



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:03 PM JST

PDB ID : 6JLM / pdb_00006jlm
Title : XFEL structure of cyanobacterial photosystem II (dark state, dataset2)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2019-03-06
Resolution : 2.35 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:

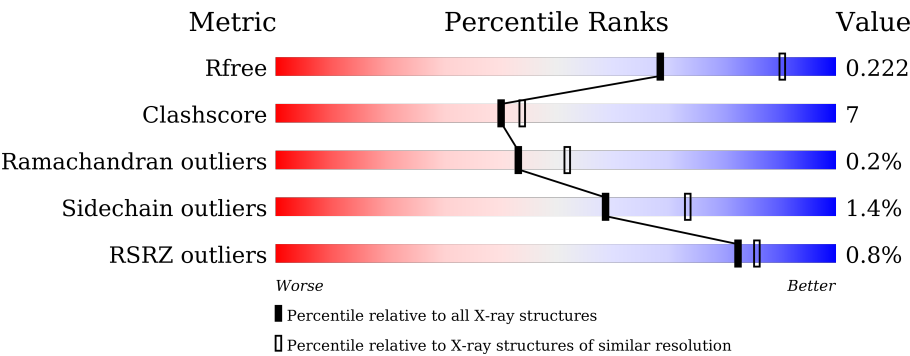
MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
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 2.35 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.



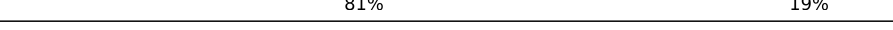
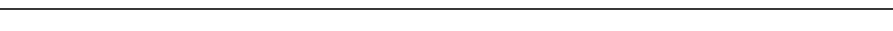
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	344	84%12%.
1	a	344	86%11%.
2	B	505	86%13%
2	b	505	% 88%12%
3	C	455	89%10%..
3	c	455	87%12%.

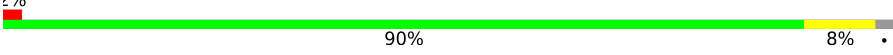
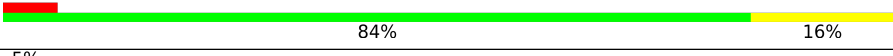
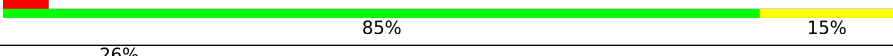
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Mol	Chain	Length	Quality of chain
4	D	342	 88% 12%
4	d	342	 89% 10%
5	E	84	 73% 24% .
5	e	84	 77% 19% .
6	F	44	 64% 14% 23%
6	f	44	 57% 16% 27%
7	H	65	 89% 9% .
7	h	65	 91% 9%
8	I	38	 79% 18% .
8	i	38	 87% 11% .
9	J	39	 90% 8% .
9	j	39	 90% 10%
10	K	37	 78% 22%
10	k	37	 81% 19%
11	L	37	 89% 8% .
11	l	37	 86% 14%
12	M	36	 64% 25% 6% 6%
12	m	36	 69% 25% 6%
13	O	244	 86% 13%
13	o	244	 83% 17%
14	T	32	 69% 25% 6%
14	t	32	 84% 6% . 6%
15	U	104	 81% 12% 7%
15	u	104	 88% 6% 7%
16	V	137	 93% 7%

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Mol	Chain	Length	Quality of chain
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	34	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	HEC	V	202	X	-	-	-
40	HEC	v	202	X	-	-	-

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 54101 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
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	6	0
			2645	1737	432	461	15			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4021	2639	667	702	13			
2	b	503	Total	C	N	O	S	0	12	0
			4022	2644	664	701	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	6	0
			3544	2323	589	619	13			

There are 8 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	See sequence details	UNP D0VWR7
C	22	PHE	-	See sequence details	UNP D0VWR7
c	19	ASN	-	See sequence details	UNP D0VWR7
c	20	SER	-	See sequence details	UNP D0VWR7
c	21	ILE	-	See sequence details	UNP D0VWR7
c	22	PHE	-	See sequence details	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	1	0
			519	346	85	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			
14	t	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

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

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

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

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

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

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

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

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

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

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

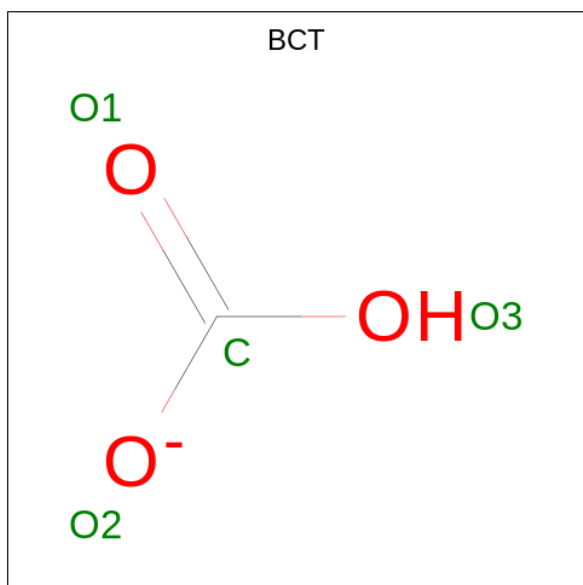
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	U	1	Total	Cl	0	0
			1	1		

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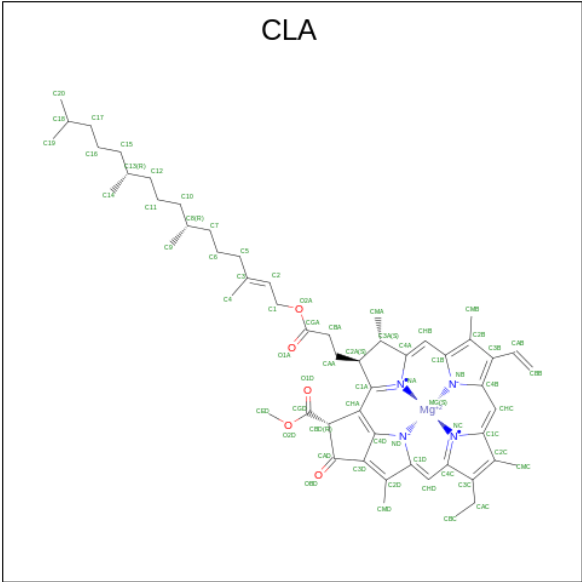
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	2	Total	Cl	0	0
			2	2		
22	v	1	Total	Cl	0	0
			1	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			4	1	3		
23	d	1	Total	C	O	0	0
			4	1	3		

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



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

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

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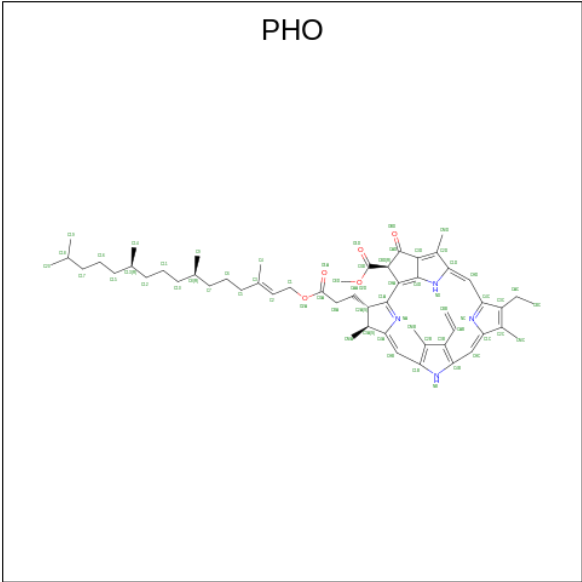
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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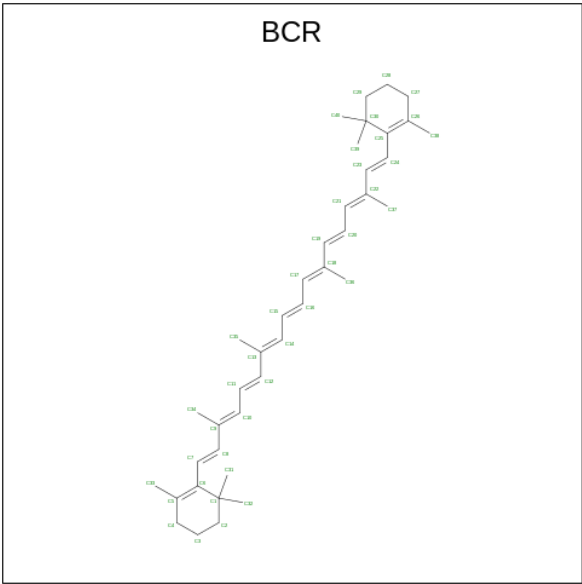
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N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

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



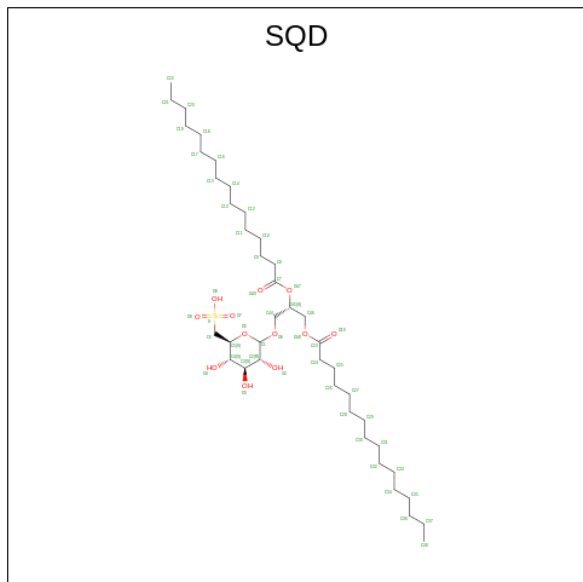
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



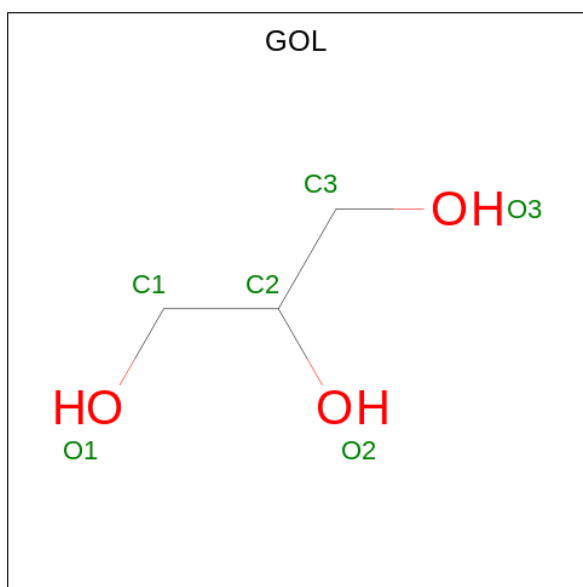
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			43	30	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			43	30	12	1		

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



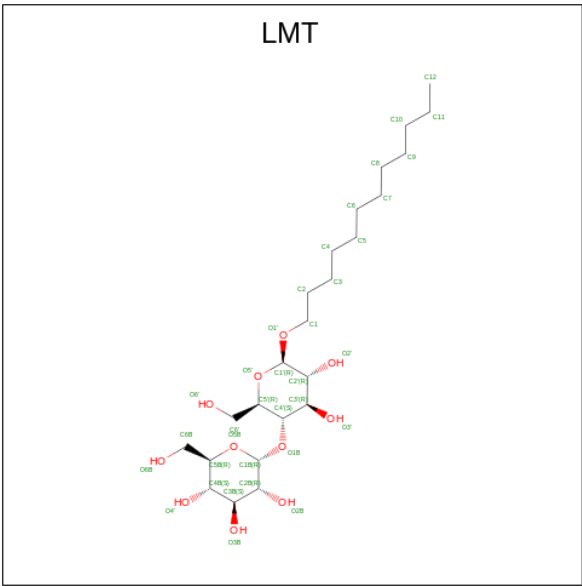
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28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

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

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



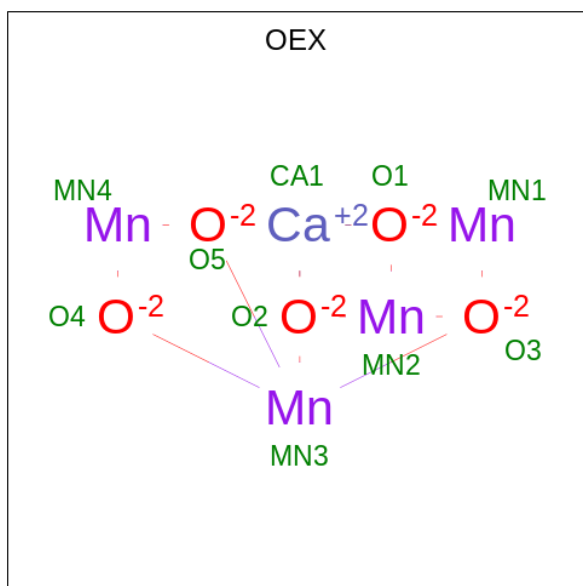
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	C	1	Total	C	O	0	0
			35	24	11		
29	D	1	Total	C	O	0	0
			35	24	11		
29	F	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	b	1	Total	C	O	0	0
			25	19	6		
29	b	1	Total	C	O	0	0
			25	19	6		
29	e	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		

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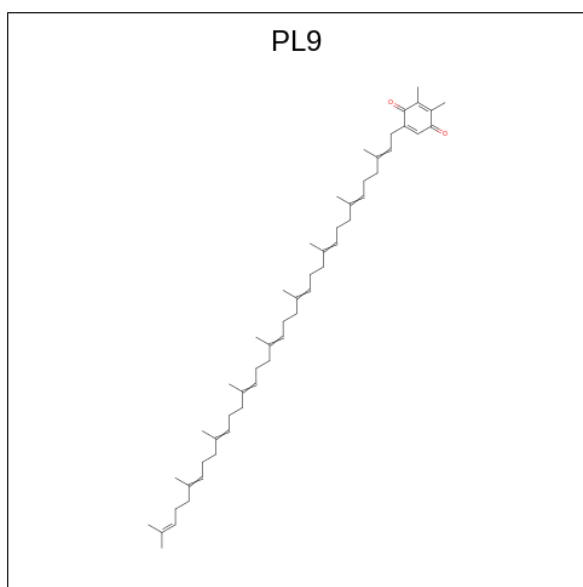
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	t	1	Total	C	O	0	0
			25	19	6		

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



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

- Molecule 31 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



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

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

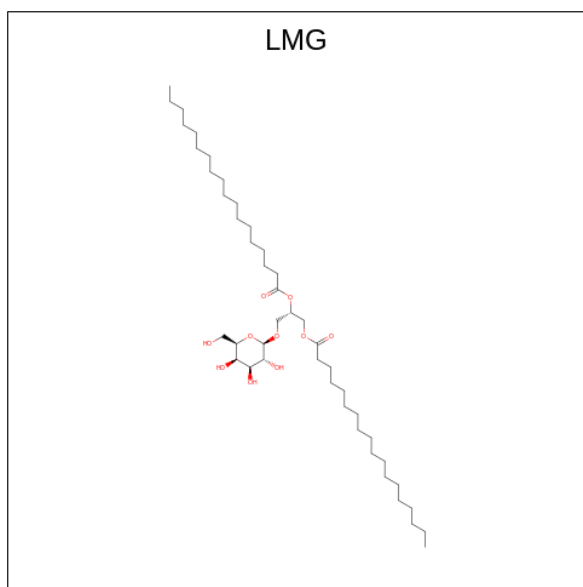
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			28	23	5		
32	B	1	Total	C	O	0	0
			33	28	5		
32	C	1	Total	C	O	0	0
			34	29	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	I	1	Total	C	O	0	0
			40	35	5		
32	J	1	Total	C		0	0
			10	10			
32	M	1	Total	C		0	0
			10	10			
32	X	1	Total	C	O	0	0
		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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	a	1	Total	C	O	0	0
			30	25	5		
32	b	1	Total	C	O	0	0
			33	28	5		
32	c	1	Total	C	O	0	0
			32	27	5		
32	d	2	Total	C	O	0	0
			53	47	6		
32	i	1	Total	C	O	0	0
			40	35	5		
32	j	1	Total	C		0	0
			10	10			
32	m	1	Total	C		0	0
			10	10			
32	x	1	Total	C	O	0	0
			18	16	2		

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



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

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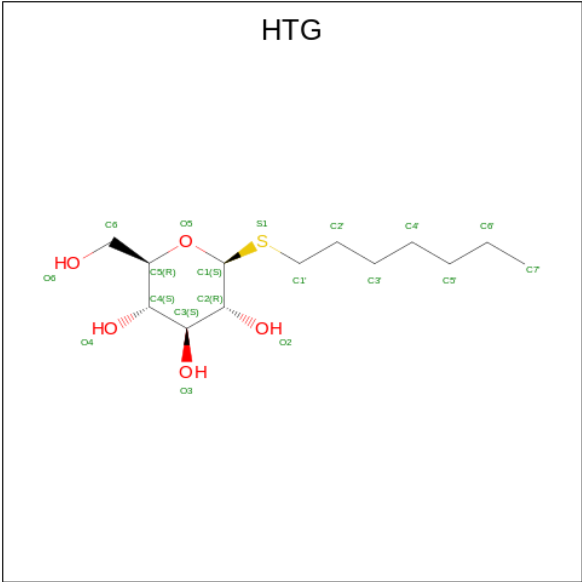
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	J	1	Total C O 51 41 10	0	0
33	Y	1	Total C O 51 41 10	0	0
33	Z	1	Total C O 37 27 10	0	0
33	a	1	Total C O 51 41 10	0	0
33	b	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0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

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

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

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



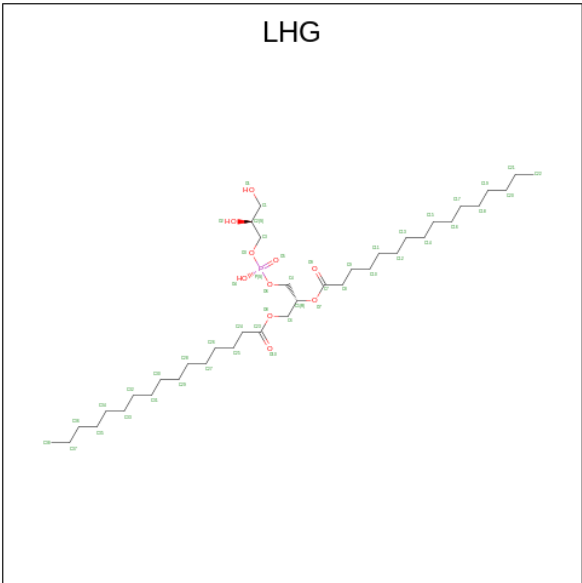
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19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

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

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



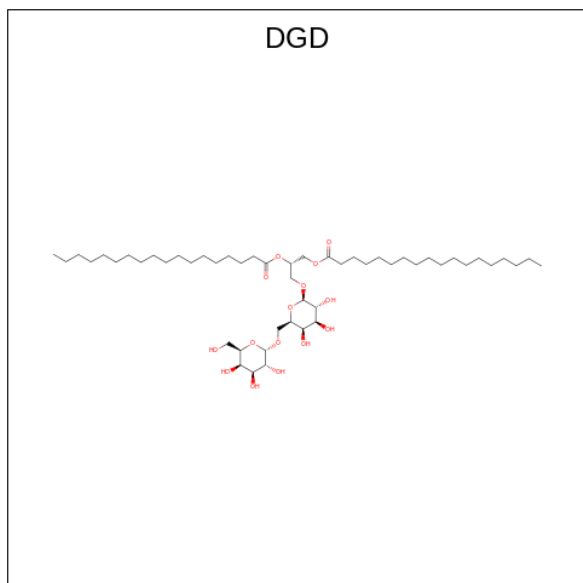
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	E	1	Total	C	O	P	0	0
			42	31	10	1		
36	L	1	Total	C	O	P	0	0
			49	38	10	1		
36	a	1	Total	C	O	P	0	0
			42	31	10	1		
36	b	1	Total	C	O	P	0	0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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



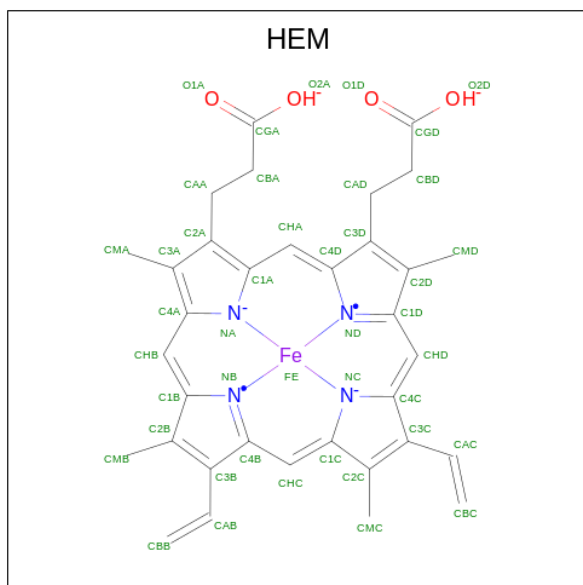
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	D	1	Total	C	O	0	0
			52	42	10		
37	H	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total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

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

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

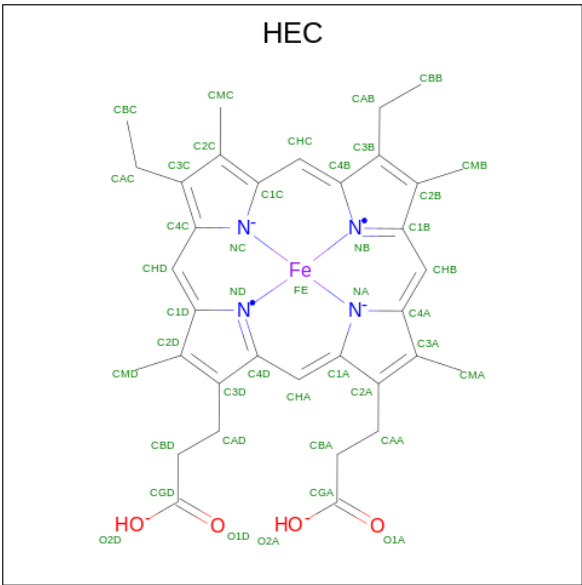


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	164	Total	O	0	3
			167	167		
41	B	295	Total	O	0	4
			299	299		
41	C	232	Total	O	0	2
			234	234		
41	D	140	Total	O	0	4
			144	144		
41	E	30	Total	O	0	1
			31	31		
41	F	10	Total	O	0	0
			10	10		
41	H	48	Total	O	0	0
			48	48		
41	I	6	Total	O	0	0
			6	6		
41	J	12	Total	O	0	0
			12	12		
41	K	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	14	Total O 15 15	0	1
41	M	13	Total O 13 13	0	0
41	O	179	Total O 181 181	0	2
41	T	16	Total O 17 17	0	1
41	U	80	Total O 80 80	0	0
41	V	114	Total O 116 116	0	2
41	Y	4	Total O 4 4	0	0
41	X	9	Total O 9 9	0	0
41	Z	1	Total O 1 1	0	0
41	a	158	Total O 159 159	0	1
41	b	262	Total O 265 265	0	3
41	c	207	Total O 210 210	0	3
41	d	129	Total O 132 132	0	3
41	e	19	Total O 19 19	0	0
41	f	6	Total O 6 6	0	0
41	h	40	Total O 40 40	0	0
41	i	4	Total O 4 4	0	0
41	j	6	Total O 6 6	0	0
41	k	7	Total O 7 7	0	0
41	l	10	Total O 10 10	0	0
41	m	15	Total O 15 15	0	0

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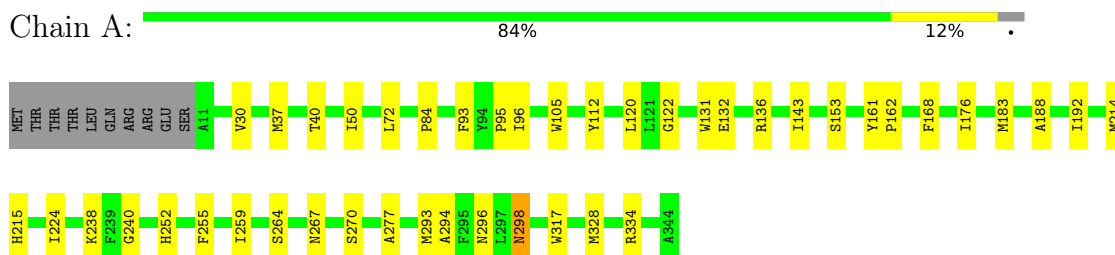
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	o	155	Total 155	O 155	0	0
41	t	11	Total 11	O 11	0	0
41	u	97	Total 97	O 97	0	0
41	v	77	Total 78	O 78	0	1
41	y	2	Total 2	O 2	0	0
41	x	6	Total 6	O 6	0	0

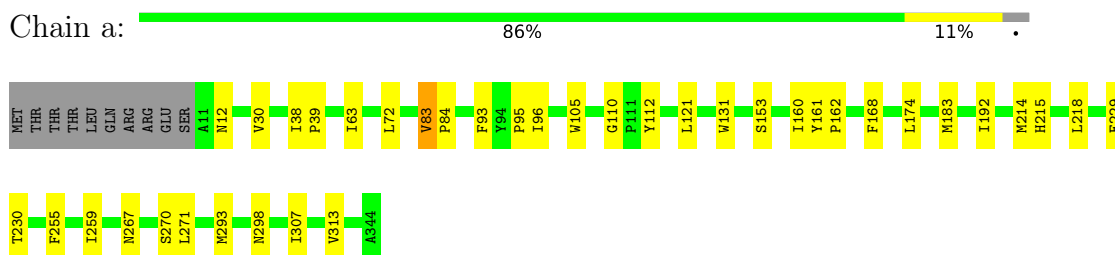
3 Residue-property plots

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

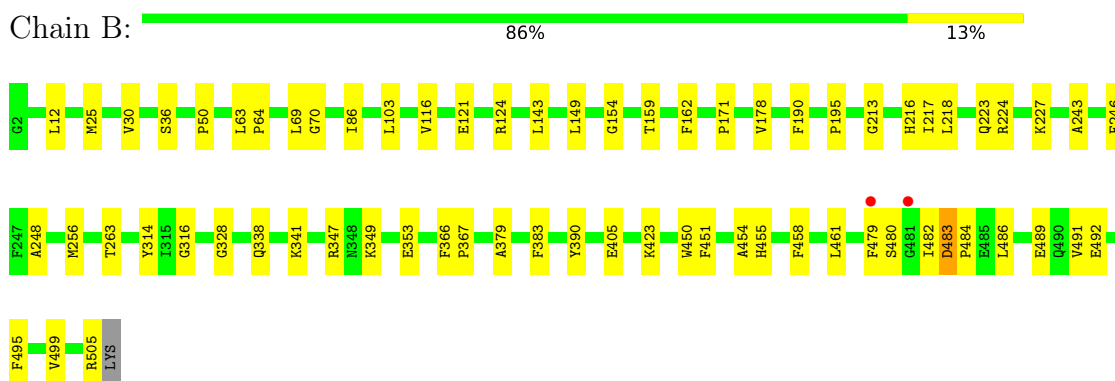
- Molecule 1: Photosystem II protein D1



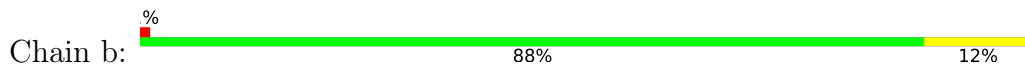
- Molecule 1: Photosystem II protein D1

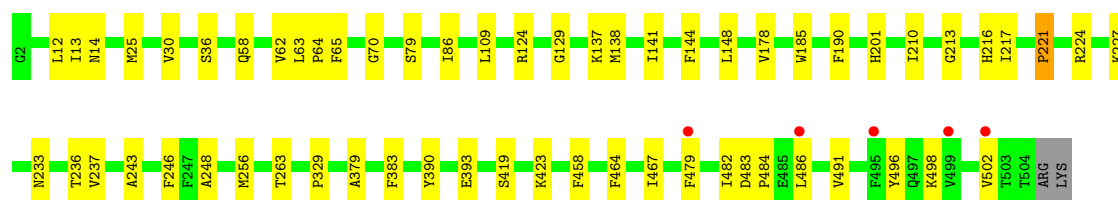


- Molecule 2: Photosystem II CP47 reaction center protein



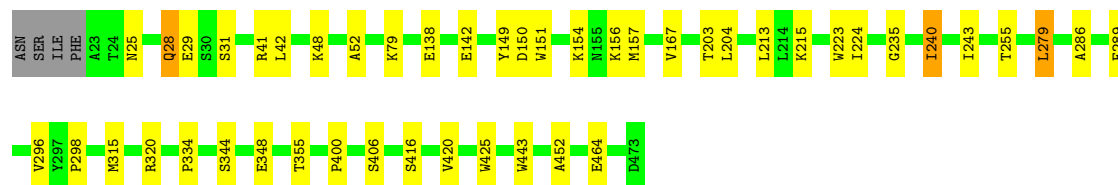
- Molecule 2: Photosystem II CP47 reaction center protein





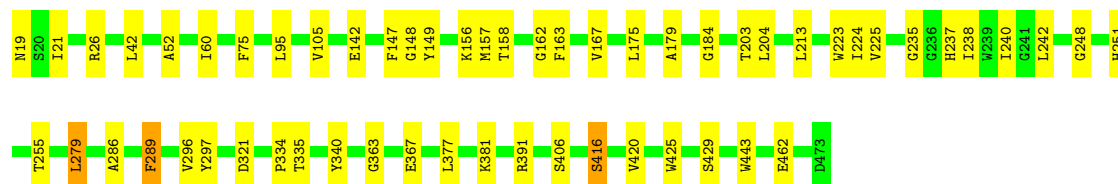
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 89% 10% ..



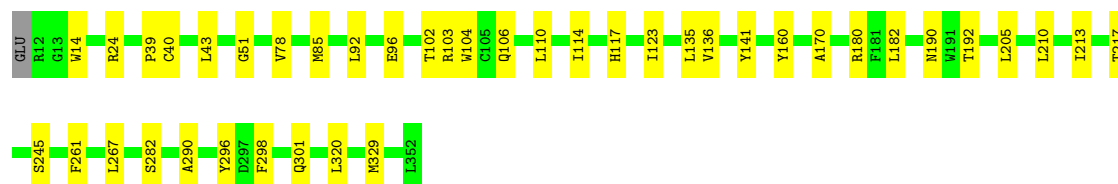
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 87% 12% .



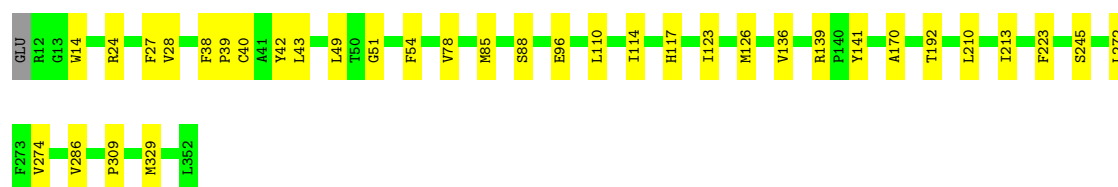
• Molecule 4: Photosystem II D2 protein

Chain D: 88% 12%

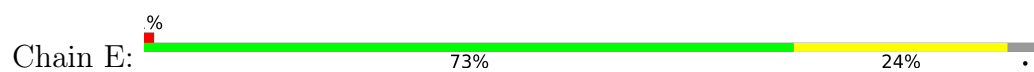


• Molecule 4: Photosystem II D2 protein

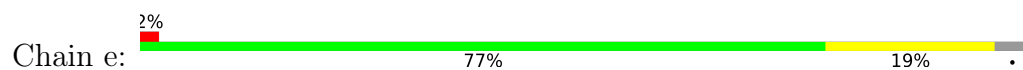
Chain d: 89% 10%



• Molecule 5: Cytochrome b559 subunit alpha



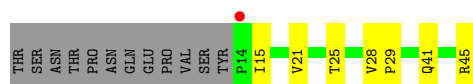
- Molecule 5: Cytochrome b559 subunit alpha



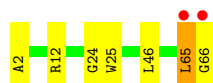
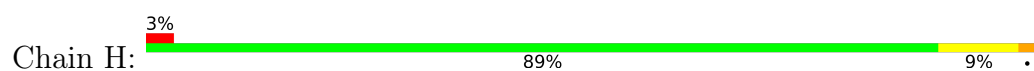
- Molecule 6: Cytochrome b559 subunit beta



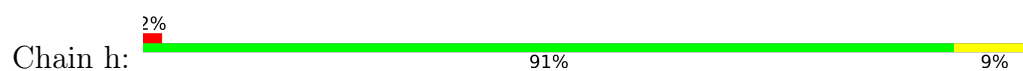
- Molecule 6: Cytochrome b559 subunit beta



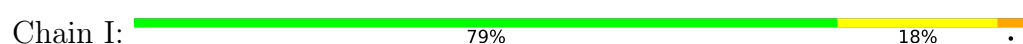
- Molecule 7: Photosystem II reaction center protein H



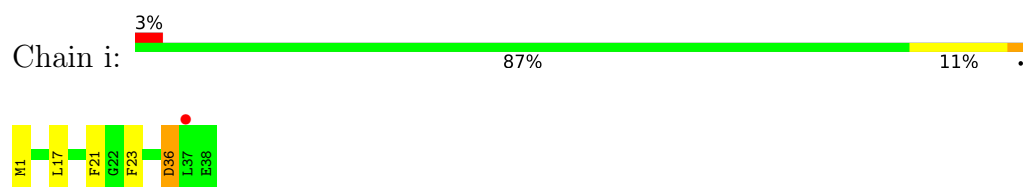
- Molecule 7: Photosystem II reaction center protein H



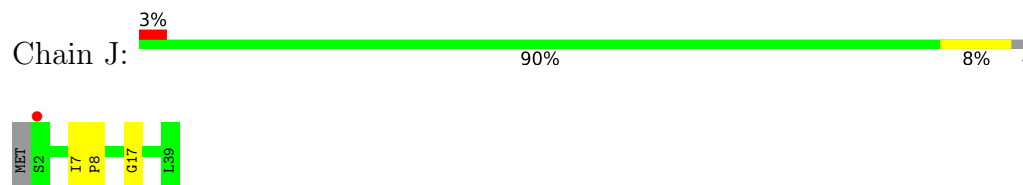
- Molecule 8: Photosystem II reaction center protein I



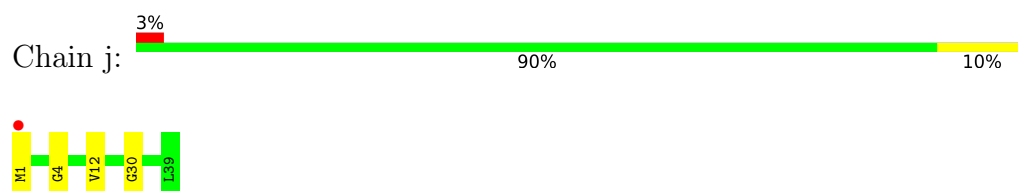
- Molecule 8: Photosystem II reaction center protein I



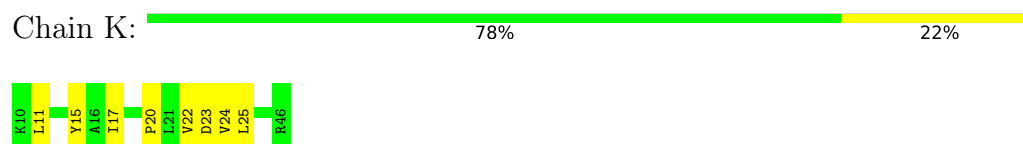
- Molecule 9: Photosystem II reaction center protein J



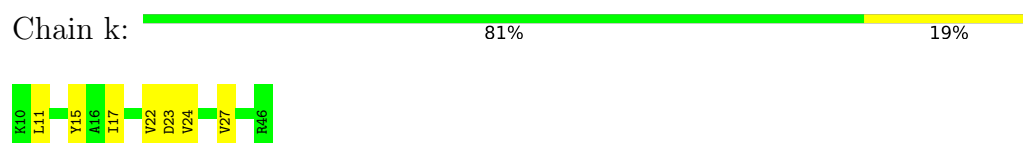
- Molecule 9: Photosystem II reaction center protein J



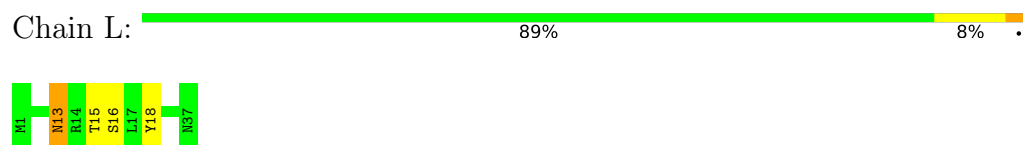
- Molecule 10: Photosystem II reaction center protein K



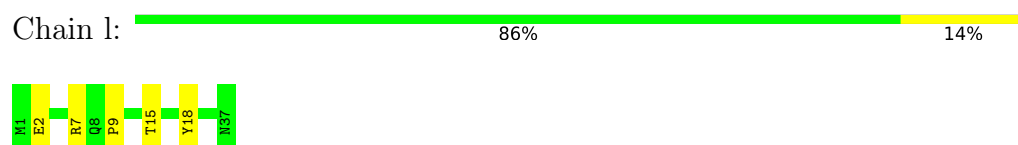
- Molecule 10: Photosystem II reaction center protein K



- 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:  64% 25% 6% 6%



- Molecule 12: Photosystem II reaction center protein M

Chain m:  69% 25% 6%



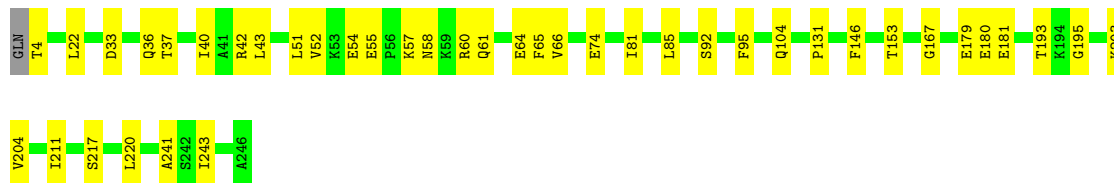
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  86% 13%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  83% 17%



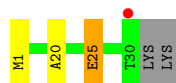
- Molecule 14: Photosystem II reaction center protein T

Chain T:  3% 69% 25% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 84% 6% 6%

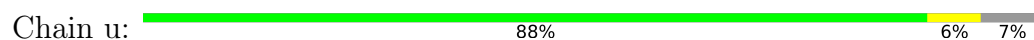


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  81% 12% 7%



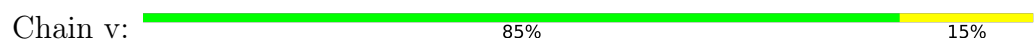
- Molecule 15: Photosystem II 12 kDa extrinsic protein



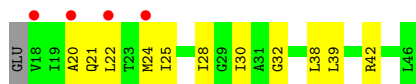
- Molecule 16: Cytochrome c-550



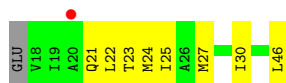
- Molecule 16: Cytochrome c-550



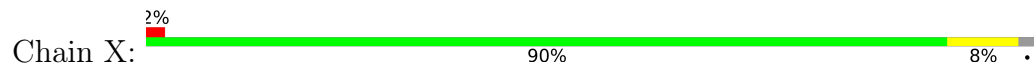
- Molecule 17: Photosystem II reaction center protein Ycf12



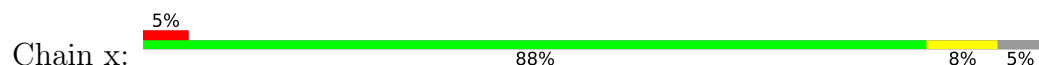
- Molecule 17: Photosystem II reaction center protein Ycf12

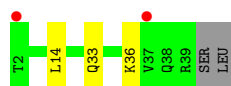


- Molecule 18: Photosystem II reaction center protein X

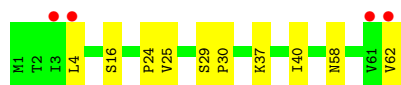
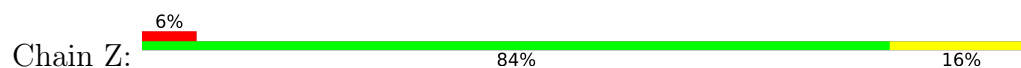


- Molecule 18: Photosystem II reaction center protein X

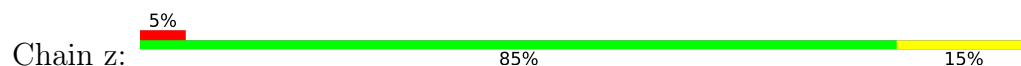




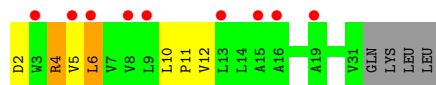
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.04Å 228.84Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.35 19.99 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.35) 99.8 (19.99-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.153 , 0.209 0.172 , 0.222	Depositor DCC
R_{free} test set	17809 reflections (3.30%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 95.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	54101	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.59	0/2728	0.87	1/3719 (0.0%)
1	a	0.59	0/2748	0.88	2/3746 (0.1%)
2	B	0.54	0/4191	0.84	4/5709 (0.1%)
2	b	0.54	0/4198	0.83	2/5720 (0.0%)
3	C	0.50	0/3626	0.82	0/4936
3	c	0.49	0/3676	0.81	0/5004
4	D	0.58	0/2818	0.84	2/3840 (0.1%)
4	d	0.57	1/2818 (0.0%)	0.84	4/3840 (0.1%)
5	E	0.51	0/693	0.81	0/944
5	e	0.47	0/695	0.87	0/948
6	F	0.59	0/284	0.83	0/387
6	f	0.55	0/265	0.80	0/360
7	H	0.47	0/535	0.87	0/728
7	h	0.47	0/524	0.79	0/713
8	I	0.47	0/311	0.76	0/419
8	i	0.52	0/311	0.76	0/419
9	J	0.47	0/278	0.77	0/376
9	j	0.44	0/286	0.77	0/386
10	K	0.48	0/303	0.85	0/416
10	k	0.55	0/303	0.83	0/416
11	L	0.53	0/319	0.77	0/433
11	l	0.53	0/319	0.71	0/433
12	M	0.68	0/270	1.15	3/368 (0.8%)
12	m	0.65	0/262	1.02	2/357 (0.6%)
13	O	0.47	0/1958	0.80	2/2654 (0.1%)
13	o	0.47	0/1937	0.84	4/2625 (0.2%)
14	T	0.54	0/266	0.77	0/362
14	t	0.59	0/266	0.74	0/362
15	U	0.50	0/785	0.76	0/1064
15	u	0.48	0/785	0.77	0/1064
16	V	0.50	0/1096	0.83	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.49	0/1085	0.85	1/1473 (0.1%)
17	Y	0.51	0/216	0.89	0/289
17	y	0.46	0/216	0.78	0/289
18	X	0.45	0/290	0.79	0/392
18	x	0.45	0/284	0.73	0/384
19	Z	0.42	0/490	0.81	0/669
19	z	0.43	0/490	0.86	0/669
20	R	0.35	0/245	0.69	0/338
All	All	0.53	1/43170 (0.0%)	0.83	27/58738 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	274	VAL	CA-C	5.03	1.58	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	170	ALA	CA-C-N	-7.52	112.24	119.76
4	d	170	ALA	C-N-CA	-7.52	112.24	119.76
4	D	170	ALA	CA-C-N	-6.39	113.37	119.76
4	D	170	ALA	C-N-CA	-6.39	113.37	119.76
16	v	105	ARG	N-CA-C	6.12	118.46	111.11
12	m	17	VAL	CA-C-N	-5.85	112.47	118.85
12	m	17	VAL	C-N-CA	-5.85	112.47	118.85
2	B	483	ASP	CA-C-N	5.59	125.43	119.28
2	B	483	ASP	C-N-CA	5.59	125.43	119.28
1	a	110	GLY	O-C-N	5.53	123.06	121.07
2	B	328	GLY	CA-C-N	5.35	125.33	120.03
2	B	328	GLY	C-N-CA	5.35	125.33	120.03
12	M	17	VAL	CA-C-N	-5.31	113.06	118.85
12	M	17	VAL	C-N-CA	-5.31	113.06	118.85
13	O	55	GLU	CA-C-N	5.21	125.50	119.92
13	O	55	GLU	C-N-CA	5.21	125.50	119.92
4	d	38	PHE	CA-C-N	-5.20	113.27	119.05
4	d	38	PHE	C-N-CA	-5.20	113.27	119.05
12	M	9	ILE	N-CA-C	-5.17	105.35	110.62
13	o	55	GLU	CA-C-N	5.11	125.83	120.11
13	o	55	GLU	C-N-CA	5.11	125.83	120.11
2	b	13	ILE	N-CA-C	5.09	115.81	110.62
2	b	221	PRO	O-C-N	5.06	123.53	121.15
13	o	104	GLN	CA-C-N	-5.05	114.71	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	104	GLN	C-N-CA	-5.05	114.71	119.76
1	a	83	VAL	N-CA-C	5.04	112.97	108.63
1	A	298	ASN	N-CA-C	5.00	117.80	109.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2634	0	2546	33	0
1	a	2645	0	2567	27	0
2	B	4021	0	3898	56	0
2	b	4022	0	3908	49	0
3	C	3501	0	3428	33	0
3	c	3544	0	3479	33	0
4	D	2720	0	2626	29	0
4	d	2720	0	2626	27	0
5	E	668	0	658	13	0
5	e	670	0	664	13	0
6	F	275	0	282	5	0
6	f	257	0	269	5	0
7	H	519	0	545	10	0
7	h	511	0	532	8	0
8	I	314	0	328	5	0
8	i	314	0	328	2	0
9	J	272	0	279	3	0
9	j	280	0	291	3	0
10	K	293	0	305	7	0
10	k	293	0	305	6	0
11	L	309	0	327	3	0
11	l	309	0	327	5	0
12	M	274	0	299	8	0
12	m	269	0	288	7	0
13	O	1903	0	1886	18	0
13	o	1891	0	1870	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	T	264	0	267	6	0
14	t	264	0	267	2	0
15	U	774	0	773	6	1
15	u	774	0	773	4	0
16	V	1072	0	1086	6	0
16	v	1064	0	1073	11	0
17	Y	215	0	246	9	0
17	y	215	0	246	6	0
18	X	287	0	317	3	0
18	x	281	0	312	2	0
19	Z	479	0	516	8	0
19	z	479	0	516	10	0
20	R	239	0	262	5	0
21	A	1	0	0	0	0
21	d	1	0	0	0	0
22	A	2	0	0	0	0
22	U	1	0	0	1	0
22	a	2	0	0	0	0
22	v	1	0	0	0	0
23	A	4	0	0	0	0
23	d	4	0	0	0	0
24	A	260	0	288	12	0
24	B	1040	0	1152	42	0
24	C	845	0	936	38	0
24	D	130	0	144	5	0
24	a	195	0	216	7	0
24	b	1040	0	1152	42	0
24	c	845	0	936	44	0
24	d	195	0	216	11	0
25	A	64	0	74	2	0
25	D	64	0	74	3	0
25	a	64	0	74	3	0
25	d	64	0	74	3	0
26	A	40	0	56	1	0
26	B	120	0	168	10	0
26	C	80	0	112	9	0
26	D	40	0	56	1	0
26	H	40	0	56	4	0
26	K	40	0	56	2	0
26	T	40	0	56	4	0
26	Y	40	0	56	6	0
26	a	40	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	b	120	0	168	5	0
26	c	80	0	112	8	0
26	d	40	0	56	4	0
26	h	40	0	56	5	0
26	k	40	0	56	1	0
26	t	40	0	56	5	0
26	y	40	0	56	1	0
27	A	108	0	156	7	0
27	B	54	0	78	3	0
27	F	43	0	53	3	0
27	L	54	0	78	4	0
27	a	108	0	156	5	0
27	f	43	0	53	2	1
28	A	12	0	16	0	0
28	B	42	0	56	1	0
28	C	12	0	16	1	0
28	D	6	0	8	1	0
28	O	6	0	8	0	0
28	T	12	0	16	4	0
28	V	30	0	39	1	0
28	a	18	0	23	2	0
28	b	30	0	40	2	0
28	c	18	0	24	0	0
28	l	6	0	8	1	0
28	v	18	0	24	1	0
29	A	35	0	46	3	0
29	C	35	0	46	1	0
29	D	35	0	46	1	0
29	F	35	0	46	0	0
29	M	70	0	92	4	0
29	a	70	0	92	2	0
29	b	50	0	70	2	0
29	e	35	0	46	1	0
29	m	70	0	92	5	0
29	t	25	0	35	0	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	A	55	0	80	7	0
31	D	55	0	80	0	0
31	a	55	0	80	11	0
31	d	55	0	80	1	0
32	A	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	B	33	0	0	0	0
32	C	34	0	0	0	0
32	D	57	0	0	0	0
32	I	40	0	0	0	0
32	J	10	0	0	0	0
32	M	10	0	0	0	0
32	X	18	0	0	0	0
32	a	30	0	0	0	0
32	b	33	0	0	0	0
32	c	32	0	0	0	0
32	d	53	0	0	0	0
32	i	40	0	0	0	0
32	j	10	0	0	0	0
32	m	10	0	0	0	0
32	x	18	0	0	0	0
33	A	51	0	72	6	0
33	B	51	0	72	3	0
33	C	51	0	72	2	0
33	J	51	0	72	0	0
33	Y	51	0	72	2	0
33	Z	37	0	44	3	0
33	a	51	0	72	2	0
33	b	51	0	72	4	0
33	c	102	0	144	6	0
33	d	51	0	72	3	0
33	z	39	0	48	5	0
34	B	1	0	0	0	0
34	C	1	0	0	0	0
34	F	1	0	0	0	0
34	O	1	0	0	0	0
34	b	1	0	0	0	0
34	c	2	0	0	0	0
34	f	1	0	0	0	0
34	o	1	0	0	0	0
35	B	95	0	130	0	0
35	C	38	0	52	0	0
35	D	16	0	17	3	0
35	V	19	0	26	2	0
35	b	95	0	130	3	0
35	c	38	0	52	1	0
35	d	16	0	17	2	0
36	B	49	0	74	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	D	98	0	148	8	0
36	E	42	0	57	1	0
36	L	49	0	74	0	0
36	a	42	0	57	6	0
36	b	49	0	74	5	0
36	d	147	0	222	10	0
37	C	186	0	246	7	0
37	D	52	0	71	4	0
37	H	62	0	82	1	0
37	c	186	0	246	9	0
37	e	62	0	82	5	0
37	h	62	0	82	2	0
38	F	43	0	30	3	0
38	f	43	0	30	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	167	0	0	3	0
41	B	299	0	0	3	0
41	C	234	0	0	4	0
41	D	144	0	0	1	0
41	E	31	0	0	1	0
41	F	10	0	0	0	0
41	H	48	0	0	0	0
41	I	6	0	0	1	0
41	J	12	0	0	0	0
41	K	7	0	0	1	0
41	L	15	0	0	0	0
41	M	13	0	0	1	0
41	O	181	0	0	4	0
41	T	17	0	0	1	0
41	U	80	0	0	1	0
41	V	116	0	0	1	0
41	X	9	0	0	0	0
41	Y	4	0	0	0	0
41	Z	1	0	0	0	0
41	a	159	0	0	1	0
41	b	265	0	0	1	0
41	c	210	0	0	0	0
41	d	132	0	0	3	0
41	e	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	f	6	0	0	1	0
41	h	40	0	0	1	0
41	i	4	0	0	0	0
41	j	6	0	0	0	0
41	k	7	0	0	0	0
41	l	10	0	0	1	0
41	m	15	0	0	2	0
41	o	155	0	0	4	0
41	t	11	0	0	0	0
41	u	97	0	0	1	0
41	v	78	0	0	1	0
41	x	6	0	0	0	0
41	y	2	0	0	0	0
All	All	54101	0	52737	685	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (685) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:MET:HG2	31:A:417:PL9:H102	1.42	0.99
24:B:616:CLA:H71	24:B:617:CLA:H192	1.51	0.90
24:c:904:CLA:HBB1	24:c:913:CLA:H41	1.58	0.84
24:c:914:CLA:HHC	24:c:914:CLA:HBB1	1.65	0.78
33:a:411:LMG:H221	37:c:916:DGD:HA81	1.66	0.77
14:T:25[A]:GLU:HG3	28:T:101:GOL:H2	1.66	0.77
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.66	0.76
41:B:989:HOH:O	22:U:201:CL:CL	2.41	0.75
26:T:102:BCR:H19C	26:b:623:BCR:H363	1.69	0.75
3:c:279:LEU:HD22	24:c:910:CLA:HED2	1.68	0.75
6:f:45:ARG:OXT	41:f:201:HOH:O	2.03	0.75
24:c:906:CLA:HHC	24:c:906:CLA:HBB1	1.68	0.74
28:D:402:GOL:H11	12:M:1:FME:HG2	1.69	0.73
26:t:102:BCR:HC8	26:t:102:BCR:H321	1.70	0.73
36:d:411:LHG:H342	36:d:411:LHG:H151	1.69	0.73
24:c:902:CLA:H202	24:c:908:CLA:HBB1	1.69	0.73
3:C:149:TYR:HB2	3:C:157:MET:HE1	1.70	0.73
4:d:192:THR:HG23	24:d:405:CLA:HBC2	1.70	0.71
24:d:406:CLA:H162	7:h:33:VAL:HG13	1.71	0.71
36:a:418:LHG:HC31	5:e:9:PRO:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:505:CLA:CMD	24:C:507:CLA:HAB	2.21	0.70
2:B:248:ALA:HA	24:B:604:CLA:H42	1.72	0.70
24:B:615:CLA:H18	33:B:622:LMG:H421	1.74	0.70
1:a:215:HIS:ND1	31:a:415:PL9:O1	2.24	0.70
1:a:307[B]:ILE:HG22	1:a:313:VAL:HA	1.73	0.69
24:b:620:CLA:H2	24:b:621:CLA:HBB2	1.75	0.69
1:a:214:MET:HG2	31:a:415:PL9:H102	1.75	0.69
24:c:914:CLA:H171	26:c:927:BCR:H373	1.75	0.69
24:b:610:CLA:HHC	24:b:610:CLA:HBB1	1.74	0.68
2:B:480[B]:SER:OG	41:B:701:HOH:O	2.11	0.68
33:c:919:LMG:H181	10:k:27:VAL:HG11	1.76	0.68
15:u:51:LYS:NZ	41:u:201:HOH:O	2.25	0.68
28:a:419:GOL:H11	16:v:27:LEU:HD21	1.75	0.67
24:b:616:CLA:H142	36:b:635:LHG:H361	1.76	0.67
41:C:602:HOH:O	15:U:51:LYS:NZ	2.26	0.67
24:D:405:CLA:H171	18:X:15:LEU:HD13	1.77	0.67
28:b:631:GOL:H11	16:v:51:SER:HA	1.77	0.67
16:v:71:GLY:HA2	28:v:203:GOL:H31	1.77	0.67
2:B:30:VAL:HG12	24:B:606:CLA:HHD	1.77	0.67
4:D:192:THR:HG23	24:D:404:CLA:HBC2	1.76	0.66
1:a:72:LEU:HD11	29:a:401:LMT:H52	1.77	0.66
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.77	0.66
26:T:102:BCR:H321	26:T:102:BCR:HC8	1.77	0.66
24:c:906:CLA:CMD	24:c:908:CLA:HAB	2.25	0.66
24:B:617:CLA:HED2	24:B:617:CLA:H43	1.79	0.65
24:C:505:CLA:HBB1	24:C:505:CLA:HHC	1.79	0.65
13:O:27:ARG:NH1	13:O:202:ALA:O	2.30	0.65
33:b:625:LMG:O2	41:b:702:HOH:O	2.15	0.65
12:m:6:LEU:HD11	29:m:103:LMT:H11	1.78	0.65
2:b:248:ALA:HA	24:b:608:CLA:H42	1.79	0.65
16:V:96:ARG:HH21	35:V:203:HTG:H6'1	1.62	0.64
24:c:909:CLA:HBC3	24:c:911:CLA:H71	1.79	0.64
4:D:14:TRP:CD1	35:D:413:HTG:HO6	2.15	0.64
24:a:406:CLA:H203	33:d:415:LMG:H412	1.78	0.64
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.29	0.63
28:T:103:GOL:O1	41:T:201:HOH:O	2.15	0.63
11:L:13:ASN:ND2	11:L:16:SER:H	1.96	0.63
29:M:101:LMT:H6'2	11:l:9:PRO:HB3	1.81	0.63
2:B:341:LYS:HA	2:B:405[A]:GLU:HG2	1.80	0.62
2:b:62:VAL:HB	24:b:610:CLA:HED3	1.81	0.62
24:C:503:CLA:HBB1	24:C:512:CLA:H41	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:213[B]:LEU:HD11	26:c:915:BCR:H373	1.81	0.62
36:D:410:LHG:H151	36:D:410:LHG:H352	1.82	0.62
24:C:513:CLA:H171	26:C:514:BCR:H373	1.81	0.61
3:c:26:ARG:NH2	17:y:46:LEU:OXT	2.33	0.61
31:a:415:PL9:H262	36:a:418:LHG:H201	1.82	0.61
36:D:410:LHG:H132	36:D:410:LHG:H372	1.83	0.61
1:A:298:ASN:ND2	41:A:503:HOH:O	2.33	0.60
24:B:609:CLA:HAB	4:D:123:ILE:HG12	1.83	0.60
5:E:59:GLU:OE2	41:E:201:HOH:O	2.17	0.60
1:a:271:LEU:HD11	31:a:415:PL9:HC8	1.83	0.60
2:B:482:ILE:HD12	2:B:486:LEU:HD22	1.84	0.60
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.37	0.60
24:C:505:CLA:HMD3	24:C:507:CLA:HAB	1.83	0.60
2:b:12:LEU:HB2	24:b:617:CLA:HMC2	1.83	0.60
27:A:414:SQD:H272	2:b:109:LEU:HD13	1.84	0.60
5:E:40:THR:HB	20:R:4:ARG:HG2	1.83	0.60
10:K:15:TYR:OH	19:Z:58:ASN:ND2	2.34	0.60
3:c:148:GLY:O	3:c:156:LYS:NZ	2.28	0.60
3:C:48:LYS:HG3	3:C:138:GLU:HG3	1.84	0.59
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.84	0.59
13:o:74[B]:GLU:OE1	41:o:401:HOH:O	2.16	0.59
24:b:606:CLA:HBA2	24:b:606:CLA:H101	1.84	0.59
10:k:15:TYR:OH	19:z:58:ASN:ND2	2.31	0.59
24:c:905:CLA:H201	36:d:411:LHG:H352	1.85	0.59
27:A:411:SQD:H251	36:D:410:LHG:H131	1.83	0.59
24:c:909:CLA:H141	24:c:911:CLA:H203	1.83	0.59
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.84	0.59
19:z:47:TRP:CE2	33:z:101:LMG:H241	2.38	0.59
20:R:2:ASP:HB3	20:R:5:VAL:HG23	1.84	0.58
24:b:613:CLA:HAB	4:d:123:ILE:HG12	1.85	0.58
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.85	0.58
2:B:12:LEU:HB2	24:B:613:CLA:HMC2	1.85	0.58
13:O:99[A]:ASP:OD1	41:O:401:HOH:O	2.17	0.58
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.84	0.58
24:B:615:CLA:H42	29:m:102:LMT:H61	1.85	0.58
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.86	0.58
24:B:605:CLA:H43	24:B:606:CLA:H2	1.85	0.58
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.86	0.58
27:a:410:SQD:H301	24:c:909:CLA:H71	1.86	0.58
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.86	0.58
1:a:84:PRO:HA	1:a:112:TYR:CG	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:d:407:BCR:H313	37:e:101:DGD:HA91	1.86	0.57
13:o:180:GLU:OE2	41:o:402:HOH:O	2.17	0.57
33:A:419:LMG:H382	37:C:516:DGD:HB42	1.87	0.57
27:a:410:SQD:H271	36:d:411:LHG:H141	1.86	0.57
37:e:101:DGD:HAW1	27:f:102:SQD:H382	1.86	0.57
36:D:410:LHG:H112	36:D:410:LHG:H382	1.86	0.57
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.40	0.56
3:C:286:ALA:HB2	24:C:502:CLA:HMD1	1.87	0.56
31:a:415:PL9:H28	36:a:418:LHG:H222	1.85	0.56
3:c:213[A]:LEU:HG	24:c:907:CLA:H202	1.86	0.56
26:b:622:BCR:H12C	33:b:625:LMG:C43	2.36	0.56
1:A:240:GLY:HA3	14:T:29:ILE:HG23	1.88	0.56
24:b:618:CLA:HMB1	24:b:618:CLA:HBB1	1.86	0.56
3:c:406:SER:HA	3:c:420:VAL:HG23	1.87	0.56
1:A:72:LEU:HD13	29:A:415:LMT:H11	1.87	0.56
1:a:183:MET:HA	24:a:405:CLA:HMD1	1.88	0.56
2:B:171:PRO:HD3	7:H:66:GLY:HA2	1.87	0.56
1:A:238[A]:LYS:HG2	14:T:30:THR:HG21	1.87	0.56
2:b:30:VAL:HG12	24:b:610:CLA:HHD	1.87	0.56
2:B:195:PRO:HD2	7:H:65:LEU:HD11	1.88	0.56
3:C:279:LEU:HD22	24:C:509:CLA:HED2	1.87	0.55
24:B:607:CLA:H191	26:B:620:BCR:H363	1.88	0.55
24:c:912:CLA:H171	19:z:20:VAL:HA	1.88	0.55
37:C:517:DGD:HB51	33:Y:101:LMG:H392	1.89	0.55
24:C:506:CLA:HBA2	24:C:507:CLA:H202	1.89	0.55
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.89	0.55
3:C:79:LYS:HG2	16:V:103:LYS:HD3	1.87	0.55
33:c:920:LMG:H321	26:c:927:BCR:H342	1.88	0.55
24:A:407:CLA:HMD3	4:D:182:LEU:HD11	1.88	0.55
33:a:411:LMG:H242	24:c:906:CLA:H92	1.89	0.55
37:e:101:DGD:HE3	37:e:101:DGD:HD4	1.89	0.55
25:A:408:PHO:HAB	4:D:205:LEU:HD13	1.88	0.54
3:c:429:SER:HA	37:c:917:DGD:HBW1	1.88	0.54
24:c:909:CLA:H191	33:c:919:LMG:H232	1.89	0.54
2:B:349:LYS:NZ	41:B:823[B]:HOH:O	2.39	0.54
4:d:139:ARG:NH2	41:d:504:HOH:O	2.39	0.54
12:m:5:GLN:OE1	41:m:201:HOH:O	2.18	0.54
26:y:101:BCR:H321	26:y:101:BCR:HC8	1.89	0.54
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.43	0.54
1:a:153:SER:HB2	24:a:405:CLA:H43	1.90	0.54
31:a:415:PL9:H512	27:f:102:SQD:H302	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:902:CLA:C4D	24:c:904:CLA:H2	2.38	0.54
4:d:141:TYR:OH	36:d:409:LHG:O4	2.22	0.53
16:v:81:THR:HG21	16:v:86:GLN:HE21	1.73	0.53
9:J:17:GLY:HA3	26:Y:102:BCR:H371	1.91	0.53
3:c:321:ASP:OD2	3:c:340:TYR:OH	2.24	0.53
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.90	0.53
2:B:36[A]:SER:OG	26:B:619:BCR:H362	2.08	0.53
13:O:204:VAL:HG22	13:O:211:ILE:HG22	1.89	0.53
24:C:501:CLA:C4D	24:C:503:CLA:H2	2.39	0.53
2:B:50:PRO:HB2	28:B:630:GOL:H12	1.91	0.53
24:D:405:CLA:HAC1	27:F:103:SQD:H383	1.91	0.53
13:O:180:GLU:CD	13:O:180:GLU:H	2.16	0.53
8:I:37:LEU:O	41:I:201:HOH:O	2.19	0.53
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.08	0.53
3:C:334:PRO:HA	13:O:153:THR:OG1	2.09	0.52
31:A:417:PL9:H261	36:E:101:LHG:H223	1.92	0.52
26:B:618:BCR:H383	27:B:621:SQD:H101	1.92	0.52
28:T:103:GOL:H2	29:m:103:LMT:H6D	1.90	0.52
37:e:101:DGD:HB71	37:e:101:DGD:HBW2	1.90	0.52
4:d:85:MET:CE	4:d:96:GLU:HG2	2.40	0.52
24:d:406:CLA:H142	7:h:36:GLY:HA3	1.92	0.52
24:A:405:CLA:CBD	24:A:406:CLA:HAC2	2.39	0.52
24:A:407:CLA:H122	31:A:417:PL9:H252	1.91	0.52
24:b:616:CLA:H141	36:b:635:LHG:H382	1.89	0.52
16:V:30:LYS:NZ	41:V:302:HOH:O	2.27	0.52
2:B:190:PHE:HZ	24:B:603:CLA:HBB1	1.75	0.52
2:B:216:HIS:HE1	24:B:610:CLA:C1A	2.22	0.52
3:C:320:ARG:HB2	28:C:523:GOL:H32	1.91	0.52
2:B:149:LEU:HD21	24:B:607:CLA:HBB2	1.91	0.52
2:b:216:HIS:HE1	24:b:614:CLA:C1A	2.22	0.52
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.45	0.52
31:a:415:PL9:HC2	31:a:415:PL9:H103	1.92	0.52
15:U:16:LYS:NZ	41:U:303:HOH:O	2.43	0.52
28:a:413:GOL:H2	5:e:63[A]:ILE:HD11	1.92	0.52
24:c:910:CLA:HMB1	24:c:910:CLA:HBB1	1.91	0.52
33:Y:101:LMG:H161	33:Y:101:LMG:H292	1.92	0.51
24:d:406:CLA:H2	18:x:14:LEU:HA	1.90	0.51
16:v:23:GLU:OE1	41:v:301:HOH:O	2.19	0.51
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.44	0.51
4:D:78:VAL:HG11	4:D:114:ILE:HD12	1.92	0.51
3:c:363:GLY:O	3:c:367:GLU:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:LEU:HD21	24:C:511:CLA:H2A	1.92	0.51
24:C:510:CLA:HBC3	24:C:510:CLA:H192	1.92	0.51
2:B:116:VAL:HG21	26:B:620:BCR:H292	1.92	0.51
3:C:215:LYS:NZ	41:C:607:HOH:O	2.42	0.51
3:C:223:TRP:CG	3:C:224:ILE:H	2.29	0.51
35:D:413:HTG:H1'2	7:H:25:TRP:CD2	2.45	0.51
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.92	0.51
33:A:419:LMG:C25	24:C:505:CLA:HBB2	2.41	0.51
24:c:909:CLA:H162	37:c:918:DGD:HBN2	1.93	0.51
10:K:25:LEU:HD22	26:Y:102:BCR:H332	1.91	0.51
1:A:183:MET:HA	24:A:405:CLA:HMD1	1.93	0.51
6:F:21:VAL:O	6:F:25:THR:HG23	2.11	0.51
27:A:411:SQD:H291	24:C:508:CLA:H71	1.92	0.51
2:b:464:PHE:CZ	36:d:409:LHG:H252	2.45	0.51
24:b:609:CLA:H43	24:b:610:CLA:H2	1.93	0.51
24:c:911:CLA:H41	36:d:411:LHG:H383	1.93	0.51
1:A:153:SER:HB2	24:A:405:CLA:H43	1.92	0.51
29:A:415:LMT:H6E	35:b:601:HTG:O4	2.11	0.51
24:c:903:CLA:H61	24:c:913:CLA:H42	1.93	0.51
1:a:267:ASN:HB3	1:a:270[B]:SER:OG	2.11	0.50
3:c:377:LEU:HG	3:c:381:LYS:HE3	1.94	0.50
3:c:60:ILE:HG22	24:c:904:CLA:HHD	1.93	0.50
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.93	0.50
4:d:286:VAL:HG21	24:d:405:CLA:HED2	1.93	0.50
1:A:215:HIS:ND1	31:A:417:PL9:O1	2.36	0.50
2:B:458:PHE:HB3	24:B:605:CLA:HBC2	1.94	0.50
13:O:137:THR:C	13:O:139:SER:H	2.20	0.50
13:o:40:ILE:HG12	13:o:243:ILE:HD13	1.92	0.50
13:o:58:ASN:HD21	13:o:61:GLN:HB2	1.77	0.50
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.47	0.50
4:D:85:MET:CE	4:D:96:GLU:HG2	2.42	0.50
19:Z:40:ILE:HG22	33:Z:101:LMG:H121	1.94	0.50
3:c:223:TRP:CG	3:c:224:ILE:H	2.30	0.50
4:d:110:LEU:HB2	41:d:578:HOH:O	2.12	0.50
36:d:409:LHG:H212	12:m:18:PRO:HG3	1.94	0.50
13:o:179[B]:GLU:OE2	41:o:403:HOH:O	2.18	0.50
33:A:419:LMG:H221	37:C:516:DGD:HAE1	1.94	0.50
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.45	0.50
26:Y:102:BCR:HC8	26:Y:102:BCR:H321	1.93	0.50
24:b:620:CLA:H2	24:b:621:CLA:CBB	2.40	0.50
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:606:CLA:H193	26:h:101:BCR:H353	1.94	0.50
3:c:42:LEU:HD21	24:c:912:CLA:H2A	1.94	0.50
3:c:286:ALA:HB2	24:c:903:CLA:HMD1	1.93	0.50
24:a:405:CLA:HMB3	24:a:405:CLA:HBB1	1.94	0.49
4:D:39:PRO:O	4:D:43:LEU:HG	2.12	0.49
2:b:148[B]:LEU:HD23	24:b:609:CLA:H191	1.94	0.49
4:d:14:TRP:CD1	35:d:414:HTG:H61	2.47	0.49
33:d:415:LMG:H142	33:d:415:LMG:H292	1.94	0.49
2:B:405[B]:GLU:OE1	13:o:60:ARG:HD3	2.11	0.49
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.48	0.49
33:A:419:LMG:H191	37:C:516:DGD:HA62	1.94	0.49
2:B:454:ALA:HB2	33:B:622:LMG:H172	1.93	0.49
37:D:408:DGD:O1B	37:D:408:DGD:O2D	2.30	0.49
3:c:149:TYR:HB2	3:c:157:MET:HE1	1.92	0.49
3:c:443:TRP:CZ2	24:c:909:CLA:HMD1	2.47	0.49
24:B:607:CLA:H151	24:B:617:CLA:H142	1.95	0.49
13:O:54:GLU:HG2	13:O:64:GLU:O	2.13	0.49
4:d:309:PRO:HA	41:d:525[B]:HOH:O	2.13	0.49
2:b:227:LYS:NZ	29:b:626:LMT:O6'	2.46	0.49
10:K:20:PRO:HG2	17:Y:20:ALA:HB3	1.95	0.49
12:M:33:GLN:HB2	12:m:33:GLN:HB2	1.94	0.49
2:b:256:MET:HA	2:b:263:THR:HG21	1.94	0.49
24:b:610:CLA:HAA1	24:b:610:CLA:HBD	1.94	0.49
10:k:24:VAL:HG13	17:y:25:ILE:HD13	1.94	0.49
1:A:238[A]:LYS:NZ	41:A:505:HOH:O	2.46	0.49
33:A:419:LMG:H211	37:C:516:DGD:HA61	1.95	0.49
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.47	0.49
24:C:510:CLA:H43	36:D:410:LHG:H383	1.94	0.49
17:Y:32:GLY:HA3	26:Y:102:BCR:C15	2.43	0.49
13:o:181[A]:GLU:HG3	41:o:449:HOH:O	2.13	0.49
3:C:443:TRP:CZ2	24:C:508:CLA:HMD1	2.48	0.48
12:M:30:GLU:OE2	41:M:201:HOH:O	2.20	0.48
24:B:614:CLA:HBB1	24:B:614:CLA:HMB1	1.94	0.48
8:i:36:ASP:OD1	8:i:36:ASP:N	2.46	0.48
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.48	0.48
1:A:296:ASN:HB2	3:C:400:PRO:O	2.13	0.48
8:I:2:GLU:O	8:I:6:ILE:HG12	2.12	0.48
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.48	0.48
17:Y:39:LEU:HD21	19:Z:25:VAL:HA	1.95	0.48
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.48	0.48
13:o:204:VAL:HG22	13:o:211:ILE:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:513:CLA:HBB1	26:C:514:BCR:H371	1.95	0.48
1:a:131:TRP:CH2	24:c:906:CLA:HAA2	2.48	0.48
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.49	0.48
1:A:267:ASN:HB3	1:A:270:SER:HB3	1.95	0.48
36:D:409:LHG:H02	28:T:101:GOL:HO1	1.62	0.48
26:k:101:BCR:H371	26:k:101:BCR:H24C	1.70	0.48
24:a:406:CLA:HMB2	24:d:405:CLA:H122	1.95	0.48
13:o:92:SER:HB3	13:o:131:PRO:HA	1.96	0.48
1:A:132:GLU:O	1:A:136:ARG:HG2	2.14	0.48
29:M:101:LMT:H6D	11:l:9:PRO:HA	1.95	0.48
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.49	0.48
2:B:223:GLN:NE2	2:B:227:LYS:HD3	2.29	0.47
24:B:608:CLA:H2	33:B:622:LMG:H152	1.96	0.47
24:B:611:CLA:H152	24:B:611:CLA:OBD	2.14	0.47
3:c:175:LEU:HD23	3:c:237:HIS:CG	2.48	0.47
26:D:406:BCR:H313	37:D:408:DGD:HAE2	1.95	0.47
3:c:225:VAL:HG13	3:c:289:PHE:HA	1.96	0.47
25:d:403:PHO:H61	24:d:405:CLA:H111	1.96	0.47
3:C:452:ALA:HB1	8:I:37:LEU:HD22	1.96	0.47
3:C:344:SER:OG	3:C:348:GLU:OE2	2.32	0.47
20:R:10:LEU:HB3	20:R:11:PRO:HD3	1.97	0.47
29:e:102:LMT:O3'	29:e:102:LMT:O2B	2.28	0.47
13:o:42:ARG:O	13:o:241:ALA:HA	2.14	0.47
24:A:405:CLA:HMB3	24:A:405:CLA:HBB1	1.96	0.47
16:V:68:ASN:ND2	28:V:207:GOL:O1	2.37	0.47
24:B:616:CLA:H2	24:B:617:CLA:HBB2	1.96	0.47
5:E:73:LYS:NZ	5:E:77:GLU:OE2	2.47	0.47
27:L:102:SQD:H62	11:l:7:ARG:NH1	2.30	0.47
24:c:913:CLA:O2D	24:c:914:CLA:HBB2	2.15	0.47
6:f:21:VAL:O	6:f:25:THR:HG23	2.15	0.47
1:A:277:ALA:HB1	27:A:411:SQD:H142	1.96	0.47
2:b:419:SER:HB3	35:b:627:HTG:H2'1	1.96	0.47
24:c:914:CLA:H61	26:c:927:BCR:H281	1.97	0.47
10:k:23:ASP:OD2	17:y:21:GLN:NE2	2.48	0.47
1:A:238[B]:LYS:NZ	41:A:508:HOH:O	2.47	0.47
4:d:123:ILE:HD11	37:h:102:DGD:HAE2	1.97	0.47
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.49	0.47
24:c:907:CLA:H143	37:c:916:DGD:HAN2	1.96	0.47
24:c:909:CLA:H203	24:c:909:CLA:H161	1.78	0.47
13:o:40:ILE:HD12	13:o:95:PHE:CD1	2.49	0.47
6:F:27:ALA:HB1	38:F:102:HEM:HAC	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:K:202:HOH:O	19:Z:62:VAL:HG22	2.15	0.46
24:c:914:CLA:H202	33:c:920:LMG:H402	1.98	0.46
8:i:17:LEU:HD22	8:i:21:PHE:HE2	1.79	0.46
2:b:137:LYS:O	2:b:141:ILE:HG13	2.15	0.46
24:c:902:CLA:C3D	24:c:904:CLA:H2	2.45	0.46
5:e:37:PHE:HD1	5:e:42:LEU:HD23	1.80	0.46
31:A:417:PL9:H221	25:D:401:PHO:HMA2	1.98	0.46
27:L:102:SQD:H1	27:L:102:SQD:H462	1.97	0.46
2:B:423:LYS:HA	2:B:423:LYS:HD3	1.77	0.46
12:M:18:PRO:O	12:M:21:PHE:HB3	2.16	0.46
2:b:201:HIS:HB2	24:b:607:CLA:CHB	2.46	0.46
24:b:611:CLA:H192	24:b:611:CLA:H161	1.75	0.46
13:o:33:ASP:HB3	13:o:36:GLN:HG3	1.96	0.46
3:C:25:ASN:O	3:C:41:ARG:HD3	2.15	0.46
26:K:101:BCR:H24C	26:K:101:BCR:H371	1.70	0.46
33:b:625:LMG:H421	36:b:635:LHG:H371	1.98	0.46
1:A:334:ARG:HD3	4:D:320:LEU:HD13	1.97	0.46
4:D:51:GLY:HA3	4:D:78:VAL:HG22	1.97	0.46
2:b:138:MET:HE1	24:b:615:CLA:H192	1.96	0.46
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.70	0.46
24:b:610:CLA:H62	24:b:610:CLA:H41	1.72	0.46
3:c:163:PHE:O	3:c:167:VAL:HG23	2.16	0.46
1:A:176:ILE:HD13	24:A:406:CLA:HED3	1.97	0.46
3:C:243:ILE:HG22	24:C:506:CLA:HMC3	1.97	0.46
37:C:517:DGD:HA62	37:C:517:DGD:HA31	1.66	0.46
2:b:233:ASN:O	2:b:236:THR:HG22	2.16	0.46
3:c:334:PRO:HA	13:o:153:THR:OG1	2.15	0.46
2:B:69:LEU:HD12	24:B:606:CLA:HBA1	1.98	0.46
2:B:461:LEU:HD22	36:B:635:LHG:H301	1.98	0.46
27:B:621:SQD:H223	26:t:102:BCR:H351	1.98	0.46
10:K:11:LEU:HD11	10:K:22:VAL:HG21	1.97	0.46
2:B:162:PHE:O	24:B:607:CLA:HHD	2.16	0.46
24:B:604:CLA:H3A	24:B:604:CLA:CGA	2.46	0.46
31:d:408:PL9:H401	36:d:410:LHG:H211	1.98	0.46
26:t:102:BCR:H382	26:t:102:BCR:H23C	1.97	0.46
24:C:502:CLA:H61	24:C:512:CLA:H42	1.98	0.46
2:b:213:GLY:O	2:b:217:ILE:HG13	2.16	0.46
24:c:906:CLA:H43	26:c:915:BCR:HC7	1.97	0.46
36:B:635:LHG:O4	4:D:141:TYR:OH	2.20	0.45
26:c:927:BCR:H15C	26:c:927:BCR:H351	1.79	0.45
4:d:40:CYS:HB3	4:d:117:HIS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:MET:HA	2:B:263:THR:HG21	1.98	0.45
24:B:602:CLA:CGA	24:B:602:CLA:H72	2.47	0.45
4:D:160:TYR:HA	4:D:290:ALA:HB2	1.99	0.45
13:o:146:PHE:CE1	13:o:195:GLY:HA3	2.51	0.45
19:z:47:TRP:CD2	33:z:101:LMG:H241	2.51	0.45
1:A:84:PRO:HA	1:A:112:TYR:CG	2.51	0.45
24:C:513:CLA:H202	33:C:519:LMG:H402	1.98	0.45
13:O:39:ARG:HB2	13:O:246:ALA:HB2	1.98	0.45
26:T:102:BCR:H331	26:T:102:BCR:HC7	1.64	0.45
17:Y:38:LEU:O	17:Y:42:ARG:HD3	2.15	0.45
24:b:618:CLA:OBD	24:b:619:CLA:HHC	2.16	0.45
24:B:613:CLA:CMB	24:B:615:CLA:HBB1	2.47	0.45
3:C:156:LYS:HE3	41:C:792:HOH:O	2.17	0.45
3:C:406:SER:HA	3:C:420:VAL:HG23	1.98	0.45
12:M:20:VAL:HG22	12:m:20:VAL:HG11	1.98	0.45
13:O:163:GLY:HA2	13:O:188:LYS:HG3	1.98	0.45
2:b:63:LEU:N	2:b:64:PRO:HD2	2.31	0.45
4:d:42:TYR:OH	6:f:25:THR:O	2.26	0.45
1:A:143:ILE:HD11	4:D:217:THR:HA	1.99	0.45
3:C:425:TRP:CD1	24:C:504:CLA:HMA3	2.52	0.45
24:b:616:CLA:H112	24:b:616:CLA:H72	1.80	0.45
2:B:213:GLY:O	2:B:217:ILE:HG13	2.17	0.45
3:C:52:ALA:HB2	24:C:511:CLA:HMA2	1.99	0.45
5:E:36:LEU:HA	5:E:39:SER:OG	2.17	0.45
12:M:27:VAL:HG12	12:m:28:GLN:HB3	1.98	0.45
13:O:194:LYS:NZ	41:O:417:HOH:O	2.50	0.45
26:h:101:BCR:H371	26:h:101:BCR:H24C	1.75	0.45
16:v:95:LEU:HD11	16:v:112:LEU:HD11	1.98	0.45
2:B:154:GLY:O	2:B:159:THR:HG23	2.17	0.45
26:B:620:BCR:H331	26:B:620:BCR:C8	2.47	0.45
24:C:512:CLA:HMB2	24:C:512:CLA:H202	1.98	0.45
31:a:415:PL9:H151	31:a:415:PL9:H171	1.70	0.45
4:d:78:VAL:HG11	4:d:114:ILE:HD12	1.99	0.45
5:e:53:ASP:O	16:v:1:ALA:N	2.49	0.45
28:l:101:GOL:H2	14:t:25[A]:GLU:HG3	1.99	0.45
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.98	0.45
3:C:203:THR:O	3:C:235:GLY:HA3	2.17	0.45
37:D:408:DGD:HB31	37:D:408:DGD:HA61	1.97	0.45
2:b:224:ARG:HH11	29:b:626:LMT:H1'	1.81	0.45
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.52	0.45
10:k:15:TYR:HE2	19:z:62:VAL:HG21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:GLU:HA	7:H:2:ALA:HB1	1.99	0.45
5:E:60:GLN:HG2	5:E:61:ARG:N	2.31	0.45
29:M:103:LMT:O2B	29:M:103:LMT:O3'	2.23	0.45
5:e:60:GLN:HG2	5:e:61:ARG:N	2.30	0.45
10:k:11:LEU:HD11	10:k:22:VAL:HG21	1.98	0.45
24:B:616:CLA:H192	24:B:616:CLA:H162	1.77	0.44
5:E:15:THR:HB	9:J:7:ILE:O	2.17	0.44
5:E:26:THR:HB	38:F:102:HEM:HAB	1.99	0.44
14:T:20:ALA:O	14:T:24:ARG:HB3	2.17	0.44
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.97	0.44
1:a:298:ASN:ND2	41:a:506:HOH:O	2.42	0.44
24:b:612:CLA:C4A	24:b:612:CLA:HBA2	2.47	0.44
4:d:49:LEU:HD13	26:d:407:BCR:C15	2.46	0.44
4:d:286:VAL:CG2	24:d:405:CLA:HED2	2.47	0.44
2:B:103:LEU:HD21	24:B:606:CLA:HMC3	2.00	0.44
25:D:401:PHO:HBC2	25:D:401:PHO:HHD	1.99	0.44
13:O:121:THR:OG1	13:O:123:LYS:HG3	2.17	0.44
1:a:229:GLU:HG3	1:a:230:THR:HG23	1.99	0.44
2:b:482:ILE:HD12	2:b:486:LEU:HD12	1.98	0.44
26:d:407:BCR:C8	26:d:407:BCR:H331	2.47	0.44
26:t:102:BCR:HC7	26:t:102:BCR:H331	1.76	0.44
1:a:38:ILE:HB	1:a:39:PRO:HD3	1.98	0.44
1:a:162:PRO:HB3	1:a:168:PHE:HA	2.00	0.44
2:b:190:PHE:CZ	24:b:607:CLA:HBB1	2.53	0.44
24:b:609:CLA:HMD2	24:b:617:CLA:H203	1.99	0.44
3:c:52:ALA:HB2	24:c:912:CLA:HMA2	1.99	0.44
4:d:51:GLY:HA3	4:d:78:VAL:HG22	1.98	0.44
27:A:411:SQD:H192	36:D:410:LHG:H201	1.99	0.44
2:B:143:LEU:HB2	24:B:611:CLA:HED1	1.99	0.44
24:B:608:CLA:C4A	24:B:608:CLA:HBA2	2.47	0.44
2:b:36:SER:OG	26:b:623:BCR:H362	2.17	0.44
24:b:620:CLA:H52	24:b:621:CLA:HBB1	2.00	0.44
7:h:38:PHE:HB2	26:h:101:BCR:C10	2.48	0.44
19:z:7:LEU:HD23	19:z:7:LEU:HA	1.79	0.44
31:A:417:PL9:H503	18:X:24:THR:OG1	2.16	0.44
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.99	0.44
1:a:63:ILE:HB	3:c:335:THR:HG21	2.00	0.44
24:b:606:CLA:H93	24:b:606:CLA:H111	1.77	0.44
15:U:64:ILE:O	15:U:67:LEU:HG	2.17	0.44
1:a:160:ILE:HD11	37:c:916:DGD:HBE1	2.00	0.44
3:c:179:ALA:O	3:c:184:GLY:HA2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:MET:HG2	26:B:618:BCR:H23C	2.00	0.44
11:L:18:TYR:OH	27:L:102:SQD:H241	2.18	0.44
20:R:6:LEU:O	20:R:10:LEU:HB2	2.16	0.44
2:b:14:ASN:ND2	28:b:633:GOL:H12	2.33	0.44
2:b:498:LYS:HA	4:d:24:ARG:HA	2.00	0.44
25:d:403:PHO:NC	25:d:403:PHO:ND	2.65	0.44
5:e:47:PHE:HZ	37:e:101:DGD:HBT2	1.81	0.44
13:o:51:LEU:HB3	13:o:65:PHE:HB3	1.99	0.44
24:A:405:CLA:HBD	24:A:406:CLA:HAC2	2.00	0.44
24:B:602:CLA:H52	24:B:602:CLA:H12	1.88	0.44
3:C:154:LYS:NZ	41:C:604:HOH:O	2.36	0.44
26:C:515:BCR:H11C	26:C:515:BCR:H341	1.88	0.44
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.00	0.44
17:y:22:LEU:HA	17:y:25:ILE:HG22	1.99	0.44
31:A:417:PL9:H101	31:A:417:PL9:H13	2.00	0.43
24:B:605:CLA:HBB1	24:B:605:CLA:HMB1	1.99	0.43
11:l:2:GLU:HB2	41:l:208:HOH:O	2.18	0.43
26:C:514:BCR:H20C	26:C:514:BCR:H361	1.86	0.43
35:D:413:HTG:H1	7:H:25:TRP:CD1	2.53	0.43
5:E:30:LEU:HD23	20:R:12:VAL:HG22	2.00	0.43
5:E:60:GLN:HG2	5:E:62[A]:SER:H	1.83	0.43
5:E:60:GLN:HG2	5:E:62[B]:SER:H	1.83	0.43
12:M:5:GLN:NE2	41:m:201:HOH:O	2.51	0.43
24:c:914:CLA:C4B	26:c:927:BCR:H383	2.47	0.43
24:d:404:CLA:H162	24:d:404:CLA:H203	1.71	0.43
16:v:41:HIS:HA	16:v:45:ILE:O	2.18	0.43
1:A:224:ILE:HG23	2:B:484:PRO:HA	1.99	0.43
33:A:419:LMG:H191	33:A:419:LMG:H161	1.80	0.43
19:Z:37:LYS:NZ	33:Z:101:LMG:O6	2.43	0.43
17:y:23:THR:O	17:y:27:MET:HG3	2.18	0.43
17:y:27:MET:HE2	17:y:27:MET:HB3	1.90	0.43
36:B:635:LHG:H321	36:B:635:LHG:H291	1.81	0.43
27:a:410:SQD:H321	24:c:909:CLA:H71	2.00	0.43
31:a:415:PL9:H272	31:a:415:PL9:H251	1.87	0.43
2:b:467:ILE:HG13	4:d:126:MET:HE1	1.99	0.43
2:b:483:ASP:HA	2:b:484:PRO:HD3	1.88	0.43
24:c:909:CLA:H162	24:c:909:CLA:H122	1.66	0.43
37:C:517:DGD:HA81	37:C:517:DGD:HAF1	2.00	0.43
17:Y:28:ILE:HG23	26:Y:102:BCR:H10C	2.00	0.43
1:a:174:LEU:HD22	25:a:407:PHO:H151	2.00	0.43
3:c:162:GLY:HA2	3:c:248:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:238:ILE:O	3:c:242:LEU:HG	2.19	0.43
26:A:410:BCR:H24C	26:A:410:BCR:H371	1.75	0.43
2:B:124:ARG:O	7:H:12[A]:ARG:NH1	2.47	0.43
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.53	0.43
4:D:282:SER:OG	24:D:404:CLA:HED3	2.18	0.43
1:a:161:TYR:HB3	1:a:162:PRO:HD3	2.00	0.43
24:b:607:CLA:H41	7:h:46:LEU:HA	2.00	0.43
33:c:920:LMG:H391	33:c:920:LMG:H232	2.01	0.43
2:B:347[B]:ARG:HG2	2:B:353:GLU:HA	2.00	0.43
24:B:605:CLA:H192	24:B:605:CLA:H162	1.91	0.43
8:I:33:LYS:HB3	8:I:34:ARG:H	1.53	0.43
15:U:73:GLN:O	15:U:77:GLU:HG3	2.18	0.43
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.54	0.43
1:a:215:HIS:HA	31:a:415:PL9:HC71	2.01	0.43
2:b:237:VAL:HG11	24:b:615:CLA:H201	2.00	0.43
4:d:27:PHE:HD2	4:d:28:VAL:HG23	1.84	0.43
35:d:414:HTG:H1	7:h:25:TRP:CD1	2.53	0.43
1:A:120:LEU:HD23	1:A:120:LEU:HA	1.93	0.43
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.01	0.43
24:B:615:CLA:H93	29:m:102:LMT:H112	2.01	0.43
29:C:520:LMT:H61	29:C:520:LMT:H32	1.76	0.43
36:D:409:LHG:H192	14:T:17:PHE:HZ	1.83	0.43
5:E:51:ARG:N	5:E:54[B]:SER:OG	2.52	0.43
13:O:40:ILE:HG12	13:O:243:ILE:HD13	2.01	0.43
13:O:179[B]:GLU:OE1	41:O:402:HOH:O	2.21	0.43
3:c:147:PHE:CD1	24:c:914:CLA:HHB	2.54	0.43
2:B:499:VAL:HG12	4:D:135:LEU:HB3	2.00	0.43
24:C:513:CLA:HBB1	26:C:514:BCR:H24C	2.00	0.43
4:d:39:PRO:O	4:d:43:LEU:HG	2.18	0.43
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.99	0.43
27:A:411:SQD:H152	27:A:411:SQD:H122	1.50	0.43
24:B:602:CLA:H91	26:H:101:BCR:H21C	2.01	0.43
8:I:3:THR:O	8:I:7:THR:OG1	2.31	0.43
2:b:221:PRO:HA	24:b:614:CLA:HED3	2.01	0.43
24:b:616:CLA:C14	36:b:635:LHG:H382	2.49	0.43
1:A:131:TRP:CH2	24:C:505:CLA:HAA2	2.54	0.42
3:C:31:SER:HB2	3:C:41:ARG:HG2	2.00	0.42
3:C:464:GLU:OE2	4:D:245:SER:OG	2.35	0.42
16:V:41:HIS:HA	16:V:45:ILE:O	2.19	0.42
2:b:58:GLN:C	2:b:329:PRO:HB3	2.44	0.42
2:b:379:ALA:HA	2:b:390:TYR:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:43:LEU:HB3	13:o:81:ILE:HB	2.00	0.42
19:z:37:LYS:HZ2	33:z:101:LMG:HC4	1.84	0.42
24:B:603:CLA:H41	7:H:46:LEU:HA	2.02	0.42
24:C:511:CLA:HMB1	26:K:101:BCR:H382	2.00	0.42
24:b:612:CLA:H42	33:b:625:LMG:H311	2.01	0.42
24:b:618:CLA:H18	36:d:409:LHG:H202	2.00	0.42
4:d:223:PHE:CZ	4:d:245:SER:HB2	2.53	0.42
2:B:224:ARG:HH11	29:D:403:LMT:H2'	1.84	0.42
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.54	0.42
1:a:93:PHE:CD1	1:a:95:PRO:HD3	2.54	0.42
1:a:121[A]:LEU:HD11	24:c:906:CLA:H152	2.02	0.42
2:b:124:ARG:HD2	2:b:129:GLY:O	2.18	0.42
2:b:190:PHE:HZ	24:b:607:CLA:HBB1	1.84	0.42
24:C:513:CLA:CBB	26:C:514:BCR:H371	2.49	0.42
1:a:72:LEU:HD22	29:a:401:LMT:O2'	2.20	0.42
33:c:920:LMG:H131	35:c:921:HTG:H2'1	2.00	0.42
25:d:403:PHO:HBC2	25:d:403:PHO:HHD	2.01	0.42
13:o:193:THR:HG21	13:o:220:LEU:HD12	2.00	0.42
16:v:109:GLU:O	16:v:113:VAL:HG23	2.19	0.42
24:C:501:CLA:H151	24:C:507:CLA:HMB3	2.01	0.42
24:C:511:CLA:H111	19:Z:24:PRO:HB3	2.00	0.42
14:T:14:ILE:HG22	26:T:102:BCR:H10C	2.01	0.42
27:a:410:SQD:H202	27:a:410:SQD:H171	1.75	0.42
24:b:607:CLA:H171	37:h:102:DGD:HAT2	2.02	0.42
1:A:40:THR:HG23	24:A:409:CLA:HBB1	2.01	0.42
26:B:619:BCR:H24C	26:B:619:BCR:H371	1.75	0.42
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.55	0.42
24:D:404:CLA:HAA2	24:D:404:CLA:HBD	2.02	0.42
12:m:18:PRO:O	12:m:21:PHE:HB3	2.19	0.42
13:o:180:GLU:CD	13:o:180:GLU:H	2.28	0.42
1:A:161:TYR:CD1	1:A:294:ALA:HA	2.55	0.42
2:b:65:PHE:CE2	24:b:609:CLA:HMA1	2.54	0.42
3:c:158:THR:O	3:c:251:HIS:HB3	2.20	0.42
5:e:17:VAL:O	5:e:21:VAL:HG23	2.20	0.42
26:h:101:BCR:H331	26:h:101:BCR:C8	2.49	0.42
24:B:602:CLA:H91	24:B:602:CLA:H111	1.75	0.42
3:C:213:LEU:HD21	26:C:515:BCR:C20	2.50	0.42
4:D:210:LEU:HA	4:D:213:ILE:HG22	2.02	0.42
26:b:624:BCR:H331	26:b:624:BCR:C8	2.49	0.42
2:B:63:LEU:N	2:B:64:PRO:HD2	2.35	0.42
4:D:92:LEU:HA	4:D:104:TRP:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:103:ARG:NH1	4:D:106:GLN:OE1	2.48	0.42
6:F:18:VAL:N	27:F:103:SQD:O9	2.38	0.42
26:H:101:BCR:H24C	26:H:101:BCR:H371	1.68	0.42
13:O:138:THR:HG23	41:O:462:HOH:O	2.20	0.42
1:a:218:LEU:HD12	31:a:415:PL9:HC72	2.02	0.42
1:A:252:HIS:CE1	1:A:264:SER:HB3	2.55	0.42
3:C:167:VAL:HG13	24:C:512:CLA:H102	2.02	0.42
16:V:12:LEU:HD12	16:V:69:ILE:HB	2.00	0.42
36:a:418:LHG:H262	36:a:418:LHG:HC61	2.02	0.42
24:b:608:CLA:CGA	24:b:608:CLA:H3A	2.49	0.42
5:e:12:ASP:O	9:j:4:GLY:HA2	2.20	0.42
11:l:18:TYR:CE2	14:t:20:ALA:HA	2.54	0.42
13:o:85:LEU:HD12	13:o:85:LEU:HA	1.79	0.42
2:B:224:ARG:HG3	7:H:24:GLY:C	2.45	0.41
26:B:620:BCR:H24C	26:B:620:BCR:H371	1.90	0.41
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.83	0.41
3:C:296:VAL:C	3:C:298:PRO:HD3	2.45	0.41
3:c:95:LEU:HD21	24:c:902:CLA:OBD	2.19	0.41
24:c:906:CLA:HAA1	24:c:906:CLA:HBD	2.02	0.41
19:z:37:LYS:NZ	33:z:101:LMG:HC4	2.34	0.41
1:A:50:ILE:HG12	29:A:415:LMT:H101	2.02	0.41
27:A:411:SQD:O7	3:C:28:GLN:NE2	2.53	0.41
25:a:407:PHO:H141	24:d:404:CLA:HBB1	2.00	0.41
36:a:418:LHG:H201	36:a:418:LHG:H171	1.88	0.41
26:h:101:BCR:H20C	26:h:101:BCR:H361	1.93	0.41
1:A:37:MET:HG3	1:A:122:GLY:O	2.21	0.41
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.03	0.41
2:B:216:HIS:CE1	24:B:610:CLA:C1A	3.03	0.41
24:B:616:CLA:H61	24:B:617:CLA:HBB1	2.01	0.41
24:C:501:CLA:H201	24:C:507:CLA:H13	2.02	0.41
4:D:102:THR:OG1	37:D:408:DGD:HG31	2.21	0.41
10:K:24:VAL:HG13	17:Y:25:ILE:HD13	2.02	0.41
19:Z:29:SER:HA	19:Z:30:PRO:HD3	1.80	0.41
2:b:144:PHE:CE1	2:b:210:ILE:HG23	2.56	0.41
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.49	0.41
24:B:603:CLA:H171	37:H:102:DGD:HA72	2.02	0.41
26:B:620:BCR:H15C	26:B:620:BCR:H351	1.90	0.41
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	2.01	0.41
33:Z:101:LMG:H111	33:Z:101:LMG:HC8	1.64	0.41
24:a:405:CLA:H111	24:a:405:CLA:H72	1.81	0.41
24:b:611:CLA:H162	24:b:611:CLA:H122	1.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:425:TRP:CD1	24:c:905:CLA:HMA2	2.55	0.41
2:B:218:LEU:HA	2:B:218:LEU:HD23	1.86	0.41
24:B:615:CLA:HAA1	24:B:615:CLA:HBD	2.03	0.41
5:E:8:ARG:HD3	5:E:13:ILE:HG12	2.02	0.41
2:B:70:GLY:HA2	2:B:178:VAL:HG21	2.02	0.41
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.55	0.41
2:B:450:TRP:CD1	24:B:608:CLA:HBA1	2.55	0.41
24:C:505:CLA:HAA1	24:C:505:CLA:HBD	2.03	0.41
24:C:506:CLA:H142	24:C:506:CLA:H112	1.93	0.41
4:D:40:CYS:HB3	4:D:117:HIS:O	2.21	0.41
26:H:101:BCR:H20C	26:H:101:BCR:H361	1.93	0.41
11:L:13:ASN:HD22	11:L:16:SER:H	1.68	0.41
3:c:296:VAL:HG23	3:c:297:TYR:CD2	2.56	0.41
26:c:915:BCR:H11C	26:c:915:BCR:H341	1.92	0.41
2:B:338:GLN:HA	13:o:57:LYS:HE3	2.01	0.41
24:C:510:CLA:H3A	24:C:510:CLA:HBA1	1.89	0.41
24:C:512:CLA:O2D	24:C:513:CLA:HBB2	2.20	0.41
27:a:410:SQD:H342	27:a:410:SQD:H312	1.86	0.41
2:b:185:TRP:CZ2	35:b:628:HTG:H2'1	2.56	0.41
2:b:393:GLU:HB3	15:u:18:GLY:CA	2.51	0.41
2:b:467:ILE:HD13	2:b:467:ILE:HA	1.82	0.41
24:b:620:CLA:H112	24:b:620:CLA:H91	1.88	0.41
5:e:14:ILE:HD12	9:j:12:VAL:HG11	2.03	0.41
2:B:451:PHE:CE1	2:B:455:HIS:CE1	3.09	0.41
24:C:505:CLA:HHC	24:C:505:CLA:CBB	2.49	0.41
15:U:32:ILE:HG13	15:U:46:ALA:HB1	2.03	0.41
2:b:458:PHE:HB3	24:b:609:CLA:HBC2	2.02	0.41
37:c:916:DGD:HAN1	37:c:916:DGD:HAW2	1.92	0.41
24:A:406:CLA:H162	24:A:406:CLA:H203	1.83	0.41
2:B:483:ASP:HA	2:B:484:PRO:HD3	1.77	0.41
26:B:619:BCR:H363	26:t:102:BCR:H19C	2.03	0.41
27:B:621:SQD:H352	27:B:621:SQD:H383	1.80	0.41
26:C:514:BCR:H15C	26:C:514:BCR:H351	1.83	0.41
4:D:298:PHE:O	4:D:301:GLN:HB2	2.20	0.41
27:L:102:SQD:H312	27:L:102:SQD:H341	1.97	0.41
13:O:29:ALA:HB1	13:O:135:SER:HB3	2.02	0.41
35:V:203:HTG:H6'2	35:V:203:HTG:H3'2	1.85	0.41
25:a:407:PHO:H2	25:a:407:PHO:H61	1.86	0.41
2:b:216:HIS:CE1	24:b:614:CLA:NA	2.88	0.41
2:b:496:TYR:OH	2:b:502:VAL:HG13	2.21	0.41
36:b:635:LHG:HC81	36:d:409:LHG:O9	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:203:THR:O	3:c:235:GLY:HA3	2.20	0.41
24:c:906:CLA:HHC	24:c:906:CLA:CBB	2.46	0.41
37:c:916:DGD:HA52	37:c:916:DGD:HA21	1.63	0.41
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.56	0.41
33:C:519:LMG:H411	33:C:519:LMG:H381	1.92	0.41
12:M:34:LYS:HG2	29:M:101:LMT:O3B	2.20	0.41
1:a:83:VAL:HA	1:a:84:PRO:HD3	1.99	0.41
24:a:405:CLA:CBD	24:d:404:CLA:HAC2	2.51	0.41
37:c:917:DGD:HB61	37:c:917:DGD:HB32	1.48	0.41
24:B:615:CLA:C9	29:m:102:LMT:H112	2.52	0.40
3:C:150:ASP:O	3:C:157:MET:HE3	2.21	0.40
2:b:79[A]:SER:HB3	2:b:86[A]:ILE:HG12	2.03	0.40
4:d:54:PHE:HB3	5:e:47:PHE:CD1	2.56	0.40
15:u:38:TYR:HB2	15:u:41:LEU:HD12	2.03	0.40
18:x:33:GLN:O	18:x:36:LYS:HG3	2.21	0.40
2:B:491:VAL:HG12	4:D:136:VAL:HG13	2.03	0.40
3:C:151:TRP:HH2	24:C:509:CLA:H193	1.87	0.40
24:C:509:CLA:H161	24:C:509:CLA:H141	1.86	0.40
4:D:110:LEU:HB2	41:D:585:HOH:O	2.20	0.40
27:F:103:SQD:H342	27:F:103:SQD:H311	1.96	0.40
36:a:418:LHG:H181	36:a:418:LHG:H151	1.97	0.40
3:c:204:LEU:HD23	3:c:204:LEU:HA	1.90	0.40
37:c:917:DGD:HBF2	37:c:917:DGD:HBE1	1.89	0.40
26:d:407:BCR:H11C	26:d:407:BCR:H341	1.98	0.40
24:A:405:CLA:H192	24:A:405:CLA:H161	1.72	0.40
26:H:101:BCR:H15C	26:H:101:BCR:H351	1.92	0.40
26:Y:102:BCR:H312	19:Z:16:SER:HB3	2.04	0.40
24:c:914:CLA:HBB1	24:c:914:CLA:CHC	2.44	0.40
33:d:415:LMG:H392	33:d:415:LMG:H362	1.82	0.40
19:z:47:TRP:CE3	33:z:101:LMG:H221	2.57	0.40
2:B:216:HIS:CE1	24:B:610:CLA:NA	2.90	0.40
3:C:149:TYR:HB2	3:C:157:MET:CE	2.47	0.40
26:C:514:BCR:H11C	26:C:514:BCR:H341	1.89	0.40
4:D:261:PHE:CE1	4:D:267:LEU:HA	2.57	0.40
6:F:27:ALA:HB1	38:F:102:HEM:CAC	2.51	0.40
9:J:7:ILE:HA	9:J:8:PRO:HD3	1.95	0.40
2:b:25:MET:HG2	26:b:622:BCR:H23C	2.03	0.40
24:c:904:CLA:H101	24:c:904:CLA:H62	1.82	0.40
4:d:210:LEU:HA	4:d:213:ILE:HG22	2.03	0.40
5:e:8:ARG:HA	5:e:9:PRO:HD3	1.99	0.40
13:o:52:VAL:O	13:o:66:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:405:CLA:H143	25:A:408:PHO:H61	2.03	0.40
2:B:366:PHE:CG	2:B:367:PRO:HD2	2.56	0.40
2:B:489:GLU:HB3	2:B:495:PHE:CD1	2.56	0.40
3:C:204:LEU:HD23	3:C:204:LEU:HA	1.88	0.40
25:D:401:PHO:NC	25:D:401:PHO:ND	2.69	0.40
4:d:272:LEU:HD23	4:d:272:LEU:C	2.47	0.40
7:h:20:LYS:HG3	41:h:223:HOH:O	2.22	0.40
13:o:22:LEU:O	13:o:203:LYS:NZ	2.54	0.40
13:o:54:GLU:HG2	13:o:64:GLU:O	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:69:GLU:OE1	27:f:102:SQD:O3[2_554]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	328 (98%)	5 (2%)	2 (1%)	21	24
1	a	338/344 (98%)	331 (98%)	5 (2%)	2 (1%)	21	24
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	513/505 (102%)	504 (98%)	9 (2%)	0	100	100
3	C	453/455 (100%)	442 (98%)	9 (2%)	2 (0%)	30	34
3	c	459/455 (101%)	448 (98%)	9 (2%)	2 (0%)	30	34
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	31 (97%)	1 (3%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	58 (91%)	6 (9%)	0	100	100
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	2
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	33 (89%)	4 (11%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	242 (97%)	6 (2%)	1 (0%)	30	34
13	o	246/244 (101%)	240 (98%)	6 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
17	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
17	y	27/30 (90%)	24 (89%)	3 (11%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
All	All	5282/5384 (98%)	5151 (98%)	121 (2%)	10 (0%)	43	52

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
8	I	34	ARG
1	a	259	ILE
13	O	138	THR
1	A	30	VAL
1	A	259	ILE
1	a	30	VAL

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	272/279 (98%)	272 (100%)	0	100	100
1	a	275/279 (99%)	274 (100%)	1 (0%)	84	91
2	B	412/403 (102%)	408 (99%)	4 (1%)	68	81
2	b	413/403 (102%)	412 (100%)	1 (0%)	87	94
3	C	356/356 (100%)	347 (98%)	9 (2%)	42	55
3	c	362/356 (102%)	350 (97%)	12 (3%)	33	44
4	D	277/277 (100%)	276 (100%)	1 (0%)	84	91
4	d	277/277 (100%)	276 (100%)	1 (0%)	84	91
5	E	74/73 (101%)	72 (97%)	2 (3%)	39	52
5	e	74/73 (101%)	74 (100%)	0	100	100
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	25 (96%)	1 (4%)	29	39
7	H	55/54 (102%)	54 (98%)	1 (2%)	51	66
7	h	54/54 (100%)	54 (100%)	0	100	100
8	I	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	i	34/34 (100%)	32 (94%)	2 (6%)	18	22
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	30	40
10	K	30/30 (100%)	29 (97%)	1 (3%)	33	44
10	k	30/30 (100%)	29 (97%)	1 (3%)	33	44
11	L	36/35 (103%)	34 (94%)	2 (6%)	19	23
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	51
12	M	31/32 (97%)	30 (97%)	1 (3%)	34	46
12	m	30/32 (94%)	29 (97%)	1 (3%)	33	44
13	O	214/207 (103%)	211 (99%)	3 (1%)	59	73
13	o	211/207 (102%)	207 (98%)	4 (2%)	50	65
14	T	27/28 (96%)	27 (100%)	0	100	100
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	14
15	U	84/89 (94%)	82 (98%)	2 (2%)	43	57
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	118/117 (101%)	116 (98%)	2 (2%)	53	68
16	v	117/117 (100%)	115 (98%)	2 (2%)	53	68
17	Y	22/23 (96%)	20 (91%)	2 (9%)	9	9
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	9
18	X	32/33 (97%)	32 (100%)	0	100	100
18	x	31/33 (94%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	50	65
19	z	52/52 (100%)	51 (98%)	1 (2%)	50	65
20	R	25/29 (86%)	23 (92%)	2 (8%)	11	12
All	All	4387/4403 (100%)	4321 (98%)	66 (2%)	59	72

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	86	ILE
2	B	479	PHE
2	B	492	GLU
2	B	505	ARG
3	C	28	GLN

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Mol	Chain	Res	Type
3	C	29	GLU
3	C	142	GLU
3	C	240	ILE
3	C	255	THR
3	C	279	LEU
3	C	289	PHE
3	C	315	MET
3	C	355	THR
4	D	329	MET
5	E	14	ILE
5	E	17	VAL
7	H	65	LEU
10	K	17	ILE
11	L	13	ASN
11	L	15	THR
12	M	5	GLN
13	O	4	THR
13	O	34	SER
13	O	69	LYS
15	U	59	GLU
15	U	70	ARG
16	V	42	VAL
16	V	85	GLU
17	Y	24	MET
17	Y	30	ILE
19	Z	4	LEU
20	R	4	ARG
20	R	6	LEU
1	a	12	ASN
2	b	479	PHE
3	c	19	ASN
3	c	21	ILE
3	c	142	GLU
3	c	240	ILE
3	c	255	THR
3	c	279	LEU
3	c	289	PHE
3	c	391	ARG
3	c	416[A]	SER
3	c	416[B]	SER
3	c	462[A]	GLU
3	c	462[B]	GLU

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Mol	Chain	Res	Type
4	d	329	MET
6	f	15	ILE
8	i	23	PHE
8	i	36	ASP
9	j	1	MET
10	k	17	ILE
11	l	15	THR
12	m	2	GLU
13	o	4	THR
13	o	37	THR
13	o	217[A]	SER
13	o	217[B]	SER
14	t	25[A]	GLU
14	t	25[B]	GLU
16	v	2	GLU
16	v	42	VAL
17	y	24	MET
17	y	30	ILE
19	z	34	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
2	B	53	ASN
3	C	44	ASN
3	C	201	ASN
4	D	83	ASN
4	D	332	GLN
11	L	13	ASN
13	O	124	ASN
13	O	130	GLN
13	O	147	ASN
13	O	200	ASN
13	O	231	HIS
19	Z	58	ASN
1	a	75	ASN
1	a	165	GLN
1	a	315	ASN
2	b	14	ASN
2	b	53	ASN
2	b	179	GLN

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Mol	Chain	Res	Type
2	b	331	ASN
3	c	44	ASN
3	c	201	ASN
3	c	373	ASN
3	c	418	ASN
4	d	83	ASN
4	d	186	GLN
4	d	332	GLN
5	e	82	GLN
13	o	124	ASN
13	o	130	GLN
13	o	147	ASN
15	u	73	GLN
15	u	81	HIS
16	v	86	GLN
19	z	31	GLN
19	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	FME	t	1	14	8,9,10	0.80	0	7,9,11	2.51	5 (71%)
12	FME	M	1	12	8,9,10	0.64	0	7,9,11	1.16	1 (14%)
8	FME	I	1	8	8,9,10	0.75	0	7,9,11	1.26	1 (14%)
14	FME	T	1	14	8,9,10	0.69	0	7,9,11	1.44	1 (14%)
12	FME	m	1	12	8,9,10	0.67	0	7,9,11	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	i	1	8	8,9,10	0.66	0	7,9,11	1.23	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	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-4.15	116.44	122.82
14	t	1	FME	C-CA-N	3.05	115.23	109.73
14	T	1	FME	O-C-CA	-2.50	118.21	124.78
14	t	1	FME	O-C-CA	-2.47	118.31	124.78
14	t	1	FME	CE-SD-CG	-2.19	92.88	100.40
8	I	1	FME	O-C-CA	-2.15	119.14	124.78
14	t	1	FME	O1-CN-N	-2.10	119.73	125.27
12	M	1	FME	O-C-CA	-2.08	119.34	124.78
8	i	1	FME	CA-N-CN	-2.04	119.68	122.82

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	O1-CN-N-CA
14	T	1	FME	N-CA-CB-CG
12	m	1	FME	N-CA-CB-CG
14	t	1	FME	N-CA-CB-CG
14	t	1	FME	C-CA-CB-CG
14	t	1	FME	CB-CA-N-CN
12	m	1	FME	O1-CN-N-CA

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Mol	Chain	Res	Type	Atoms
14	T	1	FME	CB-CG-SD-CE
12	M	1	FME	CA-CB-CG-SD

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 251 ligands modelled in this entry, 19 are monoatomic and 18 are unknown - leaving 214 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$
26	BCR	c	927	-	41,41,41	1.02	1 (2%)	56,56,56	1.59	11 (19%)
28	GOL	T	101	-	5,5,5	0.38	0	5,5,5	0.22	0
35	HTG	b	601	-	19,19,19	1.03	1 (5%)	23,24,24	1.28	1 (4%)
29	LMT	a	417	-	36,36,36	0.42	0	47,47,47	0.79	1 (2%)
24	CLA	B	614	2	69,73,73	2.08	19 (27%)	83,113,113	2.78	33 (39%)
29	LMT	M	103	-	36,36,36	0.59	1 (2%)	47,47,47	1.08	4 (8%)
35	HTG	c	921	-	19,19,19	1.00	2 (10%)	23,24,24	1.56	1 (4%)
28	GOL	v	204	-	5,5,5	0.36	0	5,5,5	0.34	0
28	GOL	b	632	-	5,5,5	0.38	0	5,5,5	0.33	0
24	CLA	b	619	2	69,73,73	2.04	20 (28%)	83,113,113	2.89	33 (39%)
24	CLA	C	505	3	69,73,73	1.98	20 (28%)	83,113,113	2.69	29 (34%)
24	CLA	B	612	2	69,73,73	1.97	20 (28%)	83,113,113	2.93	33 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LHG	L	101	-	48,48,48	0.95	3 (6%)	51,54,54	1.13	5 (9%)
24	CLA	b	618	2	69,73,73	2.03	20 (28%)	83,113,113	2.75	30 (36%)
24	CLA	c	905	41	69,73,73	2.03	19 (27%)	83,113,113	2.85	32 (38%)
28	GOL	a	412	-	5,5,5	0.39	0	5,5,5	0.53	0
28	GOL	a	413	-	5,5,5	0.41	0	5,5,5	0.26	0
28	GOL	T	103	-	5,5,5	0.40	0	5,5,5	0.30	0
28	GOL	B	636	-	5,5,5	0.41	0	5,5,5	0.47	0
26	BCR	B	619	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	9 (16%)
27	SQD	B	621	-	53,54,54	1.03	3 (5%)	62,65,65	1.44	8 (12%)
24	CLA	C	511	3	69,73,73	2.07	20 (28%)	83,113,113	2.75	29 (34%)
24	CLA	c	914	3	69,73,73	2.06	20 (28%)	83,113,113	2.88	29 (34%)
28	GOL	V	201	34	5,5,5	0.34	0	5,5,5	0.26	0
35	HTG	B	623	-	19,19,19	1.20	1 (5%)	23,24,24	1.28	1 (4%)
24	CLA	a	406	41	69,73,73	2.03	19 (27%)	83,113,113	2.90	30 (36%)
33	LMG	a	411	-	51,51,55	0.91	2 (3%)	59,59,63	1.16	5 (8%)
37	DGD	C	517	-	63,63,67	0.88	3 (4%)	77,77,81	1.07	7 (9%)
36	LHG	B	635	-	48,48,48	0.91	2 (4%)	51,54,54	1.11	5 (9%)
28	GOL	V	206	-	5,5,5	0.43	0	5,5,5	0.32	0
24	CLA	c	907	3	69,73,73	2.00	20 (28%)	83,113,113	2.77	30 (36%)
24	CLA	c	906	3	69,73,73	2.01	19 (27%)	83,113,113	2.68	29 (34%)
28	GOL	D	402	-	5,5,5	0.43	0	5,5,5	0.35	0
23	BCT	d	402	21	2,3,3	0.67	0	2,3,3	0.71	0
24	CLA	C	510	3	69,73,73	2.09	20 (28%)	83,113,113	2.76	29 (34%)
35	HTG	C	521	-	19,19,19	1.02	2 (10%)	23,24,24	1.76	3 (13%)
24	CLA	b	615	41	69,73,73	2.06	21 (30%)	83,113,113	2.74	32 (38%)
24	CLA	C	507	41	69,73,73	2.04	20 (28%)	83,113,113	2.78	29 (34%)
29	LMT	C	520	-	36,36,36	0.48	0	47,47,47	1.17	4 (8%)
26	BCR	k	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.46	14 (25%)
25	PHO	A	408	-	58,69,69	2.70	14 (24%)	56,99,99	2.70	12 (21%)
24	CLA	C	506	3	69,73,73	2.05	20 (28%)	83,113,113	2.75	29 (34%)
30	OEX	a	416	41,1,3	0,14,14	-	-	-	-	-
38	HEM	F	102	6,5	50,50,50	1.56	6 (12%)	66,82,82	1.85	15 (22%)
35	HTG	B	625	-	19,19,19	1.05	2 (10%)	23,24,24	1.64	2 (8%)
24	CLA	b	606	41	69,73,73	2.09	19 (27%)	83,113,113	2.82	26 (31%)
26	BCR	K	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.47	12 (21%)
37	DGD	e	101	-	63,63,67	0.93	2 (3%)	77,77,81	1.24	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMT	e	102	-	36,36,36	0.48	0	47,47,47	0.86	1 (2%)
28	GOL	V	205	-	5,5,5	0.37	0	5,5,5	0.57	0
24	CLA	C	501	3	69,73,73	2.07	20 (28%)	83,113,113	2.83	30 (36%)
33	LMG	Y	101	-	51,51,55	0.95	2 (3%)	59,59,63	1.00	4 (6%)
24	CLA	C	503	3	69,73,73	2.09	20 (28%)	83,113,113	2.82	27 (32%)
28	GOL	V	204	-	5,5,5	0.38	0	5,5,5	0.37	0
31	PL9	a	415	-	55,55,55	0.64	2 (3%)	68,69,69	1.88	21 (30%)
29	LMT	m	102	-	36,36,36	0.46	0	47,47,47	0.85	1 (2%)
26	BCR	T	102	-	41,41,41	1.03	1 (2%)	56,56,56	1.85	17 (30%)
26	BCR	D	406	-	41,41,41	1.06	1 (2%)	56,56,56	1.74	10 (17%)
26	BCR	c	915	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	10 (17%)
35	HTG	D	413	-	16,16,19	1.07	2 (12%)	20,21,24	1.52	1 (5%)
36	LHG	d	411	-	48,48,48	0.94	2 (4%)	51,54,54	1.08	3 (5%)
36	LHG	D	409	-	48,48,48	0.89	2 (4%)	51,54,54	0.89	3 (5%)
35	HTG	b	627	-	19,19,19	0.81	1 (5%)	23,24,24	1.54	3 (13%)
26	BCR	h	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.37	8 (14%)
27	SQD	a	402	-	53,54,54	1.07	3 (5%)	62,65,65	1.19	6 (9%)
24	CLA	B	603	2	69,73,73	2.02	21 (30%)	83,113,113	2.94	31 (37%)
24	CLA	c	911	3	69,73,73	2.05	20 (28%)	83,113,113	2.77	30 (36%)
26	BCR	C	514	-	41,41,41	1.08	1 (2%)	56,56,56	1.52	9 (16%)
37	DGD	c	918	-	63,63,67	0.90	2 (3%)	77,77,81	1.04	5 (6%)
27	SQD	f	102	-	42,43,54	1.20	3 (7%)	51,54,65	1.45	6 (11%)
28	GOL	B	629	-	5,5,5	0.35	0	5,5,5	0.31	0
26	BCR	t	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.68	13 (23%)
31	PL9	d	408	-	55,55,55	0.67	2 (3%)	68,69,69	1.69	16 (23%)
35	HTG	b	604	-	19,19,19	0.99	2 (10%)	23,24,24	1.11	1 (4%)
29	LMT	b	602	-	25,25,36	0.57	1 (4%)	30,30,47	1.12	2 (6%)
33	LMG	Z	101	-	37,37,55	0.97	2 (5%)	45,45,63	1.39	6 (13%)
24	CLA	D	405	4	69,73,73	2.02	20 (28%)	83,113,113	2.82	29 (34%)
36	LHG	b	635	-	48,48,48	0.96	2 (4%)	51,54,54	1.12	3 (5%)
28	GOL	b	630	-	5,5,5	0.40	0	5,5,5	0.14	0
24	CLA	B	604	2	69,73,73	2.06	19 (27%)	83,113,113	2.88	28 (33%)
37	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	0.96	5 (6%)
35	HTG	b	603	-	19,19,19	1.00	2 (10%)	23,24,24	1.55	4 (17%)
37	DGD	C	516	-	63,63,67	0.87	2 (3%)	77,77,81	1.12	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMG	J	101	39	51,51,55	0.90	2 (3%)	59,59,63	0.97	3 (5%)
24	CLA	B	615	2	69,73,73	2.05	20 (28%)	83,113,113	2.87	31 (37%)
36	LHG	a	418	-	41,41,48	1.04	2 (4%)	44,47,54	0.95	2 (4%)
27	SQD	A	411	-	53,54,54	0.98	3 (5%)	62,65,65	1.57	11 (17%)
24	CLA	d	406	4	69,73,73	2.08	20 (28%)	83,113,113	2.85	30 (36%)
24	CLA	b	611	2	69,73,73	2.03	20 (28%)	83,113,113	2.86	28 (33%)
26	BCR	B	620	-	41,41,41	1.02	1 (2%)	56,56,56	1.48	10 (17%)
28	GOL	B	630	-	5,5,5	0.39	0	5,5,5	0.21	0
28	GOL	c	924	-	5,5,5	0.37	0	5,5,5	0.61	0
24	CLA	c	902	3	69,73,73	2.04	19 (27%)	83,113,113	2.79	30 (36%)
28	GOL	b	631	-	5,5,5	0.32	0	5,5,5	0.26	0
24	CLA	B	608	41	69,73,73	2.01	20 (28%)	83,113,113	2.72	29 (34%)
27	SQD	A	414	-	53,54,54	1.03	3 (5%)	62,65,65	1.12	6 (9%)
27	SQD	a	410	-	53,54,54	0.98	3 (5%)	62,65,65	1.64	11 (17%)
24	CLA	B	617	2	69,73,73	2.01	19 (27%)	83,113,113	2.85	29 (34%)
37	DGD	c	916	-	63,63,67	0.84	2 (3%)	77,77,81	1.07	7 (9%)
24	CLA	B	602	41	69,73,73	2.06	21 (30%)	83,113,113	2.85	27 (32%)
24	CLA	C	513	3	69,73,73	2.05	19 (27%)	83,113,113	2.84	30 (36%)
31	PL9	A	417	-	55,55,55	0.66	2 (3%)	68,69,69	1.80	23 (33%)
36	LHG	d	409	-	48,48,48	0.92	3 (6%)	51,54,54	1.11	6 (11%)
25	PHO	d	403	-	58,69,69	2.78	12 (20%)	56,99,99	2.91	17 (30%)
24	CLA	b	617	2	69,73,73	2.00	20 (28%)	83,113,113	2.81	33 (39%)
29	LMT	F	101	-	36,36,36	0.46	0	47,47,47	0.90	1 (2%)
28	GOL	C	524	-	5,5,5	0.41	0	5,5,5	0.57	0
24	CLA	c	903	3	69,73,73	2.07	20 (28%)	83,113,113	2.78	27 (32%)
36	LHG	D	410	-	48,48,48	0.97	2 (4%)	51,54,54	1.20	4 (7%)
24	CLA	B	611	41	69,73,73	2.07	19 (27%)	83,113,113	2.90	32 (38%)
24	CLA	b	612	41	69,73,73	2.05	18 (26%)	83,113,113	2.74	29 (34%)
26	BCR	B	618	-	41,41,41	1.00	1 (2%)	56,56,56	1.40	9 (16%)
24	CLA	d	404	41	69,73,73	2.05	19 (27%)	83,113,113	2.83	32 (38%)
24	CLA	b	610	2	69,73,73	2.01	20 (28%)	83,113,113	2.94	27 (32%)
35	HTG	d	414	-	16,16,19	1.14	2 (12%)	20,21,24	1.76	1 (5%)
26	BCR	H	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.41	9 (16%)
24	CLA	c	912	3	69,73,73	1.98	20 (28%)	83,113,113	2.79	27 (32%)
30	OEX	A	416	41,1,3	0,14,14	-	-	-	-	-
27	SQD	L	102	-	53,54,54	1.04	3 (5%)	62,65,65	1.55	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	610	2	69,73,73	2.03	19 (27%)	83,113,113	2.74	28 (33%)
24	CLA	B	616	2	69,73,73	2.05	19 (27%)	83,113,113	2.77	28 (33%)
35	HTG	c	922	-	19,19,19	1.00	2 (10%)	23,24,24	1.45	3 (13%)
33	LMG	A	419	-	51,51,55	0.96	2 (3%)	59,59,63	1.12	4 (6%)
37	DGD	c	917	-	63,63,67	0.90	2 (3%)	77,77,81	1.02	6 (7%)
28	GOL	A	412	-	5,5,5	0.39	0	5,5,5	0.29	0
24	CLA	b	607	2	69,73,73	2.06	21 (30%)	83,113,113	2.93	32 (38%)
24	CLA	b	616	2	69,73,73	1.96	20 (28%)	83,113,113	2.81	31 (37%)
28	GOL	B	627	-	5,5,5	0.36	0	5,5,5	0.49	0
29	LMT	D	403	-	36,36,36	0.47	0	47,47,47	1.04	3 (6%)
37	DGD	H	102	-	63,63,67	0.87	2 (3%)	77,77,81	1.02	6 (7%)
24	CLA	a	405	1	69,73,73	2.00	20 (28%)	83,113,113	2.82	31 (37%)
26	BCR	b	622	-	41,41,41	1.01	1 (2%)	56,56,56	1.53	9 (16%)
28	GOL	b	629	-	5,5,5	0.38	0	5,5,5	0.49	0
33	LMG	c	920	-	51,51,55	0.95	2 (3%)	59,59,63	1.30	7 (11%)
28	GOL	C	523	-	5,5,5	0.37	0	5,5,5	0.88	0
24	CLA	c	913	3	69,73,73	2.05	19 (27%)	83,113,113	2.95	31 (37%)
37	DGD	D	408	-	52,52,67	1.04	3 (5%)	60,60,81	1.17	5 (8%)
29	LMT	b	626	-	25,25,36	0.47	0	30,30,47	0.58	0
24	CLA	C	508	3	69,73,73	2.08	20 (28%)	83,113,113	2.80	29 (34%)
28	GOL	O	302	-	5,5,5	0.33	0	5,5,5	0.39	0
35	HTG	B	632	-	19,19,19	0.96	2 (10%)	23,24,24	1.37	2 (8%)
28	GOL	B	626	-	5,5,5	0.41	0	5,5,5	0.34	0
35	HTG	C	522	-	19,19,19	1.00	1 (5%)	23,24,24	1.71	4 (17%)
24	CLA	B	607	2	69,73,73	2.06	19 (27%)	83,113,113	2.93	31 (37%)
24	CLA	b	614	2	69,73,73	2.04	18 (26%)	83,113,113	2.86	29 (34%)
35	HTG	b	628	-	19,19,19	1.21	2 (10%)	23,24,24	1.69	3 (13%)
24	CLA	a	408	1	69,73,73	2.03	19 (27%)	83,113,113	2.91	31 (37%)
24	CLA	b	609	2	69,73,73	2.06	21 (30%)	83,113,113	2.69	26 (31%)
40	HEC	v	202	16	50,50,50	1.66	9 (18%)	68,82,82	1.77	17 (25%)
24	CLA	C	502	3	69,73,73	2.06	20 (28%)	83,113,113	2.75	29 (34%)
35	HTG	V	203	-	19,19,19	1.02	2 (10%)	23,24,24	1.31	3 (13%)
33	LMG	C	519	-	51,51,55	0.96	2 (3%)	59,59,63	1.25	8 (13%)
26	BCR	A	410	-	41,41,41	1.11	1 (2%)	56,56,56	1.11	4 (7%)
33	LMG	c	919	-	51,51,55	0.88	2 (3%)	59,59,63	1.18	4 (6%)
24	CLA	B	606	2	69,73,73	2.03	18 (26%)	83,113,113	2.88	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMT	a	401	-	36,36,36	0.51	1 (2%)	47,47,47	1.15	3 (6%)
25	PHO	D	401	-	58,69,69	2.81	14 (24%)	56,99,99	2.80	15 (26%)
36	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.11	4 (9%)
24	CLA	b	608	2	69,73,73	2.02	20 (28%)	83,113,113	2.83	29 (34%)
24	CLA	c	904	3	69,73,73	2.04	19 (27%)	83,113,113	2.82	27 (32%)
26	BCR	b	624	-	41,41,41	1.09	2 (4%)	56,56,56	1.21	4 (7%)
24	CLA	A	409	1	69,73,73	2.10	19 (27%)	83,113,113	2.75	32 (38%)
28	GOL	A	413	-	5,5,5	0.38	0	5,5,5	0.22	0
28	GOL	v	203	-	5,5,5	0.35	0	5,5,5	0.27	0
24	CLA	D	404	4	69,73,73	1.97	20 (28%)	83,113,113	2.93	33 (39%)
27	SQD	F	103	-	42,43,54	1.17	3 (7%)	51,54,65	1.58	9 (17%)
24	CLA	A	406	41	69,73,73	2.04	20 (28%)	83,113,113	2.96	32 (38%)
24	CLA	c	909	3	69,73,73	2.03	20 (28%)	83,113,113	2.81	29 (34%)
29	LMT	A	415	-	36,36,36	0.67	1 (2%)	47,47,47	1.43	5 (10%)
28	GOL	v	205	-	5,5,5	0.33	0	5,5,5	0.47	0
40	HEC	V	202	16	50,50,50	1.69	10 (20%)	68,82,82	1.81	19 (27%)
29	LMT	m	103	-	36,36,36	0.49	0	47,47,47	1.08	3 (6%)
26	BCR	y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.48	9 (16%)
26	BCR	Y	102	-	41,41,41	1.07	1 (2%)	56,56,56	1.67	11 (19%)
24	CLA	B	605	2	69,73,73	1.97	20 (28%)	83,113,113	2.81	31 (37%)
24	CLA	B	613	2	69,73,73	1.98	18 (26%)	83,113,113	2.78	28 (33%)
28	GOL	B	631	-	5,5,5	0.33	0	5,5,5	0.43	0
29	LMT	t	101	-	25,25,36	0.50	0	30,30,47	0.77	1 (3%)
24	CLA	b	620	2	69,73,73	2.04	20 (28%)	83,113,113	2.77	32 (38%)
26	BCR	C	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.53	10 (17%)
35	HTG	B	633	-	19,19,19	1.04	2 (10%)	23,24,24	1.39	2 (8%)
35	HTG	B	624	-	19,19,19	0.82	1 (5%)	23,24,24	1.74	4 (17%)
37	DGD	h	102	-	63,63,67	0.91	3 (4%)	77,77,81	1.02	4 (5%)
24	CLA	B	609	2	69,73,73	2.06	20 (28%)	83,113,113	2.70	28 (33%)
28	GOL	B	628	-	5,5,5	0.38	0	5,5,5	0.47	0
28	GOL	a	419	34	5,5,5	0.31	0	5,5,5	0.40	0
33	LMG	B	622	-	51,51,55	0.94	2 (3%)	59,59,63	1.02	3 (5%)
33	LMG	d	415	39	51,51,55	0.94	2 (3%)	59,59,63	1.01	3 (5%)
28	GOL	b	633	-	5,5,5	0.37	0	5,5,5	0.41	0
28	GOL	c	928	-	5,5,5	0.41	0	5,5,5	0.25	0
25	PHO	a	407	-	58,69,69	2.74	14 (24%)	56,99,99	2.89	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	512	3	69,73,73	2.07	20 (28%)	83,113,113	2.81	30 (36%)
23	BCT	A	404	21	2,3,3	0.65	0	2,3,3	1.14	0
24	CLA	C	504	41	69,73,73	2.06	20 (28%)	83,113,113	2.82	28 (33%)
26	BCR	d	407	-	41,41,41	1.06	1 (2%)	56,56,56	1.66	15 (26%)
31	PL9	D	407	-	55,55,55	0.64	2 (3%)	68,69,69	1.89	22 (32%)
33	LMG	b	625	-	51,51,55	0.89	2 (3%)	59,59,63	1.11	5 (8%)
38	HEM	f	101	6,5	50,50,50	1.53	8 (16%)	66,82,82	1.77	13 (19%)
29	LMT	M	101	-	36,36,36	0.46	0	47,47,47	0.92	0
28	GOL	c	923	-	5,5,5	0.37	0	5,5,5	0.22	0
24	CLA	b	621	2	69,73,73	2.04	19 (27%)	83,113,113	2.82	32 (38%)
24	CLA	A	405	1	69,73,73	2.04	20 (28%)	83,113,113	2.81	31 (37%)
24	CLA	C	509	3	69,73,73	2.10	20 (28%)	83,113,113	2.78	30 (36%)
24	CLA	d	405	4	69,73,73	1.96	20 (28%)	83,113,113	2.88	29 (34%)
28	GOL	V	207	-	5,5,5	0.34	0	5,5,5	0.30	0
36	LHG	d	410	-	48,48,48	0.87	2 (4%)	51,54,54	1.03	4 (7%)
24	CLA	c	910	3	69,73,73	2.12	20 (28%)	83,113,113	2.80	29 (34%)
26	BCR	a	409	-	41,41,41	1.05	1 (2%)	56,56,56	1.28	2 (3%)
24	CLA	b	613	2	69,73,73	2.09	20 (28%)	83,113,113	2.72	31 (37%)
24	CLA	A	407	41	69,73,73	2.05	19 (27%)	83,113,113	2.83	31 (37%)
26	BCR	b	623	-	41,41,41	1.02	1 (2%)	56,56,56	1.29	7 (12%)
33	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.10	4 (8%)
28	GOL	l	101	-	5,5,5	0.47	0	5,5,5	0.24	0
24	CLA	c	908	41	69,73,73	2.01	20 (28%)	83,113,113	2.74	28 (33%)

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
26	BCR	c	927	-	-	0/29/63/63	0/2/2/2
28	GOL	T	101	-	-	0/4/4/4	-
35	HTG	b	601	-	-	3/10/30/30	0/1/1/1
29	LMT	a	417	-	-	4/21/61/61	0/2/2/2
24	CLA	B	614	2	-	8/39/115/115	-
29	LMT	M	103	-	-	11/21/61/61	0/2/2/2
35	HTG	c	921	-	-	4/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	v	204	-	-	2/4/4/4	-
28	GOL	b	632	-	-	2/4/4/4	-
24	CLA	b	619	2	-	20/39/115/115	-
24	CLA	C	505	3	-	6/39/115/115	-
24	CLA	B	612	2	-	1/39/115/115	-
36	LHG	L	101	-	-	16/53/53/53	-
24	CLA	b	618	2	-	3/39/115/115	-
24	CLA	c	905	41	-	6/39/115/115	-
28	GOL	a	412	-	-	4/4/4/4	-
28	GOL	a	413	-	-	2/4/4/4	-
28	GOL	T	103	-	-	2/4/4/4	-
28	GOL	B	636	-	-	2/4/4/4	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
24	CLA	C	511	3	-	4/39/115/115	-
24	CLA	c	914	3	-	5/39/115/115	-
28	GOL	V	201	34	-	2/4/4/4	-
35	HTG	B	623	-	-	3/10/30/30	0/1/1/1
24	CLA	a	406	41	-	11/39/115/115	-
33	LMG	a	411	-	-	14/46/66/70	0/1/1/1
37	DGD	C	517	-	-	19/51/91/95	0/2/2/2
36	LHG	B	635	-	-	13/53/53/53	-
28	GOL	V	206	-	-	2/4/4/4	-
24	CLA	c	907	3	-	13/39/115/115	-
24	CLA	c	906	3	-	8/39/115/115	-
28	GOL	D	402	-	-	4/4/4/4	-
24	CLA	C	510	3	-	8/39/115/115	-
35	HTG	C	521	-	-	0/10/30/30	0/1/1/1
24	CLA	b	615	41	-	5/39/115/115	-
24	CLA	C	507	41	-	5/39/115/115	-
29	LMT	C	520	-	-	6/21/61/61	0/2/2/2
26	BCR	k	101	-	-	0/29/63/63	0/2/2/2
25	PHO	A	408	-	-	2/37/103/103	0/5/6/6
24	CLA	C	506	3	-	6/39/115/115	-
38	HEM	F	102	6,5	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	B	625	-	-	5/10/30/30	0/1/1/1
24	CLA	b	606	41	-	16/39/115/115	-
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
37	DGD	e	101	-	-	26/51/91/95	0/2/2/2
29	LMT	e	102	-	-	9/21/61/61	0/2/2/2
28	GOL	V	205	-	-	0/4/4/4	-
24	CLA	C	501	3	-	7/39/115/115	-
33	LMG	Y	101	-	-	10/46/66/70	0/1/1/1
24	CLA	C	503	3	-	2/39/115/115	-
28	GOL	V	204	-	-	2/4/4/4	-
31	PL9	a	415	-	-	15/53/73/73	0/1/1/1
29	LMT	m	102	-	-	6/21/61/61	0/2/2/2
26	BCR	T	102	-	-	1/29/63/63	0/2/2/2
26	BCR	D	406	-	-	8/29/63/63	0/2/2/2
26	BCR	c	915	-	-	4/29/63/63	0/2/2/2
35	HTG	D	413	-	-	0/7/27/30	0/1/1/1
36	LHG	d	411	-	-	12/53/53/53	-
36	LHG	D	409	-	-	11/53/53/53	-
35	HTG	b	627	-	-	2/10/30/30	0/1/1/1
26	BCR	h	101	-	-	2/29/63/63	0/2/2/2
27	SQD	a	402	-	-	10/49/69/69	0/1/1/1
24	CLA	B	603	2	-	5/39/115/115	-
24	CLA	c	911	3	-	7/39/115/115	-
26	BCR	C	514	-	-	1/29/63/63	0/2/2/2
37	DGD	c	918	-	-	13/51/91/95	0/2/2/2
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
28	GOL	B	629	-	-	3/4/4/4	-
26	BCR	t	102	-	-	5/29/63/63	0/2/2/2
31	PL9	d	408	-	-	3/53/73/73	0/1/1/1
35	HTG	b	604	-	-	1/10/30/30	0/1/1/1
29	LMT	b	602	-	-	7/17/37/61	0/1/1/2
33	LMG	Z	101	-	-	13/31/51/70	0/1/1/1
24	CLA	D	405	4	-	6/39/115/115	-
36	LHG	b	635	-	-	20/53/53/53	-
28	GOL	b	630	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	604	2	-	6/39/115/115	-
37	DGD	C	518	-	-	10/51/91/95	0/2/2/2
35	HTG	b	603	-	-	1/10/30/30	0/1/1/1
37	DGD	C	516	-	-	16/51/91/95	0/2/2/2
33	LMG	J	101	39	-	11/46/66/70	0/1/1/1
24	CLA	B	615	2	-	18/39/115/115	-
36	LHG	a	418	-	-	15/46/46/53	-
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1
24	CLA	d	406	4	-	8/39/115/115	-
24	CLA	b	611	2	-	14/39/115/115	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
28	GOL	B	630	-	-	4/4/4/4	-
28	GOL	c	924	-	-	2/4/4/4	-
24	CLA	c	902	3	-	7/39/115/115	-
28	GOL	b	631	-	-	4/4/4/4	-
24	CLA	B	608	41	-	6/39/115/115	-
27	SQD	A	414	-	-	13/49/69/69	0/1/1/1
27	SQD	a	410	-	-	14/49/69/69	0/1/1/1
24	CLA	B	617	2	-	8/39/115/115	-
37	DGD	c	916	-	-	12/51/91/95	0/2/2/2
24	CLA	B	602	41	-	15/39/115/115	-
24	CLA	C	513	3	-	8/39/115/115	-
31	PL9	A	417	-	-	13/53/73/73	0/1/1/1
36	LHG	d	409	-	-	18/53/53/53	-
25	PHO	d	403	-	-	3/37/103/103	0/5/6/6
24	CLA	b	617	2	-	4/39/115/115	-
29	LMT	F	101	-	-	6/21/61/61	0/2/2/2
28	GOL	C	524	-	-	2/4/4/4	-
24	CLA	c	903	3	-	7/39/115/115	-
36	LHG	D	410	-	-	18/53/53/53	-
24	CLA	B	611	41	-	4/39/115/115	-
24	CLA	b	612	41	-	3/39/115/115	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
24	CLA	d	404	41	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	610	2	-	4/39/115/115	-
35	HTG	d	414	-	-	0/7/27/30	0/1/1/1
26	BCR	H	101	-	-	2/29/63/63	0/2/2/2
24	CLA	c	912	3	-	6/39/115/115	-
27	SQD	L	102	-	-	22/49/69/69	0/1/1/1
24	CLA	B	610	2	-	5/39/115/115	-
24	CLA	B	616	2	-	13/39/115/115	-
35	HTG	c	922	-	-	0/10/30/30	0/1/1/1
33	LMG	A	419	-	-	21/46/66/70	0/1/1/1
37	DGD	c	917	-	-	18/51/91/95	0/2/2/2
28	GOL	A	412	-	-	0/4/4/4	-
24	CLA	b	607	2	-	7/39/115/115	-
24	CLA	b	616	2	-	3/39/115/115	-
28	GOL	B	627	-	-	2/4/4/4	-
29	LMT	D	403	-	-	10/21/61/61	0/2/2/2
37	DGD	H	102	-	-	9/51/91/95	0/2/2/2
24	CLA	a	405	1	-	4/39/115/115	-
26	BCR	b	622	-	-	2/29/63/63	0/2/2/2
28	GOL	b	629	-	-	0/4/4/4	-
33	LMG	c	920	-	-	5/46/66/70	0/1/1/1
28	GOL	C	523	-	-	2/4/4/4	-
24	CLA	c	913	3	-	14/39/115/115	-
37	DGD	D	408	-	-	18/47/67/95	0/1/1/2
29	LMT	b	626	-	-	5/17/37/61	0/1/1/2
24	CLA	C	508	3	-	5/39/115/115	-
28	GOL	O	302	-	-	0/4/4/4	-
35	HTG	B	632	-	-	0/10/30/30	0/1/1/1
28	GOL	B	626	-	-	2/4/4/4	-
35	HTG	C	522	-	-	3/10/30/30	0/1/1/1
24	CLA	B	607	2	-	7/39/115/115	-
24	CLA	b	614	2	-	3/39/115/115	-
35	HTG	b	628	-	-	4/10/30/30	0/1/1/1
24	CLA	a	408	1	-	10/39/115/115	-
24	CLA	b	609	2	-	3/39/115/115	-
40	HEC	v	202	16	1/1/3/7	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	502	3	-	10/39/115/115	-
35	HTG	V	203	-	-	5/10/30/30	0/1/1/1
33	LMG	C	519	-	-	10/46/66/70	0/1/1/1
26	BCR	A	410	-	-	4/29/63/63	0/2/2/2
33	LMG	c	919	-	-	12/46/66/70	0/1/1/1
24	CLA	B	606	2	-	6/39/115/115	-
29	LMT	a	401	-	-	7/21/61/61	0/2/2/2
25	PHO	D	401	-	-	3/37/103/103	0/5/6/6
36	LHG	E	101	-	-	19/46/46/53	-
24	CLA	b	608	2	-	5/39/115/115	-
24	CLA	c	904	3	-	8/39/115/115	-
26	BCR	b	624	-	-	0/29/63/63	0/2/2/2
24	CLA	A	409	1	-	12/39/115/115	-
28	GOL	A	413	-	-	2/4/4/4	-
28	GOL	v	203	-	-	2/4/4/4	-
24	CLA	D	404	4	-	2/39/115/115	-
27	SQD	F	103	-	-	15/38/58/69	0/1/1/1
24	CLA	A	406	41	-	4/39/115/115	-
24	CLA	c	909	3	-	7/39/115/115	-
29	LMT	A	415	-	-	5/21/61/61	0/2/2/2
28	GOL	v	205	-	-	2/4/4/4	-
40	HEC	V	202	16	1/1/3/7	6/14/54/54	-
29	LMT	m	103	-	-	8/21/61/61	0/2/2/2
26	BCR	y	101	-	-	4/29/63/63	0/2/2/2
26	BCR	Y	102	-	-	4/29/63/63	0/2/2/2
24	CLA	B	605	2	-	4/39/115/115	-
24	CLA	B	613	2	-	5/39/115/115	-
28	GOL	B	631	-	-	1/4/4/4	-
29	LMT	t	101	-	-	7/17/37/61	0/1/1/2
24	CLA	b	620	2	-	9/39/115/115	-
26	BCR	C	515	-	-	4/29/63/63	0/2/2/2
35	HTG	B	633	-	-	0/10/30/30	0/1/1/1
35	HTG	B	624	-	-	4/10/30/30	0/1/1/1
37	DGD	h	102	-	-	9/51/91/95	0/2/2/2
24	CLA	B	609	2	-	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	B	628	-	-	2/4/4/4	-
28	GOL	a	419	34	-	3/4/4/4	-
33	LMG	B	622	-	-	8/46/66/70	0/1/1/1
33	LMG	d	415	39	-	10/46/66/70	0/1/1/1
28	GOL	b	633	-	-	2/4/4/4	-
28	GOL	c	928	-	-	2/4/4/4	-
25	PHO	a	407	-	-	4/37/103/103	0/5/6/6
24	CLA	C	512	3	-	9/39/115/115	-
24	CLA	C	504	41	-	7/39/115/115	-
26	BCR	d	407	-	-	4/29/63/63	0/2/2/2
31	PL9	D	407	-	-	9/53/73/73	0/1/1/1
33	LMG	b	625	-	-	8/46/66/70	0/1/1/1
38	HEM	f	101	6,5	-	10/14/54/54	-
29	LMT	M	101	-	-	6/21/61/61	0/2/2/2
28	GOL	c	923	-	-	0/4/4/4	-
24	CLA	b	621	2	-	9/39/115/115	-
24	CLA	A	405	1	-	4/39/115/115	-
24	CLA	C	509	3	-	14/39/115/115	-
24	CLA	d	405	4	-	7/39/115/115	-
28	GOL	V	207	-	-	4/4/4/4	-
36	LHG	d	410	-	-	9/53/53/53	-
24	CLA	c	910	3	-	15/39/115/115	-
26	BCR	a	409	-	-	2/29/63/63	0/2/2/2
24	CLA	b	613	2	-	1/39/115/115	-
24	CLA	A	407	41	-	8/39/115/115	-
26	BCR	b	623	-	-	1/29/63/63	0/2/2/2
33	LMG	z	101	-	-	11/34/54/70	0/1/1/1
28	GOL	l	101	-	-	0/4/4/4	-
24	CLA	c	908	41	-	6/39/115/115	-

