Full wwPDB EM Validation Report ⓘ

Oct 7, 2023 – 01:17 PM EDT

PDB ID	:	8HLV
EMDB ID	:	EMD-34883
Title	:	Bry-LHCII homotrimer of Bryopsis corticulans
Authors	:	Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on	:	2022-12-01
Resolution	:	2.55 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.55 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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	306	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	A	318	X	-	-	-
5	CHL	B	305	X	-	-	-
5	CHL	B	306	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	B	318	X	-	-	-
5	CHL	C	305	X	-	-	-
5	CHL	C	306	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	-	-	-
5	CHL	C	318	X	-	-	-
6	CLA	A	307	X	-	-	-
6	CLA	A	308	X	-	-	-
6	CLA	A	314	X	-	-	-
6	CLA	A	315	X	-	-	-
6	CLA	A	316	X	-	-	-
6	CLA	A	317	X	-	-	-
6	CLA	B	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CLA	B	308	X	-	-	-
6	CLA	B	314	X	-	-	-
6	CLA	B	315	X	-	-	-
6	CLA	B	316	X	-	-	-
6	CLA	B	317	X	-	-	-
6	CLA	C	307	X	-	-	-
6	CLA	C	308	X	-	-	-
6	CLA	C	314	X	-	-	-
6	CLA	C	315	X	-	-	-
6	CLA	C	316	X	-	-	-
6	CLA	C	317	X	-	-	-

2 Entry composition

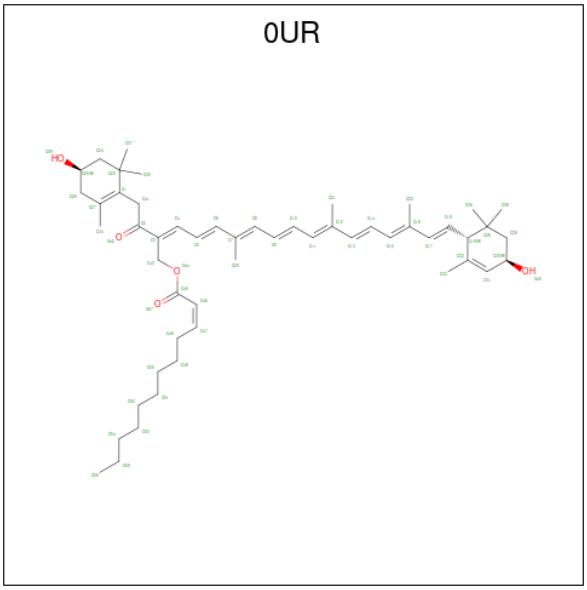
There are 7 unique types of molecules in this entry. The entry contains 8136 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1.

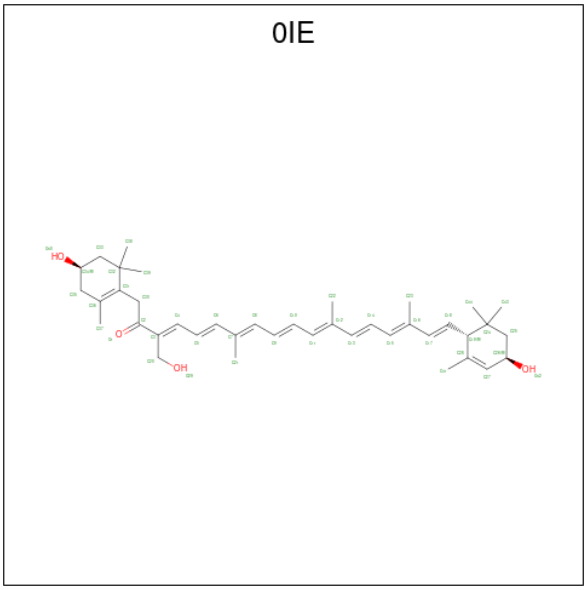
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	223	Total	C	N	O	S	0	0
			1690	1097	268	315	10		
1	B	223	Total	C	N	O	S	0	0
			1690	1097	268	315	10		
1	C	223	Total	C	N	O	S	0	0
			1690	1097	268	315	10		

- Molecule 2 is Siphonein (three-letter code: 0UR) (formula: $C_{52}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



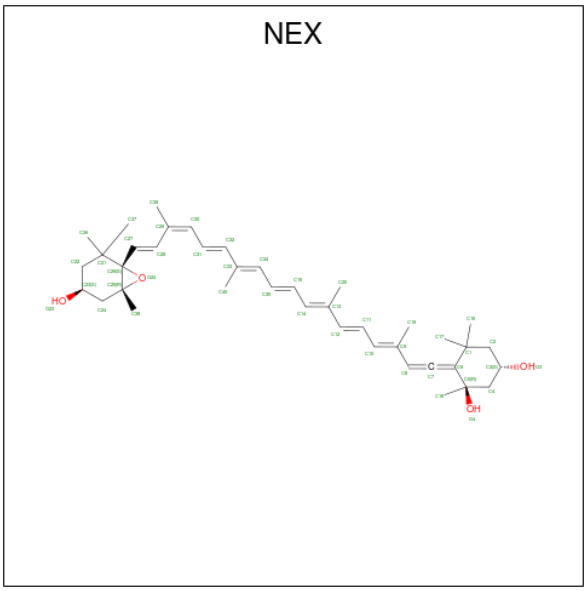
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O		0
			52	47	5		
2	B	1	Total	C	O		0
			52	47	5		
2	C	1	Total	C	O		0
			52	47	5		

- Molecule 3 is Siphonaxanthin (three-letter code: 0IE) (formula: $C_{40}H_{56}O_4$).



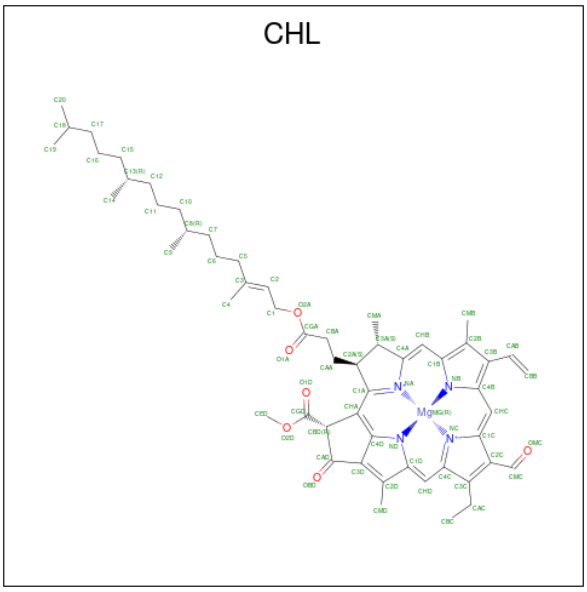
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C O 44 40 4	0
3	A	1	Total C O 44 40 4	0
3	B	1	Total C O 44 40 4	0
3	B	1	Total C O 44 40 4	0
3	C	1	Total C O 44 40 4	0
3	C	1	Total C O 44 40 4	0

- Molecule 4 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: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
5	A	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
5	A	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
5	A	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
5	A	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
5	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
5	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
5	A	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
5	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
5	B	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
5	B	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
5	B	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
5	B	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
5	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
5	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
5	B	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
5	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
5	C	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
5	C	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
5	C	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
5	C	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
5	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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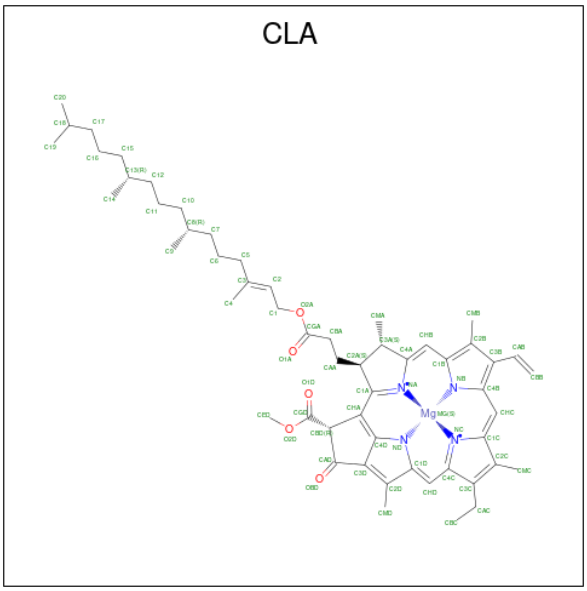
Mol	Chain	Residues	Atoms					AltConf
5	C	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	C	1	Total 44	C 35	Mg 1	N 4	O 4	0

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



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

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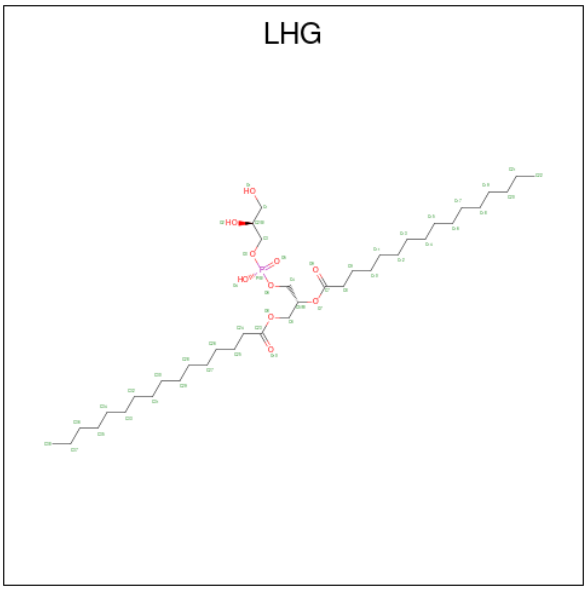
Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
6	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
6	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
6	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
6	C	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
6	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
6	C	1	Total	C	Mg	N	O	0
			63	53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

- Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	O	P	0
			43	32	10	1	
7	B	1	Total	C	O	P	0
			43	32	10	1	

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Mol	Chain	Residues	Atoms				AltConf
7	C	1	Total	C	O	P	0
			43	32	10	1	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	614955	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.903	Depositor
Minimum map value	-0.282	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.207	Depositor
Map size (Å)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

57 ligands are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	CHL	C	312	-	66,74,74	1.95	14 (21%)	73,114,114	3.10	27 (36%)
3	0IE	C	303	-	42,45,45	1.42	6 (14%)	49,63,63	1.60	9 (18%)
5	CHL	A	318	-	44,52,74	2.31	13 (29%)	46,87,114	3.68	23 (50%)
2	0UR	A	301	-	50,53,58	0.98	1 (2%)	58,72,77	1.67	12 (20%)
4	NEX	B	304	-	38,46,46	0.97	2 (5%)	50,70,70	1.20	6 (12%)
4	NEX	C	304	-	38,46,46	0.98	2 (5%)	50,70,70	1.28	6 (12%)
6	CLA	A	316	1	45,53,73	1.76	7 (15%)	52,89,113	1.60	6 (11%)
2	0UR	B	301	-	50,53,58	0.97	1 (2%)	58,72,77	1.75	14 (24%)
5	CHL	C	310	-	51,59,74	2.24	14 (27%)	55,96,114	3.51	27 (49%)
5	CHL	A	311	-	61,69,74	2.06	13 (21%)	66,107,114	3.25	30 (45%)
5	CHL	B	312	-	66,74,74	1.96	14 (21%)	73,114,114	3.11	27 (36%)
3	0IE	B	303	-	42,45,45	1.43	6 (14%)	49,63,63	1.61	9 (18%)
5	CHL	A	310	-	51,59,74	2.24	15 (29%)	55,96,114	3.50	27 (49%)
6	CLA	B	308	-	50,58,73	1.67	6 (12%)	58,95,113	1.57	9 (15%)
5	CHL	B	305	1	66,74,74	1.96	13 (19%)	73,114,114	3.03	27 (36%)
5	CHL	C	305	1	66,74,74	1.96	14 (21%)	73,114,114	3.03	27 (36%)
6	CLA	B	307	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	8 (10%)
5	CHL	C	311	-	61,69,74	2.06	14 (22%)	66,107,114	3.25	30 (45%)
3	0IE	B	302	-	42,45,45	1.41	6 (14%)	49,63,63	1.63	9 (18%)
5	CHL	C	318	-	44,52,74	2.31	13 (29%)	46,87,114	3.68	24 (52%)
2	0UR	C	301	-	50,53,58	0.97	1 (2%)	58,72,77	1.72	13 (22%)
7	LHG	C	319	6	42,42,48	1.16	5 (11%)	45,48,54	1.33	4 (8%)
5	CHL	B	313	1	66,74,74	2.00	14 (21%)	73,114,114	2.96	29 (39%)
5	CHL	C	306	1	64,72,74	2.03	15 (23%)	70,111,114	3.11	28 (40%)
5	CHL	C	313	1	66,74,74	2.00	15 (22%)	73,114,114	2.96	29 (39%)
6	CLA	B	316	1	45,53,73	1.76	7 (15%)	52,89,113	1.60	6 (11%)
6	CLA	B	317	1	55,63,73	1.59	6 (10%)	63,100,113	1.47	6 (9%)
6	CLA	C	315	7	63,71,73	1.48	6 (9%)	73,110,113	1.40	6 (8%)
6	CLA	A	315	7	63,71,73	1.48	6 (9%)	73,110,113	1.41	7 (9%)
6	CLA	C	316	1	45,53,73	1.75	7 (15%)	52,89,113	1.60	6 (11%)
7	LHG	B	319	6	42,42,48	1.16	5 (11%)	45,48,54	1.34	4 (8%)
6	CLA	B	315	7	63,71,73	1.48	6 (9%)	73,110,113	1.40	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CLA	C	308	-	50,58,73	1.67	6 (12%)	58,95,113	1.57	7 (12%)
5	CHL	A	309	1	43,51,74	2.33	13 (30%)	45,86,114	3.71	24 (53%)
5	CHL	B	309	1	43,51,74	2.34	14 (32%)	45,86,114	3.72	24 (53%)
5	CHL	B	318	-	47,55,74	2.35	15 (31%)	50,91,114	3.60	24 (48%)
6	CLA	B	314	1	55,63,73	1.61	6 (10%)	64,101,113	1.50	8 (12%)
6	CLA	C	314	1	55,63,73	1.61	6 (10%)	64,101,113	1.49	8 (12%)
6	CLA	A	308	-	50,58,73	1.65	6 (12%)	58,95,113	1.57	8 (13%)
5	CHL	A	306	1	64,72,74	2.03	15 (23%)	70,111,114	3.11	28 (40%)
5	CHL	B	306	1	64,72,74	2.01	15 (23%)	70,111,114	3.08	27 (38%)
3	0IE	C	302	-	42,45,45	1.41	6 (14%)	49,63,63	1.64	9 (18%)
4	NEX	A	304	-	38,46,46	0.90	1 (2%)	50,70,70	1.16	5 (10%)
5	CHL	B	311	-	61,69,74	2.06	13 (21%)	66,107,114	3.26	30 (45%)
3	0IE	A	302	-	42,45,45	1.41	6 (14%)	49,63,63	1.67	10 (20%)
5	CHL	A	312	-	66,74,74	1.96	14 (21%)	73,114,114	3.11	27 (36%)
6	CLA	A	307	-	65,73,73	1.46	6 (9%)	76,113,113	1.43	8 (10%)
3	0IE	A	303	-	42,45,45	1.43	6 (14%)	49,63,63	1.63	9 (18%)
6	CLA	C	307	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	7 (9%)
5	CHL	A	313	1	66,74,74	2.00	15 (22%)	73,114,114	2.95	29 (39%)
6	CLA	C	317	1	55,63,73	1.59	6 (10%)	63,100,113	1.50	6 (9%)
6	CLA	A	317	1	55,63,73	1.61	6 (10%)	63,100,113	1.47	7 (11%)
6	CLA	A	314	1	55,63,73	1.61	6 (10%)	64,101,113	1.50	8 (12%)
5	CHL	C	309	1	43,51,74	2.34	14 (32%)	45,86,114	3.72	24 (53%)
5	CHL	B	310	-	51,59,74	2.24	14 (27%)	55,96,114	3.51	26 (47%)
5	CHL	A	305	1	66,74,74	1.96	14 (21%)	73,114,114	3.03	27 (36%)
7	LHG	A	319	6	42,42,48	1.16	5 (11%)	45,48,54	1.36	4 (8%)

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
5	CHL	C	312	-	3/3/20/26	15/39/137/137	-
3	0IE	C	303	-	-	9/33/72/72	0/2/2/2
5	CHL	A	318	-	3/3/15/26	3/13/111/137	-
2	0UR	A	301	-	-	9/42/81/86	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NEX	B	304	-	-	2/27/83/83	0/3/3/3
4	NEX	C	304	-	-	2/27/83/83	0/3/3/3
6	CLA	A	316	1	1/1/11/20	4/13/91/115	-
2	0UR	B	301	-	-	9/42/81/86	0/2/2/2
5	CHL	C	310	-	3/3/17/26	8/21/119/137	-
5	CHL	A	311	-	3/3/18/26	19/33/131/137	-
5	CHL	B	312	-	3/3/20/26	14/39/137/137	-
3	0IE	B	303	-	-	9/33/72/72	0/2/2/2
5	CHL	A	310	-	3/3/17/26	8/21/119/137	-
6	CLA	B	308	-	1/1/12/20	6/19/97/115	-
5	CHL	B	305	1	3/3/20/26	17/39/137/137	-
5	CHL	C	305	1	3/3/20/26	15/39/137/137	-
6	CLA	B	307	-	1/1/15/20	7/37/115/115	-
5	CHL	C	311	-	3/3/18/26	19/33/131/137	-
3	0IE	B	302	-	-	6/33/72/72	0/2/2/2
5	CHL	C	318	-	3/3/15/26	3/13/111/137	-
2	0UR	C	301	-	-	9/42/81/86	0/2/2/2
7	LHG	C	319	6	-	22/47/47/53	-
5	CHL	B	313	1	3/3/20/26	15/39/137/137	-
5	CHL	C	306	1	3/3/19/26	17/37/135/137	-
5	CHL	C	313	1	3/3/20/26	15/39/137/137	-
6	CLA	B	316	1	1/1/11/20	3/13/91/115	-
6	CLA	B	317	1	1/1/12/20	6/25/103/115	-
6	CLA	C	315	7	1/1/14/20	5/35/113/115	-
6	CLA	A	315	7	1/1/14/20	9/35/113/115	-
6	CLA	C	316	1	1/1/11/20	2/13/91/115	-
7	LHG	B	319	6	-	24/47/47/53	-
6	CLA	B	315	7	1/1/14/20	8/35/113/115	-
6	CLA	C	308	-	1/1/12/20	7/19/97/115	-
5	CHL	A	309	1	3/3/15/26	2/12/110/137	-
5	CHL	B	309	1	3/3/15/26	2/12/110/137	-
5	CHL	B	318	-	3/3/16/26	7/17/115/137	-
6	CLA	B	314	1	1/1/13/20	4/25/103/115	-
6	CLA	C	314	1	1/1/13/20	4/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLA	A	308	-	1/1/12/20	8/19/97/115	-
5	CHL	A	306	1	3/3/19/26	17/37/135/137	-
5	CHL	B	306	1	3/3/19/26	14/37/135/137	-
3	0IE	C	302	-	-	8/33/72/72	0/2/2/2
4	NEX	A	304	-	-	3/27/83/83	0/3/3/3
5	CHL	B	311	-	3/3/18/26	19/33/131/137	-
3	0IE	A	302	-	-	8/33/72/72	0/2/2/2
5	CHL	A	312	-	3/3/20/26	14/39/137/137	-
6	CLA	A	307	-	1/1/15/20	6/37/115/115	-
3	0IE	A	303	-	-	6/33/72/72	0/2/2/2
6	CLA	C	307	-	1/1/15/20	7/37/115/115	-
5	CHL	A	313	1	3/3/20/26	15/39/137/137	-
6	CLA	C	317	1	1/1/12/20	8/25/103/115	-
6	CLA	A	317	1	1/1/12/20	7/25/103/115	-
6	CLA	A	314	1	1/1/13/20	4/25/103/115	-
5	CHL	C	309	1	3/3/15/26	2/12/110/137	-
5	CHL	B	310	-	3/3/17/26	8/21/119/137	-
5	CHL	A	305	1	3/3/20/26	16/39/137/137	-
7	LHG	A	319	6	-	24/47/47/53	-

All (507) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	314	CLA	C4B-NB	7.31	1.41	1.35
6	A	317	CLA	C4B-NB	7.30	1.41	1.35
6	A	314	CLA	C4B-NB	7.26	1.41	1.35
6	C	308	CLA	C4B-NB	7.26	1.41	1.35
6	B	307	CLA	C4B-NB	7.25	1.41	1.35
6	B	308	CLA	C4B-NB	7.25	1.41	1.35
6	B	314	CLA	C4B-NB	7.23	1.41	1.35
6	C	317	CLA	C4B-NB	7.19	1.41	1.35
6	B	316	CLA	C4B-NB	7.18	1.41	1.35
6	B	317	CLA	C4B-NB	7.18	1.41	1.35
6	A	316	CLA	C4B-NB	7.18	1.41	1.35
6	C	307	CLA	C4B-NB	7.17	1.41	1.35
6	A	315	CLA	C4B-NB	7.15	1.41	1.35
6	A	307	CLA	C4B-NB	7.15	1.41	1.35
6	C	316	CLA	C4B-NB	7.12	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	315	CLA	C4B-NB	7.08	1.41	1.35
6	B	315	CLA	C4B-NB	7.08	1.41	1.35
6	A	308	CLA	C4B-NB	7.05	1.41	1.35
5	A	306	CHL	C3B-C2B	5.58	1.48	1.40
5	C	306	CHL	C3B-C2B	5.57	1.48	1.40
5	A	310	CHL	C3B-C2B	5.33	1.47	1.40
5	A	318	CHL	C3B-C2B	5.33	1.47	1.40
5	C	310	CHL	C3B-C2B	5.32	1.47	1.40
5	B	313	CHL	C3B-C2B	5.30	1.47	1.40
5	A	309	CHL	C3B-C2B	5.29	1.47	1.40
5	B	309	CHL	C3B-C2B	5.28	1.47	1.40
5	B	310	CHL	C3B-C2B	5.28	1.47	1.40
5	C	309	CHL	C3B-C2B	5.28	1.47	1.40
5	B	318	CHL	C2C-C3C	5.27	1.48	1.36
5	C	318	CHL	C2C-C3C	5.27	1.48	1.36
5	A	306	CHL	C2C-C3C	5.27	1.48	1.36
5	B	306	CHL	C2C-C3C	5.27	1.48	1.36
5	C	306	CHL	C2C-C3C	5.27	1.48	1.36
5	B	306	CHL	C3B-C2B	5.26	1.47	1.40
5	C	318	CHL	C3B-C2B	5.26	1.47	1.40
5	C	311	CHL	C3B-C2B	5.26	1.47	1.40
5	A	313	CHL	C3B-C2B	5.24	1.47	1.40
5	A	318	CHL	C2C-C3C	5.23	1.48	1.36
5	B	311	CHL	C3B-C2B	5.22	1.47	1.40
5	A	311	CHL	C3B-C2B	5.22	1.47	1.40
5	C	313	CHL	C3B-C2B	5.22	1.47	1.40
5	B	318	CHL	C3B-C2B	5.20	1.47	1.40
5	C	312	CHL	C3B-C2B	5.20	1.47	1.40
5	B	312	CHL	C3B-C2B	5.19	1.47	1.40
5	A	312	CHL	C3B-C2B	5.15	1.47	1.40
5	A	305	CHL	C3B-C2B	5.15	1.47	1.40
5	B	305	CHL	C3B-C2B	5.14	1.47	1.40
5	C	309	CHL	O2D-CGD	5.13	1.45	1.33
5	B	309	CHL	O2D-CGD	5.12	1.45	1.33
5	B	306	CHL	O2D-CGD	5.11	1.45	1.33
5	B	310	CHL	O2D-CGD	5.11	1.45	1.33
5	C	311	CHL	O2D-CGD	5.11	1.45	1.33
5	C	310	CHL	O2D-CGD	5.10	1.45	1.33
5	C	306	CHL	O2D-CGD	5.10	1.45	1.33
5	A	306	CHL	O2D-CGD	5.10	1.45	1.33
5	A	305	CHL	O2D-CGD	5.10	1.45	1.33
5	A	309	CHL	O2D-CGD	5.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	311	CHL	O2D-CGD	5.09	1.45	1.33
5	A	310	CHL	O2D-CGD	5.09	1.45	1.33
5	A	311	CHL	O2D-CGD	5.08	1.45	1.33
5	C	312	CHL	O2D-CGD	5.08	1.45	1.33
5	C	305	CHL	O2D-CGD	5.08	1.45	1.33
5	A	312	CHL	O2D-CGD	5.08	1.45	1.33
5	C	313	CHL	C2C-C3C	5.06	1.47	1.36
5	B	312	CHL	O2D-CGD	5.05	1.45	1.33
5	C	305	CHL	C3B-C2B	5.05	1.47	1.40
5	B	305	CHL	O2D-CGD	5.05	1.45	1.33
5	B	318	CHL	O2D-CGD	5.05	1.45	1.33
5	B	313	CHL	C2C-C3C	5.03	1.47	1.36
5	A	313	CHL	C2C-C3C	5.02	1.47	1.36
5	A	313	CHL	O2D-CGD	4.99	1.45	1.33
5	B	312	CHL	C2C-C3C	4.99	1.47	1.36
5	C	310	CHL	CHC-C1C	4.99	1.47	1.35
5	C	313	CHL	O2D-CGD	4.98	1.45	1.33
5	A	309	CHL	C2C-C3C	4.97	1.47	1.36
5	C	311	CHL	C2C-C3C	4.97	1.47	1.36
5	A	311	CHL	C2C-C3C	4.96	1.47	1.36
5	B	313	CHL	O2D-CGD	4.96	1.45	1.33
5	B	309	CHL	C2C-C3C	4.96	1.47	1.36
5	B	311	CHL	C2C-C3C	4.96	1.47	1.36
5	C	309	CHL	C2C-C3C	4.95	1.47	1.36
5	C	318	CHL	O2D-CGD	4.95	1.45	1.33
5	A	310	CHL	CHC-C1C	4.94	1.47	1.35
5	B	305	CHL	C2C-C3C	4.94	1.47	1.36
5	C	305	CHL	C2C-C3C	4.94	1.47	1.36
5	A	318	CHL	O2D-CGD	4.94	1.45	1.33
5	B	310	CHL	CHC-C1C	4.94	1.47	1.35
5	B	310	CHL	C2C-C3C	4.93	1.47	1.36
5	A	312	CHL	C2C-C3C	4.92	1.47	1.36
5	A	305	CHL	C2C-C3C	4.91	1.47	1.36
5	C	312	CHL	C2C-C3C	4.91	1.47	1.36
5	C	310	CHL	C2C-C3C	4.90	1.47	1.36
5	A	310	CHL	C2C-C3C	4.89	1.47	1.36
5	A	311	CHL	CHC-C1C	4.88	1.47	1.35
5	A	309	CHL	CHC-C1C	4.87	1.47	1.35
5	B	311	CHL	CHC-C1C	4.86	1.47	1.35
5	B	309	CHL	CHC-C1C	4.86	1.47	1.35
5	B	306	CHL	CHC-C1C	4.86	1.47	1.35
5	C	311	CHL	CHC-C1C	4.85	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	309	CHL	CHC-C1C	4.84	1.47	1.35
5	B	312	CHL	CHC-C1C	4.83	1.47	1.35
5	A	306	CHL	CHC-C1C	4.81	1.47	1.35
5	C	306	CHL	CHC-C1C	4.80	1.47	1.35
5	B	305	CHL	CHC-C1C	4.78	1.47	1.35
5	C	313	CHL	CHC-C1C	4.78	1.47	1.35
5	A	305	CHL	CHC-C1C	4.78	1.47	1.35
5	B	313	CHL	CHC-C1C	4.78	1.47	1.35
5	C	312	CHL	CHC-C1C	4.78	1.47	1.35
5	A	313	CHL	CHC-C1C	4.77	1.47	1.35
5	A	312	CHL	CHC-C1C	4.76	1.47	1.35
5	C	305	CHL	CHC-C1C	4.74	1.47	1.35
5	B	318	CHL	CHC-C1C	4.73	1.47	1.35
5	C	318	CHL	CHC-C1C	4.72	1.47	1.35
5	A	318	CHL	CHC-C1C	4.68	1.47	1.35
5	B	318	CHL	CHD-C1D	4.54	1.47	1.38
5	B	310	CHL	C1D-ND	-4.53	1.32	1.37
5	B	313	CHL	CHD-C1D	4.48	1.47	1.38
5	A	313	CHL	CHD-C1D	4.47	1.47	1.38
5	A	310	CHL	C1D-ND	-4.46	1.32	1.37
5	C	313	CHL	CHD-C1D	4.45	1.47	1.38
5	C	310	CHL	C1D-ND	-4.42	1.32	1.37
5	C	318	CHL	CHD-C1D	4.41	1.47	1.38
5	A	313	CHL	O2A-CGA	4.39	1.46	1.33
5	B	313	CHL	O2A-CGA	4.39	1.46	1.33
5	B	313	CHL	C1D-ND	-4.38	1.32	1.37
5	C	313	CHL	O2A-CGA	4.37	1.46	1.33
5	A	311	CHL	O2A-CGA	4.36	1.46	1.33
5	A	309	CHL	C1D-ND	-4.36	1.32	1.37
5	A	318	CHL	CHD-C1D	4.36	1.46	1.38
5	C	309	CHL	C1D-ND	-4.36	1.32	1.37
5	C	313	CHL	C1D-ND	-4.35	1.32	1.37
5	C	311	CHL	O2A-CGA	4.35	1.46	1.33
5	B	311	CHL	O2A-CGA	4.35	1.46	1.33
5	C	306	CHL	C1D-ND	-4.35	1.32	1.37
5	A	306	CHL	C1D-ND	-4.34	1.32	1.37
5	B	306	CHL	C1D-ND	-4.34	1.32	1.37
5	C	305	CHL	C1D-ND	-4.33	1.32	1.37
5	B	309	CHL	C1D-ND	-4.32	1.32	1.37
5	B	305	CHL	O2A-CGA	4.31	1.45	1.33
5	B	311	CHL	C1D-ND	-4.31	1.32	1.37
5	C	311	CHL	C1D-ND	-4.30	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	311	CHL	CHD-C1D	4.29	1.46	1.38
5	A	313	CHL	C1D-ND	-4.29	1.32	1.37
5	A	305	CHL	O2A-CGA	4.29	1.45	1.33
5	A	305	CHL	CHD-C1D	4.29	1.46	1.38
5	C	311	CHL	CHD-C1D	4.28	1.46	1.38
5	A	305	CHL	C1D-ND	-4.28	1.32	1.37
5	B	311	CHL	CHD-C1D	4.28	1.46	1.38
5	A	306	CHL	CHD-C1D	4.27	1.46	1.38
5	C	310	CHL	O2A-CGA	4.27	1.45	1.33
5	B	312	CHL	C1D-ND	-4.27	1.32	1.37
5	A	311	CHL	C1D-ND	-4.27	1.32	1.37
5	B	305	CHL	C1D-ND	-4.27	1.32	1.37
5	C	305	CHL	CHD-C1D	4.27	1.46	1.38
5	C	312	CHL	O2A-CGA	4.27	1.45	1.33
5	B	312	CHL	O2A-CGA	4.27	1.45	1.33
5	A	310	CHL	O2A-CGA	4.27	1.45	1.33
5	B	310	CHL	O2A-CGA	4.25	1.45	1.33
5	A	312	CHL	C1D-ND	-4.25	1.32	1.37
5	C	305	CHL	O2A-CGA	4.25	1.45	1.33
5	B	306	CHL	CHD-C1D	4.24	1.46	1.38
5	A	312	CHL	O2A-CGA	4.24	1.45	1.33
5	C	306	CHL	CHD-C1D	4.24	1.46	1.38
5	B	305	CHL	CHD-C1D	4.23	1.46	1.38
5	C	309	CHL	CHD-C1D	4.23	1.46	1.38
5	A	309	CHL	CHD-C1D	4.22	1.46	1.38
5	A	312	CHL	CHD-C1D	4.21	1.46	1.38
5	B	309	CHL	CHD-C1D	4.20	1.46	1.38
5	C	306	CHL	O2A-CGA	4.20	1.45	1.33
5	C	312	CHL	CHD-C1D	4.20	1.46	1.38
5	C	312	CHL	C1D-ND	-4.20	1.32	1.37
5	A	306	CHL	O2A-CGA	4.19	1.45	1.33
5	B	312	CHL	CHD-C1D	4.18	1.46	1.38
5	B	306	CHL	O2A-CGA	4.17	1.45	1.33
5	B	318	CHL	C1D-ND	-4.14	1.32	1.37
5	B	310	CHL	CHD-C1D	4.12	1.46	1.38
2	B	301	0UR	O44-C45	4.11	1.44	1.34
5	C	318	CHL	C1D-ND	-4.11	1.32	1.37
5	A	310	CHL	CHD-C1D	4.11	1.46	1.38
4	B	304	NEX	C7-C8	4.10	1.38	1.32
5	A	318	CHL	C1D-ND	-4.09	1.32	1.37
2	C	301	0UR	O44-C45	4.08	1.44	1.34
2	A	301	0UR	O44-C45	4.08	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	310	CHL	CHD-C1D	4.08	1.46	1.38
5	B	318	CHL	O2A-CGA	4.08	1.46	1.33
5	B	318	CHL	CHD-C4C	4.07	1.48	1.39
3	A	303	0IE	C15-C16	4.02	1.41	1.35
5	C	313	CHL	CHD-C4C	3.99	1.48	1.39
5	B	313	CHL	CHD-C4C	3.98	1.48	1.39
3	A	302	0IE	C8-C7	3.97	1.41	1.35
5	A	313	CHL	CHD-C4C	3.97	1.48	1.39
3	B	303	0IE	C15-C16	3.96	1.41	1.35
3	A	303	0IE	C11-C12	3.96	1.41	1.35
4	C	304	NEX	C7-C8	3.95	1.38	1.32
5	C	318	CHL	CHD-C4C	3.94	1.48	1.39
3	A	303	0IE	C8-C7	3.94	1.41	1.35
3	C	303	0IE	C15-C16	3.93	1.41	1.35
3	B	303	0IE	C8-C7	3.93	1.41	1.35
5	A	318	CHL	CHD-C4C	3.91	1.48	1.39
3	B	302	0IE	C8-C7	3.89	1.40	1.35
3	C	302	0IE	C11-C12	3.89	1.40	1.35
3	B	303	0IE	C11-C12	3.88	1.40	1.35
5	C	306	CHL	CHD-C4C	3.87	1.48	1.39
5	A	306	CHL	CHD-C4C	3.86	1.48	1.39
5	B	311	CHL	CHD-C4C	3.85	1.48	1.39
3	C	302	0IE	C8-C7	3.85	1.40	1.35
3	A	302	0IE	C11-C12	3.84	1.40	1.35
3	C	302	0IE	C15-C16	3.84	1.40	1.35
5	C	311	CHL	CHD-C4C	3.84	1.48	1.39
5	A	311	CHL	CHD-C4C	3.83	1.48	1.39
3	B	302	0IE	C11-C12	3.83	1.40	1.35
5	A	305	CHL	CHD-C4C	3.83	1.48	1.39
5	B	306	CHL	CHD-C4C	3.82	1.48	1.39
5	C	305	CHL	CHD-C4C	3.82	1.47	1.39
3	C	303	0IE	C11-C12	3.81	1.40	1.35
3	A	302	0IE	C15-C16	3.79	1.40	1.35
5	B	312	CHL	CHD-C4C	3.79	1.47	1.39
5	B	309	CHL	CHD-C4C	3.79	1.47	1.39
5	C	312	CHL	CHD-C4C	3.79	1.47	1.39
5	B	305	CHL	CHD-C4C	3.79	1.47	1.39
3	C	303	0IE	C8-C7	3.78	1.40	1.35
5	A	312	CHL	CHD-C4C	3.78	1.47	1.39
6	B	317	CLA	C1D-ND	3.77	1.42	1.37
3	B	302	0IE	C15-C16	3.77	1.40	1.35
5	A	309	CHL	CHD-C4C	3.76	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	309	CHL	CHD-C4C	3.75	1.47	1.39
5	C	310	CHL	CHD-C4C	3.75	1.47	1.39
6	C	317	CLA	C1D-ND	3.73	1.42	1.37
5	A	310	CHL	CHD-C4C	3.73	1.47	1.39
5	B	310	CHL	CHD-C4C	3.71	1.47	1.39
6	A	317	CLA	C1D-ND	3.70	1.42	1.37
6	C	315	CLA	C1D-ND	3.70	1.42	1.37
6	C	307	CLA	C1D-ND	3.69	1.42	1.37
6	B	316	CLA	C1D-ND	3.69	1.42	1.37
5	B	305	CHL	OBD-CAD	3.68	1.28	1.22
6	A	315	CLA	C1D-ND	3.68	1.42	1.37
5	A	311	CHL	OBD-CAD	3.68	1.28	1.22
6	A	316	CLA	C1D-ND	3.67	1.42	1.37
6	B	315	CLA	C1D-ND	3.66	1.42	1.37
5	B	318	CHL	OBD-CAD	3.65	1.28	1.22
5	C	305	CHL	OBD-CAD	3.65	1.28	1.22
5	B	311	CHL	OBD-CAD	3.65	1.28	1.22
6	B	314	CLA	C1D-ND	3.65	1.42	1.37
6	B	308	CLA	C1D-ND	3.64	1.42	1.37
6	C	314	CLA	C1D-ND	3.64	1.42	1.37
6	A	307	CLA	C1D-ND	3.64	1.42	1.37
6	C	316	CLA	C1D-ND	3.64	1.42	1.37
6	B	307	CLA	C1D-ND	3.63	1.42	1.37
5	C	311	CHL	OBD-CAD	3.63	1.28	1.22
6	A	314	CLA	C1D-ND	3.63	1.42	1.37
5	A	318	CHL	OBD-CAD	3.62	1.28	1.22
5	B	309	CHL	OBD-CAD	3.62	1.28	1.22
5	C	318	CHL	OBD-CAD	3.62	1.28	1.22
5	C	309	CHL	OBD-CAD	3.62	1.28	1.22
5	A	305	CHL	OBD-CAD	3.62	1.28	1.22
6	A	308	CLA	C1D-ND	3.61	1.42	1.37
6	C	308	CLA	C1D-ND	3.60	1.42	1.37
5	A	312	CHL	OBD-CAD	3.60	1.28	1.22
5	C	312	CHL	OBD-CAD	3.59	1.28	1.22
5	A	309	CHL	OBD-CAD	3.59	1.28	1.22
5	A	313	CHL	OBD-CAD	3.57	1.28	1.22
5	C	313	CHL	OBD-CAD	3.54	1.28	1.22
5	B	313	CHL	OBD-CAD	3.54	1.28	1.22
5	B	312	CHL	OBD-CAD	3.53	1.28	1.22
5	B	313	CHL	C3D-C2D	3.52	1.48	1.39
4	A	304	NEX	C7-C8	3.51	1.37	1.32
5	B	310	CHL	OBD-CAD	3.51	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	313	CHL	C3D-C2D	3.50	1.48	1.39
5	C	310	CHL	OBD-CAD	3.49	1.28	1.22
5	C	313	CHL	C3D-C2D	3.48	1.48	1.39
5	A	310	CHL	OBD-CAD	3.46	1.28	1.22
5	A	306	CHL	C3D-C2D	3.44	1.48	1.39
5	B	306	CHL	C3D-C2D	3.44	1.48	1.39
5	A	311	CHL	C3D-C2D	3.44	1.48	1.39
5	C	306	CHL	C3D-C2D	3.43	1.48	1.39
5	B	318	CHL	C3D-C2D	3.43	1.48	1.39
5	C	311	CHL	C3D-C2D	3.41	1.48	1.39
5	B	311	CHL	C3D-C2D	3.40	1.48	1.39
5	B	309	CHL	C3D-C2D	3.39	1.48	1.39
5	A	318	CHL	C3D-C2D	3.39	1.48	1.39
5	C	305	CHL	C3D-C2D	3.39	1.48	1.39
5	C	318	CHL	C3D-C2D	3.37	1.48	1.39
5	A	306	CHL	OBD-CAD	3.37	1.28	1.22
5	C	306	CHL	OBD-CAD	3.36	1.28	1.22
6	B	314	CLA	CHC-C1C	3.36	1.43	1.35
5	B	305	CHL	C3D-C2D	3.36	1.48	1.39
6	A	314	CLA	CHC-C1C	3.36	1.43	1.35
5	A	309	CHL	C3D-C2D	3.36	1.48	1.39
5	C	309	CHL	C3D-C2D	3.35	1.48	1.39
5	A	305	CHL	C3D-C2D	3.35	1.48	1.39
5	A	312	CHL	C3D-C2D	3.33	1.48	1.39
5	B	312	CHL	C3D-C2D	3.33	1.48	1.39
6	C	314	CLA	CHC-C1C	3.33	1.43	1.35
5	C	312	CHL	C3D-C2D	3.30	1.48	1.39
5	A	310	CHL	C3D-C2D	3.30	1.48	1.39
5	B	306	CHL	OBD-CAD	3.29	1.28	1.22
5	B	310	CHL	C3D-C2D	3.29	1.48	1.39
5	C	310	CHL	C3D-C2D	3.27	1.48	1.39
6	A	317	CLA	CHC-C1C	3.12	1.43	1.35
6	B	316	CLA	C4D-ND	-3.10	1.33	1.37
6	C	308	CLA	CHC-C1C	3.09	1.42	1.35
6	B	308	CLA	CHC-C1C	3.09	1.42	1.35
6	B	315	CLA	CHC-C1C	3.08	1.42	1.35
6	A	316	CLA	CHC-C1C	3.08	1.42	1.35
6	A	315	CLA	CHC-C1C	3.07	1.42	1.35
6	A	308	CLA	CHC-C1C	3.07	1.42	1.35
6	A	307	CLA	C4D-ND	-3.07	1.33	1.37
6	B	317	CLA	C4D-ND	-3.07	1.33	1.37
6	C	308	CLA	C4D-ND	-3.06	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	308	CLA	C4D-ND	-3.06	1.33	1.37
6	A	316	CLA	C4D-ND	-3.05	1.33	1.37
6	C	316	CLA	CHC-C1C	3.04	1.42	1.35
6	C	314	CLA	C4D-ND	-3.04	1.33	1.37
6	B	316	CLA	CHC-C1C	3.04	1.42	1.35
6	C	317	CLA	CHC-C1C	3.04	1.42	1.35
6	C	316	CLA	C4D-ND	-3.04	1.33	1.37
6	C	315	CLA	CHC-C1C	3.03	1.42	1.35
6	B	314	CLA	C4D-ND	-3.03	1.33	1.37
6	C	317	CLA	C4D-ND	-3.03	1.33	1.37
6	A	308	CLA	C4D-ND	-3.02	1.33	1.37
6	B	317	CLA	CHC-C1C	3.02	1.42	1.35
6	A	314	CLA	C4D-ND	-3.01	1.33	1.37
6	B	315	CLA	C4D-ND	-3.01	1.33	1.37
6	A	315	CLA	C4D-ND	-3.00	1.33	1.37
6	C	315	CLA	C4D-ND	-2.98	1.33	1.37
6	B	307	CLA	CHC-C1C	2.98	1.42	1.35
6	A	317	CLA	C4D-ND	-2.97	1.33	1.37
6	C	307	CLA	CHC-C1C	2.95	1.42	1.35
6	C	307	CLA	C4D-ND	-2.95	1.33	1.37
6	A	307	CLA	CHC-C1C	2.94	1.42	1.35
5	C	313	CHL	MG-NA	-2.91	1.99	2.06
5	A	313	CHL	MG-NA	-2.91	1.99	2.06
5	B	313	CHL	MG-NA	-2.87	1.99	2.06
6	B	307	CLA	C4D-ND	-2.87	1.33	1.37
5	B	311	CHL	MG-NA	-2.81	1.99	2.06
7	A	319	LHG	C26-C25	-2.81	1.35	1.51
5	C	306	CHL	MG-NA	-2.81	1.99	2.06
7	C	319	LHG	C26-C25	-2.80	1.35	1.51
5	A	306	CHL	MG-NA	-2.80	1.99	2.06
7	B	319	LHG	C26-C25	-2.79	1.35	1.51
5	A	311	CHL	MG-NA	-2.79	1.99	2.06
5	C	311	CHL	MG-NA	-2.79	1.99	2.06
5	B	306	CHL	MG-NA	-2.76	1.99	2.06
5	B	312	CHL	MG-NA	-2.72	1.99	2.06
5	C	312	CHL	MG-NA	-2.70	1.99	2.06
5	A	312	CHL	MG-NA	-2.69	1.99	2.06
5	B	310	CHL	MG-NA	-2.69	1.99	2.06
5	A	309	CHL	MG-NA	-2.69	1.99	2.06
5	B	309	CHL	MG-NA	-2.68	1.99	2.06
5	B	305	CHL	MG-NA	-2.68	1.99	2.06
5	C	310	CHL	MG-NA	-2.67	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	309	CHL	MG-NA	-2.67	1.99	2.06
5	B	318	CHL	MG-NA	-2.67	1.99	2.06
5	A	310	CHL	MG-NA	-2.66	1.99	2.06
5	C	305	CHL	MG-NA	-2.66	2.00	2.06
5	A	305	CHL	MG-NA	-2.66	2.00	2.06
6	A	308	CLA	CMB-C2B	-2.62	1.46	1.51
6	B	314	CLA	CMB-C2B	-2.61	1.46	1.51
6	A	314	CLA	CMB-C2B	-2.59	1.46	1.51
6	B	308	CLA	CMB-C2B	-2.59	1.46	1.51
5	C	318	CHL	C4D-CHA	2.59	1.47	1.38
6	C	314	CLA	CMB-C2B	-2.58	1.46	1.51
5	A	305	CHL	C4D-CHA	2.57	1.47	1.38
5	A	318	CHL	C4D-CHA	2.56	1.47	1.38
5	C	305	CHL	C4D-CHA	2.56	1.47	1.38
5	B	305	CHL	C4D-CHA	2.56	1.47	1.38
5	C	309	CHL	C4D-CHA	2.56	1.47	1.38
5	B	309	CHL	C4D-CHA	2.55	1.47	1.38
6	C	308	CLA	CMB-C2B	-2.55	1.46	1.51
5	A	311	CHL	C4D-CHA	2.55	1.47	1.38
5	C	312	CHL	C4D-CHA	2.54	1.47	1.38
5	A	312	CHL	C4D-CHA	2.54	1.47	1.38
6	C	307	CLA	CMB-C2B	-2.53	1.46	1.51
5	C	311	CHL	C4D-CHA	2.53	1.47	1.38
5	A	309	CHL	C4D-CHA	2.53	1.47	1.38
5	B	311	CHL	C4D-CHA	2.53	1.47	1.38
5	B	318	CHL	C4D-CHA	2.52	1.47	1.38
5	B	312	CHL	C4D-CHA	2.52	1.47	1.38
6	A	317	CLA	CMB-C2B	-2.50	1.46	1.51
7	C	319	LHG	O8-C6	-2.50	1.39	1.45
5	B	310	CHL	C4D-CHA	2.49	1.47	1.38
7	B	319	LHG	O8-C6	-2.49	1.39	1.45
6	C	315	CLA	CMB-C2B	-2.48	1.46	1.51
5	C	310	CHL	C4D-CHA	2.48	1.47	1.38
6	A	315	CLA	CMB-C2B	-2.48	1.46	1.51
5	A	318	CHL	MG-NA	-2.47	2.00	2.06
5	A	310	CHL	C4D-CHA	2.47	1.47	1.38
6	B	316	CLA	CMB-C2B	-2.47	1.46	1.51
7	A	319	LHG	O8-C6	-2.47	1.39	1.45
5	C	306	CHL	C4D-CHA	2.47	1.47	1.38
7	A	319	LHG	O7-C5	-2.46	1.40	1.46
5	A	306	CHL	C4D-CHA	2.46	1.47	1.38
6	B	315	CLA	CMB-C2B	-2.46	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	318	CHL	MG-NA	-2.45	2.00	2.06
6	B	317	CLA	CMB-C2B	-2.45	1.46	1.51
7	B	319	LHG	O7-C5	-2.44	1.40	1.46
6	C	317	CLA	CMB-C2B	-2.44	1.46	1.51
6	C	316	CLA	CMB-C2B	-2.44	1.46	1.51
5	B	318	CHL	C4C-C3C	2.43	1.49	1.45
6	B	307	CLA	CMB-C2B	-2.43	1.46	1.51
6	A	316	CLA	CMB-C2B	-2.43	1.46	1.51
5	B	306	CHL	C4D-CHA	2.43	1.47	1.38
6	A	307	CLA	CMB-C2B	-2.43	1.46	1.51
7	C	319	LHG	O7-C5	-2.42	1.40	1.46
5	A	318	CHL	C4C-C3C	2.39	1.49	1.45
3	C	303	0IE	C6-C7	-2.37	1.40	1.45
3	B	303	0IE	C6-C7	-2.37	1.40	1.45
3	B	302	0IE	C13-C12	-2.37	1.40	1.45
5	C	318	CHL	C4C-C3C	2.36	1.49	1.45
5	A	310	CHL	C2C-C1C	2.35	1.49	1.44
3	C	302	0IE	C17-C16	-2.35	1.40	1.45
3	B	302	0IE	C17-C16	-2.34	1.40	1.45
3	C	303	0IE	C13-C12	-2.33	1.40	1.45
3	A	303	0IE	C6-C7	-2.32	1.41	1.45
3	C	302	0IE	C13-C12	-2.31	1.41	1.45
3	A	302	0IE	C13-C12	-2.31	1.41	1.45
5	A	310	CHL	C4B-CHC	2.31	1.47	1.41
3	B	303	0IE	C17-C16	-2.31	1.41	1.45
3	C	303	0IE	C17-C16	-2.31	1.41	1.45
5	B	313	CHL	C4D-CHA	2.30	1.46	1.38
5	C	313	CHL	C4D-CHA	2.30	1.46	1.38
5	A	313	CHL	C4D-CHA	2.30	1.46	1.38
5	C	310	CHL	C4B-CHC	2.29	1.47	1.41
5	B	310	CHL	C2C-C1C	2.29	1.49	1.44
5	C	310	CHL	C2C-C1C	2.29	1.49	1.44
5	B	310	CHL	C4B-CHC	2.29	1.47	1.41
3	B	303	0IE	C13-C12	-2.27	1.41	1.45
3	C	302	0IE	C6-C7	-2.27	1.41	1.45
3	A	303	0IE	C17-C16	-2.26	1.41	1.45
3	A	302	0IE	C17-C16	-2.25	1.41	1.45
5	A	312	CHL	C1B-NB	-2.24	1.33	1.35
5	B	309	CHL	C4B-CHC	2.23	1.47	1.41
5	A	309	CHL	C4B-CHC	2.23	1.47	1.41
5	C	309	CHL	C4B-CHC	2.22	1.47	1.41
3	A	303	0IE	C13-C12	-2.21	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	319	LHG	O8-C23	2.21	1.39	1.33
3	A	302	0IE	C6-C7	-2.21	1.41	1.45
3	B	302	0IE	C6-C7	-2.21	1.41	1.45
7	C	319	LHG	O8-C23	2.20	1.39	1.33
7	B	319	LHG	O8-C23	2.20	1.39	1.33
5	A	311	CHL	C4B-CHC	2.19	1.47	1.41
5	B	311	CHL	C4B-CHC	2.18	1.47	1.41
5	B	309	CHL	C2C-C1C	2.17	1.49	1.44
5	B	306	CHL	C4B-CHC	2.17	1.47	1.41
6	C	316	CLA	CMC-C2C	-2.17	1.46	1.50
5	B	313	CHL	C4C-C3C	2.16	1.48	1.45
6	B	316	CLA	CMC-C2C	-2.16	1.46	1.50
6	A	316	CLA	CMC-C2C	-2.15	1.46	1.50
5	C	311	CHL	C4B-CHC	2.15	1.47	1.41
5	B	312	CHL	C4B-CHC	2.14	1.47	1.41
5	C	306	CHL	C4C-C3C	2.13	1.48	1.45
5	A	313	CHL	C4C-C3C	2.13	1.48	1.45
7	C	319	LHG	O7-C7	2.12	1.40	1.34
5	A	305	CHL	C4B-CHC	2.12	1.46	1.41
5	C	305	CHL	C4B-CHC	2.12	1.46	1.41
5	A	309	CHL	C2C-C1C	2.12	1.49	1.44
7	A	319	LHG	O7-C7	2.12	1.40	1.34
6	A	314	CLA	CMD-C2D	-2.11	1.46	1.50
5	A	313	CHL	C1B-NB	-2.11	1.33	1.35
6	C	314	CLA	CMD-C2D	-2.11	1.46	1.50
5	C	313	CHL	C4C-C3C	2.11	1.48	1.45
5	A	312	CHL	C4B-CHC	2.11	1.46	1.41
5	C	309	CHL	C2C-C1C	2.11	1.49	1.44
5	B	305	CHL	C4B-CHC	2.11	1.46	1.41
5	A	306	CHL	C4C-C3C	2.11	1.48	1.45
7	B	319	LHG	O7-C7	2.11	1.40	1.34
5	C	312	CHL	C4B-CHC	2.10	1.46	1.41
5	B	313	CHL	C4B-CHC	2.10	1.46	1.41
6	B	316	CLA	CMD-C2D	-2.10	1.46	1.50
6	C	316	CLA	CMD-C2D	-2.10	1.46	1.50
6	B	314	CLA	CMD-C2D	-2.09	1.46	1.50
6	B	307	CLA	CMD-C2D	-2.09	1.46	1.50
6	C	308	CLA	CMD-C2D	-2.09	1.46	1.50
5	C	313	CHL	C1B-NB	-2.09	1.33	1.35
5	A	313	CHL	C4B-CHC	2.09	1.46	1.41
6	A	315	CLA	CMD-C2D	-2.09	1.46	1.50
5	C	306	CHL	C4B-CHC	2.08	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	315	CLA	CMD-C2D	-2.08	1.46	1.50
6	A	316	CLA	CMD-C2D	-2.08	1.46	1.50
6	A	308	CLA	CMD-C2D	-2.08	1.46	1.50
5	A	306	CHL	C4B-CHC	2.08	1.46	1.41
6	A	317	CLA	CMD-C2D	-2.07	1.46	1.50
6	B	308	CLA	CMD-C2D	-2.07	1.46	1.50
6	A	307	CLA	CMD-C2D	-2.07	1.46	1.50
5	C	313	CHL	C4B-CHC	2.07	1.46	1.41
5	B	306	CHL	C4C-C3C	2.06	1.48	1.45
6	C	315	CLA	CMD-C2D	-2.06	1.46	1.50
5	C	311	CHL	C4C-C3C	2.06	1.48	1.45
6	C	317	CLA	CMD-C2D	-2.05	1.46	1.50
6	B	317	CLA	CMD-C2D	-2.05	1.46	1.50
5	B	312	CHL	C1B-NB	-2.05	1.33	1.35
5	A	306	CHL	C1B-CHB	2.05	1.46	1.41
5	C	306	CHL	C1B-CHB	2.04	1.46	1.41
5	C	312	CHL	C1B-NB	-2.04	1.33	1.35
5	C	318	CHL	C4B-CHC	2.04	1.46	1.41
6	C	307	CLA	CMD-C2D	-2.03	1.46	1.50
5	A	318	CHL	C4B-CHC	2.03	1.46	1.41
4	C	304	NEX	C1-C6	2.03	1.57	1.54
5	A	310	CHL	C1B-NB	-2.03	1.33	1.35
5	C	305	CHL	C1B-NB	-2.02	1.33	1.35
5	B	306	CHL	C1B-CHB	2.02	1.46	1.41
5	B	318	CHL	C1B-CHB	2.02	1.46	1.41
4	B	304	NEX	C1-C6	2.01	1.57	1.54
5	C	309	CHL	C4C-C3C	2.01	1.48	1.45
5	A	305	CHL	C1B-NB	-2.01	1.33	1.35
5	B	318	CHL	C4B-CHC	2.00	1.46	1.41
5	B	309	CHL	C1B-CHB	2.00	1.46	1.41

