Full wwPDB EM Validation Report ⓘ

Oct 10, 2023 – 04:26 PM JST

PDB ID	:	8HPD
EMDB ID	:	EMD-34930
Title	:	Bry-LHCII heterotrimer of Bryopsis corticulans
Authors	:	Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on	:	2022-12-12
Resolution	:	2.74 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:

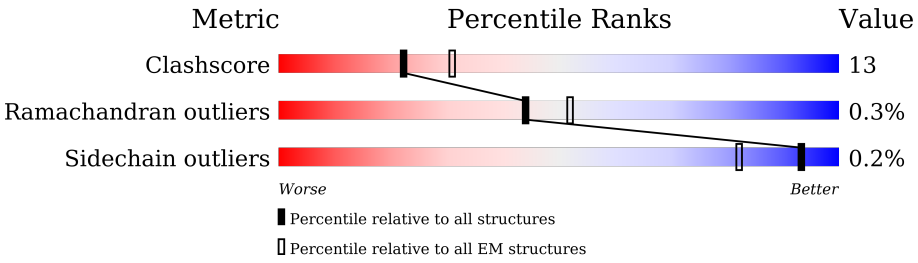
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.74 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	249	71% 14% 15%
2	B	253	71% 15% 14%
3	C	256	6% 61% 25% 14%

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
7	CHL	A	304	X	-	-	-
7	CHL	A	305	X	-	-	-
7	CHL	A	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CHL	A	309	X	-	-	-
7	CHL	A	310	X	-	-	-
7	CHL	A	311	X	-	-	-
7	CHL	A	312	X	-	-	-
7	CHL	A	317	X	-	-	-
7	CHL	B	305	X	-	-	-
7	CHL	B	306	X	-	-	-
7	CHL	B	309	X	-	-	-
7	CHL	B	310	X	-	-	-
7	CHL	B	311	X	-	-	-
7	CHL	B	312	X	-	-	-
7	CHL	B	313	X	-	-	-
7	CHL	B	318	X	-	-	-
7	CHL	C	305	X	-	-	-
7	CHL	C	306	X	-	-	-
7	CHL	C	309	X	-	-	-
7	CHL	C	310	X	-	-	-
7	CHL	C	311	X	-	-	-
7	CHL	C	312	X	-	-	-
7	CHL	C	313	X	-	-	-
7	CHL	C	318	X	-	-	-
8	CLA	A	306	X	-	-	-
8	CLA	A	307	X	-	-	-
8	CLA	A	313	X	-	-	-
8	CLA	A	314	X	-	-	-
8	CLA	A	315	X	-	-	-
8	CLA	A	316	X	-	-	-
8	CLA	B	307	X	-	-	-
8	CLA	B	308	X	-	-	-
8	CLA	B	314	X	-	-	-
8	CLA	B	315	X	-	-	-
8	CLA	B	316	X	-	-	-
8	CLA	B	317	X	-	-	-
8	CLA	C	307	X	-	-	-
8	CLA	C	308	X	-	-	-
8	CLA	C	314	X	-	-	-
8	CLA	C	315	X	-	-	-
8	CLA	C	316	X	-	-	-
8	CLA	C	317	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7949 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	212	Total	C	N	O	S	0	0
			1609	1038	255	306	10		

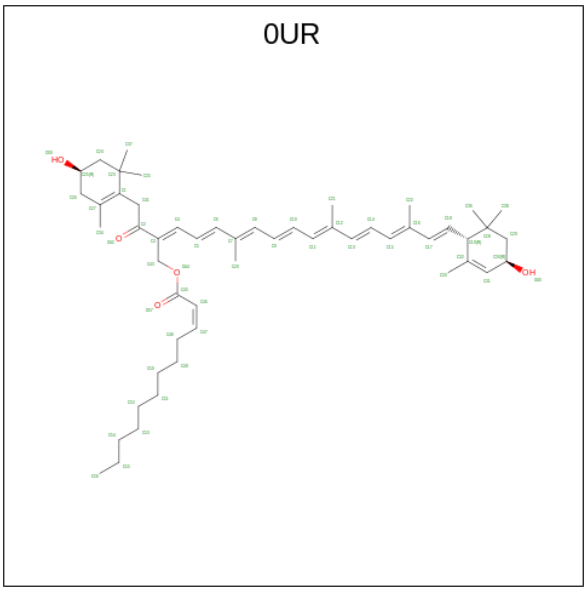
- Molecule 2 is a protein called siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	218	Total	C	N	O	S	0	0
			1658	1074	265	307	12		

- Molecule 3 is a protein called siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb2.

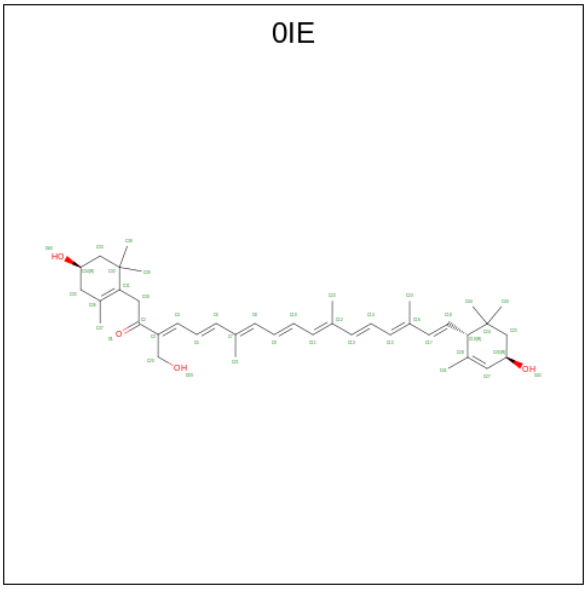
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	221	Total	C	N	O	S	0	0
			1716	1111	279	318	8		

- Molecule 4 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
4	A	1	Total C O 52 47 5	0
4	B	1	Total C O 52 47 5	0
4	C	1	Total C O 52 47 5	0

- Molecule 5 is Siphonaxanthin (three-letter code: 0IE) (formula: $C_{40}H_{56}O_4$).



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

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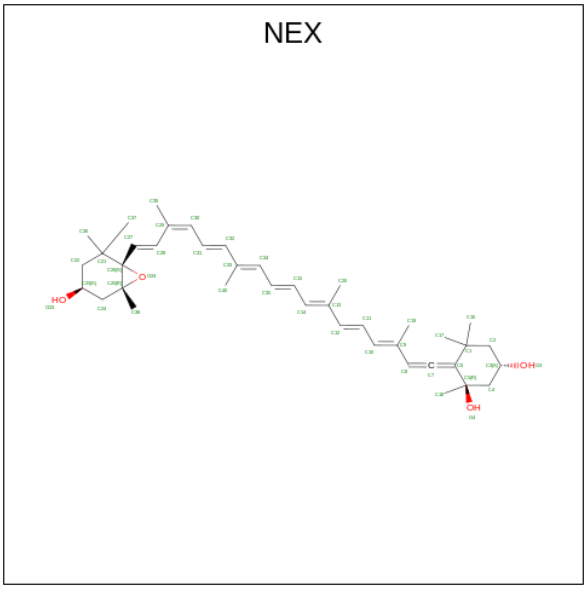
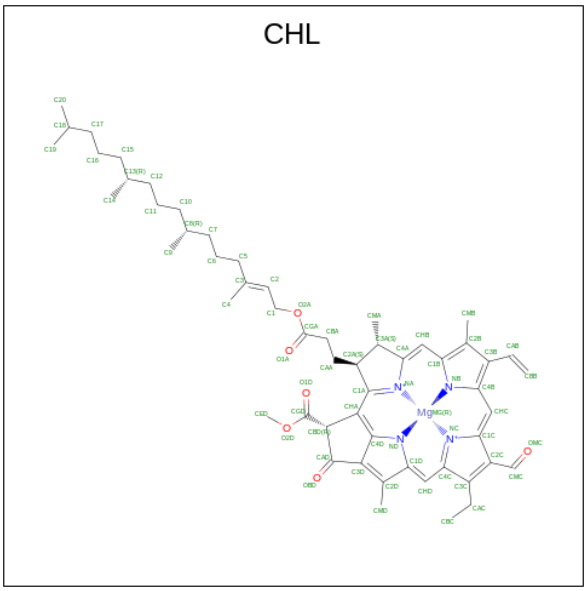
Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total C O 44 40 4	0
5	B	1	Total C O 44 40 4	0
5	C	1	Total C O 44 40 4	0
5	C	1	Total C O 44 40 4	0

- Molecule 6 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
6	A	1	Total C O 44 40 4	0
6	B	1	Total C O 44 40 4	0
6	C	1	Total C O 44 40 4	0

- Molecule 7 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
7	A	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
7	A	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
7	A	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
7	A	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
7	A	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
7	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	A	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
7	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	B	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
7	B	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
7	B	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
7	B	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
7	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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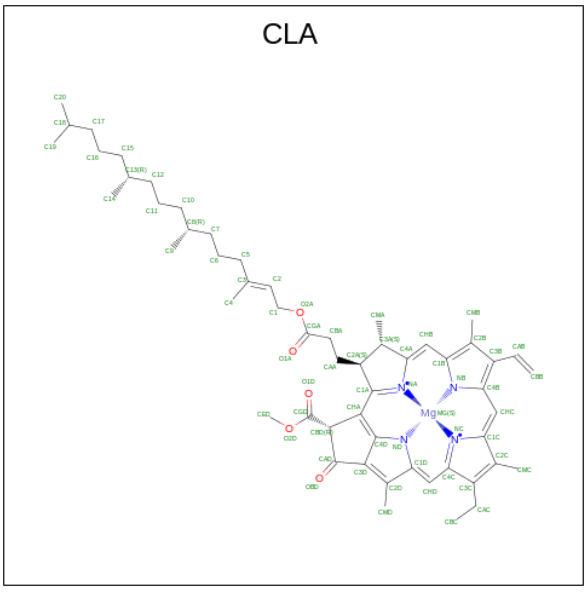
Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	B	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
7	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	C	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
7	C	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
7	C	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
7	C	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
7	C	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
7	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	C	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 8 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
8	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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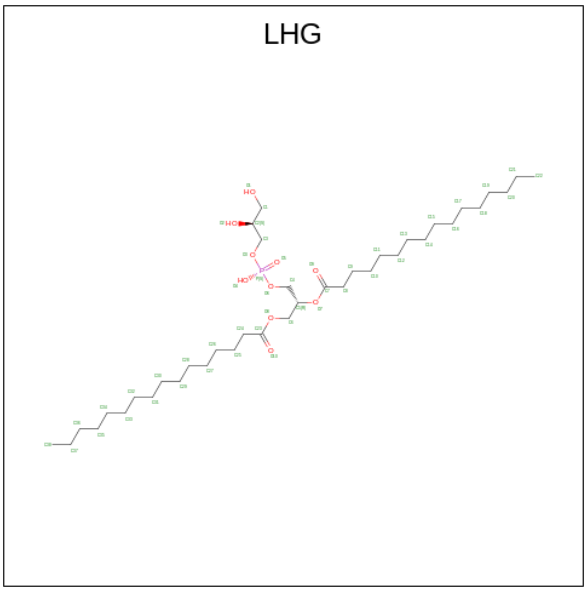
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			50	40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

- Molecule 9 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



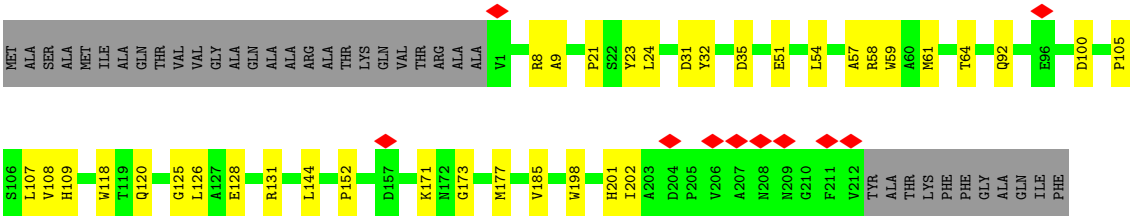
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	O	P	0
			42	31	10	1	
9	B	1	Total	C	O	P	0
			44	33	10	1	
9	C	1	Total	C	O	P	0
			43	32	10	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

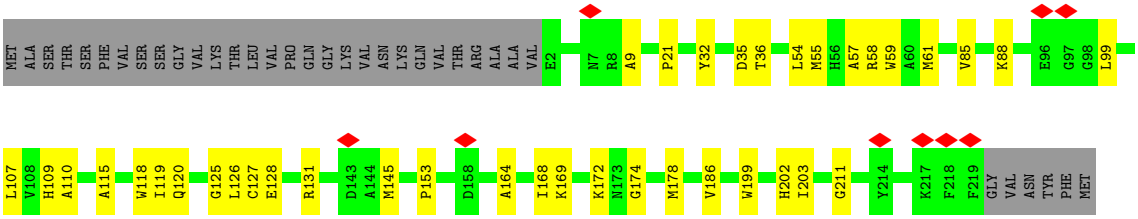
• Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1

Chain A:



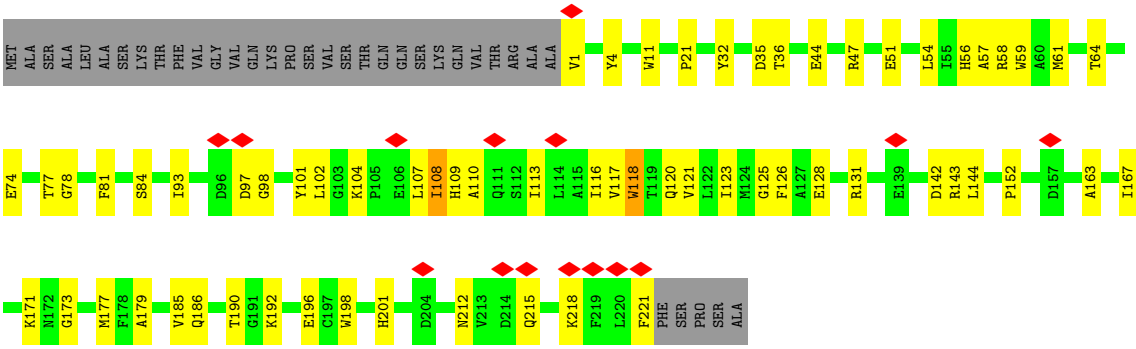
• Molecule 2: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb3

Chain B:



• Molecule 3: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb2

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1298053	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	0.986	Depositor
Minimum map value	-0.318	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.228	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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, 0IE, NEX, 0UR, LHG, CHL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/1658	0.42	0/2257
2	B	0.26	0/1711	0.43	0/2326
3	C	0.26	0/1769	0.47	0/2402
All	All	0.26	0/5138	0.44	0/6985

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1609	0	1517	35	0
2	B	1658	0	1556	37	0
3	C	1716	0	1627	62	0
4	A	52	0	0	3	0
4	B	52	0	0	2	0
4	C	52	0	0	4	0
5	A	44	0	0	0	0
5	B	88	0	0	1	0
5	C	88	0	0	1	0
6	A	44	0	56	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	44	0	56	7	0
6	C	44	0	56	14	0
7	A	450	0	400	27	0
7	B	445	0	397	28	0
7	C	435	0	374	31	0
8	A	333	0	305	13	0
8	B	333	0	305	15	0
8	C	333	0	305	13	0
9	A	42	0	54	3	0
9	B	44	0	58	2	0
9	C	43	0	56	3	0
All	All	7949	0	7122	191	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (191) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:304:NEX:H403	7:B:310:CHL:HBA2	1.33	1.07
6:B:304:NEX:H403	7:B:310:CHL:CBA	2.01	0.90
3:C:123:ILE:HG23	6:C:304:NEX:C15	2.05	0.87
1:A:57:ALA:HB1	1:A:173:GLY:HA3	1.65	0.79
6:C:304:NEX:H403	7:C:310:CHL:HBA2	1.65	0.77
6:A:303:NEX:H403	7:A:309:CHL:HBA2	1.66	0.77
3:C:123:ILE:HG23	6:C:304:NEX:H15	1.68	0.76
3:C:57:ALA:HB1	3:C:173:GLY:HA3	1.67	0.75
6:A:303:NEX:H403	7:A:309:CHL:CBA	2.17	0.74
2:B:57:ALA:HB1	2:B:174:GLY:HA3	1.69	0.74
2:B:55:MET:SD	2:B:131:ARG:NH1	2.62	0.73
3:C:131:ARG:NH2	7:C:313:CHL:O1D	2.23	0.70
3:C:128:GLU:OE1	3:C:131:ARG:NH1	2.25	0.69
3:C:126:PHE:HB2	6:C:304:NEX:C20	2.23	0.69
8:C:307:CLA:HBB1	7:C:313:CHL:H161	1.73	0.68
1:A:131:ARG:NH2	7:A:312:CHL:O1D	2.27	0.68
6:C:304:NEX:H403	7:C:310:CHL:CBA	2.24	0.66
2:B:99:LEU:HB3	2:B:110:ALA:HB3	1.78	0.66
1:A:128:GLU:OE1	1:A:131:ARG:NH1	2.29	0.65
7:B:312:CHL:H192	7:B:312:CHL:HAA2	1.79	0.64
3:C:32:TYR:HB2	7:C:306:CHL:HMD1	1.80	0.63
1:A:171:LYS:NZ	9:A:318:LHG:O5	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:307:CLA:H91	7:C:313:CHL:H143	1.81	0.62
2:B:172:LYS:NZ	9:B:319:LHG:O4	2.31	0.61
1:A:9:ALA:HB1	7:A:304:CHL:HBC1	1.83	0.61
2:B:85:VAL:HG21	2:B:88:LYS:HE2	1.83	0.60
8:B:307:CLA:H91	7:B:313:CHL:H143	1.82	0.60
1:A:152:PRO:HD2	4:A:301:0UR:C30	2.31	0.60
3:C:171:LYS:NZ	9:C:319:LHG:O4	2.31	0.60
2:B:128:GLU:OE1	2:B:131:ARG:NH2	2.35	0.60
1:A:8:ARG:NH1	1:A:31:ASP:O	2.34	0.60
8:C:307:CLA:H2	8:C:307:CLA:HMA2	1.83	0.60
1:A:32:TYR:HB2	7:A:305:CHL:HMD1	1.83	0.59
2:B:54:LEU:HD23	2:B:145:MET:HB3	1.85	0.59
8:B:307:CLA:H72	7:C:306:CHL:H91	1.85	0.59
2:B:127:CYS:SG	6:B:304:NEX:H15	2.43	0.58
3:C:44:GLU:OE2	3:C:47:ARG:NH2	2.34	0.58
3:C:126:PHE:HB2	6:C:304:NEX:H203	1.84	0.58
8:A:306:CLA:HBB1	7:A:312:CHL:H162	1.86	0.57
7:A:310:CHL:H121	7:B:305:CHL:H202	1.86	0.57
8:B:308:CLA:HBD	8:B:308:CLA:HBA1	1.86	0.57
7:C:310:CHL:HBB2	7:C:311:CHL:HBB1	1.87	0.57
2:B:32:TYR:HB2	7:B:306:CHL:HMD1	1.87	0.57
6:B:304:NEX:C35	7:B:312:CHL:HMB3	2.35	0.56
3:C:116:ILE:HD11	7:C:310:CHL:HMD3	1.87	0.56
3:C:61:MET:HE3	8:C:314:CLA:HMC3	1.86	0.56
3:C:97:ASP:OD1	3:C:109:HIS:NE2	2.38	0.56
9:A:318:LHG:H261	9:A:318:LHG:HC82	1.86	0.56
8:A:316:CLA:HMB1	8:A:316:CLA:HBB1	1.88	0.56
1:A:21:PRO:HG3	1:A:35:ASP:HB3	1.87	0.56
5:B:303:0IE:C23	9:B:319:LHG:H101	2.36	0.56
6:A:303:NEX:C35	7:A:311:CHL:HMB3	2.38	0.54
1:A:54:LEU:HD23	1:A:144:LEU:HB3	1.89	0.54
4:A:301:0UR:C15	8:A:313:CLA:H72	2.37	0.54
3:C:201:HIS:CG	8:C:317:CLA:HAA2	2.43	0.54
6:A:303:NEX:H362	8:A:307:CLA:CHC	2.38	0.54
3:C:54:LEU:HD23	3:C:144:LEU:HD22	1.90	0.53
1:A:58:ARG:NH1	7:A:311:CHL:OBD	2.42	0.53
2:B:57:ALA:O	2:B:61:MET:HG3	2.08	0.52
2:B:21:PRO:HG2	2:B:35:ASP:HB3	1.91	0.52
8:C:315:CLA:HAC1	9:C:319:LHG:H301	1.91	0.52
7:A:304:CHL:HMD3	9:A:318:LHG:HC41	1.91	0.52
1:A:59:TRP:CD1	7:A:312:CHL:HMD3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:MET:SD	7:B:306:CHL:HBB1	2.49	0.52
2:B:186:VAL:HG12	8:B:317:CLA:HMD3	1.91	0.51
3:C:131:ARG:HG3	7:C:312:CHL:C1D	2.40	0.51
8:B:317:CLA:H2	7:B:318:CHL:HMD1	1.93	0.51
4:C:301:0UR:C15	8:C:314:CLA:H72	2.40	0.51
8:C:317:CLA:H2	7:C:318:CHL:HMD1	1.92	0.51
2:B:118:TRP:HZ2	7:C:318:CHL:HBD	1.76	0.51
3:C:123:ILE:CG2	6:C:304:NEX:C34	2.89	0.51
3:C:126:PHE:CB	6:C:304:NEX:C20	2.89	0.51
3:C:107:LEU:O	3:C:109:HIS:N	2.44	0.50
3:C:51:GLU:HA	3:C:144:LEU:HD21	1.93	0.50
1:A:177:MET:SD	7:A:305:CHL:HBB1	2.51	0.50
3:C:212:ASN:HB2	3:C:215:GLN:HB2	1.93	0.50
2:B:115:ALA:O	2:B:119:ILE:HG12	2.11	0.50
2:B:59:TRP:CD1	7:B:313:CHL:HMD3	2.46	0.49
1:A:61:MET:HE3	8:A:313:CLA:HMC3	1.95	0.48
7:B:305:CHL:H12	7:B:305:CHL:H51	1.65	0.48
1:A:185:VAL:HG12	8:A:316:CLA:HMD3	1.96	0.48
7:A:304:CHL:HHB	7:C:313:CHL:HMB2	1.96	0.48
7:A:312:CHL:HAA2	2:B:36:THR:HG21	1.94	0.48
2:B:58:ARG:NH1	7:B:312:CHL:OBD	2.41	0.48
8:B:307:CLA:HMA2	8:B:307:CLA:H2	1.95	0.48
3:C:11:TRP:HB3	3:C:32:TYR:HB3	1.95	0.48
3:C:59:TRP:CD1	7:C:313:CHL:HMD3	2.48	0.48
7:B:305:CHL:H121	7:B:305:CHL:H162	1.42	0.48
1:A:23:TYR:HE2	3:C:44:GLU:HG2	1.78	0.48
3:C:118:TRP:O	3:C:121:VAL:HG22	2.14	0.48
3:C:185:VAL:HG12	8:C:317:CLA:HMD3	1.96	0.47
7:B:313:CHL:HAA2	3:C:36:THR:HG21	1.97	0.47
7:C:305:CHL:H61	7:C:305:CHL:H41	1.62	0.47
2:B:153:PRO:HD2	4:B:301:0UR:C30	2.45	0.47
3:C:58:ARG:NH1	7:C:312:CHL:OBD	2.46	0.46
2:B:199:TRP:O	2:B:203:ILE:HG12	2.16	0.46
3:C:21:PRO:HG2	3:C:35:ASP:HB3	1.96	0.46
3:C:218:LYS:HD2	3:C:221:PHE:HA	1.97	0.46
7:B:312:CHL:H141	7:B:312:CHL:H162	1.71	0.46
3:C:1:VAL:HG23	3:C:4:TYR:H	1.80	0.46
3:C:123:ILE:HG23	6:C:304:NEX:C35	2.42	0.46
1:A:51:GLU:HA	1:A:144:LEU:HD21	1.97	0.46
3:C:117:VAL:HG22	7:C:311:CHL:HBC1	1.98	0.46
3:C:186:GLN:O	3:C:190:THR:OG1	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:PRO:HG2	1:A:24:LEU:HG	1.97	0.46
3:C:59:TRP:CE2	7:C:312:CHL:HED2	2.51	0.46
2:B:9:ALA:HB1	7:B:305:CHL:HBC1	1.98	0.46
3:C:118:TRP:HA	3:C:121:VAL:HG22	1.97	0.46
6:C:304:NEX:H362	8:C:308:CLA:CHC	2.46	0.46
2:B:202:HIS:CG	8:B:317:CLA:HAA2	2.51	0.45
1:A:131:ARG:HG3	7:A:311:CHL:C1D	2.47	0.45
3:C:198:TRP:HE1	7:C:318:CHL:HMC	1.80	0.45
3:C:101:TYR:HB2	3:C:108:ILE:HD13	1.99	0.45
3:C:152:PRO:HD2	4:C:301:0UR:C30	2.46	0.45
2:B:169:LYS:HD3	8:B:316:CLA:HBD	1.99	0.45
2:B:107:LEU:O	2:B:109:HIS:N	2.49	0.45
7:B:312:CHL:H91	7:B:312:CHL:H112	1.71	0.45
1:A:201:HIS:CG	8:A:316:CLA:HAA2	2.52	0.45
2:B:125:GLY:CA	7:B:313:CHL:HAB	2.46	0.45
3:C:93:ILE:HG21	3:C:113:ILE:HD13	1.99	0.45
3:C:128:GLU:HG3	7:C:313:CHL:NB	2.32	0.45
5:C:303:0IE:C23	9:C:319:LHG:H101	2.47	0.45
1:A:61:MET:SD	8:A:313:CLA:HAB	2.57	0.45
7:A:311:CHL:H143	7:A:311:CHL:H162	1.72	0.45
3:C:192:LYS:HD3	3:C:196:GLU:HG2	1.99	0.45
3:C:177:MET:SD	7:C:306:CHL:HBB1	2.56	0.45
1:A:107:LEU:O	1:A:109:HIS:N	2.49	0.45
2:B:125:GLY:HA2	7:B:313:CHL:HAB	1.99	0.45
1:A:64:THR:HG21	4:A:301:0UR:C6	2.47	0.44
1:A:125:GLY:HA2	7:A:312:CHL:HAB	2.00	0.44
3:C:120:GLN:HE22	7:C:311:CHL:CMC	2.31	0.44
7:C:305:CHL:H112	7:C:305:CHL:H91	1.72	0.44
3:C:56:HIS:CD2	7:C:306:CHL:HBB2	2.52	0.44
3:C:116:ILE:HG13	7:C:309:CHL:HAC1	2.00	0.44
6:C:304:NEX:H28	7:C:310:CHL:O1A	2.18	0.44
3:C:77:THR:HG22	3:C:78:GLY:H	1.83	0.43
3:C:142:ASP:OD1	3:C:143:ARG:N	2.51	0.43
7:A:304:CHL:H41	7:A:304:CHL:H61	1.55	0.43
2:B:211:GLY:N	8:B:317:CLA:O1A	2.51	0.43
7:B:305:CHL:H91	7:B:305:CHL:H111	1.77	0.43
3:C:77:THR:HG22	3:C:78:GLY:N	2.33	0.43
7:C:305:CHL:HBA1	7:C:305:CHL:H3A	1.79	0.43
1:A:120:GLN:HE22	7:A:310:CHL:CMC	2.32	0.43
6:C:304:NEX:H241	8:C:308:CLA:O2A	2.19	0.43
1:A:92:GLN:HE22	8:A:307:CLA:HED2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:314:CLA:H142	8:A:314:CLA:H112	1.74	0.42
7:B:306:CHL:H141	7:B:306:CHL:H161	1.84	0.42
7:C:313:CHL:H92	7:C:313:CHL:H62	1.71	0.42
3:C:168:LYS:HD3	8:C:316:CLA:HAA2	2.02	0.42
3:C:179:ALA:HB1	4:C:301:0UR:O42	2.19	0.42
6:C:304:NEX:H403	7:C:310:CHL:CGA	2.49	0.42
7:A:311:CHL:H91	7:A:311:CHL:H112	1.81	0.42
2:B:169:LYS:HD3	8:B:316:CLA:HAA2	2.01	0.42
3:C:81:PHE:CE1	3:C:102:LEU:HA	2.55	0.42
7:A:304:CHL:H3A	7:A:304:CHL:HBA1	1.75	0.42
2:B:59:TRP:CE2	7:B:312:CHL:HED2	2.55	0.42
2:B:126:LEU:CD1	6:B:304:NEX:H203	2.49	0.42
3:C:51:GLU:HA	3:C:144:LEU:HD11	2.01	0.42
1:A:128:GLU:HG3	7:A:312:CHL:NB	2.35	0.42
1:A:59:TRP:CE2	7:A:311:CHL:HED2	2.55	0.42
8:A:306:CLA:H72	7:B:306:CHL:H91	2.02	0.42
2:B:126:LEU:HB2	6:B:304:NEX:C20	2.50	0.42
3:C:125:GLY:CA	7:C:313:CHL:HAB	2.50	0.42
1:A:125:GLY:CA	7:A:312:CHL:HAB	2.50	0.41
1:A:107:LEU:HD23	7:A:308:CHL:HED2	2.01	0.41
2:B:120:GLN:HE22	7:B:311:CHL:CMC	2.34	0.41
3:C:64:THR:HG21	4:C:301:0UR:C6	2.51	0.41
3:C:98:GLY:HA3	3:C:110:ALA:O	2.21	0.41
8:A:306:CLA:CAD	7:A:312:CHL:H2	2.50	0.41
2:B:120:GLN:OE1	7:B:311:CHL:HMC	2.20	0.41
2:B:127:CYS:HG	6:B:304:NEX:H15	1.85	0.41
8:B:308:CLA:H42	7:B:310:CHL:HBD	2.03	0.41
3:C:104:LYS:N	3:C:104:LYS:HD3	2.36	0.41
1:A:100:ASP:OD2	1:A:105:PRO:HA	2.20	0.41
8:B:307:CLA:H72	8:B:307:CLA:H112	1.89	0.41
1:A:198:TRP:O	1:A:202:ILE:HG12	2.21	0.41
2:B:119:ILE:HD12	7:B:310:CHL:HED2	2.02	0.41
2:B:164:ALA:O	2:B:168:ILE:HG12	2.21	0.41
4:B:301:0UR:C15	8:B:314:CLA:H72	2.51	0.41
1:A:126:LEU:CB	6:A:303:NEX:C20	2.99	0.41
1:A:126:LEU:HB3	6:A:303:NEX:C20	2.51	0.41
3:C:74:GLU:OE1	3:C:84:SER:OG	2.37	0.41
3:C:163:ALA:O	3:C:167:ILE:HG12	2.21	0.41
8:A:306:CLA:H2	8:A:306:CLA:H61	1.67	0.40
2:B:99:LEU:HD21	8:B:308:CLA:HBA2	2.03	0.40
3:C:185:VAL:HG21	8:C:317:CLA:HAC2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:311:CHL:HBB1	7:A:311:CHL:HHC	2.02	0.40
3:C:126:PHE:CB	6:C:304:NEX:H203	2.48	0.40
8:B:315:CLA:H141	8:B:315:CLA:H162	1.89	0.40
3:C:128:GLU:HG3	7:C:313:CHL:C1B	2.51	0.40
1:A:118:TRP:HZ2	7:B:318:CHL:HBD	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	210/249 (84%)	205 (98%)	4 (2%)	1 (0%)	29 48
2	B	216/253 (85%)	203 (94%)	13 (6%)	0	100 100
3	C	219/256 (86%)	212 (97%)	6 (3%)	1 (0%)	29 48
All	All	645/758 (85%)	620 (96%)	23 (4%)	2 (0%)	44 61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	VAL
3	C	108	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	160/184 (87%)	160 (100%)	0	100	100
2	B	161/191 (84%)	161 (100%)	0	100	100
3	C	170/199 (85%)	169 (99%)	1 (1%)	86	91
All	All	491/574 (86%)	490 (100%)	1 (0%)	93	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	118	TRP