All (1621) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	403	PHO	C1B-C2B	9.34	1.49	1.39
25	a	407	PHO	C1B-C2B	8.98	1.49	1.39
25	D	401	PHO	C1B-C2B	8.94	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	401	PHO	C1D-C2D	8.68	1.49	1.39
25	A	408	PHO	C1B-C2B	8.33	1.48	1.39
25	A	408	PHO	C1D-C2D	8.28	1.48	1.39
25	d	403	PHO	C1D-C2D	8.21	1.48	1.39
25	a	407	PHO	C1D-C2D	7.95	1.48	1.39
25	D	401	PHO	C3B-C4B	7.20	1.49	1.41
25	d	403	PHO	C3B-C4B	7.11	1.49	1.41
25	a	407	PHO	C3B-C4B	6.98	1.49	1.41
25	d	403	PHO	C3C-C2C	6.64	1.50	1.36
25	A	408	PHO	C3B-C4B	6.60	1.49	1.41
25	A	408	PHO	C4D-CHA	6.52	1.50	1.39
25	D	401	PHO	C4D-CHA	6.51	1.50	1.39
25	d	403	PHO	C3B-C2B	6.22	1.49	1.40
25	a	407	PHO	C4D-CHA	6.16	1.49	1.39
25	d	403	PHO	C4D-CHA	6.15	1.49	1.39
25	D	401	PHO	C3B-C2B	6.06	1.48	1.40
25	A	408	PHO	C3C-C2C	5.99	1.49	1.36
24	B	614	CLA	C1D-ND	5.96	1.45	1.37
25	A	408	PHO	C3B-C2B	5.93	1.48	1.40
25	a	407	PHO	C3B-C2B	5.93	1.48	1.40
25	D	401	PHO	C3C-C2C	5.88	1.49	1.36
24	B	605	CLA	C1D-ND	5.83	1.45	1.37
24	B	604	CLA	C3C-C2C	5.78	1.49	1.36
24	C	503	CLA	C1D-ND	5.72	1.44	1.37
24	b	606	CLA	C3C-C2C	5.70	1.48	1.36
24	d	404	CLA	C3C-C2C	5.70	1.48	1.36
25	a	407	PHO	C3D-C2D	5.66	1.49	1.39
24	a	408	CLA	C3C-C2C	5.63	1.48	1.36
24	B	607	CLA	C3C-C2C	5.62	1.48	1.36
24	c	903	CLA	O2D-CGD	5.62	1.46	1.33
24	C	510	CLA	C3C-C2C	5.61	1.48	1.36
24	b	610	CLA	C3C-C2C	5.59	1.48	1.36
24	b	620	CLA	C1D-ND	5.59	1.44	1.37
24	B	611	CLA	C3C-C2C	5.57	1.48	1.36
24	c	904	CLA	C3C-C2C	5.56	1.48	1.36
25	A	408	PHO	C3D-C2D	5.56	1.49	1.39
24	c	903	CLA	C3C-C2C	5.55	1.48	1.36
24	d	406	CLA	C1D-ND	5.55	1.44	1.37
24	c	910	CLA	C1D-ND	5.53	1.44	1.37
24	c	911	CLA	C1D-ND	5.51	1.44	1.37
24	A	406	CLA	C3C-C2C	5.49	1.48	1.36
25	a	407	PHO	C3C-C2C	5.47	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	C3C-C2C	5.46	1.48	1.36
24	C	512	CLA	C3C-C2C	5.46	1.48	1.36
24	B	612	CLA	C3C-C2C	5.45	1.48	1.36
24	b	606	CLA	C1D-ND	5.44	1.44	1.37
38	f	101	HEM	FE-NB	5.42	2.11	1.94
25	D	401	PHO	C3D-C2D	5.41	1.49	1.39
24	c	913	CLA	C3C-C2C	5.41	1.48	1.36
24	c	911	CLA	C3C-C2C	5.39	1.48	1.36
24	B	606	CLA	C1D-ND	5.39	1.44	1.37
24	C	509	CLA	C3C-C2C	5.38	1.48	1.36
24	c	914	CLA	C3C-C2C	5.37	1.48	1.36
24	C	509	CLA	C1D-ND	5.36	1.44	1.37
24	B	602	CLA	C3C-C2C	5.36	1.48	1.36
24	C	503	CLA	C3C-C2C	5.36	1.48	1.36
24	B	602	CLA	C1D-ND	5.35	1.44	1.37
24	B	603	CLA	C3C-C2C	5.34	1.48	1.36
24	A	407	CLA	C3C-C2C	5.33	1.48	1.36
24	b	607	CLA	C3C-C2C	5.33	1.48	1.36
24	b	619	CLA	C3C-C2C	5.33	1.48	1.36
24	b	618	CLA	O2D-CGD	5.33	1.46	1.33
24	b	617	CLA	C3C-C2C	5.33	1.48	1.36
24	b	618	CLA	C3C-C2C	5.32	1.48	1.36
24	a	405	CLA	C3C-C2C	5.32	1.48	1.36
24	C	513	CLA	C3C-C2C	5.32	1.48	1.36
24	C	508	CLA	C3C-C2C	5.31	1.48	1.36
24	c	906	CLA	C3C-C2C	5.31	1.48	1.36
24	b	611	CLA	C3C-C2C	5.30	1.48	1.36
24	B	616	CLA	C1D-ND	5.30	1.44	1.37
24	C	510	CLA	C1D-ND	5.29	1.44	1.37
24	c	902	CLA	C1D-ND	5.29	1.44	1.37
24	C	507	CLA	C3C-C2C	5.29	1.48	1.36
24	d	406	CLA	O2D-CGD	5.27	1.46	1.33
24	C	501	CLA	C1D-ND	5.26	1.44	1.37
25	D	401	PHO	O2D-CGD	5.26	1.46	1.33
24	b	618	CLA	C1D-ND	5.25	1.44	1.37
24	A	406	CLA	C1D-ND	5.25	1.44	1.37
24	C	511	CLA	C1D-ND	5.25	1.44	1.37
24	c	909	CLA	O2D-CGD	5.25	1.46	1.33
24	C	504	CLA	C1D-ND	5.24	1.44	1.37
24	c	904	CLA	C1D-ND	5.24	1.44	1.37
26	b	624	BCR	C23-C22	-5.24	1.34	1.45
38	F	102	HEM	FE-NB	5.24	2.11	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	909	CLA	C3C-C2C	5.24	1.47	1.36
24	B	616	CLA	O2D-CGD	5.24	1.46	1.33
25	a	407	PHO	O2D-CGD	5.23	1.46	1.33
24	b	619	CLA	C1D-ND	5.23	1.44	1.37
24	A	409	CLA	C1D-ND	5.23	1.44	1.37
24	b	615	CLA	C3C-C2C	5.23	1.47	1.36
24	b	609	CLA	C3C-C2C	5.21	1.47	1.36
26	Y	102	BCR	C23-C22	-5.21	1.34	1.45
24	c	905	CLA	C1D-ND	5.21	1.44	1.37
24	c	910	CLA	C3C-C2C	5.20	1.47	1.36
24	c	902	CLA	C3C-C2C	5.20	1.47	1.36
24	C	502	CLA	C3C-C2C	5.20	1.47	1.36
24	B	617	CLA	C3C-C2C	5.20	1.47	1.36
24	B	609	CLA	C3C-C2C	5.20	1.47	1.36
24	c	914	CLA	O2D-CGD	5.19	1.45	1.33
26	C	514	BCR	C23-C22	-5.19	1.34	1.45
24	b	613	CLA	C3C-C2C	5.19	1.47	1.36
24	B	608	CLA	C3C-C2C	5.19	1.47	1.36
24	B	606	CLA	C3C-C2C	5.18	1.47	1.36
24	c	903	CLA	C1D-ND	5.18	1.44	1.37
26	k	101	BCR	C23-C22	-5.18	1.34	1.45
24	C	502	CLA	C1D-ND	5.18	1.44	1.37
24	b	619	CLA	O2D-CGD	5.17	1.45	1.33
24	B	617	CLA	O2D-CGD	5.17	1.45	1.33
24	a	408	CLA	O2D-CGD	5.16	1.45	1.33
24	B	610	CLA	O2D-CGD	5.16	1.45	1.33
24	c	905	CLA	O2D-CGD	5.15	1.45	1.33
24	B	610	CLA	C3C-C2C	5.15	1.47	1.36
24	d	404	CLA	C1D-ND	5.15	1.44	1.37
24	B	611	CLA	C1D-ND	5.15	1.44	1.37
24	d	406	CLA	C3C-C2C	5.14	1.47	1.36
24	b	608	CLA	C3C-C2C	5.14	1.47	1.36
24	D	404	CLA	C3C-C2C	5.14	1.47	1.36
24	c	908	CLA	C3C-C2C	5.14	1.47	1.36
24	d	405	CLA	C3C-C2C	5.14	1.47	1.36
24	c	907	CLA	C3C-C2C	5.14	1.47	1.36
24	b	607	CLA	C1D-ND	5.14	1.44	1.37
26	H	101	BCR	C23-C22	-5.13	1.34	1.45
24	c	907	CLA	O2D-CGD	5.12	1.45	1.33
24	C	507	CLA	CHC-C1C	5.12	1.48	1.38
24	a	406	CLA	C1D-ND	5.12	1.44	1.37
24	c	909	CLA	C1D-ND	5.11	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	C1D-ND	5.11	1.44	1.37
24	b	616	CLA	O2D-CGD	5.11	1.45	1.33
24	C	501	CLA	C3C-C2C	5.10	1.47	1.36
24	A	409	CLA	C3C-C2C	5.10	1.47	1.36
24	b	614	CLA	C3C-C2C	5.10	1.47	1.36
24	C	510	CLA	O2D-CGD	5.10	1.45	1.33
24	b	611	CLA	C1D-ND	5.10	1.44	1.37
40	v	202	HEC	FE-NB	5.10	2.10	1.94
24	C	503	CLA	CHC-C1C	5.09	1.48	1.38
24	b	621	CLA	O2D-CGD	5.09	1.45	1.33
24	C	505	CLA	C3C-C2C	5.09	1.47	1.36
24	b	620	CLA	C3C-C2C	5.09	1.47	1.36
25	d	403	PHO	O2D-CGD	5.08	1.45	1.33
26	t	102	BCR	C23-C22	-5.08	1.35	1.45
24	B	615	CLA	O2D-CGD	5.08	1.45	1.33
24	a	408	CLA	C1D-ND	5.07	1.44	1.37
24	b	614	CLA	CHC-C1C	5.07	1.48	1.38
24	b	609	CLA	C1D-ND	5.06	1.44	1.37
24	C	511	CLA	O2D-CGD	5.06	1.45	1.33
24	C	513	CLA	C1D-ND	5.06	1.44	1.37
24	C	508	CLA	O2D-CGD	5.06	1.45	1.33
24	A	409	CLA	O2D-CGD	5.05	1.45	1.33
24	b	614	CLA	O2D-CGD	5.05	1.45	1.33
24	B	602	CLA	O2D-CGD	5.05	1.45	1.33
24	c	914	CLA	C1D-ND	5.05	1.44	1.37
25	a	407	PHO	OBD-CAD	5.04	1.29	1.22
24	B	614	CLA	O2D-CGD	5.04	1.45	1.33
24	C	512	CLA	O2D-CGD	5.04	1.45	1.33
24	C	506	CLA	C1D-ND	5.04	1.44	1.37
24	B	605	CLA	C3C-C2C	5.04	1.47	1.36
24	C	508	CLA	C1D-ND	5.04	1.44	1.37
24	C	501	CLA	CHC-C1C	5.04	1.48	1.38
24	C	513	CLA	O2D-CGD	5.03	1.45	1.33
24	b	621	CLA	C3C-C2C	5.03	1.47	1.36
24	b	613	CLA	O2D-CGD	5.03	1.45	1.33
24	C	507	CLA	C1D-ND	5.02	1.44	1.37
24	c	905	CLA	C3C-C2C	5.01	1.47	1.36
25	d	403	PHO	C3D-C2D	5.01	1.48	1.39
24	B	612	CLA	O2D-CGD	5.00	1.45	1.33
24	b	613	CLA	C1D-ND	5.00	1.43	1.37
24	C	504	CLA	C3C-C2C	5.00	1.47	1.36
24	b	606	CLA	O2D-CGD	5.00	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	C1D-ND	5.00	1.43	1.37
24	B	607	CLA	O2D-CGD	4.99	1.45	1.33
24	c	910	CLA	O2D-CGD	4.99	1.45	1.33
24	c	902	CLA	O2D-CGD	4.99	1.45	1.33
24	c	907	CLA	C1D-ND	4.99	1.43	1.37
24	A	405	CLA	C1D-ND	4.98	1.43	1.37
24	A	409	CLA	CHC-C1C	4.97	1.48	1.38
24	D	405	CLA	C1D-ND	4.97	1.43	1.37
24	C	511	CLA	C3C-C2C	4.97	1.47	1.36
40	V	202	HEC	FE-NB	4.97	2.10	1.94
24	b	612	CLA	O2D-CGD	4.96	1.45	1.33
24	b	616	CLA	C3C-C2C	4.96	1.47	1.36
24	C	502	CLA	O2D-CGD	4.96	1.45	1.33
24	c	913	CLA	C1D-ND	4.95	1.43	1.37
24	C	509	CLA	O2D-CGD	4.95	1.45	1.33
24	B	607	CLA	CHC-C1C	4.95	1.48	1.38
24	B	606	CLA	O2D-CGD	4.95	1.45	1.33
26	K	101	BCR	C23-C22	-4.94	1.35	1.45
24	b	612	CLA	C3C-C2C	4.93	1.47	1.36
24	C	506	CLA	O2D-CGD	4.93	1.45	1.33
24	D	404	CLA	O2D-CGD	4.93	1.45	1.33
26	y	101	BCR	C23-C22	-4.93	1.35	1.45
24	C	506	CLA	C3C-C2C	4.92	1.47	1.36
24	c	912	CLA	C3C-C2C	4.91	1.47	1.36
24	b	607	CLA	CHC-C1C	4.91	1.48	1.38
24	c	913	CLA	O2D-CGD	4.91	1.45	1.33
24	a	406	CLA	CHC-C1C	4.91	1.48	1.38
24	b	609	CLA	O2D-CGD	4.90	1.45	1.33
24	b	610	CLA	O2D-CGD	4.89	1.45	1.33
24	b	614	CLA	C1D-ND	4.89	1.43	1.37
24	B	609	CLA	O2D-CGD	4.89	1.45	1.33
24	B	617	CLA	C1D-ND	4.89	1.43	1.37
24	A	407	CLA	CHD-C1D	4.89	1.47	1.38
24	D	405	CLA	C3C-C2C	4.89	1.47	1.36
24	c	904	CLA	CHC-C1C	4.88	1.48	1.38
24	b	615	CLA	CHC-C1C	4.88	1.48	1.38
24	b	610	CLA	CHC-C1C	4.88	1.48	1.38
24	C	512	CLA	CHC-C1C	4.87	1.48	1.38
26	b	623	BCR	C23-C22	-4.87	1.35	1.45
24	a	405	CLA	C1D-ND	4.87	1.43	1.37
24	b	620	CLA	O2D-CGD	4.87	1.45	1.33
24	D	405	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	607	CLA	C1D-ND	4.87	1.43	1.37
24	A	405	CLA	C3C-C2C	4.87	1.47	1.36
24	A	405	CLA	CHC-C1C	4.86	1.48	1.38
24	C	504	CLA	O2D-CGD	4.86	1.45	1.33
24	b	617	CLA	O2D-CGD	4.85	1.45	1.33
24	a	406	CLA	O2D-CGD	4.85	1.45	1.33
24	A	407	CLA	C1D-ND	4.84	1.43	1.37
24	B	613	CLA	C3C-C2C	4.83	1.47	1.36
24	B	604	CLA	O2D-CGD	4.83	1.45	1.33
26	C	515	BCR	C23-C22	-4.82	1.35	1.45
24	c	906	CLA	O2D-CGD	4.82	1.45	1.33
24	B	616	CLA	C3C-C2C	4.81	1.47	1.36
24	C	502	CLA	CHC-C1C	4.81	1.48	1.38
24	A	407	CLA	O2D-CGD	4.81	1.44	1.33
24	b	615	CLA	O2D-CGD	4.81	1.44	1.33
24	B	603	CLA	CHC-C1C	4.81	1.48	1.38
26	a	409	BCR	C23-C22	-4.81	1.35	1.45
24	d	406	CLA	CHC-C1C	4.80	1.48	1.38
25	A	408	PHO	O2D-CGD	4.80	1.44	1.33
24	B	604	CLA	C1D-ND	4.80	1.43	1.37
24	B	614	CLA	C3C-C2C	4.80	1.46	1.36
24	C	511	CLA	CHC-C1C	4.80	1.48	1.38
26	T	102	BCR	C23-C22	-4.79	1.35	1.45
24	c	908	CLA	O2D-CGD	4.79	1.44	1.33
24	a	406	CLA	C3C-C2C	4.79	1.46	1.36
24	c	914	CLA	CHC-C1C	4.78	1.48	1.38
26	A	410	BCR	C23-C22	-4.78	1.35	1.45
24	b	611	CLA	O2D-CGD	4.78	1.44	1.33
24	b	615	CLA	C1D-ND	4.78	1.43	1.37
35	B	623	HTG	C1'-S1	-4.77	1.75	1.81
24	d	405	CLA	CHC-C1C	4.77	1.48	1.38
24	B	604	CLA	CHC-C1C	4.76	1.48	1.38
24	B	602	CLA	O2A-CGA	4.76	1.47	1.33
24	c	905	CLA	CHC-C1C	4.76	1.48	1.38
24	c	913	CLA	CHC-C1C	4.76	1.48	1.38
24	C	504	CLA	CHC-C1C	4.76	1.48	1.38
26	B	620	BCR	C23-C22	-4.76	1.35	1.45
24	B	613	CLA	CHC-C1C	4.75	1.48	1.38
24	B	611	CLA	O2D-CGD	4.75	1.44	1.33
24	b	608	CLA	O2D-CGD	4.74	1.44	1.33
26	d	407	BCR	C23-C22	-4.74	1.35	1.45
24	A	406	CLA	O2D-CGD	4.74	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	CLA	CHD-C1D	4.74	1.47	1.38
24	C	509	CLA	CHC-C1C	4.74	1.48	1.38
24	b	613	CLA	CHC-C1C	4.73	1.48	1.38
24	c	910	CLA	CHC-C1C	4.73	1.48	1.38
24	C	506	CLA	CHD-C1D	4.73	1.47	1.38
24	B	613	CLA	O2D-CGD	4.72	1.44	1.33
26	c	927	BCR	C23-C22	-4.72	1.35	1.45
24	b	621	CLA	C1D-ND	4.72	1.43	1.37
24	b	610	CLA	C1D-ND	4.71	1.43	1.37
24	b	621	CLA	CHC-C1C	4.71	1.48	1.38
24	C	501	CLA	O2D-CGD	4.71	1.44	1.33
26	h	101	BCR	C23-C22	-4.71	1.35	1.45
24	c	911	CLA	O2D-CGD	4.71	1.44	1.33
24	B	610	CLA	CHC-C1C	4.70	1.48	1.38
24	C	513	CLA	CHC-C1C	4.70	1.48	1.38
24	B	603	CLA	O2D-CGD	4.70	1.44	1.33
24	b	619	CLA	CHC-C1C	4.70	1.48	1.38
24	c	908	CLA	C1D-ND	4.70	1.43	1.37
24	b	607	CLA	O2D-CGD	4.69	1.44	1.33
24	B	608	CLA	C1D-ND	4.69	1.43	1.37
24	c	912	CLA	O2D-CGD	4.69	1.44	1.33
24	b	616	CLA	C1D-ND	4.69	1.43	1.37
24	C	503	CLA	O2D-CGD	4.68	1.44	1.33
24	C	508	CLA	CHD-C1D	4.68	1.47	1.38
24	B	617	CLA	CHC-C1C	4.68	1.48	1.38
24	C	507	CLA	O2D-CGD	4.68	1.44	1.33
24	c	904	CLA	O2D-CGD	4.66	1.44	1.33
24	D	404	CLA	C1D-ND	4.66	1.43	1.37
24	d	404	CLA	O2D-CGD	4.66	1.44	1.33
24	b	606	CLA	CHC-C1C	4.66	1.48	1.38
24	b	612	CLA	CHC-C1C	4.65	1.48	1.38
24	c	912	CLA	CHC-C1C	4.65	1.48	1.38
24	B	614	CLA	CHC-C1C	4.64	1.48	1.38
24	b	608	CLA	CHC-C1C	4.63	1.47	1.38
24	C	505	CLA	O2D-CGD	4.63	1.44	1.33
24	A	405	CLA	O2D-CGD	4.63	1.44	1.33
24	B	616	CLA	CHC-C1C	4.63	1.47	1.38
24	B	605	CLA	O2D-CGD	4.62	1.44	1.33
24	c	906	CLA	CHC-C1C	4.61	1.47	1.38
24	c	910	CLA	CHD-C1D	4.61	1.47	1.38
37	D	408	DGD	O1G-C1A	4.60	1.46	1.33
24	a	405	CLA	CHC-C1C	4.60	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	C1D-ND	4.60	1.43	1.37
27	A	414	SQD	O48-C23	4.60	1.46	1.33
24	b	608	CLA	C1D-ND	4.59	1.43	1.37
24	B	608	CLA	O2D-CGD	4.59	1.44	1.33
24	c	908	CLA	CHC-C1C	4.59	1.47	1.38
24	A	407	CLA	CHC-C1C	4.59	1.47	1.38
33	z	101	LMG	O8-C28	4.59	1.46	1.33
24	c	909	CLA	CHC-C1C	4.58	1.47	1.38
24	C	501	CLA	CHD-C1D	4.58	1.47	1.38
24	b	617	CLA	CHC-C1C	4.57	1.47	1.38
24	c	912	CLA	C1D-ND	4.57	1.43	1.37
24	C	510	CLA	CHC-C1C	4.57	1.47	1.38
24	a	406	CLA	O2A-CGA	4.55	1.46	1.33
24	B	609	CLA	CHD-C1D	4.55	1.47	1.38
24	B	606	CLA	CHC-C1C	4.55	1.47	1.38
24	a	408	CLA	CHC-C1C	4.54	1.47	1.38
24	a	405	CLA	O2D-CGD	4.54	1.44	1.33
24	c	903	CLA	CHC-C1C	4.54	1.47	1.38
24	C	505	CLA	CHC-C1C	4.54	1.47	1.38
26	c	915	BCR	C23-C22	-4.53	1.36	1.45
27	a	402	SQD	O48-C23	4.53	1.46	1.33
27	f	102	SQD	O47-C7	4.52	1.47	1.34
24	c	910	CLA	O2A-CGA	4.51	1.46	1.33
24	B	613	CLA	C1D-ND	4.51	1.43	1.37
24	C	508	CLA	O2A-CGA	4.51	1.46	1.33
24	b	609	CLA	O2A-CGA	4.51	1.46	1.33
37	e	101	DGD	O2G-C1B	4.50	1.47	1.34
24	B	609	CLA	CHC-C1C	4.49	1.47	1.38
24	b	620	CLA	CHC-C1C	4.49	1.47	1.38
24	C	509	CLA	O2A-CGA	4.48	1.46	1.33
24	B	610	CLA	C1D-ND	4.48	1.43	1.37
37	D	408	DGD	O2G-C1B	4.48	1.46	1.34
24	b	606	CLA	CHD-C1D	4.47	1.47	1.38
24	b	611	CLA	CHC-C1C	4.47	1.47	1.38
24	B	610	CLA	O2A-CGA	4.47	1.46	1.33
24	B	602	CLA	CHC-C1C	4.46	1.47	1.38
24	C	506	CLA	CHC-C1C	4.46	1.47	1.38
27	F	103	SQD	O47-C7	4.45	1.46	1.34
26	b	622	BCR	C23-C22	-4.44	1.36	1.45
24	b	612	CLA	CHD-C1D	4.44	1.47	1.38
24	B	604	CLA	O2A-CGA	4.44	1.46	1.33
24	D	405	CLA	CHC-C1C	4.44	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	O2A-CGA	4.44	1.46	1.33
24	B	612	CLA	C1D-ND	4.43	1.43	1.37
24	B	609	CLA	C1D-ND	4.42	1.43	1.37
26	D	406	BCR	C23-C22	-4.42	1.36	1.45
24	b	621	CLA	O2A-CGA	4.42	1.46	1.33
24	B	611	CLA	CHC-C1C	4.42	1.47	1.38
25	A	408	PHO	OBD-CAD	4.42	1.28	1.22
24	C	502	CLA	CHD-C1D	4.41	1.47	1.38
33	Y	101	LMG	O8-C28	4.41	1.46	1.33
33	A	419	LMG	O7-C10	4.41	1.46	1.34
24	c	907	CLA	CHC-C1C	4.40	1.47	1.38
26	B	618	BCR	C23-C22	-4.40	1.36	1.45
24	c	911	CLA	CHD-C1D	4.40	1.46	1.38
24	D	405	CLA	CHD-C1D	4.40	1.46	1.38
24	B	610	CLA	CHD-C1D	4.39	1.46	1.38
24	B	608	CLA	CHC-C1C	4.39	1.47	1.38
36	a	418	LHG	O8-C23	4.39	1.46	1.33
24	b	615	CLA	CHD-C1D	4.39	1.46	1.38
36	D	410	LHG	O7-C7	4.38	1.46	1.34
24	B	603	CLA	C1D-ND	4.38	1.43	1.37
24	A	406	CLA	O2A-CGA	4.38	1.46	1.33
24	b	606	CLA	O2A-CGA	4.37	1.46	1.33
27	f	102	SQD	O48-C23	4.37	1.46	1.33
36	L	101	LHG	O8-C23	4.37	1.46	1.33
24	d	405	CLA	O2D-CGD	4.37	1.43	1.33
24	c	906	CLA	C1D-ND	4.37	1.43	1.37
24	B	609	CLA	O2A-CGA	4.35	1.46	1.33
24	C	505	CLA	C1D-ND	4.35	1.43	1.37
33	B	622	LMG	O8-C28	4.35	1.46	1.33
24	b	607	CLA	CHD-C1D	4.35	1.46	1.38
25	D	401	PHO	OBD-CAD	4.35	1.28	1.22
33	C	519	LMG	O7-C10	4.34	1.46	1.34
24	c	912	CLA	O2A-CGA	4.34	1.46	1.33
24	B	615	CLA	O2A-CGA	4.34	1.46	1.33
24	C	508	CLA	CHC-C1C	4.33	1.47	1.38
24	d	404	CLA	CHD-C1D	4.33	1.46	1.38
24	d	404	CLA	O2A-CGA	4.33	1.46	1.33
24	C	509	CLA	CHD-C1D	4.33	1.46	1.38
24	b	613	CLA	CHD-C1D	4.32	1.46	1.38
24	b	621	CLA	CHD-C1D	4.32	1.46	1.38
24	c	908	CLA	O2A-CGA	4.32	1.46	1.33
33	A	419	LMG	O8-C28	4.32	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	CHD-C1D	4.31	1.46	1.38
36	E	101	LHG	O8-C23	4.31	1.45	1.33
24	C	503	CLA	CHD-C1D	4.31	1.46	1.38
24	c	904	CLA	CHD-C1D	4.31	1.46	1.38
24	C	506	CLA	O2A-CGA	4.31	1.45	1.33
24	b	614	CLA	CHD-C1D	4.30	1.46	1.38
24	B	607	CLA	CHD-C1D	4.30	1.46	1.38
24	b	608	CLA	CHD-C1D	4.30	1.46	1.38
24	c	909	CLA	O2A-CGA	4.30	1.45	1.33
24	B	616	CLA	O2A-CGA	4.30	1.45	1.33
27	L	102	SQD	O47-C7	4.30	1.46	1.34
33	a	411	LMG	O8-C28	4.29	1.45	1.33
24	C	512	CLA	CHD-C1D	4.29	1.46	1.38
37	e	101	DGD	O1G-C1A	4.29	1.45	1.33
24	b	612	CLA	O2A-CGA	4.29	1.45	1.33
24	c	911	CLA	CHC-C1C	4.29	1.47	1.38
37	c	918	DGD	O1G-C1A	4.29	1.45	1.33
24	b	620	CLA	O2A-CGA	4.28	1.45	1.33
36	b	635	LHG	O8-C23	4.28	1.45	1.33
24	b	609	CLA	CHC-C1C	4.28	1.47	1.38
27	a	402	SQD	O47-C7	4.28	1.46	1.34
27	B	621	SQD	O47-C7	4.28	1.46	1.34
24	b	609	CLA	CHD-C1D	4.27	1.46	1.38
24	C	510	CLA	O2A-CGA	4.27	1.45	1.33
24	C	510	CLA	CHD-C1D	4.27	1.46	1.38
24	d	404	CLA	CHC-C1C	4.27	1.47	1.38
24	d	406	CLA	O2A-CGA	4.26	1.45	1.33
35	b	628	HTG	C1'-S1	-4.26	1.76	1.81
24	C	506	CLA	CHD-C4C	4.26	1.49	1.39
24	c	902	CLA	CHD-C1D	4.26	1.46	1.38
24	c	912	CLA	CHD-C1D	4.25	1.46	1.38
37	c	917	DGD	O1G-C1A	4.25	1.45	1.33
24	b	619	CLA	O2A-CGA	4.25	1.45	1.33
24	C	507	CLA	CHD-C1D	4.25	1.46	1.38
24	c	913	CLA	O2A-CGA	4.25	1.45	1.33
24	b	617	CLA	C1D-ND	4.25	1.43	1.37
37	C	518	DGD	O1G-C1A	4.24	1.45	1.33
24	B	612	CLA	CHC-C1C	4.24	1.47	1.38
24	c	902	CLA	CHC-C1C	4.24	1.47	1.38
24	B	607	CLA	O2A-CGA	4.24	1.45	1.33
24	B	615	CLA	CHD-C1D	4.24	1.46	1.38
24	B	608	CLA	CHD-C1D	4.24	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	619	BCR	C23-C22	-4.23	1.36	1.45
24	c	903	CLA	O2A-CGA	4.23	1.45	1.33
24	C	513	CLA	CHD-C1D	4.23	1.46	1.38
24	C	505	CLA	CHD-C1D	4.22	1.46	1.38
24	b	606	CLA	C3D-C2D	4.22	1.50	1.39
24	B	614	CLA	CHD-C4C	4.22	1.48	1.39
33	c	920	LMG	O7-C10	4.21	1.46	1.34
36	B	635	LHG	O8-C23	4.21	1.45	1.33
24	b	620	CLA	C3D-C2D	4.21	1.50	1.39
24	C	511	CLA	O2A-CGA	4.21	1.45	1.33
24	B	617	CLA	CHD-C1D	4.20	1.46	1.38
33	d	415	LMG	O7-C10	4.20	1.46	1.34
24	A	405	CLA	CHD-C4C	4.20	1.48	1.39
24	C	504	CLA	CHD-C1D	4.20	1.46	1.38
36	d	411	LHG	O7-C7	4.19	1.46	1.34
25	D	401	PHO	O2A-CGA	4.19	1.45	1.33
24	B	617	CLA	O2A-CGA	4.19	1.45	1.33
24	B	614	CLA	CHD-C1D	4.19	1.46	1.38
24	B	613	CLA	CHB-C1B	4.19	1.48	1.39
24	C	501	CLA	O2A-CGA	4.19	1.45	1.33
38	F	102	HEM	FE-NC	4.19	2.09	1.95
24	C	503	CLA	O2A-CGA	4.19	1.45	1.33
24	b	616	CLA	CHC-C1C	4.19	1.47	1.38
33	c	920	LMG	O8-C28	4.18	1.45	1.33
24	B	610	CLA	C3D-C2D	4.18	1.50	1.39
27	a	410	SQD	O48-C23	4.18	1.45	1.33
24	b	613	CLA	CHB-C1B	4.18	1.48	1.39
24	C	504	CLA	C3D-C2D	4.18	1.50	1.39
24	c	908	CLA	CHD-C1D	4.18	1.46	1.38
24	C	507	CLA	O2A-CGA	4.18	1.45	1.33
36	D	410	LHG	O8-C23	4.18	1.45	1.33
24	b	614	CLA	O2A-CGA	4.18	1.45	1.33
33	C	519	LMG	O8-C28	4.18	1.45	1.33
36	a	418	LHG	O7-C7	4.17	1.46	1.34
24	B	605	CLA	CHC-C1C	4.17	1.47	1.38
24	B	606	CLA	O2A-CGA	4.17	1.45	1.33
24	B	608	CLA	O2A-CGA	4.17	1.45	1.33
24	B	614	CLA	O2A-CGA	4.17	1.45	1.33
24	C	511	CLA	CHD-C4C	4.17	1.48	1.39
24	b	607	CLA	O2A-CGA	4.16	1.45	1.33
24	B	615	CLA	CHC-C1C	4.16	1.47	1.38
33	z	101	LMG	O7-C10	4.16	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	d	411	LHG	O8-C23	4.16	1.45	1.33
25	d	403	PHO	O2A-CGA	4.15	1.45	1.33
27	L	102	SQD	O48-C23	4.15	1.45	1.33
24	d	406	CLA	CHD-C1D	4.15	1.46	1.38
38	f	101	HEM	FE-NC	4.15	2.09	1.95
33	Z	101	LMG	O7-C10	4.15	1.46	1.34
27	B	621	SQD	O48-C23	4.14	1.45	1.33
24	A	405	CLA	CHD-C1D	4.14	1.46	1.38
24	d	405	CLA	CHD-C1D	4.14	1.46	1.38
24	D	404	CLA	CHC-C1C	4.14	1.46	1.38
24	B	603	CLA	OBD-CAD	4.14	1.29	1.22
24	C	505	CLA	CHB-C1B	4.14	1.48	1.39
24	C	513	CLA	O2A-CGA	4.13	1.45	1.33
24	C	501	CLA	CHD-C4C	4.13	1.48	1.39
24	c	906	CLA	O2A-CGA	4.13	1.45	1.33
24	B	612	CLA	CHD-C1D	4.13	1.46	1.38
24	C	507	CLA	CHC-C4B	4.13	1.48	1.39
24	b	611	CLA	O2A-CGA	4.13	1.45	1.33
37	C	517	DGD	O1G-C1A	4.13	1.45	1.33
24	c	914	CLA	O2A-CGA	4.12	1.45	1.33
33	d	415	LMG	O8-C28	4.12	1.45	1.33
24	b	606	CLA	CHD-C4C	4.12	1.48	1.39
24	A	407	CLA	C3D-C2D	4.12	1.50	1.39
25	A	408	PHO	O2A-CGA	4.12	1.45	1.33
24	B	611	CLA	CHD-C1D	4.12	1.46	1.38
24	B	613	CLA	O2A-CGA	4.12	1.45	1.33
24	c	902	CLA	CHD-C4C	4.12	1.48	1.39
24	B	616	CLA	C3D-C2D	4.12	1.50	1.39
37	C	516	DGD	O1G-C1A	4.12	1.45	1.33
24	a	408	CLA	O2A-CGA	4.12	1.45	1.33
37	h	102	DGD	O1G-C1A	4.11	1.45	1.33
40	v	202	HEC	FE-NC	4.10	2.09	1.95
37	C	516	DGD	O2G-C1B	4.10	1.45	1.34
24	c	911	CLA	CHD-C4C	4.10	1.48	1.39
25	d	403	PHO	OBD-CAD	4.10	1.28	1.22
24	D	405	CLA	O2A-CGA	4.10	1.45	1.33
24	A	406	CLA	CHC-C1C	4.09	1.46	1.38
24	c	913	CLA	CHD-C1D	4.09	1.46	1.38
24	B	614	CLA	C3D-C2D	4.09	1.50	1.39
24	d	404	CLA	C3D-C2D	4.09	1.50	1.39
24	B	606	CLA	CHD-C1D	4.08	1.46	1.38
24	C	511	CLA	CHD-C1D	4.08	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	907	CLA	CHD-C1D	4.08	1.46	1.38
24	d	406	CLA	CHC-C4B	4.08	1.48	1.39
37	H	102	DGD	O1G-C1A	4.08	1.45	1.33
24	C	513	CLA	CHD-C4C	4.08	1.48	1.39
36	E	101	LHG	O7-C7	4.07	1.45	1.34
24	b	613	CLA	O2A-CGA	4.07	1.45	1.33
36	b	635	LHG	O7-C7	4.07	1.45	1.34
24	c	905	CLA	CHD-C1D	4.07	1.46	1.38
24	A	409	CLA	O2A-CGA	4.07	1.45	1.33
24	C	504	CLA	CHD-C4C	4.07	1.48	1.39
24	b	615	CLA	CHD-C4C	4.07	1.48	1.39
24	C	503	CLA	CHD-C4C	4.07	1.48	1.39
24	c	911	CLA	O2A-CGA	4.06	1.45	1.33
24	B	613	CLA	CHD-C1D	4.06	1.46	1.38
24	B	606	CLA	CHC-C4B	4.06	1.48	1.39
24	B	611	CLA	CHD-C4C	4.06	1.48	1.39
27	F	103	SQD	O48-C23	4.06	1.45	1.33
24	B	611	CLA	O2A-CGA	4.06	1.45	1.33
24	B	605	CLA	CHD-C1D	4.05	1.46	1.38
24	B	604	CLA	CHD-C1D	4.05	1.46	1.38
24	C	504	CLA	CHB-C1B	4.05	1.48	1.39
24	c	903	CLA	CHD-C1D	4.05	1.46	1.38
24	A	407	CLA	CHD-C4C	4.05	1.48	1.39
24	a	405	CLA	CHD-C4C	4.05	1.48	1.39
24	b	616	CLA	O2A-CGA	4.05	1.45	1.33
24	b	613	CLA	C3D-C2D	4.05	1.50	1.39
24	C	508	CLA	CHD-C4C	4.05	1.48	1.39
24	B	616	CLA	CHD-C1D	4.05	1.46	1.38
24	c	914	CLA	CHD-C4C	4.04	1.48	1.39
33	c	919	LMG	O8-C28	4.04	1.45	1.33
24	A	409	CLA	CHC-C4B	4.04	1.48	1.39
24	c	910	CLA	CHB-C1B	4.04	1.48	1.39
24	c	909	CLA	CHD-C1D	4.04	1.46	1.38
24	C	511	CLA	C3D-C2D	4.04	1.50	1.39
24	b	613	CLA	CHC-C4B	4.04	1.48	1.39
24	c	913	CLA	CHD-C4C	4.04	1.48	1.39
24	A	406	CLA	C3D-C2D	4.03	1.50	1.39
24	a	406	CLA	CHD-C1D	4.03	1.46	1.38
24	b	611	CLA	CHD-C1D	4.03	1.46	1.38
24	c	903	CLA	C3D-C2D	4.03	1.50	1.39
24	C	502	CLA	CHD-C4C	4.03	1.48	1.39
24	D	404	CLA	O2A-CGA	4.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	405	CLA	O2A-CGA	4.02	1.45	1.33
24	C	512	CLA	CHD-C4C	4.02	1.48	1.39
24	B	602	CLA	CHD-C1D	4.02	1.46	1.38
36	d	409	LHG	O8-C23	4.01	1.45	1.33
24	b	616	CLA	CHB-C1B	4.01	1.48	1.39
33	B	622	LMG	O7-C10	4.01	1.45	1.34
24	c	910	CLA	OBD-CAD	4.01	1.29	1.22
24	b	618	CLA	O2A-CGA	4.01	1.45	1.33
24	C	504	CLA	O2A-CGA	4.00	1.45	1.33
27	a	410	SQD	O47-C7	4.00	1.45	1.34
24	b	617	CLA	CHB-C1B	4.00	1.48	1.39
24	c	903	CLA	CHB-C1B	4.00	1.48	1.39
27	A	411	SQD	O47-C7	4.00	1.45	1.34
24	A	409	CLA	CHD-C4C	4.00	1.48	1.39
24	b	615	CLA	CHB-C1B	4.00	1.48	1.39
24	C	510	CLA	CHD-C4C	4.00	1.48	1.39
24	b	620	CLA	CHB-C1B	4.00	1.48	1.39
24	c	910	CLA	CHD-C4C	4.00	1.48	1.39
24	b	617	CLA	O2A-CGA	3.99	1.45	1.33
24	C	508	CLA	C3D-C2D	3.99	1.50	1.39
24	B	609	CLA	CHD-C4C	3.99	1.48	1.39
24	C	502	CLA	O2A-CGA	3.99	1.45	1.33
24	A	407	CLA	O2A-CGA	3.99	1.45	1.33
37	c	916	DGD	O2G-C1B	3.99	1.45	1.34
24	d	404	CLA	CHD-C4C	3.98	1.48	1.39
24	c	913	CLA	OBD-CAD	3.98	1.29	1.22
24	B	615	CLA	OBD-CAD	3.98	1.29	1.22
24	B	615	CLA	CHD-C4C	3.98	1.48	1.39
24	B	608	CLA	CHD-C4C	3.97	1.48	1.39
24	b	617	CLA	C3D-C2D	3.97	1.50	1.39
24	C	510	CLA	CHB-C1B	3.97	1.48	1.39
33	Y	101	LMG	O7-C10	3.97	1.45	1.34
24	c	905	CLA	O2A-CGA	3.96	1.44	1.33
24	b	614	CLA	CHD-C4C	3.96	1.48	1.39
24	c	906	CLA	CHB-C1B	3.96	1.48	1.39
24	C	503	CLA	CHC-C4B	3.96	1.48	1.39
37	H	102	DGD	O2G-C1B	3.95	1.45	1.34
24	D	405	CLA	CHD-C4C	3.95	1.48	1.39
24	C	506	CLA	C3D-C2D	3.95	1.49	1.39
24	c	914	CLA	CHD-C1D	3.95	1.46	1.38
24	A	409	CLA	C3D-C2D	3.95	1.49	1.39
37	c	917	DGD	O2G-C1B	3.95	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	CHD-C1D	3.95	1.46	1.38
24	c	909	CLA	C3D-C2D	3.95	1.49	1.39
37	h	102	DGD	O2G-C1B	3.95	1.45	1.34
33	J	101	LMG	O8-C28	3.95	1.44	1.33
24	c	902	CLA	O2A-CGA	3.95	1.44	1.33
24	C	501	CLA	CHC-C4B	3.95	1.48	1.39
36	D	409	LHG	O8-C23	3.94	1.44	1.33
24	b	620	CLA	CHD-C1D	3.94	1.46	1.38
24	b	618	CLA	CHB-C1B	3.94	1.48	1.39
24	A	406	CLA	OBD-CAD	3.94	1.29	1.22
24	c	907	CLA	C1B-NB	-3.94	1.32	1.37
24	a	406	CLA	OBD-CAD	3.94	1.29	1.22
24	C	509	CLA	C3D-C2D	3.94	1.49	1.39
24	b	613	CLA	CHD-C4C	3.93	1.48	1.39
24	A	405	CLA	O2A-CGA	3.93	1.44	1.33
24	C	505	CLA	O2A-CGA	3.93	1.44	1.33
24	B	615	CLA	CHB-C1B	3.93	1.48	1.39
33	J	101	LMG	O7-C10	3.93	1.45	1.34
24	B	609	CLA	OBD-CAD	3.93	1.29	1.22
40	v	202	HEC	CBC-CAC	-3.93	1.34	1.51
24	C	509	CLA	CHD-C4C	3.93	1.48	1.39
24	c	904	CLA	O2A-CGA	3.92	1.44	1.33
24	B	616	CLA	CHD-C4C	3.92	1.48	1.39
24	b	618	CLA	CHC-C1C	3.92	1.46	1.38
24	b	619	CLA	CHD-C4C	3.92	1.48	1.39
37	C	518	DGD	O2G-C1B	3.92	1.45	1.34
24	c	907	CLA	O2A-CGA	3.92	1.44	1.33
24	c	911	CLA	OBD-CAD	3.91	1.29	1.22
24	b	615	CLA	OBD-CAD	3.91	1.29	1.22
24	c	911	CLA	CHB-C1B	3.91	1.48	1.39
33	a	411	LMG	O7-C10	3.91	1.45	1.34
24	b	615	CLA	O2A-CGA	3.91	1.44	1.33
40	V	202	HEC	FE-NC	3.91	2.08	1.95
24	A	405	CLA	OBD-CAD	3.91	1.29	1.22
24	C	510	CLA	OBD-CAD	3.91	1.29	1.22
37	c	918	DGD	O2G-C1B	3.91	1.45	1.34
24	C	501	CLA	C3D-C2D	3.91	1.49	1.39
33	b	625	LMG	O8-C28	3.91	1.44	1.33
24	B	612	CLA	O2A-CGA	3.91	1.44	1.33
24	B	604	CLA	CHD-C4C	3.90	1.48	1.39
24	C	503	CLA	C3D-C2D	3.90	1.49	1.39
24	b	608	CLA	O2A-CGA	3.90	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	C4B-NB	-3.90	1.33	1.37
24	C	512	CLA	C3D-C2D	3.90	1.49	1.39
24	b	610	CLA	CHD-C1D	3.90	1.46	1.38
24	c	906	CLA	CHD-C1D	3.90	1.46	1.38
24	c	904	CLA	CHD-C4C	3.89	1.48	1.39
24	B	603	CLA	O2A-CGA	3.89	1.44	1.33
24	c	904	CLA	CHC-C4B	3.89	1.48	1.39
27	A	414	SQD	O47-C7	3.89	1.45	1.34
24	c	905	CLA	CHD-C4C	3.89	1.48	1.39
24	b	619	CLA	C3D-C2D	3.89	1.49	1.39
40	V	202	HEC	CBB-CAB	-3.89	1.34	1.51
24	B	607	CLA	CHD-C4C	3.88	1.48	1.39
24	b	621	CLA	CHB-C1B	3.88	1.48	1.39
24	C	511	CLA	CHB-C1B	3.88	1.48	1.39
24	c	911	CLA	C3D-C2D	3.88	1.49	1.39
24	C	505	CLA	CHC-C4B	3.87	1.48	1.39
24	b	614	CLA	CHB-C1B	3.87	1.48	1.39
24	d	406	CLA	C3D-C2D	3.87	1.49	1.39
24	c	908	CLA	CHD-C4C	3.86	1.48	1.39
24	c	909	CLA	CHB-C1B	3.86	1.48	1.39
24	B	608	CLA	CHB-C1B	3.86	1.48	1.39
40	v	202	HEC	CBB-CAB	-3.85	1.34	1.51
24	C	512	CLA	CHC-C4B	3.85	1.48	1.39
24	c	902	CLA	CHB-C1B	3.85	1.48	1.39
24	C	510	CLA	C3D-C2D	3.85	1.49	1.39
33	c	919	LMG	O7-C10	3.85	1.45	1.34
24	b	619	CLA	CHB-C1B	3.85	1.48	1.39
24	C	502	CLA	C3D-C2D	3.85	1.49	1.39
24	c	913	CLA	C3D-C2D	3.84	1.49	1.39
24	b	621	CLA	C3D-C2D	3.84	1.49	1.39
24	B	605	CLA	CHD-C4C	3.84	1.48	1.39
24	b	607	CLA	CHD-C4C	3.84	1.48	1.39
24	b	618	CLA	C3D-C2D	3.84	1.49	1.39
24	c	914	CLA	CHC-C4B	3.84	1.48	1.39
24	B	608	CLA	C1B-NB	-3.84	1.33	1.37
24	a	405	CLA	CHD-C1D	3.84	1.45	1.38
24	D	405	CLA	C3D-C2D	3.84	1.49	1.39
24	b	617	CLA	CHC-C4B	3.84	1.48	1.39
24	b	611	CLA	OBD-CAD	3.83	1.29	1.22
24	B	608	CLA	CHC-C4B	3.83	1.48	1.39
24	B	616	CLA	CHC-C4B	3.83	1.48	1.39
24	a	405	CLA	OBD-CAD	3.83	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	CHB-C1B	3.83	1.48	1.39
24	c	910	CLA	C3D-C2D	3.83	1.49	1.39
24	c	905	CLA	C3D-C2D	3.83	1.49	1.39
24	b	619	CLA	CHC-C4B	3.83	1.48	1.39
24	a	408	CLA	C3D-C2D	3.83	1.49	1.39
24	b	614	CLA	C3D-C2D	3.83	1.49	1.39
24	c	909	CLA	OBD-CAD	3.83	1.29	1.22
24	b	617	CLA	OBD-CAD	3.82	1.29	1.22
24	b	619	CLA	CHD-C1D	3.82	1.45	1.38
24	d	405	CLA	C3D-C2D	3.82	1.49	1.39
24	B	614	CLA	OBD-CAD	3.82	1.29	1.22
37	C	517	DGD	O2G-C1B	3.82	1.45	1.34
24	C	504	CLA	CHC-C4B	3.82	1.48	1.39
24	b	616	CLA	CHD-C1D	3.81	1.45	1.38
24	C	513	CLA	C3D-C2D	3.81	1.49	1.39
24	b	610	CLA	CHC-C4B	3.81	1.48	1.39
24	b	610	CLA	O2A-CGA	3.81	1.44	1.33
24	b	618	CLA	CHD-C1D	3.81	1.45	1.38
24	c	902	CLA	C3D-C2D	3.81	1.49	1.39
33	b	625	LMG	O7-C10	3.81	1.45	1.34
24	b	621	CLA	CHC-C4B	3.81	1.47	1.39
27	A	411	SQD	O48-C23	3.81	1.44	1.33
24	B	615	CLA	C3D-C2D	3.81	1.49	1.39
24	b	608	CLA	CHD-C4C	3.81	1.47	1.39
24	B	605	CLA	O2A-CGA	3.80	1.44	1.33
37	c	916	DGD	O1G-C1A	3.80	1.44	1.33
24	B	609	CLA	C3D-C2D	3.80	1.49	1.39
24	B	603	CLA	CHC-C4B	3.80	1.47	1.39
40	V	202	HEC	CBC-CAC	-3.80	1.34	1.51
24	A	409	CLA	OBD-CAD	3.80	1.29	1.22
24	C	507	CLA	CHD-C4C	3.80	1.47	1.39
24	c	906	CLA	CHC-C4B	3.80	1.47	1.39
24	d	405	CLA	CHC-C4B	3.80	1.47	1.39
24	a	406	CLA	CHD-C4C	3.80	1.47	1.39
24	d	405	CLA	CHD-C4C	3.79	1.47	1.39
24	B	604	CLA	C3D-C2D	3.79	1.49	1.39
24	c	906	CLA	OBD-CAD	3.79	1.29	1.22
24	c	907	CLA	CHB-C1B	3.78	1.47	1.39
24	D	404	CLA	CHD-C1D	3.78	1.45	1.38
24	a	405	CLA	CHC-C4B	3.78	1.47	1.39
24	c	908	CLA	C3D-C2D	3.78	1.49	1.39
24	C	509	CLA	CHC-C4B	3.78	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	CHB-C1B	3.78	1.47	1.39
24	b	615	CLA	C3D-C2D	3.78	1.49	1.39
24	b	609	CLA	C1B-NB	-3.78	1.33	1.37
36	d	410	LHG	O7-C7	3.78	1.45	1.34
24	B	602	CLA	C3D-C2D	3.77	1.49	1.39
24	b	607	CLA	CHB-C1B	3.77	1.47	1.39
24	C	509	CLA	CHB-C1B	3.77	1.47	1.39
24	C	501	CLA	OBD-CAD	3.77	1.29	1.22
24	C	510	CLA	CHC-C4B	3.77	1.47	1.39
24	B	611	CLA	C3D-C2D	3.77	1.49	1.39
24	C	502	CLA	CHB-C1B	3.77	1.47	1.39
24	d	405	CLA	C1D-ND	3.76	1.42	1.37
24	a	406	CLA	CHC-C4B	3.76	1.47	1.39
24	B	606	CLA	C3D-C2D	3.76	1.49	1.39
24	b	620	CLA	CHD-C4C	3.76	1.47	1.39
24	c	903	CLA	CHD-C4C	3.76	1.47	1.39
24	B	605	CLA	CHB-C1B	3.76	1.47	1.39
24	B	606	CLA	CHD-C4C	3.76	1.47	1.39
24	B	611	CLA	CHB-C1B	3.75	1.47	1.39
24	A	407	CLA	OBD-CAD	3.75	1.28	1.22
24	D	404	CLA	C1B-NB	-3.74	1.33	1.37
24	c	914	CLA	C3D-C2D	3.74	1.49	1.39
24	c	908	CLA	CHC-C4B	3.74	1.47	1.39
24	A	406	CLA	CHD-C4C	3.74	1.47	1.39
24	B	602	CLA	CHB-C1B	3.74	1.47	1.39
24	B	611	CLA	CHC-C4B	3.74	1.47	1.39
24	d	406	CLA	CHB-C1B	3.74	1.47	1.39
24	B	617	CLA	CHC-C4B	3.74	1.47	1.39
24	b	615	CLA	CHC-C4B	3.74	1.47	1.39
24	b	612	CLA	C3D-C2D	3.74	1.49	1.39
24	C	513	CLA	CHC-C4B	3.73	1.47	1.39
24	b	620	CLA	OBD-CAD	3.73	1.28	1.22
24	B	606	CLA	CHB-C1B	3.73	1.47	1.39
24	B	612	CLA	CHB-C1B	3.73	1.47	1.39
24	d	406	CLA	CHD-C4C	3.73	1.47	1.39
24	a	408	CLA	CHD-C4C	3.73	1.47	1.39
24	b	612	CLA	CHD-C4C	3.72	1.47	1.39
24	C	506	CLA	CHB-C1B	3.72	1.47	1.39
24	b	609	CLA	CHD-C4C	3.72	1.47	1.39
24	b	606	CLA	CHC-C4B	3.72	1.47	1.39
24	b	614	CLA	OBD-CAD	3.72	1.28	1.22
24	a	406	CLA	C3D-C2D	3.72	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	406	CLA	CHD-C1D	3.72	1.45	1.38
24	B	602	CLA	CHD-C4C	3.71	1.47	1.39
24	c	905	CLA	CHC-C4B	3.71	1.47	1.39
24	B	613	CLA	CHC-C4B	3.71	1.47	1.39
24	A	405	CLA	C3D-C2D	3.71	1.49	1.39
24	C	509	CLA	OBD-CAD	3.70	1.28	1.22
24	c	907	CLA	CHD-C4C	3.70	1.47	1.39
24	c	909	CLA	CHD-C4C	3.70	1.47	1.39
24	D	404	CLA	CHD-C4C	3.70	1.47	1.39
36	L	101	LHG	O7-C7	3.70	1.44	1.34
24	b	610	CLA	CHB-C1B	3.70	1.47	1.39
24	b	610	CLA	CHD-C4C	3.70	1.47	1.39
24	b	611	CLA	CHD-C4C	3.70	1.47	1.39
24	b	607	CLA	CHC-C4B	3.70	1.47	1.39
24	B	607	CLA	OBD-CAD	3.70	1.28	1.22
24	c	912	CLA	OBD-CAD	3.69	1.28	1.22
25	a	407	PHO	O2A-CGA	3.69	1.44	1.33
24	b	612	CLA	OBD-CAD	3.69	1.28	1.22
24	b	606	CLA	OBD-CAD	3.69	1.28	1.22
35	d	414	HTG	C1'-S1	-3.69	1.76	1.81
24	c	904	CLA	OBD-CAD	3.69	1.28	1.22
24	b	611	CLA	CHB-C1B	3.69	1.47	1.39
24	b	607	CLA	OBD-CAD	3.69	1.28	1.22
24	C	502	CLA	CHC-C4B	3.68	1.47	1.39
24	a	408	CLA	CHC-C4B	3.68	1.47	1.39
24	b	618	CLA	CHD-C4C	3.68	1.47	1.39
24	B	604	CLA	CHB-C1B	3.68	1.47	1.39
24	B	613	CLA	C3D-C2D	3.68	1.49	1.39
24	B	607	CLA	CHB-C1B	3.68	1.47	1.39
24	b	608	CLA	C3D-C2D	3.68	1.49	1.39
24	c	912	CLA	CHD-C4C	3.68	1.47	1.39
35	b	603	HTG	C1'-S1	-3.68	1.76	1.81
24	b	620	CLA	CHC-C4B	3.67	1.47	1.39
24	d	406	CLA	OBD-CAD	3.67	1.28	1.22
24	b	616	CLA	C3D-C2D	3.67	1.49	1.39
24	a	405	CLA	C3D-C2D	3.67	1.49	1.39
24	C	508	CLA	OBD-CAD	3.66	1.28	1.22
24	c	913	CLA	CHC-C4B	3.66	1.47	1.39
24	B	603	CLA	CHD-C4C	3.66	1.47	1.39
24	B	610	CLA	CHD-C4C	3.66	1.47	1.39
24	c	905	CLA	C1B-NB	-3.66	1.33	1.37
24	c	910	CLA	CHC-C4B	3.66	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	b	601	HTG	C1'-S1	-3.66	1.76	1.81
24	B	616	CLA	OBD-CAD	3.65	1.28	1.22
24	C	508	CLA	CHB-C1B	3.65	1.47	1.39
35	B	633	HTG	C1'-S1	-3.65	1.76	1.81
24	c	912	CLA	C3D-C2D	3.65	1.49	1.39
24	C	512	CLA	OBD-CAD	3.65	1.28	1.22
24	a	408	CLA	C4B-NB	-3.65	1.33	1.37
24	C	507	CLA	C3D-C2D	3.65	1.49	1.39
24	b	609	CLA	C3D-C2D	3.65	1.49	1.39
24	B	604	CLA	C1B-NB	-3.65	1.33	1.37
24	a	408	CLA	CHD-C1D	3.65	1.45	1.38
24	B	609	CLA	CHB-C1B	3.65	1.47	1.39
36	d	410	LHG	O8-C23	3.64	1.44	1.33
24	C	512	CLA	CHB-C1B	3.64	1.47	1.39
24	B	602	CLA	OBD-CAD	3.64	1.28	1.22
24	C	502	CLA	OBD-CAD	3.64	1.28	1.22
24	B	616	CLA	CHB-C1B	3.64	1.47	1.39
24	B	610	CLA	CHC-C4B	3.64	1.47	1.39
24	a	406	CLA	CHB-C1B	3.64	1.47	1.39
24	B	617	CLA	CHB-C1B	3.63	1.47	1.39
24	b	611	CLA	C3D-C2D	3.63	1.49	1.39
36	D	409	LHG	O7-C7	3.63	1.44	1.34
24	a	408	CLA	CHB-C1B	3.63	1.47	1.39
24	b	612	CLA	CHB-C1B	3.63	1.47	1.39
24	b	611	CLA	CHC-C4B	3.63	1.47	1.39
24	C	513	CLA	CHB-C1B	3.63	1.47	1.39
24	D	405	CLA	CHB-C1B	3.62	1.47	1.39
24	A	405	CLA	CHB-C1B	3.62	1.47	1.39
24	A	407	CLA	CHC-C4B	3.62	1.47	1.39
24	B	612	CLA	C3D-C2D	3.62	1.49	1.39
24	b	613	CLA	OBD-CAD	3.61	1.28	1.22
24	B	607	CLA	CHC-C4B	3.61	1.47	1.39
24	d	404	CLA	OBD-CAD	3.61	1.28	1.22
24	C	507	CLA	CHB-C1B	3.61	1.47	1.39
24	a	405	CLA	O2A-CGA	3.60	1.43	1.33
24	b	608	CLA	C1B-NB	-3.60	1.33	1.37
24	b	621	CLA	OBD-CAD	3.60	1.28	1.22
24	b	621	CLA	CHD-C4C	3.60	1.47	1.39
24	B	614	CLA	CHC-C4B	3.60	1.47	1.39
24	c	904	CLA	C3D-C2D	3.60	1.48	1.39
35	V	203	HTG	C1'-S1	-3.60	1.76	1.81
24	c	914	CLA	OBD-CAD	3.59	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	CHC-C4B	3.59	1.47	1.39
24	C	513	CLA	OBD-CAD	3.59	1.28	1.22
24	b	616	CLA	C1B-NB	-3.58	1.33	1.37
35	B	625	HTG	C1'-S1	-3.58	1.76	1.81
24	c	908	CLA	CHB-C1B	3.58	1.47	1.39
24	B	613	CLA	CHD-C4C	3.58	1.47	1.39
24	b	612	CLA	CHC-C4B	3.57	1.47	1.39
24	B	603	CLA	C1B-NB	-3.57	1.33	1.37
24	c	908	CLA	OBD-CAD	3.57	1.28	1.22
24	b	609	CLA	CHC-C4B	3.57	1.47	1.39
24	B	604	CLA	CHC-C4B	3.56	1.47	1.39
24	C	503	CLA	OBD-CAD	3.56	1.28	1.22
24	d	405	CLA	C1B-NB	-3.56	1.33	1.37
24	C	503	CLA	CHB-C1B	3.56	1.47	1.39
24	c	905	CLA	CHB-C1B	3.56	1.47	1.39
24	B	611	CLA	OBD-CAD	3.56	1.28	1.22
24	B	602	CLA	CHC-C4B	3.55	1.47	1.39
24	B	614	CLA	CHB-C1B	3.55	1.47	1.39
24	B	613	CLA	C1B-NB	-3.55	1.33	1.37
24	B	603	CLA	C3D-C2D	3.54	1.48	1.39
24	c	914	CLA	CHB-C1B	3.54	1.47	1.39
24	A	407	CLA	CHB-C1B	3.54	1.47	1.39
24	B	607	CLA	C3D-C2D	3.54	1.48	1.39
24	c	912	CLA	CHB-C1B	3.54	1.47	1.39
24	B	608	CLA	C3D-C2D	3.54	1.48	1.39
24	c	906	CLA	C3D-C2D	3.54	1.48	1.39
24	A	406	CLA	CHC-C4B	3.53	1.47	1.39
24	D	404	CLA	CHC-C4B	3.53	1.47	1.39
24	c	907	CLA	C3D-C2D	3.53	1.48	1.39
24	b	611	CLA	C1B-NB	-3.53	1.33	1.37
24	B	617	CLA	CHD-C4C	3.53	1.47	1.39
24	c	904	CLA	CHB-C1B	3.53	1.47	1.39
24	C	511	CLA	OBD-CAD	3.53	1.28	1.22
24	a	405	CLA	CHB-C1B	3.52	1.47	1.39
24	c	913	CLA	CHB-C1B	3.52	1.47	1.39
24	C	504	CLA	OBD-CAD	3.52	1.28	1.22
24	B	617	CLA	C3D-C2D	3.52	1.48	1.39
35	c	922	HTG	C1'-S1	-3.52	1.76	1.81
24	b	608	CLA	OBD-CAD	3.51	1.28	1.22
24	c	902	CLA	C1B-NB	-3.51	1.33	1.37
24	c	907	CLA	OBD-CAD	3.51	1.28	1.22
24	c	907	CLA	CHC-C4B	3.51	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	CHD-C4C	3.50	1.47	1.39
24	b	612	CLA	C1B-NB	-3.50	1.33	1.37
24	b	610	CLA	C3D-C2D	3.50	1.48	1.39
24	D	404	CLA	CHB-C1B	3.50	1.47	1.39
24	C	508	CLA	CHC-C4B	3.50	1.47	1.39
24	b	615	CLA	C1B-NB	-3.49	1.33	1.37
24	B	610	CLA	OBD-CAD	3.49	1.28	1.22
24	b	607	CLA	C3D-C2D	3.49	1.48	1.39
24	B	617	CLA	OBD-CAD	3.49	1.28	1.22
24	B	612	CLA	CHD-C4C	3.48	1.47	1.39
38	F	102	HEM	C4D-ND	-3.48	1.34	1.40
24	b	608	CLA	CHC-C4B	3.48	1.47	1.39
36	B	635	LHG	O7-C7	3.48	1.44	1.34
24	b	606	CLA	CHB-C1B	3.47	1.47	1.39
24	C	506	CLA	CHC-C4B	3.47	1.47	1.39
24	D	404	CLA	C3D-C2D	3.47	1.48	1.39
24	D	405	CLA	C4B-NB	-3.47	1.33	1.37
24	B	605	CLA	C3D-C2D	3.47	1.48	1.39
24	C	501	CLA	CHB-C1B	3.47	1.47	1.39
36	d	409	LHG	O7-C7	3.47	1.44	1.34
24	b	616	CLA	CHD-C4C	3.47	1.47	1.39
24	C	505	CLA	C3D-C2D	3.47	1.48	1.39
24	C	511	CLA	CHC-C4B	3.46	1.47	1.39
24	B	612	CLA	CHC-C4B	3.46	1.47	1.39
35	C	522	HTG	C1'-S1	-3.45	1.77	1.81
24	c	902	CLA	OBD-CAD	3.45	1.28	1.22
24	B	608	CLA	OBD-CAD	3.45	1.28	1.22
24	A	409	CLA	CHB-C1B	3.45	1.47	1.39
24	D	405	CLA	CHC-C4B	3.44	1.47	1.39
35	C	521	HTG	C1'-S1	-3.44	1.77	1.81
35	D	413	HTG	C1'-S1	-3.44	1.77	1.81
40	v	202	HEC	C1D-ND	-3.44	1.34	1.40
24	B	609	CLA	CHC-C4B	3.44	1.47	1.39
24	b	608	CLA	CHB-C1B	3.43	1.47	1.39
24	c	911	CLA	CHC-C4B	3.43	1.47	1.39
24	d	404	CLA	CHB-C1B	3.43	1.47	1.39
24	A	405	CLA	C1B-NB	-3.42	1.33	1.37
24	c	909	CLA	C1B-NB	-3.42	1.33	1.37
24	a	406	CLA	C1B-NB	-3.42	1.33	1.37
24	A	405	CLA	CHC-C4B	3.38	1.47	1.39
24	c	902	CLA	C4B-NB	-3.38	1.33	1.37
24	C	507	CLA	OBD-CAD	3.38	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	906	CLA	CHD-C4C	3.38	1.46	1.39
38	F	102	HEM	C1B-NB	-3.37	1.34	1.40
24	c	912	CLA	CHC-C4B	3.36	1.47	1.39
24	d	405	CLA	CHB-C1B	3.36	1.47	1.39
35	B	632	HTG	C1'-S1	-3.36	1.77	1.81
24	c	910	CLA	C1B-NB	-3.36	1.33	1.37
24	B	606	CLA	OBD-CAD	3.36	1.28	1.22
24	b	618	CLA	OBD-CAD	3.36	1.28	1.22
24	d	406	CLA	C1B-NB	-3.35	1.33	1.37
24	B	613	CLA	OBD-CAD	3.34	1.28	1.22
24	B	606	CLA	C3B-C4B	3.34	1.50	1.42
24	c	903	CLA	OBD-CAD	3.34	1.28	1.22
40	V	202	HEC	C1D-ND	-3.34	1.34	1.40
24	c	905	CLA	C4B-NB	-3.34	1.33	1.37
38	f	101	HEM	C4D-ND	-3.33	1.34	1.40
35	b	604	HTG	C1'-S1	-3.33	1.77	1.81
24	c	903	CLA	CHC-C4B	3.32	1.46	1.39
24	b	617	CLA	CHD-C4C	3.32	1.46	1.39
24	C	505	CLA	OBD-CAD	3.32	1.28	1.22
24	A	405	CLA	C4C-C3C	3.31	1.50	1.45
24	C	506	CLA	OBD-CAD	3.31	1.28	1.22
24	b	612	CLA	C3B-C4B	3.30	1.50	1.42
24	A	407	CLA	C3B-C4B	3.30	1.50	1.42
24	b	614	CLA	C1B-NB	-3.30	1.33	1.37
24	d	404	CLA	CHC-C4B	3.30	1.46	1.39
24	d	404	CLA	C4B-NB	-3.30	1.33	1.37
35	c	921	HTG	C1'-S1	-3.29	1.77	1.81
24	B	615	CLA	CHC-C4B	3.29	1.46	1.39
24	b	613	CLA	C4B-NB	-3.29	1.33	1.37
24	c	909	CLA	CHC-C4B	3.28	1.46	1.39
38	f	101	HEM	C1B-NB	-3.27	1.34	1.40
24	b	618	CLA	C1B-NB	-3.27	1.33	1.37
24	b	609	CLA	OBD-CAD	3.26	1.28	1.22
24	c	913	CLA	C4B-NB	-3.26	1.33	1.37
40	V	202	HEC	C4B-NB	-3.25	1.34	1.40
24	c	902	CLA	CHC-C4B	3.25	1.46	1.39
24	C	503	CLA	C1B-NB	-3.25	1.33	1.37
24	A	406	CLA	C4B-NB	-3.25	1.33	1.37
24	b	606	CLA	C3B-C4B	3.24	1.50	1.42
24	d	405	CLA	OBD-CAD	3.24	1.28	1.22
24	C	501	CLA	C1B-NB	-3.24	1.33	1.37
24	b	607	CLA	C1B-NB	-3.24	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	C1B-NB	-3.24	1.33	1.37
24	B	616	CLA	C1B-NB	-3.23	1.33	1.37
24	B	609	CLA	C1B-NB	-3.23	1.33	1.37
24	A	406	CLA	CHB-C1B	3.23	1.46	1.39
24	A	406	CLA	C1B-NB	-3.23	1.33	1.37
24	a	408	CLA	C1B-NB	-3.23	1.33	1.37
24	B	611	CLA	C1B-NB	-3.22	1.33	1.37
24	C	506	CLA	C4B-NB	-3.22	1.33	1.37
24	B	604	CLA	OBD-CAD	3.22	1.28	1.22
24	C	510	CLA	C1B-NB	-3.22	1.33	1.37
24	a	408	CLA	OBD-CAD	3.21	1.28	1.22
24	B	614	CLA	C4B-NB	-3.20	1.33	1.37
24	C	508	CLA	C1B-NB	-3.19	1.33	1.37
24	B	612	CLA	C1B-NB	-3.18	1.33	1.37
24	C	509	CLA	C1B-NB	-3.18	1.33	1.37
24	b	616	CLA	OBD-CAD	3.18	1.28	1.22
24	b	616	CLA	CHC-C4B	3.18	1.46	1.39
24	a	405	CLA	C1B-NB	-3.18	1.33	1.37
24	A	409	CLA	C3B-C4B	3.18	1.50	1.42
24	B	617	CLA	C4B-NB	-3.17	1.33	1.37
24	C	507	CLA	C1B-NB	-3.17	1.33	1.37
24	b	608	CLA	C4B-NB	-3.16	1.33	1.37
24	b	619	CLA	OBD-CAD	3.16	1.27	1.22
24	c	905	CLA	OBD-CAD	3.16	1.27	1.22
24	B	610	CLA	C1B-NB	-3.16	1.33	1.37
24	D	404	CLA	OBD-CAD	3.16	1.27	1.22
24	D	405	CLA	OBD-CAD	3.15	1.27	1.22
24	C	504	CLA	C1B-NB	-3.15	1.33	1.37
24	C	505	CLA	C1B-NB	-3.15	1.33	1.37
24	B	603	CLA	CHB-C1B	3.14	1.46	1.39
24	C	503	CLA	C3B-C4B	3.14	1.50	1.42
24	C	512	CLA	C3B-C4B	3.14	1.50	1.42
24	B	607	CLA	C4B-NB	-3.13	1.33	1.37
24	B	612	CLA	C4B-NB	-3.13	1.33	1.37
24	B	606	CLA	C1C-C2C	3.13	1.50	1.44
24	b	610	CLA	OBD-CAD	3.13	1.27	1.22
24	b	612	CLA	C1B-C2B	3.12	1.50	1.43
24	c	914	CLA	C3B-C4B	3.12	1.50	1.42
24	c	903	CLA	C4B-NB	-3.12	1.34	1.37
24	c	914	CLA	C1B-NB	-3.11	1.34	1.37
24	B	614	CLA	C1B-NB	-3.11	1.34	1.37
24	c	906	CLA	C1B-NB	-3.10	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	CHC-C4B	3.10	1.46	1.39
24	c	910	CLA	C4B-NB	-3.10	1.34	1.37
24	b	618	CLA	CHC-C4B	3.10	1.46	1.39
24	b	619	CLA	C1B-NB	-3.10	1.34	1.37
24	C	513	CLA	C3B-C4B	3.10	1.50	1.42
24	c	913	CLA	C1B-NB	-3.09	1.34	1.37
24	b	610	CLA	C3B-C4B	3.09	1.50	1.42
24	b	618	CLA	C4B-NB	-3.09	1.34	1.37
24	c	914	CLA	C4B-NB	-3.09	1.34	1.37
24	b	610	CLA	C1B-NB	-3.09	1.34	1.37
24	c	906	CLA	C3B-C4B	3.08	1.50	1.42
24	c	908	CLA	C4B-NB	-3.08	1.34	1.37
24	C	505	CLA	C1B-C2B	3.07	1.50	1.43
24	B	612	CLA	OBD-CAD	3.06	1.27	1.22
24	C	502	CLA	C4B-NB	-3.06	1.34	1.37
24	B	615	CLA	C1B-NB	-3.06	1.34	1.37
35	B	624	HTG	C1'-S1	-3.06	1.77	1.81
24	b	614	CLA	C3B-C4B	3.05	1.49	1.42
24	C	504	CLA	C4B-NB	-3.05	1.34	1.37
24	C	501	CLA	C3B-C4B	3.05	1.49	1.42
24	D	405	CLA	C1B-NB	-3.04	1.34	1.37
24	B	609	CLA	C4B-NB	-3.04	1.34	1.37
24	c	911	CLA	C1B-NB	-3.03	1.34	1.37
24	b	617	CLA	C3B-C4B	3.02	1.49	1.42
24	d	404	CLA	C1B-NB	-3.01	1.34	1.37
24	b	621	CLA	C1B-C2B	3.01	1.50	1.43
24	B	605	CLA	OBD-CAD	3.01	1.27	1.22
24	B	605	CLA	C1B-C2B	3.01	1.50	1.43
24	B	602	CLA	C1B-NB	-3.00	1.34	1.37
24	C	510	CLA	C4B-NB	-3.00	1.34	1.37
24	b	611	CLA	C4B-NB	-2.99	1.34	1.37
24	b	617	CLA	C1B-C2B	2.99	1.50	1.43
24	C	512	CLA	C1B-NB	-2.99	1.34	1.37
24	C	507	CLA	C1C-C2C	2.98	1.50	1.44
24	C	513	CLA	C4B-NB	-2.97	1.34	1.37
24	c	903	CLA	C3B-C4B	2.97	1.49	1.42
24	c	903	CLA	C1B-C2B	2.97	1.50	1.43
24	a	408	CLA	C3B-C4B	2.96	1.49	1.42
27	f	102	SQD	C6-S	-2.96	1.66	1.77
24	C	502	CLA	C3B-C4B	2.96	1.49	1.42
24	B	611	CLA	C3B-C4B	2.95	1.49	1.42
24	a	406	CLA	C3B-C4B	2.95	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	C4C-C3C	2.95	1.50	1.45
24	C	513	CLA	C1B-NB	-2.95	1.34	1.37
24	B	607	CLA	C1B-NB	-2.95	1.34	1.37
24	C	509	CLA	C4B-NB	-2.95	1.34	1.37
24	B	602	CLA	C3B-C4B	2.94	1.49	1.42
24	C	508	CLA	C4C-C3C	2.94	1.50	1.45
24	B	603	CLA	C3B-C4B	2.94	1.49	1.42
24	C	505	CLA	C3B-C4B	2.93	1.49	1.42
24	D	405	CLA	C3B-C4B	2.93	1.49	1.42
24	c	911	CLA	C4B-NB	-2.92	1.34	1.37
24	B	617	CLA	C1B-NB	-2.92	1.34	1.37
24	b	607	CLA	C4B-NB	-2.92	1.34	1.37
24	c	906	CLA	C1B-C2B	2.92	1.50	1.43
27	A	411	SQD	C6-S	-2.92	1.66	1.77
24	c	911	CLA	C1B-C2B	2.92	1.50	1.43
24	b	609	CLA	C4D-CHA	2.91	1.48	1.38
24	C	511	CLA	C1B-C2B	2.91	1.50	1.43
24	B	613	CLA	C1C-C2C	2.91	1.50	1.44
27	A	414	SQD	C6-S	-2.90	1.66	1.77
29	A	415	LMT	O1'-C1'	2.90	1.45	1.40
24	B	605	CLA	C1B-NB	-2.90	1.34	1.37
24	c	910	CLA	C1C-C2C	2.90	1.50	1.44
24	b	617	CLA	C4B-NB	-2.90	1.34	1.37
24	c	908	CLA	C4D-CHA	2.90	1.48	1.38
24	A	409	CLA	C1B-NB	-2.89	1.34	1.37
24	C	511	CLA	C4C-C3C	2.89	1.50	1.45
24	b	613	CLA	C1B-NB	-2.89	1.34	1.37
24	b	621	CLA	C1B-NB	-2.88	1.34	1.37
24	b	609	CLA	C1C-C2C	2.88	1.50	1.44
24	c	902	CLA	C4C-C3C	2.88	1.50	1.45
24	C	511	CLA	C3B-C4B	2.88	1.49	1.42
24	C	511	CLA	C4B-NB	-2.87	1.34	1.37
24	b	617	CLA	C1C-C2C	2.87	1.50	1.44
24	b	606	CLA	C1B-NB	-2.87	1.34	1.37
40	v	202	HEC	C4B-NB	-2.87	1.35	1.40
24	B	610	CLA	C3B-C4B	2.87	1.49	1.42
24	C	508	CLA	C4B-NB	-2.86	1.34	1.37
24	d	405	CLA	C4B-NB	-2.86	1.34	1.37
24	b	618	CLA	C1B-C2B	2.86	1.50	1.43
27	a	402	SQD	C6-S	-2.86	1.66	1.77
24	A	409	CLA	C4B-NB	-2.86	1.34	1.37
24	c	913	CLA	C3B-C4B	2.84	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	912	CLA	C4B-NB	-2.84	1.34	1.37
24	B	616	CLA	C4B-NB	-2.83	1.34	1.37
24	C	511	CLA	C4D-CHA	2.83	1.48	1.38
24	b	620	CLA	C1B-C2B	2.83	1.49	1.43
27	F	103	SQD	C6-S	-2.83	1.67	1.77
38	F	102	HEM	C1C-C2C	-2.83	1.39	1.45
24	B	602	CLA	C1B-C2B	2.82	1.49	1.43
24	b	610	CLA	C1C-C2C	2.82	1.50	1.44
24	B	604	CLA	C1C-C2C	2.82	1.50	1.44
24	d	404	CLA	C1B-C2B	2.82	1.49	1.43
24	A	407	CLA	C1B-NB	-2.82	1.34	1.37
24	b	616	CLA	C1B-C2B	2.81	1.49	1.43
24	C	507	CLA	C4D-CHA	2.81	1.48	1.38
24	B	615	CLA	C4C-C3C	2.81	1.49	1.45
24	a	405	CLA	C4C-C3C	2.80	1.49	1.45
24	B	613	CLA	C1B-C2B	2.80	1.49	1.43
24	B	606	CLA	C1B-C2B	2.79	1.49	1.43
24	c	904	CLA	C3B-C4B	2.79	1.49	1.42
24	b	608	CLA	C3B-C4B	2.79	1.49	1.42
24	B	605	CLA	C4D-CHA	2.78	1.48	1.38
24	b	620	CLA	C4D-CHA	2.78	1.48	1.38
24	B	611	CLA	C4D-CHA	2.78	1.48	1.38
24	B	610	CLA	C1B-C2B	2.78	1.49	1.43
24	C	509	CLA	C1B-C2B	2.77	1.49	1.43
24	c	912	CLA	C3B-C4B	2.77	1.49	1.42
24	B	604	CLA	C4B-NB	-2.77	1.34	1.37
24	b	613	CLA	C3B-C4B	2.77	1.49	1.42
24	b	621	CLA	C3B-C4B	2.77	1.49	1.42
24	c	908	CLA	C1C-C2C	2.77	1.49	1.44
24	c	904	CLA	C1B-NB	-2.77	1.34	1.37
24	c	908	CLA	C1B-NB	-2.77	1.34	1.37
24	C	501	CLA	C1C-C2C	2.76	1.49	1.44
24	b	620	CLA	C3B-C4B	2.76	1.49	1.42
24	D	404	CLA	C1C-C2C	2.76	1.49	1.44
24	C	507	CLA	C3B-C4B	2.76	1.49	1.42
24	c	903	CLA	C4D-CHA	2.75	1.48	1.38
24	C	509	CLA	C1C-C2C	2.75	1.49	1.44
24	c	909	CLA	C1B-C2B	2.75	1.49	1.43
24	C	508	CLA	C3B-C4B	2.75	1.49	1.42
24	B	617	CLA	C1B-C2B	2.75	1.49	1.43
24	b	607	CLA	C3B-C4B	2.74	1.49	1.42
24	A	405	CLA	C1C-C2C	2.74	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	C4B-NB	-2.74	1.34	1.37
24	b	621	CLA	C4B-NB	-2.74	1.34	1.37
24	A	405	CLA	C1B-C2B	2.74	1.49	1.43
24	b	611	CLA	C1C-C2C	2.74	1.49	1.44
24	c	907	CLA	C4B-NB	-2.73	1.34	1.37
24	d	406	CLA	C3B-C4B	2.73	1.49	1.42
24	B	604	CLA	C3B-C4B	2.73	1.49	1.42
24	A	405	CLA	C4B-NB	-2.73	1.34	1.37
24	B	609	CLA	C3B-C4B	2.73	1.49	1.42
24	c	904	CLA	C1C-C2C	2.72	1.49	1.44
24	C	510	CLA	C1C-C2C	2.72	1.49	1.44
24	b	612	CLA	C4D-CHA	2.72	1.48	1.38
24	B	605	CLA	C4B-NB	-2.72	1.34	1.37
24	B	615	CLA	C1B-C2B	2.72	1.49	1.43
24	B	602	CLA	C4B-NB	-2.71	1.34	1.37
24	c	912	CLA	C1B-NB	-2.71	1.34	1.37
24	A	407	CLA	C4D-CHA	2.71	1.48	1.38
24	b	619	CLA	C1C-C2C	2.71	1.49	1.44
24	C	509	CLA	C4D-CHA	2.70	1.48	1.38
24	c	902	CLA	C1B-C2B	2.70	1.49	1.43
24	b	610	CLA	C1B-C2B	2.70	1.49	1.43
33	Z	101	LMG	O8-C28	2.70	1.46	1.33
24	d	406	CLA	C1C-C2C	2.69	1.49	1.44
24	b	616	CLA	C4B-NB	-2.69	1.34	1.37
24	A	409	CLA	C1B-C2B	2.69	1.49	1.43
24	b	612	CLA	C3D-C4D	-2.69	1.38	1.44
24	A	409	CLA	C4C-C3C	2.69	1.49	1.45
24	C	503	CLA	C1C-C2C	2.68	1.49	1.44
24	c	910	CLA	C4D-CHA	2.68	1.47	1.38
24	B	616	CLA	C3B-C4B	2.68	1.49	1.42
24	C	502	CLA	C1B-C2B	2.67	1.49	1.43
24	B	612	CLA	C3B-C4B	2.67	1.49	1.42
24	B	614	CLA	C4D-CHA	2.67	1.47	1.38
24	b	611	CLA	C3B-C4B	2.67	1.49	1.42
24	C	502	CLA	C1B-NB	-2.67	1.34	1.37
24	B	607	CLA	C1C-C2C	2.67	1.49	1.44
24	d	406	CLA	C1B-C2B	2.67	1.49	1.43
24	A	409	CLA	C4D-CHA	2.67	1.47	1.38
24	B	607	CLA	C3B-C4B	2.66	1.49	1.42
24	b	621	CLA	C4D-CHA	2.66	1.47	1.38
24	C	504	CLA	C4D-CHA	2.66	1.47	1.38
24	b	616	CLA	C4D-CHA	2.66	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	C4D-CHA	2.66	1.47	1.38
24	B	606	CLA	C4B-NB	-2.66	1.34	1.37
24	A	407	CLA	C4B-NB	-2.66	1.34	1.37
24	b	607	CLA	C1C-C2C	2.65	1.49	1.44
24	d	405	CLA	C3B-C4B	2.65	1.49	1.42
24	b	615	CLA	C4C-C3C	2.65	1.49	1.45
24	B	611	CLA	C1B-C2B	2.65	1.49	1.43
24	C	512	CLA	C1C-C2C	2.64	1.49	1.44
24	b	611	CLA	C4D-CHA	2.64	1.47	1.38
24	b	608	CLA	C1C-C2C	2.64	1.49	1.44
35	b	628	HTG	C1-S1	-2.64	1.76	1.80
27	L	102	SQD	C6-S	-2.64	1.67	1.77
24	B	610	CLA	C4D-CHA	2.63	1.47	1.38
24	b	615	CLA	C4B-NB	-2.63	1.34	1.37
24	C	502	CLA	C1C-C2C	2.63	1.49	1.44
24	b	615	CLA	C3B-C4B	2.63	1.48	1.42
24	D	405	CLA	C1B-C2B	2.63	1.49	1.43
24	c	914	CLA	C1C-C2C	2.63	1.49	1.44
24	b	606	CLA	C4D-CHA	2.63	1.47	1.38
24	A	407	CLA	C1B-C2B	2.63	1.49	1.43
24	C	502	CLA	C4D-CHA	2.63	1.47	1.38
24	d	406	CLA	C4B-NB	-2.62	1.34	1.37
27	B	621	SQD	C6-S	-2.62	1.67	1.77
24	C	509	CLA	C3B-C4B	2.62	1.48	1.42
24	b	609	CLA	C1B-C2B	2.62	1.49	1.43
24	C	506	CLA	C4C-C3C	2.62	1.49	1.45
24	C	508	CLA	C4D-CHA	2.62	1.47	1.38
24	B	615	CLA	C1C-C2C	2.62	1.49	1.44
24	b	619	CLA	C1B-C2B	2.62	1.49	1.43
24	c	906	CLA	C4B-NB	-2.62	1.34	1.37
35	b	627	HTG	C1'-S1	-2.62	1.78	1.81
24	c	905	CLA	C4D-CHA	2.62	1.47	1.38
24	C	504	CLA	C1C-C2C	2.62	1.49	1.44
24	D	405	CLA	C4D-CHA	2.61	1.47	1.38
24	b	613	CLA	C4D-CHA	2.61	1.47	1.38
24	B	607	CLA	C4D-CHA	2.61	1.47	1.38
24	C	512	CLA	C1B-C2B	2.61	1.49	1.43
24	B	608	CLA	C1B-C2B	2.61	1.49	1.43
31	A	417	PL9	C6-C5	2.61	1.48	1.35
24	b	609	CLA	C4B-NB	-2.61	1.34	1.37
24	b	617	CLA	C4D-CHA	2.60	1.47	1.38
24	c	902	CLA	C4D-CHA	2.60	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	C1B-C2B	2.60	1.49	1.43
24	D	404	CLA	C4C-C3C	2.60	1.49	1.45
24	c	911	CLA	C4D-CHA	2.60	1.47	1.38
24	B	614	CLA	C1C-C2C	2.59	1.49	1.44
38	f	101	HEM	C1C-C2C	-2.59	1.40	1.45
24	B	613	CLA	C4D-CHA	2.59	1.47	1.38
24	b	618	CLA	C4D-CHA	2.59	1.47	1.38
24	b	610	CLA	C4D-CHA	2.59	1.47	1.38
24	C	510	CLA	C4D-CHA	2.59	1.47	1.38
24	c	910	CLA	C1B-C2B	2.59	1.49	1.43
24	b	613	CLA	C4C-C3C	2.59	1.49	1.45
24	B	609	CLA	C4D-CHA	2.59	1.47	1.38
24	c	904	CLA	C4D-CHA	2.59	1.47	1.38
24	b	608	CLA	C4D-CHA	2.58	1.47	1.38
24	D	404	CLA	C4B-NB	-2.58	1.34	1.37
24	D	404	CLA	C1B-C2B	2.58	1.49	1.43
24	b	609	CLA	C3D-C4D	-2.58	1.38	1.44
24	C	502	CLA	C4C-C3C	2.58	1.49	1.45
24	a	405	CLA	C4B-NB	-2.58	1.34	1.37
24	c	910	CLA	C3B-C4B	2.58	1.48	1.42
24	c	908	CLA	C1B-C2B	2.58	1.49	1.43
24	A	409	CLA	C1C-C2C	2.57	1.49	1.44
24	C	511	CLA	C1B-NB	-2.57	1.34	1.37
31	a	415	PL9	C6-C5	2.57	1.48	1.35
24	c	904	CLA	C1B-C2B	2.57	1.49	1.43
24	B	616	CLA	C4D-CHA	2.57	1.47	1.38
24	a	406	CLA	C1B-C2B	2.56	1.49	1.43
24	C	509	CLA	C4C-C3C	2.56	1.49	1.45
24	c	906	CLA	C1C-C2C	2.56	1.49	1.44
25	a	407	PHO	CHA-CBD	-2.56	1.48	1.51
24	C	510	CLA	C1B-C2B	2.56	1.49	1.43
24	C	512	CLA	C4D-CHA	2.56	1.47	1.38
24	B	610	CLA	C4B-NB	-2.56	1.34	1.37
24	B	602	CLA	C4D-CHA	2.56	1.47	1.38
24	C	505	CLA	C4D-CHA	2.56	1.47	1.38
24	c	913	CLA	C4D-CHA	2.55	1.47	1.38
24	C	503	CLA	C1B-C2B	2.55	1.49	1.43
24	B	612	CLA	C1C-C2C	2.55	1.49	1.44
24	B	616	CLA	C1B-C2B	2.55	1.49	1.43
24	b	610	CLA	C4B-NB	-2.55	1.34	1.37
24	c	904	CLA	C4B-NB	-2.54	1.34	1.37
24	C	513	CLA	C4D-CHA	2.54	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	C4D-CHA	2.54	1.47	1.38
24	d	404	CLA	C4D-CHA	2.54	1.47	1.38
24	B	606	CLA	C4D-CHA	2.54	1.47	1.38
24	B	615	CLA	C4D-CHA	2.54	1.47	1.38
24	B	603	CLA	C4B-NB	-2.53	1.34	1.37
24	a	408	CLA	C4D-CHA	2.53	1.47	1.38
24	C	507	CLA	C1B-C2B	2.53	1.49	1.43
25	D	401	PHO	C4B-NB	-2.53	1.33	1.38
24	B	617	CLA	C3D-C4D	-2.53	1.38	1.44
27	a	410	SQD	C6-S	-2.53	1.68	1.77
24	c	911	CLA	C3B-C4B	2.53	1.48	1.42
40	V	202	HEC	C4B-C3B	2.53	1.49	1.45
24	C	501	CLA	C4D-CHA	2.52	1.47	1.38
24	B	614	CLA	C4C-C3C	2.52	1.49	1.45
24	C	504	CLA	C1B-C2B	2.52	1.49	1.43
24	c	913	CLA	C1C-C2C	2.52	1.49	1.44
24	B	613	CLA	C4C-C3C	2.52	1.49	1.45
40	V	202	HEC	C4D-ND	-2.52	1.33	1.38
24	C	506	CLA	C4D-CHA	2.52	1.47	1.38
24	b	615	CLA	C1B-C2B	2.52	1.49	1.43
24	B	603	CLA	C4D-CHA	2.52	1.47	1.38
24	B	604	CLA	C1B-C2B	2.52	1.49	1.43
24	a	408	CLA	C1B-C2B	2.52	1.49	1.43
24	b	613	CLA	C1C-C2C	2.52	1.49	1.44
31	d	408	PL9	C6-C5	2.51	1.48	1.35
24	C	505	CLA	C4B-NB	-2.51	1.34	1.37
24	D	405	CLA	C3D-C4D	-2.51	1.38	1.44
24	B	609	CLA	C1C-C2C	2.51	1.49	1.44
24	b	606	CLA	C4B-NB	-2.51	1.34	1.37
24	d	404	CLA	C3B-C4B	2.51	1.48	1.42
24	A	406	CLA	C3B-C4B	2.51	1.48	1.42
24	C	505	CLA	C1C-C2C	2.50	1.49	1.44
24	C	507	CLA	C4B-NB	-2.50	1.34	1.37
24	B	617	CLA	C3B-C4B	2.50	1.48	1.42
24	B	608	CLA	C4C-C3C	2.50	1.49	1.45
24	B	608	CLA	C1C-C2C	2.50	1.49	1.44
24	C	510	CLA	C4C-C3C	2.50	1.49	1.45
24	B	612	CLA	C1B-C2B	2.50	1.49	1.43
24	c	910	CLA	C3B-C2B	2.50	1.49	1.41
24	A	406	CLA	C3B-C2B	2.49	1.49	1.41
24	b	607	CLA	C1B-C2B	2.49	1.49	1.43
24	B	603	CLA	C3D-C4D	-2.49	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	609	CLA	C1B-C2B	2.49	1.49	1.43
24	b	615	CLA	C4D-CHA	2.49	1.47	1.38
24	C	511	CLA	C1C-C2C	2.49	1.49	1.44
24	b	613	CLA	C1B-C2B	2.48	1.49	1.43
24	B	617	CLA	C4D-CHA	2.48	1.47	1.38
24	b	608	CLA	C4C-C3C	2.48	1.49	1.45
24	c	912	CLA	C3B-C2B	2.48	1.49	1.41
24	a	405	CLA	C4D-CHA	2.48	1.47	1.38
24	C	506	CLA	C3D-C4D	-2.48	1.38	1.44
24	B	615	CLA	C4B-NB	-2.48	1.34	1.37
24	b	618	CLA	C3D-C4D	-2.48	1.38	1.44
24	C	506	CLA	C3B-C4B	2.47	1.48	1.42
24	b	618	CLA	C3B-C4B	2.47	1.48	1.42
24	B	603	CLA	C1C-C2C	2.47	1.49	1.44
24	b	620	CLA	C1C-C2C	2.47	1.49	1.44
24	b	619	CLA	C4B-NB	-2.47	1.34	1.37
24	B	603	CLA	C1B-C2B	2.47	1.49	1.43
35	c	921	HTG	C1-S1	-2.47	1.76	1.80
24	c	912	CLA	C1B-C2B	2.46	1.49	1.43
24	b	614	CLA	C1B-C2B	2.46	1.49	1.43
24	c	906	CLA	C4C-C3C	2.46	1.49	1.45
24	C	510	CLA	C3B-C4B	2.46	1.48	1.42
24	c	909	CLA	C4D-CHA	2.46	1.47	1.38
24	B	610	CLA	C3D-C4D	-2.46	1.38	1.44
24	c	909	CLA	C3B-C4B	2.46	1.48	1.42
24	a	405	CLA	C3B-C4B	2.46	1.48	1.42
24	C	509	CLA	C3B-C2B	2.46	1.49	1.41
24	B	609	CLA	C4C-C3C	2.46	1.49	1.45
24	D	405	CLA	C4C-C3C	2.45	1.49	1.45
24	b	619	CLA	C3D-C4D	-2.45	1.38	1.44
24	c	912	CLA	C4D-CHA	2.45	1.47	1.38
24	c	905	CLA	C1C-C2C	2.45	1.49	1.44
24	c	914	CLA	C4D-CHA	2.45	1.47	1.38
24	c	907	CLA	C3B-C4B	2.45	1.48	1.42
24	A	406	CLA	C1B-C2B	2.44	1.49	1.43
24	A	406	CLA	C1C-C2C	2.44	1.49	1.44
40	v	202	HEC	C4B-C3B	2.44	1.49	1.45
24	c	911	CLA	C4C-C3C	2.44	1.49	1.45
24	B	614	CLA	C3B-C4B	2.44	1.48	1.42
24	b	606	CLA	C1B-C2B	2.44	1.49	1.43
24	b	620	CLA	C4B-NB	-2.44	1.34	1.37
24	B	604	CLA	C4D-CHA	2.44	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	621	CLA	C4C-C3C	2.44	1.49	1.45
24	b	608	CLA	C1B-C2B	2.44	1.49	1.43
24	c	906	CLA	C3D-C4D	-2.43	1.38	1.44
24	c	909	CLA	C4B-NB	-2.43	1.34	1.37
24	C	501	CLA	C4B-NB	-2.43	1.34	1.37
24	b	619	CLA	C4D-CHA	2.43	1.47	1.38
24	C	508	CLA	C1B-C2B	2.43	1.49	1.43
24	c	906	CLA	C4D-CHA	2.42	1.47	1.38
24	b	612	CLA	C4B-NB	-2.42	1.34	1.37
24	b	607	CLA	C4D-CHA	2.42	1.47	1.38
24	C	505	CLA	C3D-C4D	-2.42	1.38	1.44
24	c	907	CLA	C1B-C2B	2.42	1.49	1.43
24	D	404	CLA	C3B-C4B	2.42	1.48	1.42
24	b	607	CLA	C4C-C3C	2.41	1.49	1.45
24	c	907	CLA	C3D-C4D	-2.41	1.38	1.44
24	b	609	CLA	C3B-C4B	2.41	1.48	1.42
24	b	609	CLA	C4C-C3C	2.41	1.49	1.45
24	D	405	CLA	C1C-C2C	2.41	1.49	1.44
24	A	406	CLA	C4D-CHA	2.41	1.47	1.38
24	b	608	CLA	C3D-C4D	-2.41	1.38	1.44
35	C	521	HTG	C1-S1	-2.40	1.77	1.80
24	C	504	CLA	C3B-C2B	2.40	1.49	1.41
24	a	406	CLA	C4D-CHA	2.40	1.46	1.38
24	B	611	CLA	C4C-C3C	2.40	1.49	1.45
24	d	405	CLA	C1C-C2C	2.40	1.49	1.44
25	D	401	PHO	CHA-CBD	-2.40	1.48	1.51
24	B	613	CLA	C3B-C2B	2.40	1.49	1.41
24	B	617	CLA	C3B-C2B	2.40	1.49	1.41
24	B	602	CLA	C1C-C2C	2.40	1.49	1.44
24	b	615	CLA	C1C-C2C	2.39	1.49	1.44
24	B	607	CLA	C4C-C3C	2.39	1.49	1.45
24	c	905	CLA	C3B-C4B	2.39	1.48	1.42
24	b	611	CLA	C1B-C2B	2.39	1.48	1.43
24	b	610	CLA	C3D-C4D	-2.39	1.38	1.44
24	d	406	CLA	C4D-CHA	2.39	1.46	1.38
24	B	607	CLA	C1B-C2B	2.39	1.48	1.43
24	c	907	CLA	C4D-CHA	2.38	1.46	1.38
24	d	405	CLA	C3D-C4D	-2.38	1.38	1.44
24	C	504	CLA	C4C-C3C	2.38	1.49	1.45
24	D	404	CLA	C4D-CHA	2.38	1.46	1.38
24	c	914	CLA	C1B-C2B	2.38	1.48	1.43
24	b	614	CLA	C4B-NB	-2.38	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	C4D-CHA	2.37	1.46	1.38
24	D	404	CLA	C3B-C2B	2.37	1.49	1.41
31	D	407	PL9	C6-C5	2.37	1.47	1.35
37	D	408	DGD	O3G-C1D	2.37	1.44	1.40
24	b	612	CLA	C1C-C2C	2.37	1.49	1.44
24	b	607	CLA	C3D-C4D	-2.37	1.38	1.44
24	c	910	CLA	C3D-C4D	-2.36	1.38	1.44
25	D	401	PHO	C1B-NB	-2.36	1.34	1.38
24	C	504	CLA	C3B-C4B	2.36	1.48	1.42
24	d	405	CLA	C4C-C3C	2.36	1.49	1.45
24	C	501	CLA	C4C-C3C	2.35	1.49	1.45
24	d	405	CLA	C4D-CHA	2.35	1.46	1.38
24	c	904	CLA	C3D-C4D	-2.35	1.38	1.44
24	a	406	CLA	C1C-C2C	2.35	1.49	1.44
24	A	405	CLA	C4D-CHA	2.35	1.46	1.38
24	c	910	CLA	C4C-C3C	2.35	1.49	1.45
25	a	407	PHO	C4B-NB	-2.35	1.34	1.38
24	b	614	CLA	C1C-C2C	2.35	1.49	1.44
24	B	615	CLA	C3B-C2B	2.35	1.49	1.41
24	B	605	CLA	C1C-C2C	2.35	1.49	1.44
24	C	513	CLA	C3D-C4D	-2.35	1.38	1.44
24	B	612	CLA	C4C-C3C	2.34	1.49	1.45
24	B	614	CLA	C1B-C2B	2.34	1.48	1.43
24	b	619	CLA	C3B-C4B	2.33	1.48	1.42
24	c	911	CLA	C3B-C2B	2.33	1.49	1.41
24	C	513	CLA	C1C-C2C	2.33	1.49	1.44
25	d	403	PHO	CHA-CBD	-2.33	1.48	1.51
24	B	612	CLA	C4D-CHA	2.33	1.46	1.38
24	d	404	CLA	C3B-C2B	2.33	1.49	1.41
24	c	913	CLA	C1B-C2B	2.33	1.48	1.43
24	a	406	CLA	C3D-C4D	-2.32	1.38	1.44
24	c	914	CLA	C3D-C4D	-2.32	1.38	1.44
24	B	614	CLA	C3B-C2B	2.32	1.49	1.41
24	B	609	CLA	C3D-C4D	-2.32	1.38	1.44
24	B	609	CLA	C3B-C2B	2.32	1.49	1.41
24	C	508	CLA	C1C-C2C	2.32	1.49	1.44
24	A	405	CLA	C3B-C4B	2.32	1.48	1.42
24	C	511	CLA	C3B-C2B	2.32	1.49	1.41
24	b	618	CLA	C3B-C2B	2.32	1.49	1.41
24	B	603	CLA	C4C-C3C	2.31	1.49	1.45
24	c	908	CLA	C4C-C3C	2.31	1.49	1.45
24	b	613	CLA	C3D-C4D	-2.31	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	C3D-C4D	-2.31	1.39	1.44
24	B	608	CLA	C3B-C4B	2.31	1.48	1.42
24	b	619	CLA	C4C-C3C	2.31	1.49	1.45
24	A	405	CLA	C3B-C2B	2.31	1.49	1.41
24	A	409	CLA	C3D-C4D	-2.30	1.39	1.44
24	b	621	CLA	C3B-C2B	2.30	1.49	1.41
24	C	504	CLA	C3D-C4D	-2.30	1.39	1.44
24	B	616	CLA	C1C-C2C	2.30	1.49	1.44
24	c	909	CLA	C3B-C2B	2.30	1.49	1.41
24	b	619	CLA	C3B-C2B	2.30	1.49	1.41
24	a	405	CLA	C1C-C2C	2.29	1.49	1.44
35	B	625	HTG	C1-S1	-2.29	1.77	1.80
24	d	404	CLA	C3D-C4D	-2.29	1.39	1.44
24	C	512	CLA	C4C-C3C	2.29	1.49	1.45
24	b	616	CLA	C4C-C3C	2.29	1.49	1.45
25	a	407	PHO	C3A-C2A	-2.29	1.52	1.54
24	B	608	CLA	C4B-NB	-2.29	1.35	1.37
24	b	611	CLA	C4C-C3C	2.29	1.49	1.45
24	a	405	CLA	C1B-C2B	2.29	1.48	1.43
24	C	512	CLA	C4B-NB	-2.28	1.35	1.37
25	A	408	PHO	C4B-NB	-2.28	1.34	1.38
35	V	203	HTG	C1-S1	-2.28	1.77	1.80
24	c	903	CLA	C1C-C2C	2.28	1.49	1.44
24	B	605	CLA	C4C-C3C	2.28	1.49	1.45
24	C	501	CLA	C3D-C4D	-2.27	1.39	1.44
37	h	102	DGD	O5D-C1E	2.27	1.44	1.40
24	B	612	CLA	C3D-C4D	-2.27	1.39	1.44
24	B	605	CLA	C3B-C4B	2.27	1.48	1.42
24	C	507	CLA	C3D-C4D	-2.27	1.39	1.44
24	C	503	CLA	C4B-NB	-2.27	1.35	1.37
24	c	909	CLA	C3D-C4D	-2.27	1.39	1.44
24	b	611	CLA	C3D-C4D	-2.27	1.39	1.44
24	c	908	CLA	C3B-C4B	2.26	1.48	1.42
24	b	615	CLA	C3B-C2B	2.26	1.48	1.41
24	C	502	CLA	C3D-C4D	-2.26	1.39	1.44
24	c	905	CLA	C3B-C2B	2.26	1.48	1.41
24	b	616	CLA	C3B-C2B	2.26	1.48	1.41
24	b	616	CLA	C1C-C2C	2.26	1.48	1.44
35	d	414	HTG	C1-S1	-2.25	1.77	1.80
24	c	909	CLA	C4C-C3C	2.25	1.48	1.45
24	B	611	CLA	C3D-C4D	-2.25	1.39	1.44
24	A	407	CLA	C1C-C2C	2.25	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	C3D-C4D	-2.25	1.39	1.44
24	B	605	CLA	C3B-C2B	2.24	1.48	1.41
24	B	610	CLA	C1C-C2C	2.23	1.48	1.44
25	A	408	PHO	CHA-CBD	-2.23	1.48	1.51
24	A	407	CLA	C3D-C4D	-2.23	1.39	1.44
24	c	912	CLA	C1C-C2C	2.23	1.48	1.44
24	d	405	CLA	C3B-C2B	2.23	1.48	1.41
24	B	608	CLA	C3B-C2B	2.23	1.48	1.41
24	C	510	CLA	C3D-C4D	-2.22	1.39	1.44
24	b	616	CLA	C3D-C4D	-2.22	1.39	1.44
24	B	604	CLA	C3B-C2B	2.21	1.48	1.41
24	a	405	CLA	C3D-C4D	-2.21	1.39	1.44
24	b	606	CLA	C1C-C2C	2.21	1.48	1.44
24	B	607	CLA	C3D-C4D	-2.21	1.39	1.44
24	A	406	CLA	C4C-C3C	2.21	1.48	1.45
24	d	405	CLA	C1B-C2B	2.21	1.48	1.43
24	D	404	CLA	C3D-C4D	-2.21	1.39	1.44
24	d	404	CLA	C1C-NC	-2.20	1.34	1.37
24	A	406	CLA	C3D-C4D	-2.20	1.39	1.44
24	b	617	CLA	C3B-C2B	2.20	1.48	1.41
40	v	202	HEC	C4A-C3A	-2.20	1.41	1.45
24	D	405	CLA	C1C-NC	-2.20	1.34	1.37
24	c	907	CLA	C3B-C2B	2.20	1.48	1.41
24	B	602	CLA	C3B-C2B	2.20	1.48	1.41
24	a	408	CLA	C1C-C2C	2.20	1.48	1.44
24	c	902	CLA	C3D-C4D	-2.20	1.39	1.44
24	C	501	CLA	C1B-C2B	2.19	1.48	1.43
40	V	202	HEC	C1B-NB	-2.19	1.34	1.38
24	B	602	CLA	C1C-NC	-2.19	1.34	1.37
24	b	618	CLA	C1C-C2C	2.19	1.48	1.44
24	A	407	CLA	C4C-C3C	2.19	1.48	1.45
24	b	606	CLA	C3B-C2B	2.19	1.48	1.41
29	M	103	LMT	O1'-C1'	2.19	1.43	1.40
24	C	511	CLA	C3D-C4D	-2.19	1.39	1.44
24	c	905	CLA	C3D-C4D	-2.18	1.39	1.44
24	C	510	CLA	C3B-C2B	2.18	1.48	1.41
24	B	615	CLA	C3B-C4B	2.18	1.47	1.42
24	b	607	CLA	C1D-C2D	2.18	1.49	1.45
24	b	617	CLA	C1B-NB	-2.18	1.35	1.37
24	c	903	CLA	C1B-NB	-2.18	1.35	1.37
24	a	405	CLA	C3B-C2B	2.18	1.48	1.41
35	c	922	HTG	C1-S1	-2.18	1.77	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C3D-C4D	-2.18	1.39	1.44
35	D	413	HTG	C1-S1	-2.18	1.77	1.80
24	b	620	CLA	C1B-NB	-2.17	1.35	1.37
24	B	610	CLA	C4C-C3C	2.17	1.48	1.45
24	b	621	CLA	C1C-C2C	2.17	1.48	1.44
24	c	908	CLA	C3D-C4D	-2.17	1.39	1.44
24	b	607	CLA	C3B-C2B	2.17	1.48	1.41
24	B	615	CLA	C3D-C4D	-2.17	1.39	1.44
24	a	406	CLA	C4B-NB	-2.17	1.35	1.37
24	C	506	CLA	C1C-C2C	2.16	1.48	1.44
24	b	610	CLA	C4C-C3C	2.16	1.48	1.45
24	B	616	CLA	C4C-C3C	2.16	1.48	1.45
24	b	620	CLA	C3B-C2B	2.16	1.48	1.41
24	c	911	CLA	C3D-C4D	-2.16	1.39	1.44
25	a	407	PHO	C1D-ND	-2.16	1.34	1.38
36	d	409	LHG	O7-C5	-2.16	1.41	1.46
26	b	624	BCR	C30-C25	-2.16	1.50	1.53
24	b	615	CLA	C3D-C4D	-2.15	1.39	1.44
24	C	506	CLA	C1B-C2B	2.15	1.48	1.43
24	C	506	CLA	C3B-C2B	2.15	1.48	1.41
24	B	608	CLA	C3D-C4D	-2.15	1.39	1.44
24	c	902	CLA	C3B-C2B	2.14	1.48	1.41
25	D	401	PHO	C1D-ND	-2.14	1.34	1.38
24	c	903	CLA	C3B-C2B	2.14	1.48	1.41
24	C	508	CLA	C3B-C2B	2.14	1.48	1.41
24	b	620	CLA	C3D-C4D	-2.14	1.39	1.44
24	c	904	CLA	C3B-C2B	2.14	1.48	1.41
24	B	604	CLA	C3D-C4D	-2.13	1.39	1.44
24	c	905	CLA	C1B-C2B	2.13	1.48	1.43
24	b	609	CLA	C3B-C2B	2.13	1.48	1.41
24	c	909	CLA	C1C-C2C	2.13	1.48	1.44
24	b	616	CLA	C3B-C4B	2.13	1.47	1.42
24	C	505	CLA	C4C-C3C	2.13	1.48	1.45
24	C	505	CLA	C3B-C2B	2.13	1.48	1.41
24	c	908	CLA	C3B-C2B	2.13	1.48	1.41
25	A	408	PHO	C3A-C2A	-2.13	1.52	1.54
24	b	617	CLA	C1C-NC	-2.12	1.34	1.37
24	b	620	CLA	C4C-C3C	2.12	1.48	1.45
29	b	602	LMT	O1'-C1'	2.12	1.43	1.40
24	b	613	CLA	C3B-C2B	2.12	1.48	1.41
24	C	512	CLA	C3B-C2B	2.11	1.48	1.41
24	d	406	CLA	C3D-C4D	-2.11	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	610	CLA	C3B-C2B	2.11	1.48	1.41
38	f	101	HEM	C3C-C4C	-2.11	1.42	1.46
24	B	616	CLA	C3D-C4D	-2.11	1.39	1.44
24	c	912	CLA	C1D-C2D	2.11	1.49	1.45
35	b	603	HTG	C1-S1	-2.11	1.77	1.80
25	A	408	PHO	C1D-ND	-2.11	1.34	1.38
24	b	617	CLA	C3D-C4D	-2.11	1.39	1.44
29	a	401	LMT	O1'-C1'	2.11	1.43	1.40
24	c	903	CLA	C3D-C4D	-2.10	1.39	1.44
24	C	502	CLA	C3B-C2B	2.10	1.48	1.41
35	b	604	HTG	C1-S1	-2.10	1.77	1.80
38	F	102	HEM	C1D-ND	-2.10	1.34	1.38
24	b	611	CLA	C3B-C2B	2.10	1.48	1.41
31	A	417	PL9	C2-C3	2.10	1.40	1.34
35	B	633	HTG	C1-S1	-2.10	1.77	1.80
24	b	608	CLA	C3B-C2B	2.10	1.48	1.41
24	C	503	CLA	C4C-C3C	2.10	1.48	1.45
24	c	902	CLA	C1C-C2C	2.09	1.48	1.44
24	c	907	CLA	C1C-C2C	2.09	1.48	1.44
24	C	501	CLA	C3B-C2B	2.09	1.48	1.41
24	c	913	CLA	C3B-C2B	2.09	1.48	1.41
24	c	912	CLA	C3D-C4D	-2.09	1.39	1.44
24	B	603	CLA	C3B-C2B	2.09	1.48	1.41
24	B	605	CLA	C1A-CHA	2.08	1.51	1.43
24	b	614	CLA	C3D-C4D	-2.08	1.39	1.44
24	b	606	CLA	C3D-C4D	-2.08	1.39	1.44
25	d	403	PHO	C4B-NB	-2.08	1.34	1.38
31	a	415	PL9	C2-C3	2.07	1.40	1.34
24	B	606	CLA	C3B-C2B	2.07	1.48	1.41
24	c	914	CLA	C3B-C2B	2.07	1.48	1.41
24	c	914	CLA	C4C-C3C	2.06	1.48	1.45
24	B	606	CLA	C3D-C4D	-2.06	1.39	1.44
24	a	408	CLA	C3B-C2B	2.06	1.48	1.41
24	c	903	CLA	C1C-NC	-2.06	1.34	1.37
24	c	913	CLA	C3D-C4D	-2.06	1.39	1.44
24	a	408	CLA	C3D-C4D	-2.05	1.39	1.44
40	v	202	HEC	C1B-NB	-2.05	1.34	1.38
37	C	517	DGD	O5D-C1E	2.04	1.43	1.40
24	d	406	CLA	C3B-C2B	2.04	1.48	1.41
24	B	617	CLA	C1C-C2C	2.04	1.48	1.44
24	c	911	CLA	C1C-C2C	2.04	1.48	1.44
24	C	513	CLA	C3B-C2B	2.04	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	C3B-C2B	2.04	1.48	1.41
24	C	512	CLA	C3D-C4D	-2.04	1.39	1.44
40	V	202	HEC	C1A-C2A	-2.04	1.41	1.45
24	B	603	CLA	C1D-C2D	2.03	1.49	1.45
24	A	405	CLA	C3D-C4D	-2.03	1.39	1.44
24	a	406	CLA	C3B-C2B	2.03	1.48	1.41
38	f	101	HEM	C3B-C4B	2.03	1.48	1.44
35	B	632	HTG	C1-S1	-2.03	1.77	1.80
24	B	602	CLA	C4C-C3C	2.03	1.48	1.45
24	C	507	CLA	C3B-C2B	2.03	1.48	1.41
24	b	609	CLA	MG-NA	2.02	2.11	2.06
38	f	101	HEM	C1D-ND	-2.02	1.34	1.38
24	B	611	CLA	C1C-NC	-2.02	1.34	1.37
24	d	406	CLA	C1D-C2D	2.02	1.49	1.45
24	B	602	CLA	C3D-C4D	-2.02	1.39	1.44
24	C	503	CLA	C3B-C2B	2.02	1.48	1.41
31	d	408	PL9	C2-C3	2.01	1.39	1.34
31	D	407	PL9	C2-C3	2.01	1.39	1.34
24	C	507	CLA	C4C-C3C	2.01	1.48	1.45
24	b	615	CLA	C1D-C2D	2.01	1.49	1.45
24	c	907	CLA	C4C-C3C	2.01	1.48	1.45
36	L	101	LHG	O7-C5	-2.00	1.41	1.46