All (896) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	310	CHL	C4D-CHA-C1A	-9.69	109.45	121.25
5	A	310	CHL	C4D-CHA-C1A	-9.68	109.47	121.25
5	C	310	CHL	C4D-CHA-C1A	-9.64	109.51	121.25
5	C	309	CHL	C4D-CHA-C1A	-9.58	109.59	121.25
5	A	309	CHL	C4D-CHA-C1A	-9.53	109.65	121.25
5	B	309	CHL	C4D-CHA-C1A	-9.52	109.66	121.25
5	B	312	CHL	C4D-CHA-C1A	-9.49	109.70	121.25
5	A	312	CHL	C4D-CHA-C1A	-9.48	109.72	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	312	CHL	C4D-CHA-C1A	-9.47	109.73	121.25
5	B	305	CHL	C4D-CHA-C1A	-9.44	109.76	121.25
5	C	311	CHL	C4D-CHA-C1A	-9.44	109.76	121.25
5	A	305	CHL	C4D-CHA-C1A	-9.44	109.76	121.25
5	C	305	CHL	C4D-CHA-C1A	-9.41	109.79	121.25
5	C	311	CHL	C1D-ND-C4D	9.38	113.00	106.33
5	B	311	CHL	C4D-CHA-C1A	-9.36	109.86	121.25
5	A	311	CHL	C4D-CHA-C1A	-9.34	109.89	121.25
5	B	311	CHL	C1D-ND-C4D	9.30	112.94	106.33
5	B	318	CHL	C4D-CHA-C1A	-9.28	109.96	121.25
5	C	306	CHL	C4D-CHA-C1A	-9.27	109.97	121.25
5	A	306	CHL	C4D-CHA-C1A	-9.26	109.98	121.25
5	A	311	CHL	C1D-ND-C4D	9.26	112.91	106.33
5	C	318	CHL	C1D-ND-C4D	9.22	112.88	106.33
5	A	305	CHL	C1D-ND-C4D	9.18	112.86	106.33
5	C	312	CHL	C1D-ND-C4D	9.17	112.85	106.33
5	C	305	CHL	C1D-ND-C4D	9.15	112.84	106.33
5	B	312	CHL	C1D-ND-C4D	9.15	112.83	106.33
5	A	312	CHL	C1D-ND-C4D	9.15	112.83	106.33
5	B	306	CHL	C4D-CHA-C1A	-9.13	110.14	121.25
5	B	318	CHL	C1D-ND-C4D	9.13	112.82	106.33
5	A	318	CHL	C1D-ND-C4D	9.12	112.82	106.33
5	C	318	CHL	C4D-CHA-C1A	-9.09	110.19	121.25
5	B	305	CHL	C1D-ND-C4D	9.08	112.79	106.33
5	B	310	CHL	C1D-ND-C4D	9.02	112.74	106.33
5	C	310	CHL	C1D-ND-C4D	9.01	112.74	106.33
5	B	309	CHL	C1D-ND-C4D	9.00	112.73	106.33
5	B	306	CHL	C1D-ND-C4D	8.99	112.72	106.33
5	A	309	CHL	C1D-ND-C4D	8.98	112.72	106.33
5	A	318	CHL	C4D-CHA-C1A	-8.98	110.32	121.25
5	C	309	CHL	C1D-ND-C4D	8.98	112.71	106.33
5	A	310	CHL	C1D-ND-C4D	8.89	112.65	106.33
5	A	306	CHL	C1D-ND-C4D	8.87	112.64	106.33
5	C	306	CHL	C1D-ND-C4D	8.86	112.63	106.33
5	B	313	CHL	C1D-ND-C4D	8.75	112.55	106.33
5	C	313	CHL	C1D-ND-C4D	8.73	112.54	106.33
5	A	313	CHL	C1D-ND-C4D	8.67	112.49	106.33
5	C	313	CHL	C4D-CHA-C1A	-7.63	111.96	121.25
5	B	313	CHL	C4D-CHA-C1A	-7.61	111.99	121.25
5	A	313	CHL	C4D-CHA-C1A	-7.59	112.01	121.25
5	B	313	CHL	C1B-CHB-C4A	-6.85	116.56	130.12
5	C	313	CHL	C1B-CHB-C4A	-6.84	116.56	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	313	CHL	C1B-CHB-C4A	-6.84	116.57	130.12
5	A	311	CHL	CHB-C4A-NA	6.82	133.94	124.51
5	B	311	CHL	CHB-C4A-NA	6.81	133.93	124.51
6	B	317	CLA	C4A-NA-C1A	6.74	109.74	106.71
6	B	316	CLA	C4A-NA-C1A	6.73	109.73	106.71
5	C	311	CHL	CHB-C4A-NA	6.71	133.79	124.51
6	A	317	CLA	C4A-NA-C1A	6.71	109.72	106.71
6	C	316	CLA	C4A-NA-C1A	6.67	109.70	106.71
6	A	316	CLA	C4A-NA-C1A	6.66	109.70	106.71
6	C	317	CLA	C4A-NA-C1A	6.62	109.68	106.71
5	C	305	CHL	CHB-C4A-NA	6.57	133.59	124.51
5	B	305	CHL	CHB-C4A-NA	6.51	133.51	124.51
5	A	305	CHL	CHB-C4A-NA	6.49	133.49	124.51
6	B	308	CLA	C4A-NA-C1A	6.47	109.61	106.71
6	C	315	CLA	C4A-NA-C1A	6.46	109.61	106.71
5	C	310	CHL	CHD-C1D-ND	6.46	130.39	124.45
6	A	315	CLA	C4A-NA-C1A	6.43	109.60	106.71
5	A	310	CHL	CHD-C1D-ND	6.43	130.36	124.45
5	C	309	CHL	CHB-C4A-NA	6.42	133.40	124.51
5	A	306	CHL	CHB-C4A-NA	6.42	133.39	124.51
6	C	308	CLA	C4A-NA-C1A	6.41	109.59	106.71
5	C	306	CHL	CHB-C4A-NA	6.41	133.37	124.51
5	B	310	CHL	CHD-C1D-ND	6.39	130.33	124.45
5	A	318	CHL	CHB-C4A-NA	6.37	133.32	124.51
6	A	308	CLA	C4A-NA-C1A	6.36	109.56	106.71
5	A	309	CHL	CHB-C4A-NA	6.36	133.30	124.51
5	A	318	CHL	CMD-C2D-C1D	6.35	135.91	124.71
5	B	309	CHL	CHB-C4A-NA	6.34	133.28	124.51
5	A	312	CHL	CHB-C4A-NA	6.34	133.28	124.51
5	C	318	CHL	CHB-C4A-NA	6.33	133.26	124.51
5	B	318	CHL	CMD-C2D-C1D	6.33	135.86	124.71
5	A	311	CHL	C1B-CHB-C4A	-6.33	117.59	130.12
5	B	313	CHL	CMD-C2D-C1D	6.32	135.86	124.71
5	C	311	CHL	C1B-CHB-C4A	-6.32	117.60	130.12
5	A	313	CHL	CMD-C2D-C1D	6.32	135.85	124.71
5	C	313	CHL	CMD-C2D-C1D	6.32	135.85	124.71
5	C	312	CHL	C1B-CHB-C4A	-6.31	117.62	130.12
5	C	318	CHL	CMD-C2D-C1D	6.31	135.84	124.71
6	A	307	CLA	C4A-NA-C1A	6.31	109.54	106.71
5	B	311	CHL	C1B-CHB-C4A	-6.30	117.64	130.12
5	A	312	CHL	CHD-C1D-ND	6.30	130.24	124.45
5	B	312	CHL	C1B-CHB-C4A	-6.30	117.65	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	312	CHL	CHB-C4A-NA	6.29	133.21	124.51
5	B	306	CHL	CHB-C4A-NA	6.28	133.19	124.51
5	A	312	CHL	C1B-CHB-C4A	-6.27	117.69	130.12
5	B	312	CHL	CHB-C4A-NA	6.27	133.18	124.51
5	B	312	CHL	CMD-C2D-C1D	6.27	135.76	124.71
5	C	312	CHL	CMD-C2D-C1D	6.26	135.75	124.71
5	A	310	CHL	CHB-C4A-NA	6.26	133.17	124.51
6	B	315	CLA	C4A-NA-C1A	6.25	109.51	106.71
5	C	305	CHL	CHD-C1D-ND	6.23	130.18	124.45
5	C	312	CHL	CHD-C1D-ND	6.23	130.18	124.45
5	B	311	CHL	CHD-C1D-ND	6.23	130.18	124.45
6	C	307	CLA	C4A-NA-C1A	6.21	109.50	106.71
5	A	312	CHL	CMD-C2D-C1D	6.21	135.66	124.71
5	B	312	CHL	CHD-C1D-ND	6.21	130.16	124.45
5	B	305	CHL	CMD-C2D-C1D	6.20	135.64	124.71
5	B	309	CHL	CMD-C2D-C1D	6.20	135.64	124.71
5	B	310	CHL	CHB-C4A-NA	6.20	133.08	124.51
5	C	311	CHL	CHD-C1D-ND	6.19	130.15	124.45
5	A	309	CHL	C1B-CHB-C4A	-6.19	117.87	130.12
5	B	309	CHL	C1B-CHB-C4A	-6.18	117.88	130.12
5	C	309	CHL	CMD-C2D-C1D	6.18	135.61	124.71
5	C	309	CHL	C1B-CHB-C4A	-6.18	117.88	130.12
5	C	310	CHL	CHB-C4A-NA	6.17	133.04	124.51
5	A	309	CHL	CMD-C2D-C1D	6.16	135.58	124.71
5	C	305	CHL	CMD-C2D-C1D	6.16	135.58	124.71
5	B	306	CHL	C1B-CHB-C4A	-6.16	117.91	130.12
5	A	305	CHL	CMD-C2D-C1D	6.15	135.55	124.71
6	B	307	CLA	C4A-NA-C1A	6.15	109.47	106.71
5	B	310	CHL	CMD-C2D-C1D	6.15	135.55	124.71
5	A	311	CHL	CHD-C1D-ND	6.15	130.10	124.45
5	A	310	CHL	C1B-CHB-C4A	-6.13	117.97	130.12
5	C	310	CHL	C1B-CHB-C4A	-6.13	117.98	130.12
5	B	305	CHL	CHD-C1D-ND	6.13	130.09	124.45
5	B	318	CHL	C1B-CHB-C4A	-6.12	118.00	130.12
5	A	305	CHL	CHD-C1D-ND	6.11	130.07	124.45
5	B	310	CHL	C1B-CHB-C4A	-6.09	118.06	130.12
5	A	318	CHL	CHD-C1D-ND	6.09	130.05	124.45
5	C	310	CHL	CMD-C2D-C1D	6.08	135.43	124.71
5	C	318	CHL	C1B-CHB-C4A	-6.07	118.10	130.12
5	A	310	CHL	CMD-C2D-C1D	6.06	135.40	124.71
5	C	306	CHL	CHD-C1D-ND	6.05	130.01	124.45
5	C	318	CHL	CHD-C1D-ND	6.03	130.00	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	318	CHL	C1B-CHB-C4A	-6.03	118.18	130.12
5	B	306	CHL	CHD-C1D-ND	6.02	129.99	124.45
5	A	306	CHL	C1B-CHB-C4A	-6.02	118.20	130.12
5	A	306	CHL	CHD-C1D-ND	6.02	129.99	124.45
5	B	318	CHL	CHB-C4A-NA	6.00	132.81	124.51
5	C	306	CHL	C1B-CHB-C4A	-6.00	118.24	130.12
5	A	311	CHL	CMD-C2D-C1D	5.99	135.27	124.71
5	C	309	CHL	CHD-C1D-ND	5.98	129.95	124.45
5	B	306	CHL	CMD-C2D-C1D	5.98	135.25	124.71
5	A	309	CHL	CHD-C1D-ND	5.97	129.94	124.45
5	A	305	CHL	C1B-CHB-C4A	-5.97	118.30	130.12
5	B	311	CHL	CMD-C2D-C1D	5.95	135.20	124.71
5	B	309	CHL	CHD-C1D-ND	5.94	129.91	124.45
5	A	306	CHL	CMD-C2D-C1D	5.93	135.17	124.71
5	C	306	CHL	CMD-C2D-C1D	5.93	135.16	124.71
5	C	311	CHL	CMD-C2D-C1D	5.92	135.15	124.71
5	C	305	CHL	C1B-CHB-C4A	-5.89	118.46	130.12
5	B	305	CHL	C1B-CHB-C4A	-5.88	118.47	130.12
5	C	313	CHL	C2A-C1A-CHA	-5.80	113.72	123.86
5	A	313	CHL	C2A-C1A-CHA	-5.78	113.76	123.86
5	B	313	CHL	C2A-C1A-CHA	-5.77	113.78	123.86
5	B	313	CHL	CHB-C4A-NA	5.76	132.48	124.51
5	C	313	CHL	CHB-C4A-NA	5.76	132.47	124.51
5	A	313	CHL	CHB-C4A-NA	5.76	132.47	124.51
5	B	318	CHL	O2D-CGD-CBD	5.72	121.43	111.27
5	A	312	CHL	C6-C7-C8	-5.70	97.49	115.92
5	B	312	CHL	C6-C7-C8	-5.65	97.66	115.92
5	B	310	CHL	C2A-C1A-CHA	-5.62	114.03	123.86
5	C	310	CHL	C2A-C1A-CHA	-5.61	114.05	123.86
5	B	318	CHL	C2A-C1A-CHA	-5.60	114.07	123.86
5	B	318	CHL	CHD-C1D-ND	5.60	129.60	124.45
5	A	310	CHL	C2A-C1A-CHA	-5.59	114.08	123.86
5	C	312	CHL	C6-C7-C8	-5.58	97.88	115.92
5	A	306	CHL	C2A-C1A-CHA	-5.53	114.18	123.86
5	A	318	CHL	O2D-CGD-CBD	5.53	121.09	111.27
5	C	306	CHL	C2A-C1A-CHA	-5.52	114.20	123.86
5	B	318	CHL	C2D-C1D-ND	-5.48	106.07	110.10
5	B	306	CHL	C2A-C1A-CHA	-5.47	114.30	123.86
5	C	310	CHL	C1D-CHD-C4C	-5.44	114.33	126.06
5	C	318	CHL	O2D-CGD-CBD	5.43	120.92	111.27
5	B	310	CHL	CHD-C4C-C3C	-5.42	116.88	124.84
5	A	310	CHL	C1D-CHD-C4C	-5.41	114.38	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	314	CLA	C4A-NA-C1A	5.39	109.13	106.71
5	B	310	CHL	C1D-CHD-C4C	-5.38	114.45	126.06
5	A	310	CHL	CHD-C4C-C3C	-5.37	116.94	124.84
5	C	312	CHL	C1D-CHD-C4C	-5.34	114.53	126.06
5	A	312	CHL	C1D-CHD-C4C	-5.33	114.55	126.06
5	C	310	CHL	CHD-C4C-C3C	-5.33	117.00	124.84
5	A	311	CHL	C1D-CHD-C4C	-5.32	114.58	126.06
5	B	312	CHL	C1D-CHD-C4C	-5.32	114.59	126.06
5	B	311	CHL	C1D-CHD-C4C	-5.31	114.60	126.06
6	A	314	CLA	C4A-NA-C1A	5.31	109.09	106.71
5	C	311	CHL	C1D-CHD-C4C	-5.29	114.64	126.06
2	B	301	0UR	C43-C3-C4	-5.29	118.63	125.02
5	C	306	CHL	O2D-CGD-CBD	5.29	120.66	111.27
6	C	314	CLA	C4A-NA-C1A	5.28	109.08	106.71
5	A	306	CHL	O2D-CGD-CBD	5.28	120.65	111.27
5	C	305	CHL	C1D-CHD-C4C	-5.27	114.69	126.06
7	A	319	LHG	C11-C10-C9	-5.27	87.68	114.42
5	B	305	CHL	C1D-CHD-C4C	-5.26	114.71	126.06
5	A	318	CHL	C1D-CHD-C4C	-5.24	114.75	126.06
5	B	306	CHL	C1D-CHD-C4C	-5.23	114.77	126.06
5	A	305	CHL	C1D-CHD-C4C	-5.23	114.78	126.06
5	A	313	CHL	C4A-NA-C1A	-5.23	104.36	106.71
5	B	313	CHL	C1D-CHD-C4C	-5.23	114.79	126.06
5	C	306	CHL	C1D-CHD-C4C	-5.22	114.80	126.06
5	B	309	CHL	C2A-C1A-CHA	-5.21	114.75	123.86
5	C	313	CHL	C1D-CHD-C4C	-5.21	114.82	126.06
5	C	313	CHL	C4A-NA-C1A	-5.21	104.36	106.71
5	B	312	CHL	C2A-C1A-CHA	-5.20	114.76	123.86
5	A	313	CHL	C1D-CHD-C4C	-5.20	114.83	126.06
5	A	306	CHL	C1D-CHD-C4C	-5.20	114.84	126.06
5	C	309	CHL	C2A-C1A-CHA	-5.20	114.77	123.86
5	B	306	CHL	CHD-C4C-C3C	-5.19	117.20	124.84
5	B	313	CHL	C4A-NA-C1A	-5.19	104.37	106.71
2	C	301	0UR	C43-C3-C4	-5.18	118.76	125.02
5	A	309	CHL	C2A-C1A-CHA	-5.17	114.81	123.86
5	A	305	CHL	C2A-C1A-CHA	-5.16	114.83	123.86
5	A	312	CHL	C2A-C1A-CHA	-5.16	114.83	123.86
5	C	318	CHL	C2D-C1D-ND	-5.15	106.31	110.10
5	C	305	CHL	C2A-C1A-CHA	-5.14	114.87	123.86
5	C	312	CHL	C2A-C1A-CHA	-5.14	114.88	123.86
5	C	306	CHL	CHD-C4C-C3C	-5.13	117.30	124.84
5	C	309	CHL	CHD-C4C-C3C	-5.12	117.31	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	309	CHL	C1D-CHD-C4C	-5.12	115.01	126.06
5	B	305	CHL	C2A-C1A-CHA	-5.12	114.91	123.86
5	C	318	CHL	C1D-CHD-C4C	-5.12	115.01	126.06
5	C	311	CHL	C2D-C1D-ND	-5.12	106.33	110.10
5	A	306	CHL	CHD-C4C-C3C	-5.11	117.33	124.84
5	A	309	CHL	C1D-CHD-C4C	-5.11	115.03	126.06
5	B	309	CHL	C1D-CHD-C4C	-5.11	115.03	126.06
5	A	309	CHL	CHD-C4C-C3C	-5.10	117.34	124.84
5	C	313	CHL	C2D-C1D-ND	-5.10	106.35	110.10
5	B	306	CHL	O2D-CGD-CBD	5.09	120.32	111.27
5	C	310	CHL	C2D-C1D-ND	-5.09	106.35	110.10
5	B	312	CHL	CHD-C4C-C3C	-5.09	117.36	124.84
5	B	313	CHL	C2D-C1D-ND	-5.09	106.36	110.10
5	B	310	CHL	C1C-C2C-C3C	-5.09	103.08	107.11
5	C	311	CHL	O2D-CGD-CBD	5.09	120.31	111.27
5	B	311	CHL	C2D-C1D-ND	-5.08	106.36	110.10
5	B	309	CHL	CHD-C4C-C3C	-5.08	117.37	124.84
5	A	310	CHL	C1C-C2C-C3C	-5.08	103.08	107.11
5	A	305	CHL	C2D-C1D-ND	-5.08	106.36	110.10
5	A	313	CHL	C2D-C1D-ND	-5.07	106.37	110.10
5	A	310	CHL	O2D-CGD-CBD	5.06	120.27	111.27
5	C	310	CHL	O2D-CGD-CBD	5.06	120.25	111.27
5	A	311	CHL	O2D-CGD-CBD	5.05	120.24	111.27
5	B	305	CHL	O2D-CGD-CBD	5.04	120.23	111.27
5	B	305	CHL	CHD-C4C-C3C	-5.03	117.44	124.84
5	B	311	CHL	O2D-CGD-CBD	5.03	120.21	111.27
5	C	305	CHL	O2D-CGD-CBD	5.03	120.20	111.27
5	A	311	CHL	C2D-C1D-ND	-5.02	106.40	110.10
5	B	309	CHL	O2D-CGD-CBD	5.01	120.18	111.27
5	B	310	CHL	O2D-CGD-CBD	5.01	120.18	111.27
5	A	312	CHL	CHD-C4C-C3C	-5.01	117.47	124.84
5	C	312	CHL	CHD-C4C-C3C	-5.01	117.48	124.84
5	A	305	CHL	O2D-CGD-CBD	5.01	120.16	111.27
5	A	318	CHL	C2D-C1D-ND	-5.00	106.42	110.10
5	C	305	CHL	CHD-C4C-C3C	-5.00	117.49	124.84
5	C	311	CHL	C2A-C1A-CHA	-5.00	115.12	123.86
2	A	301	0UR	C43-C3-C4	-4.99	118.98	125.02
5	B	306	CHL	C2D-C1D-ND	-4.99	106.42	110.10
5	C	312	CHL	C2D-C1D-ND	-4.99	106.43	110.10
5	C	305	CHL	C2D-C1D-ND	-4.98	106.43	110.10
5	B	311	CHL	C2A-C1A-CHA	-4.98	115.14	123.86
5	B	311	CHL	CHD-C4C-C3C	-4.98	117.52	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	312	CHL	C2D-C1D-ND	-4.98	106.44	110.10
5	C	310	CHL	C1C-C2C-C3C	-4.98	103.16	107.11
5	A	311	CHL	C2A-C1A-CHA	-4.97	115.17	123.86
5	A	306	CHL	C2D-C1D-ND	-4.97	106.44	110.10
5	A	311	CHL	CHD-C4C-C3C	-4.97	117.54	124.84
5	C	306	CHL	C2D-C1D-ND	-4.96	106.45	110.10
5	A	309	CHL	O2D-CGD-CBD	4.96	120.08	111.27
5	B	318	CHL	C1D-CHD-C4C	-4.96	115.36	126.06
5	B	305	CHL	C1C-C2C-C3C	-4.95	103.18	107.11
5	C	309	CHL	O2D-CGD-CBD	4.95	120.06	111.27
5	B	310	CHL	C2D-C1D-ND	-4.94	106.46	110.10
5	C	311	CHL	CHD-C4C-C3C	-4.94	117.58	124.84
5	C	318	CHL	C2A-C1A-CHA	-4.93	115.24	123.86
5	B	318	CHL	CHC-C1C-NC	4.93	131.68	124.20
5	B	312	CHL	C2D-C1D-ND	-4.92	106.48	110.10
6	A	314	CLA	CMB-C2B-C1B	-4.92	120.90	128.46
5	A	305	CHL	C1C-C2C-C3C	-4.92	103.21	107.11
5	A	305	CHL	CHD-C4C-C3C	-4.92	117.61	124.84
6	C	314	CLA	CMB-C2B-C1B	-4.91	120.92	128.46
6	B	314	CLA	CMB-C2B-C1B	-4.91	120.92	128.46
5	C	305	CHL	C1C-C2C-C3C	-4.89	103.23	107.11
5	B	305	CHL	C2D-C1D-ND	-4.88	106.51	110.10
4	C	304	NEX	C5-C4-C3	4.87	117.51	111.75
5	A	310	CHL	C2D-C1D-ND	-4.87	106.52	110.10
5	A	318	CHL	CHD-C4C-C3C	-4.85	117.71	124.84
5	A	318	CHL	C2A-C1A-CHA	-4.83	115.42	123.86
7	B	319	LHG	C11-C10-C9	-4.82	89.98	114.42
5	A	311	CHL	C11-C10-C8	-4.79	100.43	115.92
7	C	319	LHG	C11-C10-C9	-4.78	90.16	114.42
5	B	311	CHL	C11-C10-C8	-4.76	100.53	115.92
5	C	318	CHL	CHD-C4C-C3C	-4.76	117.84	124.84
5	B	309	CHL	C2D-C1D-ND	-4.76	106.60	110.10
5	C	309	CHL	C2D-C1D-ND	-4.74	106.61	110.10
5	B	318	CHL	C4A-NA-C1A	-4.73	104.58	106.71
3	A	302	0IE	C20-C3-C4	-4.72	118.76	124.83
5	A	309	CHL	C2D-C1D-ND	-4.71	106.63	110.10
5	B	309	CHL	C1C-C2C-C3C	-4.70	103.38	107.11
4	A	304	NEX	C5-C4-C3	4.70	117.31	111.75
5	C	313	CHL	CHD-C4C-C3C	-4.68	117.96	124.84
5	B	313	CHL	CHD-C4C-C3C	-4.68	117.96	124.84
5	C	309	CHL	C1C-C2C-C3C	-4.68	103.40	107.11
5	A	309	CHL	C1C-C2C-C3C	-4.67	103.41	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	313	CHL	C1C-C2C-C3C	-4.67	103.41	107.11
5	B	313	CHL	CHD-C1D-ND	4.66	128.74	124.45
5	A	313	CHL	CHD-C4C-C3C	-4.66	117.99	124.84
5	A	318	CHL	CHC-C1C-NC	4.66	131.27	124.20
5	C	313	CHL	C1C-C2C-C3C	-4.66	103.42	107.11
5	C	313	CHL	CHD-C1D-ND	4.63	128.71	124.45
5	A	313	CHL	C1C-C2C-C3C	-4.62	103.45	107.11
5	A	313	CHL	CHD-C1D-ND	4.62	128.70	124.45
5	B	318	CHL	CMD-C2D-C3D	-4.59	117.06	127.61
5	C	311	CHL	C11-C10-C8	-4.58	101.10	115.92
5	C	318	CHL	CHC-C1C-NC	4.57	131.13	124.20
5	B	312	CHL	C1C-C2C-C3C	-4.54	103.51	107.11
5	A	312	CHL	O2D-CGD-CBD	4.54	119.34	111.27
5	B	312	CHL	O2D-CGD-CBD	4.53	119.31	111.27
5	A	318	CHL	C2C-C3C-C4C	-4.51	103.28	106.49
5	C	318	CHL	C2C-C3C-C4C	-4.47	103.31	106.49
5	A	312	CHL	CHC-C1C-NC	4.46	130.97	124.20
5	A	312	CHL	C1C-C2C-C3C	-4.45	103.58	107.11
5	C	318	CHL	CMD-C2D-C3D	-4.45	117.38	127.61
5	A	313	CHL	CHC-C1C-NC	4.45	130.95	124.20
5	A	313	CHL	O2D-CGD-CBD	4.44	119.16	111.27
5	C	306	CHL	C2C-C3C-C4C	-4.44	103.33	106.49
5	C	312	CHL	O2D-CGD-CBD	4.43	119.15	111.27
5	C	312	CHL	CHC-C1C-NC	4.43	130.93	124.20
5	A	318	CHL	CMD-C2D-C3D	-4.43	117.42	127.61
5	B	313	CHL	CMD-C2D-C3D	-4.43	117.43	127.61
3	C	302	0IE	C20-C3-C4	-4.43	119.14	124.83
5	C	313	CHL	CMD-C2D-C3D	-4.42	117.44	127.61
5	C	313	CHL	CHC-C1C-NC	4.42	130.91	124.20
5	B	306	CHL	C2C-C3C-C4C	-4.42	103.34	106.49
5	B	313	CHL	CHC-C1C-NC	4.41	130.90	124.20
5	A	306	CHL	C2C-C3C-C4C	-4.41	103.35	106.49
5	C	313	CHL	O2D-CGD-CBD	4.41	119.10	111.27
5	A	313	CHL	CMD-C2D-C3D	-4.41	117.48	127.61
5	B	318	CHL	CHD-C4C-C3C	-4.40	118.37	124.84
5	B	313	CHL	O2D-CGD-CBD	4.40	119.08	111.27
5	C	312	CHL	C1C-C2C-C3C	-4.38	103.64	107.11
5	C	311	CHL	CHC-C1C-NC	4.37	130.84	124.20
5	B	311	CHL	CHC-C1C-NC	4.37	130.83	124.20
5	B	312	CHL	CHC-C1C-NC	4.37	130.83	124.20
5	B	305	CHL	CHC-C1C-NC	4.36	130.81	124.20
5	B	318	CHL	C2C-C3C-C4C	-4.36	103.38	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	305	CHL	CHC-C1C-NC	4.35	130.81	124.20
5	A	306	CHL	CHC-C1C-NC	4.35	130.80	124.20
5	C	305	CHL	CHC-C1C-NC	4.35	130.80	124.20
5	C	306	CHL	CHC-C1C-NC	4.34	130.79	124.20
5	C	312	CHL	CMD-C2D-C3D	-4.34	117.63	127.61
5	A	311	CHL	CHC-C1C-NC	4.34	130.78	124.20
5	B	306	CHL	CHC-C1C-NC	4.34	130.78	124.20
5	B	310	CHL	CMD-C2D-C3D	-4.33	117.65	127.61
3	B	302	0IE	C20-C3-C4	-4.33	119.26	124.83
5	B	312	CHL	CMD-C2D-C3D	-4.32	117.67	127.61
5	C	310	CHL	CMD-C2D-C3D	-4.32	117.67	127.61
5	B	305	CHL	CMD-C2D-C3D	-4.30	117.71	127.61
3	C	303	0IE	C23-C16-C15	-4.30	116.90	122.92
5	A	305	CHL	CMD-C2D-C3D	-4.29	117.74	127.61
5	A	312	CHL	CMD-C2D-C3D	-4.29	117.74	127.61
4	B	304	NEX	C5-C4-C3	4.29	116.83	111.75
5	C	305	CHL	CMD-C2D-C3D	-4.28	117.77	127.61
5	A	310	CHL	CMD-C2D-C3D	-4.27	117.80	127.61
3	B	303	0IE	C23-C16-C15	-4.26	116.96	122.92
5	B	309	CHL	CMD-C2D-C3D	-4.25	117.83	127.61
3	A	303	0IE	C23-C16-C15	-4.25	116.97	122.92
5	C	309	CHL	CMD-C2D-C3D	-4.24	117.85	127.61
5	A	309	CHL	CMD-C2D-C3D	-4.23	117.88	127.61
5	C	312	CHL	CHA-C4D-ND	4.19	141.27	132.50
5	B	310	CHL	CHA-C4D-ND	4.18	141.25	132.50
5	C	305	CHL	CHA-C4D-ND	4.18	141.25	132.50
5	B	305	CHL	CHA-C4D-ND	4.18	141.25	132.50
5	A	305	CHL	CHA-C4D-ND	4.18	141.24	132.50
5	B	312	CHL	CHA-C4D-ND	4.17	141.23	132.50
5	A	306	CHL	CMD-C2D-C3D	-4.17	118.02	127.61
5	B	306	CHL	CMD-C2D-C3D	-4.17	118.02	127.61
5	C	306	CHL	CMD-C2D-C3D	-4.17	118.02	127.61
5	A	311	CHL	CMD-C2D-C3D	-4.17	118.03	127.61
3	A	302	0IE	C23-C16-C15	-4.16	117.09	122.92
5	C	309	CHL	CHA-C4D-ND	4.16	141.21	132.50
3	B	302	0IE	C23-C16-C15	-4.16	117.09	122.92
5	C	318	CHL	CHA-C4D-ND	4.16	141.20	132.50
5	B	309	CHL	CHA-C4D-ND	4.16	141.20	132.50
5	B	311	CHL	CMD-C2D-C3D	-4.15	118.06	127.61
5	C	310	CHL	CHA-C4D-ND	4.15	141.18	132.50
5	A	312	CHL	CHA-C4D-ND	4.15	141.17	132.50
5	C	311	CHL	CMD-C2D-C3D	-4.14	118.09	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	303	0IE	C20-C3-C4	-4.14	119.50	124.83
5	A	309	CHL	CHA-C4D-ND	4.14	141.16	132.50
5	A	318	CHL	CHA-C4D-ND	4.14	141.15	132.50
5	A	310	CHL	CHA-C4D-ND	4.13	141.14	132.50
5	C	311	CHL	CHA-C4D-ND	4.12	141.12	132.50
5	C	311	CHL	C1C-C2C-C3C	-4.11	103.85	107.11
5	B	309	CHL	CHC-C1C-NC	4.11	130.44	124.20
5	A	309	CHL	CHC-C1C-NC	4.10	130.42	124.20
5	B	311	CHL	CHA-C4D-ND	4.10	141.07	132.50
6	A	308	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
5	A	306	CHL	C1C-C2C-C3C	-4.09	103.87	107.11
5	A	311	CHL	CHA-C4D-ND	4.09	141.05	132.50
5	B	311	CHL	C1C-C2C-C3C	-4.09	103.87	107.11
5	C	309	CHL	CHC-C1C-NC	4.09	130.40	124.20
5	A	311	CHL	C1C-C2C-C3C	-4.09	103.87	107.11
5	C	306	CHL	C1C-C2C-C3C	-4.06	103.89	107.11
6	A	314	CLA	CMB-C2B-C3B	4.06	132.27	124.68
5	B	318	CHL	CHA-C4D-ND	4.05	140.97	132.50
3	C	302	0IE	C23-C16-C15	-4.05	117.25	122.92
6	B	314	CLA	CMB-C2B-C3B	4.03	132.23	124.68
5	A	318	CHL	C1C-C2C-C3C	-4.03	103.92	107.11
5	B	306	CHL	C1C-C2C-C3C	-4.03	103.92	107.11
5	B	306	CHL	CHA-C4D-ND	4.03	140.93	132.50
6	C	314	CLA	CMB-C2B-C3B	4.03	132.21	124.68
6	C	308	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
5	C	306	CHL	CHA-C4D-ND	4.02	140.91	132.50
3	B	303	0IE	C20-C3-C4	-4.02	119.66	124.83
6	B	308	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
5	A	306	CHL	CHA-C4D-ND	4.02	140.90	132.50
5	C	318	CHL	C1C-C2C-C3C	-3.98	103.95	107.11
3	B	303	0IE	C10-C9-C8	3.97	131.61	123.47
5	B	318	CHL	C1C-C2C-C3C	-3.93	104.00	107.11
5	B	310	CHL	CHD-C4C-NC	3.92	130.37	124.20
3	A	303	0IE	C10-C9-C8	3.91	131.49	123.47
3	C	302	0IE	C9-C10-C11	3.90	131.47	123.47
5	A	310	CHL	CHD-C4C-NC	3.89	130.33	124.20
3	C	303	0IE	C20-C3-C4	-3.88	119.83	124.83
3	A	302	0IE	C10-C9-C8	3.87	131.40	123.47
5	C	311	CHL	C2C-C3C-C4C	-3.85	103.75	106.49
6	C	317	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
5	C	310	CHL	CHD-C4C-NC	3.82	130.23	124.20
5	C	318	CHL	C4A-NA-C1A	-3.80	105.00	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	0UR	C29-C30-C31	-3.80	107.42	111.74
5	B	311	CHL	C2C-C3C-C4C	-3.80	103.78	106.49
5	A	306	CHL	C4-C3-C5	3.79	121.64	115.27
6	B	317	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
5	A	311	CHL	C2C-C3C-C4C	-3.78	103.80	106.49
5	C	306	CHL	C4-C3-C5	3.77	121.62	115.27
5	A	310	CHL	CHC-C1C-NC	3.76	129.91	124.20
5	B	306	CHL	C4A-NA-C1A	-3.76	105.02	106.71
6	A	315	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
7	C	319	LHG	O7-C7-C8	3.75	119.58	111.50
5	C	310	CHL	CHC-C1C-NC	3.74	129.88	124.20
6	B	315	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
2	A	301	0UR	C29-C30-C31	-3.73	107.49	111.74
6	C	315	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
7	B	319	LHG	O7-C7-C8	3.73	119.54	111.50
5	B	312	CHL	CHD-C4C-NC	3.70	130.04	124.20
6	A	307	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
6	B	307	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
5	B	310	CHL	CHC-C1C-NC	3.69	129.81	124.20
5	B	305	CHL	CHD-C4C-NC	3.69	130.02	124.20
6	A	316	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
2	B	301	0UR	C29-C30-C31	-3.67	107.56	111.74
5	C	312	CHL	CHD-C4C-NC	3.67	129.98	124.20
5	A	312	CHL	CHD-C4C-NC	3.66	129.97	124.20
5	C	313	CHL	CHA-C4D-ND	3.66	140.15	132.50
6	C	316	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
5	B	313	CHL	CHA-C4D-ND	3.65	140.14	132.50
5	C	309	CHL	CHD-C4C-NC	3.64	129.94	124.20
5	C	305	CHL	CHD-C4C-NC	3.63	129.93	124.20
5	A	313	CHL	CHD-C4C-NC	3.63	129.92	124.20
5	B	309	CHL	CHD-C4C-NC	3.63	129.92	124.20
5	B	313	CHL	CHD-C4C-NC	3.63	129.92	124.20
5	A	313	CHL	CHA-C4D-ND	3.63	140.09	132.50
6	B	316	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
3	C	303	0IE	C9-C10-C11	3.63	130.90	123.47
7	A	319	LHG	C18-C17-C16	-3.62	96.02	114.42
5	A	305	CHL	CHD-C4C-NC	3.62	129.90	124.20
5	C	313	CHL	CHD-C4C-NC	3.61	129.90	124.20
5	A	309	CHL	CHD-C4C-NC	3.60	129.88	124.20
5	A	311	CHL	CHD-C4C-NC	3.60	129.88	124.20
5	B	306	CHL	CHD-C4C-NC	3.60	129.87	124.20
7	B	319	LHG	C18-C17-C16	-3.60	96.16	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	311	CHL	CHD-C4C-NC	3.59	129.86	124.20
3	B	302	0IE	C9-C10-C11	3.59	130.82	123.47
5	C	311	CHL	CHD-C4C-NC	3.57	129.83	124.20
7	A	319	LHG	O7-C7-C8	3.56	119.18	111.50
7	C	319	LHG	C18-C17-C16	-3.56	96.34	114.42
5	A	318	CHL	C4A-NA-C1A	-3.55	105.11	106.71
6	C	307	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
5	C	312	CHL	C2C-C3C-C4C	-3.54	103.96	106.49
3	B	302	0IE	C10-C9-C8	3.54	130.72	123.47
5	B	312	CHL	C2C-C3C-C4C	-3.53	103.97	106.49
5	A	312	CHL	C2C-C3C-C4C	-3.52	103.98	106.49
2	B	301	0UR	C10-C11-C12	-3.52	122.29	127.31
2	C	301	0UR	C34-C27-C1	-3.52	119.88	124.49
5	C	306	CHL	CHD-C4C-NC	3.51	129.74	124.20
2	A	301	0UR	C34-C27-C1	-3.51	119.89	124.49
5	A	306	CHL	CHD-C4C-NC	3.50	129.71	124.20
3	C	303	0IE	C10-C9-C8	3.49	130.63	123.47
2	C	301	0UR	C10-C11-C12	-3.45	122.39	127.31
3	C	303	0IE	C22-C12-C11	-3.45	118.09	122.92
3	C	302	0IE	C22-C12-C11	-3.44	118.10	122.92
3	A	303	0IE	C9-C10-C11	3.44	130.51	123.47
5	A	309	CHL	C2C-C3C-C4C	-3.43	104.04	106.49
2	B	301	0UR	C34-C27-C1	-3.42	120.00	124.49
6	A	317	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
3	B	302	0IE	C22-C12-C11	-3.41	118.15	122.92
3	B	303	0IE	C21-C7-C8	-3.41	118.15	122.92
5	C	309	CHL	C2C-C3C-C4C	-3.41	104.06	106.49
3	B	303	0IE	C22-C12-C11	-3.38	118.18	122.92
3	A	303	0IE	C21-C7-C8	-3.38	118.19	122.92
3	A	303	0IE	C22-C12-C11	-3.38	118.19	122.92
3	A	302	0IE	C21-C7-C8	-3.38	118.19	122.92
5	B	309	CHL	C2C-C3C-C4C	-3.37	104.09	106.49
3	C	302	0IE	C10-C9-C8	3.36	130.37	123.47
5	A	312	CHL	C1-C2-C3	-3.35	120.24	126.04
5	B	310	CHL	C4A-NA-C1A	-3.35	105.20	106.71
6	A	308	CLA	CMB-C2B-C3B	3.35	130.94	124.68
5	C	312	CHL	C1-C2-C3	-3.34	120.26	126.04
3	A	302	0IE	C22-C12-C11	-3.34	118.24	122.92
2	B	301	0UR	O44-C45-C46	3.34	120.44	111.55
5	A	310	CHL	C1-C2-C3	-3.34	121.35	126.75
3	C	302	0IE	C21-C7-C8	-3.34	118.25	122.92
5	C	310	CHL	C4A-NA-C1A	-3.34	105.21	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	309	CHL	C4A-NA-C1A	-3.33	105.21	106.71
5	B	310	CHL	C1-C2-C3	-3.33	121.36	126.75
3	B	302	0IE	C21-C7-C8	-3.33	118.26	122.92
3	A	302	0IE	C9-C10-C11	3.33	130.29	123.47
5	B	312	CHL	C1-C2-C3	-3.33	120.29	126.04
5	C	310	CHL	C1-C2-C3	-3.33	121.37	126.75
5	C	312	CHL	OBD-CAD-C3D	-3.31	120.55	128.52
3	C	303	0IE	C21-C7-C8	-3.30	118.30	122.92
6	C	308	CLA	CMB-C2B-C3B	3.29	130.84	124.68
3	B	303	0IE	C9-C10-C11	3.29	130.22	123.47
2	A	301	0UR	O44-C45-C46	3.29	120.29	111.55
5	B	306	CHL	C4-C3-C5	3.28	120.78	115.27
5	C	306	CHL	C4A-NA-C1A	-3.27	105.23	106.71
2	C	301	0UR	O44-C45-C46	3.27	120.25	111.55
6	B	308	CLA	CMB-C2B-C3B	3.27	130.80	124.68
5	A	318	CHL	CHD-C4C-NC	3.27	129.35	124.20
5	A	306	CHL	C4A-NA-C1A	-3.24	105.25	106.71
5	B	312	CHL	OBD-CAD-C3D	-3.23	120.74	128.52
6	C	317	CLA	CMB-C2B-C3B	3.22	130.71	124.68
5	C	313	CHL	C2C-C3C-C4C	-3.22	104.19	106.49
5	C	318	CHL	CHD-C4C-NC	3.22	129.28	124.20
5	A	310	CHL	C4A-NA-C1A	-3.21	105.26	106.71
5	A	312	CHL	OBD-CAD-C3D	-3.21	120.80	128.52
5	A	309	CHL	C4A-NA-C1A	-3.19	105.27	106.71
6	B	315	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
6	A	315	CLA	CMB-C2B-C3B	3.18	130.63	124.68
5	A	313	CHL	C2C-C3C-C4C	-3.18	104.22	106.49
5	B	313	CHL	C2C-C3C-C4C	-3.17	104.23	106.49
5	B	313	CHL	C1-C2-C3	-3.16	120.58	126.04
5	C	311	CHL	OBD-CAD-C3D	-3.16	120.92	128.52
5	C	313	CHL	C1-C2-C3	-3.16	120.59	126.04
5	C	305	CHL	C2C-C3C-C4C	-3.15	104.24	106.49
5	A	313	CHL	C1-C2-C3	-3.15	120.60	126.04
6	C	315	CLA	CMB-C2B-C3B	3.14	130.56	124.68
6	B	315	CLA	CMB-C2B-C3B	3.14	130.56	124.68
6	A	315	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
5	B	305	CHL	C2C-C3C-C4C	-3.13	104.26	106.49
3	B	303	0IE	C6-C7-C8	3.12	123.73	118.94
6	B	317	CLA	CMB-C2B-C3B	3.12	130.51	124.68
5	C	312	CHL	C4A-NA-C1A	-3.11	105.31	106.71
3	C	302	0IE	C13-C12-C11	3.11	123.71	118.94
5	B	318	CHL	CHD-C4C-NC	3.10	129.09	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	305	CHL	C2C-C3C-C4C	-3.10	104.28	106.49
5	B	311	CHL	OBD-CAD-C3D	-3.10	121.06	128.52
6	A	307	CLA	CMB-C2B-C3B	3.10	130.47	124.68
5	B	305	CHL	OBD-CAD-C3D	-3.10	121.06	128.52
6	A	316	CLA	CMB-C2B-C3B	3.10	130.47	124.68
5	B	312	CHL	C4A-NA-C1A	-3.09	105.32	106.71
6	A	307	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
3	A	303	0IE	C6-C7-C8	3.08	123.66	118.94
5	C	305	CHL	C1-C2-C3	-3.07	120.72	126.04
5	A	310	CHL	OBD-CAD-C3D	-3.07	121.13	128.52
6	C	316	CLA	CMB-C2B-C3B	3.06	130.41	124.68
3	C	303	0IE	C13-C12-C11	3.06	123.64	118.94
6	B	307	CLA	CMB-C2B-C3B	3.06	130.40	124.68
5	B	305	CHL	C1-C2-C3	-3.05	120.76	126.04
5	A	305	CHL	C1-C2-C3	-3.05	120.77	126.04
6	B	316	CLA	CMB-C2B-C3B	3.04	130.37	124.68
5	A	311	CHL	OBD-CAD-C3D	-3.03	121.22	128.52
5	C	310	CHL	C2C-C3C-C4C	-3.03	104.33	106.49
5	B	310	CHL	OBD-CAD-C3D	-3.03	121.23	128.52
5	C	310	CHL	OBD-CAD-C3D	-3.02	121.24	128.52
5	B	309	CHL	OBD-CAD-C3D	-3.01	121.27	128.52
6	C	315	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
5	A	305	CHL	OBD-CAD-C3D	-3.01	121.28	128.52
5	B	318	CHL	CHC-C1C-C2C	-3.01	115.21	126.11
6	B	308	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
5	A	309	CHL	OBD-CAD-C3D	-3.00	121.29	128.52
3	B	302	0IE	C13-C12-C11	3.00	123.54	118.94
5	A	312	CHL	C4A-NA-C1A	-2.98	105.36	106.71
3	C	303	0IE	C6-C7-C8	2.97	123.50	118.94
6	A	308	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
3	A	303	0IE	C13-C12-C11	2.97	123.50	118.94
5	C	305	CHL	OBD-CAD-C3D	-2.97	121.37	128.52
6	C	307	CLA	CMB-C2B-C3B	2.97	130.23	124.68
5	A	313	CHL	OBD-CAD-C3D	-2.96	121.39	128.52
5	C	309	CHL	C4A-NA-C1A	-2.96	105.38	106.71
5	B	313	CHL	OBD-CAD-C3D	-2.96	121.41	128.52
5	C	313	CHL	OBD-CAD-C3D	-2.96	121.41	128.52
5	C	309	CHL	OBD-CAD-C3D	-2.95	121.41	128.52
6	C	308	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
5	A	318	CHL	CHC-C1C-C2C	-2.95	115.43	126.11
5	B	311	CHL	O2A-CGA-CBA	2.94	121.13	111.91
3	A	302	0IE	C13-C12-C11	2.93	123.44	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	303	0IE	C13-C12-C11	2.93	123.44	118.94
5	A	310	CHL	C2C-C3C-C4C	-2.93	104.40	106.49
2	C	301	0UR	C48-C47-C46	-2.93	119.57	125.85
5	B	310	CHL	C2C-C3C-C4C	-2.93	104.40	106.49
2	A	301	0UR	C48-C47-C46	-2.92	119.58	125.85
2	B	301	0UR	C9-C8-C7	-2.91	123.15	127.31
5	A	311	CHL	O2A-CGA-CBA	2.89	120.99	111.91
5	C	318	CHL	CHC-C1C-C2C	-2.89	115.64	126.11
6	C	307	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
6	A	316	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
5	B	305	CHL	C4-C3-C5	2.88	120.11	115.27
3	A	302	0IE	C6-C7-C8	2.87	123.34	118.94
6	B	307	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
6	A	317	CLA	CMB-C2B-C3B	2.87	130.04	124.68
6	C	317	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
5	C	306	CHL	C11-C10-C8	-2.86	106.68	115.92
5	A	306	CHL	C11-C10-C8	-2.85	106.69	115.92
5	C	311	CHL	O2A-CGA-CBA	2.85	120.86	111.91
6	A	317	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
6	B	316	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
2	B	301	0UR	C48-C47-C46	-2.82	119.79	125.85
5	C	305	CHL	C4-C3-C5	2.82	120.02	115.27
6	B	314	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
2	A	301	0UR	O42-C2-C41	-2.81	116.51	120.58
5	A	305	CHL	C4-C3-C5	2.81	120.00	115.27
3	C	302	0IE	C6-C7-C8	2.81	123.26	118.94
6	C	316	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
5	A	305	CHL	CHC-C1C-C2C	-2.81	115.93	126.11
5	B	305	CHL	CHC-C1C-C2C	-2.81	115.94	126.11
6	A	314	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
6	A	314	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
6	B	314	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
5	C	305	CHL	CHC-C1C-C2C	-2.80	115.97	126.11
5	C	306	CHL	OBD-CAD-C3D	-2.79	121.80	128.52
6	C	314	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
5	B	318	CHL	O2D-CGD-O1D	-2.78	118.40	123.84
5	A	306	CHL	OBD-CAD-C3D	-2.78	121.84	128.52
5	C	313	CHL	CHC-C1C-C2C	-2.77	116.05	126.11
5	A	312	CHL	CHC-C1C-C2C	-2.77	116.06	126.11
5	B	313	CHL	CHC-C1C-C2C	-2.77	116.06	126.11
3	B	302	0IE	C6-C7-C8	2.77	123.19	118.94
5	A	313	CHL	CHC-C1C-C2C	-2.77	116.08	126.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	314	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
5	A	305	CHL	C4A-NA-C1A	-2.76	105.46	106.71
7	B	319	LHG	O8-C23-C24	2.76	120.58	111.91
5	B	306	CHL	OBD-CAD-C3D	-2.76	121.89	128.52
5	B	312	CHL	CHC-C1C-C2C	-2.75	116.13	126.11
6	B	317	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
5	C	312	CHL	CHC-C1C-C2C	-2.75	116.14	126.11
2	C	301	0UR	O42-C2-C41	-2.75	116.60	120.58
7	C	319	LHG	O8-C23-C24	2.74	120.51	111.91
5	C	312	CHL	OMC-CMC-C2C	-2.74	119.49	125.69
5	B	312	CHL	OMC-CMC-C2C	-2.74	119.50	125.69
5	A	306	CHL	CHC-C1C-C2C	-2.73	116.20	126.11
5	C	306	CHL	CHC-C1C-C2C	-2.72	116.23	126.11
5	A	318	CHL	O2D-CGD-O1D	-2.72	118.51	123.84
3	A	303	0IE	C17-C16-C15	2.72	123.12	118.94
2	B	301	0UR	C5-C4-C3	-2.72	123.73	127.00
2	B	301	0UR	C28-C19-C18	-2.72	109.26	112.70
5	C	312	CHL	O2A-CGA-CBA	2.72	120.44	111.91
4	C	304	NEX	C16-C1-C6	2.72	112.90	110.47
5	A	312	CHL	O2A-CGA-CBA	2.71	120.42	111.91
2	C	301	0UR	C5-C4-C3	-2.71	123.75	127.00
5	A	312	CHL	OMC-CMC-C2C	-2.71	119.56	125.69
7	A	319	LHG	O8-C23-C24	2.70	120.37	111.91
5	B	306	CHL	CHC-C1C-C2C	-2.69	116.35	126.11
5	A	306	CHL	C1-C2-C3	-2.68	121.40	126.04
5	C	311	CHL	CHC-C1C-C2C	-2.68	116.39	126.11
5	B	312	CHL	O2A-CGA-CBA	2.68	120.31	111.91
3	B	303	0IE	C17-C16-C15	2.67	123.04	118.94
5	A	313	CHL	C6-C7-C8	-2.66	107.32	115.92
5	B	313	CHL	C6-C7-C8	-2.66	107.33	115.92
5	B	311	CHL	CHC-C1C-C2C	-2.66	116.48	126.11
5	C	305	CHL	C4A-NA-C1A	-2.65	105.52	106.71
5	C	313	CHL	C6-C7-C8	-2.65	107.36	115.92
5	C	306	CHL	C1-C2-C3	-2.65	121.47	126.04
5	A	311	CHL	CHC-C1C-C2C	-2.64	116.53	126.11
5	C	309	CHL	CHC-C1C-C2C	-2.64	116.53	126.11
5	B	309	CHL	CHC-C1C-C2C	-2.64	116.54	126.11
5	A	309	CHL	CHC-C1C-C2C	-2.64	116.55	126.11
6	A	316	CLA	CHB-C4A-NA	2.63	128.15	124.51
4	B	304	NEX	C16-C1-C6	2.63	112.83	110.47
5	C	318	CHL	O2D-CGD-O1D	-2.63	118.69	123.84
6	A	307	CLA	CHB-C4A-NA	2.63	128.15	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	305	CHL	C4A-NA-C1A	-2.63	105.52	106.71
5	C	310	CHL	O2A-CGA-CBA	2.61	120.11	111.91
5	B	305	CHL	C3B-C4B-NB	2.61	112.59	109.21
5	B	310	CHL	O2A-CGA-CBA	2.61	120.10	111.91
3	C	303	0IE	C17-C16-C15	2.61	122.94	118.94
6	B	316	CLA	CHB-C4A-NA	2.60	128.11	124.51
5	A	310	CHL	O2A-CGA-CBA	2.60	120.07	111.91
6	C	316	CLA	CHB-C4A-NA	2.60	128.10	124.51
5	A	309	CHL	OMC-CMC-C2C	-2.59	119.83	125.69
5	C	309	CHL	OMC-CMC-C2C	-2.59	119.83	125.69
4	C	304	NEX	C24-C23-C22	2.58	115.77	110.77
5	B	309	CHL	OMC-CMC-C2C	-2.57	119.87	125.69
5	C	306	CHL	O2A-CGA-CBA	2.57	119.97	111.91
5	B	311	CHL	C1-C2-C3	-2.57	121.60	126.04
5	A	305	CHL	C3B-C4B-NB	2.57	112.53	109.21
5	A	306	CHL	O2A-CGA-CBA	2.57	119.96	111.91
5	C	313	CHL	CAC-C3C-C4C	2.57	128.14	124.81
5	C	306	CHL	O2D-CGD-O1D	-2.57	118.82	123.84
5	C	311	CHL	C1-C2-C3	-2.56	121.61	126.04
5	C	311	CHL	OMC-CMC-C2C	-2.56	119.89	125.69
6	B	308	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
5	C	312	CHL	C3B-C4B-NB	2.56	112.52	109.21
5	C	305	CHL	C3B-C4B-NB	2.55	112.51	109.21
6	C	307	CLA	CHB-C4A-NA	2.55	128.04	124.51
5	A	313	CHL	CAC-C3C-C4C	2.55	128.12	124.81
5	A	305	CHL	OMC-CMC-C2C	-2.55	119.92	125.69
2	C	301	0UR	C9-C8-C7	-2.55	123.67	127.31
2	A	301	0UR	C5-C4-C3	-2.55	123.94	127.00
5	B	312	CHL	C3B-C4B-NB	2.55	112.50	109.21
5	A	311	CHL	C1-C2-C3	-2.54	121.64	126.04
5	B	311	CHL	OMC-CMC-C2C	-2.54	119.94	125.69
6	C	317	CLA	CHB-C4A-NA	2.54	128.03	124.51
6	A	317	CLA	CHB-C4A-NA	2.54	128.03	124.51
5	A	306	CHL	O2D-CGD-O1D	-2.54	118.88	123.84
5	B	305	CHL	OMC-CMC-C2C	-2.53	119.96	125.69
4	A	304	NEX	C16-C1-C6	2.53	112.74	110.47
2	B	301	0UR	C24-C25-C26	-2.53	106.84	110.30
5	C	313	CHL	O2A-CGA-CBA	2.53	119.84	111.91
5	B	313	CHL	CAC-C3C-C4C	2.52	128.09	124.81
5	A	318	CHL	C3B-C4B-NB	2.52	112.47	109.21
5	C	311	CHL	C7-C6-C5	-2.52	106.50	113.36
6	A	308	CLA	C1B-CHB-C4A	-2.52	125.12	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	305	CHL	O2D-CGD-O1D	-2.52	118.91	123.84
5	A	313	CHL	O2A-CGA-CBA	2.52	119.81	111.91
3	A	302	0IE	C4-C3-C2	2.52	122.24	120.08
5	B	313	CHL	O2A-CGA-CBA	2.52	119.81	111.91
6	C	308	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
6	B	307	CLA	CHB-C4A-NA	2.51	127.98	124.51
5	A	312	CHL	C3B-C4B-NB	2.51	112.45	109.21
5	A	310	CHL	CHC-C1C-C2C	-2.51	117.02	126.11
2	A	301	0UR	C24-C25-C26	-2.51	106.87	110.30
5	C	310	CHL	CHC-C1C-C2C	-2.50	117.05	126.11
5	C	311	CHL	CAC-C3C-C4C	2.50	128.05	124.81
5	A	311	CHL	OMC-CMC-C2C	-2.50	120.04	125.69
5	C	305	CHL	OMC-CMC-C2C	-2.50	120.04	125.69
5	B	311	CHL	CAC-C3C-C4C	2.49	128.05	124.81
5	B	310	CHL	CHC-C1C-C2C	-2.49	117.08	126.11
5	A	311	CHL	CAC-C3C-C4C	2.49	128.04	124.81
5	B	306	CHL	O2D-CGD-O1D	-2.48	118.98	123.84
6	B	317	CLA	CHB-C4A-NA	2.48	127.94	124.51
5	C	305	CHL	O2D-CGD-O1D	-2.48	118.99	123.84
5	A	306	CHL	C3B-C4B-NB	2.48	112.41	109.21
5	B	306	CHL	C1-C2-C3	-2.48	121.76	126.04
5	B	311	CHL	C7-C6-C5	-2.47	106.64	113.36
5	A	318	CHL	OBD-CAD-C3D	-2.46	122.59	128.52
5	C	306	CHL	C3B-C4B-NB	2.45	112.38	109.21
4	B	304	NEX	C24-C23-C22	2.45	115.50	110.77
5	A	305	CHL	O2D-CGD-O1D	-2.44	119.06	123.84
6	A	315	CLA	CHB-C4A-NA	2.44	127.89	124.51
5	A	311	CHL	C7-C6-C5	-2.44	106.73	113.36
6	A	307	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
6	A	317	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
6	B	308	CLA	CHB-C4A-NA	2.43	127.88	124.51
6	C	308	CLA	CHB-C4A-NA	2.43	127.88	124.51
5	C	310	CHL	CAC-C3C-C4C	2.43	127.96	124.81
6	C	315	CLA	CHB-C4A-NA	2.43	127.87	124.51
6	A	308	CLA	CHB-C4A-NA	2.42	127.86	124.51
5	B	313	CHL	OMC-CMC-C2C	-2.42	120.22	125.69
5	B	305	CHL	O2A-CGA-CBA	2.42	119.49	111.91
5	A	310	CHL	O2D-CGD-O1D	-2.41	119.12	123.84
5	B	306	CHL	O2A-CGA-CBA	2.41	119.48	111.91
5	C	310	CHL	O2D-CGD-O1D	-2.40	119.14	123.84
3	B	302	0IE	C17-C16-C15	2.40	122.63	118.94
5	B	311	CHL	C4-C3-C5	2.40	119.31	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	310	CHL	C5-C3-C4	2.40	119.91	114.60
5	C	318	CHL	C3B-C4B-NB	2.40	112.31	109.21
5	C	313	CHL	OMC-CMC-C2C	-2.40	120.26	125.69
5	C	310	CHL	OMC-CMC-C2C	-2.40	120.26	125.69
5	A	313	CHL	OMC-CMC-C2C	-2.40	120.27	125.69
5	C	311	CHL	O2D-CGD-O1D	-2.40	119.15	123.84
5	B	318	CHL	C3B-C4B-NB	2.40	112.31	109.21
5	A	310	CHL	C5-C3-C4	2.39	119.89	114.60
5	B	310	CHL	C5-C3-C4	2.39	119.89	114.60
5	C	312	CHL	CAC-C3C-C4C	2.39	127.91	124.81
5	C	305	CHL	O2A-CGA-CBA	2.39	119.40	111.91
6	C	308	CLA	C1-C2-C3	-2.38	122.89	126.75
6	B	315	CLA	CHB-C4A-NA	2.38	127.80	124.51
6	B	308	CLA	C1-C2-C3	-2.38	122.90	126.75
5	A	310	CHL	OMC-CMC-C2C	-2.38	120.31	125.69
5	B	310	CHL	O2D-CGD-O1D	-2.37	119.20	123.84
6	B	314	CLA	CHB-C4A-NA	2.37	127.79	124.51
6	A	314	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
6	A	315	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
2	A	301	0UR	C9-C8-C7	-2.37	123.93	127.31
6	C	314	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
6	C	317	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
5	B	310	CHL	OMC-CMC-C2C	-2.36	120.34	125.69
5	A	311	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
5	A	305	CHL	O2A-CGA-CBA	2.36	119.32	111.91
6	B	314	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
6	C	307	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
5	B	309	CHL	O2D-CGD-O1D	-2.36	119.23	123.84
5	C	318	CHL	OBD-CAD-C3D	-2.36	122.85	128.52
2	B	301	0UR	O42-C2-C41	-2.35	117.17	120.58
5	B	306	CHL	C3B-C4B-NB	2.35	112.25	109.21
5	A	313	CHL	O2D-CGD-O1D	-2.35	119.24	123.84
5	A	310	CHL	CAC-C3C-C4C	2.35	127.86	124.81
6	A	308	CLA	C1-C2-C3	-2.35	122.96	126.75
5	A	312	CHL	CAC-C3C-C4C	2.35	127.85	124.81
5	A	311	CHL	C4-C3-C5	2.34	119.21	115.27
2	C	301	0UR	C28-C19-C18	-2.34	109.74	112.70
6	A	314	CLA	CHB-C4A-NA	2.34	127.75	124.51
5	C	313	CHL	O2D-CGD-O1D	-2.34	119.27	123.84
2	A	301	0UR	C10-C11-C12	-2.33	123.98	127.31
6	B	315	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
5	B	311	CHL	O2D-CGD-O1D	-2.32	119.29	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	314	CLA	CHB-C4A-NA	2.32	127.72	124.51
4	C	304	NEX	C38-C25-C24	-2.32	111.67	114.28
5	C	309	CHL	O2D-CGD-O1D	-2.32	119.31	123.84
5	A	309	CHL	O2D-CGD-O1D	-2.32	119.31	123.84
6	B	317	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
4	B	304	NEX	C1-C2-C3	2.31	118.86	113.64
3	A	302	0IE	C17-C16-C15	2.31	122.48	118.94
5	B	309	CHL	CAC-C3C-C4C	2.31	127.81	124.81
6	B	316	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
2	A	301	0UR	C28-C19-C18	-2.30	109.79	112.70
5	C	311	CHL	C4-C3-C5	2.30	119.14	115.27
6	C	316	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
5	B	313	CHL	O2D-CGD-O1D	-2.30	119.34	123.84
6	A	316	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
5	A	305	CHL	CAC-C3C-C4C	2.30	127.79	124.81
5	A	309	CHL	CAC-C3C-C4C	2.30	127.79	124.81
6	C	315	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
5	B	310	CHL	CAC-C3C-C4C	2.29	127.78	124.81
5	C	305	CHL	CAC-C3C-C4C	2.29	127.78	124.81
6	B	307	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
5	B	312	CHL	CAC-C3C-C4C	2.28	127.77	124.81
5	C	309	CHL	CAC-C3C-C4C	2.28	127.77	124.81
5	A	311	CHL	C4A-NA-C1A	-2.26	105.69	106.71
2	C	301	0UR	C24-C25-C26	-2.26	107.20	110.30
3	C	302	0IE	C17-C16-C15	2.26	122.41	118.94
5	B	311	CHL	C4A-NA-C1A	-2.26	105.69	106.71
5	B	305	CHL	CAC-C3C-C4C	2.24	127.71	124.81
5	A	311	CHL	C1-O2A-CGA	2.23	122.30	116.44
2	B	301	0UR	O44-C45-O57	-2.22	118.06	122.93
5	B	309	CHL	C3B-C4B-NB	2.22	112.07	109.21
5	C	309	CHL	C3B-C4B-NB	2.21	112.07	109.21
4	C	304	NEX	C1-C2-C3	2.21	118.63	113.64
5	B	311	CHL	C3B-C4B-NB	2.21	112.06	109.21
5	B	318	CHL	OBD-CAD-C3D	-2.20	123.22	128.52
5	A	309	CHL	C3B-C4B-NB	2.20	112.05	109.21
2	C	301	0UR	O44-C45-O57	-2.20	118.10	122.93
4	A	304	NEX	O24-C25-C24	2.18	115.02	113.38
5	C	311	CHL	C3B-C4B-NB	2.17	112.02	109.21
5	A	312	CHL	O2D-CGD-O1D	-2.17	119.60	123.84
5	C	311	CHL	C1-O2A-CGA	2.17	122.13	116.44
4	B	304	NEX	C38-C25-C24	-2.17	111.84	114.28
5	A	311	CHL	C3B-C4B-NB	2.17	112.01	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	0UR	O44-C45-O57	-2.16	118.17	122.93
4	A	304	NEX	C24-C23-C22	2.16	114.95	110.77
5	C	306	CHL	CMB-C2B-C3B	2.15	128.70	124.68
5	B	312	CHL	O2D-CGD-O1D	-2.15	119.64	123.84
5	B	311	CHL	C1-O2A-CGA	2.15	122.07	116.44
5	B	306	CHL	C1-O2A-CGA	2.14	122.05	116.44
6	A	315	CLA	C1-C2-C3	-2.14	122.35	126.04
6	B	315	CLA	C1-C2-C3	-2.14	122.35	126.04
5	B	313	CHL	C3B-C4B-NB	2.13	111.97	109.21
5	C	306	CHL	C3C-C4C-NC	2.13	112.97	110.57
6	A	314	CLA	CHD-C1D-ND	-2.13	122.49	124.45
5	A	306	CHL	C3C-C4C-NC	2.13	112.96	110.57
5	A	306	CHL	CMB-C2B-C3B	2.12	128.65	124.68
5	A	318	CHL	C3C-C4C-NC	2.12	112.94	110.57
5	C	312	CHL	O2D-CGD-O1D	-2.11	119.72	123.84
5	A	310	CHL	C3B-C4B-NB	2.11	111.93	109.21
5	B	318	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
5	B	306	CHL	C3C-C4C-NC	2.10	112.92	110.57
6	B	314	CLA	CHD-C1D-ND	-2.10	122.53	124.45
6	A	307	CLA	O2D-CGD-CBD	2.10	114.99	111.27
6	A	307	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
6	A	317	CLA	CHD-C1D-ND	-2.09	122.53	124.45
4	C	304	NEX	O24-C25-C24	2.09	114.95	113.38
6	B	308	CLA	CHD-C1D-ND	-2.08	122.54	124.45
6	C	314	CLA	CHD-C1D-ND	-2.08	122.54	124.45
5	B	313	CHL	CMB-C2B-C3B	2.08	128.57	124.68
5	C	313	CHL	CMB-C2B-C3B	2.08	128.56	124.68
5	A	313	CHL	C3B-C4B-NB	2.08	111.89	109.21
4	A	304	NEX	C1-C2-C3	2.07	118.33	113.64
5	C	311	CHL	C4A-NA-C1A	-2.07	105.77	106.71
5	C	313	CHL	C3B-C4B-NB	2.07	111.89	109.21
6	B	307	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
5	A	313	CHL	CMB-C2B-C3B	2.06	128.54	124.68
5	C	313	CHL	C4-C3-C5	2.06	118.74	115.27
5	B	313	CHL	C4-C3-C5	2.06	118.74	115.27
6	C	307	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
2	C	301	0UR	C15-C14-C13	-2.06	116.79	123.22
5	C	318	CHL	C3C-C4C-NC	2.06	112.88	110.57
6	B	307	CLA	CHD-C1D-ND	-2.05	122.57	124.45
5	A	313	CHL	C4-C3-C5	2.04	118.70	115.27
5	C	310	CHL	C3B-C4B-NB	2.03	111.83	109.21
5	B	318	CHL	CAA-CBA-CGA	-2.03	107.33	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	0UR	C15-C14-C13	-2.02	116.90	123.22
4	B	304	NEX	O24-C25-C24	2.02	114.90	113.38
2	B	301	0UR	C20-C7-C8	-2.02	120.10	122.92
6	B	308	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
6	A	308	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
5	C	318	CHL	O1D-CGD-CBD	-2.00	120.39	124.48

