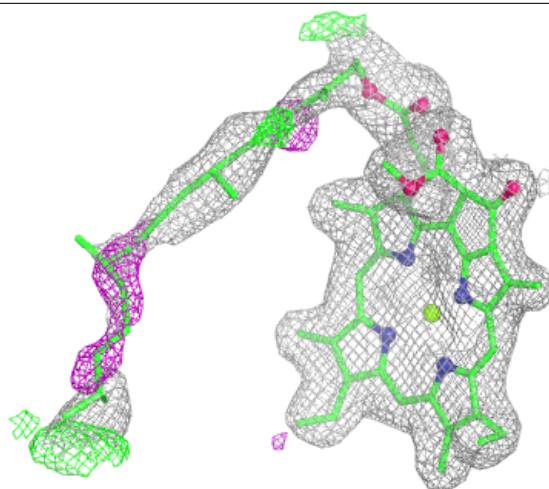
Electron density around BCR d 406:

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



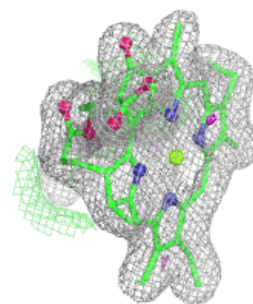
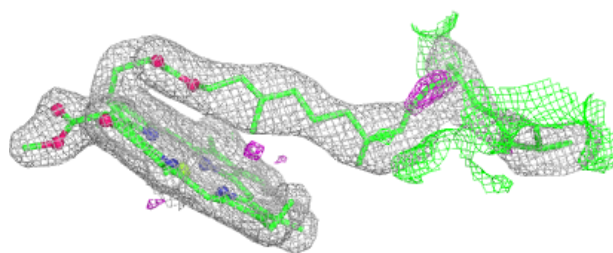
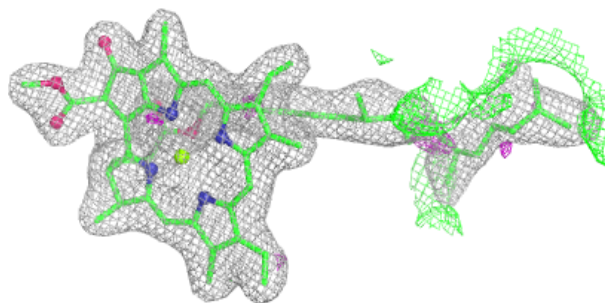
Electron density around CLA B 617:

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



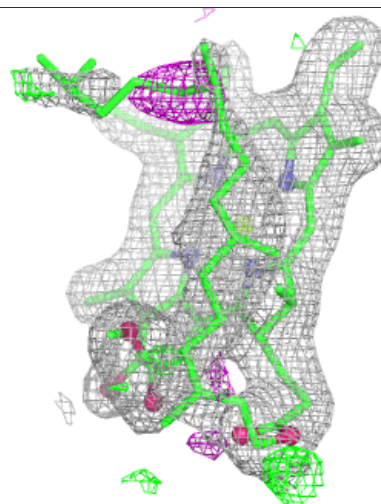
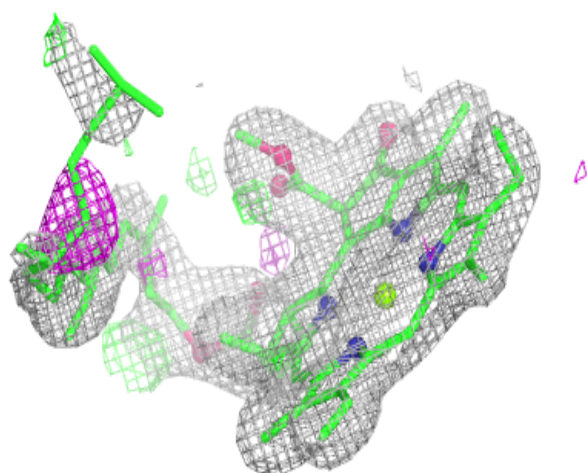
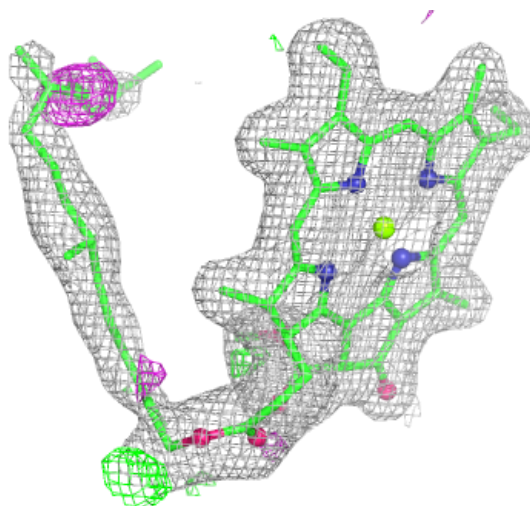
Electron density around CLA b 618:

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



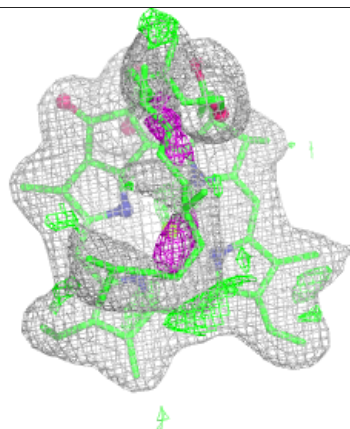
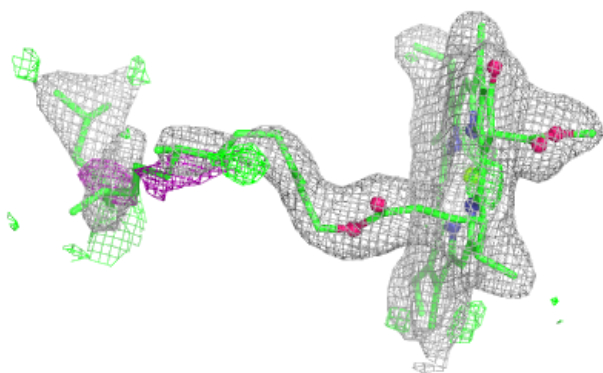
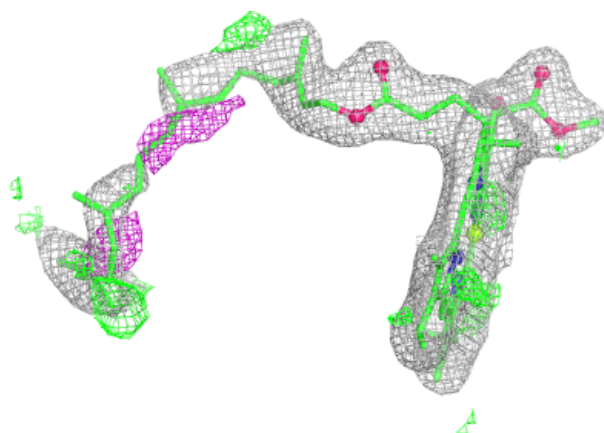
Electron density around CLA b 620:

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

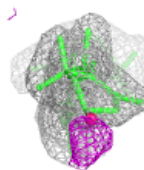
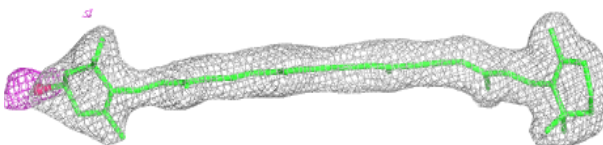
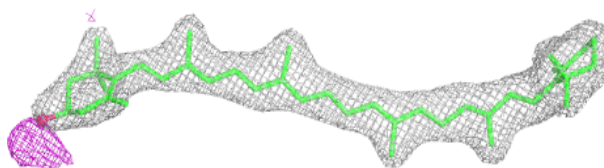


Electron density around CLA c 907:

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

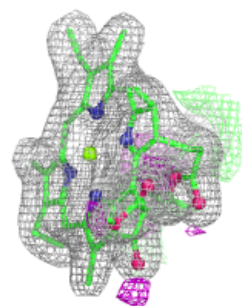
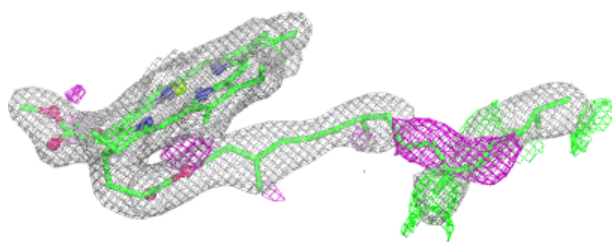
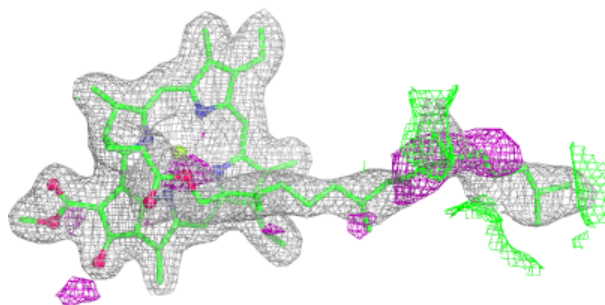
**Electron density around RRX h 101:**

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



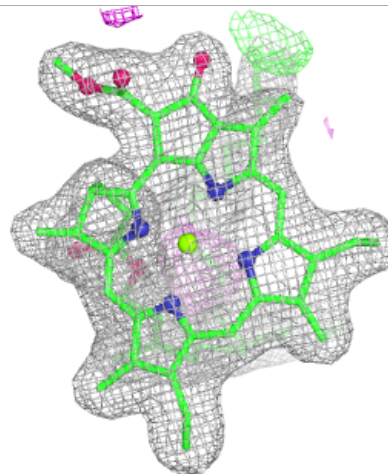
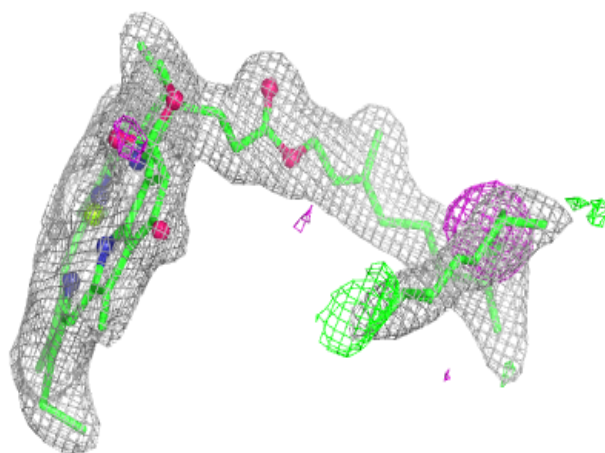
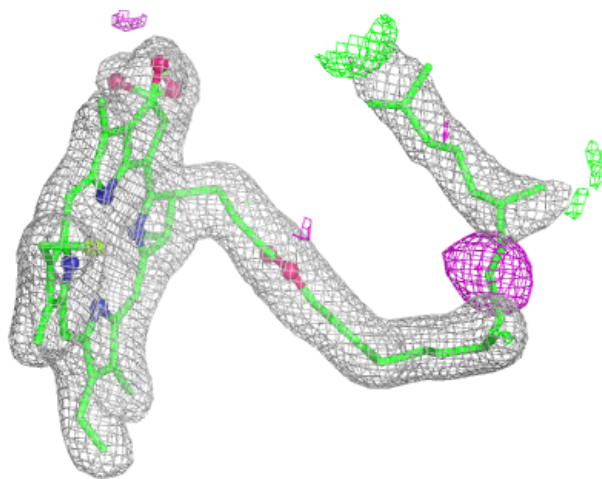
Electron density around CLA B 615:

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



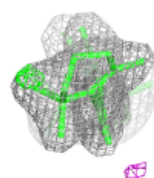
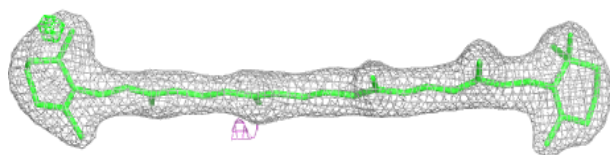
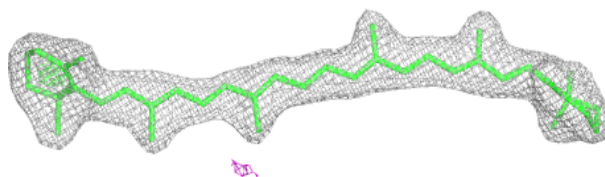
Electron density around CLA b 610:

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

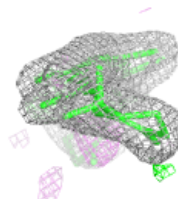
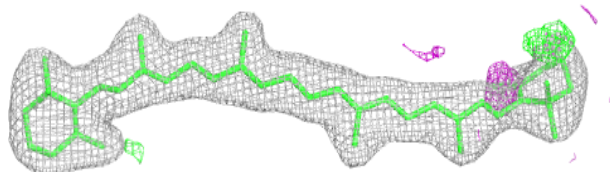
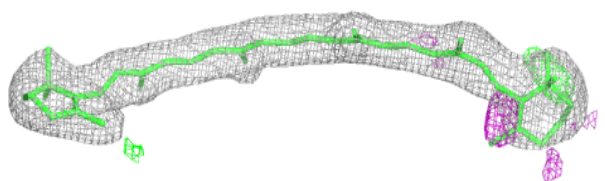


Electron density around BCR C 514:

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

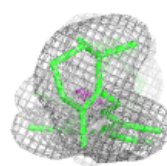
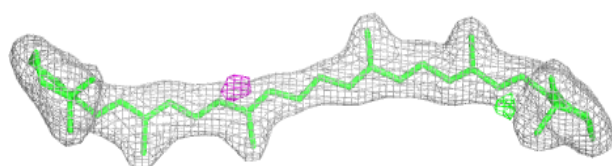
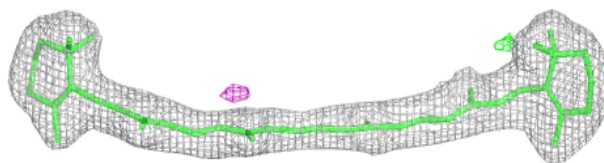
**Electron density around BCR D 404:**

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

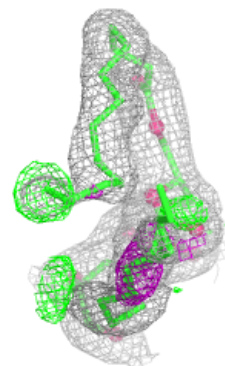
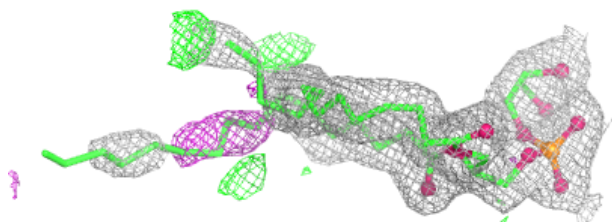
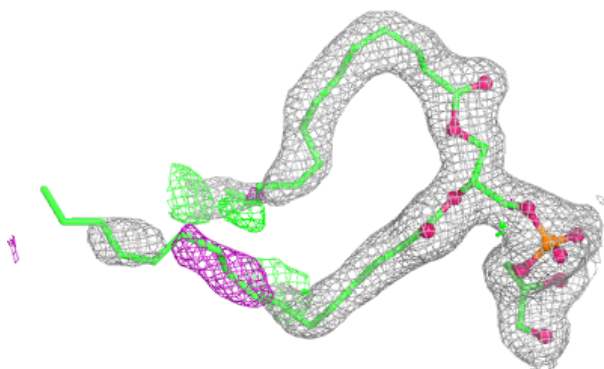


Electron density around BCR K 101:

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

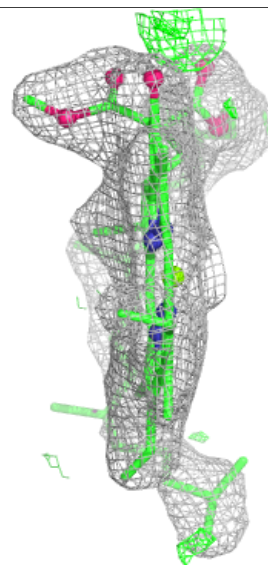
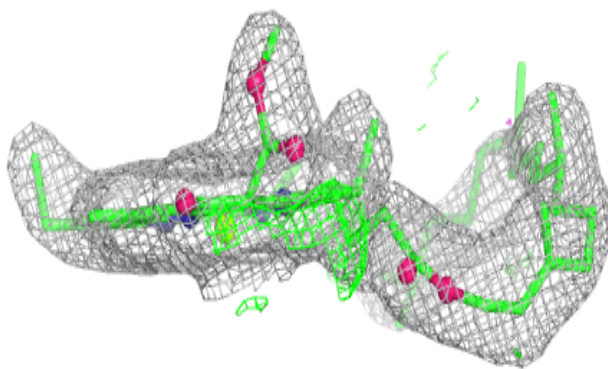
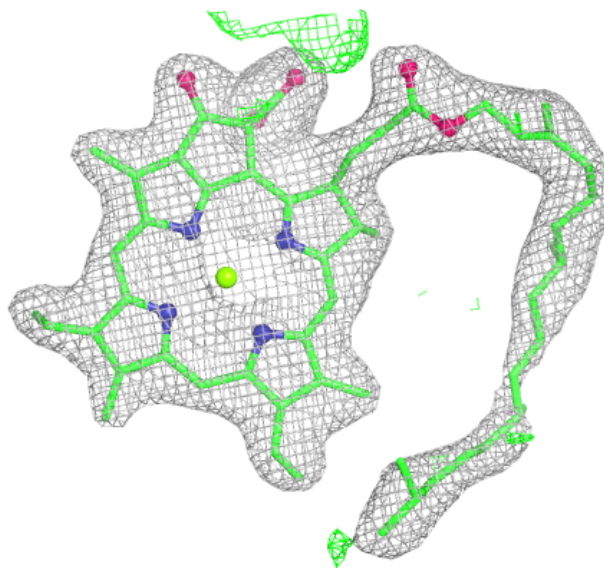
**Electron density around LHG D 409:**

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



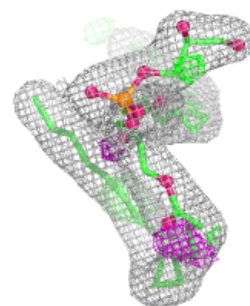
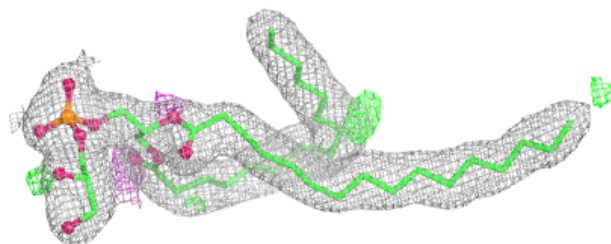
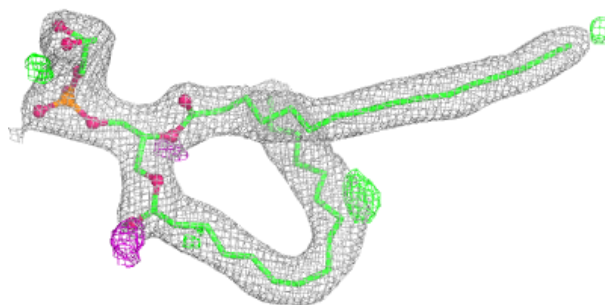
Electron density around CLA C 512:

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

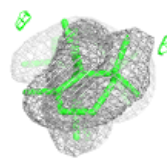
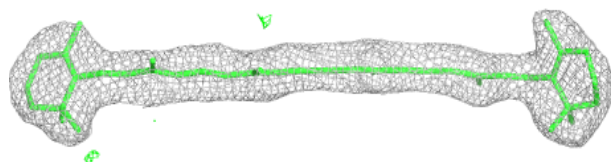
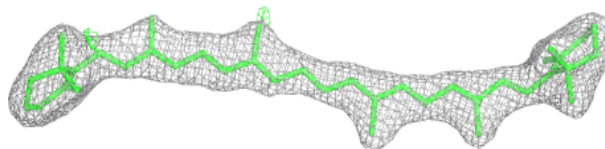


Electron density around LHG d 408:

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

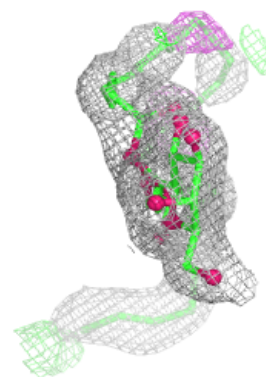
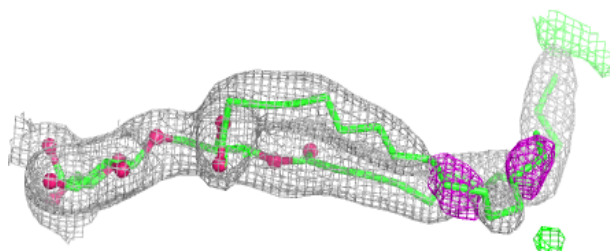
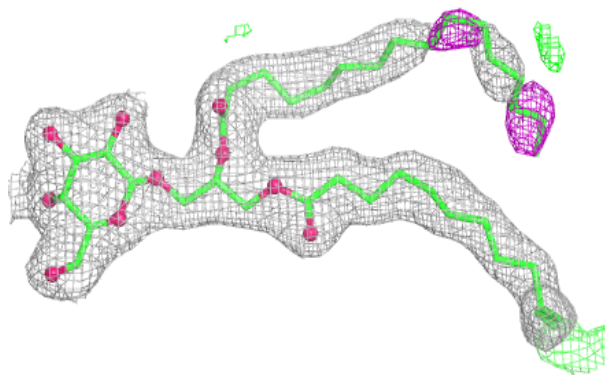
**Electron density around BCR c 915:**