All (2792) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	407	PHO	C2D-C1D-ND	11.94	117.77	109.53
25	d	403	PHO	C2D-C1D-ND	11.93	117.76	109.53
25	D	401	PHO	C2D-C1D-ND	11.53	117.49	109.53
25	A	408	PHO	C2D-C1D-ND	11.16	117.23	109.53
24	c	914	CLA	C1D-ND-C4D	-10.25	99.05	106.33
24	b	610	CLA	C1D-ND-C4D	-10.21	99.08	106.33
24	D	404	CLA	C1D-ND-C4D	-10.09	99.16	106.33
24	B	602	CLA	C1D-ND-C4D	-9.98	99.24	106.33
24	a	406	CLA	C1D-ND-C4D	-9.97	99.25	106.33
24	a	408	CLA	C1D-ND-C4D	-9.95	99.26	106.33
24	B	604	CLA	C1D-ND-C4D	-9.89	99.31	106.33
24	B	615	CLA	C1D-ND-C4D	-9.87	99.32	106.33
24	B	612	CLA	C1D-ND-C4D	-9.85	99.34	106.33
24	b	614	CLA	C1D-ND-C4D	-9.73	99.43	106.33
24	c	912	CLA	C1D-ND-C4D	-9.70	99.44	106.33
24	B	606	CLA	C1D-ND-C4D	-9.66	99.47	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	C1D-ND-C4D	-9.61	99.51	106.33
24	c	904	CLA	C1D-ND-C4D	-9.61	99.51	106.33
24	c	903	CLA	C1D-ND-C4D	-9.58	99.53	106.33
24	c	913	CLA	C1D-ND-C4D	-9.57	99.53	106.33
24	b	607	CLA	C1D-ND-C4D	-9.52	99.57	106.33
24	A	407	CLA	C1D-ND-C4D	-9.51	99.58	106.33
24	A	406	CLA	C1D-ND-C4D	-9.51	99.58	106.33
24	b	619	CLA	C1D-ND-C4D	-9.49	99.59	106.33
24	B	607	CLA	C1D-ND-C4D	-9.48	99.60	106.33
24	B	613	CLA	C1D-ND-C4D	-9.43	99.64	106.33
24	d	406	CLA	C1D-ND-C4D	-9.40	99.66	106.33
24	B	608	CLA	C1D-ND-C4D	-9.39	99.66	106.33
24	c	905	CLA	C1D-ND-C4D	-9.36	99.68	106.33
24	B	603	CLA	C1D-ND-C4D	-9.33	99.71	106.33
24	b	621	CLA	C1D-ND-C4D	-9.31	99.72	106.33
24	b	617	CLA	C1D-ND-C4D	-9.29	99.73	106.33
24	A	405	CLA	C1D-ND-C4D	-9.29	99.73	106.33
24	C	503	CLA	C1D-ND-C4D	-9.29	99.74	106.33
24	C	512	CLA	C1D-ND-C4D	-9.26	99.76	106.33
24	d	405	CLA	C1D-ND-C4D	-9.25	99.77	106.33
24	B	617	CLA	C1D-ND-C4D	-9.24	99.77	106.33
24	D	404	CLA	C2D-C1D-ND	9.19	116.88	110.10
24	B	611	CLA	C1D-ND-C4D	-9.18	99.81	106.33
24	C	501	CLA	C1D-ND-C4D	-9.18	99.82	106.33
24	a	405	CLA	C1D-ND-C4D	-9.14	99.85	106.33
24	C	502	CLA	C1D-ND-C4D	-9.12	99.86	106.33
24	b	616	CLA	C1D-ND-C4D	-9.09	99.88	106.33
24	C	511	CLA	C1D-ND-C4D	-9.08	99.89	106.33
24	c	902	CLA	C1D-ND-C4D	-9.06	99.90	106.33
24	c	909	CLA	C1D-ND-C4D	-9.06	99.90	106.33
24	B	609	CLA	C1D-ND-C4D	-9.05	99.90	106.33
24	B	616	CLA	C1D-ND-C4D	-9.02	99.92	106.33
24	b	608	CLA	C1D-ND-C4D	-9.01	99.93	106.33
24	b	606	CLA	C1D-ND-C4D	-9.00	99.94	106.33
24	C	508	CLA	C1D-ND-C4D	-8.99	99.95	106.33
24	B	613	CLA	C2D-C1D-ND	8.92	116.68	110.10
24	C	510	CLA	C1D-ND-C4D	-8.90	100.01	106.33
24	c	907	CLA	C1D-ND-C4D	-8.90	100.01	106.33
24	b	610	CLA	C2D-C1D-ND	8.81	116.60	110.10
24	A	406	CLA	C2D-C1D-ND	8.80	116.59	110.10
24	b	619	CLA	C2D-C1D-ND	8.80	116.59	110.10
24	a	408	CLA	C2D-C1D-ND	8.80	116.59	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	620	CLA	C1D-ND-C4D	-8.79	100.09	106.33
24	b	615	CLA	C1D-ND-C4D	-8.78	100.10	106.33
24	C	507	CLA	C1D-ND-C4D	-8.75	100.12	106.33
24	c	910	CLA	C1D-ND-C4D	-8.73	100.13	106.33
24	D	405	CLA	C1D-ND-C4D	-8.73	100.13	106.33
24	b	617	CLA	C2D-C1D-ND	8.72	116.53	110.10
24	b	616	CLA	C2D-C1D-ND	8.70	116.52	110.10
24	b	611	CLA	C1D-ND-C4D	-8.69	100.16	106.33
24	B	602	CLA	C2D-C1D-ND	8.65	116.48	110.10
24	c	911	CLA	C1D-ND-C4D	-8.63	100.21	106.33
24	B	610	CLA	C1D-ND-C4D	-8.61	100.22	106.33
24	b	613	CLA	C1D-ND-C4D	-8.57	100.25	106.33
24	c	906	CLA	C1D-ND-C4D	-8.56	100.25	106.33
24	C	509	CLA	C1D-ND-C4D	-8.55	100.26	106.33
24	d	404	CLA	C1D-ND-C4D	-8.53	100.27	106.33
24	C	505	CLA	C1D-ND-C4D	-8.52	100.28	106.33
24	B	604	CLA	C2D-C1D-ND	8.48	116.35	110.10
24	C	506	CLA	C1D-ND-C4D	-8.47	100.31	106.33
24	b	614	CLA	C2D-C1D-ND	8.47	116.35	110.10
24	B	614	CLA	C1D-ND-C4D	-8.47	100.32	106.33
24	B	605	CLA	C1D-ND-C4D	-8.46	100.33	106.33
24	B	615	CLA	C2D-C1D-ND	8.44	116.32	110.10
24	C	504	CLA	C1D-ND-C4D	-8.43	100.34	106.33
24	c	905	CLA	C2D-C1D-ND	8.43	116.31	110.10
24	B	605	CLA	C2D-C1D-ND	8.38	116.28	110.10
24	c	903	CLA	C2D-C1D-ND	8.35	116.26	110.10
24	c	904	CLA	C2D-C1D-ND	8.35	116.26	110.10
24	c	914	CLA	C2D-C1D-ND	8.34	116.25	110.10
24	A	409	CLA	C2B-C1B-NB	8.32	115.81	110.23
24	B	606	CLA	C2D-C1D-ND	8.32	116.23	110.10
24	C	512	CLA	C2D-C1D-ND	8.31	116.23	110.10
24	c	908	CLA	C1D-ND-C4D	-8.29	100.45	106.33
24	B	608	CLA	C2D-C1D-ND	8.28	116.21	110.10
24	a	406	CLA	C2D-C1D-ND	8.26	116.19	110.10
24	b	621	CLA	C2D-C1D-ND	8.25	116.19	110.10
24	B	611	CLA	C2D-C1D-ND	8.23	116.17	110.10
24	c	913	CLA	C2D-C1D-ND	8.22	116.16	110.10
24	A	409	CLA	C1D-ND-C4D	-8.21	100.50	106.33
24	c	909	CLA	C2D-C1D-ND	8.19	116.14	110.10
24	d	406	CLA	C2D-C1D-ND	8.16	116.12	110.10
24	B	614	CLA	C2D-C1D-ND	8.15	116.11	110.10
24	c	913	CLA	C2B-C1B-NB	8.13	115.68	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	C2B-C1B-NB	8.12	115.68	110.23
24	B	612	CLA	C2D-C1D-ND	8.10	116.07	110.10
24	B	611	CLA	C2B-C1B-NB	8.09	115.65	110.23
24	B	617	CLA	C2D-C1D-ND	8.08	116.06	110.10
24	A	407	CLA	C2D-C1D-ND	8.08	116.06	110.10
24	C	511	CLA	C2D-C1D-ND	8.06	116.04	110.10
24	C	503	CLA	C2D-C1D-ND	8.01	116.01	110.10
24	B	607	CLA	C2D-C1D-ND	8.00	116.00	110.10
24	c	912	CLA	C2D-C1D-ND	8.00	116.00	110.10
24	b	611	CLA	C2B-C1B-NB	7.99	115.59	110.23
24	B	616	CLA	C2D-C1D-ND	7.95	115.96	110.10
24	B	603	CLA	C2B-C1B-NB	7.91	115.53	110.23
24	C	513	CLA	C2D-C1D-ND	7.90	115.92	110.10
24	b	620	CLA	C2D-C1D-ND	7.87	115.91	110.10
24	C	507	CLA	C2D-C1D-ND	7.87	115.90	110.10
24	c	902	CLA	C2D-C1D-ND	7.86	115.90	110.10
24	C	504	CLA	C2D-C1D-ND	7.84	115.88	110.10
24	c	907	CLA	C2D-C1D-ND	7.84	115.88	110.10
24	C	513	CLA	C2B-C1B-NB	7.83	115.48	110.23
24	c	908	CLA	C2D-C1D-ND	7.78	115.84	110.10
24	B	610	CLA	C2D-C1D-ND	7.77	115.83	110.10
24	d	405	CLA	C4A-NA-C1A	-7.75	103.22	106.71
24	C	502	CLA	C2D-C1D-ND	7.75	115.81	110.10
24	d	404	CLA	C2D-C1D-ND	7.73	115.80	110.10
24	b	612	CLA	C1D-ND-C4D	-7.71	100.86	106.33
24	B	614	CLA	C2B-C1B-NB	7.71	115.40	110.23
24	C	508	CLA	C2D-C1D-ND	7.67	115.76	110.10
24	C	508	CLA	C2B-C1B-NB	7.66	115.37	110.23
24	b	611	CLA	C2D-C1D-ND	7.66	115.75	110.10
24	B	603	CLA	C2D-C1D-ND	7.66	115.75	110.10
24	C	501	CLA	C2D-C1D-ND	7.65	115.74	110.10
24	d	405	CLA	C2D-C1D-ND	7.64	115.73	110.10
24	b	607	CLA	CMD-C2D-C1D	7.63	138.17	124.71
25	A	408	PHO	O2D-CGD-CBD	7.63	120.66	111.00
24	C	503	CLA	C2B-C1B-NB	7.62	115.34	110.23
24	a	405	CLA	C2D-C1D-ND	7.61	115.71	110.10
24	b	606	CLA	C2D-C1D-ND	7.61	115.71	110.10
25	d	403	PHO	O2D-CGD-CBD	7.59	120.62	111.00
24	b	607	CLA	C2D-C1D-ND	7.59	115.70	110.10
24	D	405	CLA	C2B-C1B-NB	7.58	115.31	110.23
24	b	606	CLA	C2B-C1B-NB	7.57	115.31	110.23
24	a	408	CLA	C2B-C1B-NB	7.56	115.30	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	618	CLA	C1D-ND-C4D	-7.54	100.98	106.33
24	C	501	CLA	C2B-C1B-NB	7.53	115.28	110.23
24	C	512	CLA	C2B-C1B-NB	7.52	115.27	110.23
24	C	510	CLA	C2D-C1D-ND	7.49	115.63	110.10
24	c	910	CLA	C2D-C1D-ND	7.48	115.62	110.10
24	A	407	CLA	C2B-C1B-NB	7.48	115.25	110.23
24	c	912	CLA	C2B-C1B-NB	7.47	115.24	110.23
24	D	405	CLA	C2D-C1D-ND	7.47	115.61	110.10
25	a	407	PHO	O2D-CGD-CBD	7.45	120.44	111.00
24	c	914	CLA	C2B-C1B-NB	7.37	115.17	110.23
24	b	607	CLA	C2B-C1B-NB	7.35	115.16	110.23
24	C	509	CLA	C2D-C1D-ND	7.35	115.52	110.10
24	b	613	CLA	C2D-C1D-ND	7.33	115.51	110.10
24	A	405	CLA	C2D-C1D-ND	7.31	115.49	110.10
24	b	618	CLA	C2D-C1D-ND	7.31	115.49	110.10
24	b	608	CLA	C2B-C1B-NB	7.29	115.12	110.23
24	B	609	CLA	C2B-C1B-NB	7.25	115.09	110.23
24	b	609	CLA	C1D-ND-C4D	-7.25	101.18	106.33
24	A	405	CLA	C2B-C1B-NB	7.25	115.09	110.23
24	C	511	CLA	C2B-C1B-NB	7.23	115.08	110.23
24	b	615	CLA	C2D-C1D-ND	7.18	115.39	110.10
24	B	607	CLA	C2B-C1B-NB	7.16	115.03	110.23
24	c	911	CLA	C2D-C1D-ND	7.14	115.37	110.10
24	b	608	CLA	C4A-NA-C1A	-7.14	103.50	106.71
24	a	406	CLA	C2B-C1B-NB	7.13	115.01	110.23
24	B	606	CLA	CHD-C4C-C3C	-7.13	114.36	124.84
24	d	406	CLA	C2B-C1B-NB	7.13	115.01	110.23
24	C	505	CLA	C2D-C1D-ND	7.12	115.35	110.10
24	C	509	CLA	C2B-C1B-NB	7.08	114.98	110.23
24	b	618	CLA	C2B-C1B-NB	7.08	114.98	110.23
24	B	606	CLA	C2B-C1B-NB	7.07	114.97	110.23
24	C	506	CLA	C2B-C1B-NB	7.07	114.97	110.23
24	B	616	CLA	C2B-C1B-NB	7.06	114.97	110.23
24	B	604	CLA	C2B-C1B-NB	7.06	114.97	110.23
24	c	904	CLA	C2B-C1B-NB	7.06	114.97	110.23
24	b	608	CLA	C2D-C1D-ND	7.05	115.30	110.10
24	B	615	CLA	C2B-C1B-NB	7.05	114.96	110.23
25	d	403	PHO	C2B-C1B-NB	7.04	114.39	109.53
24	B	607	CLA	C4A-NA-C1A	-7.03	103.54	106.71
24	b	612	CLA	C2D-C1D-ND	7.02	115.28	110.10
24	d	405	CLA	C2B-C1B-NB	7.02	114.94	110.23
24	d	404	CLA	C2B-C1B-NB	7.02	114.94	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	910	CLA	C2B-C1B-NB	7.01	114.93	110.23
24	B	617	CLA	C2B-C1B-NB	6.98	114.91	110.23
24	B	605	CLA	CMD-C2D-C1D	6.96	136.98	124.71
24	c	904	CLA	CMD-C2D-C1D	6.96	136.98	124.71
24	a	405	CLA	C2B-C1B-NB	6.93	114.88	110.23
24	b	610	CLA	CMD-C2D-C1D	6.91	136.90	124.71
24	B	607	CLA	CMD-C2D-C1D	6.91	136.90	124.71
24	c	903	CLA	C2B-C1B-NB	6.90	114.86	110.23
24	B	609	CLA	C2D-C1D-ND	6.90	115.19	110.10
24	b	609	CLA	C2D-C1D-ND	6.90	115.19	110.10
24	b	611	CLA	CMD-C2D-C1D	6.88	136.84	124.71
24	C	506	CLA	C2D-C1D-ND	6.86	115.16	110.10
24	b	612	CLA	C2B-C1B-NB	6.86	114.83	110.23
24	A	409	CLA	C2D-C1D-ND	6.85	115.16	110.10
35	d	414	HTG	C1'-S1-C1	6.85	112.91	100.09
35	C	521	HTG	C1'-S1-C1	6.85	112.91	100.09
24	b	607	CLA	CHD-C1D-ND	-6.84	118.16	124.45
24	b	606	CLA	O2D-CGD-CBD	6.83	123.40	111.27
24	B	617	CLA	CMD-C2D-C1D	6.83	136.74	124.71
24	c	905	CLA	C2B-C1B-NB	6.82	114.81	110.23
24	c	907	CLA	CMD-C2D-C1D	6.82	136.73	124.71
24	C	502	CLA	C2B-C1B-NB	6.82	114.80	110.23
24	B	610	CLA	C2B-C1B-NB	6.81	114.80	110.23
24	b	617	CLA	CHD-C4C-C3C	-6.81	114.84	124.84
24	b	612	CLA	CMD-C2D-C1D	6.80	136.69	124.71
24	D	404	CLA	C2B-C1B-NB	6.79	114.79	110.23
25	d	403	PHO	C4D-ND-C1D	-6.79	101.92	108.83
24	b	621	CLA	C2B-C1B-NB	6.79	114.78	110.23
24	b	614	CLA	C2B-C1B-NB	6.76	114.76	110.23
24	B	603	CLA	CMD-C2D-C1D	6.76	136.62	124.71
24	C	507	CLA	CMD-C2D-C1D	6.76	136.62	124.71
24	B	602	CLA	C2B-C1B-NB	6.76	114.76	110.23
24	a	406	CLA	CMD-C2D-C1D	6.74	136.59	124.71
24	B	607	CLA	CHD-C1D-ND	-6.73	118.27	124.45
24	b	617	CLA	C2B-C1B-NB	6.73	114.74	110.23
24	b	618	CLA	C2C-C1C-NC	6.72	116.27	109.97
24	b	609	CLA	CMD-C2D-C1D	6.71	136.54	124.71
24	b	615	CLA	C2B-C1B-NB	6.71	114.73	110.23
24	a	405	CLA	CMD-C2D-C1D	6.70	136.52	124.71
24	d	406	CLA	CMD-C2D-C1D	6.69	136.51	124.71
24	C	507	CLA	CHD-C4C-C3C	-6.69	115.00	124.84
24	B	611	CLA	CMD-C2D-C1D	6.68	136.49	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	407	PHO	C4D-ND-C1D	-6.67	102.05	108.83
24	c	906	CLA	C2D-C1D-ND	6.66	115.02	110.10
25	D	401	PHO	C4D-ND-C1D	-6.66	102.05	108.83
24	B	616	CLA	C4A-NA-C1A	-6.66	103.71	106.71
24	C	507	CLA	C2B-C1B-NB	6.65	114.69	110.23
24	B	612	CLA	C2B-C1B-NB	6.63	114.68	110.23
24	b	613	CLA	C2B-C1B-NB	6.63	114.68	110.23
24	c	912	CLA	CHD-C1D-ND	-6.62	118.37	124.45
24	b	610	CLA	CHD-C4C-C3C	-6.61	115.12	124.84
24	b	619	CLA	C2B-C1B-NB	6.61	114.66	110.23
24	D	405	CLA	CMD-C2D-C1D	6.61	136.36	124.71
24	c	909	CLA	C2B-C1B-NB	6.57	114.64	110.23
24	C	504	CLA	C2B-C1B-NB	6.56	114.63	110.23
24	a	405	CLA	CHD-C1D-ND	-6.55	118.43	124.45
24	B	612	CLA	CHD-C1D-ND	-6.55	118.44	124.45
24	b	610	CLA	C2B-C1B-NB	6.54	114.62	110.23
24	c	905	CLA	CMD-C2D-C1D	6.52	136.21	124.71
24	A	405	CLA	CMD-C2D-C1D	6.52	136.20	124.71
24	B	604	CLA	CHD-C4C-C3C	-6.52	115.26	124.84
24	D	404	CLA	CHD-C1D-ND	-6.52	118.47	124.45
24	B	602	CLA	CMD-C2D-C1D	6.52	136.20	124.71
24	b	620	CLA	CHD-C4C-C3C	-6.51	115.28	124.84
24	B	603	CLA	C4A-NA-C1A	-6.50	103.78	106.71
24	b	607	CLA	C4A-NA-C1A	-6.50	103.78	106.71
24	b	610	CLA	CHD-C1D-ND	-6.50	118.48	124.45
24	c	906	CLA	CHD-C4C-C3C	-6.49	115.30	124.84
24	c	914	CLA	CMD-C2D-C1D	6.46	136.10	124.71
24	C	503	CLA	CMD-C2D-C1D	6.45	136.08	124.71
24	D	404	CLA	CMD-C2D-C1D	6.44	136.07	124.71
24	c	914	CLA	CHD-C1D-ND	-6.43	118.54	124.45
24	c	907	CLA	C2B-C1B-NB	6.43	114.54	110.23
24	b	618	CLA	CMD-C2D-C1D	6.43	136.04	124.71
24	A	406	CLA	CHD-C4C-C3C	-6.42	115.41	124.84
24	c	911	CLA	C2B-C1B-NB	6.41	114.53	110.23
24	C	510	CLA	C2B-C1B-NB	6.40	114.52	110.23
24	A	407	CLA	CHD-C1D-ND	-6.40	118.57	124.45
24	B	617	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
24	b	614	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
24	C	510	CLA	CMD-C2D-C1D	6.39	135.97	124.71
24	a	406	CLA	CHD-C1D-ND	-6.38	118.59	124.45
24	c	902	CLA	CMD-C2D-C1D	6.38	135.95	124.71
24	c	906	CLA	C2B-C1B-NB	6.37	114.50	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	PHO	C4D-ND-C1D	-6.37	102.35	108.83
24	c	904	CLA	CHD-C4C-C3C	-6.37	115.48	124.84
24	b	615	CLA	CMD-C2D-C1D	6.35	135.91	124.71
24	B	602	CLA	CHD-C4C-C3C	-6.35	115.51	124.84
24	c	908	CLA	CHD-C4C-C3C	-6.35	115.51	124.84
24	C	504	CLA	O2D-CGD-CBD	6.35	122.54	111.27
24	c	903	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
24	A	409	CLA	C4A-NA-C1A	-6.34	103.86	106.71
25	D	401	PHO	C2B-C1B-NB	6.32	113.89	109.53
24	B	605	CLA	C2C-C1C-NC	6.32	115.90	109.97
24	b	614	CLA	CHD-C1D-ND	-6.32	118.65	124.45
24	b	613	CLA	C4A-NA-C1A	-6.31	103.87	106.71
24	D	405	CLA	CHD-C1D-ND	-6.31	118.66	124.45
24	C	503	CLA	CHD-C4C-C3C	-6.31	115.57	124.84
24	c	910	CLA	CMD-C2D-C1D	6.30	135.81	124.71
24	B	614	CLA	CMD-C2D-C1D	6.30	135.81	124.71
25	D	401	PHO	O2D-CGD-CBD	6.29	118.97	111.00
24	B	603	CLA	CHD-C4C-C3C	-6.29	115.59	124.84
25	a	407	PHO	C1C-C2C-C3C	-6.29	103.38	108.61
24	C	508	CLA	CHD-C1D-ND	-6.28	118.68	124.45
24	d	405	CLA	CHD-C1D-ND	-6.28	118.68	124.45
25	a	407	PHO	C2B-C1B-NB	6.28	113.86	109.53
24	B	611	CLA	CHD-C1D-ND	-6.27	118.69	124.45
24	c	908	CLA	C2B-C1B-NB	6.27	114.44	110.23
24	B	612	CLA	CHD-C4C-C3C	-6.26	115.63	124.84
24	C	506	CLA	CMD-C2D-C1D	6.26	135.75	124.71
24	b	619	CLA	CMD-C2D-C1D	6.24	135.72	124.71
24	C	506	CLA	CHD-C1D-ND	-6.24	118.72	124.45
24	b	609	CLA	C4A-NA-C1A	-6.23	103.90	106.71
24	b	620	CLA	C2B-C1B-NB	6.22	114.40	110.23
24	c	912	CLA	CMD-C2D-C1D	6.21	135.66	124.71
24	c	910	CLA	CHD-C4C-C3C	-6.21	115.71	124.84
24	C	501	CLA	O2D-CGD-CBD	6.21	122.30	111.27
24	d	406	CLA	CHD-C4C-C3C	-6.20	115.73	124.84
24	C	508	CLA	C4A-NA-C1A	-6.20	103.92	106.71
24	c	905	CLA	CHD-C1D-ND	-6.20	118.76	124.45
24	b	609	CLA	C2C-C1C-NC	6.20	115.78	109.97
24	b	608	CLA	CMD-C2D-C1D	6.19	135.63	124.71
24	b	611	CLA	CHD-C4C-C3C	-6.19	115.74	124.84
24	C	501	CLA	CMD-C2D-C1D	6.19	135.63	124.71
24	c	902	CLA	C2C-C1C-NC	6.19	115.77	109.97
24	C	505	CLA	CHD-C4C-C3C	-6.19	115.74	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	617	CLA	O2D-CGD-CBD	6.18	122.26	111.27
24	b	616	CLA	C2C-C1C-NC	6.18	115.76	109.97
24	b	620	CLA	CMD-C2D-C1D	6.18	135.60	124.71
24	a	408	CLA	CHD-C4C-C3C	-6.16	115.78	124.84
24	b	606	CLA	CHD-C4C-C3C	-6.16	115.78	124.84
24	C	505	CLA	C4A-NA-C1A	-6.16	103.94	106.71
24	c	902	CLA	C2B-C1B-NB	6.15	114.36	110.23
24	c	912	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
24	B	615	CLA	CMD-C2D-C1D	6.15	135.55	124.71
24	c	908	CLA	O2D-CGD-CBD	6.14	122.19	111.27
24	C	509	CLA	CMD-C2D-C1D	6.14	135.53	124.71
24	C	513	CLA	CHD-C1D-ND	-6.13	118.82	124.45
35	c	921	HTG	C1'-S1-C1	6.12	111.54	100.09
24	B	616	CLA	CHD-C4C-C3C	-6.12	115.85	124.84
24	d	404	CLA	CHD-C1D-ND	-6.11	118.83	124.45
24	B	606	CLA	CMD-C2D-C1D	6.11	135.48	124.71
24	A	409	CLA	CMD-C2D-C1D	6.11	135.48	124.71
24	C	504	CLA	CMD-C2D-C1D	6.11	135.48	124.71
24	b	611	CLA	CHD-C1D-ND	-6.11	118.84	124.45
24	c	913	CLA	CHD-C1D-ND	-6.11	118.84	124.45
24	c	904	CLA	CHD-C1D-ND	-6.10	118.85	124.45
24	a	406	CLA	CHD-C4C-C3C	-6.10	115.88	124.84
24	c	913	CLA	O2D-CGD-CBD	6.09	122.09	111.27
24	c	911	CLA	CMD-C2D-C1D	6.09	135.44	124.71
24	B	613	CLA	CHD-C4C-C3C	-6.08	115.91	124.84
24	d	406	CLA	CHD-C1D-ND	-6.07	118.87	124.45
24	B	608	CLA	CMD-C2D-C1D	6.07	135.41	124.71
24	b	614	CLA	C4A-NA-C1A	-6.05	103.98	106.71
24	c	911	CLA	C2C-C1C-NC	6.05	115.64	109.97
35	D	413	HTG	C1'-S1-C1	6.05	111.40	100.09
24	B	612	CLA	CMD-C2D-C1D	6.04	135.36	124.71
24	b	620	CLA	C4A-NA-C1A	-6.04	103.99	106.71
24	C	502	CLA	CMD-C2D-C1D	6.03	135.35	124.71
24	c	913	CLA	C4A-NA-C1A	-6.02	104.00	106.71
24	c	907	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
24	C	512	CLA	CHD-C4C-C3C	-6.02	116.00	124.84
24	b	616	CLA	CHD-C4C-C3C	-6.02	116.00	124.84
24	B	616	CLA	CMD-C2D-C1D	6.02	135.31	124.71
24	c	913	CLA	CMD-C2D-C1D	6.01	135.30	124.71
24	d	405	CLA	CMD-C2D-C1D	6.01	135.30	124.71
24	A	406	CLA	CMD-C2D-C1D	6.00	135.29	124.71
24	C	501	CLA	CHD-C1D-ND	-6.00	118.94	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	C4A-NA-C1A	-6.00	104.01	106.71
24	b	621	CLA	CHD-C4C-C3C	-6.00	116.03	124.84
24	C	513	CLA	CMD-C2D-C1D	5.99	135.28	124.71
24	c	902	CLA	CHD-C1D-ND	-5.99	118.95	124.45
24	B	612	CLA	C4A-NA-C1A	-5.99	104.02	106.71
24	C	504	CLA	CHD-C1D-ND	-5.98	118.95	124.45
24	c	909	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
24	B	602	CLA	CHD-C1D-ND	-5.98	118.96	124.45
24	d	406	CLA	C4A-NA-C1A	-5.97	104.02	106.71
24	a	405	CLA	C2C-C1C-NC	5.96	115.55	109.97
25	A	408	PHO	C1C-C2C-C3C	-5.95	103.66	108.61
24	c	913	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
24	B	605	CLA	C2B-C1B-NB	5.95	114.22	110.23
24	C	504	CLA	C4A-NA-C1A	-5.94	104.03	106.71
24	b	619	CLA	CHD-C1D-ND	-5.94	119.00	124.45
24	C	510	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
24	b	606	CLA	CHD-C1D-ND	-5.94	119.00	124.45
24	a	408	CLA	CHD-C1D-ND	-5.93	119.00	124.45
24	b	619	CLA	CHD-C4C-C3C	-5.93	116.13	124.84
24	C	507	CLA	CHD-C1D-ND	-5.93	119.01	124.45
24	b	608	CLA	CHD-C1D-ND	-5.91	119.02	124.45
24	c	909	CLA	C2C-C1C-NC	5.91	115.51	109.97
24	b	614	CLA	CMD-C2D-C1D	5.91	135.13	124.71
24	b	606	CLA	CMD-C2D-C1D	5.91	135.13	124.71
24	B	610	CLA	C4A-NA-C1A	-5.91	104.05	106.71
24	B	607	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
24	D	404	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
24	B	602	CLA	O2D-CGD-CBD	5.89	121.74	111.27
24	D	404	CLA	C2C-C1C-NC	5.89	115.49	109.97
24	B	608	CLA	CHD-C1D-ND	-5.88	119.05	124.45
24	B	603	CLA	CHD-C1D-ND	-5.88	119.05	124.45
24	c	914	CLA	CHD-C4C-C3C	-5.87	116.20	124.84
24	B	604	CLA	CHD-C1D-ND	-5.85	119.07	124.45
24	d	404	CLA	C2C-C1C-NC	5.85	115.45	109.97
24	D	404	CLA	C4A-NA-C1A	-5.85	104.08	106.71
24	b	616	CLA	C2B-C1B-NB	5.84	114.15	110.23
24	C	509	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
24	b	609	CLA	O2D-CGD-CBD	5.84	121.65	111.27
24	B	615	CLA	CHD-C1D-ND	-5.84	119.08	124.45
24	C	513	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
24	C	505	CLA	C2B-C1B-NB	5.83	114.14	110.23
24	b	609	CLA	C2B-C1B-NB	5.83	114.14	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	CHD-C1D-ND	-5.82	119.11	124.45
24	C	506	CLA	C4A-NA-C1A	-5.81	104.09	106.71
24	b	609	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
24	c	908	CLA	CMD-C2D-C1D	5.81	134.95	124.71
24	c	907	CLA	CHD-C1D-ND	-5.81	119.12	124.45
24	B	614	CLA	C2C-C1C-NC	5.80	115.41	109.97
24	C	502	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
26	D	406	BCR	C7-C8-C9	-5.80	117.47	126.23
24	c	905	CLA	CHD-C4C-C3C	-5.80	116.32	124.84
24	b	612	CLA	CHD-C1D-ND	-5.80	119.12	124.45
24	b	612	CLA	CHD-C4C-C3C	-5.80	116.32	124.84
24	b	621	CLA	C4A-NA-C1A	-5.79	104.10	106.71
24	c	906	CLA	C2C-C1C-NC	5.79	115.39	109.97
24	B	613	CLA	O2D-CGD-CBD	5.78	121.55	111.27
24	B	616	CLA	CHD-C1D-ND	-5.77	119.15	124.45
24	B	610	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
24	C	508	CLA	CMD-C2D-C1D	5.77	134.88	124.71
24	A	405	CLA	CHD-C1D-ND	-5.76	119.16	124.45
24	b	611	CLA	C2C-C1C-NC	5.76	115.36	109.97
25	A	408	PHO	C2B-C1B-NB	5.75	113.50	109.53
24	C	505	CLA	CMD-C2D-C1D	5.75	134.85	124.71
24	C	511	CLA	CMD-C2D-C1D	5.75	134.84	124.71
24	A	405	CLA	C2C-C1C-NC	5.75	115.36	109.97
24	d	404	CLA	CMD-C2D-C1D	5.74	134.83	124.71
24	b	607	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
24	D	405	CLA	C4A-NA-C1A	-5.73	104.13	106.71
24	b	619	CLA	O2D-CGD-CBD	5.72	121.42	111.27
24	b	606	CLA	C4A-NA-C1A	-5.71	104.14	106.71
24	C	503	CLA	CHD-C1D-ND	-5.71	119.20	124.45
24	C	512	CLA	CMD-C2D-C1D	5.71	134.78	124.71
24	b	621	CLA	O2D-CGD-CBD	5.71	121.42	111.27
24	B	605	CLA	CHD-C1D-ND	-5.71	119.21	124.45
24	b	616	CLA	CMD-C2D-C1D	5.70	134.76	124.71
24	B	605	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
24	d	405	CLA	C2C-C1C-NC	5.66	115.28	109.97
24	c	908	CLA	C2C-C1C-NC	5.66	115.27	109.97
24	c	907	CLA	C2C-C1C-NC	5.66	115.27	109.97
24	B	611	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
24	A	406	CLA	C2C-C1C-NC	5.63	115.25	109.97
24	C	506	CLA	C2C-C1C-NC	5.63	115.25	109.97
24	C	512	CLA	CHD-C1D-ND	-5.63	119.28	124.45
24	B	605	CLA	O2D-CGD-CBD	5.63	121.27	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	501	CLA	C4A-NA-C1A	-5.62	104.18	106.71
24	a	408	CLA	CMD-C2D-C1D	5.62	134.61	124.71
24	B	604	CLA	CMD-C2D-C1D	5.61	134.60	124.71
24	c	911	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
24	C	504	CLA	C2C-C1C-NC	5.60	115.22	109.97
35	B	624	HTG	C1'-S1-C1	5.60	110.56	100.09
24	C	507	CLA	O2D-CGD-CBD	5.60	121.21	111.27
24	C	505	CLA	C2C-C1C-NC	5.60	115.22	109.97
24	B	608	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
24	b	620	CLA	CHD-C1D-ND	-5.59	119.31	124.45
24	B	609	CLA	CMD-C2D-C1D	5.59	134.57	124.71
24	C	509	CLA	C4A-NA-C1A	-5.59	104.19	106.71
24	B	614	CLA	CHD-C4C-C3C	-5.59	116.63	124.84
24	B	606	CLA	C4A-NA-C1A	-5.59	104.19	106.71
24	C	502	CLA	CHD-C1D-ND	-5.58	119.32	124.45
24	B	611	CLA	C2C-C1C-NC	5.58	115.20	109.97
24	b	618	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
24	B	609	CLA	CHD-C1D-ND	-5.56	119.34	124.45
24	b	610	CLA	O2D-CGD-CBD	5.56	121.14	111.27
27	f	102	SQD	O47-C7-C8	5.56	123.48	111.50
24	b	615	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
24	d	404	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
25	D	401	PHO	C1C-C2C-C3C	-5.55	104.00	108.61
24	C	510	CLA	O2D-CGD-CBD	5.54	121.11	111.27
24	c	909	CLA	O2D-CGD-CBD	5.53	121.10	111.27
24	b	615	CLA	CHD-C1D-ND	-5.53	119.37	124.45
38	F	102	HEM	CHC-C4B-NB	5.53	130.43	124.42
24	b	612	CLA	C2C-C1C-NC	5.53	115.15	109.97
24	B	603	CLA	O2D-CGD-CBD	5.53	121.09	111.27
24	b	618	CLA	C4A-NA-C1A	-5.52	104.22	106.71
24	B	612	CLA	O2D-CGD-CBD	5.51	121.06	111.27
24	a	406	CLA	C4A-NA-C1A	-5.51	104.23	106.71
24	b	608	CLA	O2D-CGD-CBD	5.50	121.05	111.27
24	b	610	CLA	C4A-NA-C1A	-5.50	104.23	106.71
24	b	615	CLA	C4A-NA-C1A	-5.50	104.23	106.71
24	B	612	CLA	C2C-C1C-NC	5.49	115.11	109.97
24	B	610	CLA	CHD-C1D-ND	-5.49	119.41	124.45
24	B	615	CLA	C2C-C1C-NC	5.48	115.11	109.97
24	B	615	CLA	O2D-CGD-CBD	5.47	120.99	111.27
24	c	914	CLA	C4A-NA-C1A	-5.47	104.25	106.71
24	B	606	CLA	CHD-C1D-ND	-5.47	119.43	124.45
24	b	608	CLA	C2C-C1C-NC	5.45	115.08	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	614	CLA	C4A-NA-C1A	-5.45	104.25	106.71
24	C	501	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
35	B	633	HTG	C1'-S1-C1	5.45	110.28	100.09
25	d	403	PHO	C1C-C2C-C3C	-5.45	104.08	108.61
24	C	511	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
24	c	902	CLA	O2D-CGD-CBD	5.44	120.94	111.27
24	C	510	CLA	CHD-C1D-ND	-5.43	119.46	124.45
24	B	609	CLA	C2C-C1C-NC	5.43	115.06	109.97
25	d	403	PHO	C1-C2-C3	-5.43	116.65	126.04
24	b	613	CLA	CMD-C2D-C1D	5.43	134.28	124.71
24	c	910	CLA	C2C-C1C-NC	5.43	115.06	109.97
24	c	906	CLA	CMD-C2D-C1D	5.43	134.28	124.71
24	c	903	CLA	CHD-C1D-ND	-5.42	119.47	124.45
24	b	613	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
24	d	405	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
24	c	910	CLA	O2D-CGD-CBD	5.41	120.88	111.27
24	B	615	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
24	B	604	CLA	O2D-CGD-CBD	5.40	120.86	111.27
24	B	613	CLA	CHD-C1D-ND	-5.40	119.49	124.45
24	B	610	CLA	C2C-C1C-NC	5.40	115.03	109.97
24	B	608	CLA	C2C-C1C-NC	5.38	115.01	109.97
24	a	406	CLA	O2D-CGD-CBD	5.38	120.83	111.27
24	B	609	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
24	b	611	CLA	C4A-NA-C1A	-5.36	104.30	106.71
24	A	407	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
24	c	906	CLA	C4A-NA-C1A	-5.36	104.30	106.71
24	B	610	CLA	CMD-C2D-C1D	5.36	134.15	124.71
24	A	407	CLA	CMD-C2D-C1D	5.35	134.15	124.71
24	b	621	CLA	CMD-C2D-C1D	5.34	134.13	124.71
24	B	613	CLA	CMD-C2D-C1D	5.33	134.10	124.71
24	B	614	CLA	CHD-C1D-ND	-5.32	119.56	124.45
24	d	404	CLA	C4A-NA-C1A	-5.31	104.32	106.71
24	B	617	CLA	CHD-C1D-ND	-5.31	119.58	124.45
24	B	613	CLA	C2C-C1C-NC	5.30	114.94	109.97
24	b	616	CLA	CHD-C1D-ND	-5.30	119.58	124.45
24	c	909	CLA	CMD-C2D-C1D	5.30	134.05	124.71
24	C	504	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
24	A	407	CLA	O2D-CGD-CBD	5.29	120.68	111.27
24	c	912	CLA	C4A-NA-C1A	-5.28	104.33	106.71
24	C	503	CLA	O2D-CGD-CBD	5.28	120.66	111.27
24	C	508	CLA	C2C-C1C-NC	5.28	114.92	109.97
24	b	608	CLA	CHD-C4C-C3C	-5.27	117.10	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	609	CLA	CHD-C1D-ND	-5.26	119.62	124.45
35	C	522	HTG	C1'-S1-C1	5.26	109.93	100.09
24	B	607	CLA	O2D-CGD-CBD	5.25	120.59	111.27
24	C	508	CLA	O2D-CGD-CBD	5.25	120.59	111.27
24	C	510	CLA	C2C-C1C-NC	5.25	114.89	109.97
24	A	409	CLA	CHD-C1D-ND	-5.24	119.64	124.45
24	c	911	CLA	O2D-CGD-CBD	5.24	120.58	111.27
24	c	906	CLA	C3C-C4C-NC	5.24	116.45	110.57
27	L	102	SQD	O6-C1-C2	5.23	116.48	108.30
24	c	903	CLA	CMD-C2D-C1D	5.23	133.94	124.71
35	b	627	HTG	C1'-S1-C1	5.23	109.88	100.09
24	C	501	CLA	C2C-C1C-NC	5.23	114.87	109.97
24	b	621	CLA	CHD-C1D-ND	-5.23	119.65	124.45
24	C	508	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
24	c	908	CLA	CHD-C1D-ND	-5.23	119.65	124.45
24	b	619	CLA	C3D-C2D-C1D	-5.22	98.70	105.83
24	C	512	CLA	O2D-CGD-CBD	5.20	120.51	111.27
24	C	509	CLA	CHD-C1D-ND	-5.20	119.68	124.45
24	b	614	CLA	O2D-CGD-CBD	5.20	120.50	111.27
24	c	905	CLA	O2D-CGD-CBD	5.20	120.50	111.27
24	a	405	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
24	C	513	CLA	C2C-C1C-NC	5.19	114.83	109.97
24	B	617	CLA	C4A-NA-C1A	-5.18	104.38	106.71
27	a	410	SQD	O6-C1-C2	5.18	116.39	108.30
24	B	608	CLA	C2B-C1B-NB	5.18	113.70	110.23
24	b	620	CLA	C2C-C1C-NC	5.18	114.82	109.97
26	Y	102	BCR	C33-C5-C6	-5.17	118.72	124.53
24	b	617	CLA	C3C-C4C-NC	5.17	116.37	110.57
24	b	613	CLA	C2C-C1C-NC	5.16	114.81	109.97
24	B	609	CLA	C4A-NA-C1A	-5.16	104.39	106.71
24	B	605	CLA	C3D-C2D-C1D	-5.16	98.80	105.83
24	B	611	CLA	C3B-C2B-C1B	-5.15	100.95	107.16
24	C	505	CLA	O2D-CGD-CBD	5.14	120.41	111.27
24	D	405	CLA	C2C-C1C-NC	5.14	114.78	109.97
24	C	511	CLA	CHD-C1D-ND	-5.14	119.73	124.45
24	b	613	CLA	CHD-C1D-ND	-5.14	119.73	124.45
24	c	913	CLA	C3B-C2B-C1B	-5.13	100.97	107.16
24	c	911	CLA	CHD-C1D-ND	-5.13	119.74	124.45
24	c	904	CLA	C4A-NA-C1A	-5.13	104.40	106.71
29	A	415	LMT	C1'-O5'-C5'	5.13	123.75	113.69
24	A	406	CLA	C3B-C2B-C1B	-5.13	100.97	107.16
24	D	404	CLA	C3D-C2D-C1D	-5.12	98.84	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	509	CLA	C2C-C1C-NC	5.12	114.77	109.97
24	c	909	CLA	CHD-C1D-ND	-5.12	119.75	124.45
24	A	409	CLA	CHD-C4C-C3C	-5.12	117.32	124.84
24	c	905	CLA	C4A-NA-C1A	-5.12	104.41	106.71
24	B	603	CLA	C2C-C1C-NC	5.11	114.75	109.97
24	b	607	CLA	O2D-CGD-CBD	5.10	120.33	111.27
24	B	608	CLA	O2D-CGD-CBD	5.09	120.32	111.27
24	d	405	CLA	O2D-CGD-CBD	5.09	120.32	111.27
24	b	611	CLA	O2D-CGD-CBD	5.09	120.31	111.27
24	D	405	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
24	a	405	CLA	C4A-NA-C1A	-5.08	104.42	106.71
25	D	401	PHO	C1-C2-C3	-5.07	117.27	126.04
27	F	103	SQD	O47-C7-C8	5.07	122.43	111.50
24	A	409	CLA	C3B-C2B-C1B	-5.06	101.05	107.16
24	c	913	CLA	C2C-C1C-NC	5.06	114.71	109.97
24	A	406	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
24	B	604	CLA	C4A-NA-C1A	-5.06	104.43	106.71
24	b	619	CLA	C4A-NA-C1A	-5.05	104.44	106.71
24	C	512	CLA	C2C-C1C-NC	5.04	114.69	109.97
24	C	511	CLA	C2C-C1C-NC	5.04	114.69	109.97
24	b	612	CLA	C4A-NA-C1A	-5.03	104.44	106.71
25	A	408	PHO	C3D-C4D-ND	5.03	114.58	107.72
24	c	908	CLA	C3B-C2B-C1B	-5.03	101.09	107.16
25	a	407	PHO	C3D-C4D-ND	5.03	114.58	107.72
35	B	625	HTG	C1'-S1-C1	5.03	109.49	100.09
24	A	405	CLA	CHD-C4C-C3C	-5.02	117.46	124.84
24	b	610	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
24	B	613	CLA	C2B-C1B-NB	5.02	113.60	110.23
24	C	507	CLA	C4A-NA-C1A	-5.01	104.45	106.71
24	b	615	CLA	C2C-C1C-NC	5.01	114.66	109.97
24	c	910	CLA	C4A-NA-C1A	-5.00	104.46	106.71
24	c	906	CLA	O2D-CGD-CBD	5.00	120.15	111.27
24	C	505	CLA	C3C-C4C-NC	5.00	116.18	110.57
24	B	607	CLA	C2C-C1C-NC	4.99	114.65	109.97
24	a	408	CLA	C4A-NA-C1A	-4.99	104.46	106.71
24	D	405	CLA	O2D-CGD-CBD	4.99	120.14	111.27
24	c	912	CLA	C3B-C2B-C1B	-4.99	101.14	107.16
35	b	603	HTG	C1'-S1-C1	4.98	109.41	100.09
24	C	512	CLA	C4A-NA-C1A	-4.97	104.47	106.71
24	b	616	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
24	c	905	CLA	C2C-C1C-NC	4.96	114.62	109.97
24	C	503	CLA	C2C-C1C-NC	4.96	114.61	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	c	922	HTG	C1'-S1-C1	4.95	109.35	100.09
35	b	628	HTG	C1'-S1-C1	4.95	109.35	100.09
24	C	509	CLA	C1-C2-C3	-4.95	117.48	126.04
24	C	502	CLA	C2C-C1C-NC	4.95	114.61	109.97
24	B	604	CLA	C2C-C1C-NC	4.95	114.61	109.97
24	A	406	CLA	O2D-CGD-CBD	4.94	120.05	111.27
27	A	411	SQD	O47-C7-C8	4.94	122.15	111.50
24	c	903	CLA	C3B-C2B-C1B	-4.94	101.20	107.16
24	C	513	CLA	C3B-C2B-C1B	-4.93	101.21	107.16
24	B	611	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
24	c	910	CLA	CHD-C1D-ND	-4.92	119.93	124.45
24	B	616	CLA	C2C-C1C-NC	4.91	114.57	109.97
24	B	617	CLA	C3B-C2B-C1B	-4.91	101.24	107.16
40	V	202	HEC	C4B-NB-C1B	4.91	110.14	105.07
24	b	619	CLA	C2C-C1C-NC	4.90	114.57	109.97
24	c	905	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
24	A	406	CLA	C4A-NA-C1A	-4.90	104.50	106.71
24	c	907	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
24	C	509	CLA	C3B-C2B-C1B	-4.90	101.25	107.16
36	D	410	LHG	O7-C7-C8	4.89	122.04	111.50
25	D	401	PHO	C3D-C4D-ND	4.88	114.37	107.72
35	B	632	HTG	C1'-S1-C1	4.88	109.21	100.09
24	b	613	CLA	O2D-CGD-CBD	4.87	119.93	111.27
24	c	904	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
24	a	408	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
24	b	607	CLA	C3B-C2B-C1B	-4.86	101.30	107.16
24	c	908	CLA	C3C-C4C-NC	4.86	116.02	110.57
24	b	611	CLA	C3B-C2B-C1B	-4.86	101.30	107.16
24	C	510	CLA	C4A-NA-C1A	-4.86	104.52	106.71
24	C	506	CLA	O2D-CGD-CBD	4.85	119.89	111.27
24	d	406	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
24	b	617	CLA	C2C-C1C-NC	4.84	114.51	109.97
24	A	407	CLA	C4A-NA-C1A	-4.84	104.53	106.71
24	c	911	CLA	C1-C2-C3	-4.83	117.68	126.04
24	b	617	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
24	C	504	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
24	c	914	CLA	C3D-C4D-ND	4.82	118.04	110.24
24	B	617	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
24	c	904	CLA	C3B-C2B-C1B	-4.82	101.35	107.16
24	c	903	CLA	C2C-C1C-NC	4.81	114.48	109.97
24	B	614	CLA	C3B-C2B-C1B	-4.81	101.36	107.16
24	C	513	CLA	C4A-NA-C1A	-4.81	104.55	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	405	CLA	C3D-C4D-ND	4.81	118.01	110.24
24	B	606	CLA	C2C-C1C-NC	4.80	114.47	109.97
24	B	613	CLA	C3C-C4C-NC	4.80	115.96	110.57
24	c	914	CLA	C2C-C1C-NC	4.80	114.47	109.97
24	b	618	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
24	B	614	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
24	B	602	CLA	C2C-C1C-NC	4.79	114.46	109.97
24	b	610	CLA	C2C-C1C-NC	4.79	114.46	109.97
24	B	606	CLA	C3B-C2B-C1B	-4.79	101.38	107.16
24	C	503	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
24	C	506	CLA	CHD-C4C-C3C	-4.78	117.81	124.84
24	b	619	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
24	B	613	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
24	b	614	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
24	c	909	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
24	C	509	CLA	O2D-CGD-CBD	4.77	119.75	111.27
27	L	102	SQD	O47-C7-C8	4.76	121.76	111.50
24	C	507	CLA	C3B-C2B-C1B	-4.76	101.41	107.16
24	B	603	CLA	C3B-C2B-C1B	-4.76	101.41	107.16
24	A	407	CLA	C3D-C4D-ND	4.76	117.94	110.24
24	B	617	CLA	C2C-C1C-NC	4.75	114.42	109.97
24	b	614	CLA	C2C-C1C-NC	4.75	114.42	109.97
24	C	507	CLA	C3D-C2D-C1D	-4.75	99.36	105.83
24	b	621	CLA	C2C-C1C-NC	4.74	114.42	109.97
24	c	902	CLA	CHD-C4C-C3C	-4.74	117.87	124.84
24	B	602	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
24	B	606	CLA	C3C-C4C-NC	4.74	115.89	110.57
27	B	621	SQD	O47-C7-C8	4.74	121.71	111.50
24	b	606	CLA	C2C-C1C-NC	4.74	114.41	109.97
24	B	609	CLA	O2D-CGD-CBD	4.73	119.68	111.27
24	d	406	CLA	C2C-C1C-NC	4.73	114.40	109.97
24	c	914	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
24	c	910	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
24	c	902	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
24	d	404	CLA	C1C-C2C-C3C	-4.70	102.01	106.96
24	b	609	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
24	d	404	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
24	D	405	CLA	C3B-C2B-C1B	-4.70	101.49	107.16
24	a	408	CLA	C2C-C1C-NC	4.70	114.37	109.97
24	A	407	CLA	C2C-C1C-NC	4.70	114.37	109.97
24	b	612	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
24	a	408	CLA	C3D-C2D-C1D	-4.70	99.42	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	512	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
37	e	101	DGD	O2G-C1B-C2B	4.69	121.61	111.50
24	B	615	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
24	A	409	CLA	C2C-C1C-NC	4.68	114.36	109.97
24	A	405	CLA	C3D-C4D-ND	4.68	117.81	110.24
24	C	502	CLA	C4A-NA-C1A	-4.68	104.60	106.71
24	c	905	CLA	C3B-C2B-C1B	-4.68	101.51	107.16
24	C	511	CLA	C3B-C2B-C1B	-4.68	101.51	107.16
24	D	405	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
27	B	621	SQD	O7-S-C6	4.68	112.50	106.94
27	a	410	SQD	O47-C7-C8	4.67	121.57	111.50
24	c	902	CLA	C4A-NA-C1A	-4.67	104.61	106.71
24	B	609	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
24	c	912	CLA	C3D-C4D-ND	4.66	117.78	110.24
24	b	611	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
24	B	608	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
24	B	615	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
24	b	616	CLA	C3C-C4C-NC	4.66	115.80	110.57
37	C	516	DGD	O2G-C1B-C2B	4.66	121.53	111.50
24	b	607	CLA	C2C-C1C-NC	4.65	114.33	109.97
24	B	609	CLA	C3D-C4D-ND	4.64	117.75	110.24
24	b	618	CLA	C3C-C4C-NC	4.64	115.78	110.57
24	b	607	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
24	d	404	CLA	C3B-C2B-C1B	-4.64	101.56	107.16
24	b	620	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
24	C	507	CLA	C3C-C4C-NC	4.64	115.77	110.57
24	b	609	CLA	C3C-C4C-NC	4.63	115.77	110.57
24	d	406	CLA	C3B-C2B-C1B	-4.63	101.57	107.16
24	B	612	CLA	C3D-C4D-ND	4.63	117.73	110.24
24	B	616	CLA	C3B-C2B-C1B	-4.63	101.57	107.16
24	B	604	CLA	C3D-C4D-ND	4.63	117.72	110.24
24	B	611	CLA	C4A-NA-C1A	-4.62	104.63	106.71
24	B	607	CLA	C3B-C2B-C1B	-4.62	101.59	107.16
24	a	406	CLA	C3D-C4D-ND	4.61	117.70	110.24
24	a	408	CLA	O2D-CGD-CBD	4.61	119.47	111.27
26	t	102	BCR	C33-C5-C6	-4.61	119.35	124.53
24	c	908	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
24	B	606	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
24	b	614	CLA	C3D-C4D-ND	4.61	117.69	110.24
27	B	621	SQD	O6-C1-C2	4.60	115.49	108.30
24	b	621	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
24	B	606	CLA	O2D-CGD-CBD	4.60	119.44	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	612	CLA	O2D-CGD-CBD	4.60	119.43	111.27
24	C	513	CLA	C3D-C4D-ND	4.59	117.67	110.24
24	d	406	CLA	O2D-CGD-CBD	4.59	119.42	111.27
24	a	406	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
24	b	617	CLA	CHD-C1D-ND	-4.59	120.24	124.45
29	A	415	LMT	O5'-C5'-C4'	4.59	119.42	109.75
27	A	411	SQD	O6-C1-C2	4.58	115.46	108.30
24	C	502	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
24	b	608	CLA	C3D-C4D-ND	4.58	117.64	110.24
24	B	610	CLA	C3D-C2D-C1D	-4.58	99.59	105.83
24	C	508	CLA	C3B-C2B-C1B	-4.57	101.64	107.16
24	C	511	CLA	CAC-C3C-C4C	4.57	130.74	124.81
24	d	405	CLA	C3B-C2B-C1B	-4.57	101.65	107.16
33	a	411	LMG	O7-C10-C11	4.57	121.34	111.50
37	e	101	DGD	O6E-C5E-C4E	4.57	117.99	109.69
25	d	403	PHO	C3D-C4D-ND	4.57	113.94	107.72
24	c	904	CLA	C2C-C1C-NC	4.56	114.25	109.97
26	B	618	BCR	C33-C5-C6	-4.56	119.40	124.53
24	b	621	CLA	CAC-C3C-C4C	4.56	130.72	124.81
24	B	605	CLA	C3C-C4C-NC	4.56	115.68	110.57
24	B	616	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
24	c	904	CLA	C3C-C4C-NC	4.56	115.68	110.57
24	A	405	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
24	c	910	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
38	f	101	HEM	CHC-C4B-NB	4.55	129.36	124.42
24	B	612	CLA	C3C-C4C-NC	4.55	115.67	110.57
24	C	510	CLA	C1-C2-C3	-4.55	118.18	126.04
24	C	502	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
24	b	610	CLA	C3D-C4D-ND	4.54	117.58	110.24
24	b	618	CLA	C3B-C2B-C1B	-4.53	101.69	107.16
24	b	607	CLA	C3D-C4D-ND	4.53	117.56	110.24
24	B	607	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	B	604	CLA	C3B-C2B-C1B	-4.52	101.70	107.16
24	b	616	CLA	O2D-CGD-CBD	4.52	119.30	111.27
24	c	902	CLA	C3B-C2B-C1B	-4.52	101.71	107.16
24	b	621	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
24	C	507	CLA	C2C-C1C-NC	4.52	114.20	109.97
38	F	102	HEM	CAD-CBD-CGD	4.52	123.32	113.60
24	B	605	CLA	C3B-C4B-NB	4.52	114.70	110.52
24	B	615	CLA	C3D-C4D-ND	4.51	117.54	110.24
24	C	511	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
24	c	903	CLA	C4A-NA-C1A	-4.50	104.68	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	914	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
24	b	610	CLA	C3C-C4C-NC	4.49	115.61	110.57
24	C	512	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
24	a	408	CLA	C3D-C4D-ND	4.49	117.50	110.24
24	c	913	CLA	C3D-C4D-ND	4.49	117.50	110.24
33	c	920	LMG	O7-C10-C11	4.49	121.17	111.50
37	c	918	DGD	O2G-C1B-C2B	4.49	121.17	111.50
24	b	618	CLA	C3B-C4B-NB	4.49	114.68	110.52
24	C	508	CLA	C3D-C4D-ND	4.48	117.49	110.24
24	C	501	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
24	C	503	CLA	C1D-CHD-C4C	-4.48	116.40	126.06
26	b	622	BCR	C15-C14-C13	-4.48	120.92	127.31
24	b	615	CLA	C3D-C4D-ND	4.47	117.48	110.24
24	A	407	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
24	b	613	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
24	D	404	CLA	C3D-C4D-ND	4.47	117.46	110.24
24	A	407	CLA	C3B-C2B-C1B	-4.46	101.77	107.16
24	C	513	CLA	O2D-CGD-CBD	4.46	119.20	111.27
24	b	606	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
24	C	511	CLA	O2D-CGD-CBD	4.46	119.19	111.27
24	b	617	CLA	O2D-CGD-CBD	4.46	119.19	111.27
24	C	508	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
24	c	903	CLA	C3D-C4D-ND	4.45	117.44	110.24
35	C	522	HTG	C1-O5-C5	4.45	120.79	112.58
24	C	501	CLA	C3D-C4D-ND	4.45	117.44	110.24
24	C	504	CLA	C3B-C2B-C1B	-4.45	101.79	107.16
24	a	405	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
24	a	406	CLA	C2C-C1C-NC	4.44	114.14	109.97
24	C	510	CLA	C3B-C2B-C1B	-4.44	101.81	107.16
33	C	519	LMG	O7-C10-C11	4.44	121.06	111.50
24	c	913	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
24	C	505	CLA	CHD-C1D-ND	-4.43	120.38	124.45
24	b	612	CLA	C3C-C4C-NC	4.43	115.54	110.57
24	c	912	CLA	C2C-C1C-NC	4.43	114.12	109.97
24	B	603	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
24	B	602	CLA	C3D-C4D-ND	4.42	117.39	110.24
24	B	604	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
24	C	513	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
24	C	506	CLA	C3D-C4D-ND	4.42	117.38	110.24
24	b	615	CLA	C3B-C2B-C1B	-4.41	101.83	107.16
24	b	608	CLA	C3B-C2B-C1B	-4.41	101.83	107.16
24	b	621	CLA	C3C-C4C-NC	4.41	115.52	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	911	CLA	C4A-NA-C1A	-4.41	104.72	106.71
24	b	620	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
24	B	603	CLA	C3D-C4D-ND	4.41	117.37	110.24
24	C	503	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
24	D	404	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
24	c	903	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
24	c	909	CLA	C4A-NA-C1A	-4.40	104.73	106.71
26	K	101	BCR	C7-C8-C9	-4.40	119.59	126.23
24	d	404	CLA	O2D-CGD-CBD	4.40	119.08	111.27
24	b	609	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
24	C	501	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
24	c	910	CLA	C1D-CHD-C4C	-4.39	116.59	126.06
24	a	406	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
24	b	606	CLA	C3D-C4D-ND	4.38	117.33	110.24
24	b	621	CLA	C3D-C4D-ND	4.38	117.32	110.24
24	C	505	CLA	C3B-C2B-C1B	-4.38	101.88	107.16
24	b	617	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
35	b	628	HTG	O5-C1-C2	4.38	115.82	110.31
24	C	506	CLA	C3B-C2B-C1B	-4.37	101.88	107.16
24	c	911	CLA	C3B-C2B-C1B	-4.37	101.89	107.16
24	B	606	CLA	C3D-C4D-ND	4.36	117.29	110.24
24	b	606	CLA	O2D-CGD-O1D	-4.36	115.32	123.84
27	A	411	SQD	C45-O47-C7	-4.36	107.06	117.79
24	c	903	CLA	C3C-C4C-NC	4.35	115.45	110.57
24	A	409	CLA	O2D-CGD-CBD	4.35	119.00	111.27
24	b	616	CLA	C1-C2-C3	-4.35	118.51	126.04
24	b	611	CLA	C3C-C4C-NC	4.35	115.45	110.57
24	B	603	CLA	C3C-C4C-NC	4.35	115.45	110.57
24	a	405	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
24	B	612	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
24	A	405	CLA	C3B-C4B-NB	4.34	114.54	110.52
24	C	502	CLA	O2D-CGD-CBD	4.33	118.97	111.27
24	b	610	CLA	C3B-C2B-C1B	-4.33	101.93	107.16
24	B	606	CLA	C1D-CHD-C4C	-4.33	116.71	126.06
24	c	912	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
26	b	622	BCR	C33-C5-C6	-4.33	119.67	124.53
37	D	408	DGD	O2G-C1B-C2B	4.33	120.83	111.50
24	C	510	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
35	B	625	HTG	O5-C1-C2	4.33	115.76	110.31
24	C	502	CLA	C3D-C4D-ND	4.33	117.24	110.24
24	C	509	CLA	C3C-C4C-NC	4.33	115.42	110.57
24	B	602	CLA	C3B-C2B-C1B	-4.33	101.94	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	909	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
24	C	506	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
24	a	405	CLA	C3D-C2D-C1D	-4.32	99.94	105.83
24	c	906	CLA	C3B-C2B-C1B	-4.32	101.95	107.16
24	A	406	CLA	C1C-C2C-C3C	-4.32	102.42	106.96
33	c	920	LMG	C3-C4-C5	4.31	117.93	110.24
24	B	610	CLA	C3D-C4D-ND	4.31	117.21	110.24
24	B	602	CLA	C3C-C4C-NC	4.31	115.40	110.57
24	C	509	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
24	b	611	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
24	b	610	CLA	O2D-CGD-O1D	-4.30	115.42	123.84
24	b	620	CLA	C1D-CHD-C4C	-4.30	116.78	126.06
24	B	607	CLA	C3C-C4C-NC	4.30	115.39	110.57
24	d	406	CLA	C3D-C4D-ND	4.30	117.19	110.24
24	C	512	CLA	C3D-C4D-ND	4.29	117.19	110.24
24	d	404	CLA	C3B-C4B-NB	4.29	114.50	110.52
24	a	405	CLA	C3D-C4D-ND	4.29	117.18	110.24
24	c	910	CLA	C3C-C4C-NC	4.29	115.38	110.57
24	C	503	CLA	C3C-C4C-NC	4.29	115.38	110.57
24	b	614	CLA	C3C-C4C-NC	4.29	115.38	110.57
24	B	611	CLA	O2D-CGD-CBD	4.28	118.88	111.27
24	b	615	CLA	O2D-CGD-CBD	4.28	118.88	111.27
24	c	904	CLA	C1-C2-C3	-4.28	118.64	126.04
24	A	406	CLA	C3D-C4D-ND	4.28	117.16	110.24
24	B	616	CLA	C3D-C4D-ND	4.28	117.16	110.24
24	b	620	CLA	C3C-C4C-NC	4.27	115.36	110.57
24	C	505	CLA	CMB-C2B-C1B	4.27	131.88	125.37
24	b	606	CLA	C3D-C2D-C1D	-4.27	100.01	105.83
24	C	510	CLA	C3D-C4D-ND	4.26	117.14	110.24
24	b	618	CLA	CHD-C1D-ND	-4.26	120.54	124.45
33	A	419	LMG	O7-C10-C11	4.26	120.69	111.50
24	c	909	CLA	C3D-C4D-ND	4.26	117.13	110.24
24	b	616	CLA	C4A-NA-C1A	-4.26	104.79	106.71
24	B	617	CLA	C3C-C4C-NC	4.26	115.34	110.57
37	e	101	DGD	C3E-C4E-C5E	4.25	117.83	110.24
24	c	906	CLA	C3D-C4D-ND	4.25	117.12	110.24
24	c	906	CLA	C1D-CHD-C4C	-4.25	116.88	126.06
24	B	607	CLA	C3D-C4D-ND	4.25	117.12	110.24
24	c	904	CLA	C3D-C4D-ND	4.24	117.10	110.24
24	B	603	CLA	O2D-CGD-O1D	-4.24	115.54	123.84
24	c	906	CLA	CHD-C1D-ND	-4.24	120.56	124.45
24	c	907	CLA	C4A-NA-C1A	-4.23	104.80	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	405	CLA	C3D-C4D-ND	4.23	117.08	110.24
24	C	503	CLA	C3D-C4D-ND	4.23	117.08	110.24
24	c	909	CLA	C3B-C4B-NB	4.23	114.44	110.52
26	H	101	BCR	C38-C26-C25	-4.23	119.78	124.53
24	A	409	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
24	b	613	CLA	C3C-C4C-NC	4.22	115.31	110.57
24	B	612	CLA	C3B-C2B-C1B	-4.22	102.06	107.16
24	c	902	CLA	C3D-C4D-ND	4.22	117.06	110.24
26	y	101	BCR	C33-C5-C6	-4.22	119.79	124.53
24	B	604	CLA	C3C-C4C-NC	4.22	115.30	110.57
24	B	608	CLA	C3C-C4C-NC	4.21	115.30	110.57
24	c	903	CLA	O2D-CGD-CBD	4.21	118.75	111.27
24	b	617	CLA	C3D-C4D-ND	4.21	117.05	110.24
24	C	502	CLA	C1-C2-C3	-4.21	118.77	126.04
24	B	617	CLA	C1D-CHD-C4C	-4.21	116.99	126.06
24	b	613	CLA	C3D-C2D-C1D	-4.20	100.09	105.83
24	B	613	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
24	B	608	CLA	C3D-C4D-ND	4.20	117.03	110.24
24	c	911	CLA	C3D-C4D-ND	4.19	117.02	110.24
24	c	911	CLA	C4-C3-C5	4.19	122.32	115.27
26	b	622	BCR	C7-C8-C9	-4.19	119.91	126.23
31	D	407	PL9	C7-C8-C9	-4.19	119.82	126.79
24	C	512	CLA	C3C-C4C-NC	4.19	115.27	110.57
24	B	617	CLA	C3D-C4D-ND	4.18	117.00	110.24
24	b	612	CLA	CMB-C2B-C1B	4.18	131.74	125.37
24	b	615	CLA	C3D-C2D-C1D	-4.18	100.13	105.83
24	c	911	CLA	C3D-C2D-C1D	-4.18	100.13	105.83
24	B	606	CLA	CMC-C2C-C1C	4.18	131.40	125.04
24	A	409	CLA	C3D-C4D-ND	4.17	116.99	110.24
24	B	610	CLA	C3B-C2B-C1B	-4.17	102.12	107.16
24	B	614	CLA	C3C-C4C-NC	4.17	115.25	110.57
24	b	613	CLA	C3D-C4D-ND	4.16	116.97	110.24
31	a	415	PL9	C7-C3-C4	4.16	120.26	116.88
26	T	102	BCR	C11-C10-C9	-4.16	121.38	127.31
24	B	611	CLA	C3D-C4D-ND	4.16	116.96	110.24
24	b	612	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
24	b	619	CLA	C3D-C4D-ND	4.15	116.95	110.24
36	b	635	LHG	O7-C7-C8	4.15	120.44	111.50
24	C	511	CLA	C3D-C4D-ND	4.14	116.94	110.24
24	B	610	CLA	CMB-C2B-C1B	4.14	131.68	125.37
24	B	613	CLA	C3D-C4D-ND	4.14	116.94	110.24
24	d	404	CLA	C3D-C4D-ND	4.14	116.94	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	404	CLA	C3C-C4C-NC	4.14	115.21	110.57
26	C	515	BCR	C7-C8-C9	-4.14	119.98	126.23
24	b	616	CLA	C3B-C4B-NB	4.13	114.35	110.52
24	C	513	CLA	C1D-CHD-C4C	-4.13	117.15	126.06
24	c	905	CLA	C3D-C4D-ND	4.11	116.89	110.24
24	b	612	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
24	b	606	CLA	C1D-CHD-C4C	-4.11	117.19	126.06
24	B	605	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
24	d	405	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
24	c	909	CLA	C3C-C4C-NC	4.10	115.17	110.57
24	C	511	CLA	C4A-NA-C1A	-4.09	104.86	106.71
24	d	405	CLA	C3C-C4C-NC	4.09	115.16	110.57
24	b	617	CLA	CMD-C2D-C1D	4.09	131.92	124.71
24	A	406	CLA	C1D-CHD-C4C	-4.09	117.24	126.06
24	d	406	CLA	C3C-C4C-NC	4.09	115.16	110.57
24	B	616	CLA	C3C-C4C-NC	4.08	115.15	110.57
24	C	511	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
38	f	101	HEM	CAD-CBD-CGD	4.08	122.39	113.60
24	B	616	CLA	C1D-CHD-C4C	-4.08	117.26	126.06
24	b	608	CLA	C1D-CHD-C4C	-4.08	117.26	126.06
24	c	907	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
24	c	903	CLA	C1D-CHD-C4C	-4.07	117.27	126.06
24	A	409	CLA	CAC-C3C-C4C	4.07	130.09	124.81
24	B	605	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
24	c	911	CLA	C3B-C4B-NB	4.06	114.29	110.52
24	c	904	CLA	C1D-CHD-C4C	-4.06	117.29	126.06
24	c	909	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
24	b	616	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
24	C	504	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
24	B	614	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
24	c	902	CLA	CAC-C3C-C4C	4.05	130.07	124.81
24	B	610	CLA	C3C-C4C-NC	4.05	115.11	110.57
24	b	620	CLA	C3D-C4D-ND	4.05	116.79	110.24
24	C	510	CLA	C3C-C4C-NC	4.05	115.11	110.57
24	C	506	CLA	CAC-C3C-C4C	4.05	130.06	124.81
24	b	610	CLA	C1D-CHD-C4C	-4.05	117.33	126.06
24	A	405	CLA	C1D-CHD-C4C	-4.05	117.33	126.06
24	a	408	CLA	C1-C2-C3	-4.05	119.05	126.04
24	B	604	CLA	C1D-CHD-C4C	-4.04	117.33	126.06
24	C	501	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	D	404	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	b	617	CLA	C4A-NA-C1A	-4.04	104.89	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	V	202	HEC	CBC-CAC-C3C	4.04	123.56	112.43
24	c	911	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	b	616	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	C	505	CLA	C3D-C4D-ND	4.03	116.76	110.24
24	c	902	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
24	A	409	CLA	CMB-C2B-C1B	4.03	131.51	125.37
29	D	403	LMT	O1B-C4'-C3'	4.03	118.00	107.28
24	b	619	CLA	C3C-C4C-NC	4.03	115.09	110.57
24	A	405	CLA	C3D-C2D-C1D	-4.03	100.33	105.83
24	b	607	CLA	O2D-CGD-O1D	-4.03	115.97	123.84
24	b	621	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
24	c	911	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
24	C	502	CLA	C3C-C4C-NC	4.02	115.08	110.57
26	c	927	BCR	C15-C14-C13	-4.01	121.58	127.31
29	a	401	LMT	O5'-C5'-C4'	4.01	118.21	109.75
24	d	405	CLA	C3D-C2D-C1D	-4.01	100.36	105.83
24	B	602	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
24	D	404	CLA	O2D-CGD-CBD	4.00	118.38	111.27
36	E	101	LHG	O7-C7-C8	4.00	120.12	111.50
24	c	902	CLA	O2D-CGD-O1D	-4.00	116.03	123.84
24	c	907	CLA	C3D-C4D-ND	3.99	116.70	110.24
24	b	611	CLA	C1D-CHD-C4C	-3.99	117.45	126.06
24	C	502	CLA	C1D-CHD-C4C	-3.99	117.45	126.06
24	a	408	CLA	C1D-CHD-C4C	-3.99	117.45	126.06
40	V	202	HEC	CHB-C1B-NB	3.99	128.75	124.42
24	b	608	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
24	A	405	CLA	C4A-NA-C1A	-3.99	104.91	106.71
24	c	913	CLA	C1C-C2C-C3C	-3.99	102.77	106.96
24	C	504	CLA	C3D-C4D-ND	3.98	116.68	110.24
40	v	202	HEC	CHC-C4B-NB	3.98	129.28	124.37
24	B	607	CLA	C1D-CHD-C4C	-3.98	117.48	126.06
24	B	602	CLA	C4A-NA-C1A	-3.97	104.92	106.71
38	F	102	HEM	C1B-NB-C4B	3.97	109.18	105.07
24	c	902	CLA	C3B-C4B-NB	3.97	114.20	110.52
24	C	509	CLA	C3D-C4D-ND	3.97	116.66	110.24
24	c	914	CLA	O2D-CGD-CBD	3.97	118.31	111.27
24	c	914	CLA	C1D-CHD-C4C	-3.96	117.51	126.06
24	B	603	CLA	C1D-CHD-C4C	-3.96	117.51	126.06
24	c	910	CLA	C3D-C4D-ND	3.96	116.64	110.24
24	c	906	CLA	CMB-C2B-C1B	3.95	131.39	125.37
24	C	513	CLA	C3C-C4C-NC	3.95	115.00	110.57
24	d	405	CLA	C1-C2-C3	-3.95	119.21	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	414	SQD	O48-C23-C24	3.95	124.31	111.91
24	B	615	CLA	C3C-C4C-NC	3.95	115.00	110.57
33	c	920	LMG	O6-C5-C4	3.95	116.86	109.69
24	b	615	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	B	606	CLA	CMB-C2B-C1B	3.94	131.37	125.37
26	T	102	BCR	C15-C16-C17	-3.94	115.41	123.47
24	b	607	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	c	905	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	a	405	CLA	CAA-C2A-C3A	-3.93	102.00	112.78
24	B	604	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
24	c	909	CLA	C1-C2-C3	-3.93	119.24	126.04
24	b	618	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
24	C	501	CLA	O2D-CGD-O1D	-3.93	116.16	123.84
24	b	608	CLA	C3D-C2D-C1D	-3.93	100.47	105.83
24	b	616	CLA	C3D-C4D-ND	3.93	116.59	110.24
24	C	504	CLA	C3C-C4C-NC	3.92	114.97	110.57
29	b	602	LMT	C1'-O5'-C5'	3.92	121.39	113.69
38	f	101	HEM	C4C-NC-C1C	3.92	109.19	105.35
24	b	614	CLA	C3B-C2B-C1B	-3.92	102.43	107.16
24	c	907	CLA	C3C-C4C-NC	3.92	114.97	110.57
24	c	907	CLA	C3B-C2B-C1B	-3.92	102.43	107.16
24	d	405	CLA	O2D-CGD-O1D	-3.92	116.18	123.84
24	a	408	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
24	C	505	CLA	C3D-C2D-C1D	-3.91	100.49	105.83
24	C	505	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
25	a	407	PHO	O1D-CGD-CBD	-3.91	118.23	124.74
24	c	913	CLA	C1D-CHD-C4C	-3.90	117.63	126.06
24	c	907	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
24	A	405	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
26	a	409	BCR	C33-C5-C6	-3.90	120.15	124.53
24	b	617	CLA	CMB-C2B-C1B	3.89	131.30	125.37
38	f	101	HEM	CHD-C1D-ND	3.89	128.65	124.42
24	c	907	CLA	O2D-CGD-CBD	3.89	118.18	111.27
26	t	102	BCR	C15-C14-C13	3.89	132.86	127.31
29	a	401	LMT	C1'-O5'-C5'	3.89	121.32	113.69
24	B	609	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
24	B	615	CLA	C3B-C4B-NB	3.88	114.12	110.52
31	D	407	PL9	C37-C38-C39	-3.88	118.31	127.66
40	v	202	HEC	CBC-CAC-C3C	3.88	123.14	112.43
24	b	617	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
35	B	623	HTG	C1'-S1-C1	3.88	107.35	100.09
24	b	611	CLA	C3D-C4D-ND	3.88	116.51	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	b	601	HTG	C1'-S1-C1	3.88	107.34	100.09
33	Z	101	LMG	O7-C10-C11	3.87	119.85	111.50
24	b	618	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
24	c	908	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
36	d	411	LHG	O7-C7-C8	3.87	119.84	111.50
24	b	617	CLA	C1-C2-C3	-3.87	119.35	126.04
24	A	405	CLA	CAC-C3C-C4C	3.87	129.82	124.81
40	v	202	HEC	C4B-NB-C1B	3.86	109.06	105.07
24	C	509	CLA	C1D-CHD-C4C	-3.86	117.72	126.06
24	C	512	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
24	C	507	CLA	C3D-C4D-ND	3.86	116.48	110.24
24	c	905	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
24	c	903	CLA	CMB-C2B-C1B	3.86	131.24	125.37
24	B	611	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
24	a	406	CLA	O2D-CGD-O1D	-3.85	116.31	123.84
27	a	410	SQD	C1-C2-C3	-3.85	101.98	110.00
35	V	203	HTG	C1'-S1-C1	3.84	107.27	100.09
24	B	613	CLA	C4-C3-C5	3.84	121.73	115.27
26	t	102	BCR	C15-C16-C17	-3.84	115.62	123.47
24	A	406	CLA	C3C-C4C-NC	3.83	114.87	110.57
24	b	620	CLA	CMB-C2B-C1B	3.83	131.21	125.37
24	b	609	CLA	C3B-C4B-NB	3.83	114.07	110.52
24	C	504	CLA	C1D-CHD-C4C	-3.82	117.81	126.06
24	d	404	CLA	C1D-CHD-C4C	-3.82	117.82	126.06
27	a	410	SQD	O8-S-C6	3.82	111.83	105.74
35	b	604	HTG	C1'-S1-C1	3.82	107.23	100.09
26	y	101	BCR	C15-C14-C13	-3.81	121.87	127.31
24	B	615	CLA	C4A-NA-C1A	-3.81	104.99	106.71
37	C	517	DGD	O2G-C1B-C2B	3.81	119.71	111.50
24	c	909	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
24	B	616	CLA	CMB-C2B-C1B	3.81	131.17	125.37
31	D	407	PL9	C42-C43-C44	-3.80	118.50	127.66
24	c	907	CLA	C3B-C4B-NB	3.80	114.04	110.52
24	d	406	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
24	C	506	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
24	A	409	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
24	C	511	CLA	C3B-C4B-NB	3.80	114.04	110.52
24	B	613	CLA	C4A-NA-C1A	-3.80	105.00	106.71
24	C	511	CLA	C1-C2-C3	-3.80	119.48	126.04
24	c	912	CLA	C3C-C4C-NC	3.79	114.82	110.57
24	c	912	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
24	c	914	CLA	C1C-C2C-C3C	-3.79	102.97	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	514	BCR	C7-C8-C9	-3.78	120.53	126.23
24	B	614	CLA	C3B-C4B-NB	3.78	114.02	110.52
26	d	407	BCR	C24-C23-C22	-3.78	120.53	126.23
24	C	511	CLA	C3C-C4C-NC	3.77	114.80	110.57
37	H	102	DGD	O2G-C1B-C2B	3.77	119.62	111.50
24	b	609	CLA	CMC-C2C-C1C	3.77	130.78	125.04
26	H	101	BCR	C24-C23-C22	-3.77	120.55	126.23
37	c	917	DGD	O2G-C1B-C2B	3.77	119.62	111.50
31	a	415	PL9	C15-C14-C16	3.77	121.61	115.27
24	c	905	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	B	612	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	b	615	CLA	C1-C2-C3	-3.76	119.53	126.04
24	a	405	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
24	A	406	CLA	C3B-C4B-NB	3.75	113.99	110.52
24	C	510	CLA	C1D-CHD-C4C	-3.74	118.00	126.06
24	b	609	CLA	C3B-C2B-C1B	-3.74	102.65	107.16
24	c	908	CLA	C3D-C4D-ND	3.73	116.27	110.24
24	D	405	CLA	C3C-C4C-NC	3.73	114.75	110.57
24	c	911	CLA	C3C-C4C-NC	3.73	114.75	110.57
29	C	520	LMT	O1B-C4'-C3'	3.73	117.20	107.28
24	c	908	CLA	CMC-C2C-C1C	3.73	130.71	125.04
26	D	406	BCR	C33-C5-C6	-3.73	120.34	124.53
24	C	508	CLA	C3C-C4C-NC	3.72	114.75	110.57
37	D	408	DGD	C1D-C2D-C3D	3.72	117.74	110.00
24	C	507	CLA	C1D-CHD-C4C	-3.71	118.04	126.06
33	c	919	LMG	O7-C10-C11	3.71	119.50	111.50
24	C	504	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
24	c	908	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
24	A	405	CLA	O2D-CGD-CBD	3.71	117.86	111.27
24	C	513	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
24	b	614	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
27	L	102	SQD	C3-C4-C5	3.71	116.85	110.24
24	c	910	CLA	C1-O2A-CGA	3.71	126.17	116.44
24	c	913	CLA	C1-C2-C3	-3.70	119.64	126.04
24	b	615	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
24	C	504	CLA	C3B-C4B-NB	3.70	113.95	110.52
24	A	406	CLA	CBC-CAC-C3C	-3.70	102.23	112.43
24	b	619	CLA	C1-C2-C3	-3.70	119.65	126.04
26	d	407	BCR	C38-C26-C25	-3.70	120.38	124.53
24	c	913	CLA	C3C-C4C-NC	3.70	114.72	110.57
24	b	619	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
24	c	903	CLA	C1-C2-C3	-3.69	119.66	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	417	PL9	C20-C19-C21	3.69	121.48	115.27
24	B	614	CLA	C3D-C4D-ND	3.69	116.21	110.24
24	C	501	CLA	C3C-C4C-NC	3.69	114.71	110.57
31	A	417	PL9	C37-C38-C39	-3.69	118.78	127.66
24	a	406	CLA	C3C-C4C-NC	3.69	114.71	110.57
24	D	404	CLA	C1-C2-C3	-3.68	119.67	126.04
24	c	910	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
24	b	618	CLA	O2D-CGD-CBD	3.68	117.80	111.27
24	C	510	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
24	b	608	CLA	C3C-C4C-NC	3.68	114.69	110.57
24	C	502	CLA	CAC-C3C-C4C	3.67	129.58	124.81
36	B	635	LHG	O8-C23-C24	3.67	123.43	111.91
27	a	402	SQD	O47-C7-C8	3.67	119.41	111.50
24	B	615	CLA	O2D-CGD-O1D	-3.67	116.67	123.84
24	b	613	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
24	B	616	CLA	CAC-C3C-C4C	3.66	129.56	124.81
24	B	616	CLA	O2D-CGD-CBD	3.66	117.77	111.27
24	b	616	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
24	B	611	CLA	CAA-C2A-C3A	-3.66	102.76	112.78
24	a	406	CLA	C1D-CHD-C4C	-3.65	118.17	126.06
36	B	635	LHG	O7-C7-C8	3.65	119.37	111.50
24	B	612	CLA	C1-C2-C3	-3.65	119.73	126.04
26	T	102	BCR	C16-C17-C18	-3.65	122.10	127.31
24	B	610	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
24	b	613	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
24	A	407	CLA	O2D-CGD-O1D	-3.64	116.73	123.84
24	c	902	CLA	C3C-C4C-NC	3.63	114.65	110.57
24	b	621	CLA	C4C-C3C-C2C	-3.63	101.60	106.90
24	B	612	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
24	c	914	CLA	C3C-C4C-NC	3.63	114.65	110.57
25	A	408	PHO	C1A-C2A-C3A	-3.63	99.38	102.84
24	B	609	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
37	c	916	DGD	O2G-C1B-C2B	3.63	119.32	111.50
24	b	618	CLA	C1-C2-C3	-3.63	119.77	126.04
24	b	606	CLA	C3C-C4C-NC	3.63	114.64	110.57
24	B	610	CLA	O2D-CGD-CBD	3.62	117.71	111.27
24	B	608	CLA	C3B-C2B-C1B	-3.62	102.79	107.16
24	d	404	CLA	CAA-C2A-C3A	-3.62	102.86	112.78
24	b	606	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
24	b	612	CLA	C3D-C4D-ND	3.62	116.09	110.24
24	B	609	CLA	C3C-C4C-NC	3.62	114.63	110.57
26	h	101	BCR	C38-C26-C25	-3.62	120.46	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	102	BCR	C12-C13-C14	-3.62	113.39	118.94
24	B	608	CLA	C4A-NA-C1A	-3.61	105.08	106.71
24	c	907	CLA	C1-C2-C3	-3.61	119.80	126.04
24	D	405	CLA	CAC-C3C-C4C	3.61	129.50	124.81
24	B	603	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	b	615	CLA	CAC-C3C-C4C	3.61	129.49	124.81
24	c	904	CLA	O2D-CGD-CBD	3.61	117.68	111.27
33	b	625	LMG	O7-C10-C11	3.61	119.28	111.50
24	B	611	CLA	C1D-CHD-C4C	-3.61	118.28	126.06
24	B	614	CLA	C1-C2-C3	-3.61	119.81	126.04
40	V	202	HEC	CHC-C4B-NB	3.60	128.81	124.37
25	D	401	PHO	C1A-C2A-C3A	-3.60	99.41	102.84
24	b	617	CLA	C4C-C3C-C2C	-3.60	101.65	106.90
24	b	621	CLA	C3B-C4B-NB	3.60	113.85	110.52
24	b	619	CLA	O2D-CGD-O1D	-3.59	116.81	123.84
24	b	608	CLA	CAA-C2A-C3A	-3.59	102.95	112.78
31	d	408	PL9	C10-C9-C11	3.59	121.31	115.27
24	B	614	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
24	d	406	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
40	v	202	HEC	C4C-NC-C1C	3.59	108.86	105.35
29	C	520	LMT	C1'-O5'-C5'	3.59	120.73	113.69
24	b	613	CLA	CAC-C3C-C4C	3.58	129.46	124.81
24	D	405	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
24	B	611	CLA	C3C-C4C-NC	3.57	114.58	110.57
24	b	619	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
24	a	406	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
35	B	624	HTG	C1-O5-C5	3.57	119.16	112.58
24	B	610	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
25	d	403	PHO	C4-C3-C5	3.57	121.27	115.27
24	c	906	CLA	C4C-C3C-C2C	-3.57	101.70	106.90
26	T	102	BCR	C33-C5-C6	-3.56	120.53	124.53
24	D	404	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
24	A	407	CLA	CMB-C2B-C1B	3.56	130.80	125.37
24	b	620	CLA	O2D-CGD-CBD	3.56	117.60	111.27
24	C	501	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
24	c	910	CLA	C1-C2-C3	-3.56	119.88	126.04
24	B	608	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
24	a	405	CLA	C3C-C4C-NC	3.56	114.56	110.57
24	C	505	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
40	V	202	HEC	C4C-NC-C1C	3.56	108.83	105.35
24	A	405	CLA	O2A-CGA-CBA	3.56	123.07	111.91
24	D	405	CLA	C3B-C4B-NB	3.56	113.81	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	CMB-C2B-C1B	3.56	130.78	125.37
26	B	618	BCR	C7-C8-C9	-3.56	120.86	126.23
38	f	101	HEM	C4D-ND-C1D	3.56	108.75	105.07
24	a	405	CLA	C4-C3-C5	3.55	121.25	115.27
31	D	407	PL9	C10-C9-C11	3.55	121.25	115.27
33	C	519	LMG	C3-C4-C5	3.55	116.58	110.24
24	B	609	CLA	C3D-C2D-C1D	-3.55	100.99	105.83
24	A	409	CLA	C3C-C4C-NC	3.55	114.55	110.57
33	Y	101	LMG	O7-C10-C11	3.55	119.15	111.50
33	z	101	LMG	O7-C10-C11	3.55	119.14	111.50
26	C	514	BCR	C33-C5-C6	-3.54	120.55	124.53
38	f	101	HEM	C1B-NB-C4B	3.54	108.73	105.07
24	A	407	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
24	B	615	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
24	B	607	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
26	D	406	BCR	C29-C30-C25	3.53	115.91	110.48
31	a	415	PL9	C32-C33-C34	-3.53	119.17	127.66
24	B	613	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
36	d	410	LHG	O7-C7-C8	3.52	119.09	111.50
24	B	606	CLA	CHD-C4C-NC	3.52	129.75	124.20
33	B	622	LMG	O8-C28-C29	3.52	122.94	111.91
24	B	612	CLA	C3B-C4B-NB	3.52	113.78	110.52
24	C	508	CLA	C3B-C4B-NB	3.52	113.78	110.52
24	C	505	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
26	C	514	BCR	C20-C21-C22	-3.51	122.30	127.31
33	J	101	LMG	O7-C10-C11	3.51	119.07	111.50
24	a	408	CLA	C3C-C4C-NC	3.51	114.51	110.57
24	c	908	CLA	C4A-NA-C1A	-3.51	105.13	106.71
24	B	613	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
31	d	408	PL9	C20-C19-C21	3.50	121.16	115.27
24	C	512	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
24	A	405	CLA	C3C-C4C-NC	3.50	114.50	110.57
24	b	618	CLA	CHC-C1C-C2C	-3.50	117.01	126.73
24	b	610	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
24	a	408	CLA	CHD-C4C-NC	3.50	129.71	124.20
24	A	406	CLA	CHD-C4C-NC	3.49	129.71	124.20
24	C	506	CLA	C3B-C4B-NB	3.49	113.75	110.52
24	b	608	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
24	B	608	CLA	C1D-CHD-C4C	-3.49	118.54	126.06
26	d	407	BCR	C28-C27-C26	-3.48	107.86	114.08
24	b	608	CLA	C3B-C4B-NB	3.48	113.75	110.52
27	A	411	SQD	O8-S-C6	3.48	111.29	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	411	LMG	C8-O7-C10	-3.48	109.22	117.79
24	C	504	CLA	CMC-C2C-C1C	3.48	130.34	125.04
24	c	904	CLA	CMB-C2B-C1B	3.48	130.66	125.37
26	C	514	BCR	C15-C14-C13	-3.48	122.35	127.31
24	D	404	CLA	C3B-C4B-NB	3.48	113.74	110.52
24	a	405	CLA	O2A-CGA-O1A	-3.47	114.82	123.59
26	B	619	BCR	C28-C27-C26	-3.47	107.88	114.08
26	t	102	BCR	C11-C10-C9	-3.47	122.36	127.31
24	C	508	CLA	CAC-C3C-C4C	3.47	129.31	124.81
24	B	617	CLA	C3B-C4B-NB	3.47	113.73	110.52
26	k	101	BCR	C20-C21-C22	-3.47	122.36	127.31
24	c	906	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
24	B	613	CLA	CMC-C2C-C1C	3.47	130.32	125.04
40	v	202	HEC	C1D-ND-C4D	3.47	108.65	105.07
24	C	510	CLA	C4-C3-C5	3.46	121.10	115.27
24	B	602	CLA	C4C-C3C-C2C	-3.46	101.86	106.90
24	c	903	CLA	C4C-C3C-C2C	-3.46	101.86	106.90
26	A	410	BCR	C33-C5-C6	-3.46	120.65	124.53
24	A	406	CLA	CAA-C2A-C3A	-3.45	103.33	112.78
24	C	508	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
24	B	608	CLA	C4-C3-C5	3.45	121.07	115.27
24	B	602	CLA	C3B-C4B-NB	3.45	113.71	110.52
31	a	415	PL9	C42-C43-C44	-3.45	119.36	127.66
27	F	103	SQD	O7-S-C6	3.45	111.03	106.94
31	a	415	PL9	C20-C19-C21	3.45	121.07	115.27
24	b	607	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
37	h	102	DGD	O2G-C1B-C2B	3.44	118.92	111.50
24	c	906	CLA	C3D-C2D-C1D	-3.44	101.14	105.83
24	D	405	CLA	C4-C3-C5	3.44	121.06	115.27
38	F	102	HEM	C4A-NA-C1A	3.44	108.71	105.35
24	B	615	CLA	C4-C3-C5	3.44	121.05	115.27
24	b	609	CLA	C1D-CHD-C4C	-3.44	118.65	126.06
31	A	417	PL9	C8-C7-C3	3.43	121.68	111.98
27	f	102	SQD	C1-O5-C5	3.43	120.42	113.69
24	C	501	CLA	CBC-CAC-C3C	-3.43	102.97	112.43
24	D	405	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
24	d	404	CLA	CBC-CAC-C3C	-3.43	102.98	112.43
24	A	405	CLA	CAA-C2A-C3A	-3.43	103.40	112.78
31	d	408	PL9	C42-C43-C44	-3.42	119.41	127.66
24	d	405	CLA	O2A-CGA-CBA	3.42	122.65	111.91
24	B	605	CLA	C1D-CHD-C4C	-3.42	118.67	126.06
24	B	605	CLA	C1-C2-C3	-3.42	120.13	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	501	CLA	C1-C2-C3	-3.42	120.13	126.04
31	D	407	PL9	C40-C39-C41	3.42	121.02	115.27
24	c	912	CLA	O2D-CGD-CBD	3.41	117.34	111.27
24	c	910	CLA	C3B-C4B-NB	3.41	113.68	110.52
24	b	606	CLA	CHD-C4C-NC	3.41	129.58	124.20
24	C	506	CLA	C3C-C4C-NC	3.41	114.39	110.57
31	a	415	PL9	C22-C23-C24	-3.40	119.46	127.66
24	B	604	CLA	CAA-C2A-C3A	-3.40	103.46	112.78
27	a	402	SQD	O48-C23-C24	3.40	122.59	111.91
24	A	407	CLA	C3C-C4C-NC	3.40	114.39	110.57
24	D	405	CLA	CMB-C2B-C1B	3.40	130.55	125.37
38	f	101	HEM	CHD-C4C-NC	3.40	128.12	124.44
24	d	406	CLA	CMB-C2B-C1B	3.40	130.55	125.37
24	B	611	CLA	C3B-C4B-NB	3.40	113.67	110.52
31	a	415	PL9	C7-C8-C9	-3.40	121.14	126.79
26	c	927	BCR	C16-C17-C18	-3.40	122.46	127.31
24	B	607	CLA	CMB-C2B-C1B	3.39	130.54	125.37
24	c	908	CLA	CMB-C2B-C1B	3.39	130.54	125.37
24	b	618	CLA	C3D-C4D-ND	3.39	115.72	110.24
40	v	202	HEC	CHA-C4D-ND	3.39	128.10	124.42
24	c	902	CLA	CHC-C1C-C2C	-3.38	117.34	126.73
24	C	504	CLA	CBC-CAC-C3C	-3.38	103.11	112.43
24	b	612	CLA	CBC-CAC-C3C	-3.38	103.12	112.43
36	L	101	LHG	O7-C7-C8	3.38	118.78	111.50
24	C	513	CLA	CMB-C2B-C1B	3.37	130.50	125.37
24	C	507	CLA	CMC-C2C-C1C	3.37	130.17	125.04
38	F	102	HEM	CHD-C1D-ND	3.37	128.07	124.42
24	B	615	CLA	CAC-C3C-C4C	3.36	129.18	124.81
27	F	103	SQD	C1-O5-C5	3.36	120.29	113.69
24	B	610	CLA	C3B-C4B-NB	3.36	113.63	110.52
24	B	611	CLA	CMB-C2B-C1B	3.36	130.49	125.37
24	c	904	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
24	B	613	CLA	C1-C2-C3	-3.35	120.24	126.04
24	C	503	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
24	c	902	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
24	C	506	CLA	C1D-CHD-C4C	-3.35	118.84	126.06
24	B	608	CLA	C3B-C4B-NB	3.35	113.62	110.52
26	B	619	BCR	C33-C5-C6	-3.34	120.77	124.53
24	b	617	CLA	C4-C3-C5	3.34	120.90	115.27
24	b	618	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
24	C	507	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
24	B	607	CLA	C1-C2-C3	-3.34	120.27	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
24	a	405	CLA	O2A-CGA-CBA	3.34	122.38	111.91
27	F	103	SQD	O5-C5-C4	3.34	115.75	109.69
26	D	406	BCR	C28-C27-C26	-3.34	108.12	114.08
24	C	505	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
24	B	617	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
24	B	611	CLA	O2A-CGA-CBA	3.32	122.34	111.91
24	B	604	CLA	CHD-C4C-NC	3.32	129.44	124.20
24	B	607	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
31	d	408	PL9	C40-C39-C41	3.31	120.85	115.27
24	D	405	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
24	B	611	CLA	CHC-C1C-C2C	-3.31	117.55	126.73
24	c	908	CLA	O2D-CGD-O1D	-3.31	117.38	123.84
24	B	613	CLA	C1D-CHD-C4C	-3.31	118.93	126.06
36	d	409	LHG	O7-C7-C8	3.31	118.62	111.50
24	a	406	CLA	CHD-C4C-NC	3.30	129.41	124.20
24	B	612	CLA	CMB-C2B-C1B	3.30	130.40	125.37
24	C	508	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
25	a	407	PHO	CBC-CAC-C3C	-3.30	108.05	112.88
24	b	617	CLA	O2A-CGA-CBA	3.30	122.26	111.91
26	C	515	BCR	C24-C23-C22	-3.30	121.25	126.23
24	a	406	CLA	CMC-C2C-C1C	3.30	130.06	125.04
24	b	612	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
26	c	915	BCR	C15-C14-C13	-3.29	122.61	127.31
24	B	605	CLA	CMB-C2B-C1B	3.29	130.38	125.37
31	a	415	PL9	C27-C28-C29	-3.29	119.74	127.66
38	F	102	HEM	CBA-CAA-C2A	-3.29	103.50	112.63
26	D	406	BCR	C38-C26-C25	-3.29	120.84	124.53
24	B	615	CLA	C1D-CHD-C4C	-3.28	118.97	126.06
24	B	615	CLA	CHC-C1C-C2C	-3.28	117.61	126.73
24	a	408	CLA	C4-C3-C5	3.28	120.79	115.27
24	c	912	CLA	CHD-C4C-NC	3.28	129.38	124.20
40	V	202	HEC	CHA-C4D-ND	3.28	127.98	124.42
24	B	617	CLA	CBC-CAC-C3C	-3.28	103.38	112.43
31	d	408	PL9	C27-C28-C29	-3.28	119.76	127.66
24	C	507	CLA	C1-C2-C3	-3.28	120.37	126.04
24	b	616	CLA	CHC-C1C-C2C	-3.27	117.63	126.73
24	A	409	CLA	C4-C3-C5	3.27	120.78	115.27
24	d	404	CLA	C3C-C4C-NC	3.27	114.24	110.57
24	a	405	CLA	O2D-CGD-CBD	3.27	117.08	111.27
24	b	620	CLA	CHD-C4C-NC	3.27	129.36	124.20
24	B	606	CLA	C1C-C2C-C3C	-3.27	103.52	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	621	CLA	O2A-CGA-CBA	3.27	122.17	111.91
24	A	407	CLA	C1D-CHD-C4C	-3.27	119.01	126.06
24	b	617	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
24	A	407	CLA	C4-C3-C5	3.27	120.76	115.27
27	A	414	SQD	O47-C7-C8	3.26	118.53	111.50
24	B	610	CLA	C1-C2-C3	-3.26	120.40	126.04
24	b	613	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
24	b	610	CLA	C2A-C1A-CHA	-3.26	118.17	123.86
33	d	415	LMG	O7-C10-C11	3.25	118.52	111.50
31	A	417	PL9	C32-C33-C34	-3.25	119.83	127.66
24	a	405	CLA	C3B-C4B-NB	3.25	113.53	110.52
24	C	509	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
38	F	102	HEM	C4C-NC-C1C	3.25	108.53	105.35
24	c	912	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
24	b	612	CLA	CAA-C2A-C3A	-3.25	103.89	112.78
31	D	407	PL9	C53-C6-C1	3.24	121.62	114.99
24	b	620	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
24	B	605	CLA	C4A-NA-C1A	-3.24	105.25	106.71
24	b	619	CLA	CMC-C2C-C1C	3.24	129.97	125.04
24	A	405	CLA	O2A-CGA-O1A	-3.24	115.42	123.59
24	b	607	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
27	a	402	SQD	O8-S-C6	3.24	110.90	105.74
24	c	905	CLA	CMC-C2C-C1C	3.24	129.97	125.04
24	c	912	CLA	CMC-C2C-C1C	3.24	129.97	125.04
24	b	611	CLA	C3B-C4B-NB	3.23	113.52	110.52
38	f	101	HEM	CBD-CAD-C3D	-3.23	103.66	112.63
24	c	905	CLA	C4-C3-C5	3.23	120.70	115.27
31	a	415	PL9	C35-C34-C36	3.23	120.70	115.27
24	c	911	CLA	CHC-C1C-C2C	-3.23	117.77	126.73
24	C	509	CLA	C3B-C4B-NB	3.23	113.51	110.52
24	b	612	CLA	C3B-C4B-NB	3.23	113.51	110.52
24	b	614	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
24	C	509	CLA	CAC-C3C-C4C	3.22	128.99	124.81
24	B	609	CLA	C3B-C4B-NB	3.22	113.50	110.52
24	b	613	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
40	v	202	HEC	CHB-C1B-NB	3.22	127.92	124.42
24	b	610	CLA	CHD-C4C-NC	3.22	129.28	124.20
33	b	625	LMG	O8-C28-C29	3.22	122.01	111.91
24	d	404	CLA	CHC-C1C-C2C	-3.22	117.80	126.73
26	Y	102	BCR	C15-C14-C13	-3.21	122.72	127.31
24	b	611	CLA	C4-C3-C5	3.21	120.67	115.27
24	B	602	CLA	O2A-CGA-CBA	3.21	121.98	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	511	CLA	CMC-C2C-C1C	3.21	129.93	125.04
24	C	510	CLA	C3B-C4B-NB	3.21	113.49	110.52
24	B	602	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
24	C	502	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
24	B	613	CLA	C3B-C4B-NB	3.20	113.49	110.52
24	B	608	CLA	CAA-C2A-C3A	-3.20	104.00	112.78
24	C	502	CLA	CMB-C2B-C1B	3.20	130.25	125.37
24	c	913	CLA	C4-C3-C5	3.20	120.66	115.27
24	B	612	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
24	B	613	CLA	C4C-C3C-C2C	-3.20	102.24	106.90
26	b	623	BCR	C24-C23-C22	-3.20	121.41	126.23
36	a	418	LHG	O7-C7-C8	3.20	118.39	111.50
24	B	605	CLA	CHC-C1C-C2C	-3.19	117.86	126.73
24	A	409	CLA	CAA-C2A-C3A	-3.19	104.03	112.78
24	B	616	CLA	CMC-C2C-C1C	3.19	129.90	125.04
24	C	504	CLA	CAC-C3C-C4C	3.19	128.95	124.81
24	b	609	CLA	C3D-C4D-ND	3.19	115.39	110.24
24	b	610	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
26	Y	102	BCR	C16-C17-C18	-3.19	122.76	127.31
38	F	102	HEM	CHD-C4C-NC	3.18	127.88	124.44
24	b	615	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
24	C	507	CLA	CHD-C4C-NC	3.18	129.22	124.20
24	C	509	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
27	f	102	SQD	O7-S-C6	3.18	110.72	106.94
24	a	406	CLA	CMB-C2B-C1B	3.18	130.22	125.37
24	B	617	CLA	CHD-C4C-NC	3.18	129.22	124.20
24	B	605	CLA	C3D-C4D-ND	3.18	115.38	110.24
26	b	623	BCR	C15-C14-C13	-3.18	122.77	127.31
24	B	605	CLA	O2A-CGA-O1A	-3.18	115.57	123.59
24	C	506	CLA	CBC-CAC-C3C	-3.18	103.67	112.43
24	c	907	CLA	CBC-CAC-C3C	-3.17	103.68	112.43
24	c	914	CLA	CMC-C2C-C1C	3.17	129.87	125.04
24	c	909	CLA	CHC-C1C-C2C	-3.17	117.93	126.73
24	c	913	CLA	CHD-C4C-NC	3.17	129.19	124.20
24	a	405	CLA	CHC-C1C-C2C	-3.17	117.94	126.73
26	Y	102	BCR	C24-C23-C22	-3.16	121.45	126.23
24	A	406	CLA	CHC-C1C-C2C	-3.16	117.95	126.73
24	b	615	CLA	CAA-C2A-C3A	-3.16	104.12	112.78
24	b	614	CLA	CHD-C4C-NC	3.16	129.18	124.20
24	b	611	CLA	CBC-CAC-C3C	-3.16	103.73	112.43
31	A	417	PL9	C7-C8-C9	-3.16	121.54	126.79
36	D	410	LHG	O8-C23-C24	3.15	121.81	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	907	CLA	CHC-C1C-C2C	-3.15	117.97	126.73
31	A	417	PL9	C22-C23-C24	-3.15	120.08	127.66
24	c	913	CLA	CMB-C2B-C1B	3.15	130.16	125.37
24	b	608	CLA	CAC-C3C-C4C	3.15	128.89	124.81
24	C	501	CLA	CMC-C2C-C1C	3.14	129.83	125.04
24	B	604	CLA	O2A-CGA-CBA	3.14	121.77	111.91
24	B	613	CLA	CAC-C3C-C4C	3.14	128.88	124.81
26	H	101	BCR	C16-C17-C18	-3.14	122.83	127.31
24	c	914	CLA	CHD-C4C-NC	3.14	129.15	124.20
24	d	406	CLA	CMC-C2C-C1C	3.13	129.81	125.04
24	C	508	CLA	CHC-C1C-C2C	-3.13	118.03	126.73
26	B	620	BCR	C28-C27-C26	-3.13	108.48	114.08
24	B	606	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
24	B	607	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
24	b	618	CLA	CAC-C3C-C4C	3.13	128.87	124.81
24	B	614	CLA	O2D-CGD-CBD	3.13	116.82	111.27
27	F	103	SQD	C3-C4-C5	3.13	115.81	110.24
24	B	604	CLA	C2A-C1A-CHA	-3.12	118.39	123.86
24	B	612	CLA	C4C-C3C-C2C	-3.12	102.34	106.90
26	k	101	BCR	C11-C10-C9	-3.12	122.85	127.31
31	A	417	PL9	C7-C3-C4	3.12	119.41	116.88
31	a	415	PL9	C17-C18-C19	-3.12	120.15	127.66
24	d	405	CLA	C1D-CHD-C4C	-3.12	119.33	126.06
24	b	615	CLA	O2A-CGA-CBA	3.12	121.69	111.91
26	b	624	BCR	C24-C23-C22	-3.12	121.52	126.23
26	c	915	BCR	C33-C5-C6	-3.12	121.03	124.53
24	d	406	CLA	CHD-C4C-NC	3.12	129.11	124.20
33	C	519	LMG	C4-C3-C2	3.11	116.26	110.82
26	D	406	BCR	C15-C14-C13	-3.11	122.87	127.31
24	b	617	CLA	O2A-CGA-O1A	-3.11	115.74	123.59
24	C	503	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
24	C	508	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
24	a	408	CLA	CAA-C2A-C3A	-3.11	104.27	112.78
36	L	101	LHG	O8-C23-C24	3.10	121.65	111.91
24	A	407	CLA	C1-C2-C3	-3.10	120.68	126.04
24	A	409	CLA	C1C-C2C-C3C	-3.10	103.69	106.96
33	Z	101	LMG	C1-O6-C5	3.10	119.78	113.69
24	B	604	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
24	C	503	CLA	CMB-C2B-C1B	3.10	130.09	125.37
24	b	619	CLA	C2A-C1A-CHA	-3.10	118.44	123.86
31	D	407	PL9	C36-C37-C38	-3.10	101.69	111.88
24	B	602	CLA	CHD-C4C-NC	3.10	129.09	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	CHC-C1C-C2C	-3.10	118.12	126.73
33	Y	101	LMG	O8-C28-C29	3.09	121.62	111.91
40	V	202	HEC	CHA-C1A-NA	3.09	127.78	124.44
24	d	404	CLA	CHD-C4C-NC	3.09	129.07	124.20
24	B	616	CLA	C1C-C2C-C3C	-3.09	103.71	106.96
24	B	610	CLA	CAC-C3C-C4C	3.09	128.82	124.81
24	C	502	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
24	b	611	CLA	CMC-C2C-C1C	3.09	129.74	125.04
24	B	606	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
24	C	511	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
24	B	616	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
26	Y	102	BCR	C40-C30-C25	-3.08	105.30	110.30
24	A	405	CLA	CHC-C1C-C2C	-3.08	118.18	126.73
24	c	908	CLA	C4C-C3C-C2C	-3.08	102.42	106.90
24	b	616	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
38	f	101	HEM	CHA-C4D-ND	3.07	128.16	124.37
24	B	608	CLA	CAC-C3C-C4C	3.07	128.80	124.81
24	B	608	CLA	CMC-C2C-C1C	3.07	129.72	125.04
24	b	614	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
24	B	606	CLA	C2A-C1A-CHA	-3.07	118.49	123.86
31	a	415	PL9	C10-C9-C11	3.07	120.44	115.27
37	C	518	DGD	O1G-C1A-C2A	3.07	121.55	111.91
24	a	408	CLA	C3B-C4B-NB	3.07	113.36	110.52
24	b	620	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
24	c	907	CLA	CHD-C4C-NC	3.07	129.04	124.20
35	b	603	HTG	O5-C5-C4	3.07	115.27	109.69
24	b	607	CLA	CAA-C2A-C3A	-3.07	104.37	112.78
33	B	622	LMG	O7-C10-C11	3.06	118.11	111.50
31	A	417	PL9	C27-C28-C29	-3.06	120.28	127.66
24	C	503	CLA	CHD-C4C-NC	3.06	129.03	124.20
24	c	910	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
24	c	903	CLA	CHD-C4C-NC	3.06	129.02	124.20
24	b	615	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
24	C	511	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
24	B	609	CLA	CMA-C3A-C4A	-3.05	103.56	111.77
26	B	619	BCR	C37-C22-C21	-3.05	118.65	122.92
24	b	614	CLA	CMB-C2B-C1B	3.05	130.01	125.37
24	B	603	CLA	CMA-C3A-C4A	-3.05	103.58	111.77
24	B	616	CLA	CHD-C4C-NC	3.05	129.00	124.20
24	d	405	CLA	C2A-C1A-CHA	-3.04	118.54	123.86
24	b	606	CLA	C4-C3-C5	3.04	120.39	115.27
24	C	507	CLA	C4C-C3C-C2C	-3.04	102.47	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	d	410	LHG	O8-C23-O10	-3.04	115.92	123.59
24	C	505	CLA	CMC-C2C-C1C	3.04	129.67	125.04
24	C	507	CLA	CMB-C2B-C1B	3.04	130.00	125.37
26	d	407	BCR	C7-C8-C9	-3.04	121.64	126.23
31	A	417	PL9	C45-C44-C46	3.04	120.38	115.27
25	a	407	PHO	C1A-C2A-C3A	-3.04	99.95	102.84
24	B	605	CLA	CAC-C3C-C4C	3.03	128.74	124.81
24	a	406	CLA	C2A-C1A-CHA	-3.03	118.56	123.86
24	B	615	CLA	O2A-CGA-CBA	3.03	121.42	111.91
24	B	615	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
24	c	903	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
24	C	503	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
24	c	910	CLA	CMC-C2C-C1C	3.03	129.65	125.04
24	b	607	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
24	b	613	CLA	C3B-C4B-NB	3.02	113.32	110.52
24	C	512	CLA	CMB-C2B-C1B	3.02	129.97	125.37
24	C	506	CLA	C1-C2-C3	-3.02	120.82	126.04
24	B	603	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
24	B	603	CLA	CHD-C4C-NC	3.02	128.96	124.20
24	B	607	CLA	C3B-C4B-NB	3.02	113.31	110.52
26	B	619	BCR	C29-C30-C25	3.02	115.12	110.48
26	d	407	BCR	C29-C30-C25	3.02	115.12	110.48
24	C	512	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
24	C	511	CLA	CMB-C2B-C1B	3.01	129.96	125.37
37	C	518	DGD	O2G-C1B-C2B	3.01	117.99	111.50
24	C	509	CLA	C4-C3-C5	3.01	120.34	115.27
26	T	102	BCR	C15-C14-C13	3.01	131.60	127.31
24	b	611	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
24	B	612	CLA	CMC-C2C-C1C	3.01	129.62	125.04
24	B	604	CLA	C1-O2A-CGA	3.01	124.33	116.44
24	b	618	CLA	O2A-CGA-CBA	3.01	121.34	111.91
37	D	408	DGD	O1G-C1A-C2A	3.00	121.33	111.91
24	b	620	CLA	C4-C3-C5	3.00	120.32	115.27
24	c	913	CLA	CBA-CAA-C2A	-3.00	105.01	113.86
24	C	506	CLA	C4-C3-C5	3.00	120.32	115.27
24	C	512	CLA	C1-C2-C3	-3.00	120.86	126.04
24	b	612	CLA	CHC-C1C-C2C	-3.00	118.40	126.73
24	C	511	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
24	c	914	CLA	C1-C2-C3	-2.99	120.86	126.04
24	B	604	CLA	C3B-C4B-NB	2.99	113.29	110.52
24	b	609	CLA	O2A-CGA-CBA	2.99	121.30	111.91
24	C	513	CLA	C1-C2-C3	-2.99	120.87	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608	CLA	CMC-C2C-C1C	2.99	129.59	125.04
24	A	407	CLA	CAA-C2A-C3A	-2.99	104.60	112.78
24	c	910	CLA	CHD-C4C-NC	2.99	128.91	124.20
26	C	515	BCR	C33-C5-C6	-2.99	121.17	124.53
29	M	103	LMT	O1B-C1B-C2B	2.98	115.83	108.10
24	D	404	CLA	CHC-C1C-C2C	-2.98	118.44	126.73
24	a	408	CLA	CMA-C3A-C2A	-2.98	101.80	113.83
24	a	408	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
24	c	904	CLA	C1C-C2C-C3C	-2.98	103.82	106.96
31	D	407	PL9	C45-C44-C46	2.98	120.28	115.27
26	D	406	BCR	C24-C23-C22	-2.98	121.73	126.23
37	c	918	DGD	O1G-C1A-C2A	2.98	121.25	111.91
24	b	606	CLA	CHC-C1C-C2C	-2.98	118.46	126.73
36	B	635	LHG	O8-C23-O10	-2.97	116.09	123.59
24	D	405	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
24	B	614	CLA	CBC-CAC-C3C	-2.97	104.24	112.43
24	B	611	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
36	E	101	LHG	O8-C23-C24	2.97	121.22	111.91
24	B	608	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
24	b	613	CLA	O2A-CGA-CBA	2.97	121.22	111.91
35	c	922	HTG	C1-O5-C5	2.96	118.05	112.58
24	d	405	CLA	O2A-CGA-O1A	-2.96	116.11	123.59
24	c	912	CLA	CBC-CAC-C3C	-2.96	104.26	112.43
24	a	406	CLA	CBC-CAC-C3C	-2.96	104.26	112.43
24	b	614	CLA	C3B-C4B-NB	2.96	113.26	110.52
24	a	405	CLA	C1-C2-C3	-2.96	120.92	126.04
24	B	612	CLA	C2A-C1A-CHA	-2.96	118.68	123.86
24	B	611	CLA	CHD-C4C-NC	2.96	128.87	124.20
24	B	610	CLA	CHC-C1C-C2C	-2.95	118.52	126.73
24	C	506	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
24	C	504	CLA	C4-C3-C5	2.95	120.23	115.27
24	c	910	CLA	O2A-CGA-CBA	2.95	121.16	111.91
24	C	510	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
31	d	408	PL9	C17-C18-C19	-2.95	120.56	127.66
24	C	505	CLA	CAC-C3C-C4C	2.94	128.63	124.81
24	c	903	CLA	C3B-C4B-NB	2.94	113.24	110.52
24	B	605	CLA	O2A-CGA-CBA	2.94	121.14	111.91
24	b	614	CLA	O2A-CGA-CBA	2.94	121.14	111.91
24	b	620	CLA	C3B-C4B-NB	2.94	113.24	110.52
36	b	635	LHG	O8-C23-C24	2.94	121.13	111.91
26	b	623	BCR	C29-C30-C25	2.94	115.01	110.48
24	c	904	CLA	CHD-C4C-NC	2.94	128.83	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	919	LMG	C8-O7-C10	-2.94	110.56	117.79
24	B	609	CLA	CAC-C3C-C4C	2.94	128.62	124.81
24	B	603	CLA	CMB-C2B-C1B	2.94	129.84	125.37
24	B	604	CLA	O2A-CGA-O1A	-2.94	116.18	123.59
24	B	617	CLA	C1C-C2C-C3C	-2.93	103.87	106.96
31	d	408	PL9	C12-C13-C14	-2.93	120.60	127.66
24	b	611	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
26	K	101	BCR	C20-C21-C22	-2.93	123.12	127.31
24	c	906	CLA	C1-C2-C3	-2.93	120.97	126.04
24	b	616	CLA	CAC-C3C-C4C	2.93	128.61	124.81
24	D	405	CLA	CBC-CAC-C3C	-2.93	104.35	112.43
24	C	503	CLA	C1-C2-C3	-2.93	120.98	126.04
26	K	101	BCR	C33-C5-C6	-2.93	121.24	124.53
36	D	409	LHG	O7-C7-C8	2.93	117.81	111.50
24	b	613	CLA	C1-C2-C3	-2.93	120.98	126.04
24	b	615	CLA	C3B-C4B-NB	2.93	113.23	110.52
25	d	403	PHO	CMB-C2B-C3B	2.93	130.15	124.68
24	C	507	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
40	v	202	HEC	CHA-C1A-NA	2.92	127.60	124.44
24	b	611	CLA	CHD-C4C-NC	2.92	128.81	124.20
24	b	611	CLA	C1-O2A-CGA	2.92	124.11	116.44
27	L	102	SQD	O7-S-C6	2.92	110.41	106.94
27	a	410	SQD	C1-O5-C5	-2.92	107.96	113.69
24	b	607	CLA	C2A-C1A-CHA	-2.92	118.75	123.86
24	c	913	CLA	CBC-CAC-C3C	-2.92	104.39	112.43
27	A	414	SQD	O9-S-C6	2.92	110.41	106.94
24	c	912	CLA	C1-C2-C3	-2.92	121.00	126.04
24	A	409	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
24	C	508	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	d	404	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	b	617	CLA	CHD-C4C-NC	2.91	128.79	124.20
24	c	906	CLA	CHC-C1C-C2C	-2.91	118.64	126.73
24	C	502	CLA	C3B-C4B-NB	2.91	113.22	110.52
33	c	919	LMG	O8-C28-C29	2.91	121.04	111.91
24	B	602	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
24	B	605	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
24	a	405	CLA	CAA-C2A-C1A	-2.91	102.44	111.97
24	b	619	CLA	CHD-C4C-NC	2.91	128.78	124.20
24	C	501	CLA	CAC-C3C-C4C	2.91	128.58	124.81
31	d	408	PL9	C7-C8-C9	-2.90	121.96	126.79
24	c	909	CLA	CHD-C4C-NC	2.90	128.78	124.20
26	h	101	BCR	C7-C8-C9	-2.90	121.85	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	CHD-C4C-NC	2.90	128.78	124.20
24	c	914	CLA	CMB-C2B-C1B	2.90	129.79	125.37
24	a	408	CLA	CBC-CAC-C3C	-2.90	104.44	112.43
24	A	407	CLA	C3B-C4B-NB	2.90	113.20	110.52
24	B	606	CLA	O2A-CGA-O1A	-2.90	116.28	123.59
24	B	617	CLA	CMB-C2B-C1B	2.89	129.77	125.37
24	B	610	CLA	CMC-C2C-C1C	2.89	129.44	125.04
24	b	621	CLA	C1-C2-C3	-2.89	121.04	126.04
24	c	910	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
24	b	616	CLA	CMB-C2B-C1B	2.89	129.77	125.37
24	B	617	CLA	O1D-CGD-CBD	-2.89	118.58	124.48
24	d	406	CLA	C3B-C4B-NB	2.89	113.19	110.52
24	B	607	CLA	C4-C3-C5	2.89	120.13	115.27
24	c	914	CLA	C2A-C1A-CHA	-2.88	118.82	123.86
24	B	608	CLA	C1-C2-C3	-2.88	121.06	126.04
24	b	621	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
24	B	602	CLA	CAC-C3C-C4C	2.88	128.55	124.81
24	B	609	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
24	C	512	CLA	CHD-C4C-NC	2.88	128.74	124.20
24	b	612	CLA	CMC-C2C-C1C	2.88	129.42	125.04
24	b	614	CLA	CBC-CAC-C3C	-2.88	104.50	112.43
24	c	912	CLA	CAC-C3C-C4C	2.88	128.54	124.81
24	C	501	CLA	CMB-C2B-C1B	2.88	129.75	125.37
27	L	102	SQD	O48-C23-C24	2.88	120.93	111.91
31	a	415	PL9	C53-C6-C1	2.87	120.86	114.99
24	C	513	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
24	A	407	CLA	CHC-C1C-C2C	-2.87	118.76	126.73
24	A	405	CLA	CMC-C2C-C1C	2.87	129.41	125.04
24	c	903	CLA	O2A-C1-C2	2.87	116.17	108.64
24	d	406	CLA	CAA-C2A-C3A	-2.87	104.92	112.78
24	b	610	CLA	C4-C3-C5	2.87	120.09	115.27
24	B	609	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
24	b	619	CLA	O2A-CGA-CBA	2.87	120.90	111.91
24	A	407	CLA	CBC-CAC-C3C	-2.86	104.53	112.43
24	b	607	CLA	C4-C3-C5	2.86	120.09	115.27
37	C	517	DGD	C1E-O6E-C5E	-2.86	108.07	113.69
27	a	410	SQD	O9-S-C6	2.86	110.34	106.94
24	C	513	CLA	CHD-C4C-NC	2.86	128.71	124.20
24	C	503	CLA	C3B-C4B-NB	2.86	113.17	110.52
24	C	506	CLA	CAA-C2A-C3A	-2.86	104.95	112.78
24	D	405	CLA	CAA-C2A-C3A	-2.86	104.95	112.78
40	V	202	HEC	C3B-C4B-NB	-2.86	106.98	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	102	BCR	C35-C13-C12	2.85	122.57	118.08
26	C	514	BCR	C38-C26-C25	-2.85	121.33	124.53
31	A	417	PL9	C53-C6-C1	2.85	120.82	114.99
24	b	619	CLA	CAA-C2A-C3A	-2.85	104.97	112.78
26	T	102	BCR	C21-C20-C19	-2.85	114.32	123.22
24	C	512	CLA	C3B-C4B-NB	2.85	113.16	110.52
40	v	202	HEC	C2A-C1A-NA	-2.85	107.55	110.32
24	c	905	CLA	CHD-C4C-NC	2.85	128.69	124.20
36	d	409	LHG	O7-C7-O9	-2.85	116.81	123.70
24	c	907	CLA	CAA-C2A-C3A	-2.85	104.97	112.78
24	B	612	CLA	CHD-C4C-NC	2.85	128.69	124.20
24	C	511	CLA	O2A-CGA-CBA	2.85	120.84	111.91
24	c	912	CLA	C4-C3-C5	2.85	120.06	115.27
26	C	515	BCR	C3-C4-C5	-2.85	109.00	114.08
24	c	903	CLA	O2A-CGA-CBA	2.84	120.83	111.91
24	c	912	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
24	B	604	CLA	CMC-C2C-C1C	2.84	129.37	125.04
31	a	415	PL9	C37-C38-C39	-2.84	120.82	127.66
24	c	903	CLA	CHC-C1C-C2C	-2.84	118.84	126.73
25	D	401	PHO	CED-O2D-CGD	2.84	122.36	115.94
24	B	614	CLA	CMC-C2C-C1C	2.84	129.36	125.04
24	B	604	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
24	b	608	CLA	C2A-C1A-CHA	-2.84	118.90	123.86
24	B	607	CLA	O2A-CGA-O1A	-2.83	116.44	123.59
24	b	608	CLA	CHC-C1C-C2C	-2.83	118.86	126.73
24	B	614	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
27	F	103	SQD	C44-O6-C1	-2.83	108.21	113.74
24	c	902	CLA	O2A-CGA-CBA	2.83	120.79	111.91
24	b	615	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
38	F	102	HEM	CHA-C1A-NA	2.83	129.05	123.85
24	c	909	CLA	O2A-CGA-CBA	2.83	120.78	111.91
24	b	607	CLA	CMB-C2B-C1B	2.83	129.68	125.37
24	C	511	CLA	CHC-C1C-C2C	-2.83	118.88	126.73
24	B	613	CLA	C2A-C1A-CHA	-2.83	118.92	123.86
24	B	613	CLA	CMB-C2B-C1B	2.83	129.67	125.37
24	a	408	CLA	O2A-CGA-CBA	2.83	120.78	111.91
31	D	407	PL9	C36-C34-C33	-2.83	115.40	121.12
24	B	603	CLA	C1-O2A-CGA	2.83	123.86	116.44
24	C	502	CLA	CMC-C2C-C1C	2.83	129.34	125.04
24	B	602	CLA	CMB-C2B-C1B	2.82	129.67	125.37
24	c	911	CLA	CHD-C4C-NC	2.82	128.65	124.20
24	B	603	CLA	CHC-C1C-C2C	-2.82	118.89	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407	CLA	CHD-C4C-NC	2.82	128.65	124.20
27	A	411	SQD	O9-S-C6	2.82	110.29	106.94
24	B	605	CLA	CMC-C2C-C1C	2.82	129.33	125.04
26	C	514	BCR	C11-C10-C9	-2.82	123.29	127.31
24	c	905	CLA	C2A-C1A-CHA	-2.82	118.93	123.86
24	B	602	CLA	CHC-C1C-C2C	-2.82	118.91	126.73
24	b	618	CLA	CHB-C1B-NB	-2.82	121.28	124.26
24	b	617	CLA	C3B-C4B-NB	2.81	113.13	110.52
24	b	613	CLA	C2A-C1A-CHA	-2.81	118.94	123.86
31	D	407	PL9	C12-C13-C14	-2.81	120.89	127.66
24	C	508	CLA	O2A-CGA-CBA	2.81	120.73	111.91
24	C	509	CLA	O2A-CGA-CBA	2.81	120.73	111.91
33	Z	101	LMG	C9-O8-C28	2.81	124.17	117.10
24	B	609	CLA	CMC-C2C-C1C	2.81	129.32	125.04
40	V	202	HEC	CAB-C3B-C4B	2.81	128.46	124.81
24	b	606	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
31	A	417	PL9	C12-C13-C14	-2.81	120.90	127.66
24	B	615	CLA	C2A-C1A-CHA	-2.81	118.95	123.86
26	k	101	BCR	C24-C23-C22	-2.81	122.00	126.23
24	b	609	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
24	B	615	CLA	CMB-C2B-C1B	2.81	129.64	125.37
24	B	603	CLA	C1-C2-C3	-2.81	121.19	126.04
24	B	610	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
27	a	410	SQD	C44-O6-C1	-2.80	108.26	113.74
24	a	406	CLA	CAC-C3C-C4C	2.80	128.44	124.81
27	L	102	SQD	O8-S-C6	2.80	110.20	105.74
24	B	606	CLA	O2A-CGA-CBA	2.80	120.69	111.91
24	b	609	CLA	CHC-C1C-C2C	-2.80	118.95	126.73
35	V	203	HTG	C1-C2-C3	-2.80	105.06	110.59
24	C	502	CLA	CHD-C4C-NC	2.80	128.61	124.20
31	D	407	PL9	C51-C49-C50	2.80	120.78	114.60
24	b	607	CLA	CHD-C4C-NC	2.80	128.61	124.20
26	y	101	BCR	C24-C23-C22	-2.79	122.01	126.23
24	B	608	CLA	C1-O2A-CGA	2.79	123.78	116.44
24	d	404	CLA	C4-C3-C5	2.79	119.97	115.27
24	D	404	CLA	CHD-C4C-NC	2.79	128.60	124.20
24	C	502	CLA	CHC-C1C-C2C	-2.79	118.97	126.73
24	c	906	CLA	C4-C3-C5	2.79	119.97	115.27
27	A	414	SQD	O48-C23-O10	-2.79	116.55	123.59
31	a	415	PL9	C7-C3-C2	-2.79	119.63	123.30
26	c	927	BCR	C11-C10-C9	-2.79	123.33	127.31
26	C	515	BCR	C11-C10-C9	-2.79	123.33	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	909	CLA	CBC-CAC-C3C	-2.79	104.74	112.43
24	c	908	CLA	C1-C2-C3	-2.79	121.22	126.04
24	b	620	CLA	CAC-C3C-C4C	2.79	128.43	124.81
24	c	913	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
24	D	405	CLA	CHC-C1C-C2C	-2.79	118.99	126.73
24	D	404	CLA	CMC-C2C-C1C	2.79	129.28	125.04
24	c	902	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
24	C	502	CLA	O2A-CGA-CBA	2.79	120.65	111.91
33	Z	101	LMG	O6-C5-C4	2.78	114.75	109.69
24	d	406	CLA	CBC-CAC-C3C	-2.78	104.76	112.43
27	f	102	SQD	O5-C5-C4	2.78	114.75	109.69
24	A	409	CLA	C3B-C4B-NB	2.78	113.10	110.52
26	c	927	BCR	C28-C27-C26	-2.78	109.11	114.08
24	C	503	CLA	C4-C3-C5	2.78	119.95	115.27
24	B	608	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
40	V	202	HEC	C1D-ND-C4D	2.78	107.94	105.07
24	c	906	CLA	CAC-C3C-C4C	2.78	128.41	124.81
24	c	908	CLA	C4-C3-C5	2.78	119.94	115.27
31	a	415	PL9	C40-C39-C41	2.78	119.94	115.27
24	c	902	CLA	C4C-C3C-C2C	-2.77	102.85	106.90
40	v	202	HEC	CHD-C1D-ND	2.77	127.79	124.37
37	C	517	DGD	O1G-C1A-C2A	2.77	120.61	111.91
24	B	612	CLA	CHC-C1C-C2C	-2.77	119.03	126.73
24	c	905	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
24	d	404	CLA	CMA-C3A-C2A	-2.77	102.65	113.83
24	b	608	CLA	O2A-CGA-CBA	2.77	120.61	111.91
27	a	410	SQD	O48-C23-C24	2.77	120.61	111.91
24	a	408	CLA	CMB-C2B-C1B	2.77	129.59	125.37
24	c	910	CLA	C4-C3-C5	2.77	119.93	115.27
24	b	606	CLA	C3B-C4B-NB	2.77	113.08	110.52
24	C	509	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
24	b	613	CLA	CHC-C1C-C2C	-2.77	119.05	126.73
24	C	509	CLA	C1-O2A-CGA	2.77	123.70	116.44
24	B	616	CLA	C3B-C4B-NB	2.77	113.08	110.52
24	B	617	CLA	CHC-C1C-C2C	-2.76	119.05	126.73
24	B	608	CLA	CHC-C1C-C2C	-2.76	119.05	126.73
26	B	620	BCR	C38-C26-C25	-2.76	121.43	124.53
29	M	103	LMT	O5'-C5'-C4'	2.76	115.57	109.75
24	d	406	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
24	B	615	CLA	C1-O2A-CGA	2.76	123.68	116.44
24	b	621	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
24	B	614	CLA	CAC-C3C-C4C	2.75	128.38	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	402	SQD	C3-C4-C5	2.75	115.14	110.24
29	A	415	LMT	C4B-C3B-C2B	-2.75	106.02	110.82
24	B	607	CLA	CHC-C1C-C2C	-2.75	119.09	126.73
24	c	909	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
35	C	521	HTG	C1-O5-C5	2.75	117.65	112.58
24	c	909	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
24	d	405	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
24	C	513	CLA	CHC-C1C-C2C	-2.75	119.10	126.73
27	F	103	SQD	O6-C1-C2	2.74	112.59	108.30
24	B	610	CLA	CHD-C4C-NC	2.74	128.53	124.20
24	b	620	CLA	CMC-C2C-C1C	2.74	129.22	125.04
24	B	607	CLA	CAA-C2A-C3A	-2.74	105.27	112.78
24	B	607	CLA	O2A-CGA-CBA	2.74	120.51	111.91
24	c	905	CLA	CAC-C3C-C4C	2.74	128.37	124.81
24	c	912	CLA	C3B-C4B-NB	2.74	113.06	110.52
24	c	902	CLA	CMB-C2B-C1B	2.74	129.53	125.37
24	D	404	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
24	b	612	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
24	b	614	CLA	CHC-C1C-C2C	-2.73	119.14	126.73
24	c	911	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
24	C	504	CLA	CHC-C1C-C2C	-2.73	119.14	126.73
24	B	606	CLA	CAC-C3C-C4C	2.73	128.35	124.81
24	A	405	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
24	C	501	CLA	CHC-C1C-C2C	-2.73	119.15	126.73
36	d	409	LHG	O8-C23-C24	2.73	120.47	111.91
24	a	408	CLA	CHC-C1C-C2C	-2.73	119.15	126.73
24	A	409	CLA	CHC-C1C-C2C	-2.73	119.15	126.73
24	b	607	CLA	C1-C2-C3	-2.73	121.33	126.04
24	A	407	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
25	d	403	PHO	C1A-C2A-C3A	-2.73	100.25	102.84
24	c	905	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
24	C	510	CLA	CMC-C2C-C1C	2.72	129.19	125.04
26	t	102	BCR	C12-C13-C14	-2.72	114.76	118.94
24	C	512	CLA	CHC-C1C-C2C	-2.72	119.17	126.73
27	L	102	SQD	O47-C7-O49	-2.72	117.13	123.70
24	b	620	CLA	CHC-C1C-C2C	-2.72	119.18	126.73
26	c	927	BCR	C33-C5-C6	-2.72	121.48	124.53
24	B	609	CLA	CBC-CAC-C3C	-2.71	104.95	112.43
24	b	619	CLA	CBC-CAC-C3C	-2.71	104.95	112.43
24	B	616	CLA	CHC-C1C-C2C	-2.71	119.20	126.73
24	C	513	CLA	CBC-CAC-C3C	-2.71	104.96	112.43
26	b	624	BCR	C2-C1-C6	2.71	114.65	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	913	CLA	C3B-C4B-NB	2.71	113.03	110.52
24	b	619	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
24	c	910	CLA	CHC-C1C-C2C	-2.71	119.21	126.73
24	c	911	CLA	O2A-CGA-CBA	2.71	120.40	111.91
26	k	101	BCR	C34-C9-C8	2.71	122.34	118.08
24	c	905	CLA	CAA-C2A-C3A	-2.71	105.37	112.78
24	C	513	CLA	C3B-C4B-NB	2.71	113.03	110.52
25	D	401	PHO	CMB-C2B-C3B	2.71	129.74	124.68
24	c	907	CLA	C4-C3-C5	2.71	119.82	115.27
24	c	914	CLA	CED-O2D-CGD	2.70	122.05	115.94
24	B	614	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
24	C	501	CLA	CHD-C4C-NC	2.70	128.46	124.20
24	C	513	CLA	CMC-C2C-C1C	2.70	129.15	125.04
24	D	404	CLA	CAA-C2A-C3A	-2.70	105.38	112.78
37	h	102	DGD	O1G-C1A-C2A	2.70	120.39	111.91
24	c	914	CLA	CBC-CAC-C3C	-2.70	104.98	112.43
24	B	603	CLA	C3B-C4B-NB	2.70	113.02	110.52
24	c	904	CLA	C4-C3-C5	2.70	119.81	115.27
24	C	507	CLA	O2A-CGA-CBA	2.70	120.38	111.91
26	c	915	BCR	C16-C17-C18	-2.70	123.46	127.31
24	b	621	CLA	CHD-C4C-NC	2.69	128.45	124.20
24	c	908	CLA	CHD-C4C-NC	2.69	128.45	124.20
25	D	401	PHO	C4-C3-C5	2.69	119.80	115.27
24	c	910	CLA	CAC-C3C-C4C	2.69	128.30	124.81
25	A	408	PHO	C1-O2A-CGA	2.69	123.50	116.44
24	A	405	CLA	CHB-C1B-NB	-2.69	121.41	124.26
33	A	419	LMG	O1-C1-C2	2.69	112.50	108.30
24	B	607	CLA	CHD-C4C-NC	2.69	128.44	124.20
24	c	908	CLA	CAC-C3C-C4C	2.69	128.29	124.81
27	f	102	SQD	O47-C7-O49	-2.69	117.21	123.70
24	B	609	CLA	C4C-C3C-C2C	-2.68	102.98	106.90
24	C	510	CLA	CHC-C1C-C2C	-2.68	119.28	126.73
24	a	406	CLA	O2A-CGA-CBA	2.68	120.32	111.91
24	d	405	CLA	C4-C3-C5	2.68	119.78	115.27
26	B	619	BCR	C31-C1-C6	-2.68	105.95	110.30
24	c	914	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
24	C	503	CLA	CHC-C1C-C2C	-2.68	119.29	126.73
33	z	101	LMG	O8-C28-C29	2.68	120.30	111.91
24	B	613	CLA	O2A-CGA-CBA	2.67	120.30	111.91
24	B	609	CLA	CHD-C4C-NC	2.67	128.42	124.20
35	C	522	HTG	O5-C5-C4	2.67	114.55	109.69
24	d	405	CLA	CHC-C1C-C2C	-2.67	119.31	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
24	C	508	CLA	C1-C2-C3	-2.67	121.42	126.04
24	a	406	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
24	a	408	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
24	c	913	CLA	CHC-C1C-C2C	-2.67	119.32	126.73
24	b	612	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
24	d	404	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
24	A	409	CLA	C1-C2-C3	-2.67	121.43	126.04
24	c	905	CLA	CHC-C1C-C2C	-2.67	119.32	126.73
24	c	912	CLA	CHC-C1C-C2C	-2.66	119.33	126.73
38	F	102	HEM	CHB-C1B-NB	2.66	127.66	124.37
24	d	406	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
31	D	407	PL9	C35-C34-C36	2.66	119.75	115.27
26	K	101	BCR	C24-C23-C22	-2.66	122.22	126.23
26	b	623	BCR	C38-C26-C25	-2.66	121.54	124.53
24	C	505	CLA	CHC-C1C-C2C	-2.66	119.34	126.73
31	D	407	PL9	C42-C41-C39	-2.66	104.24	112.98
24	b	616	CLA	O2A-CGA-CBA	2.65	120.24	111.91
24	b	609	CLA	CAC-C3C-C4C	2.65	128.25	124.81
33	b	625	LMG	O8-C28-O10	-2.65	116.89	123.59
38	f	101	HEM	C4A-NA-C1A	2.65	107.95	105.35
24	B	617	CLA	CHB-C1B-NB	-2.65	121.45	124.26
36	D	410	LHG	O8-C23-O10	-2.65	116.90	123.59
24	C	509	CLA	CMC-C2C-C1C	2.65	129.07	125.04
24	b	607	CLA	C3B-C4B-NB	2.65	112.97	110.52
26	B	620	BCR	C32-C1-C6	-2.65	106.01	110.30
24	c	914	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
24	C	511	CLA	CHD-C4C-NC	2.64	128.37	124.20
24	b	618	CLA	O2A-CGA-O1A	-2.64	116.92	123.59
24	b	606	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
24	a	405	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
24	c	906	CLA	C3B-C4B-NB	2.64	112.96	110.52
33	a	411	LMG	O8-C28-C29	2.64	120.19	111.91
24	b	619	CLA	C3B-C4B-NB	2.64	112.96	110.52
29	M	103	LMT	O1'-C1'-C2'	2.64	112.42	108.30
24	C	503	CLA	O2A-CGA-CBA	2.64	120.18	111.91
24	d	406	CLA	O2A-CGA-CBA	2.63	120.17	111.91
24	c	907	CLA	CMC-C2C-C1C	2.63	129.05	125.04
26	B	620	BCR	C15-C14-C13	-2.63	123.56	127.31
24	C	512	CLA	C4-C3-C5	2.63	119.69	115.27
24	c	913	CLA	CMC-C2C-C1C	2.63	129.04	125.04
25	d	403	PHO	O2D-CGD-O1D	-2.63	118.70	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	101	BCR	C24-C23-C22	-2.62	122.27	126.23
26	T	102	BCR	C34-C9-C10	-2.62	119.25	122.92
24	C	512	CLA	C1-O2A-CGA	2.62	123.33	116.44
26	y	101	BCR	C10-C11-C12	-2.62	115.03	123.22
24	C	509	CLA	CHC-C1C-C2C	-2.62	119.45	126.73
24	b	615	CLA	CHD-C4C-NC	2.62	128.34	124.20
24	B	614	CLA	O2A-CGA-CBA	2.62	120.13	111.91
27	F	103	SQD	O48-C23-C24	2.62	120.13	111.91
24	C	513	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
26	B	619	BCR	C24-C23-C22	-2.62	122.28	126.23
24	B	611	CLA	CBC-CAC-C3C	-2.62	105.21	112.43
24	c	907	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
24	B	603	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
26	B	620	BCR	C10-C11-C12	-2.62	115.05	123.22
24	C	506	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
24	C	509	CLA	CHD-C4C-NC	2.62	128.33	124.20
26	h	101	BCR	C11-C10-C9	-2.62	123.58	127.31
40	V	202	HEC	CMD-C2D-C1D	2.62	129.02	125.04
31	D	407	PL9	C40-C39-C38	-2.62	116.97	123.68
24	d	405	CLA	CMC-C2C-C1C	2.61	129.02	125.04
24	A	407	CLA	CAC-C3C-C4C	2.61	128.20	124.81
24	A	409	CLA	CMC-C2C-C1C	2.61	129.02	125.04
24	b	606	CLA	CMB-C2B-C1B	2.61	129.35	125.37
24	b	607	CLA	CHC-C1C-C2C	-2.61	119.48	126.73
24	A	406	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
24	C	512	CLA	O2A-CGA-CBA	2.61	120.10	111.91
24	c	911	CLA	CMB-C2B-C1B	2.61	129.34	125.37
24	D	404	CLA	O2A-CGA-CBA	2.61	120.09	111.91
24	c	912	CLA	O2A-CGA-CBA	2.61	120.09	111.91
36	L	101	LHG	O8-C23-O10	-2.61	117.01	123.59
24	b	613	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
24	b	615	CLA	C4-C3-C5	2.61	119.66	115.27
24	A	406	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
33	Z	101	LMG	C1-C2-C3	2.61	115.42	110.00
26	B	620	BCR	C29-C30-C25	2.60	114.49	110.48
24	c	905	CLA	C3B-C4B-NB	2.60	112.93	110.52
24	d	404	CLA	O2A-CGA-O1A	-2.60	117.02	123.59
37	C	516	DGD	C3G-C2G-C1G	-2.60	105.63	111.79
24	b	607	CLA	CAC-C3C-C4C	2.60	128.19	124.81
24	a	406	CLA	C4C-C3C-C2C	-2.60	103.10	106.90
24	a	406	CLA	CHC-C1C-C2C	-2.60	119.51	126.73
24	d	406	CLA	CAC-C3C-C4C	2.60	128.18	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	c	916	DGD	C2G-O2G-C1B	-2.60	111.39	117.79
24	B	617	CLA	O2A-CGA-CBA	2.60	120.06	111.91
26	A	410	BCR	C8-C7-C6	-2.60	119.90	127.20
29	m	103	LMT	O5'-C5'-C4'	2.60	115.23	109.75
24	B	613	CLA	CHB-C1B-NB	-2.60	121.51	124.26
24	C	507	CLA	O2A-CGA-O1A	-2.60	117.04	123.59
24	c	909	CLA	C4-C3-C5	2.60	119.64	115.27
24	c	914	CLA	C4-C3-C5	2.60	119.64	115.27
24	c	902	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
26	Y	102	BCR	C21-C20-C19	-2.59	115.12	123.22
26	d	407	BCR	C10-C11-C12	-2.59	115.12	123.22
24	C	512	CLA	CMC-C2C-C1C	2.59	128.99	125.04
24	b	620	CLA	O2A-CGA-CBA	2.59	120.04	111.91
24	c	913	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
35	B	624	HTG	O5-C1-C2	2.59	113.57	110.31
37	c	917	DGD	O1G-C1A-C2A	2.59	120.04	111.91
27	A	411	SQD	O48-C23-C24	2.59	120.04	111.91
24	b	614	CLA	C1-C2-C3	-2.59	121.56	126.04
24	C	503	CLA	CAC-C3C-C4C	2.59	128.17	124.81
27	A	411	SQD	C1-C2-C3	-2.59	104.61	110.00
24	a	408	CLA	C2A-C1A-CHA	-2.59	119.34	123.86
37	c	918	DGD	C2G-O2G-C1B	-2.59	111.43	117.79
24	B	603	CLA	CMC-C2C-C1C	2.58	128.97	125.04
24	b	613	CLA	CMC-C2C-C1C	2.58	128.97	125.04
24	C	513	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
24	A	407	CLA	C2A-C1A-CHA	-2.58	119.34	123.86
24	b	611	CLA	C4C-C3C-C2C	-2.58	103.13	106.90
31	D	407	PL9	C27-C28-C29	-2.58	121.44	127.66
37	e	101	DGD	O5D-C1E-C2E	2.58	112.33	108.30
24	b	614	CLA	C4-C3-C5	2.58	119.61	115.27
37	C	516	DGD	O3G-C3G-C2G	-2.58	104.67	110.90
35	b	603	HTG	C1-O5-C5	2.58	117.33	112.58
26	b	624	BCR	C3-C4-C5	-2.58	109.48	114.08
25	a	407	PHO	CMC-C2C-C1C	2.58	129.59	124.73
26	C	515	BCR	C28-C27-C26	-2.58	109.48	114.08
24	d	406	CLA	C4-C3-C5	2.57	119.60	115.27
25	A	408	PHO	O1D-CGD-CBD	-2.57	120.45	124.74
24	b	615	CLA	CMC-C2C-C1C	2.57	128.96	125.04
24	b	608	CLA	O2A-CGA-O1A	-2.57	117.11	123.59
24	d	405	CLA	CAC-C3C-C4C	2.57	128.14	124.81
24	b	616	CLA	CBC-CAC-C3C	-2.57	105.35	112.43
24	D	405	CLA	C2A-C1A-CHA	-2.57	119.37	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608	CLA	CBC-CAC-C3C	-2.57	105.35	112.43
24	C	513	CLA	C4-C3-C5	2.57	119.59	115.27
27	a	410	SQD	C45-O47-C7	-2.57	111.47	117.79
36	d	409	LHG	O8-C23-O10	-2.57	117.11	123.59
24	c	906	CLA	CHD-C4C-NC	2.57	128.25	124.20
24	C	513	CLA	O2A-CGA-CBA	2.57	119.96	111.91
24	b	615	CLA	CMA-C3A-C4A	-2.56	104.88	111.77
38	f	101	HEM	CHB-C1B-NB	2.56	127.54	124.37
26	Y	102	BCR	C10-C11-C12	-2.56	115.22	123.22
24	A	405	CLA	C4C-C3C-C2C	-2.56	103.16	106.90
35	C	522	HTG	O5-C1-C2	2.56	113.54	110.31
24	a	406	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
36	L	101	LHG	C5-O7-C7	-2.56	111.48	117.79
27	A	414	SQD	O8-S-C6	2.56	109.82	105.74
24	c	909	CLA	O2A-CGA-O1A	-2.56	117.13	123.59
24	C	502	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
24	D	405	CLA	CMC-C2C-C1C	2.56	128.94	125.04
24	b	621	CLA	CHB-C1B-NB	-2.56	121.55	124.26
24	A	405	CLA	CMA-C3A-C4A	-2.55	104.91	111.77
33	A	419	LMG	C7-O1-C1	-2.55	108.75	113.74
24	A	409	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
26	K	101	BCR	C10-C11-C12	-2.55	115.26	123.22
24	a	406	CLA	C3B-C4B-NB	2.55	112.88	110.52
24	b	616	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
36	d	409	LHG	C5-O7-C7	-2.55	111.52	117.79
26	C	514	BCR	C16-C17-C18	-2.55	123.67	127.31
26	c	915	BCR	C7-C8-C9	-2.55	122.39	126.23
31	A	417	PL9	C30-C29-C31	2.55	119.56	115.27
31	A	417	PL9	C17-C18-C19	-2.55	121.53	127.66
29	t	101	LMT	C1'-O5'-C5'	2.55	118.68	113.69
24	B	611	CLA	C4-C3-C5	2.54	119.55	115.27
26	t	102	BCR	C29-C28-C27	-2.54	105.69	111.38
24	c	908	CLA	CHC-C1C-C2C	-2.54	119.66	126.73
24	b	621	CLA	CMB-C2B-C1B	2.54	129.24	125.37
35	b	627	HTG	C1-C2-C3	2.54	115.61	110.59
24	B	612	CLA	CAC-C3C-C4C	2.54	128.11	124.81
24	b	616	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
24	b	616	CLA	CHD-C4C-NC	2.54	128.21	124.20
24	d	406	CLA	CHC-C1C-C2C	-2.54	119.67	126.73
24	c	913	CLA	O2A-CGA-CBA	2.54	119.88	111.91
24	b	608	CLA	C4C-C3C-C2C	-2.54	103.19	106.90
24	b	608	CLA	CHD-C4C-NC	2.54	128.21	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	602	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
27	B	621	SQD	O48-C23-C24	2.54	119.87	111.91
24	a	405	CLA	CHD-C4C-NC	2.54	128.20	124.20
25	A	408	PHO	O2D-CGD-O1D	-2.54	118.88	123.84
24	c	911	CLA	CAC-C3C-C4C	2.54	128.10	124.81
40	V	202	HEC	CHD-C1D-ND	2.53	127.50	124.37
24	b	620	CLA	O2A-CGA-O1A	-2.53	117.20	123.59
24	C	506	CLA	CMC-C2C-C1C	2.53	128.89	125.04
26	h	101	BCR	C10-C11-C12	-2.53	115.33	123.22
24	b	619	CLA	CHC-C1C-C2C	-2.53	119.71	126.73
25	d	403	PHO	C4A-C3A-C2A	-2.53	100.44	102.84
27	L	102	SQD	C1-C2-C3	-2.52	104.74	110.00
24	d	406	CLA	O2A-CGA-O1A	-2.52	117.22	123.59
26	t	102	BCR	C1-C6-C7	2.52	122.91	115.78
31	A	417	PL9	C15-C14-C16	2.52	119.51	115.27
31	a	415	PL9	C30-C29-C31	2.52	119.51	115.27
24	B	612	CLA	CMA-C3A-C4A	-2.52	105.00	111.77
26	B	619	BCR	C2-C1-C6	2.52	114.36	110.48
24	b	617	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
24	b	609	CLA	O1D-CGD-CBD	-2.52	119.33	124.48
38	F	102	HEM	C4D-ND-C1D	2.52	107.67	105.07
24	B	612	CLA	C4-C3-C5	2.51	119.50	115.27
24	b	610	CLA	CMC-C2C-C1C	2.51	128.86	125.04
24	C	513	CLA	CAC-C3C-C4C	2.51	128.07	124.81
31	a	415	PL9	C25-C24-C26	2.51	119.49	115.27
26	C	515	BCR	C21-C20-C19	-2.51	115.38	123.22
24	b	609	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
24	c	904	CLA	O2A-CGA-CBA	2.51	119.78	111.91
24	C	503	CLA	CMC-C2C-C1C	2.51	128.86	125.04
24	b	610	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
24	B	612	CLA	CBC-CAC-C3C	-2.51	105.52	112.43
24	B	605	CLA	CHB-C1B-NB	-2.51	121.60	124.26
24	C	512	CLA	CAC-C3C-C4C	2.51	128.06	124.81
24	B	614	CLA	CHB-C1B-NB	-2.51	121.61	124.26
24	b	607	CLA	CMA-C3A-C2A	-2.50	103.74	113.83
24	c	905	CLA	CBC-CAC-C3C	-2.50	105.54	112.43
24	B	605	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
24	B	613	CLA	CHC-C1C-C2C	-2.50	119.79	126.73
36	D	409	LHG	O8-C23-O10	-2.50	117.29	123.59
24	B	612	CLA	C11-C12-C13	-2.50	107.85	115.92
24	A	406	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
24	C	511	CLA	CHB-C1B-NB	-2.50	121.61	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	516	DGD	O6D-C5D-C6D	2.49	111.70	106.67
26	C	515	BCR	C15-C16-C17	-2.49	118.37	123.47
24	C	510	CLA	CAC-C3C-C4C	2.49	128.04	124.81
24	A	409	CLA	CHD-C4C-NC	2.49	128.13	124.20
24	b	610	CLA	C3B-C4B-NB	2.49	112.83	110.52
24	b	612	CLA	CHD-C4C-NC	2.49	128.13	124.20
24	B	613	CLA	CHD-C4C-NC	2.49	128.12	124.20
24	B	614	CLA	CHD-C4C-NC	2.49	128.12	124.20
24	B	614	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	b	620	CLA	C11-C10-C8	-2.49	107.88	115.92
24	A	406	CLA	O2A-CGA-CBA	2.48	119.71	111.91
24	b	607	CLA	O2A-CGA-CBA	2.48	119.70	111.91
24	c	904	CLA	CMC-C2C-C1C	2.48	128.82	125.04
25	a	407	PHO	CMA-C3A-C4A	-2.48	108.94	114.38
27	B	621	SQD	O47-C7-O49	-2.48	117.70	123.70
36	d	411	LHG	O8-C23-C24	2.48	119.70	111.91
31	A	417	PL9	C25-C24-C26	2.48	119.45	115.27
24	C	504	CLA	C4C-C3C-C2C	-2.48	103.28	106.90
24	D	404	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
37	H	102	DGD	O1G-C1A-C2A	2.48	119.69	111.91
36	a	418	LHG	O8-C23-C24	2.48	119.69	111.91
24	b	612	CLA	CAC-C3C-C4C	2.48	128.02	124.81
24	C	501	CLA	C3B-C4B-NB	2.47	112.81	110.52
24	c	911	CLA	O1D-CGD-CBD	-2.47	119.42	124.48
24	B	617	CLA	C4-C3-C5	2.47	119.43	115.27
24	B	614	CLA	CMA-C3A-C4A	-2.47	105.12	111.77
36	d	410	LHG	O8-C23-C24	2.47	119.67	111.91
24	c	914	CLA	O2A-CGA-CBA	2.47	119.67	111.91
33	c	920	LMG	O8-C28-C29	2.47	119.66	111.91
24	b	617	CLA	CHC-C1C-C2C	-2.47	119.87	126.73
24	C	508	CLA	CHD-C4C-NC	2.47	128.09	124.20
27	L	102	SQD	C44-O6-C1	-2.47	108.92	113.74
24	c	914	CLA	CHC-C1C-C2C	-2.47	119.88	126.73
24	d	405	CLA	C3B-C4B-NB	2.47	112.80	110.52
24	C	510	CLA	O1D-CGD-CBD	-2.47	119.44	124.48
24	C	508	CLA	C2A-C1A-CHA	-2.47	119.55	123.86
26	H	101	BCR	C16-C15-C14	-2.47	118.42	123.47
24	a	406	CLA	C4-C3-C5	2.46	119.42	115.27
24	c	905	CLA	C1-C2-C3	-2.46	121.78	126.04
24	b	610	CLA	CHC-C1C-C2C	-2.46	119.89	126.73
26	c	927	BCR	C20-C21-C22	-2.46	123.80	127.31
24	C	505	CLA	CHD-C4C-NC	2.46	128.08	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	604	CLA	CHC-C1C-C2C	-2.46	119.89	126.73
24	B	608	CLA	CHD-C4C-NC	2.46	128.08	124.20
37	D	408	DGD	O6D-C5D-C6D	2.46	111.63	106.67
24	B	615	CLA	CHD-C4C-NC	2.46	128.08	124.20
25	D	401	PHO	C4D-CHA-CBD	2.46	109.63	108.52
24	b	620	CLA	C1-C2-C3	-2.46	121.80	126.04
24	A	405	CLA	CAA-C2A-C1A	-2.45	103.93	111.97
24	b	617	CLA	CMC-C2C-C1C	2.45	128.78	125.04
24	C	501	CLA	C4C-C3C-C2C	-2.45	103.33	106.90
37	e	101	DGD	C1E-O6E-C5E	2.45	118.49	113.69
24	C	505	CLA	C3B-C4B-NB	2.45	112.78	110.52
24	b	621	CLA	C1C-C2C-C3C	-2.45	104.39	106.96
24	d	406	CLA	CHB-C1B-NB	-2.45	121.67	124.26
24	C	504	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
24	c	909	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
27	a	402	SQD	O48-C23-O10	-2.44	117.43	123.59
31	d	408	PL9	C36-C37-C38	-2.44	103.87	111.88
24	B	614	CLA	CED-O2D-CGD	2.44	121.45	115.94
25	a	407	PHO	CBA-CAA-C2A	-2.44	106.69	113.81
37	e	101	DGD	O1G-C1A-C2A	2.44	119.56	111.91
24	C	510	CLA	CMB-C2B-C1B	2.44	129.08	125.37
24	b	621	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
25	d	403	PHO	O1D-CGD-CBD	-2.44	120.68	124.74
26	b	624	BCR	C38-C26-C25	-2.44	121.79	124.53
24	B	604	CLA	C4-C3-C5	2.44	119.37	115.27
24	c	907	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
38	F	102	HEM	CBD-CAD-C3D	-2.43	105.87	112.63
24	c	903	CLA	CAC-C3C-C4C	2.43	127.97	124.81
24	c	902	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
24	B	609	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
24	b	612	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
26	c	927	BCR	C38-C26-C25	-2.43	121.80	124.53
24	c	913	CLA	O1D-CGD-CBD	-2.43	119.52	124.48
37	H	102	DGD	O6D-C5D-C6D	2.42	111.56	106.67
24	C	510	CLA	O2A-CGA-CBA	2.42	119.51	111.91
27	A	411	SQD	O47-C7-O49	-2.42	117.85	123.70
31	d	408	PL9	C30-C29-C31	2.42	119.35	115.27
26	C	515	BCR	C37-C22-C23	2.42	121.89	118.08
24	D	404	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
24	b	613	CLA	CMB-C2B-C1B	2.42	129.06	125.37
24	B	608	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
26	Y	102	BCR	C38-C26-C25	-2.42	121.81	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	101	BCR	C11-C10-C9	-2.42	123.86	127.31
24	C	510	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
24	c	907	CLA	CAC-C3C-C4C	2.42	127.95	124.81
26	y	101	BCR	C40-C30-C25	-2.42	106.38	110.30
24	d	404	CLA	CMB-C2B-C1B	2.42	129.05	125.37
24	A	409	CLA	O2A-CGA-CBA	2.42	119.50	111.91
24	c	911	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
37	h	102	DGD	O6E-C5E-C6E	2.41	112.44	106.44
31	a	415	PL9	C51-C49-C50	2.41	119.93	114.60
24	c	906	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
24	A	405	CLA	CHD-C4C-NC	2.41	128.00	124.20
37	C	517	DGD	O1G-C1A-O1A	-2.41	117.52	123.59
31	d	408	PL9	C45-C44-C46	2.41	119.32	115.27
31	D	407	PL9	C31-C32-C33	-2.40	103.98	111.88
24	b	617	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
35	b	627	HTG	O2-C2-C3	-2.40	104.80	110.35
24	b	615	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
33	d	415	LMG	O6-C5-C4	2.40	114.05	109.69
27	L	102	SQD	O5-C5-C4	2.40	114.05	109.69
35	c	922	HTG	O5-C5-C4	2.40	114.04	109.69
24	B	614	CLA	C4-C3-C5	2.39	119.30	115.27
24	C	504	CLA	CHD-C4C-NC	2.39	127.97	124.20
24	b	612	CLA	CAA-CBA-CGA	2.39	120.24	113.25
24	b	619	CLA	C1-O2A-CGA	2.39	122.72	116.44
24	B	617	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
31	d	408	PL9	C51-C49-C50	2.39	119.88	114.60
31	D	407	PL9	C7-C3-C4	2.39	118.82	116.88
24	C	506	CLA	C2A-C1A-CHA	-2.39	119.69	123.86
24	c	904	CLA	CAC-C3C-C4C	2.39	127.91	124.81
25	D	401	PHO	O2A-CGA-CBA	2.39	119.39	111.91
24	A	405	CLA	CHB-C4A-NA	2.38	127.81	124.51
24	a	405	CLA	C4C-C3C-C2C	-2.38	103.42	106.90
24	b	617	CLA	CED-O2D-CGD	2.38	121.33	115.94
24	b	615	CLA	CMB-C2B-C1B	2.38	129.00	125.37
24	A	406	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
31	d	408	PL9	C22-C23-C24	-2.38	121.93	127.66
37	h	102	DGD	O1G-C1A-O1A	-2.38	117.58	123.59
27	F	103	SQD	O47-C7-O49	-2.38	117.95	123.70
36	D	410	LHG	C6-C5-C4	-2.38	106.16	111.79
37	c	916	DGD	C3G-C2G-C1G	-2.38	106.16	111.79
24	d	404	CLA	C1-C2-C3	-2.38	121.93	126.04
27	f	102	SQD	O48-C23-C24	2.38	119.38	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	CLA	C4C-C3C-C2C	-2.38	103.43	106.90
33	J	101	LMG	O8-C28-O10	-2.38	117.59	123.59
26	c	915	BCR	C38-C26-C25	-2.38	121.86	124.53
24	B	603	CLA	C4-C3-C5	2.38	119.27	115.27
24	B	612	CLA	C1-O2A-CGA	2.37	122.67	116.44
24	A	406	CLA	CMA-C3A-C2A	-2.37	104.25	113.83
24	d	405	CLA	CHD-C4C-NC	2.37	127.94	124.20
24	B	616	CLA	C4-C3-C5	2.37	119.26	115.27
24	c	908	CLA	O2A-CGA-CBA	2.37	119.35	111.91
26	B	620	BCR	C37-C22-C23	2.37	121.81	118.08
24	B	609	CLA	O2A-CGA-CBA	2.37	119.35	111.91
26	T	102	BCR	C1-C6-C7	2.37	122.48	115.78
27	a	410	SQD	O47-C7-O49	-2.37	117.98	123.70
24	B	611	CLA	C1-C2-C3	-2.37	121.95	126.04
24	b	609	CLA	C1-C2-C3	-2.37	121.95	126.04
26	c	915	BCR	C3-C4-C5	-2.37	109.85	114.08
24	c	908	CLA	CHB-C4A-NA	2.37	127.79	124.51
26	t	102	BCR	C21-C20-C19	-2.37	115.83	123.22
24	c	903	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
24	B	607	CLA	CAC-C3C-C4C	2.37	127.88	124.81
24	b	609	CLA	CHD-C4C-NC	2.37	127.93	124.20
31	A	417	PL9	C40-C39-C41	2.37	119.25	115.27
24	c	914	CLA	CAC-C3C-C4C	2.36	127.88	124.81
24	D	404	CLA	CAC-C3C-C4C	2.36	127.88	124.81
24	A	406	CLA	CED-O2D-CGD	2.36	121.28	115.94
24	A	407	CLA	CMC-C2C-C1C	2.36	128.63	125.04
24	B	610	CLA	O2A-CGA-CBA	2.36	119.31	111.91
24	b	619	CLA	CAC-C3C-C4C	2.36	127.87	124.81
24	c	904	CLA	C2A-C1A-CHA	-2.36	119.74	123.86
26	b	622	BCR	C10-C11-C12	-2.36	115.86	123.22
24	C	504	CLA	C1-O2A-CGA	2.36	122.63	116.44
24	d	404	CLA	O2A-CGA-CBA	2.36	119.30	111.91
26	K	101	BCR	C29-C30-C25	2.36	114.11	110.48
24	B	605	CLA	O1D-CGD-CBD	-2.36	119.66	124.48
24	c	904	CLA	CHC-C1C-C2C	-2.36	120.19	126.73
31	A	417	PL9	C10-C9-C11	2.35	119.23	115.27
24	B	607	CLA	CMC-C2C-C1C	2.35	128.62	125.04
26	H	101	BCR	C10-C11-C12	-2.35	115.87	123.22
24	C	505	CLA	CHB-C1B-NB	-2.35	121.77	124.26
24	d	404	CLA	CHB-C1B-NB	-2.35	121.77	124.26
24	d	406	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
26	b	622	BCR	C36-C18-C17	-2.35	119.63	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	621	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
24	c	911	CLA	C4-C3-C2	-2.35	117.65	123.68
38	F	102	HEM	C2A-C1A-NA	-2.35	107.52	110.15
26	y	101	BCR	C38-C26-C25	-2.35	121.89	124.53
26	k	101	BCR	C7-C8-C9	-2.35	122.69	126.23
33	C	519	LMG	O8-C28-C29	2.35	119.27	111.91
26	d	407	BCR	C37-C22-C23	2.34	121.77	118.08
24	D	404	CLA	CBC-CAC-C3C	-2.34	105.97	112.43
24	B	603	CLA	CAC-C3C-C4C	2.34	127.85	124.81
24	C	508	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
26	c	915	BCR	C37-C22-C23	2.34	121.77	118.08
27	A	411	SQD	C44-O6-C1	-2.34	109.17	113.74
24	C	502	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
37	c	918	DGD	O1G-C1A-O1A	-2.34	117.70	123.59
24	c	902	CLA	C1-O2A-CGA	2.33	122.57	116.44
24	A	409	CLA	CHB-C4A-NA	2.33	127.74	124.51
24	B	616	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
26	B	618	BCR	C16-C17-C18	-2.33	123.98	127.31
24	D	405	CLA	CHD-C4C-NC	2.33	127.88	124.20
29	m	103	LMT	C1B-O5B-C5B	2.33	118.26	113.69
24	B	611	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
24	B	617	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
26	c	915	BCR	C21-C20-C19	-2.33	115.95	123.22
24	C	501	CLA	C4-C3-C5	2.33	119.19	115.27
24	b	608	CLA	CMA-C3A-C2A	-2.33	104.44	113.83
25	A	408	PHO	CMB-C2B-C3B	2.33	129.03	124.68
27	A	411	SQD	O48-C23-O10	-2.33	117.72	123.59
24	b	613	CLA	CMA-C3A-C2A	-2.32	104.46	113.83
24	C	507	CLA	CHC-C1C-C2C	-2.32	120.28	126.73
24	B	606	CLA	CAA-C2A-C3A	-2.32	106.42	112.78
24	B	603	CLA	OBd-CAD-C3D	-2.32	122.94	128.52
24	B	615	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
40	v	202	HEC	C4A-NA-C1A	2.32	107.62	105.35
31	D	407	PL9	C22-C23-C24	-2.32	122.08	127.66
26	D	406	BCR	C10-C11-C12	-2.32	115.99	123.22
24	c	906	CLA	CMC-C2C-C1C	2.32	128.56	125.04
27	a	410	SQD	O5-C1-C2	-2.31	105.45	110.35
24	D	405	CLA	CHB-C4A-NA	2.31	127.71	124.51
26	C	514	BCR	C37-C22-C23	2.31	121.72	118.08
24	B	605	CLA	CHD-C4C-NC	2.31	127.85	124.20
24	B	615	CLA	CHB-C1B-NB	-2.31	121.81	124.26
24	c	904	CLA	C3B-C4B-NB	2.31	112.66	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	920	LMG	C8-O7-C10	-2.31	112.10	117.79
26	c	927	BCR	C11-C12-C13	-2.31	119.92	126.42
31	A	417	PL9	C42-C43-C44	-2.31	122.10	127.66
24	C	512	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
33	A	419	LMG	O8-C28-C29	2.31	119.15	111.91
37	C	518	DGD	O3G-C3G-C2G	-2.31	105.33	110.90
24	a	408	CLA	CMC-C2C-C1C	2.31	128.55	125.04
38	f	101	HEM	CHA-C1A-NA	2.30	128.09	123.85
24	c	909	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
24	C	512	CLA	CHB-C4A-NA	2.30	127.70	124.51
26	d	407	BCR	C33-C5-C6	-2.30	121.94	124.53
24	D	404	CLA	CED-O2D-CGD	2.30	121.14	115.94
26	d	407	BCR	C15-C14-C13	-2.30	124.03	127.31
26	T	102	BCR	C37-C22-C23	2.30	121.70	118.08
24	b	607	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
26	b	622	BCR	C33-C5-C4	2.30	118.03	113.62
26	d	407	BCR	C39-C30-C25	-2.30	106.57	110.30
37	C	517	DGD	C2G-O2G-C1B	-2.30	112.14	117.79
37	H	102	DGD	C2G-O2G-C1B	-2.29	112.14	117.79
26	T	102	BCR	C3-C4-C5	-2.29	109.98	114.08
24	a	408	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
26	B	618	BCR	C38-C26-C25	-2.29	121.95	124.53
26	h	101	BCR	C16-C15-C14	-2.29	118.78	123.47
24	B	612	CLA	CHB-C1B-NB	-2.29	121.83	124.26
24	B	606	CLA	C3B-C4B-NB	2.29	112.64	110.52
37	c	918	DGD	O2G-C1B-O1B	-2.29	118.16	123.70
24	C	506	CLA	O2A-CGA-CBA	2.29	119.10	111.91
24	C	508	CLA	C4-C3-C5	2.29	119.12	115.27
24	b	613	CLA	CHD-C4C-NC	2.29	127.81	124.20
38	F	102	HEM	C4B-C3B-C2B	-2.29	105.30	107.11
24	B	610	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
24	C	510	CLA	C4-C3-C2	-2.29	117.81	123.68
33	B	622	LMG	O8-C28-O10	-2.29	117.82	123.59
24	C	505	CLA	O2A-CGA-CBA	2.29	119.08	111.91
24	c	914	CLA	C3B-C4B-NB	2.29	112.64	110.52
24	C	507	CLA	C4-C3-C5	2.29	119.11	115.27
36	D	409	LHG	O8-C23-C24	2.28	119.07	111.91
26	b	622	BCR	C16-C17-C18	-2.28	124.05	127.31
24	B	603	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
24	C	506	CLA	CHD-C4C-NC	2.28	127.80	124.20
37	c	916	DGD	C4D-C3D-C2D	-2.28	106.84	110.82
27	B	621	SQD	C44-O6-C1	-2.28	109.28	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	b	628	HTG	C1-O5-C5	2.28	116.79	112.58
24	B	615	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
24	C	513	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
26	H	101	BCR	C7-C8-C9	-2.28	122.79	126.23
26	d	407	BCR	C21-C20-C19	-2.28	116.11	123.22
26	C	514	BCR	C23-C24-C25	-2.28	120.80	127.20
24	c	909	CLA	CHB-C1B-NB	-2.28	121.85	124.26
26	B	618	BCR	C37-C22-C21	-2.28	119.74	122.92
24	d	405	CLA	CMB-C2B-C1B	2.27	128.83	125.37
24	b	614	CLA	CMA-C3A-C4A	-2.27	105.66	111.77
33	J	101	LMG	O8-C28-C29	2.27	119.03	111.91
24	C	505	CLA	C1-O2A-CGA	2.27	122.39	116.44
24	B	609	CLA	CHB-C4A-NA	2.27	127.65	124.51
26	D	406	BCR	C39-C30-C25	-2.27	106.62	110.30
24	a	408	CLA	CHB-C4A-NA	2.26	127.64	124.51
24	b	618	CLA	C4-C3-C5	2.26	119.08	115.27
24	b	607	CLA	CMC-C2C-C1C	2.26	128.49	125.04
31	D	407	PL9	C15-C14-C16	2.26	119.08	115.27
24	b	616	CLA	CMC-C2C-C1C	2.26	128.49	125.04
24	b	607	CLA	CBC-CAC-C3C	-2.26	106.19	112.43
24	B	605	CLA	C4-C3-C5	2.26	119.08	115.27
24	B	611	CLA	CHB-C4A-NA	2.26	127.64	124.51
24	A	409	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
26	B	618	BCR	C21-C20-C19	-2.26	116.16	123.22
33	Z	101	LMG	C8-O7-C10	-2.26	112.22	117.79
24	B	614	CLA	CMB-C2B-C1B	2.26	128.81	125.37
24	A	409	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
24	C	504	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
24	D	404	CLA	CMB-C2B-C1B	2.26	128.81	125.37
26	d	407	BCR	C29-C28-C27	-2.26	106.33	111.38
37	c	916	DGD	O3G-C3G-C2G	-2.26	105.45	110.90
24	B	607	CLA	C11-C10-C8	-2.26	108.63	115.92
26	c	927	BCR	C29-C30-C25	2.26	113.95	110.48
26	c	915	BCR	C35-C13-C14	-2.25	119.77	122.92
24	D	404	CLA	CMA-C3A-C4A	-2.25	105.71	111.77
24	b	621	CLA	C4-C3-C5	2.25	119.06	115.27
24	b	617	CLA	CMA-C3A-C4A	-2.25	105.72	111.77
26	d	407	BCR	C38-C26-C27	2.25	117.94	113.62
38	f	101	HEM	C2A-C1A-NA	-2.25	107.63	110.15
24	B	617	CLA	C1-O2A-CGA	2.25	122.35	116.44
24	b	618	CLA	CMB-C2B-C1B	2.25	128.80	125.37
24	C	505	CLA	C2A-C1A-CHA	-2.25	119.92	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	405	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
24	b	616	CLA	OBD-CAD-C3D	-2.25	123.10	128.52
24	b	619	CLA	CMB-C2B-C1B	2.25	128.80	125.37
26	B	619	BCR	C32-C1-C6	-2.25	106.65	110.30
24	b	615	CLA	C11-C12-C13	-2.25	108.65	115.92
36	B	635	LHG	C5-O7-C7	-2.25	112.25	117.79
26	c	927	BCR	C35-C13-C14	-2.25	119.77	122.92
24	C	510	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
26	B	619	BCR	C37-C22-C23	2.25	121.62	118.08
33	a	411	LMG	O7-C10-O9	-2.25	118.27	123.70
24	b	614	CLA	CMC-C2C-C1C	2.25	128.46	125.04
24	B	614	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
37	C	517	DGD	C3G-O3G-C1D	-2.24	109.36	113.74
26	k	101	BCR	C10-C11-C12	-2.24	116.22	123.22
40	V	202	HEC	CHB-C1B-C2B	-2.24	121.48	124.98
33	Y	101	LMG	C8-O7-C10	-2.24	112.28	117.79
24	b	613	CLA	C4-C3-C5	2.24	119.04	115.27
24	c	913	CLA	C1-O2A-CGA	2.24	122.31	116.44
24	c	902	CLA	CMC-C2C-C1C	2.24	128.44	125.04
38	F	102	HEM	O2A-CGA-CBA	2.24	121.21	114.03
25	a	407	PHO	C1-O2A-CGA	2.24	122.31	116.44
24	C	501	CLA	O2A-CGA-CBA	2.23	118.92	111.91
27	L	102	SQD	O48-C23-O10	-2.23	117.96	123.59
37	C	518	DGD	O6D-C5D-C6D	2.23	111.17	106.67
26	H	101	BCR	C31-C1-C6	-2.23	106.68	110.30
24	C	502	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
33	a	411	LMG	C7-O1-C1	-2.23	109.38	113.74
24	b	617	CLA	CHB-C4A-NA	2.23	127.60	124.51
24	C	502	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
24	c	903	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
29	a	417	LMT	C1B-O1B-C4'	-2.23	112.45	117.96
24	B	606	CLA	CHC-C1C-C2C	-2.23	120.54	126.73
24	a	406	CLA	CMA-C3A-C2A	-2.23	104.84	113.83
24	b	617	CLA	CHB-C1B-NB	-2.22	121.90	124.26
26	T	102	BCR	C37-C22-C21	-2.22	119.81	122.92
26	b	623	BCR	C28-C27-C26	-2.22	110.11	114.08
24	B	612	CLA	CHB-C4A-NA	2.22	127.58	124.51
24	B	611	CLA	CAC-C3C-C4C	2.22	127.69	124.81
40	v	202	HEC	C3B-C4B-NB	-2.21	107.70	110.17
24	d	404	CLA	CAA-CBA-CGA	2.21	119.72	113.25
29	C	520	LMT	O5'-C5'-C4'	2.21	114.42	109.75
27	a	402	SQD	O5-C5-C4	2.21	113.71	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	405	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
24	c	903	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
24	b	616	CLA	C4-C3-C5	2.21	118.99	115.27
24	b	607	CLA	CMA-C3A-C4A	-2.21	105.83	111.77
26	T	102	BCR	C7-C8-C9	-2.21	122.89	126.23
24	b	610	CLA	O2A-CGA-CBA	2.21	118.84	111.91
25	A	408	PHO	C1-C2-C3	-2.21	122.22	126.04
25	a	407	PHO	CED-O2D-CGD	2.21	120.93	115.94
40	V	202	HEC	CHD-C4C-NC	2.21	127.91	123.85
24	b	609	CLA	CHA-C1A-NA	-2.21	121.34	126.40
25	d	403	PHO	CAC-C3C-C2C	2.21	131.30	127.53
33	C	519	LMG	O6-C5-C4	2.20	113.70	109.69
29	A	415	LMT	C1B-O5B-C5B	2.20	118.01	113.69
37	C	517	DGD	O6E-C5E-C6E	2.20	111.91	106.44
24	b	618	CLA	CHA-C1A-NA	-2.20	121.36	126.40
26	t	102	BCR	C7-C6-C5	-2.20	116.13	121.46
36	d	409	LHG	O4-P-O5	2.20	123.12	112.24
29	a	401	LMT	O1B-C1B-C2B	2.20	113.80	108.10
24	c	902	CLA	C4-C3-C5	2.20	118.97	115.27
26	B	618	BCR	C11-C10-C9	-2.20	124.17	127.31
24	B	610	CLA	C1-O2A-CGA	2.20	122.21	116.44
40	V	202	HEC	CBB-CAB-C3B	2.20	118.48	112.43
24	B	606	CLA	OBD-CAD-C3D	-2.20	123.24	128.52
24	d	405	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
24	B	616	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
33	Y	101	LMG	O8-C28-O10	-2.19	118.06	123.59
33	d	415	LMG	C1-O6-C5	2.19	117.98	113.69
26	T	102	BCR	C2-C1-C6	2.19	113.85	110.48
24	C	501	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
24	D	405	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
26	k	101	BCR	C38-C26-C25	-2.19	122.07	124.53
24	b	613	CLA	C11-C12-C13	-2.19	108.85	115.92
27	B	621	SQD	C3-C4-C5	2.19	114.14	110.24
24	c	909	CLA	C11-C10-C8	-2.19	108.86	115.92
24	B	611	CLA	CHB-C1B-NB	-2.18	121.94	124.26
24	c	908	CLA	C3B-C4B-NB	2.18	112.54	110.52
24	B	602	CLA	CHB-C4A-NA	2.18	127.53	124.51
33	b	625	LMG	O7-C10-O9	-2.18	118.43	123.70
35	C	521	HTG	C4-C3-C2	-2.18	107.01	110.82
36	E	101	LHG	C5-O7-C7	-2.18	112.42	117.79
31	D	407	PL9	C30-C29-C31	2.18	118.94	115.27
26	B	620	BCR	C36-C18-C19	2.18	121.51	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	501	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
24	c	906	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
25	a	407	PHO	C4-C3-C5	2.18	118.93	115.27
27	B	621	SQD	C1-C2-C3	-2.18	105.46	110.00
24	d	404	CLA	C1-O2A-CGA	2.18	122.15	116.44
24	C	511	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
24	c	904	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
26	y	101	BCR	C21-C20-C19	-2.17	116.43	123.22
24	b	621	CLA	CMC-C2C-C1C	2.17	128.35	125.04
26	k	101	BCR	C3-C4-C5	-2.17	110.20	114.08
25	a	407	PHO	C1-C2-C3	-2.17	122.28	126.04
24	B	615	CLA	CMC-C2C-C1C	2.17	128.35	125.04
26	d	407	BCR	C16-C15-C14	-2.17	119.03	123.47
24	D	404	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
24	B	616	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
26	B	620	BCR	C37-C22-C21	-2.17	119.89	122.92
24	C	512	CLA	C11-C12-C13	-2.16	108.93	115.92
24	b	620	CLA	CED-O2D-CGD	2.16	120.83	115.94
33	c	919	LMG	O8-C28-O10	-2.16	118.14	123.59
35	B	632	HTG	C6-C5-C4	-2.16	107.94	113.00
24	b	615	CLA	CMA-C3A-C2A	-2.16	105.12	113.83
24	b	619	CLA	C4-C3-C5	2.16	118.90	115.27
24	C	504	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
31	A	417	PL9	C47-C48-C49	-2.16	120.37	127.75
40	v	202	HEC	O2A-CGA-CBA	2.16	120.96	114.03
24	C	509	CLA	CMB-C2B-C1B	2.16	128.66	125.37
24	B	614	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
24	b	616	CLA	CHB-C1B-NB	-2.16	121.97	124.26
26	c	927	BCR	C37-C22-C21	-2.16	119.90	122.92
24	b	610	CLA	OBD-CAD-C3D	-2.16	123.33	128.52
33	z	101	LMG	C7-O1-C1	-2.15	109.53	113.74
24	b	620	CLA	CHA-C1A-NA	-2.15	121.47	126.40
26	C	515	BCR	C15-C14-C13	-2.15	124.24	127.31
24	c	907	CLA	OBD-CAD-C3D	-2.15	123.35	128.52
24	C	507	CLA	CBC-CAC-C3C	-2.15	106.51	112.43
24	b	619	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
37	H	102	DGD	O1G-C1A-O1A	-2.15	118.17	123.59
24	B	608	CLA	CMB-C2B-C1B	2.15	128.64	125.37
24	C	508	CLA	CMB-C2B-C1B	2.15	128.64	125.37
24	b	617	CLA	C11-C10-C8	-2.15	108.98	115.92
29	A	415	LMT	O5'-C5'-C6'	2.15	111.77	106.44
24	C	509	CLA	C2A-C1A-CHA	-2.14	120.11	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	V	202	HEC	CBA-CAA-C2A	-2.14	106.67	112.63
40	V	202	HEC	C4A-NA-C1A	2.14	107.45	105.35
24	c	907	CLA	CHB-C4A-NA	2.14	127.47	124.51
24	b	620	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
26	T	102	BCR	C7-C6-C5	-2.14	116.27	121.46
40	V	202	HEC	O2D-CGD-CBD	2.14	120.91	114.03
24	B	611	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
24	B	611	CLA	CAA-CBA-CGA	-2.14	107.00	113.25
36	L	101	LHG	O7-C7-O9	-2.14	118.53	123.70
24	a	405	CLA	CHB-C4A-NA	2.14	127.47	124.51
24	b	612	CLA	O2A-CGA-CBA	2.14	118.61	111.91
26	k	101	BCR	C36-C18-C19	2.14	121.44	118.08
25	a	407	PHO	O2A-CGA-CBA	2.13	118.61	111.91
24	c	906	CLA	CHB-C1B-NB	-2.13	122.00	124.26
24	b	618	CLA	CHD-C4C-NC	2.13	127.57	124.20
26	h	101	BCR	C16-C17-C18	-2.13	124.27	127.31
24	c	912	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
24	A	406	CLA	CHB-C1B-NB	-2.13	122.00	124.26
26	k	101	BCR	C34-C9-C10	-2.13	119.94	122.92
24	C	508	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
24	b	619	CLA	C4-C3-C2	-2.13	118.22	123.68
24	b	614	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
24	b	621	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
24	b	611	CLA	CAA-C2A-C3A	-2.12	106.96	112.78
25	d	403	PHO	O2A-CGA-CBA	2.12	118.57	111.91
24	b	617	CLA	CAC-C3C-C2C	2.12	131.16	127.53
26	Y	102	BCR	C15-C16-C17	-2.12	119.13	123.47
31	d	408	PL9	C53-C6-C1	2.12	119.33	114.99
24	C	503	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
24	b	611	CLA	O2A-CGA-CBA	2.12	118.56	111.91
26	D	406	BCR	C38-C26-C27	2.12	117.69	113.62
35	B	624	HTG	C1-C2-C3	2.12	114.77	110.59
24	B	607	CLA	C2A-C1A-CHA	-2.12	120.16	123.86
25	D	401	PHO	O1D-CGD-CBD	-2.12	121.21	124.74
37	c	917	DGD	O6E-C1E-O5D	-2.12	104.96	109.97
24	C	502	CLA	C4-C3-C5	2.12	118.83	115.27
24	c	905	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
24	C	505	CLA	C4-C3-C5	2.12	118.83	115.27
26	y	101	BCR	C16-C17-C18	-2.12	124.29	127.31
31	d	408	PL9	C11-C9-C8	-2.12	116.83	121.12
24	a	405	CLA	CAC-C3C-C4C	2.12	127.56	124.81
24	B	605	CLA	C11-C10-C8	-2.11	109.08	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	635	LHG	O4-P-O5	2.11	122.69	112.24
24	D	404	CLA	C4-C3-C5	2.11	118.83	115.27
24	c	911	CLA	C2A-C1A-CHA	-2.11	120.16	123.86
31	a	415	PL9	C45-C44-C46	2.11	118.83	115.27
37	D	408	DGD	C4D-C3D-C2D	2.11	114.51	110.82
26	H	101	BCR	C21-C20-C19	-2.11	116.63	123.22
24	C	511	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
24	b	615	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
26	T	102	BCR	C36-C18-C19	2.11	121.40	118.08
26	k	101	BCR	C2-C1-C6	2.11	113.72	110.48
24	c	912	CLA	CMB-C2B-C1B	2.11	128.58	125.37
24	B	616	CLA	CHA-C1A-NA	-2.11	121.58	126.40
31	A	417	PL9	C7-C3-C2	-2.11	120.53	123.30
24	a	405	CLA	CHB-C1B-C2B	-2.10	121.29	127.24
31	a	415	PL9	C8-C7-C3	2.10	117.92	111.98
24	C	512	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
24	c	913	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
25	a	407	PHO	C16-C15-C13	-2.10	109.14	115.92
24	B	605	CLA	OBD-CAD-C3D	-2.10	123.47	128.52
26	a	409	BCR	C8-C7-C6	-2.10	121.31	127.20
24	c	902	CLA	CAA-C2A-C3A	-2.10	107.04	112.78
24	c	910	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
26	b	622	BCR	C29-C30-C25	2.09	113.70	110.48
26	Y	102	BCR	C37-C22-C23	2.09	121.37	118.08
24	b	621	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
24	A	407	CLA	CMA-C3A-C4A	-2.09	106.15	111.77
27	A	414	SQD	O6-C44-C45	-2.09	105.86	110.90
26	t	102	BCR	C28-C27-C26	-2.09	110.35	114.08
40	v	202	HEC	CHB-C4A-NA	2.09	126.70	124.44
33	C	519	LMG	C8-O7-C10	-2.09	112.65	117.79
26	K	101	BCR	C31-C1-C6	-2.09	106.91	110.30
31	A	417	PL9	C16-C17-C18	-2.09	105.02	111.88
24	A	407	CLA	CHB-C4A-NA	2.09	127.40	124.51
24	B	612	CLA	O2A-CGA-CBA	2.09	118.46	111.91
24	c	905	CLA	OBD-CAD-C3D	-2.09	123.50	128.52
24	b	606	CLA	O2A-CGA-CBA	2.09	118.46	111.91
35	b	603	HTG	C6-C5-C4	-2.09	108.12	113.00
24	C	513	CLA	CHB-C4A-NA	2.09	127.40	124.51
24	B	609	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
24	C	511	CLA	C4-C3-C5	2.09	118.78	115.27
24	b	618	CLA	CMA-C3A-C4A	-2.08	106.17	111.77
24	A	406	CLA	OBD-CAD-C3D	-2.08	123.50	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	C	519	LMG	O7-C10-O9	-2.08	118.67	123.70
24	c	902	CLA	CHD-C4C-NC	2.08	127.48	124.20
26	b	623	BCR	C7-C8-C9	-2.08	123.09	126.23
33	c	920	LMG	O8-C28-O10	-2.08	118.34	123.59
24	b	618	CLA	CED-O2D-CGD	2.08	120.64	115.94
37	c	916	DGD	O1G-C1A-C2A	2.08	118.43	111.91
25	d	403	PHO	O2A-CGA-O1A	-2.08	118.35	123.59
24	C	507	CLA	OBD-CAD-C3D	-2.08	123.52	128.52
29	D	403	LMT	O5B-C5B-C4B	2.08	113.47	109.69
37	c	917	DGD	O6E-C5E-C6E	2.08	111.60	106.44
26	d	407	BCR	C3-C4-C5	-2.08	110.37	114.08
24	C	509	CLA	C11-C12-C13	-2.08	109.21	115.92
37	e	101	DGD	O2G-C1B-O1B	-2.08	118.68	123.70
37	H	102	DGD	C3G-C2G-C1G	-2.07	106.88	111.79
37	c	917	DGD	O1G-C1A-O1A	-2.07	118.36	123.59
24	C	506	CLA	C1-O2A-CGA	2.07	121.89	116.44
37	c	917	DGD	C3B-C2B-C1B	-2.07	106.08	113.62
26	k	101	BCR	C15-C16-C17	-2.07	119.23	123.47
24	C	509	CLA	CHB-C1B-NB	-2.07	122.06	124.26
29	F	101	LMT	O5'-C5'-C4'	2.07	114.12	109.75
24	C	501	CLA	C2A-C3A-C4A	-2.07	98.52	101.87
24	c	907	CLA	CMA-C3A-C4A	-2.07	106.21	111.77
24	c	905	CLA	C11-C10-C8	-2.07	109.23	115.92
37	C	516	DGD	O6E-C5E-C4E	2.07	113.45	109.69
24	b	611	CLA	C1-C2-C3	-2.07	122.47	126.04
33	b	625	LMG	O6-C5-C6	2.07	111.58	106.44
24	b	615	CLA	C2A-C1A-CHA	-2.07	120.25	123.86
40	V	202	HEC	C2A-C1A-NA	-2.07	108.31	110.32
37	C	516	DGD	O2G-C1B-O1B	-2.07	118.71	123.70
26	k	101	BCR	C39-C30-C25	-2.07	106.95	110.30
24	b	613	CLA	CAA-C2A-C3A	-2.06	107.12	112.78
24	a	405	CLA	CMC-C2C-C1C	2.06	128.18	125.04
31	D	407	PL9	C25-C24-C26	2.06	118.74	115.27
26	H	101	BCR	C15-C14-C13	-2.06	124.37	127.31
29	e	102	LMT	C1B-O5B-C5B	2.06	117.74	113.69
40	v	202	HEC	O2D-CGD-CBD	2.06	120.66	114.03
24	b	616	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
24	B	610	CLA	CMA-C3A-C4A	-2.06	106.23	111.77
31	d	408	PL9	C40-C39-C38	-2.06	118.39	123.68
24	b	612	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
24	c	905	CLA	CMB-C2B-C1B	2.06	128.51	125.37
26	t	102	BCR	C35-C13-C12	2.06	121.32	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	913	CLA	CHB-C1B-C2B	-2.06	121.42	127.24
31	A	417	PL9	C35-C34-C36	2.06	118.73	115.27
24	C	508	CLA	CHB-C1B-C2B	-2.06	121.42	127.24
25	D	401	PHO	O2D-CGD-O1D	-2.06	119.81	123.84
24	b	608	CLA	CHB-C1B-C2B	-2.06	121.42	127.24
24	B	614	CLA	CHA-C1A-NA	-2.06	121.69	126.40
26	K	101	BCR	C36-C18-C19	2.06	121.32	118.08
24	A	407	CLA	CMA-C3A-C2A	-2.06	105.54	113.83
33	C	519	LMG	C1-C2-C3	2.05	114.28	110.00
24	A	409	CLA	CHB-C1B-C2B	-2.05	121.44	127.24
24	B	608	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
24	b	618	CLA	OBD-CAD-C3D	-2.05	123.58	128.52
26	b	622	BCR	C31-C1-C6	-2.05	106.97	110.30
35	B	633	HTG	C1-O5-C5	2.05	116.36	112.58
24	A	406	CLA	C1-C2-C3	-2.05	122.50	126.04
27	A	411	SQD	C1-O5-C5	-2.05	109.67	113.69
24	b	619	CLA	CHB-C4A-NA	2.05	127.34	124.51
24	D	404	CLA	CHB-C4A-NA	2.05	127.34	124.51
24	b	621	CLA	CMA-C3A-C2A	-2.05	105.58	113.83
26	B	618	BCR	C34-C9-C10	-2.05	120.06	122.92
24	B	606	CLA	C1-O2A-CGA	2.04	121.81	116.44
26	t	102	BCR	C3-C4-C5	-2.04	110.43	114.08
24	B	603	CLA	CAA-CBA-CGA	-2.04	107.28	113.25
24	c	911	CLA	CMC-C2C-C1C	2.04	128.15	125.04
24	A	406	CLA	CAC-C3C-C2C	2.04	131.02	127.53
24	B	610	CLA	CHA-C1A-NA	-2.04	121.73	126.40
24	b	620	CLA	C6-C7-C8	-2.04	109.33	115.92
29	C	520	LMT	C1B-O5B-C5B	2.04	117.69	113.69
24	b	606	CLA	CBC-CAC-C3C	-2.04	106.82	112.43
25	d	403	PHO	C4-C3-C2	-2.03	118.46	123.68
24	c	910	CLA	CHB-C1B-NB	-2.03	122.11	124.26
24	b	606	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
26	t	102	BCR	C34-C9-C10	-2.03	120.08	122.92
31	D	407	PL9	C17-C18-C19	-2.03	122.77	127.66
26	B	618	BCR	C37-C22-C23	2.03	121.28	118.08
29	D	403	LMT	C1B-O5B-C5B	2.03	117.67	113.69
24	C	505	CLA	CHA-C1A-NA	-2.03	121.75	126.40
24	b	620	CLA	C11-C12-C13	-2.03	109.37	115.92
26	K	101	BCR	C15-C14-C13	-2.03	124.42	127.31
36	E	101	LHG	O8-C23-O10	-2.03	118.48	123.59
24	B	617	CLA	CAC-C3C-C4C	2.03	127.44	124.81
24	B	615	CLA	CHC-C1C-NC	2.02	127.28	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	C4-C3-C5	2.02	118.68	115.27
24	B	602	CLA	CHB-C1B-NB	-2.02	122.11	124.26
33	c	920	LMG	O7-C10-O9	-2.02	118.81	123.70
33	z	101	LMG	C8-O7-C10	-2.02	112.81	117.79
40	v	202	HEC	CHB-C1B-C2B	-2.02	121.82	124.98
26	K	101	BCR	C38-C26-C25	-2.02	122.26	124.53
37	C	518	DGD	O6E-C5E-C6E	2.02	111.47	106.44
36	B	635	LHG	O7-C7-O9	-2.02	118.81	123.70
35	V	203	HTG	O5-C1-C2	-2.02	107.77	110.31
24	B	607	CLA	C7-C6-C5	-2.02	107.87	113.36
26	h	101	BCR	C3-C2-C1	-2.02	107.38	114.60
26	b	623	BCR	C21-C20-C19	-2.02	116.91	123.22
36	d	410	LHG	O7-C7-O9	-2.02	118.82	123.70
31	A	417	PL9	C47-C46-C44	-2.02	106.33	112.98
24	B	604	CLA	CHB-C1B-C2B	-2.02	121.54	127.24
24	b	611	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
40	v	202	HEC	CBB-CAB-C3B	2.01	117.99	112.43
24	B	602	CLA	C4-C3-C5	2.01	118.66	115.27
26	c	915	BCR	C11-C10-C9	-2.01	124.44	127.31
37	c	916	DGD	O1G-C1A-O1A	-2.01	118.51	123.59
24	B	616	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
24	c	905	CLA	O2A-CGA-CBA	2.01	118.22	111.91
26	k	101	BCR	C29-C30-C25	2.01	113.58	110.48
29	m	102	LMT	C1B-O5B-C5B	2.01	117.64	113.69
29	m	103	LMT	C1'-O5'-C5'	2.01	117.64	113.69
31	a	415	PL9	C35-C34-C33	-2.01	118.52	123.68
24	c	907	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
24	B	611	CLA	CHC-C1C-NC	2.01	127.25	124.20
29	M	103	LMT	C1B-O5B-C5B	2.01	117.63	113.69
24	C	507	CLA	CAC-C3C-C4C	2.01	127.41	124.81
36	d	411	LHG	O8-C23-O10	-2.01	118.53	123.59
24	c	906	CLA	C1-O2A-CGA	2.01	121.71	116.44
26	A	410	BCR	C7-C8-C9	-2.01	123.20	126.23
26	B	620	BCR	C16-C15-C14	-2.01	119.36	123.47
24	c	906	CLA	C2A-C1A-CHA	-2.01	120.35	123.86
24	A	405	CLA	C7-C6-C5	-2.01	107.91	113.36
26	A	410	BCR	C3-C4-C5	-2.01	110.50	114.08
24	c	910	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
24	A	409	CLA	CED-O2D-CGD	2.00	120.47	115.94
26	Y	102	BCR	C35-C13-C12	2.00	121.23	118.08
29	b	602	LMT	C6'-C5'-C4'	-2.00	107.50	113.33
24	c	911	CLA	CBC-CAC-C3C	-2.00	106.91	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	101	BCR	C3-C4-C5	-2.00	110.50	114.08
26	y	101	BCR	C32-C1-C6	-2.00	107.05	110.30
24	c	908	CLA	OBD-CAD-C3D	-2.00	123.70	128.52
24	C	507	CLA	CHB-C1B-C2B	-2.00	121.59	127.24