All (90) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	305	CHL	ND
5	A	305	CHL	NA
5	A	305	CHL	NC
5	A	306	CHL	ND
5	A	306	CHL	NA
5	A	306	CHL	NC
5	A	309	CHL	ND
5	A	309	CHL	NA
5	A	309	CHL	NC
5	A	310	CHL	ND
5	A	310	CHL	NA
5	A	310	CHL	NC
5	A	311	CHL	ND
5	A	311	CHL	NA
5	A	311	CHL	NC
5	A	312	CHL	ND
5	A	312	CHL	NA
5	A	312	CHL	NC
5	A	313	CHL	ND
5	A	313	CHL	NA
5	A	313	CHL	NC
5	A	318	CHL	ND
5	A	318	CHL	NA
5	A	318	CHL	NC
5	B	305	CHL	ND
5	B	305	CHL	NA
5	B	305	CHL	NC
5	B	306	CHL	ND
5	B	306	CHL	NA
5	B	306	CHL	NC
5	B	309	CHL	ND
5	B	309	CHL	NA

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Mol	Chain	Res	Type	Atom
5	B	309	CHL	NC
5	B	310	CHL	ND
5	B	310	CHL	NA
5	B	310	CHL	NC
5	B	311	CHL	ND
5	B	311	CHL	NA
5	B	311	CHL	NC
5	B	312	CHL	ND
5	B	312	CHL	NA
5	B	312	CHL	NC
5	B	313	CHL	ND
5	B	313	CHL	NA
5	B	313	CHL	NC
5	B	318	CHL	ND
5	B	318	CHL	NA
5	B	318	CHL	NC
5	C	305	CHL	ND
5	C	305	CHL	NA
5	C	305	CHL	NC
5	C	306	CHL	ND
5	C	306	CHL	NA
5	C	306	CHL	NC
5	C	309	CHL	ND
5	C	309	CHL	NA
5	C	309	CHL	NC
5	C	310	CHL	ND
5	C	310	CHL	NA
5	C	310	CHL	NC
5	C	311	CHL	ND
5	C	311	CHL	NA
5	C	311	CHL	NC
5	C	312	CHL	ND
5	C	312	CHL	NA
5	C	312	CHL	NC
5	C	313	CHL	ND
5	C	313	CHL	NA
5	C	313	CHL	NC
5	C	318	CHL	ND
5	C	318	CHL	NA
5	C	318	CHL	NC
6	A	307	CLA	ND
6	A	308	CLA	ND

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Mol	Chain	Res	Type	Atom
6	A	314	CLA	ND
6	A	315	CLA	ND
6	A	316	CLA	ND
6	A	317	CLA	ND
6	B	307	CLA	ND
6	B	308	CLA	ND
6	B	314	CLA	ND
6	B	315	CLA	ND
6	B	316	CLA	ND
6	B	317	CLA	ND
6	C	307	CLA	ND
6	C	308	CLA	ND
6	C	314	CLA	ND
6	C	315	CLA	ND
6	C	316	CLA	ND
6	C	317	CLA	ND

All (539) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	0UR	C5-C6-C7-C20
2	A	301	0UR	C46-C45-O44-C43
2	A	301	0UR	O57-C45-O44-C43
2	B	301	0UR	C46-C45-O44-C43
2	B	301	0UR	O57-C45-O44-C43
2	C	301	0UR	C5-C6-C7-C20
2	C	301	0UR	C46-C45-O44-C43
2	C	301	0UR	O57-C45-O44-C43
3	A	302	0IE	O1-C2-C3-C20
3	A	303	0IE	C14-C15-C16-C17
3	A	303	0IE	C14-C15-C16-C23
3	B	302	0IE	O1-C2-C3-C20
3	B	303	0IE	C14-C15-C16-C23
3	C	302	0IE	O1-C2-C3-C20
3	C	302	0IE	C15-C16-C17-C18
3	C	302	0IE	C23-C16-C17-C18
3	C	303	0IE	C14-C15-C16-C17
3	C	303	0IE	C14-C15-C16-C23
3	C	303	0IE	C16-C17-C18-C19
5	A	306	CHL	CHA-CBD-CGD-O2D
5	A	312	CHL	C2A-CAA-CBA-CGA
5	A	312	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
5	A	313	CHL	CBD-CGD-O2D-CED
5	B	312	CHL	C2A-CAA-CBA-CGA
5	B	312	CHL	CBD-CGD-O2D-CED
5	B	313	CHL	CBD-CGD-O2D-CED
5	C	306	CHL	CHA-CBD-CGD-O2D
5	C	312	CHL	CBD-CGD-O2D-CED
5	C	313	CHL	CBD-CGD-O2D-CED
6	A	317	CLA	CHA-CBD-CGD-O1D
6	A	317	CLA	CHA-CBD-CGD-O2D
6	B	317	CLA	CHA-CBD-CGD-O1D
6	B	317	CLA	CHA-CBD-CGD-O2D
6	C	317	CLA	CHA-CBD-CGD-O1D
6	C	317	CLA	CHA-CBD-CGD-O2D
7	A	319	LHG	C3-O3-P-O5
7	A	319	LHG	C3-O3-P-O6
7	A	319	LHG	C4-O6-P-O5
7	B	319	LHG	C3-O3-P-O5
7	B	319	LHG	C3-O3-P-O6
7	C	319	LHG	C3-O3-P-O5
7	C	319	LHG	C3-O3-P-O6
5	A	313	CHL	O1D-CGD-O2D-CED
5	B	313	CHL	O1D-CGD-O2D-CED
5	C	313	CHL	O1D-CGD-O2D-CED
6	A	314	CLA	CBD-CGD-O2D-CED
6	B	314	CLA	CBD-CGD-O2D-CED
6	C	314	CLA	CBD-CGD-O2D-CED
6	C	317	CLA	CBD-CGD-O2D-CED
5	A	312	CHL	O1D-CGD-O2D-CED
5	B	312	CHL	O1D-CGD-O2D-CED
6	A	308	CLA	CBD-CGD-O2D-CED
6	A	317	CLA	CBD-CGD-O2D-CED
7	A	319	LHG	O10-C23-O8-C6
7	B	319	LHG	O10-C23-O8-C6
7	C	319	LHG	O10-C23-O8-C6
5	C	312	CHL	O1D-CGD-O2D-CED
5	A	311	CHL	C3-C5-C6-C7
5	B	311	CHL	C3-C5-C6-C7
5	C	311	CHL	C3-C5-C6-C7
7	B	319	LHG	C24-C23-O8-C6
7	C	319	LHG	C24-C23-O8-C6
5	A	310	CHL	C2A-CAA-CBA-CGA
5	B	310	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
5	C	310	CHL	C2A-CAA-CBA-CGA
5	C	312	CHL	C2A-CAA-CBA-CGA
7	A	319	LHG	C24-C25-C26-C27
7	B	319	LHG	C24-C25-C26-C27
7	C	319	LHG	C24-C25-C26-C27
7	A	319	LHG	C24-C23-O8-C6
5	A	309	CHL	CBD-CGD-O2D-CED
5	C	309	CHL	CBD-CGD-O2D-CED
5	C	318	CHL	CBD-CGD-O2D-CED
6	B	317	CLA	CBD-CGD-O2D-CED
6	C	317	CLA	O1D-CGD-O2D-CED
6	A	314	CLA	O1D-CGD-O2D-CED
6	B	314	CLA	O1D-CGD-O2D-CED
6	C	314	CLA	O1D-CGD-O2D-CED
5	A	305	CHL	CBD-CGD-O2D-CED
5	A	318	CHL	CBD-CGD-O2D-CED
5	B	305	CHL	CBD-CGD-O2D-CED
5	B	309	CHL	CBD-CGD-O2D-CED
6	B	308	CLA	CBD-CGD-O2D-CED
6	C	308	CLA	CBD-CGD-O2D-CED
6	A	315	CLA	C3-C5-C6-C7
6	B	315	CLA	C3-C5-C6-C7
6	C	315	CLA	C3-C5-C6-C7
6	A	317	CLA	O1D-CGD-O2D-CED
5	A	311	CHL	CBD-CGD-O2D-CED
5	B	311	CHL	C8-C10-C11-C12
5	A	305	CHL	C11-C12-C13-C14
5	A	306	CHL	C11-C12-C13-C14
5	A	311	CHL	C6-C7-C8-C9
5	A	313	CHL	C11-C10-C8-C9
5	A	313	CHL	C11-C12-C13-C14
5	B	305	CHL	C11-C10-C8-C9
5	B	305	CHL	C11-C12-C13-C14
5	B	306	CHL	C6-C7-C8-C9
5	B	311	CHL	C6-C7-C8-C9
5	B	313	CHL	C11-C10-C8-C9
5	B	313	CHL	C11-C12-C13-C14
5	C	306	CHL	C11-C12-C13-C14
5	C	311	CHL	C6-C7-C8-C9
5	C	313	CHL	C11-C10-C8-C9
5	C	313	CHL	C11-C12-C13-C14
5	C	311	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	B	301	0UR	C5-C6-C7-C20
5	A	311	CHL	C5-C6-C7-C8
5	A	311	CHL	C8-C10-C11-C12
5	C	305	CHL	C13-C15-C16-C17
5	C	312	CHL	C8-C10-C11-C12
5	A	306	CHL	C5-C6-C7-C8
5	B	311	CHL	C5-C6-C7-C8
5	C	306	CHL	C5-C6-C7-C8
5	A	312	CHL	C8-C10-C11-C12
5	B	312	CHL	C8-C10-C11-C12
5	C	311	CHL	C5-C6-C7-C8
6	A	308	CLA	O1D-CGD-O2D-CED
7	A	319	LHG	C7-C8-C9-C10
7	A	319	LHG	C23-C24-C25-C26
7	C	319	LHG	C23-C24-C25-C26
7	B	319	LHG	C7-C8-C9-C10
7	B	319	LHG	C23-C24-C25-C26
5	A	305	CHL	C13-C15-C16-C17
6	A	315	CLA	C6-C7-C8-C10
6	B	315	CLA	C6-C7-C8-C10
6	B	308	CLA	C2A-CAA-CBA-CGA
6	C	308	CLA	C2A-CAA-CBA-CGA
5	A	312	CHL	C15-C16-C17-C18
5	A	313	CHL	C5-C6-C7-C8
5	B	306	CHL	C5-C6-C7-C8
5	B	313	CHL	C5-C6-C7-C8
5	C	313	CHL	C5-C6-C7-C8
5	C	305	CHL	CBD-CGD-O2D-CED
3	C	303	0IE	C4-C5-C6-C7
5	B	305	CHL	C13-C15-C16-C17
5	C	312	CHL	C15-C16-C17-C18
6	B	307	CLA	C8-C10-C11-C12
5	A	312	CHL	C13-C15-C16-C17
5	B	312	CHL	C13-C15-C16-C17
5	C	312	CHL	C13-C15-C16-C17
5	B	312	CHL	C15-C16-C17-C18
5	A	318	CHL	C2A-CAA-CBA-CGA
5	C	318	CHL	C2A-CAA-CBA-CGA
5	A	306	CHL	C8-C10-C11-C12
5	C	306	CHL	C8-C10-C11-C12
3	A	302	0IE	C14-C15-C16-C23
3	B	302	0IE	C14-C15-C16-C23

