Full wwPDB X-ray Structure Validation Report (i)

Aug 17, 2022 – 05:23 PM EDT

PDB ID	:	4LCZ
Title	:	Crystal structure of a multilayer-packed major light-harvesting complex
Authors	:	Wan, T.; Li, M.; Chang, W.R.
Deposited on	:	2013-06-24
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 (i) 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 (i)) were used in the production of this report:

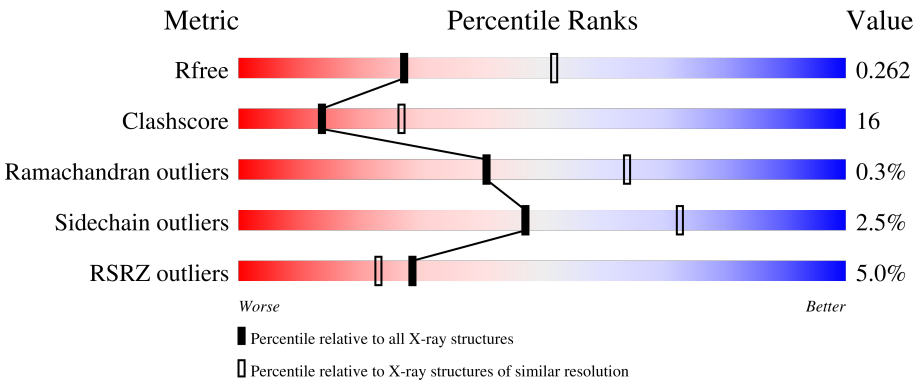
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	224	6% 75% 17% • 7%
1	B	224	3% 75% 18% 7%
1	C	224	4% 79% 14% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CHL	A	305	X	-	-	-
5	CHL	A	309	X	-	-	-
5	CHL	A	310	X	-	-	-
5	CHL	A	311	X	-	-	-
5	CHL	A	312	X	-	-	-
5	CHL	A	313	X	-	-	-
5	CHL	B	305	X	-	-	-
5	CHL	B	309	X	-	-	-
5	CHL	B	310	X	-	-	-
5	CHL	B	311	X	-	-	-
5	CHL	B	312	X	-	-	-
5	CHL	B	313	X	-	-	-
5	CHL	C	305	X	-	-	-
5	CHL	C	309	X	-	-	-
5	CHL	C	310	X	-	-	-
5	CHL	C	311	X	-	-	-
5	CHL	C	312	X	-	-	-
5	CHL	C	313	X	-	-	-
6	CLA	A	307	X	-	-	-
6	CLA	B	316	X	-	-	-
6	CLA	C	307	-	-	X	-

2 Entry composition (i)

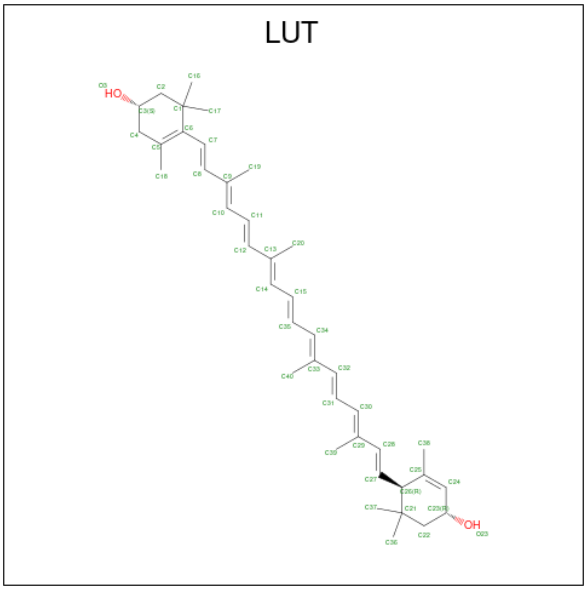
There are 10 unique types of molecules in this entry. The entry contains 8016 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Major chlorophyll a/b binding protein LHCb1.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	1579	1023	257	292	7	0	0	0
1	B	208	1579	1023	257	292	7	0	0	0
1	C	208	1579	1023	257	292	7	0	0	0

- Molecule 2 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	42	40	2	0	0
2	A	1	42	40	2	0	0
2	B	1	42	40	2	0	0

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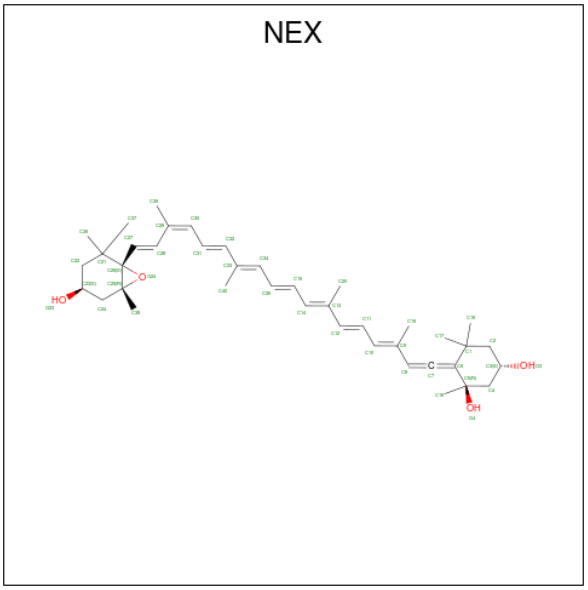
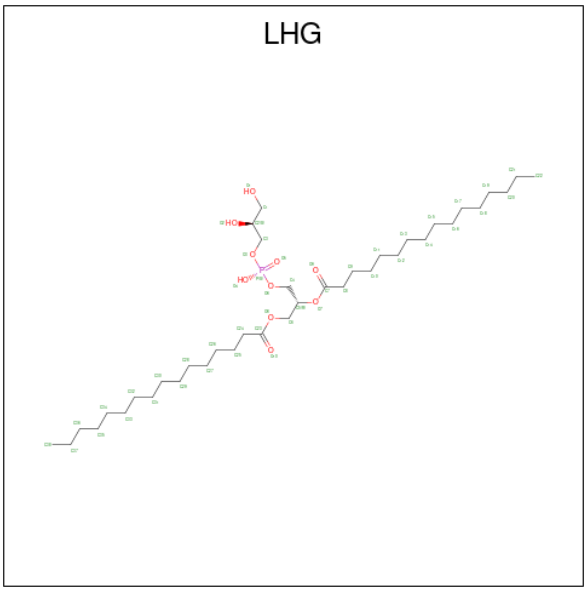
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	42	40	2	0	0
			Total	C	O		
2	C	1	42	40	2	0	0
			Total	C	O		
2	C	1	42	40	2	0	0

- 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 (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$).



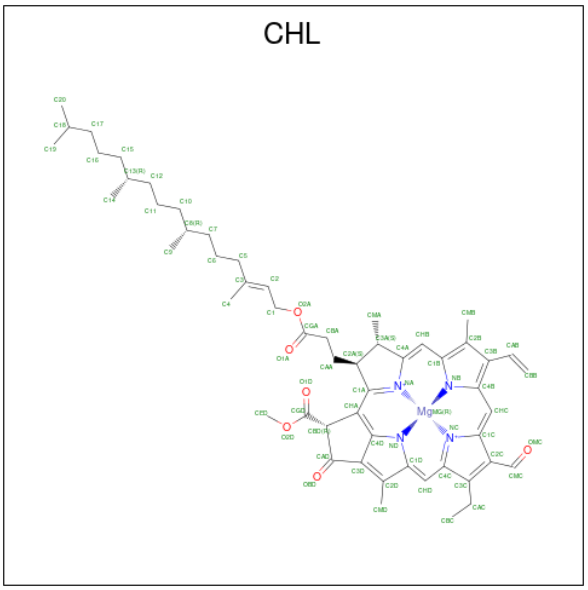
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	44	40	4	0	0
			Total	C	O		
3	B	1	44	40	4	0	0
			Total	C	O		
3	C	1	44	40	4	0	0

- Molecule 4 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

- Molecule 5 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
5	A	1	66	55	1	4	6	0	0

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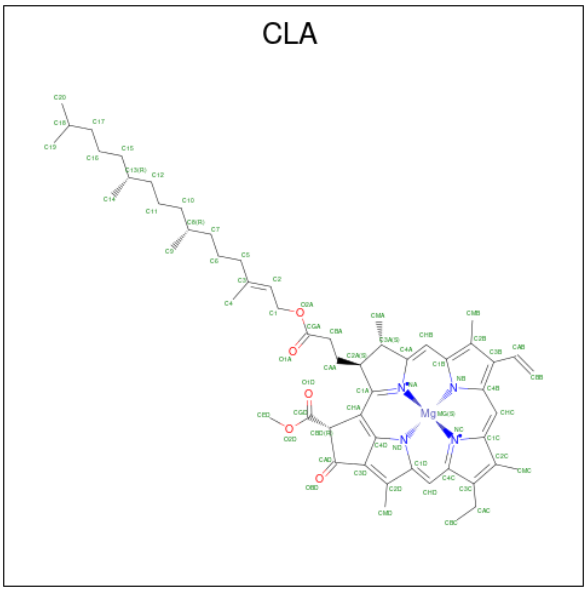
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
5	A	1	48	37	1	4	6	0	0
			Total	C	Mg	N	O		
5	A	1	51	40	1	4	6	0	0
			Total	C	Mg	N	O		
5	A	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	A	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	A	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	B	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	B	1	48	37	1	4	6	0	0
			Total	C	Mg	N	O		
5	B	1	51	40	1	4	6	0	0
			Total	C	Mg	N	O		
5	B	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	B	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	B	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	C	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	C	1	48	37	1	4	6	0	0
			Total	C	Mg	N	O		
5	C	1	51	40	1	4	6	0	0
			Total	C	Mg	N	O		
5	C	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	C	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	C	1	66	55	1	4	6	0	0

- Molecule 6 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
6	A	1	65	55	1	4	5	0	0
6	A	1	65	55	1	4	5	0	0
6	A	1	62	52	1	4	5	0	0
6	A	1	65	55	1	4	5	0	0
6	A	1	65	55	1	4	5	0	0
6	A	1	65	55	1	4	5	0	0
6	A	1	65	55	1	4	5	0	0
6	A	1	41	33	1	4	3	0	0
6	B	1	65	55	1	4	5	0	0
6	B	1	65	55	1	4	5	0	0
6	B	1	62	52	1	4	5	0	0
6	B	1	65	55	1	4	5	0	0
6	B	1	65	55	1	4	5	0	0
6	B	1	65	55	1	4	5	0	0

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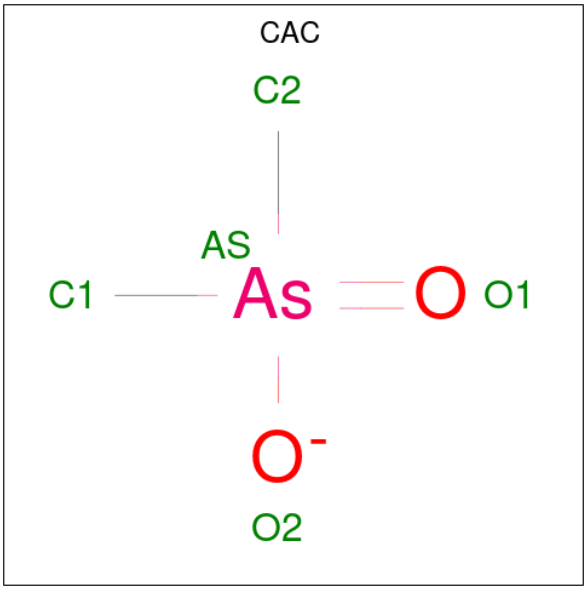
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
6	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	B	1	41	33	1	4	3	0	0
			Total	C	Mg	N	O		
6	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	C	1	62	52	1	4	5	0	0
			Total	C	Mg	N	O		
6	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	C	1	40	32	1	4	3	0	0

- Molecule 7 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	As	C	O		
7	A	1	5	1	2	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	As	C	O		
7	B	1	5	1	2	2	0	0
7	C	1	5	1	2	2	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
8	A	3	3	3	0	0
8	B	1	1	1	0	0
8	C	1	1	1	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
9	B	2	2	2	0	0
9	C	3	3	3	0	0

- Molecule 10 is water.

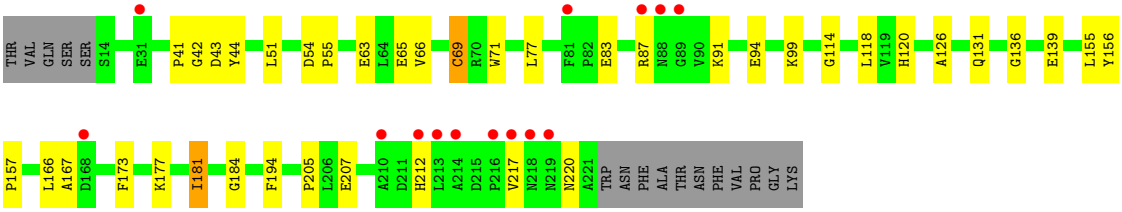
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	58	58	58	0	0
10	B	46	46	46	0	0
10	C	52	52	52	0	0

3 Residue-property plots (i)

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

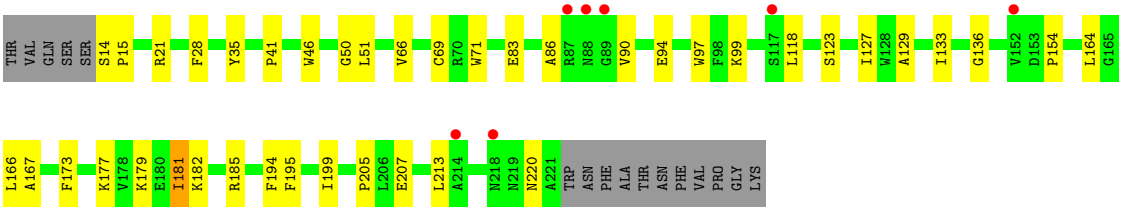
• Molecule 1: Major chlorophyll a/b binding protein LHCb1.3

Chain A:



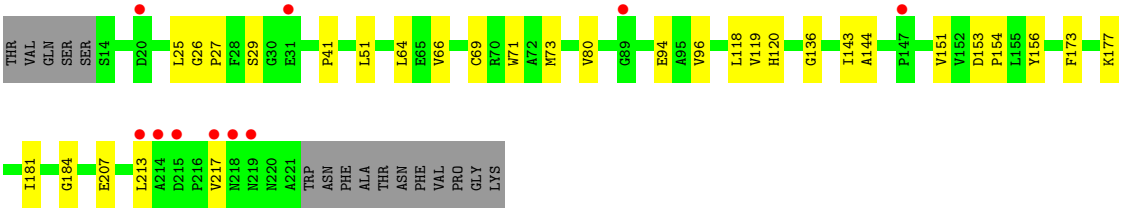
• Molecule 1: Major chlorophyll a/b binding protein LHCb1.3

Chain B:



• Molecule 1: Major chlorophyll a/b binding protein LHCb1.3

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	199.19Å 115.10Å 109.60Å 90.00° 113.23° 90.00°	Depositor
Resolution (Å)	43.45 – 2.60 49.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.4 (43.45-2.60) 83.4 (49.97-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.69 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.250 , 0.258 0.241 , 0.262	Depositor DCC
R_{free} test set	3046 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 75.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	8016	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NEX, NA, LUT, CAC, ZN, CHL, LHG, CLA

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	0.51	1/1626 (0.1%)	0.60	0/2212
1	B	0.53	0/1626	0.60	0/2212
1	C	0.53	0/1626	0.64	0/2212
All	All	0.52	1/4878 (0.0%)	0.61	0/6636

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	CYS	CB-SG	-5.30	1.73	1.81

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	1579	0	1520	33	0
1	B	1579	0	1521	31	0
1	C	1579	0	1521	20	0
2	A	84	0	112	6	0
2	B	84	0	112	15	0
2	C	84	0	112	7	0
3	A	44	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	56	3	0
3	C	44	0	56	3	0
4	A	49	0	74	9	0
4	B	49	0	74	5	0
4	C	49	0	74	5	0
5	A	363	0	350	23	0
5	B	363	0	350	22	0
5	C	363	0	350	21	0
6	A	493	0	522	43	0
6	B	493	0	524	43	0
6	C	492	0	521	47	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
8	A	3	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	B	2	0	0	0	0
9	C	3	0	0	0	0
10	A	58	0	0	1	0
10	B	46	0	0	2	0
10	C	52	0	0	2	0
All	All	8016	0	7905	250	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 16.

All (250) 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)
4:C:304:LHG:C14	6:C:317:CLA:H93	1.72	1.19
6:C:306:CLA:H92	6:C:307:CLA:HMA1	1.20	1.14
4:A:304:LHG:H142	6:A:317:CLA:H93	1.22	1.12
4:A:304:LHG:C14	6:A:317:CLA:H93	1.83	1.08
6:B:306:CLA:H92	6:B:307:CLA:HMA1	1.32	1.08
6:A:307:CLA:C9	6:C:307:CLA:H92	1.85	1.06
4:B:304:LHG:H142	6:B:317:CLA:H93	1.37	1.06
4:C:304:LHG:H142	6:C:317:CLA:H93	1.05	1.03
6:A:307:CLA:H92	6:C:307:CLA:H92	1.40	1.03
4:C:304:LHG:H142	6:C:317:CLA:C9	1.96	0.95
6:A:306:CLA:H92	6:A:307:CLA:HMA1	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:307:CLA:C9	6:C:307:CLA:C9	2.52	0.87
4:B:304:LHG:C14	6:B:317:CLA:H93	2.03	0.87
6:B:306:CLA:C9	6:B:307:CLA:HMA1	2.03	0.87
6:C:306:CLA:C9	6:C:307:CLA:HMA1	2.05	0.85
2:C:301:LUT:H30	6:C:314:CLA:H52	1.65	0.78
6:A:306:CLA:H93	6:A:307:CLA:HMB3	1.67	0.77
6:B:306:CLA:H92	6:B:307:CLA:CMA	2.15	0.76
6:B:315:CLA:HBA1	6:B:315:CLA:HBD	1.69	0.75
6:C:306:CLA:H92	6:C:307:CLA:CMA	2.10	0.75
6:A:307:CLA:HHC	6:A:307:CLA:HBB1	1.69	0.75
6:B:307:CLA:H92	6:C:307:CLA:H93	1.70	0.73
1:B:136:GLY:HA2	5:B:313:CHL:HAB	1.72	0.70
6:B:306:CLA:C9	6:B:307:CLA:HHB	2.22	0.70
5:A:310:CHL:HBA2	5:A:310:CHL:HBD	1.72	0.69
5:B:311:CHL:O1A	10:B:446:HOH:O	2.11	0.69
6:C:316:CLA:HHC	6:C:316:CLA:HBB1	1.73	0.68
5:B:305:CHL:HHC	5:B:305:CHL:HBB1	1.76	0.67
6:A:306:CLA:H93	6:A:307:CLA:CMB	2.25	0.66
1:A:136:GLY:HA2	5:A:313:CHL:HAB	1.77	0.66
5:B:305:CHL:H2	5:C:311:CHL:H201	1.78	0.65
5:B:310:CHL:HBA2	5:B:310:CHL:HBD	1.77	0.65
1:C:41:PRO:HG3	1:C:177:LYS:HB3	1.78	0.65
4:A:304:LHG:H141	6:A:317:CLA:H93	1.76	0.65
1:B:28:PHE:O	1:C:144:ALA:HB2	1.97	0.64
1:C:136:GLY:HA2	5:C:313:CHL:HAB	1.79	0.64
6:A:307:CLA:H92	6:C:307:CLA:C9	2.22	0.63
6:B:307:CLA:HHC	6:B:307:CLA:HBB1	1.80	0.63
6:A:318:CLA:HHC	6:A:318:CLA:HBB1	1.81	0.63
5:A:305:CHL:HHC	5:A:305:CHL:HBB1	1.80	0.62
5:B:312:CHL:HHC	5:B:312:CHL:HBB1	1.81	0.62
6:C:315:CLA:HBD	6:C:315:CLA:HBA1	1.82	0.61
1:A:41:PRO:HG3	1:A:177:LYS:HB3	1.82	0.61
5:A:312:CHL:HHC	5:A:312:CHL:HBB1	1.82	0.60
6:A:315:CLA:H18	6:A:316:CLA:H193	1.83	0.60
1:A:156:TYR:CE2	1:A:177:LYS:HE2	2.36	0.60
6:C:307:CLA:HHC	6:C:307:CLA:HBB1	1.83	0.59
1:B:66:VAL:O	1:B:69:CYS:HB2	2.02	0.59
6:B:307:CLA:C9	6:C:307:CLA:H93	2.32	0.59
5:C:312:CHL:HHC	5:C:312:CHL:HBB1	1.83	0.59
4:C:304:LHG:H141	6:C:317:CLA:H93	1.80	0.59
1:A:66:VAL:O	1:A:69:CYS:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LYS:HA	5:B:311:CHL:HED2	1.84	0.59
2:B:301:LUT:H34	6:B:314:CLA:CBB	2.32	0.59
5:B:305:CHL:H91	5:B:305:CHL:H142	1.84	0.58
5:C:310:CHL:HBA2	5:C:310:CHL:HBD	1.84	0.58
2:B:301:LUT:C31	6:B:314:CLA:HMC2	2.33	0.58
5:C:305:CHL:HBB1	5:C:305:CHL:HHC	1.84	0.58
1:A:156:TYR:CD2	1:A:177:LYS:HE2	2.39	0.58
1:A:51:LEU:HD12	2:A:302:LUT:H221	1.86	0.58
1:C:173:PHE:CZ	1:C:177:LYS:HE3	2.39	0.58
6:B:306:CLA:H93	6:B:307:CLA:HHB	1.85	0.57
1:A:71:TRP:CD1	5:A:313:CHL:HMD3	2.38	0.57
5:B:310:CHL:HBB2	5:B:311:CHL:HBB1	1.85	0.57
6:C:306:CLA:H93	6:C:307:CLA:HHB	1.87	0.57
1:C:71:TRP:CD1	5:C:313:CHL:HMD3	2.39	0.57
5:A:309:CHL:HHD	5:A:310:CHL:OBD	2.05	0.56
6:A:316:CLA:HHC	6:A:316:CLA:HBB1	1.87	0.56
1:B:46:TRP:CE3	2:B:302:LUT:H383	2.41	0.56
6:C:306:CLA:H93	6:C:307:CLA:HMB3	1.88	0.55
6:B:307:CLA:H92	6:C:307:CLA:C9	2.36	0.55
1:A:139:GLU:HG3	5:A:313:CHL:C4B	2.38	0.54
6:C:306:CLA:C9	6:C:307:CLA:HHB	2.38	0.54
5:C:305:CHL:H141	5:C:305:CHL:H193	1.89	0.54
4:A:304:LHG:C14	6:A:317:CLA:C9	2.73	0.53
6:A:315:CLA:HBD	6:A:315:CLA:HBA1	1.90	0.53
6:A:306:CLA:H92	6:A:307:CLA:HHB	1.90	0.53
6:B:315:CLA:H18	6:B:316:CLA:H193	1.91	0.53
5:A:313:CHL:HBB1	5:C:305:CHL:H51	1.89	0.53
6:B:316:CLA:HHC	6:B:316:CLA:HBB1	1.92	0.52
4:A:304:LHG:H222	6:B:307:CLA:H201	1.91	0.52
1:A:194:PHE:HE2	2:A:301:LUT:H41	1.73	0.52
6:C:306:CLA:HHC	6:C:306:CLA:HBB1	1.92	0.52
5:A:305:CHL:H193	5:A:305:CHL:H141	1.92	0.52
6:A:307:CLA:H93	6:C:307:CLA:H92	1.86	0.52
1:B:166:LEU:HD12	6:B:314:CLA:CGA	2.39	0.51
2:C:302:LUT:H32	6:C:306:CLA:CBB	2.40	0.51
1:C:118:LEU:O	1:C:120:HIS:N	2.44	0.51
1:A:131:GLN:OE1	5:A:311:CHL:HMC	2.10	0.50
6:A:314:CLA:HBB1	6:A:314:CLA:HHC	1.93	0.50
5:C:312:CHL:O1A	6:C:314:CLA:HMD2	2.11	0.50
1:A:99:LYS:HA	5:A:311:CHL:HED2	1.92	0.50
6:B:307:CLA:HAC2	5:B:311:CHL:H162	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:305:CHL:H141	5:B:305:CHL:H193	1.94	0.50
6:B:306:CLA:H92	6:B:307:CLA:HHB	1.94	0.50
1:B:182:LYS:HE2	6:B:315:CLA:O1D	2.11	0.50
1:A:166:LEU:HD12	6:A:314:CLA:CGA	2.40	0.49
1:B:41:PRO:HG3	1:B:177:LYS:HB3	1.92	0.49
1:B:164:LEU:HD12	2:B:301:LUT:H222	1.95	0.49
6:A:307:CLA:H91	6:C:307:CLA:C9	2.41	0.49
1:A:173:PHE:CZ	1:A:177:LYS:HE3	2.48	0.49
1:B:167:ALA:HB1	1:B:173:PHE:CD1	2.48	0.49
2:C:302:LUT:H382	6:C:306:CLA:HBA1	1.95	0.48
1:A:42:GLY:O	1:A:44:TYR:HD1	1.96	0.48
1:A:65:GLU:HG2	1:A:181:ILE:HD11	1.95	0.48
6:C:314:CLA:H12	6:C:314:CLA:HMB2	1.95	0.48
1:C:25:LEU:HB2	1:C:29:SER:HA	1.96	0.48
1:A:51:LEU:HD13	6:A:306:CLA:H42	1.96	0.48
4:A:304:LHG:H281	4:A:304:LHG:HC91	1.96	0.48
1:C:173:PHE:CE1	6:C:314:CLA:HED3	2.48	0.48
1:A:220:ASN:HB2	6:A:317:CLA:O1A	2.14	0.48
1:B:173:PHE:CZ	1:B:177:LYS:HE3	2.48	0.48
3:B:303:NEX:H192	3:B:303:NEX:H183	1.95	0.48
1:A:63:GLU:HA	1:A:155:LEU:HD21	1.96	0.47
1:B:21:ARG:HH11	1:B:21:ARG:HG2	1.78	0.47
4:B:304:LHG:H142	6:B:317:CLA:C9	2.27	0.47
5:B:305:CHL:H13	5:B:305:CHL:H172	1.47	0.47
1:A:139:GLU:HG3	5:A:313:CHL:NB	2.30	0.47
5:A:312:CHL:O1A	6:A:314:CLA:HMD2	2.14	0.47
2:B:301:LUT:H34	6:B:314:CLA:HBB2	1.95	0.47
1:B:71:TRP:CD1	5:B:313:CHL:HMD3	2.50	0.47
1:C:69:CYS:SG	1:C:184:GLY:HA3	2.55	0.47
2:C:302:LUT:H11	2:C:302:LUT:H191	1.78	0.47
6:B:306:CLA:H93	6:B:307:CLA:CMB	2.45	0.47
1:B:118:LEU:HD23	5:B:309:CHL:HED2	1.96	0.46
6:B:307:CLA:H92	6:B:307:CLA:H62	1.78	0.46
1:C:64:LEU:HD23	5:C:313:CHL:OBD	2.15	0.46
1:C:66:VAL:O	1:C:69:CYS:HB2	2.15	0.46
5:A:305:CHL:H62	5:A:305:CHL:H41	1.70	0.46
6:A:307:CLA:C9	6:C:307:CLA:H91	2.44	0.46
6:B:306:CLA:H41	6:B:306:CLA:H61	1.71	0.46
1:A:83:GLU:OE1	1:A:205:PRO:HD2	2.14	0.46
6:A:314:CLA:H12	6:A:314:CLA:HMB2	1.96	0.46
6:B:314:CLA:HMB1	6:B:314:CLA:HAB	1.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LYS:O	1:A:114:GLY:HA3	2.15	0.46
2:A:301:LUT:C33	6:A:316:CLA:HMB2	2.46	0.46
5:A:311:CHL:H152	5:A:313:CHL:H71	1.98	0.46
1:B:83:GLU:OE1	1:B:205:PRO:HD2	2.16	0.46
6:C:314:CLA:H43	6:C:316:CLA:HBA1	1.97	0.46
1:B:14:SER:HA	1:B:15:PRO:HD3	1.83	0.46
6:A:307:CLA:H92	6:A:307:CLA:H62	1.67	0.46
5:A:305:CHL:HBA1	5:A:305:CHL:H3A	1.53	0.45
1:C:156:TYR:CE1	1:C:177:LYS:HG2	2.51	0.45
5:C:312:CHL:HMB1	5:C:312:CHL:HAB	1.60	0.45
1:C:51:LEU:HD13	6:C:306:CLA:H42	1.98	0.45
6:C:318:CLA:HHC	6:C:318:CLA:HBB1	1.98	0.45
2:C:302:LUT:C31	6:C:306:CLA:HMC2	2.47	0.45
2:A:301:LUT:C31	6:A:314:CLA:HMC2	2.47	0.45
1:B:179:LYS:HD3	6:B:316:CLA:HAA2	1.99	0.45
1:A:77:LEU:HD12	1:A:77:LEU:O	2.16	0.45
1:A:94:GLU:HG2	1:A:99:LYS:CB	2.45	0.45
2:B:301:LUT:C34	6:B:316:CLA:HMB2	2.47	0.45
5:B:305:CHL:HBA1	5:B:305:CHL:H3A	1.65	0.45
2:B:301:LUT:H31	6:B:314:CLA:HMC2	1.99	0.45
1:A:69:CYS:SG	1:A:184:GLY:HA3	2.57	0.44
2:A:301:LUT:H34	6:A:314:CLA:CBB	2.47	0.44
1:B:136:GLY:CA	5:B:313:CHL:HAB	2.43	0.44
1:A:173:PHE:CZ	6:A:314:CLA:HED3	2.52	0.44
3:C:303:NEX:H402	5:C:312:CHL:H152	2.00	0.44
1:B:35:TYR:HH	1:B:50:GLY:HA2	1.83	0.44
2:C:302:LUT:H32	6:C:306:CLA:HBB1	1.99	0.44
3:C:303:NEX:H191	3:C:303:NEX:H11	1.76	0.44
2:B:301:LUT:H11	2:B:301:LUT:H191	1.75	0.44
6:B:308:CLA:HMB1	6:B:308:CLA:HAB	1.68	0.44
5:A:312:CHL:CAD	6:A:314:CLA:HMD3	2.48	0.44
5:A:305:CHL:H172	5:A:305:CHL:H13	1.57	0.44
1:C:151:VAL:HG11	10:C:406:HOH:O	2.18	0.44
6:B:307:CLA:H41	6:C:307:CLA:H51	1.99	0.44
6:B:315:CLA:C1D	6:B:316:CLA:HMD2	2.48	0.43
2:A:301:LUT:H11	2:A:301:LUT:H191	1.81	0.43
5:B:305:CHL:H61	5:B:305:CHL:H101	1.46	0.43
5:B:305:CHL:H62	5:B:305:CHL:H41	1.78	0.43
1:C:73:MET:SD	6:C:314:CLA:HBB1	2.58	0.43
5:C:305:CHL:HBA1	5:C:305:CHL:H3A	1.47	0.43
6:A:307:CLA:H41	6:A:307:CLA:H61	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:314:CLA:H93	6:A:316:CLA:H102	2.01	0.43
6:B:314:CLA:HHC	6:B:314:CLA:HBB1	2.00	0.43
1:C:143:ILE:HD11	5:C:313:CHL:HMA3	2.00	0.43
6:C:306:CLA:H93	6:C:307:CLA:CMB	2.48	0.43
1:A:94:GLU:HG2	1:A:99:LYS:HB3	1.99	0.43
6:B:315:CLA:HBD	6:B:316:CLA:OBD	2.18	0.43
4:A:304:LHG:H182	4:A:304:LHG:H151	1.80	0.43
1:B:86:ALA:HA	1:B:90:VAL:O	2.19	0.43
3:B:303:NEX:H11	3:B:303:NEX:H191	1.78	0.43
4:A:304:LHG:H171	5:A:305:CHL:H42	2.00	0.43
1:B:181:ILE:HD12	1:B:185:ARG:NE	2.34	0.43
2:B:302:LUT:C31	6:B:306:CLA:HMC2	2.49	0.43
5:C:312:CHL:HHC	5:C:312:CHL:OMC	2.17	0.43
1:B:35:TYR:OH	1:B:50:GLY:HA2	2.19	0.42
5:B:312:CHL:C4A	5:B:312:CHL:HBA2	2.49	0.42
3:C:303:NEX:H35	3:C:303:NEX:H401	1.78	0.42
6:C:306:CLA:HMB1	6:C:306:CLA:HAB	1.73	0.42
5:A:312:CHL:H143	5:A:312:CHL:H161	1.74	0.42
6:A:314:CLA:HMB1	6:A:314:CLA:HAB	1.65	0.42
1:B:129:ALA:O	1:B:133:ILE:HG12	2.19	0.42
2:B:302:LUT:H11	2:B:302:LUT:H191	1.84	0.42
6:C:306:CLA:H141	6:C:306:CLA:H161	1.80	0.42
1:A:87:ARG:NH1	10:A:402:HOH:O	2.53	0.42
6:A:307:CLA:HBB1	6:A:307:CLA:CHC	2.46	0.42
6:A:307:CLA:H42	6:A:307:CLA:HMA2	2.01	0.42
6:A:306:CLA:HAB	6:A:306:CLA:HMB1	1.81	0.42
1:B:213:LEU:HD21	6:B:318:CLA:HHC	2.00	0.42
2:B:302:LUT:H35	2:B:302:LUT:H401	1.88	0.42
1:C:153:ASP:HA	1:C:154:PRO:HD2	1.86	0.42
3:A:303:NEX:H35	3:A:303:NEX:H401	1.73	0.42
6:B:314:CLA:H51	6:B:316:CLA:HMA1	2.01	0.42
6:C:307:CLA:HMA2	6:C:307:CLA:H42	2.00	0.42
6:B:306:CLA:H141	6:B:306:CLA:H161	1.73	0.42
1:A:157:PRO:HD3	5:A:312:CHL:HMD2	2.02	0.42
1:B:194:PHE:HE2	2:B:301:LUT:H41	1.85	0.41
5:C:305:CHL:HAB	5:C:305:CHL:HMB1	1.78	0.41
1:A:167:ALA:HB1	1:A:173:PHE:CD1	2.54	0.41
1:A:118:LEU:O	1:A:120:HIS:N	2.52	0.41
6:A:315:CLA:HBA1	6:A:315:CLA:CHA	2.50	0.41
1:B:123:SER:O	1:B:127:ILE:HG13	2.21	0.41
5:C:305:CHL:H43	5:C:305:CHL:HMA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:305:CHL:H143	5:A:305:CHL:H111	1.73	0.41
1:B:51:LEU:HD13	6:B:306:CLA:H42	2.02	0.41
2:B:301:LUT:H15	2:B:301:LUT:H201	1.93	0.41
6:B:306:CLA:H92	6:B:306:CLA:H62	1.66	0.41
5:C:311:CHL:H152	5:C:313:CHL:H71	2.01	0.41
3:B:303:NEX:H15	3:B:303:NEX:H201	1.90	0.41
6:C:315:CLA:HHC	6:C:315:CLA:HBB1	2.01	0.41
1:A:212:HIS:CG	6:A:317:CLA:HAA2	2.56	0.41
1:B:154:PRO:HG2	10:B:437:HOH:O	2.20	0.41
5:B:312:CHL:CAD	6:B:314:CLA:HMD3	2.50	0.41
1:C:26:GLY:HA3	1:C:27:PRO:HD2	1.93	0.41
3:A:303:NEX:H183	3:A:303:NEX:H192	2.03	0.41
1:B:94:GLU:HG2	1:B:99:LYS:CB	2.50	0.41
2:B:302:LUT:H15	2:B:302:LUT:H201	1.94	0.41
1:C:120:HIS:HE1	10:C:409:HOH:O	2.03	0.41
1:C:213:LEU:HD21	6:C:318:CLA:HHC	2.03	0.41
5:C:305:CHL:H143	5:C:305:CHL:H111	1.65	0.41
6:C:307:CLA:HAC2	5:C:311:CHL:H162	2.03	0.41
1:B:97:TRP:O	2:B:302:LUT:O3	2.39	0.41
1:A:126:ALA:HB3	5:A:309:CHL:HMC	2.03	0.40
3:A:303:NEX:H11	3:A:303:NEX:H191	1.87	0.40
4:B:304:LHG:H151	4:B:304:LHG:H182	1.77	0.40
6:A:306:CLA:C9	6:A:307:CLA:HHB	2.49	0.40
1:B:195:PHE:O	1:B:199:ILE:HG13	2.21	0.40
4:B:304:LHG:H171	5:B:305:CHL:H42	2.04	0.40
6:C:314:CLA:HBB1	6:C:314:CLA:HHC	2.01	0.40
4:A:304:LHG:H141	6:A:317:CLA:C9	2.45	0.40
6:B:307:CLA:C9	6:C:307:CLA:C9	2.97	0.40
2:C:301:LUT:H35	2:C:301:LUT:H401	1.75	0.40
4:C:304:LHG:H182	4:C:304:LHG:H151	1.81	0.40
5:C:305:CHL:H13	5:C:305:CHL:H172	1.51	0.40
1:A:54:ASP:HA	1:A:55:PRO:HD3	1.87	0.40
6:A:307:CLA:H91	6:C:307:CLA:H91	2.03	0.40
5:B:305:CHL:HMB1	5:B:305:CHL:HAB	1.79	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	206/224 (92%)	199 (97%)	6 (3%)	1 (0%)	29	52
1	B	206/224 (92%)	199 (97%)	7 (3%)	0	100	100
1	C	206/224 (92%)	198 (96%)	7 (3%)	1 (0%)	29	52
All	All	618/672 (92%)	596 (96%)	20 (3%)	2 (0%)	41	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	C	119	VAL

5.3.2 Protein sidechains (i)

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	160/174 (92%)	157 (98%)	3 (2%)	57	79
1	B	160/174 (92%)	157 (98%)	3 (2%)	57	79
1	C	160/174 (92%)	154 (96%)	6 (4%)	33	59
All	All	480/522 (92%)	468 (98%)	12 (2%)	47	73

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	ILE

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Mol	Chain	Res	Type
1	A	207	GLU
1	A	217	VAL
1	B	181	ILE
1	B	207	GLU
1	B	220	ASN
1	C	80	VAL
1	C	94	GLU
1	C	96	VAL
1	C	181	ILE
1	C	207	GLU
1	C	217	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 67 ligands modelled in this entry, 10 are monoatomic - leaving 57 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	$\#\|Z\| > 2$
2	LUT	A	301	-	42,43,43	0.89	1 (2%)	51,60,60	1.53	10 (19%)
5	CHL	B	311	10	66,74,74	1.98	15 (22%)	73,114,114	2.00	16 (21%)
6	CLA	B	308	10	62,70,73	2.71	15 (24%)	72,109,113	1.91	13 (18%)
5	CHL	C	312	10	66,74,74	2.32	15 (22%)	73,114,114	2.02	20 (27%)
4	LHG	A	304	6	48,48,48	0.93	2 (4%)	51,54,54	1.01	2 (3%)
6	CLA	C	314	1	65,73,73	2.36	15 (23%)	76,113,113	1.87	19 (25%)
5	CHL	A	312	10	66,74,74	2.27	14 (21%)	73,114,114	1.92	16 (21%)
6	CLA	A	317	1	65,73,73	2.16	14 (21%)	76,113,113	1.63	14 (18%)
6	CLA	A	306	1	65,73,73	2.14	15 (23%)	76,113,113	1.96	15 (19%)
6	CLA	A	308	10	62,70,73	2.70	14 (22%)	72,109,113	1.98	18 (25%)
6	CLA	C	315	4	65,73,73	2.60	16 (24%)	76,113,113	1.80	19 (25%)
5	CHL	C	311	10	66,74,74	1.99	15 (22%)	73,114,114	2.00	18 (24%)
6	CLA	B	315	4	65,73,73	2.48	15 (23%)	76,113,113	2.11	20 (26%)
6	CLA	C	318	1	39,48,73	3.01	16 (41%)	45,82,113	2.08	15 (33%)
6	CLA	B	307	1	65,73,73	2.47	16 (24%)	76,113,113	2.04	18 (23%)
5	CHL	C	305	1	66,74,74	2.12	15 (22%)	73,114,114	1.96	19 (26%)
5	CHL	B	305	1	66,74,74	2.38	15 (22%)	73,114,114	2.10	18 (24%)
5	CHL	A	310	10	51,59,74	2.78	14 (27%)	55,96,114	2.14	16 (29%)
6	CLA	B	316	1	65,73,73	2.63	14 (21%)	76,113,113	2.07	16 (21%)
2	LUT	C	302	-	42,43,43	0.82	1 (2%)	51,60,60	1.69	11 (21%)
2	LUT	B	302	-	42,43,43	0.99	3 (7%)	51,60,60	1.69	13 (25%)
6	CLA	A	315	4	65,73,73	2.53	15 (23%)	76,113,113	1.94	20 (26%)
6	CLA	C	317	1	65,73,73	2.40	17 (26%)	76,113,113	1.79	19 (25%)
6	CLA	A	318	1	41,49,73	3.06	17 (41%)	47,84,113	2.01	12 (25%)
6	CLA	A	307	1	65,73,73	2.19	15 (23%)	76,113,113	2.06	23 (30%)
5	CHL	A	305	1	66,74,74	1.99	14 (21%)	73,114,114	1.99	19 (26%)
6	CLA	A	316	1	65,73,73	2.88	14 (21%)	76,113,113	1.87	14 (18%)
5	CHL	B	309	1	48,56,74	2.55	13 (27%)	51,92,114	2.05	13 (25%)
3	NEX	B	303	-	38,46,46	0.97	2 (5%)	50,70,70	3.01	16 (32%)
3	NEX	C	303	-	38,46,46	1.02	1 (2%)	50,70,70	3.13	17 (34%)
2	LUT	A	302	-	42,43,43	0.88	1 (2%)	51,60,60	1.53	8 (15%)
3	NEX	A	303	-	38,46,46	0.97	2 (5%)	50,70,70	3.03	17 (34%)
4	LHG	B	304	6	48,48,48	0.98	2 (4%)	51,54,54	1.10	3 (5%)
4	LHG	C	304	6	48,48,48	0.95	2 (4%)	51,54,54	1.03	4 (7%)
6	CLA	C	306	1	65,73,73	2.56	16 (24%)	76,113,113	1.95	22 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	CLA	B	314	1	65,73,73	2.26	15 (23%)	76,113,113	1.72	15 (19%)
6	CLA	C	307	1	65,73,73	2.24	16 (24%)	76,113,113	2.02	24 (31%)
5	CHL	B	310	10	51,59,74	2.55	13 (25%)	55,96,114	2.16	14 (25%)
6	CLA	C	308	10	62,70,73	2.19	14 (22%)	72,109,113	1.85	17 (23%)
7	CAC	A	319	8	0,4,4	-	-	0,6,6	-	-
5	CHL	C	310	10	51,59,74	2.48	15 (29%)	55,96,114	2.16	16 (29%)
5	CHL	A	309	1	48,56,74	2.59	15 (31%)	51,92,114	2.23	14 (27%)
5	CHL	B	313	1	66,74,74	2.25	11 (16%)	73,114,114	1.71	15 (20%)
5	CHL	C	309	1	48,56,74	2.62	16 (33%)	51,92,114	2.06	15 (29%)
2	LUT	B	301	-	42,43,43	0.88	0	51,60,60	1.71	14 (27%)
5	CHL	C	313	1	66,74,74	2.13	15 (22%)	73,114,114	1.79	18 (24%)
6	CLA	A	314	1	65,73,73	2.44	15 (23%)	76,113,113	1.81	17 (22%)
6	CLA	C	316	1	65,73,73	2.56	13 (20%)	76,113,113	1.96	17 (22%)
7	CAC	B	319	8	0,4,4	-	-	0,6,6	-	-
7	CAC	C	319	8	0,4,4	-	-	0,6,6	-	-
2	LUT	C	301	-	42,43,43	1.02	1 (2%)	51,60,60	1.89	15 (29%)
5	CHL	A	313	1	66,74,74	2.22	14 (21%)	73,114,114	1.71	13 (17%)
5	CHL	A	311	10	66,74,74	2.23	12 (18%)	73,114,114	1.82	13 (17%)
5	CHL	B	312	10	66,74,74	2.08	16 (24%)	73,114,114	1.78	18 (24%)
6	CLA	B	318	1	41,49,73	3.10	17 (41%)	47,84,113	2.01	12 (25%)
6	CLA	B	306	1	65,73,73	2.21	15 (23%)	76,113,113	1.92	18 (23%)
6	CLA	B	317	1	65,73,73	2.21	11 (16%)	76,113,113	1.63	15 (19%)

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
2	LUT	A	301	-	-	2/29/67/67	0/2/2/2
5	CHL	B	311	10	4/4/20/26	22/39/137/137	-
6	CLA	B	308	10	-	13/34/112/115	-
5	CHL	C	312	10	4/4/20/26	13/39/137/137	-
4	LHG	A	304	6	-	17/53/53/53	-
6	CLA	C	314	1	-	9/37/115/115	-
5	CHL	A	312	10	4/4/20/26	11/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLA	A	317	1	-	18/37/115/115	-
6	CLA	A	306	1	-	7/37/115/115	-
6	CLA	A	308	10	-	16/34/112/115	-
6	CLA	C	315	4	-	10/37/115/115	-
5	CHL	C	311	10	4/4/20/26	20/39/137/137	-
6	CLA	B	315	4	-	12/37/115/115	-
6	CLA	C	318	1	-	1/8/82/115	-
6	CLA	B	307	1	-	13/37/115/115	-
5	CHL	C	305	1	4/4/20/26	26/39/137/137	-
5	CHL	B	305	1	4/4/20/26	27/39/137/137	-
5	CHL	A	310	10	3/3/17/26	8/21/119/137	-
6	CLA	B	316	1	1/1/15/20	12/37/115/115	-
2	LUT	C	302	-	-	3/29/67/67	0/2/2/2
2	LUT	B	302	-	-	1/29/67/67	0/2/2/2
6	CLA	A	315	4	-	14/37/115/115	-
6	CLA	C	317	1	-	11/37/115/115	-
6	CLA	A	318	1	-	1/8/86/115	-
6	CLA	A	307	1	1/1/15/20	14/37/115/115	-
5	CHL	A	305	1	4/4/20/26	27/39/137/137	-
6	CLA	A	316	1	-	13/37/115/115	-
5	CHL	B	309	1	3/3/16/26	7/18/116/137	-
3	NEX	B	303	-	-	4/27/83/83	0/3/3/3
3	NEX	C	303	-	-	5/27/83/83	0/3/3/3
2	LUT	A	302	-	-	3/29/67/67	0/2/2/2
3	NEX	A	303	-	-	4/27/83/83	0/3/3/3
4	LHG	B	304	6	-	17/53/53/53	-
4	LHG	C	304	6	-	14/53/53/53	-
6	CLA	C	306	1	-	9/37/115/115	-
6	CLA	B	314	1	-	4/37/115/115	-
6	CLA	C	307	1	-	13/37/115/115	-
5	CHL	B	310	10	3/3/17/26	7/21/119/137	-
6	CLA	C	308	10	-	11/34/112/115	-
5	CHL	C	310	10	3/3/17/26	6/21/119/137	-
5	CHL	A	309	1	3/3/16/26	5/18/116/137	-
5	CHL	B	313	1	4/4/20/26	13/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CHL	C	309	1	3/3/16/26	1/18/116/137	-
2	LUT	B	301	-	-	1/29/67/67	0/2/2/2
5	CHL	C	313	1	4/4/20/26	15/39/137/137	-
6	CLA	A	314	1	-	3/37/115/115	-
6	CLA	C	316	1	-	12/37/115/115	-
5	CHL	A	313	1	4/4/20/26	14/39/137/137	-
2	LUT	C	301	-	-	3/29/67/67	0/2/2/2
5	CHL	A	311	10	4/4/20/26	21/39/137/137	-
5	CHL	B	312	10	4/4/20/26	13/39/137/137	-
6	CLA	B	318	1	-	1/8/86/115	-
6	CLA	B	306	1	-	6/37/115/115	-
6	CLA	B	317	1	-	20/37/115/115	-