All (2) chirality outliers are listed below:

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

All (1380) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	406	CLA	CHA-CBD-CGD-O1D
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	B	602	CLA	C11-C10-C8-C9
24	B	603	CLA	C2B-C3B-CAB-CBB
24	B	603	CLA	C4B-C3B-CAB-CBB
24	B	606	CLA	C2-C3-C5-C6
24	B	606	CLA	C4-C3-C5-C6
24	B	607	CLA	C2B-C3B-CAB-CBB
24	B	607	CLA	C4B-C3B-CAB-CBB
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	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	B	616	CLA	C4B-C3B-CAB-CBB
24	C	502	CLA	C2B-C3B-CAB-CBB
24	C	502	CLA	C4B-C3B-CAB-CBB
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	C2-C1-O2A-CGA
24	b	610	CLA	C2-C3-C5-C6
24	b	610	CLA	C4-C3-C5-C6
24	b	611	CLA	CHA-CBD-CGD-O1D
24	b	611	CLA	CHA-CBD-CGD-O2D
24	b	612	CLA	C2B-C3B-CAB-CBB
24	b	612	CLA	C4B-C3B-CAB-CBB
24	b	619	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	b	619	CLA	CHA-CBD-CGD-O2D
24	b	619	CLA	CAD-CBD-CGD-O1D
24	b	619	CLA	CAD-CBD-CGD-O2D
24	b	619	CLA	C2-C3-C5-C6
24	b	619	CLA	C4-C3-C5-C6
24	c	908	CLA	C2B-C3B-CAB-CBB
24	c	908	CLA	C4B-C3B-CAB-CBB
24	c	909	CLA	CHA-CBD-CGD-O1D
24	c	909	CLA	CHA-CBD-CGD-O2D
24	c	910	CLA	C2-C1-O2A-CGA
24	c	913	CLA	C2B-C3B-CAB-CBB
24	c	913	CLA	C4B-C3B-CAB-CBB
26	D	406	BCR	C7-C8-C9-C10
26	D	406	BCR	C7-C8-C9-C34
26	D	406	BCR	C21-C22-C23-C24
26	D	406	BCR	C37-C22-C23-C24
26	Y	102	BCR	C1-C6-C7-C8
26	Y	102	BCR	C5-C6-C7-C8
26	d	407	BCR	C21-C22-C23-C24
26	d	407	BCR	C37-C22-C23-C24
26	y	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
26	y	101	BCR	C21-C22-C23-C24
26	y	101	BCR	C37-C22-C23-C24
27	A	414	SQD	O6-C44-C45-O47
27	A	414	SQD	O5-C5-C6-S
27	B	621	SQD	O5-C1-O6-C44
27	B	621	SQD	O49-C7-O47-C45
27	F	103	SQD	O49-C7-O47-C45
27	F	103	SQD	C5-C6-S-O7
27	F	103	SQD	C5-C6-S-O8
27	F	103	SQD	C5-C6-S-O9
27	L	102	SQD	O5-C1-O6-C44
27	L	102	SQD	O49-C7-O47-C45
27	a	402	SQD	O6-C44-C45-O47
27	a	402	SQD	O5-C5-C6-S
27	f	102	SQD	O49-C7-O47-C45
27	f	102	SQD	C8-C7-O47-C45
27	f	102	SQD	C5-C6-S-O7
27	f	102	SQD	C5-C6-S-O8
27	f	102	SQD	C5-C6-S-O9
28	A	413	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
28	B	627	GOL	O1-C1-C2-O2
28	B	627	GOL	O1-C1-C2-C3
28	B	628	GOL	O1-C1-C2-C3
28	B	630	GOL	C1-C2-C3-O3
28	B	630	GOL	O2-C2-C3-O3
28	C	523	GOL	O1-C1-C2-C3
28	D	402	GOL	C1-C2-C3-O3
28	D	402	GOL	O2-C2-C3-O3
28	T	103	GOL	O1-C1-C2-C3
28	V	201	GOL	O1-C1-C2-C3
28	V	204	GOL	C1-C2-C3-O3
28	V	206	GOL	C1-C2-C3-O3
28	V	207	GOL	C1-C2-C3-O3
28	a	412	GOL	C1-C2-C3-O3
28	a	412	GOL	O2-C2-C3-O3
28	a	419	GOL	O1-C1-C2-C3
28	b	632	GOL	O1-C1-C2-C3
28	b	633	GOL	O1-C1-C2-C3
28	c	924	GOL	O1-C1-C2-C3
28	v	203	GOL	O1-C1-C2-C3
28	v	204	GOL	O1-C1-C2-C3
28	v	205	GOL	O1-C1-C2-C3
29	A	415	LMT	C2'-C1'-O1'-C1
29	A	415	LMT	O5'-C1'-O1'-C1
29	C	520	LMT	C2'-C1'-O1'-C1
29	C	520	LMT	O5'-C1'-O1'-C1
29	F	101	LMT	C2'-C1'-O1'-C1
29	F	101	LMT	O5'-C1'-O1'-C1
29	M	103	LMT	O5'-C1'-O1'-C1
29	a	401	LMT	C2'-C1'-O1'-C1
29	a	401	LMT	O5'-C1'-O1'-C1
29	a	417	LMT	C2'-C1'-O1'-C1
29	a	417	LMT	O5'-C1'-O1'-C1
29	b	602	LMT	C2'-C1'-O1'-C1
29	b	602	LMT	O5'-C1'-O1'-C1
29	b	626	LMT	C2'-C1'-O1'-C1
29	b	626	LMT	O5'-C1'-O1'-C1
29	e	102	LMT	C2'-C1'-O1'-C1
29	e	102	LMT	O5'-C1'-O1'-C1
29	t	101	LMT	C2'-C1'-O1'-C1
29	t	101	LMT	O5'-C1'-O1'-C1
31	a	415	PL9	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	a	415	PL9	C23-C24-C26-C27
31	a	415	PL9	C25-C24-C26-C27
33	C	519	LMG	C11-C10-O7-C8
33	Z	101	LMG	O6-C1-O1-C7
33	Z	101	LMG	O9-C10-O7-C8
33	Z	101	LMG	C11-C10-O7-C8
33	z	101	LMG	O6-C1-O1-C7
33	z	101	LMG	O9-C10-O7-C8
33	z	101	LMG	C11-C10-O7-C8
35	B	624	HTG	C2'-C1'-S1-C1
35	B	625	HTG	O5-C1-S1-C1'
35	c	921	HTG	C2'-C1'-S1-C1
36	D	409	LHG	C3-O3-P-O6
36	D	409	LHG	C4-O6-P-O4
36	D	410	LHG	C4-O6-P-O4
36	E	101	LHG	C4-O6-P-O5
36	L	101	LHG	C4-O6-P-O4
36	L	101	LHG	C4-O6-P-O5
36	a	418	LHG	C3-O3-P-O5
36	a	418	LHG	C3-O3-P-O6
36	a	418	LHG	C4-O6-P-O3
36	a	418	LHG	C4-O6-P-O5
36	a	418	LHG	O10-C23-O8-C6
36	a	418	LHG	C24-C23-O8-C6
36	b	635	LHG	C4-O6-P-O4
36	b	635	LHG	C4-O6-P-O5
36	d	410	LHG	C3-O3-P-O4
37	D	408	DGD	C2B-C1B-O2G-C2G
37	D	408	DGD	O1B-C1B-O2G-C2G
37	D	408	DGD	C2D-C1D-O3G-C3G
37	D	408	DGD	O6D-C1D-O3G-C3G
37	e	101	DGD	C2B-C1B-O2G-C2G
37	e	101	DGD	O1B-C1B-O2G-C2G
37	e	101	DGD	C2D-C1D-O3G-C3G
37	e	101	DGD	O6D-C1D-O3G-C3G
37	e	101	DGD	O6E-C1E-O5D-C6D
38	F	102	HEM	C2B-C3B-CAB-CBB
38	F	102	HEM	C2C-C3C-CAC-CBC
38	F	102	HEM	C4C-C3C-CAC-CBC
29	D	403	LMT	C3'-C4'-O1B-C1B
29	C	520	LMT	C3'-C4'-O1B-C1B
24	C	509	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	E	101	LHG	O10-C23-O8-C6
33	C	519	LMG	O9-C10-O7-C8
24	B	602	CLA	C3-C5-C6-C7
24	b	619	CLA	C3-C5-C6-C7
36	E	101	LHG	C24-C23-O8-C6
27	B	621	SQD	C8-C7-O47-C45
27	F	103	SQD	C8-C7-O47-C45
27	L	102	SQD	C8-C7-O47-C45
37	e	101	DGD	O6E-C5E-C6E-O5E
24	A	409	CLA	C3-C5-C6-C7
24	c	907	CLA	C3-C5-C6-C7
36	D	410	LHG	C24-C23-O8-C6
35	b	628	HTG	S1-C1'-C2'-C3'
26	T	102	BCR	C13-C14-C15-C16
29	M	103	LMT	O5'-C5'-C6'-O6'
29	m	102	LMT	O5'-C5'-C6'-O6'
37	h	102	DGD	O6E-C5E-C6E-O5E
24	c	912	CLA	CBD-CGD-O2D-CED
24	d	406	CLA	CBD-CGD-O2D-CED
36	d	410	LHG	O2-C2-C3-O3
24	B	615	CLA	C3-C5-C6-C7
36	D	410	LHG	O10-C23-O8-C6
33	z	101	LMG	O6-C5-C6-O5
35	B	625	HTG	O5-C5-C6-O6
33	C	519	LMG	O6-C5-C6-O5
33	a	411	LMG	C17-C18-C19-C20
24	C	512	CLA	CBD-CGD-O2D-CED
29	m	102	LMT	C4'-C5'-C6'-O6'
29	M	101	LMT	O5B-C5B-C6B-O6B
31	A	417	PL9	C25-C24-C26-C27
31	a	415	PL9	C15-C14-C16-C17
31	a	415	PL9	C20-C19-C21-C22
31	a	415	PL9	C30-C29-C31-C32
31	A	417	PL9	C23-C24-C26-C27
31	a	415	PL9	C13-C14-C16-C17
31	a	415	PL9	C18-C19-C21-C22
24	B	607	CLA	C2A-CAA-CBA-CGA
31	A	417	PL9	C44-C46-C47-C48
31	D	407	PL9	C39-C41-C42-C43
31	d	408	PL9	C39-C41-C42-C43
29	M	103	LMT	C4'-C5'-C6'-O6'
29	e	102	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
36	E	101	LHG	C1-C2-C3-O3
33	z	101	LMG	C4-C5-C6-O5
24	C	509	CLA	O1A-CGA-O2A-C1
24	C	509	CLA	CBA-CGA-O2A-C1
24	a	408	CLA	CBA-CGA-O2A-C1
24	c	910	CLA	CBA-CGA-O2A-C1
37	e	101	DGD	C2A-C1A-O1G-C1G
37	h	102	DGD	C4E-C5E-C6E-O5E
33	d	415	LMG	C19-C20-C21-C22
24	B	614	CLA	C13-C15-C16-C17
37	e	101	DGD	C4E-C5E-C6E-O5E
27	a	402	SQD	C18-C19-C20-C21
24	C	506	CLA	C5-C6-C7-C8
33	Z	101	LMG	C2-C1-O1-C7
37	e	101	DGD	C2E-C1E-O5D-C6D
24	B	602	CLA	C14-C13-C15-C16
24	B	617	CLA	C6-C7-C8-C9
24	C	501	CLA	C11-C12-C13-C14
24	c	907	CLA	C6-C7-C8-C9
24	c	910	CLA	C11-C10-C8-C9
24	B	615	CLA	C10-C11-C12-C13
26	Y	102	BCR	C37-C22-C23-C24
26	c	915	BCR	C7-C8-C9-C34
24	A	407	CLA	C13-C15-C16-C17
24	B	617	CLA	C3-C5-C6-C7
24	B	616	CLA	C8-C10-C11-C12
24	C	508	CLA	C10-C11-C12-C13
24	c	913	CLA	C15-C16-C17-C18
29	C	520	LMT	O5B-C5B-C6B-O6B
33	J	101	LMG	O6-C5-C6-O5
37	c	918	DGD	C1A-C2A-C3A-C4A
35	b	628	HTG	C1'-C2'-C3'-C4'
24	A	409	CLA	C10-C11-C12-C13
24	B	617	CLA	C10-C11-C12-C13
24	C	509	CLA	C13-C15-C16-C17
24	b	606	CLA	C8-C10-C11-C12
28	B	626	GOL	O2-C2-C3-O3
28	a	419	GOL	O1-C1-C2-O2
28	c	924	GOL	O1-C1-C2-O2
27	A	414	SQD	C23-C24-C25-C26
33	C	519	LMG	C10-C11-C12-C13
33	Z	101	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	b	611	CLA	C10-C11-C12-C13
24	b	619	CLA	C5-C6-C7-C8
24	c	909	CLA	C15-C16-C17-C18
24	d	406	CLA	C15-C16-C17-C18
24	c	910	CLA	C3-C5-C6-C7
29	m	103	LMT	O5'-C5'-C6'-O6'
35	C	522	HTG	O5-C5-C6-O6
24	b	611	CLA	C15-C16-C17-C18
24	b	620	CLA	C10-C11-C12-C13
37	c	917	DGD	C3B-C4B-C5B-C6B
24	C	501	CLA	C15-C16-C17-C18
24	C	509	CLA	O1D-CGD-O2D-CED
24	B	614	CLA	C11-C10-C8-C7
24	C	505	CLA	C11-C12-C13-C15
24	b	611	CLA	C12-C13-C15-C16
24	b	621	CLA	C11-C12-C13-C15
24	a	408	CLA	O1A-CGA-O2A-C1
37	e	101	DGD	O1A-C1A-O1G-C1G
37	H	102	DGD	C3B-C4B-C5B-C6B
26	t	102	BCR	C13-C14-C15-C16
24	B	614	CLA	C8-C10-C11-C12
24	B	615	CLA	C8-C10-C11-C12
24	C	506	CLA	C13-C15-C16-C17
35	B	624	HTG	C1'-C2'-C3'-C4'
29	M	101	LMT	C4B-C5B-C6B-O6B
27	L	102	SQD	C31-C32-C33-C34
29	D	403	LMT	O1'-C1-C2-C3
24	c	910	CLA	O1A-CGA-O2A-C1
33	a	411	LMG	C10-C11-C12-C13
24	B	602	CLA	C10-C11-C12-C13
24	B	614	CLA	C15-C16-C17-C18
24	b	606	CLA	C10-C11-C12-C13
24	c	910	CLA	C15-C16-C17-C18
35	B	625	HTG	C4-C5-C6-O6
24	A	409	CLA	C13-C15-C16-C17
24	a	406	CLA	CBD-CGD-O2D-CED
33	c	919	LMG	C11-C10-O7-C8
33	d	415	LMG	C36-C37-C38-C39
24	a	408	CLA	C15-C16-C17-C18
36	E	101	LHG	C3-O3-P-O6
36	L	101	LHG	C4-O6-P-O3
36	b	635	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
36	d	410	LHG	C3-O3-P-O6
33	C	519	LMG	C28-C29-C30-C31
24	D	405	CLA	C3-C5-C6-C7
24	A	409	CLA	CBA-CGA-O2A-C1
35	b	601	HTG	C1'-C2'-C3'-C4'
35	c	921	HTG	C1'-C2'-C3'-C4'
24	b	619	CLA	C13-C15-C16-C17
24	c	910	CLA	C13-C15-C16-C17
24	B	615	CLA	C4-C3-C5-C6
31	a	415	PL9	C12-C11-C9-C10
24	b	608	CLA	C5-C6-C7-C8
24	b	611	CLA	C2A-CAA-CBA-CGA
24	b	620	CLA	C16-C17-C18-C20
29	e	102	LMT	O5'-C5'-C6'-O6'
24	b	609	CLA	C13-C15-C16-C17
27	A	411	SQD	C12-C13-C14-C15
36	a	418	LHG	C11-C12-C13-C14
33	A	419	LMG	C11-C10-O7-C8
24	B	605	CLA	C3-C5-C6-C7
29	b	602	LMT	C11-C10-C9-C8
33	a	411	LMG	C30-C31-C32-C33
37	C	516	DGD	C6A-C7A-C8A-C9A
37	D	408	DGD	C7A-C8A-C9A-CAA
37	e	101	DGD	C8B-C9B-CAB-CBB
27	a	402	SQD	C25-C26-C27-C28
33	d	415	LMG	C35-C36-C37-C38
33	A	419	LMG	O9-C10-O7-C8
33	c	919	LMG	O9-C10-O7-C8
24	C	513	CLA	CBD-CGD-O2D-CED
27	F	103	SQD	C26-C27-C28-C29
29	t	101	LMT	C3-C4-C5-C6
29	t	101	LMT	C7-C8-C9-C10
33	Y	101	LMG	C11-C12-C13-C14
36	E	101	LHG	C24-C25-C26-C27
27	F	103	SQD	C31-C32-C33-C34
27	L	102	SQD	C28-C29-C30-C31
36	E	101	LHG	O2-C2-C3-O3
37	C	517	DGD	C9A-CAA-CBA-CCA
37	C	517	DGD	CBB-CCB-CDB-CEB
24	C	509	CLA	C3-C5-C6-C7
24	a	408	CLA	C3-C5-C6-C7
27	B	621	SQD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
37	C	517	DGD	C2E-C1E-O5D-C6D
37	c	917	DGD	C2E-C1E-O5D-C6D
33	B	622	LMG	C35-C36-C37-C38
37	c	916	DGD	C9A-CAA-CBA-CCA
37	c	918	DGD	C7A-C8A-C9A-CAA
24	A	409	CLA	O1A-CGA-O2A-C1
31	D	407	PL9	C45-C44-C46-C47
27	A	411	SQD	C9-C10-C11-C12
36	d	411	LHG	C29-C30-C31-C32
37	H	102	DGD	CBB-CCB-CDB-CEB
37	c	917	DGD	C9B-CAB-CBB-CCB
24	B	604	CLA	C6-C7-C8-C9
24	a	406	CLA	C14-C13-C15-C16
24	b	615	CLA	C11-C12-C13-C14
24	c	909	CLA	C11-C10-C8-C9
24	c	914	CLA	C11-C10-C8-C9
24	a	405	CLA	C2C-C3C-CAC-CBC
27	a	410	SQD	C15-C16-C17-C18
33	C	519	LMG	C14-C15-C16-C17
33	c	919	LMG	C32-C33-C34-C35
37	H	102	DGD	C7A-C8A-C9A-CAA
24	C	504	CLA	C15-C16-C17-C18
29	b	626	LMT	C3'-C4'-O1B-C1B
33	B	622	LMG	C29-C30-C31-C32
36	a	418	LHG	C24-C25-C26-C27
36	b	635	LHG	C10-C11-C12-C13
37	c	918	DGD	C6A-C7A-C8A-C9A
28	B	626	GOL	C1-C2-C3-O3
28	B	629	GOL	O1-C1-C2-C3
28	B	630	GOL	O1-C1-C2-C3
28	B	631	GOL	O1-C1-C2-C3
28	B	636	GOL	O1-C1-C2-C3
28	a	413	GOL	O1-C1-C2-C3
28	b	631	GOL	O1-C1-C2-C3
28	b	631	GOL	C1-C2-C3-O3
36	B	635	LHG	O1-C1-C2-C3
36	d	411	LHG	O1-C1-C2-C3
24	c	912	CLA	O1D-CGD-O2D-CED
24	a	406	CLA	C10-C11-C12-C13
27	B	621	SQD	C34-C35-C36-C37
27	a	410	SQD	C30-C31-C32-C33
33	A	419	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	A	419	LMG	C13-C14-C15-C16
36	D	409	LHG	C32-C33-C34-C35
27	L	102	SQD	C12-C13-C14-C15
27	a	410	SQD	C11-C12-C13-C14
33	A	419	LMG	C14-C15-C16-C17
33	J	101	LMG	C19-C20-C21-C22
33	c	919	LMG	C36-C37-C38-C39
37	D	408	DGD	C2A-C3A-C4A-C5A
24	C	507	CLA	C4B-C3B-CAB-CBB
24	b	607	CLA	C4B-C3B-CAB-CBB
24	c	903	CLA	C4B-C3B-CAB-CBB
24	d	405	CLA	C4B-C3B-CAB-CBB
24	a	408	CLA	C16-C17-C18-C19
24	a	408	CLA	C16-C17-C18-C20
37	C	517	DGD	O6E-C1E-O5D-C6D
31	D	407	PL9	C9-C11-C12-C13
27	A	411	SQD	C13-C14-C15-C16
36	D	409	LHG	C13-C14-C15-C16
36	D	410	LHG	C29-C30-C31-C32
36	b	635	LHG	C27-C28-C29-C30
27	A	411	SQD	C15-C16-C17-C18
33	c	919	LMG	C39-C40-C41-C42
36	d	409	LHG	C16-C17-C18-C19
37	C	516	DGD	C4B-C5B-C6B-C7B
37	D	408	DGD	C8B-C9B-CAB-CBB
36	B	635	LHG	C23-C24-C25-C26
27	F	103	SQD	C34-C35-C36-C37
33	b	625	LMG	C30-C31-C32-C33
36	B	635	LHG	C24-C25-C26-C27
37	C	516	DGD	C7B-C8B-C9B-CAB
29	C	520	LMT	O5'-C5'-C6'-O6'
29	M	103	LMT	C2-C1-O1'-C1'
29	a	401	LMT	C7-C8-C9-C10
35	b	601	HTG	C3'-C4'-C5'-C6'
36	B	635	LHG	C28-C29-C30-C31
37	c	917	DGD	C9A-CAA-CBA-CCA
37	c	918	DGD	C6B-C7B-C8B-C9B
37	C	517	DGD	C4B-C5B-C6B-C7B
37	C	516	DGD	O6D-C5D-C6D-O5D
37	c	916	DGD	O6D-C5D-C6D-O5D
37	e	101	DGD	O6D-C5D-C6D-O5D
24	d	406	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	a	407	PHO	C4-C3-C5-C6
24	B	615	CLA	C2-C3-C5-C6
25	a	407	PHO	C2-C3-C5-C6
31	D	407	PL9	C43-C44-C46-C47
31	a	415	PL9	C28-C29-C31-C32
29	b	602	LMT	C3-C4-C5-C6
36	L	101	LHG	C14-C15-C16-C17
28	A	413	GOL	O2-C2-C3-O3
28	B	628	GOL	O1-C1-C2-O2
28	B	630	GOL	O1-C1-C2-O2
28	T	103	GOL	O1-C1-C2-O2
28	V	201	GOL	O1-C1-C2-O2
28	V	204	GOL	O2-C2-C3-O3
28	V	207	GOL	O2-C2-C3-O3
28	b	632	GOL	O1-C1-C2-O2
28	b	633	GOL	O1-C1-C2-O2
28	v	203	GOL	O1-C1-C2-O2
28	v	204	GOL	O1-C1-C2-O2
28	v	205	GOL	O1-C1-C2-O2
37	C	517	DGD	CAB-CBB-CCB-CDB
33	c	919	LMG	C10-C11-C12-C13
36	d	410	LHG	C11-C10-C9-C8
24	B	616	CLA	C2B-C3B-CAB-CBB
24	C	507	CLA	C2B-C3B-CAB-CBB
24	D	404	CLA	C2B-C3B-CAB-CBB
24	b	607	CLA	C2B-C3B-CAB-CBB
24	c	903	CLA	C2B-C3B-CAB-CBB
24	d	405	CLA	C2B-C3B-CAB-CBB
36	d	409	LHG	O2-C2-C3-O3
24	d	404	CLA	C2C-C3C-CAC-CBC
33	J	101	LMG	C34-C35-C36-C37
29	b	602	LMT	C4-C5-C6-C7
33	B	622	LMG	C30-C31-C32-C33
36	d	409	LHG	C25-C26-C27-C28
24	B	617	CLA	C2-C1-O2A-CGA
36	b	635	LHG	C11-C12-C13-C14
37	c	916	DGD	C4D-C5D-C6D-O5D
27	F	103	SQD	C30-C31-C32-C33
33	A	419	LMG	C36-C37-C38-C39
33	z	101	LMG	C13-C14-C15-C16
37	e	101	DGD	C2A-C3A-C4A-C5A
26	B	618	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	B	618	BCR	C5-C6-C7-C8
26	C	515	BCR	C1-C6-C7-C8
26	t	102	BCR	C1-C6-C7-C8
26	t	102	BCR	C5-C6-C7-C8
36	d	409	LHG	C32-C33-C34-C35
24	A	405	CLA	C13-C15-C16-C17
37	c	918	DGD	C5B-C6B-C7B-C8B
37	e	101	DGD	C2B-C3B-C4B-C5B
37	C	516	DGD	C1B-C2B-C3B-C4B
24	B	615	CLA	C5-C6-C7-C8
29	a	401	LMT	C2-C3-C4-C5
36	L	101	LHG	C10-C11-C12-C13
24	C	510	CLA	C4-C3-C5-C6
24	B	604	CLA	C6-C7-C8-C10
24	B	616	CLA	C11-C12-C13-C15
24	B	617	CLA	C6-C7-C8-C10
24	C	510	CLA	C2-C3-C5-C6
24	C	510	CLA	C6-C7-C8-C10
24	a	406	CLA	C6-C7-C8-C10
24	a	406	CLA	C12-C13-C15-C16
24	b	608	CLA	C6-C7-C8-C10
24	c	909	CLA	C11-C10-C8-C7
24	c	910	CLA	C6-C7-C8-C10
24	c	911	CLA	C2-C3-C5-C6
24	c	914	CLA	C11-C10-C8-C7
33	C	519	LMG	C13-C14-C15-C16
24	B	615	CLA	CBA-CGA-O2A-C1
33	A	419	LMG	C29-C28-O8-C9
27	a	402	SQD	C28-C29-C30-C31
36	E	101	LHG	C7-C8-C9-C10
24	C	512	CLA	O1D-CGD-O2D-CED
24	a	408	CLA	C10-C11-C12-C13
24	b	611	CLA	C8-C10-C11-C12
24	b	611	CLA	C13-C15-C16-C17
25	D	401	PHO	C2C-C3C-CAC-CBC
27	B	621	SQD	C31-C32-C33-C34
33	z	101	LMG	C12-C13-C14-C15
36	d	410	LHG	C32-C33-C34-C35
37	c	917	DGD	O6E-C1E-O5D-C6D
24	B	616	CLA	C5-C6-C7-C8
24	c	904	CLA	C8-C10-C11-C12
29	M	103	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
37	D	408	DGD	C6A-C7A-C8A-C9A
33	A	419	LMG	C10-C11-C12-C13
29	M	103	LMT	C2-C3-C4-C5
38	F	102	HEM	C4B-C3B-CAB-CBB
33	Z	101	LMG	O1-C7-C8-O7
36	D	410	LHG	O7-C5-C6-O8
29	t	101	LMT	C2-C3-C4-C5
37	C	517	DGD	C8B-C9B-CAB-CBB
24	b	620	CLA	C16-C17-C18-C19
29	e	102	LMT	C2-C3-C4-C5
37	D	408	DGD	C3B-C4B-C5B-C6B
37	c	916	DGD	O6E-C5E-C6E-O5E
24	c	911	CLA	C4-C3-C5-C6
37	H	102	DGD	C4E-C5E-C6E-O5E
24	B	610	CLA	C2-C3-C5-C6
31	A	417	PL9	C4-C3-C7-C8
31	a	415	PL9	C4-C3-C7-C8
24	B	614	CLA	C11-C10-C8-C9
24	B	615	CLA	C14-C13-C15-C16
24	C	505	CLA	C11-C12-C13-C14
24	C	510	CLA	C6-C7-C8-C9
24	a	406	CLA	C6-C7-C8-C9
24	a	406	CLA	C11-C12-C13-C14
24	b	608	CLA	C6-C7-C8-C9
24	b	619	CLA	C11-C12-C13-C14
24	b	621	CLA	C11-C12-C13-C14
24	c	910	CLA	C6-C7-C8-C9
29	M	103	LMT	O5B-C5B-C6B-O6B
27	A	414	SQD	C30-C31-C32-C33
37	c	916	DGD	CAB-CBB-CCB-CDB
24	c	914	CLA	C10-C11-C12-C13
27	A	414	SQD	C24-C25-C26-C27
37	c	918	DGD	C2A-C3A-C4A-C5A
24	B	615	CLA	O1A-CGA-O2A-C1
24	C	511	CLA	C1A-C2A-CAA-CBA
24	c	909	CLA	C1A-C2A-CAA-CBA
24	B	611	CLA	C16-C17-C18-C19
24	B	611	CLA	C16-C17-C18-C20
37	c	917	DGD	C4A-C5A-C6A-C7A
24	c	905	CLA	C15-C16-C17-C18
36	D	410	LHG	C4-O6-P-O3
36	B	635	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
24	c	914	CLA	C3-C5-C6-C7
27	a	410	SQD	C34-C35-C36-C37
33	Y	101	LMG	C12-C13-C14-C15
33	d	415	LMG	C16-C17-C18-C19
29	b	602	LMT	C7-C8-C9-C10
29	C	520	LMT	O1'-C1-C2-C3
37	h	102	DGD	C5B-C6B-C7B-C8B
24	B	616	CLA	C15-C16-C17-C18
35	C	522	HTG	S1-C1'-C2'-C3'
24	C	510	CLA	CBA-CGA-O2A-C1
29	D	403	LMT	O5B-C5B-C6B-O6B
36	d	409	LHG	C1-C2-C3-O3
36	d	410	LHG	C1-C2-C3-O3
31	D	407	PL9	C15-C14-C16-C17
31	D	407	PL9	C13-C14-C16-C17
27	L	102	SQD	C27-C28-C29-C30
33	a	411	LMG	C14-C15-C16-C17
33	d	415	LMG	C14-C15-C16-C17
36	B	635	LHG	C34-C35-C36-C37
37	c	917	DGD	C5B-C6B-C7B-C8B
36	d	409	LHG	O10-C23-O8-C6
27	B	621	SQD	C11-C10-C9-C8
27	B	621	SQD	C44-C45-C46-O48
27	F	103	SQD	C44-C45-C46-O48
27	L	102	SQD	C44-C45-C46-O48
27	a	402	SQD	O6-C44-C45-C46
36	D	410	LHG	C4-C5-C6-O8
37	D	408	DGD	O1G-C1G-C2G-C3G
37	c	916	DGD	C2A-C3A-C4A-C5A
37	c	917	DGD	C2B-C3B-C4B-C5B
24	C	509	CLA	C5-C6-C7-C8
35	b	601	HTG	C2'-C3'-C4'-C5'
24	C	510	CLA	O1A-CGA-O2A-C1
33	A	419	LMG	O10-C28-O8-C9
33	C	519	LMG	C8-C7-O1-C1
37	c	917	DGD	C2G-C3G-O3G-C1D
37	c	917	DGD	C5D-C6D-O5D-C1E
33	A	419	LMG	C39-C40-C41-C42
33	Y	101	LMG	C31-C32-C33-C34
35	b	628	HTG	O5-C5-C6-O6
27	A	411	SQD	C7-C8-C9-C10
24	C	508	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	A	417	PL9	C19-C21-C22-C23
31	a	415	PL9	C14-C16-C17-C18
33	z	101	LMG	C16-C17-C18-C19
37	C	516	DGD	O6E-C5E-C6E-O5E
28	C	523	GOL	O1-C1-C2-O2
33	C	519	LMG	C4-C5-C6-O5
37	e	101	DGD	C9B-CAB-CBB-CCB
24	D	405	CLA	C8-C10-C11-C12
33	Z	101	LMG	O6-C5-C6-O5
33	d	415	LMG	O6-C5-C6-O5
27	B	621	SQD	C30-C31-C32-C33
37	C	517	DGD	C4A-C5A-C6A-C7A
24	C	511	CLA	CBA-CGA-O2A-C1
36	d	409	LHG	C24-C23-O8-C6
29	A	415	LMT	O5B-C5B-C6B-O6B
27	a	410	SQD	C9-C10-C11-C12
33	b	625	LMG	C40-C41-C42-C43
35	B	624	HTG	C4'-C5'-C6'-C7'
37	c	916	DGD	C8B-C9B-CAB-CBB
24	C	501	CLA	CBD-CGD-O2D-CED
40	V	202	HEC	C2C-C3C-CAC-CBC
36	D	410	LHG	C27-C28-C29-C30
24	a	408	CLA	C8-C10-C11-C12
24	C	513	CLA	C2-C1-O2A-CGA
24	b	606	CLA	C2-C1-O2A-CGA
37	e	101	DGD	C5A-C6A-C7A-C8A
29	A	415	LMT	O1'-C1-C2-C3
37	c	917	DGD	C2A-C3A-C4A-C5A
37	H	102	DGD	O6E-C5E-C6E-O5E
24	C	511	CLA	O1A-CGA-O2A-C1
36	d	409	LHG	C29-C30-C31-C32
29	M	103	LMT	C2'-C1'-O1'-C1
27	f	102	SQD	O6-C44-C45-O47
36	d	411	LHG	C31-C32-C33-C34
24	B	613	CLA	C8-C10-C11-C12
31	A	417	PL9	C45-C44-C46-C47
24	A	409	CLA	C6-C7-C8-C10
24	B	602	CLA	C11-C10-C8-C7
24	B	602	CLA	C12-C13-C15-C16
24	B	615	CLA	C12-C13-C15-C16
24	b	611	CLA	C11-C10-C8-C7
24	b	619	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	c	903	CLA	C11-C12-C13-C15
24	c	907	CLA	C6-C7-C8-C10
24	d	405	CLA	C11-C12-C13-C15
33	B	622	LMG	C38-C39-C40-C41
24	A	409	CLA	C6-C7-C8-C9
24	B	614	CLA	C11-C12-C13-C14
24	C	504	CLA	C11-C12-C13-C14
24	b	611	CLA	C11-C10-C8-C9
24	b	619	CLA	C11-C10-C8-C9
24	c	910	CLA	C14-C13-C15-C16
33	A	419	LMG	C32-C33-C34-C35
33	J	101	LMG	C13-C14-C15-C16
33	a	411	LMG	C12-C13-C14-C15
27	B	621	SQD	C24-C23-O48-C46
36	d	411	LHG	C24-C23-O8-C6
27	L	102	SQD	C32-C33-C34-C35
27	f	102	SQD	C25-C26-C27-C28
33	d	415	LMG	C17-C18-C19-C20
37	C	516	DGD	C4D-C5D-C6D-O5D
36	d	409	LHG	O1-C1-C2-C3
26	Y	102	BCR	C21-C22-C23-C24
29	D	403	LMT	C2-C3-C4-C5
37	C	517	DGD	C5A-C6A-C7A-C8A
24	A	409	CLA	C15-C16-C17-C18
27	L	102	SQD	C24-C23-O48-C46
24	c	907	CLA	C15-C16-C17-C18
36	d	409	LHG	C30-C31-C32-C33
24	A	409	CLA	C4B-C3B-CAB-CBB
24	B	608	CLA	C4B-C3B-CAB-CBB
24	D	404	CLA	C4B-C3B-CAB-CBB
24	D	405	CLA	C4B-C3B-CAB-CBB
24	c	902	CLA	C4B-C3B-CAB-CBB
24	d	406	CLA	C4B-C3B-CAB-CBB
29	m	103	LMT	O5'-C1'-O1'-C1
24	A	409	CLA	C8-C10-C11-C12
36	b	635	LHG	O6-C4-C5-C6
27	B	621	SQD	C16-C17-C18-C19
29	m	102	LMT	C5-C6-C7-C8
27	L	102	SQD	C7-C8-C9-C10
33	c	920	LMG	C10-C11-C12-C13
37	D	408	DGD	C1B-C2B-C3B-C4B
33	A	419	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
27	A	414	SQD	C24-C23-O48-C46
24	C	505	CLA	C2-C3-C5-C6
31	A	417	PL9	C43-C44-C46-C47
37	C	517	DGD	C1A-C2A-C3A-C4A
36	b	635	LHG	C31-C32-C33-C34
37	e	101	DGD	C4D-C5D-C6D-O5D
24	C	502	CLA	C16-C17-C18-C20
24	a	405	CLA	C4C-C3C-CAC-CBC
24	c	912	CLA	CBA-CGA-O2A-C1
27	L	102	SQD	C29-C30-C31-C32
33	B	622	LMG	C37-C38-C39-C40
37	h	102	DGD	CAA-CBA-CCA-CDA
24	B	608	CLA	C3A-C2A-CAA-CBA
24	b	614	CLA	C3A-C2A-CAA-CBA
33	A	419	LMG	C12-C13-C14-C15
35	B	624	HTG	C3'-C4'-C5'-C6'
33	Z	101	LMG	C13-C14-C15-C16
24	a	406	CLA	O1D-CGD-O2D-CED
36	d	409	LHG	C26-C27-C28-C29
38	f	101	HEM	C2A-CAA-CBA-CGA
24	b	619	CLA	C10-C11-C12-C13
27	A	414	SQD	O6-C44-C45-C46
27	a	410	SQD	O6-C44-C45-C46
33	A	419	LMG	C7-C8-C9-O8
33	Z	101	LMG	O1-C7-C8-C9
33	a	411	LMG	C7-C8-C9-O8
33	c	919	LMG	C7-C8-C9-O8
36	E	101	LHG	C4-C5-C6-O8
37	e	101	DGD	O1G-C1G-C2G-C3G
29	D	403	LMT	C5-C6-C7-C8
37	C	518	DGD	CBA-CCA-CDA-CEA
37	c	917	DGD	C6A-C7A-C8A-C9A
24	C	509	CLA	C10-C11-C12-C13
36	b	635	LHG	C28-C29-C30-C31
37	C	518	DGD	C8B-C9B-CAB-CBB
36	d	411	LHG	O10-C23-O8-C6
24	C	505	CLA	C4-C3-C5-C6
31	a	415	PL9	C12-C11-C9-C8
27	a	410	SQD	C27-C28-C29-C30
24	C	513	CLA	O1D-CGD-O2D-CED
24	B	604	CLA	C5-C6-C7-C8
36	E	101	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
29	a	401	LMT	C9-C10-C11-C12
29	e	102	LMT	C9-C10-C11-C12
28	B	636	GOL	O1-C1-C2-O2
28	V	206	GOL	O2-C2-C3-O3
28	V	207	GOL	O1-C1-C2-O2
28	b	631	GOL	O1-C1-C2-O2
24	b	621	CLA	C10-C11-C12-C13
33	B	622	LMG	C16-C17-C18-C19
37	c	916	DGD	C7B-C8B-C9B-CAB
36	D	410	LHG	O6-C4-C5-O7
33	b	625	LMG	C17-C18-C19-C20
24	d	406	CLA	C2B-C3B-CAB-CBB
27	A	411	SQD	C16-C17-C18-C19
36	D	410	LHG	C12-C13-C14-C15
40	V	202	HEC	C2B-C3B-CAB-CBB
27	L	102	SQD	O47-C45-C46-O48
27	a	410	SQD	O6-C44-C45-O47
33	A	419	LMG	O7-C8-C9-O8
33	Z	101	LMG	O7-C8-C9-O8
33	c	920	LMG	O7-C8-C9-O8
36	E	101	LHG	O7-C5-C6-O8
27	L	102	SQD	C11-C10-C9-C8
27	f	102	SQD	C24-C25-C26-C27
37	c	916	DGD	O6E-C1E-O5D-C6D
24	A	405	CLA	C15-C16-C17-C18
27	A	411	SQD	C18-C19-C20-C21
37	C	516	DGD	C4A-C5A-C6A-C7A
37	h	102	DGD	CDA-CEA-CFA-CGA
36	b	635	LHG	C17-C18-C19-C20
24	C	512	CLA	C11-C10-C8-C9
24	b	606	CLA	C6-C7-C8-C9
24	c	903	CLA	C11-C12-C13-C14
33	b	625	LMG	C33-C34-C35-C36
36	D	410	LHG	C2-C3-O3-P
29	m	103	LMT	C1-C2-C3-C4
33	a	411	LMG	C32-C33-C34-C35
37	e	101	DGD	C4A-C5A-C6A-C7A
24	c	902	CLA	C2A-CAA-CBA-CGA
36	E	101	LHG	C23-C24-C25-C26
26	D	406	BCR	C5-C6-C7-C8
26	H	101	BCR	C23-C24-C25-C26
26	H	101	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
26	a	409	BCR	C1-C6-C7-C8
26	b	622	BCR	C1-C6-C7-C8
26	b	622	BCR	C5-C6-C7-C8
26	c	915	BCR	C1-C6-C7-C8
26	c	915	BCR	C5-C6-C7-C8
26	d	407	BCR	C23-C24-C25-C26
26	d	407	BCR	C23-C24-C25-C30
24	B	602	CLA	C8-C10-C11-C12
36	d	411	LHG	C35-C36-C37-C38
33	b	625	LMG	C36-C37-C38-C39
37	C	518	DGD	C6B-C7B-C8B-C9B
35	V	203	HTG	S1-C1'-C2'-C3'
36	d	410	LHG	C16-C17-C18-C19
37	H	102	DGD	CDB-CEB-CFB-CGB
25	d	403	PHO	C2C-C3C-CAC-CBC
27	A	411	SQD	C8-C7-O47-C45
37	H	102	DGD	CDA-CEA-CFA-CGA
24	C	506	CLA	C16-C17-C18-C20
36	a	418	LHG	C7-C8-C9-C10
27	B	621	SQD	C35-C36-C37-C38
27	a	410	SQD	C29-C30-C31-C32
27	f	102	SQD	C31-C32-C33-C34
27	B	621	SQD	O10-C23-O48-C46
33	A	419	LMG	C30-C31-C32-C33
24	B	602	CLA	C11-C12-C13-C15
24	C	512	CLA	C11-C10-C8-C7
24	a	406	CLA	C11-C10-C8-C7
24	b	606	CLA	C6-C7-C8-C10
24	b	621	CLA	C12-C13-C15-C16
24	c	910	CLA	C12-C13-C15-C16
24	c	913	CLA	C11-C10-C8-C7
24	d	404	CLA	C15-C16-C17-C18
24	c	910	CLA	CBD-CGD-O2D-CED
24	b	615	CLA	C16-C17-C18-C19
24	b	615	CLA	C16-C17-C18-C20
33	J	101	LMG	C12-C13-C14-C15
37	e	101	DGD	CCA-CDA-CEA-CFA
24	B	602	CLA	C2A-CAA-CBA-CGA
35	V	203	HTG	O5-C1-S1-C1'
35	V	203	HTG	C2'-C1'-S1-C1
35	b	604	HTG	O5-C1-S1-C1'
35	b	628	HTG	C2'-C1'-S1-C1

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Mol	Chain	Res	Type	Atoms
33	Y	101	LMG	C29-C28-O8-C9
37	C	518	DGD	C2A-C1A-O1G-C1G
37	H	102	DGD	O2G-C1B-C2B-C3B
27	B	621	SQD	C19-C20-C21-C22
33	A	419	LMG	C19-C20-C21-C22
33	Y	101	LMG	C30-C31-C32-C33
27	L	102	SQD	O10-C23-O48-C46
24	B	611	CLA	CAD-CBD-CGD-O2D
24	B	617	CLA	CAD-CBD-CGD-O2D
24	C	512	CLA	CAD-CBD-CGD-O2D
24	D	405	CLA	CAD-CBD-CGD-O2D
24	b	618	CLA	CAD-CBD-CGD-O2D
24	c	902	CLA	CAD-CBD-CGD-O2D
25	A	408	PHO	CAD-CBD-CGD-O2D
25	a	407	PHO	CAD-CBD-CGD-O2D
27	B	621	SQD	C46-C45-O47-C7
38	f	101	HEM	C2C-C3C-CAC-CBC
36	L	101	LHG	C9-C10-C11-C12
24	c	913	CLA	CBA-CGA-O2A-C1
31	A	417	PL9	C15-C14-C16-C17
33	Z	101	LMG	C7-C8-C9-O8
33	z	101	LMG	O1-C7-C8-C9
36	d	409	LHG	C4-C5-C6-O8
24	c	912	CLA	O1A-CGA-O2A-C1
36	b	635	LHG	O6-C4-C5-O7
24	c	911	CLA	C13-C15-C16-C17
24	B	616	CLA	C10-C11-C12-C13
36	b	635	LHG	C9-C10-C11-C12
24	A	405	CLA	C16-C17-C18-C19
29	M	103	LMT	C2B-C1B-O1B-C4'
24	B	606	CLA	CHA-CBD-CGD-O1D
24	B	608	CLA	CHA-CBD-CGD-O1D
24	C	502	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	b	606	CLA	CHA-CBD-CGD-O1D
24	b	606	CLA	CHA-CBD-CGD-O2D
24	c	903	CLA	CHA-CBD-CGD-O1D
24	c	907	CLA	CHA-CBD-CGD-O1D
24	c	910	CLA	CHA-CBD-CGD-O1D
24	c	913	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	c	904	CLA	CBD-CGD-O2D-CED
27	A	414	SQD	O10-C23-O48-C46
29	D	403	LMT	C2'-C1'-O1'-C1
33	J	101	LMG	C30-C31-C32-C33
36	b	635	LHG	C33-C34-C35-C36
36	d	410	LHG	C34-C35-C36-C37
33	A	419	LMG	O1-C7-C8-O7
33	c	919	LMG	O7-C8-C9-O8
37	D	408	DGD	O1G-C1G-C2G-O2G
33	Y	101	LMG	O10-C28-O8-C9
27	a	402	SQD	C29-C30-C31-C32
24	c	907	CLA	C16-C17-C18-C19
28	B	629	GOL	O1-C1-C2-O2
28	D	402	GOL	O1-C1-C2-O2
24	B	610	CLA	C4-C3-C5-C6
24	c	913	CLA	O1A-CGA-O2A-C1
27	A	411	SQD	O49-C7-O47-C45
24	A	407	CLA	C11-C10-C8-C9
24	a	406	CLA	C11-C10-C8-C9
24	c	913	CLA	C11-C10-C8-C9
36	B	635	LHG	C33-C34-C35-C36
36	d	411	LHG	C9-C10-C11-C12
24	b	620	CLA	CBD-CGD-O2D-CED
37	h	102	DGD	O2G-C1B-C2B-C3B
24	c	911	CLA	C8-C10-C11-C12
36	a	418	LHG	C25-C26-C27-C28
36	d	409	LHG	C18-C19-C20-C21
26	t	102	BCR	C7-C8-C9-C34
28	D	402	GOL	O1-C1-C2-C3
37	c	917	DGD	C4B-C5B-C6B-C7B
26	c	915	BCR	C7-C8-C9-C10
24	C	502	CLA	C3-C5-C6-C7
24	C	501	CLA	C1A-C2A-CAA-CBA
24	b	616	CLA	C16-C17-C18-C20
33	Y	101	LMG	C16-C17-C18-C19
33	b	625	LMG	C37-C38-C39-C40
36	L	101	LHG	C29-C30-C31-C32
37	C	517	DGD	C8A-C9A-CAA-CBA
29	b	602	LMT	C2-C3-C4-C5
36	d	411	LHG	C28-C29-C30-C31
36	d	411	LHG	C2-C3-O3-P
24	A	407	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	B	610	CLA	C4B-C3B-CAB-CBB
24	c	904	CLA	C4B-C3B-CAB-CBB
36	D	410	LHG	C4-O6-P-O5
36	E	101	LHG	C3-O3-P-O5
36	d	410	LHG	C3-O3-P-O5
24	b	619	CLA	C16-C17-C18-C19
29	D	403	LMT	O5'-C1'-O1'-C1
24	b	617	CLA	C8-C10-C11-C12
36	L	101	LHG	O6-C4-C5-C6
40	V	202	HEC	C4C-C3C-CAC-CBC
24	C	508	CLA	C3-C5-C6-C7
35	b	603	HTG	C2'-C3'-C4'-C5'
37	c	917	DGD	C7A-C8A-C9A-CAA
37	C	518	DGD	O1A-C1A-O1G-C1G
24	d	406	CLA	C16-C17-C18-C19
24	B	602	CLA	CAD-CBD-CGD-O1D
24	B	606	CLA	CAD-CBD-CGD-O1D
24	B	608	CLA	CAD-CBD-CGD-O1D
24	B	610	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	b	606	CLA	CAD-CBD-CGD-O1D
24	b	610	CLA	CAD-CBD-CGD-O1D
24	c	903	CLA	CAD-CBD-CGD-O1D
24	c	905	CLA	CAD-CBD-CGD-O1D
24	c	907	CLA	CAD-CBD-CGD-O1D
24	c	913	CLA	CAD-CBD-CGD-O1D
24	d	404	CLA	C4C-C3C-CAC-CBC
24	c	909	CLA	C10-C11-C12-C13
35	c	921	HTG	S1-C1'-C2'-C3'
24	A	406	CLA	C2C-C3C-CAC-CBC
27	a	410	SQD	C10-C11-C12-C13
37	C	517	DGD	CBA-CCA-CDA-CEA
37	C	517	DGD	C1B-C2B-C3B-C4B
24	A	407	CLA	C11-C10-C8-C7
24	B	616	CLA	C12-C13-C15-C16
24	C	504	CLA	C12-C13-C15-C16
24	c	907	CLA	C11-C10-C8-C7
35	B	625	HTG	C2-C1-S1-C1'
35	V	203	HTG	C2-C1-S1-C1'
35	c	921	HTG	C2-C1-S1-C1'
29	t	101	LMT	C11-C10-C9-C8
36	L	101	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
36	d	411	LHG	C33-C34-C35-C36
37	C	517	DGD	C3A-C4A-C5A-C6A
27	B	621	SQD	C14-C15-C16-C17
27	f	102	SQD	C26-C27-C28-C29
37	e	101	DGD	CAA-CBA-CCA-CDA
37	h	102	DGD	C6A-C7A-C8A-C9A
24	B	615	CLA	C16-C17-C18-C19
33	d	415	LMG	C38-C39-C40-C41
27	L	102	SQD	C18-C19-C20-C21
33	c	919	LMG	C17-C18-C19-C20
27	B	621	SQD	O47-C45-C46-O48
27	F	103	SQD	O47-C45-C46-O48
33	a	411	LMG	O7-C8-C9-O8
37	e	101	DGD	O1G-C1G-C2G-O2G
27	A	414	SQD	C17-C18-C19-C20
33	c	920	LMG	C37-C38-C39-C40
36	B	635	LHG	C25-C26-C27-C28
29	A	415	LMT	C5-C6-C7-C8
36	L	101	LHG	C32-C33-C34-C35
29	t	101	LMT	C4-C5-C6-C7
37	C	517	DGD	C5D-C6D-O5D-C1E
24	C	502	CLA	C16-C17-C18-C19
27	B	621	SQD	C17-C18-C19-C20
29	a	417	LMT	C7-C8-C9-C10
29	m	103	LMT	C2-C3-C4-C5
33	b	625	LMG	C34-C35-C36-C37
24	B	607	CLA	C10-C11-C12-C13
24	b	621	CLA	C4-C3-C5-C6
27	L	102	SQD	C10-C11-C12-C13
37	C	517	DGD	CAA-CBA-CCA-CDA
37	c	918	DGD	C4A-C5A-C6A-C7A
31	d	408	PL9	C13-C14-C16-C17
24	b	606	CLA	CAA-CBA-CGA-O2A
27	L	102	SQD	C11-C12-C13-C14
24	A	407	CLA	C6-C7-C8-C9
24	B	602	CLA	C11-C12-C13-C14
24	B	615	CLA	C6-C7-C8-C9
24	b	606	CLA	C11-C10-C8-C9
24	b	621	CLA	C14-C13-C15-C16
24	b	619	CLA	C16-C17-C18-C20
27	A	414	SQD	C25-C26-C27-C28
27	A	414	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
27	A	411	SQD	C14-C15-C16-C17
36	d	411	LHG	C11-C12-C13-C14
24	C	512	CLA	O1A-CGA-O2A-C1
28	C	524	GOL	O1-C1-C2-O2
28	a	413	GOL	O1-C1-C2-O2
28	a	419	GOL	O2-C2-C3-O3
36	B	635	LHG	O1-C1-C2-O2
29	a	401	LMT	C3-C4-C5-C6
33	A	419	LMG	C33-C34-C35-C36
37	e	101	DGD	C7B-C8B-C9B-CAB
27	a	402	SQD	C24-C25-C26-C27
24	A	407	CLA	C2B-C3B-CAB-CBB
24	A	409	CLA	C2B-C3B-CAB-CBB
24	B	608	CLA	C2B-C3B-CAB-CBB
24	D	405	CLA	C2B-C3B-CAB-CBB
24	c	902	CLA	C2B-C3B-CAB-CBB
27	a	410	SQD	C16-C17-C18-C19
31	d	408	PL9	C15-C14-C16-C17
37	H	102	DGD	CCA-CDA-CEA-CFA
29	M	101	LMT	C7-C8-C9-C10
27	a	410	SQD	C33-C34-C35-C36
36	D	410	LHG	C28-C29-C30-C31
27	L	102	SQD	C46-C45-O47-C7
24	B	603	CLA	C2A-CAA-CBA-CGA
24	b	607	CLA	C2A-CAA-CBA-CGA
24	b	610	CLA	C8-C10-C11-C12
24	b	613	CLA	C13-C15-C16-C17
24	C	511	CLA	C2-C1-O2A-CGA
24	c	904	CLA	C2-C1-O2A-CGA
33	C	519	LMG	C29-C30-C31-C32
36	E	101	LHG	C19-C20-C21-C22
36	b	635	LHG	C5-C6-O8-C23
29	F	101	LMT	C2-C3-C4-C5
37	c	918	DGD	C7B-C8B-C9B-CAB
24	B	617	CLA	C16-C17-C18-C19
29	m	103	LMT	O1'-C1-C2-C3
24	b	620	CLA	O1D-CGD-O2D-CED
26	A	410	BCR	C1-C6-C7-C8
26	C	515	BCR	C5-C6-C7-C8
26	D	406	BCR	C1-C6-C7-C8
26	a	409	BCR	C5-C6-C7-C8
31	A	417	PL9	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
24	B	616	CLA	C13-C15-C16-C17
27	a	402	SQD	C31-C32-C33-C34
36	D	409	LHG	C17-C18-C19-C20
29	m	103	LMT	C11-C10-C9-C8
40	V	202	HEC	C4B-C3B-CAB-CBB
27	A	414	SQD	C2-C1-O6-C44
29	m	103	LMT	C2'-C1'-O1'-C1
37	c	916	DGD	C2E-C1E-O5D-C6D
37	h	102	DGD	C9B-CAB-CBB-CCB
33	z	101	LMG	O1-C7-C8-O7
25	d	403	PHO	CHA-CBD-CGD-O2D
27	f	102	SQD	O6-C44-C45-C46
33	c	920	LMG	C7-C8-C9-O8
24	A	407	CLA	C6-C7-C8-C10
24	C	504	CLA	C11-C12-C13-C15
24	c	906	CLA	C11-C12-C13-C14
24	d	405	CLA	C11-C12-C13-C14
29	D	403	LMT	O5B-C1B-O1B-C4'
24	b	616	CLA	C16-C17-C18-C19
29	e	102	LMT	C5-C6-C7-C8
36	B	635	LHG	C11-C10-C9-C8
29	e	102	LMT	C2B-C1B-O1B-C4'
37	C	518	DGD	C3B-C4B-C5B-C6B
24	C	513	CLA	O1A-CGA-O2A-C1
24	c	907	CLA	C16-C17-C18-C20
37	C	518	DGD	C2A-C3A-C4A-C5A
28	c	928	GOL	C1-C2-C3-O3
36	D	410	LHG	C17-C18-C19-C20
24	C	501	CLA	O1D-CGD-O2D-CED
24	B	606	CLA	CBD-CGD-O2D-CED
24	C	506	CLA	C16-C17-C18-C19
24	C	512	CLA	CBA-CGA-O2A-C1
24	C	513	CLA	CBA-CGA-O2A-C1
24	b	606	CLA	CBA-CGA-O2A-C1
24	b	606	CLA	O1A-CGA-O2A-C1
24	B	602	CLA	CAA-CBA-CGA-O2A
33	d	415	LMG	C29-C30-C31-C32
24	b	616	CLA	C8-C10-C11-C12
24	B	604	CLA	C4B-C3B-CAB-CBB
24	b	620	CLA	C4B-C3B-CAB-CBB
24	B	611	CLA	C2A-CAA-CBA-CGA
24	B	615	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	b	607	CLA	C16-C17-C18-C19
29	M	101	LMT	O5'-C1'-O1'-C1
27	B	621	SQD	C12-C13-C14-C15
24	C	513	CLA	C3-C5-C6-C7
36	a	418	LHG	C28-C29-C30-C31
27	A	414	SQD	C11-C12-C13-C14
24	b	606	CLA	C13-C15-C16-C17
38	f	101	HEM	C4C-C3C-CAC-CBC
24	c	911	CLA	C3-C5-C6-C7
36	D	409	LHG	C9-C10-C11-C12
31	D	407	PL9	C28-C29-C31-C32
38	f	101	HEM	CAA-CBA-CGA-O1A
29	D	403	LMT	C2B-C1B-O1B-C4'
24	b	618	CLA	C2-C1-O2A-CGA
24	c	913	CLA	C2-C1-O2A-CGA
33	b	625	LMG	C32-C33-C34-C35
36	d	409	LHG	O7-C5-C6-O8
24	c	904	CLA	O1D-CGD-O2D-CED
24	c	912	CLA	C3-C5-C6-C7
29	m	102	LMT	C11-C10-C9-C8
24	a	408	CLA	C4-C3-C5-C6
24	b	621	CLA	C16-C17-C18-C19
37	e	101	DGD	C6A-C7A-C8A-C9A
29	F	101	LMT	C1-C2-C3-C4
33	B	622	LMG	C15-C16-C17-C18
24	C	509	CLA	C15-C16-C17-C18
37	c	916	DGD	C6A-C7A-C8A-C9A
24	B	617	CLA	C16-C17-C18-C20
24	d	406	CLA	C16-C17-C18-C20
37	C	516	DGD	O6E-C1E-O5D-C6D
26	A	410	BCR	C36-C18-C19-C20
27	a	410	SQD	C26-C27-C28-C29
36	d	409	LHG	C11-C10-C9-C8
24	A	406	CLA	C1A-C2A-CAA-CBA
24	C	506	CLA	C1A-C2A-CAA-CBA
24	c	902	CLA	C1A-C2A-CAA-CBA
24	d	404	CLA	C1A-C2A-CAA-CBA
24	a	406	CLA	C11-C12-C13-C15
24	b	611	CLA	C11-C12-C13-C15
24	c	911	CLA	C12-C13-C15-C16
29	M	101	LMT	O5'-C5'-C6'-O6'
26	h	101	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	a	411	LMG	C29-C30-C31-C32
37	c	916	DGD	C5B-C6B-C7B-C8B
36	B	635	LHG	C15-C16-C17-C18
37	D	408	DGD	C2B-C3B-C4B-C5B
24	b	619	CLA	C2A-CAA-CBA-CGA
24	b	619	CLA	C15-C16-C17-C18
24	c	913	CLA	C13-C15-C16-C17
29	b	626	LMT	C6-C7-C8-C9
36	D	410	LHG	C10-C11-C12-C13
37	D	408	DGD	CBA-CCA-CDA-CEA
36	L	101	LHG	O6-C4-C5-O7
38	F	102	HEM	CAD-CBD-CGD-O1D
37	c	918	DGD	CBA-CCA-CDA-CEA
37	c	917	DGD	C3A-C4A-C5A-C6A
31	a	415	PL9	C45-C44-C46-C47
24	B	604	CLA	C2B-C3B-CAB-CBB
24	B	610	CLA	C2B-C3B-CAB-CBB
24	b	620	CLA	C2B-C3B-CAB-CBB
24	c	904	CLA	C2B-C3B-CAB-CBB
38	f	101	HEM	CAA-CBA-CGA-O2A
33	a	411	LMG	C35-C36-C37-C38
24	b	620	CLA	C5-C6-C7-C8
29	M	101	LMT	C2'-C1'-O1'-C1
37	D	408	DGD	O2G-C2G-C3G-O3G
27	F	103	SQD	C24-C23-O48-C46
24	c	904	CLA	C5-C6-C7-C8
35	B	625	HTG	C3'-C4'-C5'-C6'
37	C	516	DGD	C9A-CAA-CBA-CCA
37	C	517	DGD	C6B-C7B-C8B-C9B
29	F	101	LMT	C4'-C5'-C6'-O6'
24	a	405	CLA	C2-C1-O2A-CGA
24	b	619	CLA	C2-C1-O2A-CGA
24	c	907	CLA	C2-C1-O2A-CGA
24	a	408	CLA	C2-C3-C5-C6
24	b	621	CLA	C2-C3-C5-C6
24	C	509	CLA	C8-C10-C11-C12
24	C	502	CLA	C11-C12-C13-C14
24	b	611	CLA	C14-C13-C15-C16
33	J	101	LMG	C20-C21-C22-C23
29	M	103	LMT	O5B-C1B-O1B-C4'
24	A	405	CLA	C16-C17-C18-C20
38	F	102	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	F	103	SQD	O10-C23-O48-C46
26	A	410	BCR	C5-C6-C7-C8
26	C	514	BCR	C1-C6-C7-C8
26	D	406	BCR	C23-C24-C25-C26
26	D	406	BCR	C23-C24-C25-C30
26	h	101	BCR	C23-C24-C25-C30
24	C	513	CLA	C8-C10-C11-C12
33	A	419	LMG	O1-C7-C8-C9
33	Y	101	LMG	C35-C36-C37-C38
36	D	409	LHG	C33-C34-C35-C36
28	B	629	GOL	C1-C2-C3-O3
28	C	524	GOL	O1-C1-C2-C3
28	c	928	GOL	O1-C1-C2-C3
36	b	635	LHG	O1-C1-C2-C3
31	D	407	PL9	C30-C29-C31-C32
33	J	101	LMG	C8-C7-O1-C1
37	C	516	DGD	C5D-C6D-O5D-C1E
37	C	517	DGD	C2G-C3G-O3G-C1D
27	a	410	SQD	C35-C36-C37-C38
33	B	622	LMG	O8-C28-C29-C30
29	m	102	LMT	C9-C10-C11-C12
24	b	609	CLA	C16-C17-C18-C19
24	C	501	CLA	C2A-CAA-CBA-CGA
24	C	507	CLA	C2A-CAA-CBA-CGA
24	c	907	CLA	C13-C15-C16-C17
27	F	103	SQD	C32-C33-C34-C35
33	c	919	LMG	C20-C21-C22-C23
24	c	905	CLA	C4B-C3B-CAB-CBB
36	D	410	LHG	O6-C4-C5-C6
24	b	606	CLA	C4-C3-C5-C6
31	A	417	PL9	C20-C19-C21-C22
24	B	612	CLA	C2-C3-C5-C6
24	c	906	CLA	C11-C12-C13-C15
24	B	609	CLA	C13-C15-C16-C17
24	b	620	CLA	C13-C15-C16-C17
28	b	631	GOL	O2-C2-C3-O3
36	b	635	LHG	O1-C1-C2-O2
33	Z	101	LMG	O7-C10-C11-C12
24	d	405	CLA	C16-C17-C18-C20
29	a	417	LMT	C6-C7-C8-C9
35	B	623	HTG	C4-C5-C6-O6
24	C	510	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	F	101	LMT	O1'-C1-C2-C3
33	d	415	LMG	C11-C12-C13-C14
36	L	101	LHG	C28-C29-C30-C31
37	c	917	DGD	C6B-C7B-C8B-C9B
35	B	623	HTG	C2'-C1'-S1-C1
37	C	518	DGD	C7A-C8A-C9A-CAA
24	C	512	CLA	CAA-CBA-CGA-O2A
27	f	102	SQD	O47-C7-C8-C9
37	c	917	DGD	O2G-C1B-C2B-C3B
35	B	623	HTG	C4'-C5'-C6'-C7'
24	B	607	CLA	C4-C3-C5-C6
24	B	616	CLA	C4-C3-C5-C6
24	c	914	CLA	C4-C3-C5-C6
31	A	417	PL9	C30-C29-C31-C32
31	A	417	PL9	C40-C39-C41-C42
40	V	202	HEC	CAD-CBD-CGD-O2D
37	C	516	DGD	O1A-C1A-O1G-C1G
31	a	415	PL9	C43-C44-C46-C47
24	B	616	CLA	C14-C13-C15-C16
24	C	504	CLA	C14-C13-C15-C16
24	c	907	CLA	C11-C10-C8-C9
27	a	402	SQD	C12-C13-C14-C15
24	A	409	CLA	C3A-C2A-CAA-CBA
24	B	613	CLA	O1A-CGA-O2A-C1
33	a	411	LMG	O8-C28-C29-C30
36	a	418	LHG	C14-C15-C16-C17
24	B	605	CLA	CAD-CBD-CGD-O2D
24	B	613	CLA	CAD-CBD-CGD-O2D
24	C	501	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	b	608	CLA	CAD-CBD-CGD-O2D
24	b	609	CLA	CAD-CBD-CGD-O2D
24	b	615	CLA	CAD-CBD-CGD-O2D
24	b	617	CLA	CAD-CBD-CGD-O2D
24	b	621	CLA	CAD-CBD-CGD-O2D
24	c	904	CLA	CAD-CBD-CGD-O2D
24	c	911	CLA	CAD-CBD-CGD-O2D
38	f	101	HEM	C2B-C3B-CAB-CBB
33	J	101	LMG	C15-C16-C17-C18
24	b	615	CLA	C2A-CAA-CBA-CGA
24	c	912	CLA	C2-C1-O2A-CGA
29	a	401	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
37	C	516	DGD	O2G-C1B-C2B-C3B
24	c	908	CLA	C5-C6-C7-C8
24	c	913	CLA	CAA-CBA-CGA-O2A
36	b	635	LHG	O7-C7-C8-C9
37	c	918	DGD	O1G-C1A-C2A-C3A
26	A	410	BCR	C17-C18-C19-C20
26	C	515	BCR	C7-C8-C9-C10
36	b	635	LHG	C34-C35-C36-C37
33	c	919	LMG	O1-C7-C8-C9
40	v	202	HEC	CAD-CBD-CGD-O2D
36	a	418	LHG	C18-C19-C20-C21
37	D	408	DGD	O1G-C1A-C2A-C3A
27	F	103	SQD	C33-C34-C35-C36
24	B	605	CLA	O2A-C1-C2-C3
24	B	614	CLA	O2A-C1-C2-C3
24	d	406	CLA	O2A-C1-C2-C3
25	A	408	PHO	O2A-C1-C2-C3
25	a	407	PHO	O2A-C1-C2-C3
27	L	102	SQD	C16-C17-C18-C19
27	L	102	SQD	C30-C31-C32-C33
27	f	102	SQD	C33-C34-C35-C36
38	f	101	HEM	C4B-C3B-CAB-CBB
24	B	606	CLA	C2A-CAA-CBA-CGA
24	c	908	CLA	C2A-CAA-CBA-CGA
33	a	411	LMG	C22-C23-C24-C25
36	D	410	LHG	C33-C34-C35-C36
36	a	418	LHG	O8-C23-C24-C25
40	V	202	HEC	CAD-CBD-CGD-O1D
36	D	410	LHG	C30-C31-C32-C33
37	c	918	DGD	C3A-C4A-C5A-C6A
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
24	B	608	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O2D
24	C	502	CLA	CHA-CBD-CGD-O2D
24	C	504	CLA	CHA-CBD-CGD-O1D
24	C	505	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	b	607	CLA	CHA-CBD-CGD-O1D
24	b	607	CLA	CHA-CBD-CGD-O2D
24	c	903	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	c	905	CLA	CHA-CBD-CGD-O1D
24	c	906	CLA	CHA-CBD-CGD-O1D
24	c	906	CLA	CHA-CBD-CGD-O2D
24	c	907	CLA	CHA-CBD-CGD-O2D
24	c	908	CLA	CHA-CBD-CGD-O1D
24	c	908	CLA	CHA-CBD-CGD-O2D
24	c	910	CLA	CHA-CBD-CGD-O2D
24	c	913	CLA	CHA-CBD-CGD-O2D
24	d	404	CLA	CHA-CBD-CGD-O1D
24	d	404	CLA	CHA-CBD-CGD-O2D
36	B	635	LHG	C11-C12-C13-C14
24	B	616	CLA	C2-C3-C5-C6
40	v	202	HEC	CAD-CBD-CGD-O1D
29	D	403	LMT	C6-C7-C8-C9
36	B	635	LHG	C29-C30-C31-C32
24	b	606	CLA	C16-C17-C18-C20
31	A	417	PL9	C2-C3-C7-C8
33	J	101	LMG	O1-C7-C8-O7
33	c	919	LMG	O1-C7-C8-O7
24	B	613	CLA	C13-C15-C16-C17
27	f	102	SQD	C35-C36-C37-C38
36	E	101	LHG	O8-C23-C24-C25
36	L	101	LHG	O7-C7-C8-C9
37	C	516	DGD	CAA-CBA-CCA-CDA
24	C	502	CLA	C11-C12-C13-C15
38	f	101	HEM	CAD-CBD-CGD-O1D
24	B	616	CLA	C11-C12-C13-C14
24	D	405	CLA	C11-C10-C8-C9
24	b	611	CLA	C11-C12-C13-C14
25	D	401	PHO	C14-C13-C15-C16
29	m	103	LMT	C9-C10-C11-C12
24	c	905	CLA	C2B-C3B-CAB-CBB
33	a	411	LMG	C18-C19-C20-C21
36	b	635	LHG	C12-C13-C14-C15
37	C	516	DGD	C2A-C1A-O1G-C1G
24	b	607	CLA	C16-C17-C18-C20
24	d	405	CLA	C16-C17-C18-C19
24	b	617	CLA	O1A-CGA-O2A-C1
37	D	408	DGD	O1A-C1A-C2A-C3A
33	c	920	LMG	C12-C13-C14-C15
24	B	613	CLA	CBA-CGA-O2A-C1
38	f	101	HEM	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
24	C	509	CLA	C16-C17-C18-C19
37	C	518	DGD	CAB-CBB-CCB-CDB
28	V	207	GOL	O1-C1-C2-C3
28	a	412	GOL	O1-C1-C2-C3
24	C	510	CLA	CAA-CBA-CGA-O2A
37	D	408	DGD	C4B-C5B-C6B-C7B
24	b	614	CLA	C1A-C2A-CAA-CBA
24	d	405	CLA	C1A-C2A-CAA-CBA
36	d	409	LHG	C33-C34-C35-C36
24	C	512	CLA	CAA-CBA-CGA-O1A
27	A	411	SQD	C30-C31-C32-C33
24	a	405	CLA	C2A-CAA-CBA-CGA
24	b	608	CLA	C2A-CAA-CBA-CGA
24	c	902	CLA	CBD-CGD-O2D-CED
36	D	409	LHG	C4-O6-P-O3
29	e	102	LMT	O5B-C1B-O1B-C4'
33	Z	101	LMG	O9-C10-C11-C12
33	Y	101	LMG	C29-C30-C31-C32
33	a	411	LMG	O9-C10-O7-C8
36	E	101	LHG	O9-C7-O7-C5
27	f	102	SQD	O49-C7-C8-C9
37	c	918	DGD	O1A-C1A-C2A-C3A
37	C	516	DGD	C2E-C1E-O5D-C6D
24	c	905	CLA	C8-C10-C11-C12
27	L	102	SQD	C13-C14-C15-C16
24	B	602	CLA	C4B-C3B-CAB-CBB
36	D	409	LHG	C3-O3-P-O4
36	D	409	LHG	C4-O6-P-O5
24	c	913	CLA	CAA-CBA-CGA-O1A
24	C	503	CLA	C10-C11-C12-C13
26	b	623	BCR	C23-C24-C25-C30
24	C	513	CLA	C5-C6-C7-C8
37	e	101	DGD	C1A-C2A-C3A-C4A
36	L	101	LHG	O9-C7-C8-C9
36	d	409	LHG	O8-C23-C24-C25
37	e	101	DGD	O2G-C1B-C2B-C3B
24	b	611	CLA	C16-C17-C18-C19
36	b	635	LHG	O9-C7-C8-C9
35	b	627	HTG	C4'-C5'-C6'-C7'
36	E	101	LHG	C25-C26-C27-C28
37	C	518	DGD	CCB-CDB-CEB-CFB
33	J	101	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
33	z	101	LMG	C10-C11-C12-C13
36	a	418	LHG	O10-C23-C24-C25
36	d	409	LHG	O10-C23-C24-C25
37	c	917	DGD	O1B-C1B-C2B-C3B
24	B	604	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	C	506	CLA	CAD-CBD-CGD-O1D
24	b	612	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O1D
24	c	906	CLA	CAD-CBD-CGD-O1D
27	B	621	SQD	C5-C6-S-O7
24	c	906	CLA	O1A-CGA-O2A-C1
24	b	618	CLA	CAA-CBA-CGA-O2A
37	c	918	DGD	O6D-C5D-C6D-O5D
24	B	605	CLA	C6-C7-C8-C9
28	a	412	GOL	O1-C1-C2-O2
38	f	101	HEM	CAD-CBD-CGD-O2D
36	D	409	LHG	C31-C32-C33-C34
24	C	505	CLA	CAA-CBA-CGA-O2A
29	b	626	LMT	C5-C6-C7-C8
35	C	522	HTG	C1'-C2'-C3'-C4'
24	c	906	CLA	CAA-CBA-CGA-O2A
36	d	411	LHG	O8-C23-C24-C25
36	E	101	LHG	C15-C16-C17-C18
24	A	407	CLA	C10-C11-C12-C13
24	b	606	CLA	C11-C10-C8-C7
24	b	619	CLA	C12-C13-C15-C16
24	c	902	CLA	C11-C12-C13-C15
24	c	910	CLA	C11-C10-C8-C7
25	D	401	PHO	C12-C13-C15-C16
37	h	102	DGD	C7B-C8B-C9B-CAB
33	Y	101	LMG	O7-C10-C11-C12
37	C	517	DGD	O2G-C1B-C2B-C3B
26	C	515	BCR	C21-C22-C23-C24
26	t	102	BCR	C7-C8-C9-C10
29	m	102	LMT	C2-C1-O1'-C1'
24	B	614	CLA	CAA-CBA-CGA-O2A
29	M	103	LMT	C3-C4-C5-C6
35	b	627	HTG	C2'-C3'-C4'-C5'
36	L	101	LHG	C16-C17-C18-C19
35	V	203	HTG	C4-C5-C6-O6
24	b	619	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	c	906	CLA	CAA-CBA-CGA-O1A
24	b	617	CLA	CBA-CGA-O2A-C1
31	D	407	PL9	C34-C36-C37-C38
36	L	101	LHG	C13-C14-C15-C16
33	A	419	LMG	O7-C10-C11-C12
25	d	403	PHO	C8-C10-C11-C12
36	E	101	LHG	O10-C23-C24-C25
24	B	615	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

162 monomers are involved in 391 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	927	BCR	5	0
28	T	101	GOL	2	0
35	b	601	HTG	1	0
24	B	614	CLA	1	0
29	M	103	LMT	1	0
35	c	921	HTG	1	0
24	b	619	CLA	1	0
24	C	505	CLA	7	0
24	b	618	CLA	3	0
24	c	905	CLA	2	0
28	a	413	GOL	1	0
28	T	103	GOL	2	0
26	B	619	BCR	3	0
27	B	621	SQD	3	0
24	C	511	CLA	4	0
24	c	914	CLA	8	0
24	a	406	CLA	2	0
33	a	411	LMG	2	0
37	C	517	DGD	3	0
36	B	635	LHG	3	0
24	c	907	CLA	2	0
24	c	906	CLA	8	0
28	D	402	GOL	1	0
24	C	510	CLA	3	0
24	b	615	CLA	2	0
24	C	507	CLA	5	0
29	C	520	LMT	1	0
26	k	101	BCR	1	0
25	A	408	PHO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	506	CLA	3	0
38	F	102	HEM	3	0
24	b	606	CLA	3	0
26	K	101	BCR	2	0
37	e	101	DGD	5	0
29	e	102	LMT	1	0
24	C	501	CLA	3	0
33	Y	101	LMG	2	0
24	C	503	CLA	2	0
31	a	415	PL9	11	0
29	m	102	LMT	3	0
26	T	102	BCR	4	0
26	D	406	BCR	1	0
26	c	915	BCR	3	0
35	D	413	HTG	3	0
36	d	411	LHG	4	0
36	D	409	LHG	2	0
35	b	627	HTG	1	0
26	h	101	BCR	5	0
24	B	603	CLA	3	0
24	c	911	CLA	3	0
26	C	514	BCR	7	0
37	c	918	DGD	1	0
27	f	102	SQD	2	1
26	t	102	BCR	5	0
31	d	408	PL9	1	0
33	Z	101	LMG	3	0
24	D	405	CLA	2	0
36	b	635	LHG	5	0
24	B	604	CLA	2	0
37	C	516	DGD	4	0
24	B	615	CLA	6	0
36	a	418	LHG	6	0
27	A	411	SQD	6	0
24	d	406	CLA	3	0
24	b	611	CLA	2	0
26	B	620	BCR	5	0
28	B	630	GOL	1	0
24	c	902	CLA	4	0
28	b	631	GOL	1	0
24	B	608	CLA	3	0
27	A	414	SQD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	410	SQD	5	0
24	B	617	CLA	5	0
37	c	916	DGD	5	0
24	B	602	CLA	4	0
24	C	513	CLA	6	0
31	A	417	PL9	7	0
36	d	409	LHG	5	0
25	d	403	PHO	3	0
24	b	617	CLA	2	0
24	c	903	CLA	2	0
36	D	410	LHG	6	0
24	B	611	CLA	2	0
24	b	612	CLA	2	0
26	B	618	BCR	2	0
24	d	404	CLA	3	0
24	b	610	CLA	6	0
35	d	414	HTG	2	0
26	H	101	BCR	4	0
24	c	912	CLA	3	0
27	L	102	SQD	4	0
24	B	610	CLA	3	0
24	B	616	CLA	4	0
33	A	419	LMG	6	0
37	c	917	DGD	3	0
24	b	607	CLA	5	0
24	b	616	CLA	4	0
29	D	403	LMT	1	0
37	H	102	DGD	1	0
24	a	405	CLA	5	0
26	b	622	BCR	2	0
33	c	920	LMG	4	0
28	C	523	GOL	1	0
24	c	913	CLA	3	0
37	D	408	DGD	4	0
29	b	626	LMT	2	0
24	C	508	CLA	2	0
24	B	607	CLA	4	0
24	b	614	CLA	3	0
35	b	628	HTG	1	0
24	b	609	CLA	5	0
24	C	502	CLA	2	0
35	V	203	HTG	2	0

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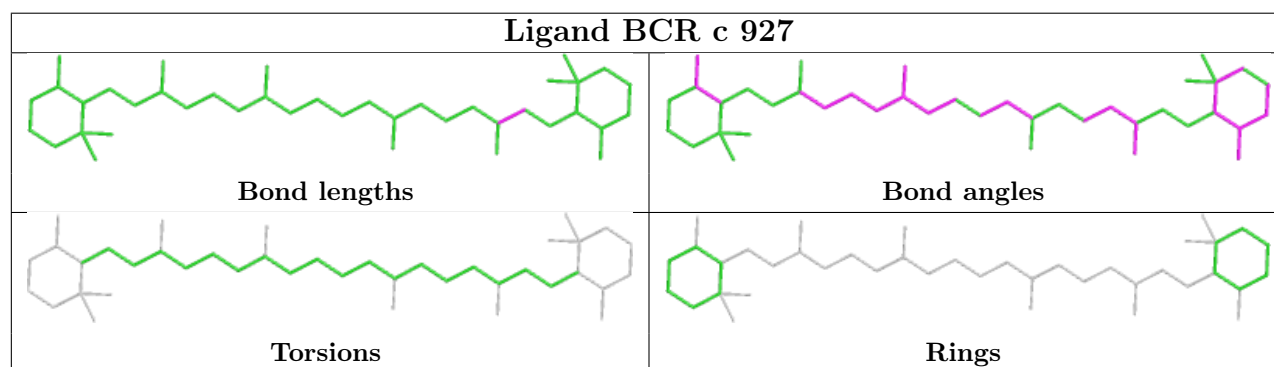
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	C	519	LMG	2	0
26	A	410	BCR	1	0
33	c	919	LMG	2	0
24	B	606	CLA	4	0
29	a	401	LMT	2	0
25	D	401	PHO	3	0
36	E	101	LHG	1	0
24	b	608	CLA	2	0
24	c	904	CLA	5	0
26	b	624	BCR	1	0
24	A	409	CLA	1	0
28	v	203	GOL	1	0
24	D	404	CLA	3	0
27	F	103	SQD	3	0
24	A	406	CLA	4	0
24	c	909	CLA	9	0
29	A	415	LMT	3	0
29	m	103	LMT	2	0
26	y	101	BCR	1	0
26	Y	102	BCR	6	0
24	B	605	CLA	4	0
24	B	613	CLA	2	0
24	b	620	CLA	4	0
26	C	515	BCR	2	0
37	h	102	DGD	2	0
24	B	609	CLA	1	0
28	a	419	GOL	1	0
33	B	622	LMG	3	0
33	d	415	LMG	3	0
28	b	633	GOL	1	0
25	a	407	PHO	3	0
24	C	512	CLA	5	0
24	C	504	CLA	1	0
26	d	407	BCR	4	0
33	b	625	LMG	4	0
29	M	101	LMT	3	0
24	b	621	CLA	3	0
24	A	405	CLA	7	0
24	C	509	CLA	4	0
24	d	405	CLA	5	0
28	V	207	GOL	1	0
36	d	410	LHG	1	0

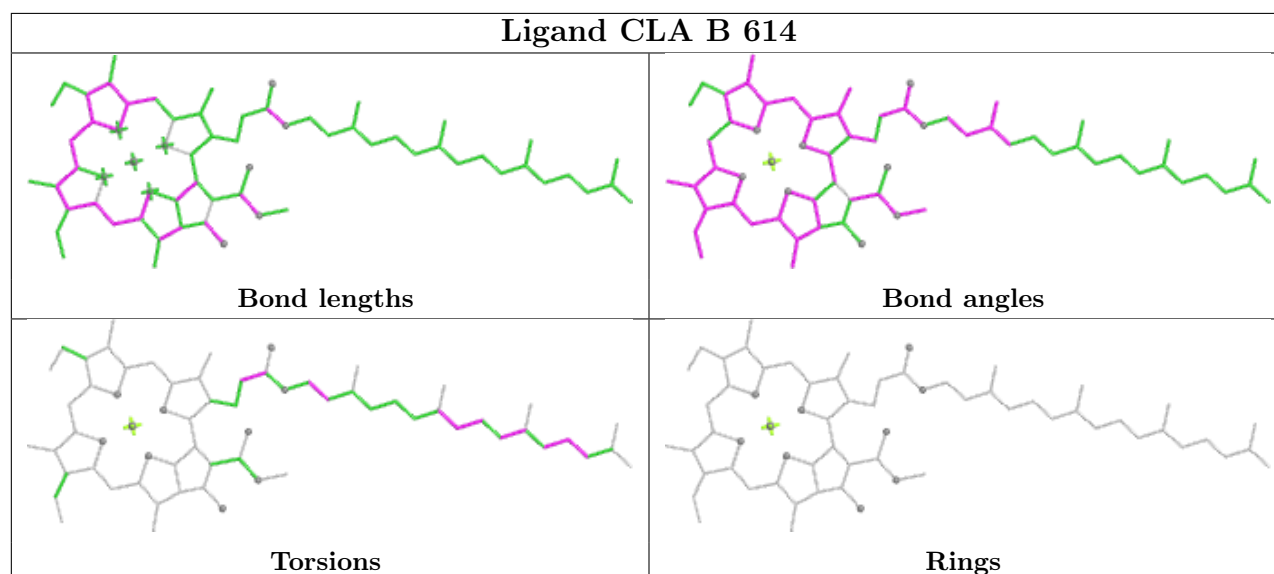
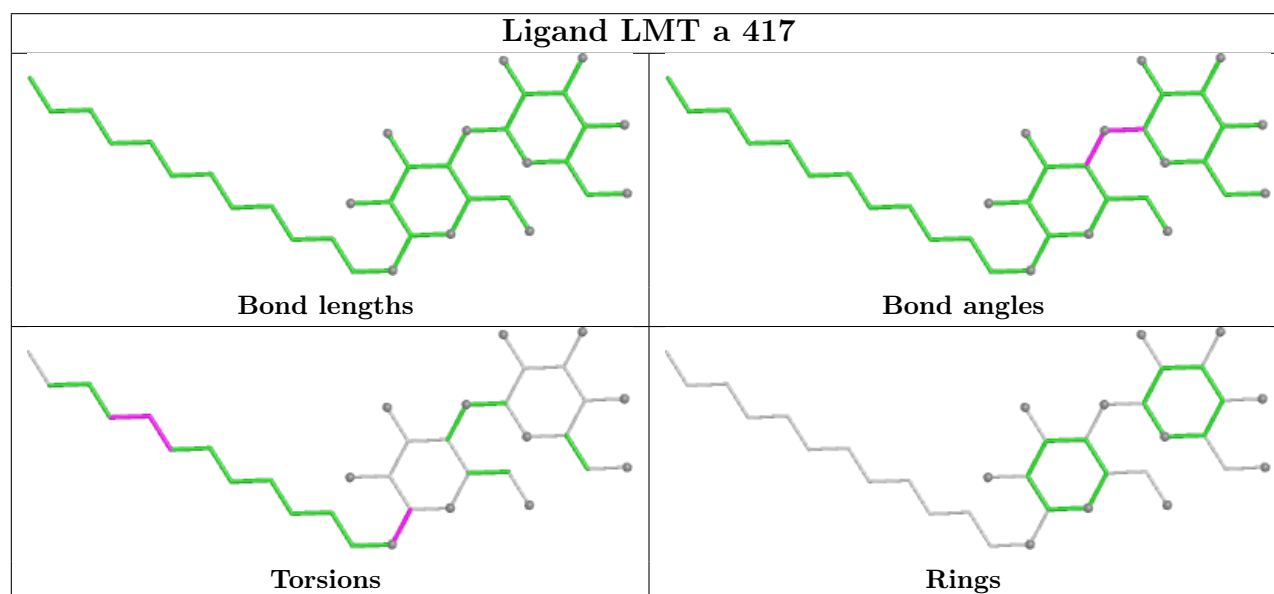
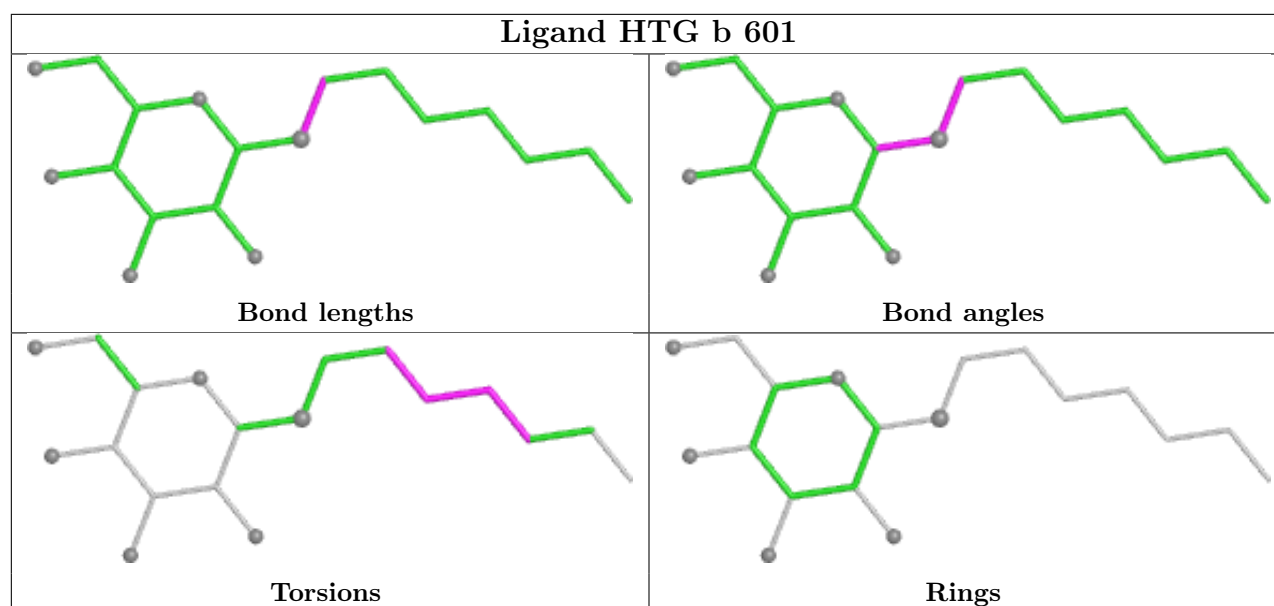
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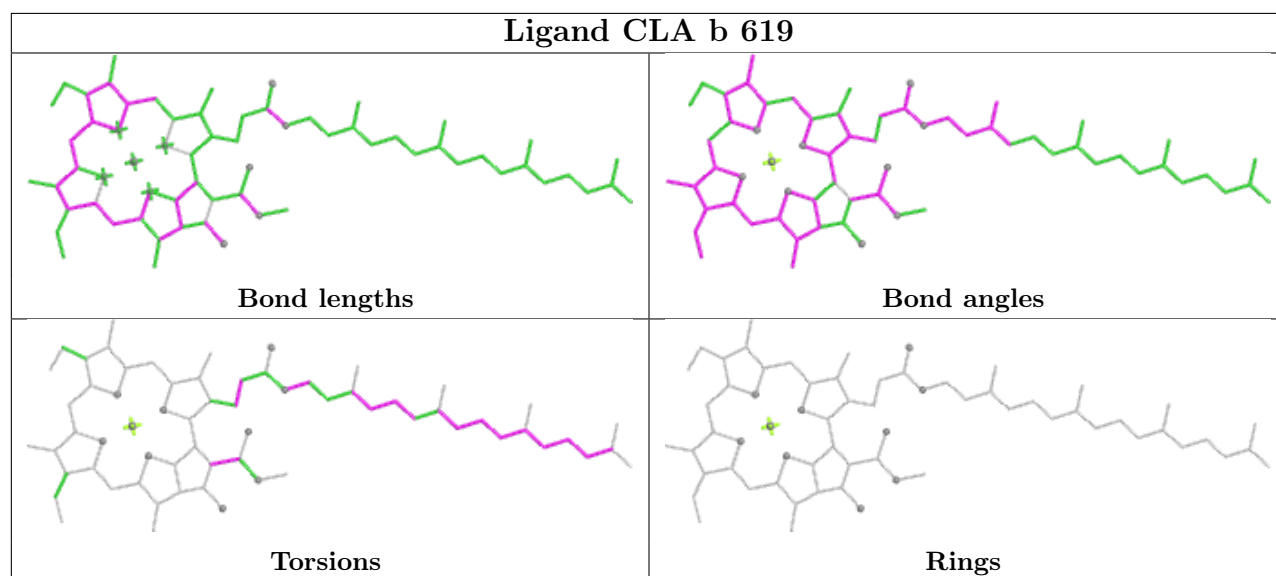
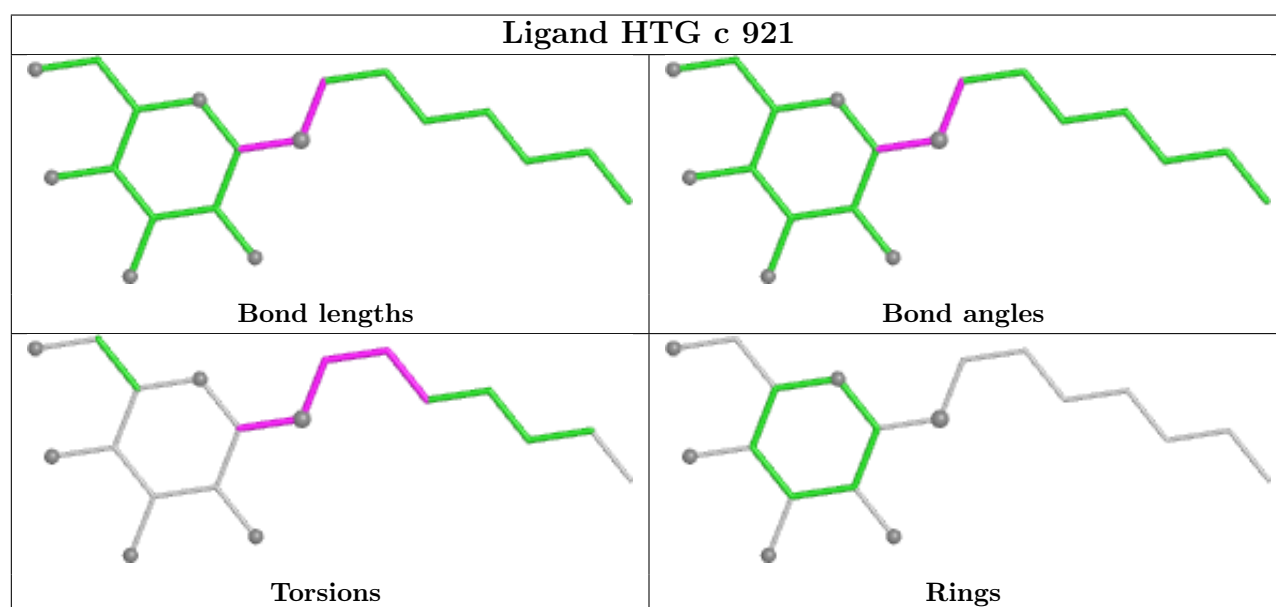
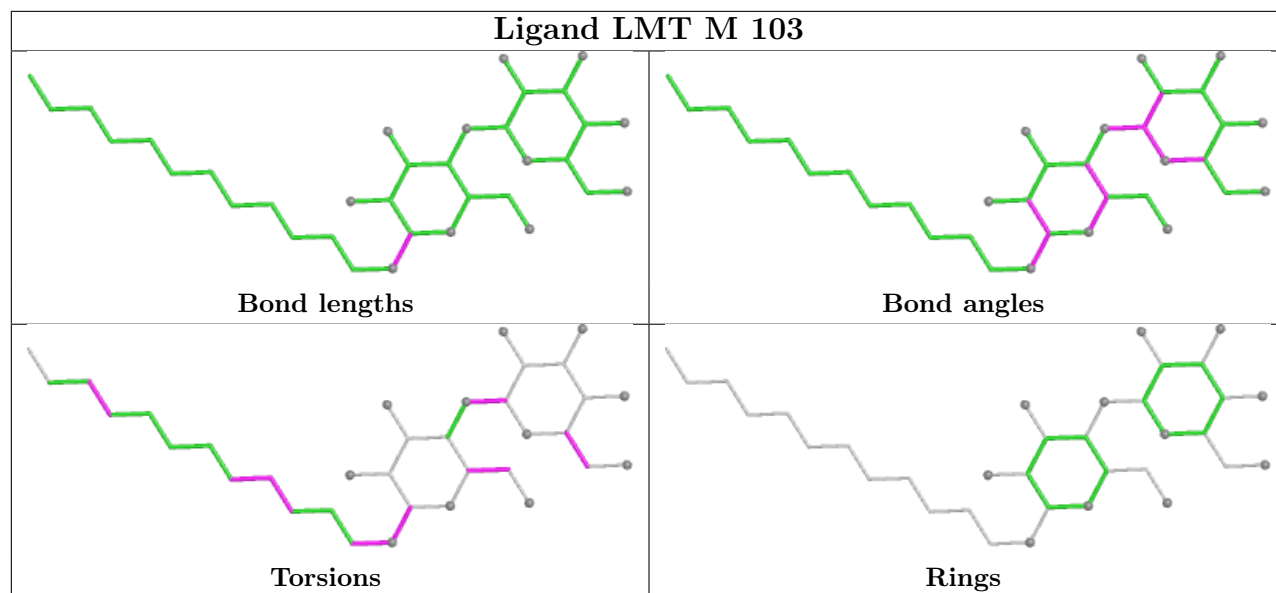
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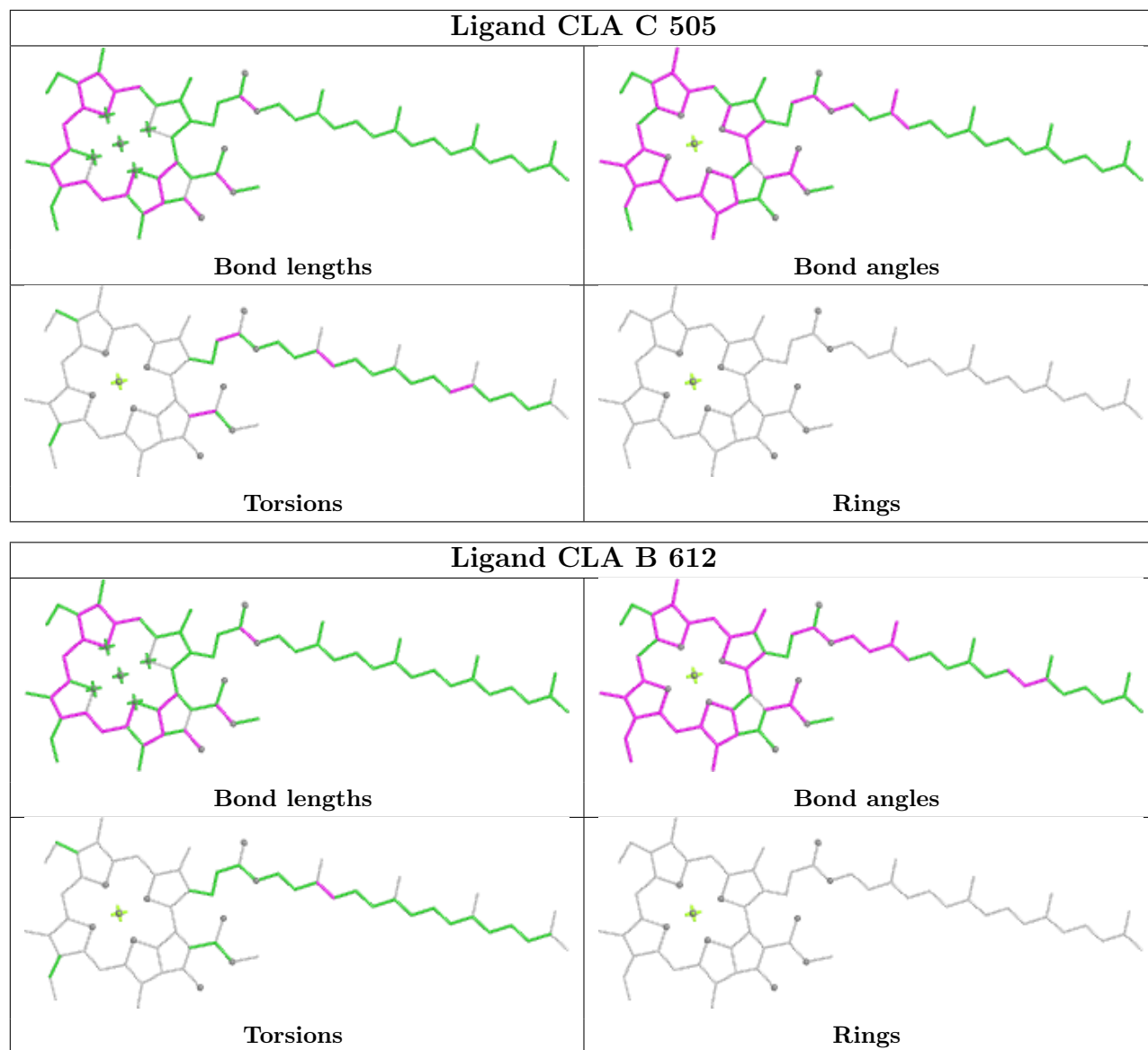
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	910	CLA	2	0
24	b	613	CLA	1	0
24	A	407	CLA	2	0
26	b	623	BCR	2	0
33	z	101	LMG	5	0
28	l	101	GOL	1	0
24	c	908	CLA	2	0

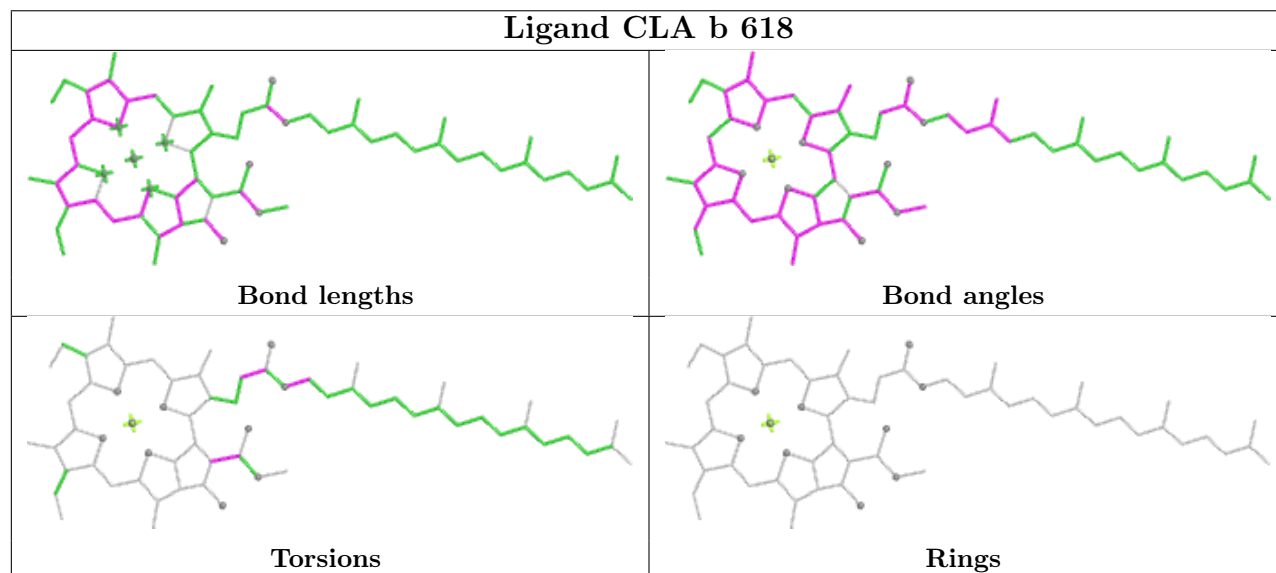
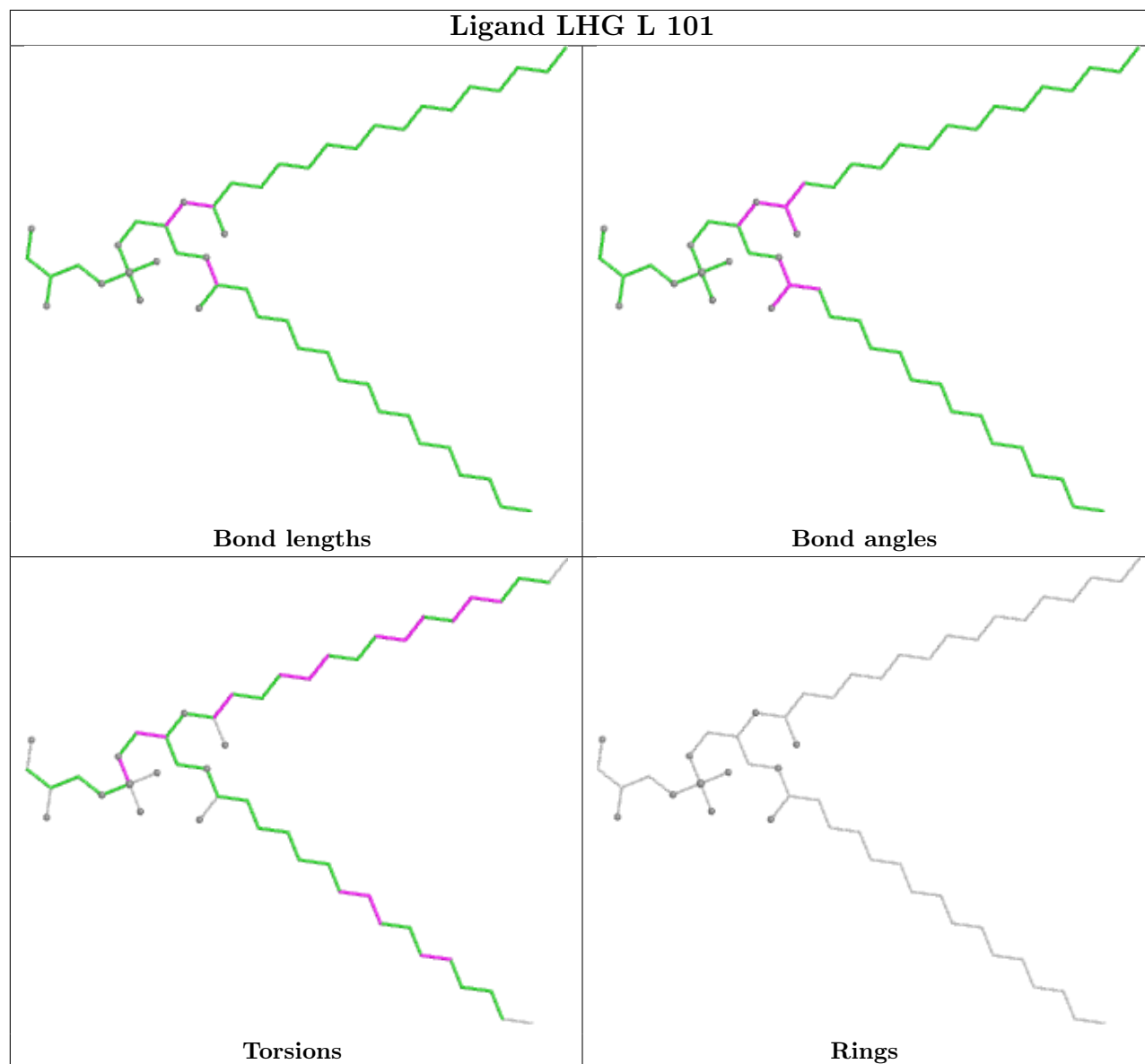
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

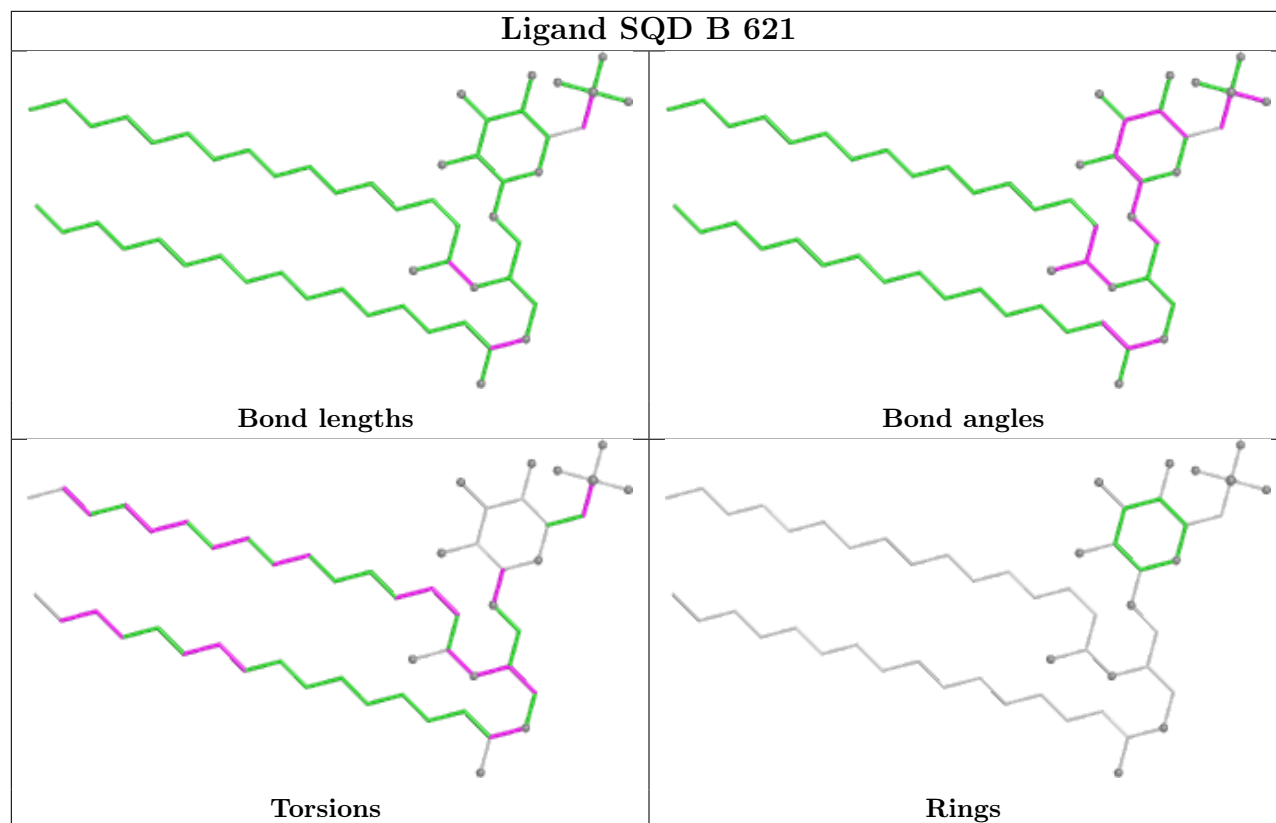
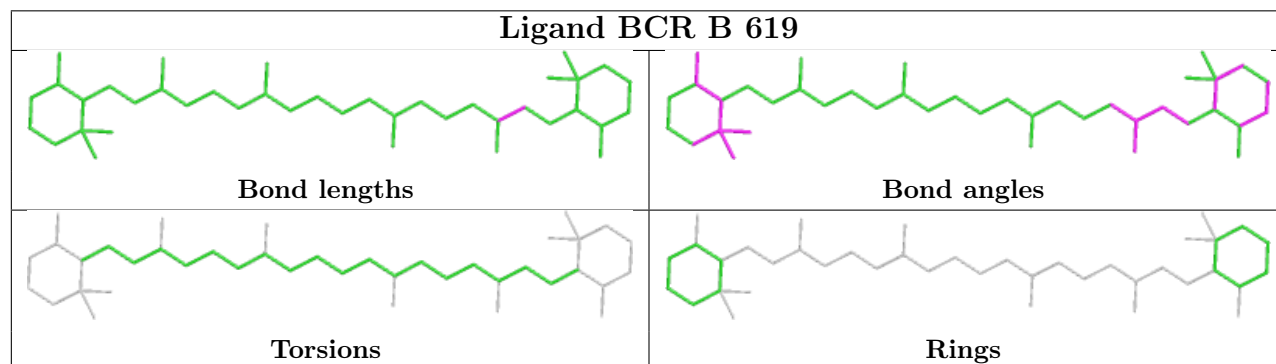
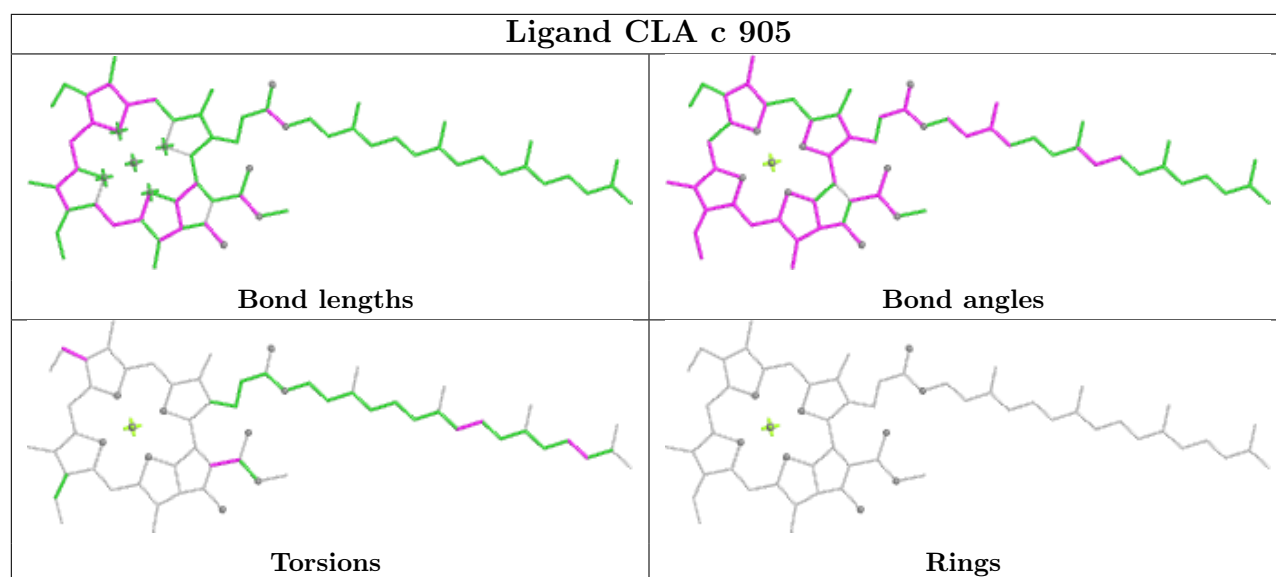


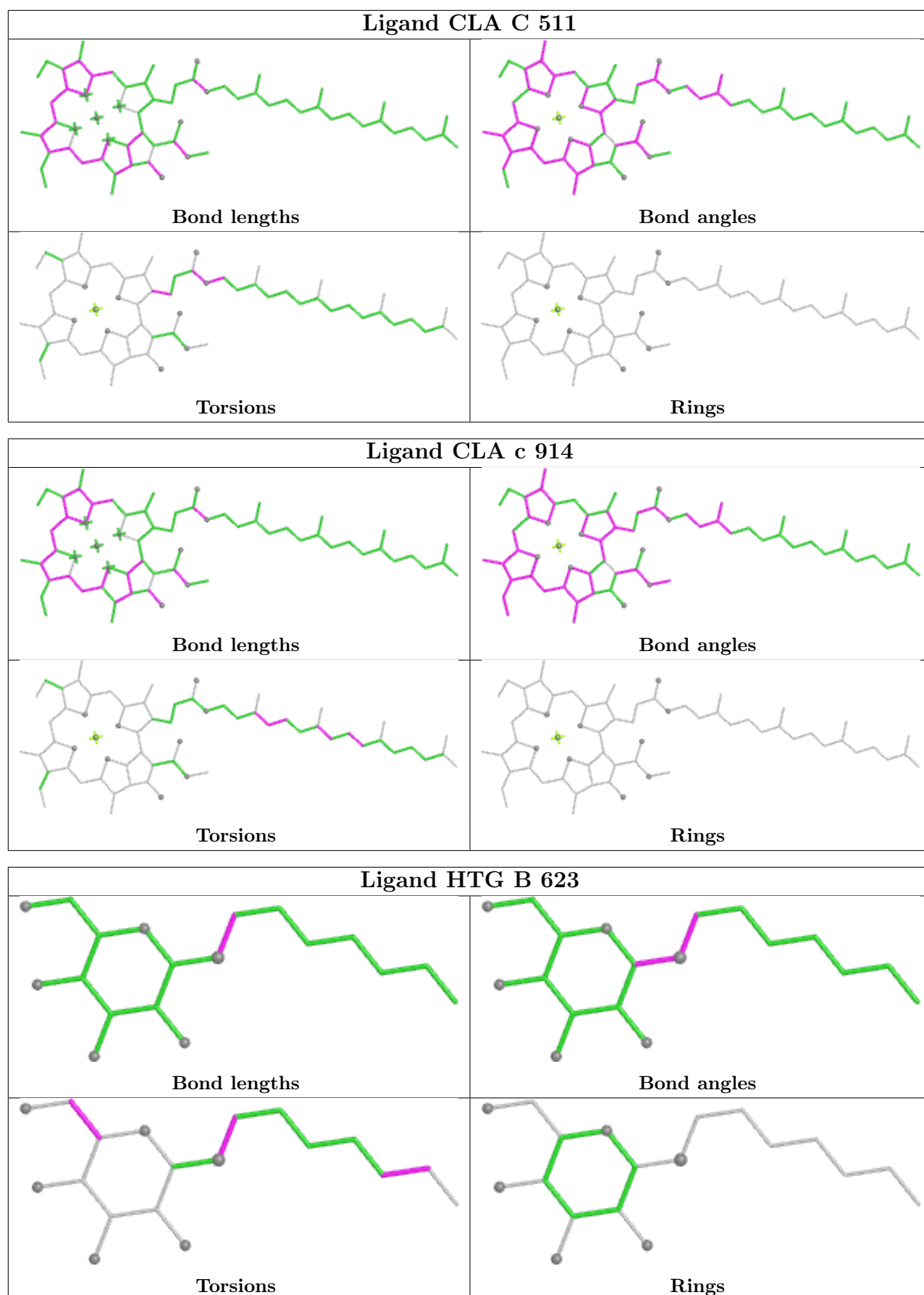


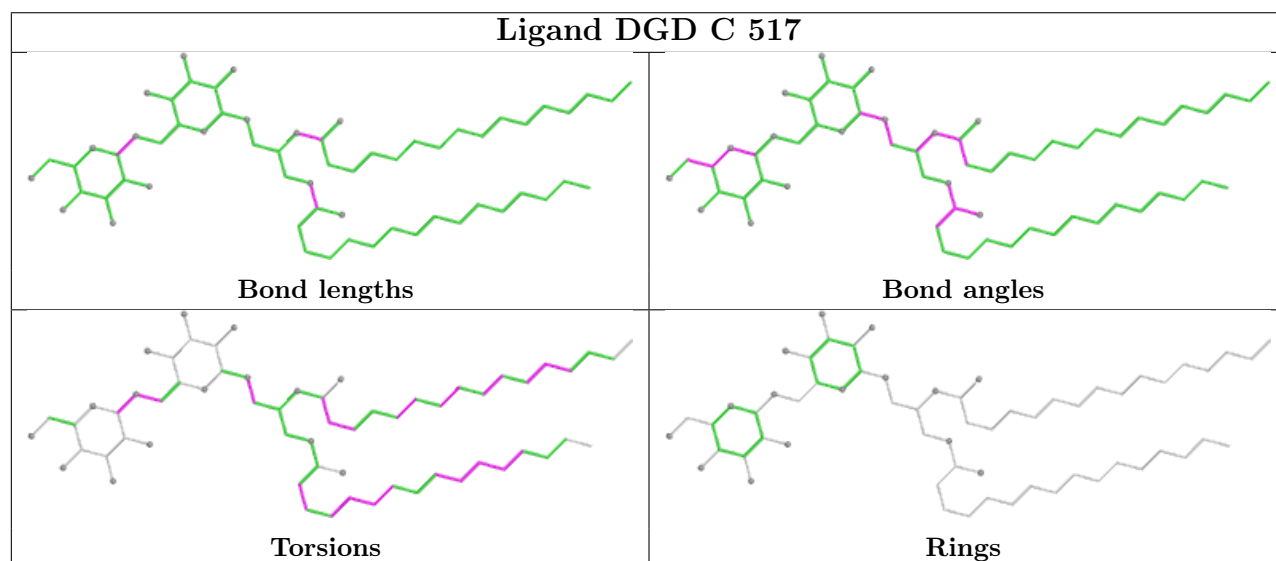
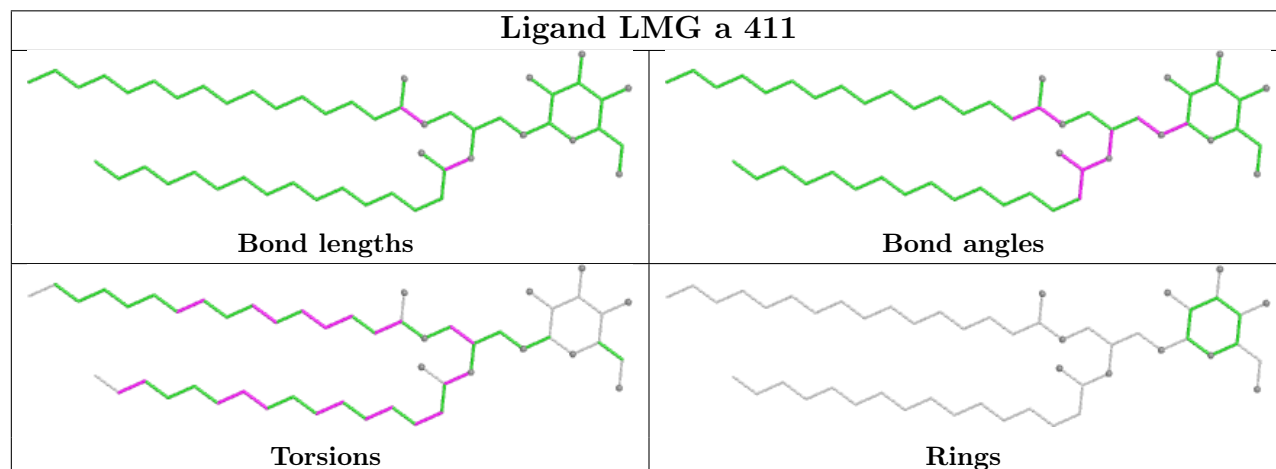
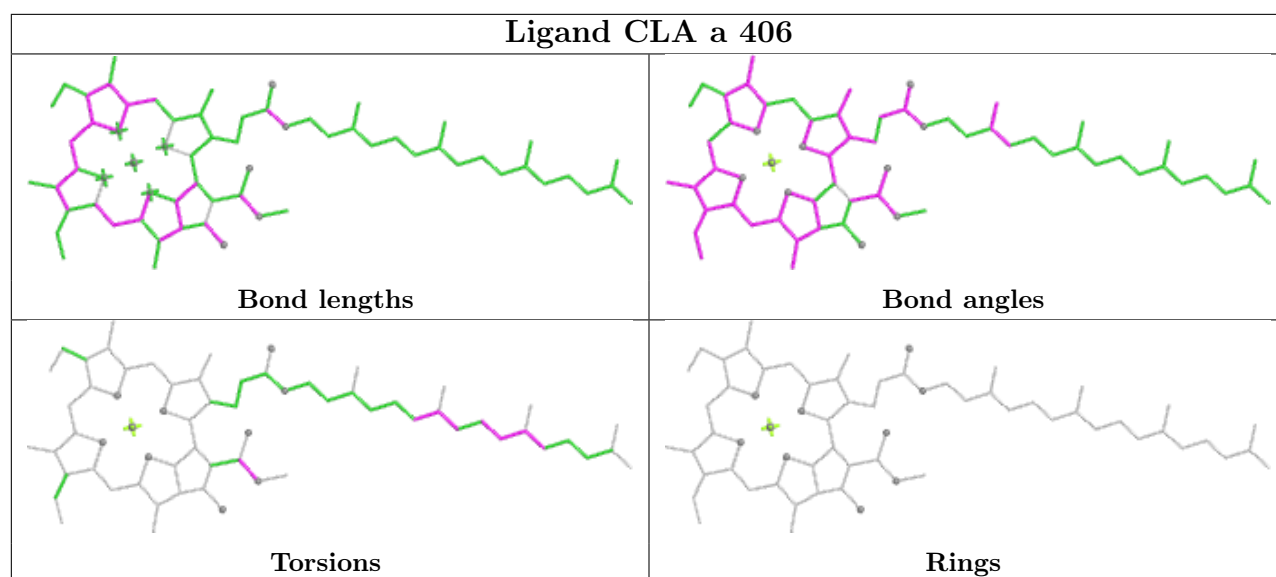


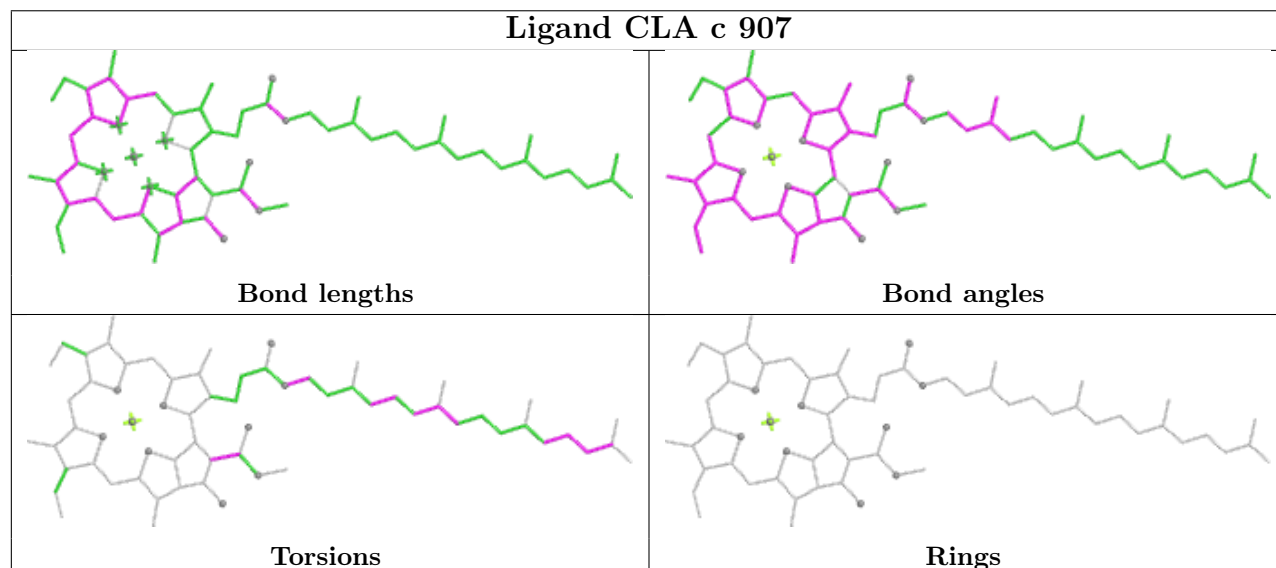
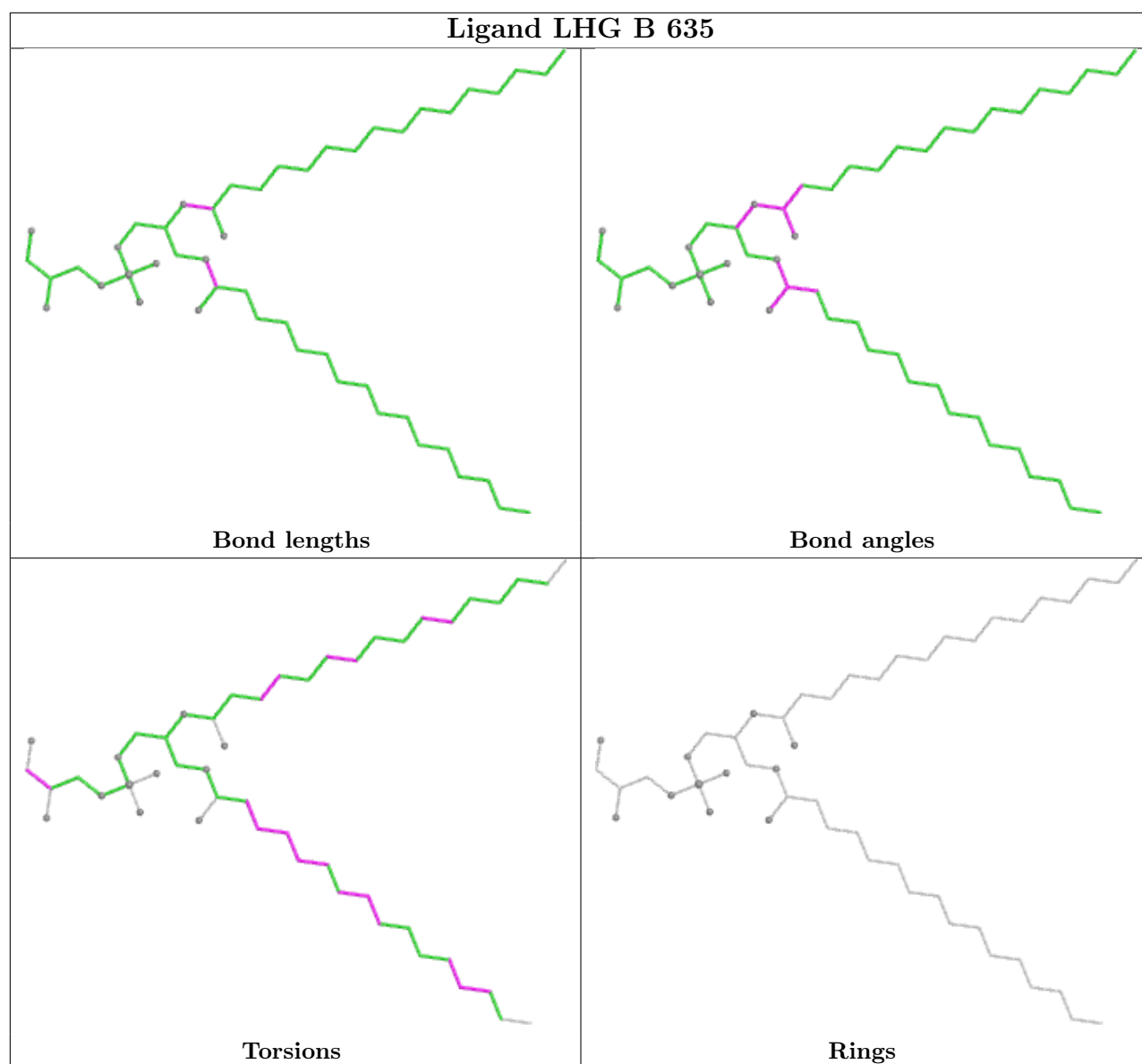