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Mol	Chain	Res	Type	Atoms
3	B	303	0IE	C10-C11-C12-C22
3	C	302	0IE	C14-C15-C16-C23
6	A	315	CLA	CBA-CGA-O2A-C1
7	C	319	LHG	C27-C28-C29-C30
5	C	309	CHL	O1D-CGD-O2D-CED
6	A	307	CLA	C8-C10-C11-C12
6	C	307	CLA	C8-C10-C11-C12
5	A	309	CHL	O1D-CGD-O2D-CED
5	C	318	CHL	O1D-CGD-O2D-CED
6	B	317	CLA	O1D-CGD-O2D-CED
6	C	308	CLA	O1D-CGD-O2D-CED
3	A	302	0IE	C14-C15-C16-C17
3	B	302	0IE	C14-C15-C16-C17
3	B	303	0IE	C10-C11-C12-C13
3	B	303	0IE	C14-C15-C16-C17
3	C	302	0IE	C14-C15-C16-C17
5	A	305	CHL	C11-C10-C8-C9
6	C	315	CLA	C6-C7-C8-C9
5	B	305	CHL	O1D-CGD-O2D-CED
7	C	319	LHG	C12-C13-C14-C15
6	B	308	CLA	O1D-CGD-O2D-CED
7	B	319	LHG	O1-C1-C2-C3
7	C	319	LHG	O1-C1-C2-C3
2	A	301	0UR	C5-C6-C7-C8
2	C	301	0UR	C5-C6-C7-C8
5	A	305	CHL	O1D-CGD-O2D-CED
7	C	319	LHG	C26-C27-C28-C29
5	A	305	CHL	C16-C17-C18-C19
5	A	305	CHL	C16-C17-C18-C20
5	A	313	CHL	C16-C17-C18-C19
5	B	305	CHL	C16-C17-C18-C19
5	B	305	CHL	C16-C17-C18-C20
5	B	313	CHL	C16-C17-C18-C19
5	C	305	CHL	C16-C17-C18-C19
5	C	305	CHL	C16-C17-C18-C20
5	C	313	CHL	C16-C17-C18-C19
5	B	309	CHL	O1D-CGD-O2D-CED
7	A	319	LHG	C27-C28-C29-C30
6	B	308	CLA	CBA-CGA-O2A-C1
6	B	315	CLA	CBA-CGA-O2A-C1
5	A	318	CHL	O1D-CGD-O2D-CED
5	A	311	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
5	B	311	CHL	C3A-C2A-CAA-CBA
5	C	311	CHL	C3A-C2A-CAA-CBA
7	B	319	LHG	C12-C13-C14-C15
5	A	313	CHL	C16-C17-C18-C20
5	B	313	CHL	C16-C17-C18-C20
5	C	313	CHL	C16-C17-C18-C20
6	C	317	CLA	C6-C7-C8-C10
3	C	303	0IE	C11-C10-C9-C8
5	B	313	CHL	C2-C3-C5-C6
7	A	319	LHG	C10-C11-C12-C13
6	A	315	CLA	O1A-CGA-O2A-C1
7	A	319	LHG	C11-C10-C9-C8
7	C	319	LHG	C10-C11-C12-C13
5	A	311	CHL	CBA-CGA-O2A-C1
5	C	311	CHL	CBA-CGA-O2A-C1
5	A	306	CHL	C10-C11-C12-C13
5	C	305	CHL	C15-C16-C17-C18
5	C	306	CHL	C10-C11-C12-C13
5	A	313	CHL	C4-C3-C5-C6
5	B	313	CHL	C4-C3-C5-C6
5	C	313	CHL	C4-C3-C5-C6
5	A	313	CHL	C2-C3-C5-C6
5	B	306	CHL	C6-C7-C8-C10
5	C	313	CHL	C2-C3-C5-C6
6	C	315	CLA	C6-C7-C8-C10
6	B	308	CLA	O1A-CGA-O2A-C1
6	B	315	CLA	O1A-CGA-O2A-C1
7	C	319	LHG	C7-C8-C9-C10
5	B	311	CHL	CBA-CGA-O2A-C1
5	A	306	CHL	C2A-CAA-CBA-CGA
5	C	306	CHL	C2A-CAA-CBA-CGA
5	A	305	CHL	C15-C16-C17-C18
7	A	319	LHG	C26-C27-C28-C29
5	B	311	CHL	C10-C11-C12-C13
7	A	319	LHG	C12-C13-C14-C15
7	B	319	LHG	C10-C11-C12-C13
7	B	319	LHG	C27-C28-C29-C30
5	A	311	CHL	O1A-CGA-O2A-C1
5	C	311	CHL	O1A-CGA-O2A-C1
5	B	318	CHL	CBD-CGD-O2D-CED
5	B	312	CHL	C16-C17-C18-C20
5	A	311	CHL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
5	B	310	CHL	CBD-CGD-O2D-CED
5	A	310	CHL	CBA-CGA-O2A-C1
6	A	315	CLA	C6-C7-C8-C9
6	B	315	CLA	C6-C7-C8-C9
5	B	311	CHL	CBD-CGD-O2D-CED
5	C	311	CHL	C10-C11-C12-C13
6	A	308	CLA	C2A-CAA-CBA-CGA
5	A	311	CHL	O1D-CGD-O2D-CED
5	C	311	CHL	C11-C12-C13-C15
5	B	311	CHL	O1A-CGA-O2A-C1
5	A	305	CHL	C1A-C2A-CAA-CBA
5	A	306	CHL	C1A-C2A-CAA-CBA
5	A	311	CHL	C1A-C2A-CAA-CBA
5	B	305	CHL	C1A-C2A-CAA-CBA
5	B	306	CHL	C1A-C2A-CAA-CBA
5	B	311	CHL	C1A-C2A-CAA-CBA
5	C	305	CHL	C1A-C2A-CAA-CBA
5	C	306	CHL	C1A-C2A-CAA-CBA
5	C	311	CHL	C1A-C2A-CAA-CBA
5	B	312	CHL	C16-C17-C18-C19
5	B	310	CHL	CBA-CGA-O2A-C1
5	C	310	CHL	CBA-CGA-O2A-C1
5	A	311	CHL	C11-C12-C13-C15
5	C	312	CHL	C16-C17-C18-C20
5	B	311	CHL	C12-C13-C15-C16
5	B	311	CHL	C11-C12-C13-C15
5	C	311	CHL	C12-C13-C15-C16
5	A	311	CHL	C12-C13-C15-C16
7	C	319	LHG	O1-C1-C2-O2
7	B	319	LHG	C26-C27-C28-C29
5	C	305	CHL	C4-C3-C5-C6
7	C	319	LHG	C13-C14-C15-C16
5	A	312	CHL	C16-C17-C18-C20
5	C	311	CHL	CBD-CGD-O2D-CED
5	B	306	CHL	C15-C16-C17-C18
5	A	306	CHL	C15-C16-C17-C18
5	C	306	CHL	C15-C16-C17-C18
3	A	303	0IE	C16-C17-C18-C19
5	A	310	CHL	O1A-CGA-O2A-C1
5	B	310	CHL	O1A-CGA-O2A-C1
5	B	305	CHL	C15-C16-C17-C18
5	C	310	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
5	A	311	CHL	C6-C7-C8-C10
5	A	313	CHL	C11-C12-C13-C15
5	B	305	CHL	C6-C7-C8-C10
5	B	305	CHL	C11-C12-C13-C15
5	B	311	CHL	C6-C7-C8-C10
5	B	313	CHL	C11-C12-C13-C15
5	C	313	CHL	C11-C12-C13-C15
2	A	301	0UR	C46-C47-C48-C49
5	B	306	CHL	C11-C12-C13-C14
5	C	305	CHL	O1D-CGD-O2D-CED
3	B	302	0IE	C13-C14-C15-C16
7	B	319	LHG	C13-C14-C15-C16
6	B	317	CLA	C6-C7-C8-C10
5	C	312	CHL	C16-C17-C18-C19
7	A	319	LHG	O6-C4-C5-C6
7	B	319	LHG	O6-C4-C5-C6
7	C	319	LHG	O6-C4-C5-C6
2	A	301	0UR	O44-C45-C46-C47
5	A	305	CHL	C3A-C2A-CAA-CBA
5	B	305	CHL	C3A-C2A-CAA-CBA
5	C	305	CHL	C3A-C2A-CAA-CBA
7	A	319	LHG	C13-C14-C15-C16
5	A	305	CHL	C3-C5-C6-C7
5	A	305	CHL	C4-C3-C5-C6
5	B	305	CHL	C4-C3-C5-C6
7	B	319	LHG	O6-C4-C5-O7
7	C	319	LHG	O6-C4-C5-O7
6	C	308	CLA	CBA-CGA-O2A-C1
5	A	312	CHL	C16-C17-C18-C19
7	C	319	LHG	O2-C2-C3-O3
5	A	310	CHL	C2-C1-O2A-CGA
5	B	310	CHL	C2-C1-O2A-CGA
5	C	311	CHL	C2-C1-O2A-CGA
6	A	315	CLA	C2-C1-O2A-CGA
5	B	310	CHL	O1D-CGD-O2D-CED
5	B	306	CHL	C11-C10-C8-C9
5	C	305	CHL	C11-C10-C8-C9
5	C	305	CHL	C11-C12-C13-C14
6	A	317	CLA	C2A-CAA-CBA-CGA
2	C	301	0UR	C46-C47-C48-C49
5	B	318	CHL	O1D-CGD-O2D-CED
2	B	301	0UR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
7	B	319	LHG	C9-C10-C11-C12
5	A	305	CHL	C11-C12-C13-C15
5	A	311	CHL	C11-C10-C8-C7
5	A	312	CHL	C6-C7-C8-C10
5	B	311	CHL	C11-C10-C8-C7
5	B	312	CHL	C6-C7-C8-C10
5	C	311	CHL	C6-C7-C8-C10
5	C	311	CHL	C11-C10-C8-C7
5	C	312	CHL	C6-C7-C8-C10
3	C	302	0IE	C13-C14-C15-C16
5	B	311	CHL	O1D-CGD-O2D-CED
2	A	301	0UR	O42-C2-C3-C4
2	B	301	0UR	O42-C2-C3-C4
2	C	301	0UR	O42-C2-C3-C4
3	A	302	0IE	O1-C2-C3-C4
3	B	302	0IE	O1-C2-C3-C4
3	C	302	0IE	O1-C2-C3-C4
5	C	305	CHL	C3-C5-C6-C7
2	B	301	0UR	O44-C45-C46-C47
5	B	318	CHL	CAA-CBA-CGA-O2A
7	A	319	LHG	O6-C4-C5-O7
6	A	308	CLA	CBA-CGA-O2A-C1
5	A	306	CHL	CHA-CBD-CGD-O1D
5	B	306	CHL	CHA-CBD-CGD-O1D
5	B	306	CHL	CHA-CBD-CGD-O2D
5	B	318	CHL	CHA-CBD-CGD-O1D
5	B	318	CHL	CHA-CBD-CGD-O2D
5	C	306	CHL	CHA-CBD-CGD-O1D
6	A	308	CLA	CHA-CBD-CGD-O1D
6	A	308	CLA	CHA-CBD-CGD-O2D
6	B	307	CLA	C10-C11-C12-C13
6	C	308	CLA	O1A-CGA-O2A-C1
7	B	319	LHG	O1-C1-C2-O2
5	C	311	CHL	O1D-CGD-O2D-CED
5	B	312	CHL	C4-C3-C5-C6
5	C	312	CHL	C4-C3-C5-C6
6	A	307	CLA	C10-C11-C12-C13
6	C	307	CLA	C10-C11-C12-C13
6	A	316	CLA	CBD-CGD-O2D-CED
6	A	314	CLA	C1A-C2A-CAA-CBA
6	B	314	CLA	C1A-C2A-CAA-CBA
6	C	314	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
7	A	319	LHG	C4-O6-P-O3
5	B	305	CHL	C3-C5-C6-C7
7	A	319	LHG	C4-O6-P-O4
7	B	319	LHG	C4-O6-P-O4
6	A	317	CLA	C11-C10-C8-C7
5	B	318	CHL	CAD-CBD-CGD-O1D
6	A	308	CLA	CAD-CBD-CGD-O1D
2	A	301	0UR	O42-C2-C3-C43
5	A	313	CHL	C11-C10-C8-C7
5	B	313	CHL	C11-C10-C8-C7
5	C	313	CHL	C11-C10-C8-C7
3	A	303	0IE	C13-C14-C15-C16
6	A	308	CLA	O1A-CGA-O2A-C1
5	C	305	CHL	C5-C6-C7-C8
5	C	305	CHL	C2-C3-C5-C6
5	B	312	CHL	C14-C13-C15-C16
5	C	312	CHL	C14-C13-C15-C16
2	A	301	0UR	O57-C45-C46-C47
7	B	319	LHG	O2-C2-C3-O3
7	B	319	LHG	C29-C30-C31-C32
5	A	312	CHL	C4-C3-C5-C6
7	A	319	LHG	C25-C26-C27-C28
5	C	306	CHL	O1A-CGA-O2A-C1
5	B	306	CHL	C2A-CAA-CBA-CGA
5	A	306	CHL	O1A-CGA-O2A-C1
6	C	317	CLA	CBA-CGA-O2A-C1
6	A	316	CLA	O1D-CGD-O2D-CED
5	A	311	CHL	C2-C1-O2A-CGA
5	B	311	CHL	C2-C1-O2A-CGA
5	C	310	CHL	C2-C1-O2A-CGA
5	B	306	CHL	C13-C15-C16-C17
3	B	303	0IE	C16-C17-C18-C19
3	C	302	0IE	C16-C17-C18-C19
5	B	312	CHL	C2-C3-C5-C6
5	C	312	CHL	C2-C3-C5-C6
5	A	306	CHL	CBA-CGA-O2A-C1
5	C	306	CHL	CBA-CGA-O2A-C1
6	A	317	CLA	C6-C7-C8-C10
4	A	304	NEX	C11-C10-C9-C8
7	B	319	LHG	C31-C32-C33-C34
6	C	317	CLA	O1A-CGA-O2A-C1
7	C	319	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
5	A	305	CHL	C6-C7-C8-C10
5	C	305	CHL	C6-C7-C8-C10
5	A	311	CHL	C11-C10-C8-C9
5	A	312	CHL	C6-C7-C8-C9
5	B	311	CHL	C11-C10-C8-C9
5	C	311	CHL	C11-C10-C8-C9
3	A	303	0IE	C3-C4-C5-C6
5	A	305	CHL	C5-C6-C7-C8
2	B	301	0UR	O57-C45-C46-C47
2	B	301	0UR	C46-C47-C48-C49
5	B	305	CHL	C2-C3-C5-C6
7	C	319	LHG	C11-C10-C9-C8
6	C	317	CLA	C2A-CAA-CBA-CGA
3	A	302	0IE	C13-C14-C15-C16
3	B	303	0IE	C13-C14-C15-C16
5	C	310	CHL	O1D-CGD-O2D-CED
7	A	319	LHG	C29-C30-C31-C32
5	A	310	CHL	O1D-CGD-O2D-CED
7	C	319	LHG	C29-C30-C31-C32
2	C	301	0UR	C47-C48-C49-C50
5	A	306	CHL	C4-C3-C5-C6
5	C	306	CHL	C4-C3-C5-C6
5	A	312	CHL	C14-C13-C15-C16
6	A	307	CLA	C11-C12-C13-C14
6	B	307	CLA	C11-C12-C13-C14
6	C	307	CLA	C11-C12-C13-C14
7	A	319	LHG	C15-C16-C17-C18
3	C	303	0IE	C10-C11-C12-C22
4	A	304	NEX	C39-C29-C30-C31
4	B	304	NEX	C39-C29-C30-C31
4	C	304	NEX	C39-C29-C30-C31
3	A	302	0IE	C5-C6-C7-C21
5	A	313	CHL	C10-C11-C12-C13
5	A	306	CHL	C11-C12-C13-C15
5	A	313	CHL	C12-C13-C15-C16
5	B	313	CHL	C12-C13-C15-C16
5	C	306	CHL	C11-C12-C13-C15
5	C	313	CHL	C12-C13-C15-C16
7	B	319	LHG	C4-O6-P-O3
2	C	301	0UR	O44-C45-C46-C47
5	B	313	CHL	C10-C11-C12-C13
6	B	317	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
5	B	305	CHL	C5-C6-C7-C8
5	C	313	CHL	C10-C11-C12-C13
4	A	304	NEX	C28-C29-C30-C31
4	B	304	NEX	C28-C29-C30-C31
4	C	304	NEX	C28-C29-C30-C31
3	B	303	0IE	C3-C4-C5-C6
5	A	313	CHL	C13-C15-C16-C17
5	B	313	CHL	C13-C15-C16-C17
5	C	313	CHL	C13-C15-C16-C17
6	B	315	CLA	C2-C1-O2A-CGA
5	A	305	CHL	C2-C3-C5-C6
5	A	312	CHL	C2-C3-C5-C6
5	B	306	CHL	C14-C13-C15-C16
5	A	311	CHL	CAA-CBA-CGA-O2A
7	A	319	LHG	C9-C10-C11-C12
5	B	311	CHL	CAA-CBA-CGA-O2A
5	C	311	CHL	CAA-CBA-CGA-O2A
7	B	319	LHG	C11-C10-C9-C8
6	C	316	CLA	CAA-CBA-CGA-O2A
7	A	319	LHG	C2-C3-O3-P
3	B	303	0IE	C20-C3-C4-C5
3	C	303	0IE	C20-C3-C4-C5
5	C	312	CHL	C10-C11-C12-C13
7	A	319	LHG	C31-C32-C33-C34
5	B	312	CHL	C6-C7-C8-C9
5	C	310	CHL	CBD-CGD-O2D-CED
6	C	315	CLA	C3A-C2A-CAA-CBA
5	A	306	CHL	CAA-CBA-CGA-O2A
5	C	306	CHL	CAA-CBA-CGA-O2A
6	C	316	CLA	CAA-CBA-CGA-O1A
5	A	313	CHL	CAD-CBD-CGD-O2D
5	B	313	CHL	CAD-CBD-CGD-O2D
5	C	313	CHL	CAD-CBD-CGD-O2D
5	A	312	CHL	C10-C11-C12-C13
6	B	316	CLA	CAA-CBA-CGA-O2A
5	A	310	CHL	CBD-CGD-O2D-CED
5	C	310	CHL	CAA-CBA-CGA-O2A
3	B	303	0IE	C12-C13-C14-C15
6	A	307	CLA	O2A-C1-C2-C3
6	B	307	CLA	O2A-C1-C2-C3
6	C	307	CLA	O2A-C1-C2-C3
5	B	311	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
5	C	311	CHL	C2A-CAA-CBA-CGA
6	A	316	CLA	CAA-CBA-CGA-O2A
6	A	307	CLA	CHA-CBD-CGD-O1D
6	A	307	CLA	CHA-CBD-CGD-O2D
6	A	315	CLA	CHA-CBD-CGD-O1D
6	A	315	CLA	CHA-CBD-CGD-O2D
6	B	307	CLA	CHA-CBD-CGD-O1D
6	B	307	CLA	CHA-CBD-CGD-O2D
6	B	315	CLA	CHA-CBD-CGD-O1D
6	B	315	CLA	CHA-CBD-CGD-O2D
6	B	316	CLA	CHA-CBD-CGD-O1D
6	C	307	CLA	CHA-CBD-CGD-O1D
6	C	307	CLA	CHA-CBD-CGD-O2D
6	C	308	CLA	CHA-CBD-CGD-O1D
6	A	316	CLA	CAA-CBA-CGA-O1A
6	B	316	CLA	CAA-CBA-CGA-O1A
5	A	310	CHL	CAA-CBA-CGA-O2A
5	B	310	CHL	CAA-CBA-CGA-O2A
6	C	314	CLA	C2A-CAA-CBA-CGA
5	C	312	CHL	C6-C7-C8-C9
3	C	303	0IE	C3-C4-C5-C6
6	A	314	CLA	C2A-CAA-CBA-CGA
6	B	314	CLA	C2A-CAA-CBA-CGA
5	A	306	CHL	C2-C3-C5-C6
5	C	306	CHL	C2-C3-C5-C6
3	A	302	0IE	C5-C6-C7-C8
3	B	302	0IE	C15-C16-C17-C18
6	C	315	CLA	C1A-C2A-CAA-CBA
7	C	319	LHG	C2-C3-O3-P
5	B	310	CHL	CAA-CBA-CGA-O1A
5	C	310	CHL	CAA-CBA-CGA-O1A
7	B	319	LHG	C4-O6-P-O5
7	C	319	LHG	C4-O6-P-O4
5	C	306	CHL	CAA-CBA-CGA-O1A
5	A	306	CHL	CAA-CBA-CGA-O1A
5	A	310	CHL	CAA-CBA-CGA-O1A
5	B	318	CHL	CAA-CBA-CGA-O1A
6	A	315	CLA	CAD-CBD-CGD-O1D
6	B	308	CLA	CAD-CBD-CGD-O1D
6	C	308	CLA	CAD-CBD-CGD-O1D
5	A	311	CHL	C2A-CAA-CBA-CGA
2	B	301	0UR	O42-C2-C3-C43

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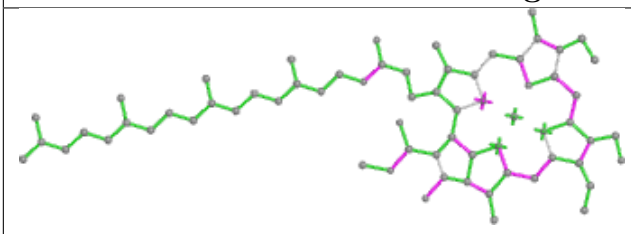
Mol	Chain	Res	Type	Atoms
2	C	301	0UR	O42-C2-C3-C43
3	C	303	0IE	C2-C3-C4-C5
5	B	305	CHL	C11-C10-C8-C7
5	B	312	CHL	C12-C13-C15-C16
5	C	312	CHL	C12-C13-C15-C16
6	B	307	CLA	C11-C10-C8-C7
6	C	307	CLA	C11-C10-C8-C7
5	B	306	CHL	CAA-CBA-CGA-O2A
3	A	302	0IE	C15-C16-C17-C18
3	A	303	0IE	C5-C6-C7-C8
5	B	306	CHL	CAA-CBA-CGA-O1A
5	A	306	CHL	C13-C15-C16-C17
5	C	306	CHL	C13-C15-C16-C17

There are no ring outliers.

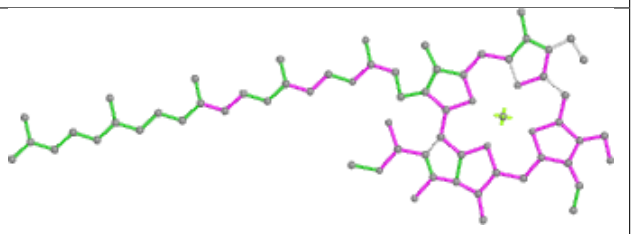
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

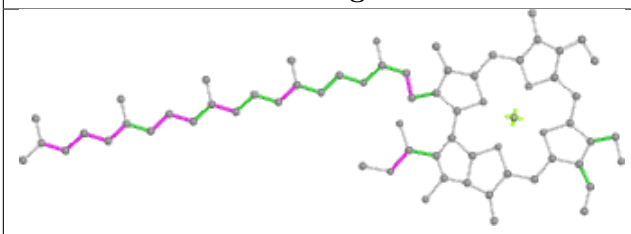
Ligand CHL C 312



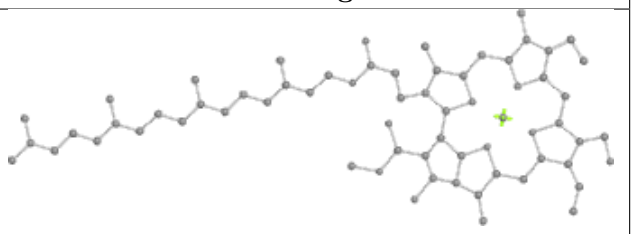
Bond lengths



Bond angles

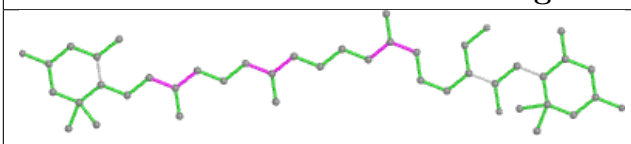


Torsions

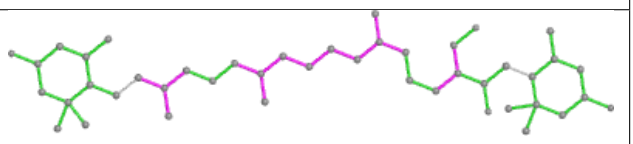


Rings

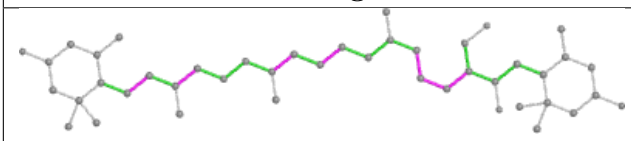
Ligand 0IE C 303



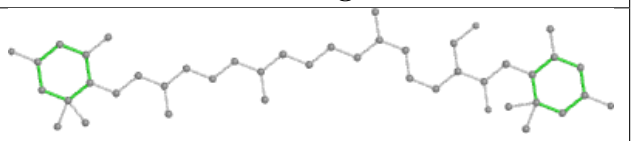
Bond lengths



Bond angles

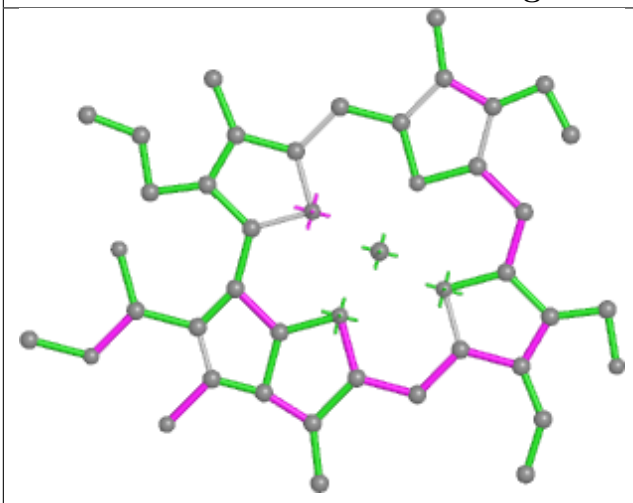


Torsions

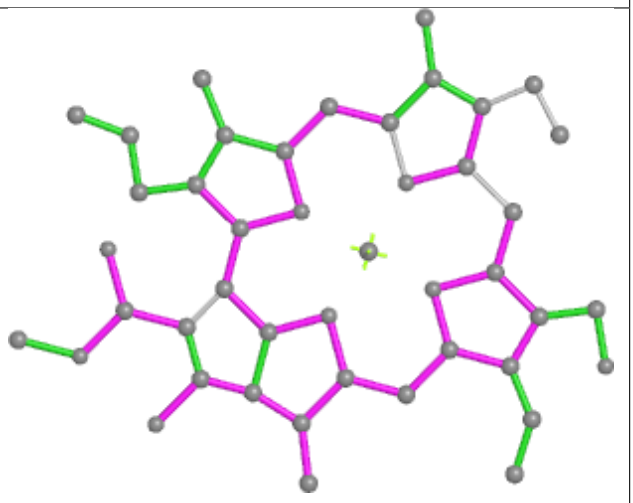


Rings

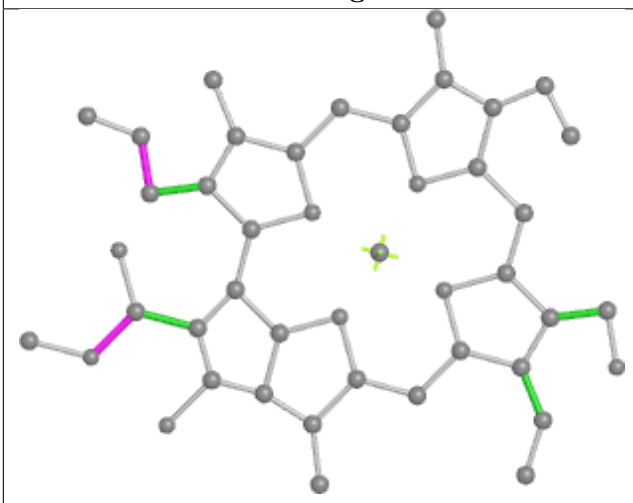
Ligand CHL A 318



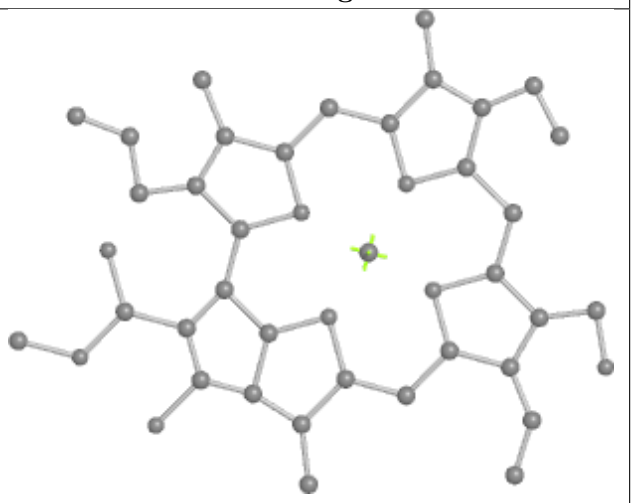
Bond lengths



Bond angles

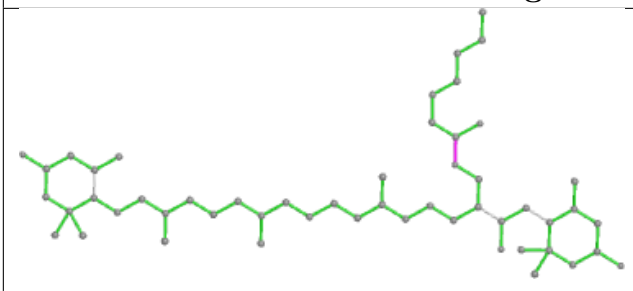


Torsions

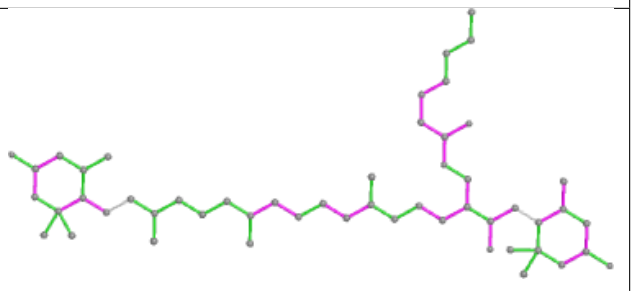


Rings

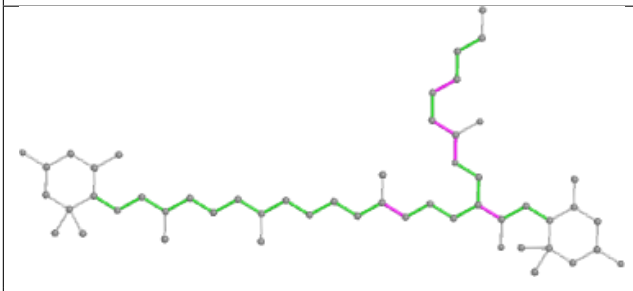
Ligand 0UR A 301



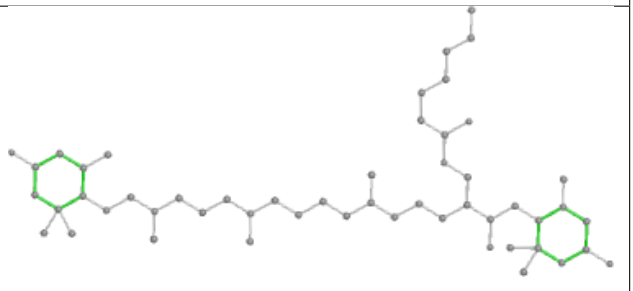
Bond lengths



Bond angles

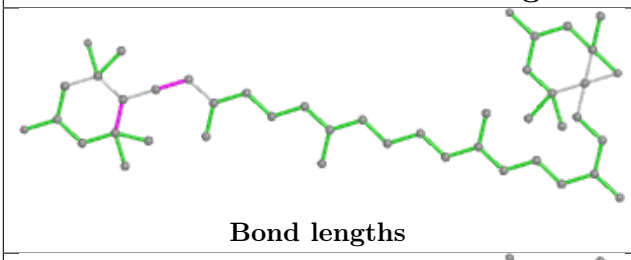


Torsions

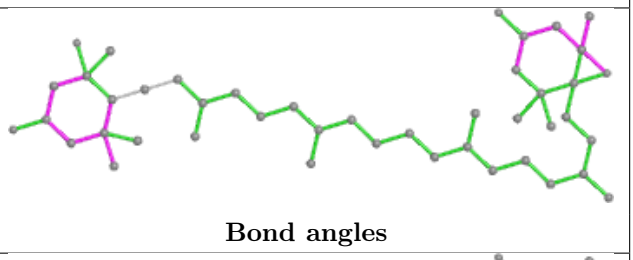


Rings

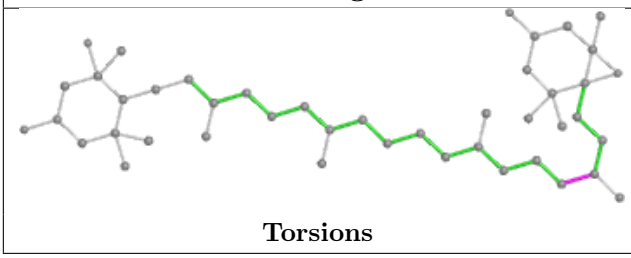
Ligand NEX B 304



Bond lengths



Bond angles



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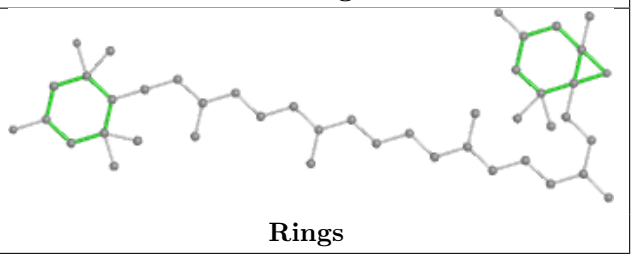
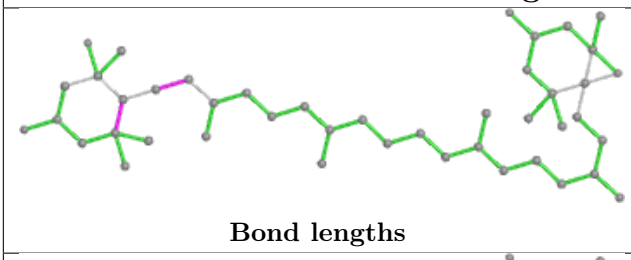
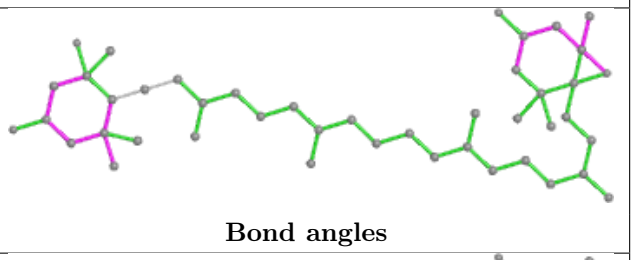


Rings

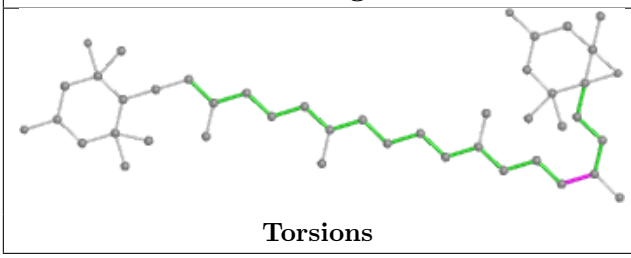
Ligand NEX C 304



Bond lengths



Bond angles



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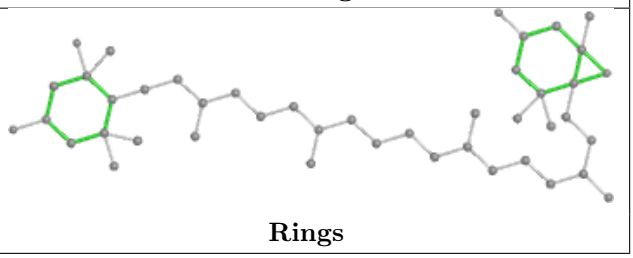
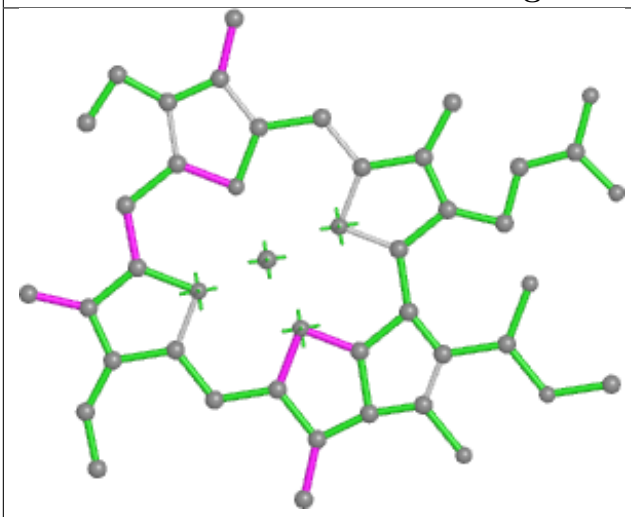
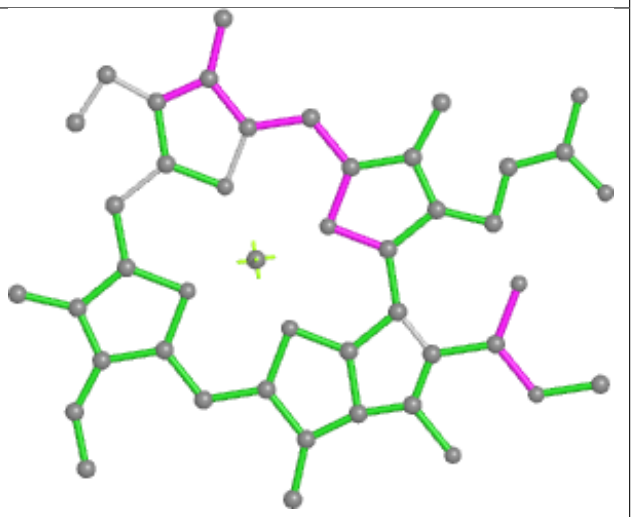


Rings

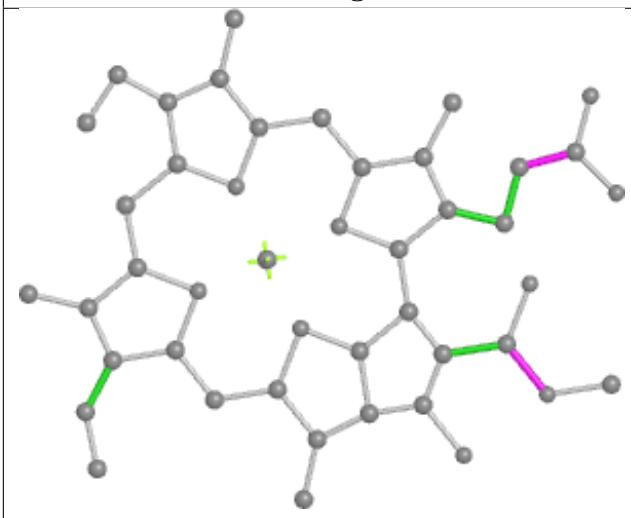
Ligand CLA A 316



Bond lengths



Bond angles



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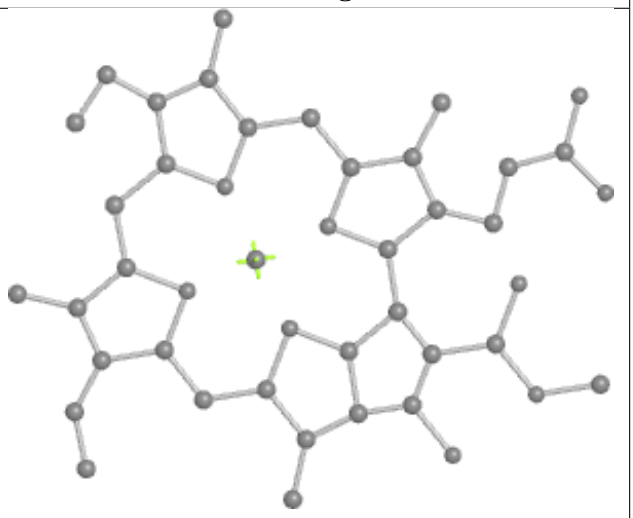
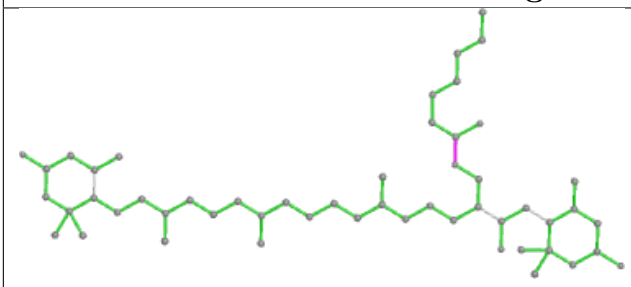
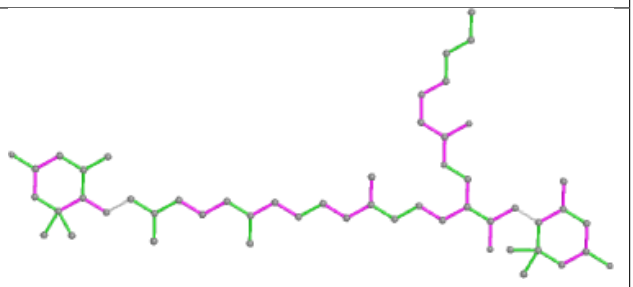