All (635) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	316	CLA	MG-NA	18.03	2.49	2.06
6	A	308	CLA	MG-NA	15.46	2.43	2.06
6	B	316	CLA	MG-NA	15.07	2.42	2.06
6	C	316	CLA	MG-NA	14.04	2.39	2.06
5	A	310	CHL	MG-NA	13.49	2.38	2.06
6	C	315	CLA	MG-NA	13.34	2.38	2.06
6	B	308	CLA	MG-NA	12.75	2.36	2.06
6	A	315	CLA	MG-NA	12.54	2.36	2.06
6	B	315	CLA	MG-NA	12.40	2.35	2.06
6	C	306	CLA	MG-NA	12.39	2.35	2.06
6	B	318	CLA	MG-NA	11.94	2.34	2.06
5	B	313	CHL	MG-NA	11.84	2.34	2.06
5	B	310	CHL	MG-NA	11.37	2.33	2.06
6	A	318	CLA	MG-NA	11.22	2.32	2.06
6	C	318	CLA	MG-NA	11.03	2.32	2.06
5	A	312	CHL	MG-NA	10.80	2.31	2.06
6	A	314	CLA	MG-NA	10.61	2.31	2.06
5	A	311	CHL	MG-NA	10.59	2.31	2.06
5	A	313	CHL	MG-NA	10.46	2.31	2.06
6	C	317	CLA	MG-NA	10.43	2.31	2.06
6	C	314	CLA	MG-NA	10.36	2.30	2.06
5	B	305	CHL	MG-NA	10.26	2.30	2.06
5	C	310	CHL	MG-NA	10.05	2.30	2.06
6	B	307	CLA	MG-NA	9.86	2.29	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	309	CHL	MG-NA	9.79	2.29	2.06
5	C	305	CHL	MG-NA	9.77	2.29	2.06
6	C	307	CLA	MG-NA	9.75	2.29	2.06
5	B	309	CHL	MG-NA	9.60	2.29	2.06
5	C	313	CHL	MG-NA	9.57	2.29	2.06
6	B	317	CLA	MG-NA	9.49	2.28	2.06
5	C	312	CHL	C3B-C2B	-9.45	1.27	1.40
5	A	309	CHL	MG-NA	9.11	2.27	2.06
6	B	306	CLA	MG-NA	9.06	2.27	2.06
6	C	308	CLA	MG-NA	8.74	2.27	2.06
5	B	305	CHL	C3B-C2B	-8.64	1.28	1.40
5	C	312	CHL	MG-NA	8.56	2.26	2.06
6	A	317	CLA	MG-NA	8.56	2.26	2.06
5	A	305	CHL	MG-NA	8.45	2.26	2.06
6	B	314	CLA	MG-NA	8.22	2.25	2.06
6	B	307	CLA	C3B-C2B	-8.09	1.29	1.40
6	B	308	CLA	C3B-C2B	-8.04	1.29	1.40
6	A	306	CLA	MG-NA	7.63	2.24	2.06
5	B	312	CHL	MG-NA	7.53	2.24	2.06
5	A	309	CHL	C3B-C2B	-6.94	1.30	1.40
5	B	311	CHL	MG-NA	6.64	2.22	2.06
6	B	314	CLA	C3B-C2B	-6.64	1.31	1.40
5	C	311	CHL	MG-NA	6.62	2.22	2.06
6	A	314	CLA	C3B-C2B	-6.47	1.31	1.40
6	A	307	CLA	MG-NA	6.32	2.21	2.06
6	B	307	CLA	C1D-ND	6.22	1.45	1.37
6	B	316	CLA	C1D-ND	6.19	1.45	1.37
6	B	314	CLA	O2D-CGD	6.14	1.48	1.33
5	B	310	CHL	CHC-C1C	6.11	1.50	1.35
6	A	307	CLA	C1D-ND	6.08	1.45	1.37
6	A	318	CLA	MG-NC	6.06	2.20	2.06
6	B	306	CLA	CHC-C1C	6.06	1.50	1.35
6	C	315	CLA	C1D-ND	6.02	1.45	1.37
6	C	316	CLA	C1D-ND	6.01	1.45	1.37
6	A	318	CLA	C1D-ND	6.00	1.45	1.37
6	C	306	CLA	CHC-C1C	5.96	1.50	1.35
6	B	308	CLA	CHC-C1C	5.95	1.50	1.35
6	A	315	CLA	C1D-ND	5.95	1.45	1.37
5	A	311	CHL	CHC-C1C	5.92	1.50	1.35
6	C	317	CLA	C1D-ND	5.91	1.45	1.37
5	B	312	CHL	O2D-CGD	5.88	1.47	1.33
6	C	318	CLA	C1D-ND	5.88	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	318	CLA	C1D-ND	5.88	1.45	1.37
5	C	309	CHL	C3B-C2B	-5.87	1.32	1.40
6	B	315	CLA	C1D-ND	5.85	1.45	1.37
6	B	318	CLA	MG-NC	5.84	2.20	2.06
6	C	314	CLA	CHC-C1C	5.84	1.49	1.35
6	A	306	CLA	CHC-C1C	5.81	1.49	1.35
5	C	313	CHL	CHC-C1C	5.77	1.49	1.35
5	B	313	CHL	CHC-C1C	5.73	1.49	1.35
5	C	310	CHL	CHC-C1C	5.72	1.49	1.35
6	B	317	CLA	C1D-ND	5.72	1.44	1.37
6	B	317	CLA	CHC-C1C	5.70	1.49	1.35
6	B	315	CLA	CHC-C1C	5.68	1.49	1.35
5	A	312	CHL	CHC-C1C	5.66	1.49	1.35
5	A	310	CHL	CHC-C1C	5.65	1.49	1.35
6	C	306	CLA	C3B-C2B	-5.64	1.32	1.40
6	A	315	CLA	CHC-C1C	5.64	1.49	1.35
6	A	317	CLA	C1D-ND	5.61	1.44	1.37
5	A	312	CHL	C3B-C2B	-5.60	1.32	1.40
5	C	305	CHL	CHC-C1C	5.58	1.49	1.35
6	C	307	CLA	C1D-ND	5.58	1.44	1.37
5	B	309	CHL	C3B-C2B	-5.57	1.32	1.40
6	A	317	CLA	CHC-C1C	5.55	1.49	1.35
6	B	314	CLA	CHC-C1C	5.54	1.49	1.35
5	A	313	CHL	CHC-C1C	5.53	1.49	1.35
6	A	314	CLA	CHC-C1C	5.51	1.49	1.35
6	A	308	CLA	CHC-C1C	5.51	1.49	1.35
5	A	310	CHL	O2D-CGD	5.49	1.46	1.33
6	B	315	CLA	MG-NC	5.47	2.19	2.06
5	C	309	CHL	CHC-C1C	5.44	1.48	1.35
6	C	317	CLA	O2D-CGD	5.44	1.46	1.33
6	C	315	CLA	CHC-C1C	5.43	1.48	1.35
6	A	307	CLA	O2D-CGD	5.41	1.46	1.33
6	C	317	CLA	CHC-C1C	5.41	1.48	1.35
6	A	314	CLA	O2D-CGD	5.41	1.46	1.33
6	C	316	CLA	CHC-C1C	5.40	1.48	1.35
6	B	316	CLA	O2D-CGD	5.39	1.46	1.33
6	B	307	CLA	CHC-C1C	5.36	1.48	1.35
5	B	312	CHL	CHC-C1C	5.33	1.48	1.35
6	C	317	CLA	CHD-C4C	5.33	1.51	1.39
6	C	318	CLA	MG-NC	5.32	2.18	2.06
5	C	310	CHL	O2D-CGD	5.29	1.46	1.33
5	C	311	CHL	CHC-C1C	5.29	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	309	CHL	CHC-C1C	5.27	1.48	1.35
5	A	313	CHL	O2D-CGD	5.27	1.46	1.33
5	B	311	CHL	CHC-C1C	5.26	1.48	1.35
6	B	318	CLA	O2D-CGD	5.25	1.46	1.33
6	B	307	CLA	O2D-CGD	5.25	1.46	1.33
6	A	318	CLA	CHC-C1C	5.24	1.48	1.35
5	B	311	CHL	O2D-CGD	5.23	1.46	1.33
6	C	315	CLA	C3B-C2B	-5.20	1.33	1.40
6	C	318	CLA	O2D-CGD	5.20	1.45	1.33
6	A	316	CLA	CHC-C1C	5.19	1.48	1.35
6	C	308	CLA	CHC-C1C	5.19	1.48	1.35
5	B	309	CHL	CHC-C1C	5.19	1.48	1.35
6	C	318	CLA	CHC-C1C	5.18	1.48	1.35
5	C	311	CHL	O2A-CGA	5.18	1.48	1.33
5	C	312	CHL	CHC-C1C	5.17	1.48	1.35
6	C	306	CLA	O2D-CGD	5.16	1.45	1.33
6	C	307	CLA	CHC-C1C	5.16	1.48	1.35
6	C	314	CLA	O2D-CGD	5.15	1.45	1.33
6	A	308	CLA	O2D-CGD	5.15	1.45	1.33
5	A	311	CHL	O2D-CGD	5.15	1.45	1.33
5	A	305	CHL	CHC-C1C	5.14	1.48	1.35
6	C	306	CLA	C1D-ND	5.11	1.44	1.37
6	A	306	CLA	MG-NC	5.11	2.18	2.06
6	C	308	CLA	O2D-CGD	5.10	1.45	1.33
6	C	308	CLA	C3B-C2B	-5.09	1.33	1.40
6	C	306	CLA	CHD-C4C	5.08	1.50	1.39
5	B	305	CHL	O2D-CGD	5.08	1.45	1.33
6	B	316	CLA	CHC-C1C	5.08	1.48	1.35
6	C	317	CLA	C3B-C2B	-5.08	1.33	1.40
5	A	309	CHL	O2D-CGD	5.07	1.45	1.33
6	B	314	CLA	O2A-CGA	5.06	1.48	1.33
6	C	314	CLA	C3B-C2B	-5.06	1.33	1.40
6	A	306	CLA	O2D-CGD	5.05	1.45	1.33
6	A	318	CLA	O2D-CGD	5.05	1.45	1.33
5	C	311	CHL	O2D-CGD	5.04	1.45	1.33
6	A	317	CLA	O2D-CGD	5.04	1.45	1.33
6	B	306	CLA	O2D-CGD	5.04	1.45	1.33
6	B	315	CLA	O2D-CGD	5.02	1.45	1.33
6	B	318	CLA	CHC-C1C	5.02	1.47	1.35
6	B	317	CLA	O2D-CGD	5.02	1.45	1.33
5	B	305	CHL	CHC-C1C	5.01	1.47	1.35
5	C	313	CHL	O2D-CGD	5.00	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	307	CLA	MG-NC	4.99	2.18	2.06
5	C	312	CHL	O2D-CGD	4.99	1.45	1.33
5	B	311	CHL	O2A-CGA	4.99	1.47	1.33
6	A	314	CLA	O2A-CGA	4.97	1.47	1.33
5	A	312	CHL	O2D-CGD	4.94	1.45	1.33
6	C	307	CLA	O2D-CGD	4.94	1.45	1.33
5	A	311	CHL	O2A-CGA	4.93	1.47	1.33
5	C	305	CHL	O2D-CGD	4.90	1.45	1.33
6	A	307	CLA	CHC-C1C	4.90	1.47	1.35
6	B	307	CLA	CHD-C4C	4.88	1.50	1.39
6	A	315	CLA	MG-NC	4.88	2.17	2.06
6	C	314	CLA	C1D-ND	4.83	1.43	1.37
6	C	315	CLA	CHD-C4C	4.83	1.50	1.39
5	C	313	CHL	C1D-ND	-4.82	1.31	1.37
6	B	317	CLA	CHD-C4C	4.79	1.50	1.39
6	B	308	CLA	C1D-ND	4.79	1.43	1.37
5	B	313	CHL	O2D-CGD	4.78	1.44	1.33
6	C	307	CLA	O2A-CGA	4.75	1.47	1.33
5	A	313	CHL	C1D-ND	-4.75	1.31	1.37
6	B	306	CLA	MG-NC	4.75	2.17	2.06
5	B	312	CHL	C3B-C2B	-4.74	1.33	1.40
6	C	314	CLA	O2A-CGA	4.74	1.47	1.33
6	A	318	CLA	CHD-C4C	4.74	1.50	1.39
5	C	309	CHL	O2D-CGD	4.73	1.44	1.33
4	B	304	LHG	O8-C23	4.71	1.47	1.33
5	C	312	CHL	CHD-C4C	4.71	1.50	1.39
6	A	317	CLA	MG-NC	4.71	2.17	2.06
6	A	317	CLA	CHD-C4C	4.71	1.50	1.39
6	A	316	CLA	O2D-CGD	4.70	1.44	1.33
6	B	307	CLA	O2A-CGA	4.69	1.47	1.33
6	B	306	CLA	C3B-C2B	-4.68	1.33	1.40
6	A	307	CLA	CHD-C4C	4.68	1.49	1.39
6	A	316	CLA	CHD-C4C	4.66	1.49	1.39
6	A	315	CLA	CHD-C4C	4.65	1.49	1.39
5	C	311	CHL	C3B-C2B	-4.65	1.33	1.40
6	B	317	CLA	MG-NC	4.64	2.17	2.06
5	B	312	CHL	CHD-C4C	4.63	1.49	1.39
6	C	318	CLA	CHD-C4C	4.61	1.49	1.39
6	C	316	CLA	O2D-CGD	4.59	1.44	1.33
6	C	315	CLA	O2D-CGD	4.58	1.44	1.33
5	B	309	CHL	O2D-CGD	4.56	1.44	1.33
5	C	309	CHL	O2A-CGA	4.55	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	308	CLA	O2A-CGA	4.53	1.46	1.33
5	A	305	CHL	O2D-CGD	4.53	1.44	1.33
6	C	308	CLA	O2A-CGA	4.51	1.46	1.33
5	B	305	CHL	O2A-CGA	4.50	1.46	1.33
6	A	308	CLA	O2A-CGA	4.50	1.46	1.33
6	B	308	CLA	O2D-CGD	4.49	1.44	1.33
5	B	309	CHL	O2A-CGA	4.49	1.46	1.33
6	A	308	CLA	C1D-ND	4.49	1.43	1.37
6	C	308	CLA	C1D-ND	4.49	1.43	1.37
4	A	304	LHG	O8-C23	4.48	1.46	1.33
5	A	310	CHL	O2A-CGA	4.48	1.46	1.33
6	B	318	CLA	CHD-C4C	4.47	1.49	1.39
5	A	305	CHL	CHD-C4C	4.46	1.49	1.39
6	B	314	CLA	C3D-C2D	4.46	1.51	1.39
6	A	315	CLA	O2D-CGD	4.45	1.44	1.33
6	A	307	CLA	O2A-CGA	4.45	1.46	1.33
5	B	310	CHL	O2A-CGA	4.44	1.46	1.33
6	A	314	CLA	C1D-ND	4.44	1.43	1.37
6	C	314	CLA	CHD-C4C	4.43	1.49	1.39
5	A	313	CHL	O2A-CGA	4.43	1.46	1.33
5	B	310	CHL	O2D-CGD	4.43	1.44	1.33
6	A	306	CLA	C1D-ND	4.41	1.43	1.37
6	C	317	CLA	MG-NC	4.41	2.16	2.06
5	A	309	CHL	O2A-CGA	4.40	1.46	1.33
5	A	312	CHL	O2A-CGA	4.40	1.46	1.33
5	C	310	CHL	C1D-ND	-4.40	1.32	1.37
4	C	304	LHG	O8-C23	4.39	1.46	1.33
6	A	315	CLA	O2A-CGA	4.39	1.46	1.33
6	A	316	CLA	C1D-ND	4.38	1.43	1.37
5	A	311	CHL	CHD-C4C	4.38	1.49	1.39
6	A	306	CLA	C3D-C2D	4.36	1.51	1.39
6	C	316	CLA	CHD-C4C	4.36	1.49	1.39
5	C	310	CHL	O2A-CGA	4.35	1.46	1.33
6	C	315	CLA	O2A-CGA	4.35	1.46	1.33
5	B	309	CHL	C1D-ND	-4.34	1.32	1.37
6	A	315	CLA	C3D-C2D	4.34	1.51	1.39
6	A	316	CLA	O2A-CGA	4.34	1.46	1.33
6	B	308	CLA	CHD-C4C	4.33	1.49	1.39
6	B	318	CLA	C3D-C2D	4.30	1.50	1.39
6	A	314	CLA	CHD-C4C	4.30	1.49	1.39
6	C	316	CLA	O2A-CGA	4.29	1.45	1.33
5	B	313	CHL	C1D-ND	-4.28	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	316	CLA	C3B-C2B	-4.28	1.34	1.40
5	A	310	CHL	C1D-ND	-4.28	1.32	1.37
6	B	308	CLA	C3D-C2D	4.27	1.50	1.39
5	B	310	CHL	C1D-ND	-4.24	1.32	1.37
5	A	305	CHL	O2A-CGA	4.23	1.45	1.33
5	B	313	CHL	O2A-CGA	4.23	1.45	1.33
6	B	315	CLA	O2A-CGA	4.22	1.45	1.33
6	B	315	CLA	C3D-C2D	4.21	1.50	1.39
5	A	310	CHL	CHD-C4C	4.21	1.48	1.39
6	A	317	CLA	O2A-CGA	4.20	1.45	1.33
6	B	314	CLA	CHD-C4C	4.20	1.48	1.39
6	C	306	CLA	C3D-C2D	4.19	1.50	1.39
5	B	305	CHL	C3D-C2D	4.19	1.50	1.39
6	B	316	CLA	O2A-CGA	4.18	1.45	1.33
5	C	312	CHL	O2A-CGA	4.18	1.45	1.33
6	B	316	CLA	CHD-C4C	4.17	1.48	1.39
6	C	314	CLA	C3D-C2D	4.15	1.50	1.39
6	A	314	CLA	C3D-C2D	4.14	1.50	1.39
6	B	306	CLA	CHD-C4C	4.13	1.48	1.39
6	C	307	CLA	CHD-C4C	4.12	1.48	1.39
6	B	317	CLA	C3D-C2D	4.12	1.50	1.39
5	A	309	CHL	CHD-C4C	4.11	1.48	1.39
6	A	307	CLA	C3B-C2B	-4.10	1.34	1.40
4	C	304	LHG	O7-C7	4.09	1.45	1.34
6	B	306	CLA	C3D-C2D	4.09	1.50	1.39
5	A	313	CHL	CHD-C4C	4.09	1.48	1.39
5	C	305	CHL	O2A-CGA	4.07	1.45	1.33
6	A	308	CLA	CHD-C4C	4.06	1.48	1.39
5	B	309	CHL	CHD-C4C	4.05	1.48	1.39
5	C	310	CHL	CHD-C4C	4.03	1.48	1.39
6	A	317	CLA	C3D-C2D	4.03	1.50	1.39
5	B	312	CHL	O2A-CGA	4.02	1.45	1.33
6	C	308	CLA	MG-NC	4.02	2.15	2.06
6	C	317	CLA	O2A-CGA	4.01	1.45	1.33
5	A	305	CHL	C3D-C2D	4.01	1.50	1.39
6	A	318	CLA	C3D-C2D	4.01	1.50	1.39
6	B	317	CLA	O2A-CGA	4.00	1.45	1.33
5	C	309	CHL	C1D-ND	-4.00	1.32	1.37
6	B	316	CLA	C3D-C2D	3.99	1.50	1.39
5	A	312	CHL	CHD-C4C	3.99	1.48	1.39
6	A	306	CLA	CHD-C4C	3.99	1.48	1.39
6	C	306	CLA	C4B-CHC	3.98	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	315	CLA	CHD-C4C	3.96	1.48	1.39
6	B	306	CLA	C4B-CHC	3.94	1.51	1.41
6	A	316	CLA	C3D-C2D	3.92	1.49	1.39
5	A	311	CHL	C1D-ND	-3.90	1.33	1.37
6	B	307	CLA	C1B-NB	-3.90	1.31	1.35
5	A	311	CHL	C3D-C2D	3.89	1.49	1.39
5	C	309	CHL	CHD-C4C	3.88	1.48	1.39
6	A	308	CLA	C3B-C2B	-3.88	1.35	1.40
5	B	310	CHL	C3D-C2D	3.87	1.49	1.39
6	C	307	CLA	C3D-C2D	3.85	1.49	1.39
6	C	315	CLA	C3D-C2D	3.84	1.49	1.39
5	C	311	CHL	CHD-C4C	3.84	1.48	1.39
5	C	305	CHL	CHD-C4C	3.84	1.48	1.39
6	B	314	CLA	C1D-ND	3.83	1.42	1.37
6	C	318	CLA	C3D-C2D	3.83	1.49	1.39
6	A	307	CLA	C3D-C2D	3.83	1.49	1.39
6	C	314	CLA	C1C-C2C	3.81	1.51	1.44
5	C	310	CHL	C3D-C2D	3.81	1.49	1.39
6	A	314	CLA	MG-NC	3.80	2.15	2.06
4	B	304	LHG	O7-C7	3.79	1.45	1.34
5	A	312	CHL	C3D-C2D	3.78	1.49	1.39
5	A	309	CHL	C3D-C2D	3.77	1.49	1.39
5	C	313	CHL	O2A-CGA	3.77	1.44	1.33
5	C	312	CHL	C3D-C2D	3.76	1.49	1.39
6	C	308	CLA	C3D-C2D	3.74	1.49	1.39
5	B	310	CHL	CHD-C4C	3.73	1.47	1.39
6	A	308	CLA	C3D-C2D	3.73	1.49	1.39
5	C	305	CHL	C3D-C2D	3.73	1.49	1.39
5	B	313	CHL	CHD-C4C	3.72	1.47	1.39
5	B	305	CHL	C4D-CHA	3.71	1.51	1.38
5	C	313	CHL	CHD-C4C	3.69	1.47	1.39
5	B	311	CHL	C1D-ND	-3.69	1.33	1.37
5	B	312	CHL	C1D-ND	-3.68	1.33	1.37
5	C	311	CHL	C1D-ND	-3.68	1.33	1.37
6	C	316	CLA	C3D-C2D	3.68	1.49	1.39
6	C	317	CLA	C3D-C2D	3.68	1.49	1.39
6	A	306	CLA	C3B-C2B	-3.66	1.35	1.40
6	A	318	CLA	C3B-C2B	-3.66	1.35	1.40
4	A	304	LHG	O7-C7	3.65	1.44	1.34
5	B	309	CHL	C3D-C2D	3.65	1.49	1.39
6	B	306	CLA	O2A-CGA	3.63	1.43	1.33
2	C	301	LUT	C22-C21	-3.63	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	306	CLA	O2A-CGA	3.62	1.43	1.33
5	B	313	CHL	C3D-C2D	3.60	1.48	1.39
6	B	308	CLA	MG-NC	3.59	2.14	2.06
5	C	311	CHL	C3D-C2D	3.58	1.48	1.39
5	B	312	CHL	C3D-C2D	3.57	1.48	1.39
5	C	309	CHL	C3D-C2D	3.56	1.48	1.39
5	B	305	CHL	CHD-C4C	3.54	1.47	1.39
6	C	316	CLA	C4D-CHA	3.53	1.50	1.38
5	A	309	CHL	C1D-ND	-3.53	1.33	1.37
6	C	306	CLA	O2A-CGA	3.53	1.43	1.33
5	B	311	CHL	C3D-C2D	3.53	1.48	1.39
5	C	309	CHL	C4B-CHC	3.53	1.50	1.41
6	A	306	CLA	C4B-CHC	3.53	1.50	1.41
5	B	311	CHL	MG-NC	3.53	2.14	2.06
6	C	315	CLA	MG-NC	3.52	2.14	2.06
5	C	305	CHL	C3B-C2B	-3.52	1.35	1.40
6	A	307	CLA	C4C-C3C	3.50	1.51	1.45
6	A	315	CLA	C4D-CHA	3.49	1.50	1.38
6	B	318	CLA	C3B-C2B	-3.48	1.35	1.40
6	C	316	CLA	C1B-CHB	3.46	1.50	1.41
6	C	306	CLA	C1B-CHB	3.45	1.50	1.41
5	B	311	CHL	CHD-C4C	3.44	1.47	1.39
6	C	318	CLA	C3B-C2B	-3.44	1.35	1.40
5	C	305	CHL	C1C-NC	-3.41	1.32	1.37
5	A	310	CHL	C3D-C2D	3.41	1.48	1.39
6	B	316	CLA	C1B-CHB	3.40	1.50	1.41
6	A	316	CLA	C1C-NC	-3.39	1.32	1.37
6	B	308	CLA	C1C-C2C	3.34	1.51	1.44
5	A	312	CHL	C4D-CHA	3.34	1.50	1.38
6	B	308	CLA	C4B-CHC	3.34	1.50	1.41
6	C	307	CLA	C4C-C3C	3.33	1.50	1.45
5	B	313	CHL	C4B-CHC	3.33	1.50	1.41
6	C	314	CLA	C4D-CHA	3.33	1.50	1.38
5	C	310	CHL	C4D-CHA	3.32	1.50	1.38
6	B	307	CLA	C3D-C2D	3.29	1.48	1.39
6	B	306	CLA	C1D-ND	3.28	1.41	1.37
6	A	314	CLA	C1B-CHB	3.27	1.50	1.41
5	A	310	CHL	C4D-CHA	3.26	1.50	1.38
5	C	312	CHL	C1C-NC	-3.24	1.33	1.37
5	B	305	CHL	C1D-ND	-3.22	1.33	1.37
3	C	303	NEX	C7-C8	-3.21	1.26	1.32
6	A	316	CLA	MG-NC	-3.19	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	315	CLA	C4D-CHA	3.19	1.49	1.38
5	C	313	CHL	C2C-C1C	3.19	1.51	1.44
6	B	315	CLA	C4D-CHA	3.18	1.49	1.38
5	A	312	CHL	C1D-ND	-3.18	1.33	1.37
5	A	305	CHL	C1D-ND	-3.17	1.33	1.37
5	A	305	CHL	C4D-CHA	3.17	1.49	1.38
6	C	306	CLA	MG-NC	3.15	2.13	2.06
3	A	303	NEX	C7-C8	-3.15	1.26	1.32
5	B	311	CHL	C4B-CHC	3.14	1.49	1.41
6	A	307	CLA	C1C-C2C	3.13	1.50	1.44
6	A	316	CLA	C4B-CHC	3.12	1.49	1.41
6	A	306	CLA	C1B-CHB	3.12	1.49	1.41
6	C	317	CLA	C4D-CHA	3.11	1.49	1.38
6	A	308	CLA	C4D-CHA	3.11	1.49	1.38
5	B	310	CHL	C4D-CHA	3.10	1.49	1.38
5	C	305	CHL	C1D-ND	-3.09	1.34	1.37
6	A	315	CLA	C3B-C2B	-3.08	1.36	1.40
5	A	312	CHL	C2C-C1C	3.08	1.51	1.44
5	B	311	CHL	C3B-C2B	-3.08	1.36	1.40
5	A	313	CHL	C3D-C2D	3.08	1.47	1.39
5	B	313	CHL	C2C-C1C	3.08	1.51	1.44
6	B	308	CLA	C4D-ND	3.06	1.41	1.37
6	B	317	CLA	C4D-CHA	3.06	1.49	1.38
6	C	307	CLA	C1C-C2C	3.06	1.50	1.44
5	A	313	CHL	C4D-CHA	3.06	1.49	1.38
6	C	308	CLA	C1C-C2C	3.05	1.50	1.44
5	A	310	CHL	C4B-CHC	3.05	1.49	1.41
6	C	318	CLA	C1B-CHB	3.05	1.49	1.41
5	C	313	CHL	C4B-CHC	3.04	1.49	1.41
5	B	309	CHL	C4B-CHC	3.04	1.49	1.41
6	C	316	CLA	C4B-CHC	3.04	1.49	1.41
6	B	318	CLA	C4D-CHA	3.04	1.49	1.38
6	A	318	CLA	C4D-CHA	3.04	1.49	1.38
6	B	306	CLA	C1B-CHB	3.03	1.49	1.41
6	A	318	CLA	C4B-CHC	3.03	1.49	1.41
6	B	316	CLA	C4D-CHA	3.02	1.49	1.38
5	C	312	CHL	C4D-CHA	3.02	1.49	1.38
6	B	315	CLA	C4B-CHC	3.02	1.49	1.41
5	A	311	CHL	C4D-CHA	3.01	1.49	1.38
5	A	310	CHL	C1B-CHB	3.01	1.49	1.41
5	A	311	CHL	C1B-CHB	3.01	1.49	1.41
5	C	309	CHL	C4D-CHA	3.00	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	310	CHL	C2C-C1C	3.00	1.50	1.44
6	A	316	CLA	C1B-CHB	3.00	1.49	1.41
6	A	315	CLA	C1B-CHB	3.00	1.49	1.41
5	A	311	CHL	C4B-CHC	3.00	1.49	1.41
6	C	314	CLA	C4C-C3C	3.00	1.50	1.45
5	C	313	CHL	C4D-CHA	2.99	1.49	1.38
2	A	301	LUT	C22-C21	-2.99	1.51	1.54
6	B	308	CLA	C4D-CHA	2.99	1.49	1.38
5	A	313	CHL	C4B-CHC	2.99	1.49	1.41
5	B	310	CHL	C4B-CHC	2.98	1.49	1.41
6	A	307	CLA	C4D-CHA	2.97	1.49	1.38
3	B	303	NEX	C7-C8	-2.97	1.27	1.32
6	B	318	CLA	C1B-CHB	2.97	1.49	1.41
6	C	307	CLA	C4D-CHA	2.96	1.48	1.38
5	B	310	CHL	C2C-C1C	2.95	1.50	1.44
6	A	315	CLA	C4D-ND	2.95	1.41	1.37
6	A	314	CLA	C4D-CHA	2.95	1.48	1.38
6	C	318	CLA	C4D-CHA	2.94	1.48	1.38
6	B	314	CLA	C4D-CHA	2.93	1.48	1.38
5	B	309	CHL	C4D-CHA	2.93	1.48	1.38
5	C	309	CHL	C1B-CHB	2.91	1.49	1.41
5	A	309	CHL	C1C-NC	-2.91	1.33	1.37
5	C	311	CHL	C4D-CHA	2.90	1.48	1.38
5	A	309	CHL	C4D-CHA	2.90	1.48	1.38
5	B	310	CHL	C1B-CHB	2.90	1.49	1.41
6	A	317	CLA	C3B-C2B	-2.89	1.36	1.40
5	C	311	CHL	C1B-CHB	2.89	1.49	1.41
5	A	313	CHL	C2C-C1C	2.88	1.50	1.44
6	A	318	CLA	C1C-NC	-2.88	1.33	1.37
5	A	313	CHL	C4C-C3C	2.87	1.50	1.45
6	B	316	CLA	C1C-NC	-2.87	1.33	1.37
6	C	308	CLA	CHD-C4C	2.87	1.45	1.39
6	B	314	CLA	C4C-C3C	2.87	1.50	1.45
6	C	315	CLA	C4C-C3C	2.87	1.50	1.45
6	B	317	CLA	C4B-CHC	2.87	1.49	1.41
5	C	310	CHL	C1B-CHB	2.86	1.49	1.41
6	A	308	CLA	C1B-CHB	2.86	1.48	1.41
6	A	314	CLA	C4C-C3C	2.85	1.50	1.45
6	C	306	CLA	C4D-CHA	2.85	1.48	1.38
6	B	307	CLA	C4D-CHA	2.85	1.48	1.38
6	A	315	CLA	C4B-CHC	2.85	1.48	1.41
6	A	318	CLA	C1B-CHB	2.85	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	305	CHL	C4D-CHA	2.84	1.48	1.38
5	A	305	CHL	C2C-C1C	2.84	1.50	1.44
6	A	318	CLA	C3A-C2A	-2.84	1.51	1.54
6	B	306	CLA	C1C-C2C	2.84	1.50	1.44
6	A	317	CLA	C4D-CHA	2.83	1.48	1.38
5	A	313	CHL	MG-NC	2.83	2.13	2.06
5	B	312	CHL	C4B-CHC	2.83	1.48	1.41
6	A	316	CLA	C4D-CHA	2.83	1.48	1.38
5	C	305	CHL	C1B-CHB	2.83	1.48	1.41
6	B	318	CLA	C4C-C3C	2.82	1.49	1.45
5	B	311	CHL	C4D-CHA	2.82	1.48	1.38
5	A	312	CHL	C4B-CHC	2.82	1.48	1.41
5	A	309	CHL	C4B-CHC	2.82	1.48	1.41
5	C	310	CHL	C4B-CHC	2.82	1.48	1.41
5	A	309	CHL	C4C-C3C	2.82	1.49	1.45
5	A	312	CHL	C1B-CHB	2.82	1.48	1.41
6	B	318	CLA	C4B-CHC	2.81	1.48	1.41
5	B	312	CHL	C1B-CHB	2.81	1.48	1.41
6	C	315	CLA	C4B-CHC	2.81	1.48	1.41
5	B	313	CHL	C4D-CHA	2.80	1.48	1.38
5	C	313	CHL	C3D-C2D	2.80	1.46	1.39
6	A	316	CLA	C4D-ND	2.79	1.41	1.37
6	B	315	CLA	C1B-CHB	2.79	1.48	1.41
6	A	318	CLA	C4C-C3C	2.79	1.49	1.45
6	A	307	CLA	C1B-NB	-2.78	1.32	1.35
6	C	316	CLA	C1C-NC	-2.78	1.33	1.37
5	B	309	CHL	C1B-CHB	2.78	1.48	1.41
5	B	310	CHL	C3B-C2B	-2.77	1.36	1.40
6	C	315	CLA	C1C-C2C	2.77	1.49	1.44
5	A	309	CHL	C1B-CHB	2.76	1.48	1.41
6	B	316	CLA	C1B-NB	-2.76	1.32	1.35
5	C	313	CHL	MG-NC	2.75	2.12	2.06
5	B	312	CHL	C4D-CHA	2.75	1.48	1.38
6	C	318	CLA	C4C-C3C	2.75	1.49	1.45
6	C	308	CLA	C4B-CHC	2.75	1.48	1.41
6	B	317	CLA	C1B-CHB	2.74	1.48	1.41
5	B	305	CHL	C4B-NB	-2.74	1.32	1.35
6	C	306	CLA	C1C-C2C	2.74	1.49	1.44
5	A	305	CHL	C4B-CHC	2.74	1.48	1.41
6	A	308	CLA	C4B-CHC	2.73	1.48	1.41
6	C	307	CLA	C1B-CHB	2.73	1.48	1.41
5	B	305	CHL	C4B-CHC	2.73	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	311	CHL	C4B-CHC	2.72	1.48	1.41
5	A	310	CHL	C4C-C3C	2.72	1.49	1.45
6	C	317	CLA	C4C-C3C	2.72	1.49	1.45
5	C	312	CHL	C1D-C2D	2.72	1.50	1.45
6	A	314	CLA	C1C-C2C	2.72	1.49	1.44
5	C	310	CHL	C4C-C3C	2.71	1.49	1.45
6	B	314	CLA	C1B-CHB	2.70	1.48	1.41
6	C	317	CLA	C1B-CHB	2.69	1.48	1.41
6	B	306	CLA	C4D-CHA	2.69	1.47	1.38
5	C	312	CHL	C4B-CHC	2.68	1.48	1.41
5	A	305	CHL	C1C-NC	-2.68	1.33	1.37
5	C	312	CHL	CHD-C1D	2.68	1.43	1.38
5	B	311	CHL	C2C-C1C	2.67	1.50	1.44
6	A	314	CLA	C4D-ND	2.66	1.41	1.37
6	C	314	CLA	C1B-CHB	2.66	1.48	1.41
6	B	318	CLA	C1C-NC	-2.65	1.33	1.37
5	C	309	CHL	C2C-C1C	2.65	1.50	1.44
5	C	312	CHL	C2C-C1C	2.65	1.50	1.44
6	A	306	CLA	C1C-NC	-2.65	1.33	1.37
6	B	308	CLA	C1B-CHB	2.65	1.48	1.41
6	C	308	CLA	C4D-CHA	2.65	1.47	1.38
5	B	309	CHL	C1C-NC	-2.65	1.33	1.37
5	C	305	CHL	C4B-CHC	2.64	1.48	1.41
6	B	318	CLA	C4D-ND	2.64	1.41	1.37
6	C	317	CLA	C1C-C2C	2.63	1.49	1.44
6	C	318	CLA	C4B-CHC	2.63	1.48	1.41
5	B	313	CHL	C1B-CHB	2.63	1.48	1.41
6	B	307	CLA	C1C-C2C	2.61	1.49	1.44
5	B	305	CHL	C1C-NC	-2.61	1.33	1.37
5	A	312	CHL	C1D-C2D	2.61	1.50	1.45
6	C	308	CLA	C1B-CHB	2.60	1.48	1.41
5	A	313	CHL	C1B-CHB	2.60	1.48	1.41
6	C	315	CLA	C1B-CHB	2.60	1.48	1.41
6	B	307	CLA	C4C-C3C	2.59	1.49	1.45
5	C	313	CHL	C3B-C2B	-2.58	1.36	1.40
6	A	306	CLA	C4D-CHA	2.58	1.47	1.38
5	C	312	CHL	C4B-NB	-2.57	1.32	1.35
6	B	314	CLA	C4D-ND	2.57	1.41	1.37
6	B	318	CLA	C3A-C2A	-2.57	1.52	1.54
6	A	308	CLA	C4D-ND	2.57	1.41	1.37
5	A	311	CHL	C4C-C3C	2.57	1.49	1.45
2	C	302	LUT	C1-C6	-2.56	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	305	CHL	C3B-C2B	-2.53	1.36	1.40
2	B	302	LUT	C26-C27	2.52	1.54	1.50
5	C	309	CHL	C4C-C3C	2.52	1.49	1.45
6	A	307	CLA	C4B-CHC	2.51	1.48	1.41
5	B	312	CHL	C2C-C1C	2.50	1.49	1.44
5	B	305	CHL	C1B-CHB	2.50	1.47	1.41
6	C	316	CLA	C1C-C2C	2.50	1.49	1.44
5	B	311	CHL	C1B-CHB	2.49	1.47	1.41
6	C	318	CLA	C1C-NC	-2.48	1.34	1.37
5	B	312	CHL	C4C-C3C	2.48	1.49	1.45
6	C	306	CLA	C4D-ND	2.47	1.41	1.37
6	B	316	CLA	C4B-CHC	2.47	1.47	1.41
5	B	312	CHL	MG-NC	2.47	2.12	2.06
5	C	313	CHL	C1C-NC	-2.47	1.34	1.37
5	B	310	CHL	C4C-C3C	2.47	1.49	1.45
6	A	307	CLA	C1B-CHB	2.46	1.47	1.41
6	C	315	CLA	C4D-ND	2.45	1.41	1.37
6	B	307	CLA	C1D-C2D	2.45	1.50	1.45
5	A	310	CHL	C4D-ND	2.45	1.41	1.37
5	C	313	CHL	C1B-NB	-2.44	1.33	1.35
5	A	305	CHL	C1B-CHB	2.44	1.47	1.41
6	B	307	CLA	C1B-CHB	2.43	1.47	1.41
6	A	318	CLA	C1C-C2C	2.43	1.49	1.44
5	C	310	CHL	C2C-C1C	2.43	1.49	1.44
5	B	311	CHL	C1C-NC	-2.43	1.34	1.37
6	B	315	CLA	C4D-ND	2.42	1.41	1.37
6	B	318	CLA	C1C-C2C	2.42	1.49	1.44
6	C	314	CLA	C4B-CHC	2.42	1.47	1.41
6	C	308	CLA	C1C-NC	-2.42	1.34	1.37
5	C	309	CHL	C1C-NC	-2.41	1.34	1.37
6	B	307	CLA	C1C-NC	-2.41	1.34	1.37
6	A	317	CLA	C4B-CHC	2.40	1.47	1.41
6	C	307	CLA	MG-ND	-2.40	2.01	2.05
5	C	309	CHL	C1D-C2D	2.40	1.50	1.45
5	B	311	CHL	C3D-C4D	-2.39	1.38	1.44
6	B	307	CLA	C4B-CHC	2.38	1.47	1.41
6	C	315	CLA	C1C-NC	-2.38	1.34	1.37
6	C	307	CLA	C4B-CHC	2.37	1.47	1.41
5	A	311	CHL	C2C-C1C	2.36	1.49	1.44
6	B	314	CLA	C1B-NB	-2.36	1.33	1.35
5	B	305	CHL	C1B-NB	-2.35	1.33	1.35
6	A	306	CLA	C1C-C2C	2.35	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	311	CHL	C4C-C3C	2.35	1.49	1.45
6	C	317	CLA	C4B-CHC	2.34	1.47	1.41
5	A	309	CHL	C3D-C4D	-2.34	1.38	1.44
6	C	318	CLA	C1D-C2D	2.33	1.49	1.45
5	C	313	CHL	C1B-CHB	2.33	1.47	1.41
5	B	312	CHL	C1C-NC	-2.33	1.34	1.37
5	C	310	CHL	MG-NC	2.33	2.11	2.06
5	C	311	CHL	C2C-C1C	2.32	1.49	1.44
6	A	315	CLA	C1C-NC	-2.32	1.34	1.37
6	A	317	CLA	C1B-CHB	2.32	1.47	1.41
3	B	303	NEX	O24-C25	-2.31	1.42	1.46
6	A	306	CLA	C4D-ND	2.30	1.40	1.37
6	B	315	CLA	C1C-NC	-2.28	1.34	1.37
6	A	314	CLA	C4B-CHC	2.28	1.47	1.41
5	B	305	CHL	C2C-C1C	2.27	1.49	1.44
5	C	305	CHL	C2C-C1C	2.27	1.49	1.44
6	C	317	CLA	C1D-C2D	2.27	1.49	1.45
6	A	317	CLA	C1C-NC	-2.24	1.34	1.37
6	A	317	CLA	C4C-C3C	2.24	1.48	1.45
6	A	308	CLA	C1C-C2C	2.24	1.48	1.44
6	A	318	CLA	C4D-ND	2.24	1.40	1.37
6	A	316	CLA	C4B-NB	-2.23	1.33	1.35
6	C	307	CLA	C1C-NC	-2.23	1.34	1.37
6	C	318	CLA	C4D-ND	2.22	1.40	1.37
6	B	314	CLA	C4B-CHC	2.22	1.47	1.41
5	A	312	CHL	C1C-NC	-2.22	1.34	1.37
5	A	313	CHL	CMC-C2C	2.22	1.49	1.45
6	B	316	CLA	C4C-C3C	2.22	1.48	1.45
5	B	309	CHL	C4C-C3C	2.21	1.48	1.45
6	C	306	CLA	C1D-C2D	2.21	1.49	1.45
5	A	309	CHL	C2C-C1C	2.21	1.49	1.44
6	A	315	CLA	C4C-C3C	2.20	1.48	1.45
5	C	312	CHL	C1B-CHB	2.20	1.47	1.41
6	C	317	CLA	CHD-C1D	2.20	1.42	1.38
6	C	307	CLA	C3B-C2B	-2.19	1.37	1.40
6	B	308	CLA	C1C-NC	-2.18	1.34	1.37
6	A	318	CLA	C1D-C2D	2.18	1.49	1.45
5	C	310	CHL	C3B-C2B	-2.18	1.37	1.40
6	C	314	CLA	C4D-ND	2.18	1.40	1.37
2	B	302	LUT	C23-C24	2.16	1.53	1.50
6	B	315	CLA	C1D-C2D	2.15	1.49	1.45
6	C	318	CLA	C1C-C2C	2.15	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	314	CLA	MG-NC	2.13	2.11	2.06
5	C	311	CHL	C3D-C4D	-2.13	1.39	1.44
5	C	311	CHL	C1C-NC	-2.13	1.34	1.37
5	C	305	CHL	MG-NC	2.12	2.11	2.06
6	B	318	CLA	C1D-C2D	2.12	1.49	1.45
6	B	316	CLA	C1C-C2C	2.10	1.48	1.44
6	C	307	CLA	CAA-C2A	-2.10	1.50	1.54
5	C	310	CHL	C1C-NC	-2.10	1.34	1.37
5	C	305	CHL	C3D-C4D	-2.10	1.39	1.44
5	B	312	CHL	C3D-C4D	-2.09	1.39	1.44
6	C	314	CLA	C1B-NB	-2.09	1.33	1.35
6	A	308	CLA	C4C-C3C	2.08	1.48	1.45
5	A	310	CHL	CMC-C2C	2.08	1.49	1.45
5	C	309	CHL	C3D-C4D	-2.07	1.39	1.44
3	A	303	NEX	O24-C25	-2.05	1.43	1.46
2	B	302	LUT	C1-C6	-2.05	1.50	1.53
6	C	306	CLA	C4C-C3C	2.05	1.48	1.45
6	B	315	CLA	C1C-C2C	2.04	1.48	1.44
6	C	317	CLA	C1C-NC	-2.03	1.34	1.37
6	B	306	CLA	C3D-C4D	-2.02	1.39	1.44
2	A	302	LUT	C24-C25	2.02	1.35	1.33
6	B	306	CLA	C1C-NC	-2.01	1.34	1.37
5	A	305	CHL	CMC-C2C	2.00	1.49	1.45