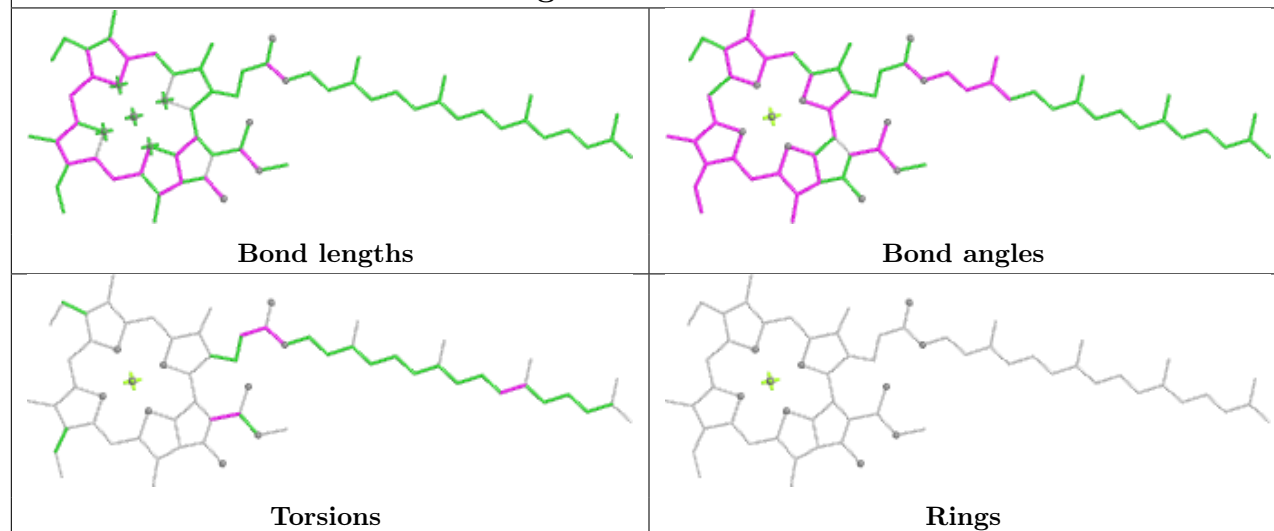




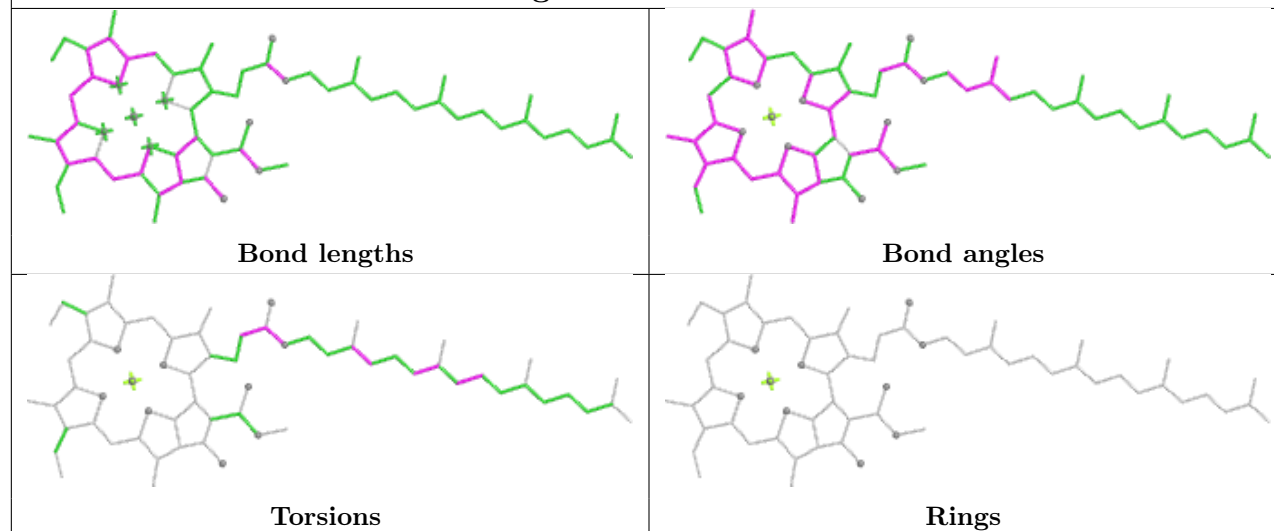




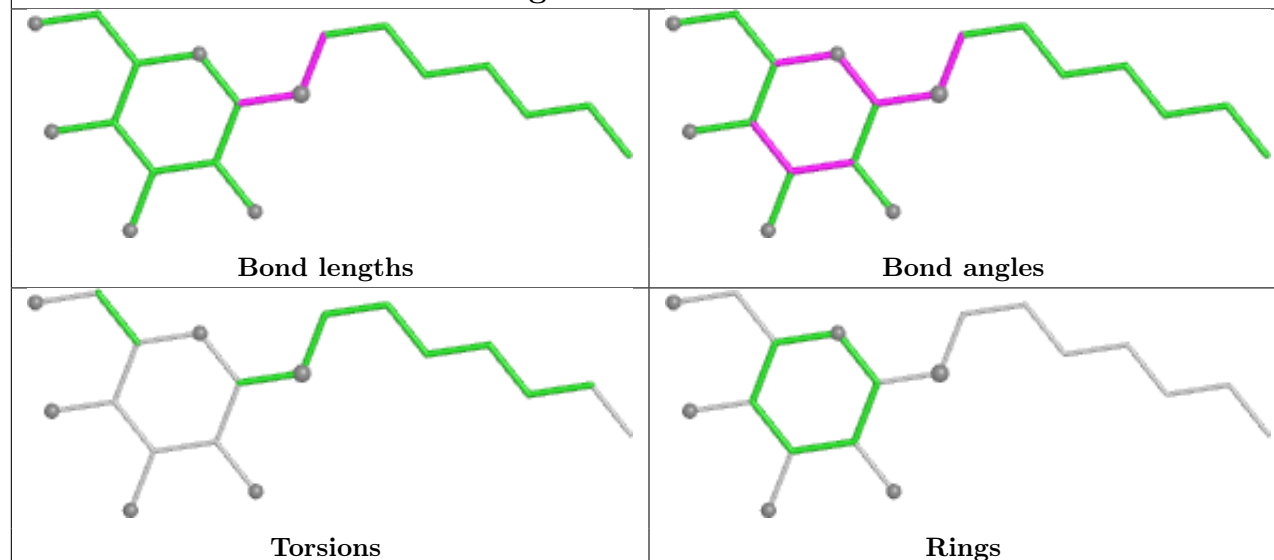
Ligand CLA c 906

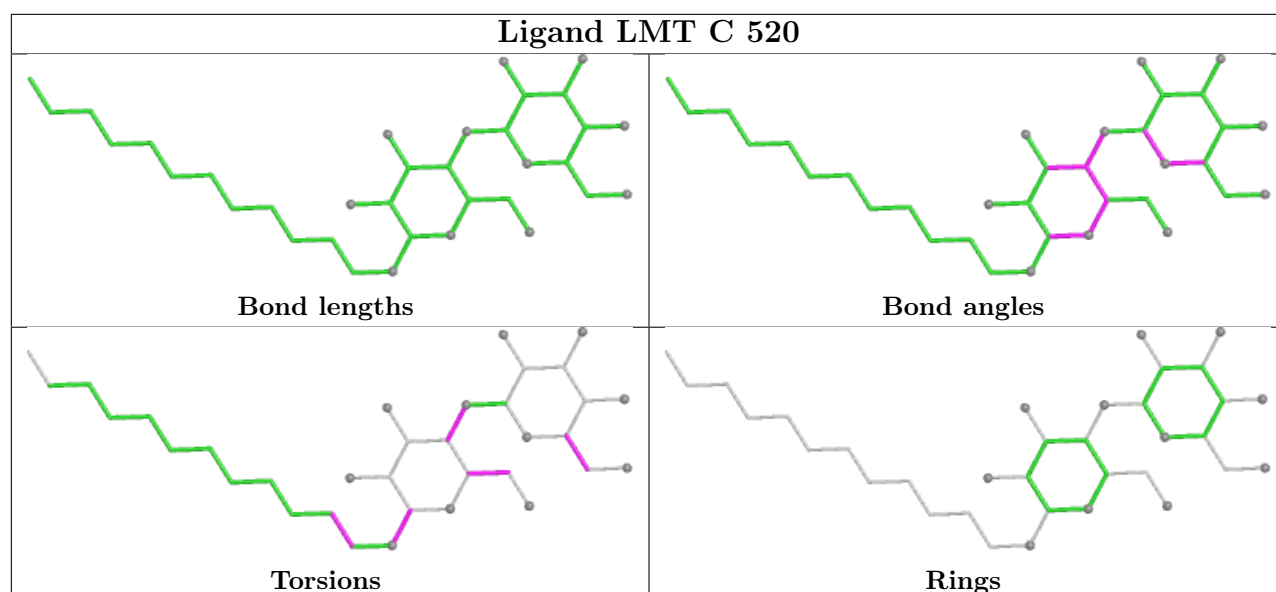
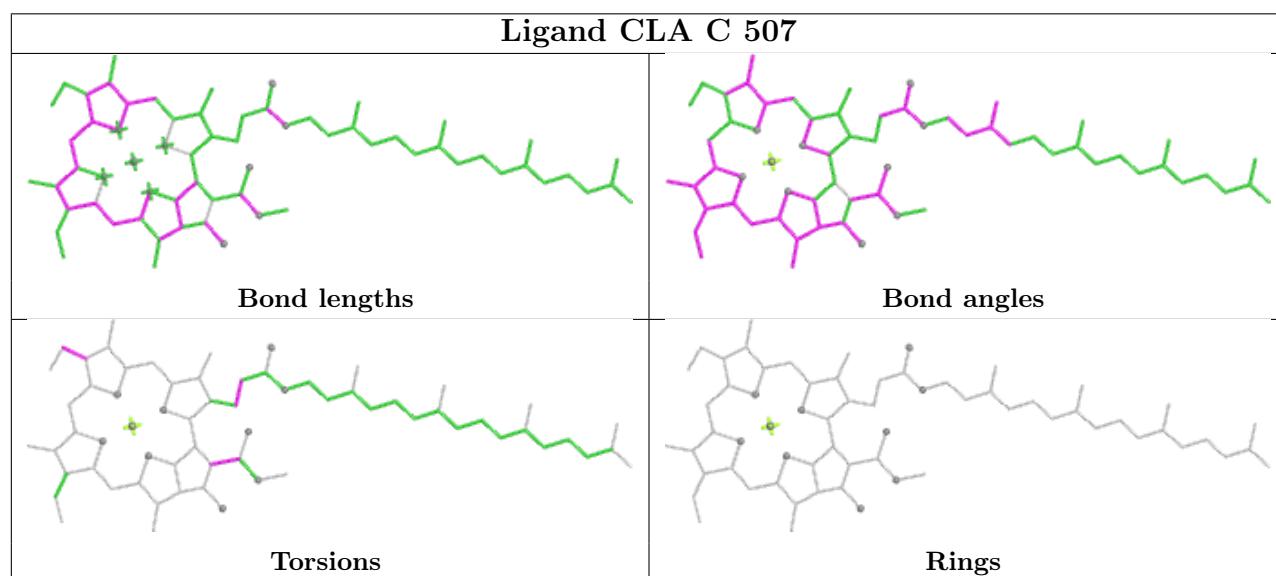
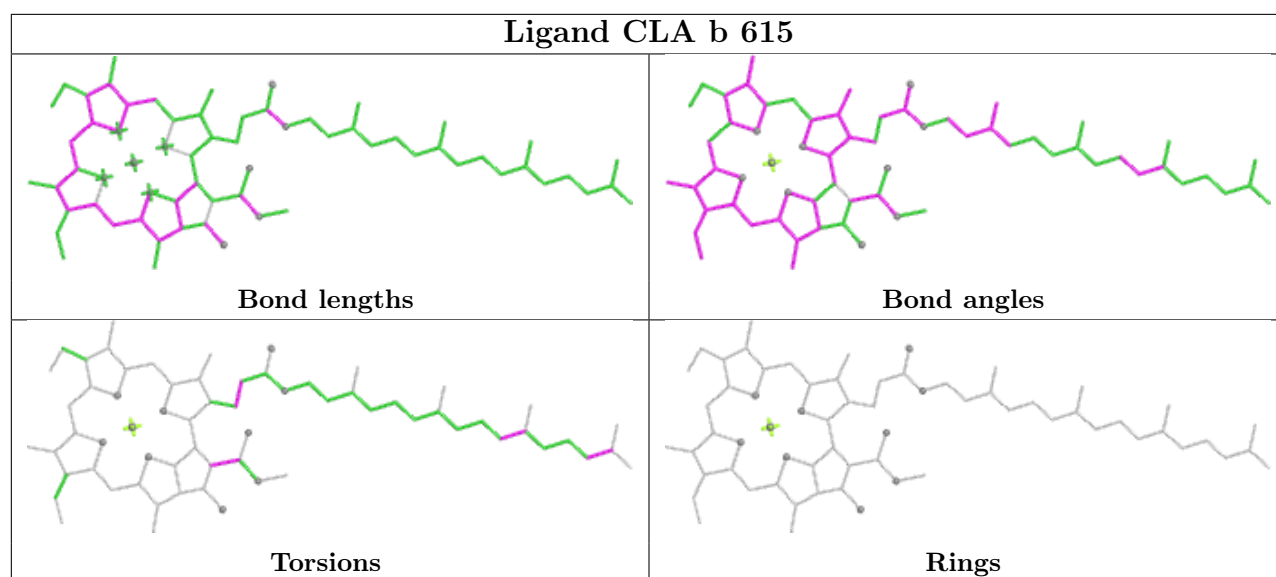


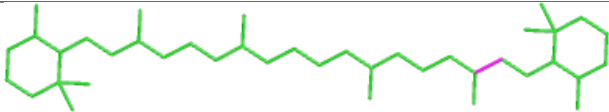
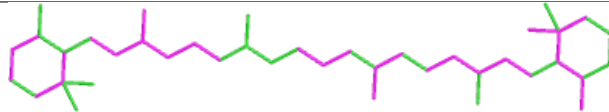
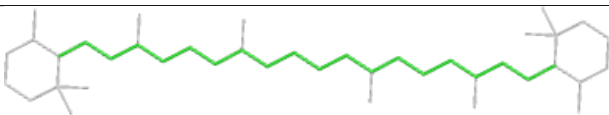
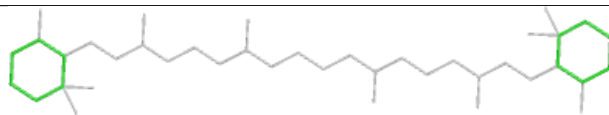
Ligand CLA C 510

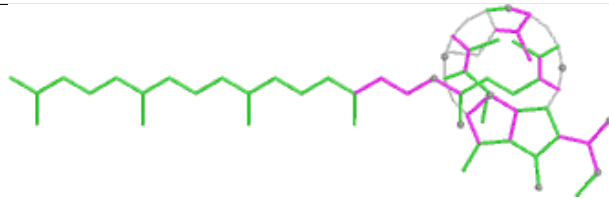
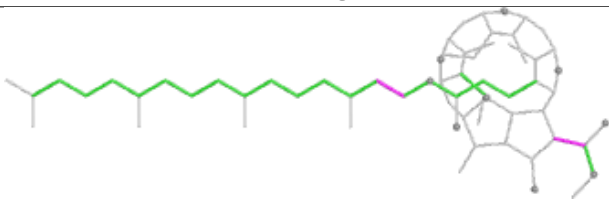
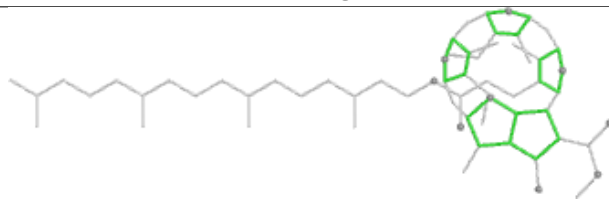


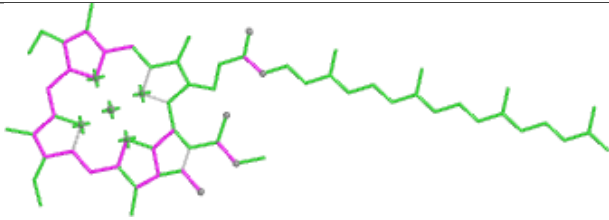
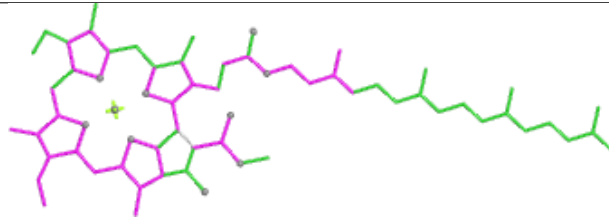
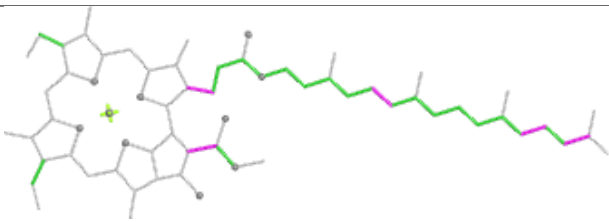
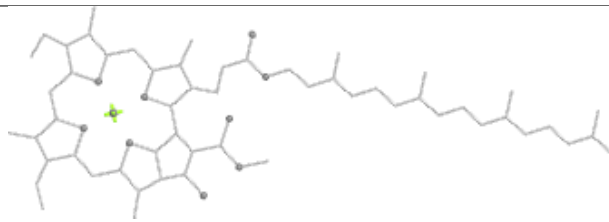
Ligand HTG C 521

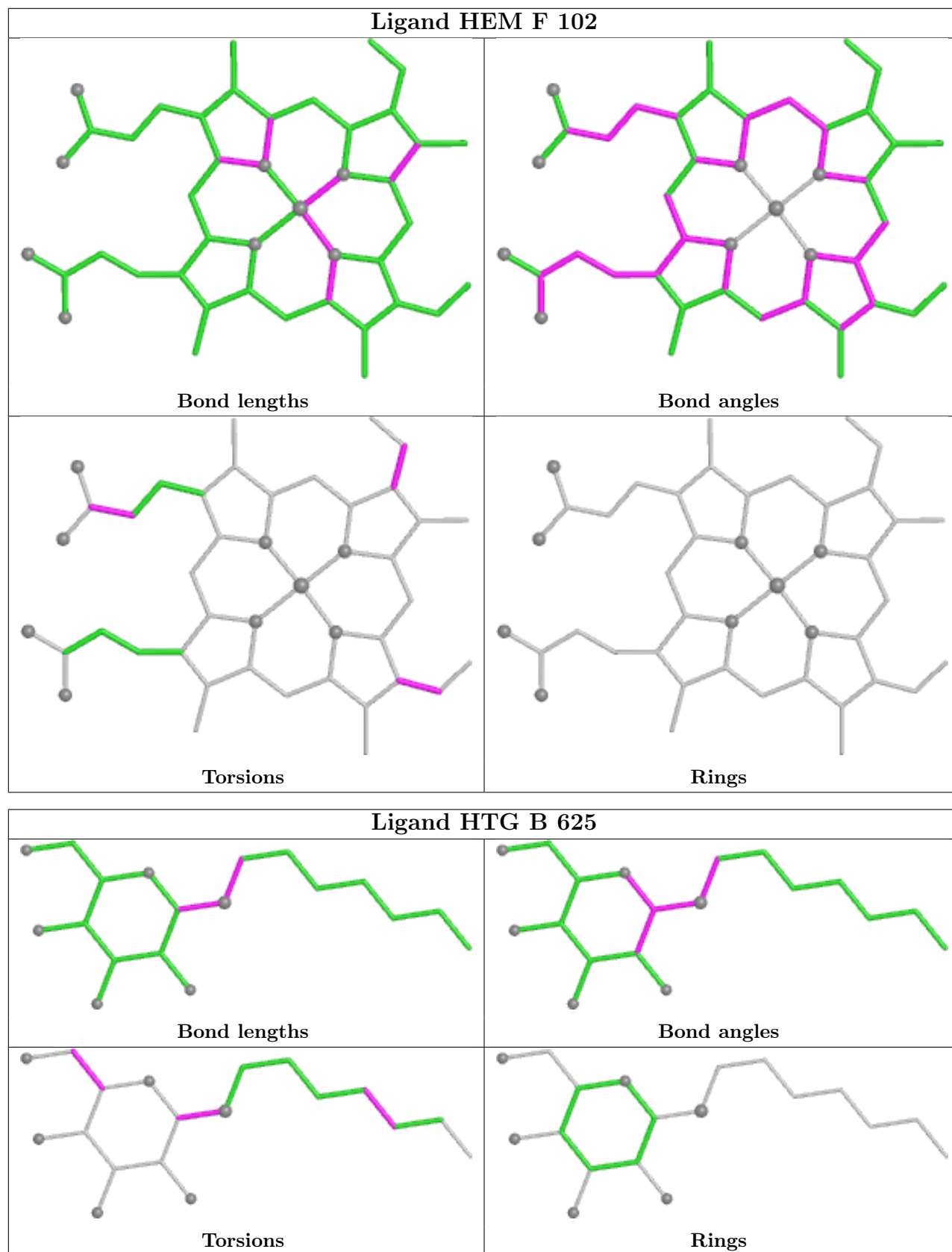


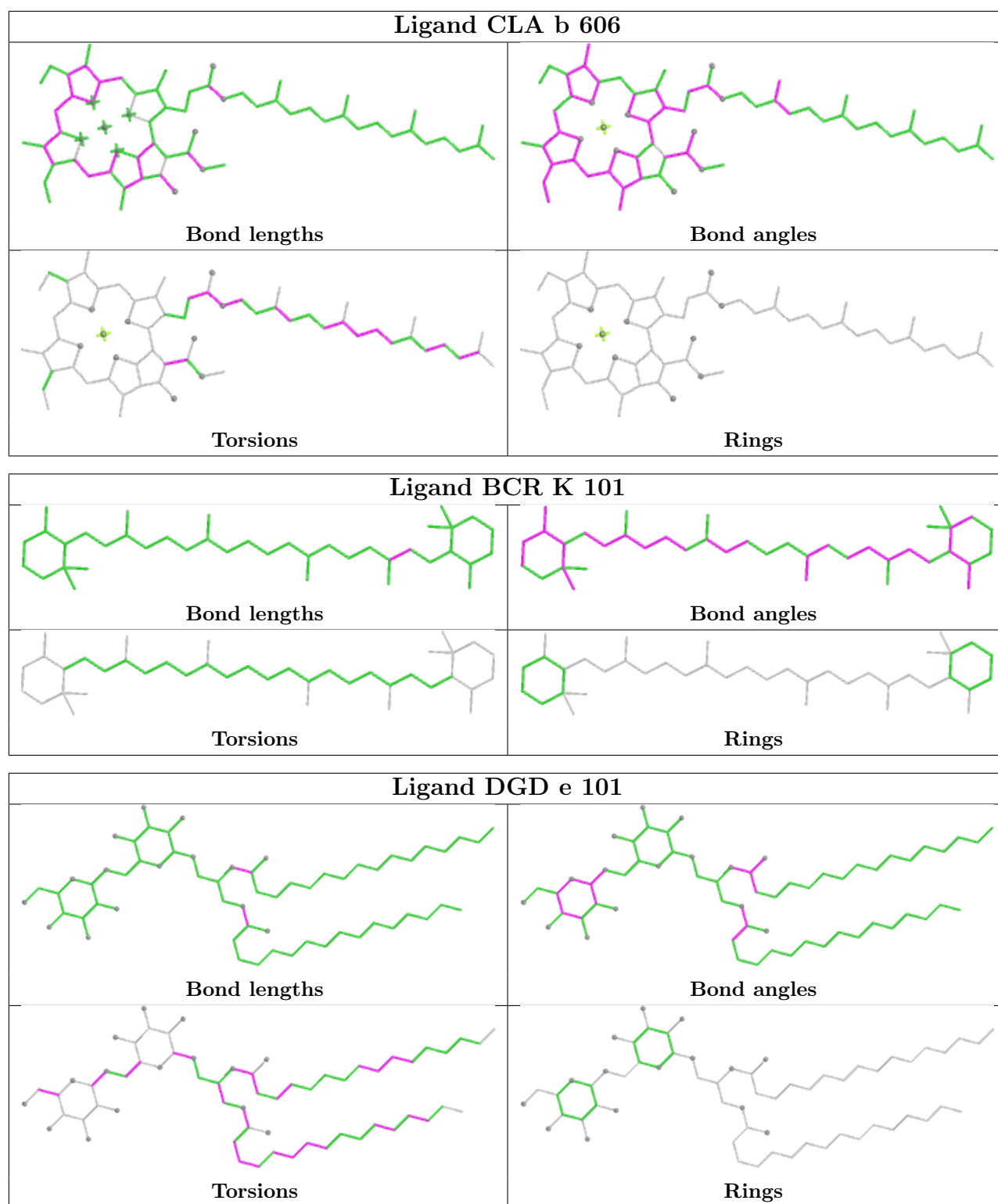


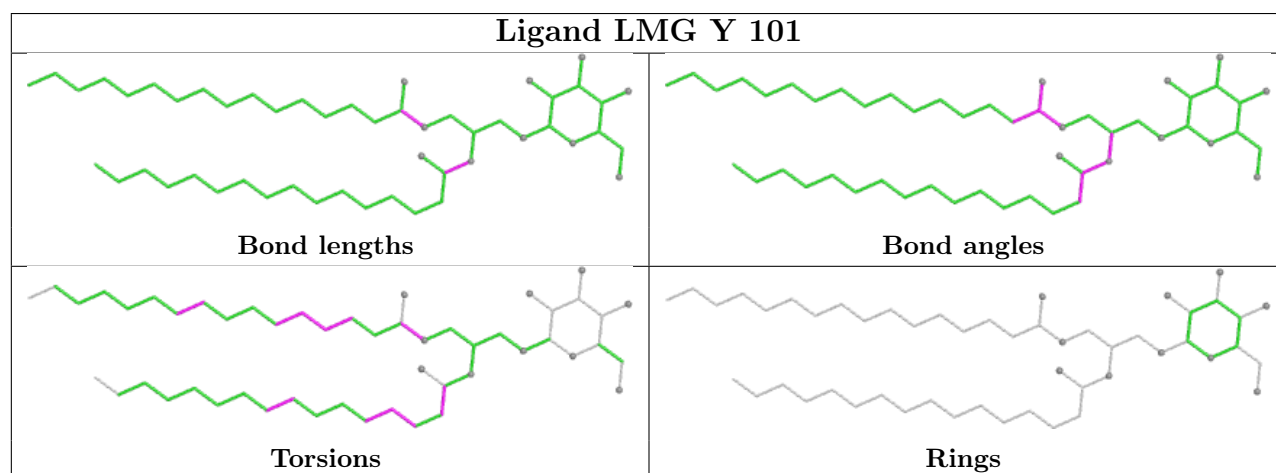
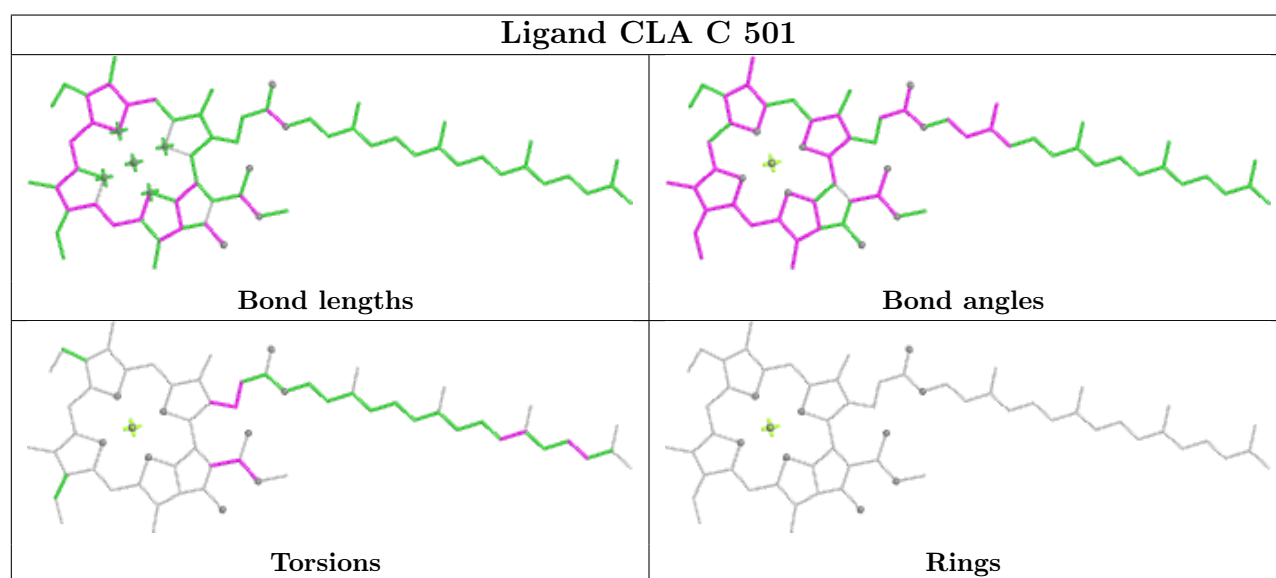
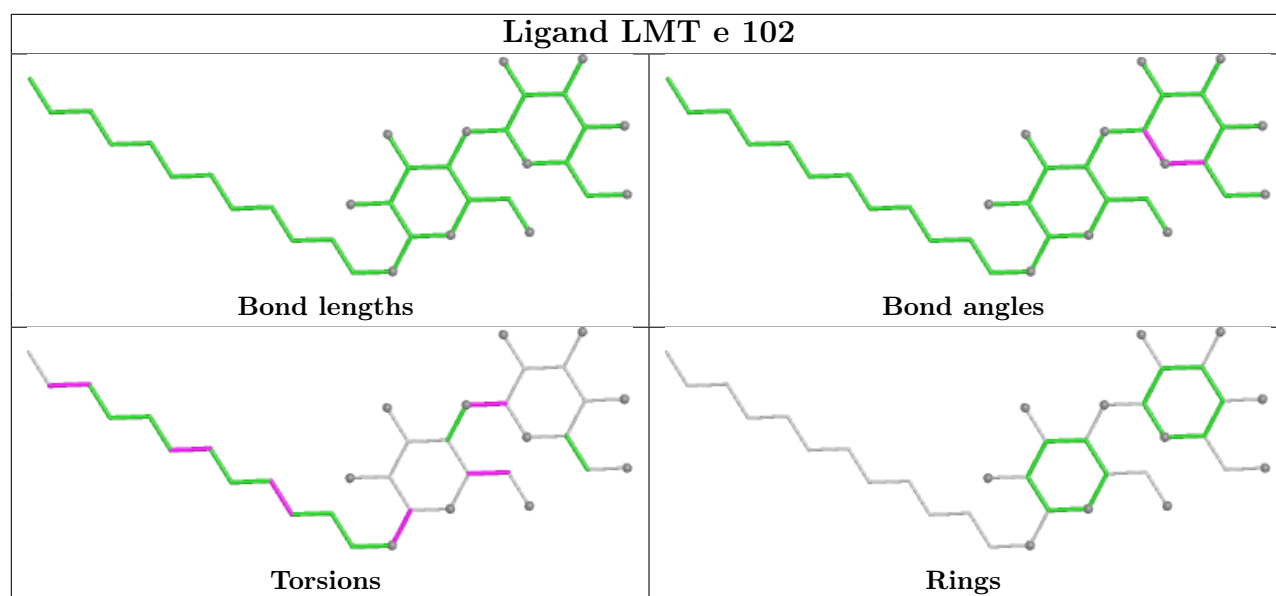
Ligand BCR k 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

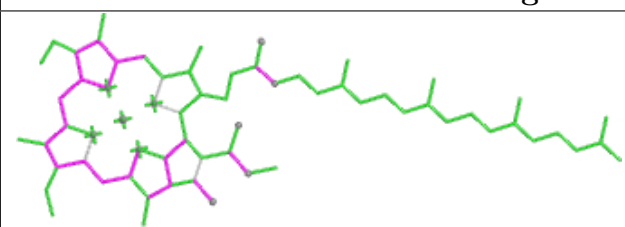
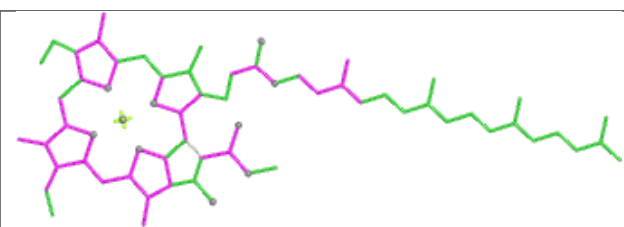
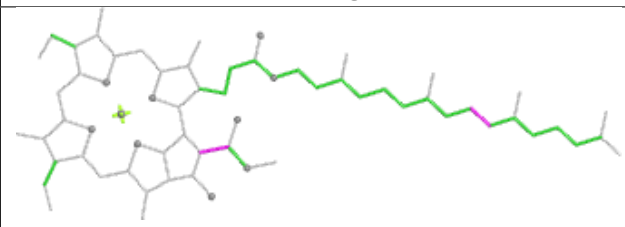
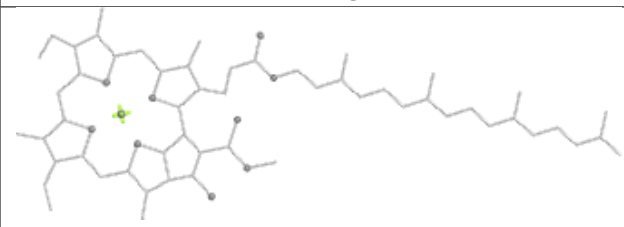
Ligand PHO A 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

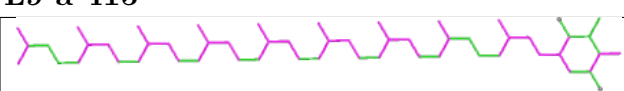
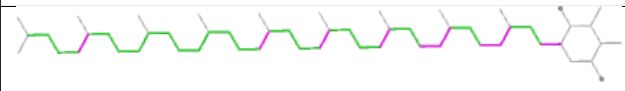
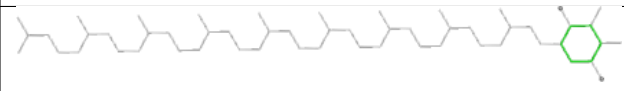
Ligand CLA C 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

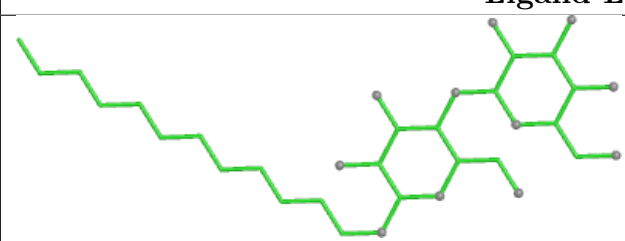
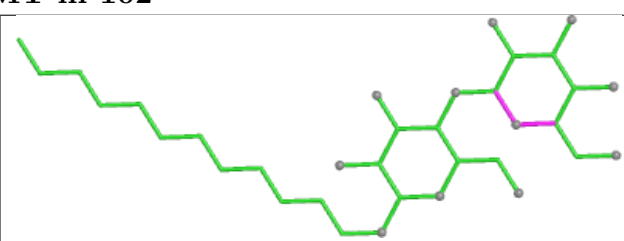
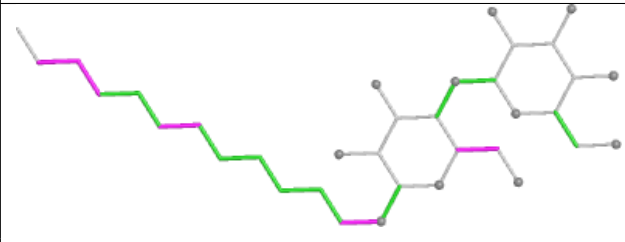
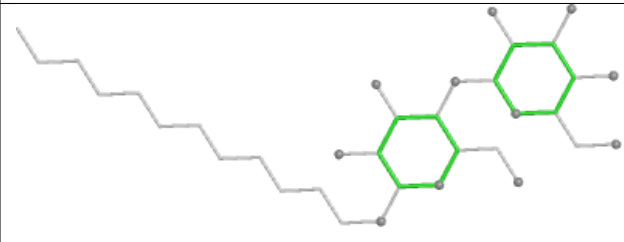


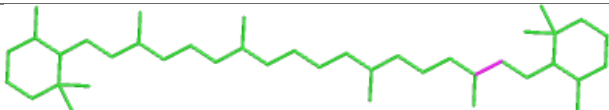
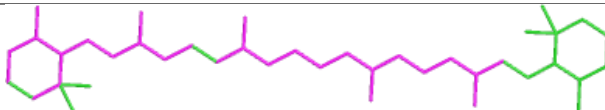
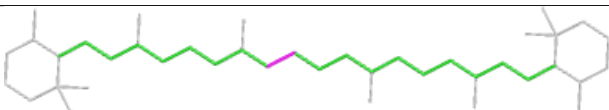
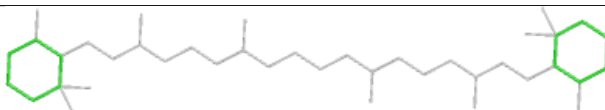


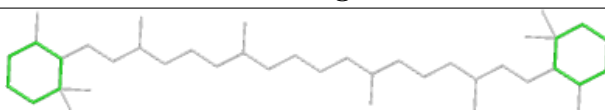


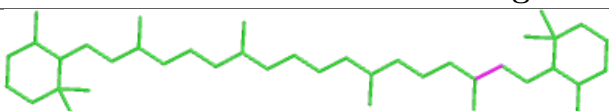
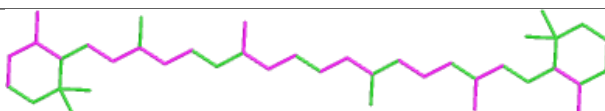
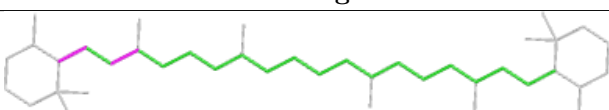
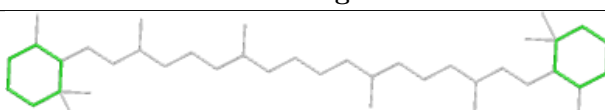
Ligand CLA C 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

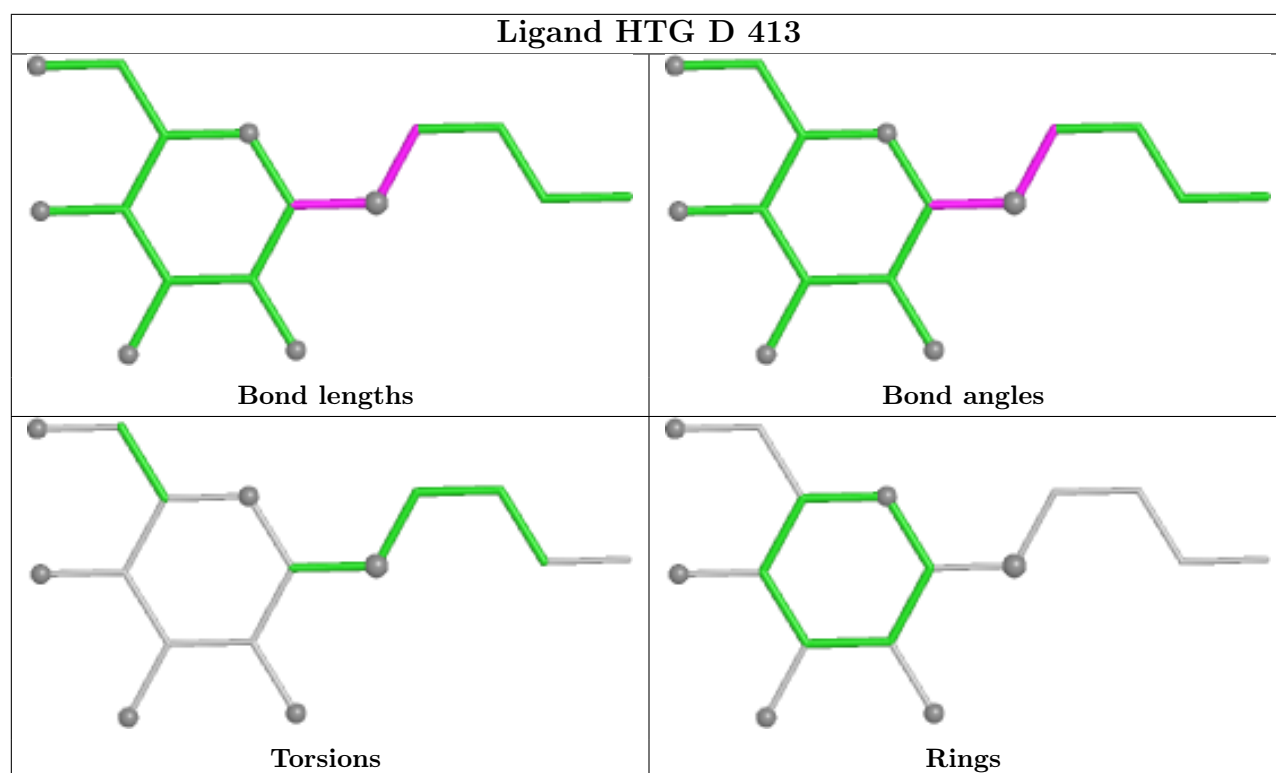
Ligand PL9 a 415	
	
Bond lengths	Bond angles
	
Torsions	Rings

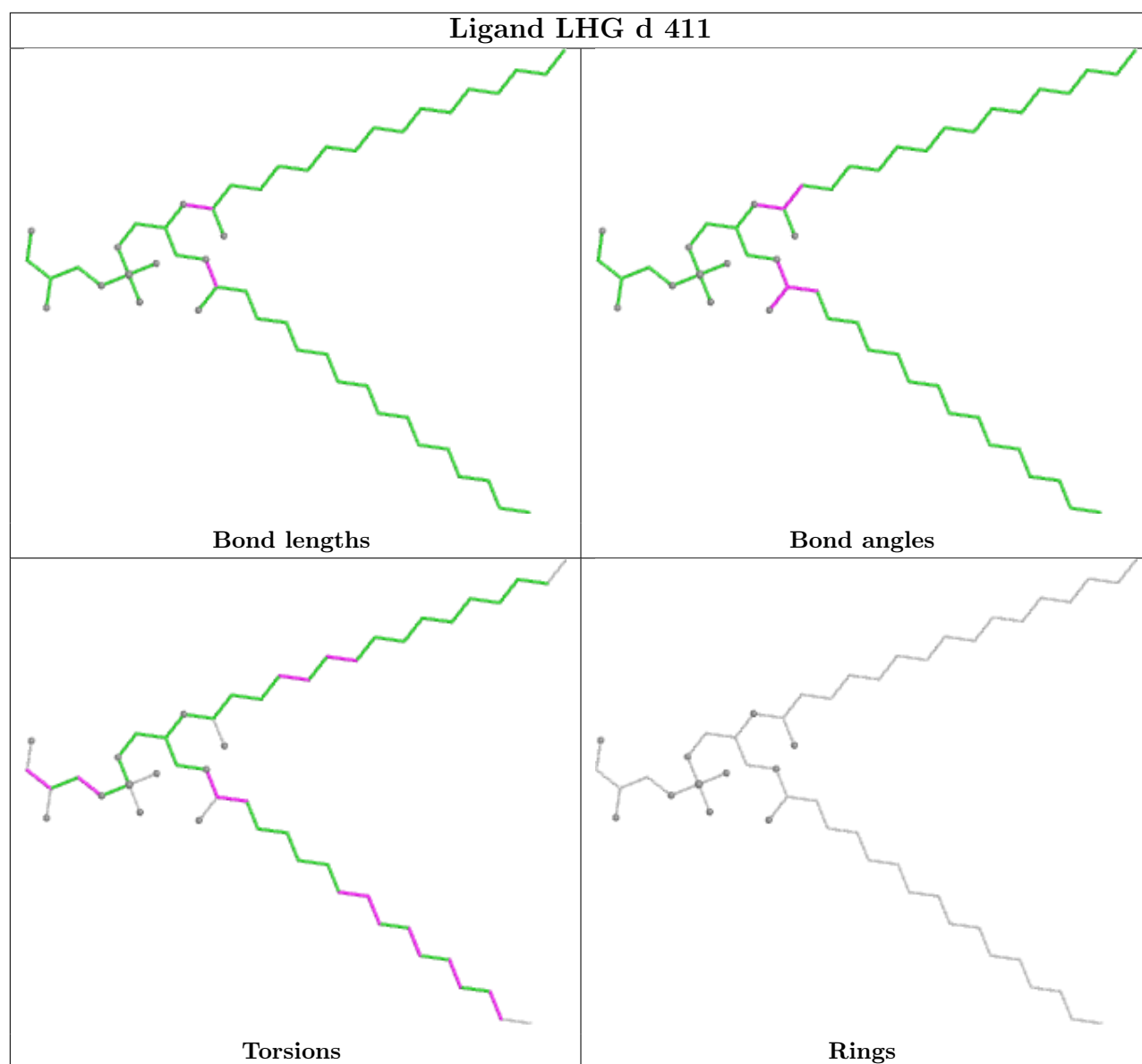
Ligand LMT m 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

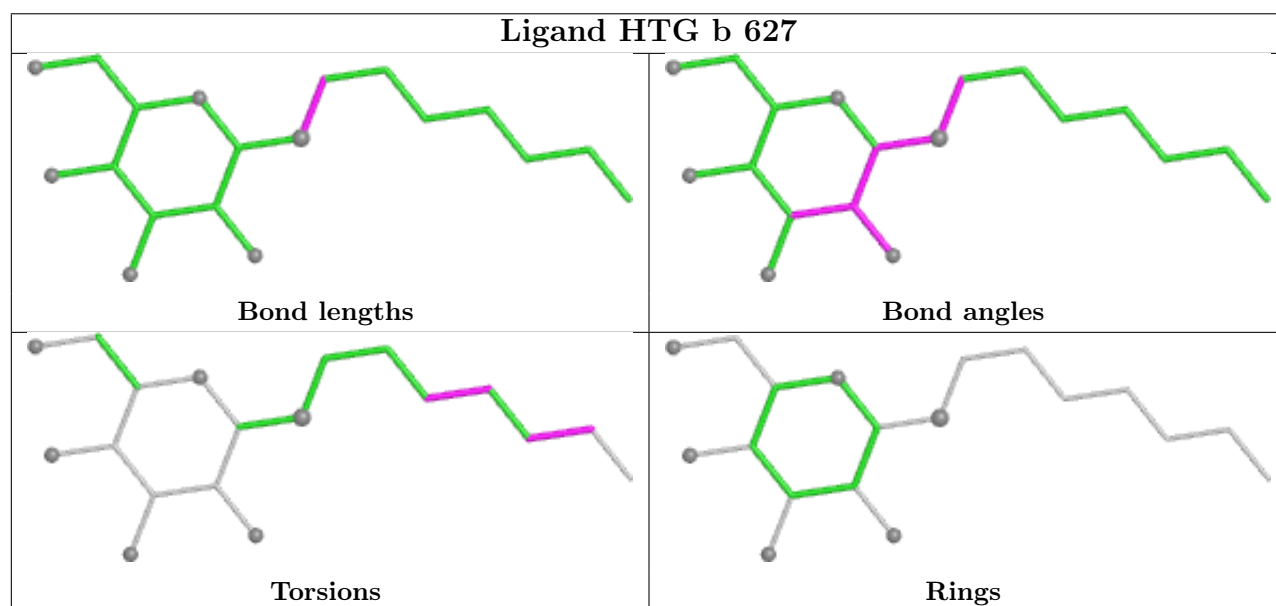
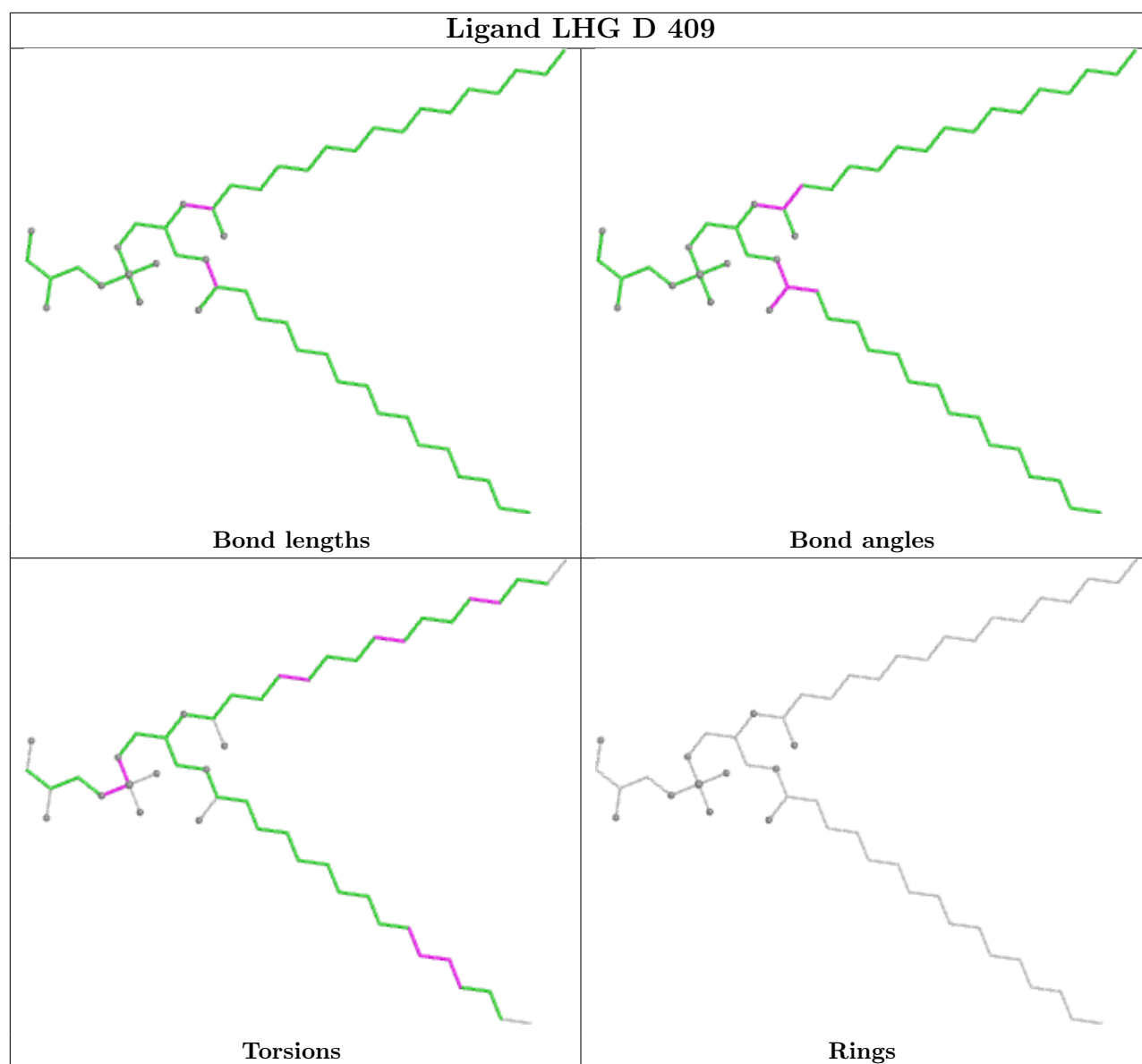
Ligand BCR T 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

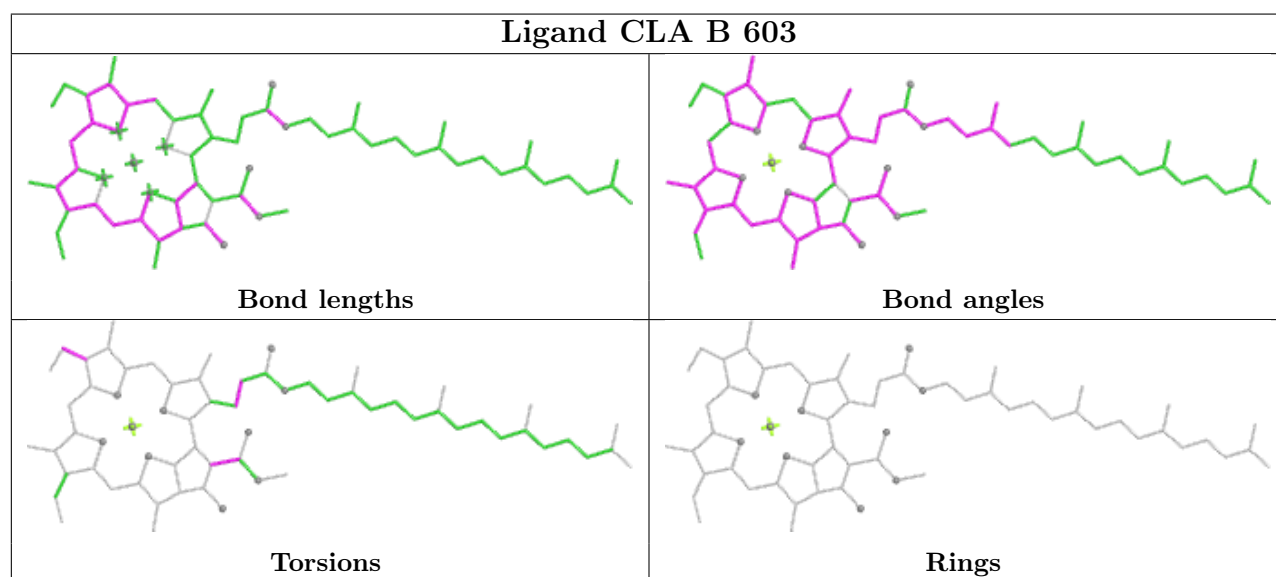
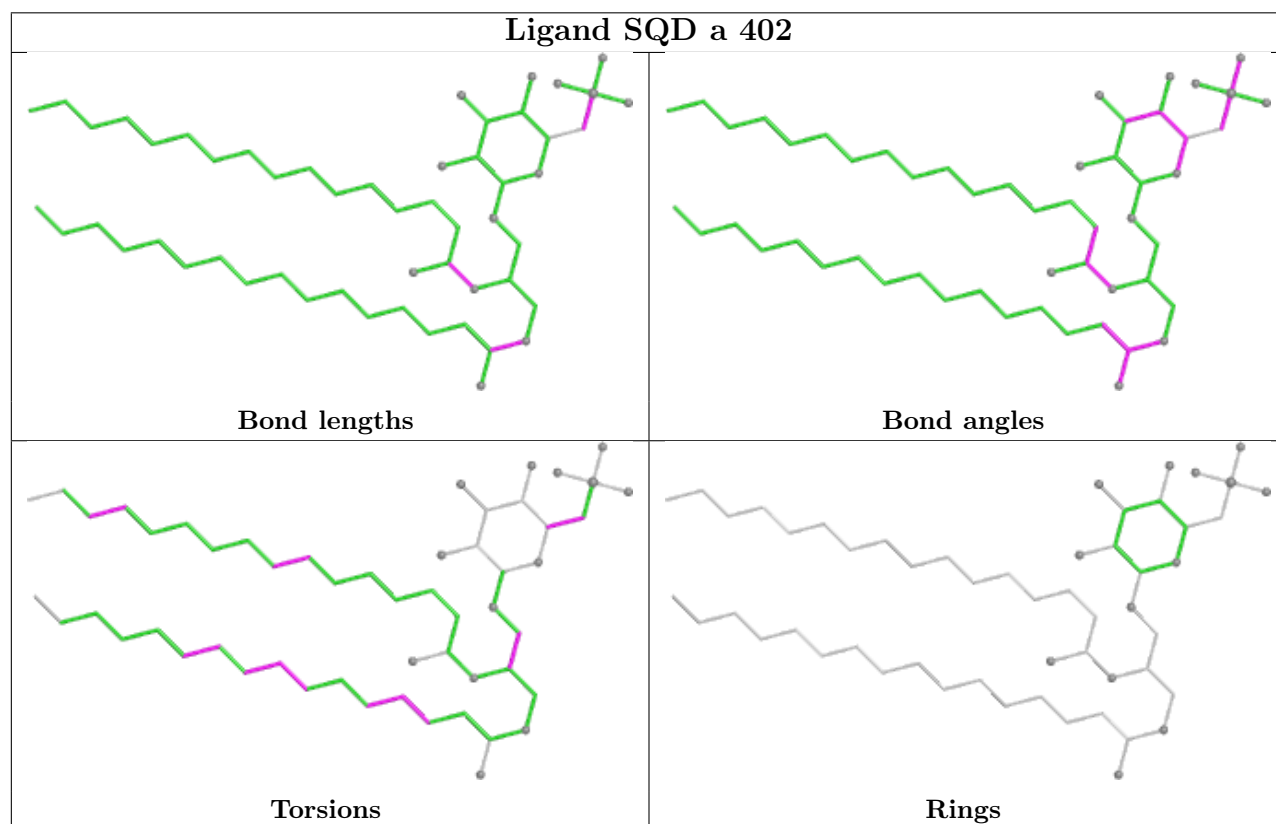
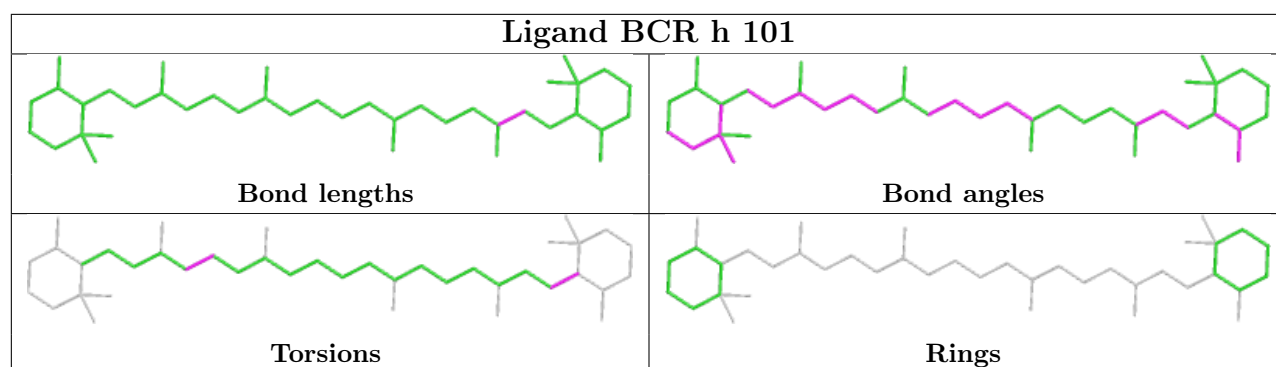
Ligand BCR D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

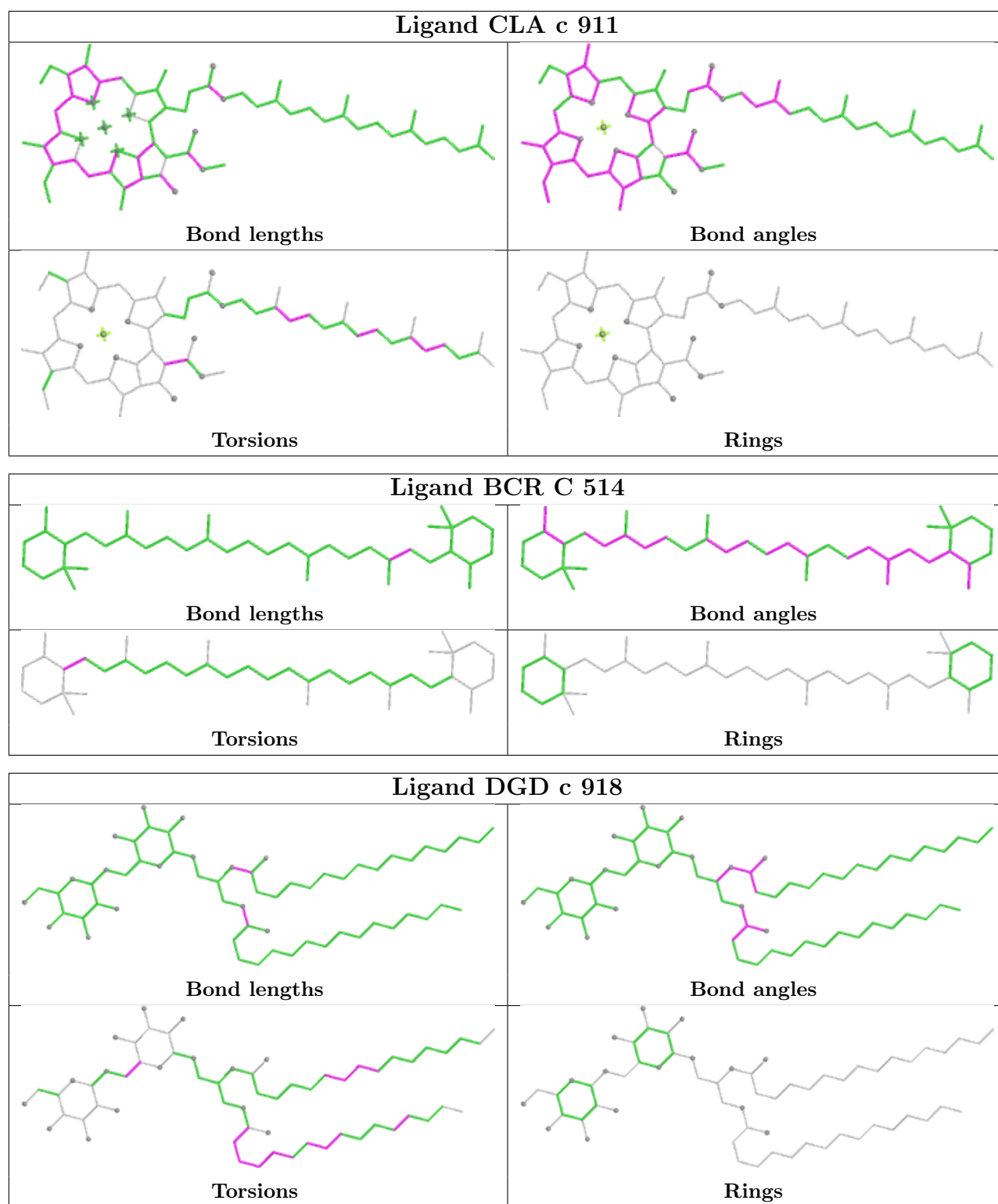
Ligand BCR c 915	
 Bond lengths	 Bond angles
 Torsions	 Rings

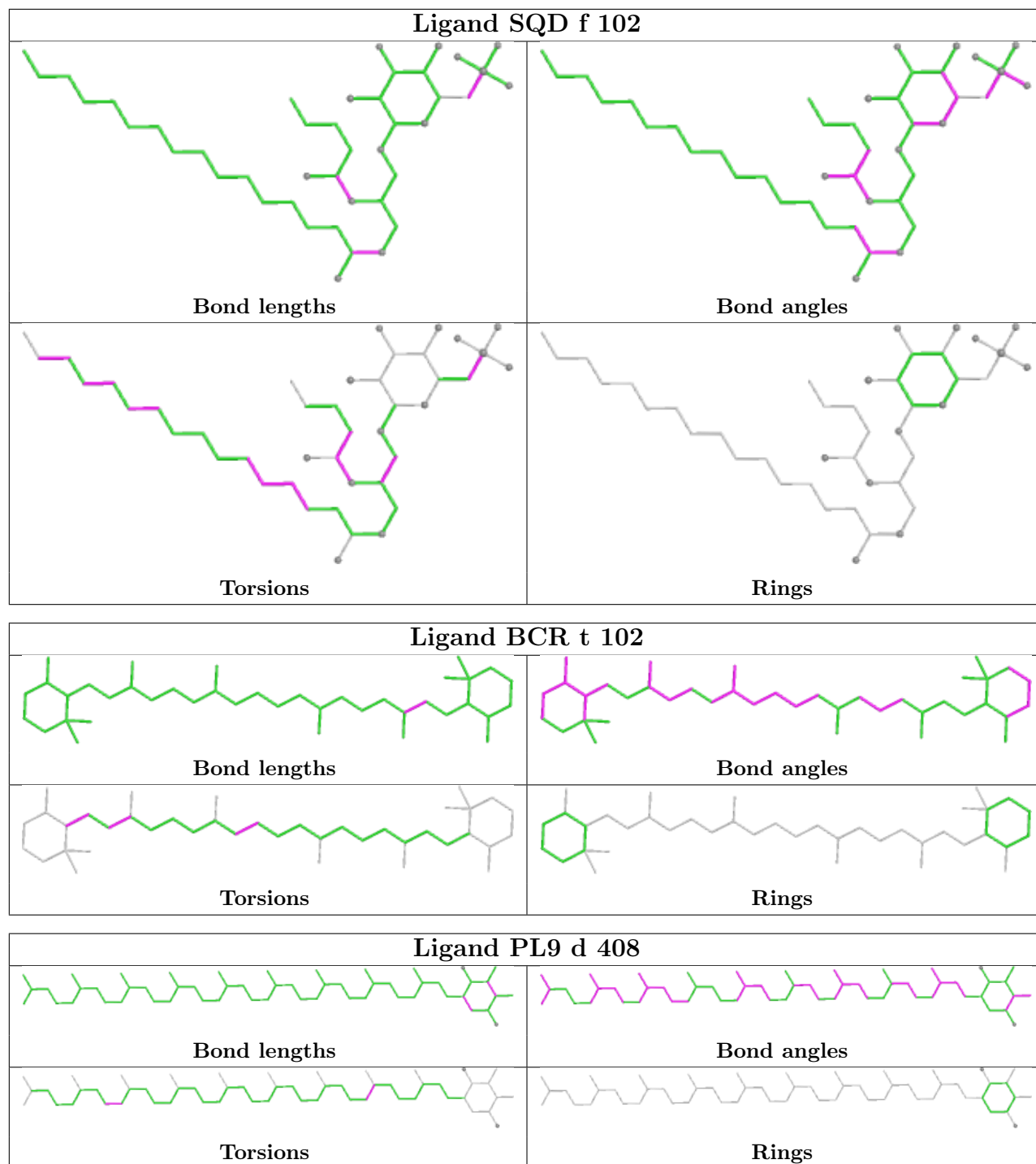


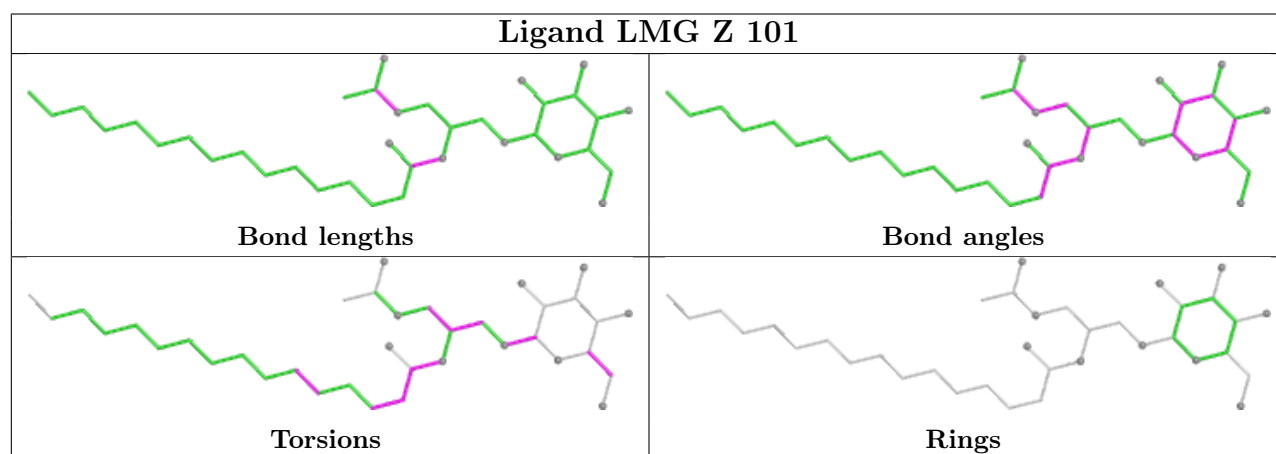
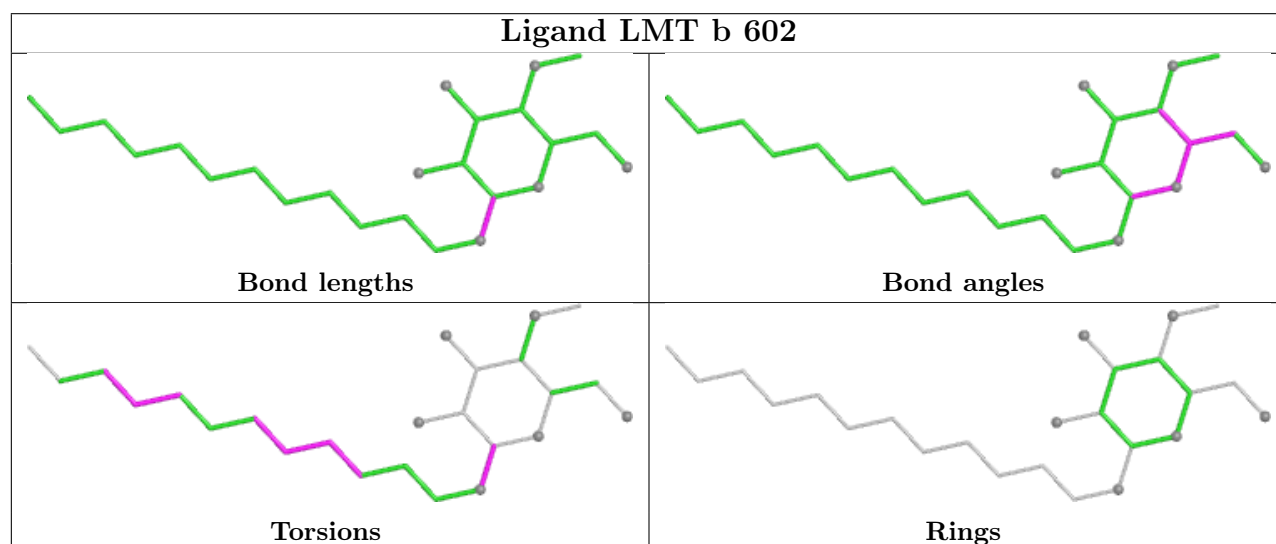
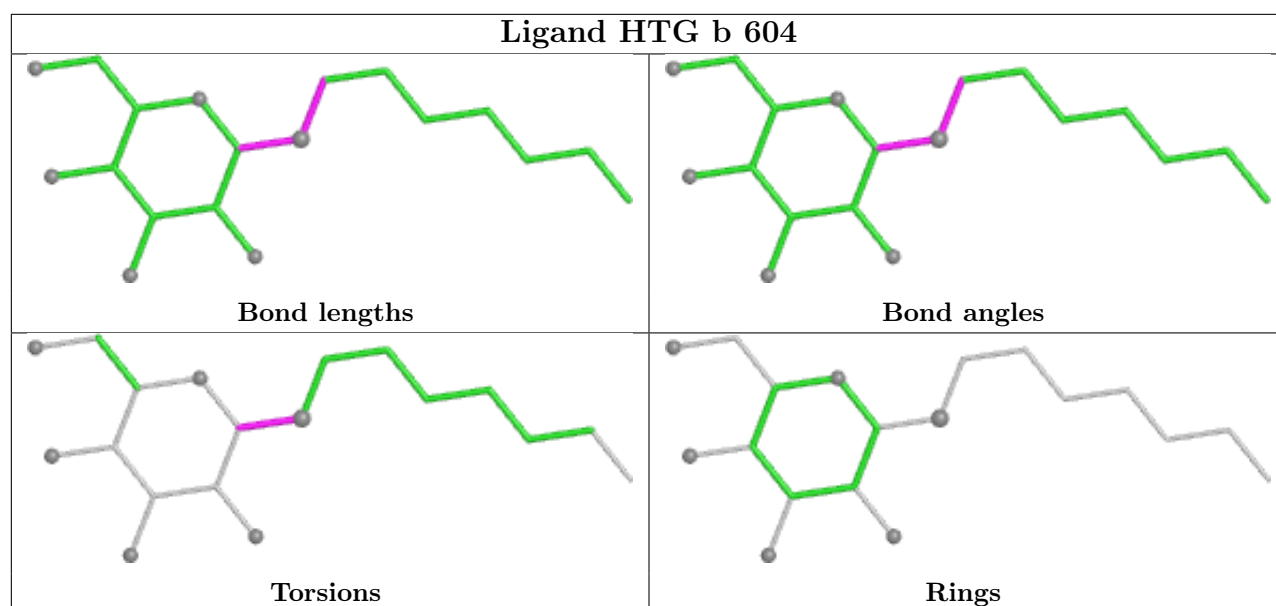


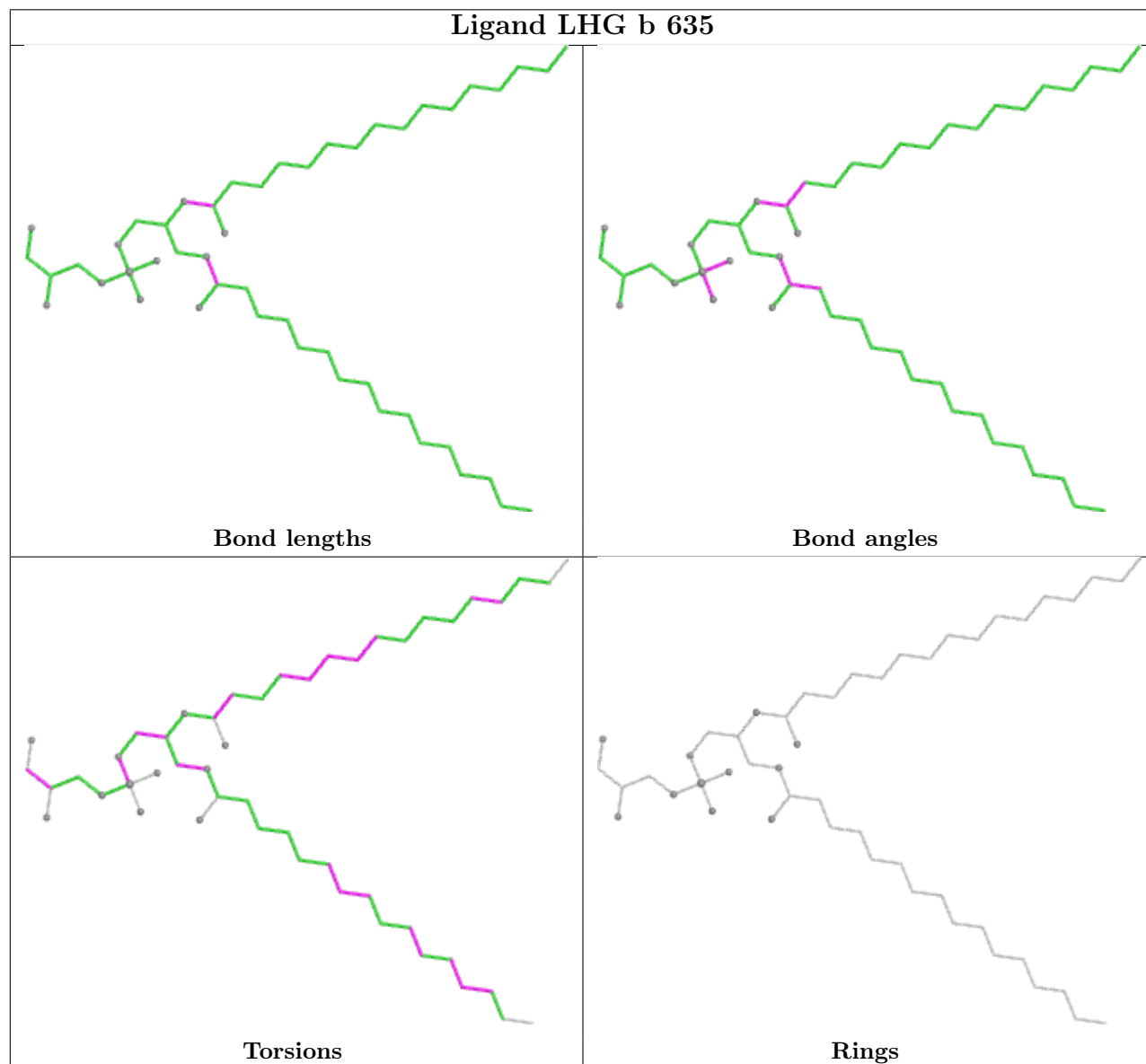
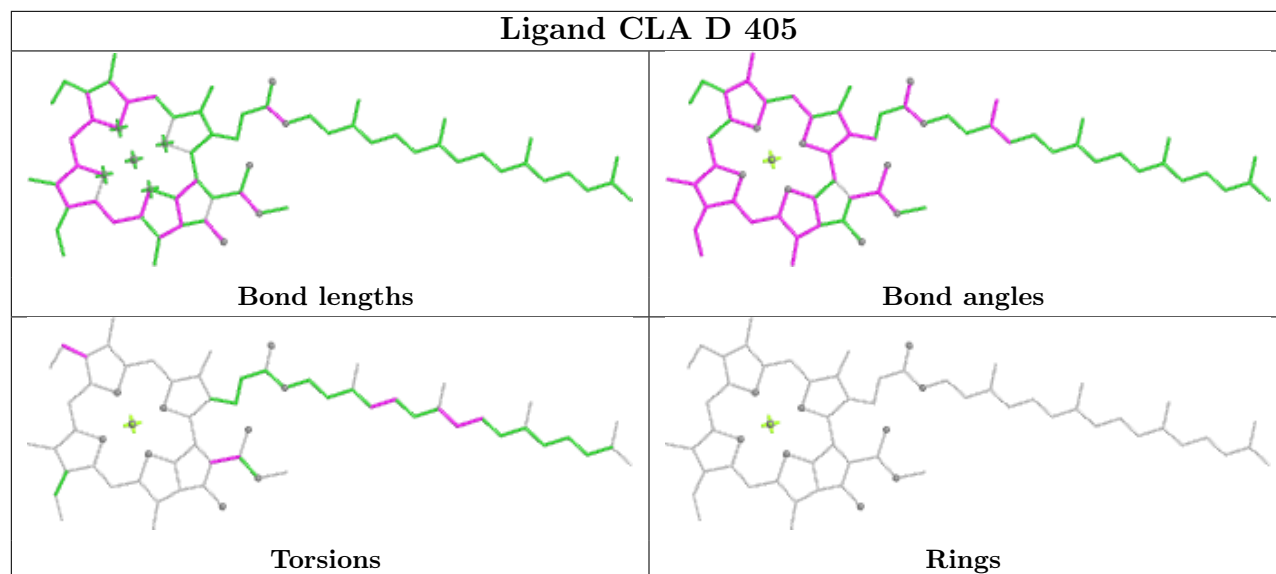


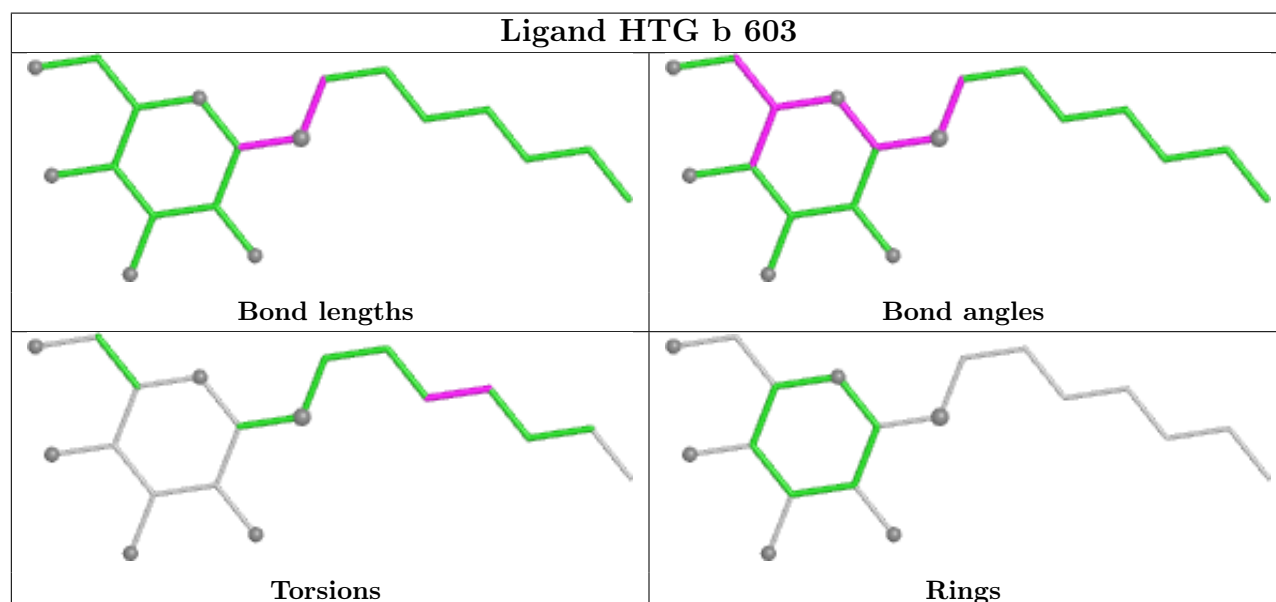
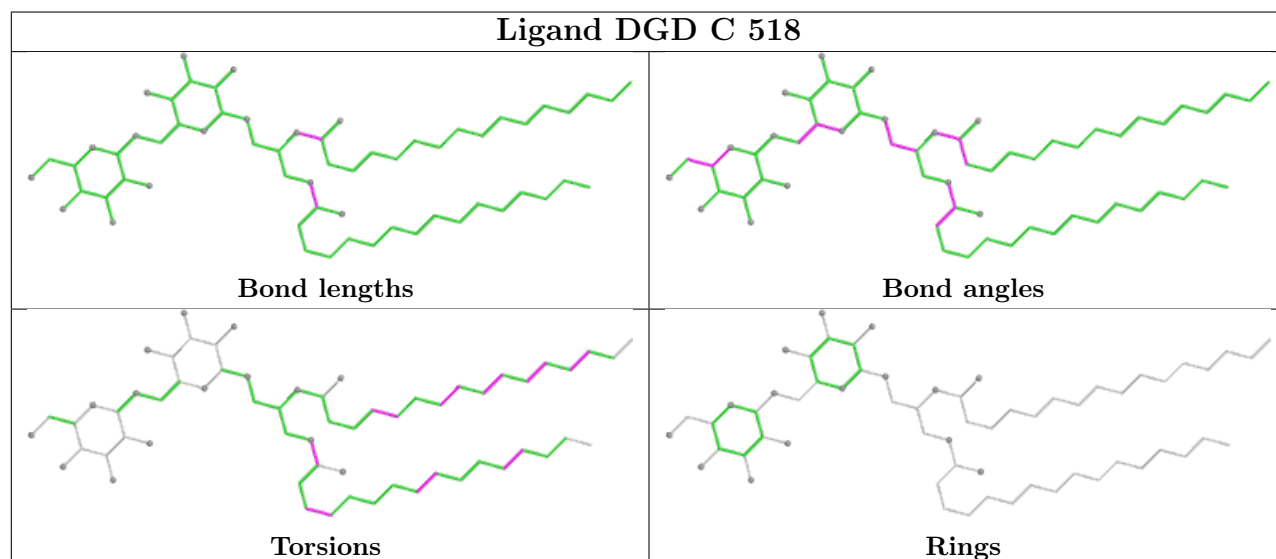
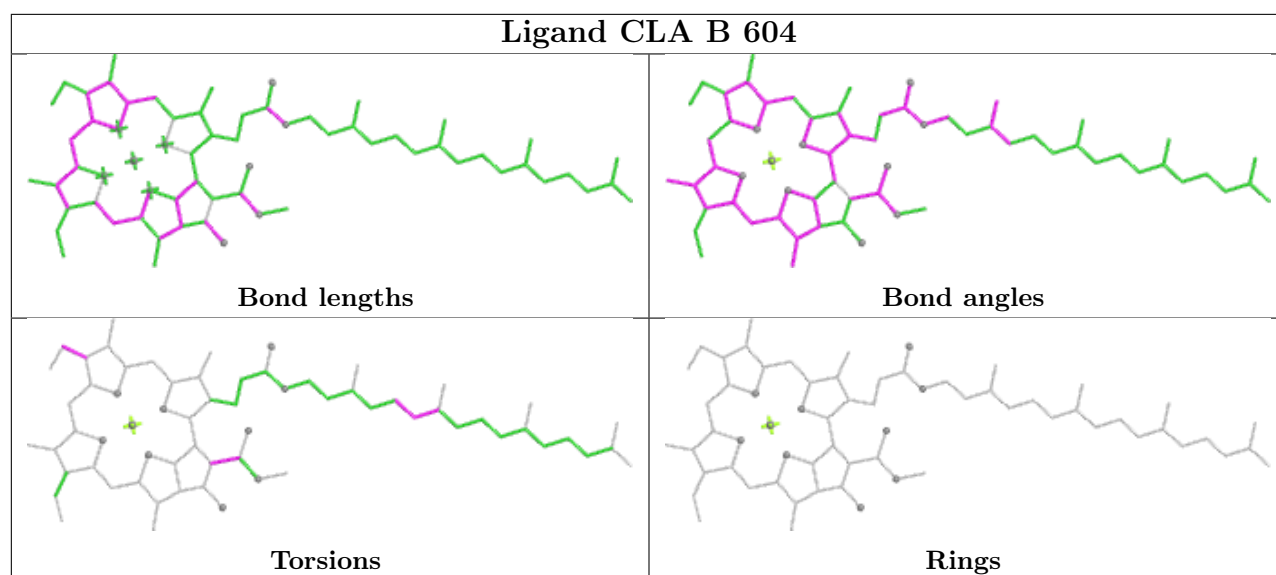


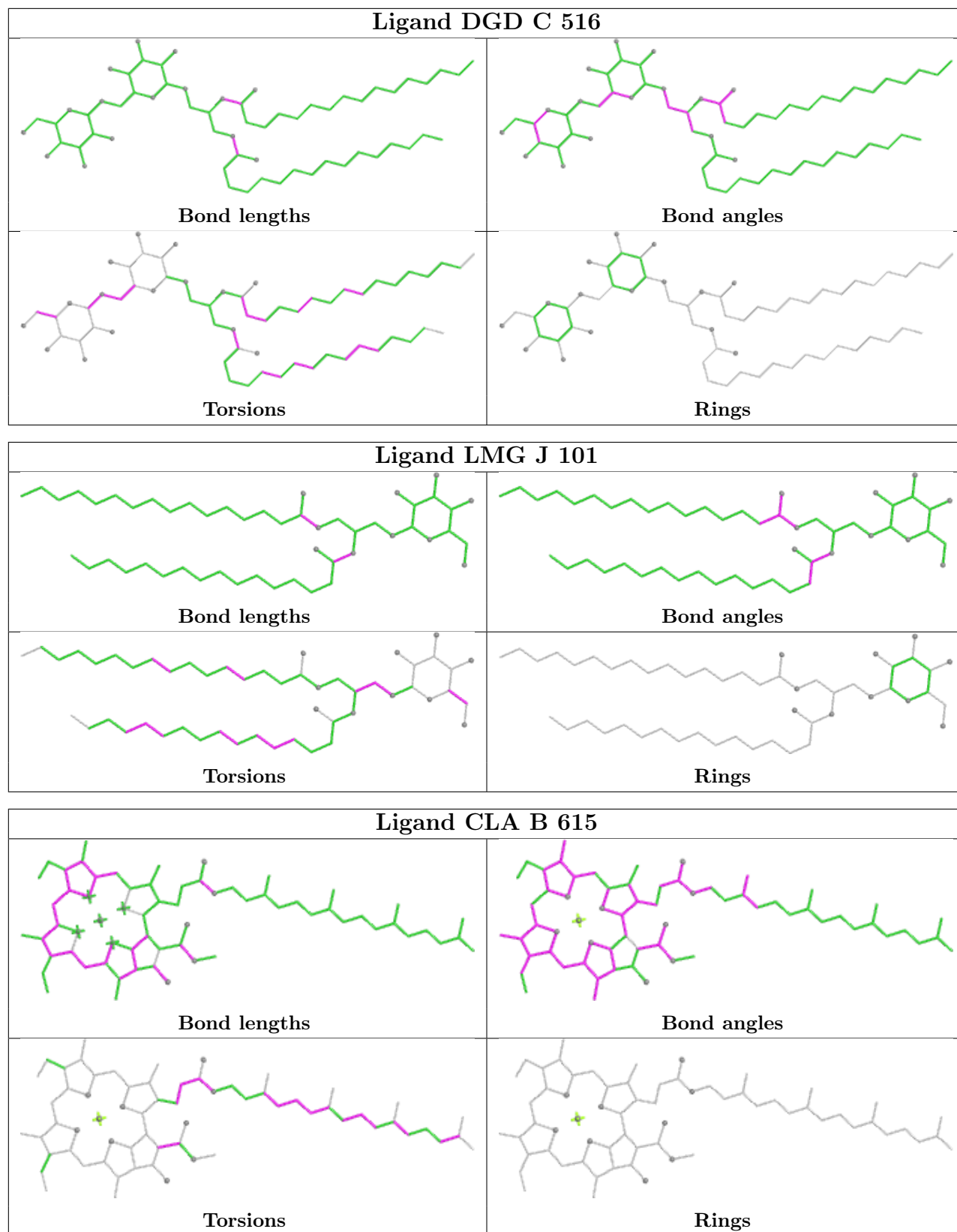


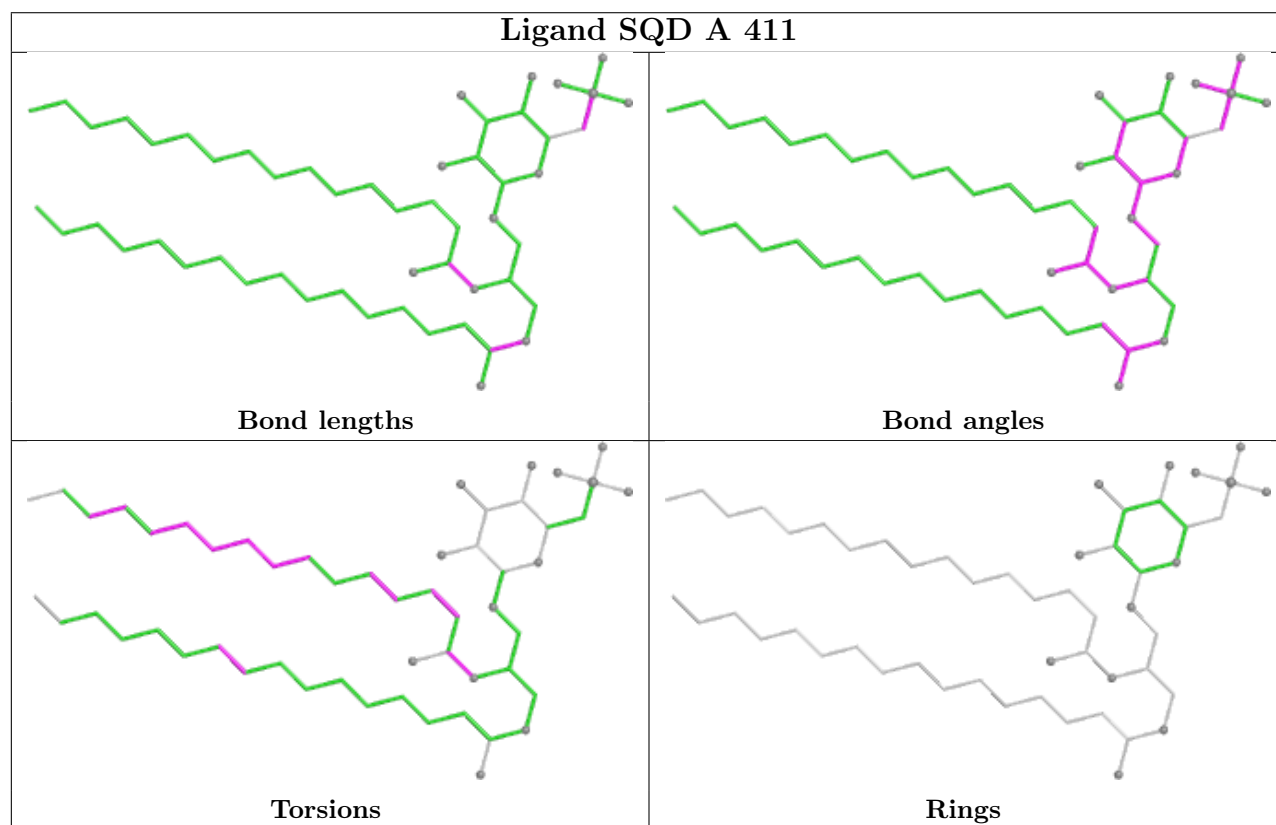
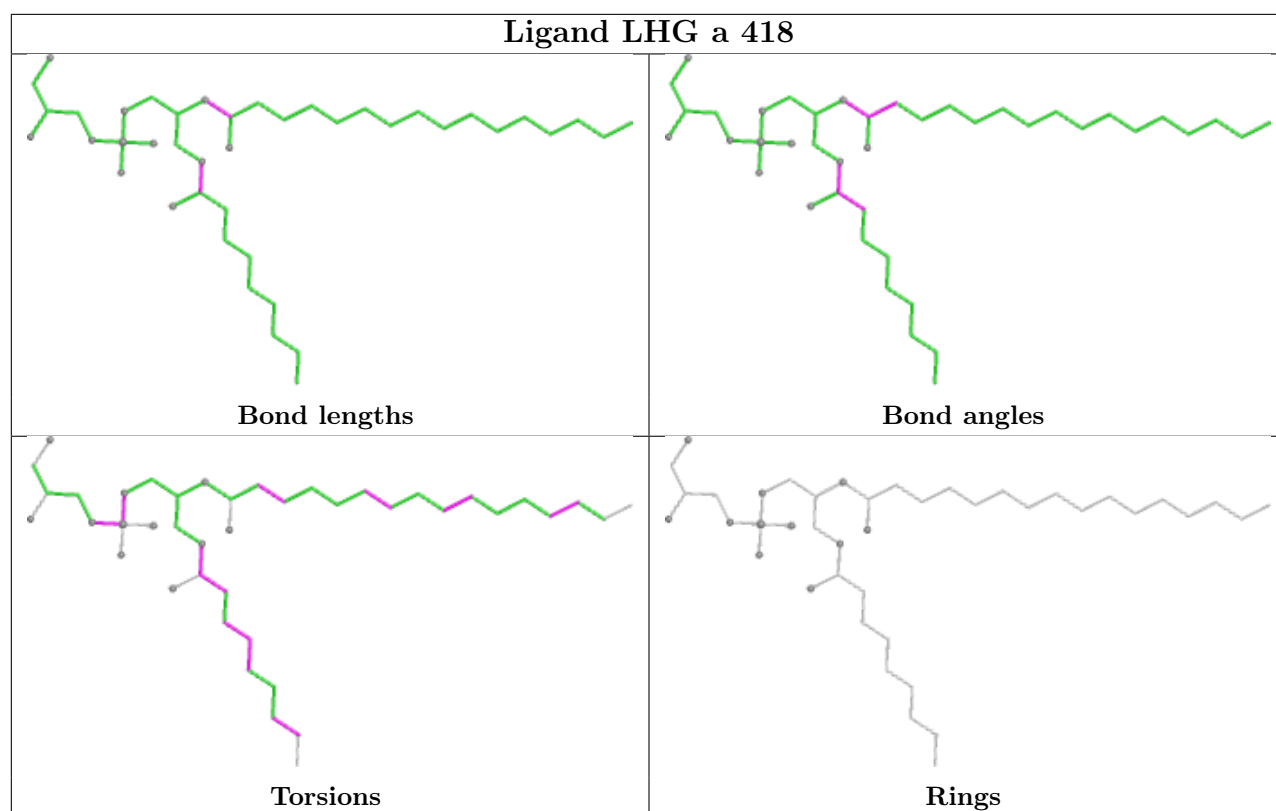


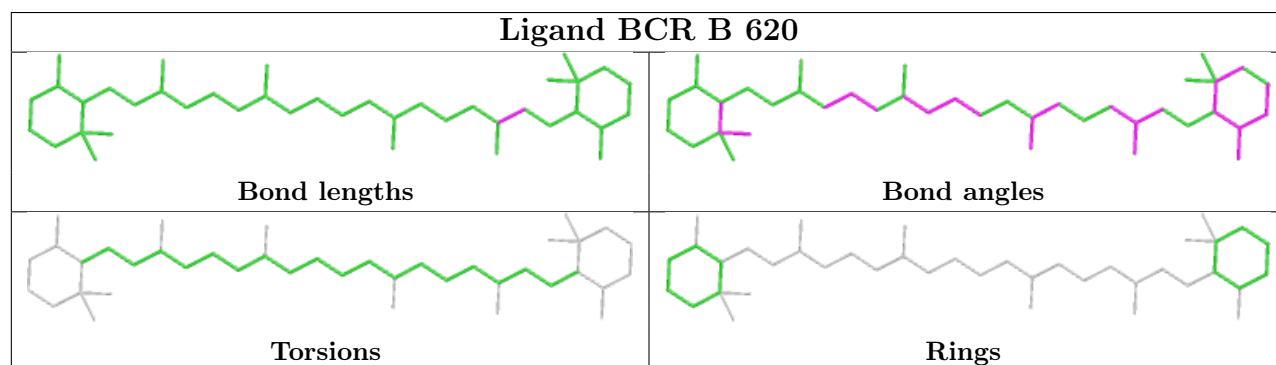
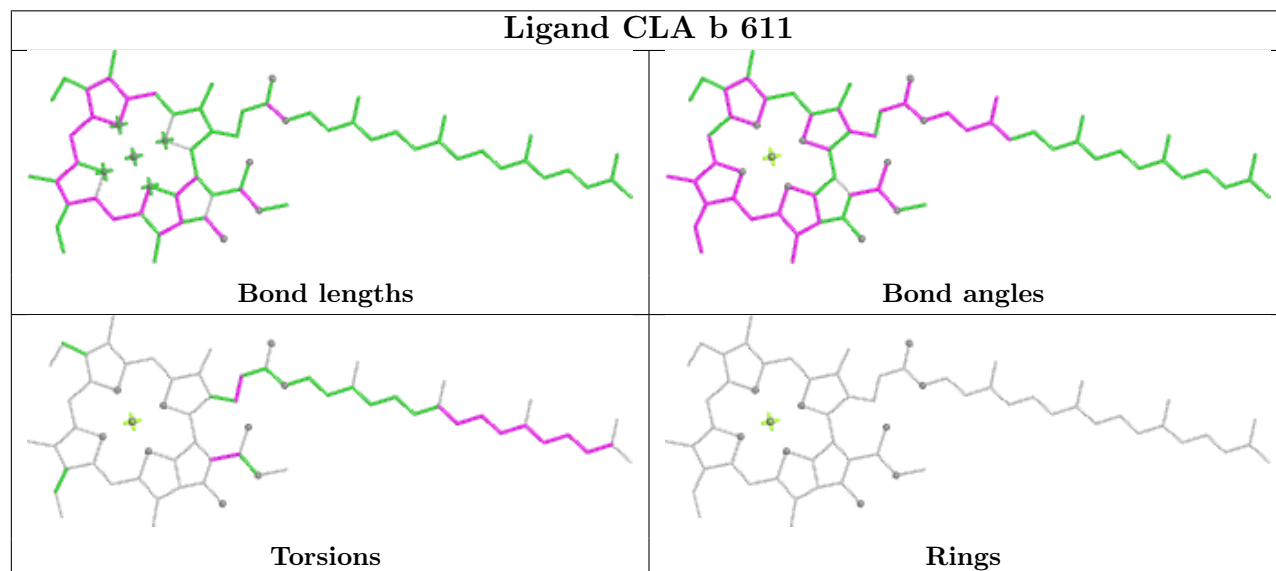
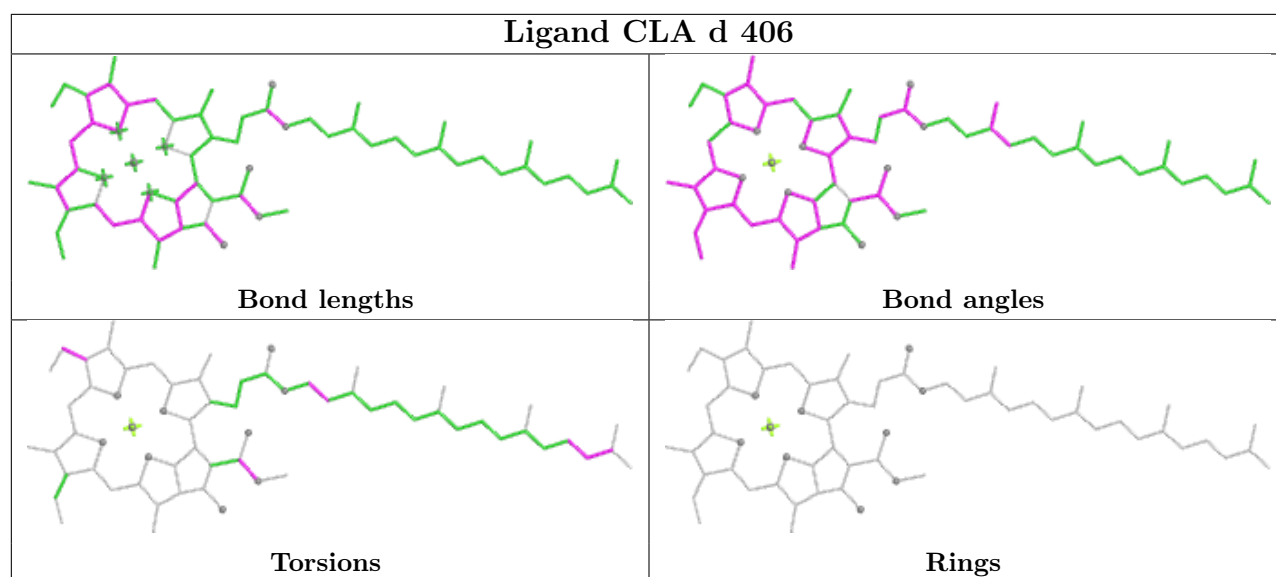




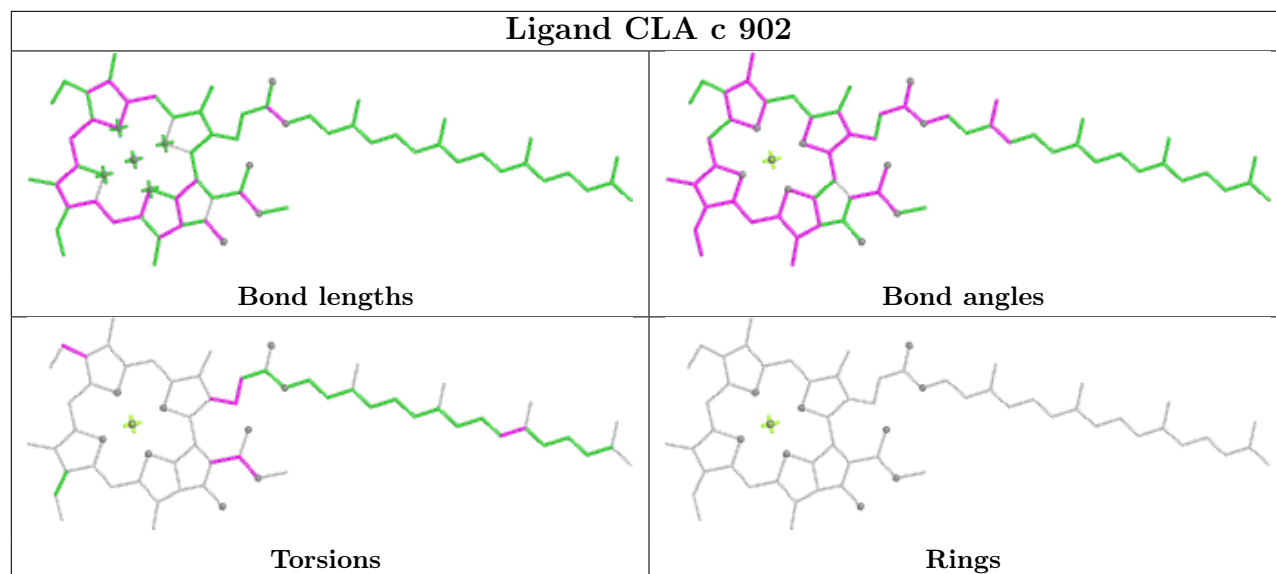




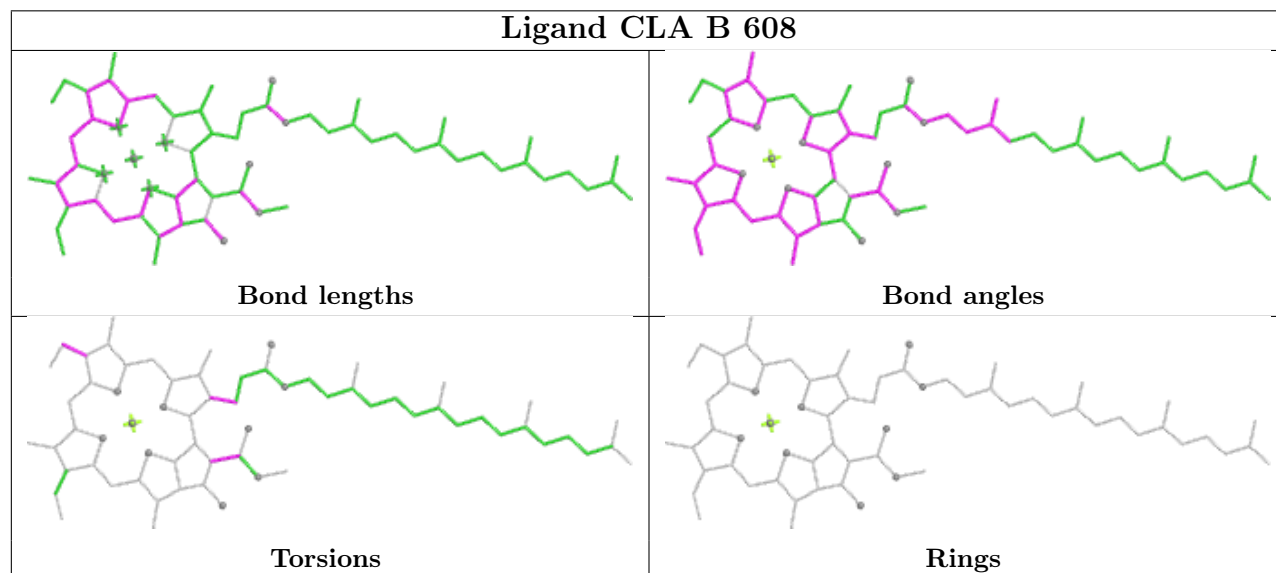


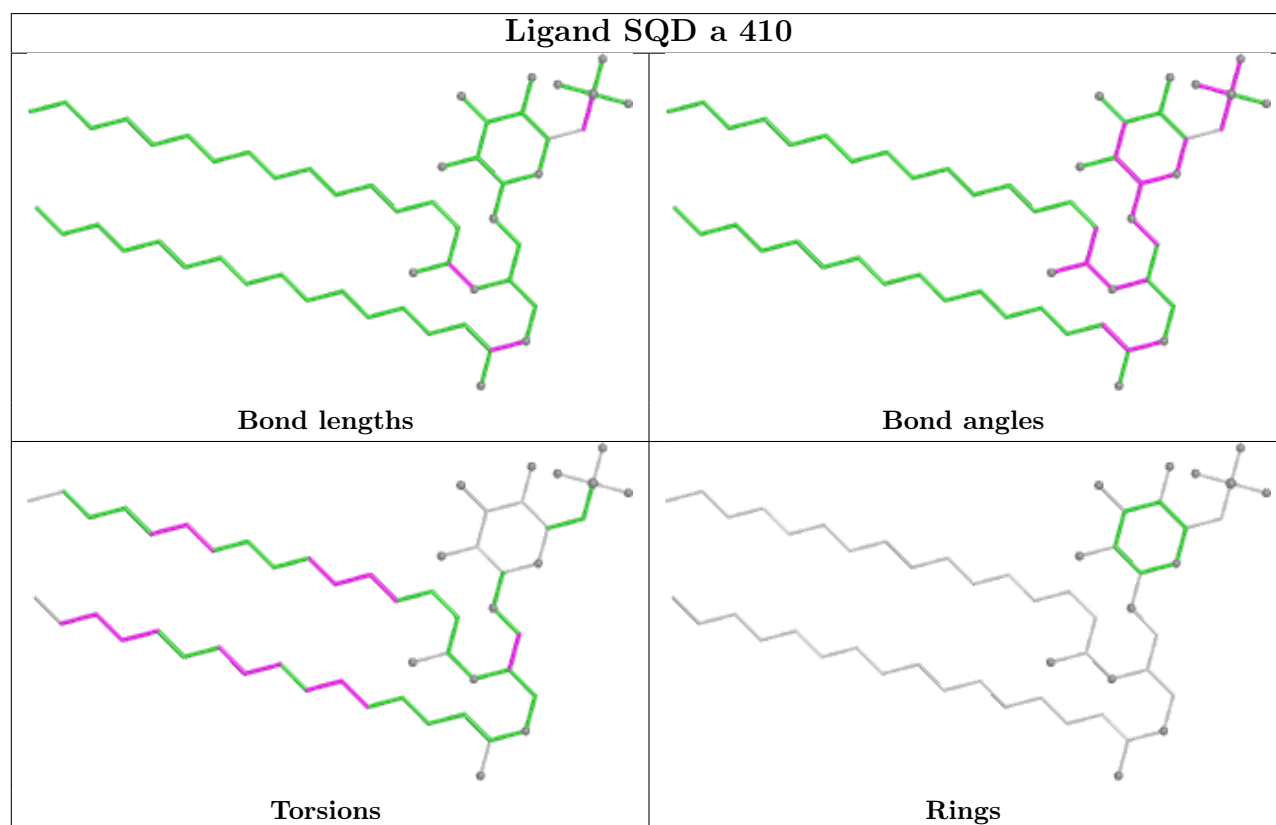
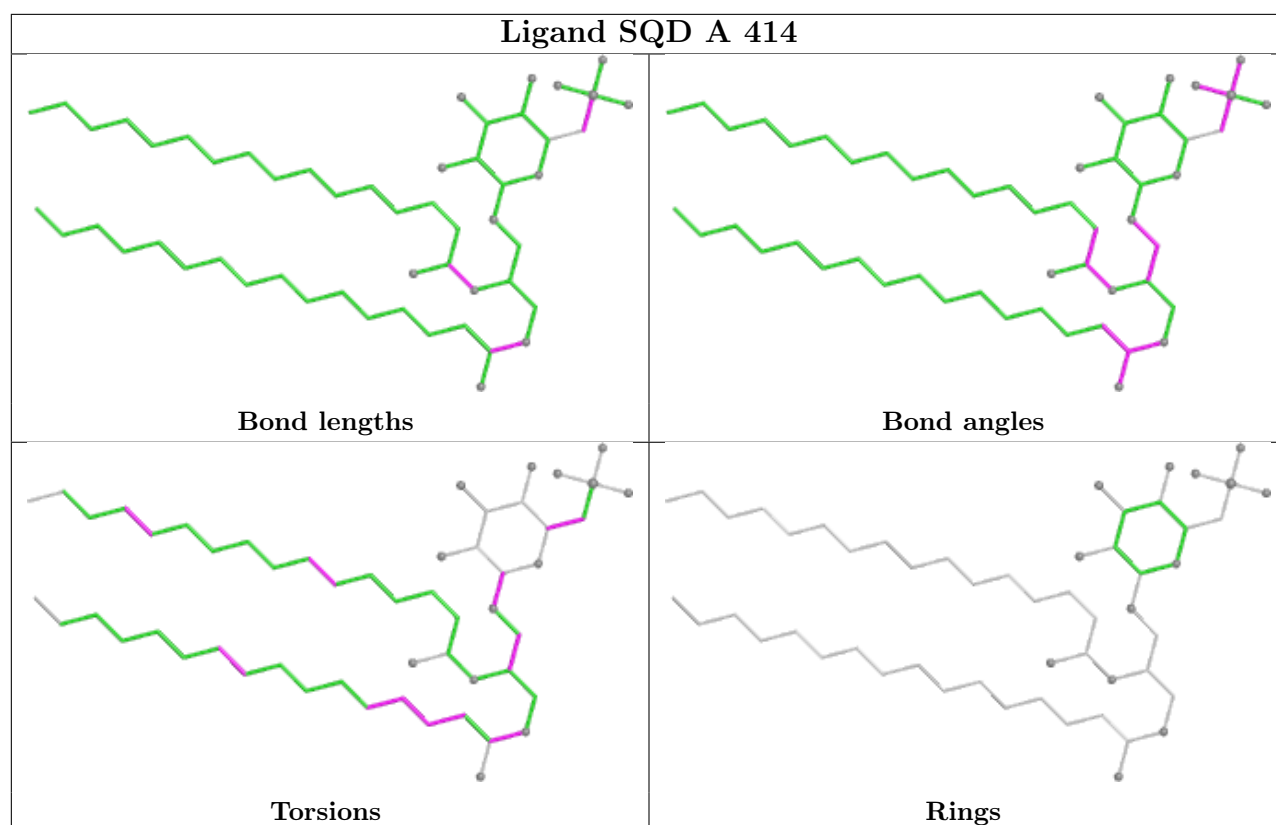


Ligand CLA c 902

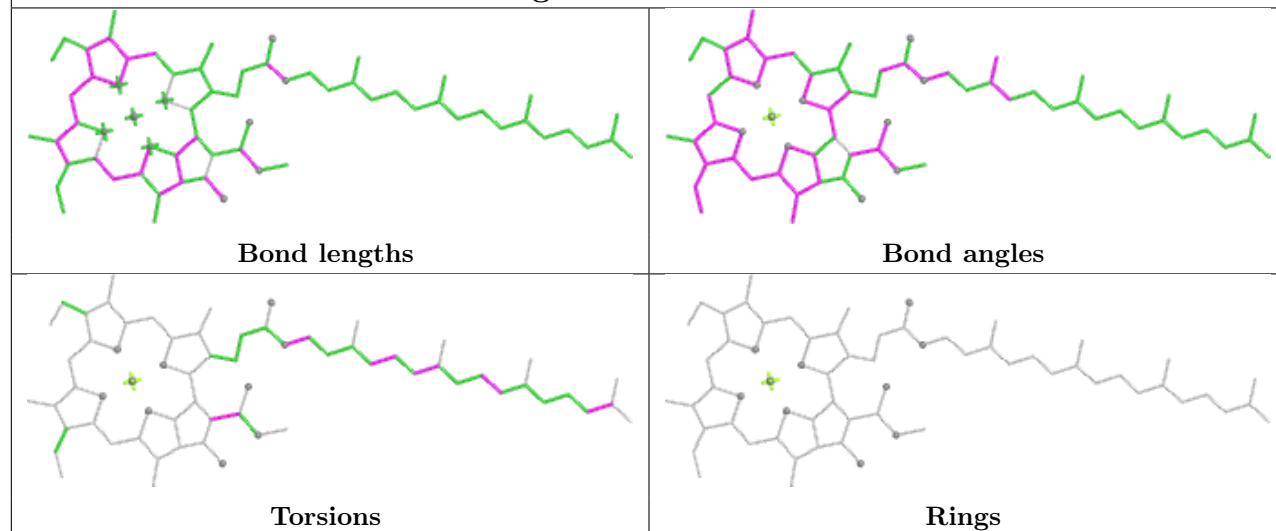


Ligand CLA B 608

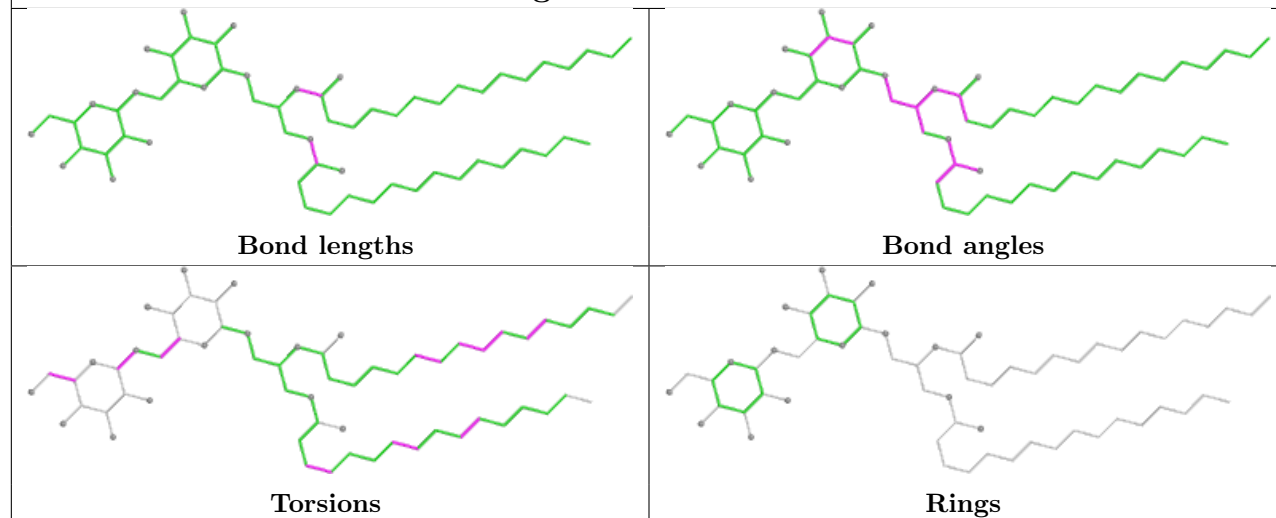




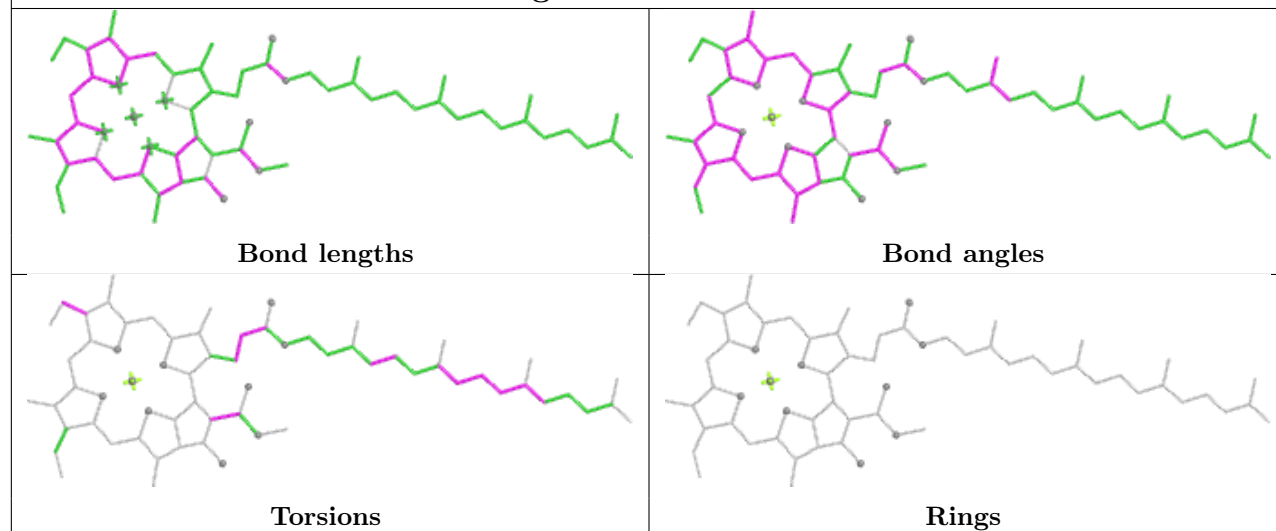
Ligand CLA B 617

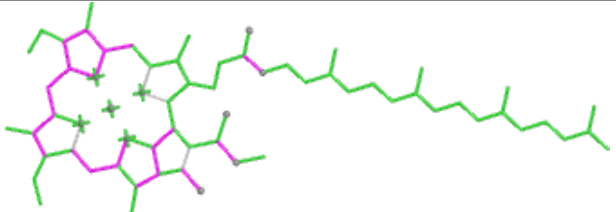
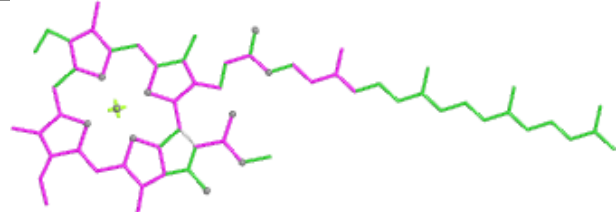
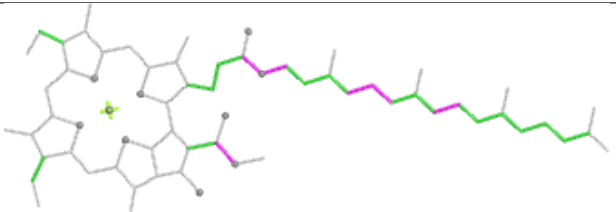
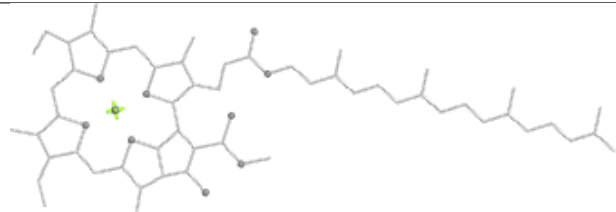


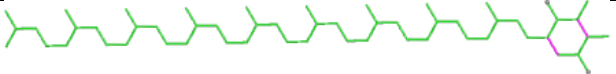
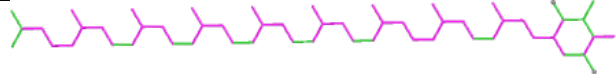
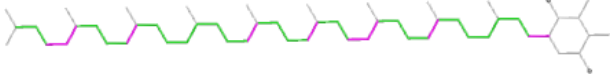
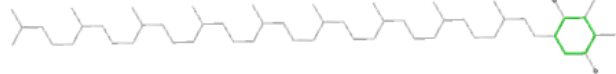
Ligand DGD c 916

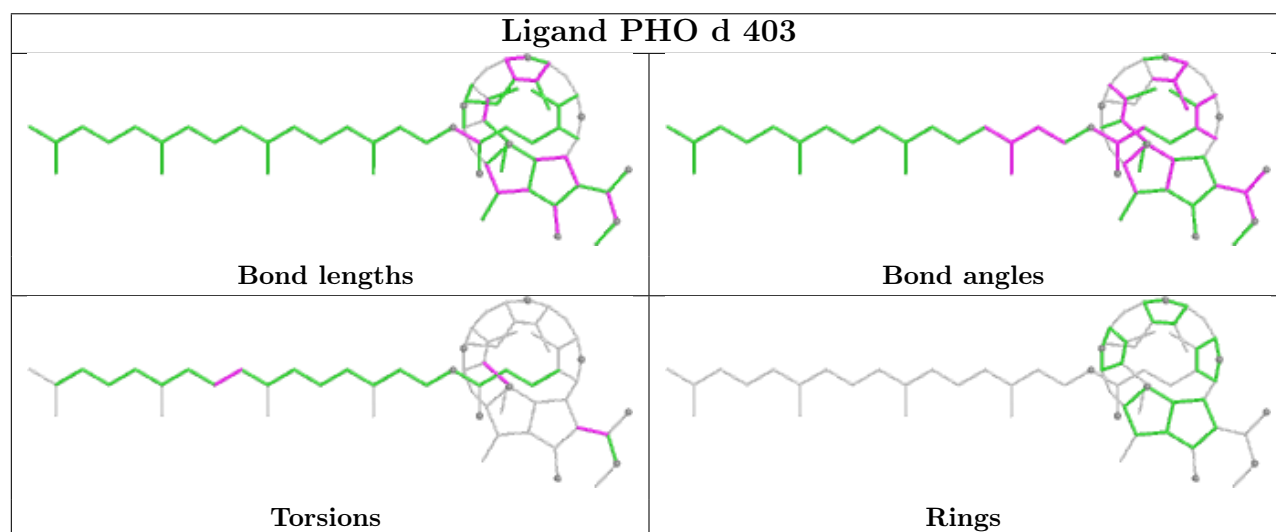
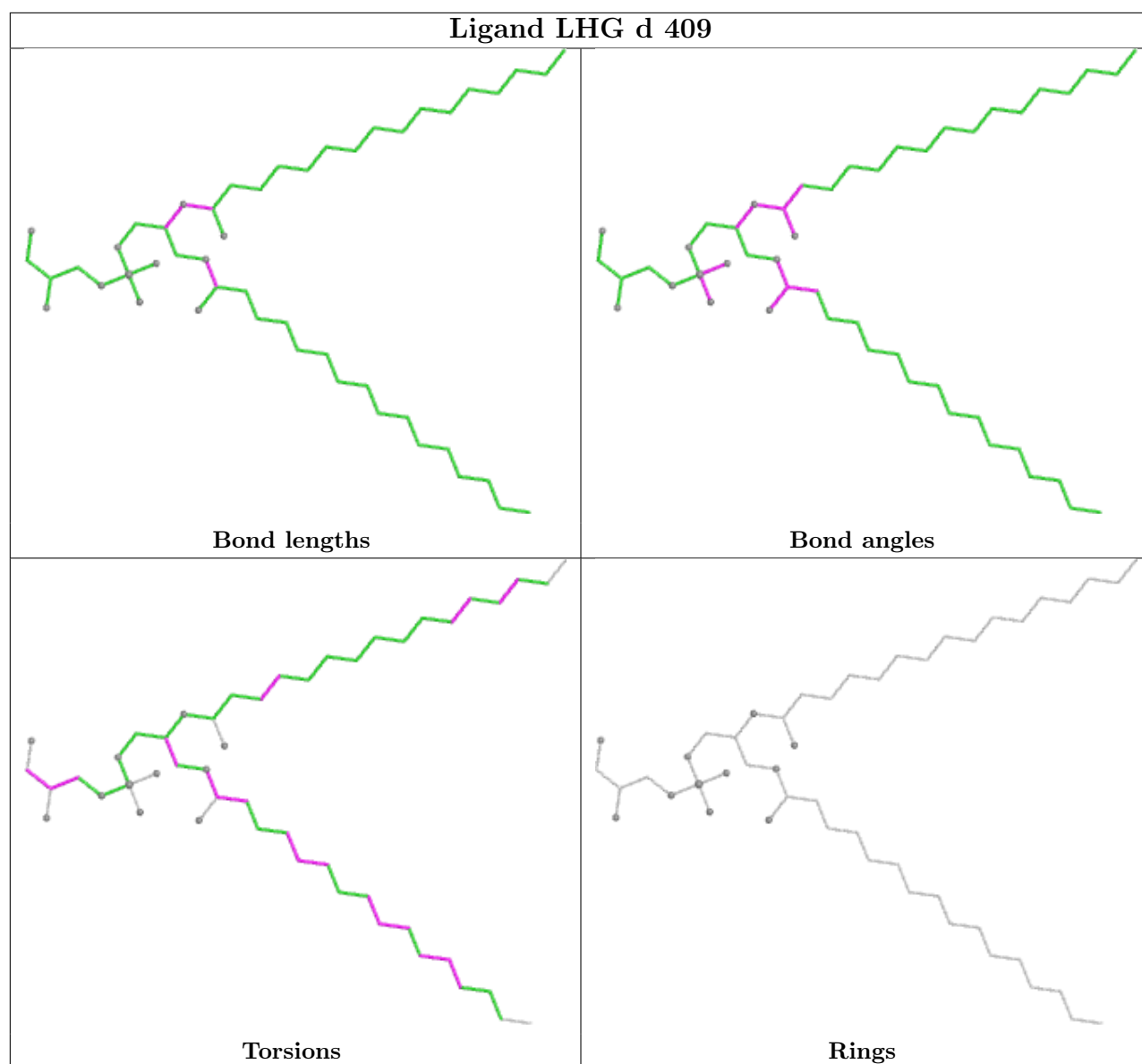


Ligand CLA B 602

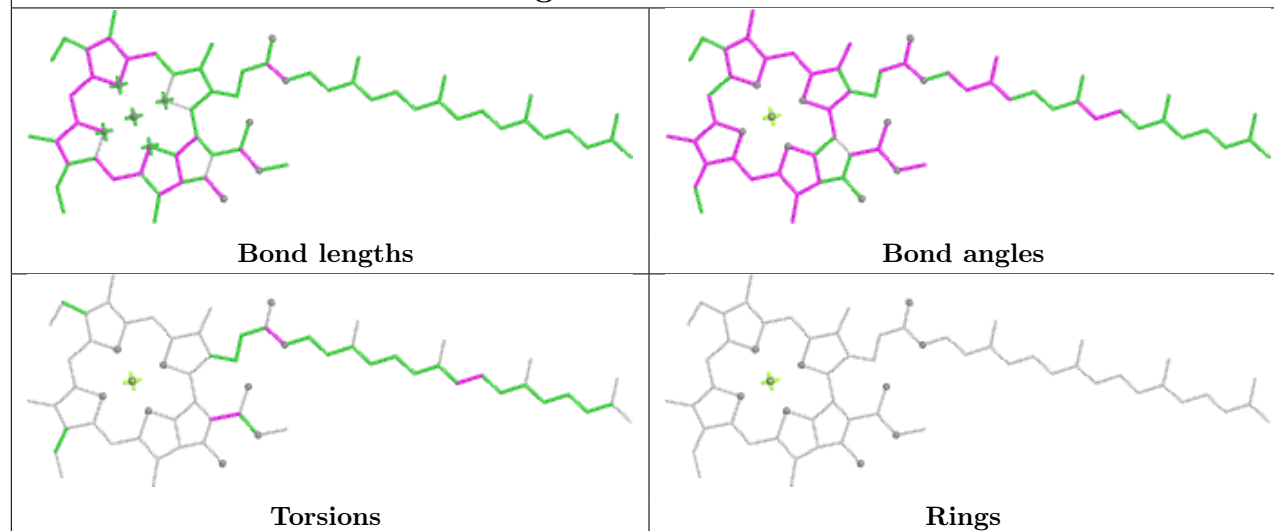


Ligand CLA C 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

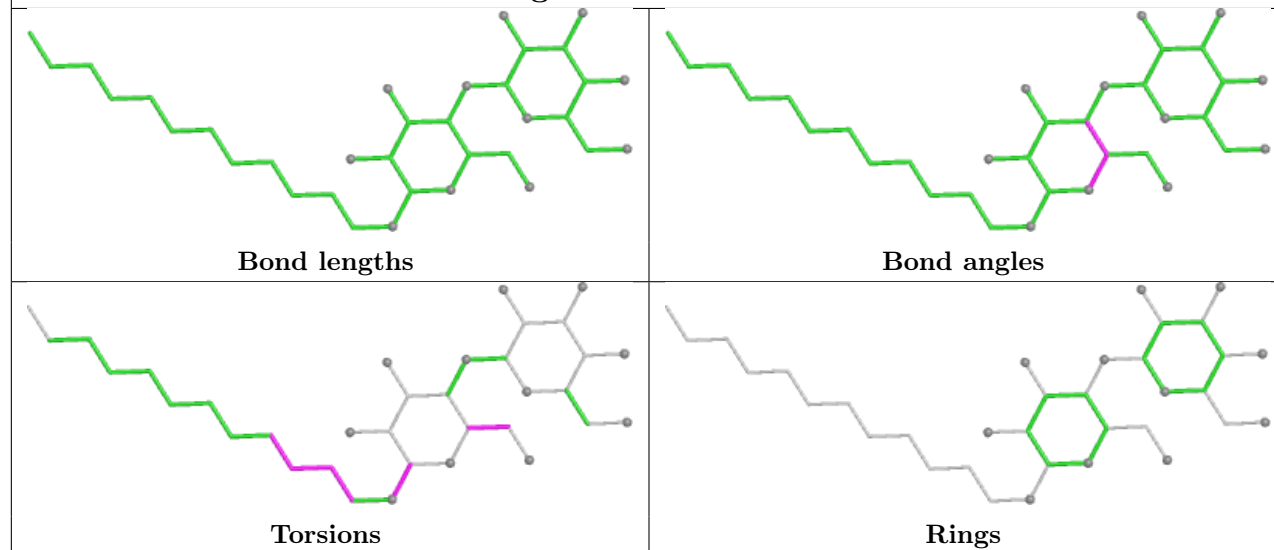
Ligand PL9 A 417	
	
Bond lengths	Bond angles
	
Torsions	Rings



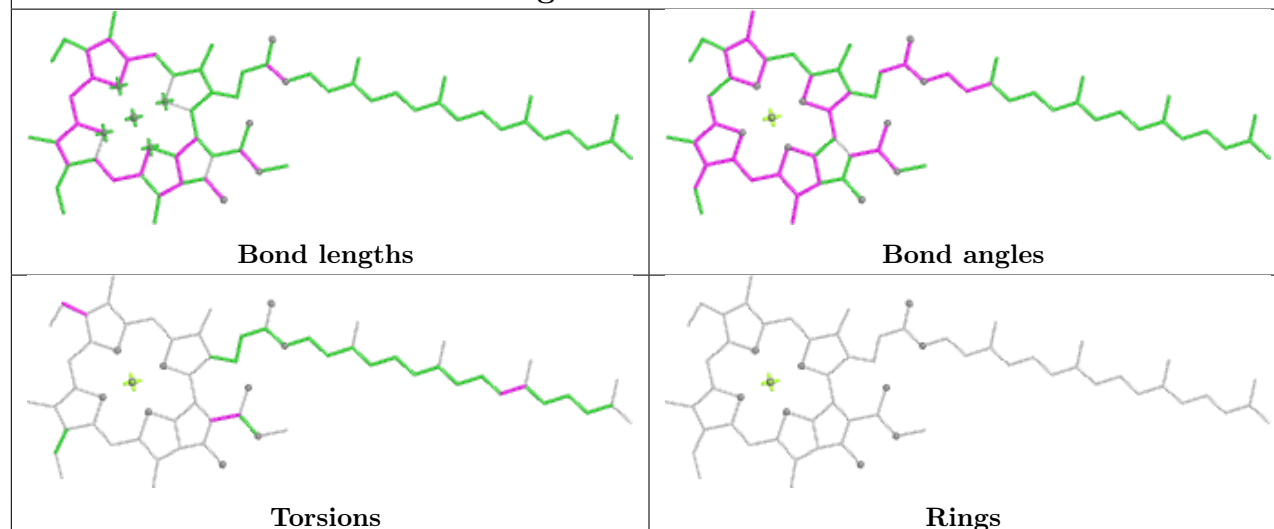
Ligand CLA b 617

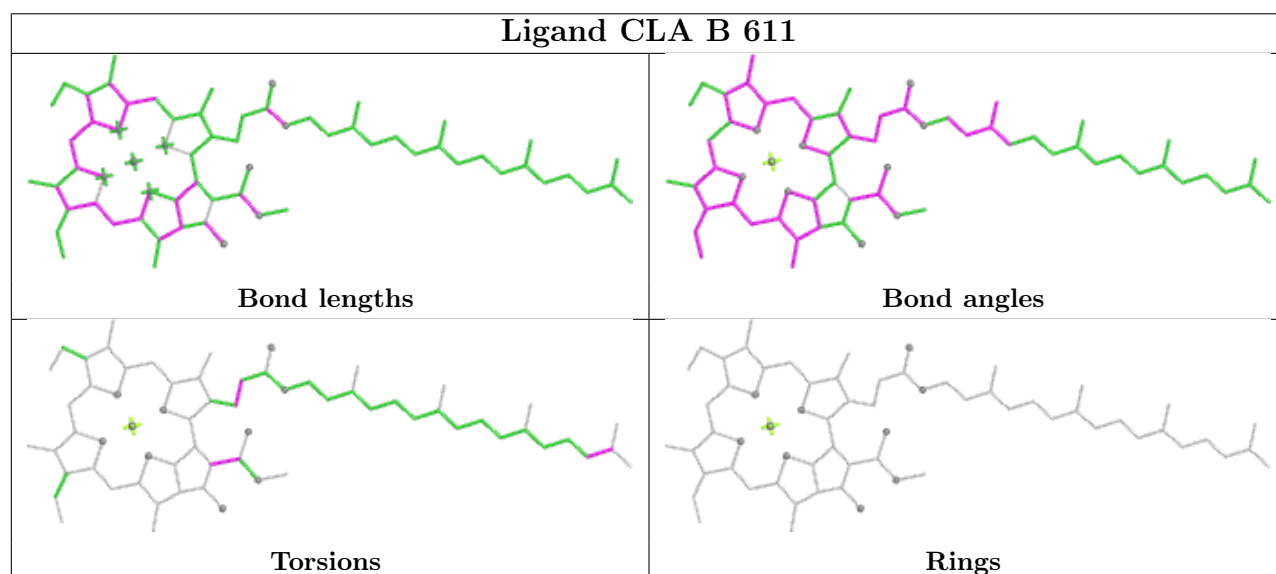
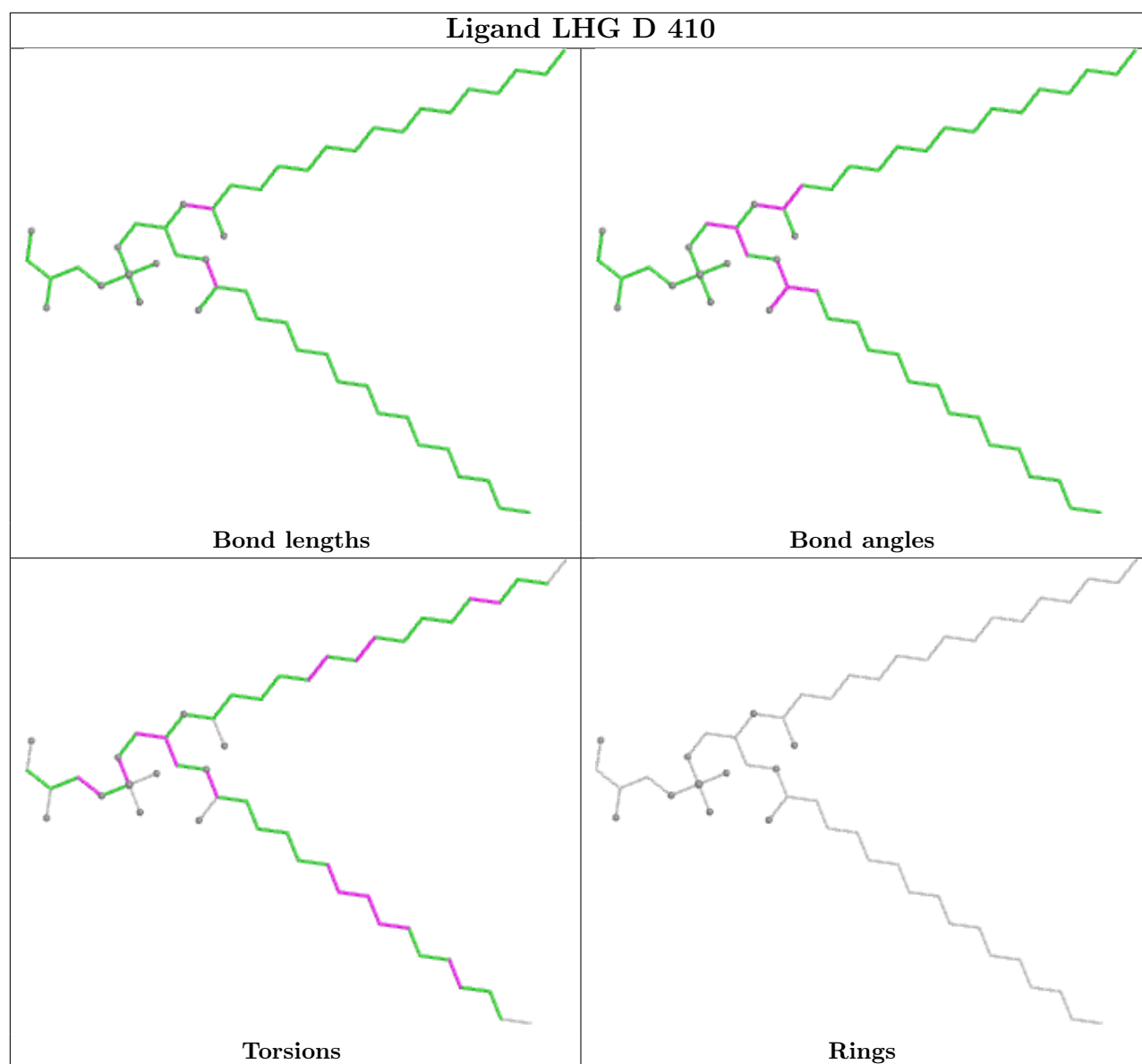


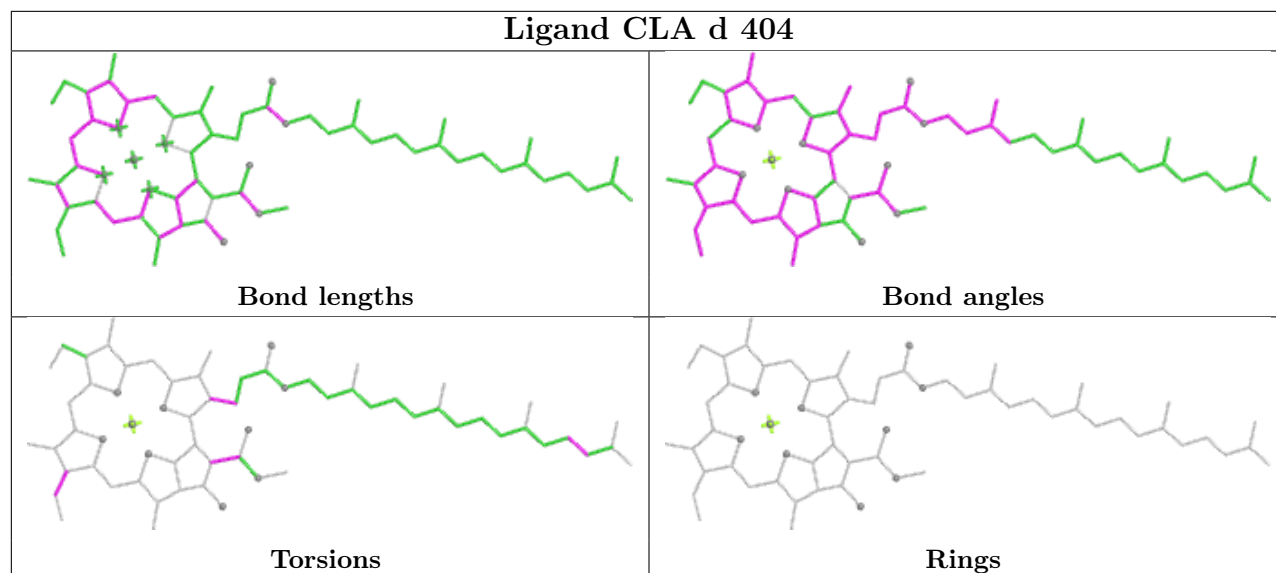
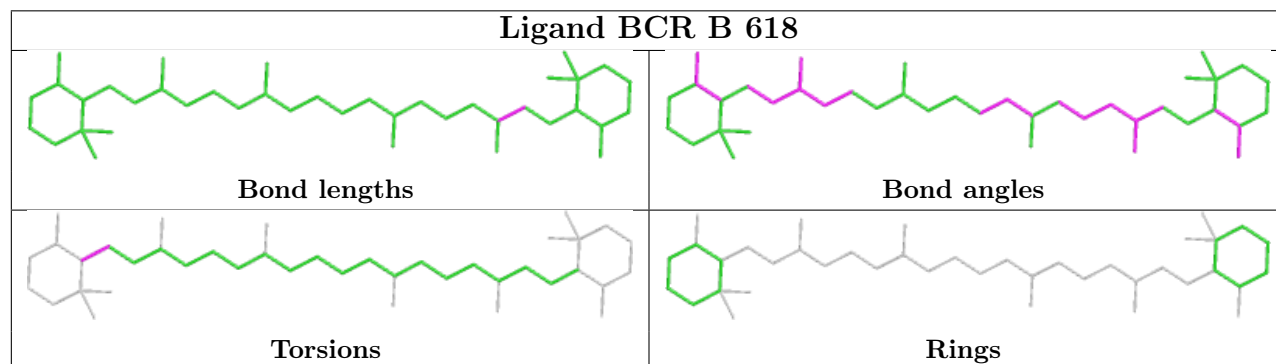
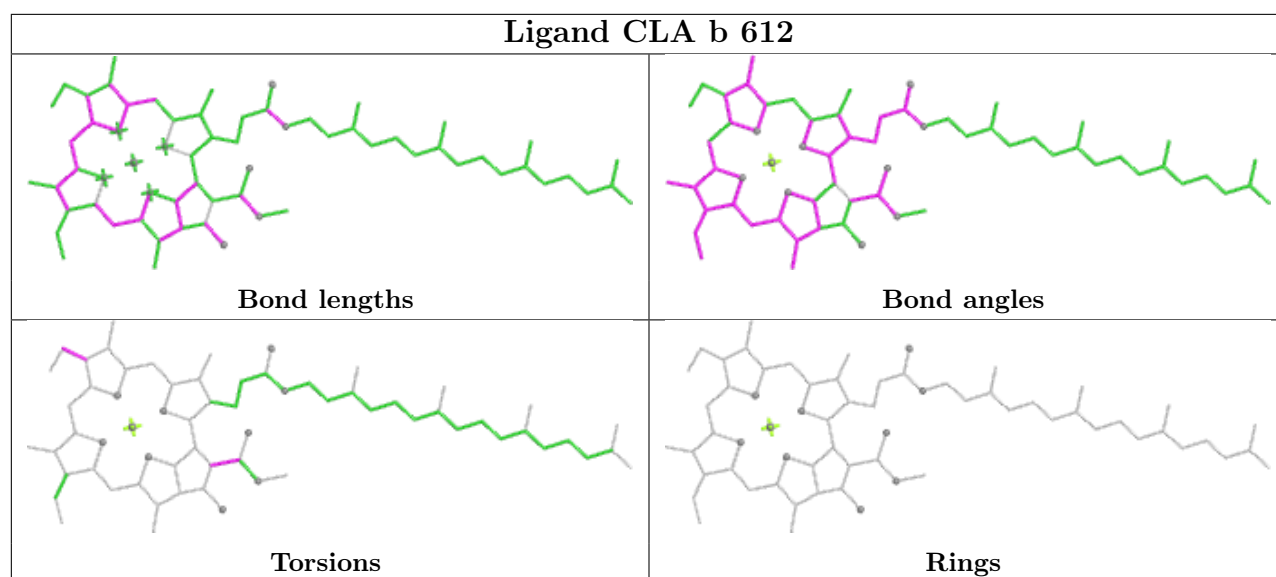
Ligand LMT F 101