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

56 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	$\#\|Z\| > 2$
8	CLA	B	307	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	CHL	B	305	2	66,74,74	1.97	15 (22%)	73,114,114	3.01	27 (36%)
6	NEX	C	304	-	38,46,46	0.99	2 (5%)	50,70,70	1.27	6 (12%)
5	0IE	C	302	-	42,45,45	1.44	6 (14%)	49,63,63	1.71	10 (20%)
8	CLA	A	306	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	7 (9%)
5	0IE	B	302	-	42,45,45	1.47	5 (11%)	49,63,63	1.82	10 (20%)
7	CHL	C	312	-	56,64,74	2.12	15 (26%)	61,102,114	3.30	27 (44%)
4	0UR	B	301	-	50,53,58	0.96	1 (2%)	58,72,77	1.80	13 (22%)
7	CHL	B	313	-	66,74,74	1.99	16 (24%)	73,114,114	3.01	27 (36%)
5	0IE	C	303	-	42,45,45	1.46	6 (14%)	49,63,63	1.64	9 (18%)
7	CHL	B	309	2	43,51,74	2.37	15 (34%)	45,86,114	3.69	24 (53%)
8	CLA	C	316	3	45,53,73	1.78	7 (15%)	52,89,113	1.60	6 (11%)
8	CLA	C	317	-	55,63,73	1.61	6 (10%)	63,100,113	1.48	8 (12%)
9	LHG	C	319	-	42,42,48	0.66	1 (2%)	45,48,54	1.27	5 (11%)
7	CHL	C	305	3	66,74,74	1.98	15 (22%)	73,114,114	3.02	27 (36%)
8	CLA	B	316	2	45,53,73	1.77	6 (13%)	52,89,113	1.59	6 (11%)
8	CLA	B	317	-	55,63,73	1.61	6 (10%)	63,100,113	1.47	7 (11%)
7	CHL	B	306	2	64,72,74	2.01	14 (21%)	70,111,114	3.10	27 (38%)
7	CHL	A	312	-	66,74,74	1.99	16 (24%)	73,114,114	3.00	27 (36%)
4	0UR	C	301	-	50,53,58	0.97	1 (2%)	58,72,77	1.75	14 (24%)
8	CLA	A	316	-	55,63,73	1.59	6 (10%)	63,100,113	1.51	8 (12%)
6	NEX	B	304	-	38,46,46	0.97	2 (5%)	50,70,70	1.20	6 (12%)
7	CHL	A	304	1	57,65,74	2.13	16 (28%)	62,103,114	3.25	27 (43%)
8	CLA	A	314	-	63,71,73	1.52	5 (7%)	73,110,113	1.38	6 (8%)
7	CHL	C	313	-	66,74,74	2.01	16 (24%)	73,114,114	2.98	27 (36%)
6	NEX	A	303	-	38,46,46	0.90	1 (2%)	50,70,70	1.17	5 (10%)
5	0IE	B	303	-	42,45,45	1.47	6 (14%)	49,63,63	1.69	9 (18%)
8	CLA	B	315	-	63,71,73	1.52	6 (9%)	73,110,113	1.38	6 (8%)
7	CHL	B	312	-	66,74,74	1.97	16 (24%)	73,114,114	3.02	27 (36%)
7	CHL	A	310	-	61,69,74	2.07	16 (26%)	66,107,114	3.15	26 (39%)
7	CHL	A	309	-	51,59,74	2.25	15 (29%)	55,96,114	3.45	27 (49%)
7	CHL	C	311	-	47,55,74	2.35	16 (34%)	50,91,114	3.52	25 (50%)
7	CHL	C	310	-	51,59,74	2.26	16 (31%)	55,96,114	3.46	27 (49%)
8	CLA	C	308	-	50,58,73	1.69	5 (10%)	58,95,113	1.56	8 (13%)
7	CHL	A	311	-	66,74,74	1.97	16 (24%)	73,114,114	3.03	27 (36%)
7	CHL	B	318	-	42,50,74	2.49	16 (38%)	44,85,114	3.77	25 (56%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	CHL	C	306	-	64,72,74	2.01	16 (25%)	70,111,114	3.08	27 (38%)
8	CLA	A	313	-	55,63,73	1.60	6 (10%)	64,101,113	1.46	8 (12%)
7	CHL	A	308	1	43,51,74	2.36	15 (34%)	45,86,114	3.71	24 (53%)
7	CHL	B	310	-	51,59,74	2.27	16 (31%)	55,96,114	3.45	28 (50%)
8	CLA	A	315	1	45,53,73	1.79	7 (15%)	52,89,113	1.58	6 (11%)
8	CLA	B	308	-	50,58,73	1.70	5 (10%)	58,95,113	1.59	8 (13%)
8	CLA	B	314	2	55,63,73	1.60	6 (10%)	64,101,113	1.47	8 (12%)
9	LHG	B	319	-	43,43,48	0.65	1 (2%)	46,49,54	1.27	5 (10%)
4	0UR	A	301	-	50,53,58	0.96	1 (2%)	58,72,77	1.73	13 (22%)
7	CHL	B	311	-	47,55,74	2.34	15 (31%)	50,91,114	3.53	24 (48%)
7	CHL	A	305	-	64,72,74	2.01	15 (23%)	70,111,114	3.09	27 (38%)
7	CHL	A	317	-	42,50,74	2.48	16 (38%)	44,85,114	3.77	25 (56%)
7	CHL	C	309	3	43,51,74	2.39	15 (34%)	45,86,114	3.68	24 (53%)
8	CLA	C	314	-	55,63,73	1.60	6 (10%)	64,101,113	1.46	8 (12%)
8	CLA	C	315	-	63,71,73	1.51	5 (7%)	73,110,113	1.41	7 (9%)
8	CLA	A	307	-	50,58,73	1.69	6 (12%)	58,95,113	1.58	9 (15%)
9	LHG	A	318	-	41,41,48	0.65	1 (2%)	44,47,54	1.24	3 (6%)
7	CHL	C	318	-	42,50,74	2.49	16 (38%)	44,85,114	3.77	25 (56%)
8	CLA	C	307	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	6 (7%)
5	0IE	A	302	-	42,45,45	1.44	6 (14%)	49,63,63	1.75	9 (18%)

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
8	CLA	B	307	-	1/1/15/20	8/37/115/115	-
7	CHL	B	305	2	3/3/20/26	12/39/137/137	-
6	NEX	C	304	-	-	2/27/83/83	0/3/3/3
5	0IE	C	302	-	-	9/33/72/72	0/2/2/2
8	CLA	A	306	-	1/1/15/20	4/37/115/115	-
7	CHL	C	312	-	3/3/18/26	10/27/125/137	-
5	0IE	B	302	-	-	9/33/72/72	0/2/2/2
4	0UR	B	301	-	-	9/42/81/86	0/2/2/2
7	CHL	B	313	-	3/3/20/26	16/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLA	C	317	-	1/1/12/20	8/25/103/115	-
7	CHL	B	309	2	3/3/15/26	2/12/110/137	-
8	CLA	C	316	3	1/1/11/20	6/13/91/115	-
5	0IE	C	303	-	-	11/33/72/72	0/2/2/2
9	LHG	C	319	-	-	17/47/47/53	-
7	CHL	C	305	3	3/3/20/26	17/39/137/137	-
8	CLA	B	316	2	1/1/11/20	3/13/91/115	-
8	CLA	B	317	-	1/1/12/20	8/25/103/115	-
7	CHL	B	306	2	3/3/19/26	19/37/135/137	-
7	CHL	A	312	-	3/3/20/26	18/39/137/137	-
4	0UR	C	301	-	-	8/42/81/86	0/2/2/2
8	CLA	A	316	-	1/1/12/20	9/25/103/115	-
7	CHL	A	304	1	3/3/18/26	7/29/127/137	-
8	CLA	A	314	-	1/1/14/20	6/35/113/115	-
6	NEX	B	304	-	-	2/27/83/83	0/3/3/3
7	CHL	C	313	-	3/3/20/26	16/39/137/137	-
6	NEX	A	303	-	-	3/27/83/83	0/3/3/3
8	CLA	B	315	-	1/1/14/20	6/35/113/115	-
5	0IE	B	303	-	-	5/33/72/72	0/2/2/2
7	CHL	B	312	-	3/3/20/26	16/39/137/137	-
7	CHL	A	310	-	3/3/18/26	18/33/131/137	-
7	CHL	A	309	-	3/3/17/26	8/21/119/137	-
7	CHL	C	311	-	3/3/16/26	7/17/115/137	-
7	CHL	C	310	-	3/3/17/26	2/21/119/137	-
8	CLA	C	308	-	1/1/12/20	7/19/97/115	-
7	CHL	A	311	-	3/3/20/26	14/39/137/137	-
7	CHL	C	306	-	3/3/19/26	19/37/135/137	-
7	CHL	B	318	-	3/3/15/26	6/10/108/137	-
8	CLA	A	313	-	1/1/13/20	5/25/103/115	-
7	CHL	A	308	1	3/3/15/26	2/12/110/137	-
7	CHL	B	310	-	3/3/17/26	9/21/119/137	-
8	CLA	A	315	1	1/1/11/20	6/13/91/115	-
8	CLA	B	308	-	1/1/12/20	9/19/97/115	-
8	CLA	B	314	2	1/1/13/20	5/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	LHG	B	319	-	-	12/48/48/53	-
8	CLA	C	314	-	1/1/13/20	3/25/103/115	-
7	CHL	B	311	-	3/3/16/26	5/17/115/137	-
7	CHL	A	305	-	3/3/19/26	23/37/135/137	-
7	CHL	A	317	-	3/3/15/26	6/10/108/137	-
7	CHL	C	309	3	3/3/15/26	2/12/110/137	-
8	CLA	C	315	-	1/1/14/20	6/35/113/115	-
4	0UR	A	301	-	-	9/42/81/86	0/2/2/2
8	CLA	A	307	-	1/1/12/20	7/19/97/115	-
9	LHG	A	318	-	-	28/46/46/53	-
7	CHL	C	318	-	3/3/15/26	6/10/108/137	-
8	CLA	C	307	-	1/1/15/20	6/37/115/115	-
5	0IE	A	302	-	-	10/33/72/72	0/2/2/2

All (519) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	314	CLA	C4B-NB	7.61	1.42	1.35
8	B	308	CLA	C4B-NB	7.50	1.41	1.35
8	A	315	CLA	C4B-NB	7.48	1.41	1.35
8	B	315	CLA	C4B-NB	7.46	1.41	1.35
8	B	307	CLA	C4B-NB	7.46	1.41	1.35
8	C	308	CLA	C4B-NB	7.43	1.41	1.35
8	A	307	CLA	C4B-NB	7.35	1.41	1.35
8	C	316	CLA	C4B-NB	7.34	1.41	1.35
8	B	316	CLA	C4B-NB	7.33	1.41	1.35
8	C	317	CLA	C4B-NB	7.33	1.41	1.35
8	C	315	CLA	C4B-NB	7.33	1.41	1.35
8	B	317	CLA	C4B-NB	7.30	1.41	1.35
8	C	307	CLA	C4B-NB	7.28	1.41	1.35
8	B	314	CLA	C4B-NB	7.26	1.41	1.35
8	C	314	CLA	C4B-NB	7.25	1.41	1.35
8	A	313	CLA	C4B-NB	7.23	1.41	1.35
8	A	316	CLA	C4B-NB	7.23	1.41	1.35
8	A	306	CLA	C4B-NB	7.23	1.41	1.35
7	C	309	CHL	C3B-C2B	5.59	1.48	1.40
7	A	310	CHL	C3B-C2B	5.48	1.48	1.40
7	B	309	CHL	C3B-C2B	5.48	1.48	1.40
7	B	311	CHL	C3B-C2B	5.48	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	311	CHL	C3B-C2B	5.48	1.48	1.40
7	C	313	CHL	C3B-C2B	5.47	1.48	1.40
7	B	310	CHL	C3B-C2B	5.46	1.48	1.40
7	C	318	CHL	C3B-C2B	5.46	1.47	1.40
7	A	305	CHL	C3B-C2B	5.46	1.47	1.40
7	B	318	CHL	C3B-C2B	5.42	1.47	1.40
7	C	310	CHL	C3B-C2B	5.41	1.47	1.40
7	A	317	CHL	C3B-C2B	5.41	1.47	1.40
7	B	306	CHL	C3B-C2B	5.40	1.47	1.40
7	A	308	CHL	C3B-C2B	5.39	1.47	1.40
7	A	312	CHL	C3B-C2B	5.37	1.47	1.40
7	A	311	CHL	C3B-C2B	5.36	1.47	1.40
7	B	313	CHL	C3B-C2B	5.36	1.47	1.40
7	A	309	CHL	C3B-C2B	5.36	1.47	1.40
7	C	305	CHL	C3B-C2B	5.35	1.47	1.40
7	B	305	CHL	C3B-C2B	5.34	1.47	1.40
7	C	306	CHL	C3B-C2B	5.34	1.47	1.40
7	A	304	CHL	C3B-C2B	5.33	1.47	1.40
7	B	312	CHL	C3B-C2B	5.28	1.47	1.40
7	C	312	CHL	C3B-C2B	5.28	1.47	1.40
7	C	310	CHL	O2D-CGD	5.18	1.45	1.33
7	B	310	CHL	O2D-CGD	5.16	1.45	1.33
7	C	309	CHL	O2D-CGD	5.16	1.45	1.33
7	B	309	CHL	O2D-CGD	5.16	1.45	1.33
7	A	308	CHL	O2D-CGD	5.15	1.45	1.33
7	B	306	CHL	O2D-CGD	5.15	1.45	1.33
7	B	313	CHL	O2D-CGD	5.15	1.45	1.33
7	A	309	CHL	O2D-CGD	5.15	1.45	1.33
7	C	313	CHL	C2C-C3C	5.15	1.47	1.36
7	B	305	CHL	O2D-CGD	5.14	1.45	1.33
7	B	311	CHL	O2D-CGD	5.14	1.45	1.33
7	C	313	CHL	O2D-CGD	5.14	1.45	1.33
7	A	312	CHL	C2C-C3C	5.14	1.47	1.36
7	C	306	CHL	O2D-CGD	5.13	1.45	1.33
7	C	311	CHL	O2D-CGD	5.13	1.45	1.33
7	C	309	CHL	C2C-C3C	5.13	1.47	1.36
7	A	317	CHL	O2D-CGD	5.13	1.45	1.33
7	A	305	CHL	O2D-CGD	5.12	1.45	1.33
7	A	310	CHL	O2D-CGD	5.12	1.45	1.33
7	B	313	CHL	C2C-C3C	5.12	1.47	1.36
7	C	305	CHL	O2D-CGD	5.12	1.45	1.33
7	A	304	CHL	O2D-CGD	5.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	318	CHL	O2D-CGD	5.11	1.45	1.33
7	C	312	CHL	O2D-CGD	5.10	1.45	1.33
7	B	312	CHL	O2D-CGD	5.10	1.45	1.33
7	A	312	CHL	O2D-CGD	5.10	1.45	1.33
7	A	311	CHL	O2D-CGD	5.09	1.45	1.33
7	B	318	CHL	O2D-CGD	5.09	1.45	1.33
7	B	318	CHL	C2C-C3C	5.06	1.47	1.36
7	C	305	CHL	C2C-C3C	5.06	1.47	1.36
7	A	304	CHL	C2C-C3C	5.06	1.47	1.36
7	A	317	CHL	C2C-C3C	5.05	1.47	1.36
7	B	318	CHL	C3A-C2A	-5.05	1.49	1.54
7	B	311	CHL	C2C-C3C	5.05	1.47	1.36
7	C	311	CHL	C2C-C3C	5.05	1.47	1.36
7	A	308	CHL	C2C-C3C	5.04	1.47	1.36
7	B	309	CHL	C2C-C3C	5.04	1.47	1.36
7	B	312	CHL	C2C-C3C	5.03	1.47	1.36
7	A	310	CHL	C2C-C3C	5.03	1.47	1.36
7	C	318	CHL	C2C-C3C	5.02	1.47	1.36
7	A	311	CHL	C2C-C3C	5.01	1.47	1.36
7	B	306	CHL	C2C-C3C	5.01	1.47	1.36
7	C	318	CHL	C3A-C2A	-5.00	1.49	1.54
7	B	306	CHL	CHC-C1C	5.00	1.47	1.35
7	C	309	CHL	CHC-C1C	5.00	1.47	1.35
7	B	305	CHL	C2C-C3C	4.99	1.47	1.36
7	B	310	CHL	C2C-C3C	4.99	1.47	1.36
7	C	310	CHL	C2C-C3C	4.98	1.47	1.36
7	C	312	CHL	C2C-C3C	4.98	1.47	1.36
7	A	305	CHL	CHC-C1C	4.98	1.47	1.35
7	A	305	CHL	C2C-C3C	4.97	1.47	1.36
7	C	306	CHL	C2C-C3C	4.97	1.47	1.36
7	C	310	CHL	CHC-C1C	4.97	1.47	1.35
7	A	317	CHL	C3A-C2A	-4.96	1.49	1.54
7	A	317	CHL	CHC-C1C	4.96	1.47	1.35
7	C	306	CHL	CHC-C1C	4.95	1.47	1.35
7	A	309	CHL	C2C-C3C	4.94	1.47	1.36
7	B	318	CHL	CHC-C1C	4.94	1.47	1.35
7	C	313	CHL	CHC-C1C	4.93	1.47	1.35
7	A	309	CHL	CHC-C1C	4.93	1.47	1.35
7	B	310	CHL	CHC-C1C	4.93	1.47	1.35
7	A	310	CHL	CHC-C1C	4.92	1.47	1.35
7	C	311	CHL	CHC-C1C	4.92	1.47	1.35
7	B	311	CHL	CHC-C1C	4.91	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	312	CHL	CHC-C1C	4.91	1.47	1.35
7	A	308	CHL	CHC-C1C	4.90	1.47	1.35
7	C	318	CHL	CHC-C1C	4.90	1.47	1.35
7	B	309	CHL	CHC-C1C	4.89	1.47	1.35
7	A	311	CHL	CHC-C1C	4.88	1.47	1.35
7	C	305	CHL	CHC-C1C	4.87	1.47	1.35
7	B	313	CHL	CHC-C1C	4.87	1.47	1.35
7	A	312	CHL	CHC-C1C	4.87	1.47	1.35
7	A	304	CHL	CHC-C1C	4.86	1.47	1.35
7	B	305	CHL	CHC-C1C	4.85	1.47	1.35
7	C	312	CHL	CHC-C1C	4.84	1.47	1.35
7	C	313	CHL	CHD-C1D	4.51	1.47	1.38
7	A	312	CHL	CHD-C1D	4.46	1.47	1.38
7	B	313	CHL	CHD-C1D	4.42	1.47	1.38
7	C	309	CHL	CHD-C1D	4.42	1.47	1.38
7	B	309	CHL	CHD-C1D	4.40	1.46	1.38
7	A	304	CHL	CHD-C1D	4.37	1.46	1.38
7	C	311	CHL	CHD-C1D	4.35	1.46	1.38
7	A	310	CHL	CHD-C1D	4.35	1.46	1.38
7	C	318	CHL	CHD-C1D	4.33	1.46	1.38
7	A	310	CHL	O2A-CGA	4.32	1.46	1.33
7	C	313	CHL	O2A-CGA	4.32	1.46	1.33
7	A	317	CHL	CHD-C1D	4.32	1.46	1.38
7	B	318	CHL	CHD-C1D	4.32	1.46	1.38
7	C	305	CHL	CHD-C1D	4.31	1.46	1.38
7	A	308	CHL	CHD-C1D	4.31	1.46	1.38
7	A	304	CHL	O2A-CGA	4.31	1.45	1.33
7	B	306	CHL	CHD-C1D	4.31	1.46	1.38
7	B	312	CHL	CHD-C1D	4.31	1.46	1.38
7	C	306	CHL	C1D-ND	-4.30	1.32	1.37
7	B	310	CHL	O2A-CGA	4.30	1.45	1.33
7	A	312	CHL	O2A-CGA	4.30	1.45	1.33
7	C	310	CHL	CHD-C1D	4.30	1.46	1.38
7	B	305	CHL	CHD-C1D	4.30	1.46	1.38
7	A	305	CHL	C1D-ND	-4.29	1.32	1.37
7	C	306	CHL	CHD-C1D	4.29	1.46	1.38
7	B	310	CHL	C1D-ND	-4.29	1.32	1.37
7	B	305	CHL	O2A-CGA	4.29	1.45	1.33
5	B	302	0IE	C8-C7	4.29	1.41	1.35
7	B	306	CHL	C1D-ND	-4.28	1.32	1.37
7	B	310	CHL	CHD-C1D	4.28	1.46	1.38
7	A	311	CHL	CHD-C1D	4.28	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	311	CHL	CHD-C1D	4.28	1.46	1.38
7	B	313	CHL	O2A-CGA	4.28	1.45	1.33
7	A	309	CHL	CHD-C1D	4.27	1.46	1.38
7	C	305	CHL	O2A-CGA	4.27	1.45	1.33
7	A	305	CHL	CHD-C1D	4.27	1.46	1.38
7	B	312	CHL	O2A-CGA	4.26	1.45	1.33
7	A	309	CHL	O2A-CGA	4.26	1.45	1.33
7	C	312	CHL	O2A-CGA	4.26	1.45	1.33
7	A	311	CHL	O2A-CGA	4.25	1.45	1.33
7	C	310	CHL	O2A-CGA	4.25	1.45	1.33
7	A	310	CHL	C1D-ND	-4.24	1.32	1.37
7	C	312	CHL	CHD-C1D	4.24	1.46	1.38
7	A	309	CHL	C1D-ND	-4.24	1.32	1.37
5	B	303	0IE	C15-C16	4.23	1.41	1.35
7	A	305	CHL	O2A-CGA	4.23	1.45	1.33
7	C	311	CHL	C1D-ND	-4.20	1.32	1.37
7	C	318	CHL	C1D-ND	-4.20	1.32	1.37
7	A	308	CHL	C1D-ND	-4.19	1.32	1.37
5	B	302	0IE	C11-C12	4.19	1.41	1.35
7	C	310	CHL	C1D-ND	-4.19	1.32	1.37
7	B	306	CHL	O2A-CGA	4.19	1.45	1.33
5	C	303	0IE	C8-C7	4.19	1.41	1.35
7	C	306	CHL	O2A-CGA	4.19	1.45	1.33
7	B	305	CHL	C1D-ND	-4.17	1.32	1.37
7	C	313	CHL	C1D-ND	-4.16	1.32	1.37
5	B	303	0IE	C8-C7	4.16	1.41	1.35
7	B	309	CHL	C1D-ND	-4.15	1.32	1.37
7	B	311	CHL	C1D-ND	-4.15	1.32	1.37
7	C	309	CHL	C1D-ND	-4.15	1.32	1.37
7	B	313	CHL	C1D-ND	-4.15	1.32	1.37
7	B	318	CHL	C1D-ND	-4.15	1.32	1.37
7	C	312	CHL	C1D-ND	-4.14	1.32	1.37
7	A	311	CHL	C1D-ND	-4.14	1.32	1.37
5	C	303	0IE	C11-C12	4.13	1.41	1.35
7	A	312	CHL	C1D-ND	-4.11	1.32	1.37
7	A	304	CHL	C1D-ND	-4.11	1.32	1.37
5	B	303	0IE	C11-C12	4.10	1.41	1.35
5	A	302	0IE	C15-C16	4.10	1.41	1.35
7	B	312	CHL	C1D-ND	-4.09	1.32	1.37
6	B	304	NEX	C7-C8	4.09	1.38	1.32
4	A	301	0UR	O44-C45	4.09	1.44	1.34
7	A	317	CHL	C1D-ND	-4.07	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	305	CHL	C1D-ND	-4.07	1.32	1.37
5	C	302	0IE	C8-C7	4.06	1.41	1.35
5	C	302	0IE	C15-C16	4.06	1.41	1.35
4	C	301	0UR	O44-C45	4.05	1.44	1.34
5	A	302	0IE	C11-C12	4.05	1.41	1.35
5	C	303	0IE	C15-C16	4.04	1.41	1.35
5	A	302	0IE	C8-C7	4.04	1.41	1.35
5	B	302	0IE	C15-C16	4.04	1.41	1.35
7	C	311	CHL	O2A-CGA	4.03	1.45	1.33
7	B	311	CHL	O2A-CGA	4.02	1.45	1.33
7	A	312	CHL	CHD-C4C	4.01	1.48	1.39
4	B	301	0UR	O44-C45	4.00	1.44	1.34
6	C	304	NEX	C7-C8	3.99	1.38	1.32
7	C	313	CHL	CHD-C4C	3.97	1.48	1.39
7	B	313	CHL	CHD-C4C	3.97	1.48	1.39
7	A	304	CHL	CHD-C4C	3.96	1.48	1.39
5	C	302	0IE	C11-C12	3.95	1.41	1.35
7	C	309	CHL	CHD-C4C	3.92	1.48	1.39
7	A	317	CHL	CHD-C4C	3.91	1.48	1.39
7	B	311	CHL	CHD-C4C	3.91	1.48	1.39
8	B	317	CLA	C1D-ND	3.91	1.42	1.37
7	B	309	CHL	CHD-C4C	3.90	1.48	1.39
8	C	315	CLA	C1D-ND	3.89	1.42	1.37
7	C	311	CHL	CHD-C4C	3.89	1.48	1.39
7	B	312	CHL	CHD-C4C	3.89	1.48	1.39
7	C	318	CHL	CHD-C4C	3.88	1.48	1.39
7	B	310	CHL	CHD-C4C	3.88	1.48	1.39
7	B	305	CHL	CHD-C4C	3.88	1.48	1.39
8	C	316	CLA	C1D-ND	3.88	1.42	1.37
7	B	318	CHL	CHD-C4C	3.87	1.48	1.39
7	A	308	CHL	CHD-C4C	3.87	1.48	1.39
7	C	306	CHL	CHD-C4C	3.87	1.48	1.39
8	C	317	CLA	C1D-ND	3.86	1.42	1.37
8	A	316	CLA	C1D-ND	3.86	1.42	1.37
7	A	309	CHL	CHD-C4C	3.86	1.48	1.39
7	A	311	CHL	CHD-C4C	3.86	1.48	1.39
7	C	310	CHL	CHD-C4C	3.86	1.48	1.39
8	A	306	CLA	C1D-ND	3.86	1.42	1.37
7	C	305	CHL	CHD-C4C	3.86	1.48	1.39
7	B	306	CHL	CHD-C4C	3.86	1.48	1.39
7	A	310	CHL	CHD-C4C	3.85	1.48	1.39
7	A	305	CHL	CHD-C4C	3.84	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	314	CLA	C1D-ND	3.84	1.42	1.37
8	A	307	CLA	C1D-ND	3.83	1.42	1.37
8	B	315	CLA	C1D-ND	3.82	1.42	1.37
8	B	314	CLA	C1D-ND	3.81	1.42	1.37
8	A	314	CLA	C1D-ND	3.81	1.42	1.37
7	C	312	CHL	CHD-C4C	3.80	1.47	1.39
8	A	313	CLA	C1D-ND	3.80	1.42	1.37
8	C	308	CLA	C1D-ND	3.79	1.42	1.37
8	B	308	CLA	C1D-ND	3.77	1.42	1.37
8	C	307	CLA	C1D-ND	3.76	1.42	1.37
8	B	307	CLA	C1D-ND	3.76	1.42	1.37
8	B	316	CLA	C1D-ND	3.75	1.42	1.37
8	A	315	CLA	C1D-ND	3.74	1.42	1.37
7	A	317	CHL	OBD-CAD	3.74	1.28	1.22
7	A	310	CHL	OBD-CAD	3.73	1.28	1.22
7	A	308	CHL	OBD-CAD	3.73	1.28	1.22
7	B	318	CHL	OBD-CAD	3.72	1.28	1.22
7	C	309	CHL	OBD-CAD	3.72	1.28	1.22
7	C	305	CHL	OBD-CAD	3.72	1.28	1.22
7	C	318	CHL	OBD-CAD	3.71	1.28	1.22
7	C	310	CHL	OBD-CAD	3.70	1.28	1.22
7	B	311	CHL	OBD-CAD	3.69	1.28	1.22
7	B	309	CHL	OBD-CAD	3.68	1.28	1.22
7	C	311	CHL	OBD-CAD	3.68	1.28	1.22
7	A	304	CHL	OBD-CAD	3.67	1.28	1.22
7	B	310	CHL	OBD-CAD	3.67	1.28	1.22
7	B	305	CHL	OBD-CAD	3.65	1.28	1.22
7	A	309	CHL	OBD-CAD	3.64	1.28	1.22
7	A	311	CHL	OBD-CAD	3.62	1.28	1.22
7	B	313	CHL	OBD-CAD	3.61	1.28	1.22
7	B	312	CHL	OBD-CAD	3.61	1.28	1.22
7	C	312	CHL	OBD-CAD	3.57	1.28	1.22
7	A	312	CHL	OBD-CAD	3.56	1.28	1.22
7	C	313	CHL	OBD-CAD	3.55	1.28	1.22
7	A	305	CHL	OBD-CAD	3.53	1.28	1.22
7	B	306	CHL	OBD-CAD	3.53	1.28	1.22
7	C	313	CHL	C3D-C2D	3.53	1.48	1.39
7	C	306	CHL	OBD-CAD	3.51	1.28	1.22
6	A	303	NEX	C7-C8	3.49	1.37	1.32
7	C	309	CHL	C3D-C2D	3.48	1.48	1.39
7	C	311	CHL	C3D-C2D	3.46	1.48	1.39
7	C	306	CHL	C3D-C2D	3.45	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	318	CHL	C3D-C2D	3.45	1.48	1.39
7	A	310	CHL	C3D-C2D	3.45	1.48	1.39
7	A	312	CHL	C3D-C2D	3.45	1.48	1.39
7	B	313	CHL	C3D-C2D	3.44	1.48	1.39
7	B	309	CHL	C3D-C2D	3.44	1.48	1.39
7	A	308	CHL	C3D-C2D	3.43	1.48	1.39
7	C	305	CHL	C3D-C2D	3.43	1.48	1.39
7	B	311	CHL	C3D-C2D	3.43	1.48	1.39
7	A	305	CHL	C3D-C2D	3.43	1.48	1.39
7	C	318	CHL	C3D-C2D	3.42	1.48	1.39
7	B	306	CHL	C3D-C2D	3.42	1.48	1.39
7	A	317	CHL	C3D-C2D	3.42	1.48	1.39
7	B	305	CHL	C3D-C2D	3.41	1.48	1.39
7	A	309	CHL	C3D-C2D	3.39	1.48	1.39
7	A	304	CHL	C3D-C2D	3.39	1.48	1.39
7	B	310	CHL	C3D-C2D	3.39	1.48	1.39
7	C	312	CHL	C3D-C2D	3.37	1.48	1.39
7	A	311	CHL	C3D-C2D	3.37	1.48	1.39
7	C	310	CHL	C3D-C2D	3.35	1.48	1.39
7	B	312	CHL	C3D-C2D	3.33	1.48	1.39
8	C	314	CLA	CHC-C1C	3.17	1.43	1.35
8	B	314	CLA	CHC-C1C	3.17	1.43	1.35
8	A	313	CLA	CHC-C1C	3.16	1.43	1.35
8	B	315	CLA	CHC-C1C	3.16	1.43	1.35
8	B	308	CLA	CHC-C1C	3.15	1.43	1.35
8	A	307	CLA	CHC-C1C	3.14	1.43	1.35
8	C	315	CLA	CHC-C1C	3.14	1.43	1.35
8	A	315	CLA	CHC-C1C	3.13	1.43	1.35
8	A	314	CLA	CHC-C1C	3.13	1.43	1.35
8	C	308	CLA	CHC-C1C	3.13	1.43	1.35
8	A	316	CLA	CHC-C1C	3.13	1.43	1.35
8	C	317	CLA	CHC-C1C	3.12	1.43	1.35
8	B	316	CLA	CHC-C1C	3.12	1.43	1.35
8	B	317	CLA	CHC-C1C	3.11	1.42	1.35
8	C	316	CLA	CHC-C1C	3.11	1.42	1.35
8	C	307	CLA	CHC-C1C	3.10	1.42	1.35
8	B	307	CLA	CHC-C1C	3.08	1.42	1.35
8	A	307	CLA	C4D-ND	-2.99	1.33	1.37
8	A	306	CLA	CHC-C1C	2.98	1.42	1.35
8	A	313	CLA	C4D-ND	-2.95	1.33	1.37
8	C	316	CLA	C4D-ND	-2.94	1.33	1.37
8	C	308	CLA	C4D-ND	-2.93	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	308	CLA	C4D-ND	-2.93	1.33	1.37
8	A	306	CLA	C4D-ND	-2.93	1.33	1.37
8	C	315	CLA	C4D-ND	-2.92	1.33	1.37
8	B	314	CLA	C4D-ND	-2.91	1.33	1.37
8	A	316	CLA	C4D-ND	-2.90	1.33	1.37
8	B	316	CLA	C4D-ND	-2.90	1.33	1.37
8	A	315	CLA	C4D-ND	-2.90	1.33	1.37
8	C	314	CLA	C4D-ND	-2.88	1.33	1.37
8	B	317	CLA	C4D-ND	-2.88	1.33	1.37
8	C	317	CLA	C4D-ND	-2.87	1.33	1.37
8	C	307	CLA	C4D-ND	-2.87	1.33	1.37
8	B	307	CLA	C4D-ND	-2.86	1.33	1.37
8	B	315	CLA	C4D-ND	-2.86	1.33	1.37
8	A	314	CLA	C4D-ND	-2.85	1.33	1.37
7	B	309	CHL	MG-NA	-2.79	1.99	2.06
7	C	309	CHL	MG-NA	-2.77	1.99	2.06
7	B	311	CHL	MG-NA	-2.75	1.99	2.06
7	C	311	CHL	MG-NA	-2.74	1.99	2.06
7	A	310	CHL	MG-NA	-2.73	1.99	2.06
7	C	313	CHL	MG-NA	-2.72	1.99	2.06
7	C	318	CHL	MG-NA	-2.69	1.99	2.06
7	A	304	CHL	MG-NA	-2.69	1.99	2.06
7	A	312	CHL	MG-NA	-2.68	1.99	2.06
7	B	312	CHL	MG-NA	-2.68	1.99	2.06
7	A	308	CHL	MG-NA	-2.66	2.00	2.06
7	B	318	CHL	MG-NA	-2.66	2.00	2.06
7	A	305	CHL	MG-NA	-2.66	2.00	2.06
7	C	306	CHL	MG-NA	-2.66	2.00	2.06
7	B	306	CHL	MG-NA	-2.65	2.00	2.06
7	B	310	CHL	MG-NA	-2.65	2.00	2.06
7	C	305	CHL	MG-NA	-2.63	2.00	2.06
7	B	313	CHL	MG-NA	-2.63	2.00	2.06
7	A	311	CHL	MG-NA	-2.63	2.00	2.06
7	A	309	CHL	MG-NA	-2.63	2.00	2.06
7	B	305	CHL	MG-NA	-2.62	2.00	2.06
7	C	309	CHL	C4D-CHA	2.61	1.47	1.38
7	A	317	CHL	MG-NA	-2.61	2.00	2.06
7	C	310	CHL	MG-NA	-2.60	2.00	2.06
7	C	312	CHL	C4D-CHA	2.59	1.47	1.38
7	A	311	CHL	C4D-CHA	2.59	1.47	1.38
7	C	312	CHL	MG-NA	-2.58	2.00	2.06
7	B	309	CHL	C4D-CHA	2.58	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	304	CHL	C4D-CHA	2.58	1.47	1.38
7	A	317	CHL	C4D-CHA	2.57	1.47	1.38
7	B	318	CHL	C4D-CHA	2.57	1.47	1.38
7	C	318	CHL	C4D-CHA	2.57	1.47	1.38
8	A	306	CLA	CMB-C2B	-2.57	1.46	1.51
7	B	305	CHL	C4D-CHA	2.56	1.47	1.38
7	C	305	CHL	C4D-CHA	2.56	1.47	1.38
7	A	310	CHL	C4D-CHA	2.55	1.47	1.38
7	B	312	CHL	C4D-CHA	2.55	1.47	1.38
7	B	311	CHL	C4D-CHA	2.55	1.47	1.38
7	C	313	CHL	C4D-CHA	2.54	1.47	1.38
7	A	312	CHL	C4D-CHA	2.54	1.47	1.38
7	C	311	CHL	C4D-CHA	2.54	1.47	1.38
7	B	313	CHL	C4D-CHA	2.54	1.47	1.38
7	A	308	CHL	C4D-CHA	2.53	1.47	1.38
7	A	309	CHL	C4D-CHA	2.53	1.47	1.38
7	C	310	CHL	C4D-CHA	2.51	1.47	1.38
7	B	310	CHL	C4D-CHA	2.51	1.47	1.38
7	C	306	CHL	C4D-CHA	2.51	1.47	1.38
7	A	305	CHL	C4D-CHA	2.50	1.47	1.38
8	B	308	CLA	CMB-C2B	-2.50	1.46	1.51
7	B	306	CHL	C4D-CHA	2.49	1.47	1.38
8	A	307	CLA	CMB-C2B	-2.49	1.46	1.51
8	C	308	CLA	CMB-C2B	-2.46	1.46	1.51
8	A	315	CLA	CMB-C2B	-2.45	1.46	1.51
8	B	314	CLA	CMB-C2B	-2.45	1.46	1.51
8	B	307	CLA	CMB-C2B	-2.44	1.46	1.51
8	C	314	CLA	CMB-C2B	-2.44	1.46	1.51
8	A	313	CLA	CMB-C2B	-2.44	1.46	1.51
8	B	315	CLA	CMB-C2B	-2.43	1.46	1.51
8	B	316	CLA	CMB-C2B	-2.43	1.46	1.51
8	C	307	CLA	CMB-C2B	-2.43	1.46	1.51
8	A	314	CLA	CMB-C2B	-2.43	1.46	1.51
8	C	315	CLA	CMB-C2B	-2.42	1.46	1.51
8	B	317	CLA	CMB-C2B	-2.41	1.46	1.51
8	C	317	CLA	CMB-C2B	-2.39	1.46	1.51
8	C	316	CLA	CMB-C2B	-2.39	1.46	1.51
8	A	316	CLA	CMB-C2B	-2.37	1.46	1.51
7	C	310	CHL	C4B-CHC	2.32	1.47	1.41
7	A	305	CHL	C4B-CHC	2.32	1.47	1.41
7	B	306	CHL	C4B-CHC	2.32	1.47	1.41
5	C	303	0IE	C17-C16	-2.30	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	310	CHL	C4B-CHC	2.30	1.47	1.41
7	C	306	CHL	C4B-CHC	2.30	1.47	1.41
7	C	313	CHL	C4C-C3C	2.29	1.49	1.45
7	C	309	CHL	C4B-CHC	2.27	1.47	1.41
7	C	306	CHL	C2C-C1C	2.27	1.49	1.44
7	B	306	CHL	C2C-C1C	2.26	1.49	1.44
5	B	303	0IE	C6-C7	-2.26	1.41	1.45
5	C	303	0IE	C6-C7	-2.25	1.41	1.45
7	B	309	CHL	C4B-CHC	2.25	1.47	1.41
7	B	313	CHL	C4C-C3C	2.25	1.48	1.45
7	A	309	CHL	C4B-CHC	2.25	1.47	1.41
7	B	310	CHL	C2C-C1C	2.24	1.49	1.44
7	C	318	CHL	C4B-CHC	2.24	1.47	1.41
7	C	310	CHL	C2C-C1C	2.24	1.49	1.44
5	B	303	0IE	C17-C16	-2.24	1.41	1.45
7	A	309	CHL	C2C-C1C	2.24	1.49	1.44
7	A	305	CHL	C2C-C1C	2.24	1.49	1.44
7	A	308	CHL	C4B-CHC	2.24	1.47	1.41
7	A	312	CHL	C4C-C3C	2.24	1.48	1.45
5	B	302	0IE	C13-C12	-2.23	1.41	1.45
7	C	311	CHL	C4B-CHC	2.23	1.47	1.41
7	B	312	CHL	C4B-CHC	2.23	1.47	1.41
5	B	302	0IE	C17-C16	-2.23	1.41	1.45
7	B	311	CHL	C4B-CHC	2.23	1.47	1.41
7	A	311	CHL	C4B-CHC	2.22	1.47	1.41
7	A	317	CHL	C4B-CHC	2.22	1.47	1.41
7	B	318	CHL	C4B-CHC	2.22	1.47	1.41
7	A	310	CHL	C4B-CHC	2.22	1.47	1.41
7	A	304	CHL	C4B-CHC	2.21	1.47	1.41
7	C	305	CHL	C4B-CHC	2.21	1.47	1.41
7	C	309	CHL	C2C-C1C	2.20	1.49	1.44
7	B	305	CHL	C4B-CHC	2.20	1.47	1.41
7	A	317	CHL	C2C-C1C	2.19	1.49	1.44
9	C	319	LHG	O7-C5	-2.19	1.41	1.46
7	C	318	CHL	C2C-C1C	2.19	1.49	1.44
5	C	302	0IE	C17-C16	-2.19	1.41	1.45
7	B	318	CHL	C2C-C1C	2.18	1.49	1.44
5	C	302	0IE	C6-C7	-2.16	1.41	1.45
9	B	319	LHG	O7-C5	-2.16	1.41	1.46
5	C	302	0IE	C13-C12	-2.16	1.41	1.45
7	B	313	CHL	C4B-CHC	2.16	1.47	1.41
7	C	305	CHL	C4C-C3C	2.15	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	309	CHL	C1B-CHB	2.15	1.47	1.41
7	C	309	CHL	C4C-C3C	2.15	1.48	1.45
5	A	302	0IE	C17-C16	-2.15	1.41	1.45
7	A	308	CHL	C2C-C1C	2.15	1.49	1.44
7	C	313	CHL	C4B-CHC	2.14	1.47	1.41
7	A	312	CHL	C4B-CHC	2.14	1.47	1.41
5	C	303	0IE	C13-C12	-2.14	1.41	1.45
7	B	309	CHL	C2C-C1C	2.13	1.49	1.44
7	C	313	CHL	C1B-CHB	2.13	1.46	1.41
7	B	309	CHL	C1B-CHB	2.13	1.46	1.41
9	A	318	LHG	O7-C5	-2.13	1.41	1.46
7	C	311	CHL	C1B-CHB	2.13	1.46	1.41
7	B	312	CHL	C2C-C1C	2.12	1.49	1.44
7	C	312	CHL	C4B-CHC	2.11	1.46	1.41
7	C	305	CHL	C2C-C1C	2.10	1.49	1.44
7	C	311	CHL	C4C-C3C	2.10	1.48	1.45
7	B	318	CHL	C4C-C3C	2.10	1.48	1.45
7	B	305	CHL	C2C-C1C	2.09	1.49	1.44
7	A	317	CHL	C4C-C3C	2.09	1.48	1.45
7	A	310	CHL	C4C-C3C	2.09	1.48	1.45
7	C	310	CHL	C1B-CHB	2.08	1.46	1.41
7	B	318	CHL	C1B-CHB	2.08	1.46	1.41
7	B	311	CHL	C1B-CHB	2.08	1.46	1.41
5	A	302	0IE	C6-C7	-2.08	1.41	1.45
8	C	307	CLA	CMD-C2D	-2.07	1.46	1.50
7	B	309	CHL	C4C-C3C	2.07	1.48	1.45
7	A	304	CHL	C2C-C1C	2.07	1.49	1.44
7	C	318	CHL	C1B-CHB	2.07	1.46	1.41
5	B	303	0IE	C13-C12	-2.07	1.41	1.45
7	C	318	CHL	C4C-C3C	2.06	1.48	1.45
7	A	304	CHL	C4C-C3C	2.06	1.48	1.45
7	A	308	CHL	C4C-C3C	2.06	1.48	1.45
7	B	312	CHL	C4C-C3C	2.06	1.48	1.45
7	C	312	CHL	C1B-CHB	2.06	1.46	1.41
7	A	311	CHL	C2C-C1C	2.05	1.49	1.44
8	A	315	CLA	CMC-C2C	-2.05	1.46	1.50
7	B	312	CHL	C1B-CHB	2.05	1.46	1.41
7	A	310	CHL	C2C-C1C	2.05	1.49	1.44
6	C	304	NEX	C1-C6	2.05	1.58	1.54
5	A	302	0IE	C13-C12	-2.05	1.41	1.45
7	B	313	CHL	C2C-C1C	2.05	1.49	1.44
7	A	312	CHL	C1B-CHB	2.05	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	306	CLA	CMD-C2D	-2.05	1.46	1.50
7	C	312	CHL	C4C-C3C	2.04	1.48	1.45
7	A	311	CHL	C4C-C3C	2.04	1.48	1.45
7	A	308	CHL	C1B-CHB	2.04	1.46	1.41
7	C	306	CHL	C1B-CHB	2.04	1.46	1.41
7	C	313	CHL	C2C-C1C	2.04	1.48	1.44
7	B	310	CHL	C1B-CHB	2.04	1.46	1.41
8	B	307	CLA	CMD-C2D	-2.04	1.46	1.50
8	B	314	CLA	CMD-C2D	-2.04	1.46	1.50
7	A	311	CHL	C1B-CHB	2.04	1.46	1.41
7	A	305	CHL	C1B-CHB	2.04	1.46	1.41
7	C	311	CHL	C2C-C1C	2.04	1.48	1.44
7	B	310	CHL	C4C-C3C	2.04	1.48	1.45
7	B	305	CHL	C4C-C3C	2.03	1.48	1.45
8	A	315	CLA	CMD-C2D	-2.03	1.46	1.50
7	A	317	CHL	C1B-CHB	2.03	1.46	1.41
7	A	309	CHL	C1B-CHB	2.03	1.46	1.41
7	B	313	CHL	C1B-CHB	2.03	1.46	1.41
8	C	316	CLA	CMD-C2D	-2.03	1.46	1.50
7	C	310	CHL	C4C-C3C	2.03	1.48	1.45
8	C	316	CLA	CMC-C2C	-2.03	1.46	1.50
7	A	304	CHL	C1B-CHB	2.02	1.46	1.41
8	A	313	CLA	CMD-C2D	-2.02	1.46	1.50
7	A	312	CHL	C2C-C1C	2.02	1.48	1.44
6	B	304	NEX	C1-C6	2.02	1.57	1.54
8	C	314	CLA	CMD-C2D	-2.02	1.46	1.50
8	B	316	CLA	CMC-C2C	-2.01	1.46	1.50
7	A	310	CHL	C1B-CHB	2.01	1.46	1.41
8	B	317	CLA	CMD-C2D	-2.01	1.46	1.50
7	B	311	CHL	C2C-C1C	2.01	1.48	1.44
8	B	315	CLA	CMD-C2D	-2.01	1.46	1.50
8	C	317	CLA	CMD-C2D	-2.01	1.46	1.50
8	A	307	CLA	CMD-C2D	-2.01	1.46	1.50
7	C	306	CHL	C4C-C3C	2.01	1.48	1.45
8	A	316	CLA	CMD-C2D	-2.01	1.46	1.50

