



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2026 – 06:04 AM JST

PDB ID : 8HQ8 / pdb_00008hq8
Title : Bry-LHCII homotrimer of Bryopsis corticulans
Authors : Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on : 2022-12-13
Resolution : 2.60 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

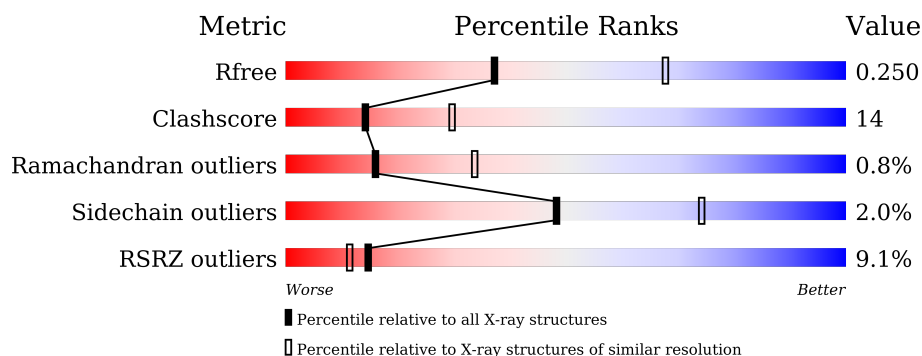
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	249	9% 69% 20% 10%
1	B	249	7% 70% 19% 10%
1	C	249	5% 72% 17% 11%
1	D	249	7% 72% 17% 10%
1	E	249	12% 65% 23% 10%
1	F	249	8% 71% 18% 10%

2 Entry composition [i](#)

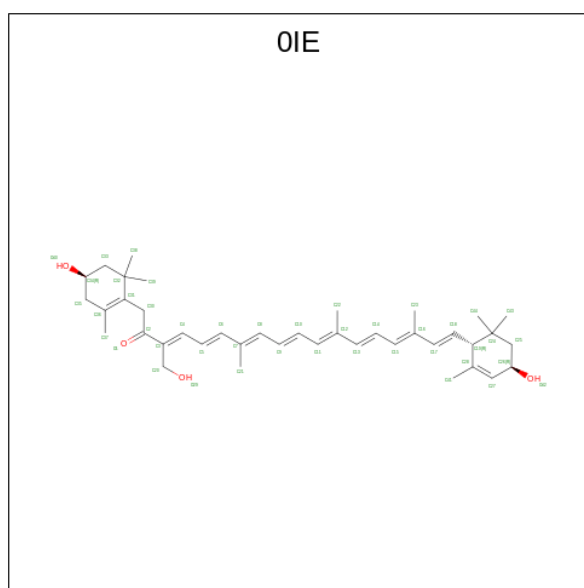
There are 12 unique types of molecules in this entry. The entry contains 16480 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1.

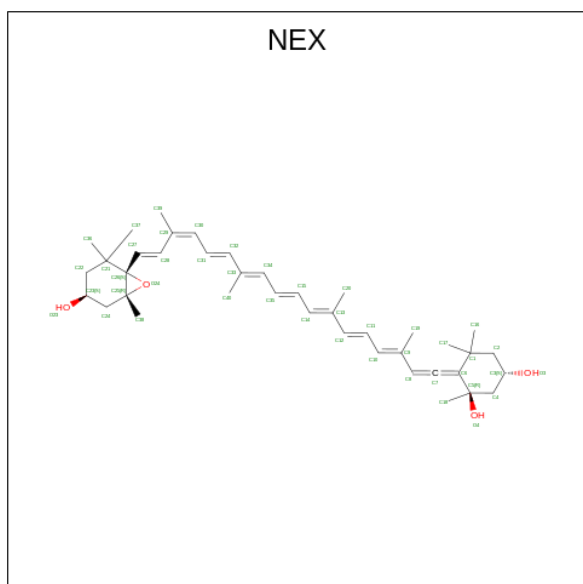
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1672	1083	265	314	10			
1	B	223	Total	C	N	O	S	0	0	0
			1669	1083	266	310	10			
1	C	222	Total	C	N	O	S	0	0	0
			1659	1075	264	310	10			
1	D	223	Total	C	N	O	S	0	0	0
			1682	1090	267	315	10			
1	E	223	Total	C	N	O	S	0	0	0
			1684	1095	267	312	10			
1	F	223	Total	C	N	O	S	0	0	0
			1685	1094	267	314	10			

- Molecule 2 is Siphonaxanthin (CCD ID: 01E) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



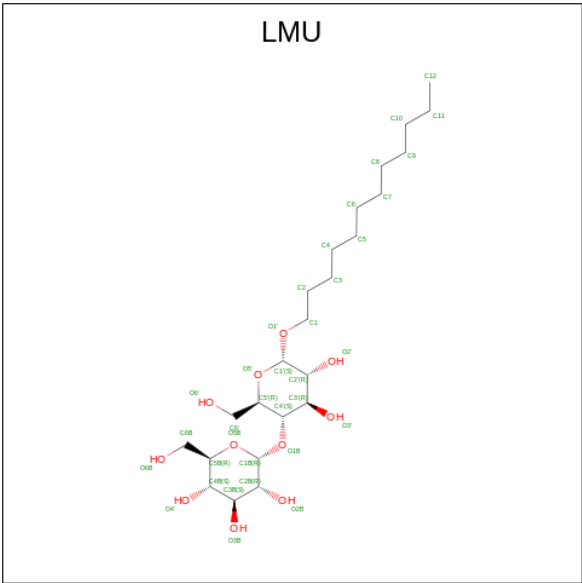
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 44 40 4	0	0
2	A	1	Total C O 44 40 4	0	0
2	B	1	Total C O 44 40 4	0	0
2	C	1	Total C O 44 40 4	0	0
2	C	1	Total C O 44 40 4	0	0
2	D	1	Total C O 44 40 4	0	0
2	D	1	Total C O 44 40 4	0	0
2	E	1	Total C O 44 40 4	0	0
2	E	1	Total C O 44 40 4	0	0
2	F	1	Total C O 44 40 4	0	0
2	F	1	Total C O 44 40 4	0	0

- Molecule 3 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



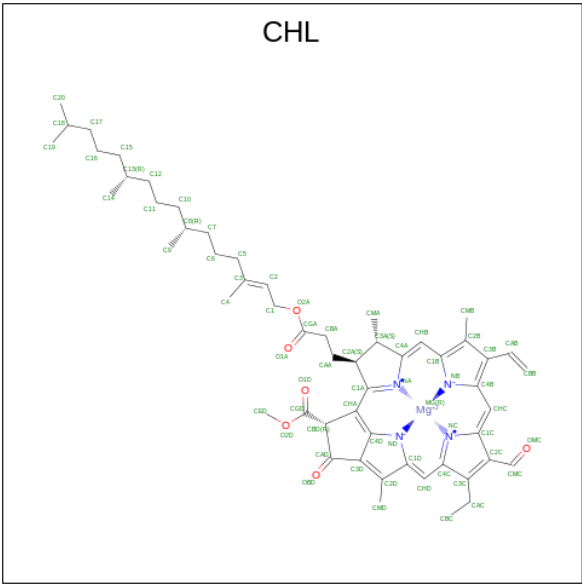
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			44	40	4		
3	B	1	Total	C	O	0	0
			44	40	4		
3	C	1	Total	C	O	0	0
			44	40	4		
3	D	1	Total	C	O	0	0
			44	40	4		
3	E	1	Total	C	O	0	0
			44	40	4		
3	F	1	Total	C	O	0	0
			44	40	4		

- Molecule 4 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	24	11		
4	B	1	Total	C	O	0	0
			33	23	10		
4	B	1	Total	C	O	0	0
			35	24	11		
4	D	1	Total	C	O	0	0
			35	24	11		
4	E	1	Total	C	O	0	0
			35	24	11		

- Molecule 5 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	A	1	Total 64	C 53	Mg 1	N 4	O 6	0	0
5	A	1	Total 43	C 34	Mg 1	N 4	O 4	0	0
5	A	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
5	A	1	Total 61	C 50	Mg 1	N 4	O 6	0	0
5	A	1	Total 56	C 45	Mg 1	N 4	O 6	0	0
5	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	A	1	Total 42	C 33	Mg 1	N 4	O 4	0	0
5	B	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	B	1	Total 65	C 54	Mg 1	N 4	O 6	0	0
5	B	1	Total 43	C 34	Mg 1	N 4	O 4	0	0
5	B	1	Total 51	C 40	Mg 1	N 4	O 6	0	0

Continued on next page...

Continued from previous page...

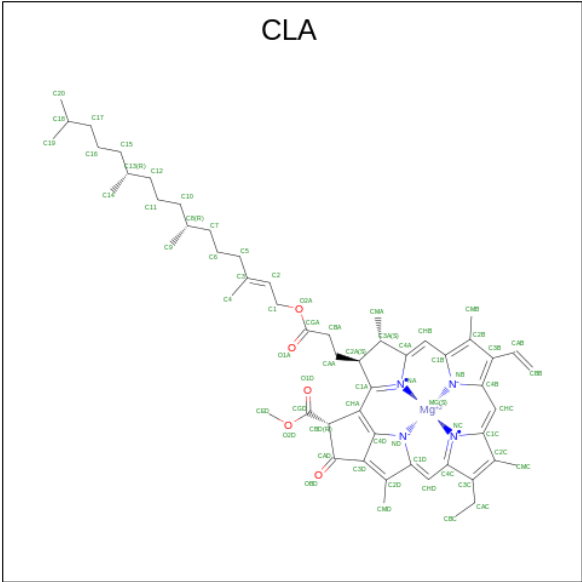
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	Mg	N	O	0	0
			62	51	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			57	46	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
5	C	1	Total	C	Mg	N	O	0	0
			44	35	1	4	4		
5	C	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			44	35	1	4	4		
5	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	D	1	Total	C	Mg	N	O	0	0
			65	54	1	4	6		
5	D	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
5	D	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
5	D	1	Total	C	Mg	N	O	0	0
			62	51	1	4	6		
5	D	1	Total	C	Mg	N	O	0	0
			57	46	1	4	6		
5	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	D	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
5	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	Mg	N	O	0	0
			64	53	1	4	6		
5	E	1	Total	C	Mg	N	O	0	0
			41	32	1	4	4		
5	E	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
5	E	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
5	E	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
5	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	E	1	Total	C	Mg	N	O	0	0
			41	32	1	4	4		
5	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	F	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
5	F	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
5	F	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
5	F	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
5	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	F	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		

- Molecule 6 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			63	53	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

Continued on next page...

Continued from previous page...

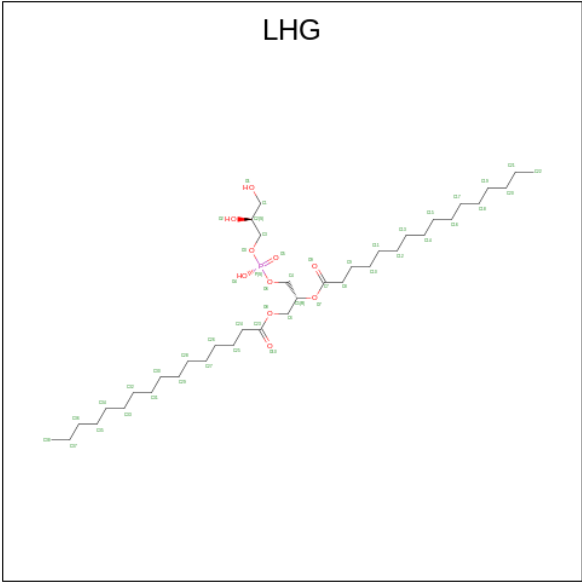
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
6	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	D	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
6	D	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
6	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	D	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
6	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	E	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	E	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
6	E	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
6	E	1	Total	C	Mg	N	O	0	0
			63	53	1	4	5		
6	E	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
6	E	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
6	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	F	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
6	F	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
6	F	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
6	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	F	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		

- Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).

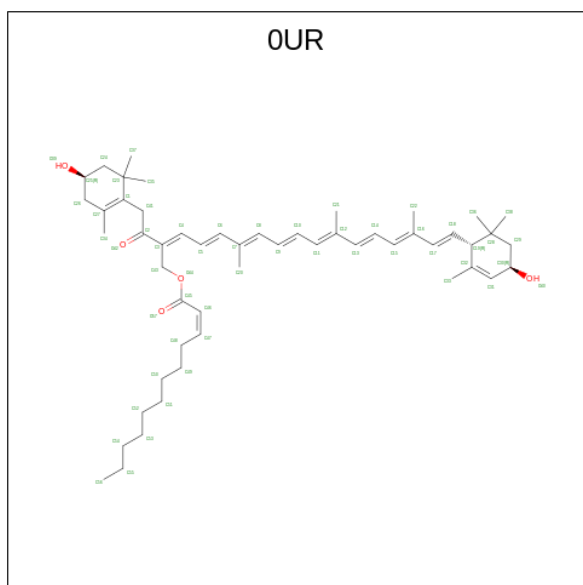


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			47	36	10	1		
7	B	1	Total	C	O	P	0	0
			46	35	10	1		
7	B	1	Total	C	O	P	0	0
			31	20	10	1		
7	C	1	Total	C	O	P	0	0
			25	14	10	1		
7	C	1	Total	C	O	P	0	0
			45	34	10	1		
7	D	1	Total	C	O	P	0	0
			46	35	10	1		
7	E	1	Total	C	O	P	0	0
			41	30	10	1		
7	F	1	Total	C	O	P	0	0
			45	34	10	1		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

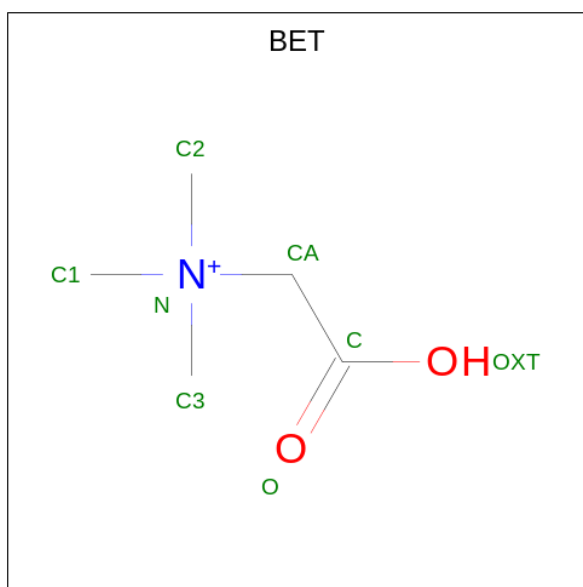
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Mg 2 2	0	0
8	D	1	Total Mg 1 1	0	0

- Molecule 9 is Siphonein (CCD ID: 0UR) (formula: $C_{52}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



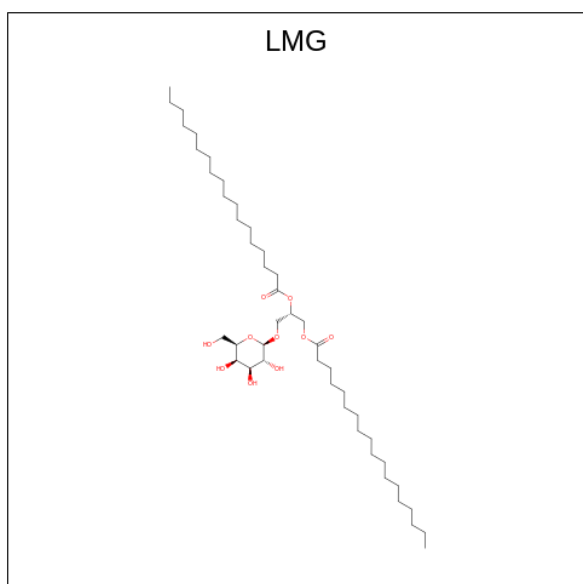
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 52 47 5	0	0
9	B	1	Total C O 50 45 5	0	0
9	B	1	Total C O 52 47 5	0	0
9	C	1	Total C O 52 47 5	0	0
9	D	1	Total C O 52 47 5	0	0
9	E	1	Total C O 52 47 5	0	0
9	F	1	Total C O 52 47 5	0	0

- Molecule 10 is TRIMETHYL GLYCINE (CCD ID: BET) (formula: $C_5H_{12}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			8	5	1	2		
10	B	1	Total	C	N	O	0	0
			8	5	1	2		
10	C	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 11 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			30	20	10		
11	F	1	Total	C	O	0	0
			30	20	10		

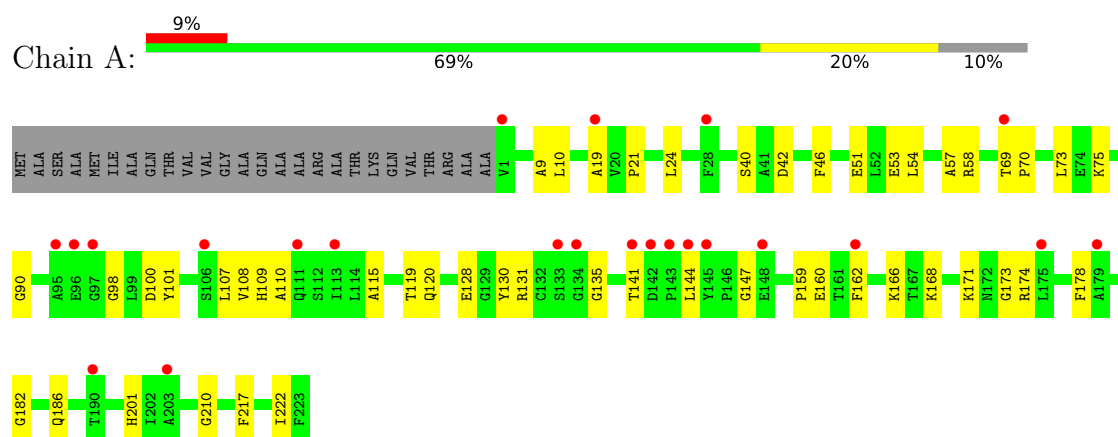
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	8	Total	O	0	0
			8	8		
12	B	7	Total	O	0	0
			7	7		
12	C	8	Total	O	0	0
			8	8		
12	D	4	Total	O	0	0
			4	4		
12	E	6	Total	O	0	0
			6	6		
12	F	8	Total	O	0	0
			8	8		

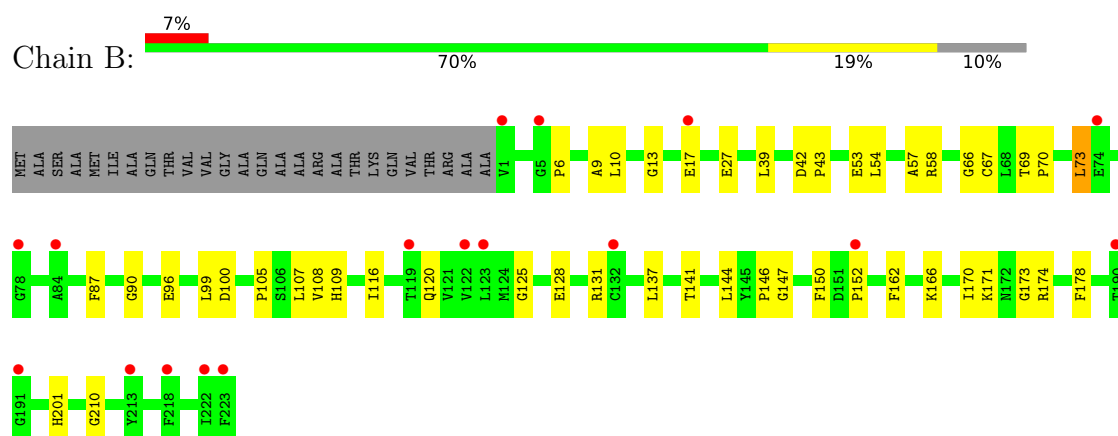
3 Residue-property plots [i](#)

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

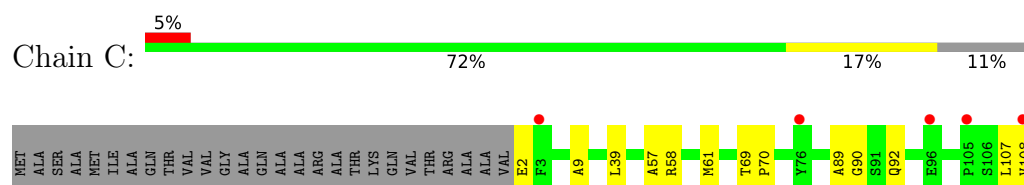
- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1



- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1

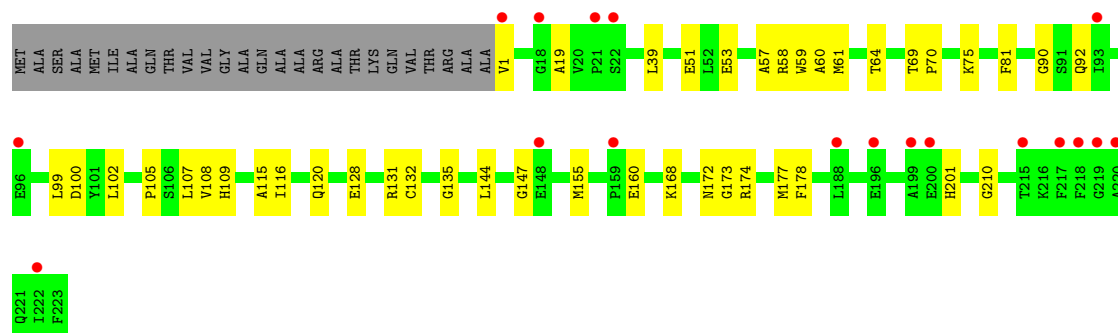
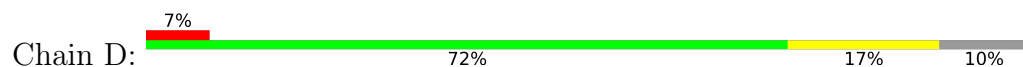


- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1

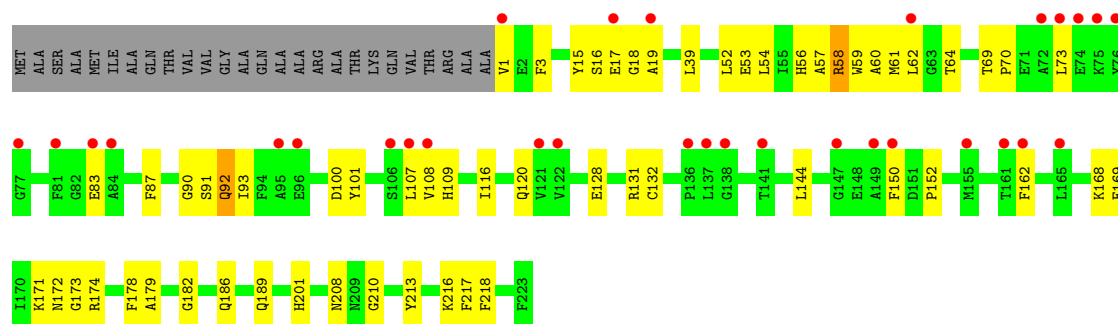




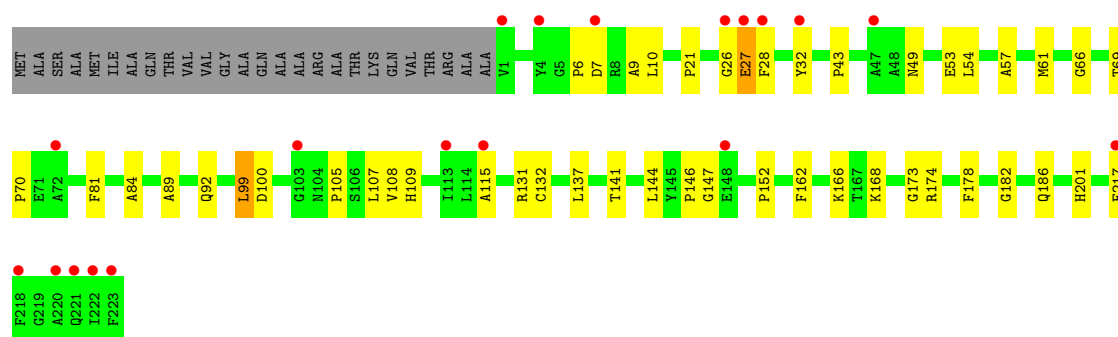
- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1



- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1



- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.72Å 91.61Å 169.22Å 90.00° 103.52° 90.00°	Depositor
Resolution (Å)	39.90 – 2.60 39.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	66.2 (39.90-2.60) 66.2 (39.90-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.18_3861: ???)	Depositor
R, R_{free}	0.207 , 0.249 0.216 , 0.250	Depositor DCC
R_{free} test set	2000 reflections (2.93%)	wwPDB-VP
Wilson B-factor (Å ²)	75.7	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16480	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NEX, LMG, LMU, OIE, LHG, OUR, CHL, CLA, BET

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	0.18	0/1725	0.38	0/2350
1	B	0.18	0/1722	0.37	0/2345
1	C	0.19	0/1712	0.35	0/2332
1	D	0.17	0/1735	0.37	0/2361
1	E	0.16	0/1737	0.36	0/2364
1	F	0.20	0/1738	0.40	0/2366
All	All	0.18	0/10369	0.37	0/14118

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1672	0	1547	42	0
1	B	1669	0	1552	44	0
1	C	1659	0	1523	43	0
1	D	1682	0	1572	36	0
1	E	1684	0	1581	52	0
1	F	1685	0	1579	41	0
2	A	88	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	0	1	0
2	C	88	0	0	2	0
2	D	88	0	0	0	0
2	E	88	0	0	1	0
2	F	88	0	0	0	0
3	A	44	0	56	3	0
3	B	44	0	54	4	0
3	C	44	0	55	4	0
3	D	44	0	55	4	0
3	E	44	0	55	3	0
3	F	44	0	53	1	0
4	A	35	0	46	4	0
4	B	68	0	85	3	0
4	D	35	0	46	3	0
4	E	35	0	46	3	0
5	A	449	0	397	25	0
5	B	457	0	407	35	0
5	C	445	0	403	35	0
5	D	449	0	402	34	0
5	E	438	0	384	29	0
5	F	445	0	397	29	0
6	A	333	0	305	22	0
6	B	344	0	337	22	0
6	C	330	0	306	25	0
6	D	344	0	337	22	0
6	E	333	0	305	19	0
6	F	325	0	293	23	0
7	A	47	0	67	3	0
7	B	77	0	97	13	0
7	C	70	0	83	4	0
7	D	46	0	65	4	0
7	E	41	0	52	7	0
7	F	45	0	63	8	0
8	A	2	0	0	0	0
8	D	1	0	0	0	0
9	A	52	0	0	0	0
9	B	102	0	0	5	0
9	C	52	0	0	4	0
9	D	52	0	0	0	0
9	E	52	0	0	4	0
9	F	52	0	0	3	0
10	B	16	0	22	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	8	0	11	0	0
11	B	30	0	30	0	0
11	F	30	0	30	1	0
12	A	8	0	0	0	0
12	B	7	0	0	1	0
12	C	8	0	0	1	0
12	D	4	0	0	1	0
12	E	6	0	0	0	0
12	F	8	0	0	2	0
All	All	16480	0	14698	441	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (441) 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:E:83:GLU:H	1:E:92:GLN:HE21	1.12	0.94
6:F:313:CLA:H43	6:F:315:CLA:HBA1	1.50	0.89
3:D:303:NEX:H42	4:D:304:LMU:H6'2	1.56	0.88
5:D:311:CHL:H62	5:D:313:CHL:H193	1.61	0.81
1:B:150:PHE:HD1	5:B:313:CHL:H2	1.47	0.79
1:B:42:ASP:OD2	7:B:324:LHG:O3	2.02	0.78
1:D:135:GLY:HA2	4:D:304:LMU:H3B	1.68	0.75
1:E:150:PHE:HA	5:E:311:CHL:H51	1.67	0.75
6:F:306:CLA:HAC2	5:F:310:CHL:H142	1.69	0.75
1:F:57:ALA:HB1	1:F:173:GLY:HA3	1.69	0.74
1:C:131:ARG:NH2	5:C:313:CHL:O1D	2.20	0.74
1:A:42:ASP:OD2	7:B:324:LHG:HC41	1.87	0.74
1:C:119:THR:HG21	5:C:310:CHL:HED2	1.71	0.73
1:B:57:ALA:HB1	1:B:173:GLY:HA3	1.71	0.73
5:F:305:CHL:CHB	5:F:305:CHL:H11	2.19	0.73
5:D:311:CHL:H93	5:D:313:CHL:H152	1.71	0.72
1:A:57:ALA:HB1	1:A:173:GLY:HA3	1.71	0.72
1:C:111:GLN:HG3	5:C:309:CHL:HAB	1.69	0.72
1:C:125:GLY:HA2	5:C:313:CHL:HAB	1.72	0.72
5:B:311:CHL:HAB	5:B:312:CHL:HMC	1.70	0.71
1:C:198:TRP:HE1	5:C:318:CHL:CMC	2.04	0.71
1:E:171:LYS:NZ	7:E:318:LHG:O4	2.24	0.71
1:D:57:ALA:HB1	1:D:173:GLY:HA3	1.72	0.70
1:E:131:ARG:NH2	5:E:312:CHL:O1D	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:SER:O	1:E:18:GLY:N	2.24	0.70
1:F:26:GLY:O	1:F:28:PHE:N	2.24	0.69
1:E:57:ALA:HB1	1:E:173:GLY:HA3	1.73	0.69
1:B:152:PRO:HD2	9:B:325:OUR:O40	1.93	0.69
5:E:312:CHL:HHC	5:E:312:CHL:HBB1	1.75	0.69
1:E:58:ARG:NH1	1:E:169:GLU:OE2	2.27	0.68
6:C:307:CLA:HBB1	5:C:313:CHL:H172	1.76	0.68
6:A:307:CLA:H91	5:A:313:CHL:H121	1.75	0.67
1:D:131:ARG:NH2	5:D:313:CHL:O1D	2.27	0.66
1:C:58:ARG:NH1	5:C:312:CHL:OBD	2.27	0.66
1:A:90:GLY:HA2	5:A:310:CHL:HAC2	1.78	0.66
1:A:201:HIS:CG	6:A:317:CLA:HAA2	2.31	0.66
1:F:92:GLN:HG3	1:F:99:LEU:HG	1.78	0.66
1:B:120:GLN:NE2	5:B:314:CHL:OMC	2.26	0.66
1:B:131:ARG:NH2	5:B:314:CHL:O1D	2.28	0.66
1:C:137:LEU:HD13	5:C:312:CHL:HAB	1.77	0.66
6:F:315:CLA:HMC3	9:F:320:OUR:C43	2.26	0.65
1:A:100:ASP:OD1	1:A:109:HIS:ND1	2.25	0.65
1:F:132:CYS:SG	12:F:406:HOH:O	2.53	0.65
1:E:100:ASP:OD1	1:E:109:HIS:ND1	2.25	0.65
1:A:147:GLY:HA3	6:A:314:CLA:HED1	1.78	0.65
6:C:307:CLA:CBB	5:C:313:CHL:H172	2.27	0.64
1:B:150:PHE:CD1	5:B:313:CHL:H2	2.30	0.64
1:B:120:GLN:NE2	5:B:312:CHL:OMC	2.30	0.63
1:B:43:PRO:HB2	1:F:6:PRO:HB3	1.80	0.63
1:F:201:HIS:CG	6:F:316:CLA:HAA2	2.33	0.63
1:E:168:LYS:O	1:E:172:ASN:ND2	2.26	0.63
2:A:302:OIE:C25	6:A:315:CLA:HBB1	2.28	0.62
6:F:316:CLA:H93	7:F:318:LHG:H142	1.80	0.62
5:A:305:CHL:H52	5:C:313:CHL:HBB1	1.82	0.61
1:E:90:GLY:HA2	5:E:309:CHL:HAC2	1.81	0.61
5:D:311:CHL:H71	5:D:313:CHL:H171	1.82	0.61
1:B:66:GLY:O	12:B:401:HOH:O	2.16	0.61
5:D:310:CHL:HAB	5:D:311:CHL:HMC	1.82	0.61
5:E:317:CHL:HHC	5:E:317:CHL:HBB1	1.82	0.61
6:A:308:CLA:HBA1	6:A:308:CLA:HBD	1.82	0.61
6:E:315:CLA:HMC2	9:E:320:OUR:C43	2.31	0.60
1:F:131:ARG:NH2	5:F:312:CHL:O1D	2.35	0.60
5:D:306:CHL:H141	5:E:312:CHL:H42	1.83	0.60
1:A:131:ARG:NH2	5:A:313:CHL:O1D	2.34	0.60
1:F:147:GLY:HA3	6:F:313:CLA:HED1	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:314:CLA:HAB	9:C:321:0UR:C13	2.31	0.60
1:B:147:GLY:HA3	6:B:315:CLA:HED1	1.84	0.59
1:B:152:PRO:HD2	9:B:325:0UR:C30	2.32	0.59
1:D:147:GLY:HA3	6:D:314:CLA:HED1	1.85	0.59
1:E:1:VAL:HG22	1:E:3:PHE:H	1.67	0.59
1:F:178:PHE:CD1	5:F:305:CHL:H191	2.38	0.59
5:E:312:CHL:H202	6:F:306:CLA:H141	1.85	0.59
1:E:39:LEU:HD12	5:E:305:CHL:H11	1.85	0.59
6:E:316:CLA:HBB	5:E:317:CHL:HHD	1.84	0.59
1:D:132:CYS:SG	12:D:404:HOH:O	2.57	0.58
1:B:90:GLY:HA2	5:B:311:CHL:HAC2	1.84	0.58
6:F:313:CLA:O1D	6:F:313:CLA:H2A	2.02	0.58
1:C:92:GLN:NE2	6:C:308:CLA:O1D	2.37	0.58
5:D:310:CHL:CAB	5:D:311:CHL:HMC	2.35	0.57
1:E:83:GLU:N	1:E:92:GLN:HE21	1.93	0.57
1:D:201:HIS:CG	6:D:317:CLA:HAA2	2.39	0.57
1:C:201:HIS:ND1	1:C:208:ASN:O	2.34	0.57
1:C:115:ALA:HB3	5:C:309:CHL:HMC	1.86	0.57
1:E:201:HIS:ND1	1:E:208:ASN:O	2.29	0.57
5:A:311:CHL:H62	5:A:313:CHL:H193	1.87	0.56
1:B:201:HIS:CG	6:B:318:CLA:HAA2	2.40	0.56
6:D:307:CLA:H51	5:F:305:CHL:H91	1.86	0.56
1:B:42:ASP:OD2	7:B:324:LHG:C3	2.53	0.56
6:F:314:CLA:H2	6:F:315:CLA:HMD2	1.86	0.56
6:E:315:CLA:HED2	6:E:315:CLA:H2A	1.88	0.56
1:B:137:LEU:HD13	5:B:313:CHL:HAB	1.87	0.56
5:F:312:CHL:HHC	5:F:312:CHL:HBB1	1.88	0.56
1:C:201:HIS:CG	6:C:317:CLA:HAA2	2.39	0.56
5:C:305:CHL:HBB1	5:C:305:CHL:HHC	1.87	0.56
6:B:317:CLA:HMC3	9:B:325:0UR:C43	2.36	0.56
1:B:9:ALA:HA	10:B:322:BET:H23	1.88	0.55
6:B:315:CLA:HHD	6:B:315:CLA:HBC2	1.88	0.55
6:B:316:CLA:NC	7:B:320:LHG:HC42	2.21	0.55
6:C:317:CLA:H2	5:C:318:CHL:HMD1	1.88	0.55
7:F:318:LHG:HC62	7:F:318:LHG:H281	1.89	0.55
1:D:51:GLU:HA	1:D:144:LEU:HD11	1.89	0.54
1:A:168:LYS:HD3	6:A:316:CLA:HAA2	1.90	0.54
6:C:317:CLA:H91	7:C:319:LHG:H322	1.88	0.54
1:E:182:GLY:O	1:E:186:GLN:HB2	2.07	0.54
6:B:318:CLA:H8	5:B:319:CHL:HMD3	1.90	0.54
1:C:111:GLN:CG	5:C:309:CHL:HAB	2.36	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:HIS:CG	6:E:316:CLA:HAA2	2.42	0.54
1:D:120:GLN:NE2	5:D:313:CHL:OMC	2.32	0.53
6:D:308:CLA:HMB2	5:D:310:CHL:HBB1	1.90	0.53
1:F:9:ALA:HB1	5:F:304:CHL:HBC1	1.89	0.53
6:F:314:CLA:C4C	7:F:318:LHG:HC61	2.38	0.53
1:A:9:ALA:HB1	5:A:305:CHL:HBC1	1.91	0.53
1:C:198:TRP:NE1	5:C:318:CHL:OMC	2.35	0.53
1:F:53:GLU:OE2	1:F:174:ARG:NE	2.38	0.53
1:B:58:ARG:NH1	5:B:313:CHL:OBD	2.34	0.53
6:B:315:CLA:H2A	6:B:315:CLA:O1D	2.08	0.53
1:E:15:TYR:OH	4:E:319:LMU:H1B	2.08	0.53
1:C:125:GLY:CA	5:C:313:CHL:HAB	2.38	0.53
1:B:125:GLY:HA2	5:B:314:CHL:HAB	1.90	0.53
1:E:101:TYR:CE2	6:E:307:CLA:H2	2.44	0.53
1:F:32:TYR:OH	7:F:318:LHG:O5	2.18	0.53
1:B:6:PRO:HB3	1:F:43:PRO:HB2	1.91	0.52
1:D:120:GLN:NE2	5:D:311:CHL:OMC	2.42	0.52
1:D:168:LYS:O	1:D:172:ASN:ND2	2.31	0.52
1:E:150:PHE:HD1	5:E:311:CHL:H2	1.74	0.52
1:A:42:ASP:OD2	7:B:324:LHG:O4	2.28	0.52
1:B:67:CYS:SG	2:B:301:OIE:C39	2.98	0.52
1:D:58:ARG:NH1	5:D:312:CHL:OBD	2.35	0.52
1:F:100:ASP:CG	1:F:105:PRO:HA	2.35	0.52
1:B:53:GLU:OE2	1:B:174:ARG:NE	2.40	0.52
6:A:307:CLA:H51	5:B:307:CHL:H91	1.92	0.52
1:E:128:GLU:HG3	5:E:312:CHL:NB	2.24	0.52
1:D:115:ALA:HB3	5:D:309:CHL:HMC	1.90	0.51
5:D:310:CHL:HAA2	5:D:310:CHL:HBD	1.93	0.51
1:E:54:LEU:O	1:E:58:ARG:HG2	2.11	0.51
6:F:306:CLA:O1A	6:F:306:CLA:H2A	2.01	0.51
1:A:58:ARG:NH1	5:A:312:CHL:OBD	2.43	0.51
1:B:152:PRO:CD	9:B:325:OUR:O40	2.58	0.51
1:C:61:MET:HE3	1:C:173:GLY:N	2.25	0.51
6:C:317:CLA:H101	7:C:319:LHG:H142	1.91	0.51
1:F:92:GLN:HE22	6:F:307:CLA:HED2	1.76	0.51
1:E:162:PHE:CZ	6:E:313:CLA:HED3	2.46	0.51
1:E:213:TYR:O	1:E:216:LYS:HG2	2.10	0.51
1:F:61:MET:HE3	1:F:173:GLY:N	2.25	0.51
1:C:57:ALA:HB1	1:C:173:GLY:HA3	1.93	0.51
1:B:54:LEU:HD23	1:B:144:LEU:HD13	1.92	0.50
6:D:317:CLA:H92	7:D:319:LHG:H151	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:LEU:O	1:E:56:HIS:ND1	2.43	0.50
1:A:53:GLU:OE2	1:A:174:ARG:NE	2.44	0.50
1:F:54:LEU:HD23	1:F:144:LEU:HD13	1.93	0.50
1:F:178:PHE:HE1	5:F:305:CHL:H201	1.76	0.50
6:E:307:CLA:HBD	6:E:307:CLA:HBA1	1.93	0.50
1:A:128:GLU:HG3	5:A:313:CHL:NB	2.26	0.49
1:C:92:GLN:HE22	6:C:308:CLA:HED3	1.76	0.49
3:D:303:NEX:H42	4:D:304:LMU:C6B	2.37	0.49
1:A:210:GLY:HA2	6:A:317:CLA:OBD	2.13	0.49
6:B:308:CLA:O1A	6:B:308:CLA:H2A	2.12	0.49
1:C:90:GLY:HA2	5:C:310:CHL:HAC2	1.94	0.49
6:C:307:CLA:CAD	5:C:313:CHL:H2	2.41	0.49
1:D:116:ILE:HG12	5:D:309:CHL:HAC1	1.92	0.49
5:D:305:CHL:HAC1	7:D:319:LHG:HC2	1.93	0.49
5:E:304:CHL:HED3	7:E:318:LHG:H141	1.95	0.49
6:F:316:CLA:HHB	5:F:317:CHL:HHD	1.94	0.49
1:F:66:GLY:O	12:F:401:HOH:O	2.19	0.49
6:C:308:CLA:HMB1	5:C:310:CHL:HBB1	1.93	0.49
6:D:317:CLA:H122	7:D:319:LHG:H322	1.95	0.49
5:D:311:CHL:O1A	1:F:217:PHE:HB2	2.13	0.49
1:F:89:ALA:O	1:F:92:GLN:HG2	2.13	0.49
6:B:318:CLA:H111	7:B:320:LHG:H312	1.93	0.49
6:D:314:CLA:HMB1	6:D:314:CLA:HBB1	1.94	0.49
1:C:152:PRO:HD2	9:C:321:OUR:C30	2.43	0.49
1:A:159:PRO:HD2	1:D:1:VAL:HB	1.94	0.49
1:A:21:PRO:HD2	1:A:24:LEU:HD12	1.95	0.48
1:B:116:ILE:HG12	5:B:310:CHL:HAC1	1.94	0.48
1:D:53:GLU:OE2	1:D:174:ARG:NE	2.45	0.48
1:C:201:HIS:CD2	6:C:317:CLA:HAA2	2.49	0.48
1:E:152:PRO:HD2	9:E:320:OUR:C30	2.43	0.48
1:A:69:THR:HB	1:A:70:PRO:HD3	1.95	0.48
5:F:309:CHL:CAB	5:F:310:CHL:HMC	2.43	0.48
1:A:19:ALA:HB2	1:C:132:CYS:HB3	1.95	0.48
5:B:314:CHL:H141	5:B:314:CHL:H161	1.57	0.48
1:E:201:HIS:CD2	6:E:316:CLA:HAA2	2.49	0.48
1:A:201:HIS:CD2	6:A:317:CLA:HAA2	2.48	0.48
7:F:318:LHG:H272	7:F:318:LHG:H242	1.49	0.48
1:B:152:PRO:HD2	9:B:325:OUR:C31	2.44	0.48
5:B:312:CHL:H142	5:B:314:CHL:H102	1.95	0.48
1:B:107:LEU:O	1:B:109:HIS:N	2.47	0.48
5:E:308:CHL:HHC	5:E:308:CHL:HBB1	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:304:CHL:HBA1	5:E:304:CHL:H3A	1.63	0.47
1:D:59:TRP:CD1	5:D:313:CHL:HMD3	2.49	0.47
5:E:308:CHL:HHD	5:E:309:CHL:OBD	2.14	0.47
6:C:316:CLA:HMC2	9:C:321:OUR:C43	2.44	0.47
1:A:130:TYR:CE1	4:A:304:LMU:H6D	2.49	0.47
5:F:311:CHL:HHC	5:F:311:CHL:HMC	1.60	0.47
1:D:39:LEU:HD11	6:E:306:CLA:H12	1.97	0.47
1:D:201:HIS:CD2	6:D:317:CLA:HAA2	2.49	0.47
4:B:304:LMU:H1B	4:B:304:LMU:H6'2	1.59	0.47
7:B:324:LHG:H272	7:B:324:LHG:H241	1.50	0.47
1:D:19:ALA:HB2	1:E:132:CYS:HB3	1.97	0.47
4:E:319:LMU:O2'	3:F:303:NEX:H193	2.15	0.47
1:F:182:GLY:O	1:F:186:GLN:HB2	2.15	0.47
5:A:306:CHL:H121	5:A:306:CHL:H8	1.51	0.47
5:D:311:CHL:HAB	5:D:311:CHL:H151	1.97	0.47
1:E:58:ARG:NH2	1:E:144:LEU:O	2.47	0.47
3:B:303:NEX:H15	3:B:303:NEX:H201	1.65	0.47
1:C:107:LEU:HD23	5:C:309:CHL:HED2	1.97	0.47
1:D:210:GLY:HA2	6:D:317:CLA:OBD	2.15	0.47
1:F:9:ALA:HB1	5:F:304:CHL:CBC	2.44	0.47
5:B:307:CHL:H72	5:B:307:CHL:H111	1.62	0.47
1:F:137:LEU:HD13	5:F:311:CHL:HAB	1.96	0.47
1:F:146:PRO:HD2	6:F:313:CLA:OBD	2.15	0.47
6:F:313:CLA:H72	9:F:320:OUR:C15	2.45	0.47
1:B:171:LYS:NZ	7:B:320:LHG:O4	2.44	0.46
6:C:307:CLA:H91	5:C:313:CHL:H143	1.97	0.46
4:A:304:LMU:H91	4:A:304:LMU:H62	1.45	0.46
1:C:182:GLY:O	1:C:186:GLN:HB2	2.14	0.46
3:C:303:NEX:O24	5:C:310:CHL:HAA2	2.16	0.46
1:E:120:GLN:OE1	5:E:310:CHL:HMC	2.16	0.46
1:F:107:LEU:O	1:F:109:HIS:N	2.48	0.46
5:B:314:CHL:H91	5:B:314:CHL:H112	1.62	0.46
6:C:315:CLA:H151	6:C:316:CLA:HBB1	1.97	0.46
5:A:306:CHL:H92	5:A:306:CHL:H61	1.52	0.46
5:B:306:CHL:HBA1	5:B:306:CHL:H3A	1.59	0.46
5:C:309:CHL:HHD	5:C:310:CHL:OBD	2.16	0.46
1:F:178:PHE:HD1	5:F:305:CHL:H191	1.76	0.46
1:C:89:ALA:O	1:C:92:GLN:HG2	2.16	0.46
6:D:315:CLA:C4D	6:D:316:CLA:HMD3	2.46	0.46
6:F:306:CLA:CAC	5:F:310:CHL:H142	2.41	0.46
5:A:305:CHL:H61	5:A:305:CHL:H41	1.35	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:307:CLA:H202	6:A:307:CLA:H161	1.80	0.46
1:E:19:ALA:HB2	1:F:132:CYS:HB3	1.97	0.46
6:E:314:CLA:C4C	7:E:318:LHG:HC61	2.46	0.46
1:D:128:GLU:HG3	5:D:313:CHL:NB	2.31	0.46
1:B:58:ARG:HB3	6:B:315:CLA:HAC2	1.97	0.46
5:B:306:CHL:HMD1	7:B:320:LHG:H251	1.98	0.46
3:D:303:NEX:H32	5:D:312:CHL:HMA1	1.97	0.46
5:D:313:CHL:CMB	5:F:304:CHL:HHB	2.46	0.46
6:D:315:CLA:HBD	6:D:316:CLA:OBD	2.16	0.46
6:A:307:CLA:H12	1:B:39:LEU:HD11	1.98	0.45
1:B:162:PHE:CZ	1:B:166:LYS:HE3	2.51	0.45
1:A:51:GLU:HA	1:A:144:LEU:HD11	1.99	0.45
3:A:303:NEX:H401	3:A:303:NEX:H35	1.58	0.45
1:D:61:MET:SD	6:D:314:CLA:HHC	2.56	0.45
6:D:307:CLA:H91	5:D:313:CHL:H121	1.99	0.45
5:A:306:CHL:H101	6:C:307:CLA:H72	1.97	0.45
5:F:304:CHL:H111	7:F:318:LHG:H211	1.98	0.45
6:A:314:CLA:HBB1	6:A:314:CLA:HMB1	1.97	0.45
1:B:27:GLU:CD	1:F:27:GLU:HB2	2.41	0.45
5:C:305:CHL:H41	5:C:305:CHL:H61	1.58	0.45
1:C:107:LEU:O	1:C:109:HIS:N	2.50	0.45
5:C:305:CHL:O1A	5:C:305:CHL:H3A	2.16	0.45
6:C:315:CLA:H162	6:C:315:CLA:H141	1.69	0.45
1:E:59:TRP:NE1	5:E:311:CHL:HED2	2.31	0.45
7:E:318:LHG:HC62	7:E:318:LHG:H272	1.99	0.45
1:F:186:GLN:HB2	1:F:186:GLN:HE21	1.65	0.45
1:F:201:HIS:CD2	6:F:316:CLA:HAA2	2.51	0.45
4:B:305:LMU:H32	4:B:305:LMU:H61	1.48	0.45
3:C:303:NEX:H191	3:C:303:NEX:H11	1.73	0.45
5:B:313:CHL:HAA1	6:B:315:CLA:HBC1	1.99	0.45
1:C:209:ASN:HB2	5:C:318:CHL:HED1	1.97	0.45
1:D:81:PHE:CE2	1:D:102:LEU:HD23	2.52	0.45
1:C:210:GLY:HA2	6:C:317:CLA:OBD	2.16	0.45
5:F:304:CHL:H143	5:F:304:CHL:H161	1.67	0.45
1:A:178:PHE:HE2	6:A:317:CLA:HAB	1.82	0.44
5:D:306:CHL:H172	5:D:306:CHL:H13	1.44	0.44
7:F:318:LHG:H182	7:F:318:LHG:H151	1.72	0.44
3:B:303:NEX:H362	6:B:309:CLA:HAB	1.99	0.44
5:B:312:CHL:H101	5:B:314:CHL:H152	2.00	0.44
6:C:317:CLA:H2	6:C:317:CLA:H61	1.66	0.44
1:D:60:ALA:O	1:D:64:THR:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:MET:HE2	1:D:155:MET:HB3	1.91	0.44
5:E:305:CHL:H41	6:E:306:CLA:HBA1	1.99	0.44
1:F:69:THR:HB	1:F:70:PRO:HD3	1.98	0.44
1:A:130:TYR:HE1	4:A:304:LMU:H6D	1.82	0.44
1:B:178:PHE:HD1	5:B:307:CHL:H191	1.83	0.44
5:B:306:CHL:HMD3	7:B:320:LHG:HC62	1.99	0.44
1:C:132:CYS:SG	12:C:405:HOH:O	2.62	0.44
1:E:107:LEU:O	1:E:109:HIS:N	2.51	0.44
1:C:162:PHE:CZ	6:C:314:CLA:HED3	2.52	0.44
1:D:92:GLN:HG3	1:D:99:LEU:HD13	1.99	0.44
6:A:314:CLA:H43	6:A:316:CLA:HBA1	1.99	0.44
7:F:318:LHG:H223	7:F:318:LHG:H191	1.75	0.44
1:C:181:PHE:HD1	6:C:307:CLA:HBB2	1.83	0.44
5:D:313:CHL:HBB1	5:F:304:CHL:H52	2.00	0.44
6:E:314:CLA:HBD	6:E:315:CLA:OBD	2.18	0.44
5:E:304:CHL:H202	5:E:304:CHL:H161	1.64	0.44
5:A:306:CHL:H72	6:A:307:CLA:HMB1	2.00	0.44
3:D:303:NEX:H191	3:D:303:NEX:H11	1.70	0.44
1:E:61:MET:SD	6:E:313:CLA:HHC	2.58	0.44
5:C:312:CHL:HHC	5:C:312:CHL:HMC	1.53	0.43
6:F:313:CLA:HMB3	6:F:313:CLA:HBB1	1.99	0.43
6:B:308:CLA:H12	1:C:39:LEU:HD11	2.00	0.43
5:B:319:CHL:HHC	5:B:319:CHL:HMC	1.77	0.43
4:E:319:LMU:H101	4:E:319:LMU:H71	1.67	0.43
1:A:171:LYS:NZ	7:A:319:LHG:O4	2.52	0.43
1:C:9:ALA:HB1	5:C:305:CHL:HBC1	2.01	0.43
1:A:135:GLY:HA2	4:A:304:LMU:H12	2.00	0.43
5:B:307:CHL:H41	6:B:308:CLA:HBA1	2.00	0.43
7:B:324:LHG:H261	7:B:324:LHG:H292	1.35	0.43
1:C:128:GLU:HG3	5:C:313:CHL:NB	2.33	0.43
1:E:91:SER:C	1:E:93:ILE:H	2.26	0.43
1:F:115:ALA:HB3	5:F:308:CHL:HMC	1.99	0.43
1:A:101:TYR:CE2	6:A:308:CLA:H2	2.54	0.43
5:A:306:CHL:H111	6:C:307:CLA:H121	2.01	0.43
1:D:69:THR:HB	1:D:70:PRO:HD3	2.01	0.43
1:E:178:PHE:HZ	7:E:318:LHG:H142	1.83	0.43
1:F:53:GLU:HB2	5:F:305:CHL:C1B	2.49	0.43
1:A:178:PHE:CE2	6:A:317:CLA:HAB	2.54	0.43
6:B:316:CLA:H2	6:B:317:CLA:HMD2	2.01	0.43
3:C:303:NEX:H31	3:C:303:NEX:H28	1.93	0.43
1:E:179:ALA:HB1	9:E:320:OUR:O42	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:311:CHL:HAC2	5:B:311:CHL:HMC	1.58	0.43
1:D:61:MET:SD	6:D:314:CLA:HAB	2.59	0.43
1:E:116:ILE:HG12	5:E:308:CHL:HAC1	2.01	0.43
1:A:162:PHE:CZ	1:A:166:LYS:HE3	2.54	0.43
1:A:182:GLY:O	1:A:186:GLN:HB2	2.18	0.43
5:D:305:CHL:H41	5:D:305:CHL:H61	1.47	0.43
3:A:303:NEX:H241	6:A:308:CLA:C2	2.48	0.42
5:B:312:CHL:HMC	5:B:312:CHL:HHC	1.63	0.42
1:C:152:PRO:HD2	9:C:321:OUR:O40	2.18	0.42
1:D:210:GLY:HA2	6:D:317:CLA:CAD	2.49	0.42
5:E:310:CHL:H62	5:E:312:CHL:H192	2.01	0.42
3:A:303:NEX:H201	3:A:303:NEX:H15	1.62	0.42
1:B:100:ASP:CG	1:B:105:PRO:HA	2.45	0.42
1:B:128:GLU:HG3	5:B:314:CHL:NB	2.34	0.42
1:C:186:GLN:HE21	1:C:197:CYS:HB3	1.84	0.42
6:D:316:CLA:O1A	6:D:316:CLA:H2A	2.18	0.42
6:D:317:CLA:H143	6:D:317:CLA:H161	1.89	0.42
1:E:150:PHE:CE1	5:E:311:CHL:H92	2.55	0.42
1:F:162:PHE:CZ	1:F:166:LYS:HE3	2.53	0.42
2:C:302:OIE:C15	7:C:319:LHG:H111	2.50	0.42
6:A:307:CLA:HBB1	5:A:313:CHL:H161	2.01	0.42
5:B:314:CHL:HMC	5:B:314:CHL:HHC	1.75	0.42
1:C:158:ASP:HB3	1:C:161:THR:OG1	2.19	0.42
1:E:59:TRP:HE1	5:E:311:CHL:HED2	1.84	0.42
5:B:311:CHL:CAB	5:B:312:CHL:HMC	2.45	0.42
3:E:303:NEX:H35	3:E:303:NEX:H401	1.42	0.42
5:F:305:CHL:HMD3	5:F:305:CHL:HHD	1.52	0.42
1:C:2:GLU:O	1:C:9:ALA:N	2.50	0.42
1:D:90:GLY:HA2	5:D:310:CHL:HAC2	2.02	0.42
1:E:53:GLU:OE2	1:E:174:ARG:NE	2.46	0.42
1:A:9:ALA:HB1	5:A:305:CHL:CBC	2.49	0.42
5:A:310:CHL:HBB2	5:A:311:CHL:CBB	2.49	0.42
3:B:303:NEX:H191	3:B:303:NEX:H11	1.73	0.42
3:C:303:NEX:H15	3:C:303:NEX:H201	1.57	0.42
1:D:174:ARG:HA	1:D:177:MET:HE3	2.01	0.42
5:D:306:CHL:H122	5:D:306:CHL:H8	1.55	0.42
5:A:312:CHL:HHD	5:A:312:CHL:HMD3	1.72	0.42
7:A:319:LHG:H341	7:A:319:LHG:H312	1.91	0.42
1:B:13:GLY:C	10:B:322:BET:H11	2.45	0.42
6:B:308:CLA:H51	5:C:306:CHL:H91	2.01	0.42
5:B:312:CHL:H151	5:B:312:CHL:HAB	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:GLY:HA2	6:E:316:CLA:CAD	2.50	0.42
6:E:314:CLA:H112	6:E:314:CLA:H142	1.76	0.42
1:F:81:PHE:CD2	6:F:307:CLA:HED3	2.55	0.42
1:A:54:LEU:HD23	1:A:144:LEU:HB3	2.02	0.42
1:B:69:THR:HB	1:B:70:PRO:HD3	2.01	0.42
1:B:210:GLY:HA2	6:B:318:CLA:OBD	2.20	0.42
5:C:313:CHL:H91	5:C:313:CHL:H112	1.77	0.42
1:F:49:ASN:C	5:F:305:CHL:HMA1	2.45	0.42
11:F:319:LMG:HC92	11:F:319:LMG:H291	1.70	0.42
1:A:217:PHE:HB2	5:C:311:CHL:O1A	2.20	0.42
5:B:312:CHL:H122	5:B:312:CHL:H8	1.83	0.42
1:C:69:THR:HB	1:C:70:PRO:HD3	2.02	0.42
1:D:39:LEU:HD12	5:D:306:CHL:H11	2.02	0.42
1:D:178:PHE:HE1	5:D:306:CHL:H191	1.85	0.42
5:D:313:CHL:CHC	5:F:304:CHL:H52	2.50	0.42
6:B:316:CLA:H112	6:B:316:CLA:H151	1.82	0.41
1:E:62:LEU:HB3	6:E:307:CLA:HAB	2.02	0.41
1:E:189:GLN:HG3	1:E:213:TYR:HB2	2.02	0.41
1:F:152:PRO:HD2	9:F:320:OUR:C30	2.50	0.41
6:F:316:CLA:H2	6:F:316:CLA:H61	1.74	0.41
1:A:128:GLU:OE2	1:A:131:ARG:NH1	2.53	0.41
5:A:305:CHL:H202	5:A:305:CHL:H161	1.67	0.41
5:A:305:CHL:H3A	5:A:305:CHL:HBA1	1.56	0.41
1:B:147:GLY:HA3	6:B:315:CLA:CED	2.50	0.41
1:D:107:LEU:O	1:D:109:HIS:N	2.53	0.41
1:E:60:ALA:O	1:E:64:THR:HG23	2.21	0.41
1:F:168:LYS:HD3	6:F:315:CLA:HAA2	2.03	0.41
1:A:42:ASP:OD2	7:B:324:LHG:C4	2.61	0.41
1:A:98:GLY:HA3	1:A:110:ALA:O	2.19	0.41
1:A:115:ALA:O	1:A:119:THR:OG1	2.30	0.41
5:B:307:CHL:HHD	5:B:307:CHL:HMD3	1.80	0.41
2:C:302:OIE:C8	5:C:305:CHL:H91	2.50	0.41
6:D:308:CLA:HMA2	5:D:310:CHL:C3C	2.50	0.41
6:D:315:CLA:H112	6:D:315:CLA:H151	1.79	0.41
3:E:303:NEX:H11	3:E:303:NEX:H191	1.68	0.41
6:E:313:CLA:H72	9:E:320:OUR:C15	2.50	0.41
1:A:120:GLN:HE22	5:A:311:CHL:CMC	2.32	0.41
1:B:137:LEU:CD1	5:B:313:CHL:HAB	2.51	0.41
5:C:306:CHL:HHD	5:C:306:CHL:HMD3	1.72	0.41
5:E:305:CHL:H161	5:E:305:CHL:H141	1.81	0.41
1:A:101:TYR:HB3	1:A:107:LEU:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:303:NEX:H12	4:B:304:LMU:H82	2.03	0.41
6:B:318:CLA:H111	6:B:318:CLA:H91	1.69	0.41
1:D:168:LYS:HD3	6:D:316:CLA:HAA2	2.02	0.41
1:E:69:THR:HB	1:E:70:PRO:HD3	2.02	0.41
1:E:87:PHE:O	5:E:310:CHL:HED3	2.19	0.41
5:E:304:CHL:HAC1	7:E:318:LHG:HC32	2.02	0.41
1:A:75:LYS:HB2	1:A:75:LYS:HE3	1.66	0.41
1:B:73:LEU:HD12	1:B:73:LEU:HA	1.90	0.41
7:B:324:LHG:H262	1:F:21:PRO:HA	2.01	0.41
1:C:197:CYS:HB3	6:C:317:CLA:O1D	2.20	0.41
5:D:313:CHL:HMB3	5:F:304:CHL:HHB	2.01	0.41
1:C:168:LYS:HD3	6:C:316:CLA:HAA2	2.03	0.41
5:A:318:CHL:HMA2	1:C:114:LEU:HD13	2.03	0.41
1:B:87:PHE:O	5:B:312:CHL:HED3	2.21	0.41
1:E:58:ARG:HG2	1:E:58:ARG:H	1.67	0.41
1:A:120:GLN:OE1	5:A:311:CHL:HMC	2.21	0.41
6:A:315:CLA:HBD	6:A:316:CLA:OBD	2.21	0.41
1:B:170:ILE:HD12	1:B:170:ILE:HA	1.89	0.41
1:C:189:GLN:HG3	1:C:213:TYR:HB2	2.03	0.41
5:C:311:CHL:H91	5:C:311:CHL:H112	1.77	0.41
6:D:317:CLA:H61	6:D:317:CLA:H101	1.86	0.41
1:E:52:LEU:HD23	5:E:312:CHL:OBD	2.21	0.41
1:E:120:GLN:HE21	5:E:312:CHL:CMC	2.34	0.41
5:F:317:CHL:HMC	5:F:317:CHL:HHC	1.85	0.41
6:A:315:CLA:H142	6:A:315:CLA:H112	1.75	0.41
5:D:311:CHL:H61	5:D:311:CHL:H2	1.80	0.41
3:E:303:NEX:C31	5:E:309:CHL:H3A	2.51	0.41
6:F:306:CLA:HBB1	5:F:312:CHL:H162	2.03	0.41
1:A:107:LEU:O	1:A:109:HIS:N	2.54	0.40
1:D:100:ASP:CG	1:D:105:PRO:HA	2.46	0.40
1:E:218:PHE:N	2:E:302:OIE:O40	2.51	0.40
1:A:40:SER:HB3	1:A:46:PHE:CD1	2.56	0.40
5:A:306:CHL:H62	5:A:306:CHL:H41	1.86	0.40
6:A:314:CLA:O1D	6:A:314:CLA:H2A	2.20	0.40
6:C:315:CLA:H151	6:C:316:CLA:CBB	2.51	0.40
6:D:315:CLA:HAC1	7:D:319:LHG:H301	2.02	0.40
1:E:210:GLY:HA2	6:E:316:CLA:OBD	2.21	0.40
1:F:81:PHE:HB2	1:F:84:ALA:HB2	2.04	0.40
6:F:314:CLA:C4D	6:F:315:CLA:HMD3	2.51	0.40
1:B:146:PRO:HD2	6:B:315:CLA:OBD	2.21	0.40
5:A:311:CHL:HHH	5:A:311:CHL:HMD3	1.74	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:319:LHG:H272	7:A:319:LHG:H242	1.77	0.40
5:D:310:CHL:HAA2	5:D:310:CHL:CBD	2.52	0.40
5:F:310:CHL:H41	5:F:310:CHL:H62	1.83	0.40
6:B:308:CLA:H162	6:B:308:CLA:H122	1.60	0.40
1:C:178:PHE:CD2	7:C:319:LHG:H291	2.56	0.40
1:E:217:PHE:CE1	5:F:310:CHL:H2	2.56	0.40
6:E:316:CLA:HBB2	7:E:318:LHG:H311	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/249 (89%)	213 (96%)	7 (3%)	1 (0%)	24	46
1	B	221/249 (89%)	213 (96%)	6 (3%)	2 (1%)	14	30
1	C	220/249 (88%)	212 (96%)	7 (3%)	1 (0%)	24	46
1	D	221/249 (89%)	214 (97%)	6 (3%)	1 (0%)	24	46
1	E	221/249 (89%)	211 (96%)	7 (3%)	3 (1%)	9	19
1	F	221/249 (89%)	214 (97%)	5 (2%)	2 (1%)	14	30
All	All	1325/1494 (89%)	1277 (96%)	38 (3%)	10 (1%)	16	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	17	GLU
1	F	27	GLU
1	B	17	GLU
1	C	108	VAL
1	E	92	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	108	VAL
1	A	108	VAL
1	B	108	VAL
1	F	108	VAL
1	D	108	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	160/184 (87%)	155 (97%)	5 (3%)	35	63
1	B	159/184 (86%)	154 (97%)	5 (3%)	35	63
1	C	156/184 (85%)	155 (99%)	1 (1%)	78	91
1	D	163/184 (89%)	161 (99%)	2 (1%)	63	83
1	E	162/184 (88%)	160 (99%)	2 (1%)	63	83
1	F	163/184 (89%)	159 (98%)	4 (2%)	42	69
All	All	963/1104 (87%)	944 (98%)	19 (2%)	48	74

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	73	LEU
1	A	141	THR
1	A	160	GLU
1	A	222	ILE
1	B	10	LEU
1	B	73	LEU
1	B	96	GLU
1	B	99	LEU
1	B	141	THR
1	C	141	THR
1	D	75	LYS
1	D	160	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	58	ARG
1	E	73	LEU
1	F	7	ASP
1	F	10	LEU
1	F	99	LEU
1	F	141	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	GLN
1	B	186	GLN
1	E	92	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 129 ligands modelled in this entry, 3 are monoatomic - leaving 126 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
4	LMU	A	304	-	36,36,36	0.40	0	47,47,47	0.91	1 (2%)
5	CHL	A	318	1	46,50,74	3.29	22 (47%)	51,85,114	3.41	28 (54%)
5	CHL	E	312	1	70,74,74	2.49	23 (32%)	80,114,114	3.08	33 (41%)
2	OIE	D	301	-	42,45,45	1.43	5 (11%)	49,63,63	1.86	10 (20%)
4	LMU	B	305	-	36,36,36	0.38	0	47,47,47	1.09	5 (10%)
6	CLA	A	307	1	69,73,73	1.27	8 (11%)	83,113,113	1.32	7 (8%)
6	CLA	C	307	1	69,73,73	1.26	7 (10%)	83,113,113	1.42	8 (9%)
9	OUR	F	320	-	50,53,58	1.09	3 (6%)	58,72,77	1.89	16 (27%)
6	CLA	A	314	1	59,63,73	1.43	11 (18%)	71,101,113	1.55	15 (21%)
6	CLA	C	317	-	60,64,73	1.41	9 (15%)	72,102,113	1.43	9 (12%)
5	CHL	B	312	12	66,70,74	2.84	21 (31%)	75,109,114	2.97	33 (44%)
5	CHL	C	318	1	48,52,74	3.16	22 (45%)	53,87,114	4.05	27 (50%)
6	CLA	A	315	7	67,71,73	1.29	7 (10%)	80,110,113	1.32	7 (8%)
6	CLA	C	315	7	69,73,73	1.26	6 (8%)	83,113,113	1.27	7 (8%)
5	CHL	C	306	1	70,74,74	2.34	21 (30%)	80,114,114	2.86	33 (41%)
4	LMU	D	304	-	36,36,36	0.50	0	47,47,47	1.19	4 (8%)
6	CLA	C	314	1	57,61,73	1.38	6 (10%)	68,98,113	1.41	10 (14%)
10	BET	B	322	-	7,7,7	1.02	0	10,10,10	0.87	1 (10%)
2	OIE	B	301	-	42,45,45	1.41	6 (14%)	49,63,63	1.70	9 (18%)
2	OIE	C	301	-	42,45,45	1.47	6 (14%)	49,63,63	1.71	9 (18%)
5	CHL	A	310	-	55,59,74	3.11	21 (38%)	62,96,114	3.39	30 (48%)
5	CHL	C	312	12	60,64,74	2.97	22 (36%)	68,102,114	2.96	30 (44%)
5	CHL	B	310	1	47,51,74	3.12	21 (44%)	52,86,114	3.67	26 (50%)
5	CHL	F	304	1	70,74,74	2.53	22 (31%)	80,114,114	3.45	35 (43%)
3	NEX	D	303	-	38,46,46	0.95	2 (5%)	50,70,70	5.96	20 (40%)
9	OUR	A	322	-	50,53,58	1.01	2 (4%)	58,72,77	2.10	21 (36%)
5	CHL	F	312	1	70,74,74	2.26	20 (28%)	80,114,114	2.53	32 (40%)
5	CHL	F	311	12	60,64,74	2.55	23 (38%)	68,102,114	3.80	32 (47%)
6	CLA	A	308	12	54,58,73	1.43	7 (12%)	65,95,113	1.42	7 (10%)
5	CHL	B	306	1	70,74,74	2.73	23 (32%)	80,114,114	3.66	32 (40%)
5	CHL	F	308	1	46,50,74	3.18	22 (47%)	51,85,114	4.04	30 (58%)
7	LHG	C	319	6	44,44,48	0.73	1 (2%)	47,50,54	1.30	7 (14%)
5	CHL	B	319	1	51,55,74	3.15	23 (45%)	57,91,114	4.16	28 (49%)
6	CLA	B	308	1	69,73,73	1.26	8 (11%)	83,113,113	1.39	7 (8%)
5	CHL	D	305	1	70,74,74	2.92	23 (32%)	80,114,114	2.90	30 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CLA	E	313	1	59,63,73	1.36	6 (10%)	71,101,113	1.31	9 (12%)
5	CHL	F	310	12	65,69,74	2.77	25 (38%)	74,108,114	3.27	29 (39%)
5	CHL	B	313	12	61,65,74	2.69	23 (37%)	69,103,114	3.50	30 (43%)
5	CHL	A	313	1	70,74,74	2.44	22 (31%)	80,114,114	2.57	26 (32%)
5	CHL	B	314	1	70,74,74	2.26	22 (31%)	80,114,114	2.73	29 (36%)
6	CLA	D	308	12	50,54,73	1.48	8 (16%)	60,90,113	1.41	7 (11%)
5	CHL	D	311	-	66,70,74	2.78	20 (30%)	75,109,114	2.92	34 (45%)
6	CLA	D	315	7	69,73,73	1.26	8 (11%)	83,113,113	1.26	8 (9%)
7	LHG	B	320	6	45,45,48	0.67	1 (2%)	48,51,54	1.30	6 (12%)
7	LHG	F	318	6	44,44,48	0.67	1 (2%)	47,50,54	1.33	8 (17%)
6	CLA	D	314	1	62,66,73	1.39	10 (16%)	74,104,113	1.41	13 (17%)
6	CLA	C	308	12	50,54,73	1.47	8 (16%)	60,90,113	1.39	7 (11%)
10	BET	C	320	-	7,7,7	1.01	0	10,10,10	0.75	0
11	LMG	B	323	-	30,30,55	1.05	0	38,38,63	1.12	5 (13%)
6	CLA	B	309	12	50,54,73	1.50	9 (18%)	60,90,113	1.41	7 (11%)
9	OUR	B	325	-	50,53,58	1.01	2 (4%)	58,72,77	2.09	18 (31%)
6	CLA	E	315	1	49,53,73	1.48	8 (16%)	59,89,113	1.45	5 (8%)
6	CLA	D	317	1	69,73,73	1.27	8 (11%)	83,113,113	1.28	6 (7%)
5	CHL	D	309	1	46,50,74	3.20	22 (47%)	51,85,114	5.51	31 (60%)
6	CLA	F	306	1	69,73,73	1.27	8 (11%)	83,113,113	1.34	6 (7%)
6	CLA	E	306	1	69,73,73	1.28	7 (10%)	83,113,113	1.32	8 (9%)
6	CLA	F	315	1	49,53,73	1.49	8 (16%)	59,89,113	1.49	7 (11%)
11	LMG	F	319	-	30,30,55	0.93	0	38,38,63	1.21	3 (7%)
5	CHL	E	311	12	60,64,74	2.81	24 (40%)	68,102,114	3.00	31 (45%)
5	CHL	C	310	-	48,52,74	3.10	22 (45%)	53,87,114	3.36	24 (45%)
3	NEX	F	303	-	38,46,46	0.96	1 (2%)	50,70,70	6.25	22 (44%)
5	CHL	C	311	12	65,69,74	3.11	22 (33%)	74,108,114	3.03	31 (41%)
6	CLA	E	314	7	67,71,73	1.30	6 (8%)	80,110,113	1.28	6 (7%)
2	OIE	C	302	-	42,45,45	1.45	6 (14%)	49,63,63	1.67	9 (18%)
6	CLA	D	316	1	49,53,73	1.50	9 (18%)	59,89,113	1.47	6 (10%)
10	BET	B	321	-	7,7,7	1.03	0	10,10,10	0.85	1 (10%)
5	CHL	E	304	1	70,74,74	2.41	23 (32%)	80,114,114	3.65	35 (43%)
5	CHL	E	309	-	47,51,74	3.18	20 (42%)	52,86,114	5.80	28 (53%)
7	LHG	C	304	-	24,24,48	0.87	0	27,30,54	1.22	2 (7%)
9	OUR	C	321	-	50,53,58	0.97	1 (2%)	58,72,77	1.98	16 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CHL	E	317	1	44,49,74	3.28	20 (45%)	49,83,114	5.17	26 (53%)
2	OIE	F	302	-	42,45,45	1.43	6 (14%)	49,63,63	1.71	9 (18%)
5	CHL	F	305	1	70,74,74	2.13	19 (27%)	80,114,114	3.31	35 (43%)
7	LHG	D	319	6	45,45,48	0.69	1 (2%)	48,51,54	1.28	7 (14%)
2	OIE	E	301	-	42,45,45	1.46	5 (11%)	49,63,63	1.79	10 (20%)
2	OIE	F	301	-	42,45,45	1.44	6 (14%)	49,63,63	1.74	10 (20%)
5	CHL	D	312	12	61,65,74	2.69	24 (39%)	69,103,114	3.03	32 (46%)
4	LMU	E	319	-	36,36,36	0.38	0	47,47,47	0.91	1 (2%)
3	NEX	A	303	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
6	CLA	C	316	1	49,53,73	1.49	8 (16%)	59,89,113	1.46	5 (8%)
5	CHL	C	313	1	70,74,74	2.46	22 (31%)	80,114,114	2.67	29 (36%)
4	LMU	B	304	-	34,34,36	0.39	0	42,44,47	1.07	3 (7%)
5	CHL	C	309	1	46,50,74	3.17	20 (43%)	51,85,114	3.59	28 (54%)
3	NEX	C	303	-	38,46,46	0.96	1 (2%)	50,70,70	6.57	19 (38%)
5	CHL	D	318	1	50,54,74	3.15	22 (44%)	56,90,114	3.29	27 (48%)
6	CLA	A	317	1	59,63,73	1.39	8 (13%)	70,100,113	1.36	9 (12%)
5	CHL	D	310	12	49,53,74	3.06	20 (40%)	53,88,114	3.42	24 (45%)
5	CHL	F	317	1	50,54,74	3.32	23 (46%)	56,90,114	3.76	30 (53%)
7	LHG	B	324	-	30,30,48	1.18	2 (6%)	33,36,54	1.40	4 (12%)
6	CLA	B	317	1	49,53,73	1.48	8 (16%)	59,89,113	1.45	7 (11%)
2	OIE	A	301	-	42,45,45	1.50	10 (23%)	49,63,63	2.07	13 (26%)
5	CHL	A	312	12	60,64,74	2.77	23 (38%)	68,102,114	3.16	32 (47%)
6	CLA	B	315	1	62,66,73	1.45	9 (14%)	74,104,113	1.61	12 (16%)
6	CLA	F	307	12	50,54,73	1.47	8 (16%)	60,90,113	1.43	4 (6%)
5	CHL	C	305	1	70,74,74	2.53	24 (34%)	80,114,114	2.88	30 (37%)
2	OIE	A	302	-	42,45,45	1.53	7 (16%)	49,63,63	2.04	10 (20%)
6	CLA	B	318	1	69,73,73	1.24	8 (11%)	83,113,113	1.29	7 (8%)
5	CHL	F	309	-	46,50,74	3.48	21 (45%)	51,85,114	3.64	31 (60%)
3	NEX	E	303	-	38,46,46	0.94	1 (2%)	50,70,70	6.17	19 (38%)
9	OUR	D	321	-	50,53,58	0.88	1 (2%)	58,72,77	1.92	14 (24%)
5	CHL	B	311	-	55,59,74	2.99	22 (40%)	62,96,114	5.09	33 (53%)
9	OUR	B	302	-	48,51,58	1.14	3 (6%)	56,70,77	2.80	19 (33%)
5	CHL	E	305	1	68,72,74	2.39	21 (30%)	77,111,114	2.55	31 (40%)
5	CHL	E	310	-	65,69,74	3.07	23 (35%)	73,107,114	2.95	32 (43%)
5	CHL	E	308	1	44,49,74	3.44	21 (47%)	49,83,114	3.36	23 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OIE	E	302	-	42,45,45	1.49	5 (11%)	49,63,63	1.76	9 (18%)
2	OIE	D	302	-	42,45,45	1.43	6 (14%)	49,63,63	1.68	11 (22%)
5	CHL	A	305	1	70,74,74	2.72	23 (32%)	80,114,114	3.35	35 (43%)
5	CHL	A	306	1	68,72,74	2.34	20 (29%)	77,111,114	2.69	33 (42%)
6	CLA	F	313	1	62,66,73	1.42	10 (16%)	74,104,113	1.57	13 (17%)
6	CLA	E	316	1	59,63,73	1.34	8 (13%)	70,100,113	1.35	6 (8%)
3	NEX	B	303	-	38,46,46	0.94	2 (5%)	50,70,70	5.77	22 (44%)
6	CLA	F	314	7	59,63,73	1.39	7 (11%)	71,101,113	1.34	8 (11%)
7	LHG	A	319	6	46,46,48	0.64	1 (2%)	49,52,54	1.22	3 (6%)
5	CHL	D	313	1	70,74,74	2.60	20 (28%)	80,114,114	2.78	31 (38%)
5	CHL	A	311	12	65,69,74	2.86	23 (35%)	73,107,114	3.83	33 (45%)
5	CHL	B	307	1	69,73,74	2.22	20 (28%)	78,112,114	3.07	32 (41%)
6	CLA	E	307	-	54,58,73	1.42	8 (14%)	65,95,113	1.47	9 (13%)
6	CLA	A	316	1	49,53,73	1.51	8 (16%)	59,89,113	1.49	5 (8%)
6	CLA	D	307	1	69,73,73	1.24	8 (11%)	83,113,113	1.36	6 (7%)
7	LHG	E	318	6	40,40,48	0.67	1 (2%)	43,46,54	1.30	6 (13%)
5	CHL	A	309	1	47,51,74	3.17	22 (46%)	52,86,114	3.78	28 (53%)
5	CHL	D	306	1	69,73,74	2.29	20 (28%)	78,112,114	2.91	34 (43%)
6	CLA	B	316	7	69,73,73	1.28	7 (10%)	83,113,113	1.33	7 (8%)
6	CLA	F	316	-	60,64,73	1.35	9 (15%)	72,102,113	1.36	7 (9%)
9	OUR	E	320	-	50,53,58	0.99	1 (2%)	58,72,77	2.05	19 (32%)

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
4	LMU	A	304	-	-	14/21/61/61	0/2/2/2
5	CHL	A	318	1	-	6/12/88/117	-
5	CHL	E	312	1	-	9/41/117/117	-
2	OIE	D	301	-	-	14/33/72/72	0/2/2/2
4	LMU	B	305	-	-	14/21/61/61	0/2/2/2
6	CLA	A	307	1	-	15/39/115/115	-
6	CLA	C	307	1	-	9/39/115/115	-
9	OUR	F	320	-	-	7/42/81/86	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLA	A	314	1	-	6/27/103/115	-
6	CLA	C	317	-	-	7/29/105/115	-
5	CHL	B	312	12	-	11/37/113/117	-
5	CHL	C	318	1	-	4/15/91/117	-
6	CLA	A	315	7	-	11/37/113/115	-
6	CLA	C	315	7	-	15/39/115/115	-
5	CHL	C	306	1	-	18/41/117/117	-
4	LMU	D	304	-	-	14/21/61/61	0/2/2/2
6	CLA	C	314	1	-	5/25/101/115	-
10	BET	B	322	-	-	5/5/5/5	-
2	OIE	B	301	-	-	11/33/72/72	0/2/2/2
2	OIE	C	301	-	-	9/33/72/72	0/2/2/2
5	CHL	A	310	-	-	6/23/99/117	-
5	CHL	C	312	12	-	13/29/105/117	-
5	CHL	B	310	1	-	6/14/90/117	-
5	CHL	F	304	1	-	16/41/117/117	-
3	NEX	D	303	-	-	6/27/83/83	0/3/3/3
9	OUR	A	322	-	-	8/42/81/86	0/2/2/2
5	CHL	F	312	1	-	16/41/117/117	-
5	CHL	F	311	12	-	14/29/105/117	-
6	CLA	A	308	12	-	6/21/97/115	-
5	CHL	B	306	1	-	16/41/117/117	-
5	CHL	F	308	1	-	6/12/88/117	-
7	LHG	C	319	6	-	18/49/49/53	-
5	CHL	B	319	1	-	7/19/95/117	-
6	CLA	B	308	1	-	16/39/115/115	-
5	CHL	D	305	1	-	20/41/117/117	-
6	CLA	E	313	1	-	4/27/103/115	-
5	CHL	F	310	12	-	19/35/111/117	-
5	CHL	B	313	12	-	9/31/107/117	-
5	CHL	A	313	1	-	14/41/117/117	-
5	CHL	B	314	1	-	19/41/117/117	-
6	CLA	D	308	12	-	6/17/93/115	-
5	CHL	D	311	-	-	17/37/113/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLA	D	315	7	-	9/39/115/115	-
7	LHG	B	320	6	-	24/50/50/53	-
7	LHG	F	318	6	-	23/49/49/53	-
6	CLA	D	314	1	-	9/31/107/115	-
6	CLA	C	308	12	-	7/17/93/115	-
10	BET	C	320	-	-	5/5/5/5	-
11	LMG	B	323	-	-	9/25/45/70	0/1/1/1
6	CLA	B	309	12	-	4/17/93/115	-
9	OUR	B	325	-	-	7/42/81/86	0/2/2/2
6	CLA	E	315	1	-	8/15/91/115	-
6	CLA	D	317	1	-	10/39/115/115	-
5	CHL	D	309	1	-	4/12/88/117	-
6	CLA	F	306	1	-	17/39/115/115	-
6	CLA	E	306	1	-	12/39/115/115	-
6	CLA	F	315	1	-	4/15/91/115	-
11	LMG	F	319	-	-	11/25/45/70	0/1/1/1
5	CHL	E	311	12	-	10/29/105/117	-
5	CHL	C	310	-	-	9/15/91/117	-
3	NEX	F	303	-	-	3/27/83/83	0/3/3/3
5	CHL	C	311	12	-	17/35/111/117	-
6	CLA	E	314	7	-	11/37/113/115	-
2	OIE	C	302	-	-	14/33/72/72	0/2/2/2
6	CLA	D	316	1	-	2/15/91/115	-
10	BET	B	321	-	-	5/5/5/5	-
5	CHL	E	304	1	-	17/41/117/117	-
5	CHL	E	309	-	-	6/14/90/117	-
7	LHG	C	304	-	-	16/29/29/53	-
9	OUR	C	321	-	-	7/42/81/86	0/2/2/2
5	CHL	E	317	1	-	3/12/84/117	-
2	OIE	F	302	-	-	12/33/72/72	0/2/2/2
5	CHL	F	305	1	-	20/41/117/117	-
7	LHG	D	319	6	-	16/50/50/53	-
2	OIE	E	301	-	-	7/33/72/72	0/2/2/2
2	OIE	F	301	-	-	12/33/72/72	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CHL	D	312	12	-	7/31/107/117	-
4	LMU	E	319	-	-	15/21/61/61	0/2/2/2
3	NEX	A	303	-	-	5/27/83/83	0/3/3/3
6	CLA	C	316	1	-	4/15/91/115	-
5	CHL	C	313	1	-	13/41/117/117	-
4	LMU	B	304	-	-	9/20/56/61	1/2/2/2
5	CHL	C	309	1	-	6/12/88/117	-
3	NEX	C	303	-	-	2/27/83/83	0/3/3/3
5	CHL	D	318	1	-	4/17/93/117	-
6	CLA	A	317	1	-	10/27/103/115	-
5	CHL	D	310	12	-	4/15/92/117	-
5	CHL	F	317	1	-	7/17/93/117	-
7	LHG	B	324	-	-	24/35/35/53	-
6	CLA	B	317	1	-	3/15/91/115	-
2	OIE	A	301	-	-	10/33/72/72	0/2/2/2
5	CHL	A	312	12	-	9/29/105/117	-
6	CLA	B	315	1	-	6/31/107/115	-
6	CLA	F	307	12	-	4/17/93/115	-
5	CHL	C	305	1	-	24/41/117/117	-
2	OIE	A	302	-	-	11/33/72/72	0/2/2/2
6	CLA	B	318	1	-	18/39/115/115	-
5	CHL	F	309	-	-	5/12/88/117	-
3	NEX	E	303	-	-	4/27/83/83	0/3/3/3
9	OUR	D	321	-	-	7/42/81/86	0/2/2/2
5	CHL	B	311	-	-	7/23/99/117	-
9	OUR	B	302	-	-	16/40/79/86	0/2/2/2
5	CHL	E	305	1	-	12/39/115/117	-
5	CHL	E	310	-	-	16/35/111/117	-
5	CHL	E	308	1	-	4/12/84/117	-
2	OIE	E	302	-	-	12/33/72/72	0/2/2/2
2	OIE	D	302	-	-	16/33/72/72	0/2/2/2
5	CHL	A	305	1	-	23/41/117/117	-
5	CHL	A	306	1	-	17/39/115/117	-
6	CLA	F	313	1	-	12/31/107/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLA	E	316	1	-	9/27/103/115	-
3	NEX	B	303	-	-	2/27/83/83	0/3/3/3
6	CLA	F	314	7	-	4/27/103/115	-
7	LHG	A	319	6	-	18/51/51/53	-
5	CHL	D	313	1	-	18/41/117/117	-
5	CHL	A	311	12	-	16/35/111/117	-
5	CHL	B	307	1	-	15/40/116/117	-
6	CLA	E	307	-	-	2/21/97/115	-
6	CLA	A	316	1	-	6/15/91/115	-
6	CLA	D	307	1	-	12/39/115/115	-
7	LHG	E	318	6	-	15/45/45/53	-
5	CHL	A	309	1	-	7/14/90/117	-
5	CHL	D	306	1	-	20/40/116/117	-
6	CLA	B	316	7	-	8/39/115/115	-
6	CLA	F	316	-	-	7/29/105/115	-
9	OUR	E	320	-	-	6/42/81/86	0/2/2/2