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



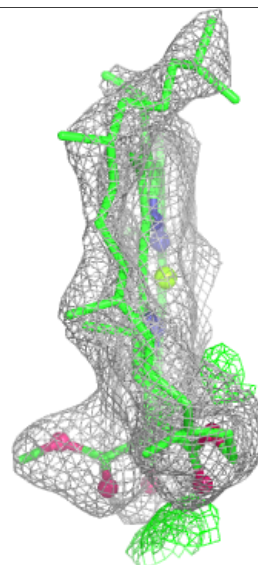
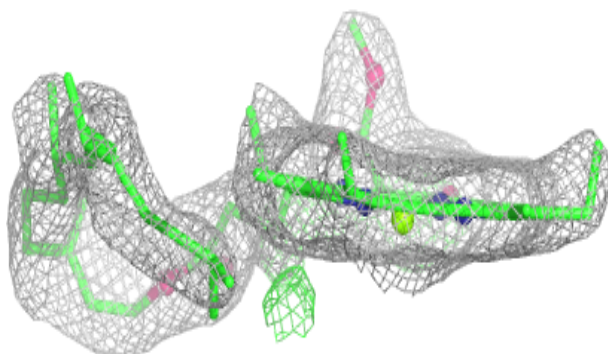
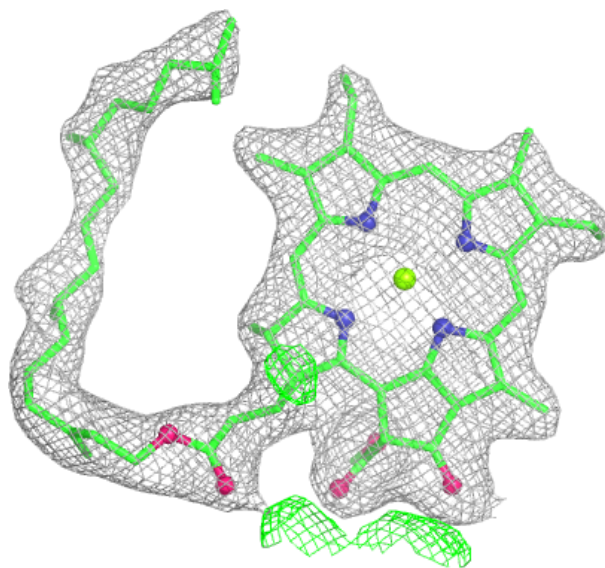
Electron density around LMG D 410:

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



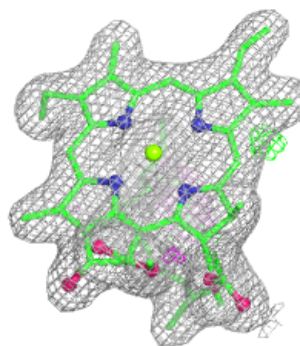
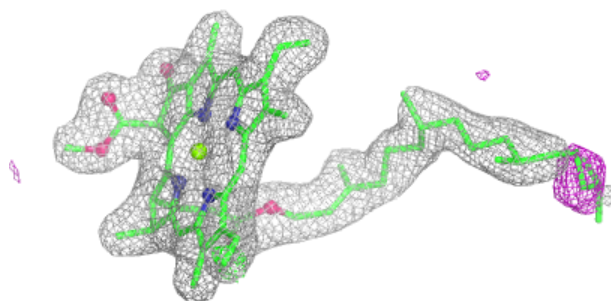
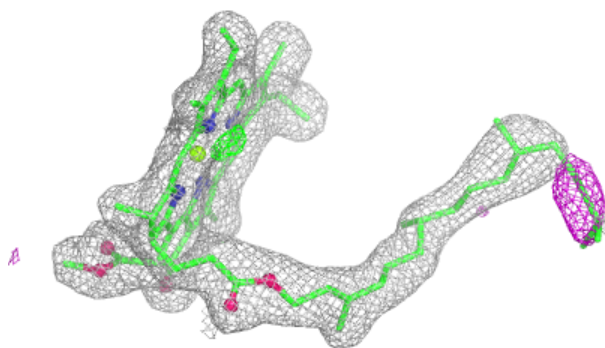
Electron density around CLA c 913:

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

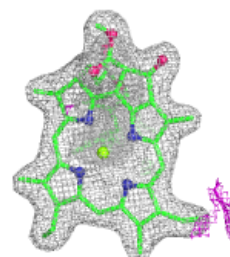
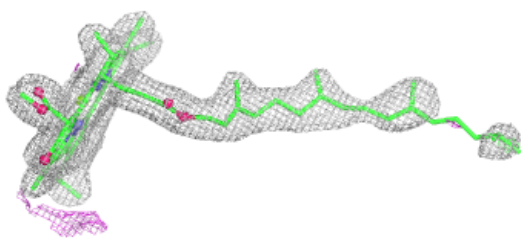
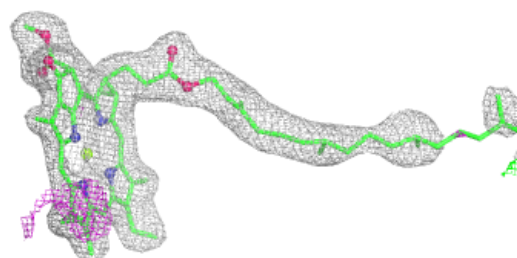


Electron density around CLA C 508:

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

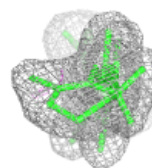
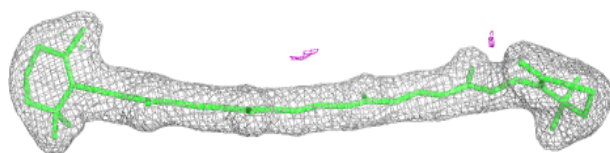
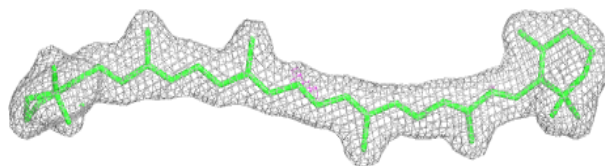
**Electron density around CLA d 405:**

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

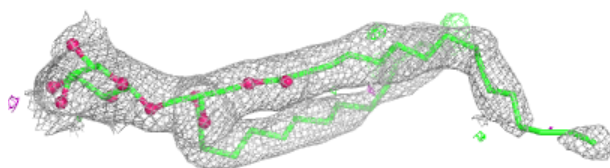
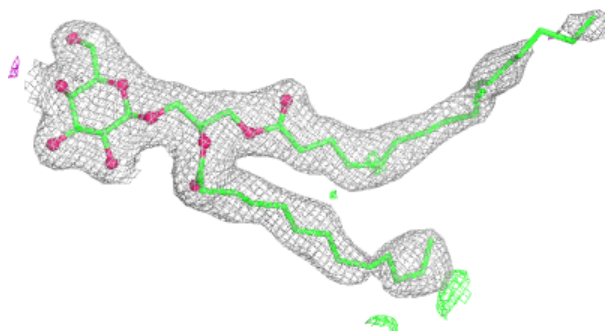


Electron density around BCR B 618:

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

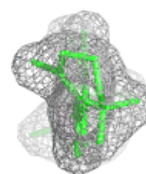
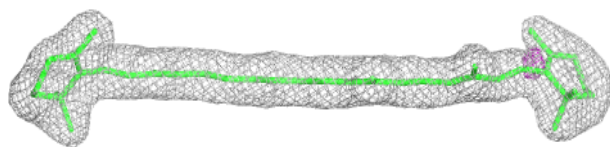
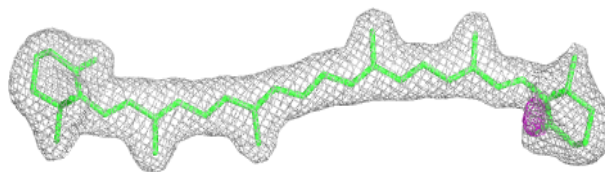
**Electron density around LMG d 411:**

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



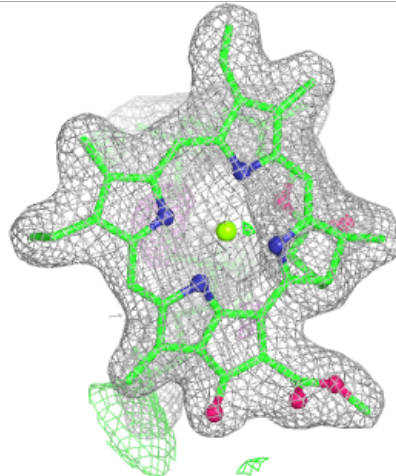
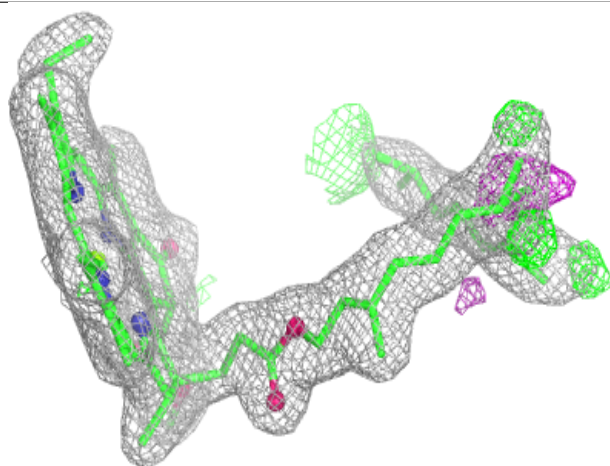
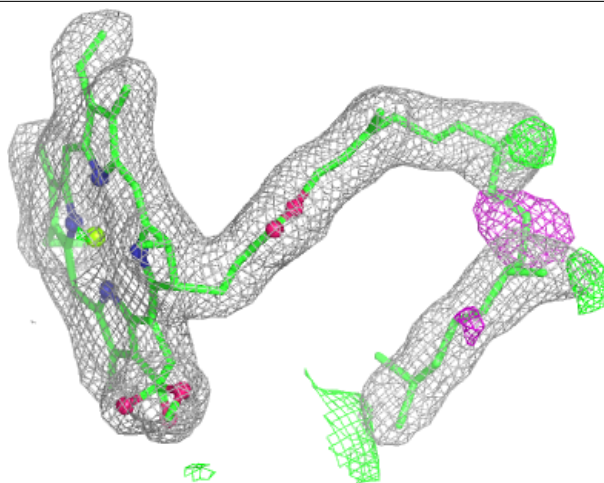
Electron density around BCR B 619:

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



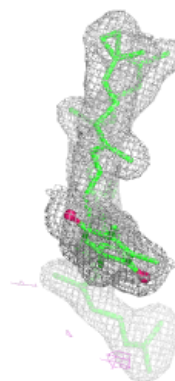
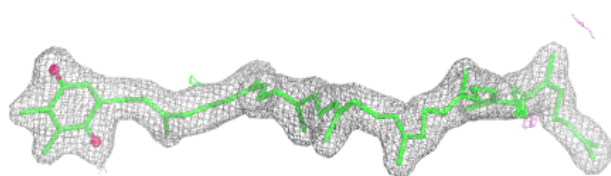
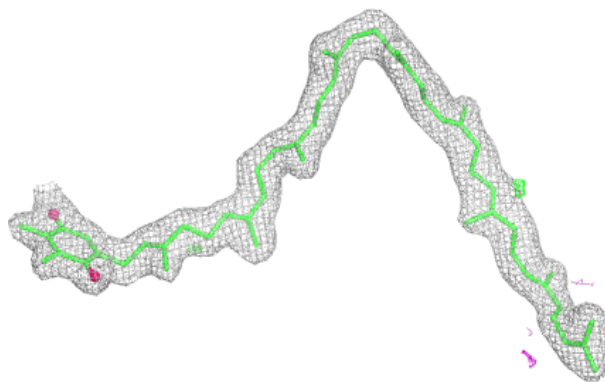
Electron density around CLA B 607:

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

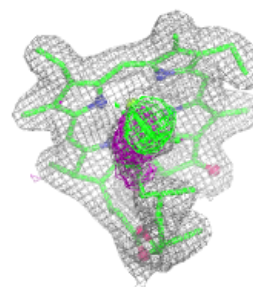
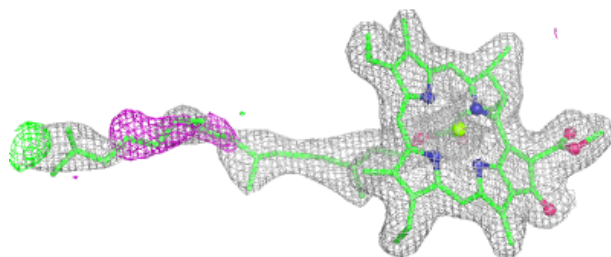
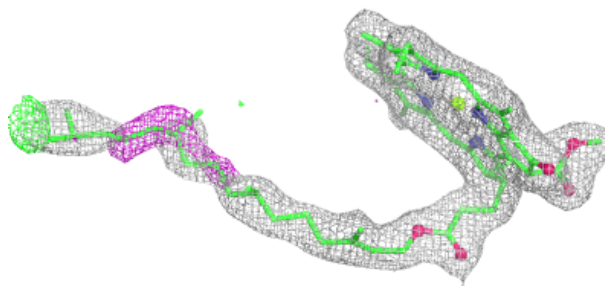


Electron density around PL9 d 407:

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

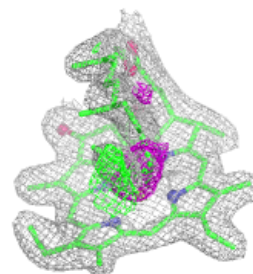
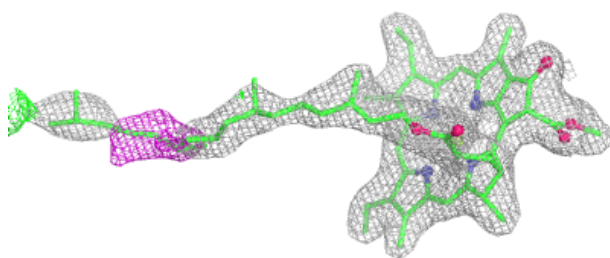
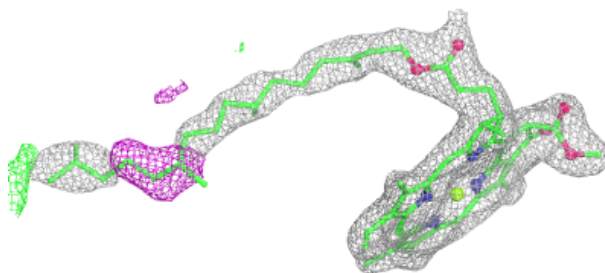
**Electron density around CLA C 504:**

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

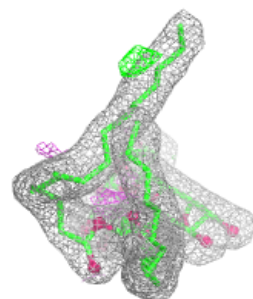
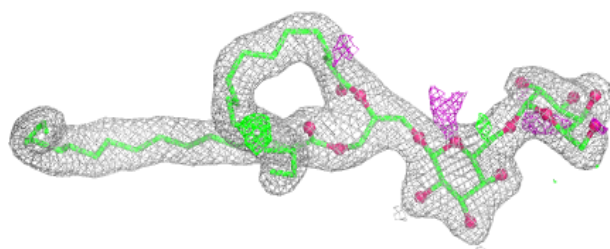
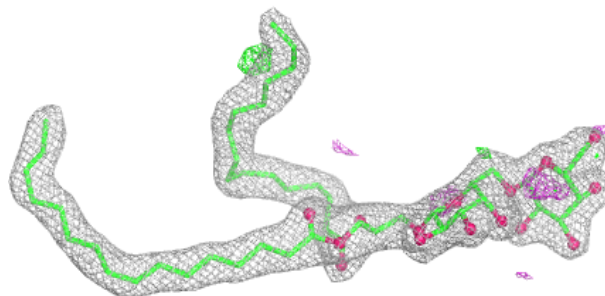


Electron density around CLA c 905:

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

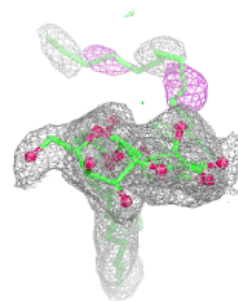
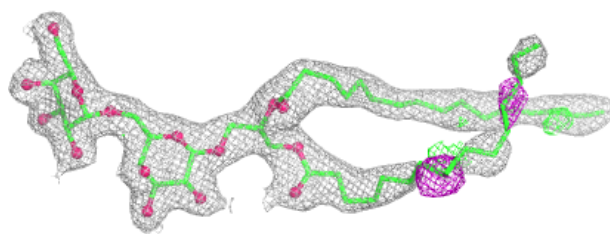
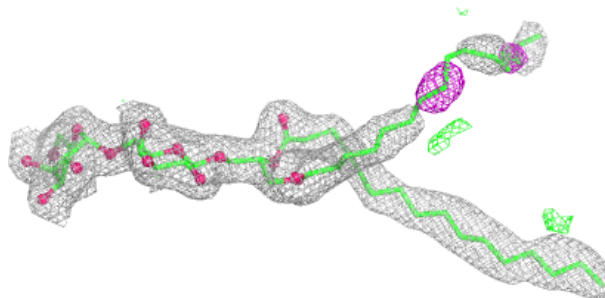
**Electron density around DGD H 103:**

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

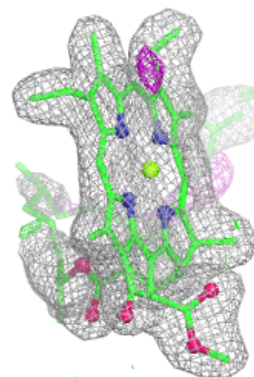
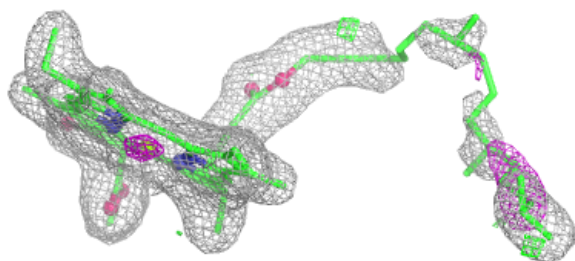
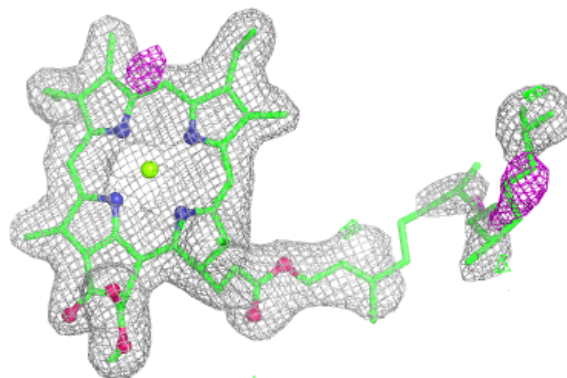


Electron density around DGD c 917:

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

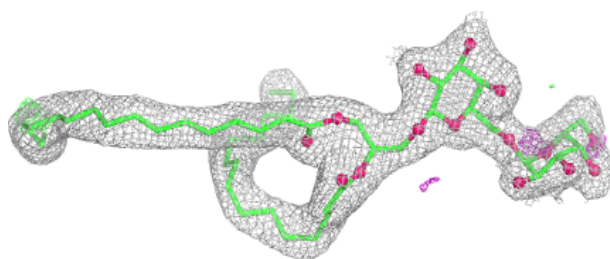
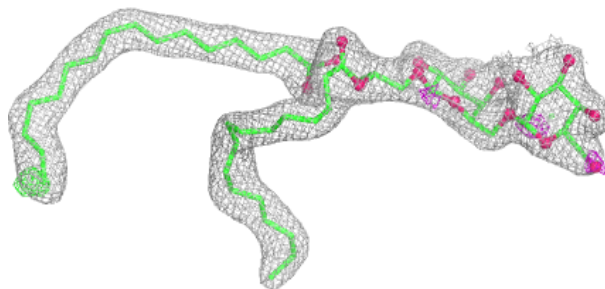
**Electron density around CLA a 413:**

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

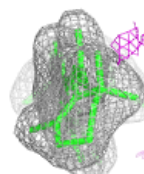
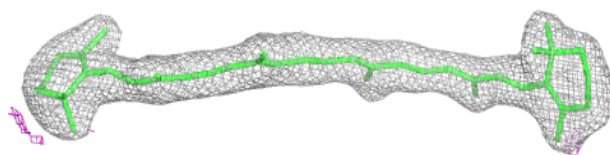
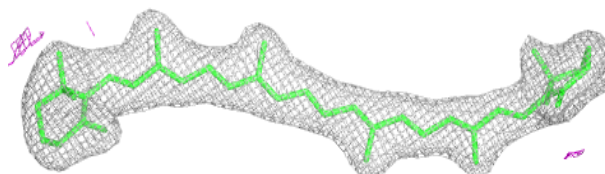


Electron density around DGD h 102:

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

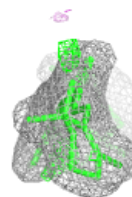
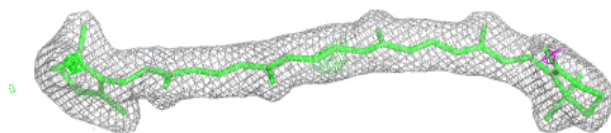
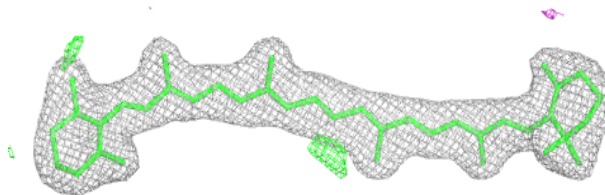
**Electron density around BCR Y 101:**

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



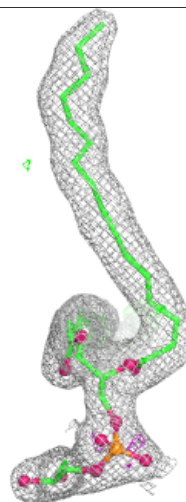
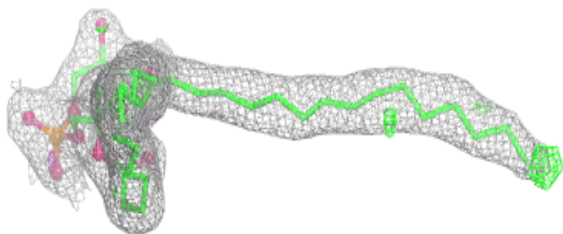
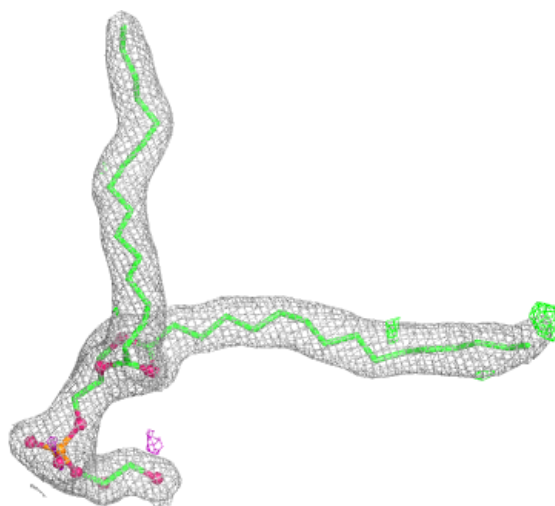
Electron density around BCR b 623:

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



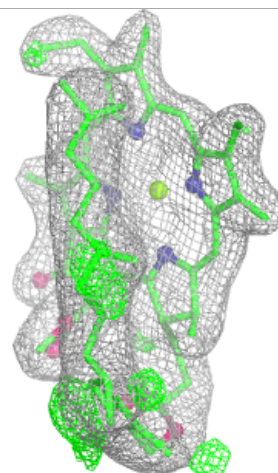
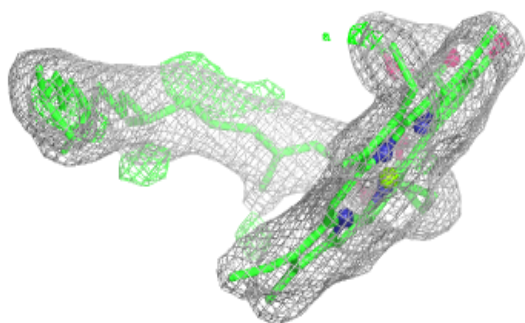
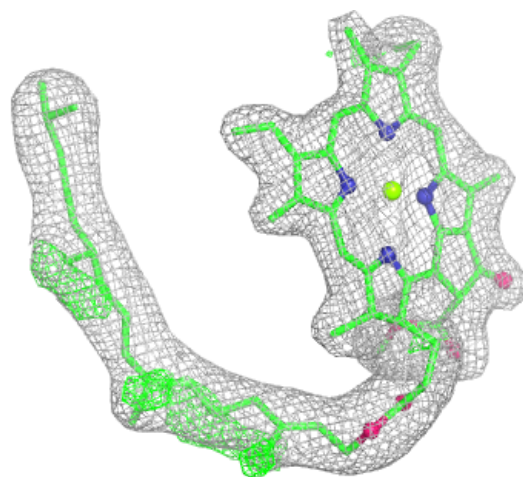
Electron density around LHG b 639:

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



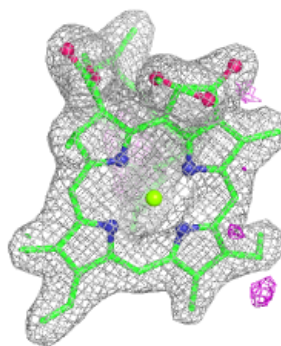
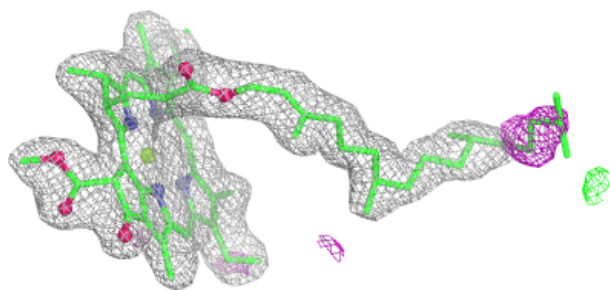
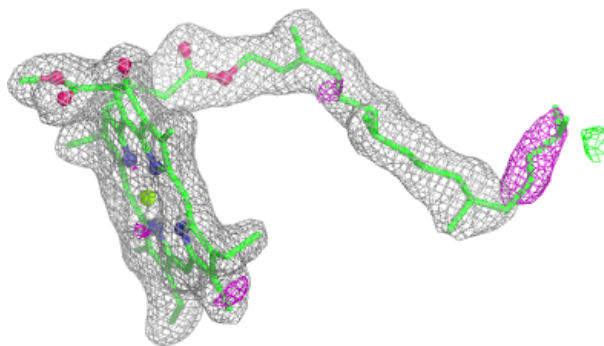
Electron density around CLA c 908:

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

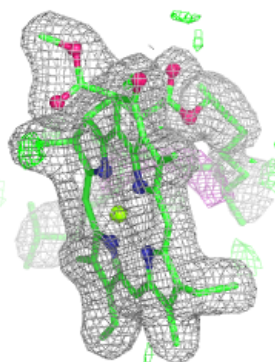
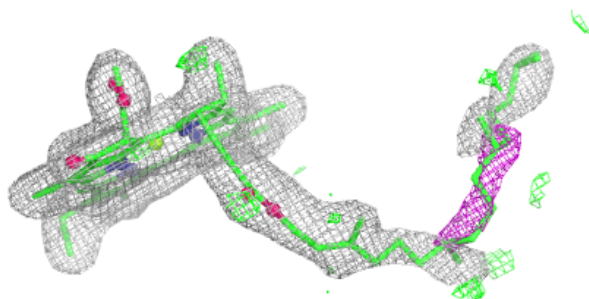
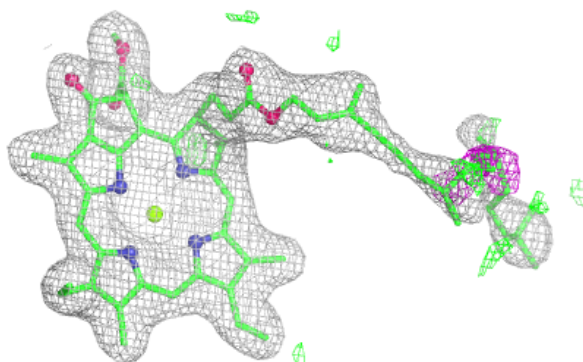


Electron density around CLA c 909:

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

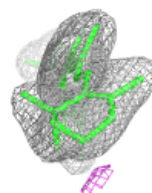
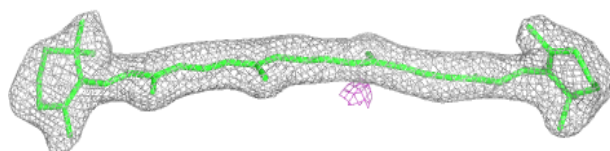
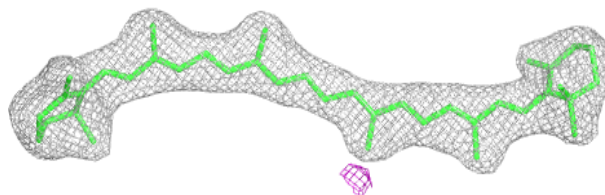
**Electron density around CLA A 410:**

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

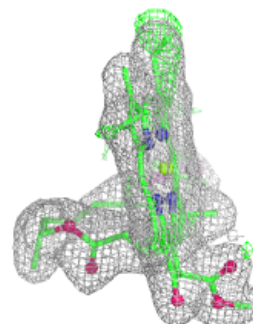
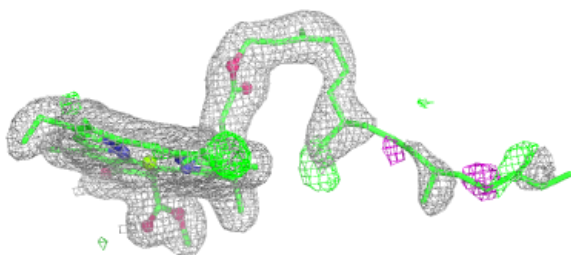
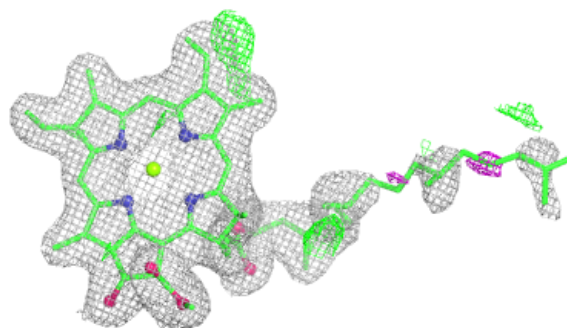


Electron density around BCR y 101:

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

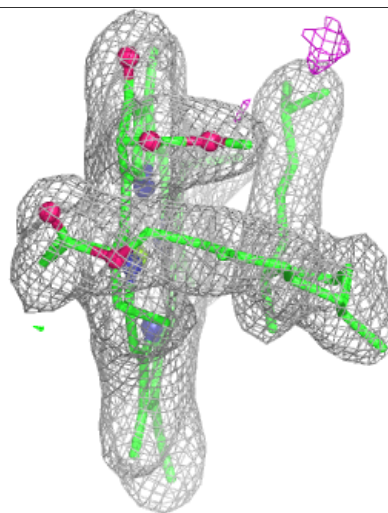
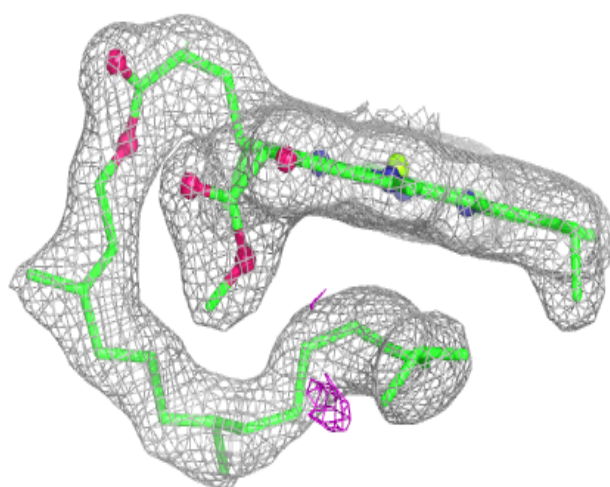
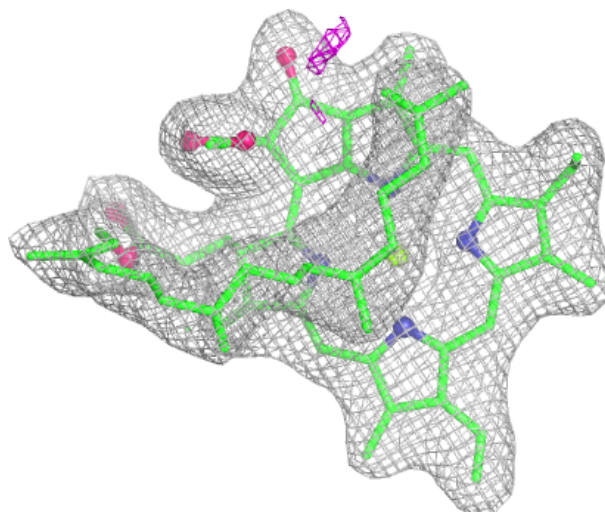
**Electron density around CLA a 410:**

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



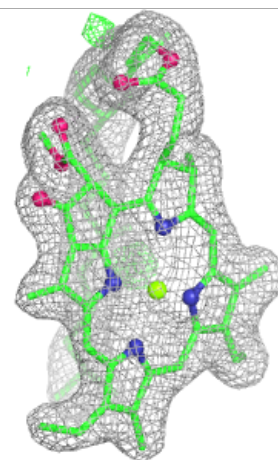
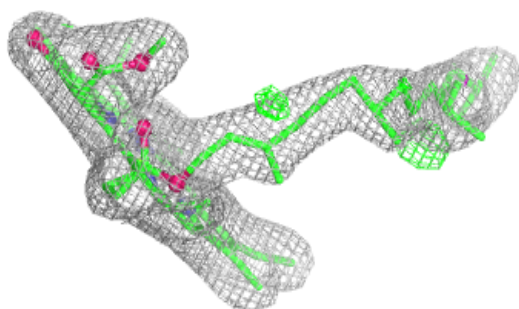
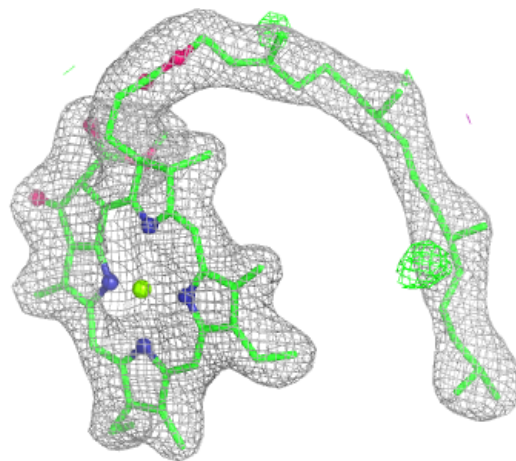
Electron density around CLA c 911:

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



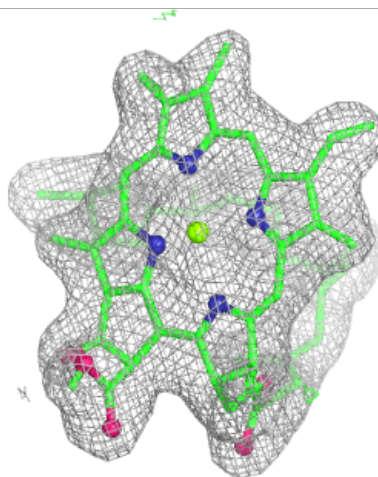
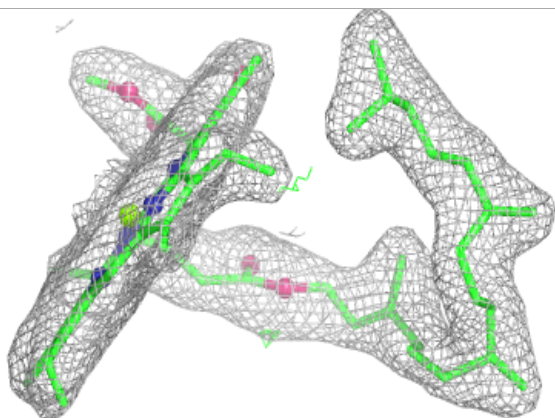
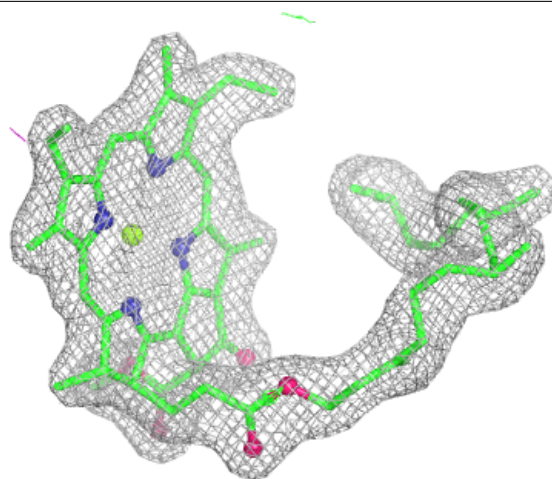
Electron density around CLA C 507:

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



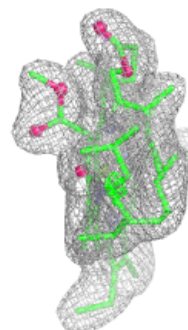
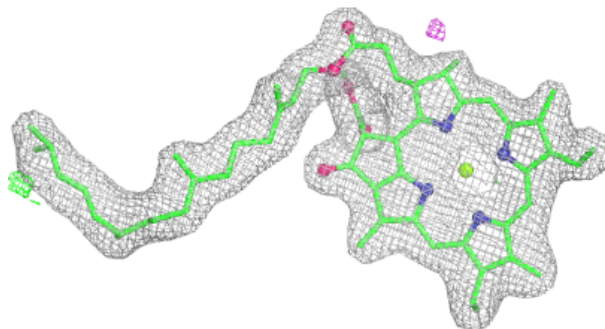
Electron density around CLA C 503:

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



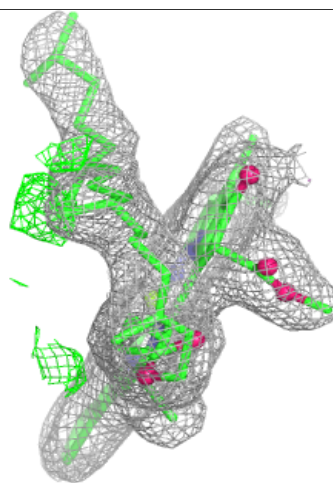
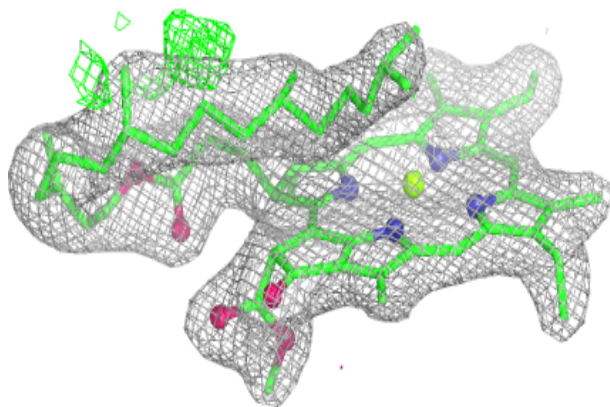
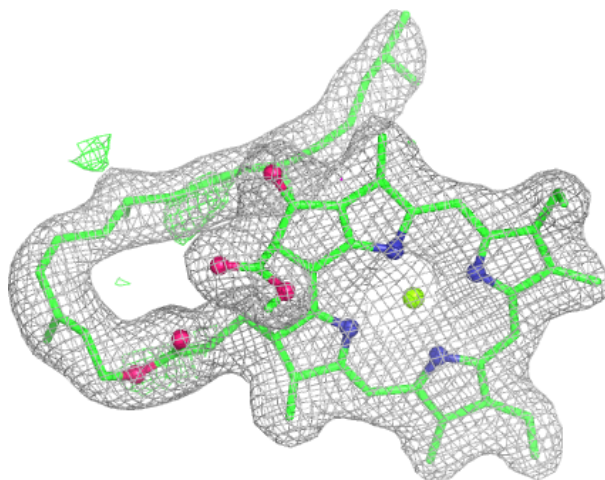
Electron density around CLA b 606:

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



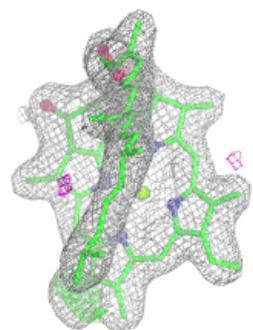
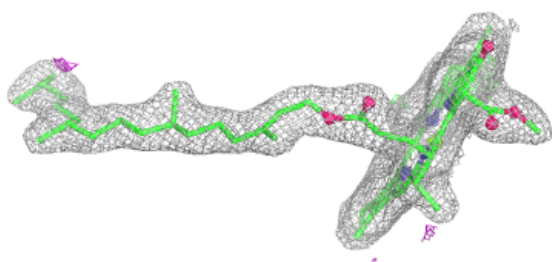
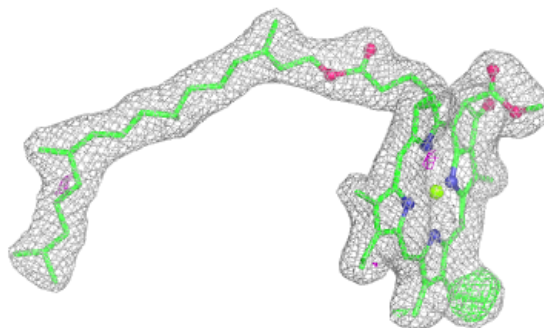
Electron density around CLA C 509:

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

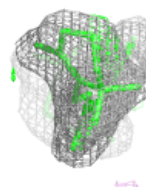
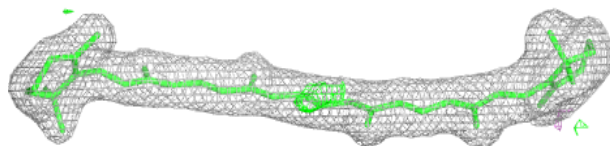
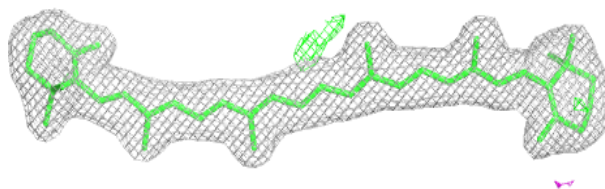


Electron density around CLA b 613:

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

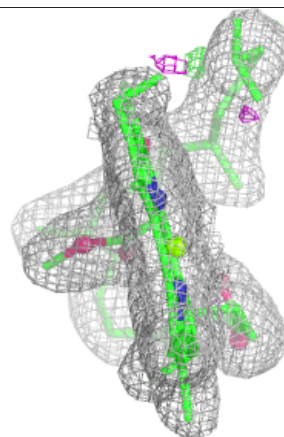
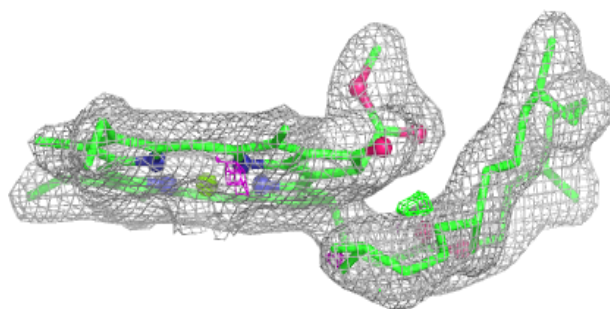
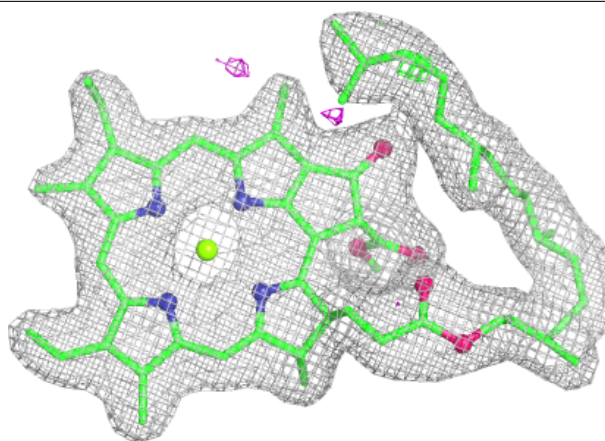
**Electron density around BCR B 620:**

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

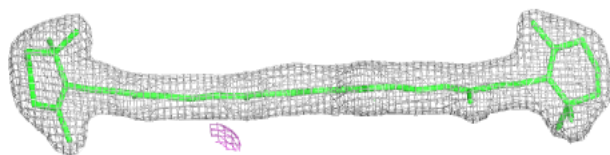
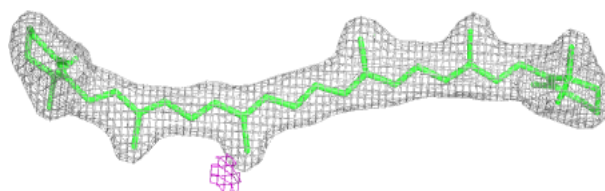