All (874) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	317	CHL	C4D-CHA-C1A	-9.58	109.59	121.25
7	C	310	CHL	C4D-CHA-C1A	-9.57	109.61	121.25
7	B	312	CHL	C4D-CHA-C1A	-9.56	109.61	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	318	CHL	C4D-CHA-C1A	-9.53	109.66	121.25
7	C	312	CHL	C4D-CHA-C1A	-9.51	109.67	121.25
7	C	318	CHL	C4D-CHA-C1A	-9.50	109.69	121.25
7	A	309	CHL	C4D-CHA-C1A	-9.49	109.70	121.25
7	A	311	CHL	C4D-CHA-C1A	-9.47	109.73	121.25
7	A	308	CHL	C4D-CHA-C1A	-9.46	109.73	121.25
7	B	310	CHL	C4D-CHA-C1A	-9.46	109.74	121.25
7	C	309	CHL	C4D-CHA-C1A	-9.46	109.74	121.25
7	B	305	CHL	C4D-CHA-C1A	-9.45	109.74	121.25
7	B	309	CHL	C4D-CHA-C1A	-9.45	109.75	121.25
7	B	311	CHL	C4D-CHA-C1A	-9.43	109.77	121.25
7	C	313	CHL	C4D-CHA-C1A	-9.43	109.78	121.25
7	C	311	CHL	C4D-CHA-C1A	-9.43	109.78	121.25
7	A	310	CHL	C4D-CHA-C1A	-9.42	109.78	121.25
7	A	312	CHL	C4D-CHA-C1A	-9.42	109.79	121.25
7	B	313	CHL	C4D-CHA-C1A	-9.41	109.80	121.25
7	A	304	CHL	C4D-CHA-C1A	-9.41	109.80	121.25
7	A	305	CHL	C4D-CHA-C1A	-9.40	109.80	121.25
7	B	306	CHL	C4D-CHA-C1A	-9.40	109.81	121.25
7	C	305	CHL	C4D-CHA-C1A	-9.40	109.81	121.25
7	C	306	CHL	C4D-CHA-C1A	-9.34	109.88	121.25
7	C	313	CHL	C1D-ND-C4D	9.22	112.89	106.33
7	C	312	CHL	C1D-ND-C4D	9.17	112.85	106.33
7	C	309	CHL	C1D-ND-C4D	9.14	112.83	106.33
7	B	311	CHL	C1D-ND-C4D	9.10	112.80	106.33
7	A	304	CHL	C1D-ND-C4D	9.09	112.80	106.33
7	C	311	CHL	C1D-ND-C4D	9.09	112.79	106.33
7	B	313	CHL	C1D-ND-C4D	9.08	112.79	106.33
7	A	312	CHL	C1D-ND-C4D	9.08	112.79	106.33
7	C	305	CHL	C1D-ND-C4D	9.07	112.78	106.33
7	A	311	CHL	C1D-ND-C4D	9.03	112.75	106.33
7	A	310	CHL	C1D-ND-C4D	9.03	112.75	106.33
7	C	318	CHL	C1D-ND-C4D	8.96	112.70	106.33
7	B	309	CHL	C1D-ND-C4D	8.96	112.70	106.33
7	B	310	CHL	C1D-ND-C4D	8.95	112.69	106.33
7	B	318	CHL	C1D-ND-C4D	8.93	112.68	106.33
7	A	308	CHL	C1D-ND-C4D	8.89	112.65	106.33
7	C	306	CHL	C1D-ND-C4D	8.89	112.65	106.33
7	B	305	CHL	C1D-ND-C4D	8.87	112.64	106.33
7	B	312	CHL	C1D-ND-C4D	8.87	112.63	106.33
7	A	317	CHL	C1D-ND-C4D	8.80	112.59	106.33
7	A	309	CHL	C1D-ND-C4D	8.80	112.58	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	306	CHL	C1D-ND-C4D	8.78	112.57	106.33
7	A	305	CHL	C1D-ND-C4D	8.76	112.56	106.33
7	C	310	CHL	C1D-ND-C4D	8.75	112.55	106.33
8	A	315	CLA	C4A-NA-C1A	6.74	109.73	106.71
7	C	309	CHL	C1B-CHB-C4A	-6.72	116.82	130.12
8	C	316	CLA	C4A-NA-C1A	6.71	109.72	106.71
8	A	306	CLA	C4A-NA-C1A	6.69	109.71	106.71
8	C	317	CLA	C4A-NA-C1A	6.68	109.71	106.71
8	B	316	CLA	C4A-NA-C1A	6.65	109.70	106.71
8	A	307	CLA	C4A-NA-C1A	6.58	109.66	106.71
8	C	315	CLA	C4A-NA-C1A	6.57	109.66	106.71
7	A	310	CHL	CHB-C4A-NA	6.56	133.58	124.51
8	C	308	CLA	C4A-NA-C1A	6.56	109.65	106.71
8	B	315	CLA	C4A-NA-C1A	6.55	109.65	106.71
8	A	316	CLA	C4A-NA-C1A	6.53	109.64	106.71
7	B	305	CHL	CHB-C4A-NA	6.53	133.54	124.51
7	C	305	CHL	CHB-C4A-NA	6.51	133.51	124.51
8	C	307	CLA	C4A-NA-C1A	6.51	109.63	106.71
8	B	317	CLA	C4A-NA-C1A	6.50	109.63	106.71
8	B	307	CLA	C4A-NA-C1A	6.49	109.62	106.71
8	A	314	CLA	C4A-NA-C1A	6.47	109.62	106.71
7	B	311	CHL	CHB-C4A-NA	6.47	133.45	124.51
7	B	309	CHL	C1B-CHB-C4A	-6.45	117.34	130.12
7	B	312	CHL	CMD-C2D-C1D	6.44	136.06	124.71
7	A	304	CHL	CMD-C2D-C1D	6.44	136.06	124.71
7	C	310	CHL	CMD-C2D-C1D	6.40	135.99	124.71
7	A	317	CHL	CHB-C4A-NA	6.38	133.33	124.51
7	A	312	CHL	CMD-C2D-C1D	6.36	135.93	124.71
7	B	312	CHL	CHB-C4A-NA	6.34	133.28	124.51
7	C	312	CHL	CHD-C1D-ND	6.34	130.28	124.45
7	C	312	CHL	CHB-C4A-NA	6.34	133.27	124.51
7	B	313	CHL	CMD-C2D-C1D	6.32	135.85	124.71
7	B	313	CHL	CHB-C4A-NA	6.31	133.24	124.51
7	B	306	CHL	CHB-C4A-NA	6.31	133.24	124.51
8	B	314	CLA	C4A-NA-C1A	6.30	109.54	106.71
7	A	311	CHL	CHB-C4A-NA	6.29	133.21	124.51
7	A	311	CHL	CMD-C2D-C1D	6.27	135.77	124.71
7	A	305	CHL	CHB-C4A-NA	6.26	133.17	124.51
7	A	309	CHL	CHB-C4A-NA	6.25	133.16	124.51
7	C	318	CHL	CMD-C2D-C1D	6.25	135.73	124.71
7	C	312	CHL	CMD-C2D-C1D	6.25	135.72	124.71
7	A	317	CHL	CMD-C2D-C1D	6.24	135.71	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	304	CHL	C1B-CHB-C4A	-6.24	117.76	130.12
7	B	309	CHL	CMD-C2D-C1D	6.23	135.69	124.71
7	C	313	CHL	C1B-CHB-C4A	-6.23	117.78	130.12
7	B	310	CHL	CMD-C2D-C1D	6.23	135.69	124.71
7	C	306	CHL	CHB-C4A-NA	6.22	133.12	124.51
7	A	311	CHL	C1B-CHB-C4A	-6.22	117.79	130.12
8	A	313	CLA	C4A-NA-C1A	6.22	109.50	106.71
7	A	312	CHL	CHB-C4A-NA	6.21	133.10	124.51
7	C	309	CHL	CMD-C2D-C1D	6.21	135.66	124.71
8	C	314	CLA	C4A-NA-C1A	6.19	109.49	106.71
7	C	313	CHL	CMD-C2D-C1D	6.19	135.62	124.71
7	A	308	CHL	CMD-C2D-C1D	6.18	135.61	124.71
7	B	305	CHL	CMD-C2D-C1D	6.18	135.61	124.71
7	C	318	CHL	C1B-CHB-C4A	-6.18	117.88	130.12
7	C	305	CHL	CMD-C2D-C1D	6.18	135.60	124.71
7	B	318	CHL	CMD-C2D-C1D	6.17	135.59	124.71
7	A	308	CHL	C1B-CHB-C4A	-6.17	117.90	130.12
7	B	312	CHL	C1B-CHB-C4A	-6.17	117.91	130.12
7	B	318	CHL	CHB-C4A-NA	6.16	133.03	124.51
7	C	313	CHL	CHB-C4A-NA	6.15	133.02	124.51
7	A	309	CHL	CMD-C2D-C1D	6.15	135.56	124.71
7	C	311	CHL	C1B-CHB-C4A	-6.14	117.96	130.12
7	A	312	CHL	C1B-CHB-C4A	-6.12	117.99	130.12
7	B	310	CHL	CHB-C4A-NA	6.12	132.97	124.51
7	A	311	CHL	CHD-C1D-ND	6.11	130.07	124.45
7	B	306	CHL	C1B-CHB-C4A	-6.11	118.02	130.12
7	A	310	CHL	C1B-CHB-C4A	-6.11	118.03	130.12
7	C	311	CHL	CMD-C2D-C1D	6.10	135.47	124.71
7	C	318	CHL	CHB-C4A-NA	6.10	132.95	124.51
7	B	318	CHL	C1B-CHB-C4A	-6.10	118.04	130.12
7	A	304	CHL	CHB-C4A-NA	6.10	132.94	124.51
7	B	311	CHL	C1B-CHB-C4A	-6.10	118.05	130.12
7	C	310	CHL	CHB-C4A-NA	6.10	132.94	124.51
7	A	310	CHL	CHD-C1D-ND	6.09	130.05	124.45
7	B	313	CHL	C1B-CHB-C4A	-6.09	118.05	130.12
8	B	308	CLA	C4A-NA-C1A	6.09	109.44	106.71
7	A	308	CHL	CHB-C4A-NA	6.08	132.91	124.51
7	C	312	CHL	C1B-CHB-C4A	-6.08	118.09	130.12
7	C	306	CHL	C1B-CHB-C4A	-6.07	118.10	130.12
7	A	317	CHL	C1B-CHB-C4A	-6.06	118.12	130.12
7	A	310	CHL	CMD-C2D-C1D	6.06	135.39	124.71
7	C	305	CHL	C1B-CHB-C4A	-6.06	118.12	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	311	CHL	CMD-C2D-C1D	6.03	135.33	124.71
7	B	310	CHL	C1B-CHB-C4A	-6.02	118.19	130.12
7	A	305	CHL	C1B-CHB-C4A	-6.02	118.20	130.12
7	A	309	CHL	CHD-C1D-ND	6.02	129.98	124.45
7	C	310	CHL	C1B-CHB-C4A	-6.02	118.21	130.12
7	A	309	CHL	C1B-CHB-C4A	-6.01	118.22	130.12
7	B	305	CHL	CHD-C1D-ND	6.00	129.97	124.45
7	A	305	CHL	CMD-C2D-C1D	5.99	135.28	124.71
7	B	306	CHL	CMD-C2D-C1D	5.99	135.27	124.71
7	C	311	CHL	CHB-C4A-NA	5.99	132.79	124.51
7	B	311	CHL	CHD-C1D-ND	5.98	129.94	124.45
7	C	305	CHL	CHD-C1D-ND	5.97	129.94	124.45
7	C	306	CHL	CHD-C1D-ND	5.95	129.93	124.45
7	A	305	CHL	CHD-C1D-ND	5.95	129.92	124.45
7	B	306	CHL	CHD-C1D-ND	5.94	129.91	124.45
7	C	306	CHL	CMD-C2D-C1D	5.94	135.17	124.71
7	B	318	CHL	CHD-C1D-ND	5.93	129.91	124.45
7	B	310	CHL	CHD-C1D-ND	5.92	129.90	124.45
7	C	311	CHL	CHD-C1D-ND	5.91	129.89	124.45
7	B	305	CHL	C1B-CHB-C4A	-5.90	118.43	130.12
7	C	318	CHL	CHD-C1D-ND	5.88	129.86	124.45
7	C	310	CHL	CHD-C1D-ND	5.87	129.85	124.45
7	B	312	CHL	CHD-C1D-ND	5.87	129.85	124.45
7	A	317	CHL	CHD-C1D-ND	5.85	129.83	124.45
7	A	308	CHL	CHD-C1D-ND	5.84	129.82	124.45
7	B	309	CHL	CHB-C4A-NA	5.79	132.51	124.51
7	A	304	CHL	CHD-C1D-ND	5.71	129.70	124.45
7	B	309	CHL	CHD-C1D-ND	5.71	129.70	124.45
7	C	309	CHL	CHD-C1D-ND	5.58	129.58	124.45
7	B	313	CHL	CHD-C1D-ND	5.57	129.57	124.45
7	C	309	CHL	CHB-C4A-NA	5.54	132.17	124.51
7	B	306	CHL	C2A-C1A-CHA	-5.53	114.18	123.86
7	C	310	CHL	C2A-C1A-CHA	-5.53	114.18	123.86
7	C	313	CHL	CHD-C1D-ND	5.49	129.50	124.45
7	A	305	CHL	C2A-C1A-CHA	-5.49	114.27	123.86
7	A	312	CHL	CHD-C1D-ND	5.46	129.47	124.45
7	C	306	CHL	C2A-C1A-CHA	-5.46	114.32	123.86
7	A	309	CHL	C2A-C1A-CHA	-5.45	114.33	123.86
4	C	301	0UR	C43-C3-C4	-5.45	118.44	125.02
7	B	310	CHL	C2A-C1A-CHA	-5.39	114.43	123.86
7	B	313	CHL	C2A-C1A-CHA	-5.36	114.48	123.86
7	B	312	CHL	C2A-C1A-CHA	-5.33	114.54	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	306	CHL	O2D-CGD-CBD	5.31	120.70	111.27
5	B	302	0IE	C20-C3-C4	-5.30	118.01	124.83
7	A	312	CHL	C2A-C1A-CHA	-5.30	114.60	123.86
4	B	301	0UR	C43-C3-C4	-5.29	118.62	125.02
7	A	310	CHL	C1D-CHD-C4C	-5.29	114.64	126.06
7	B	311	CHL	C1D-CHD-C4C	-5.29	114.65	126.06
7	C	312	CHL	C1D-CHD-C4C	-5.28	114.66	126.06
7	A	308	CHL	C2A-C1A-CHA	-5.28	114.63	123.86
7	C	311	CHL	C1D-CHD-C4C	-5.25	114.73	126.06
7	A	305	CHL	O2D-CGD-CBD	5.25	120.59	111.27
7	A	317	CHL	C2A-C1A-CHA	-5.24	114.70	123.85
7	A	311	CHL	C1D-CHD-C4C	-5.24	114.76	126.06
7	C	306	CHL	C1D-CHD-C4C	-5.23	114.77	126.06
7	A	305	CHL	C1D-CHD-C4C	-5.23	114.77	126.06
7	A	309	CHL	C1D-CHD-C4C	-5.23	114.78	126.06
7	B	306	CHL	C1D-CHD-C4C	-5.23	114.78	126.06
7	C	310	CHL	C1D-CHD-C4C	-5.22	114.79	126.06
7	C	313	CHL	C2A-C1A-CHA	-5.22	114.73	123.86
7	C	313	CHL	C2D-C1D-ND	-5.22	106.26	110.10
7	B	305	CHL	C2A-C1A-CHA	-5.21	114.74	123.86
7	C	318	CHL	C2A-C1A-CHA	-5.21	114.76	123.85
7	B	312	CHL	C1D-CHD-C4C	-5.20	114.83	126.06
7	B	310	CHL	C1D-CHD-C4C	-5.20	114.84	126.06
7	B	318	CHL	C2A-C1A-CHA	-5.19	114.80	123.85
7	B	306	CHL	CHD-C4C-C3C	-5.18	117.23	124.84
7	C	311	CHL	O2D-CGD-CBD	5.18	120.47	111.27
7	B	305	CHL	C1D-CHD-C4C	-5.18	114.89	126.06
7	A	305	CHL	CHD-C4C-C3C	-5.17	117.23	124.84
7	C	318	CHL	C1D-CHD-C4C	-5.17	114.90	126.06
7	C	306	CHL	O2D-CGD-CBD	5.16	120.44	111.27
7	B	309	CHL	C1D-CHD-C4C	-5.16	114.93	126.06
7	A	311	CHL	C2A-C1A-CHA	-5.16	114.84	123.86
4	A	301	0UR	C43-C3-C4	-5.15	118.80	125.02
7	C	310	CHL	CHD-C4C-C3C	-5.14	117.28	124.84
7	C	305	CHL	C1D-CHD-C4C	-5.14	114.98	126.06
7	A	317	CHL	C1D-CHD-C4C	-5.13	114.99	126.06
7	B	318	CHL	C1D-CHD-C4C	-5.13	114.99	126.06
7	B	313	CHL	C2D-C1D-ND	-5.13	106.32	110.10
7	A	304	CHL	O2D-CGD-CBD	5.13	120.38	111.27
7	A	308	CHL	C1D-CHD-C4C	-5.12	115.01	126.06
7	C	309	CHL	C1D-CHD-C4C	-5.12	115.01	126.06
7	C	305	CHL	C2A-C1A-CHA	-5.12	114.90	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	312	CHL	C2D-C1D-ND	-5.12	106.33	110.10
7	C	311	CHL	C2A-C1A-CHA	-5.12	114.91	123.86
7	B	310	CHL	O2D-CGD-CBD	5.11	120.35	111.27
7	C	306	CHL	CHD-C4C-C3C	-5.11	117.33	124.84
7	A	310	CHL	C2A-C1A-CHA	-5.11	114.93	123.86
7	A	304	CHL	C1D-CHD-C4C	-5.11	115.04	126.06
7	A	309	CHL	O2D-CGD-CBD	5.10	120.33	111.27
7	A	317	CHL	CHD-C4C-C3C	-5.09	117.36	124.84
7	C	312	CHL	CHD-C4C-C3C	-5.08	117.37	124.84
7	C	312	CHL	C2A-C1A-CHA	-5.08	114.98	123.86
7	A	312	CHL	C1D-CHD-C4C	-5.07	115.12	126.06
7	C	310	CHL	O2D-CGD-CBD	5.07	120.28	111.27
7	B	313	CHL	C1D-CHD-C4C	-5.06	115.13	126.06
7	C	318	CHL	CHD-C4C-C3C	-5.06	117.40	124.84
7	A	304	CHL	C2D-C1D-ND	-5.05	106.38	110.10
7	C	313	CHL	C1D-CHD-C4C	-5.05	115.17	126.06
7	B	312	CHL	CHD-C4C-C3C	-5.05	117.42	124.84
7	C	309	CHL	O2D-CGD-CBD	5.04	120.23	111.27
7	B	318	CHL	CHD-C4C-C3C	-5.04	117.43	124.84
7	B	305	CHL	CHD-C4C-C3C	-5.04	117.43	124.84
7	A	308	CHL	CHD-C4C-C3C	-5.04	117.44	124.84
7	A	309	CHL	CHD-C4C-C3C	-5.03	117.44	124.84
7	C	311	CHL	C2D-C1D-ND	-5.03	106.40	110.10
7	B	305	CHL	O2D-CGD-CBD	5.03	120.20	111.27
7	B	310	CHL	C2D-C1D-ND	-5.02	106.40	110.10
7	C	305	CHL	C2D-C1D-ND	-5.02	106.41	110.10
7	B	311	CHL	C2A-C1A-CHA	-5.02	115.09	123.86
7	A	309	CHL	C1C-C2C-C3C	-5.01	103.14	107.11
7	A	310	CHL	CHD-C4C-C3C	-5.01	117.48	124.84
7	B	318	CHL	O2D-CGD-CBD	5.01	120.17	111.27
7	B	311	CHL	C2D-C1D-ND	-5.00	106.42	110.10
7	A	308	CHL	O2D-CGD-CBD	5.00	120.16	111.27
7	C	309	CHL	C2D-C1D-ND	-5.00	106.42	110.10
7	A	311	CHL	CHD-C4C-C3C	-5.00	117.50	124.84
7	A	310	CHL	O2D-CGD-CBD	4.99	120.14	111.27
7	B	309	CHL	C2A-C1A-CHA	-4.99	115.13	123.86
7	C	305	CHL	O2D-CGD-CBD	4.99	120.14	111.27
7	B	311	CHL	O2D-CGD-CBD	4.98	120.12	111.27
7	B	310	CHL	CHD-C4C-C3C	-4.98	117.52	124.84
7	A	317	CHL	O2D-CGD-CBD	4.98	120.11	111.27
7	B	309	CHL	O2D-CGD-CBD	4.96	120.08	111.27
7	A	304	CHL	C2A-C1A-CHA	-4.96	115.19	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	313	CHL	O2D-CGD-CBD	4.96	120.08	111.27
7	B	311	CHL	CHD-C4C-C3C	-4.95	117.56	124.84
7	C	305	CHL	CHD-C4C-C3C	-4.94	117.58	124.84
7	C	311	CHL	CHD-C4C-C3C	-4.92	117.61	124.84
7	C	318	CHL	O2D-CGD-CBD	4.92	120.00	111.27
7	A	311	CHL	C2D-C1D-ND	-4.91	106.49	110.10
7	B	309	CHL	CHD-C4C-C3C	-4.89	117.65	124.84
7	B	313	CHL	O2D-CGD-CBD	4.89	119.95	111.27
7	B	305	CHL	C1C-C2C-C3C	-4.89	103.24	107.11
7	B	309	CHL	C2D-C1D-ND	-4.88	106.51	110.10
7	A	304	CHL	C1C-C2C-C3C	-4.88	103.24	107.11
7	B	309	CHL	C1C-C2C-C3C	-4.88	103.24	107.11
7	B	310	CHL	C1C-C2C-C3C	-4.87	103.25	107.11
7	C	310	CHL	C1C-C2C-C3C	-4.87	103.25	107.11
7	A	312	CHL	O2D-CGD-CBD	4.86	119.90	111.27
7	B	305	CHL	C2D-C1D-ND	-4.85	106.53	110.10
7	A	309	CHL	C2D-C1D-ND	-4.85	106.53	110.10
7	A	310	CHL	C2D-C1D-ND	-4.85	106.53	110.10
7	B	312	CHL	C2D-C1D-ND	-4.84	106.53	110.10
7	C	318	CHL	C2D-C1D-ND	-4.84	106.53	110.10
7	C	310	CHL	C2D-C1D-ND	-4.84	106.54	110.10
7	B	318	CHL	C2D-C1D-ND	-4.83	106.54	110.10
7	C	312	CHL	C2D-C1D-ND	-4.83	106.55	110.10
7	A	308	CHL	C2D-C1D-ND	-4.82	106.55	110.10
6	C	304	NEX	C5-C4-C3	4.82	117.45	111.75
7	A	317	CHL	C1C-C2C-C3C	-4.81	103.30	107.11
7	C	305	CHL	C1C-C2C-C3C	-4.81	103.30	107.11
7	A	312	CHL	C1C-C2C-C3C	-4.81	103.30	107.11
7	C	306	CHL	C2D-C1D-ND	-4.81	106.56	110.10
7	A	304	CHL	CHD-C4C-C3C	-4.80	117.78	124.84
7	A	317	CHL	C2D-C1D-ND	-4.80	106.57	110.10
7	C	309	CHL	CHD-C4C-C3C	-4.80	117.78	124.84
7	C	309	CHL	C1C-C2C-C3C	-4.79	103.31	107.11
7	B	306	CHL	C2D-C1D-ND	-4.79	106.57	110.10
7	C	309	CHL	C2A-C1A-CHA	-4.79	115.49	123.86
7	B	318	CHL	C1C-C2C-C3C	-4.79	103.31	107.11
7	B	313	CHL	C1C-C2C-C3C	-4.78	103.32	107.11
7	C	318	CHL	C1C-C2C-C3C	-4.78	103.32	107.11
7	A	305	CHL	C1C-C2C-C3C	-4.75	103.35	107.11
7	C	313	CHL	C1C-C2C-C3C	-4.75	103.35	107.11
7	A	305	CHL	C2D-C1D-ND	-4.73	106.62	110.10
7	C	306	CHL	C1C-C2C-C3C	-4.72	103.36	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	313	CHL	CHD-C4C-C3C	-4.72	117.91	124.84
7	B	306	CHL	C1C-C2C-C3C	-4.71	103.38	107.11
7	A	308	CHL	C1C-C2C-C3C	-4.71	103.38	107.11
6	A	303	NEX	C5-C4-C3	4.70	117.31	111.75
5	A	302	0IE	C20-C3-C4	-4.67	118.82	124.83
7	A	312	CHL	CHD-C4C-C3C	-4.65	118.01	124.84
7	B	312	CHL	C1C-C2C-C3C	-4.63	103.44	107.11
7	C	313	CHL	CHD-C4C-C3C	-4.61	118.07	124.84
5	C	302	0IE	C20-C3-C4	-4.59	118.92	124.83
7	A	311	CHL	O2D-CGD-CBD	4.59	119.43	111.27
7	C	312	CHL	C1C-C2C-C3C	-4.58	103.48	107.11
7	A	311	CHL	C1C-C2C-C3C	-4.49	103.55	107.11
7	A	304	CHL	CMD-C2D-C3D	-4.49	117.28	127.61
7	B	312	CHL	O2D-CGD-CBD	4.48	119.23	111.27
7	C	310	CHL	CMD-C2D-C3D	-4.47	117.34	127.61
7	B	312	CHL	CMD-C2D-C3D	-4.47	117.34	127.61
7	B	313	CHL	CMD-C2D-C3D	-4.46	117.35	127.61
7	A	312	CHL	CMD-C2D-C3D	-4.46	117.35	127.61
7	C	312	CHL	O2D-CGD-CBD	4.46	119.20	111.27
7	B	311	CHL	C1C-C2C-C3C	-4.42	103.60	107.11
7	B	310	CHL	CMD-C2D-C3D	-4.41	117.46	127.61
7	C	313	CHL	CMD-C2D-C3D	-4.38	117.55	127.61
7	A	311	CHL	CMD-C2D-C3D	-4.34	117.63	127.61
7	C	318	CHL	CMD-C2D-C3D	-4.33	117.64	127.61
7	A	317	CHL	CMD-C2D-C3D	-4.33	117.65	127.61
5	B	302	0IE	C9-C10-C11	4.33	132.34	123.47
7	B	309	CHL	CMD-C2D-C3D	-4.32	117.67	127.61
7	C	309	CHL	CMD-C2D-C3D	-4.32	117.68	127.61
7	C	311	CHL	C1C-C2C-C3C	-4.32	103.69	107.11
7	C	305	CHL	CMD-C2D-C3D	-4.32	117.69	127.61
7	A	309	CHL	CMD-C2D-C3D	-4.31	117.70	127.61
6	B	304	NEX	C5-C4-C3	4.31	116.84	111.75
7	B	305	CHL	CMD-C2D-C3D	-4.31	117.71	127.61
7	B	318	CHL	CMD-C2D-C3D	-4.30	117.72	127.61
7	A	308	CHL	CMD-C2D-C3D	-4.30	117.73	127.61
7	B	311	CHL	CHC-C1C-NC	4.30	130.72	124.20
7	A	311	CHL	CHC-C1C-NC	4.29	130.72	124.20
7	C	312	CHL	CHC-C1C-NC	4.28	130.69	124.20
7	C	311	CHL	CMD-C2D-C3D	-4.27	117.78	127.61
7	C	312	CHL	CMD-C2D-C3D	-4.27	117.79	127.61
8	A	316	CLA	CMB-C2B-C1B	-4.27	121.91	128.46
7	A	310	CHL	CHC-C1C-NC	4.27	130.67	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	303	0IE	C23-C16-C15	-4.26	116.95	122.92
5	A	302	0IE	C23-C16-C15	-4.26	116.95	122.92
7	B	312	CHL	CHC-C1C-NC	4.26	130.66	124.20
7	A	310	CHL	C1C-C2C-C3C	-4.25	103.74	107.11
7	C	305	CHL	CHC-C1C-NC	4.24	130.64	124.20
7	C	311	CHL	CHC-C1C-NC	4.24	130.64	124.20
5	B	303	0IE	C23-C16-C15	-4.24	116.98	122.92
4	B	301	0UR	C29-C30-C31	-4.24	106.92	111.74
7	A	304	CHL	CHC-C1C-NC	4.23	130.62	124.20
9	A	318	LHG	O4-P-O5	4.22	133.12	112.24
7	B	311	CHL	CMD-C2D-C3D	-4.22	117.90	127.61
7	B	313	CHL	CHC-C1C-NC	4.22	130.61	124.20
7	A	312	CHL	CHC-C1C-NC	4.21	130.59	124.20
7	C	312	CHL	CHA-C4D-ND	4.21	141.30	132.50
5	C	302	0IE	C23-C16-C15	-4.20	117.03	122.92
7	B	305	CHL	CHC-C1C-NC	4.20	130.57	124.20
7	A	310	CHL	CMD-C2D-C3D	-4.20	117.95	127.61
9	C	319	LHG	O4-P-O5	4.20	132.99	112.24
9	B	319	LHG	O4-P-O5	4.20	132.98	112.24
7	B	306	CHL	CMD-C2D-C3D	-4.18	118.00	127.61
7	B	312	CHL	CHA-C4D-ND	4.18	141.24	132.50
7	A	304	CHL	CHA-C4D-ND	4.16	141.20	132.50
7	A	305	CHL	CMD-C2D-C3D	-4.15	118.06	127.61
7	C	318	CHL	CHA-C4D-ND	4.15	141.17	132.50
7	C	313	CHL	CHC-C1C-NC	4.14	130.48	124.20
8	A	307	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
7	A	311	CHL	CHA-C4D-ND	4.14	141.15	132.50
7	C	305	CHL	CHA-C4D-ND	4.13	141.15	132.50
5	B	302	0IE	C23-C16-C15	-4.13	117.14	122.92
7	C	306	CHL	CMD-C2D-C3D	-4.12	118.13	127.61
7	B	309	CHL	CHC-C1C-NC	4.12	130.46	124.20
7	C	318	CHL	CHC-C1C-NC	4.12	130.45	124.20
7	C	310	CHL	CHA-C4D-ND	4.11	141.10	132.50
7	B	313	CHL	CHA-C4D-ND	4.10	141.09	132.50
7	A	308	CHL	CHA-C4D-ND	4.10	141.08	132.50
7	A	317	CHL	CHA-C4D-ND	4.10	141.07	132.50
7	B	318	CHL	CHA-C4D-ND	4.10	141.07	132.50
7	B	305	CHL	CHA-C4D-ND	4.09	141.06	132.50
7	B	318	CHL	CHC-C1C-NC	4.09	130.41	124.20
7	C	309	CHL	CHA-C4D-ND	4.09	141.06	132.50
7	A	312	CHL	CHA-C4D-ND	4.09	141.06	132.50
7	B	309	CHL	CHA-C4D-ND	4.08	141.04	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	317	CHL	CHC-C1C-NC	4.08	130.39	124.20
4	C	301	0UR	C29-C30-C31	-4.07	107.10	111.74
7	A	308	CHL	CHC-C1C-NC	4.07	130.38	124.20
7	B	310	CHL	CHA-C4D-ND	4.07	141.02	132.50
7	A	309	CHL	CHA-C4D-ND	4.06	140.99	132.50
7	A	310	CHL	CHA-C4D-ND	4.06	140.99	132.50
7	B	306	CHL	CHA-C4D-ND	4.05	140.97	132.50
7	C	306	CHL	CHA-C4D-ND	4.05	140.97	132.50
7	A	305	CHL	CHA-C4D-ND	4.05	140.97	132.50
7	C	313	CHL	CHA-C4D-ND	4.05	140.97	132.50
7	B	311	CHL	CHA-C4D-ND	4.04	140.96	132.50
7	C	311	CHL	CHA-C4D-ND	4.03	140.93	132.50
7	A	309	CHL	CHC-C1C-NC	4.03	130.31	124.20
5	B	303	0IE	C20-C3-C4	-4.01	119.67	124.83
7	B	306	CHL	CHC-C1C-NC	4.00	130.27	124.20
5	C	303	0IE	C10-C9-C8	3.99	131.65	123.47
7	B	310	CHL	CHC-C1C-NC	3.99	130.25	124.20
8	B	308	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
7	A	305	CHL	CHC-C1C-NC	3.99	130.25	124.20
8	C	314	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
5	A	302	0IE	C10-C9-C8	3.96	131.58	123.47
7	C	309	CHL	CHC-C1C-NC	3.96	130.20	124.20
7	C	306	CHL	CHC-C1C-NC	3.95	130.19	124.20
5	B	302	0IE	C13-C12-C11	3.93	124.97	118.94
8	B	314	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
8	A	313	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
7	C	310	CHL	CHC-C1C-NC	3.91	130.14	124.20
5	C	303	0IE	C20-C3-C4	-3.88	119.84	124.83
5	B	303	0IE	C10-C9-C8	3.87	131.41	123.47
8	C	308	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
5	A	302	0IE	C9-C10-C11	3.81	131.27	123.47
7	B	306	CHL	CHD-C4C-NC	3.79	130.18	124.20
5	C	302	0IE	C9-C10-C11	3.78	131.21	123.47
5	B	303	0IE	C9-C10-C11	3.77	131.21	123.47
4	B	301	0UR	C34-C27-C1	-3.77	119.55	124.49
7	A	305	CHL	CHD-C4C-NC	3.76	130.13	124.20
5	C	302	0IE	C10-C9-C8	3.76	131.17	123.47
7	C	310	CHL	CHD-C4C-NC	3.75	130.12	124.20
8	B	317	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
8	B	316	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
8	C	317	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
7	A	310	CHL	C2C-C3C-C4C	-3.73	103.83	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	309	CHL	CHD-C4C-NC	3.71	130.06	124.20
8	C	315	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
5	B	302	0IE	C22-C12-C11	-3.71	117.73	122.92
7	C	306	CHL	CHD-C4C-NC	3.70	130.04	124.20
7	C	318	CHL	CHD-C4C-NC	3.70	130.03	124.20
7	B	312	CHL	CHD-C4C-NC	3.69	130.01	124.20
7	A	308	CHL	C4A-NA-C1A	-3.68	105.05	106.71
7	A	317	CHL	CHD-C4C-NC	3.67	129.99	124.20
7	B	305	CHL	CHD-C4C-NC	3.67	129.99	124.20
5	B	302	0IE	C10-C9-C8	3.67	130.99	123.47
7	B	309	CHL	CHD-C4C-NC	3.67	129.98	124.20
8	C	316	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
7	B	318	CHL	CHD-C4C-NC	3.66	129.96	124.20
7	B	306	CHL	C4A-NA-C1A	-3.65	105.06	106.71
7	A	308	CHL	CHD-C4C-NC	3.63	129.93	124.20
7	B	310	CHL	CHD-C4C-NC	3.63	129.93	124.20
7	C	311	CHL	CHD-C4C-NC	3.63	129.92	124.20
7	B	311	CHL	CHD-C4C-NC	3.61	129.90	124.20
7	C	312	CHL	CHD-C4C-NC	3.61	129.88	124.20
7	C	305	CHL	CHD-C4C-NC	3.60	129.88	124.20
7	C	306	CHL	C4A-NA-C1A	-3.60	105.09	106.71
5	B	303	0IE	C22-C12-C11	-3.60	117.89	122.92
7	A	311	CHL	CHD-C4C-NC	3.59	129.87	124.20
7	A	304	CHL	CHD-C4C-NC	3.59	129.86	124.20
7	A	310	CHL	CHD-C4C-NC	3.59	129.86	124.20
8	A	316	CLA	CMB-C2B-C3B	3.57	131.36	124.68
7	C	309	CHL	CHD-C4C-NC	3.56	129.82	124.20
4	A	301	0UR	C10-C11-C12	-3.55	122.24	127.31
4	B	301	0UR	C10-C11-C12	-3.55	122.25	127.31
7	C	311	CHL	C2C-C3C-C4C	-3.55	103.96	106.49
5	A	302	0IE	C22-C12-C11	-3.54	117.96	122.92
7	B	318	CHL	C4A-NA-C1A	-3.53	105.12	106.71
8	A	306	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
7	C	312	CHL	C2C-C3C-C4C	-3.51	103.98	106.49
5	C	303	0IE	C9-C10-C11	3.51	130.65	123.47
7	C	312	CHL	OBD-CAD-C3D	-3.50	120.09	128.52
7	B	311	CHL	C2C-C3C-C4C	-3.50	104.00	106.49
7	A	311	CHL	C2C-C3C-C4C	-3.50	104.00	106.49
5	C	302	0IE	C22-C12-C11	-3.50	118.03	122.92
7	A	305	CHL	C1-C2-C3	-3.49	120.00	126.04
5	A	302	0IE	C21-C7-C8	-3.48	118.04	122.92
4	C	301	0UR	C10-C11-C12	-3.47	122.35	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	318	CHL	C4A-NA-C1A	-3.47	105.15	106.71
4	B	301	0UR	O44-C45-C46	3.47	120.77	111.55
5	B	302	0IE	C21-C7-C8	-3.47	118.07	122.92
7	B	313	CHL	CHD-C4C-NC	3.46	129.66	124.20
7	A	305	CHL	C4A-NA-C1A	-3.45	105.16	106.71
7	A	309	CHL	C1-C2-C3	-3.43	121.21	126.75
8	A	315	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
5	C	303	0IE	C22-C12-C11	-3.42	118.14	122.92
7	C	313	CHL	CHD-C4C-NC	3.41	129.58	124.20
7	A	312	CHL	CHD-C4C-NC	3.41	129.57	124.20
5	B	303	0IE	C21-C7-C8	-3.41	118.15	122.92
7	B	306	CHL	C1-C2-C3	-3.41	120.15	126.04
8	A	314	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
4	A	301	0UR	C29-C30-C31	-3.40	107.87	111.74
8	A	307	CLA	CMB-C2B-C3B	3.40	131.05	124.68
8	B	315	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
7	B	310	CHL	C1-C2-C3	-3.40	121.25	126.75
4	A	301	0UR	C34-C27-C1	-3.39	120.04	124.49
5	C	302	0IE	C21-C7-C8	-3.39	118.18	122.92
7	C	310	CHL	C1-C2-C3	-3.38	121.28	126.75
5	C	303	0IE	C21-C7-C8	-3.38	118.19	122.92
8	C	307	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
8	C	314	CLA	CMB-C2B-C3B	3.33	130.91	124.68
7	A	311	CHL	OBD-CAD-C3D	-3.33	120.51	128.52
7	B	312	CHL	C2C-C3C-C4C	-3.32	104.12	106.49
5	A	302	0IE	C13-C12-C11	3.32	124.03	118.94
8	B	307	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
7	C	310	CHL	C4A-NA-C1A	-3.31	105.22	106.71
4	A	301	0UR	O44-C45-C46	3.30	120.33	111.55
4	C	301	0UR	O44-C45-C46	3.30	120.32	111.55
7	B	309	CHL	C4A-NA-C1A	-3.30	105.22	106.71
7	A	312	CHL	C2C-C3C-C4C	-3.29	104.14	106.49
8	B	308	CLA	CMB-C2B-C3B	3.28	130.82	124.68
8	A	313	CLA	CMB-C2B-C3B	3.28	130.82	124.68
7	A	308	CHL	C2C-C3C-C4C	-3.28	104.15	106.49
7	C	313	CHL	C2C-C3C-C4C	-3.28	104.15	106.49
7	B	313	CHL	C2C-C3C-C4C	-3.27	104.16	106.49
7	C	305	CHL	C2C-C3C-C4C	-3.25	104.17	106.49
5	B	303	0IE	C17-C16-C15	3.24	123.92	118.94
7	B	318	CHL	C2C-C3C-C4C	-3.24	104.18	106.49
4	C	301	0UR	C34-C27-C1	-3.24	120.24	124.49
8	B	314	CLA	CMB-C2B-C3B	3.23	130.73	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	302	0IE	C13-C12-C11	3.23	123.89	118.94
7	A	317	CHL	C2C-C3C-C4C	-3.22	104.19	106.49
7	B	310	CHL	C4A-NA-C1A	-3.22	105.26	106.71
7	B	312	CHL	C4A-NA-C1A	-3.22	105.26	106.71
7	C	306	CHL	C2C-C3C-C4C	-3.21	104.20	106.49
5	B	303	0IE	C6-C7-C8	3.20	123.85	118.94
5	B	303	0IE	C13-C12-C11	3.19	123.83	118.94
7	B	306	CHL	C2C-C3C-C4C	-3.18	104.22	106.49
7	B	312	CHL	OBD-CAD-C3D	-3.18	120.86	128.52
4	B	301	0UR	C5-C4-C3	-3.18	123.18	127.00
7	A	311	CHL	C4A-NA-C1A	-3.18	105.28	106.71
7	C	318	CHL	C2C-C3C-C4C	-3.18	104.22	106.49
7	A	305	CHL	C2C-C3C-C4C	-3.16	104.23	106.49
8	C	308	CLA	CMB-C2B-C3B	3.16	130.59	124.68
7	C	306	CHL	C1-C2-C3	-3.15	120.60	126.04
5	B	302	0IE	C6-C7-C8	3.13	123.75	118.94
8	B	317	CLA	CMB-C2B-C3B	3.13	130.54	124.68
7	C	309	CHL	C2C-C3C-C4C	-3.13	104.26	106.49
5	A	302	0IE	C6-C7-C8	3.13	123.74	118.94
7	B	305	CHL	C2C-C3C-C4C	-3.12	104.27	106.49
8	C	317	CLA	CMB-C2B-C3B	3.10	130.49	124.68
8	C	315	CLA	CMB-C2B-C3B	3.10	130.48	124.68
7	A	309	CHL	C4A-NA-C1A	-3.10	105.31	106.71
8	B	316	CLA	CMB-C2B-C3B	3.09	130.47	124.68
7	B	305	CHL	C1-C2-C3	-3.08	120.72	126.04
7	A	317	CHL	C4A-NA-C1A	-3.07	105.33	106.71
5	C	303	0IE	C6-C7-C8	3.07	123.64	118.94
7	B	313	CHL	C1-C2-C3	-3.06	120.76	126.04
7	C	310	CHL	C2C-C3C-C4C	-3.06	104.31	106.49
7	C	313	CHL	C1-C2-C3	-3.05	120.77	126.04
4	A	301	0UR	C28-C19-C18	-3.04	108.85	112.70
7	C	309	CHL	C4A-NA-C1A	-3.04	105.34	106.71
7	B	310	CHL	C2C-C3C-C4C	-3.04	104.32	106.49
8	A	314	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
8	C	316	CLA	CMB-C2B-C3B	3.04	130.36	124.68
7	A	304	CHL	C2C-C3C-C4C	-3.03	104.33	106.49
7	C	305	CHL	OBD-CAD-C3D	-3.02	121.24	128.52
5	C	303	0IE	C13-C12-C11	3.02	123.57	118.94
7	B	305	CHL	OBD-CAD-C3D	-3.01	121.27	128.52
7	A	304	CHL	OBD-CAD-C3D	-3.01	121.28	128.52
7	A	304	CHL	C4A-NA-C1A	-2.99	105.36	106.71
4	C	301	0UR	C48-C47-C46	-2.99	119.44	125.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	312	CHL	C1-C2-C3	-2.98	120.88	126.04
7	C	311	CHL	OBD-CAD-C3D	-2.98	121.34	128.52
7	B	309	CHL	C2C-C3C-C4C	-2.98	104.37	106.49
7	A	310	CHL	OBD-CAD-C3D	-2.98	121.36	128.52
7	B	310	CHL	OBD-CAD-C3D	-2.96	121.39	128.52
7	B	309	CHL	OBD-CAD-C3D	-2.96	121.40	128.52
5	C	302	0IE	C6-C7-C8	2.95	123.47	118.94
7	B	313	CHL	C4A-NA-C1A	-2.95	105.38	106.71
7	A	308	CHL	OBD-CAD-C3D	-2.95	121.42	128.52
7	B	311	CHL	OBD-CAD-C3D	-2.94	121.43	128.52
7	C	309	CHL	OBD-CAD-C3D	-2.94	121.43	128.52
7	A	309	CHL	OBD-CAD-C3D	-2.94	121.45	128.52
8	C	315	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
7	C	310	CHL	OBD-CAD-C3D	-2.92	121.50	128.52
8	A	307	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
8	B	308	CLA	CAA-C2A-C3A	-2.91	104.82	112.78
7	C	305	CHL	C1-C2-C3	-2.90	121.02	126.04
8	B	308	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
4	B	301	0UR	C48-C47-C46	-2.89	119.64	125.85
7	A	317	CHL	OBD-CAD-C3D	-2.88	121.59	128.52
4	A	301	0UR	C48-C47-C46	-2.88	119.67	125.85
7	C	305	CHL	C4-C3-C5	2.88	120.12	115.27
8	B	317	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
7	C	305	CHL	C4A-NA-C1A	-2.87	105.42	106.71
7	A	309	CHL	C2C-C3C-C4C	-2.87	104.45	106.49
7	A	312	CHL	C4A-NA-C1A	-2.86	105.42	106.71
7	C	306	CHL	C4-C3-C5	2.86	120.08	115.27
8	C	314	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
8	A	316	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
7	A	310	CHL	C4-C3-C5	2.85	120.07	115.27
8	A	306	CLA	CMB-C2B-C3B	2.85	130.01	124.68
8	A	306	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
7	C	306	CHL	OBD-CAD-C3D	-2.85	121.67	128.52
8	B	314	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
8	A	313	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
8	C	308	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
8	B	315	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
7	B	318	CHL	OBD-CAD-C3D	-2.83	121.70	128.52
8	C	316	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
5	C	303	0IE	C17-C16-C15	2.83	123.28	118.94
7	A	304	CHL	C1-C2-C3	-2.83	121.15	126.04
7	C	310	CHL	O2A-CGA-CBA	2.82	120.77	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	312	CHL	O2A-CGA-CBA	2.82	120.77	111.91
8	B	307	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
8	A	315	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
8	C	317	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
7	B	306	CHL	C4-C3-C5	2.80	119.98	115.27
7	C	312	CHL	C4-C3-C5	2.80	119.98	115.27
8	C	307	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
7	A	305	CHL	OBD-CAD-C3D	-2.79	121.79	128.52
8	A	314	CLA	CMB-C2B-C3B	2.79	129.89	124.68
7	A	312	CHL	OBD-CAD-C3D	-2.78	121.82	128.52
4	A	301	0UR	C5-C4-C3	-2.78	123.66	127.00
8	C	307	CLA	CMB-C2B-C3B	2.78	129.88	124.68
8	B	315	CLA	CMB-C2B-C3B	2.78	129.88	124.68
7	B	305	CHL	C4-C3-C5	2.77	119.94	115.27
8	A	315	CLA	CMB-C2B-C3B	2.76	129.84	124.68
7	A	305	CHL	C4-C3-C5	2.76	119.91	115.27
8	B	316	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
7	B	313	CHL	OBD-CAD-C3D	-2.75	121.89	128.52
7	C	312	CHL	CHC-C1C-C2C	-2.75	116.13	126.11
7	B	312	CHL	C1-C2-C3	-2.75	121.29	126.04
7	C	305	CHL	CHC-C1C-C2C	-2.75	116.15	126.11
7	A	311	CHL	C1-C2-C3	-2.75	121.29	126.04
7	B	313	CHL	CHC-C1C-C2C	-2.74	116.16	126.11
7	B	306	CHL	OBD-CAD-C3D	-2.74	121.92	128.52
7	A	312	CHL	CHC-C1C-C2C	-2.74	116.18	126.11
4	C	301	0UR	C5-C4-C3	-2.73	123.72	127.00
7	B	305	CHL	CHC-C1C-C2C	-2.73	116.22	126.11
7	C	318	CHL	OBD-CAD-C3D	-2.73	121.95	128.52
7	B	305	CHL	C4A-NA-C1A	-2.73	105.48	106.71
7	A	304	CHL	C4-C3-C5	2.72	119.85	115.27
7	C	313	CHL	C4A-NA-C1A	-2.71	105.49	106.71
7	A	304	CHL	CHC-C1C-C2C	-2.71	116.28	126.11
7	A	312	CHL	O2A-CGA-CBA	2.71	120.40	111.91
8	B	307	CLA	CMB-C2B-C3B	2.71	129.74	124.68
7	A	317	CHL	O2D-CGD-O1D	-2.70	118.55	123.84
7	A	311	CHL	CHC-C1C-C2C	-2.70	116.31	126.11
7	B	313	CHL	O2A-CGA-CBA	2.70	120.39	111.91
7	A	311	CHL	C4-C3-C5	2.70	119.81	115.27
7	A	310	CHL	O2A-CGA-CBA	2.70	120.38	111.91
7	A	311	CHL	O2A-CGA-CBA	2.69	120.34	111.91
7	B	312	CHL	CHC-C1C-C2C	-2.69	116.37	126.11
7	C	313	CHL	CHC-C1C-C2C	-2.68	116.40	126.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	304	NEX	C16-C1-C6	2.68	112.87	110.47
7	B	311	CHL	CHC-C1C-C2C	-2.67	116.44	126.11
7	C	312	CHL	OMC-CMC-C2C	-2.66	119.67	125.69
7	B	312	CHL	O2A-CGA-CBA	2.66	120.26	111.91
4	C	301	0UR	C9-C8-C7	-2.66	123.51	127.31
7	A	310	CHL	CHC-C1C-C2C	-2.66	116.47	126.11
7	A	317	CHL	CHC-C1C-C2C	-2.66	116.48	126.11
7	B	318	CHL	CHC-C1C-C2C	-2.66	116.48	126.11
7	B	312	CHL	OMC-CMC-C2C	-2.65	119.69	125.69
7	A	312	CHL	C4-C3-C5	2.65	119.73	115.27
7	C	318	CHL	CHC-C1C-C2C	-2.65	116.50	126.11
7	B	309	CHL	CHC-C1C-C2C	-2.65	116.51	126.11
7	C	312	CHL	C4A-NA-C1A	-2.64	105.52	106.71
7	B	313	CHL	C4-C3-C5	2.64	119.71	115.27
7	A	309	CHL	CHC-C1C-C2C	-2.64	116.54	126.11
7	B	312	CHL	C4-C3-C5	2.64	119.71	115.27
9	B	319	LHG	O8-C23-C24	2.64	120.18	111.91
7	A	308	CHL	CHC-C1C-C2C	-2.63	116.56	126.11
4	C	301	0UR	C24-C25-C26	-2.63	106.70	110.30
6	B	304	NEX	C16-C1-C6	2.63	112.83	110.47
7	A	311	CHL	OMC-CMC-C2C	-2.63	119.74	125.69
7	C	311	CHL	CHC-C1C-C2C	-2.63	116.58	126.11
9	C	319	LHG	O8-C23-C24	2.62	120.14	111.91
7	A	310	CHL	C1-C2-C3	-2.62	121.51	126.04
7	C	313	CHL	O2A-CGA-CBA	2.60	120.06	111.91
9	A	318	LHG	O8-C23-C24	2.60	120.06	111.91
7	B	310	CHL	O2A-CGA-CBA	2.60	120.05	111.91
5	C	302	0IE	C17-C16-C15	2.59	122.92	118.94
6	C	304	NEX	C24-C23-C22	2.59	115.78	110.77
7	B	310	CHL	CHC-C1C-C2C	-2.59	116.73	126.11
7	A	309	CHL	O2A-CGA-CBA	2.58	120.00	111.91
8	B	308	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
7	C	312	CHL	C1-C2-C3	-2.58	121.58	126.04
7	C	310	CHL	CHC-C1C-C2C	-2.57	116.78	126.11
7	C	306	CHL	O2A-CGA-CBA	2.56	119.96	111.91
7	A	309	CHL	CAC-C3C-C4C	2.56	128.14	124.81
4	A	301	0UR	C24-C25-C26	-2.56	106.80	110.30
7	A	305	CHL	CHC-C1C-C2C	-2.56	116.82	126.11
7	C	309	CHL	CHC-C1C-C2C	-2.56	116.82	126.11
4	B	301	0UR	C24-C25-C26	-2.56	106.80	110.30
7	A	305	CHL	O2A-CGA-CBA	2.56	119.93	111.91
7	B	306	CHL	CHC-C1C-C2C	-2.56	116.85	126.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	306	CHL	CHC-C1C-C2C	-2.55	116.86	126.11
5	A	302	0IE	C17-C16-C15	2.55	122.85	118.94
7	B	310	CHL	CAC-C3C-C4C	2.55	128.12	124.81
8	A	315	CLA	CHB-C4A-NA	2.55	128.03	124.51
8	C	316	CLA	CHB-C4A-NA	2.55	128.03	124.51
7	B	306	CHL	O2D-CGD-O1D	-2.54	118.86	123.84
4	C	301	0UR	C28-C19-C18	-2.54	109.49	112.70
6	A	303	NEX	C16-C1-C6	2.54	112.75	110.47
8	C	307	CLA	CHB-C4A-NA	2.54	128.02	124.51
8	C	317	CLA	CHB-C4A-NA	2.53	128.01	124.51
7	B	306	CHL	OMC-CMC-C2C	-2.53	119.97	125.69
7	B	313	CHL	CAC-C3C-C4C	2.52	128.09	124.81
7	B	306	CHL	O2A-CGA-CBA	2.52	119.82	111.91
7	A	305	CHL	OMC-CMC-C2C	-2.52	119.99	125.69
8	B	316	CLA	CHB-C4A-NA	2.52	127.99	124.51
9	A	318	LHG	C11-C10-C9	-2.52	101.65	114.42
7	B	318	CHL	OMC-CMC-C2C	-2.52	120.00	125.69
7	A	312	CHL	CAC-C3C-C4C	2.51	128.07	124.81
7	B	305	CHL	O2D-CGD-O1D	-2.51	118.93	123.84
7	A	310	CHL	OMC-CMC-C2C	-2.51	120.01	125.69
8	B	307	CLA	CHB-C4A-NA	2.51	127.98	124.51
8	B	308	CLA	CHB-C4A-NA	2.51	127.98	124.51
7	C	306	CHL	OMC-CMC-C2C	-2.51	120.02	125.69
7	B	305	CHL	OMC-CMC-C2C	-2.50	120.03	125.69
7	A	311	CHL	C3B-C4B-NB	2.50	112.44	109.21
7	B	311	CHL	OMC-CMC-C2C	-2.50	120.03	125.69
7	A	308	CHL	OMC-CMC-C2C	-2.50	120.03	125.69
8	A	316	CLA	CHB-C4A-NA	2.49	127.96	124.51
8	B	317	CLA	CHB-C4A-NA	2.49	127.96	124.51
8	A	314	CLA	CHB-C4A-NA	2.49	127.96	124.51
8	A	306	CLA	CHB-C4A-NA	2.49	127.95	124.51
7	C	311	CHL	OMC-CMC-C2C	-2.49	120.06	125.69
7	A	305	CHL	O2D-CGD-O1D	-2.49	118.98	123.84
7	B	318	CHL	O2D-CGD-O1D	-2.49	118.98	123.84
7	C	318	CHL	OMC-CMC-C2C	-2.48	120.07	125.69
7	C	305	CHL	O2D-CGD-O1D	-2.48	118.99	123.84
9	B	319	LHG	C11-C10-C9	-2.48	101.84	114.42
7	C	313	CHL	CAC-C3C-C4C	2.48	128.02	124.81
8	A	307	CLA	CHB-C4A-NA	2.48	127.94	124.51
9	C	319	LHG	C11-C10-C9	-2.47	101.87	114.42
7	A	304	CHL	O2A-CGA-CBA	2.47	119.67	111.91
8	B	315	CLA	CHB-C4A-NA	2.47	127.93	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	306	CHL	O2D-CGD-O1D	-2.47	119.01	123.84
8	A	313	CLA	CHB-C4A-NA	2.47	127.93	124.51
8	C	315	CLA	CHB-C4A-NA	2.47	127.92	124.51
7	A	304	CHL	OMC-CMC-C2C	-2.47	120.11	125.69
7	C	311	CHL	O2D-CGD-O1D	-2.46	119.02	123.84
7	C	313	CHL	C4-C3-C5	2.46	119.41	115.27
7	A	317	CHL	OMC-CMC-C2C	-2.46	120.13	125.69
4	A	301	0UR	C9-C8-C7	-2.46	123.80	127.31
7	C	305	CHL	OMC-CMC-C2C	-2.46	120.13	125.69
7	C	305	CHL	O2A-CGA-CBA	2.46	119.61	111.91
8	B	314	CLA	CHB-C4A-NA	2.46	127.91	124.51
8	C	308	CLA	CHB-C4A-NA	2.45	127.90	124.51
7	B	309	CHL	OMC-CMC-C2C	-2.45	120.15	125.69
8	A	307	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
7	C	309	CHL	OMC-CMC-C2C	-2.44	120.16	125.69
8	A	313	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
7	A	309	CHL	O2D-CGD-O1D	-2.44	119.07	123.84
7	C	313	CHL	OMC-CMC-C2C	-2.44	120.17	125.69
6	B	304	NEX	C24-C23-C22	2.44	115.48	110.77
8	B	314	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
7	A	304	CHL	O2D-CGD-O1D	-2.43	119.08	123.84
7	B	310	CHL	OMC-CMC-C2C	-2.43	120.19	125.69
4	A	301	0UR	O42-C2-C41	-2.43	117.06	120.58
7	A	309	CHL	OMC-CMC-C2C	-2.43	120.20	125.69
7	A	310	CHL	CAC-C3C-C4C	2.43	127.96	124.81
7	C	309	CHL	O2D-CGD-O1D	-2.42	119.10	123.84
8	C	314	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
8	C	314	CLA	CHB-C4A-NA	2.42	127.86	124.51
7	C	318	CHL	O2D-CGD-O1D	-2.42	119.11	123.84
7	C	310	CHL	OMC-CMC-C2C	-2.41	120.23	125.69
8	C	308	CLA	C1-C2-C3	-2.41	122.84	126.75
7	C	305	CHL	C3B-C4B-NB	2.41	112.32	109.21
7	B	313	CHL	OMC-CMC-C2C	-2.41	120.25	125.69
5	B	302	0IE	C17-C16-C15	2.40	122.63	118.94
7	B	305	CHL	O2A-CGA-CBA	2.40	119.44	111.91
7	B	310	CHL	C5-C3-C4	2.40	119.90	114.60
7	C	313	CHL	OBD-CAD-C3D	-2.39	122.77	128.52
7	C	310	CHL	C5-C3-C4	2.39	119.88	114.60
7	B	312	CHL	C3B-C4B-NB	2.39	112.30	109.21
8	C	308	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
7	A	312	CHL	OMC-CMC-C2C	-2.39	120.29	125.69
7	A	309	CHL	C5-C3-C4	2.38	119.86	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	311	CHL	CAC-C3C-C4C	2.38	127.90	124.81
7	C	312	CHL	C3B-C4B-NB	2.37	112.28	109.21
4	B	301	0UR	C21-C12-C11	-2.37	119.61	122.92
7	A	305	CHL	CAC-C3C-C4C	2.37	127.88	124.81
7	A	311	CHL	CAC-C3C-C4C	2.37	127.88	124.81
7	B	306	CHL	CAC-C3C-C4C	2.36	127.87	124.81
7	B	311	CHL	CAC-C3C-C4C	2.36	127.87	124.81
7	C	305	CHL	CAC-C3C-C4C	2.36	127.87	124.81
6	C	304	NEX	C38-C25-C24	-2.36	111.63	114.28
7	B	305	CHL	C3B-C4B-NB	2.36	112.25	109.21
8	A	307	CLA	C1-C2-C3	-2.35	122.95	126.75
4	B	301	0UR	C9-C8-C7	-2.35	123.96	127.31
7	A	308	CHL	O2D-CGD-O1D	-2.35	119.25	123.84
7	A	310	CHL	O2D-CGD-O1D	-2.35	119.25	123.84
7	C	310	CHL	CAC-C3C-C4C	2.34	127.85	124.81
7	B	311	CHL	O2D-CGD-O1D	-2.33	119.28	123.84
7	A	304	CHL	C3B-C4B-NB	2.33	112.23	109.21
7	B	311	CHL	C3B-C4B-NB	2.33	112.23	109.21
7	B	309	CHL	O2D-CGD-O1D	-2.33	119.28	123.84
7	C	306	CHL	CAC-C3C-C4C	2.33	127.83	124.81
7	C	310	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
7	B	318	CHL	CAC-C3C-C4C	2.33	127.83	124.81
7	C	313	CHL	O2D-CGD-O1D	-2.32	119.29	123.84
7	A	304	CHL	CAC-C3C-C4C	2.31	127.81	124.81
8	C	317	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
6	B	304	NEX	C1-C2-C3	2.31	118.86	113.64
7	B	313	CHL	O2D-CGD-O1D	-2.31	119.32	123.84
7	A	312	CHL	O2D-CGD-O1D	-2.31	119.33	123.84
7	C	312	CHL	CAC-C3C-C4C	2.31	127.80	124.81
8	B	317	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
8	A	306	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
7	B	310	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
7	C	311	CHL	C4A-NA-C1A	-2.28	105.68	106.71
8	A	314	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
7	A	310	CHL	C3B-C4B-NB	2.28	112.16	109.21
8	C	315	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
8	B	307	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
8	C	307	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
5	B	302	0IE	C4-C3-C2	2.27	122.02	120.08
7	A	305	CHL	C3B-C4B-NB	2.27	112.14	109.21
8	A	316	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
7	C	311	CHL	C3B-C4B-NB	2.26	112.14	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	317	CHL	C3B-C4B-NB	2.26	112.14	109.21
8	B	315	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
7	B	310	CHL	C3B-C4B-NB	2.26	112.13	109.21
8	B	314	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
8	A	315	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
7	A	309	CHL	C3B-C4B-NB	2.25	112.12	109.21
7	B	305	CHL	CAC-C3C-C4C	2.25	127.73	124.81
7	A	308	CHL	CAC-C3C-C4C	2.25	127.73	124.81
8	B	308	CLA	C1-C2-C3	-2.25	123.12	126.75
4	B	301	0UR	O44-C45-O57	-2.25	117.99	122.93
8	C	316	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
8	C	314	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
7	C	318	CHL	CAC-C3C-C4C	2.23	127.71	124.81
7	A	317	CHL	CAC-C3C-C4C	2.23	127.70	124.81
8	B	316	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
6	A	303	NEX	O24-C25-C24	2.22	115.05	113.38
7	A	312	CHL	C3B-C4B-NB	2.21	112.07	109.21
7	B	313	CHL	C3B-C4B-NB	2.21	112.07	109.21
7	B	318	CHL	C3B-C4B-NB	2.21	112.06	109.21
7	B	309	CHL	C3B-C4B-NB	2.21	112.06	109.21
7	C	318	CHL	C3B-C4B-NB	2.21	112.06	109.21
6	C	304	NEX	C1-C2-C3	2.21	118.63	113.64
7	B	306	CHL	C3B-C4B-NB	2.20	112.06	109.21
9	B	319	LHG	C18-C17-C16	-2.20	103.27	114.42
7	B	312	CHL	CAC-C3C-C4C	2.19	127.66	124.81
7	A	308	CHL	C3B-C4B-NB	2.19	112.04	109.21
9	C	319	LHG	C18-C17-C16	-2.18	103.34	114.42
4	A	301	0UR	O44-C45-O57	-2.18	118.14	122.93
7	C	309	CHL	CAC-C3C-C4C	2.18	127.64	124.81
7	A	311	CHL	O2D-CGD-O1D	-2.17	119.59	123.84
6	A	303	NEX	C24-C23-C22	2.17	114.96	110.77
7	C	313	CHL	C3B-C4B-NB	2.17	112.01	109.21
8	A	313	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
7	C	310	CHL	C3B-C4B-NB	2.16	112.00	109.21
7	B	312	CHL	O2D-CGD-O1D	-2.16	119.62	123.84
7	C	306	CHL	C3B-C4B-NB	2.15	111.99	109.21
7	C	312	CHL	O2D-CGD-O1D	-2.15	119.63	123.84
7	B	309	CHL	CAC-C3C-C4C	2.14	127.59	124.81
6	B	304	NEX	C38-C25-C24	-2.14	111.87	114.28
7	C	318	CHL	CAA-C2A-C3A	-2.14	111.10	116.10
4	C	301	0UR	C15-C14-C13	-2.13	116.57	123.22
7	B	311	CHL	O2A-CGA-CBA	2.12	120.61	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	301	0UR	O44-C45-O57	-2.12	118.28	122.93
7	C	309	CHL	C3B-C4B-NB	2.11	111.94	109.21
8	C	317	CLA	CHD-C1D-ND	-2.11	122.51	124.45
4	C	301	0UR	C21-C12-C11	-2.11	119.96	122.92
8	B	317	CLA	CHD-C1D-ND	-2.11	122.51	124.45
8	A	306	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
4	B	301	0UR	C28-C19-C18	-2.09	110.05	112.70
4	A	301	0UR	C21-C12-C11	-2.09	119.99	122.92
7	B	318	CHL	CAA-C2A-C3A	-2.09	111.22	116.10
6	A	303	NEX	C1-C2-C3	2.09	118.36	113.64
8	C	308	CLA	CHD-C1D-ND	-2.09	122.54	124.45
6	C	304	NEX	O24-C25-C24	2.08	114.95	113.38
8	B	314	CLA	C1-C2-C3	-2.08	122.44	126.04
4	B	301	0UR	C15-C14-C13	-2.08	116.72	123.22
8	A	307	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
4	C	301	0UR	O42-C2-C41	-2.08	117.57	120.58
5	C	302	0IE	C4-C3-C2	2.08	121.86	120.08
8	B	307	CLA	CHD-C1D-ND	-2.07	122.56	124.45
7	C	311	CHL	O2A-CGA-CBA	2.06	120.37	112.23
7	A	317	CHL	CAA-C2A-C3A	-2.05	111.30	116.10
7	B	310	CHL	O1D-CGD-CBD	-2.05	120.28	124.48
8	A	313	CLA	C1-C2-C3	-2.05	122.50	126.04
8	A	307	CLA	CHD-C1D-ND	-2.04	122.58	124.45
8	A	316	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
9	C	319	LHG	C27-C26-C25	-2.04	104.07	114.42
6	B	304	NEX	O24-C25-C24	2.04	114.91	113.38
8	C	314	CLA	C1-C2-C3	-2.02	122.54	126.04
8	C	317	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
8	C	315	CLA	CHD-C1D-ND	-2.01	122.60	124.45
9	B	319	LHG	C27-C26-C25	-2.00	104.27	114.42
8	A	316	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (90) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	304	CHL	NA
7	A	304	CHL	NC
7	A	304	CHL	ND
7	A	305	CHL	NA
7	A	305	CHL	NC
7	A	305	CHL	ND
7	A	308	CHL	NA