All (833) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	303	NEX	O24-C25-C24	16.37	125.68	113.38
3	B	303	NEX	O24-C25-C24	15.85	125.29	113.38
3	A	303	NEX	O24-C25-C24	14.75	124.46	113.38
6	A	314	CLA	C4A-NA-C1A	7.55	110.10	106.71
5	A	312	CHL	C4A-NA-C1A	7.47	110.06	106.71
6	B	307	CLA	O2D-CGD-CBD	7.27	124.18	111.27
6	A	316	CLA	C4A-NA-C1A	7.25	109.97	106.71
6	B	316	CLA	C4A-NA-C1A	7.14	109.92	106.71
6	C	316	CLA	C4A-NA-C1A	6.97	109.84	106.71
5	B	305	CHL	C1D-ND-C4D	6.94	111.27	106.33
5	A	313	CHL	C4A-NA-C1A	6.83	109.78	106.71
6	B	308	CLA	O2D-CGD-CBD	6.82	123.39	111.27
6	A	306	CLA	O2D-CGD-CBD	6.82	123.38	111.27
5	A	310	CHL	C4A-NA-C1A	6.78	109.75	106.71
5	C	305	CHL	C4A-NA-C1A	6.73	109.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	316	CLA	O2D-CGD-CBD	6.66	123.09	111.27
3	A	303	NEX	C35-C34-C33	-6.56	117.94	127.31
5	B	305	CHL	C4A-NA-C1A	6.56	109.65	106.71
5	A	309	CHL	C4A-NA-C1A	6.50	109.63	106.71
5	C	311	CHL	C4A-NA-C1A	6.48	109.62	106.71
6	B	306	CLA	O2D-CGD-CBD	6.46	122.74	111.27
5	B	311	CHL	C4A-NA-C1A	6.41	109.59	106.71
6	B	315	CLA	O2D-CGD-CBD	6.40	122.64	111.27
5	C	312	CHL	O2D-CGD-CBD	6.39	122.62	111.27
6	B	315	CLA	C4A-NA-C1A	6.37	109.57	106.71
5	C	310	CHL	C4A-NA-C1A	6.25	109.52	106.71
6	C	306	CLA	O2D-CGD-CBD	6.23	122.35	111.27
6	B	318	CLA	C4A-NA-C1A	6.23	109.51	106.71
6	A	307	CLA	C2D-C1D-ND	-6.22	105.52	110.10
6	C	316	CLA	O2D-CGD-CBD	6.18	122.24	111.27
5	C	311	CHL	O2D-CGD-CBD	6.16	122.22	111.27
3	B	303	NEX	C38-C25-C26	-6.11	112.03	122.26
5	A	309	CHL	O2D-CGD-CBD	6.07	122.06	111.27
5	A	311	CHL	C4A-NA-C1A	6.07	109.44	106.71
6	A	318	CLA	O2D-CGD-CBD	6.07	122.05	111.27
6	B	318	CLA	O2D-CGD-CBD	6.05	122.02	111.27
5	B	311	CHL	O2D-CGD-CBD	6.04	122.00	111.27
6	C	317	CLA	C4A-NA-C1A	5.99	109.40	106.71
5	C	312	CHL	C4A-NA-C1A	5.98	109.40	106.71
6	A	318	CLA	C4A-NA-C1A	5.98	109.39	106.71
6	C	314	CLA	C4A-NA-C1A	5.96	109.39	106.71
6	B	307	CLA	C2D-C1D-ND	-5.96	105.72	110.10
3	C	303	NEX	C35-C34-C33	-5.95	118.82	127.31
5	B	310	CHL	C4A-NA-C1A	5.92	109.37	106.71
6	C	307	CLA	O2D-CGD-CBD	5.90	121.75	111.27
6	A	307	CLA	O2D-CGD-CBD	5.88	121.72	111.27
6	C	308	CLA	O2D-CGD-CBD	5.87	121.71	111.27
5	C	305	CHL	C1D-ND-C4D	5.86	110.50	106.33
5	B	310	CHL	O2D-CGD-CBD	5.83	121.63	111.27
6	A	307	CLA	C1D-ND-C4D	5.81	110.46	106.33
5	C	310	CHL	O2D-CGD-CBD	5.75	121.48	111.27
5	C	312	CHL	C1D-ND-C4D	5.72	110.40	106.33
6	A	307	CLA	C4A-NA-C1A	5.71	109.27	106.71
6	A	315	CLA	C4A-NA-C1A	5.71	109.27	106.71
6	C	315	CLA	C4A-NA-C1A	5.70	109.27	106.71
5	A	309	CHL	C1D-ND-C4D	5.69	110.38	106.33
5	A	305	CHL	C4A-NA-C1A	5.61	109.23	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	318	CLA	O2D-CGD-CBD	5.60	121.22	111.27
5	B	309	CHL	O2D-CGD-CBD	5.57	121.17	111.27
6	A	306	CLA	C9-C8-C7	5.55	131.39	111.29
6	B	316	CLA	C1D-ND-C4D	5.53	110.26	106.33
5	C	310	CHL	C1D-ND-C4D	5.52	110.25	106.33
6	A	308	CLA	C4A-NA-C1A	5.50	109.18	106.71
6	A	308	CLA	O2D-CGD-CBD	5.45	120.95	111.27
5	B	309	CHL	C4A-NA-C1A	5.42	109.14	106.71
3	A	303	NEX	C38-C25-C26	-5.40	113.22	122.26
3	C	303	NEX	C38-C25-C26	-5.34	113.32	122.26
5	B	309	CHL	C1D-ND-C4D	5.33	110.12	106.33
6	B	315	CLA	C1D-ND-C4D	5.32	110.11	106.33
5	A	310	CHL	C1D-ND-C4D	5.31	110.11	106.33
5	C	309	CHL	O2D-CGD-CBD	5.26	120.61	111.27
5	A	305	CHL	C1D-ND-C4D	5.23	110.05	106.33
6	C	308	CLA	C4A-NA-C1A	5.22	109.05	106.71
5	B	311	CHL	C1D-ND-C4D	5.21	110.04	106.33
3	A	303	NEX	C27-C28-C29	-5.20	117.47	125.53
5	C	311	CHL	C1D-ND-C4D	5.18	110.01	106.33
5	A	311	CHL	C1D-ND-C4D	5.17	110.01	106.33
6	C	308	CLA	CHD-C4C-C3C	-5.16	117.25	124.84
6	C	306	CLA	C4A-NA-C1A	5.16	109.03	106.71
5	B	312	CHL	C1D-ND-C4D	5.15	109.99	106.33
5	A	311	CHL	O2D-CGD-CBD	5.14	120.40	111.27
3	B	303	NEX	C35-C34-C33	-5.13	119.98	127.31
5	A	305	CHL	CHD-C4C-NC	5.13	132.28	124.20
6	B	307	CLA	C1D-ND-C4D	5.12	109.97	106.33
5	C	309	CHL	C1D-ND-C4D	5.11	109.97	106.33
5	A	312	CHL	C1D-ND-C4D	5.10	109.95	106.33
6	A	315	CLA	O2D-CGD-CBD	5.09	120.31	111.27
5	C	313	CHL	C4A-NA-C1A	5.06	108.98	106.71
5	B	310	CHL	O2D-CGD-O1D	-5.03	114.01	123.84
5	C	313	CHL	CHD-C4C-C3C	-5.02	117.47	124.84
6	B	316	CLA	C2D-C1D-ND	-5.00	106.42	110.10
5	A	305	CHL	CHD-C4C-C3C	-4.96	117.55	124.84
6	B	308	CLA	C4A-NA-C1A	4.96	108.94	106.71
5	B	305	CHL	C1D-CHD-C4C	-4.95	115.38	126.06
6	A	316	CLA	CHD-C4C-NC	4.94	131.99	124.20
5	B	312	CHL	C4A-NA-C1A	4.94	108.93	106.71
6	C	315	CLA	O2D-CGD-CBD	4.92	120.01	111.27
6	A	316	CLA	O2D-CGD-CBD	4.90	119.98	111.27
6	C	318	CLA	C4A-NA-C1A	4.88	108.90	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	310	CHL	O2D-CGD-CBD	4.88	119.93	111.27
5	B	305	CHL	CHD-C4C-C3C	-4.86	117.70	124.84
5	B	312	CHL	O2D-CGD-CBD	4.86	119.90	111.27
6	A	308	CLA	C1D-CHD-C4C	-4.85	115.58	126.06
6	B	314	CLA	C1D-CHD-C4C	-4.85	115.60	126.06
6	C	314	CLA	O2D-CGD-CBD	4.84	119.87	111.27
6	C	307	CLA	C1D-ND-C4D	4.84	109.77	106.33
5	B	305	CHL	CHD-C4C-NC	4.83	131.82	124.20
2	C	301	LUT	C18-C5-C6	-4.82	119.11	124.53
6	B	315	CLA	C2D-C1D-ND	-4.81	106.56	110.10
2	C	302	LUT	C11-C10-C9	-4.79	120.47	127.31
6	A	308	CLA	CHD-C4C-NC	4.76	131.70	124.20
6	C	307	CLA	C2D-C1D-ND	-4.75	106.60	110.10
6	B	306	CLA	CHD-C4C-NC	4.73	131.65	124.20
6	C	308	CLA	C1D-CHD-C4C	-4.72	115.88	126.06
6	B	308	CLA	CHD-C4C-C3C	-4.70	117.94	124.84
5	B	310	CHL	CHD-C4C-C3C	-4.69	117.94	124.84
6	B	307	CLA	O2D-CGD-O1D	-4.69	114.68	123.84
5	C	313	CHL	O2D-CGD-CBD	4.66	119.54	111.27
2	B	301	LUT	C11-C10-C9	-4.65	120.67	127.31
6	B	306	CLA	CHD-C4C-C3C	-4.65	118.01	124.84
6	A	306	CLA	CHD-C4C-NC	4.64	131.51	124.20
6	B	316	CLA	C1D-CHD-C4C	-4.59	116.17	126.06
6	B	308	CLA	O2D-CGD-O1D	-4.58	114.89	123.84
5	A	305	CHL	C1-C2-C3	-4.56	118.15	126.04
6	A	308	CLA	CHD-C4C-C3C	-4.54	118.16	124.84
6	B	315	CLA	O2D-CGD-O1D	-4.53	114.97	123.84
5	C	309	CHL	C4A-NA-C1A	4.52	108.74	106.71
5	B	313	CHL	C1D-ND-C4D	4.51	109.54	106.33
6	A	315	CLA	C1D-ND-C4D	4.51	109.54	106.33
5	B	313	CHL	O2D-CGD-CBD	4.50	119.26	111.27
5	A	312	CHL	O2D-CGD-CBD	4.46	119.19	111.27
6	A	315	CLA	C2D-C1D-ND	-4.44	106.83	110.10
5	B	310	CHL	C1D-ND-C4D	4.43	109.48	106.33
6	B	314	CLA	CHD-C4C-NC	4.43	131.18	124.20
6	B	308	CLA	CHD-C4C-NC	4.42	131.18	124.20
6	C	308	CLA	CHD-C4C-NC	4.42	131.17	124.20
2	B	302	LUT	C11-C10-C9	-4.41	121.01	127.31
6	C	317	CLA	O2D-CGD-CBD	4.40	119.08	111.27
5	B	311	CHL	CHD-C4C-C3C	-4.40	118.38	124.84
6	B	317	CLA	CHD-C4C-NC	4.39	131.12	124.20
6	A	306	CLA	O2D-CGD-O1D	-4.39	115.26	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	305	CHL	C1-C2-C3	-4.38	118.46	126.04
6	C	307	CLA	C4A-NA-C1A	4.37	108.67	106.71
2	C	301	LUT	C15-C35-C34	-4.37	114.53	123.47
6	B	314	CLA	CHD-C4C-C3C	-4.35	118.44	124.84
5	C	311	CHL	CAA-CBA-CGA	-4.34	100.56	113.25
6	A	317	CLA	C1-C2-C3	-4.34	118.54	126.04
6	B	308	CLA	C1D-CHD-C4C	-4.33	116.72	126.06
6	A	315	CLA	O2D-CGD-O1D	-4.33	115.38	123.84
5	C	313	CHL	CHD-C4C-NC	4.33	131.02	124.20
3	B	303	NEX	C39-C29-C30	-4.32	116.87	122.92
5	A	313	CHL	C1D-ND-C4D	4.32	109.40	106.33
6	A	306	CLA	CHD-C4C-C3C	-4.30	118.51	124.84
6	B	317	CLA	C1-C2-C3	-4.29	118.62	126.04
6	A	316	CLA	CHD-C4C-C3C	-4.29	118.54	124.84
6	C	316	CLA	CHD-C4C-NC	4.29	130.96	124.20
6	C	307	CLA	C1D-CHD-C4C	-4.28	116.83	126.06
6	B	316	CLA	CHD-C4C-NC	4.28	130.94	124.20
5	C	312	CHL	C1D-CHD-C4C	-4.27	116.85	126.06
6	A	306	CLA	C4A-NA-C1A	4.24	108.61	106.71
5	C	310	CHL	C1-C2-C3	-4.24	119.89	126.75
6	A	315	CLA	C1D-CHD-C4C	-4.23	116.92	126.06
6	A	314	CLA	C1-O2A-CGA	4.22	127.51	116.44
2	B	301	LUT	C31-C30-C29	4.21	133.31	127.31
5	A	305	CHL	O2D-CGD-CBD	4.20	118.74	111.27
2	A	301	LUT	C31-C30-C29	4.20	133.31	127.31
6	C	316	CLA	O2D-CGD-O1D	-4.20	115.64	123.84
5	B	310	CHL	CHD-C4C-NC	4.19	130.81	124.20
6	A	308	CLA	CHC-C1C-NC	4.19	130.56	124.20
6	C	316	CLA	C1D-CHD-C4C	-4.19	117.02	126.06
5	C	305	CHL	C1-C2-C3	-4.18	118.82	126.04
5	B	311	CHL	C1D-CHD-C4C	-4.18	117.05	126.06
5	B	313	CHL	CHD-C4C-C3C	-4.16	118.72	124.84
6	A	314	CLA	O2D-CGD-CBD	4.16	118.66	111.27
6	C	306	CLA	C9-C8-C7	4.16	126.34	111.29
6	C	317	CLA	C1-C2-C3	-4.15	118.86	126.04
6	B	318	CLA	O2D-CGD-O1D	-4.15	115.73	123.84
5	A	305	CHL	C1D-CHD-C4C	-4.15	117.11	126.06
6	B	317	CLA	O2D-CGD-CBD	4.14	118.63	111.27
6	A	316	CLA	C1D-CHD-C4C	-4.13	117.14	126.06
6	A	306	CLA	C6-C5-C3	-4.13	102.62	113.45
5	C	305	CHL	C1D-CHD-C4C	-4.13	117.15	126.06
6	B	307	CLA	CHD-C4C-NC	4.13	130.70	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	317	CLA	C1D-CHD-C4C	-4.12	117.17	126.06
6	C	314	CLA	O2D-CGD-O1D	-4.11	115.80	123.84
6	B	314	CLA	C1-O2A-CGA	4.10	127.21	116.44
6	A	314	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
6	B	315	CLA	CAA-C2A-C3A	-4.08	101.60	112.78
6	C	314	CLA	CHD-C4C-NC	4.08	130.63	124.20
5	B	311	CHL	CHD-C4C-NC	4.07	130.62	124.20
6	A	318	CLA	O2D-CGD-O1D	-4.06	115.90	123.84
6	B	316	CLA	CHD-C4C-C3C	-4.04	118.89	124.84
3	C	303	NEX	C39-C29-C30	-4.04	117.27	122.92
6	A	315	CLA	CHC-C1C-NC	4.03	130.32	124.20
5	C	312	CHL	CHD-C4C-NC	4.03	130.55	124.20
2	C	302	LUT	C7-C8-C9	4.03	132.32	126.23
5	B	309	CHL	O2D-CGD-O1D	-4.02	115.98	123.84
6	A	307	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
5	A	313	CHL	O2D-CGD-CBD	4.01	118.39	111.27
2	B	302	LUT	C1-C2-C3	3.97	122.62	113.64
5	A	312	CHL	CHD-C4C-NC	3.97	130.46	124.20
6	C	316	CLA	C1D-ND-C4D	3.95	109.14	106.33
6	A	317	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
6	B	307	CLA	C4A-NA-C1A	3.94	108.48	106.71
6	B	315	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
3	A	303	NEX	C24-C23-C22	-3.92	103.20	110.77
5	A	312	CHL	CHD-C4C-C3C	-3.92	119.08	124.84
6	C	314	CLA	CHD-C4C-C3C	-3.91	119.09	124.84
2	C	301	LUT	C40-C33-C34	-3.91	117.45	122.92
5	C	311	CHL	C1D-CHD-C4C	-3.91	117.63	126.06
2	C	301	LUT	C40-C33-C32	3.91	124.23	118.08
6	C	306	CLA	C2D-C1D-ND	-3.90	107.23	110.10
4	B	304	LHG	O8-C23-C24	3.90	124.14	111.91
6	B	314	CLA	CHC-C1C-NC	3.89	130.10	124.20
6	B	314	CLA	O2D-CGD-CBD	3.89	118.18	111.27
5	B	311	CHL	CAA-CBA-CGA	-3.89	101.90	113.25
6	C	306	CLA	CHD-C4C-NC	3.89	130.32	124.20
5	C	311	CHL	CHD-C4C-C3C	-3.88	119.13	124.84
5	B	305	CHL	O2A-CGA-CBA	3.87	124.07	111.91
6	C	315	CLA	CHD-C4C-NC	3.87	130.30	124.20
2	B	301	LUT	C20-C13-C14	-3.86	117.51	122.92
5	A	310	CHL	CHD-C4C-C3C	-3.85	119.18	124.84
6	C	315	CLA	C1D-CHD-C4C	-3.85	117.76	126.06
5	B	313	CHL	CHD-C4C-NC	3.84	130.25	124.20
6	C	317	CLA	CHD-C4C-NC	3.82	130.22	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	310	CHL	CHD-C4C-NC	3.82	130.22	124.20
6	A	317	CLA	CHD-C4C-NC	3.81	130.21	124.20
6	C	307	CLA	CHD-C4C-NC	3.80	130.20	124.20
6	A	317	CLA	C4A-NA-C1A	3.80	108.42	106.71
5	B	311	CHL	O2D-CGD-O1D	-3.79	116.43	123.84
2	B	302	LUT	C20-C13-C14	-3.79	117.61	122.92
6	A	317	CLA	O2D-CGD-CBD	3.78	117.99	111.27
3	C	303	NEX	C26-C27-C28	-3.78	118.00	125.99
5	C	312	CHL	O2A-CGA-CBA	3.78	123.76	111.91
2	A	302	LUT	C1-C2-C3	3.78	122.17	113.64
2	C	302	LUT	C15-C14-C13	3.77	132.69	127.31
5	C	305	CHL	O2A-CGA-CBA	3.77	123.74	111.91
6	C	316	CLA	CHD-C4C-C3C	-3.77	119.30	124.84
6	B	306	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
6	B	315	CLA	CHD-C4C-NC	3.76	130.12	124.20
6	C	318	CLA	CBD-CHA-C1A	3.75	132.92	128.50
5	A	311	CHL	CHD-C4C-NC	3.75	130.11	124.20
6	B	307	CLA	C1D-CHD-C4C	-3.74	117.98	126.06
6	C	314	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
6	A	314	CLA	CHD-C4C-C3C	-3.74	119.35	124.84
6	A	307	CLA	CHD-C4C-NC	3.73	130.09	124.20
5	C	305	CHL	O2D-CGD-CBD	3.73	117.90	111.27
5	A	310	CHL	C1-C2-C3	-3.73	120.72	126.75
5	C	311	CHL	CHD-C4C-NC	3.73	130.07	124.20
5	C	309	CHL	CHD-C4C-C3C	-3.72	119.37	124.84
5	B	312	CHL	CHD-C4C-NC	3.71	130.06	124.20
2	C	302	LUT	C1-C2-C3	3.71	122.03	113.64
6	A	318	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
6	C	318	CLA	C1D-CHD-C4C	-3.69	118.09	126.06
5	A	309	CHL	C1D-CHD-C4C	-3.69	118.09	126.06
5	C	313	CHL	C1D-ND-C4D	3.69	108.96	106.33
5	C	312	CHL	CHD-C4C-C3C	-3.69	119.42	124.84
6	C	315	CLA	C1-C2-C3	-3.69	119.67	126.04
5	B	313	CHL	C1D-CHD-C4C	-3.68	118.11	126.06
6	A	315	CLA	CHD-C4C-NC	3.68	130.00	124.20
5	B	309	CHL	CHD-C4C-NC	3.68	130.00	124.20
6	A	314	CLA	CHD-C4C-NC	3.68	130.00	124.20
3	C	303	NEX	C11-C10-C9	-3.67	122.07	127.31
5	B	313	CHL	C4A-NA-C1A	3.67	108.36	106.71
5	C	305	CHL	OMC-CMC-C2C	-3.66	117.41	125.69
6	C	316	CLA	C2D-C1D-ND	-3.65	107.41	110.10
6	A	316	CLA	C1D-ND-C4D	3.65	108.93	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	311	CHL	CAA-CBA-CGA	-3.65	102.59	113.25
6	A	308	CLA	C1-O2A-CGA	3.64	125.99	116.44
5	C	305	CHL	CHD-C4C-C3C	-3.63	119.50	124.84
6	B	317	CLA	CHD-C4C-C3C	-3.63	119.50	124.84
6	B	318	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
5	C	309	CHL	CHD-C4C-NC	3.62	129.91	124.20
6	C	306	CLA	C4-C3-C5	3.62	121.35	115.27
2	C	302	LUT	C16-C1-C6	-3.62	104.43	110.30
6	B	306	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
5	B	310	CHL	C1D-CHD-C4C	-3.61	118.27	126.06
6	B	306	CLA	C6-C7-C8	-3.61	104.26	115.92
5	C	313	CHL	C1D-CHD-C4C	-3.61	118.28	126.06
5	A	312	CHL	C1D-CHD-C4C	-3.60	118.28	126.06
6	A	308	CLA	C1-C2-C3	-3.60	119.81	126.04
2	A	302	LUT	C16-C1-C6	-3.59	104.47	110.30
5	B	309	CHL	CHD-C4C-C3C	-3.57	119.59	124.84
5	C	310	CHL	CHD-C4C-C3C	-3.56	119.61	124.84
5	A	305	CHL	O2A-CGA-CBA	3.56	123.06	111.91
6	B	306	CLA	C4A-NA-C1A	3.55	108.30	106.71
3	C	303	NEX	C24-C23-C22	-3.54	103.93	110.77
5	C	310	CHL	C1D-CHD-C4C	-3.53	118.44	126.06
5	B	311	CHL	C1-O2A-CGA	3.53	125.69	116.44
5	A	311	CHL	CHD-C4C-C3C	-3.52	119.66	124.84
5	C	309	CHL	C1D-CHD-C4C	-3.52	118.47	126.06
6	C	318	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
5	C	310	CHL	CHD-C4C-NC	3.50	129.71	124.20
3	B	303	NEX	C27-C28-C29	-3.49	120.11	125.53
6	C	306	CLA	C1D-ND-C4D	3.49	108.81	106.33
6	C	314	CLA	C1D-ND-C4D	3.49	108.81	106.33
5	C	305	CHL	CHD-C4C-NC	3.48	129.69	124.20
5	C	313	CHL	O2A-CGA-CBA	3.47	122.80	111.91
4	B	304	LHG	O7-C7-C8	3.46	118.96	111.50
6	C	318	CLA	CHD-C4C-NC	3.46	129.65	124.20
6	A	306	CLA	C1D-CHD-C4C	-3.46	118.60	126.06
5	C	309	CHL	O2D-CGD-O1D	-3.45	117.09	123.84
6	C	314	CLA	O2A-CGA-CBA	3.44	122.71	111.91
6	B	314	CLA	C4A-NA-C1A	3.44	108.25	106.71
6	C	317	CLA	CHC-C1C-NC	3.44	129.42	124.20
6	B	308	CLA	C9-C8-C10	3.42	123.67	111.29
5	B	310	CHL	C1-C2-C3	-3.41	121.24	126.75
3	A	303	NEX	C25-C24-C23	-3.40	106.01	112.75
6	C	306	CLA	C1-C2-C3	-3.40	120.17	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	310	CHL	C1D-CHD-C4C	-3.40	118.73	126.06
6	C	307	CLA	CAA-C2A-C3A	-3.40	103.48	112.78
6	C	317	CLA	C2D-C1D-ND	-3.39	107.60	110.10
6	B	306	CLA	C6-C5-C3	-3.39	104.57	113.45
5	B	305	CHL	CHA-C4D-ND	3.37	139.56	132.50
5	A	309	CHL	O2D-CGD-O1D	-3.37	117.25	123.84
5	B	309	CHL	C1D-CHD-C4C	-3.37	118.79	126.06
6	B	308	CLA	C1-O2A-CGA	3.36	125.27	116.44
5	B	313	CHL	C1-C2-C3	-3.36	120.23	126.04
5	C	311	CHL	O2D-CGD-O1D	-3.36	117.28	123.84
6	B	315	CLA	C1-C2-C3	-3.35	120.24	126.04
5	A	309	CHL	C2C-C3C-C4C	-3.34	104.11	106.49
6	A	307	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
6	C	316	CLA	O2A-CGA-CBA	3.33	122.36	111.91
3	C	303	NEX	C27-C28-C29	-3.33	120.37	125.53
3	A	303	NEX	C26-C27-C28	-3.33	118.96	125.99
6	A	308	CLA	C9-C8-C10	-3.32	99.26	111.29
3	A	303	NEX	C39-C29-C30	-3.32	118.28	122.92
5	C	310	CHL	O2D-CGD-O1D	-3.31	117.36	123.84
6	C	314	CLA	C1-O2A-CGA	3.31	125.13	116.44
6	A	314	CLA	C1D-ND-C4D	3.31	108.69	106.33
6	A	317	CLA	CHD-C4C-C3C	-3.30	119.98	124.84
6	A	307	CLA	CHD-C4C-C3C	-3.30	119.99	124.84
6	A	318	CLA	CHD-C4C-NC	3.29	129.39	124.20
5	A	313	CHL	C1D-CHD-C4C	-3.29	118.97	126.06
6	B	307	CLA	CHC-C1C-NC	3.28	129.17	124.20
6	A	308	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
2	C	301	LUT	C16-C1-C6	-3.26	105.01	110.30
3	B	303	NEX	C11-C10-C9	-3.26	122.66	127.31
2	C	301	LUT	C35-C34-C33	-3.25	122.67	127.31
6	C	307	CLA	CHD-C4C-C3C	-3.25	120.06	124.84
6	C	306	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
6	C	317	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
5	A	305	CHL	O2D-CGD-O1D	-3.23	117.53	123.84
5	B	312	CHL	C1D-CHD-C4C	-3.23	119.10	126.06
6	B	307	CLA	CHD-C4C-C3C	-3.22	120.11	124.84
6	A	317	CLA	O2A-CGA-CBA	3.22	122.01	111.91
5	C	311	CHL	CHC-C1C-NC	3.21	129.08	124.20
6	C	317	CLA	C1D-ND-C4D	3.21	108.61	106.33
5	A	313	CHL	CHD-C4C-NC	3.20	129.25	124.20
5	A	312	CHL	OMC-CMC-C2C	-3.20	118.45	125.69
6	C	315	CLA	CAA-C2A-C3A	-3.20	104.02	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	302	LUT	C12-C13-C14	3.19	123.84	118.94
5	A	313	CHL	C1-C2-C3	-3.19	120.53	126.04
6	C	307	CLA	CBC-CAC-C3C	-3.18	103.67	112.43
2	A	301	LUT	C16-C1-C6	-3.17	105.17	110.30
6	C	318	CLA	C2D-C1D-ND	-3.16	107.77	110.10
6	B	315	CLA	CHC-C1C-NC	3.16	129.00	124.20
6	B	306	CLA	O2A-CGA-O1A	-3.15	115.63	123.59
5	A	310	CHL	CHA-C4D-ND	3.15	139.10	132.50
5	A	311	CHL	C1D-CHD-C4C	-3.15	119.26	126.06
5	C	310	CHL	O2A-CGA-CBA	3.15	121.79	111.91
6	B	316	CLA	O1D-CGD-CBD	-3.15	118.05	124.48
5	B	313	CHL	C4-C3-C5	3.15	120.56	115.27
5	B	305	CHL	CHC-C1C-NC	3.14	128.97	124.20
6	A	307	CLA	C4-C3-C5	3.14	120.56	115.27
6	C	315	CLA	CHD-C4C-C3C	-3.14	120.23	124.84
5	A	309	CHL	CHD-C4C-C3C	-3.14	120.23	124.84
5	C	309	CHL	C1B-CHB-C4A	-3.13	123.91	130.12
2	A	301	LUT	C11-C10-C9	-3.13	122.84	127.31
6	B	318	CLA	CHD-C4C-NC	3.13	129.13	124.20
6	A	317	CLA	CHC-C1C-NC	3.12	128.94	124.20
5	C	312	CHL	O2D-CGD-O1D	-3.12	117.73	123.84
2	C	301	LUT	C36-C21-C26	3.11	114.26	109.55
6	C	307	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
5	A	312	CHL	O2A-CGA-CBA	3.11	121.66	111.91
5	B	309	CHL	OMC-CMC-C2C	-3.10	118.67	125.69
5	A	312	CHL	C3D-C2D-C1D	-3.10	101.60	105.83
5	B	312	CHL	CHD-C4C-C3C	-3.10	120.29	124.84
5	A	310	CHL	O2A-CGA-CBA	3.10	121.62	111.91
6	C	315	CLA	CAA-C2A-C1A	3.10	122.12	111.97
5	A	311	CHL	O2D-CGD-O1D	-3.09	117.79	123.84
6	A	315	CLA	CAA-C2A-C3A	-3.09	104.31	112.78
6	C	314	CLA	C1-C2-C3	-3.09	120.70	126.04
6	C	307	CLA	C1-C2-C3	-3.09	120.70	126.04
6	A	315	CLA	C1-C2-C3	-3.09	120.70	126.04
5	A	311	CHL	CHC-C1C-NC	3.08	128.87	124.20
6	B	307	CLA	C1-C2-C3	-3.07	120.72	126.04
5	A	313	CHL	C1C-C2C-C3C	-3.07	104.67	107.11
3	A	303	NEX	C37-C21-C36	3.06	111.89	107.37
6	C	307	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
6	A	316	CLA	C4-C3-C5	3.06	120.42	115.27
6	C	307	CLA	O2A-CGA-CBA	3.06	121.52	111.91
3	C	303	NEX	C11-C12-C13	-3.06	117.83	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	309	CHL	CHD-C4C-NC	3.05	129.02	124.20
5	C	305	CHL	CHC-C1C-NC	3.05	128.83	124.20
2	A	302	LUT	C8-C7-C6	-3.04	118.67	127.20
5	C	311	CHL	C1-O2A-CGA	3.03	124.39	116.44
5	B	313	CHL	CHA-C4D-ND	3.03	138.84	132.50
5	A	309	CHL	CHC-C1C-NC	3.02	128.79	124.20
2	B	301	LUT	C1-C2-C3	3.02	120.46	113.64
6	C	306	CLA	CHD-C4C-C3C	-3.02	120.41	124.84
6	C	307	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
5	B	313	CHL	O2A-CGA-CBA	3.00	121.34	111.91
6	C	306	CLA	O2A-CGA-O1A	-3.00	116.01	123.59
5	C	305	CHL	CHA-C4D-ND	3.00	138.78	132.50
6	B	316	CLA	O2A-CGA-CBA	3.00	121.32	111.91
6	C	316	CLA	CHA-C4D-ND	2.98	138.74	132.50
5	C	309	CHL	C2C-C3C-C4C	-2.98	104.36	106.49
6	B	315	CLA	CHA-C4D-ND	2.98	138.72	132.50
6	C	314	CLA	CGD-CBD-CAD	2.97	120.36	110.73
5	C	309	CHL	CHA-C4D-ND	2.97	138.70	132.50
6	B	308	CLA	C1-C2-C3	-2.96	120.92	126.04
6	B	317	CLA	CHC-C1C-NC	2.96	128.70	124.20
5	B	311	CHL	C1B-CHB-C4A	-2.96	124.25	130.12
6	A	316	CLA	CHA-C4D-ND	2.96	138.69	132.50
6	C	308	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
3	B	303	NEX	C15-C14-C13	-2.96	123.09	127.31
5	B	305	CHL	O2D-CGD-CBD	2.96	116.52	111.27
6	A	307	CLA	O2A-CGA-CBA	2.95	121.16	111.91
6	B	314	CLA	CED-O2D-CGD	2.94	122.59	115.94
5	A	309	CHL	OMC-CMC-C2C	-2.94	119.03	125.69
6	C	317	CLA	O2A-CGA-CBA	2.94	121.14	111.91
6	A	318	CLA	C2D-C1D-ND	-2.94	107.94	110.10
5	C	312	CHL	C3D-C2D-C1D	-2.93	101.83	105.83
6	C	317	CLA	C4-C3-C5	2.93	120.20	115.27
5	A	313	CHL	CHD-C4C-C3C	-2.93	120.53	124.84
5	A	309	CHL	O2A-CGA-CBA	2.93	121.10	111.91
5	A	305	CHL	CBC-CAC-C3C	-2.93	104.37	112.43
6	C	318	CLA	CHD-C4C-C3C	-2.92	120.54	124.84
6	B	314	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
2	B	301	LUT	C35-C34-C33	-2.91	123.16	127.31
4	A	304	LHG	O8-C23-C24	2.91	121.03	111.91
5	A	305	CHL	C1B-CHB-C4A	-2.91	124.36	130.12
2	A	302	LUT	C11-C10-C9	-2.90	123.17	127.31
5	C	310	CHL	CHA-C4D-ND	2.90	138.56	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	303	NEX	C25-C24-C23	-2.89	107.03	112.75
6	A	308	CLA	C4-C3-C5	2.89	120.14	115.27
6	A	314	CLA	O2A-CGA-CBA	2.89	120.97	111.91
5	B	310	CHL	O2A-CGA-CBA	2.88	120.94	111.91
6	B	306	CLA	C1-C2-C3	-2.87	121.07	126.04
6	B	316	CLA	CHC-C1C-NC	2.87	128.56	124.20
6	C	306	CLA	C1D-CHD-C4C	-2.87	119.86	126.06
2	C	302	LUT	C18-C5-C6	-2.87	121.31	124.53
6	C	308	CLA	CHC-C1C-NC	2.86	128.54	124.20
6	C	318	CLA	CMD-C2D-C1D	2.86	129.75	124.71
6	A	317	CLA	C4-C3-C5	2.86	120.08	115.27
5	C	309	CHL	CHC-C1C-NC	2.85	128.53	124.20
6	B	306	CLA	O2A-CGA-CBA	2.85	120.86	111.91
6	C	306	CLA	CMC-C2C-C1C	2.85	129.38	125.04
6	A	314	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
3	B	303	NEX	C15-C35-C34	-2.84	117.65	123.47
6	C	315	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
3	A	303	NEX	C15-C14-C13	-2.84	123.26	127.31
5	B	309	CHL	CHA-C4D-ND	2.84	138.44	132.50
3	B	303	NEX	C26-C27-C28	-2.84	119.99	125.99
6	B	306	CLA	C4-C3-C5	2.84	120.04	115.27
3	C	303	NEX	C30-C31-C32	-2.83	114.38	123.22
6	B	316	CLA	C4-C3-C5	2.83	120.03	115.27
5	C	309	CHL	O2A-CGA-CBA	2.83	120.78	111.91
6	A	318	CLA	C1D-ND-C4D	2.83	108.34	106.33
6	A	316	CLA	O2A-CGA-CBA	2.82	120.77	111.91
6	A	308	CLA	C9-C8-C7	-2.82	101.07	111.29
5	A	309	CHL	CHA-C4D-ND	2.82	138.40	132.50
5	B	312	CHL	CHA-C4D-ND	2.81	138.38	132.50
6	B	307	CLA	O2A-CGA-CBA	2.81	120.73	111.91
6	C	318	CLA	CHC-C1C-NC	2.81	128.46	124.20
5	A	311	CHL	CHA-C4D-ND	2.81	138.37	132.50
6	B	315	CLA	C4-C3-C5	2.81	119.99	115.27
5	B	310	CHL	CHA-C4D-ND	2.81	138.37	132.50
6	A	318	CLA	CHD-C4C-C3C	-2.80	120.72	124.84
6	C	315	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
6	C	308	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
5	A	305	CHL	CAA-CBA-CGA	-2.80	105.08	113.25
5	C	311	CHL	O2A-CGA-CBA	2.79	120.66	111.91
6	B	315	CLA	CGD-CBD-CAD	-2.78	101.74	110.73
5	C	311	CHL	C1B-CHB-C4A	-2.78	124.62	130.12
4	C	304	LHG	O7-C7-C8	2.77	117.48	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	309	CHL	CHC-C1C-NC	2.77	128.41	124.20
5	A	309	CHL	C1B-CHB-C4A	-2.77	124.63	130.12
6	C	306	CLA	C6-C5-C3	-2.77	106.19	113.45
4	B	304	LHG	O8-C23-O10	-2.77	116.61	123.59
2	B	302	LUT	C8-C7-C6	-2.77	119.43	127.20
5	B	311	CHL	O2A-CGA-CBA	2.77	120.59	111.91
6	A	315	CLA	CAA-C2A-C1A	2.77	121.04	111.97
5	B	311	CHL	CHD-C1D-ND	2.77	127.00	124.45
6	A	318	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
5	B	312	CHL	CHC-C1C-NC	2.76	128.40	124.20
5	A	312	CHL	C6-C5-C3	-2.76	106.22	113.45
6	A	306	CLA	C1D-ND-C4D	2.76	108.30	106.33
6	B	314	CLA	C1-C2-C3	-2.75	121.28	126.04
4	A	304	LHG	O7-C7-C8	2.75	117.43	111.50
6	B	315	CLA	CHD-C4C-C3C	-2.75	120.80	124.84
6	A	306	CLA	C2D-C1D-ND	-2.75	108.08	110.10
5	A	305	CHL	CMB-C2B-C1B	-2.74	124.25	128.46
5	C	313	CHL	CAA-C2A-C3A	-2.74	105.27	112.78
5	A	311	CHL	C1-O2A-CGA	2.74	123.64	116.44
5	B	309	CHL	O2A-CGA-CBA	2.74	120.51	111.91
6	B	317	CLA	C1D-ND-C4D	2.74	108.28	106.33
5	B	313	CHL	O2D-CGD-O1D	-2.73	118.49	123.84
6	A	308	CLA	CHA-C4D-ND	2.73	138.21	132.50
5	B	312	CHL	O1D-CGD-CBD	-2.73	118.90	124.48
6	B	308	CLA	C4-C3-C5	2.73	119.86	115.27
6	C	315	CLA	C2D-C1D-ND	-2.73	108.09	110.10
2	A	302	LUT	C31-C32-C33	-2.72	118.76	126.42
6	A	307	CLA	C6-C7-C8	-2.72	107.12	115.92
2	B	302	LUT	C38-C25-C24	-2.72	117.74	123.56
2	C	302	LUT	C38-C25-C24	-2.72	117.74	123.56
4	C	304	LHG	O8-C23-C24	2.71	120.43	111.91
5	C	312	CHL	CHC-C1C-NC	2.71	128.32	124.20
6	A	307	CLA	CHA-C4D-ND	2.71	138.17	132.50
5	C	305	CHL	CAA-CBA-CGA	-2.71	105.33	113.25
4	C	304	LHG	C5-O7-C7	-2.70	111.13	117.79
2	B	302	LUT	C15-C35-C34	-2.70	117.93	123.47
5	A	312	CHL	CHA-C4D-ND	2.70	138.15	132.50
6	C	307	CLA	CHA-C4D-ND	2.70	138.15	132.50
6	C	306	CLA	O2A-C1-C2	-2.70	101.55	108.64
6	B	316	CLA	CHA-C4D-ND	2.70	138.14	132.50
6	C	314	CLA	CHC-C1C-NC	2.69	128.29	124.20
5	B	311	CHL	CHA-C4D-ND	2.68	138.11	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	303	NEX	C24-C23-C22	-2.68	105.60	110.77
2	A	302	LUT	C18-C5-C6	-2.68	121.52	124.53
5	C	313	CHL	O1D-CGD-CBD	-2.68	119.00	124.48
6	C	317	CLA	CHD-C4C-C3C	-2.67	120.91	124.84
6	C	314	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
5	C	310	CHL	C5-C3-C4	2.67	120.49	114.60
5	B	305	CHL	C1B-CHB-C4A	-2.66	124.84	130.12
5	C	309	CHL	OMC-CMC-C2C	-2.66	119.67	125.69
6	C	316	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
5	A	313	CHL	CHA-C4D-ND	2.66	138.06	132.50
6	A	314	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
5	B	305	CHL	CED-O2D-CGD	2.66	121.94	115.94
6	A	314	CLA	CMA-C3A-C4A	-2.66	104.64	111.77
5	A	310	CHL	CHC-C1C-NC	2.65	128.23	124.20
5	C	311	CHL	CHA-C4D-ND	2.65	138.05	132.50
2	B	302	LUT	C35-C34-C33	-2.65	123.53	127.31
5	C	312	CHL	C1B-CHB-C4A	-2.64	124.88	130.12
5	B	312	CHL	O2A-CGA-CBA	2.64	120.20	111.91
5	B	310	CHL	CHC-C1C-NC	2.64	128.21	124.20
2	C	301	LUT	C1-C2-C3	2.64	119.60	113.64
6	A	314	CLA	CGD-CBD-CAD	2.64	119.28	110.73
6	C	317	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
6	B	314	CLA	C1D-ND-C4D	2.63	108.21	106.33
5	A	310	CHL	OMC-CMC-C2C	-2.63	119.73	125.69
6	A	306	CLA	C1-C2-C3	-2.63	121.49	126.04
5	C	309	CHL	CMD-C2D-C1D	2.62	129.34	124.71
3	B	303	NEX	C19-C9-C10	-2.62	119.25	122.92
6	A	308	CLA	CHC-C1C-C2C	-2.62	119.46	126.72
6	C	315	CLA	C1D-ND-C4D	2.62	108.20	106.33
6	A	315	CLA	CHA-C4D-ND	2.62	137.99	132.50
5	B	312	CHL	C1B-CHB-C4A	-2.62	124.93	130.12
5	C	313	CHL	O2A-CGA-O1A	-2.62	116.98	123.59
5	C	305	CHL	C2C-C3C-C4C	-2.62	104.62	106.49
5	C	310	CHL	CHC-C1C-NC	2.61	128.17	124.20
5	C	305	CHL	CHD-C1D-ND	2.61	126.85	124.45
5	A	313	CHL	O2A-CGA-CBA	2.61	120.09	111.91
6	A	316	CLA	CHC-C1C-NC	2.60	128.15	124.20
6	B	317	CLA	O2A-CGA-CBA	2.60	120.06	111.91
2	A	301	LUT	C18-C5-C6	-2.60	121.61	124.53
5	A	305	CHL	CMB-C2B-C3B	2.58	129.51	124.68
6	A	315	CLA	C9-C8-C10	2.58	120.65	111.29
6	B	314	CLA	CHC-C1C-C2C	-2.58	119.58	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	306	CLA	C1D-ND-C4D	2.58	108.17	106.33
6	B	318	CLA	CHD-C4C-C3C	-2.57	121.06	124.84
5	C	312	CHL	O2A-CGA-O1A	-2.57	117.10	123.59
6	C	306	CLA	O2A-CGA-CBA	2.57	119.98	111.91
5	C	313	CHL	C1-O2A-CGA	2.57	123.19	116.44
2	A	301	LUT	C1-C2-C3	2.57	119.44	113.64
5	C	313	CHL	CHA-C4D-ND	2.56	137.86	132.50
6	C	314	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
5	C	312	CHL	C11-C10-C8	-2.56	107.66	115.92
6	B	316	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
6	A	314	CLA	CHC-C1C-NC	2.55	128.07	124.20
5	A	305	CHL	CHA-C4D-ND	2.55	137.83	132.50
3	A	303	NEX	C19-C9-C10	-2.54	119.37	122.92
6	C	307	CLA	C9-C8-C10	2.53	120.45	111.29
6	B	307	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
6	C	318	CLA	CHA-C4D-ND	2.52	137.77	132.50
6	C	316	CLA	C4-C3-C5	2.52	119.51	115.27
6	B	317	CLA	C4-C3-C5	2.52	119.50	115.27
6	B	307	CLA	CHC-C1C-C2C	-2.51	119.78	126.72
6	C	318	CLA	C1D-ND-C4D	2.51	108.12	106.33
2	C	301	LUT	C36-C21-C22	-2.51	104.69	109.44
5	B	312	CHL	C4-C3-C5	2.50	119.47	115.27
5	A	312	CHL	CHC-C1C-NC	2.50	127.99	124.20
6	B	314	CLA	CBC-CAC-C3C	-2.49	105.56	112.43
6	C	306	CLA	C7-C6-C5	-2.48	106.61	113.36
3	C	303	NEX	C19-C9-C10	-2.48	119.45	122.92
6	A	317	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
5	B	310	CHL	OMC-CMC-C2C	-2.47	120.09	125.69
5	A	313	CHL	C4-C3-C5	2.47	119.43	115.27
5	C	312	CHL	C6-C5-C3	-2.47	106.98	113.45
6	C	314	CLA	CMA-C3A-C4A	-2.47	105.13	111.77
6	B	318	CLA	C2D-C1D-ND	-2.47	108.28	110.10
6	A	307	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
6	C	308	CLA	CMA-C3A-C4A	-2.46	105.17	111.77
6	C	315	CLA	O2A-CGA-CBA	2.45	119.61	111.91
6	C	306	CLA	C6-C7-C8	-2.45	107.99	115.92
5	C	312	CHL	CAA-CBA-CGA	-2.44	106.12	113.25
2	C	301	LUT	C20-C13-C12	2.44	121.92	118.08
5	A	305	CHL	CHC-C1C-NC	2.44	127.90	124.20
6	B	307	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
5	B	309	CHL	C1B-CHB-C4A	-2.44	125.29	130.12
6	B	317	CLA	O2A-CGA-O1A	-2.43	117.45	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	316	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
5	B	305	CHL	CBC-CAC-C3C	-2.43	105.73	112.43
6	C	315	CLA	C4-C3-C5	2.43	119.36	115.27
5	C	305	CHL	CED-O2D-CGD	2.43	121.43	115.94
6	C	307	CLA	CHC-C1C-NC	2.43	127.88	124.20
2	A	302	LUT	C31-C30-C29	2.43	130.77	127.31
2	C	301	LUT	C38-C25-C24	-2.43	118.37	123.56
6	A	317	CLA	C6-C7-C8	-2.42	108.09	115.92
5	C	312	CHL	CMD-C2D-C1D	2.42	128.98	124.71
6	A	306	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
6	C	317	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
5	B	312	CHL	CMD-C2D-C1D	2.42	128.98	124.71
6	A	308	CLA	CBC-CAC-C3C	-2.41	105.78	112.43
6	B	306	CLA	CAA-C2A-C3A	2.41	119.38	112.78
6	C	315	CLA	CHC-C1C-NC	2.40	127.85	124.20
5	C	310	CHL	OMC-CMC-C2C	-2.40	120.26	125.69
6	B	317	CLA	CHA-C4D-ND	2.40	137.52	132.50
6	C	315	CLA	CHA-C4D-ND	2.39	137.51	132.50
6	C	307	CLA	CMC-C2C-C1C	2.39	128.68	125.04
6	B	307	CLA	C1C-C2C-C3C	-2.39	104.44	106.96
2	B	302	LUT	C7-C8-C9	2.39	129.84	126.23
6	A	307	CLA	CMA-C3A-C4A	-2.39	105.36	111.77
3	C	303	NEX	C15-C35-C34	-2.39	118.59	123.47
5	A	309	CHL	CAC-C3C-C4C	2.38	127.90	124.81
6	B	307	CLA	CMB-C2B-C1B	-2.38	124.80	128.46
5	A	310	CHL	C5-C3-C4	2.38	119.86	114.60
5	C	313	CHL	C1B-CHB-C4A	-2.38	125.41	130.12
5	B	305	CHL	OMC-CMC-C2C	-2.38	120.31	125.69
6	A	307	CLA	C1-C2-C3	-2.38	121.94	126.04
6	B	314	CLA	O2A-CGA-CBA	2.37	119.36	111.91
2	C	302	LUT	C8-C7-C6	-2.37	120.54	127.20
6	C	316	CLA	CAA-CBA-CGA	-2.37	106.32	113.25
6	C	317	CLA	CHA-C4D-ND	2.37	137.46	132.50
5	B	312	CHL	C6-C5-C3	-2.37	107.24	113.45
6	B	308	CLA	CHC-C1C-NC	2.37	127.80	124.20
5	C	305	CHL	C1B-CHB-C4A	-2.37	125.42	130.12
5	A	310	CHL	CGD-CBD-CAD	-2.37	103.06	110.73
6	B	318	CLA	C1D-ND-C4D	2.36	108.01	106.33
5	C	312	CHL	O1D-CGD-CBD	-2.36	119.65	124.48
6	A	307	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
6	C	307	CLA	CHC-C1C-C2C	-2.36	120.20	126.72
6	C	308	CLA	CBC-CAC-C3C	-2.35	105.95	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	317	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
6	C	308	CLA	C1-O2A-CGA	2.35	122.60	116.44
2	C	301	LUT	C7-C8-C9	2.35	129.78	126.23
6	B	315	CLA	CAA-CBA-CGA	-2.34	106.40	113.25
5	B	305	CHL	O2A-CGA-O1A	-2.34	117.68	123.59
5	A	311	CHL	OMC-CMC-C2C	-2.34	120.39	125.69
6	A	316	CLA	C1-C2-C3	-2.34	122.00	126.04
6	A	307	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
3	A	303	NEX	O24-C25-C38	2.33	117.85	115.06
6	B	315	CLA	O2A-CGA-CBA	2.33	119.23	111.91
2	B	301	LUT	C20-C13-C12	2.33	121.75	118.08
2	B	301	LUT	C8-C7-C6	-2.33	120.66	127.20
5	B	313	CHL	C1B-CHB-C4A	-2.33	125.51	130.12
3	A	303	NEX	C11-C10-C9	-2.32	123.99	127.31
6	A	316	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
6	B	316	CLA	CHD-C1D-ND	2.32	126.59	124.45
6	C	316	CLA	CHC-C1C-NC	2.32	127.72	124.20
6	B	318	CLA	CAC-C3C-C4C	2.32	127.82	124.81
6	A	315	CLA	O2A-CGA-CBA	2.31	119.17	111.91
6	C	318	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
5	A	305	CHL	C1C-C2C-C3C	-2.31	105.28	107.11
6	C	314	CLA	C2D-C1D-ND	-2.31	108.40	110.10
6	A	318	CLA	CHA-C4D-ND	2.31	137.33	132.50
6	A	315	CLA	CHD-C1D-ND	2.31	126.58	124.45
6	C	317	CLA	CHC-C1C-C2C	-2.31	120.34	126.72
5	B	305	CHL	CHD-C1D-ND	2.30	126.57	124.45
6	B	318	CLA	CHA-C4D-ND	2.30	137.32	132.50
5	B	310	CHL	C5-C3-C4	2.30	119.69	114.60
6	A	315	CLA	CHC-C1C-C2C	-2.30	120.36	126.72
5	C	311	CHL	CHB-C4A-NA	2.30	127.69	124.51
3	A	303	NEX	O24-C25-C26	-2.30	57.06	58.96
6	B	316	CLA	C1-C2-C3	-2.29	122.08	126.04
6	B	317	CLA	C4A-NA-C1A	2.29	107.74	106.71
6	A	306	CLA	CHC-C1C-NC	2.29	127.68	124.20
6	B	307	CLA	CHA-C4D-ND	2.29	137.29	132.50
6	C	316	CLA	CMD-C2D-C1D	2.29	128.75	124.71
6	A	308	CLA	C2D-C1D-ND	-2.29	108.42	110.10
5	A	312	CHL	CMD-C2D-C1D	2.29	128.75	124.71
2	A	301	LUT	C8-C7-C6	-2.29	120.78	127.20
3	B	303	NEX	C19-C9-C8	2.28	124.22	118.93
5	A	312	CHL	CBC-CAC-C3C	-2.28	106.15	112.43
6	B	315	CLA	CAA-C2A-C1A	2.27	119.43	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	LUT	C21-C26-C27	-2.27	109.83	112.70
3	C	303	NEX	C37-C21-C36	2.27	110.72	107.37
6	C	308	CLA	C1-C2-C3	-2.27	122.12	126.04
6	A	317	CLA	C6-C5-C3	-2.27	107.51	113.45
2	C	302	LUT	C19-C9-C8	2.27	121.65	118.08
6	A	306	CLA	C6-C7-C8	-2.27	108.59	115.92
2	C	301	LUT	C20-C13-C14	-2.27	119.75	122.92
6	C	306	CLA	CHC-C1C-NC	2.27	127.64	124.20
5	A	305	CHL	OMC-CMC-C2C	-2.27	120.56	125.69
6	A	317	CLA	O2A-CGA-O1A	-2.27	117.88	123.59
3	A	303	NEX	C20-C13-C12	2.26	121.64	118.08
6	A	307	CLA	CHC-C1C-NC	2.26	127.63	124.20
6	B	307	CLA	CMD-C2D-C1D	2.26	128.69	124.71
6	B	317	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
2	C	301	LUT	C8-C7-C6	-2.25	120.87	127.20
6	A	307	CLA	CHC-C1C-C2C	-2.25	120.49	126.72
3	B	303	NEX	C31-C32-C33	-2.25	120.09	126.42
5	C	312	CHL	CHA-C4D-ND	2.25	137.20	132.50
5	C	310	CHL	C2C-C3C-C4C	-2.24	104.89	106.49
6	C	317	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
5	C	311	CHL	CMA-C3A-C4A	-2.24	105.76	111.77
6	B	308	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
2	B	301	LUT	C18-C5-C4	2.24	118.50	114.36
6	A	314	CLA	C2D-C1D-ND	-2.23	108.46	110.10
6	C	308	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
2	B	301	LUT	C19-C9-C10	-2.23	119.80	122.92
2	B	302	LUT	C19-C9-C10	-2.23	119.80	122.92
6	B	315	CLA	CMB-C2B-C3B	2.22	128.84	124.68
5	B	312	CHL	C11-C10-C8	-2.22	108.73	115.92
5	B	313	CHL	O2A-CGA-O1A	-2.22	117.99	123.59
5	B	305	CHL	C3D-C2D-C1D	-2.22	102.80	105.83
6	B	306	CLA	C11-C10-C8	-2.22	108.75	115.92
2	B	302	LUT	C18-C5-C6	-2.22	122.04	124.53
6	C	308	CLA	C4-C3-C5	2.21	118.99	115.27
5	A	311	CHL	O2A-CGA-CBA	2.21	118.85	111.91
5	C	310	CHL	CHD-C1D-ND	2.21	126.48	124.45
5	C	311	CHL	C2C-C3C-C4C	-2.20	104.92	106.49
5	A	310	CHL	CED-O2D-CGD	2.20	120.91	115.94
6	A	315	CLA	CHD-C4C-C3C	-2.20	121.61	124.84
6	A	314	CLA	C4-C3-C5	2.20	118.97	115.27
5	C	310	CHL	O2A-CGA-O1A	-2.19	118.05	123.59
6	B	308	CLA	CHA-C4D-ND	2.19	137.09	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	317	CLA	CHC-C1C-C2C	-2.19	120.66	126.72
6	A	306	CLA	O2A-CGA-CBA	2.19	118.79	111.91
5	B	309	CHL	C2C-C3C-C4C	-2.19	104.93	106.49
5	C	305	CHL	C4-C3-C5	2.19	118.95	115.27
6	B	306	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
6	A	307	CLA	CMC-C2C-C1C	2.18	128.36	125.04
6	C	308	CLA	CHD-C1D-ND	2.18	126.46	124.45
6	C	308	CLA	O2A-CGA-CBA	2.18	118.75	111.91
6	C	314	CLA	CMC-C2C-C1C	2.18	128.36	125.04
5	C	311	CHL	OMC-CMC-C2C	-2.18	120.76	125.69
2	C	301	LUT	O3-C3-C2	-2.18	105.48	109.80
5	B	313	CHL	OMC-CMC-C2C	-2.17	120.77	125.69
3	B	303	NEX	C28-C29-C30	2.17	122.27	118.94
6	A	316	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
6	C	306	CLA	CHA-C4D-ND	2.17	137.04	132.50
6	B	318	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
6	C	318	CLA	CHC-C1C-C2C	-2.17	120.73	126.72
6	B	314	CLA	C2D-C1D-ND	-2.16	108.51	110.10
2	B	302	LUT	C11-C12-C13	2.16	132.49	126.42
6	A	315	CLA	CAC-C3C-C4C	2.16	127.62	124.81
5	A	313	CHL	C1B-CHB-C4A	-2.16	125.83	130.12
2	B	301	LUT	C11-C12-C13	2.16	132.49	126.42
6	C	317	CLA	CMD-C2D-C1D	2.16	128.52	124.71
2	B	301	LUT	C8-C9-C10	2.15	122.24	118.94
3	B	303	NEX	O24-C25-C26	-2.15	57.18	58.96
2	B	301	LUT	C30-C31-C32	-2.15	116.51	123.22
5	C	305	CHL	O2D-CGD-O1D	-2.15	119.64	123.84
6	C	307	CLA	C9-C8-C7	2.14	119.06	111.29
6	B	318	CLA	CHC-C1C-NC	2.14	127.45	124.20
5	A	310	CHL	O2D-CGD-O1D	-2.14	119.66	123.84
5	C	313	CHL	C4-C3-C5	2.14	118.87	115.27
5	B	312	CHL	OMC-CMC-C2C	-2.14	120.86	125.69
6	A	307	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
3	C	303	NEX	C35-C15-C14	-2.14	119.10	123.47
6	A	318	CLA	CHC-C1C-NC	2.14	127.44	124.20
6	C	315	CLA	CMD-C2D-C1D	2.14	128.48	124.71
5	C	305	CHL	CAC-C3C-C4C	2.13	127.58	124.81
6	C	306	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
6	C	308	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
2	C	302	LUT	C36-C21-C26	2.13	112.77	109.55
6	C	314	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
2	B	302	LUT	C40-C33-C34	-2.13	119.94	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	314	CLA	CBC-CAC-C3C	-2.13	106.57	112.43
6	C	318	CLA	CMB-C2B-C1B	-2.12	125.20	128.46
3	A	303	NEX	C20-C13-C14	-2.12	119.96	122.92
6	C	306	CLA	C5-C3-C2	-2.12	116.83	121.12
2	A	301	LUT	C19-C9-C10	-2.12	119.96	122.92
6	A	308	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
5	C	312	CHL	C7-C6-C5	-2.11	107.62	113.36
5	C	313	CHL	C3D-C2D-C1D	-2.11	102.95	105.83
5	C	309	CHL	C1-O2A-CGA	2.11	122.86	116.73
6	C	307	CLA	C6-C7-C8	-2.11	109.11	115.92
5	C	313	CHL	C7-C6-C5	-2.10	107.65	113.36
6	C	316	CLA	CAC-C3C-C2C	2.10	131.12	127.53
5	C	313	CHL	CMD-C2D-C1D	2.10	128.41	124.71
3	C	303	NEX	C19-C9-C8	2.10	123.78	118.93
5	A	312	CHL	O2A-CGA-O1A	-2.09	118.31	123.59
6	C	307	CLA	C4-C3-C5	2.09	118.79	115.27
6	C	315	CLA	CHA-C1A-NA	-2.09	121.60	126.40
2	B	302	LUT	C31-C30-C29	2.09	130.30	127.31
3	A	303	NEX	C15-C35-C34	-2.09	119.19	123.47
5	A	313	CHL	O2A-CGA-O1A	-2.09	118.32	123.59
6	A	315	CLA	CGD-CBD-CAD	-2.09	103.97	110.73
6	A	318	CLA	CMD-C2D-C1D	2.08	128.38	124.71
2	B	301	LUT	C22-C23-C24	-2.08	109.38	111.74
6	A	316	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
5	B	313	CHL	CHC-C1C-NC	2.08	127.35	124.20
6	A	315	CLA	C4-C3-C5	2.08	118.76	115.27
6	B	317	CLA	C2D-C1D-ND	-2.07	108.58	110.10
2	A	301	LUT	C15-C35-C34	-2.07	119.23	123.47
3	C	303	NEX	C28-C29-C30	2.07	122.12	118.94
6	B	306	CLA	CMA-C3A-C4A	-2.07	106.20	111.77
5	B	311	CHL	C3D-C2D-C1D	-2.07	103.00	105.83
6	C	307	CLA	C2C-C1C-NC	2.07	111.91	109.97
3	B	303	NEX	C40-C33-C34	-2.07	120.03	122.92
6	A	308	CLA	C1D-ND-C4D	2.07	107.80	106.33
5	B	312	CHL	C16-C15-C13	-2.06	109.27	115.92
5	B	310	CHL	C2C-C3C-C4C	-2.06	105.02	106.49
5	B	311	CHL	CHC-C1C-NC	2.05	127.31	124.20
5	B	311	CHL	C2C-C3C-C4C	-2.05	105.03	106.49
5	C	311	CHL	O1A-CGA-CBA	-2.05	115.75	123.73
5	A	305	CHL	C3D-C2D-C1D	-2.04	103.04	105.83
6	A	314	CLA	CHA-C4D-ND	2.04	136.77	132.50
2	B	301	LUT	C16-C1-C6	-2.04	106.99	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	302	LUT	C31-C30-C29	2.04	130.22	127.31
6	C	315	CLA	C9-C8-C10	2.04	118.67	111.29
6	B	315	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
4	C	304	LHG	O7-C7-O9	-2.04	118.78	123.70
5	C	313	CHL	OMC-CMC-C2C	-2.04	121.08	125.69
2	A	301	LUT	C20-C13-C12	2.04	121.28	118.08
6	B	317	CLA	CHC-C1C-C2C	-2.03	121.10	126.72
5	C	312	CHL	OMC-CMC-C2C	-2.03	121.09	125.69
6	A	307	CLA	C2C-C1C-NC	2.03	111.88	109.97
6	A	314	CLA	C1-C2-C3	-2.03	122.53	126.04
6	C	316	CLA	C1-C2-C3	-2.03	122.54	126.04
5	B	312	CHL	C1C-C2C-C3C	-2.03	105.51	107.11
6	C	317	CLA	C11-C10-C8	-2.03	109.37	115.92
6	A	307	CLA	CHD-C1D-ND	2.02	126.31	124.45
5	B	305	CHL	CHA-C1A-NA	-2.02	121.77	126.40
5	A	310	CHL	O1D-CGD-CBD	-2.01	120.36	124.48
6	B	315	CLA	CMD-C2D-C1D	2.01	128.26	124.71
6	B	306	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
5	A	312	CHL	C1-O2A-CGA	2.00	121.70	116.44
6	C	307	CLA	O1D-CGD-CBD	-2.00	120.39	124.48

All (68) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	305	CHL	NA
5	A	305	CHL	C8
5	A	305	CHL	ND
5	A	305	CHL	NC
5	A	309	CHL	NA
5	A	309	CHL	ND
5	A	309	CHL	NC
5	A	310	CHL	NA
5	A	310	CHL	ND
5	A	310	CHL	NC
5	A	311	CHL	NA
5	A	311	CHL	C8
5	A	311	CHL	ND
5	A	311	CHL	NC
5	A	312	CHL	NA
5	A	312	CHL	C8
5	A	312	CHL	ND
5	A	312	CHL	NC

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Mol	Chain	Res	Type	Atom
5	A	313	CHL	NA
5	A	313	CHL	C8
5	A	313	CHL	ND
5	A	313	CHL	NC
5	B	305	CHL	NA
5	B	305	CHL	C8
5	B	305	CHL	ND
5	B	305	CHL	NC
5	B	309	CHL	NA
5	B	309	CHL	ND
5	B	309	CHL	NC
5	B	310	CHL	NA
5	B	310	CHL	ND
5	B	310	CHL	NC
5	B	311	CHL	NA
5	B	311	CHL	C8
5	B	311	CHL	ND
5	B	311	CHL	NC
5	B	312	CHL	NA
5	B	312	CHL	C8
5	B	312	CHL	ND
5	B	312	CHL	NC
5	B	313	CHL	NA
5	B	313	CHL	C8
5	B	313	CHL	ND
5	B	313	CHL	NC
5	C	305	CHL	NA
5	C	305	CHL	C8
5	C	305	CHL	ND
5	C	305	CHL	NC
5	C	309	CHL	NA
5	C	309	CHL	ND
5	C	309	CHL	NC
5	C	310	CHL	NA
5	C	310	CHL	ND
5	C	310	CHL	NC
5	C	311	CHL	NA
5	C	311	CHL	C8
5	C	311	CHL	ND
5	C	311	CHL	NC
5	C	312	CHL	NA
5	C	312	CHL	C8

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Mol	Chain	Res	Type	Atom
5	C	312	CHL	ND
5	C	312	CHL	NC
5	C	313	CHL	NA
5	C	313	CHL	C8
5	C	313	CHL	ND
5	C	313	CHL	NC
6	A	307	CLA	ND
6	B	316	CLA	ND