All (1431) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	310	CHL	MG-ND	-13.99	1.78	2.05
5	C	311	CHL	MG-ND	-13.00	1.80	2.05
5	E	308	CHL	MG-NA	12.97	2.37	2.06
5	C	311	CHL	MG-NA	12.90	2.36	2.06
5	D	313	CHL	MG-NA	12.84	2.36	2.06
5	F	309	CHL	MG-NA	12.49	2.35	2.06
5	D	305	CHL	MG-NA	12.35	2.35	2.06
5	C	309	CHL	MG-NA	12.24	2.35	2.06
5	E	317	CHL	MG-NA	12.19	2.35	2.06
5	C	318	CHL	MG-NA	12.06	2.34	2.06
5	A	305	CHL	MG-NA	11.91	2.34	2.06
5	B	306	CHL	MG-NA	11.91	2.34	2.06
5	D	305	CHL	MG-ND	-11.66	1.82	2.05
5	B	312	CHL	MG-NA	11.61	2.33	2.06
5	A	313	CHL	MG-NA	11.61	2.33	2.06
5	F	317	CHL	MG-NA	11.56	2.33	2.06
5	A	311	CHL	MG-ND	-11.55	1.82	2.05
5	B	319	CHL	MG-NA	11.41	2.33	2.06
5	A	310	CHL	MG-ND	-11.36	1.83	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	309	CHL	MG-NA	11.28	2.33	2.06
5	D	311	CHL	MG-ND	-11.12	1.83	2.05
5	F	308	CHL	MG-NA	11.08	2.32	2.06
5	B	311	CHL	MG-NA	11.05	2.32	2.06
5	C	305	CHL	MG-NA	10.98	2.32	2.06
5	A	318	CHL	MG-NA	10.91	2.32	2.06
5	B	310	CHL	MG-NA	10.60	2.31	2.06
5	D	312	CHL	MG-NA	10.59	2.31	2.06
5	F	309	CHL	MG-ND	-10.43	1.85	2.05
5	D	310	CHL	MG-NA	10.42	2.31	2.06
5	C	310	CHL	MG-NA	10.27	2.30	2.06
5	A	309	CHL	MG-NA	10.20	2.30	2.06
5	C	312	CHL	MG-NA	10.02	2.30	2.06
5	F	310	CHL	MG-ND	-9.98	1.86	2.05
5	B	312	CHL	MG-ND	-9.90	1.86	2.05
5	F	317	CHL	MG-ND	-9.82	1.86	2.05
5	F	304	CHL	MG-NA	9.68	2.29	2.06
5	C	312	CHL	MG-ND	-9.58	1.86	2.05
5	D	318	CHL	MG-NA	9.57	2.29	2.06
5	F	310	CHL	MG-NA	9.53	2.28	2.06
5	C	313	CHL	MG-NA	9.41	2.28	2.06
5	A	311	CHL	MG-NA	9.38	2.28	2.06
5	E	310	CHL	MG-NA	9.21	2.28	2.06
5	E	309	CHL	MG-NA	9.20	2.28	2.06
5	B	306	CHL	MG-ND	-9.08	1.87	2.05
5	A	305	CHL	MG-ND	-8.95	1.88	2.05
5	A	312	CHL	MG-NA	8.95	2.27	2.06
5	D	311	CHL	MG-NA	8.78	2.27	2.06
5	A	318	CHL	MG-ND	-8.76	1.88	2.05
5	E	308	CHL	MG-ND	-8.67	1.88	2.05
5	E	304	CHL	MG-NA	8.64	2.26	2.06
5	A	309	CHL	MG-ND	-8.51	1.88	2.05
5	F	304	CHL	MG-ND	-8.48	1.89	2.05
5	E	311	CHL	MG-ND	-8.46	1.89	2.05
5	D	318	CHL	MG-ND	-8.45	1.89	2.05
5	A	312	CHL	MG-ND	-8.43	1.89	2.05
5	E	309	CHL	MG-ND	-8.41	1.89	2.05
5	B	314	CHL	MG-NA	8.26	2.25	2.06
5	E	312	CHL	MG-ND	-8.11	1.89	2.05
5	E	312	CHL	MG-NA	8.11	2.25	2.06
5	E	311	CHL	MG-NA	8.10	2.25	2.06
5	C	310	CHL	MG-ND	-8.06	1.89	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	310	CHL	MG-NA	7.99	2.25	2.06
5	B	310	CHL	MG-ND	-7.90	1.90	2.05
5	B	313	CHL	MG-NA	7.85	2.24	2.06
5	F	308	CHL	MG-ND	-7.61	1.90	2.05
5	B	319	CHL	MG-ND	-7.54	1.90	2.05
5	E	317	CHL	MG-ND	-7.49	1.90	2.05
5	D	309	CHL	MG-ND	-7.43	1.91	2.05
5	A	306	CHL	MG-NA	7.26	2.23	2.06
5	E	309	CHL	MG-NC	7.19	2.23	2.06
5	D	310	CHL	MG-ND	-7.17	1.91	2.05
5	B	313	CHL	MG-ND	-7.15	1.91	2.05
5	D	306	CHL	MG-ND	-6.98	1.91	2.05
5	E	305	CHL	MG-NA	6.94	2.22	2.06
5	B	307	CHL	MG-NA	6.77	2.22	2.06
5	B	311	CHL	MG-ND	-6.72	1.92	2.05
5	F	311	CHL	MG-NC	6.56	2.21	2.06
5	C	318	CHL	MG-ND	-6.53	1.92	2.05
5	C	306	CHL	MG-NA	6.49	2.21	2.06
5	C	312	CHL	MG-NC	6.44	2.21	2.06
5	D	318	CHL	MG-NC	6.38	2.21	2.06
5	E	310	CHL	MG-NB	6.35	2.18	2.05
5	F	311	CHL	MG-NA	6.28	2.21	2.06
5	F	305	CHL	MG-NA	6.23	2.21	2.06
5	A	310	CHL	MG-NC	6.06	2.20	2.06
5	C	306	CHL	MG-ND	-6.04	1.93	2.05
5	F	312	CHL	MG-NA	6.03	2.20	2.06
5	F	312	CHL	MG-NC	5.99	2.20	2.06
5	B	313	CHL	MG-NC	5.96	2.20	2.06
5	C	309	CHL	MG-ND	-5.91	1.94	2.05
5	B	311	CHL	C2C-C3C	5.88	1.49	1.36
5	E	304	CHL	MG-ND	-5.81	1.94	2.05
5	D	309	CHL	C2C-C3C	5.78	1.49	1.36
5	D	306	CHL	MG-NA	5.76	2.19	2.06
5	E	305	CHL	C2C-C3C	5.75	1.49	1.36
5	B	312	CHL	C2C-C3C	5.73	1.49	1.36
5	B	310	CHL	C2C-C3C	5.73	1.49	1.36
5	E	305	CHL	MG-ND	-5.70	1.94	2.05
5	D	318	CHL	C2C-C3C	5.69	1.48	1.36
5	F	308	CHL	C2C-C3C	5.68	1.48	1.36
5	A	306	CHL	C2C-C3C	5.67	1.48	1.36
5	A	309	CHL	C2C-C3C	5.64	1.48	1.36
5	F	310	CHL	C2C-C3C	5.63	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	310	CHL	C2C-C3C	5.63	1.48	1.36
5	D	305	CHL	C2C-C3C	5.63	1.48	1.36
5	E	308	CHL	C2C-C3C	5.63	1.48	1.36
5	E	317	CHL	C2C-C3C	5.62	1.48	1.36
5	E	309	CHL	C2C-C3C	5.62	1.48	1.36
5	A	318	CHL	C2C-C3C	5.61	1.48	1.36
5	D	310	CHL	C2C-C3C	5.60	1.48	1.36
5	D	313	CHL	C2C-C3C	5.59	1.48	1.36
5	D	311	CHL	C2C-C3C	5.59	1.48	1.36
5	E	311	CHL	MG-NC	5.58	2.19	2.06
5	C	306	CHL	C2C-C3C	5.57	1.48	1.36
5	A	310	CHL	C2C-C3C	5.57	1.48	1.36
5	C	310	CHL	C2C-C3C	5.55	1.48	1.36
5	C	318	CHL	C2C-C3C	5.55	1.48	1.36
5	C	309	CHL	C2C-C3C	5.54	1.48	1.36
5	F	317	CHL	C2C-C3C	5.54	1.48	1.36
5	C	311	CHL	C2C-C3C	5.53	1.48	1.36
5	F	312	CHL	C2C-C3C	5.52	1.48	1.36
5	A	311	CHL	C2C-C3C	5.52	1.48	1.36
5	E	311	CHL	C2C-C3C	5.52	1.48	1.36
5	B	306	CHL	C2C-C3C	5.51	1.48	1.36
5	F	317	CHL	MG-NC	5.50	2.19	2.06
5	E	312	CHL	C2C-C3C	5.50	1.48	1.36
5	F	309	CHL	C2C-C3C	5.49	1.48	1.36
5	B	314	CHL	C2C-C3C	5.49	1.48	1.36
5	C	313	CHL	C2C-C3C	5.47	1.48	1.36
5	C	312	CHL	C2C-C3C	5.45	1.48	1.36
5	C	305	CHL	C2C-C3C	5.45	1.48	1.36
5	A	318	CHL	MG-NC	5.43	2.19	2.06
5	C	312	CHL	CHD-C1D	5.42	1.48	1.38
5	B	319	CHL	C2C-C3C	5.42	1.48	1.36
5	D	311	CHL	O2D-CGD	5.41	1.46	1.33
5	B	313	CHL	C2C-C3C	5.40	1.48	1.36
5	C	310	CHL	MG-NC	5.37	2.19	2.06
5	B	319	CHL	CHD-C1D	5.37	1.48	1.38
5	E	304	CHL	C2C-C3C	5.37	1.48	1.36
5	D	311	CHL	CHD-C1D	5.36	1.48	1.38
6	B	315	CLA	C4D-ND	-5.36	1.30	1.37
5	F	311	CHL	C2C-C3C	5.36	1.48	1.36
5	B	311	CHL	MG-NC	5.35	2.19	2.06
5	E	305	CHL	O2D-CGD	5.34	1.46	1.33
5	A	305	CHL	C2C-C3C	5.33	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	312	CHL	C2C-C3C	5.31	1.48	1.36
5	A	313	CHL	C2C-C3C	5.31	1.48	1.36
5	D	306	CHL	C2C-C3C	5.30	1.48	1.36
5	A	312	CHL	CHD-C1D	5.30	1.48	1.38
5	D	310	CHL	O2D-CGD	5.30	1.46	1.33
5	B	311	CHL	CHD-C1D	5.29	1.48	1.38
5	F	317	CHL	CHD-C1D	5.29	1.48	1.38
5	A	306	CHL	O2D-CGD	5.29	1.46	1.33
5	E	311	CHL	O2D-CGD	5.27	1.46	1.33
5	B	310	CHL	CHD-C1D	5.27	1.48	1.38
5	F	304	CHL	C2C-C3C	5.27	1.48	1.36
5	D	310	CHL	CHD-C1D	5.27	1.48	1.38
5	D	318	CHL	CHD-C1D	5.26	1.48	1.38
5	F	305	CHL	C2C-C3C	5.26	1.48	1.36
5	F	309	CHL	O2D-CGD	5.26	1.46	1.33
5	D	312	CHL	MG-NC	5.25	2.18	2.06
5	A	318	CHL	CHD-C1D	5.24	1.48	1.38
5	C	312	CHL	O2D-CGD	5.23	1.46	1.33
5	B	311	CHL	O2D-CGD	5.23	1.46	1.33
5	A	318	CHL	O2D-CGD	5.23	1.45	1.33
5	F	309	CHL	CHD-C1D	5.22	1.48	1.38
5	F	308	CHL	O2D-CGD	5.22	1.45	1.33
5	A	309	CHL	CHD-C1D	5.22	1.48	1.38
5	B	306	CHL	CHD-C1D	5.22	1.48	1.38
5	E	308	CHL	CHD-C1D	5.21	1.48	1.38
5	B	313	CHL	CHD-C1D	5.21	1.48	1.38
5	C	309	CHL	CHD-C1D	5.21	1.48	1.38
5	F	308	CHL	CHD-C1D	5.21	1.48	1.38
5	D	312	CHL	C2C-C3C	5.21	1.47	1.36
5	D	310	CHL	MG-NC	5.20	2.18	2.06
5	D	312	CHL	CHD-C1D	5.19	1.48	1.38
5	C	313	CHL	O2D-CGD	5.19	1.45	1.33
5	E	309	CHL	CHD-C1D	5.19	1.48	1.38
5	B	312	CHL	O2D-CGD	5.18	1.45	1.33
5	A	309	CHL	O2D-CGD	5.18	1.45	1.33
5	D	309	CHL	O2D-CGD	5.18	1.45	1.33
5	B	319	CHL	O2D-CGD	5.18	1.45	1.33
5	F	311	CHL	CHD-C1D	5.17	1.48	1.38
5	B	306	CHL	O2D-CGD	5.17	1.45	1.33
5	F	312	CHL	O2D-CGD	5.17	1.45	1.33
5	C	313	CHL	CHD-C1D	5.17	1.48	1.38
5	D	311	CHL	CHC-C1C	5.16	1.49	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	305	CHL	O2D-CGD	5.16	1.45	1.33
5	F	310	CHL	CHD-C1D	5.16	1.48	1.38
5	A	305	CHL	O2D-CGD	5.15	1.45	1.33
5	E	310	CHL	O2D-CGD	5.15	1.45	1.33
5	F	311	CHL	O2D-CGD	5.15	1.45	1.33
5	A	312	CHL	O2D-CGD	5.15	1.45	1.33
5	B	313	CHL	O2D-CGD	5.15	1.45	1.33
5	D	309	CHL	CHD-C1D	5.15	1.48	1.38
5	A	311	CHL	CHD-C1D	5.15	1.48	1.38
5	E	304	CHL	O2D-CGD	5.14	1.45	1.33
5	D	305	CHL	CHD-C1D	5.14	1.48	1.38
5	F	304	CHL	O2D-CGD	5.13	1.45	1.33
5	D	313	CHL	O2D-CGD	5.13	1.45	1.33
5	C	309	CHL	O2D-CGD	5.13	1.45	1.33
5	E	308	CHL	O2D-CGD	5.12	1.45	1.33
5	E	305	CHL	CHD-C1D	5.12	1.48	1.38
5	F	317	CHL	O2D-CGD	5.12	1.45	1.33
5	A	310	CHL	CHD-C1D	5.12	1.48	1.38
5	B	311	CHL	CHC-C1C	5.11	1.48	1.38
5	C	318	CHL	CHD-C1D	5.11	1.48	1.38
5	B	312	CHL	CHC-C1C	5.11	1.48	1.38
5	B	312	CHL	CHD-C1D	5.09	1.48	1.38
5	D	312	CHL	O2D-CGD	5.09	1.45	1.33
5	E	304	CHL	CHD-C1D	5.09	1.48	1.38
5	D	318	CHL	O2D-CGD	5.08	1.45	1.33
5	C	310	CHL	CHD-C1D	5.07	1.48	1.38
5	C	305	CHL	O2D-CGD	5.07	1.45	1.33
5	C	305	CHL	CHD-C1D	5.07	1.48	1.38
5	B	310	CHL	O2D-CGD	5.07	1.45	1.33
5	C	311	CHL	CHD-C1D	5.06	1.48	1.38
5	B	307	CHL	C2C-C3C	5.06	1.47	1.36
5	A	310	CHL	CHC-C1C	5.05	1.48	1.38
5	A	311	CHL	O2D-CGD	5.04	1.45	1.33
5	E	309	CHL	O2D-CGD	5.03	1.45	1.33
5	E	312	CHL	CHD-C1D	5.03	1.48	1.38
5	B	310	CHL	CHC-C1C	5.03	1.48	1.38
5	B	307	CHL	O2D-CGD	5.03	1.45	1.33
5	E	311	CHL	CHD-C1D	5.03	1.48	1.38
5	A	311	CHL	CHC-C1C	5.03	1.48	1.38
5	D	306	CHL	O2D-CGD	5.02	1.45	1.33
5	C	309	CHL	CHC-C1C	5.02	1.48	1.38
5	E	311	CHL	CHC-C1C	5.01	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	305	CHL	CHC-C1C	5.00	1.48	1.38
5	C	313	CHL	CHC-C1C	4.99	1.48	1.38
5	F	304	CHL	CHD-C1D	4.98	1.48	1.38
5	E	312	CHL	O2D-CGD	4.98	1.45	1.33
5	E	317	CHL	CHD-C1D	4.98	1.48	1.38
5	C	312	CHL	CHC-C1C	4.98	1.48	1.38
5	B	319	CHL	MG-NC	4.97	2.18	2.06
5	C	311	CHL	O2D-CGD	4.97	1.45	1.33
5	A	313	CHL	CHC-C1C	4.96	1.48	1.38
5	C	306	CHL	O2D-CGD	4.96	1.45	1.33
5	A	305	CHL	CHD-C1D	4.96	1.48	1.38
5	E	310	CHL	CHD-C1D	4.95	1.48	1.38
5	C	306	CHL	CHC-C1C	4.94	1.48	1.38
5	E	309	CHL	CHC-C1C	4.93	1.48	1.38
5	C	311	CHL	CHC-C1C	4.93	1.48	1.38
5	F	312	CHL	CHD-C1D	4.93	1.48	1.38
5	F	305	CHL	O2D-CGD	4.93	1.45	1.33
5	B	307	CHL	CHD-C1D	4.93	1.48	1.38
5	D	306	CHL	CHC-C1C	4.92	1.48	1.38
5	D	313	CHL	MG-ND	-4.92	1.96	2.05
5	F	311	CHL	MG-ND	-4.92	1.96	2.05
5	D	309	CHL	CHC-C1C	4.90	1.48	1.38
5	C	306	CHL	CHD-C1D	4.90	1.47	1.38
5	B	314	CHL	CHC-C1C	4.90	1.48	1.38
5	E	308	CHL	CHC-C1C	4.89	1.48	1.38
5	D	311	CHL	MG-NC	4.89	2.17	2.06
5	B	313	CHL	CHC-C1C	4.89	1.48	1.38
5	A	306	CHL	MG-ND	-4.89	1.96	2.05
5	A	309	CHL	CHC-C1C	4.88	1.48	1.38
5	D	310	CHL	CHC-C1C	4.88	1.48	1.38
5	B	314	CHL	O2D-CGD	4.87	1.45	1.33
5	F	309	CHL	CHC-C1C	4.87	1.48	1.38
5	F	317	CHL	CHC-C1C	4.86	1.48	1.38
5	D	305	CHL	CHC-C1C	4.86	1.48	1.38
5	C	305	CHL	MG-ND	-4.86	1.96	2.05
5	C	318	CHL	O2D-CGD	4.85	1.45	1.33
5	F	312	CHL	CHC-C1C	4.84	1.48	1.38
5	E	304	CHL	CHC-C1C	4.84	1.48	1.38
5	E	312	CHL	CHC-C1C	4.82	1.48	1.38
5	A	313	CHL	O2D-CGD	4.82	1.45	1.33
5	A	305	CHL	CHC-C1C	4.82	1.48	1.38
5	E	317	CHL	O2D-CGD	4.81	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	310	CHL	CHC-C1C	4.80	1.48	1.38
5	D	318	CHL	CHC-C1C	4.79	1.48	1.38
5	F	308	CHL	CHC-C1C	4.79	1.48	1.38
5	E	310	CHL	CHC-C1C	4.78	1.48	1.38
5	F	311	CHL	CHC-C1C	4.78	1.48	1.38
5	B	306	CHL	CHC-C1C	4.78	1.48	1.38
5	A	306	CHL	CHC-C1C	4.77	1.48	1.38
5	C	310	CHL	CHC-C1C	4.76	1.48	1.38
5	D	313	CHL	CHC-C1C	4.75	1.48	1.38
5	F	310	CHL	MG-NC	4.74	2.17	2.06
5	F	310	CHL	O2D-CGD	4.74	1.44	1.33
5	A	312	CHL	CHC-C1C	4.72	1.48	1.38
5	F	304	CHL	CHC-C1C	4.72	1.48	1.38
5	A	306	CHL	CHD-C1D	4.71	1.47	1.38
5	F	305	CHL	CHD-C1D	4.70	1.47	1.38
5	B	319	CHL	CHC-C1C	4.70	1.48	1.38
5	A	312	CHL	MG-NC	4.69	2.17	2.06
5	C	305	CHL	CHC-C1C	4.68	1.48	1.38
5	E	317	CHL	CHC-C1C	4.68	1.48	1.38
5	B	314	CHL	CHD-C1D	4.67	1.47	1.38
5	A	318	CHL	CHC-C1C	4.66	1.48	1.38
5	C	318	CHL	CHC-C1C	4.66	1.48	1.38
5	A	313	CHL	CHD-C1D	4.65	1.47	1.38
5	C	313	CHL	MG-NC	4.65	2.17	2.06
5	B	307	CHL	CHC-C1C	4.62	1.47	1.38
5	D	318	CHL	O2A-CGA	4.62	1.46	1.30
5	D	306	CHL	CHD-C1D	4.61	1.47	1.38
5	D	313	CHL	CHD-C1D	4.61	1.47	1.38
5	F	309	CHL	MG-NC	4.60	2.17	2.06
5	C	313	CHL	MG-ND	-4.59	1.96	2.05
5	F	317	CHL	O2A-CGA	4.58	1.46	1.30
5	F	305	CHL	CHC-C1C	4.55	1.47	1.38
6	D	314	CLA	C4D-ND	-4.53	1.31	1.37
5	D	312	CHL	CHC-C1C	4.53	1.47	1.38
5	C	306	CHL	MG-NC	4.52	2.17	2.06
5	D	305	CHL	MG-NC	4.50	2.17	2.06
5	F	309	CHL	CHB-C1B	4.46	1.49	1.39
5	D	313	CHL	O2A-CGA	4.45	1.46	1.33
5	E	310	CHL	O2A-CGA	4.44	1.46	1.33
5	E	317	CHL	CHB-C1B	4.44	1.49	1.39
2	A	302	0IE	C15-C16	4.43	1.41	1.35
5	C	313	CHL	O2A-CGA	4.43	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	310	CHL	CHB-C1B	4.43	1.49	1.39
6	F	313	CLA	C4D-ND	-4.42	1.31	1.37
5	B	311	CHL	CHB-C1B	4.41	1.49	1.39
5	C	318	CHL	MG-NC	4.40	2.16	2.06
5	F	312	CHL	O2A-CGA	4.39	1.46	1.33
5	D	312	CHL	O2A-CGA	4.39	1.46	1.33
5	E	312	CHL	O2A-CGA	4.38	1.46	1.33
5	E	311	CHL	O2A-CGA	4.38	1.46	1.33
5	A	311	CHL	MG-NC	4.36	2.16	2.06
6	A	314	CLA	C4D-ND	-4.36	1.31	1.37
2	E	302	OIE	C15-C16	4.35	1.41	1.35
5	B	306	CHL	CHB-C1B	4.34	1.49	1.39
5	E	309	CHL	CHB-C1B	4.34	1.49	1.39
5	D	309	CHL	CHB-C1B	4.33	1.49	1.39
5	D	312	CHL	CHB-C1B	4.32	1.49	1.39
5	B	311	CHL	O2A-CGA	4.32	1.46	1.33
2	E	302	OIE	C8-C7	4.32	1.41	1.35
5	B	311	CHL	CHC-C4B	4.32	1.49	1.39
5	C	311	CHL	O2A-CGA	4.30	1.45	1.33
5	A	311	CHL	O2A-CGA	4.30	1.45	1.33
5	F	310	CHL	O2A-CGA	4.30	1.45	1.33
5	B	306	CHL	O2A-CGA	4.29	1.45	1.33
7	B	324	LHG	O8-C23	4.28	1.45	1.33
5	E	309	CHL	CHC-C4B	4.28	1.49	1.39
5	A	305	CHL	CHB-C1B	4.28	1.49	1.39
5	B	319	CHL	CHB-C1B	4.28	1.49	1.39
5	C	313	CHL	CHC-C4B	4.27	1.49	1.39
5	A	310	CHL	CHB-C1B	4.26	1.49	1.39
5	B	314	CHL	O2A-CGA	4.26	1.45	1.33
9	B	302	OUE	O44-C45	4.26	1.44	1.34
5	D	305	CHL	CHB-C1B	4.25	1.48	1.39
5	A	310	CHL	CHC-C4B	4.25	1.48	1.39
5	E	308	CHL	CHB-C1B	4.25	1.48	1.39
5	A	305	CHL	O2A-CGA	4.25	1.45	1.33
5	C	309	CHL	CHB-C1B	4.25	1.48	1.39
5	C	312	CHL	O2A-CGA	4.25	1.45	1.33
5	D	311	CHL	O2A-CGA	4.25	1.45	1.33
5	B	319	CHL	CHD-C4C	4.24	1.48	1.39
5	C	311	CHL	CHB-C1B	4.23	1.48	1.39
5	D	313	CHL	CHB-C1B	4.23	1.48	1.39
5	D	312	CHL	CHD-C4C	4.22	1.48	1.39
5	F	304	CHL	CHB-C1B	4.22	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	312	CHL	CHD-C4C	4.22	1.48	1.39
5	B	312	CHL	CHB-C1B	4.22	1.48	1.39
5	E	305	CHL	CHC-C4B	4.21	1.48	1.39
2	C	301	0IE	C15-C16	4.21	1.41	1.35
5	F	311	CHL	O2A-CGA	4.21	1.45	1.33
5	B	312	CHL	O2A-CGA	4.21	1.45	1.33
5	D	318	CHL	CHC-C4B	4.20	1.48	1.39
5	E	304	CHL	O2A-CGA	4.20	1.45	1.33
5	D	306	CHL	O2A-CGA	4.20	1.45	1.33
5	A	313	CHL	O2A-CGA	4.20	1.45	1.33
5	C	310	CHL	CHB-C1B	4.20	1.48	1.39
5	A	306	CHL	CHB-C1B	4.20	1.48	1.39
5	E	311	CHL	CHC-C4B	4.20	1.48	1.39
5	C	305	CHL	CHB-C1B	4.19	1.48	1.39
5	B	310	CHL	CHB-C1B	4.19	1.48	1.39
5	F	308	CHL	CHB-C1B	4.19	1.48	1.39
5	C	318	CHL	CHB-C1B	4.18	1.48	1.39
2	E	301	0IE	C11-C12	4.17	1.41	1.35
5	F	317	CHL	CHB-C1B	4.17	1.48	1.39
5	F	312	CHL	CHC-C4B	4.17	1.48	1.39
5	D	312	CHL	MG-ND	-4.17	1.97	2.05
5	E	317	CHL	CHC-C4B	4.17	1.48	1.39
5	A	306	CHL	O2A-CGA	4.17	1.45	1.33
5	B	307	CHL	CHD-C4C	4.17	1.48	1.39
5	B	312	CHL	CHC-C4B	4.17	1.48	1.39
5	C	312	CHL	CHC-C4B	4.17	1.48	1.39
5	C	313	CHL	CHD-C4C	4.16	1.48	1.39
5	A	312	CHL	O2A-CGA	4.16	1.45	1.33
5	A	318	CHL	CHB-C1B	4.16	1.48	1.39
5	C	318	CHL	CHC-C4B	4.16	1.48	1.39
5	A	312	CHL	CHD-C4C	4.15	1.48	1.39
6	C	317	CLA	C4D-ND	-4.15	1.32	1.37
5	C	310	CHL	O2D-CGD	4.15	1.43	1.33
5	C	309	CHL	CHC-C4B	4.15	1.48	1.39
5	D	310	CHL	CHC-C4B	4.15	1.48	1.39
5	A	318	CHL	CHC-C4B	4.14	1.48	1.39
5	F	308	CHL	CHC-C4B	4.14	1.48	1.39
5	F	317	CHL	CHC-C4B	4.14	1.48	1.39
5	B	313	CHL	O2A-CGA	4.14	1.45	1.33
5	D	305	CHL	O2A-CGA	4.14	1.45	1.33
5	F	309	CHL	CHC-C4B	4.14	1.48	1.39
2	E	301	0IE	C15-C16	4.13	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	319	CHL	O2A-CGA	4.13	1.46	1.33
5	D	318	CHL	CHB-C1B	4.13	1.48	1.39
5	A	310	CHL	O2A-CGA	4.13	1.45	1.33
6	D	308	CLA	C1D-ND	4.13	1.42	1.37
6	F	306	CLA	C1D-ND	4.13	1.42	1.37
6	E	306	CLA	C1D-ND	4.13	1.42	1.37
5	E	304	CHL	CHD-C4C	4.12	1.48	1.39
2	C	301	0IE	C8-C7	4.12	1.41	1.35
5	C	305	CHL	CHD-C4C	4.12	1.48	1.39
6	B	316	CLA	C1D-ND	4.11	1.42	1.37
2	E	302	0IE	C11-C12	4.11	1.41	1.35
5	C	312	CHL	CHB-C1B	4.11	1.48	1.39
5	E	311	CHL	CHB-C1B	4.11	1.48	1.39
5	A	312	CHL	CHB-C1B	4.10	1.48	1.39
2	C	301	0IE	C11-C12	4.10	1.41	1.35
5	B	313	CHL	CHD-C4C	4.10	1.48	1.39
6	E	313	CLA	C1D-ND	4.10	1.42	1.37
6	F	307	CLA	C1D-ND	4.09	1.42	1.37
5	B	307	CHL	O2A-CGA	4.09	1.45	1.33
5	B	314	CHL	CHB-C1B	4.09	1.48	1.39
5	D	309	CHL	CHD-C4C	4.08	1.48	1.39
5	E	305	CHL	MG-NC	4.08	2.16	2.06
6	C	307	CLA	C1D-ND	4.08	1.42	1.37
5	B	313	CHL	CHC-C4B	4.08	1.48	1.39
5	D	305	CHL	CHC-C4B	4.08	1.48	1.39
2	D	302	0IE	C15-C16	4.07	1.41	1.35
5	B	319	CHL	CHC-C4B	4.07	1.48	1.39
5	C	311	CHL	CHC-C4B	4.07	1.48	1.39
5	F	311	CHL	CHD-C4C	4.07	1.48	1.39
5	C	310	CHL	CHC-C4B	4.07	1.48	1.39
5	C	313	CHL	CHB-C1B	4.07	1.48	1.39
5	C	306	CHL	CHC-C4B	4.07	1.48	1.39
5	E	304	CHL	CHC-C4B	4.06	1.48	1.39
5	A	309	CHL	CHB-C1B	4.06	1.48	1.39
5	E	308	CHL	CHC-C4B	4.06	1.48	1.39
5	E	308	CHL	CHD-C4C	4.06	1.48	1.39
5	A	311	CHL	CHC-C4B	4.06	1.48	1.39
5	F	311	CHL	CHB-C1B	4.06	1.48	1.39
5	C	306	CHL	O2A-CGA	4.05	1.45	1.33
5	B	313	CHL	OBD-CAD	4.05	1.29	1.22
5	A	318	CHL	CHD-C4C	4.05	1.48	1.39
5	B	314	CHL	CHC-C4B	4.05	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	302	0IE	C15-C16	4.05	1.41	1.35
2	E	301	0IE	C8-C7	4.05	1.41	1.35
5	B	311	CHL	CHD-C4C	4.04	1.48	1.39
5	E	311	CHL	CHD-C4C	4.04	1.48	1.39
5	A	309	CHL	CHD-C4C	4.04	1.48	1.39
5	D	311	CHL	CHC-C4B	4.04	1.48	1.39
5	B	310	CHL	CHC-C4B	4.04	1.48	1.39
5	E	312	CHL	CHC-C4B	4.04	1.48	1.39
5	F	308	CHL	CHD-C4C	4.03	1.48	1.39
6	A	308	CLA	C1D-ND	4.03	1.42	1.37
6	A	316	CLA	C1D-ND	4.03	1.42	1.37
2	F	301	0IE	C8-C7	4.03	1.41	1.35
5	E	312	CHL	CHB-C1B	4.03	1.48	1.39
6	D	317	CLA	C1D-ND	4.03	1.42	1.37
5	C	309	CHL	CHD-C4C	4.03	1.48	1.39
5	D	318	CHL	CHD-C4C	4.03	1.48	1.39
5	E	305	CHL	CHD-C4C	4.02	1.48	1.39
6	B	309	CLA	C1D-ND	4.02	1.42	1.37
6	E	314	CLA	C1D-ND	4.01	1.42	1.37
5	B	313	CHL	CHB-C1B	4.01	1.48	1.39
5	A	313	CHL	CHC-C4B	4.01	1.48	1.39
5	A	306	CHL	OBD-CAD	4.01	1.29	1.22
5	D	311	CHL	CHD-C4C	4.01	1.48	1.39
2	F	302	0IE	C11-C12	4.00	1.41	1.35
5	E	304	CHL	CHB-C1B	4.00	1.48	1.39
5	A	306	CHL	CHD-C4C	4.00	1.48	1.39
5	F	311	CHL	CHC-C4B	4.00	1.48	1.39
5	B	306	CHL	CHC-C4B	4.00	1.48	1.39
5	A	305	CHL	CHD-C4C	4.00	1.48	1.39
2	C	302	0IE	C11-C12	4.00	1.41	1.35
5	E	312	CHL	MG-NC	3.99	2.15	2.06
5	A	309	CHL	CHC-C4B	3.99	1.48	1.39
5	D	309	CHL	CHC-C4B	3.98	1.48	1.39
5	F	317	CHL	CHD-C4C	3.98	1.48	1.39
5	C	305	CHL	CHC-C4B	3.98	1.48	1.39
7	B	324	LHG	O7-C7	3.97	1.45	1.34
6	A	317	CLA	C1D-ND	3.97	1.42	1.37
5	D	310	CHL	CHD-C4C	3.97	1.48	1.39
2	D	301	0IE	C15-C16	3.97	1.41	1.35
5	E	309	CHL	CHD-C4C	3.96	1.48	1.39
5	A	306	CHL	CHC-C4B	3.96	1.48	1.39
6	E	307	CLA	C1D-ND	3.96	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	0IE	C11-C12	3.96	1.41	1.35
9	B	325	0UR	O44-C45	3.95	1.43	1.34
5	B	314	CHL	CHD-C4C	3.95	1.48	1.39
5	A	313	CHL	CHD-C4C	3.95	1.48	1.39
5	C	306	CHL	CHB-C1B	3.95	1.48	1.39
5	F	310	CHL	CHC-C4B	3.94	1.48	1.39
5	C	306	CHL	CHD-C4C	3.94	1.48	1.39
5	F	309	CHL	CHD-C4C	3.93	1.48	1.39
5	B	306	CHL	CHD-C4C	3.93	1.48	1.39
5	B	310	CHL	CHD-C4C	3.93	1.48	1.39
9	E	320	0UR	O44-C45	3.93	1.43	1.34
5	D	313	CHL	CHC-C4B	3.92	1.48	1.39
5	D	313	CHL	CHD-C4C	3.92	1.48	1.39
9	A	322	0UR	O44-C45	3.92	1.43	1.34
5	A	311	CHL	CHB-C1B	3.91	1.48	1.39
6	D	316	CLA	C1D-ND	3.91	1.42	1.37
5	F	308	CHL	MG-NC	3.91	2.15	2.06
2	D	302	0IE	C11-C12	3.91	1.41	1.35
5	E	310	CHL	CHB-C1B	3.89	1.48	1.39
5	F	312	CHL	CHB-C1B	3.89	1.48	1.39
5	A	305	CHL	CHC-C4B	3.89	1.48	1.39
5	F	305	CHL	O2A-CGA	3.89	1.44	1.33
5	A	312	CHL	CHC-C4B	3.89	1.48	1.39
5	F	304	CHL	CHD-C4C	3.89	1.48	1.39
5	C	310	CHL	CHD-C4C	3.88	1.48	1.39
6	C	314	CLA	C1D-ND	3.88	1.42	1.37
9	C	321	0UR	O44-C45	3.88	1.43	1.34
5	A	309	CHL	OBD-CAD	3.88	1.29	1.22
6	F	314	CLA	C1D-ND	3.88	1.42	1.37
6	C	308	CLA	C1D-ND	3.88	1.42	1.37
5	E	310	CHL	CHC-C4B	3.87	1.48	1.39
5	B	310	CHL	OBD-CAD	3.87	1.29	1.22
2	D	301	0IE	C8-C7	3.87	1.40	1.35
5	D	311	CHL	CHB-C1B	3.87	1.48	1.39
5	E	305	CHL	O2A-CGA	3.86	1.44	1.33
5	D	309	CHL	OBD-CAD	3.86	1.29	1.22
5	D	312	CHL	CHC-C4B	3.85	1.48	1.39
9	F	320	0UR	O44-C45	3.85	1.43	1.34
5	B	319	CHL	OBD-CAD	3.85	1.29	1.22
5	E	305	CHL	OBD-CAD	3.84	1.29	1.22
2	C	302	0IE	C8-C7	3.84	1.40	1.35
5	F	310	CHL	CHB-C1B	3.84	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	313	CHL	CHB-C1B	3.83	1.48	1.39
5	F	312	CHL	CHD-C4C	3.83	1.48	1.39
5	F	305	CHL	CHB-C1B	3.83	1.48	1.39
5	D	305	CHL	CHD-C4C	3.83	1.48	1.39
6	C	315	CLA	C1D-ND	3.82	1.42	1.37
5	E	308	CHL	OBD-CAD	3.82	1.29	1.22
5	E	311	CHL	OBD-CAD	3.82	1.29	1.22
5	C	318	CHL	CHD-C4C	3.81	1.47	1.39
6	B	318	CLA	C1D-ND	3.81	1.42	1.37
5	E	305	CHL	CHB-C1B	3.81	1.48	1.39
6	B	308	CLA	C1D-ND	3.81	1.42	1.37
5	F	310	CHL	CHD-C4C	3.81	1.47	1.39
5	E	312	CHL	CHD-C4C	3.81	1.47	1.39
5	F	305	CHL	CHD-C4C	3.81	1.47	1.39
5	C	305	CHL	OBD-CAD	3.81	1.29	1.22
6	F	316	CLA	C1D-ND	3.80	1.42	1.37
5	F	305	CHL	CHC-C4B	3.80	1.47	1.39
6	F	315	CLA	C1D-ND	3.80	1.42	1.37
5	B	307	CHL	CHB-C1B	3.79	1.47	1.39
5	A	305	CHL	OBD-CAD	3.79	1.29	1.22
6	A	307	CLA	C1D-ND	3.79	1.42	1.37
5	F	312	CHL	OBD-CAD	3.79	1.29	1.22
5	A	310	CHL	CHD-C4C	3.79	1.47	1.39
5	F	304	CHL	CHC-C4B	3.78	1.47	1.39
2	D	301	0IE	C11-C12	3.78	1.40	1.35
5	D	318	CHL	OBD-CAD	3.77	1.29	1.22
5	D	306	CHL	OBD-CAD	3.77	1.29	1.22
5	F	317	CHL	OBD-CAD	3.77	1.29	1.22
5	B	307	CHL	OBD-CAD	3.77	1.29	1.22
2	F	302	0IE	C8-C7	3.76	1.40	1.35
5	C	306	CHL	C3D-C2D	3.76	1.49	1.39
5	A	318	CHL	OBD-CAD	3.75	1.28	1.22
6	B	317	CLA	C1D-ND	3.75	1.42	1.37
5	B	307	CHL	C3D-C2D	3.75	1.49	1.39
2	B	301	0IE	C11-C12	3.75	1.40	1.35
5	C	318	CHL	OBD-CAD	3.75	1.28	1.22
5	F	309	CHL	OBD-CAD	3.75	1.28	1.22
6	A	315	CLA	C1D-ND	3.74	1.42	1.37
5	D	306	CHL	CHB-C1B	3.74	1.47	1.39
5	E	304	CHL	OBD-CAD	3.74	1.28	1.22
5	E	310	CHL	OBD-CAD	3.74	1.28	1.22
6	D	315	CLA	C1D-ND	3.74	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	317	CHL	OBD-CAD	3.73	1.28	1.22
6	E	315	CLA	C1D-ND	3.72	1.42	1.37
5	A	312	CHL	OBD-CAD	3.72	1.28	1.22
5	E	310	CHL	CHD-C4C	3.72	1.47	1.39
5	C	312	CHL	OBD-CAD	3.72	1.28	1.22
5	C	309	CHL	C3D-C2D	3.72	1.49	1.39
6	C	316	CLA	C1D-ND	3.72	1.42	1.37
5	E	317	CHL	CHD-C4C	3.71	1.47	1.39
5	F	305	CHL	OBD-CAD	3.71	1.28	1.22
5	E	309	CHL	OBD-CAD	3.71	1.28	1.22
2	D	302	OIE	C8-C7	3.71	1.40	1.35
5	D	306	CHL	CHC-C4B	3.70	1.47	1.39
5	A	311	CHL	CHD-C4C	3.70	1.47	1.39
5	F	308	CHL	OBD-CAD	3.70	1.28	1.22
2	F	302	OIE	C15-C16	3.70	1.40	1.35
5	B	306	CHL	OBD-CAD	3.70	1.28	1.22
5	B	319	CHL	C3D-C2D	3.70	1.49	1.39
5	A	309	CHL	C3D-C2D	3.69	1.49	1.39
5	D	306	CHL	CHD-C4C	3.69	1.47	1.39
5	C	313	CHL	OBD-CAD	3.69	1.28	1.22
6	F	313	CLA	C1B-NB	-3.68	1.33	1.37
5	C	306	CHL	OBD-CAD	3.68	1.28	1.22
5	E	312	CHL	OBD-CAD	3.67	1.28	1.22
6	F	314	CLA	C4B-NB	3.67	1.42	1.37
5	B	312	CHL	CHD-C4C	3.66	1.47	1.39
5	F	310	CHL	OBD-CAD	3.66	1.28	1.22
2	F	301	OIE	C15-C16	3.66	1.40	1.35
5	B	307	CHL	CHC-C4B	3.65	1.47	1.39
5	A	311	CHL	OBD-CAD	3.65	1.28	1.22
5	E	304	CHL	C3D-C2D	3.65	1.49	1.39
5	C	312	CHL	C3D-C2D	3.65	1.49	1.39
5	F	317	CHL	C3D-C2D	3.65	1.49	1.39
5	D	305	CHL	OBD-CAD	3.64	1.28	1.22
2	B	301	OIE	C8-C7	3.64	1.40	1.35
5	C	313	CHL	C3D-C2D	3.64	1.49	1.39
6	B	315	CLA	C1B-NB	-3.63	1.33	1.37
6	E	316	CLA	C1D-ND	3.63	1.42	1.37
6	E	314	CLA	C4B-NB	3.63	1.42	1.37
5	A	310	CHL	OBD-CAD	3.63	1.28	1.22
6	B	309	CLA	C4B-NB	3.62	1.42	1.37
5	D	309	CHL	C3D-C2D	3.62	1.49	1.39
5	F	304	CHL	O2A-CGA	3.61	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	314	CHL	C3D-C2D	3.61	1.49	1.39
5	E	308	CHL	C3D-C2D	3.61	1.49	1.39
5	D	311	CHL	OBD-CAD	3.61	1.28	1.22
5	F	311	CHL	OBD-CAD	3.60	1.28	1.22
5	F	305	CHL	C3D-C2D	3.60	1.49	1.39
5	D	312	CHL	C3D-C2D	3.59	1.48	1.39
5	A	309	CHL	MG-NC	3.59	2.14	2.06
5	F	311	CHL	C3D-C2D	3.59	1.48	1.39
5	C	309	CHL	OBD-CAD	3.59	1.28	1.22
6	D	307	CLA	C1D-ND	3.59	1.42	1.37
5	B	311	CHL	OBD-CAD	3.59	1.28	1.22
5	A	311	CHL	C3D-C2D	3.58	1.48	1.39
5	C	311	CHL	OBD-CAD	3.58	1.28	1.22
5	B	311	CHL	C3D-C2D	3.58	1.48	1.39
5	C	305	CHL	C3D-C2D	3.57	1.48	1.39
5	C	311	CHL	CHD-C4C	3.57	1.47	1.39
5	A	312	CHL	C3D-C2D	3.57	1.48	1.39
5	B	314	CHL	OBD-CAD	3.57	1.28	1.22
2	A	301	OIE	C17-C16	-3.57	1.38	1.45
5	A	318	CHL	C3D-C2D	3.56	1.48	1.39
5	E	312	CHL	C3D-C2D	3.56	1.48	1.39
5	D	311	CHL	C3D-C2D	3.56	1.48	1.39
5	C	318	CHL	C3D-C2D	3.56	1.48	1.39
5	B	310	CHL	C3D-C2D	3.56	1.48	1.39
5	A	305	CHL	C3D-C2D	3.56	1.48	1.39
5	A	310	CHL	O2D-CGD	3.55	1.41	1.33
5	E	305	CHL	C3D-C2D	3.55	1.48	1.39
5	B	313	CHL	C3D-C2D	3.54	1.48	1.39
5	E	309	CHL	C3D-C2D	3.54	1.48	1.39
5	D	310	CHL	C3D-C2D	3.54	1.48	1.39
5	D	318	CHL	C3D-C2D	3.54	1.48	1.39
5	F	312	CHL	C3D-C2D	3.54	1.48	1.39
5	A	310	CHL	C3D-C2D	3.53	1.48	1.39
5	A	306	CHL	C3D-C2D	3.53	1.48	1.39
5	D	313	CHL	C3D-C2D	3.53	1.48	1.39
5	E	317	CHL	C3D-C2D	3.52	1.48	1.39
5	D	312	CHL	OBD-CAD	3.51	1.28	1.22
6	E	306	CLA	C4B-NB	3.51	1.42	1.37
5	E	311	CHL	C3D-C2D	3.50	1.48	1.39
5	D	306	CHL	C3D-C2D	3.49	1.48	1.39
5	F	308	CHL	C3D-C2D	3.49	1.48	1.39
5	F	304	CHL	OBD-CAD	3.49	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	305	CHL	C3D-C2D	3.49	1.48	1.39
5	B	312	CHL	OBD-CAD	3.49	1.28	1.22
5	C	310	CHL	C3D-C2D	3.49	1.48	1.39
5	F	305	CHL	C1D-ND	-3.49	1.33	1.37
5	E	310	CHL	MG-NC	3.48	2.14	2.06
5	F	304	CHL	C3D-C2D	3.48	1.48	1.39
6	C	314	CLA	C4B-NB	3.48	1.42	1.37
2	B	301	0IE	C15-C16	3.47	1.40	1.35
5	F	310	CHL	C3D-C2D	3.46	1.48	1.39
5	C	311	CHL	MG-NC	3.45	2.14	2.06
5	E	311	CHL	MG-NB	3.45	2.12	2.05
5	F	309	CHL	C3D-C2D	3.45	1.48	1.39
5	A	313	CHL	C3D-C2D	3.44	1.48	1.39
5	B	306	CHL	C3D-C2D	3.44	1.48	1.39
6	C	315	CLA	C4B-NB	3.43	1.42	1.37
6	A	315	CLA	C4B-NB	3.42	1.42	1.37
5	A	313	CHL	MG-ND	-3.41	1.99	2.05
3	C	303	NEX	C7-C8	-3.40	1.26	1.32
5	A	313	CHL	OBD-CAD	3.40	1.28	1.22
6	D	316	CLA	C4B-NB	3.39	1.42	1.37
6	B	316	CLA	C4B-NB	3.38	1.41	1.37
5	C	311	CHL	C3D-C2D	3.38	1.48	1.39
5	B	312	CHL	C3D-C2D	3.38	1.48	1.39
5	C	318	CHL	MG-NB	-3.38	1.99	2.05
5	E	310	CHL	C3D-C2D	3.38	1.48	1.39
6	E	316	CLA	C4B-NB	3.37	1.41	1.37
6	A	308	CLA	C4B-NB	3.37	1.41	1.37
5	A	310	CHL	MG-NB	3.36	2.12	2.05
6	D	315	CLA	C4B-NB	3.36	1.41	1.37
6	F	313	CLA	MG-NB	-3.35	1.99	2.05
3	F	303	NEX	C7-C8	-3.35	1.26	1.32
6	B	308	CLA	C4B-NB	3.35	1.41	1.37
5	A	305	CHL	MG-NB	3.35	2.12	2.05
5	A	309	CHL	MG-NB	3.34	2.12	2.05
3	A	303	NEX	C7-C8	-3.34	1.26	1.32
2	A	302	0IE	C11-C12	3.33	1.40	1.35
5	D	313	CHL	OBD-CAD	3.33	1.28	1.22
6	D	307	CLA	C4B-NB	3.33	1.41	1.37
6	A	317	CLA	C4B-NB	3.32	1.41	1.37
6	A	316	CLA	C4B-NB	3.31	1.41	1.37
2	A	302	0IE	C6-C7	-3.30	1.38	1.45
5	B	306	CHL	C4D-CHA	3.30	1.50	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	307	CHL	C1D-ND	-3.29	1.33	1.37
6	C	316	CLA	C4B-NB	3.28	1.41	1.37
5	A	313	CHL	C1D-ND	-3.28	1.33	1.37
6	B	317	CLA	C4B-NB	3.27	1.41	1.37
5	D	306	CHL	C1D-ND	-3.26	1.33	1.37
6	B	315	CLA	MG-NB	-3.25	1.99	2.05
6	F	306	CLA	C4B-NB	3.25	1.41	1.37
6	C	307	CLA	C4B-NB	3.24	1.41	1.37
5	B	307	CHL	MG-ND	-3.24	1.99	2.05
6	E	307	CLA	C4B-NB	3.23	1.41	1.37
6	A	307	CLA	C4B-NB	3.23	1.41	1.37
3	D	303	NEX	C7-C8	-3.23	1.26	1.32
5	F	311	CHL	C1D-ND	-3.22	1.33	1.37
6	F	316	CLA	C4B-NB	3.22	1.41	1.37
5	C	305	CHL	C1D-ND	-3.21	1.33	1.37
6	C	308	CLA	C4B-NB	3.19	1.41	1.37
3	E	303	NEX	C7-C8	-3.19	1.26	1.32
6	D	317	CLA	C4B-NB	3.19	1.41	1.37
6	A	314	CLA	MG-ND	-3.18	1.99	2.05
6	B	318	CLA	C4B-NB	3.17	1.41	1.37
6	F	315	CLA	C4B-NB	3.17	1.41	1.37
5	D	309	CHL	C1D-ND	-3.16	1.33	1.37
5	F	317	CHL	C4D-CHA	3.16	1.49	1.38
3	B	303	NEX	C7-C8	-3.16	1.26	1.32
5	E	308	CHL	C4D-CHA	3.16	1.49	1.38
5	B	307	CHL	C1B-NB	-3.15	1.33	1.37
5	C	311	CHL	C4D-CHA	3.14	1.49	1.38
5	B	319	CHL	C4D-CHA	3.13	1.49	1.38
5	B	307	CHL	C4D-CHA	3.13	1.49	1.38
5	D	313	CHL	C1D-ND	-3.13	1.33	1.37
6	D	308	CLA	C4B-NB	3.13	1.41	1.37
2	A	301	OIE	C15-C16	3.12	1.39	1.35
5	A	305	CHL	C4D-CHA	3.12	1.49	1.38
6	B	309	CLA	C3B-C4B	3.12	1.50	1.42
6	E	313	CLA	C3B-C4B	3.12	1.50	1.42
5	F	312	CHL	C1B-NB	-3.09	1.34	1.37
6	E	314	CLA	C3B-C4B	3.09	1.50	1.42
5	A	306	CHL	C1D-ND	-3.09	1.34	1.37
5	C	309	CHL	C1D-ND	-3.08	1.34	1.37
5	D	305	CHL	C4D-CHA	3.08	1.49	1.38
5	C	318	CHL	C1D-ND	-3.08	1.34	1.37
5	C	318	CHL	C4D-CHA	3.08	1.49	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	305	CHL	C1D-ND	-3.07	1.34	1.37
5	A	311	CHL	C4D-CHA	3.07	1.49	1.38
6	F	307	CLA	C4B-NB	3.07	1.41	1.37
5	C	305	CHL	C4D-CHA	3.07	1.49	1.38
5	E	310	CHL	C4D-CHA	3.07	1.49	1.38
5	C	313	CHL	C4D-CHA	3.06	1.49	1.38
5	E	305	CHL	C3B-C4B	3.05	1.49	1.42
5	D	318	CHL	C4D-CHA	3.05	1.49	1.38
6	E	313	CLA	C4B-NB	3.05	1.41	1.37
6	E	315	CLA	C4B-NB	3.05	1.41	1.37
5	B	312	CHL	C4D-CHA	3.05	1.49	1.38
6	F	315	CLA	C3B-C4B	3.05	1.49	1.42
6	C	317	CLA	MG-NB	-3.04	1.99	2.05
5	B	313	CHL	C1D-ND	-3.04	1.34	1.37
5	E	308	CHL	C1D-ND	-3.04	1.34	1.37
5	A	318	CHL	C4D-CHA	3.04	1.49	1.38
5	B	310	CHL	C4D-CHA	3.04	1.49	1.38
6	B	308	CLA	C3B-C4B	3.04	1.49	1.42
5	A	311	CHL	MG-NB	3.04	2.11	2.05
6	E	307	CLA	C3B-C4B	3.04	1.49	1.42
5	F	308	CHL	C4D-CHA	3.04	1.49	1.38
5	B	314	CHL	MG-ND	-3.03	1.99	2.05
5	A	305	CHL	C1D-ND	-3.03	1.34	1.37
5	B	310	CHL	C1D-ND	-3.03	1.34	1.37
5	B	312	CHL	MG-NC	3.03	2.13	2.06
6	A	314	CLA	MG-NB	-3.03	1.99	2.05
5	D	312	CHL	C4D-CHA	3.02	1.49	1.38
5	A	306	CHL	C3B-C4B	3.02	1.49	1.42
5	C	309	CHL	C4D-CHA	3.02	1.49	1.38
5	D	310	CHL	C4D-CHA	3.01	1.49	1.38
5	E	317	CHL	C1D-ND	-3.01	1.34	1.37
5	F	309	CHL	C3B-C4B	3.01	1.49	1.42
5	C	310	CHL	C4D-CHA	3.00	1.49	1.38
5	A	309	CHL	C4D-CHA	3.00	1.49	1.38
5	E	317	CHL	C4D-CHA	3.00	1.49	1.38
6	B	308	CLA	C4D-ND	-3.00	1.33	1.37
5	C	310	CHL	OBD-CAD	3.00	1.27	1.22
5	F	310	CHL	C4D-CHA	3.00	1.49	1.38
5	D	318	CHL	C3B-C4B	3.00	1.49	1.42
6	C	307	CLA	C1B-C2B	2.99	1.50	1.43
5	D	311	CHL	C4D-CHA	2.99	1.49	1.38
5	C	306	CHL	C3B-C4B	2.98	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	310	CHL	C4D-CHA	2.98	1.49	1.38
6	D	307	CLA	C3B-C4B	2.98	1.49	1.42
6	E	306	CLA	C3B-C4B	2.98	1.49	1.42
5	C	306	CHL	C1D-ND	-2.98	1.34	1.37
5	F	309	CHL	C4D-CHA	2.98	1.49	1.38
6	D	315	CLA	C3B-C4B	2.98	1.49	1.42
5	D	309	CHL	C4D-CHA	2.97	1.49	1.38
5	C	313	CHL	C3B-C4B	2.97	1.49	1.42
6	A	317	CLA	C4D-ND	-2.97	1.33	1.37
5	D	306	CHL	C3B-C4B	2.97	1.49	1.42
5	F	312	CHL	C3B-C4B	2.97	1.49	1.42
6	D	315	CLA	C4D-ND	-2.97	1.33	1.37
6	C	314	CLA	C3B-C4B	2.97	1.49	1.42
5	C	312	CHL	C4D-CHA	2.97	1.48	1.38
5	F	304	CHL	C4D-CHA	2.97	1.48	1.38
5	F	304	CHL	MG-NB	2.96	2.11	2.05
6	F	316	CLA	C3B-C4B	2.96	1.49	1.42
6	B	316	CLA	C3B-C4B	2.96	1.49	1.42
5	E	317	CHL	C3B-C4B	2.96	1.49	1.42
5	B	307	CHL	C3B-C4B	2.95	1.49	1.42
6	D	316	CLA	C3B-C4B	2.95	1.49	1.42
6	C	315	CLA	C3B-C4B	2.95	1.49	1.42
5	A	312	CHL	C4D-CHA	2.94	1.48	1.38
5	E	312	CHL	C4D-CHA	2.94	1.48	1.38
6	A	315	CLA	C3B-C4B	2.94	1.49	1.42
6	C	308	CLA	C4D-ND	-2.94	1.33	1.37
5	E	304	CHL	MG-NB	2.94	2.11	2.05
6	E	316	CLA	C4D-ND	-2.94	1.33	1.37
6	B	318	CLA	C3B-C4B	2.93	1.49	1.42
5	F	308	CHL	C1D-ND	-2.93	1.34	1.37
6	A	314	CLA	CMC-C2C	-2.93	1.44	1.50
5	B	312	CHL	C1D-ND	-2.93	1.34	1.37
5	E	311	CHL	C1D-ND	-2.93	1.34	1.37
6	A	308	CLA	C3B-C4B	2.92	1.49	1.42
5	E	309	CHL	C4D-CHA	2.92	1.48	1.38
6	D	314	CLA	MG-NB	-2.92	2.00	2.05
6	A	316	CLA	C3B-C4B	2.92	1.49	1.42
5	A	312	CHL	C1D-ND	-2.92	1.34	1.37
6	F	314	CLA	C3B-C4B	2.92	1.49	1.42
5	E	311	CHL	C4D-CHA	2.92	1.48	1.38
6	F	306	CLA	C4D-ND	-2.92	1.33	1.37
5	B	314	CHL	C4D-CHA	2.91	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	311	CHL	C4D-CHA	2.91	1.48	1.38
6	A	307	CLA	C4D-ND	-2.91	1.33	1.37
5	D	309	CHL	MG-NC	2.91	2.13	2.06
5	B	313	CHL	C4D-CHA	2.90	1.48	1.38
2	A	301	0IE	C23-C16	-2.90	1.44	1.50
5	A	309	CHL	C1D-ND	-2.90	1.34	1.37
6	C	316	CLA	C4D-ND	-2.90	1.33	1.37
5	C	306	CHL	C1B-NB	-2.90	1.34	1.37
5	B	311	CHL	C4D-CHA	2.90	1.48	1.38
6	E	315	CLA	C3B-C4B	2.90	1.49	1.42
5	E	311	CHL	C3B-C4B	2.90	1.49	1.42
5	D	306	CHL	C1B-NB	-2.89	1.34	1.37
6	F	314	CLA	C4D-ND	-2.88	1.33	1.37
2	A	302	0IE	C8-C7	2.88	1.39	1.35
5	F	304	CHL	C1D-ND	-2.88	1.34	1.37
5	E	304	CHL	C4D-CHA	2.88	1.48	1.38
6	E	313	CLA	C4D-ND	-2.88	1.33	1.37
5	E	304	CHL	MG-NC	2.88	2.13	2.06
6	C	308	CLA	C3B-C4B	2.88	1.49	1.42
6	E	307	CLA	C4D-ND	-2.87	1.33	1.37
6	A	317	CLA	C3B-C4B	2.87	1.49	1.42
5	B	313	CHL	C1B-NB	-2.87	1.34	1.37
5	D	313	CHL	C4D-CHA	2.86	1.48	1.38
5	C	309	CHL	C3B-C4B	2.86	1.49	1.42
5	A	313	CHL	C3B-C4B	2.86	1.49	1.42
5	E	317	CHL	MG-NC	2.86	2.13	2.06
2	A	301	0IE	C21-C7	-2.86	1.45	1.50
5	F	305	CHL	C1B-NB	-2.86	1.34	1.37
5	C	305	CHL	O2A-CGA	2.86	1.41	1.33
5	A	313	CHL	C4D-CHA	2.86	1.48	1.38
2	A	301	0IE	C22-C12	-2.85	1.45	1.50
6	D	308	CLA	C3B-C4B	2.85	1.49	1.42
5	F	310	CHL	C3B-C4B	2.85	1.49	1.42
5	E	305	CHL	C4D-CHA	2.84	1.48	1.38
6	E	306	CLA	C4D-ND	-2.84	1.33	1.37
6	F	316	CLA	C4D-ND	-2.84	1.33	1.37
5	D	311	CHL	C3B-C4B	2.84	1.49	1.42
5	E	312	CHL	C1B-NB	-2.84	1.34	1.37
6	E	315	CLA	C4D-ND	-2.84	1.33	1.37
6	F	307	CLA	C3B-C4B	2.84	1.49	1.42
6	E	314	CLA	C4D-ND	-2.84	1.33	1.37
5	B	314	CHL	C3B-C4B	2.84	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	306	CHL	C4D-CHA	2.83	1.48	1.38
5	E	304	CHL	C3B-C4B	2.83	1.49	1.42
6	E	316	CLA	C3B-C4B	2.83	1.49	1.42
5	D	306	CHL	C4D-CHA	2.83	1.48	1.38
5	F	305	CHL	C4D-CHA	2.82	1.48	1.38
5	F	317	CHL	C3B-C4B	2.82	1.49	1.42
6	B	316	CLA	C4D-ND	-2.82	1.33	1.37
6	D	317	CLA	C1B-C2B	2.82	1.49	1.43
5	E	311	CHL	C1B-NB	-2.82	1.34	1.37
5	B	312	CHL	C3B-C4B	2.82	1.49	1.42
6	A	307	CLA	C3B-C4B	2.81	1.49	1.42
6	D	317	CLA	C4D-ND	-2.81	1.33	1.37
5	C	318	CHL	C3B-C4B	2.81	1.49	1.42
6	D	316	CLA	C4D-ND	-2.80	1.33	1.37
5	D	309	CHL	C3B-C4B	2.80	1.49	1.42
5	C	305	CHL	C3B-C4B	2.80	1.49	1.42
6	B	318	CLA	C4D-ND	-2.79	1.33	1.37
6	E	306	CLA	C1B-C2B	2.79	1.49	1.43
5	C	306	CHL	C4D-CHA	2.79	1.48	1.38
5	F	305	CHL	C1B-C2B	2.79	1.49	1.43
5	B	310	CHL	MG-NC	2.79	2.12	2.06
5	F	312	CHL	C4D-CHA	2.79	1.48	1.38
5	A	306	CHL	C1B-NB	-2.79	1.34	1.37
5	E	304	CHL	C1D-ND	-2.79	1.34	1.37
6	B	317	CLA	C3B-C4B	2.79	1.49	1.42
6	A	317	CLA	C1B-C2B	2.79	1.49	1.43
5	C	311	CHL	C3B-C4B	2.78	1.49	1.42
5	E	308	CHL	C3B-C4B	2.78	1.49	1.42
6	F	315	CLA	C4D-ND	-2.78	1.33	1.37
5	D	312	CHL	C1D-ND	-2.78	1.34	1.37
5	C	305	CHL	C1B-C2B	2.78	1.49	1.43
5	B	312	CHL	C2C-C1C	2.78	1.50	1.44
5	F	309	CHL	C2C-C1C	2.78	1.50	1.44
6	C	316	CLA	C3B-C4B	2.78	1.49	1.42
5	F	304	CHL	C1B-C2B	2.78	1.49	1.43
5	D	313	CHL	C3B-C4B	2.77	1.49	1.42
5	E	309	CHL	C3B-C4B	2.77	1.49	1.42
5	C	311	CHL	C1D-ND	-2.77	1.34	1.37
5	B	314	CHL	C1D-ND	-2.77	1.34	1.37
5	D	313	CHL	MG-NB	-2.76	2.00	2.05
5	C	312	CHL	C3B-C4B	2.76	1.49	1.42
5	D	310	CHL	C3B-C4B	2.76	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	314	CLA	C1B-C2B	2.76	1.49	1.43
5	B	307	CHL	C1B-C2B	2.76	1.49	1.43
6	D	308	CLA	C4D-ND	-2.75	1.33	1.37
5	C	310	CHL	C3B-C4B	2.75	1.49	1.42
6	B	315	CLA	CMC-C2C	-2.75	1.45	1.50
6	D	317	CLA	C3B-C4B	2.75	1.49	1.42
6	C	317	CLA	MG-ND	-2.75	2.00	2.05
6	F	306	CLA	C3B-C4B	2.75	1.49	1.42
5	F	317	CHL	C1D-ND	-2.75	1.34	1.37
6	C	317	CLA	C1B-NB	-2.74	1.34	1.37
6	A	315	CLA	C4D-ND	-2.74	1.33	1.37
5	D	305	CHL	C1D-ND	-2.74	1.34	1.37
5	B	319	CHL	C3B-C4B	2.74	1.49	1.42
5	F	305	CHL	C3B-C4B	2.73	1.49	1.42
5	F	312	CHL	C1D-ND	-2.73	1.34	1.37
6	C	316	CLA	C1B-C2B	2.73	1.49	1.43
6	C	307	CLA	C4D-ND	-2.73	1.33	1.37
6	C	307	CLA	C3B-C4B	2.73	1.49	1.42
5	A	318	CHL	C3B-C4B	2.73	1.49	1.42
6	A	316	CLA	C4D-ND	-2.73	1.33	1.37
9	B	302	OUR	C19-C18	2.72	1.54	1.50
5	B	306	CHL	C3B-C4B	2.72	1.49	1.42
5	E	310	CHL	C3B-C4B	2.72	1.49	1.42
5	E	309	CHL	C1D-ND	-2.72	1.34	1.37
5	C	310	CHL	C1D-ND	-2.71	1.34	1.37
5	A	318	CHL	C1D-ND	-2.71	1.34	1.37
5	A	306	CHL	C1B-C2B	2.71	1.49	1.43
5	B	314	CHL	MG-NC	2.71	2.12	2.06
5	E	310	CHL	C1D-ND	-2.71	1.34	1.37
6	F	313	CLA	C1D-ND	2.71	1.41	1.37
5	E	317	CHL	C1B-C2B	2.70	1.49	1.43
5	B	311	CHL	C3B-C4B	2.70	1.49	1.42
5	C	306	CHL	C1B-C2B	2.70	1.49	1.43
5	D	310	CHL	C1D-ND	-2.70	1.34	1.37
6	C	315	CLA	C1B-C2B	2.70	1.49	1.43
6	D	314	CLA	CMC-C2C	-2.70	1.45	1.50
5	A	305	CHL	C3B-C4B	2.70	1.49	1.42
5	A	305	CHL	C1B-C2B	2.70	1.49	1.43
6	F	314	CLA	C1B-C2B	2.70	1.49	1.43
6	B	308	CLA	C1B-C2B	2.70	1.49	1.43
5	D	310	CHL	C1B-C2B	2.69	1.49	1.43
5	A	311	CHL	C3B-C4B	2.69	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	0IE	C13-C12	-2.69	1.40	1.45
5	C	313	CHL	C1B-NB	-2.69	1.34	1.37
6	B	317	CLA	C4D-ND	-2.69	1.34	1.37
5	A	310	CHL	C3B-C4B	2.69	1.49	1.42
6	B	309	CLA	C4D-ND	-2.69	1.34	1.37
6	A	308	CLA	C4D-ND	-2.68	1.34	1.37
6	A	316	CLA	C1B-C2B	2.68	1.49	1.43
5	C	313	CHL	C1D-ND	-2.68	1.34	1.37
5	F	311	CHL	C3B-C4B	2.68	1.49	1.42
5	C	312	CHL	C1B-NB	-2.68	1.34	1.37
6	C	314	CLA	C4D-ND	-2.68	1.34	1.37
6	D	314	CLA	MG-ND	-2.67	2.00	2.05
5	F	304	CHL	C3B-C4B	2.67	1.49	1.42
6	A	307	CLA	C1B-C2B	2.67	1.49	1.43
6	B	315	CLA	CMD-C2D	-2.67	1.45	1.50
6	F	307	CLA	C4D-ND	-2.66	1.34	1.37
5	C	312	CHL	C1D-ND	-2.66	1.34	1.37
5	E	310	CHL	C4B-NB	-2.66	1.34	1.37
5	F	309	CHL	C1D-ND	-2.66	1.34	1.37
6	C	315	CLA	C4D-ND	-2.66	1.34	1.37
5	F	310	CHL	C1C-NC	-2.65	1.33	1.37
5	A	309	CHL	C3B-C4B	2.65	1.49	1.42
5	B	306	CHL	C1B-C2B	2.65	1.49	1.43
5	B	312	CHL	C1B-C2B	2.65	1.49	1.43
6	F	307	CLA	C1B-C2B	2.64	1.49	1.43
5	B	319	CHL	C1D-ND	-2.64	1.34	1.37
6	C	314	CLA	C1B-C2B	2.63	1.49	1.43
5	B	313	CHL	C3B-C4B	2.63	1.48	1.42
5	B	314	CHL	C1B-NB	-2.63	1.34	1.37
6	F	306	CLA	C1B-C2B	2.63	1.49	1.43
6	A	314	CLA	CMB-C2B	-2.63	1.45	1.50
5	D	305	CHL	C3B-C4B	2.63	1.48	1.42
6	B	316	CLA	C1B-C2B	2.63	1.49	1.43
5	C	309	CHL	C2C-C1C	2.62	1.50	1.44
5	E	312	CHL	MG-NB	2.62	2.11	2.05
5	F	310	CHL	C2C-C1C	2.62	1.50	1.44
5	B	310	CHL	C2C-C1C	2.62	1.50	1.44
5	D	311	CHL	C2C-C1C	2.62	1.50	1.44
5	F	305	CHL	MG-ND	-2.62	2.00	2.05
5	E	312	CHL	C3B-C4B	2.61	1.48	1.42
5	E	312	CHL	C1D-ND	-2.61	1.34	1.37
6	D	314	CLA	C1B-NB	-2.61	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	311	CHL	C1D-ND	-2.61	1.34	1.37
6	D	314	CLA	CMD-C2D	-2.61	1.45	1.50
5	A	310	CHL	C1B-C2B	2.60	1.49	1.43
5	A	310	CHL	C2C-C1C	2.60	1.50	1.44
5	A	310	CHL	C1D-ND	-2.60	1.34	1.37
5	E	310	CHL	C1B-C2B	2.60	1.49	1.43
5	E	304	CHL	C1B-C2B	2.60	1.49	1.43
5	B	310	CHL	C3B-C4B	2.60	1.48	1.42
6	A	314	CLA	C1B-NB	-2.60	1.34	1.37
6	A	315	CLA	C1B-C2B	2.59	1.49	1.43
5	E	305	CHL	C1B-NB	-2.59	1.34	1.37
5	E	309	CHL	C1B-C2B	2.59	1.49	1.43
5	F	309	CHL	C1B-C2B	2.59	1.49	1.43
5	E	309	CHL	C2C-C1C	2.59	1.50	1.44
5	F	311	CHL	C1B-NB	-2.58	1.34	1.37
6	D	316	CLA	C1B-C2B	2.58	1.49	1.43
5	B	306	CHL	MG-NB	2.58	2.10	2.05
5	A	312	CHL	C1B-NB	-2.58	1.34	1.37
6	B	318	CLA	C1B-C2B	2.57	1.49	1.43
6	E	313	CLA	C1B-C2B	2.57	1.49	1.43
5	E	308	CHL	C2C-C1C	2.57	1.50	1.44
6	E	315	CLA	C1B-C2B	2.57	1.49	1.43
5	A	311	CHL	C1D-ND	-2.57	1.34	1.37
5	F	312	CHL	C1B-C2B	2.56	1.49	1.43
7	C	319	LHG	O7-C5	-2.56	1.40	1.46
5	B	311	CHL	C2C-C1C	2.56	1.50	1.44
6	F	316	CLA	C1B-C2B	2.56	1.49	1.43
5	B	306	CHL	C1D-ND	-2.56	1.34	1.37
5	B	310	CHL	C4B-NB	-2.56	1.34	1.37
5	C	306	CHL	C2C-C1C	2.56	1.50	1.44
5	A	312	CHL	C3B-C4B	2.55	1.48	1.42
5	B	306	CHL	C4B-NB	-2.55	1.34	1.37
5	D	309	CHL	C2C-C1C	2.55	1.50	1.44
5	D	312	CHL	C3B-C4B	2.55	1.48	1.42
5	E	311	CHL	C1B-C2B	2.55	1.49	1.43
6	A	307	CLA	MG-NB	-2.54	2.00	2.05
5	B	307	CHL	C4C-C3C	2.54	1.49	1.45
5	C	310	CHL	C2C-C1C	2.53	1.49	1.44
5	F	317	CHL	C1B-C2B	2.53	1.49	1.43
6	A	314	CLA	CMD-C2D	-2.53	1.45	1.50
5	C	311	CHL	C2C-C1C	2.53	1.49	1.44
5	E	304	CHL	C1B-NB	-2.53	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	313	CLA	CMB-C2B	-2.53	1.45	1.50
5	A	310	CHL	C1B-NB	-2.53	1.34	1.37
2	F	301	0IE	C17-C16	-2.52	1.40	1.45
5	E	310	CHL	C2C-C1C	2.52	1.49	1.44
5	D	310	CHL	C2C-C1C	2.52	1.49	1.44
5	B	311	CHL	C1B-C2B	2.52	1.49	1.43
5	D	311	CHL	C1D-ND	-2.51	1.34	1.37
2	D	302	0IE	C6-C7	-2.51	1.40	1.45
5	E	308	CHL	C1B-C2B	2.51	1.49	1.43
6	E	316	CLA	C1B-C2B	2.51	1.49	1.43
5	F	304	CHL	MG-NC	2.51	2.12	2.06
6	B	317	CLA	C1B-C2B	2.51	1.49	1.43
5	A	306	CHL	C2C-C1C	2.51	1.49	1.44
5	D	312	CHL	C1B-C2B	2.51	1.49	1.43
5	D	306	CHL	C2C-C1C	2.51	1.49	1.44
5	A	309	CHL	C1B-NB	-2.51	1.34	1.37
6	F	313	CLA	CMC-C2C	-2.51	1.45	1.50
5	A	311	CHL	C1B-NB	-2.51	1.34	1.37
7	B	320	LHG	O7-C5	-2.51	1.40	1.46
5	C	310	CHL	C1B-C2B	2.50	1.49	1.43
5	D	305	CHL	C1B-C2B	2.50	1.49	1.43
6	D	314	CLA	C3B-C4B	2.50	1.48	1.42
5	D	318	CHL	C1B-C2B	2.50	1.49	1.43
5	D	305	CHL	C2C-C1C	2.49	1.49	1.44
5	A	311	CHL	C2C-C1C	2.49	1.49	1.44
6	D	315	CLA	CHC-C1C	2.49	1.43	1.38
5	D	318	CHL	C2C-C1C	2.49	1.49	1.44
6	C	317	CLA	CMD-C2D	-2.49	1.45	1.50
5	F	310	CHL	C1D-ND	-2.49	1.34	1.37
5	C	313	CHL	C1B-C2B	2.49	1.49	1.43
5	D	313	CHL	C1B-NB	-2.48	1.34	1.37
6	D	315	CLA	C1B-C2B	2.48	1.49	1.43
6	B	309	CLA	C1B-C2B	2.48	1.49	1.43
6	D	307	CLA	C1B-C2B	2.48	1.49	1.43
5	D	318	CHL	C1D-ND	-2.48	1.34	1.37
5	A	309	CHL	C1B-C2B	2.48	1.49	1.43
5	F	310	CHL	C1B-NB	-2.48	1.34	1.37
5	B	319	CHL	C1B-C2B	2.48	1.49	1.43
5	D	309	CHL	C1B-C2B	2.47	1.49	1.43
5	F	308	CHL	C2C-C1C	2.47	1.49	1.44
5	B	319	CHL	C4C-C3C	2.47	1.49	1.45
5	B	310	CHL	C1B-C2B	2.47	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	308	CLA	C1B-C2B	2.46	1.49	1.43
5	B	313	CHL	C1B-C2B	2.46	1.49	1.43
5	C	318	CHL	C1B-C2B	2.46	1.49	1.43
5	C	318	CHL	C1C-NC	-2.46	1.34	1.37
6	F	313	CLA	CMD-C2D	-2.45	1.45	1.50
5	F	308	CHL	C3B-C4B	2.45	1.48	1.42
6	C	317	CLA	CMB-C2B	-2.45	1.45	1.50
5	A	312	CHL	C1B-C2B	2.45	1.49	1.43
6	D	307	CLA	C4D-ND	-2.45	1.34	1.37
5	D	312	CHL	C4C-C3C	2.45	1.49	1.45
9	D	321	OUR	O44-C45	2.45	1.40	1.34
6	F	315	CLA	C1B-C2B	2.44	1.49	1.43
6	A	315	CLA	CHC-C1C	2.44	1.43	1.38
2	B	301	OIE	C13-C12	-2.44	1.40	1.45
5	C	312	CHL	C1B-C2B	2.44	1.49	1.43
5	A	318	CHL	C2C-C1C	2.43	1.49	1.44
5	E	305	CHL	C2C-C1C	2.43	1.49	1.44
2	A	301	OIE	C8-C7	2.43	1.39	1.35
6	F	315	CLA	CHC-C1C	2.43	1.43	1.38
5	E	312	CHL	C4B-NB	-2.42	1.34	1.37
5	F	311	CHL	C1B-C2B	2.42	1.49	1.43
5	E	310	CHL	C1B-NB	-2.42	1.34	1.37
5	E	317	CHL	C2C-C1C	2.42	1.49	1.44
5	A	313	CHL	C4B-NB	-2.42	1.34	1.37
6	E	307	CLA	C1B-C2B	2.42	1.49	1.43
5	D	313	CHL	C2C-C1C	2.42	1.49	1.44
5	A	318	CHL	C1C-NC	-2.41	1.34	1.37
5	C	309	CHL	C1B-C2B	2.41	1.48	1.43
5	F	304	CHL	C2C-C1C	2.40	1.49	1.44
5	A	309	CHL	C2C-C1C	2.40	1.49	1.44
5	A	318	CHL	C1B-C2B	2.40	1.48	1.43
5	D	313	CHL	C1B-C2B	2.40	1.48	1.43
5	E	317	CHL	C1C-NC	-2.40	1.34	1.37
2	C	302	OIE	C17-C16	-2.40	1.40	1.45
6	B	309	CLA	CHC-C1C	2.40	1.43	1.38
5	B	314	CHL	C1B-C2B	2.39	1.48	1.43
6	A	308	CLA	C1B-C2B	2.39	1.48	1.43
2	F	302	OIE	C13-C12	-2.39	1.40	1.45
5	C	311	CHL	C1B-C2B	2.39	1.48	1.43
2	A	302	OIE	C17-C16	-2.39	1.40	1.45
2	B	301	OIE	C17-C16	-2.39	1.40	1.45
6	B	317	CLA	CHC-C1C	2.38	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	0IE	C13-C12	-2.38	1.40	1.45
5	B	306	CHL	C2C-C1C	2.38	1.49	1.44
2	F	302	0IE	C6-C7	-2.38	1.40	1.45
5	A	311	CHL	C4B-NB	-2.38	1.34	1.37
5	C	312	CHL	C2C-C1C	2.38	1.49	1.44
5	F	308	CHL	C1B-C2B	2.38	1.48	1.43
2	F	302	0IE	C17-C16	-2.37	1.40	1.45
6	D	308	CLA	C1B-C2B	2.37	1.48	1.43
5	F	317	CHL	C2C-C1C	2.37	1.49	1.44
2	E	302	0IE	C6-C7	-2.37	1.40	1.45
5	B	319	CHL	C1C-NC	-2.37	1.34	1.37
5	E	305	CHL	C1B-C2B	2.37	1.48	1.43
6	D	307	CLA	CHC-C1C	2.36	1.43	1.38
5	B	313	CHL	C4B-NB	-2.36	1.34	1.37
6	B	315	CLA	CMB-C2B	-2.36	1.45	1.50
5	D	306	CHL	C1B-C2B	2.35	1.48	1.43
5	A	313	CHL	C2C-C1C	2.35	1.49	1.44
6	C	317	CLA	C1D-ND	2.35	1.40	1.37
5	B	319	CHL	C2C-C1C	2.35	1.49	1.44
6	C	317	CLA	CMC-C2C	-2.35	1.45	1.50
5	E	308	CHL	C4B-NB	-2.35	1.34	1.37
2	C	302	0IE	C13-C12	-2.35	1.40	1.45
6	C	314	CLA	CHC-C1C	2.35	1.43	1.38
6	B	316	CLA	CHC-C1C	2.35	1.43	1.38
5	E	312	CHL	C1B-C2B	2.34	1.48	1.43
5	D	306	CHL	C4B-NB	-2.34	1.34	1.37
5	C	318	CHL	C2C-C1C	2.34	1.49	1.44
6	A	316	CLA	CHC-C1C	2.34	1.43	1.38
5	D	305	CHL	C4B-NB	-2.33	1.34	1.37
5	D	318	CHL	C1B-NB	-2.33	1.34	1.37
5	F	317	CHL	C4C-C3C	2.33	1.49	1.45
5	A	310	CHL	C3B-C2B	2.33	1.49	1.41
2	D	301	0IE	C13-C12	-2.33	1.40	1.45
5	F	312	CHL	C1C-NC	-2.32	1.34	1.37
6	A	308	CLA	CHC-C1C	2.32	1.43	1.38
5	E	311	CHL	C2C-C1C	2.32	1.49	1.44
2	B	301	0IE	C6-C7	-2.32	1.41	1.45
5	E	308	CHL	C4C-C3C	2.32	1.49	1.45
5	A	309	CHL	C4B-NB	-2.32	1.34	1.37
5	C	311	CHL	C4B-NB	-2.32	1.34	1.37
5	D	309	CHL	C4C-C3C	2.32	1.49	1.45
5	E	304	CHL	C2C-C1C	2.32	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	312	CHL	C4B-NB	-2.31	1.34	1.37
5	C	309	CHL	C4B-NB	-2.31	1.34	1.37
2	D	302	0IE	C17-C16	-2.31	1.41	1.45
6	D	314	CLA	CMB-C2B	-2.31	1.45	1.50
5	A	313	CHL	C1B-C2B	2.30	1.48	1.43
5	C	305	CHL	C1B-NB	-2.30	1.35	1.37
5	A	305	CHL	C4B-NB	-2.30	1.35	1.37
6	E	313	CLA	CHC-C1C	2.30	1.43	1.38
5	B	311	CHL	C3B-C2B	2.30	1.49	1.41
5	C	313	CHL	C4B-NB	-2.29	1.35	1.37
6	C	316	CLA	MG-NB	-2.29	2.01	2.05
5	D	312	CHL	MG-NB	-2.29	2.01	2.05
5	C	305	CHL	O2A-C1	-2.29	1.39	1.46
6	D	316	CLA	CHC-C1C	2.29	1.43	1.38
5	F	310	CHL	C4B-NB	-2.29	1.35	1.37
5	E	304	CHL	C4B-NB	-2.28	1.35	1.37
6	B	315	CLA	CHC-C4B	-2.28	1.34	1.39
5	A	312	CHL	C4C-C3C	2.28	1.49	1.45
6	E	315	CLA	CHC-C1C	2.28	1.43	1.38
5	A	305	CHL	C1B-NB	-2.28	1.35	1.37
5	D	311	CHL	C3B-C2B	2.28	1.48	1.41
5	A	311	CHL	C1C-NC	-2.28	1.34	1.37
5	F	304	CHL	C4B-NB	-2.28	1.35	1.37
5	B	313	CHL	C2C-C1C	2.28	1.49	1.44
6	F	314	CLA	CHC-C1C	2.28	1.43	1.38
2	D	302	0IE	C13-C12	-2.27	1.41	1.45
5	F	310	CHL	C1B-C2B	2.27	1.48	1.43
5	E	309	CHL	C1C-NC	-2.27	1.34	1.37
5	F	311	CHL	C1C-NC	-2.27	1.34	1.37
5	A	306	CHL	MG-NC	2.27	2.11	2.06
5	B	314	CHL	C2C-C1C	2.27	1.49	1.44
5	C	313	CHL	C1C-NC	-2.27	1.34	1.37
5	E	309	CHL	C1B-NB	-2.27	1.35	1.37
5	F	304	CHL	C1B-NB	-2.27	1.35	1.37
5	A	306	CHL	C4B-NB	-2.27	1.35	1.37
3	D	303	NEX	O24-C25	-2.27	1.43	1.46
5	A	313	CHL	C1B-NB	-2.26	1.35	1.37
6	F	306	CLA	CHC-C1C	2.26	1.43	1.38
6	C	315	CLA	CHC-C1C	2.26	1.43	1.38
6	E	307	CLA	CHC-C1C	2.26	1.43	1.38
2	D	301	0IE	C17-C16	-2.26	1.41	1.45
5	C	306	CHL	C3B-C2B	2.25	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	305	CHL	C2A-C1A	-2.25	1.47	1.52
6	A	317	CLA	CHC-C1C	2.25	1.43	1.38
5	D	310	CHL	C4C-C3C	2.25	1.48	1.45
5	B	306	CHL	MG-NC	2.25	2.11	2.06
5	D	318	CHL	C4C-C3C	2.25	1.48	1.45
5	C	313	CHL	C2C-C1C	2.25	1.49	1.44
5	D	313	CHL	C4B-NB	-2.25	1.35	1.37
5	C	310	CHL	C1C-NC	-2.24	1.34	1.37
6	C	316	CLA	CHC-C1C	2.24	1.43	1.38
5	C	312	CHL	C4C-C3C	2.24	1.48	1.45
5	B	319	CHL	C4B-NB	-2.24	1.35	1.37
5	D	312	CHL	C1C-NC	-2.23	1.34	1.37
5	A	305	CHL	C2C-C1C	2.23	1.49	1.44
5	D	311	CHL	C4C-C3C	2.23	1.48	1.45
2	A	302	0IE	C22-C12	-2.23	1.46	1.50
6	F	316	CLA	MG-NB	-2.23	2.01	2.05
6	D	314	CLA	C4B-NB	2.23	1.40	1.37
2	A	301	0IE	C5-C6	2.22	1.40	1.34
5	B	313	CHL	C1C-NC	-2.22	1.34	1.37
5	F	308	CHL	C1C-NC	-2.22	1.34	1.37
6	A	307	CLA	CHC-C1C	2.22	1.43	1.38
6	F	316	CLA	CMB-C2B	-2.22	1.46	1.50
5	D	305	CHL	C4C-C3C	2.22	1.48	1.45
5	D	309	CHL	C4B-NB	-2.22	1.35	1.37
5	D	310	CHL	C3B-C2B	2.22	1.48	1.41
6	F	316	CLA	CMD-C2D	-2.22	1.46	1.50
6	C	308	CLA	CHC-C1C	2.21	1.43	1.38
5	E	309	CHL	C3B-C2B	2.21	1.48	1.41
5	A	312	CHL	C2C-C1C	2.21	1.49	1.44
2	C	302	0IE	C6-C7	-2.21	1.41	1.45
5	D	306	CHL	MG-NB	2.21	2.10	2.05
6	E	314	CLA	CHC-C1C	2.21	1.43	1.38
5	A	311	CHL	C1B-C2B	2.21	1.48	1.43
2	A	301	0IE	C10-C11	-2.21	1.36	1.43
9	A	322	0UR	C29-C28	-2.21	1.51	1.54
5	F	308	CHL	C4B-NB	-2.21	1.35	1.37
6	D	314	CLA	C1D-ND	2.21	1.40	1.37
5	F	312	CHL	C2C-C1C	2.20	1.49	1.44
2	C	301	0IE	C13-C12	-2.20	1.41	1.45
6	B	316	CLA	CMB-C2B	-2.20	1.46	1.50
6	D	317	CLA	CMC-C2C	-2.20	1.46	1.50
6	F	307	CLA	CHC-C1C	2.20	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	311	CHL	C4C-C3C	2.20	1.48	1.45
5	F	305	CHL	C3B-C2B	2.20	1.48	1.41
6	D	308	CLA	CMB-C2B	-2.19	1.46	1.50
5	D	305	CHL	C1B-NB	-2.18	1.35	1.37
5	A	318	CHL	C4C-C3C	2.18	1.48	1.45
5	E	312	CHL	C2C-C1C	2.18	1.49	1.44
6	F	313	CLA	CHC-C4B	-2.18	1.34	1.39
5	A	311	CHL	C3B-C2B	2.17	1.48	1.41
6	B	318	CLA	CHC-C1C	2.17	1.42	1.38
6	F	316	CLA	CHC-C1C	2.17	1.42	1.38
5	A	309	CHL	C4C-C3C	2.17	1.48	1.45
5	E	308	CHL	C3B-C2B	2.17	1.48	1.41
6	C	307	CLA	MG-NB	-2.17	2.01	2.05
5	B	306	CHL	C1B-NB	-2.17	1.35	1.37
5	D	318	CHL	C1C-NC	-2.17	1.34	1.37
5	F	311	CHL	C2C-C1C	2.16	1.49	1.44
5	C	312	CHL	C1C-NC	-2.16	1.34	1.37
5	F	310	CHL	C1D-C2D	2.16	1.49	1.45
6	B	308	CLA	CMB-C2B	-2.16	1.46	1.50
5	F	308	CHL	C1B-NB	-2.16	1.35	1.37
5	F	304	CHL	C1C-NC	-2.16	1.34	1.37
9	F	320	OUR	C31-C32	2.16	1.35	1.33
5	C	318	CHL	C4C-C3C	2.15	1.48	1.45
5	C	311	CHL	C1C-NC	-2.15	1.34	1.37
5	B	313	CHL	C4C-C3C	2.15	1.48	1.45
5	A	312	CHL	C3B-C2B	2.15	1.48	1.41
5	F	317	CHL	C1C-NC	-2.15	1.34	1.37
5	F	311	CHL	C4C-C3C	2.15	1.48	1.45
5	B	319	CHL	C3B-C2B	2.15	1.48	1.41
5	D	312	CHL	C4B-NB	-2.15	1.35	1.37
6	F	307	CLA	MG-NB	-2.15	2.01	2.05
5	A	309	CHL	C3B-C2B	2.15	1.48	1.41
5	C	318	CHL	C3B-C2B	2.15	1.48	1.41
3	A	303	NEX	O24-C25	-2.15	1.43	1.46
5	B	310	CHL	C1B-NB	-2.14	1.35	1.37
5	E	305	CHL	C3B-C2B	2.14	1.48	1.41
6	E	316	CLA	CHC-C1C	2.14	1.42	1.38
5	F	305	CHL	C2C-C1C	2.14	1.49	1.44
6	A	314	CLA	C1D-ND	2.14	1.40	1.37
5	F	309	CHL	C4C-C3C	2.14	1.48	1.45
5	B	319	CHL	C1B-NB	-2.14	1.35	1.37
6	A	308	CLA	CMB-C2B	-2.14	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	317	CHL	C3B-C2B	2.14	1.48	1.41
5	B	312	CHL	C1C-NC	-2.14	1.34	1.37
5	D	312	CHL	C2C-C1C	2.14	1.49	1.44
5	D	305	CHL	C3B-C2B	2.14	1.48	1.41
5	C	309	CHL	C4C-C3C	2.14	1.48	1.45
6	A	317	CLA	CMD-C2D	-2.14	1.46	1.50
2	C	301	0IE	C17-C16	-2.13	1.41	1.45
6	D	307	CLA	MG-NB	-2.13	2.01	2.05
5	E	304	CHL	C3B-C2B	2.13	1.48	1.41
6	F	307	CLA	CMB-C2B	-2.13	1.46	1.50
2	F	301	0IE	C13-C12	-2.13	1.41	1.45
7	E	318	LHG	O7-C5	-2.13	1.41	1.46
6	E	315	CLA	MG-NB	-2.13	2.01	2.05
6	B	315	CLA	CAC-C3C	-2.13	1.45	1.51
7	F	318	LHG	O7-C5	-2.13	1.41	1.46
5	C	310	CHL	C3B-C2B	2.13	1.48	1.41
6	F	313	CLA	C3B-C4B	2.12	1.47	1.42
5	C	305	CHL	C3B-C2B	2.12	1.48	1.41
5	D	309	CHL	C3B-C2B	2.12	1.48	1.41
6	A	314	CLA	C3B-C4B	2.12	1.47	1.42
5	F	317	CHL	C3B-C2B	2.12	1.48	1.41
6	F	313	CLA	CAC-C3C	-2.12	1.45	1.51
5	E	317	CHL	C1B-NB	-2.12	1.35	1.37
5	F	317	CHL	C1B-NB	-2.12	1.35	1.37
5	C	312	CHL	C3B-C2B	2.12	1.48	1.41
6	F	306	CLA	MG-NB	-2.12	2.01	2.05
5	B	314	CHL	C3B-C2B	2.12	1.48	1.41
6	D	308	CLA	CHC-C1C	2.12	1.42	1.38
6	E	306	CLA	CHC-C1C	2.12	1.42	1.38
5	C	306	CHL	C4C-C3C	2.12	1.48	1.45
2	A	301	0IE	C9-C8	-2.12	1.36	1.43
5	E	312	CHL	C1C-NC	-2.11	1.34	1.37
6	B	315	CLA	C1D-ND	2.11	1.40	1.37
5	D	305	CHL	C1C-NC	-2.11	1.34	1.37
6	E	307	CLA	CMB-C2B	-2.11	1.46	1.50
6	D	308	CLA	CMD-C2D	-2.11	1.46	1.50
6	D	317	CLA	CHC-C1C	2.11	1.42	1.38
5	E	311	CHL	C4B-NB	-2.11	1.35	1.37
6	D	316	CLA	MG-NB	-2.11	2.01	2.05
6	C	308	CLA	CMB-C2B	-2.11	1.46	1.50
5	E	312	CHL	C3B-C2B	2.11	1.48	1.41
6	B	308	CLA	CHC-C1C	2.11	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	305	CHL	C4B-NB	-2.11	1.35	1.37
6	D	316	CLA	CMD-C2D	-2.11	1.46	1.50
6	B	309	CLA	C1D-C2D	2.11	1.49	1.45
6	E	316	CLA	CMD-C2D	-2.10	1.46	1.50
5	C	311	CHL	C4C-C3C	2.10	1.48	1.45
5	B	310	CHL	C1C-NC	-2.10	1.34	1.37
5	C	311	CHL	C3B-C2B	2.10	1.48	1.41
6	A	314	CLA	CHC-C4B	-2.10	1.34	1.39
5	A	312	CHL	C1C-NC	-2.10	1.34	1.37
2	C	301	0IE	C6-C7	-2.10	1.41	1.45
5	E	304	CHL	C4C-C3C	2.09	1.48	1.45
5	B	313	CHL	C3B-C2B	2.09	1.48	1.41
6	A	314	CLA	CAC-C3C	-2.09	1.45	1.51
5	F	308	CHL	C4C-C3C	2.09	1.48	1.45
5	B	312	CHL	C3B-C2B	2.09	1.48	1.41
5	D	309	CHL	C1B-NB	-2.09	1.35	1.37
5	A	313	CHL	C1C-NC	-2.09	1.34	1.37
2	E	301	0IE	C17-C16	-2.09	1.41	1.45
5	C	313	CHL	C3B-C2B	2.09	1.48	1.41
5	B	307	CHL	C1D-C2D	2.09	1.49	1.45
5	E	311	CHL	C1C-NC	-2.08	1.34	1.37
5	C	305	CHL	C4C-C3C	2.08	1.48	1.45
5	A	305	CHL	C3B-C2B	2.08	1.48	1.41
2	E	302	0IE	C17-C16	-2.08	1.41	1.45
6	A	316	CLA	MG-NB	-2.08	2.01	2.05
5	E	308	CHL	C1C-NC	-2.08	1.34	1.37
5	B	310	CHL	C3B-C2B	2.08	1.48	1.41
5	A	318	CHL	C3B-C2B	2.07	1.48	1.41
5	C	309	CHL	C3B-C2B	2.07	1.48	1.41
6	E	306	CLA	CMB-C2B	-2.07	1.46	1.50
6	C	317	CLA	C3B-C4B	2.07	1.47	1.42
5	B	311	CHL	C1B-NB	-2.07	1.35	1.37
5	D	310	CHL	C1C-NC	-2.07	1.34	1.37
5	B	306	CHL	C4C-C3C	2.07	1.48	1.45
5	B	314	CHL	C4B-NB	-2.07	1.35	1.37
5	D	318	CHL	C3B-C2B	2.07	1.48	1.41
6	B	309	CLA	MG-NB	-2.07	2.01	2.05
6	C	316	CLA	CMD-C2D	-2.07	1.46	1.50
6	A	307	CLA	CMB-C2B	-2.07	1.46	1.50
6	D	316	CLA	CMC-C2C	-2.07	1.46	1.50
6	D	317	CLA	CMD-C2D	-2.07	1.46	1.50
9	F	320	0UR	C19-C18	2.07	1.53	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	311	CHL	C3B-C2B	2.07	1.48	1.41
5	E	311	CHL	C3B-C2B	2.06	1.48	1.41
5	C	310	CHL	C4C-C3C	2.06	1.48	1.45
5	A	313	CHL	C4C-C3C	2.06	1.48	1.45
5	F	309	CHL	C1B-NB	-2.06	1.35	1.37
5	F	309	CHL	C3B-C2B	2.06	1.48	1.41
6	B	309	CLA	CMB-C2B	-2.06	1.46	1.50
2	E	301	0IE	C13-C12	-2.06	1.41	1.45
5	C	310	CHL	C1B-NB	-2.06	1.35	1.37
5	B	307	CHL	C2C-C1C	2.06	1.49	1.44
5	D	311	CHL	C1B-C2B	2.06	1.48	1.43
5	F	309	CHL	C1C-NC	-2.06	1.34	1.37
5	B	312	CHL	C4B-NB	-2.06	1.35	1.37
3	B	303	NEX	O24-C25	-2.06	1.43	1.46
5	F	310	CHL	C4C-C3C	2.05	1.48	1.45
5	F	317	CHL	C4B-NB	-2.05	1.35	1.37
5	D	312	CHL	C3B-C2B	2.05	1.48	1.41
6	C	308	CLA	MG-NB	-2.05	2.01	2.05
7	A	319	LHG	P-O6	2.05	1.67	1.59
6	A	316	CLA	CMD-C2D	-2.04	1.46	1.50
6	B	318	CLA	CMB-C2B	-2.04	1.46	1.50
5	A	318	CHL	C1B-NB	-2.04	1.35	1.37
5	A	305	CHL	C4C-C3C	2.04	1.48	1.45
5	C	309	CHL	C1C-NC	-2.04	1.34	1.37
5	F	311	CHL	C1D-C2D	2.04	1.49	1.45
5	E	310	CHL	C1C-NC	-2.04	1.34	1.37
5	D	312	CHL	C1B-NB	-2.04	1.35	1.37
6	B	308	CLA	CMD-C2D	-2.04	1.46	1.50
6	D	307	CLA	CMB-C2B	-2.04	1.46	1.50
5	C	310	CHL	C4B-NB	-2.04	1.35	1.37
6	B	317	CLA	CMD-C2D	-2.03	1.46	1.50
5	E	310	CHL	C3B-C2B	2.03	1.48	1.41
5	B	314	CHL	C1C-NC	-2.03	1.34	1.37
5	F	310	CHL	CMC-C2C	2.03	1.49	1.45
6	A	317	CLA	MG-NB	-2.03	2.01	2.05
6	E	315	CLA	CMD-C2D	-2.03	1.46	1.50
9	B	302	0UR	O42-C2	-2.03	1.19	1.23
6	B	318	CLA	CMD-C2D	-2.03	1.46	1.50
6	F	306	CLA	CMB-C2B	-2.03	1.46	1.50
5	E	308	CHL	MG-NC	2.03	2.11	2.06
5	C	318	CHL	C4B-NB	-2.02	1.35	1.37
6	C	307	CLA	CMC-C2C	-2.02	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	316	CLA	CMB-C2B	-2.02	1.46	1.50
5	C	305	CHL	C2C-C1C	2.02	1.48	1.44
5	B	311	CHL	C1C-NC	-2.02	1.34	1.37
6	E	307	CLA	CMD-C2D	-2.02	1.46	1.50
6	F	315	CLA	MG-NB	-2.02	2.01	2.05
9	B	325	OUR	C19-C18	2.02	1.53	1.50
5	B	311	CHL	C4C-C3C	2.02	1.48	1.45
5	D	309	CHL	C1C-NC	-2.02	1.34	1.37
6	A	315	CLA	MG-NB	-2.02	2.01	2.05
6	D	315	CLA	CMD-C2D	-2.02	1.46	1.50
5	A	313	CHL	C3B-C2B	2.01	1.48	1.41
5	C	305	CHL	C3A-C4A	-2.01	1.45	1.51
6	F	315	CLA	CMD-C2D	-2.01	1.46	1.50
6	B	317	CLA	CMC-C2C	-2.01	1.46	1.50
5	A	318	CHL	C3A-C2A	-2.01	1.52	1.54
5	F	312	CHL	C1D-C2D	2.01	1.49	1.45
6	D	315	CLA	CMB-C2B	-2.01	1.46	1.50
5	D	310	CHL	C1B-NB	-2.01	1.35	1.37
2	F	301	OIE	C6-C7	-2.01	1.41	1.45
6	F	314	CLA	CMB-C2B	-2.01	1.46	1.50
7	D	319	LHG	P-O6	2.01	1.67	1.59
5	A	305	CHL	C4D-ND	2.00	1.40	1.37
5	F	308	CHL	C3B-C2B	2.00	1.48	1.41
5	F	310	CHL	C3B-C2B	2.00	1.48	1.41
5	B	306	CHL	C3B-C2B	2.00	1.48	1.41
5	E	305	CHL	C1C-NC	-2.00	1.34	1.37