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Mol	Chain	Res	Type	Atom
7	A	308	CHL	NC
7	A	308	CHL	ND
7	A	309	CHL	NA
7	A	309	CHL	NC
7	A	309	CHL	ND
7	A	310	CHL	NA
7	A	310	CHL	NC
7	A	310	CHL	ND
7	A	311	CHL	NA
7	A	311	CHL	NC
7	A	311	CHL	ND
7	A	312	CHL	NA
7	A	312	CHL	NC
7	A	312	CHL	ND
7	A	317	CHL	NA
7	A	317	CHL	NC
7	A	317	CHL	ND
7	B	305	CHL	NA
7	B	305	CHL	NC
7	B	305	CHL	ND
7	B	306	CHL	NA
7	B	306	CHL	NC
7	B	306	CHL	ND
7	B	309	CHL	NA
7	B	309	CHL	NC
7	B	309	CHL	ND
7	B	310	CHL	NA
7	B	310	CHL	NC
7	B	310	CHL	ND
7	B	311	CHL	NA
7	B	311	CHL	NC
7	B	311	CHL	ND
7	B	312	CHL	NA
7	B	312	CHL	NC
7	B	312	CHL	ND
7	B	313	CHL	NA
7	B	313	CHL	NC
7	B	313	CHL	ND
7	B	318	CHL	NA
7	B	318	CHL	NC
7	B	318	CHL	ND
7	C	305	CHL	NA