Rings

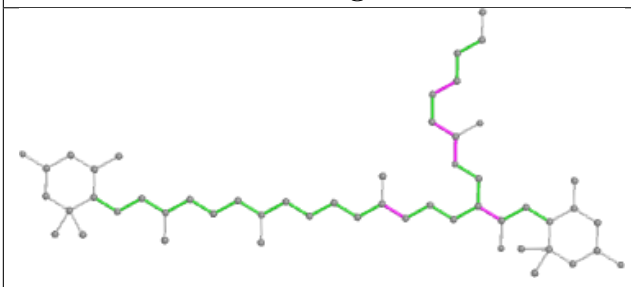
Ligand 0UR B 301



Bond lengths



Bond angles



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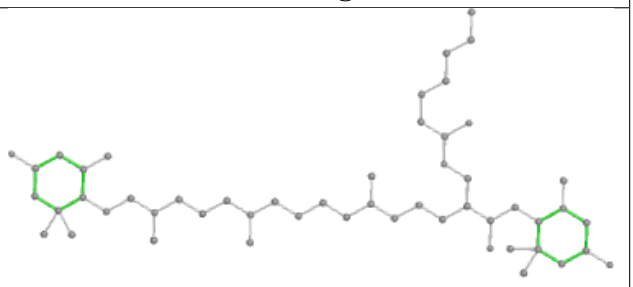
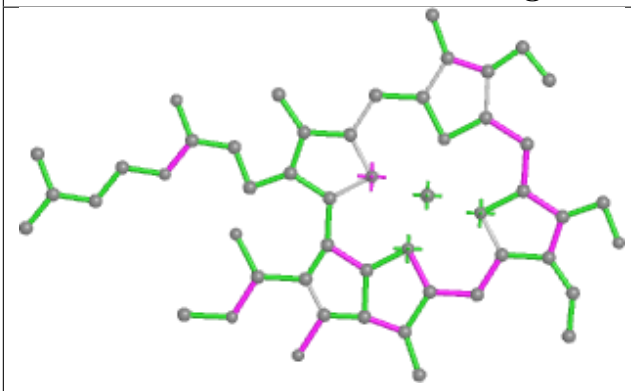
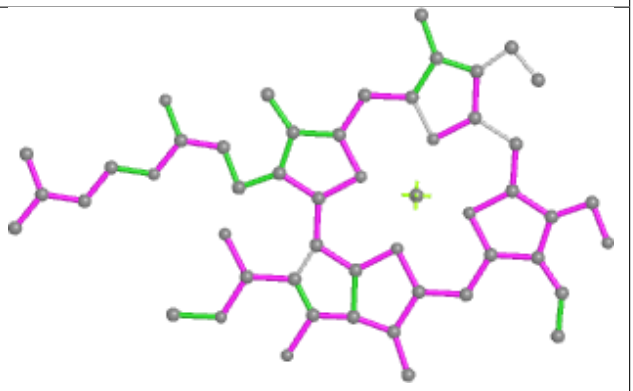


Rings

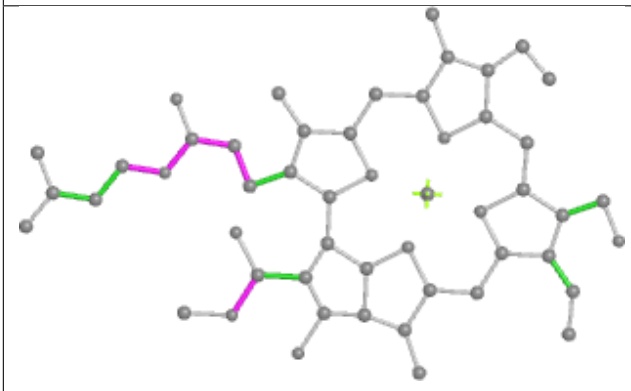
Ligand CHL C 310



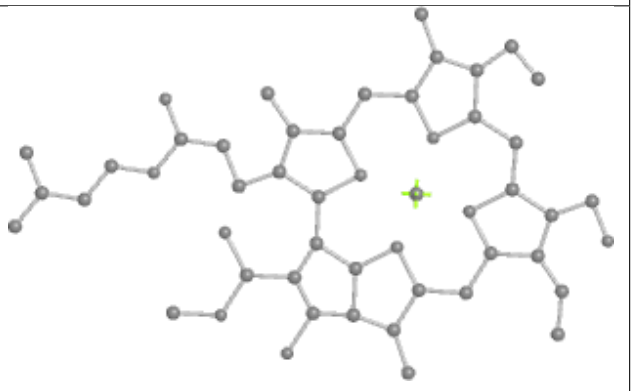
Bond lengths



Bond angles

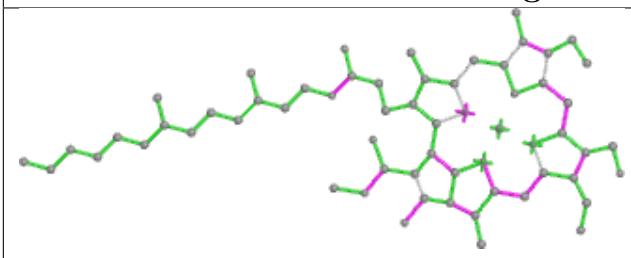


Torsions

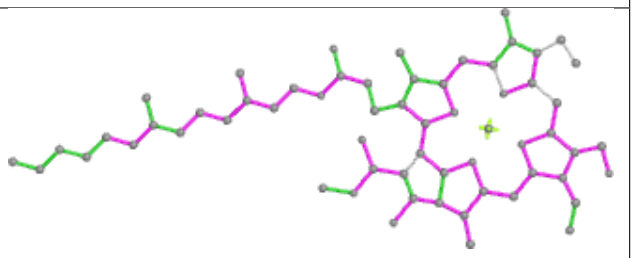


Rings

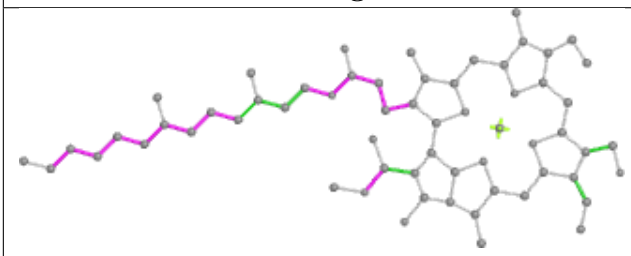
Ligand CHL A 311



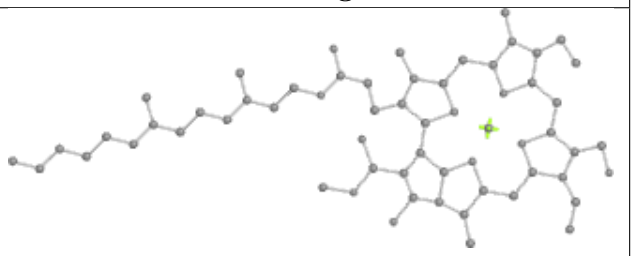
Bond lengths



Bond angles

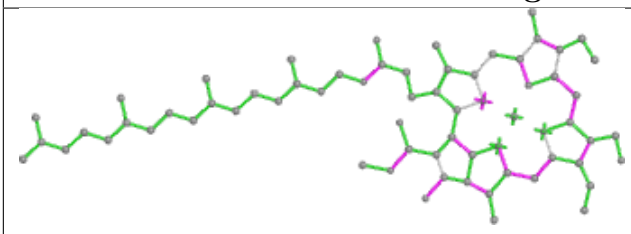


Torsions

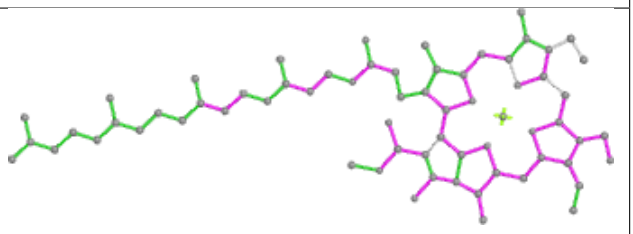


Rings

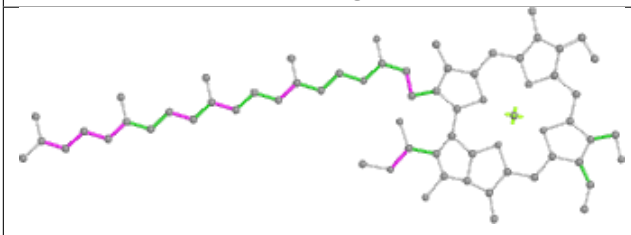
Ligand CHL B 312



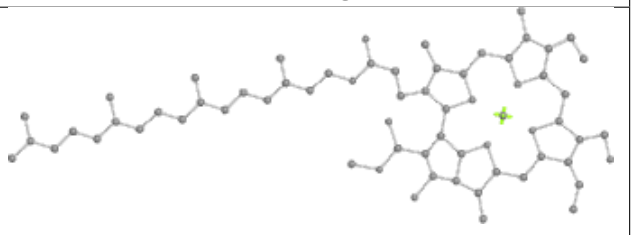
Bond lengths



Bond angles

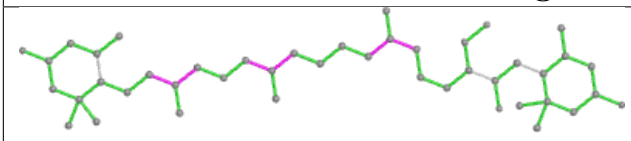


Torsions

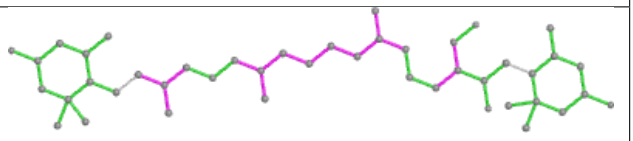


Rings

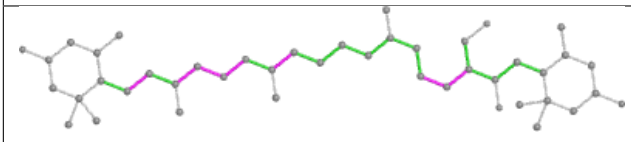
Ligand 0IE B 303



Bond lengths



Bond angles



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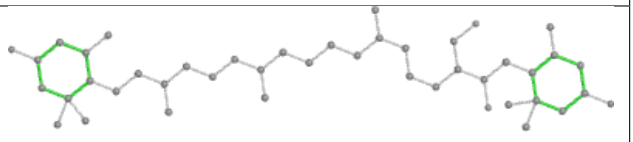
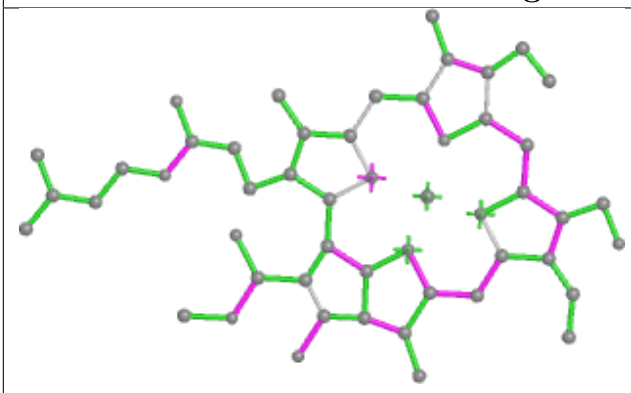
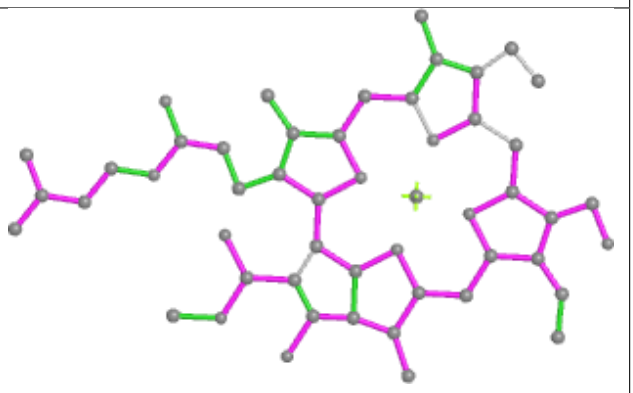


Rings

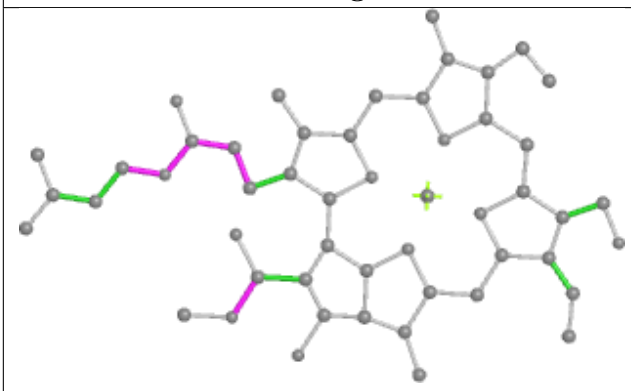
Ligand CHL A 310



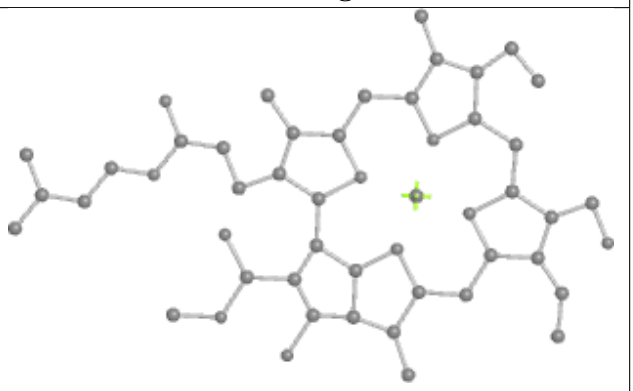
Bond lengths



Bond angles

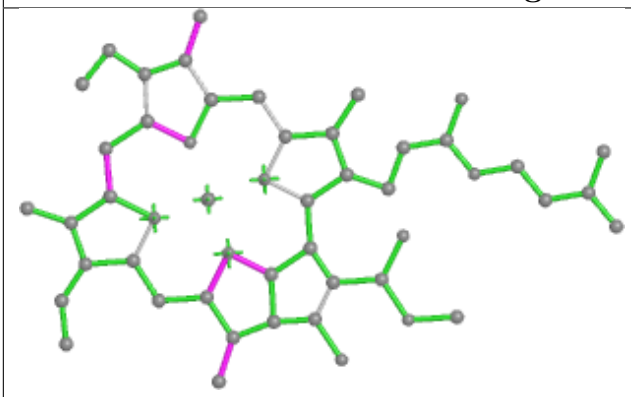


Torsions

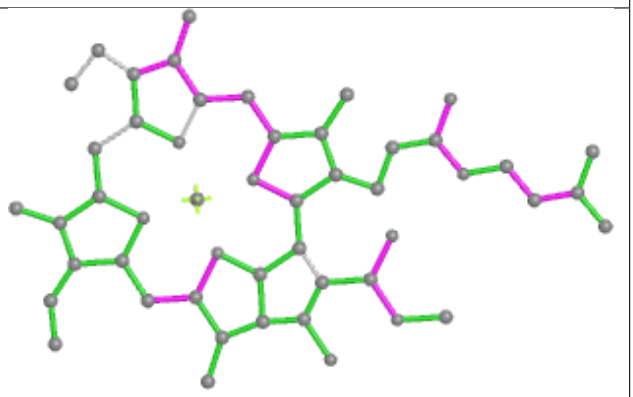


Rings

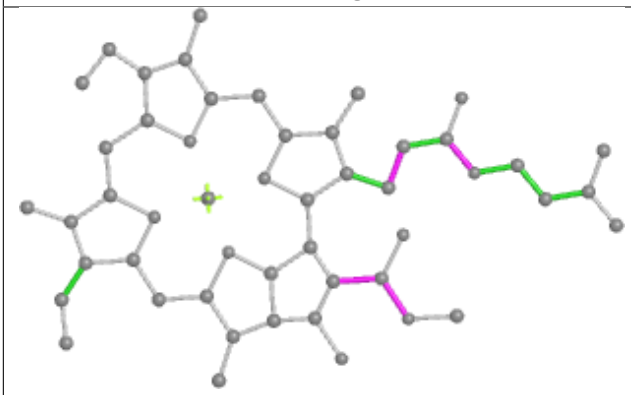
Ligand CLA B 308



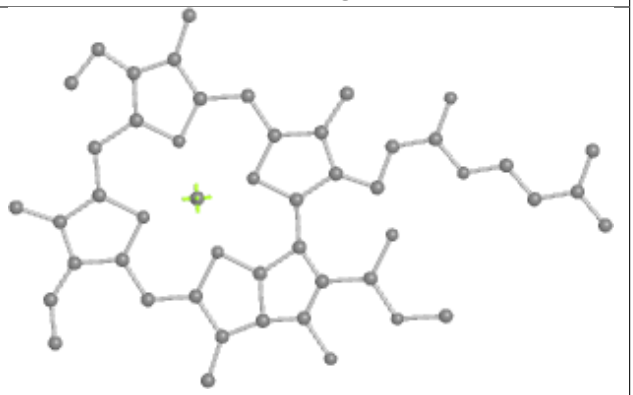
Bond lengths



Bond angles

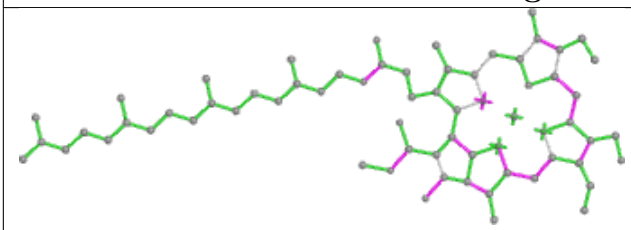


Torsions

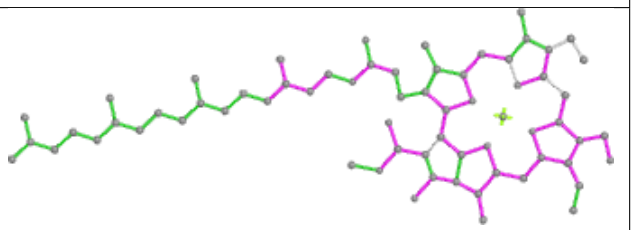


Rings

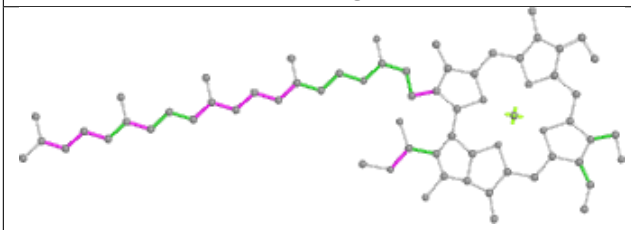
Ligand CHL B 305



Bond lengths



Bond angles



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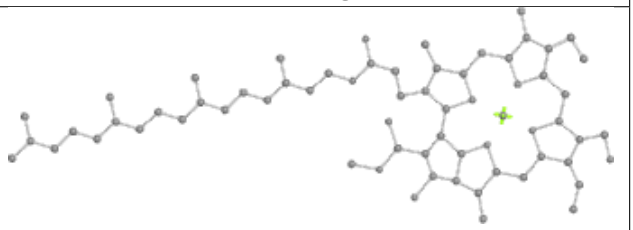
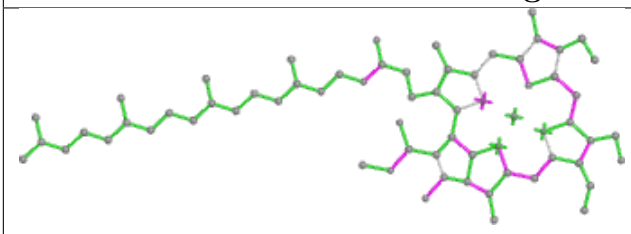
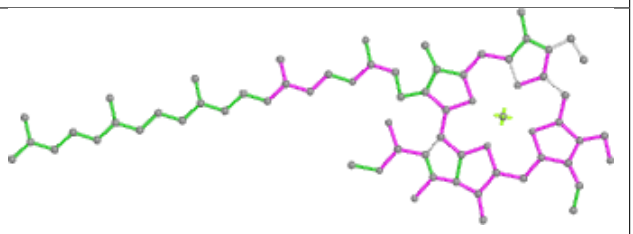


Rings

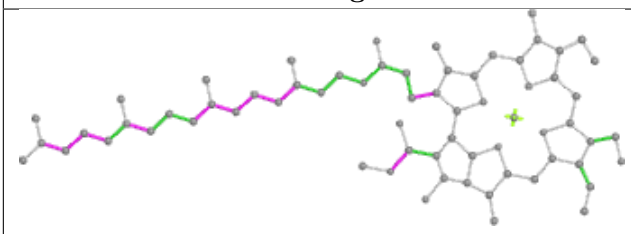
Ligand CHL C 305



Bond lengths



Bond angles



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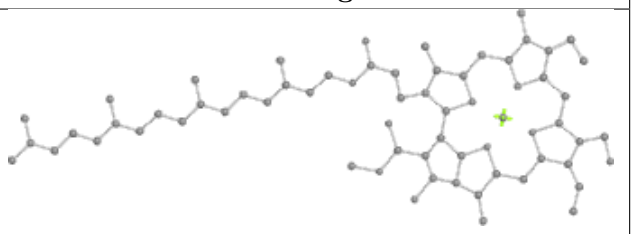
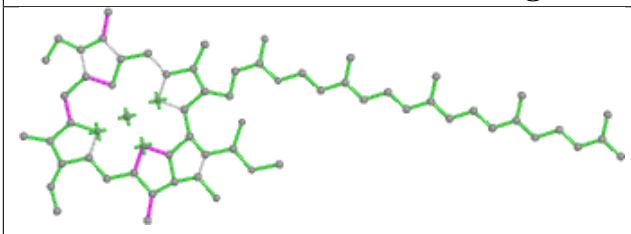


Rings

Ligand CLA B 307



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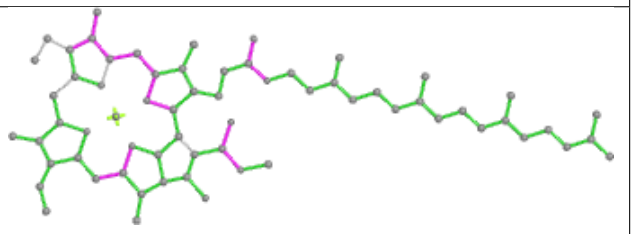
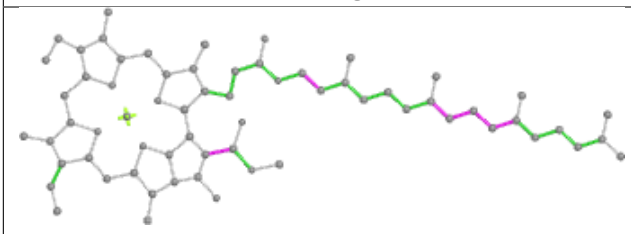


Bond angles



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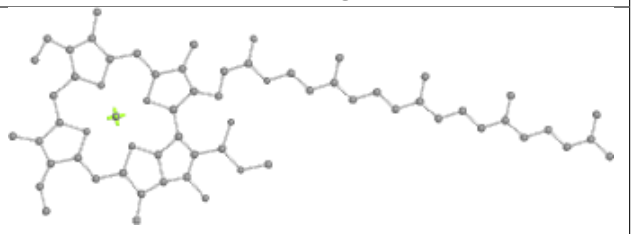
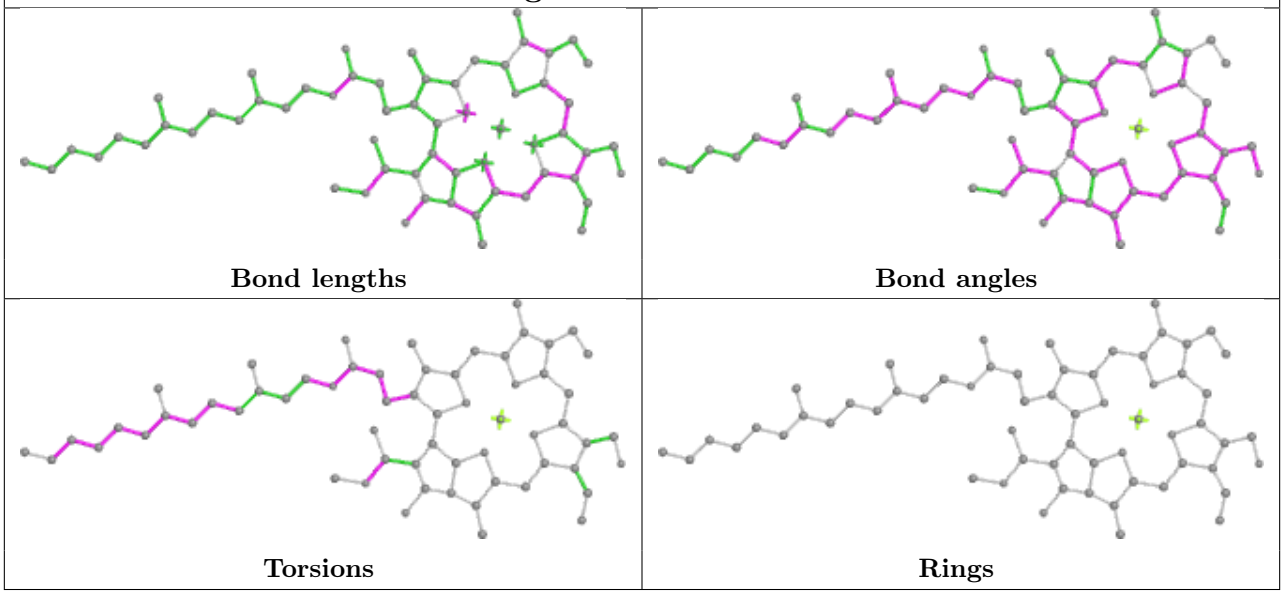
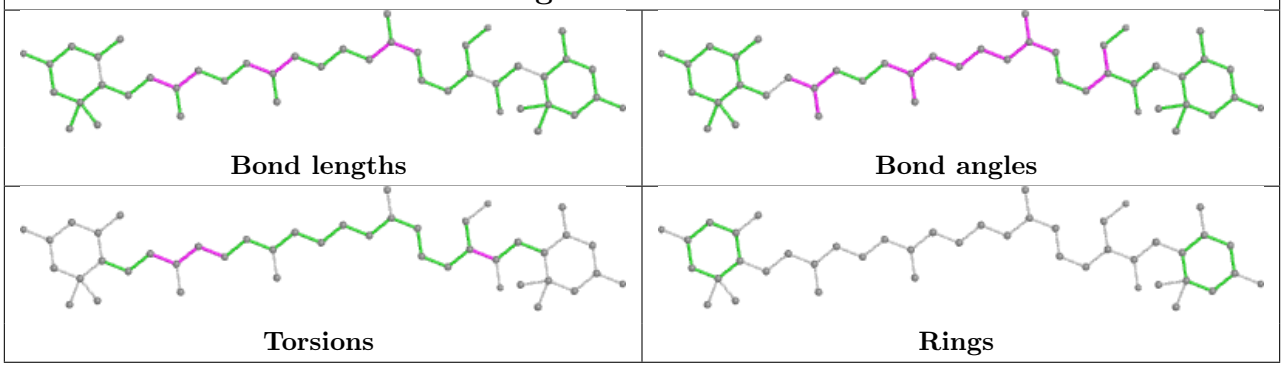


Rings

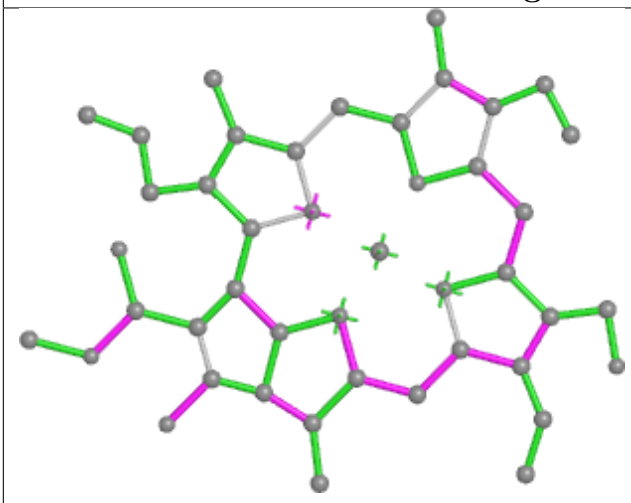
Ligand CHL C 311



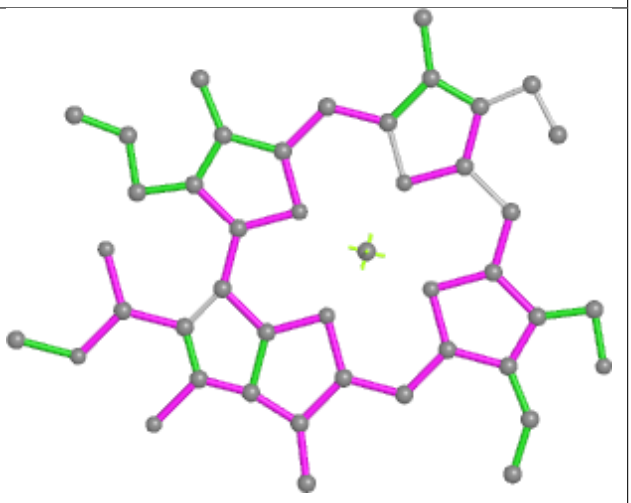
Ligand 0IE B 302



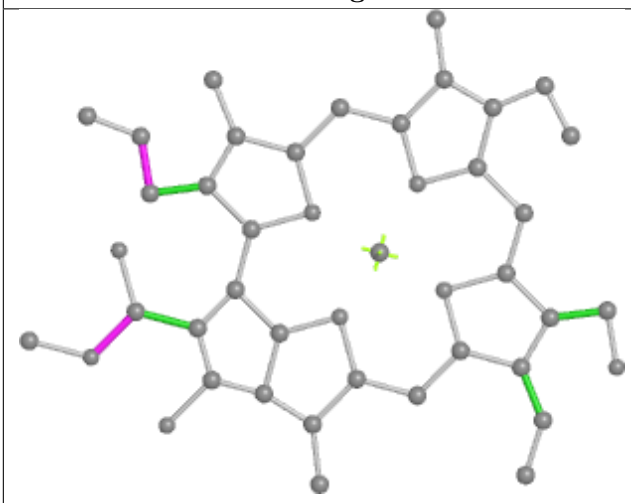
Ligand CHL C 318



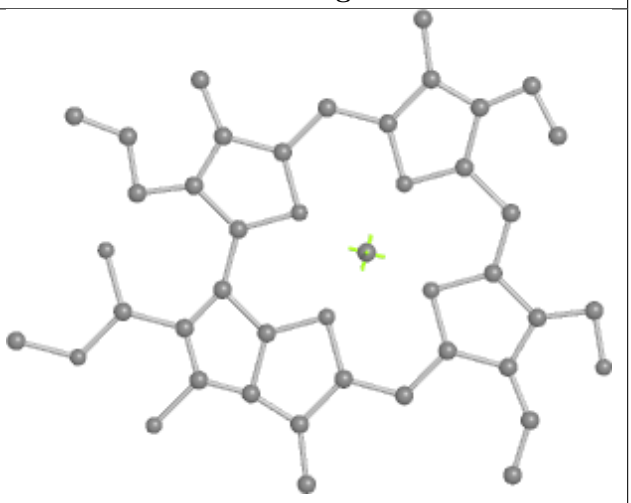
Bond lengths



Bond angles

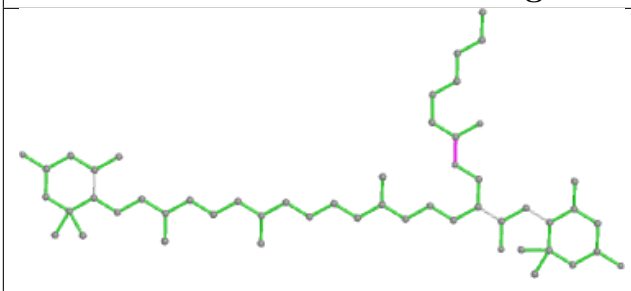


Torsions

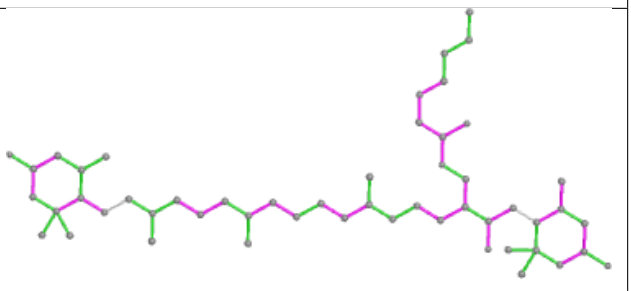


Rings

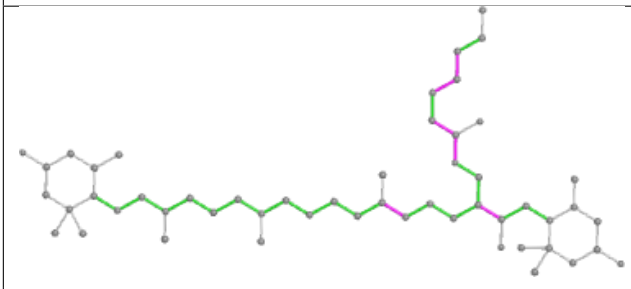
Ligand 0UR C 301



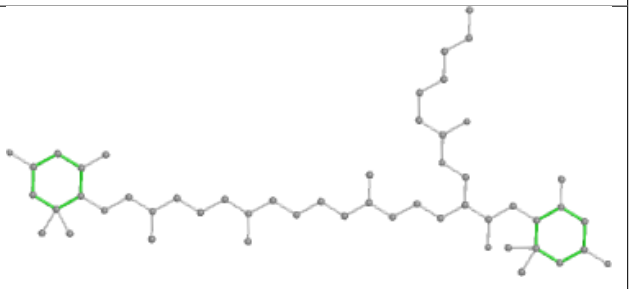
Bond lengths



Bond angles

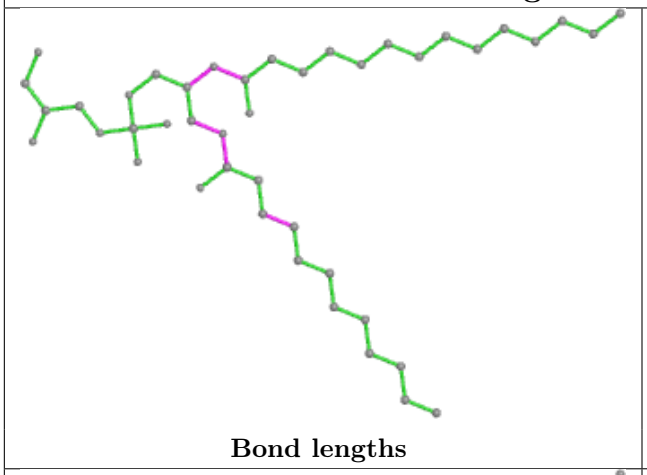


Torsions

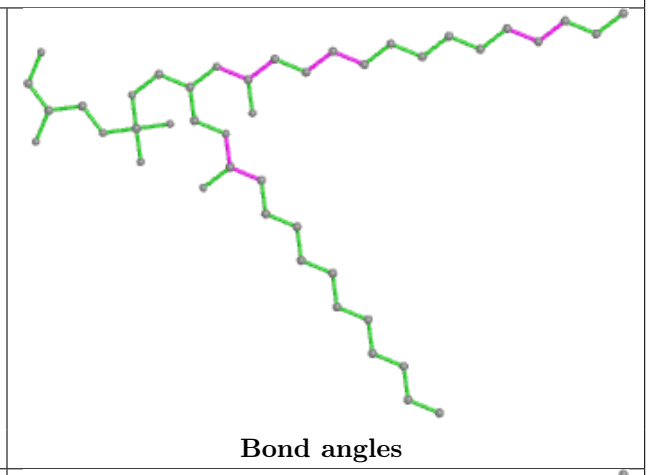


Rings

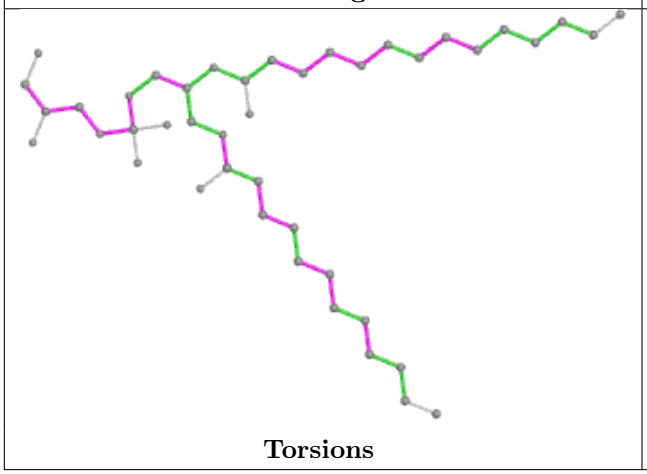
Ligand LHG C 319



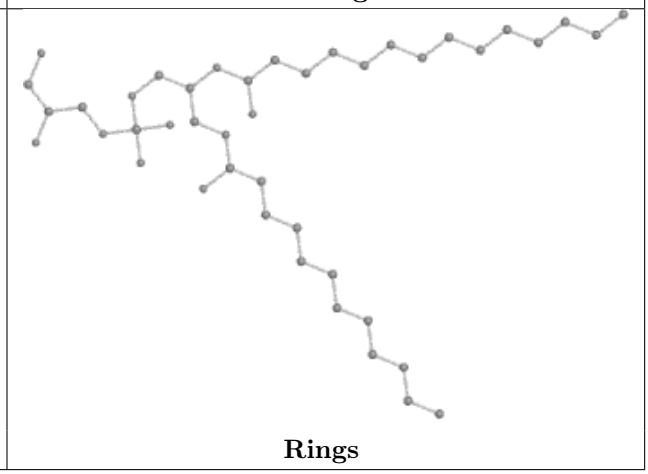
Bond lengths



Bond angles

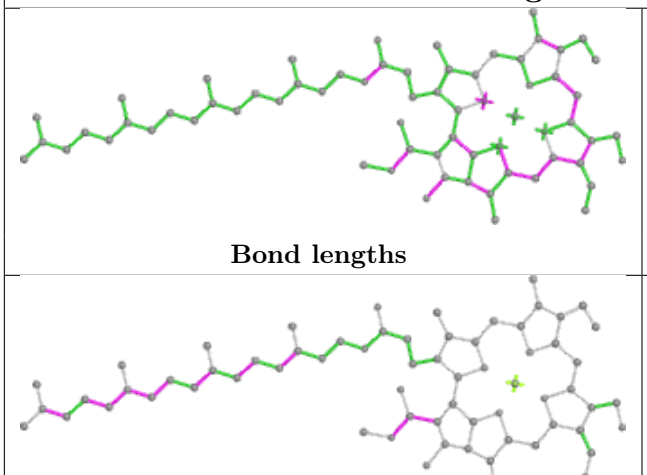


Torsions

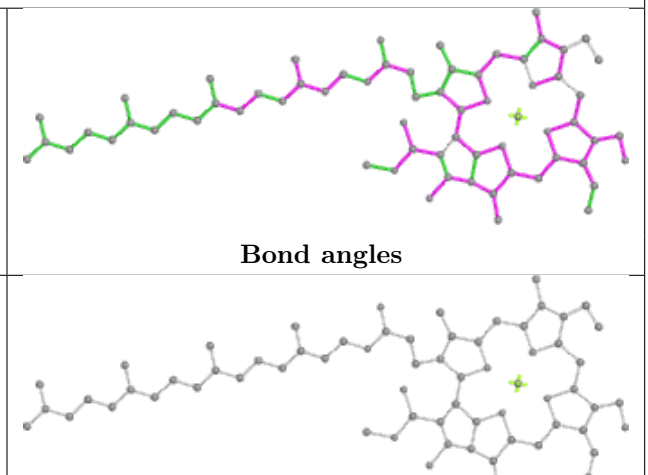


Rings

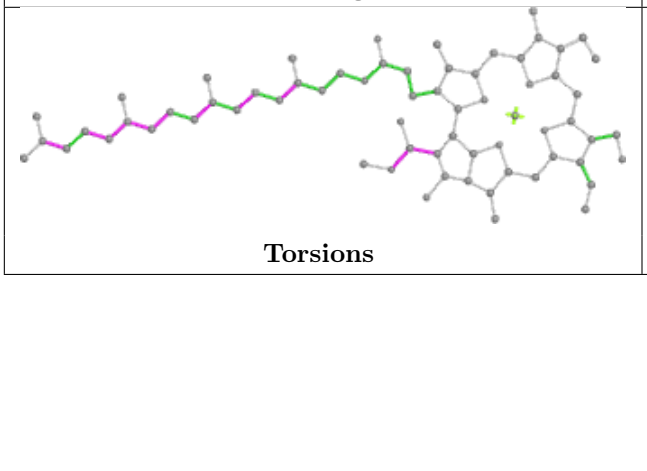
Ligand CHL B 313



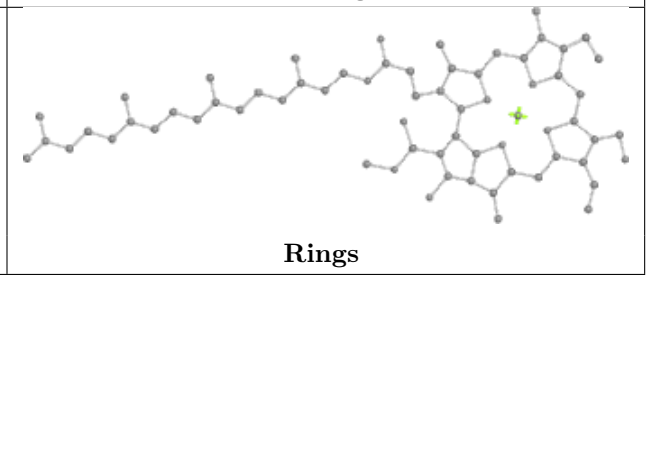
Bond lengths



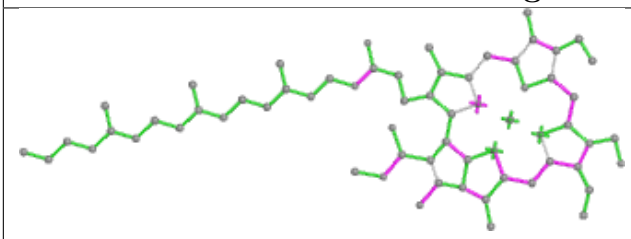
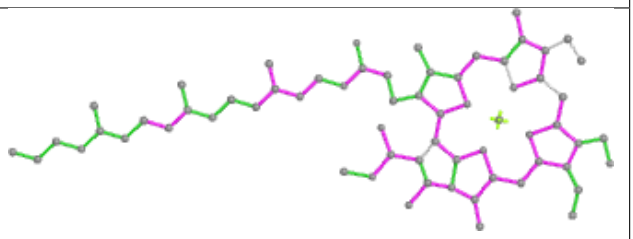
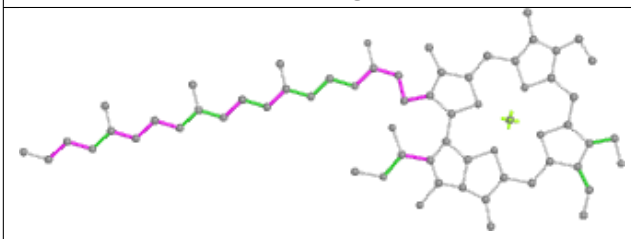
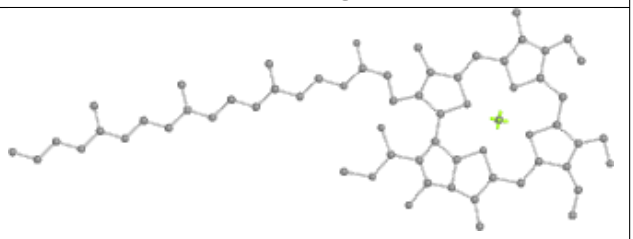
Bond angles