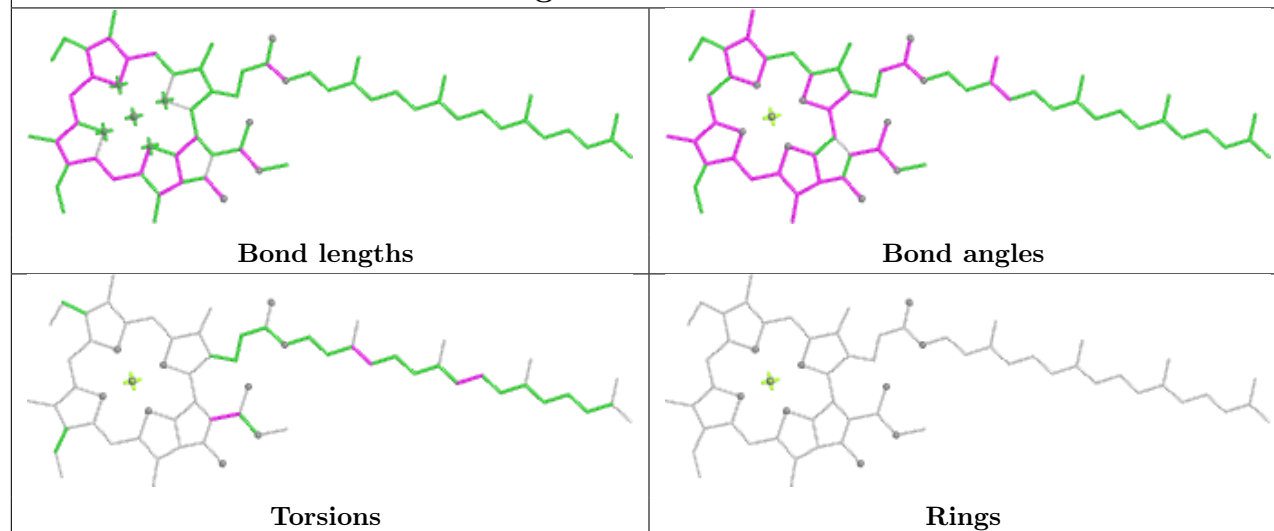
Ligand CLA c 903



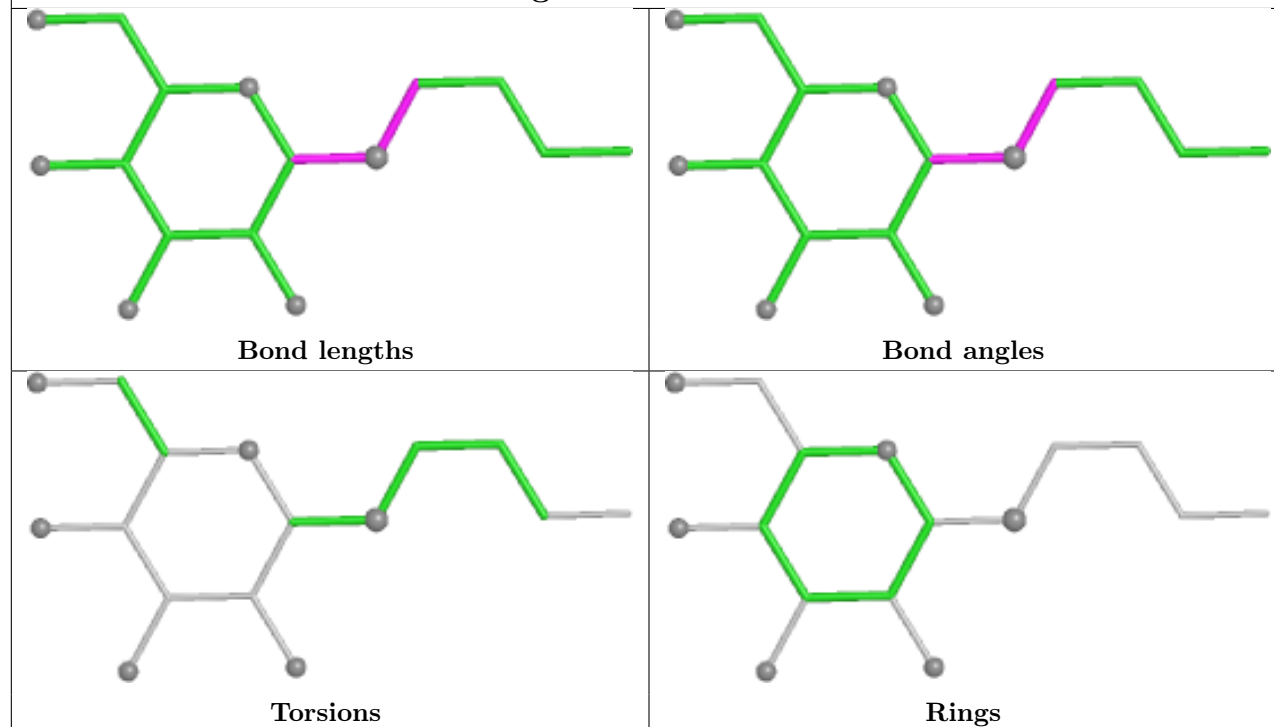




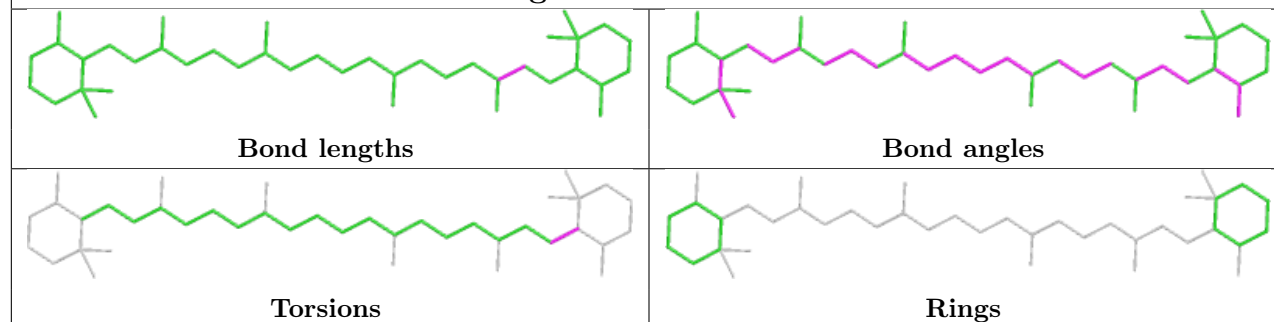
Ligand CLA b 610

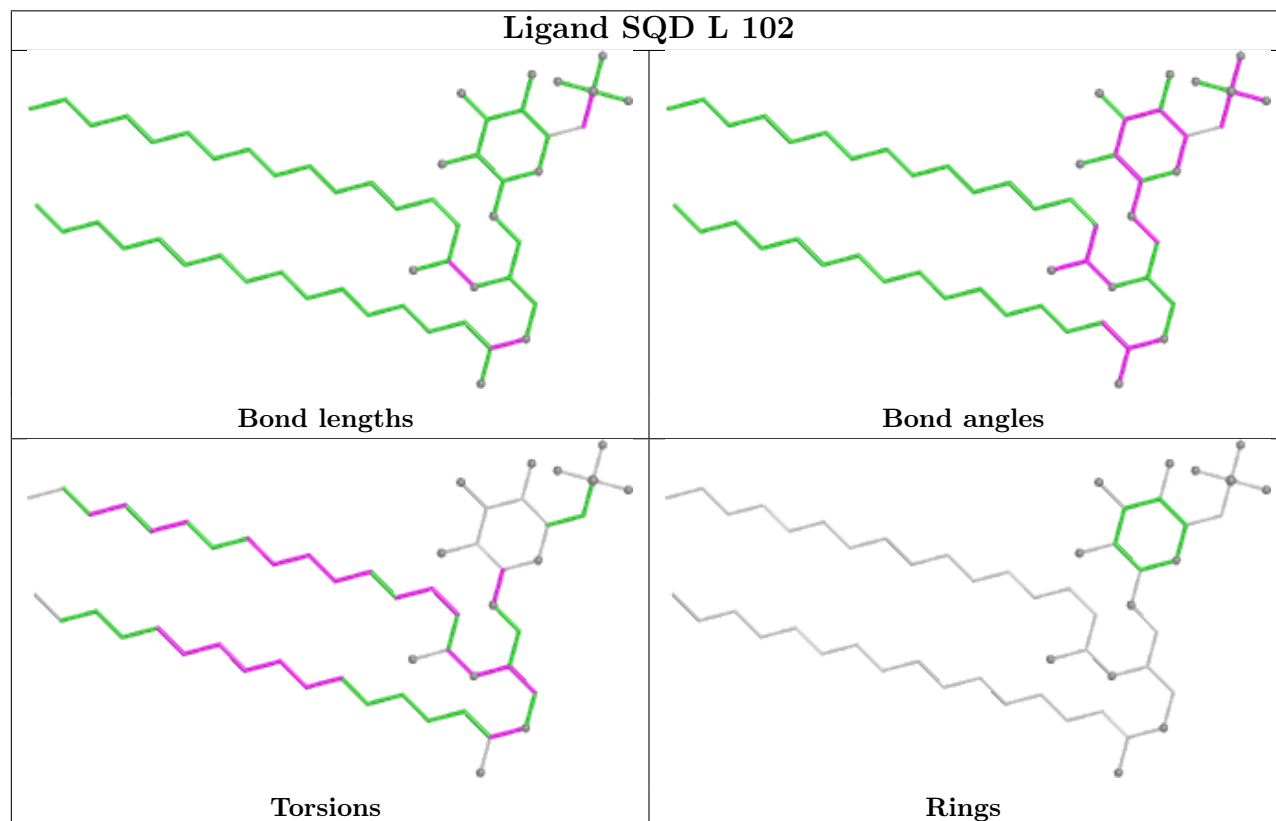
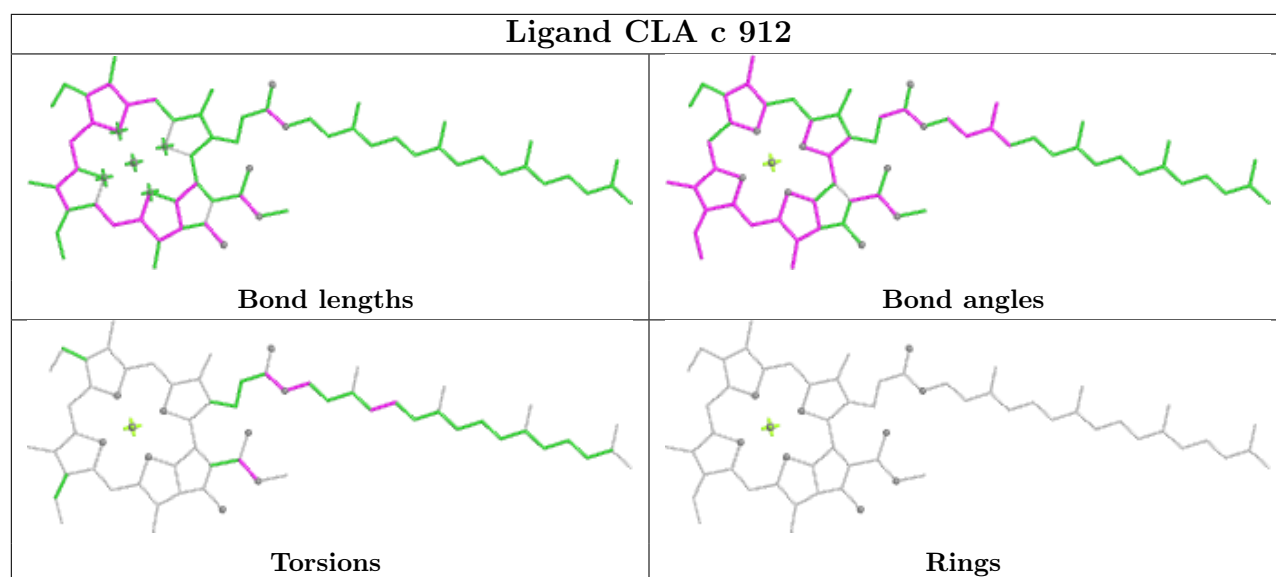


Ligand HTG d 414

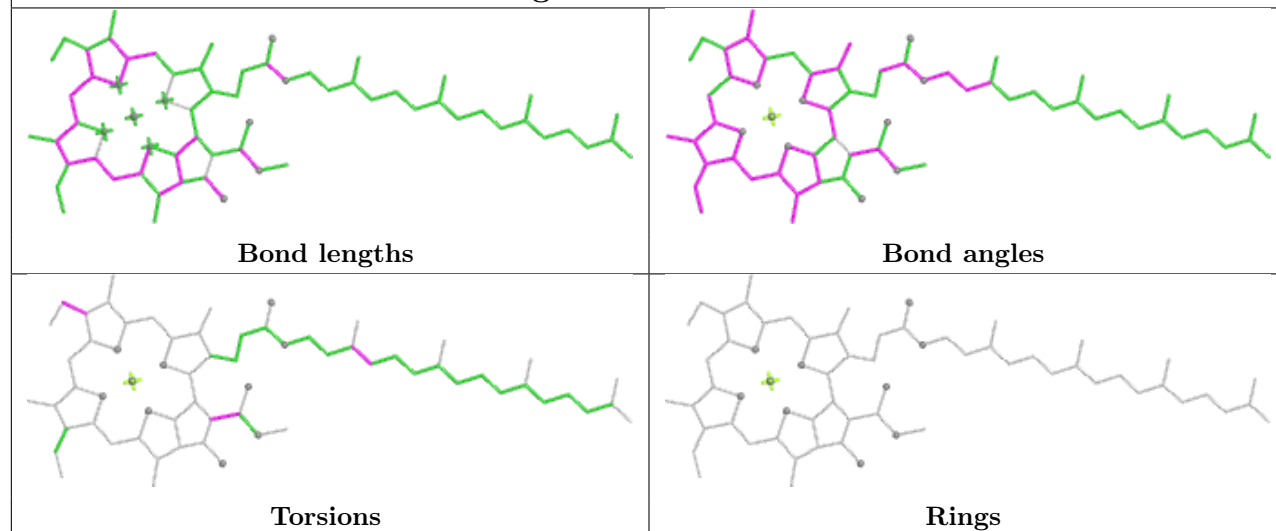


Ligand BCR H 101

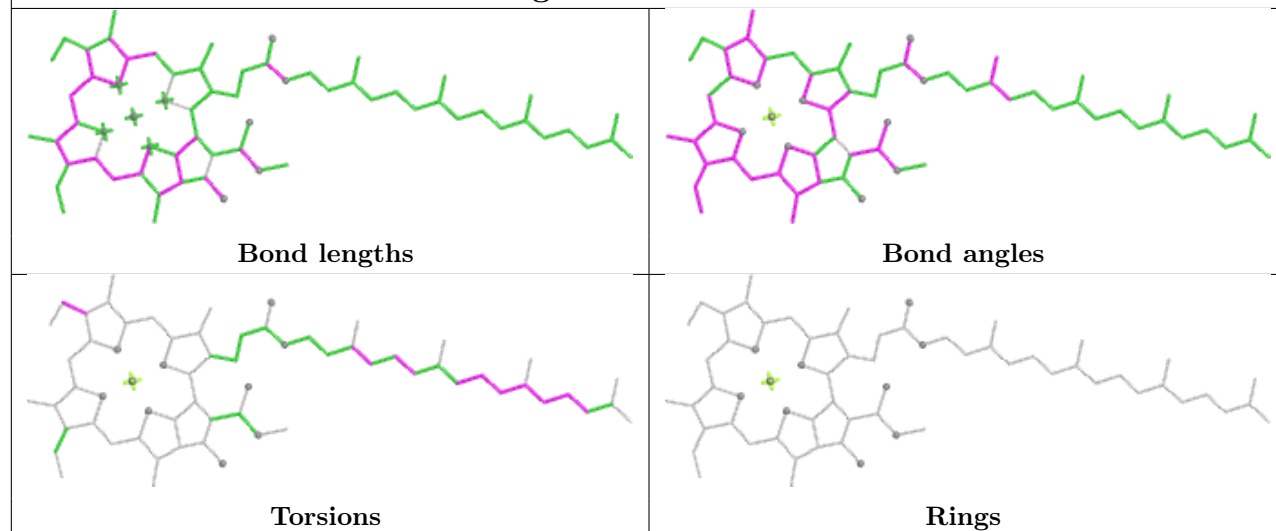




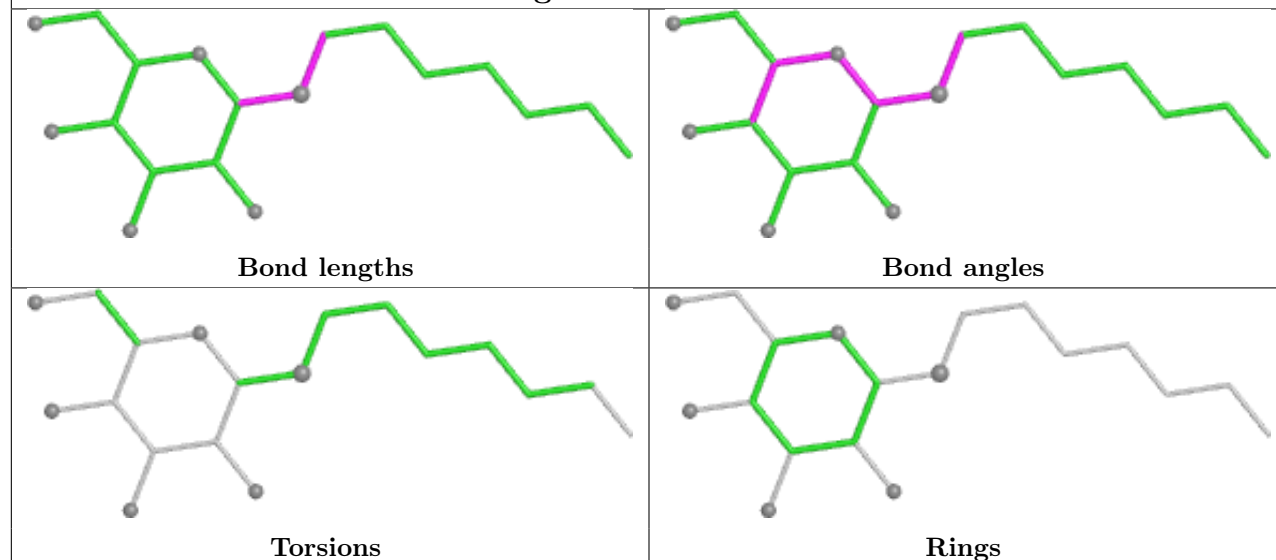
Ligand CLA B 610

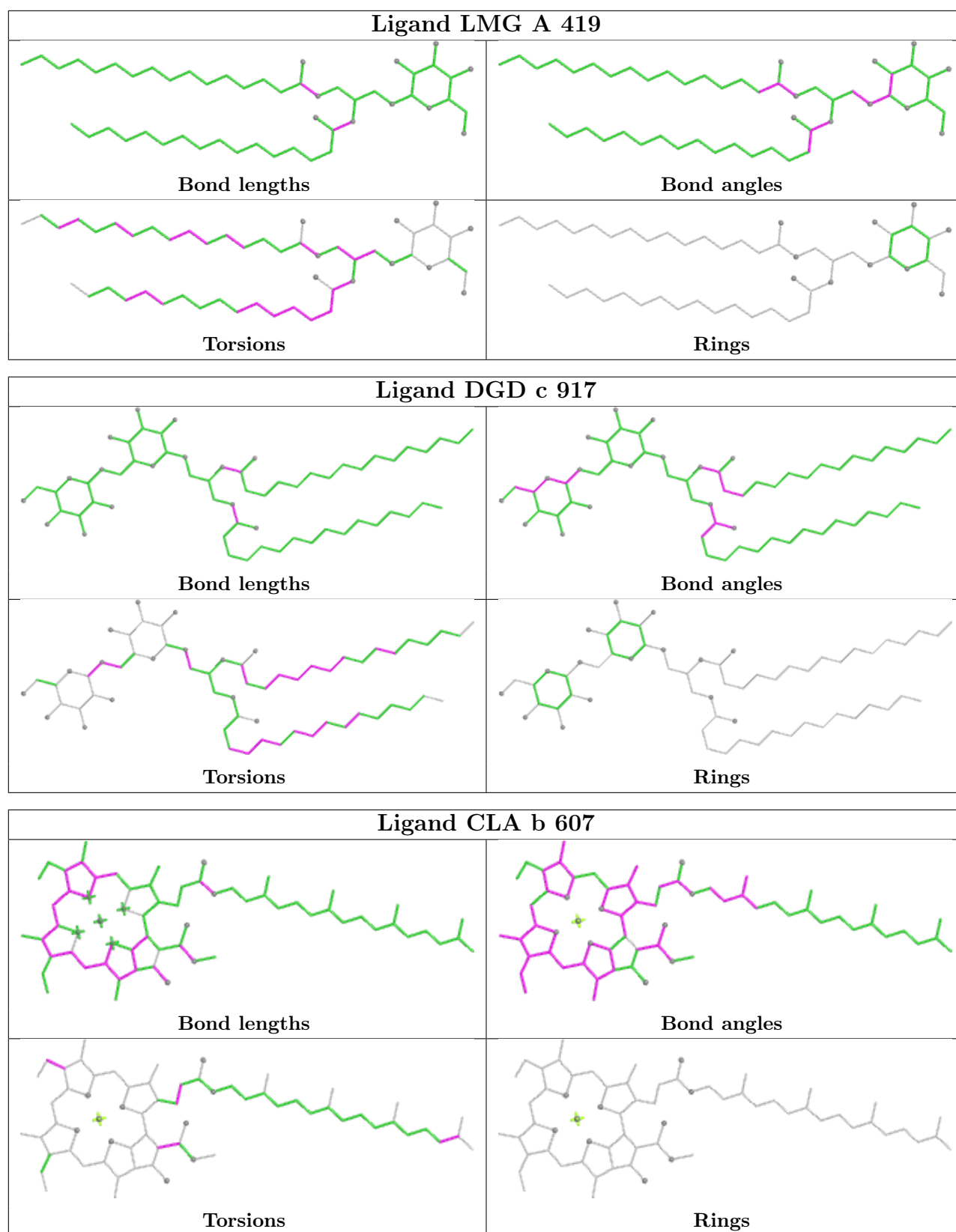


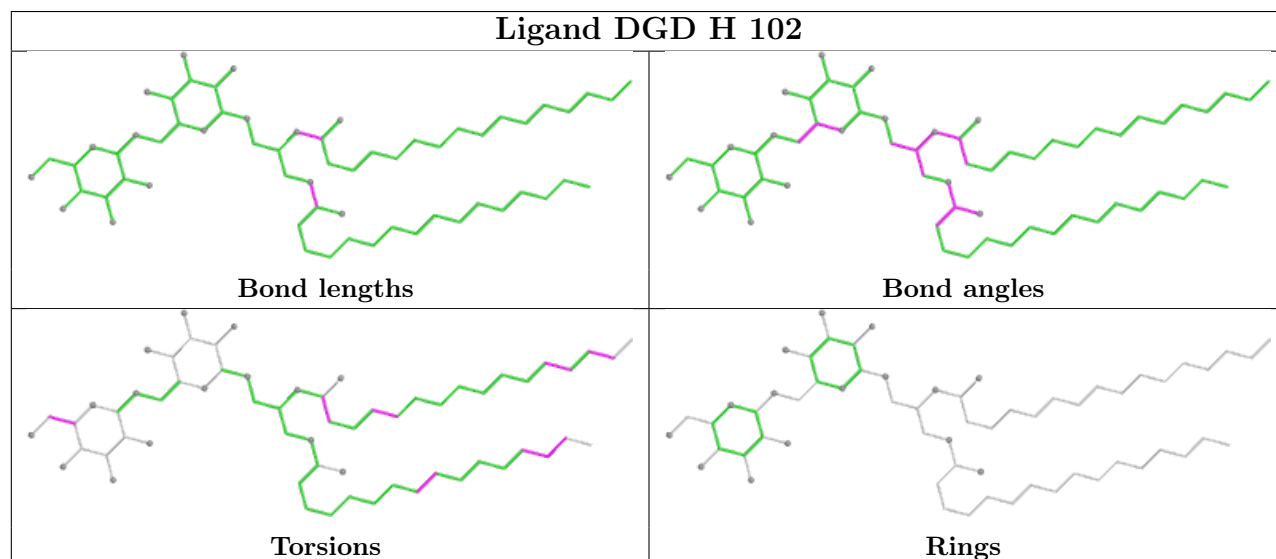
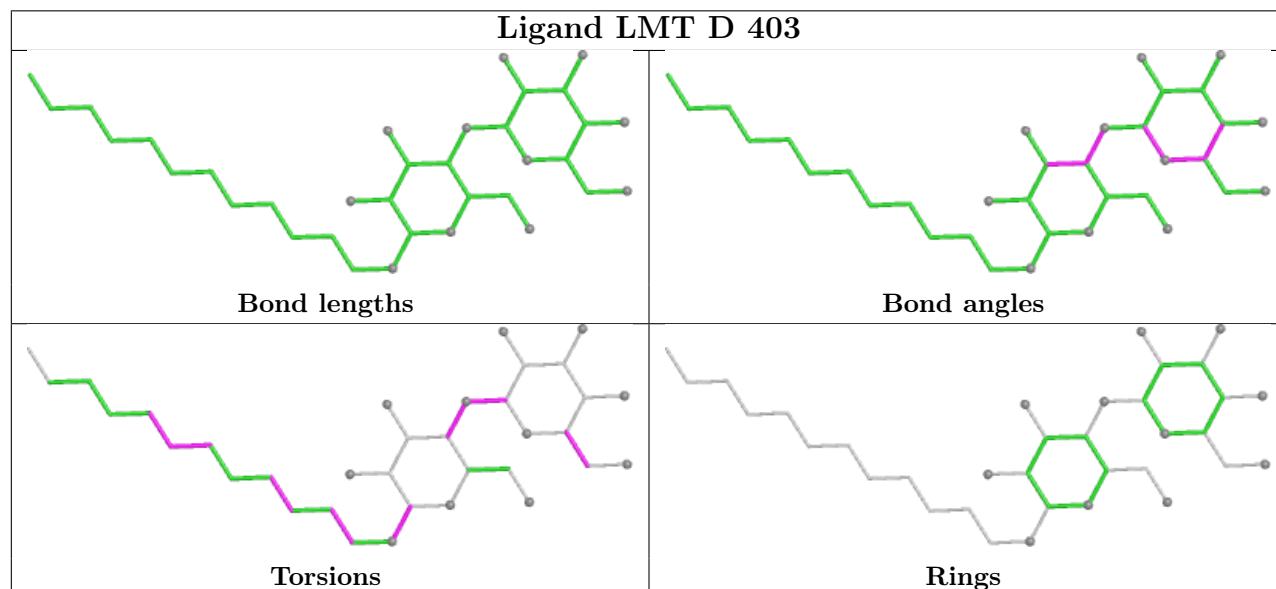
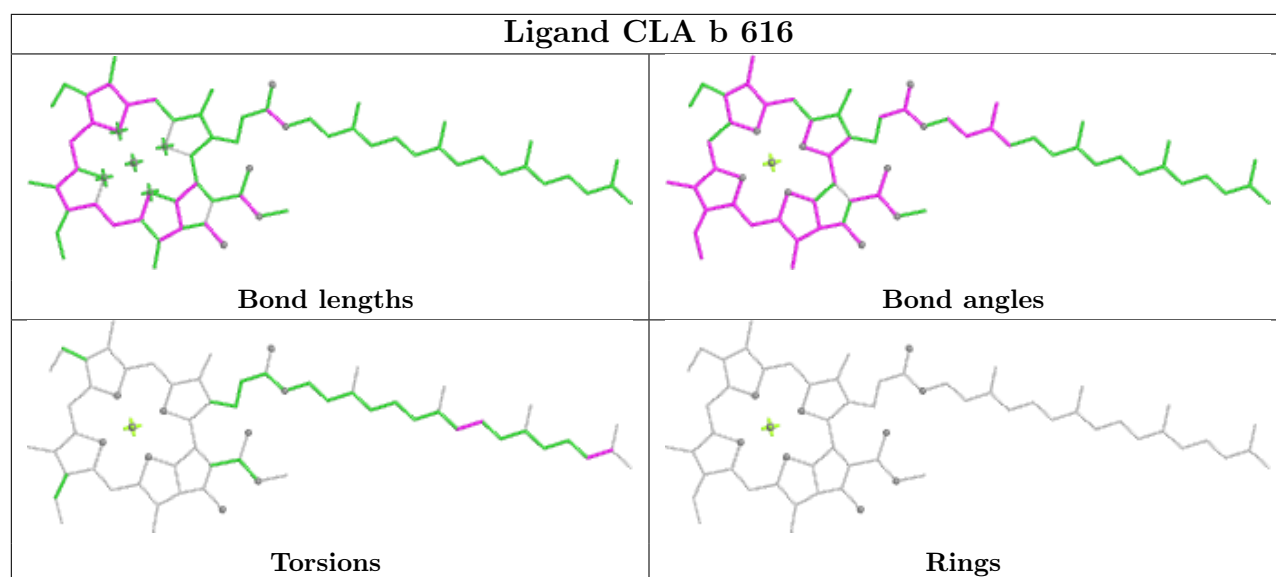
Ligand CLA B 616

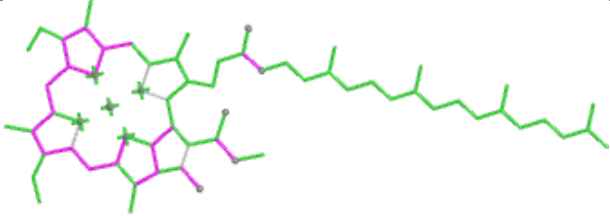
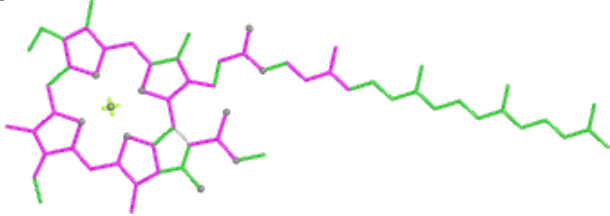
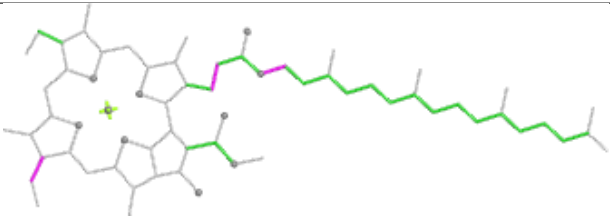
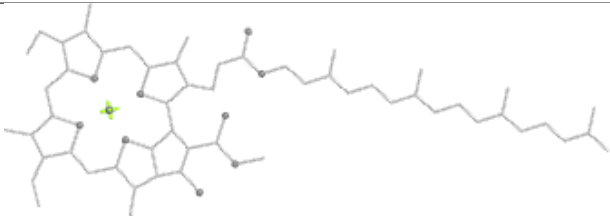
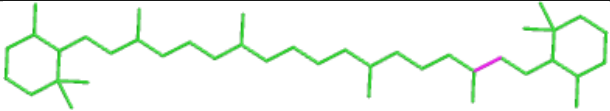
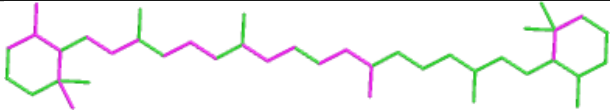
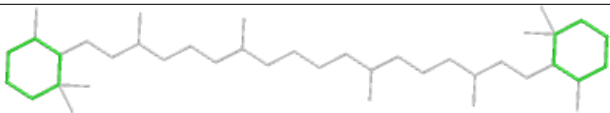
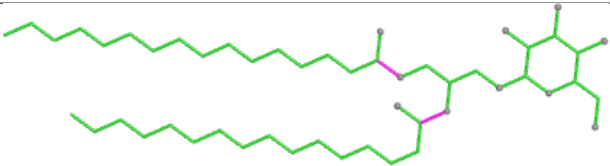
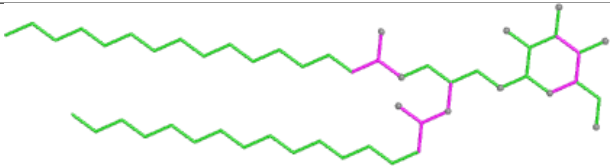
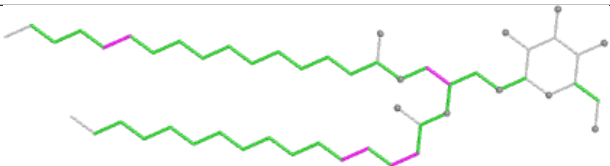
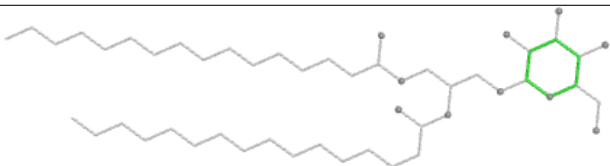


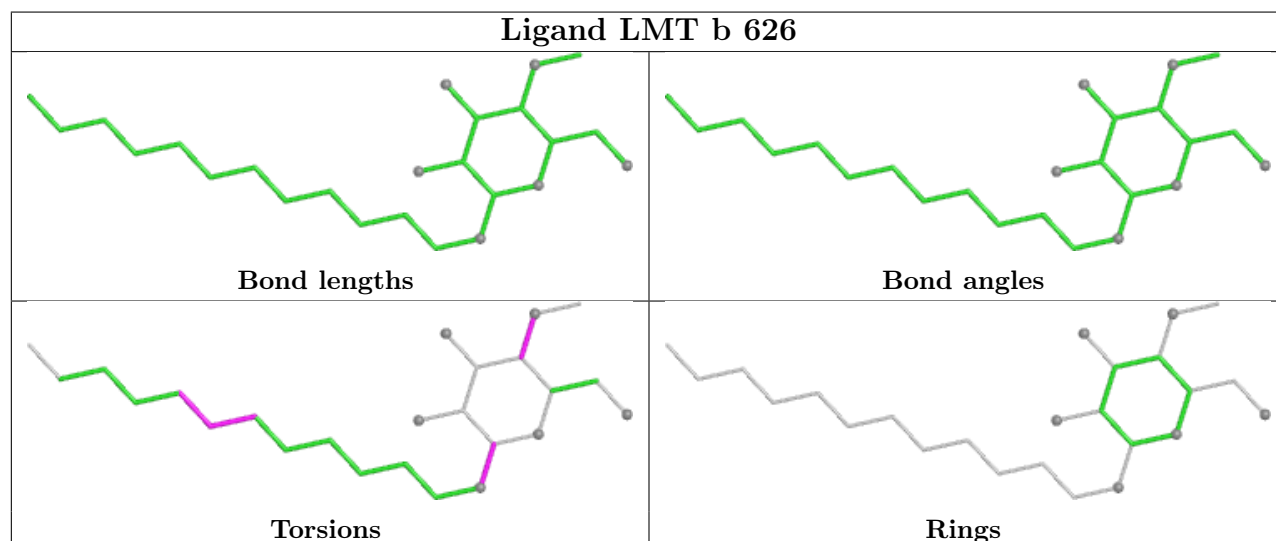
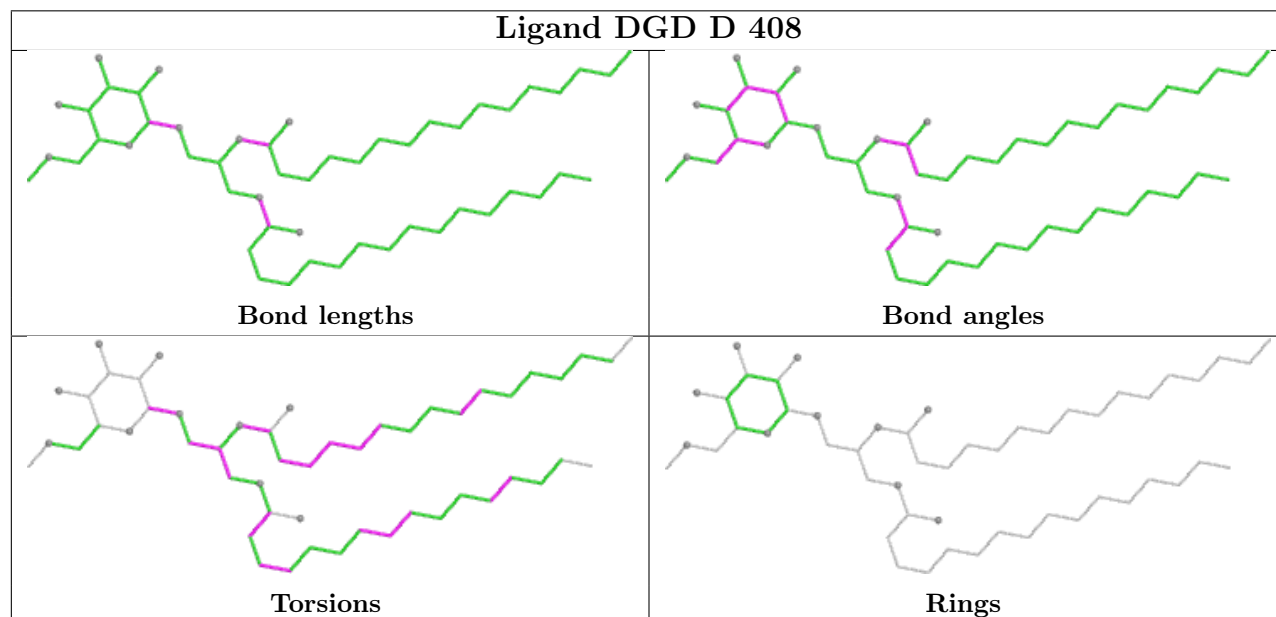
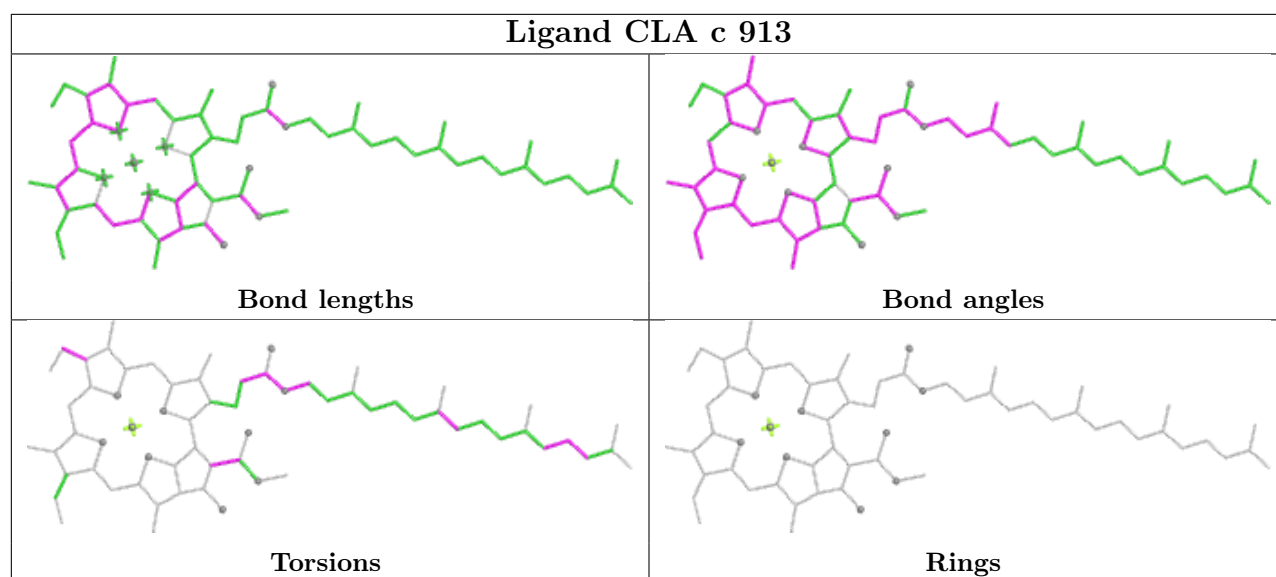
Ligand HTG c 922

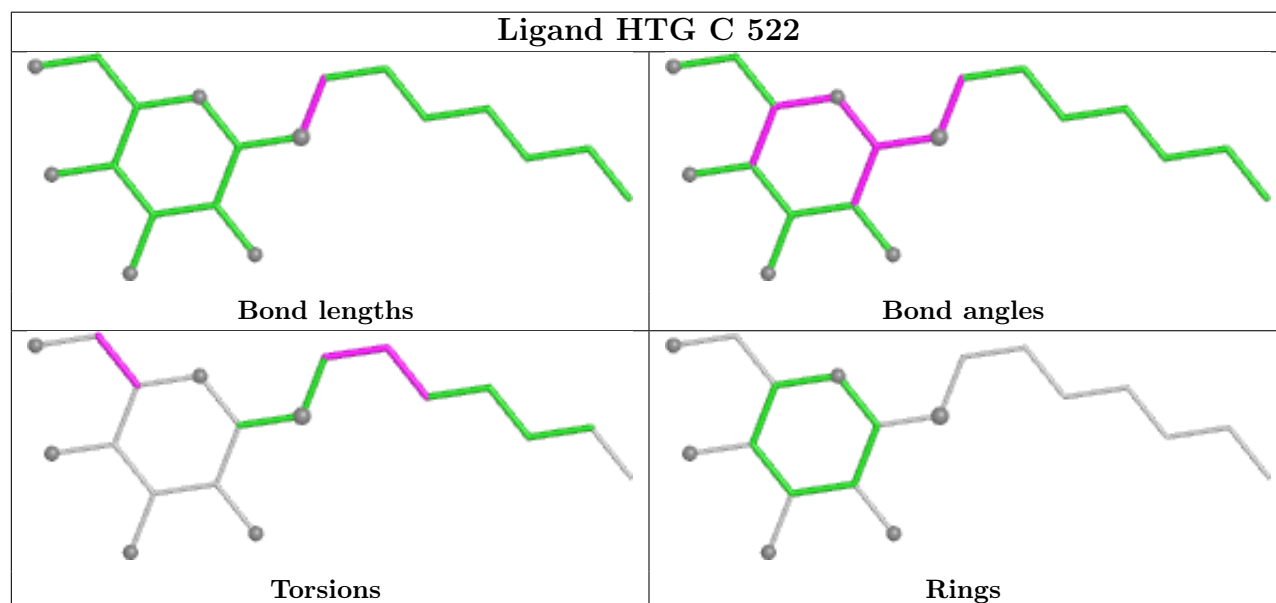
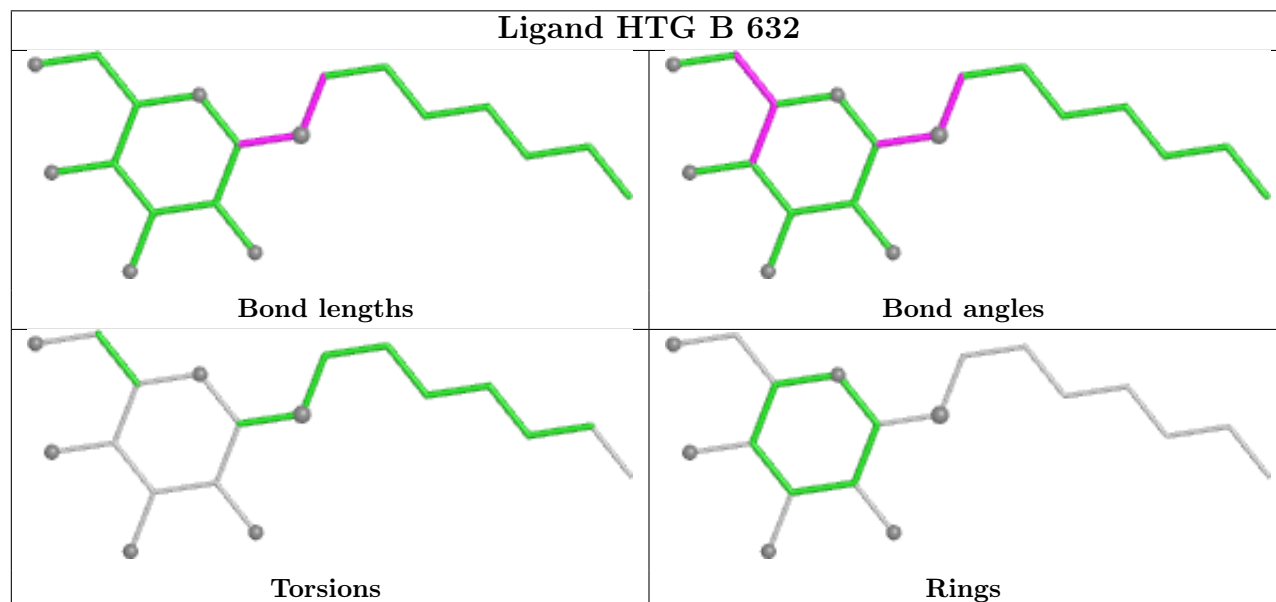
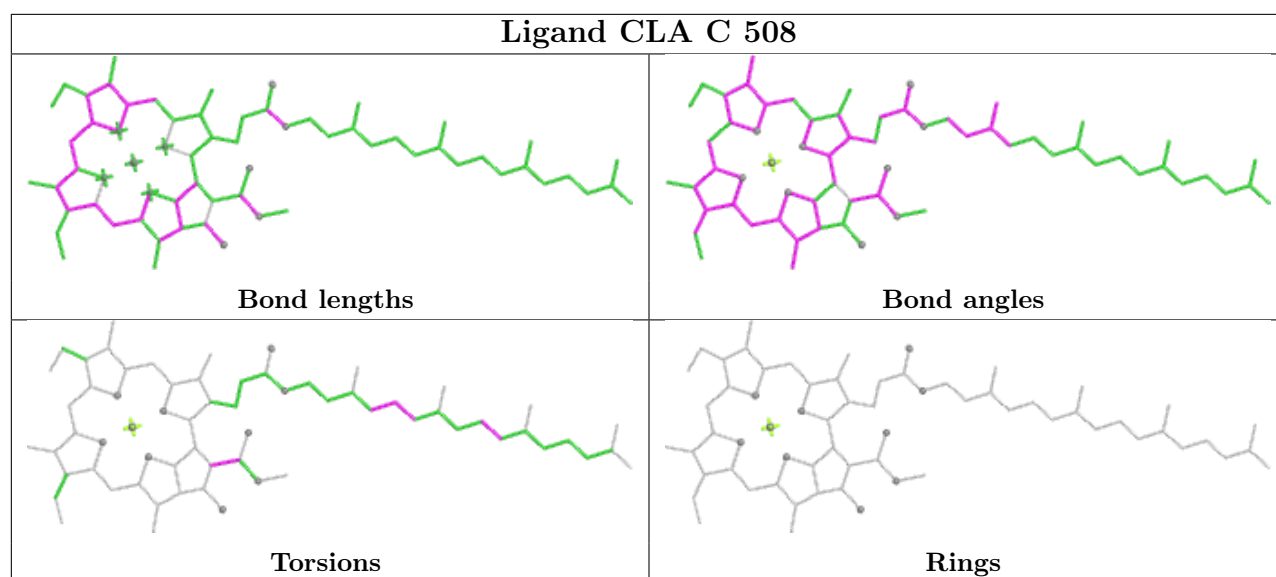


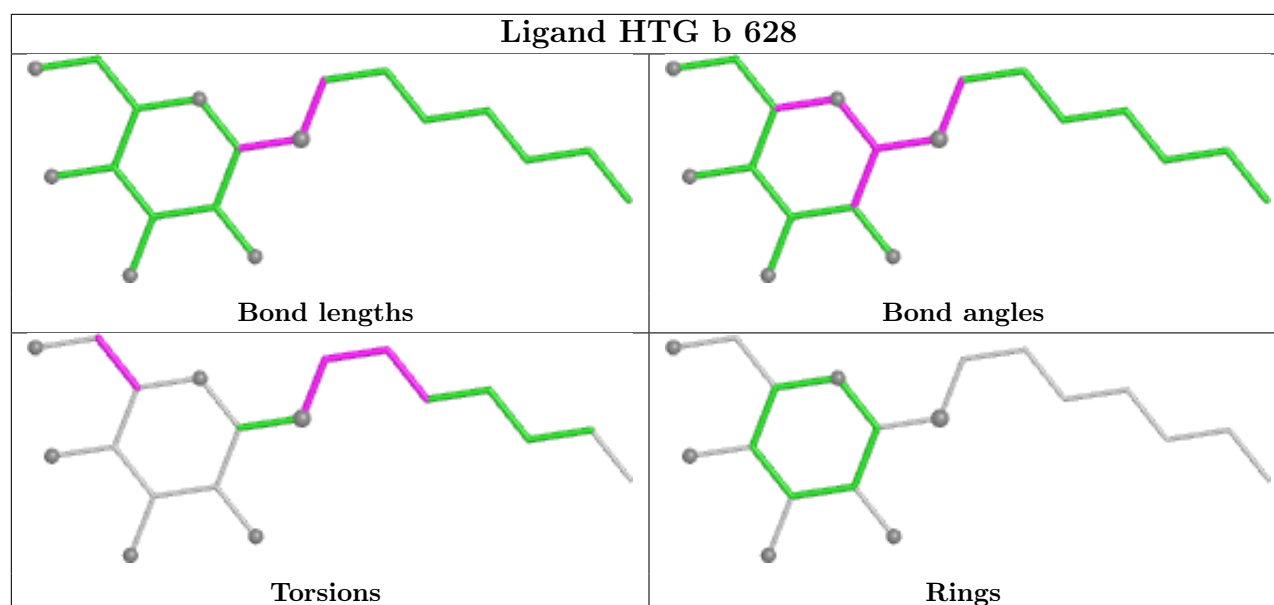
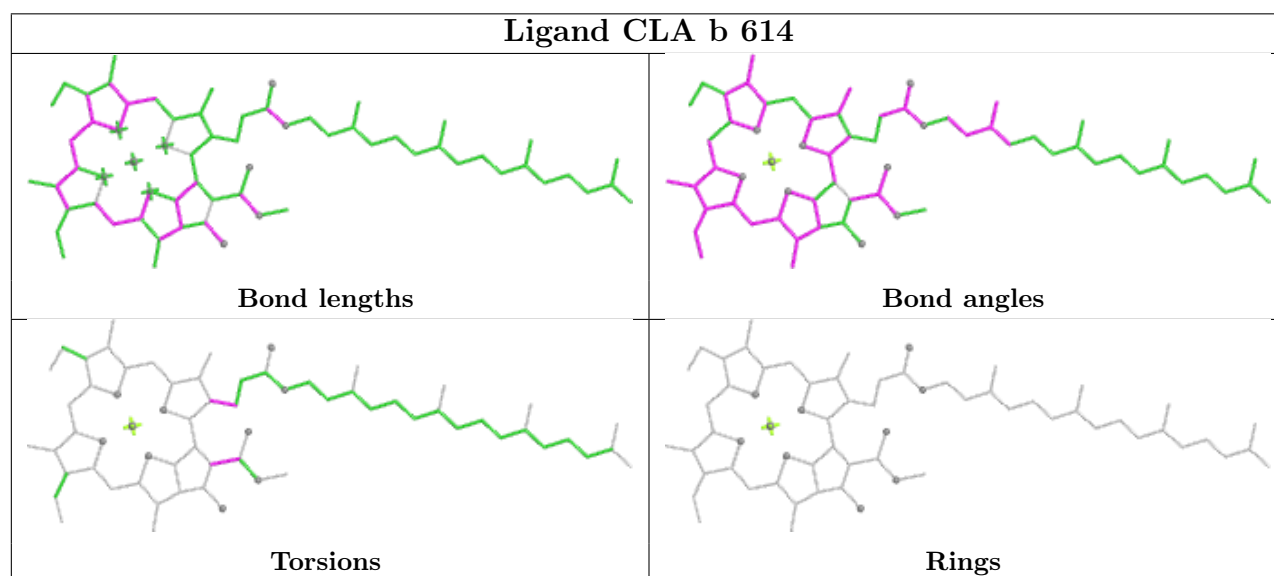
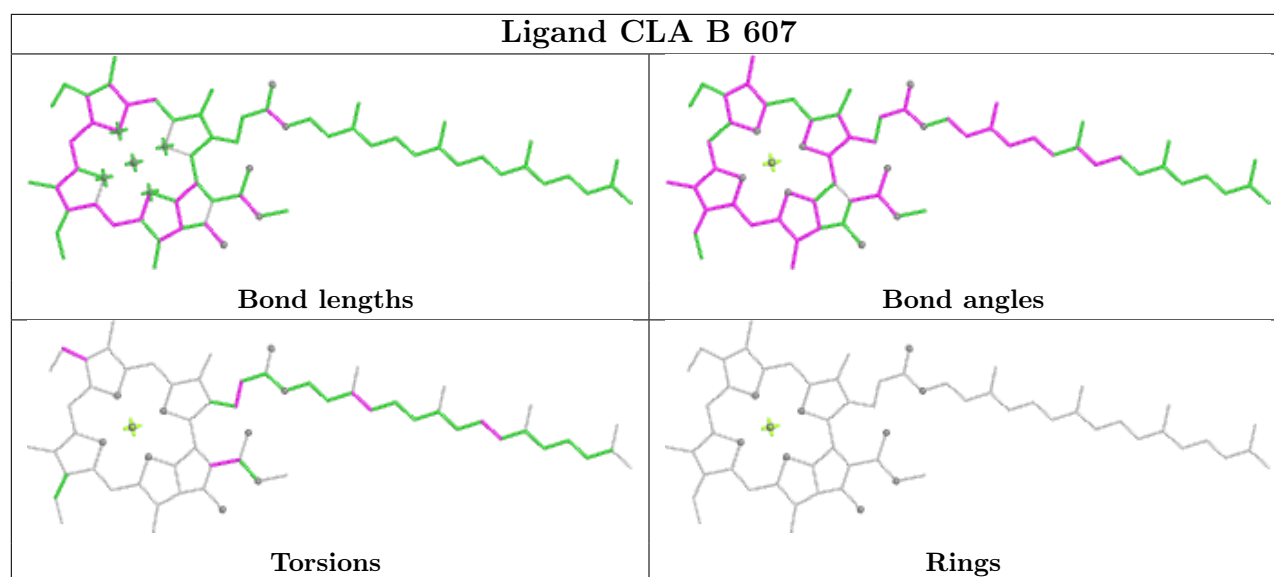




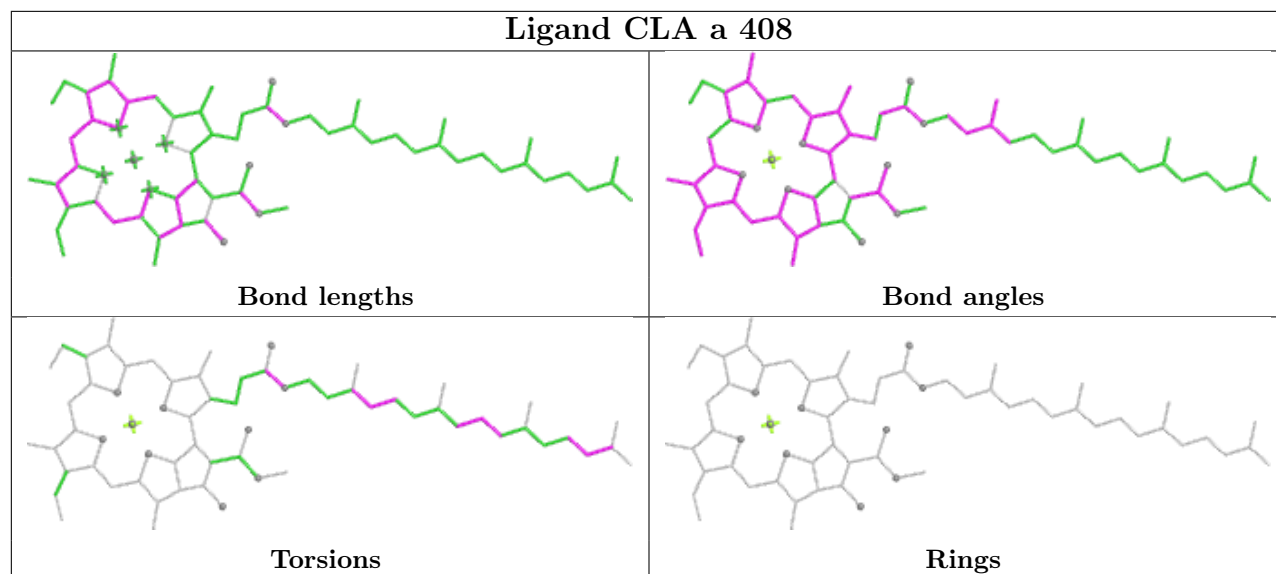
Ligand CLA a 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 622	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG c 920	
 Bond lengths	 Bond angles
 Torsions	 Rings



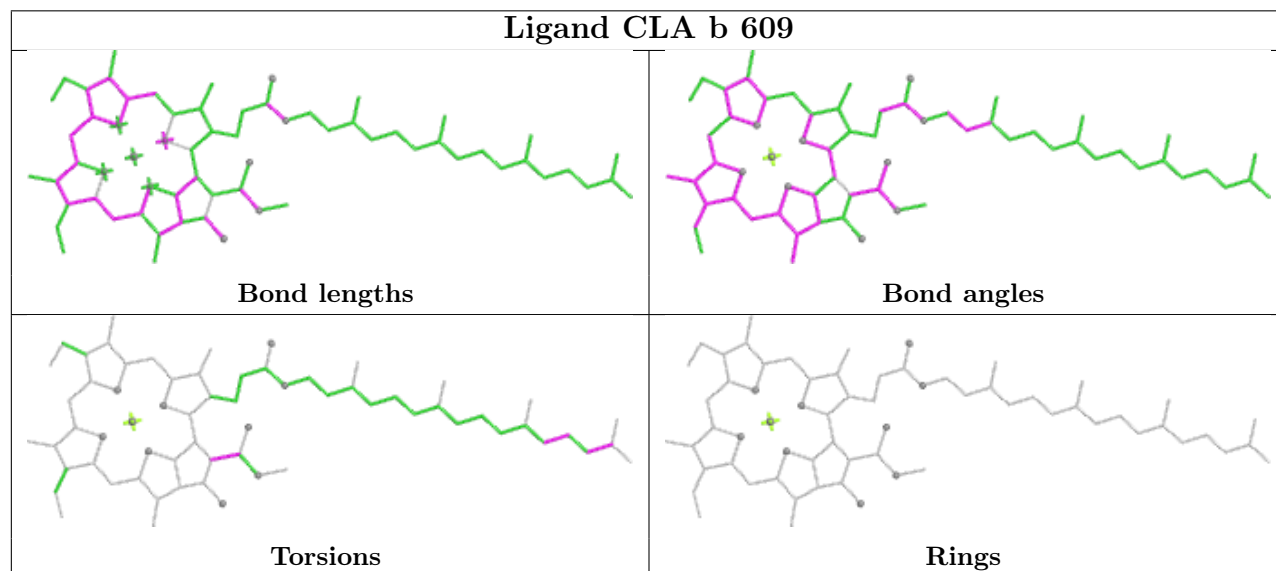




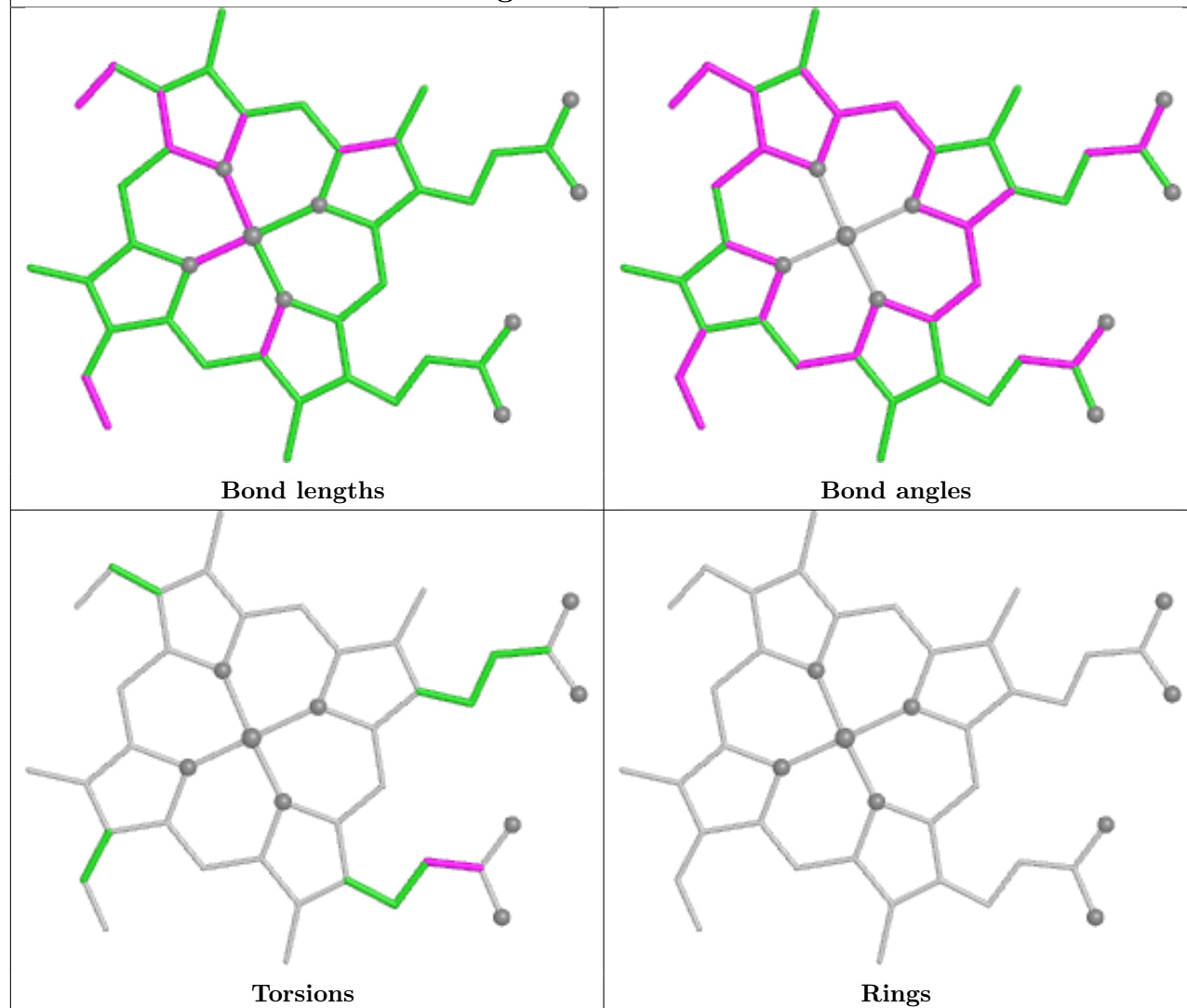
Ligand CLA a 408



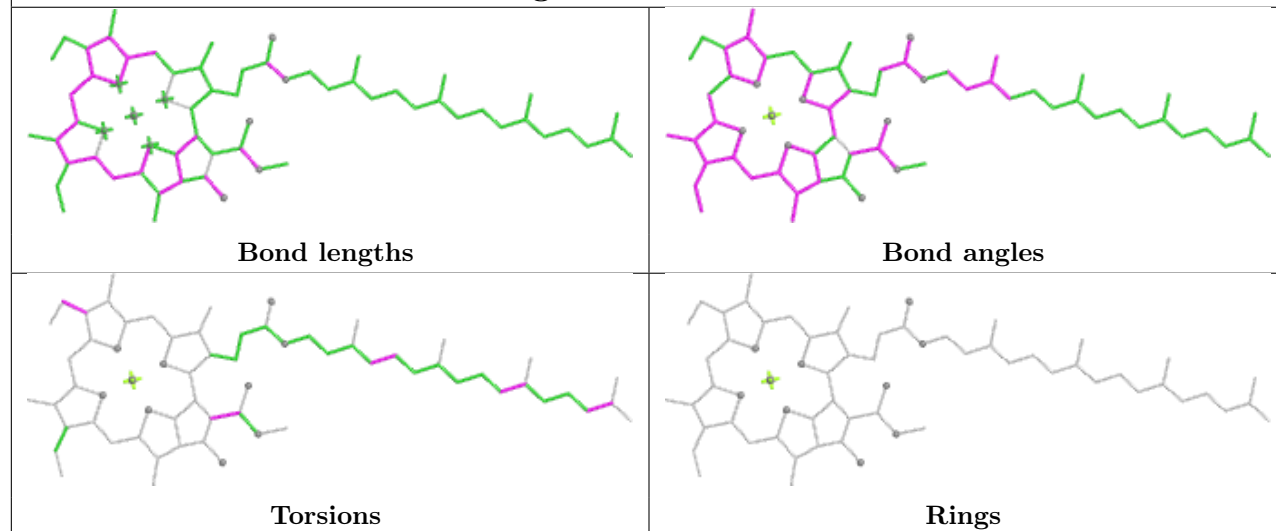
Ligand CLA b 609

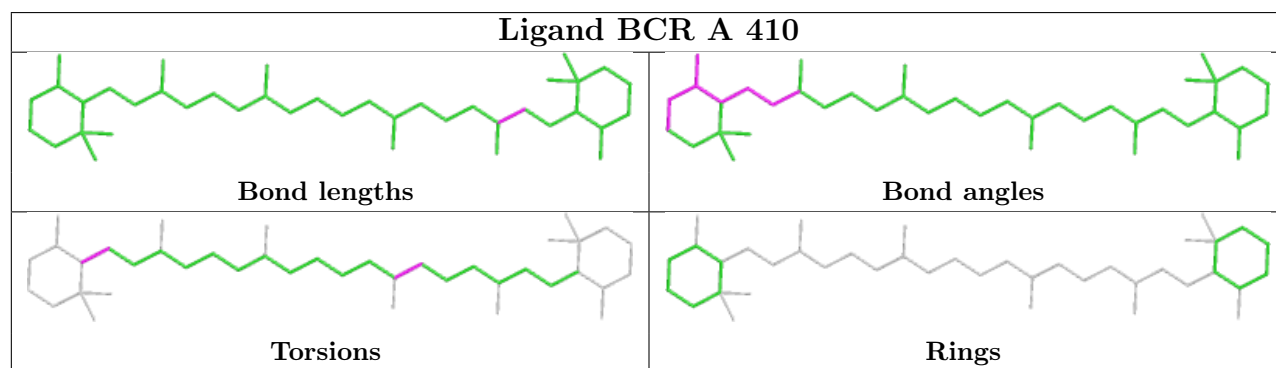
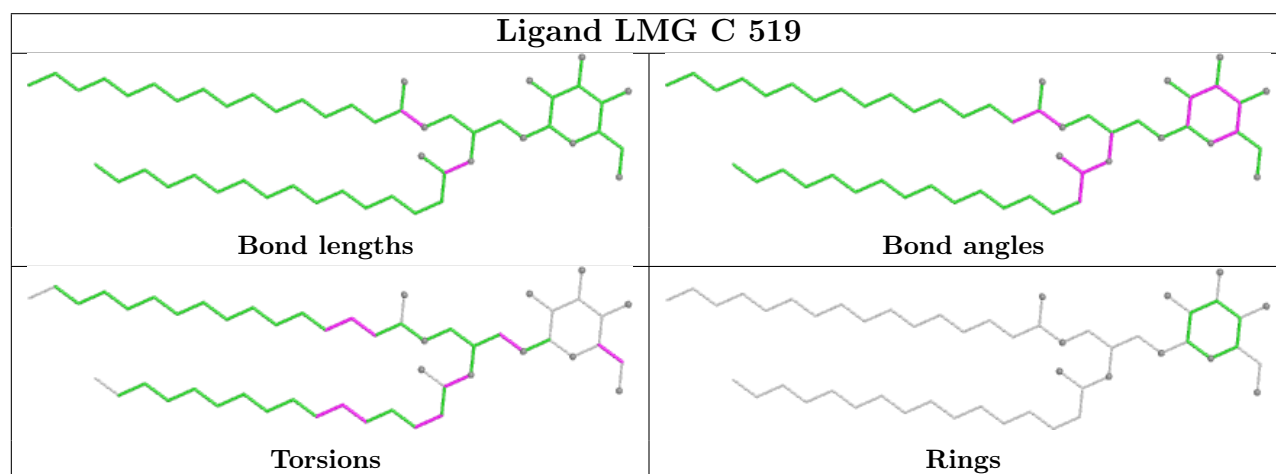
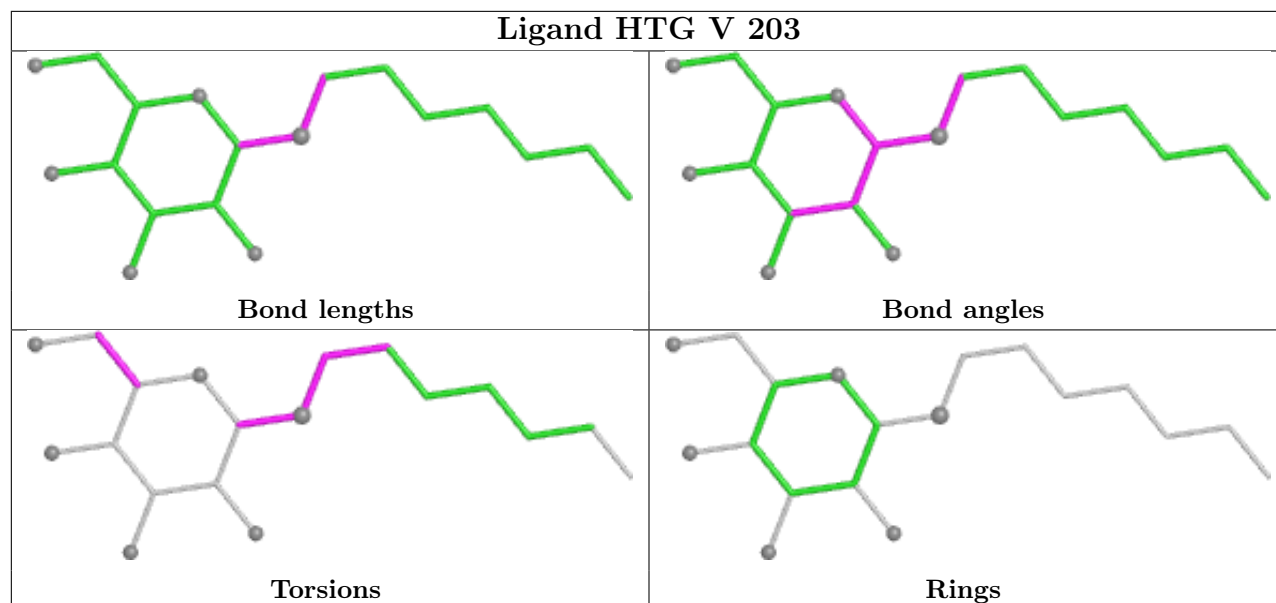


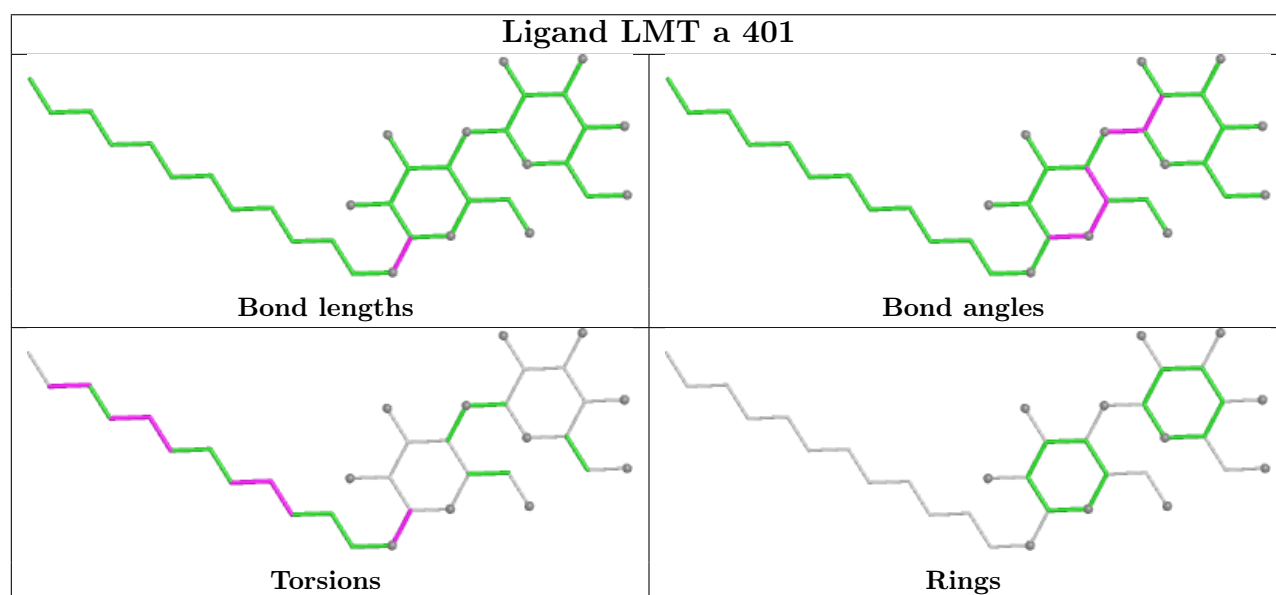
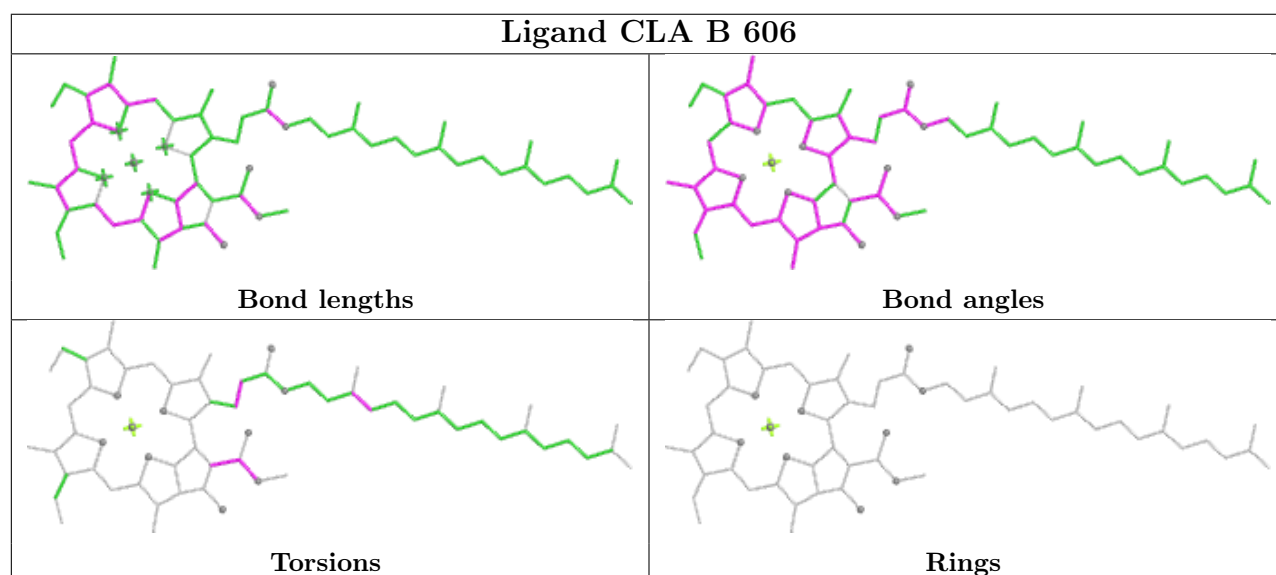
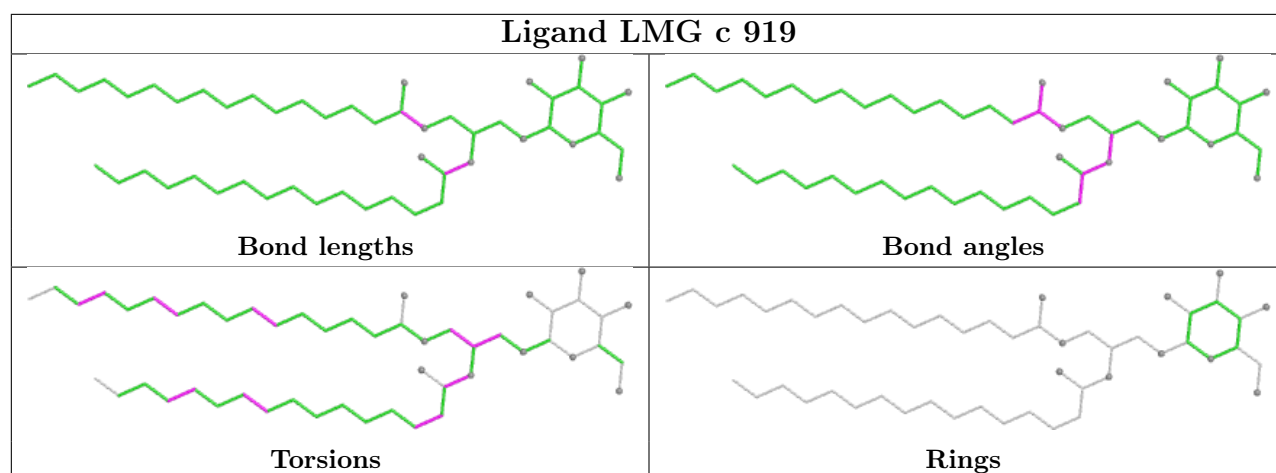
Ligand HEC v 202

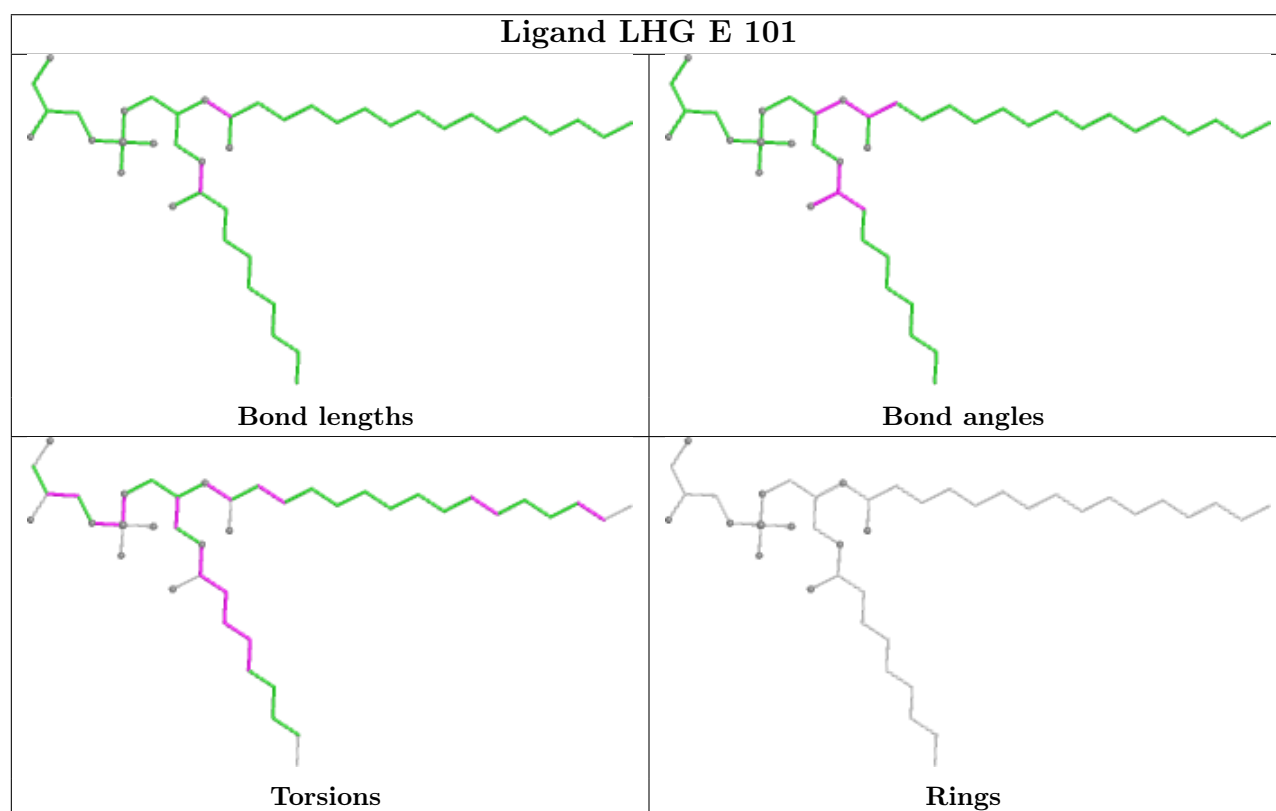
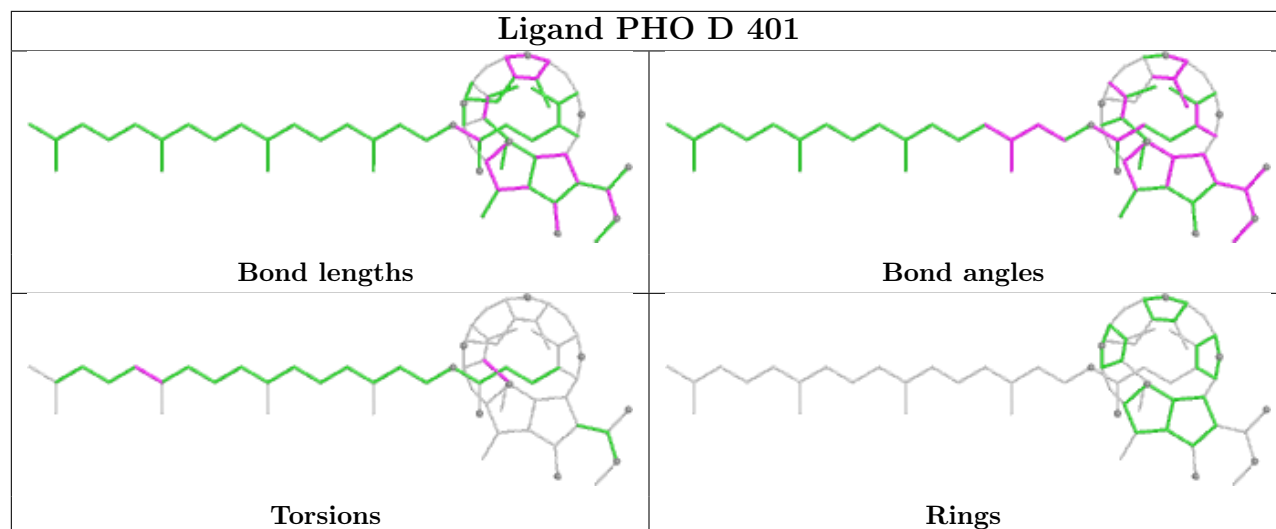


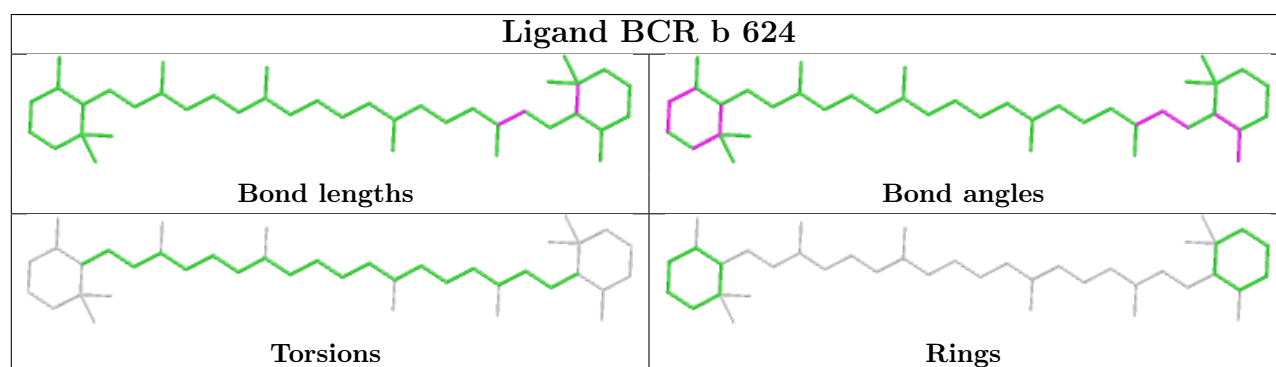
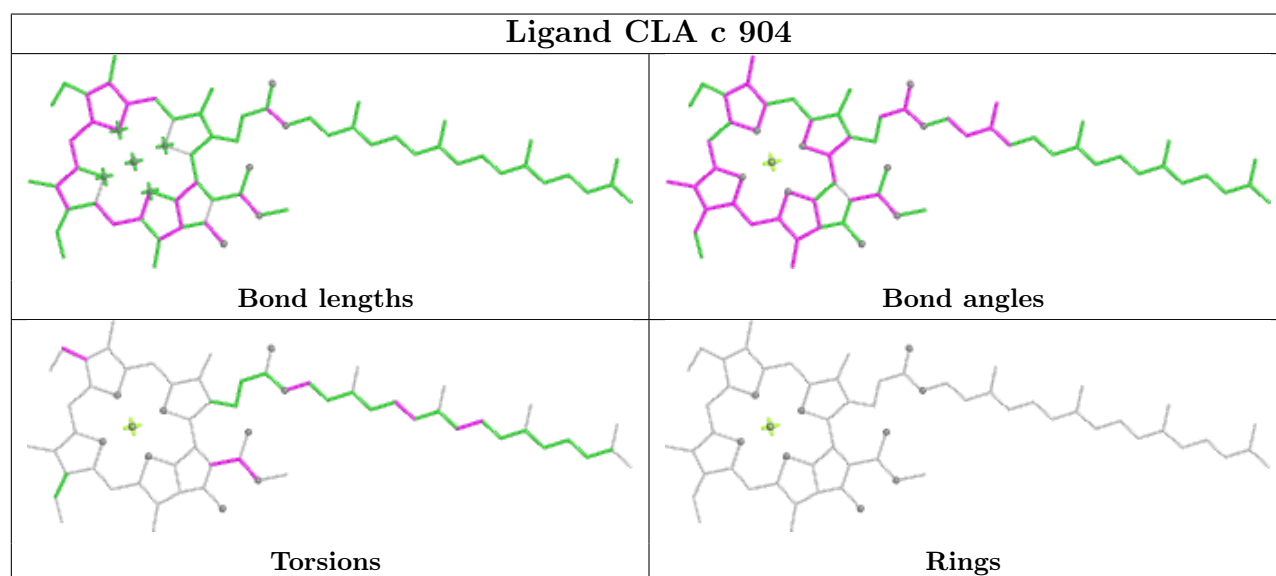
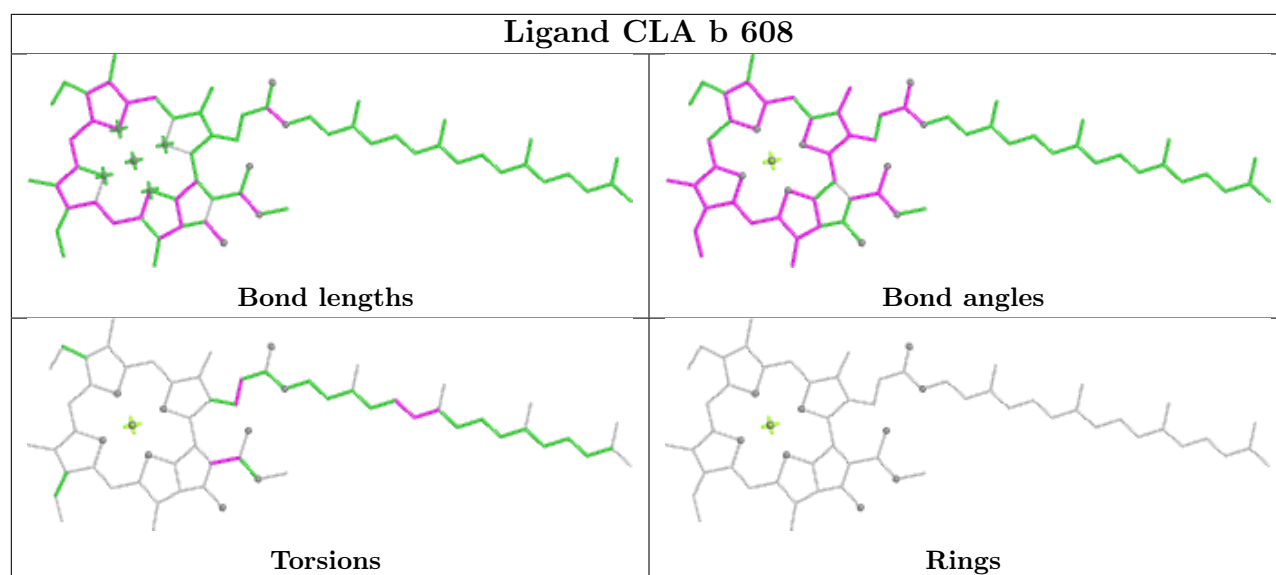
Ligand CLA C 502



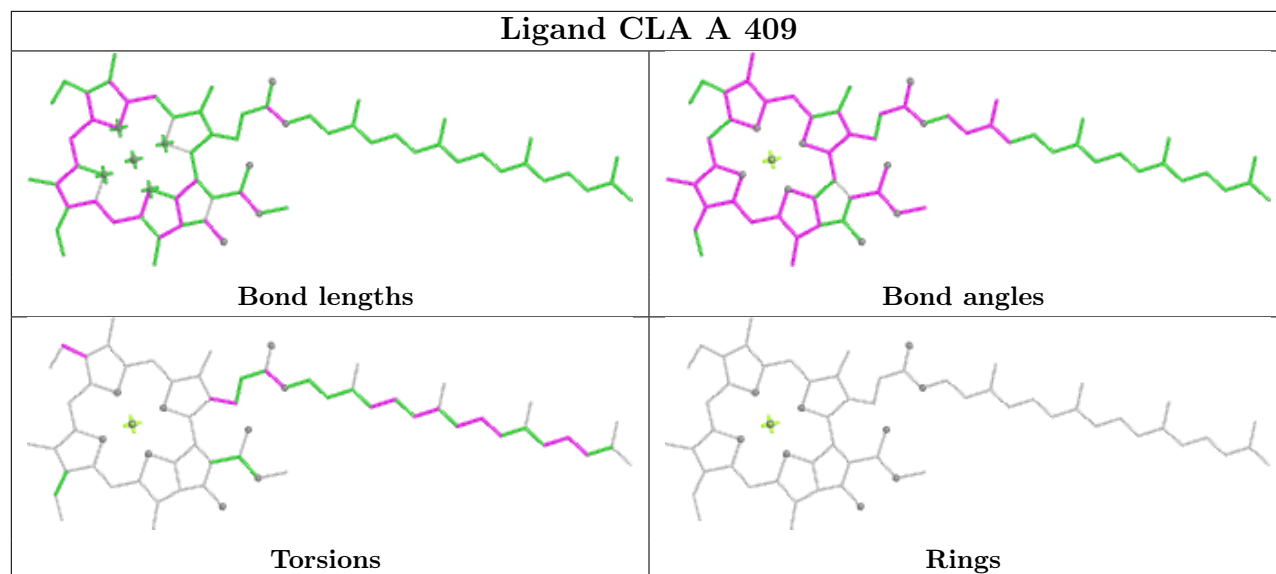




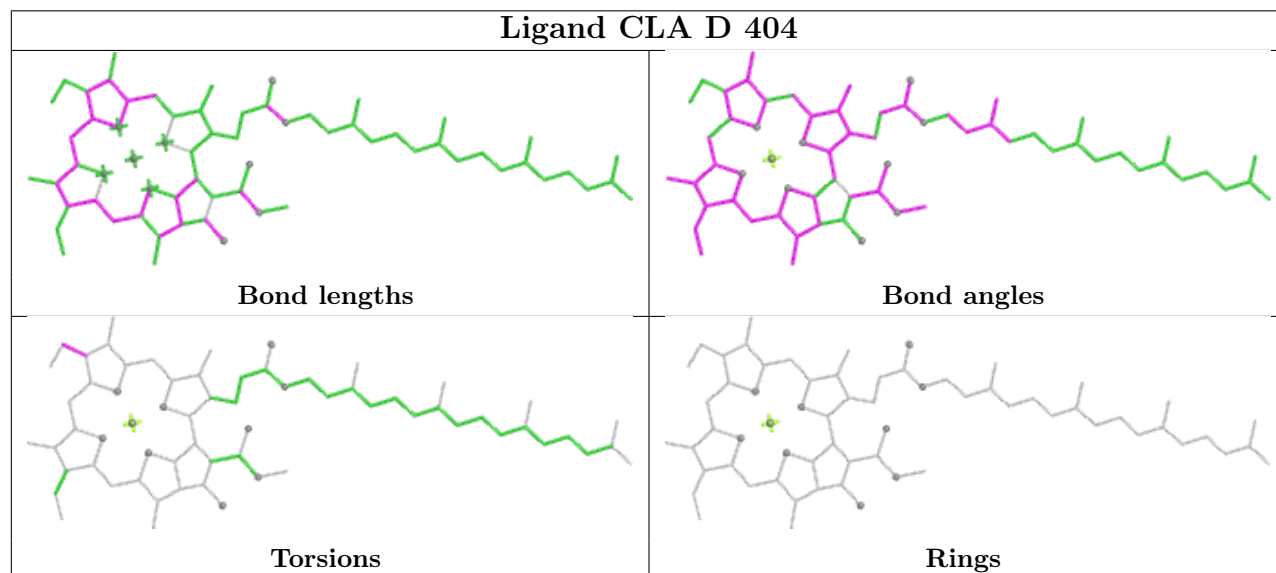


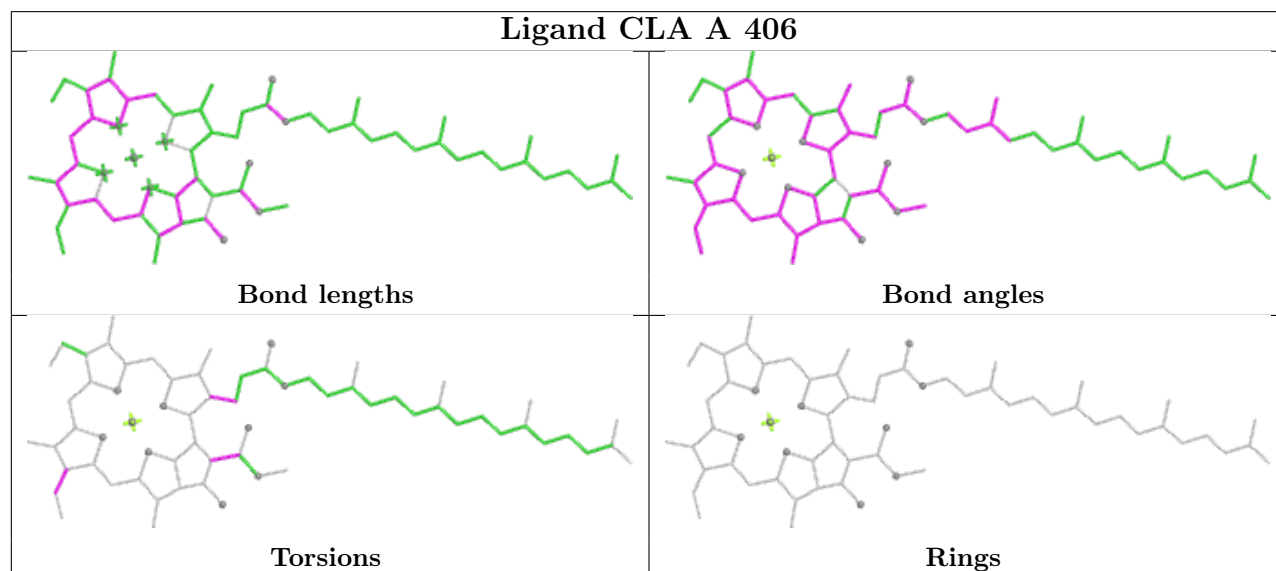
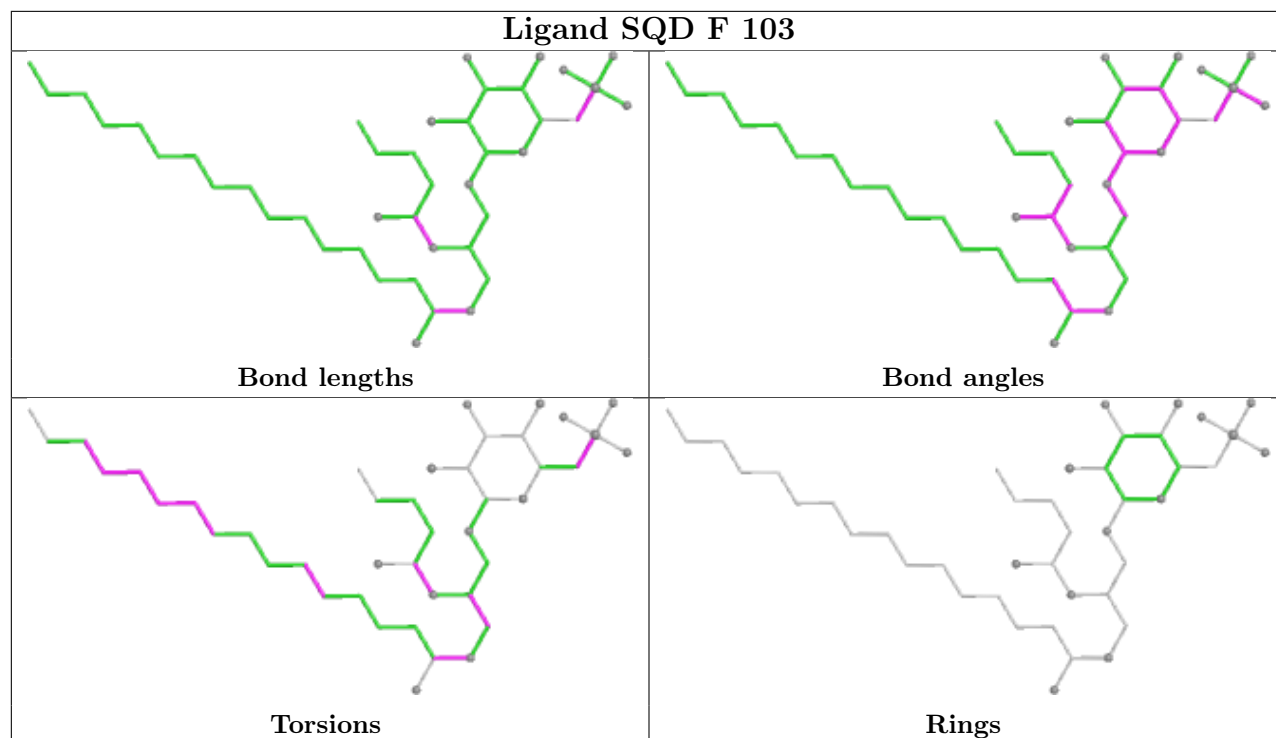


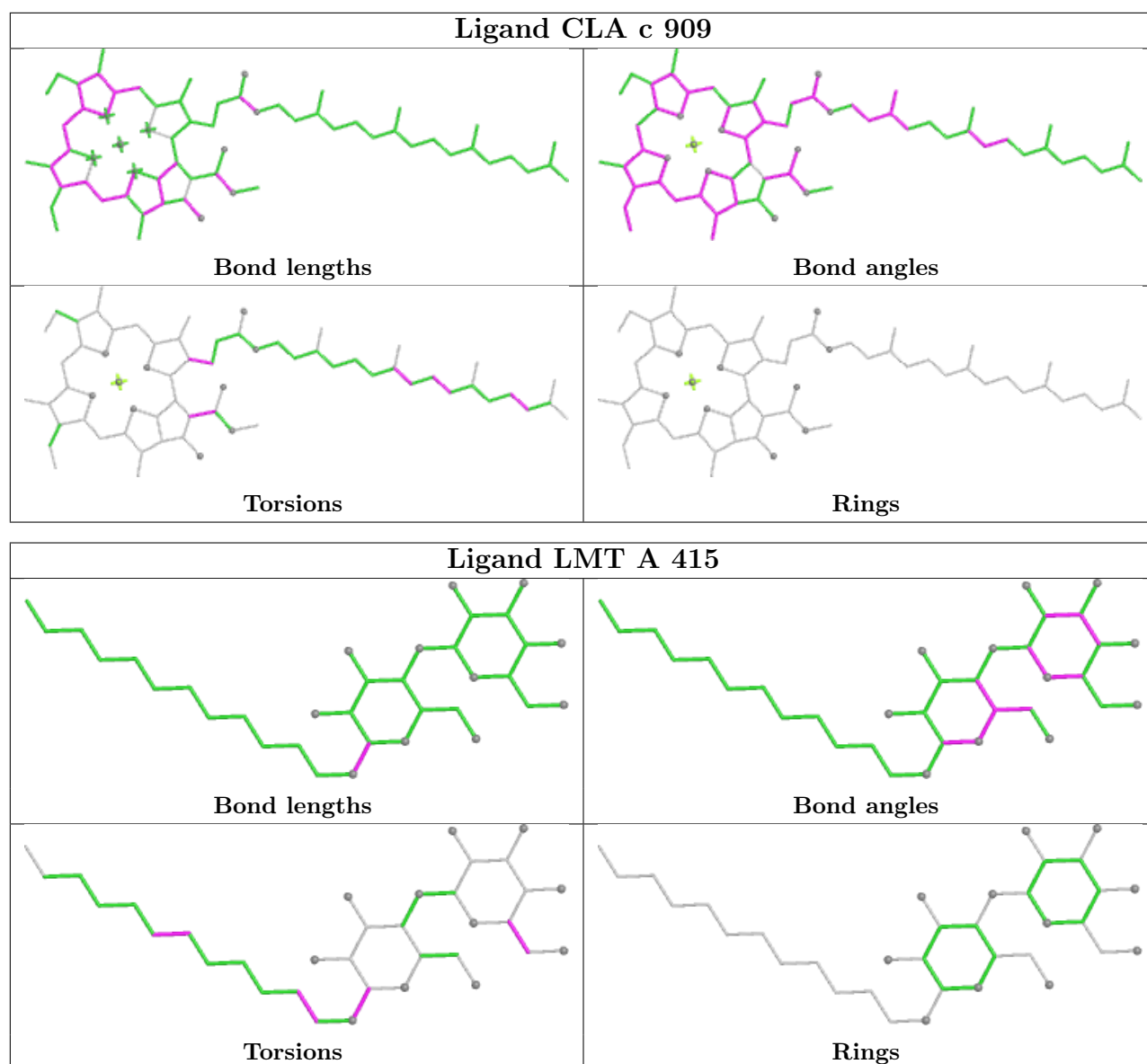
Ligand CLA A 409

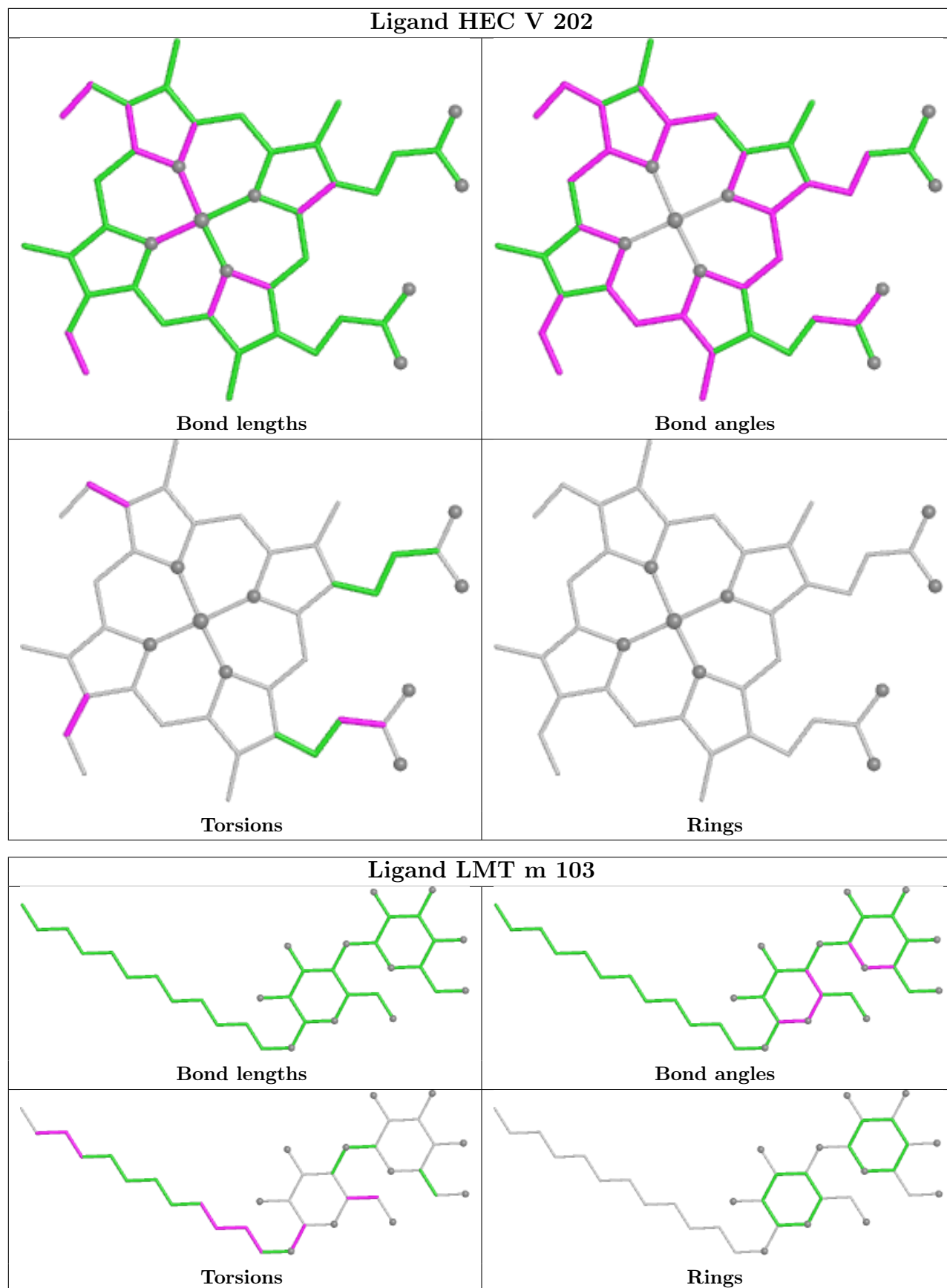


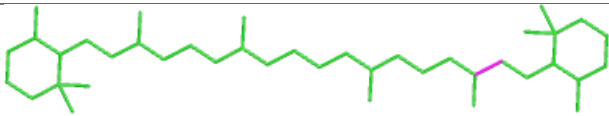
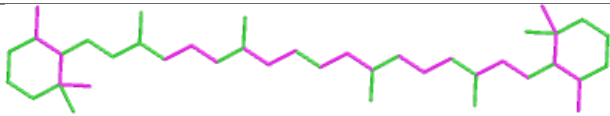
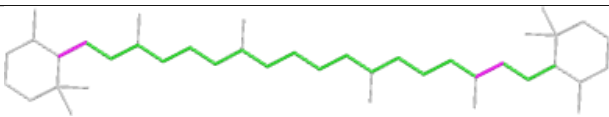
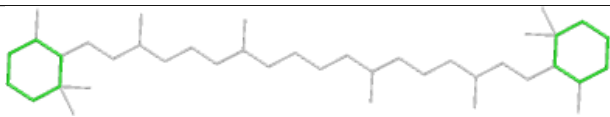
Ligand CLA D 404

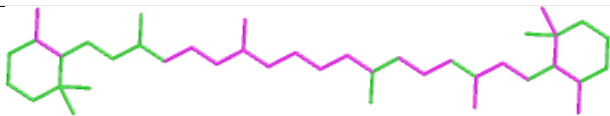
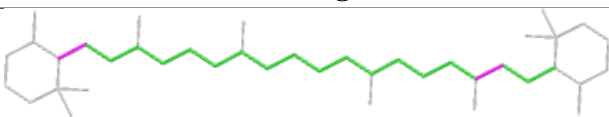
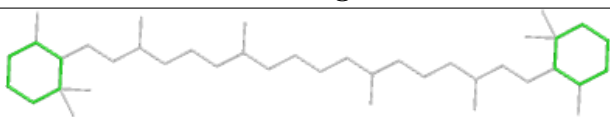


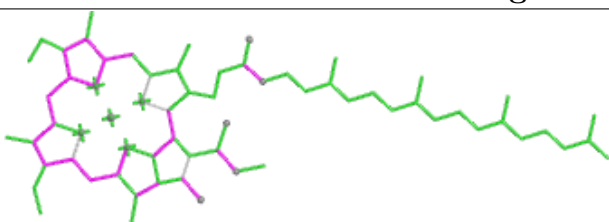
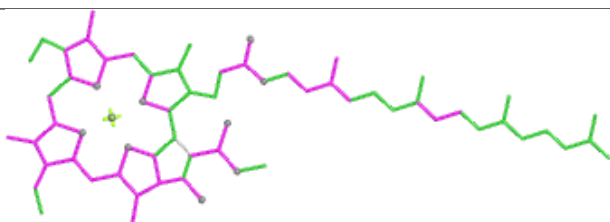
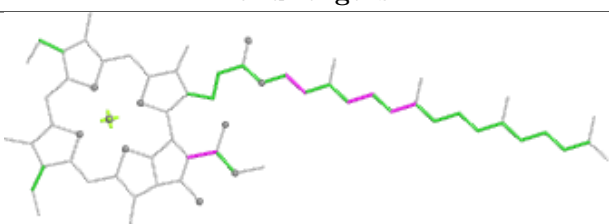
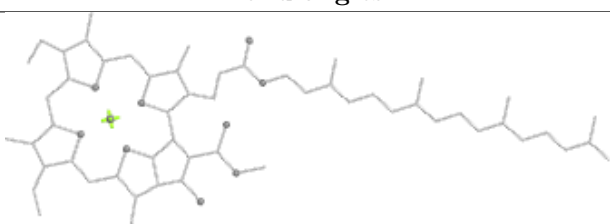


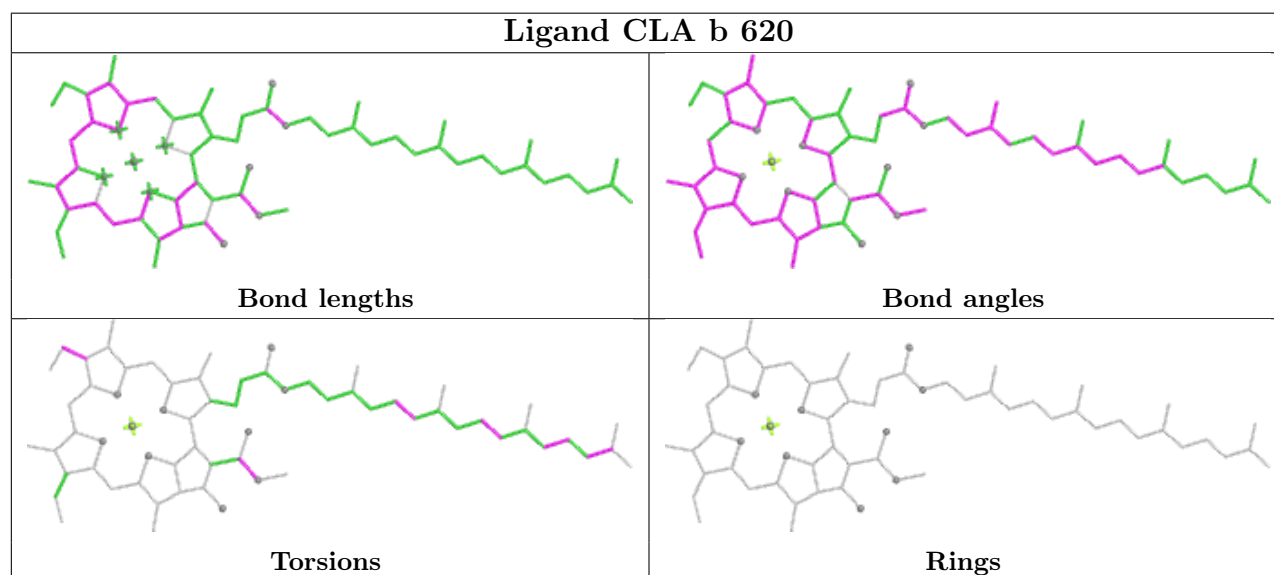
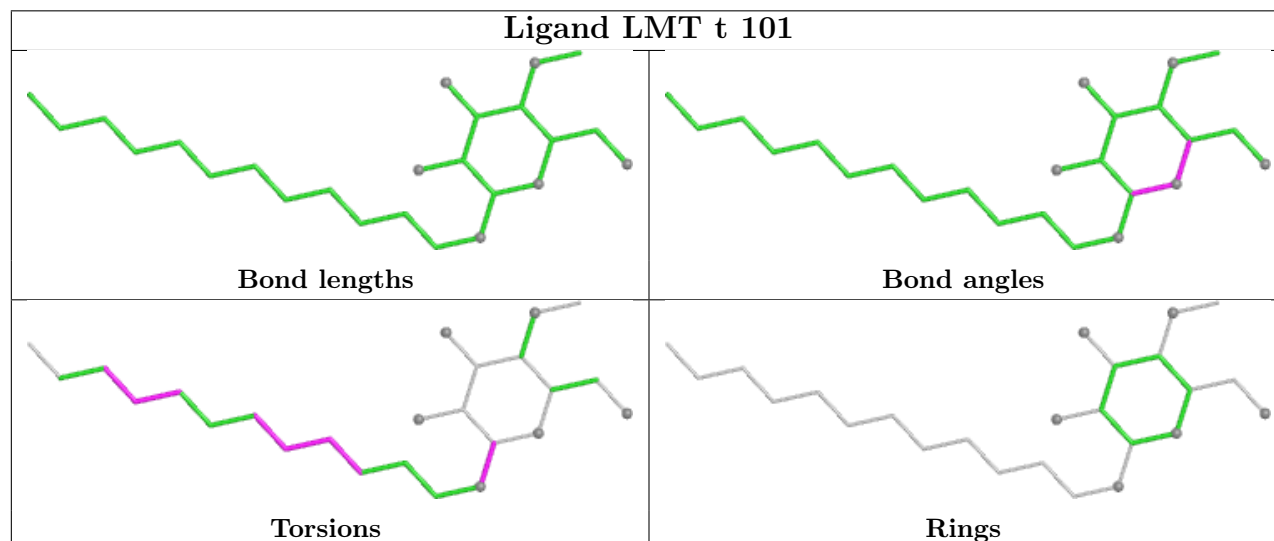
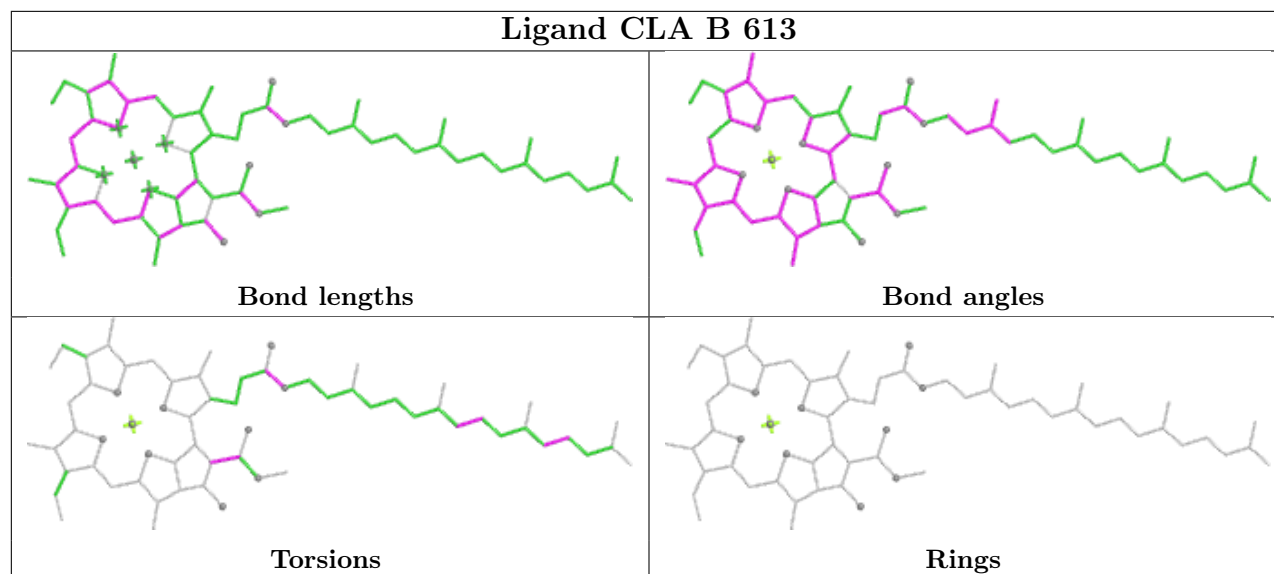


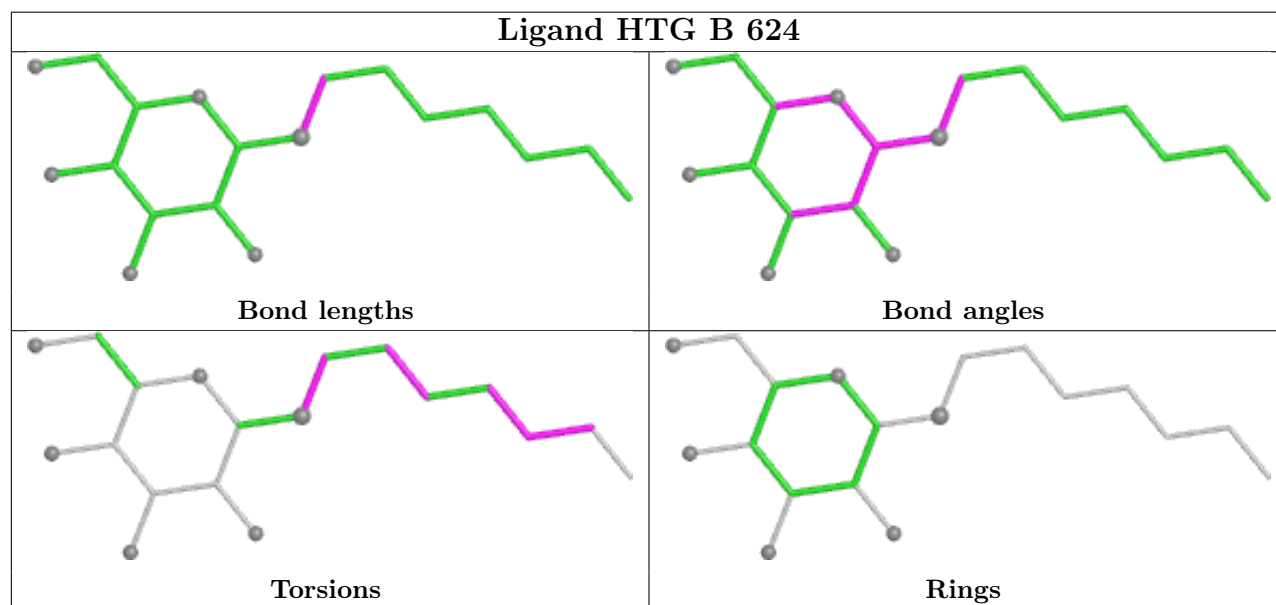
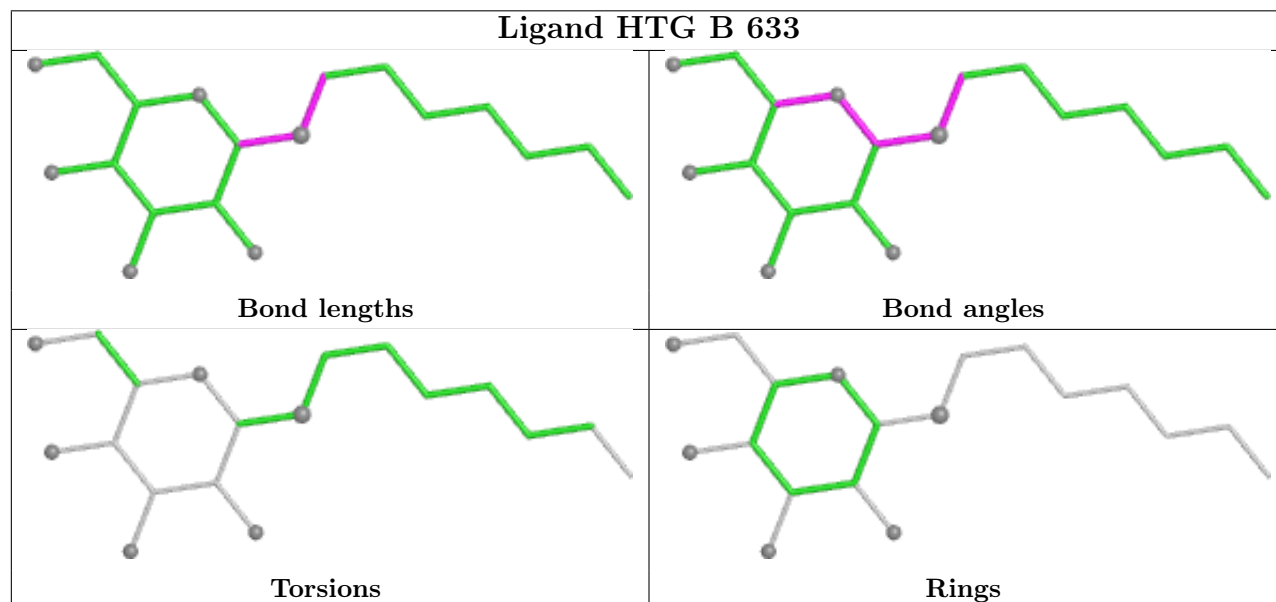
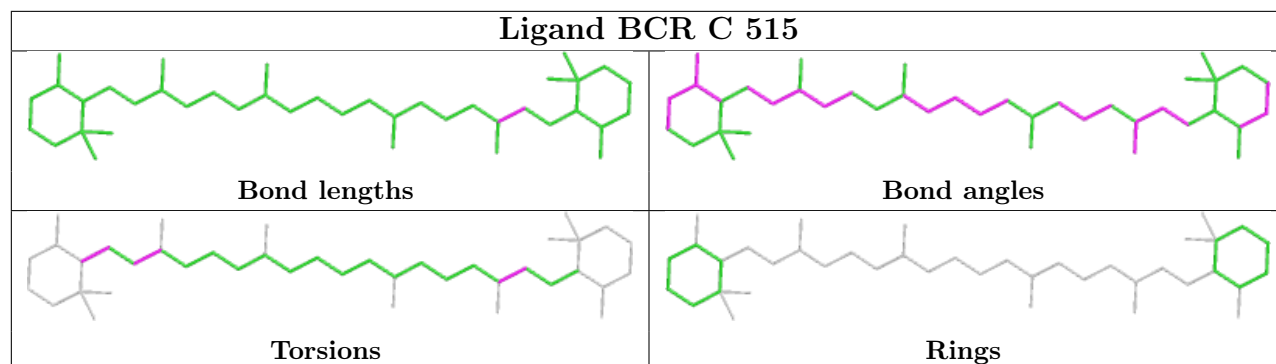


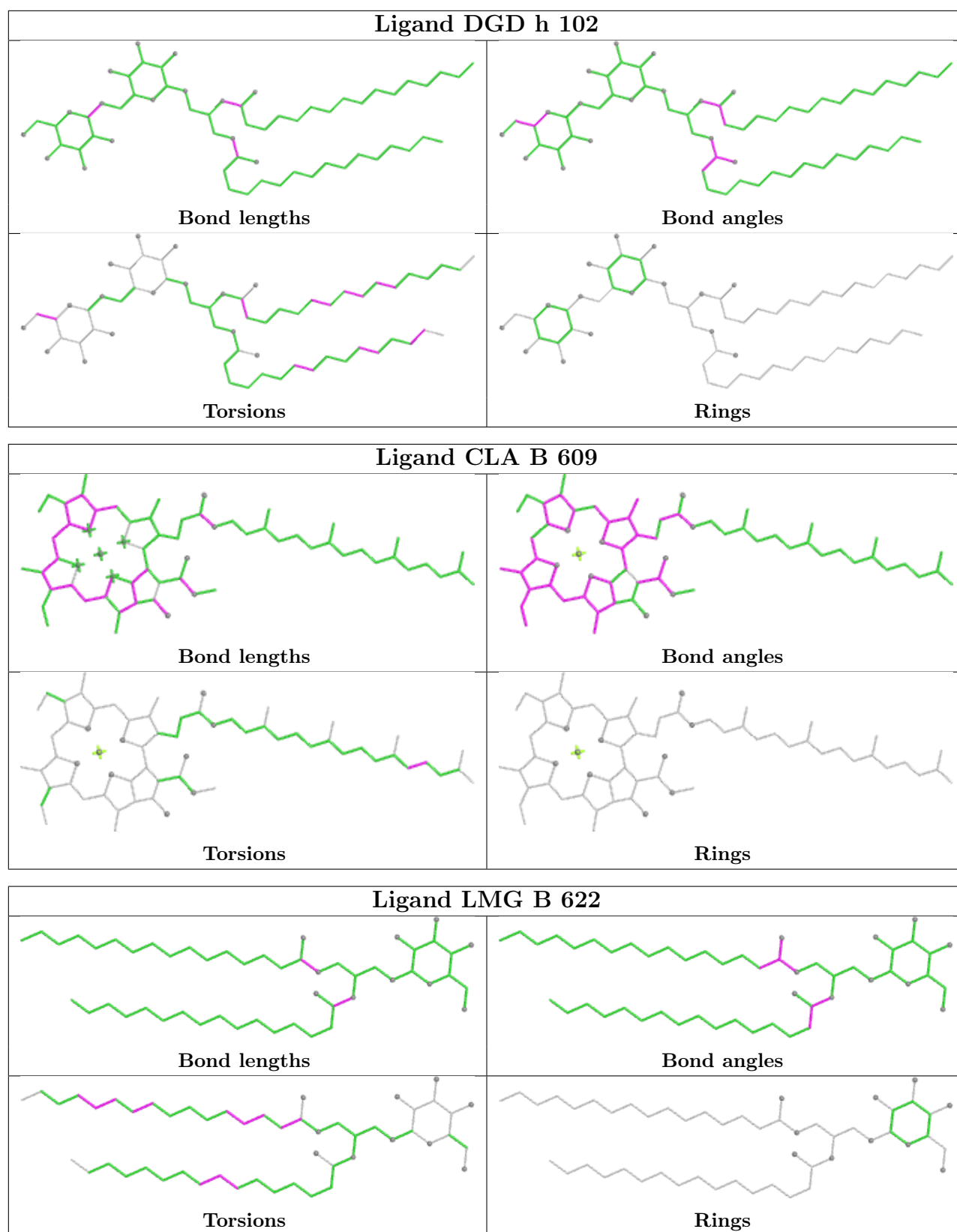
Ligand BCR y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

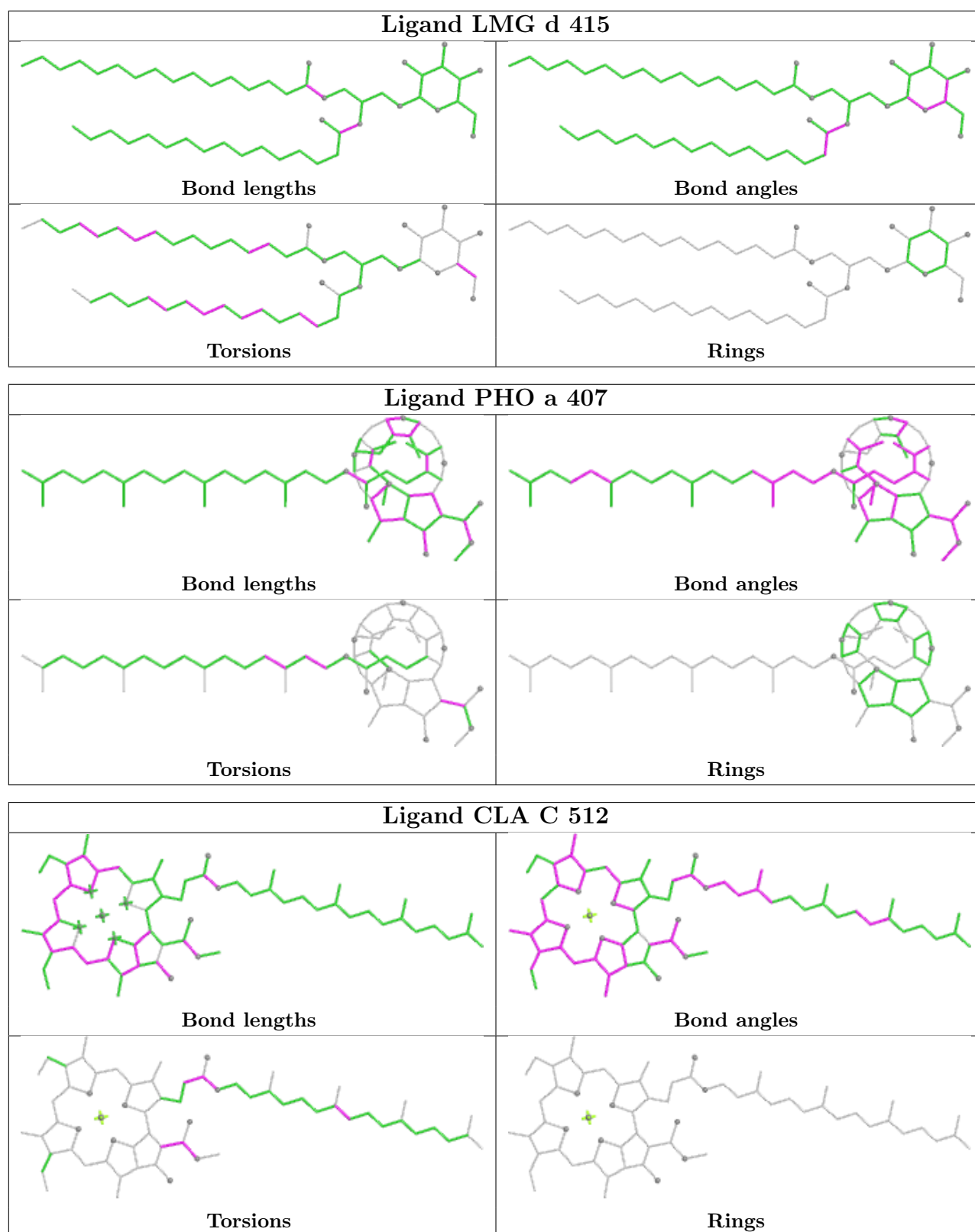
Ligand BCR Y 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

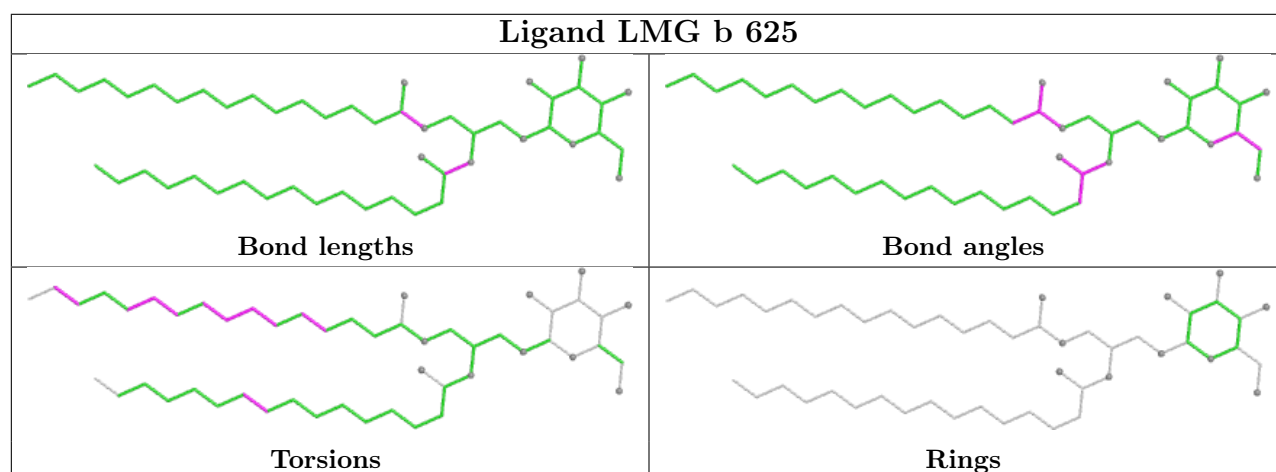
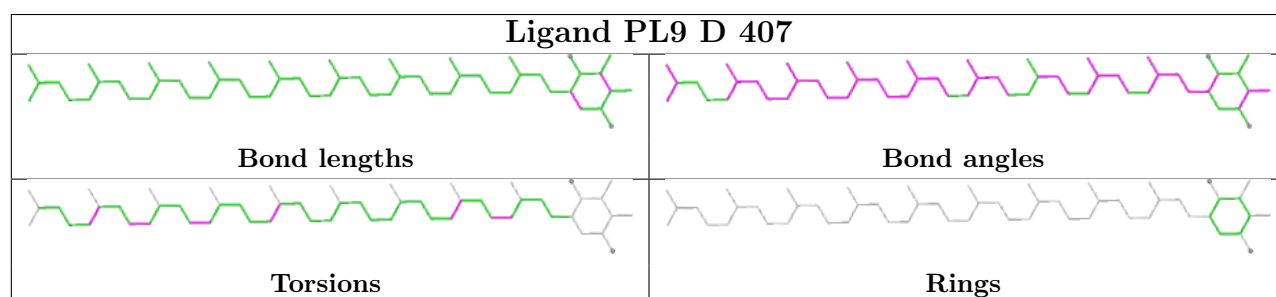
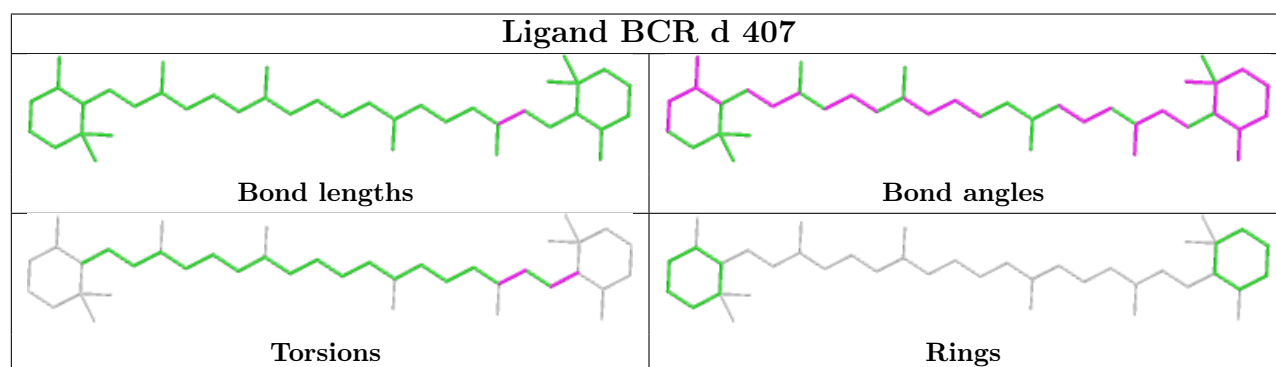
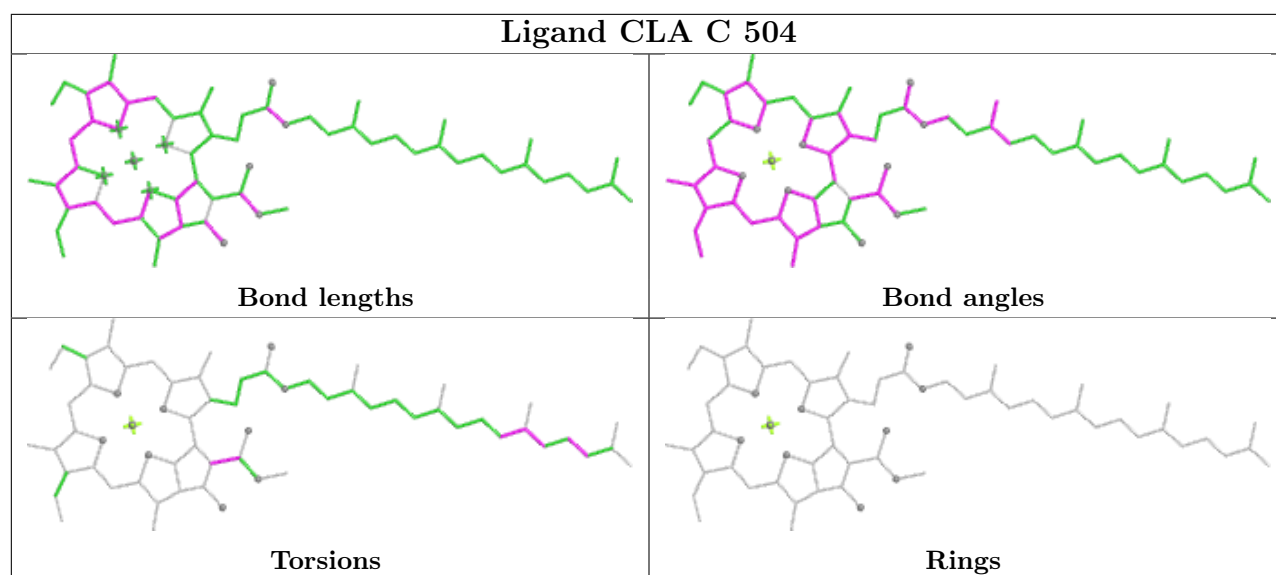
Ligand CLA B 605	
	
Bond lengths	Bond angles
	
Torsions	Rings



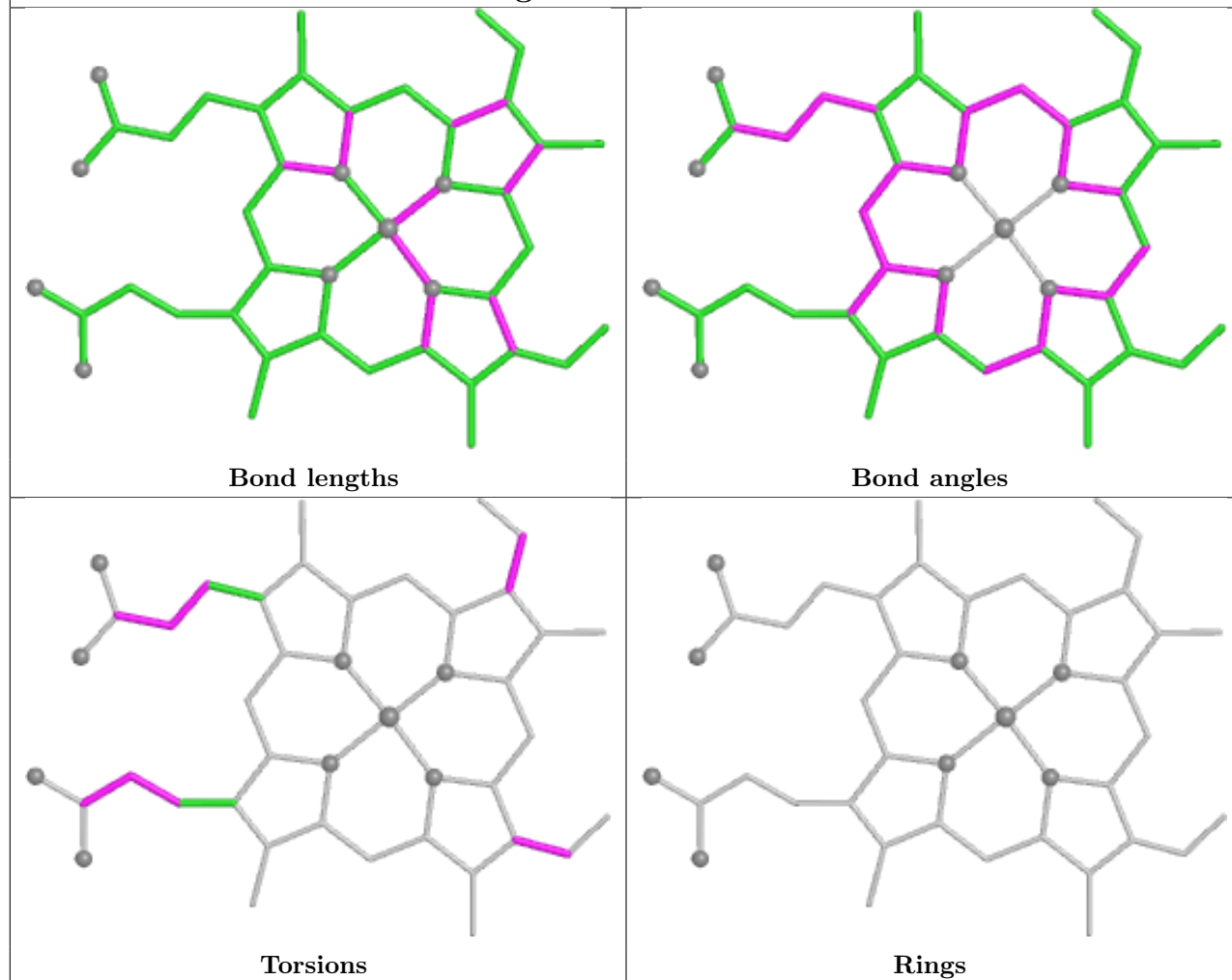




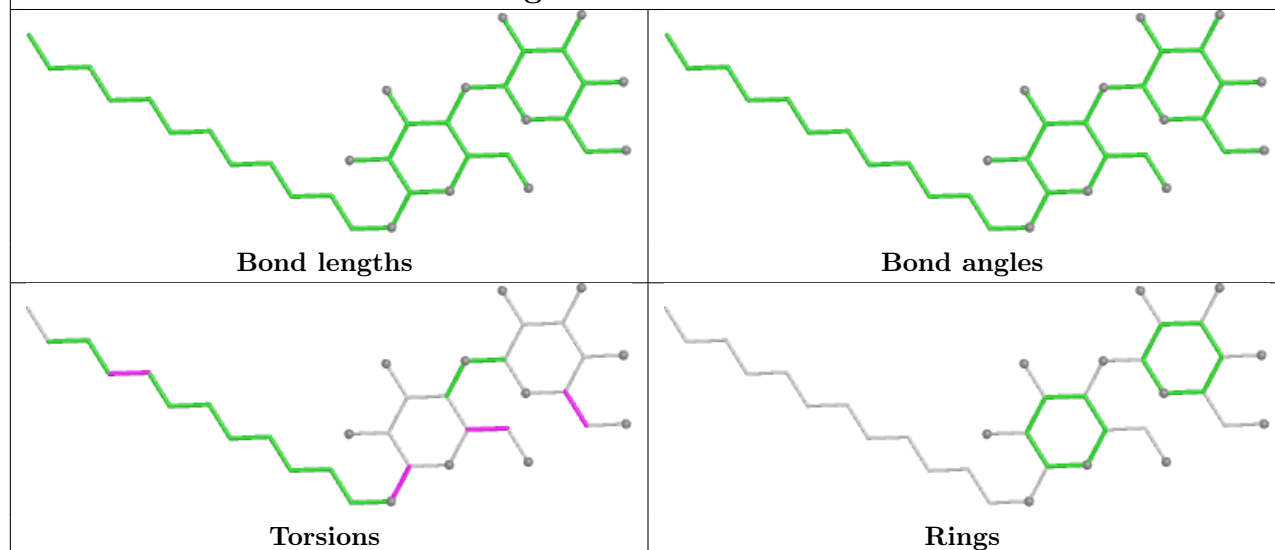




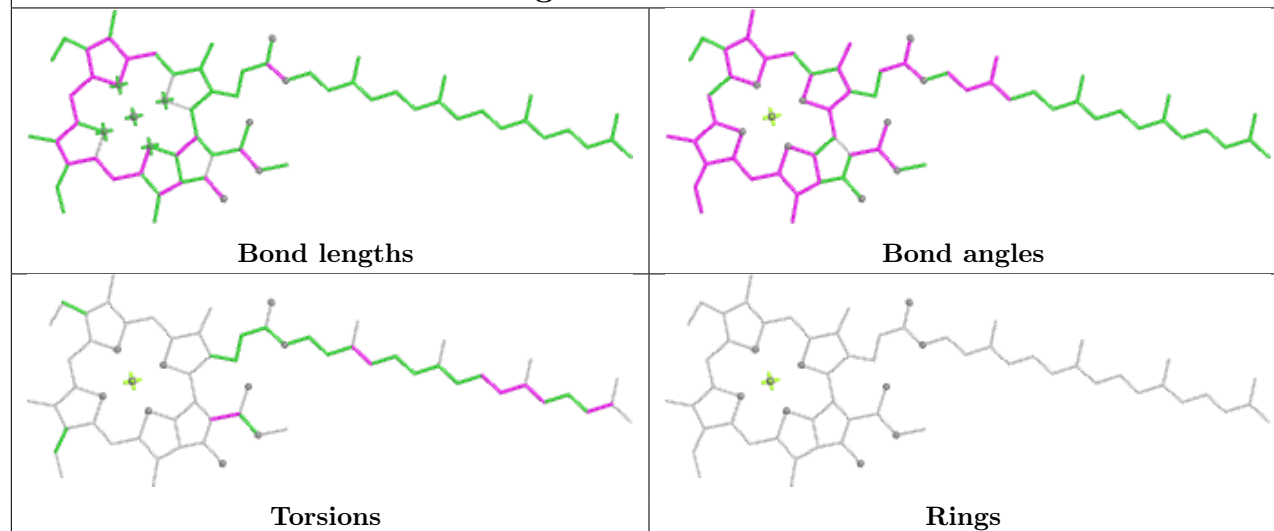
Ligand HEM f 101



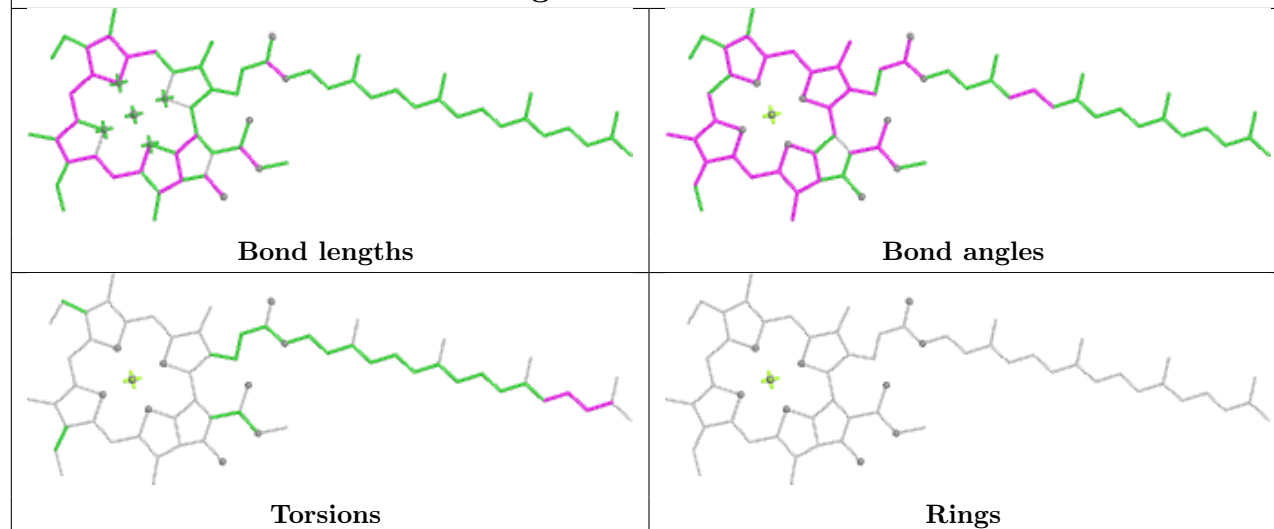
Ligand LMT M 101



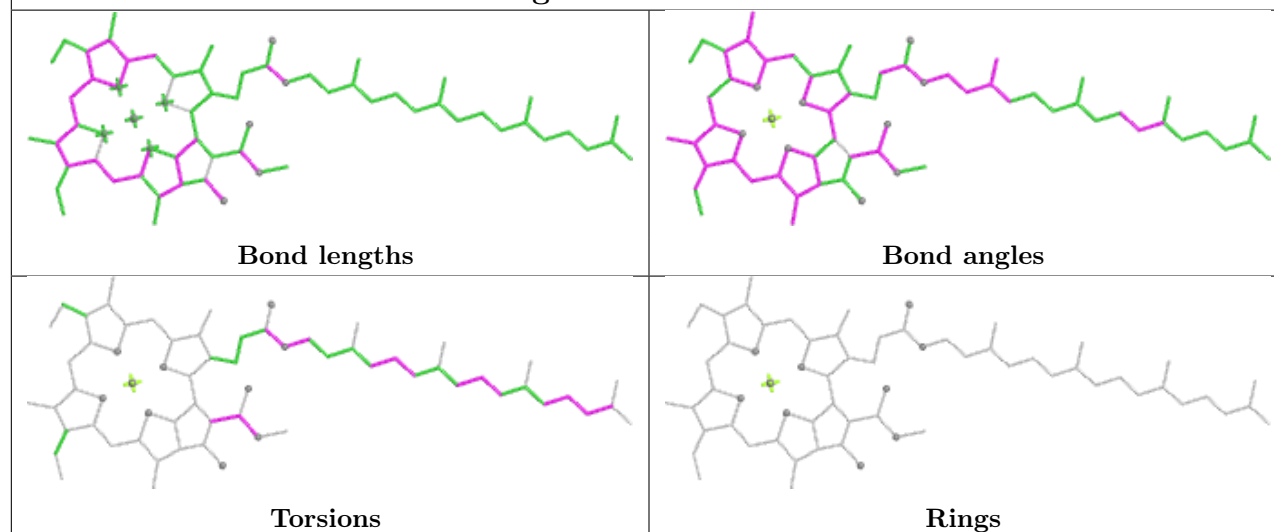
Ligand CLA b 621

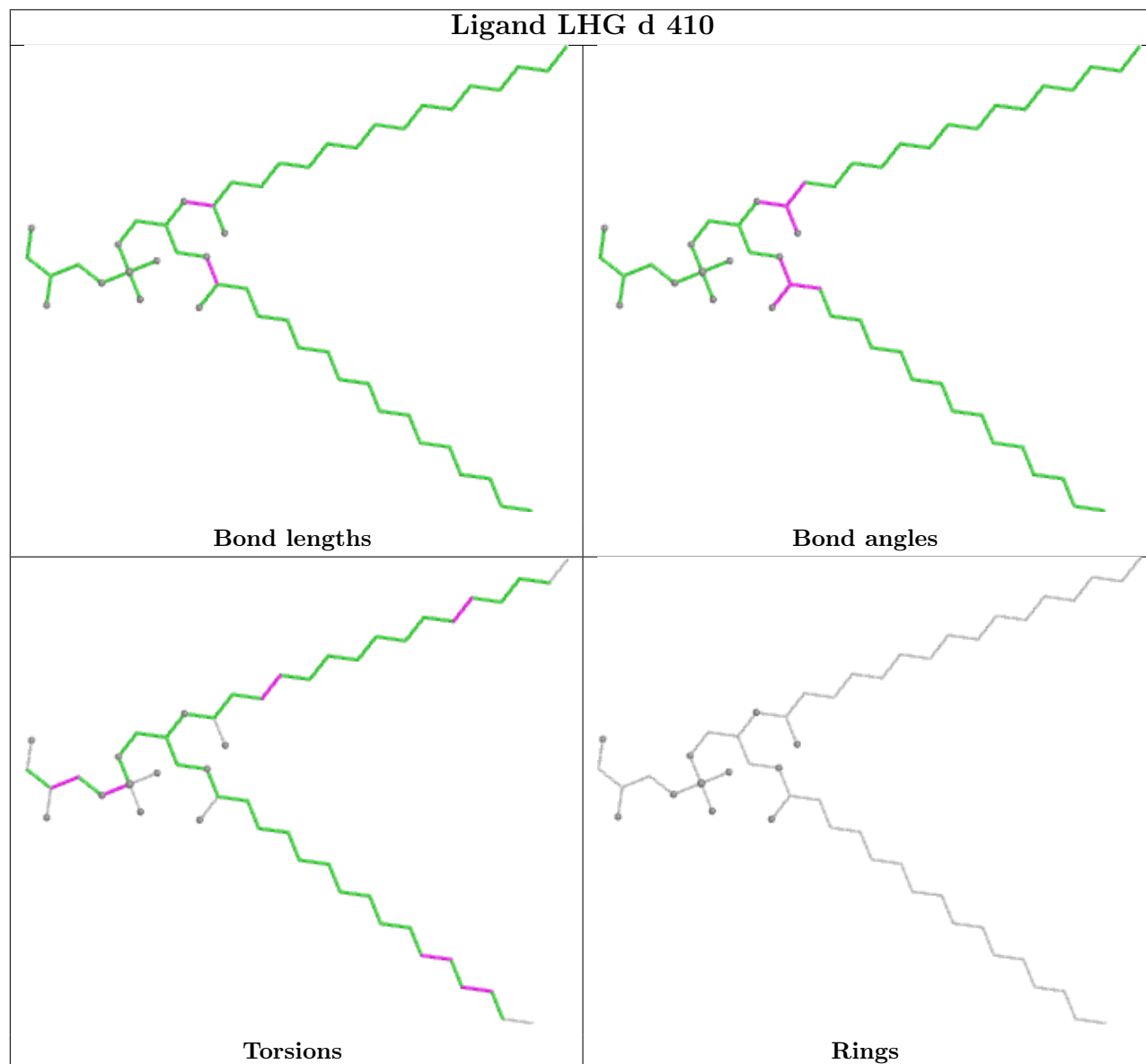
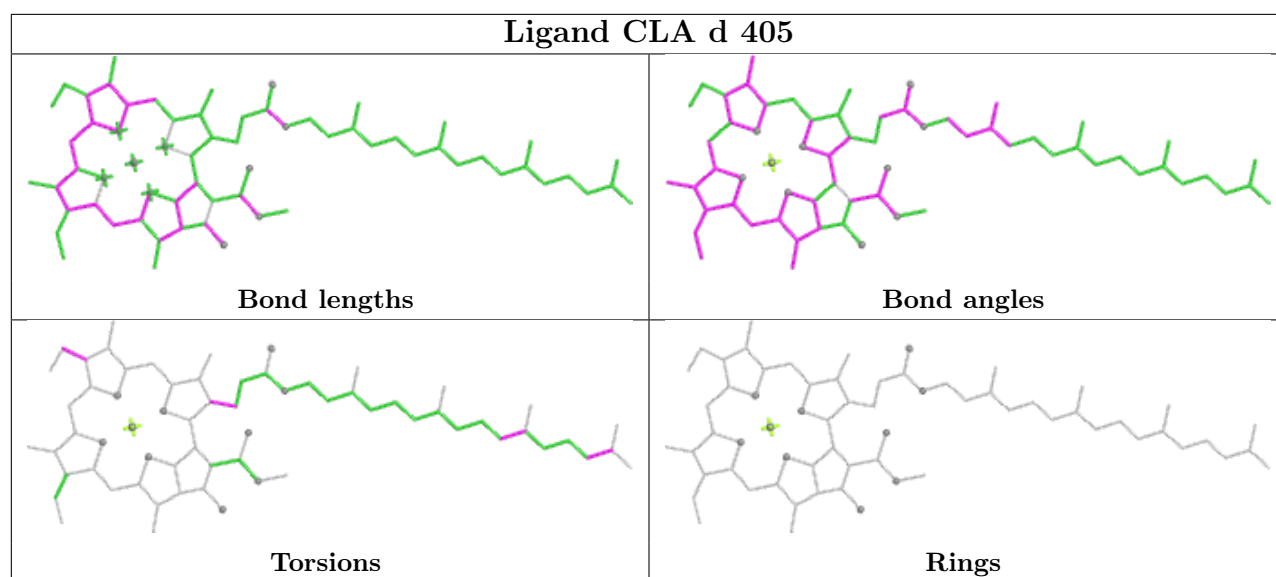