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Mol	Chain	Res	Type	Atom
7	C	305	CHL	NC
7	C	305	CHL	ND
7	C	306	CHL	NA
7	C	306	CHL	NC
7	C	306	CHL	ND
7	C	309	CHL	NA
7	C	309	CHL	NC
7	C	309	CHL	ND
7	C	310	CHL	NA
7	C	310	CHL	NC
7	C	310	CHL	ND
7	C	311	CHL	NA
7	C	311	CHL	NC
7	C	311	CHL	ND
7	C	312	CHL	NA
7	C	312	CHL	NC
7	C	312	CHL	ND
7	C	313	CHL	NA
7	C	313	CHL	NC
7	C	313	CHL	ND
7	C	318	CHL	NA
7	C	318	CHL	NC
7	C	318	CHL	ND
8	A	306	CLA	ND
8	A	307	CLA	ND
8	A	313	CLA	ND
8	A	314	CLA	ND
8	A	315	CLA	ND
8	A	316	CLA	ND
8	B	307	CLA	ND
8	B	308	CLA	ND
8	B	314	CLA	ND
8	B	315	CLA	ND
8	B	316	CLA	ND
8	B	317	CLA	ND
8	C	307	CLA	ND
8	C	308	CLA	ND
8	C	314	CLA	ND
8	C	315	CLA	ND
8	C	316	CLA	ND
8	C	317	CLA	ND

All (506) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	0UR	C5-C6-C7-C20
4	A	301	0UR	C46-C45-O44-C43
4	A	301	0UR	O57-C45-O44-C43
4	B	301	0UR	C46-C45-O44-C43
4	B	301	0UR	O57-C45-O44-C43
4	C	301	0UR	C46-C45-O44-C43
4	C	301	0UR	O57-C45-O44-C43
5	A	302	0IE	C11-C12-C13-C14
5	A	302	0IE	C22-C12-C13-C14
5	B	302	0IE	O1-C2-C3-C20
5	B	303	0IE	C14-C15-C16-C17
5	B	303	0IE	C14-C15-C16-C23
5	C	303	0IE	C14-C15-C16-C23
7	A	304	CHL	C2-C3-C5-C6
7	A	304	CHL	C4-C3-C5-C6
7	A	305	CHL	CHA-CBD-CGD-O1D
7	A	305	CHL	CHA-CBD-CGD-O2D
7	A	311	CHL	C11-C10-C8-C9
7	A	317	CHL	CAD-CBD-CGD-O1D
7	A	317	CHL	CAD-CBD-CGD-O2D
7	B	306	CHL	CHA-CBD-CGD-O1D
7	B	306	CHL	CHA-CBD-CGD-O2D
7	B	306	CHL	C14-C13-C15-C16
7	B	318	CHL	CHA-CBD-CGD-O1D
7	B	318	CHL	CHA-CBD-CGD-O2D
7	B	318	CHL	CAD-CBD-CGD-O1D
7	B	318	CHL	CAD-CBD-CGD-O2D
7	C	305	CHL	C2-C3-C5-C6
7	C	305	CHL	C4-C3-C5-C6
7	C	306	CHL	CHA-CBD-CGD-O1D
7	C	306	CHL	CHA-CBD-CGD-O2D
7	C	318	CHL	CHA-CBD-CGD-O1D
7	C	318	CHL	CHA-CBD-CGD-O2D
7	C	318	CHL	CAD-CBD-CGD-O1D
8	A	313	CLA	CBD-CGD-O2D-CED
8	A	314	CLA	C1A-C2A-CAA-CBA
8	A	314	CLA	CHA-CBD-CGD-O1D
8	A	314	CLA	CHA-CBD-CGD-O2D
8	A	316	CLA	CHA-CBD-CGD-O1D
8	A	316	CLA	CHA-CBD-CGD-O2D
8	A	316	CLA	CBD-CGD-O2D-CED
8	B	308	CLA	C1A-C2A-CAA-CBA
8	B	314	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	B	317	CLA	CHA-CBD-CGD-O1D
8	B	317	CLA	CHA-CBD-CGD-O2D
8	B	317	CLA	CBD-CGD-O2D-CED
8	C	308	CLA	C1A-C2A-CAA-CBA
8	C	314	CLA	CBD-CGD-O2D-CED
8	C	317	CLA	CHA-CBD-CGD-O1D
8	C	317	CLA	CHA-CBD-CGD-O2D
9	A	318	LHG	O1-C1-C2-C3
9	A	318	LHG	C4-O6-P-O5
9	B	319	LHG	O1-C1-C2-C3
9	C	319	LHG	C3-O3-P-O5
9	C	319	LHG	C4-O6-P-O5
7	A	311	CHL	CBD-CGD-O2D-CED
7	B	312	CHL	CBD-CGD-O2D-CED
7	C	312	CHL	CBD-CGD-O2D-CED
8	A	313	CLA	O1D-CGD-O2D-CED
8	B	314	CLA	O1D-CGD-O2D-CED
8	C	314	CLA	O1D-CGD-O2D-CED
8	B	308	CLA	CBD-CGD-O2D-CED
8	C	316	CLA	CBD-CGD-O2D-CED
8	C	317	CLA	CBD-CGD-O2D-CED
8	B	317	CLA	O1D-CGD-O2D-CED
8	A	316	CLA	O1D-CGD-O2D-CED
7	B	318	CHL	CBD-CGD-O2D-CED
7	C	312	CHL	O1D-CGD-O2D-CED
7	A	312	CHL	CBD-CGD-O2D-CED
8	A	315	CLA	CBD-CGD-O2D-CED
7	A	317	CHL	CBD-CGD-O2D-CED
7	A	309	CHL	C2A-CAA-CBA-CGA
7	A	311	CHL	C2A-CAA-CBA-CGA
7	B	310	CHL	C2A-CAA-CBA-CGA
7	A	311	CHL	O1D-CGD-O2D-CED
7	B	312	CHL	O1D-CGD-O2D-CED
5	B	303	0IE	C13-C14-C15-C16
7	B	309	CHL	CBD-CGD-O2D-CED
7	B	310	CHL	CBD-CGD-O2D-CED
7	C	309	CHL	CBD-CGD-O2D-CED
7	C	318	CHL	CBD-CGD-O2D-CED
8	A	307	CLA	CBD-CGD-O2D-CED
9	A	318	LHG	O2-C2-C3-O3
9	C	319	LHG	O2-C2-C3-O3
8	B	315	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
7	A	308	CHL	CBD-CGD-O2D-CED
7	A	310	CHL	CBD-CGD-O2D-CED
7	B	305	CHL	CBD-CGD-O2D-CED
7	B	313	CHL	CBD-CGD-O2D-CED
7	C	305	CHL	CBD-CGD-O2D-CED
7	C	313	CHL	CBD-CGD-O2D-CED
8	C	315	CLA	C3-C5-C6-C7
7	C	311	CHL	C2A-CAA-CBA-CGA
8	C	308	CLA	C2A-CAA-CBA-CGA
8	A	307	CLA	CBA-CGA-O2A-C1
8	B	308	CLA	O1D-CGD-O2D-CED
8	C	317	CLA	O1D-CGD-O2D-CED
8	A	307	CLA	O1A-CGA-O2A-C1
9	A	318	LHG	C28-C29-C30-C31
7	C	311	CHL	CBD-CGD-O2D-CED
7	B	305	CHL	C8-C10-C11-C12
7	B	312	CHL	C13-C15-C16-C17
7	A	305	CHL	C6-C7-C8-C9
7	A	310	CHL	C6-C7-C8-C9
7	A	311	CHL	C6-C7-C8-C9
7	A	311	CHL	C14-C13-C15-C16
7	B	305	CHL	C11-C12-C13-C14
7	B	312	CHL	C6-C7-C8-C9
7	B	312	CHL	C11-C10-C8-C9
7	B	312	CHL	C14-C13-C15-C16
7	C	306	CHL	C14-C13-C15-C16
7	C	313	CHL	C6-C7-C8-C9
7	A	304	CHL	CBD-CGD-O2D-CED
7	B	312	CHL	C2A-CAA-CBA-CGA
4	B	301	0UR	C5-C6-C7-C20
5	A	302	0IE	C23-C16-C17-C18
7	A	305	CHL	C8-C10-C11-C12
8	C	316	CLA	O1D-CGD-O2D-CED
9	A	318	LHG	C24-C25-C26-C27
7	A	305	CHL	C10-C11-C12-C13
7	A	310	CHL	C5-C6-C7-C8
7	A	310	CHL	C8-C10-C11-C12
7	B	306	CHL	C13-C15-C16-C17
7	B	312	CHL	C8-C10-C11-C12
7	C	313	CHL	C5-C6-C7-C8
8	B	307	CLA	C8-C10-C11-C12
4	A	301	0UR	O44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
7	C	305	CHL	C15-C16-C17-C18
7	C	313	CHL	C8-C10-C11-C12
8	A	306	CLA	C8-C10-C11-C12
8	C	307	CLA	C8-C10-C11-C12
7	C	310	CHL	CBD-CGD-O2D-CED
7	A	312	CHL	C8-C10-C11-C12
7	B	305	CHL	C15-C16-C17-C18
7	A	312	CHL	C13-C15-C16-C17
7	B	313	CHL	C8-C10-C11-C12
7	B	311	CHL	CBD-CGD-O2D-CED
9	B	319	LHG	C24-C25-C26-C27
8	C	315	CLA	C6-C7-C8-C10
7	B	318	CHL	O1D-CGD-O2D-CED
7	C	305	CHL	C8-C10-C11-C12
7	C	305	CHL	C13-C15-C16-C17
5	B	303	0IE	C4-C5-C6-C7
5	B	303	0IE	C12-C13-C14-C15
5	C	303	0IE	C12-C13-C14-C15
7	C	306	CHL	C13-C15-C16-C17
7	A	304	CHL	C5-C6-C7-C8
7	B	312	CHL	C10-C11-C12-C13
7	C	305	CHL	C5-C6-C7-C8
7	A	311	CHL	C8-C10-C11-C12
7	B	305	CHL	C13-C15-C16-C17
9	A	318	LHG	C4-O6-P-O3
7	A	311	CHL	C13-C15-C16-C17
7	A	312	CHL	O1D-CGD-O2D-CED
8	A	315	CLA	O1D-CGD-O2D-CED
7	A	305	CHL	C2A-CAA-CBA-CGA
7	B	306	CHL	C2A-CAA-CBA-CGA
7	C	306	CHL	C2A-CAA-CBA-CGA
7	C	312	CHL	C2A-CAA-CBA-CGA
9	C	319	LHG	C24-C25-C26-C27
5	C	303	0IE	C13-C14-C15-C16
5	A	302	0IE	C14-C15-C16-C23
5	B	302	0IE	C14-C15-C16-C23
5	C	302	0IE	C14-C15-C16-C23
7	A	312	CHL	C16-C17-C18-C20
7	C	313	CHL	C16-C17-C18-C19
8	C	308	CLA	CBA-CGA-O2A-C1
7	A	317	CHL	O1D-CGD-O2D-CED
7	B	309	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
7	C	305	CHL	C10-C11-C12-C13
4	A	301	0UR	O57-C45-C46-C47
5	A	302	0IE	C14-C15-C16-C17
5	B	302	0IE	C14-C15-C16-C17
5	C	302	0IE	C14-C15-C16-C17
5	C	303	0IE	C14-C15-C16-C17
8	A	316	CLA	C6-C7-C8-C10
7	A	311	CHL	C16-C17-C18-C20
7	C	305	CHL	C16-C17-C18-C19
9	A	318	LHG	C30-C31-C32-C33
7	C	318	CHL	O1D-CGD-O2D-CED
7	A	305	CHL	C13-C15-C16-C17
9	C	319	LHG	O1-C1-C2-C3
8	C	308	CLA	CBD-CGD-O2D-CED
7	A	312	CHL	C16-C17-C18-C19
7	B	305	CHL	C16-C17-C18-C19
7	B	305	CHL	C16-C17-C18-C20
7	B	310	CHL	O1D-CGD-O2D-CED
8	A	307	CLA	O1D-CGD-O2D-CED
7	A	310	CHL	C3A-C2A-CAA-CBA
7	B	311	CHL	C3A-C2A-CAA-CBA
8	A	314	CLA	C3A-C2A-CAA-CBA
5	B	302	0IE	C13-C14-C15-C16
9	C	319	LHG	C28-C29-C30-C31
7	B	313	CHL	C16-C17-C18-C19
7	B	313	CHL	C16-C17-C18-C20
7	C	313	CHL	C16-C17-C18-C20
7	C	306	CHL	CBD-CGD-O2D-CED
7	C	313	CHL	C4-C3-C5-C6
7	C	313	CHL	C2-C3-C5-C6
7	C	309	CHL	O1D-CGD-O2D-CED
9	A	318	LHG	O1-C1-C2-O2
9	B	319	LHG	O1-C1-C2-O2
9	C	319	LHG	C27-C28-C29-C30
7	A	311	CHL	C16-C17-C18-C19
7	A	311	CHL	C15-C16-C17-C18
7	A	310	CHL	O1D-CGD-O2D-CED
8	B	307	CLA	C2-C1-O2A-CGA
8	C	307	CLA	C2-C1-O2A-CGA
8	C	308	CLA	O1A-CGA-O2A-C1
7	A	312	CHL	C10-C11-C12-C13
7	A	312	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
7	C	313	CHL	C15-C16-C17-C18
7	B	313	CHL	C15-C16-C17-C18
7	B	313	CHL	O1D-CGD-O2D-CED
7	A	310	CHL	C11-C10-C8-C7
7	A	311	CHL	C12-C13-C15-C16
7	B	305	CHL	C12-C13-C15-C16
9	B	319	LHG	C27-C28-C29-C30
7	C	306	CHL	C15-C16-C17-C18
7	A	308	CHL	O1D-CGD-O2D-CED
9	A	318	LHG	C29-C30-C31-C32
7	C	305	CHL	O1D-CGD-O2D-CED
7	C	313	CHL	O1D-CGD-O2D-CED
9	A	318	LHG	C11-C10-C9-C8
7	B	305	CHL	O1D-CGD-O2D-CED
7	A	309	CHL	CBD-CGD-O2D-CED
7	B	306	CHL	CBD-CGD-O2D-CED
9	A	318	LHG	O7-C5-C6-O8
7	C	305	CHL	C16-C17-C18-C20
8	C	315	CLA	C6-C7-C8-C9
7	A	310	CHL	C2A-CAA-CBA-CGA
8	B	308	CLA	C2A-CAA-CBA-CGA
9	A	318	LHG	C27-C28-C29-C30
7	A	310	CHL	C1A-C2A-CAA-CBA
7	B	311	CHL	C1A-C2A-CAA-CBA
8	C	315	CLA	C1A-C2A-CAA-CBA
4	A	301	0UR	C46-C47-C48-C49
7	A	310	CHL	C3-C5-C6-C7
7	A	309	CHL	CBA-CGA-O2A-C1
9	C	319	LHG	C29-C30-C31-C32
7	C	311	CHL	O1D-CGD-O2D-CED
9	B	319	LHG	C29-C30-C31-C32
7	C	306	CHL	C3-C5-C6-C7
8	A	306	CLA	C3-C5-C6-C7
4	B	301	0UR	C47-C48-C49-C50
7	B	306	CHL	C15-C16-C17-C18
9	A	318	LHG	C4-C5-C6-O8
9	C	319	LHG	C4-C5-C6-O8
7	A	310	CHL	C11-C12-C13-C15
7	A	310	CHL	C12-C13-C15-C16
7	A	304	CHL	O1D-CGD-O2D-CED
9	B	319	LHG	C26-C27-C28-C29
9	B	319	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
9	A	318	LHG	C32-C33-C34-C35
7	C	310	CHL	O1D-CGD-O2D-CED
5	C	303	0IE	C10-C11-C12-C22
7	B	311	CHL	O1D-CGD-O2D-CED
8	B	307	CLA	CBA-CGA-O2A-C1
8	C	307	CLA	CBA-CGA-O2A-C1
8	A	306	CLA	C2-C1-O2A-CGA
7	B	306	CHL	C3-C5-C6-C7
4	B	301	0UR	C46-C47-C48-C49
5	B	302	0IE	C16-C17-C18-C19
9	B	319	LHG	C9-C10-C11-C12
7	A	309	CHL	O1A-CGA-O2A-C1
9	A	318	LHG	C23-C24-C25-C26
9	C	319	LHG	C23-C24-C25-C26
7	B	306	CHL	C10-C11-C12-C13
5	C	303	0IE	C10-C11-C12-C13
8	C	317	CLA	C6-C7-C8-C10
7	A	305	CHL	C12-C13-C15-C16
7	A	312	CHL	C12-C13-C15-C16
7	B	305	CHL	C11-C12-C13-C15
7	B	306	CHL	C12-C13-C15-C16
7	B	312	CHL	C6-C7-C8-C10
7	C	306	CHL	C12-C13-C15-C16
7	C	313	CHL	C11-C10-C8-C7
7	B	305	CHL	C3-C5-C6-C7
7	A	310	CHL	C11-C10-C8-C9
8	B	315	CLA	C11-C12-C13-C14
7	A	310	CHL	CBA-CGA-O2A-C1
8	C	317	CLA	CBA-CGA-O2A-C1
8	A	316	CLA	C11-C10-C8-C7
8	B	307	CLA	O1A-CGA-O2A-C1
8	C	307	CLA	O1A-CGA-O2A-C1
4	A	301	0UR	C5-C6-C7-C8
7	B	306	CHL	CBA-CGA-O2A-C1
7	B	310	CHL	CBA-CGA-O2A-C1
7	C	306	CHL	CBA-CGA-O2A-C1
7	A	305	CHL	C15-C16-C17-C18
9	A	318	LHG	O6-C4-C5-C6
9	C	319	LHG	C30-C31-C32-C33
8	B	308	CLA	CBA-CGA-O2A-C1
9	A	318	LHG	C2-C3-O3-P
9	A	318	LHG	C5-C4-O6-P