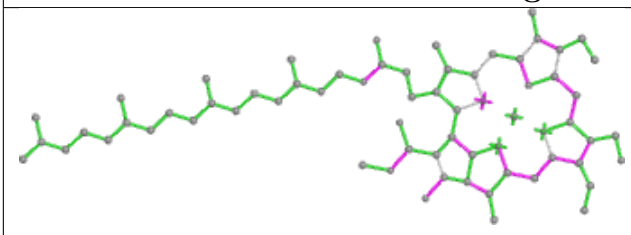
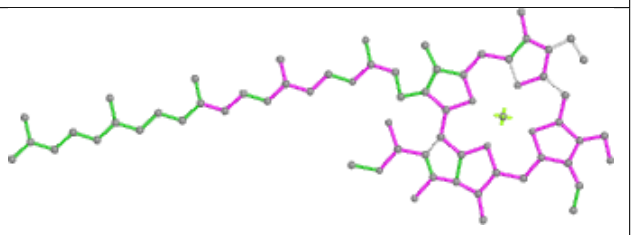
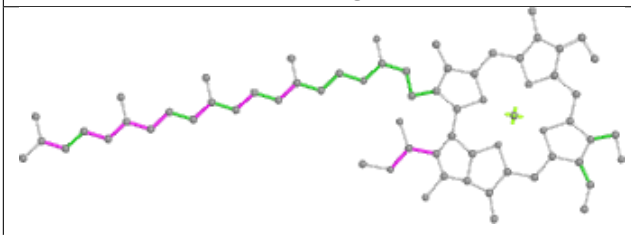
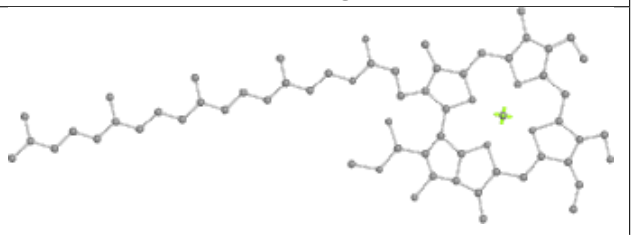


Torsions

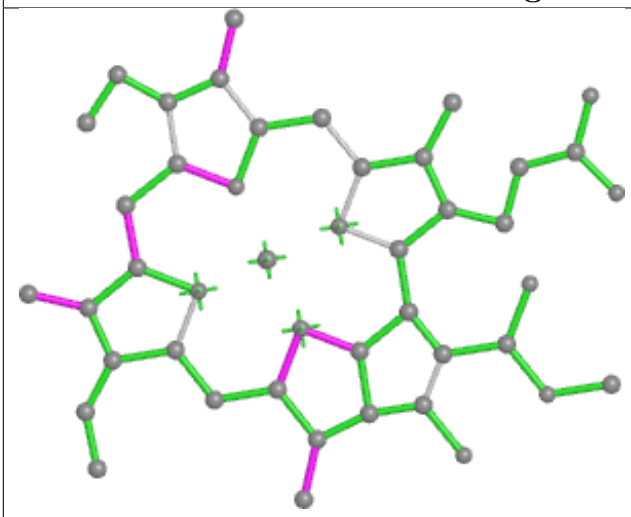


Rings

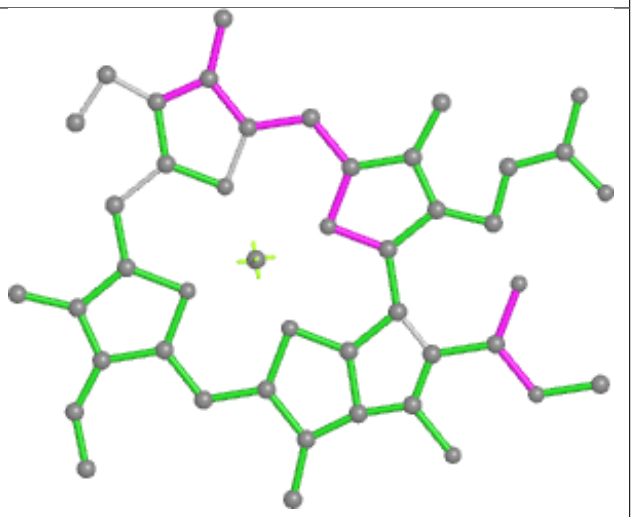
Ligand CHL C 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL C 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

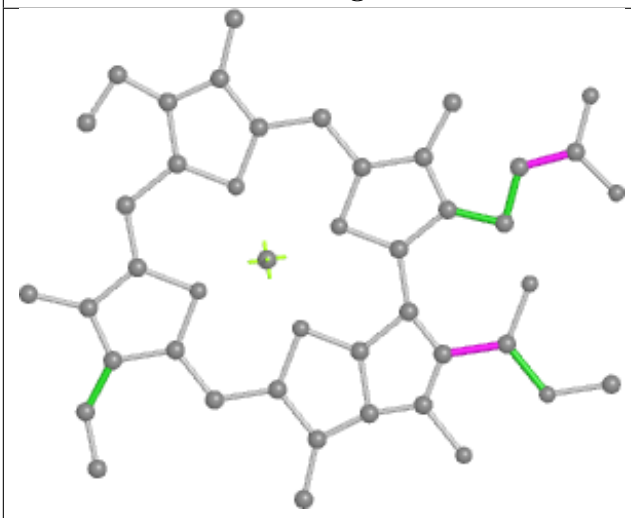
Ligand CLA B 316



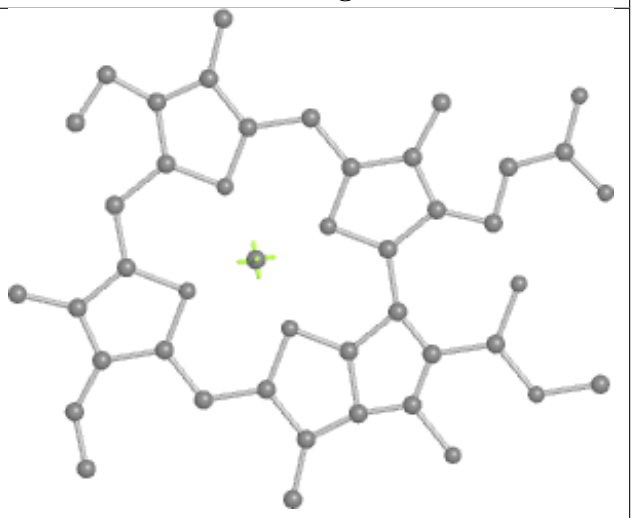
Bond lengths



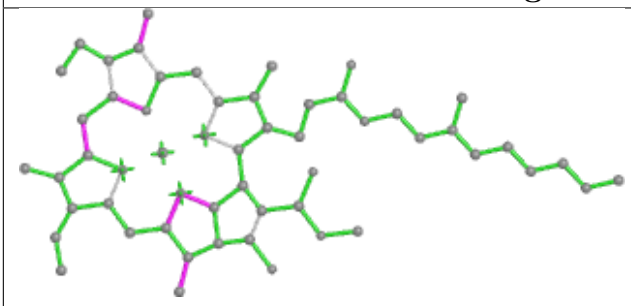
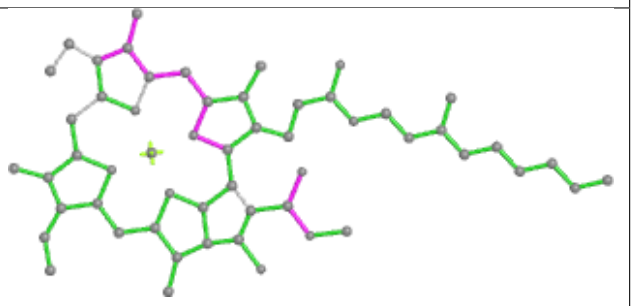
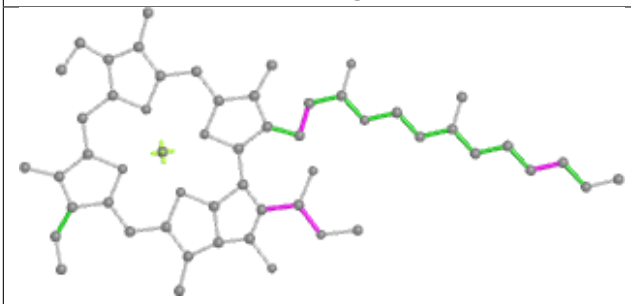
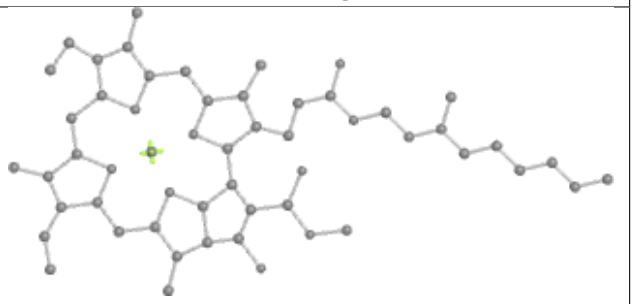
Bond angles

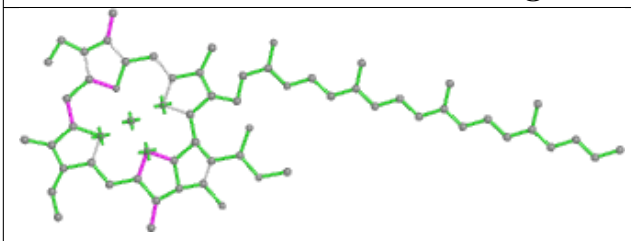
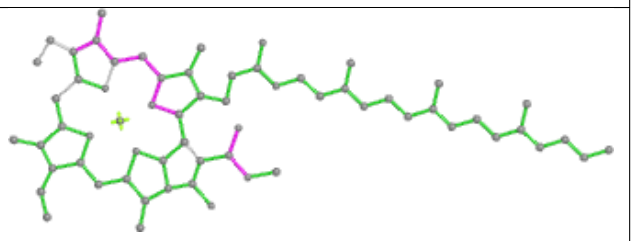
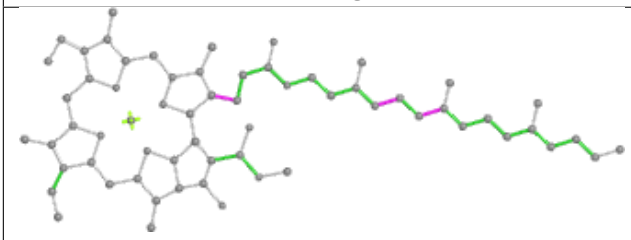
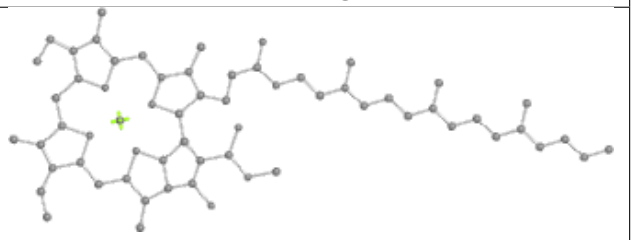


Torsions

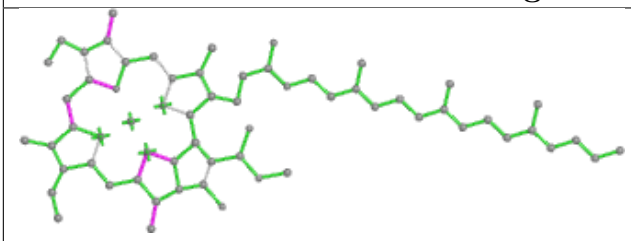


Rings

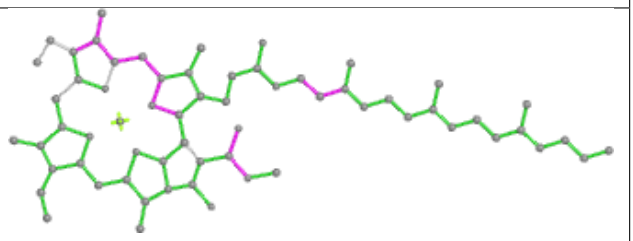
Ligand CLA B 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

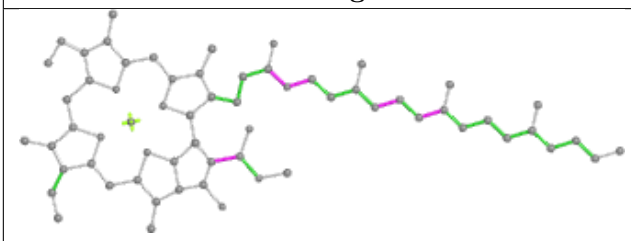
Ligand CLA A 315



Bond lengths



Bond angles



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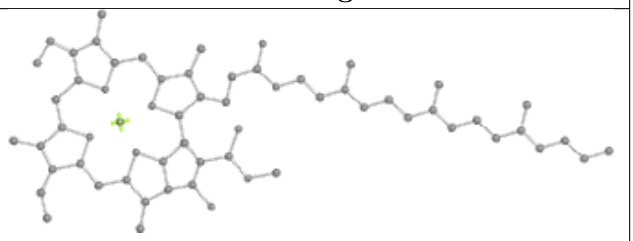
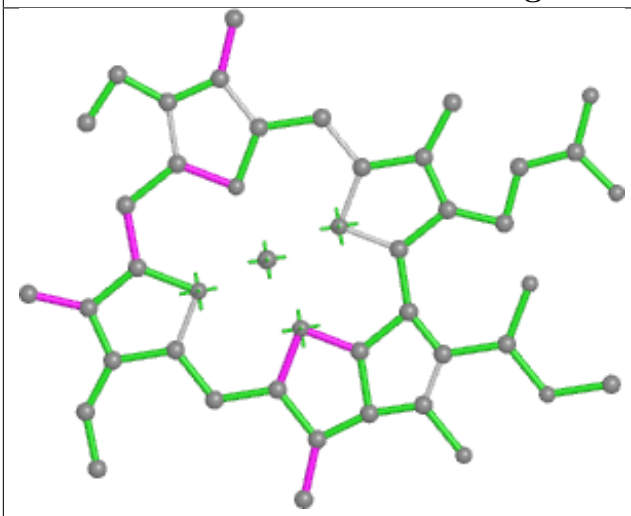
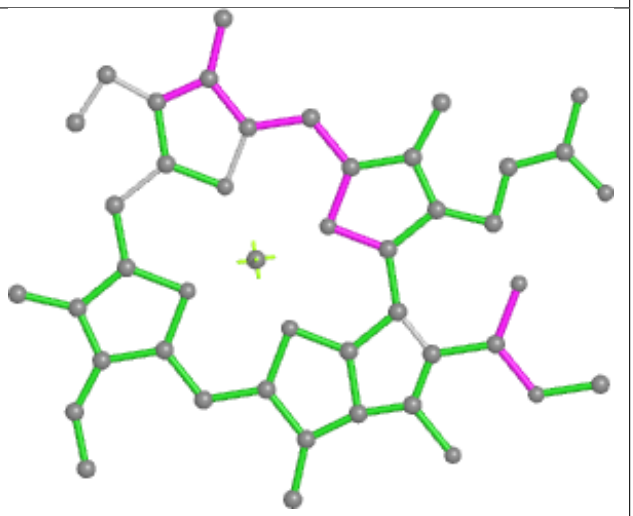


Rings

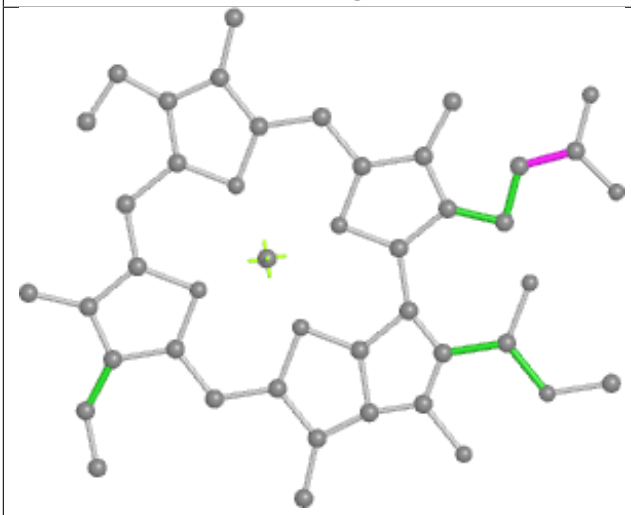
Ligand CLA C 316



Bond lengths



Bond angles



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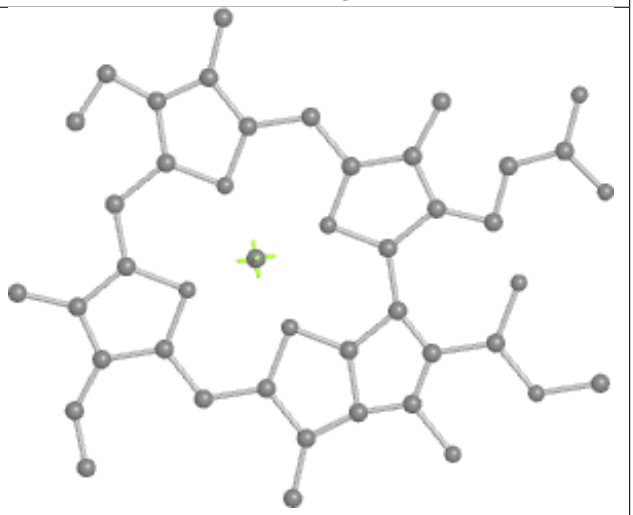
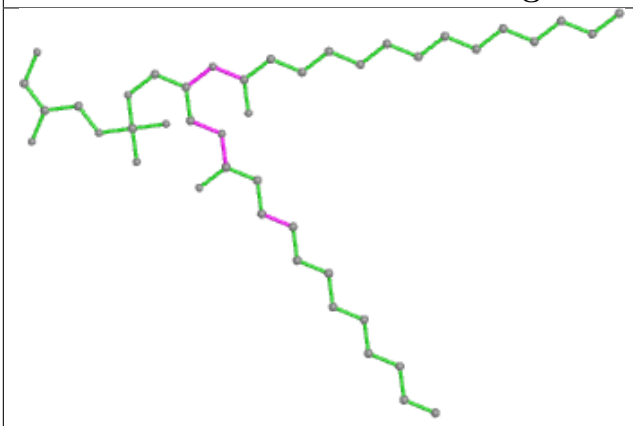
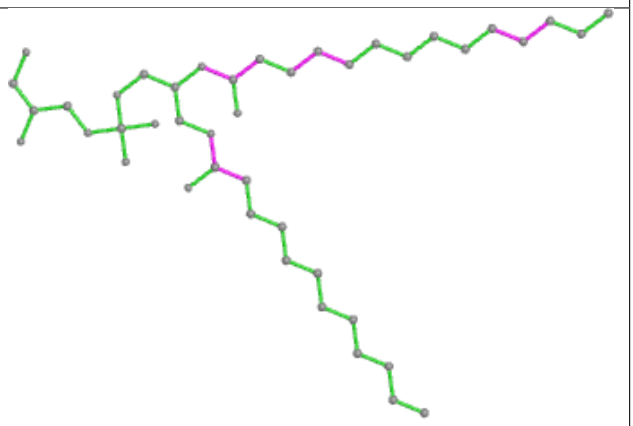


Rings

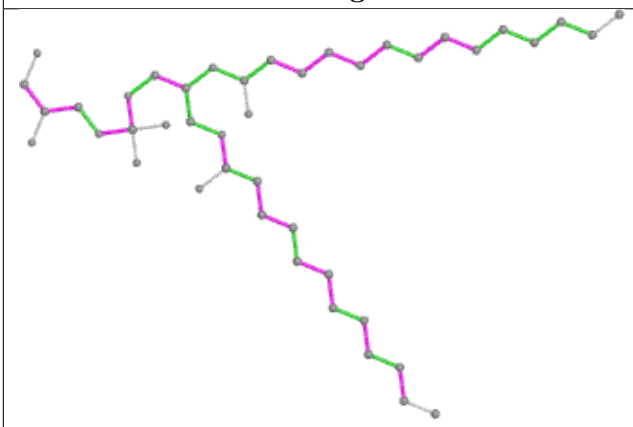
Ligand LHG B 319



Bond lengths



Bond angles



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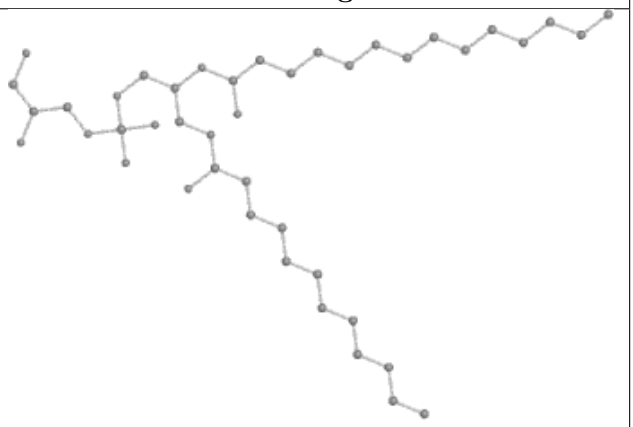
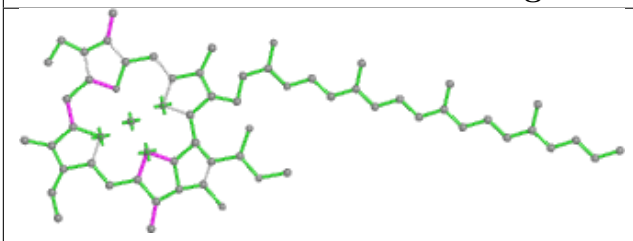
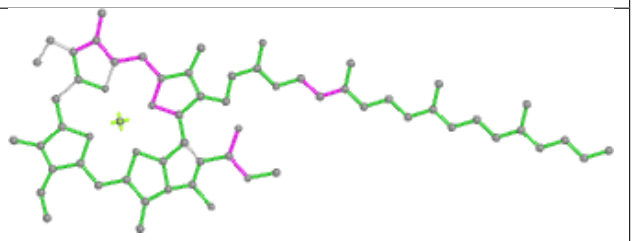


Rings

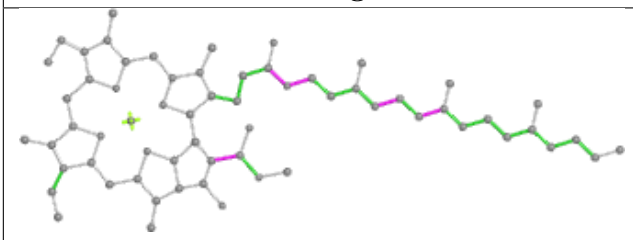
Ligand CLA B 315



Bond lengths



Bond angles



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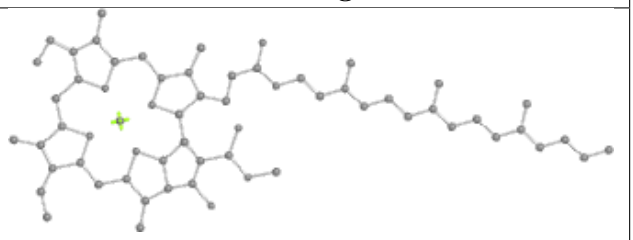
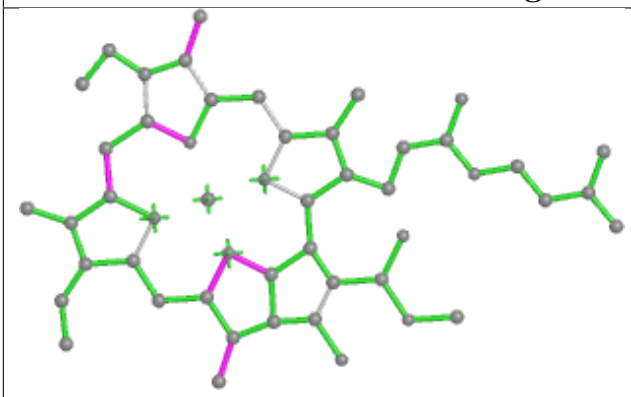
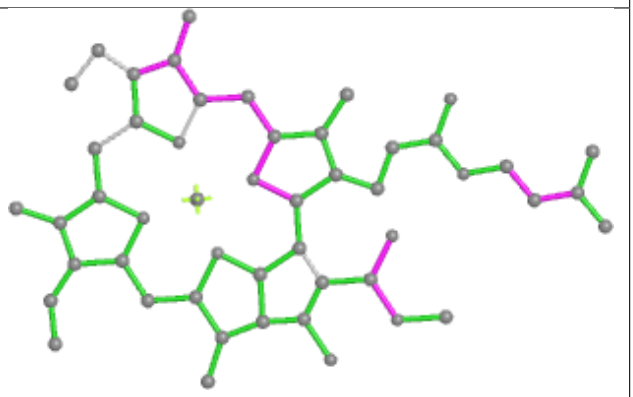


Rings

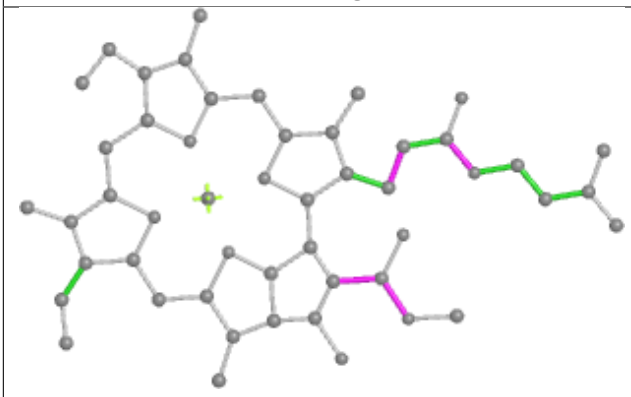
Ligand CLA C 308



Bond lengths



Bond angles



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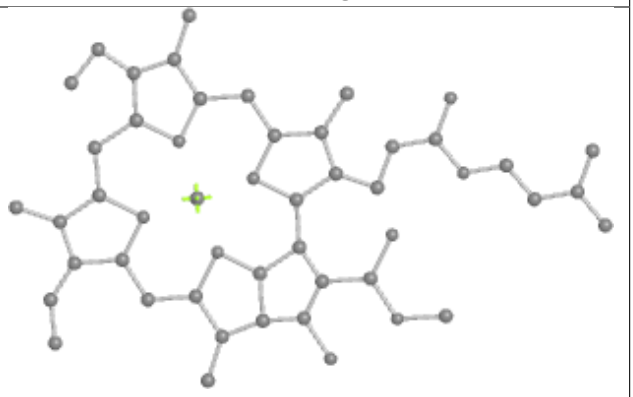
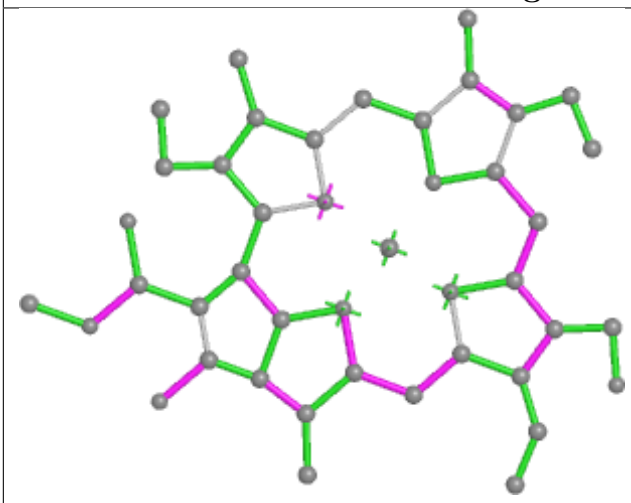
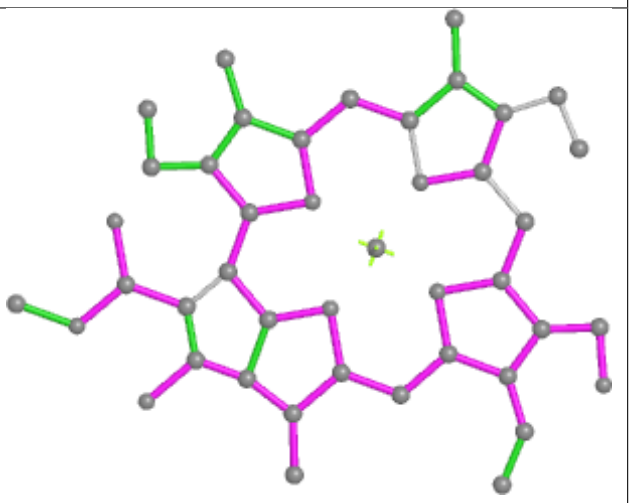


Rings

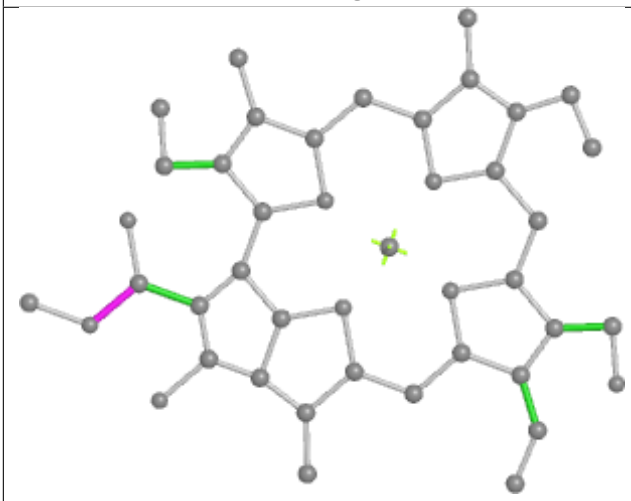
Ligand CHL A 309



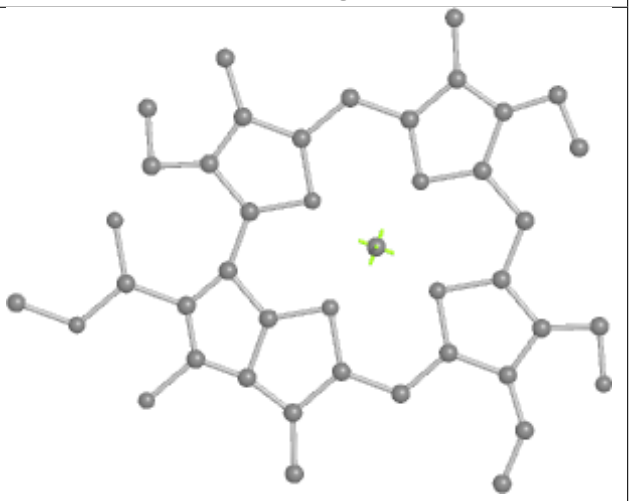
Bond lengths



Bond angles

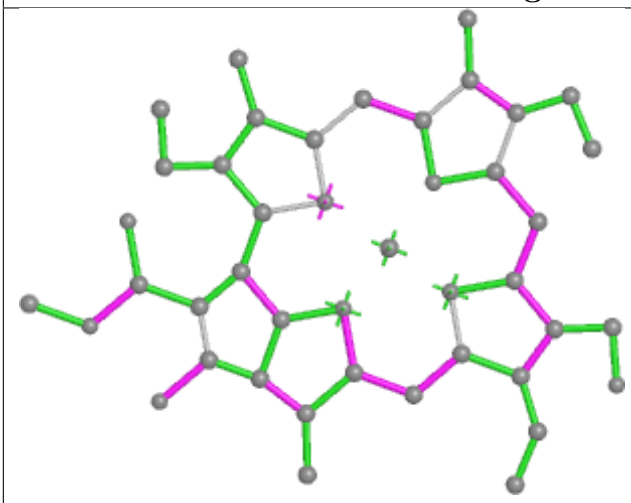


Torsions

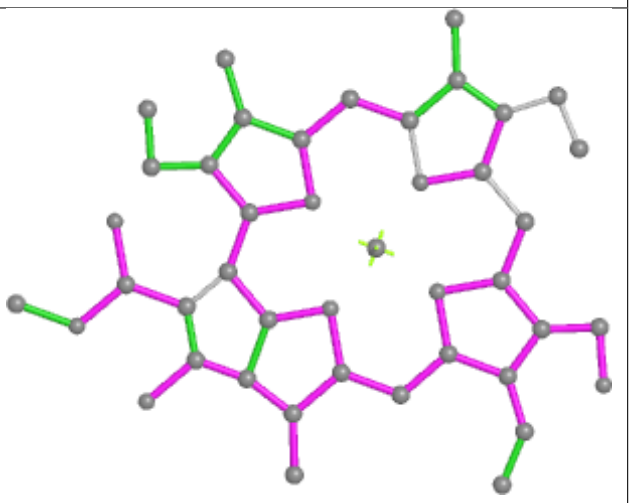


Rings

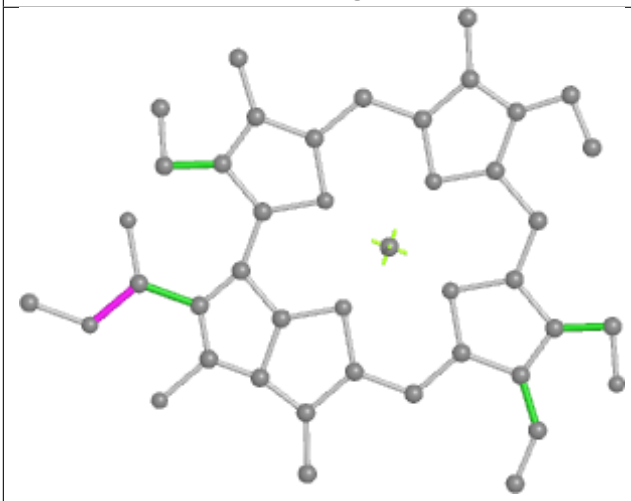
Ligand CHL B 309



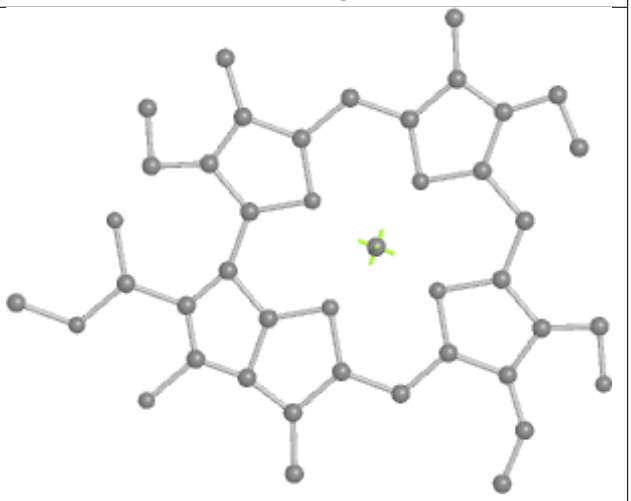
Bond lengths



Bond angles

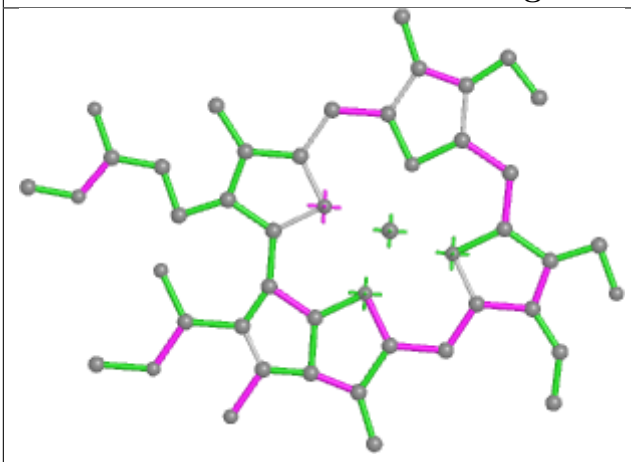


Torsions



Rings

Ligand CHL B 318



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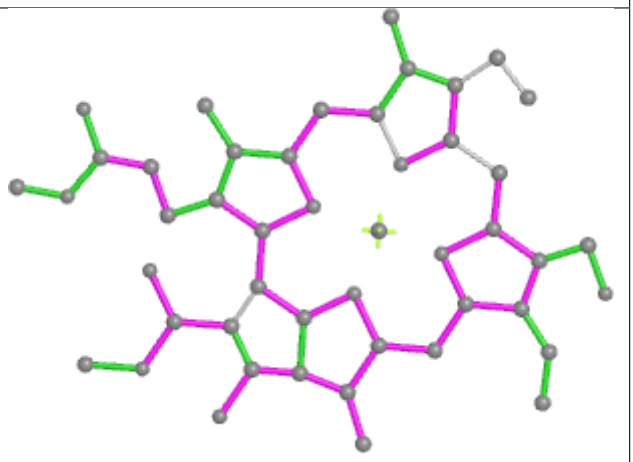
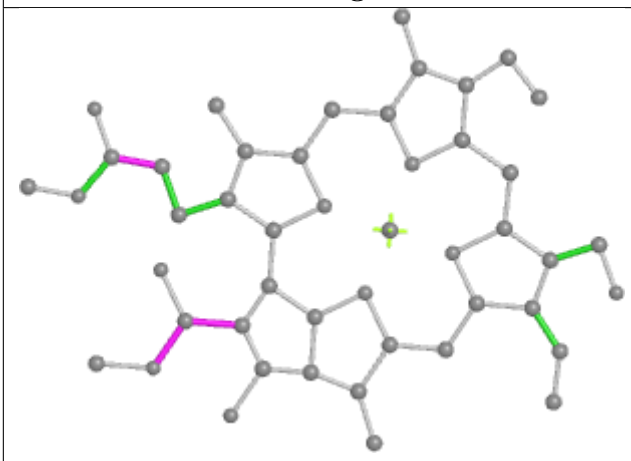


Bond angles



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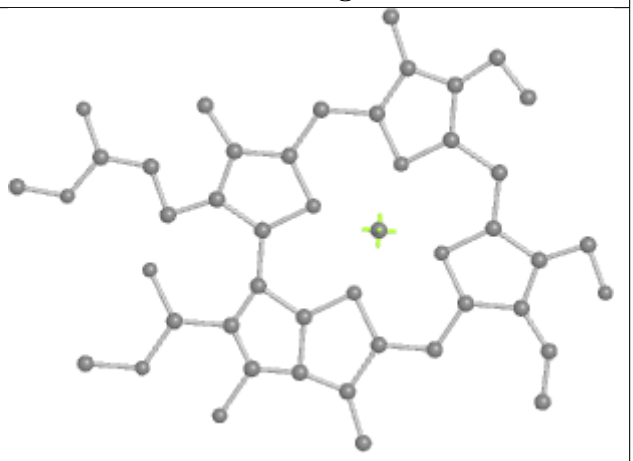
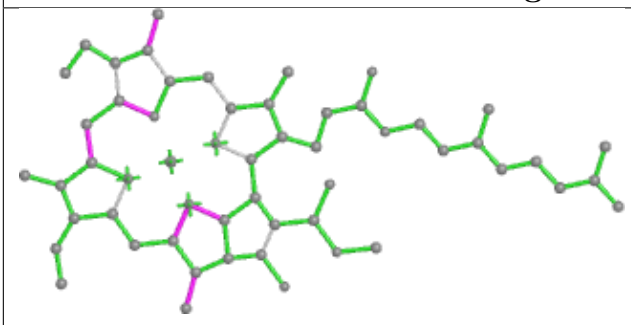


Rings

Ligand CLA B 314



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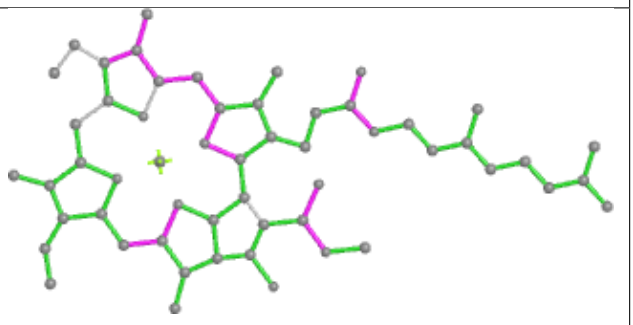
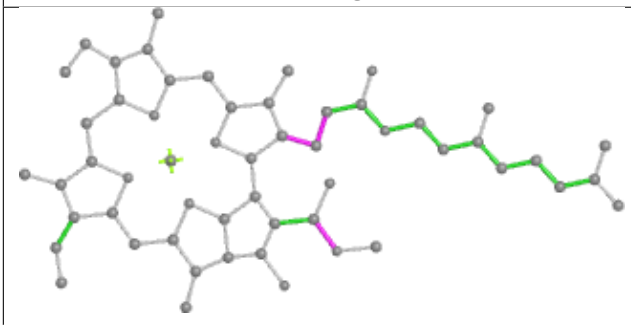


Bond angles



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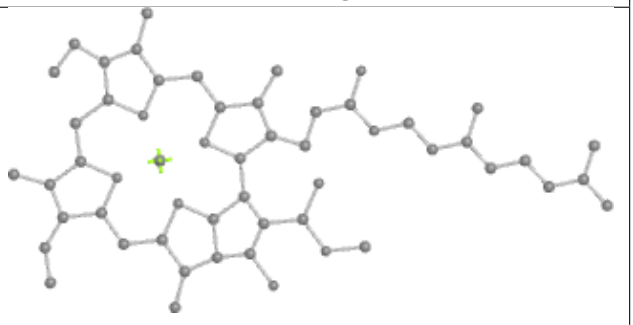
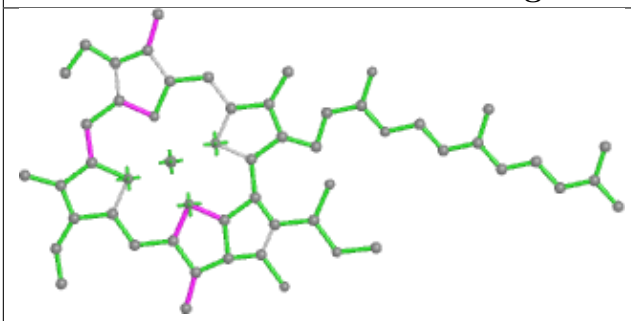
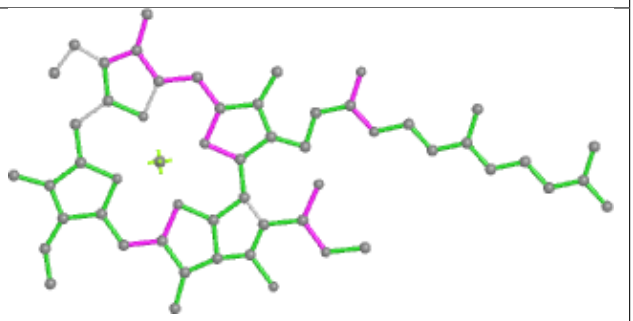