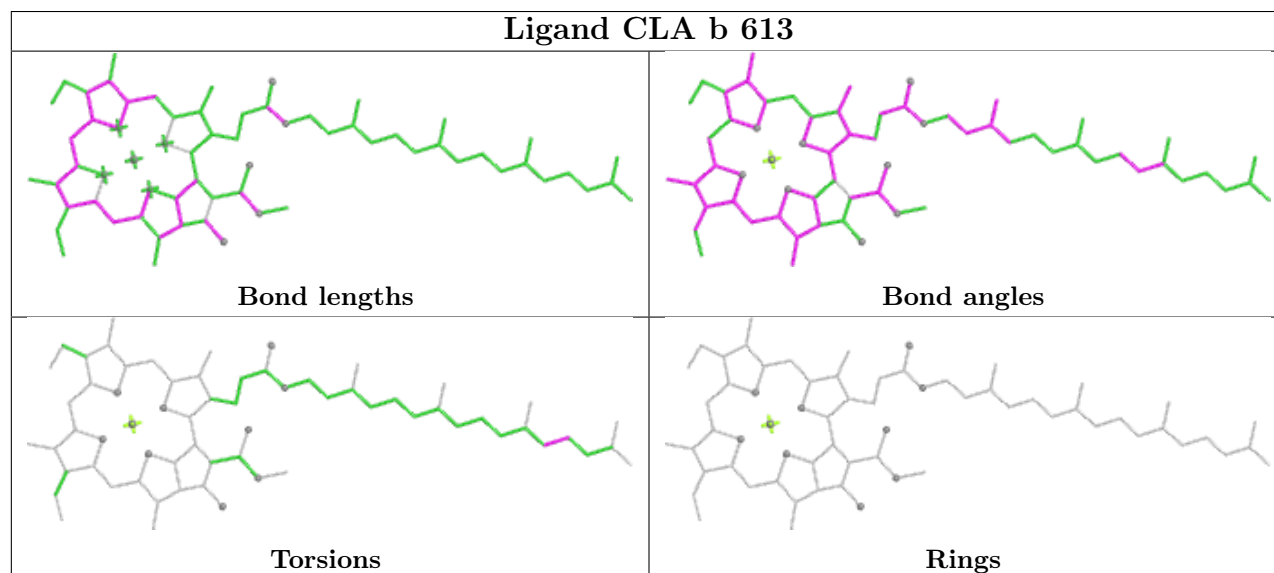
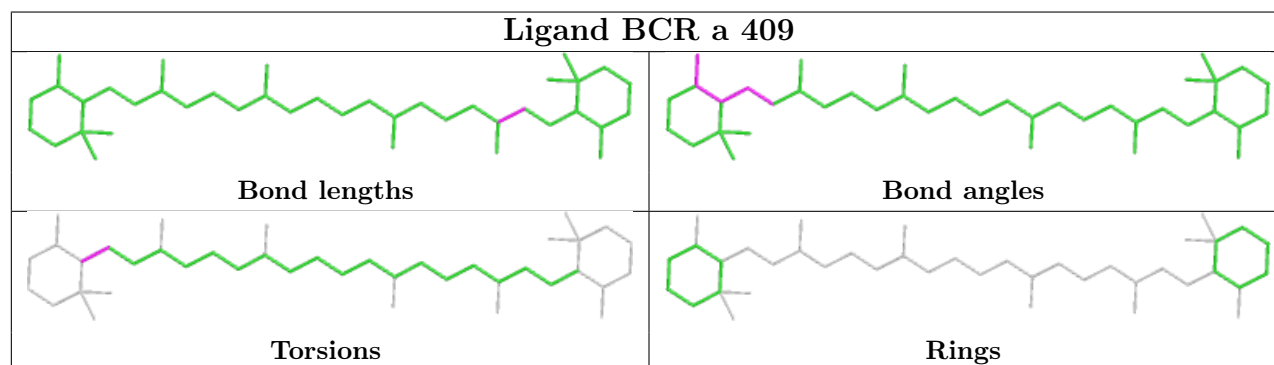
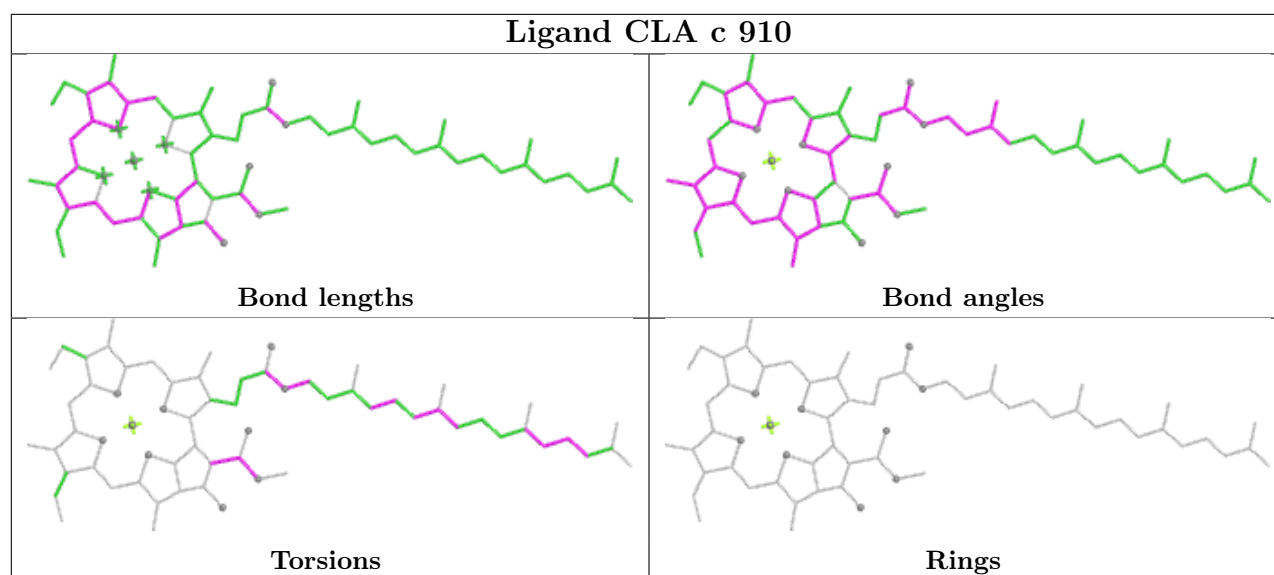
Ligand CLA A 405

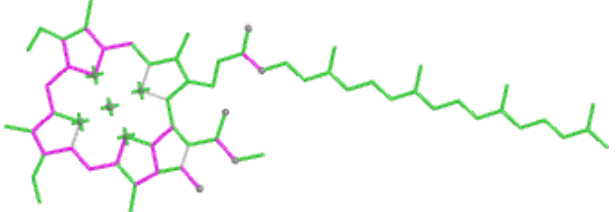
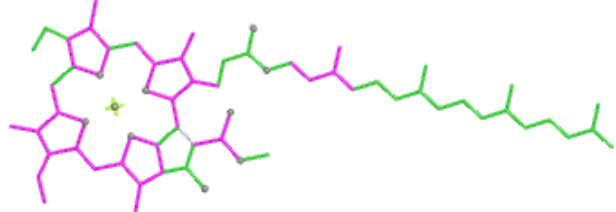
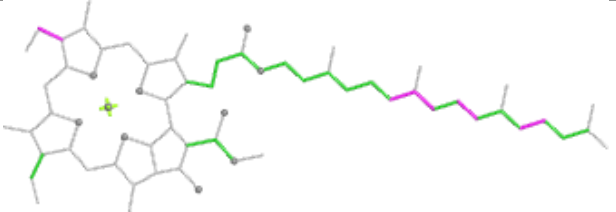
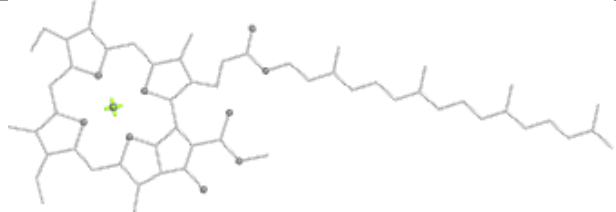
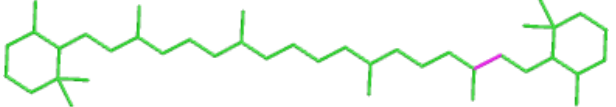
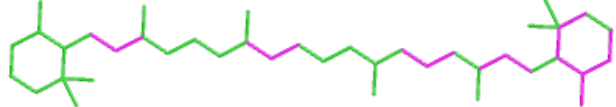
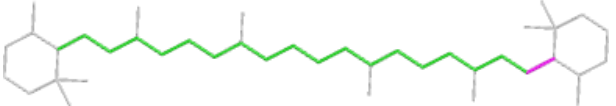
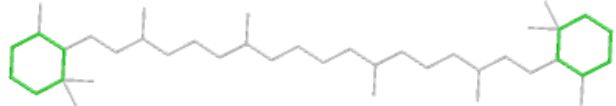
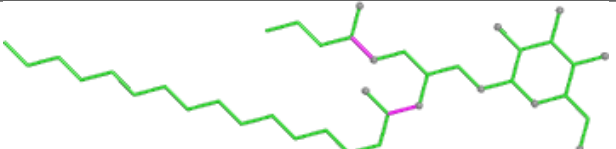
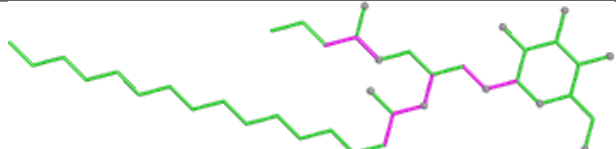
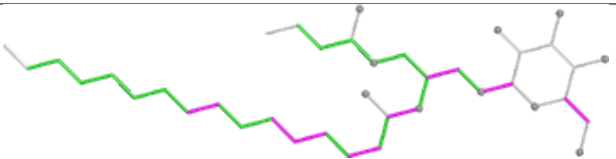


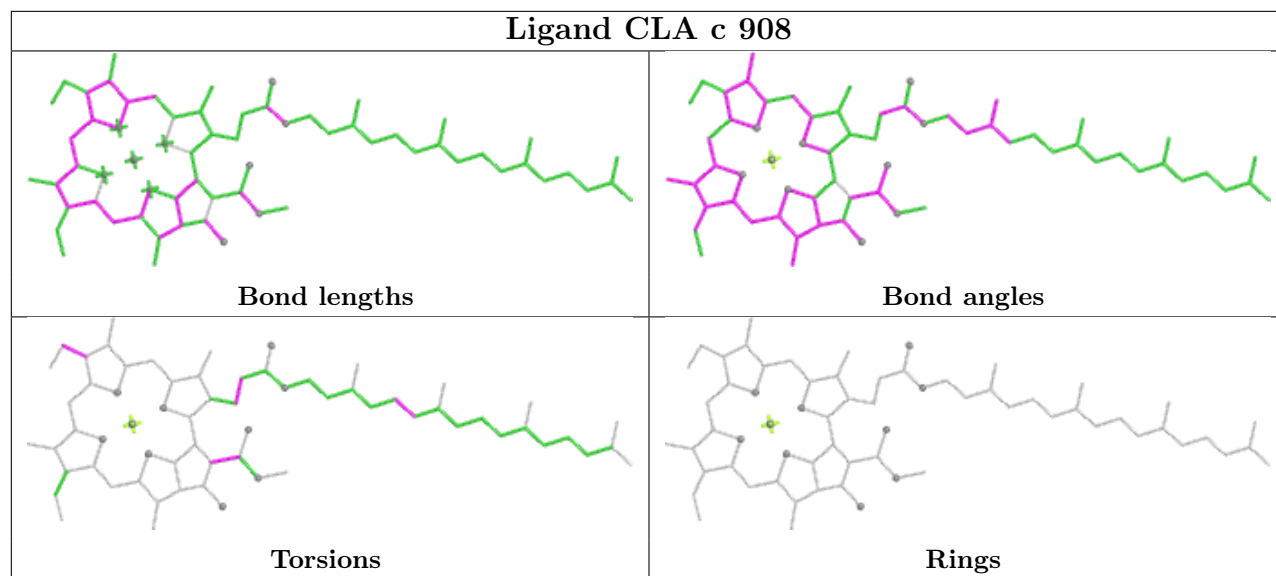
Ligand CLA C 509







Ligand CLA A 407	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 623	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.55	0 100 100	30, 43, 75, 139	3 (0%)
1	a	334/344 (97%)	-0.57	0 100 100	24, 44, 84, 146	6 (1%)
2	B	504/505 (99%)	-0.48	2 (0%) 88 91	24, 48, 86, 137	10 (1%)
2	b	503/505 (99%)	-0.44	5 (0%) 79 83	27, 48, 91, 193	12 (2%)
3	C	451/455 (99%)	-0.40	0 100 100	35, 56, 82, 134	4 (0%)
3	c	455/455 (100%)	-0.41	0 100 100	26, 58, 83, 118	6 (1%)
4	D	341/342 (99%)	-0.60	0 100 100	25, 45, 70, 129	1 (0%)
4	d	341/342 (99%)	-0.62	0 100 100	26, 45, 69, 115	1 (0%)
5	E	81/84 (96%)	0.01	1 (1%) 76 81	36, 71, 116, 150	2 (2%)
5	e	81/84 (96%)	0.03	2 (2%) 58 64	38, 71, 125, 201	2 (2%)
6	F	34/44 (77%)	-0.13	0 100 100	51, 62, 103, 104	0
6	f	32/44 (72%)	-0.16	1 (3%) 51 58	50, 62, 118, 148	0
7	H	65/65 (100%)	-0.28	2 (3%) 51 58	39, 57, 83, 145	1 (1%)
7	h	65/65 (100%)	-0.41	1 (1%) 72 77	47, 60, 83, 167	0
8	I	37/38 (97%)	-0.10	0 100 100	45, 58, 123, 187	0
8	i	37/38 (97%)	-0.15	1 (2%) 56 63	44, 57, 116, 159	0
9	J	38/39 (97%)	0.01	1 (2%) 57 63	52, 68, 151, 185	0
9	j	39/39 (100%)	0.00	1 (2%) 57 63	52, 68, 140, 190	0
10	K	37/37 (100%)	-0.20	0 100 100	60, 68, 88, 112	0
10	k	37/37 (100%)	-0.27	0 100 100	59, 67, 88, 112	0
11	L	37/37 (100%)	-0.61	0 100 100	22, 39, 101, 132	1 (2%)
11	l	37/37 (100%)	-0.49	0 100 100	23, 40, 105, 130	1 (2%)
12	M	33/36 (91%)	-0.48	0 100 100	24, 41, 75, 126	1 (3%)
12	m	33/36 (91%)	-0.52	0 100 100	35, 42, 78, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.47	0 100 100	29, 54, 102, 146	8 (3%)
13	o	243/244 (99%)	-0.42	0 100 100	28, 55, 112, 179	5 (2%)
14	T	29/32 (90%)	-0.68	1 (3%) 48 55	31, 39, 70, 142	1 (3%)
14	t	29/32 (90%)	-0.60	1 (3%) 48 55	32, 39, 68, 141	1 (3%)
15	U	97/104 (93%)	-0.54	0 100 100	39, 51, 82, 128	0
15	u	97/104 (93%)	-0.53	0 100 100	42, 52, 76, 126	0
16	V	137/137 (100%)	-0.47	0 100 100	27, 54, 88, 123	1 (0%)
16	v	137/137 (100%)	-0.46	0 100 100	43, 58, 89, 121	0
17	Y	29/30 (96%)	0.86	4 (13%) 6 7	73, 85, 162, 203	0
17	y	29/30 (96%)	0.56	1 (3%) 48 55	75, 85, 164, 202	0
18	X	39/40 (97%)	0.13	1 (2%) 57 63	52, 67, 135, 143	0
18	x	38/40 (95%)	0.31	2 (5%) 32 37	55, 67, 130, 140	0
19	Z	62/62 (100%)	0.41	4 (6%) 25 28	75, 89, 144, 191	0
19	z	62/62 (100%)	0.43	3 (4%) 35 41	75, 90, 144, 188	0
20	R	18/34 (52%)	1.99	9 (50%) 0 0	102, 135, 170, 172	0
All	All	5275/5384 (97%)	-0.40	43 (0%) 82 86	22, 52, 103, 203	67 (1%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	20	ALA	4.0
19	Z	61	VAL	3.9
18	x	37	VAL	3.8
7	H	65	LEU	3.6
20	R	15	ALA	3.5
17	y	20	ALA	3.4
19	Z	3	ILE	3.4
19	z	3	ILE	3.4
5	e	5	THR	3.4
8	i	37	LEU	3.3
2	b	486	LEU	3.2
7	h	65	LEU	3.2
18	x	2	THR	3.1
18	X	37	VAL	3.0
20	R	16	ALA	3.0
17	Y	18	VAL	2.9
20	R	9	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
14	t	30	THR	2.6
20	R	6	LEU	2.6
5	e	4	THR	2.6
20	R	3	TRP	2.5
20	R	13	LEU	2.5
14	T	30	THR	2.5
19	Z	62	VAL	2.5
20	R	19	ALA	2.5
9	J	2	SER	2.4
2	B	479	PHE	2.4
2	b	495	PHE	2.3
19	z	5	PHE	2.3
17	Y	24	MET	2.3
5	E	61	ARG	2.3
19	z	62	VAL	2.2
20	R	5	VAL	2.2
2	b	502	VAL	2.2
9	j	1	MET	2.2
2	B	481	GLY	2.2
2	b	499	VAL	2.1
20	R	8	VAL	2.1
17	Y	22	LEU	2.1
19	Z	4	LEU	2.1
6	f	14	PRO	2.1
7	H	66	GLY	2.0
2	b	479	PHE	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	0.94	0.07	26,36,47,88	0
12	FME	m	1	10/11	0.95	0.08	31,50,100,103	0
12	FME	M	1	10/11	0.96	0.08	30,50,87,93	0
14	FME	T	1	10/11	0.96	0.07	30,49,67,82	0
8	FME	I	1	10/11	0.97	0.06	28,49,62,64	0
8	FME	i	1	10/11	0.97	0.06	43,60,73,75	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
37	DGD	e	101	62/66	0.69	0.16	72,118,208,212	0
37	DGD	D	408	52/66	0.72	0.14	58,108,151,171	0
29	LMT	F	101	35/35	0.73	0.17	102,149,179,184	0
36	LHG	a	418	42/49	0.75	0.12	69,131,187,193	0
28	GOL	V	204	6/6	0.75	0.18	75,90,97,100	0
28	GOL	O	302	6/6	0.75	0.11	68,79,84,89	0
29	LMT	e	102	35/35	0.76	0.14	83,129,164,170	0
32	UNL	m	101	10/-	0.77	0.15	58,66,81,81	0
35	HTG	V	203	19/19	0.77	0.13	73,95,125,231	0
29	LMT	b	626	25/35	0.77	0.14	71,102,168,175	0
29	LMT	C	520	35/35	0.77	0.14	88,135,162,175	0
32	UNL	j	101	10/-	0.77	0.15	56,83,95,98	0
27	SQD	f	102	43/54	0.78	0.14	97,116,175,182	0
29	LMT	a	417	35/35	0.78	0.14	95,123,147,148	0
35	HTG	d	414	16/19	0.79	0.12	68,115,134,134	0
32	UNL	C	526	34/-	0.79	0.13	76,120,132,136	0
32	UNL	J	102	10/-	0.79	0.18	50,85,104,107	0
32	UNL	M	102	10/-	0.79	0.11	50,55,74,86	0
35	HTG	B	633	19/19	0.80	0.11	53,103,141,160	0
32	UNL	a	414	30/-	0.80	0.12	64,85,117,134	0
29	LMT	A	415	35/35	0.81	0.12	41,84,115,119	0
33	LMG	Z	101	37/55	0.81	0.15	55,121,146,154	0
32	UNL	i	101	40/-	0.82	0.12	48,77,140,147	0
36	LHG	E	101	42/49	0.82	0.11	59,115,138,140	0
33	LMG	z	101	39/55	0.82	0.14	65,124,153,161	0
32	UNL	D	412	40/-	0.82	0.12	51,88,141,144	0
29	LMT	M	103	35/35	0.82	0.12	47,99,150,158	0
33	LMG	c	920	51/55	0.83	0.12	50,111,142,145	0
28	GOL	a	413	6/6	0.83	0.12	73,83,95,97	0
35	HTG	B	625	19/19	0.83	0.12	75,132,140,190	0
29	LMT	D	403	35/35	0.83	0.12	58,132,172,179	0
35	HTG	D	413	16/19	0.83	0.14	76,142,160,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	GOL	c	924	6/6	0.83	0.17	81,87,97,102	0
32	UNL	A	418	28/-	0.83	0.12	59,88,108,111	0
27	SQD	F	103	43/54	0.83	0.13	77,120,145,149	0
29	LMT	a	401	35/35	0.83	0.12	52,87,118,142	0
33	LMG	C	519	51/55	0.83	0.12	53,121,145,151	0
32	UNL	I	101	40/-	0.83	0.14	42,88,155,156	0
31	PL9	A	417	55/55	0.84	0.13	61,98,125,131	0
34	CA	f	103	1/1	0.84	0.08	126,126,126,126	0
35	HTG	b	604	19/19	0.84	0.11	51,112,150,150	0
35	HTG	C	522	19/19	0.84	0.11	81,112,138,140	0
35	HTG	c	922	19/19	0.85	0.10	73,114,134,192	0
32	UNL	c	925	32/-	0.85	0.12	66,101,138,147	0
32	UNL	d	413	36/-	0.85	0.11	60,85,140,142	0
35	HTG	b	627	19/19	0.86	0.12	55,73,94,109	0
35	HTG	b	628	19/19	0.86	0.12	72,130,158,159	0
35	HTG	c	921	19/19	0.86	0.09	93,101,107,111	0
28	GOL	l	101	6/6	0.86	0.17	48,92,98,103	0
32	UNL	b	634	33/-	0.86	0.13	47,86,155,158	0
29	LMT	m	103	35/35	0.86	0.11	42,109,140,144	0
22	CL	U	201	1/1	0.86	0.12	117,117,117,117	0
27	SQD	B	621	54/54	0.86	0.11	53,88,137,156	0
32	UNL	B	634	33/-	0.86	0.12	54,73,126,134	0
28	GOL	C	523	6/6	0.87	0.15	74,80,89,92	0
29	LMT	t	101	25/35	0.87	0.12	43,92,140,150	0
29	LMT	b	602	25/35	0.87	0.13	41,91,134,149	0
31	PL9	a	415	55/55	0.87	0.13	65,110,127,130	0
27	SQD	L	102	54/54	0.87	0.10	48,79,126,149	0
35	HTG	B	624	19/19	0.87	0.12	50,73,82,92	0
28	GOL	A	413	6/6	0.87	0.10	61,79,84,86	0
27	SQD	A	414	54/54	0.88	0.10	49,75,134,141	0
22	CL	v	201	1/1	0.88	0.09	124,124,124,124	0
28	GOL	B	630	6/6	0.88	0.13	51,59,70,81	0
34	CA	b	605	1/1	0.88	0.06	124,124,124,124	0
28	GOL	b	633	6/6	0.88	0.10	68,74,80,88	0
27	SQD	a	402	54/54	0.88	0.09	45,75,125,133	0
33	LMG	Y	101	51/55	0.88	0.10	60,93,118,127	0
29	LMT	m	102	35/35	0.89	0.11	42,90,122,128	0
34	CA	B	601	1/1	0.89	0.06	138,138,138,138	0
33	LMG	A	419	51/55	0.89	0.10	54,88,107,128	0
29	LMT	M	101	35/35	0.89	0.10	45,93,118,133	0
28	GOL	T	101	6/6	0.90	0.14	60,77,82,83	0
28	GOL	T	103	6/6	0.90	0.11	103,108,112,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	GOL	c	928	6/6	0.90	0.11	75,83,90,98	0
24	CLA	C	513	65/65	0.90	0.09	53,84,113,119	0
28	GOL	v	203	6/6	0.90	0.11	72,88,91,94	0
33	LMG	a	411	51/55	0.90	0.10	51,84,96,105	0
35	HTG	C	521	19/19	0.90	0.10	70,99,121,123	0
33	LMG	c	919	51/55	0.90	0.10	51,89,123,128	0
28	GOL	v	204	6/6	0.90	0.11	84,87,94,112	0
28	GOL	B	636	6/6	0.90	0.10	49,56,64,65	0
24	CLA	b	606	65/65	0.91	0.10	39,67,123,145	0
24	CLA	c	914	65/65	0.91	0.09	68,84,105,115	0
35	HTG	B	632	19/19	0.91	0.09	48,84,110,115	0
26	BCR	d	407	40/40	0.91	0.08	39,54,85,88	0
32	UNL	X	101	18/-	0.91	0.10	53,73,112,114	0
32	UNL	x	101	18/-	0.91	0.11	51,71,116,116	0
28	GOL	b	632	6/6	0.91	0.14	77,78,102,105	0
24	CLA	C	506	65/65	0.91	0.08	41,70,114,128	0
24	CLA	B	602	65/65	0.91	0.10	43,67,119,143	0
26	BCR	C	514	40/40	0.92	0.08	50,72,86,87	0
32	UNL	d	412	17/-	0.92	0.09	47,62,95,102	0
36	LHG	D	410	49/49	0.92	0.10	47,67,121,138	0
28	GOL	a	419	6/6	0.92	0.09	73,85,94,95	0
24	CLA	C	512	65/65	0.92	0.08	49,76,99,106	0
27	SQD	A	411	54/54	0.92	0.09	43,87,114,116	0
28	GOL	A	412	6/6	0.92	0.09	49,55,57,69	0
27	SQD	a	410	54/54	0.93	0.09	51,81,110,114	0
35	HTG	b	603	19/19	0.93	0.08	47,75,92,93	0
32	UNL	D	411	17/-	0.93	0.09	40,71,92,94	0
26	BCR	y	101	40/40	0.93	0.07	47,63,74,82	0
24	CLA	c	913	65/65	0.93	0.08	47,74,93,99	0
24	CLA	B	615	65/65	0.93	0.08	26,43,97,103	0
28	GOL	B	628	6/6	0.93	0.10	62,80,83,84	0
24	CLA	C	504	65/65	0.93	0.08	36,57,79,95	0
33	LMG	J	101	51/55	0.93	0.10	44,65,120,137	0
28	GOL	B	631	6/6	0.93	0.14	40,78,87,93	0
26	BCR	D	406	40/40	0.93	0.07	39,58,89,104	0
26	BCR	c	927	40/40	0.93	0.09	54,77,91,100	0
23	BCT	d	402	4/4	0.93	0.12	70,72,76,97	0
28	GOL	b	629	6/6	0.94	0.10	57,62,67,81	0
24	CLA	c	907	65/65	0.94	0.07	44,65,104,111	0
28	GOL	B	626	6/6	0.94	0.09	44,53,66,87	0
26	BCR	k	101	40/40	0.94	0.08	51,64,75,80	0
28	GOL	B	629	6/6	0.94	0.12	56,60,69,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	c	908	65/65	0.94	0.08	45,63,74,84	0
31	PL9	D	407	55/55	0.94	0.07	29,42,52,60	0
24	CLA	c	909	65/65	0.94	0.07	38,54,125,137	0
24	CLA	B	607	65/65	0.94	0.08	31,52,95,99	0
33	LMG	B	622	51/55	0.94	0.07	38,53,78,91	0
35	HTG	b	601	19/19	0.94	0.08	42,57,82,87	0
24	CLA	b	611	65/65	0.94	0.07	37,51,97,108	0
28	GOL	D	402	6/6	0.94	0.13	52,57,83,90	0
24	CLA	b	619	65/65	0.94	0.07	25,43,86,108	0
24	CLA	b	621	65/65	0.94	0.08	33,53,103,118	0
26	BCR	H	101	40/40	0.94	0.07	33,57,78,85	0
33	LMG	b	625	51/55	0.94	0.08	40,54,73,98	0
26	BCR	K	101	40/40	0.94	0.08	43,63,79,82	0
36	LHG	B	635	49/49	0.94	0.07	30,52,68,77	0
28	GOL	V	207	6/6	0.94	0.09	81,86,89,98	0
33	LMG	d	415	51/55	0.94	0.08	38,61,112,126	0
26	BCR	Y	102	40/40	0.94	0.08	51,71,90,107	0
36	LHG	d	411	49/49	0.94	0.09	37,53,112,120	0
37	DGD	C	517	62/66	0.94	0.08	48,65,94,116	0
24	CLA	c	904	65/65	0.94	0.07	41,60,73,84	0
37	DGD	c	917	62/66	0.94	0.08	35,60,112,137	0
34	CA	F	104	1/1	0.94	0.06	107,107,107,107	0
24	CLA	b	616	65/65	0.95	0.06	29,41,54,66	0
28	GOL	V	201	6/6	0.95	0.10	88,99,104,109	0
24	CLA	B	614	65/65	0.95	0.06	29,41,64,93	0
28	GOL	V	205	6/6	0.95	0.08	45,51,58,72	0
28	GOL	V	206	6/6	0.95	0.13	52,60,67,71	0
26	BCR	h	101	40/40	0.95	0.07	36,60,79,81	0
35	HTG	B	623	19/19	0.95	0.08	38,56,78,93	0
24	CLA	C	507	65/65	0.95	0.08	41,66,77,86	0
26	BCR	t	102	40/40	0.95	0.06	33,46,62,64	0
24	CLA	c	902	65/65	0.95	0.07	44,60,72,81	0
24	CLA	C	508	65/65	0.95	0.07	35,61,138,148	0
24	CLA	c	905	65/65	0.95	0.06	31,57,74,85	0
24	CLA	C	509	65/65	0.95	0.08	53,65,82,93	0
24	CLA	C	510	65/65	0.95	0.07	40,60,77,92	0
24	CLA	C	511	65/65	0.95	0.08	48,67,85,109	0
24	CLA	c	910	65/65	0.95	0.08	43,58,77,81	0
23	BCT	A	404	4/4	0.95	0.10	59,62,74,108	0
28	GOL	v	205	6/6	0.95	0.09	48,59,69,78	0
24	CLA	B	617	65/65	0.95	0.10	34,54,130,139	0
24	CLA	d	406	65/65	0.95	0.08	40,54,106,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	PHO	d	403	64/64	0.95	0.06	27,44,54,62	0
26	BCR	A	410	40/40	0.95	0.06	32,42,54,54	0
28	GOL	B	627	6/6	0.95	0.10	54,64,88,102	0
26	BCR	B	620	40/40	0.95	0.06	36,52,64,67	0
24	CLA	D	405	65/65	0.95	0.08	39,55,106,121	0
24	CLA	a	408	65/65	0.95	0.09	32,53,122,130	0
24	CLA	A	409	65/65	0.95	0.08	33,50,116,132	0
24	CLA	C	505	65/65	0.95	0.08	41,54,71,89	0
37	DGD	C	516	62/66	0.95	0.08	32,50,88,97	0
26	BCR	T	102	40/40	0.95	0.06	29,46,64,65	0
37	DGD	C	518	62/66	0.95	0.07	39,58,92,100	0
24	CLA	b	614	65/65	0.95	0.07	39,51,61,72	0
37	DGD	c	916	62/66	0.95	0.07	38,56,100,114	0
26	BCR	b	623	40/40	0.95	0.06	29,46,66,68	0
37	DGD	c	918	62/66	0.95	0.07	41,56,90,110	0
26	BCR	c	915	40/40	0.95	0.06	32,56,67,75	0
24	CLA	b	617	65/65	0.96	0.06	25,42,53,65	0
24	CLA	b	618	65/65	0.96	0.06	24,44,60,67	0
24	CLA	A	405	65/65	0.96	0.06	24,37,51,66	0
26	BCR	a	409	40/40	0.96	0.05	28,43,54,59	0
26	BCR	b	622	40/40	0.96	0.05	32,44,56,60	0
31	PL9	d	408	55/55	0.96	0.06	22,39,53,73	0
24	CLA	b	620	65/65	0.96	0.06	36,50,64,69	0
26	BCR	b	624	40/40	0.96	0.06	39,50,61,65	0
24	CLA	B	616	65/65	0.96	0.06	37,50,65,77	0
24	CLA	B	603	65/65	0.96	0.06	38,50,57,66	0
24	CLA	c	903	65/65	0.96	0.07	39,52,76,80	0
24	CLA	C	501	65/65	0.96	0.06	39,57,85,91	0
24	CLA	C	502	65/65	0.96	0.06	42,56,69,85	0
28	GOL	b	630	6/6	0.96	0.08	50,82,94,95	0
28	GOL	b	631	6/6	0.96	0.09	58,70,81,100	0
24	CLA	c	906	65/65	0.96	0.06	36,51,70,76	0
24	CLA	C	503	65/65	0.96	0.07	36,59,72,85	0
24	CLA	a	406	65/65	0.96	0.07	31,44,118,125	0
24	CLA	B	605	65/65	0.96	0.06	28,41,72,78	0
24	CLA	A	407	65/65	0.96	0.06	28,43,106,119	0
24	CLA	c	911	65/65	0.96	0.06	43,55,69,81	0
24	CLA	c	912	65/65	0.96	0.07	43,63,83,99	0
24	CLA	b	607	65/65	0.96	0.06	30,50,60,63	0
24	CLA	b	608	65/65	0.96	0.06	38,48,58,66	0
24	CLA	b	610	65/65	0.96	0.06	31,43,53,61	0
36	LHG	L	101	49/49	0.96	0.06	36,47,56,62	0

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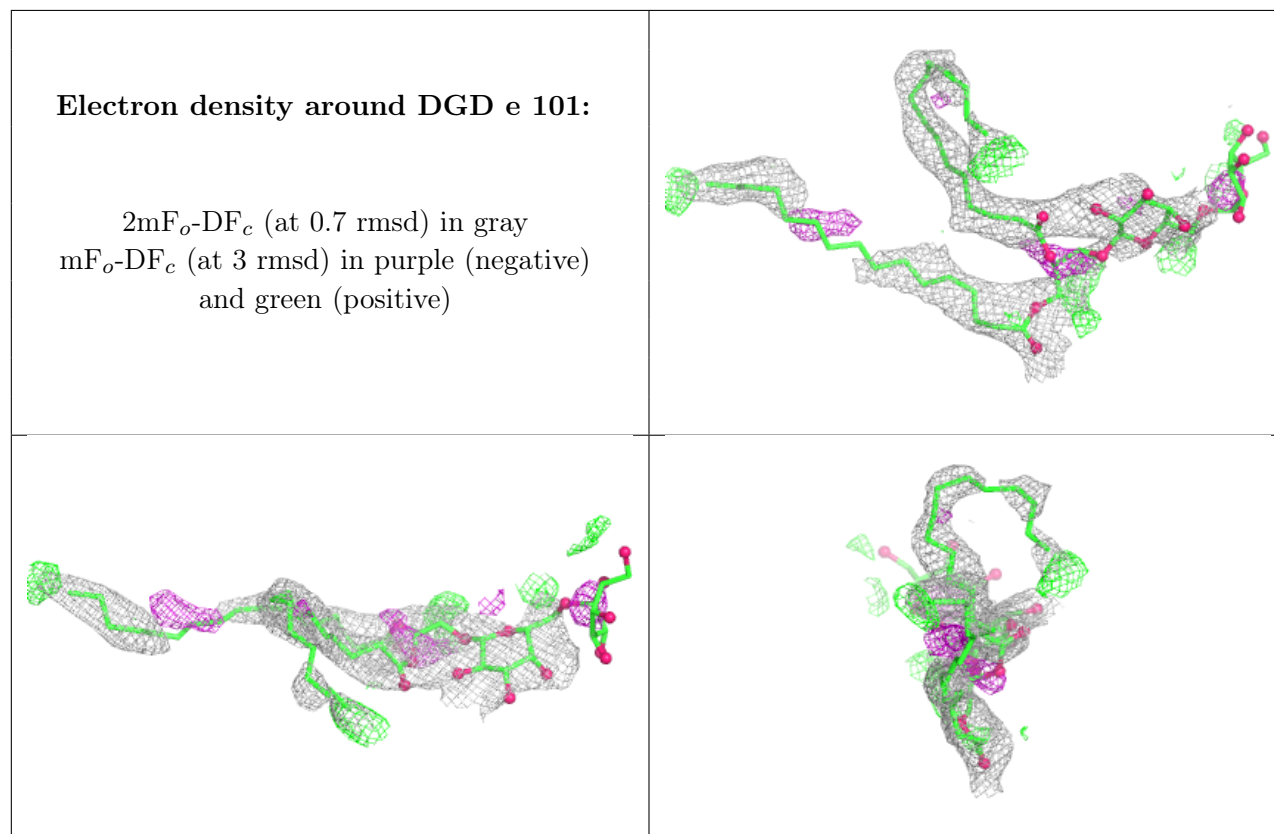
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	PHO	A	408	64/64	0.96	0.06	26,39,46,54	0
36	LHG	b	635	49/49	0.96	0.06	30,48,61,64	0
36	LHG	d	409	49/49	0.96	0.06	40,52,66,70	0
25	PHO	D	401	64/64	0.96	0.06	31,46,58,60	0
24	CLA	B	610	65/65	0.96	0.06	36,52,65,82	0
24	CLA	b	612	65/65	0.96	0.06	27,38,48,58	0
26	BCR	B	619	40/40	0.96	0.05	31,42,60,66	0
24	CLA	b	613	65/65	0.96	0.05	36,49,59,62	0
37	DGD	H	102	62/66	0.96	0.07	31,51,88,102	0
24	CLA	B	612	65/65	0.96	0.06	24,40,56,63	0
26	BCR	C	515	40/40	0.96	0.06	38,55,68,78	0
24	CLA	b	615	65/65	0.96	0.07	35,47,61,67	0
22	CL	A	403	1/1	0.96	0.09	38,38,38,38	0
37	DGD	h	102	62/66	0.96	0.07	34,52,71,82	0
39	MG	J	103	1/1	0.96	0.05	54,54,54,54	0
34	CA	c	926	1/1	0.97	0.06	77,77,77,77	0
36	LHG	D	409	49/49	0.97	0.06	31,46,67,79	0
24	CLA	a	405	65/65	0.97	0.06	24,38,53,67	0
24	CLA	B	611	65/65	0.97	0.06	31,50,62,66	0
28	GOL	a	412	6/6	0.97	0.09	54,61,67,72	0
24	CLA	d	404	65/65	0.97	0.05	29,39,48,56	0
24	CLA	d	405	65/65	0.97	0.05	24,40,55,69	0
24	CLA	B	606	65/65	0.97	0.05	28,40,55,57	0
36	LHG	d	410	49/49	0.97	0.06	29,44,63,98	0
24	CLA	B	613	65/65	0.97	0.06	26,42,50,53	0
24	CLA	B	604	65/65	0.97	0.06	35,48,60,63	0
28	GOL	C	524	6/6	0.97	0.07	39,44,53,61	0
25	PHO	a	407	64/64	0.97	0.05	28,40,48,54	0
28	GOL	c	923	6/6	0.97	0.06	41,51,54,57	0
24	CLA	B	608	65/65	0.97	0.05	25,41,51,61	0
24	CLA	b	609	65/65	0.97	0.06	27,42,74,77	0
26	BCR	B	618	40/40	0.97	0.04	29,40,51,54	0
24	CLA	B	609	65/65	0.97	0.06	32,46,59,67	0
34	CA	C	525	1/1	0.97	0.07	79,79,79,79	0
24	CLA	D	404	65/65	0.97	0.06	24,37,58,69	0
38	HEM	f	101	43/43	0.97	0.09	51,85,128,152	0
24	CLA	A	406	65/65	0.97	0.05	23,36,45,55	0
39	MG	j	102	1/1	0.97	0.08	61,61,61,61	0
34	CA	o	301	1/1	0.98	0.03	97,97,97,97	0
22	CL	a	403	1/1	0.98	0.06	37,37,37,37	0
38	HEM	F	102	43/43	0.98	0.07	53,74,105,111	0
40	HEC	V	202	43/43	0.98	0.06	31,45,54,59	0

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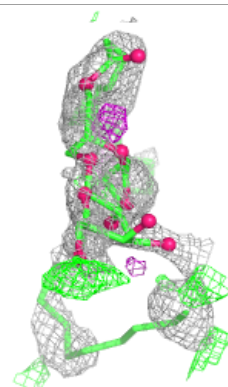
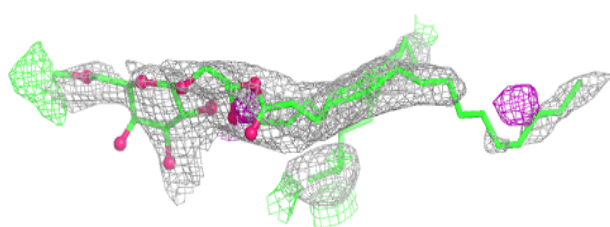
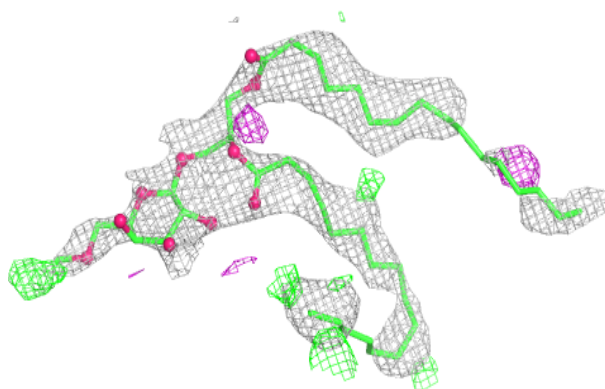
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
40	HEC	v	202	43/43	0.98	0.06	46,58,65,70	0
21	FE2	d	401	1/1	0.99	0.06	55,55,55,55	0
34	CA	c	901	1/1	0.99	0.02	74,74,74,74	0
22	CL	A	402	1/1	0.99	0.03	35,35,35,35	0
22	CL	a	404	1/1	0.99	0.02	42,42,42,42	0
30	OEX	A	416	10/10	0.99	0.03	39,45,61,77	0
30	OEX	a	416	10/10	0.99	0.04	35,45,63,74	0
21	FE2	A	401	1/1	0.99	0.02	56,56,56,56	0
34	CA	O	301	1/1	0.99	0.03	89,89,89,89	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.

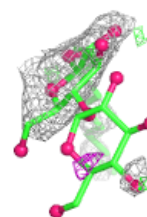
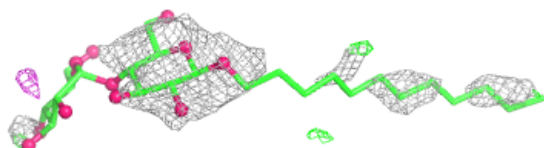
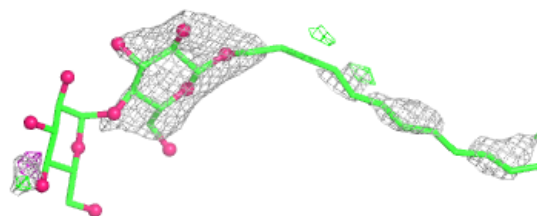


Electron density around DGD D 408:

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

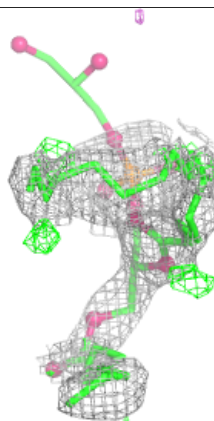
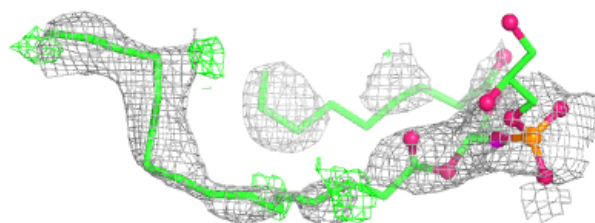
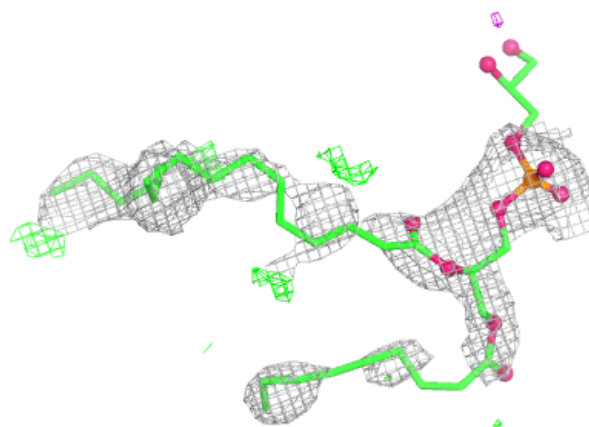
**Electron density around LMT F 101:**

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

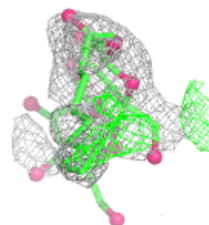
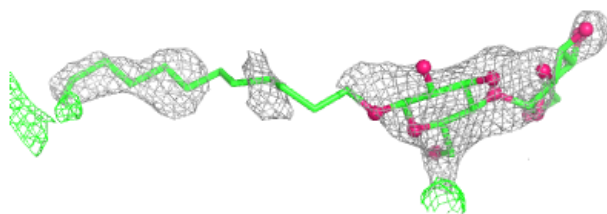
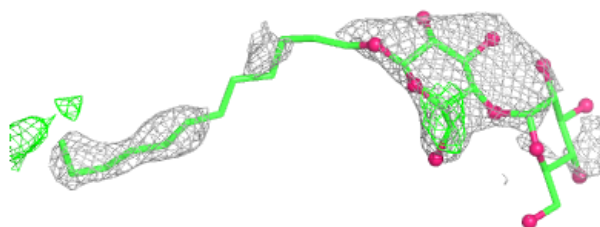


Electron density around LHG a 418:

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

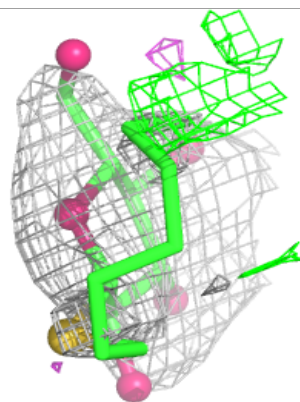
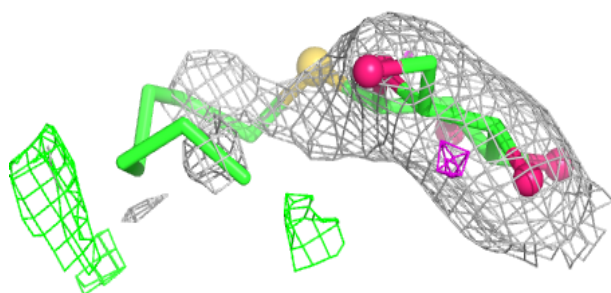
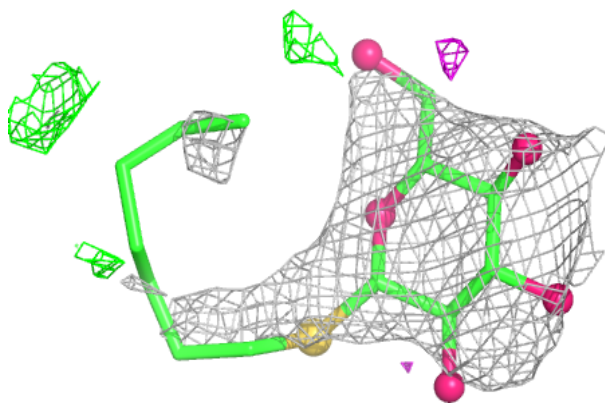
**Electron density around LMT e 102:**

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

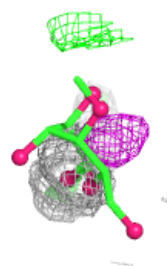
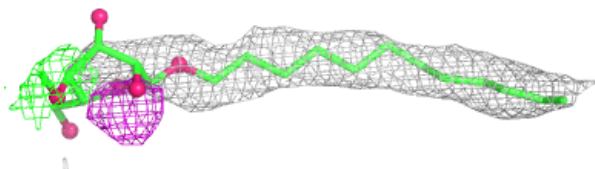
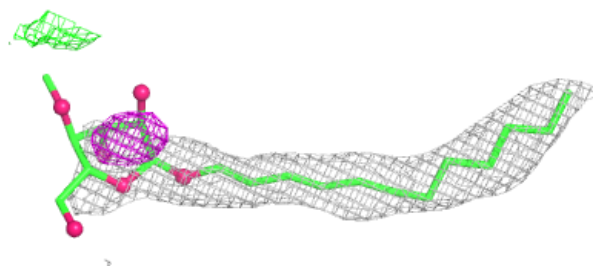


Electron density around HTG V 203:

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

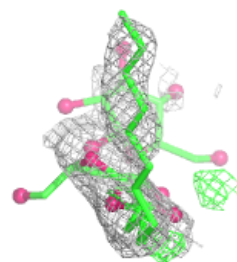
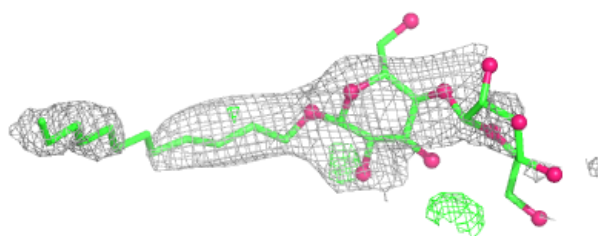
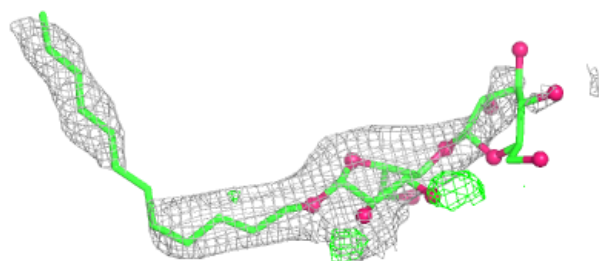
**Electron density around LMT b 626:**

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

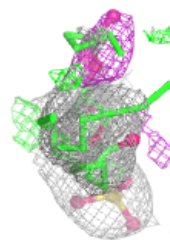
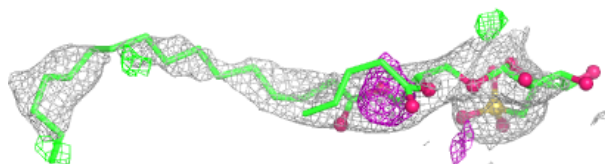
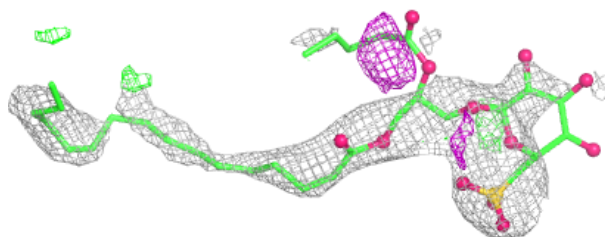


Electron density around LMT C 520:

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

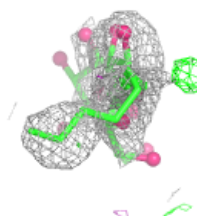
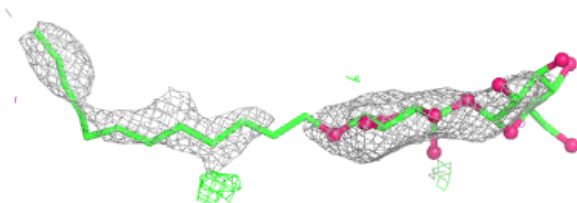
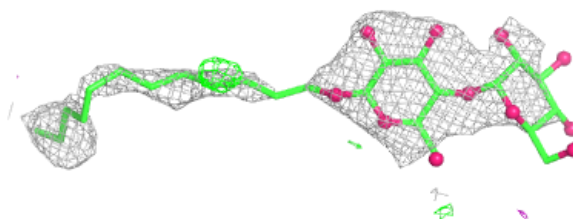
**Electron density around SQD f 102:**

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

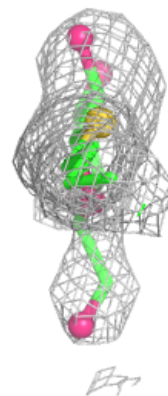
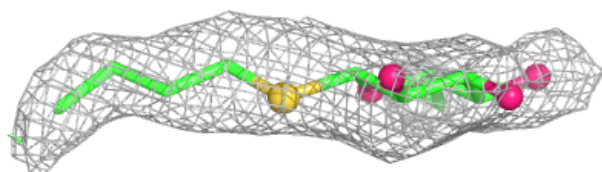
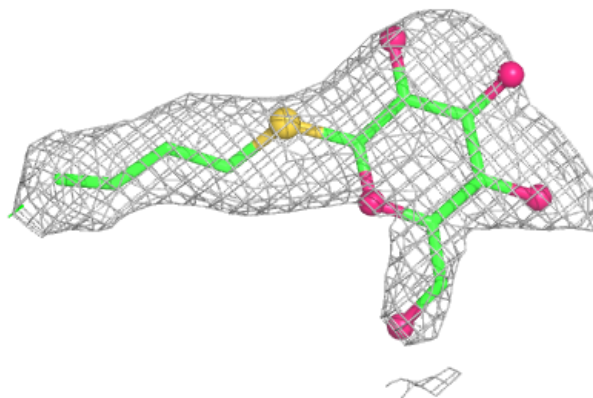


Electron density around LMT a 417:

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

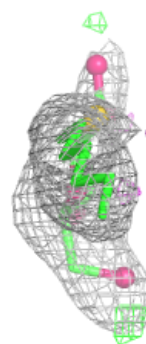
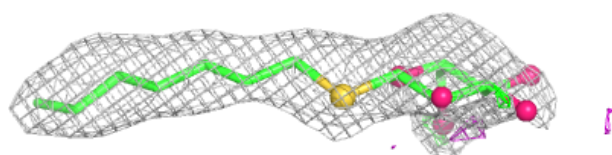
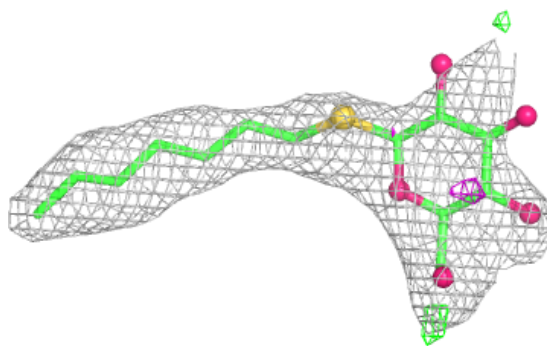
**Electron density around HTG d 414:**

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

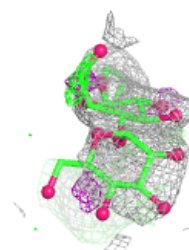
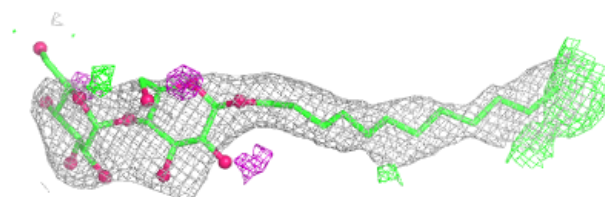
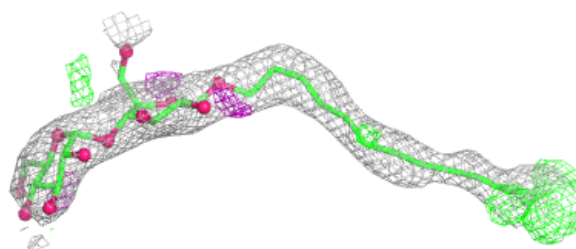


Electron density around HTG B 633:

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

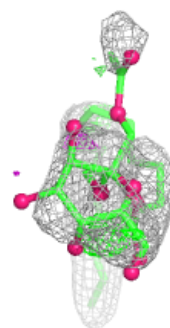
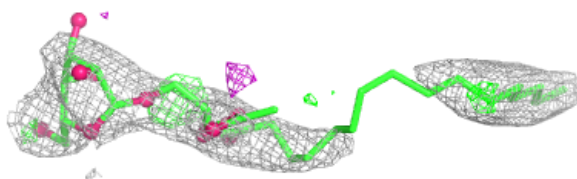
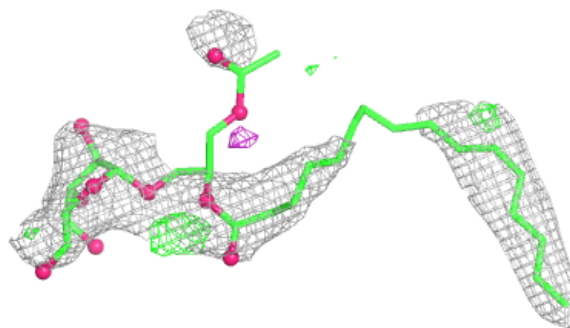
**Electron density around LMT A 415:**

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



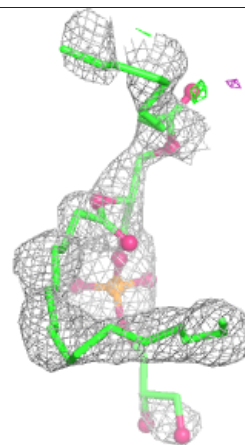
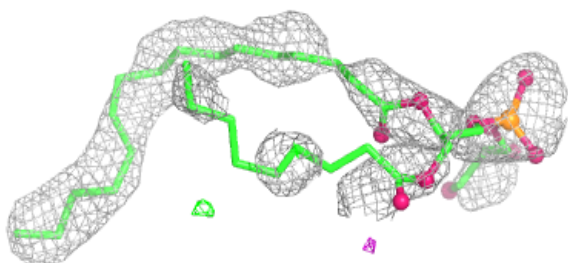
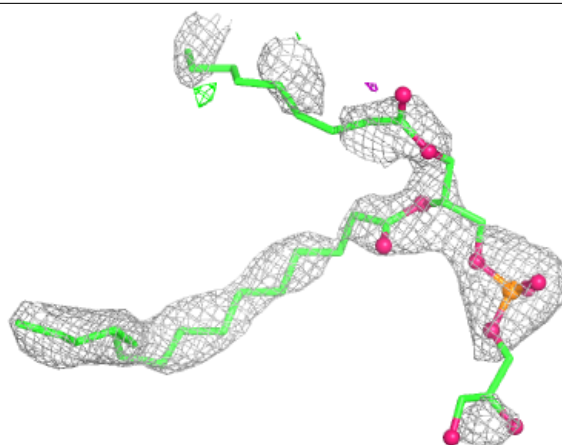
Electron density around LMG Z 101:

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



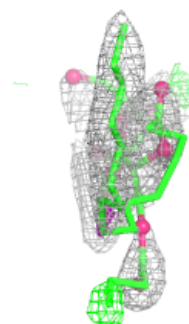
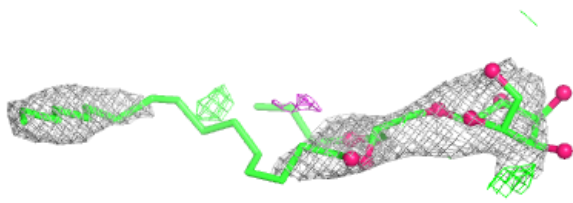
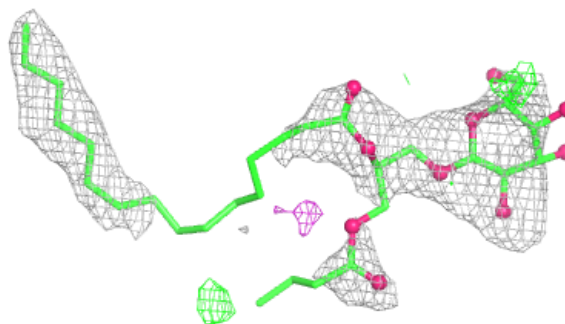
Electron density around LHG E 101:

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

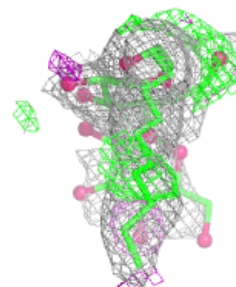
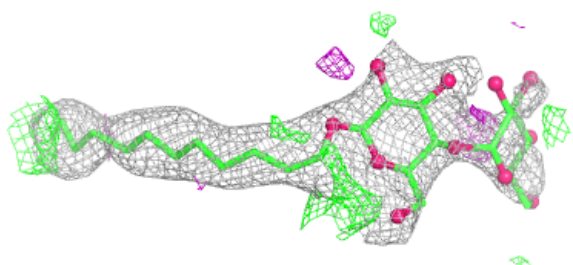
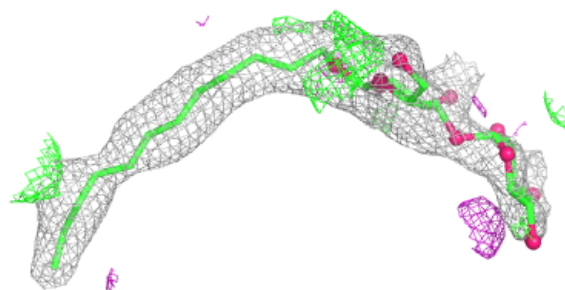


Electron density around LMG z 101:

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

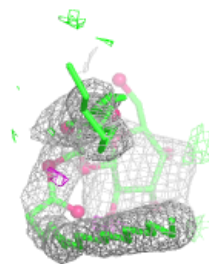
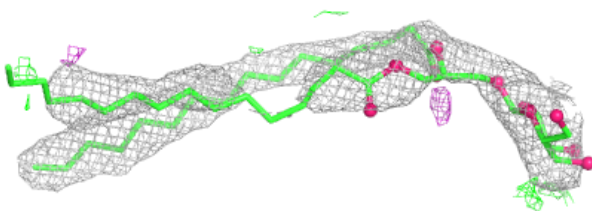
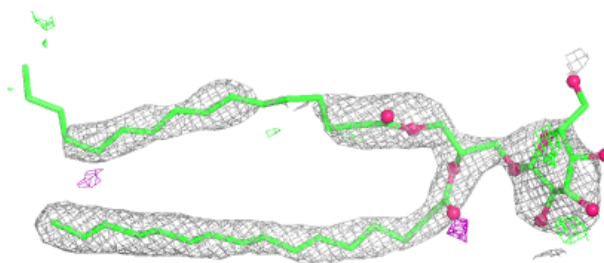
**Electron density around LMT M 103:**

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

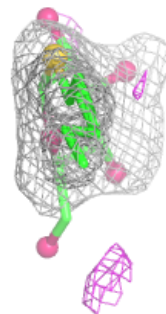
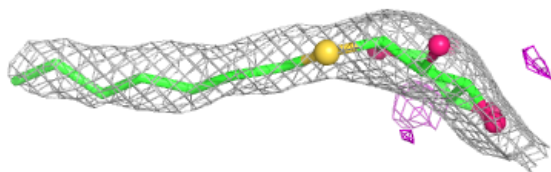
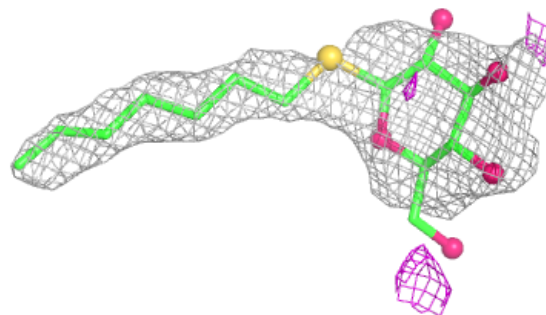


Electron density around LMG c 920:

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

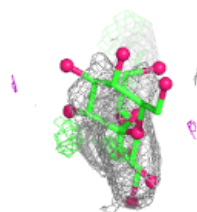
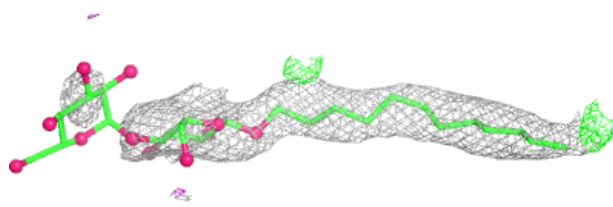
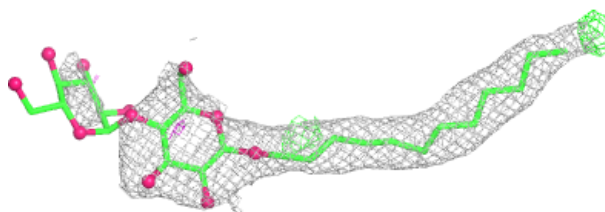
**Electron density around HTG B 625:**

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

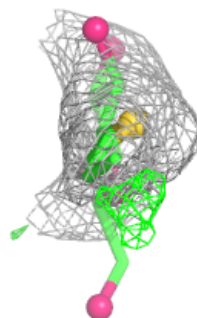
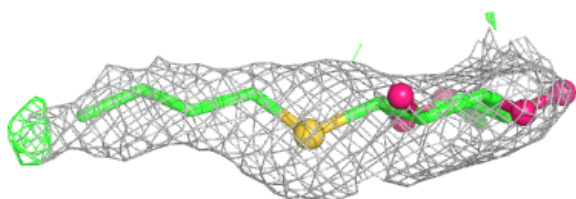
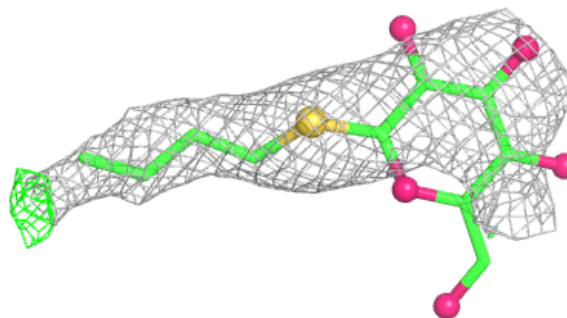


Electron density around LMT D 403:

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

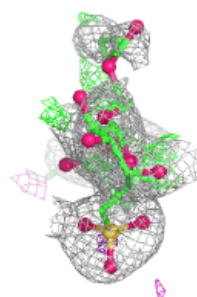
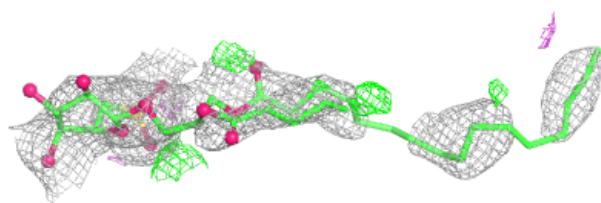
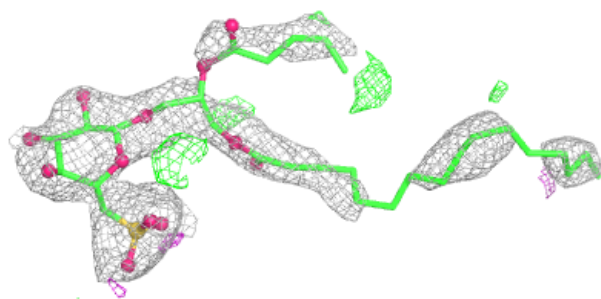
**Electron density around HTG D 413:**

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

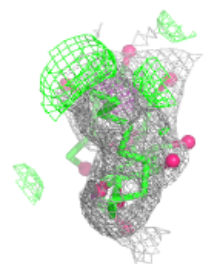
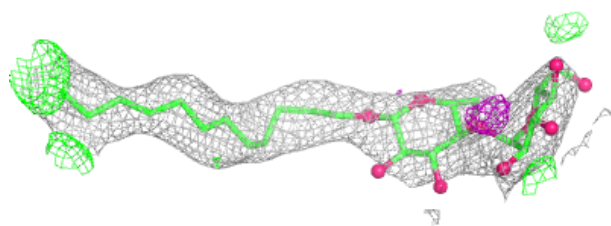
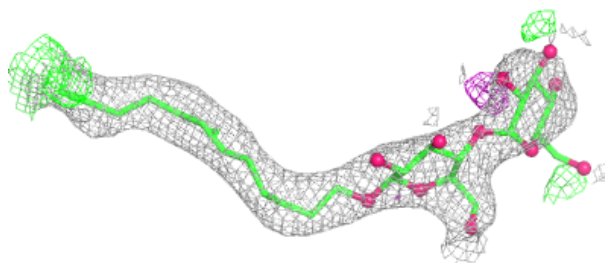


Electron density around SQD F 103:

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

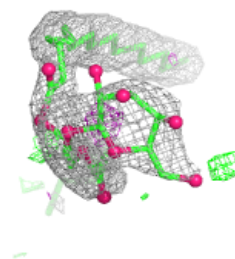
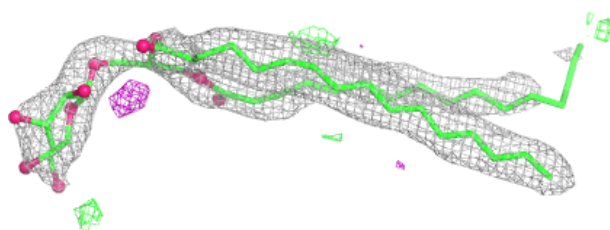
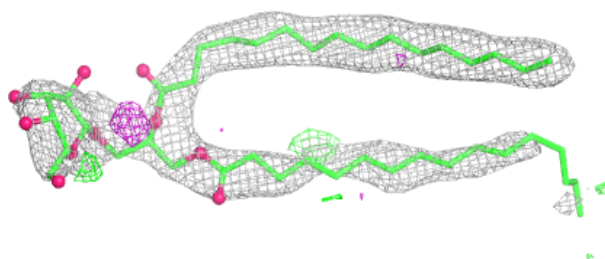
**Electron density around LMT a 401:**

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

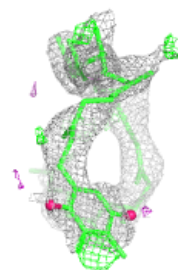
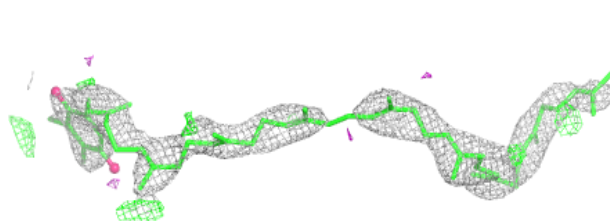
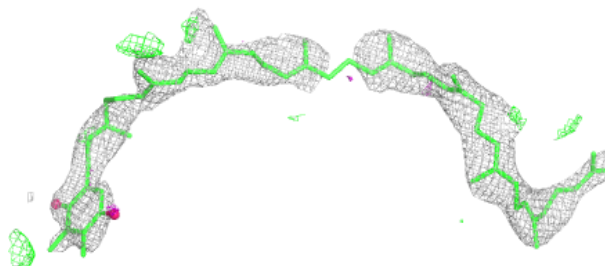


Electron density around LMG C 519:

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

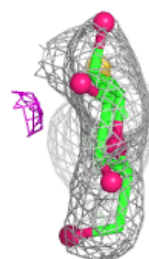
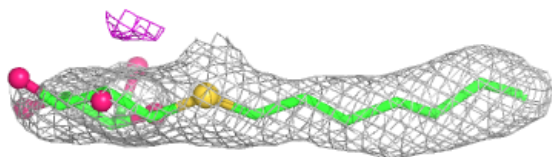
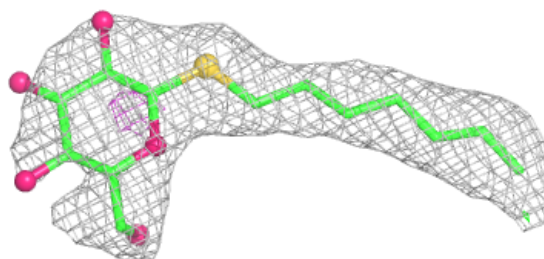
**Electron density around PL9 A 417:**

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

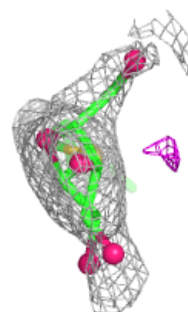
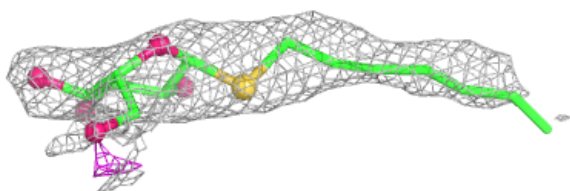
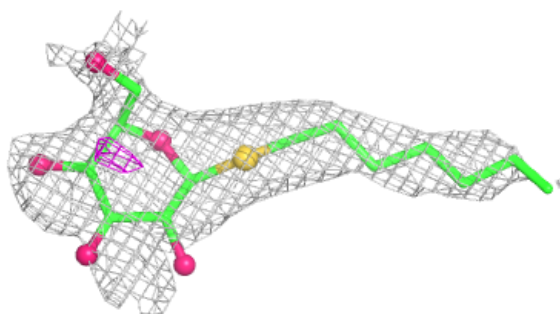


Electron density around HTG b 604:

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

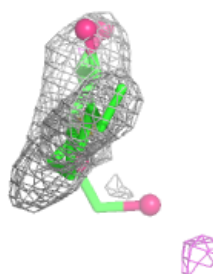
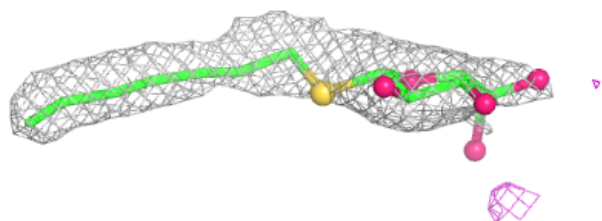
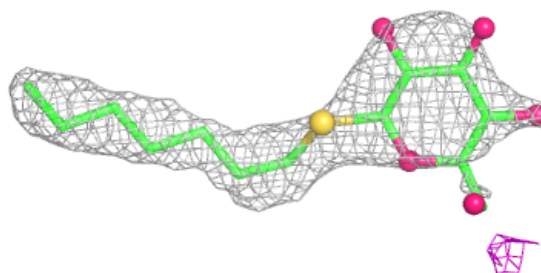
**Electron density around HTG C 522:**

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

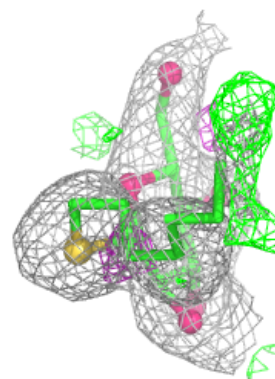
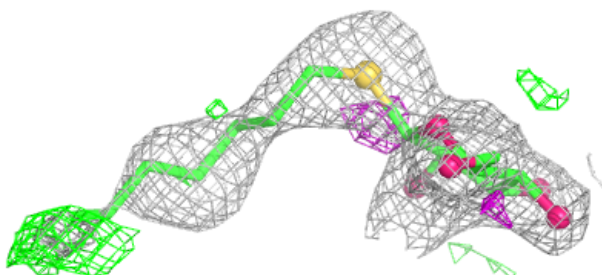
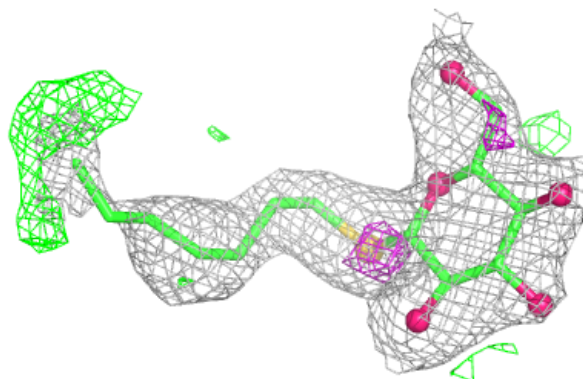


Electron density around HTG c 922:

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

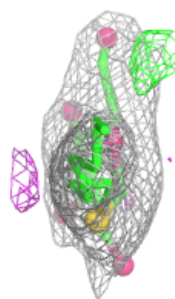
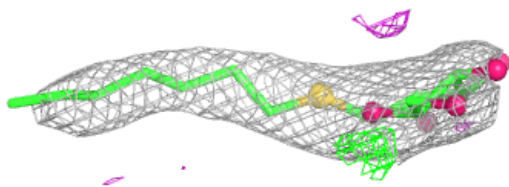
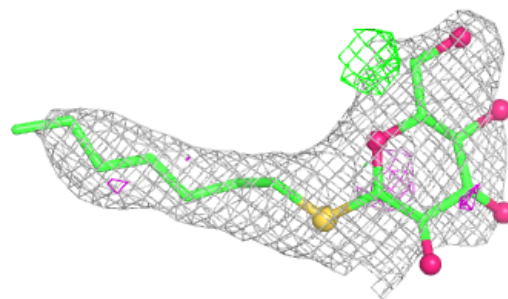
**Electron density around HTG b 627:**

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

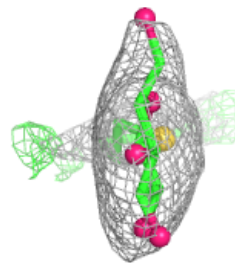
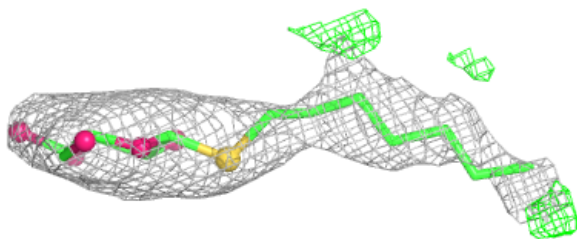
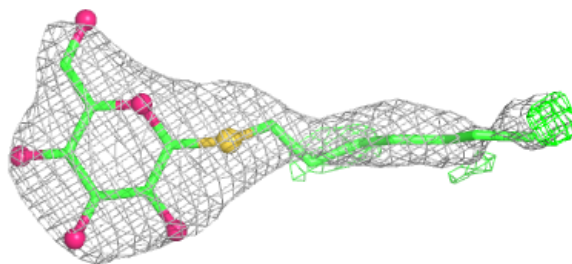


Electron density around HTG b 628:

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

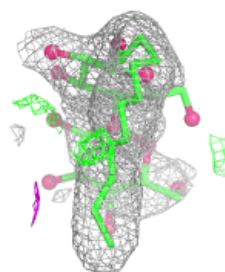
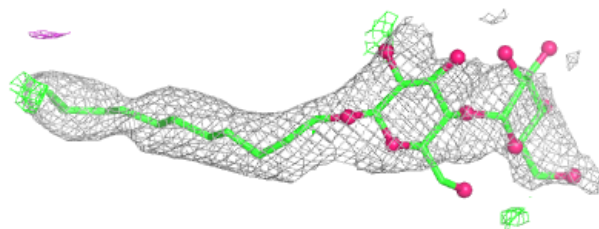
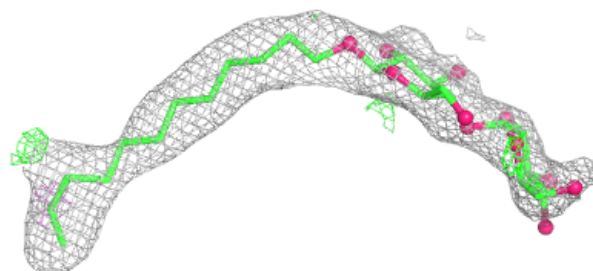
**Electron density around HTG c 921:**

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

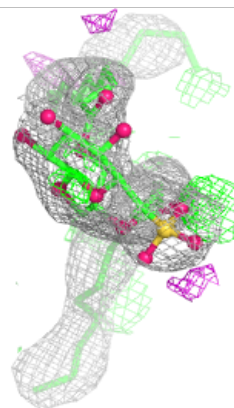
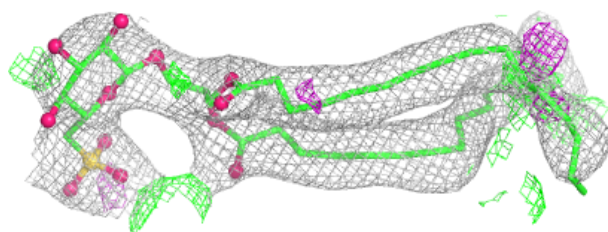
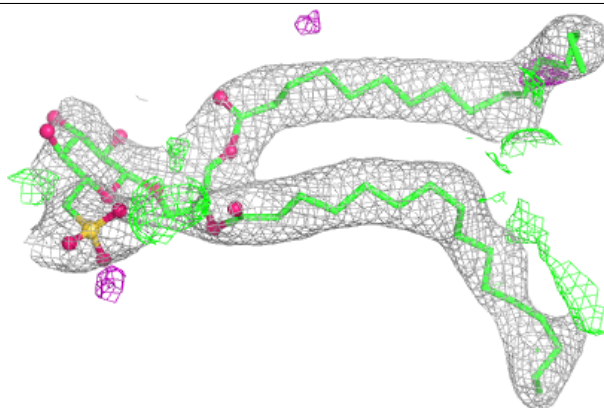


Electron density around LMT m 103:

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

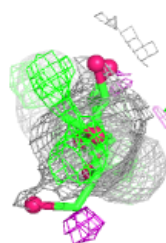
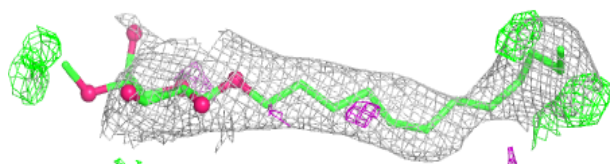
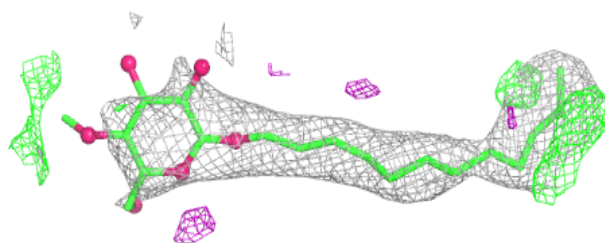
**Electron density around SQD B 621:**

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

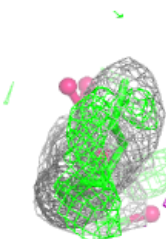
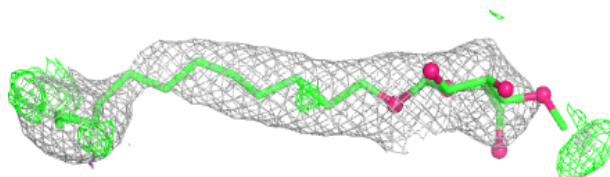
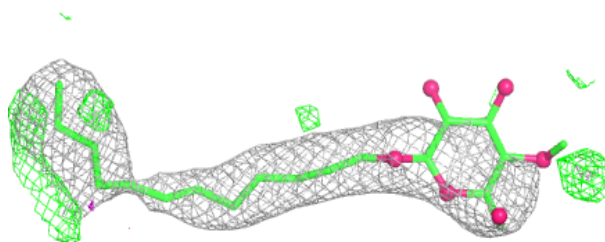


Electron density around LMT t 101:

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

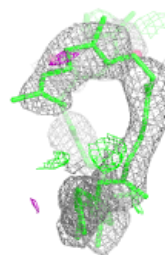
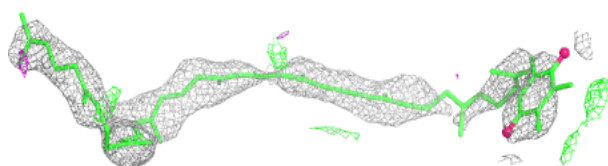
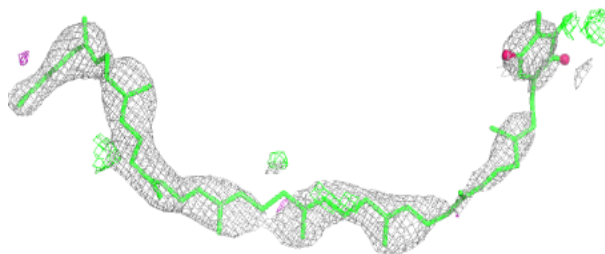
**Electron density around LMT b 602:**

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



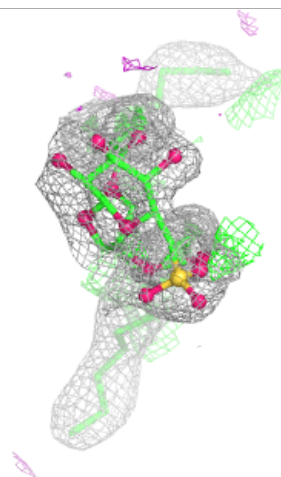
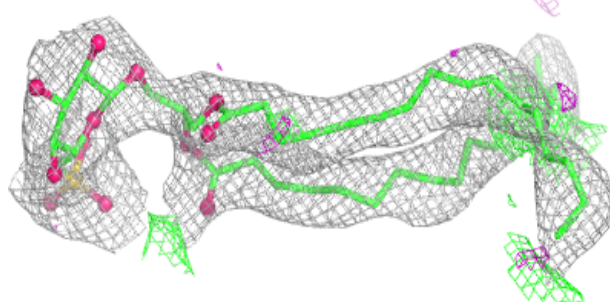
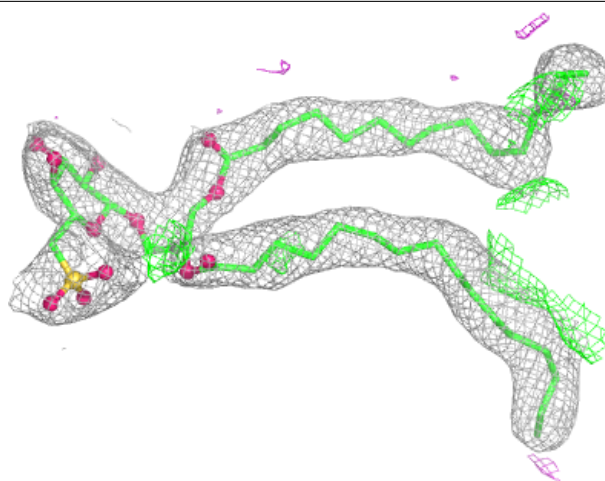
Electron density around PL9 a 415:

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



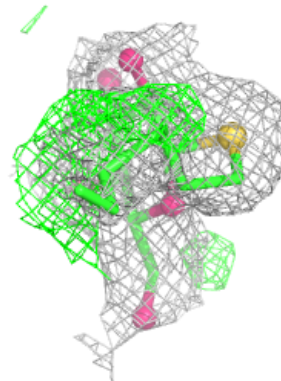
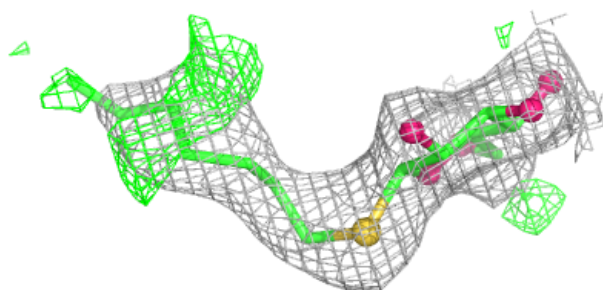
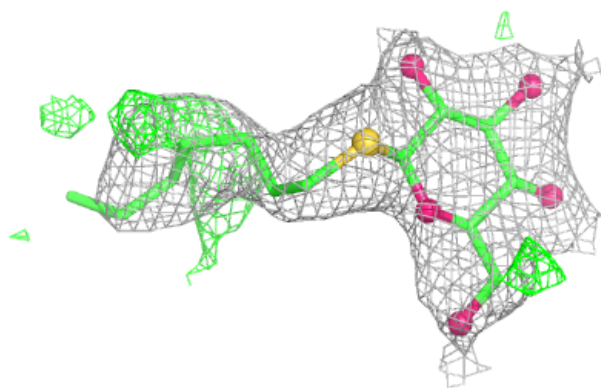
Electron density around SQD L 102:

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

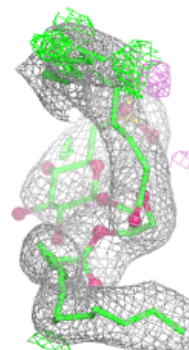
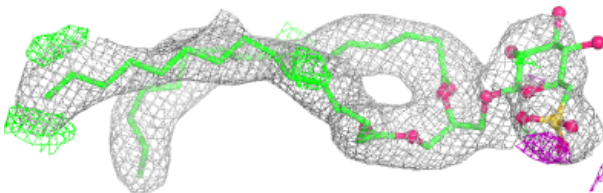
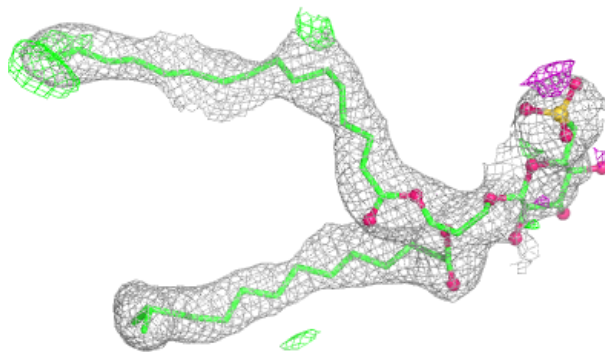


Electron density around HTG B 624:

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

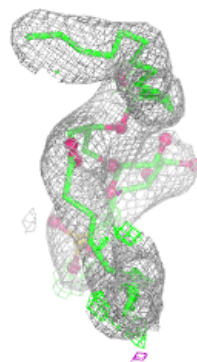
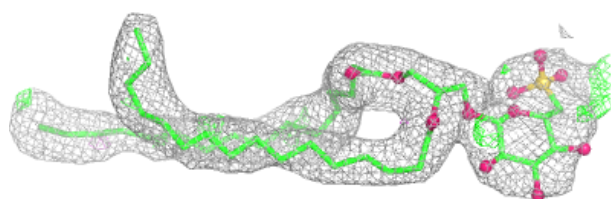
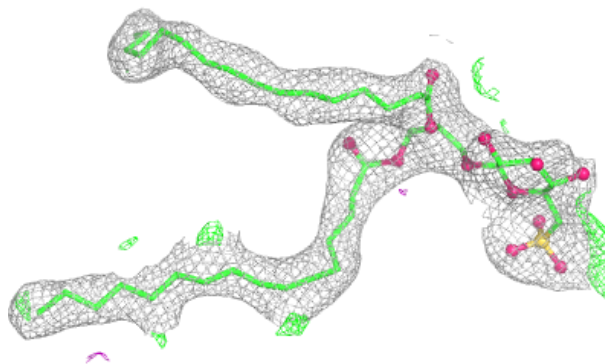
**Electron density around SQD A 414:**

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

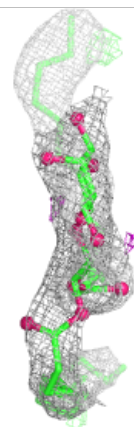
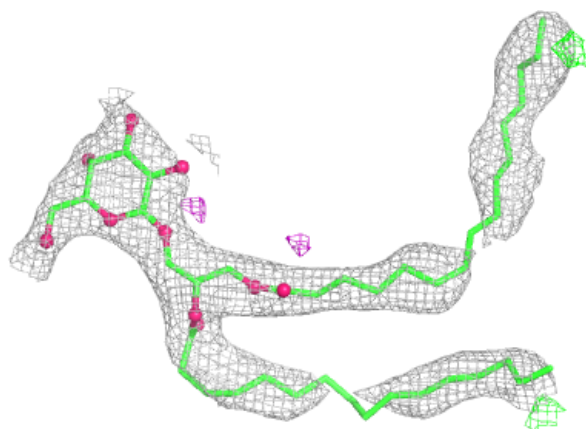


Electron density around SQD a 402:

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

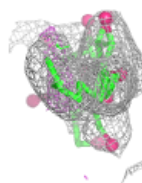
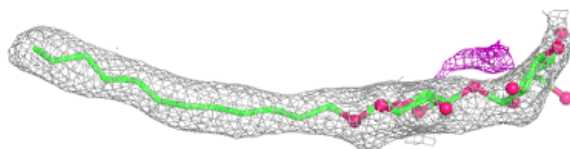
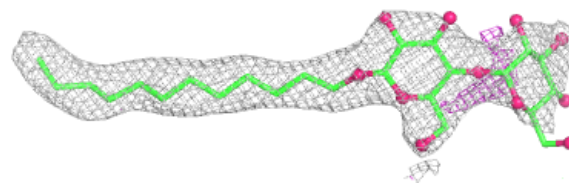
**Electron density around LMG Y 101:**

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

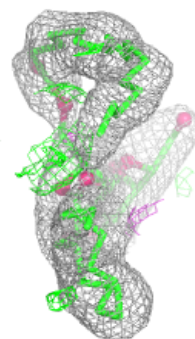
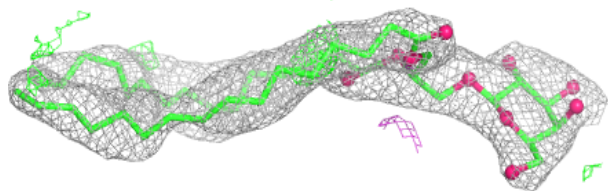
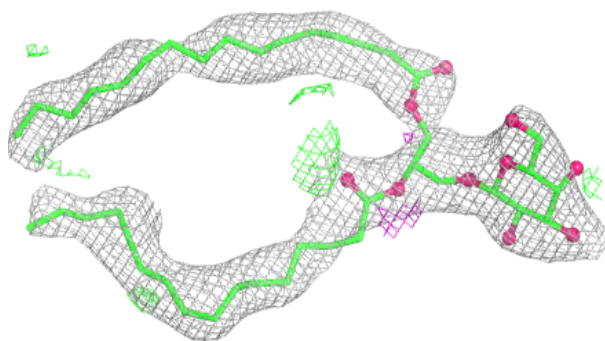


Electron density around LMT m 102:

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

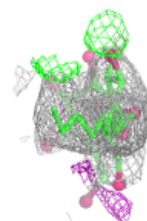
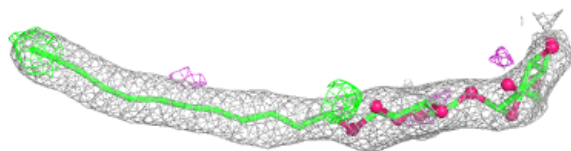
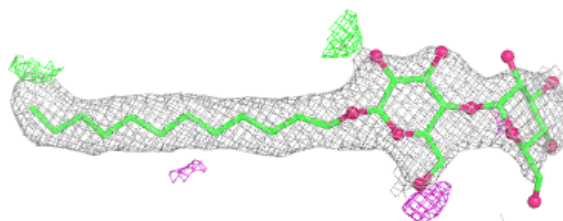
**Electron density around LMG A 419:**

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

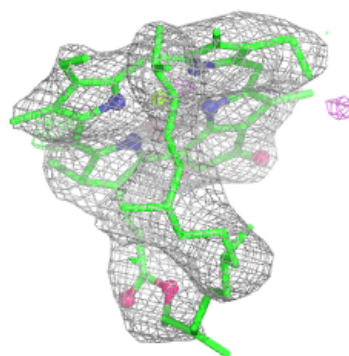
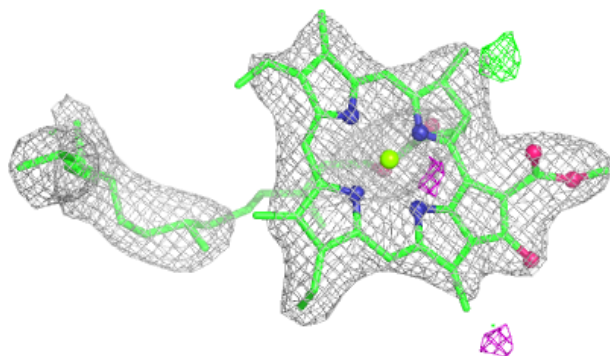
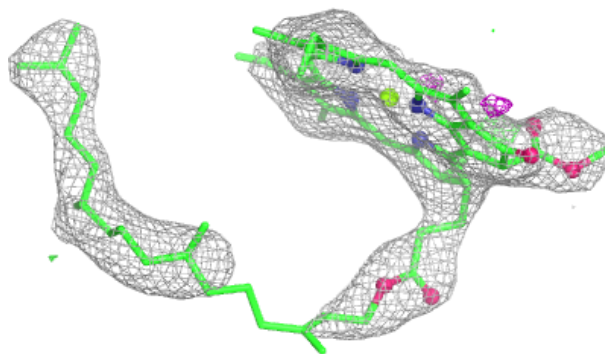


Electron density around LMT M 101:

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

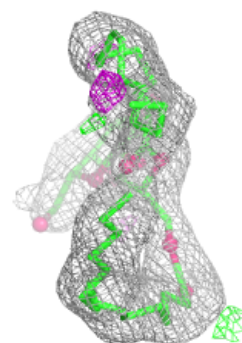
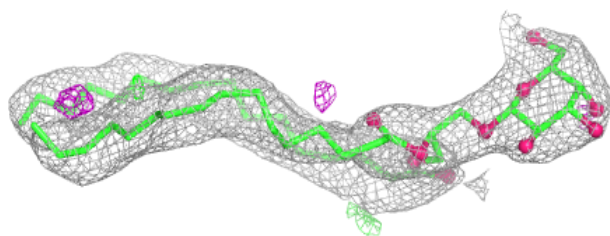
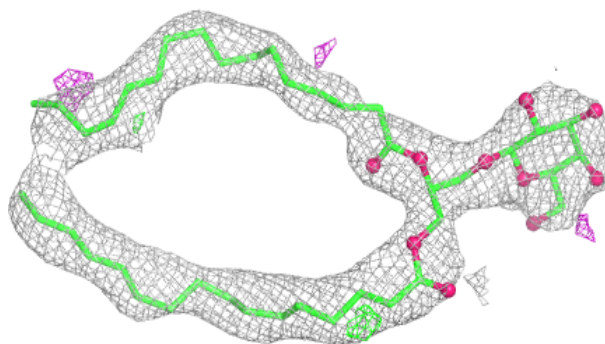
**Electron density around CLA C 513:**

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

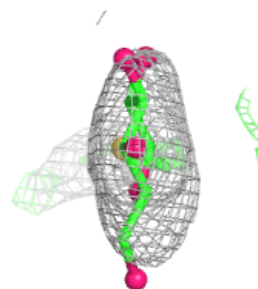
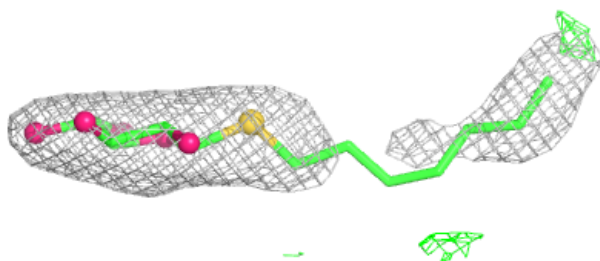
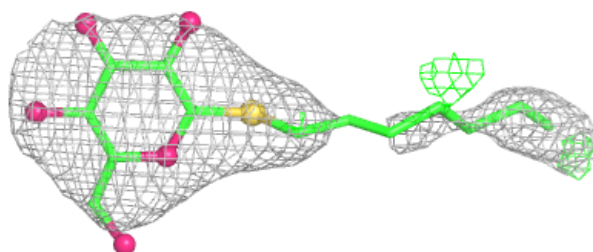


Electron density around LMG a 411:

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

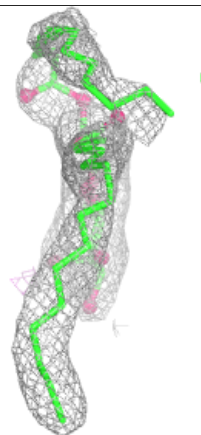
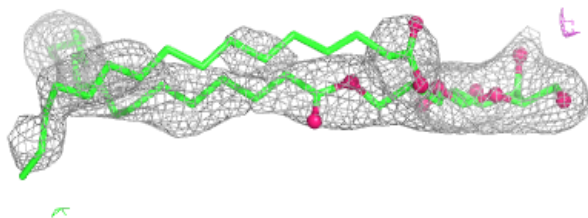
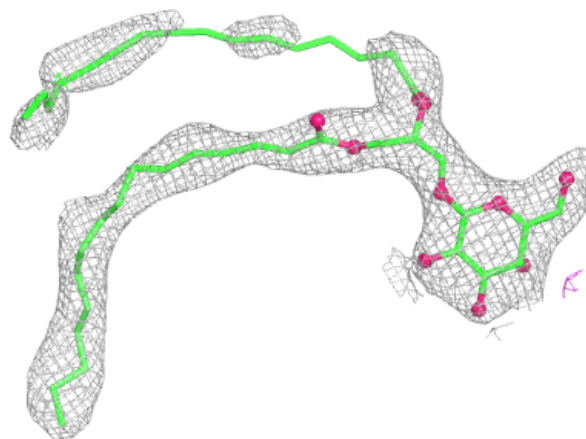
**Electron density around HTG C 521:**

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



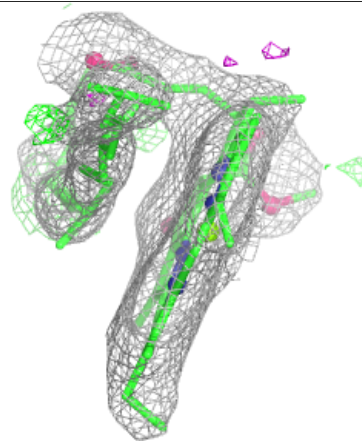
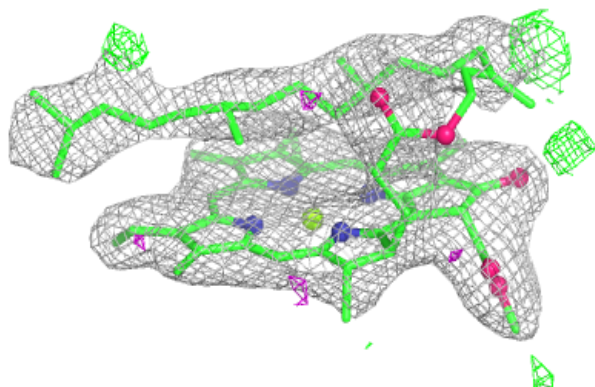
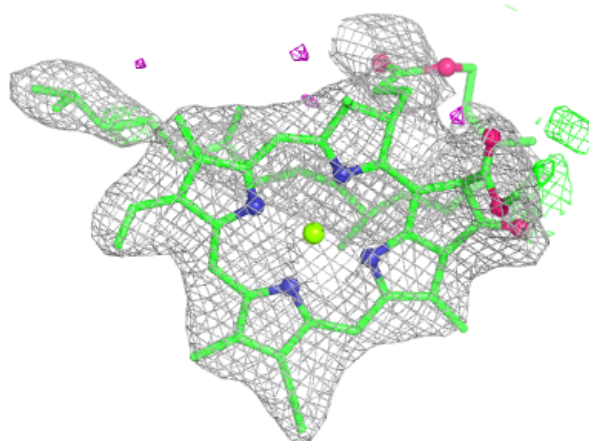
Electron density around LMG c 919:

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

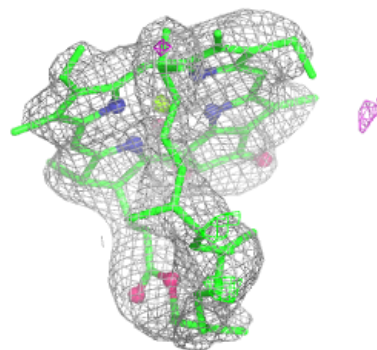
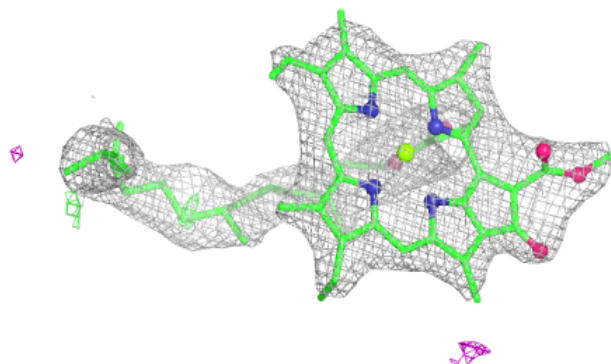
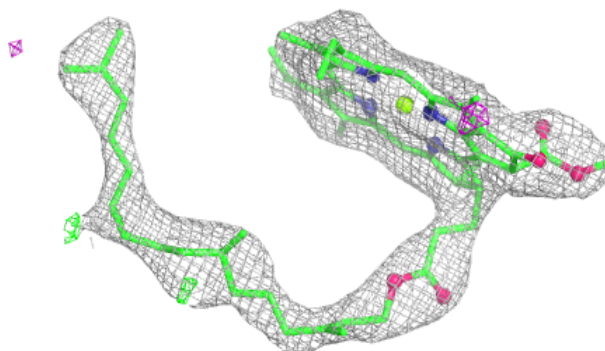


Electron density around CLA b 606:

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

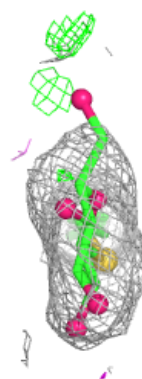
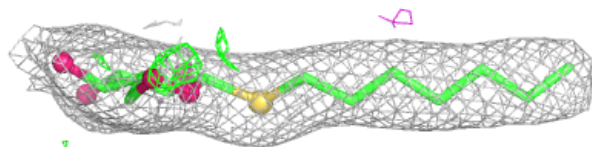
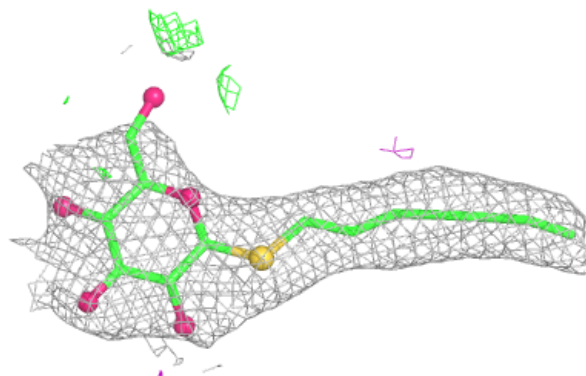
**Electron density around CLA c 914:**

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

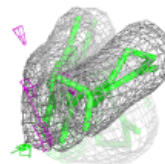
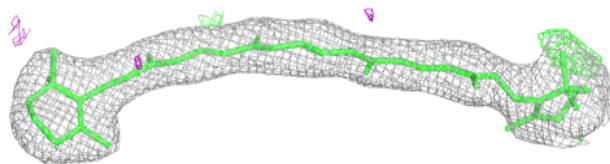
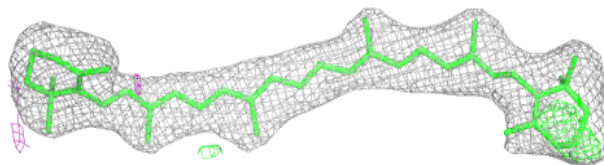


Electron density around HTG B 632:

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

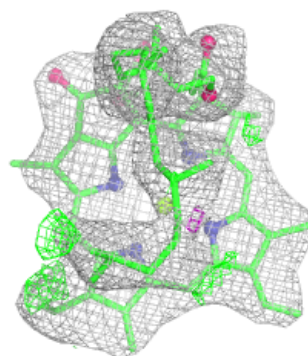
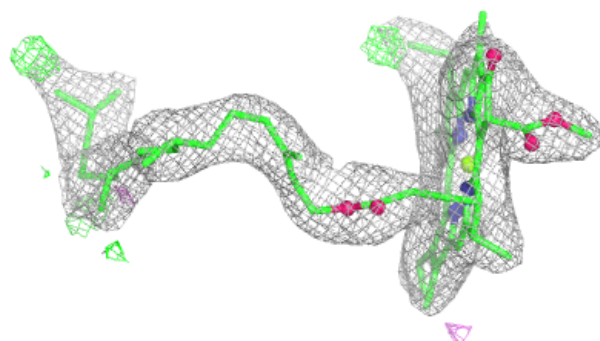
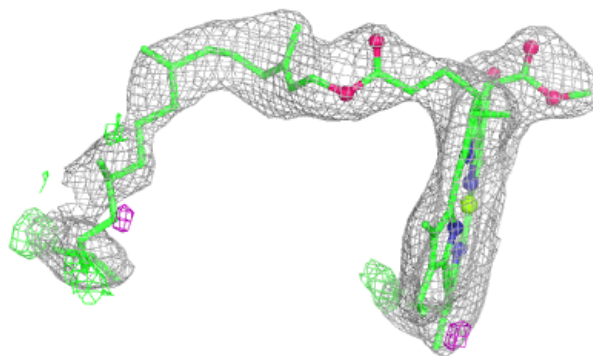
**Electron density around BCR d 407:**

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

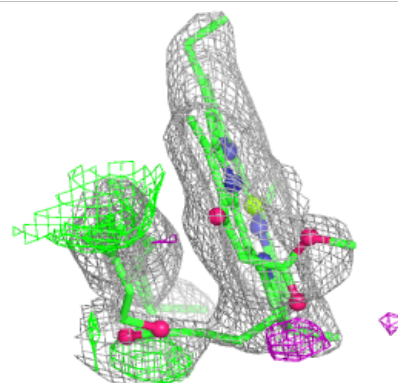
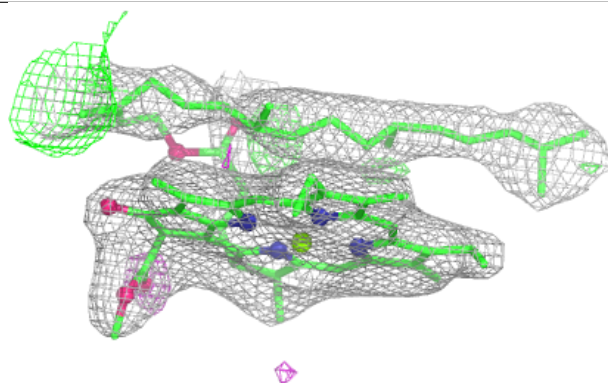
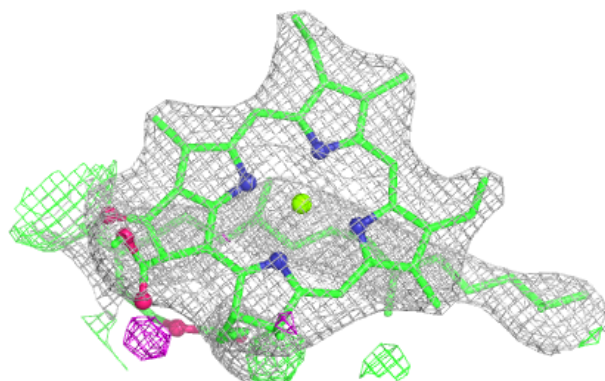


Electron density around CLA C 506:

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

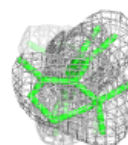
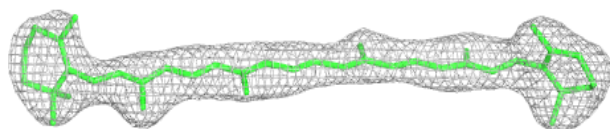
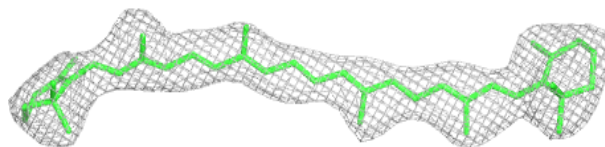
**Electron density around CLA B 602:**

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

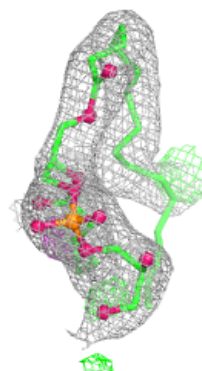
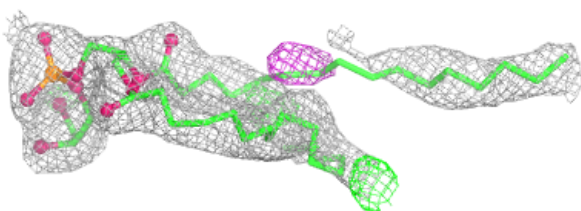
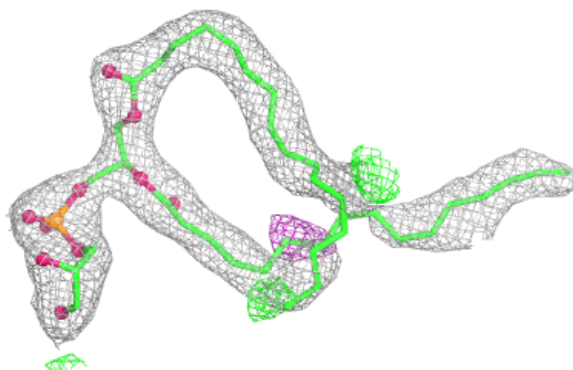


Electron density around BCR C 514:

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

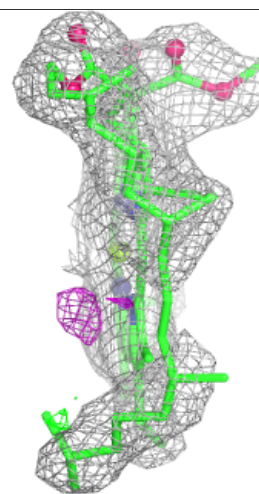
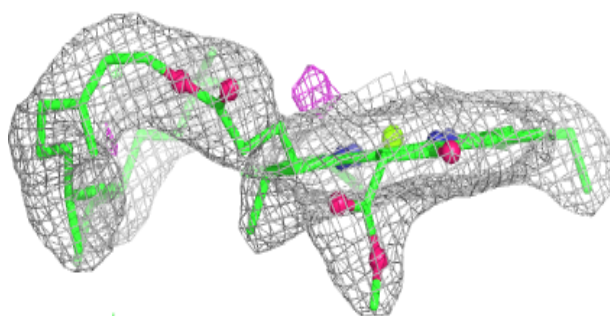
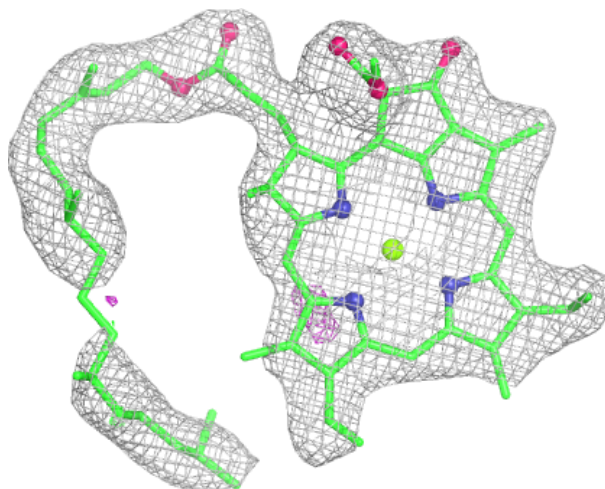
**Electron density around LHG D 410:**

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



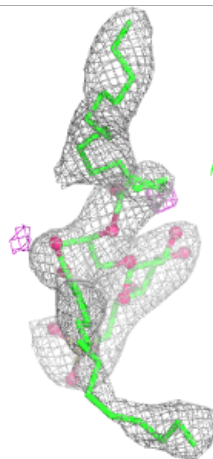
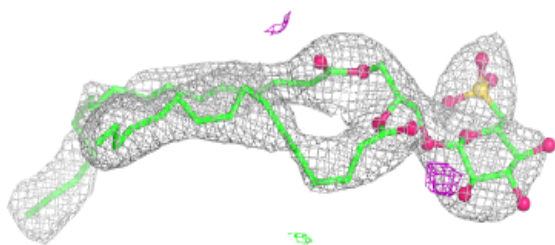
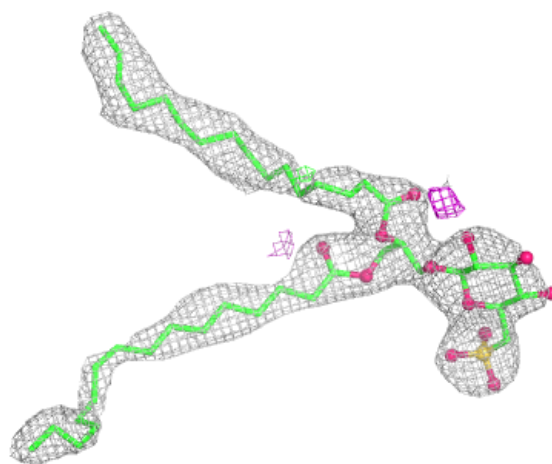
Electron density around CLA C 512:

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



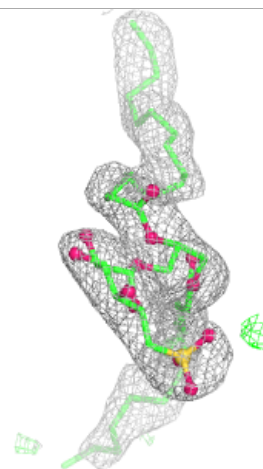
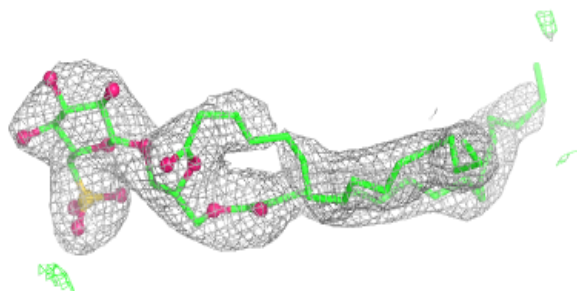
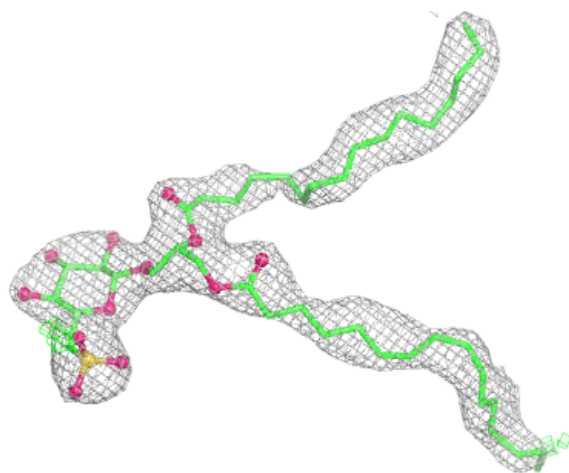
Electron density around SQD A 411:

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



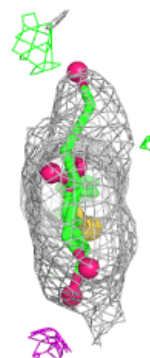
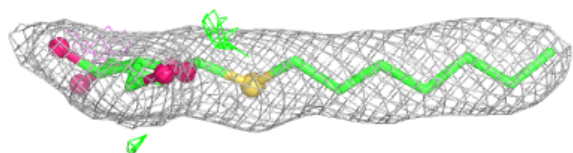
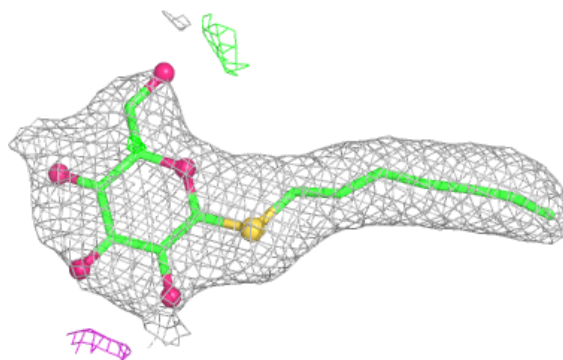
Electron density around SQD a 410:

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

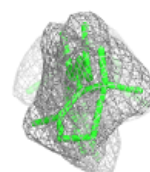
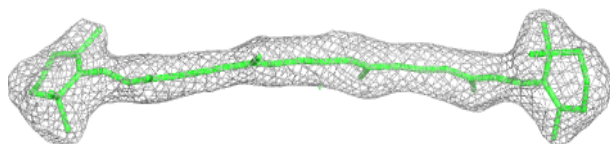
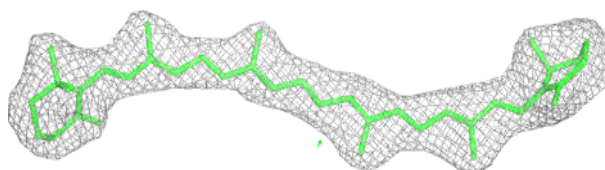


Electron density around HTG b 603:

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

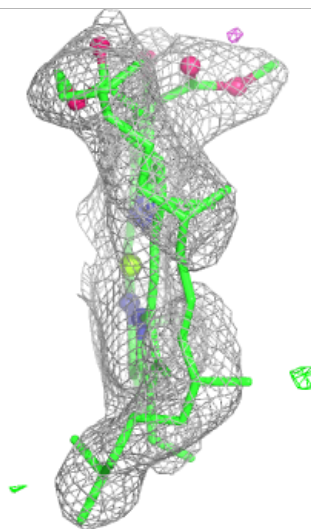
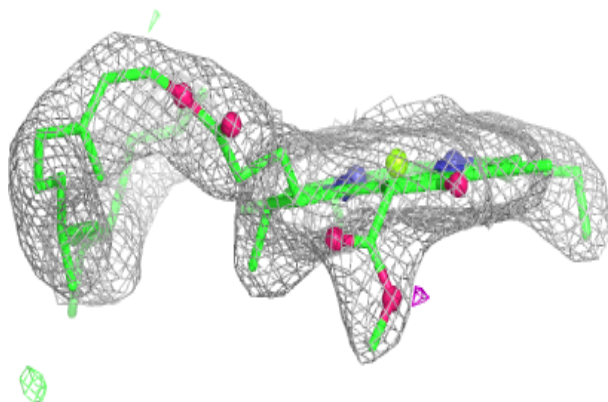
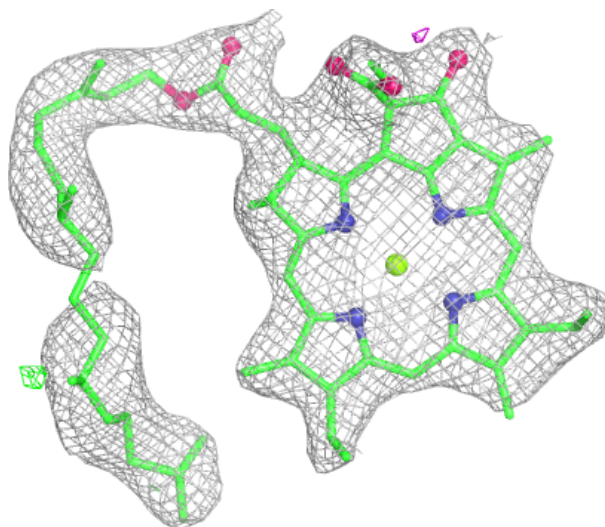
**Electron density around BCR y 101:**

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



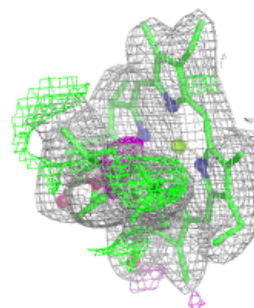
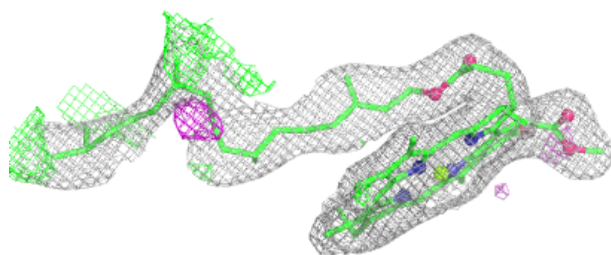
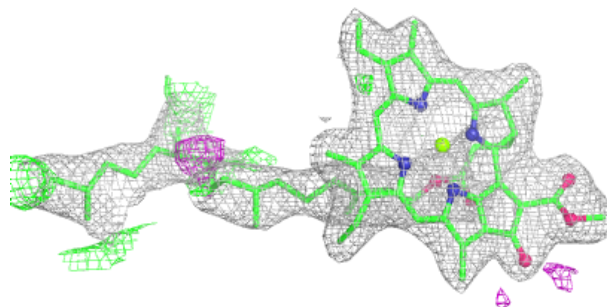
Electron density around CLA c 913:

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

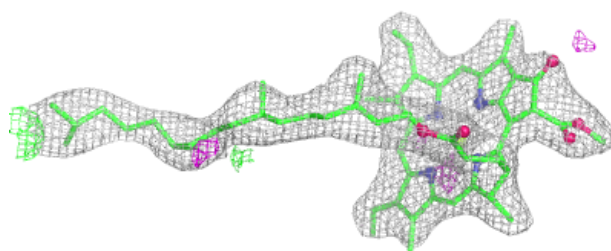
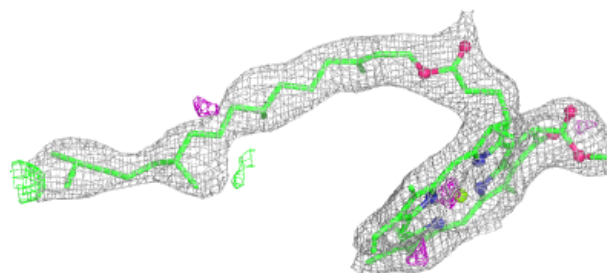


Electron density around CLA B 615:

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

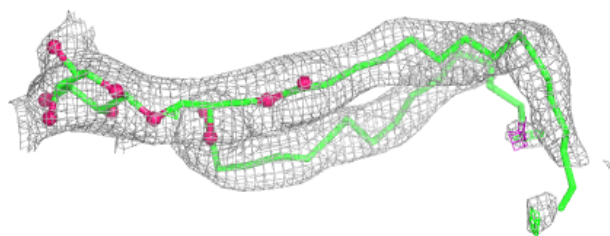
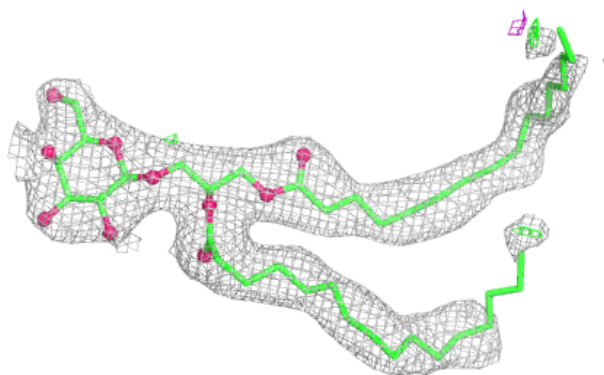
**Electron density around CLA C 504:**

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

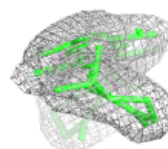
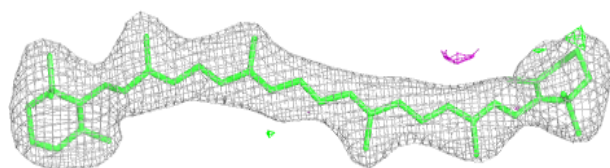
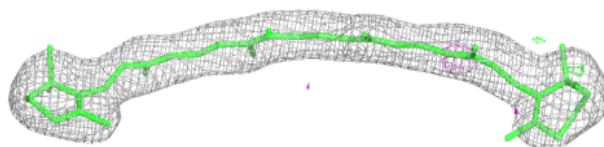


Electron density around LMG J 101:

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

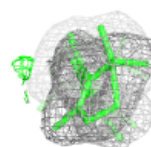
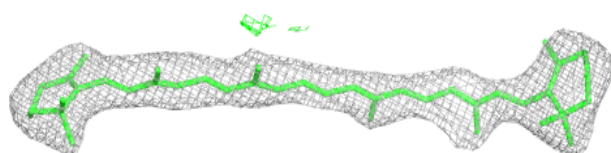
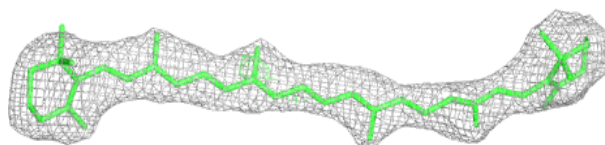
**Electron density around BCR D 406:**

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

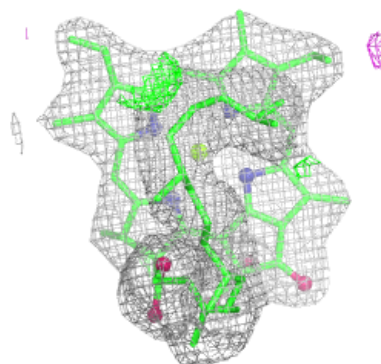
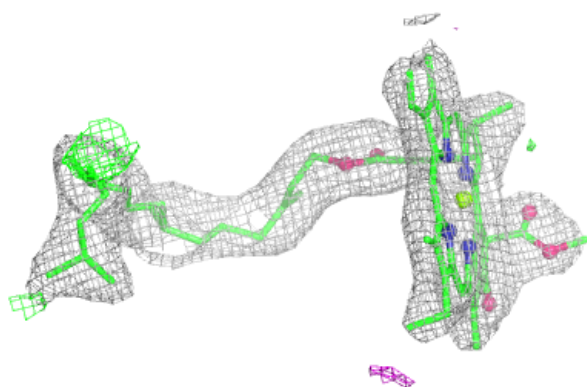
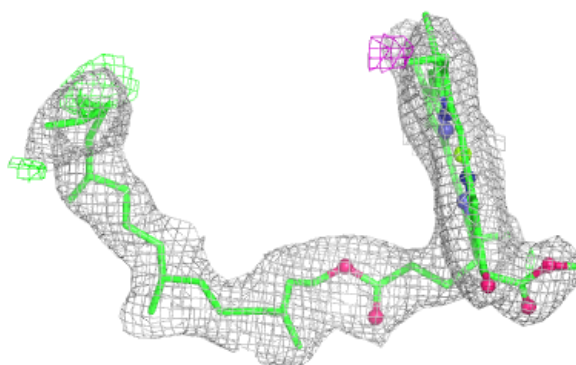


Electron density around BCR c 927:

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

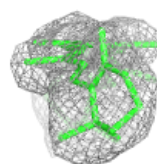
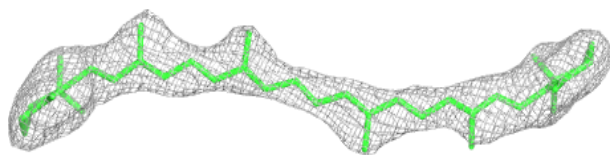
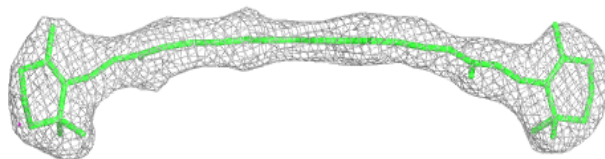
**Electron density around CLA c 907:**

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



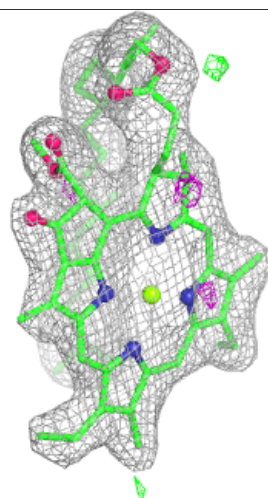
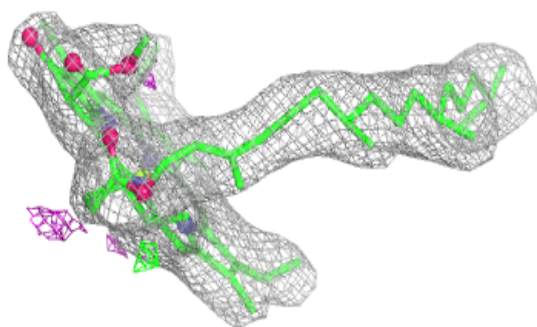
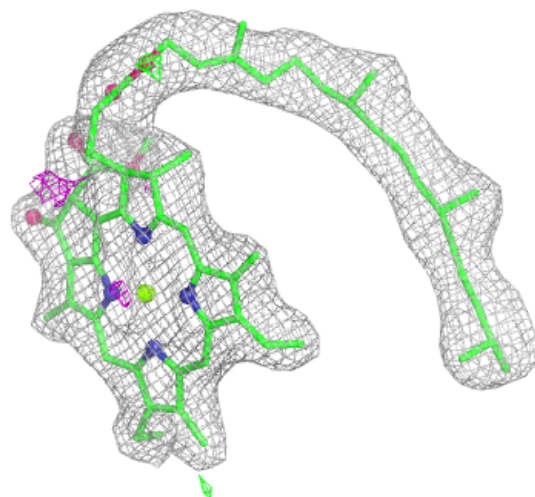
Electron density around BCR k 101:

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



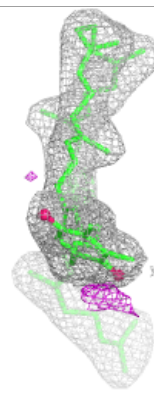
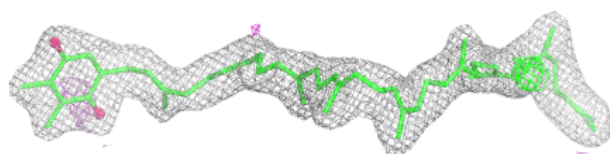
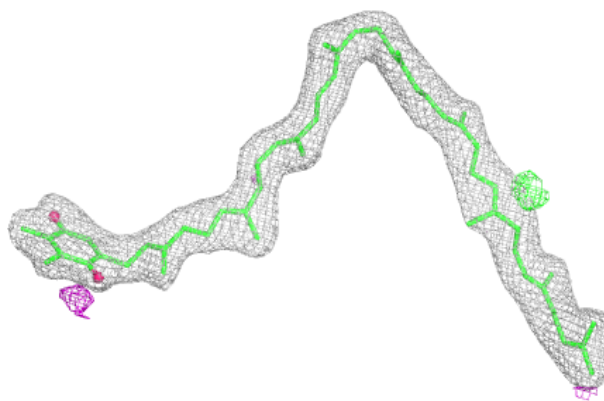
Electron density around CLA c 908:

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

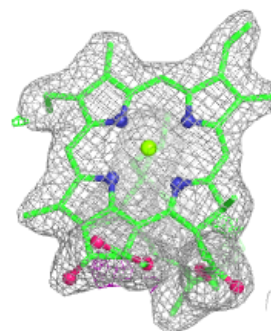
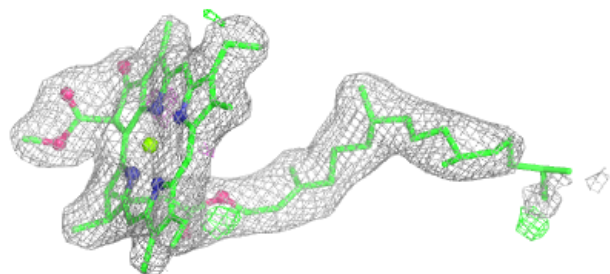
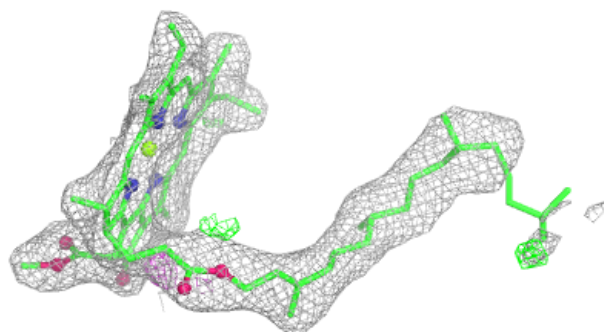


Electron density around PL9 D 407:

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

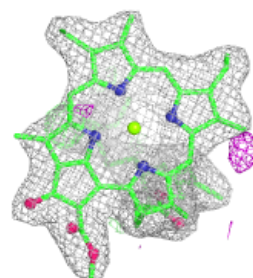
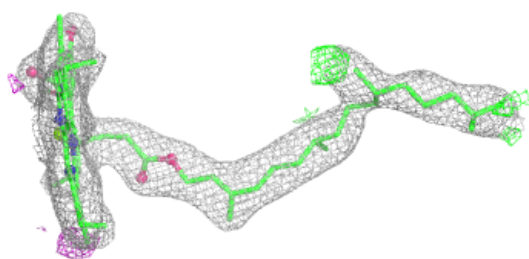
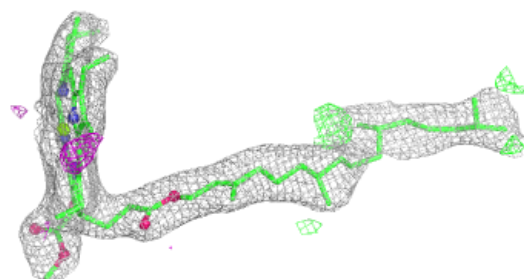
**Electron density around CLA c 909:**

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



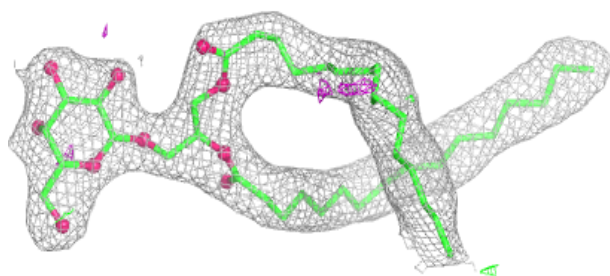
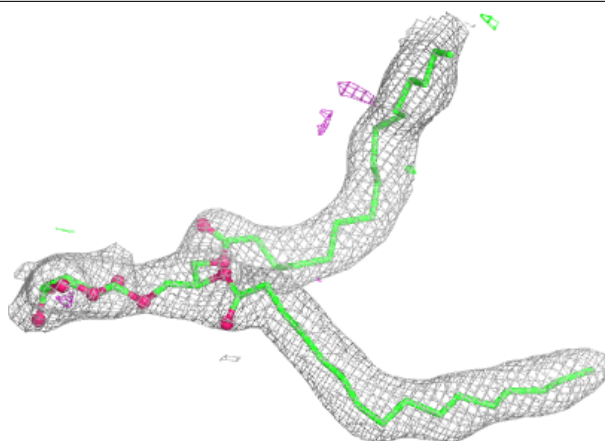
Electron density around CLA B 607:

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



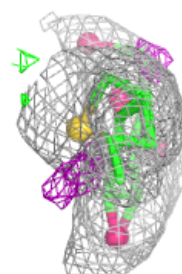
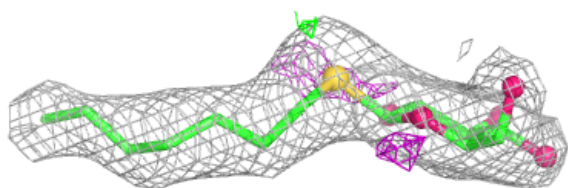
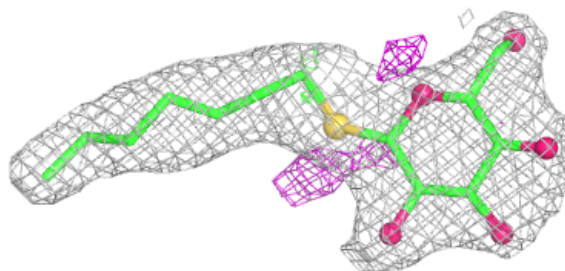
Electron density around LMG B 622:

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

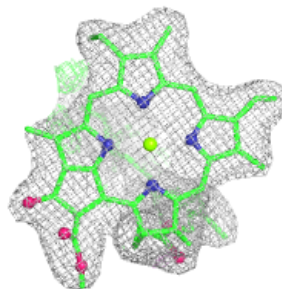
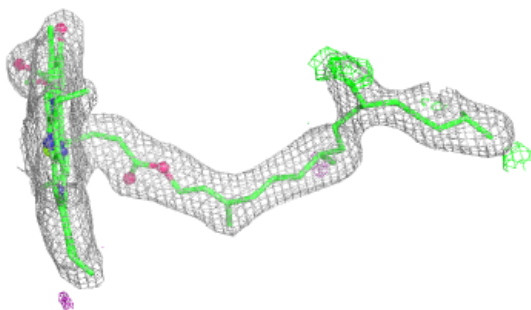
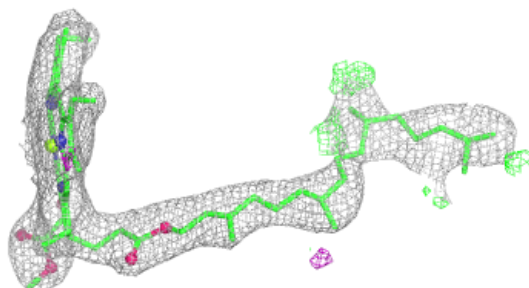


Electron density around HTG b 601:

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

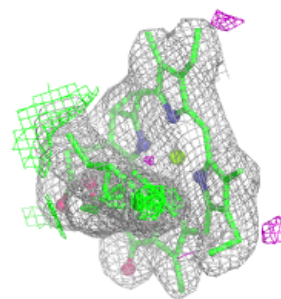
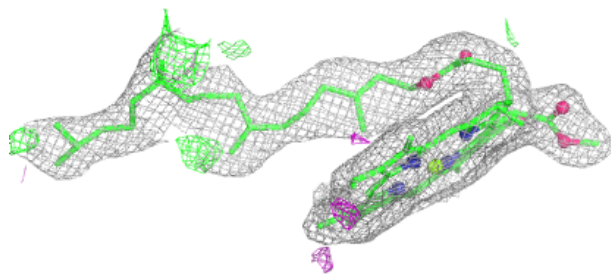
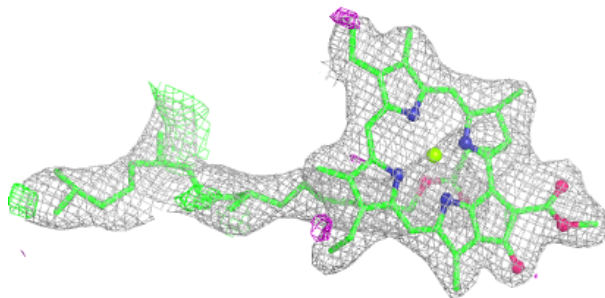
**Electron density around CLA b 611:**

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



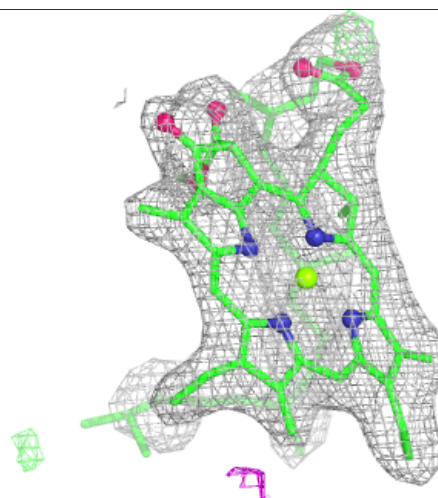
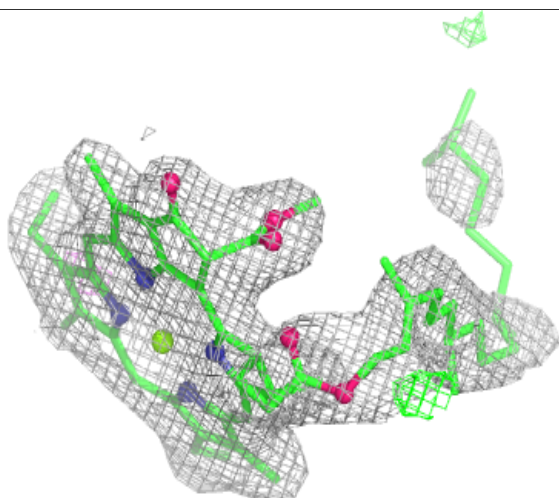
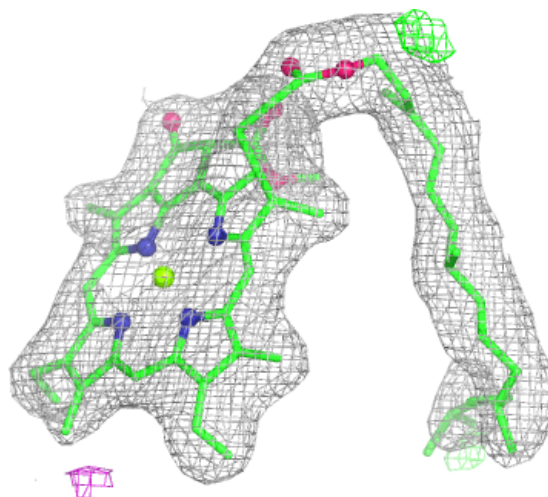
Electron density around CLA b 619:

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



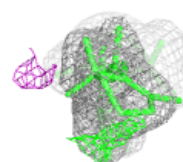
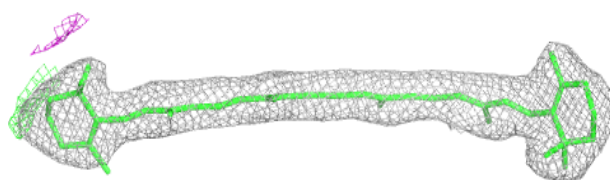
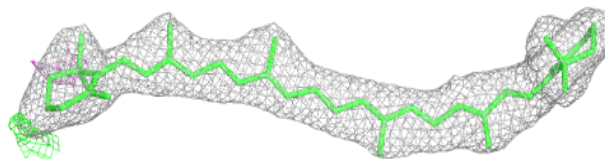
Electron density around CLA b 621:

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

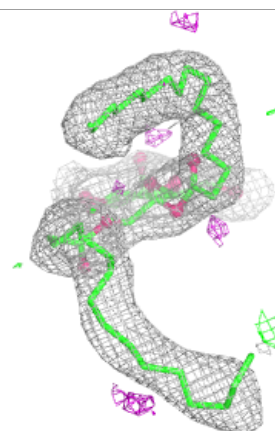
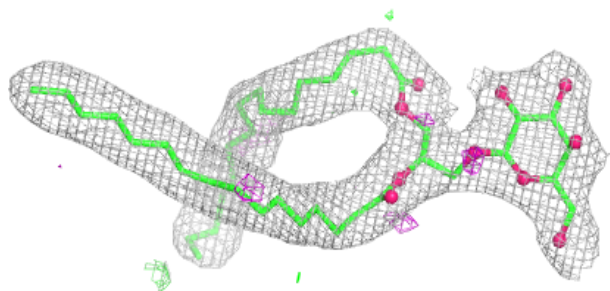
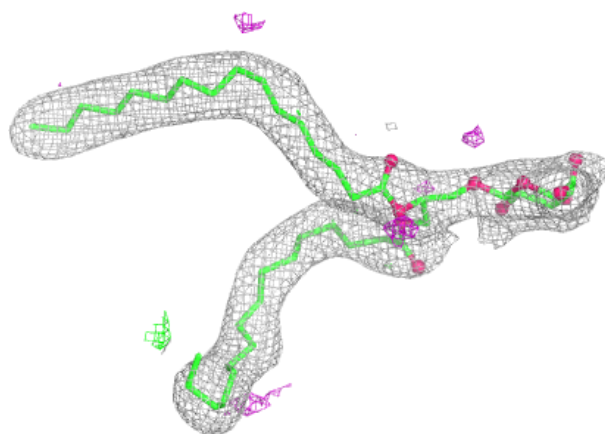


Electron density around BCR H 101:

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

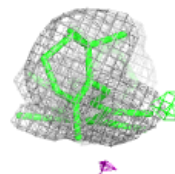
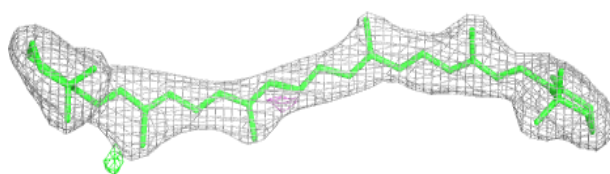
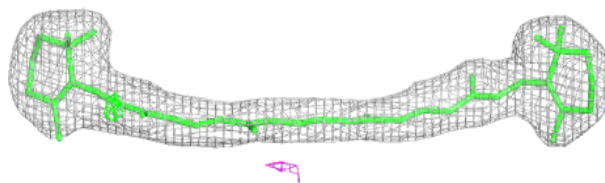
**Electron density around LMG b 625:**

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

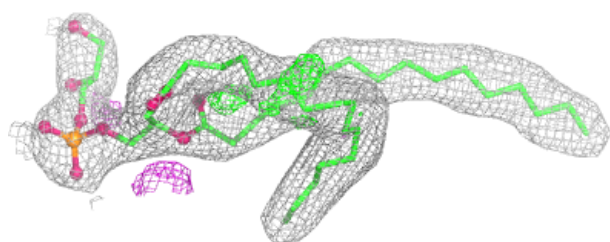
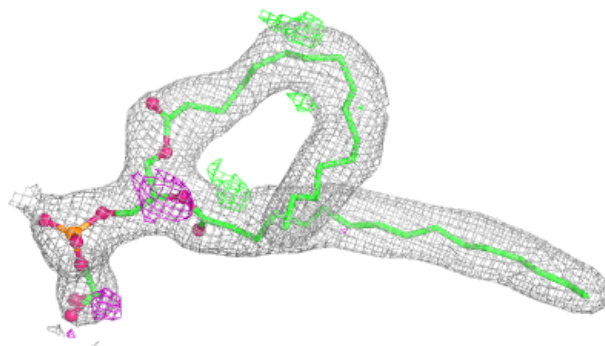


Electron density around BCR K 101:

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

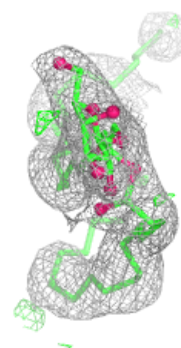
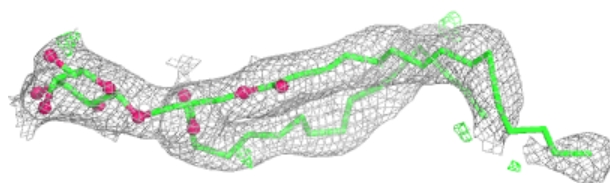
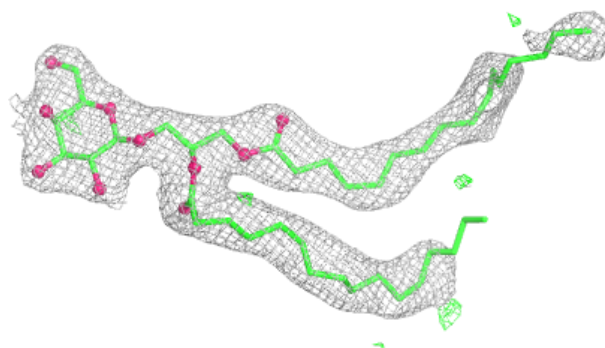
**Electron density around LHG B 635:**

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

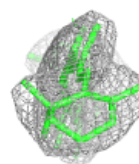
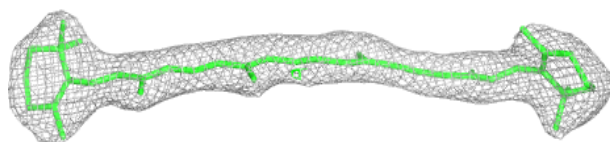
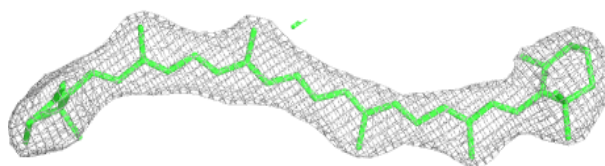


Electron density around LMG d 415:

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

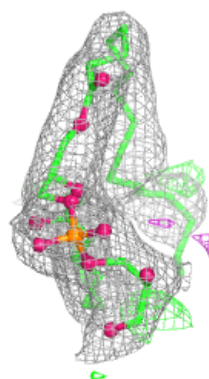
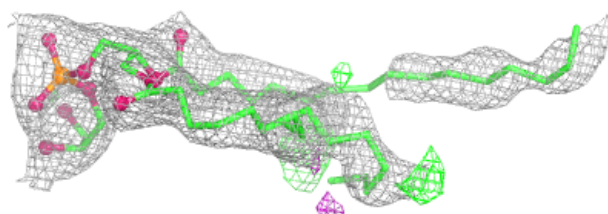
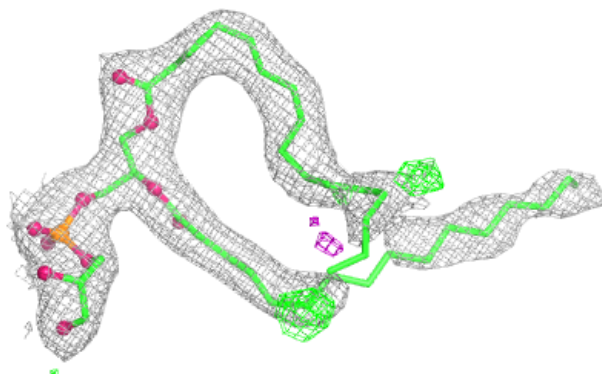
**Electron density around BCR Y 102:**

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

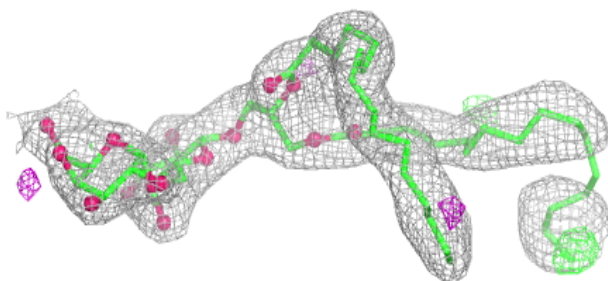
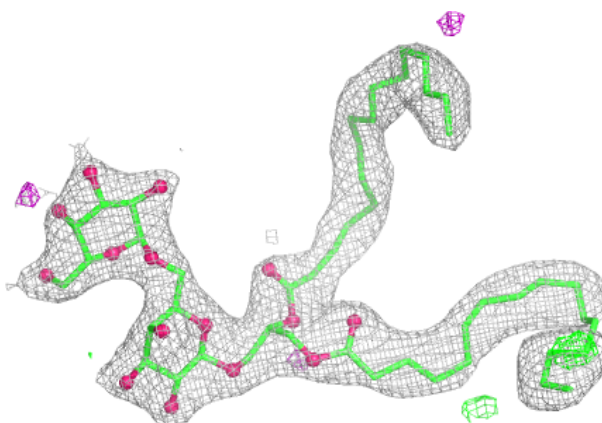


Electron density around LHG d 411:

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

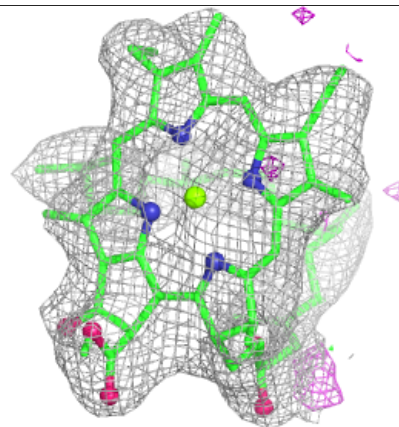
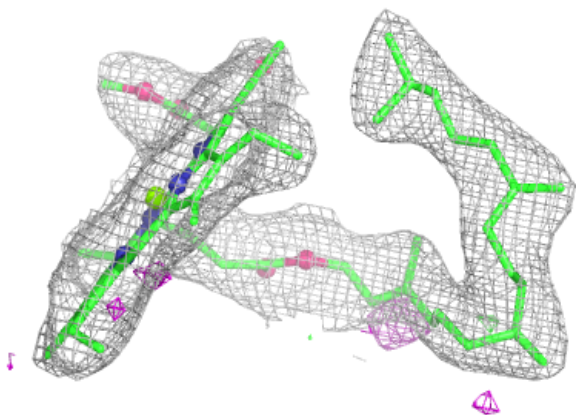
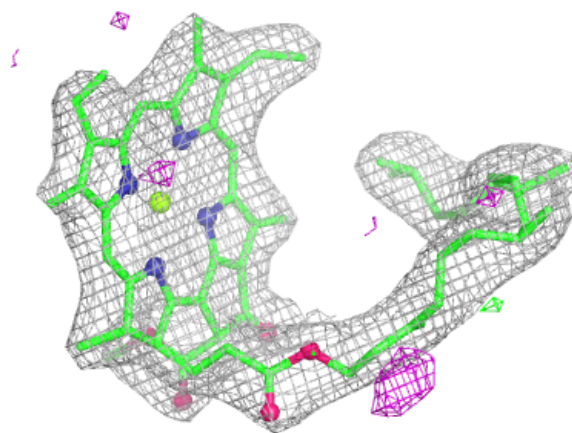
**Electron density around DGD C 517:**

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



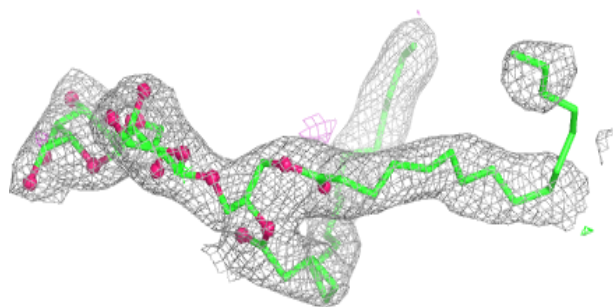
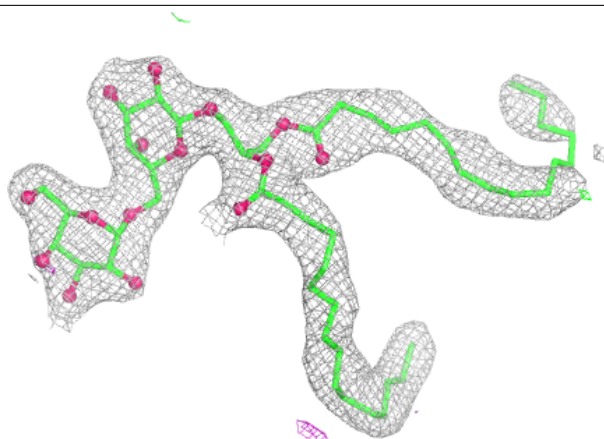
Electron density around CLA c 904:

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



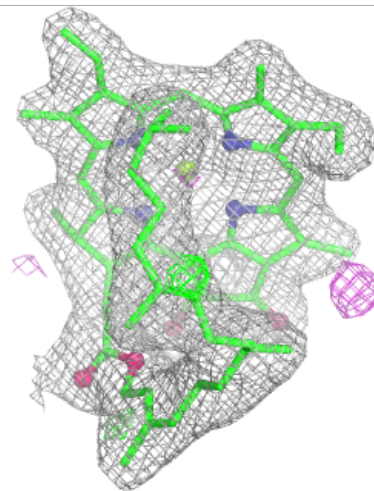
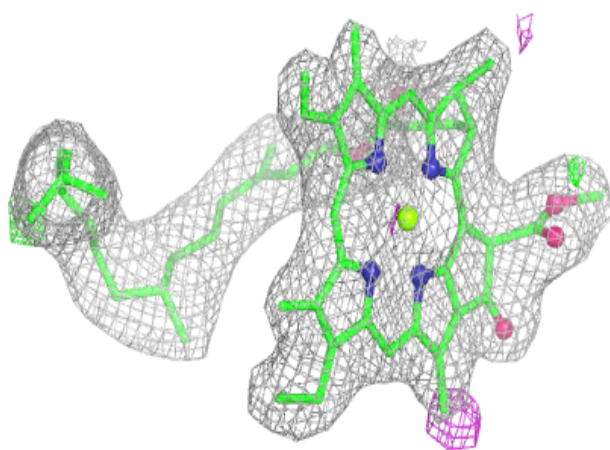
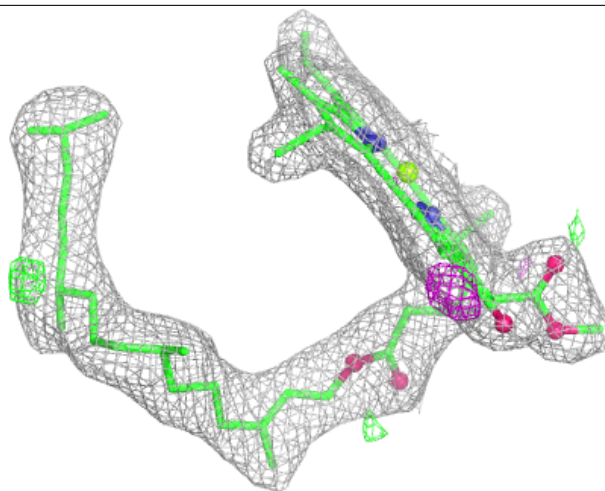
Electron density around DGD c 917:

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



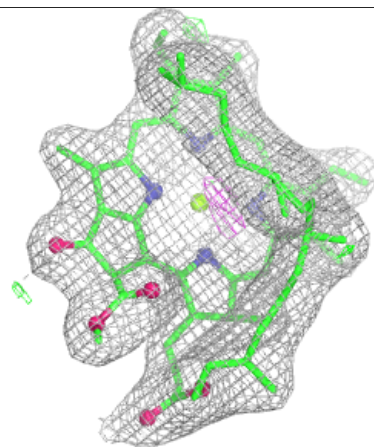
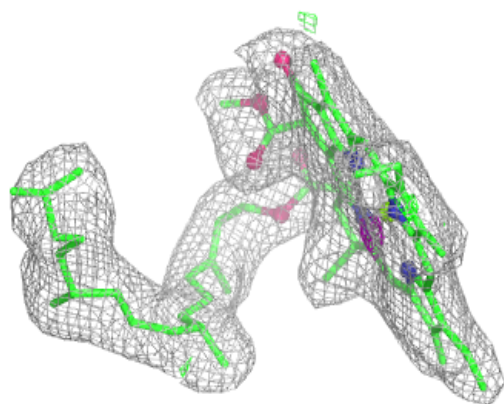
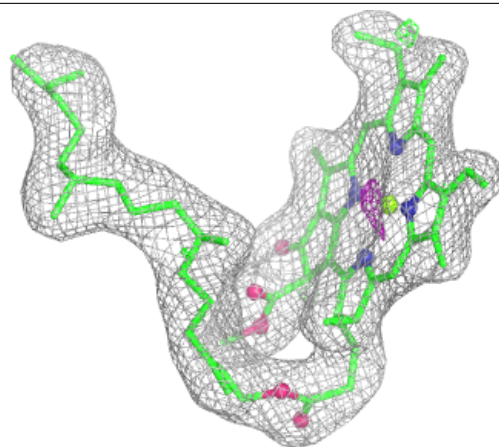
Electron density around CLA b 616:

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

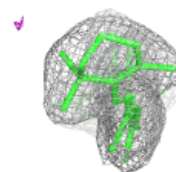
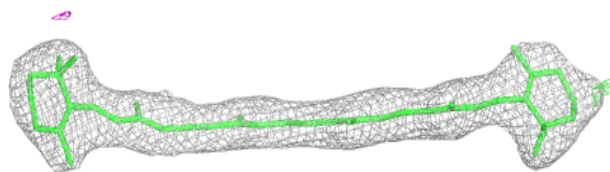
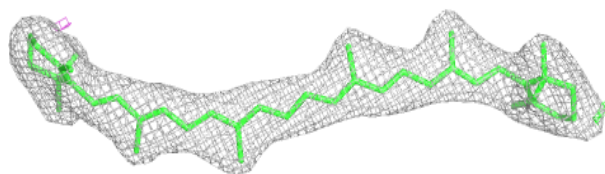


Electron density around CLA B 614:

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

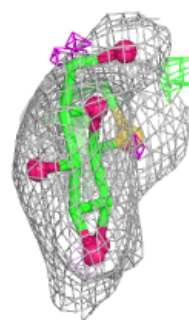
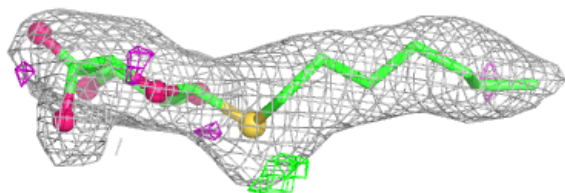
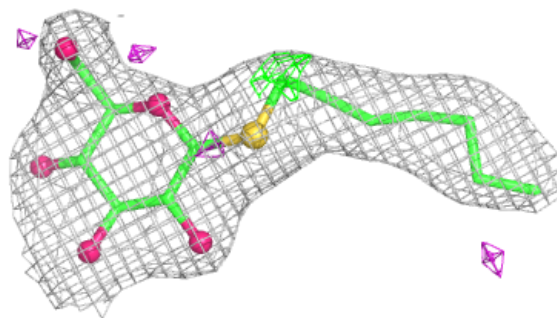
**Electron density around BCR h 101:**

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



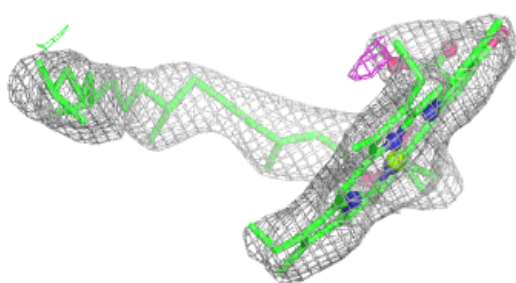
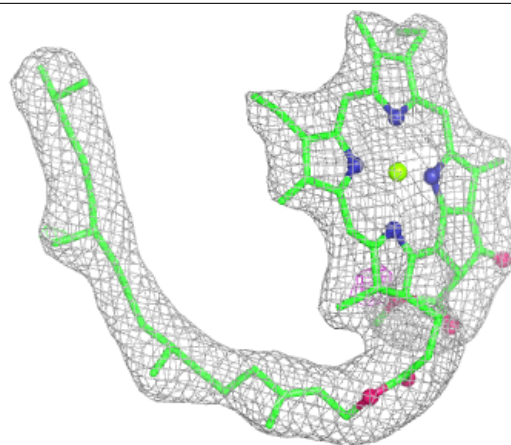
Electron density around HTG B 623:

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

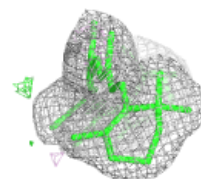
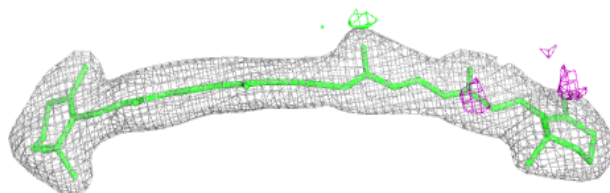
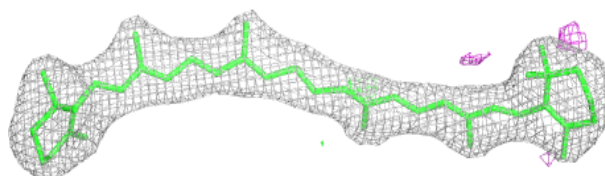


Electron density around CLA C 507:

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

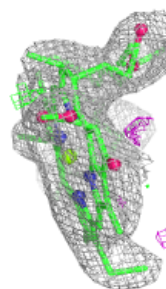
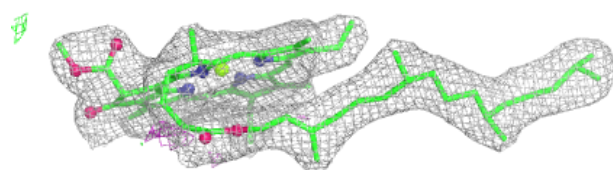
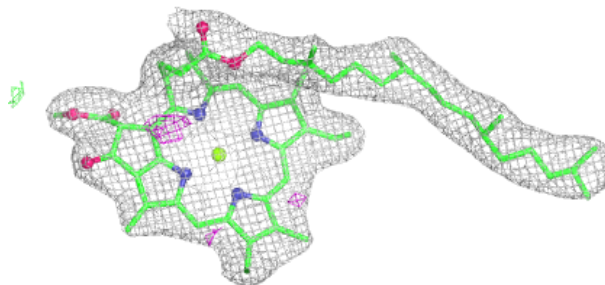
**Electron density around BCR t 102:**

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

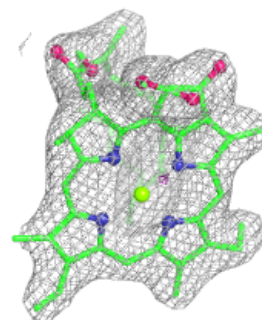
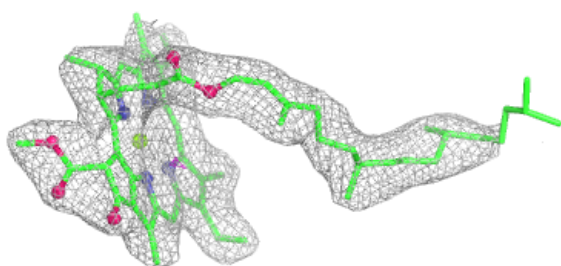
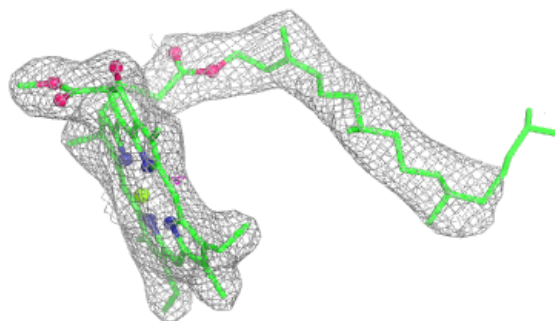


Electron density around CLA c 902:

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

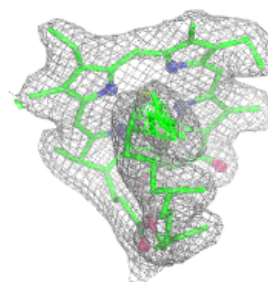
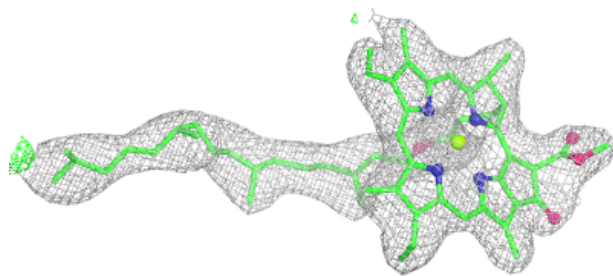
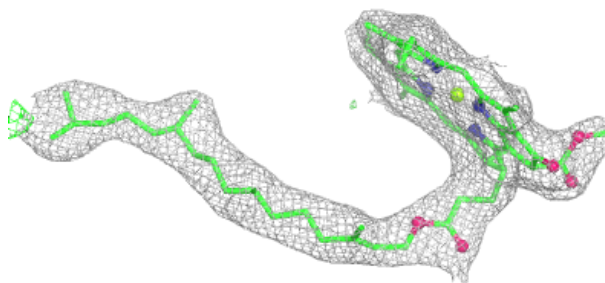
**Electron density around CLA C 508:**

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



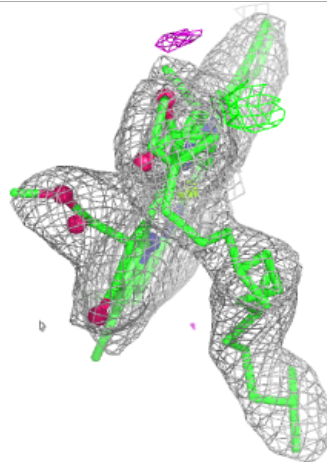
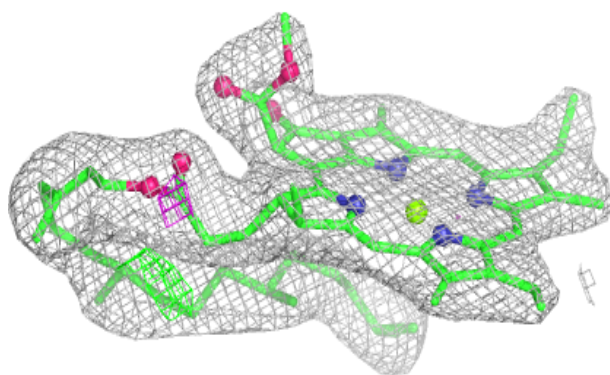
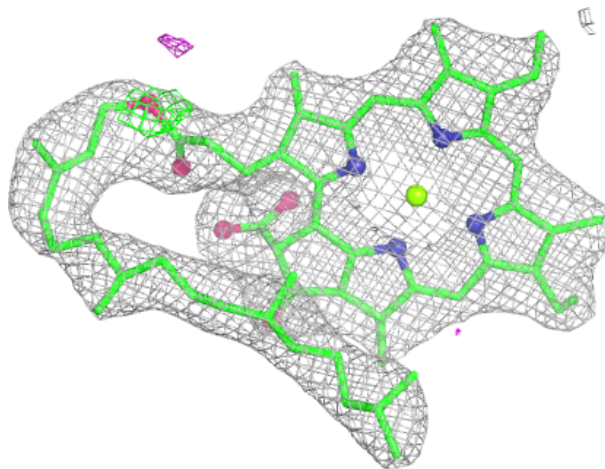
Electron density around CLA c 905:

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



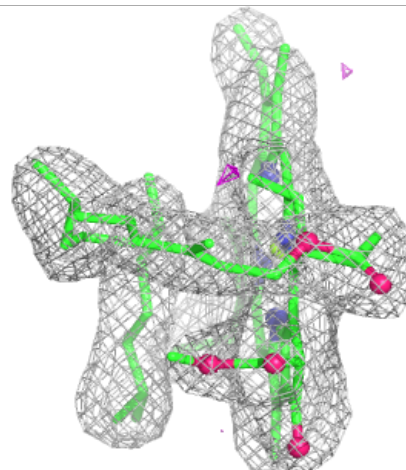
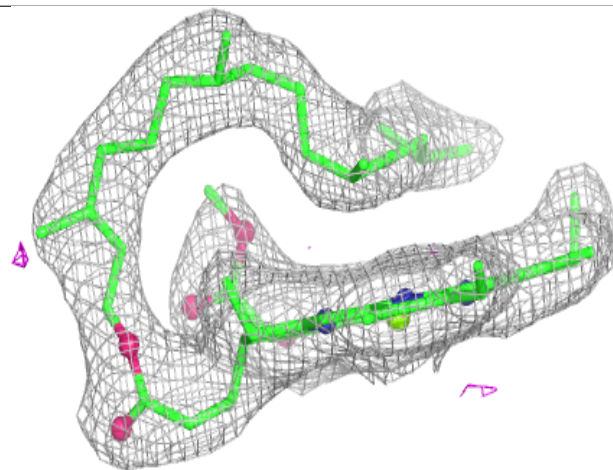
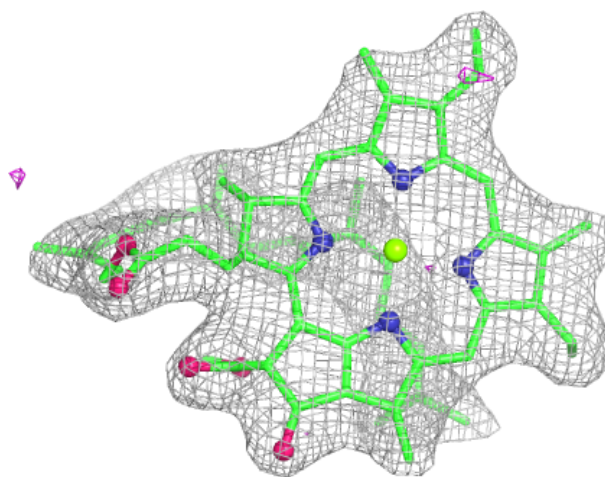
Electron density around CLA C 509:

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



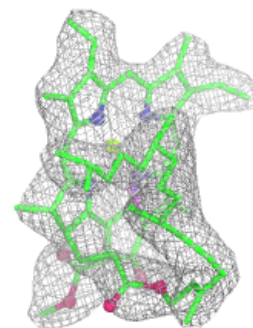
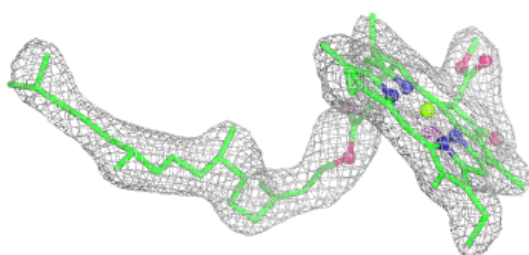
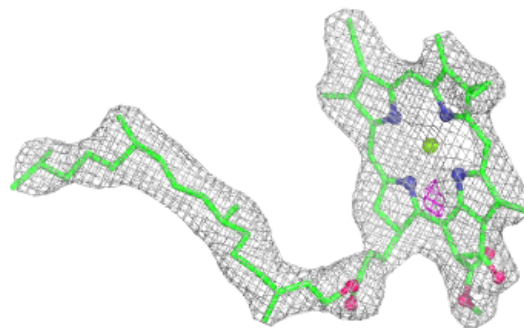
Electron density around CLA C 510:

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



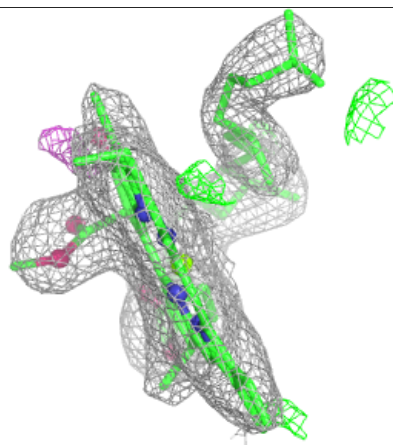
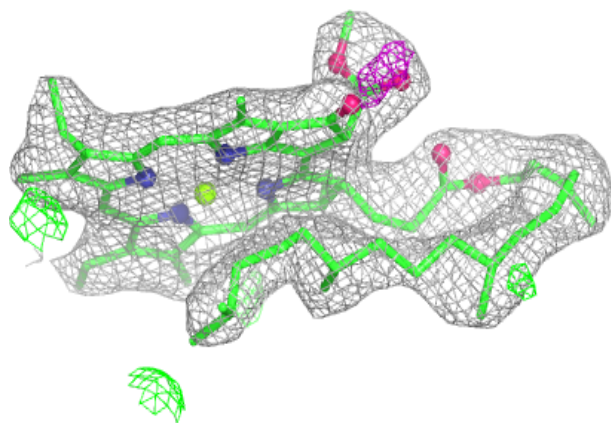
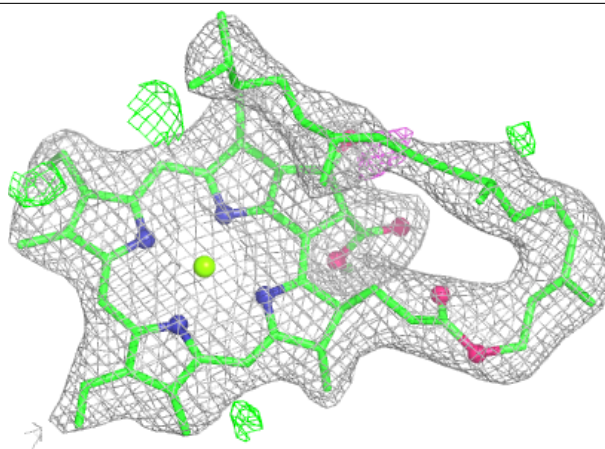
Electron density around CLA C 511:

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



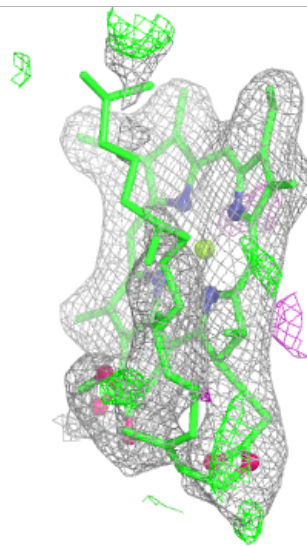
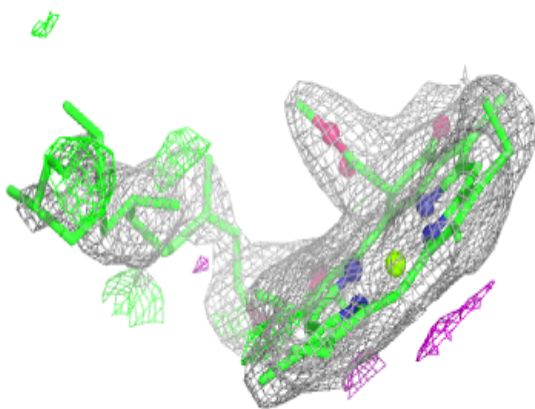
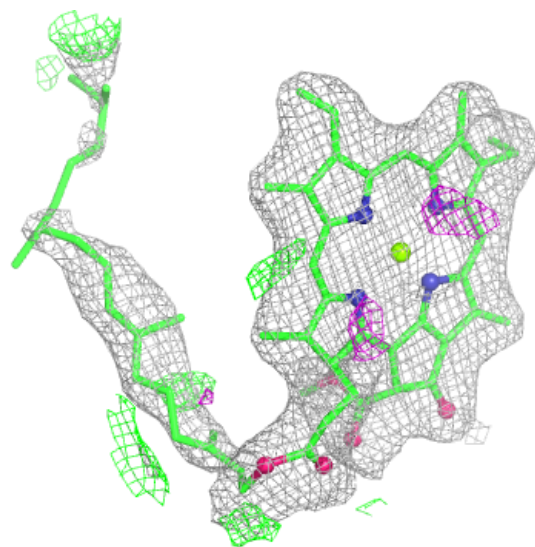
Electron density around CLA c 910:

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



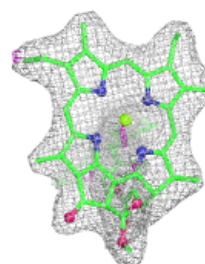
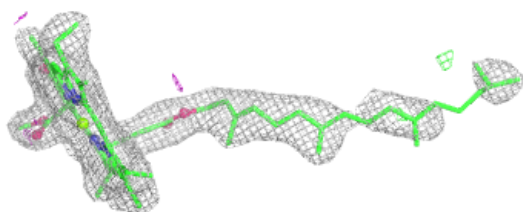
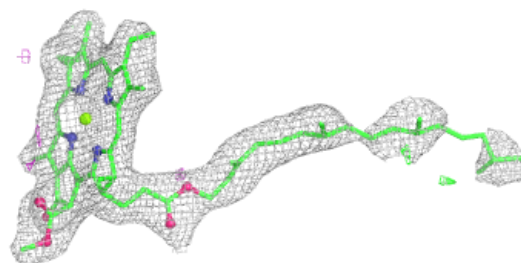
Electron density around CLA B 617:

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



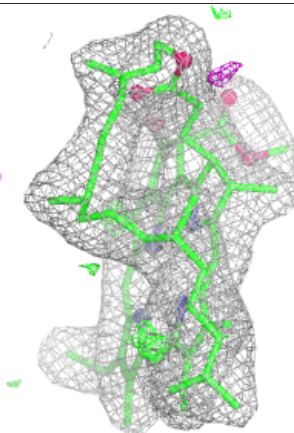
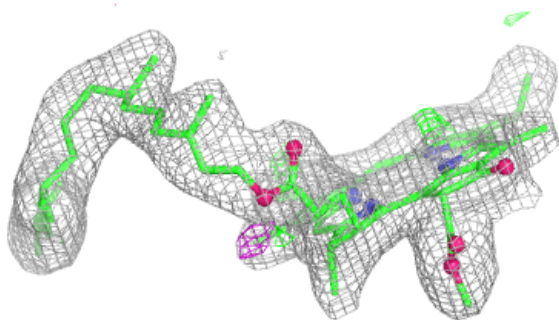
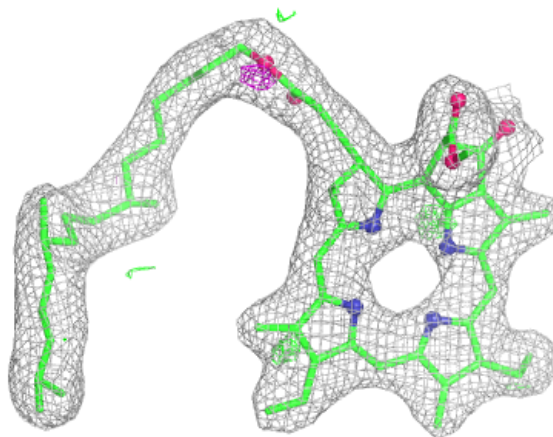
Electron density around CLA d 406:

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

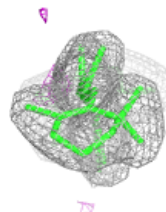
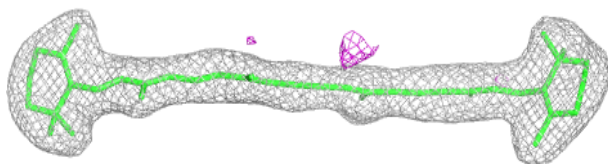
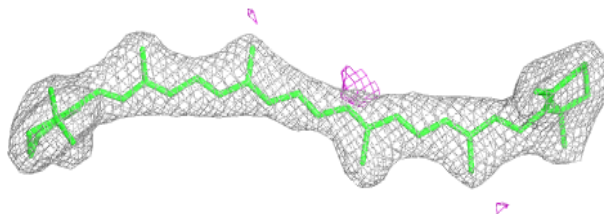


Electron density around PHO d 403:

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

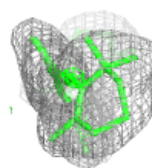
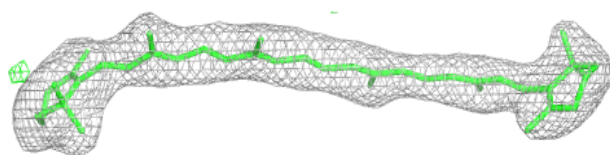
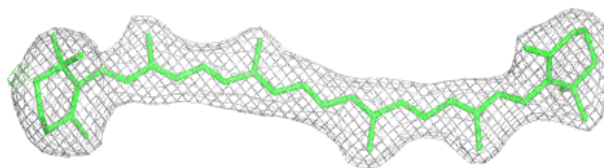
**Electron density around BCR A 410:**

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

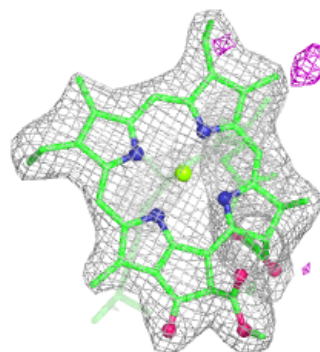
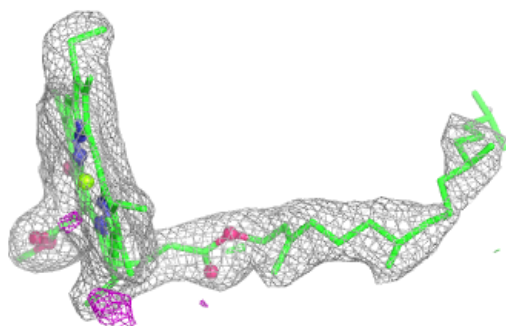
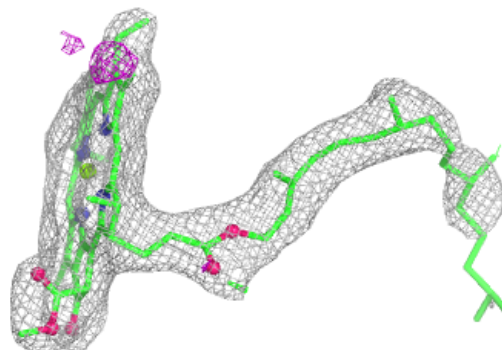


Electron density around BCR B 620:

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

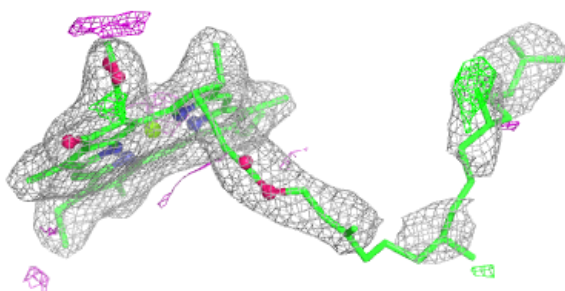
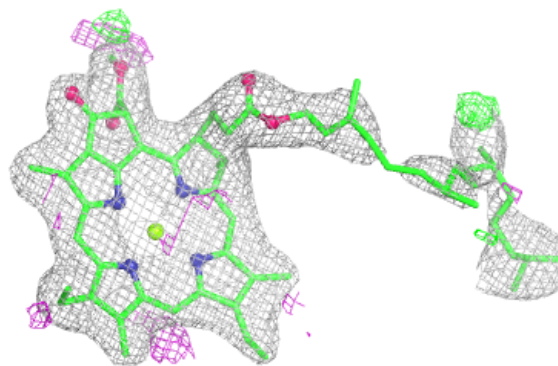
**Electron density around CLA D 405:**

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

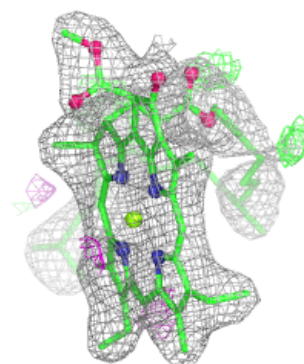
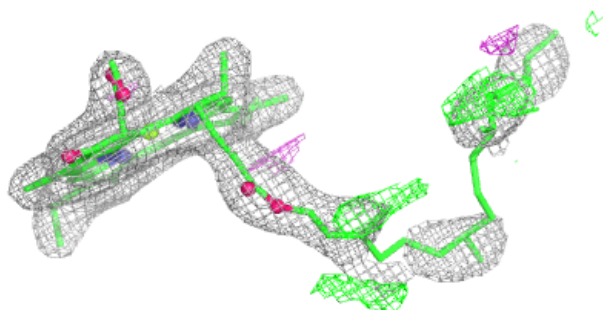
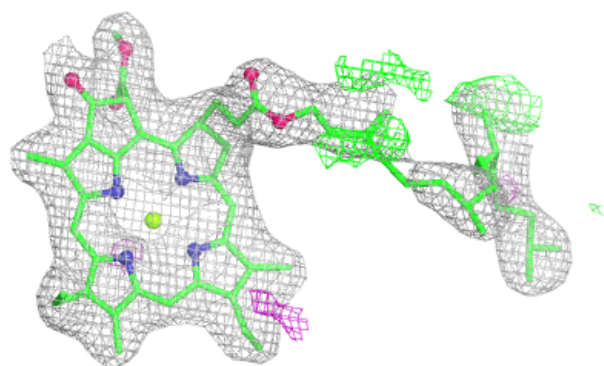


Electron density around CLA a 408:

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

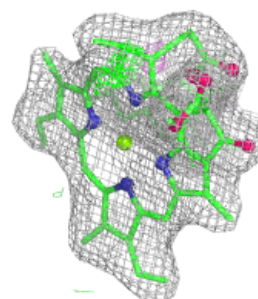
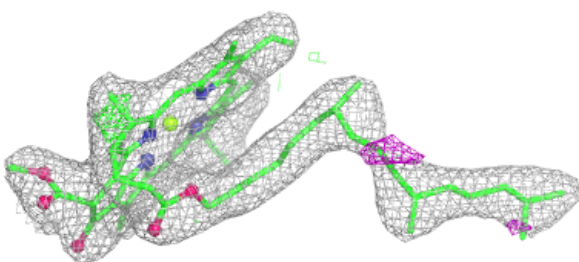
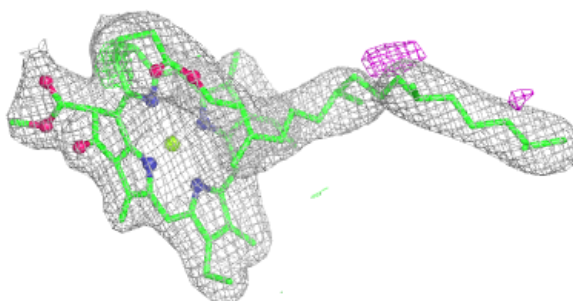
**Electron density around CLA A 409:**

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

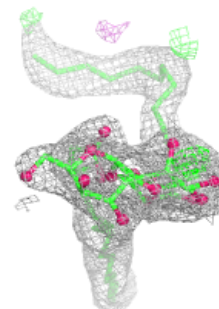
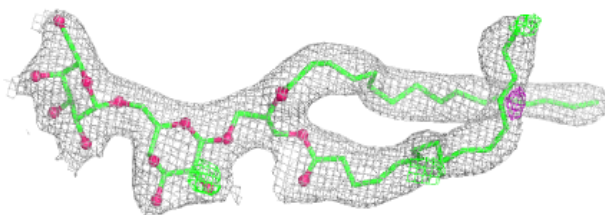
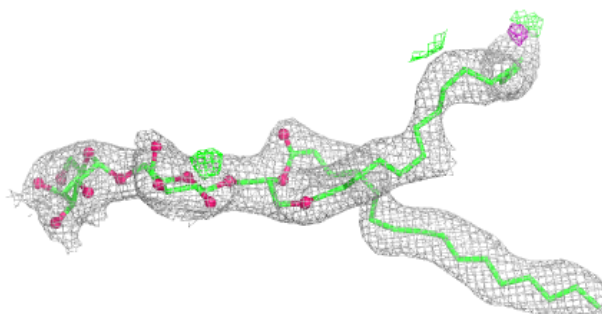


Electron density around CLA C 505:

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

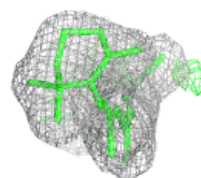
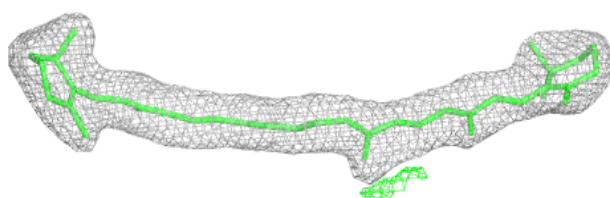
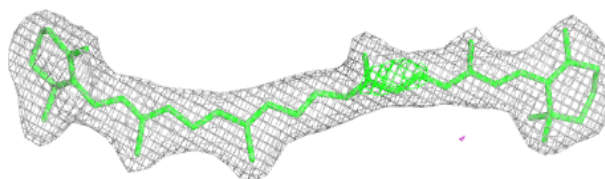
**Electron density around DGD C 516:**

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

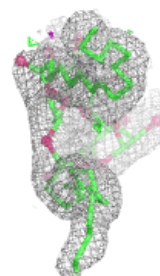
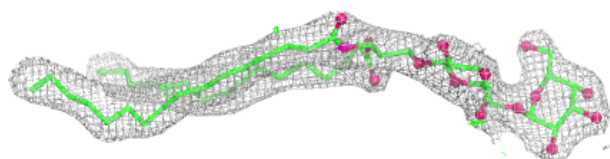
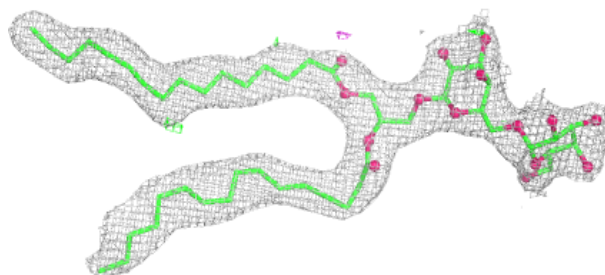


Electron density around BCR T 102:

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

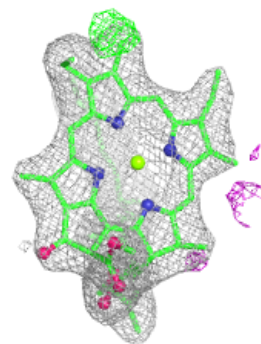
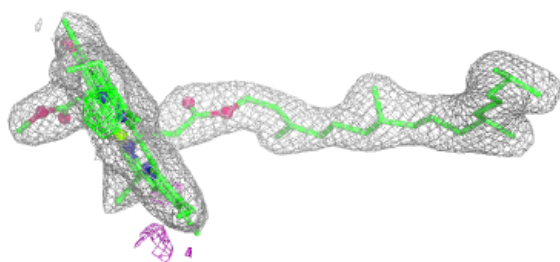
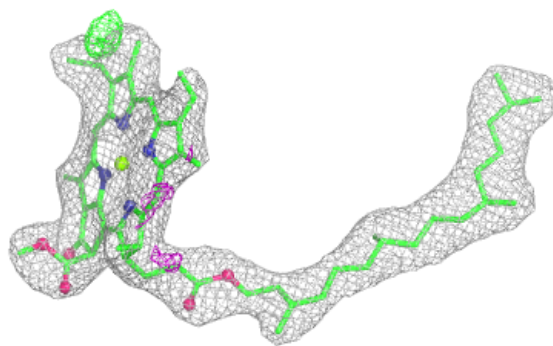
**Electron density around DGD C 518:**

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

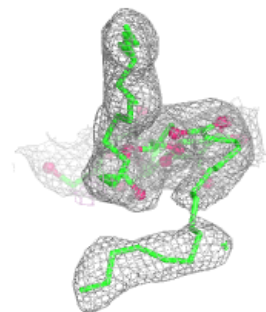
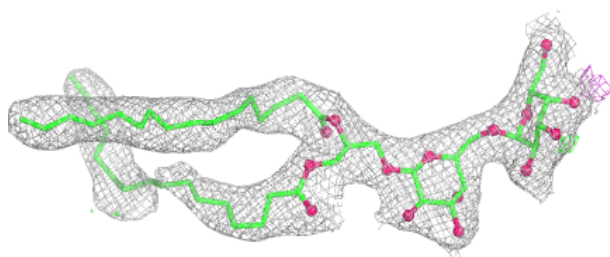
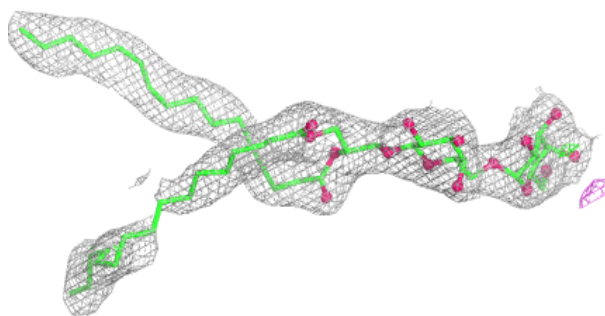


Electron density around CLA b 614:

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

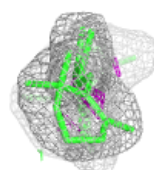
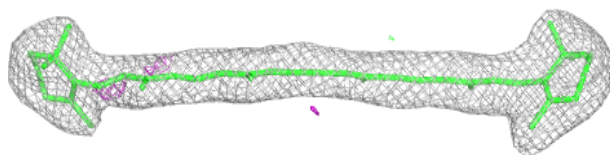
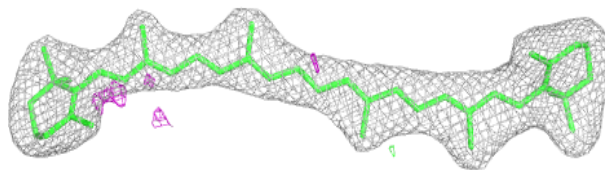
**Electron density around DGD c 916:**

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

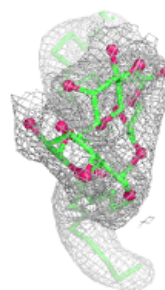
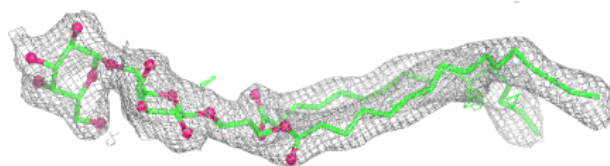
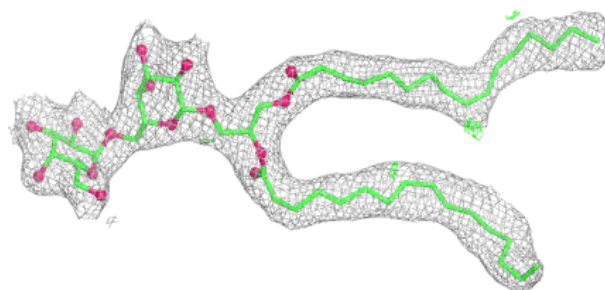


Electron density around BCR b 623:

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

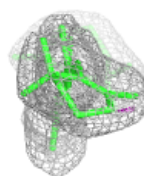
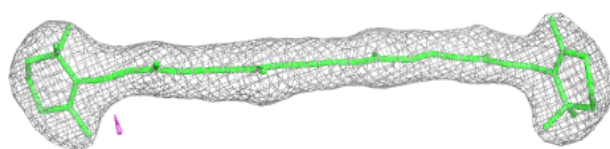
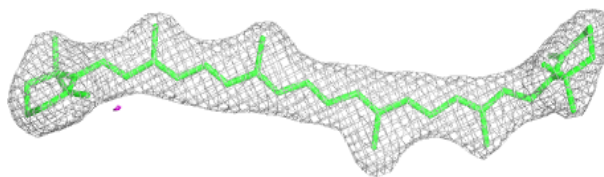
**Electron density around DGD c 918:**

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

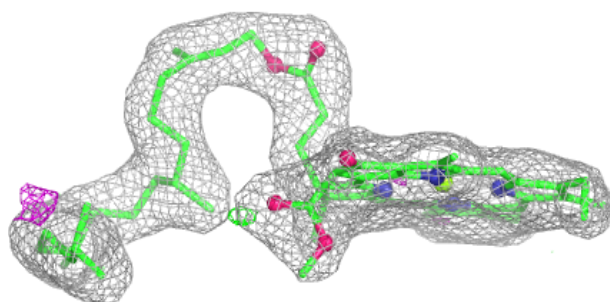
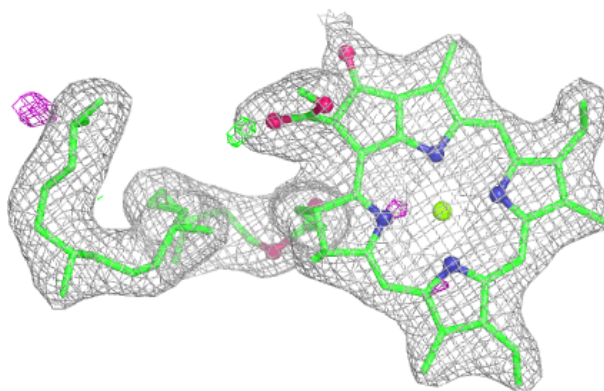


Electron density around BCR c 915:

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

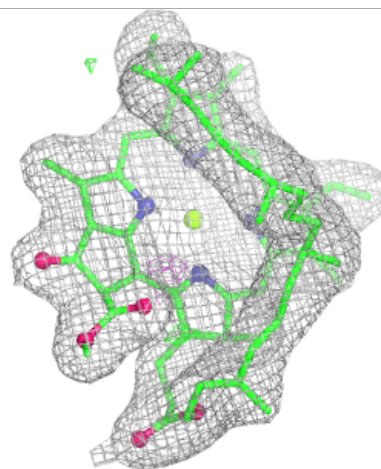
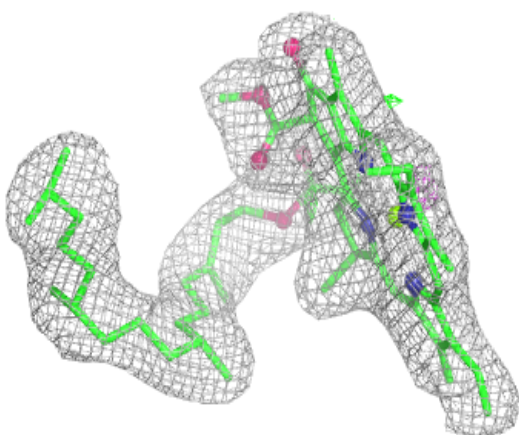
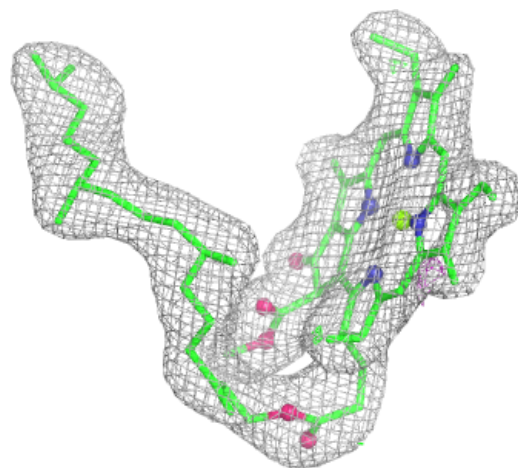
**Electron density around CLA b 617:**

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



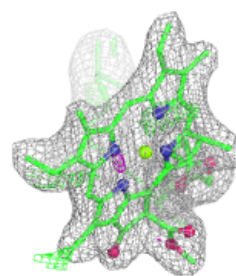
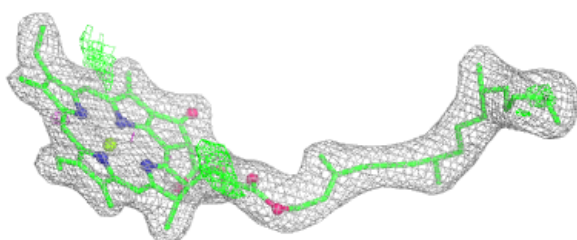
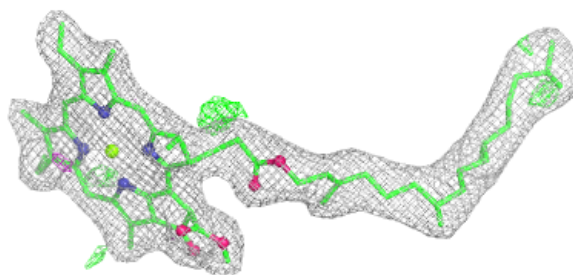
Electron density around CLA b 618:

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

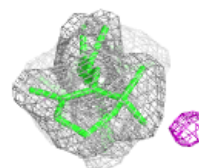
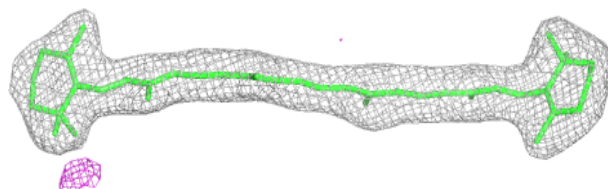
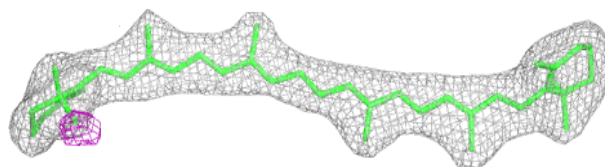


Electron density around CLA A 405:

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

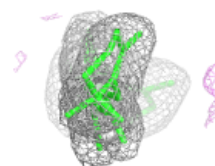
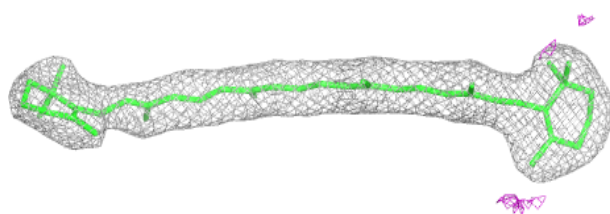
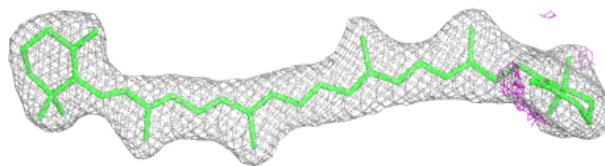
**Electron density around BCR a 409:**

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

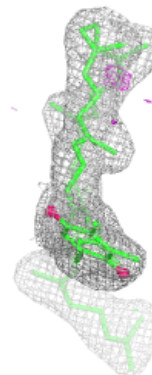
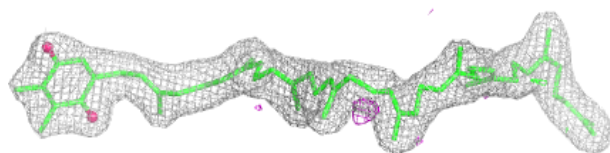
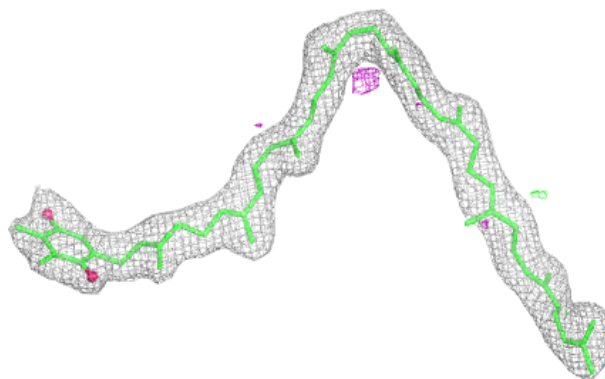


Electron density around BCR b 622:

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

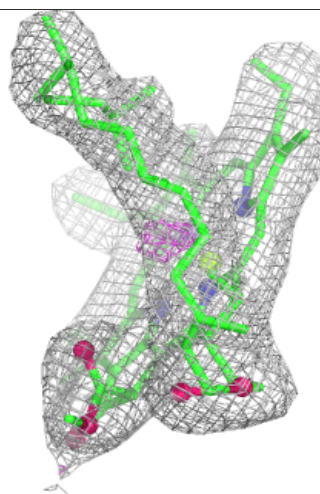
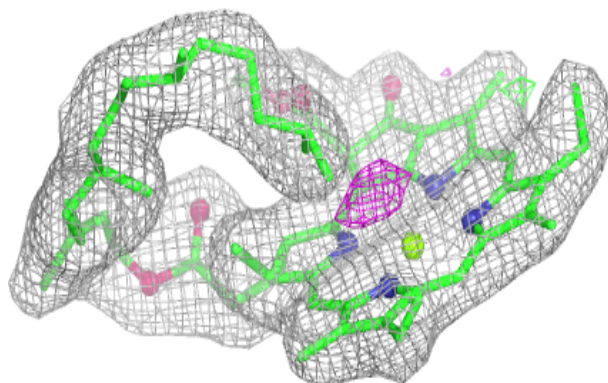
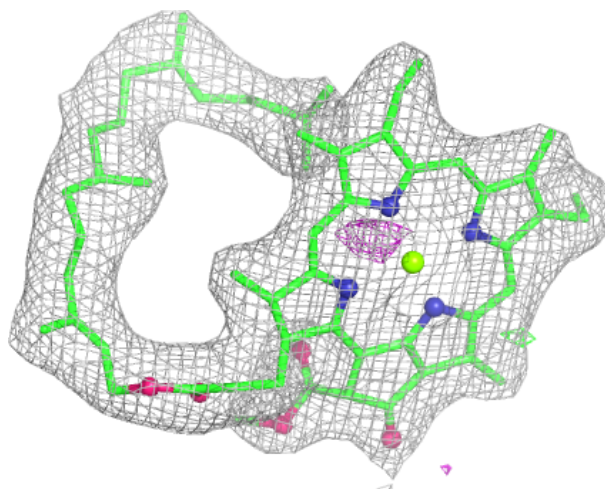
**Electron density around PL9 d 408:**

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



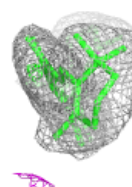
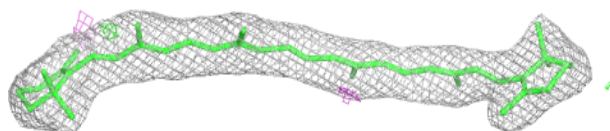
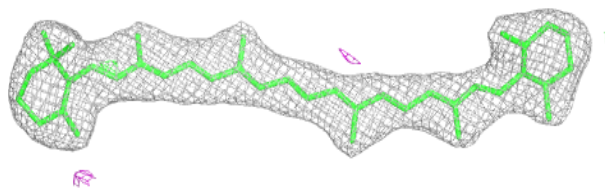
Electron density around CLA b 620:

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



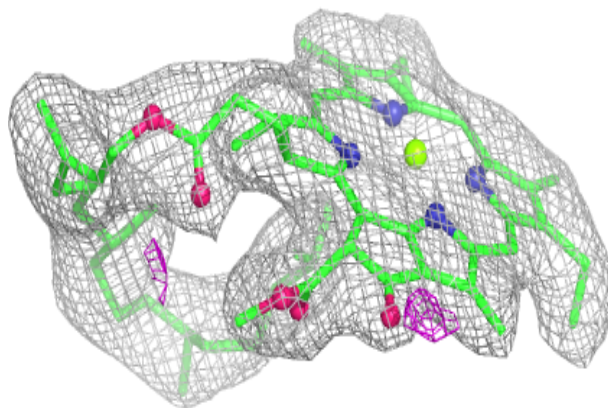
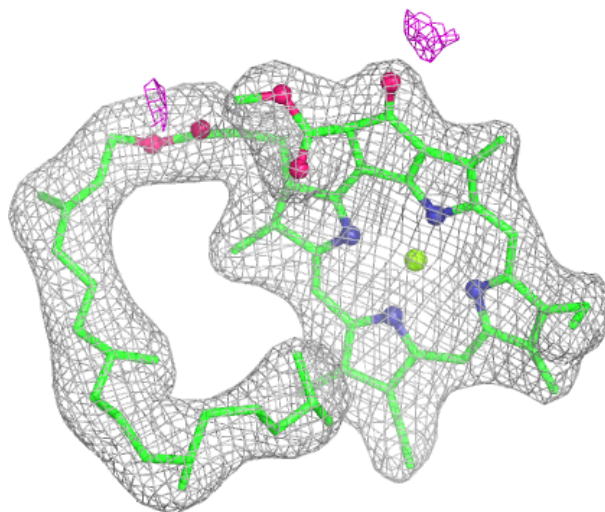
Electron density around BCR b 624:

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



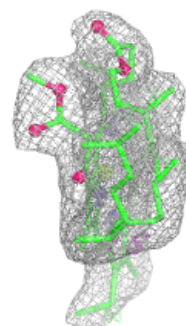
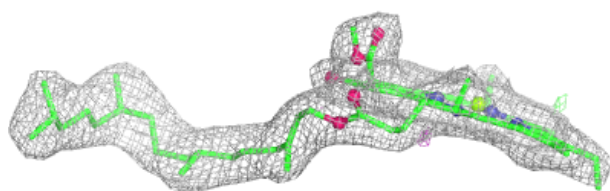
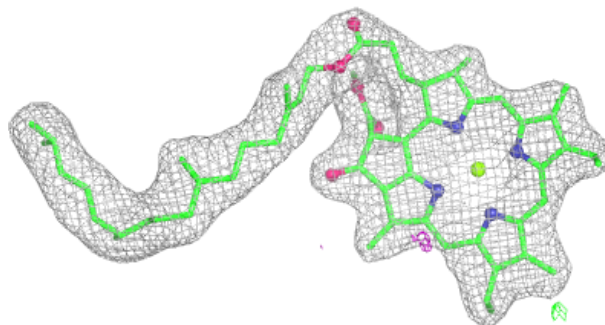
Electron density around CLA B 616:

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

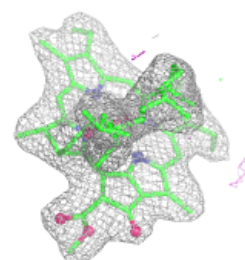
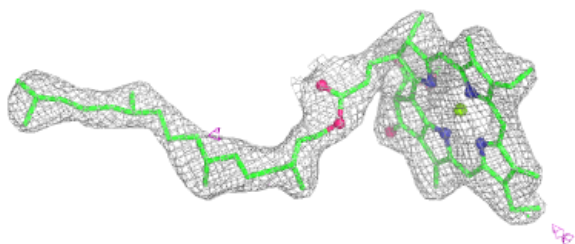
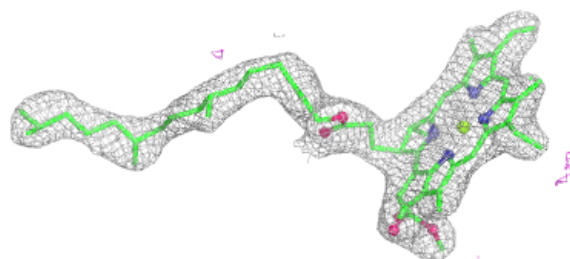


Electron density around CLA B 603:

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

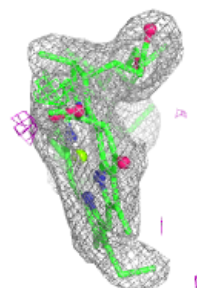
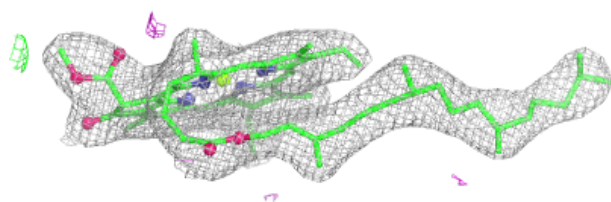
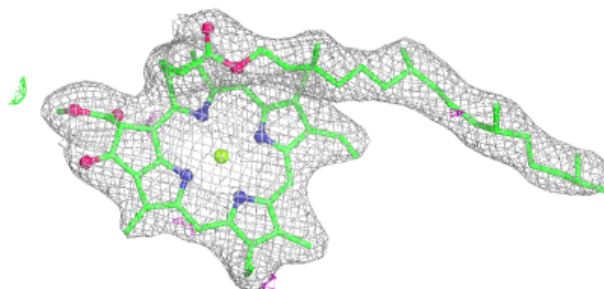
**Electron density around CLA c 903:**

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

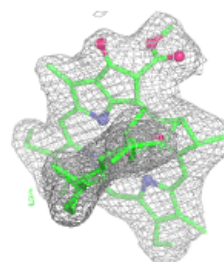
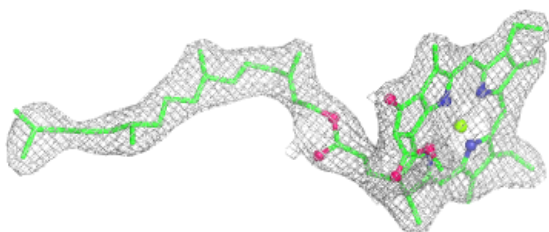
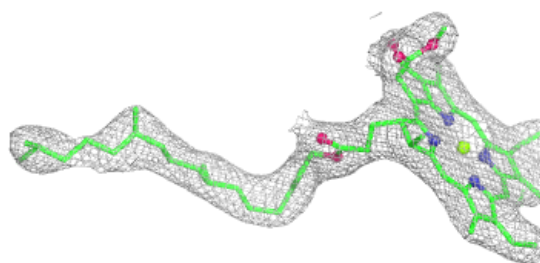


Electron density around CLA C 501:

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

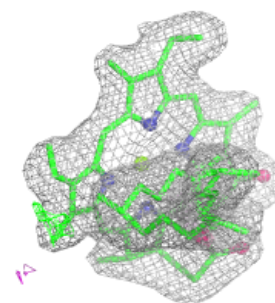
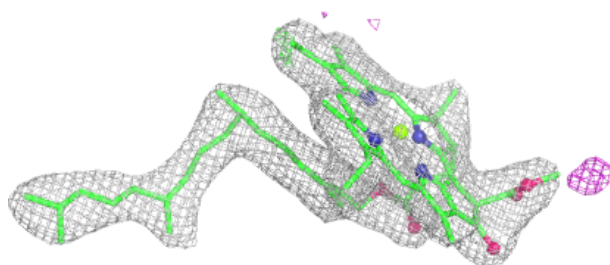
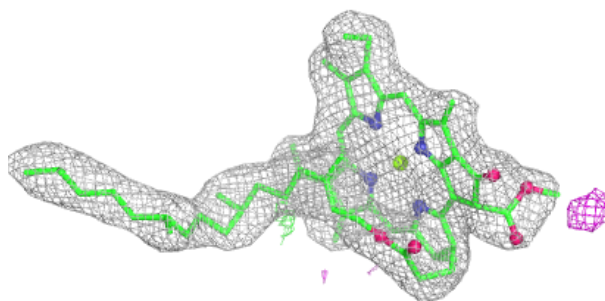
**Electron density around CLA C 502:**

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

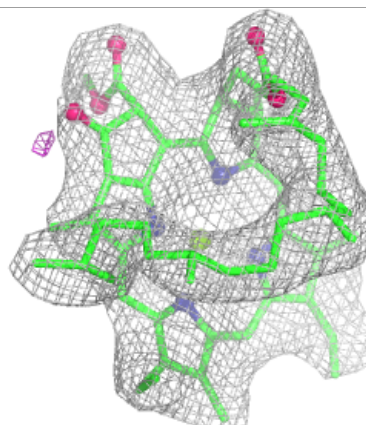
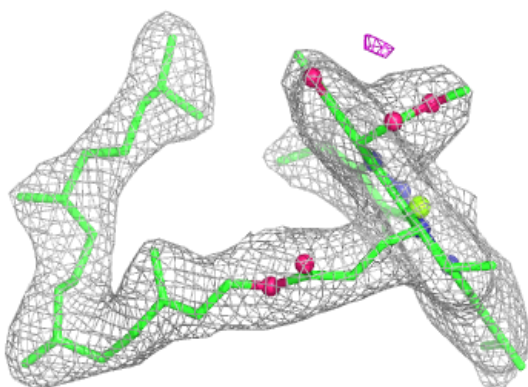
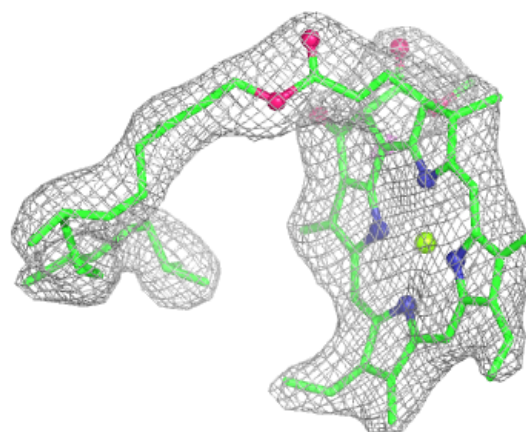


Electron density around CLA c 906:

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

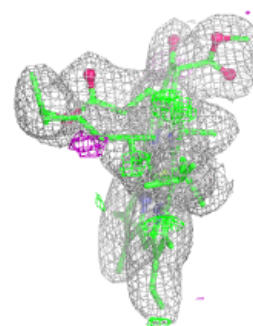
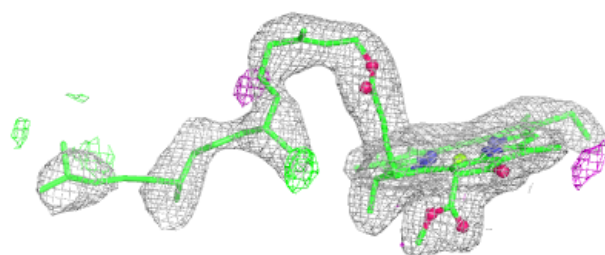
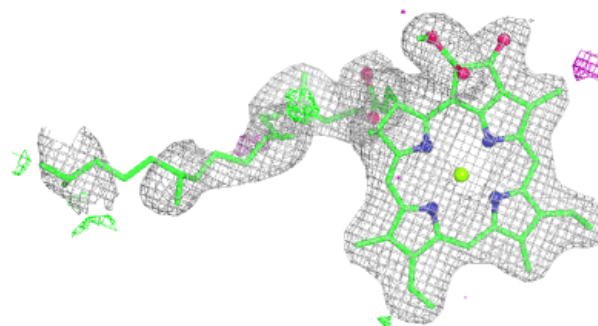
**Electron density around CLA C 503:**

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

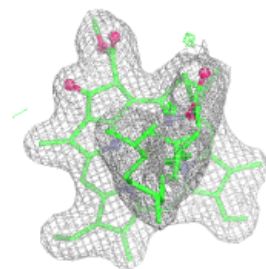
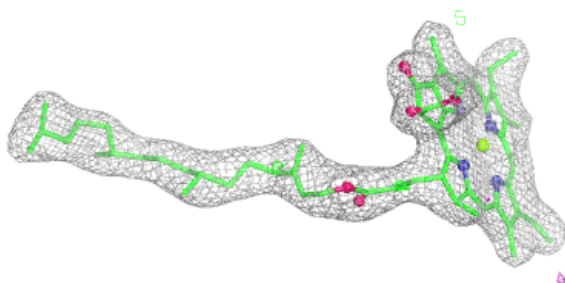
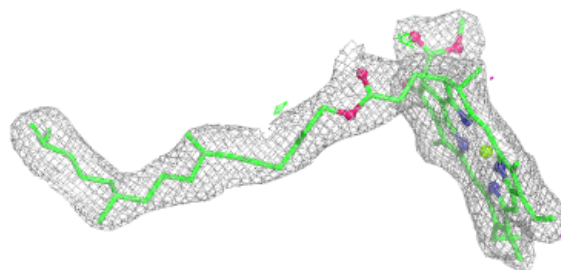


Electron density around CLA a 406:

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

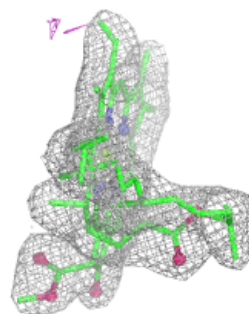
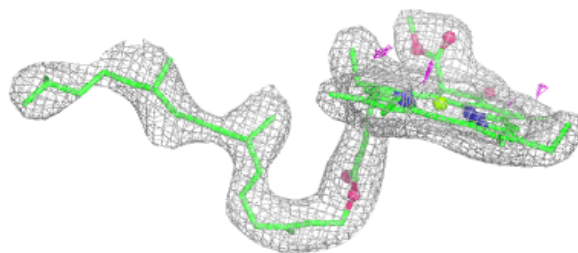
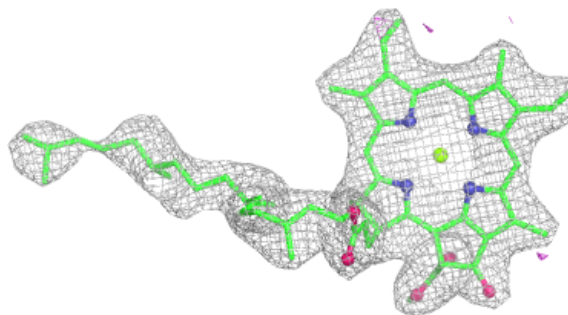
**Electron density around CLA B 605:**

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



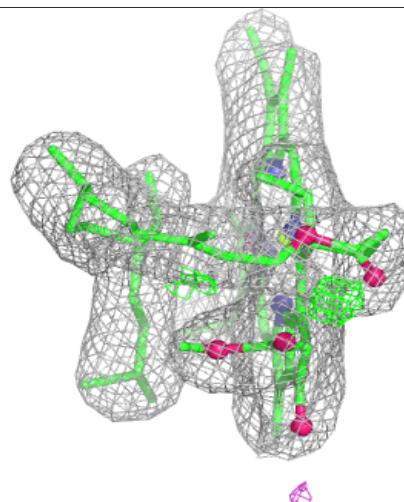
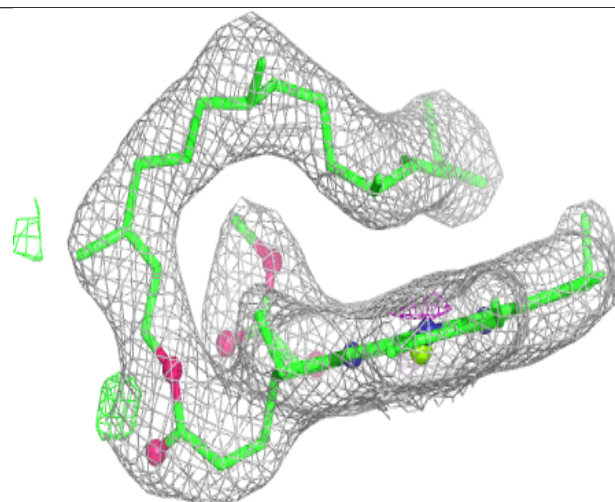
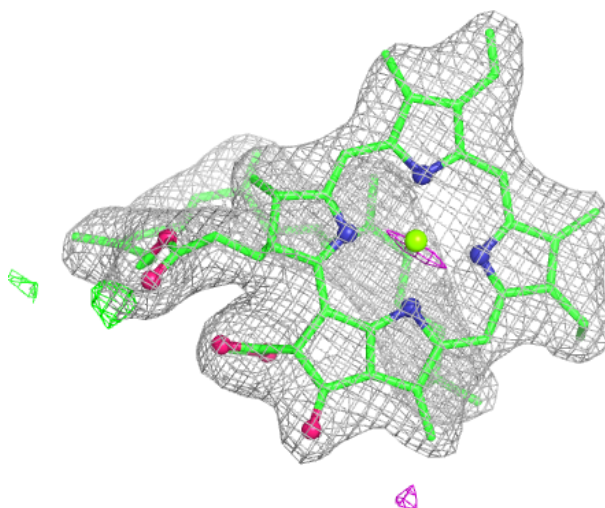
Electron density around CLA A 407:

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



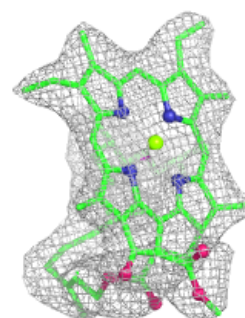
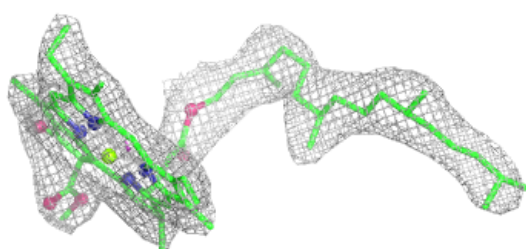
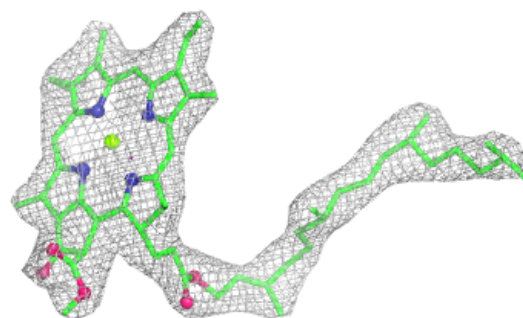
Electron density around CLA c 911:

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

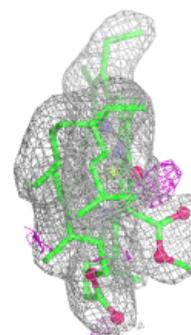
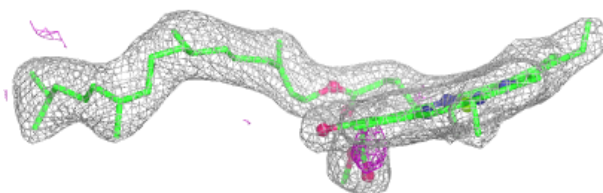
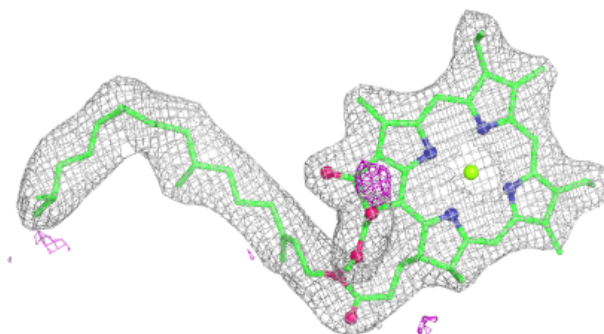


Electron density around CLA c 912:

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

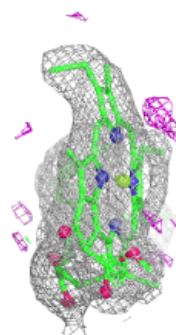
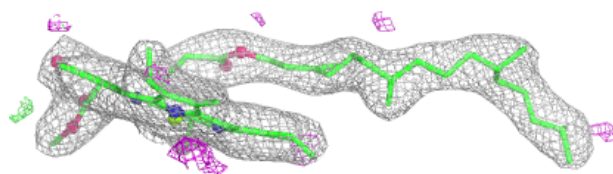
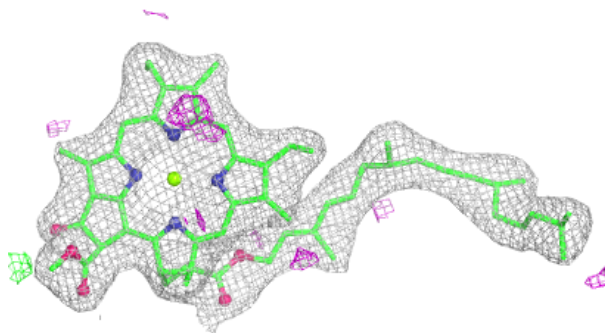
**Electron density around CLA b 607:**

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

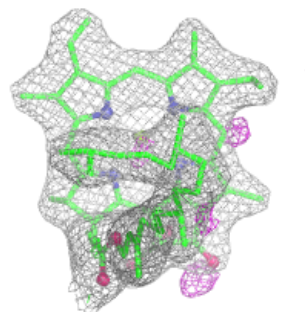
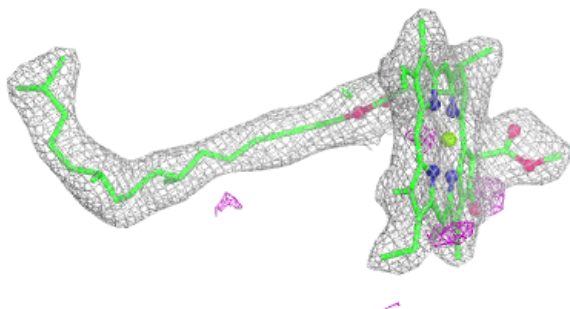
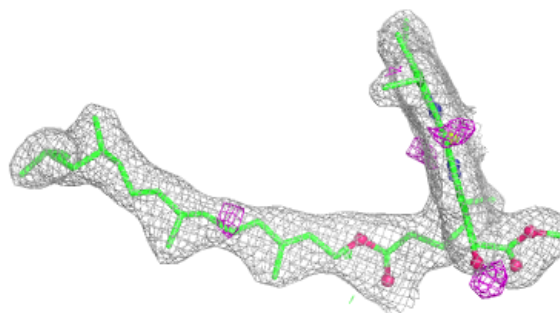


Electron density around CLA b 608:

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

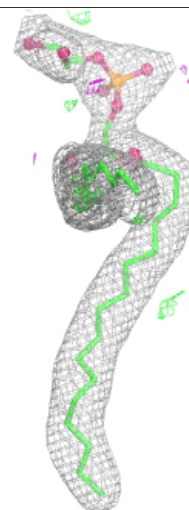
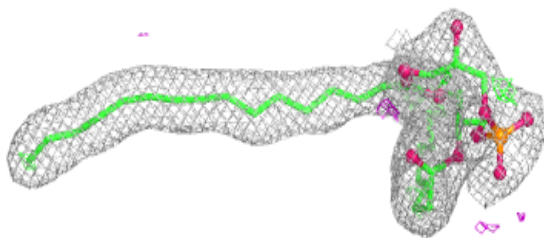
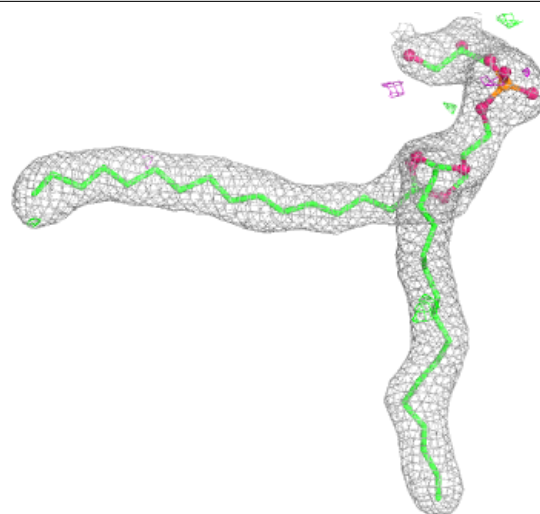
**Electron density around CLA b 610:**

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



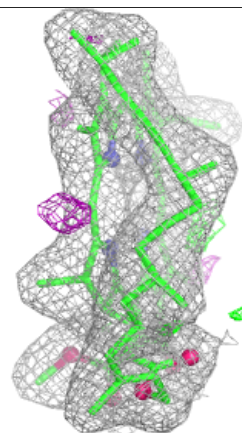
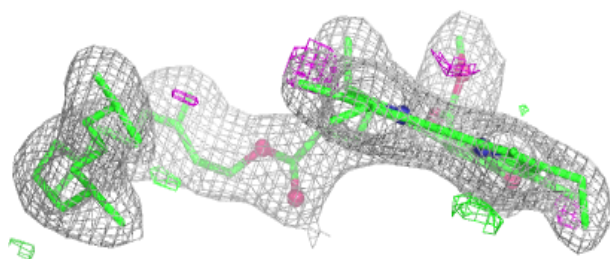
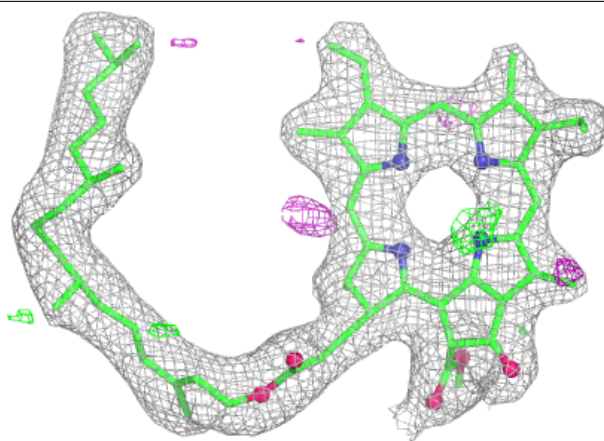
Electron density around LHG L 101:

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



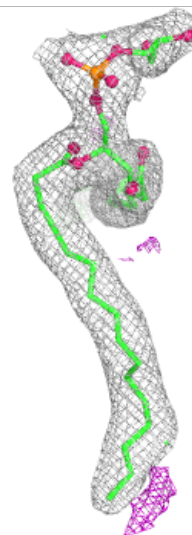
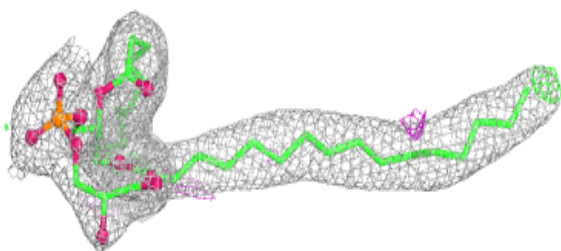
Electron density around PHO A 408:

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



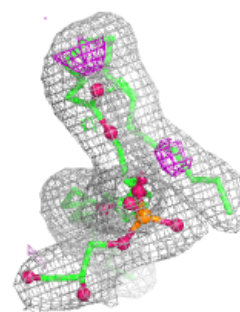
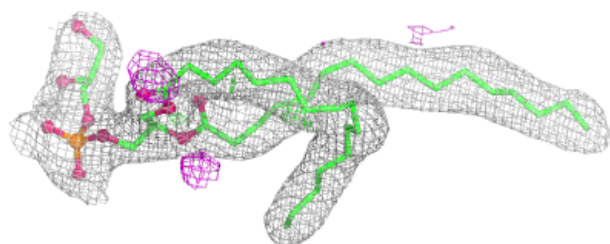
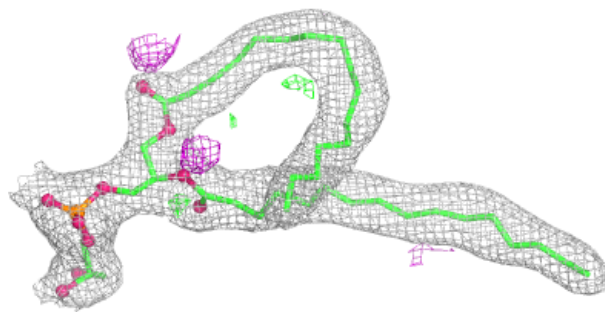
Electron density around LHG b 635:

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

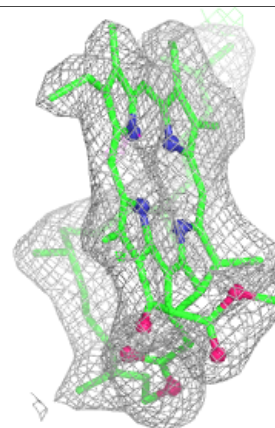
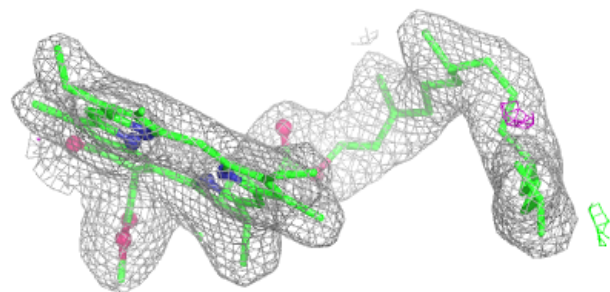
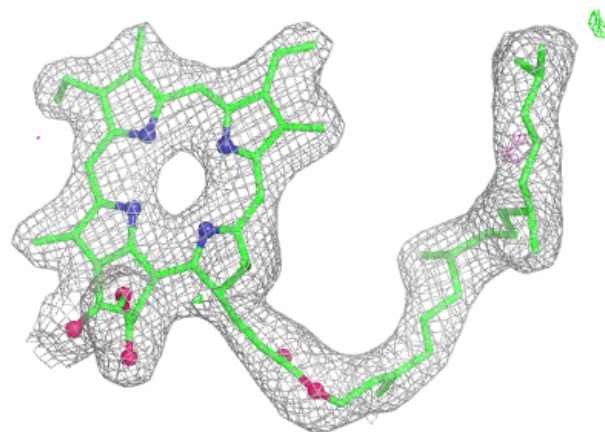


Electron density around LHG d 409:

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

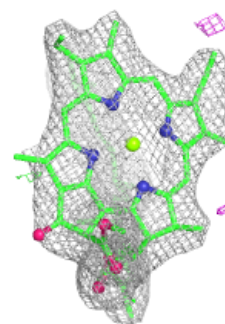
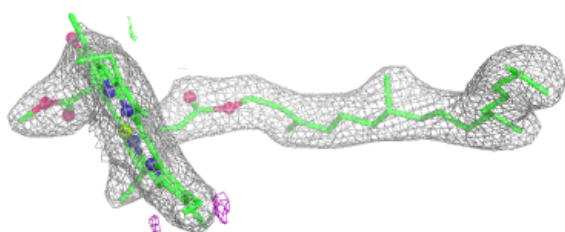
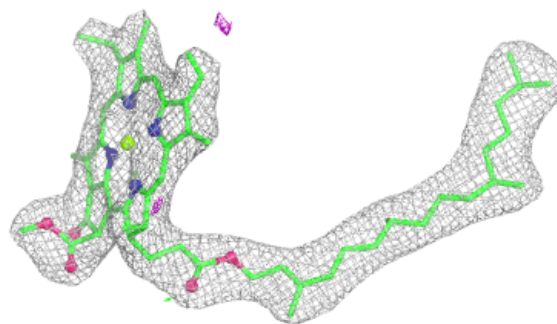
**Electron density around PHO D 401:**

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

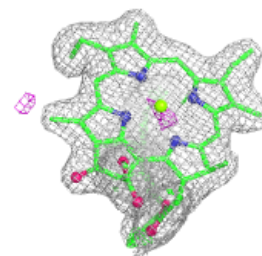
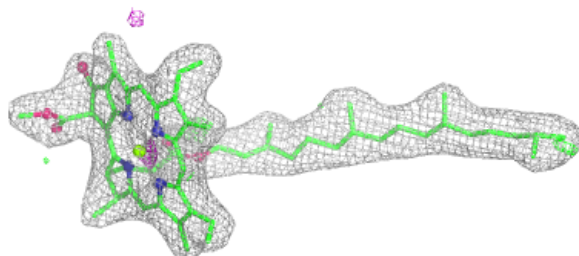
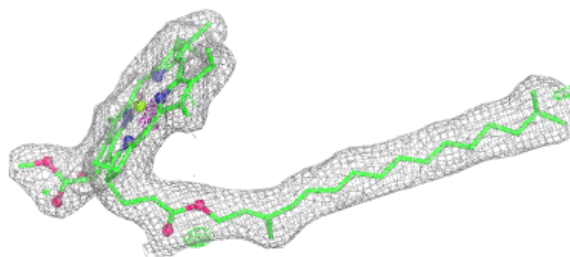


Electron density around CLA B 610:

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

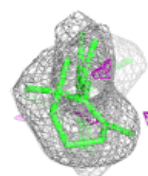
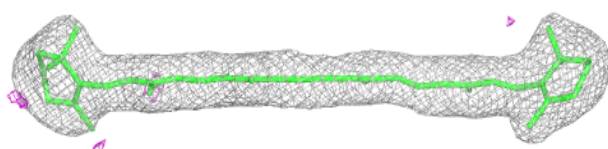
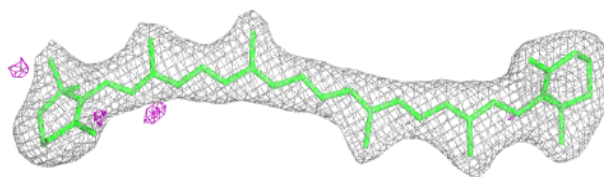
**Electron density around CLA b 612:**

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

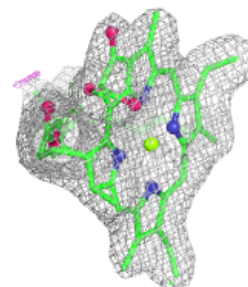
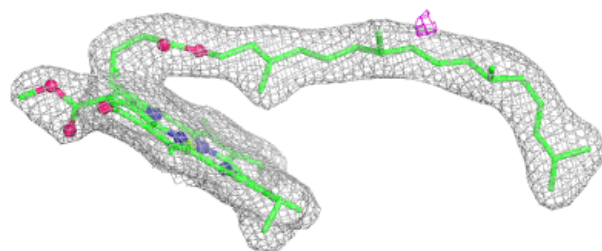
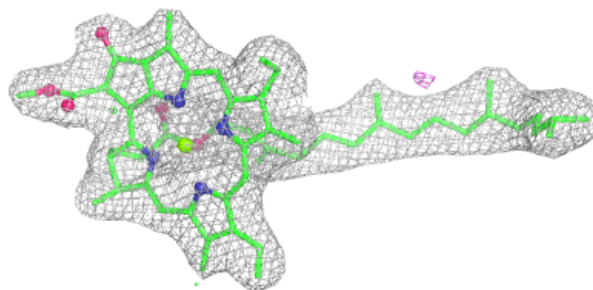


Electron density around BCR B 619:

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

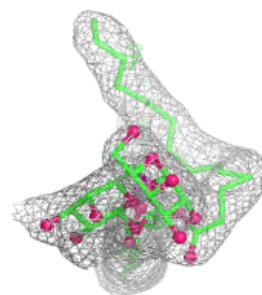
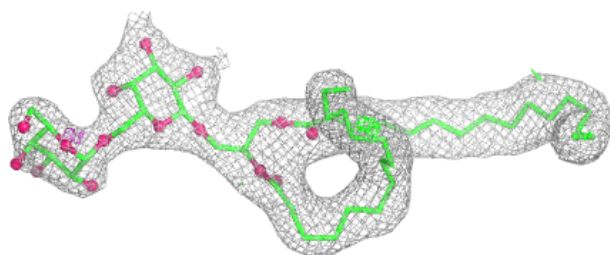
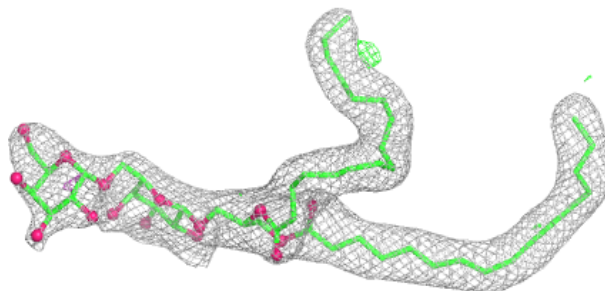
**Electron density around CLA b 613:**

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



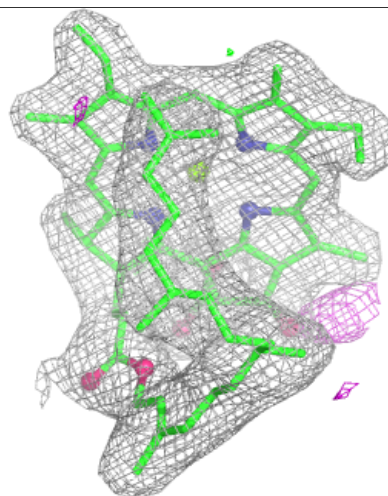
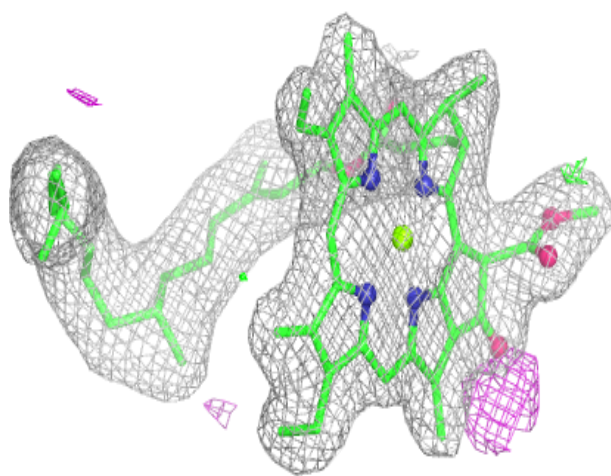
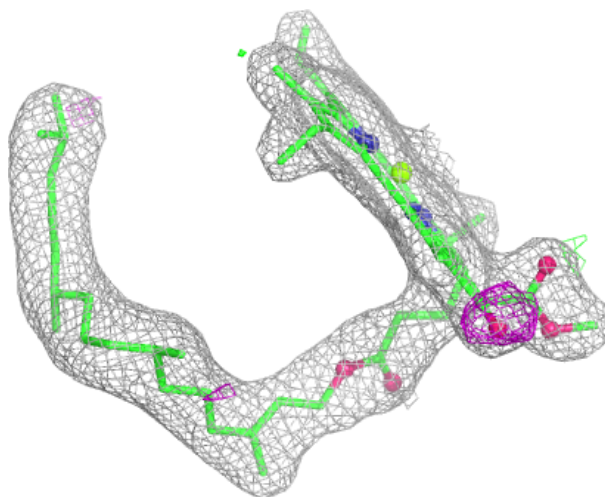
Electron density around DGD H 102:

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



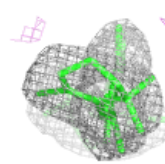
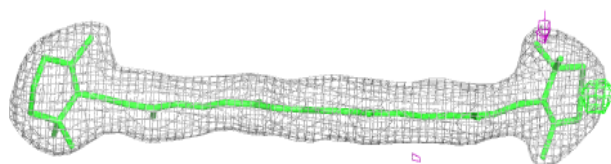
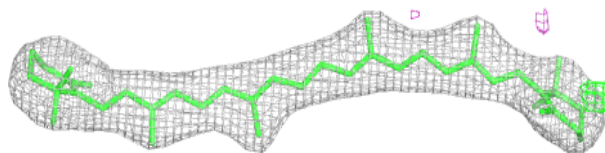
Electron density around CLA B 612:

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

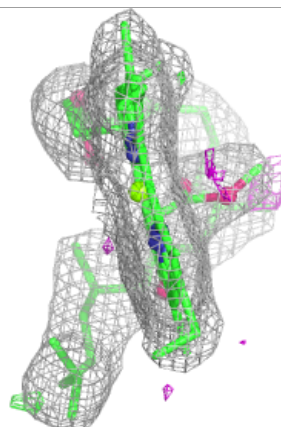
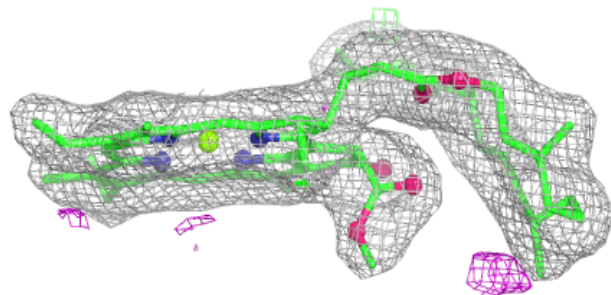
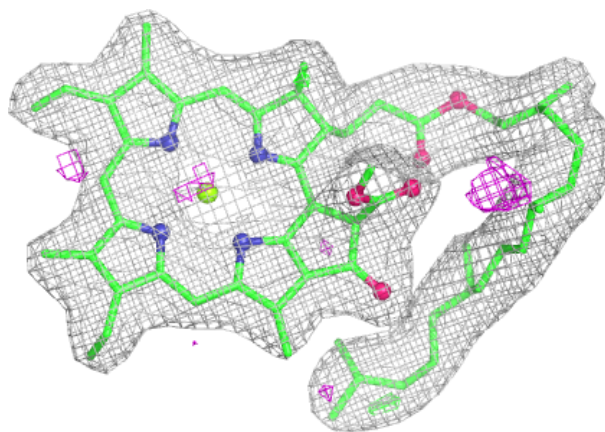


Electron density around BCR C 515:

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

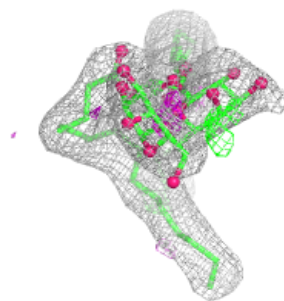
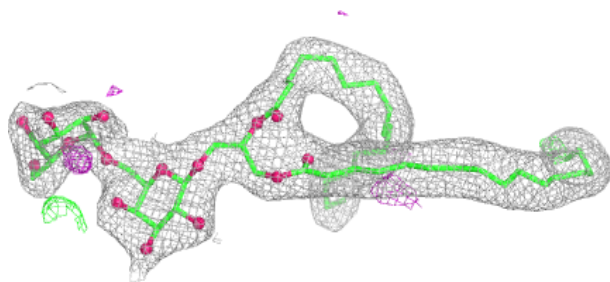
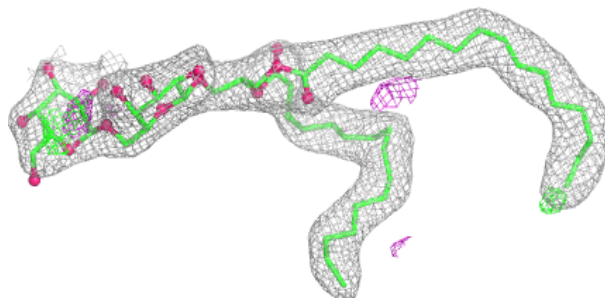
**Electron density around CLA b 615:**

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



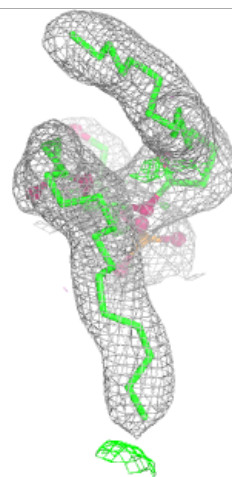
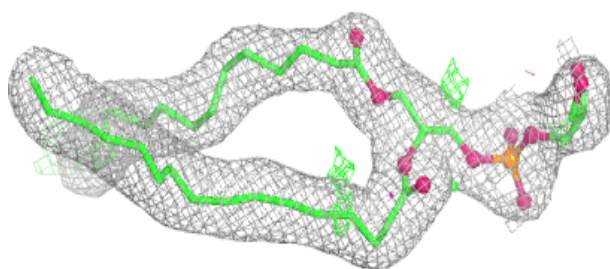
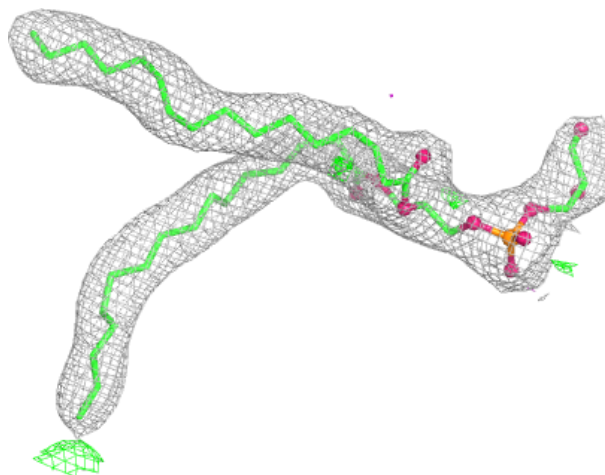
Electron density around DGD h 102:

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



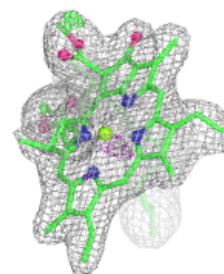
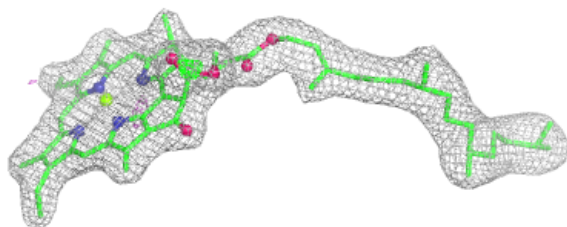
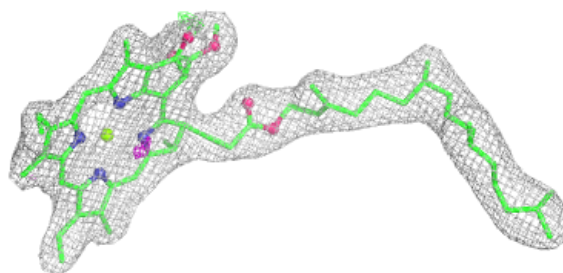
Electron density around LHG D 409:

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



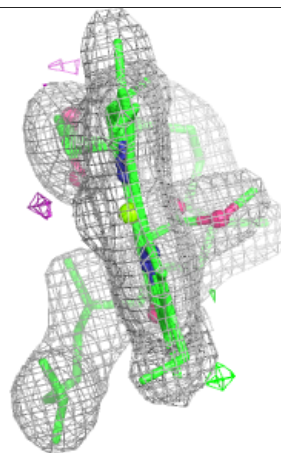
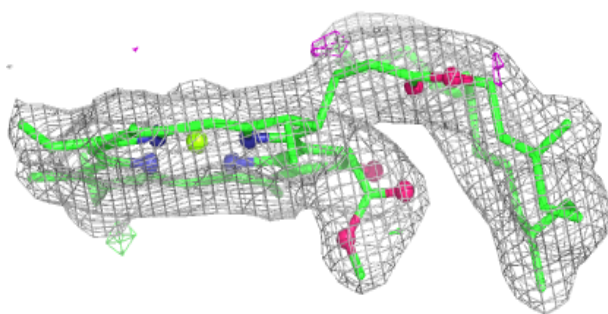
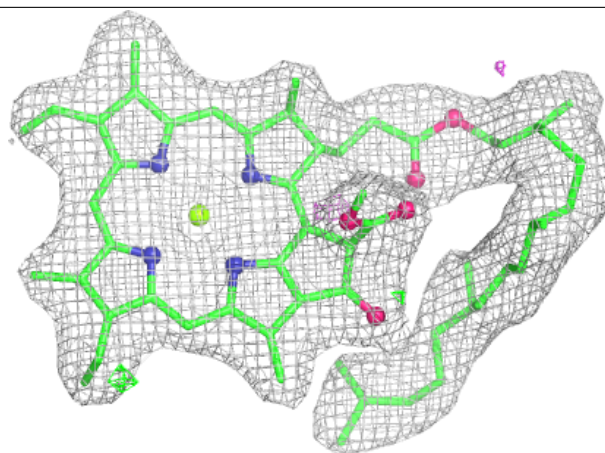
Electron density around CLA a 405:

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



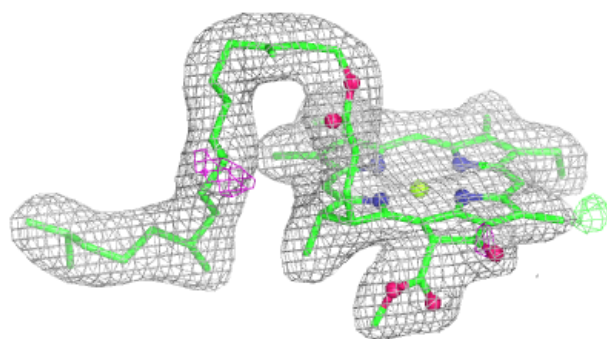
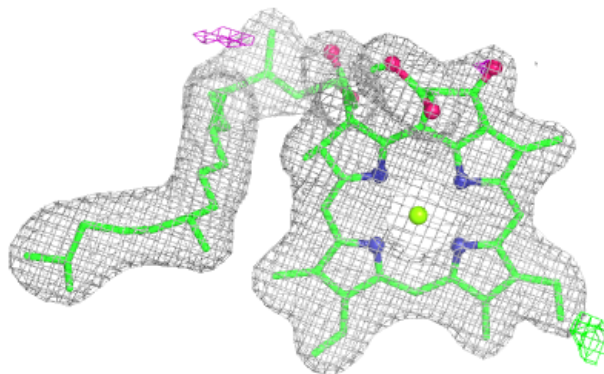
Electron density around CLA B 611:

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

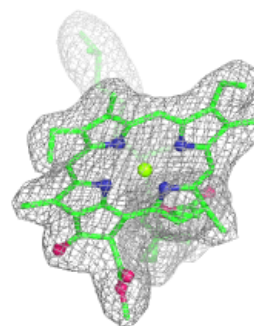
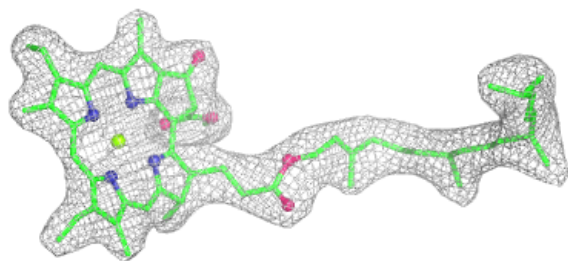
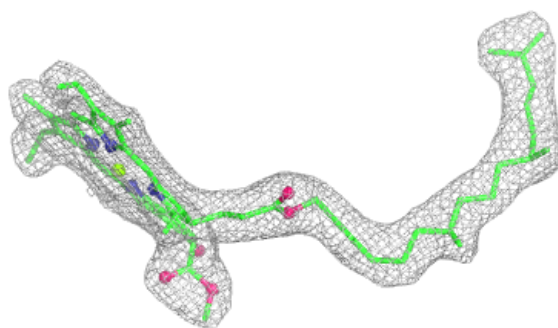


Electron density around CLA d 404:

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

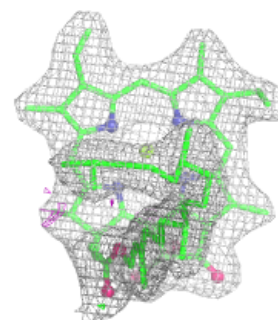
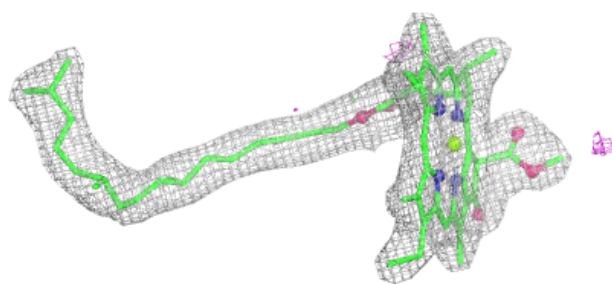
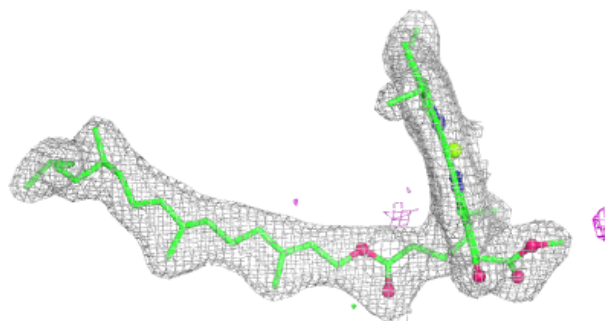
**Electron density around CLA d 405:**

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

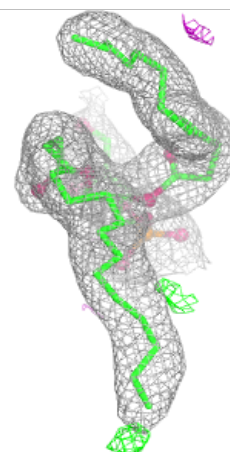
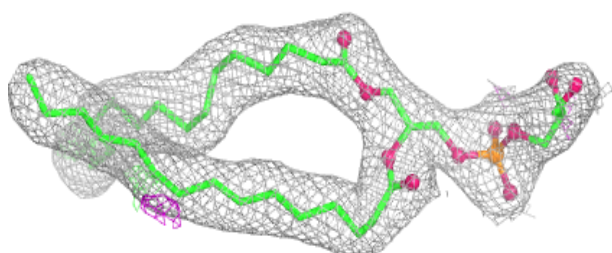
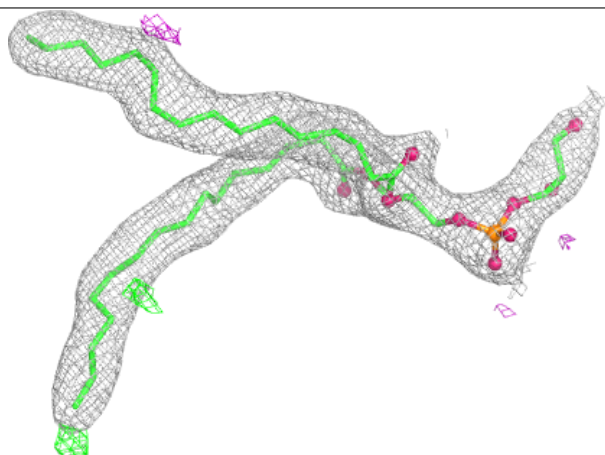


Electron density around CLA B 606:

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

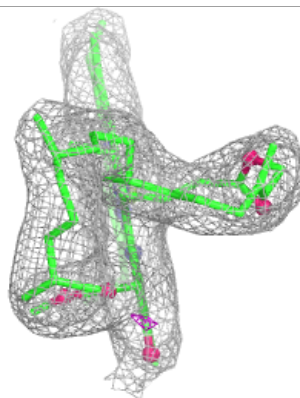
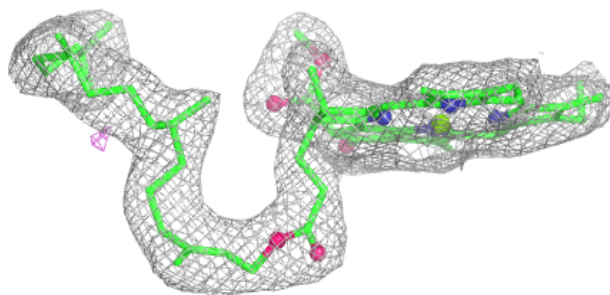
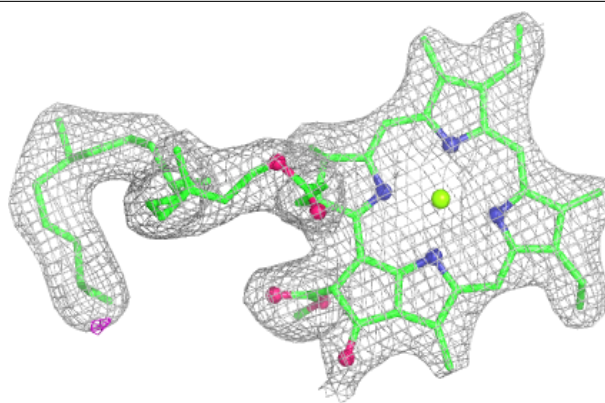
**Electron density around LHG d 410:**

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

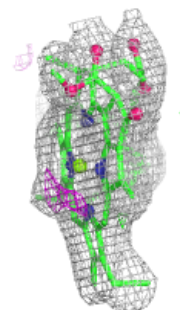
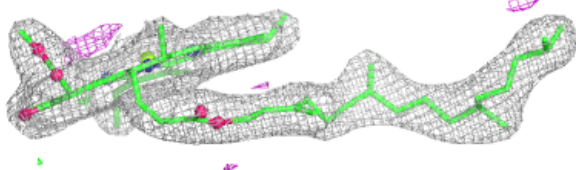
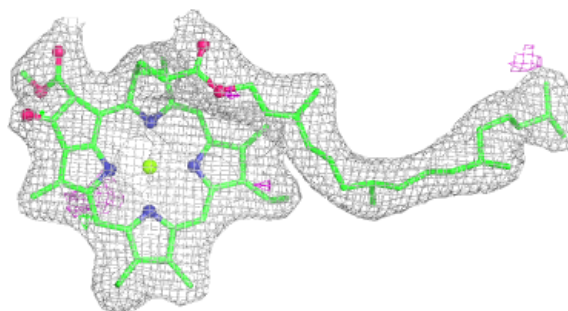


Electron density around CLA B 613:

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

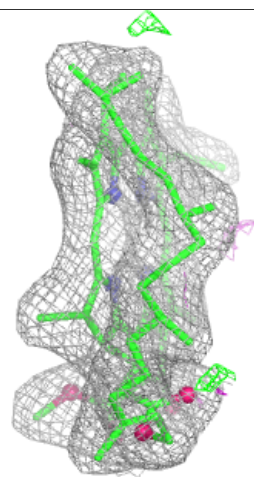
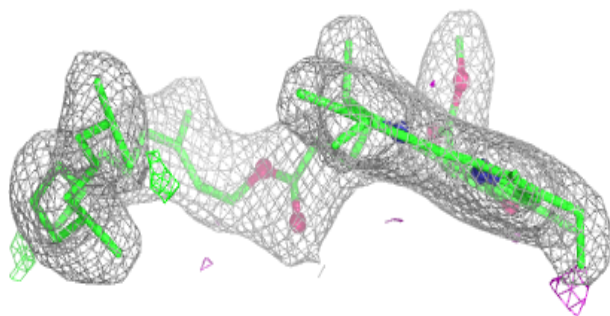
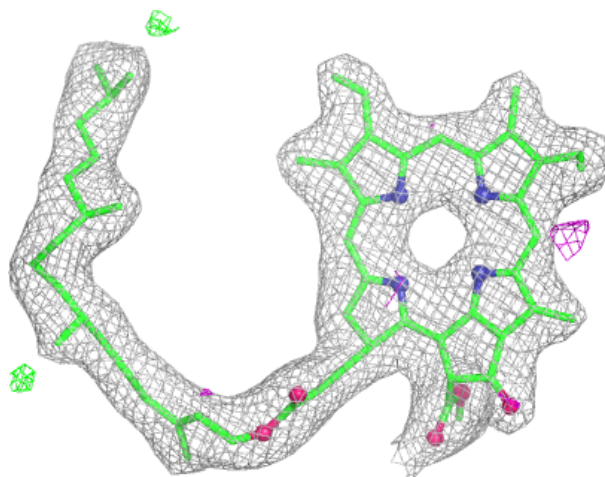
**Electron density around CLA B 604:**

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



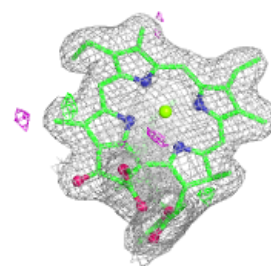
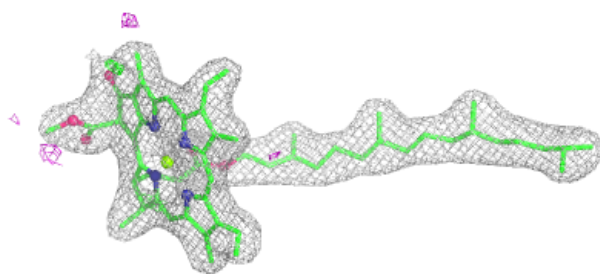
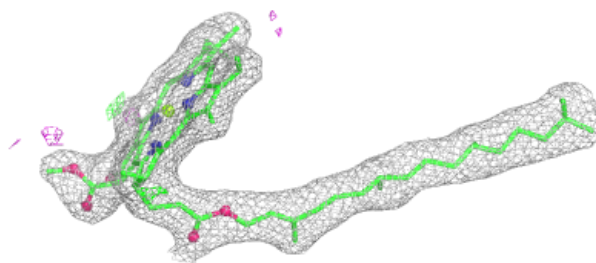
Electron density around PHO a 407:

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

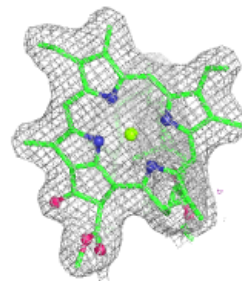
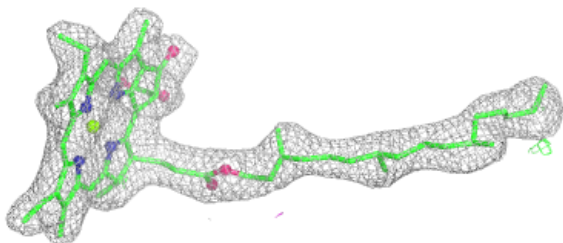
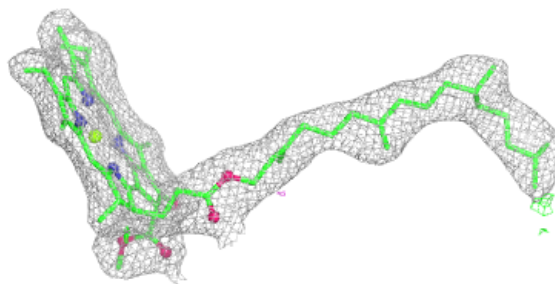


Electron density around CLA B 608:

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

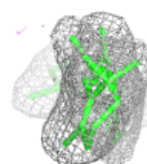
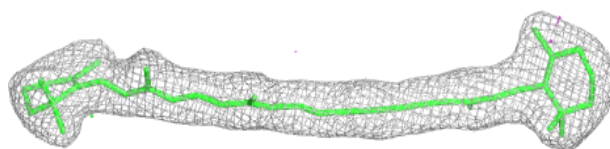
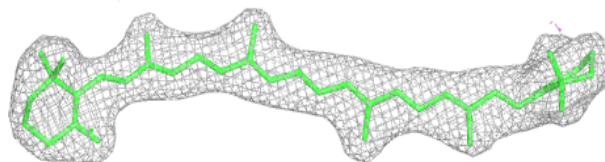
**Electron density around CLA b 609:**

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

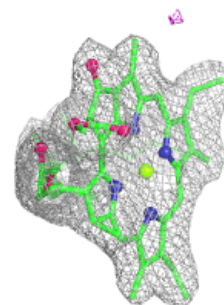
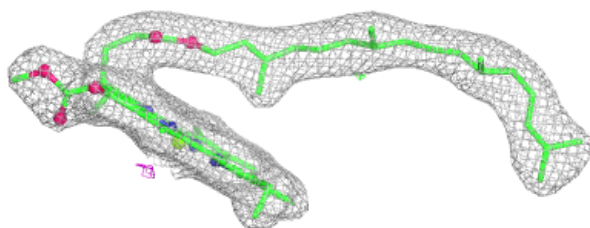
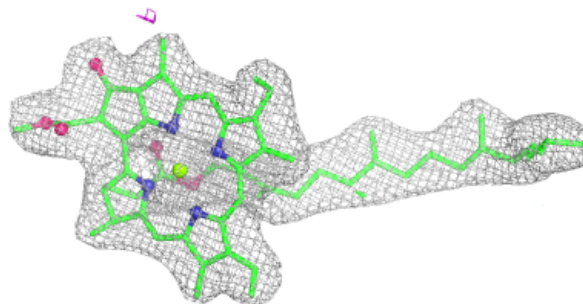


Electron density around BCR B 618:

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

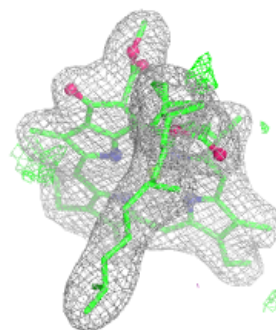
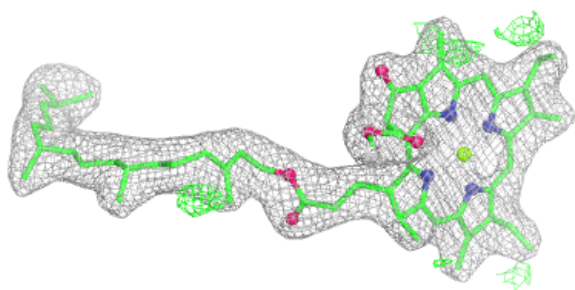
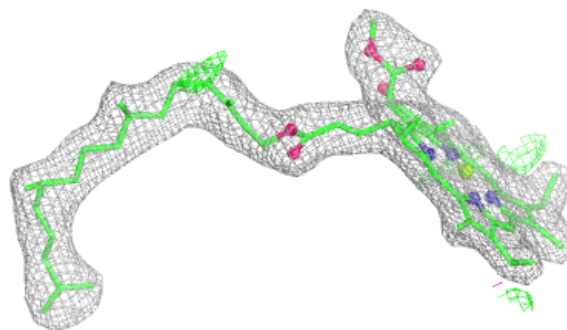
**Electron density around CLA B 609:**

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



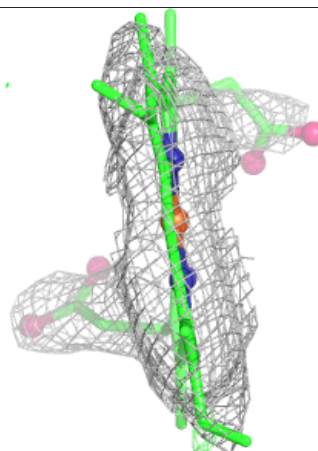
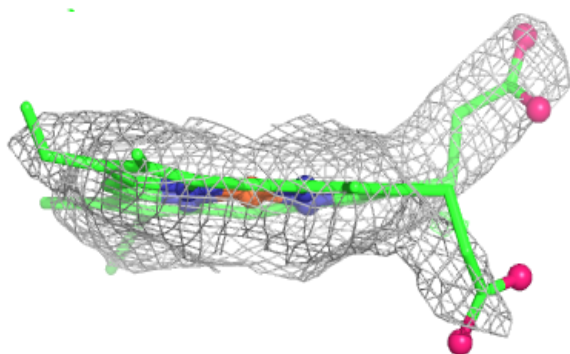
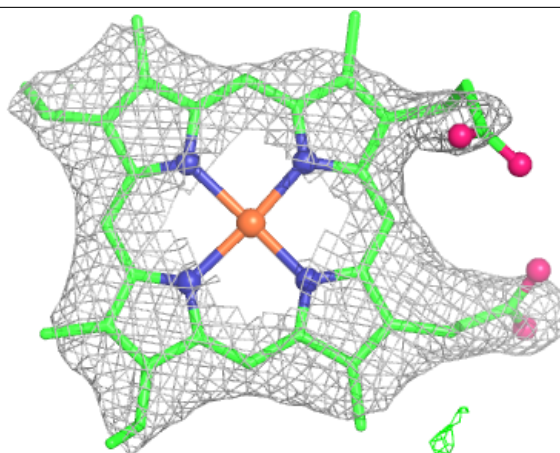
Electron density around CLA D 404:

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



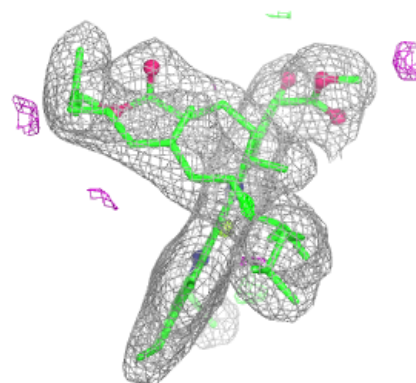
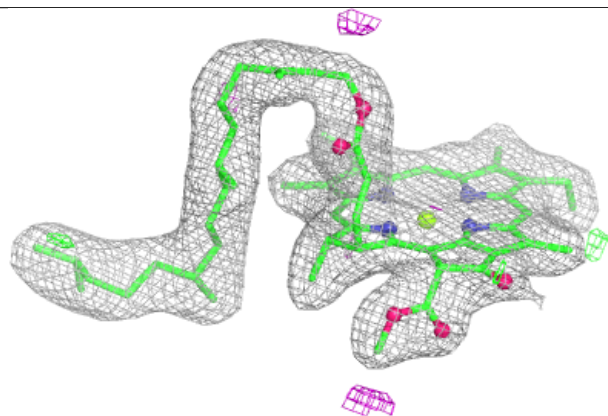
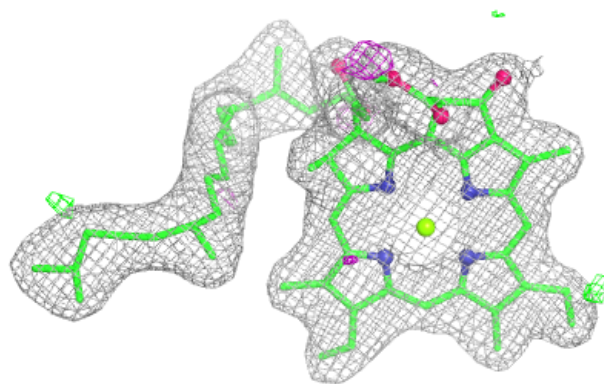
Electron density around HEM f 101:

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



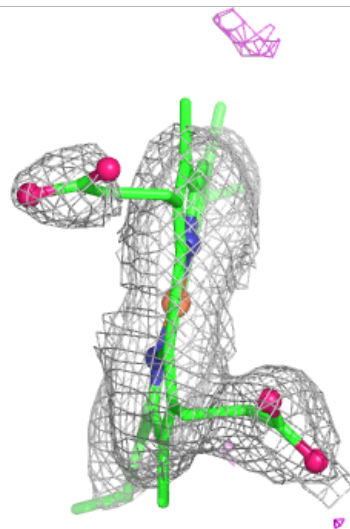
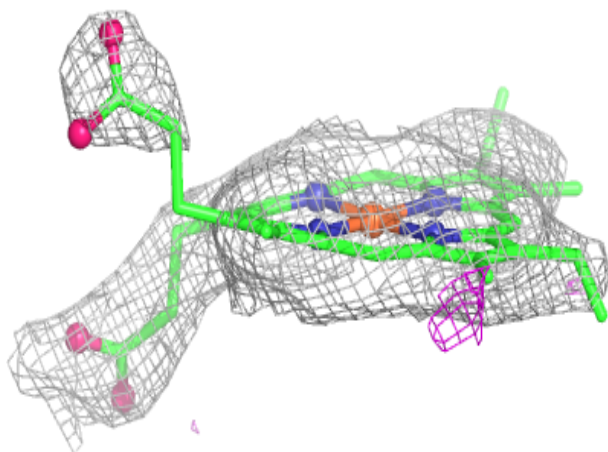
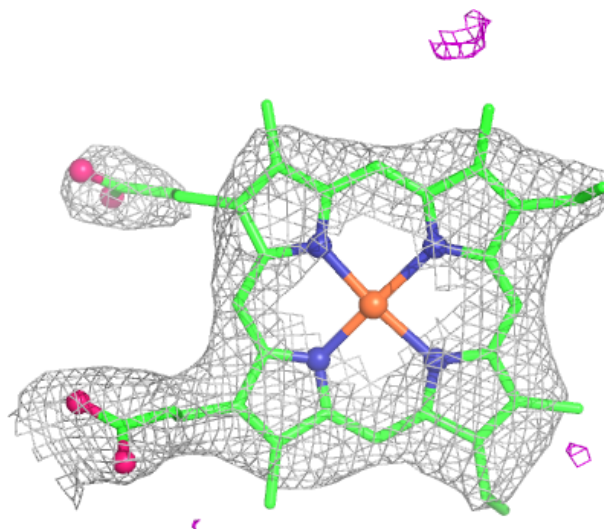
Electron density around CLA A 406:

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



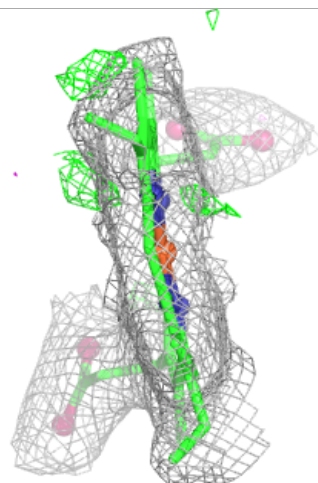
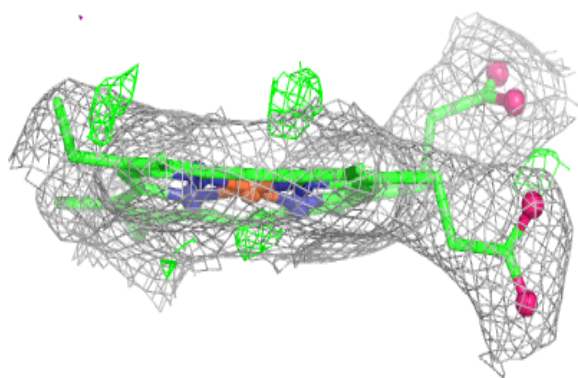
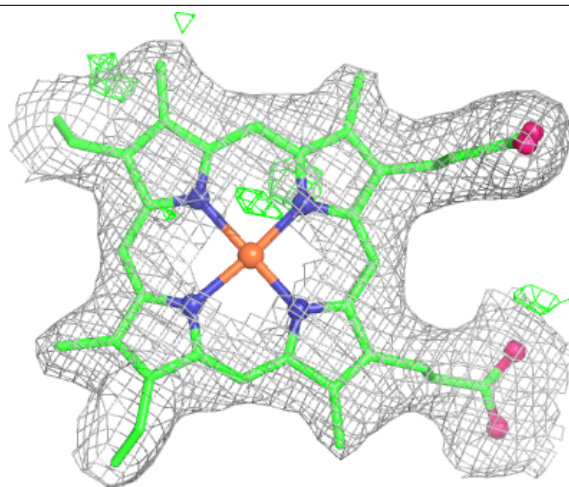
Electron density around HEM F 102:

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



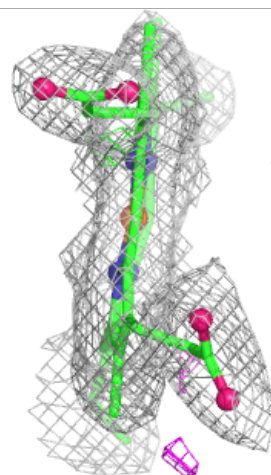
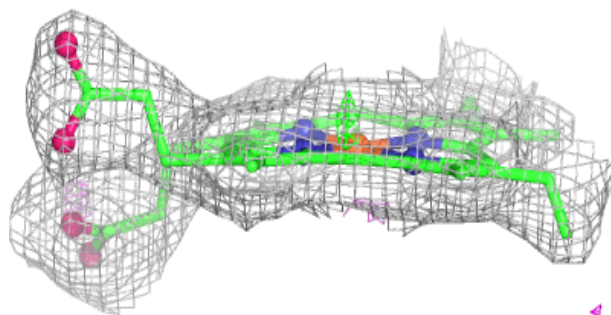
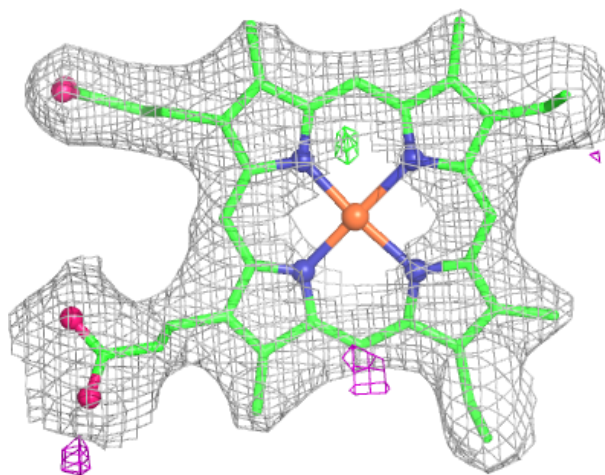
Electron density around HEC V 202:

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



Electron density around HEC v 202:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.