All (2153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	311	CHL	O2A-C1-C2	26.61	178.56	108.64
3	F	303	NEX	C15-C35-C34	26.60	177.96	123.47
3	E	303	NEX	C35-C15-C14	25.85	176.43	123.47
3	C	303	NEX	C15-C35-C34	24.82	174.32	123.47
5	E	309	CHL	CMD-C2D-C1D	24.02	167.04	124.71
3	D	303	NEX	O24-C25-C24	23.90	131.34	113.38
5	D	309	CHL	CMD-C2D-C1D	23.16	165.53	124.71
3	B	303	NEX	C15-C35-C34	22.24	169.03	123.47
3	F	303	NEX	C35-C34-C33	21.78	158.39	127.31
3	B	303	NEX	C35-C34-C33	21.67	158.24	127.31
5	E	317	CHL	CMD-C2D-C1D	20.99	161.71	124.71
3	C	303	NEX	O24-C25-C24	20.61	128.87	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	303	NEX	O24-C25-C24	20.18	128.54	113.38
3	A	303	NEX	O24-C25-C24	19.68	128.16	113.38
5	A	311	CHL	OBD-CAD-C3D	-18.98	82.85	128.52
3	D	303	NEX	C35-C34-C33	18.43	153.61	127.31
5	E	304	CHL	CMD-C2D-C1D	17.86	156.18	124.71
5	E	309	CHL	CMD-C2D-C3D	-16.99	88.53	127.61
5	B	306	CHL	CMD-C2D-C1D	16.96	154.61	124.71
5	F	311	CHL	CMD-C2D-C1D	16.49	153.78	124.71
5	D	309	CHL	CMD-C2D-C3D	-16.31	90.10	127.61
3	C	303	NEX	C27-C28-C29	16.07	150.46	125.53
3	F	303	NEX	O24-C25-C24	15.49	125.02	113.38
3	E	303	NEX	C20-C13-C12	15.30	142.18	118.08
3	D	303	NEX	C12-C13-C14	14.73	141.55	118.94
5	B	313	CHL	CMD-C2D-C1D	14.72	150.65	124.71
5	E	317	CHL	CMD-C2D-C3D	-14.38	94.53	127.61
3	E	303	NEX	C12-C13-C14	-14.14	97.24	118.94
5	F	310	CHL	OBD-CAD-C3D	-14.04	94.73	128.52
5	E	309	CHL	CAA-C2A-C1A	13.85	142.81	112.14
3	D	303	NEX	C15-C35-C34	13.80	151.74	123.47
5	C	318	CHL	CMD-C2D-C1D	13.62	148.72	124.71
3	E	303	NEX	C15-C35-C34	13.57	151.27	123.47
3	A	303	NEX	C20-C13-C12	13.48	139.31	118.08
3	F	303	NEX	C27-C28-C29	12.99	145.69	125.53
5	B	319	CHL	CMD-C2D-C1D	12.97	147.56	124.71
5	F	304	CHL	CMD-C2D-C1D	12.90	147.45	124.71
5	F	305	CHL	CMD-C2D-C1D	-12.81	102.14	124.71
5	B	319	CHL	OBD-CAD-C3D	12.75	159.19	128.52
3	D	303	NEX	C20-C13-C12	-12.31	98.68	118.08
5	F	308	CHL	OBD-CAD-C3D	12.26	158.03	128.52
3	A	303	NEX	C12-C13-C14	-12.15	100.29	118.94
5	B	311	CHL	CMD-C2D-C1D	12.11	146.05	124.71
5	E	304	CHL	CMD-C2D-C3D	-11.98	100.05	127.61
5	F	305	CHL	CMD-C2D-C3D	11.69	154.51	127.61
5	E	309	CHL	OBD-CAD-C3D	11.62	156.47	128.52
5	A	305	CHL	CMD-C2D-C1D	11.37	144.74	124.71
5	C	309	CHL	OBD-CAD-C3D	-11.30	101.33	128.52
5	F	311	CHL	CMD-C2D-C3D	-11.27	101.69	127.61
5	B	306	CHL	CMD-C2D-C3D	-11.26	101.72	127.61
3	E	303	NEX	O24-C25-C38	11.25	128.53	115.06
3	C	303	NEX	C26-C27-C28	11.04	149.34	125.99
5	D	309	CHL	CAA-C2A-C1A	11.02	139.02	111.81
5	D	309	CHL	OBD-CAD-C3D	10.92	154.80	128.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	312	CHL	CMD-C2D-C1D	10.84	143.82	124.71
5	A	309	CHL	CMD-C2D-C1D	10.79	143.73	124.71
3	C	303	NEX	C20-C13-C12	10.69	134.91	118.08
5	E	317	CHL	OBD-CAD-C3D	10.64	154.12	128.52
5	D	313	CHL	CHB-C1B-NB	10.50	135.38	124.26
5	C	318	CHL	CHB-C1B-NB	10.42	135.28	124.26
5	F	304	CHL	CAA-C2A-C1A	10.34	145.86	111.97
5	C	309	CHL	CHB-C1B-NB	10.15	135.01	124.26
5	C	311	CHL	CHB-C1B-NB	10.09	134.94	124.26
3	C	303	NEX	C30-C31-C32	-10.02	91.95	123.22
5	A	313	CHL	CHB-C1B-NB	10.01	134.85	124.26
5	F	317	CHL	CMD-C2D-C1D	9.92	142.19	124.71
5	D	306	CHL	CMD-C2D-C1D	9.88	142.12	124.71
5	B	313	CHL	CMD-C2D-C3D	-9.87	104.92	127.61
5	A	318	CHL	CHB-C1B-NB	9.86	134.70	124.26
5	A	310	CHL	CHD-C1D-ND	9.85	133.51	124.45
5	E	308	CHL	CHB-C1B-NB	9.78	134.61	124.26
5	F	317	CHL	CHB-C1B-NB	9.65	134.47	124.26
5	B	310	CHL	CMD-C2D-C1D	9.62	141.67	124.71
3	C	303	NEX	C35-C15-C14	9.60	143.15	123.47
3	E	303	NEX	C35-C34-C33	-9.57	113.65	127.31
9	B	302	OUR	C5-C4-C3	-9.55	115.53	127.00
5	F	309	CHL	CHB-C1B-NB	9.54	134.36	124.26
5	A	305	CHL	CAA-C2A-C1A	9.51	143.12	111.97
5	B	319	CHL	CHB-C1B-NB	9.50	134.32	124.26
5	C	311	CHL	CHD-C1D-ND	9.50	133.18	124.45
5	D	305	CHL	CHD-C1D-ND	9.49	133.18	124.45
5	D	309	CHL	CHB-C1B-NB	9.47	134.28	124.26
5	D	312	CHL	CHB-C1B-NB	9.47	134.28	124.26
5	F	310	CHL	CHB-C1B-NB	9.40	134.21	124.26
5	E	317	CHL	CHB-C1B-NB	9.37	134.18	124.26
5	F	308	CHL	CHB-C1B-NB	9.34	134.14	124.26
5	D	318	CHL	CHD-C1D-ND	9.28	132.98	124.45
5	C	310	CHL	CHB-C1B-NB	9.28	134.08	124.26
5	B	314	CHL	CMD-C2D-C1D	9.27	141.04	124.71
3	A	303	NEX	C30-C31-C32	-9.23	94.43	123.22
3	C	303	NEX	C12-C13-C14	-9.20	104.82	118.94
5	B	311	CHL	CHB-C1B-NB	9.14	133.93	124.26
5	D	305	CHL	CHB-C1B-NB	9.12	133.91	124.26
3	C	303	NEX	C35-C34-C33	9.07	140.25	127.31
5	E	309	CHL	CHC-C4B-NB	9.05	133.84	124.26
5	D	312	CHL	CHC-C4B-NB	9.04	133.82	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	307	CHL	CMD-C2D-C1D	-8.98	108.89	124.71
5	E	310	CHL	CHD-C1D-ND	8.97	132.70	124.45
5	D	318	CHL	CHB-C1B-NB	8.96	133.74	124.26
5	B	311	CHL	OBD-CAD-C3D	8.94	150.03	128.52
5	E	309	CHL	CHD-C1D-ND	8.91	132.64	124.45
5	B	310	CHL	CHB-C1B-NB	8.89	133.67	124.26
5	C	318	CHL	CMD-C2D-C3D	-8.87	107.20	127.61
5	C	305	CHL	C4A-NA-C1A	8.82	110.67	106.71
5	C	312	CHL	CHB-C1B-NB	8.79	133.57	124.26
5	C	310	CHL	CHC-C4B-NB	8.79	133.56	124.26
5	F	317	CHL	CHD-C1D-ND	8.75	132.49	124.45
5	F	309	CHL	CHD-C1D-ND	8.72	132.47	124.45
5	C	306	CHL	CMD-C2D-C1D	-8.70	109.39	124.71
5	F	311	CHL	CHC-C4B-NB	8.69	133.46	124.26
5	A	311	CHL	CHB-C1B-NB	8.67	133.44	124.26
5	C	305	CHL	CMD-C2D-C1D	8.65	139.95	124.71
5	F	311	CHL	OBD-CAD-C3D	8.60	149.22	128.52
5	A	318	CHL	CHC-C4B-NB	8.60	133.36	124.26
5	C	312	CHL	CHD-C1D-ND	8.59	132.35	124.45
5	B	307	CHL	CMD-C2D-C3D	8.59	147.37	127.61
5	E	309	CHL	CHB-C1B-NB	8.54	133.30	124.26
5	D	310	CHL	CHB-C1B-NB	8.51	133.26	124.26
5	F	308	CHL	CHC-C4B-NB	8.51	133.26	124.26
5	E	305	CHL	CHB-C1B-NB	8.50	133.25	124.26
5	B	311	CHL	CAA-C2A-C1A	8.47	139.74	111.97
5	D	311	CHL	OBD-CAD-C3D	-8.46	108.17	128.52
5	B	312	CHL	CHB-C1B-NB	8.45	133.20	124.26
5	B	307	CHL	OBD-CAD-C3D	8.44	148.84	128.52
5	C	313	CHL	CHB-C1B-NB	8.44	133.19	124.26
5	B	319	CHL	CMD-C2D-C3D	-8.43	108.22	127.61
5	A	312	CHL	CHB-C1B-NB	8.43	133.18	124.26
5	A	311	CHL	CHD-C1D-ND	8.40	132.17	124.45
5	E	304	CHL	CAA-C2A-C1A	8.39	139.47	111.97
5	B	314	CHL	CHB-C1B-NB	8.39	133.14	124.26
5	A	305	CHL	C4A-NA-C1A	8.38	110.47	106.71
5	C	318	CHL	CHC-C4B-NB	8.35	133.09	124.26
5	A	305	CHL	CHB-C1B-NB	8.31	133.05	124.26
5	F	304	CHL	OBD-CAD-C3D	8.26	148.39	128.52
5	B	319	CHL	CHC-C4B-NB	8.19	132.92	124.26
5	D	310	CHL	CHC-C4B-NB	8.18	132.92	124.26
5	F	317	CHL	CHC-C4B-NB	8.17	132.91	124.26
5	C	306	CHL	CMD-C2D-C3D	8.16	146.38	127.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	306	CHL	CHD-C1D-ND	8.15	131.95	124.45
5	F	304	CHL	CMD-C2D-C3D	-8.11	108.97	127.61
5	B	306	CHL	C4A-NA-C1A	8.10	110.35	106.71
5	D	318	CHL	CHC-C4B-NB	8.10	132.83	124.26
3	C	303	NEX	C11-C12-C13	-8.09	103.68	126.42
5	C	305	CHL	CHB-C1B-NB	8.08	132.81	124.26
5	D	311	CHL	CHD-C1D-ND	8.07	131.87	124.45
5	A	312	CHL	CMD-C2D-C1D	-8.05	110.52	124.71
5	A	310	CHL	CMD-C2D-C1D	8.03	138.86	124.71
5	D	310	CHL	C4A-NA-C1A	7.97	110.29	106.71
5	A	309	CHL	CHB-C1B-NB	7.97	132.70	124.26
5	F	308	CHL	CMD-C2D-C1D	7.96	138.74	124.71
5	B	306	CHL	CHB-C1B-NB	7.95	132.67	124.26
5	B	319	CHL	CHD-C1D-ND	7.94	131.75	124.45
5	B	313	CHL	CHC-C4B-NB	7.91	132.63	124.26
3	E	303	NEX	C27-C28-C29	-7.91	113.26	125.53
5	B	311	CHL	CHC-C4B-NB	7.91	132.63	124.26
5	F	310	CHL	CHD-C1D-ND	7.90	131.72	124.45
5	C	312	CHL	CHC-C4B-NB	7.89	132.61	124.26
3	E	303	NEX	O24-C25-C24	7.86	119.29	113.38
5	B	313	CHL	CHB-C1B-NB	7.85	132.57	124.26
5	B	312	CHL	CHD-C1D-ND	7.85	131.66	124.45
5	A	318	CHL	CHD-C1D-ND	7.82	131.64	124.45
5	E	311	CHL	CHB-C1B-NB	7.81	132.52	124.26
5	D	310	CHL	CHD-C1D-ND	7.79	131.61	124.45
3	F	303	NEX	C30-C31-C32	-7.78	98.94	123.22
5	D	305	CHL	C4A-NA-C1A	7.77	110.20	106.71
3	F	303	NEX	O24-C25-C38	7.75	124.35	115.06
5	A	310	CHL	CHC-C4B-NB	7.75	132.47	124.26
5	D	310	CHL	CMD-C2D-C1D	7.75	138.36	124.71
5	A	312	CHL	CMD-C2D-C3D	7.72	145.38	127.61
5	B	313	CHL	CHD-C1D-ND	7.71	131.54	124.45
6	B	315	CLA	C4A-NA-C1A	7.68	110.16	106.71
5	C	310	CHL	CHD-C1D-ND	7.67	131.51	124.45
5	B	311	CHL	CMD-C2D-C3D	-7.66	110.00	127.61
5	B	312	CHL	C4A-NA-C1A	7.65	110.15	106.71
5	B	310	CHL	CAA-C2A-C1A	7.64	129.06	112.14
5	D	305	CHL	CHC-C4B-NB	7.64	132.34	124.26
5	F	308	CHL	CAA-C2A-C1A	7.63	130.66	111.81
5	D	312	CHL	C4A-NA-C1A	7.62	110.13	106.71
5	F	312	CHL	CHC-C4B-NB	7.62	132.32	124.26
5	A	310	CHL	OBD-CAD-C3D	7.60	146.82	128.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	312	CHL	CHC-C4B-NB	7.53	132.23	124.26
6	F	313	CLA	C4A-NA-C1A	7.53	110.09	106.71
5	A	309	CHL	C4A-NA-C1A	7.52	110.09	106.71
5	E	311	CHL	CHD-C1D-ND	7.51	131.35	124.45
5	C	318	CHL	CHD-C1D-ND	7.47	131.32	124.45
5	E	310	CHL	C4A-NA-C1A	7.47	110.06	106.71
5	E	304	CHL	CHB-C1B-NB	7.43	132.12	124.26
5	D	311	CHL	C4A-NA-C1A	7.42	110.04	106.71
5	E	312	CHL	CHB-C1B-NB	7.35	132.04	124.26
5	F	310	CHL	CHC-C4B-NB	7.35	132.04	124.26
5	C	311	CHL	CHC-C4B-NB	7.34	132.03	124.26
5	B	311	CHL	C4A-NA-C1A	7.30	109.99	106.71
5	E	312	CHL	C4A-NA-C1A	7.30	109.99	106.71
5	F	304	CHL	C4A-NA-C1A	7.28	109.98	106.71
5	C	306	CHL	CHC-C4B-NB	7.27	131.95	124.26
5	E	317	CHL	CHD-C1D-ND	7.26	131.12	124.45
5	B	312	CHL	CHC-C4B-NB	7.25	131.94	124.26
5	D	306	CHL	CHB-C1B-NB	7.23	131.91	124.26
6	B	308	CLA	C4A-NA-C1A	7.22	109.95	106.71
9	B	302	OUR	C5-C6-C7	7.21	146.67	126.42
5	F	305	CHL	CHB-C1B-NB	7.21	131.89	124.26
5	E	304	CHL	C4A-NA-C1A	7.20	109.94	106.71
5	F	311	CHL	CHB-C1B-NB	7.19	131.87	124.26
5	A	305	CHL	CHD-C1D-ND	7.19	131.06	124.45
5	B	311	CHL	CHD-C1D-ND	7.18	131.05	124.45
5	A	309	CHL	CAA-C2A-C1A	7.18	128.03	112.14
5	C	306	CHL	CHB-C1B-NB	7.16	131.83	124.26
5	A	310	CHL	CHB-C1B-NB	7.15	131.83	124.26
5	F	312	CHL	CHB-C1B-NB	7.14	131.82	124.26
6	A	316	CLA	C4A-NA-C1A	7.14	109.92	106.71
5	F	309	CHL	OBD-CAD-C3D	7.14	145.70	128.52
5	E	311	CHL	CHC-C4B-NB	7.13	131.81	124.26
5	A	312	CHL	CHD-C1D-ND	7.13	131.01	124.45
5	A	311	CHL	CMD-C2D-C3D	7.12	143.98	127.61
5	A	309	CHL	CHD-C1D-ND	7.11	130.99	124.45
3	A	303	NEX	C27-C28-C29	7.10	136.54	125.53
5	A	311	CHL	CMD-C2D-C1D	-7.09	112.22	124.71
5	D	309	CHL	CHC-C4B-NB	7.08	131.75	124.26
5	F	304	CHL	CHD-C1D-ND	7.08	130.96	124.45
5	F	309	CHL	C4A-NA-C1A	7.08	109.89	106.71
5	E	312	CHL	CHD-C1D-ND	7.08	130.96	124.45
5	A	305	CHL	CMD-C2D-C3D	-7.08	111.34	127.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	308	CHL	CHD-C1D-ND	7.06	130.94	124.45
3	E	303	NEX	C26-C27-C28	7.06	140.92	125.99
5	F	304	CHL	CHC-C4B-NB	7.06	131.73	124.26
5	E	310	CHL	CHB-C4A-NA	7.00	134.19	124.51
5	C	310	CHL	CMD-C2D-C1D	6.98	137.02	124.71
5	F	309	CHL	CHC-C4B-NB	6.97	131.63	124.26
5	C	313	CHL	CMD-C2D-C1D	6.96	136.99	124.71
5	B	310	CHL	CHC-C4B-NB	6.96	131.62	124.26
5	F	305	CHL	CHC-C4B-NB	6.95	131.62	124.26
5	D	313	CHL	CHC-C4B-NB	6.94	131.60	124.26
5	E	308	CHL	CHD-C1D-ND	6.93	130.82	124.45
3	A	303	NEX	C35-C34-C33	-6.91	117.45	127.31
6	C	307	CLA	C4A-NA-C1A	6.91	109.81	106.71
5	E	309	CHL	C4A-NA-C1A	6.89	109.80	106.71
5	B	307	CHL	CHB-C1B-NB	6.88	131.54	124.26
9	A	322	OUR	C43-C3-C4	-6.88	116.71	125.02
5	F	304	CHL	CHB-C1B-NB	6.87	131.53	124.26
5	E	310	CHL	CHB-C1B-NB	6.85	131.51	124.26
5	B	306	CHL	OBD-CAD-C3D	6.85	145.00	128.52
5	A	311	CHL	C4A-NA-C1A	6.85	109.78	106.71
6	D	316	CLA	C4A-NA-C1A	6.83	109.78	106.71
5	E	312	CHL	CHC-C4B-NB	6.83	131.49	124.26
5	C	313	CHL	CHC-C4B-NB	6.82	131.48	124.26
5	E	317	CHL	CHC-C4B-NB	6.82	131.47	124.26
5	E	312	CHL	OBD-CAD-C3D	6.81	144.91	128.52
5	A	309	CHL	CHC-C4B-NB	6.81	131.46	124.26
3	A	303	NEX	C35-C15-C14	6.81	137.41	123.47
6	E	316	CLA	C4A-NA-C1A	6.80	109.76	106.71
5	B	310	CHL	CHD-C1D-ND	6.79	130.69	124.45
6	C	316	CLA	C4A-NA-C1A	6.78	109.76	106.71
5	A	311	CHL	CHC-C4B-NB	6.78	131.43	124.26
5	C	311	CHL	C4A-NA-C1A	6.77	109.75	106.71
5	A	309	CHL	CMD-C2D-C3D	-6.75	112.08	127.61
9	B	325	OUR	C43-C3-C4	-6.75	116.86	125.02
5	B	319	CHL	C4A-NA-C1A	6.72	109.72	106.71
6	F	306	CLA	C4A-NA-C1A	6.71	109.72	106.71
5	A	306	CHL	CHB-C1B-NB	6.70	131.34	124.26
5	B	314	CHL	CHC-C4B-NB	6.68	131.33	124.26
9	B	302	OUR	C4-C5-C6	6.67	144.04	123.22
5	E	308	CHL	CHC-C4B-NB	6.67	131.32	124.26
5	E	308	CHL	C4A-NA-C1A	6.67	109.70	106.71
5	B	306	CHL	CHC-C4B-NB	6.66	131.31	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	321	0UR	C43-C3-C4	-6.61	117.03	125.02
5	D	309	CHL	CHD-C1D-ND	6.58	130.50	124.45
5	E	305	CHL	CHC-C4B-NB	6.58	131.22	124.26
9	B	302	0UR	C9-C8-C7	-6.56	117.94	127.31
6	E	315	CLA	C4A-NA-C1A	6.54	109.65	106.71
3	E	303	NEX	C38-C25-C26	-6.53	111.32	122.26
5	E	312	CHL	CMD-C2D-C3D	-6.52	112.62	127.61
5	F	311	CHL	CHD-C1D-ND	6.52	130.44	124.45
6	F	316	CLA	C4A-NA-C1A	6.51	109.64	106.71
5	D	313	CHL	CMD-C2D-C1D	6.51	136.19	124.71
5	C	310	CHL	C4A-NA-C1A	6.51	109.63	106.71
5	C	318	CHL	C4A-NA-C1A	6.49	109.62	106.71
6	F	307	CLA	C4A-NA-C1A	6.49	109.62	106.71
3	D	303	NEX	C35-C15-C14	-6.48	110.20	123.47
5	E	310	CHL	CHC-C4B-NB	6.47	131.11	124.26
5	A	305	CHL	CHC-C4B-NB	6.46	131.09	124.26
6	B	316	CLA	C4A-NA-C1A	6.43	109.60	106.71
6	C	317	CLA	C4A-NA-C1A	6.41	109.59	106.71
5	D	311	CHL	CHB-C4A-NA	6.40	133.36	124.51
6	B	317	CLA	C4A-NA-C1A	6.39	109.58	106.71
5	E	311	CHL	C4A-NA-C1A	6.39	109.58	106.71
5	E	317	CHL	C4A-NA-C1A	6.38	109.57	106.71
5	C	313	CHL	C4A-NA-C1A	6.36	109.56	106.71
6	E	306	CLA	C4A-NA-C1A	6.36	109.56	106.71
5	C	309	CHL	CHC-C4B-NB	6.34	130.97	124.26
5	F	317	CHL	C1D-ND-C4D	6.33	110.83	106.33
3	A	303	NEX	C11-C12-C13	-6.33	108.62	126.42
5	E	317	CHL	CBD-CHA-C1A	6.33	135.96	128.50
6	A	307	CLA	C4A-NA-C1A	6.32	109.55	106.71
6	E	314	CLA	C4A-NA-C1A	6.31	109.54	106.71
6	C	314	CLA	C4A-NA-C1A	6.31	109.54	106.71
5	A	306	CHL	CHC-C4B-NB	6.30	130.92	124.26
5	D	318	CHL	C1D-ND-C4D	6.28	110.80	106.33
6	F	315	CLA	C4A-NA-C1A	6.27	109.53	106.71
5	E	304	CHL	CHC-C4B-NB	6.26	130.89	124.26
5	E	308	CHL	CBD-CHA-C1A	6.26	135.88	128.50
6	D	317	CLA	C4A-NA-C1A	6.24	109.51	106.71
5	D	305	CHL	C1D-ND-C4D	6.22	110.76	106.33
2	A	301	0IE	C20-C3-C4	-6.22	116.83	124.83
6	B	318	CLA	C4A-NA-C1A	6.20	109.49	106.71
5	F	312	CHL	C4A-NA-C1A	6.20	109.49	106.71
5	B	319	CHL	C1D-ND-C4D	6.19	110.73	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	307	CHL	CHC-C4B-NB	6.19	130.81	124.26
5	C	305	CHL	CHC-C4B-NB	6.17	130.79	124.26
5	F	317	CHL	CMD-C2D-C3D	-6.14	113.48	127.61
6	D	307	CLA	C4A-NA-C1A	6.13	109.46	106.71
5	C	312	CHL	C4A-NA-C1A	6.12	109.46	106.71
5	C	306	CHL	CHD-C1D-ND	6.09	130.05	124.45
3	A	303	NEX	C38-C25-C26	-6.09	112.06	122.26
5	B	314	CHL	C4A-NA-C1A	6.09	109.44	106.71
9	C	321	OUR	C43-C3-C4	-6.07	117.68	125.02
5	A	311	CHL	CHB-C4A-NA	6.07	132.90	124.51
2	A	301	OIE	C4-C3-C2	6.06	125.28	120.08
5	D	318	CHL	C4A-NA-C1A	6.06	109.43	106.71
6	A	317	CLA	C4A-NA-C1A	6.06	109.43	106.71
5	C	313	CHL	CHD-C1D-ND	6.06	130.02	124.45
5	D	312	CHL	CHD-C1D-ND	6.05	130.02	124.45
6	A	315	CLA	C4A-NA-C1A	6.05	109.43	106.71
5	B	306	CHL	C1D-ND-C4D	6.05	110.63	106.33
5	A	305	CHL	OBD-CAD-C3D	6.03	143.02	128.52
6	C	308	CLA	C4A-NA-C1A	6.03	109.42	106.71
5	F	308	CHL	C4A-NA-C1A	6.02	109.41	106.71
5	F	317	CHL	C4A-NA-C1A	6.00	109.41	106.71
5	E	311	CHL	CHB-C4A-NA	6.00	132.81	124.51
3	C	303	NEX	C38-C25-C26	-5.98	112.25	122.26
5	A	306	CHL	C4A-NA-C1A	5.95	109.38	106.71
5	D	306	CHL	CMD-C2D-C3D	-5.95	113.93	127.61
6	F	314	CLA	C4A-NA-C1A	5.94	109.38	106.71
6	D	308	CLA	C4A-NA-C1A	5.94	109.38	106.71
3	D	303	NEX	C38-C25-C26	-5.93	112.32	122.26
9	C	321	OUR	C29-C30-C31	-5.91	105.01	111.74
3	E	303	NEX	C31-C30-C29	-5.91	118.88	127.31
5	B	307	CHL	CHC-C1C-NC	5.89	133.15	124.20
5	D	306	CHL	CHB-C4A-NA	5.89	132.65	124.51
5	C	311	CHL	C2C-C3C-C4C	-5.88	102.30	106.49
3	E	303	NEX	C30-C31-C32	-5.88	104.86	123.22
5	F	305	CHL	C1-O2A-CGA	5.87	131.86	116.44
3	D	303	NEX	C27-C28-C29	-5.87	116.42	125.53
6	C	315	CLA	C4A-NA-C1A	5.86	109.34	106.71
2	A	302	OIE	C10-C9-C8	5.86	135.47	123.47
5	A	309	CHL	CHB-C4A-NA	5.85	132.60	124.51
5	C	318	CHL	O2D-CGD-CBD	5.85	121.66	111.27
6	E	307	CLA	C4A-NA-C1A	5.84	109.33	106.71
6	A	314	CLA	C4A-NA-C1A	5.83	109.33	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	319	CHL	O2D-CGD-CBD	5.82	121.61	111.27
3	B	303	NEX	C26-C27-C28	-5.81	113.70	125.99
5	D	311	CHL	CHB-C1B-NB	5.81	130.41	124.26
5	C	305	CHL	CHD-C1D-ND	5.81	129.79	124.45
5	B	310	CHL	CMD-C2D-C3D	-5.80	114.26	127.61
5	B	313	CHL	C4A-NA-C1A	5.79	109.31	106.71
3	B	303	NEX	C38-C25-C26	-5.78	112.58	122.26
6	B	309	CLA	C4A-NA-C1A	5.77	109.30	106.71
9	F	320	OUR	C43-C3-C4	-5.76	118.05	125.02
3	D	303	NEX	C15-C14-C13	-5.75	119.10	127.31
5	A	312	CHL	C4A-NA-C1A	5.75	109.29	106.71
3	F	303	NEX	C38-C25-C26	-5.74	112.64	122.26
5	D	313	CHL	C4A-NA-C1A	5.74	109.28	106.71
5	F	317	CHL	OBD-CAD-C3D	5.73	142.32	128.52
6	D	315	CLA	C4A-NA-C1A	5.69	109.27	106.71
5	D	306	CHL	CHC-C4B-NB	5.69	130.28	124.26
5	E	304	CHL	CHD-C1D-ND	5.69	129.68	124.45
5	C	312	CHL	C1D-ND-C4D	5.68	110.37	106.33
5	A	313	CHL	CHC-C4B-NB	5.67	130.26	124.26
3	E	303	NEX	C11-C10-C9	-5.66	119.23	127.31
5	E	312	CHL	CHB-C4A-NA	5.66	132.34	124.51
5	D	313	CHL	CHD-C1D-ND	5.66	129.65	124.45
5	E	304	CHL	CHB-C4A-NA	5.65	132.32	124.51
5	A	306	CHL	CHB-C4A-NA	5.65	132.32	124.51
5	F	317	CHL	CAA-C2A-C1A	5.64	130.46	111.97
5	D	306	CHL	CHD-C1D-ND	5.64	129.63	124.45
5	A	313	CHL	C1D-CHD-C4C	-5.64	113.90	126.06
5	F	310	CHL	C4A-NA-C1A	5.63	109.24	106.71
6	E	313	CLA	C4A-NA-C1A	5.63	109.24	106.71
6	A	308	CLA	C4A-NA-C1A	5.62	109.23	106.71
9	B	302	OUR	C48-C47-C46	-5.61	119.47	125.84
5	C	305	CHL	CHB-C4A-NA	5.61	132.26	124.51
5	E	311	CHL	CMD-C2D-C3D	5.60	140.50	127.61
5	C	309	CHL	CHD-C1D-ND	5.60	129.60	124.45
5	E	305	CHL	CHD-C1D-ND	5.60	129.60	124.45
5	E	308	CHL	C1D-ND-C4D	5.59	110.31	106.33
5	A	318	CHL	C1D-ND-C4D	5.59	110.31	106.33
5	F	309	CHL	CAA-C2A-C1A	5.59	125.61	111.81
5	A	318	CHL	C4A-NA-C1A	5.57	109.21	106.71
5	C	309	CHL	C4A-NA-C1A	5.57	109.21	106.71
5	A	310	CHL	C4A-NA-C1A	5.54	109.20	106.71
5	C	311	CHL	C1D-ND-C4D	5.54	110.27	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	317	CHL	O2D-CGD-CBD	5.54	121.11	111.27
5	D	313	CHL	O2D-CGD-CBD	5.53	121.10	111.27
2	D	301	0IE	C20-C3-C4	-5.52	117.73	124.83
5	F	310	CHL	O2D-CGD-CBD	5.52	121.07	111.27
5	A	309	CHL	C1D-ND-C4D	5.50	110.24	106.33
5	C	318	CHL	C1D-ND-C4D	5.50	110.24	106.33
9	E	320	0UR	C29-C30-C31	-5.47	105.51	111.74
5	C	318	CHL	OBD-CAD-C3D	5.46	141.66	128.52
5	B	312	CHL	CMD-C2D-C1D	5.45	134.32	124.71
5	B	310	CHL	O2D-CGD-CBD	5.44	120.94	111.27
5	C	313	CHL	C1D-ND-C4D	5.44	110.20	106.33
5	A	311	CHL	C2C-C3C-C4C	-5.44	102.61	106.49
5	C	309	CHL	CAA-C2A-C1A	5.41	125.17	111.81
5	D	309	CHL	O2D-CGD-CBD	5.41	120.88	111.27
5	F	305	CHL	CHD-C4C-C3C	-5.40	116.90	124.84
5	F	305	CHL	O2D-CGD-CBD	5.40	120.86	111.27
5	D	309	CHL	C4A-NA-C1A	5.39	109.13	106.71
2	A	302	0IE	C20-C3-C4	-5.39	117.90	124.83
5	B	310	CHL	CHB-C4A-NA	5.39	131.97	124.51
5	E	310	CHL	C2C-C3C-C4C	-5.38	102.65	106.49
5	D	310	CHL	C1D-ND-C4D	5.38	110.16	106.33
5	B	306	CHL	C1D-CHD-C4C	-5.36	114.49	126.06
5	E	317	CHL	O2D-CGD-CBD	5.36	120.79	111.27
5	B	314	CHL	CHD-C4C-C3C	-5.34	116.99	124.84
5	B	310	CHL	C4A-NA-C1A	5.33	109.10	106.71
5	E	309	CHL	C1D-ND-C4D	5.33	110.12	106.33
5	D	311	CHL	C1D-ND-C4D	5.32	110.12	106.33
5	D	313	CHL	C1D-CHD-C4C	-5.32	114.58	126.06
5	A	312	CHL	C1D-ND-C4D	5.31	110.10	106.33
5	F	309	CHL	C1D-ND-C4D	5.30	110.10	106.33
5	D	310	CHL	O2D-CGD-CBD	5.30	120.68	111.27
5	B	306	CHL	CHB-C4A-NA	5.28	131.81	124.51
5	E	311	CHL	CMD-C2D-C1D	-5.27	115.42	124.71
3	F	303	NEX	C38-C25-C24	-5.27	108.35	114.28
3	F	303	NEX	C15-C14-C13	-5.27	119.79	127.31
5	F	308	CHL	O2D-CGD-CBD	5.27	120.62	111.27
3	B	303	NEX	C11-C10-C9	-5.26	119.80	127.31
5	A	309	CHL	O2D-CGD-CBD	5.24	120.58	111.27
5	B	311	CHL	O2D-CGD-CBD	5.24	120.57	111.27
5	D	311	CHL	O2D-CGD-CBD	5.23	120.56	111.27
5	C	305	CHL	C1D-ND-C4D	5.22	110.04	106.33
5	F	304	CHL	C1D-CHD-C4C	-5.22	114.80	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	303	NEX	C11-C10-C9	-5.22	119.86	127.31
5	A	318	CHL	O2D-CGD-CBD	5.21	120.53	111.27
5	D	306	CHL	C1D-CHD-C4C	-5.21	114.82	126.06
5	F	310	CHL	CHB-C4A-NA	5.19	131.69	124.51
5	F	304	CHL	CHB-C4A-NA	5.19	131.69	124.51
5	A	305	CHL	C1D-ND-C4D	5.19	110.02	106.33
5	E	312	CHL	C1D-CHD-C4C	-5.19	114.87	126.06
3	C	303	NEX	C15-C14-C13	-5.18	119.91	127.31
5	C	309	CHL	O2D-CGD-CBD	5.17	120.46	111.27
6	D	314	CLA	C4A-NA-C1A	5.17	109.03	106.71
5	D	312	CHL	CMD-C2D-C3D	5.17	139.51	127.61
5	E	317	CHL	C1D-ND-C4D	5.16	110.00	106.33
9	B	302	OUR	C6-C7-C8	5.16	126.86	118.94
3	D	303	NEX	C11-C12-C13	5.16	140.91	126.42
5	A	310	CHL	C1D-CHD-C4C	-5.16	114.94	126.06
5	E	310	CHL	O2D-CGD-CBD	5.15	120.43	111.27
5	C	310	CHL	C1D-ND-C4D	5.15	110.00	106.33
5	A	310	CHL	C1D-ND-C4D	5.15	109.99	106.33
5	E	310	CHL	C1D-CHD-C4C	-5.15	114.96	126.06
5	D	312	CHL	C1D-ND-C4D	5.14	109.99	106.33
5	E	308	CHL	O2D-CGD-CBD	5.13	120.38	111.27
5	F	312	CHL	CHD-C1D-ND	5.13	129.17	124.45
5	F	311	CHL	CHB-C4A-NA	5.13	131.60	124.51
5	F	311	CHL	C4A-NA-C1A	5.12	109.01	106.71
5	B	314	CHL	C1D-CHD-C4C	-5.12	115.01	126.06
5	F	312	CHL	C1D-CHD-C4C	-5.12	115.01	126.06
5	B	311	CHL	C1D-ND-C4D	5.12	109.97	106.33
5	D	309	CHL	C1D-ND-C4D	5.12	109.97	106.33
5	A	306	CHL	CHD-C4C-C3C	-5.11	117.33	124.84
5	A	305	CHL	CHB-C4A-NA	5.10	131.57	124.51
5	F	309	CHL	CMD-C2D-C1D	5.10	133.70	124.71
3	C	303	NEX	C11-C10-C9	-5.09	120.04	127.31
5	F	309	CHL	C2C-C3C-C4C	-5.09	102.86	106.49
3	A	303	NEX	C15-C35-C34	5.09	133.90	123.47
5	F	308	CHL	C1D-ND-C4D	5.09	109.95	106.33
5	B	313	CHL	C1D-ND-C4D	5.08	109.95	106.33
5	E	312	CHL	C1D-ND-C4D	5.08	109.94	106.33
5	A	311	CHL	C1D-ND-C4D	5.08	109.94	106.33
5	B	310	CHL	C1D-ND-C4D	5.07	109.94	106.33
9	F	320	OUR	C29-C30-C31	-5.07	105.97	111.74
5	A	306	CHL	CHD-C1D-ND	5.07	129.12	124.45
5	C	311	CHL	C1D-CHD-C4C	-5.07	115.12	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	309	CHL	C1D-ND-C4D	5.06	109.93	106.33
5	A	313	CHL	O2D-CGD-CBD	5.06	120.26	111.27
9	B	325	OUR	C29-C30-C31	-5.06	105.98	111.74
2	E	301	OIE	C20-C3-C4	-5.04	118.34	124.83
5	B	307	CHL	CHB-C4A-NA	5.04	131.48	124.51
3	F	303	NEX	C11-C10-C9	-5.04	120.12	127.31
9	D	321	OUR	C29-C30-C31	-5.03	106.02	111.74
5	E	309	CHL	O2D-CGD-CBD	5.00	120.16	111.27
5	C	305	CHL	CMD-C2D-C3D	-4.99	116.13	127.61
3	B	303	NEX	C38-C25-C24	-4.99	108.66	114.28
5	E	310	CHL	C1D-ND-C4D	4.99	109.88	106.33
5	E	304	CHL	C1D-CHD-C4C	-4.98	115.31	126.06
5	B	307	CHL	O2D-CGD-CBD	4.98	120.12	111.27
5	D	306	CHL	C1-C2-C3	-4.98	117.43	126.04
9	E	320	OUR	C43-C3-C4	-4.98	119.00	125.02
5	E	304	CHL	OBD-CAD-C3D	4.98	140.50	128.52
5	D	305	CHL	CHB-C4A-NA	4.97	131.38	124.51
5	A	312	CHL	CHB-C4A-NA	4.95	131.35	124.51
5	F	311	CHL	O2D-CGD-CBD	4.94	120.04	111.27
5	A	305	CHL	C1D-CHD-C4C	-4.93	115.41	126.06
5	D	318	CHL	O2D-CGD-CBD	4.93	120.03	111.27
2	A	302	OIE	C4-C3-C2	4.93	124.30	120.08
5	B	312	CHL	O2D-CGD-CBD	4.93	120.02	111.27
5	D	313	CHL	CHD-C4C-C3C	-4.92	117.61	124.84
5	F	312	CHL	CHB-C4A-NA	4.92	131.31	124.51
5	B	307	CHL	C4B-CHC-C1C	-4.91	114.69	126.34
5	B	314	CHL	CMD-C2D-C3D	-4.91	116.32	127.61
5	B	314	CHL	CHD-C4C-NC	4.91	131.94	124.20
5	F	312	CHL	CHD-C4C-C3C	-4.91	117.62	124.84
3	B	303	NEX	C15-C14-C13	-4.91	120.30	127.31
5	C	311	CHL	O2D-CGD-CBD	4.90	119.98	111.27
5	A	306	CHL	C1D-CHD-C4C	-4.90	115.49	126.06
5	F	309	CHL	O2D-CGD-CBD	4.90	119.97	111.27
3	F	303	NEX	C35-C15-C14	4.89	133.49	123.47
7	B	324	LHG	O7-C7-C8	4.89	122.04	111.50
5	B	310	CHL	C3A-C2A-C1A	-4.89	94.02	101.34
5	A	313	CHL	CHD-C4C-C3C	-4.87	117.68	124.84
5	B	312	CHL	C1D-ND-C4D	4.87	109.79	106.33
5	E	317	CHL	C2C-C3C-C4C	-4.87	103.02	106.49
5	F	305	CHL	CHB-C4A-NA	4.86	131.24	124.51
5	C	313	CHL	C1D-CHD-C4C	-4.86	115.57	126.06
5	D	305	CHL	C1D-CHD-C4C	-4.85	115.58	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	312	CHL	O2D-CGD-CBD	4.85	119.89	111.27
5	E	317	CHL	C1D-CHD-C4C	-4.85	115.60	126.06
5	E	311	CHL	C1D-ND-C4D	4.83	109.77	106.33
5	A	310	CHL	CMD-C2D-C3D	-4.83	116.50	127.61
3	A	303	NEX	C15-C14-C13	-4.82	120.43	127.31
5	E	311	CHL	C1D-CHD-C4C	-4.81	115.67	126.06
5	B	311	CHL	C1D-CHD-C4C	-4.81	115.68	126.06
5	B	313	CHL	CHB-C4A-NA	4.81	131.16	124.51
5	E	304	CHL	C1D-ND-C4D	4.81	109.75	106.33
5	F	304	CHL	C1D-ND-C4D	4.81	109.75	106.33
5	D	306	CHL	O2D-CGD-CBD	4.81	119.81	111.27
3	C	303	NEX	C31-C30-C29	-4.80	120.47	127.31
5	C	306	CHL	CHB-C4A-NA	4.80	131.14	124.51
2	D	301	OIE	C4-C3-C2	4.79	124.19	120.08
5	F	309	CHL	C1D-CHD-C4C	-4.79	115.72	126.06
5	B	310	CHL	C1C-C2C-C3C	-4.79	103.31	107.11
5	B	312	CHL	C2C-C3C-C4C	-4.79	103.08	106.49
5	C	310	CHL	C1D-CHD-C4C	-4.78	115.74	126.06
5	D	312	CHL	C1C-C2C-C3C	-4.78	103.32	107.11
5	B	307	CHL	C4A-NA-C1A	4.78	108.85	106.71
5	C	305	CHL	C1D-CHD-C4C	-4.78	115.76	126.06
5	D	305	CHL	O2D-CGD-CBD	4.77	119.75	111.27
5	B	312	CHL	C1D-CHD-C4C	-4.77	115.77	126.06
5	C	306	CHL	C1D-ND-C4D	4.77	109.72	106.33
5	E	309	CHL	C1D-CHD-C4C	-4.76	115.78	126.06
5	E	305	CHL	CHB-C4A-NA	4.75	131.08	124.51
5	D	306	CHL	CHD-C4C-C3C	-4.75	117.86	124.84
5	B	307	CHL	CHD-C4C-NC	4.75	131.68	124.20
3	D	303	NEX	C38-C25-C24	-4.75	108.94	114.28
5	C	310	CHL	O2D-CGD-CBD	4.73	119.68	111.27
5	A	306	CHL	OBD-CAD-C3D	4.73	139.91	128.52
5	A	305	CHL	CHC-C1C-NC	4.73	131.38	124.20
5	A	311	CHL	O2D-CGD-CBD	4.73	119.67	111.27
5	B	312	CHL	CHB-C4A-NA	4.73	131.05	124.51
5	E	309	CHL	C1C-C2C-C3C	-4.72	103.37	107.11
5	F	305	CHL	C1D-CHD-C4C	-4.71	115.89	126.06
5	C	306	CHL	C1D-CHD-C4C	-4.71	115.91	126.06
9	B	325	OURL	C5-C4-C3	-4.70	121.36	127.00
5	A	310	CHL	O2D-CGD-CBD	4.69	119.61	111.27
5	C	312	CHL	CHB-C4A-NA	4.69	131.00	124.51
2	F	301	OIE	C20-C3-C4	-4.68	118.81	124.83
5	D	318	CHL	C1D-CHD-C4C	-4.68	115.97	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	313	CHL	O2D-CGD-CBD	4.68	119.58	111.27
5	C	311	CHL	CHB-C4A-NA	4.68	130.98	124.51
3	B	303	NEX	C31-C30-C29	-4.66	120.66	127.31
3	B	303	NEX	C30-C31-C32	-4.66	108.67	123.22
5	A	318	CHL	C1D-CHD-C4C	-4.66	116.01	126.06
5	D	311	CHL	C1D-CHD-C4C	-4.66	116.01	126.06
5	F	310	CHL	C1D-CHD-C4C	-4.66	116.01	126.06
5	C	305	CHL	O2D-CGD-CBD	4.65	119.53	111.27
5	E	305	CHL	O2D-CGD-CBD	4.64	119.52	111.27
5	A	305	CHL	O2D-CGD-CBD	4.64	119.50	111.27
5	D	310	CHL	C1D-CHD-C4C	-4.63	116.06	126.06
3	A	303	NEX	C31-C30-C29	-4.63	120.70	127.31
5	A	306	CHL	O2D-CGD-CBD	4.63	119.49	111.27
5	B	310	CHL	C1D-CHD-C4C	-4.62	116.10	126.06
5	B	312	CHL	OBD-CAD-C3D	-4.61	117.42	128.52
5	F	305	CHL	CHD-C4C-NC	4.61	131.47	124.20
5	D	312	CHL	CMD-C2D-C1D	-4.61	116.58	124.71
3	E	303	NEX	C15-C14-C13	-4.61	120.73	127.31
5	A	306	CHL	C1C-C2C-C3C	-4.61	103.46	107.11
5	E	312	CHL	O2D-CGD-CBD	4.61	119.45	111.27
3	C	303	NEX	C38-C25-C24	-4.61	109.10	114.28
5	E	311	CHL	OBD-CAD-C3D	-4.60	117.45	128.52
5	C	306	CHL	O2D-CGD-CBD	4.60	119.44	111.27
5	D	311	CHL	C4D-CHA-C1A	-4.60	115.66	121.25
5	B	307	CHL	C1D-CHD-C4C	-4.59	116.15	126.06
3	A	303	NEX	O24-C25-C38	4.59	120.56	115.06
5	F	305	CHL	O2A-C1-C2	4.59	120.69	108.64
5	C	313	CHL	CHB-C4A-NA	4.59	130.86	124.51
5	D	313	CHL	C1C-C2C-C3C	-4.59	103.47	107.11
5	D	311	CHL	C2C-C3C-C4C	-4.58	103.22	106.49
5	A	312	CHL	OBD-CAD-C3D	-4.58	117.50	128.52
3	A	303	NEX	C38-C25-C24	-4.58	109.13	114.28
5	F	312	CHL	CHD-C4C-NC	4.57	131.41	124.20
5	D	318	CHL	C4D-CHA-C1A	-4.57	115.69	121.25
5	F	308	CHL	C1D-CHD-C4C	-4.57	116.21	126.06
5	A	309	CHL	C1D-CHD-C4C	-4.56	116.21	126.06
5	D	305	CHL	C2C-C3C-C4C	-4.56	103.24	106.49
5	F	310	CHL	C2C-C3C-C4C	-4.56	103.24	106.49
5	B	314	CHL	CHB-C4A-NA	4.56	130.82	124.51
5	A	313	CHL	C4A-NA-C1A	4.56	108.75	106.71
5	E	311	CHL	C2C-C3C-C4C	-4.56	103.24	106.49
5	F	310	CHL	C1D-ND-C4D	4.55	109.57	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	313	CHL	C1D-ND-C4D	4.55	109.57	106.33
5	A	311	CHL	C1D-CHD-C4C	-4.55	116.25	126.06
5	D	312	CHL	C1D-CHD-C4C	-4.55	116.25	126.06
5	A	310	CHL	C2C-C3C-C4C	-4.54	103.25	106.49
5	F	308	CHL	CMD-C2D-C3D	-4.54	117.17	127.61
5	C	310	CHL	C1C-C2C-C3C	-4.54	103.51	107.11
5	B	311	CHL	C1C-C2C-C3C	-4.54	103.51	107.11
5	C	312	CHL	CMD-C2D-C1D	4.54	132.71	124.71
5	E	310	CHL	CHC-C1C-NC	4.53	131.07	124.20
5	E	305	CHL	C1D-CHD-C4C	-4.52	116.31	126.06
9	A	322	0UR	O44-C45-C46	4.51	123.54	111.55
5	B	313	CHL	C1D-CHD-C4C	-4.50	116.34	126.06
5	E	308	CHL	CHB-C4A-NA	4.50	130.73	124.51
5	F	311	CHL	C1D-CHD-C4C	-4.49	116.36	126.06
5	E	310	CHL	C4D-CHA-C1A	-4.49	115.78	121.25
2	F	301	0IE	C10-C9-C8	4.48	132.66	123.47
9	E	320	0UR	C4-C3-C2	-4.48	116.23	120.08
5	D	310	CHL	CMD-C2D-C3D	-4.48	117.31	127.61
5	F	311	CHL	C1D-ND-C4D	4.48	109.52	106.33
5	F	305	CHL	C4A-NA-C1A	4.47	108.71	106.71
5	F	311	CHL	C1C-C2C-C3C	-4.46	103.57	107.11
5	A	312	CHL	C1D-CHD-C4C	-4.44	116.47	126.06
5	F	308	CHL	C1C-C2C-C3C	-4.44	103.59	107.11
5	C	318	CHL	C2C-C3C-C4C	-4.44	103.33	106.49
5	A	311	CHL	C4D-CHA-C1A	-4.43	115.86	121.25
5	D	310	CHL	C1C-C2C-C3C	-4.43	103.60	107.11
5	D	306	CHL	CHC-C1C-NC	4.42	130.92	124.20
5	E	308	CHL	C1D-CHD-C4C	-4.42	116.53	126.06
5	F	317	CHL	C1D-CHD-C4C	-4.42	116.53	126.06
9	B	302	0UR	C43-C3-C4	-4.42	119.68	125.02
5	C	318	CHL	C1D-CHD-C4C	-4.42	116.53	126.06
5	D	309	CHL	C1C-C2C-C3C	-4.41	103.61	107.11
5	F	312	CHL	C1D-ND-C4D	4.41	109.47	106.33
5	E	308	CHL	C2C-C3C-C4C	-4.41	103.34	106.49
5	F	317	CHL	C2C-C3C-C4C	-4.40	103.36	106.49
5	A	318	CHL	CMD-C2D-C1D	4.38	132.43	124.71
5	A	305	CHL	C4D-CHA-C1A	-4.38	115.92	121.25
3	B	303	NEX	O24-C25-C38	4.38	120.30	115.06
5	E	305	CHL	C1D-ND-C4D	4.37	109.44	106.33
5	A	310	CHL	CHB-C4A-NA	4.37	130.56	124.51
5	B	307	CHL	C1-C2-C3	-4.37	118.49	126.04
5	F	317	CHL	CHB-C4A-NA	4.37	130.55	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	305	CHL	C4B-CHC-C1C	-4.37	115.98	126.34
5	C	306	CHL	C1-C2-C3	-4.37	118.49	126.04
5	A	318	CHL	C1C-C2C-C3C	-4.36	103.65	107.11
5	A	313	CHL	CHD-C4C-NC	4.36	131.08	124.20
5	B	319	CHL	C1D-CHD-C4C	-4.35	116.66	126.06
5	B	307	CHL	C1C-C2C-C3C	-4.35	103.66	107.11
9	B	302	OUR	C29-C30-C31	-4.35	106.79	111.74
2	E	301	OIE	C23-C16-C15	-4.34	116.84	122.92
5	C	309	CHL	CHB-C4A-NA	4.33	130.50	124.51
5	E	304	CHL	CHC-C1C-NC	4.32	130.76	124.20
2	F	302	OIE	C20-C3-C4	-4.32	119.28	124.83
5	D	305	CHL	OBD-CAD-C3D	-4.31	118.15	128.52
5	B	306	CHL	C4D-CHA-C1A	-4.31	116.01	121.25
5	F	312	CHL	C1C-C2C-C3C	-4.30	103.70	107.11
2	E	302	OIE	C23-C16-C15	-4.30	116.90	122.92
5	D	309	CHL	C1D-CHD-C4C	-4.30	116.78	126.06
5	C	312	CHL	C1D-CHD-C4C	-4.30	116.79	126.06
3	D	303	NEX	C31-C30-C29	-4.30	121.18	127.31
2	C	302	OIE	C20-C3-C4	-4.29	119.31	124.83
2	A	302	OIE	C6-C7-C8	4.29	125.53	118.94
9	A	322	OUR	C10-C11-C12	-4.29	121.19	127.31
5	B	307	CHL	CHD-C4C-C3C	-4.29	118.54	124.84
5	D	318	CHL	C1C-C2C-C3C	-4.27	103.72	107.11
2	F	302	OIE	C9-C10-C11	4.27	132.23	123.47
2	D	301	OIE	C23-C16-C15	-4.27	116.94	122.92
5	D	310	CHL	CHB-C4A-NA	4.27	130.41	124.51
5	C	310	CHL	CHB-C4A-NA	4.26	130.41	124.51
9	B	325	OUR	C34-C27-C1	-4.26	118.90	124.49
5	F	305	CHL	C1C-C2C-C3C	-4.26	103.73	107.11
2	B	301	OIE	C23-C16-C15	-4.26	116.96	122.92
5	F	308	CHL	CHB-C4A-NA	4.26	130.40	124.51
2	B	301	OIE	C20-C3-C4	-4.26	119.36	124.83
5	B	314	CHL	C1D-ND-C4D	4.25	109.35	106.33
9	A	322	OUR	C34-C27-C1	-4.25	118.92	124.49
5	D	309	CHL	CHB-C4A-NA	4.24	130.38	124.51
5	C	318	CHL	CHB-C1B-C2B	-4.24	115.26	127.24
7	E	318	LHG	O4-P-O5	4.24	133.19	112.24
5	C	306	CHL	C4A-NA-C1A	4.24	108.61	106.71
5	F	304	CHL	C1C-C2C-C3C	-4.23	103.75	107.11
5	A	310	CHL	C4D-CHA-C1A	-4.22	116.11	121.25
5	A	306	CHL	CHD-C4C-NC	4.21	130.84	124.20
5	C	309	CHL	C2C-C3C-C4C	-4.21	103.49	106.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	313	CHL	O2D-CGD-CBD	4.21	118.75	111.27
5	F	310	CHL	C1C-C2C-C3C	-4.21	103.78	107.11
5	C	309	CHL	C1D-CHD-C4C	-4.20	116.99	126.06
9	A	322	OUR	C5-C4-C3	-4.20	121.96	127.00
5	D	312	CHL	CHB-C4A-NA	4.19	130.31	124.51
5	A	313	CHL	CHB-C1B-C2B	-4.18	115.42	127.24
7	C	304	LHG	O4-P-O5	4.18	132.92	112.24
6	C	307	CLA	O2D-CGD-O1D	-4.18	115.66	123.84
5	E	304	CHL	C1C-C2C-C3C	-4.18	103.80	107.11
7	C	319	LHG	O4-P-O5	4.18	132.90	112.24
3	C	303	NEX	O24-C25-C38	4.18	120.06	115.06
5	D	318	CHL	CHB-C4A-NA	4.18	130.29	124.51
2	F	301	OIE	C23-C16-C15	-4.18	117.07	122.92
7	B	320	LHG	O4-P-O5	4.17	132.88	112.24
5	B	314	CHL	O2D-CGD-CBD	4.17	118.68	111.27
5	C	318	CHL	C1C-C2C-C3C	-4.17	103.81	107.11
9	E	320	OUR	C34-C27-C1	-4.16	119.02	124.49
9	B	325	OUR	O44-C45-C46	4.16	122.62	111.55
5	B	313	CHL	C1C-C2C-C3C	-4.16	103.81	107.11
9	B	302	OUR	C20-C7-C8	-4.15	117.11	122.92
5	B	306	CHL	CHA-C4D-ND	4.15	141.17	132.50
5	B	306	CHL	C1-C2-C3	-4.13	118.89	126.04
5	E	305	CHL	C1C-C2C-C3C	-4.13	103.83	107.11
5	E	311	CHL	O2D-CGD-CBD	4.13	118.60	111.27
5	F	310	CHL	CHB-C1B-C2B	-4.12	115.59	127.24
5	F	304	CHL	CHC-C1C-NC	4.12	130.46	124.20
2	D	302	OIE	C10-C9-C8	4.12	131.91	123.47
5	C	305	CHL	C1C-C2C-C3C	-4.12	103.84	107.11
5	F	312	CHL	O2D-CGD-CBD	4.12	118.58	111.27
3	F	303	NEX	C31-C30-C29	-4.12	121.44	127.31
5	C	311	CHL	CHA-C4D-ND	4.12	141.11	132.50
5	C	306	CHL	C1C-C2C-C3C	-4.11	103.85	107.11
5	E	312	CHL	C2C-C3C-C4C	-4.11	103.56	106.49
9	D	321	OUR	C34-C27-C1	-4.11	119.10	124.49
5	E	309	CHL	CHB-C4A-NA	4.11	130.19	124.51
5	A	312	CHL	O2D-CGD-CBD	4.11	118.57	111.27
5	B	306	CHL	C2C-C3C-C4C	-4.11	103.56	106.49
5	C	309	CHL	CHB-C1B-C2B	-4.10	115.65	127.24
5	C	311	CHL	C3A-C2A-C1A	-4.10	95.19	101.34
5	B	312	CHL	C4D-CHA-C1A	-4.10	116.26	121.25
5	D	305	CHL	C1C-C2C-C3C	-4.10	103.86	107.11
5	C	311	CHL	CHB-C1B-C2B	-4.10	115.67	127.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	318	CHL	C2C-C3C-C4C	-4.10	103.57	106.49
2	C	301	0IE	C23-C16-C15	-4.09	117.19	122.92
5	A	318	CHL	CHB-C1B-C2B	-4.08	115.70	127.24
5	B	314	CHL	C1C-C2C-C3C	-4.08	103.88	107.11
5	A	313	CHL	CHD-C1D-ND	4.08	128.20	124.45
7	D	319	LHG	O4-P-O5	4.08	132.41	112.24
5	E	312	CHL	CHC-C1C-NC	4.08	130.39	124.20
5	B	319	CHL	C1C-C2C-C3C	-4.08	103.88	107.11
2	E	302	0IE	C9-C10-C11	4.07	131.82	123.47
5	D	305	CHL	CHA-C4D-ND	4.06	140.99	132.50
2	F	302	0IE	C23-C16-C15	-4.05	117.25	122.92
5	D	313	CHL	CHB-C1B-C2B	-4.05	115.79	127.24
5	B	307	CHL	C1D-ND-C4D	4.05	109.21	106.33
5	B	306	CHL	O2D-CGD-CBD	4.05	118.47	111.27
7	F	318	LHG	O4-P-O5	4.04	132.23	112.24
5	A	309	CHL	CHC-C1C-NC	4.03	130.32	124.20
5	E	304	CHL	O2D-CGD-CBD	4.03	118.43	111.27
2	A	302	0IE	C23-C16-C15	-4.02	117.29	122.92
5	D	311	CHL	CHC-C1C-NC	4.02	130.31	124.20
5	B	319	CHL	CHB-C4A-NA	4.01	130.06	124.51
5	F	317	CHL	CHB-C1B-C2B	-4.01	115.92	127.24
5	D	312	CHL	O2D-CGD-CBD	4.01	118.39	111.27
5	C	312	CHL	C2C-C3C-C4C	-4.01	103.63	106.49
2	C	302	0IE	C23-C16-C15	-4.00	117.31	122.92
5	F	305	CHL	CHC-C1C-NC	4.00	130.27	124.20
5	D	306	CHL	C2C-C3C-C4C	-4.00	103.64	106.49
5	F	304	CHL	O2D-CGD-CBD	4.00	118.37	111.27
2	E	302	0IE	C10-C9-C8	4.00	131.66	123.47
5	B	306	CHL	CHC-C1C-NC	3.99	130.26	124.20
7	A	319	LHG	O4-P-O5	3.99	131.95	112.24
5	B	319	CHL	C2C-C3C-C4C	-3.99	103.65	106.49
5	A	305	CHL	C4B-CHC-C1C	-3.99	116.89	126.34
5	A	311	CHL	CHC-C1C-NC	3.98	130.25	124.20
5	D	312	CHL	OBD-CAD-C3D	-3.98	118.94	128.52
2	A	302	0IE	C21-C7-C8	-3.98	117.35	122.92
5	D	313	CHL	C4B-CHC-C1C	-3.97	116.91	126.34
5	D	318	CHL	C2C-C3C-C4C	-3.97	103.66	106.49
5	A	310	CHL	C1C-C2C-C3C	-3.97	103.97	107.11
5	D	312	CHL	C4B-CHC-C1C	-3.97	116.93	126.34
5	E	317	CHL	CHD-C4C-C3C	-3.96	119.02	124.84
5	B	312	CHL	C1C-C2C-C3C	-3.96	103.97	107.11
2	D	302	0IE	C23-C16-C15	-3.95	117.38	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	NEX	C11-C10-C9	-3.95	121.67	127.31
5	D	311	CHL	C2B-C1B-NB	3.95	112.88	110.23
5	C	305	CHL	CHC-C1C-NC	3.94	130.19	124.20
5	A	309	CHL	C2C-C3C-C4C	-3.93	103.69	106.49
2	E	301	OIE	C10-C9-C8	3.93	131.52	123.47
5	F	317	CHL	C1C-C2C-C3C	-3.92	104.00	107.11
2	C	301	OIE	C20-C3-C4	-3.92	119.78	124.83
5	F	304	CHL	CHD-C4C-C3C	-3.92	119.07	124.84
5	F	308	CHL	C2C-C3C-C4C	-3.92	103.69	106.49
5	D	318	CHL	OBD-CAD-C3D	-3.92	119.08	128.52
5	E	308	CHL	CHB-C1B-C2B	-3.92	116.17	127.24
5	A	313	CHL	C1-C2-C3	-3.92	119.27	126.04
5	D	318	CHL	CHA-C4D-ND	3.92	140.69	132.50
5	A	306	CHL	C1D-ND-C4D	3.91	109.12	106.33
5	D	313	CHL	CHD-C4C-NC	3.91	130.37	124.20
5	D	309	CHL	C2C-C3C-C4C	-3.91	103.70	106.49
5	C	312	CHL	C1C-C2C-C3C	-3.91	104.01	107.11
5	C	313	CHL	C1C-C2C-C3C	-3.90	104.02	107.11
2	C	302	OIE	C9-C10-C11	3.90	131.47	123.47
5	F	309	CHL	CHA-C4D-ND	3.90	140.66	132.50
5	A	309	CHL	C1C-C2C-C3C	-3.90	104.02	107.11
5	A	313	CHL	C1C-C2C-C3C	-3.90	104.02	107.11
2	C	301	OIE	C10-C9-C8	3.90	131.46	123.47
5	C	312	CHL	C4D-CHA-C1A	-3.90	116.50	121.25
5	C	318	CHL	CAA-C2A-C1A	3.90	124.75	111.97
5	A	313	CHL	CHC-C1C-NC	3.89	130.10	124.20
5	A	318	CHL	CHB-C4A-NA	3.88	129.88	124.51
5	A	305	CHL	C1C-C2C-C3C	-3.88	104.03	107.11
5	B	319	CHL	CAA-C2A-C1A	-3.88	99.26	111.97
5	E	317	CHL	CHB-C4A-NA	3.88	129.88	124.51
5	B	319	CHL	CHB-C1B-C2B	-3.87	116.30	127.24
5	E	305	CHL	CHD-C4C-C3C	-3.87	119.15	124.84
5	E	305	CHL	C3A-C2A-C1A	-3.87	95.55	101.34
5	C	305	CHL	CHD-C4C-C3C	-3.84	119.19	124.84
5	C	306	CHL	CHD-C4C-C3C	-3.84	119.19	124.84
2	C	301	OIE	C9-C10-C11	3.83	131.31	123.47
5	A	311	CHL	CHB-C1B-C2B	-3.83	116.43	127.24
5	D	312	CHL	CHB-C1B-C2B	-3.83	116.43	127.24
5	C	310	CHL	C2C-C3C-C4C	-3.82	103.77	106.49
5	A	313	CHL	CHB-C4A-NA	3.82	129.79	124.51
5	A	313	CHL	C1D-ND-C4D	3.82	109.05	106.33
5	A	312	CHL	C2C-C3C-C4C	-3.82	103.77	106.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	313	CHL	C4B-CHC-C1C	-3.81	117.29	126.34
5	A	309	CHL	C3A-C2A-C1A	-3.80	95.64	101.34
5	D	309	CHL	CHB-C1B-C2B	-3.80	116.50	127.24
5	A	312	CHL	C1C-C2C-C3C	-3.80	104.10	107.11
5	E	308	CHL	C1C-C2C-C3C	-3.80	104.10	107.11
5	B	306	CHL	C1C-C2C-C3C	-3.80	104.10	107.11
5	F	308	CHL	CHB-C1B-C2B	-3.80	116.52	127.24
5	A	312	CHL	CHC-C1C-NC	3.79	129.96	124.20
5	E	311	CHL	CHC-C1C-NC	3.79	129.96	124.20
5	E	312	CHL	C1C-C2C-C3C	-3.79	104.11	107.11
5	D	318	CHL	CHB-C1B-C2B	-3.79	116.53	127.24
5	D	311	CHL	CHC-C4B-NB	3.79	128.27	124.26
2	A	301	0IE	C21-C7-C8	-3.79	117.62	122.92
5	A	306	CHL	CMD-C2D-C3D	3.78	136.32	127.61
5	E	317	CHL	CHB-C1B-C2B	-3.78	116.55	127.24
2	C	302	0IE	C10-C9-C8	3.78	131.22	123.47
5	B	314	CHL	CHD-C1D-ND	3.78	127.93	124.45
5	D	306	CHL	C4B-CHC-C1C	-3.78	117.38	126.34
5	F	317	CHL	CHA-C4D-ND	3.78	140.40	132.50
5	B	314	CHL	CHC-C1C-NC	3.77	129.93	124.20
5	C	310	CHL	CHB-C1B-C2B	-3.77	116.59	127.24
5	A	306	CHL	C4D-CHA-C1A	-3.77	116.66	121.25
5	B	314	CHL	C4B-CHC-C1C	-3.77	117.40	126.34
5	F	304	CHL	C2C-C3C-C4C	-3.77	103.80	106.49
5	D	310	CHL	C2C-C3C-C4C	-3.76	103.81	106.49
5	D	306	CHL	C3A-C2A-C1A	-3.75	95.72	101.34
5	C	313	CHL	CHD-C4C-C3C	-3.75	119.33	124.84
5	F	305	CHL	CAA-C2A-C1A	3.74	124.22	111.97
5	E	317	CHL	C1C-C2C-C3C	-3.74	104.15	107.11
5	F	308	CHL	C4B-CHC-C1C	-3.74	117.47	126.34
5	E	304	CHL	CHD-C4C-C3C	-3.73	119.35	124.84
5	F	311	CHL	C4B-CHC-C1C	-3.73	117.48	126.34
5	C	305	CHL	C1-C2-C3	-3.73	119.59	126.04
5	C	318	CHL	C4B-CHC-C1C	-3.73	117.49	126.34
5	D	311	CHL	CHB-C1B-C2B	-3.73	116.71	127.24
4	B	304	LMU	C1B-O1B-C4'	-3.73	108.74	117.96
5	A	310	CHL	C1-C2-C3	-3.72	120.72	126.75
5	A	305	CHL	CHA-C4D-ND	3.72	140.29	132.50
5	A	310	CHL	CHD-C1D-C2D	-3.72	117.68	125.48
5	D	305	CHL	CHB-C1B-C2B	-3.72	116.73	127.24
5	E	305	CHL	C2C-C3C-C4C	-3.72	103.84	106.49
5	D	309	CHL	C4B-CHC-C1C	-3.71	117.53	126.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	304	LMU	C1B-O1B-C4'	-3.71	108.77	117.96
5	F	309	CHL	CHB-C4A-NA	3.71	129.65	124.51
5	A	305	CHL	C2C-C3C-C4C	-3.71	103.84	106.49
5	E	305	CHL	CHB-C1B-C2B	-3.71	116.76	127.24
5	F	304	CHL	C4B-CHC-C1C	-3.71	117.54	126.34
5	B	310	CHL	CHB-C1B-C2B	-3.71	116.76	127.24
2	E	302	0IE	C20-C3-C4	-3.71	120.06	124.83
5	D	306	CHL	C1C-C2C-C3C	-3.71	104.17	107.11
5	C	310	CHL	C4B-CHC-C1C	-3.70	117.55	126.34
2	A	301	0IE	C23-C16-C15	-3.70	117.74	122.92
9	F	320	0UR	O44-C45-C46	3.70	121.38	111.55
5	C	305	CHL	C4D-CHA-C1A	-3.70	116.75	121.25
5	A	312	CHL	C4B-CHC-C1C	-3.69	117.58	126.34
5	B	313	CHL	C2C-C3C-C4C	-3.69	103.86	106.49
5	C	309	CHL	C3A-C2A-C1A	-3.69	95.39	101.64
2	D	302	0IE	C21-C7-C8	-3.69	117.75	122.92
5	F	310	CHL	C1-O2A-CGA	3.69	126.12	116.44
5	A	318	CHL	CHA-C4D-ND	3.69	140.21	132.50
5	A	313	CHL	CMD-C2D-C1D	3.69	131.21	124.71
5	E	310	CHL	CHA-C4D-ND	3.69	140.21	132.50
5	F	309	CHL	CHB-C1B-C2B	-3.68	116.83	127.24
2	D	301	0IE	C10-C9-C8	3.68	131.02	123.47
5	D	306	CHL	CHD-C4C-NC	3.68	130.00	124.20
5	C	306	CHL	C3A-C2A-C1A	-3.68	95.83	101.34
7	B	324	LHG	O8-C23-C24	3.68	123.45	111.91
2	B	301	0IE	C10-C9-C8	3.68	131.00	123.47
5	C	310	CHL	CMD-C2D-C3D	-3.68	119.16	127.61
5	E	309	CHL	C2C-C3C-C4C	-3.67	103.87	106.49
5	C	305	CHL	CHD-C4C-NC	3.67	129.99	124.20
5	C	311	CHL	CHD-C1D-C2D	-3.67	117.78	125.48
5	C	312	CHL	CHB-C1B-C2B	-3.67	116.89	127.24
5	C	306	CHL	C4B-CHC-C1C	-3.66	117.65	126.34
5	B	319	CHL	C4B-CHC-C1C	-3.66	117.66	126.34
5	E	317	CHL	CHA-C4D-ND	3.66	140.15	132.50
5	D	306	CHL	C4A-NA-C1A	3.65	108.35	106.71
9	B	325	0UR	C10-C11-C12	-3.65	122.09	127.31
9	C	321	0UR	C5-C4-C3	-3.65	122.62	127.00
5	A	306	CHL	C4B-CHC-C1C	-3.65	117.68	126.34
5	B	319	CHL	CHA-C4D-ND	3.65	140.13	132.50
5	B	311	CHL	CHD-C4C-C3C	-3.65	119.48	124.84
2	D	302	0IE	C6-C7-C8	3.64	124.53	118.94
5	B	311	CHL	CHB-C1B-C2B	-3.64	116.95	127.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	318	CHL	C4B-CHC-C1C	-3.64	117.71	126.34
5	C	313	CHL	CMD-C2D-C3D	-3.64	119.25	127.61
5	A	318	CHL	C4B-CHC-C1C	-3.64	117.72	126.34
5	C	305	CHL	C4B-CHC-C1C	-3.64	117.72	126.34
4	E	319	LMU	C1B-O1B-C4'	-3.64	108.97	117.96
2	E	301	OIE	C9-C10-C11	3.63	130.92	123.47
5	B	307	CHL	C4D-CHA-C1A	-3.63	116.83	121.25
5	E	308	CHL	CHA-C4D-ND	3.63	140.10	132.50
5	A	312	CHL	CHB-C1B-C2B	-3.63	116.99	127.24
5	B	313	CHL	C4D-CHA-C1A	-3.63	116.84	121.25
5	C	309	CHL	C1C-C2C-C3C	-3.62	104.24	107.11
5	E	310	CHL	C3A-C2A-C1A	-3.62	95.91	101.34
5	F	304	CHL	C4D-CHA-C1A	-3.62	116.84	121.25
3	B	303	NEX	C35-C15-C14	3.62	130.89	123.47
5	C	313	CHL	CHC-C1C-NC	3.62	129.69	124.20
5	C	313	CHL	CHB-C1B-C2B	-3.61	117.04	127.24
5	D	306	CHL	C1D-ND-C4D	3.61	108.90	106.33
5	F	305	CHL	C3A-C2A-C1A	-3.60	95.95	101.34
2	E	302	OIE	C22-C12-C11	-3.60	117.88	122.92
5	F	305	CHL	C1-C2-C3	-3.59	119.83	126.04
5	A	312	CHL	C4D-CHA-C1A	-3.59	116.88	121.25
5	C	311	CHL	C4B-CHC-C1C	-3.59	117.83	126.34
2	F	301	OIE	C21-C7-C8	-3.59	117.90	122.92
5	B	312	CHL	C4B-CHC-C1C	-3.58	117.84	126.34
5	B	310	CHL	CHD-C4C-C3C	-3.58	119.58	124.84
5	D	309	CHL	C3A-C2A-C1A	-3.58	95.59	101.64
5	C	306	CHL	CHC-C1C-NC	3.58	129.63	124.20
5	B	310	CHL	C2C-C3C-C4C	-3.57	103.94	106.49
5	F	317	CHL	C4B-CHC-C1C	-3.57	117.87	126.34
5	C	309	CHL	CHD-C4C-C3C	-3.56	119.60	124.84
5	B	311	CHL	C2C-C3C-C4C	-3.56	103.95	106.49
2	D	301	OIE	C21-C7-C8	-3.56	117.93	122.92
5	E	308	CHL	C4B-CHC-C1C	-3.56	117.89	126.34
5	B	312	CHL	CHA-C4D-ND	3.56	139.95	132.50
5	B	314	CHL	CHB-C1B-C2B	-3.56	117.18	127.24
5	D	306	CHL	C4D-CHA-C1A	-3.56	116.92	121.25
5	A	309	CHL	C4B-CHC-C1C	-3.56	117.90	126.34
5	A	312	CHL	C1-C2-C3	-3.56	119.89	126.04
5	C	309	CHL	C4B-CHC-C1C	-3.56	117.90	126.34
5	D	310	CHL	C4B-CHC-C1C	-3.56	117.90	126.34
5	F	309	CHL	C1C-C2C-C3C	-3.56	104.29	107.11
5	F	310	CHL	C4-C3-C5	3.55	121.25	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	317	CHL	C4B-CHC-C1C	-3.55	117.91	126.34
9	A	322	0UR	C43-C3-C2	3.55	125.00	116.66
5	E	312	CHL	C4D-CHA-C1A	-3.55	116.93	121.25
5	E	304	CHL	CHD-C4C-NC	3.55	129.79	124.20
5	D	313	CHL	C2C-C3C-C4C	-3.55	103.96	106.49
2	B	301	0IE	C9-C10-C11	3.55	130.74	123.47
5	A	311	CHL	CHA-C4D-ND	3.54	139.91	132.50
5	C	306	CHL	C4-C3-C5	3.54	121.23	115.27
5	F	305	CHL	C2A-C1A-CHA	-3.54	117.67	123.86
9	F	320	0UR	C5-C4-C3	-3.54	122.75	127.00
5	D	311	CHL	CHA-C4D-ND	3.54	139.90	132.50
5	B	306	CHL	C4B-CHC-C1C	-3.53	117.95	126.34
5	A	311	CHL	C4B-CHC-C1C	-3.53	117.96	126.34
5	C	312	CHL	CHA-C4D-ND	3.53	139.89	132.50
5	E	311	CHL	C4D-CHA-C1A	-3.52	116.96	121.25
5	C	306	CHL	C2C-C3C-C4C	-3.52	103.98	106.49
5	B	313	CHL	C4B-CHC-C1C	-3.52	118.00	126.34
2	A	301	0IE	C10-C9-C8	3.52	130.68	123.47
2	E	302	0IE	C21-C7-C8	-3.51	118.00	122.92
4	D	304	LMU	C1'-C2'-C3'	3.51	117.31	110.00
5	E	312	CHL	CHD-C4C-C3C	-3.51	119.68	124.84
5	E	305	CHL	C4B-CHC-C1C	-3.51	118.02	126.34
5	B	312	CHL	CHB-C1B-C2B	-3.51	117.33	127.24
9	E	320	0UR	C9-C8-C7	-3.51	122.31	127.31
5	F	312	CHL	C4B-CHC-C1C	-3.51	118.02	126.34
5	F	308	CHL	C3A-C2A-C1A	-3.50	95.71	101.64
5	B	312	CHL	CHD-C4C-C3C	-3.50	119.69	124.84
5	E	309	CHL	CHB-C1B-C2B	-3.50	117.34	127.24
2	C	302	0IE	C21-C7-C8	-3.50	118.02	122.92
2	F	302	0IE	C21-C7-C8	-3.50	118.02	122.92
9	D	321	0UR	C10-C11-C12	-3.50	122.32	127.31
5	A	306	CHL	CHC-C1C-NC	3.50	129.51	124.20
5	E	312	CHL	C4B-CHC-C1C	-3.50	118.05	126.34
5	C	313	CHL	C4B-CHC-C1C	-3.49	118.05	126.34
5	E	310	CHL	CHD-C1D-C2D	-3.49	118.16	125.48
5	A	310	CHL	CHC-C1C-NC	3.49	129.50	124.20
2	C	301	0IE	C21-C7-C8	-3.49	118.04	122.92
5	B	310	CHL	C4D-CHA-C1A	-3.49	117.01	121.25
5	B	310	CHL	C4B-CHC-C1C	-3.48	118.08	126.34
2	A	301	0IE	C22-C12-C11	-3.48	118.05	122.92
2	E	301	0IE	C21-C7-C8	-3.48	118.05	122.92
5	A	306	CHL	C4-C3-C5	3.48	121.12	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	305	CHL	OBD-CAD-C3D	3.47	136.88	128.52
5	D	311	CHL	C1-C2-C3	-3.47	120.04	126.04
5	E	311	CHL	C4B-CHC-C1C	-3.47	118.10	126.34
5	C	311	CHL	C4D-CHA-C1A	-3.47	117.02	121.25
5	F	310	CHL	O2A-CGA-CBA	3.47	122.80	111.91
9	C	321	0UR	O44-C45-C46	3.47	120.77	111.55
5	F	308	CHL	CHD-C4C-C3C	-3.46	119.75	124.84
5	E	304	CHL	C4B-CHC-C1C	-3.46	118.14	126.34
5	C	313	CHL	CHD-C4C-NC	3.46	129.65	124.20
6	A	308	CLA	CAA-C2A-C3A	-3.45	103.32	112.78
9	D	321	0UR	C5-C4-C3	-3.45	122.85	127.00
9	E	320	0UR	C43-C3-C2	3.45	124.76	116.66
5	F	312	CHL	CMD-C2D-C1D	3.45	130.79	124.71
5	E	309	CHL	C4B-CHC-C1C	-3.45	118.16	126.34
9	B	325	0UR	C43-C3-C2	3.45	124.75	116.66
2	C	301	0IE	C22-C12-C11	-3.45	118.10	122.92
5	B	306	CHL	CHD-C4C-C3C	-3.45	119.78	124.84
5	D	310	CHL	CHB-C1B-C2B	-3.44	117.51	127.24
5	B	311	CHL	CHB-C4A-NA	3.44	129.26	124.51
5	A	306	CHL	C3A-C2A-C1A	-3.43	96.20	101.34
5	F	317	CHL	C3A-C2A-C1A	-3.43	96.20	101.34
5	C	311	CHL	CHC-C1C-NC	3.43	129.40	124.20
2	D	301	0IE	C22-C12-C11	-3.42	118.13	122.92
9	B	302	0UR	O44-C45-C46	3.42	120.65	111.55
5	F	310	CHL	C4D-CHA-C1A	-3.42	117.09	121.25
5	E	305	CHL	C4D-CHA-C1A	-3.42	117.09	121.25
5	F	304	CHL	CHA-C4D-ND	3.42	139.65	132.50
5	D	306	CHL	CHB-C1B-C2B	-3.42	117.59	127.24
5	B	313	CHL	CHB-C1B-C2B	-3.41	117.59	127.24
5	C	305	CHL	CHB-C1B-C2B	-3.41	117.59	127.24
5	E	308	CHL	CHC-C1C-NC	3.41	129.38	124.20
2	E	301	0IE	C22-C12-C11	-3.41	118.15	122.92
2	E	302	0IE	C6-C7-C8	3.41	124.17	118.94
5	C	310	CHL	CHA-C4D-ND	3.41	139.62	132.50
5	C	313	CHL	C2C-C3C-C4C	-3.40	104.06	106.49
5	F	309	CHL	C4D-CHA-C1A	-3.40	117.11	121.25
5	A	305	CHL	CHB-C1B-C2B	-3.40	117.62	127.24
5	C	310	CHL	CHD-C4C-C3C	-3.40	119.84	124.84
5	D	310	CHL	CHA-C4D-ND	3.40	139.60	132.50
5	F	310	CHL	C4B-CHC-C1C	-3.39	118.29	126.34
5	D	305	CHL	CHD-C1D-C2D	-3.39	118.36	125.48
6	E	306	CLA	O2D-CGD-O1D	-3.39	117.21	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	312	CHL	C4B-CHC-C1C	-3.39	118.30	126.34
5	E	305	CHL	CHC-C1C-NC	3.39	129.34	124.20
5	A	309	CHL	CHB-C1B-C2B	-3.38	117.68	127.24
5	D	311	CHL	C1C-C2C-C3C	-3.38	104.43	107.11
5	E	305	CHL	C4A-NA-C1A	3.38	108.23	106.71
5	A	313	CHL	C2C-C3C-C4C	-3.38	104.08	106.49
5	E	309	CHL	CHA-C4D-ND	3.38	139.56	132.50
5	A	306	CHL	C2C-C3C-C4C	-3.37	104.08	106.49
5	D	305	CHL	C4B-CHC-C1C	-3.37	118.34	126.34
5	D	305	CHL	C3A-C2A-C1A	-3.37	96.29	101.34
2	F	302	OIE	C22-C12-C11	-3.37	118.20	122.92
2	E	302	OIE	C13-C12-C11	3.37	124.11	118.94
2	F	302	OIE	C10-C9-C8	3.36	130.37	123.47
5	C	318	CHL	CHB-C4A-NA	3.36	129.16	124.51
5	B	307	CHL	C2A-C1A-CHA	-3.36	117.98	123.86
2	D	301	OIE	C9-C10-C11	3.36	130.36	123.47
5	A	309	CHL	CHA-C4D-ND	3.35	139.52	132.50
5	E	309	CHL	C4D-CHA-C1A	-3.35	117.17	121.25
5	A	305	CHL	CHD-C4C-C3C	-3.35	119.91	124.84
2	B	301	OIE	C21-C7-C8	-3.35	118.23	122.92
5	B	307	CHL	C3A-C2A-C1A	-3.35	96.32	101.34
5	C	305	CHL	CHA-C4D-ND	3.35	139.51	132.50
5	D	305	CHL	CAA-C2A-C1A	-3.35	101.00	111.97
5	E	311	CHL	CHB-C1B-C2B	-3.35	117.78	127.24
2	C	302	OIE	C22-C12-C11	-3.35	118.23	122.92
6	E	307	CLA	CAA-C2A-C3A	-3.35	103.61	112.78
5	A	309	CHL	C4D-CHA-C1A	-3.34	117.18	121.25
6	D	307	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
5	A	310	CHL	CHA-C4D-ND	3.34	139.49	132.50
5	C	318	CHL	CHD-C4C-C3C	-3.34	119.93	124.84
2	A	301	OIE	C17-C16-C15	3.34	124.06	118.94
5	C	306	CHL	CHB-C1B-C2B	-3.34	117.81	127.24
5	F	311	CHL	C4-C3-C5	3.33	120.88	115.27
2	F	301	OIE	C9-C10-C11	3.33	130.30	123.47
5	B	311	CHL	C4B-CHC-C1C	-3.33	118.44	126.34
5	E	310	CHL	C4B-CHC-C1C	-3.33	118.44	126.34
5	D	313	CHL	CHA-C4D-ND	3.33	139.47	132.50
5	E	309	CHL	CHD-C1D-C2D	-3.33	118.51	125.48
2	F	302	OIE	C6-C7-C8	3.32	124.04	118.94
5	C	309	CHL	CHC-C1C-NC	3.32	129.24	124.20
5	B	310	CHL	CHA-C4D-ND	3.32	139.44	132.50
5	C	318	CHL	CHA-C4D-ND	3.32	139.44	132.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	313	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
5	B	306	CHL	CHB-C1B-C2B	-3.32	117.87	127.24
5	A	312	CHL	CHA-C4D-ND	3.32	139.44	132.50
5	F	309	CHL	CHD-C1D-C2D	-3.31	118.53	125.48
5	E	305	CHL	C1-C2-C3	-3.31	120.31	126.04
5	A	310	CHL	C4B-CHC-C1C	-3.31	118.50	126.34
5	A	311	CHL	CHD-C1D-C2D	-3.31	118.55	125.48
5	A	311	CHL	C3A-C2A-C1A	-3.30	96.40	101.34
5	F	305	CHL	C2C-C3C-C4C	-3.29	104.14	106.49
5	B	312	CHL	C3A-C2A-C1A	-3.29	96.41	101.34
3	B	303	NEX	C11-C12-C13	3.29	135.66	126.42
5	F	311	CHL	CHB-C1B-C2B	-3.29	117.95	127.24
5	E	311	CHL	C1-C2-C3	-3.29	120.36	126.04
6	C	314	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
5	E	310	CHL	C1-C2-C3	-3.29	120.36	126.04
6	B	315	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
5	D	309	CHL	CHA-C4D-ND	3.28	139.37	132.50
5	F	308	CHL	CHA-C4D-ND	3.28	139.37	132.50
3	B	303	NEX	C27-C28-C29	-3.28	120.44	125.53
9	E	320	OUR	C10-C11-C12	-3.28	122.62	127.31
5	F	305	CHL	CHB-C1B-C2B	-3.28	117.97	127.24
5	D	305	CHL	CHC-C1C-NC	3.28	129.18	124.20
9	F	320	OUR	C24-C25-C26	-3.28	105.81	110.30
2	D	302	OIE	C22-C12-C11	-3.28	118.33	122.92
5	D	305	CHL	C4D-CHA-C1A	-3.28	117.26	121.25
5	B	311	CHL	CHA-C4D-ND	3.27	139.34	132.50
5	F	311	CHL	CHD-C4C-C3C	-3.26	120.04	124.84
5	B	319	CHL	C4D-CHA-C1A	-3.26	117.28	121.25
5	D	318	CHL	CHD-C1D-C2D	-3.26	118.65	125.48
2	F	301	OIE	C22-C12-C11	-3.26	118.36	122.92
5	E	312	CHL	CHB-C1B-C2B	-3.25	118.05	127.24
5	A	311	CHL	C1C-C2C-C3C	-3.25	104.53	107.11
5	D	313	CHL	CHB-C4A-NA	3.25	129.00	124.51
5	E	304	CHL	CHB-C1B-C2B	-3.25	118.06	127.24
6	A	315	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
5	A	306	CHL	C1-C2-C3	-3.25	120.43	126.04
5	E	305	CHL	C4-C3-C5	3.25	120.73	115.27
5	E	309	CHL	CHD-C4C-C3C	-3.24	120.08	124.84
5	F	309	CHL	C2A-C3A-C4A	3.23	105.91	101.78
5	C	306	CHL	CHD-C4C-NC	3.22	129.28	124.20
6	A	307	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
5	D	309	CHL	CHD-C4C-C3C	-3.22	120.11	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	310	CHL	O2D-CGD-O1D	-3.22	117.55	123.84
2	A	302	0IE	C22-C12-C11	-3.22	118.42	122.92
6	F	315	CLA	C3B-C4B-NB	-3.21	107.54	110.52
2	C	302	0IE	C6-C7-C8	3.21	123.86	118.94
5	E	311	CHL	CHA-C4D-ND	3.21	139.21	132.50
5	C	311	CHL	CAA-C2A-C1A	3.20	122.48	111.97
5	B	312	CHL	C1-C2-C3	-3.20	120.50	126.04
5	F	317	CHL	CAC-C3C-C4C	3.20	128.96	124.81
5	F	309	CHL	C4B-CHC-C1C	-3.20	118.75	126.34
4	D	304	LMU	O5'-C5'-C4'	-3.19	103.02	109.75
5	D	313	CHL	CMD-C2D-C3D	-3.19	120.28	127.61
9	E	320	0UR	O44-C45-C46	3.19	120.03	111.55
5	F	305	CHL	CHD-C1D-ND	3.19	127.38	124.45
5	D	310	CHL	CHD-C4C-C3C	-3.19	120.15	124.84
5	B	314	CHL	OMC-CMC-C2C	-3.18	118.49	125.69
5	A	312	CHL	CAC-C3C-C4C	3.18	128.94	124.81
5	E	310	CHL	CHB-C1B-C2B	-3.18	118.25	127.24
5	B	312	CHL	C1-O2A-CGA	3.18	124.79	116.44
5	F	312	CHL	CHB-C1B-C2B	-3.18	118.25	127.24
5	F	310	CHL	CHA-C4D-ND	3.18	139.15	132.50
6	A	315	CLA	C1-C2-C3	-3.18	120.54	126.04
5	A	310	CHL	O2D-CGD-O1D	-3.18	117.62	123.84
5	E	310	CHL	O2A-CGA-CBA	3.18	121.88	111.91
6	B	316	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
2	F	301	0IE	C6-C7-C8	3.18	123.81	118.94
5	E	312	CHL	C3A-C2A-C1A	-3.17	96.58	101.34
5	C	310	CHL	OBD-CAD-C3D	-3.17	120.88	128.52
5	E	317	CHL	C4D-CHA-C1A	-3.17	117.39	121.25
6	B	315	CLA	CAC-C3C-C4C	3.17	128.93	124.81
2	C	301	0IE	C6-C7-C8	3.17	123.81	118.94
5	D	311	CHL	C4B-CHC-C1C	-3.17	118.81	126.34
5	D	310	CHL	C4D-CHA-C1A	-3.17	117.39	121.25
6	B	318	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
5	E	312	CHL	CHA-C4D-ND	3.17	139.13	132.50
2	A	302	0IE	C9-C10-C11	3.17	129.96	123.47
5	D	309	CHL	CHC-C1C-NC	3.17	129.01	124.20
6	C	317	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
5	F	311	CHL	CHC-C1C-NC	3.16	129.00	124.20
5	F	310	CHL	C3A-C2A-C1A	-3.16	96.60	101.34
9	E	320	0UR	C5-C4-C3	-3.16	123.20	127.00
9	D	321	0UR	O44-C45-C46	3.16	119.96	111.55
5	C	318	CHL	O2D-CGD-O1D	-3.16	117.66	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	307	CLA	C3B-C4B-NB	-3.16	107.59	110.52
9	E	320	0UR	O42-C2-C3	-3.16	114.89	120.66
5	E	311	CHL	C1C-C2C-C3C	-3.16	104.61	107.11
5	C	309	CHL	CHA-C4D-ND	3.15	139.09	132.50
2	B	301	0IE	C22-C12-C11	-3.15	118.51	122.92
5	E	305	CHL	CHD-C4C-NC	3.14	129.15	124.20
6	C	307	CLA	O2D-CGD-CBD	3.13	116.83	111.27
5	C	312	CHL	CHC-C1C-NC	3.13	128.95	124.20
5	B	312	CHL	CHC-C1C-NC	3.13	128.95	124.20
3	E	303	NEX	C38-C25-C24	-3.13	110.76	114.28
5	F	317	CHL	CHC-C1C-NC	3.12	128.94	124.20
5	E	308	CHL	C4D-CHA-C1A	-3.12	117.45	121.25
5	F	305	CHL	O2D-CGD-O1D	-3.11	117.75	123.84
5	F	317	CHL	CHD-C1D-C2D	-3.11	118.96	125.48
5	C	305	CHL	O2A-CGA-CBA	3.11	121.65	111.91
6	A	314	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
5	B	307	CHL	CHB-C1B-C2B	-3.10	118.47	127.24
5	A	310	CHL	CHB-C1B-C2B	-3.10	118.49	127.24
5	D	311	CHL	C4-C3-C5	3.09	120.48	115.27
6	F	314	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
5	B	307	CHL	CAC-C3C-C4C	3.09	128.82	124.81
5	B	313	CHL	C4-C3-C5	3.09	120.46	115.27
5	E	310	CHL	C1C-C2C-C3C	-3.09	104.67	107.11
6	B	317	CLA	C3B-C4B-NB	-3.09	107.65	110.52
6	F	306	CLA	C3B-C4B-NB	-3.08	107.65	110.52
5	E	312	CHL	C1-C2-C3	-3.08	120.71	126.04
5	C	313	CHL	CHA-C4D-ND	3.08	138.95	132.50
5	F	311	CHL	CHD-C4C-NC	3.08	129.05	124.20
6	A	314	CLA	C1-C2-C3	-3.08	120.72	126.04
5	E	317	CHL	CHC-C1C-NC	3.08	128.87	124.20
9	F	320	0UR	O42-C2-C3	-3.08	115.04	120.66
5	D	306	CHL	C6-C7-C8	-3.07	105.98	115.92
2	D	301	0IE	C13-C12-C11	3.07	123.65	118.94
6	D	315	CLA	C3B-C4B-NB	-3.07	107.67	110.52
9	C	321	0UR	C48-C47-C46	-3.07	119.27	125.85
9	A	322	0UR	C29-C30-C31	-3.07	108.25	111.74
9	A	322	0UR	O44-C45-O57	-3.06	116.20	122.93
5	F	317	CHL	C4D-CHA-C1A	-3.06	117.52	121.25
5	C	311	CHL	CAC-C3C-C4C	3.06	128.78	124.81
2	C	301	0IE	C13-C12-C11	3.06	123.63	118.94
5	B	313	CHL	CHC-C1C-NC	3.06	128.84	124.20
6	C	317	CLA	C3B-C4B-NB	-3.05	107.68	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	306	CHL	CHD-C1D-C2D	-3.05	119.08	125.48
5	E	305	CHL	C2A-C1A-CHA	-3.05	118.53	123.86
5	F	311	CHL	C2C-C3C-C4C	-3.05	104.32	106.49
5	B	307	CHL	C4-C3-C5	3.05	120.40	115.27
5	D	309	CHL	C4D-CHA-C1A	-3.05	117.54	121.25
2	D	302	0IE	C9-C10-C11	3.05	129.72	123.47
5	F	312	CHL	C2C-C3C-C4C	-3.05	104.32	106.49
5	D	312	CHL	CHD-C4C-NC	3.04	129.00	124.20
5	B	310	CHL	CHC-C1C-NC	3.04	128.82	124.20
5	B	319	CHL	CAC-C3C-C4C	3.04	128.76	124.81
6	D	307	CLA	C3B-C4B-NB	-3.04	107.69	110.52
9	C	321	0UR	C34-C27-C1	-3.04	120.50	124.49
5	A	306	CHL	CHB-C1B-C2B	-3.04	118.66	127.24
5	B	312	CHL	CHD-C1D-C2D	-3.04	119.11	125.48
5	F	312	CHL	CHC-C1C-NC	3.03	128.80	124.20
2	A	301	0IE	C14-C15-C16	3.03	131.63	127.31
5	C	311	CHL	O2A-CGA-CBA	3.03	121.42	111.91
5	B	314	CHL	C2C-C3C-C4C	-3.03	104.33	106.49
5	E	311	CHL	CHD-C4C-C3C	-3.03	120.39	124.84
5	C	312	CHL	CHD-C1D-C2D	-3.02	119.14	125.48
2	E	301	0IE	C13-C12-C11	3.02	123.57	118.94
9	D	321	0UR	C43-C3-C2	3.02	123.75	116.66
5	D	311	CHL	O2A-CGA-CBA	3.02	121.37	111.91
6	F	306	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
3	F	303	NEX	C12-C13-C14	3.01	123.56	118.94
5	A	305	CHL	O2A-CGA-CBA	3.01	121.35	111.91
5	B	313	CHL	CHA-C4D-ND	3.01	138.79	132.50
5	C	311	CHL	C1C-C2C-C3C	-3.00	104.73	107.11
5	A	310	CHL	CBA-CAA-C2A	-3.00	105.00	113.86
5	D	306	CHL	C2A-C1A-CHA	-3.00	118.61	123.86
6	D	317	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
5	D	312	CHL	C6-C5-C3	-3.00	105.59	113.45
6	F	315	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
5	A	309	CHL	CHD-C4C-C3C	-2.99	120.44	124.84
5	C	312	CHL	C3A-C2A-C1A	-2.99	96.86	101.34
5	A	318	CHL	CHD-C4C-C3C	-2.99	120.44	124.84
5	C	310	CHL	CHD-C1D-C2D	-2.99	119.22	125.48
6	D	316	CLA	C3B-C4B-NB	-2.99	107.75	110.52
6	E	314	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
5	C	311	CHL	C2A-C3A-C4A	2.98	106.68	101.87
5	D	313	CHL	C1-C2-C3	-2.98	120.89	126.04
5	A	318	CHL	CHD-C1D-C2D	-2.98	119.24	125.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	311	CHL	OMC-CMC-C2C	-2.97	118.96	125.69
5	F	305	CHL	C1D-ND-C4D	2.97	108.45	106.33
5	F	310	CHL	CHD-C1D-C2D	-2.97	119.24	125.48
2	E	301	0IE	C6-C7-C8	2.97	123.50	118.94
5	D	311	CHL	C3A-C2A-C1A	-2.97	96.89	101.34
6	A	316	CLA	C3B-C4B-NB	-2.97	107.76	110.52
3	D	303	NEX	C24-C23-C22	-2.97	105.04	110.77
5	A	311	CHL	O2A-CGA-CBA	2.97	121.23	111.91
5	D	312	CHL	CHA-C4D-ND	2.97	138.71	132.50
5	F	304	CHL	CMB-C2B-C1B	2.97	129.89	125.37
5	F	304	CHL	CHD-C4C-NC	2.97	128.88	124.20
5	D	311	CHL	CHD-C1D-C2D	-2.96	119.27	125.48
5	F	311	CHL	C2A-C1A-CHA	-2.96	118.68	123.86
3	F	303	NEX	C39-C29-C30	-2.96	118.78	122.92
2	B	301	0IE	C6-C7-C8	2.96	123.48	118.94
5	D	310	CHL	CHC-C1C-NC	2.95	128.69	124.20
5	B	311	CHL	CHD-C4C-NC	2.95	128.86	124.20
6	F	307	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
6	E	315	CLA	C3B-C4B-NB	-2.94	107.78	110.52
5	D	312	CHL	O2A-CGA-CBA	2.94	121.14	111.91
9	A	322	0UR	C9-C8-C7	-2.94	123.11	127.31
2	D	301	0IE	C6-C7-C8	2.94	123.45	118.94
5	B	306	CHL	C4-C3-C5	2.94	120.22	115.27
5	F	309	CHL	CHC-C1C-NC	2.94	128.66	124.20
5	F	310	CHL	CHD-C4C-C3C	-2.94	120.52	124.84
5	E	308	CHL	CHD-C4C-C3C	-2.93	120.53	124.84
2	E	302	0IE	C17-C16-C15	2.93	123.44	118.94
5	F	304	CHL	CHD-C1D-C2D	-2.93	119.33	125.48
5	B	306	CHL	C3A-C2A-C1A	-2.93	96.95	101.34
5	B	319	CHL	CHC-C1C-NC	2.93	128.65	124.20
5	C	311	CHL	C4-C3-C5	2.93	120.20	115.27
5	F	304	CHL	C3A-C2A-C1A	-2.93	96.96	101.34
5	C	312	CHL	CAC-C3C-C4C	2.92	128.60	124.81
5	C	313	CHL	C1-C2-C3	-2.92	120.98	126.04
5	A	306	CHL	C2A-C1A-CHA	-2.92	118.75	123.86
5	D	312	CHL	CHC-C1C-NC	2.92	128.64	124.20
2	F	302	0IE	C13-C12-C11	2.92	123.42	118.94
5	A	312	CHL	O2A-CGA-CBA	2.92	121.07	111.91
6	F	313	CLA	O2A-CGA-O1A	-2.92	116.22	123.59
6	B	316	CLA	C3B-C4B-NB	-2.92	107.81	110.52
5	D	318	CHL	CAA-C2A-C1A	2.92	121.54	111.97
5	C	306	CHL	C4D-CHA-C1A	-2.92	117.70	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	310	CHL	O2D-CGD-O1D	-2.92	118.14	123.84
5	A	305	CHL	C1-C2-C3	-2.92	121.00	126.04
5	A	310	CHL	CHD-C4C-C3C	-2.91	120.56	124.84
5	B	312	CHL	O2A-CGA-CBA	2.91	121.05	111.91
6	A	316	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
5	E	311	CHL	CHD-C1D-C2D	-2.91	119.38	125.48
6	D	314	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
6	A	308	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
5	D	312	CHL	CHD-C4C-C3C	-2.91	120.57	124.84
5	B	312	CHL	C2A-C3A-C4A	2.90	106.56	101.87
5	B	319	CHL	O2D-CGD-O1D	-2.90	118.16	123.84
5	C	311	CHL	CMD-C2D-C3D	2.90	134.29	127.61
6	C	307	CLA	CHB-C4A-NA	2.90	128.52	124.51
5	D	309	CHL	C2A-C3A-C4A	2.90	105.48	101.78
5	C	305	CHL	C6-C5-C3	-2.90	105.86	113.45
6	C	307	CLA	O2A-CGA-O1A	-2.90	116.28	123.59
5	F	312	CHL	C3A-C2A-C1A	-2.90	97.00	101.34
5	E	317	CHL	CHD-C1D-C2D	-2.89	119.41	125.48
6	C	316	CLA	C3B-C4B-NB	-2.89	107.83	110.52
5	E	304	CHL	C2C-C3C-C4C	-2.89	104.43	106.49
5	E	304	CHL	CHA-C4D-ND	2.89	138.54	132.50
5	A	311	CHL	CAC-C3C-C4C	2.89	128.55	124.81
6	F	306	CLA	CHB-C4A-NA	2.88	128.50	124.51
5	B	313	CHL	OMC-CMC-C2C	-2.88	119.17	125.69
6	B	315	CLA	CHB-C4A-NA	2.88	128.50	124.51
6	B	308	CLA	C4-C3-C5	2.88	120.12	115.27
5	A	318	CHL	C3A-C2A-C1A	-2.88	96.76	101.64
6	D	315	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
7	B	320	LHG	C5-O7-C7	-2.88	110.71	117.79
5	C	309	CHL	CMD-C2D-C1D	2.88	129.78	124.71
5	A	306	CHL	CHA-C4D-ND	2.87	138.51	132.50
2	C	302	OIE	C13-C12-C11	2.87	123.35	118.94
5	B	313	CHL	CHD-C1D-C2D	-2.87	119.45	125.48
6	C	317	CLA	O1D-CGD-CBD	2.87	130.36	124.48
5	F	310	CHL	CHC-C1C-NC	2.87	128.56	124.20
5	B	313	CHL	O2A-CGA-CBA	2.87	120.91	111.91
6	B	309	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
5	F	305	CHL	C4D-CHA-C1A	-2.87	117.76	121.25
5	C	306	CHL	CHA-C4D-ND	2.86	138.49	132.50
5	D	312	CHL	CAC-C3C-C4C	2.86	128.53	124.81
5	A	313	CHL	CHA-C4D-ND	2.86	138.48	132.50
5	D	310	CHL	CHD-C1D-C2D	-2.86	119.49	125.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	0IE	C6-C7-C8	2.85	123.32	118.94
6	E	307	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
5	A	312	CHL	OMC-CMC-C2C	-2.85	119.24	125.69
7	A	319	LHG	O8-C23-C24	2.85	120.85	111.91
5	D	305	CHL	C2A-C3A-C4A	2.85	106.47	101.87
5	D	313	CHL	CHC-C1C-NC	2.85	128.52	124.20
5	A	313	CHL	C4-C3-C5	2.84	120.06	115.27
2	D	301	0IE	C17-C16-C15	2.84	123.30	118.94
5	C	318	CHL	OMC-CMC-C2C	-2.84	119.27	125.69
3	A	303	NEX	C26-C27-C28	2.84	131.99	125.99
5	A	309	CHL	C2A-C3A-C4A	2.84	106.45	101.87
5	D	311	CHL	CAC-C3C-C4C	2.84	128.49	124.81
5	F	304	CHL	CHB-C1B-C2B	-2.83	119.23	127.24
5	E	304	CHL	O2A-CGA-CBA	2.83	120.79	111.91
5	E	310	CHL	C2A-C3A-C4A	2.83	106.44	101.87
5	B	313	CHL	CHD-C4C-C3C	-2.83	120.68	124.84
5	A	305	CHL	CHD-C1D-C2D	-2.83	119.55	125.48
6	D	316	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
6	A	314	CLA	CHB-C1B-NB	2.82	127.25	124.26
9	C	321	0UR	C24-C25-C26	-2.82	106.44	110.30
5	F	309	CHL	C3A-C2A-C1A	-2.82	96.87	101.64
5	B	307	CHL	CHC-C1C-C2C	-2.82	115.89	126.11
7	D	319	LHG	O8-C23-C24	2.82	120.75	111.91
5	E	305	CHL	CHA-C4D-ND	2.82	138.39	132.50
9	C	321	0UR	C43-C3-C2	2.82	123.28	116.66
5	E	312	CHL	O2A-CGA-CBA	2.81	120.73	111.91
6	B	308	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
5	C	318	CHL	CHD-C1D-C2D	-2.81	119.58	125.48
9	D	321	0UR	C48-C47-C46	-2.81	119.82	125.85
5	A	311	CHL	CHD-C4C-C3C	-2.81	120.71	124.84
5	E	317	CHL	O2D-CGD-O1D	-2.81	118.35	123.84
5	B	307	CHL	O2D-CGD-O1D	-2.81	118.35	123.84
5	A	318	CHL	C4D-CHA-C1A	-2.80	117.84	121.25
6	B	308	CLA	CHB-C4A-NA	2.80	128.39	124.51
5	A	318	CHL	CAA-C2A-C3A	-2.80	109.56	116.10
2	D	302	0IE	C20-C3-C4	-2.80	121.23	124.83
5	E	312	CHL	CHD-C1D-C2D	-2.80	119.61	125.48
6	C	315	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
5	A	311	CHL	C4-C3-C5	2.80	119.98	115.27
5	B	319	CHL	CHD-C1D-C2D	-2.79	119.62	125.48
2	D	302	0IE	C4-C3-C2	-2.79	117.68	120.08
5	D	313	CHL	C3A-C2A-C1A	-2.79	97.16	101.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	313	CHL	C3A-C2A-C1A	-2.79	97.16	101.34
5	F	311	CHL	OMC-CMC-C2C	-2.79	119.38	125.69
5	E	311	CHL	CAC-C3C-C4C	2.79	128.43	124.81
5	F	311	CHL	O2A-CGA-CBA	2.79	120.66	111.91
6	A	316	CLA	CHB-C4A-NA	2.79	128.37	124.51
5	C	312	CHL	C4-C3-C5	2.79	119.96	115.27
6	B	317	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
5	C	309	CHL	OMC-CMC-C2C	-2.78	119.39	125.69
2	A	302	OIE	C13-C12-C11	2.78	123.21	118.94
5	A	306	CHL	O2A-CGA-CBA	2.78	120.64	111.91
5	F	309	CHL	CHD-C4C-C3C	-2.78	120.75	124.84
5	E	310	CHL	CHD-C4C-C3C	-2.78	120.75	124.84
5	D	306	CHL	O2A-CGA-CBA	2.78	120.63	111.91
5	A	310	CHL	O2A-CGA-CBA	2.78	120.62	111.91
2	E	301	OIE	C17-C16-C15	2.78	123.20	118.94
5	A	318	CHL	CAA-C2A-C1A	2.77	118.65	111.81
5	E	317	CHL	OMC-CMC-C2C	-2.77	119.42	125.69
5	B	314	CHL	C3A-C2A-C1A	-2.77	97.19	101.34
5	C	313	CHL	C3A-C2A-C1A	-2.76	97.20	101.34
5	C	306	CHL	C2A-C1A-CHA	-2.76	119.03	123.86
5	B	314	CHL	C1-C2-C3	-2.76	121.27	126.04
5	B	313	CHL	C1-C2-C3	-2.76	121.28	126.04
5	B	311	CHL	CHD-C1D-C2D	-2.76	119.70	125.48
2	F	301	OIE	C13-C12-C11	2.76	123.17	118.94
6	F	316	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
6	D	316	CLA	CHB-C4A-NA	2.75	128.31	124.51
5	E	304	CHL	C3A-C2A-C1A	-2.75	97.22	101.34
5	C	305	CHL	C2C-C3C-C4C	-2.75	104.53	106.49
6	C	307	CLA	C1-C2-C3	-2.75	121.29	126.04
5	D	305	CHL	CAC-C3C-C4C	2.74	128.37	124.81
5	E	308	CHL	CAC-C3C-C4C	2.74	128.37	124.81
2	B	301	OIE	C13-C12-C11	2.74	123.15	118.94
5	E	310	CHL	CAC-C3C-C4C	2.74	128.37	124.81
5	D	309	CHL	O2D-CGD-O1D	-2.74	118.48	123.84
6	E	315	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
5	D	311	CHL	C3B-C4B-NB	2.73	113.05	110.52
6	E	313	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
6	A	315	CLA	C3B-C4B-NB	-2.73	107.98	110.52
6	D	308	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
5	D	318	CHL	CHC-C1C-NC	2.73	128.34	124.20
5	D	312	CHL	OMC-CMC-C2C	-2.72	119.53	125.69
5	E	308	CHL	OMC-CMC-C2C	-2.72	119.53	125.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	309	CHL	CHD-C4C-NC	2.72	128.49	124.20
7	B	324	LHG	O7-C7-O9	-2.72	117.14	123.70
5	E	312	CHL	CHD-C4C-NC	2.72	128.48	124.20
3	E	303	NEX	C31-C32-C33	-2.71	118.80	126.42
2	D	302	OIE	C13-C12-C11	2.71	123.10	118.94
5	B	307	CHL	O2A-CGA-CBA	2.71	120.42	111.91
3	F	303	NEX	C40-C33-C34	-2.71	119.13	122.92
5	F	305	CHL	C16-C15-C13	-2.71	107.17	115.92
5	B	311	CHL	O2A-CGA-CBA	2.71	120.40	111.91
5	D	312	CHL	CHC-C4B-C3B	-2.70	115.68	127.71
5	A	313	CHL	OMC-CMC-C2C	-2.70	119.58	125.69
9	E	320	OURL	C48-C47-C46	-2.70	120.05	125.85
5	E	317	CHL	CHD-C4C-NC	2.70	128.46	124.20
4	D	304	LMU	C3'-C4'-C5'	-2.70	104.74	110.93
6	A	314	CLA	C3B-C4B-NB	-2.70	108.01	110.52
5	C	310	CHL	CHC-C1C-NC	2.70	128.30	124.20
7	F	318	LHG	C11-C10-C9	-2.70	100.74	114.42
5	E	309	CHL	C3A-C2A-C1A	-2.70	97.30	101.34
9	F	320	OURL	C10-C11-C12	-2.69	123.46	127.31
5	A	312	CHL	C4-C3-C5	2.69	119.80	115.27
5	C	312	CHL	O2A-CGA-CBA	2.69	120.36	111.91
9	F	320	OURL	C43-C3-C2	2.69	122.98	116.66
5	F	308	CHL	CHC-C1C-NC	2.69	128.28	124.20
5	E	310	CHL	C4-C3-C5	2.69	119.80	115.27
5	B	319	CHL	C3A-C2A-C1A	-2.69	97.31	101.34
6	E	306	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
6	F	313	CLA	C3B-C4B-NB	-2.69	108.02	110.52
5	E	311	CHL	C3A-C2A-C1A	-2.69	97.31	101.34
3	F	303	NEX	C17-C1-C6	-2.69	108.07	110.47
5	A	309	CHL	O2D-CGD-O1D	-2.69	118.59	123.84
5	B	310	CHL	O2D-CGD-O1D	-2.69	118.59	123.84
5	E	305	CHL	O2A-CGA-CBA	2.69	120.33	111.91
5	C	312	CHL	O2D-CGD-O1D	-2.68	118.59	123.84
6	F	316	CLA	C3B-C4B-NB	-2.68	108.03	110.52
5	F	311	CHL	C4D-CHA-C1A	-2.68	117.98	121.25
5	B	306	CHL	OMC-CMC-C2C	-2.68	119.62	125.69
5	F	310	CHL	CMD-C2D-C3D	2.68	133.78	127.61
5	D	310	CHL	CAC-C3C-C4C	2.68	128.29	124.81
5	B	313	CHL	C6-C5-C3	-2.68	106.43	113.45
5	B	310	CHL	CHD-C4C-NC	2.68	128.42	124.20
5	B	307	CHL	CHA-C4D-ND	2.68	138.10	132.50
5	A	306	CHL	CMD-C2D-C1D	-2.68	120.00	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	313	CHL	C3A-C2A-C1A	-2.67	97.33	101.34
5	A	312	CHL	CHD-C1D-C2D	-2.67	119.87	125.48
2	B	301	0IE	C39-C32-C31	2.67	113.53	109.71
5	E	304	CHL	C2A-C1A-CHA	-2.67	119.19	123.86
6	A	317	CLA	C3B-C4B-NB	-2.67	108.04	110.52
5	F	308	CHL	CHD-C1D-C2D	-2.67	119.88	125.48
6	E	306	CLA	C3B-C4B-NB	-2.67	108.04	110.52
5	F	308	CHL	C4D-CHA-C1A	-2.67	118.00	121.25
7	C	319	LHG	O8-C23-C24	2.67	120.28	111.91
5	D	306	CHL	C11-C10-C8	-2.67	107.30	115.92
6	B	315	CLA	CHD-C1D-ND	-2.67	122.00	124.45
2	A	301	0IE	C9-C10-C11	2.67	128.94	123.47
6	B	308	CLA	O2D-CGD-CBD	2.66	116.00	111.27
5	A	305	CHL	OMC-CMC-C2C	-2.66	119.67	125.69
5	F	308	CHL	C2A-C3A-C4A	2.66	105.18	101.78
9	F	320	0UR	C21-C12-C11	-2.66	119.20	122.92
5	F	311	CHL	C3A-C2A-C1A	-2.66	97.35	101.34
5	F	304	CHL	C2A-C1A-CHA	-2.66	119.21	123.86
6	B	315	CLA	C3C-C4C-NC	-2.66	107.59	110.57
5	F	317	CHL	OMC-CMC-C2C	-2.66	119.68	125.69
5	A	305	CHL	CHD-C4C-NC	2.65	128.39	124.20
9	F	320	0UR	C48-C47-C46	-2.65	120.16	125.85
6	F	306	CLA	C1-C2-C3	-2.65	121.46	126.04
5	F	304	CHL	OMC-CMC-C2C	-2.65	119.70	125.69
5	B	306	CHL	C2A-C3A-C4A	2.65	106.15	101.87
6	F	313	CLA	CHB-C4A-NA	2.65	128.17	124.51
6	F	314	CLA	C3B-C4B-NB	-2.64	108.06	110.52
5	C	312	CHL	C2A-C1A-CHA	-2.64	119.24	123.86
6	A	314	CLA	C7-C6-C5	-2.64	106.19	113.36
5	A	311	CHL	O2D-CGD-O1D	-2.64	118.68	123.84
5	E	311	CHL	O2A-CGA-CBA	2.64	120.18	111.91
5	E	304	CHL	C4D-CHA-C1A	-2.64	118.04	121.25
5	B	313	CHL	C2A-C1A-CHA	-2.63	119.25	123.86
5	D	313	CHL	OBD-CAD-C3D	-2.63	122.18	128.52
6	F	313	CLA	CHD-C1D-ND	-2.63	122.03	124.45
9	E	320	0UR	C23-C24-C25	-2.63	107.70	113.64
6	B	308	CLA	C3B-C4B-NB	-2.63	108.07	110.52
5	E	312	CHL	CAC-C3C-C4C	2.63	128.22	124.81
9	B	325	0UR	C10-C9-C8	-2.63	118.08	123.47
5	D	313	CHL	O2D-CGD-O1D	-2.63	118.69	123.84
11	F	319	LMG	O6-C1-O1	-2.63	103.75	109.97
5	B	312	CHL	CMD-C2D-C3D	-2.63	121.56	127.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	307	CLA	CHB-C4A-NA	2.63	128.15	124.51
5	B	311	CHL	C5-C3-C4	2.63	120.41	114.60
5	A	313	CHL	O2A-CGA-CBA	2.63	120.15	111.91
5	D	318	CHL	CAC-C3C-C4C	2.63	128.22	124.81
5	D	318	CHL	O2D-CGD-O1D	-2.63	118.70	123.84
5	B	311	CHL	CHC-C1C-NC	2.63	128.19	124.20
5	A	311	CHL	C2A-C3A-C4A	2.62	106.11	101.87
5	C	306	CHL	O2D-CGD-O1D	-2.62	118.72	123.84
7	A	319	LHG	C11-C10-C9	-2.62	101.15	114.42
5	E	304	CHL	OMC-CMC-C2C	-2.62	119.77	125.69
6	B	316	CLA	CHB-C4A-NA	2.61	128.13	124.51
5	F	311	CHL	O2D-CGD-O1D	-2.61	118.73	123.84
5	A	311	CHL	O2A-C1-C2	-2.61	101.77	108.64
6	B	317	CLA	CHB-C4A-NA	2.61	128.12	124.51
5	A	309	CHL	CHD-C1D-C2D	-2.60	120.02	125.48
6	D	314	CLA	CHB-C4A-NA	2.60	128.11	124.51
5	F	308	CHL	CHD-C4C-NC	2.60	128.30	124.20
6	F	313	CLA	CMB-C2B-C1B	-2.60	121.41	125.37
5	D	318	CHL	CHD-C4C-C3C	-2.60	121.02	124.84
7	B	320	LHG	C11-C10-C9	-2.59	101.25	114.42
6	D	314	CLA	CHB-C1B-NB	2.59	127.00	124.26
5	A	309	CHL	CAC-C3C-C4C	2.59	128.18	124.81
6	F	315	CLA	CHB-C4A-NA	2.59	128.10	124.51
9	A	322	OUR	O42-C2-C41	-2.59	116.83	120.58
5	F	312	CHL	C2A-C1A-CHA	-2.59	119.33	123.86
5	B	306	CHL	CHD-C4C-NC	2.59	128.28	124.20
5	C	306	CHL	CAC-C3C-C4C	2.59	128.17	124.81
9	A	322	OUR	C33-C32-C31	-2.59	118.03	123.56
5	B	313	CHL	CAC-C3C-C4C	2.58	128.16	124.81
7	C	319	LHG	C11-C10-C9	-2.58	101.32	114.42
5	F	312	CHL	C4-C3-C5	2.58	119.61	115.27
5	B	314	CHL	CHA-C4D-ND	2.58	137.90	132.50
5	D	313	CHL	OMC-CMC-C2C	-2.58	119.85	125.69
9	C	321	OUR	O42-C2-C3	-2.58	115.94	120.66
6	B	309	CLA	CHD-C1D-ND	-2.58	122.08	124.45
5	B	310	CHL	CHD-C1D-C2D	-2.58	120.07	125.48
5	C	311	CHL	CHD-C4C-C3C	-2.58	121.05	124.84
5	E	309	CHL	CHC-C4B-C3B	-2.58	116.25	127.71
6	E	313	CLA	C3B-C4B-NB	-2.58	108.12	110.52
5	C	310	CHL	CHC-C4B-C3B	-2.58	116.25	127.71
6	E	306	CLA	CHB-C4A-NA	2.58	128.07	124.51
3	E	303	NEX	C11-C12-C13	2.58	133.65	126.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	318	CHL	CAC-C3C-C4C	2.57	128.15	124.81
6	D	314	CLA	C3B-C4B-NB	-2.57	108.13	110.52
7	F	318	LHG	O8-C23-O10	-2.57	117.10	123.59
5	A	312	CHL	C3A-C2A-C1A	-2.57	97.49	101.34
2	A	301	OIE	C13-C12-C11	2.57	122.89	118.94
5	E	312	CHL	OMC-CMC-C2C	-2.57	119.88	125.69
6	C	314	CLA	C3B-C4B-NB	-2.56	108.14	110.52
9	B	302	OURL	O42-C2-C41	-2.56	116.87	120.58
9	C	321	OURL	C10-C11-C12	-2.56	123.66	127.31
6	E	307	CLA	CMB-C2B-C1B	-2.56	121.47	125.37
6	B	315	CLA	O2A-CGA-O1A	-2.56	117.14	123.59
5	D	306	CHL	CHA-C4D-ND	2.56	137.85	132.50
7	F	318	LHG	C5-O7-C7	-2.56	111.50	117.79
5	E	310	CHL	CAA-C2A-C1A	2.55	120.34	111.97
2	E	301	OIE	C4-C3-C2	2.55	122.27	120.08
5	C	309	CHL	C4D-CHA-C1A	-2.55	118.14	121.25
3	B	303	NEX	C20-C13-C14	-2.55	119.35	122.92
4	D	304	LMU	O5'-C1'-C2'	2.54	115.73	110.35
5	C	305	CHL	O2A-CGA-O1A	-2.54	117.17	123.59
5	F	309	CHL	CAC-C3C-C4C	2.54	128.11	124.81
6	C	317	CLA	CHB-C1B-NB	2.54	126.95	124.26
9	B	302	OURL	C4-C3-C2	2.54	122.26	120.08
5	B	307	CHL	CHD-C1D-ND	2.54	126.78	124.45
5	C	309	CHL	CAC-C3C-C4C	2.54	128.10	124.81
5	E	311	CHL	C4-C3-C5	2.54	119.54	115.27
5	C	311	CHL	OMC-CMC-C2C	-2.54	119.95	125.69
9	A	322	OURL	O42-C2-C3	-2.53	116.03	120.66
5	F	311	CHL	CHC-C4B-C3B	-2.53	116.44	127.71
5	A	318	CHL	CHC-C1C-NC	2.53	128.04	124.20
9	F	320	OURL	C22-C16-C15	-2.53	119.38	122.92
5	E	312	CHL	C4-C3-C5	2.53	119.52	115.27
5	E	308	CHL	CHD-C1D-C2D	-2.53	120.18	125.48
6	B	318	CLA	C3B-C4B-NB	-2.53	108.17	110.52
6	A	317	CLA	C1-C2-C3	-2.53	121.67	126.04
4	B	304	LMU	C4B-C3B-C2B	2.53	115.23	110.82
5	C	305	CHL	OMC-CMC-C2C	-2.53	119.98	125.69
5	E	309	CHL	C2A-C1A-CHA	-2.52	119.44	123.86
5	A	305	CHL	CAC-C3C-C4C	2.52	128.08	124.81
6	C	316	CLA	CHB-C4A-NA	2.52	128.00	124.51
2	A	301	OIE	C5-C4-C3	2.52	130.03	127.00
5	A	306	CHL	C1-O2A-CGA	2.52	123.05	116.44
9	D	321	OURL	C33-C32-C31	-2.51	118.18	123.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	317	CLA	CHB-C4A-NA	2.51	127.98	124.51
6	E	316	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
6	E	316	CLA	CHB-C4A-NA	2.51	127.98	124.51
5	C	310	CHL	CHD-C4C-NC	2.51	128.15	124.20
5	C	305	CHL	C4-C3-C5	2.51	119.49	115.27
5	E	310	CHL	O2D-CGD-O1D	-2.50	118.94	123.84
6	E	314	CLA	C3B-C4B-NB	-2.50	108.20	110.52
5	B	312	CHL	C2A-C1A-CHA	-2.49	119.50	123.86
2	F	301	0IE	C4-C3-C2	2.49	122.22	120.08
7	D	319	LHG	C11-C10-C9	-2.49	101.77	114.42
9	B	325	0UR	C33-C32-C31	-2.49	118.23	123.56
5	F	312	CHL	CHA-C4D-ND	2.49	137.71	132.50
6	D	307	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
4	B	305	LMU	O5'-C1'-C2'	-2.49	105.08	110.35
5	B	319	CHL	CHD-C4C-C3C	-2.49	121.19	124.84
5	F	312	CHL	O2A-CGA-CBA	2.49	119.71	111.91
4	B	305	LMU	C1B-O1B-C4'	-2.48	111.81	117.96
6	D	314	CLA	CHD-C1D-ND	-2.48	122.17	124.45
6	D	307	CLA	CHB-C4A-NA	2.48	127.95	124.51
5	C	313	CHL	OMC-CMC-C2C	-2.48	120.07	125.69
9	D	321	0UR	C21-C12-C11	-2.48	119.44	122.92
5	B	306	CHL	CAC-C3C-C4C	2.48	128.03	124.81
3	C	303	NEX	C39-C29-C30	-2.48	119.45	122.92
5	C	310	CHL	C4D-CHA-C1A	-2.48	118.23	121.25
6	D	317	CLA	C3B-C4B-NB	-2.48	108.21	110.52
7	D	319	LHG	C20-C19-C18	-2.48	101.85	114.42
5	D	310	CHL	CHC-C4B-C3B	-2.48	116.69	127.71
5	A	312	CHL	CHD-C4C-C3C	-2.48	121.20	124.84
9	A	322	0UR	C10-C9-C8	-2.47	118.41	123.47
5	A	318	CHL	CHC-C4B-C3B	-2.47	116.72	127.71
9	A	322	0UR	C15-C14-C13	-2.47	115.50	123.22
5	C	318	CHL	C3A-C2A-C1A	-2.47	97.64	101.34
5	A	318	CHL	O2D-CGD-O1D	-2.47	119.01	123.84
5	B	319	CHL	OMC-CMC-C2C	-2.47	120.11	125.69
5	C	311	CHL	C3C-C4C-NC	2.46	113.33	110.57
5	E	312	CHL	C2A-C3A-C4A	2.46	105.85	101.87
7	E	318	LHG	C11-C10-C9	-2.46	101.93	114.42
5	D	306	CHL	CHD-C1D-C2D	-2.46	120.32	125.48
5	B	319	CHL	CHC-C4B-C3B	-2.46	116.76	127.71
5	C	311	CHL	C1-O2A-CGA	2.46	122.90	116.44
5	A	318	CHL	C2A-C3A-C4A	2.46	104.92	101.78
6	A	314	CLA	CHB-C4A-NA	2.46	127.91	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	318	CHL	CHC-C4B-C3B	-2.46	116.79	127.71
6	C	314	CLA	C1-C2-C3	-2.46	121.80	126.04
5	F	305	CHL	CAC-C3C-C4C	2.45	127.99	124.81
6	E	316	CLA	C3B-C4B-NB	-2.45	108.24	110.52
9	B	302	OUR	C28-C19-C18	-2.45	109.60	112.70
5	F	304	CHL	O2A-CGA-CBA	2.45	119.60	111.91
6	E	307	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
5	D	305	CHL	O2D-CGD-O1D	-2.45	119.05	123.84
5	F	304	CHL	C2A-C3A-C4A	2.45	105.83	101.87
6	A	307	CLA	CHB-C4A-NA	2.45	127.90	124.51
5	A	313	CHL	C2A-C1A-CHA	-2.45	119.57	123.86
5	F	317	CHL	O2D-CGD-O1D	-2.45	119.05	123.84
6	E	306	CLA	O2D-CGD-CBD	2.45	115.61	111.27
5	D	318	CHL	OMC-CMC-C2C	-2.44	120.16	125.69
5	A	305	CHL	CAA-CBA-CGA	-2.44	106.11	113.25
3	D	303	NEX	C40-C33-C34	-2.44	119.50	122.92
9	B	325	OUR	C47-C46-C45	-2.44	116.69	122.92
5	F	305	CHL	CHC-C4B-C3B	-2.44	116.84	127.71
5	E	309	CHL	O2D-CGD-O1D	-2.44	119.06	123.84
6	B	309	CLA	C3B-C4B-NB	-2.44	108.25	110.52
6	E	315	CLA	CHB-C4A-NA	2.44	127.89	124.51
5	C	309	CHL	O2D-CGD-O1D	-2.44	119.06	123.84
5	B	313	CHL	CHC-C4B-C3B	-2.44	116.86	127.71
5	D	306	CHL	OMC-CMC-C2C	-2.44	120.17	125.69
3	F	303	NEX	C20-C13-C14	-2.44	119.51	122.92
6	C	316	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
5	D	309	CHL	CHD-C4C-NC	2.43	128.04	124.20
6	B	318	CLA	CHB-C4A-NA	2.43	127.87	124.51
5	F	308	CHL	CHC-C4B-C3B	-2.43	116.91	127.71
5	D	318	CHL	CHC-C4B-C3B	-2.43	116.91	127.71
4	B	304	LMU	C1B-O5B-C5B	-2.43	108.92	113.69
3	C	303	NEX	O24-C25-C26	-2.43	56.95	58.96
9	C	321	OUR	O42-C2-C41	-2.43	117.07	120.58
9	B	325	OUR	O42-C2-C41	-2.42	117.07	120.58
2	A	302	OIE	C14-C15-C16	2.42	130.77	127.31
5	F	309	CHL	CMD-C2D-C3D	-2.42	122.04	127.61
9	F	320	OUR	C25-C26-C27	-2.42	107.03	111.85
6	A	314	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
6	A	308	CLA	C3B-C4B-NB	-2.42	108.27	110.52
6	A	314	CLA	CAC-C3C-C4C	2.42	127.95	124.81
3	F	303	NEX	O24-C25-C26	-2.42	56.96	58.96
5	D	309	CHL	CHD-C1D-C2D	-2.41	120.42	125.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	311	CHL	O2D-CGD-O1D	-2.41	119.12	123.84
5	D	305	CHL	CHD-C4C-C3C	-2.41	121.29	124.84
5	D	310	CHL	CHD-C4C-NC	2.41	128.00	124.20
6	A	308	CLA	CHB-C4A-NA	2.41	127.85	124.51
4	B	305	LMU	C3'-C4'-C5'	2.41	116.45	110.93
5	F	312	CHL	OBD-CAD-C3D	2.41	134.32	128.52
5	F	312	CHL	CHC-C4B-C3B	-2.41	116.99	127.71
5	D	313	CHL	CHD-C1D-C2D	-2.41	120.42	125.48
5	A	312	CHL	C2A-C1A-CHA	-2.41	119.64	123.86
5	F	308	CHL	OMC-CMC-C2C	-2.41	120.24	125.69
5	F	317	CHL	CHC-C4B-C3B	-2.41	117.00	127.71
5	C	313	CHL	O2A-CGA-CBA	2.41	119.46	111.91
5	D	310	CHL	O2D-CGD-O1D	-2.41	119.13	123.84
5	D	305	CHL	C1-C2-C3	-2.40	121.89	126.04
5	A	313	CHL	CED-O2D-CGD	2.40	121.36	115.94
5	F	311	CHL	CHD-C1D-C2D	-2.40	120.45	125.48
5	A	312	CHL	O2D-CGD-O1D	-2.39	119.16	123.84
5	C	306	CHL	O2A-CGA-CBA	2.39	119.42	111.91
6	C	315	CLA	CHB-C4A-NA	2.39	127.82	124.51
5	D	312	CHL	C1-C2-C3	-2.39	121.91	126.04
7	F	318	LHG	C20-C19-C18	-2.39	102.31	114.42
9	E	320	OUR	O44-C43-C3	2.38	115.49	109.11
5	C	305	CHL	O2D-CGD-O1D	-2.38	119.18	123.84
6	D	314	CLA	C1-C2-C3	-2.38	121.92	126.04
9	B	302	OUR	C35-C23-C1	-2.38	106.31	109.71
5	A	318	CHL	OMC-CMC-C2C	-2.38	120.31	125.69
5	F	304	CHL	CAC-C3C-C4C	2.38	127.90	124.81
5	E	312	CHL	C2A-C1A-CHA	-2.38	119.70	123.86
5	D	312	CHL	C2C-C3C-C4C	-2.38	104.79	106.49
5	B	312	CHL	C4-C3-C5	2.38	119.27	115.27
5	C	312	CHL	CHC-C4B-C3B	-2.38	117.14	127.71
5	C	313	CHL	O1D-CGD-CBD	-2.38	119.62	124.48
6	D	308	CLA	CHB-C1B-NB	2.38	126.77	124.26
5	F	312	CHL	OMC-CMC-C2C	-2.38	120.32	125.69
5	D	311	CHL	CHD-C4C-C3C	-2.38	121.35	124.84
6	D	317	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
5	D	306	CHL	C4-C3-C5	2.37	119.26	115.27
5	E	308	CHL	O2D-CGD-O1D	-2.37	119.20	123.84
9	B	325	OUR	C21-C12-C11	-2.37	119.61	122.92
6	F	307	CLA	CHD-C1D-ND	-2.37	122.28	124.45
9	A	322	OUR	C20-C7-C6	2.37	121.81	118.08
5	D	313	CHL	CHC-C4B-C3B	-2.37	117.18	127.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	308	CLA	CHB-C4A-NA	2.37	127.78	124.51
5	E	309	CHL	CHD-C4C-NC	2.36	127.93	124.20
6	A	314	CLA	C2D-C1D-ND	-2.36	108.36	110.10
5	A	309	CHL	CHD-C4C-NC	2.36	127.93	124.20
9	E	320	0UR	C28-C19-C18	-2.36	109.72	112.70
6	A	317	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
5	F	304	CHL	C4-C3-C5	2.36	119.24	115.27
9	B	325	0UR	C48-C47-C46	-2.36	120.79	125.85
5	C	310	CHL	OMC-CMC-C2C	-2.36	120.36	125.69
5	F	304	CHL	CHC-C4B-C3B	-2.36	117.22	127.71
5	D	306	CHL	O2D-CGD-O1D	-2.36	119.23	123.84
3	B	303	NEX	C39-C29-C30	-2.36	119.62	122.92
4	B	305	LMU	C1'-O5'-C5'	-2.36	109.06	113.69
5	A	310	CHL	CHC-C4B-C3B	-2.36	117.23	127.71
5	B	312	CHL	O2D-CGD-O1D	-2.35	119.23	123.84
6	F	313	CLA	CMB-C2B-C3B	2.35	132.29	126.59
6	D	314	CLA	CMB-C2B-C1B	-2.35	121.78	125.37
5	D	318	CHL	C2D-C1D-ND	-2.35	108.37	110.10
6	D	308	CLA	CHD-C1D-ND	-2.35	122.29	124.45
5	D	311	CHL	C2A-C1A-CHA	-2.35	119.75	123.86
5	E	311	CHL	C2A-C1A-CHA	-2.35	119.75	123.86
6	B	316	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
5	F	310	CHL	CHC-C4B-C3B	-2.35	117.27	127.71
5	D	311	CHL	O2D-CGD-O1D	-2.35	119.25	123.84
6	B	318	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
5	C	318	CHL	CHC-C1C-NC	2.34	127.76	124.20
5	E	304	CHL	C2A-C3A-C4A	2.34	105.65	101.87
9	E	320	0UR	O44-C45-O57	-2.34	117.78	122.93
5	B	314	CHL	C3D-C2D-C1D	-2.34	102.64	105.83
5	D	313	CHL	C4D-CHA-C1A	-2.34	118.40	121.25
5	F	311	CHL	CHA-C4D-ND	2.34	137.39	132.50
6	D	308	CLA	CMB-C2B-C1B	-2.34	121.81	125.37
5	C	306	CHL	CHC-C4B-C3B	-2.34	117.31	127.71
6	D	315	CLA	CHB-C4A-NA	2.34	127.74	124.51
5	B	311	CHL	CHC-C4B-C3B	-2.33	117.33	127.71
6	A	317	CLA	CHD-C1D-ND	-2.33	122.31	124.45
6	B	309	CLA	CHB-C1B-NB	2.33	126.73	124.26
6	C	316	CLA	CHC-C4B-NB	2.33	126.73	124.26
6	E	313	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
5	A	305	CHL	C2A-C1A-CHA	-2.33	119.78	123.86
6	F	316	CLA	CHB-C1B-NB	2.33	126.73	124.26
5	F	304	CHL	CAA-CBA-CGA	-2.33	106.44	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	314	CLA	CMB-C2B-C1B	-2.33	121.82	125.37
6	D	314	CLA	O1D-CGD-CBD	2.33	129.25	124.48
6	A	314	CLA	CMB-C2B-C1B	-2.33	121.82	125.37
6	F	316	CLA	CHB-C4A-NA	2.33	127.73	124.51
5	E	305	CHL	O2A-CGA-O1A	-2.33	117.71	123.59
5	A	309	CHL	OMC-CMC-C2C	-2.33	120.42	125.69
6	C	308	CLA	CMB-C2B-C1B	-2.33	121.82	125.37
5	D	305	CHL	CHC-C4B-C3B	-2.33	117.35	127.71
9	B	325	OUR	O44-C43-C3	2.33	115.34	109.11
6	F	313	CLA	CHB-C1B-NB	2.33	126.72	124.26
5	A	305	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
5	A	312	CHL	CHC-C4B-C3B	-2.33	117.36	127.71
6	A	315	CLA	O2D-CGD-CBD	2.33	115.40	111.27
6	C	315	CLA	CHD-C1D-ND	-2.32	122.32	124.45
5	E	304	CHL	CAC-C3C-C4C	2.32	127.82	124.81
6	C	315	CLA	C3B-C4B-NB	-2.32	108.36	110.52
5	B	307	CHL	CMB-C2B-C1B	2.32	128.91	125.37
7	F	318	LHG	C18-C17-C16	-2.32	102.64	114.42
6	F	316	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
5	E	311	CHL	CHD-C4C-NC	2.32	127.86	124.20
5	A	306	CHL	OMC-CMC-C2C	-2.32	120.44	125.69
5	A	312	CHL	C6-C5-C3	-2.32	107.37	113.45
5	D	313	CHL	C2A-C1A-CHA	-2.32	119.80	123.86
5	B	307	CHL	OMC-CMC-C2C	-2.32	120.44	125.69
5	C	318	CHL	CHD-C4C-NC	2.32	127.86	124.20
5	F	308	CHL	O2D-CGD-O1D	-2.32	119.31	123.84
5	E	310	CHL	C3B-C2B-C1B	-2.32	104.36	107.16
6	C	317	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
6	A	317	CLA	CHB-C1B-NB	2.31	126.70	124.26
3	B	303	NEX	C20-C13-C12	2.31	121.72	118.08
6	A	308	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
6	C	307	CLA	C3B-C4B-NB	-2.31	108.37	110.52
5	A	313	CHL	O1D-CGD-CBD	-2.31	119.76	124.48
9	F	320	OUR	C21-C12-C13	2.31	121.71	118.08
6	D	308	CLA	CHB-C4A-NA	2.31	127.70	124.51
5	F	305	CHL	CBC-CAC-C3C	-2.31	106.07	112.43
5	E	305	CHL	OMC-CMC-C2C	-2.31	120.47	125.69
5	E	304	CHL	CAA-CBA-CGA	-2.30	106.52	113.25
5	A	305	CHL	CHC-C1C-C2C	-2.30	117.76	126.11
5	F	309	CHL	CMA-C3A-C2A	-2.30	110.72	116.10
6	E	313	CLA	CHB-C4A-NA	2.30	127.70	124.51
2	C	301	OIE	C17-C16-C15	2.30	122.47	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	311	CHL	C1-C2-C3	-2.30	122.06	126.04
5	D	312	CHL	CBC-CAC-C3C	-2.30	106.09	112.43
7	E	318	LHG	O8-C23-O10	-2.30	117.79	123.59
3	F	303	NEX	C31-C32-C33	-2.30	119.96	126.42
5	C	318	CHL	C4D-CHA-C1A	-2.30	118.45	121.25
6	E	313	CLA	CHB-C1B-NB	2.30	126.69	124.26
9	C	321	OUR	C28-C19-C32	-2.30	107.30	111.42
5	C	306	CHL	OMC-CMC-C2C	-2.30	120.50	125.69
5	B	313	CHL	CHD-C4C-NC	2.30	127.82	124.20
6	E	314	CLA	CHB-C4A-NA	2.29	127.68	124.51
5	E	305	CHL	C16-C15-C13	-2.29	108.50	115.92
2	C	302	OIE	C17-C16-C15	2.29	122.46	118.94
9	B	325	OUR	C15-C14-C13	-2.29	116.07	123.22
11	B	323	LMG	C1-O6-C5	-2.29	109.19	113.69
5	A	310	CHL	OMC-CMC-C2C	-2.29	120.51	125.69
5	E	305	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
6	F	315	CLA	CHB-C1B-NB	2.29	126.68	124.26
6	B	316	CLA	C1-C2-C3	-2.29	122.09	126.04
5	C	305	CHL	CMA-C3A-C4A	-2.29	105.63	111.77
5	D	312	CHL	CHD-C1D-C2D	-2.29	120.69	125.48
5	A	311	CHL	OMC-CMC-C2C	-2.29	120.52	125.69
6	F	307	CLA	CHB-C4A-NA	2.29	127.67	124.51
7	C	319	LHG	C27-C26-C25	-2.28	102.83	114.42
5	A	305	CHL	C3A-C2A-C1A	-2.28	97.92	101.34
5	F	312	CHL	C1-C2-C3	-2.28	122.09	126.04
5	B	307	CHL	CHC-C4B-C3B	-2.28	117.56	127.71
5	C	309	CHL	C2A-C3A-C4A	2.28	104.69	101.78
5	A	311	CHL	C1-C2-C3	-2.28	122.10	126.04
3	A	303	NEX	C39-C29-C30	-2.28	119.73	122.92
6	F	314	CLA	CHB-C4A-NA	2.28	127.67	124.51
5	A	306	CHL	O2A-CGA-O1A	-2.28	117.84	123.59
5	E	311	CHL	CHC-C4B-C3B	-2.28	117.57	127.71
5	C	313	CHL	CAC-C3C-C4C	2.28	127.77	124.81
5	F	304	CHL	O2A-CGA-O1A	-2.28	117.85	123.59
5	E	305	CHL	C11-C12-C13	-2.28	108.56	115.92
5	B	314	CHL	C4-C3-C5	2.27	119.10	115.27
5	C	311	CHL	O2D-CGD-O1D	-2.27	119.39	123.84
5	D	306	CHL	C16-C15-C13	-2.27	108.57	115.92
6	C	315	CLA	C1-C2-C3	-2.27	122.11	126.04
6	A	315	CLA	CHB-C4A-NA	2.27	127.66	124.51
5	C	306	CHL	CHD-C1D-C2D	-2.27	120.71	125.48
5	D	311	CHL	C2A-C3A-C4A	2.27	105.54	101.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	313	CHL	CHD-C1D-C2D	-2.27	120.72	125.48
5	D	312	CHL	C3A-C2A-C1A	-2.27	97.94	101.34
2	D	302	0IE	C39-C32-C31	2.27	112.95	109.71
5	F	317	CHL	O1D-CGD-CBD	-2.27	119.84	124.48
6	C	308	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
3	C	303	NEX	C31-C32-C33	-2.27	120.05	126.42
6	E	313	CLA	CMB-C2B-C1B	-2.27	121.92	125.37
7	C	304	LHG	O8-C23-C24	2.27	119.02	111.91
5	C	311	CHL	CHC-C4B-C3B	-2.26	117.65	127.71
5	D	318	CHL	C3A-C2A-C1A	-2.26	97.95	101.34
6	C	314	CLA	CHB-C1B-NB	2.26	126.65	124.26
5	B	306	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
7	B	320	LHG	C20-C19-C18	-2.26	102.97	114.42
5	F	311	CHL	C6-C5-C3	-2.26	107.54	113.45
5	A	318	CHL	CAC-C3C-C4C	2.25	127.73	124.81
9	B	325	0UR	C9-C8-C7	-2.25	124.10	127.31
3	D	303	NEX	C20-C13-C14	-2.25	119.77	122.92
6	C	307	CLA	CHC-C4B-NB	2.25	126.64	124.26
7	B	324	LHG	O8-C23-O10	-2.25	117.92	123.59
5	F	309	CHL	C2A-C1A-CHA	-2.24	119.94	123.85
5	D	309	CHL	CHC-C4B-C3B	-2.24	117.74	127.71
5	F	310	CHL	C2A-C3A-C4A	2.24	105.49	101.87
5	C	312	CHL	OMC-CMC-C2C	-2.24	120.62	125.69
3	F	303	NEX	C11-C12-C13	2.24	132.71	126.42
5	F	312	CHL	C4D-CHA-C1A	-2.24	118.53	121.25
5	E	305	CHL	C11-C10-C8	-2.24	108.69	115.92
6	E	307	CLA	C3B-C4B-NB	-2.24	108.44	110.52
5	D	312	CHL	O2D-CGD-O1D	-2.23	119.47	123.84
6	F	313	CLA	C3A-C2A-C1A	2.23	104.68	101.34
7	E	318	LHG	C18-C17-C16	-2.23	103.10	114.42
5	D	305	CHL	C2D-C1D-ND	-2.23	108.46	110.10
3	D	303	NEX	C39-C29-C30	-2.23	119.80	122.92
5	F	305	CHL	C2A-C3A-C4A	2.23	105.47	101.87
5	B	306	CHL	O2A-CGA-CBA	2.23	118.90	111.91
5	B	311	CHL	C2A-C1A-CHA	-2.23	119.96	123.86
5	C	312	CHL	C2A-C3A-C4A	2.23	105.47	101.87
6	F	306	CLA	CHC-C4B-NB	2.23	126.61	124.26
9	A	322	0UR	C47-C46-C45	-2.23	117.24	122.92
5	B	307	CHL	C16-C15-C13	-2.22	108.74	115.92
9	C	321	0UR	C21-C12-C13	2.22	121.58	118.08
6	A	317	CLA	CHB-C4A-NA	2.22	127.58	124.51
5	D	309	CHL	CAA-C2A-C3A	-2.22	110.92	116.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	305	CHL	OMC-CMC-C2C	-2.22	120.67	125.69
5	C	313	CHL	CHC-C4B-C3B	-2.22	117.85	127.71
6	B	317	CLA	CHB-C1B-NB	2.22	126.60	124.26
6	C	314	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
6	A	307	CLA	CHC-C4B-NB	2.22	126.60	124.26
5	B	312	CHL	CHC-C4B-C3B	-2.21	117.86	127.71
7	E	318	LHG	O8-C23-C24	2.21	118.86	111.91
5	D	309	CHL	CMA-C3A-C2A	-2.21	110.93	116.10
6	A	317	CLA	CHC-C4B-NB	2.21	126.60	124.26
5	F	311	CHL	CAC-C3C-C4C	2.21	127.68	124.81
5	F	305	CHL	OMC-CMC-C2C	-2.21	120.69	125.69
5	D	309	CHL	CAC-C3C-C4C	2.21	127.67	124.81
9	A	322	OUR	C23-C24-C25	-2.21	108.66	113.64
6	B	315	CLA	C3B-C4B-NB	-2.21	108.47	110.52
7	D	319	LHG	C18-C17-C16	-2.21	103.22	114.42
3	A	303	NEX	C31-C32-C33	-2.21	120.22	126.42
6	E	314	CLA	CHD-C1D-ND	-2.21	122.43	124.45
5	E	304	CHL	CHD-C1D-C2D	-2.21	120.85	125.48
5	F	309	CHL	CHC-C4B-C3B	-2.21	117.89	127.71
5	A	306	CHL	CHD-C1D-C2D	-2.21	120.85	125.48
5	B	310	CHL	C2A-C3A-C4A	2.20	105.43	101.87
3	F	303	NEX	C24-C23-C22	-2.20	106.52	110.77
5	D	318	CHL	O2A-CGA-CBA	2.20	121.11	114.03
5	B	314	CHL	O2A-CGA-CBA	2.20	118.81	111.91
5	E	304	CHL	C6-C5-C3	-2.20	107.69	113.45
5	B	310	CHL	OMC-CMC-C2C	-2.20	120.72	125.69
5	F	305	CHL	O2A-CGA-CBA	2.20	118.80	111.91
5	B	311	CHL	C4D-CHA-C1A	-2.20	118.58	121.25
5	F	312	CHL	CHD-C1D-C2D	-2.20	120.87	125.48
6	F	314	CLA	CHB-C1B-NB	2.20	126.58	124.26
2	D	302	OIE	C4-C5-C6	2.20	130.07	123.22
5	A	310	CHL	C5-C3-C4	2.19	119.45	114.60
5	D	312	CHL	C4-C3-C5	2.19	118.96	115.27
5	E	309	CHL	C2A-C3A-C4A	2.19	105.41	101.87
5	C	305	CHL	CHD-C1D-C2D	-2.19	120.88	125.48
5	A	306	CHL	O2D-CGD-O1D	-2.19	119.55	123.84
5	E	309	CHL	CHC-C1C-NC	2.19	127.53	124.20
5	A	310	CHL	CBC-CAC-C3C	-2.19	106.39	112.43
5	F	312	CHL	C2A-C3A-C4A	2.19	105.41	101.87
5	A	306	CHL	CHC-C4B-C3B	-2.19	117.97	127.71
5	B	311	CHL	OMC-CMC-C2C	-2.19	120.74	125.69
5	E	317	CHL	CHC-C4B-C3B	-2.19	117.98	127.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	310	CHL	O2A-CGA-O1A	-2.19	118.07	123.59
6	A	307	CLA	O2D-CGD-CBD	2.19	115.16	111.27
6	E	306	CLA	C1-C2-C3	-2.19	122.26	126.04
7	D	319	LHG	C5-O7-C7	-2.19	112.41	117.79
5	E	312	CHL	CHC-C4B-C3B	-2.19	117.99	127.71
11	B	323	LMG	O6-C1-O1	-2.18	104.80	109.97
3	B	303	NEX	O24-C25-C26	-2.18	57.15	58.96
5	D	306	CHL	O2A-CGA-O1A	-2.18	118.08	123.59
5	F	317	CHL	O2A-CGA-CBA	2.18	121.05	114.03
5	E	304	CHL	C4-C3-C5	2.18	118.94	115.27
6	D	307	CLA	CHB-C1B-NB	2.18	126.57	124.26
5	A	309	CHL	CHC-C4B-C3B	-2.18	118.00	127.71
5	B	310	CHL	CHC-C4B-C3B	-2.18	118.01	127.71
6	C	314	CLA	CHB-C4A-NA	2.18	127.53	124.51
5	A	313	CHL	CAC-C3C-C4C	2.18	127.64	124.81
6	C	308	CLA	C3B-C4B-NB	-2.18	108.49	110.52
5	E	305	CHL	CHD-C1D-C2D	-2.18	120.91	125.48
6	B	309	CLA	CHB-C4A-NA	2.18	127.52	124.51
5	A	306	CHL	C2A-C3A-C4A	2.17	105.38	101.87
6	C	315	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
5	A	305	CHL	CHC-C4B-C3B	-2.17	118.05	127.71
4	B	305	LMU	C2'-C3'-C4'	2.17	114.64	109.68
5	C	313	CHL	C4D-CHA-C1A	-2.17	118.61	121.25
9	A	322	OUR	C4-C5-C6	-2.17	116.45	123.22
5	C	311	CHL	O2A-CGA-O1A	-2.17	118.12	123.59
5	F	309	CHL	O2D-CGD-O1D	-2.17	119.60	123.84
6	D	308	CLA	C3B-C4B-NB	-2.17	108.50	110.52
5	B	306	CHL	CHC-C4B-C3B	-2.17	118.07	127.71
5	F	309	CHL	C3C-C4C-NC	2.16	113.00	110.57
5	F	310	CHL	CAC-C3C-C4C	2.16	127.62	124.81
5	F	311	CHL	C3B-C2B-C1B	-2.16	104.55	107.16
5	B	311	CHL	C1-C2-C3	-2.16	123.25	126.75
6	D	314	CLA	C7-C6-C5	-2.16	107.49	113.36
5	F	305	CHL	CHC-C1C-C2C	-2.16	118.28	126.11
6	F	313	CLA	O2D-CGD-CBD	2.16	115.11	111.27
6	B	318	CLA	CHD-C1D-ND	-2.16	122.47	124.45
6	F	315	CLA	O2A-CGA-O1A	-2.16	117.92	123.30
5	E	311	CHL	C2A-C3A-C4A	2.16	105.36	101.87
5	F	308	CHL	O1D-CGD-CBD	-2.16	120.07	124.48
5	A	311	CHL	CHC-C4B-C3B	-2.16	118.12	127.71
6	D	317	CLA	CHB-C4A-NA	2.16	127.49	124.51
3	D	303	NEX	C31-C32-C33	-2.16	120.36	126.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	302	0UR	C33-C32-C31	-2.16	118.95	123.56
3	E	303	NEX	C39-C29-C30	-2.16	119.90	122.92
6	B	317	CLA	O2A-CGA-O1A	-2.15	117.93	123.30
5	C	312	CHL	C2D-C1D-ND	-2.15	108.52	110.10
5	C	312	CHL	CMD-C2D-C3D	-2.15	122.66	127.61
9	E	320	0UR	C22-C16-C15	-2.15	119.91	122.92
6	D	316	CLA	O2A-CGA-O1A	-2.15	117.94	123.30
6	B	315	CLA	CHB-C1B-NB	2.15	126.53	124.26
6	C	317	CLA	CHD-C1D-ND	-2.15	122.48	124.45
5	E	310	CHL	CMB-C2B-C1B	2.15	128.64	125.37
5	A	318	CHL	CHD-C4C-NC	2.15	127.59	124.20
5	C	311	CHL	CHA-C1A-NA	-2.15	121.48	126.40
5	F	304	CHL	CHC-C1C-C2C	-2.15	118.33	126.11
6	B	315	CLA	CAC-C3C-C2C	-2.15	123.86	127.53
7	B	320	LHG	O8-C23-C24	2.15	118.64	111.91
5	F	305	CHL	CHA-C4D-ND	2.14	136.98	132.50
6	D	315	CLA	O2D-CGD-CBD	2.14	115.08	111.27
6	D	314	CLA	C3C-C4C-NC	-2.14	108.17	110.57
5	D	306	CHL	CHC-C1C-C2C	-2.14	118.36	126.11
5	A	311	CHL	C2A-C1A-CHA	-2.14	120.12	123.86
5	C	309	CHL	CAA-C2A-C3A	-2.14	111.11	116.10
6	E	307	CLA	CMB-C2B-C3B	2.14	131.76	126.59
9	C	321	0UR	C28-C19-C18	-2.14	110.00	112.70
5	B	314	CHL	CHC-C4B-C3B	-2.13	118.21	127.71
5	C	305	CHL	CHC-C4B-C3B	-2.13	118.22	127.71
7	C	319	LHG	C20-C19-C18	-2.13	103.60	114.42
6	E	315	CLA	CHB-C1B-NB	2.13	126.51	124.26
5	E	310	CHL	CHC-C1C-C2C	-2.13	118.38	126.11
6	C	308	CLA	CHB-C1B-NB	2.13	126.51	124.26
6	A	317	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
5	E	310	CHL	O2A-CGA-O1A	-2.13	118.22	123.59
5	F	309	CHL	C2B-C1B-NB	-2.13	108.81	110.23
5	A	311	CHL	C3C-C4C-NC	2.13	112.96	110.57
9	B	325	0UR	C21-C12-C13	2.13	121.43	118.08
5	E	311	CHL	O2D-CGD-O1D	-2.13	119.68	123.84
5	F	308	CHL	CAA-C2A-C3A	-2.13	111.14	116.10
6	E	306	CLA	C11-C12-C13	-2.13	109.05	115.92
5	B	311	CHL	C3A-C2A-C1A	-2.13	98.16	101.34
6	D	314	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
5	E	310	CHL	CHC-C4B-C3B	-2.12	118.26	127.71
7	C	319	LHG	C18-C17-C16	-2.12	103.65	114.42
9	A	322	0UR	C28-C19-C18	-2.12	110.02	112.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	315	CLA	CMB-C2B-C1B	-2.12	122.14	125.37
6	D	314	CLA	CMB-C2B-C3B	2.12	131.73	126.59
5	D	305	CHL	O2A-CGA-CBA	2.12	118.57	111.91
5	A	305	CHL	CBC-CAC-C3C	-2.12	106.59	112.43
5	F	312	CHL	CMB-C2B-C1B	2.12	128.59	125.37
6	D	315	CLA	CHB-C1B-NB	2.12	126.50	124.26
9	B	302	0UR	O44-C45-O57	-2.12	118.28	122.93
5	D	306	CHL	CAC-C3C-C4C	2.12	127.56	124.81
11	F	319	LMG	O2-C2-C1	-2.12	104.91	110.05
2	A	301	0IE	C5-C6-C7	2.12	132.36	126.42
5	F	312	CHL	C1-O2A-CGA	2.12	122.00	116.44
3	B	303	NEX	C31-C32-C33	-2.12	120.47	126.42
6	F	313	CLA	C3C-C4C-NC	-2.12	108.20	110.57
5	A	310	CHL	CAC-C3C-C4C	2.11	127.55	124.81
5	D	311	CHL	O2A-CGA-O1A	-2.11	118.26	123.59
5	C	305	CHL	CAC-C3C-C4C	2.11	127.55	124.81
5	E	305	CHL	CHC-C4B-C3B	-2.11	118.31	127.71
2	F	301	0IE	C23-C16-C17	2.11	121.40	118.08
5	E	304	CHL	CHC-C1C-C2C	-2.11	118.46	126.11
11	B	323	LMG	O3-C3-C2	-2.11	105.48	110.35
5	F	317	CHL	C2D-C1D-ND	-2.11	108.55	110.10
5	E	304	CHL	CHC-C4B-C3B	-2.11	118.34	127.71
5	F	308	CHL	CAC-C3C-C4C	2.10	127.54	124.81
9	C	321	0UR	C9-C8-C7	-2.10	124.31	127.31
5	D	311	CHL	O1D-CGD-CBD	-2.10	120.18	124.48
7	F	318	LHG	C27-C26-C25	-2.10	103.75	114.42
9	D	321	0UR	C15-C14-C13	-2.10	116.66	123.22
11	F	319	LMG	O3-C3-C2	-2.10	105.49	110.35
6	A	314	CLA	CHD-C1D-ND	-2.10	122.52	124.45
6	A	314	CLA	CMB-C2B-C3B	2.10	131.68	126.59
5	A	306	CHL	CED-O2D-CGD	2.10	120.69	115.94
5	C	309	CHL	CHD-C1D-C2D	-2.10	121.08	125.48
5	D	310	CHL	O1D-CGD-CBD	-2.10	120.19	124.48
6	C	314	CLA	O2D-CGD-CBD	2.10	115.00	111.27
6	A	307	CLA	C4-C3-C5	2.10	118.80	115.27
5	E	308	CHL	CHC-C4B-C3B	-2.10	118.38	127.71
9	E	320	0UR	C21-C12-C11	-2.10	119.98	122.92
9	F	320	0UR	C34-C27-C1	-2.10	121.74	124.49
6	D	315	CLA	CHD-C1D-ND	-2.10	122.53	124.45
6	E	314	CLA	C1-C2-C3	-2.09	122.42	126.04
6	D	316	CLA	CHB-C1B-NB	2.09	126.47	124.26
5	D	313	CHL	O1D-CGD-CBD	-2.09	120.20	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	312	CHL	O2A-CGA-O1A	-2.09	118.31	123.59
5	E	305	CHL	CED-O2D-CGD	2.09	120.67	115.94
5	E	312	CHL	C1-O2A-CGA	2.09	121.94	116.44
5	B	307	CHL	C6-C5-C3	-2.09	107.97	113.45
6	A	315	CLA	CHB-C1B-NB	2.09	126.47	124.26
5	F	309	CHL	OMC-CMC-C2C	-2.09	120.96	125.69
11	B	323	LMG	O2-C2-C1	-2.09	104.97	110.05
5	C	313	CHL	C2A-C1A-CHA	-2.09	120.21	123.86
6	A	314	CLA	O1D-CGD-CBD	2.09	128.75	124.48
6	A	308	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
3	F	303	NEX	C19-C9-C10	-2.08	120.00	122.92
5	D	313	CHL	C2B-C1B-NB	-2.08	108.83	110.23
5	B	314	CHL	C11-C10-C8	-2.08	109.18	115.92
5	B	319	CHL	O1D-CGD-CBD	-2.08	120.22	124.48
5	C	312	CHL	C6-C5-C3	-2.08	108.00	113.45
5	F	312	CHL	CED-O2D-CGD	2.08	120.64	115.94
3	B	303	NEX	C40-C33-C34	-2.08	120.01	122.92
9	A	322	OUR	C4-C3-C2	-2.08	118.29	120.08
9	F	320	OUR	O42-C2-C41	-2.08	117.57	120.58
6	A	316	CLA	O2A-CGA-O1A	-2.08	118.12	123.30
10	B	321	BET	C-CA-N	-2.08	113.48	116.34
6	F	314	CLA	CHD-C1D-ND	-2.08	122.55	124.45
6	B	315	CLA	C3A-C2A-C1A	2.08	104.45	101.34
5	F	312	CHL	C3D-C2D-C1D	-2.08	103.00	105.83
6	A	314	CLA	C6-C5-C3	2.08	118.90	113.45
9	B	302	OUR	C17-C16-C15	2.07	122.12	118.94
9	D	321	OUR	C28-C19-C18	-2.07	110.08	112.70
5	D	313	CHL	C2A-C3A-C4A	2.07	105.22	101.87
5	B	319	CHL	O2A-CGA-CBA	2.07	120.42	112.23
5	D	311	CHL	CED-O2D-CGD	2.07	120.62	115.94
3	B	303	NEX	C19-C9-C10	-2.07	120.02	122.92
3	A	303	NEX	C40-C33-C34	-2.07	120.02	122.92
5	B	312	CHL	CHD-C4C-NC	2.07	127.47	124.20
5	E	317	CHL	CAC-C3C-C4C	2.07	127.49	124.81
7	D	319	LHG	C27-C26-C25	-2.07	103.93	114.42
5	A	305	CHL	C6-C5-C3	-2.07	108.03	113.45
6	D	315	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
5	F	317	CHL	CHD-C4C-C3C	-2.07	121.80	124.84
5	D	318	CHL	C2A-C1A-CHA	-2.07	120.25	123.86
9	B	302	OUR	O42-C2-C3	-2.06	116.89	120.66
6	B	308	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
5	F	304	CHL	CBC-CAC-C3C	-2.06	106.75	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	320	0UR	C15-C14-C13	-2.06	116.79	123.22
5	A	305	CHL	C2A-C3A-C4A	2.06	105.19	101.87
5	A	311	CHL	O2A-CGA-O1A	-2.06	118.40	123.59
6	F	314	CLA	C1-C2-C3	-2.06	122.49	126.04
7	B	320	LHG	C18-C17-C16	-2.06	103.99	114.42
5	D	312	CHL	C1-O2A-CGA	2.06	121.84	116.44
3	D	303	NEX	C19-C9-C10	-2.05	120.05	122.92
3	E	303	NEX	C19-C9-C10	-2.05	120.05	122.92
9	E	320	0UR	C21-C12-C13	2.05	121.31	118.08
6	E	307	CLA	C2A-C1A-CHA	2.05	127.44	123.86
5	E	310	CHL	OMC-CMC-C2C	-2.05	121.06	125.69
5	E	304	CHL	C1-C2-C3	-2.05	122.50	126.04
9	F	320	0UR	C33-C32-C31	-2.05	119.18	123.56
5	B	312	CHL	O2A-CGA-O1A	-2.05	118.43	123.59
5	D	311	CHL	C1-O2A-CGA	2.05	121.81	116.44
7	C	319	LHG	C5-O7-C7	-2.05	112.75	117.79
5	D	309	CHL	OMC-CMC-C2C	-2.05	121.06	125.69
5	C	309	CHL	CHC-C4B-C3B	-2.05	118.61	127.71
6	E	316	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
5	E	309	CHL	OMC-CMC-C2C	-2.04	121.07	125.69
5	B	311	CHL	O1D-CGD-CBD	-2.04	120.31	124.48
9	D	321	0UR	O42-C2-C41	-2.04	117.62	120.58
6	E	313	CLA	CHD-C1D-ND	-2.04	122.58	124.45
9	A	322	0UR	C21-C12-C11	-2.04	120.07	122.92
5	C	306	CHL	C4-C3-C2	-2.04	118.45	123.68
6	C	308	CLA	CMB-C2B-C3B	2.04	131.52	126.59
5	D	305	CHL	CHA-C1A-NA	-2.04	121.73	126.40
6	E	316	CLA	CHC-C4B-NB	2.04	126.41	124.26
7	E	318	LHG	C27-C26-C25	-2.03	104.09	114.42
5	D	312	CHL	C2A-C1A-CHA	-2.03	120.30	123.86
5	B	306	CHL	CHC-C1C-C2C	-2.03	118.75	126.11
5	D	311	CHL	CHC-C4B-C3B	-2.03	118.68	127.71
6	E	313	CLA	CMB-C2B-C3B	2.03	131.50	126.59
5	B	306	CHL	C2A-C1A-CHA	-2.03	120.31	123.86
6	F	313	CLA	C1-C2-C3	-2.03	122.53	126.04
5	E	308	CHL	CHD-C4C-NC	2.03	127.40	124.20
5	E	310	CHL	C3C-C4C-NC	2.03	112.84	110.57
5	C	306	CHL	C11-C12-C13	-2.03	109.36	115.92
5	C	313	CHL	C4-C3-C5	2.03	118.68	115.27
6	D	317	CLA	CHD-C1D-ND	-2.02	122.59	124.45
5	C	306	CHL	C11-C10-C8	-2.02	109.38	115.92
5	D	309	CHL	C2A-C1A-CHA	-2.02	120.32	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	321	0UR	C25-C26-C27	2.02	115.88	111.85
6	B	315	CLA	C2D-C1D-ND	-2.02	108.61	110.10
5	F	310	CHL	C2A-C1A-CHA	-2.02	120.32	123.86
9	B	325	0UR	O44-C45-O57	-2.02	118.49	122.93
6	B	318	CLA	CHB-C1B-NB	2.02	126.40	124.26
5	B	312	CHL	C3C-C4C-NC	2.02	112.84	110.57
3	B	303	NEX	C24-C23-C22	-2.02	106.87	110.77
5	B	314	CHL	O1D-CGD-CBD	-2.02	120.36	124.48
5	E	312	CHL	CHC-C1C-C2C	-2.02	118.80	126.11
5	B	314	CHL	C2A-C1A-CHA	-2.02	120.33	123.86
5	E	312	CHL	O1D-CGD-CBD	-2.02	120.36	124.48
5	B	314	CHL	CBC-CAC-C3C	-2.01	106.88	112.43
6	B	309	CLA	CMB-C2B-C1B	-2.01	122.30	125.37
5	B	311	CHL	C2A-C3A-C4A	2.01	105.12	101.87
5	A	309	CHL	C2A-C1A-CHA	-2.01	120.34	123.86
5	D	305	CHL	C4-C3-C5	2.01	118.65	115.27
5	D	311	CHL	OMC-CMC-C2C	-2.01	121.14	125.69
6	F	314	CLA	CHC-C4B-NB	2.01	126.38	124.26
5	A	310	CHL	CMA-C3A-C4A	-2.01	106.37	111.77
5	C	306	CHL	C2A-C3A-C4A	2.01	105.11	101.87
6	C	314	CLA	CHD-C1D-ND	-2.01	122.61	124.45
9	C	321	0UR	C15-C14-C13	-2.01	116.95	123.22
11	B	323	LMG	O1-C7-C8	-2.01	106.06	110.90
6	C	317	CLA	C3A-C2A-C1A	2.01	104.34	101.34
2	F	302	0IE	C23-C16-C17	2.01	121.24	118.08
5	A	312	CHL	C3B-C2B-C1B	-2.01	104.74	107.16
5	A	312	CHL	CHD-C4C-NC	2.01	127.36	124.20
10	B	322	BET	OXT-C-O	-2.01	118.30	123.30
5	D	306	CHL	CHC-C4B-C3B	-2.01	118.79	127.71
5	B	312	CHL	CMB-C2B-C1B	2.00	128.42	125.37
5	E	304	CHL	C4-C3-C2	-2.00	118.54	123.68
9	B	302	0UR	C28-C19-C32	-2.00	107.83	111.42
5	F	317	CHL	O2A-CGA-O1A	-2.00	118.30	123.30
3	D	303	NEX	O24-C25-C38	2.00	117.46	115.06
5	A	318	CHL	CED-O2D-CGD	2.00	120.47	115.94
6	B	317	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
7	F	318	LHG	O8-C23-C24	2.00	118.19	111.91
6	F	316	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
5	B	313	CHL	O2D-CGD-O1D	-2.00	119.92	123.84
5	D	313	CHL	O2A-CGA-CBA	2.00	118.19	111.91
6	B	316	CLA	C11-C10-C8	-2.00	109.45	115.92

There are no chirality outliers.