Rings

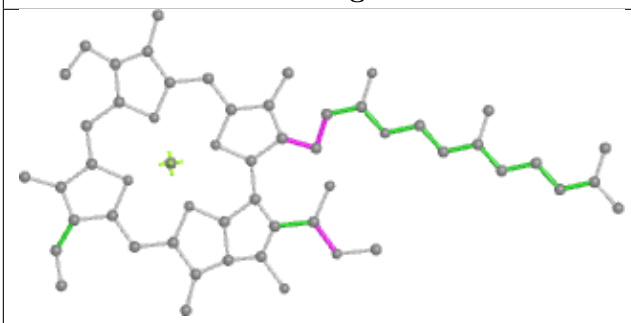
Ligand CLA C 314



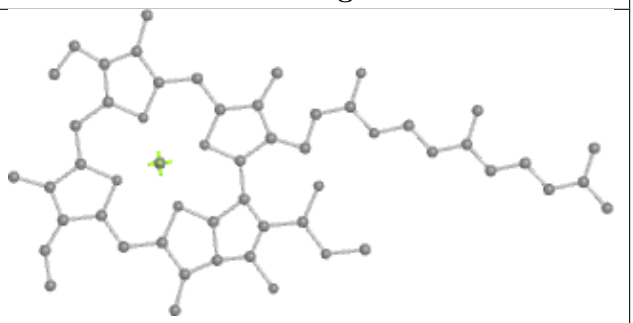
Bond lengths



Bond angles

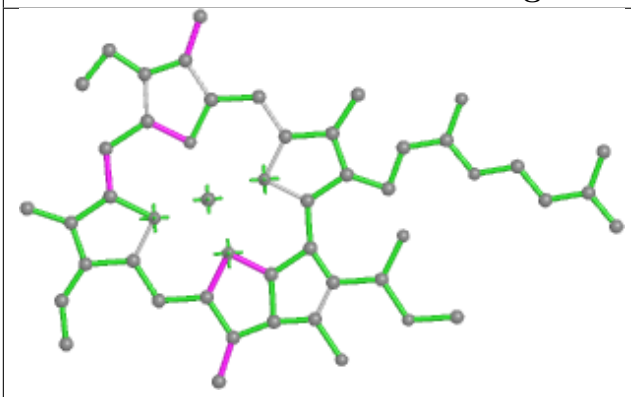


Torsions



Rings

Ligand CLA A 308



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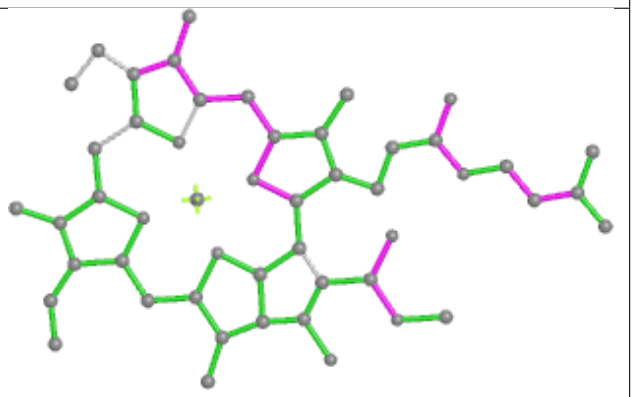
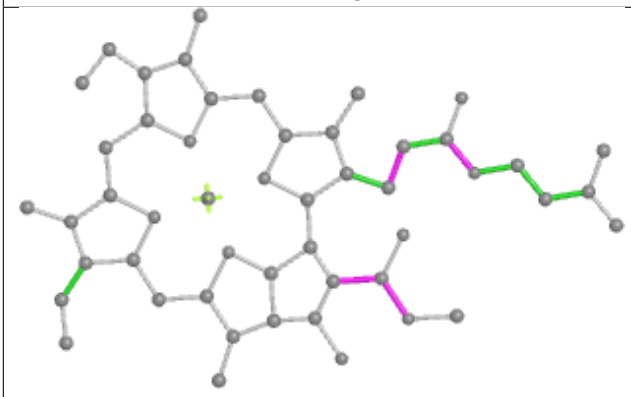


Bond angles



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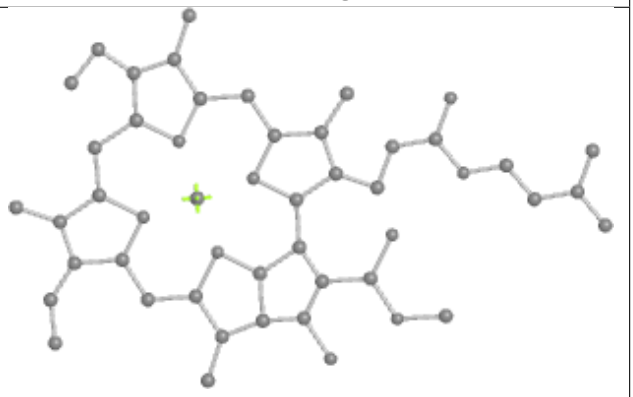
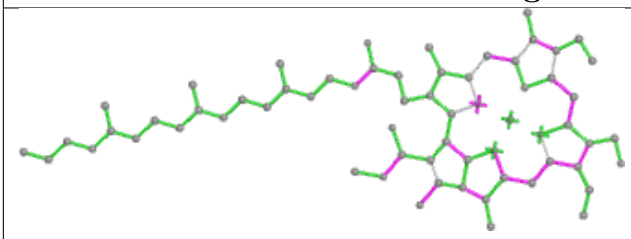
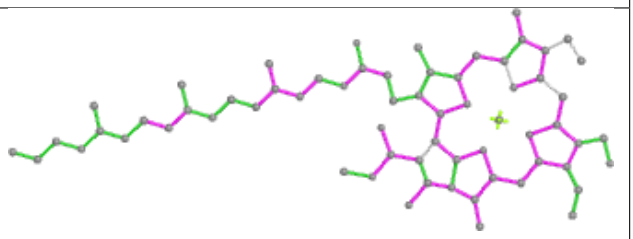


Rings

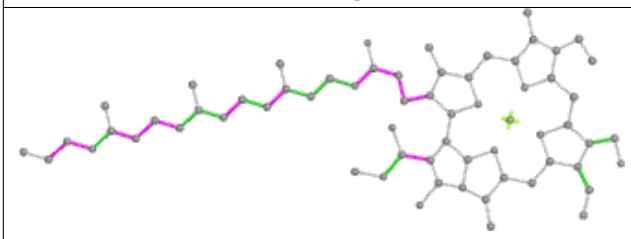
Ligand CHL A 306



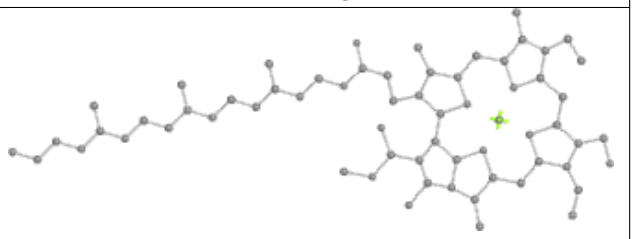
Bond lengths



Bond angles

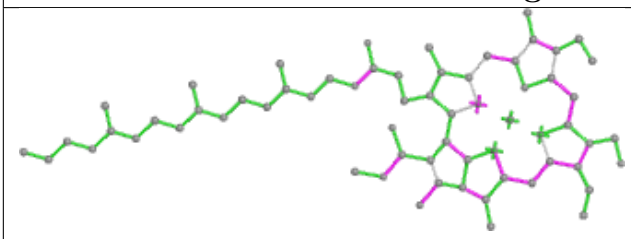


Torsions

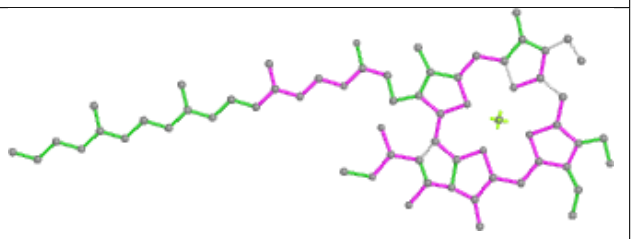


Rings

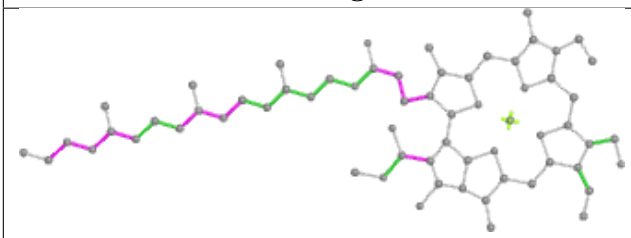
Ligand CHL B 306



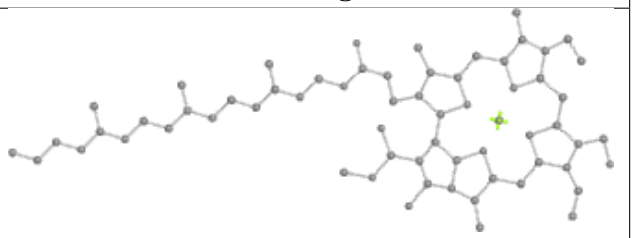
Bond lengths



Bond angles

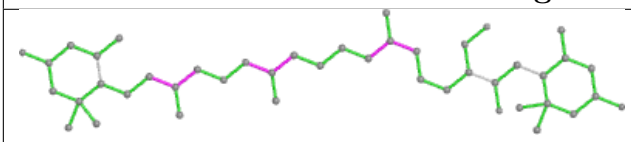


Torsions

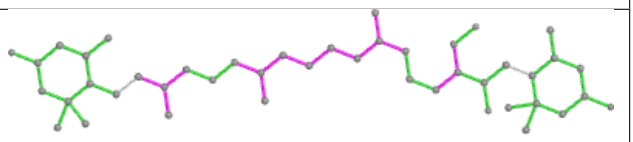


Rings

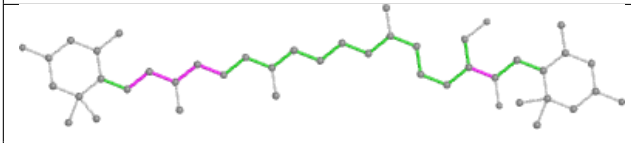
Ligand 0IE C 302



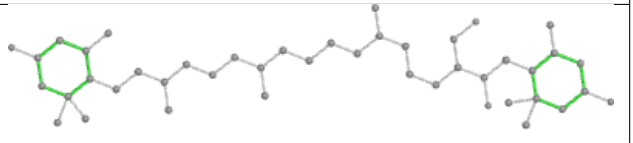
Bond lengths



Bond angles

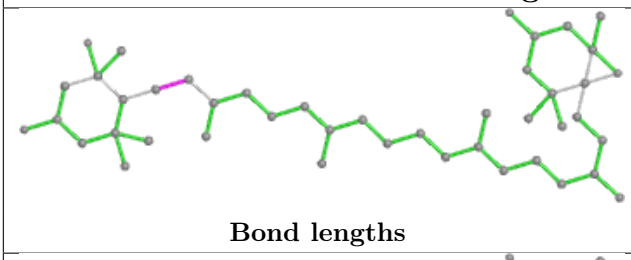


Torsions

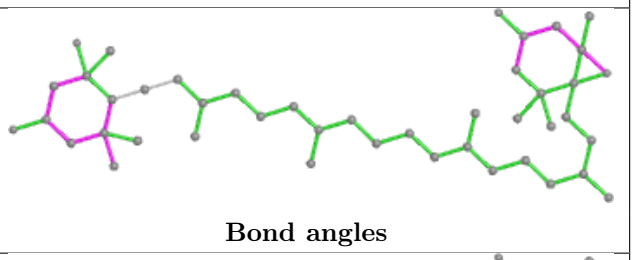


Rings

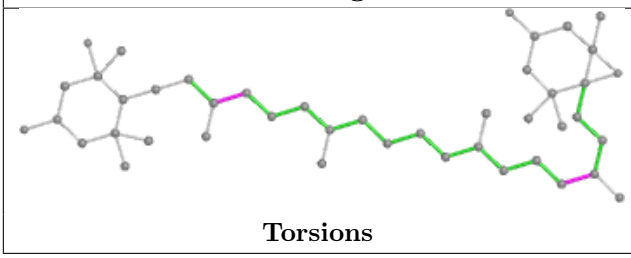
Ligand NEX A 304



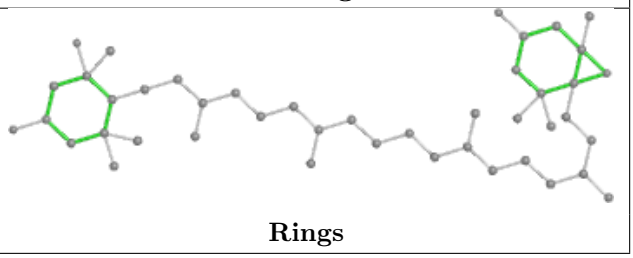
Bond lengths



Bond angles

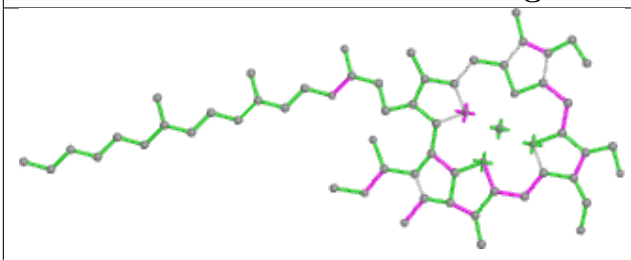


Torsions

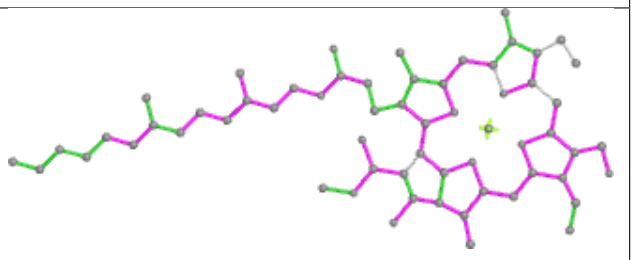


Rings

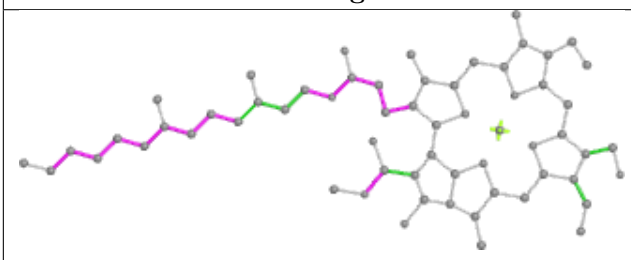
Ligand CHL B 311



Bond lengths



Bond angles



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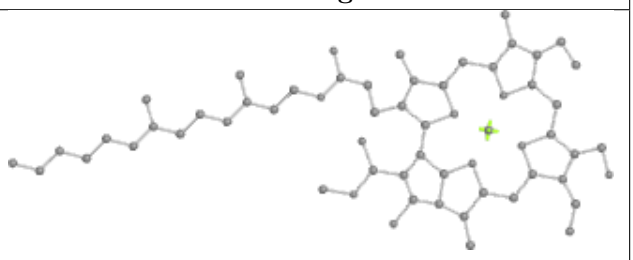
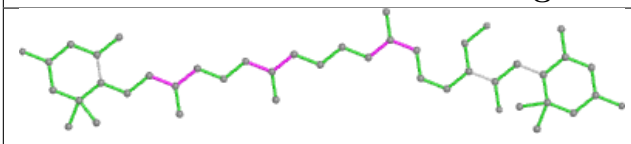
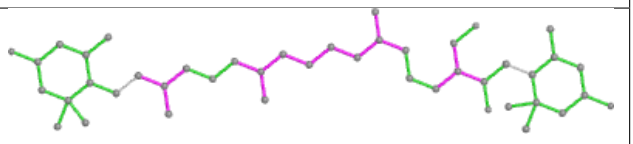


Rings

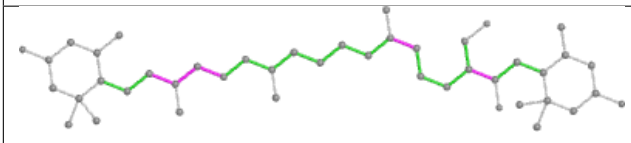
Ligand 0IE A 302



Bond lengths



Bond angles



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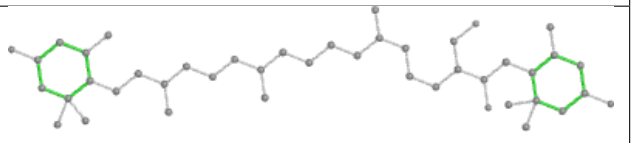
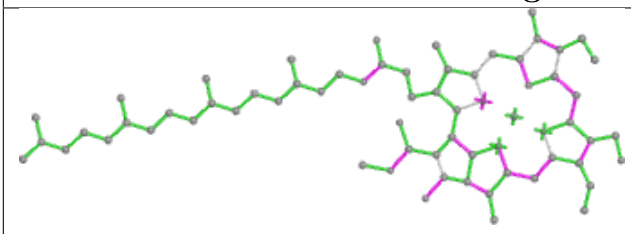
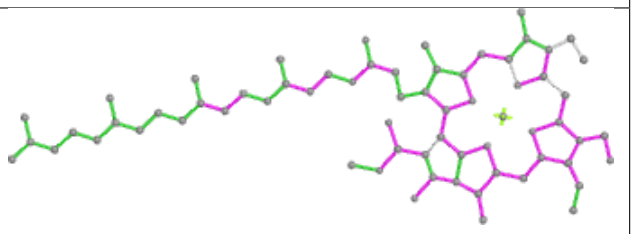


Rings

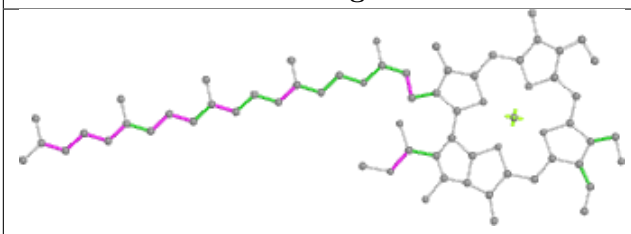
Ligand CHL A 312



Bond lengths



Bond angles



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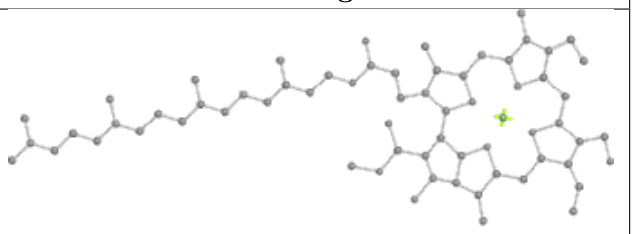
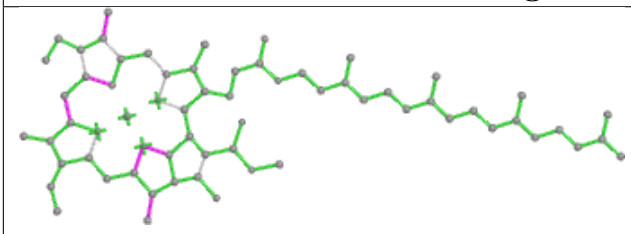
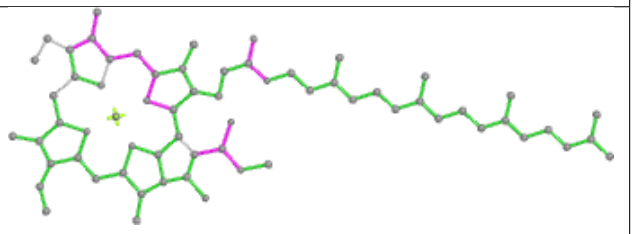


Rings

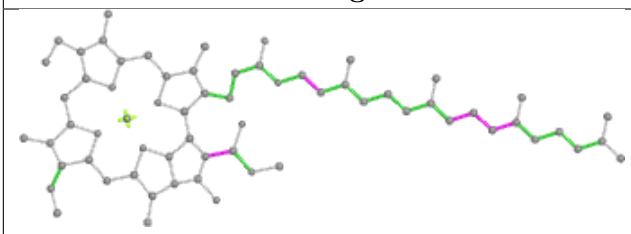
Ligand CLA A 307



Bond lengths



Bond angles



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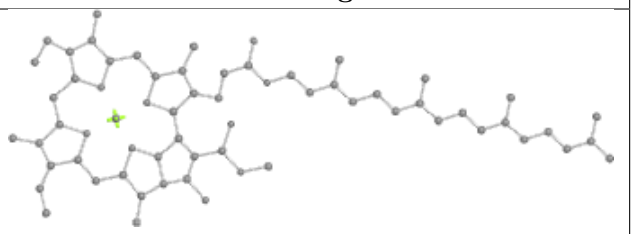
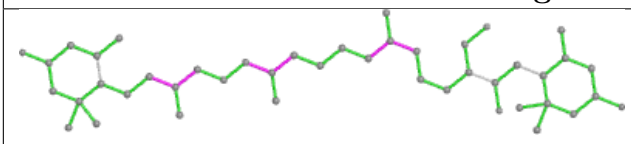
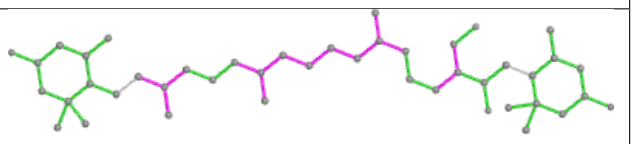


Rings

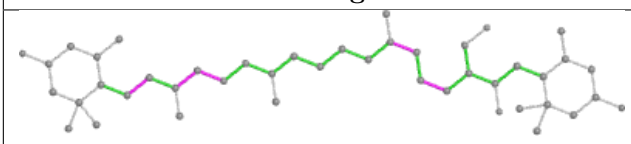
Ligand 0IE A 303



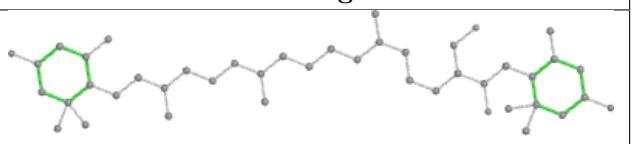
Bond lengths



Bond angles

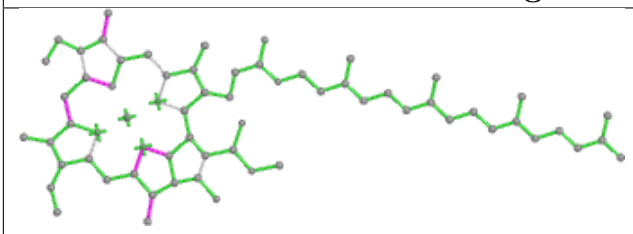


Torsions

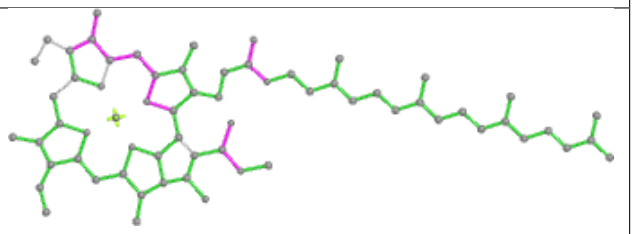


Rings

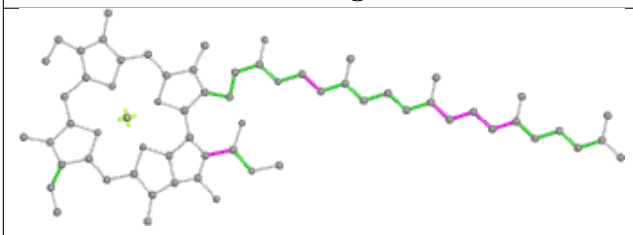
Ligand CLA C 307



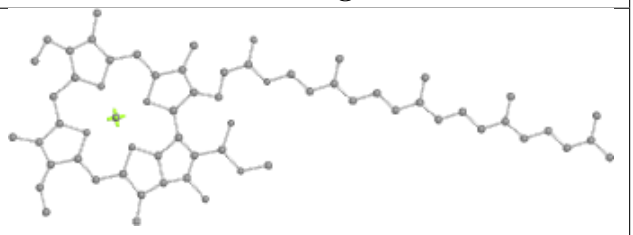
Bond lengths



Bond angles

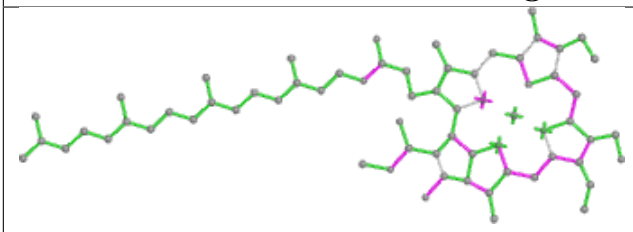


Torsions

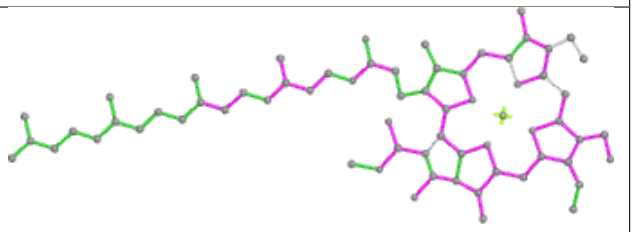


Rings

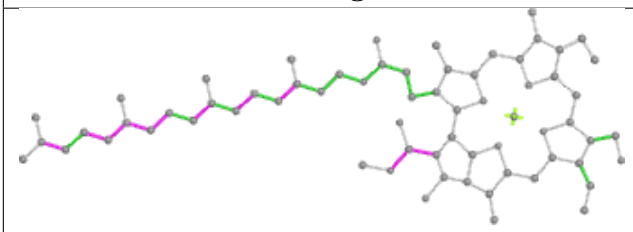
Ligand CHL A 313



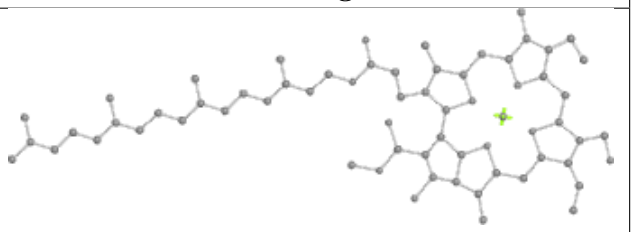
Bond lengths



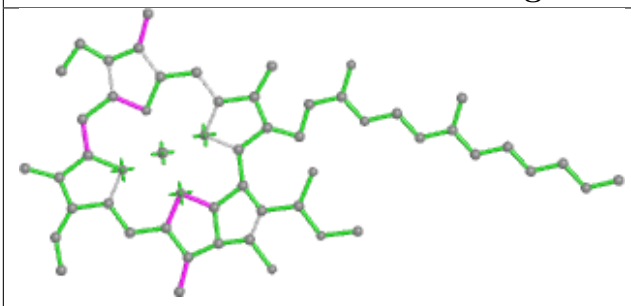
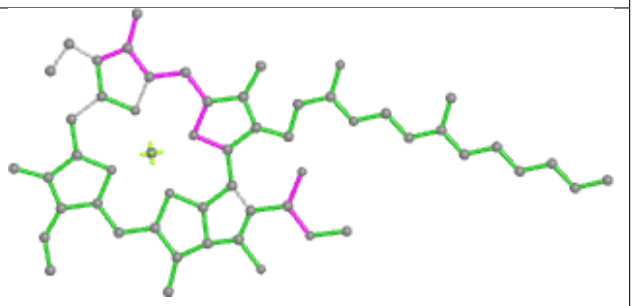
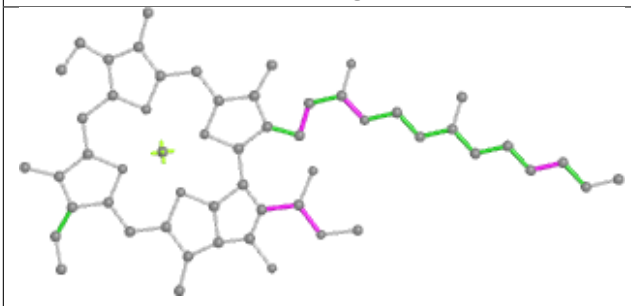
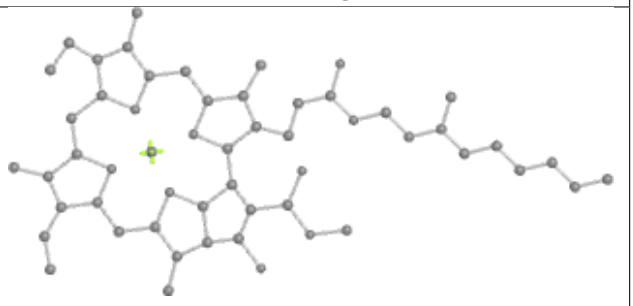
Bond angles

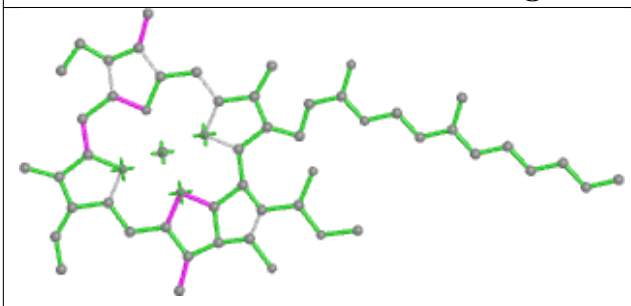
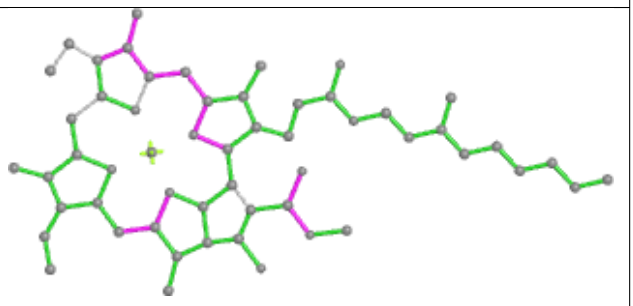
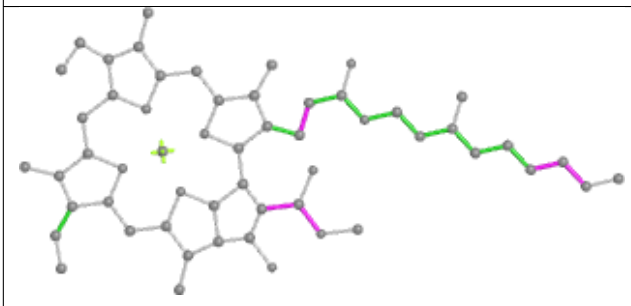
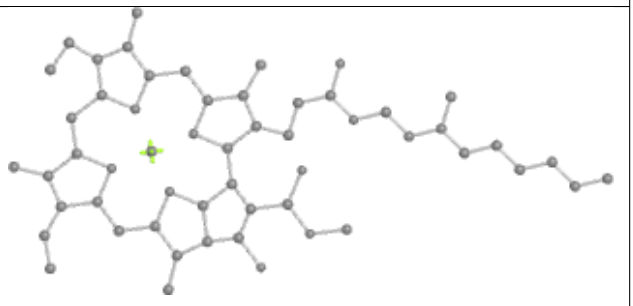


Torsions

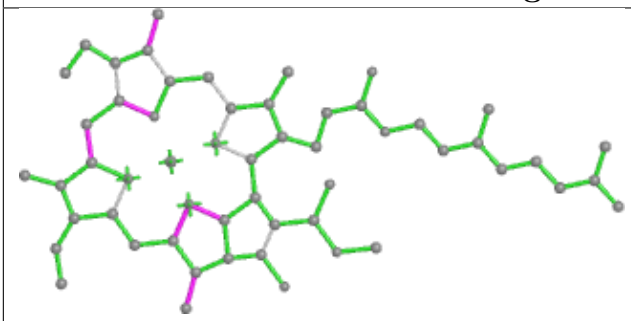


Rings

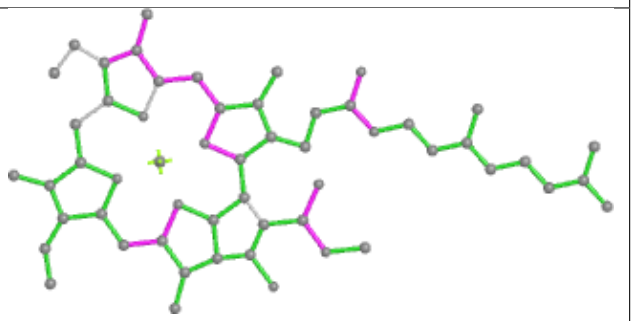
Ligand CLA C 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

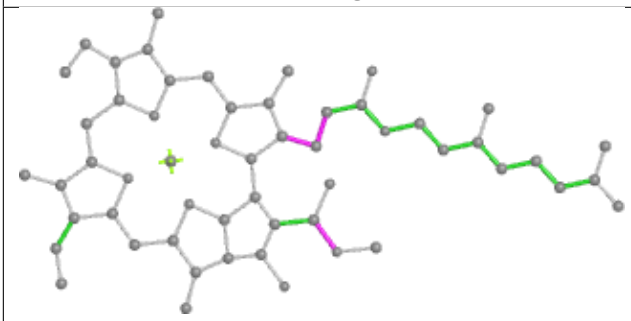
Ligand CLA A 314



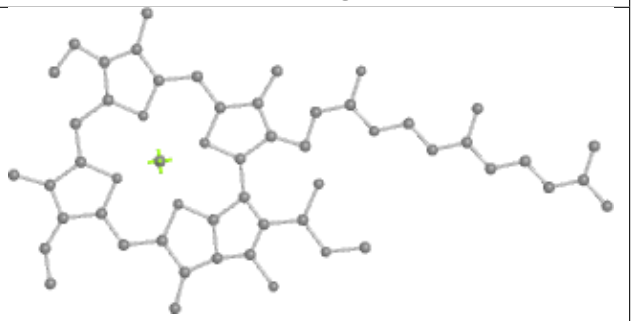
Bond lengths



Bond angles

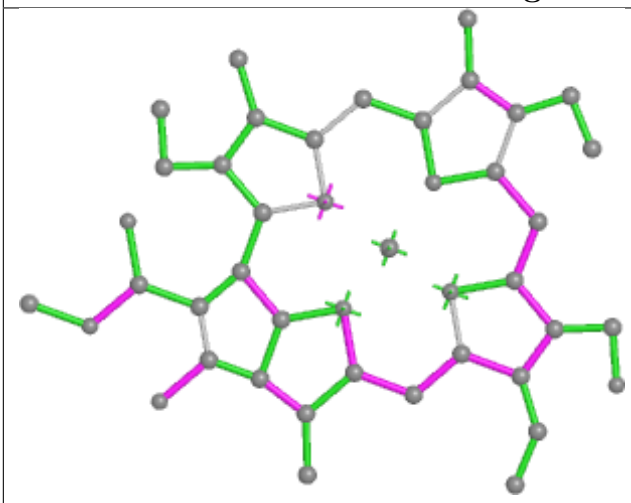


Torsions

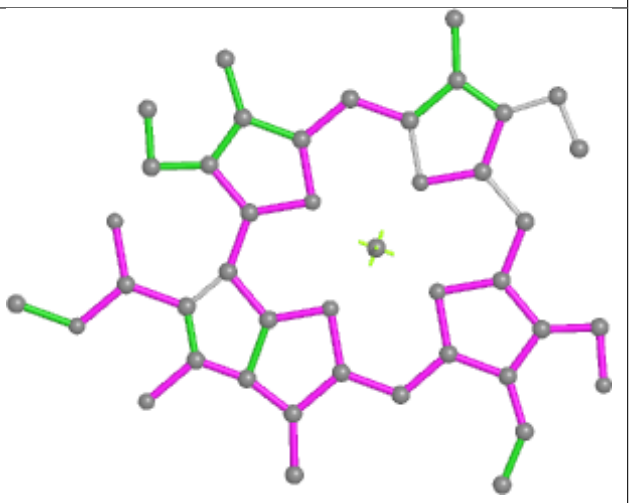


Rings

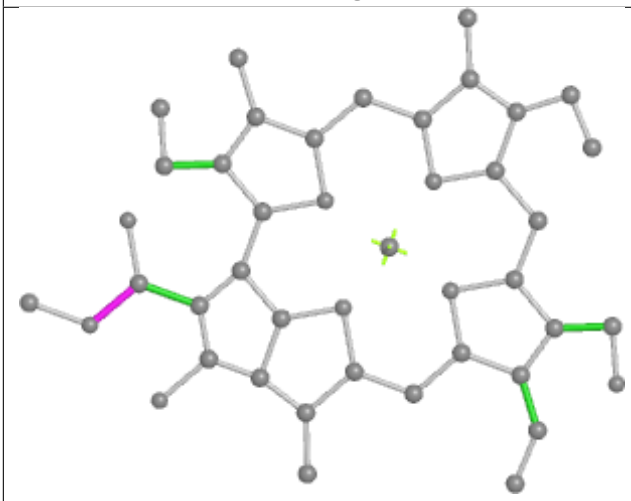
Ligand CHL C 309



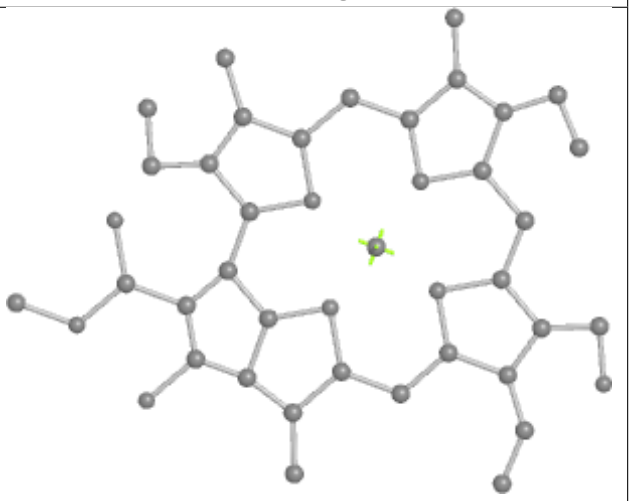
Bond lengths



Bond angles

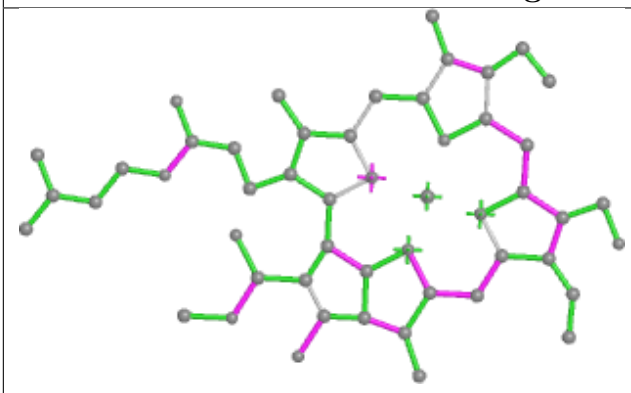


Torsions

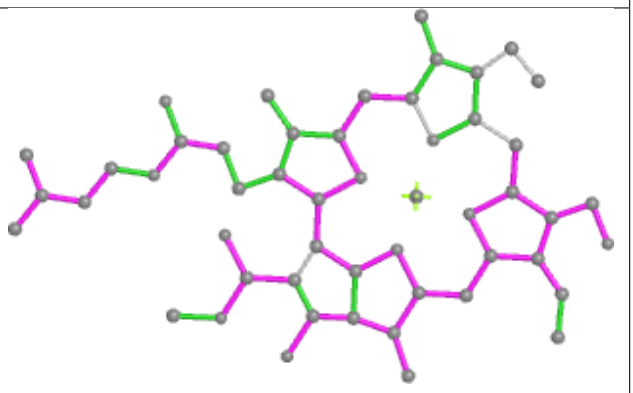


Rings

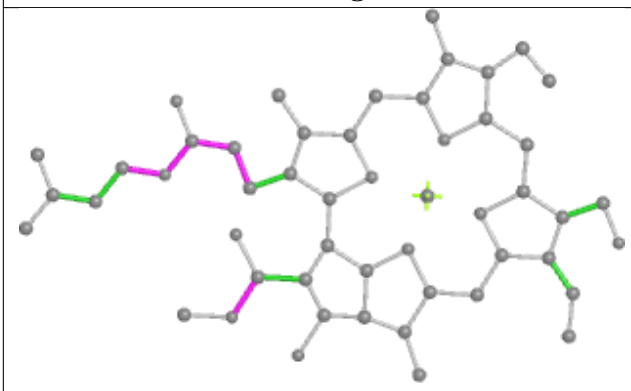
Ligand CHL B 310



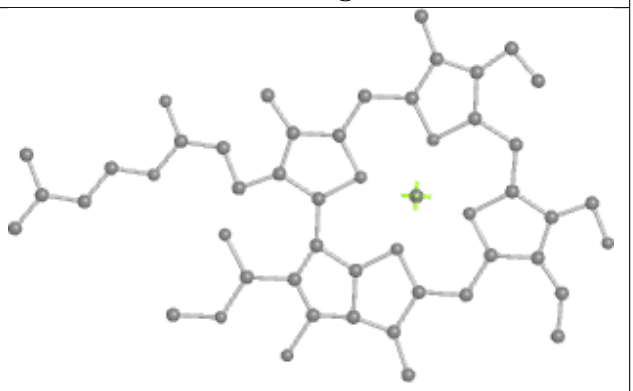
Bond lengths



Bond angles

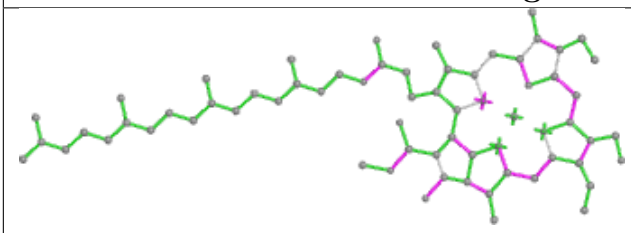


Torsions

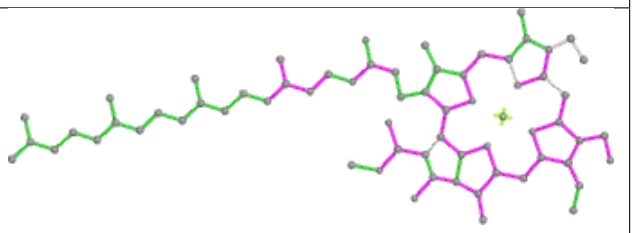


Rings

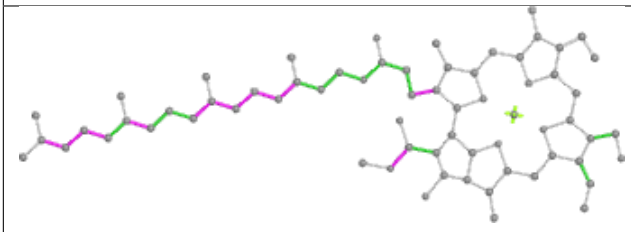
Ligand CHL A 305



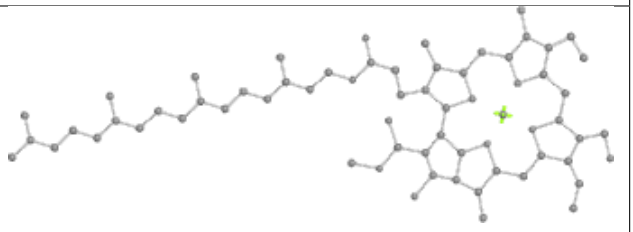
Bond lengths



Bond angles

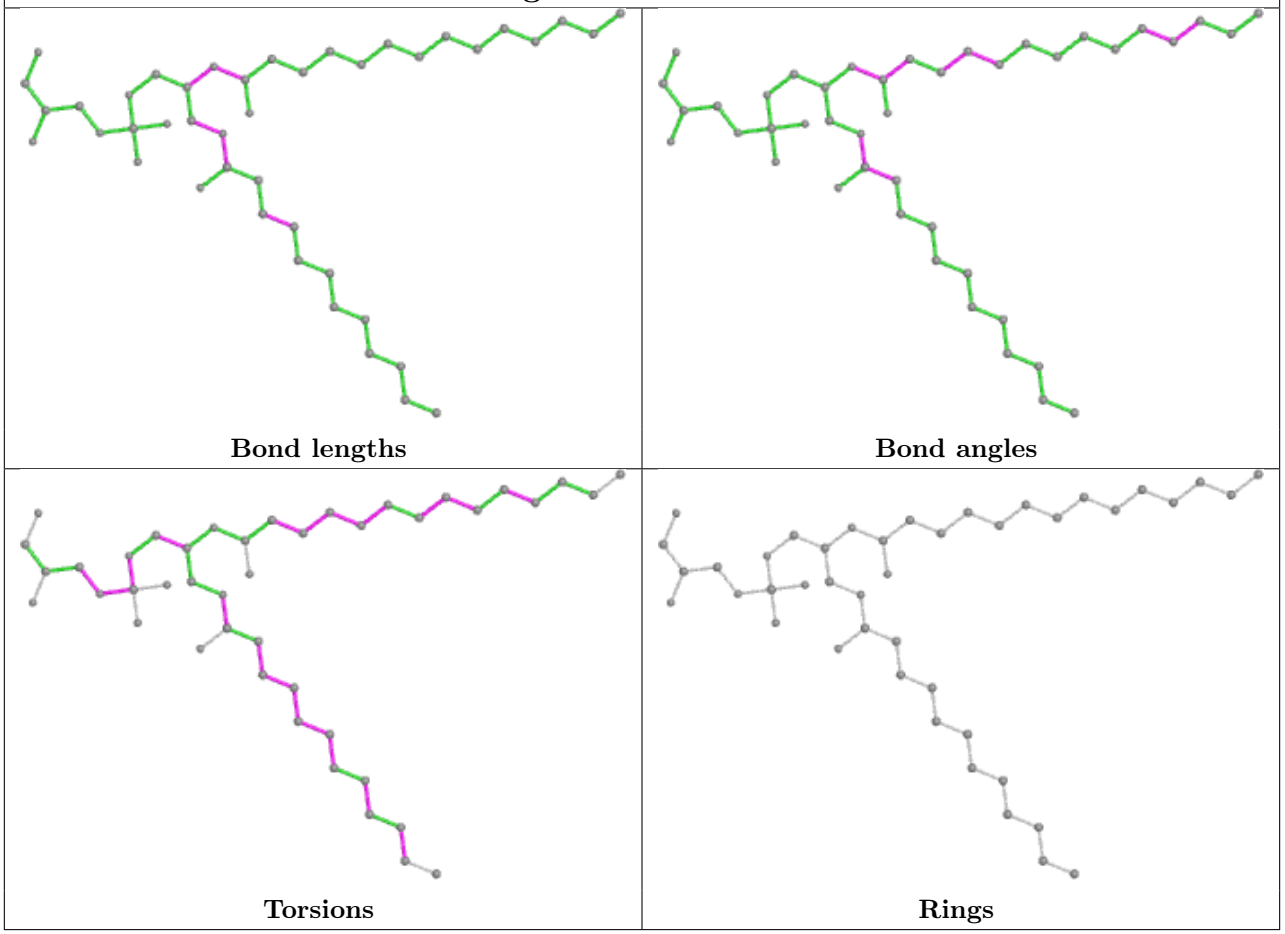


Torsions



Rings

Ligand LHG A 319



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

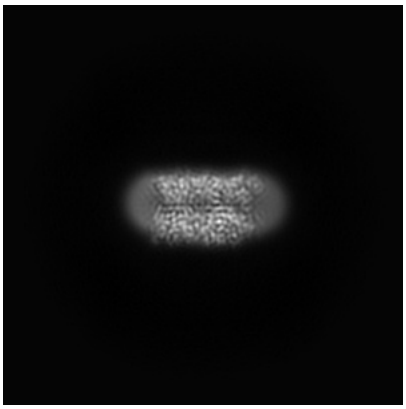
5 Map visualisation

This section contains visualisations of the EMDB entry EMD-34883. These allow visual inspection of the internal detail of the map and identification of artifacts.