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Mol	Chain	Res	Type	Atoms
8	C	308	CLA	O1D-CGD-O2D-CED
7	A	312	CHL	C3A-C2A-CAA-CBA
8	C	308	CLA	C3A-C2A-CAA-CBA
8	C	315	CLA	C3A-C2A-CAA-CBA
7	B	312	CHL	C16-C17-C18-C20
9	C	319	LHG	O1-C1-C2-O2
7	A	310	CHL	O1A-CGA-O2A-C1
9	C	319	LHG	O7-C5-C6-O8
7	B	312	CHL	C16-C17-C18-C19
9	A	318	LHG	C1-C2-C3-O3
7	A	305	CHL	C2-C1-O2A-CGA
7	C	313	CHL	C2-C1-O2A-CGA
8	C	317	CLA	O1A-CGA-O2A-C1
7	C	305	CHL	C11-C12-C13-C14
7	B	313	CHL	C5-C6-C7-C8
7	C	306	CHL	C10-C11-C12-C13
8	A	307	CLA	C2A-CAA-CBA-CGA
7	A	309	CHL	O1D-CGD-O2D-CED
7	C	306	CHL	O1D-CGD-O2D-CED
4	B	301	0UR	C5-C6-C7-C8
7	A	305	CHL	CBD-CGD-O2D-CED
7	A	311	CHL	C6-C7-C8-C10
7	A	311	CHL	C11-C10-C8-C7
7	B	312	CHL	C12-C13-C15-C16
7	C	305	CHL	C11-C12-C13-C15
7	C	306	CHL	O1A-CGA-O2A-C1
5	C	302	0IE	C13-C14-C15-C16
5	C	303	0IE	C3-C4-C5-C6
9	C	319	LHG	C9-C10-C11-C12
7	B	310	CHL	O1A-CGA-O2A-C1
4	A	301	0UR	O42-C2-C3-C4
4	B	301	0UR	O42-C2-C3-C4
4	C	301	0UR	O42-C2-C3-C4
5	A	302	0IE	O1-C2-C3-C4
5	B	302	0IE	C21-C7-C8-C9
5	B	302	0IE	O1-C2-C3-C4
5	C	302	0IE	O1-C2-C3-C4
7	C	318	CHL	CAD-CBD-CGD-O2D
8	A	306	CLA	CAD-CBD-CGD-O2D
8	A	313	CLA	CAD-CBD-CGD-O2D
8	B	308	CLA	CAD-CBD-CGD-O2D
8	B	314	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
8	C	316	CLA	CAD-CBD-CGD-O2D
9	A	318	LHG	O6-C4-C5-O7
4	C	301	0UR	C46-C47-C48-C49
9	C	319	LHG	C1-C2-C3-O3
7	B	306	CHL	O1A-CGA-O2A-C1
9	A	318	LHG	C12-C13-C14-C15
7	B	306	CHL	O1D-CGD-O2D-CED
8	B	308	CLA	O1A-CGA-O2A-C1
7	C	305	CHL	C14-C13-C15-C16
7	C	311	CHL	CAA-CBA-CGA-O2A
5	A	302	0IE	C15-C16-C17-C18
7	A	312	CHL	C1A-C2A-CAA-CBA
7	B	306	CHL	C1A-C2A-CAA-CBA
9	A	318	LHG	C3-O3-P-O6
9	C	319	LHG	C3-O3-P-O6
9	A	318	LHG	C3-O3-P-O4
9	A	318	LHG	C4-O6-P-O4
7	A	305	CHL	CBA-CGA-O2A-C1
7	C	311	CHL	CBA-CGA-O2A-C1
5	C	302	0IE	O1-C2-C3-C20
7	A	305	CHL	C11-C12-C13-C15
7	A	312	CHL	C11-C12-C13-C15
7	B	306	CHL	C11-C12-C13-C15
7	B	312	CHL	C11-C10-C8-C7
7	B	312	CHL	C11-C12-C13-C15
7	C	305	CHL	C12-C13-C15-C16
7	C	313	CHL	C11-C12-C13-C15
8	B	315	CLA	C3A-C2A-CAA-CBA
8	B	317	CLA	C6-C7-C8-C10
8	B	307	CLA	C16-C17-C18-C20
7	A	305	CHL	C11-C10-C8-C9
7	A	305	CHL	C14-C13-C15-C16
7	C	313	CHL	C11-C10-C8-C9
8	A	314	CLA	C11-C12-C13-C14
7	A	305	CHL	O1A-CGA-O2A-C1
7	C	312	CHL	C3-C5-C6-C7
7	B	311	CHL	CAA-CBA-CGA-O2A
8	A	316	CLA	C2A-CAA-CBA-CGA
8	B	317	CLA	C2A-CAA-CBA-CGA
8	C	317	CLA	C2A-CAA-CBA-CGA
7	A	309	CHL	C2-C1-O2A-CGA
7	B	306	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
7	B	310	CHL	C2-C1-O2A-CGA
7	A	305	CHL	O1D-CGD-O2D-CED
5	A	302	0IE	C16-C17-C18-C19
5	C	302	0IE	C16-C17-C18-C19
8	A	316	CLA	CBA-CGA-O2A-C1
6	A	303	NEX	C11-C10-C9-C8
9	B	319	LHG	C3-O3-P-O6
9	B	319	LHG	C28-C29-C30-C31
7	A	305	CHL	C11-C12-C13-C14
7	A	312	CHL	C14-C13-C15-C16
7	C	313	CHL	C13-C15-C16-C17
7	C	312	CHL	CBA-CGA-O2A-C1
8	A	316	CLA	O1A-CGA-O2A-C1
5	A	302	0IE	C13-C14-C15-C16
8	A	307	CLA	C2-C1-O2A-CGA
7	C	312	CHL	C6-C7-C8-C9
8	B	315	CLA	C5-C6-C7-C8
8	B	307	CLA	C16-C17-C18-C19
7	C	306	CHL	C4-C3-C5-C6
7	A	312	CHL	C6-C7-C8-C9
7	A	312	CHL	C11-C12-C13-C14
7	B	312	CHL	C11-C12-C13-C14
7	B	313	CHL	C6-C7-C8-C9
9	A	318	LHG	C11-C12-C13-C14
6	A	303	NEX	C39-C29-C30-C31
6	B	304	NEX	C39-C29-C30-C31
6	C	304	NEX	C39-C29-C30-C31
7	C	312	CHL	O1A-CGA-O2A-C1
4	C	301	0UR	C5-C6-C7-C20
5	B	302	0IE	C23-C16-C17-C18
5	C	302	0IE	C22-C12-C13-C14
7	A	304	CHL	C1A-C2A-CAA-CBA
7	A	305	CHL	C1A-C2A-CAA-CBA
8	A	313	CLA	C1A-C2A-CAA-CBA
8	B	315	CLA	C1A-C2A-CAA-CBA
7	A	310	CHL	C6-C7-C8-C10
7	B	313	CHL	C12-C13-C15-C16
8	B	315	CLA	C11-C12-C13-C15
8	B	308	CLA	CAA-CBA-CGA-O2A
7	A	310	CHL	C10-C11-C12-C13
6	A	303	NEX	C28-C29-C30-C31
6	B	304	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
6	C	304	NEX	C28-C29-C30-C31
7	A	312	CHL	C2-C1-O2A-CGA
7	B	313	CHL	C2-C1-O2A-CGA
7	C	306	CHL	C2-C1-O2A-CGA
8	A	313	CLA	C2A-CAA-CBA-CGA
8	B	317	CLA	O1A-CGA-O2A-C1
7	A	312	CHL	C4-C3-C5-C6
8	C	307	CLA	C10-C11-C12-C13
8	B	316	CLA	CAA-CBA-CGA-O2A
8	C	316	CLA	CAA-CBA-CGA-O2A
8	A	315	CLA	CAA-CBA-CGA-O2A
8	B	316	CLA	CAA-CBA-CGA-O1A
8	C	316	CLA	CAA-CBA-CGA-O1A
8	B	317	CLA	CBA-CGA-O2A-C1
7	A	305	CHL	C11-C10-C8-C7
8	C	315	CLA	C11-C10-C8-C7
7	B	306	CHL	CAA-CBA-CGA-O2A
9	A	318	LHG	O8-C23-C24-C25
4	C	301	0UR	O44-C45-C46-C47
7	C	306	CHL	CAA-CBA-CGA-O2A
7	C	312	CHL	C6-C7-C8-C10
9	C	319	LHG	C24-C23-O8-C6
5	C	303	0IE	C21-C7-C8-C9
5	C	303	0IE	C20-C3-C4-C5
5	C	303	0IE	O1-C2-C30-C31
7	A	305	CHL	CAA-CBA-CGA-O2A
4	B	301	0UR	O44-C45-C46-C47
7	B	313	CHL	C4-C3-C5-C6
7	B	313	CHL	C13-C15-C16-C17
7	B	306	CHL	C11-C12-C13-C14
7	C	313	CHL	C11-C12-C13-C14
8	A	315	CLA	CAA-CBA-CGA-O1A
7	A	304	CHL	C3A-C2A-CAA-CBA
7	B	313	CHL	C3A-C2A-CAA-CBA
7	C	305	CHL	C3A-C2A-CAA-CBA
7	B	310	CHL	CAD-CBD-CGD-O2D
8	B	316	CLA	CAD-CBD-CGD-O2D
8	C	314	CLA	CAD-CBD-CGD-O2D
7	A	312	CHL	C5-C6-C7-C8
9	B	319	LHG	C11-C12-C13-C14
8	B	307	CLA	C5-C6-C7-C8
7	A	309	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
9	A	318	LHG	C26-C27-C28-C29
5	B	302	0IE	C15-C16-C17-C18
5	C	302	0IE	C11-C12-C13-C14
7	A	317	CHL	CHA-CBD-CGD-O1D
7	A	317	CHL	CHA-CBD-CGD-O2D
8	A	307	CLA	CHA-CBD-CGD-O2D
8	A	315	CLA	CHA-CBD-CGD-O1D
8	A	315	CLA	CHA-CBD-CGD-O2D
8	B	307	CLA	CHA-CBD-CGD-O1D
8	C	307	CLA	CHA-CBD-CGD-O2D
8	C	316	CLA	CHA-CBD-CGD-O2D
7	C	311	CHL	O1A-CGA-O2A-C1
7	B	310	CHL	CAA-CBA-CGA-O2A
7	C	312	CHL	CAA-CBA-CGA-O2A
7	B	313	CHL	C2-C3-C5-C6
7	A	305	CHL	CAA-CBA-CGA-O1A
7	A	309	CHL	CAA-CBA-CGA-O1A
4	C	301	0UR	C5-C6-C7-C8
7	B	305	CHL	C1A-C2A-CAA-CBA
7	B	313	CHL	C1A-C2A-CAA-CBA
7	C	305	CHL	C1A-C2A-CAA-CBA
7	C	306	CHL	C1A-C2A-CAA-CBA
7	C	311	CHL	C1A-C2A-CAA-CBA
8	B	314	CLA	C1A-C2A-CAA-CBA
7	B	306	CHL	CAA-CBA-CGA-O1A
7	C	306	CHL	CAA-CBA-CGA-O1A
7	A	305	CHL	C5-C6-C7-C8
9	B	319	LHG	C3-O3-P-O5
9	A	318	LHG	O10-C23-C24-C25
8	A	314	CLA	C10-C11-C12-C13
8	B	314	CLA	C6-C7-C8-C10
7	B	310	CHL	CAA-CBA-CGA-O1A
7	A	310	CHL	C4-C3-C5-C6
7	B	313	CHL	C14-C13-C15-C16
7	C	312	CHL	CAA-CBA-CGA-O1A
4	A	301	0UR	O42-C2-C3-C43
4	B	301	0UR	O42-C2-C3-C43
4	C	301	0UR	O42-C2-C3-C43
5	A	302	0IE	O1-C2-C3-C20
5	C	303	0IE	C2-C3-C4-C5
7	C	306	CHL	C2-C3-C5-C6
8	B	308	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
5	C	302	0IE	C15-C16-C17-C18

There are no ring outliers.

50 monomers are involved in 141 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	307	CLA	4	0
7	B	305	CHL	5	0
6	C	304	NEX	14	0
8	A	306	CLA	4	0
7	C	312	CHL	3	0
4	B	301	0UR	2	0
7	B	313	CHL	5	0
5	C	303	0IE	1	0
8	C	316	CLA	1	0
8	C	317	CLA	4	0
9	C	319	LHG	3	0
7	C	305	CHL	3	0
8	B	316	CLA	2	0
8	B	317	CLA	4	0
7	B	306	CHL	4	0
7	A	312	CHL	8	0
4	C	301	0UR	4	0
8	A	316	CLA	3	0
6	B	304	NEX	7	0
7	A	304	CHL	5	0
8	A	314	CLA	1	0
7	C	313	CHL	9	0
6	A	303	NEX	6	0
5	B	303	0IE	1	0
8	B	315	CLA	1	0
7	B	312	CHL	6	0
7	A	310	CHL	2	0
7	A	309	CHL	2	0
7	C	311	CHL	3	0
7	C	310	CHL	6	0
8	C	308	CLA	2	0
7	A	311	CHL	7	0
7	B	318	CHL	2	0
7	C	306	CHL	4	0
8	A	313	CLA	3	0
7	A	308	CHL	1	0

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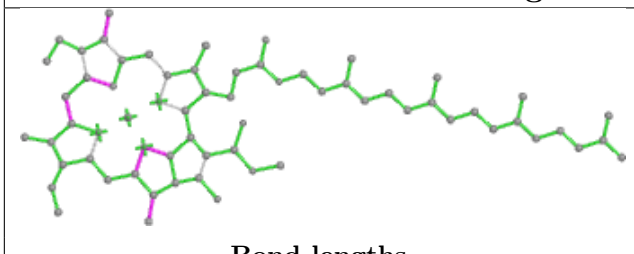
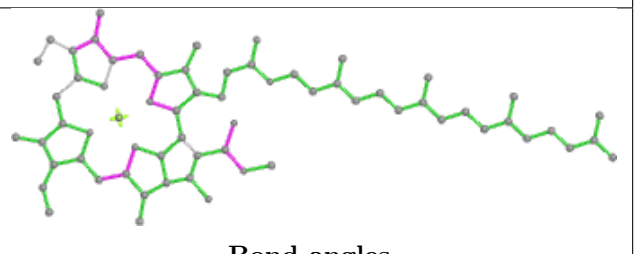
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	310	CHL	4	0
8	B	308	CLA	3	0
8	B	314	CLA	1	0
9	B	319	LHG	2	0
4	A	301	0UR	3	0
7	B	311	CHL	2	0
7	A	305	CHL	2	0
7	C	309	CHL	1	0
8	C	314	CLA	2	0
8	C	315	CLA	1	0
8	A	307	CLA	2	0
9	A	318	LHG	3	0
7	C	318	CHL	3	0
8	C	307	CLA	3	0