All (1327) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	0IE	C5-C6-C7-C21
2	A	302	0IE	C5-C6-C7-C8
2	A	302	0IE	C3-C4-C5-C6
2	A	302	0IE	C15-C16-C17-C18
2	A	302	0IE	C23-C16-C17-C18
2	B	301	0IE	C11-C12-C13-C14
2	B	301	0IE	C22-C12-C13-C14
2	C	301	0IE	C15-C16-C17-C18
2	C	301	0IE	C23-C16-C17-C18
2	C	302	0IE	C5-C6-C7-C21
2	C	302	0IE	C2-C3-C4-C5
2	C	302	0IE	C20-C3-C4-C5
2	C	302	0IE	C15-C16-C17-C18
2	C	302	0IE	C23-C16-C17-C18
2	D	301	0IE	C6-C7-C8-C9
2	D	301	0IE	C21-C7-C8-C9
2	D	301	0IE	O1-C2-C3-C20
2	D	301	0IE	C15-C16-C17-C18
2	D	301	0IE	C23-C16-C17-C18
2	D	302	0IE	C5-C6-C7-C21
2	D	302	0IE	C5-C6-C7-C8
2	D	302	0IE	C3-C4-C5-C6
2	D	302	0IE	C20-C3-C4-C5
2	D	302	0IE	O29-C20-C3-C2
2	D	302	0IE	C22-C12-C13-C14
2	D	302	0IE	C15-C16-C17-C18
2	D	302	0IE	C23-C16-C17-C18
2	E	301	0IE	C15-C16-C17-C18
2	E	301	0IE	C23-C16-C17-C18
2	E	302	0IE	C6-C7-C8-C9
2	E	302	0IE	C21-C7-C8-C9
2	E	302	0IE	C2-C3-C4-C5
2	E	302	0IE	C20-C3-C4-C5
2	E	302	0IE	C11-C10-C9-C8
2	E	302	0IE	C15-C16-C17-C18
2	E	302	0IE	C23-C16-C17-C18
2	F	301	0IE	C5-C6-C7-C21
2	F	301	0IE	C5-C6-C7-C8
2	F	301	0IE	O1-C2-C3-C20
2	F	302	0IE	C5-C6-C7-C21
2	F	302	0IE	C5-C6-C7-C8
2	F	302	0IE	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	302	0IE	C22-C12-C13-C14
2	F	302	0IE	C15-C16-C17-C18
2	F	302	0IE	C23-C16-C17-C18
3	A	303	NEX	O24-C26-C27-C28
4	A	304	LMU	C2'-C1'-O1'-C1
4	A	304	LMU	O5'-C1'-O1'-C1
4	B	304	LMU	C2'-C1'-O1'-C1
4	B	304	LMU	O5'-C1'-O1'-C1
4	B	305	LMU	O5'-C1'-O1'-C1
4	D	304	LMU	C2'-C1'-O1'-C1
4	D	304	LMU	C2-C1-O1'-C1'
4	E	319	LMU	C2'-C1'-O1'-C1
4	E	319	LMU	O5'-C1'-O1'-C1
5	A	305	CHL	C3A-C2A-CAA-CBA
5	A	305	CHL	C1C-C2C-CMC-OMC
5	A	305	CHL	C3C-C2C-CMC-OMC
5	A	305	CHL	CHA-CBD-CGD-O1D
5	A	305	CHL	CHA-CBD-CGD-O2D
5	A	305	CHL	C2-C3-C5-C6
5	A	305	CHL	C4-C3-C5-C6
5	A	306	CHL	C2B-C3B-CAB-CBB
5	A	306	CHL	C4B-C3B-CAB-CBB
5	A	309	CHL	C1A-C2A-CAA-CBA
5	A	309	CHL	C3A-C2A-CAA-CBA
5	A	309	CHL	C1C-C2C-CMC-OMC
5	A	309	CHL	C3C-C2C-CMC-OMC
5	A	311	CHL	C1A-C2A-CAA-CBA
5	A	311	CHL	C2B-C3B-CAB-CBB
5	A	311	CHL	C4B-C3B-CAB-CBB
5	A	311	CHL	C3C-C2C-CMC-OMC
5	A	312	CHL	C2A-CAA-CBA-CGA
5	A	312	CHL	C2B-C3B-CAB-CBB
5	A	313	CHL	C3C-C2C-CMC-OMC
5	A	318	CHL	C1C-C2C-CMC-OMC
5	A	318	CHL	C3C-C2C-CMC-OMC
5	B	306	CHL	C1A-C2A-CAA-CBA
5	B	306	CHL	C3A-C2A-CAA-CBA
5	B	306	CHL	C3C-C2C-CMC-OMC
5	B	307	CHL	C2B-C3B-CAB-CBB
5	B	307	CHL	C4B-C3B-CAB-CBB
5	B	310	CHL	C1A-C2A-CAA-CBA
5	B	310	CHL	C1C-C2C-CMC-OMC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	310	CHL	C3C-C2C-CMC-OMC
5	B	311	CHL	C2B-C3B-CAB-CBB
5	B	311	CHL	C4B-C3B-CAB-CBB
5	B	312	CHL	C1A-C2A-CAA-CBA
5	B	312	CHL	C2B-C3B-CAB-CBB
5	B	312	CHL	C4B-C3B-CAB-CBB
5	B	312	CHL	C1C-C2C-CMC-OMC
5	B	312	CHL	CHA-CBD-CGD-O1D
5	B	312	CHL	CHA-CBD-CGD-O2D
5	B	313	CHL	C2B-C3B-CAB-CBB
5	B	313	CHL	C4B-C3B-CAB-CBB
5	B	314	CHL	C1C-C2C-CMC-OMC
5	B	314	CHL	CBD-CGD-O2D-CED
5	B	314	CHL	C14-C13-C15-C16
5	B	319	CHL	C2B-C3B-CAB-CBB
5	B	319	CHL	C4B-C3B-CAB-CBB
5	C	305	CHL	C1C-C2C-CMC-OMC
5	C	305	CHL	C3C-C2C-CMC-OMC
5	C	306	CHL	C3C-C2C-CMC-OMC
5	C	306	CHL	C2-C3-C5-C6
5	C	306	CHL	C4-C3-C5-C6
5	C	309	CHL	C2B-C3B-CAB-CBB
5	C	309	CHL	C4B-C3B-CAB-CBB
5	C	309	CHL	C1C-C2C-CMC-OMC
5	C	309	CHL	C3C-C2C-CMC-OMC
5	C	310	CHL	C1A-C2A-CAA-CBA
5	C	310	CHL	C2B-C3B-CAB-CBB
5	C	310	CHL	C4B-C3B-CAB-CBB
5	C	310	CHL	C3C-C2C-CMC-OMC
5	C	311	CHL	C1A-C2A-CAA-CBA
5	C	311	CHL	C3A-C2A-CAA-CBA
5	C	311	CHL	C2B-C3B-CAB-CBB
5	C	311	CHL	C4B-C3B-CAB-CBB
5	C	312	CHL	C2B-C3B-CAB-CBB
5	C	312	CHL	C4B-C3B-CAB-CBB
5	C	312	CHL	C1C-C2C-CMC-OMC
5	C	312	CHL	C3C-C2C-CMC-OMC
5	D	305	CHL	C1C-C2C-CMC-OMC
5	D	305	CHL	C3C-C2C-CMC-OMC
5	D	305	CHL	CHA-CBD-CGD-O1D
5	D	305	CHL	CHA-CBD-CGD-O2D
5	D	305	CHL	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	305	CHL	C4-C3-C5-C6
5	D	306	CHL	C2B-C3B-CAB-CBB
5	D	306	CHL	C4B-C3B-CAB-CBB
5	D	306	CHL	C3C-C2C-CMC-OMC
5	D	309	CHL	C1C-C2C-CMC-OMC
5	D	309	CHL	C3C-C2C-CMC-OMC
5	D	310	CHL	C2B-C3B-CAB-CBB
5	D	310	CHL	C4B-C3B-CAB-CBB
5	D	311	CHL	C1A-C2A-CAA-CBA
5	D	311	CHL	C2B-C3B-CAB-CBB
5	D	311	CHL	C4B-C3B-CAB-CBB
5	D	311	CHL	C1C-C2C-CMC-OMC
5	D	311	CHL	C3C-C2C-CMC-OMC
5	D	312	CHL	C2B-C3B-CAB-CBB
5	D	312	CHL	C4B-C3B-CAB-CBB
5	D	313	CHL	C1C-C2C-CMC-OMC
5	D	318	CHL	CHA-CBD-CGD-O1D
5	E	304	CHL	C3A-C2A-CAA-CBA
5	E	308	CHL	C1C-C2C-CMC-OMC
5	E	308	CHL	C3C-C2C-CMC-OMC
5	E	309	CHL	C3A-C2A-CAA-CBA
5	E	309	CHL	C2B-C3B-CAB-CBB
5	E	310	CHL	C1A-C2A-CAA-CBA
5	E	310	CHL	C3A-C2A-CAA-CBA
5	E	310	CHL	C2B-C3B-CAB-CBB
5	E	310	CHL	C4B-C3B-CAB-CBB
5	E	310	CHL	C3C-C2C-CMC-OMC
5	E	311	CHL	C2B-C3B-CAB-CBB
5	E	311	CHL	C4B-C3B-CAB-CBB
5	F	304	CHL	C1A-C2A-CAA-CBA
5	F	305	CHL	C2B-C3B-CAB-CBB
5	F	305	CHL	C2-C3-C5-C6
5	F	305	CHL	C4-C3-C5-C6
5	F	308	CHL	C4B-C3B-CAB-CBB
5	F	308	CHL	C1C-C2C-CMC-OMC
5	F	308	CHL	C3C-C2C-CMC-OMC
5	F	309	CHL	C1C-C2C-CMC-OMC
5	F	309	CHL	C3C-C2C-CMC-OMC
5	F	310	CHL	C1A-C2A-CAA-CBA
5	F	310	CHL	C3A-C2A-CAA-CBA
5	F	310	CHL	C2B-C3B-CAB-CBB
5	F	310	CHL	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	F	310	CHL	C1C-C2C-CMC-OMC
5	F	310	CHL	C3C-C2C-CMC-OMC
5	F	310	CHL	C2-C3-C5-C6
5	F	310	CHL	C4-C3-C5-C6
5	F	311	CHL	C2B-C3B-CAB-CBB
5	F	311	CHL	C4B-C3B-CAB-CBB
5	F	311	CHL	C1C-C2C-CMC-OMC
5	F	311	CHL	C3C-C2C-CMC-OMC
5	F	312	CHL	C3C-C2C-CMC-OMC
6	A	307	CLA	C4B-C3B-CAB-CBB
6	A	308	CLA	C1A-C2A-CAA-CBA
6	A	315	CLA	C2B-C3B-CAB-CBB
6	A	315	CLA	C4B-C3B-CAB-CBB
6	A	316	CLA	C2B-C3B-CAB-CBB
6	A	316	CLA	C4B-C3B-CAB-CBB
6	A	317	CLA	CBD-CGD-O2D-CED
6	C	317	CLA	C2B-C3B-CAB-CBB
6	C	317	CLA	C4B-C3B-CAB-CBB
6	D	314	CLA	CBD-CGD-O2D-CED
6	D	317	CLA	CHA-CBD-CGD-O1D
6	D	317	CLA	CHA-CBD-CGD-O2D
6	D	317	CLA	CBD-CGD-O2D-CED
6	F	306	CLA	C1A-C2A-CAA-CBA
6	F	306	CLA	C3A-C2A-CAA-CBA
6	F	306	CLA	C11-C12-C13-C14
6	F	313	CLA	C4-C3-C5-C6
7	A	319	LHG	C3-O3-P-O4
7	A	319	LHG	C3-O3-P-O6
7	A	319	LHG	C4-O6-P-O5
7	B	320	LHG	O1-C1-C2-O2
7	B	320	LHG	O1-C1-C2-C3
7	B	320	LHG	O2-C2-C3-O3
7	B	320	LHG	C4-O6-P-O5
7	B	320	LHG	O6-C4-C5-O7
7	B	324	LHG	O1-C1-C2-C3
7	B	324	LHG	C3-O3-P-O5
7	B	324	LHG	C4-O6-P-O4
7	B	324	LHG	O9-C7-O7-C5
7	C	304	LHG	C3-O3-P-O4
7	C	304	LHG	C3-O3-P-O5
7	C	304	LHG	C3-O3-P-O6
7	C	304	LHG	C4-O6-P-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	C	319	LHG	C4-O6-P-O5
7	F	318	LHG	C1-C2-C3-O3
7	F	318	LHG	C4-O6-P-O3
7	F	318	LHG	C4-O6-P-O4
9	A	322	0UR	C2-C3-C43-O44
9	A	322	0UR	C4-C3-C43-O44
9	A	322	0UR	C46-C45-O44-C43
9	A	322	0UR	O57-C45-O44-C43
9	B	302	0UR	C2-C3-C43-O44
9	B	302	0UR	C4-C3-C43-O44
9	B	302	0UR	C5-C6-C7-C20
9	B	302	0UR	C5-C6-C7-C8
9	B	302	0UR	C17-C18-C19-C28
9	B	302	0UR	C17-C18-C19-C32
9	B	302	0UR	C46-C45-O44-C43
9	B	302	0UR	O57-C45-O44-C43
9	B	302	0UR	C7-C8-C9-C10
9	B	325	0UR	C2-C3-C43-O44
9	B	325	0UR	C4-C3-C43-O44
9	B	325	0UR	C46-C45-O44-C43
9	B	325	0UR	O57-C45-O44-C43
9	C	321	0UR	O57-C45-O44-C43
9	E	320	0UR	C2-C3-C43-O44
9	E	320	0UR	C4-C3-C43-O44
9	E	320	0UR	C46-C45-O44-C43
9	E	320	0UR	O57-C45-O44-C43
9	F	320	0UR	O57-C45-O44-C43
10	B	321	BET	C-CA-N-C1
10	B	321	BET	C-CA-N-C2
10	B	321	BET	C-CA-N-C3
10	B	321	BET	O-C-CA-N
10	B	321	BET	OXT-C-CA-N
10	B	322	BET	O-C-CA-N
10	B	322	BET	OXT-C-CA-N
10	C	320	BET	OXT-C-CA-N
11	B	323	LMG	O9-C10-O7-C8
11	B	323	LMG	C11-C10-O7-C8
11	F	319	LMG	C2-C1-O1-C7
11	F	319	LMG	O6-C1-O1-C7
11	F	319	LMG	O7-C8-C9-O8
11	F	319	LMG	O9-C10-O7-C8
11	F	319	LMG	C11-C10-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	313	CHL	CBD-CGD-O2D-CED
5	D	313	CHL	CBD-CGD-O2D-CED
5	F	312	CHL	CBD-CGD-O2D-CED
6	A	314	CLA	CBD-CGD-O2D-CED
6	C	308	CLA	CBD-CGD-O2D-CED
6	E	314	CLA	CBD-CGD-O2D-CED
6	E	315	CLA	CBD-CGD-O2D-CED
6	F	313	CLA	CBD-CGD-O2D-CED
11	F	319	LMG	O10-C28-O8-C9
4	D	304	LMU	O5B-C1B-O1B-C4'
4	E	319	LMU	C4'-C5'-C6'-O6'
6	E	314	CLA	O1D-CGD-O2D-CED
5	B	314	CHL	O1D-CGD-O2D-CED
6	C	315	CLA	CBA-CGA-O2A-C1
11	F	319	LMG	C29-C28-O8-C9
5	A	313	CHL	CBD-CGD-O2D-CED
5	B	306	CHL	CBD-CGD-O2D-CED
5	D	310	CHL	CBD-CGD-O2D-CED
5	E	309	CHL	CBD-CGD-O2D-CED
5	E	311	CHL	CBD-CGD-O2D-CED
5	E	312	CHL	CBD-CGD-O2D-CED
6	B	315	CLA	CBD-CGD-O2D-CED
6	B	316	CLA	CBD-CGD-O2D-CED
6	C	315	CLA	O1A-CGA-O2A-C1
7	A	319	LHG	O10-C23-O8-C6
7	E	318	LHG	O10-C23-O8-C6
7	F	318	LHG	O10-C23-O8-C6
6	A	317	CLA	O1D-CGD-O2D-CED
6	D	314	CLA	O1D-CGD-O2D-CED
6	D	317	CLA	O1D-CGD-O2D-CED
6	C	317	CLA	CBD-CGD-O2D-CED
4	E	319	LMU	C4B-C5B-C6B-O6B
6	D	308	CLA	CBA-CGA-O2A-C1
6	D	308	CLA	O1A-CGA-O2A-C1
9	D	321	OUR	O57-C45-O44-C43
5	A	311	CHL	C3-C5-C6-C7
5	B	306	CHL	C3-C5-C6-C7
5	D	312	CHL	C3-C5-C6-C7
5	E	310	CHL	C3-C5-C6-C7
5	F	310	CHL	C3-C5-C6-C7
6	A	315	CLA	C3-C5-C6-C7
6	D	315	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	E	314	CLA	C3-C5-C6-C7
9	C	321	0UR	C46-C45-O44-C43
9	F	320	0UR	C46-C45-O44-C43
7	B	324	LHG	C8-C7-O7-C5
6	C	308	CLA	CBA-CGA-O2A-C1
4	E	319	LMU	O5'-C5'-C6'-O6'
6	F	313	CLA	C2-C3-C5-C6
6	A	307	CLA	CBD-CGD-O2D-CED
6	D	307	CLA	CBD-CGD-O2D-CED
5	A	305	CHL	C2A-CAA-CBA-CGA
5	B	313	CHL	C2A-CAA-CBA-CGA
5	D	305	CHL	C2A-CAA-CBA-CGA
5	E	311	CHL	C2A-CAA-CBA-CGA
6	F	306	CLA	C2A-CAA-CBA-CGA
5	A	305	CHL	C3-C5-C6-C7
5	D	305	CHL	C3-C5-C6-C7
5	C	310	CHL	C2A-CAA-CBA-CGA
6	B	316	CLA	CBA-CGA-O2A-C1
6	F	313	CLA	CBA-CGA-O2A-C1
7	A	319	LHG	C24-C23-O8-C6
7	B	320	LHG	C24-C23-O8-C6
7	E	318	LHG	C24-C23-O8-C6
7	F	318	LHG	C24-C23-O8-C6
4	B	304	LMU	O5B-C5B-C6B-O6B
4	A	304	LMU	C4-C5-C6-C7
6	E	315	CLA	O1D-CGD-O2D-CED
6	F	313	CLA	O1A-CGA-O2A-C1
5	A	311	CHL	CBD-CGD-O2D-CED
5	A	318	CHL	CBD-CGD-O2D-CED
5	B	313	CHL	CBD-CGD-O2D-CED
5	C	311	CHL	CBD-CGD-O2D-CED
5	C	318	CHL	CBD-CGD-O2D-CED
5	D	311	CHL	CBD-CGD-O2D-CED
5	F	311	CHL	CBD-CGD-O2D-CED
6	D	315	CLA	CBD-CGD-O2D-CED
6	E	316	CLA	CBD-CGD-O2D-CED
6	F	307	CLA	CBD-CGD-O2D-CED
5	A	312	CHL	C3-C5-C6-C7
5	C	311	CHL	C3-C5-C6-C7
6	B	318	CLA	C3-C5-C6-C7
6	C	317	CLA	C3-C5-C6-C7
6	B	316	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	319	LMU	O5B-C5B-C6B-O6B
9	D	321	0UR	C46-C45-O44-C43
6	A	314	CLA	O1D-CGD-O2D-CED
6	F	313	CLA	O1D-CGD-O2D-CED
4	E	319	LMU	C1-C2-C3-C4
4	A	304	LMU	O5B-C1B-O1B-C4'
5	D	313	CHL	O1D-CGD-O2D-CED
5	C	312	CHL	CBD-CGD-O2D-CED
6	A	315	CLA	CBD-CGD-O2D-CED
6	C	308	CLA	O1D-CGD-O2D-CED
7	B	324	LHG	C24-C25-C26-C27
7	B	324	LHG	C26-C27-C28-C29
4	B	305	LMU	O5B-C5B-C6B-O6B
11	B	323	LMG	C4-C5-C6-O5
6	C	308	CLA	O1A-CGA-O2A-C1
5	C	305	CHL	C4-C3-C5-C6
5	E	304	CHL	C4-C3-C5-C6
5	C	305	CHL	C2-C3-C5-C6
5	E	304	CHL	C2-C3-C5-C6
5	F	308	CHL	CBD-CGD-O2D-CED
5	D	312	CHL	C2A-CAA-CBA-CGA
5	F	312	CHL	O1D-CGD-O2D-CED
4	B	304	LMU	C4B-C5B-C6B-O6B
6	B	315	CLA	C2C-C3C-CAC-CBC
6	F	315	CLA	CBD-CGD-O2D-CED
11	B	323	LMG	O6-C5-C6-O5
5	C	313	CHL	O1D-CGD-O2D-CED
5	D	310	CHL	O1D-CGD-O2D-CED
5	E	311	CHL	O1D-CGD-O2D-CED
6	B	316	CLA	O1D-CGD-O2D-CED
10	C	320	BET	C-CA-N-C3
5	E	312	CHL	O1D-CGD-O2D-CED
7	B	320	LHG	C1-C2-C3-O3
7	C	304	LHG	C1-C2-C3-O3
5	B	313	CHL	C3-C5-C6-C7
6	A	315	CLA	CBA-CGA-O2A-C1
6	D	315	CLA	CBA-CGA-O2A-C1
7	B	324	LHG	C24-C23-O8-C6
5	C	309	CHL	CBD-CGD-O2D-CED
2	E	302	0IE	C3-C4-C5-C6
5	E	311	CHL	C5-C6-C7-C8
6	B	315	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	320	LHG	C29-C30-C31-C32
4	A	304	LMU	C11-C10-C9-C8
5	F	305	CHL	C8-C10-C11-C12
6	D	317	CLA	C8-C10-C11-C12
7	C	304	LHG	O2-C2-C3-O3
6	D	315	CLA	O1A-CGA-O2A-C1
5	B	307	CHL	C11-C12-C13-C14
5	C	305	CHL	C14-C13-C15-C16
5	C	306	CHL	C14-C13-C15-C16
5	C	311	CHL	C11-C10-C8-C9
5	C	313	CHL	C11-C12-C13-C14
5	E	310	CHL	C11-C10-C8-C9
5	F	304	CHL	C14-C13-C15-C16
5	F	305	CHL	C11-C12-C13-C14
5	F	310	CHL	C11-C10-C8-C9
5	F	312	CHL	C11-C10-C8-C9
6	B	316	CLA	C6-C7-C8-C9
6	B	318	CLA	C11-C10-C8-C9
6	D	317	CLA	C5-C6-C7-C8
6	F	313	CLA	C5-C6-C7-C8
5	A	310	CHL	C2A-CAA-CBA-CGA
2	A	301	0IE	C5-C6-C7-C21
2	B	301	0IE	C5-C6-C7-C21
2	C	302	0IE	C5-C6-C7-C8
9	B	302	0UR	C15-C16-C17-C18
4	D	304	LMU	O5B-C5B-C6B-O6B
4	A	304	LMU	C6-C7-C8-C9
7	A	319	LHG	C24-C25-C26-C27
7	B	320	LHG	O10-C23-O8-C6
7	B	324	LHG	O10-C23-O8-C6
5	C	311	CHL	C5-C6-C7-C8
5	F	304	CHL	C13-C15-C16-C17
6	C	315	CLA	C13-C15-C16-C17
5	B	311	CHL	CBD-CGD-O2D-CED
5	D	309	CHL	CBD-CGD-O2D-CED
5	C	312	CHL	C3-C5-C6-C7
5	B	314	CHL	C13-C15-C16-C17
5	E	305	CHL	C5-C6-C7-C8
6	F	306	CLA	C10-C11-C12-C13
5	A	312	CHL	C5-C6-C7-C8
5	D	311	CHL	C8-C10-C11-C12
5	E	304	CHL	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	E	312	CHL	C15-C16-C17-C18
5	F	310	CHL	C5-C6-C7-C8
5	F	311	CHL	C5-C6-C7-C8
7	B	324	LHG	O1-C1-C2-O2
7	B	320	LHG	C23-C24-C25-C26
7	B	324	LHG	C23-C24-C25-C26
7	D	319	LHG	C7-C8-C9-C10
5	E	308	CHL	CBD-CGD-O2D-CED
5	B	313	CHL	C5-C6-C7-C8
5	C	311	CHL	C8-C10-C11-C12
5	E	304	CHL	C15-C16-C17-C18
5	F	312	CHL	C15-C16-C17-C18
6	B	318	CLA	C10-C11-C12-C13
6	C	307	CLA	C10-C11-C12-C13
6	D	317	CLA	C10-C11-C12-C13
7	C	304	LHG	C24-C23-O8-C6
5	A	313	CHL	O1D-CGD-O2D-CED
5	B	306	CHL	O1D-CGD-O2D-CED
4	D	304	LMU	O1'-C1-C2-C3
5	E	310	CHL	C5-C6-C7-C8
5	F	310	CHL	C10-C11-C12-C13
5	F	312	CHL	C13-C15-C16-C17
6	D	315	CLA	C8-C10-C11-C12
7	C	304	LHG	C5-C4-O6-P
7	A	319	LHG	C7-C8-C9-C10
5	E	317	CHL	CBD-CGD-O2D-CED
5	C	318	CHL	C2A-CAA-CBA-CGA
5	A	305	CHL	C13-C15-C16-C17
5	B	313	CHL	C6-C7-C8-C10
5	D	312	CHL	C6-C7-C8-C10
6	B	308	CLA	C12-C13-C15-C16
6	F	313	CLA	C6-C7-C8-C10
9	B	302	OUR	C9-C10-C11-C12
5	A	312	CHL	CBD-CGD-O2D-CED
6	F	314	CLA	CBA-CGA-O2A-C1
5	C	312	CHL	C2A-CAA-CBA-CGA
5	F	311	CHL	C2A-CAA-CBA-CGA
5	E	309	CHL	O1D-CGD-O2D-CED
6	D	307	CLA	O1D-CGD-O2D-CED
5	A	311	CHL	C5-C6-C7-C8
5	B	314	CHL	C10-C11-C12-C13
5	C	311	CHL	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	F	310	CHL	C8-C10-C11-C12
6	A	315	CLA	O1A-CGA-O2A-C1
5	D	305	CHL	CBD-CGD-O2D-CED
4	D	304	LMU	O5'-C1'-O1'-C1
2	D	301	OIE	C4-C5-C6-C7
4	A	304	LMU	O1'-C1-C2-C3
4	E	319	LMU	C7-C8-C9-C10
7	F	318	LHG	O2-C2-C3-O3
5	F	311	CHL	C3-C5-C6-C7
5	F	312	CHL	C5-C6-C7-C8
7	E	318	LHG	C24-C25-C26-C27
5	B	307	CHL	C5-C6-C7-C8
5	B	307	CHL	C13-C15-C16-C17
5	C	306	CHL	C15-C16-C17-C18
5	D	312	CHL	C5-C6-C7-C8
6	A	307	CLA	C15-C16-C17-C18
4	B	305	LMU	C5'-C4'-O1B-C1B
6	C	317	CLA	O1D-CGD-O2D-CED
5	C	305	CHL	CBD-CGD-O2D-CED
7	F	318	LHG	C24-C25-C26-C27
5	C	312	CHL	C5-C6-C7-C8
5	C	313	CHL	C15-C16-C17-C18
5	D	313	CHL	C13-C15-C16-C17
6	C	315	CLA	C8-C10-C11-C12
6	E	306	CLA	C10-C11-C12-C13
7	B	320	LHG	C4-O6-P-O3
7	B	324	LHG	C3-O3-P-O6
7	C	304	LHG	C4-O6-P-O3
5	C	306	CHL	C3-C5-C6-C7
6	A	317	CLA	C3-C5-C6-C7
6	F	313	CLA	C3-C5-C6-C7
4	B	305	LMU	C3'-C4'-O1B-C1B
5	E	305	CHL	CBA-CGA-O2A-C1
6	E	314	CLA	CBA-CGA-O2A-C1
10	C	320	BET	C-CA-N-C2
5	C	310	CHL	CBD-CGD-O2D-CED
5	A	306	CHL	C8-C10-C11-C12
6	B	318	CLA	C4-C3-C5-C6
5	A	306	CHL	C5-C6-C7-C8
5	F	304	CHL	C15-C16-C17-C18
5	D	305	CHL	C2C-C3C-CAC-CBC
5	F	304	CHL	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	E	306	CLA	C16-C17-C18-C19
6	C	307	CLA	C3-C5-C6-C7
5	C	306	CHL	C10-C11-C12-C13
6	B	308	CLA	C13-C15-C16-C17
4	B	305	LMU	C3-C4-C5-C6
2	F	302	0IE	C3-C4-C5-C6
9	C	321	0UR	C47-C48-C49-C50
2	A	301	0IE	C21-C7-C8-C9
2	A	302	0IE	C21-C7-C8-C9
2	A	302	0IE	C14-C15-C16-C23
2	B	301	0IE	C21-C7-C8-C9
2	C	302	0IE	C10-C11-C12-C22
2	D	301	0IE	C14-C15-C16-C23
2	D	302	0IE	C10-C11-C12-C22
2	E	301	0IE	C14-C15-C16-C23
2	F	301	0IE	C21-C7-C8-C9
2	F	302	0IE	C14-C15-C16-C23
5	D	306	CHL	C3-C5-C6-C7
5	D	313	CHL	C3-C5-C6-C7
7	D	319	LHG	C15-C16-C17-C18
7	F	318	LHG	C13-C14-C15-C16
5	A	311	CHL	O1D-CGD-O2D-CED
5	A	305	CHL	C16-C17-C18-C19
5	F	304	CHL	C16-C17-C18-C19
5	E	310	CHL	C10-C11-C12-C13
6	A	307	CLA	O1D-CGD-O2D-CED
5	A	305	CHL	C15-C16-C17-C18
4	A	304	LMU	C5-C6-C7-C8
7	A	319	LHG	C12-C13-C14-C15
7	C	319	LHG	C11-C10-C9-C8
7	E	318	LHG	C13-C14-C15-C16
6	F	314	CLA	O1A-CGA-O2A-C1
4	D	304	LMU	C3-C4-C5-C6
4	B	305	LMU	C4B-C5B-C6B-O6B
4	B	305	LMU	C6-C7-C8-C9
4	E	319	LMU	O1'-C1-C2-C3
7	D	319	LHG	C11-C10-C9-C8
2	A	301	0IE	C6-C7-C8-C9
2	A	302	0IE	C6-C7-C8-C9
2	A	302	0IE	C14-C15-C16-C17
2	B	301	0IE	C6-C7-C8-C9
2	C	302	0IE	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	301	0IE	C14-C15-C16-C17
2	D	302	0IE	C10-C11-C12-C13
2	E	301	0IE	C14-C15-C16-C17
2	F	301	0IE	C6-C7-C8-C9
2	F	302	0IE	C10-C11-C12-C13
2	F	302	0IE	C14-C15-C16-C17
5	C	305	CHL	C13-C15-C16-C17
6	E	316	CLA	C4-C3-C5-C6
7	D	319	LHG	C26-C27-C28-C29
7	F	318	LHG	C25-C26-C27-C28
6	B	318	CLA	C2-C3-C5-C6
6	F	306	CLA	C2-C3-C5-C6
5	D	305	CHL	C6-C7-C8-C9
6	C	315	CLA	C11-C12-C13-C14
6	D	314	CLA	C11-C10-C8-C9
6	F	313	CLA	C6-C7-C8-C9
10	B	322	BET	C-CA-N-C3
4	A	304	LMU	C3-C4-C5-C6
7	C	319	LHG	C24-C25-C26-C27
5	E	305	CHL	C13-C15-C16-C17
6	E	306	CLA	C2A-CAA-CBA-CGA
6	F	307	CLA	C2A-CAA-CBA-CGA
5	D	311	CHL	O1D-CGD-O2D-CED
5	E	305	CHL	O1A-CGA-O2A-C1
2	E	302	0IE	C5-C6-C7-C21
9	B	302	0UR	C22-C16-C17-C18
7	C	319	LHG	C16-C17-C18-C19
10	C	320	BET	O-C-CA-N
2	D	302	0IE	C11-C12-C13-C14
2	E	302	0IE	C5-C6-C7-C8
6	B	318	CLA	C8-C10-C11-C12
4	D	304	LMU	C4-C5-C6-C7
4	E	319	LMU	C4-C5-C6-C7
7	B	320	LHG	C27-C28-C29-C30
7	C	319	LHG	C17-C18-C19-C20
5	C	311	CHL	O1D-CGD-O2D-CED
6	E	316	CLA	O1D-CGD-O2D-CED
4	B	305	LMU	C5-C6-C7-C8
7	B	320	LHG	C9-C10-C11-C12
7	C	319	LHG	C27-C28-C29-C30
7	E	318	LHG	C12-C13-C14-C15
7	F	318	LHG	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	304	LMU	O5B-C5B-C6B-O6B
4	B	304	LMU	O5'-C5'-C6'-O6'
5	A	312	CHL	C4B-C3B-CAB-CBB
5	E	309	CHL	C4B-C3B-CAB-CBB
5	F	305	CHL	C4B-C3B-CAB-CBB
6	B	318	CLA	C4B-C3B-CAB-CBB
5	A	312	CHL	C6-C7-C8-C9
6	C	307	CLA	C16-C17-C18-C19
6	C	307	CLA	C16-C17-C18-C20
6	C	315	CLA	C16-C17-C18-C19
6	C	315	CLA	C16-C17-C18-C20
6	E	306	CLA	C16-C17-C18-C20
5	C	318	CHL	O1D-CGD-O2D-CED
4	E	319	LMU	C6-C7-C8-C9
7	B	324	LHG	C25-C26-C27-C28
6	E	313	CLA	CBD-CGD-O2D-CED
6	D	315	CLA	O1D-CGD-O2D-CED
7	D	319	LHG	C9-C10-C11-C12
7	D	319	LHG	C10-C11-C12-C13
6	E	314	CLA	O1A-CGA-O2A-C1
4	D	304	LMU	C5-C6-C7-C8
5	A	311	CHL	C3A-C2A-CAA-CBA
5	B	312	CHL	C3A-C2A-CAA-CBA
5	C	310	CHL	C3A-C2A-CAA-CBA
5	D	311	CHL	C3A-C2A-CAA-CBA
4	E	319	LMU	C2-C1-O1'-C1'
5	A	318	CHL	O1D-CGD-O2D-CED
6	F	307	CLA	O1D-CGD-O2D-CED
4	D	304	LMU	C4B-C5B-C6B-O6B
5	B	313	CHL	O1D-CGD-O2D-CED
11	F	319	LMG	O1-C7-C8-C9
7	F	318	LHG	C28-C29-C30-C31
3	F	303	NEX	C14-C15-C35-C34
6	C	315	CLA	C3-C5-C6-C7
7	B	324	LHG	C27-C28-C29-C30
6	F	306	CLA	C4-C3-C5-C6
6	E	316	CLA	C2-C3-C5-C6
6	F	316	CLA	C2-C3-C5-C6
5	E	305	CHL	C2A-CAA-CBA-CGA
5	F	305	CHL	C15-C16-C17-C18
7	C	304	LHG	C23-C24-C25-C26
10	C	320	BET	C-CA-N-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	305	CHL	C2B-C3B-CAB-CBB
5	F	308	CHL	C2B-C3B-CAB-CBB
6	A	307	CLA	C2B-C3B-CAB-CBB
6	F	306	CLA	C2B-C3B-CAB-CBB
6	A	315	CLA	C10-C11-C12-C13
4	E	319	LMU	C2-C3-C4-C5
5	A	305	CHL	CBA-CGA-O2A-C1
6	C	315	CLA	C15-C16-C17-C18
5	A	309	CHL	CBD-CGD-O2D-CED
5	F	305	CHL	C2-C1-O2A-CGA
4	A	304	LMU	O5'-C5'-C6'-O6'
5	A	310	CHL	CBA-CGA-O2A-C1
5	C	311	CHL	CBA-CGA-O2A-C1
5	F	312	CHL	CBA-CGA-O2A-C1
5	B	306	CHL	C8-C10-C11-C12
6	A	307	CLA	C10-C11-C12-C13
7	F	318	LHG	C29-C30-C31-C32
11	F	319	LMG	C11-C12-C13-C14
5	B	306	CHL	C10-C11-C12-C13
5	E	312	CHL	C4-C3-C5-C6
5	A	305	CHL	C11-C12-C13-C15
5	A	311	CHL	C2-C3-C5-C6
5	B	314	CHL	C2-C3-C5-C6
5	C	305	CHL	C6-C7-C8-C10
5	C	305	CHL	C12-C13-C15-C16
5	D	305	CHL	C6-C7-C8-C10
5	D	305	CHL	C12-C13-C15-C16
5	E	312	CHL	C2-C3-C5-C6
5	F	304	CHL	C12-C13-C15-C16
5	F	305	CHL	C11-C12-C13-C15
6	C	315	CLA	C11-C12-C13-C15
6	D	314	CLA	C6-C7-C8-C10
5	C	311	CHL	O1A-CGA-O2A-C1
2	F	302	OIE	C9-C10-C11-C12
6	F	314	CLA	CBD-CGD-O2D-CED
5	C	305	CHL	C16-C17-C18-C20
5	C	312	CHL	C6-C7-C8-C9
5	F	311	CHL	C6-C7-C8-C9
5	C	312	CHL	O1D-CGD-O2D-CED
5	F	311	CHL	O1D-CGD-O2D-CED
9	B	325	OUR	C47-C48-C49-C50
5	A	313	CHL	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	313	CHL	CBA-CGA-O2A-C1
5	E	304	CHL	CBA-CGA-O2A-C1
5	E	304	CHL	C2A-CAA-CBA-CGA
6	A	315	CLA	O1D-CGD-O2D-CED
6	D	307	CLA	C8-C10-C11-C12
6	B	315	CLA	C4C-C3C-CAC-CBC
5	A	313	CHL	C8-C10-C11-C12
4	E	319	LMU	C5-C6-C7-C8
5	B	307	CHL	C15-C16-C17-C18
5	F	308	CHL	O1D-CGD-O2D-CED
4	D	304	LMU	C11-C10-C9-C8
7	A	319	LHG	C8-C7-O7-C5
4	A	304	LMU	C1-C2-C3-C4
5	A	305	CHL	O1A-CGA-O2A-C1
5	F	312	CHL	O1A-CGA-O2A-C1
7	C	304	LHG	O7-C5-C6-O8
4	D	304	LMU	O5'-C5'-C6'-O6'
6	F	315	CLA	O1D-CGD-O2D-CED
5	F	304	CHL	C16-C17-C18-C20
4	B	305	LMU	C4-C5-C6-C7
5	B	314	CHL	C15-C16-C17-C18
9	A	322	OUR	C47-C48-C49-C50
9	D	321	OUR	C47-C48-C49-C50
5	A	306	CHL	C4-C3-C5-C6
5	B	314	CHL	C4-C3-C5-C6
6	F	316	CLA	C4-C3-C5-C6
5	A	305	CHL	C11-C12-C13-C14
5	B	313	CHL	C6-C7-C8-C9
5	C	305	CHL	C6-C7-C8-C9
5	D	305	CHL	C14-C13-C15-C16
5	D	312	CHL	C6-C7-C8-C9
5	E	305	CHL	C11-C10-C8-C9
5	E	312	CHL	C11-C12-C13-C14
6	A	307	CLA	C11-C10-C8-C9
6	A	315	CLA	C6-C7-C8-C9
2	C	302	OIE	C22-C12-C13-C14
2	F	301	OIE	C22-C12-C13-C14
3	A	303	NEX	C31-C32-C33-C40
5	A	305	CHL	C10-C11-C12-C13
5	A	305	CHL	C1A-C2A-CAA-CBA
5	A	313	CHL	C1A-C2A-CAA-CBA
5	D	313	CHL	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	318	CHL	C1A-C2A-CAA-CBA
5	E	304	CHL	C1A-C2A-CAA-CBA
5	F	305	CHL	C1A-C2A-CAA-CBA
5	F	312	CHL	C1A-C2A-CAA-CBA
6	C	315	CLA	C1A-C2A-CAA-CBA
6	D	308	CLA	C1A-C2A-CAA-CBA
6	D	314	CLA	C1A-C2A-CAA-CBA
6	D	315	CLA	C1A-C2A-CAA-CBA
5	A	312	CHL	C6-C7-C8-C10
7	B	320	LHG	C8-C7-O7-C5
4	B	305	LMU	C11-C10-C9-C8
9	F	320	OUR	C46-C47-C48-C49
2	C	302	OIE	C9-C10-C11-C12
6	E	306	CLA	C15-C16-C17-C18
5	E	312	CHL	C3-C5-C6-C7
5	C	309	CHL	O1D-CGD-O2D-CED
5	D	311	CHL	C10-C11-C12-C13
7	B	320	LHG	O6-C4-C5-C6
7	F	318	LHG	O6-C4-C5-C6
7	A	319	LHG	C34-C35-C36-C37
5	D	306	CHL	C13-C15-C16-C17
5	D	313	CHL	C8-C10-C11-C12
7	D	319	LHG	C24-C25-C26-C27
6	C	314	CLA	CBA-CGA-O2A-C1
5	A	311	CHL	C4-C3-C5-C6
5	B	310	CHL	C3A-C2A-CAA-CBA
6	D	307	CLA	C15-C16-C17-C18
7	C	319	LHG	C9-C10-C11-C12
7	E	318	LHG	C11-C10-C9-C8
5	C	305	CHL	C16-C17-C18-C19
11	F	319	LMG	C7-C8-C9-O8
4	B	304	LMU	C7-C8-C9-C10
5	E	310	CHL	C12-C13-C15-C16
7	F	318	LHG	C23-C24-C25-C26
5	B	311	CHL	O1D-CGD-O2D-CED
6	A	317	CLA	C5-C6-C7-C8
5	A	311	CHL	CAA-CBA-CGA-O2A
5	A	310	CHL	O1A-CGA-O2A-C1
5	D	313	CHL	O1A-CGA-O2A-C1
4	D	304	LMU	C1-C2-C3-C4
6	E	316	CLA	C3-C5-C6-C7
5	F	309	CHL	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	322	0UR	C46-C47-C48-C49
11	B	323	LMG	C13-C14-C15-C16
7	B	324	LHG	C7-C8-C9-C10
5	B	307	CHL	C16-C17-C18-C19
5	E	305	CHL	C15-C16-C17-C18
2	D	302	0IE	C14-C15-C16-C23
2	F	302	0IE	C10-C11-C12-C22
5	E	310	CHL	C4-C3-C5-C6
6	A	317	CLA	C4-C3-C5-C6
7	D	319	LHG	C32-C33-C34-C35
6	A	317	CLA	C2-C3-C5-C6
6	F	306	CLA	C16-C17-C18-C19
5	A	311	CHL	C12-C13-C15-C16
6	C	315	CLA	C10-C11-C12-C13
6	B	308	CLA	C2-C1-O2A-CGA
7	B	320	LHG	C11-C12-C13-C14
5	D	309	CHL	O1D-CGD-O2D-CED
5	E	308	CHL	O1D-CGD-O2D-CED
7	A	319	LHG	C28-C29-C30-C31
5	C	305	CHL	O1D-CGD-O2D-CED
9	C	321	0UR	C46-C47-C48-C49
7	C	304	LHG	O6-C4-C5-O7
5	A	313	CHL	O1A-CGA-O2A-C1
5	E	304	CHL	O1A-CGA-O2A-C1
6	A	317	CLA	C6-C7-C8-C10
2	D	302	0IE	C14-C15-C16-C17
11	B	323	LMG	C2-C1-O1-C7
4	B	304	LMU	C11-C10-C9-C8
7	D	319	LHG	C27-C28-C29-C30
5	C	305	CHL	C5-C6-C7-C8
5	F	310	CHL	C11-C12-C13-C15
5	D	305	CHL	O1D-CGD-O2D-CED
5	A	313	CHL	C4-C3-C5-C6
5	B	307	CHL	C4-C3-C5-C6
6	E	313	CLA	O1D-CGD-O2D-CED
5	F	305	CHL	C13-C15-C16-C17
5	D	306	CHL	C12-C13-C15-C16
5	D	313	CHL	C11-C12-C13-C15
5	E	305	CHL	C11-C10-C8-C7
5	E	310	CHL	C2-C3-C5-C6
5	E	310	CHL	C11-C10-C8-C7
5	F	310	CHL	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	307	CLA	C11-C10-C8-C7
6	A	315	CLA	C6-C7-C8-C10
6	D	307	CLA	C12-C13-C15-C16
6	E	314	CLA	C6-C7-C8-C10
5	A	313	CHL	C3-C5-C6-C7
5	A	306	CHL	C11-C10-C8-C9
5	B	306	CHL	C14-C13-C15-C16
5	B	314	CHL	C11-C12-C13-C14
5	D	313	CHL	C11-C12-C13-C14
5	F	304	CHL	C11-C12-C13-C14
6	B	308	CLA	C14-C13-C15-C16
6	B	318	CLA	C11-C12-C13-C14
6	E	306	CLA	C11-C10-C8-C9
6	E	314	CLA	C6-C7-C8-C9
10	B	322	BET	C-CA-N-C1
5	E	317	CHL	O1D-CGD-O2D-CED
5	D	306	CHL	C2A-CAA-CBA-CGA
5	F	317	CHL	C2A-CAA-CBA-CGA
5	C	310	CHL	O1D-CGD-O2D-CED
2	A	301	0IE	C22-C12-C13-C14
7	C	319	LHG	C7-C8-C9-C10
5	B	306	CHL	C13-C15-C16-C17
5	D	305	CHL	C5-C6-C7-C8
5	D	305	CHL	C4C-C3C-CAC-CBC
6	C	314	CLA	O1A-CGA-O2A-C1
4	E	319	LMU	C3-C4-C5-C6
5	E	312	CHL	C13-C15-C16-C17
4	A	304	LMU	C7-C8-C9-C10
7	F	318	LHG	C10-C11-C12-C13
5	A	305	CHL	C4B-C3B-CAB-CBB
5	A	310	CHL	C4B-C3B-CAB-CBB
6	B	316	CLA	C4B-C3B-CAB-CBB
6	C	307	CLA	C4B-C3B-CAB-CBB
6	D	307	CLA	C4B-C3B-CAB-CBB
6	E	316	CLA	C4B-C3B-CAB-CBB
6	F	306	CLA	C4B-C3B-CAB-CBB
5	D	313	CHL	C16-C17-C18-C19
7	C	304	LHG	O6-C4-C5-C6
5	A	313	CHL	C2-C3-C5-C6
5	B	307	CHL	C2-C3-C5-C6
5	A	312	CHL	O1D-CGD-O2D-CED
5	F	310	CHL	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	D	307	CLA	C16-C17-C18-C19
7	E	318	LHG	C11-C12-C13-C14
5	D	306	CHL	CBA-CGA-O2A-C1
7	C	319	LHG	C24-C23-O8-C6
10	B	322	BET	C-CA-N-C2
5	F	317	CHL	CBD-CGD-O2D-CED
4	B	304	LMU	C2-C1-O1'-C1'
6	D	307	CLA	C16-C17-C18-C20
7	C	304	LHG	C4-C5-C6-O8
7	C	319	LHG	C4-C5-C6-O8
7	D	319	LHG	C4-C5-C6-O8
5	D	311	CHL	CAA-CBA-CGA-O2A
6	C	314	CLA	C5-C6-C7-C8
5	B	307	CHL	C3C-C2C-CMC-OMC
5	B	312	CHL	C3C-C2C-CMC-OMC
5	B	314	CHL	C3C-C2C-CMC-OMC
5	D	313	CHL	C3C-C2C-CMC-OMC
5	A	309	CHL	O1D-CGD-O2D-CED
6	F	306	CLA	C8-C10-C11-C12
5	C	306	CHL	C2C-C3C-CAC-CBC
7	F	318	LHG	O6-C4-C5-O7
5	C	313	CHL	CBA-CGA-O2A-C1
6	F	306	CLA	C16-C17-C18-C20
5	A	310	CHL	C2B-C3B-CAB-CBB
6	B	316	CLA	C2B-C3B-CAB-CBB
6	B	318	CLA	C2B-C3B-CAB-CBB
6	C	307	CLA	C2B-C3B-CAB-CBB
6	D	307	CLA	C2B-C3B-CAB-CBB
6	E	316	CLA	C2B-C3B-CAB-CBB
7	D	319	LHG	C31-C32-C33-C34
7	B	324	LHG	O7-C5-C6-O8
7	C	319	LHG	O7-C5-C6-O8
7	D	319	LHG	O7-C5-C6-O8
11	B	323	LMG	O1-C7-C8-O7
5	F	310	CHL	CAA-CBA-CGA-O2A
6	E	316	CLA	C11-C10-C8-C7
5	D	313	CHL	C16-C17-C18-C20
5	E	312	CHL	C2-C1-O2A-CGA
5	E	304	CHL	C13-C15-C16-C17
5	A	306	CHL	C6-C7-C8-C9
5	A	311	CHL	C11-C10-C8-C9
5	A	313	CHL	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C	315	CLA	C14-C13-C15-C16
6	F	316	CLA	C6-C7-C8-C9
5	A	305	CHL	C8-C10-C11-C12
7	C	304	LHG	C2-C3-O3-P
6	D	314	CLA	C2A-CAA-CBA-CGA
5	C	312	CHL	C6-C7-C8-C10
5	F	311	CHL	C6-C7-C8-C10
5	B	319	CHL	CAA-CBA-CGA-O2A
2	B	301	0IE	C5-C6-C7-C8
6	B	308	CLA	C15-C16-C17-C18
7	A	319	LHG	O9-C7-O7-C5
2	D	301	0IE	C11-C10-C9-C8
3	E	303	NEX	C14-C15-C35-C34
5	A	305	CHL	C16-C17-C18-C20
5	D	311	CHL	C14-C13-C15-C16
5	A	305	CHL	C5-C6-C7-C8
5	F	304	CHL	C5-C6-C7-C8
7	E	318	LHG	O6-C4-C5-C6
5	D	311	CHL	C4-C3-C5-C6
5	A	306	CHL	C11-C10-C8-C7
5	A	313	CHL	C11-C12-C13-C15
5	B	306	CHL	C12-C13-C15-C16
5	B	314	CHL	C11-C12-C13-C15
5	C	306	CHL	C12-C13-C15-C16
5	C	311	CHL	C11-C10-C8-C7
5	E	304	CHL	C11-C12-C13-C15
5	E	304	CHL	C12-C13-C15-C16
5	F	304	CHL	C11-C12-C13-C15
6	B	318	CLA	C11-C10-C8-C7
6	B	318	CLA	C11-C12-C13-C15
6	E	306	CLA	C11-C10-C8-C7
6	F	306	CLA	C11-C12-C13-C15
6	F	316	CLA	C6-C7-C8-C10
6	A	307	CLA	C8-C10-C11-C12
2	A	302	0IE	C9-C10-C11-C12
2	A	302	0IE	C7-C8-C9-C10
2	D	301	0IE	C13-C14-C15-C16
2	E	301	0IE	C13-C14-C15-C16
5	B	312	CHL	CAA-CBA-CGA-O2A
2	A	301	0IE	O1-C2-C3-C4
2	B	301	0IE	C20-C3-C4-C5
2	B	301	0IE	O1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	301	0IE	O1-C2-C3-C4
2	C	301	0IE	C14-C15-C16-C23
2	C	302	0IE	C14-C15-C16-C23
2	D	301	0IE	O1-C2-C3-C4
2	E	301	0IE	O1-C2-C3-C4
2	F	301	0IE	O1-C2-C3-C4
9	A	322	0UR	O42-C2-C3-C4
9	B	302	0UR	O42-C2-C3-C4
9	B	325	0UR	O42-C2-C3-C4
9	C	321	0UR	O42-C2-C3-C4
9	D	321	0UR	O42-C2-C3-C4
9	E	320	0UR	O42-C2-C3-C4
9	F	320	0UR	O42-C2-C3-C4
5	B	314	CHL	C3-C5-C6-C7
5	B	310	CHL	CBD-CGD-O2D-CED
5	D	313	CHL	C15-C16-C17-C18
5	D	311	CHL	C12-C13-C15-C16
5	A	310	CHL	CAD-CBD-CGD-O2D
5	B	311	CHL	CAD-CBD-CGD-O2D
6	A	314	CLA	CAD-CBD-CGD-O2D
6	E	306	CLA	CAD-CBD-CGD-O2D
6	E	314	CLA	CAD-CBD-CGD-O2D
6	F	313	CLA	CAD-CBD-CGD-O2D
5	F	309	CHL	O1D-CGD-O2D-CED
11	B	323	LMG	O1-C7-C8-C9
7	E	318	LHG	O6-C4-C5-O7
6	B	318	CLA	C15-C16-C17-C18
7	E	318	LHG	C27-C28-C29-C30
6	C	315	CLA	C2A-CAA-CBA-CGA
5	B	319	CHL	CHA-CBD-CGD-O1D
5	B	319	CHL	CHA-CBD-CGD-O2D
5	D	318	CHL	CHA-CBD-CGD-O2D
5	E	305	CHL	CHA-CBD-CGD-O1D
5	E	305	CHL	CHA-CBD-CGD-O2D
5	E	311	CHL	CHA-CBD-CGD-O1D
5	E	311	CHL	CHA-CBD-CGD-O2D
5	F	305	CHL	CHA-CBD-CGD-O1D
6	A	308	CLA	CHA-CBD-CGD-O1D
6	B	309	CLA	CHA-CBD-CGD-O1D
6	B	309	CLA	CHA-CBD-CGD-O2D
6	D	308	CLA	CHA-CBD-CGD-O1D
6	D	308	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	F	314	CLA	O1D-CGD-O2D-CED
5	C	313	CHL	O1A-CGA-O2A-C1
5	D	306	CHL	O1A-CGA-O2A-C1
7	C	319	LHG	C25-C26-C27-C28
2	C	302	0IE	C14-C15-C16-C17
11	F	319	LMG	O1-C7-C8-O7
6	A	307	CLA	C3-C5-C6-C7
5	C	305	CHL	C15-C16-C17-C18
7	F	318	LHG	O9-C7-O7-C5
5	C	305	CHL	C11-C12-C13-C14
5	F	317	CHL	O1D-CGD-O2D-CED
3	D	303	NEX	C31-C32-C33-C40
6	A	307	CLA	C13-C15-C16-C17
2	A	301	0IE	C5-C6-C7-C8
5	B	314	CHL	C1A-C2A-CAA-CBA
5	D	306	CHL	C1A-C2A-CAA-CBA
6	C	314	CLA	C1A-C2A-CAA-CBA
6	E	313	CLA	C1A-C2A-CAA-CBA
6	A	307	CLA	C2-C1-O2A-CGA
6	D	307	CLA	C2-C1-O2A-CGA
2	C	302	0IE	C3-C4-C5-C6
4	A	304	LMU	C9-C10-C11-C12
5	D	306	CHL	C4-C3-C5-C6
6	F	316	CLA	C3-C5-C6-C7
5	A	306	CHL	C2-C3-C5-C6
7	C	304	LHG	O10-C23-O8-C6
5	C	313	CHL	C4B-C3B-CAB-CBB
5	F	317	CHL	C4B-C3B-CAB-CBB
6	E	306	CLA	C4B-C3B-CAB-CBB
6	E	314	CLA	C4B-C3B-CAB-CBB
7	B	324	LHG	C3-O3-P-O4
7	F	318	LHG	C4-O6-P-O5
7	A	319	LHG	C11-C12-C13-C14
5	B	319	CHL	CAD-CBD-CGD-O1D
5	D	318	CHL	CAD-CBD-CGD-O1D
6	B	309	CLA	CAD-CBD-CGD-O1D
6	D	308	CLA	CAD-CBD-CGD-O1D
5	B	310	CHL	O1D-CGD-O2D-CED
6	B	308	CLA	C4-C3-C5-C6
2	B	301	0IE	O1-C2-C3-C20
2	B	301	0IE	C3-C2-C30-C31
2	D	302	0IE	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	307	CHL	C6-C7-C8-C10
5	B	307	CHL	C11-C12-C13-C15
5	C	305	CHL	C11-C10-C8-C7
5	C	305	CHL	C11-C12-C13-C15
5	C	313	CHL	C11-C12-C13-C15
5	D	306	CHL	C11-C10-C8-C7
6	B	316	CLA	C6-C7-C8-C10
6	B	308	CLA	C10-C11-C12-C13
5	A	306	CHL	C2A-CAA-CBA-CGA
6	C	317	CLA	C2A-CAA-CBA-CGA
5	A	311	CHL	C1C-C2C-CMC-OMC
5	A	313	CHL	C1C-C2C-CMC-OMC
5	B	306	CHL	C1C-C2C-CMC-OMC
5	D	306	CHL	C1C-C2C-CMC-OMC
5	E	310	CHL	C1C-C2C-CMC-OMC
5	F	312	CHL	C1C-C2C-CMC-OMC
7	B	324	LHG	C4-C5-C6-O8
2	F	301	0IE	C11-C10-C9-C8
5	C	313	CHL	C4-C3-C5-C6
5	D	311	CHL	C2-C3-C5-C6
6	E	314	CLA	C10-C11-C12-C13
5	B	307	CHL	C6-C7-C8-C9
5	C	306	CHL	C11-C10-C8-C9
5	D	306	CHL	C14-C13-C15-C16
5	E	304	CHL	C11-C12-C13-C14
5	E	304	CHL	C14-C13-C15-C16
5	F	305	CHL	C11-C10-C8-C9
6	B	318	CLA	C14-C13-C15-C16
9	B	302	0UR	C4-C5-C6-C7
2	F	301	0IE	C11-C12-C13-C14
5	C	306	CHL	C2B-C3B-CAB-CBB
5	C	313	CHL	C2B-C3B-CAB-CBB
6	D	317	CLA	C2B-C3B-CAB-CBB
5	B	314	CHL	O1A-CGA-O2A-C1
5	F	304	CHL	CAA-CBA-CGA-O2A
7	B	324	LHG	C4-C5-O7-C7
5	C	306	CHL	C2A-CAA-CBA-CGA
6	B	309	CLA	C2A-CAA-CBA-CGA
5	C	311	CHL	C2-C1-O2A-CGA
5	D	313	CHL	C2-C1-O2A-CGA
4	B	305	LMU	C7-C8-C9-C10
2	E	302	0IE	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	314	CHL	CBA-CGA-O2A-C1
4	D	304	LMU	C9-C10-C11-C12
2	C	301	0IE	C14-C15-C16-C17
7	F	318	LHG	C11-C10-C9-C8
7	A	319	LHG	C4-O6-P-O3
7	B	320	LHG	C3-O3-P-O6
7	C	319	LHG	C3-O3-P-O6
7	D	319	LHG	C3-O3-P-O6
7	E	318	LHG	C4-O6-P-O3
7	B	320	LHG	C10-C11-C12-C13
5	A	306	CHL	C13-C15-C16-C17
5	C	306	CHL	C11-C10-C8-C7
5	D	306	CHL	C2-C3-C5-C6
5	F	305	CHL	C11-C10-C8-C7
5	F	312	CHL	C11-C10-C8-C7
6	B	308	CLA	C11-C10-C8-C7
5	D	306	CHL	C11-C10-C8-C9
6	B	308	CLA	C16-C17-C18-C20
5	F	312	CHL	C10-C11-C12-C13
7	B	324	LHG	C2-C3-O3-P
5	E	310	CHL	CAA-CBA-CGA-O2A
2	C	302	0IE	C11-C12-C13-C14
5	F	305	CHL	CBA-CGA-O2A-C1
9	F	320	0UR	C47-C48-C49-C50
7	C	319	LHG	C18-C19-C20-C21
5	C	306	CHL	C4B-C3B-CAB-CBB
6	D	317	CLA	C4B-C3B-CAB-CBB
6	E	316	CLA	C2A-CAA-CBA-CGA
2	D	302	0IE	C9-C10-C11-C12
9	F	320	0UR	C3-C4-C5-C6
6	A	308	CLA	CAA-CBA-CGA-O2A
5	A	313	CHL	C5-C6-C7-C8
5	F	305	CHL	C5-C6-C7-C8
6	B	318	CLA	C13-C15-C16-C17
6	F	313	CLA	C2A-CAA-CBA-CGA
5	C	306	CHL	C4C-C3C-CAC-CBC
6	C	307	CLA	C6-C7-C8-C9
6	F	306	CLA	C15-C16-C17-C18
2	E	302	0IE	C14-C15-C16-C23
3	A	303	NEX	C39-C29-C30-C31
3	B	303	NEX	C39-C29-C30-C31
3	C	303	NEX	C39-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	303	NEX	C39-C29-C30-C31
3	E	303	NEX	C39-C29-C30-C31
3	F	303	NEX	C39-C29-C30-C31
6	A	308	CLA	C2A-CAA-CBA-CGA
7	A	319	LHG	C33-C34-C35-C36
5	A	311	CHL	CAA-CBA-CGA-O1A
2	A	301	0IE	C23-C16-C17-C18
2	D	301	0IE	C22-C12-C13-C14
6	E	306	CLA	C5-C6-C7-C8
6	E	315	CLA	CAA-CBA-CGA-O1A
7	B	324	LHG	C6-C5-O7-C7
5	B	314	CHL	C8-C10-C11-C12
5	C	306	CHL	C5-C6-C7-C8
5	A	306	CHL	C1A-C2A-CAA-CBA
5	C	313	CHL	C1A-C2A-CAA-CBA
5	E	305	CHL	C1A-C2A-CAA-CBA
6	A	314	CLA	C1A-C2A-CAA-CBA
5	F	305	CHL	C12-C13-C15-C16
6	B	308	CLA	C6-C7-C8-C10
7	D	319	LHG	C30-C31-C32-C33
6	D	315	CLA	C10-C11-C12-C13
9	D	321	0UR	C48-C49-C50-C51
6	A	317	CLA	C2A-CAA-CBA-CGA
7	E	318	LHG	C29-C30-C31-C32
6	C	316	CLA	CAA-CBA-CGA-O2A
5	F	317	CHL	C2B-C3B-CAB-CBB
6	B	308	CLA	C2B-C3B-CAB-CBB
6	E	306	CLA	C2B-C3B-CAB-CBB
6	E	314	CLA	C2B-C3B-CAB-CBB
6	C	316	CLA	CAA-CBA-CGA-O1A
5	C	305	CHL	C3-C5-C6-C7
3	A	303	NEX	C28-C29-C30-C31
3	B	303	NEX	C28-C29-C30-C31
3	C	303	NEX	C28-C29-C30-C31
3	D	303	NEX	C28-C29-C30-C31
3	E	303	NEX	C28-C29-C30-C31
3	F	303	NEX	C28-C29-C30-C31
5	C	305	CHL	C8-C10-C11-C12
7	F	318	LHG	C16-C17-C18-C19
7	E	318	LHG	C9-C10-C11-C12
5	B	314	CHL	C2-C1-O2A-CGA
5	C	313	CHL	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	305	CHL	O1A-CGA-O2A-C1
4	B	305	LMU	C2B-C1B-O1B-C4'
6	E	315	CLA	CAA-CBA-CGA-O2A
7	A	319	LHG	C13-C14-C15-C16
6	D	316	CLA	O1D-CGD-O2D-CED
2	C	301	0IE	C3-C4-C5-C6
2	F	301	0IE	C7-C8-C9-C10
6	A	314	CLA	C4-C3-C5-C6
3	A	303	NEX	C31-C32-C33-C34
3	D	303	NEX	C31-C32-C33-C34
5	E	309	CHL	C1A-C2A-CAA-CBA
7	B	320	LHG	C13-C14-C15-C16
6	E	306	CLA	C3-C5-C6-C7
6	A	314	CLA	C6-C7-C8-C10
5	E	305	CHL	C8-C10-C11-C12
6	C	307	CLA	C15-C16-C17-C18
6	E	307	CLA	C2A-CAA-CBA-CGA
9	B	302	0UR	C46-C47-C48-C49
5	C	305	CHL	CBA-CGA-O2A-C1
6	B	317	CLA	C4B-C3B-CAB-CBB
6	E	315	CLA	C4B-C3B-CAB-CBB
6	F	316	CLA	C4B-C3B-CAB-CBB
4	B	305	LMU	O5B-C1B-O1B-C4'
5	F	304	CHL	C4-C3-C5-C6
5	F	311	CHL	C4-C3-C5-C6
5	B	314	CHL	C12-C13-C15-C16
5	F	305	CHL	O1A-CGA-O2A-C1
5	A	306	CHL	O1A-CGA-O2A-C1
7	D	319	LHG	C11-C12-C13-C14
5	C	306	CHL	C13-C15-C16-C17
2	F	301	0IE	C20-C3-C4-C5
5	D	311	CHL	CAA-CBA-CGA-O1A
5	F	312	CHL	C4-C3-C5-C6
5	D	311	CHL	C5-C6-C7-C8
6	B	308	CLA	C2-C3-C5-C6
5	C	305	CHL	C11-C10-C8-C9
5	C	313	CHL	C11-C10-C8-C9
5	F	305	CHL	C14-C13-C15-C16
6	D	307	CLA	C5-C6-C7-C8
5	E	311	CHL	O1A-CGA-O2A-C1
5	F	311	CHL	O1A-CGA-O2A-C1
5	B	307	CHL	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	310	CHL	CAD-CBD-CGD-O2D
5	C	318	CHL	CAD-CBD-CGD-O2D
5	D	313	CHL	CAD-CBD-CGD-O2D
5	E	317	CHL	CAD-CBD-CGD-O2D
5	F	309	CHL	CAD-CBD-CGD-O2D
6	A	315	CLA	CAD-CBD-CGD-O2D
6	B	315	CLA	CAD-CBD-CGD-O2D
6	C	315	CLA	CAD-CBD-CGD-O2D
6	D	307	CLA	CAD-CBD-CGD-O2D
6	D	314	CLA	CAD-CBD-CGD-O2D
6	D	315	CLA	CAD-CBD-CGD-O2D
6	F	307	CLA	CAD-CBD-CGD-O2D
6	D	314	CLA	C10-C11-C12-C13
7	B	320	LHG	C32-C33-C34-C35
5	D	305	CHL	C13-C15-C16-C17
5	C	311	CHL	C2A-CAA-CBA-CGA
4	B	305	LMU	C1-C2-C3-C4
7	A	319	LHG	C26-C27-C28-C29
5	E	304	CHL	C16-C17-C18-C20
5	F	317	CHL	CAA-CBA-CGA-O2A
5	C	311	CHL	CAA-CBA-CGA-O2A
7	F	318	LHG	C14-C15-C16-C17
2	A	301	0IE	C11-C12-C13-C14
2	D	301	0IE	C11-C12-C13-C14
4	B	304	LMU	C5-C6-C7-C8
3	D	303	NEX	O24-C26-C27-C28
3	E	303	NEX	O24-C26-C27-C28
9	D	321	0UR	C4-C3-C43-O44
6	A	316	CLA	CAA-CBA-CGA-O2A
9	C	321	0UR	C48-C49-C50-C51
5	C	305	CHL	C2A-CAA-CBA-CGA
6	B	318	CLA	C2A-CAA-CBA-CGA
6	F	316	CLA	C2A-CAA-CBA-CGA
2	C	301	0IE	C11-C10-C9-C8
5	F	310	CHL	CAA-CBA-CGA-O1A
5	F	317	CHL	CAA-CBA-CGA-O1A
6	A	316	CLA	CAA-CBA-CGA-O1A
6	B	317	CLA	CAA-CBA-CGA-O2A
6	F	315	CLA	CAA-CBA-CGA-O2A
2	C	301	0IE	C13-C14-C15-C16
5	A	306	CHL	CHA-CBD-CGD-O1D
5	B	306	CHL	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	306	CHL	CHA-CBD-CGD-O2D
5	B	307	CHL	CHA-CBD-CGD-O2D
5	C	306	CHL	CHA-CBD-CGD-O1D
5	D	306	CHL	CHA-CBD-CGD-O1D
5	E	304	CHL	CHA-CBD-CGD-O1D
5	E	304	CHL	CHA-CBD-CGD-O2D
5	F	304	CHL	CHA-CBD-CGD-O1D
5	F	304	CHL	CHA-CBD-CGD-O2D
5	F	305	CHL	CHA-CBD-CGD-O2D
6	A	307	CLA	CHA-CBD-CGD-O1D
6	A	307	CLA	CHA-CBD-CGD-O2D
6	A	308	CLA	CHA-CBD-CGD-O2D
6	A	316	CLA	CHA-CBD-CGD-O1D
6	A	316	CLA	CHA-CBD-CGD-O2D
6	A	317	CLA	CHA-CBD-CGD-O1D
6	A	317	CLA	CHA-CBD-CGD-O2D
6	B	308	CLA	CHA-CBD-CGD-O1D
6	B	308	CLA	CHA-CBD-CGD-O2D
6	B	318	CLA	CHA-CBD-CGD-O1D
6	B	318	CLA	CHA-CBD-CGD-O2D
6	C	307	CLA	CHA-CBD-CGD-O2D
6	C	308	CLA	CHA-CBD-CGD-O1D
6	C	316	CLA	CHA-CBD-CGD-O1D
6	C	316	CLA	CHA-CBD-CGD-O2D
6	E	315	CLA	CHA-CBD-CGD-O1D
6	E	315	CLA	CHA-CBD-CGD-O2D
6	F	306	CLA	CHA-CBD-CGD-O1D
6	F	306	CLA	CHA-CBD-CGD-O2D
5	F	312	CHL	C2-C3-C5-C6
7	B	320	LHG	O7-C7-C8-C9
7	F	318	LHG	O7-C7-C8-C9
6	A	307	CLA	C2A-CAA-CBA-CGA
6	D	317	CLA	C2A-CAA-CBA-CGA
5	C	312	CHL	CBA-CGA-O2A-C1
5	D	313	CHL	C2-C3-C5-C6
6	B	308	CLA	C6-C7-C8-C9
6	D	314	CLA	C6-C7-C8-C9
3	D	303	NEX	C13-C14-C15-C35
6	E	315	CLA	C2B-C3B-CAB-CBB
5	A	306	CHL	CBA-CGA-O2A-C1
5	F	311	CHL	CBA-CGA-O2A-C1
7	C	319	LHG	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B	317	CLA	CAA-CBA-CGA-O1A
6	F	315	CLA	CAA-CBA-CGA-O1A
5	B	312	CHL	CAA-CBA-CGA-O1A
5	B	319	CHL	CAA-CBA-CGA-O1A
5	E	311	CHL	CBA-CGA-O2A-C1
5	C	312	CHL	O1A-CGA-O2A-C1
6	C	308	CLA	C1A-C2A-CAA-CBA
5	F	310	CHL	C2A-CAA-CBA-CGA
6	C	314	CLA	C2A-CAA-CBA-CGA
6	E	313	CLA	C2A-CAA-CBA-CGA
7	B	324	LHG	C4-O6-P-O3
7	B	320	LHG	O10-C23-C24-C25
5	D	305	CHL	CAA-CBA-CGA-O2A
2	D	302	0IE	C11-C10-C9-C8
5	A	309	CHL	C4B-C3B-CAB-CBB
5	A	318	CHL	C4B-C3B-CAB-CBB
6	B	308	CLA	C4B-C3B-CAB-CBB
7	B	320	LHG	C3-O3-P-O5
7	B	324	LHG	C4-O6-P-O5
7	C	319	LHG	C3-O3-P-O5
7	D	319	LHG	C3-O3-P-O4
7	E	318	LHG	C4-O6-P-O5
7	C	319	LHG	O9-C7-C8-C9
5	B	311	CHL	O1A-CGA-O2A-C1
2	D	301	0IE	C10-C11-C12-C22
7	A	319	LHG	C9-C10-C11-C12
5	D	306	CHL	C5-C6-C7-C8
6	C	317	CLA	C5-C6-C7-C8
5	B	312	CHL	O1A-CGA-O2A-C1
5	E	310	CHL	C2A-CAA-CBA-CGA
5	A	318	CHL	CAD-CBD-CGD-O1D
5	F	304	CHL	CAD-CBD-CGD-O1D
6	A	308	CLA	CAD-CBD-CGD-O1D
6	B	318	CLA	CAD-CBD-CGD-O1D
6	C	308	CLA	CAD-CBD-CGD-O1D
5	B	306	CHL	C11-C12-C13-C14
5	F	312	CHL	C14-C13-C15-C16
5	B	311	CHL	CBA-CGA-O2A-C1
11	B	323	LMG	O8-C28-C29-C30
6	F	306	CLA	CAA-CBA-CGA-O2A
7	C	319	LHG	O7-C7-C8-C9
2	A	301	0IE	O1-C2-C3-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	301	0IE	C2-C3-C4-C5
2	C	301	0IE	O1-C2-C3-C20
2	E	301	0IE	O1-C2-C3-C20
2	F	301	0IE	C2-C3-C4-C5
5	B	306	CHL	C11-C12-C13-C15
6	E	307	CLA	C3A-C2A-CAA-CBA
9	A	322	0UR	O42-C2-C3-C43
9	B	302	0UR	O42-C2-C3-C43
9	B	325	0UR	O42-C2-C3-C43
9	C	321	0UR	O42-C2-C3-C43
9	D	321	0UR	O42-C2-C3-C43
9	E	320	0UR	O42-C2-C3-C43
9	F	320	0UR	O42-C2-C3-C43
5	A	306	CHL	CAA-CBA-CGA-O2A
5	D	306	CHL	CAA-CBA-CGA-O2A
2	A	301	0IE	C15-C16-C17-C18
5	D	305	CHL	CAA-CBA-CGA-O1A
7	F	318	LHG	O10-C23-C24-C25
6	B	315	CLA	C10-C11-C12-C13
7	B	324	LHG	O7-C7-C8-C9
5	A	306	CHL	CAA-CBA-CGA-O1A
7	E	318	LHG	O10-C23-C24-C25
6	D	316	CLA	CBD-CGD-O2D-CED
7	B	320	LHG	C16-C17-C18-C19
5	D	306	CHL	CAA-CBA-CGA-O1A

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	304	LMU	C1'-C2'-C3'-C4'-C5'-O5'

110 monomers are involved in 346 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304	LMU	4	0
5	A	318	CHL	1	0
5	E	312	CHL	8	0
4	B	305	LMU	1	0
6	A	307	CLA	6	0
6	C	307	CLA	7	0
9	F	320	0UR	3	0
6	A	314	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	317	CLA	8	0
5	B	312	CHL	9	0
5	C	318	CHL	4	0
6	A	315	CLA	3	0
6	C	315	CLA	3	0
5	C	306	CHL	2	0
4	D	304	LMU	3	0
6	C	314	CLA	2	0
10	B	322	BET	2	0
2	B	301	0IE	1	0
5	A	310	CHL	2	0
5	C	312	CHL	3	0
5	B	310	CHL	1	0
5	F	304	CHL	8	0
3	D	303	NEX	4	0
5	F	312	CHL	3	0
5	F	311	CHL	2	0
6	A	308	CLA	3	0
5	B	306	CHL	3	0
5	F	308	CHL	1	0
7	C	319	LHG	4	0
5	B	319	CHL	2	0
6	B	308	CLA	5	0
5	D	305	CHL	2	0
6	E	313	CLA	3	0
5	F	310	CHL	5	0
5	B	313	CHL	6	0
5	A	313	CHL	5	0
5	B	314	CHL	9	0
6	D	308	CLA	2	0
5	D	311	CHL	9	0
6	D	315	CLA	4	0
7	B	320	LHG	5	0
7	F	318	LHG	8	0
6	D	314	CLA	4	0
6	C	308	CLA	3	0
6	B	309	CLA	1	0
9	B	325	0UR	5	0
6	E	315	CLA	3	0
6	D	317	CLA	8	0
5	D	309	CHL	2	0
6	F	306	CLA	5	0

Continued on next page...

Continued from previous page...

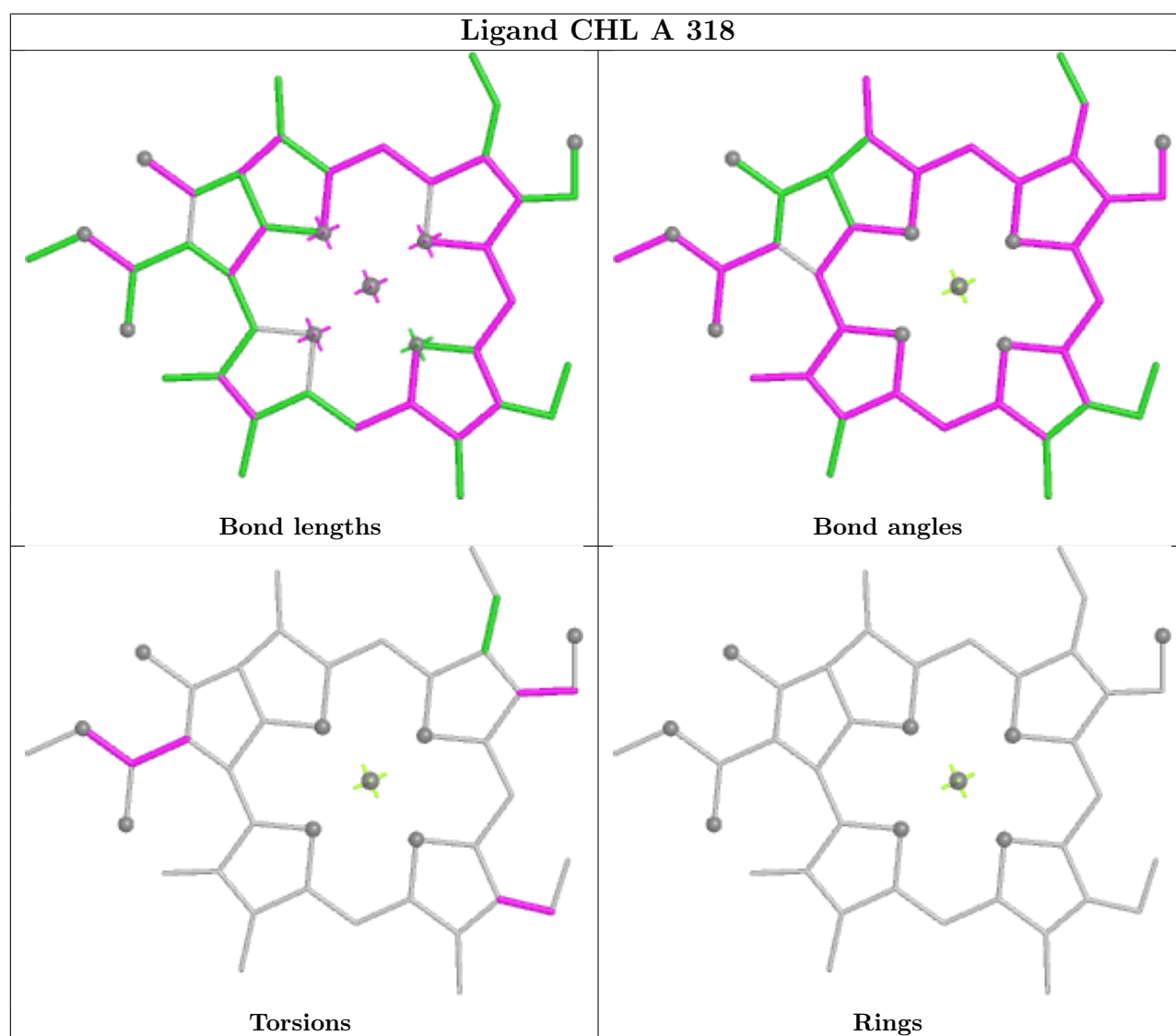
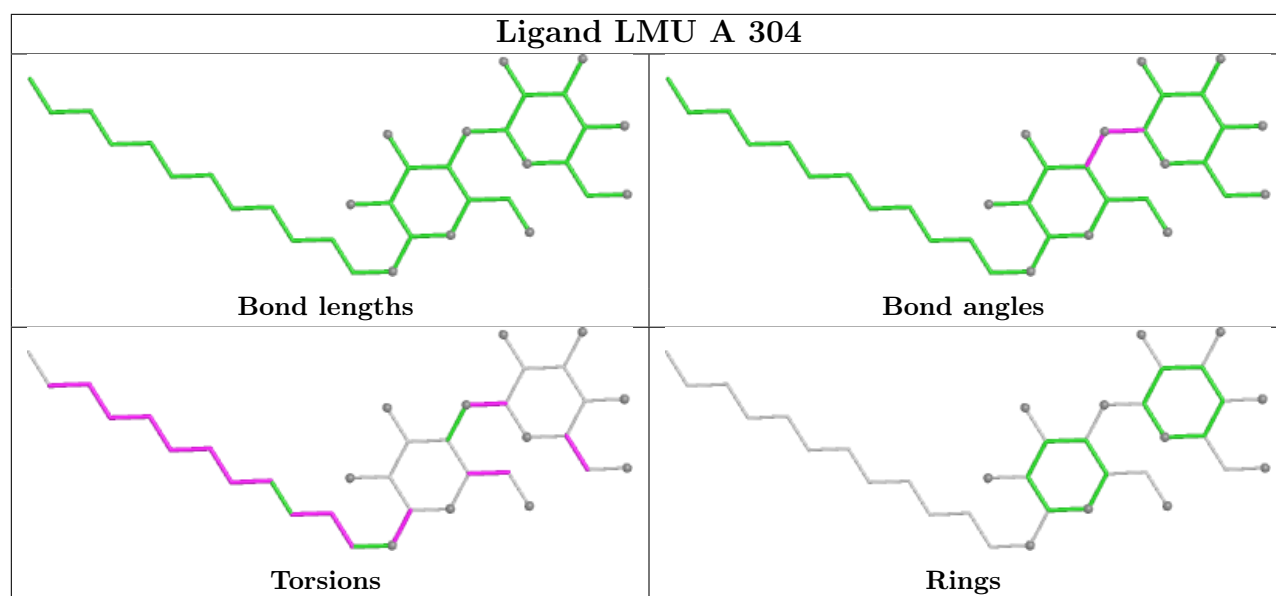
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	306	CLA	2	0
6	F	315	CLA	5	0
11	F	319	LMG	1	0
5	E	311	CHL	5	0
5	C	310	CHL	5	0
3	F	303	NEX	1	0
5	C	311	CHL	2	0
6	E	314	CLA	3	0
2	C	302	OIE	2	0
6	D	316	CLA	4	0
5	E	304	CHL	4	0
5	E	309	CHL	3	0
9	C	321	OUR	4	0
5	E	317	CHL	2	0
5	F	305	CHL	8	0
7	D	319	LHG	4	0
5	D	312	CHL	2	0
4	E	319	LMU	3	0
3	A	303	NEX	3	0
6	C	316	CLA	4	0
5	C	313	CHL	10	0
4	B	304	LMU	2	0
5	C	309	CHL	5	0
3	C	303	NEX	4	0
6	A	317	CLA	5	0
5	D	310	CHL	7	0
5	F	317	CHL	2	0
7	B	324	LHG	8	0
6	B	317	CLA	2	0
5	A	312	CHL	2	0
6	B	315	CLA	7	0
6	F	307	CLA	2	0
5	C	305	CHL	5	0
2	A	302	OIE	1	0
6	B	318	CLA	5	0
5	F	309	CHL	1	0
3	E	303	NEX	3	0
5	B	311	CHL	4	0
5	E	305	CHL	3	0
5	E	310	CHL	3	0
5	E	308	CHL	3	0
2	E	302	OIE	1	0

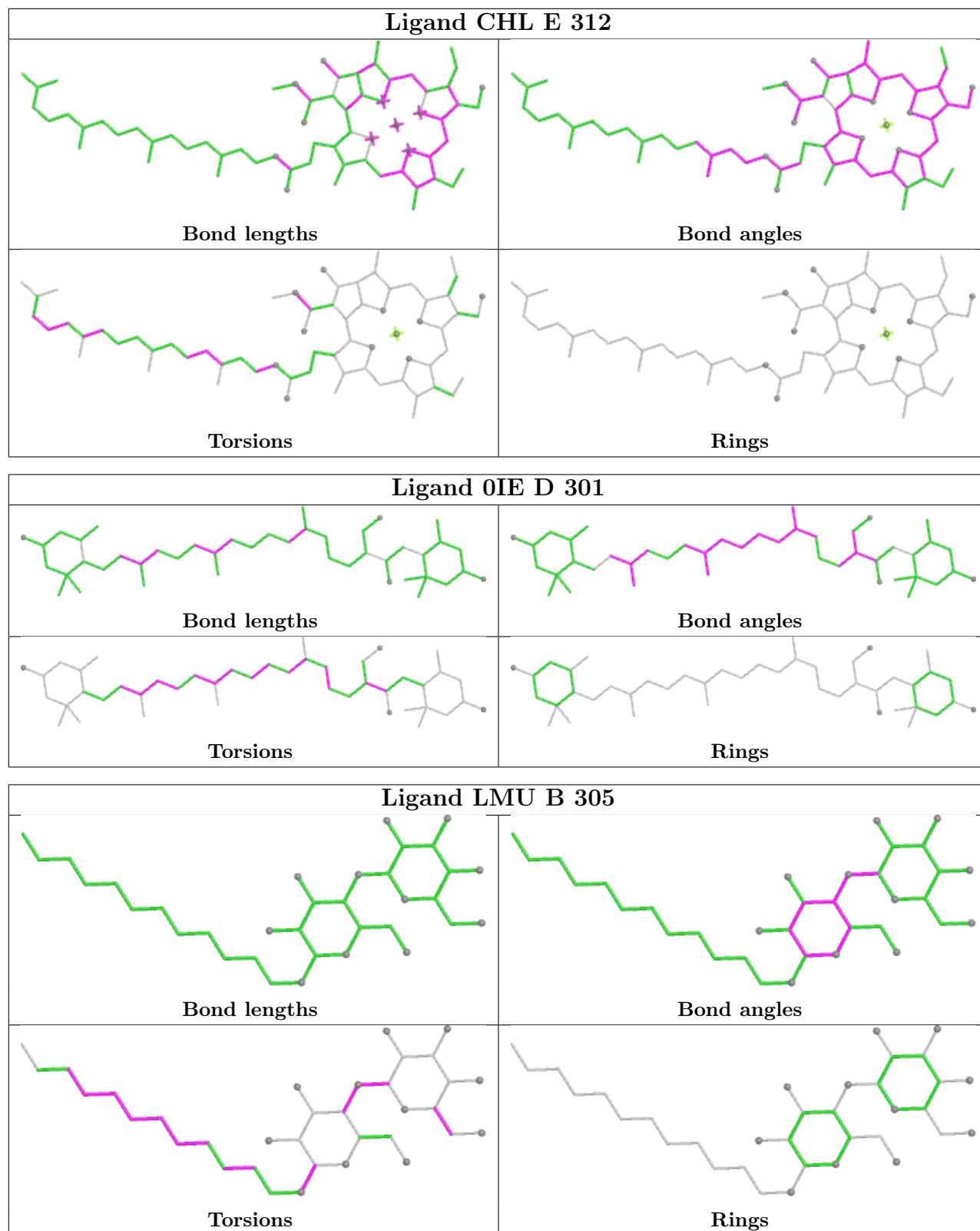
Continued on next page...

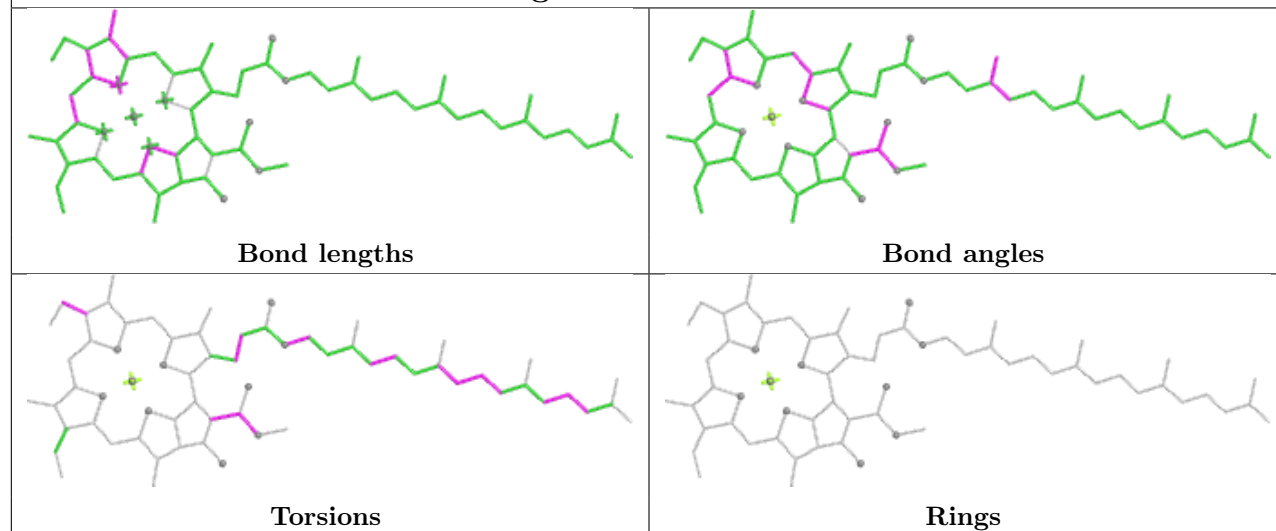
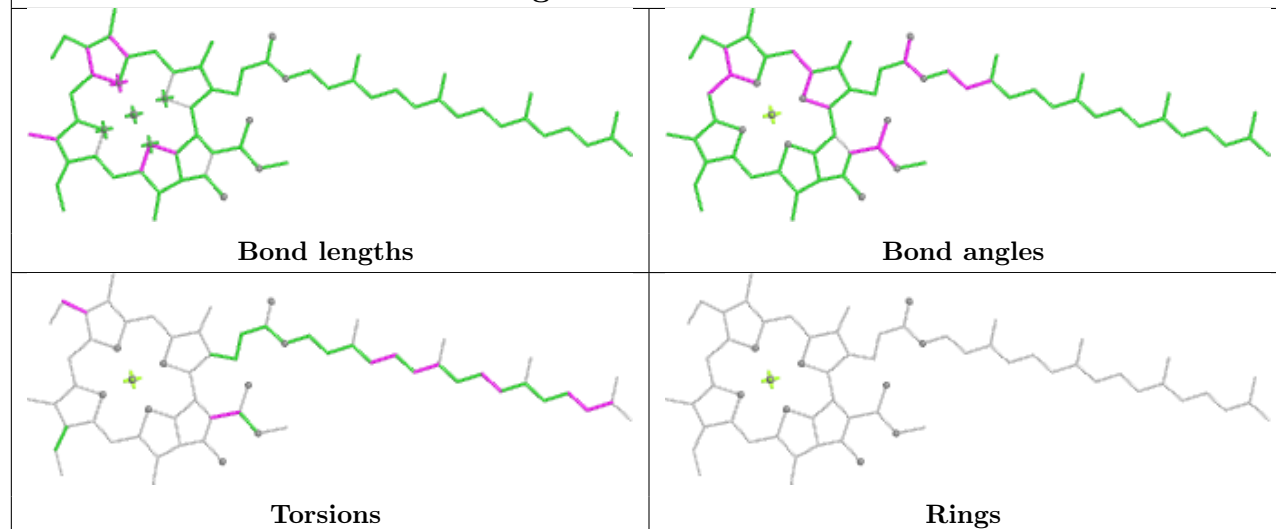
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	305	CHL	6	0
5	A	306	CHL	6	0
6	F	313	CLA	6	0
6	E	316	CLA	6	0
3	B	303	NEX	4	0
6	F	314	CLA	3	0
7	A	319	LHG	3	0
5	D	313	CHL	12	0
5	A	311	CHL	5	0
5	B	307	CHL	5	0
6	E	307	CLA	3	0
6	A	316	CLA	3	0
6	D	307	CLA	2	0
7	E	318	LHG	7	0
5	D	306	CHL	5	0
6	B	316	CLA	3	0
6	F	316	CLA	5	0
9	E	320	OUR	4	0

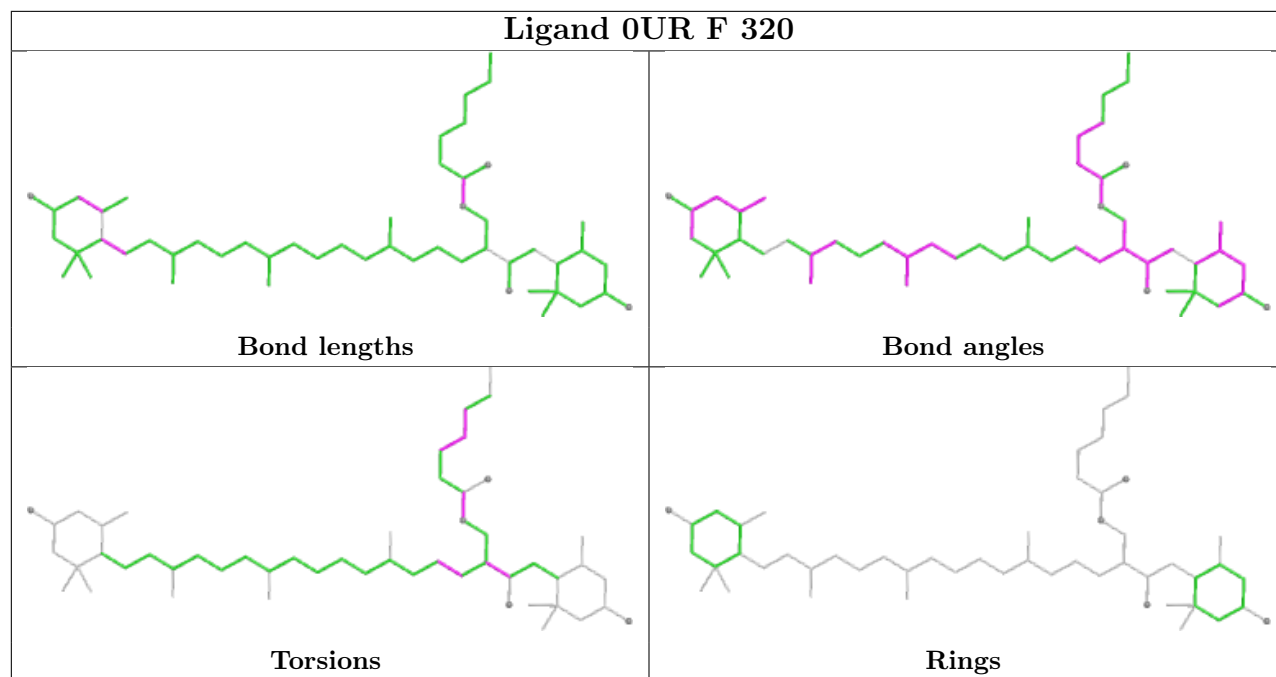
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



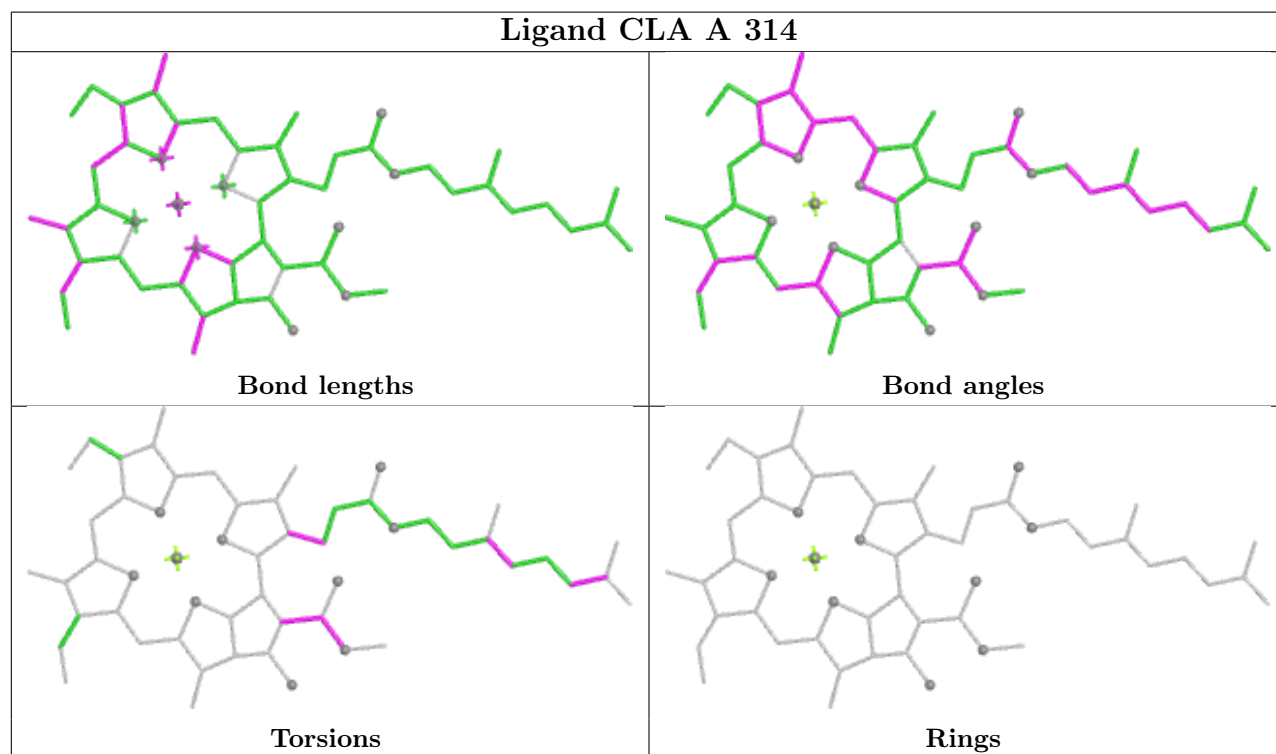


Ligand CLA A 307**Ligand CLA C 307**

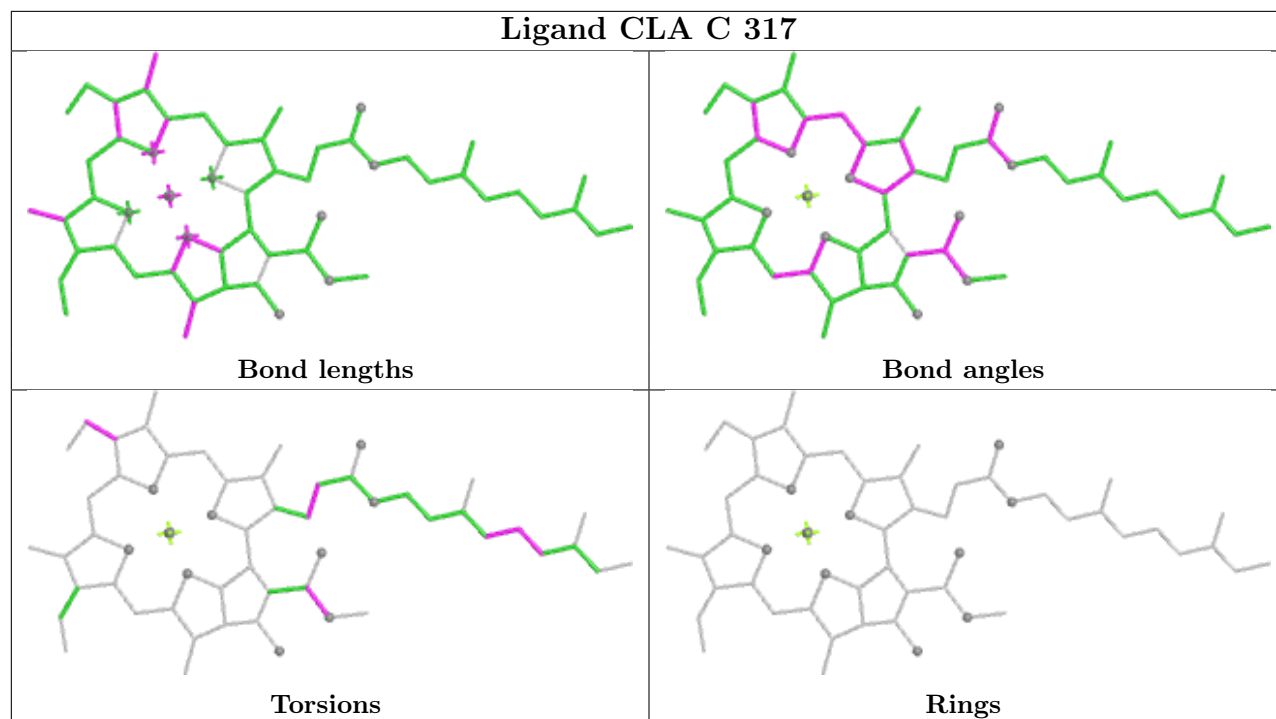
Ligand OUR F 320



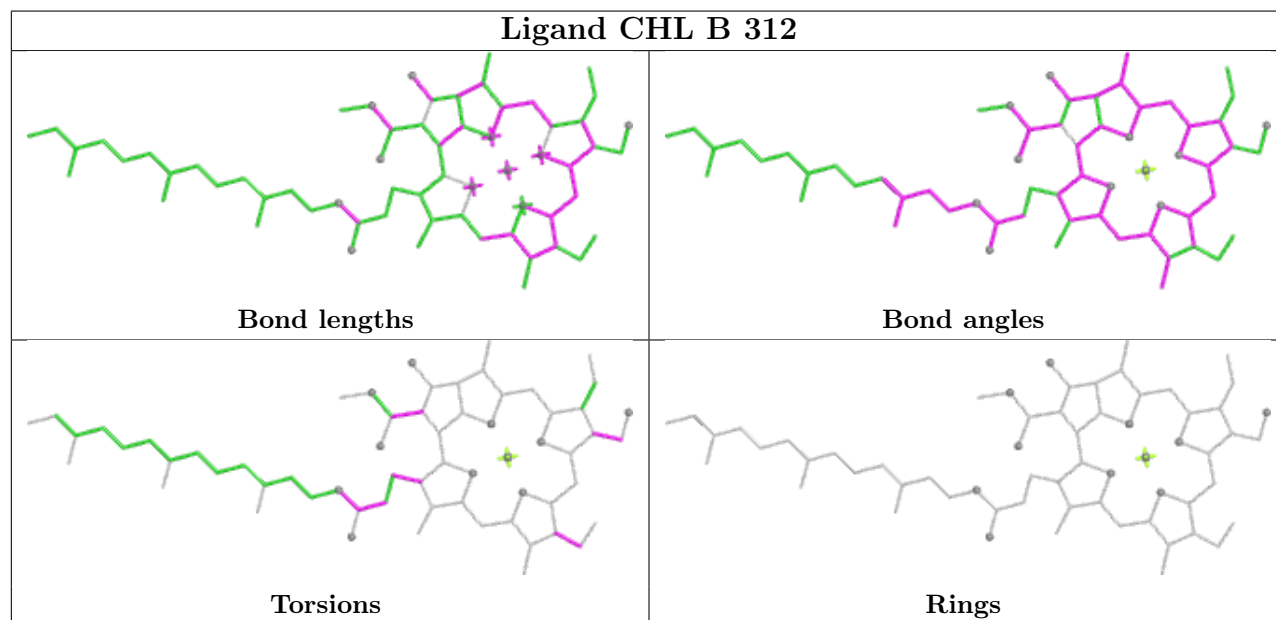
Ligand CLA A 314



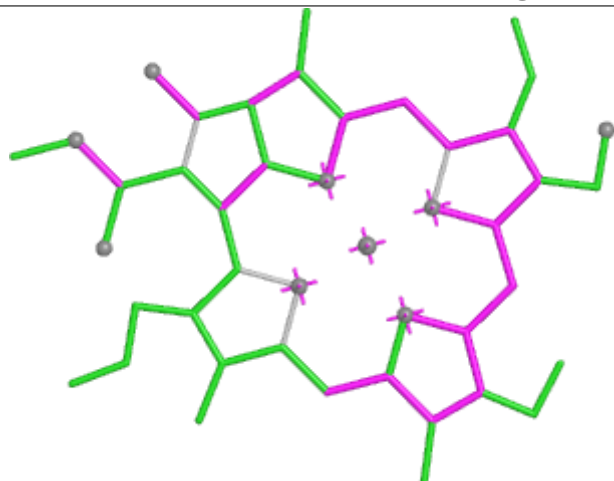
Ligand CLA C 317



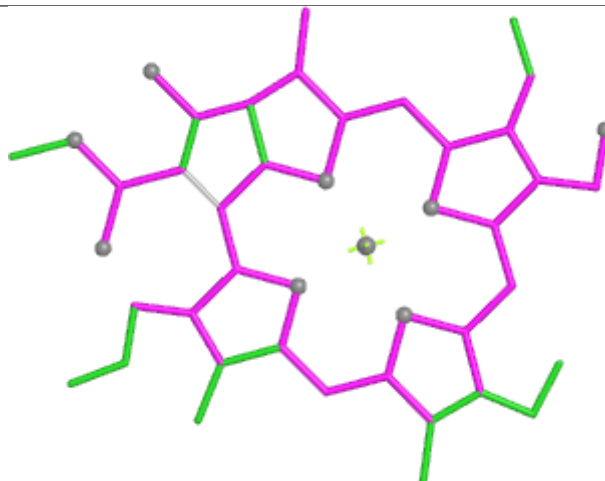
Ligand CHL B 312



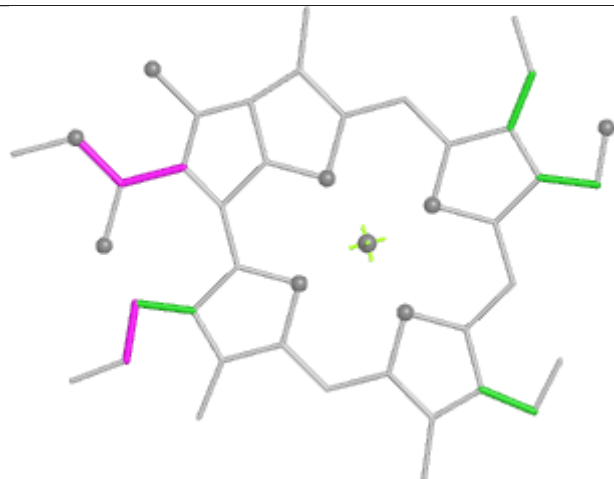
Ligand CHL C 318



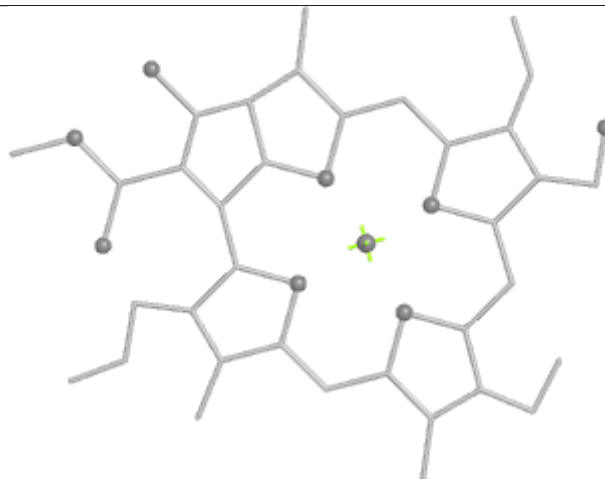
Bond lengths



Bond angles

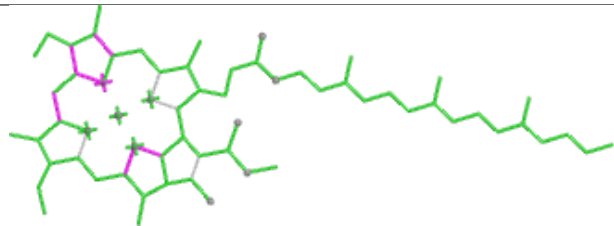


Torsions

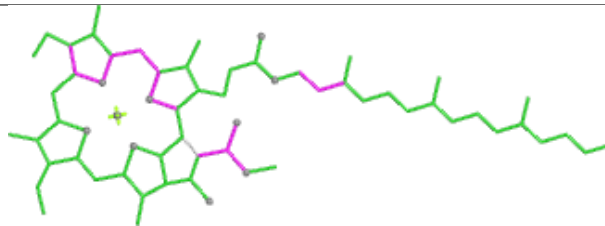


Rings

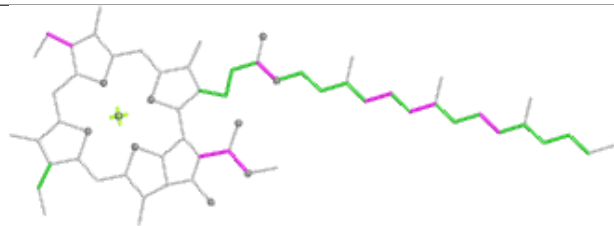
Ligand CLA A 315



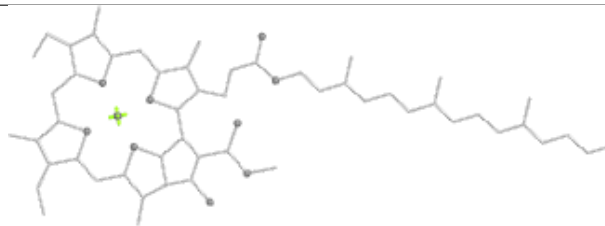
Bond lengths



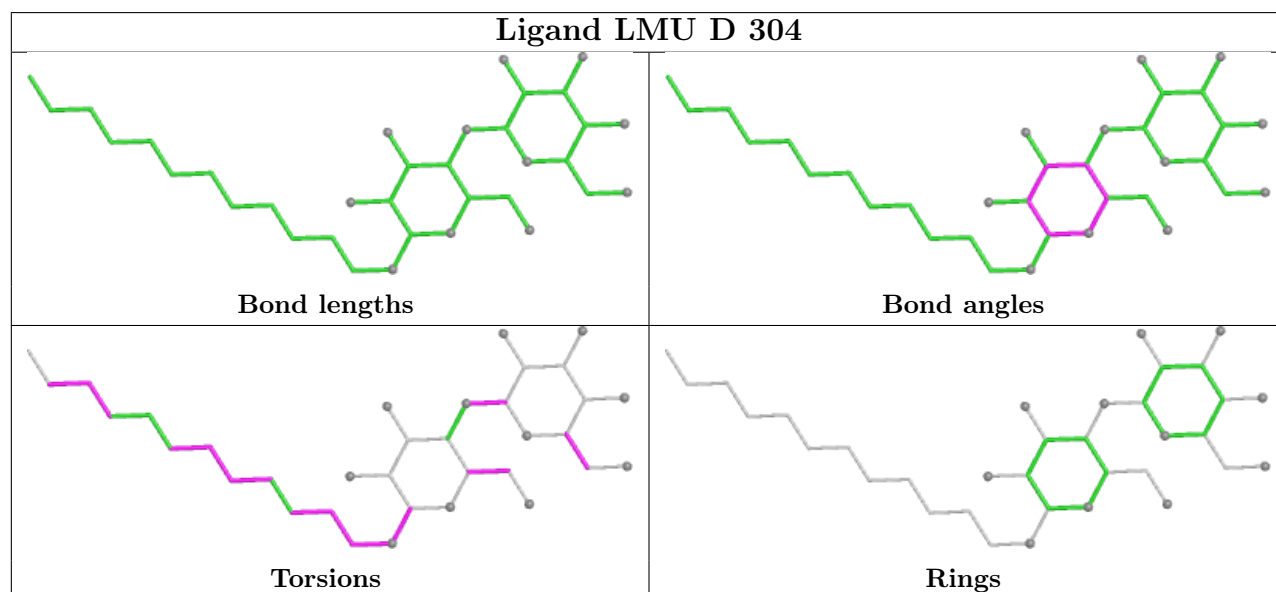
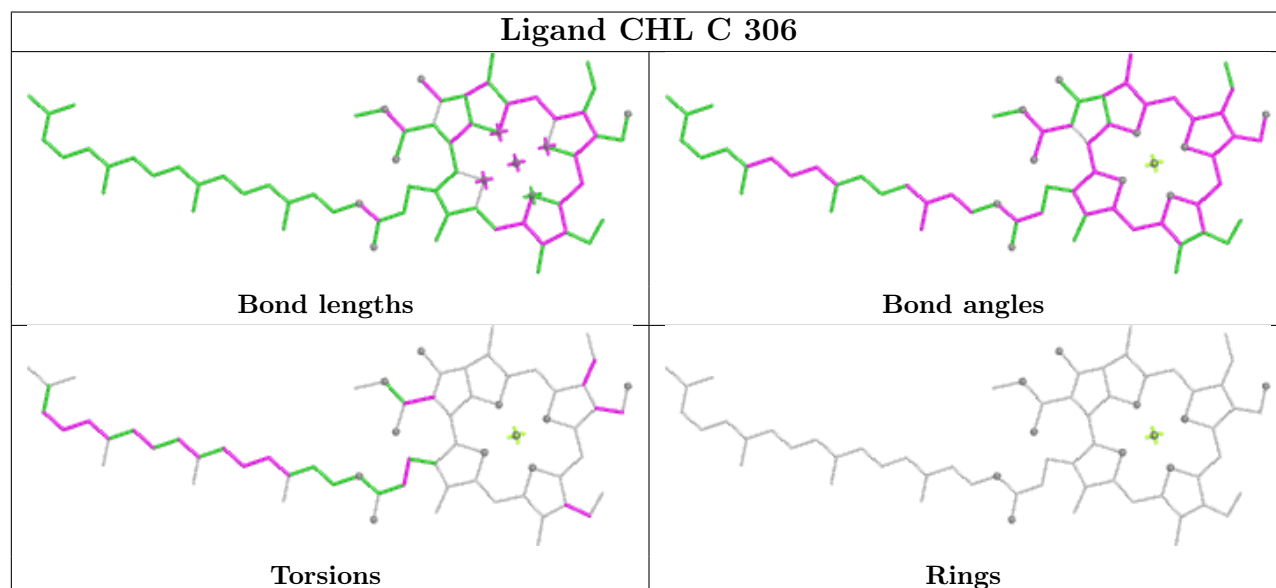
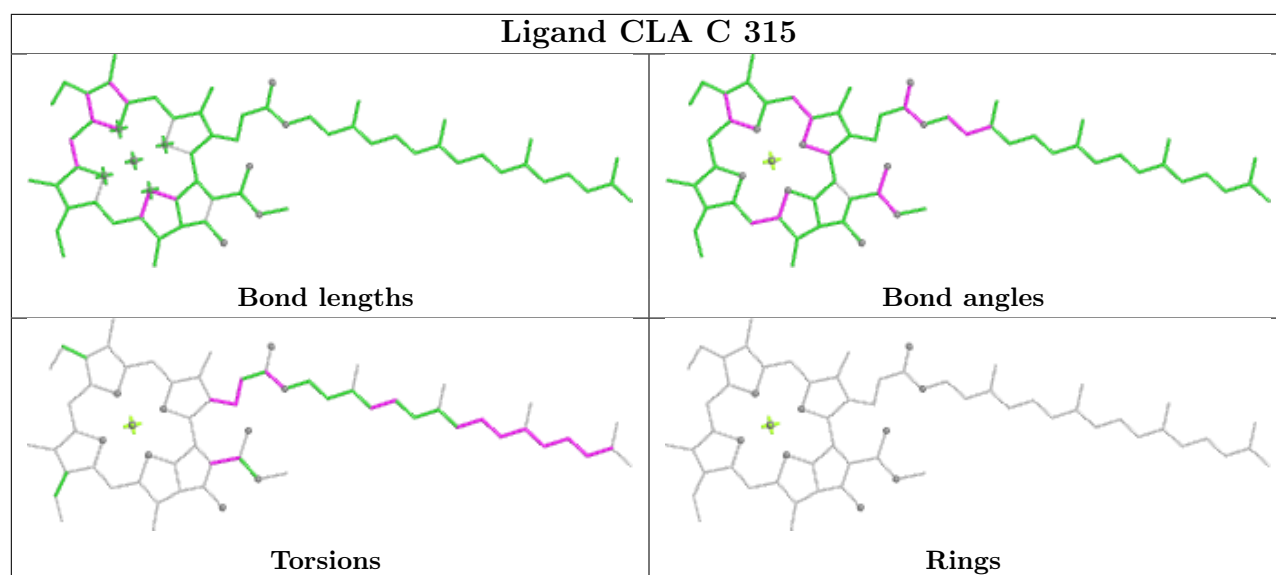
Bond angles



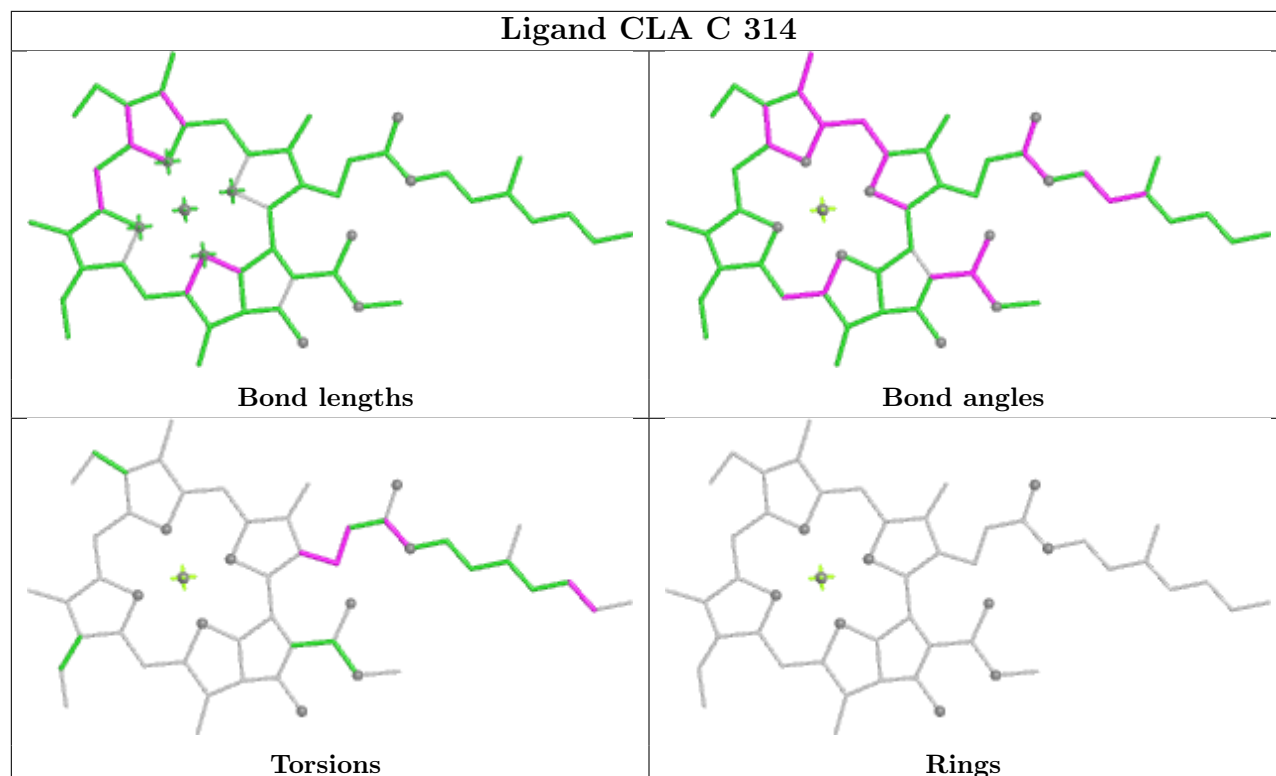
Torsions



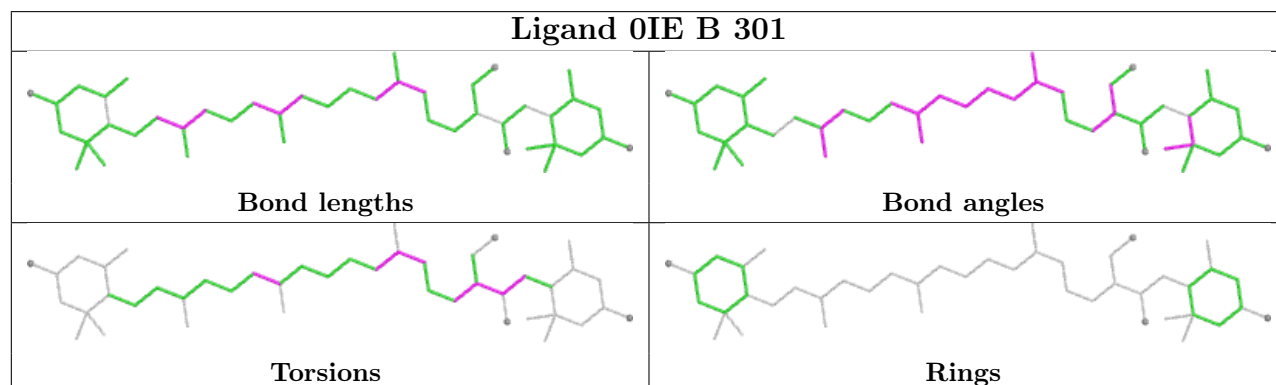
Rings



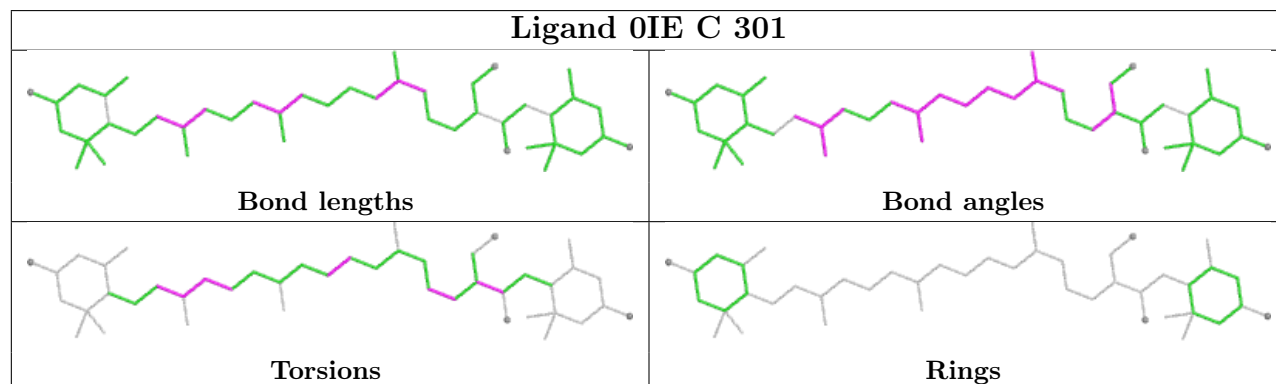
Ligand CLA C 314



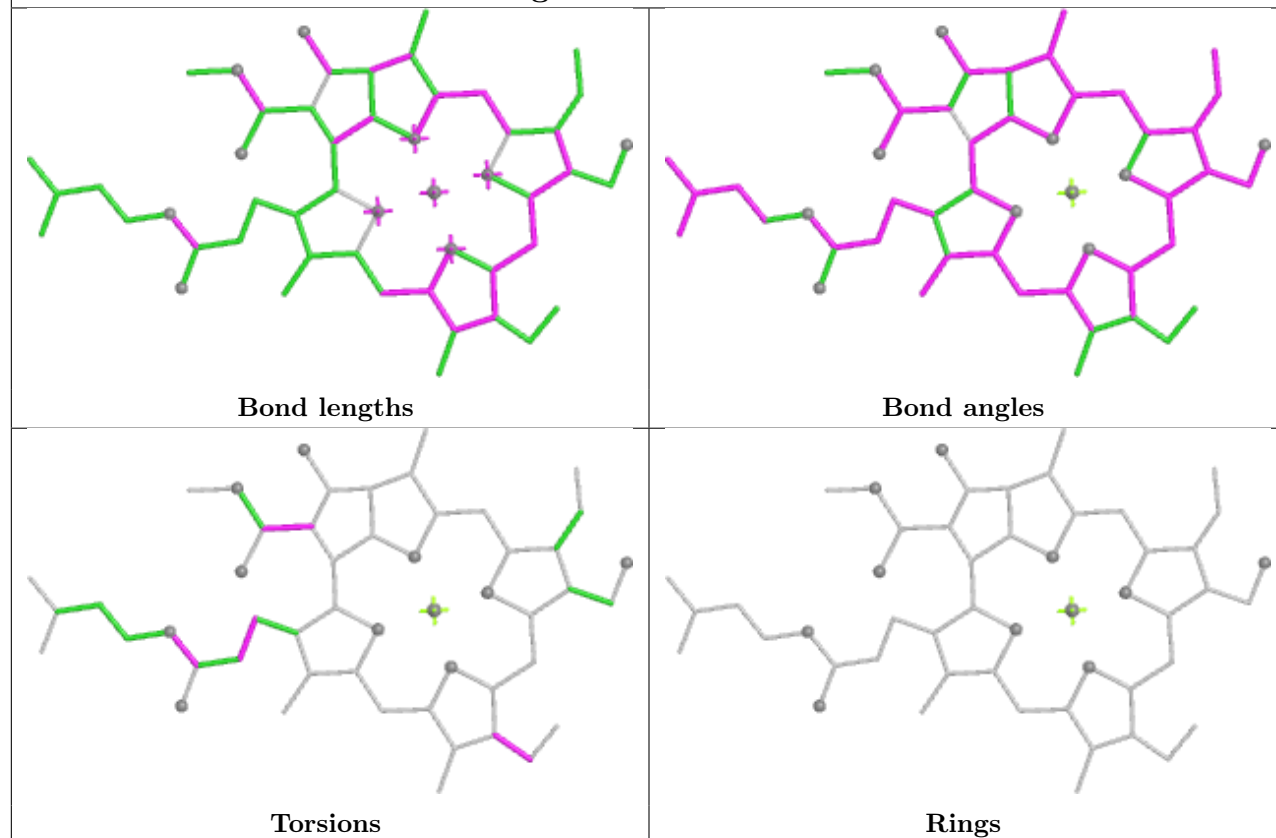
Ligand OIE B 301



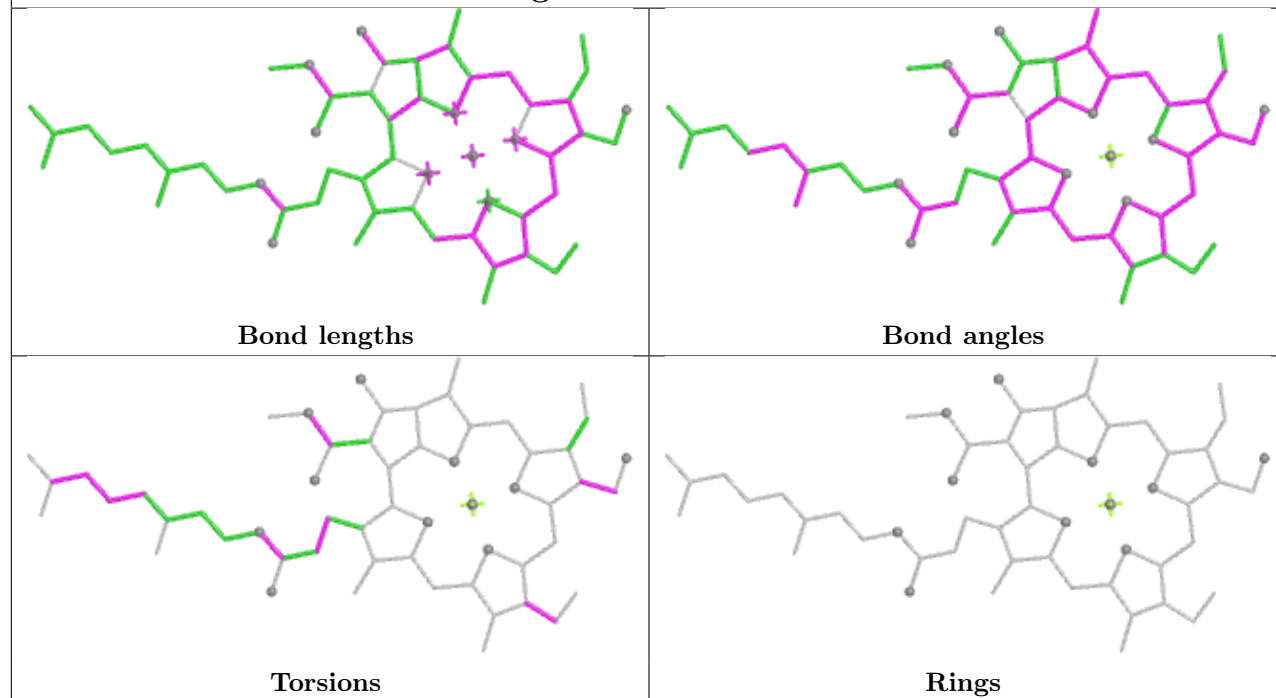
Ligand OIE C 301



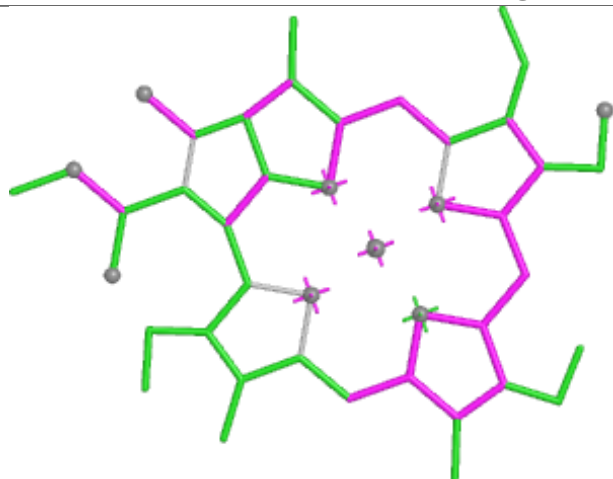
Ligand CHL A 310



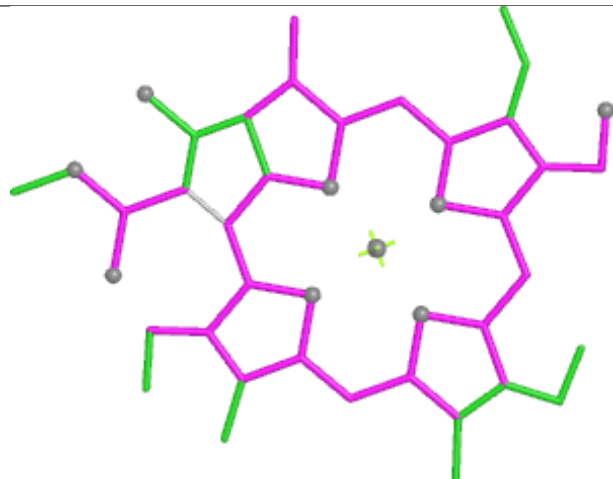
Ligand CHL C 312



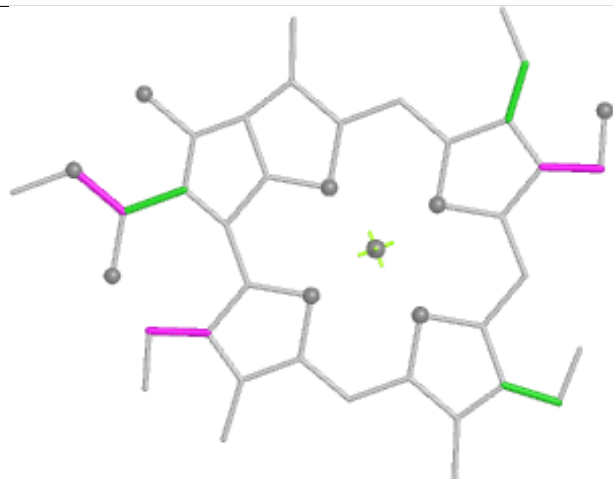
Ligand CHL B 310



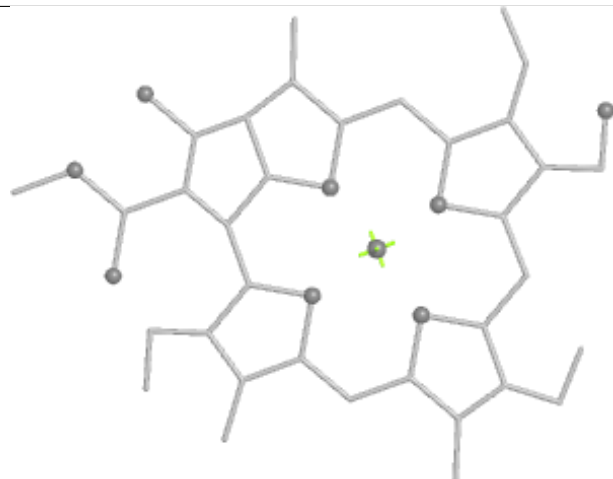
Bond lengths



Bond angles

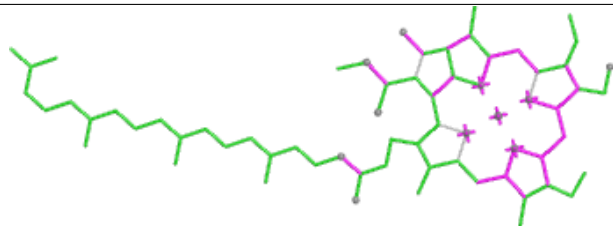


Torsions

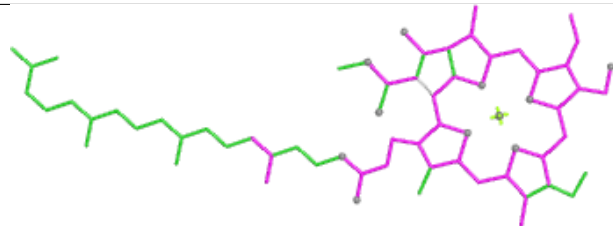


Rings

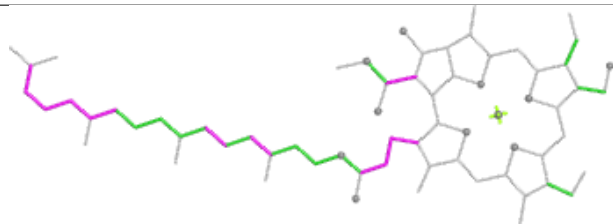
Ligand CHL F 304



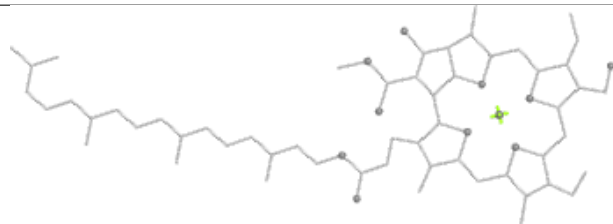
Bond lengths



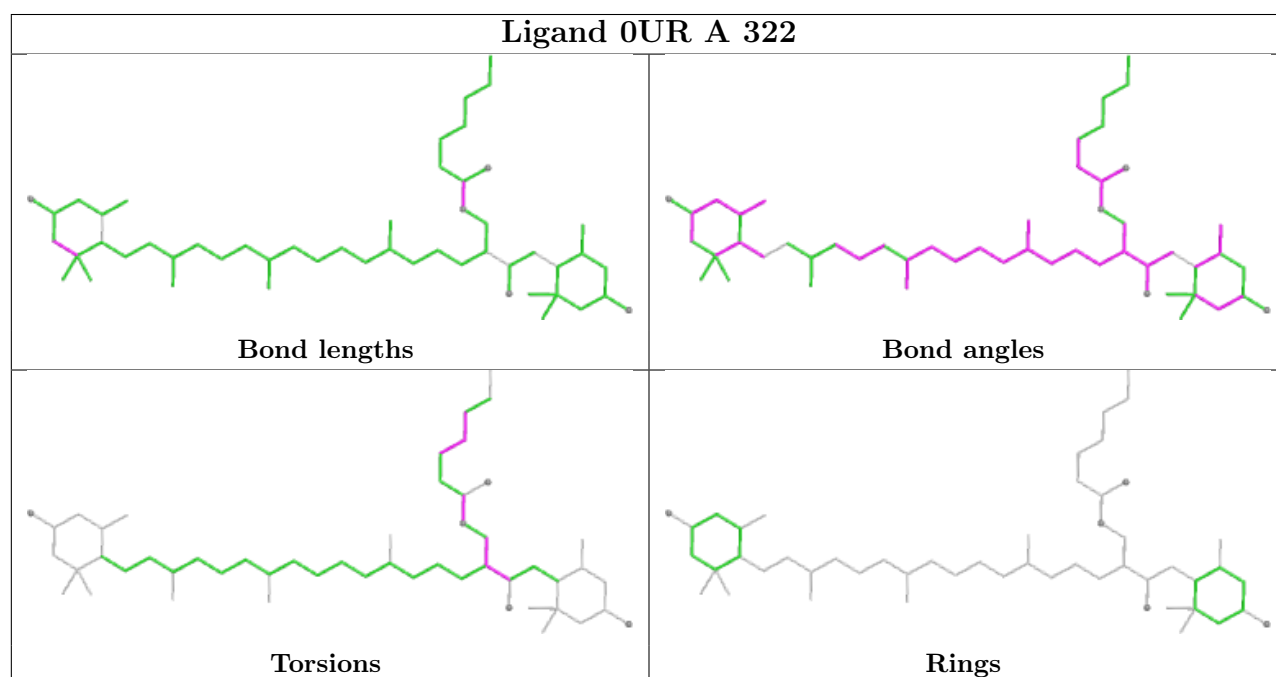
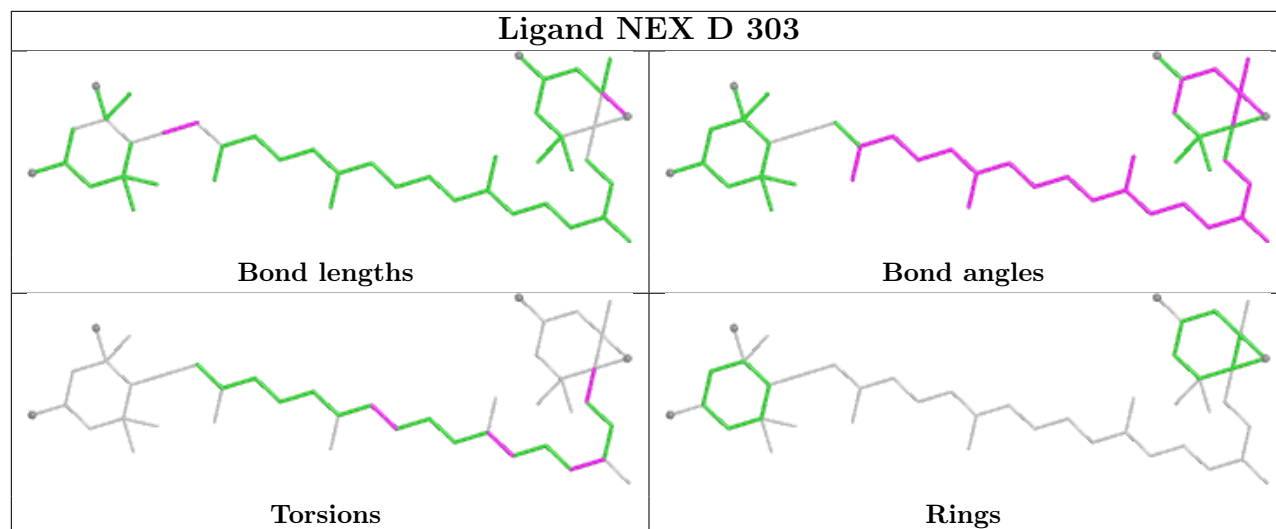
Bond angles