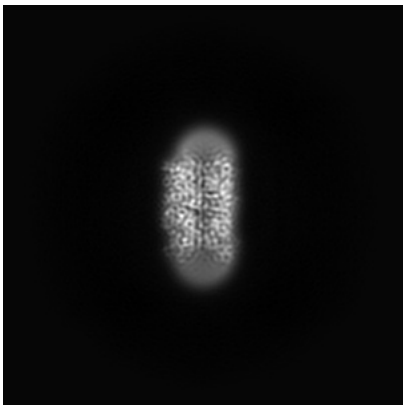
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections

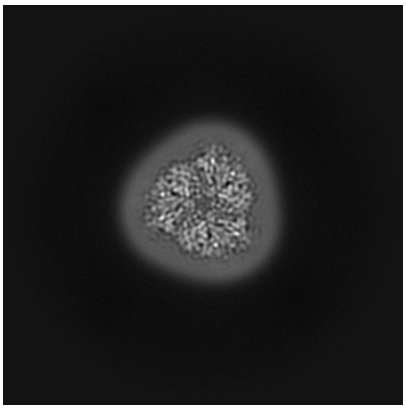
5.1.1 Primary map



X

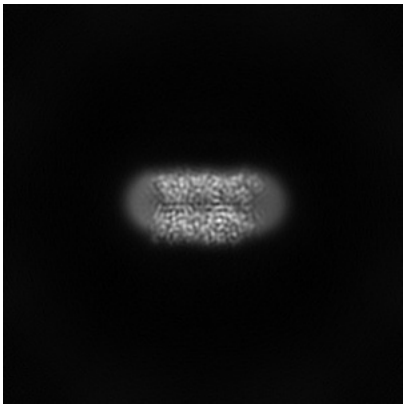


Y

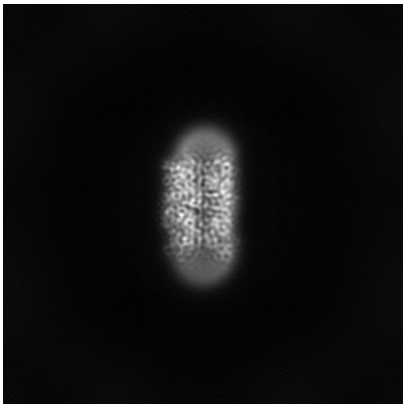


Z

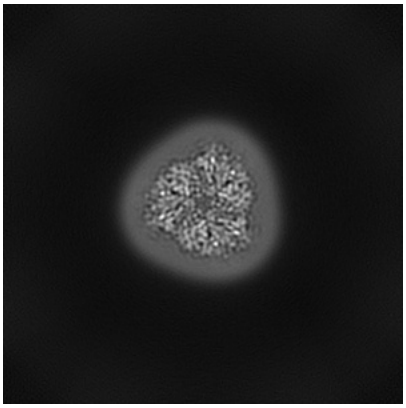
5.1.2 Raw map



X



Y

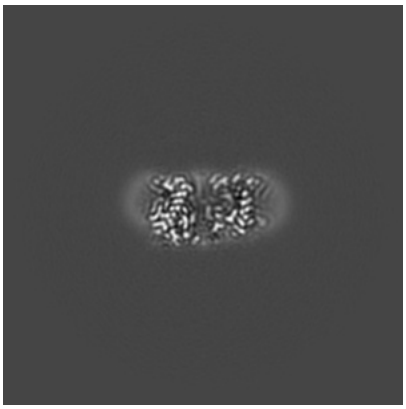


Z

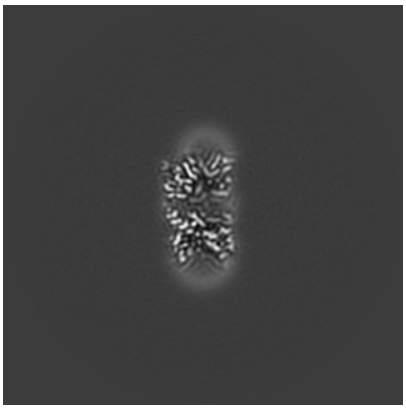
The images above show the map projected in three orthogonal directions.

5.2 Central slices (i)

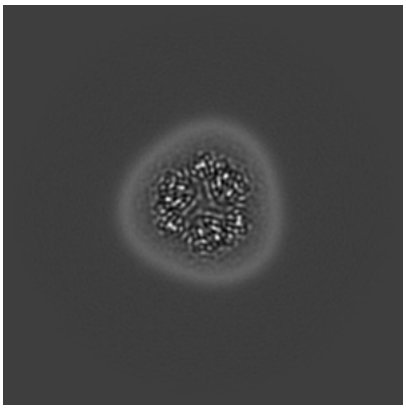
5.2.1 Primary map



X Index: 128

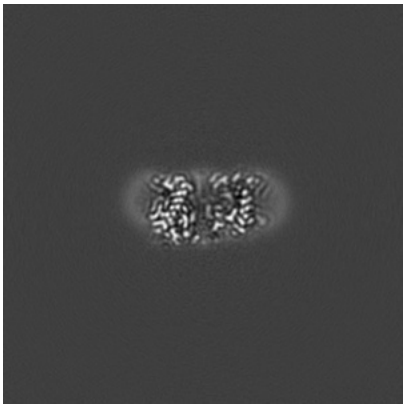


Y Index: 128

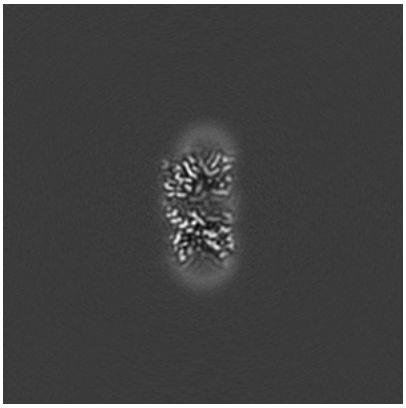


Z Index: 128

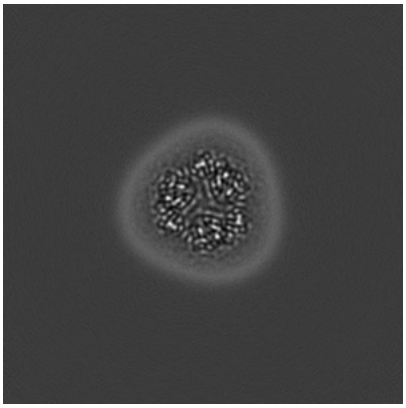
5.2.2 Raw map



X Index: 128



Y Index: 128

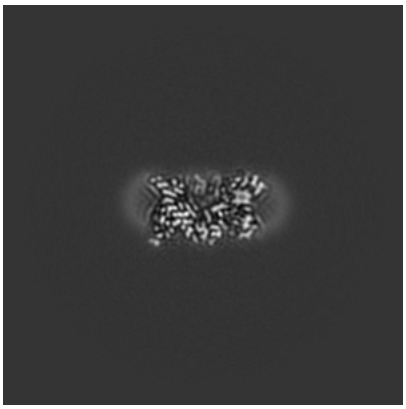


Z Index: 128

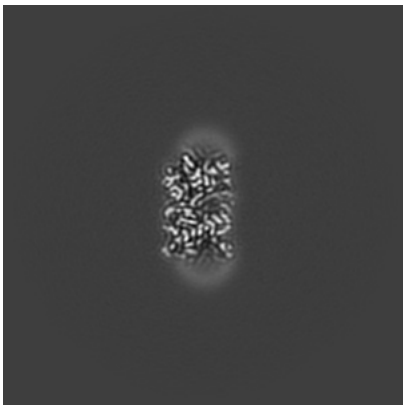
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices (i)

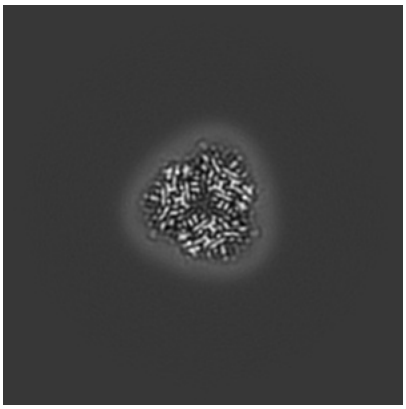
5.3.1 Primary map



X Index: 134

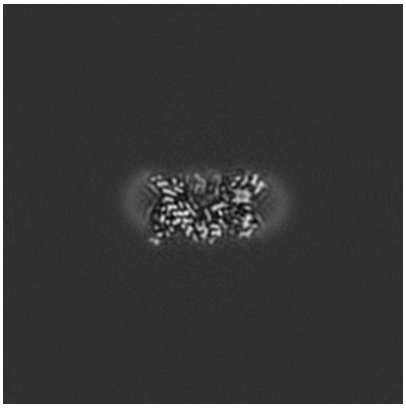


Y Index: 137

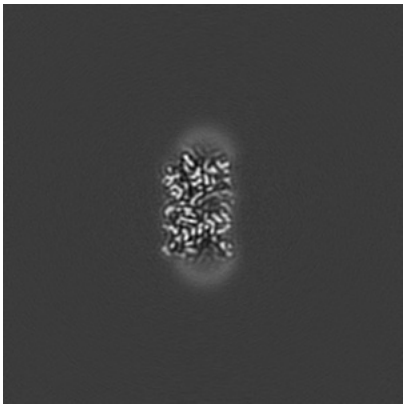


Z Index: 117

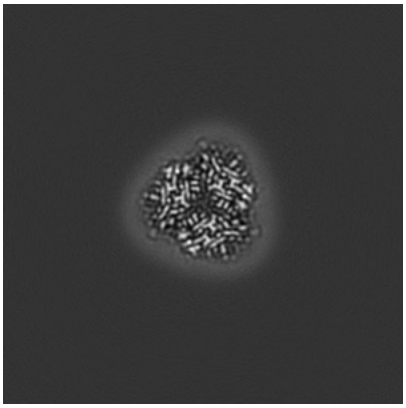
5.3.2 Raw map



X Index: 134



Y Index: 137

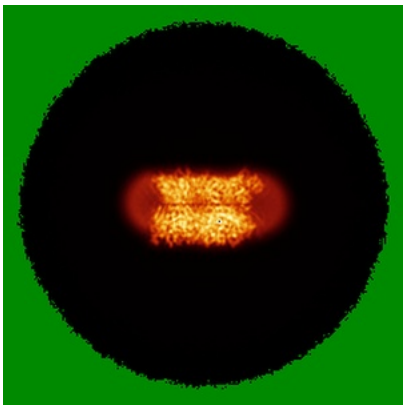


Z Index: 117

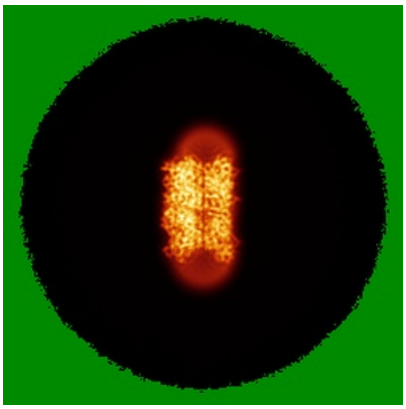
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal standard-deviation projections (False-color) (i)

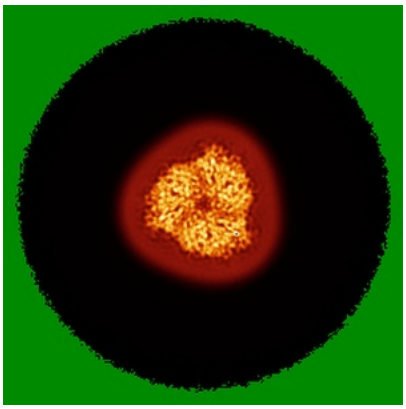
5.4.1 Primary map



X

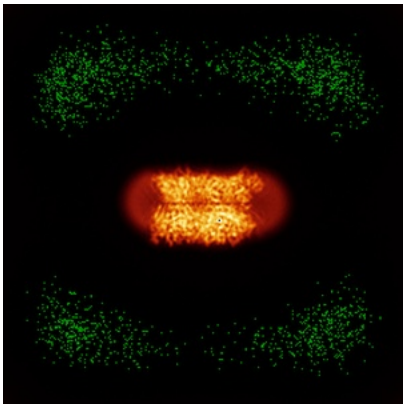


Y

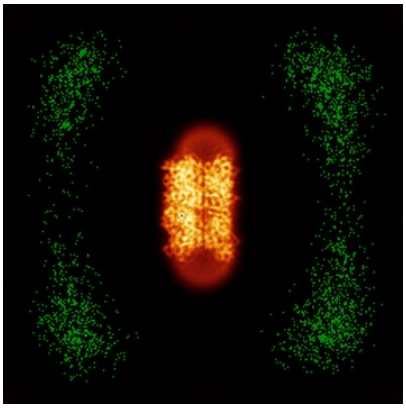


Z

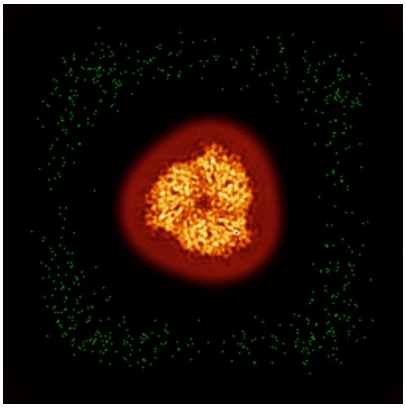
5.4.2 Raw map



X



Y

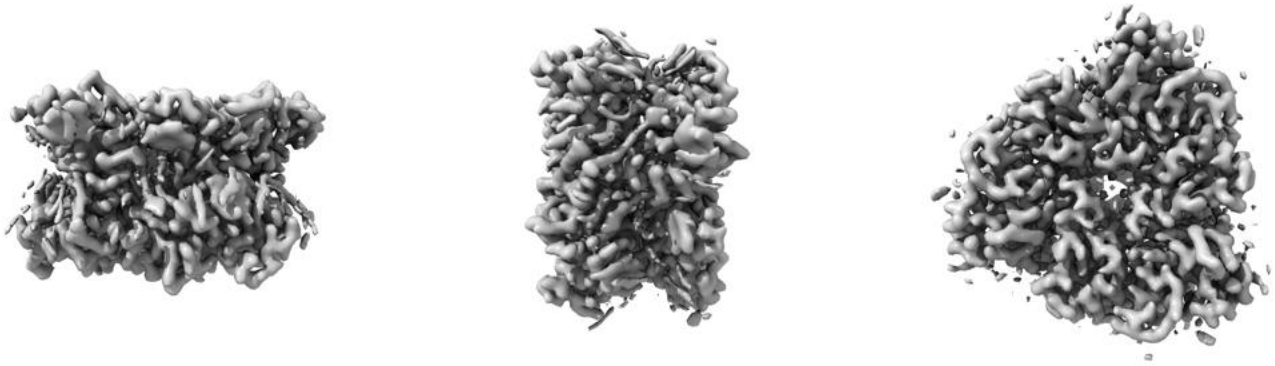


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views (i)

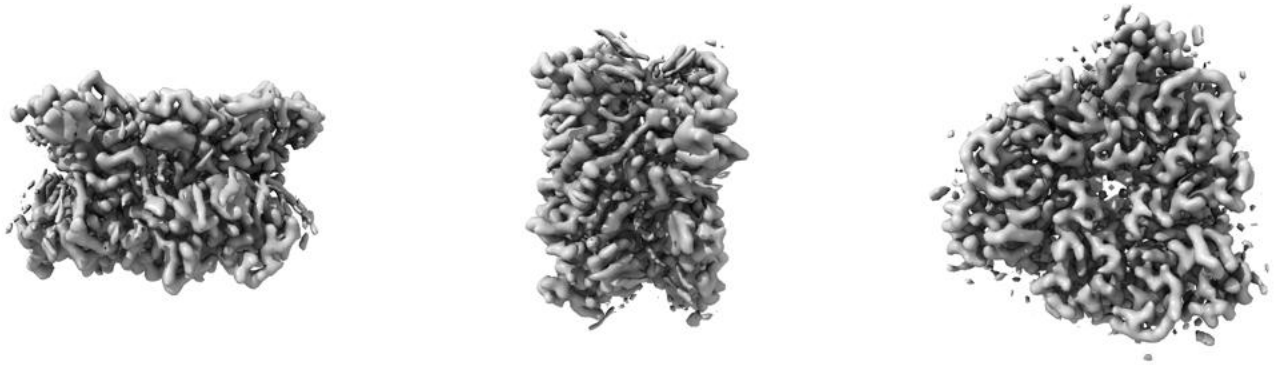
5.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.207. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

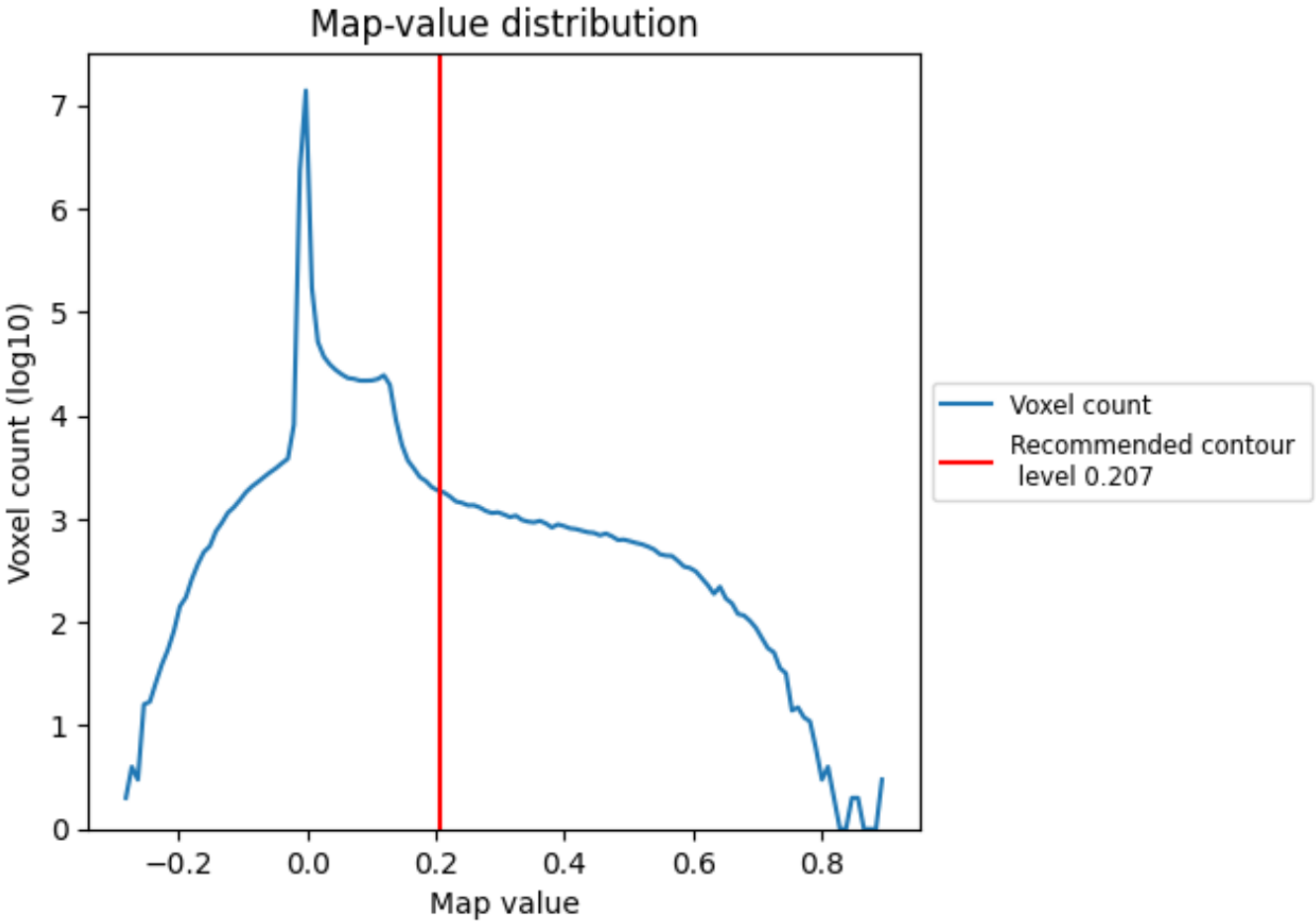
5.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

6 Map analysis

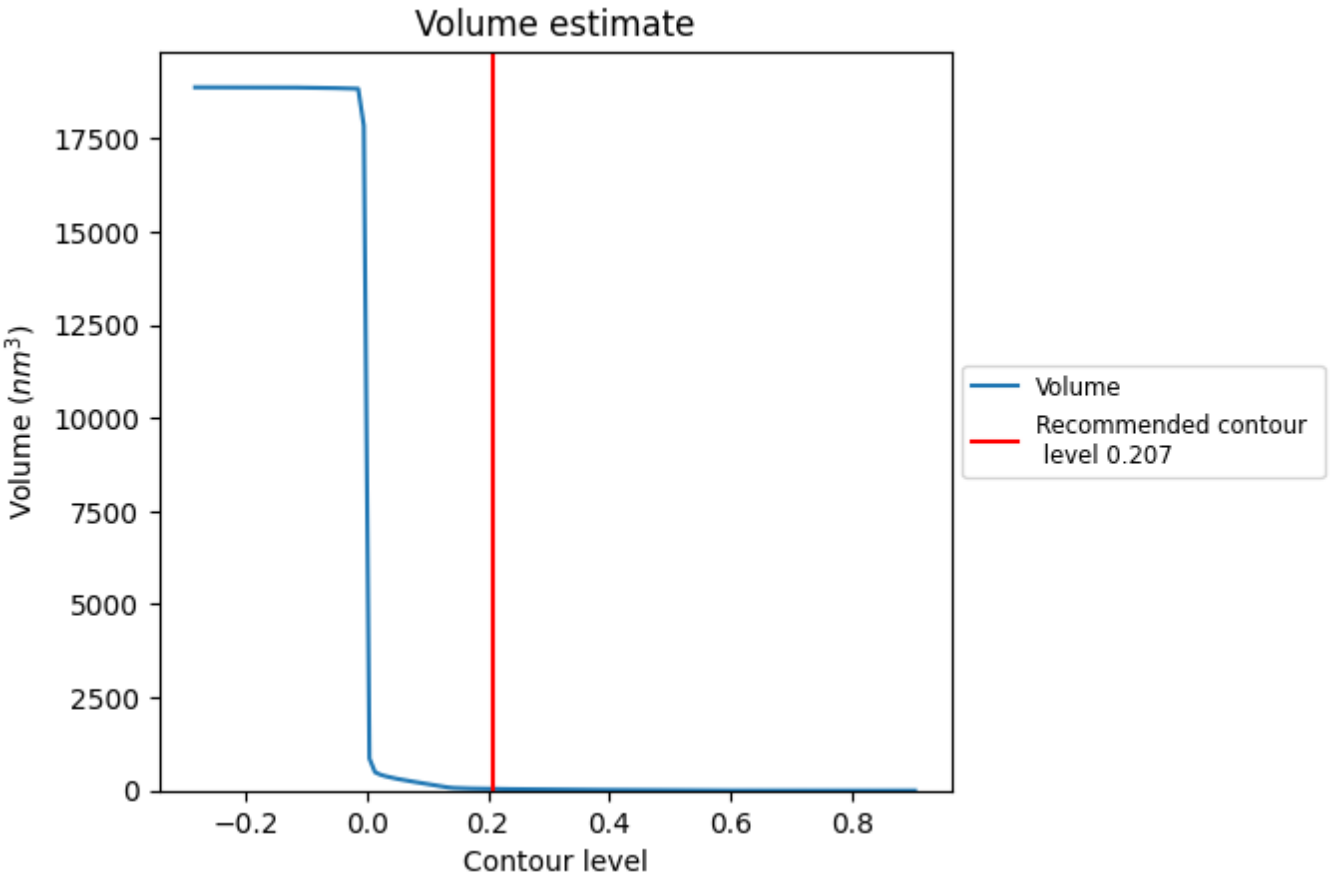
This section contains the results of statistical analysis of the map.

6.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

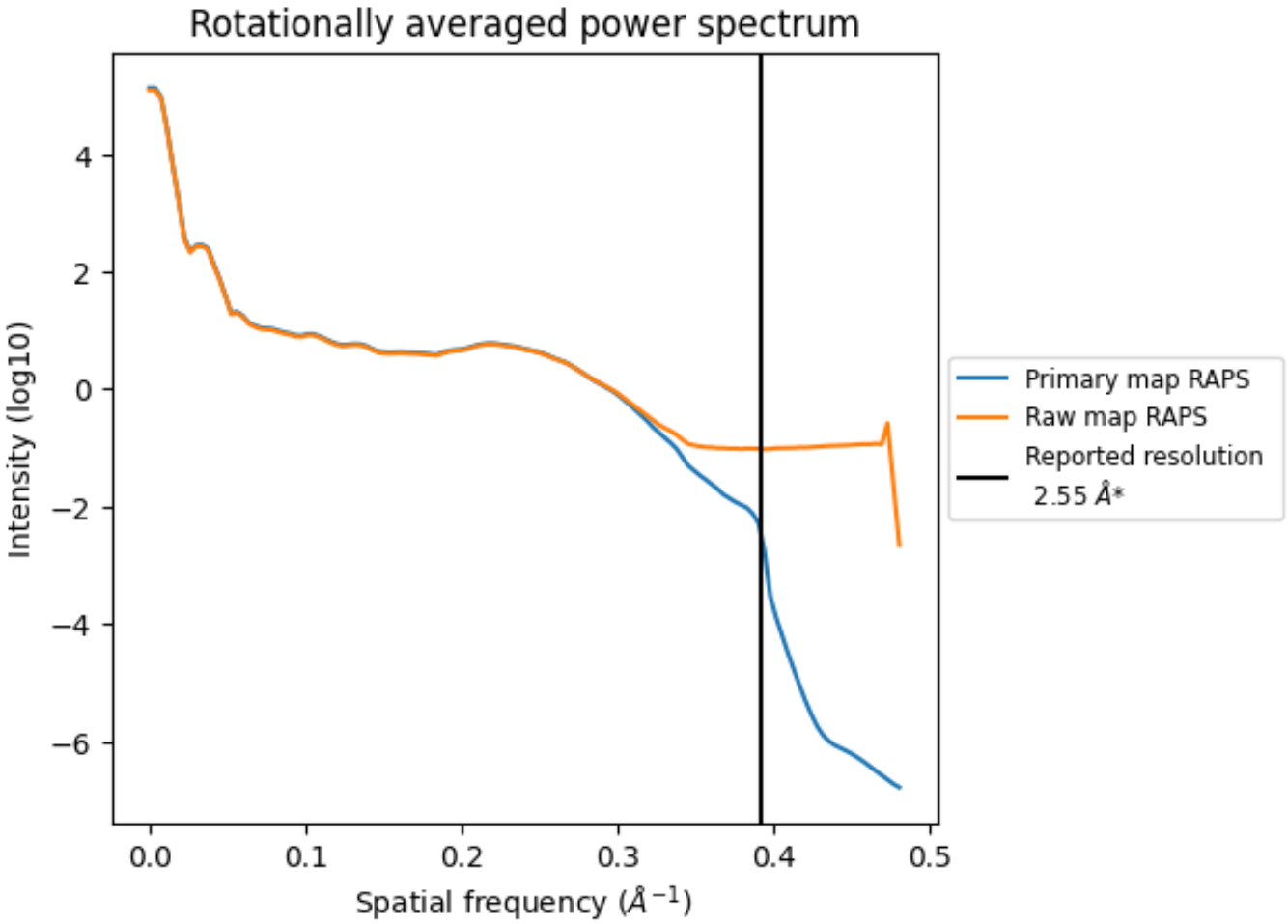
6.2 Volume estimate



The volume at the recommended contour level is 45 nm^3; this corresponds to an approximate mass of 41 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

6.3 Rotationally averaged power spectrum (i)

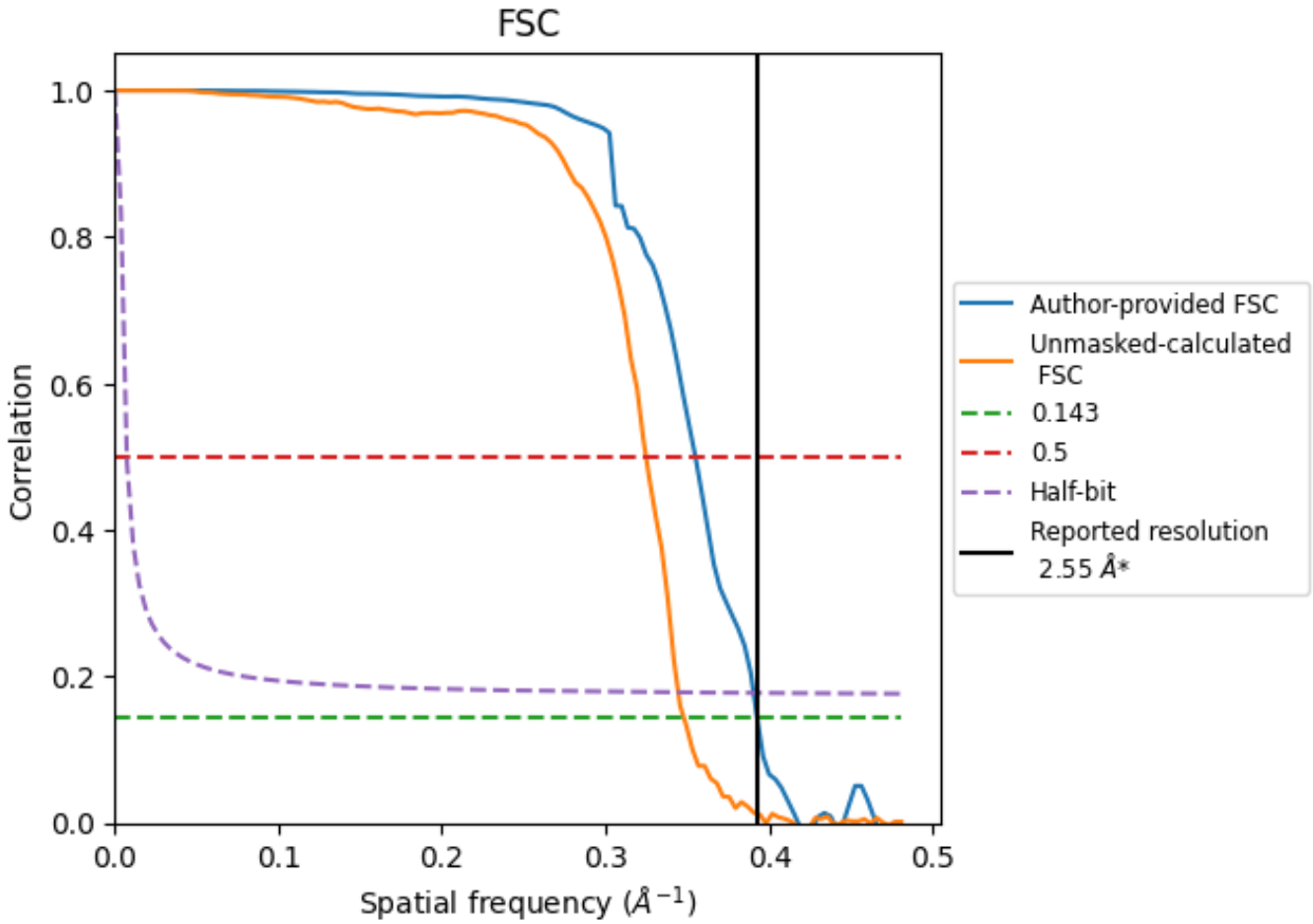


*Reported resolution corresponds to spatial frequency of 0.392 Å^{-1}

7 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

7.1 FSC



*Reported resolution corresponds to spatial frequency of 0.392 $Å^{-1}$

7.2 Resolution estimates (i)

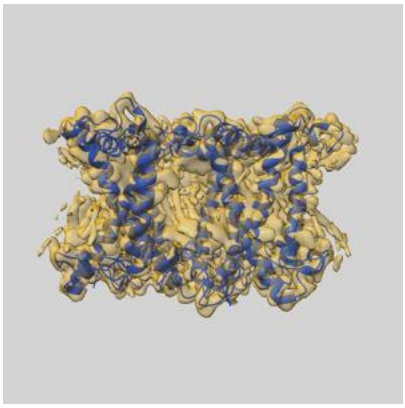
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.55	-	-
Author-provided FSC curve	2.55	2.82	2.56
Unmasked-calculated*	2.87	3.08	2.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.87 differs from the reported value 2.55 by more than 10 %

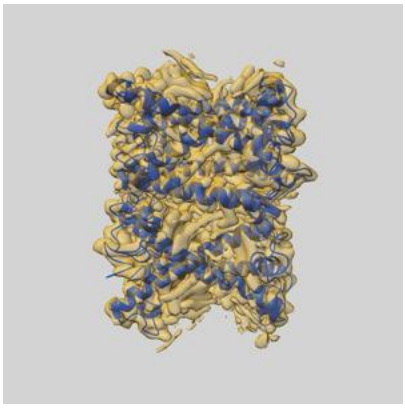
8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34883 and PDB model 8HLV. Per-residue inclusion information can be found in section ?? on page ??.

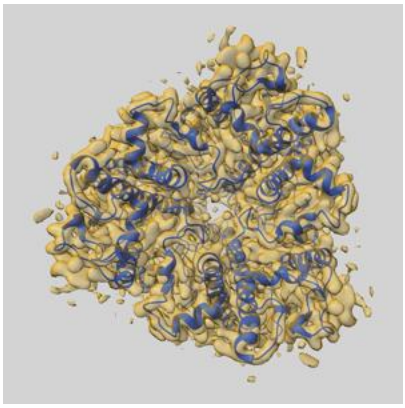
8.1 Map-model overlay



X



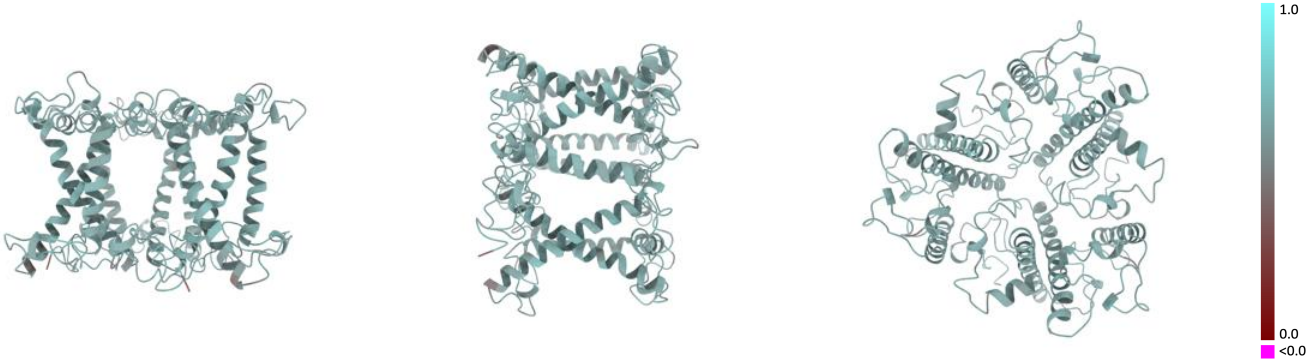
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.207 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

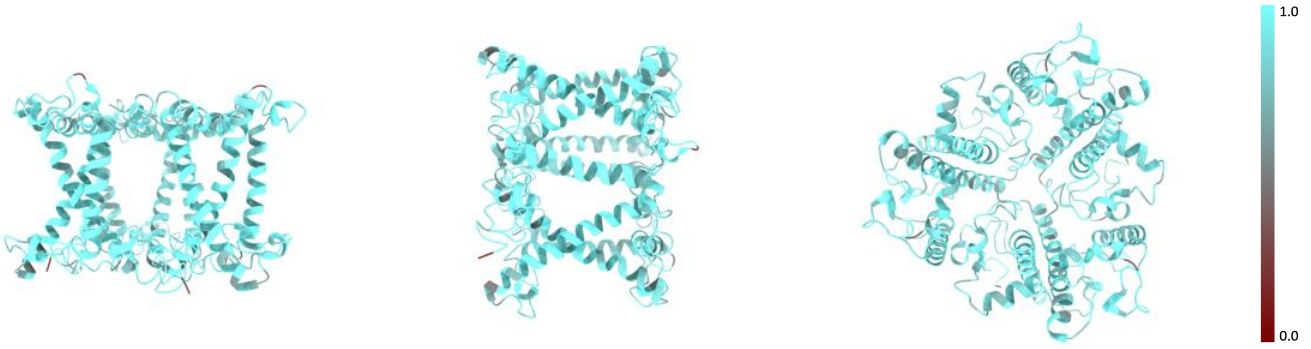
8.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

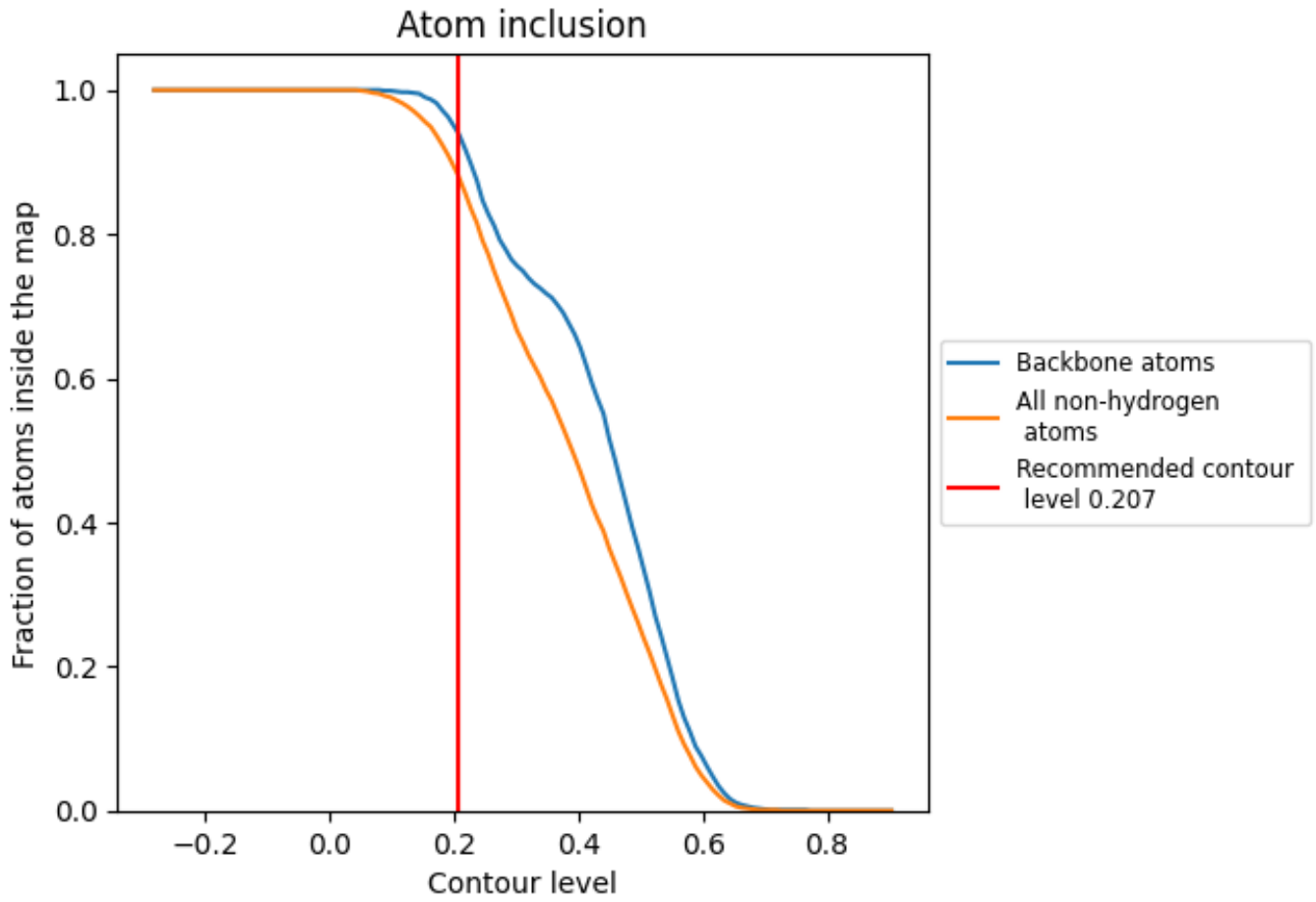
8.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.207).

8.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.207) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8810	0.6080
A	0.8820	0.6080
B	0.8820	0.6090
C	0.8790	0.6070