Electron density around CLA b 614:

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

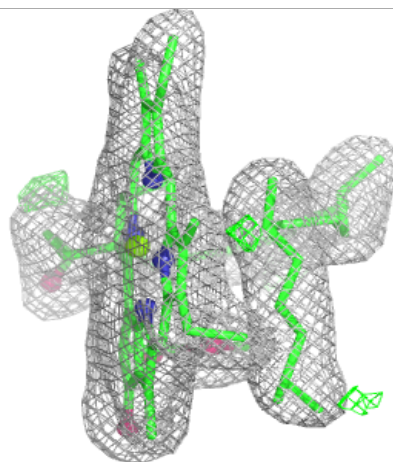
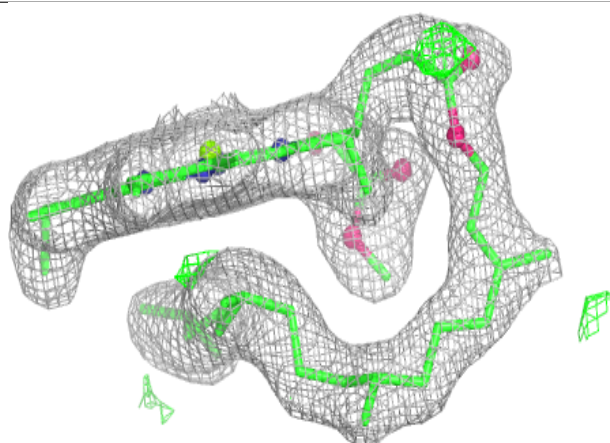
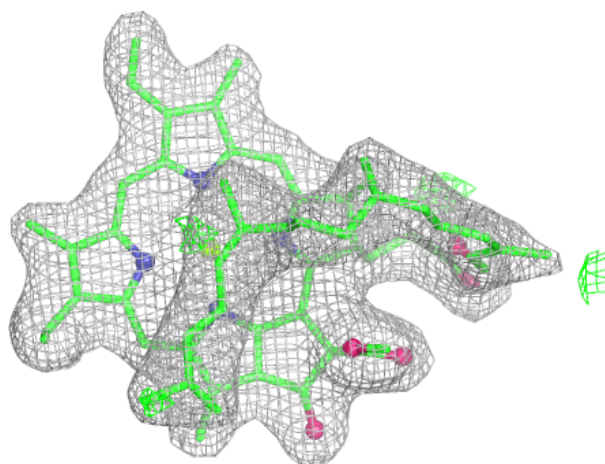
**Electron density around BCR C 515:**

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



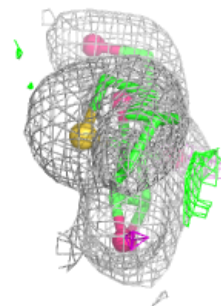
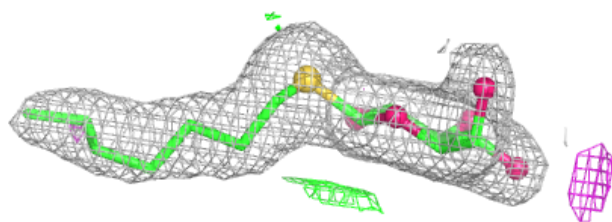
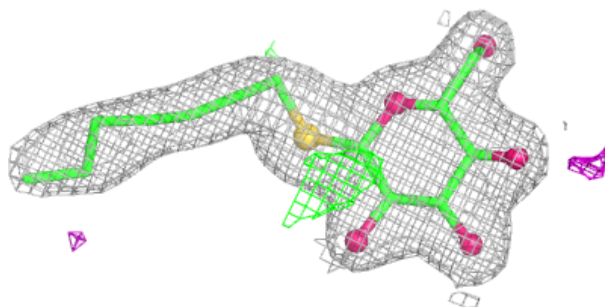
Electron density around CLA C 510:

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



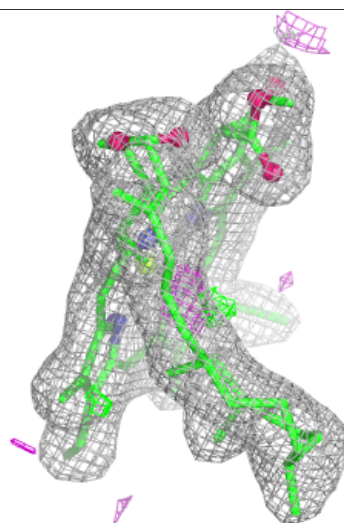
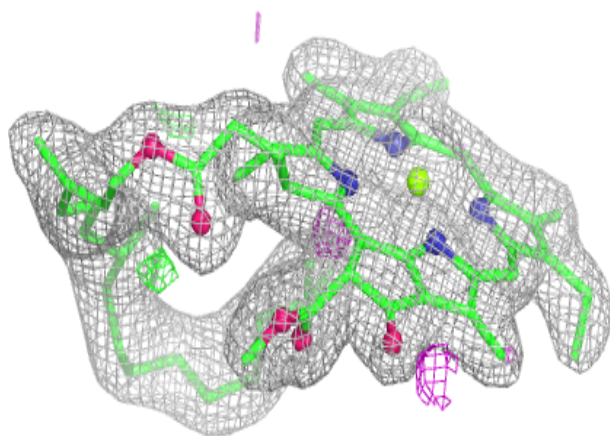
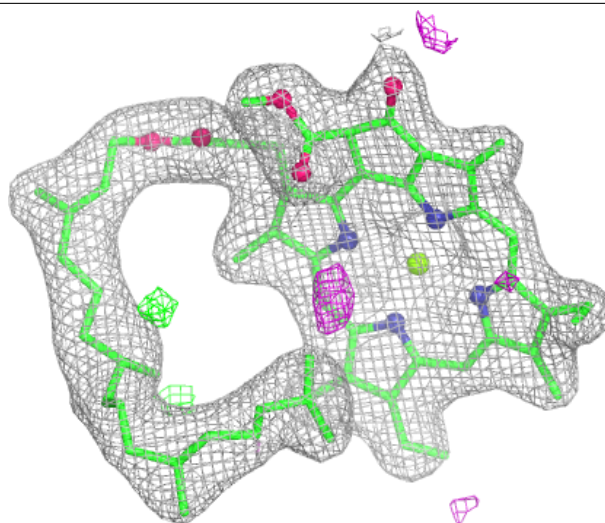
Electron density around HTG o 301:

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



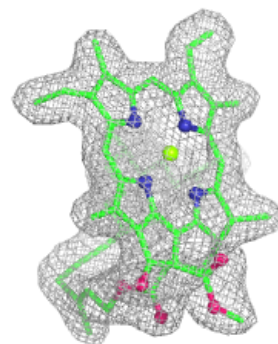
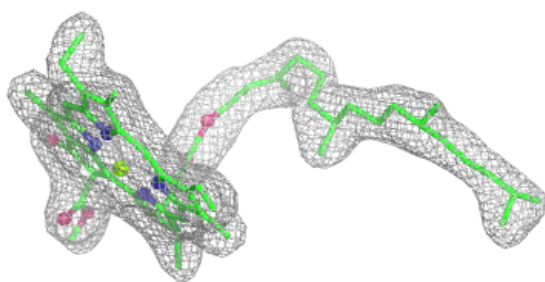
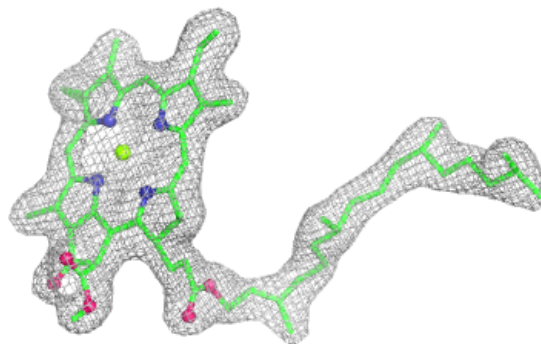
Electron density around CLA b 619:

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

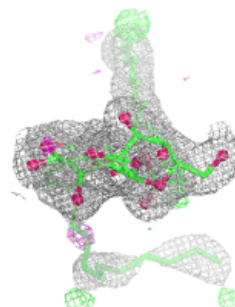
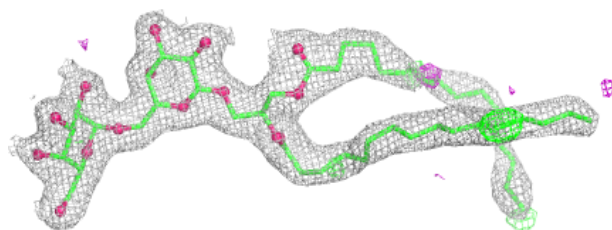
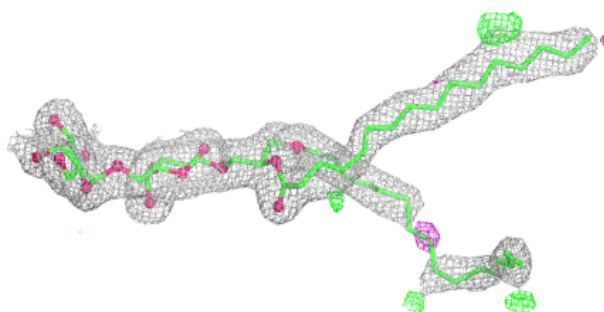


Electron density around CLA C 511:

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

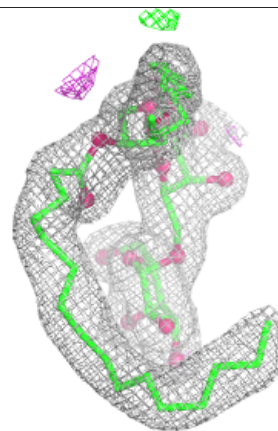
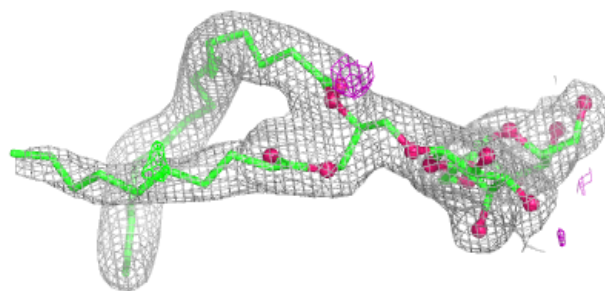
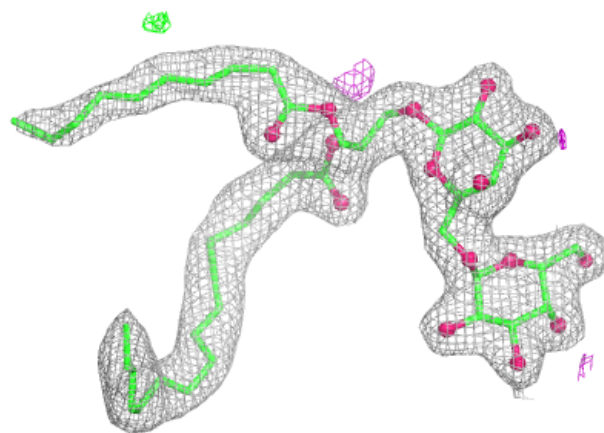
**Electron density around DGD C 516:**

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

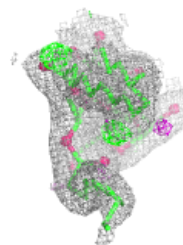
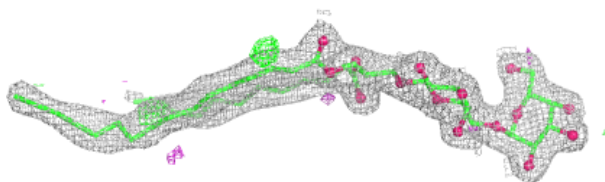
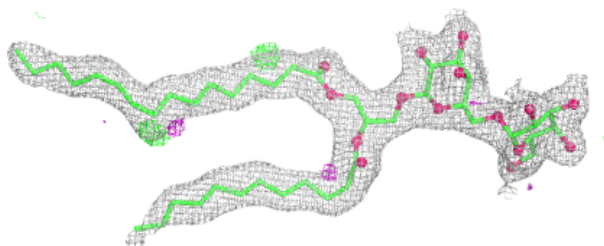


Electron density around DGD C 517:

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

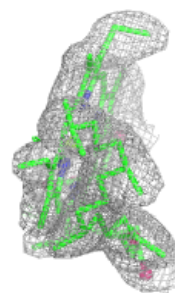
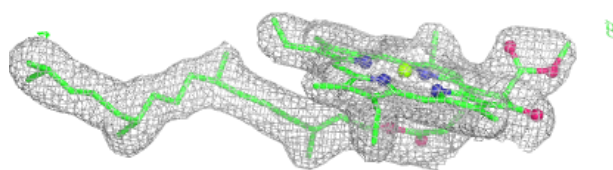
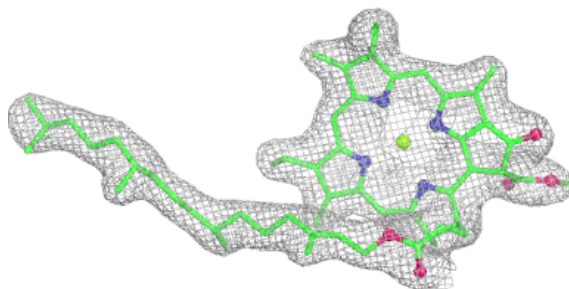
**Electron density around DGD C 518:**

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

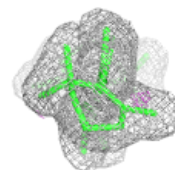
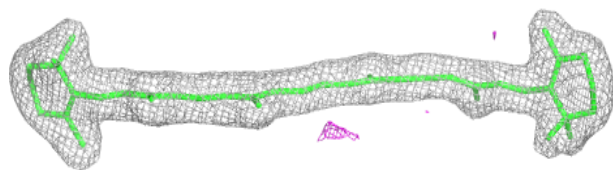
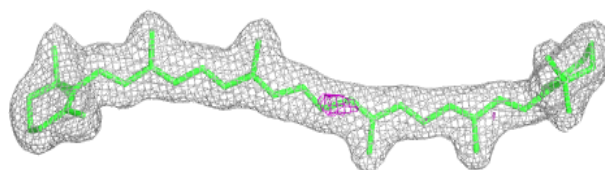


Electron density around CLA c 902:

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

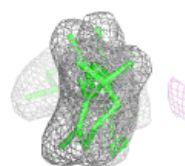
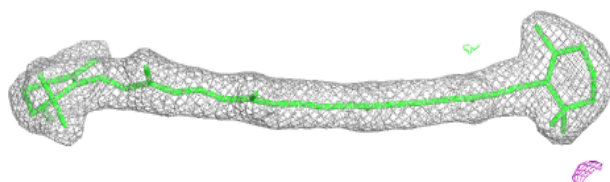
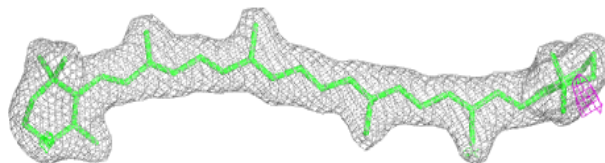
**Electron density around BCR a 414:**

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

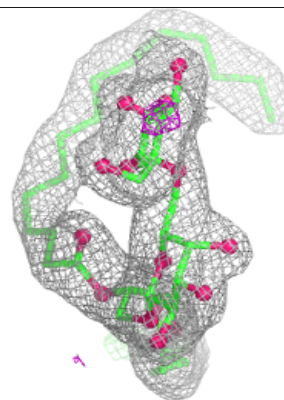
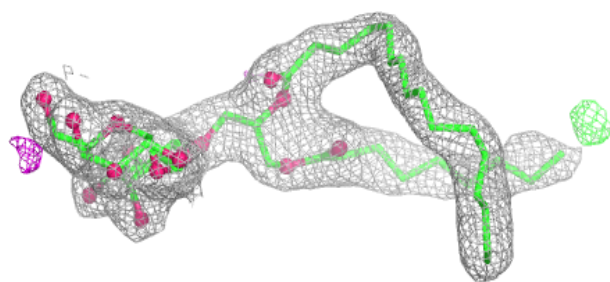
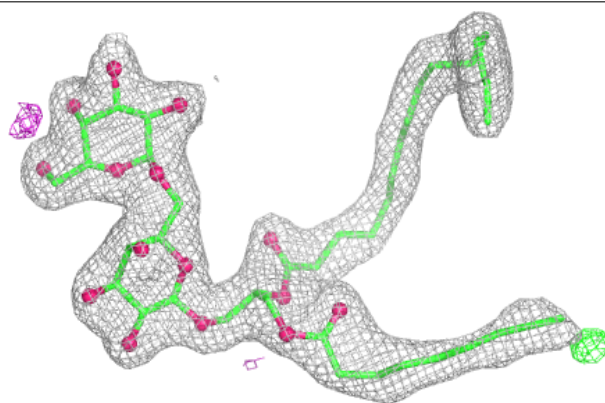


Electron density around BCR b 621:

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

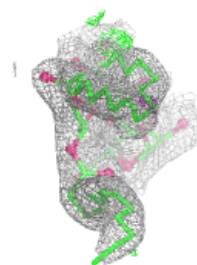
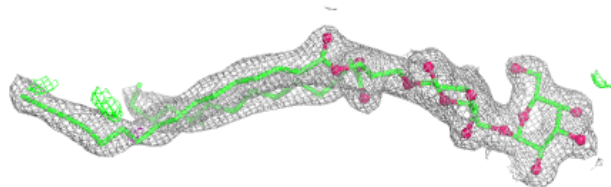
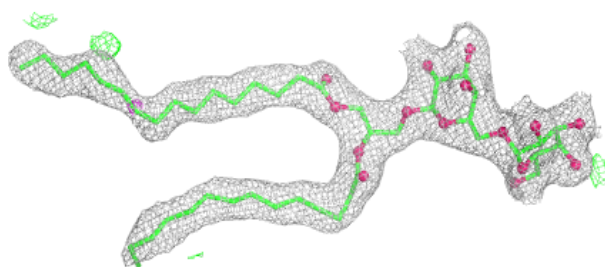
**Electron density around DGD c 918:**

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

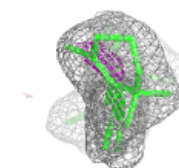
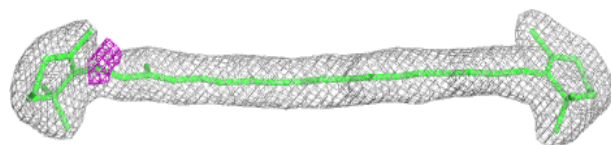
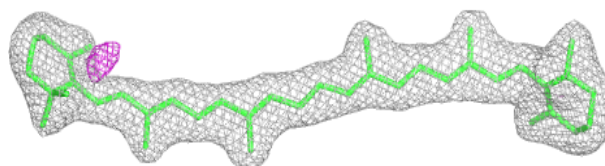


Electron density around DGD c 919:

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

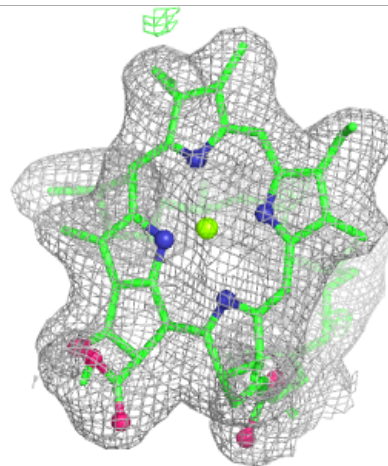
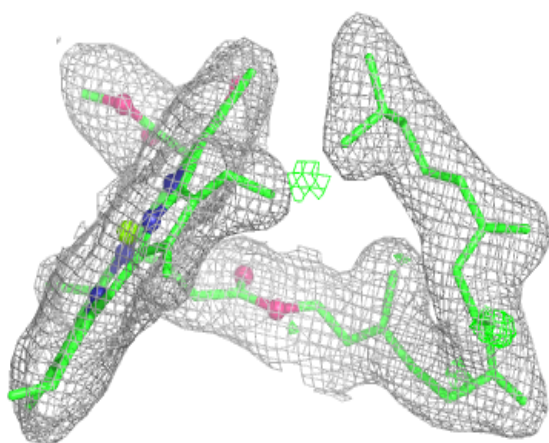
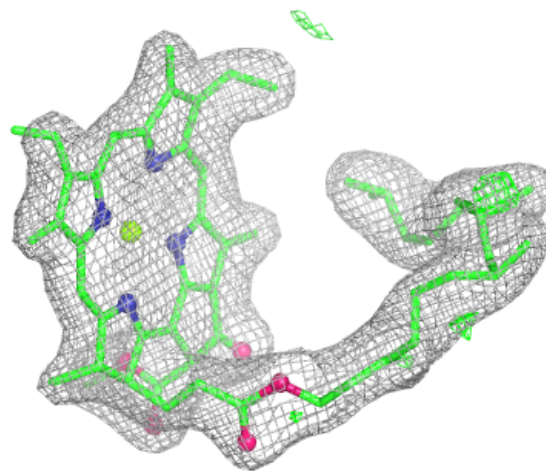
**Electron density around BCR b 622:**

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



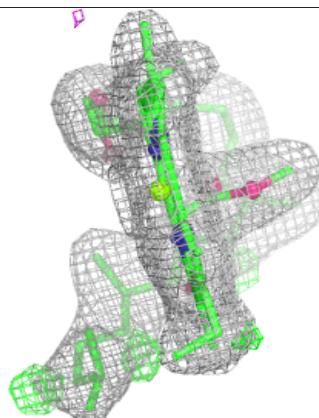
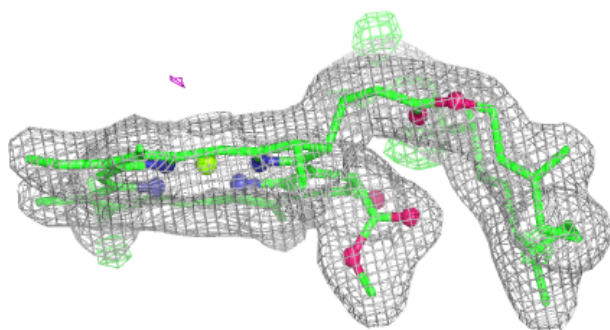
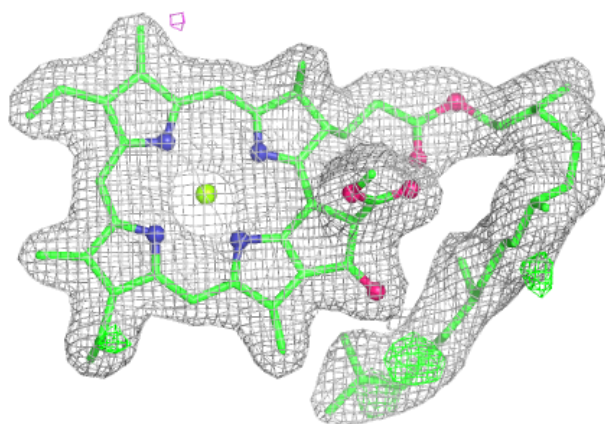
Electron density around CLA c 904:

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



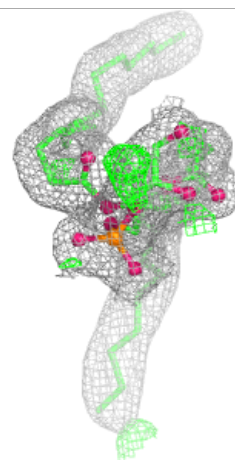
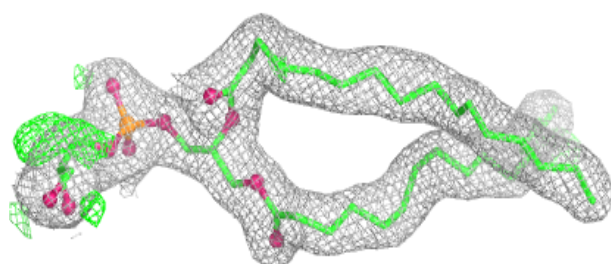
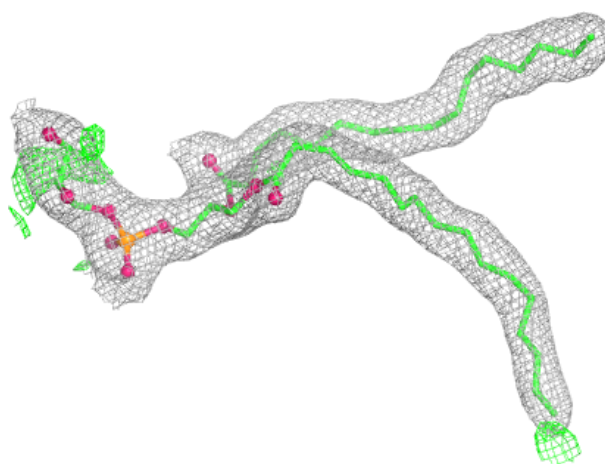
Electron density around CLA B 611:

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



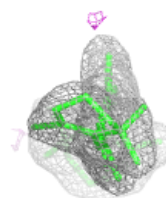
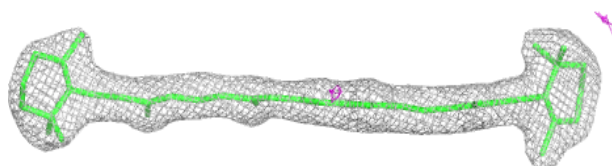
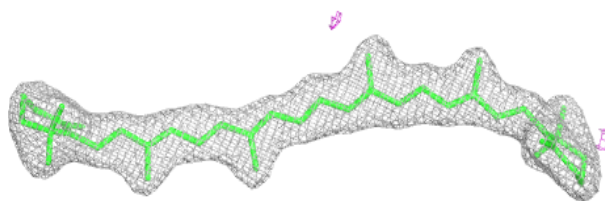
Electron density around LHG D 408:

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

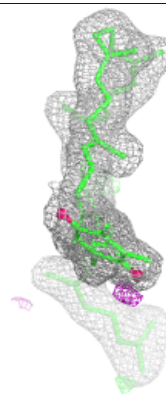
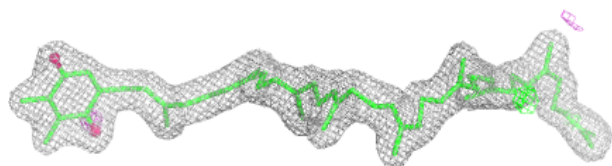
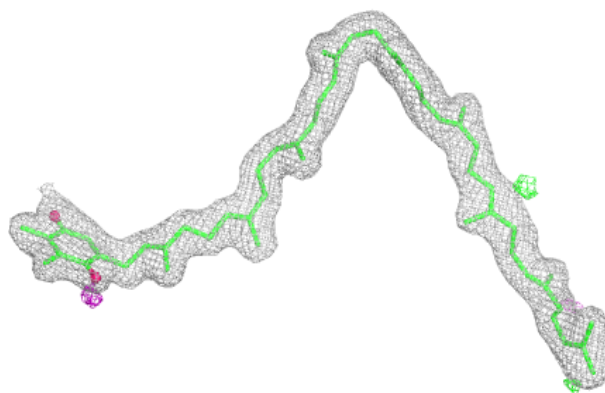


Electron density around BCR c 916:

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

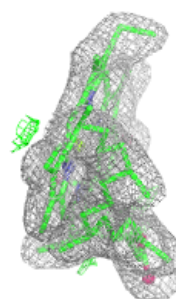
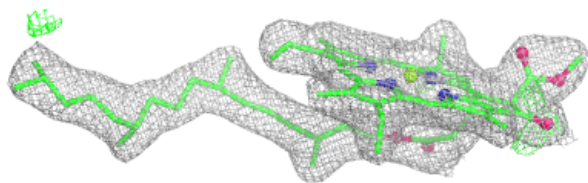
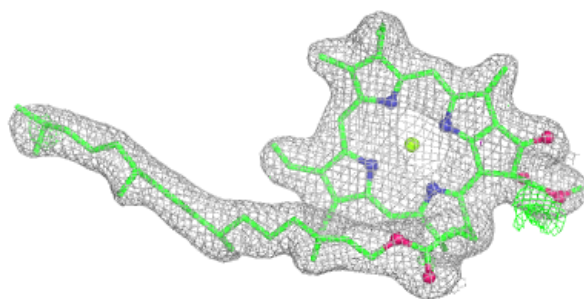
**Electron density around PL9 D 405:**

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



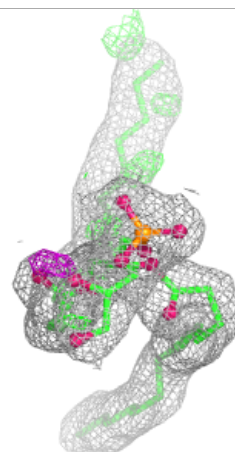
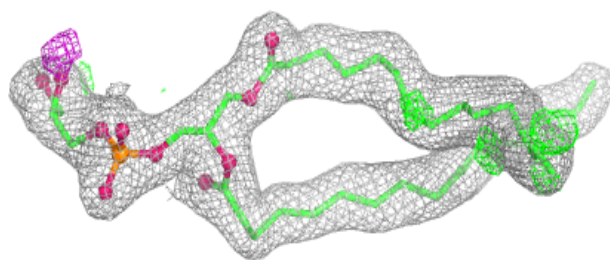
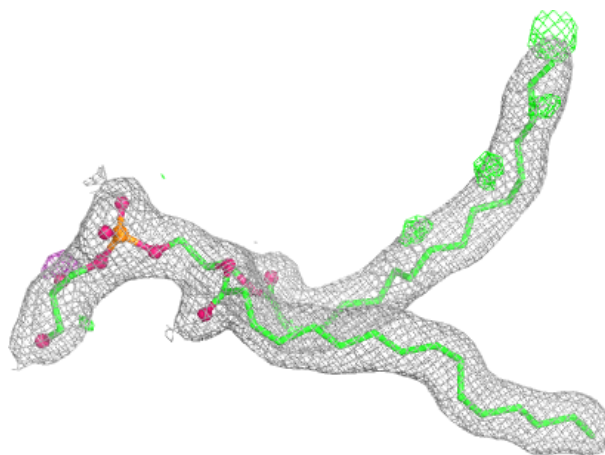
Electron density around CLA C 501:

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



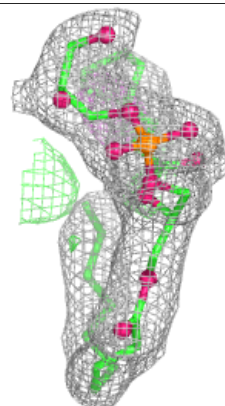
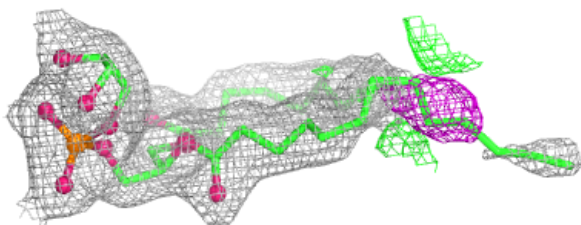
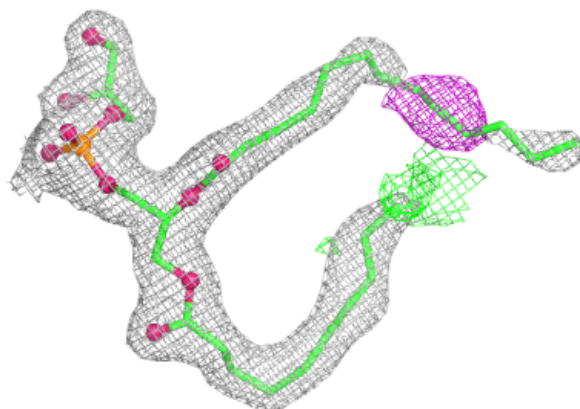
Electron density around LHG d 409:

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

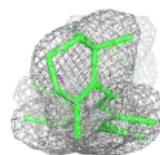
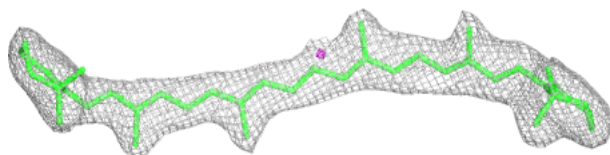
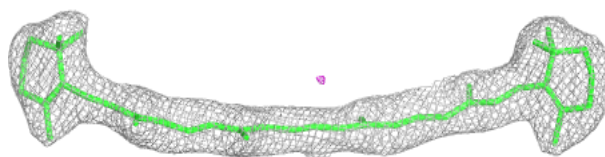


Electron density around LHG d 410:

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

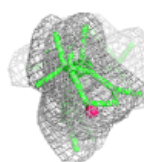
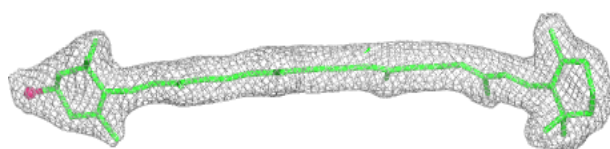
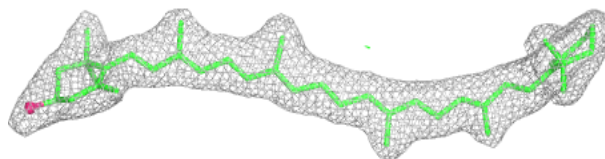
**Electron density around BCR k 101:**

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

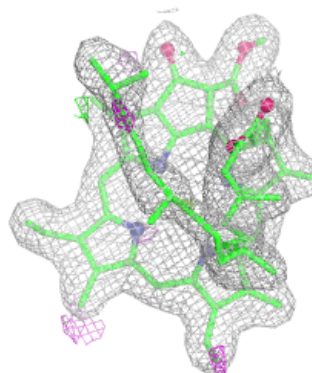
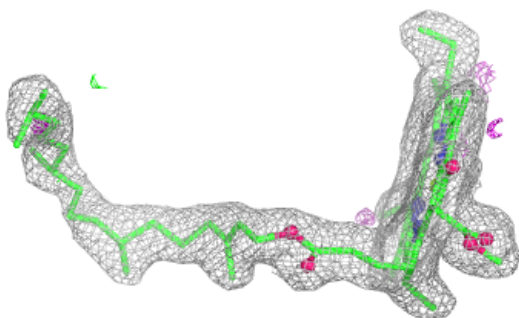
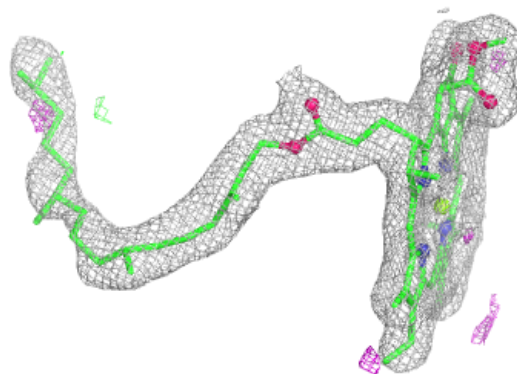


Electron density around RRX H 102:

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

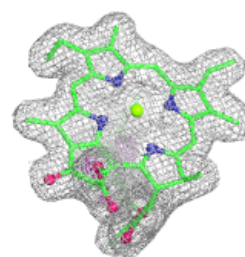
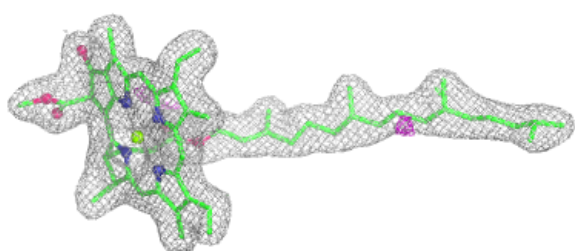
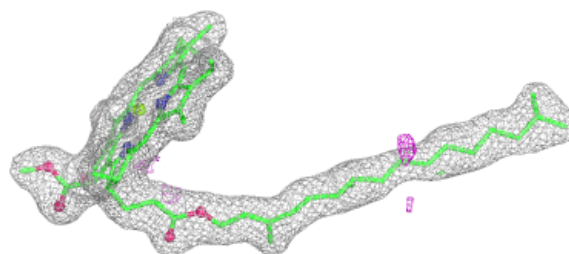
**Electron density around CLA D 403:**

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

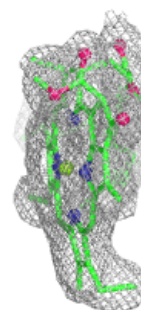
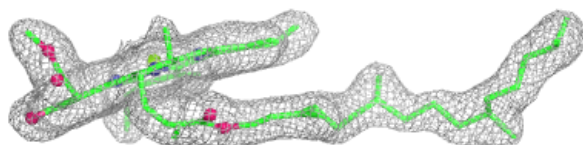
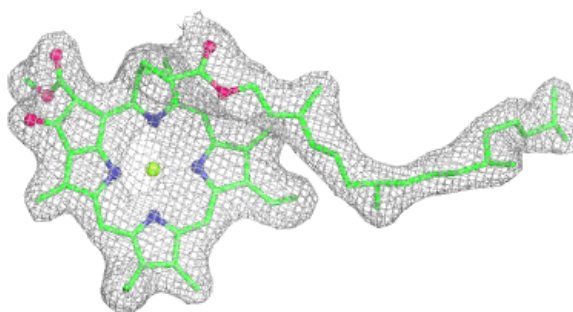


Electron density around CLA B 608:

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

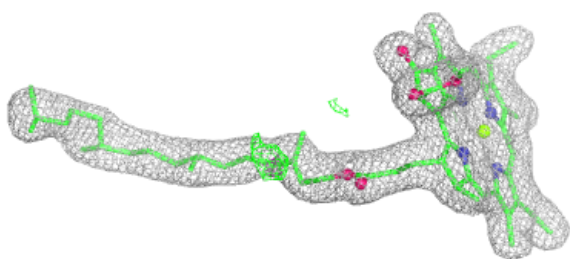
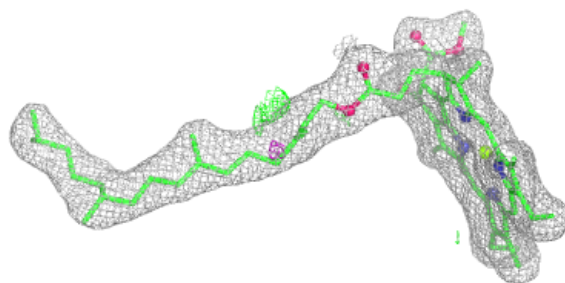
**Electron density around CLA b 607:**

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



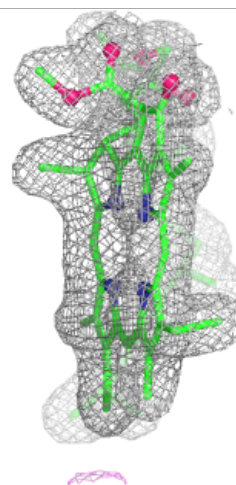
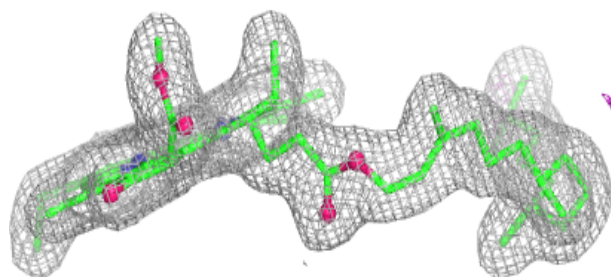
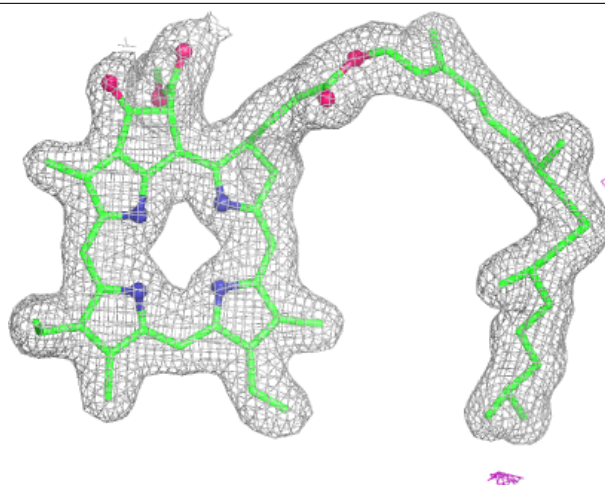
Electron density around CLA b 608:

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



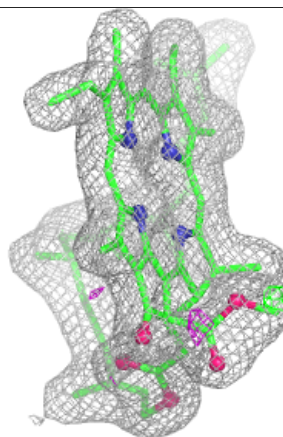
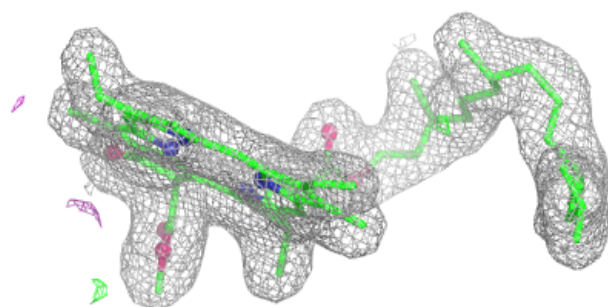
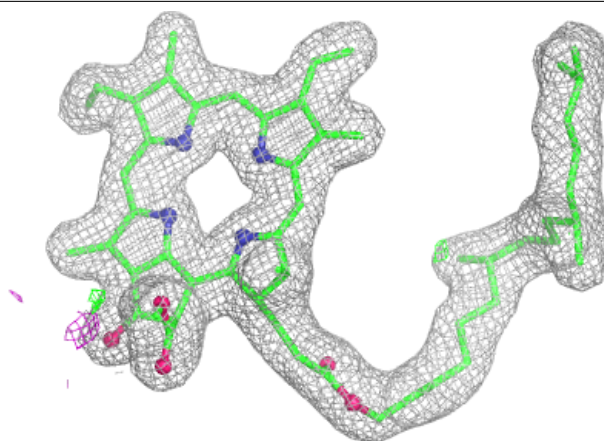
Electron density around PHO A 408:

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



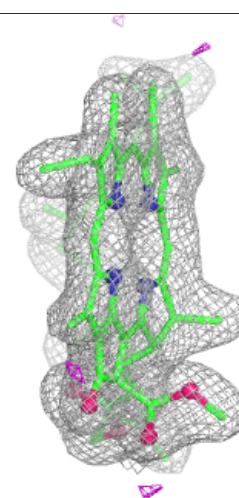
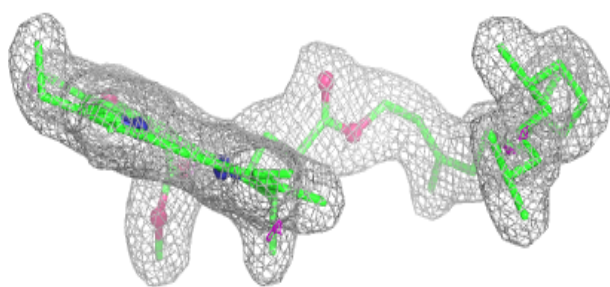
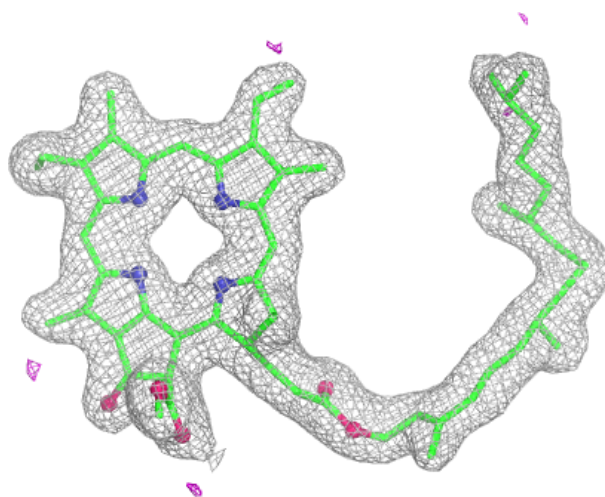
Electron density around PHO A 409:

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



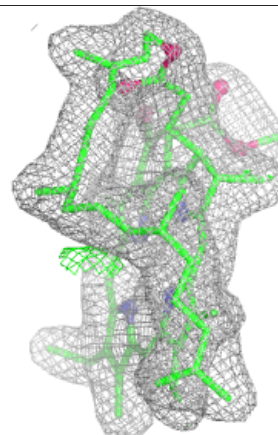
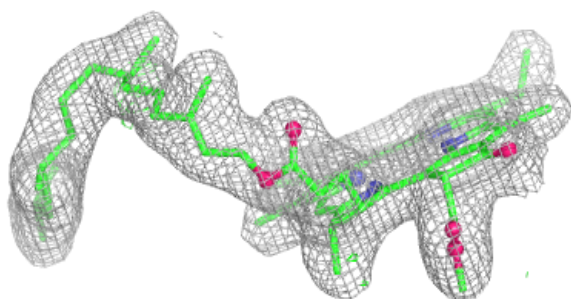
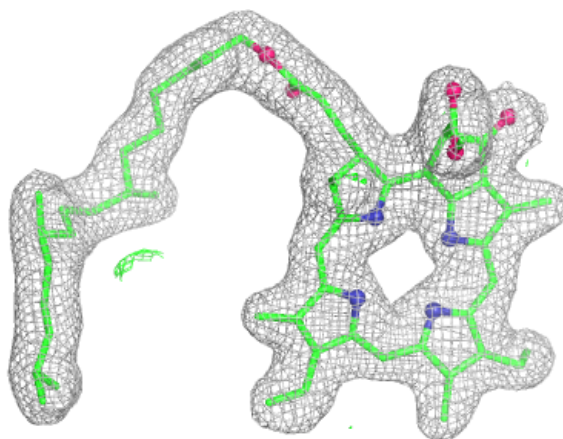
Electron density around PHO a 411:

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

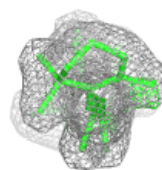
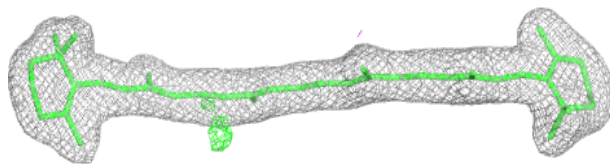
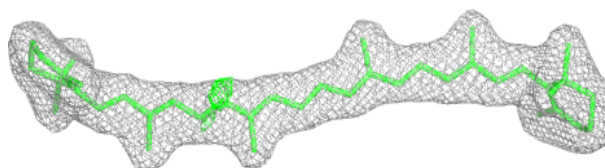


Electron density around PHO a 412:

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

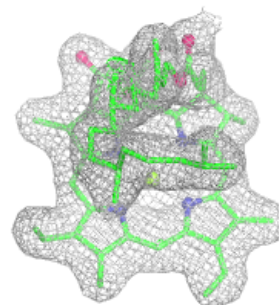
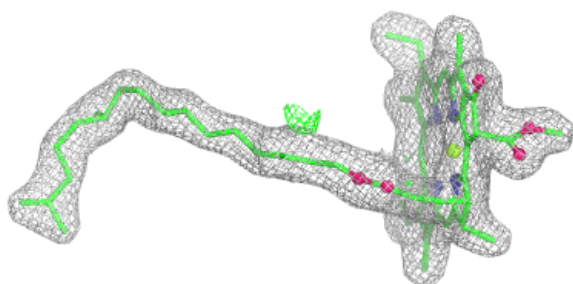
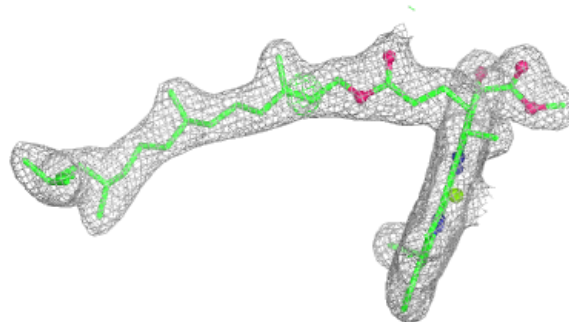
**Electron density around BCR A 411:**

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

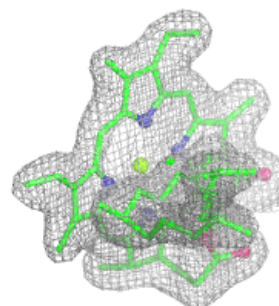
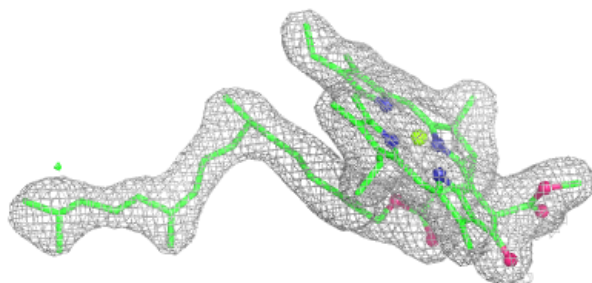
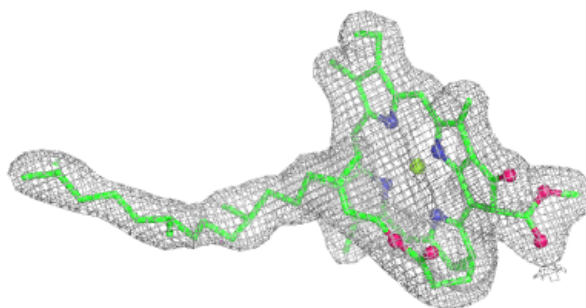


Electron density around CLA b 609:

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

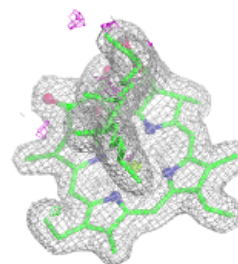
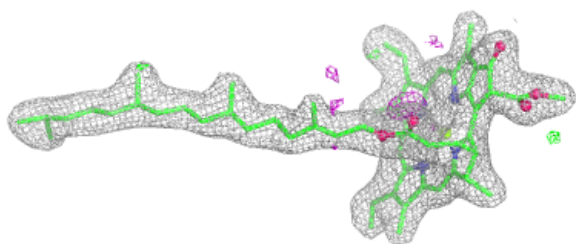
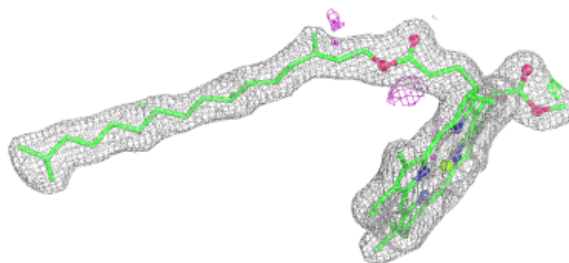
**Electron density around CLA C 505:**

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

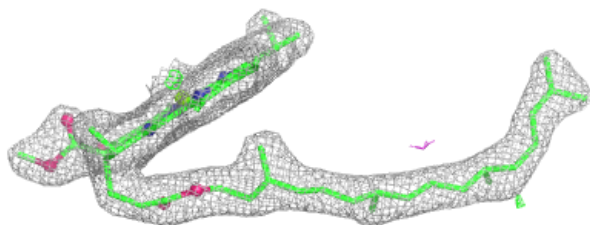
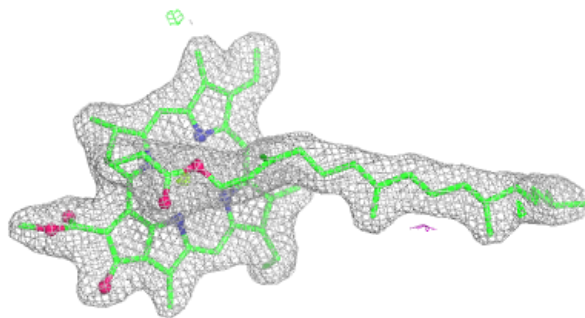


Electron density around CLA b 611:

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

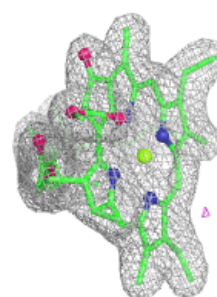
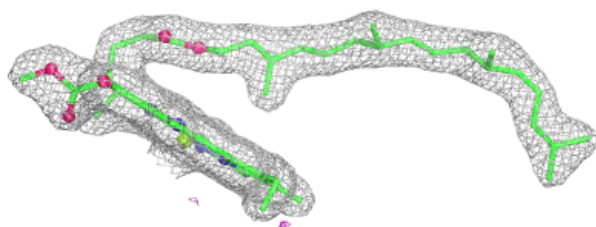
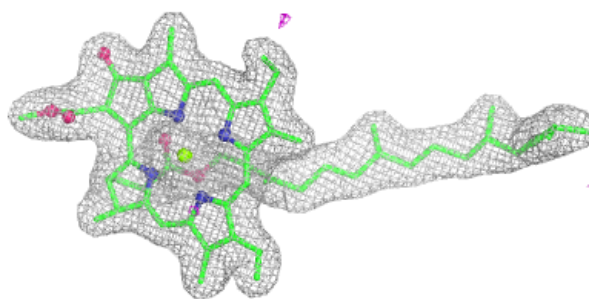
**Electron density around CLA b 612:**

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

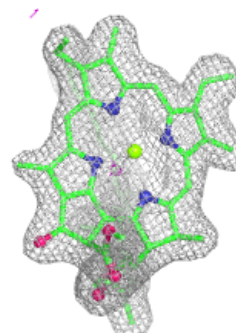
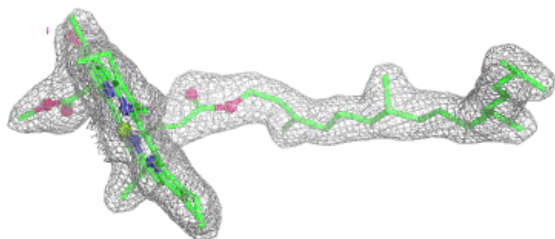
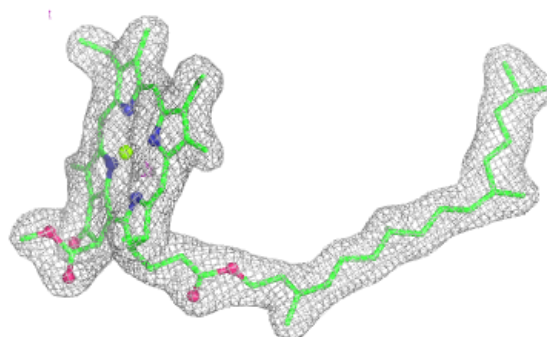


Electron density around CLA B 609:

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

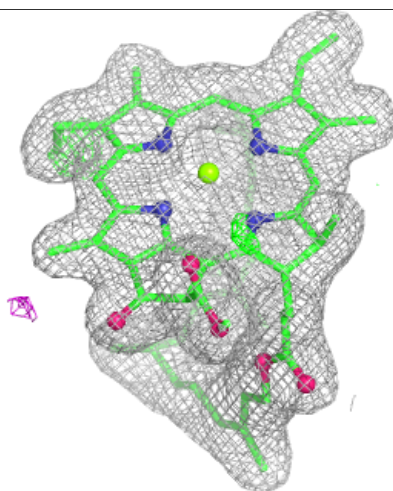
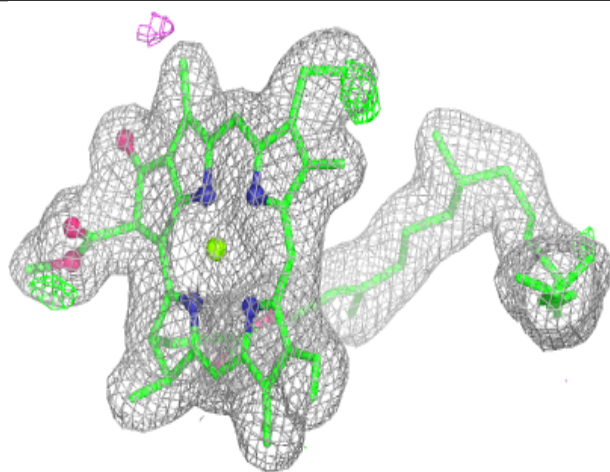
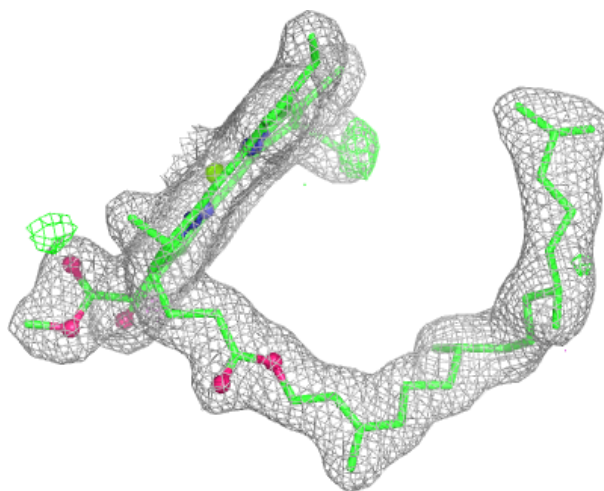
**Electron density around CLA B 610:**

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



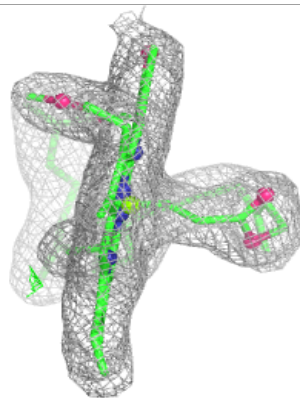
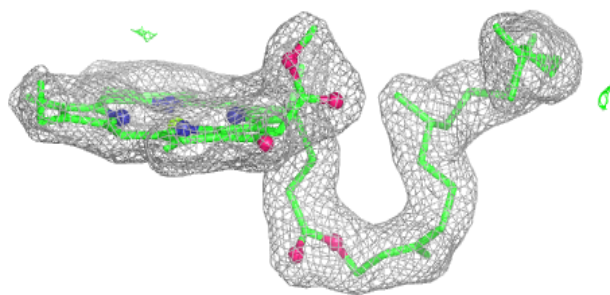
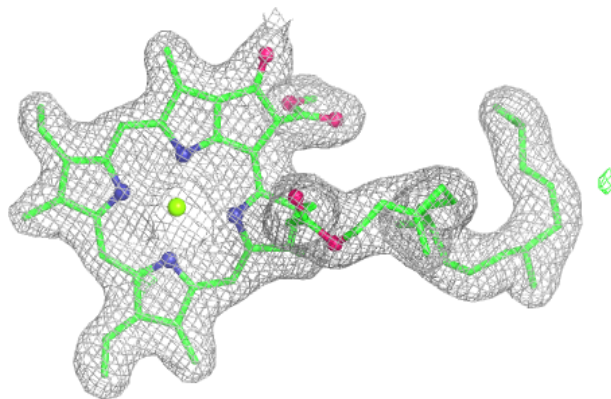
Electron density around CLA b 615:

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



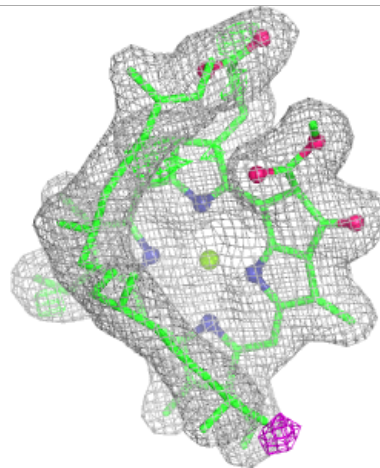
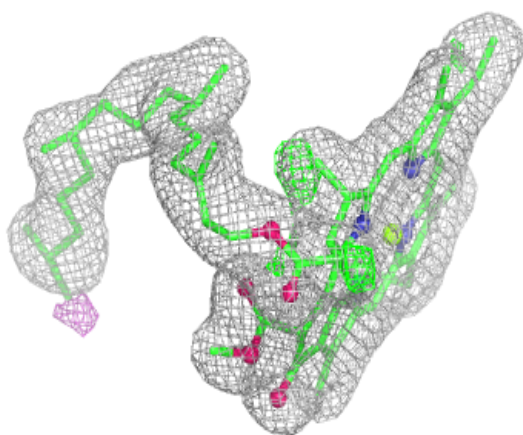
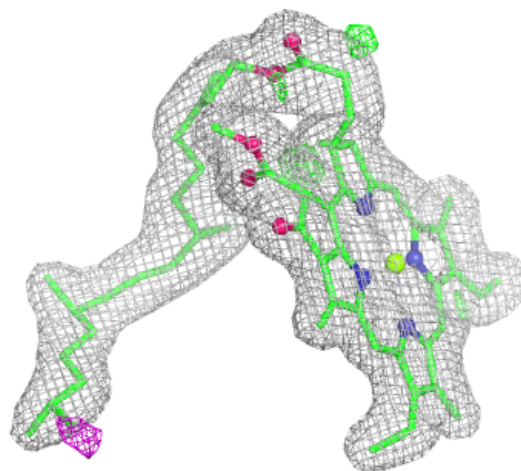
Electron density around CLA b 616:

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



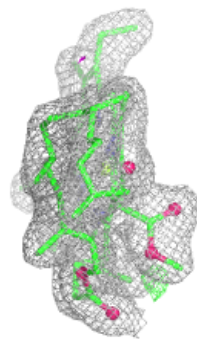
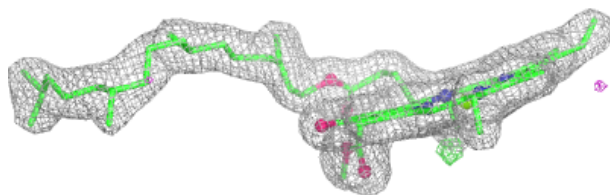
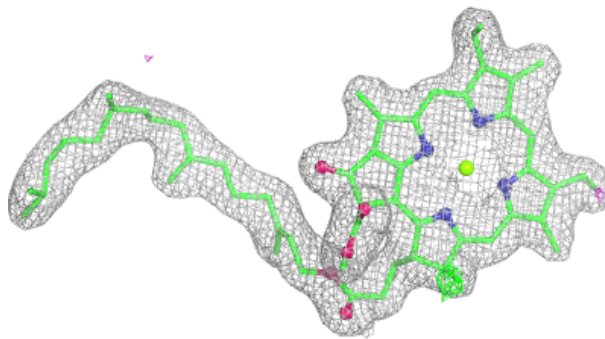
Electron density around CLA b 617:

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



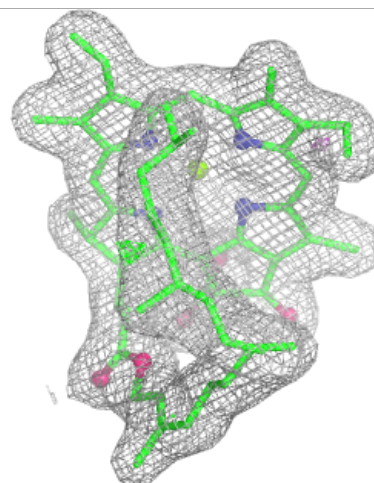
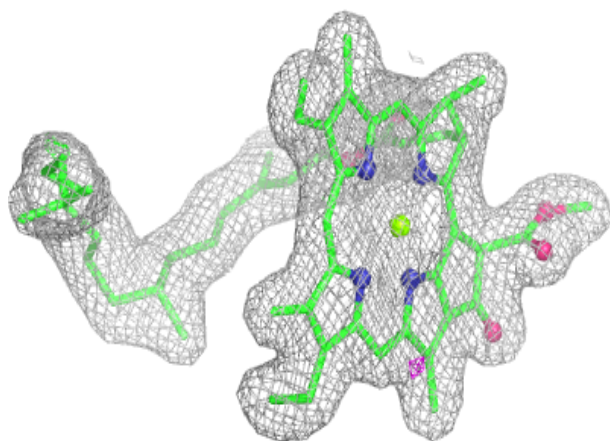
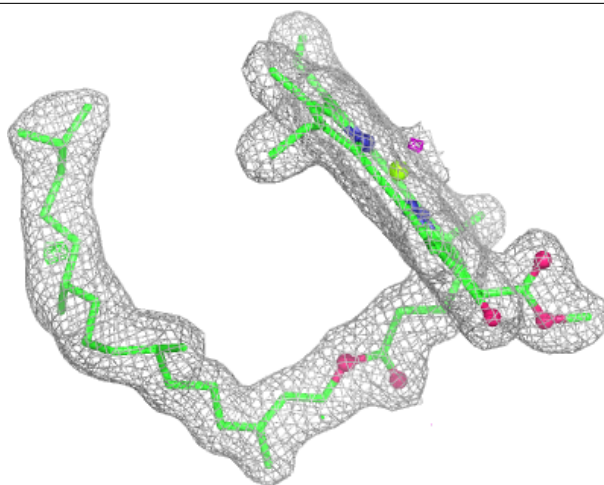
Electron density around CLA B 603:

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



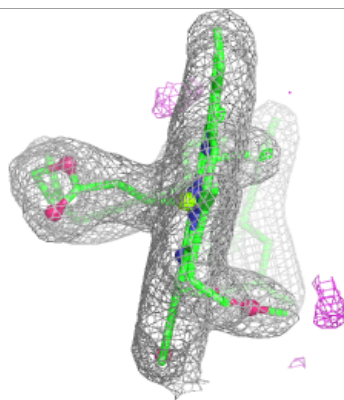
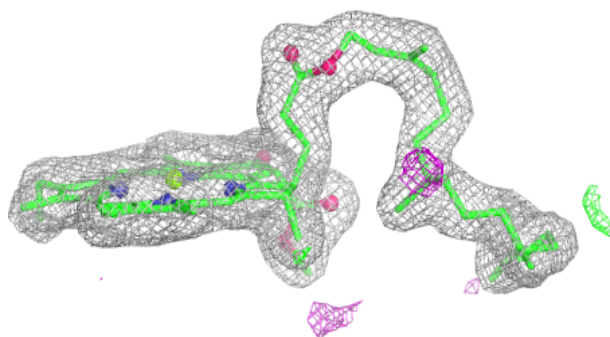
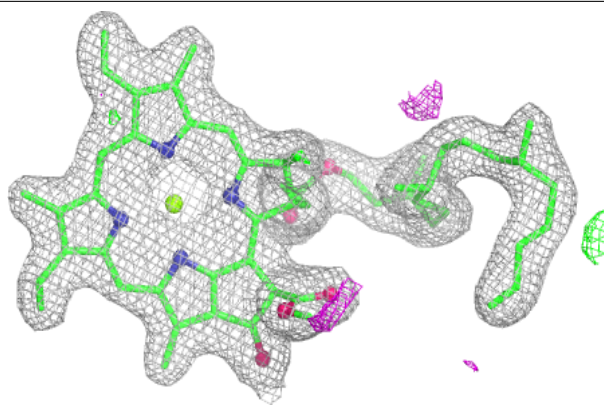
Electron density around CLA B 612:

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



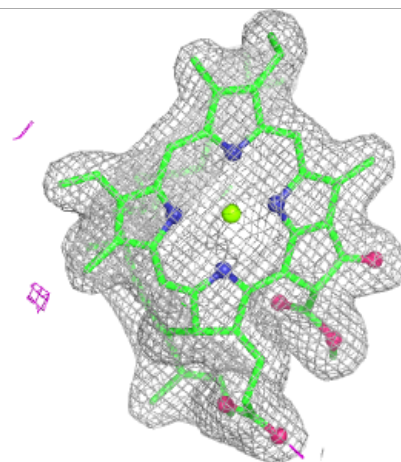
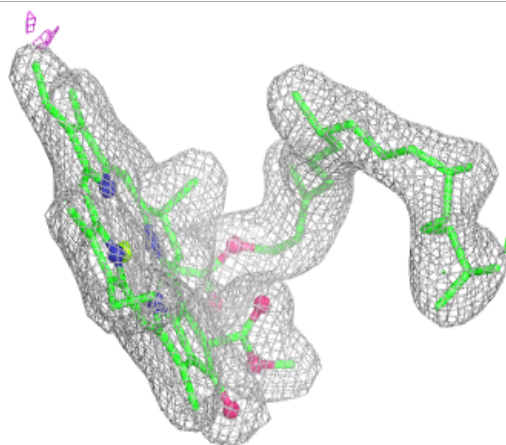
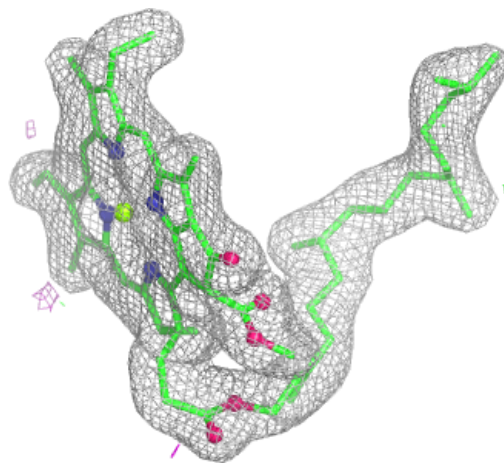
Electron density around CLA B 613:

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



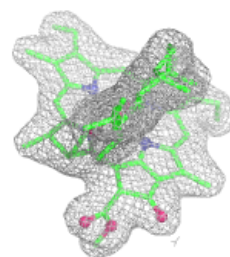
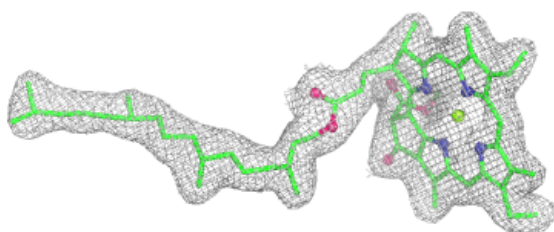
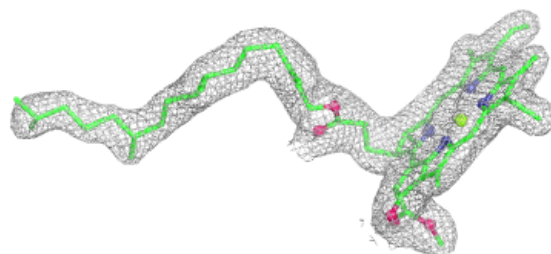
Electron density around CLA B 614:

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

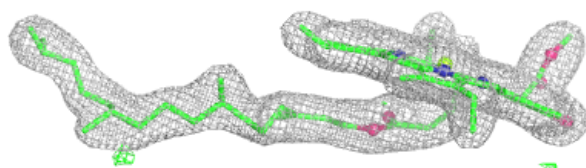
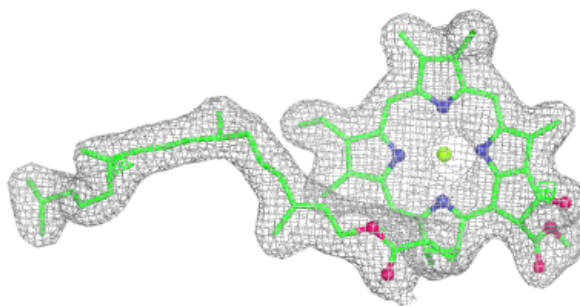


Electron density around CLA c 903:

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

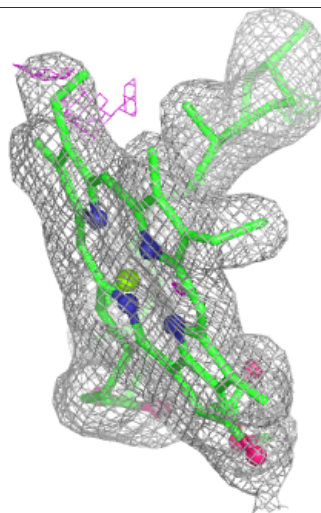
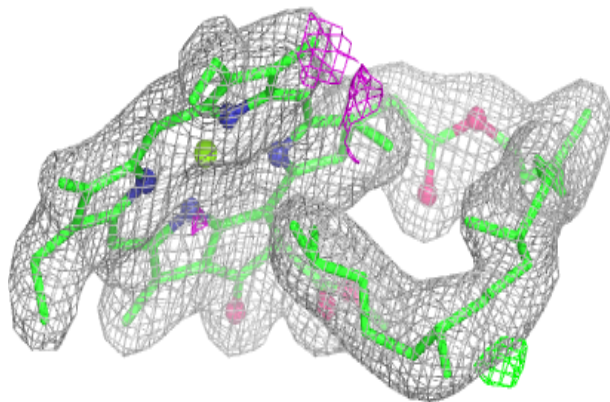
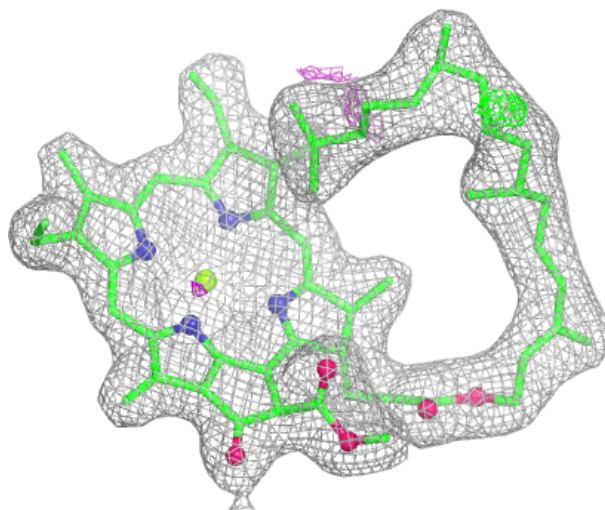
**Electron density around CLA B 604:**

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



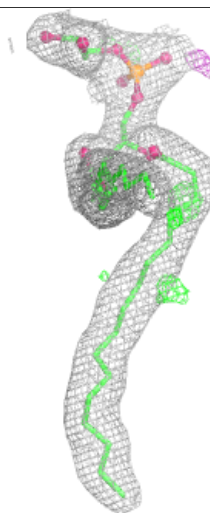
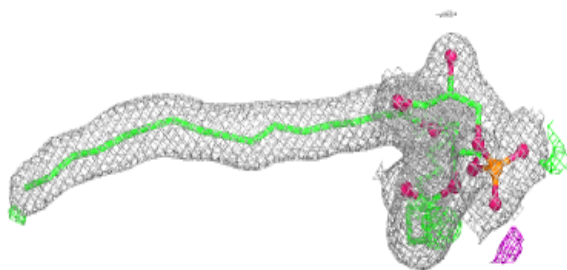
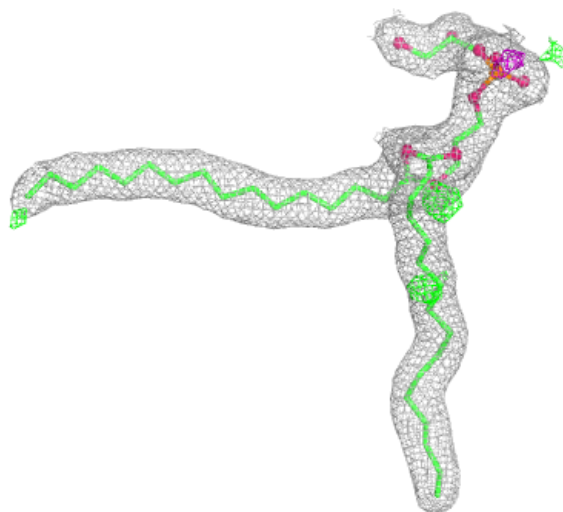
Electron density around CLA B 616:

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



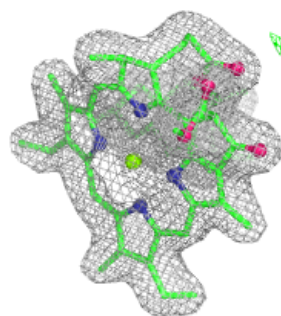
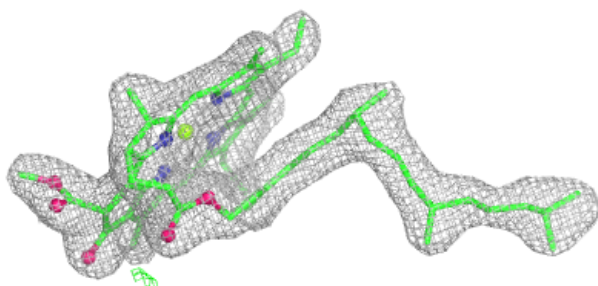
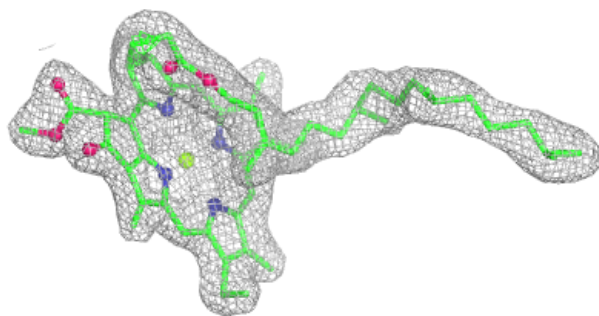
Electron density around LHG L 101:

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

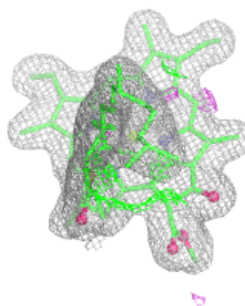
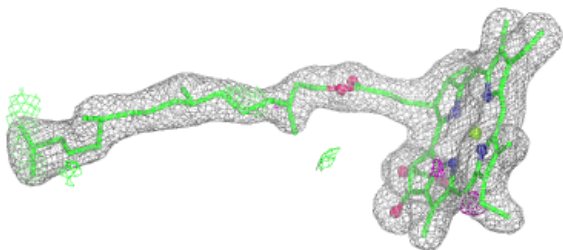
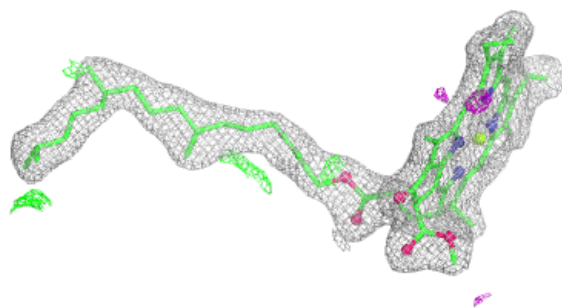


Electron density around CLA c 906:

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

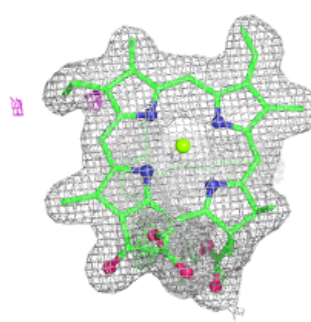
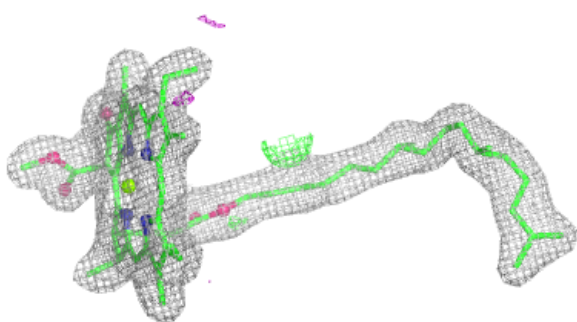
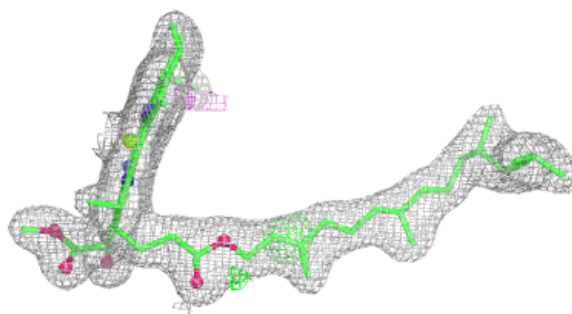
**Electron density around CLA B 605:**

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

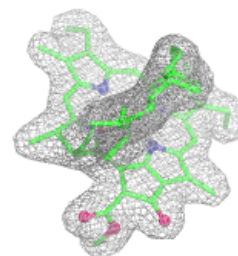
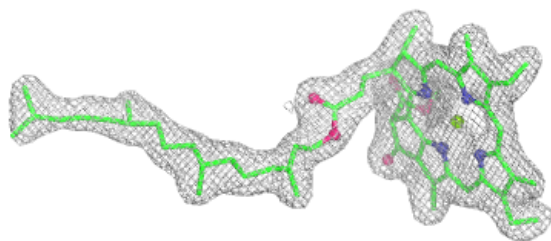
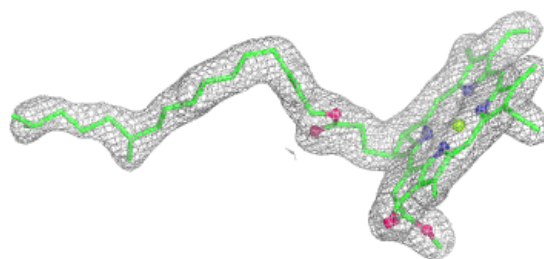


Electron density around CLA B 606:

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

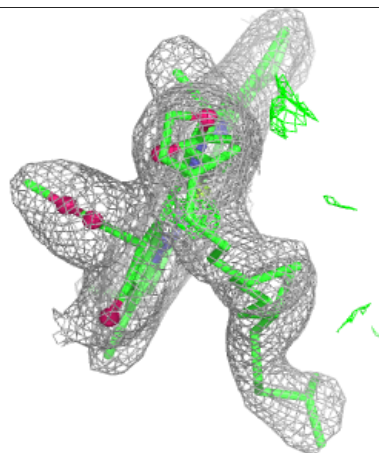
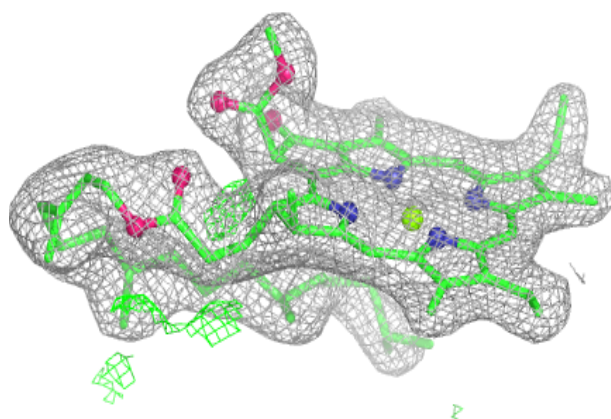
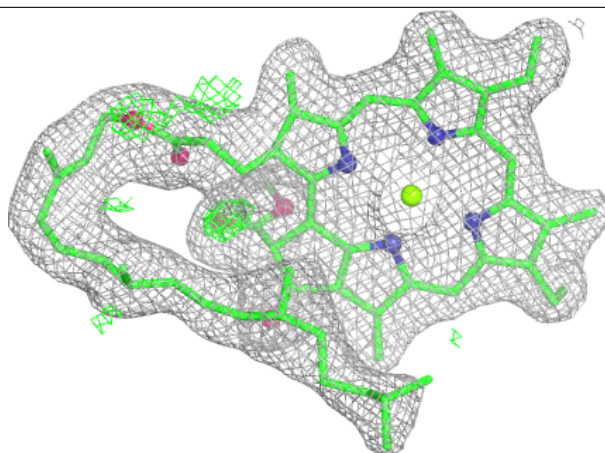
**Electron density around CLA C 502:**

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



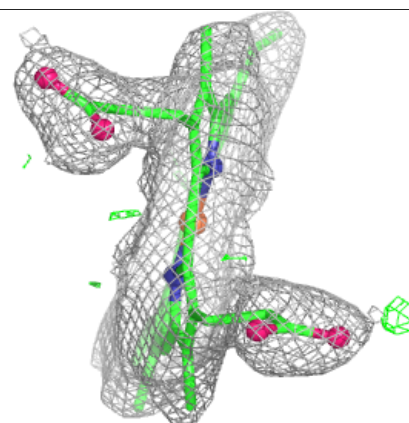
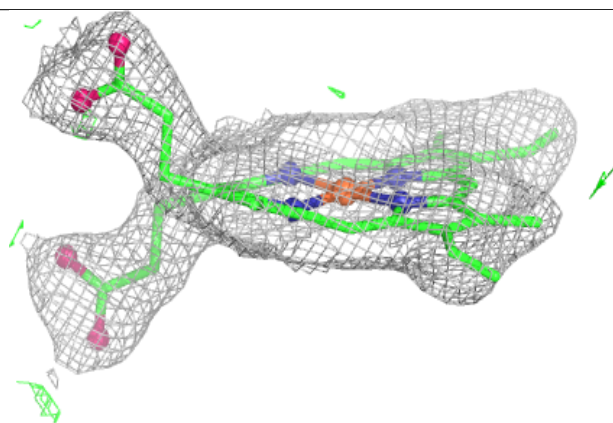
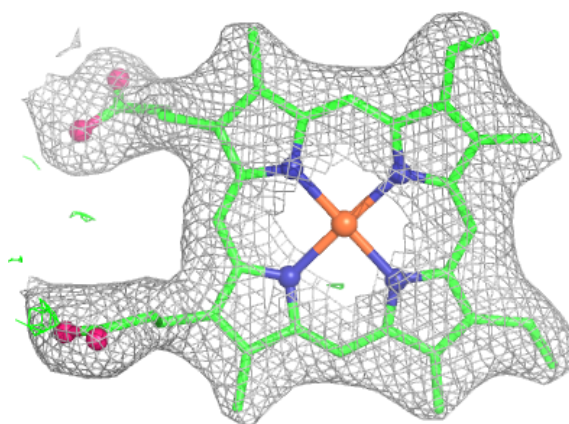
Electron density around CLA c 910:

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



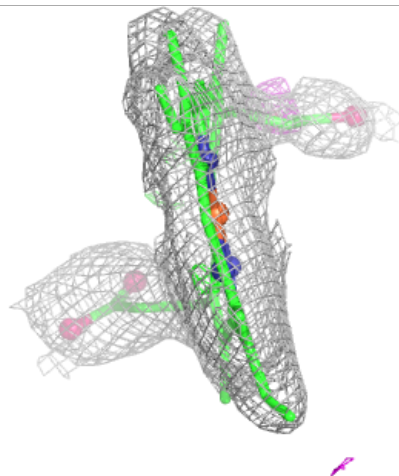
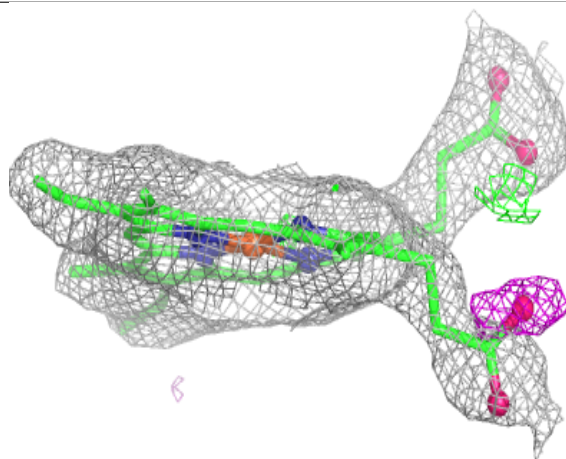
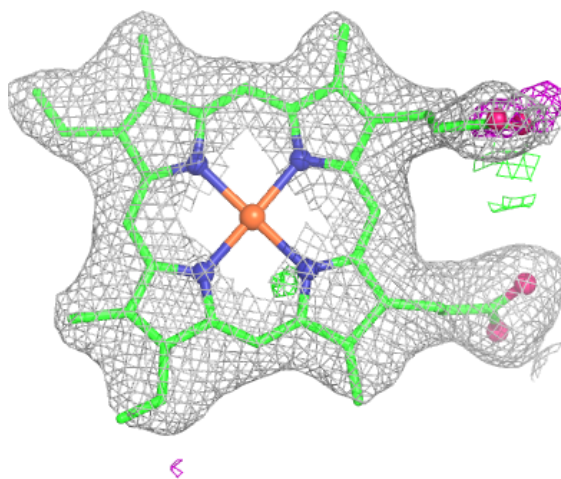
Electron density around HEM F 102:

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



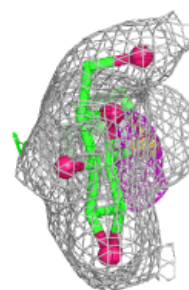
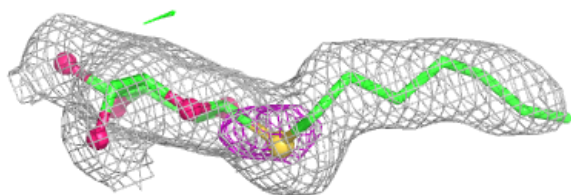
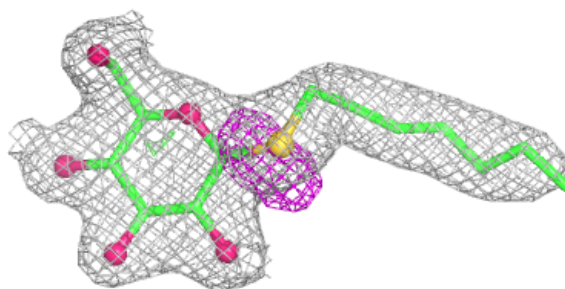
Electron density around HEM f 101:

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

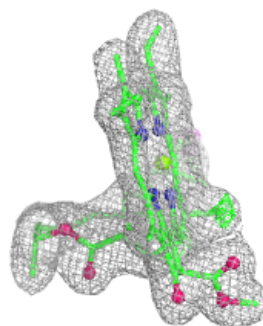
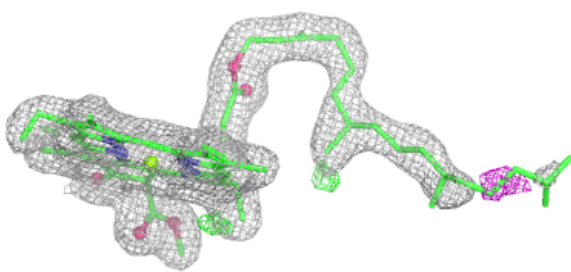
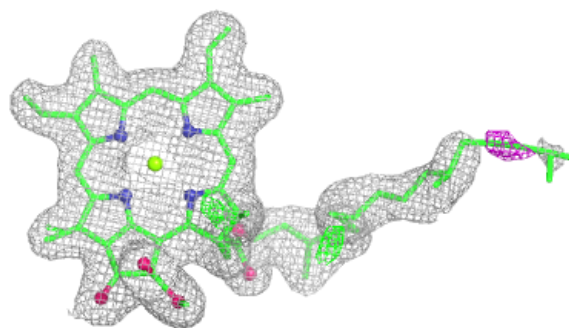


Electron density around HTG O 303:

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

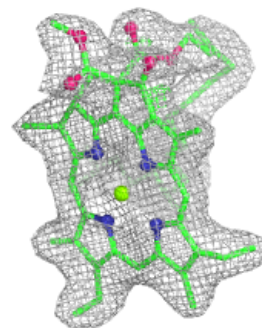
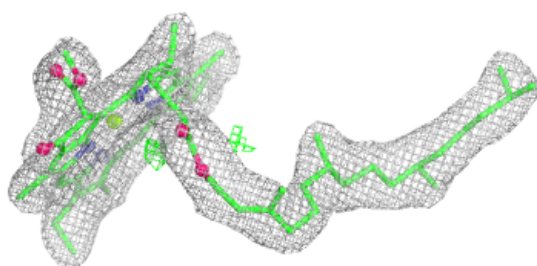
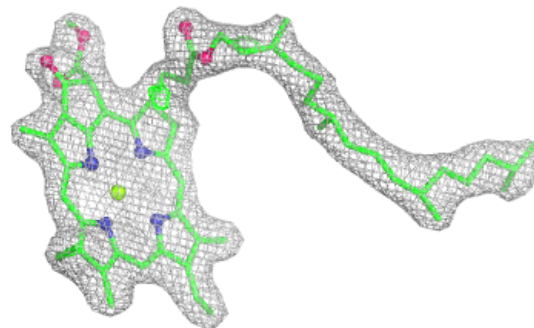
**Electron density around CLA A 407:**

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

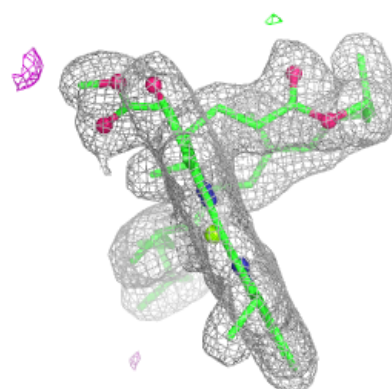
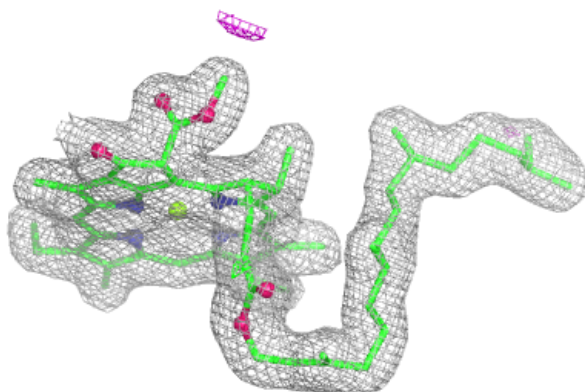
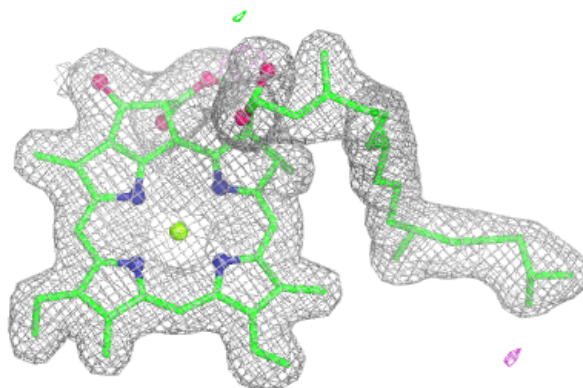


Electron density around CLA c 912:

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

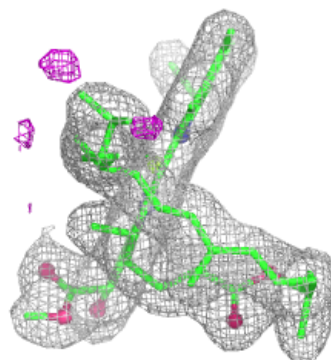
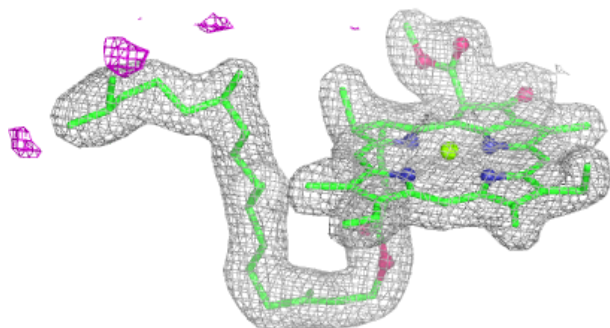
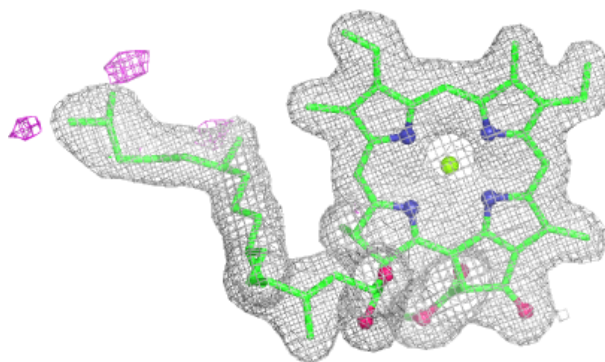
**Electron density around CLA A 406:**

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

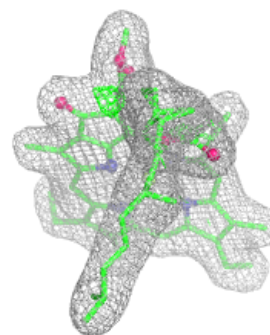
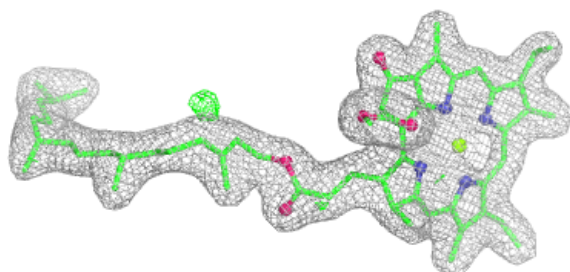
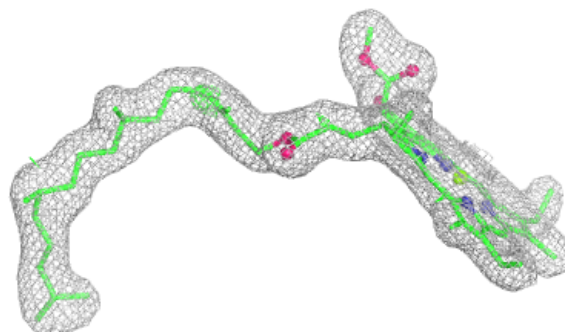


Electron density around CLA d 401:

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

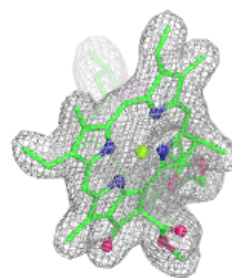
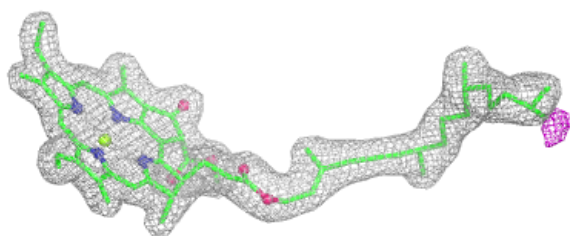
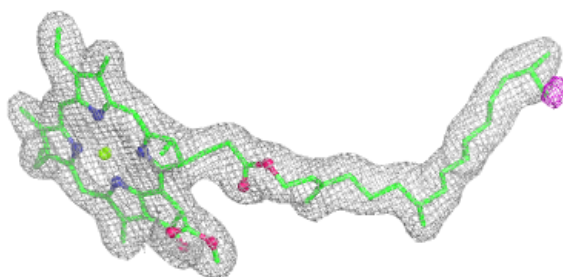
**Electron density around CLA d 404:**

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



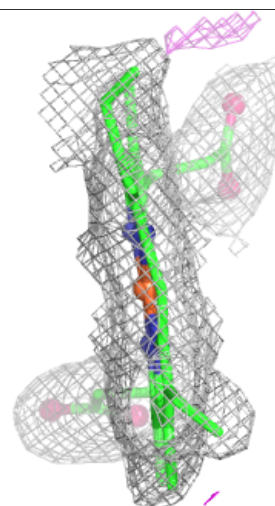
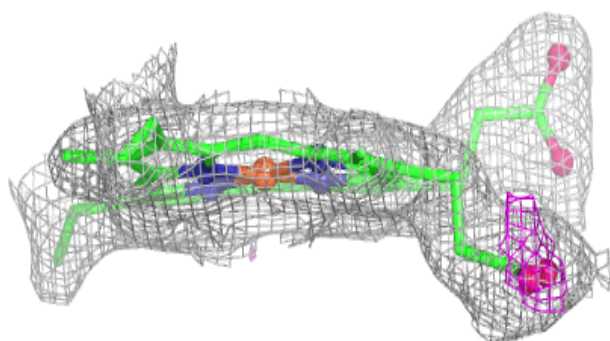
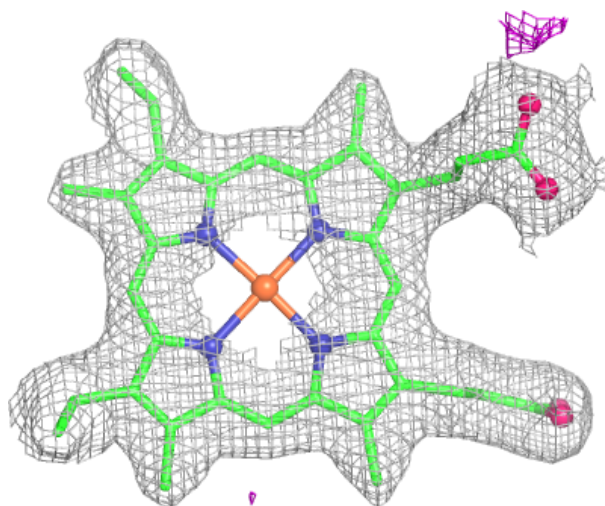
Electron density around CLA a 409:

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



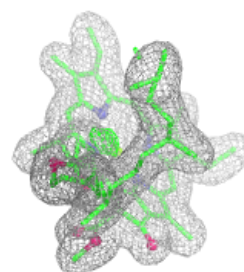
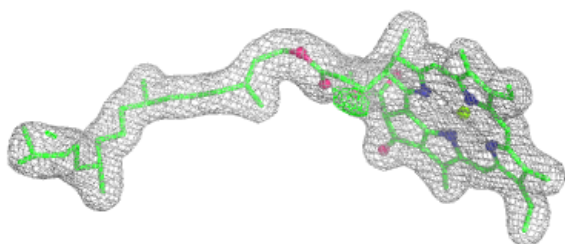
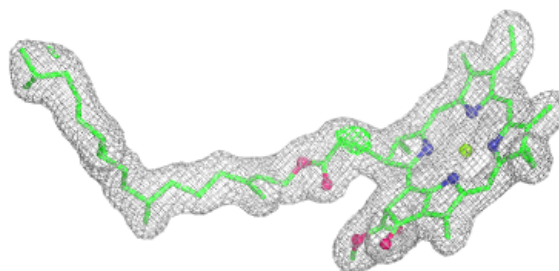
Electron density around HEM v 202:

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

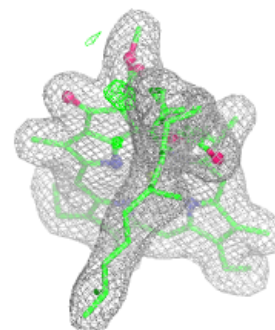
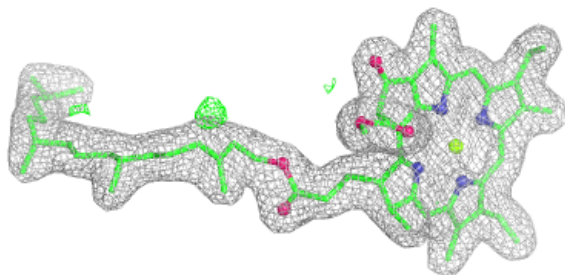
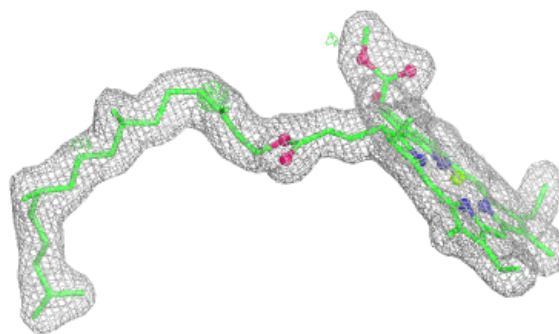


Electron density around CLA A 405:

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

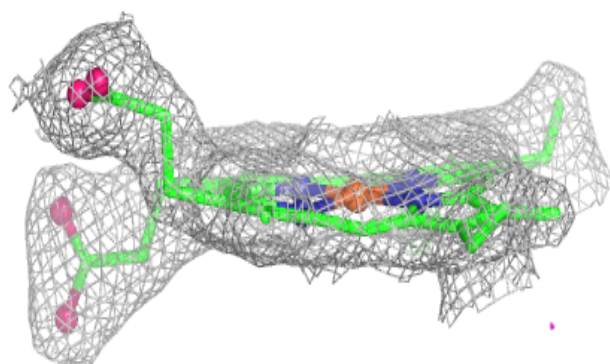
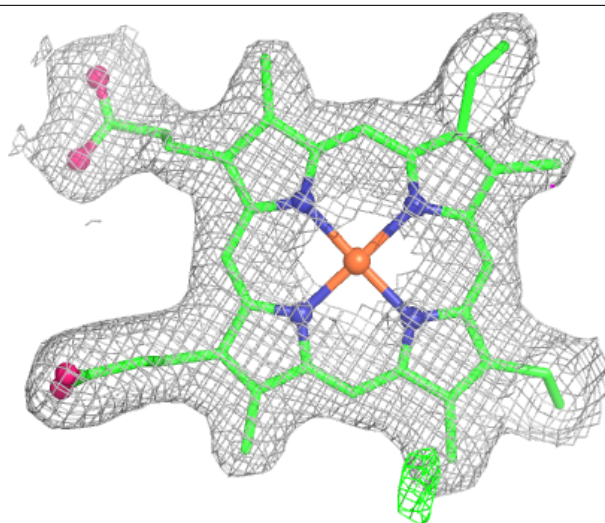
**Electron density around CLA D 402:**

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



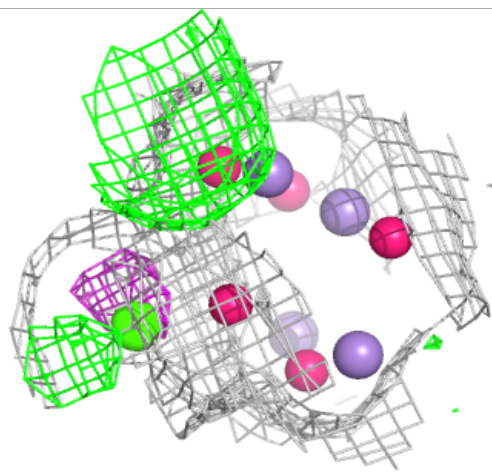
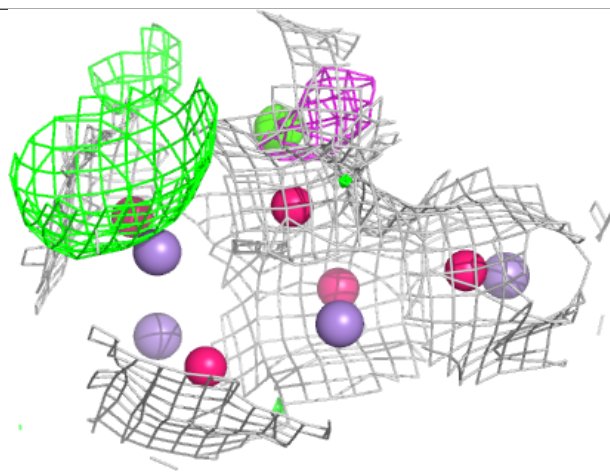
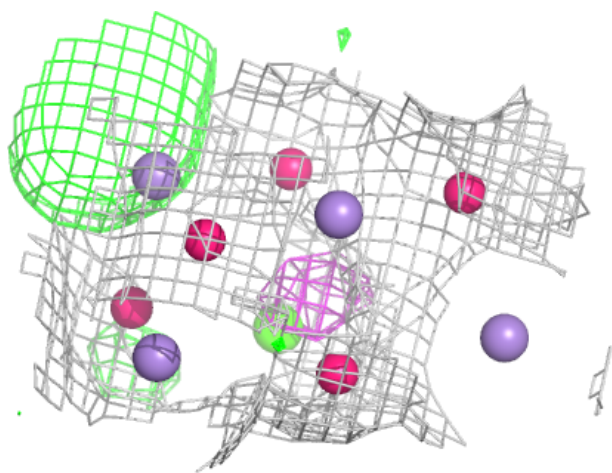
Electron density around HEM V 202:

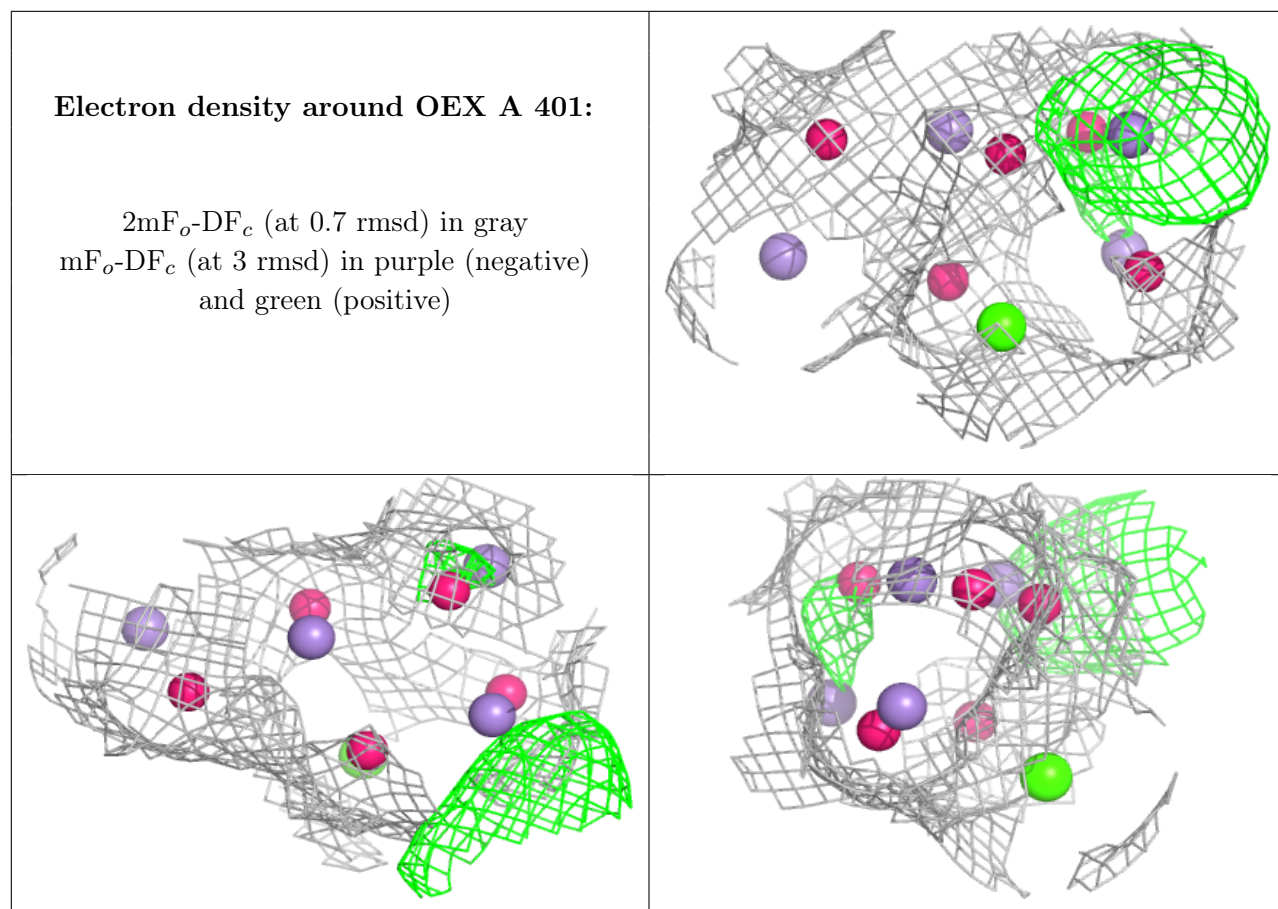
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OEX a 404:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.