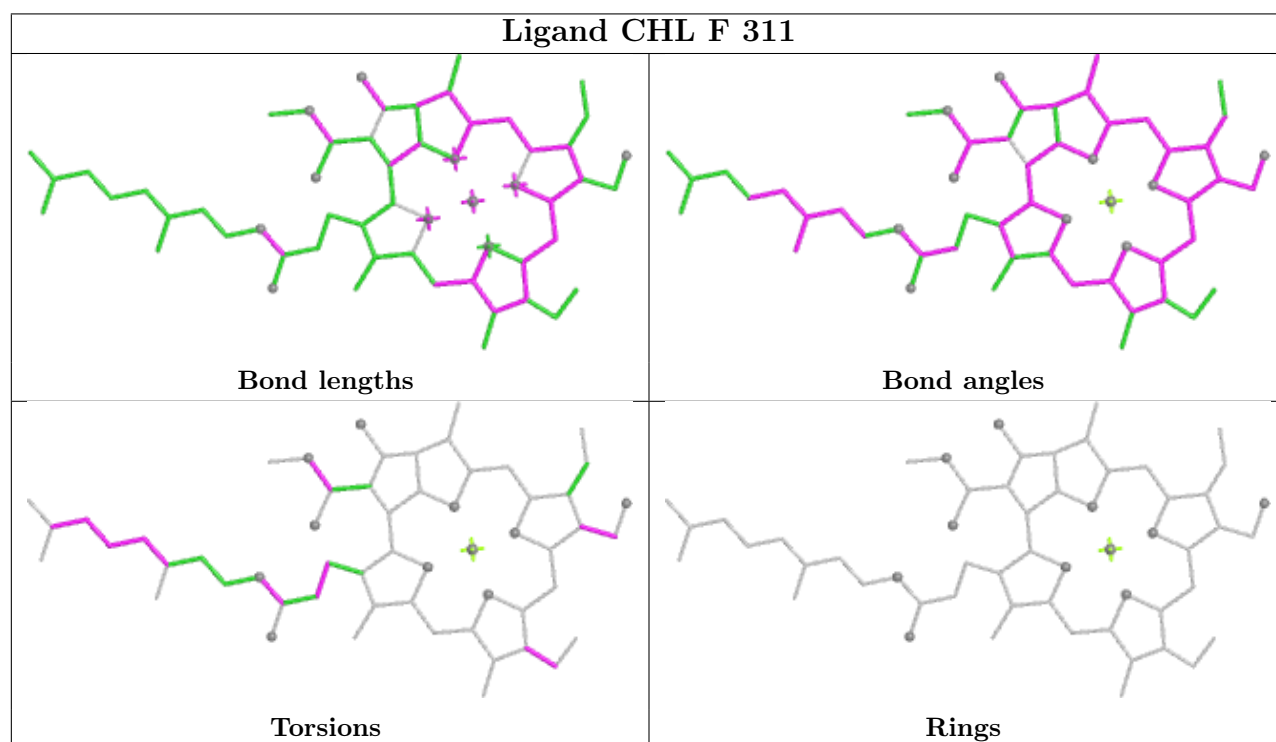
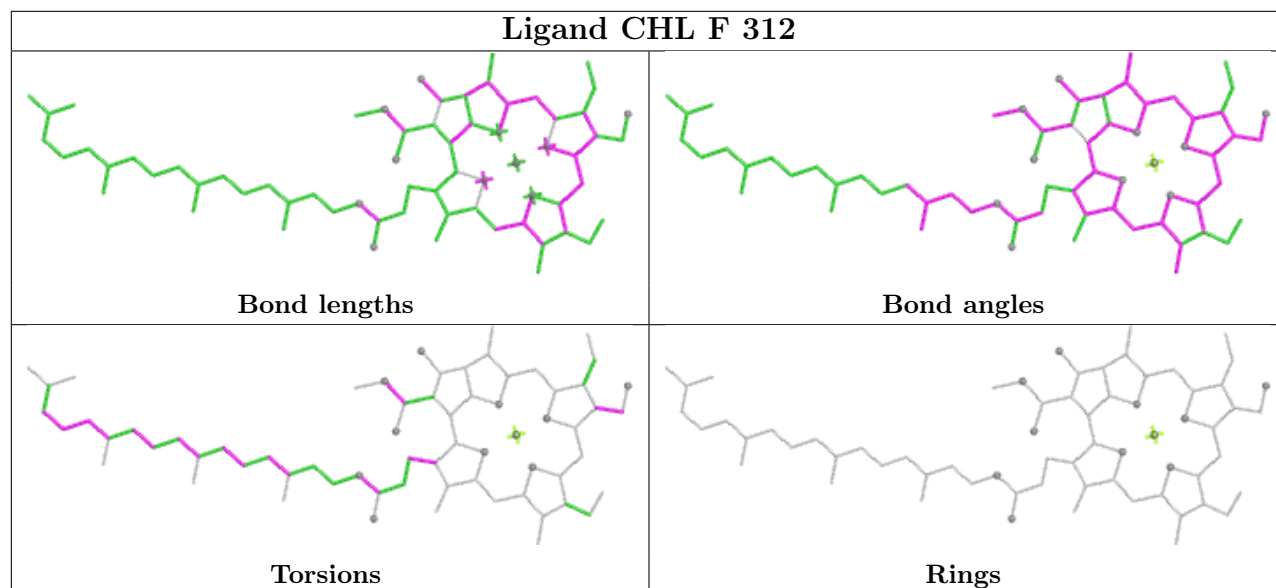


Torsions

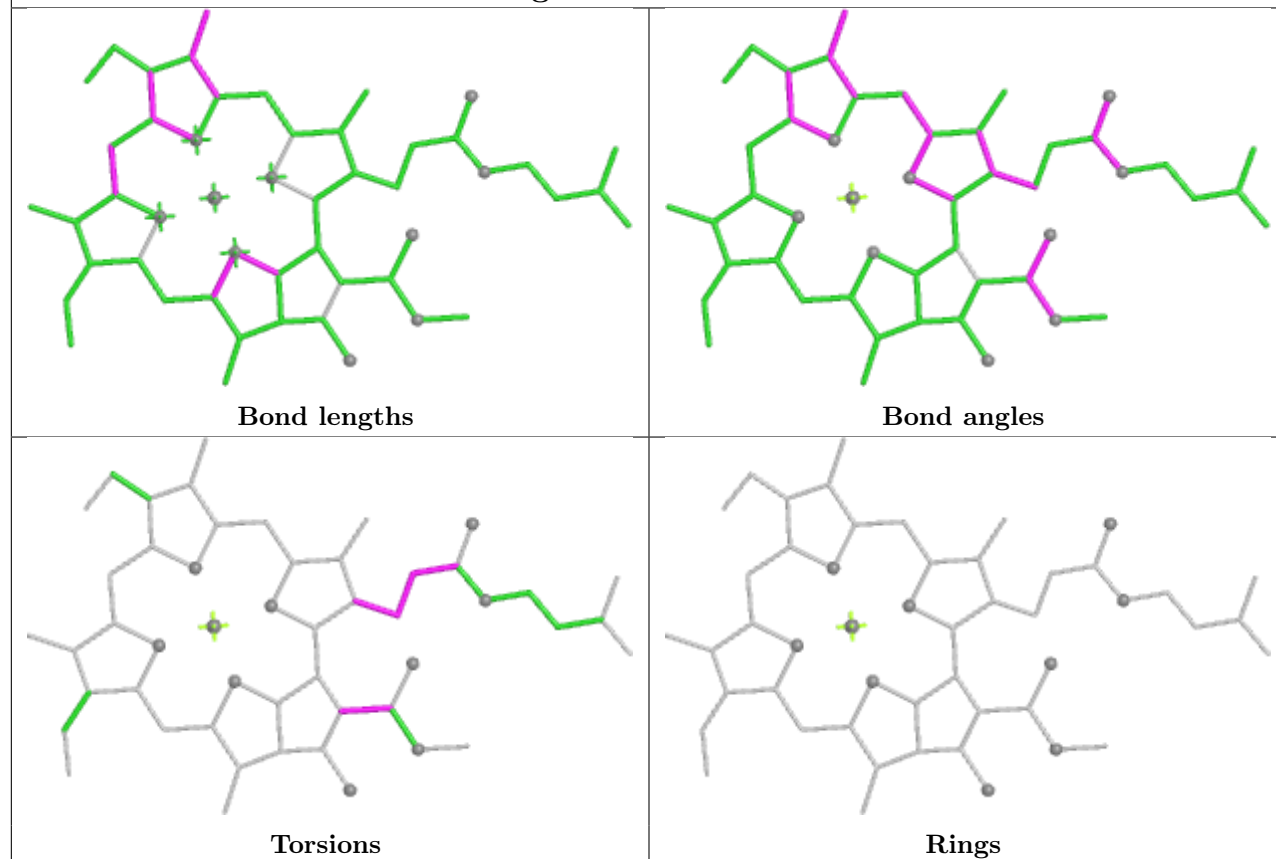


Rings

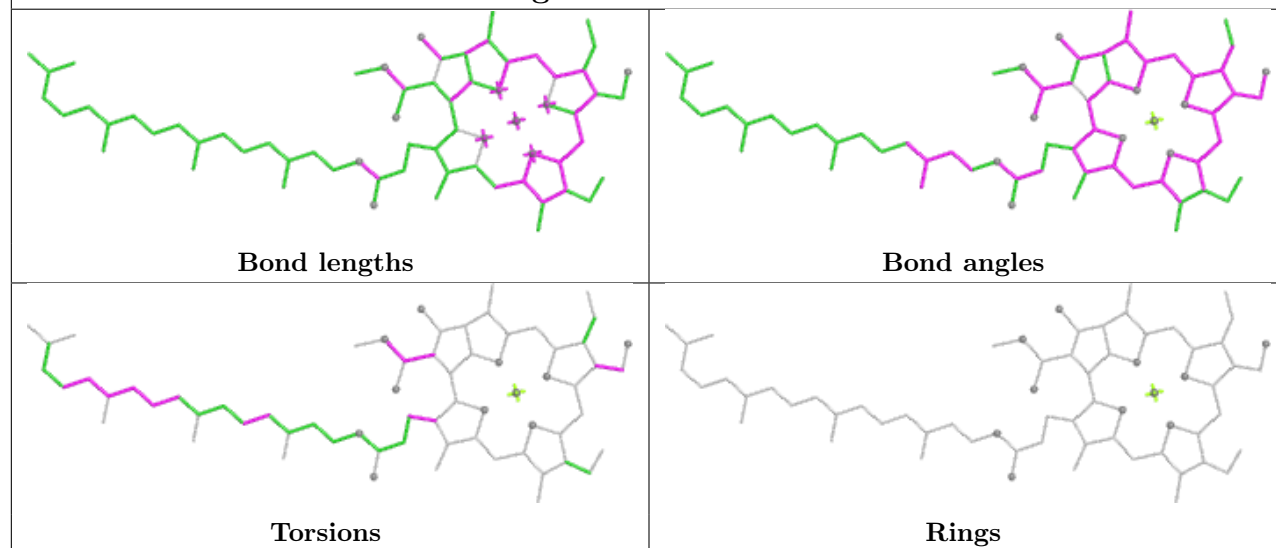




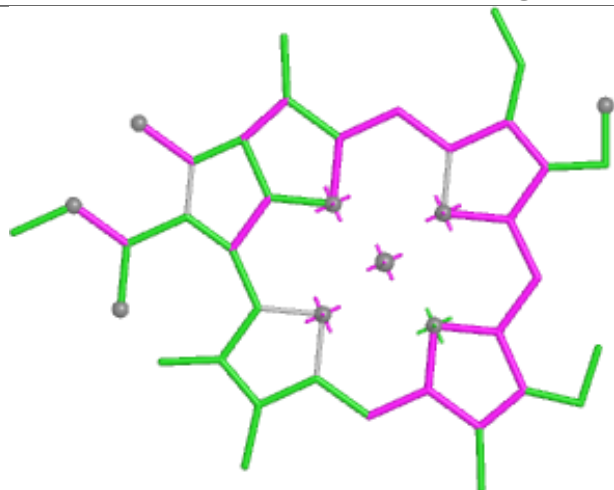
Ligand CLA A 308



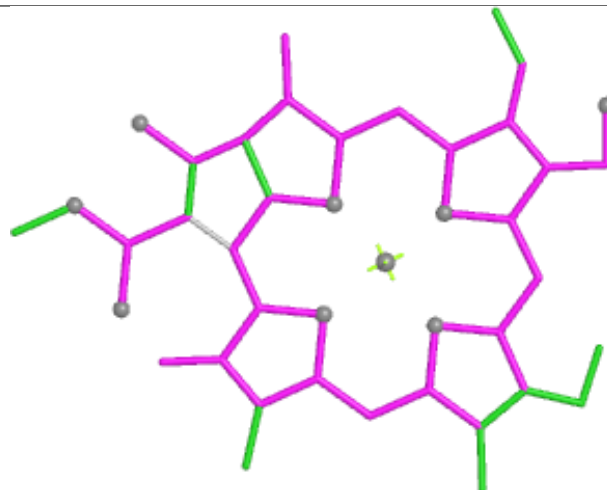
Ligand CHL B 306



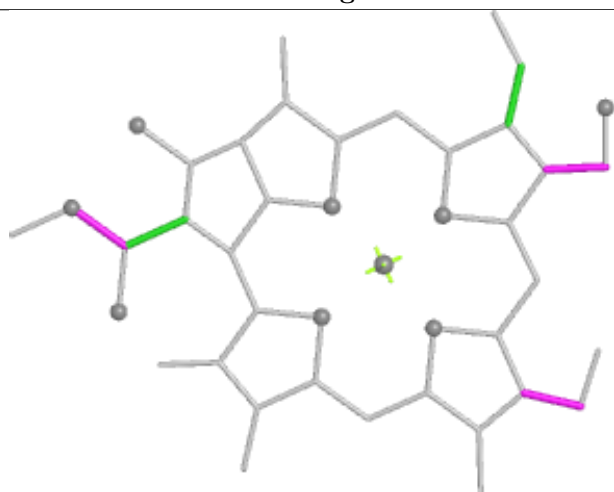
Ligand CHL F 308



Bond lengths



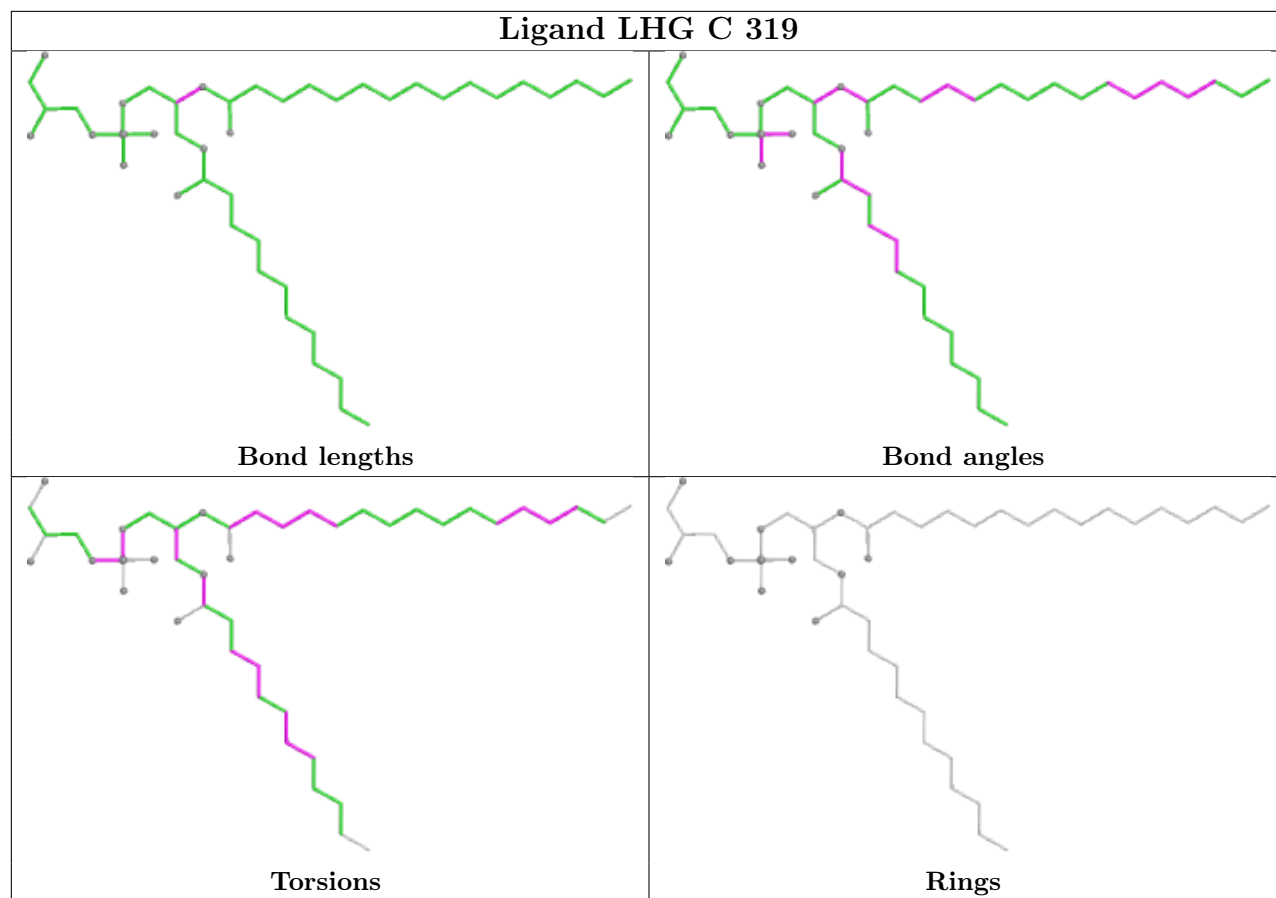
Bond angles



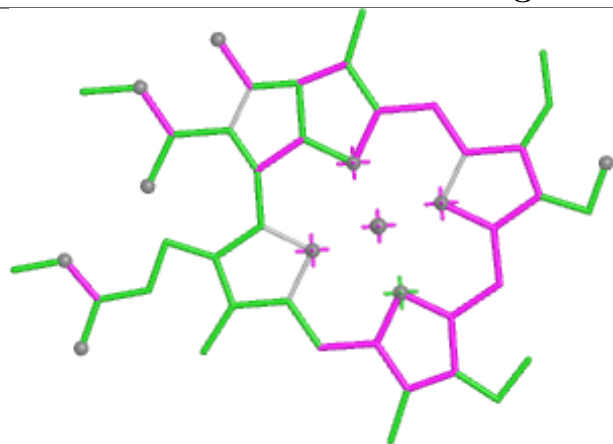
Torsions



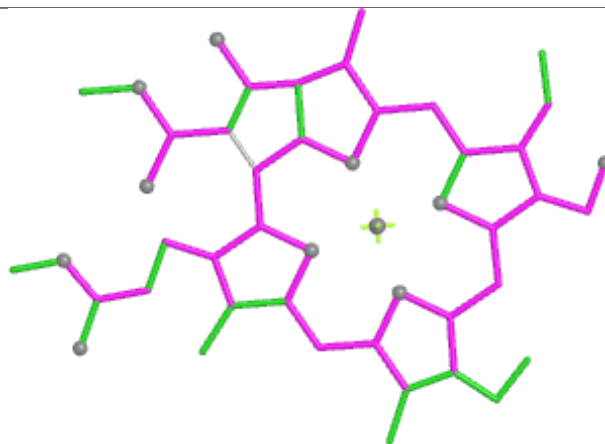
Rings



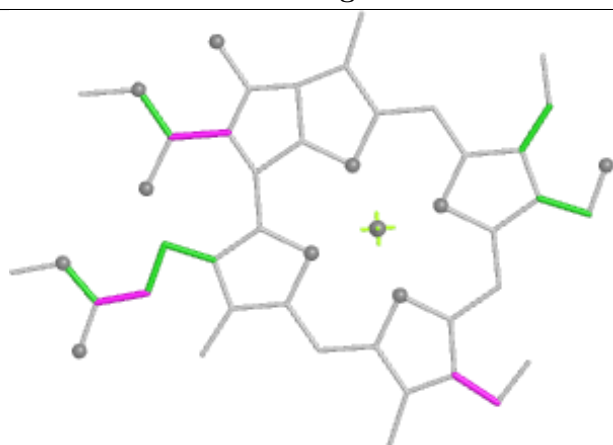
Ligand CHL B 319



Bond lengths



Bond angles

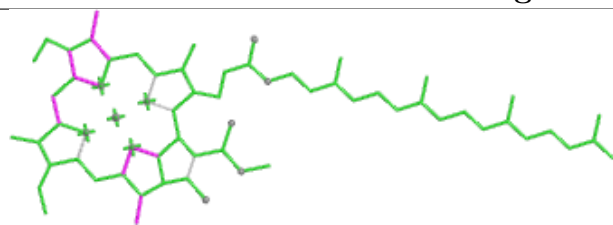


Torsions

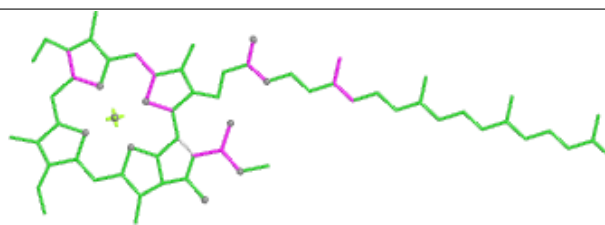


Rings

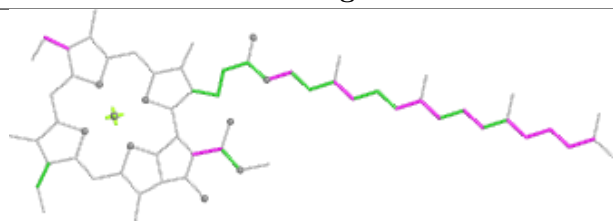
Ligand CLA B 308



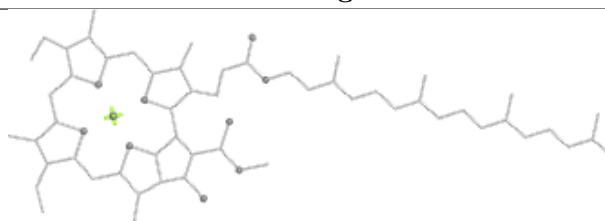
Bond lengths



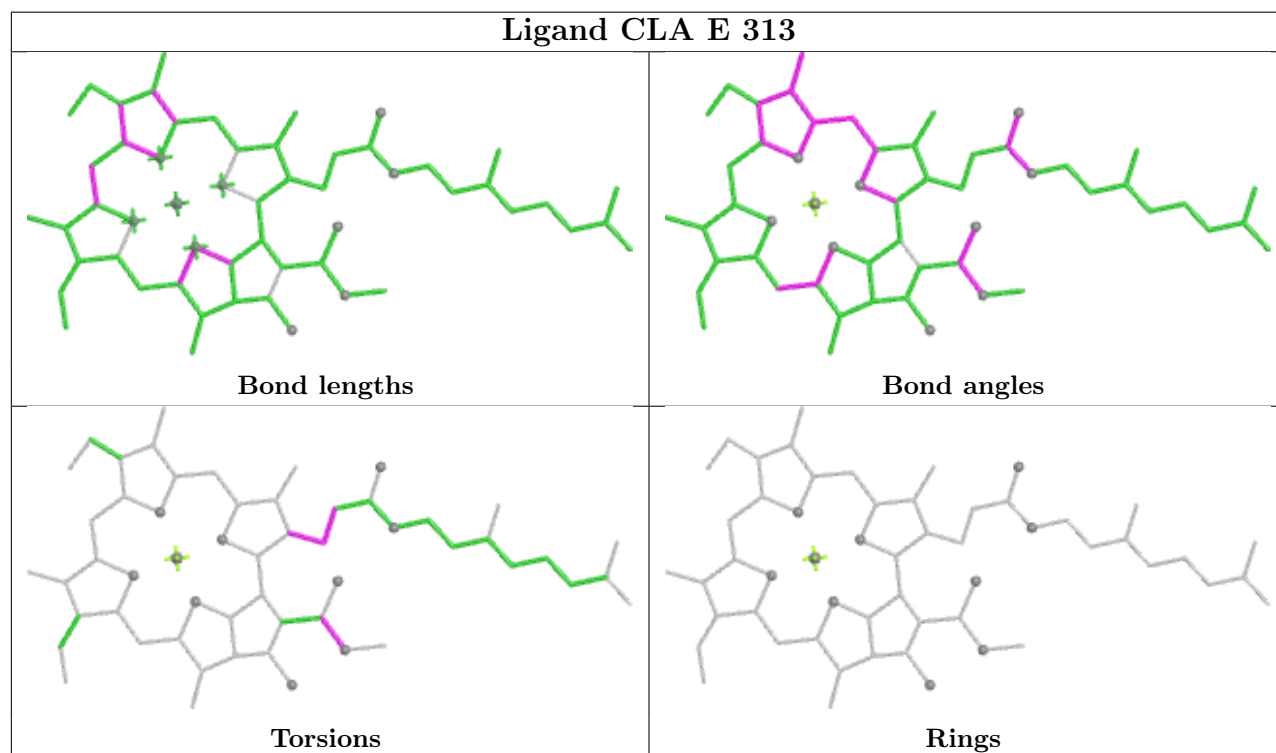
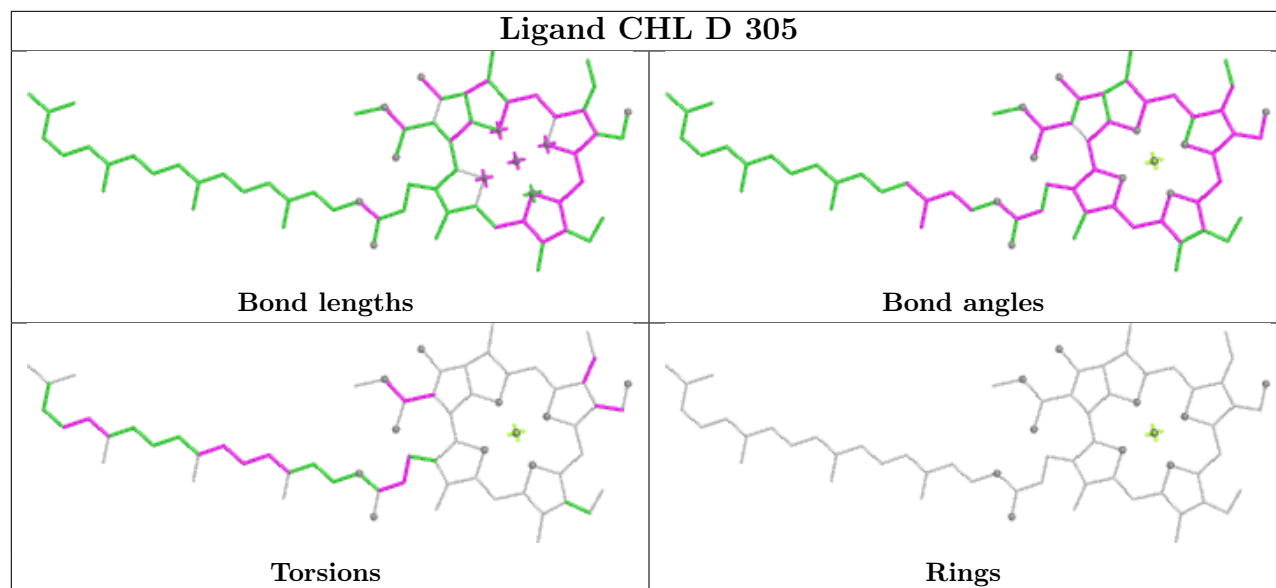
Bond angles



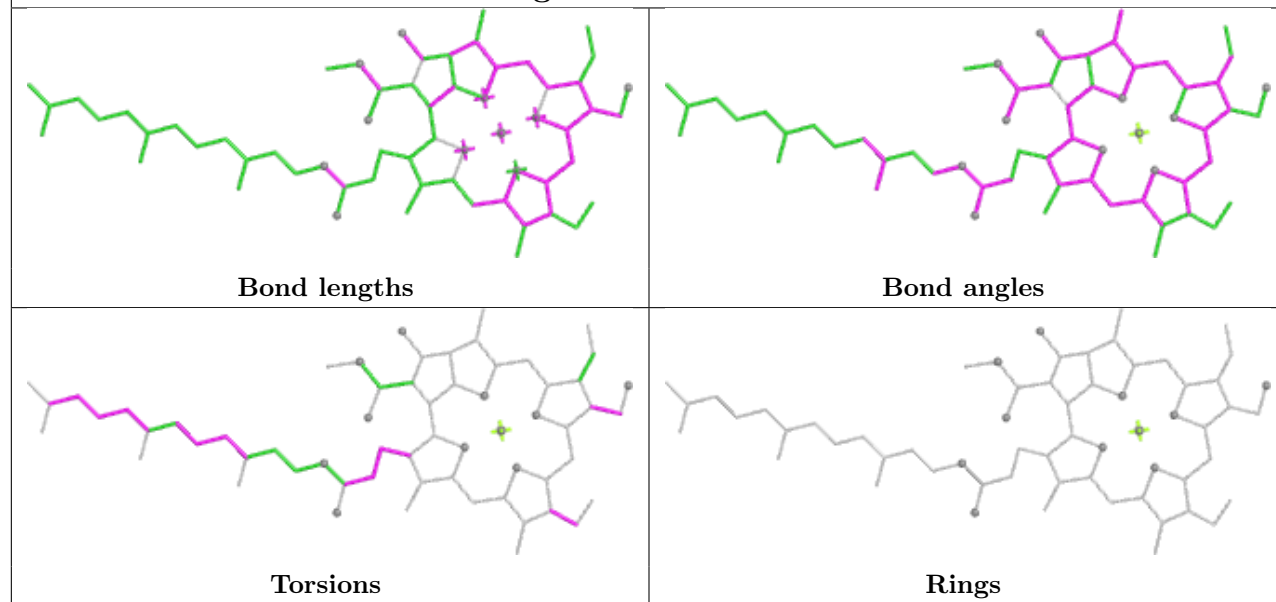
Torsions



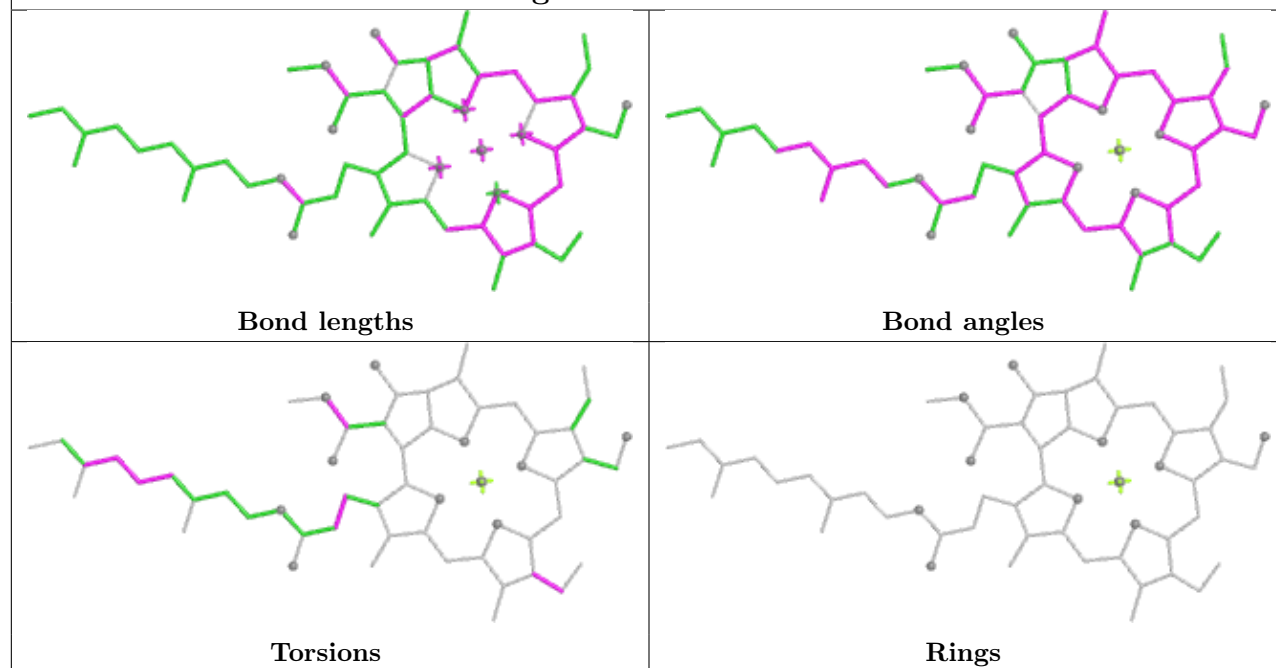
Rings

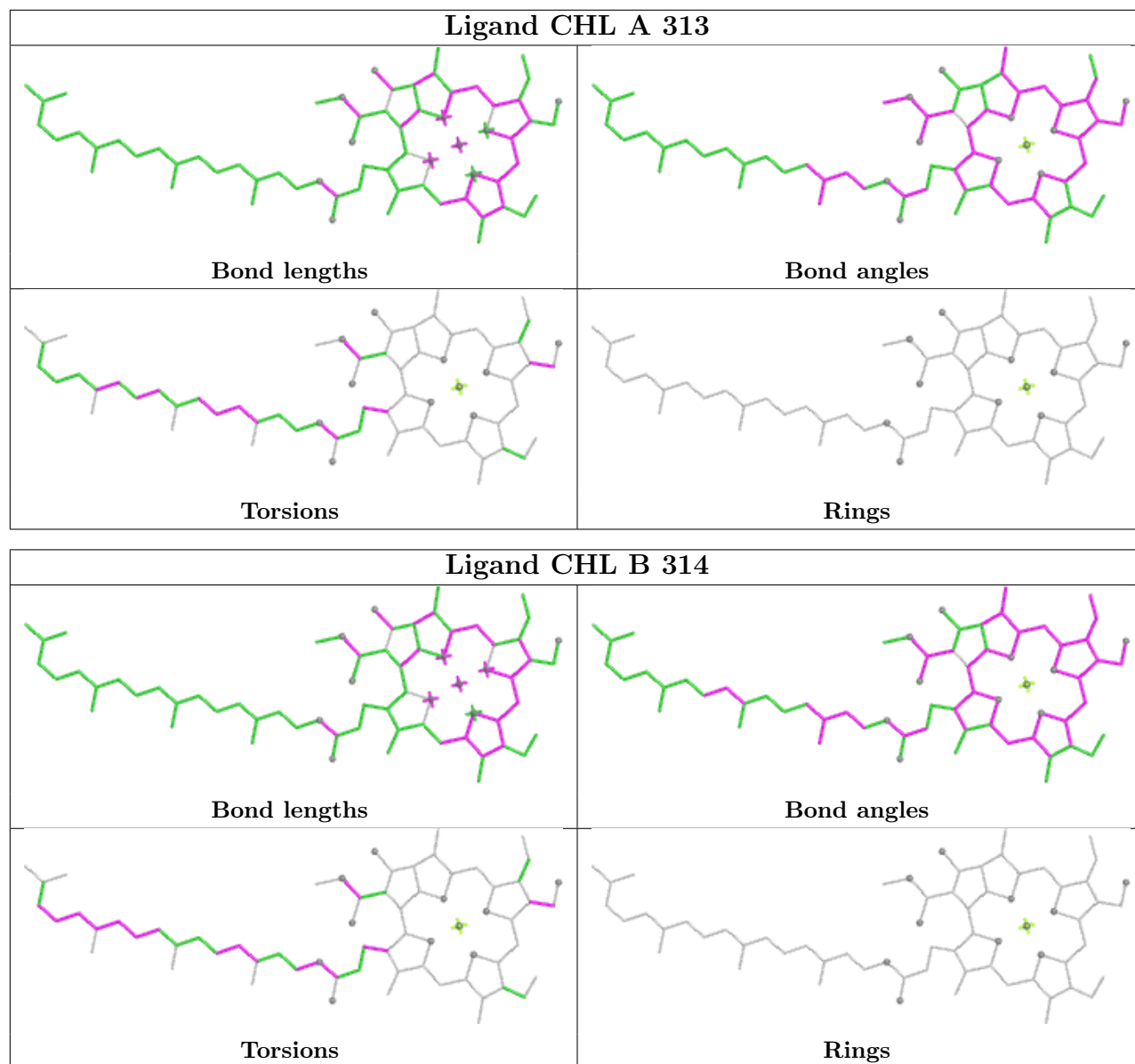


Ligand CHL F 310

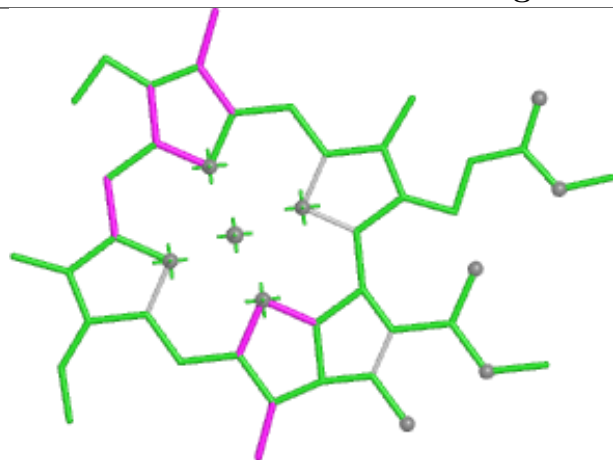


Ligand CHL B 313

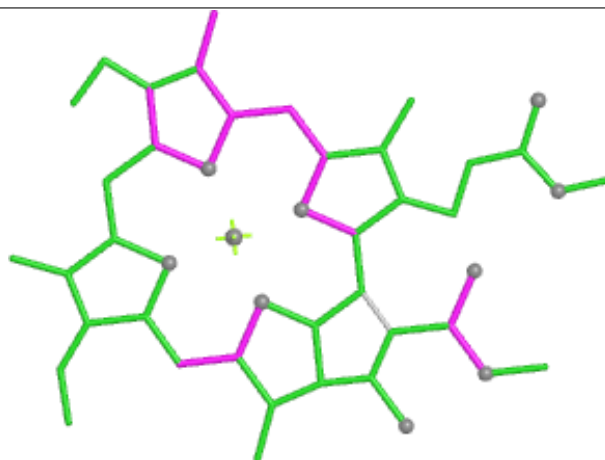




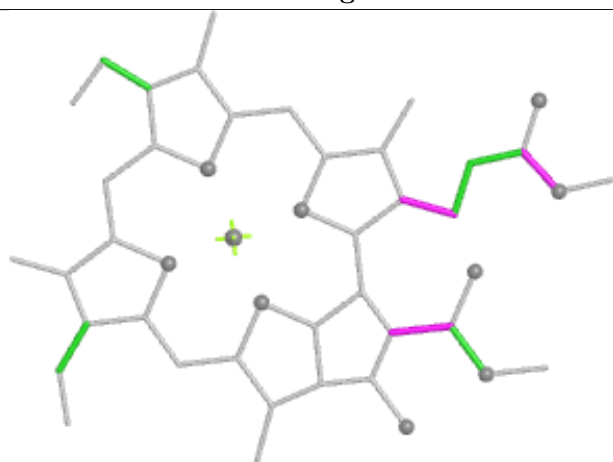
Ligand CLA D 308



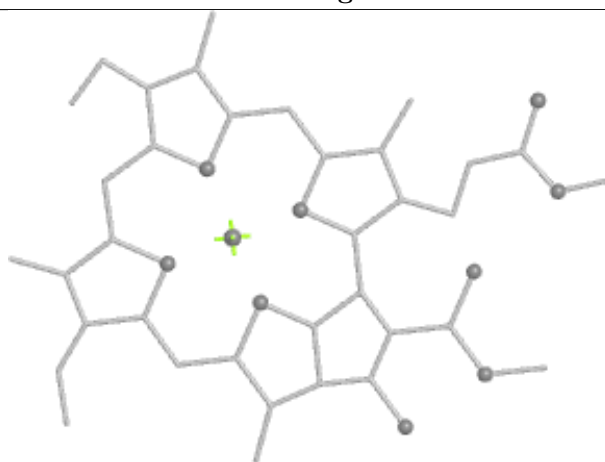
Bond lengths



Bond angles

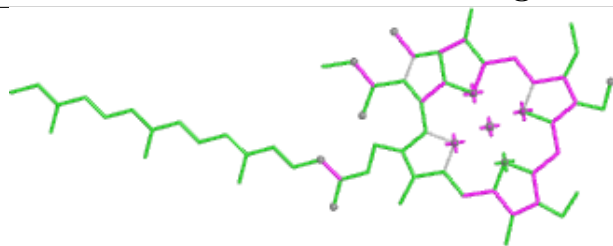


Torsions

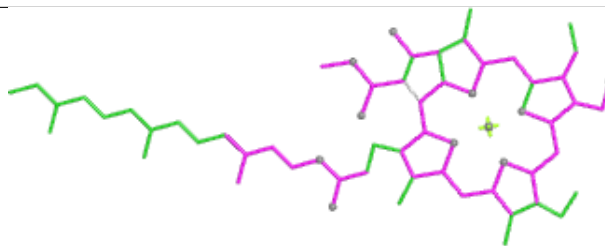


Rings

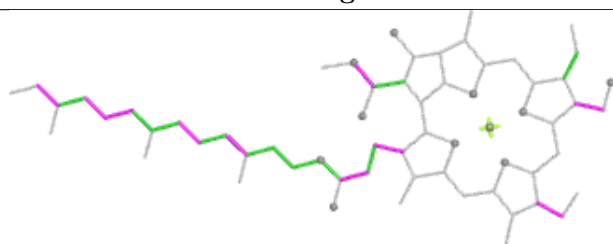
Ligand CHL D 311



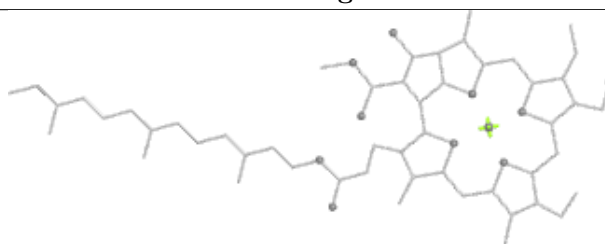
Bond lengths



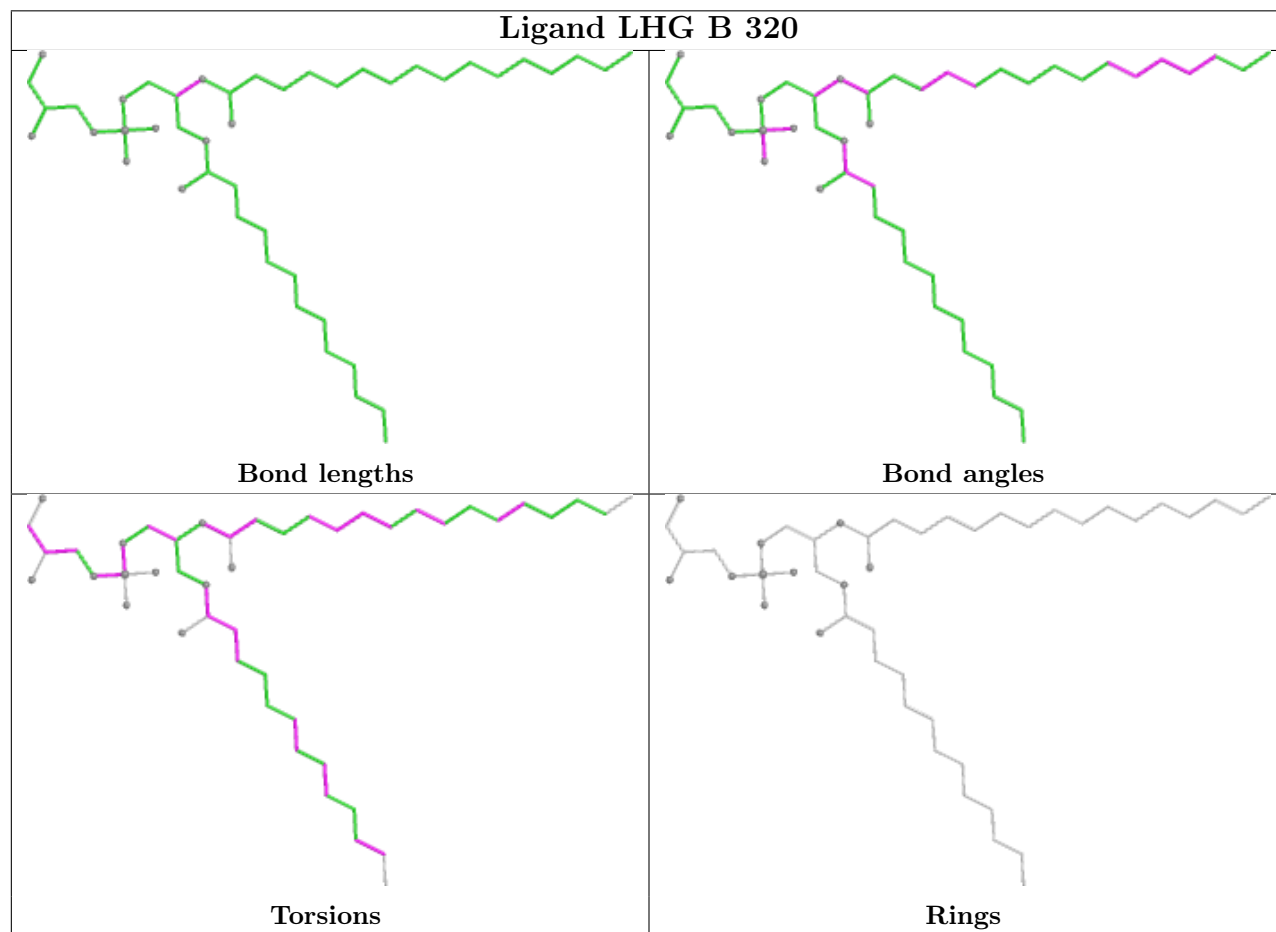
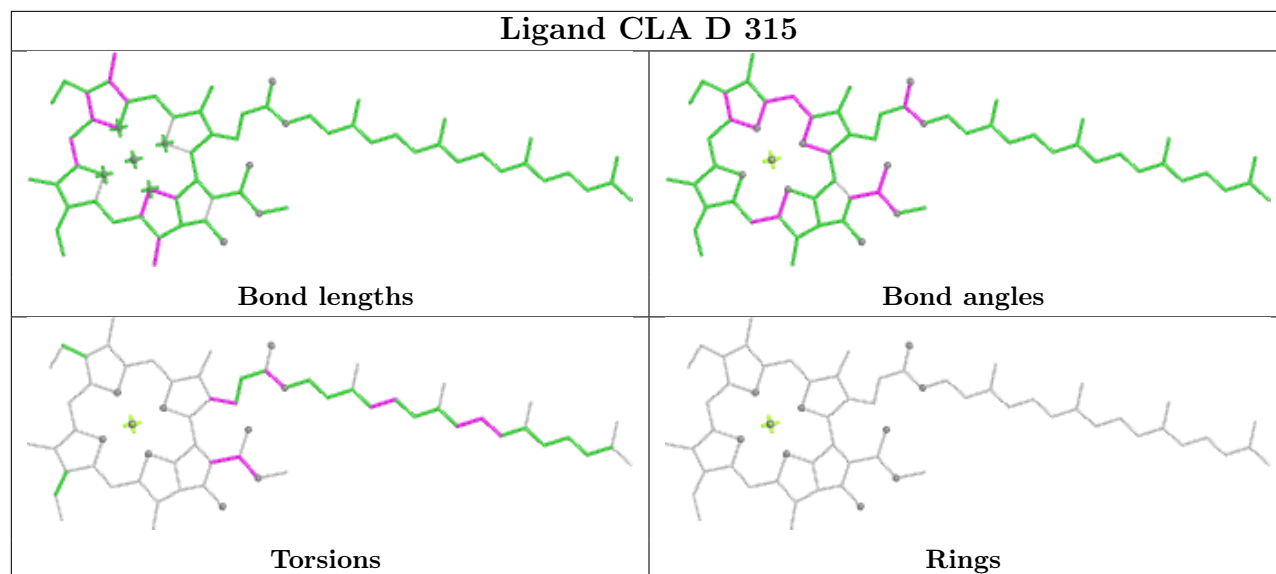
Bond angles



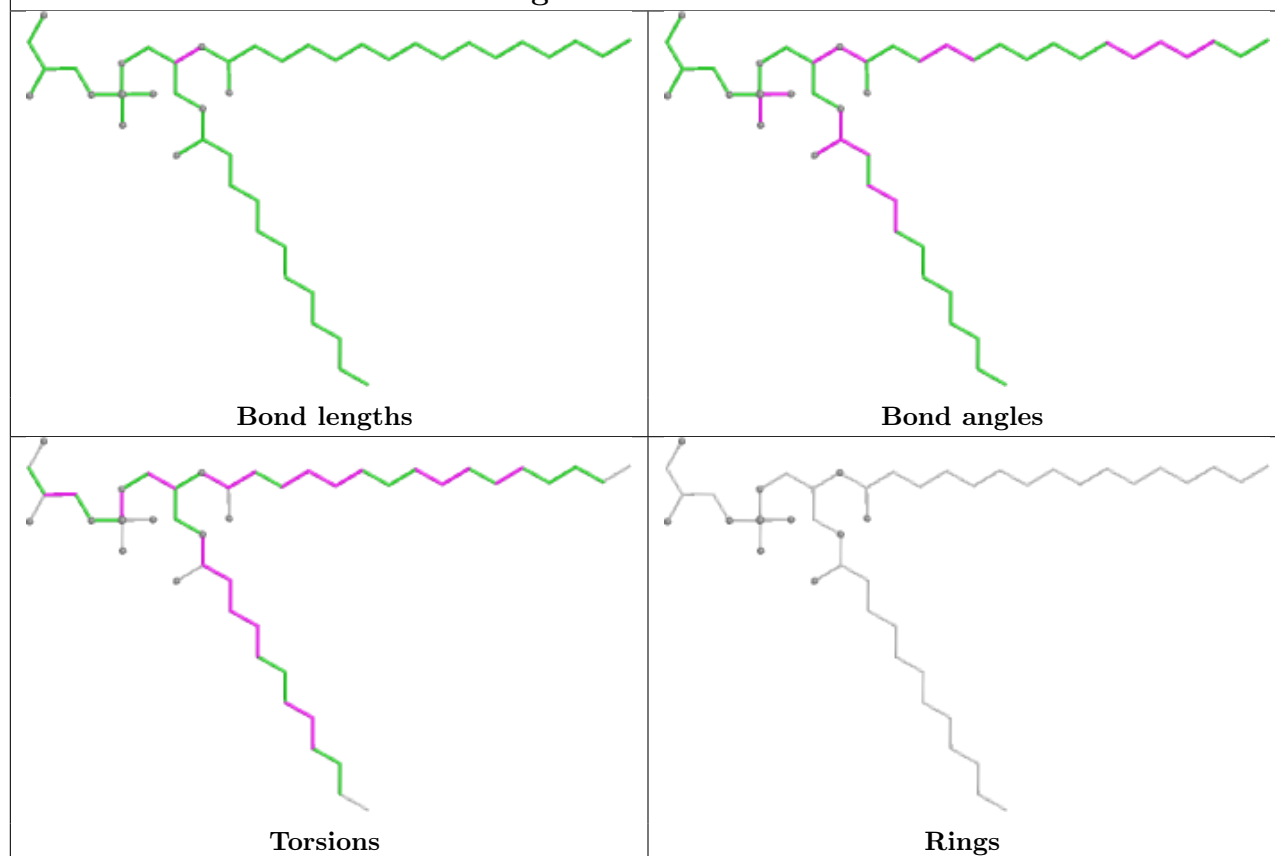
Torsions



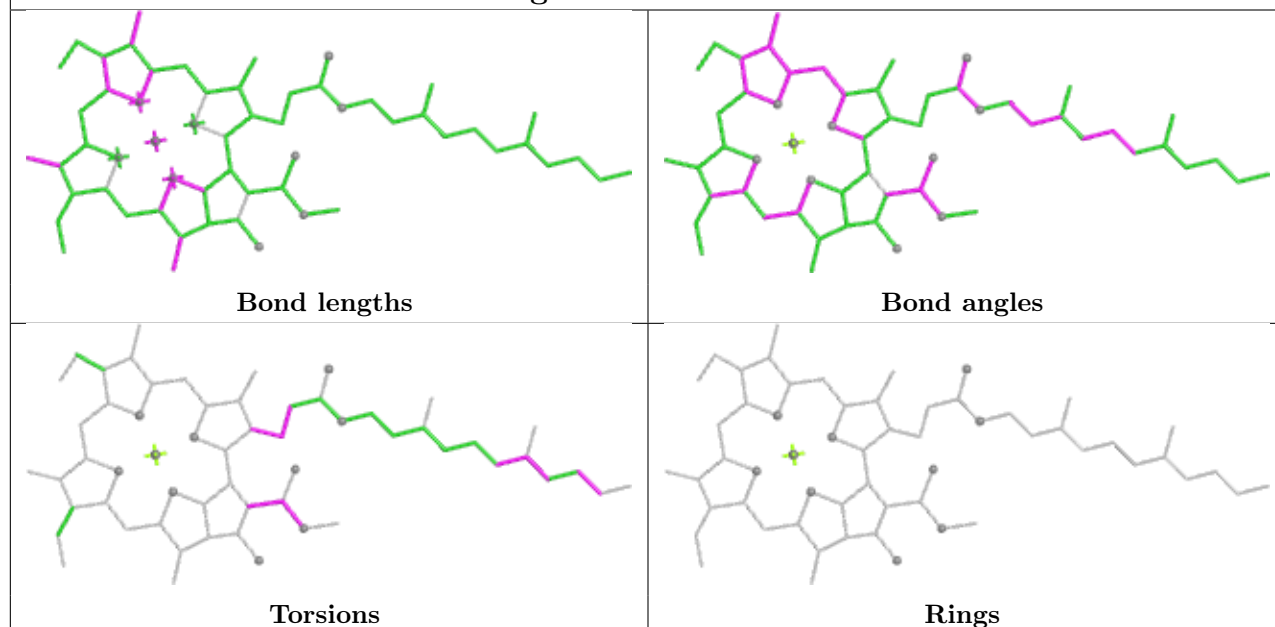
Rings



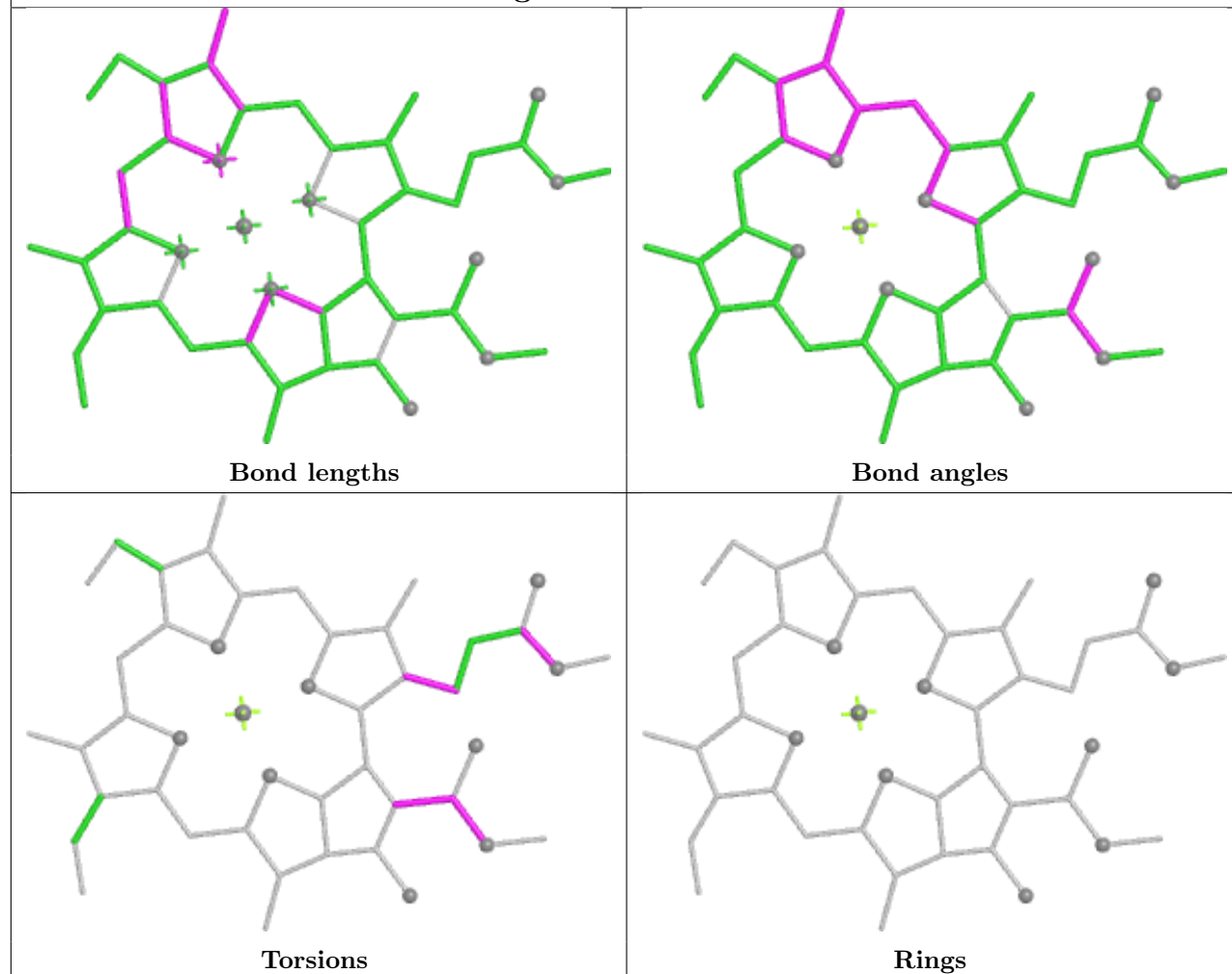
Ligand LHG F 318



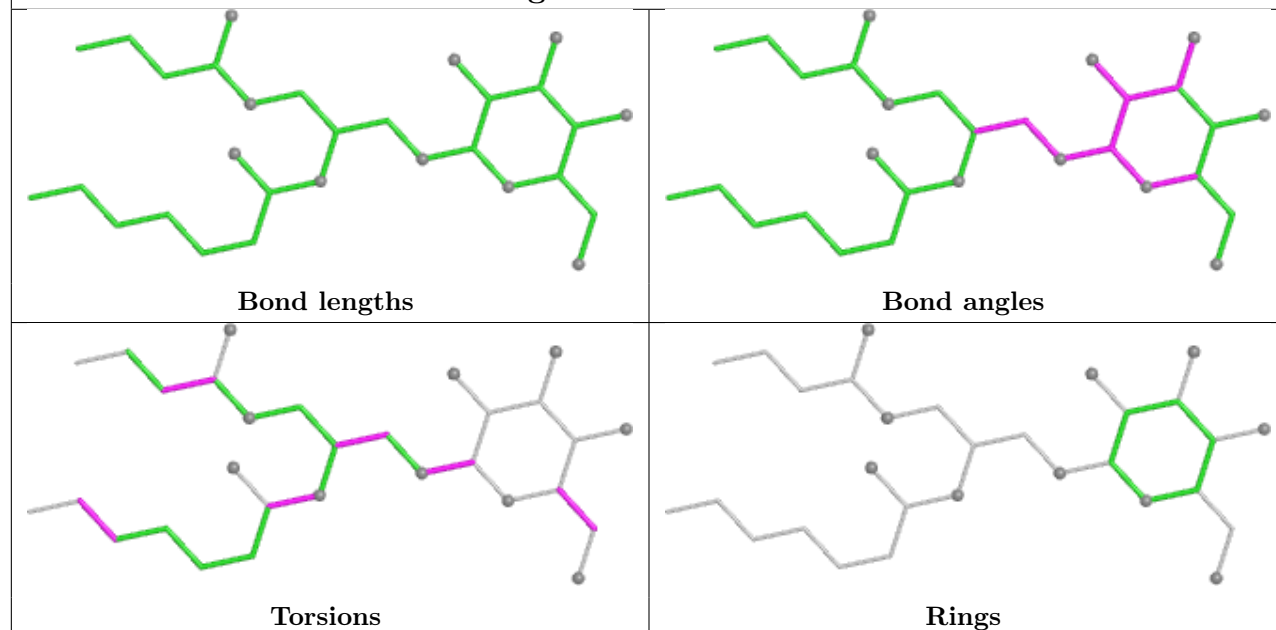
Ligand CLA D 314



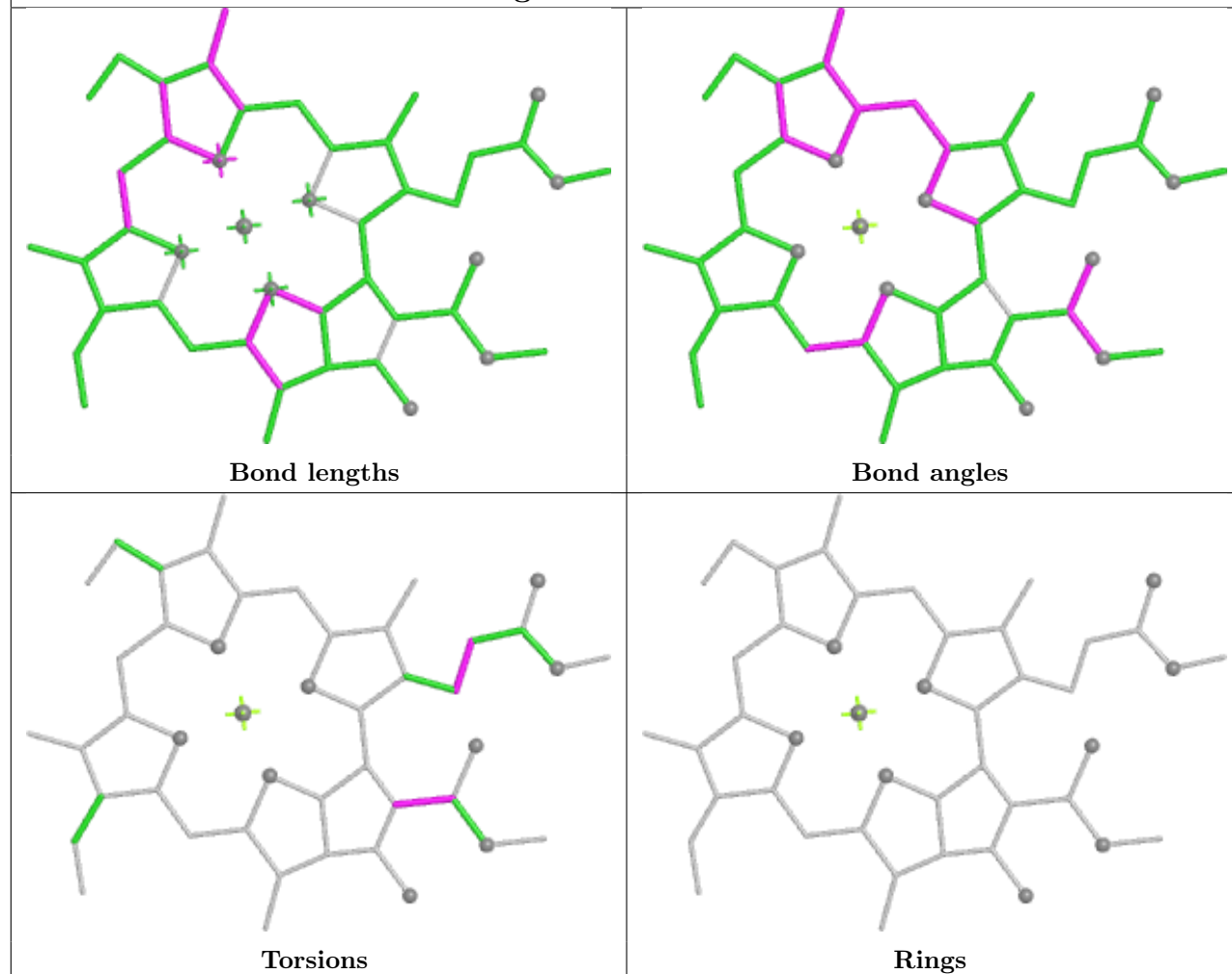
Ligand CLA C 308



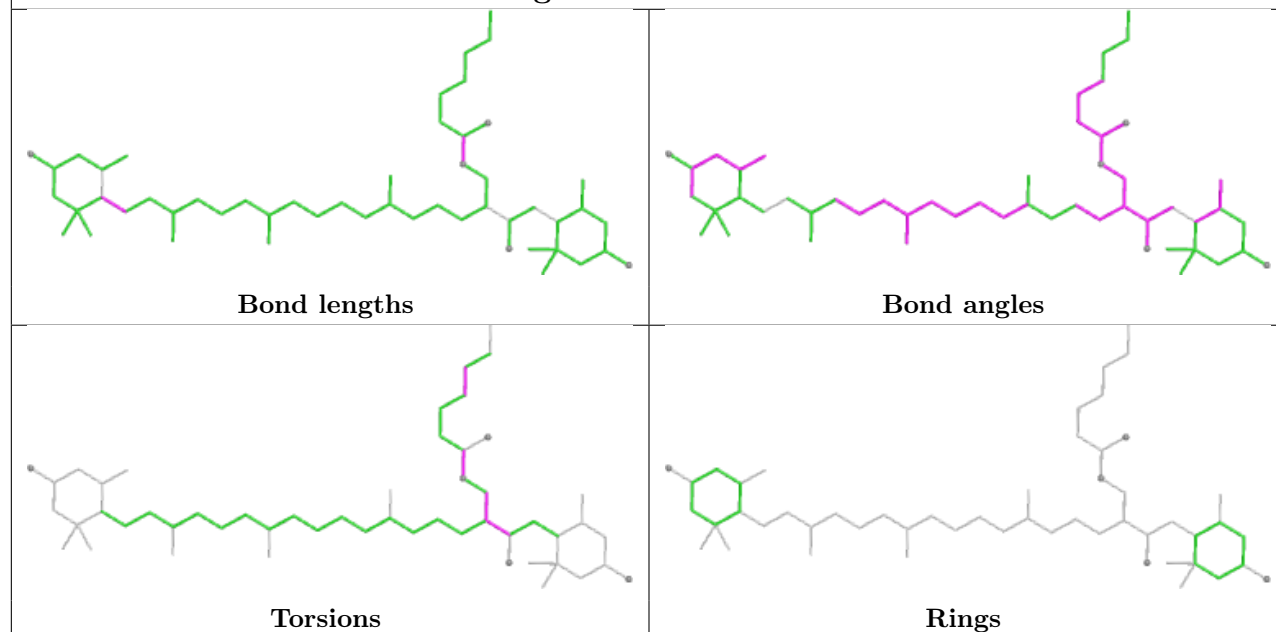
Ligand LMG B 323



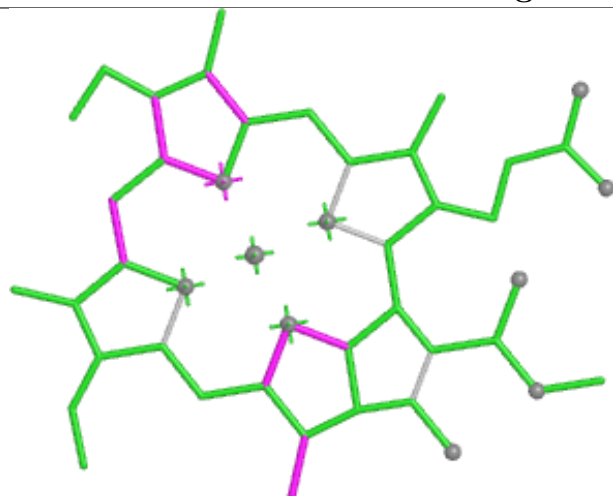
Ligand CLA B 309



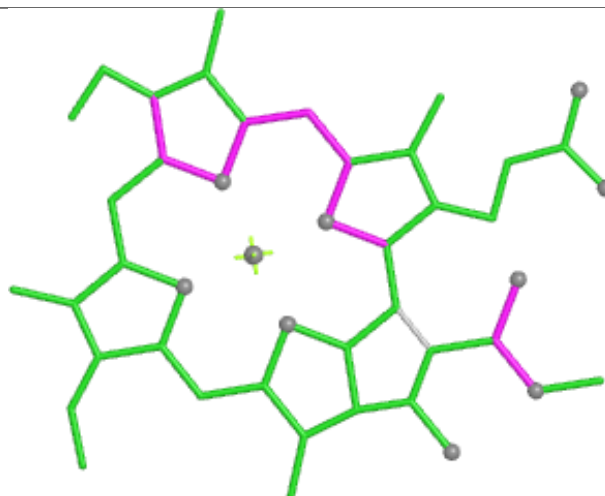
Ligand OUR B 325



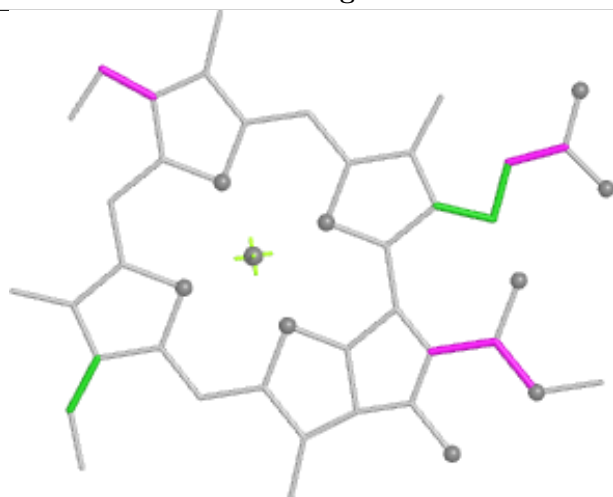
Ligand CLA E 315



Bond lengths



Bond angles

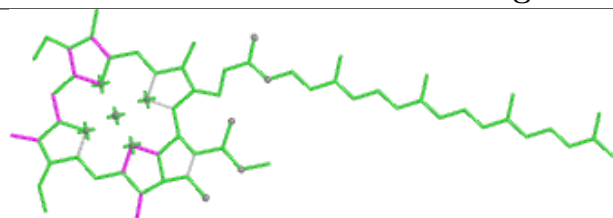


Torsions

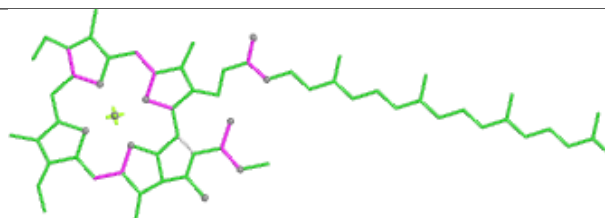


Rings

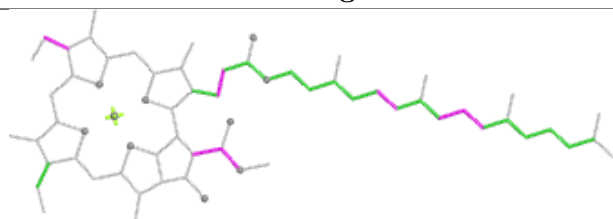
Ligand CLA D 317



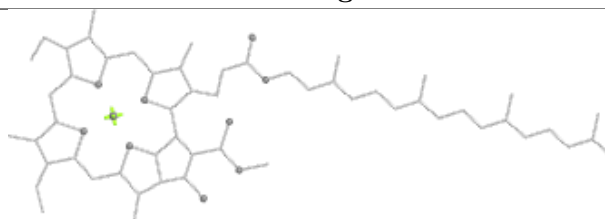
Bond lengths



Bond angles

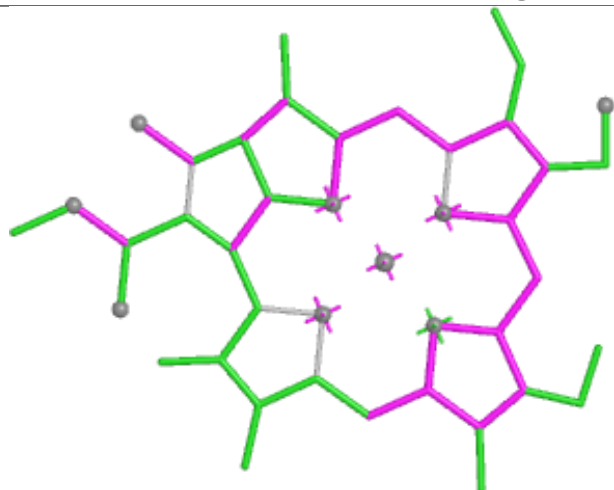


Torsions

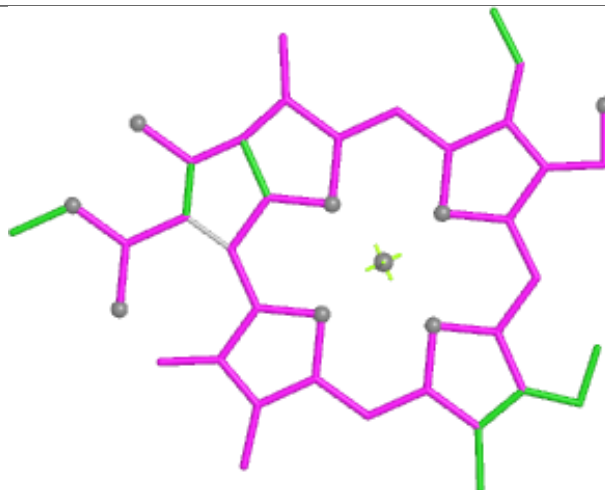


Rings

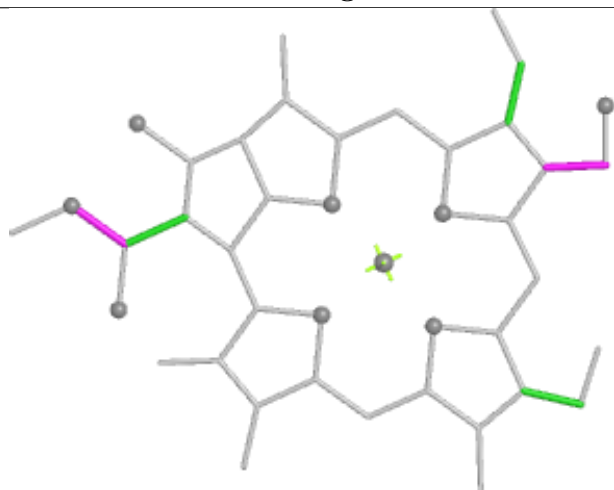
Ligand CHL D 309



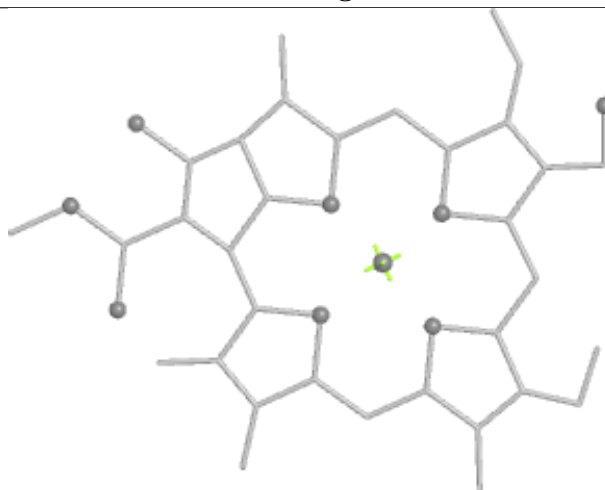
Bond lengths



Bond angles

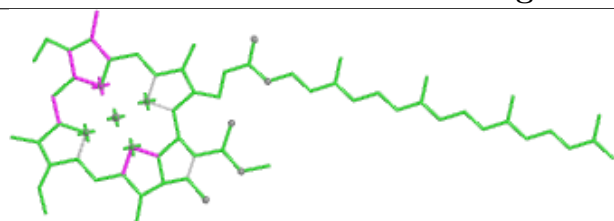


Torsions

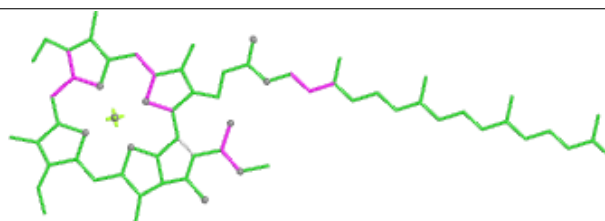


Rings

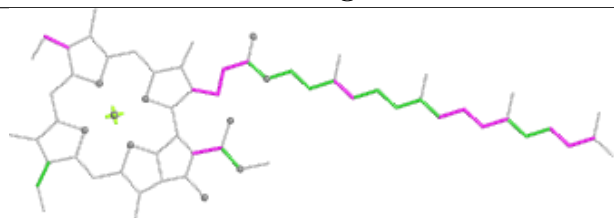
Ligand CLA F 306



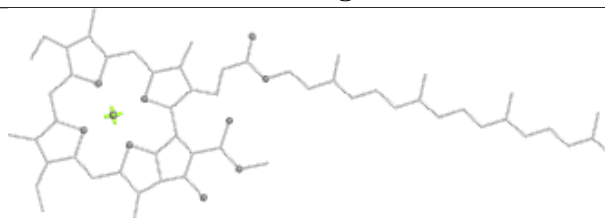
Bond lengths



Bond angles

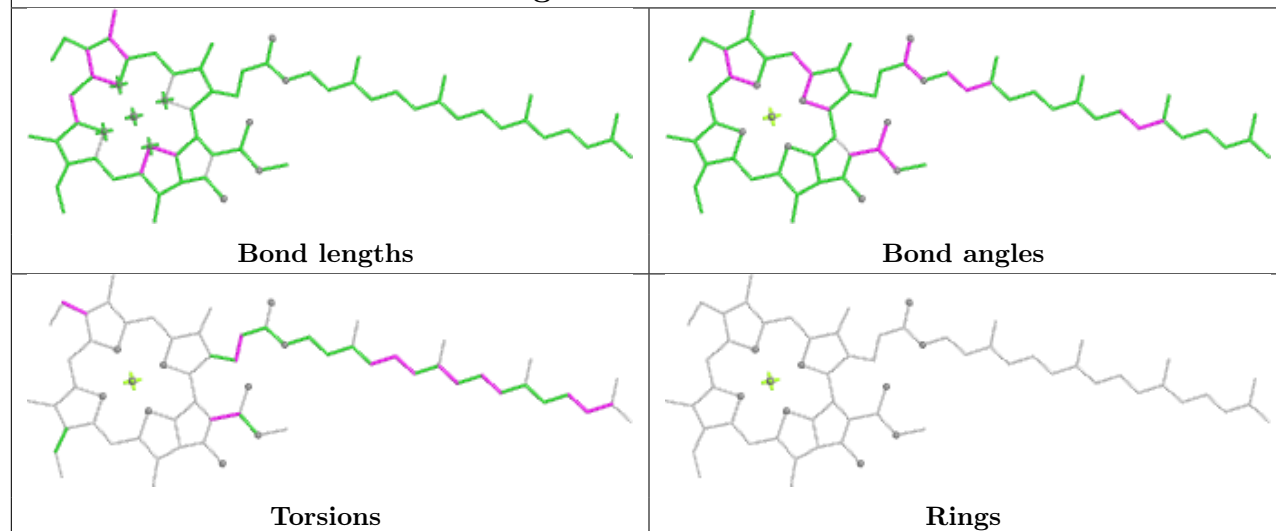


Torsions

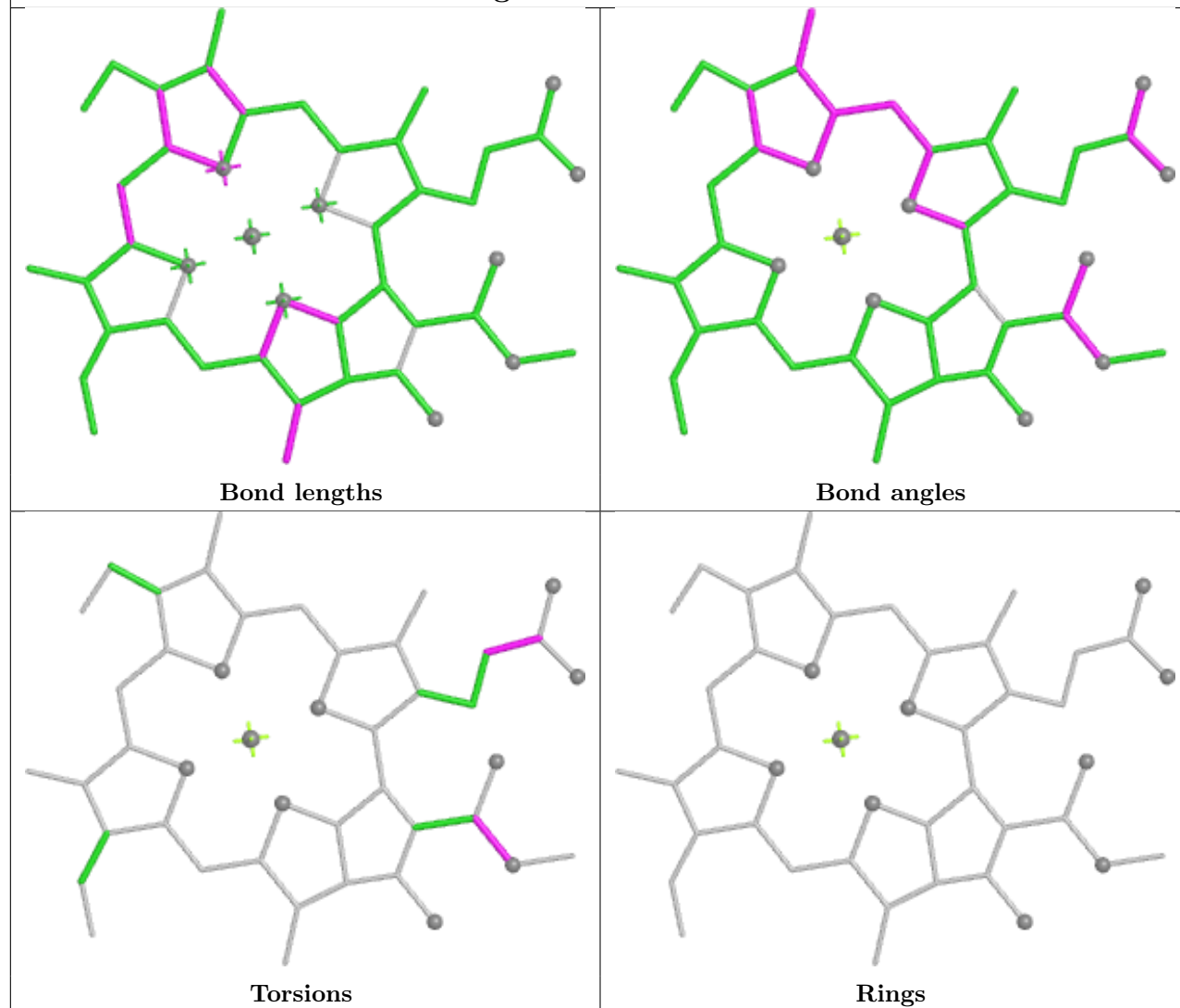


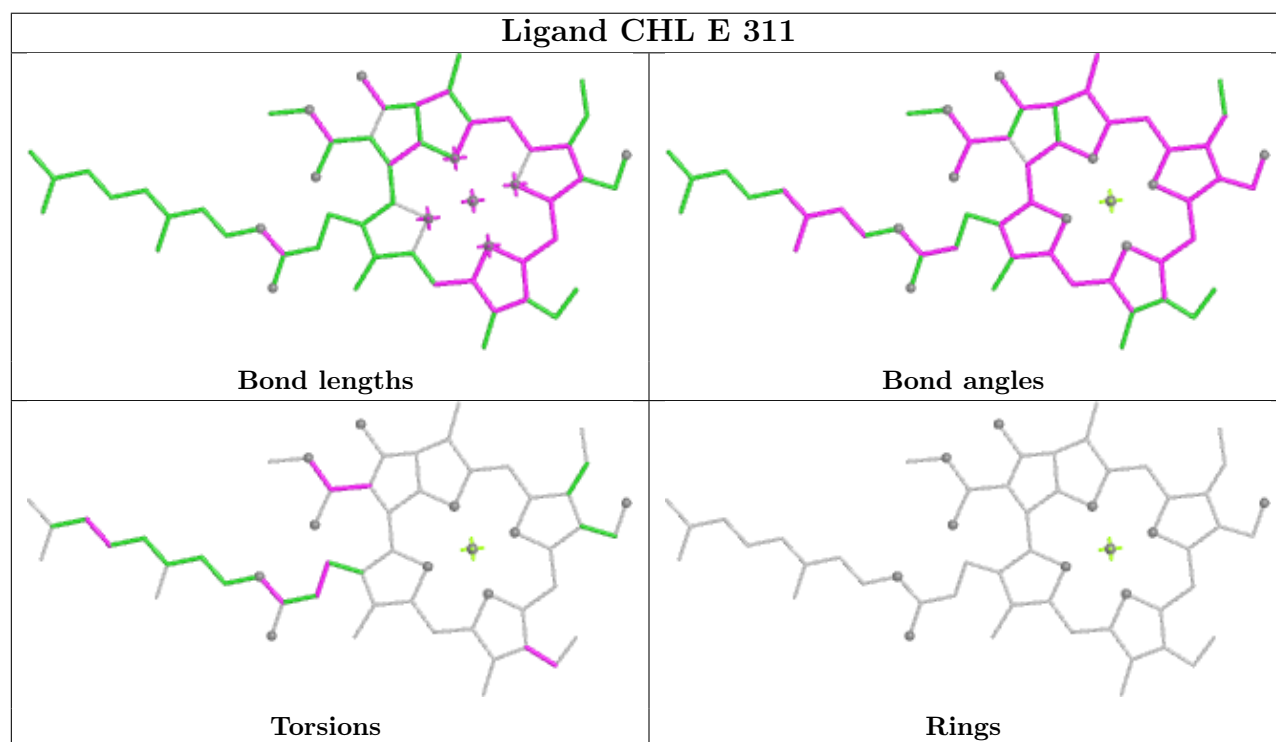
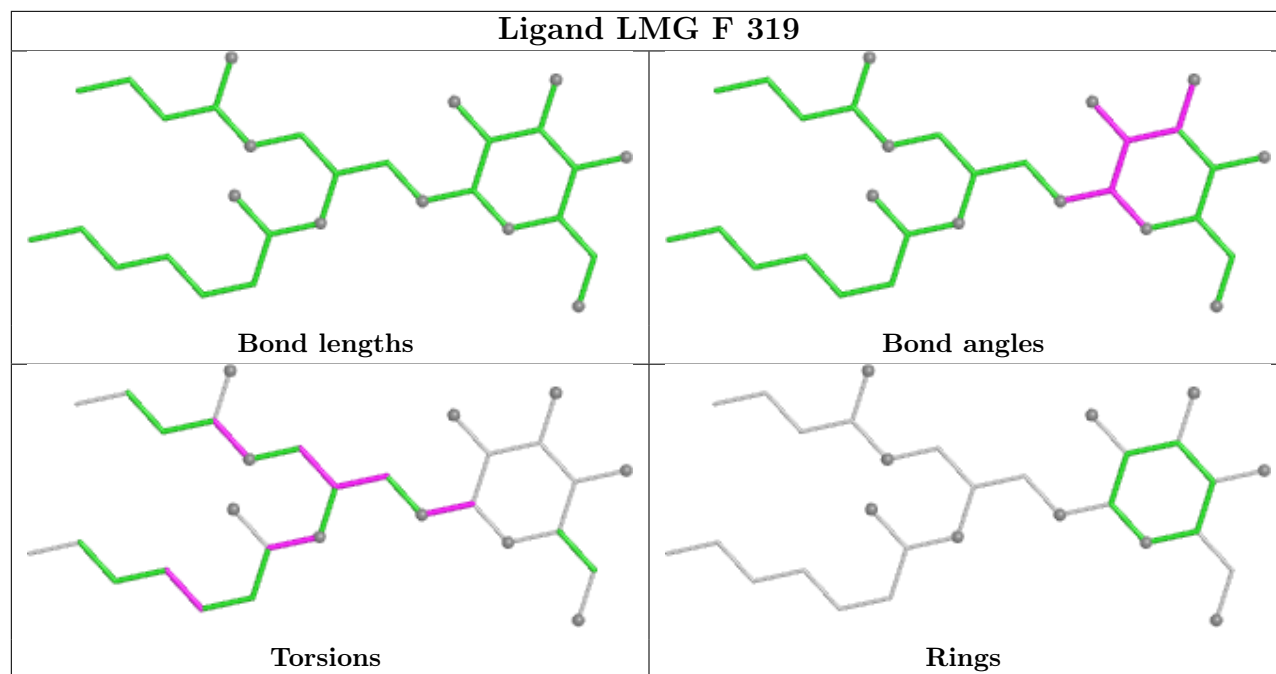
Rings

Ligand CLA E 306

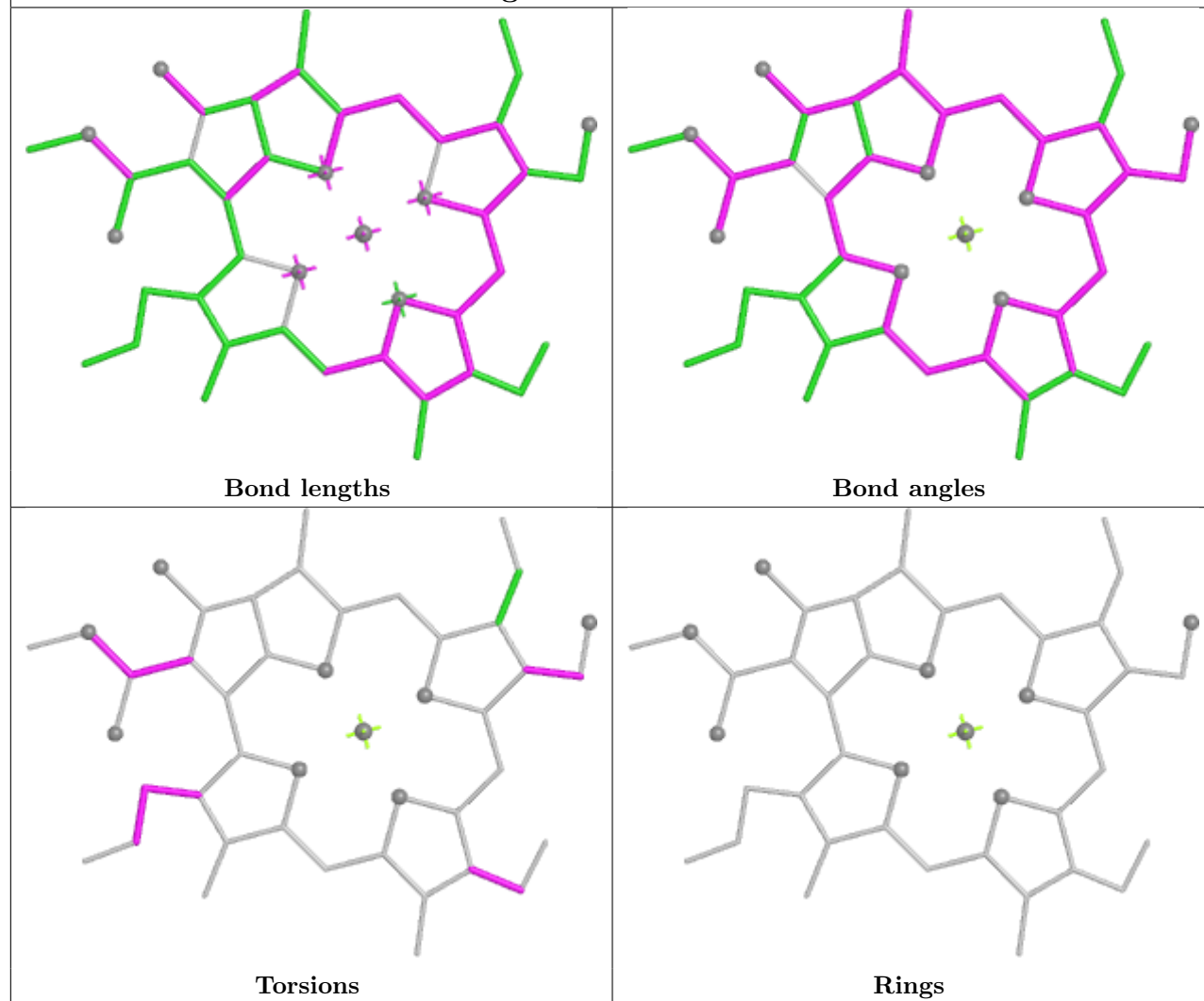


Ligand CLA F 315

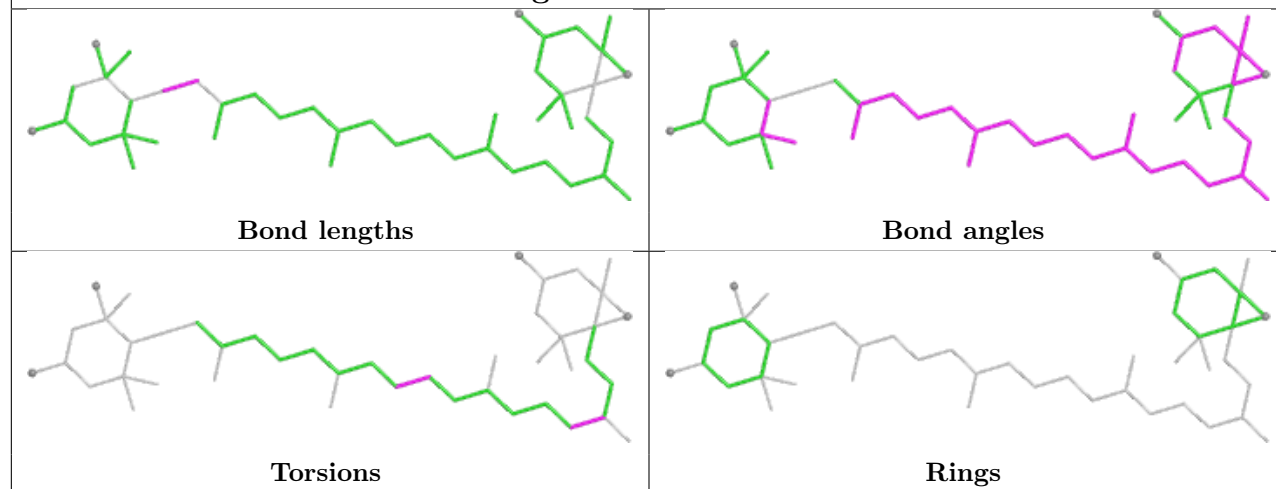


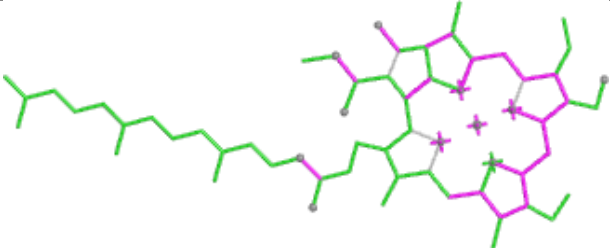
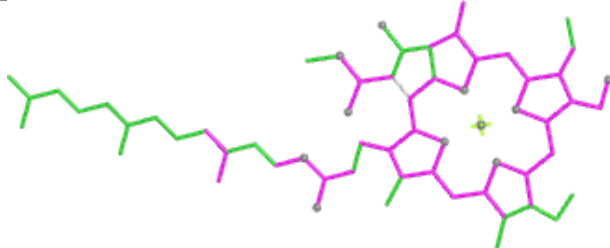
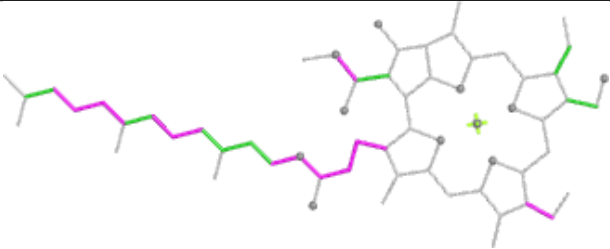
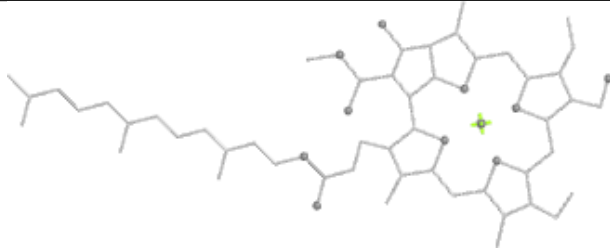
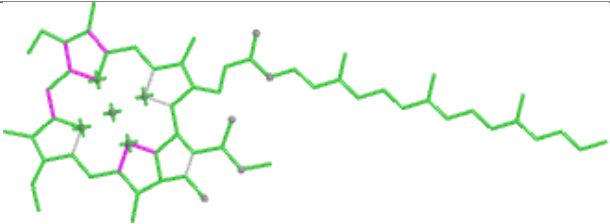
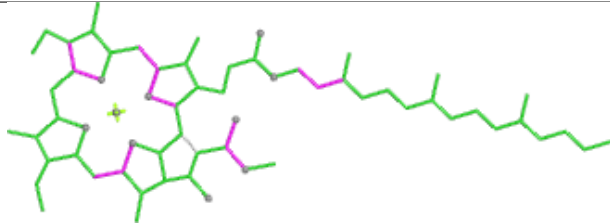
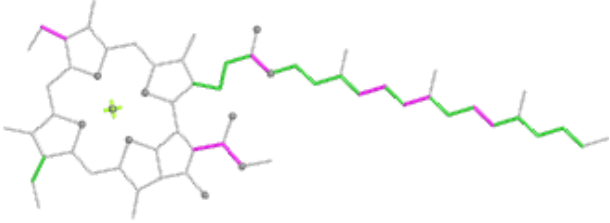
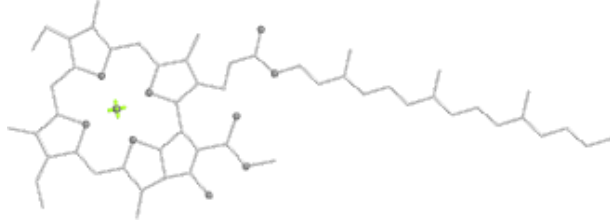
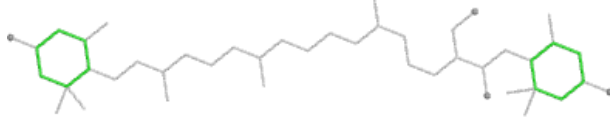


Ligand CHL C 310

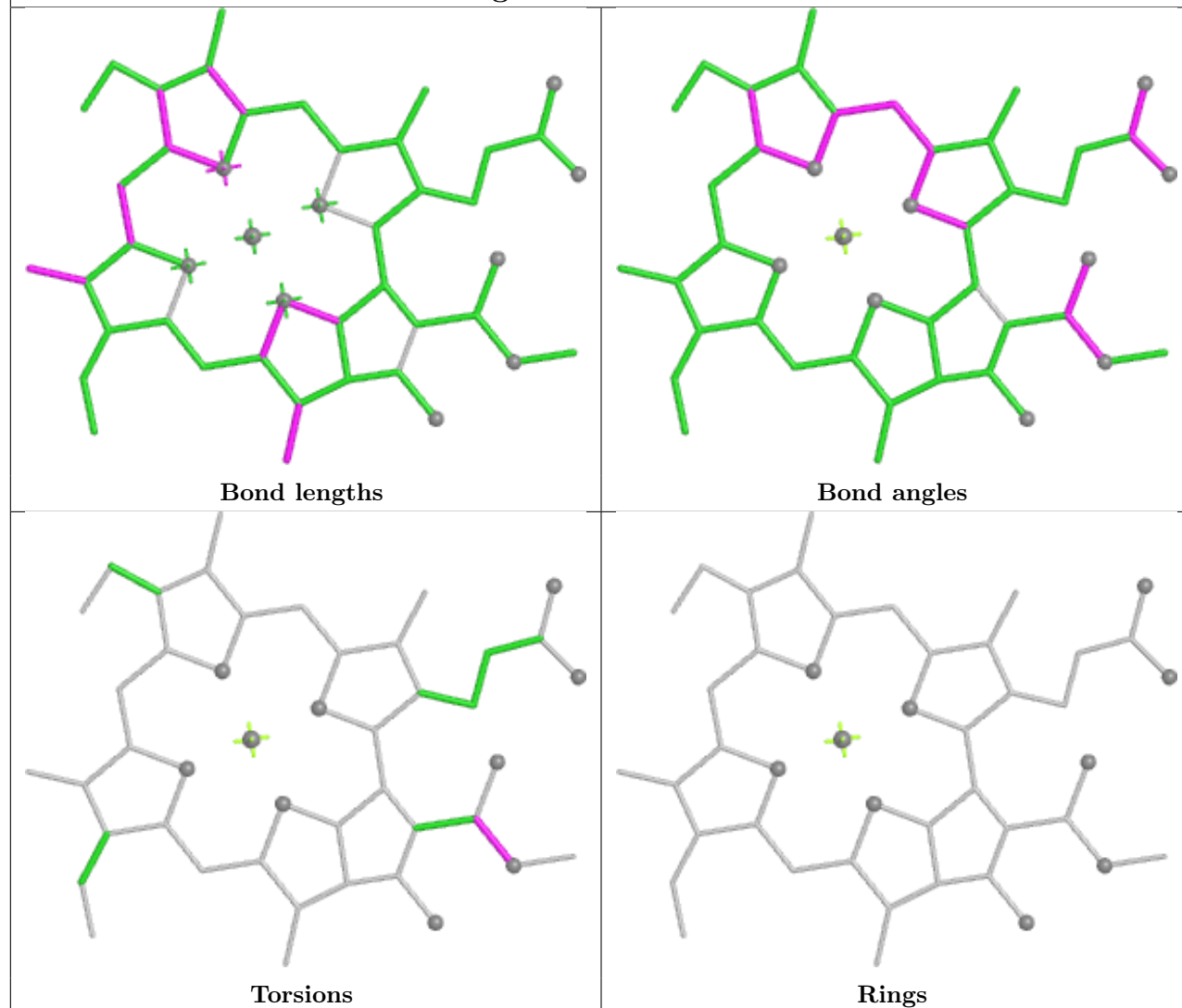


Ligand NEX F 303

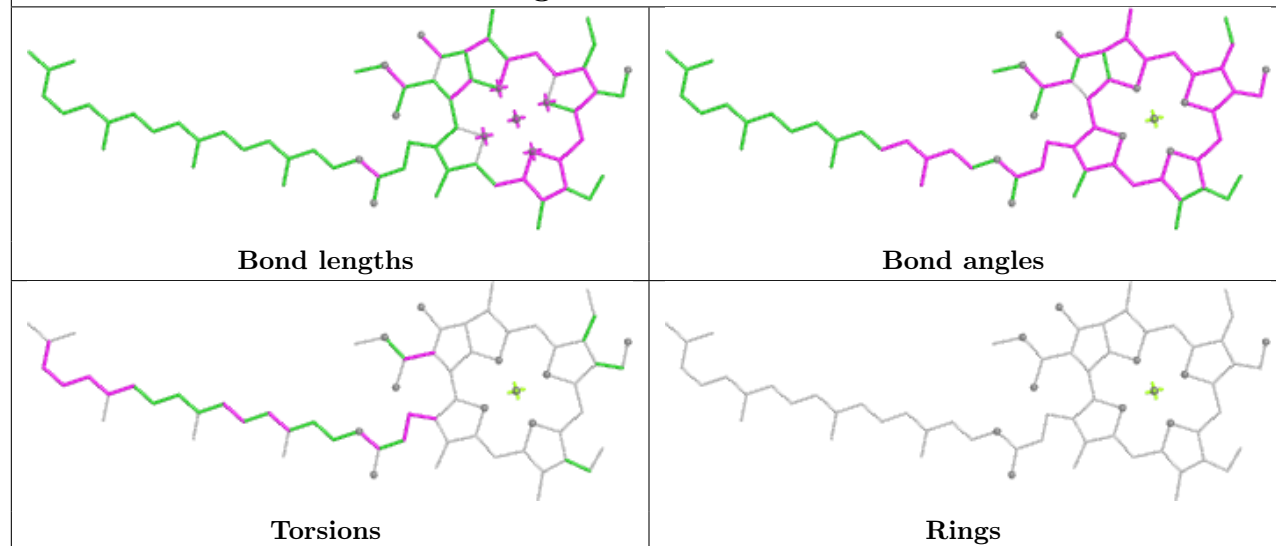


Ligand CHL C 311	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA E 314	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand OIE C 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

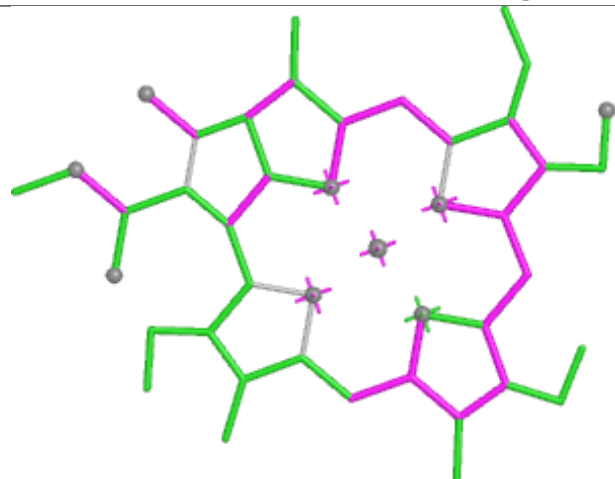
Ligand CLA D 316



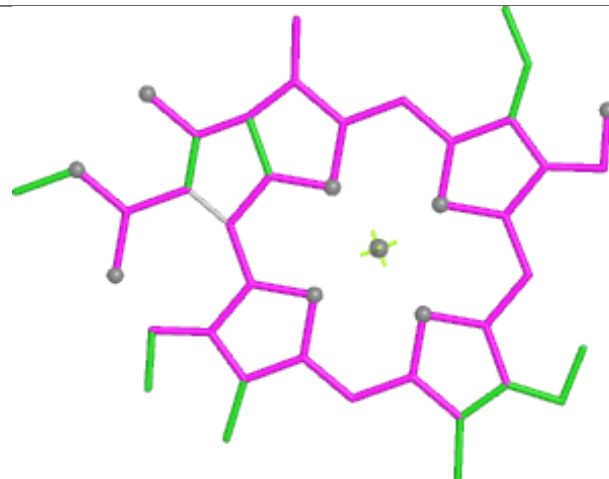
Ligand CHL E 304



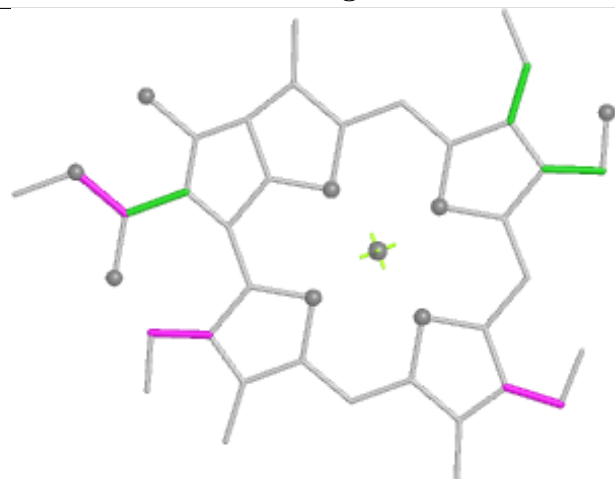
Ligand CHL E 309



Bond lengths



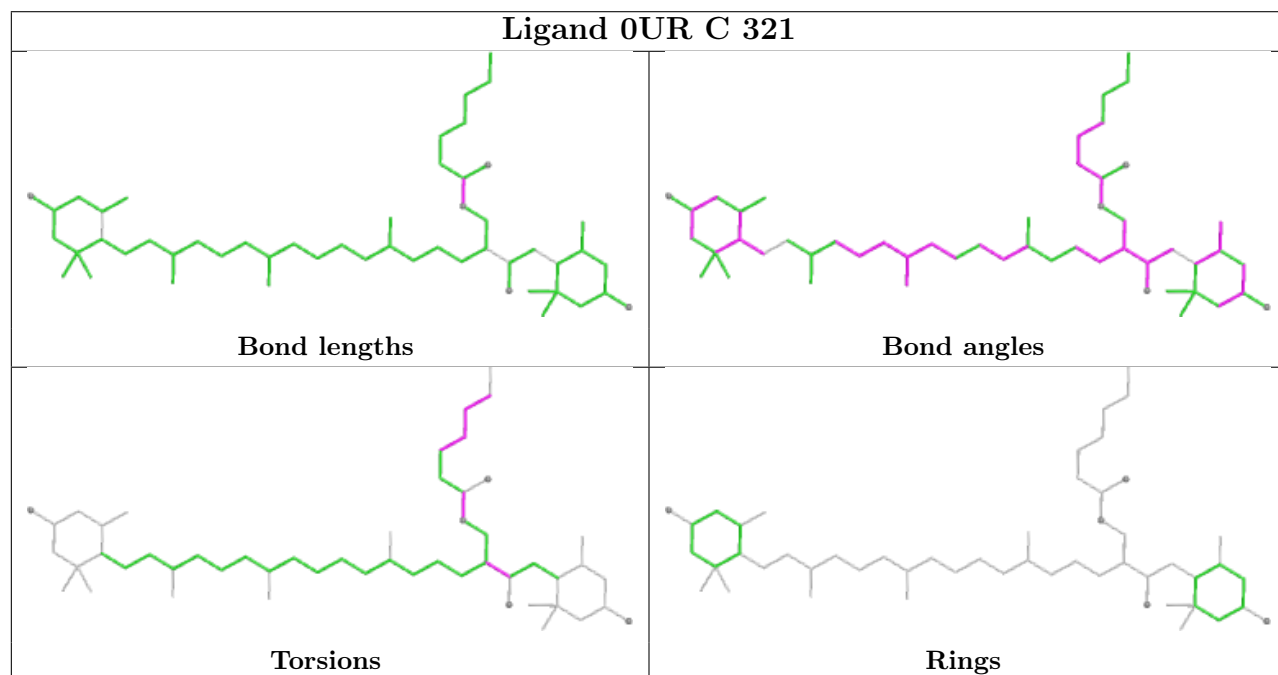
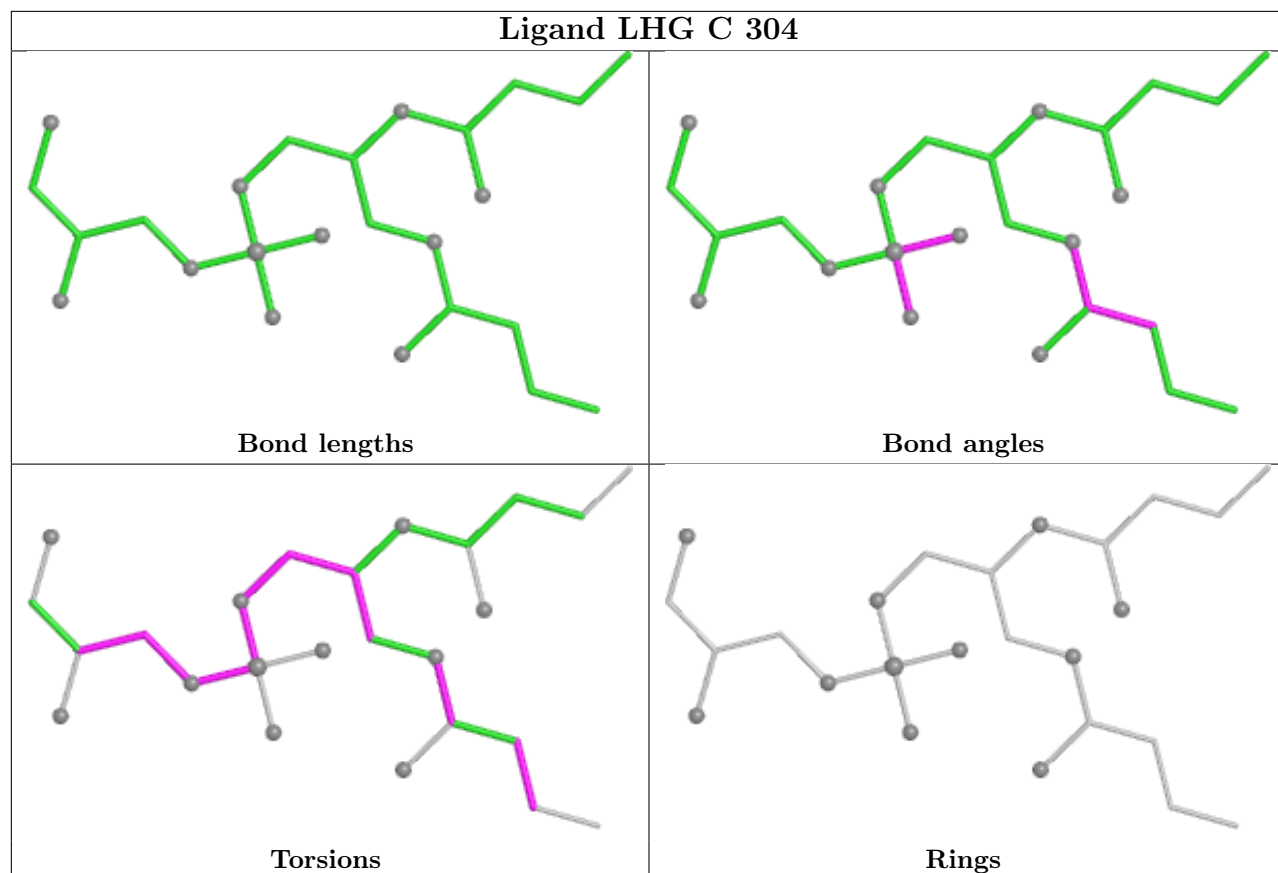
Bond angles



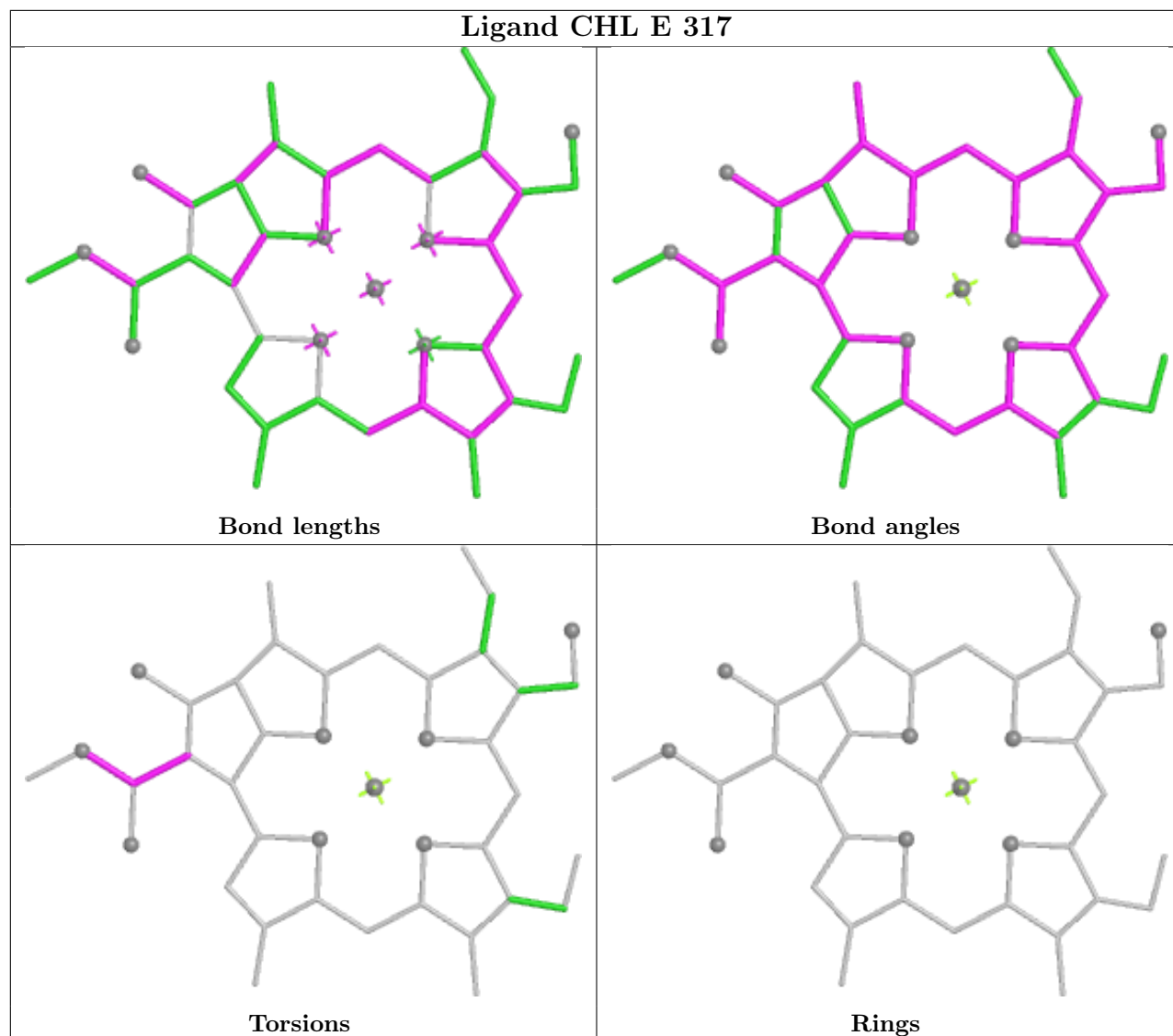
Torsions



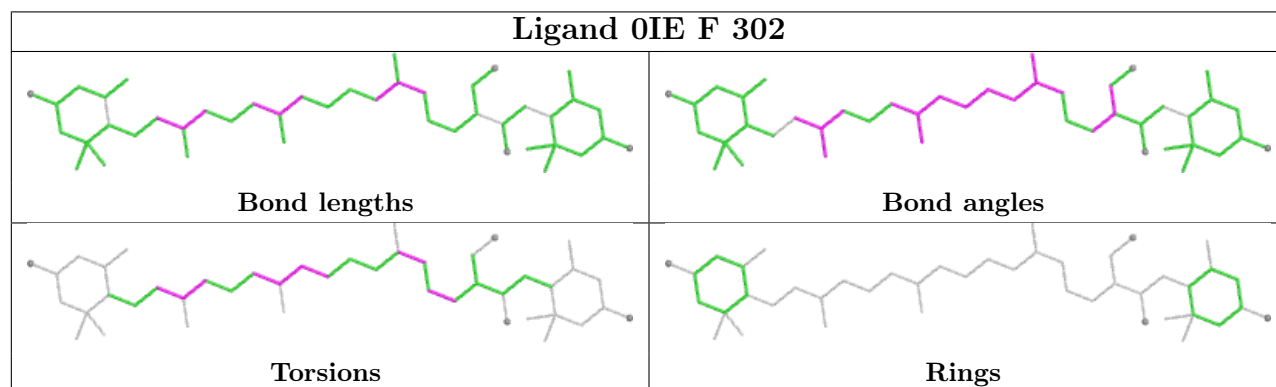
Rings

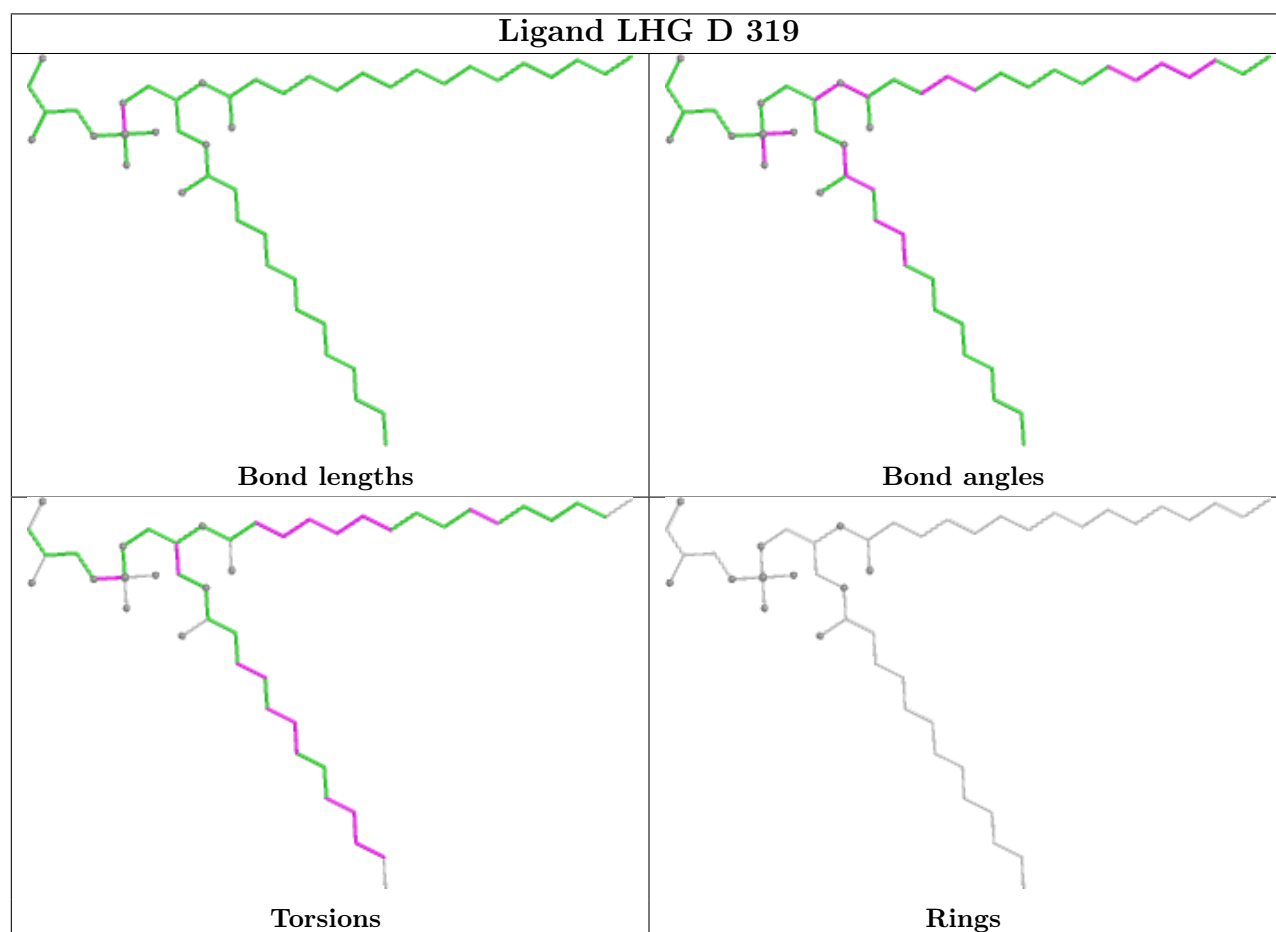
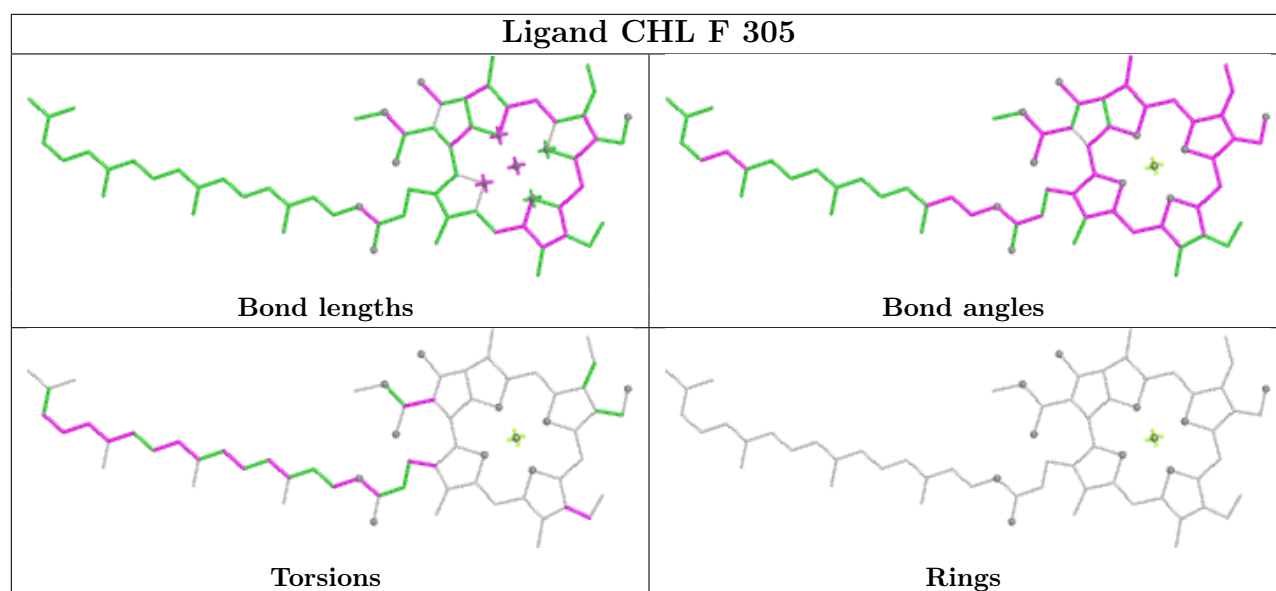