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

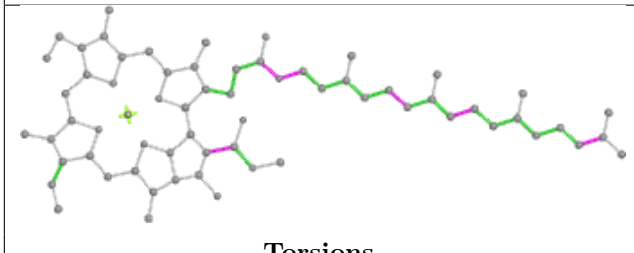
Ligand CLA B 307



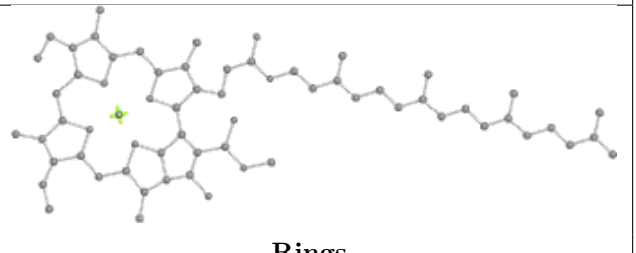
Bond lengths



Bond angles

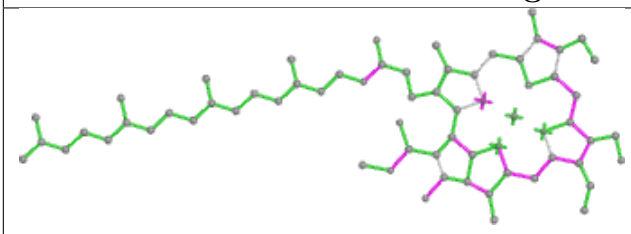


Torsions

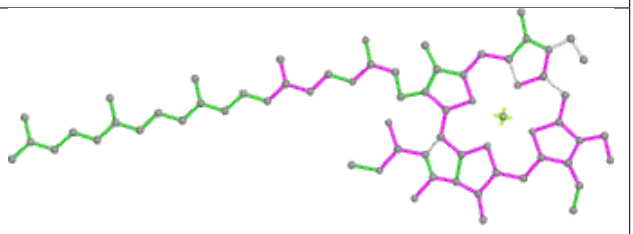


Rings

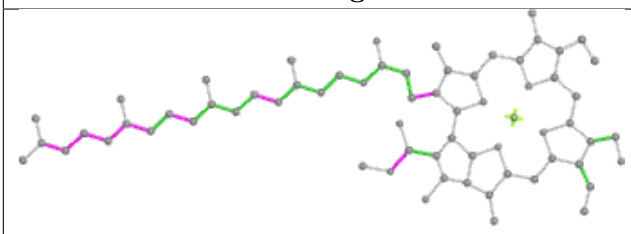
Ligand CHL B 305



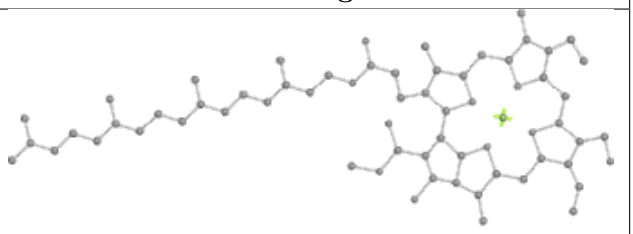
Bond lengths



Bond angles

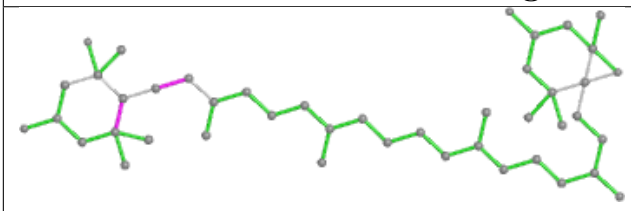


Torsions

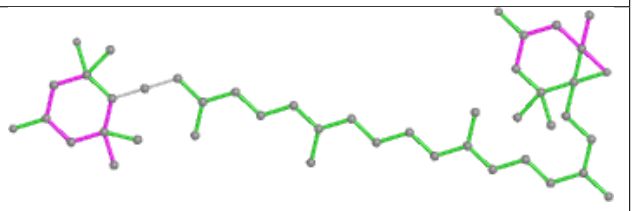


Rings

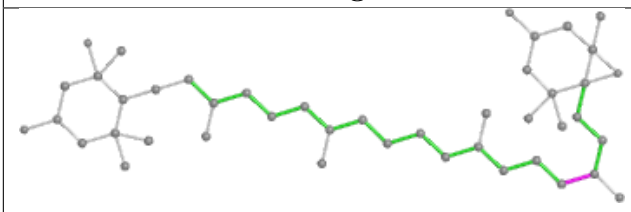
Ligand NEX C 304



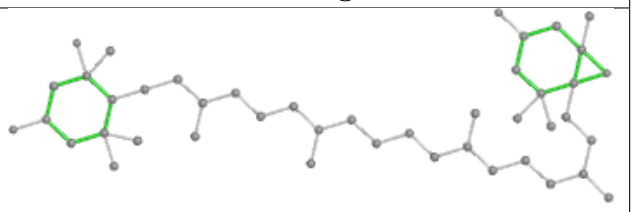
Bond lengths



Bond angles

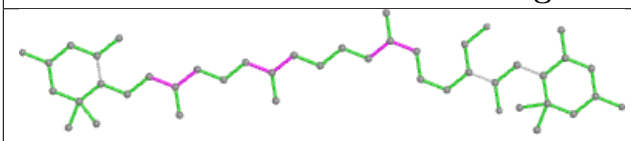


Torsions

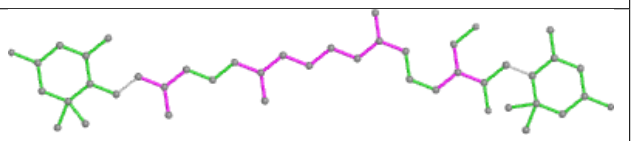


Rings

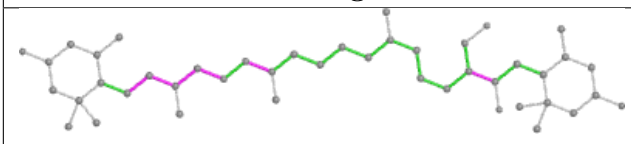
Ligand 0IE C 302



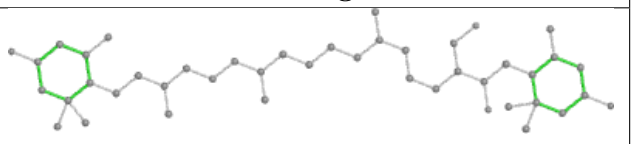
Bond lengths



Bond angles

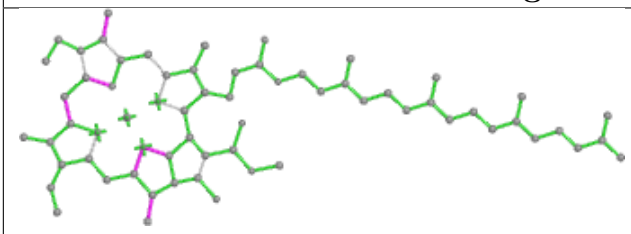


Torsions

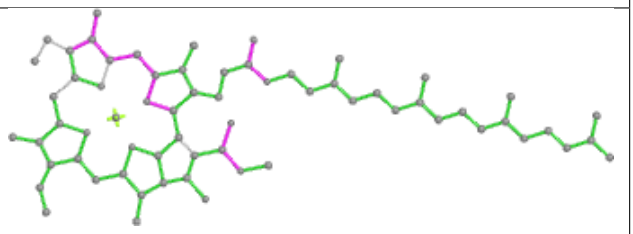


Rings

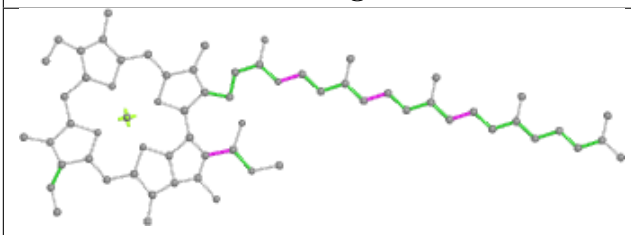
Ligand CLA A 306



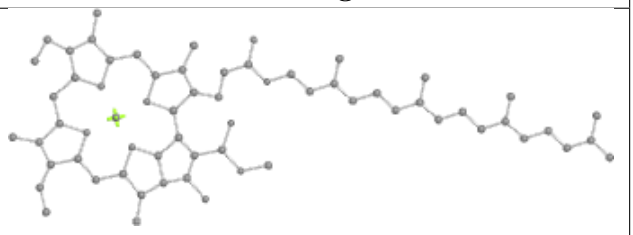
Bond lengths



Bond angles

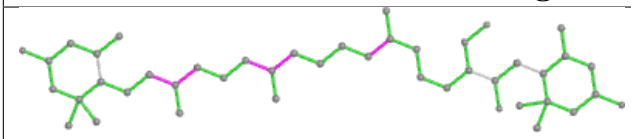


Torsions

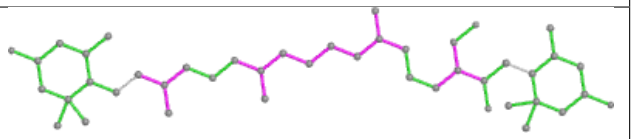


Rings

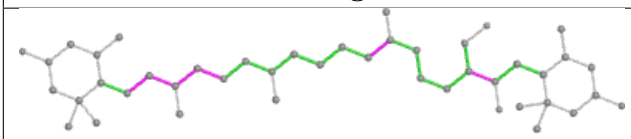
Ligand 0IE B 302



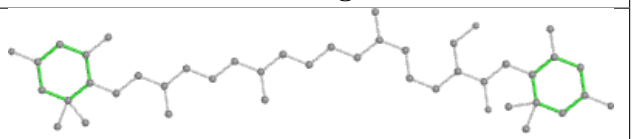
Bond lengths



Bond angles

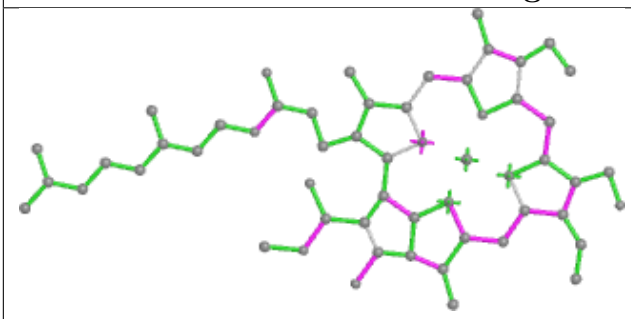


Torsions

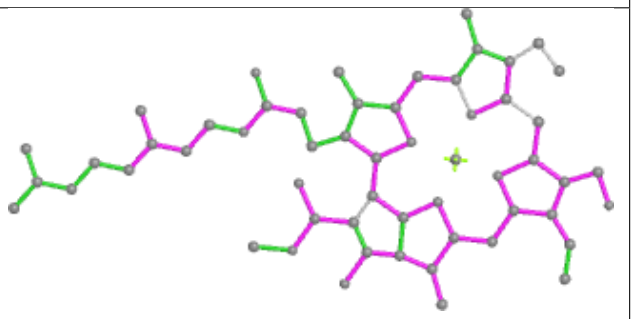


Rings

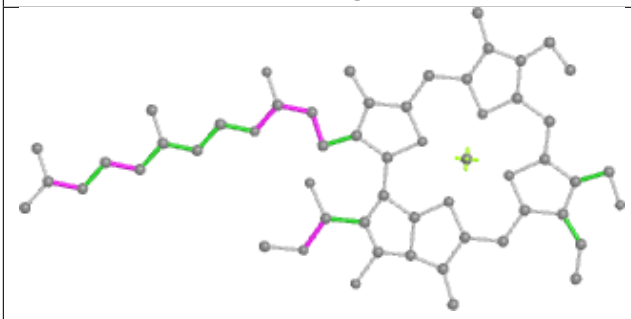
Ligand CHL C 312



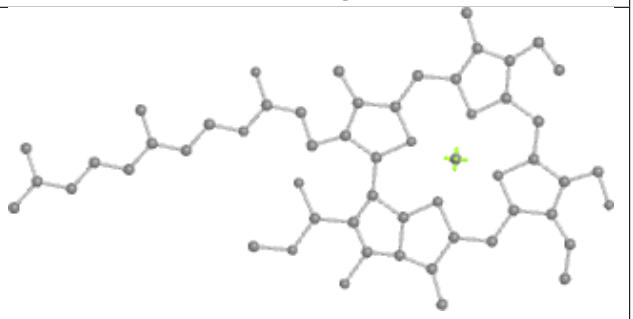
Bond lengths



Bond angles

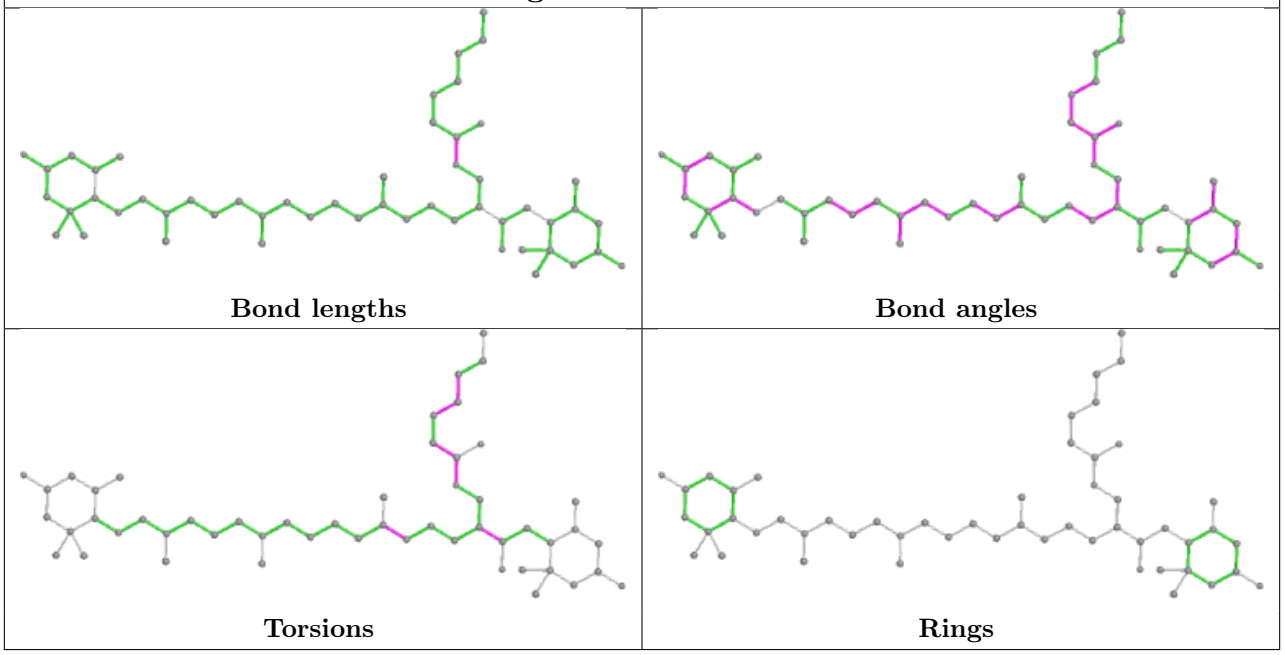


Torsions

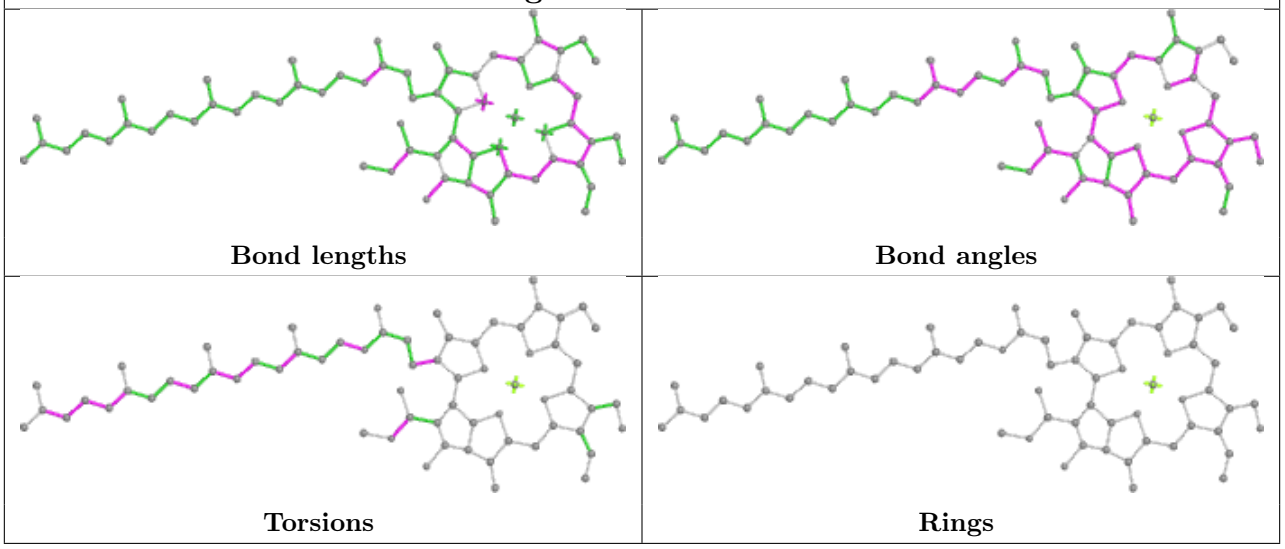


Rings

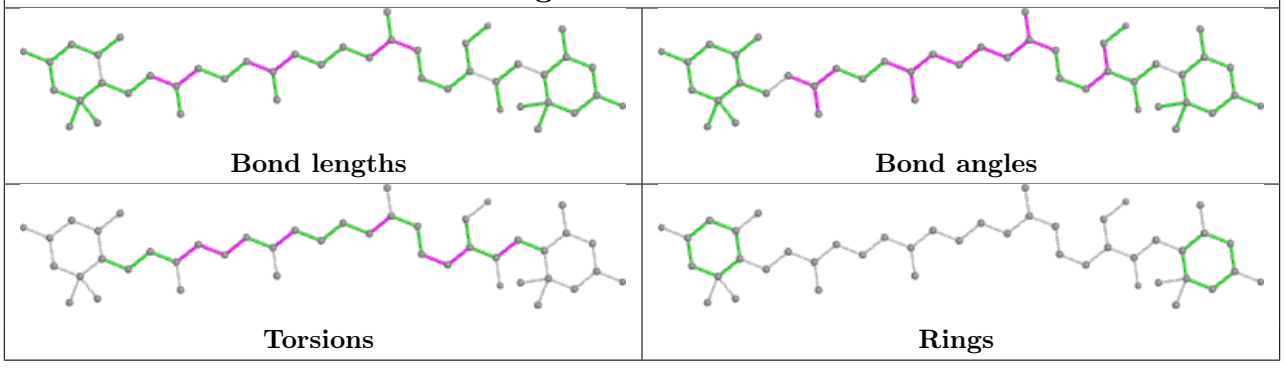
Ligand 0UR B 301



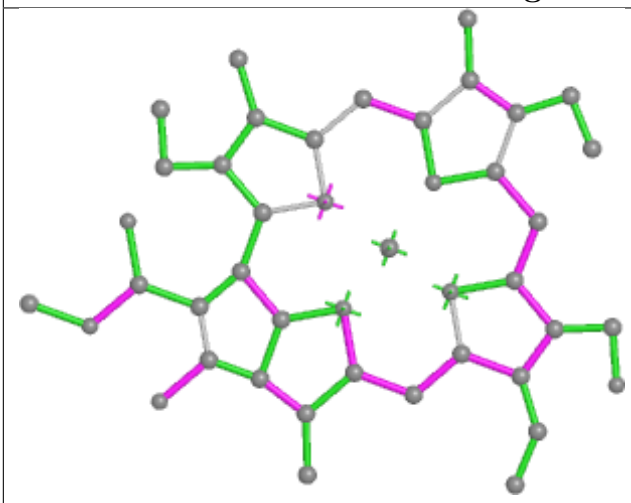
Ligand CHL B 313



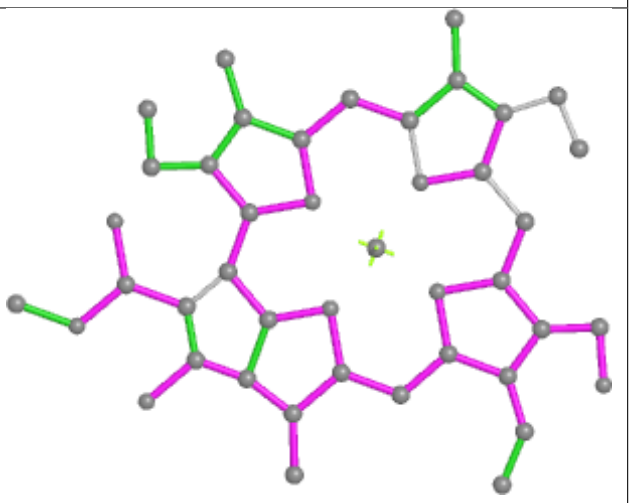
Ligand 0IE C 303



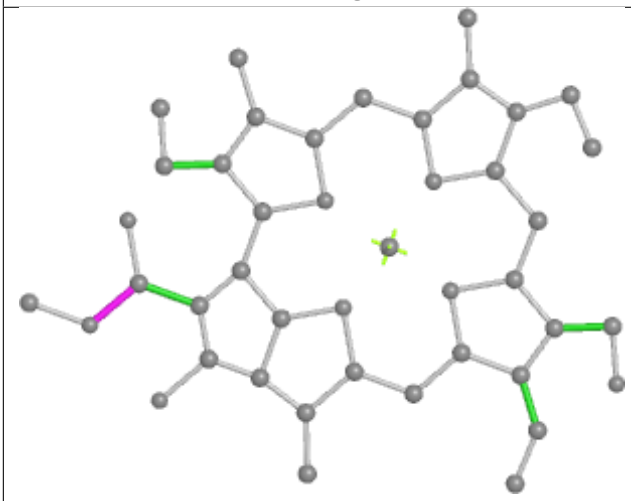
Ligand CHL B 309



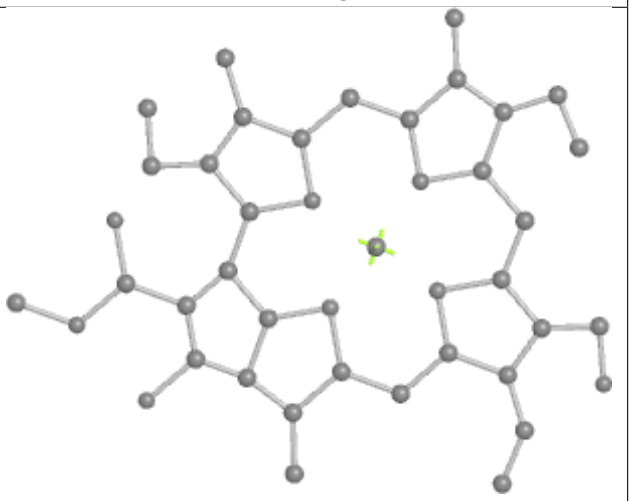
Bond lengths



Bond angles

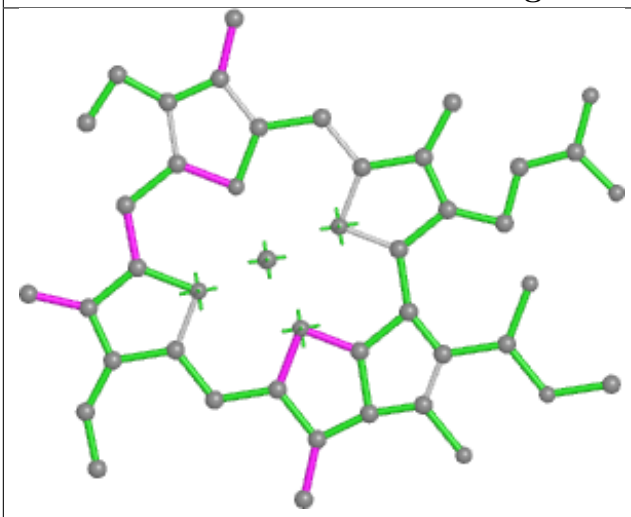


Torsions

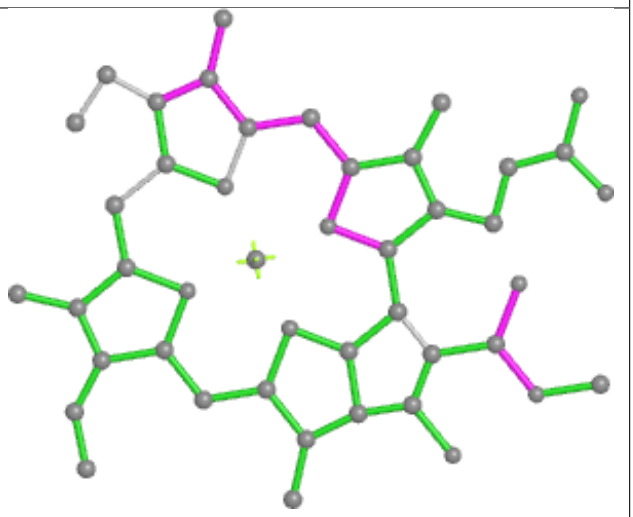


Rings

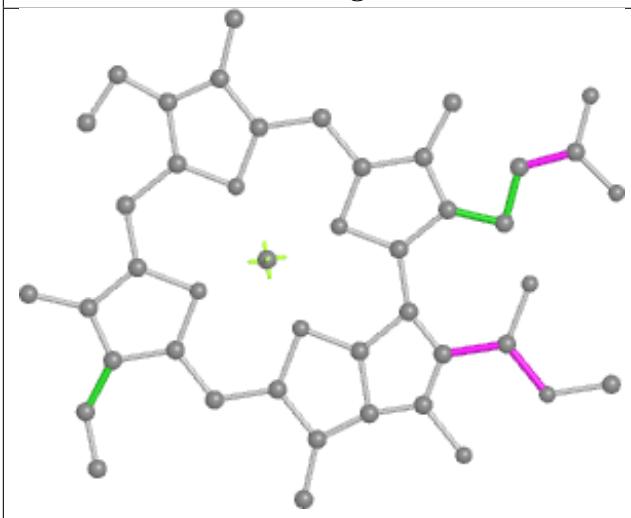
Ligand CLA C 316



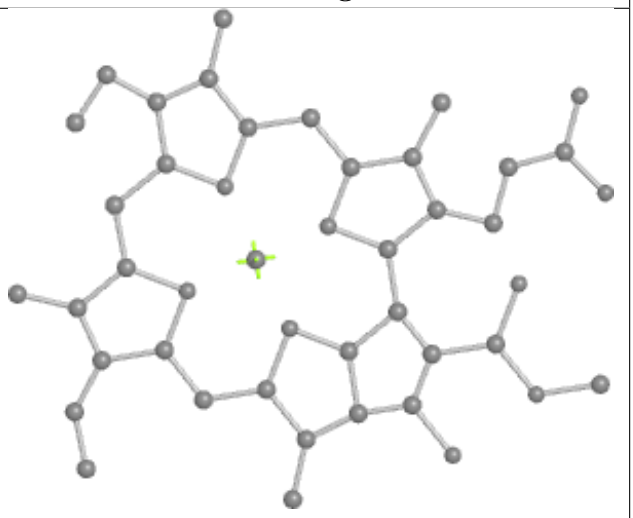
Bond lengths



Bond angles

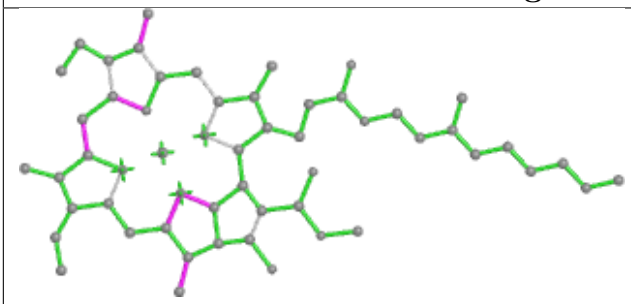


Torsions

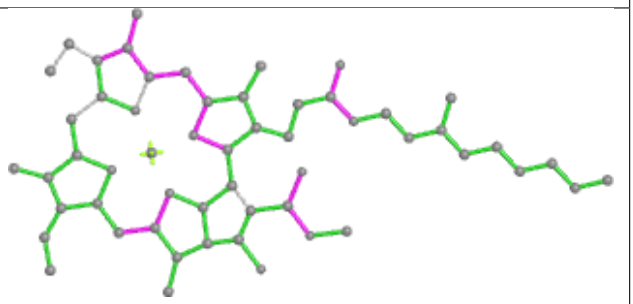


Rings

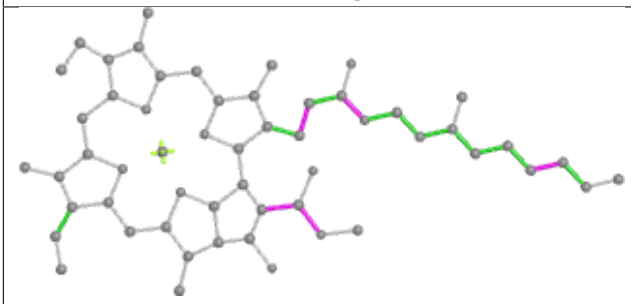
Ligand CLA C 317



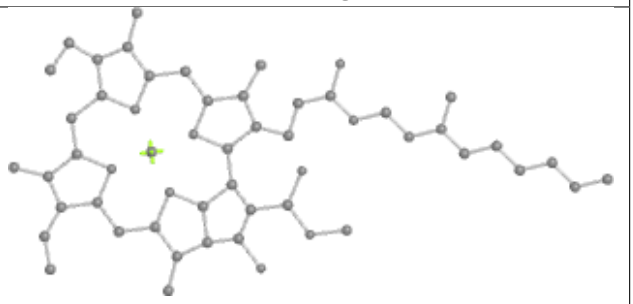
Bond lengths



Bond angles

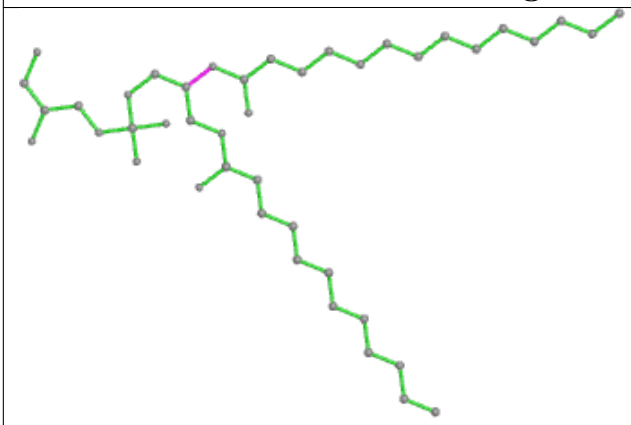


Torsions

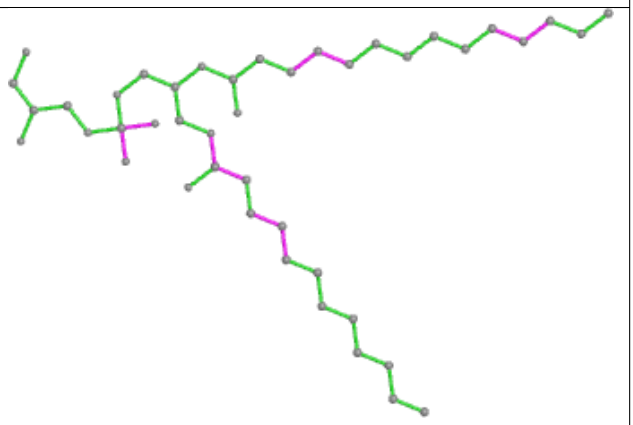


Rings

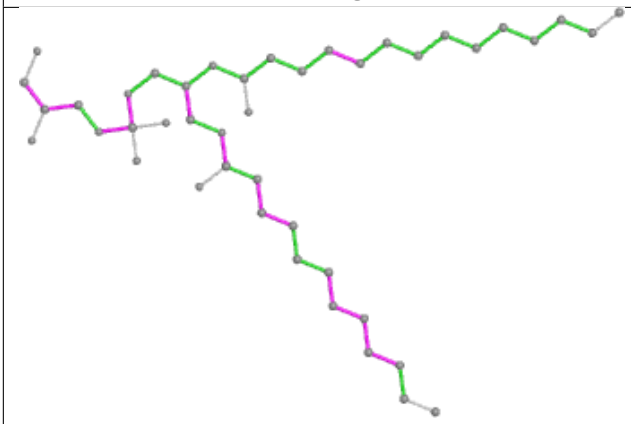
Ligand LHG C 319



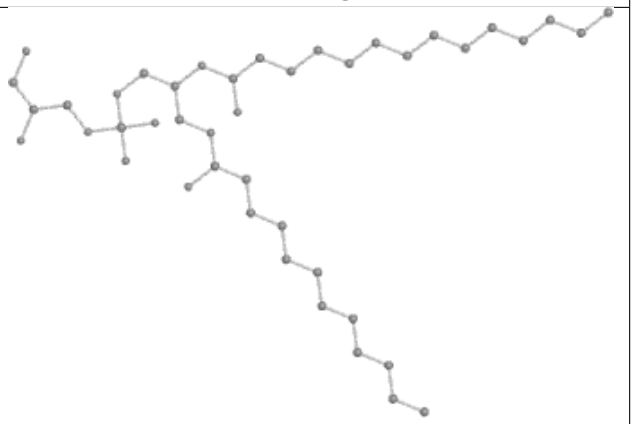
Bond lengths



Bond angles

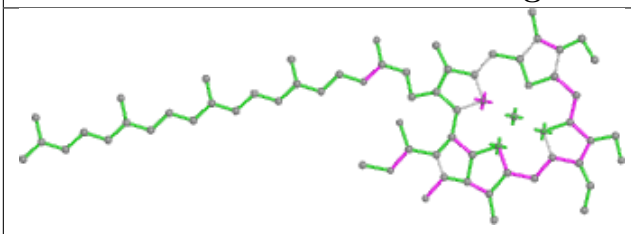


Torsions

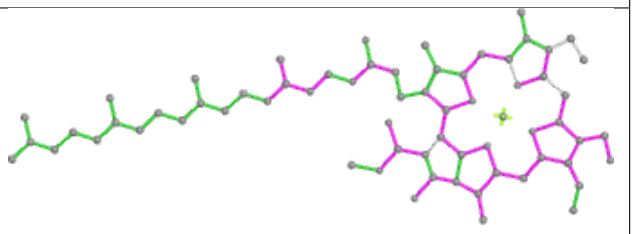


Rings

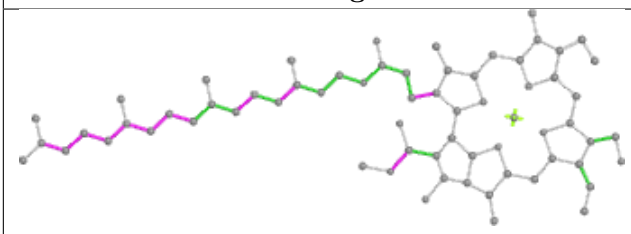
Ligand CHL C 305



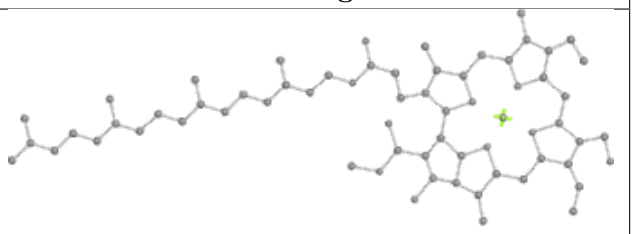
Bond lengths



Bond angles

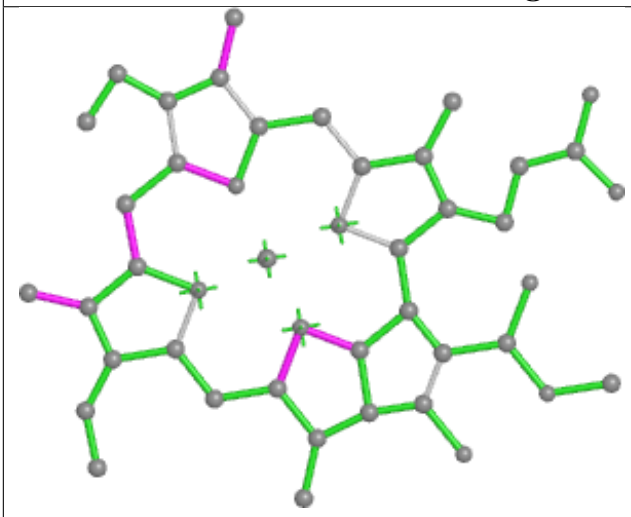


Torsions

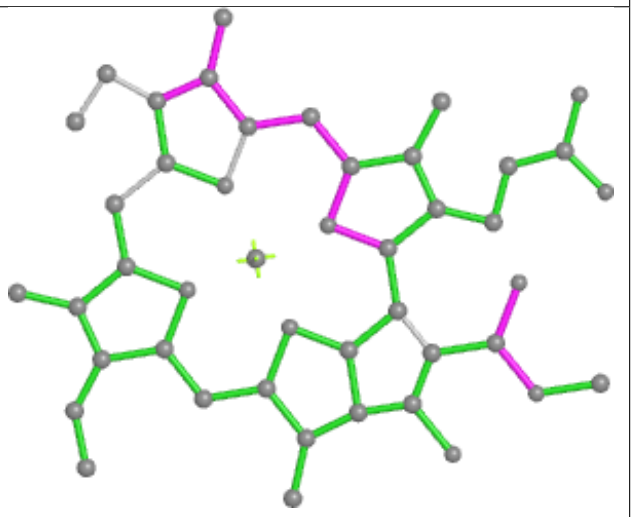


Rings

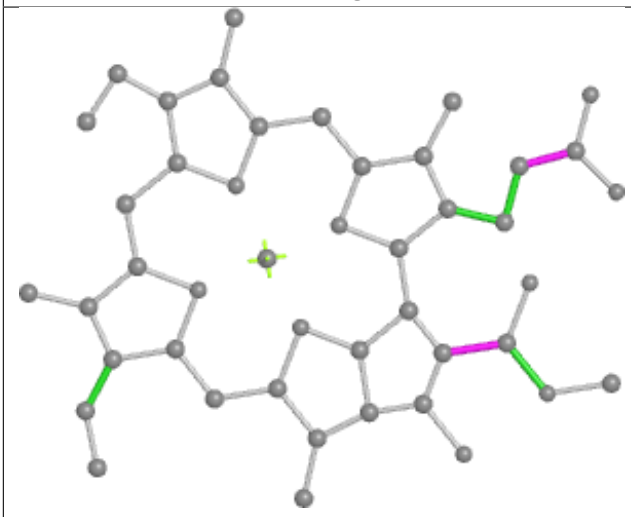
Ligand CLA B 316



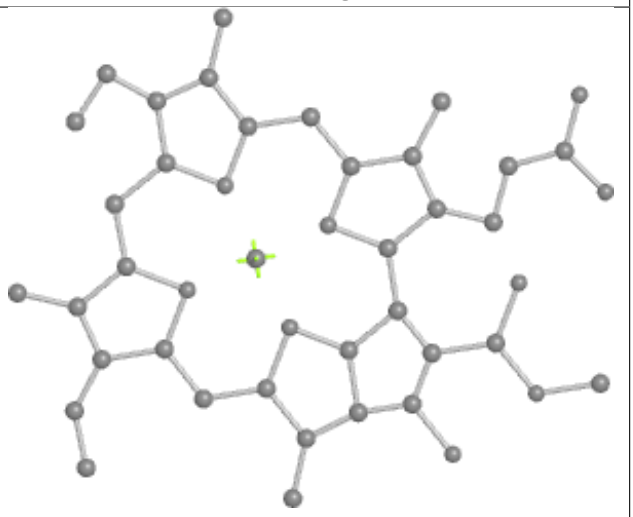
Bond lengths



Bond angles

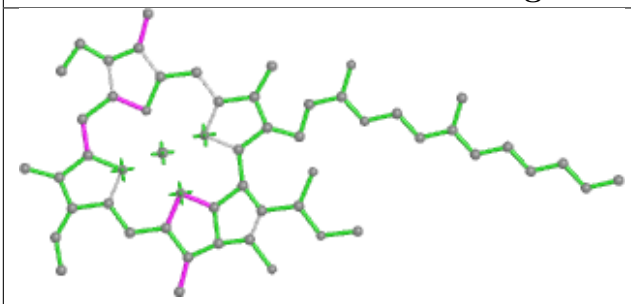


Torsions

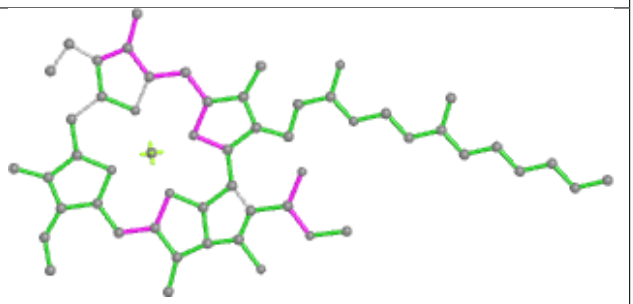


Rings

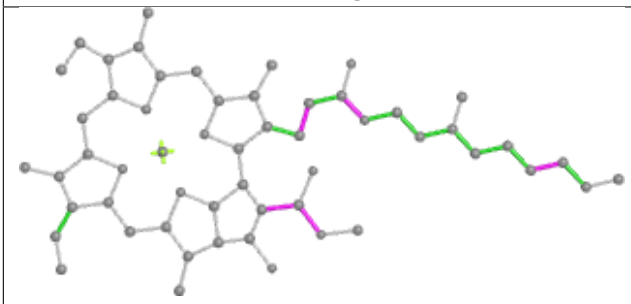
Ligand CLA B 317



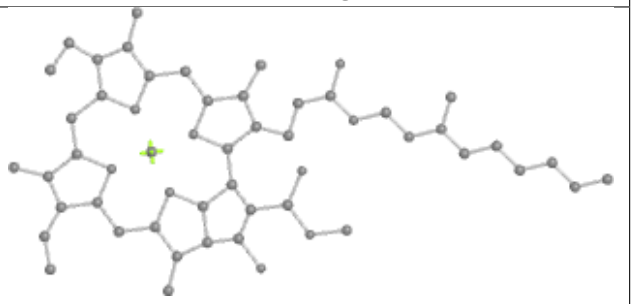
Bond lengths



Bond angles

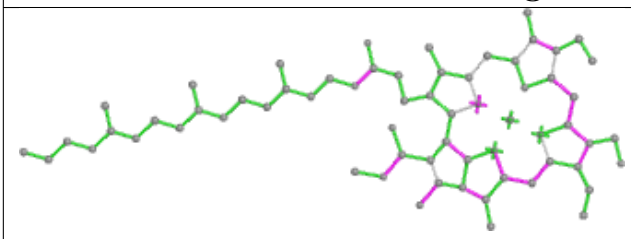


Torsions

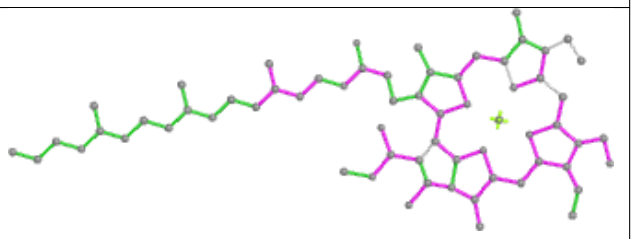


Rings

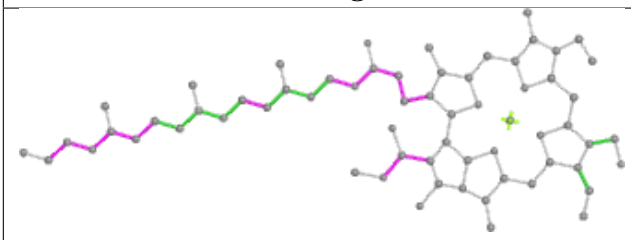
Ligand CHL B 306



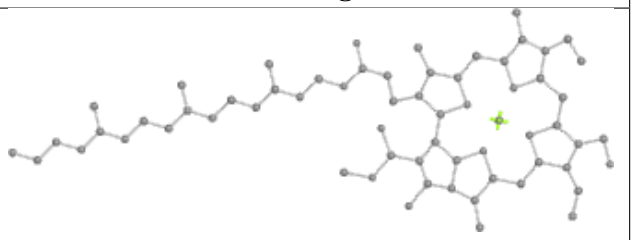
Bond lengths



Bond angles

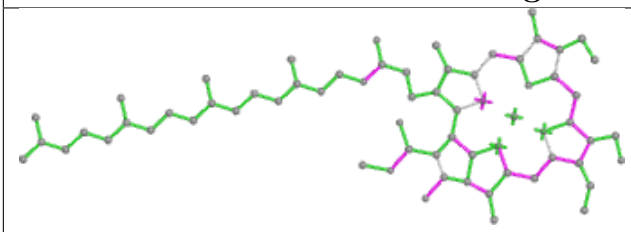


Torsions

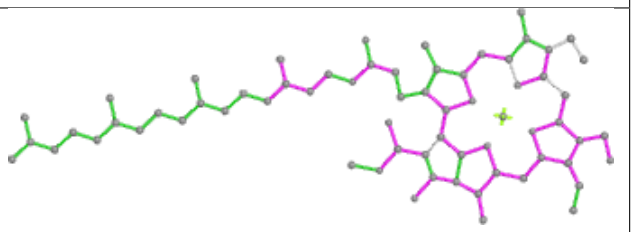


Rings

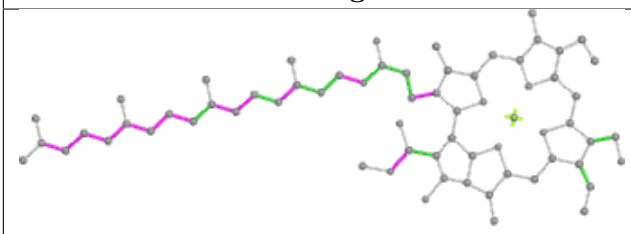
Ligand CHL A 312



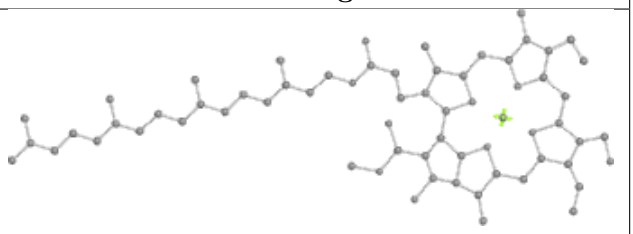
Bond lengths



Bond angles

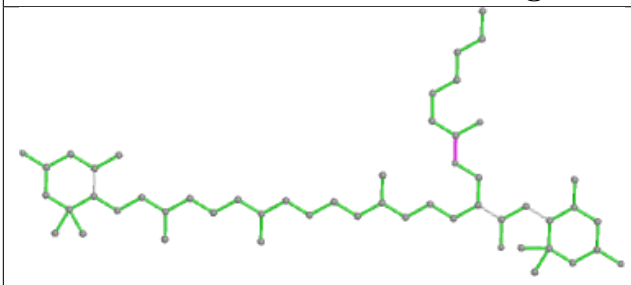


Torsions

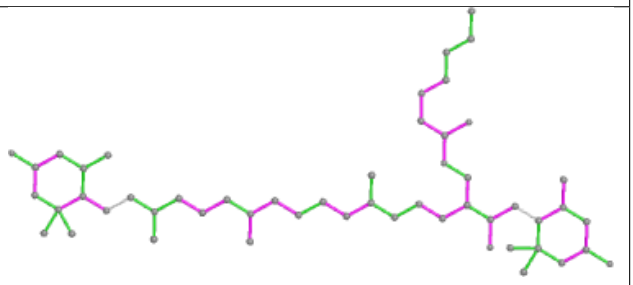


Rings

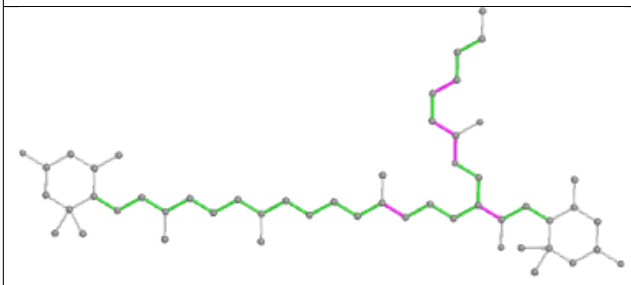
Ligand 0UR C 301



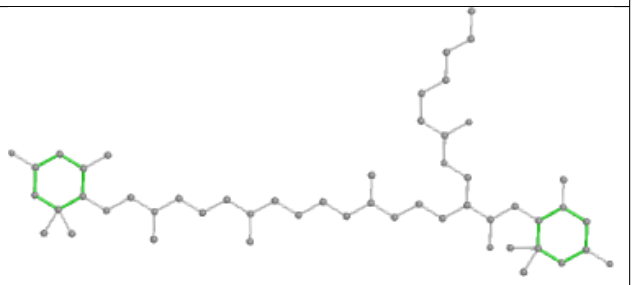
Bond lengths



Bond angles

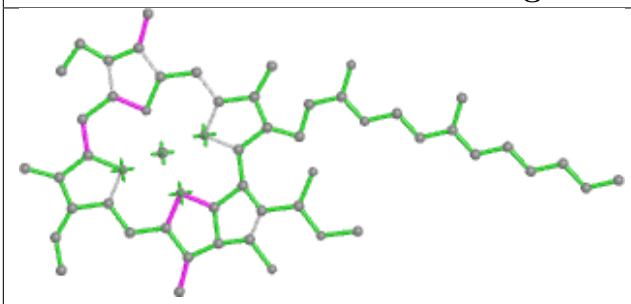


Torsions



Rings

Ligand CLA A 316



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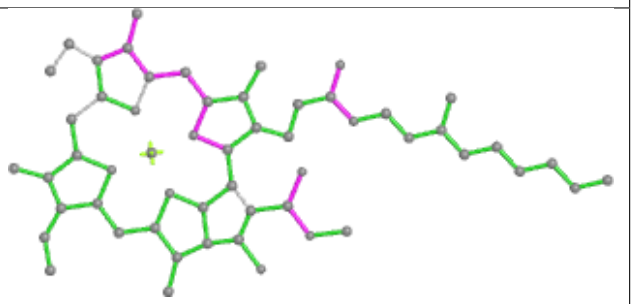
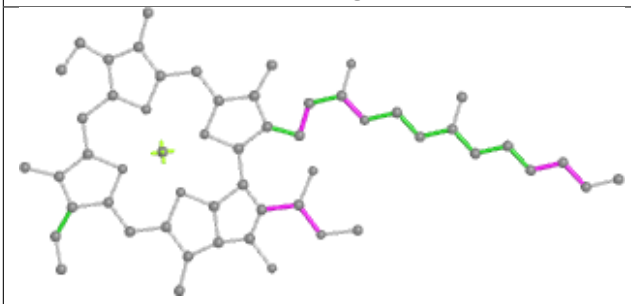
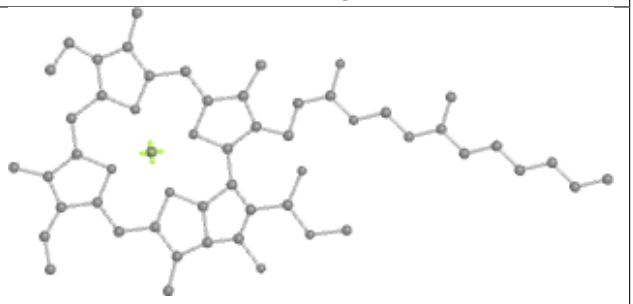