All (573) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	NEX	C11-C12-C13-C14
3	A	303	NEX	C11-C12-C13-C20
3	B	303	NEX	O24-C26-C27-C28
4	A	304	LHG	C4-O6-P-O3
4	A	304	LHG	C4-O6-P-O4
4	A	304	LHG	C4-O6-P-O5
4	B	304	LHG	C3-O3-P-O5
4	B	304	LHG	C4-O6-P-O3
4	B	304	LHG	C4-O6-P-O4
4	B	304	LHG	C4-O6-P-O5
4	C	304	LHG	C4-O6-P-O5
5	A	305	CHL	C1A-C2A-CAA-CBA
5	A	305	CHL	C3A-C2A-CAA-CBA
5	A	305	CHL	C3C-C2C-CMC-OMC
5	A	305	CHL	C2-C3-C5-C6
5	A	305	CHL	C4-C3-C5-C6
5	A	305	CHL	C6-C7-C8-C10
5	A	310	CHL	C1A-C2A-CAA-CBA
5	A	310	CHL	C1C-C2C-CMC-OMC
5	A	312	CHL	C2A-CAA-CBA-CGA
5	B	305	CHL	C1A-C2A-CAA-CBA
5	B	305	CHL	C1C-C2C-CMC-OMC
5	B	305	CHL	C3C-C2C-CMC-OMC
5	B	305	CHL	CHA-CBD-CGD-O1D
5	B	309	CHL	C3C-C2C-CMC-OMC
5	B	310	CHL	C1A-C2A-CAA-CBA
5	B	310	CHL	C1C-C2C-CMC-OMC
5	B	311	CHL	C11-C10-C8-C9
5	B	312	CHL	C2A-CAA-CBA-CGA
5	C	305	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
5	C	305	CHL	C1C-C2C-CMC-OMC
5	C	305	CHL	C3C-C2C-CMC-OMC
5	C	305	CHL	C2-C3-C5-C6
5	C	305	CHL	C4-C3-C5-C6
5	C	305	CHL	C6-C7-C8-C10
5	C	310	CHL	C1A-C2A-CAA-CBA
5	C	310	CHL	C1C-C2C-CMC-OMC
5	C	311	CHL	C11-C10-C8-C9
6	A	307	CLA	C2-C3-C5-C6
6	A	307	CLA	C4-C3-C5-C6
6	A	308	CLA	CHA-CBD-CGD-O1D
6	A	315	CLA	C1A-C2A-CAA-CBA
6	B	308	CLA	CHA-CBD-CGD-O1D
6	B	308	CLA	CHA-CBD-CGD-O2D
6	B	308	CLA	CAD-CBD-CGD-O1D
6	B	308	CLA	C11-C10-C8-C9
6	B	317	CLA	CHA-CBD-CGD-O1D
6	C	308	CLA	CHA-CBD-CGD-O1D
6	C	308	CLA	CHA-CBD-CGD-O2D
5	A	305	CHL	C13-C15-C16-C17
5	C	305	CHL	C13-C15-C16-C17
6	C	317	CLA	CBD-CGD-O2D-CED
5	B	311	CHL	O1A-CGA-O2A-C1
5	C	311	CHL	O1A-CGA-O2A-C1
5	B	305	CHL	C13-C15-C16-C17
5	C	311	CHL	CBA-CGA-O2A-C1
5	B	305	CHL	CBD-CGD-O2D-CED
6	A	317	CLA	CBD-CGD-O2D-CED
6	B	317	CLA	CBD-CGD-O2D-CED
5	A	311	CHL	O1A-CGA-O2A-C1
5	A	311	CHL	C3-C5-C6-C7
5	B	311	CHL	C3-C5-C6-C7
5	C	311	CHL	C3-C5-C6-C7
6	A	306	CLA	C3-C5-C6-C7
6	A	307	CLA	C3-C5-C6-C7
6	B	307	CLA	C3-C5-C6-C7
5	A	311	CHL	CBA-CGA-O2A-C1
5	B	311	CHL	CBA-CGA-O2A-C1
6	C	308	CLA	CBD-CGD-O2D-CED
5	A	311	CHL	C2A-CAA-CBA-CGA
5	B	311	CHL	C2A-CAA-CBA-CGA
5	C	311	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
5	C	312	CHL	C2A-CAA-CBA-CGA
6	B	315	CLA	C2A-CAA-CBA-CGA
6	A	316	CLA	C3-C5-C6-C7
6	B	316	CLA	C3-C5-C6-C7
6	C	306	CLA	C3-C5-C6-C7
5	C	310	CHL	CBA-CGA-O2A-C1
6	A	316	CLA	CBA-CGA-O2A-C1
6	A	315	CLA	CBD-CGD-O2D-CED
6	C	306	CLA	CBD-CGD-O2D-CED
6	B	306	CLA	C3-C5-C6-C7
6	C	307	CLA	C3-C5-C6-C7
6	B	316	CLA	CBA-CGA-O2A-C1
6	C	317	CLA	O1D-CGD-O2D-CED
5	A	310	CHL	CBA-CGA-O2A-C1
6	A	316	CLA	O1A-CGA-O2A-C1
6	B	316	CLA	O1A-CGA-O2A-C1
5	A	310	CHL	O1A-CGA-O2A-C1
5	C	310	CHL	O1A-CGA-O2A-C1
5	B	310	CHL	CBA-CGA-O2A-C1
5	C	305	CHL	CBD-CGD-O2D-CED
5	B	310	CHL	O1A-CGA-O2A-C1
6	C	316	CLA	CBA-CGA-O2A-C1
5	A	313	CHL	CBD-CGD-O2D-CED
5	C	313	CHL	CBD-CGD-O2D-CED
6	C	316	CLA	C3-C5-C6-C7
6	C	316	CLA	O1A-CGA-O2A-C1
5	A	305	CHL	C11-C12-C13-C14
5	A	311	CHL	C11-C10-C8-C9
5	A	311	CHL	C11-C12-C13-C14
5	A	313	CHL	C11-C12-C13-C14
5	B	305	CHL	C11-C12-C13-C14
5	B	311	CHL	C11-C12-C13-C14
5	B	313	CHL	C11-C12-C13-C14
5	C	305	CHL	C11-C12-C13-C14
5	C	311	CHL	C11-C12-C13-C14
5	C	313	CHL	C11-C12-C13-C14
6	C	307	CLA	C6-C7-C8-C9
6	C	308	CLA	C11-C10-C8-C9
6	B	306	CLA	C13-C15-C16-C17
6	A	315	CLA	C2A-CAA-CBA-CGA
3	C	303	NEX	C11-C12-C13-C20
6	B	317	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
5	A	305	CHL	C15-C16-C17-C18
5	C	305	CHL	C15-C16-C17-C18
5	C	312	CHL	C15-C16-C17-C18
6	C	315	CLA	C13-C15-C16-C17
5	B	311	CHL	CBD-CGD-O2D-CED
6	B	308	CLA	CBD-CGD-O2D-CED
5	B	305	CHL	O1D-CGD-O2D-CED
5	A	305	CHL	C10-C11-C12-C13
5	B	305	CHL	C5-C6-C7-C8
5	B	305	CHL	C10-C11-C12-C13
5	B	305	CHL	C15-C16-C17-C18
5	B	312	CHL	C15-C16-C17-C18
5	C	305	CHL	C8-C10-C11-C12
6	A	317	CLA	C10-C11-C12-C13
5	A	305	CHL	CBD-CGD-O2D-CED
5	A	312	CHL	C15-C16-C17-C18
6	A	317	CLA	C13-C15-C16-C17
6	B	317	CLA	C5-C6-C7-C8
6	A	308	CLA	C2-C1-O2A-CGA
5	A	311	CHL	C11-C12-C13-C15
5	B	305	CHL	C6-C7-C8-C10
5	C	305	CHL	C10-C11-C12-C13
6	A	315	CLA	C13-C15-C16-C17
5	A	305	CHL	C5-C6-C7-C8
5	B	305	CHL	C8-C10-C11-C12
5	B	311	CHL	C8-C10-C11-C12
6	B	317	CLA	C13-C15-C16-C17
5	B	311	CHL	C10-C11-C12-C13
5	C	305	CHL	C5-C6-C7-C8
5	C	311	CHL	C8-C10-C11-C12
6	A	317	CLA	C5-C6-C7-C8
4	C	304	LHG	C4-O6-P-O3
5	A	311	CHL	C10-C11-C12-C13
6	B	315	CLA	C13-C15-C16-C17
5	B	305	CHL	C4-C3-C5-C6
5	C	311	CHL	C15-C16-C17-C18
5	C	311	CHL	C16-C17-C18-C19
6	B	317	CLA	C10-C11-C12-C13
6	A	317	CLA	O1D-CGD-O2D-CED
4	B	304	LHG	C24-C25-C26-C27
4	C	304	LHG	C26-C27-C28-C29
6	B	316	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
6	C	308	CLA	O1D-CGD-O2D-CED
4	C	304	LHG	O2-C2-C3-O3
5	B	311	CHL	C16-C17-C18-C19
6	A	316	CLA	C16-C17-C18-C19
4	A	304	LHG	C29-C30-C31-C32
6	A	315	CLA	C6-C7-C8-C9
6	B	315	CLA	C11-C10-C8-C9
6	B	317	CLA	C11-C12-C13-C14
4	A	304	LHG	C10-C11-C12-C13
5	A	305	CHL	C8-C10-C11-C12
4	A	304	LHG	C28-C29-C30-C31
5	A	311	CHL	C16-C17-C18-C19
5	C	305	CHL	C16-C17-C18-C19
5	C	305	CHL	C16-C17-C18-C20
5	C	311	CHL	C16-C17-C18-C20
6	A	315	CLA	O1D-CGD-O2D-CED
6	A	308	CLA	CBA-CGA-O2A-C1
5	B	305	CHL	C3A-C2A-CAA-CBA
6	A	307	CLA	C3A-C2A-CAA-CBA
6	A	315	CLA	C3A-C2A-CAA-CBA
6	B	307	CLA	C3A-C2A-CAA-CBA
6	C	307	CLA	C3A-C2A-CAA-CBA
6	C	315	CLA	C3A-C2A-CAA-CBA
5	A	305	CHL	C16-C17-C18-C19
5	A	305	CHL	C16-C17-C18-C20
5	B	305	CHL	C16-C17-C18-C19
5	B	305	CHL	C16-C17-C18-C20
6	A	316	CLA	C16-C17-C18-C20
6	C	317	CLA	C4-C3-C5-C6
6	C	317	CLA	C2-C3-C5-C6
5	B	311	CHL	C16-C17-C18-C20
4	C	304	LHG	C1-C2-C3-O3
4	C	304	LHG	C24-C25-C26-C27
6	A	315	CLA	C8-C10-C11-C12
6	B	315	CLA	C10-C11-C12-C13
6	A	308	CLA	O1A-CGA-O2A-C1
4	B	304	LHG	C16-C17-C18-C19
2	A	301	LUT	C1-C6-C7-C8
6	C	316	CLA	C15-C16-C17-C18
6	B	307	CLA	C4-C3-C5-C6
6	C	306	CLA	C4-C3-C5-C6
5	A	305	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
5	C	305	CHL	C11-C12-C13-C15
5	C	311	CHL	C12-C13-C15-C16
6	B	317	CLA	C11-C12-C13-C15
6	C	315	CLA	C11-C10-C8-C7
6	B	316	CLA	C10-C11-C12-C13
5	A	311	CHL	C15-C16-C17-C18
6	A	308	CLA	C5-C6-C7-C8
6	C	306	CLA	O1D-CGD-O2D-CED
5	B	311	CHL	C15-C16-C17-C18
6	B	315	CLA	C8-C10-C11-C12
5	B	313	CHL	CBD-CGD-O2D-CED
5	A	313	CHL	C3-C5-C6-C7
5	A	311	CHL	C16-C17-C18-C20
6	C	317	CLA	C10-C11-C12-C13
6	C	307	CLA	C4-C3-C5-C6
5	B	305	CHL	C2-C3-C5-C6
6	C	306	CLA	C2-C3-C5-C6
5	A	312	CHL	C11-C12-C13-C14
5	C	305	CHL	C1A-C2A-CAA-CBA
6	A	307	CLA	C1A-C2A-CAA-CBA
6	A	308	CLA	C1A-C2A-CAA-CBA
6	B	307	CLA	C1A-C2A-CAA-CBA
6	C	307	CLA	C1A-C2A-CAA-CBA
6	C	315	CLA	C1A-C2A-CAA-CBA
6	B	316	CLA	C16-C17-C18-C20
6	A	316	CLA	C10-C11-C12-C13
5	B	313	CHL	C13-C15-C16-C17
6	C	315	CLA	C10-C11-C12-C13
4	A	304	LHG	C24-C25-C26-C27
6	C	317	CLA	C13-C15-C16-C17
5	C	305	CHL	O1D-CGD-O2D-CED
5	C	313	CHL	C16-C17-C18-C19
6	C	317	CLA	C5-C6-C7-C8
5	C	311	CHL	C10-C11-C12-C13
6	A	316	CLA	C13-C15-C16-C17
4	B	304	LHG	C29-C30-C31-C32
5	A	311	CHL	C4-C3-C5-C6
5	C	311	CHL	C4-C3-C5-C6
6	A	317	CLA	C4-C3-C5-C6
6	B	308	CLA	C4-C3-C5-C6
6	B	308	CLA	C5-C6-C7-C8
6	C	307	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
5	B	311	CHL	O1D-CGD-O2D-CED
6	A	315	CLA	C10-C11-C12-C13
6	C	308	CLA	C5-C6-C7-C8
4	C	304	LHG	C10-C11-C12-C13
6	C	314	CLA	CBA-CGA-O2A-C1
6	B	308	CLA	C10-C11-C12-C13
6	B	316	CLA	C13-C15-C16-C17
6	C	316	CLA	C13-C15-C16-C17
5	C	313	CHL	C13-C15-C16-C17
5	B	311	CHL	C4-C3-C5-C6
6	B	317	CLA	C4-C3-C5-C6
6	C	308	CLA	C4-C3-C5-C6
5	A	305	CHL	O1D-CGD-O2D-CED
5	A	311	CHL	C11-C10-C8-C7
5	A	311	CHL	C12-C13-C15-C16
5	A	312	CHL	C11-C10-C8-C7
5	A	312	CHL	C11-C12-C13-C15
5	B	305	CHL	C11-C10-C8-C7
5	B	305	CHL	C11-C12-C13-C15
5	B	311	CHL	C11-C12-C13-C15
5	B	311	CHL	C12-C13-C15-C16
5	C	311	CHL	C11-C10-C8-C7
5	C	311	CHL	C11-C12-C13-C15
6	A	315	CLA	C11-C10-C8-C7
6	A	317	CLA	C2-C3-C5-C6
6	A	317	CLA	C11-C12-C13-C15
6	B	308	CLA	C2-C3-C5-C6
6	B	315	CLA	C11-C10-C8-C7
6	B	316	CLA	C11-C12-C13-C15
6	C	306	CLA	C11-C12-C13-C15
5	A	311	CHL	C14-C13-C15-C16
5	B	305	CHL	C6-C7-C8-C9
5	B	311	CHL	C14-C13-C15-C16
5	C	311	CHL	C14-C13-C15-C16
6	A	308	CLA	C11-C10-C8-C9
6	A	316	CLA	C11-C12-C13-C14
6	A	317	CLA	C11-C12-C13-C14
6	B	306	CLA	C11-C12-C13-C14
6	B	316	CLA	C11-C12-C13-C14
6	C	306	CLA	C11-C12-C13-C14
6	C	315	CLA	C11-C10-C8-C9
6	C	315	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
6	C	316	CLA	C11-C12-C13-C14
6	C	317	CLA	C14-C13-C15-C16
5	A	310	CHL	O1D-CGD-O2D-CED
4	B	304	LHG	C17-C18-C19-C20
4	A	304	LHG	C35-C36-C37-C38
4	B	304	LHG	C10-C11-C12-C13
5	A	311	CHL	C8-C10-C11-C12
5	A	311	CHL	C2-C3-C5-C6
5	B	311	CHL	C2-C3-C5-C6
5	C	311	CHL	C2-C3-C5-C6
6	B	317	CLA	C2-C3-C5-C6
6	C	307	CLA	C2-C3-C5-C6
6	C	308	CLA	C2-C3-C5-C6
4	B	304	LHG	O2-C2-C3-O3
6	B	308	CLA	O1D-CGD-O2D-CED
6	B	307	CLA	C5-C6-C7-C8
6	B	307	CLA	C15-C16-C17-C18
4	A	304	LHG	C16-C17-C18-C19
6	B	307	CLA	C2-C3-C5-C6
4	B	304	LHG	C3-O3-P-O6
5	A	309	CHL	C3C-C2C-CMC-OMC
5	A	310	CHL	C3C-C2C-CMC-OMC
5	A	311	CHL	C3C-C2C-CMC-OMC
5	B	310	CHL	C3C-C2C-CMC-OMC
5	C	310	CHL	C3C-C2C-CMC-OMC
6	C	314	CLA	O1A-CGA-O2A-C1
5	A	313	CHL	O1D-CGD-O2D-CED
5	C	313	CHL	C16-C17-C18-C20
6	A	316	CLA	C15-C16-C17-C18
5	A	313	CHL	C2-C1-O2A-CGA
6	A	307	CLA	C2-C1-O2A-CGA
5	C	311	CHL	C13-C15-C16-C17
6	B	307	CLA	C6-C7-C8-C9
6	B	315	CLA	C6-C7-C8-C9
5	A	310	CHL	CBD-CGD-O2D-CED
6	C	316	CLA	C10-C11-C12-C13
4	B	304	LHG	C26-C27-C28-C29
6	C	316	CLA	C16-C17-C18-C19
2	A	301	LUT	C5-C6-C7-C8
2	C	301	LUT	C1-C6-C7-C8
2	C	301	LUT	C5-C6-C7-C8
6	C	314	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
3	C	303	NEX	C11-C12-C13-C14
5	A	313	CHL	C16-C17-C18-C20
5	B	313	CHL	C16-C17-C18-C20
4	C	304	LHG	C16-C17-C18-C19
5	A	313	CHL	C12-C13-C15-C16
5	B	311	CHL	C11-C10-C8-C7
5	B	313	CHL	C11-C12-C13-C15
5	C	312	CHL	C11-C12-C13-C15
5	C	313	CHL	C12-C13-C15-C16
6	A	316	CLA	C11-C12-C13-C15
6	A	317	CLA	C12-C13-C15-C16
6	B	306	CLA	C11-C12-C13-C15
6	B	317	CLA	C12-C13-C15-C16
6	C	315	CLA	C11-C12-C13-C15
6	C	316	CLA	C11-C12-C13-C15
6	C	317	CLA	C12-C13-C15-C16
6	A	315	CLA	CBA-CGA-O2A-C1
5	A	313	CHL	C13-C15-C16-C17
5	A	313	CHL	C15-C16-C17-C18
5	B	310	CHL	CAD-CBD-CGD-O2D
6	A	316	CLA	CAD-CBD-CGD-O2D
4	A	304	LHG	C4-C5-C6-O8
5	C	313	CHL	C15-C16-C17-C18
6	A	308	CLA	CHA-CBD-CGD-O2D
4	B	304	LHG	C12-C13-C14-C15
5	B	309	CHL	CBD-CGD-O2D-CED
6	A	308	CLA	C10-C11-C12-C13
5	A	305	CHL	C6-C7-C8-C9
5	B	312	CHL	C11-C12-C13-C14
5	B	313	CHL	C14-C13-C15-C16
5	C	305	CHL	C6-C7-C8-C9
5	C	312	CHL	C11-C12-C13-C14
6	A	317	CLA	C14-C13-C15-C16
6	B	317	CLA	C14-C13-C15-C16
6	B	314	CLA	C1A-C2A-CAA-CBA
5	C	313	CHL	O1D-CGD-O2D-CED
4	C	304	LHG	C4-O6-P-O4
4	C	304	LHG	C25-C26-C27-C28
6	A	315	CLA	O1A-CGA-O2A-C1
6	A	308	CLA	CAD-CBD-CGD-O1D
6	B	318	CLA	CAD-CBD-CGD-O1D
6	C	308	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
6	C	318	CLA	CAD-CBD-CGD-O1D
5	A	305	CHL	C11-C10-C8-C7
5	B	312	CHL	C6-C7-C8-C10
5	B	312	CHL	C11-C10-C8-C7
5	B	312	CHL	C11-C12-C13-C15
5	B	313	CHL	C12-C13-C15-C16
5	C	305	CHL	C12-C13-C15-C16
5	C	310	CHL	C3A-C2A-CAA-CBA
5	C	312	CHL	C11-C10-C8-C7
5	C	313	CHL	C11-C12-C13-C15
6	A	308	CLA	C11-C10-C8-C7
6	B	308	CLA	C11-C10-C8-C7
6	C	308	CLA	C11-C10-C8-C7
6	C	314	CLA	C11-C10-C8-C7
4	A	304	LHG	C11-C12-C13-C14
3	B	303	NEX	C29-C30-C31-C32
6	C	306	CLA	C13-C15-C16-C17
5	A	305	CHL	C1C-C2C-CMC-OMC
5	A	309	CHL	C1C-C2C-CMC-OMC
5	A	311	CHL	C1C-C2C-CMC-OMC
5	B	309	CHL	C1C-C2C-CMC-OMC
5	B	309	CHL	CBA-CGA-O2A-C1
5	B	309	CHL	O1D-CGD-O2D-CED
5	A	313	CHL	C14-C13-C15-C16
6	A	315	CLA	C11-C10-C8-C9
6	B	317	CLA	O1A-CGA-O2A-C1
5	B	309	CHL	O1A-CGA-O2A-C1
6	C	316	CLA	C16-C17-C18-C20
6	A	307	CLA	C15-C16-C17-C18
5	B	313	CHL	C2-C1-O2A-CGA
6	A	317	CLA	C2-C1-O2A-CGA
6	B	307	CLA	C2-C1-O2A-CGA
6	C	307	CLA	C2-C1-O2A-CGA
5	A	305	CHL	O1A-CGA-O2A-C1
6	A	317	CLA	O1A-CGA-O2A-C1
6	A	306	CLA	C4-C3-C5-C6
6	A	308	CLA	C4-C3-C5-C6
2	A	302	LUT	C1-C6-C7-C8
2	B	302	LUT	C1-C6-C7-C8
2	C	302	LUT	C1-C6-C7-C8
2	C	302	LUT	C5-C6-C7-C8
6	C	314	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
4	A	304	LHG	C3-O3-P-O6
4	C	304	LHG	C3-O3-P-O6
5	A	313	CHL	C4-C3-C5-C6
4	A	304	LHG	C17-C18-C19-C20
5	A	305	CHL	C11-C10-C8-C9
5	A	312	CHL	C11-C10-C8-C9
5	B	305	CHL	C11-C10-C8-C9
5	B	312	CHL	C6-C7-C8-C9
5	C	312	CHL	C11-C10-C8-C9
5	C	313	CHL	C14-C13-C15-C16
2	A	302	LUT	C9-C10-C11-C12
5	C	313	CHL	C3-C5-C6-C7
6	C	316	CLA	C4-C3-C5-C6
5	A	313	CHL	C16-C17-C18-C19
5	B	313	CHL	C16-C17-C18-C19
6	B	317	CLA	CBA-CGA-O2A-C1
6	C	314	CLA	C2A-CAA-CBA-CGA
4	C	304	LHG	C28-C29-C30-C31
5	B	313	CHL	C4-C3-C5-C6
5	B	311	CHL	C5-C6-C7-C8
6	B	316	CLA	C15-C16-C17-C18
5	C	313	CHL	C2-C1-O2A-CGA
6	B	317	CLA	C2-C1-O2A-CGA
6	C	315	CLA	C2A-CAA-CBA-CGA
4	C	304	LHG	C12-C13-C14-C15
5	A	310	CHL	C3A-C2A-CAA-CBA
5	B	310	CHL	C3A-C2A-CAA-CBA
6	B	315	CLA	C3A-C2A-CAA-CBA
5	B	312	CHL	C11-C10-C8-C9
5	C	311	CHL	C6-C7-C8-C9
5	C	312	CHL	C14-C13-C15-C16
6	A	307	CLA	C11-C12-C13-C14
6	A	317	CLA	C11-C10-C8-C9
6	B	307	CLA	C11-C12-C13-C14
6	B	317	CLA	C11-C10-C8-C9
3	A	303	NEX	C39-C29-C30-C31
3	B	303	NEX	C39-C29-C30-C31
3	C	303	NEX	C39-C29-C30-C31
6	B	308	CLA	C2A-CAA-CBA-CGA
5	A	312	CHL	O2A-C1-C2-C3
5	C	312	CHL	O2A-C1-C2-C3
5	A	309	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
5	A	305	CHL	C12-C13-C15-C16
5	B	305	CHL	C12-C13-C15-C16
6	B	314	CLA	C6-C7-C8-C10
6	B	314	CLA	C2A-CAA-CBA-CGA
6	A	317	CLA	CBA-CGA-O2A-C1
5	C	313	CHL	C4-C3-C5-C6
6	B	306	CLA	C4-C3-C5-C6
6	A	306	CLA	C5-C6-C7-C8
6	A	308	CLA	C2-C3-C5-C6
6	C	316	CLA	C2-C3-C5-C6
3	A	303	NEX	C28-C29-C30-C31
3	B	303	NEX	C28-C29-C30-C31
3	C	303	NEX	C28-C29-C30-C31
2	C	302	LUT	C29-C30-C31-C32
5	A	309	CHL	O1A-CGA-O2A-C1
4	B	304	LHG	C1-C2-C3-O3
6	A	315	CLA	C4-C3-C5-C6
6	C	315	CLA	C4-C3-C5-C6
5	A	313	CHL	C2-C3-C5-C6
5	B	313	CHL	C2-C3-C5-C6
6	B	315	CLA	C11-C12-C13-C14
6	C	307	CLA	C11-C12-C13-C14
2	A	302	LUT	C5-C6-C7-C8
2	B	301	LUT	C1-C6-C7-C8
4	B	304	LHG	C14-C15-C16-C17
4	B	304	LHG	C15-C16-C17-C18
6	C	317	CLA	O1A-CGA-O2A-C1
6	B	316	CLA	C4-C3-C5-C6
5	A	309	CHL	C2-C1-O2A-CGA
4	C	304	LHG	C14-C15-C16-C17
5	C	309	CHL	C2-C1-O2A-CGA
5	B	311	CHL	C13-C15-C16-C17
6	A	316	CLA	C4-C3-C5-C6
5	C	312	CHL	C6-C7-C8-C10
6	A	308	CLA	C6-C7-C8-C10
6	B	316	CLA	C2-C3-C5-C6
4	B	304	LHG	C9-C10-C11-C12
6	B	315	CLA	C4-C3-C5-C6
5	C	313	CHL	C2-C3-C5-C6
6	A	306	CLA	C2-C3-C5-C6
4	A	304	LHG	C14-C15-C16-C17
5	A	312	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
5	C	305	CHL	C14-C13-C15-C16
6	B	308	CLA	C6-C7-C8-C9
6	B	314	CLA	C6-C7-C8-C9
6	C	306	CLA	C11-C10-C8-C9
5	B	312	CHL	C3A-C2A-CAA-CBA
6	B	306	CLA	CAD-CBD-CGD-O2D
6	C	314	CLA	C16-C17-C18-C19
2	C	301	LUT	C11-C12-C13-C14
3	C	303	NEX	O24-C26-C27-C28
5	B	313	CHL	O1D-CGD-O2D-CED
5	B	309	CHL	C2-C1-O2A-CGA
5	A	305	CHL	O2A-C1-C2-C3
5	B	305	CHL	O2A-C1-C2-C3
5	B	312	CHL	O2A-C1-C2-C3
5	C	305	CHL	O2A-C1-C2-C3
6	C	317	CLA	C2A-CAA-CBA-CGA
5	C	313	CHL	C2C-C3C-CAC-CBC
6	B	315	CLA	O1D-CGD-O2D-CED
5	A	305	CHL	CHA-CBD-CGD-O2D
5	B	305	CHL	CHA-CBD-CGD-O2D
5	C	305	CHL	CHA-CBD-CGD-O1D
5	C	305	CHL	CHA-CBD-CGD-O2D
6	A	307	CLA	CHA-CBD-CGD-O1D
6	A	307	CLA	CHA-CBD-CGD-O2D
6	A	317	CLA	CHA-CBD-CGD-O1D
6	B	307	CLA	CHA-CBD-CGD-O1D
6	B	307	CLA	CHA-CBD-CGD-O2D
6	B	317	CLA	CHA-CBD-CGD-O2D
6	C	307	CLA	CHA-CBD-CGD-O1D
6	C	307	CLA	CHA-CBD-CGD-O2D
6	A	314	CLA	O1A-CGA-O2A-C1
6	A	306	CLA	C8-C10-C11-C12
5	A	305	CHL	CBA-CGA-O2A-C1
6	A	314	CLA	C11-C10-C8-C7
6	A	316	CLA	C2-C3-C5-C6
6	A	306	CLA	C11-C10-C8-C9
5	A	311	CHL	C13-C15-C16-C17
5	C	312	CHL	C8-C10-C11-C12
4	A	304	LHG	O2-C2-C3-O3
5	B	312	CHL	C1A-C2A-CAA-CBA
6	A	307	CLA	C5-C6-C7-C8
5	C	312	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
6	C	307	CLA	C5-C6-C7-C8
6	A	314	CLA	C2A-CAA-CBA-CGA
6	B	317	CLA	C2A-CAA-CBA-CGA
5	A	312	CHL	CAA-CBA-CGA-O2A
5	B	313	CHL	C2C-C3C-CAC-CBC
4	A	304	LHG	C3-O3-P-O5
6	A	308	CLA	O1D-CGD-O2D-CED
6	C	308	CLA	C10-C11-C12-C13
6	A	317	CLA	CAA-CBA-CGA-O2A
6	B	317	CLA	C15-C16-C17-C18
6	C	314	CLA	C5-C6-C7-C8
6	A	306	CLA	C13-C15-C16-C17
6	B	315	CLA	C2-C3-C5-C6
5	B	305	CHL	CAD-CBD-CGD-O1D
6	A	317	CLA	CAD-CBD-CGD-O1D
6	A	318	CLA	CAD-CBD-CGD-O1D
6	B	317	CLA	CAD-CBD-CGD-O1D
5	A	305	CHL	C14-C13-C15-C16
5	B	305	CHL	C14-C13-C15-C16
5	C	305	CHL	C11-C10-C8-C9
5	C	312	CHL	C6-C7-C8-C9
6	C	314	CLA	C11-C10-C8-C9
5	B	312	CHL	CAA-CBA-CGA-O2A
6	C	307	CLA	CAA-CBA-CGA-O2A
6	A	307	CLA	CAA-CBA-CGA-O2A
4	A	304	LHG	C1-C2-C3-O3
6	A	308	CLA	CBD-CGD-O2D-CED
5	A	312	CHL	C6-C7-C8-C10
5	A	313	CHL	C11-C12-C13-C15
5	C	305	CHL	C11-C10-C8-C7
5	C	311	CHL	C6-C7-C8-C10
6	A	307	CLA	C11-C12-C13-C15
6	B	307	CLA	C11-C12-C13-C15
5	A	312	CHL	CAA-CBA-CGA-O1A
5	C	312	CHL	CAA-CBA-CGA-O1A
5	A	311	CHL	CAA-CBA-CGA-O2A
5	B	311	CHL	CAA-CBA-CGA-O2A
6	A	307	CLA	CAA-CBA-CGA-O1A
5	B	312	CHL	CAA-CBA-CGA-O1A

There are no ring outliers.

51 monomers are involved in 204 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	LUT	5	0
5	B	311	CHL	4	0
6	B	308	CLA	1	0
5	C	312	CHL	5	0
4	A	304	LHG	9	0
6	C	314	CLA	7	0
5	A	312	CHL	5	0
6	A	317	CLA	7	0
6	A	306	CLA	7	0
6	C	315	CLA	2	0
5	C	311	CHL	3	0
6	B	315	CLA	5	0
6	C	318	CLA	2	0
6	B	307	CLA	16	0
5	C	305	CHL	8	0
5	B	305	CHL	10	0
5	A	310	CHL	2	0
6	B	316	CLA	7	0
2	C	302	LUT	5	0
2	B	302	LUT	6	0
6	A	315	CLA	3	0
6	C	317	CLA	4	0
6	A	318	CLA	1	0
6	A	307	CLA	18	0
5	A	305	CHL	7	0
6	A	316	CLA	4	0
5	B	309	CHL	1	0
3	B	303	NEX	3	0
3	C	303	NEX	3	0
2	A	302	LUT	1	0
3	A	303	NEX	3	0
4	B	304	LHG	5	0
4	C	304	LHG	5	0
6	C	306	CLA	15	0
6	B	314	CLA	9	0
6	C	307	CLA	23	0
5	B	310	CHL	2	0
5	C	310	CHL	1	0
5	A	309	CHL	2	0
5	B	313	CHL	3	0
2	B	301	LUT	9	0
5	C	313	CHL	5	0
6	A	314	CLA	10	0

Continued on next page...

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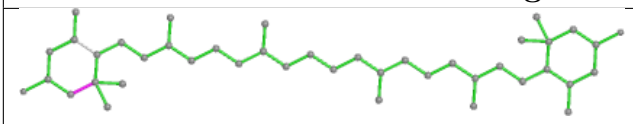
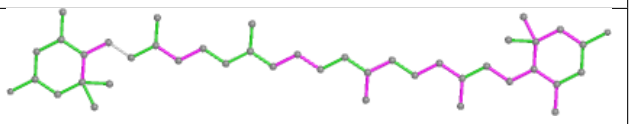
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	316	CLA	2	0
2	C	301	LUT	2	0
5	A	313	CHL	6	0
5	A	311	CHL	3	0
5	B	312	CHL	3	0
6	B	318	CLA	1	0
6	B	306	CLA	12	0
6	B	317	CLA	3	0

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 then 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.

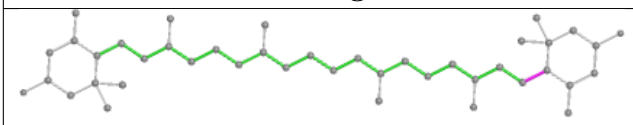
Ligand LUT A 301



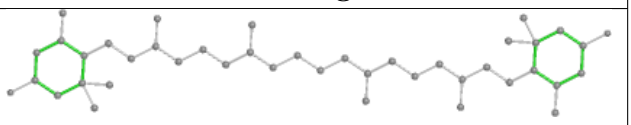
Bond lengths



Bond angles

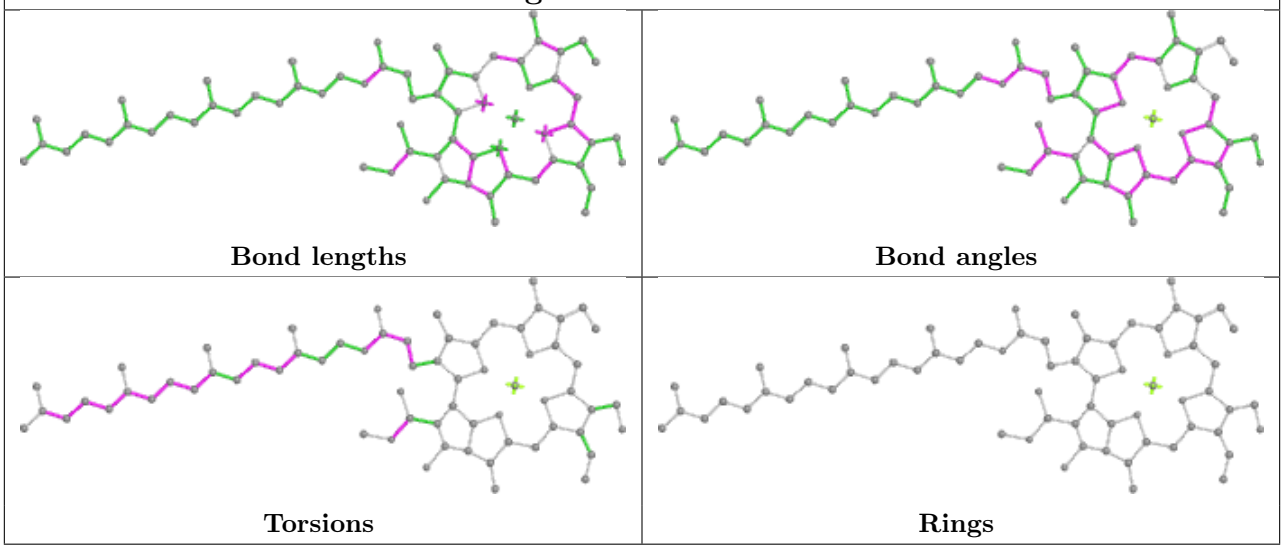


Torsions

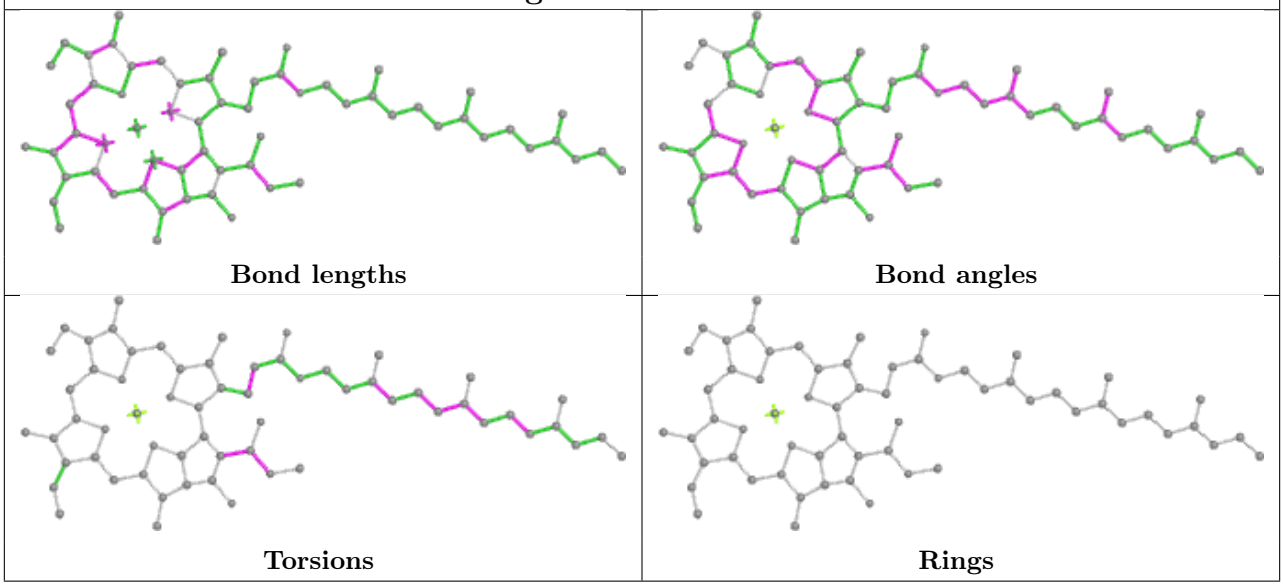


Rings

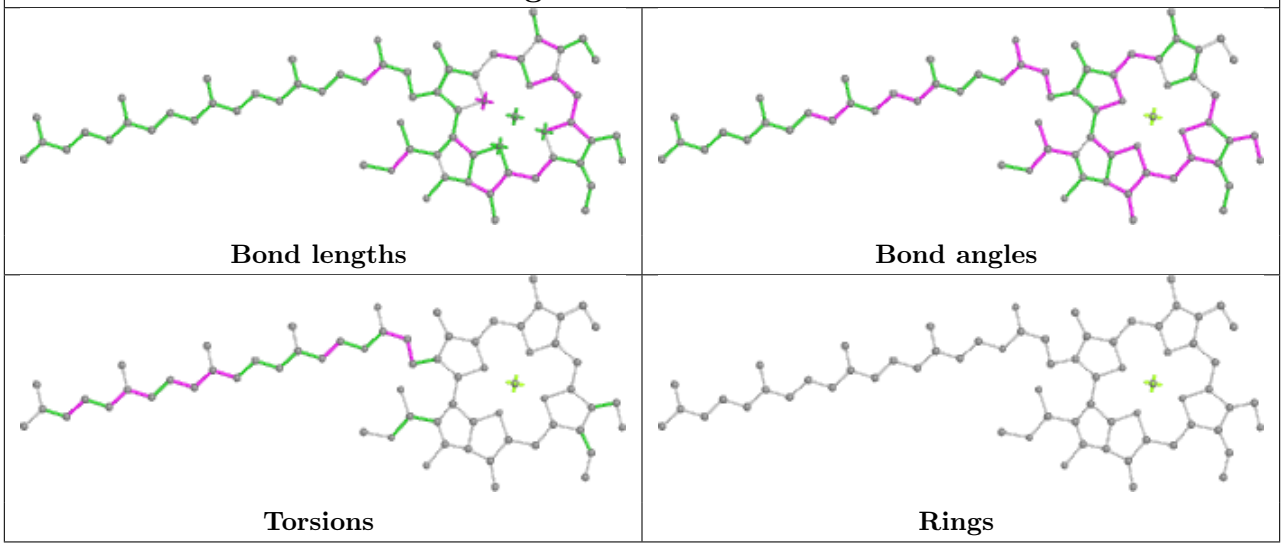
Ligand CHL B 311



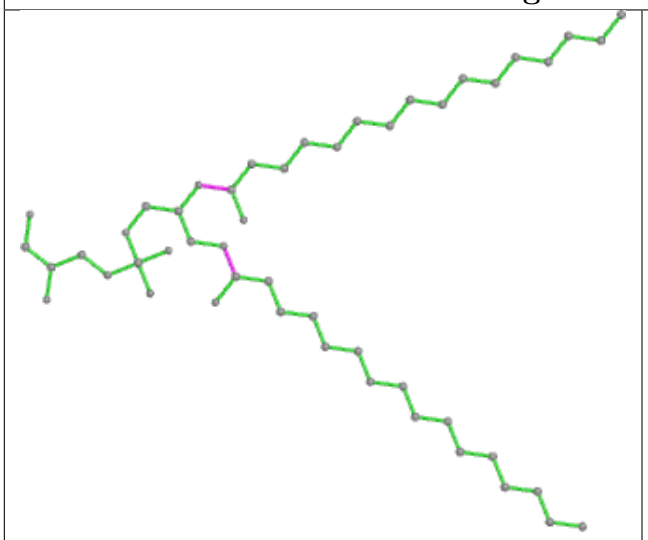
Ligand CLA B 308



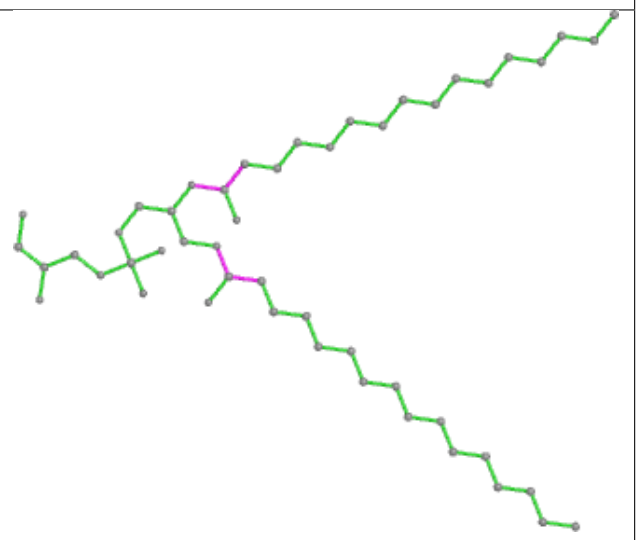
Ligand CHL C 312



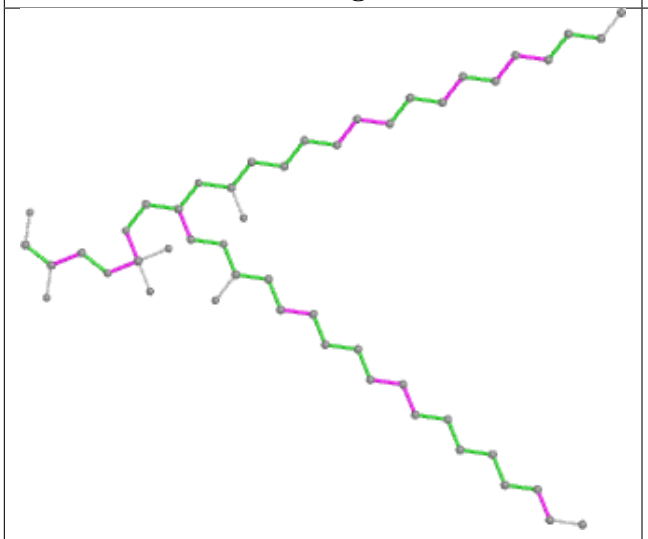
Ligand LHG A 304



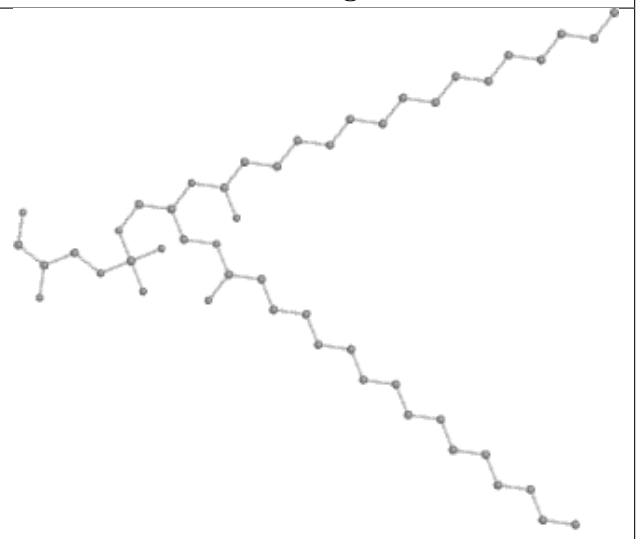
Bond lengths



Bond angles

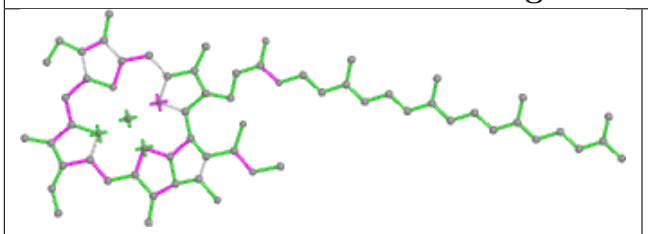


Torsions

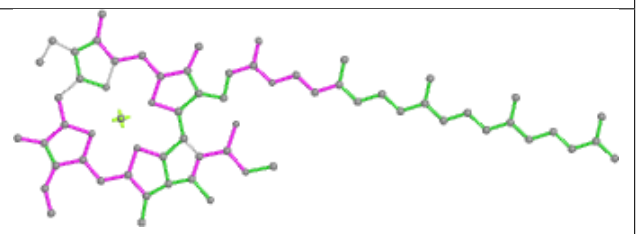


Rings

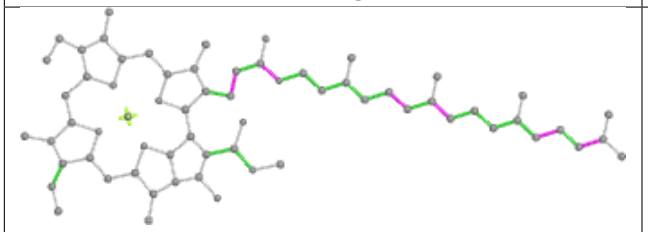
Ligand CLA C 314



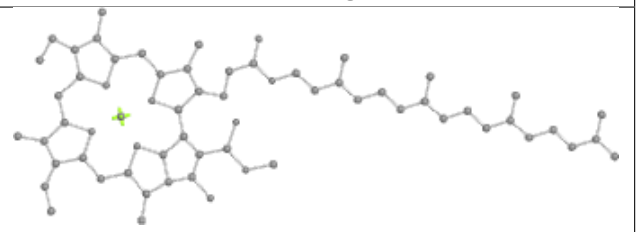
Bond lengths



Bond angles

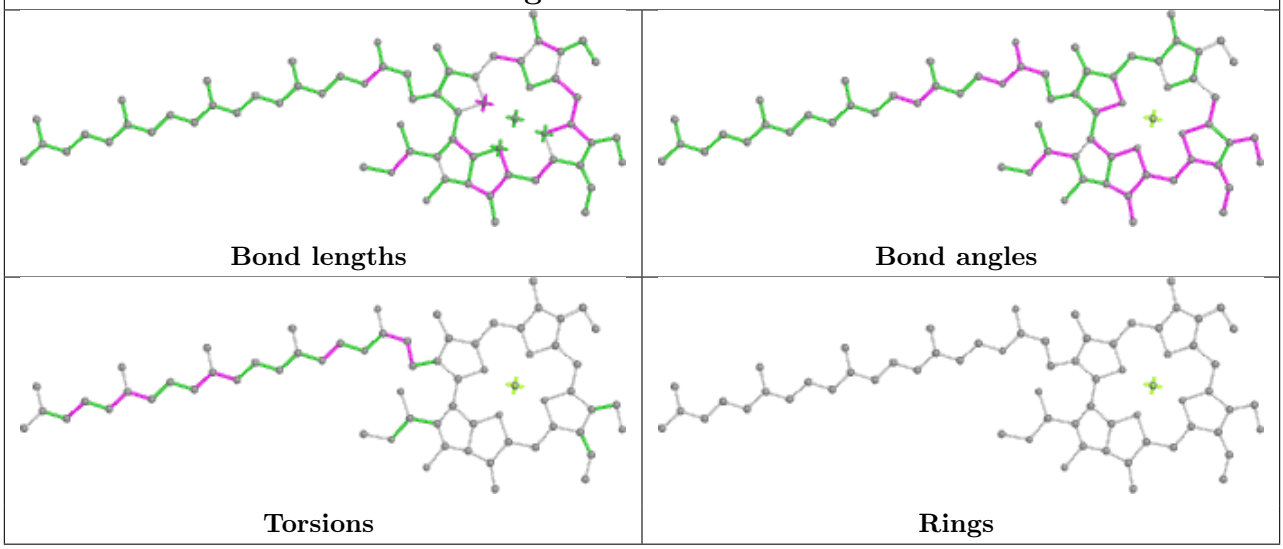


Torsions

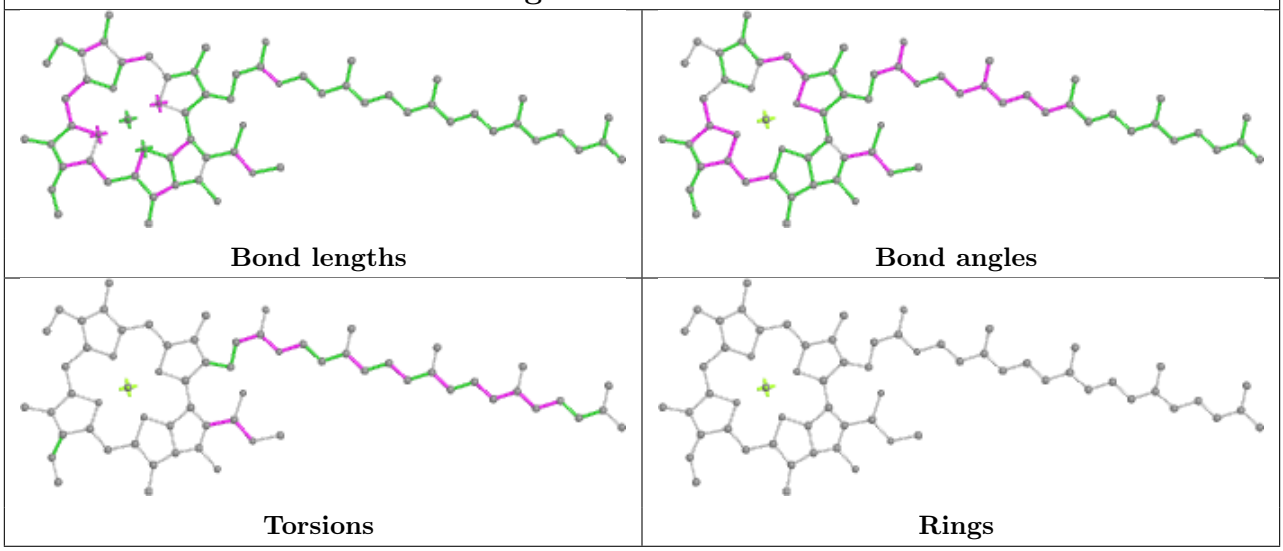


Rings

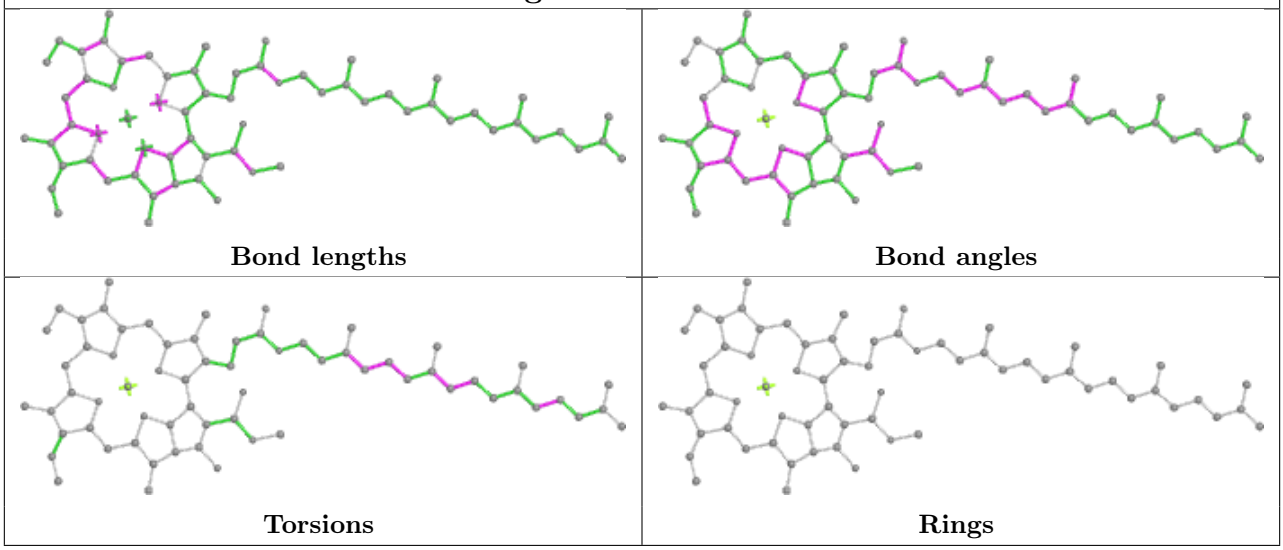
Ligand CHL A 312



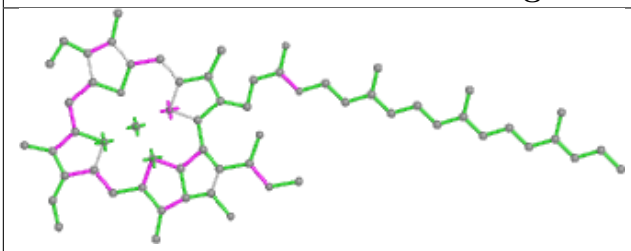
Ligand CLA A 317



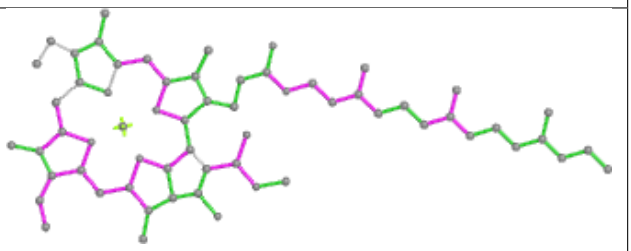
Ligand CLA A 306



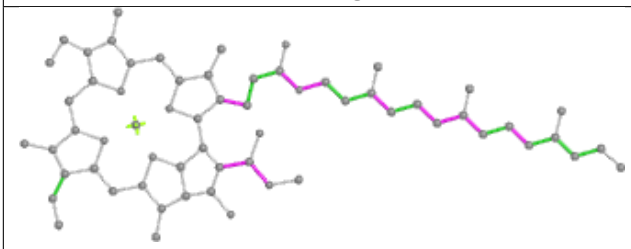
Ligand CLA A 308



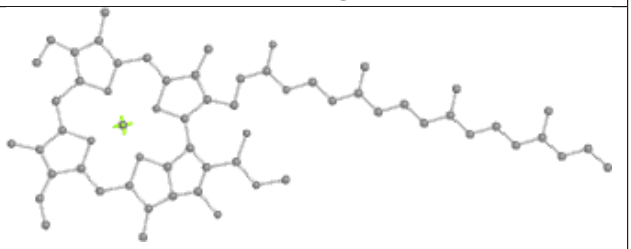
Bond lengths



Bond angles

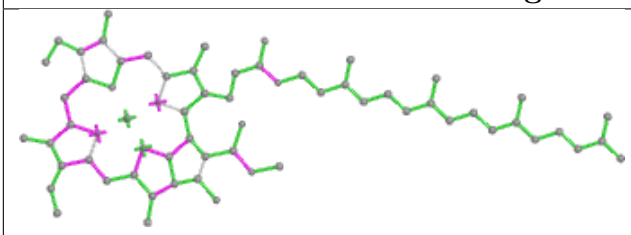


Torsions



Rings

Ligand CLA C 315



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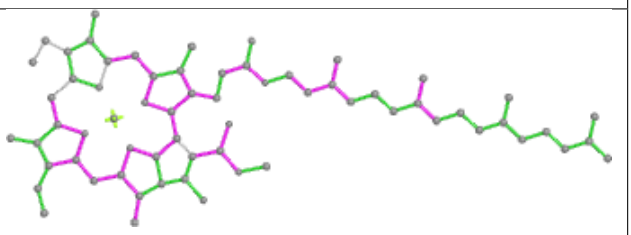
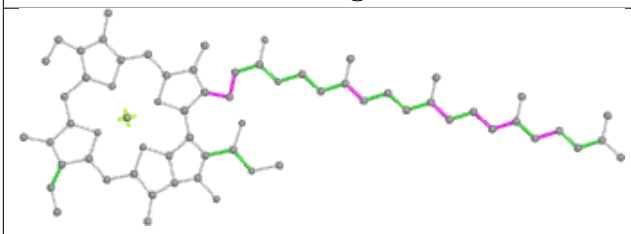


Bond angles



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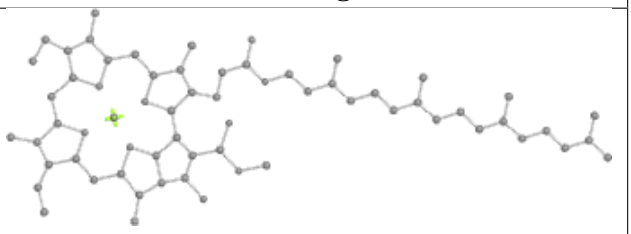
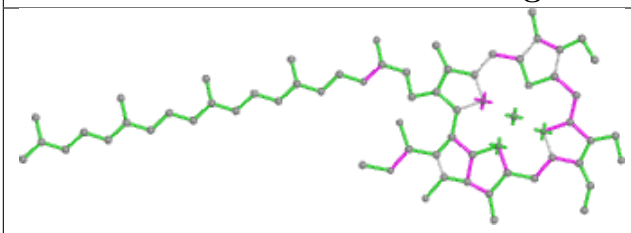


Rings

Ligand CHL C 311



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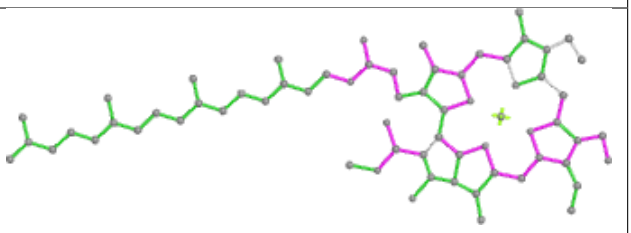
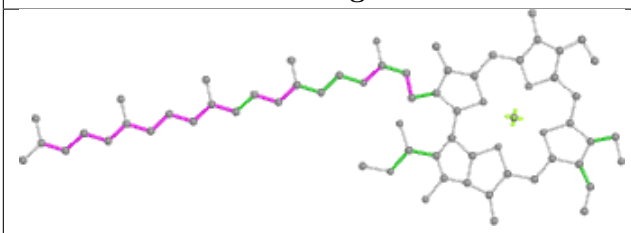
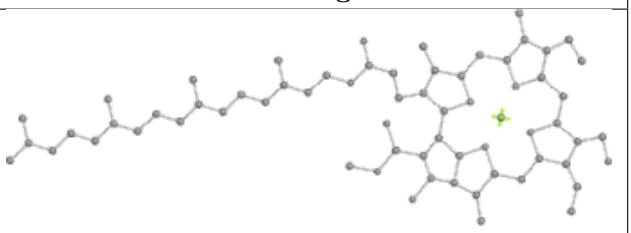


Bond angles

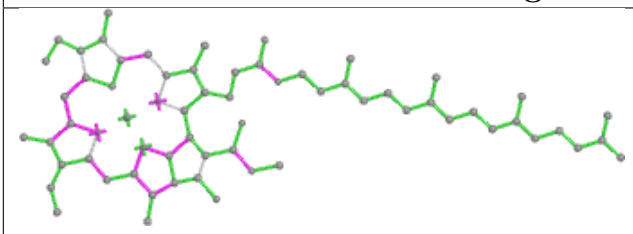


Torsions

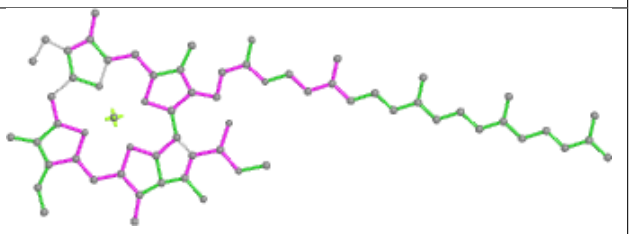


Rings

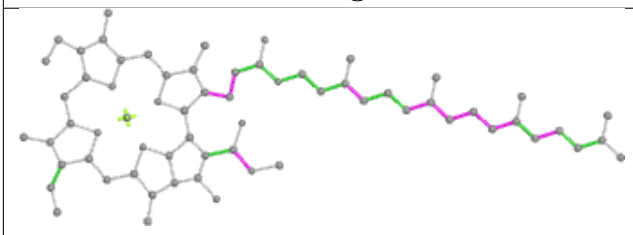
Ligand CLA B 315



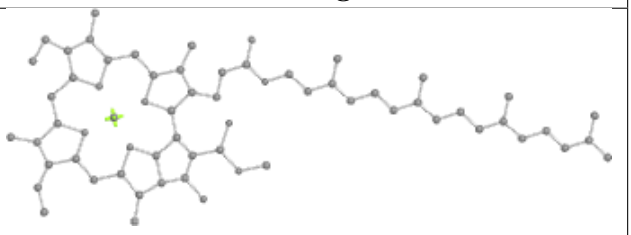
Bond lengths



Bond angles

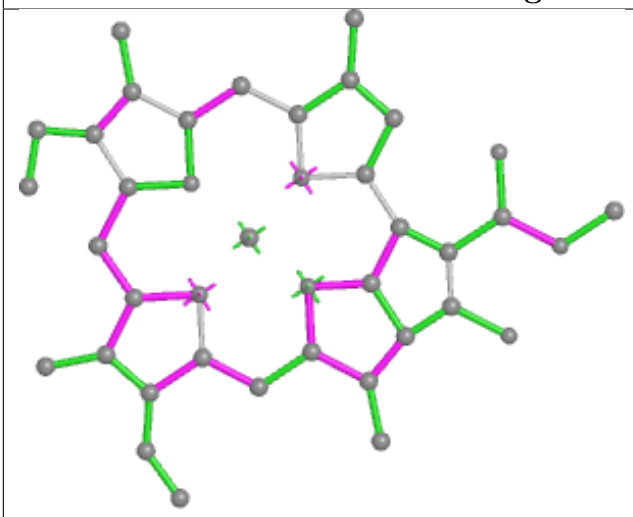


Torsions



Rings

Ligand CLA C 318



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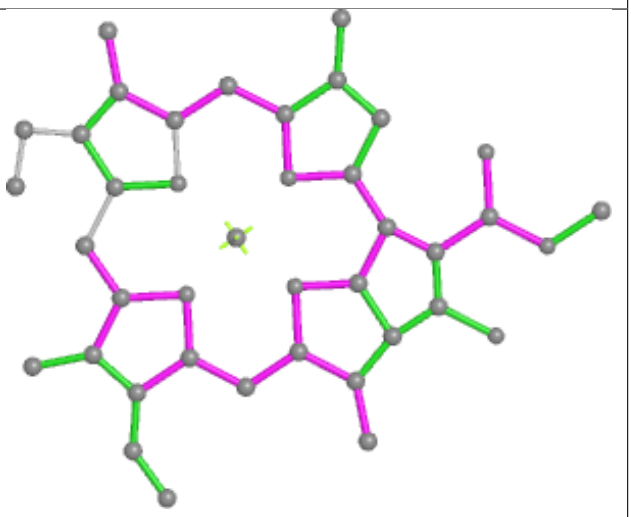
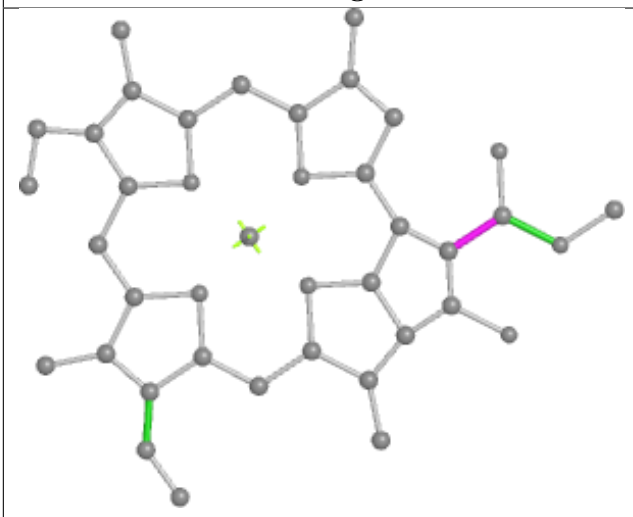
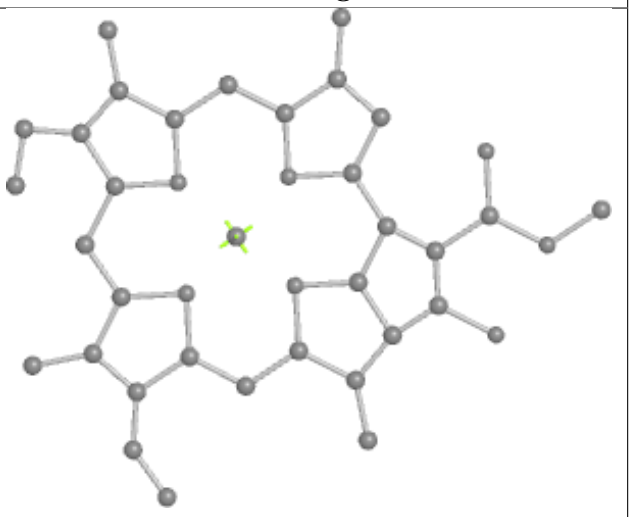