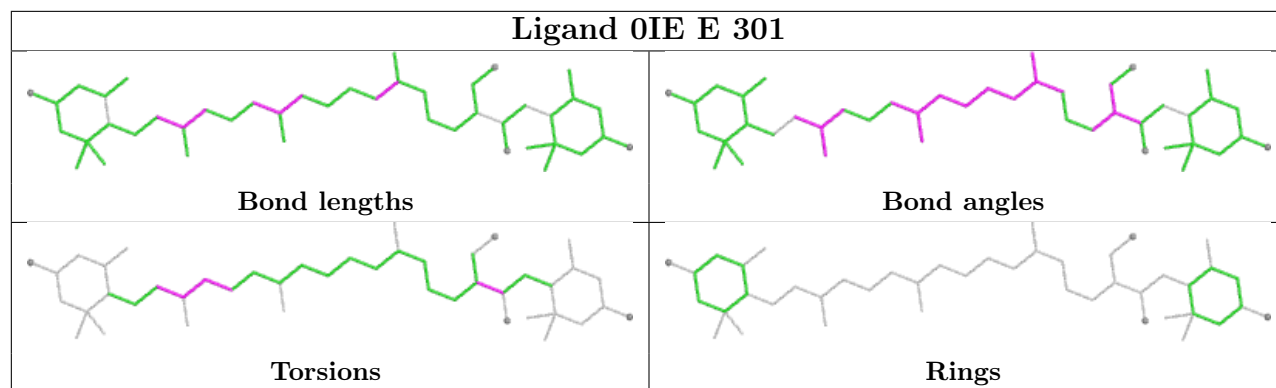
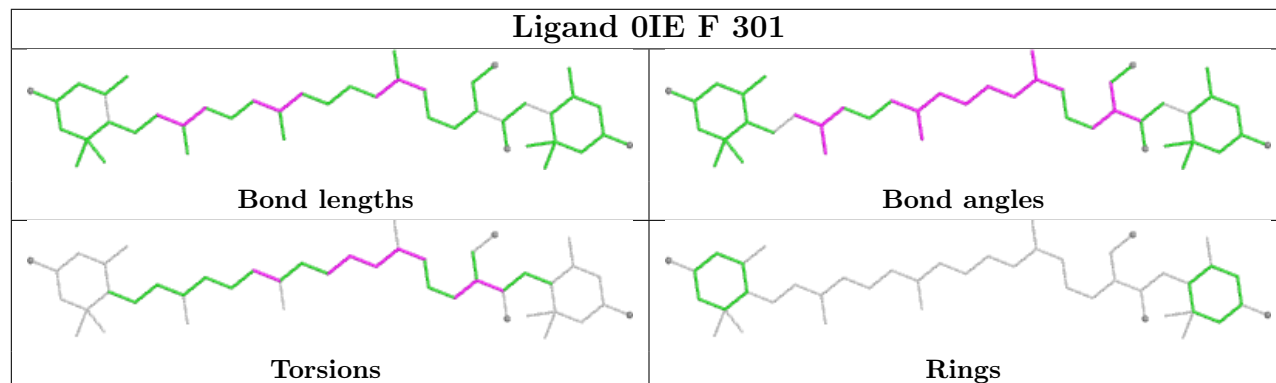
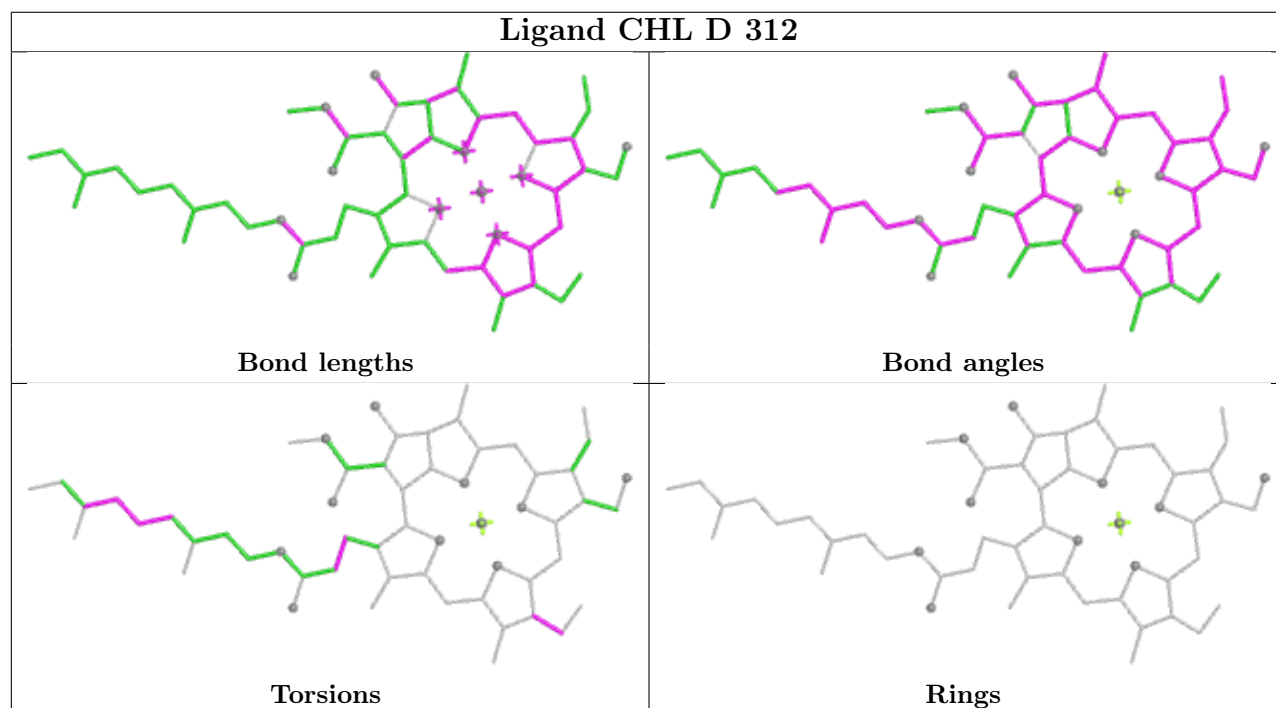
Ligand CHL E 317

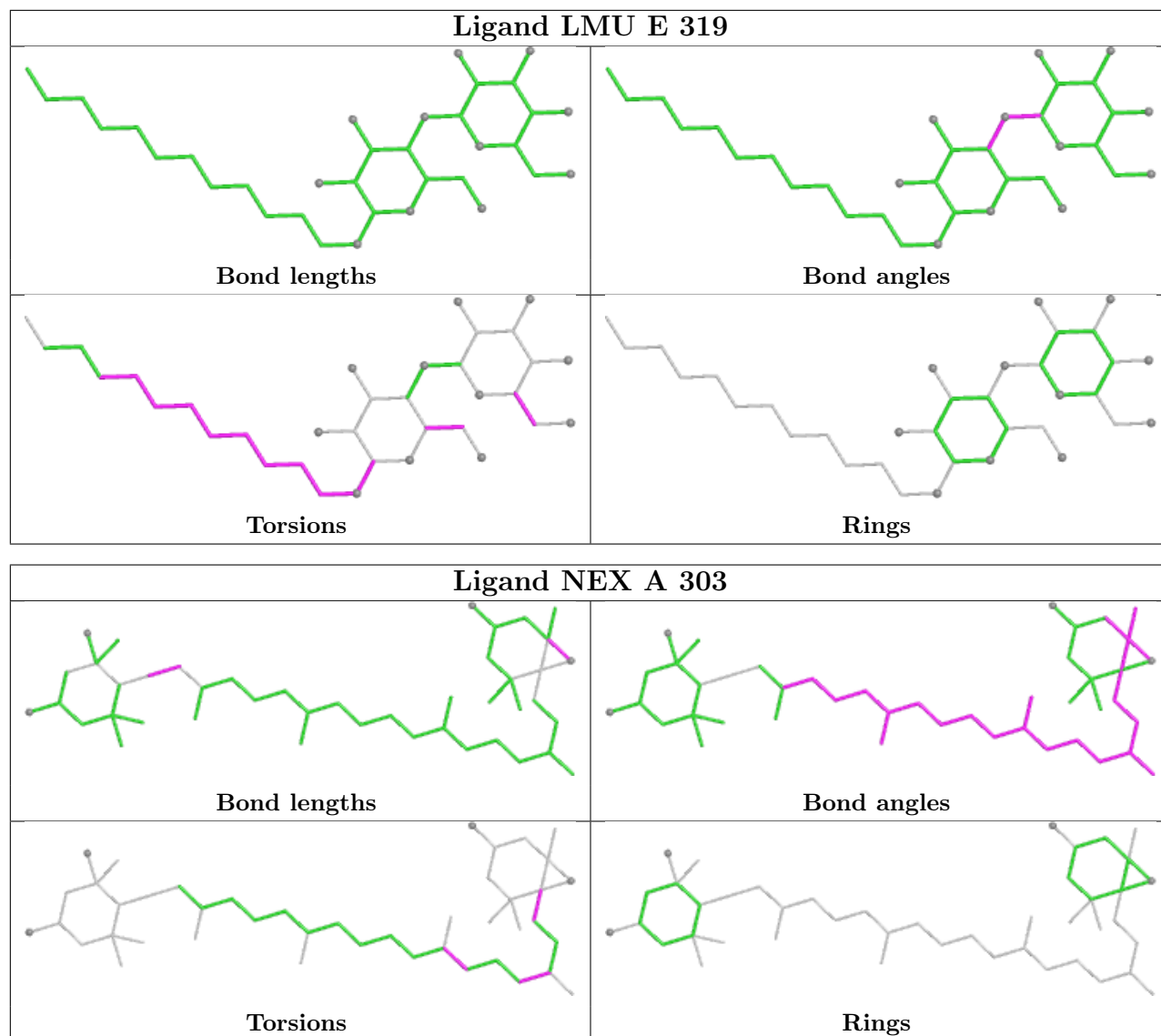


Ligand OIE F 302

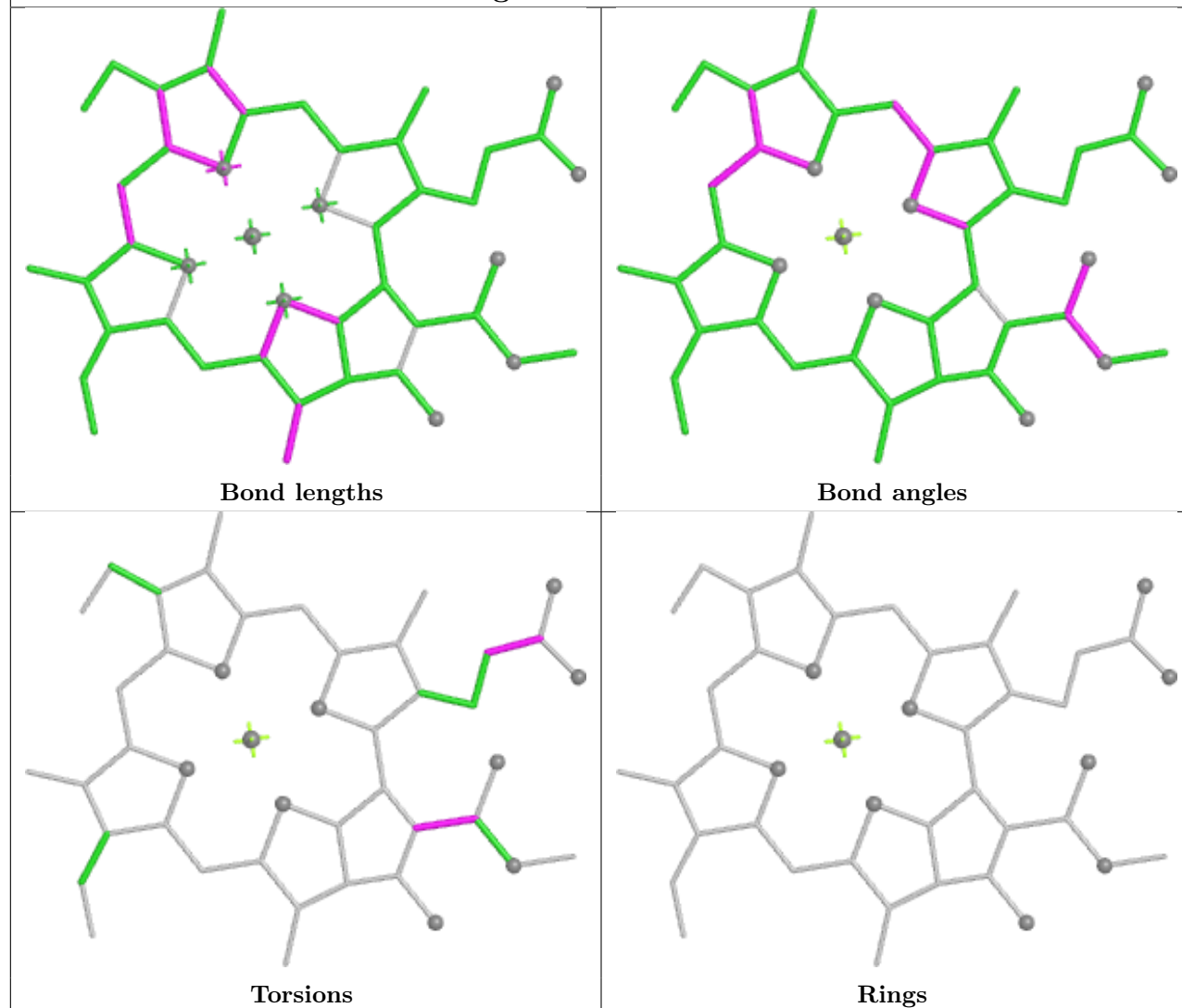




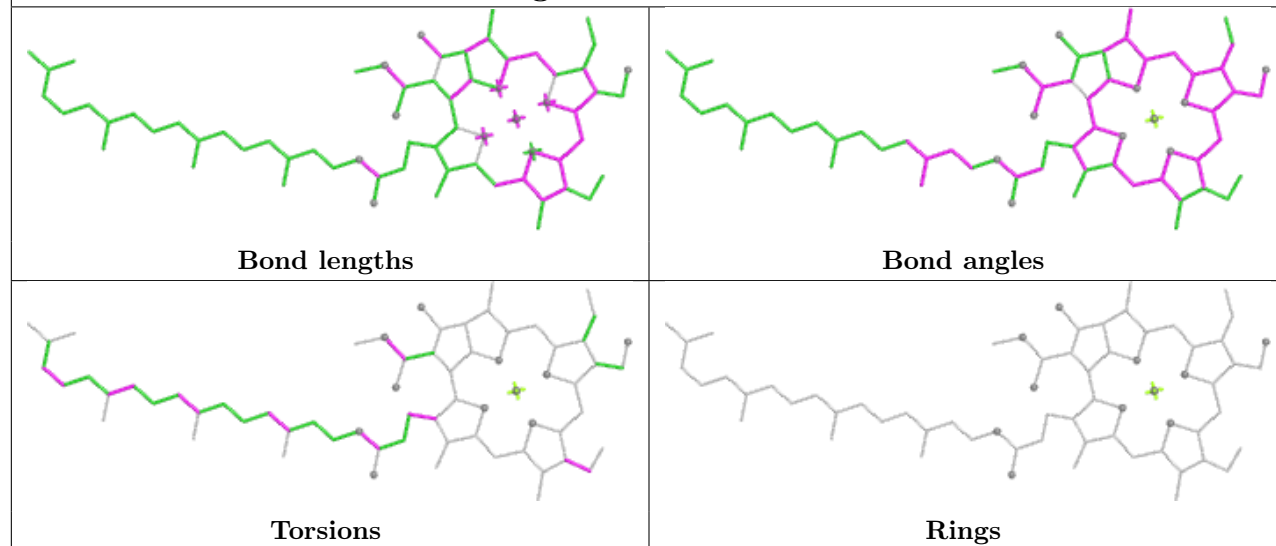
Ligand OIE E 301**Ligand OIE F 301****Ligand CHL D 312**

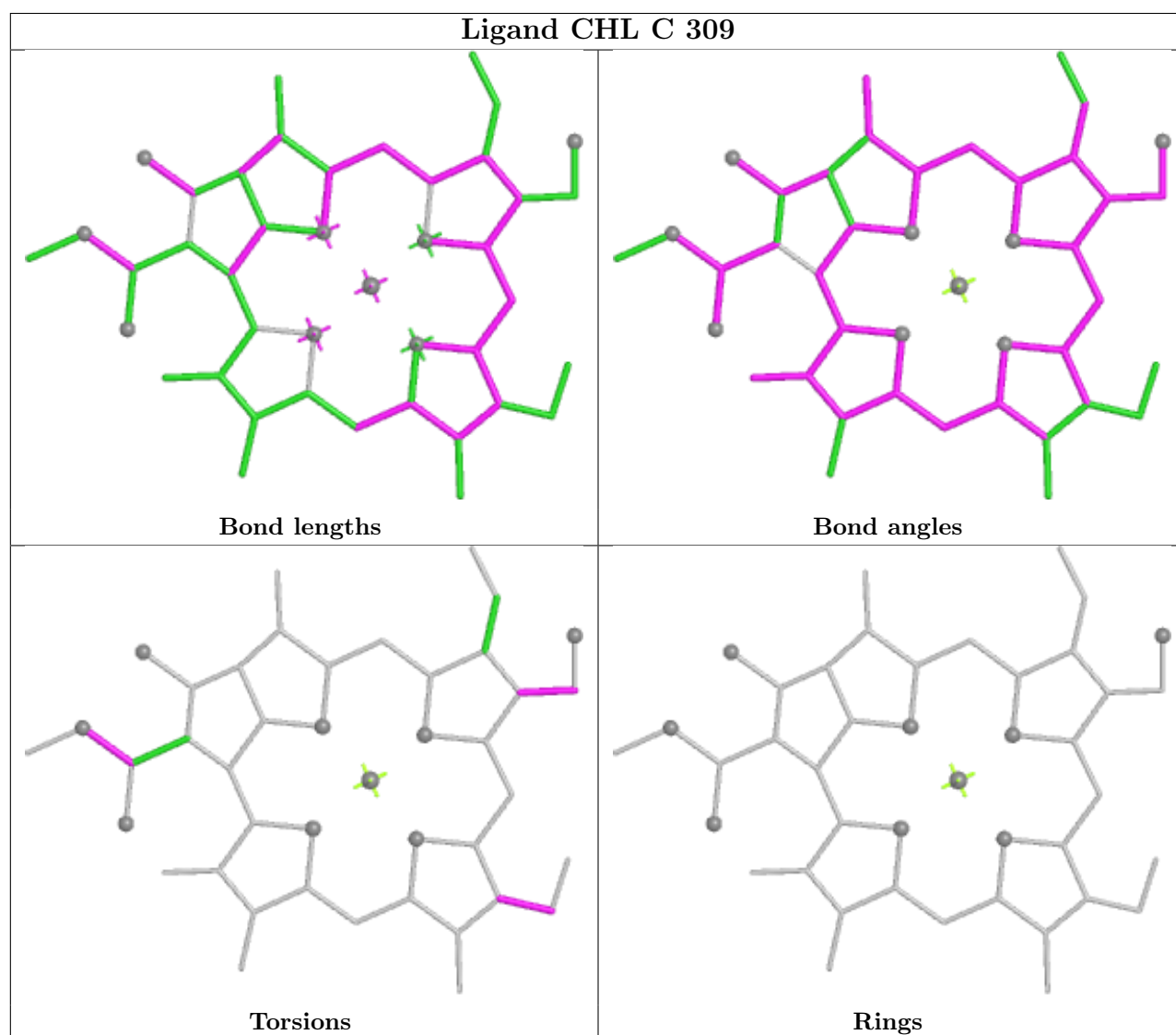
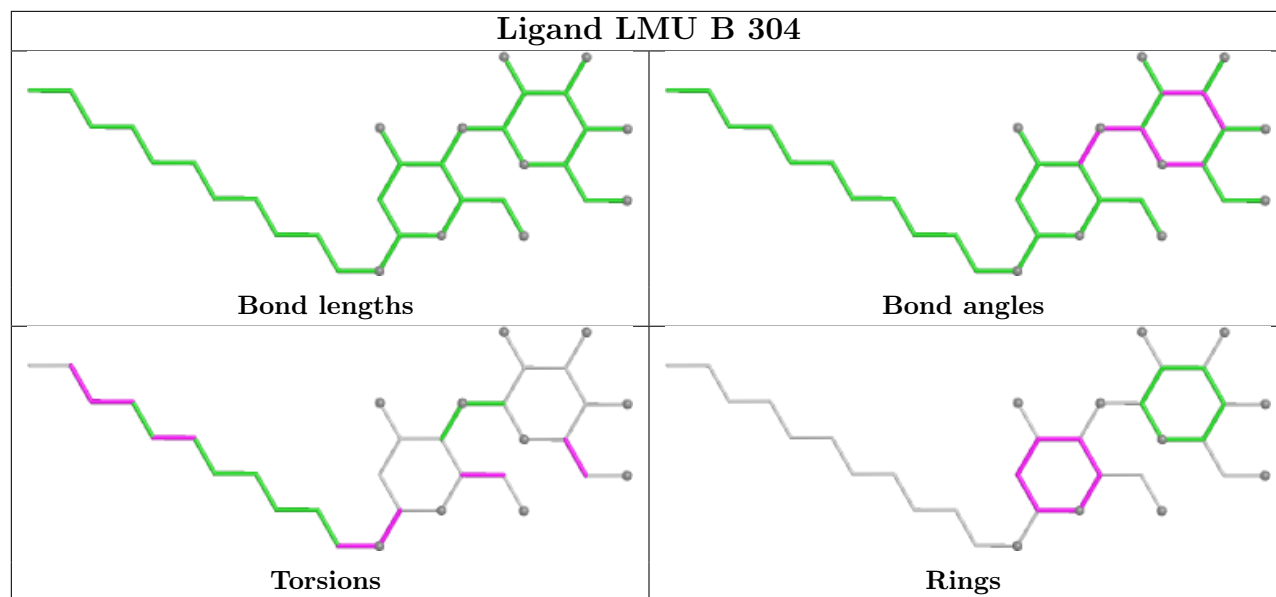


Ligand CLA C 316

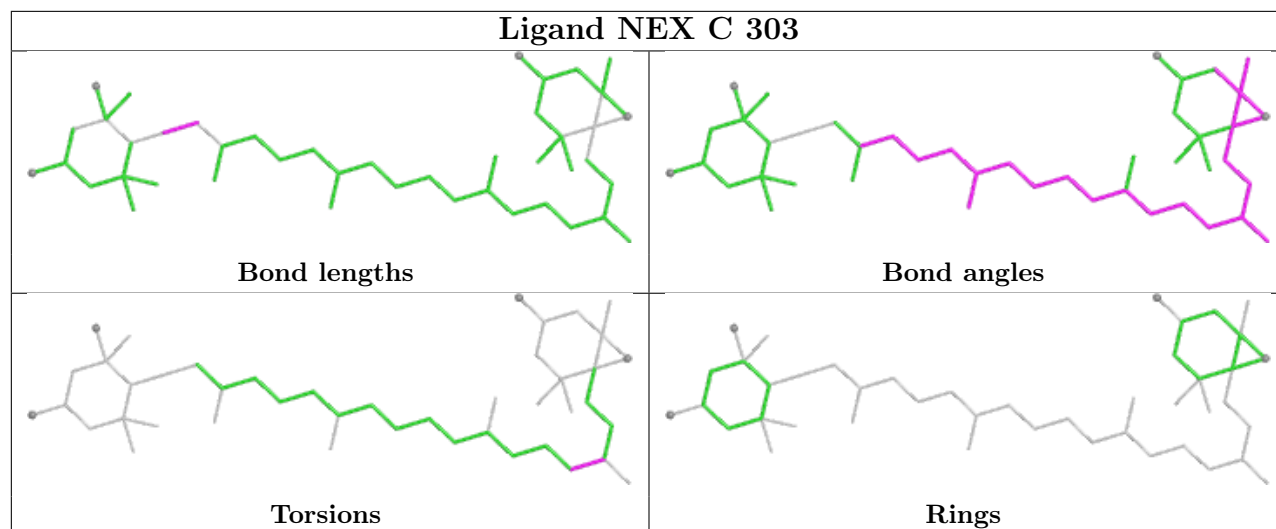


Ligand CHL C 313

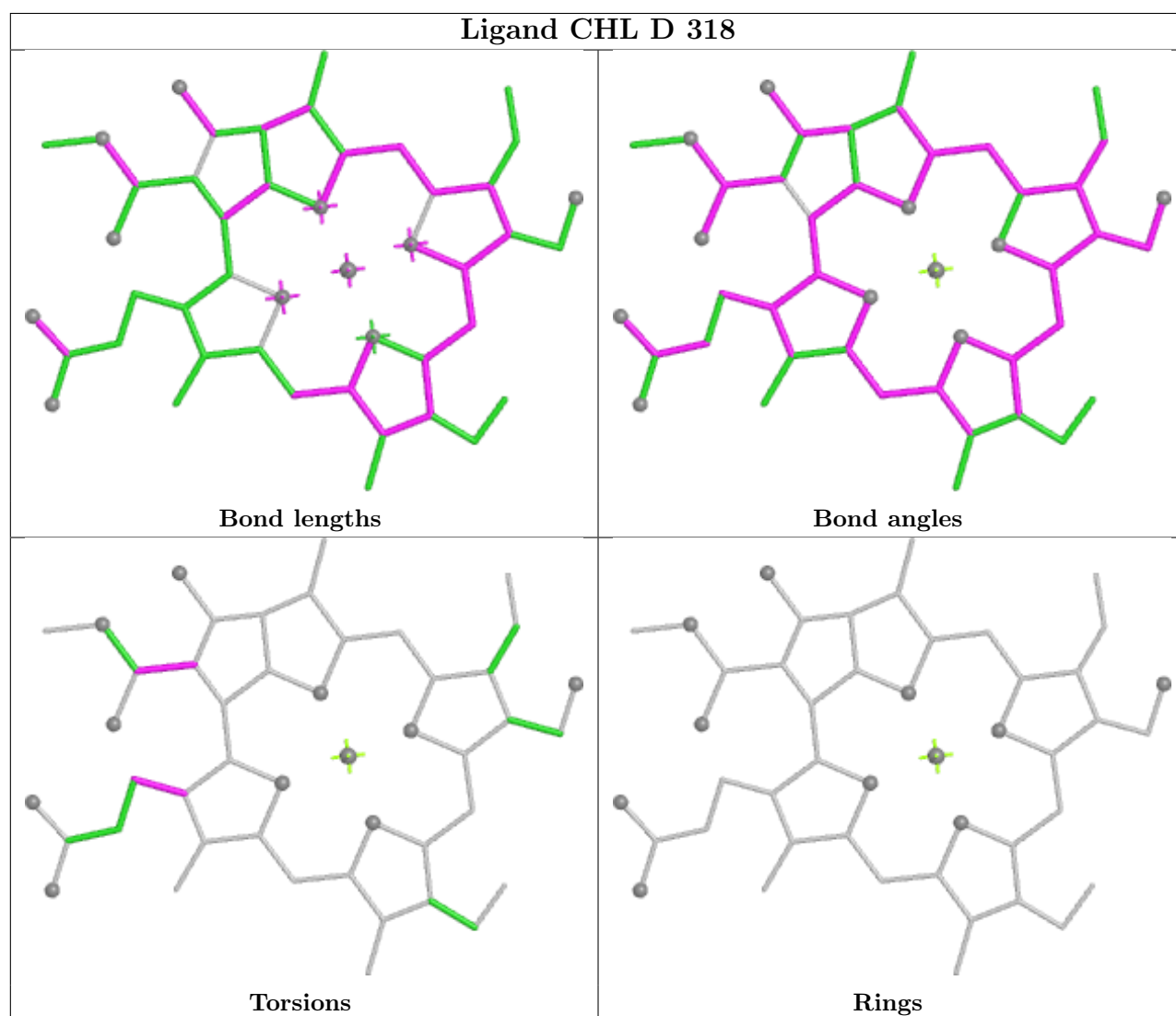


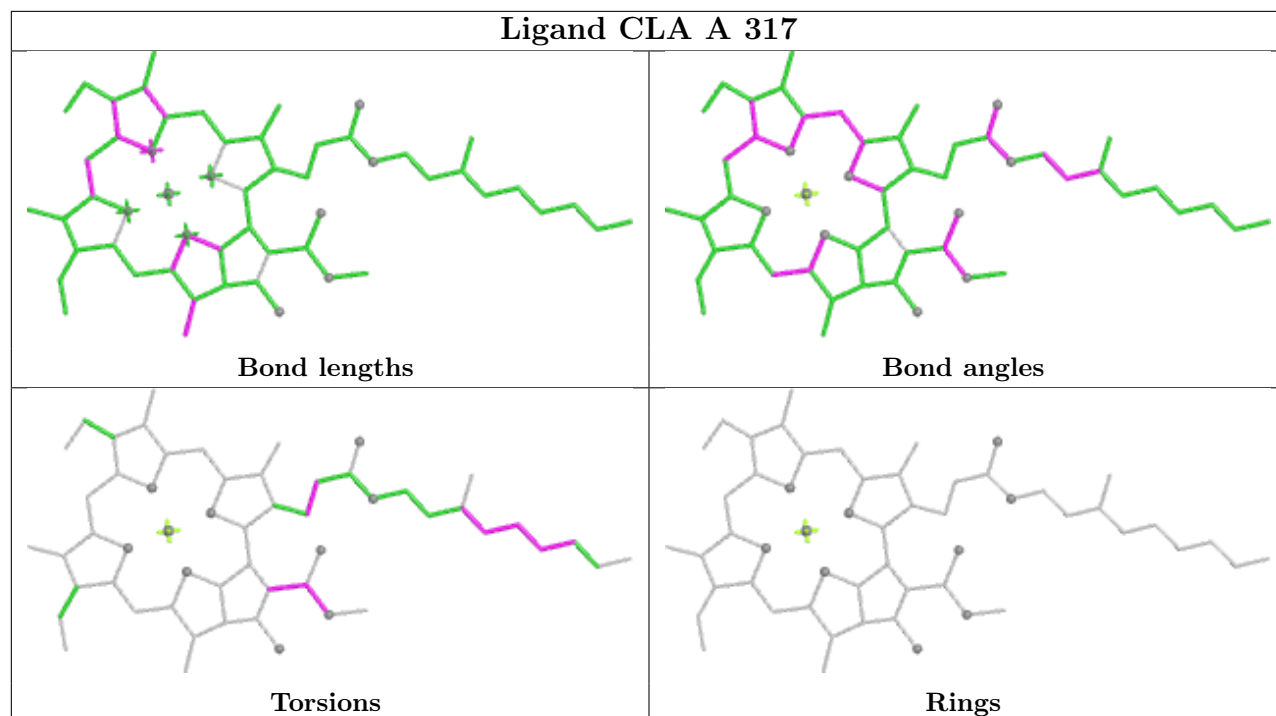


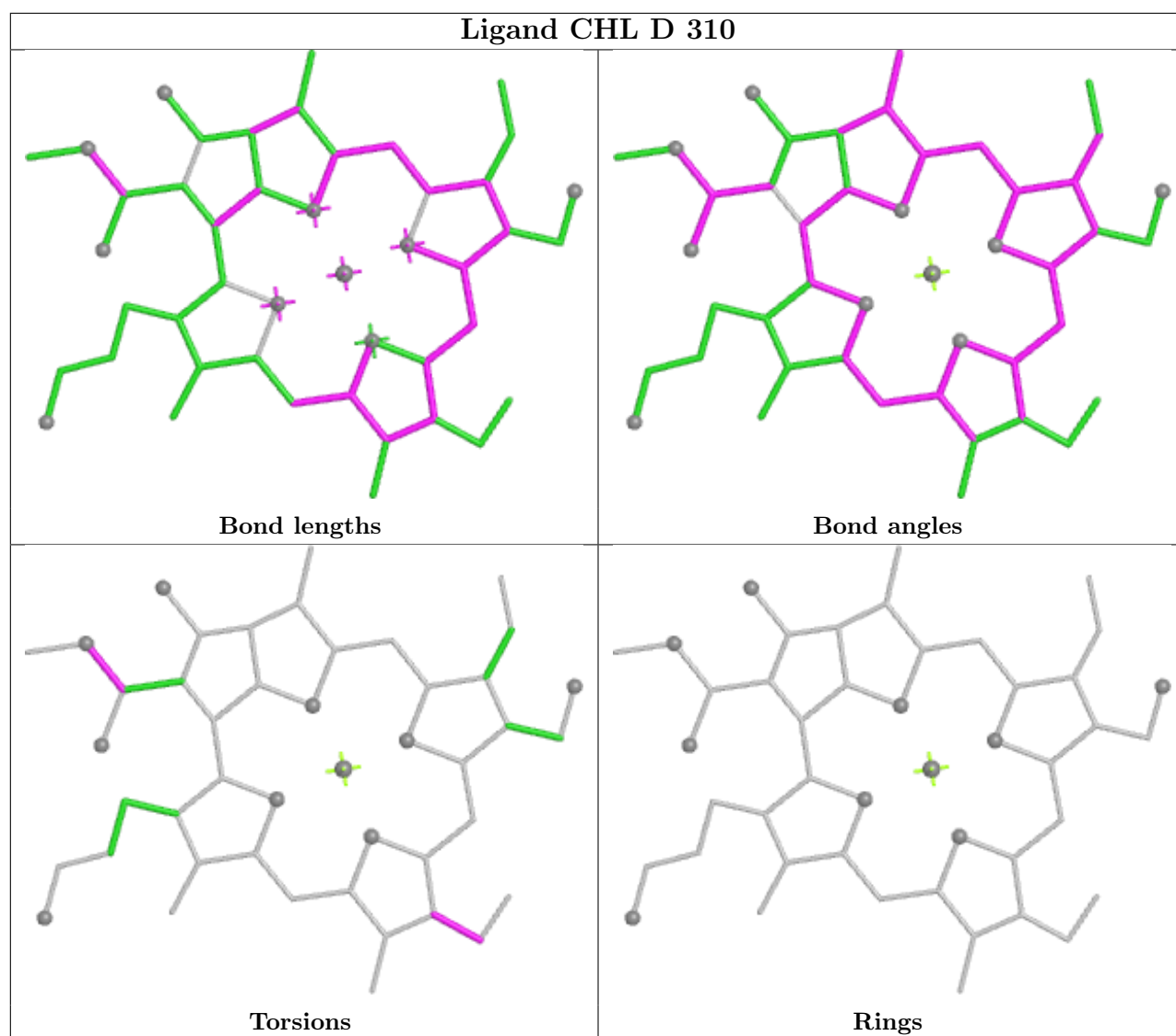
Ligand NEX C 303



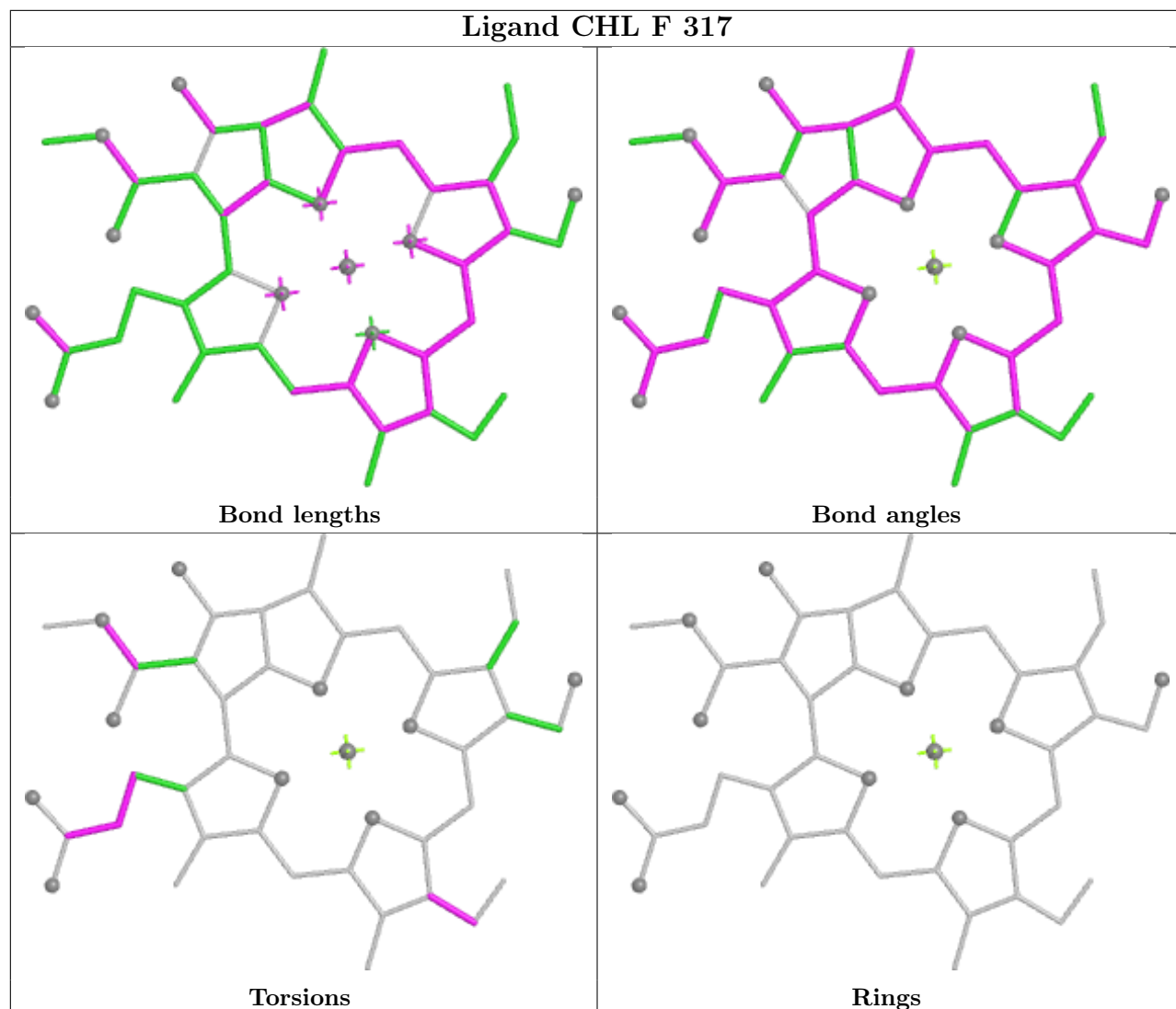
Ligand CHL D 318

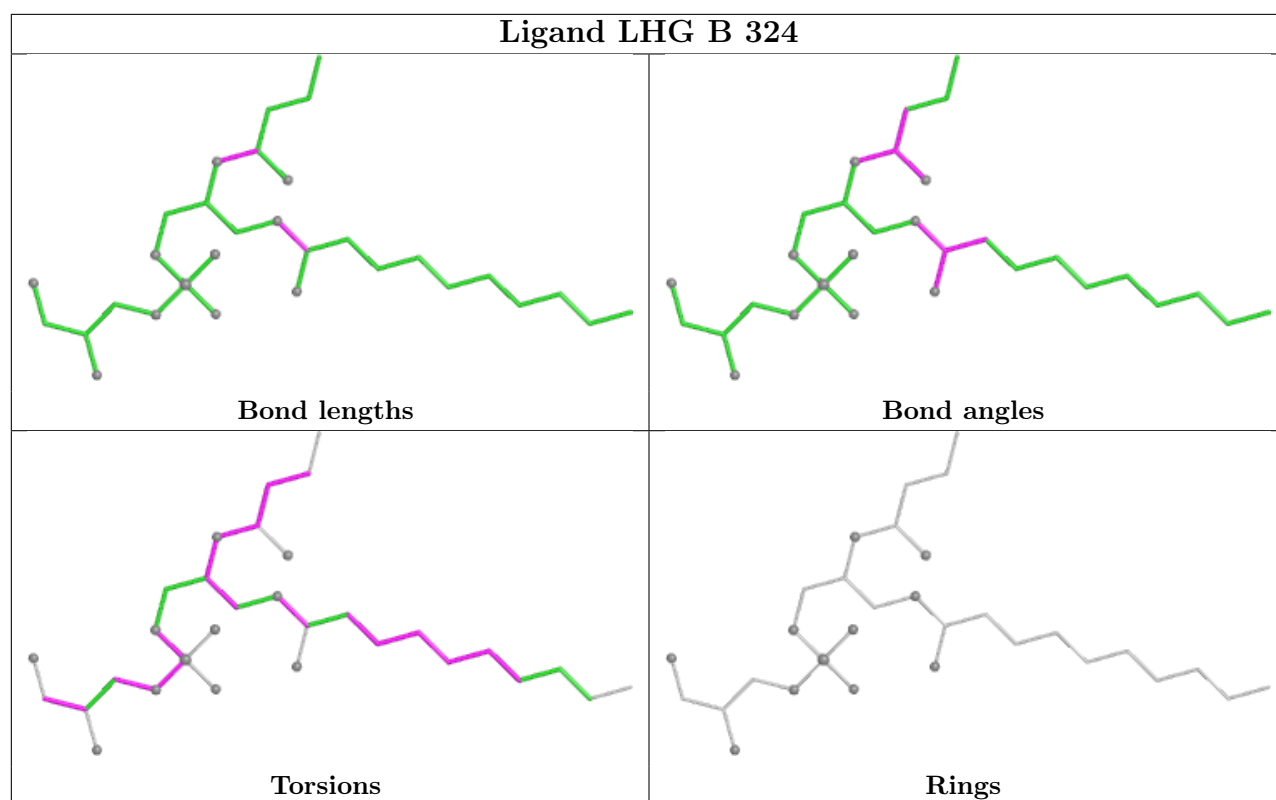




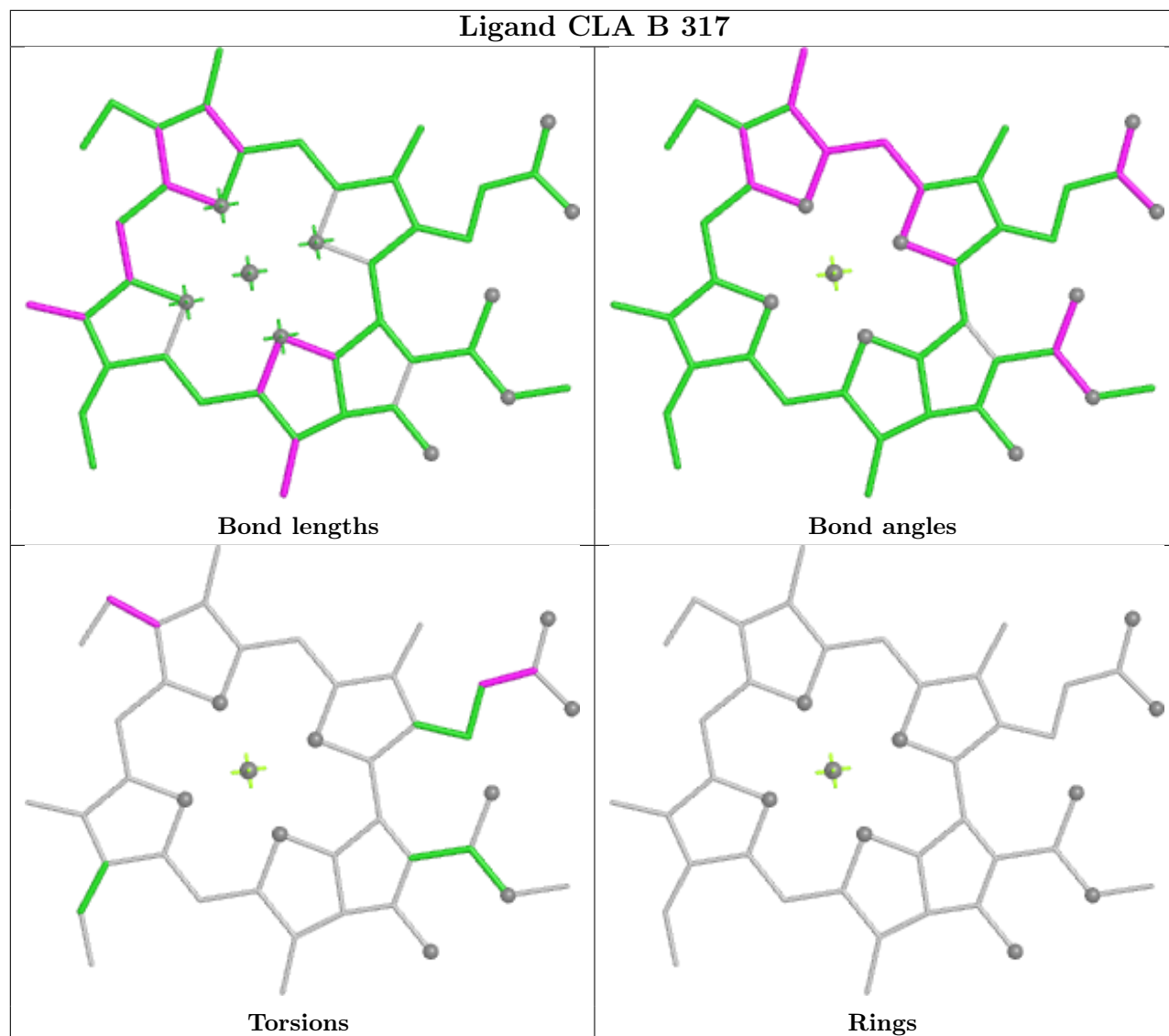


Ligand CHL F 317

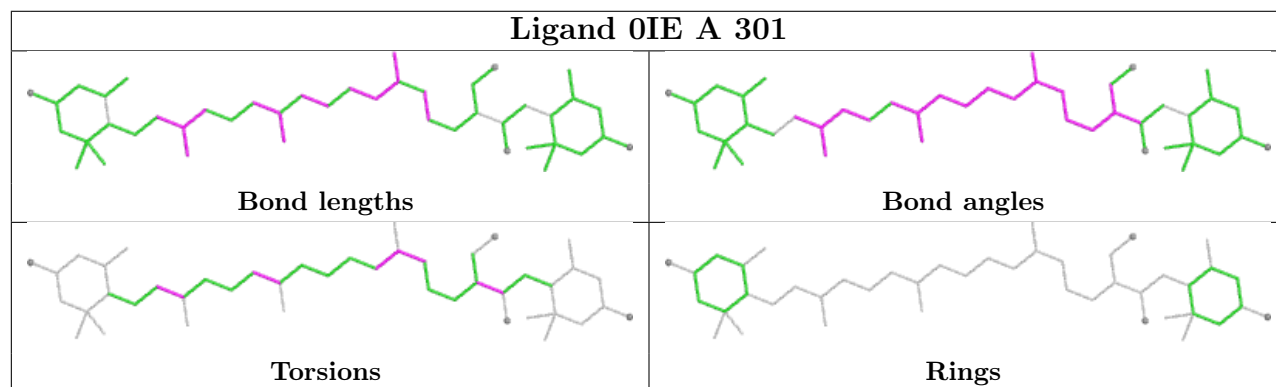




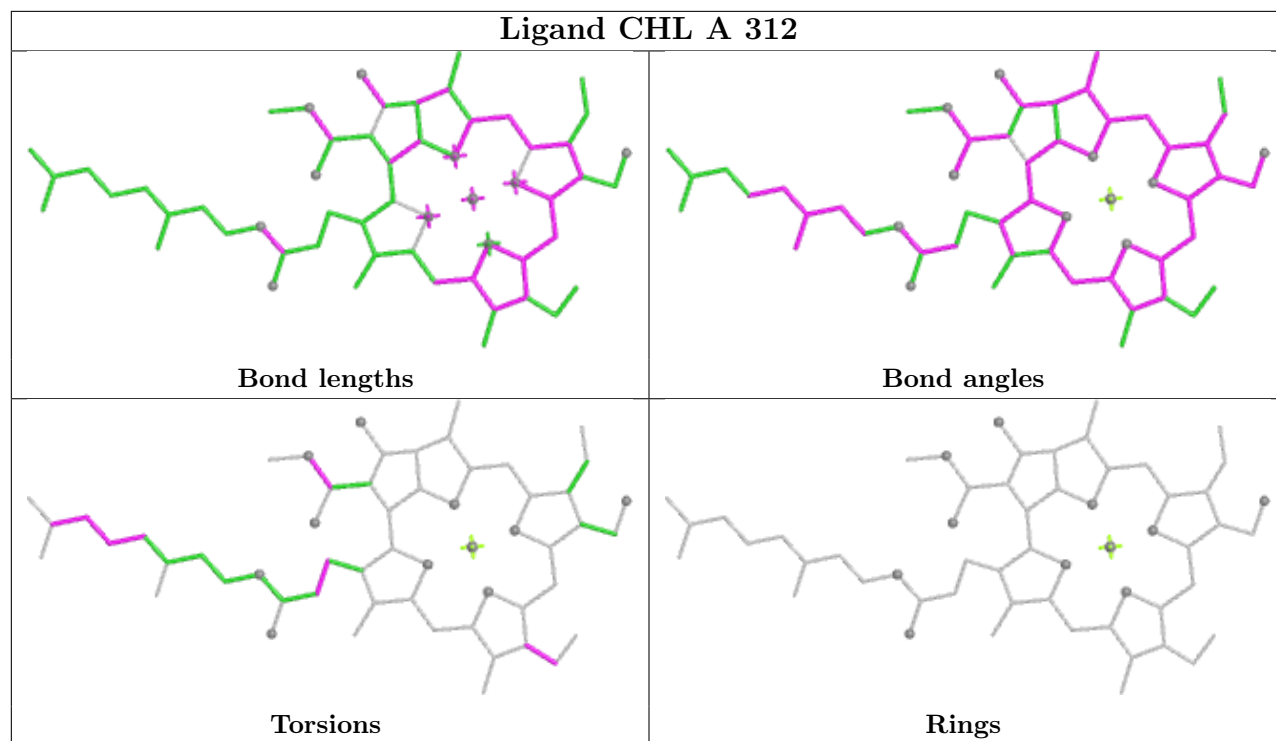
Ligand CLA B 317



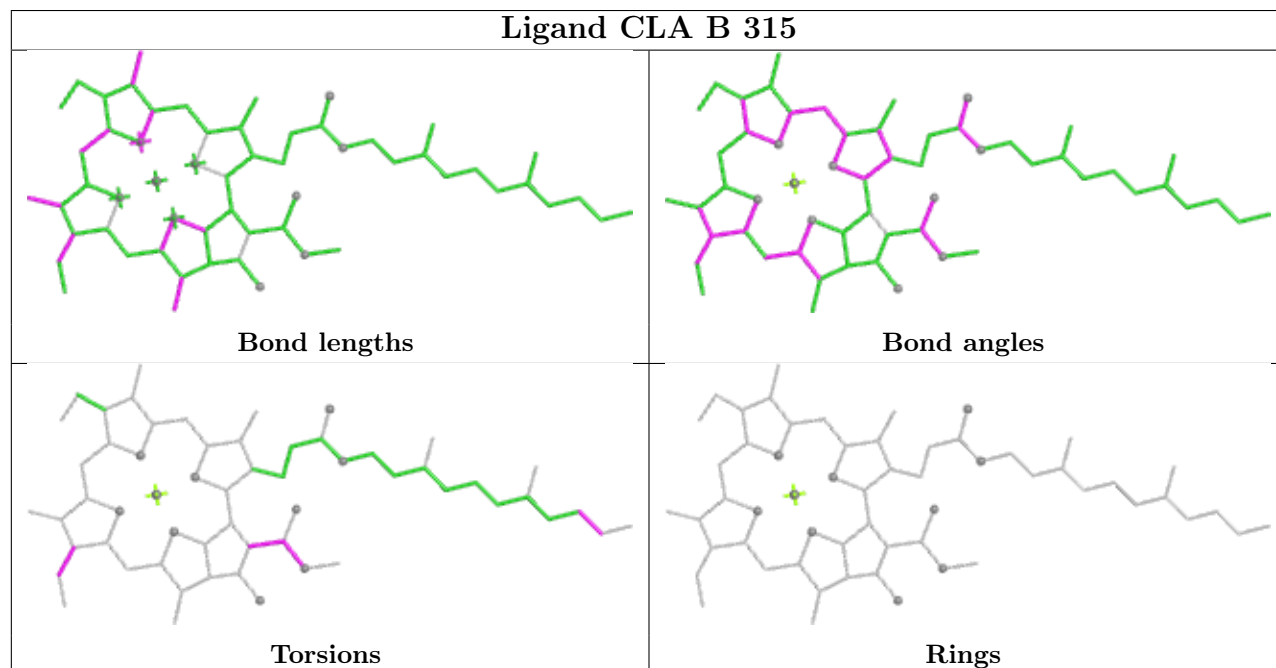
Ligand OIE A 301



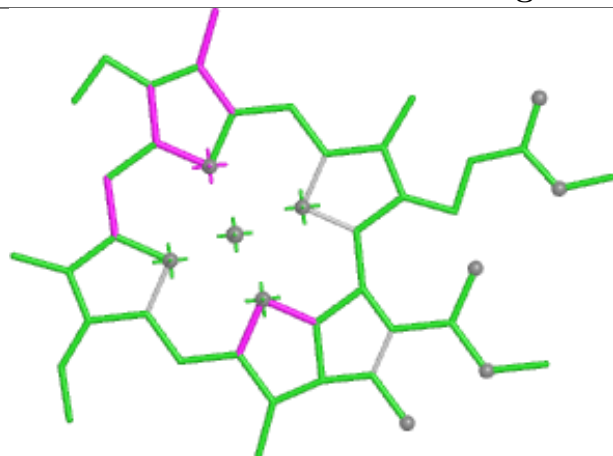
Ligand CHL A 312



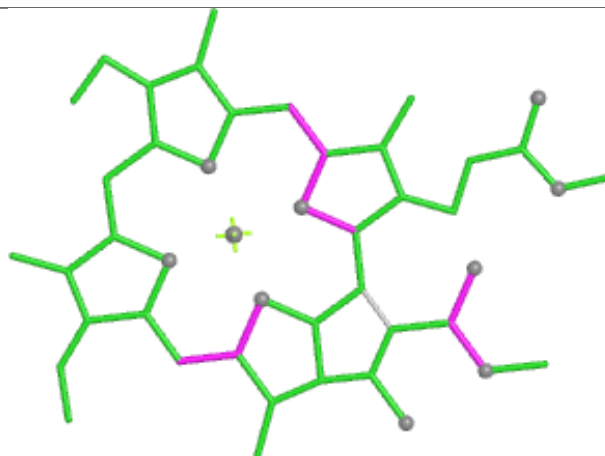
Ligand CLA B 315



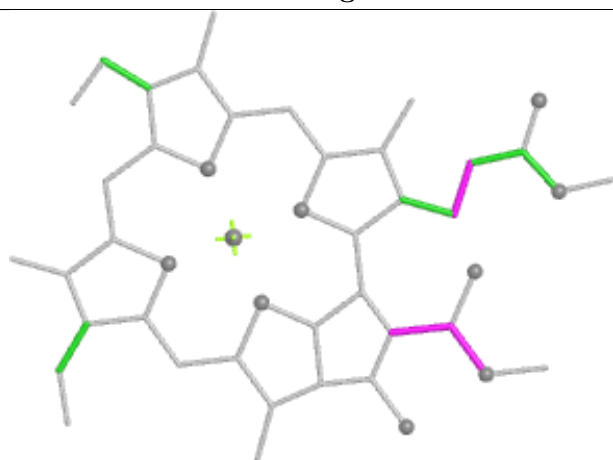
Ligand CLA F 307



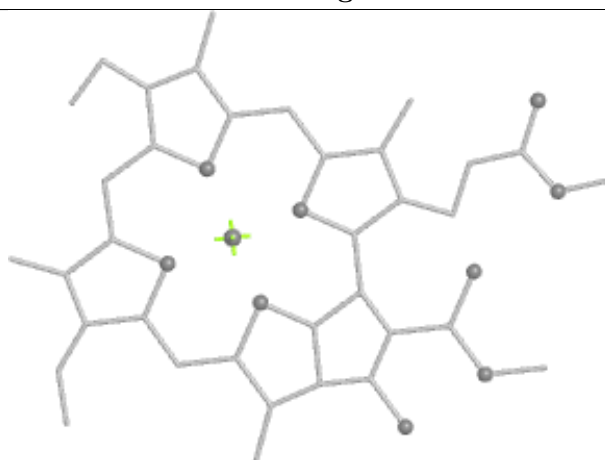
Bond lengths



Bond angles

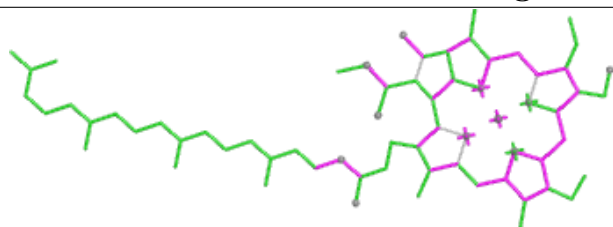


Torsions

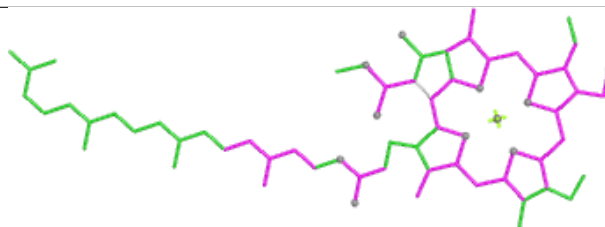


Rings

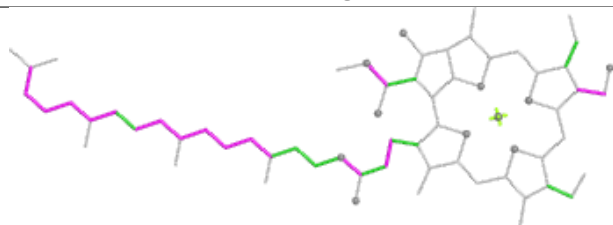
Ligand CHL C 305



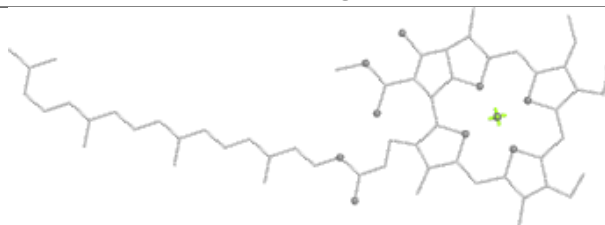
Bond lengths



Bond angles

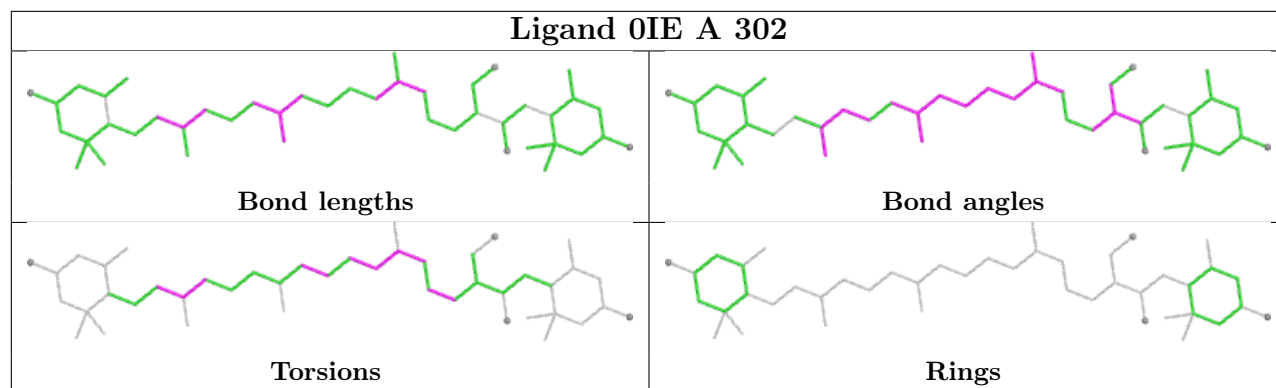


Torsions

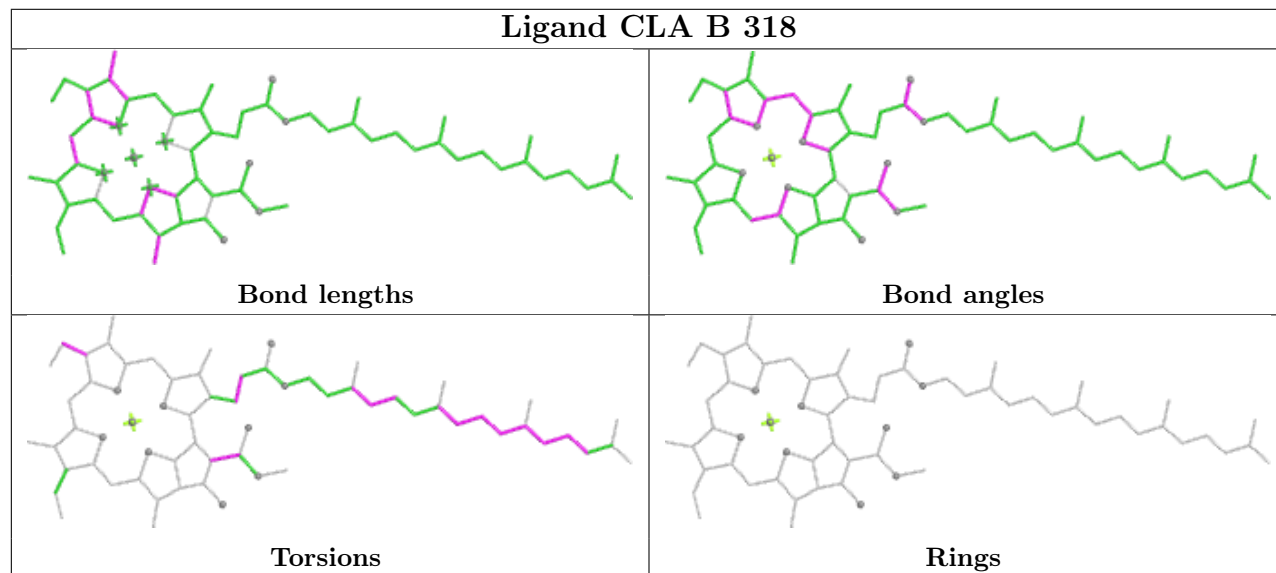


Rings

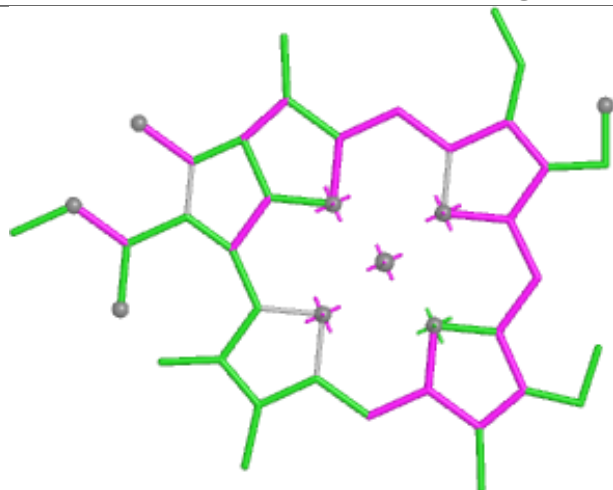
Ligand 0IE A 302



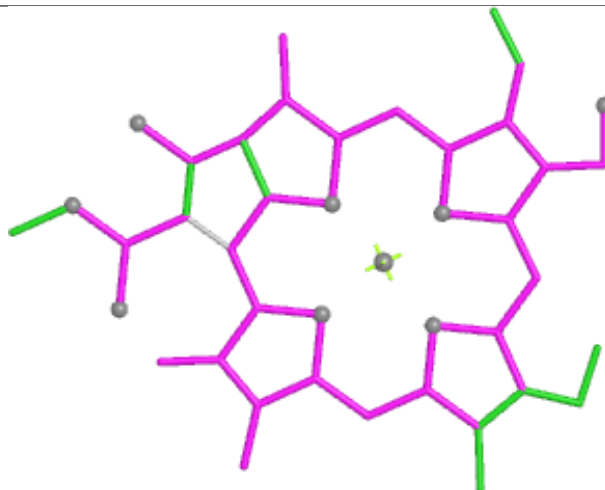
Ligand CLA B 318



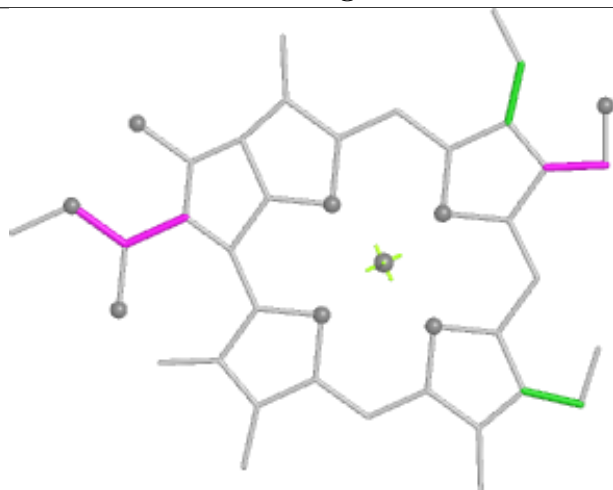
Ligand CHL F 309



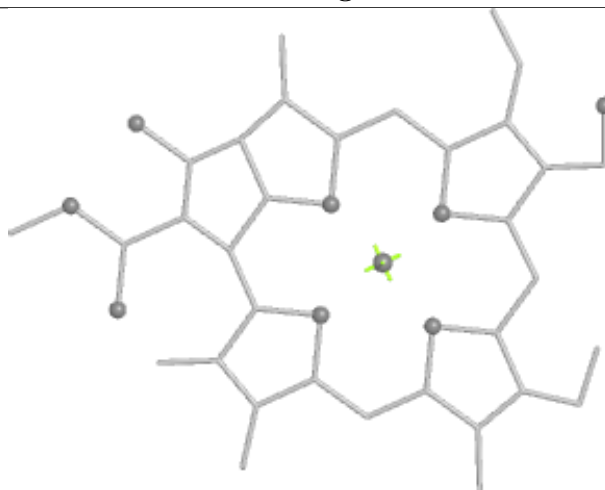
Bond lengths



Bond angles

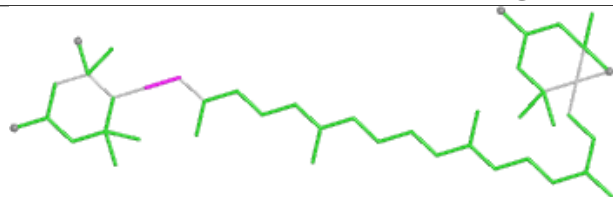


Torsions

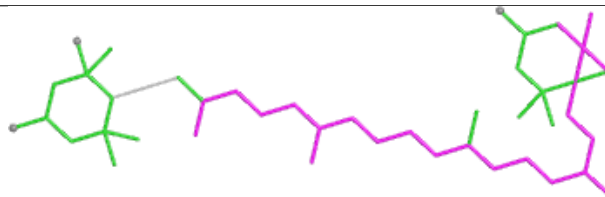


Rings

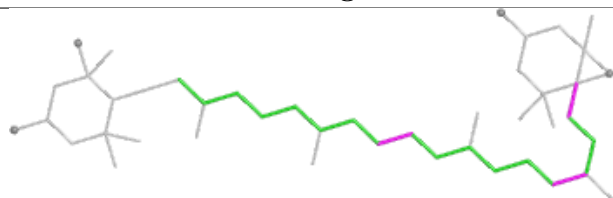
Ligand NEX E 303



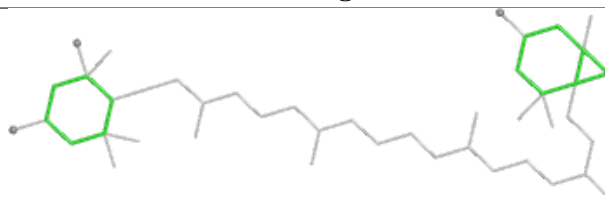
Bond lengths



Bond angles

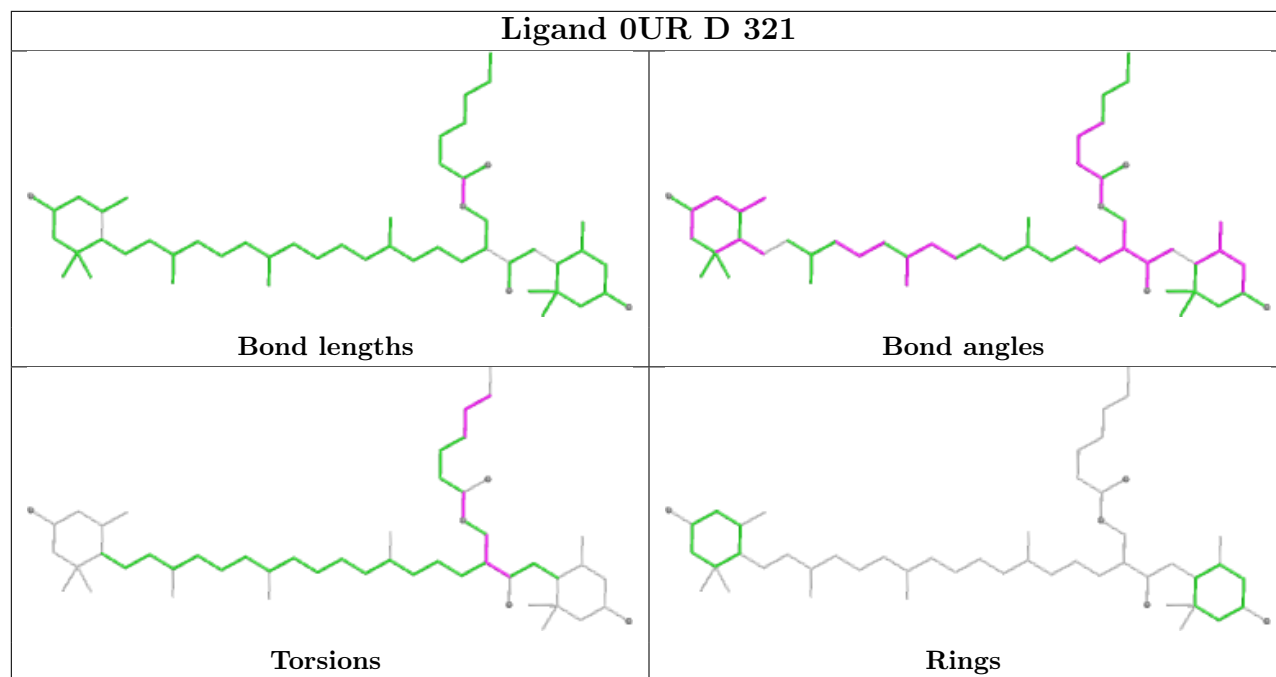


Torsions

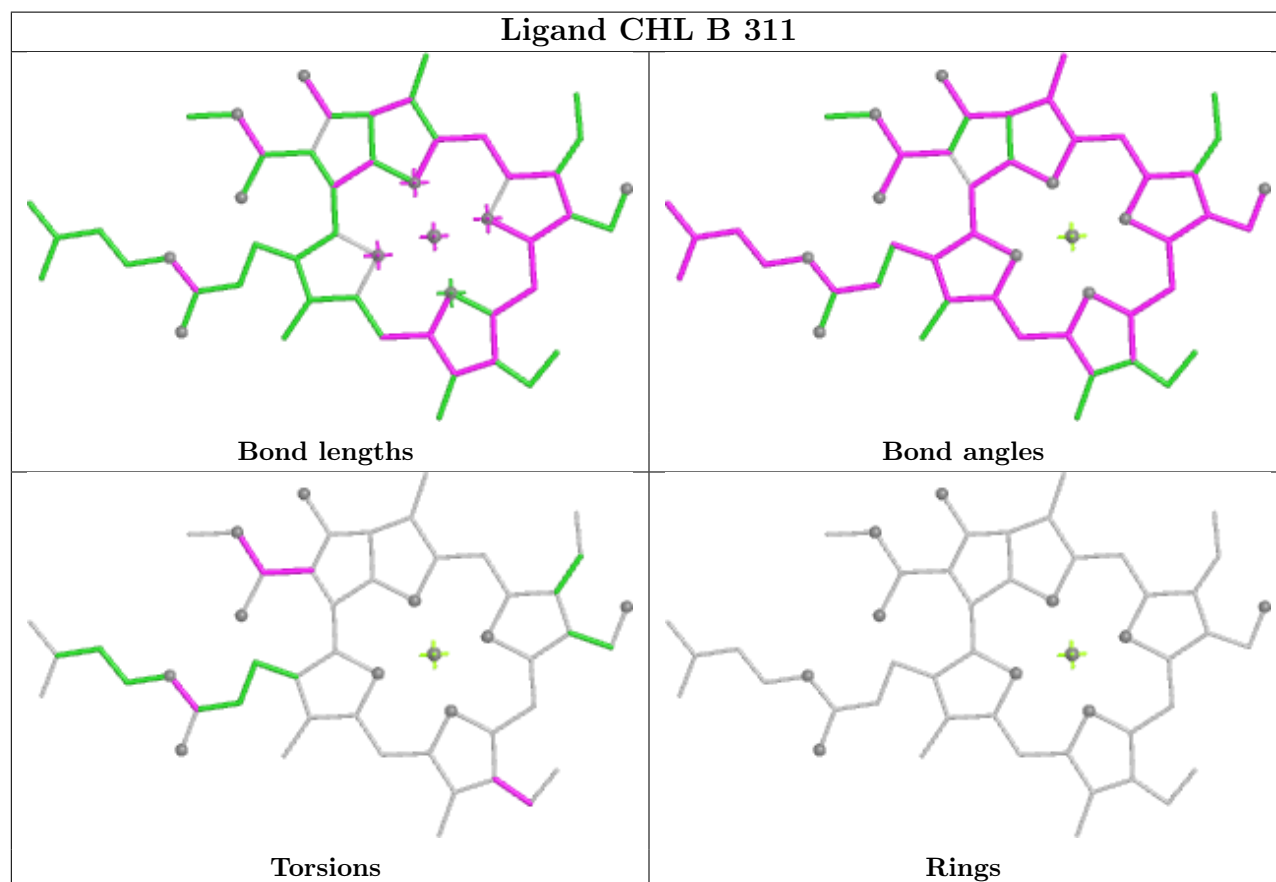


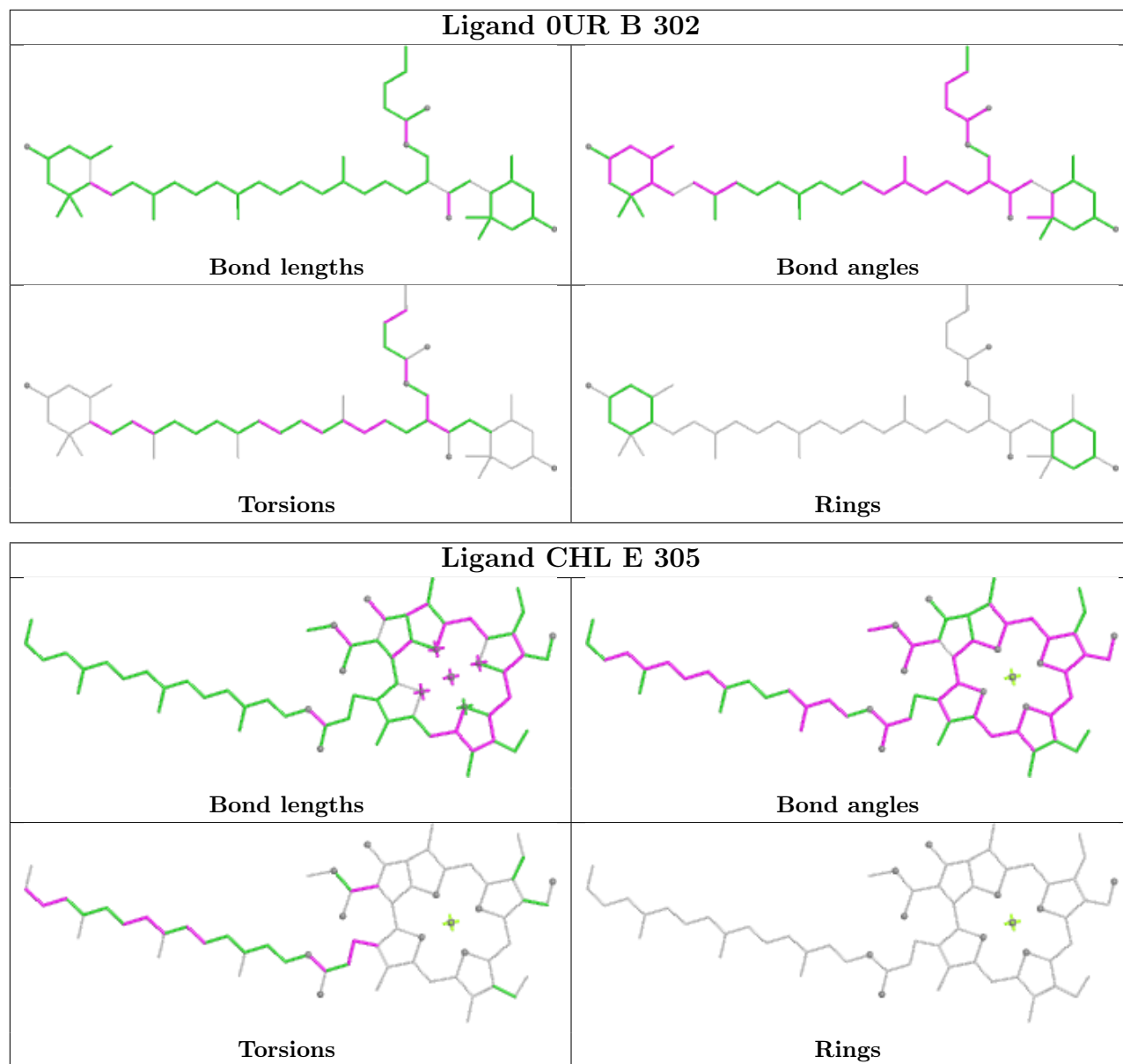
Rings

Ligand OUR D 321

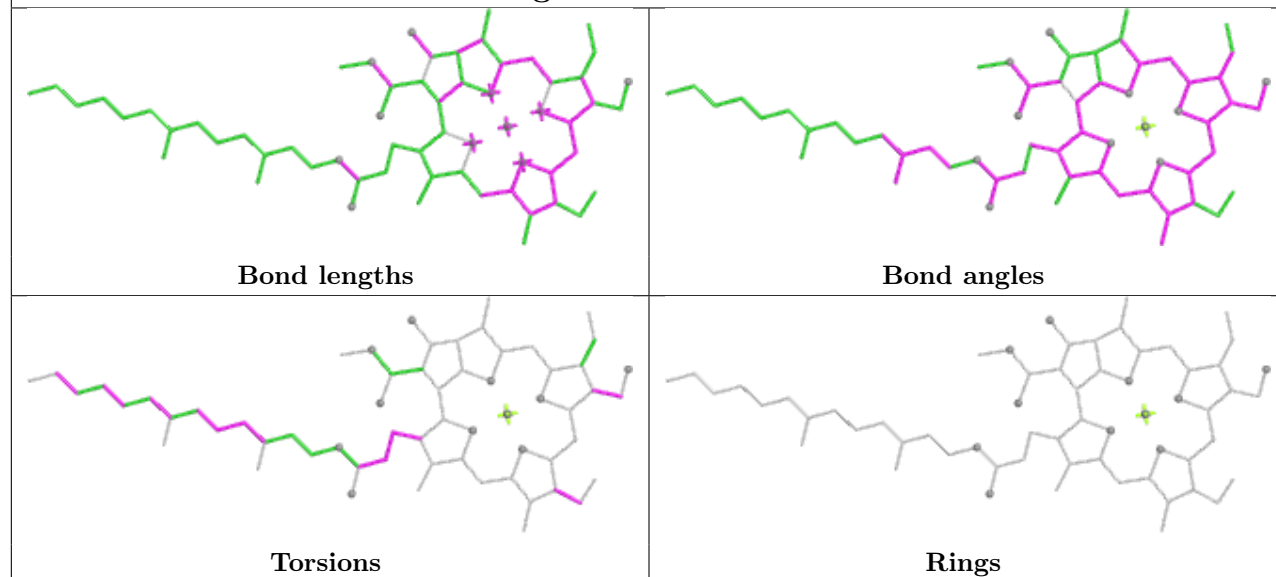


Ligand CHL B 311

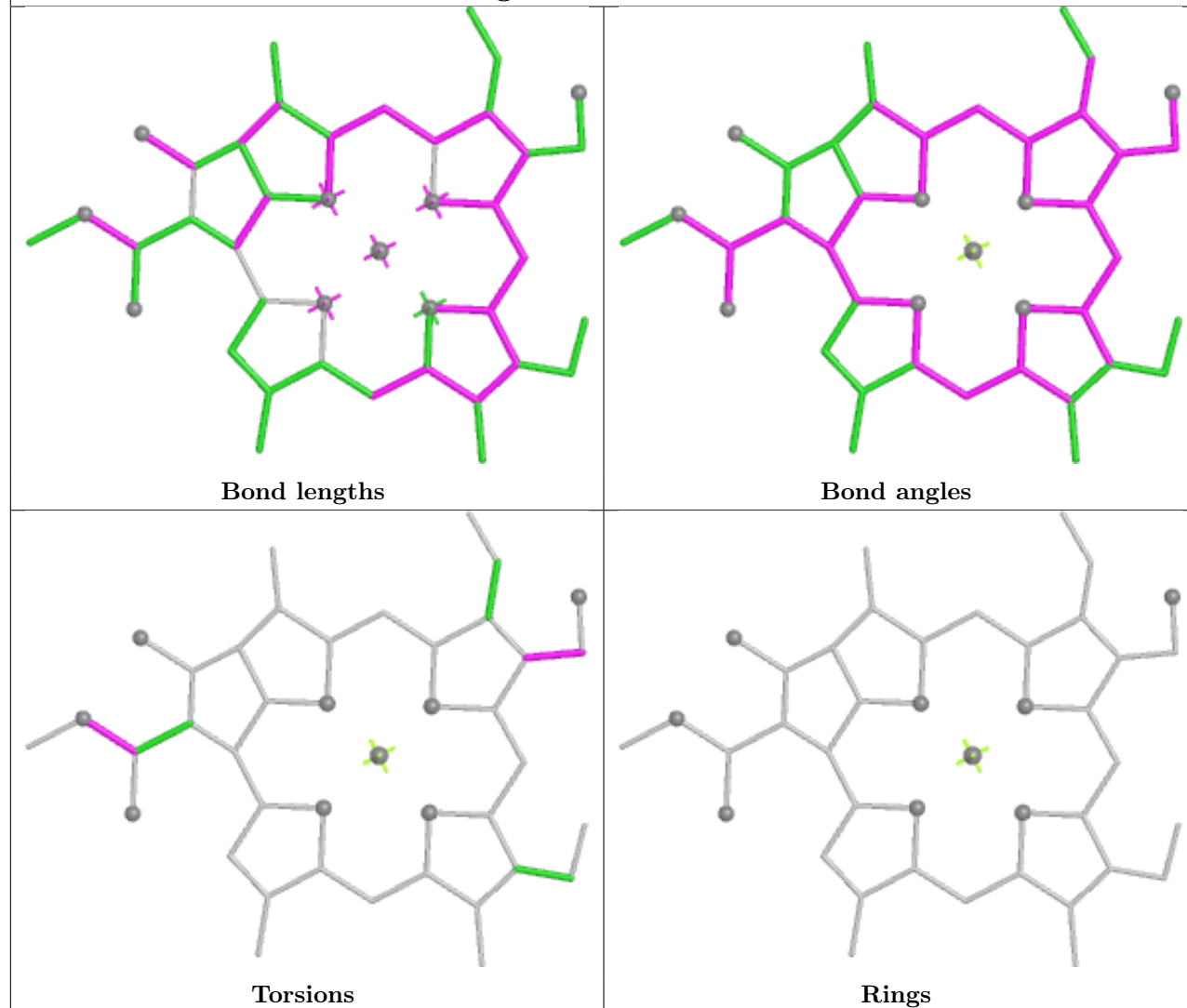


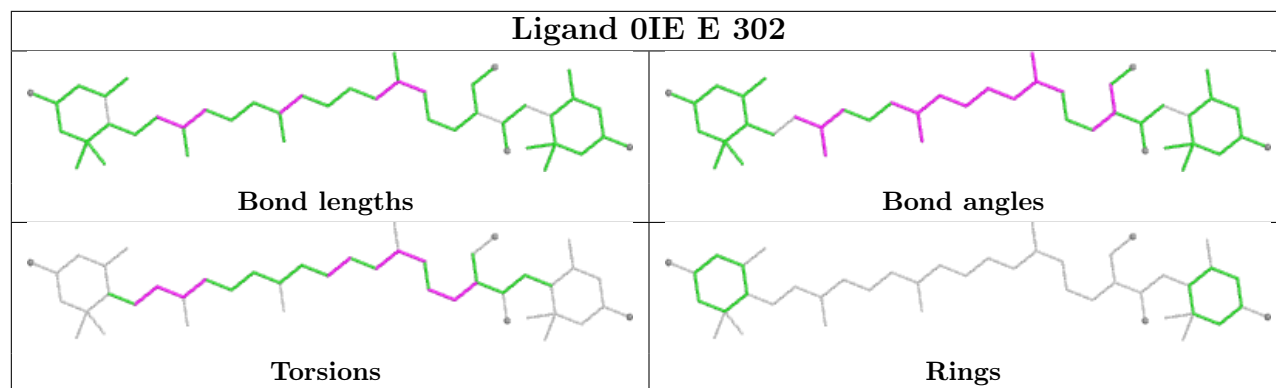
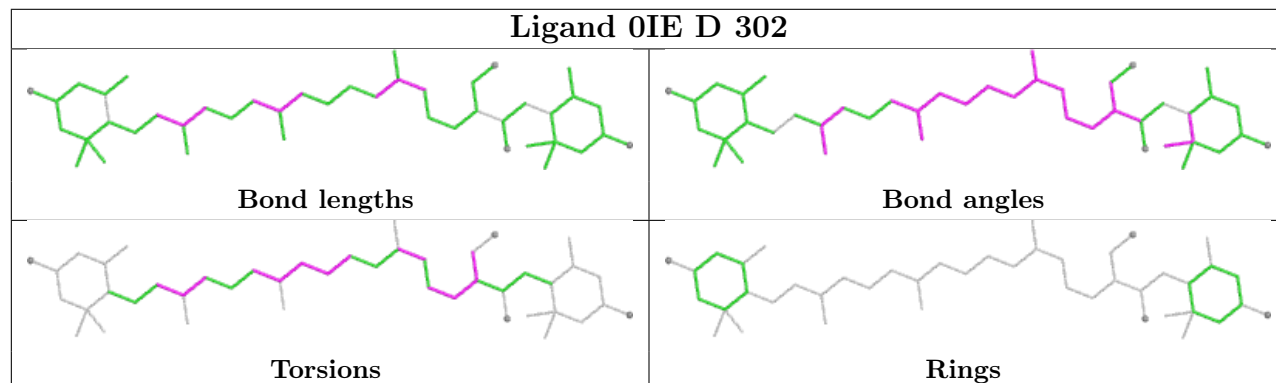
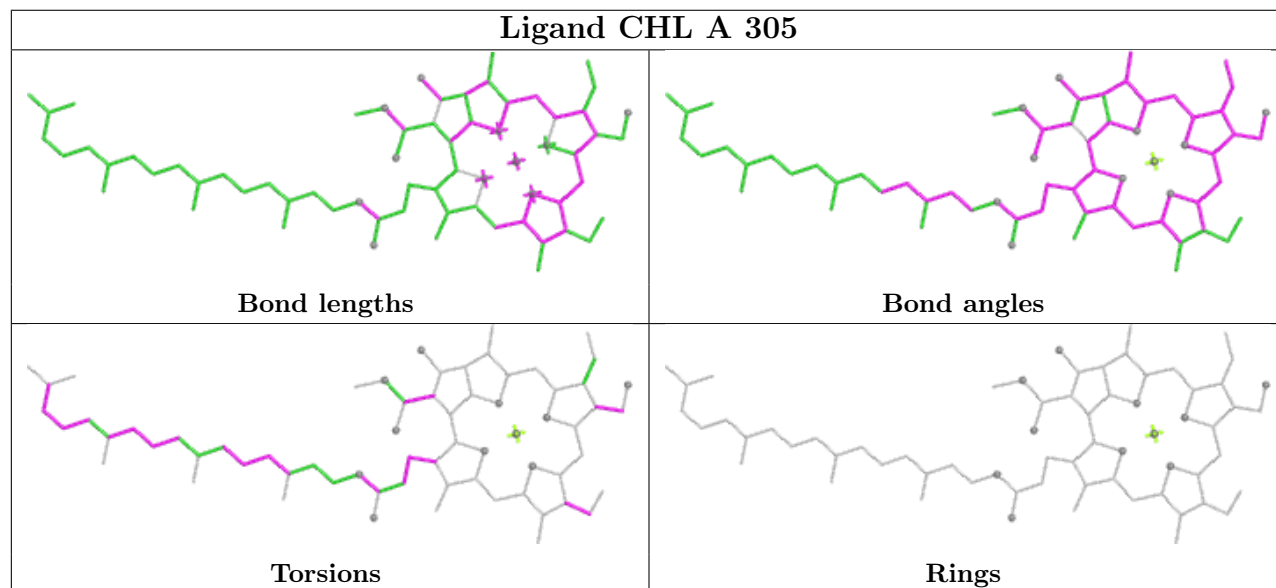


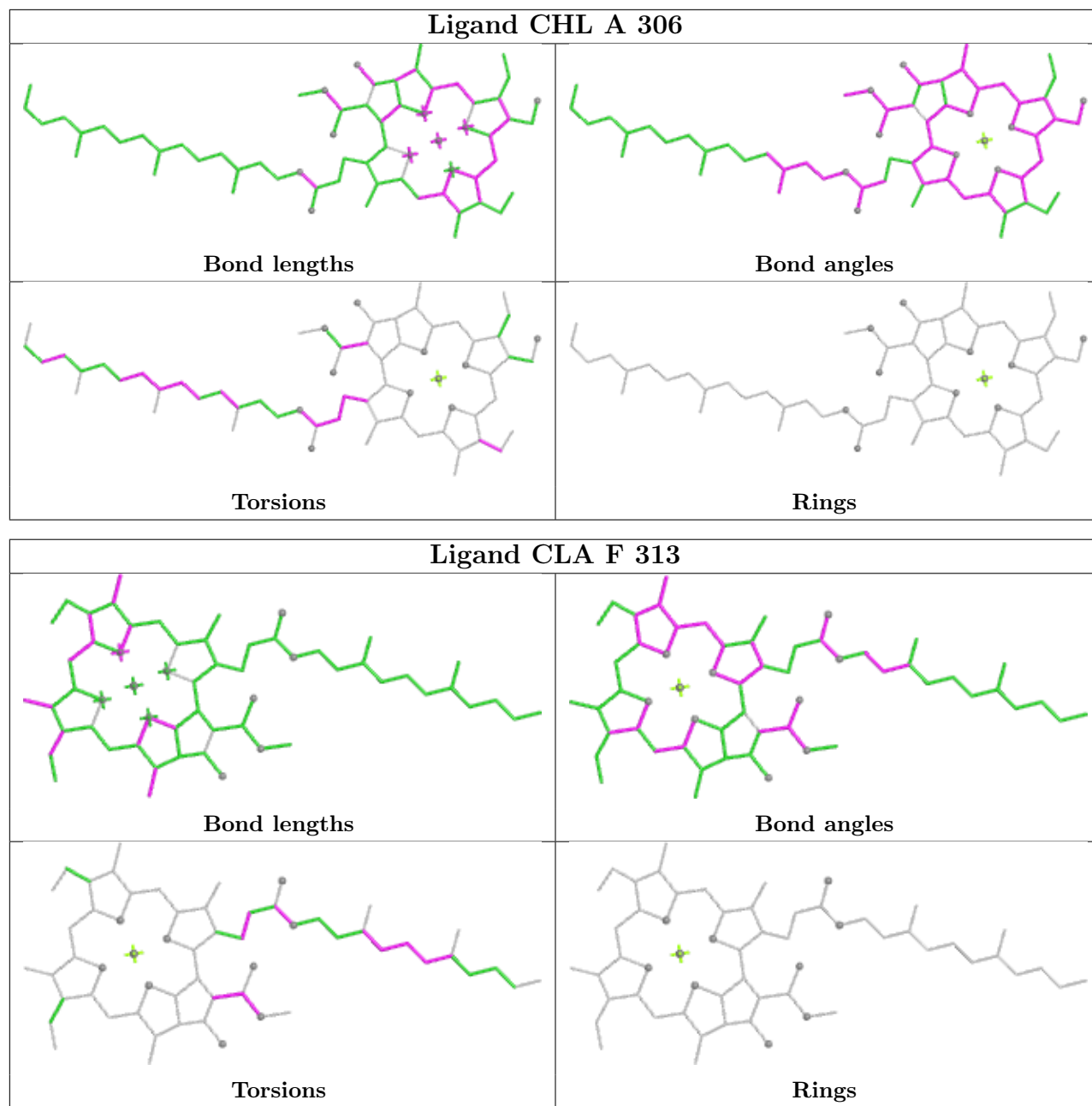
Ligand CHL E 310



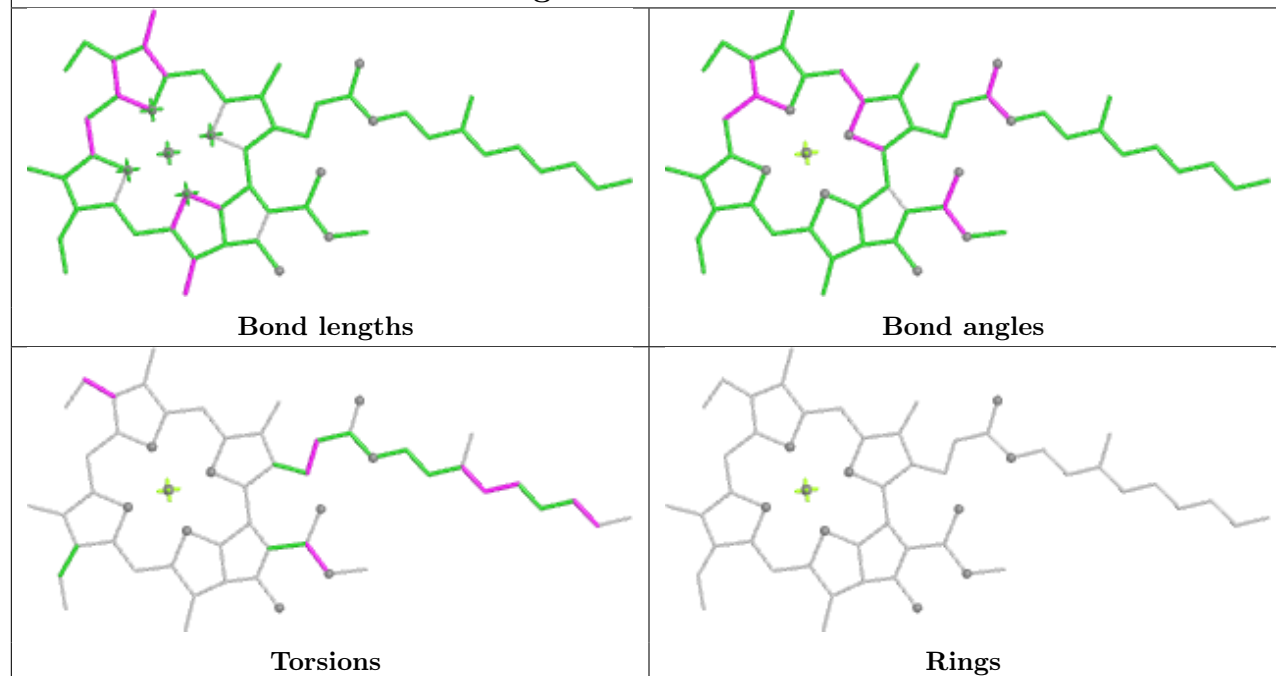
Ligand CHL E 308



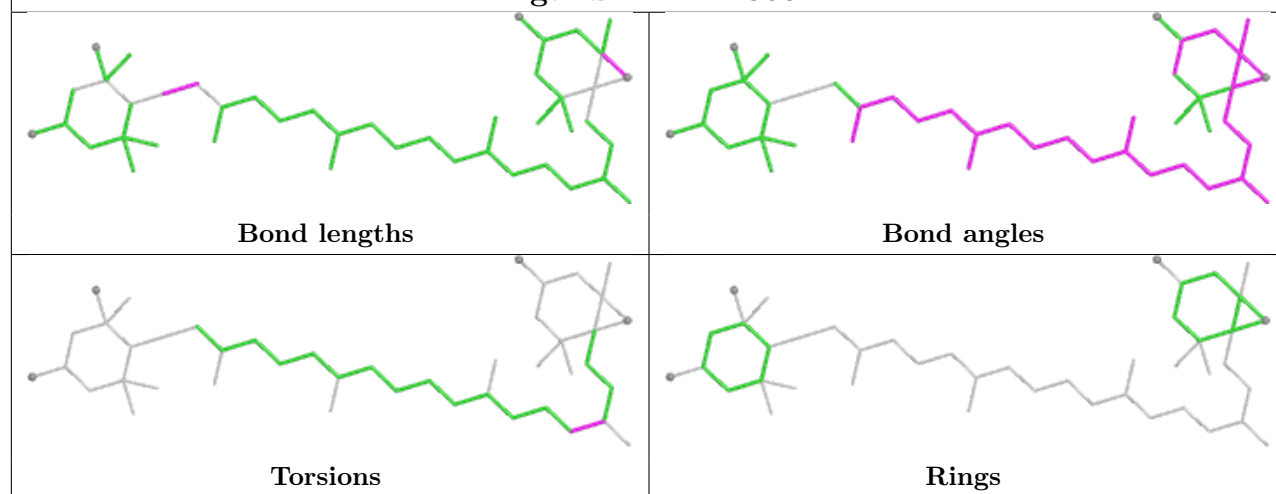
Ligand 01E E 302**Ligand 01E D 302****Ligand CHL A 305**

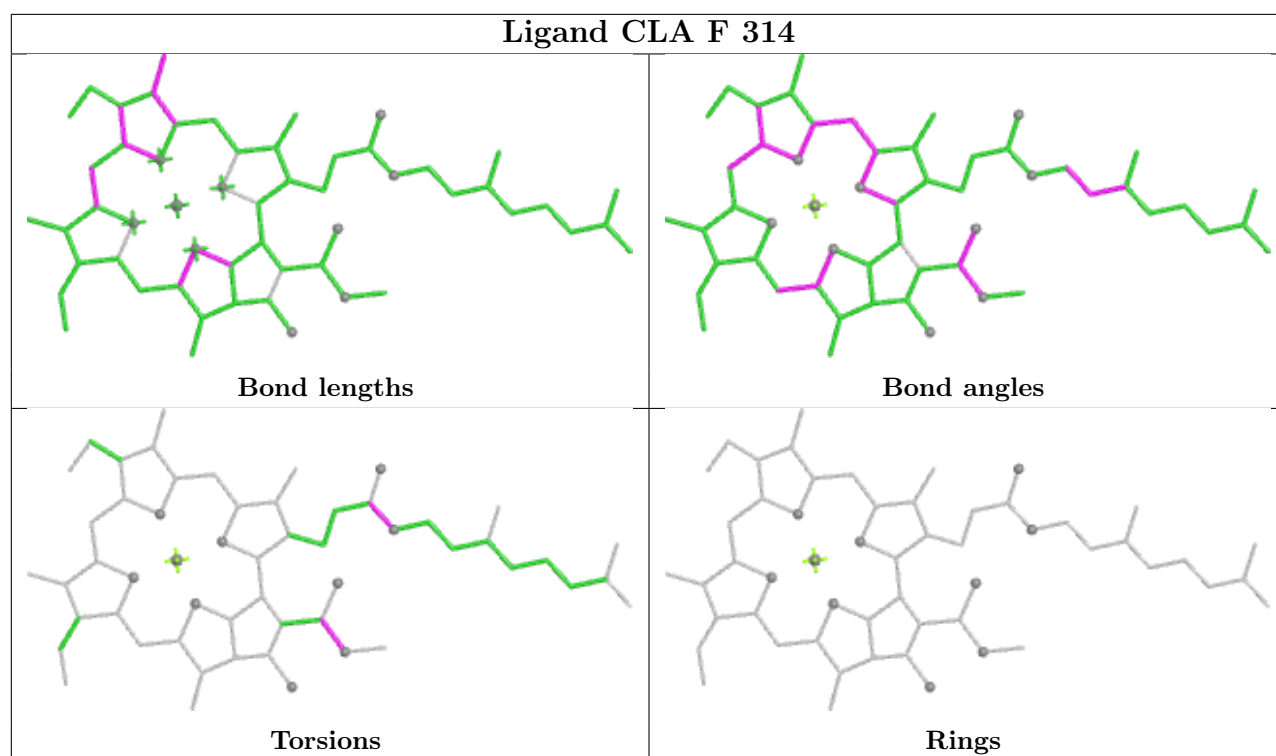


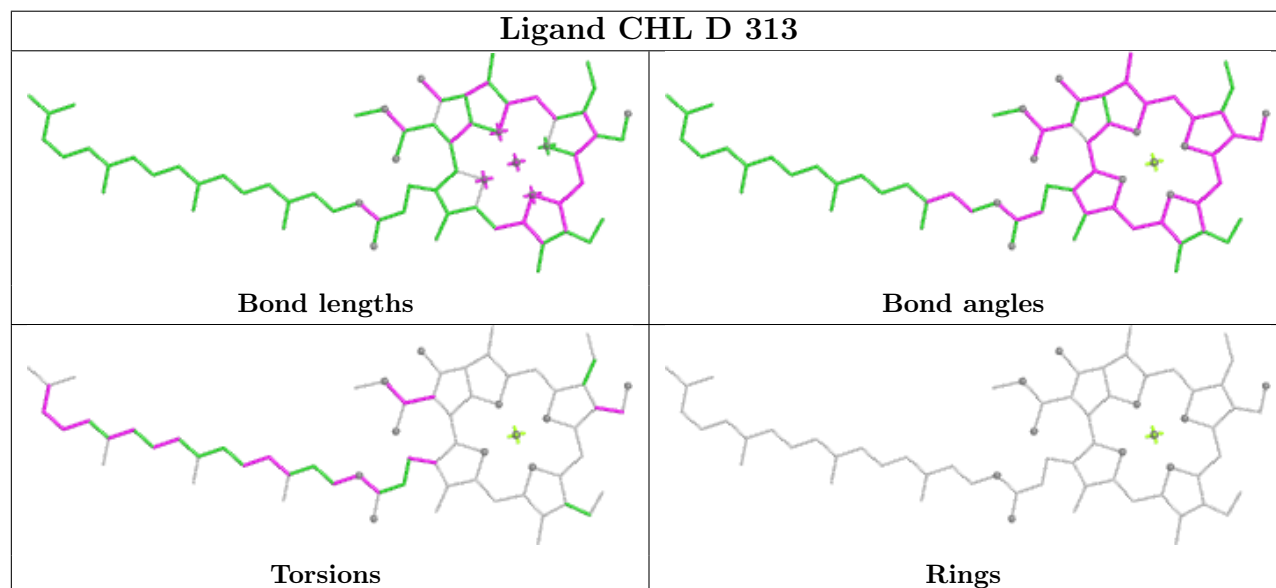
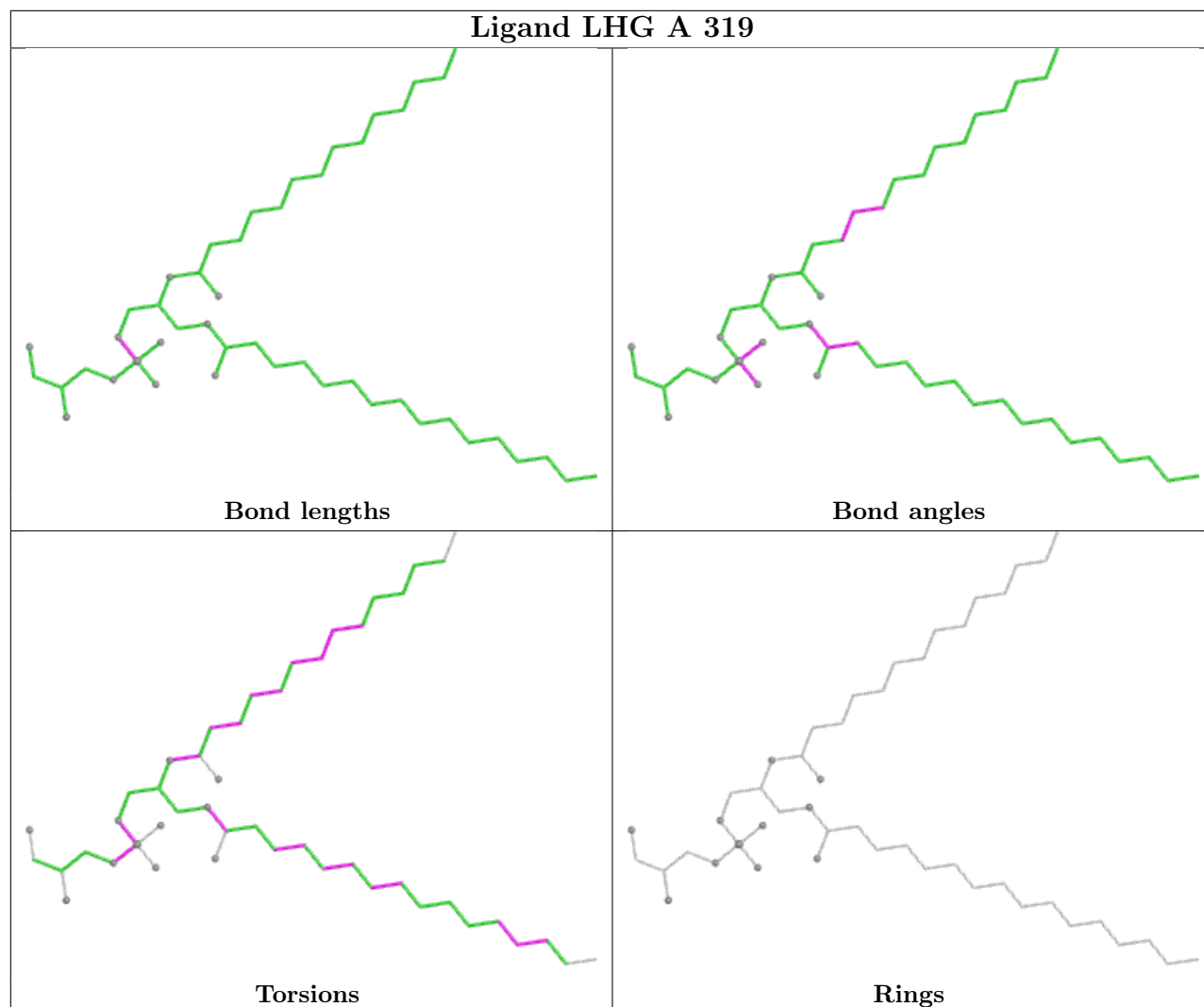
Ligand CLA E 316