Bond angles

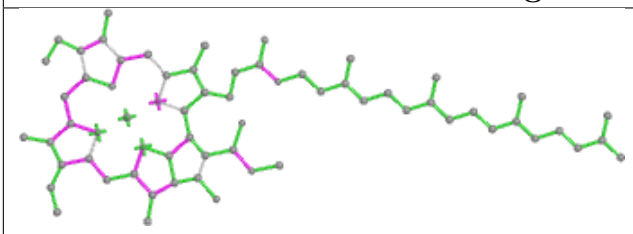


Torsions



Rings

Ligand CLA B 307



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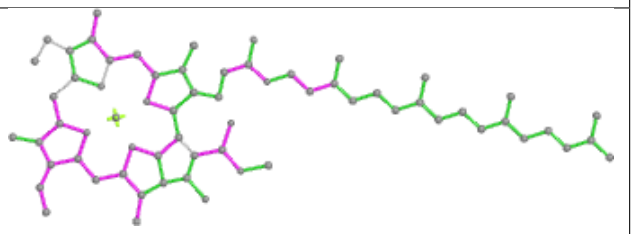
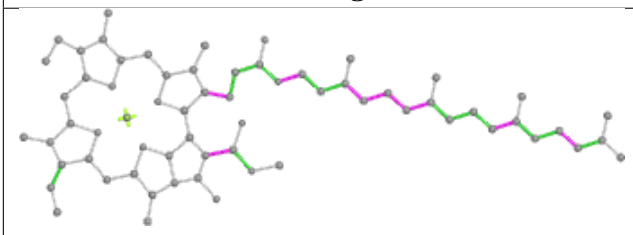
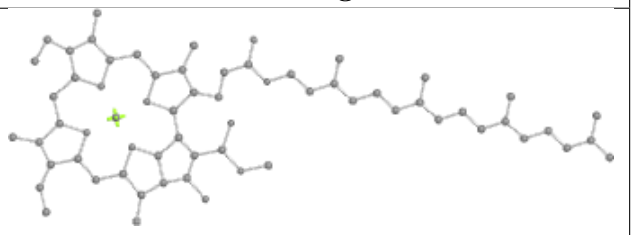


Bond angles

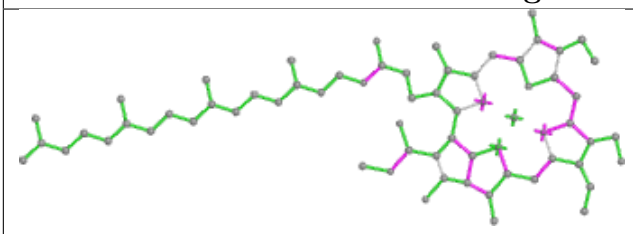


Torsions

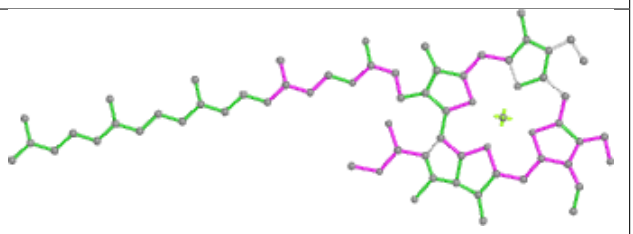


Rings

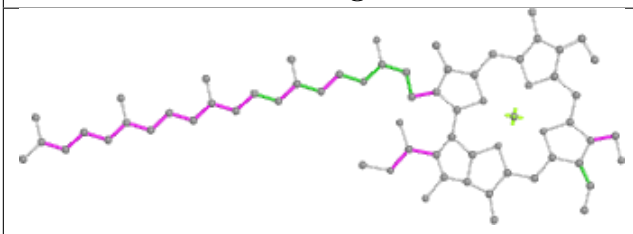
Ligand CHL C 305



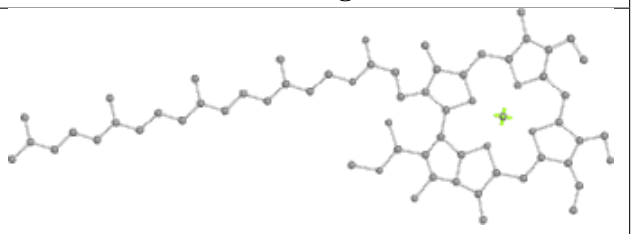
Bond lengths



Bond angles

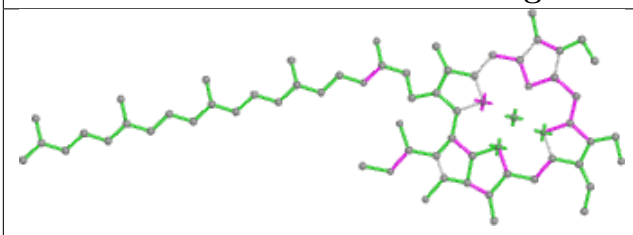


Torsions

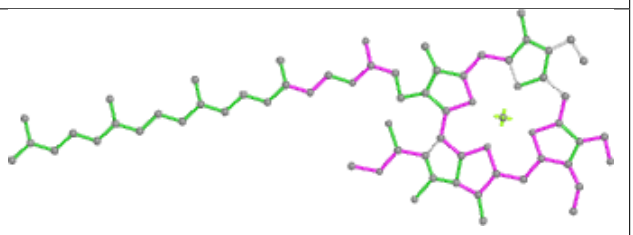


Rings

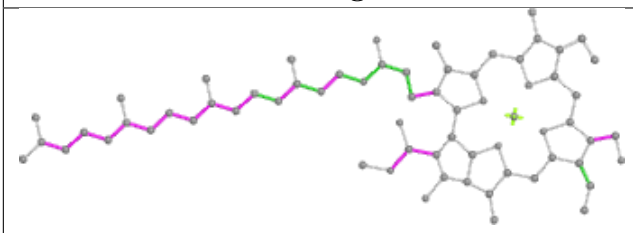
Ligand CHL B 305



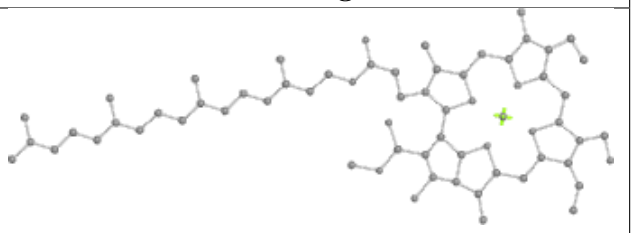
Bond lengths



Bond angles

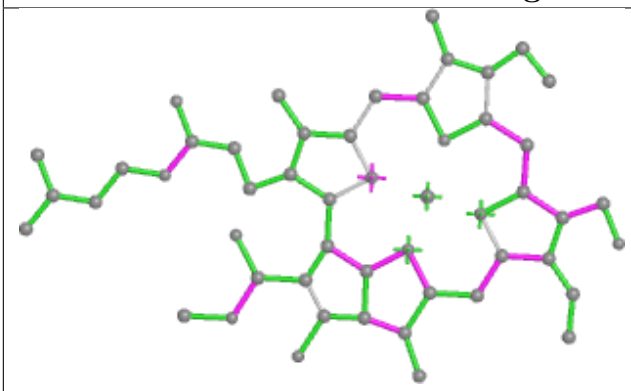


Torsions

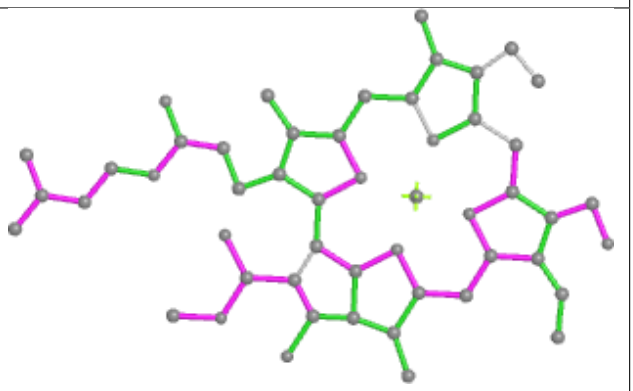


Rings

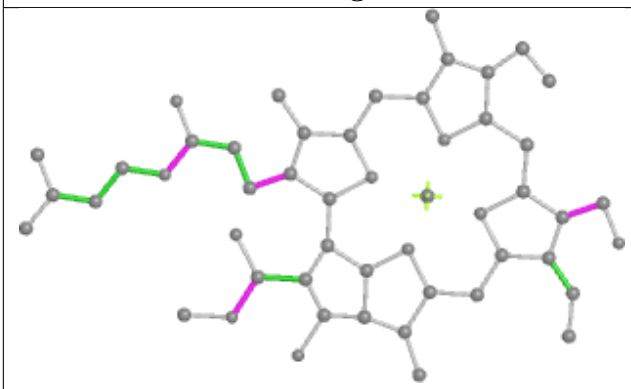
Ligand CHL A 310



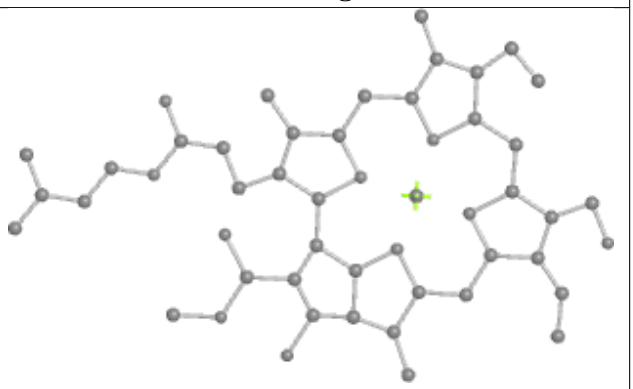
Bond lengths



Bond angles

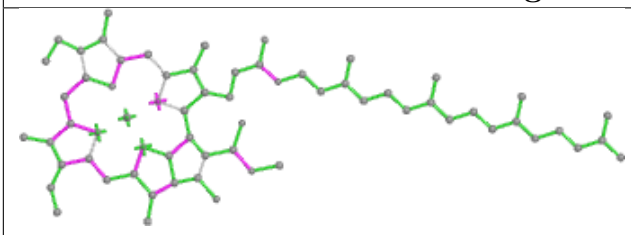


Torsions

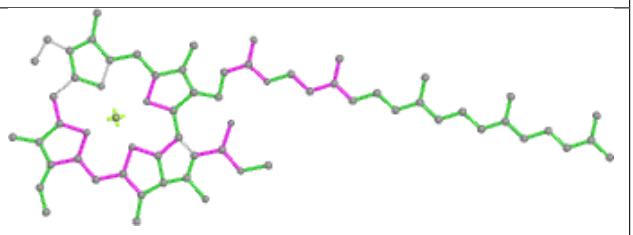


Rings

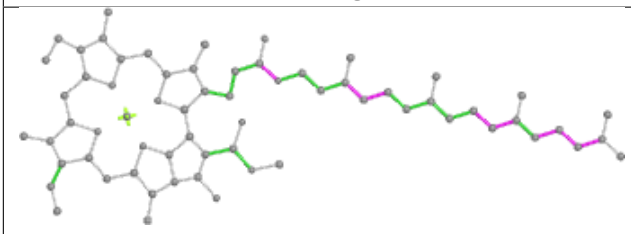
Ligand CLA B 316



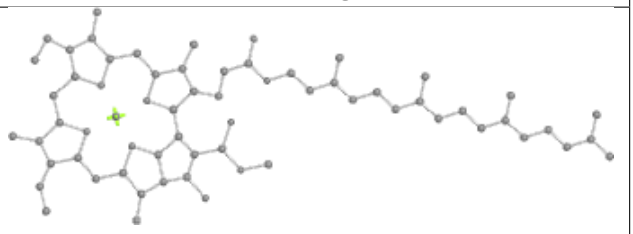
Bond lengths



Bond angles

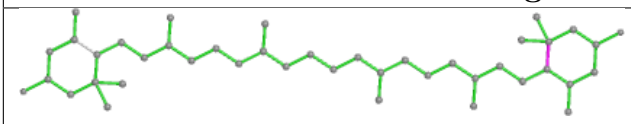


Torsions



Rings

Ligand LUT C 302



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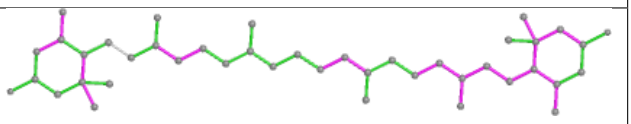
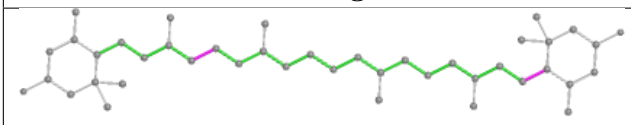


Bond angles



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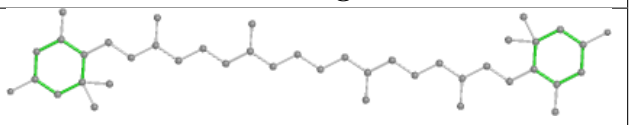
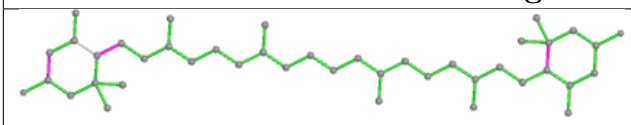


Rings

Ligand LUT B 302



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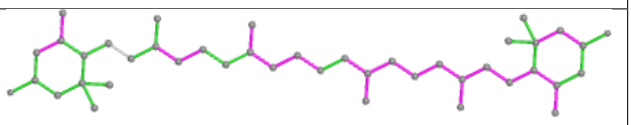
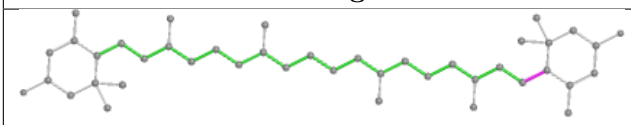


Bond angles



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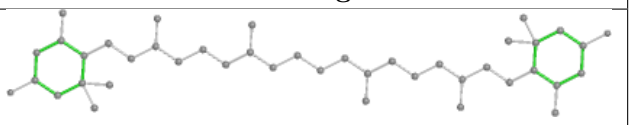
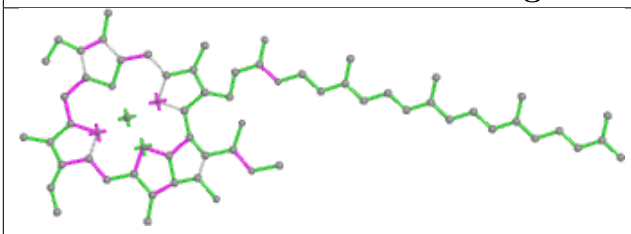


Rings

Ligand CLA A 315



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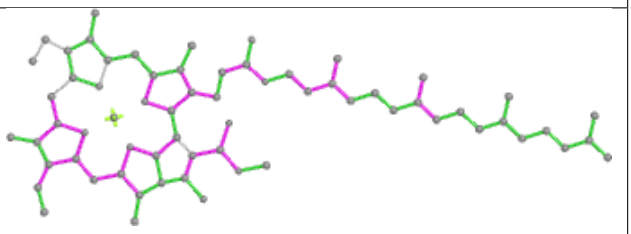
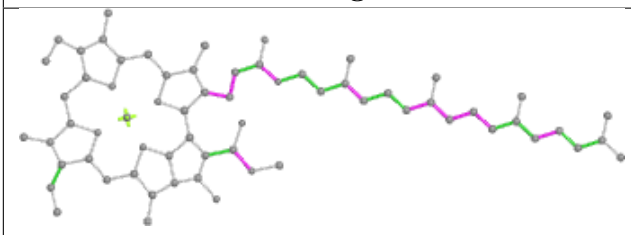


Bond angles



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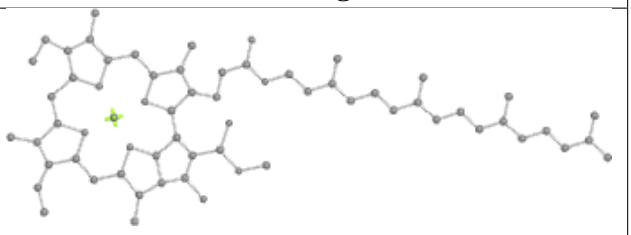
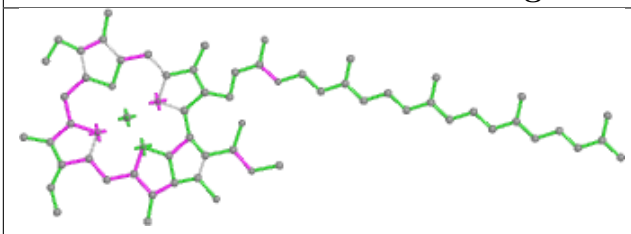


Rings

Ligand CLA C 317



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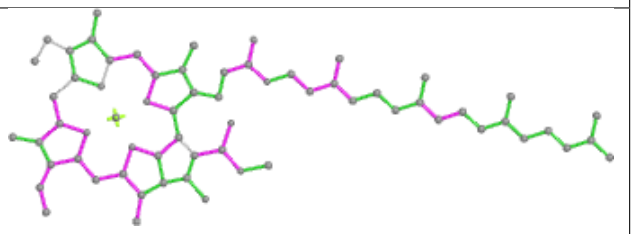
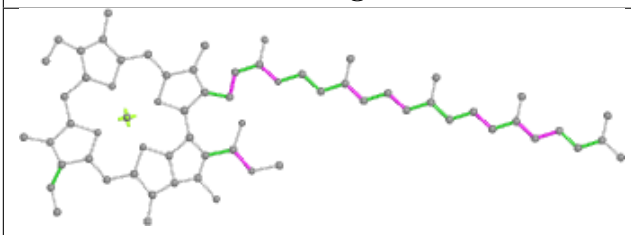


Bond angles



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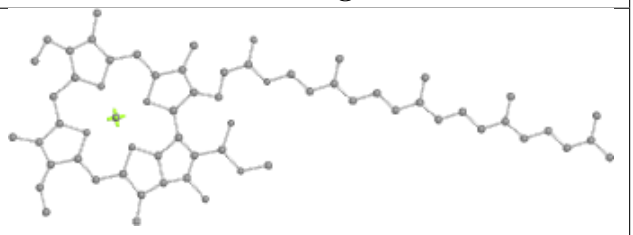
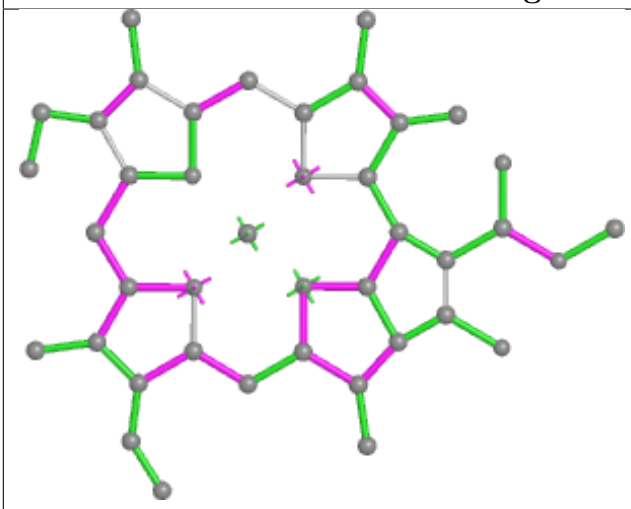


Rings

Ligand CLA A 318



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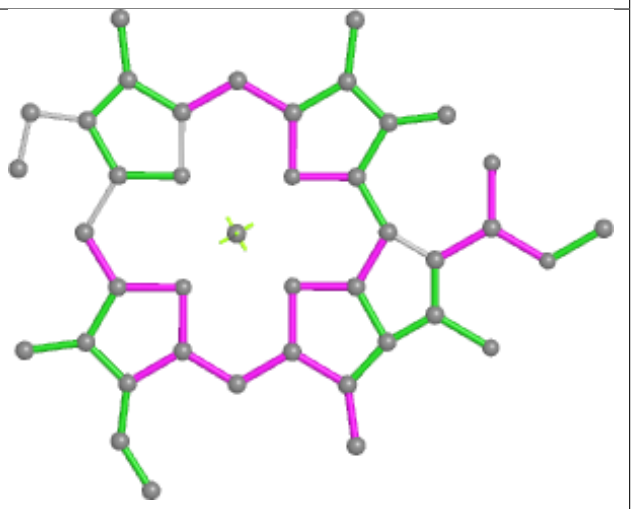
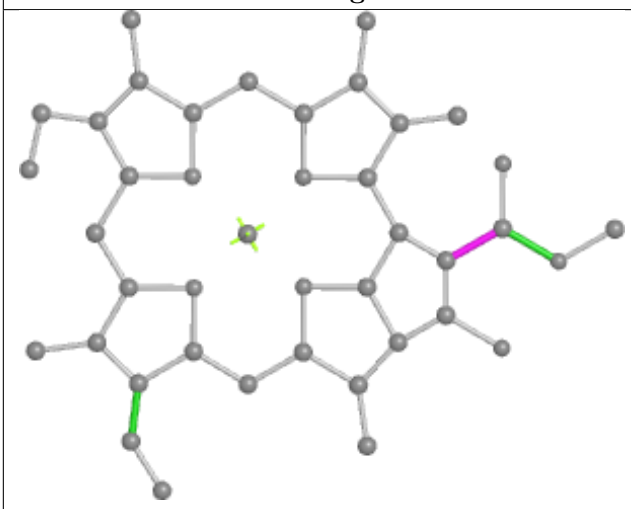


Bond angles



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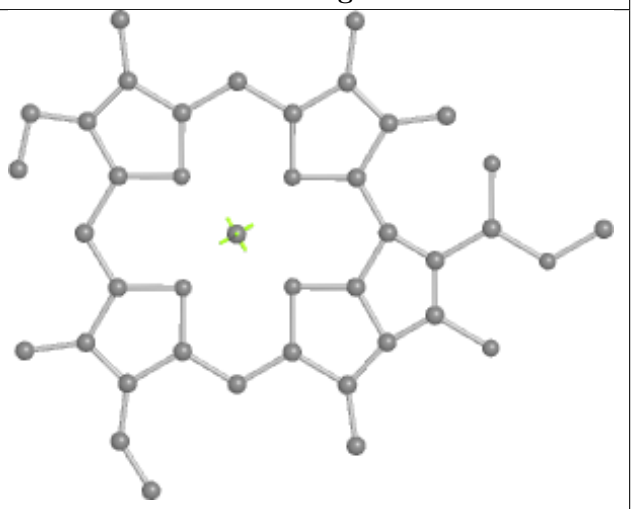
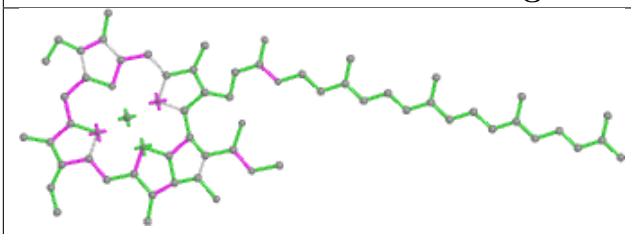


Rings

Ligand CLA A 307



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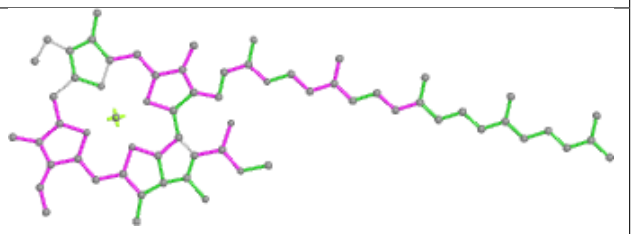
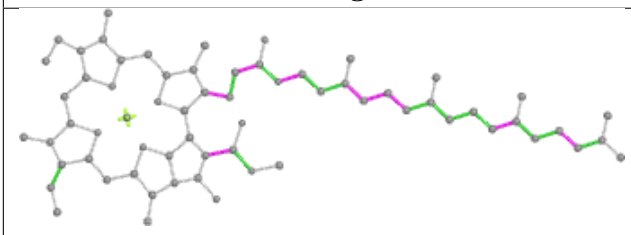
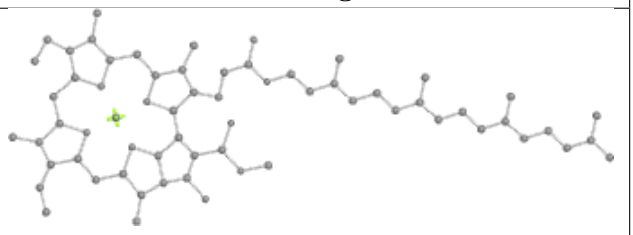


Bond angles

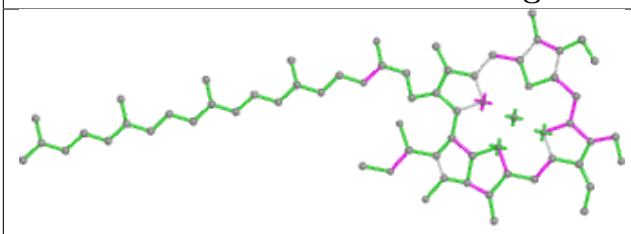


Torsions



Rings

Ligand CHL A 305



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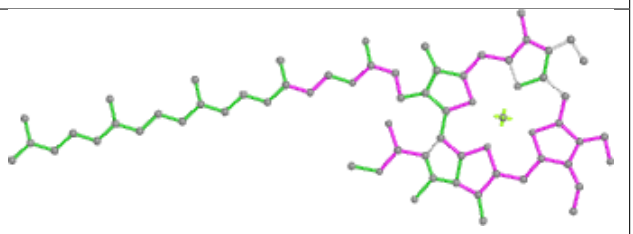
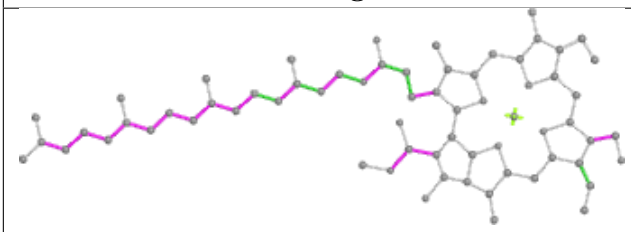


Bond angles



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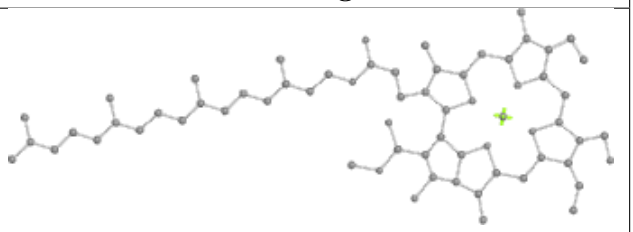
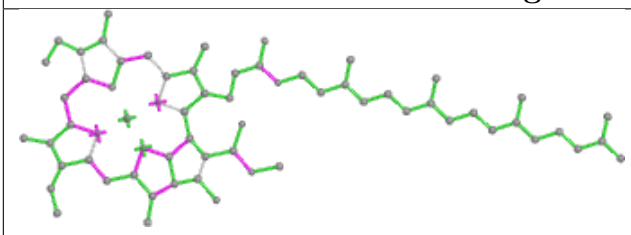


Rings

Ligand CLA A 316



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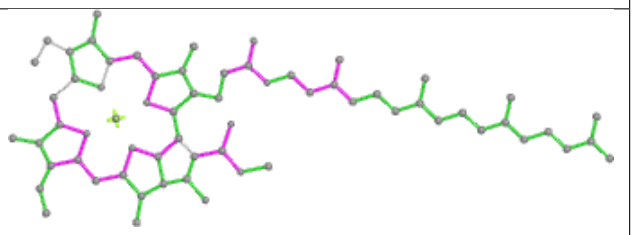
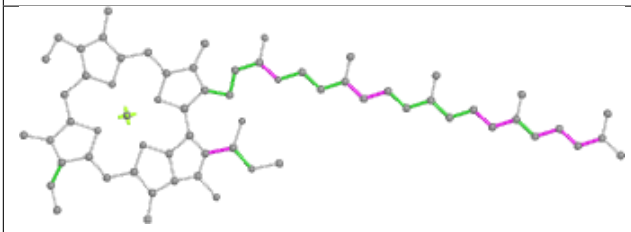
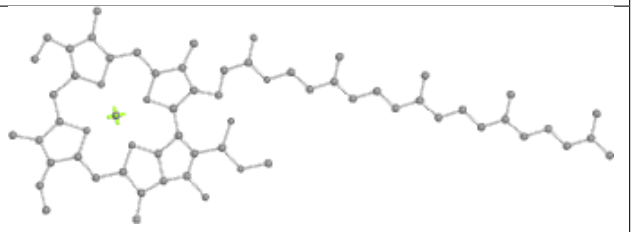


Bond angles

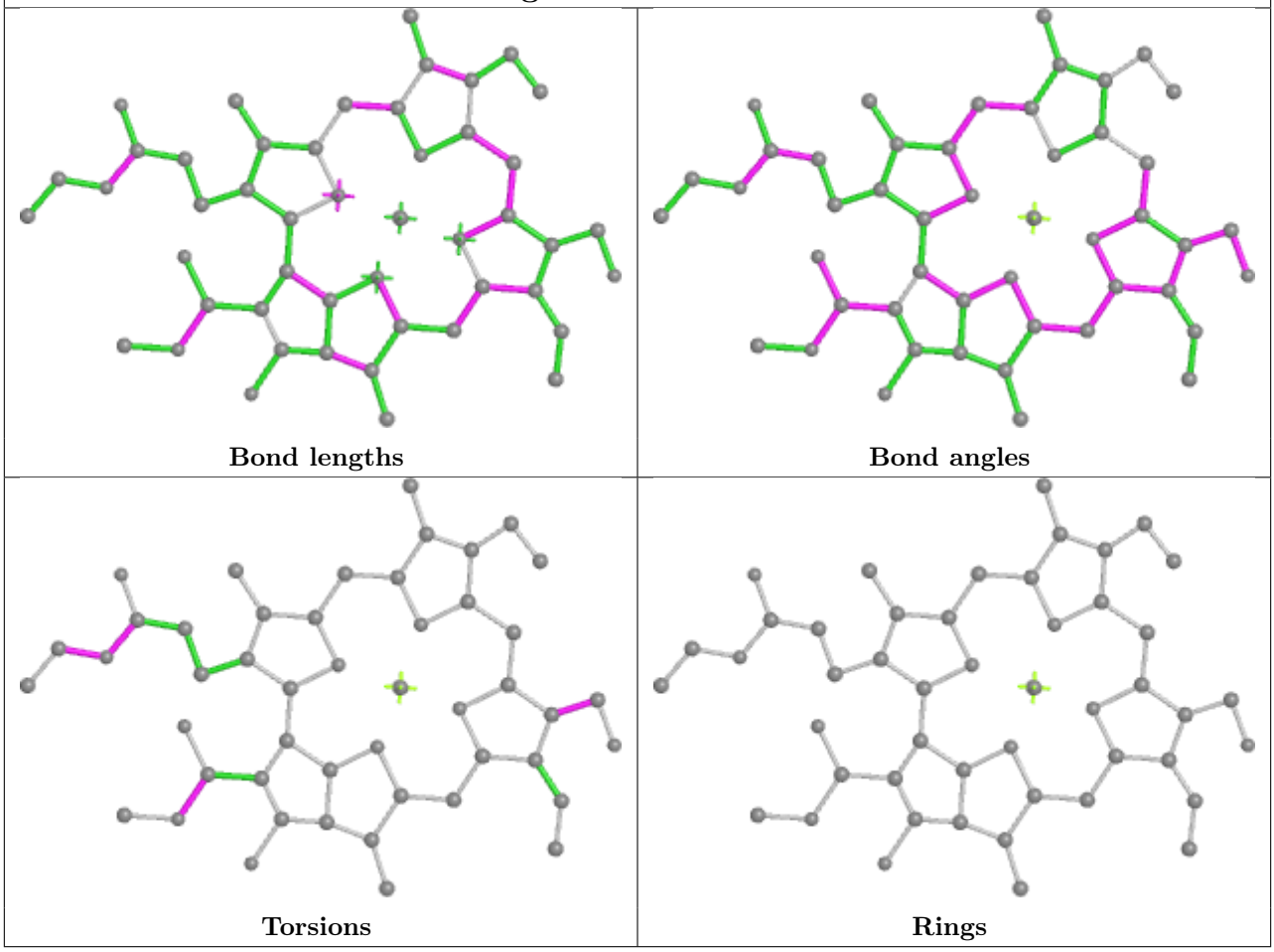


Torsions

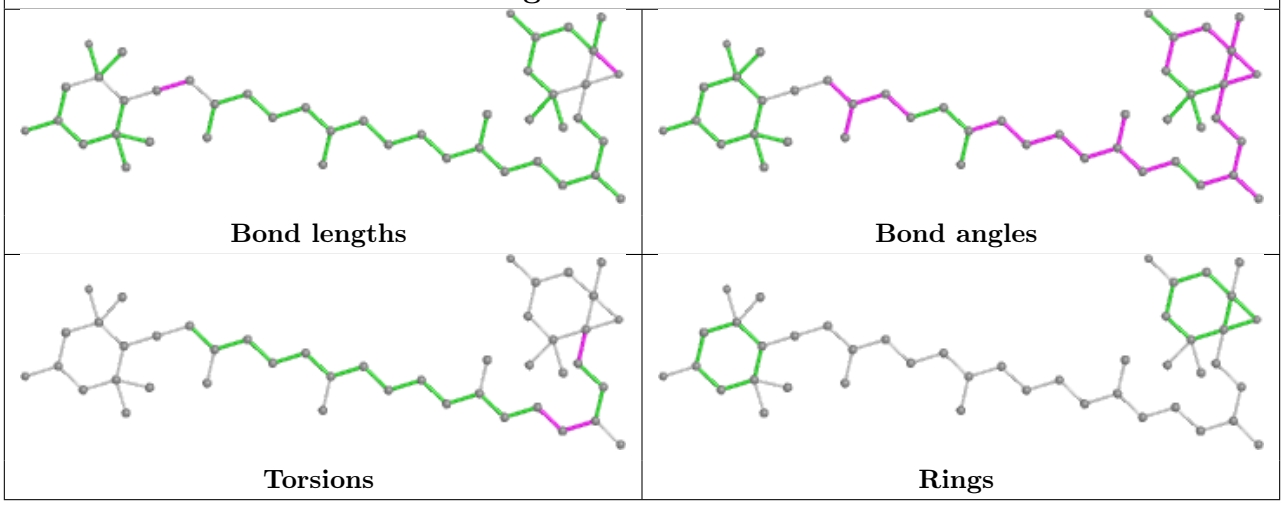


Rings

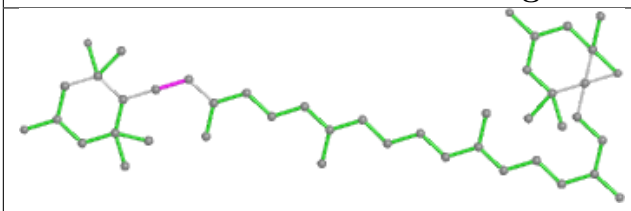
Ligand CHL B 309



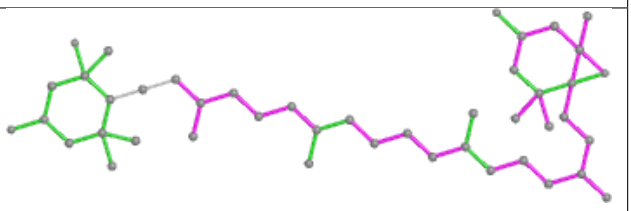
Ligand NEX B 303



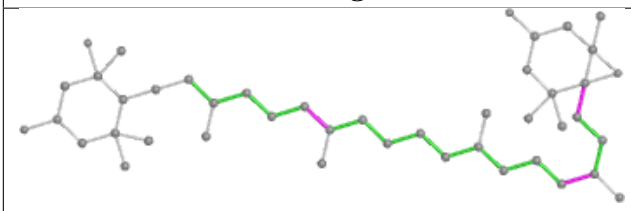
Ligand NEX C 303



Bond lengths



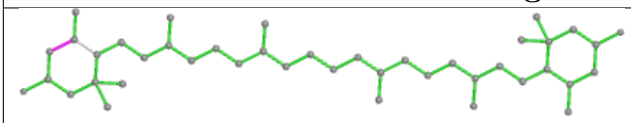
Bond angles



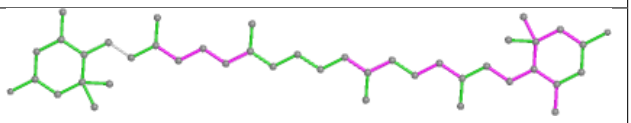
Torsions

Rings

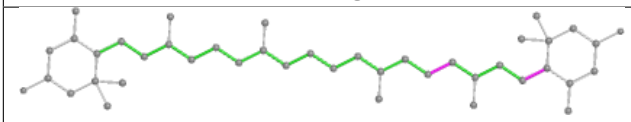
Ligand LUT A 302



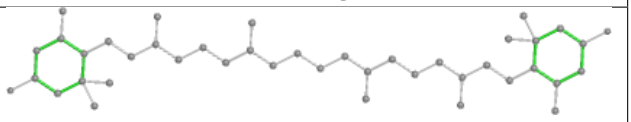
Bond lengths



Bond angles

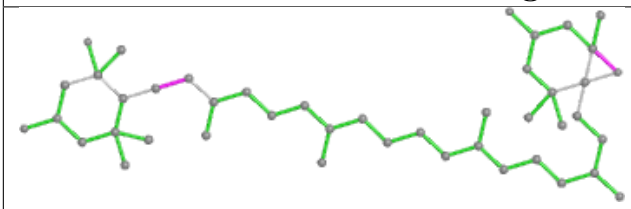


Torsions



Rings

Ligand NEX A 303



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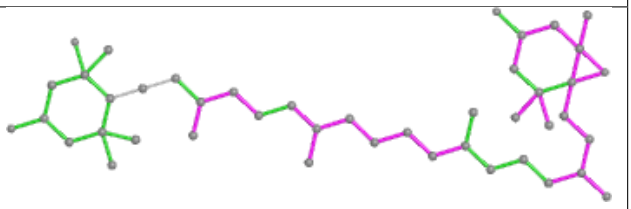
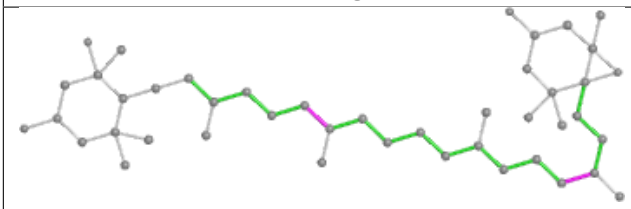


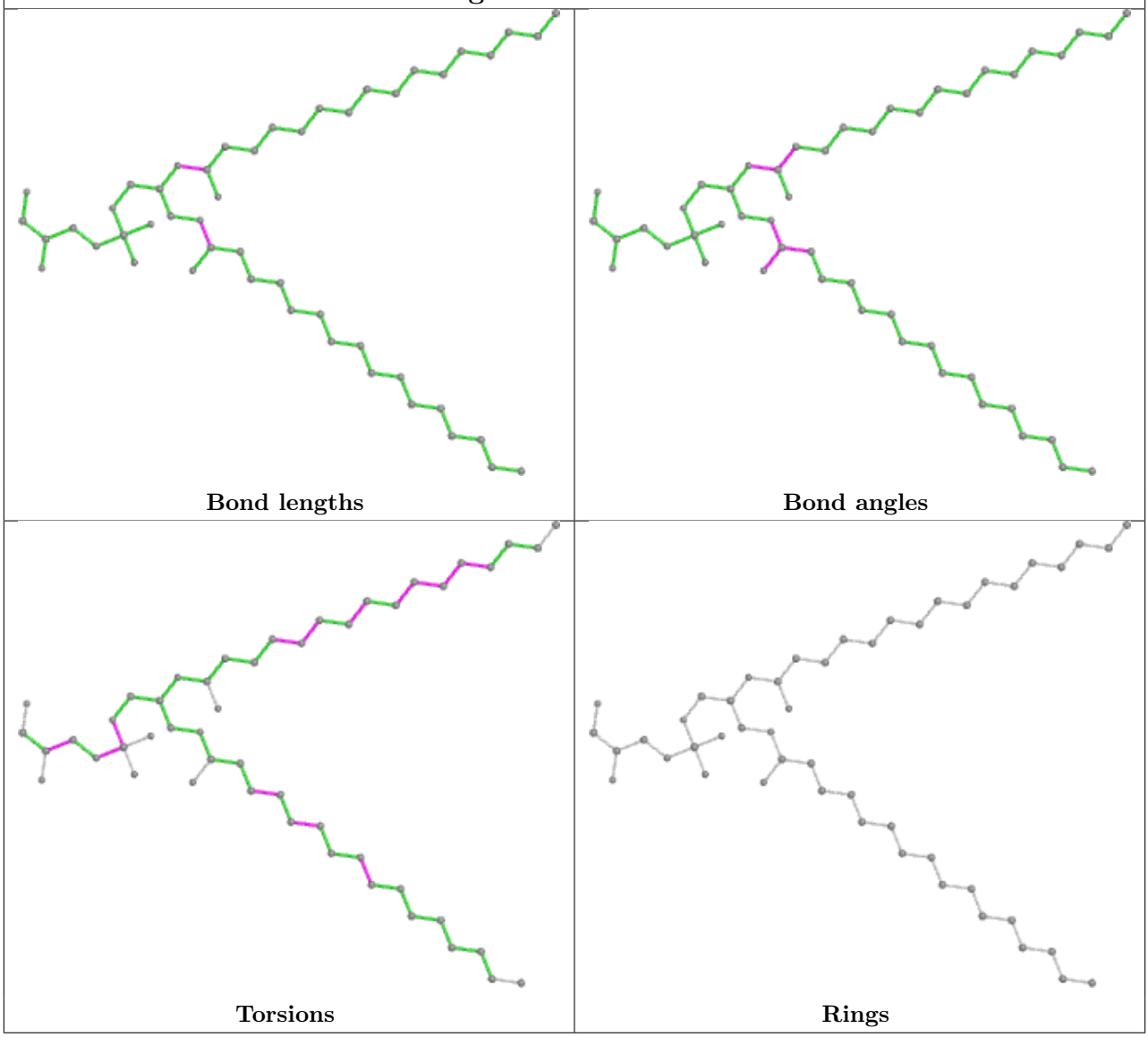
Bond angles



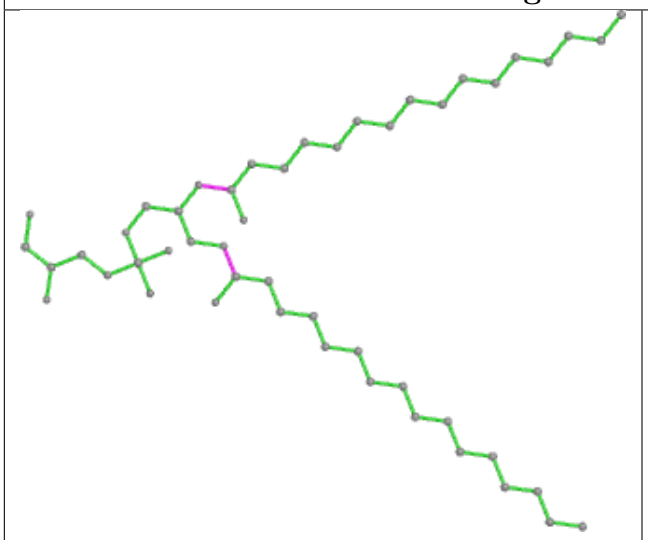
Torsions

Rings

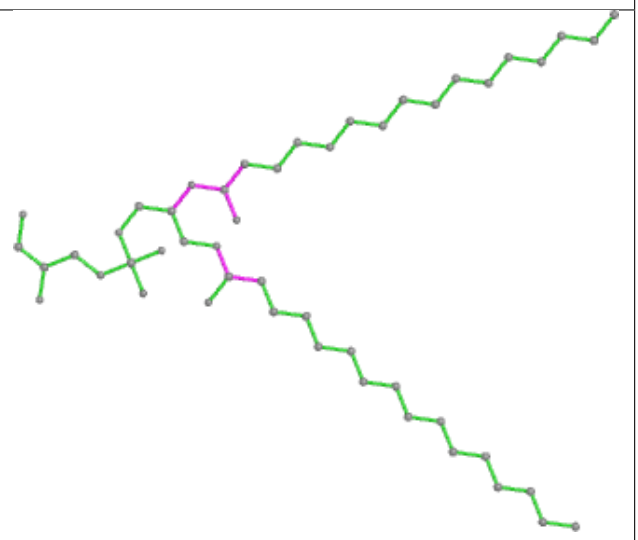
Ligand LHG B 304



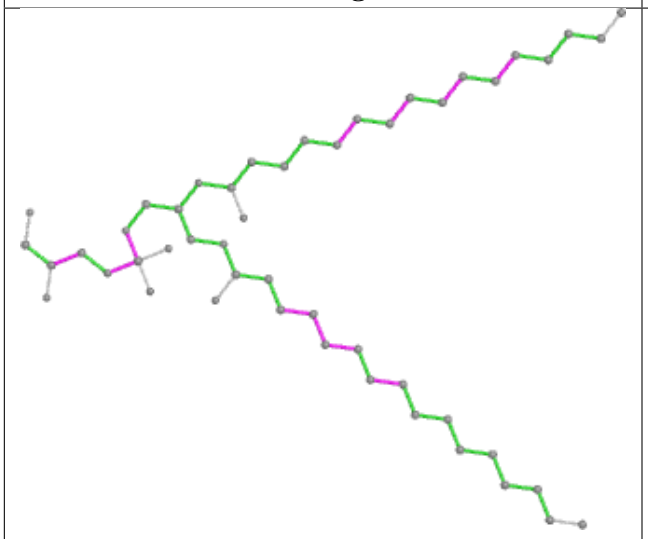
Ligand LHG C 304



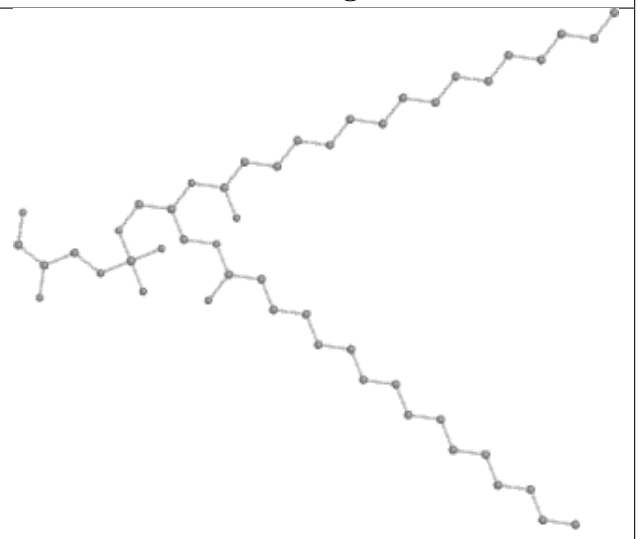
Bond lengths



Bond angles

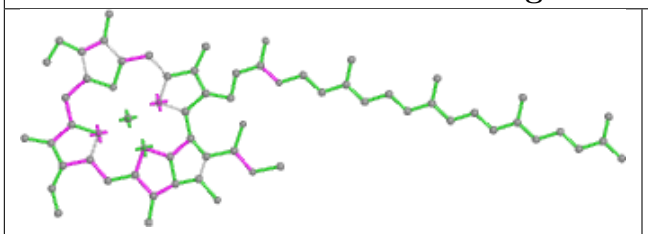


Torsions

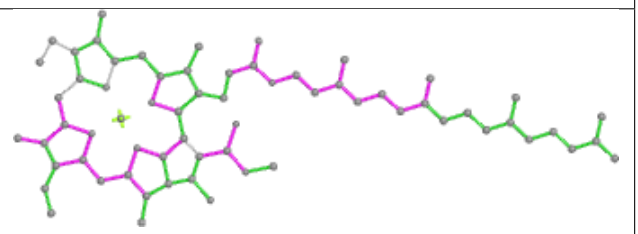


Rings

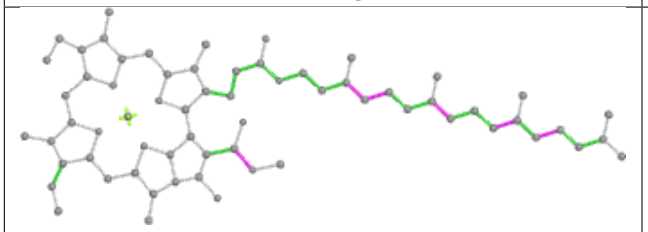
Ligand CLA C 306



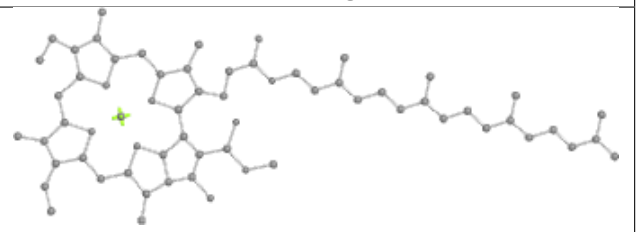
Bond lengths



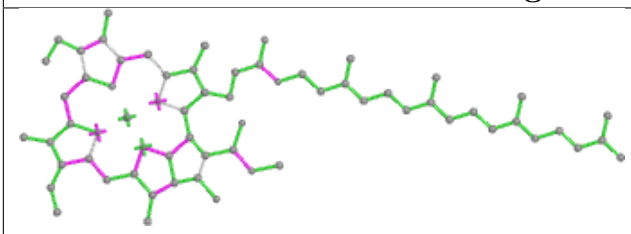
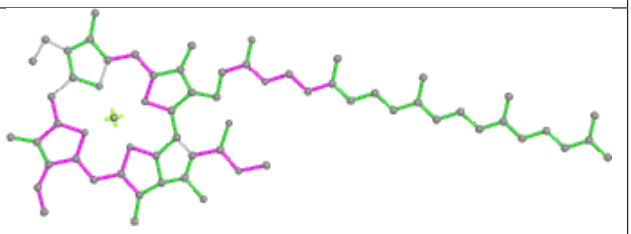
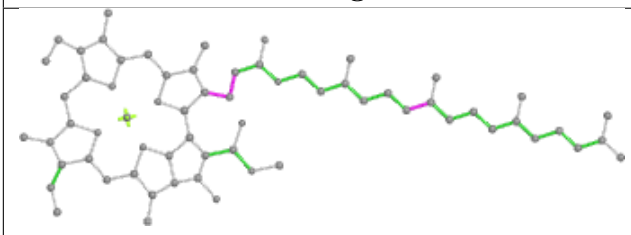
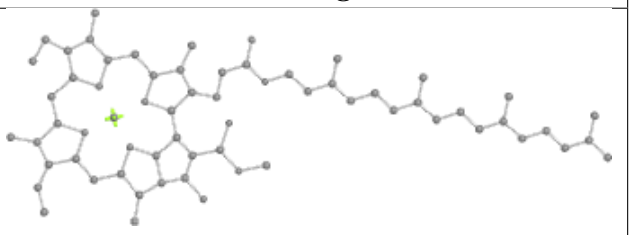
Bond angles

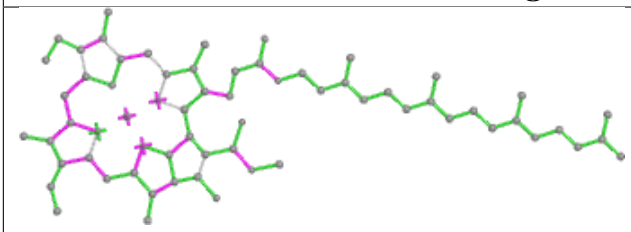
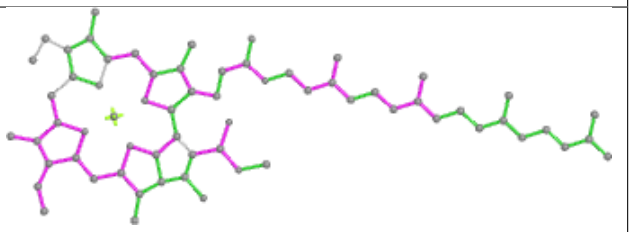
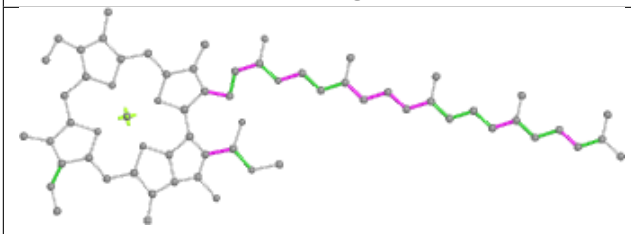
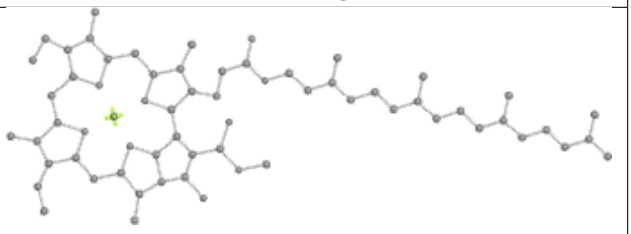


Torsions

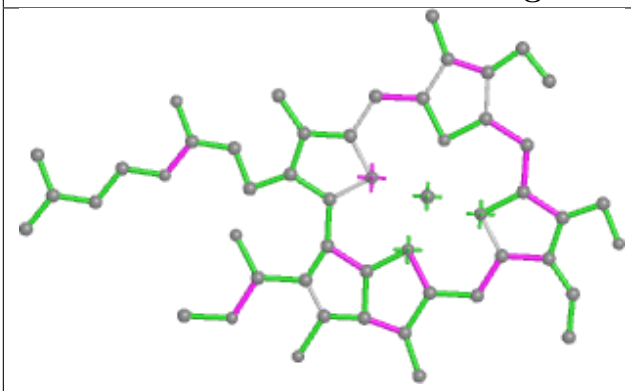


Rings

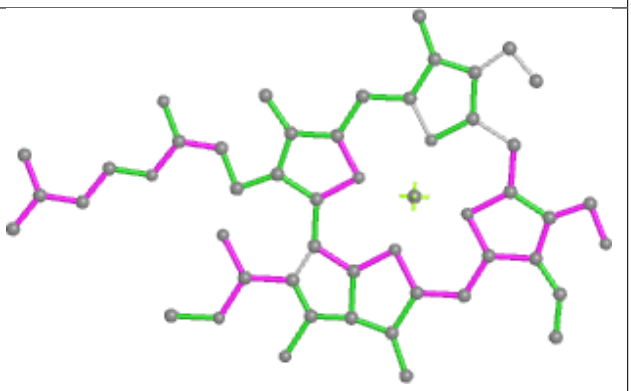
Ligand CLA B 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

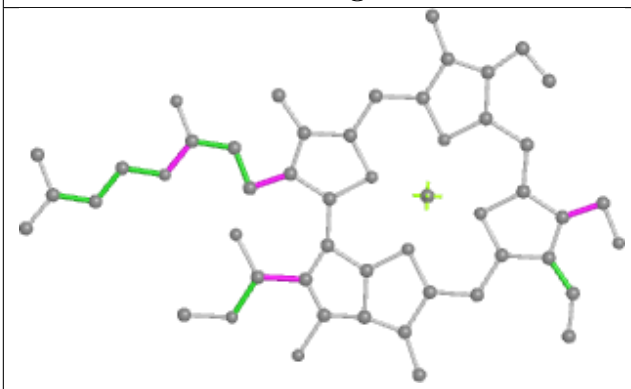
Ligand CHL B 310



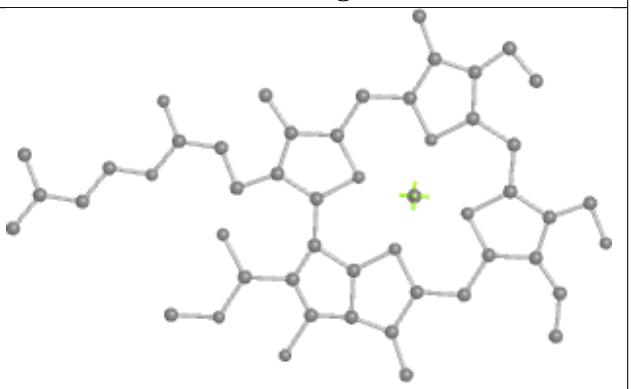
Bond lengths



Bond angles

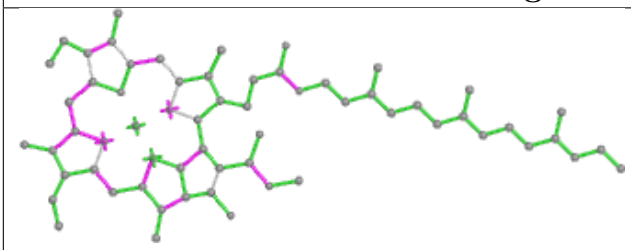


Torsions

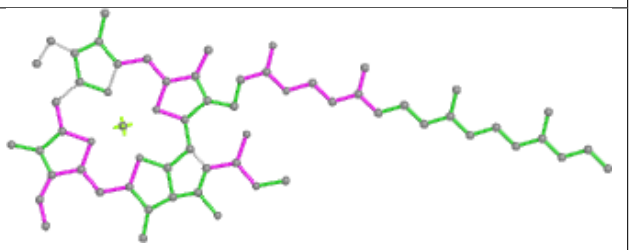


Rings

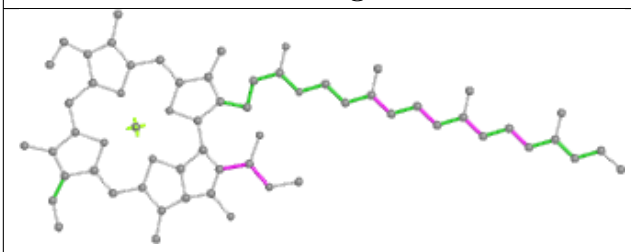
Ligand CLA C 308



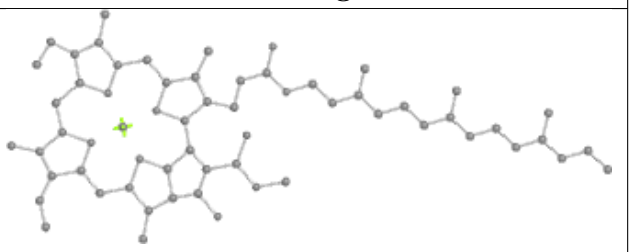
Bond lengths



Bond angles

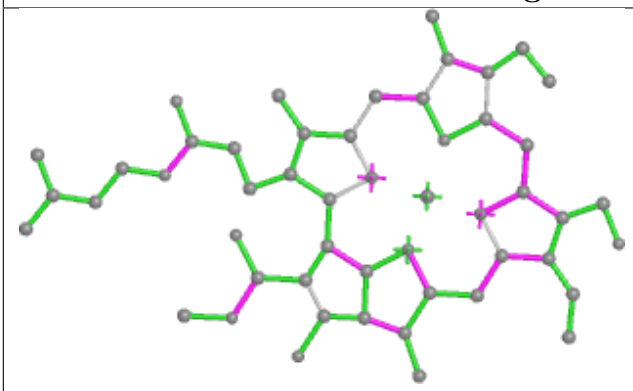


Torsions

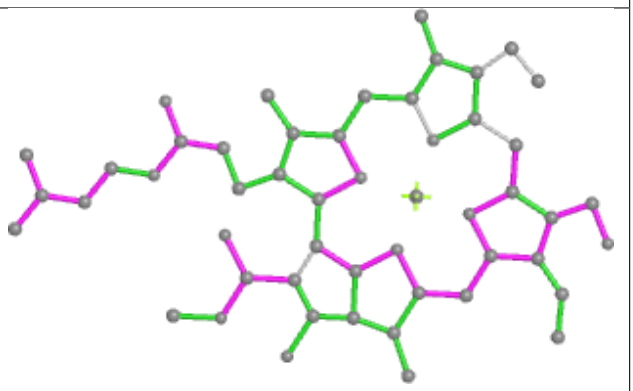


Rings

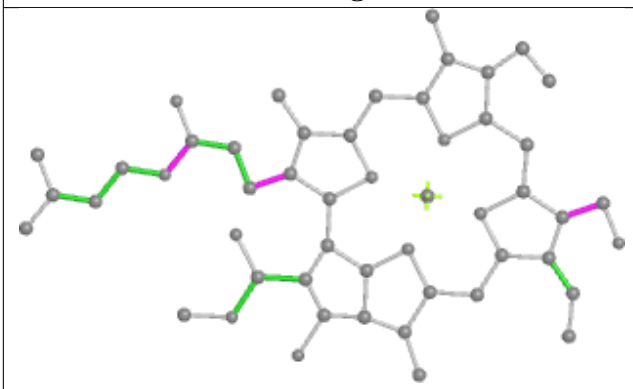
Ligand CHL C 310



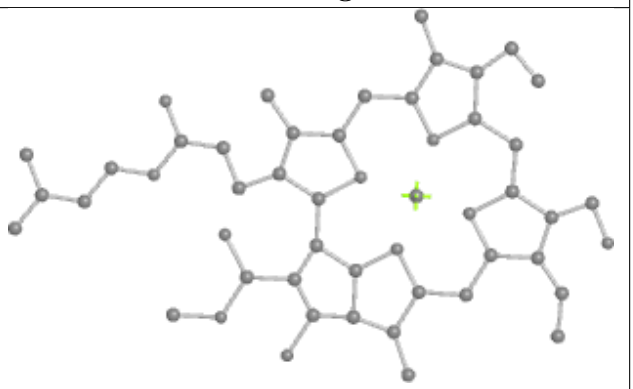
Bond lengths



Bond angles

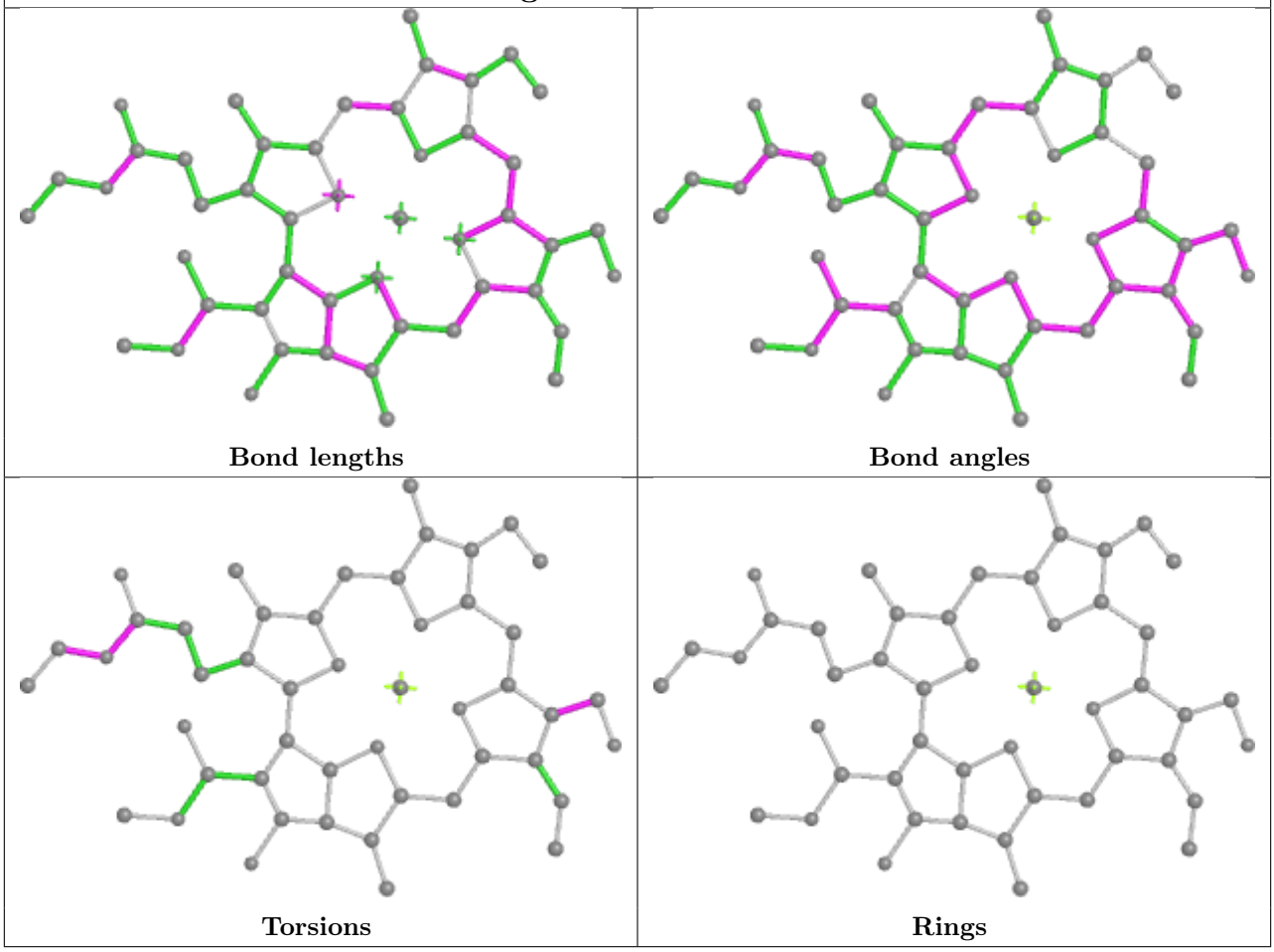


Torsions

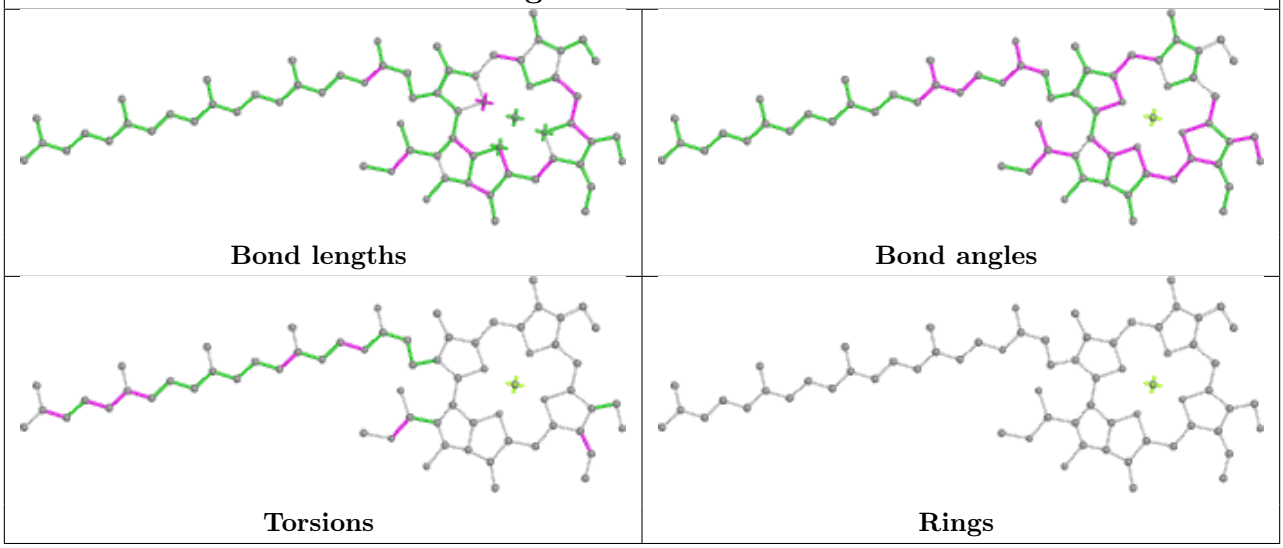


Rings

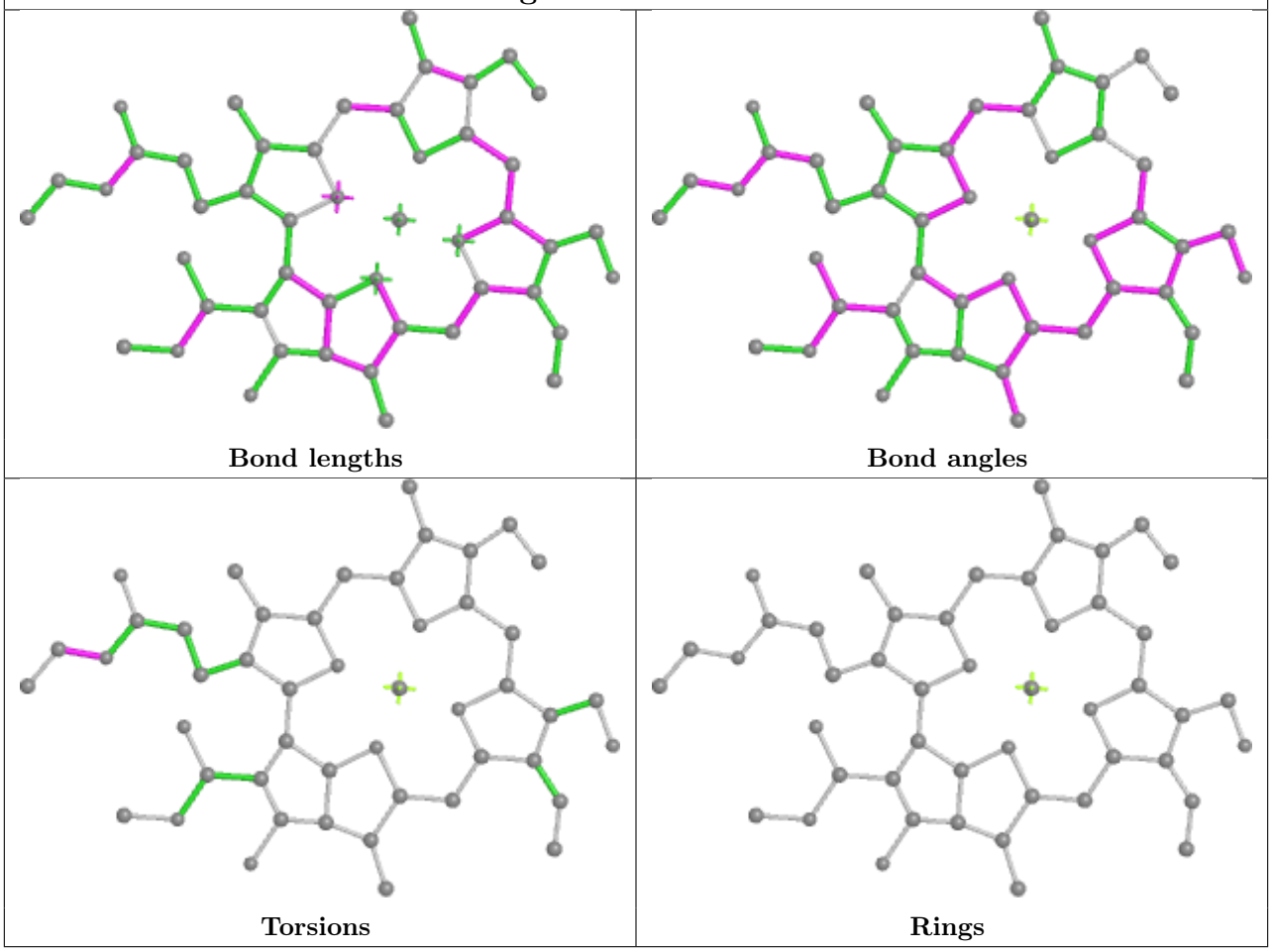
Ligand CHL A 309



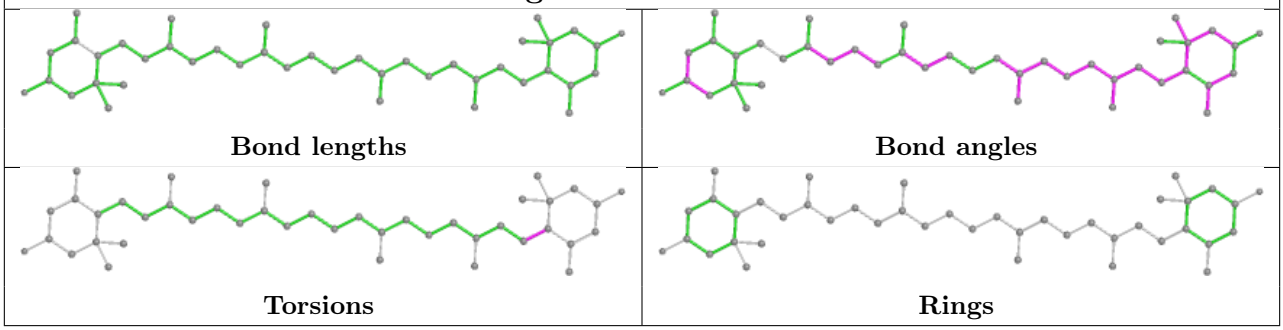
Ligand CHL B 313



Ligand CHL C 309



Ligand LUT B 301



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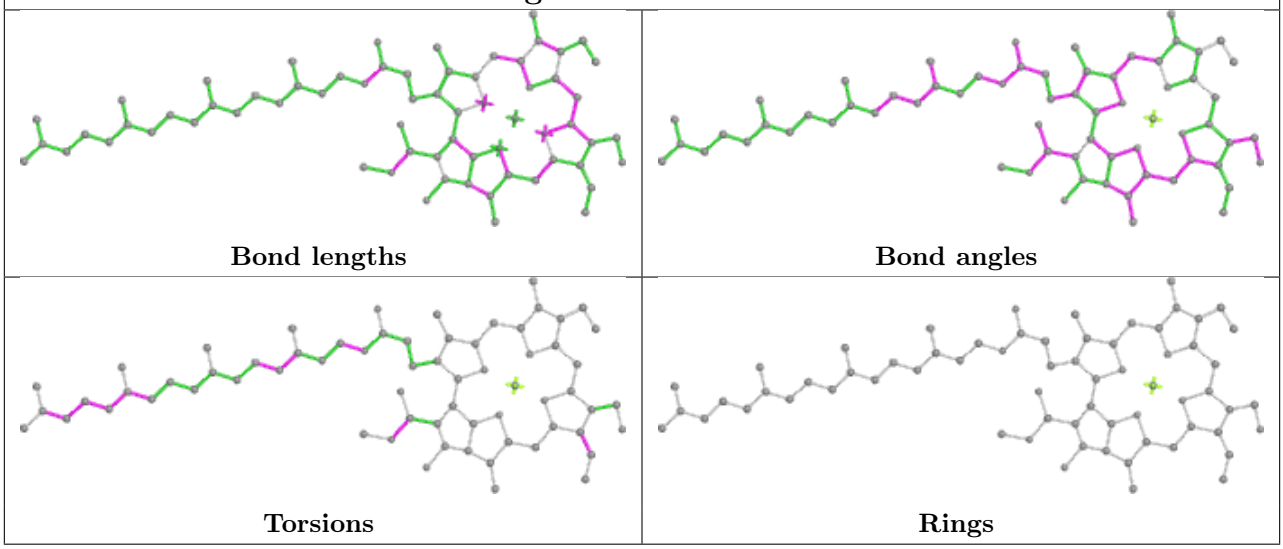
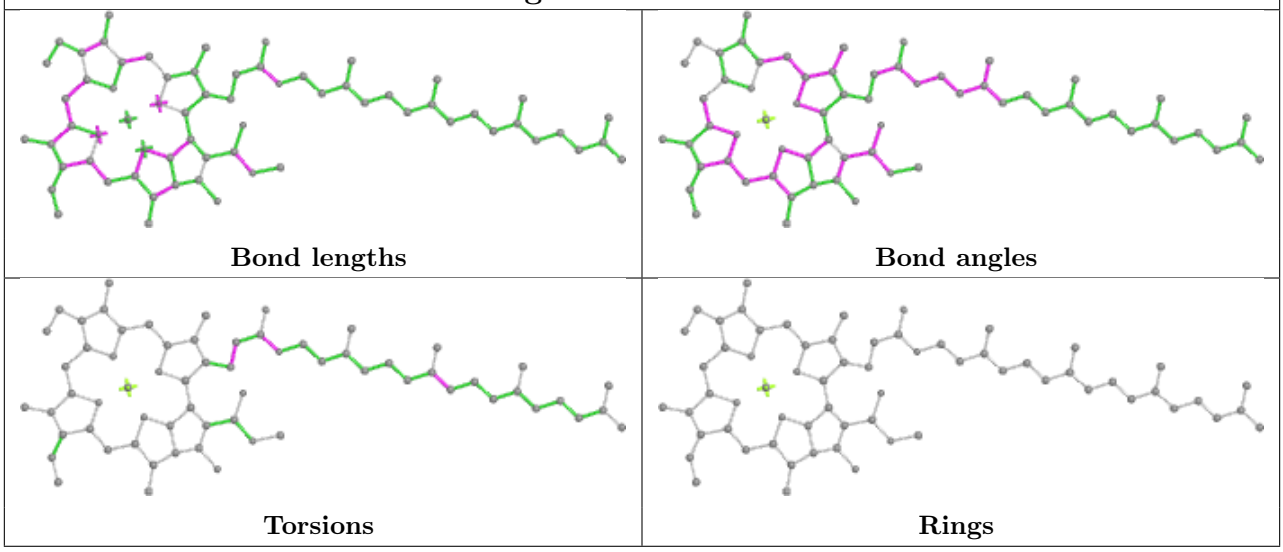
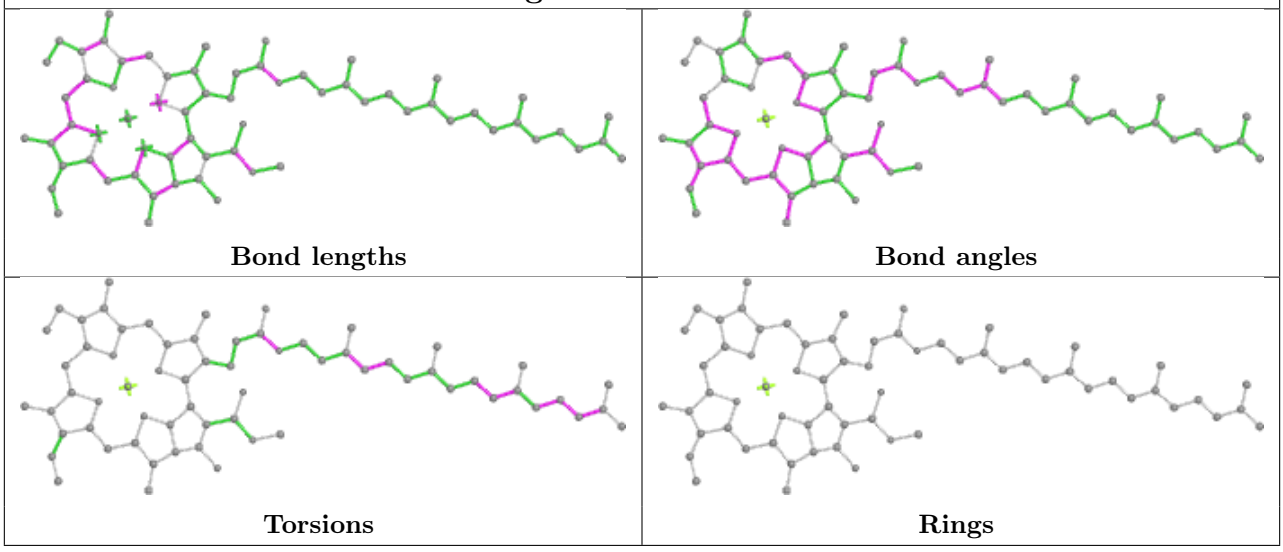


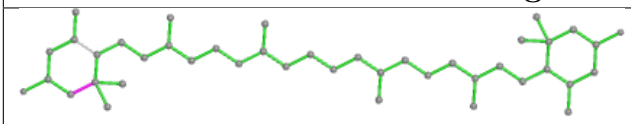
Ligand CLA A 314



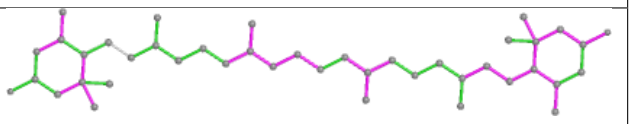
Ligand CLA C 316



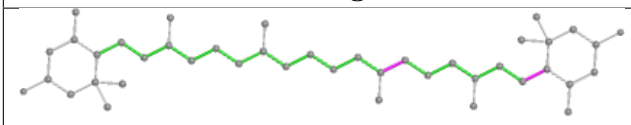
Ligand LUT C 301



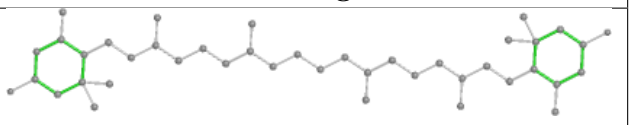
Bond lengths



Bond angles

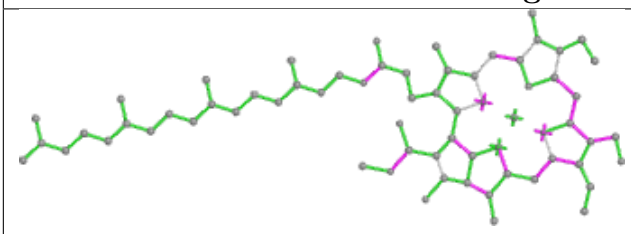


Torsions

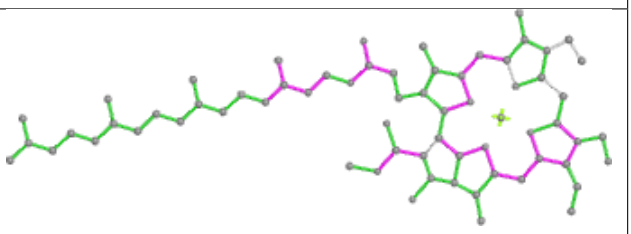


Rings

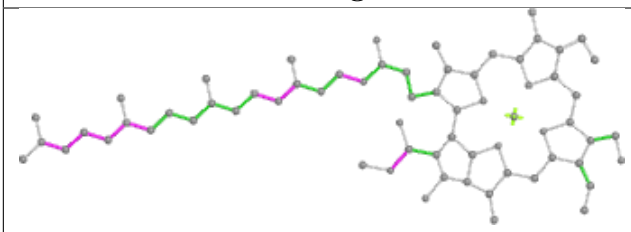
Ligand CHL A 313



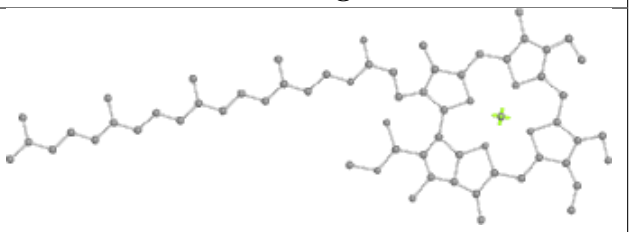
Bond lengths



Bond angles

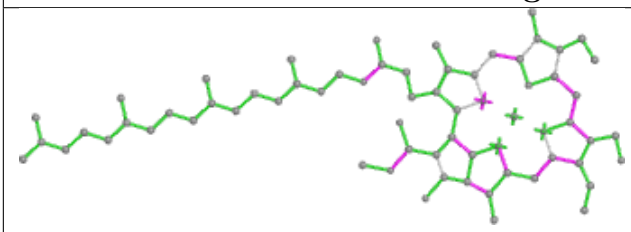


Torsions

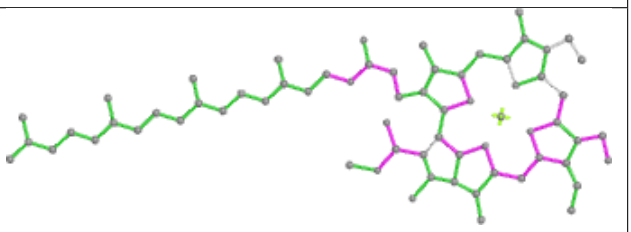


Rings

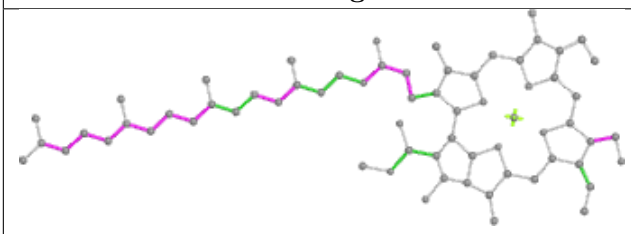
Ligand CHL A 311



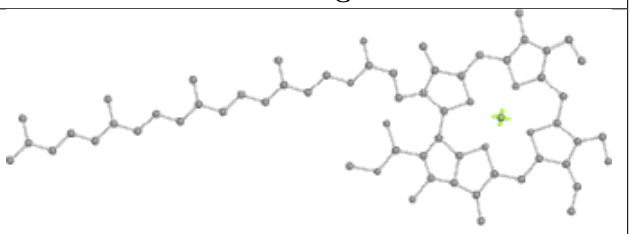
Bond lengths



Bond angles

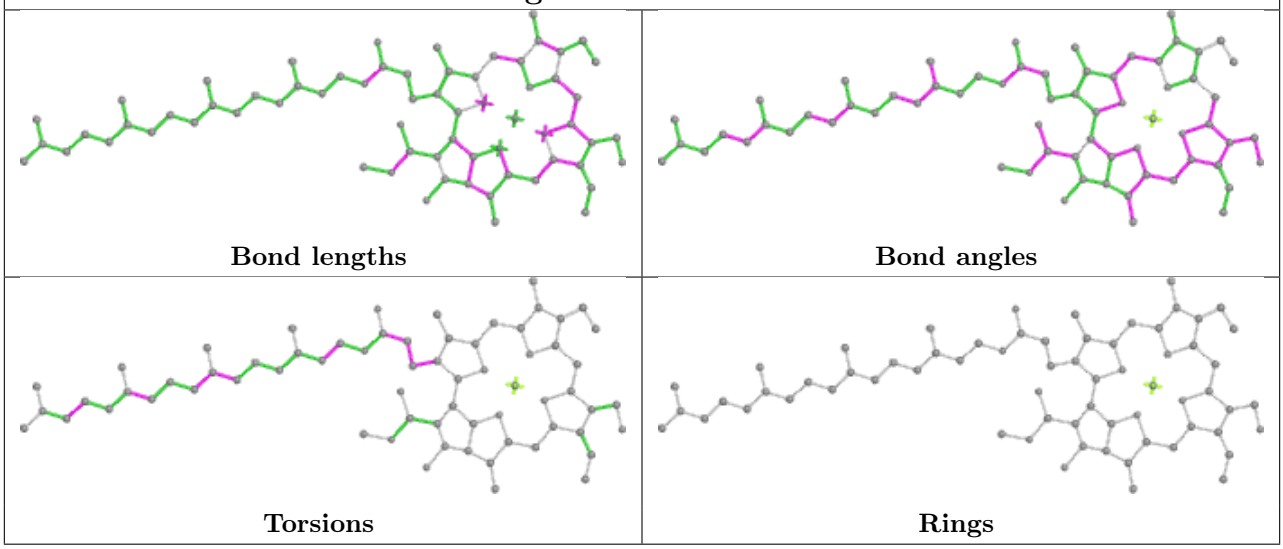


Torsions

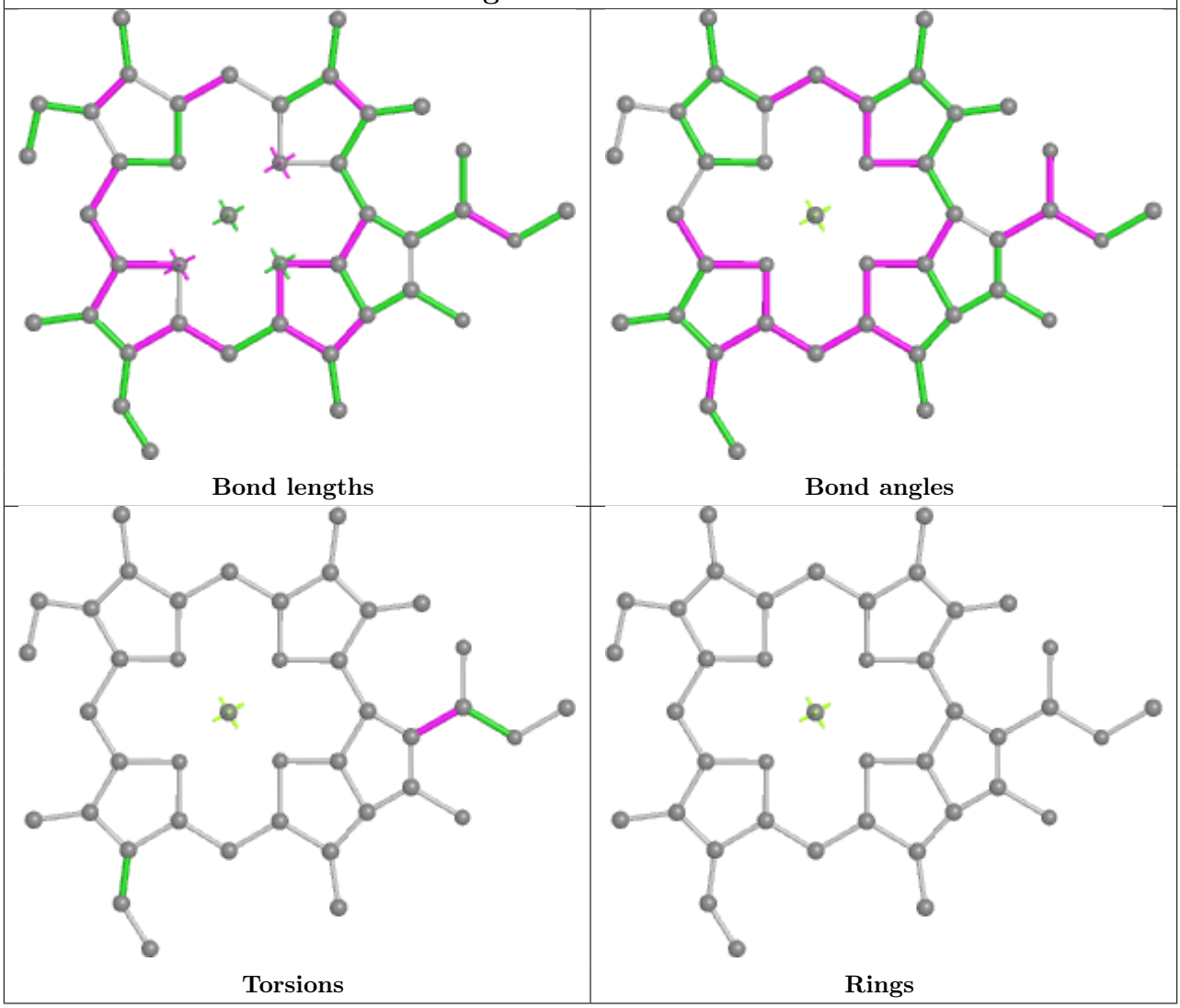


Rings

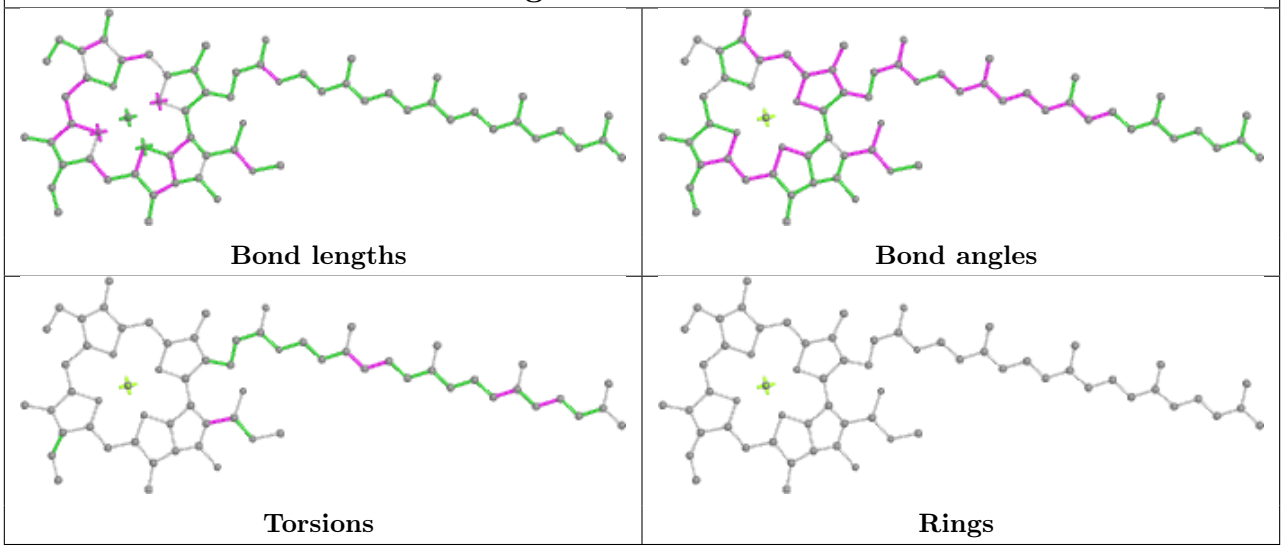
Ligand CHL B 312



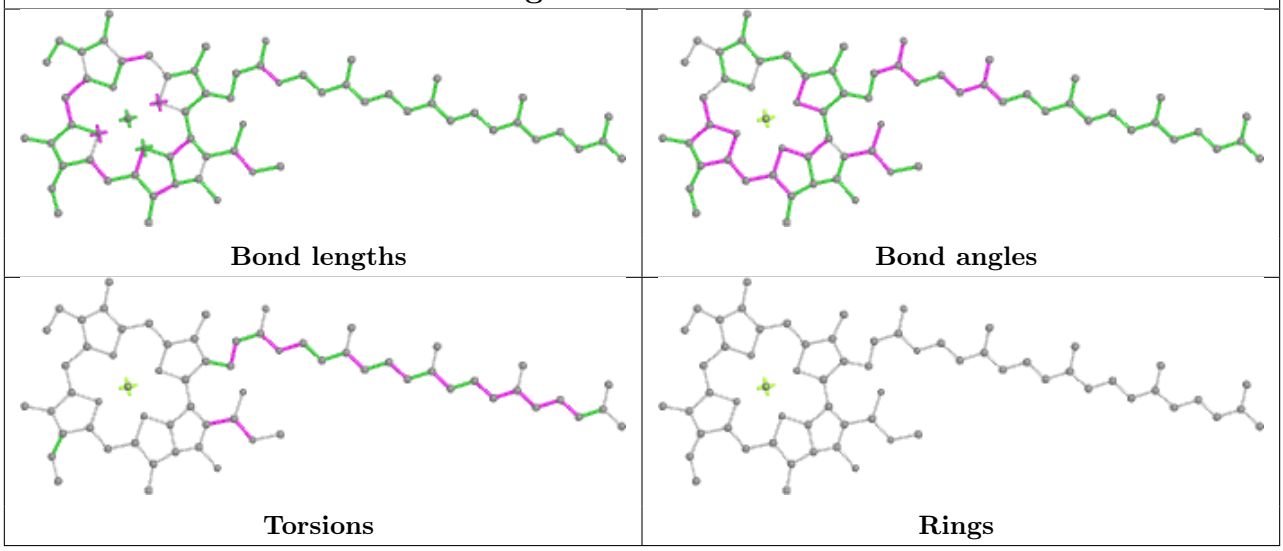
Ligand CLA B 318



Ligand CLA B 306



Ligand CLA B 317



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	208/224 (92%)	0.01	14 (6%)	17	13	6, 39, 77, 97	0
1	B	208/224 (92%)	-0.17	7 (3%)	45	38	8, 34, 67, 94	0
1	C	208/224 (92%)	-0.20	10 (4%)	30	24	6, 33, 69, 107	0
All	All	624/672 (92%)	-0.12	31 (4%)	28	23	6, 35, 70, 107	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	GLY	4.5
1	C	217	VAL	4.5
1	B	89	GLY	4.5
1	B	88	ASN	4.4
1	A	213	LEU	4.2
1	A	88	ASN	3.9
1	A	214	ALA	3.8
1	C	213	LEU	3.3
1	C	214	ALA	3.3
1	C	147	PRO	3.1
1	C	219	ASN	3.1
1	B	214	ALA	3.1
1	C	218	ASN	3.0
1	A	216	PRO	3.0
1	B	152	VAL	2.9
1	A	81	PHE	2.8
1	A	212	HIS	2.8
1	A	31	GLU	2.7
1	A	87	ARG	2.6
1	A	168	ASP	2.5
1	B	87	ARG	2.5
1	A	217	VAL	2.3
1	A	218	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	219	ASN	2.3
1	B	117	SER	2.3
1	C	89	GLY	2.1
1	A	210	ALA	2.1
1	B	218	ASN	2.1
1	C	31	GLU	2.1
1	C	20	ASP	2.1
1	C	215	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NA	C	322	1/1	-0.09	0.39	80,80,80,80	1
9	NA	C	320	1/1	0.84	0.21	60,60,60,60	0
6	CLA	A	318	41/65	0.85	0.31	44,79,96,119	0
3	NEX	B	303	44/44	0.88	0.23	26,42,94,97	0
6	CLA	B	318	41/65	0.88	0.24	44,76,92,115	0
3	NEX	C	303	44/44	0.91	0.20	14,32,90,92	0
6	CLA	C	318	40/65	0.91	0.23	36,69,91,110	0
9	NA	B	322	1/1	0.91	0.17	47,47,47,47	0
6	CLA	A	315	65/65	0.91	0.21	28,48,76,86	0
3	NEX	A	303	44/44	0.91	0.22	26,39,94,96	0
5	CHL	C	311	66/66	0.92	0.19	11,31,94,115	0
5	CHL	A	311	66/66	0.92	0.18	19,37,99,119	0
8	ZN	A	322	1/1	0.92	0.21	122,122,122,122	0
6	CLA	A	316	65/65	0.92	0.21	30,41,88,98	0
5	CHL	C	309	48/66	0.92	0.22	26,43,97,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CLA	B	315	65/65	0.92	0.23	20,43,74,83	0
6	CLA	C	315	65/65	0.93	0.20	21,45,74,87	0
6	CLA	C	316	65/65	0.93	0.20	22,37,84,97	0
5	CHL	A	305	66/66	0.93	0.18	17,32,86,104	0
5	CHL	B	309	48/66	0.93	0.23	35,52,99,105	0
6	CLA	A	308	62/65	0.93	0.17	20,35,82,89	0
6	CLA	B	316	65/65	0.93	0.25	28,41,89,99	0
5	CHL	B	311	66/66	0.93	0.18	21,38,99,119	0
4	LHG	B	304	49/49	0.94	0.20	14,40,98,107	0
6	CLA	C	308	62/65	0.94	0.16	12,28,80,87	0
6	CLA	C	314	65/65	0.94	0.19	15,27,79,93	0
4	LHG	A	304	49/49	0.94	0.18	19,42,98,108	0
6	CLA	A	317	65/65	0.94	0.18	21,37,90,99	0
5	CHL	C	312	66/66	0.94	0.16	9,32,66,79	0
6	CLA	B	308	62/65	0.94	0.18	21,37,83,91	0
6	CLA	B	314	65/65	0.94	0.20	24,31,80,96	0
5	CHL	A	309	48/66	0.94	0.26	32,48,95,101	0
6	CLA	A	314	65/65	0.94	0.18	23,34,78,93	0
5	CHL	A	310	51/66	0.95	0.16	21,36,94,100	0
5	CHL	C	313	66/66	0.95	0.18	5,21,66,80	0
2	LUT	C	301	42/42	0.95	0.17	15,22,35,57	0
6	CLA	C	317	65/65	0.95	0.16	16,31,87,95	0
5	CHL	B	312	66/66	0.95	0.15	22,40,71,83	0
5	CHL	C	305	66/66	0.95	0.16	14,34,87,104	0
6	CLA	B	317	65/65	0.95	0.17	14,30,85,94	0
5	CHL	A	312	66/66	0.95	0.14	19,36,68,81	0
5	CHL	B	305	66/66	0.95	0.16	8,26,81,100	0
2	LUT	A	302	42/42	0.96	0.16	7,21,31,37	0
5	CHL	B	313	66/66	0.96	0.17	14,28,69,85	0
4	LHG	C	304	49/49	0.96	0.18	16,42,96,107	0
5	CHL	A	313	66/66	0.96	0.16	14,25,68,82	0
5	CHL	C	310	51/66	0.96	0.13	13,27,89,94	0
6	CLA	B	307	65/65	0.96	0.20	9,20,82,94	0
2	LUT	B	301	42/42	0.96	0.15	18,26,42,62	0
2	LUT	B	302	42/42	0.96	0.16	6,19,32,35	0
8	ZN	C	321	1/1	0.96	0.13	64,64,64,64	0
5	CHL	B	310	51/66	0.96	0.13	20,32,92,97	0
6	CLA	A	306	65/65	0.96	0.17	13,21,43,63	0
2	LUT	A	301	42/42	0.96	0.15	20,25,39,61	0
9	NA	C	323	1/1	0.96	0.22	68,68,68,68	0
6	CLA	C	307	65/65	0.97	0.21	6,18,80,92	0
6	CLA	B	306	65/65	0.97	0.16	9,19,39,58	0

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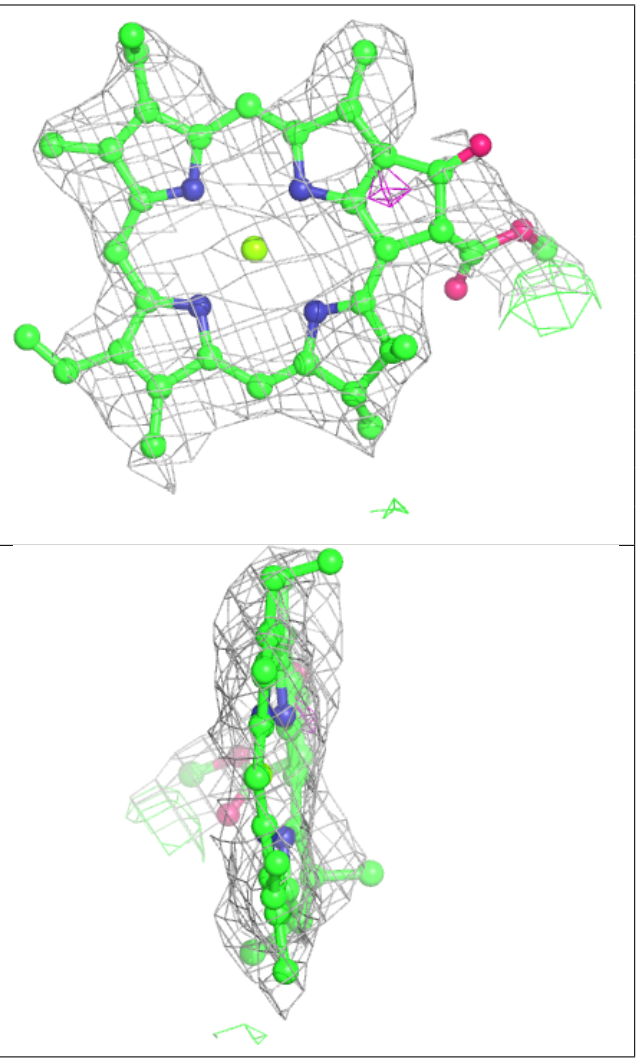
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CLA	A	307	65/65	0.97	0.21	10,20,81,93	0
7	CAC	C	319	5/5	0.97	0.18	57,62,79,156	0
6	CLA	C	306	65/65	0.97	0.17	7,19,41,60	0
8	ZN	B	321	1/1	0.98	0.12	66,66,66,66	0
7	CAC	B	319	5/5	0.98	0.17	59,62,68,97	0
2	LUT	C	302	42/42	0.98	0.15	6,16,30,35	0
8	ZN	A	320	1/1	0.98	0.09	98,98,98,98	0
8	ZN	A	321	1/1	0.98	0.09	56,56,56,56	0
7	CAC	A	319	5/5	0.98	0.17	57,59,68,81	0
9	NA	B	320	1/1	0.99	0.05	42,42,42,42	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.