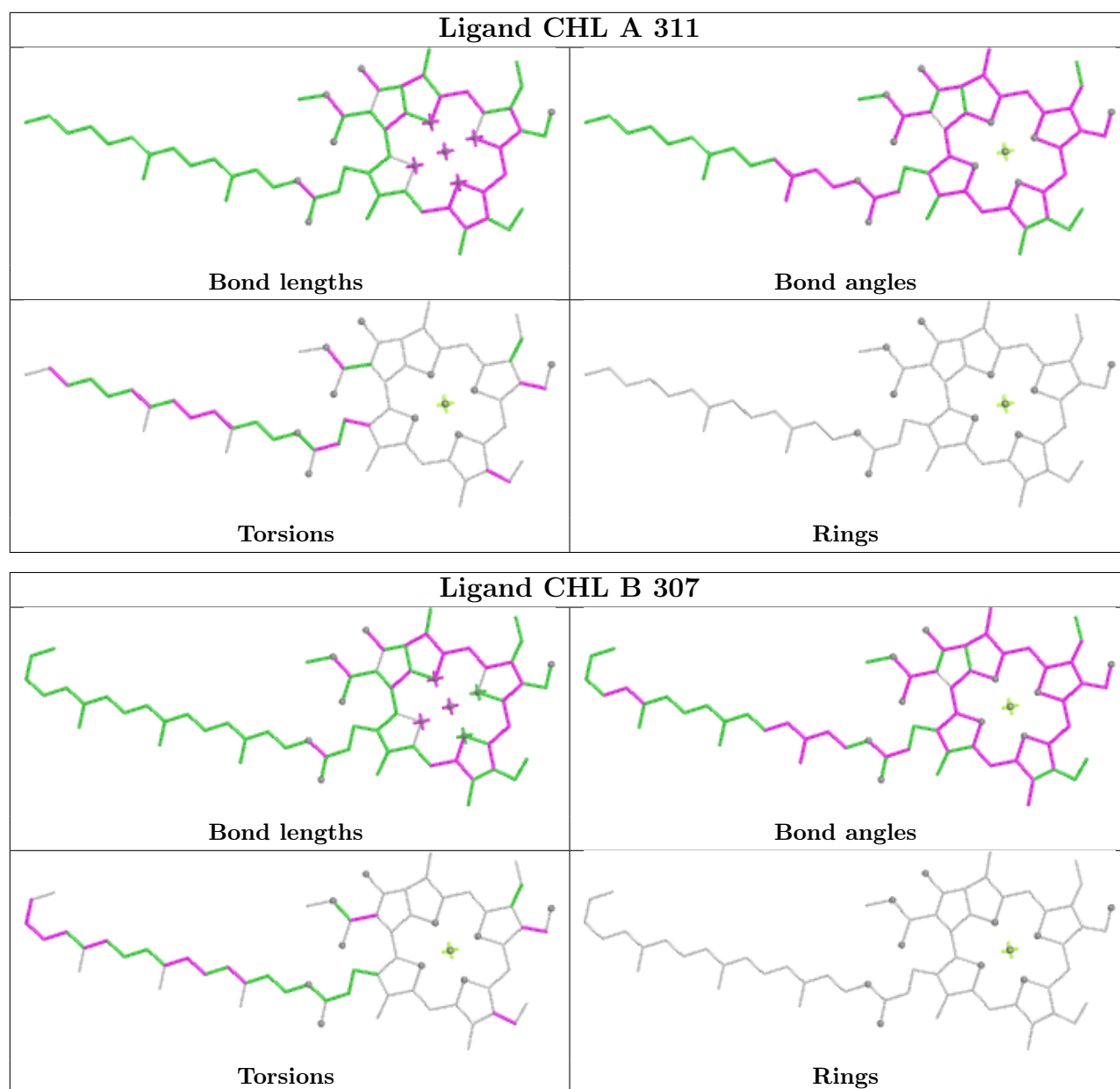


Ligand NEX B 303

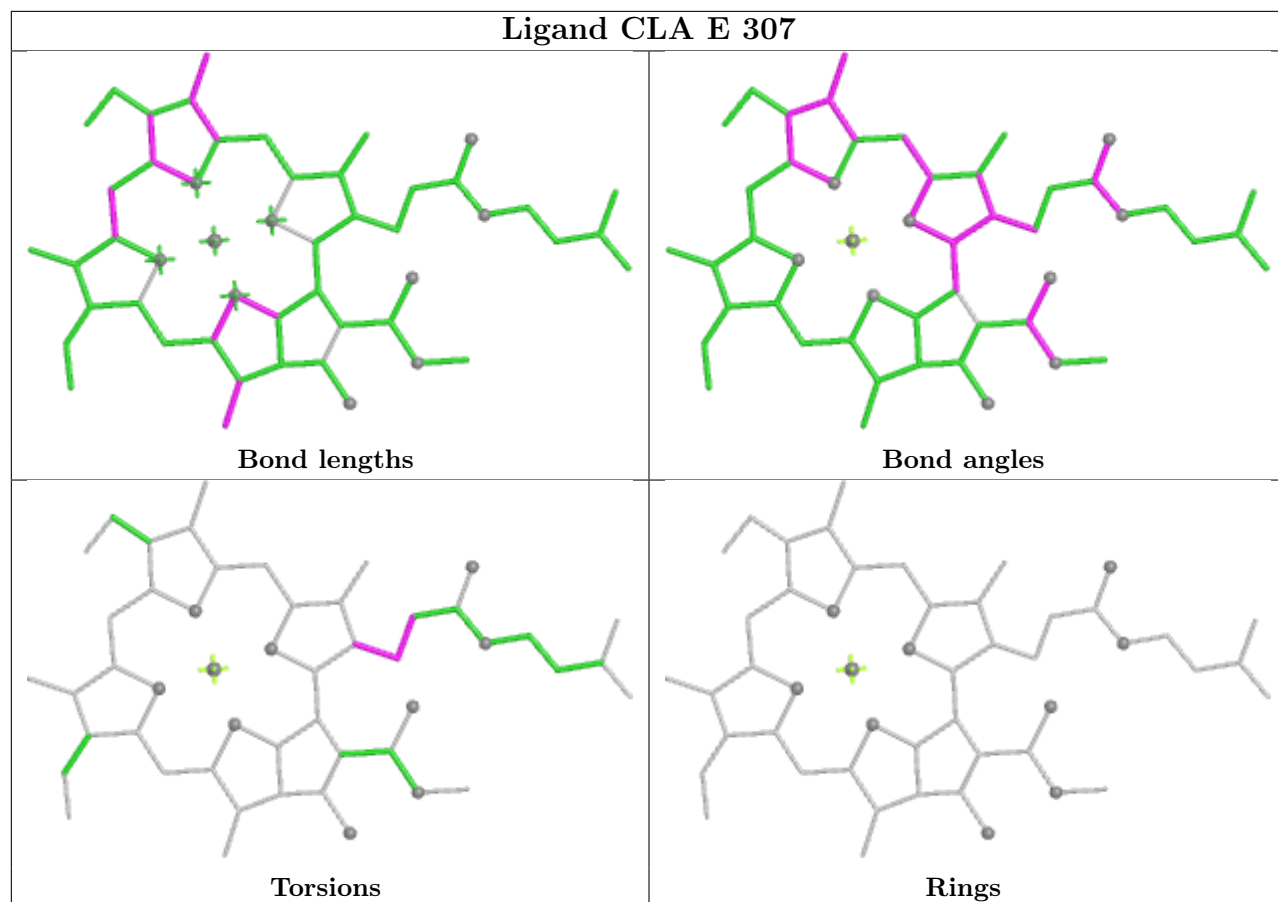




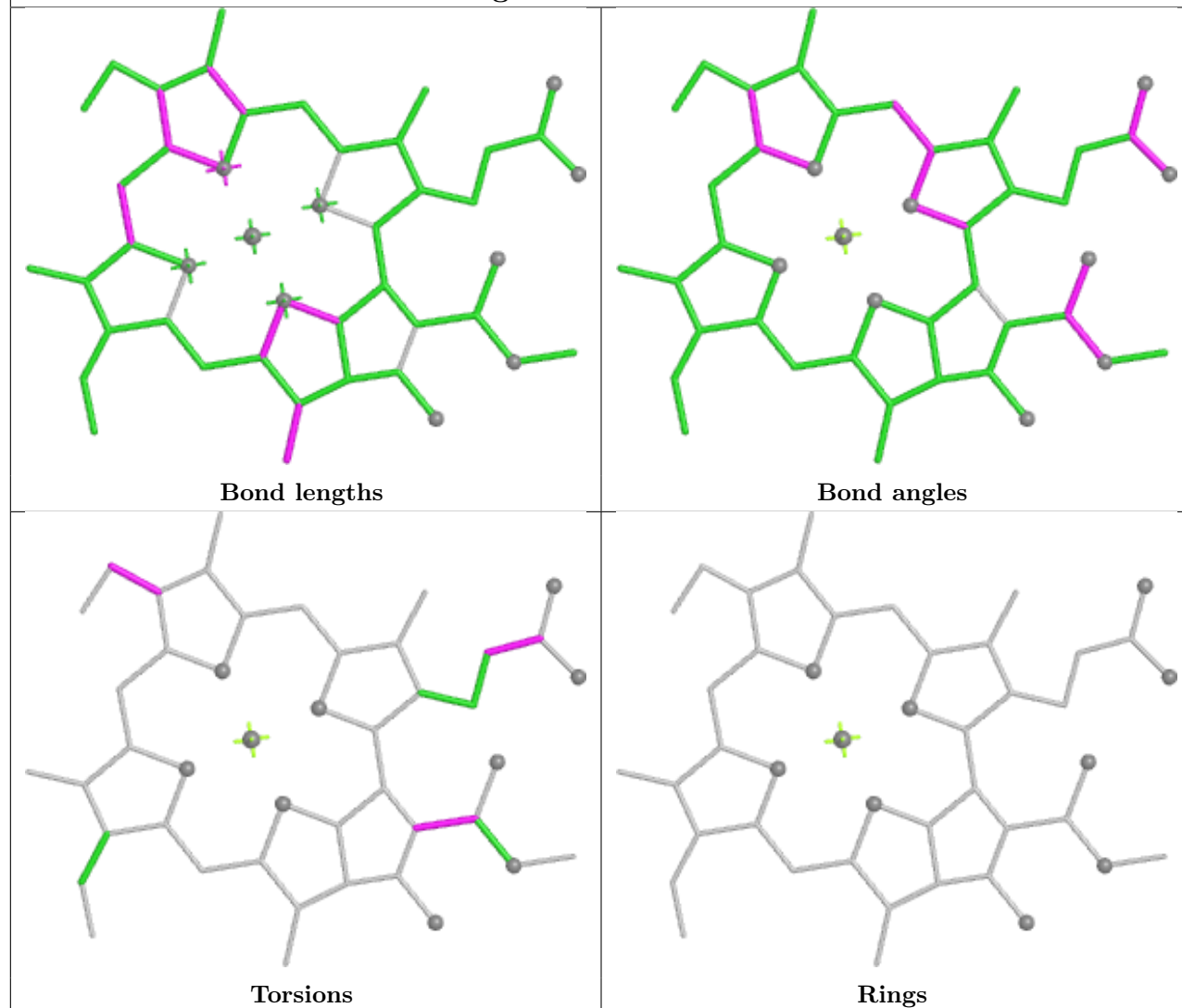




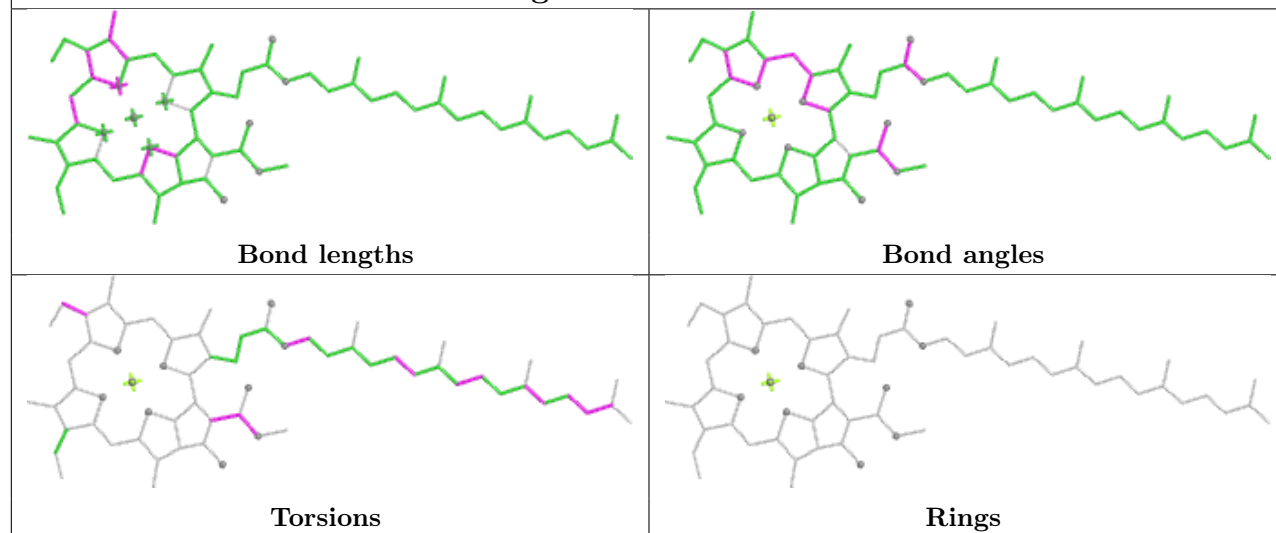
Ligand CLA E 307

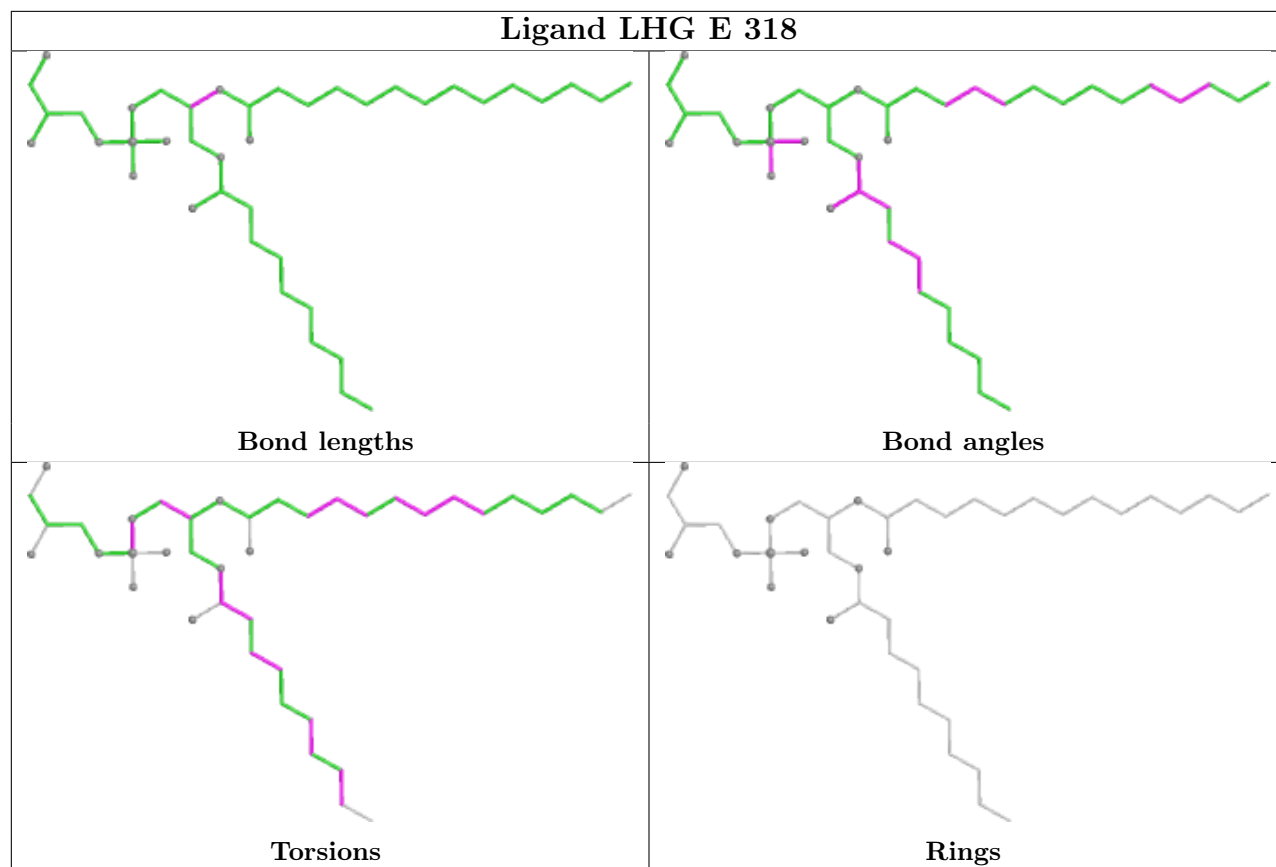


Ligand CLA A 316

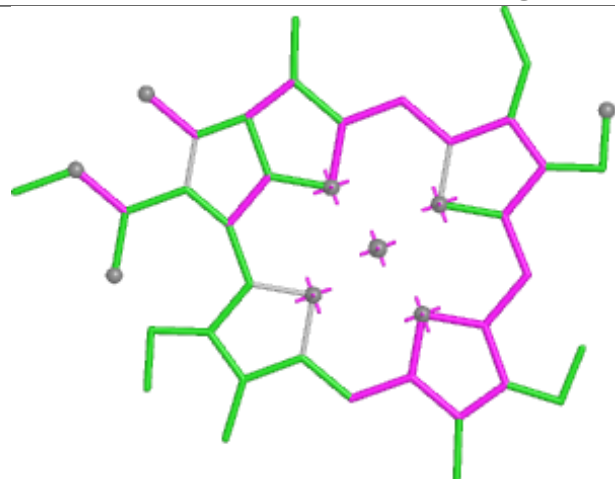


Ligand CLA D 307

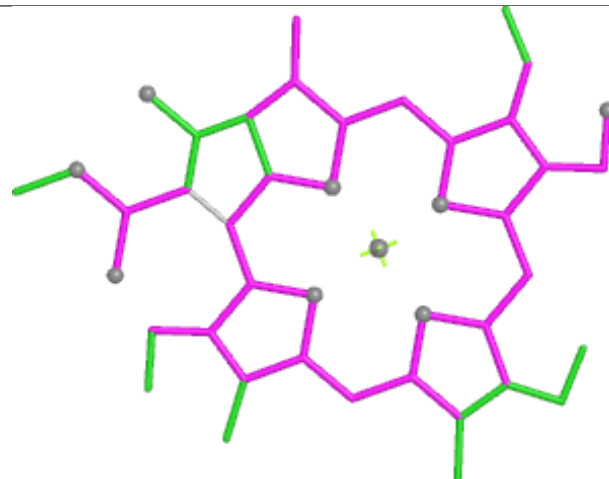




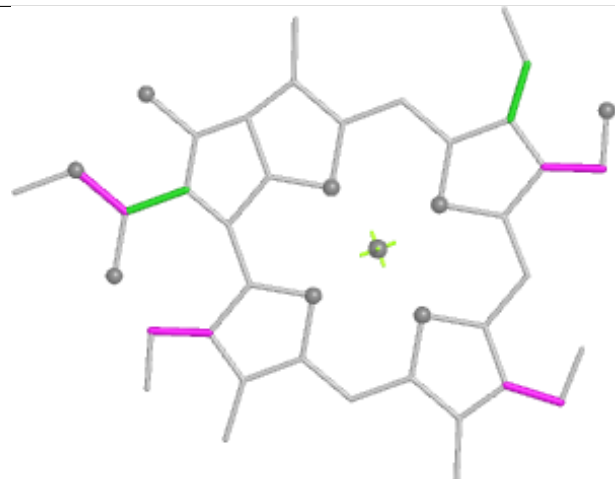
Ligand CHL A 309



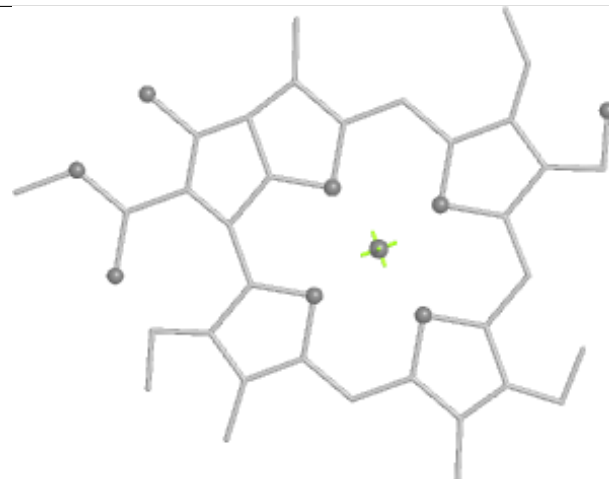
Bond lengths



Bond angles

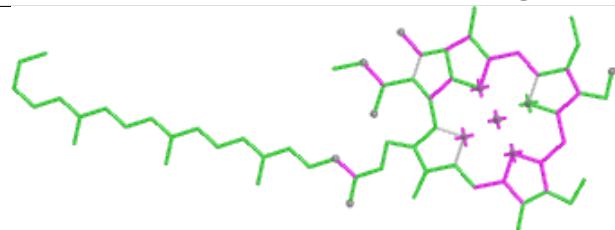


Torsions

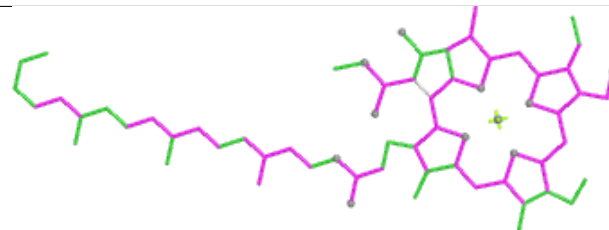


Rings

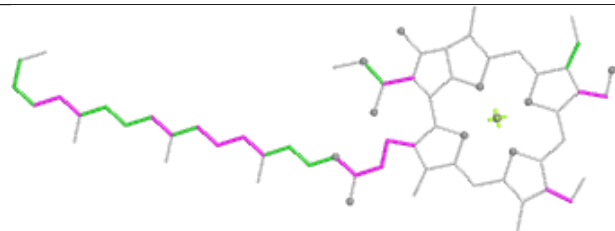
Ligand CHL D 306



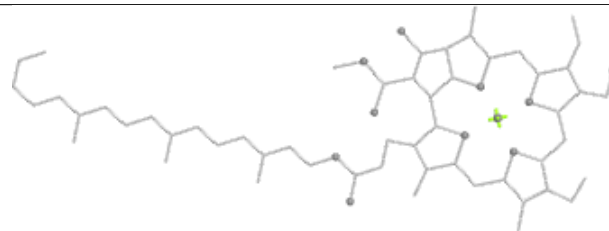
Bond lengths



Bond angles

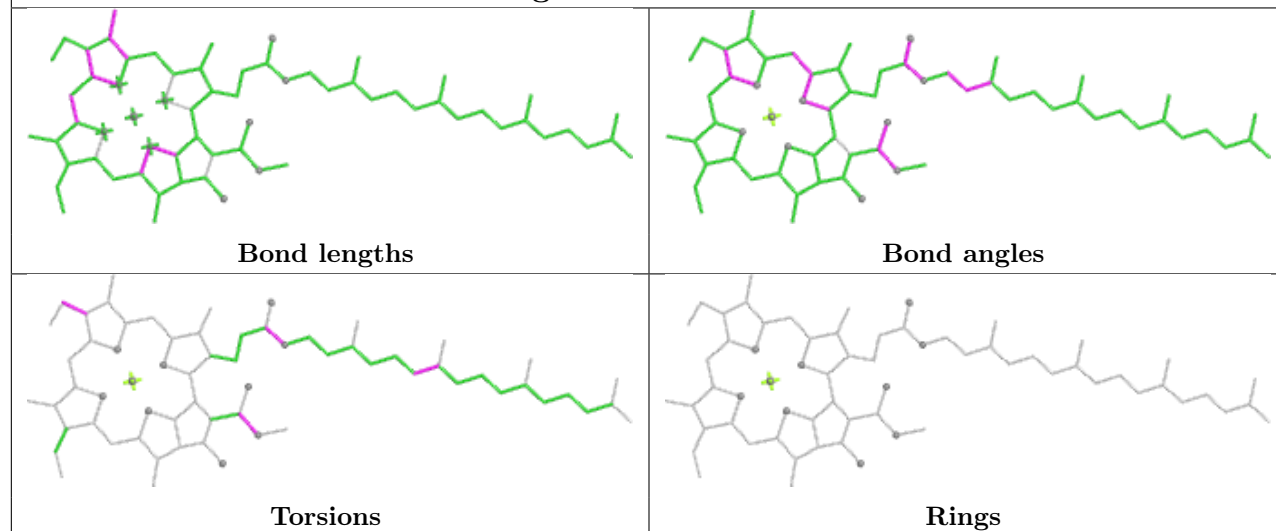


Torsions

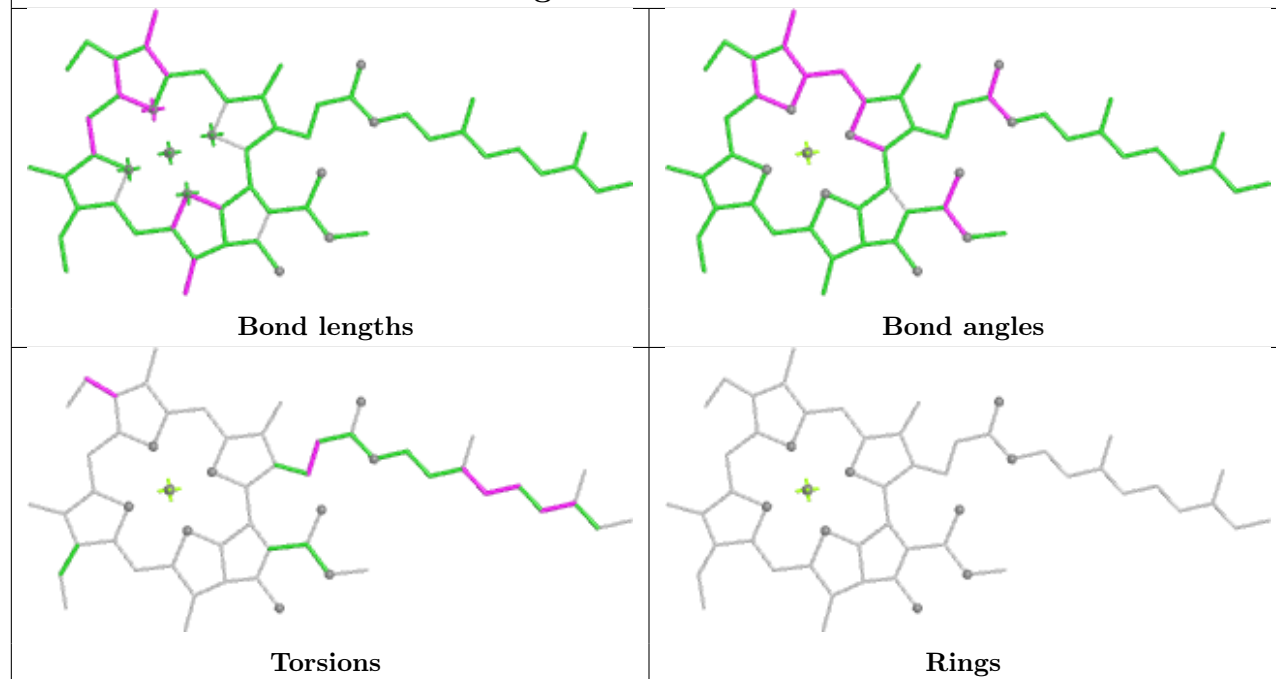


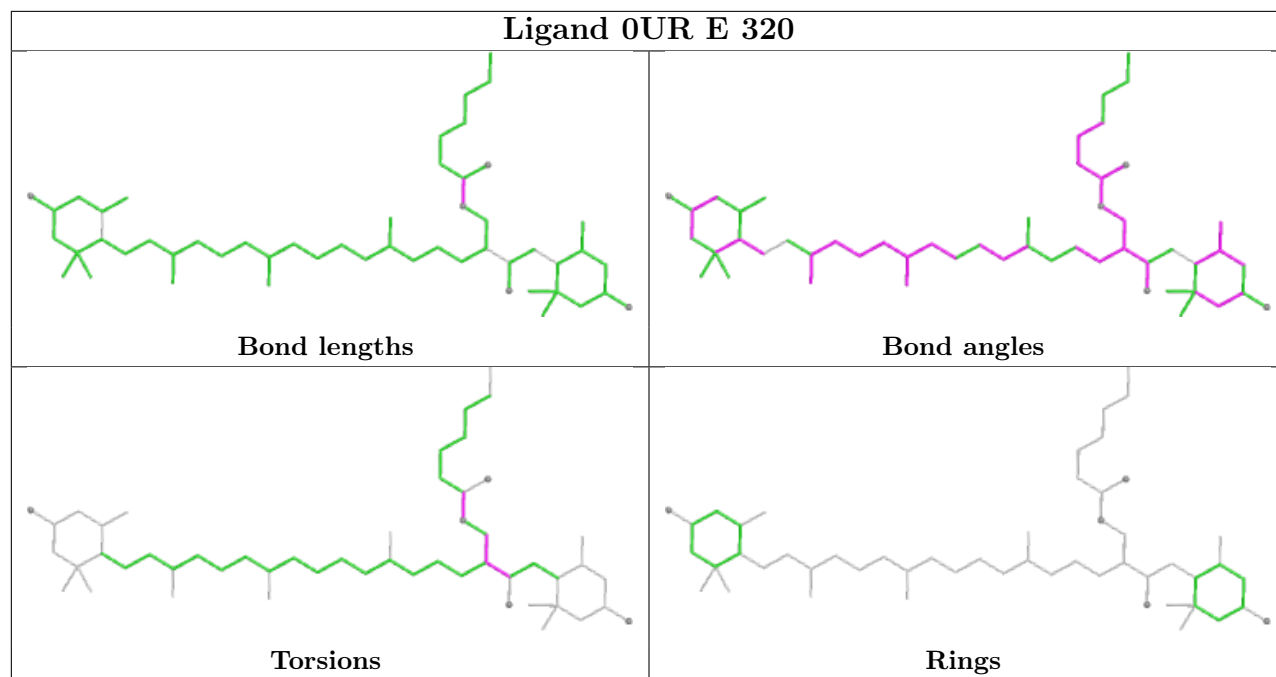
Rings

Ligand CLA B 316



Ligand CLA F 316





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	223/249 (89%)	0.55	23 (10%) 12 9	37, 79, 118, 154	0
1	B	223/249 (89%)	0.52	17 (7%) 20 16	38, 79, 117, 137	0
1	C	222/249 (89%)	0.41	13 (5%) 28 23	39, 84, 122, 158	0
1	D	223/249 (89%)	0.49	18 (8%) 18 14	43, 80, 120, 151	0
1	E	223/249 (89%)	0.78	31 (13%) 6 5	46, 100, 145, 161	0
1	F	223/249 (89%)	0.44	19 (8%) 16 13	34, 76, 109, 126	0
All	All	1337/1494 (89%)	0.53	121 (9%) 15 11	34, 83, 127, 161	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	VAL	11.1
1	F	1	VAL	7.0
1	E	74	GLU	7.0
1	E	84	ALA	6.2
1	D	219	GLY	6.1
1	B	190	THR	6.0
1	C	76	TYR	5.6
1	C	214	ALA	5.5
1	A	134	GLY	5.4
1	E	76	TYR	5.3
1	B	223	PHE	5.3
1	E	136	PRO	5.1
1	F	222	ILE	5.1
1	D	218	PHE	5.0
1	D	1	VAL	4.8
1	E	137	LEU	4.7
1	C	96	GLU	4.6
1	D	148	GLU	4.5
1	F	218	PHE	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	17	GLU	4.4
1	F	27	GLU	4.3
1	E	165	LEU	4.2
1	E	77	GLY	4.1
1	A	143	PRO	4.0
1	A	1	VAL	4.0
1	E	149	ALA	3.8
1	A	190	THR	3.8
1	F	47	ALA	3.6
1	F	221	GLN	3.6
1	D	188	LEU	3.6
1	B	152	PRO	3.5
1	C	217	PHE	3.5
1	D	93	ILE	3.5
1	A	141	THR	3.5
1	D	196	GLU	3.5
1	E	150	PHE	3.4
1	A	142	ASP	3.4
1	F	223	PHE	3.3
1	E	1	VAL	3.3
1	F	217	PHE	3.3
1	E	122	VAL	3.2
1	F	28	PHE	3.2
1	B	213	TYR	3.2
1	C	208	ASN	3.1
1	A	28	PHE	3.1
1	F	26	GLY	3.1
1	D	96	GLU	3.0
1	B	84	ALA	3.0
1	D	200	GLU	3.0
1	D	21	PRO	3.0
1	F	4	TYR	3.0
1	B	5	GLY	3.0
1	A	144	LEU	2.9
1	E	95	ALA	2.9
1	D	18	GLY	2.9
1	D	217	PHE	2.9
1	F	113	ILE	2.9
1	A	203	ALA	2.9
1	D	199	ALA	2.9
1	B	74	GLU	2.8
1	C	202	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	75	LYS	2.7
1	C	3	PHE	2.7
1	E	96	GLU	2.7
1	E	19	ALA	2.7
1	A	111	GLN	2.6
1	A	95	ALA	2.6
1	F	32	TYR	2.6
1	E	73	LEU	2.6
1	C	150	PHE	2.6
1	E	107	LEU	2.6
1	B	119	THR	2.6
1	F	7	ASP	2.5
1	E	138	GLY	2.5
1	C	223	PHE	2.5
1	D	22	SER	2.5
1	E	155	MET	2.5
1	A	113	ILE	2.5
1	F	148	GLU	2.5
1	C	108	VAL	2.5
1	C	222	ILE	2.4
1	B	78	GLY	2.4
1	B	123	LEU	2.4
1	A	106	SER	2.4
1	A	97	GLY	2.4
1	E	72	ALA	2.4
1	F	220	ALA	2.4
1	E	161	THR	2.3
1	B	191	GLY	2.3
1	E	162	PHE	2.3
1	E	106	SER	2.3
1	C	149	ALA	2.3
1	E	62	LEU	2.3
1	A	145	TYR	2.3
1	D	215	THR	2.3
1	B	132	CYS	2.3
1	F	115	ALA	2.3
1	A	96	GLU	2.3
1	D	159	PRO	2.2
1	A	175	LEU	2.2
1	E	121	VAL	2.2
1	A	19	ALA	2.2
1	B	222	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	222	ILE	2.2
1	E	81	PHE	2.2
1	C	105	PRO	2.2
1	A	69	THR	2.2
1	A	133	SER	2.2
1	D	220	ALA	2.1
1	E	141	THR	2.1
1	E	147	GLY	2.1
1	E	108	VAL	2.1
1	E	83	GLU	2.1
1	B	17	GLU	2.1
1	F	103	GLY	2.1
1	B	218	PHE	2.1
1	A	179	ALA	2.1
1	A	148	GLU	2.0
1	F	72	ALA	2.0
1	A	162	PHE	2.0
1	B	122	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	LMG	F	319	30/55	0.23	0.19	127,171,183,186	0
7	LHG	C	304	25/49	0.31	0.19	132,176,208,243	0
4	LMU	A	304	35/35	0.56	0.19	115,156,181,187	0
4	LMU	E	319	35/35	0.56	0.19	117,171,194,195	0
4	LMU	D	304	35/35	0.58	0.23	86,132,160,170	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	BET	B	321	8/8	0.60	0.28	85,102,109,114	0
4	LMU	B	305	35/35	0.64	0.16	107,181,190,195	0
10	BET	C	320	8/8	0.68	0.25	112,121,126,133	0
10	BET	B	322	8/8	0.69	0.29	90,114,123,132	0
11	LMG	B	323	30/55	0.71	0.15	122,164,179,181	0
7	LHG	B	324	31/49	0.76	0.17	56,98,121,145	0
4	LMU	B	304	33/35	0.77	0.15	116,148,174,180	0
9	OUR	E	320	52/57	0.78	0.17	66,89,116,126	0
9	OUR	B	325	52/57	0.79	0.24	66,89,116,126	0
8	MG	A	321	1/1	0.82	0.28	74,74,74,74	0
9	OUR	D	321	52/57	0.84	0.21	66,89,116,126	0
3	NEX	E	303	44/44	0.85	0.19	101,120,167,186	0
9	OUR	C	321	52/57	0.85	0.18	66,89,116,126	0
3	NEX	F	303	44/44	0.85	0.15	71,92,168,179	0
6	CLA	C	315	65/65	0.86	0.13	72,104,124,139	0
5	CHL	A	309	43/66	0.86	0.12	103,123,135,140	0
9	OUR	A	322	52/57	0.86	0.21	66,89,116,126	0
9	OUR	B	302	50/57	0.87	0.18	67,87,107,123	0
3	NEX	C	303	44/44	0.87	0.14	75,94,147,175	0
5	CHL	E	310	61/66	0.87	0.15	62,79,92,98	0
3	NEX	A	303	44/44	0.87	0.15	78,96,144,152	0
7	LHG	A	319	47/49	0.87	0.17	49,74,99,106	0
5	CHL	E	308	41/66	0.88	0.12	119,142,157,160	0
5	CHL	E	309	43/66	0.88	0.16	89,105,127,130	0
2	OIE	D	302	44/44	0.88	0.16	74,87,104,108	0
5	CHL	F	308	42/66	0.88	0.13	93,110,123,128	0
5	CHL	B	310	43/66	0.88	0.14	95,121,136,143	0
6	CLA	E	314	63/65	0.88	0.12	89,121,136,151	0
5	CHL	C	309	42/66	0.88	0.11	92,113,122,129	0
7	LHG	C	319	45/49	0.89	0.15	59,84,108,139	0
2	OIE	C	302	44/44	0.89	0.15	57,77,101,107	0
6	CLA	D	317	65/65	0.89	0.16	66,85,110,114	0
5	CHL	D	309	42/66	0.89	0.11	86,109,121,128	0
9	OUR	F	320	52/57	0.89	0.21	66,89,116,126	0
5	CHL	A	310	51/66	0.90	0.12	59,90,124,133	0
6	CLA	E	313	55/65	0.90	0.12	100,112,130,140	0
6	CLA	C	314	53/65	0.90	0.11	79,97,118,126	0
7	LHG	E	318	41/49	0.90	0.12	55,85,121,144	0
7	LHG	F	318	45/49	0.90	0.16	42,63,78,85	0
5	CHL	E	311	56/66	0.90	0.13	94,112,141,146	0
3	NEX	B	303	44/44	0.91	0.12	76,95,144,165	0
5	CHL	F	309	42/66	0.91	0.11	62,80,94,103	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CLA	A	314	55/65	0.91	0.10	60,71,85,87	0
6	CLA	B	315	58/65	0.91	0.12	65,76,100,107	0
6	CLA	E	315	45/65	0.91	0.10	100,118,132,138	0
6	CLA	E	316	55/65	0.91	0.13	65,78,89,95	0
6	CLA	F	313	58/65	0.91	0.12	58,70,101,102	0
2	OIE	F	302	44/44	0.91	0.13	50,64,77,81	0
7	LHG	B	320	46/49	0.91	0.14	50,74,88,106	0
6	CLA	A	308	50/65	0.92	0.12	68,88,102,119	0
7	LHG	D	319	46/49	0.92	0.13	66,87,101,108	0
5	CHL	C	310	44/66	0.92	0.10	66,86,104,107	0
5	CHL	C	311	61/66	0.92	0.12	51,68,84,92	0
5	CHL	C	312	56/66	0.92	0.12	62,90,116,122	0
5	CHL	C	313	66/66	0.92	0.11	46,63,80,86	0
6	CLA	C	316	45/65	0.92	0.10	77,95,118,123	0
5	CHL	C	318	44/66	0.92	0.12	70,96,112,129	0
2	OIE	A	302	44/44	0.92	0.11	55,73,85,103	0
5	CHL	A	312	56/66	0.92	0.13	51,74,104,117	0
2	OIE	C	301	44/44	0.92	0.12	35,54,75,81	0
5	CHL	B	311	51/66	0.92	0.12	71,90,122,134	0
5	CHL	B	312	62/66	0.92	0.13	51,68,84,93	0
5	CHL	B	319	47/66	0.92	0.09	80,96,112,117	0
2	OIE	E	302	44/44	0.92	0.11	57,75,105,125	0
5	CHL	F	310	61/66	0.92	0.11	49,65,80,89	0
5	CHL	F	317	46/66	0.92	0.11	63,83,106,122	0
5	CHL	E	304	66/66	0.93	0.12	54,75,102,137	0
5	CHL	E	305	64/66	0.93	0.11	44,65,79,95	0
6	CLA	A	315	63/65	0.93	0.12	66,86,99,109	0
6	CLA	B	309	46/65	0.93	0.12	72,88,99,103	0
3	NEX	D	303	44/44	0.93	0.12	65,81,126,145	0
6	CLA	B	318	65/65	0.93	0.12	58,84,98,101	0
6	CLA	C	308	46/65	0.93	0.10	65,86,94,100	0
5	CHL	B	313	57/66	0.93	0.12	59,84,104,105	0
5	CHL	A	318	42/66	0.93	0.12	66,89,100,101	0
5	CHL	A	305	66/66	0.93	0.12	45,73,91,106	0
6	CLA	D	308	46/65	0.93	0.08	68,84,96,104	0
6	CLA	D	314	58/65	0.93	0.12	60,76,97,101	0
5	CHL	E	312	66/66	0.93	0.12	46,76,90,100	0
6	CLA	E	307	50/65	0.93	0.12	89,108,130,132	0
5	CHL	E	317	41/66	0.93	0.11	83,96,113,116	0
5	CHL	D	306	65/66	0.93	0.12	42,58,76,89	0
5	CHL	A	311	61/66	0.93	0.10	51,70,82,97	0
5	CHL	D	310	45/66	0.93	0.08	52,77,90,91	0

Continued on next page...

Continued from previous page...

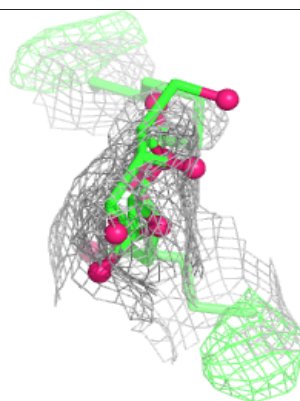
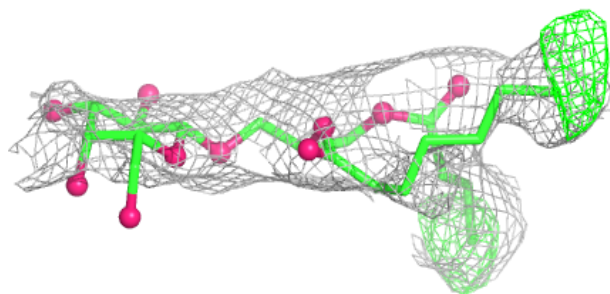
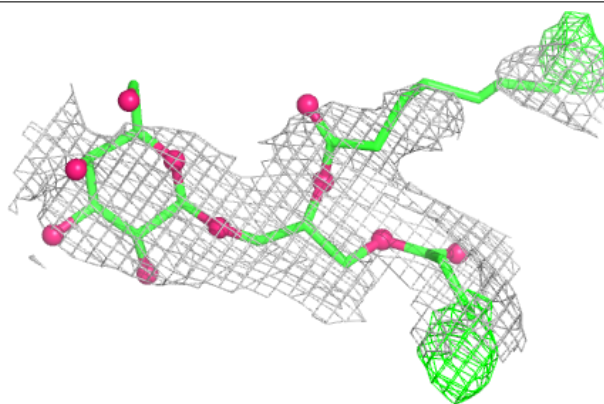
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CLA	F	307	46/65	0.93	0.09	61,79,91,96	0
5	CHL	D	311	62/66	0.93	0.12	40,72,88,94	0
6	CLA	F	315	45/65	0.93	0.09	58,74,92,100	0
5	CHL	B	306	66/66	0.94	0.12	45,63,77,93	0
5	CHL	D	305	66/66	0.94	0.12	59,85,100,108	0
6	CLA	B	316	65/65	0.94	0.11	63,79,109,139	0
5	CHL	C	305	66/66	0.94	0.11	51,71,86,102	0
6	CLA	C	307	65/65	0.94	0.09	33,51,75,92	0
5	CHL	C	306	66/66	0.94	0.12	34,58,71,87	0
2	OIE	B	301	44/44	0.94	0.10	33,46,75,79	0
5	CHL	F	304	66/66	0.94	0.11	41,58,70,84	0
5	CHL	F	305	66/66	0.94	0.10	29,43,59,71	0
6	CLA	C	317	56/65	0.94	0.11	57,75,89,96	0
2	OIE	F	301	44/44	0.94	0.11	29,43,65,81	0
8	MG	D	320	1/1	0.94	0.13	63,63,63,63	0
5	CHL	D	312	57/66	0.94	0.12	44,63,94,103	0
6	CLA	D	315	65/65	0.94	0.10	79,95,107,112	0
6	CLA	D	316	45/65	0.94	0.09	81,85,101,105	0
5	CHL	D	313	66/66	0.94	0.10	33,50,74,96	0
6	CLA	E	306	65/65	0.94	0.10	48,63,78,86	0
5	CHL	F	312	66/66	0.94	0.10	45,61,77,86	0
5	CHL	D	318	46/66	0.94	0.11	86,105,120,121	0
2	OIE	A	301	44/44	0.94	0.11	37,50,66,77	0
2	OIE	E	301	44/44	0.94	0.10	44,68,86,99	0
5	CHL	B	314	66/66	0.94	0.10	41,61,77,91	0
6	CLA	F	306	65/65	0.94	0.10	36,53,75,90	0
6	CLA	A	317	55/65	0.94	0.10	48,77,87,97	0
6	CLA	F	314	55/65	0.95	0.09	51,63,93,103	0
5	CHL	B	307	65/66	0.95	0.10	32,45,64,88	0
6	CLA	F	316	56/65	0.95	0.09	54,68,79,90	0
8	MG	A	320	1/1	0.95	0.09	83,83,83,83	0
6	CLA	A	316	45/65	0.95	0.08	74,80,98,116	0
2	OIE	D	301	44/44	0.95	0.10	44,58,74,85	0
6	CLA	D	307	65/65	0.95	0.10	34,51,81,90	0
5	CHL	A	313	66/66	0.95	0.10	43,58,76,95	0
5	CHL	F	311	56/66	0.95	0.11	55,83,110,118	0
6	CLA	A	307	65/65	0.96	0.10	31,47,79,85	0
5	CHL	A	306	64/66	0.96	0.09	30,51,64,82	0
6	CLA	B	308	65/65	0.96	0.09	35,49,75,84	0
6	CLA	B	317	45/65	0.96	0.09	74,82,99,112	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.

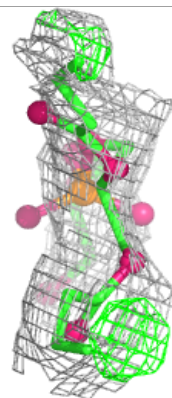
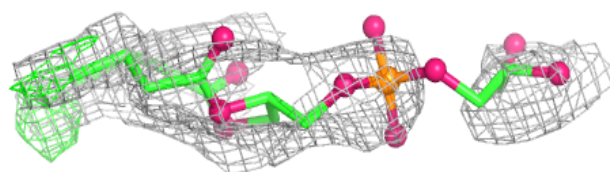
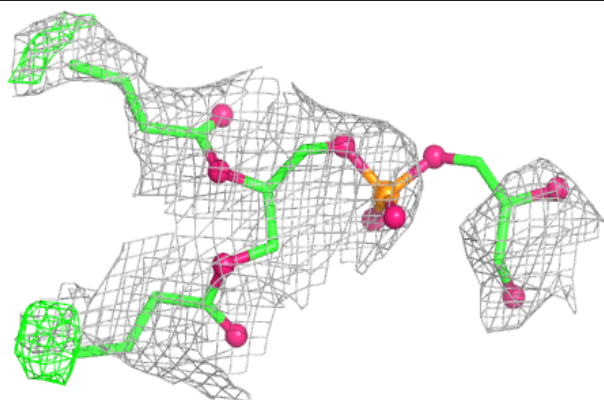
Electron density around LMG F 319:

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



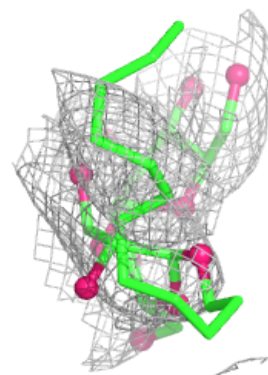
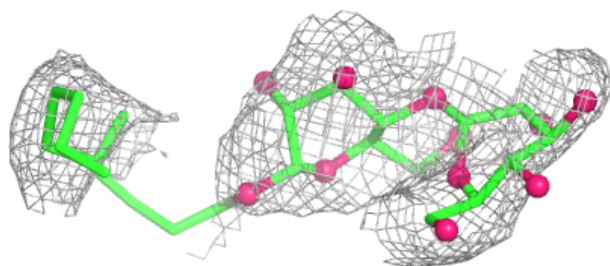
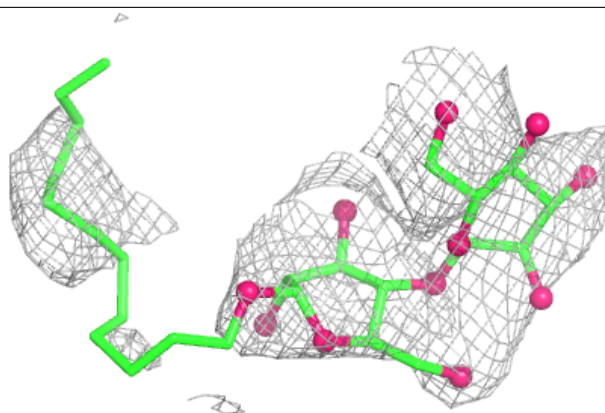
Electron density around LHG C 304:

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

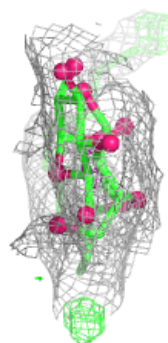
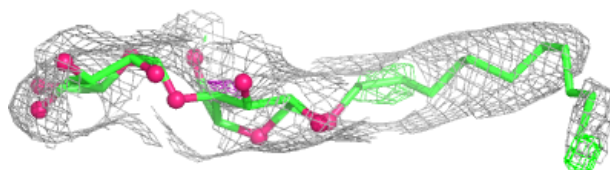
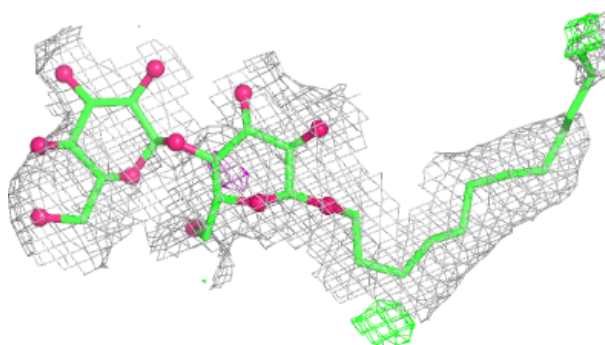


Electron density around LMU A 304:

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

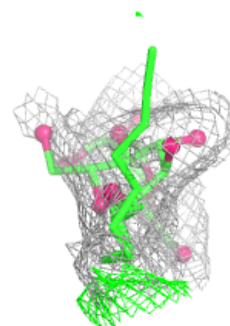
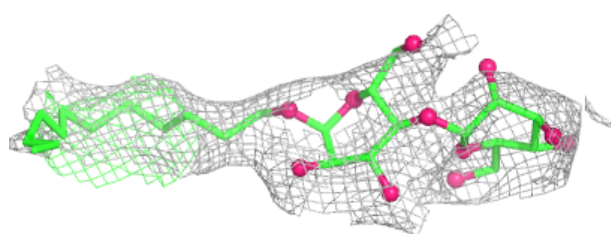
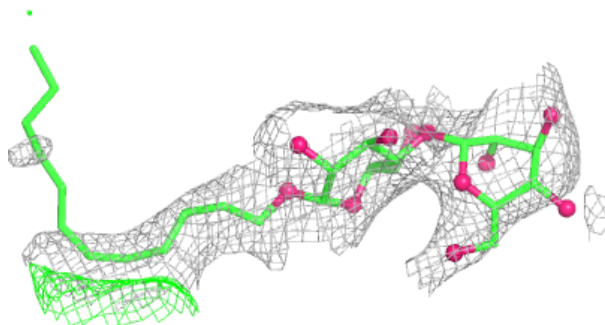
**Electron density around LMU E 319:**

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

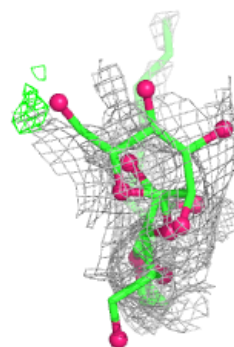
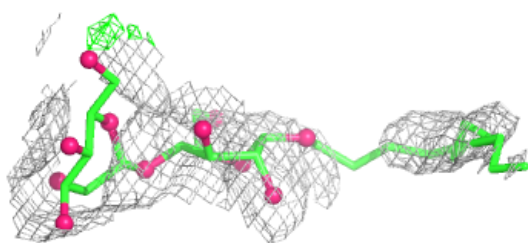
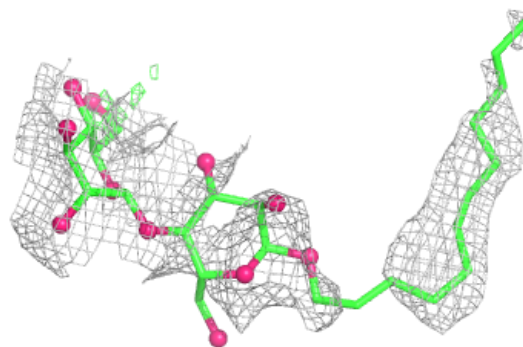


Electron density around LMU D 304:

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

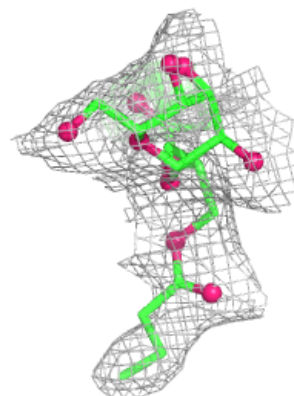
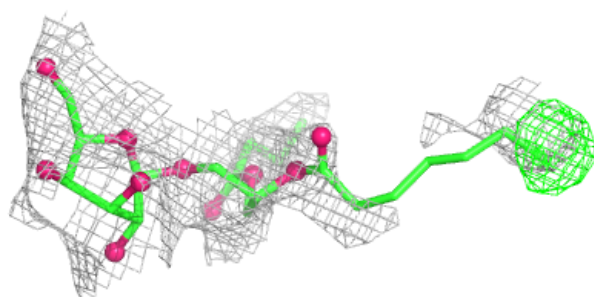
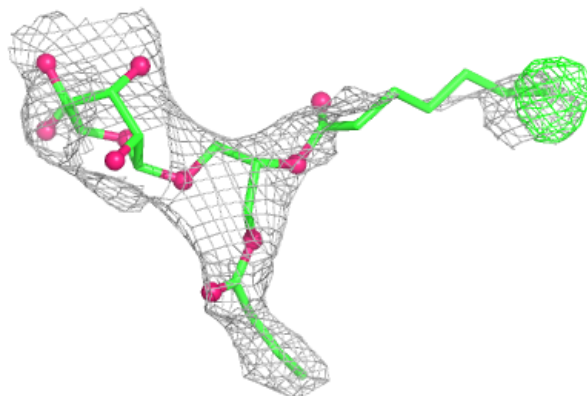
**Electron density around LMU B 305:**

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

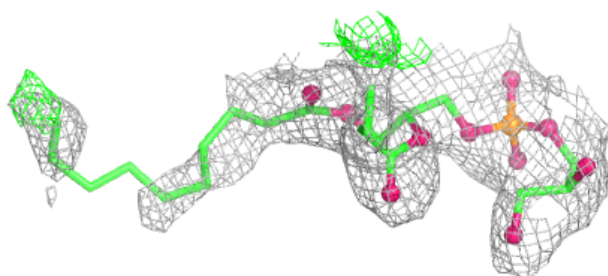
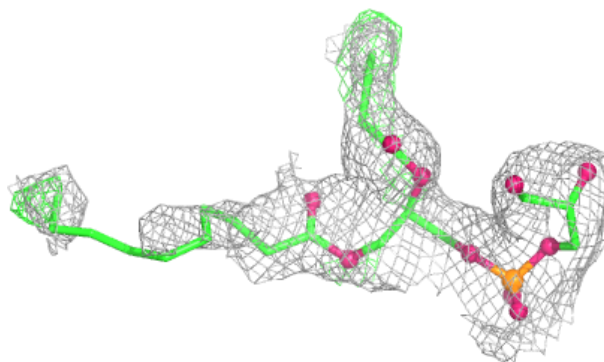


Electron density around LMG B 323:

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

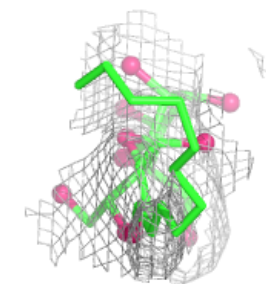
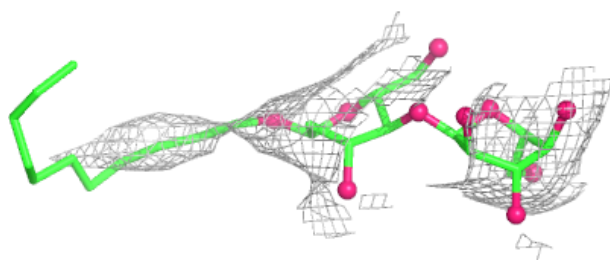
**Electron density around LHG B 324:**

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

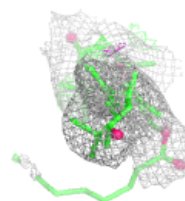
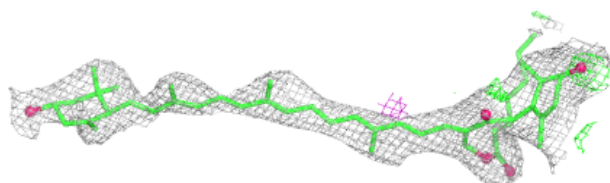
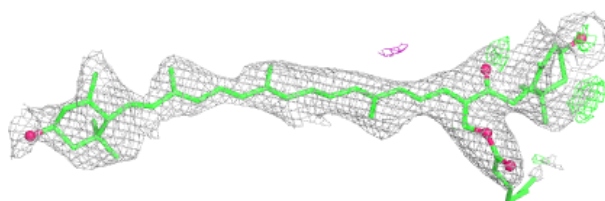


Electron density around LMU B 304:

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

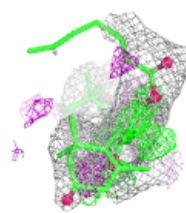
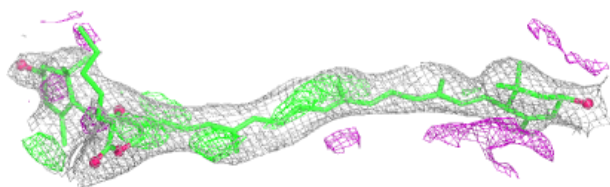
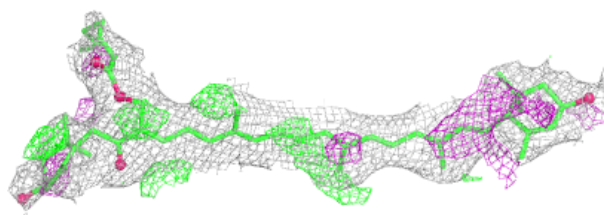
**Electron density around OUR E 320:**

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

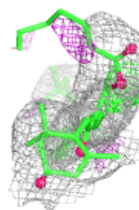
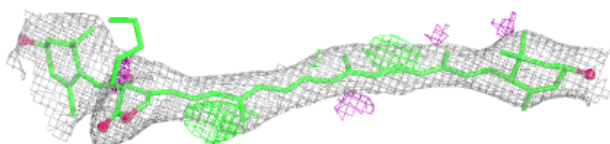
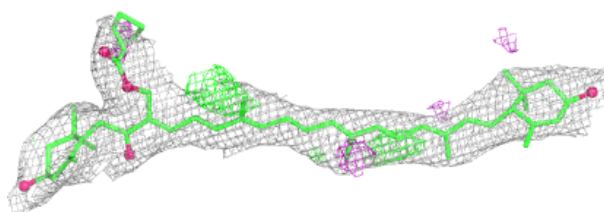


Electron density around 0UR B 325:

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

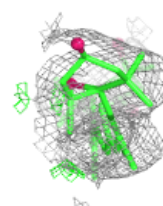
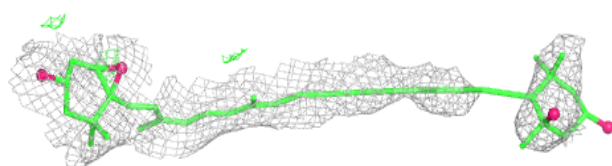
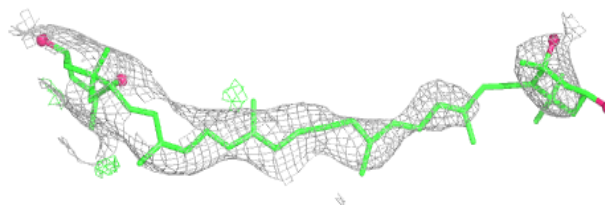
**Electron density around 0UR D 321:**

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

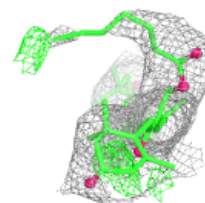
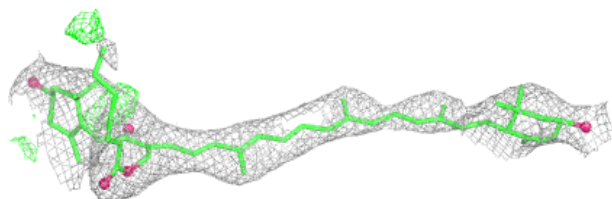
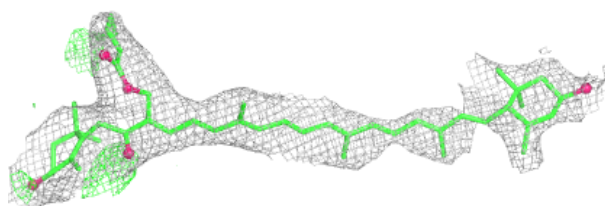


Electron density around NEX E 303:

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

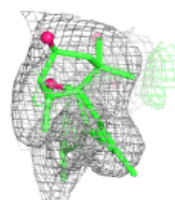
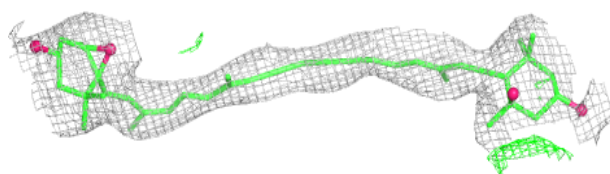
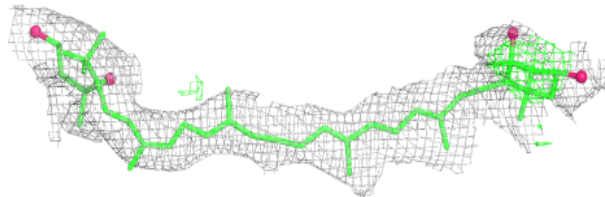
**Electron density around 0UR C 321:**

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

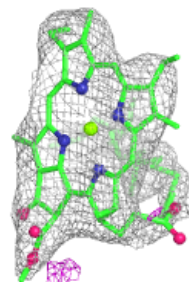
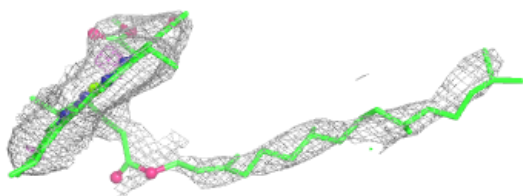
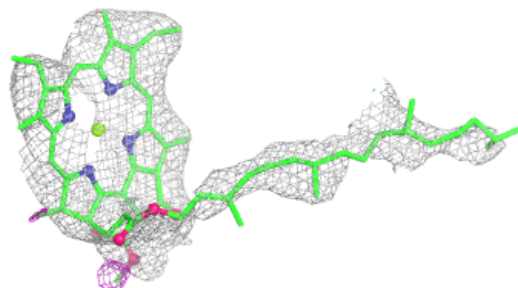


Electron density around NEX F 303:

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

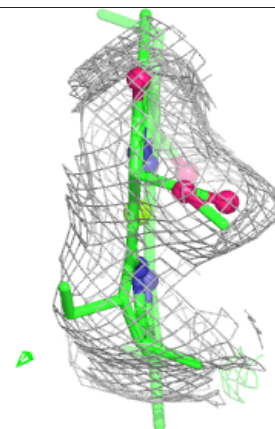
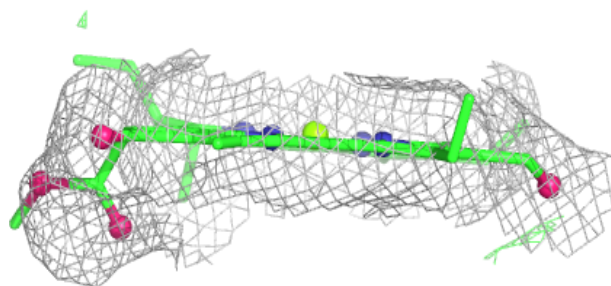
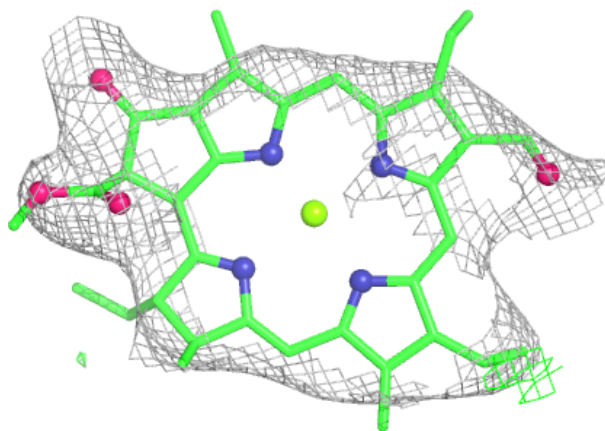
**Electron density around CLA C 315:**

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

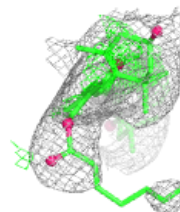
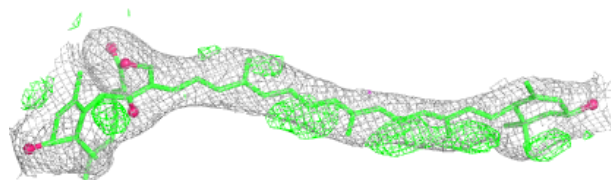
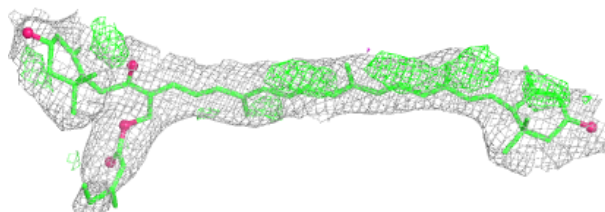


Electron density around CHL A 309:

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

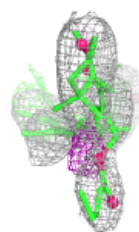
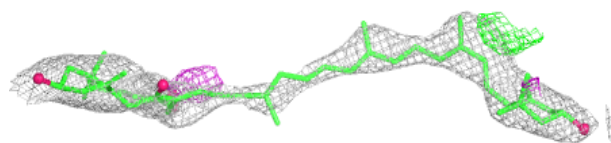
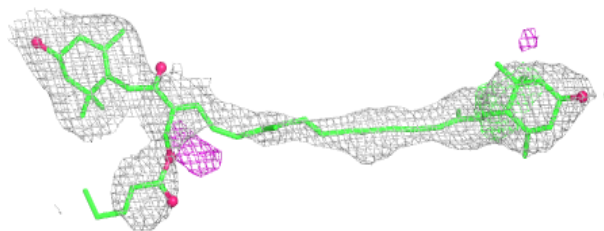
**Electron density around 0UR A 322:**

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

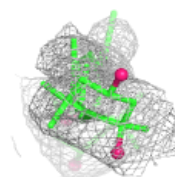
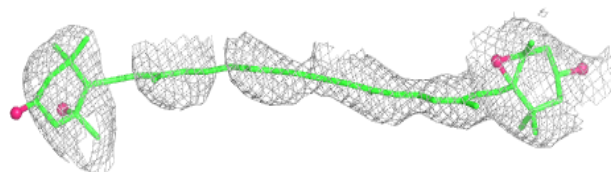
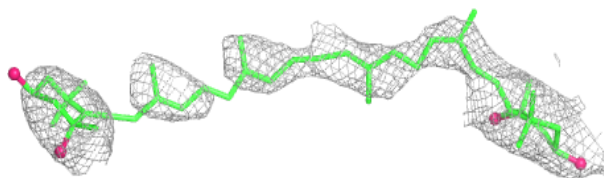


Electron density around 0UR B 302:

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

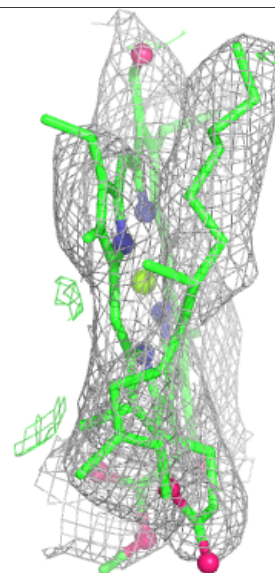
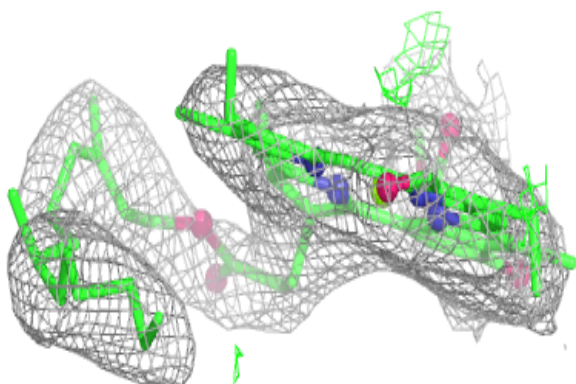
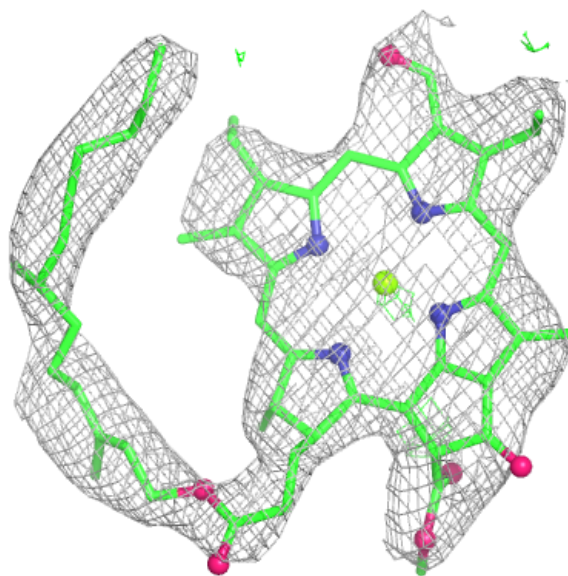
**Electron density around NEX C 303:**

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



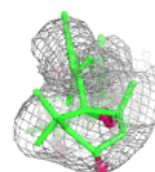
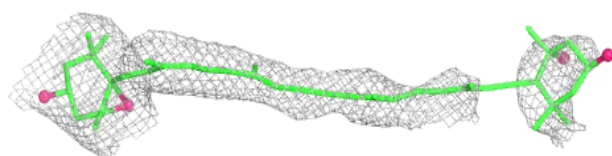
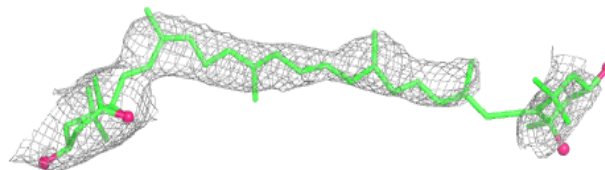
Electron density around CHL E 310:

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

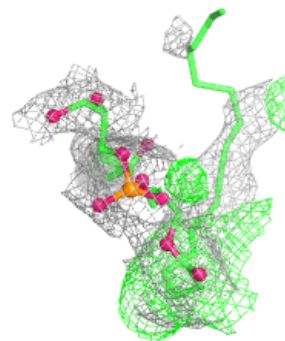
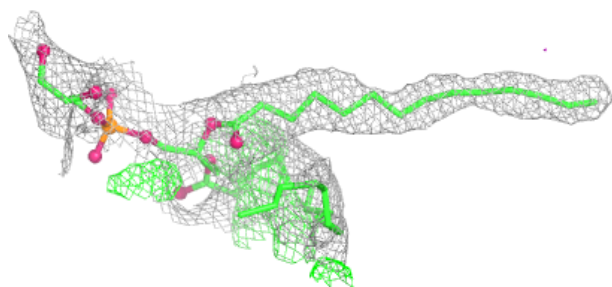
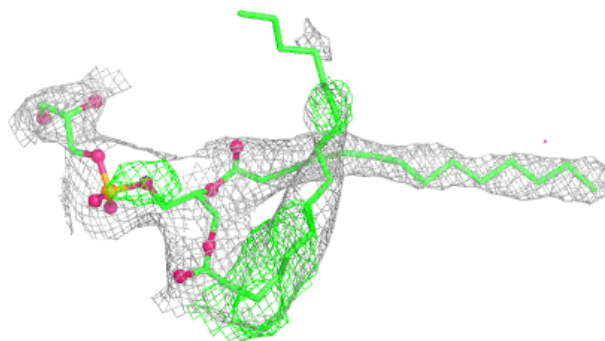


Electron density around NEX A 303:

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

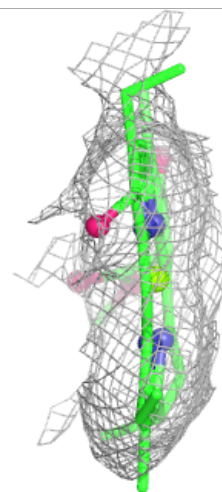
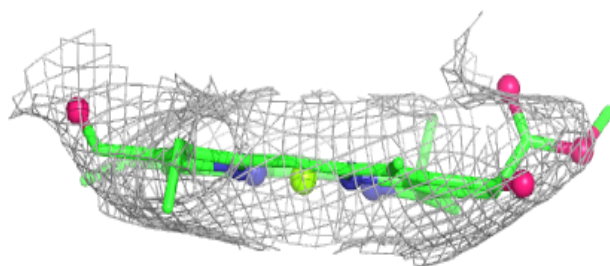
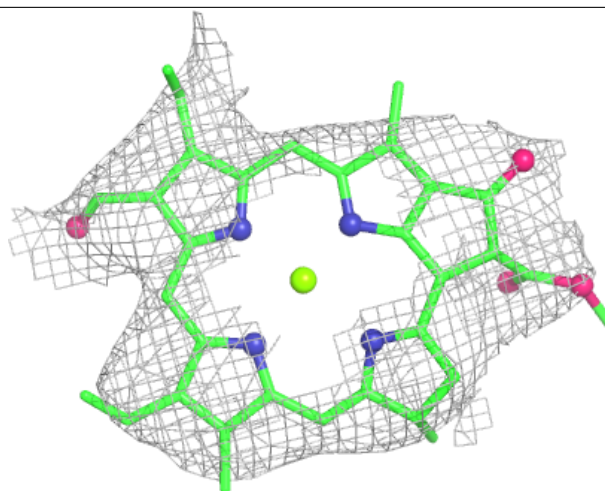
**Electron density around LHG A 319:**

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



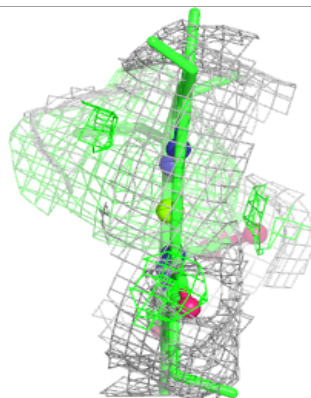
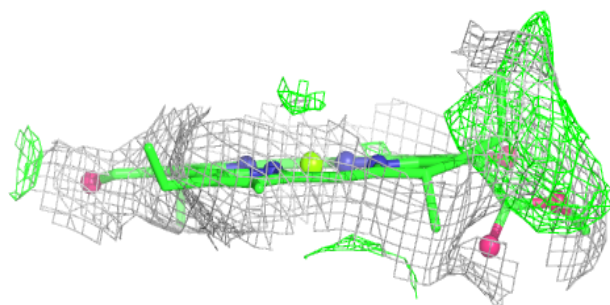
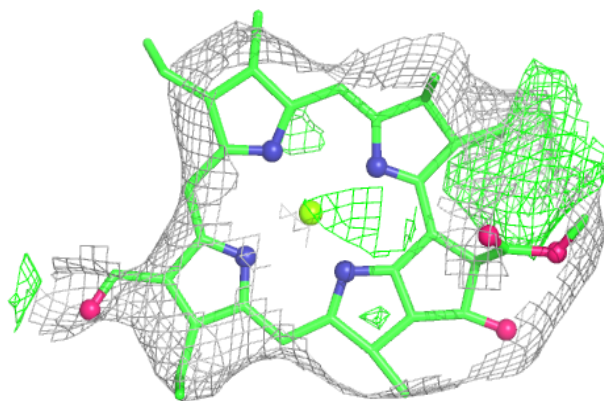
Electron density around CHL E 308:

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

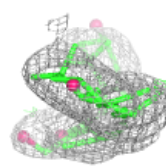
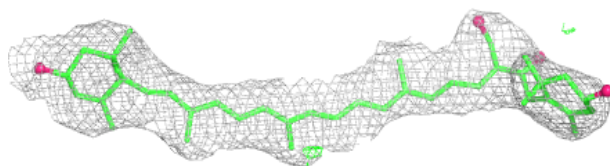
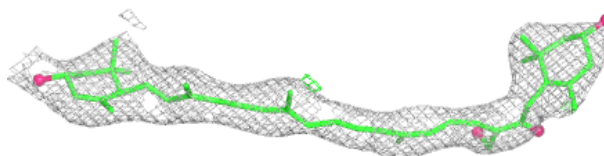


Electron density around CHL E 309:

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

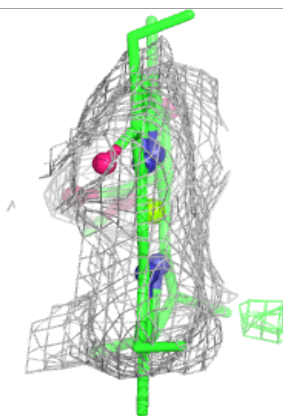
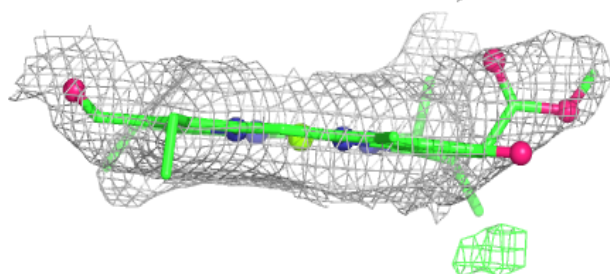
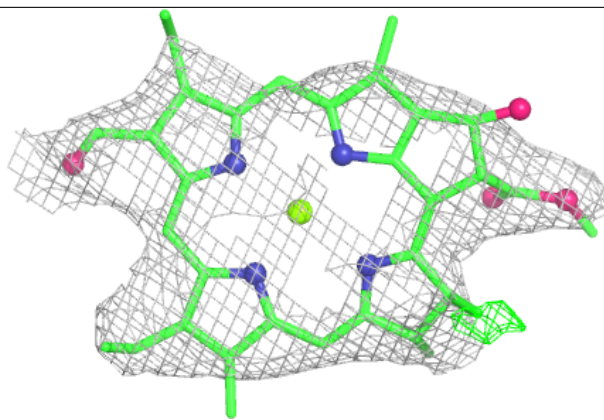
**Electron density around OIE D 302:**

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



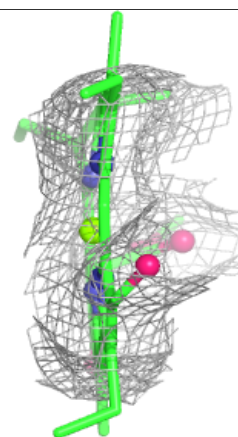
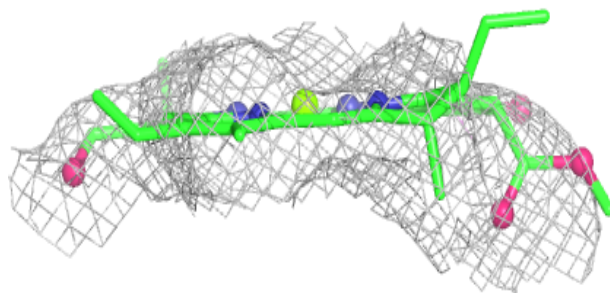
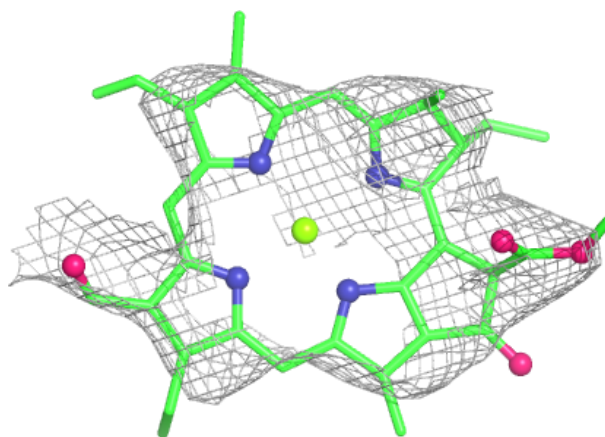
Electron density around CHL F 308:

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



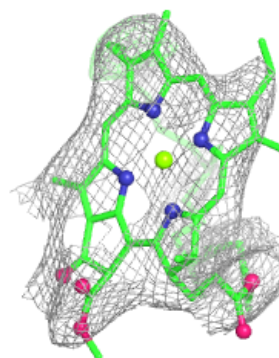
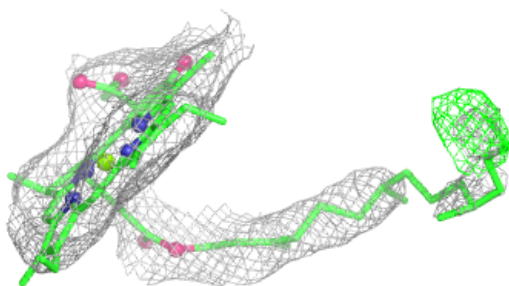
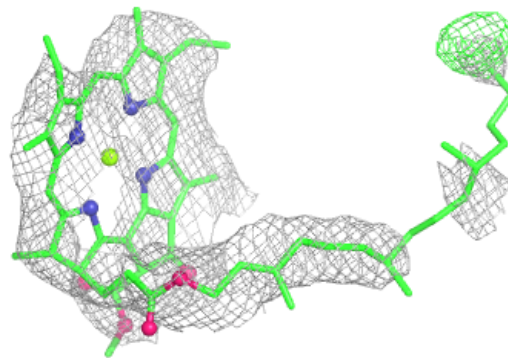
Electron density around CHL B 310:

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



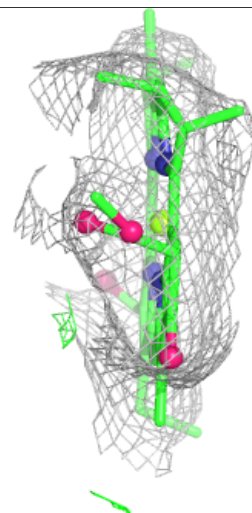
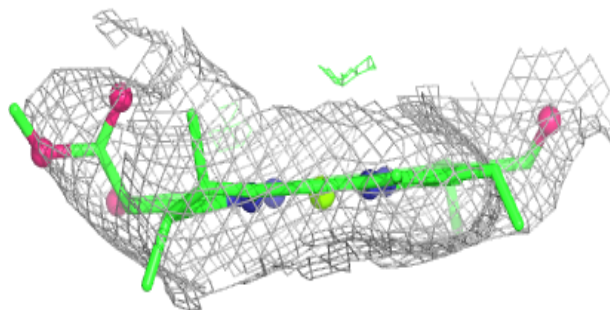
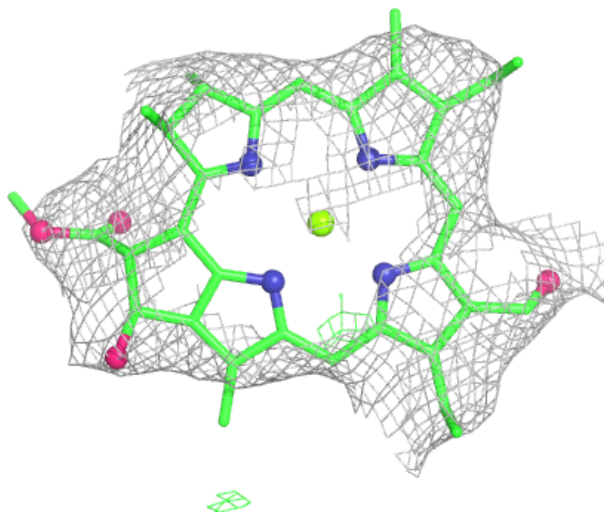
Electron density around CLA E 314:

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



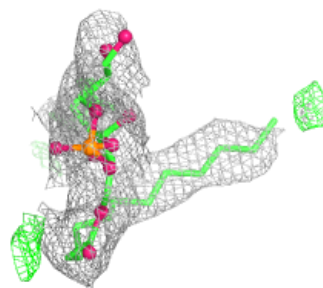
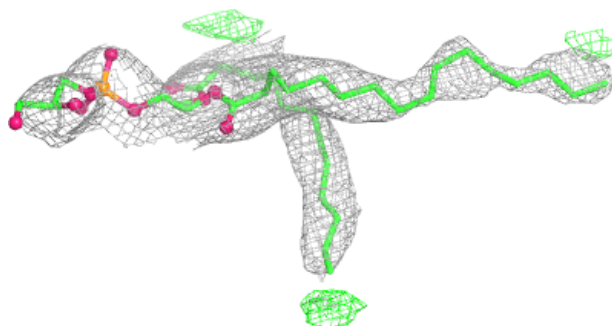
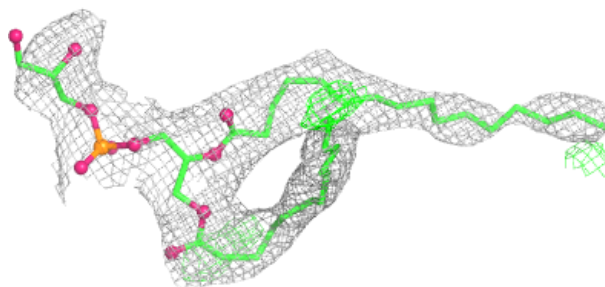
Electron density around CHL C 309:

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

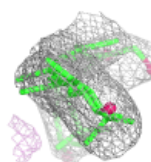
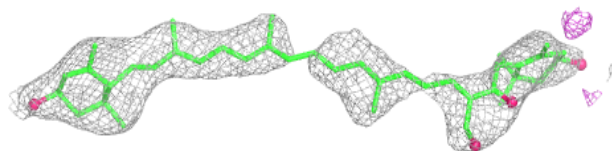
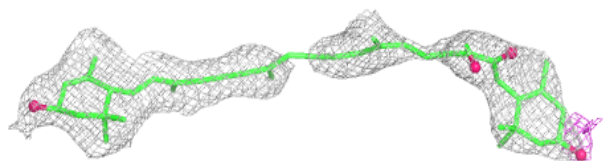


Electron density around LHG C 319:

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

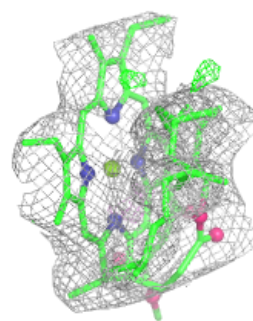
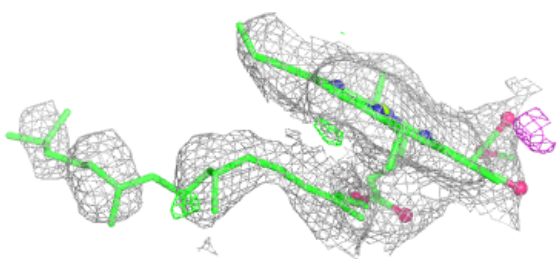
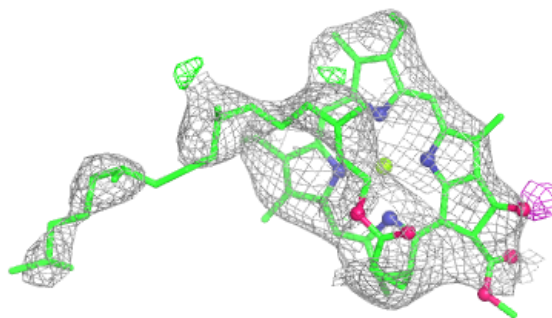
**Electron density around OIE C 302:**

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



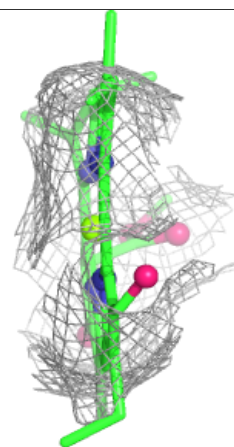
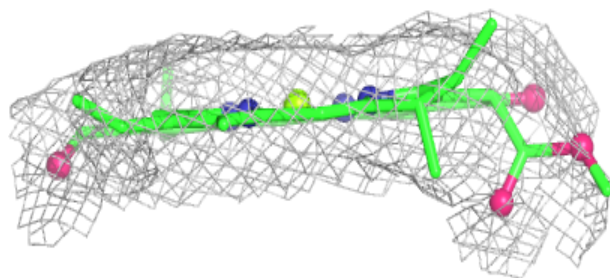
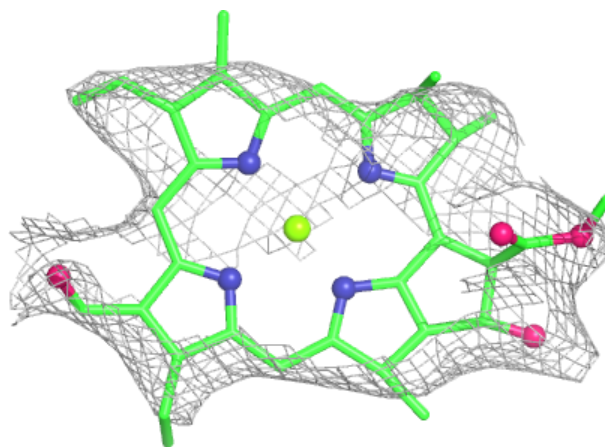
Electron density around CLA D 317:

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



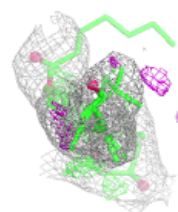
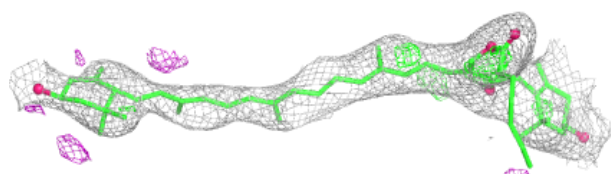
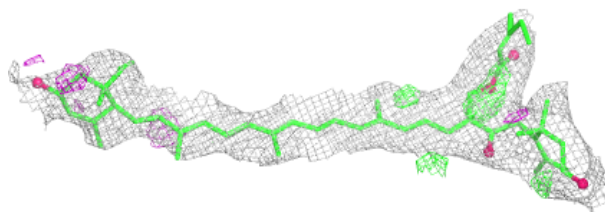
Electron density around CHL D 309:

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

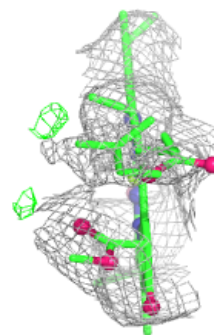
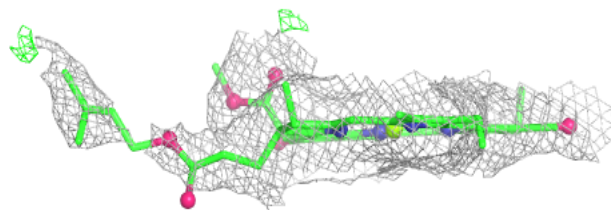
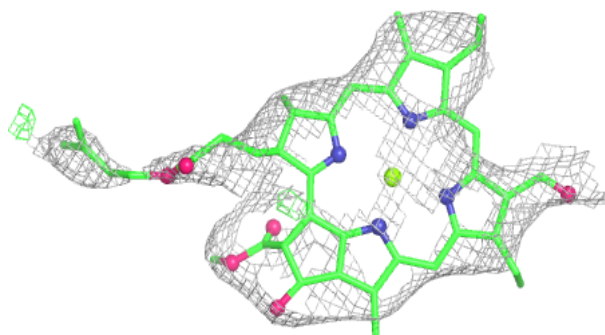


Electron density around 0UR F 320:

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

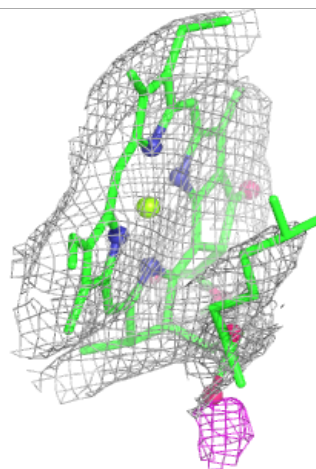
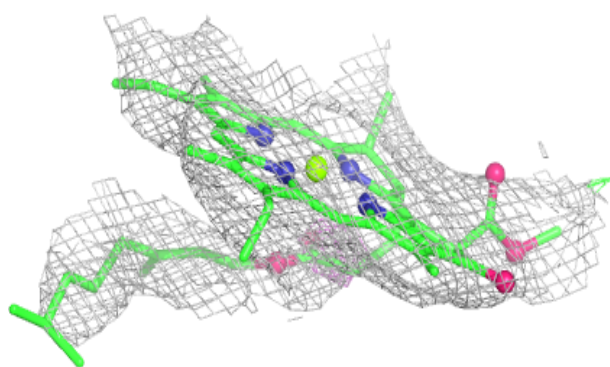
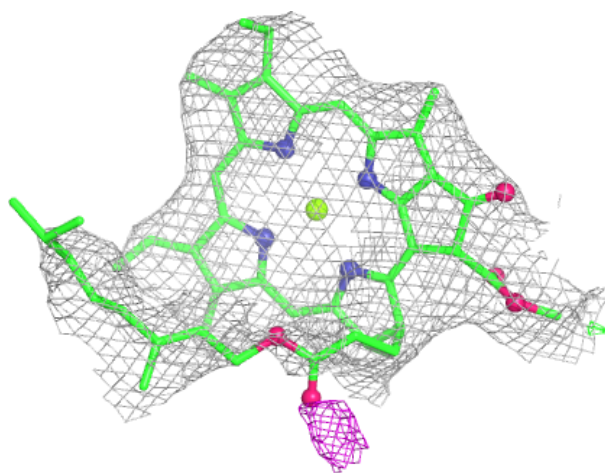
**Electron density around CHL A 310:**

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



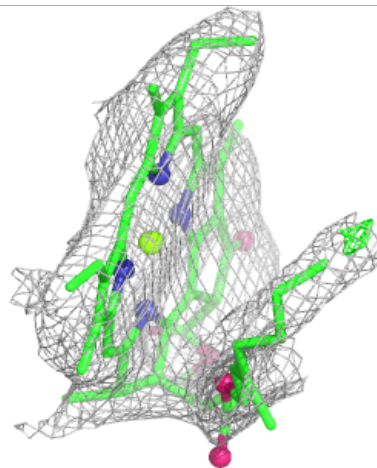
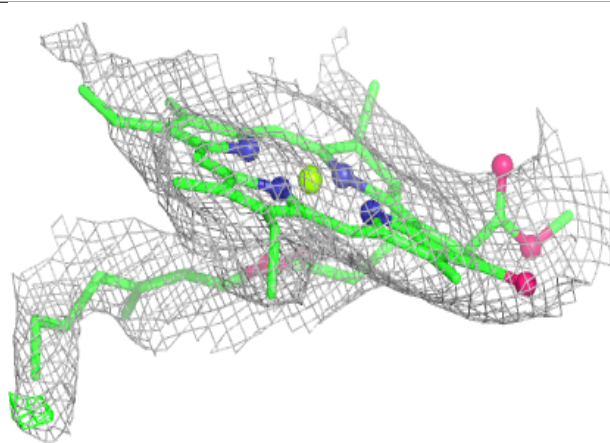
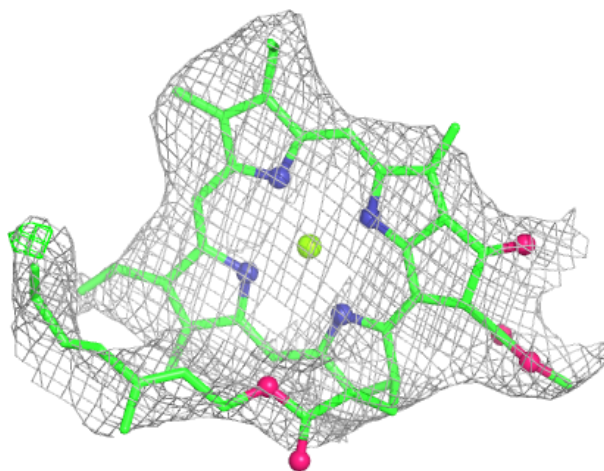
Electron density around CLA E 313:

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



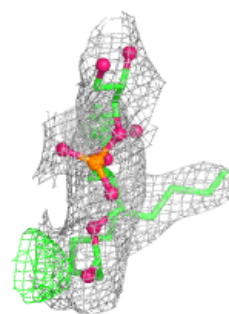
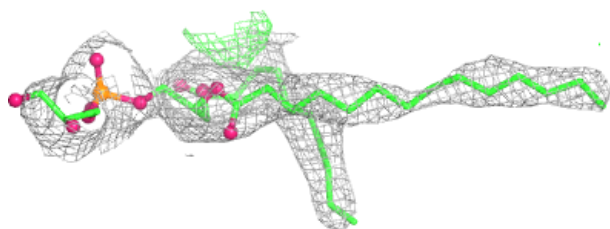
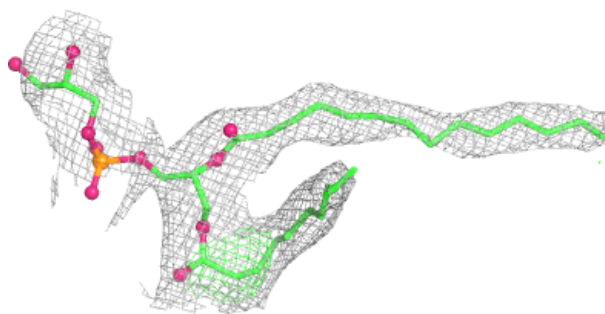
Electron density around CLA C 314:

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

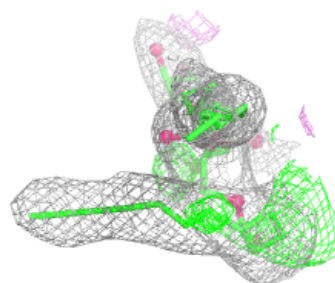
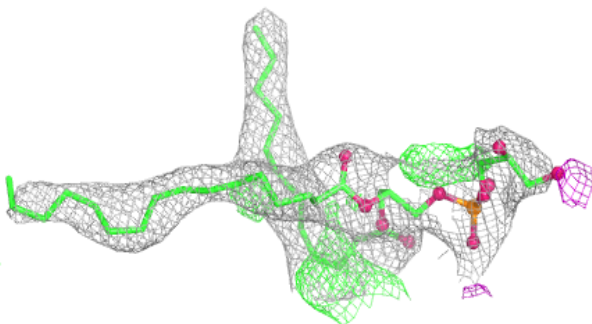
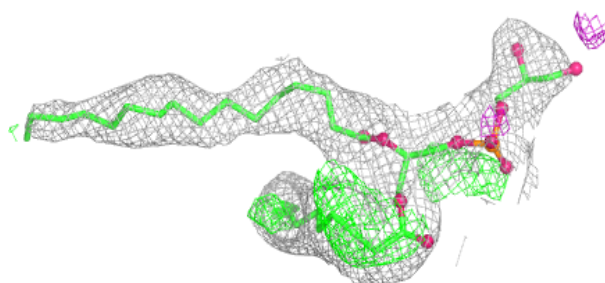


Electron density around LHG E 318:

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

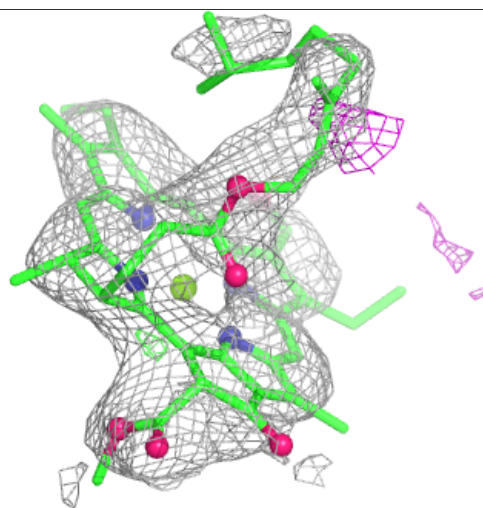
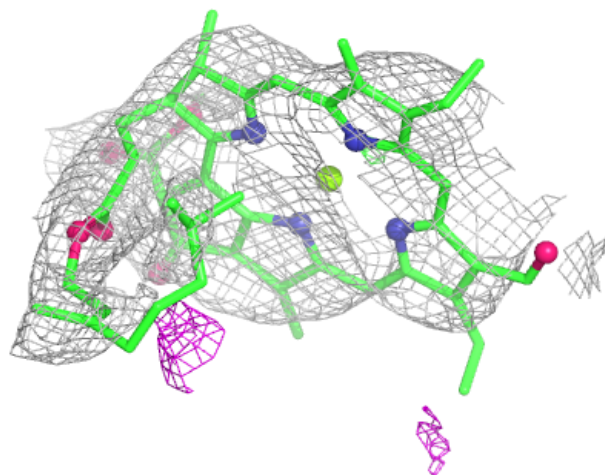
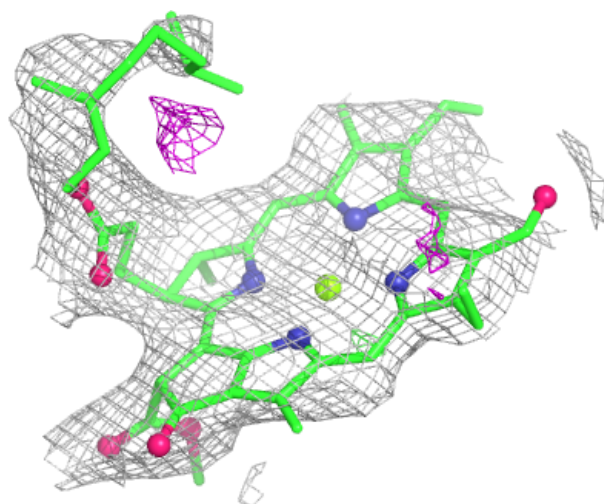
**Electron density around LHG F 318:**

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



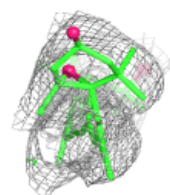
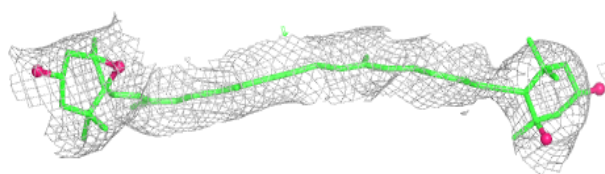
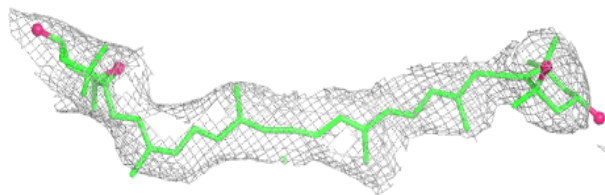
Electron density around CHL E 311:

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

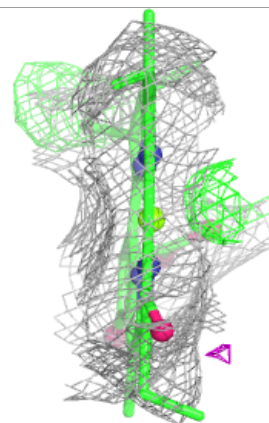
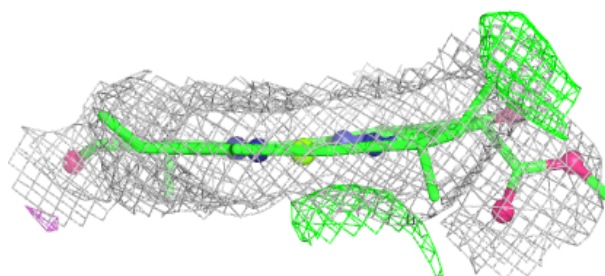
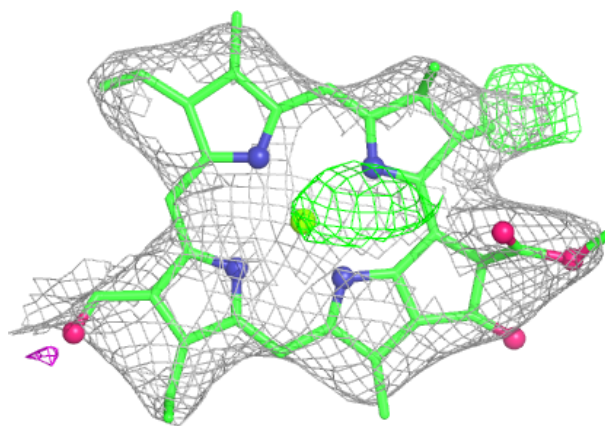


Electron density around NEX B 303:

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

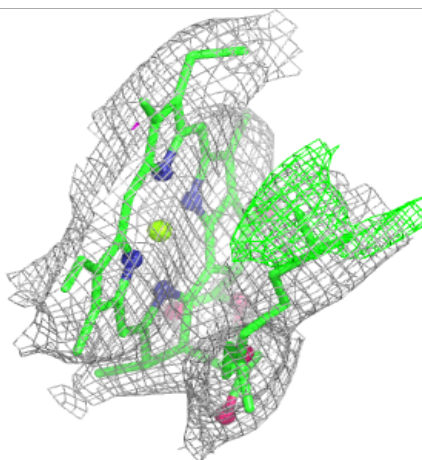
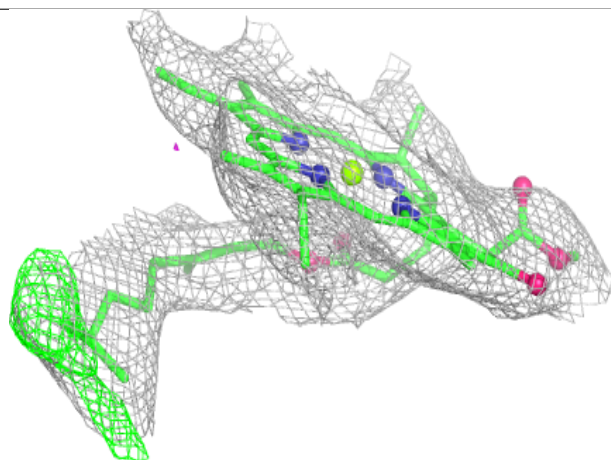
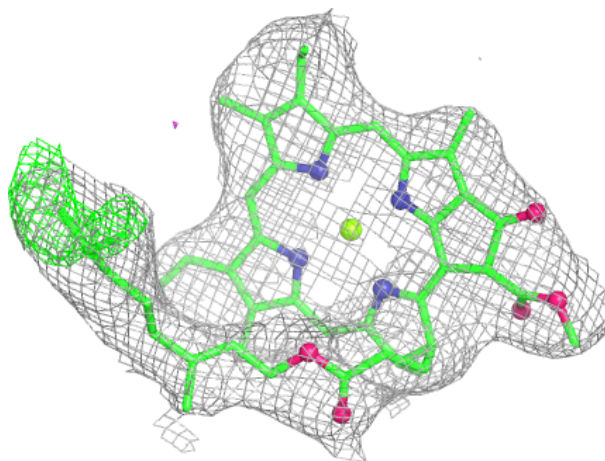
**Electron density around CHL F 309:**

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



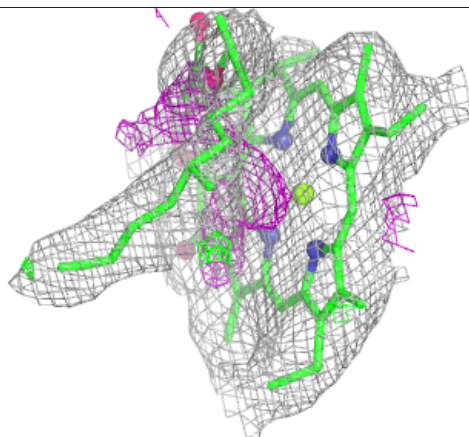
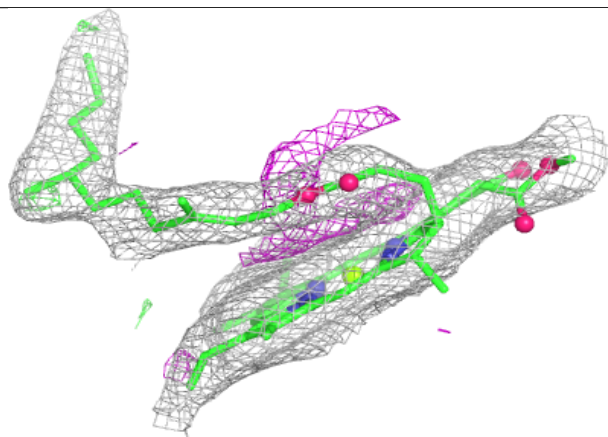
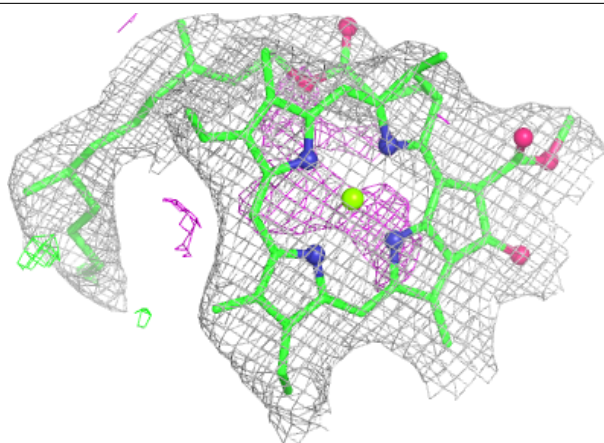
Electron density around CLA A 314:

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



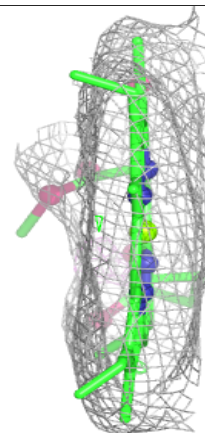
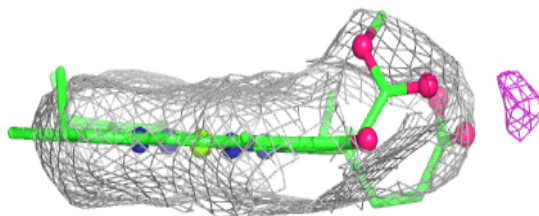
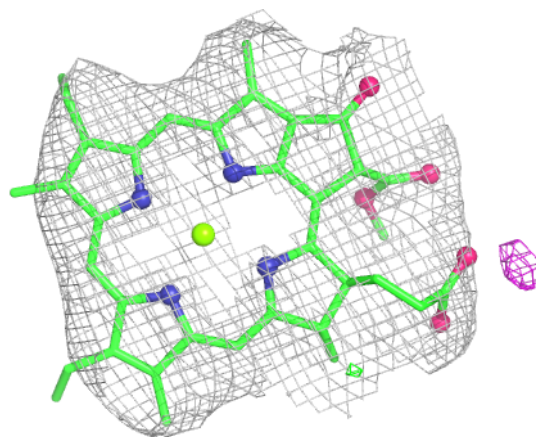
Electron density around CLA B 315:

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



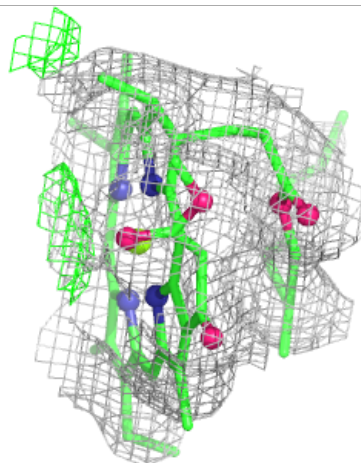
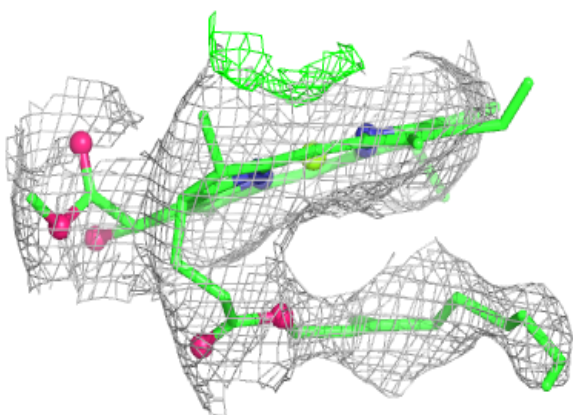
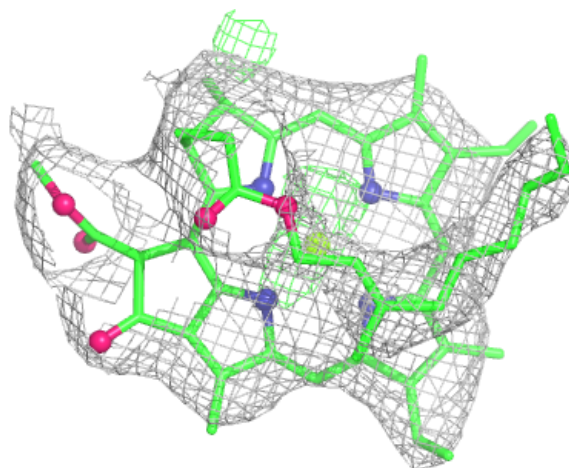
Electron density around CLA E 315:

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



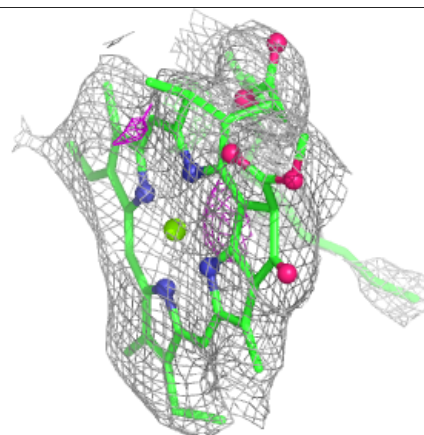
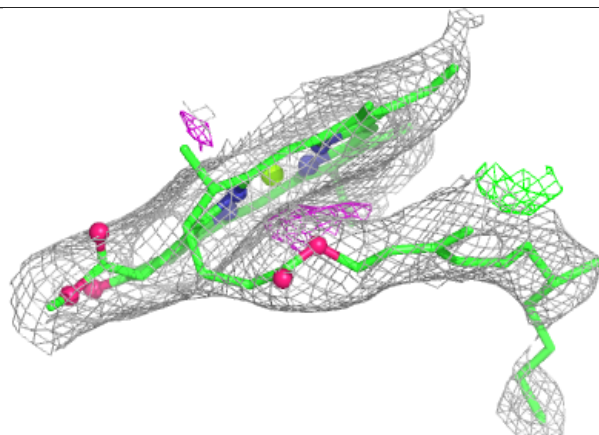
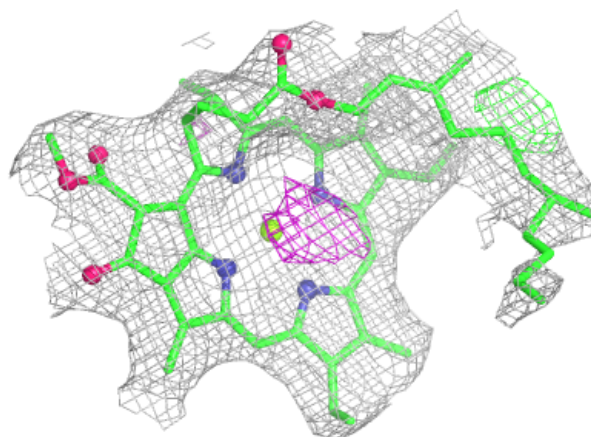
Electron density around CLA E 316:

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

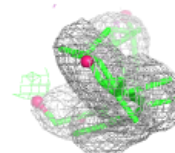
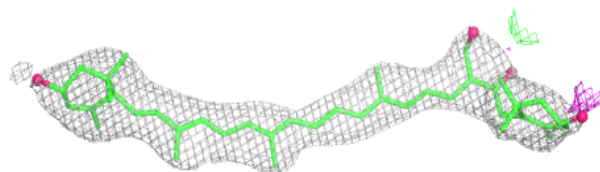
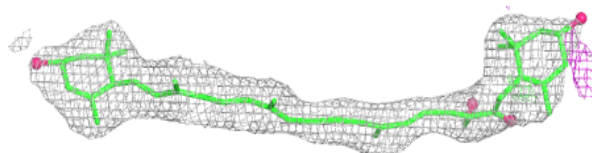


Electron density around CLA F 313:

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

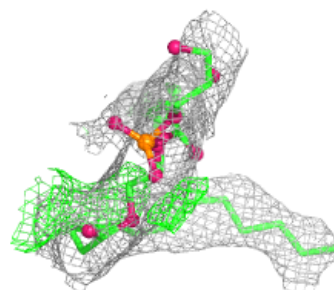
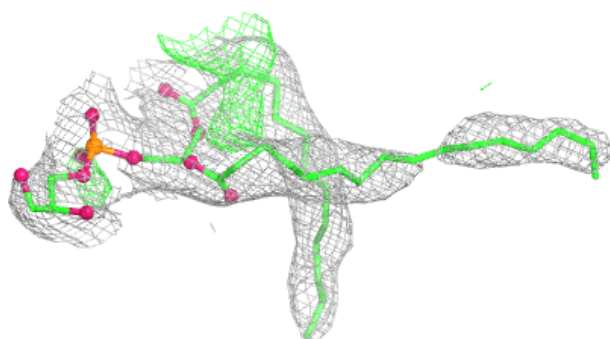
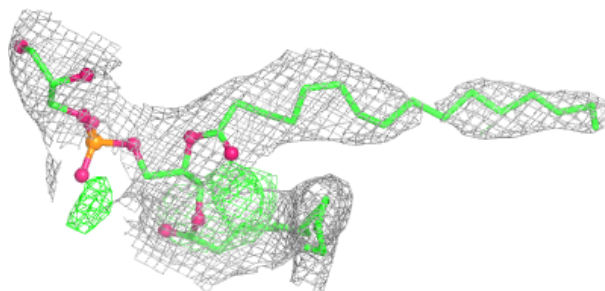
**Electron density around OIE F 302:**

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



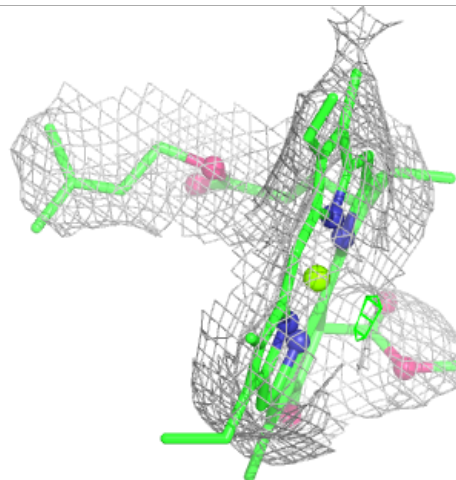
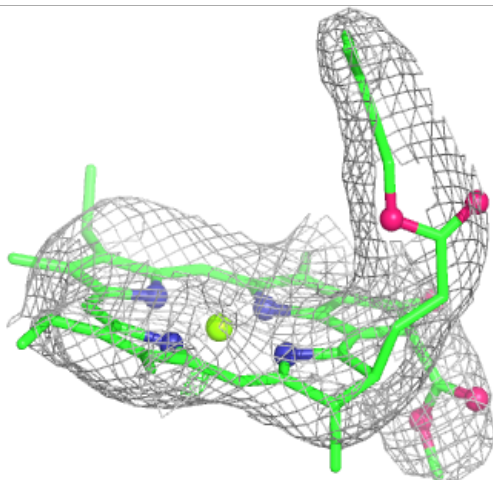
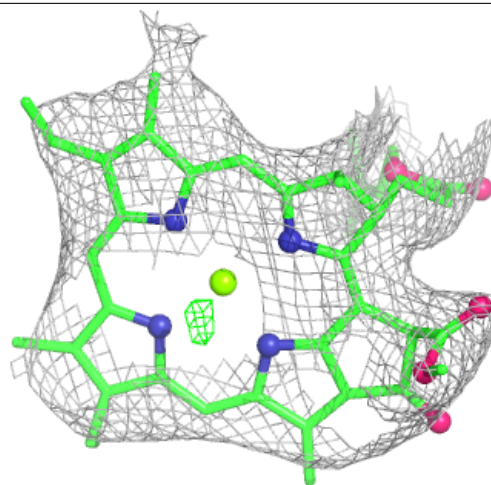
Electron density around LHG B 320:

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



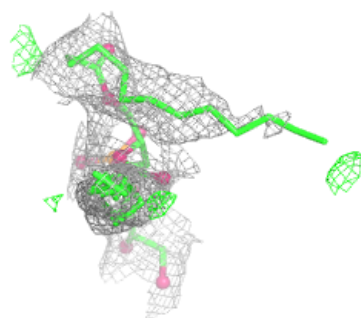
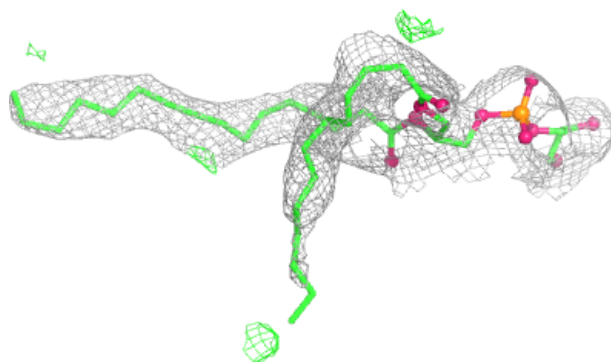
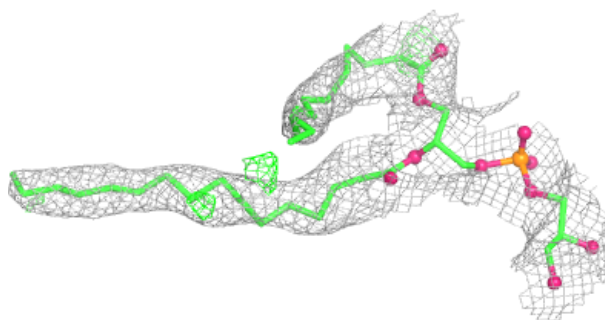
Electron density around CLA A 308:

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



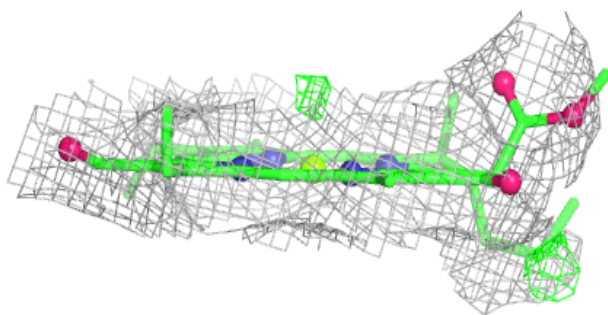
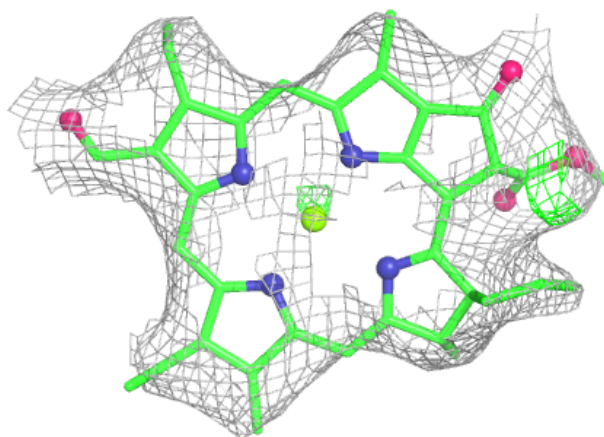
Electron density around LHG D 319:

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



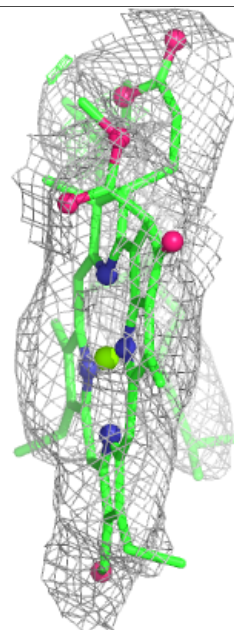
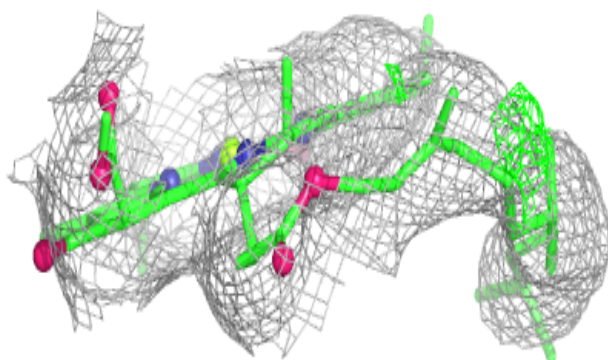
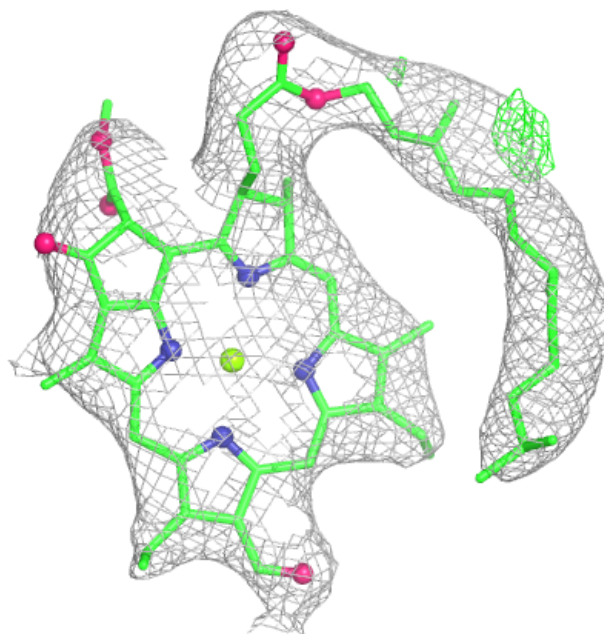
Electron density around CHL C 310:

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



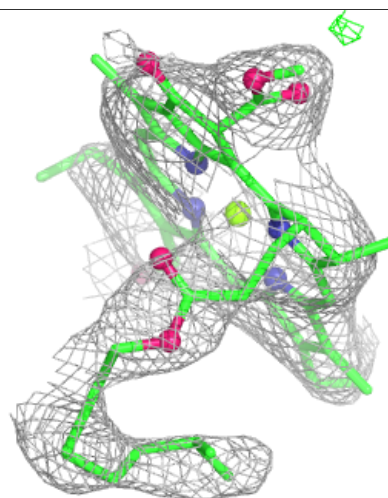
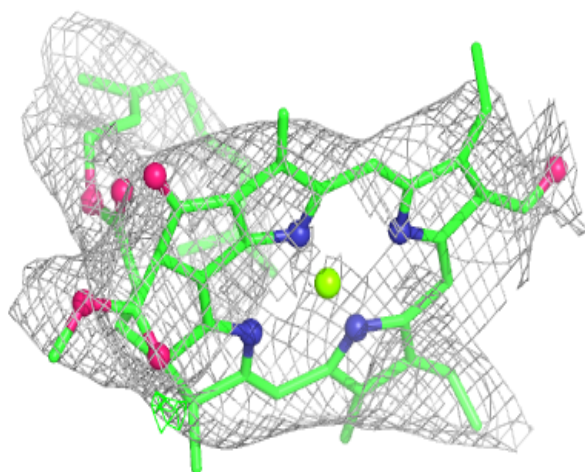
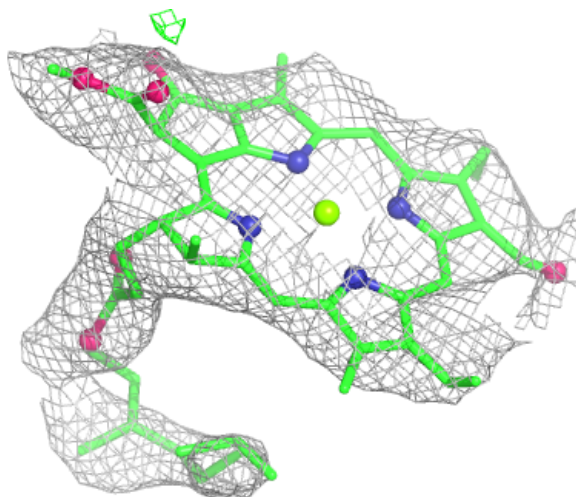
Electron density around CHL C 311:

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



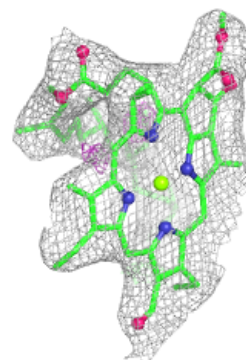
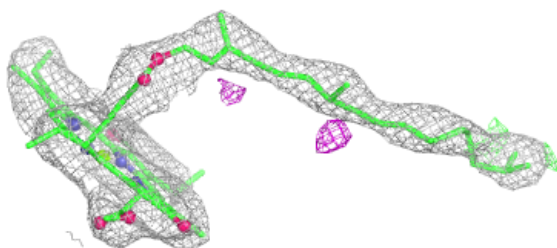
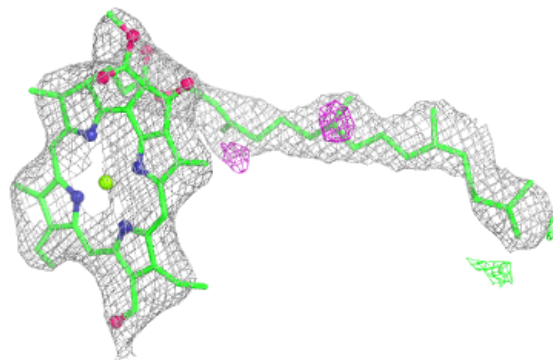
Electron density around CHL C 312:

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



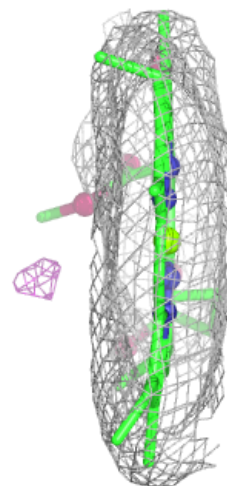
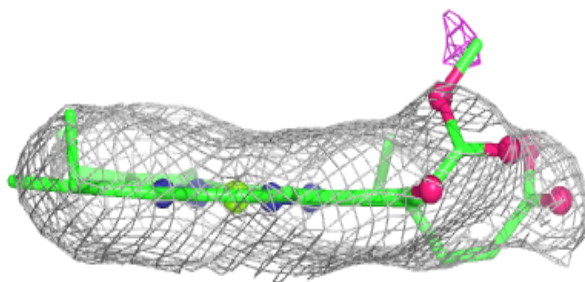
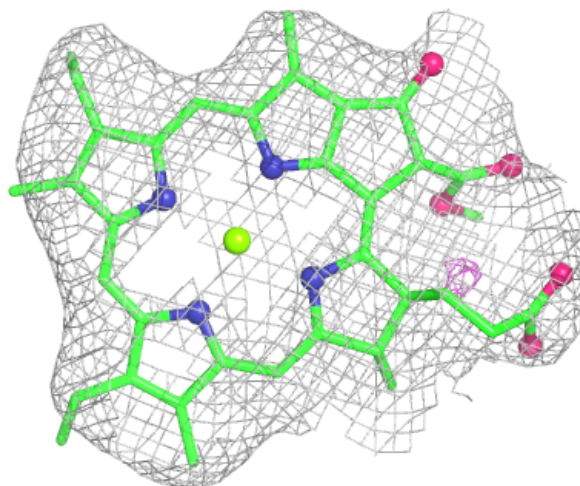
Electron density around CHL C 313:

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



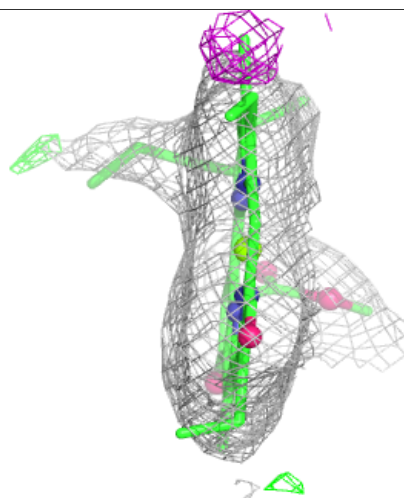
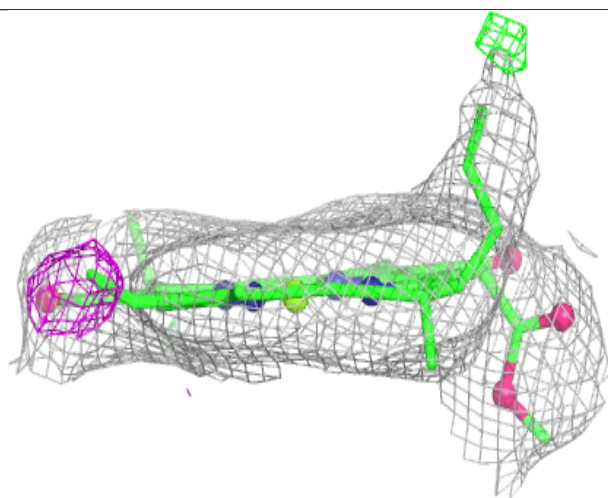
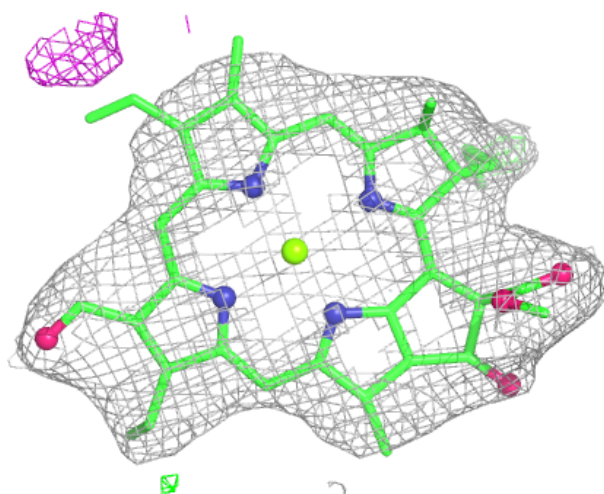
Electron density around CLA C 316:

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



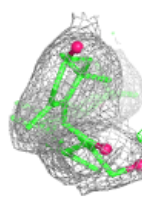
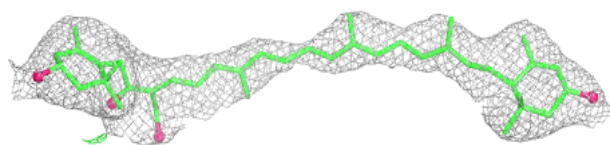
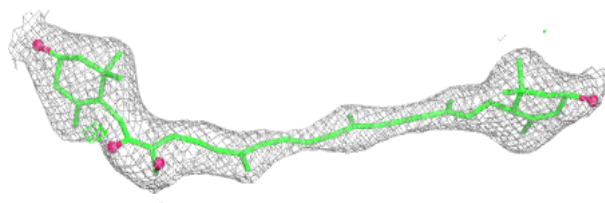
Electron density around CHL C 318:

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



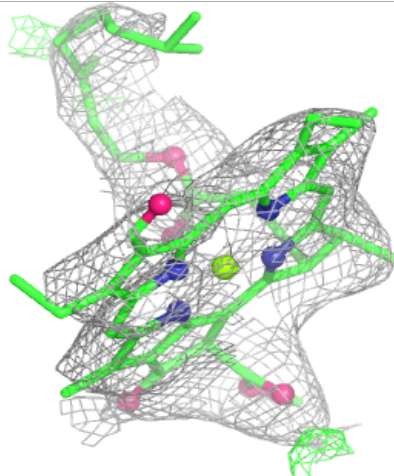
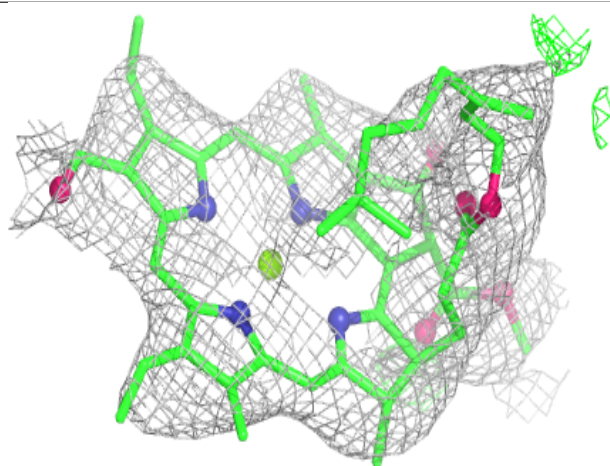
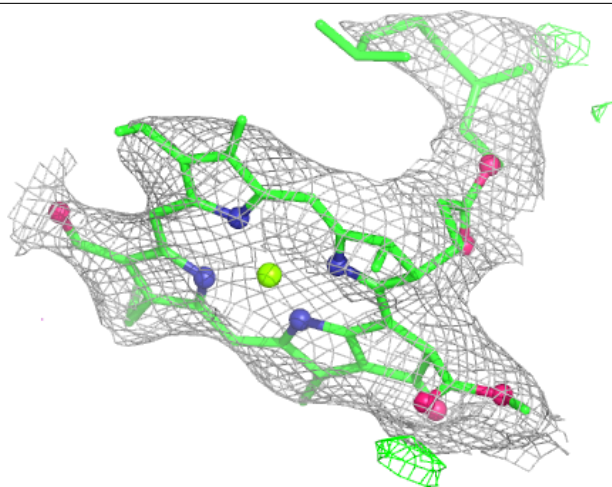
Electron density around OIE A 302:

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



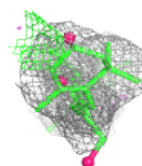
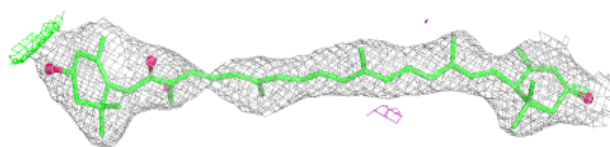
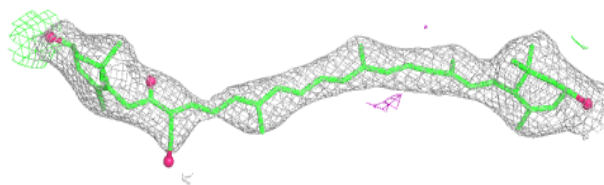
Electron density around CHL A 312:

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

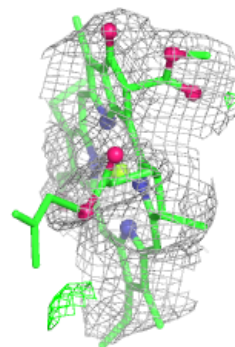
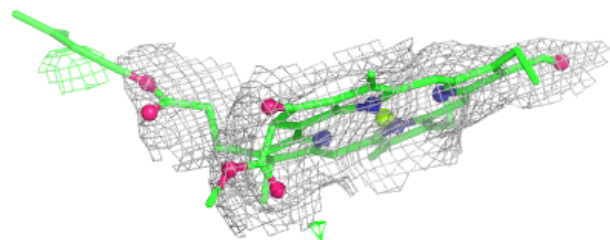
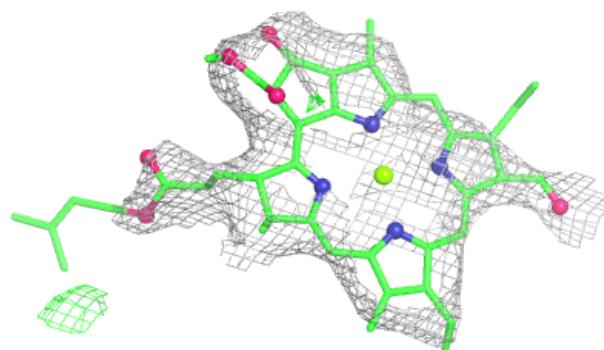


Electron density around OIE C 301:

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

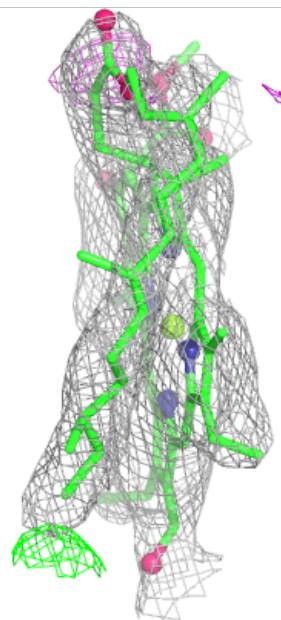
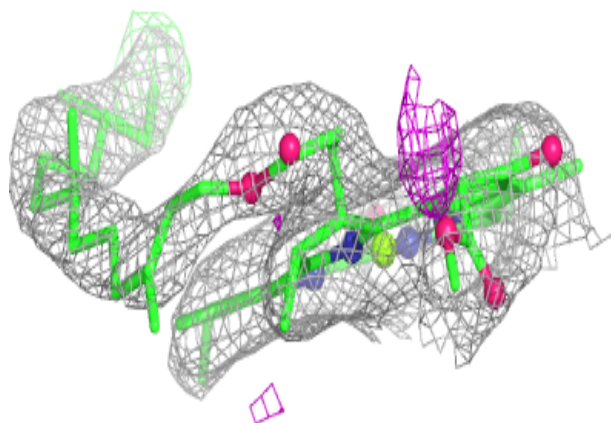
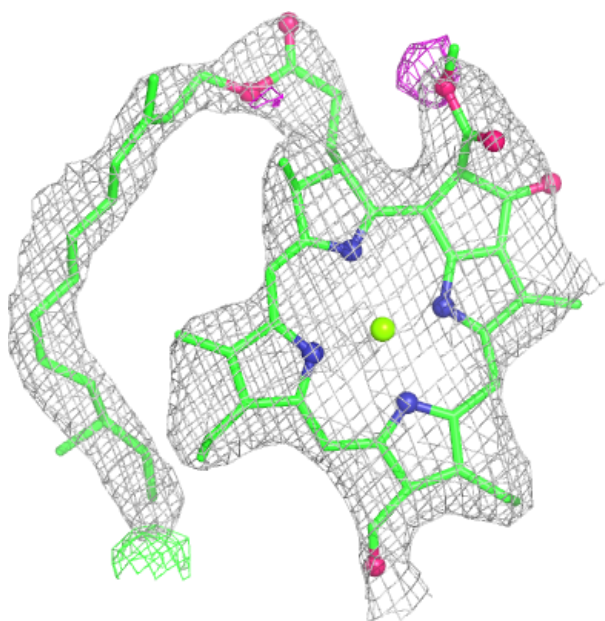
**Electron density around CHL B 311:**

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



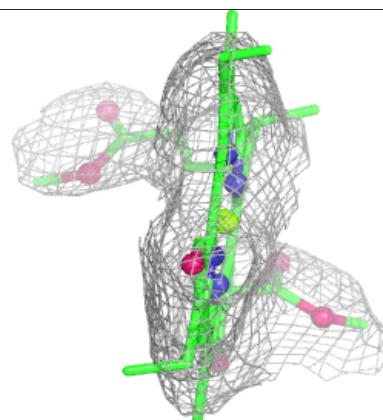
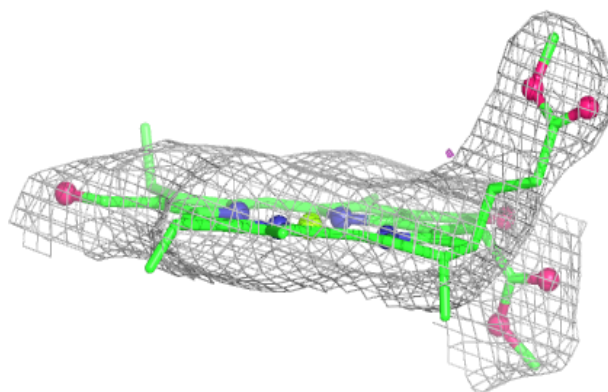
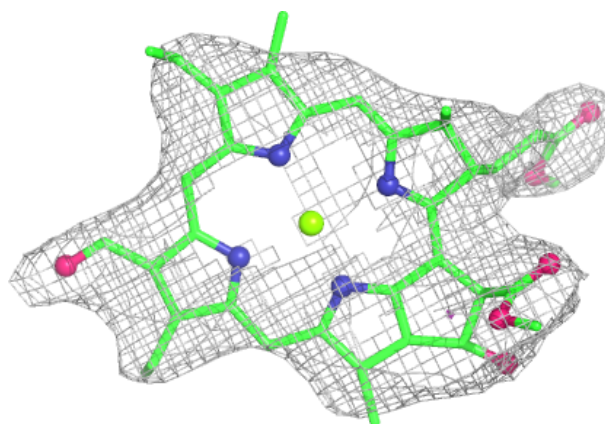
Electron density around CHL B 312:

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

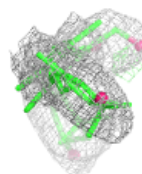
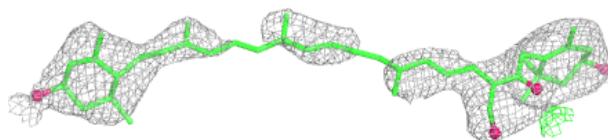
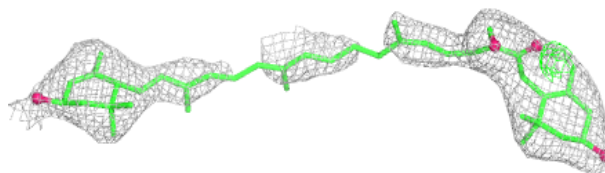


Electron density around CHL B 319:

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

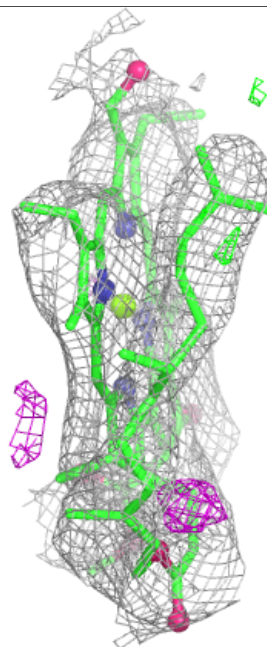
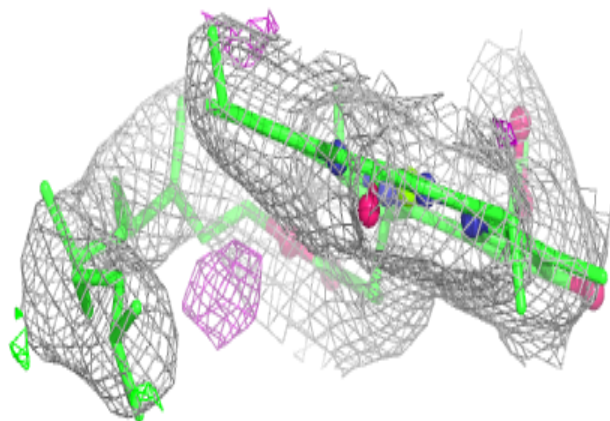
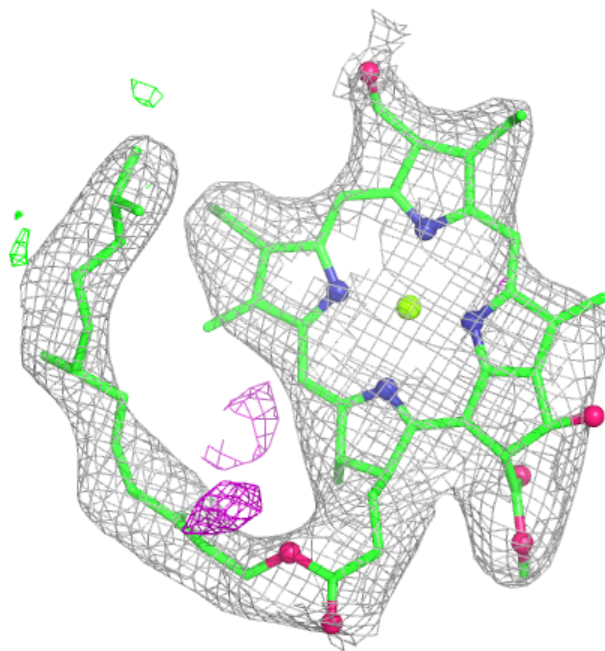
**Electron density around OIE E 302:**

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



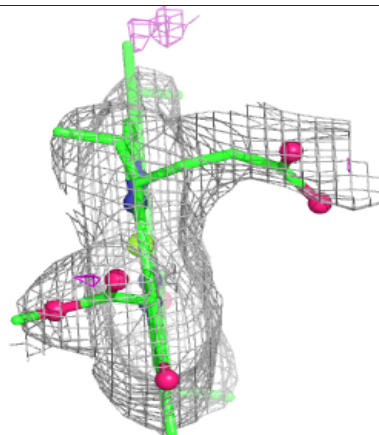
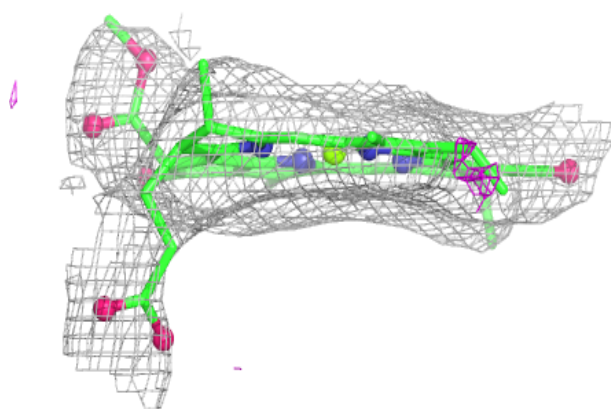
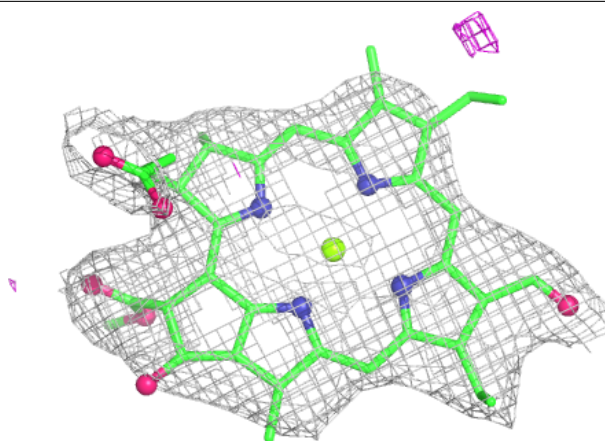
Electron density around CHL F 310:

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



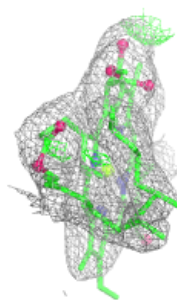
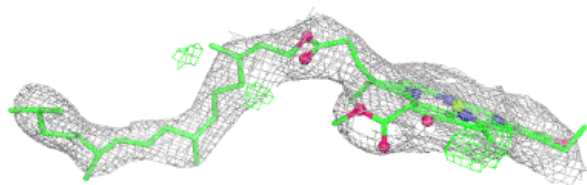
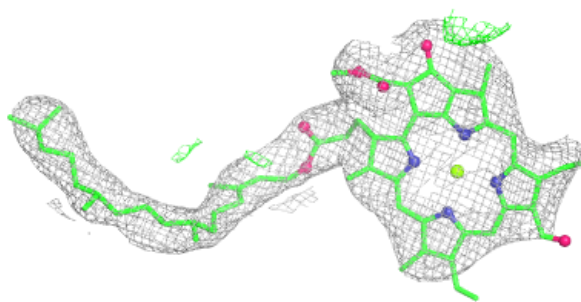
Electron density around CHL F 317:

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



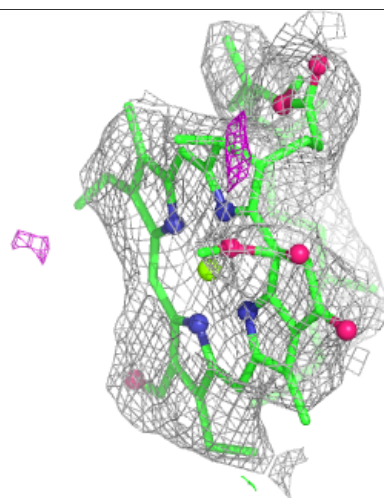
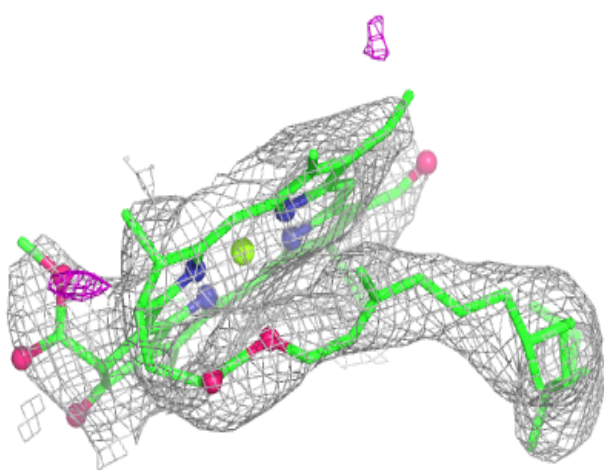
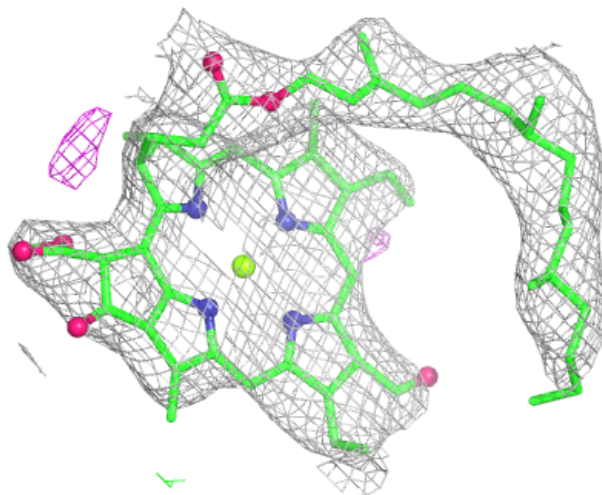
Electron density around CHL E 304:

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



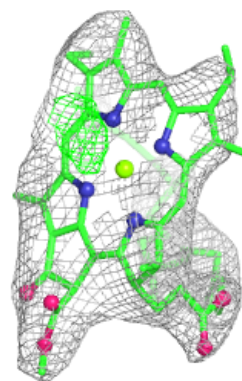
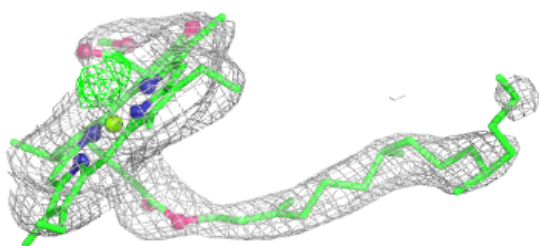
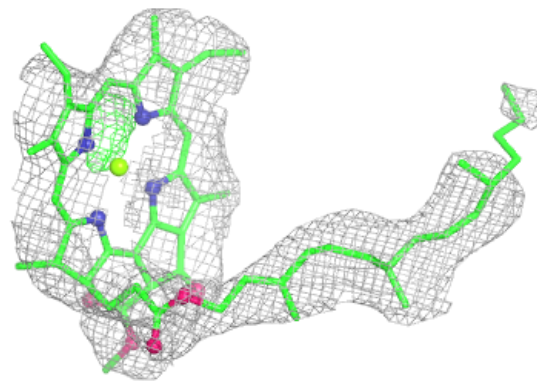
Electron density around CHL E 305:

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



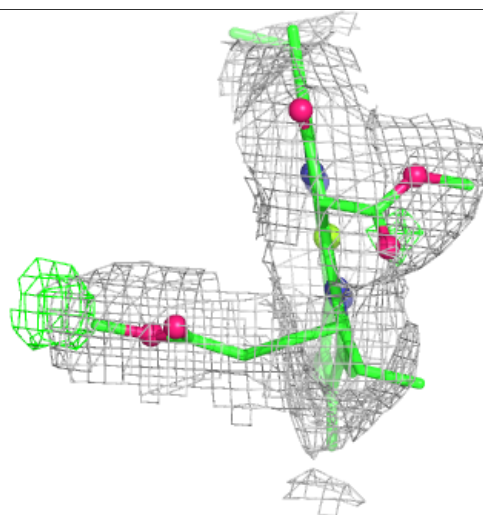
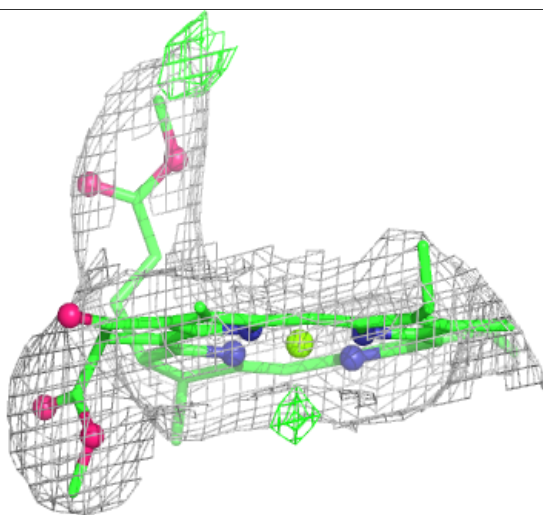
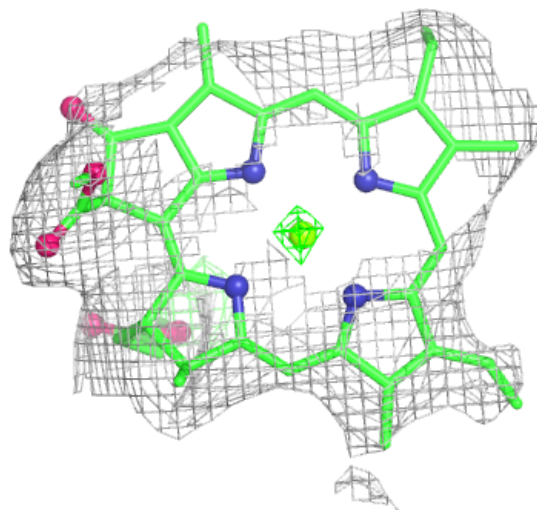
Electron density around CLA A 315:

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



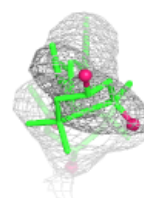
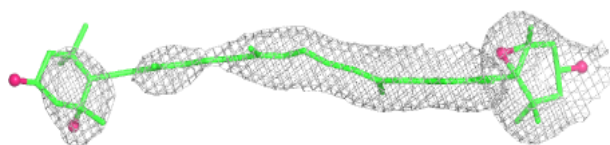
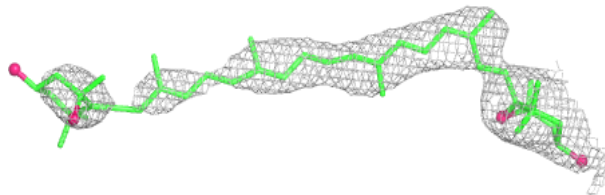
Electron density around CLA B 309:

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

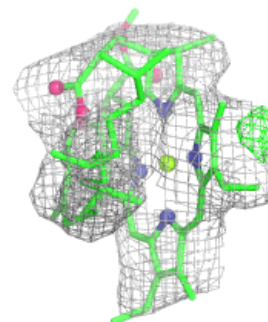
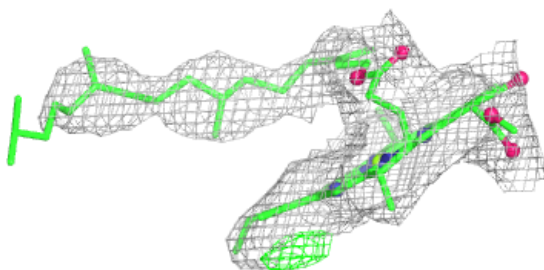
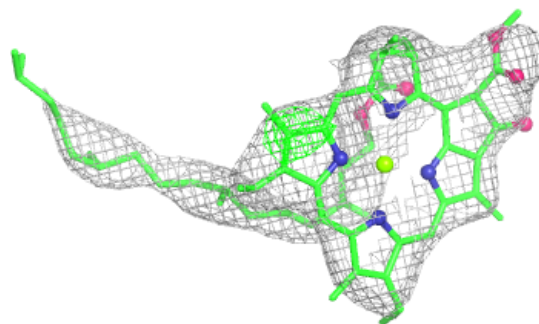


Electron density around NEX D 303:

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

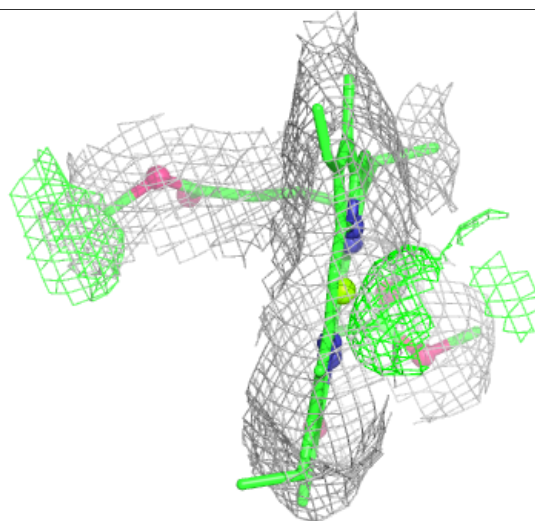
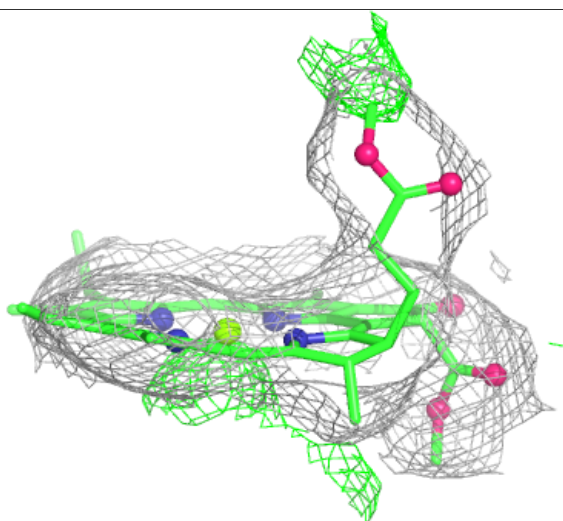
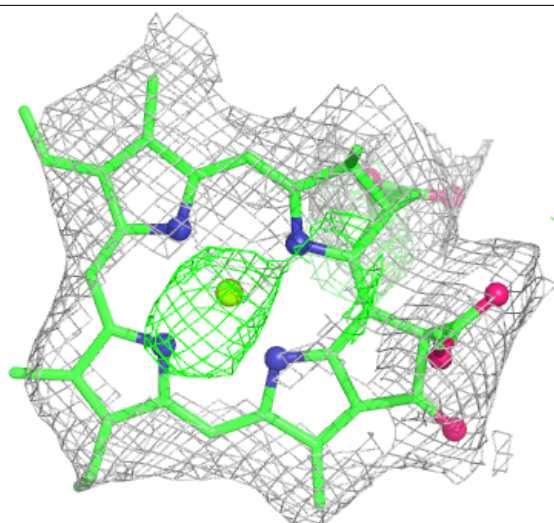
**Electron density around CLA B 318:**

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



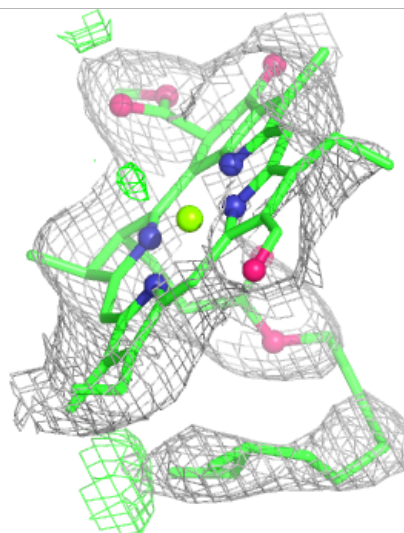
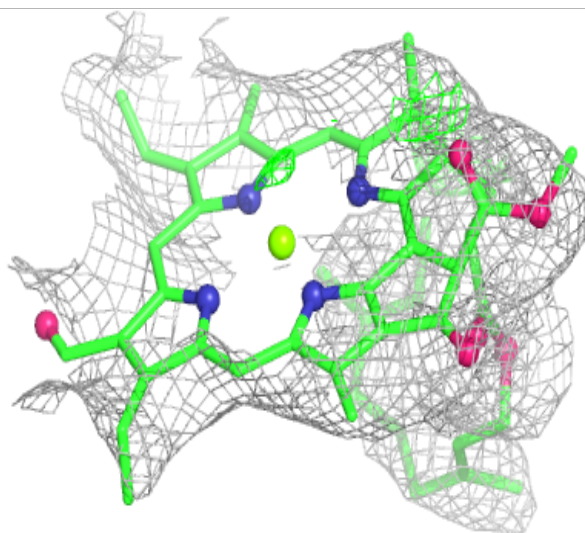
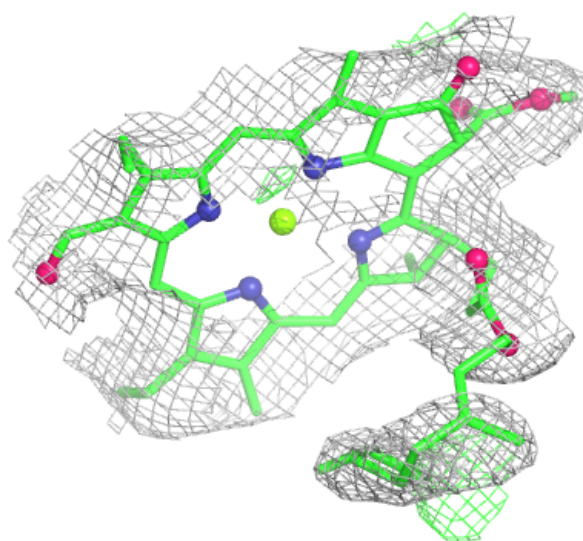
Electron density around CLA C 308:

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



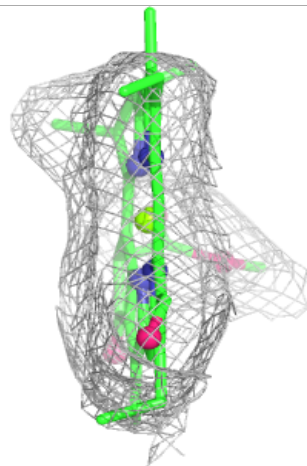
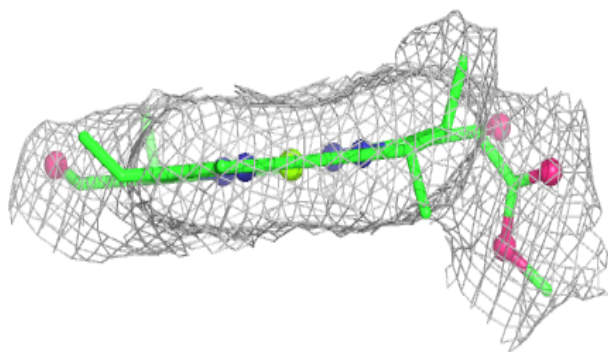
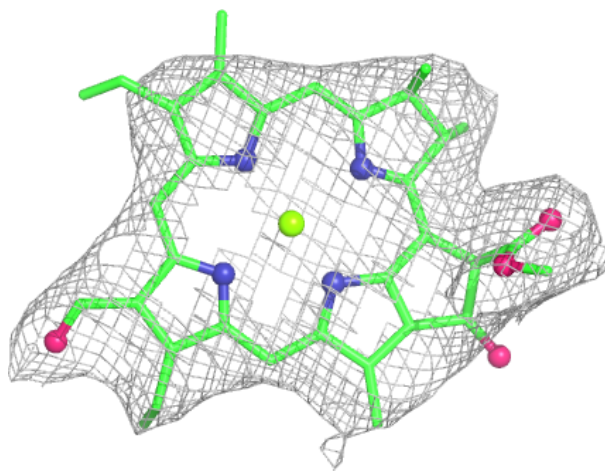
Electron density around CHL B 313:

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



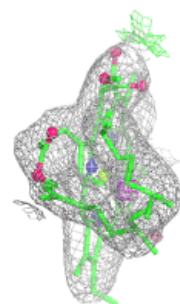
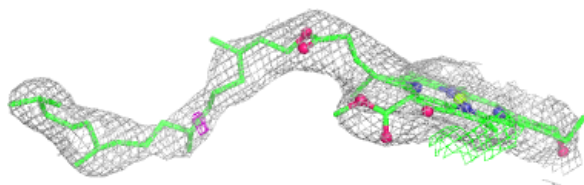
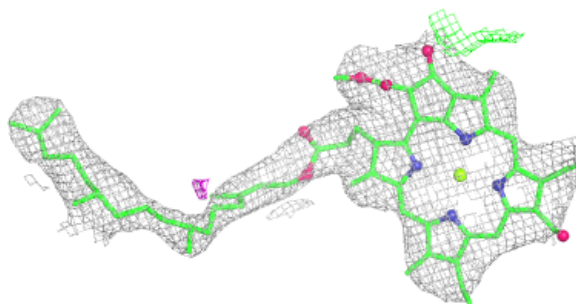
Electron density around CHL A 318:

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



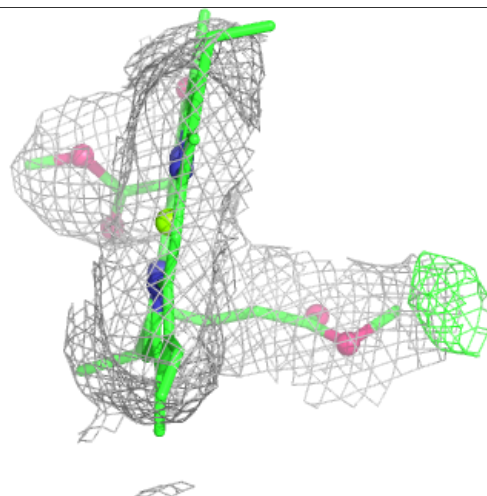
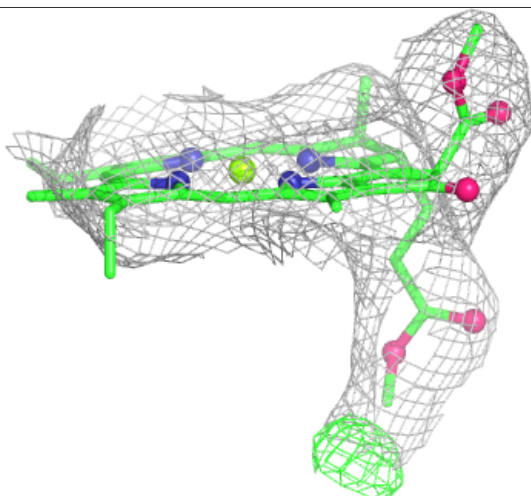
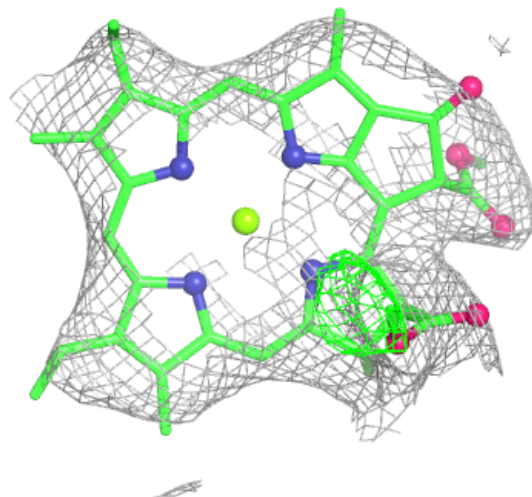
Electron density around CHL A 305:

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



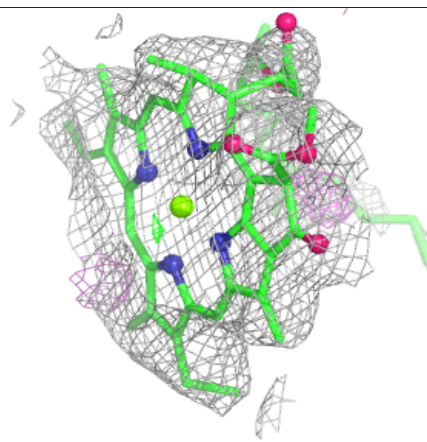
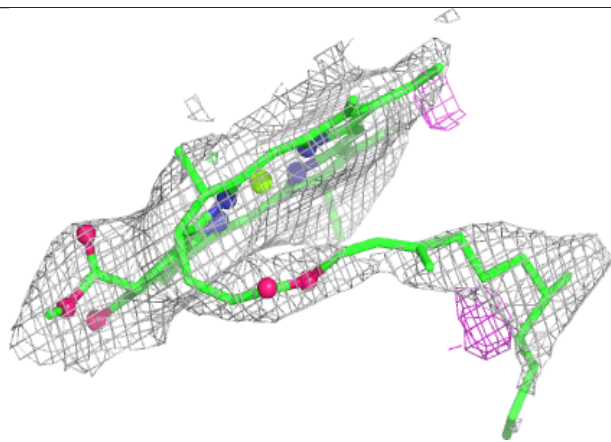
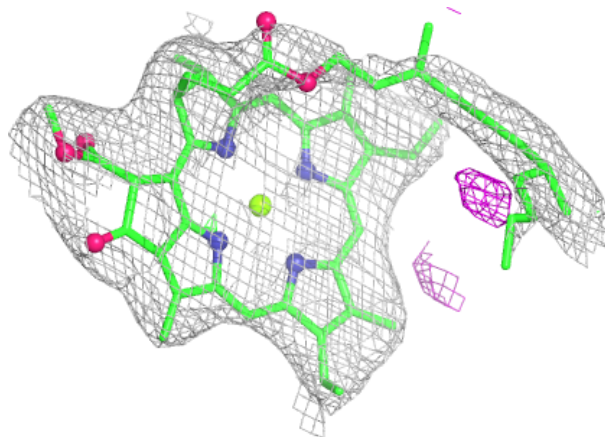
Electron density around CLA D 308:

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



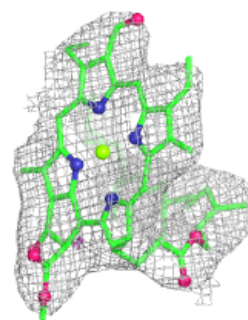
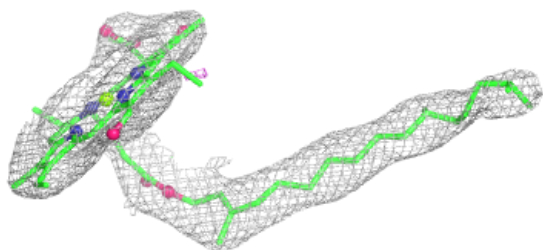
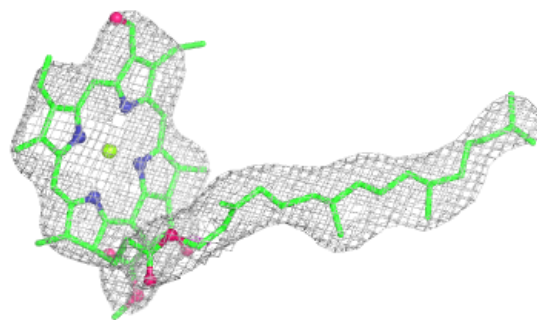
Electron density around CLA D 314:

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



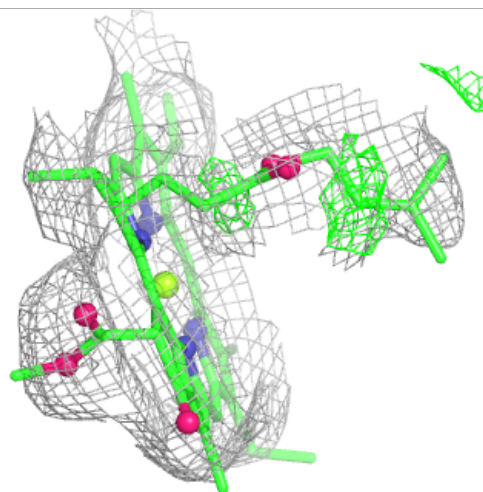
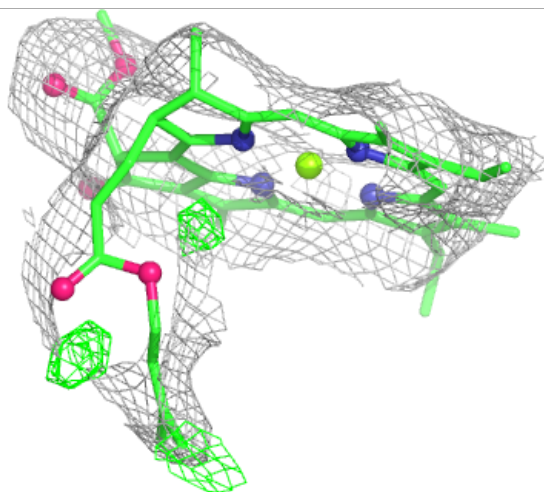
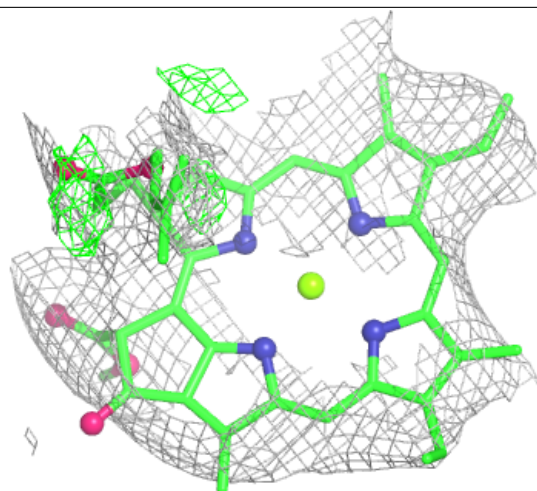
Electron density around CHL E 312:

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



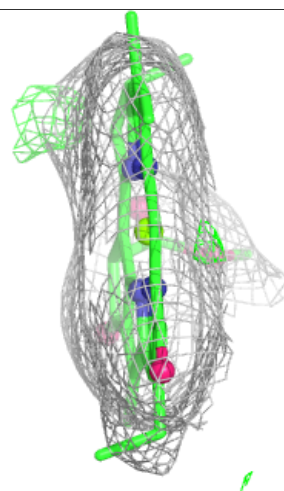
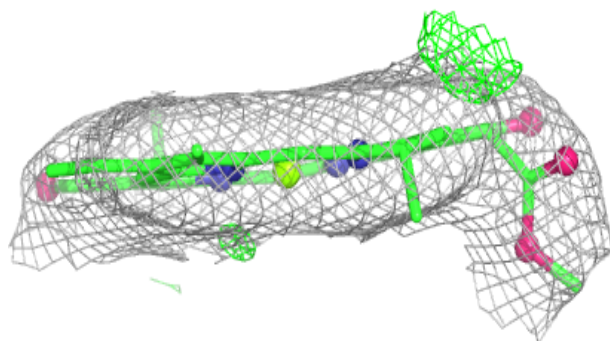
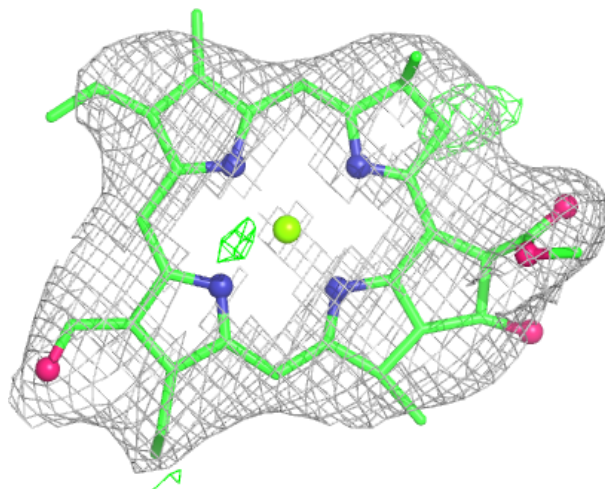
Electron density around CLA E 307:

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



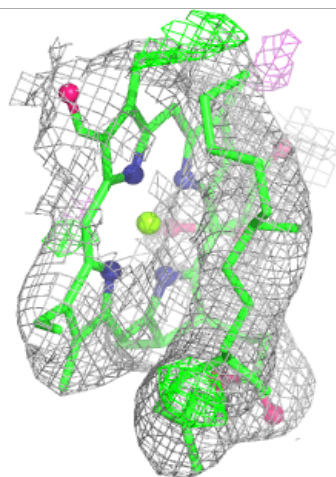
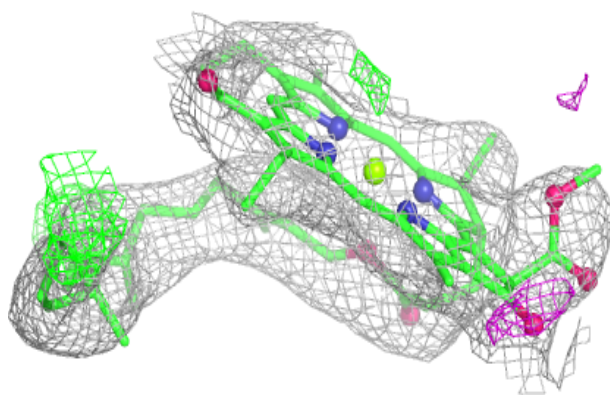
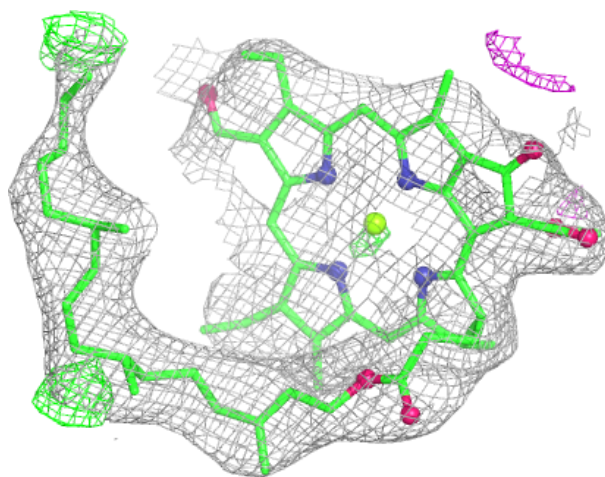
Electron density around CHL E 317:

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



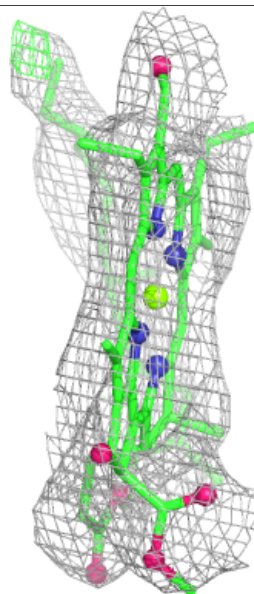
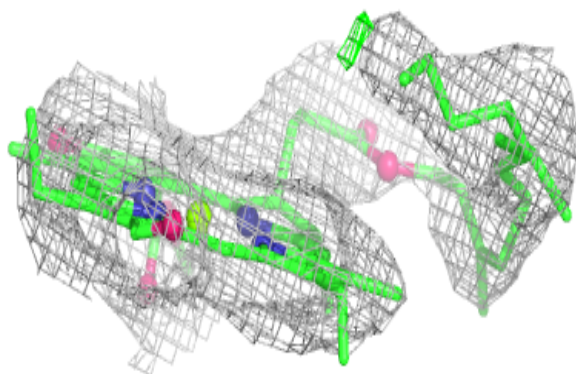
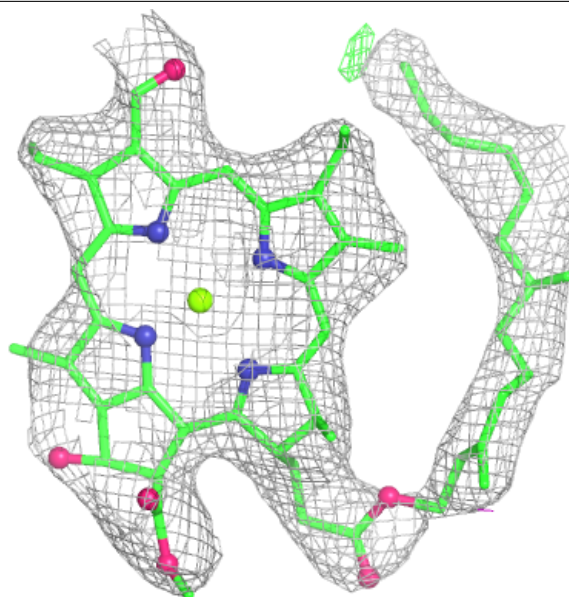
Electron density around CHL D 306:

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



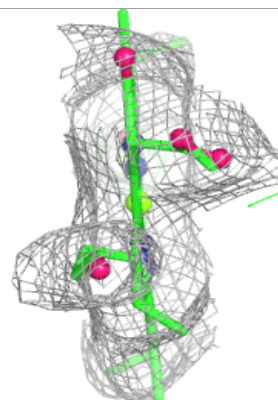
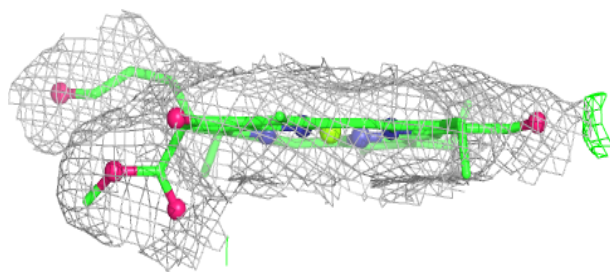
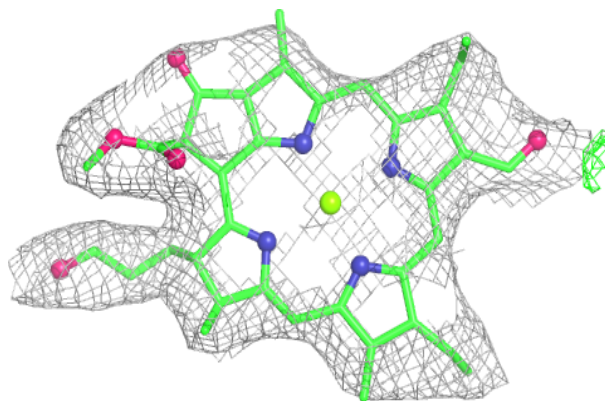
Electron density around CHL A 311:

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



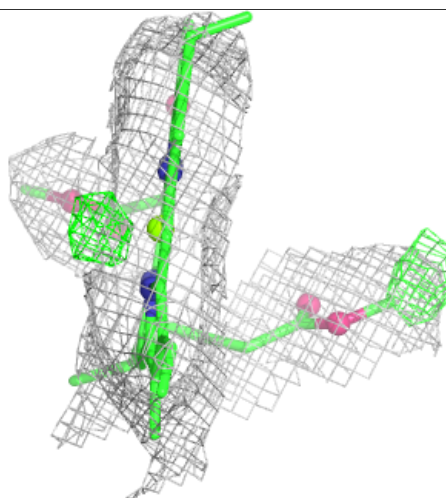
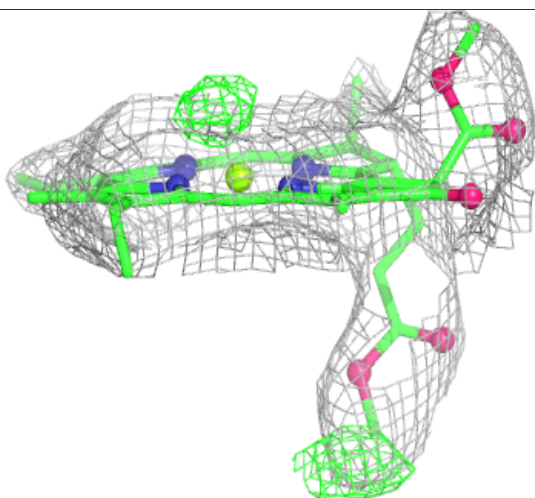
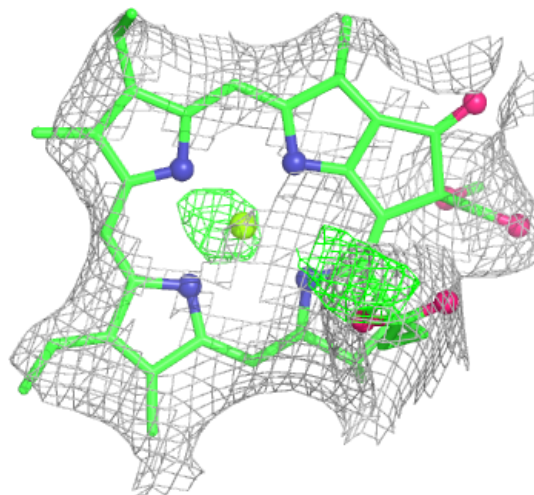
Electron density around CHL D 310:

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



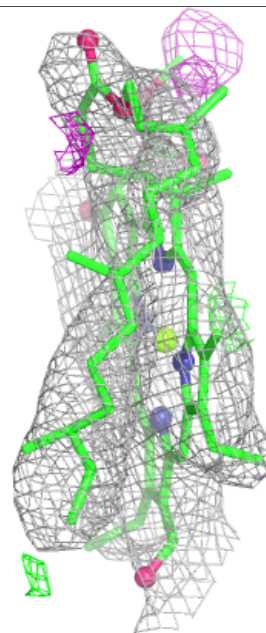
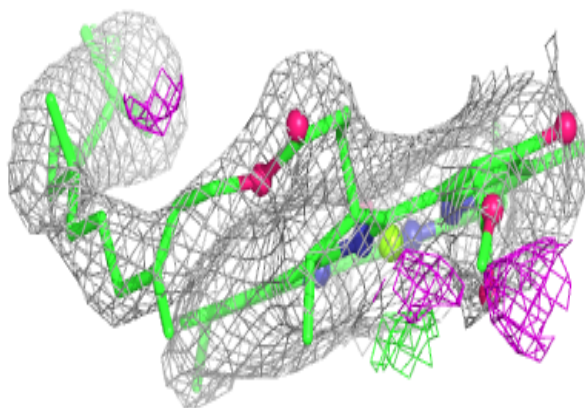
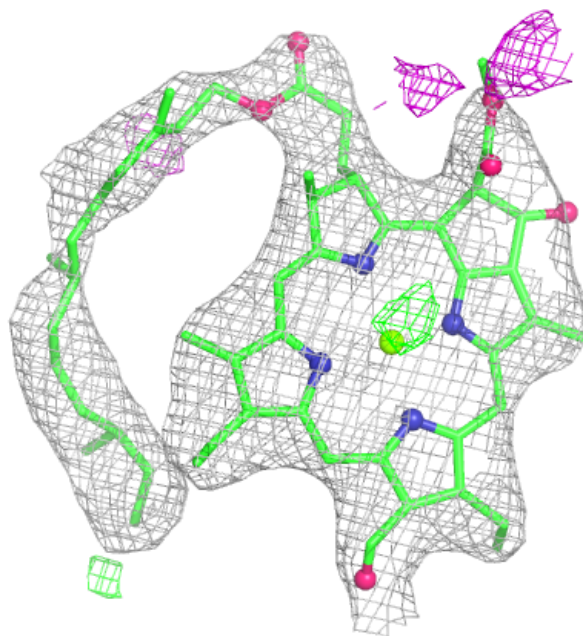
Electron density around CLA F 307:

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



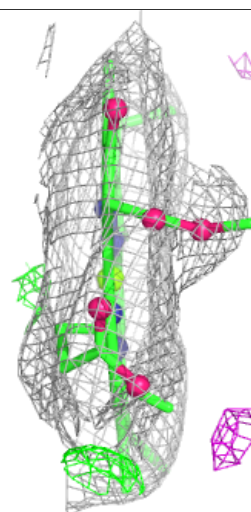
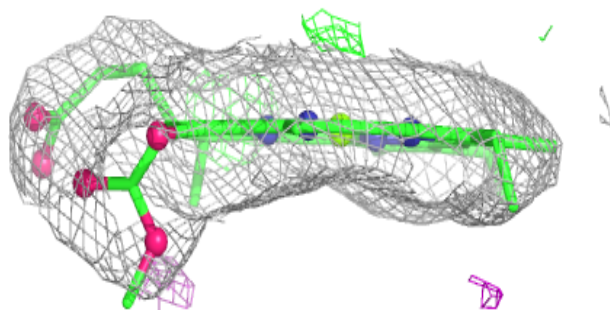
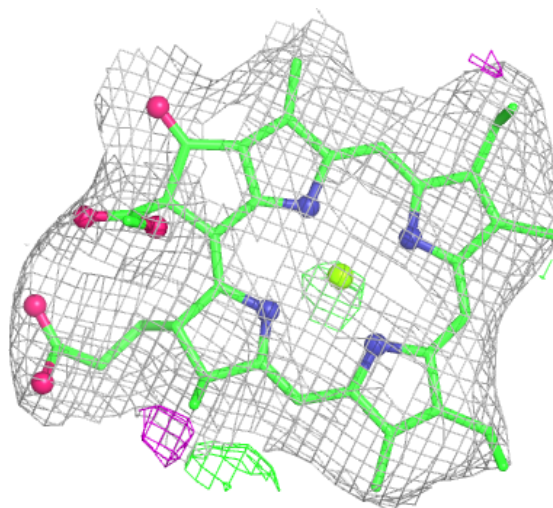
Electron density around CHL D 311:

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



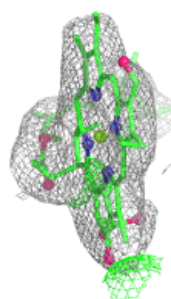
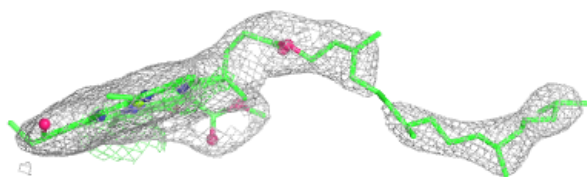
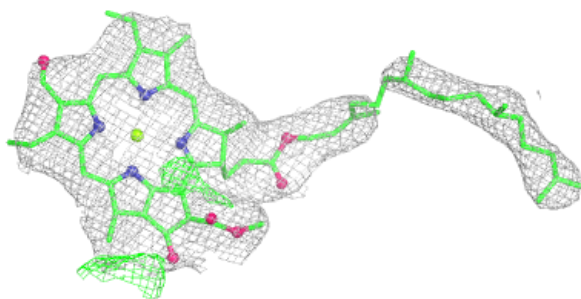
Electron density around CLA F 315:

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

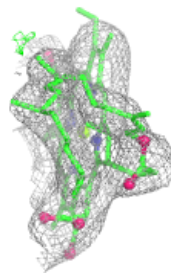
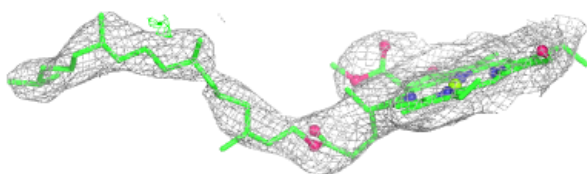
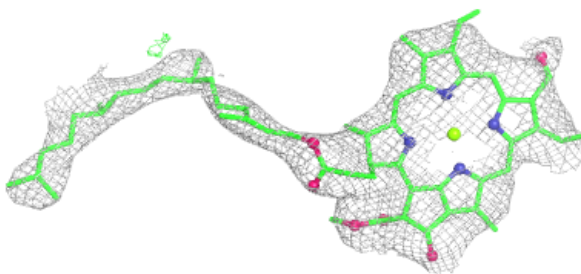


Electron density around CHL B 306:

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

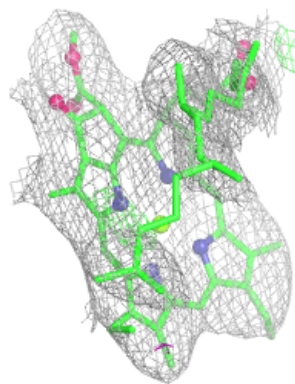
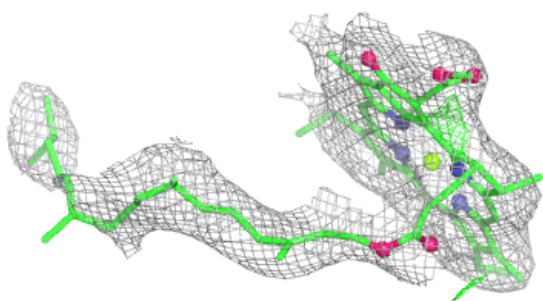
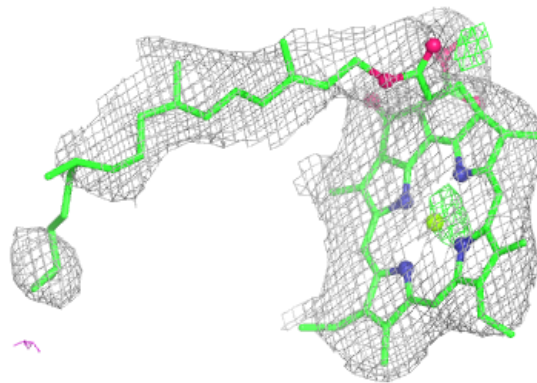
**Electron density around CHL D 305:**

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

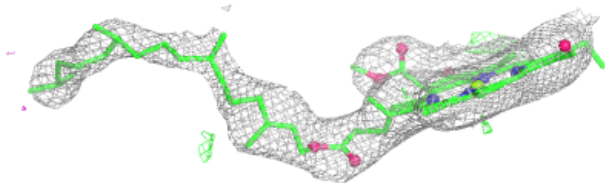
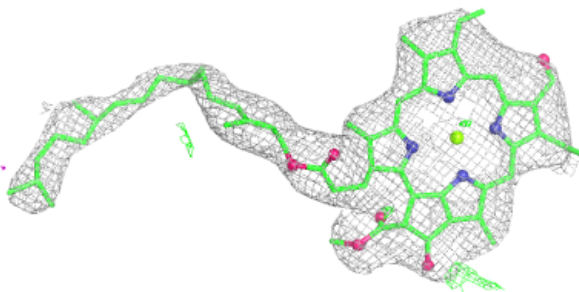


Electron density around CLA B 316:

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

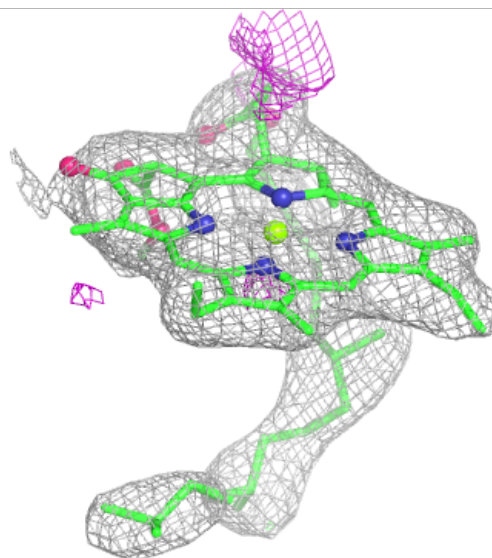
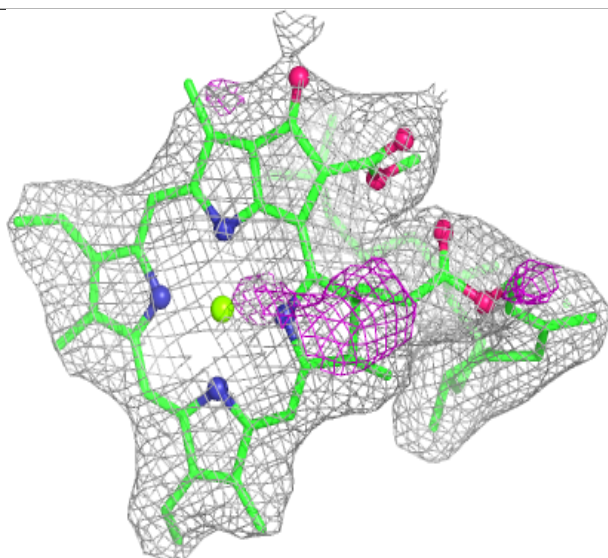
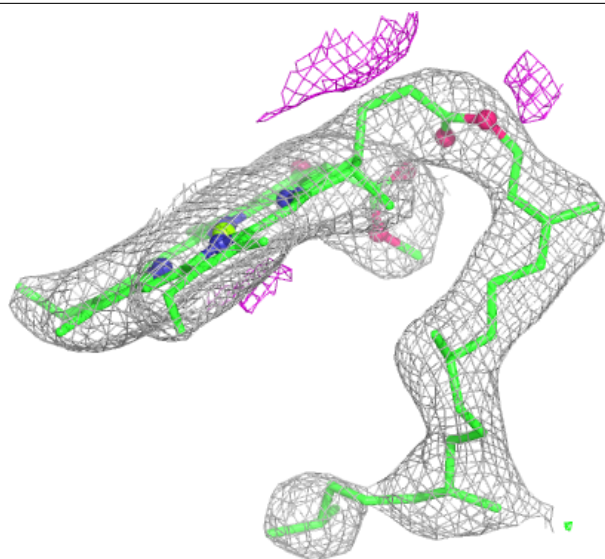
**Electron density around CHL C 305:**

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



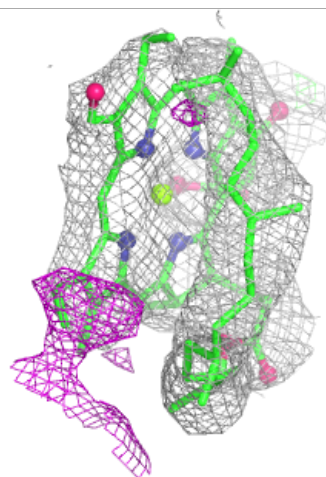
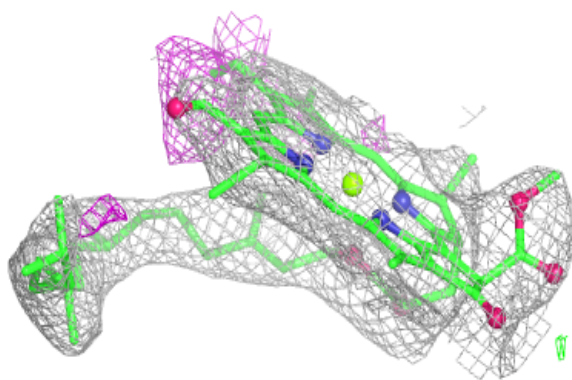
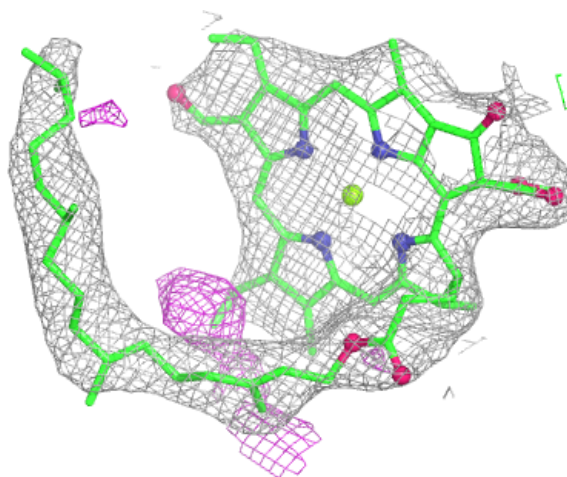
Electron density around CLA C 307:

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



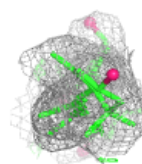
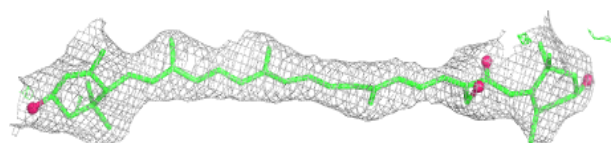
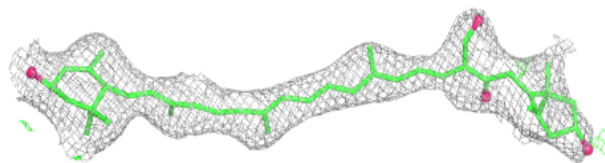
Electron density around CHL C 306:

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

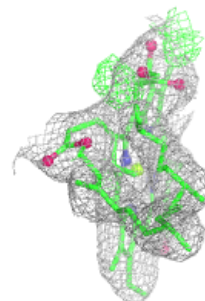
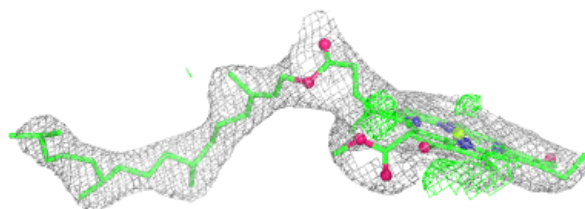
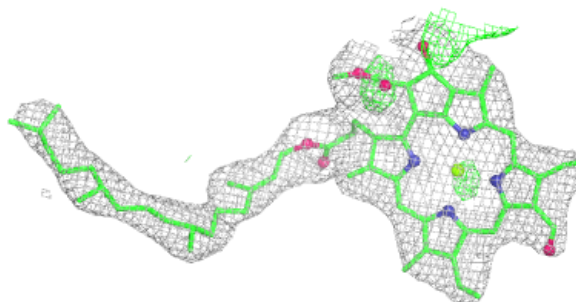


Electron density around OIE B 301:

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

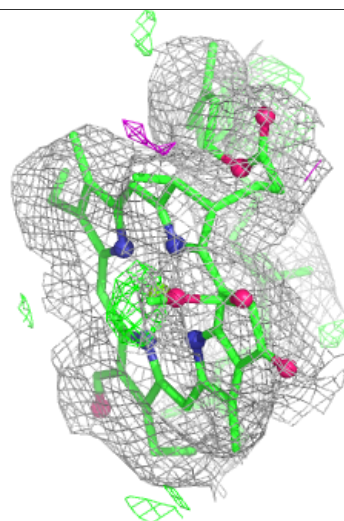
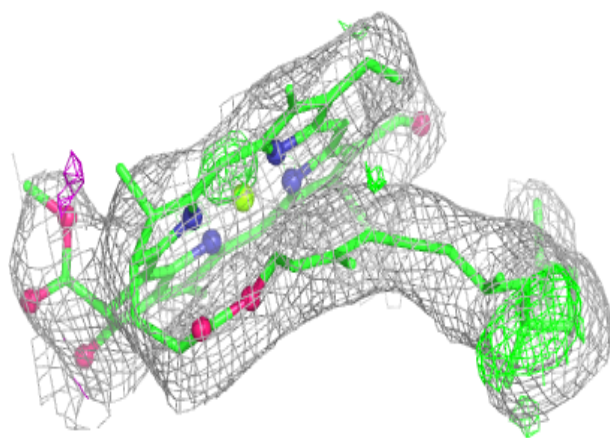
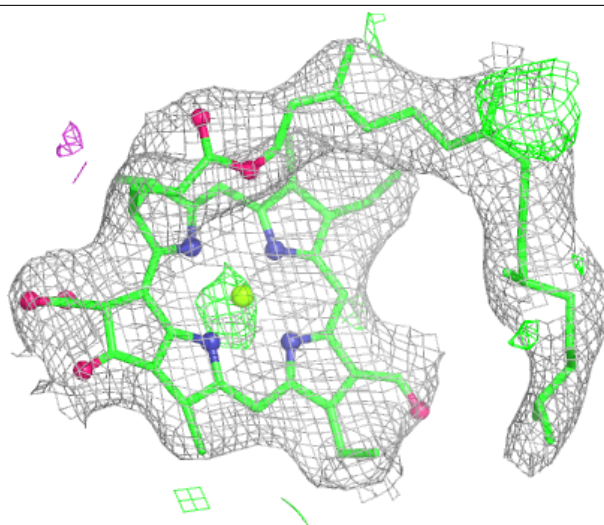
**Electron density around CHL F 304:**

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



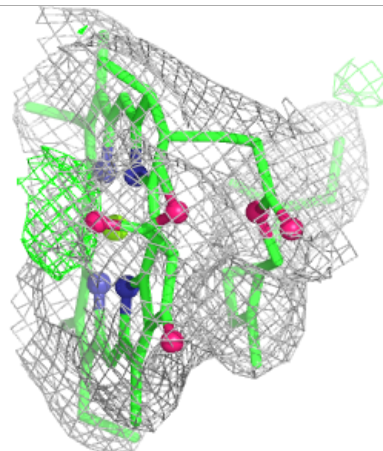
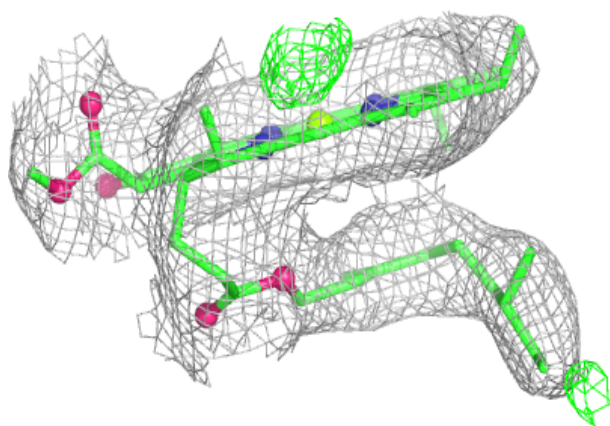
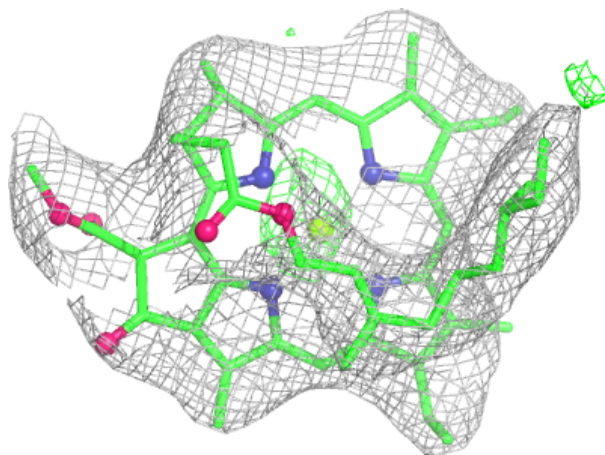
Electron density around CHL F 305:

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



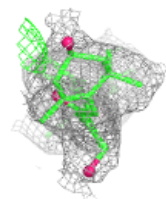
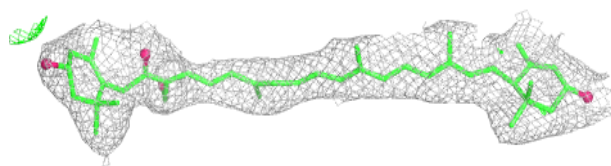
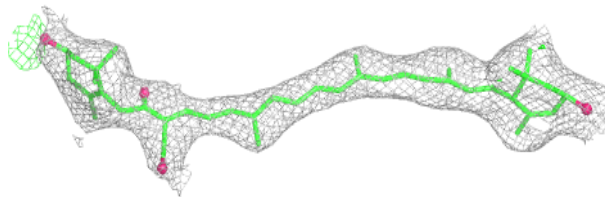
Electron density around CLA C 317:

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



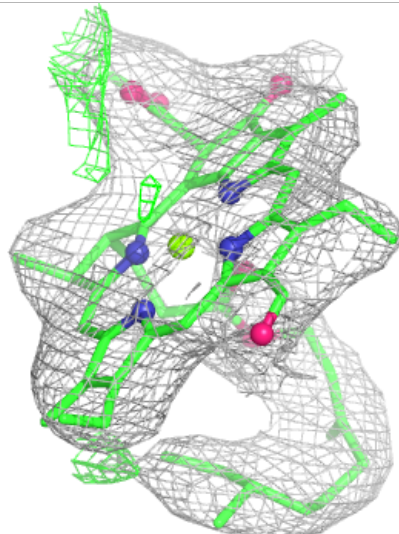
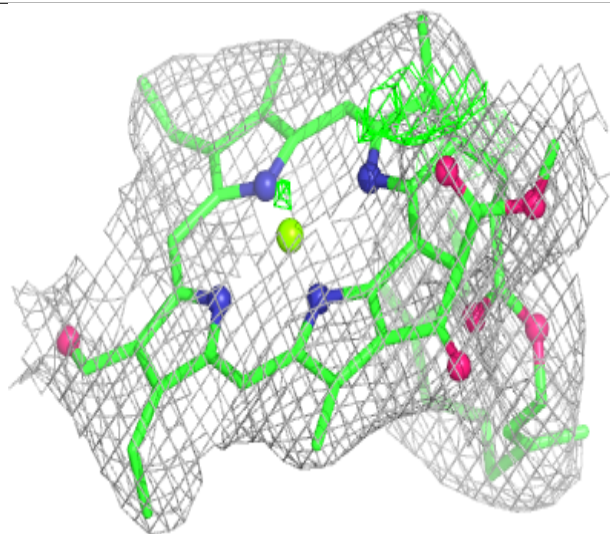
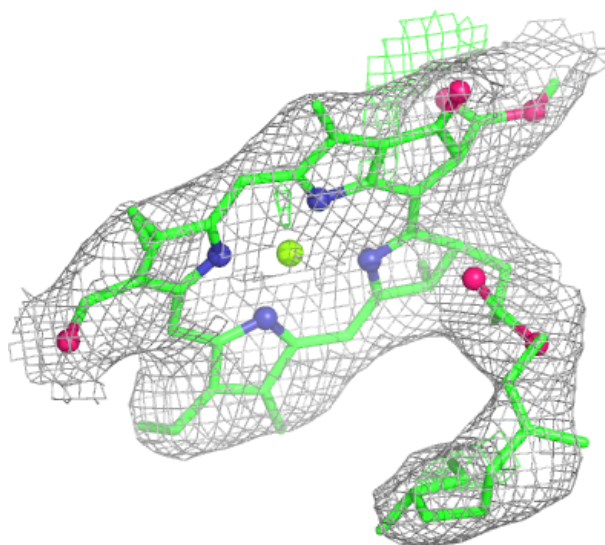
Electron density around OIE F 301:

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



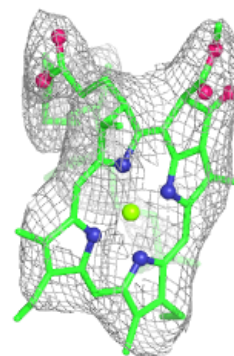
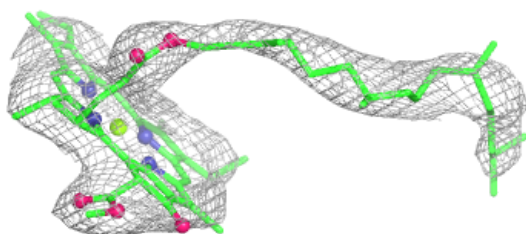
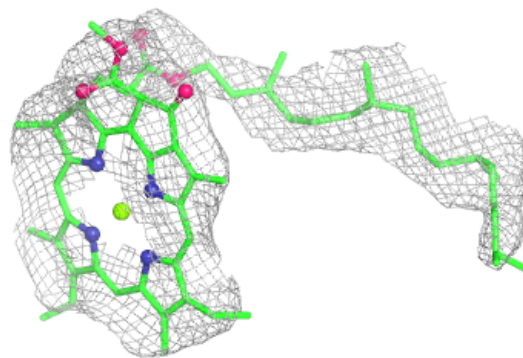
Electron density around CHL D 312:

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



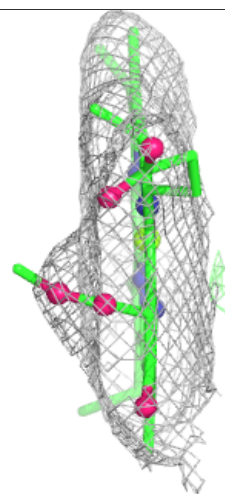
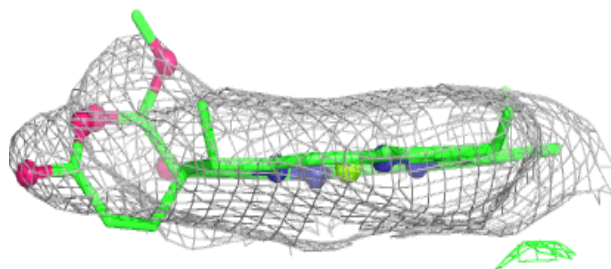
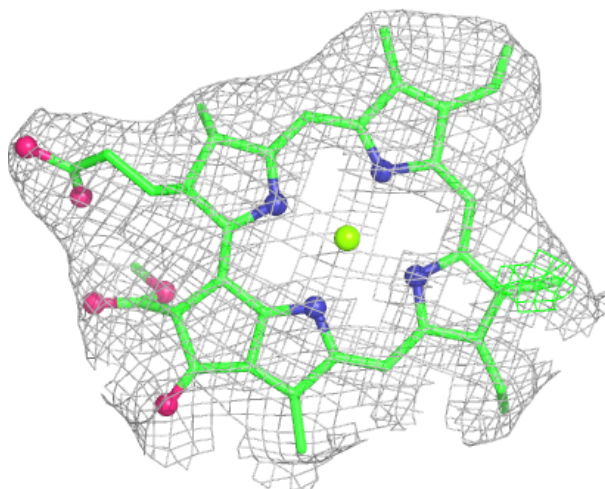
Electron density around CLA D 315:

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



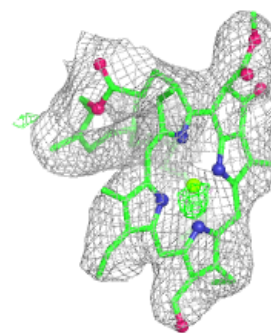
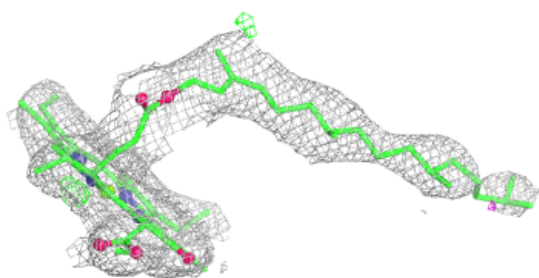
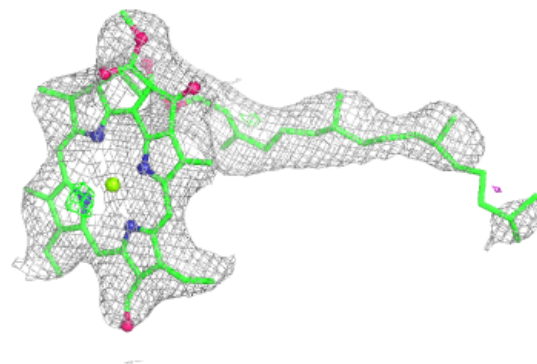
Electron density around CLA D 316:

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



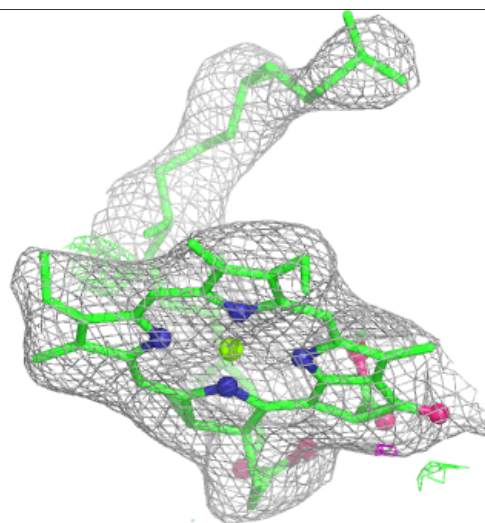
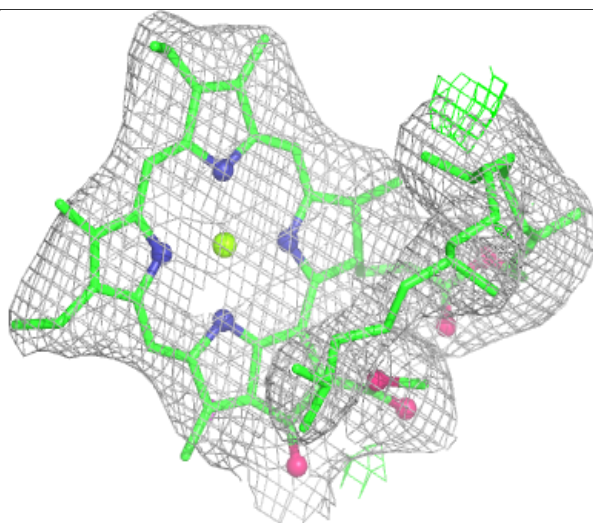
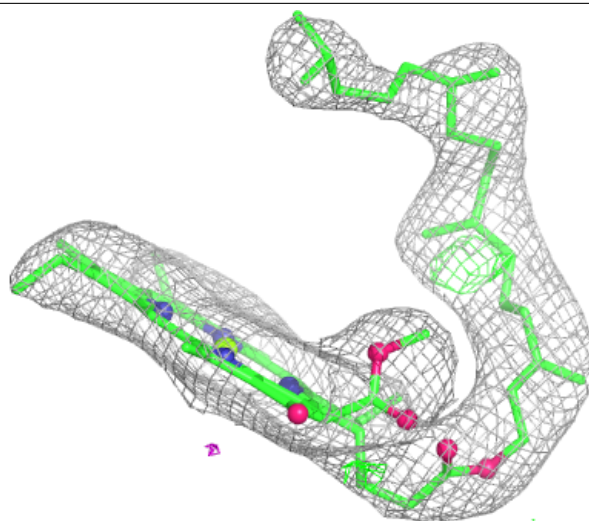
Electron density around CHL D 313:

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



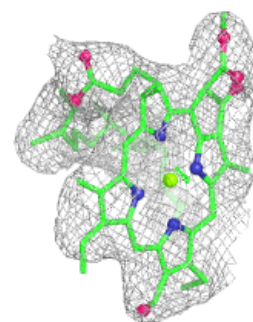
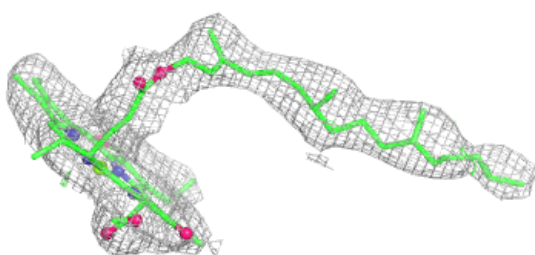
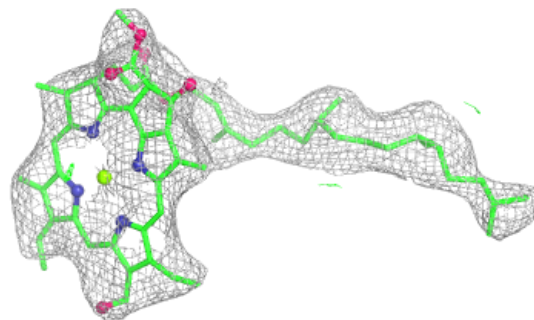
Electron density around CLA E 306:

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

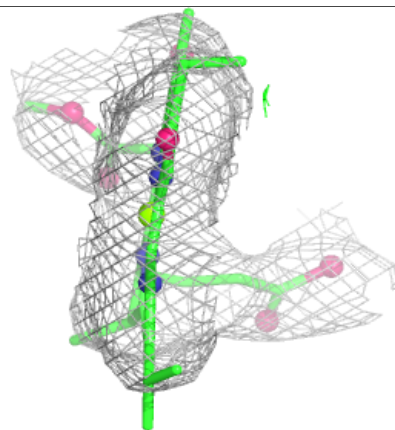
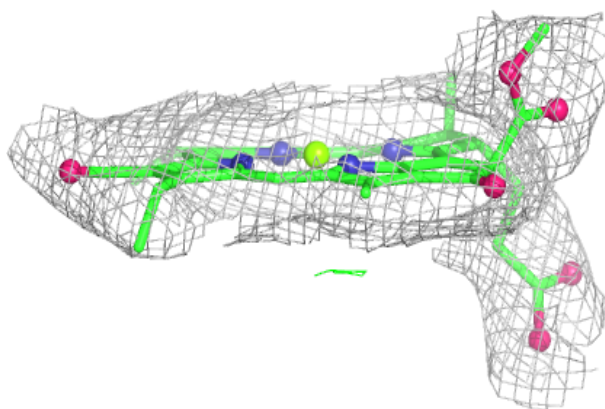
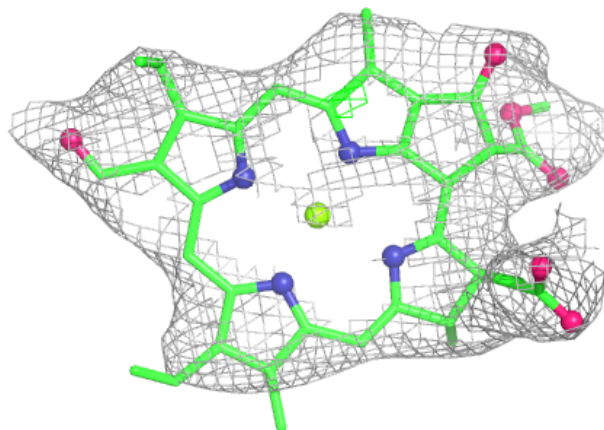


Electron density around CHL F 312:

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

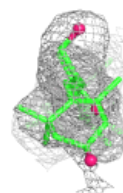
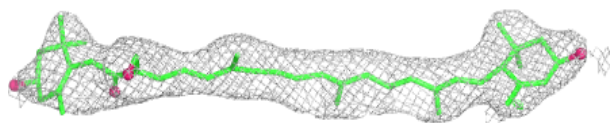
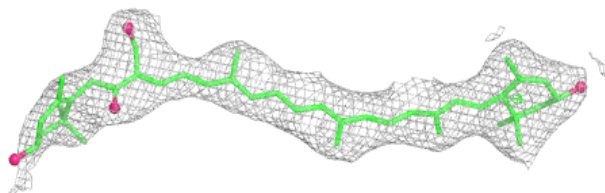
**Electron density around CHL D 318:**

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

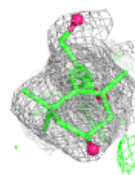
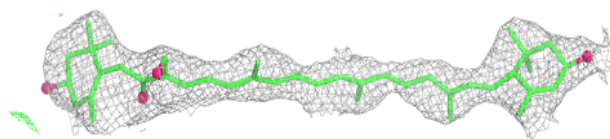
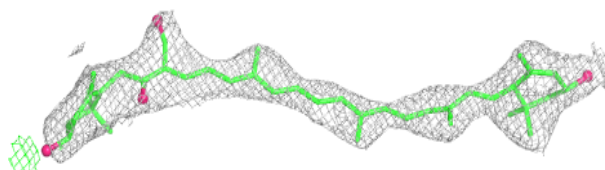


Electron density around OIE A 301:

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

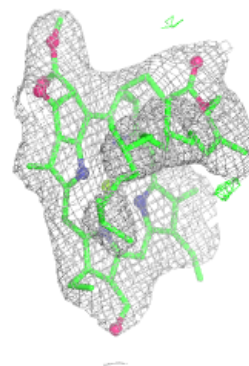
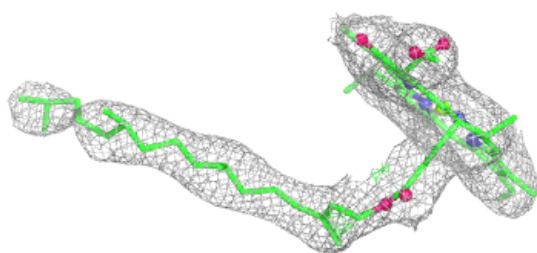
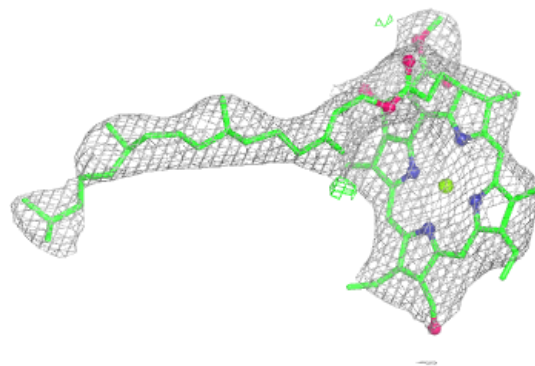
**Electron density around OIE E 301:**

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



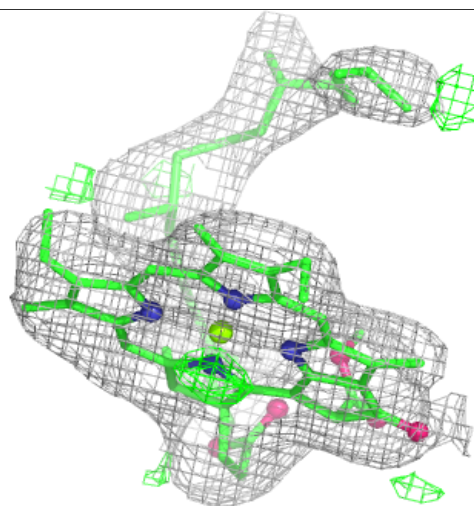
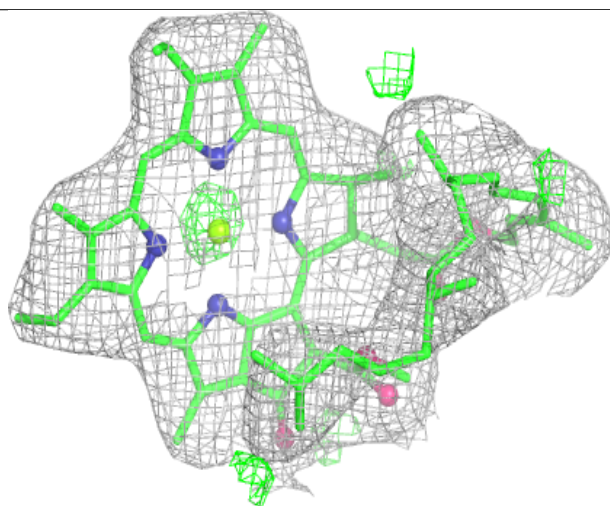
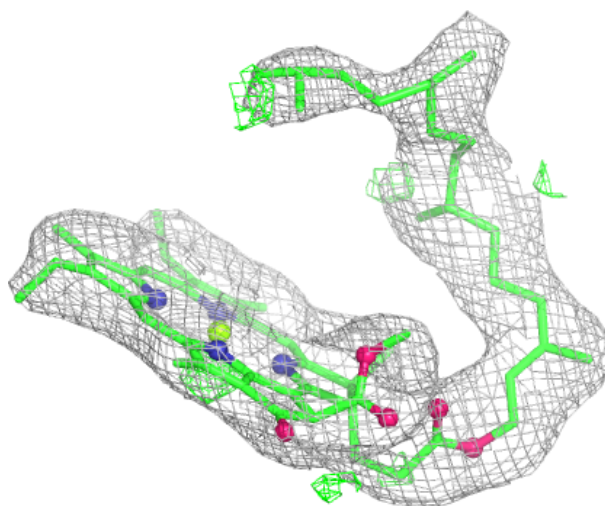
Electron density around CHL B 314:

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



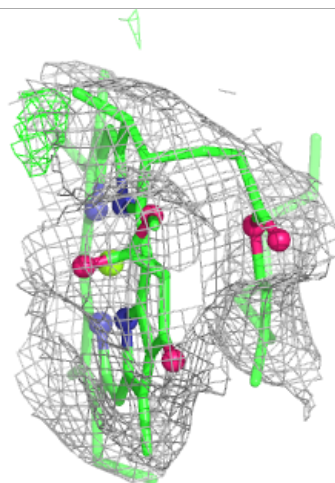
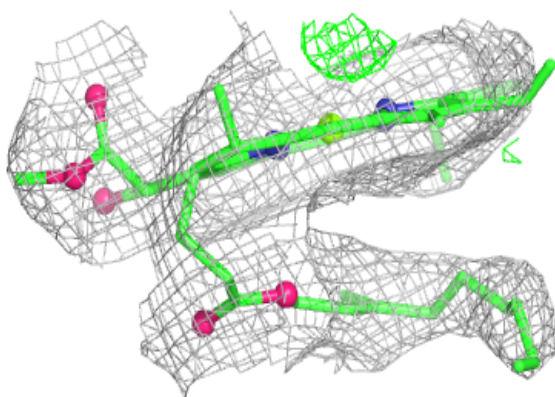
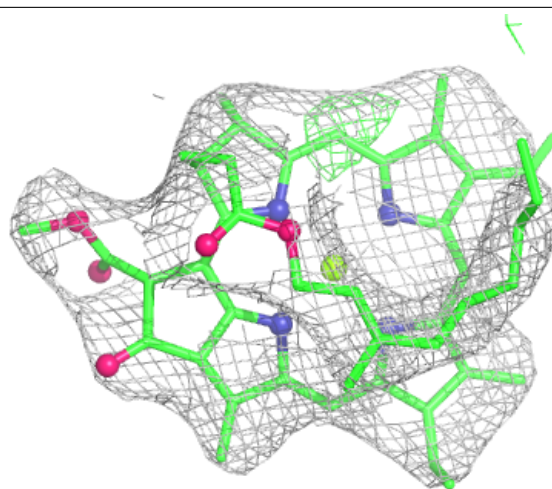
Electron density around CLA F 306:

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



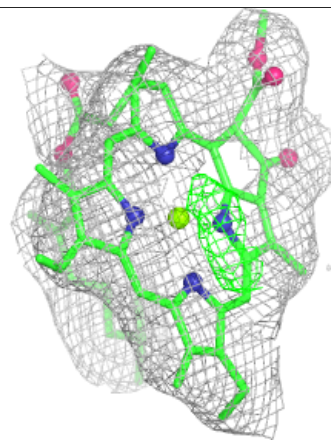
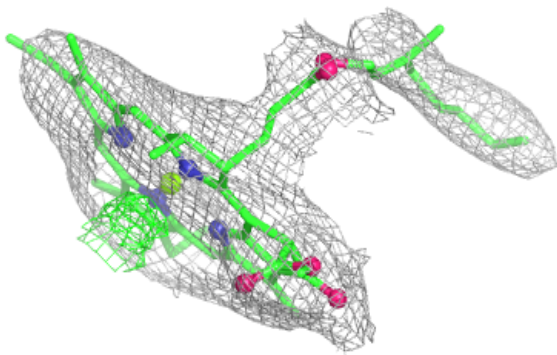
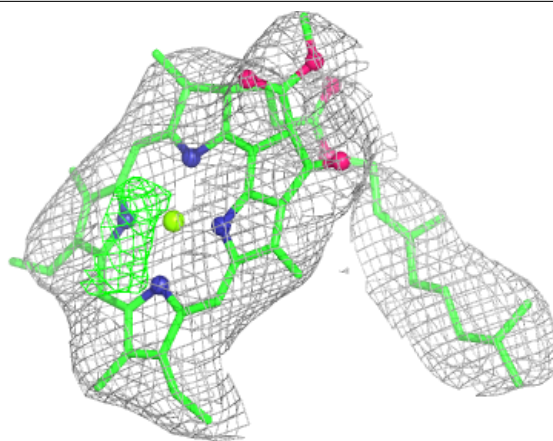
Electron density around CLA A 317:

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



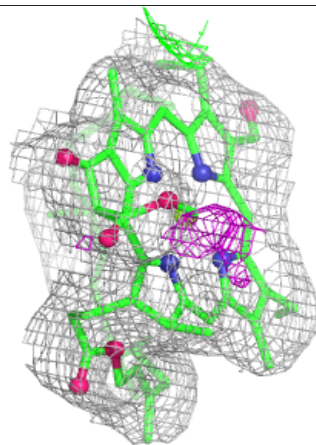
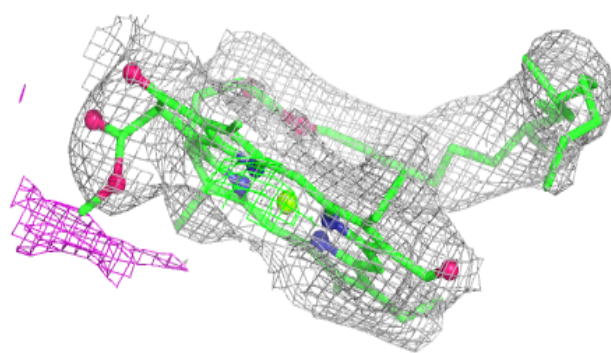
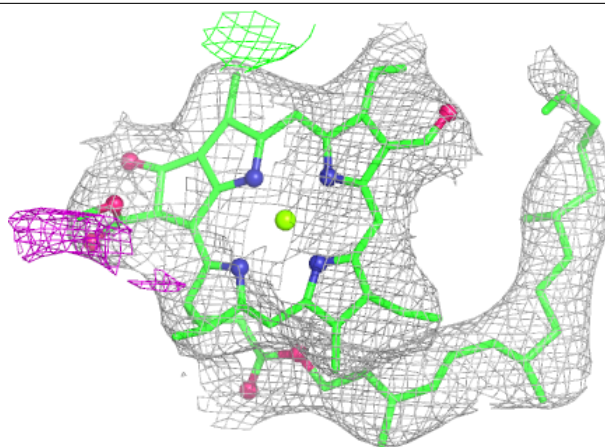
Electron density around CLA F 314:

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



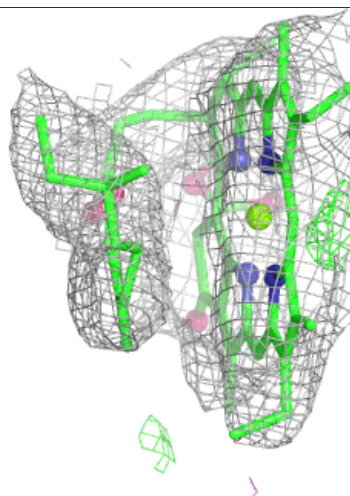
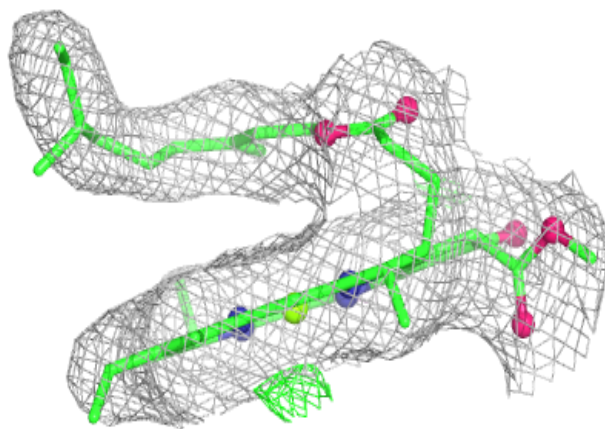
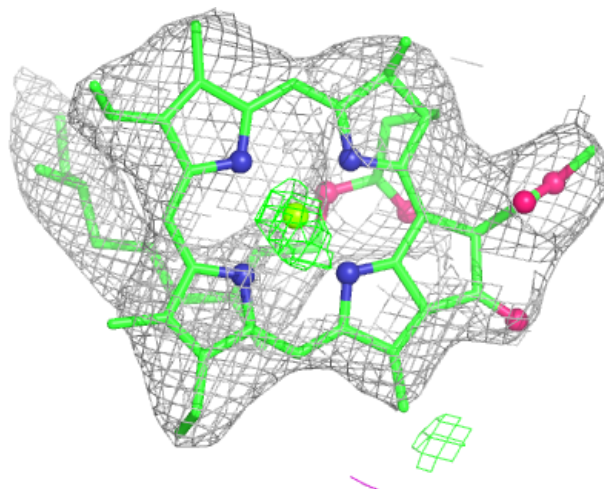
Electron density around CHL B 307:

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



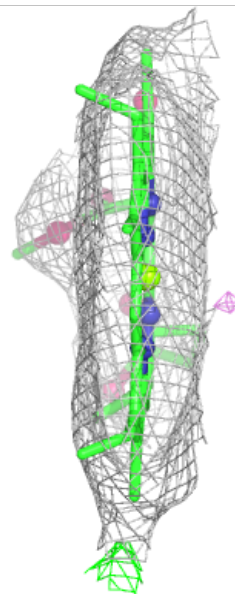
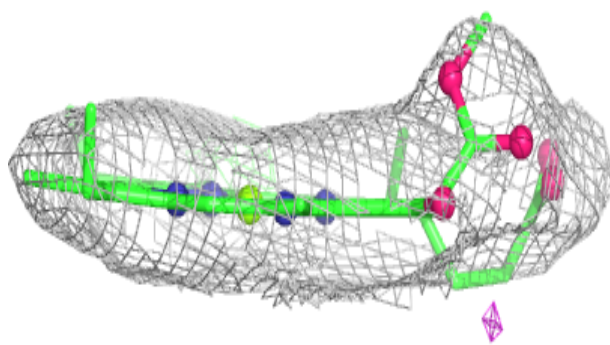
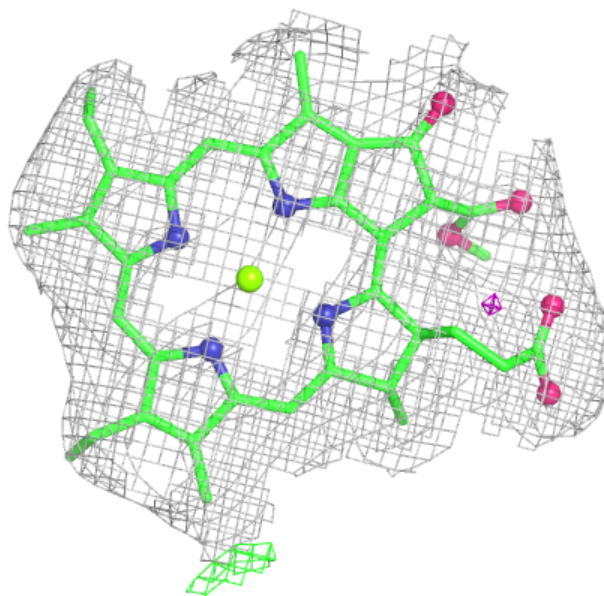
Electron density around CLA F 316:

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



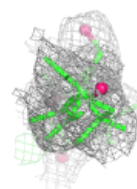
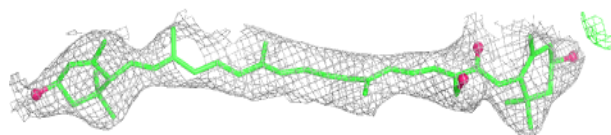
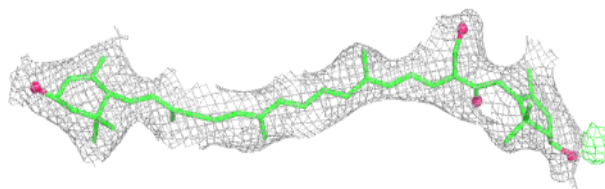
Electron density around CLA A 316:

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



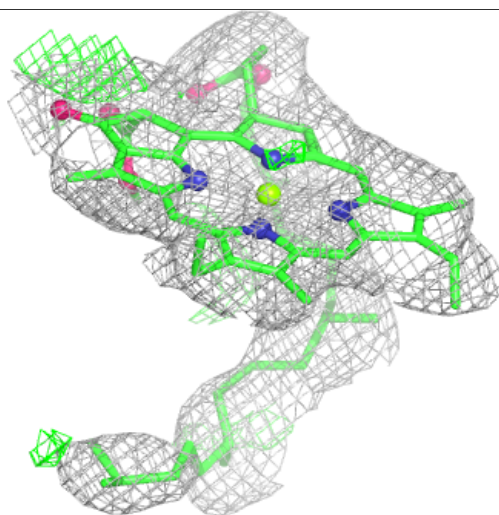
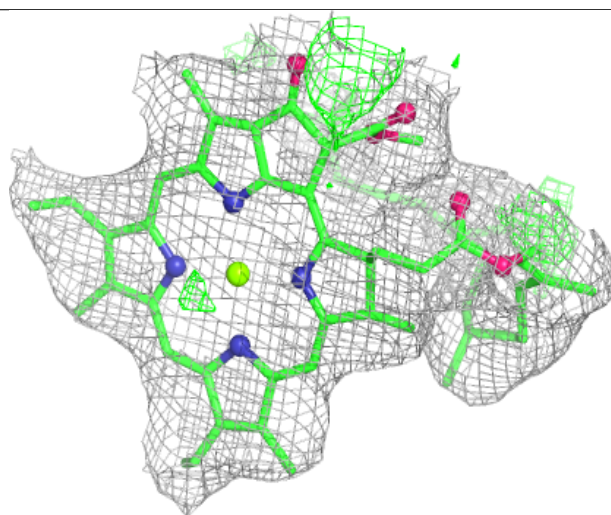
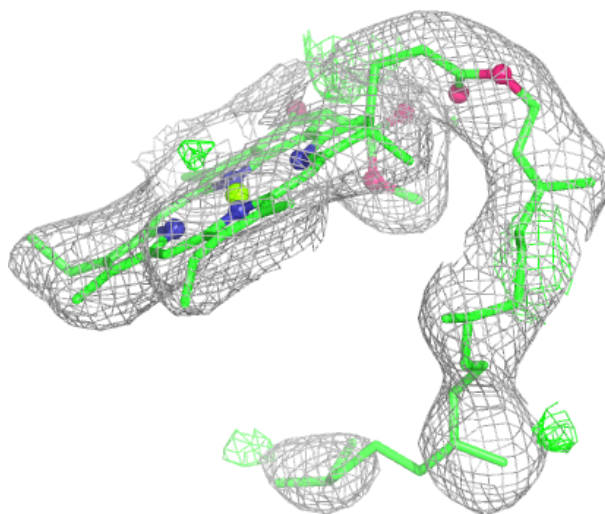
Electron density around OIE D 301:

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



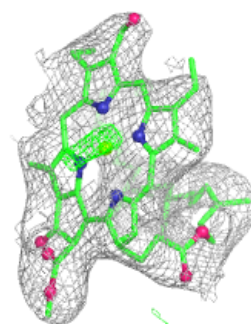
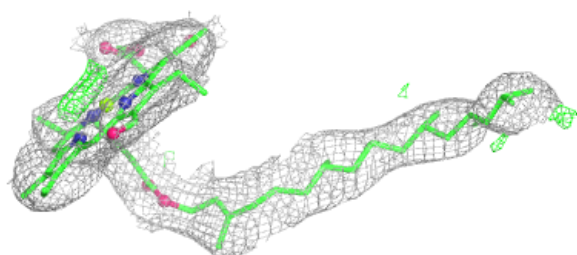
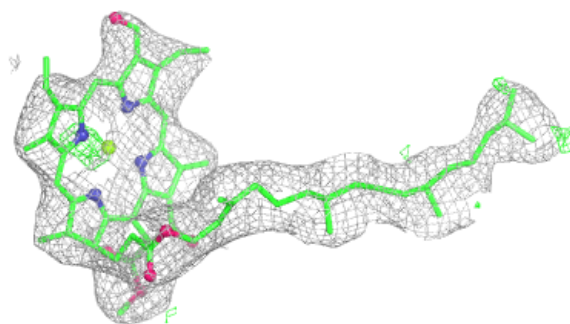
Electron density around CLA D 307:

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



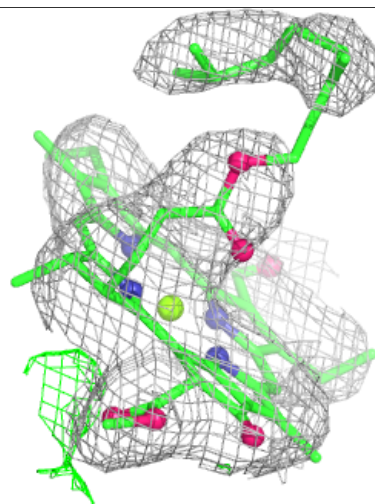
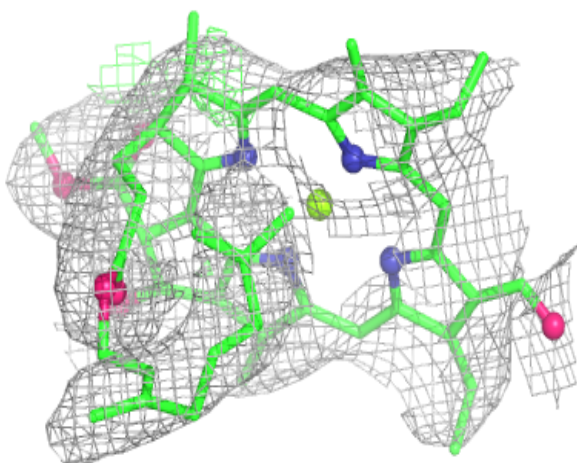
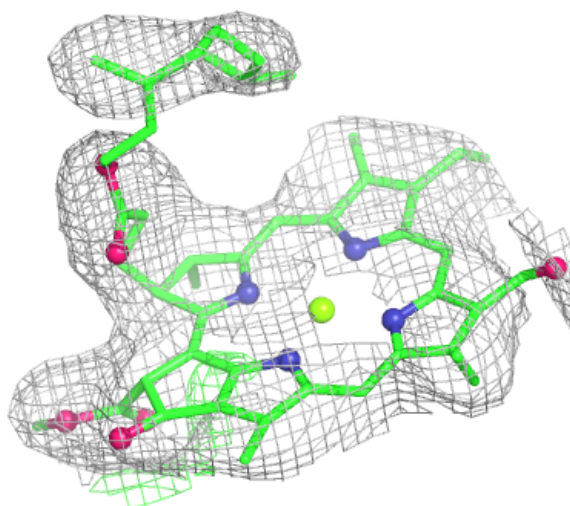
Electron density around CHL A 313:

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



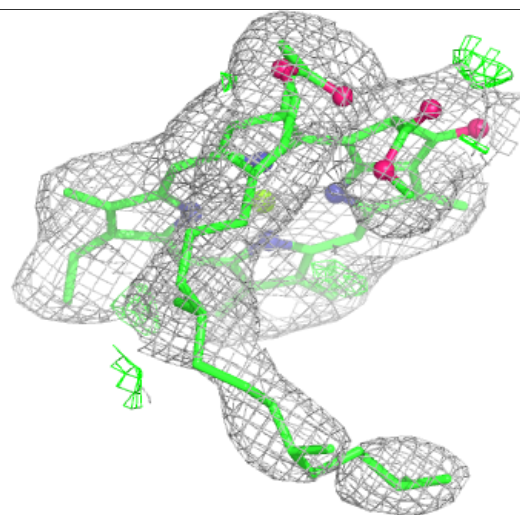
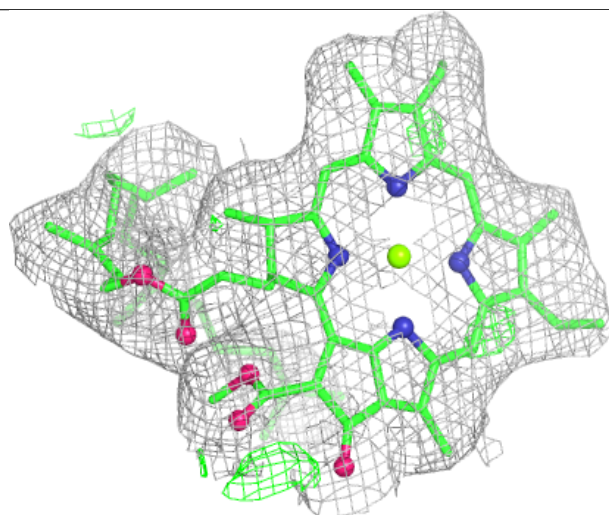
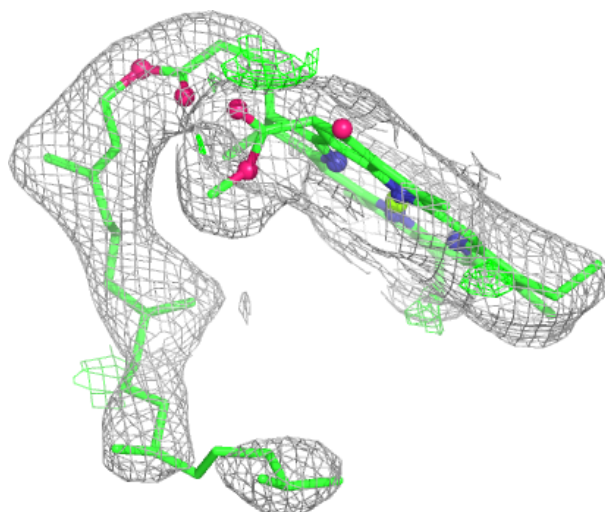
Electron density around CHL F 311:

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



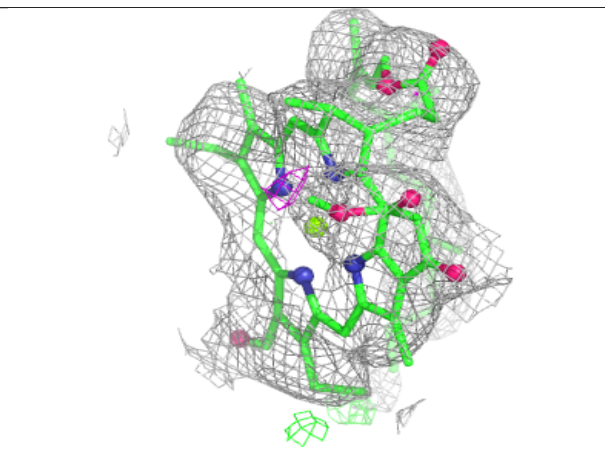
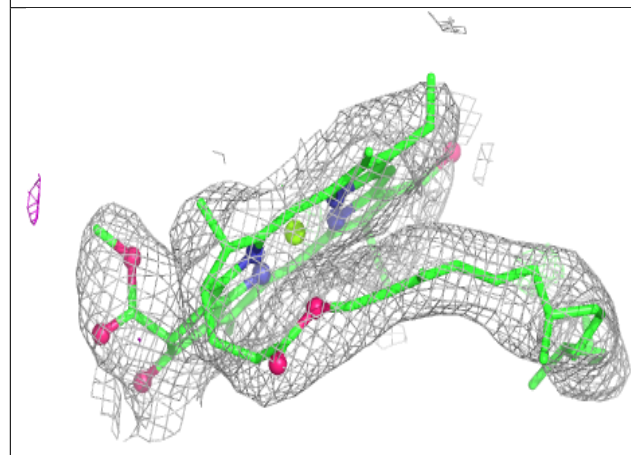
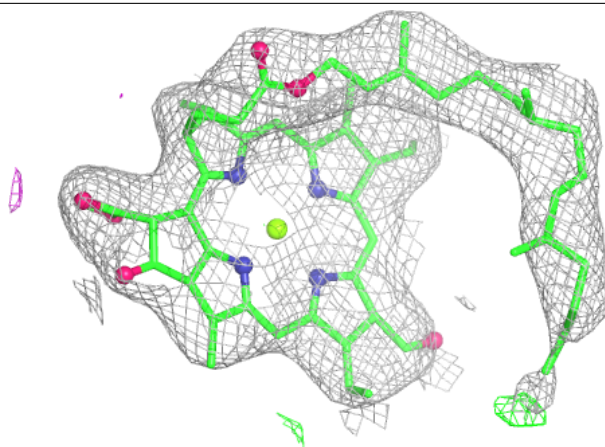
Electron density around CLA A 307:

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



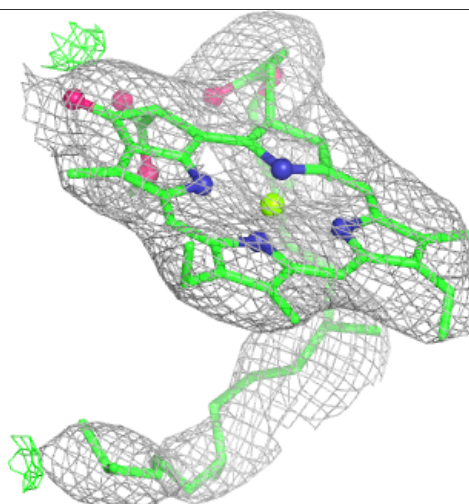
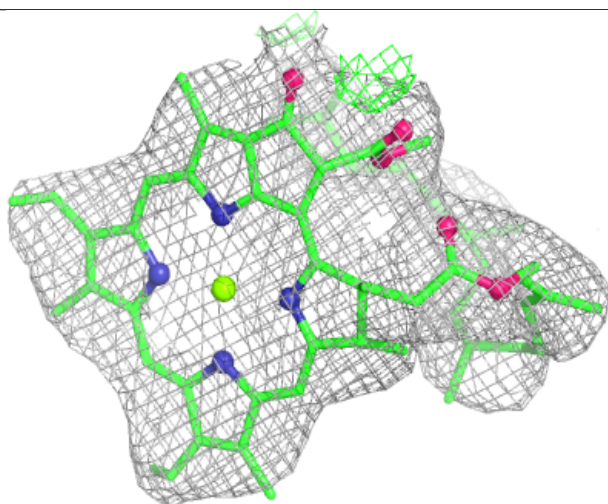
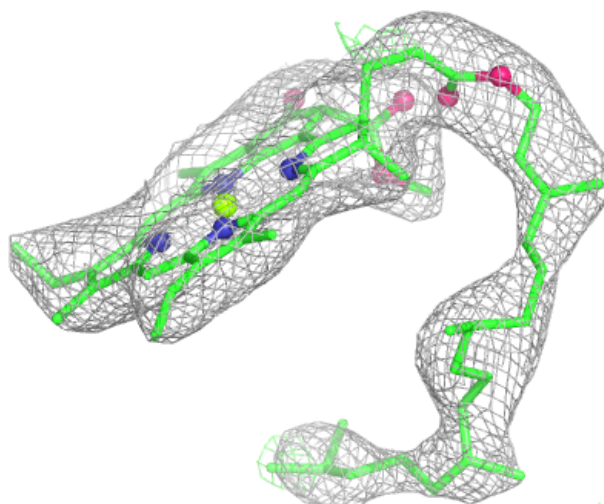
Electron density around CHL A 306:

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



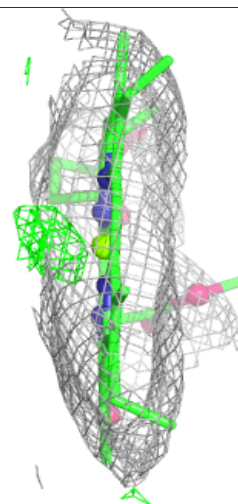
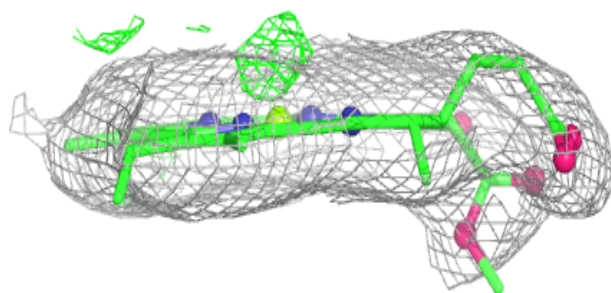
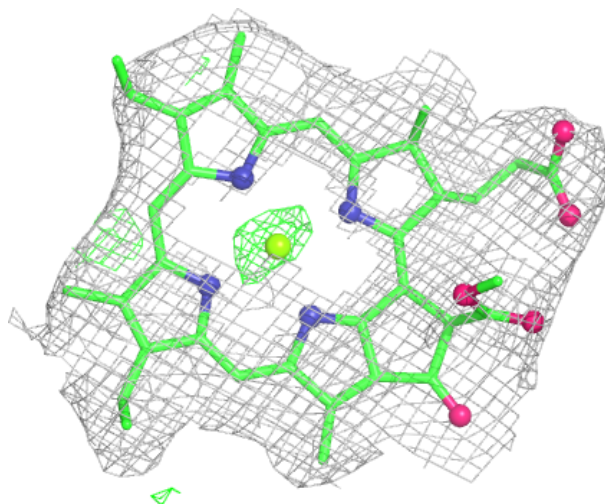
Electron density around CLA B 308:

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



Electron density around CLA B 317:

$2mF_o-DF_c$ (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.