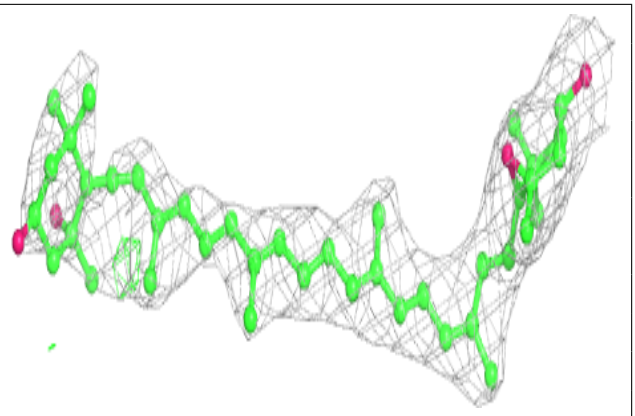
Electron density around CLA A 318:

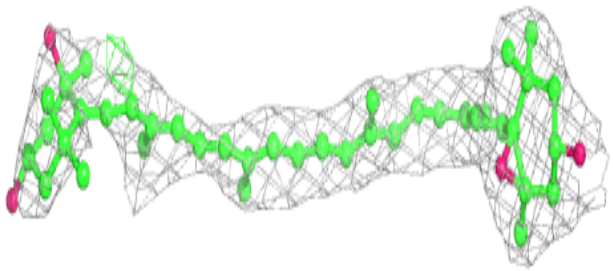
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

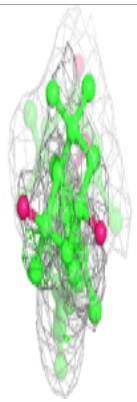


Electron density around NEX B 303:

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

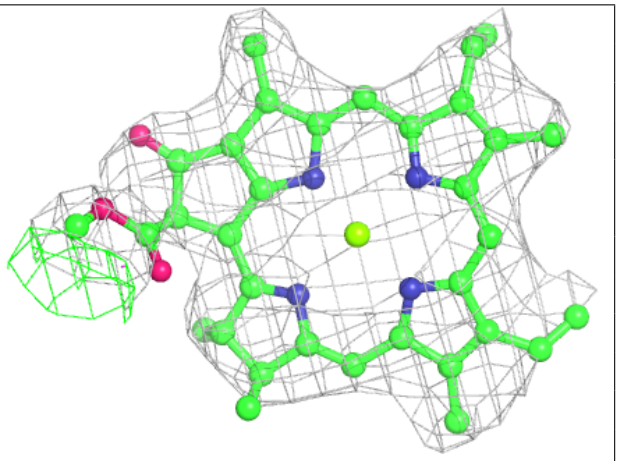


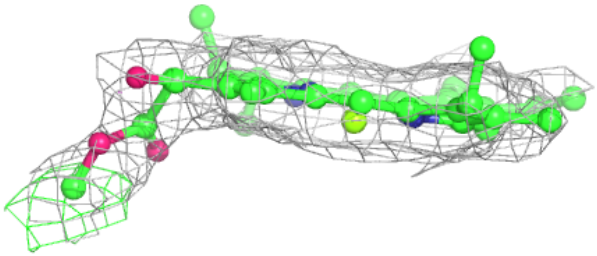


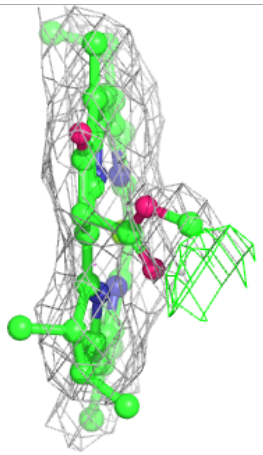


Electron density around CLA B 318:

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

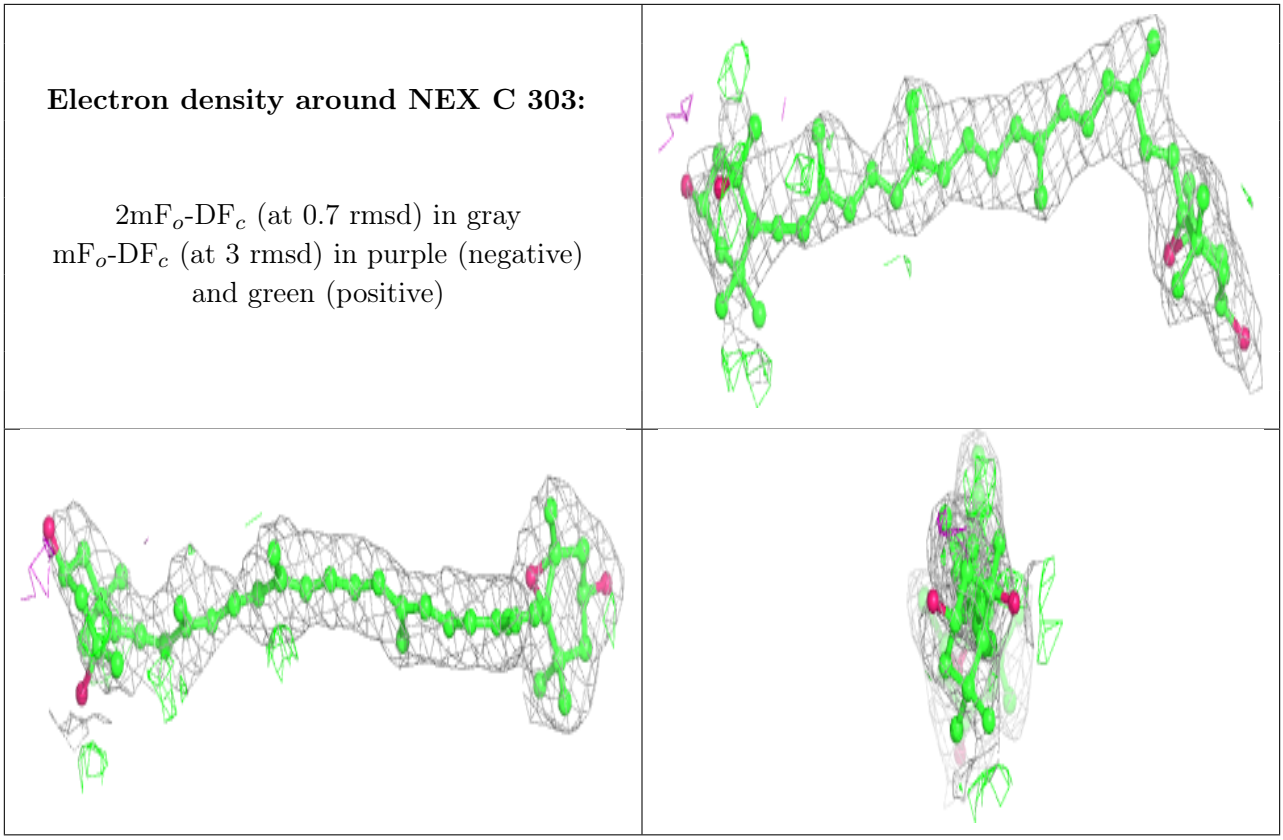






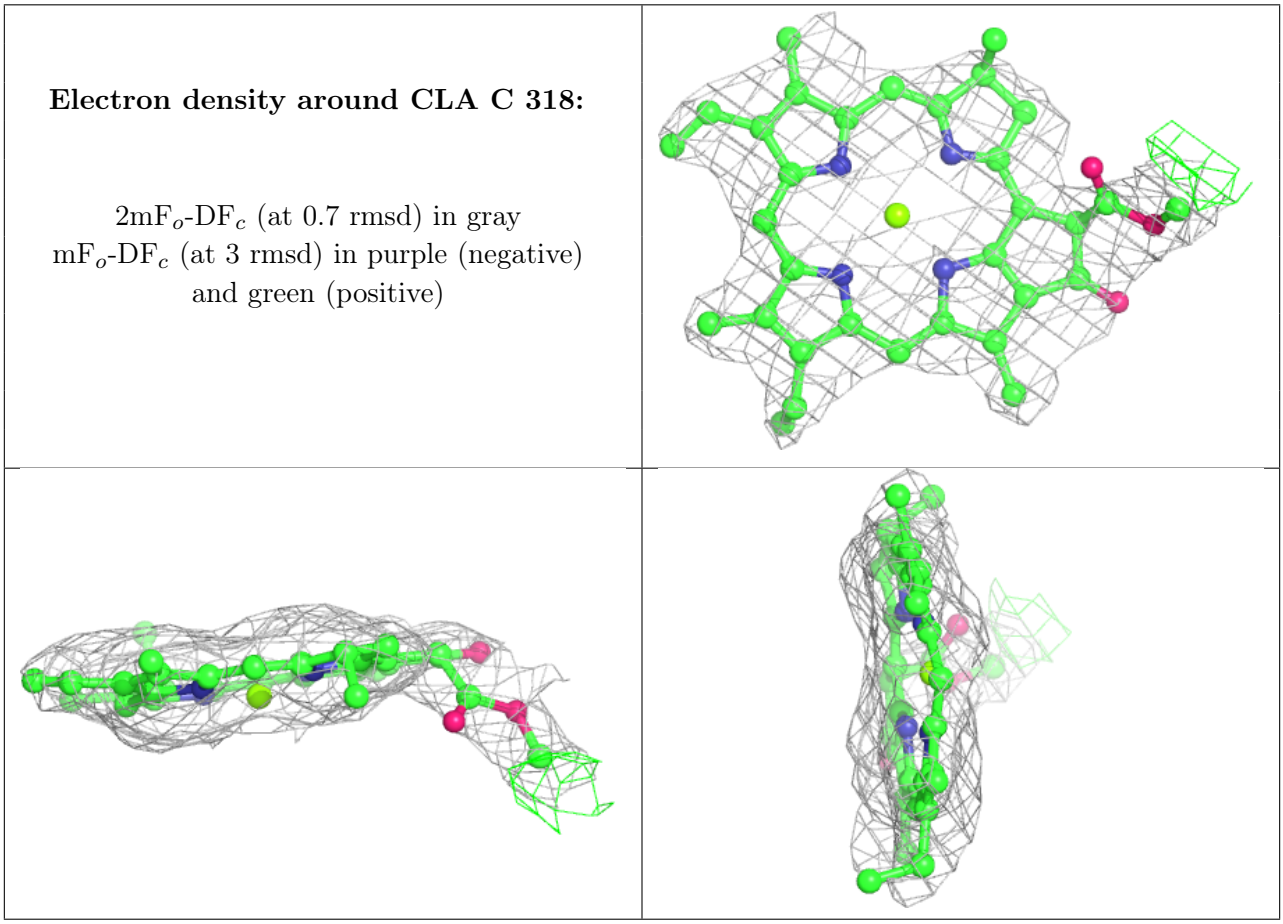
Electron density around NEX C 303:

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



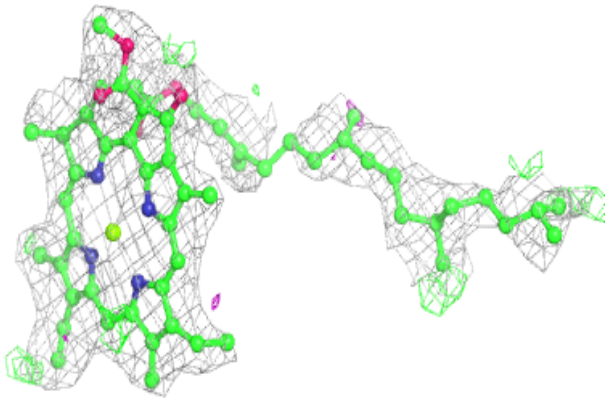
Electron density around CLA C 318:

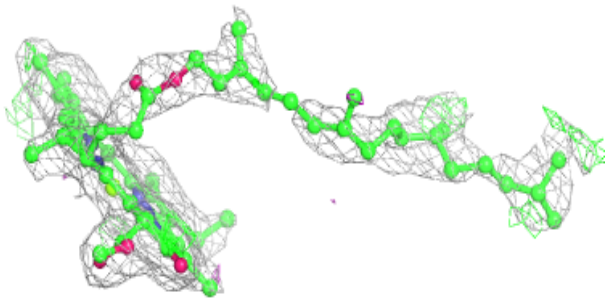
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

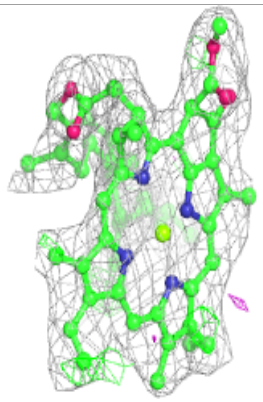


Electron density around CLA A 315:

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

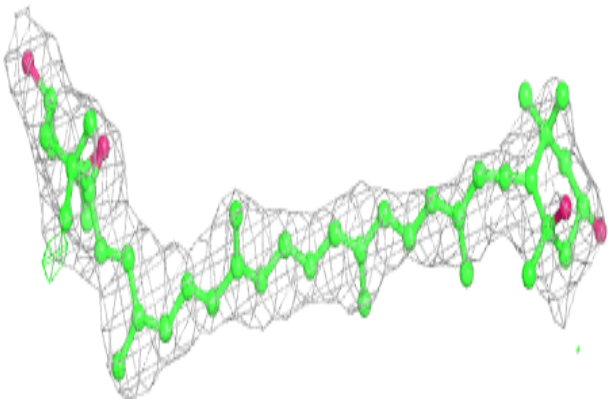


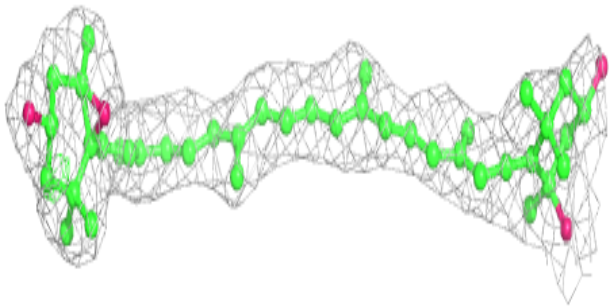


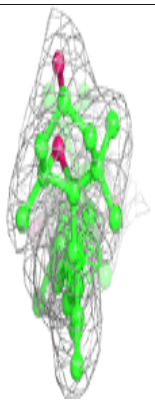


Electron density around NEX A 303:

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

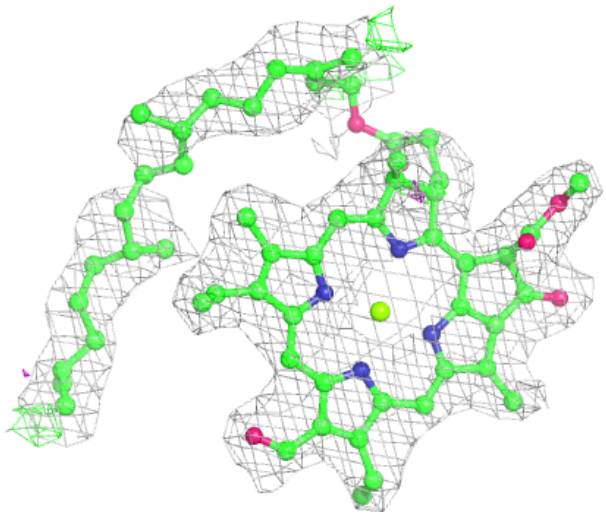


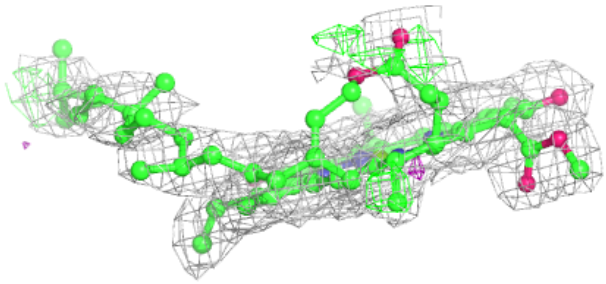


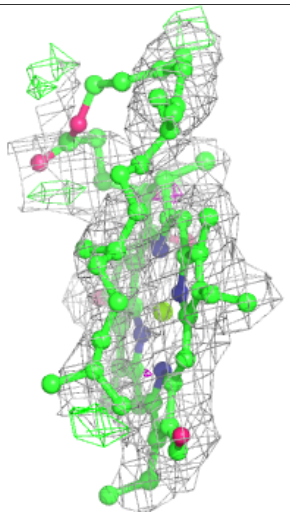


Electron density around CHL C 311:

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

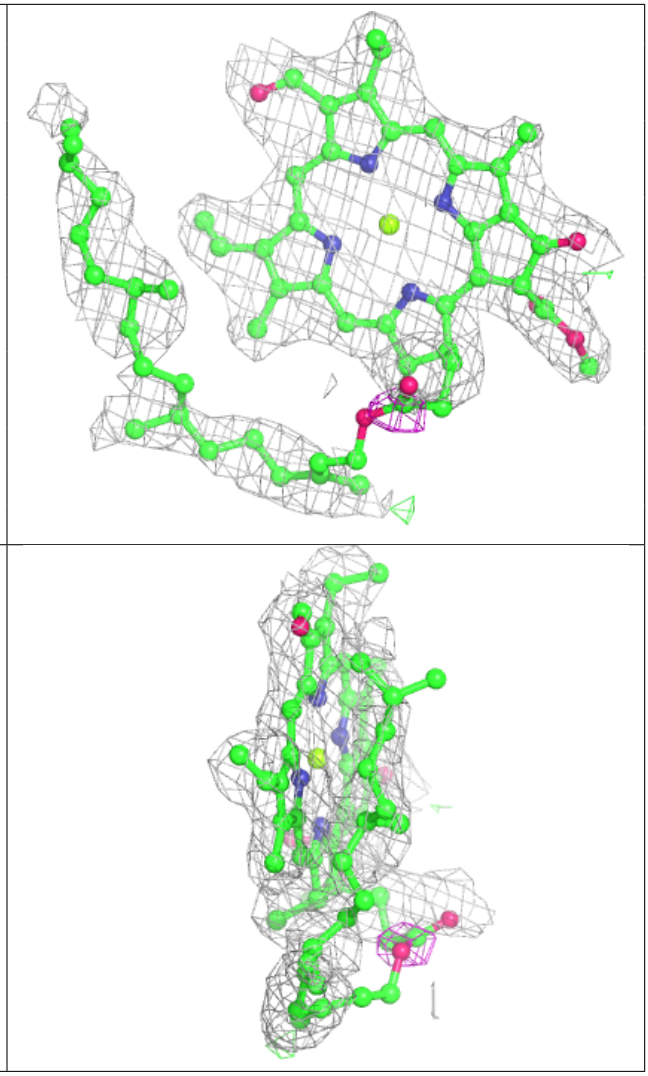






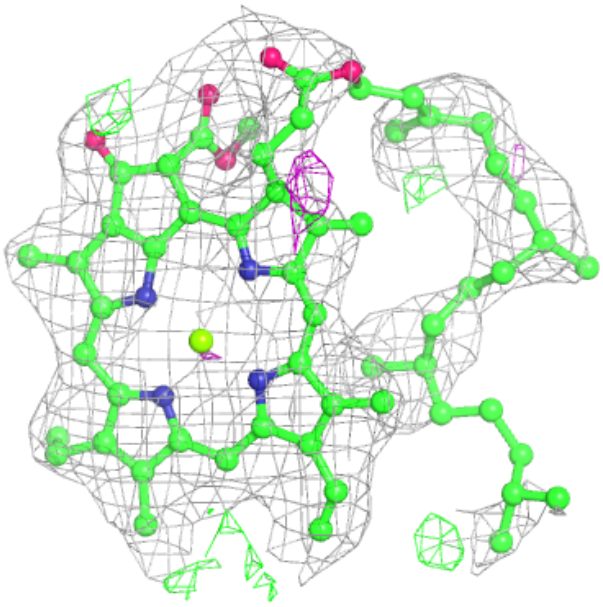
Electron density around CHL A 311:

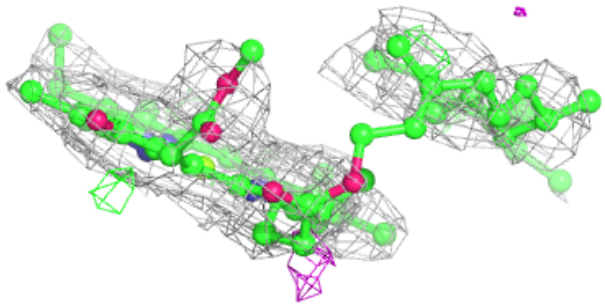
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

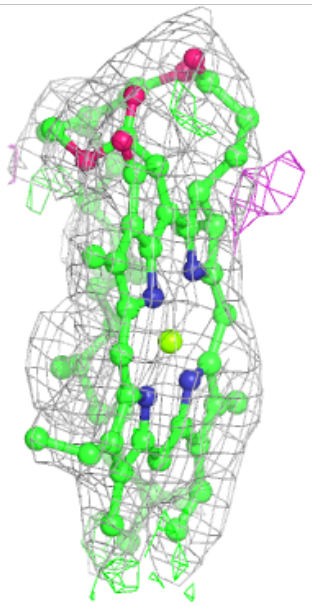


Electron density around CLA A 316:

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

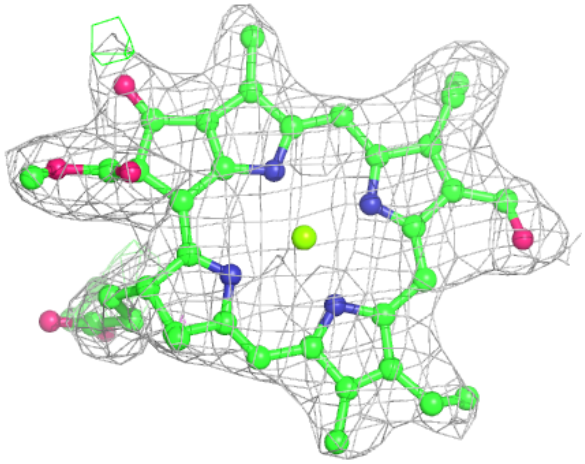


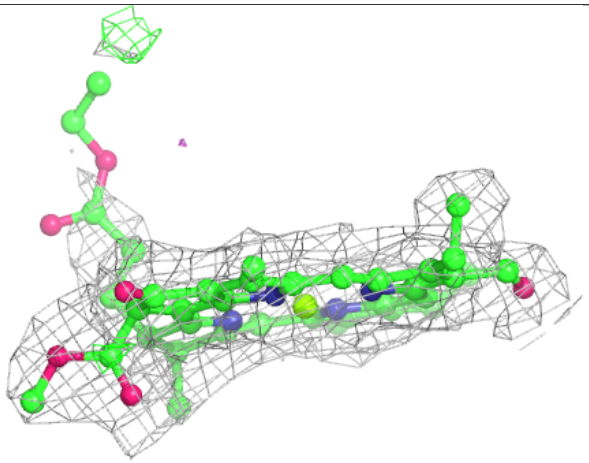


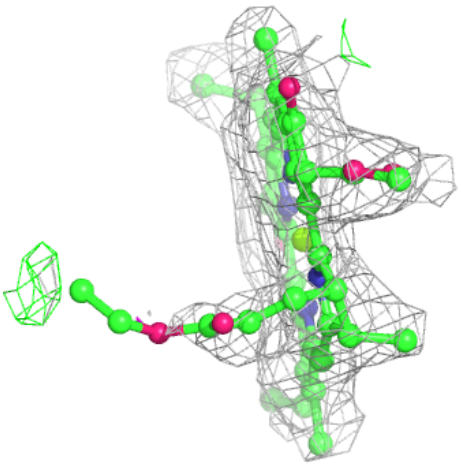


Electron density around CHL C 309:

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

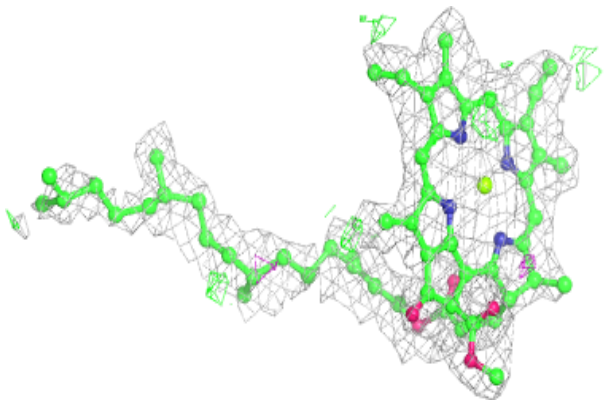


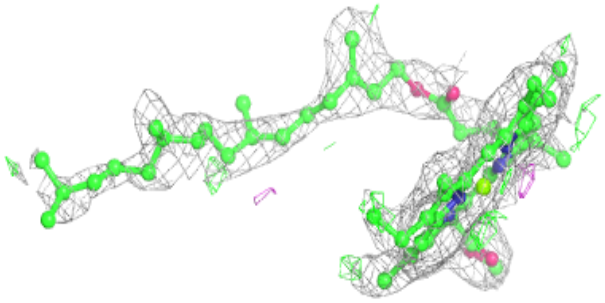


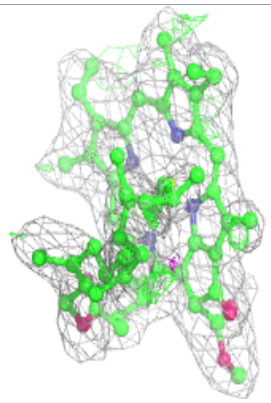


Electron density around CLA B 315:

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

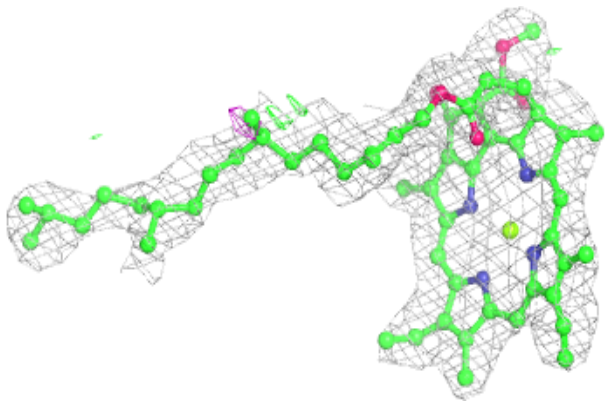


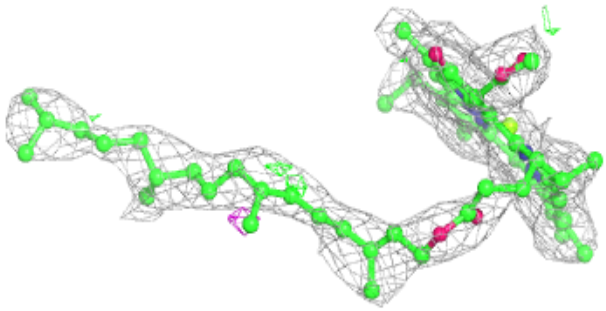


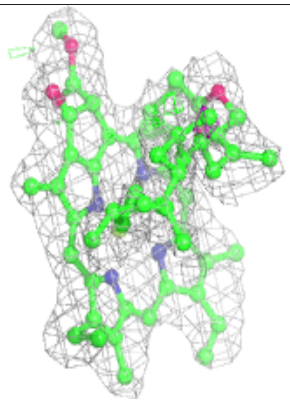


Electron density around CLA C 315:

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

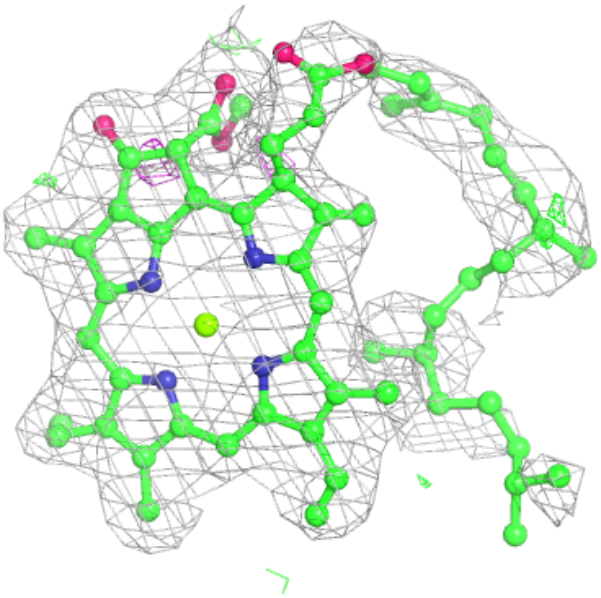


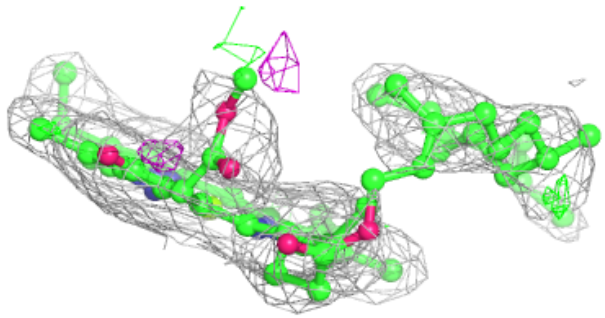


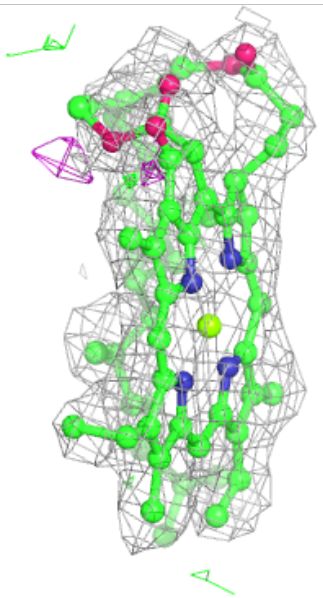


Electron density around CLA C 316:

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

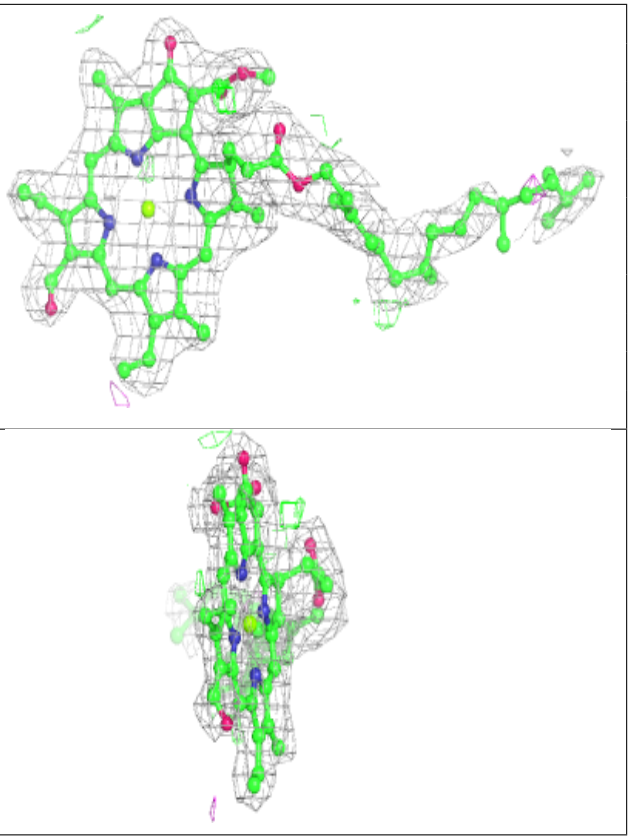


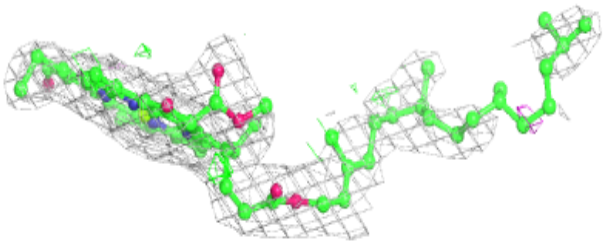




Electron density around CHL A 305:

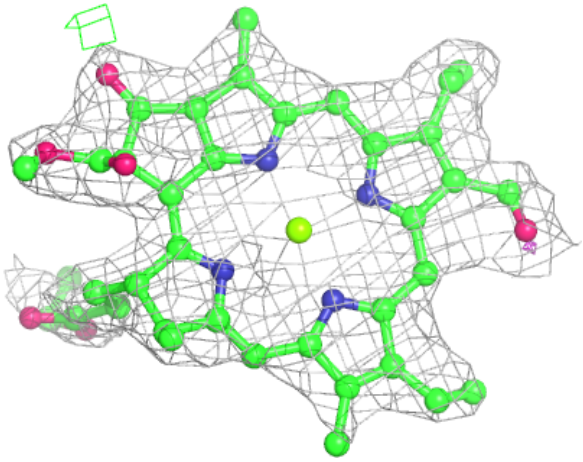
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

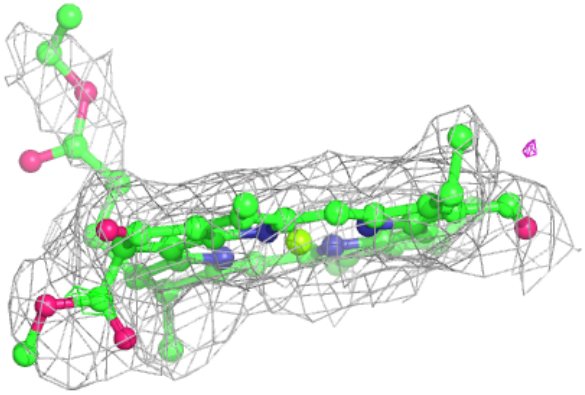


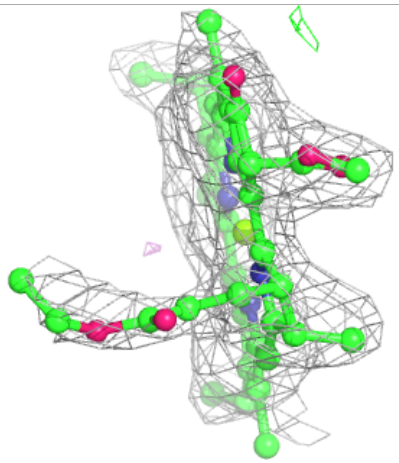


Electron density around CHL B 309:

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

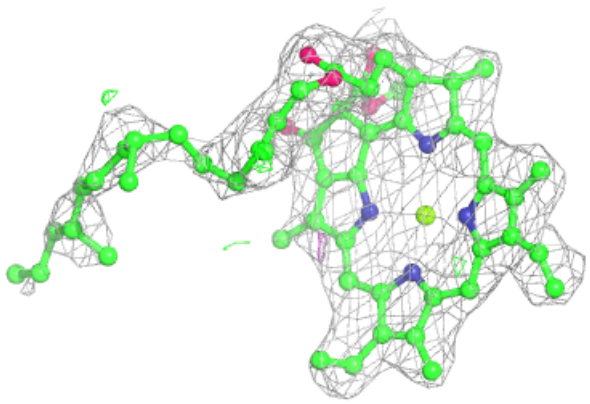


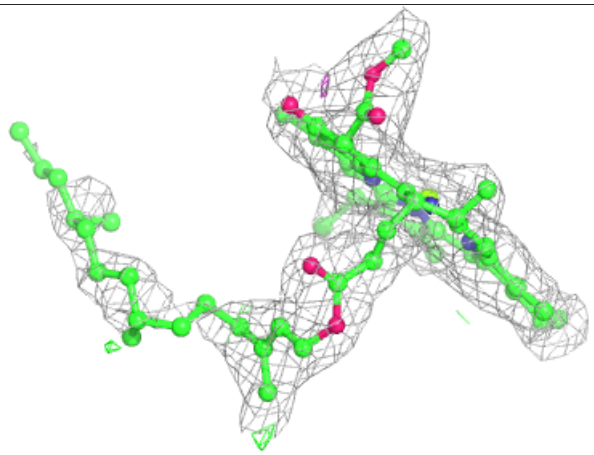


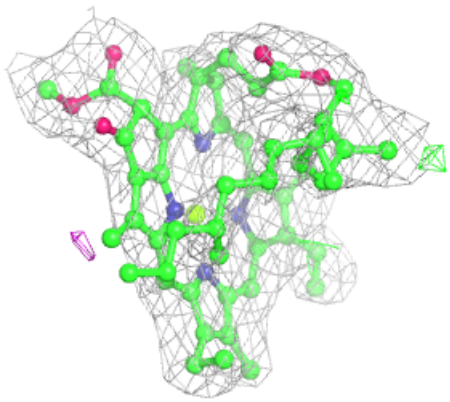


Electron density around CLA A 308:

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

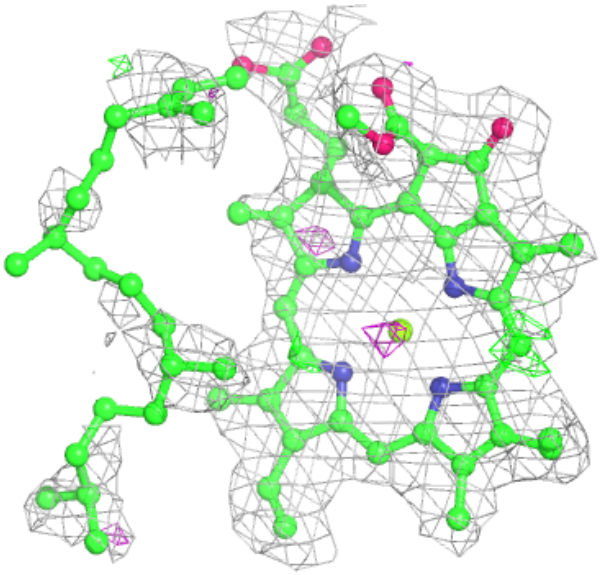


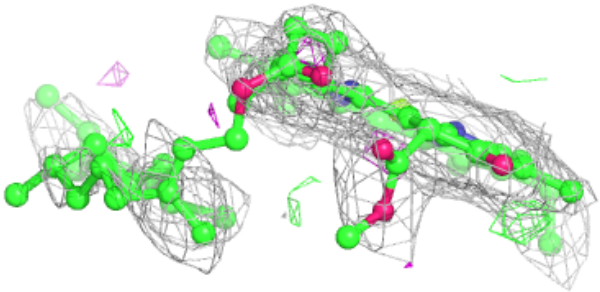


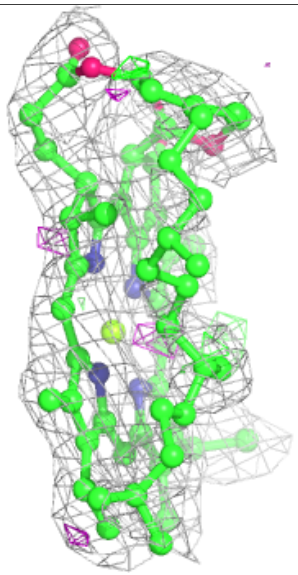


Electron density around CLA B 316:

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

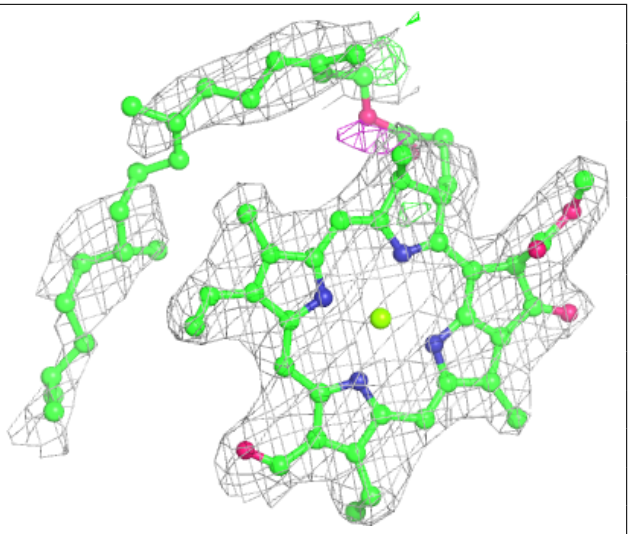


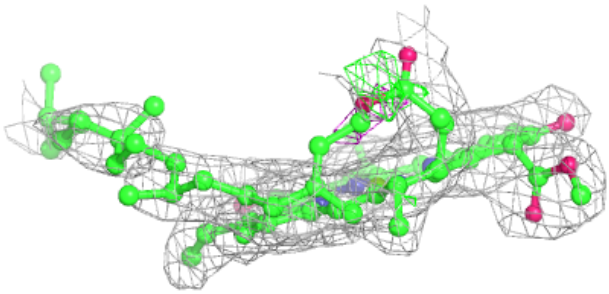


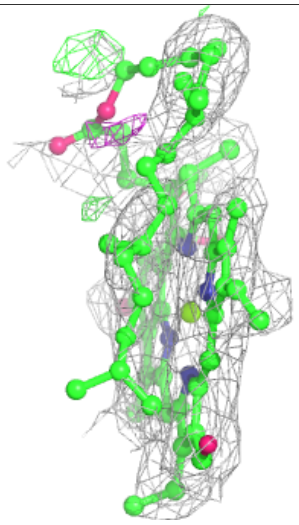


Electron density around CHL B 311:

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

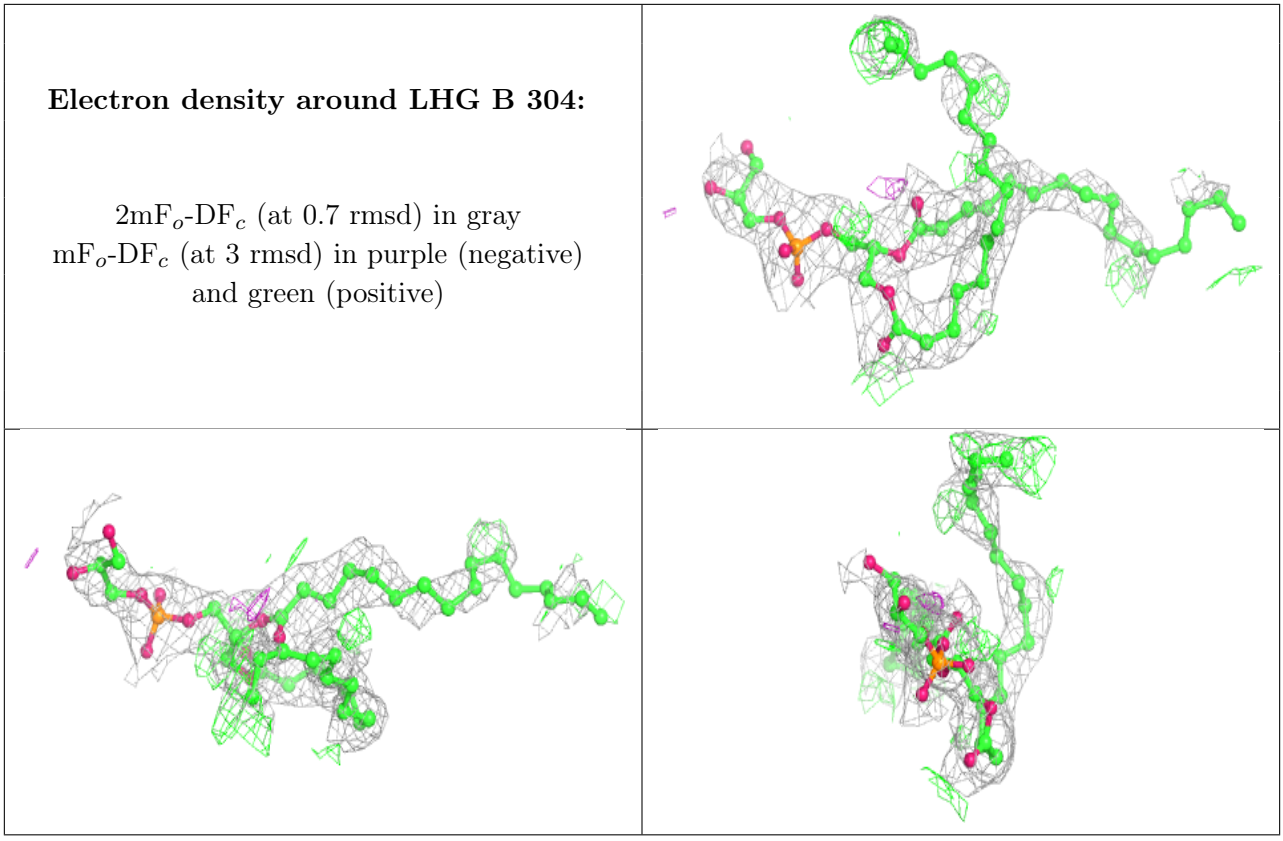






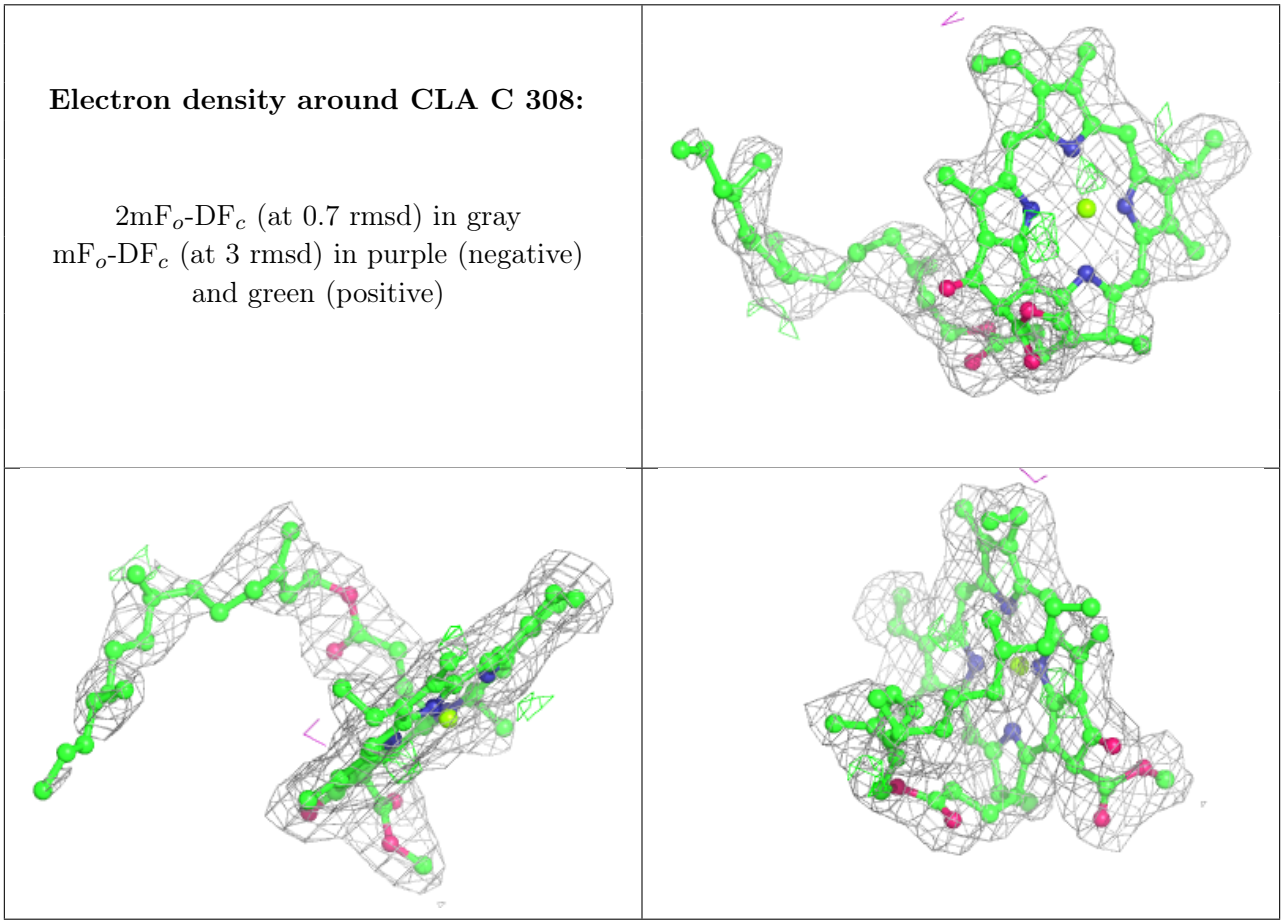
Electron density around LHG B 304:

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



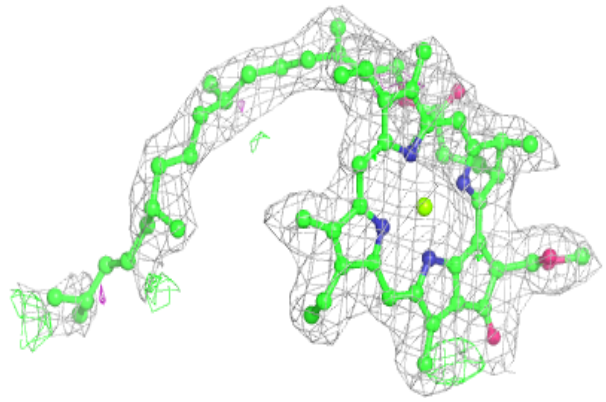
Electron density around CLA C 308:

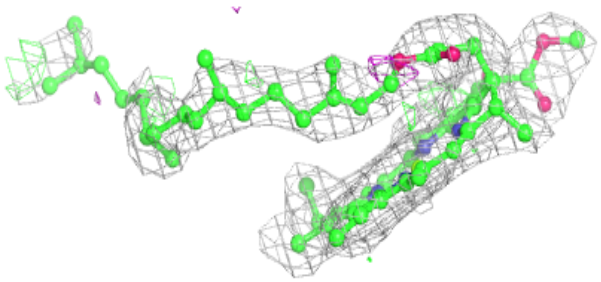
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

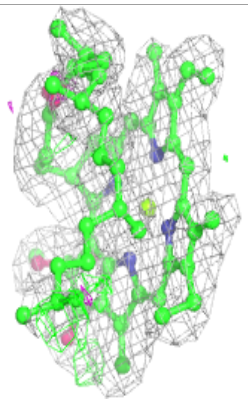


Electron density around CLA C 314:

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

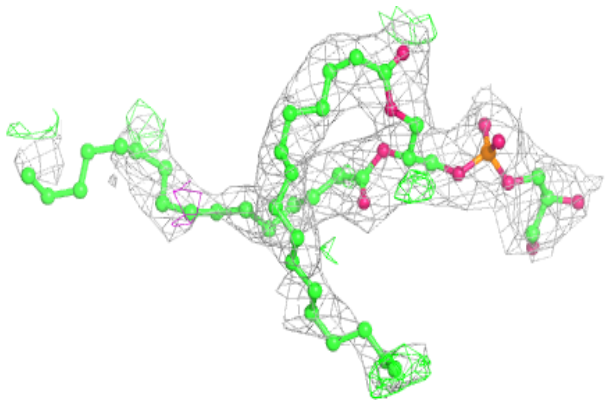


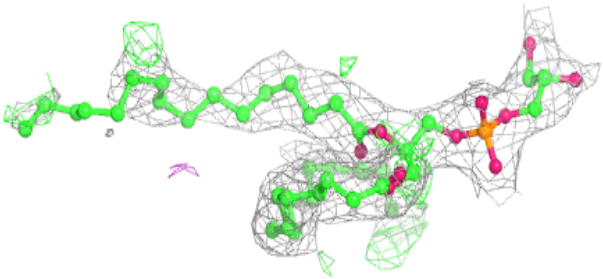


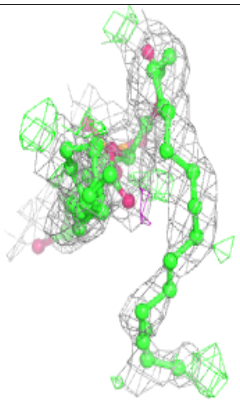


Electron density around LHG A 304:

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

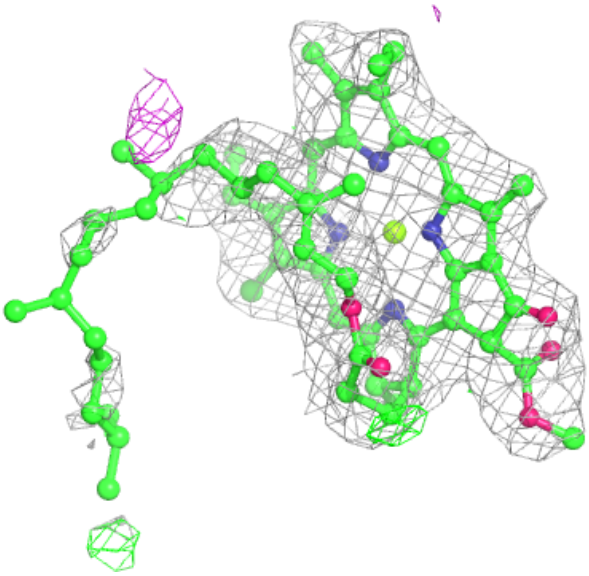


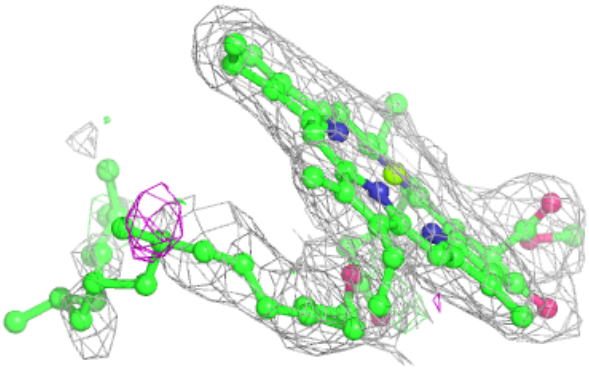


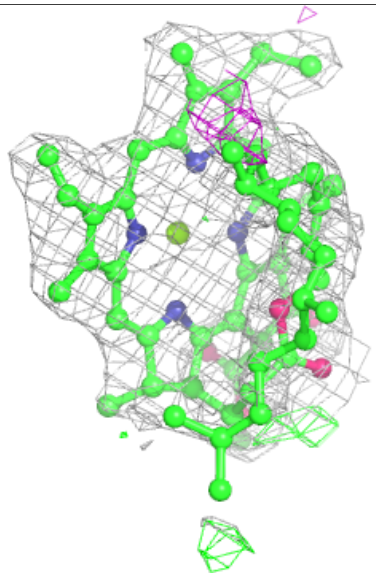


Electron density around CLA A 317:

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

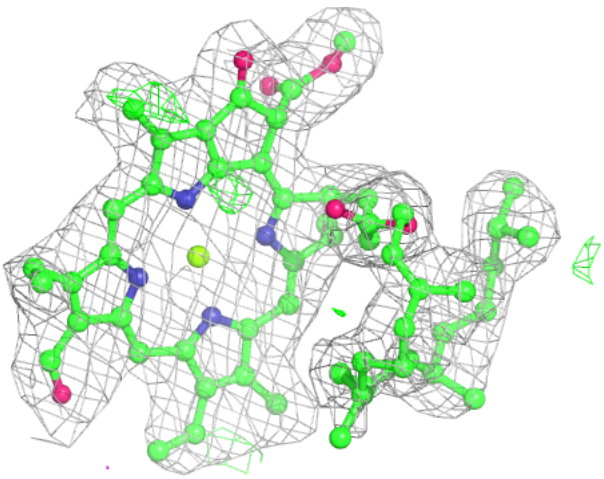


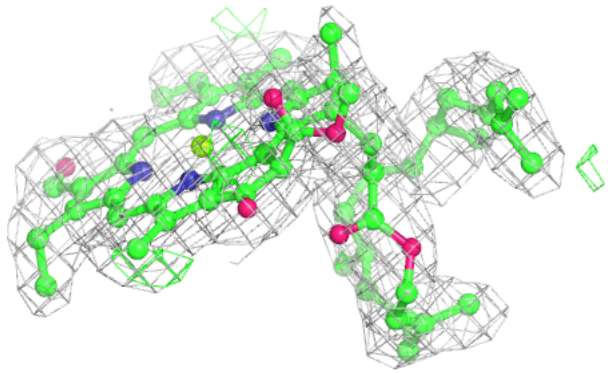


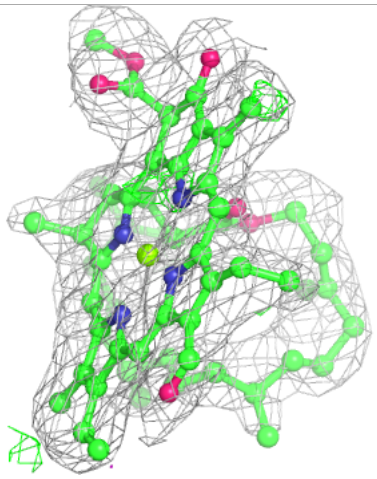


Electron density around CHL C 312:

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

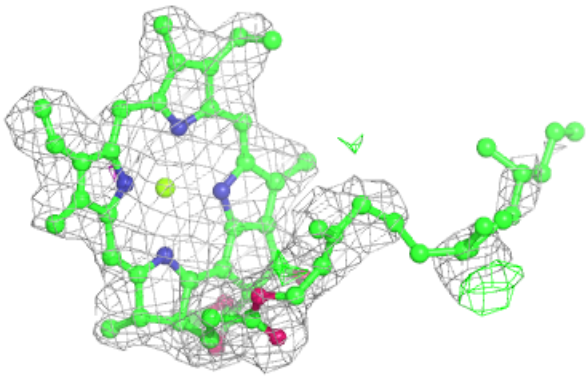


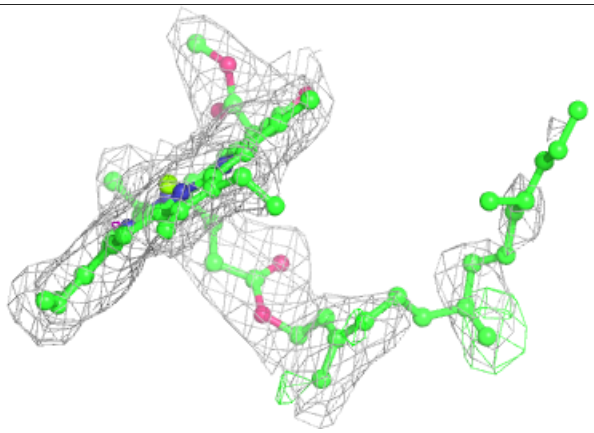


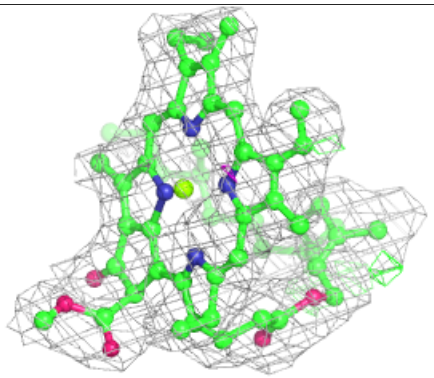


Electron density around CLA B 308:

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

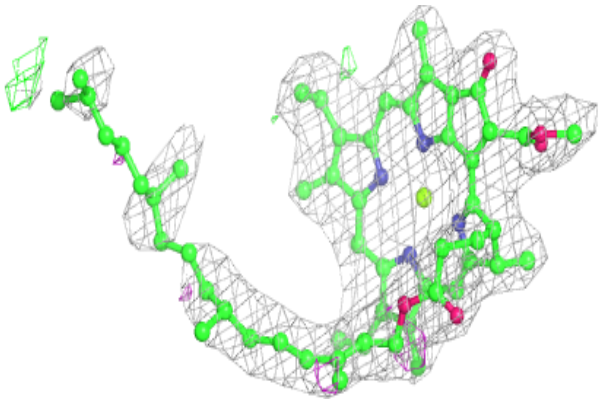


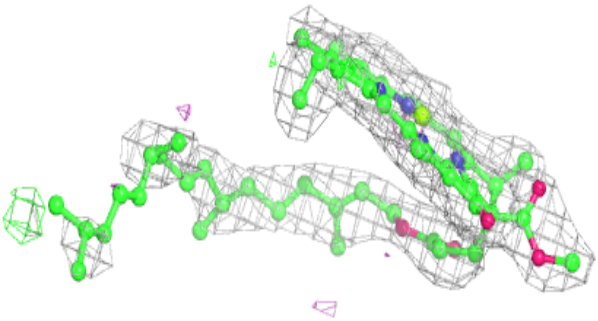


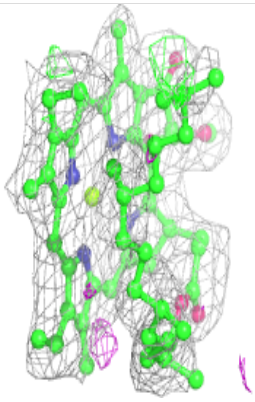


Electron density around CLA B 314:

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

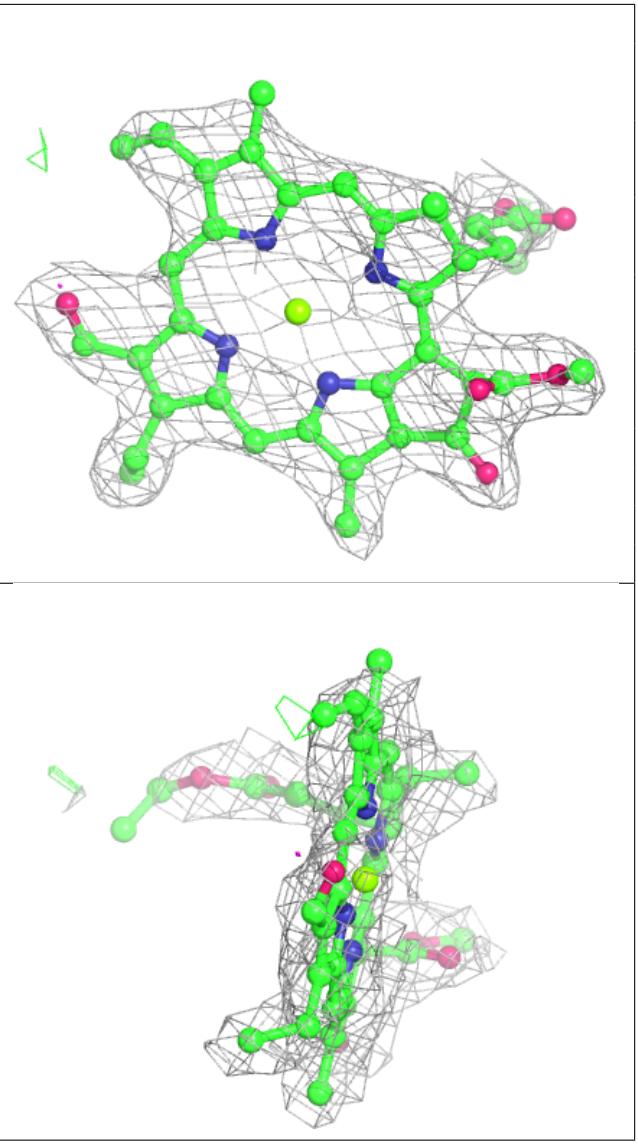






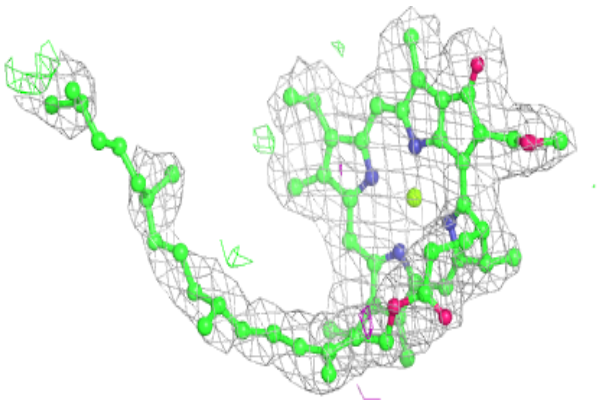
Electron density around CHL A 309:

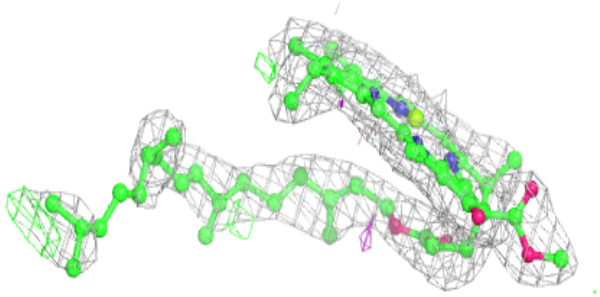
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

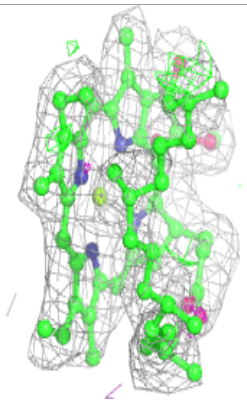


Electron density around CLA A 314:

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

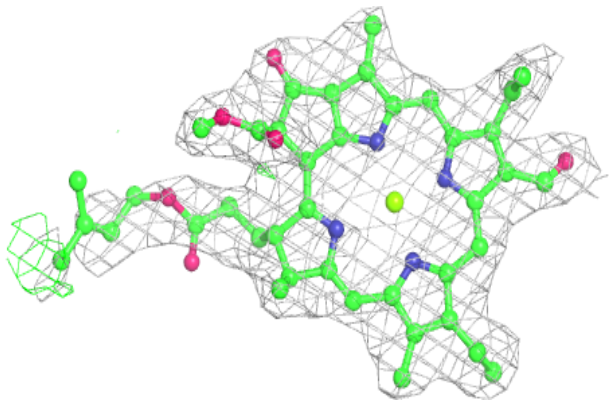


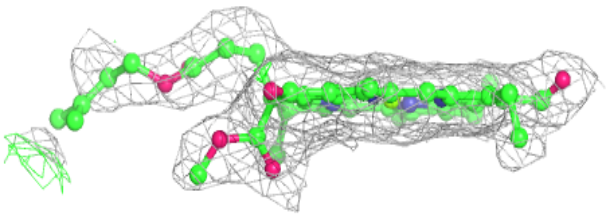


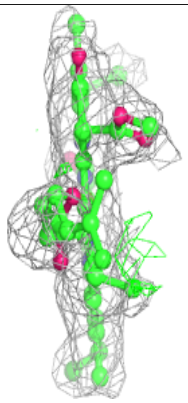


Electron density around CHL A 310:

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

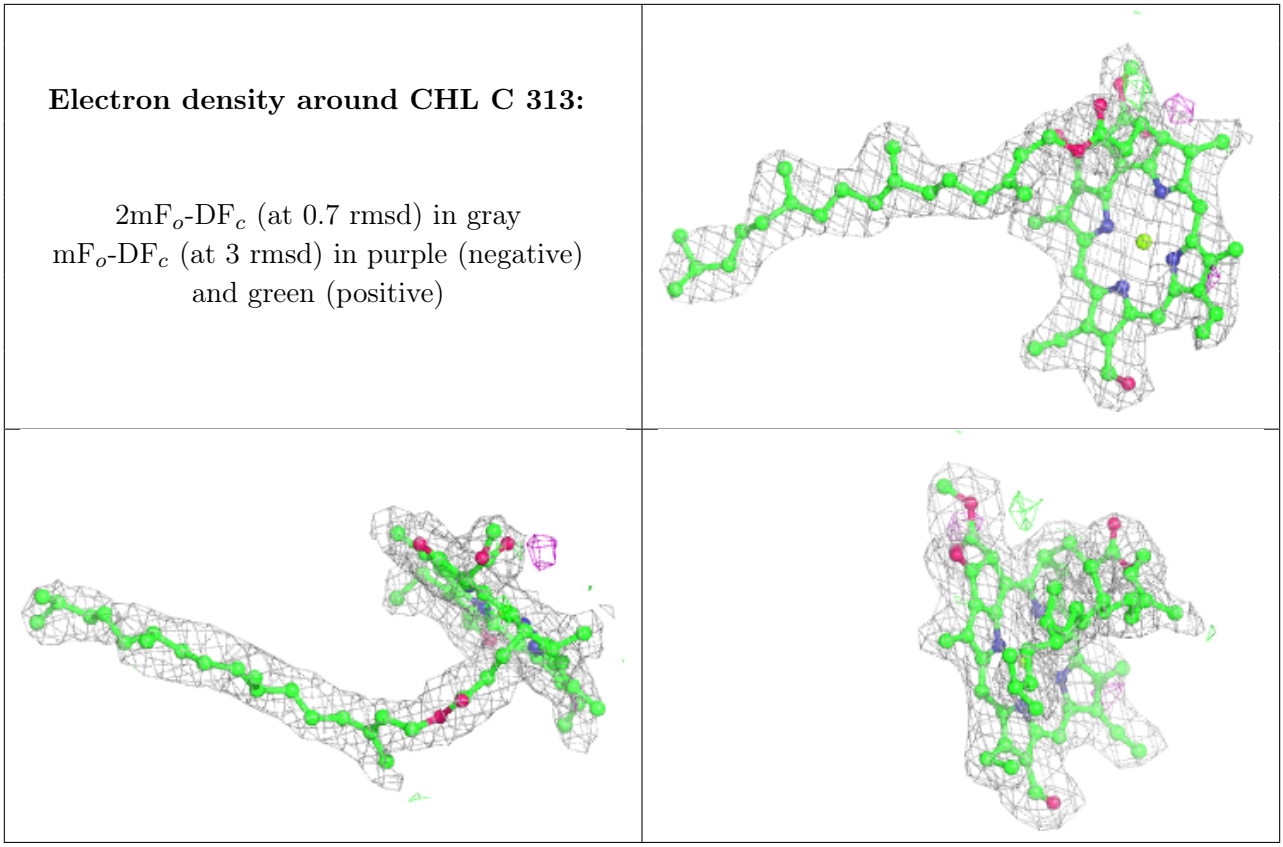






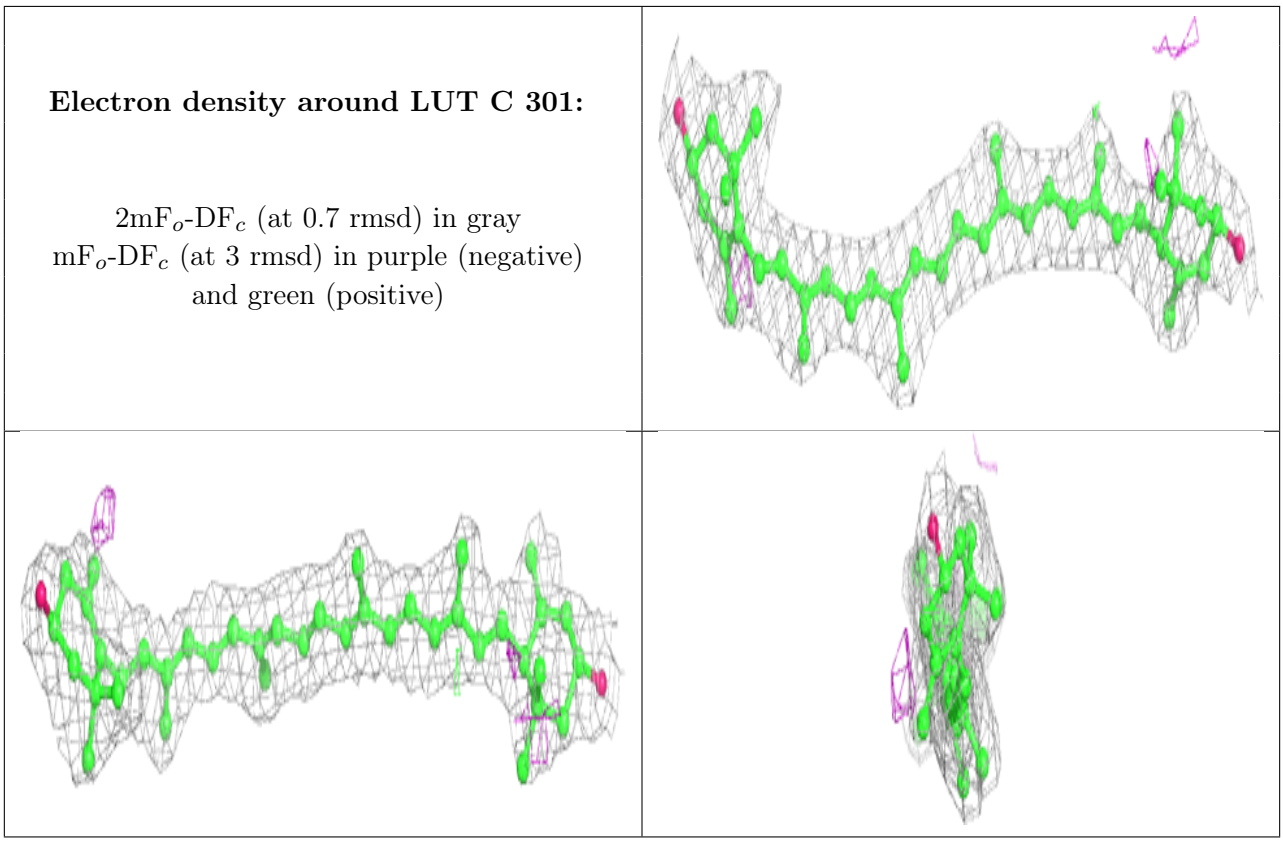
Electron density around CHL C 313:

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



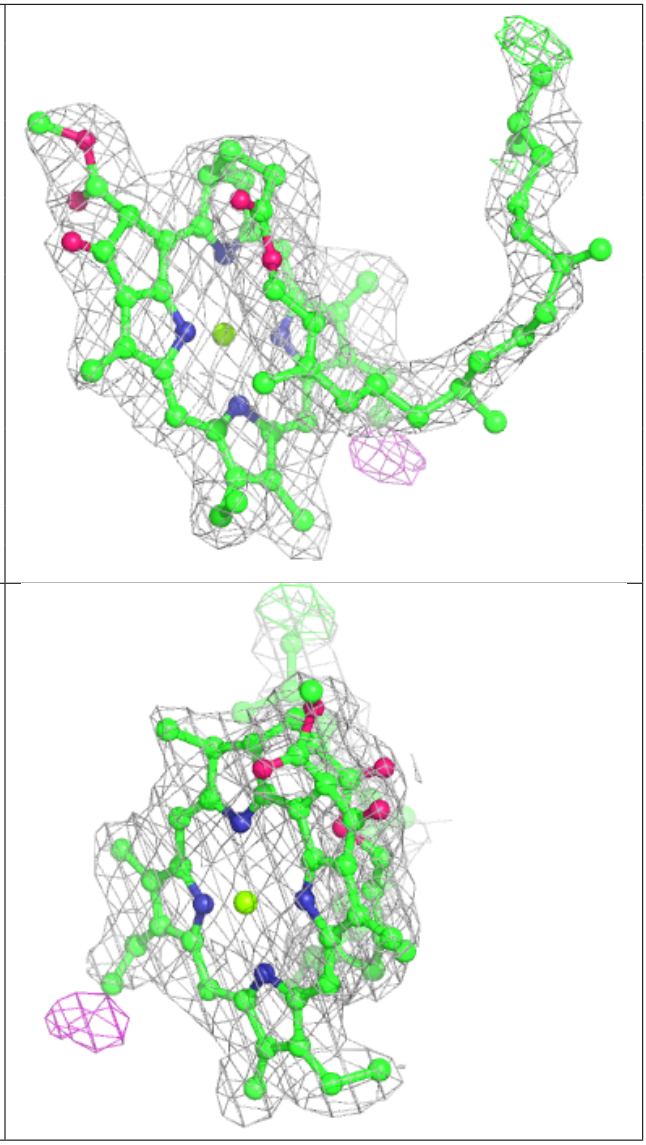
Electron density around LUT C 301:

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



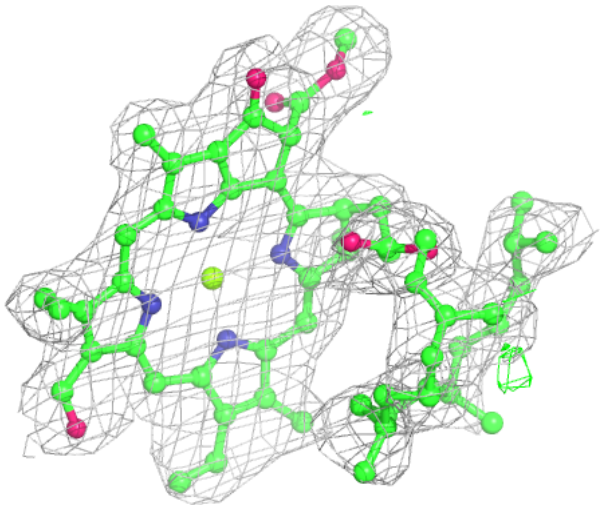
Electron density around CLA C 317:

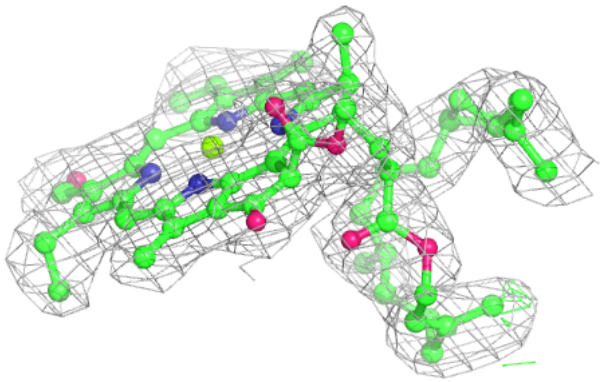
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

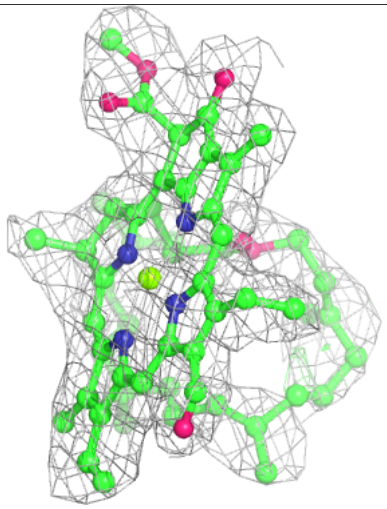


Electron density around CHL B 312:

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

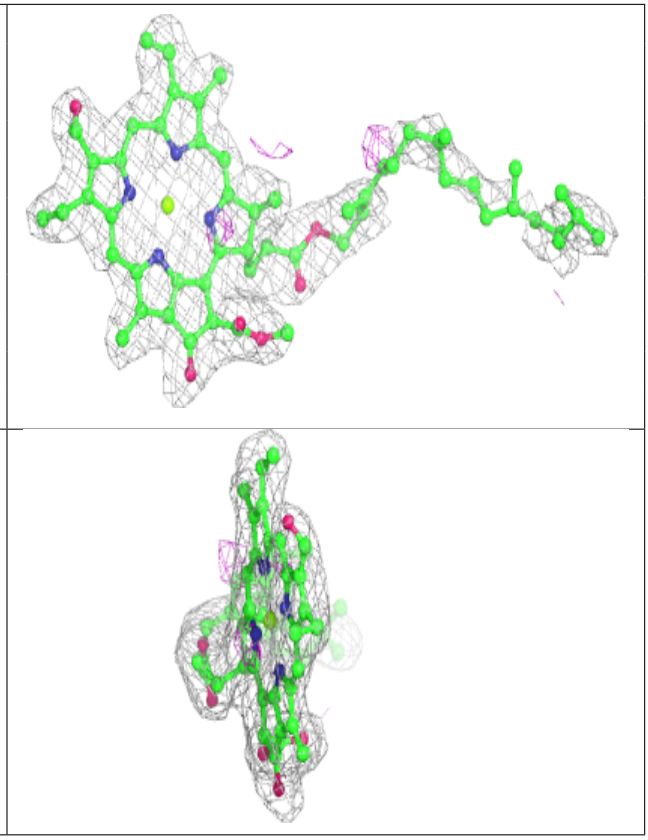






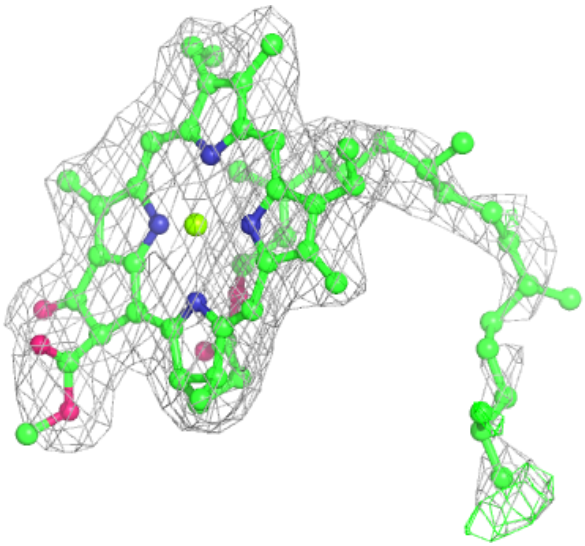
Electron density around CHL C 305:

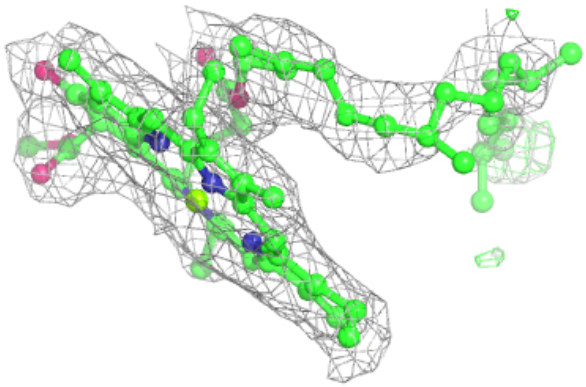
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

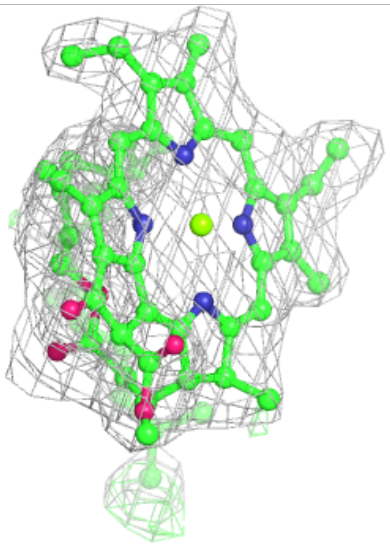


Electron density around CLA B 317:

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

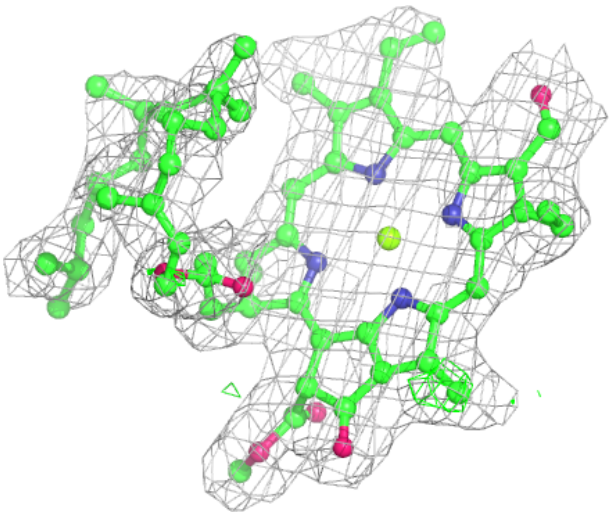


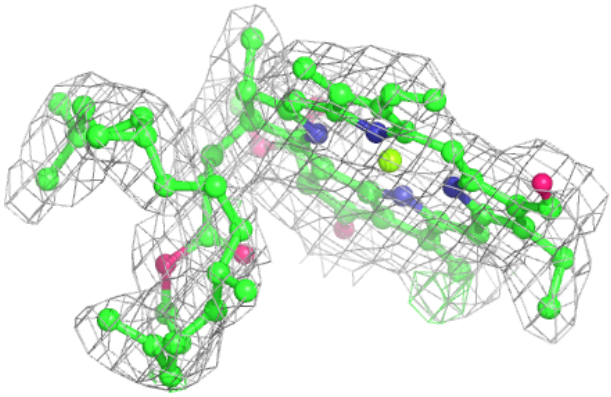


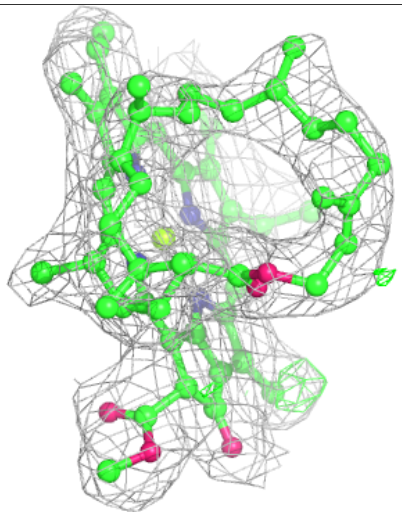


Electron density around CHL A 312:

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

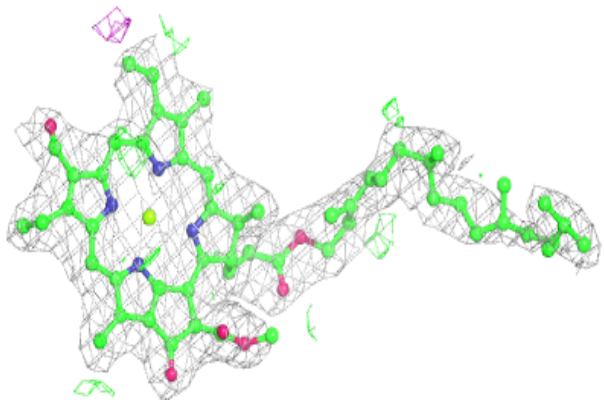


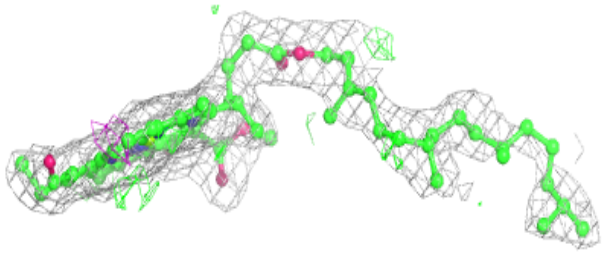


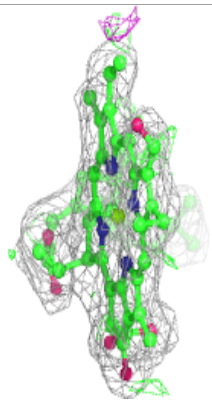


Electron density around CHL B 305:

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

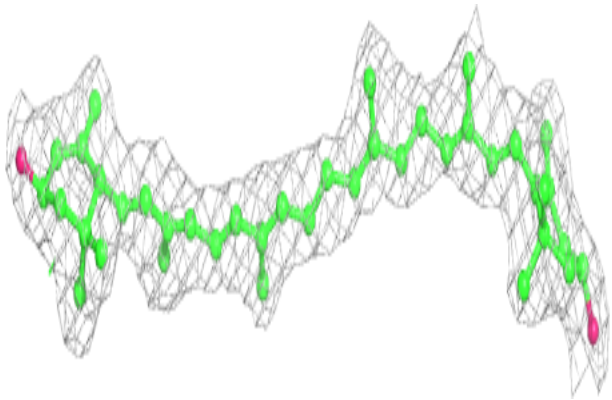


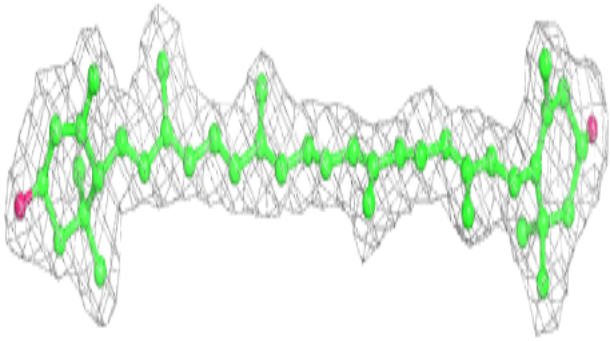




Electron density around LUT A 302:

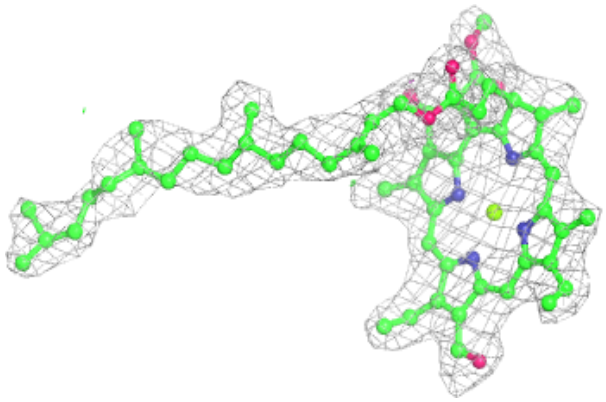
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

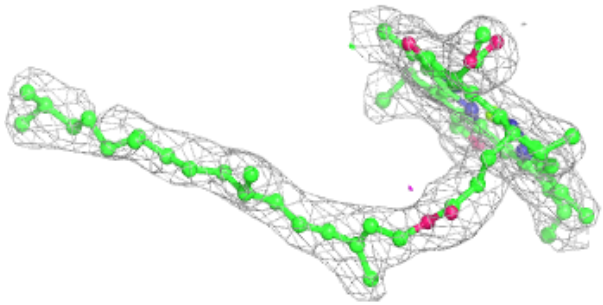


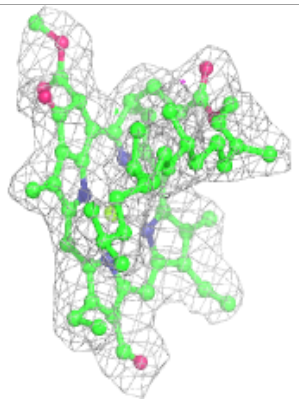


Electron density around CHL B 313:

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

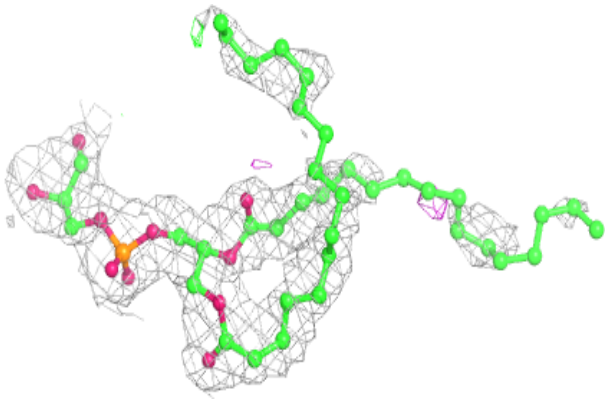


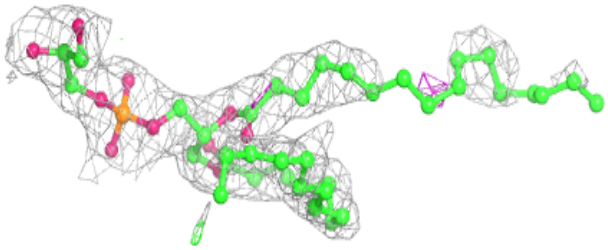


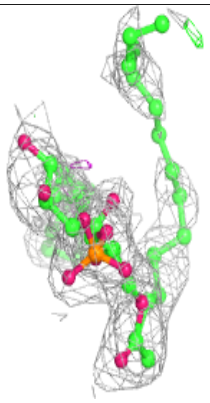


Electron density around LHG C 304:

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

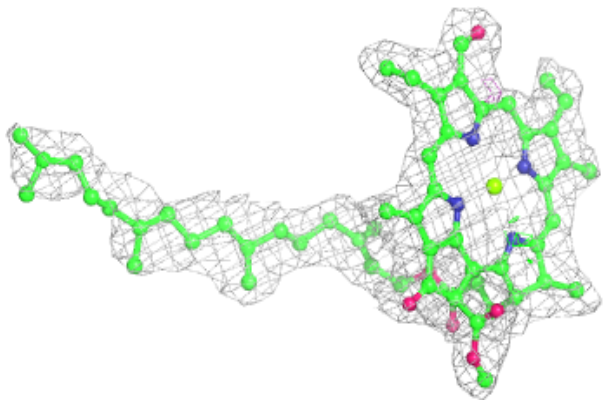


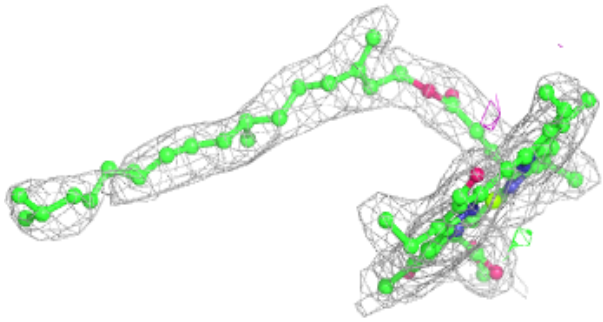


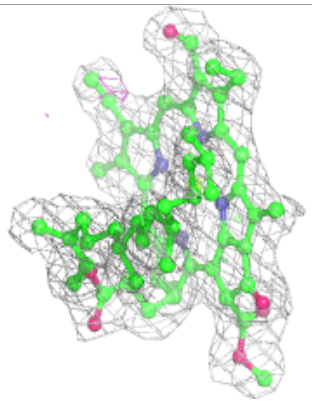


Electron density around CHL A 313:

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

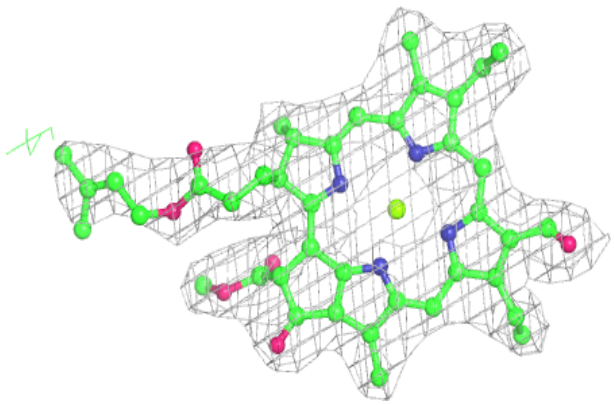


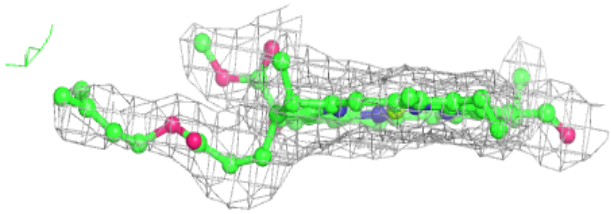




Electron density around CHL C 310:

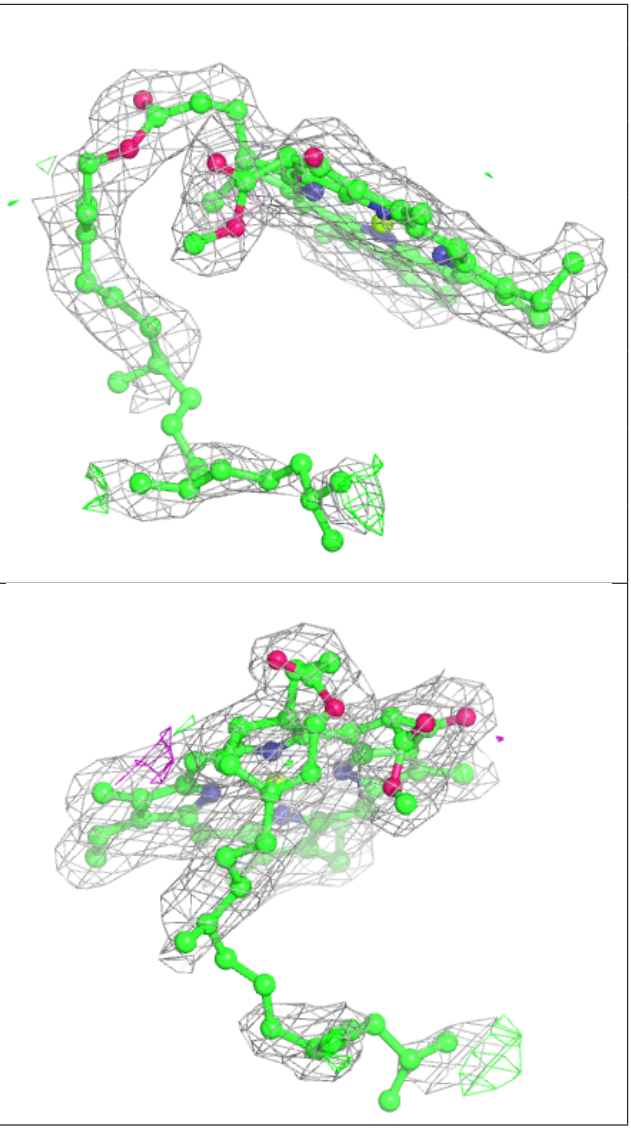
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





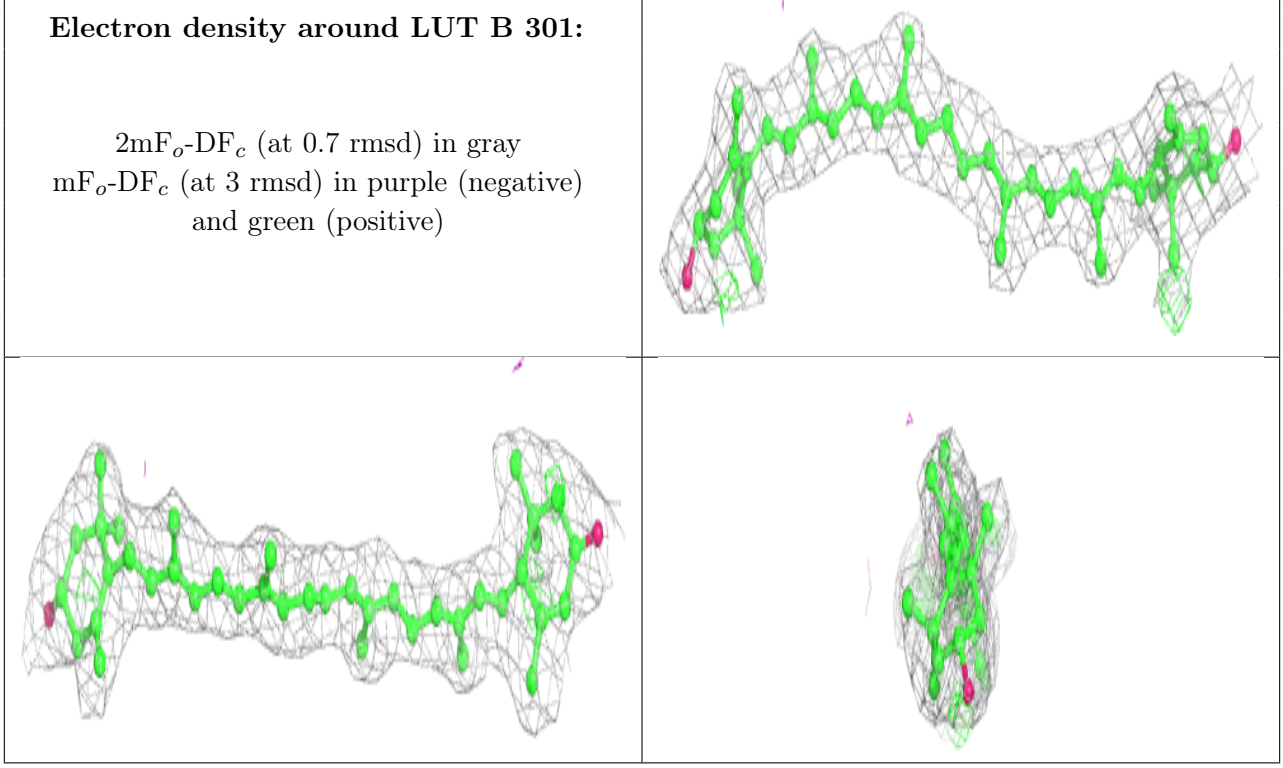
Electron density around CLA B 307:

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



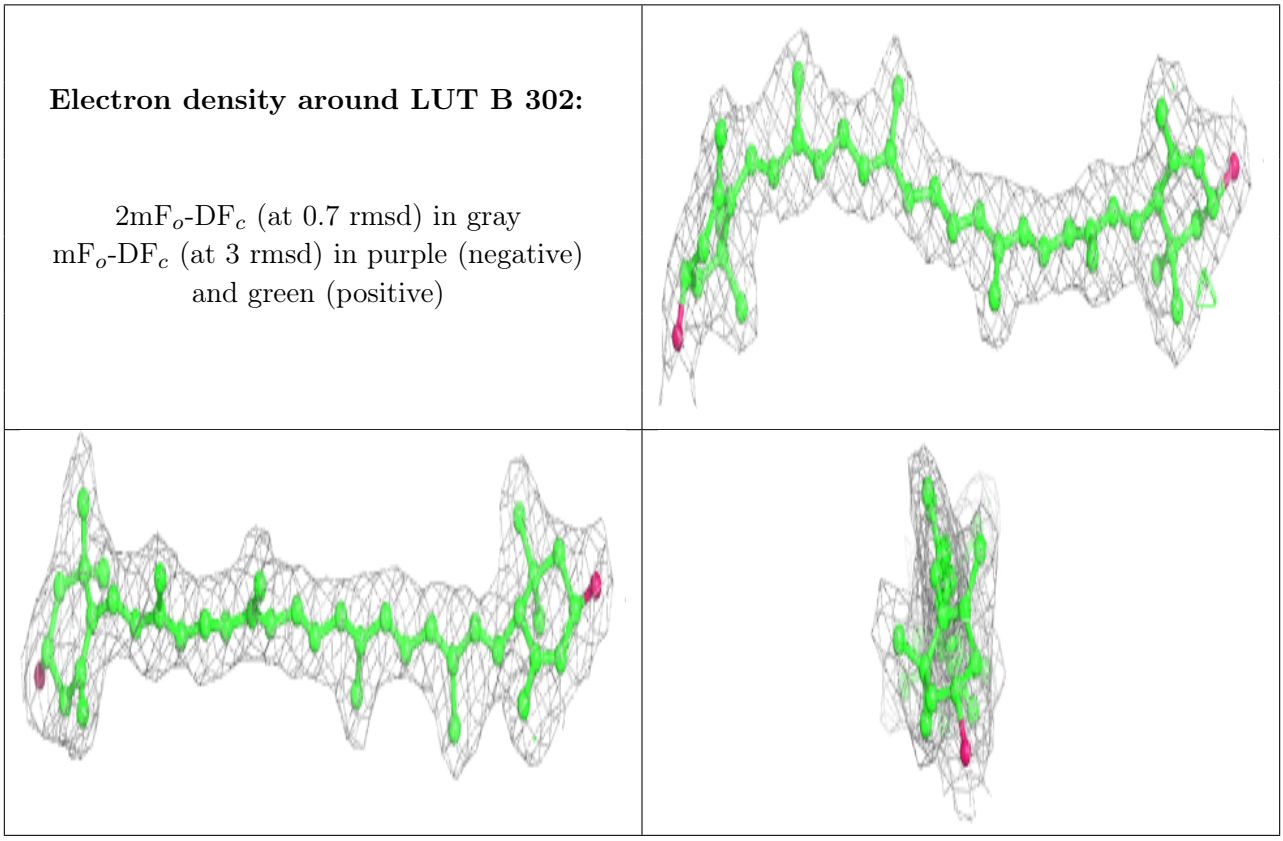
Electron density around LUT B 301:

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



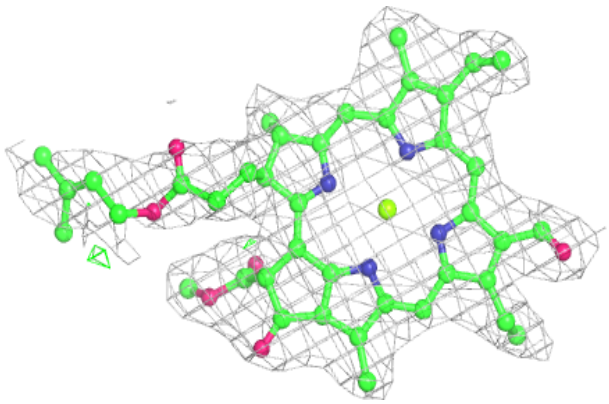
Electron density around LUT B 302:

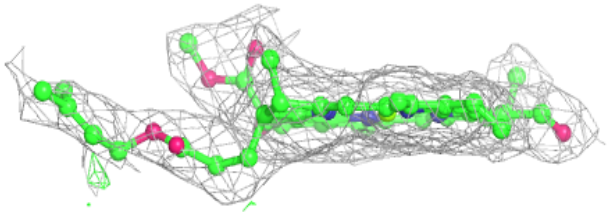
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

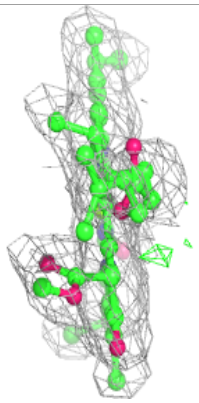


Electron density around CHL B 310:

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

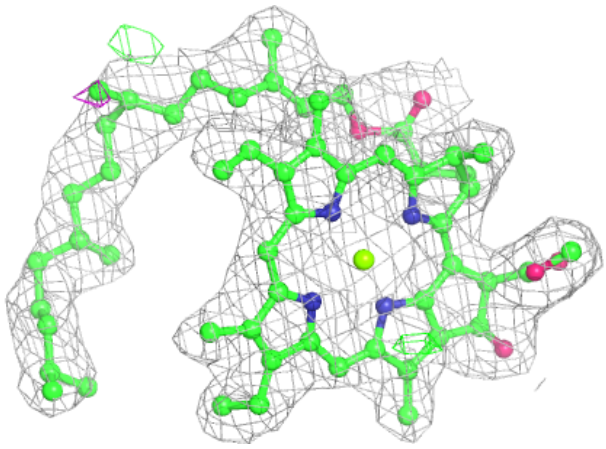


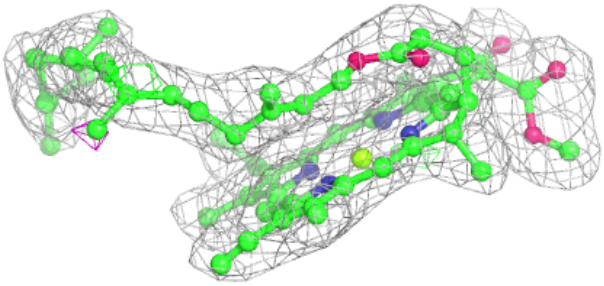


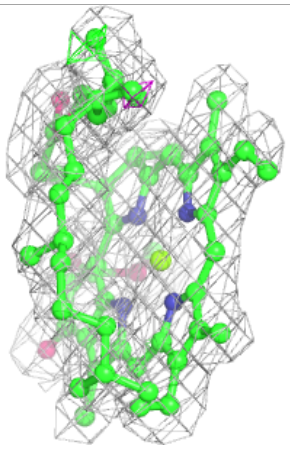


Electron density around CLA A 306:

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

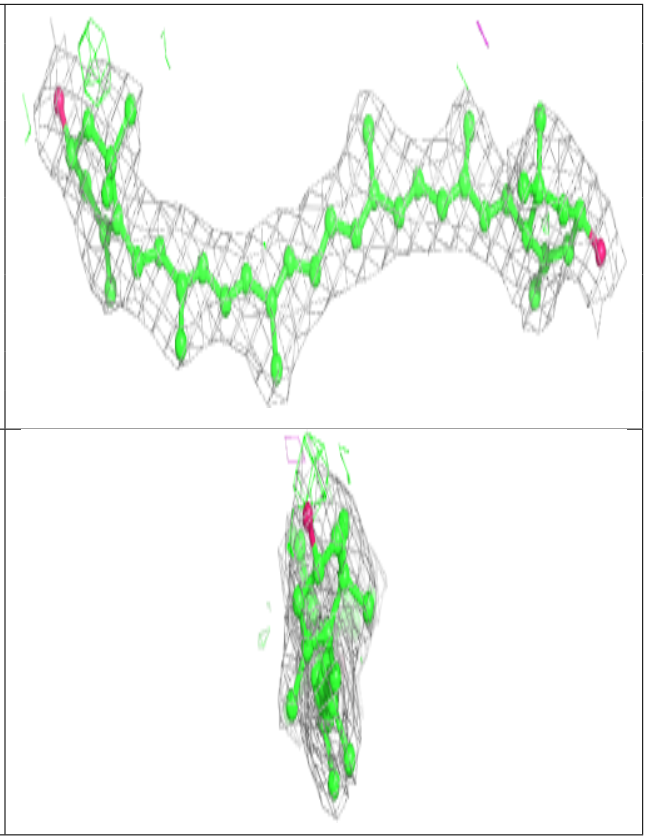






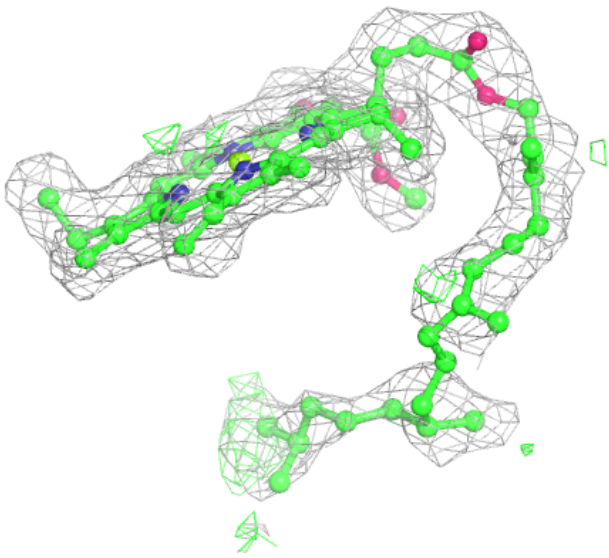
Electron density around LUT A 301:

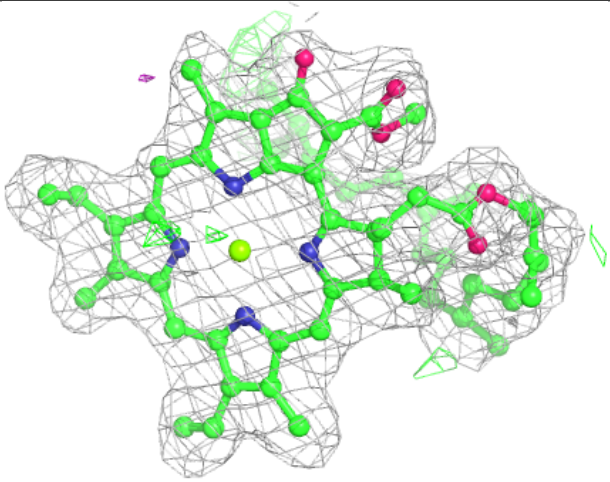
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

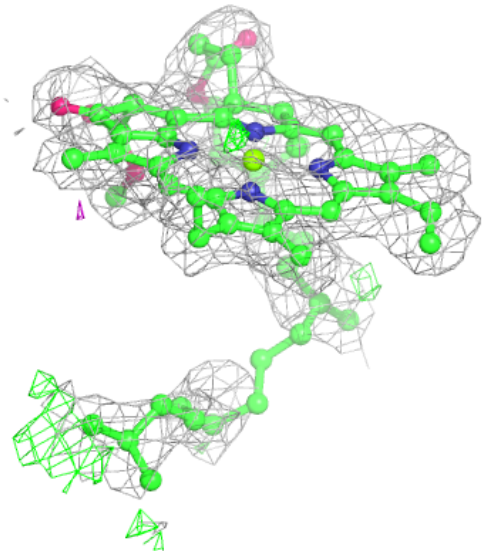


Electron density around CLA C 307:

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

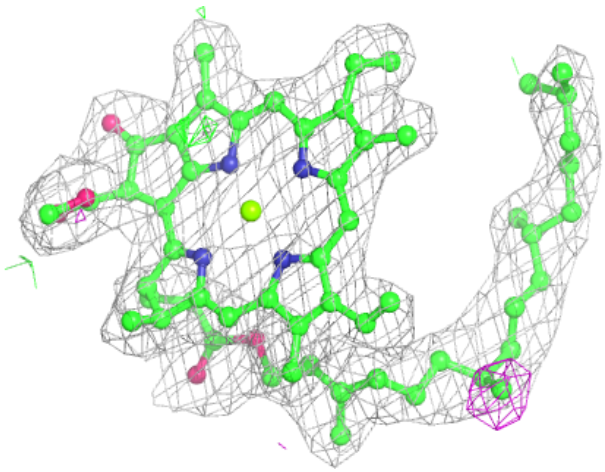


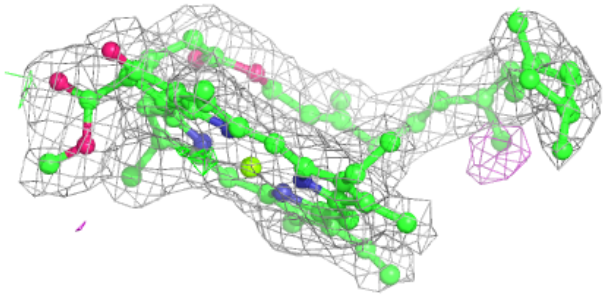


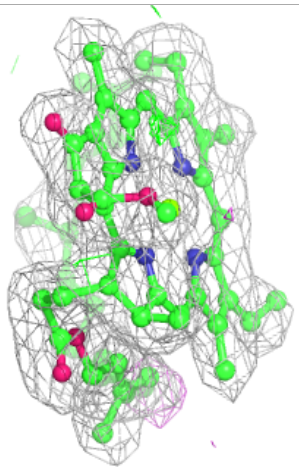


Electron density around CLA B 306:

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

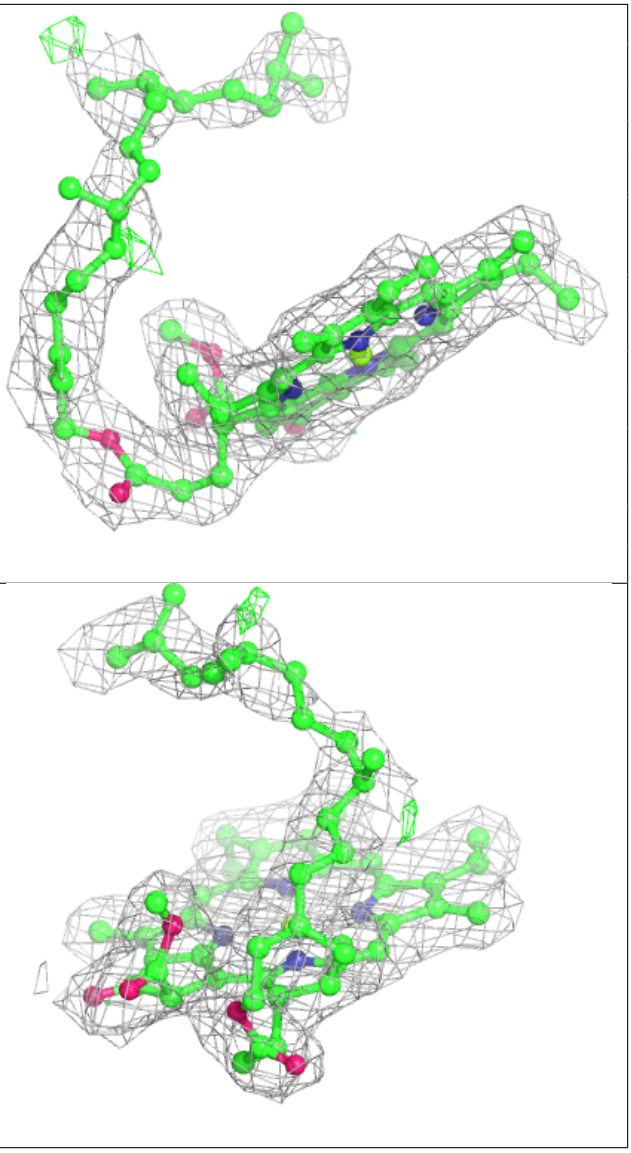






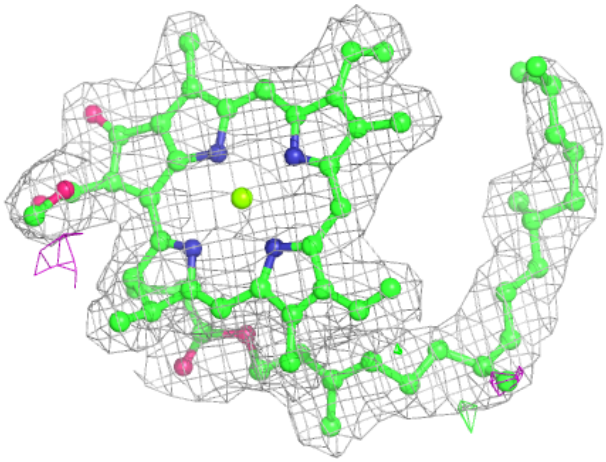
Electron density around CLA A 307:

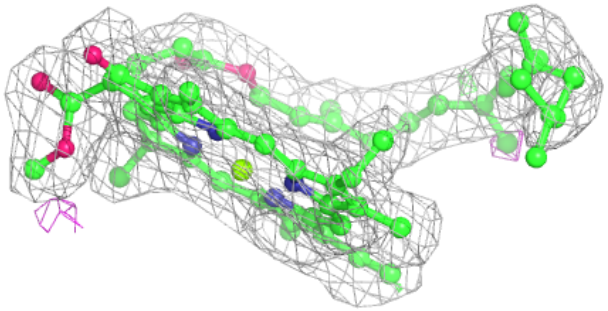
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

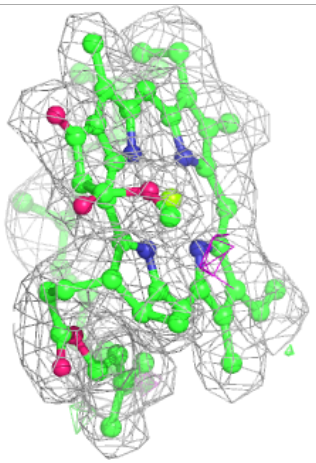


Electron density around CLA C 306:

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

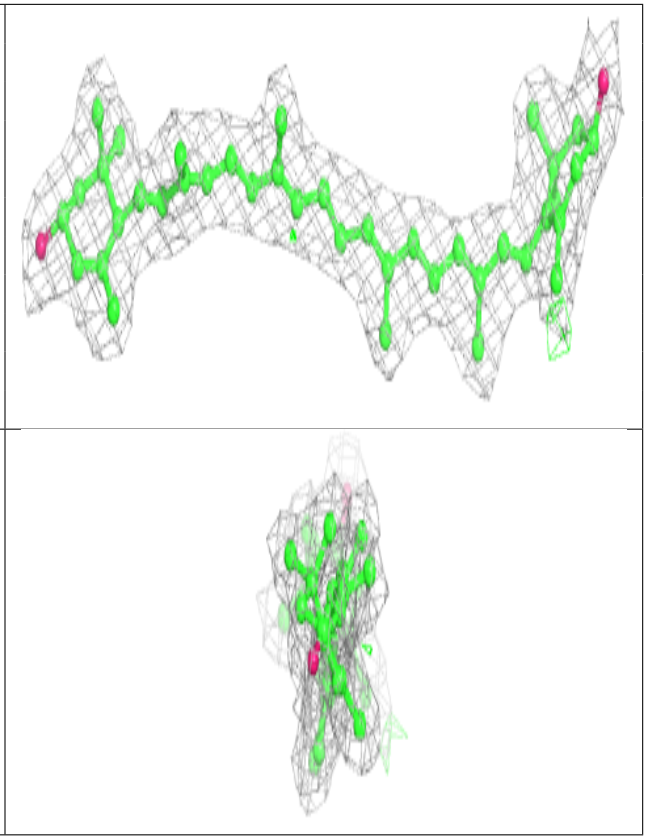






Electron density around LUT C 302:

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



6.5 Other polymers (i)

There are no such residues in this entry.