Bond angles

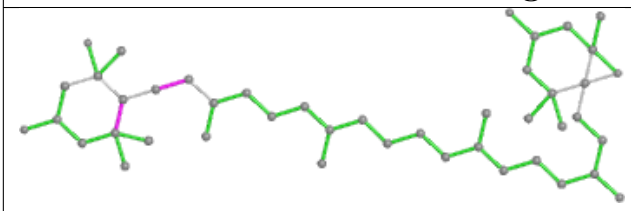


Torsions

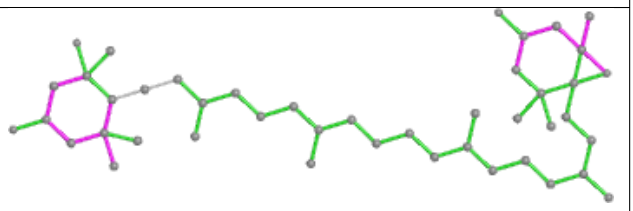


Rings

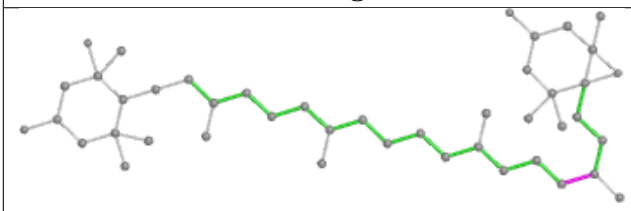
Ligand NEX B 304



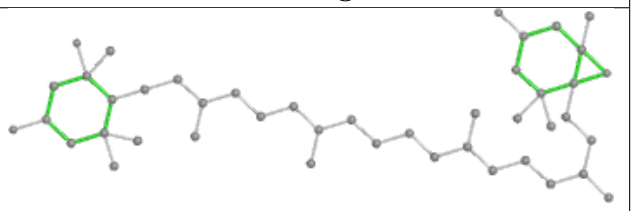
Bond lengths



Bond angles

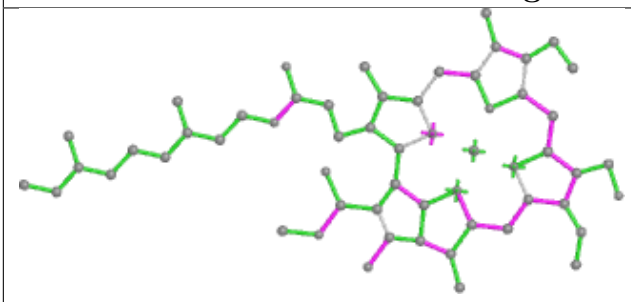


Torsions

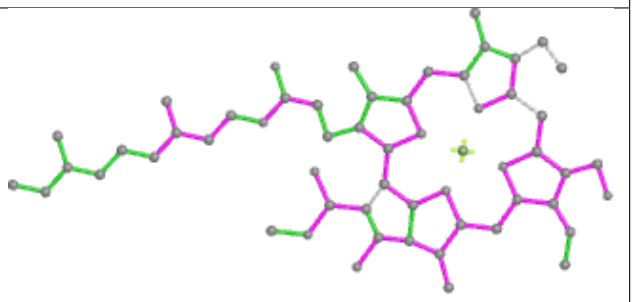


Rings

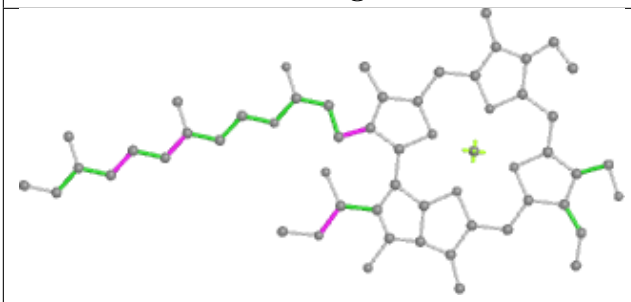
Ligand CHL A 304



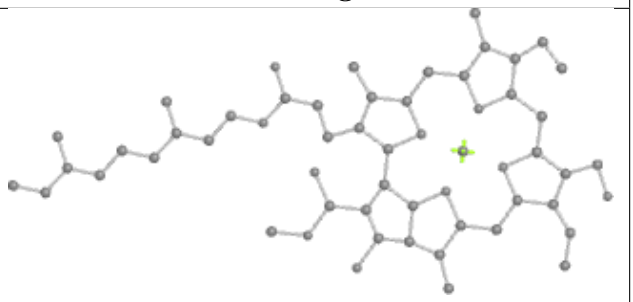
Bond lengths



Bond angles

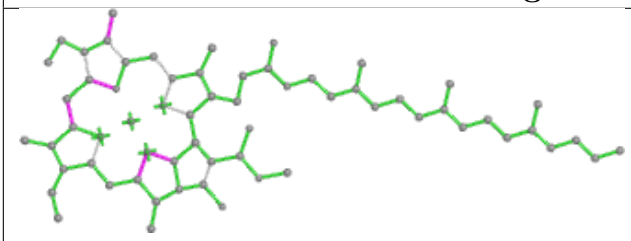


Torsions

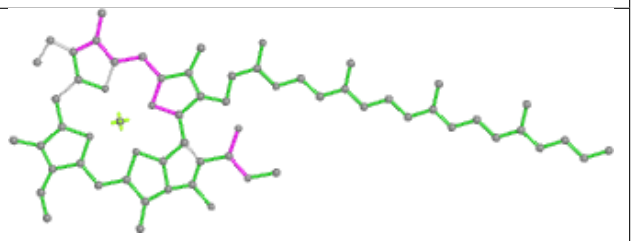


Rings

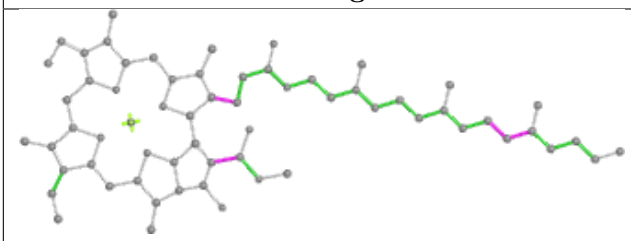
Ligand CLA A 314



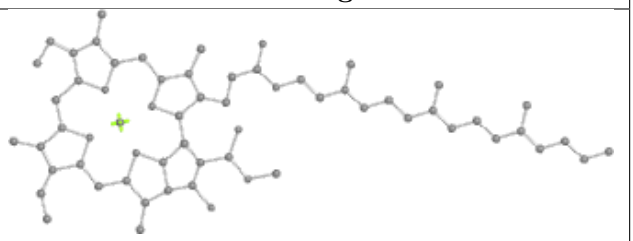
Bond lengths



Bond angles

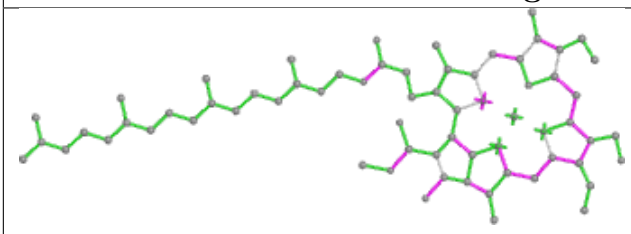


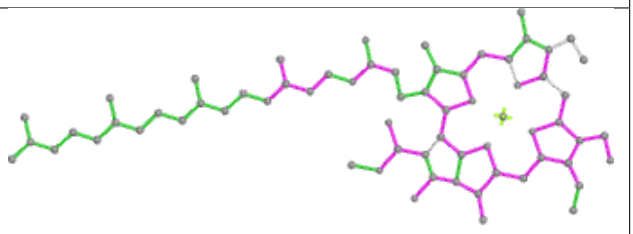
Torsions

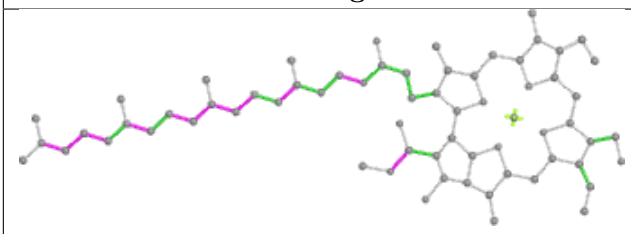


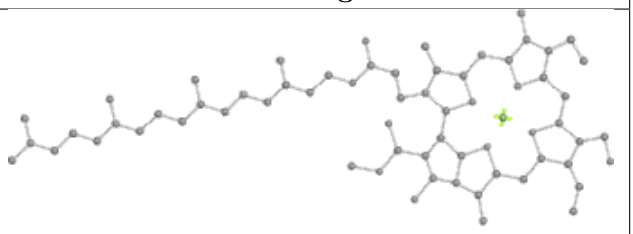
Rings

Ligand CHL C 313

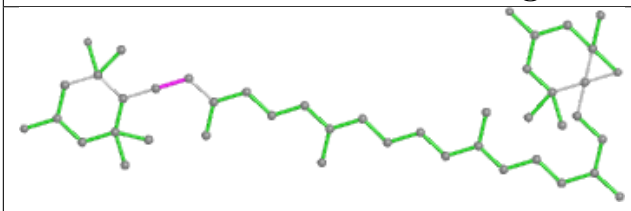

Bond lengths

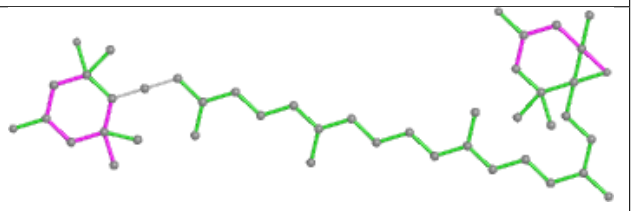

Bond angles

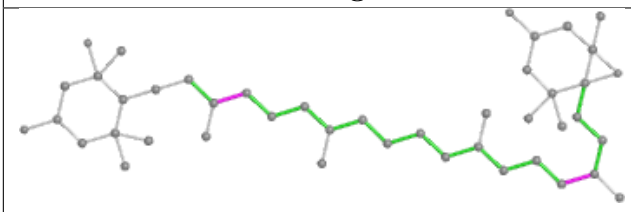

Torsions

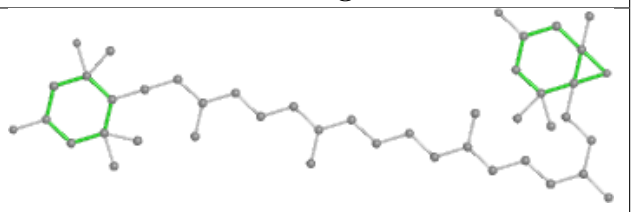

Rings

Ligand NEX A 303

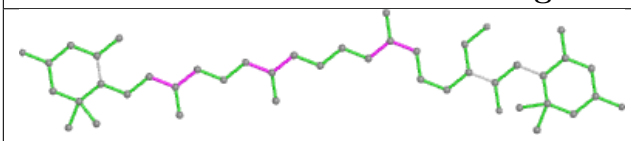

Bond lengths

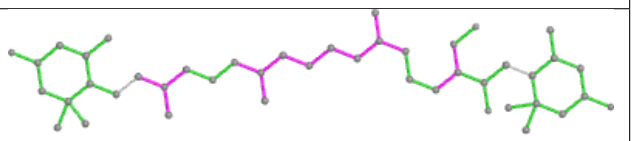

Bond angles

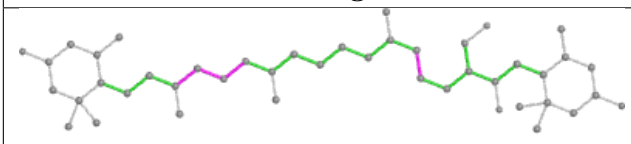

Torsions

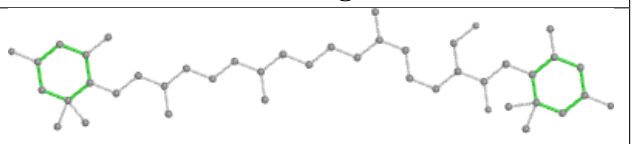

Rings

Ligand 0IE B 303

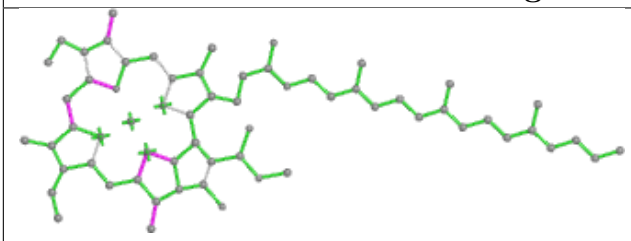

Bond lengths


Bond angles

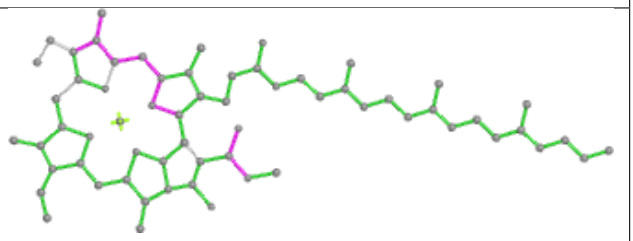

Torsions


Rings

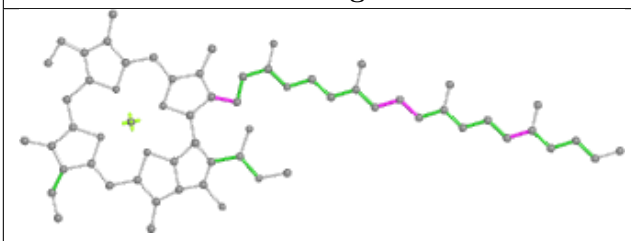
Ligand CLA B 315



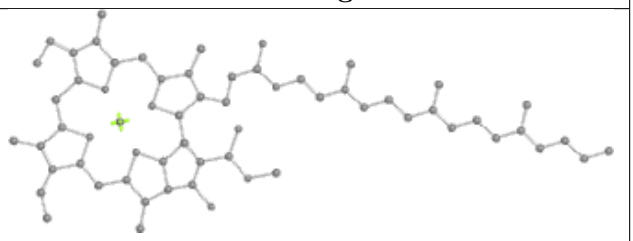
Bond lengths



Bond angles

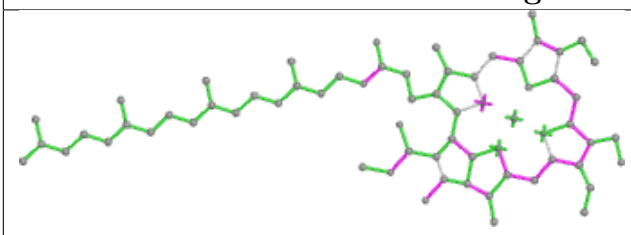


Torsions

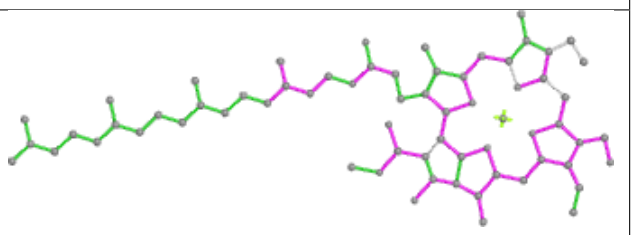


Rings

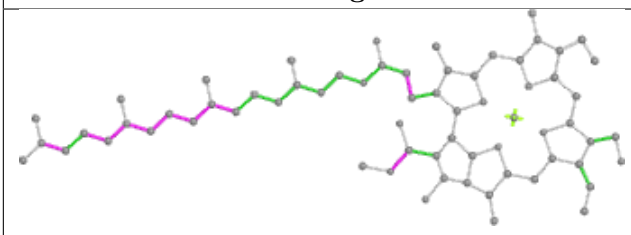
Ligand CHL B 312



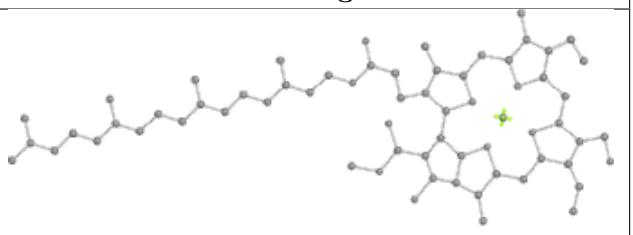
Bond lengths



Bond angles

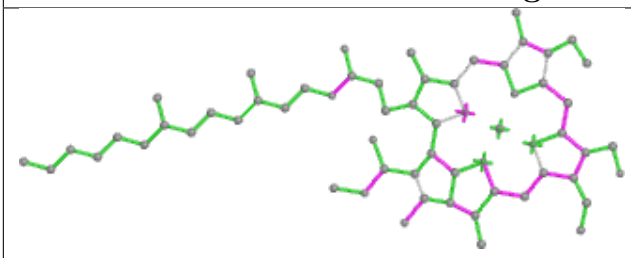


Torsions

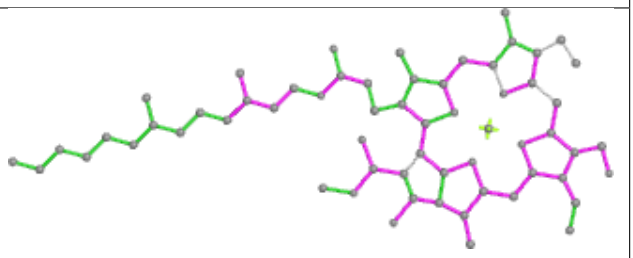


Rings

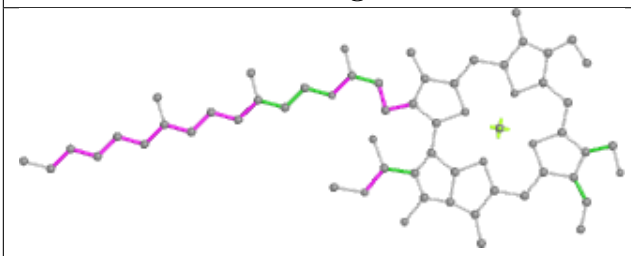
Ligand CHL A 310



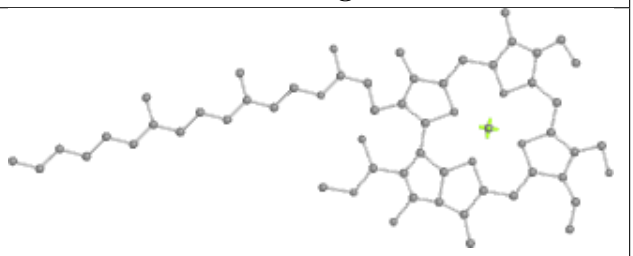
Bond lengths



Bond angles

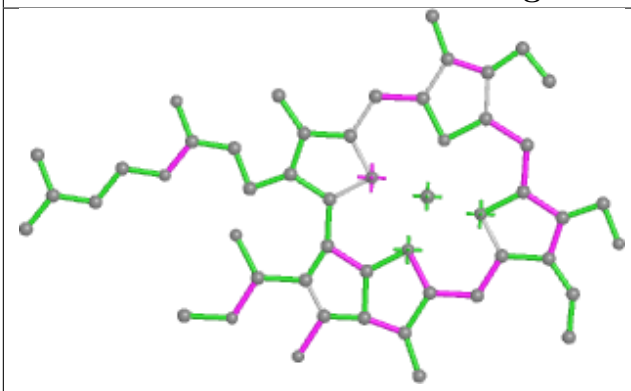


Torsions

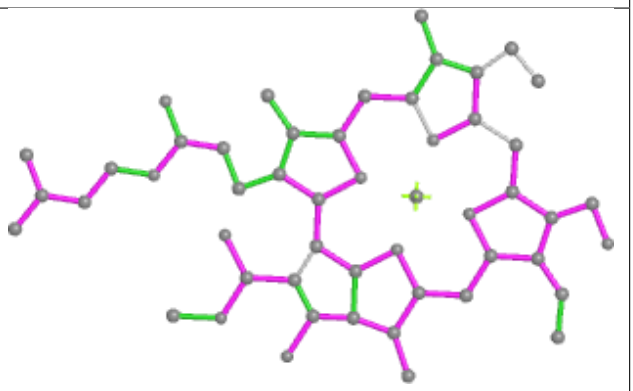


Rings

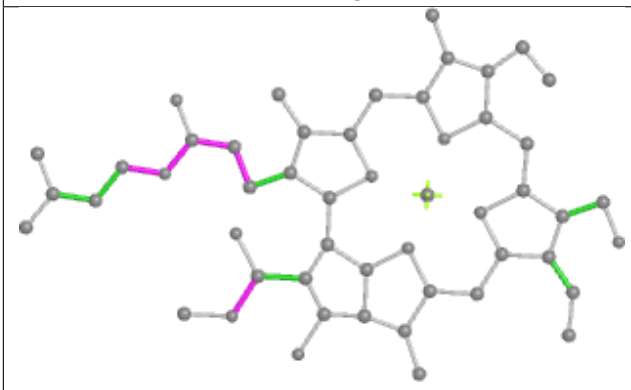
Ligand CHL A 309



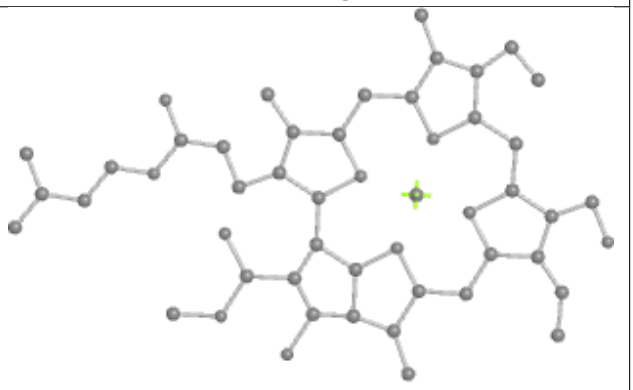
Bond lengths



Bond angles

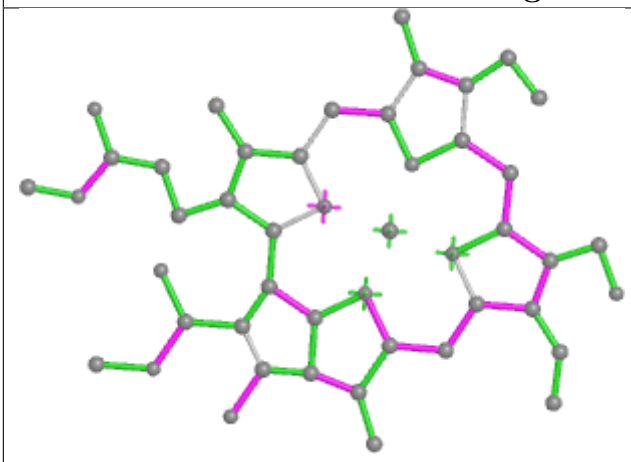


Torsions

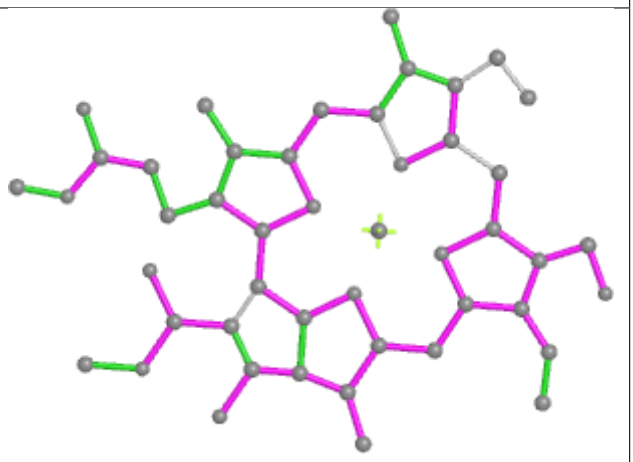


Rings

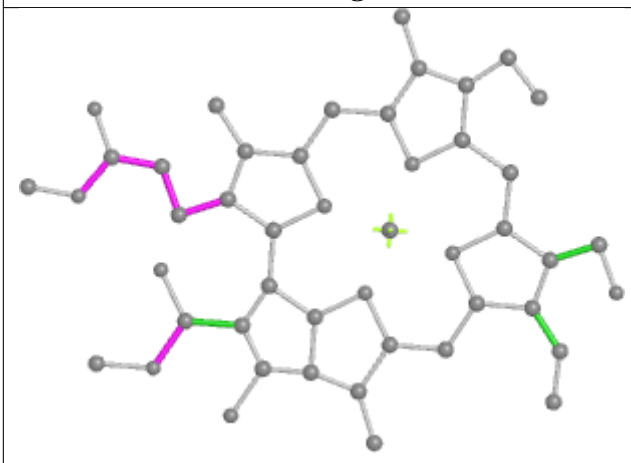
Ligand CHL C 311



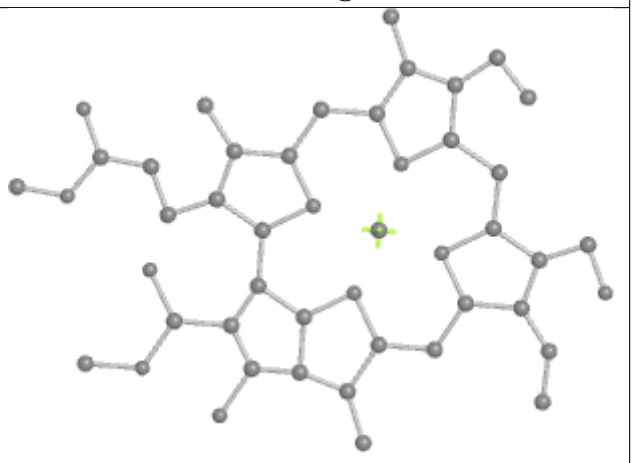
Bond lengths



Bond angles

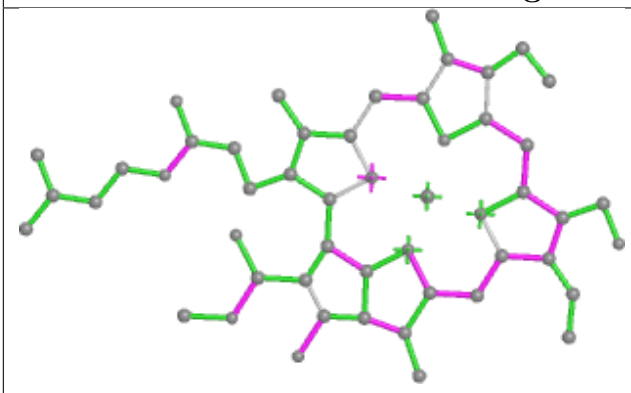


Torsions

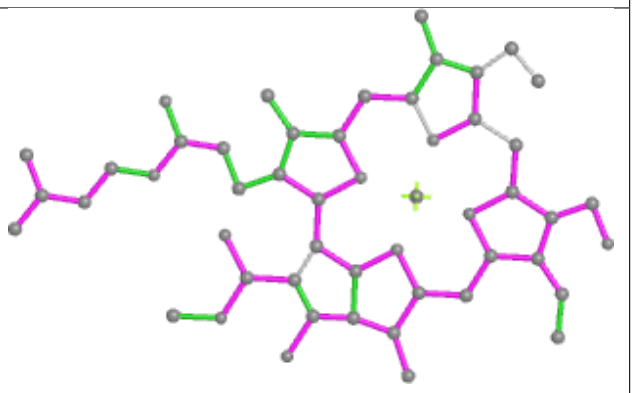


Rings

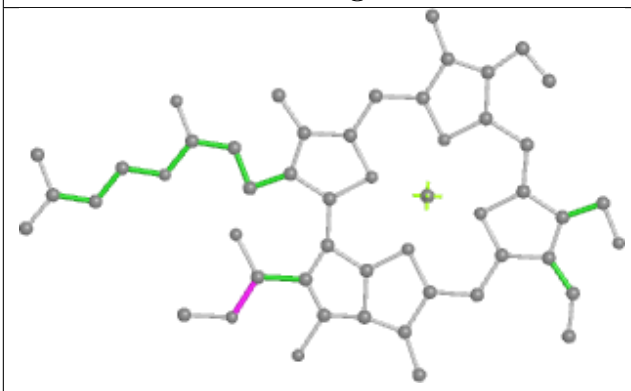
Ligand CHL C 310



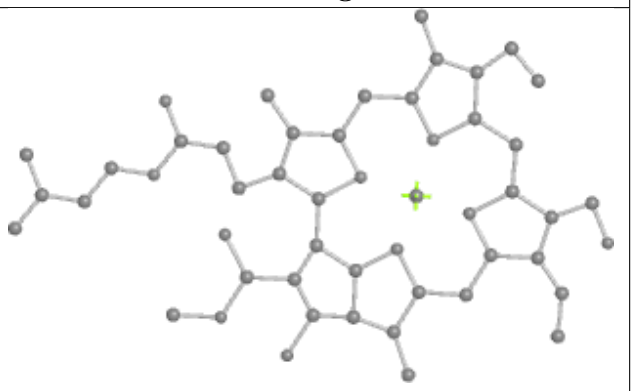
Bond lengths



Bond angles

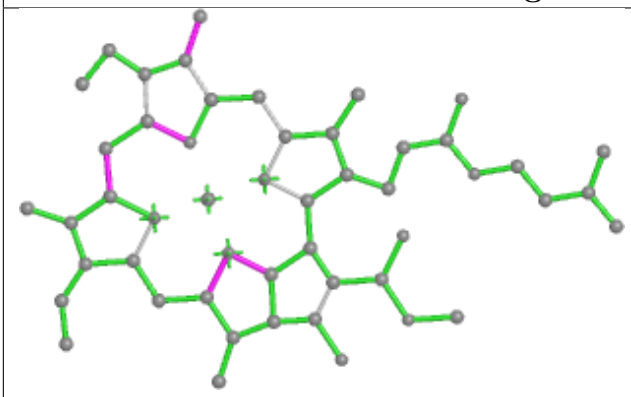


Torsions



Rings

Ligand CLA C 308



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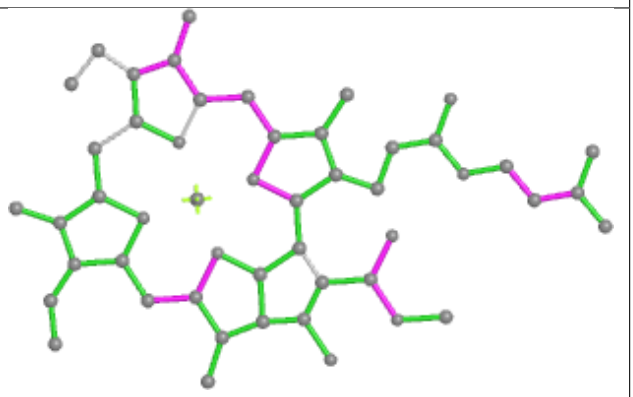
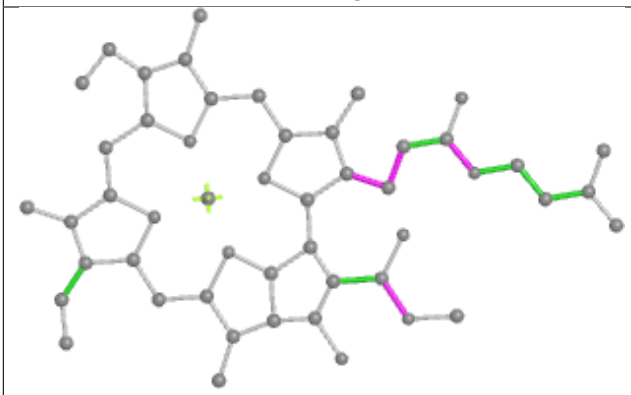
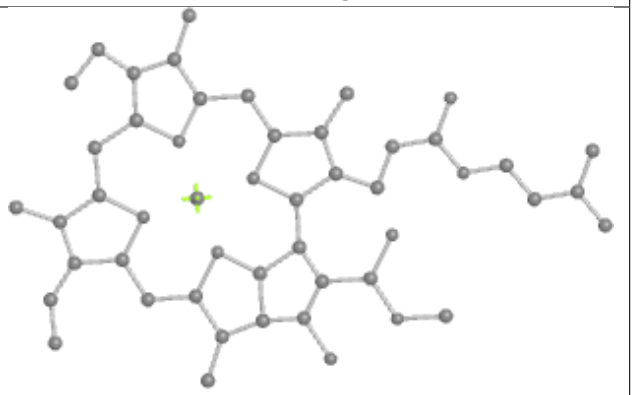


Bond angles

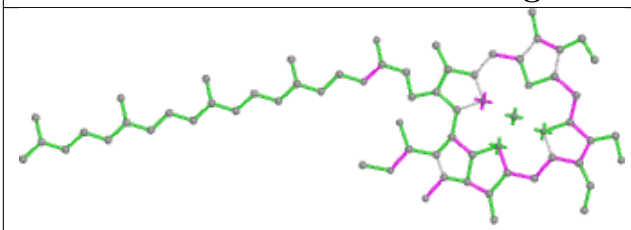


Torsions

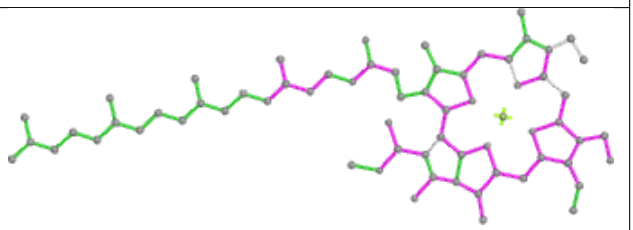


Rings

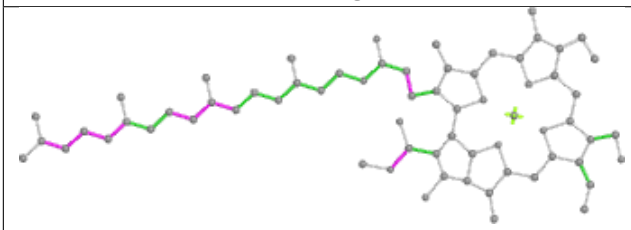
Ligand CHL A 311



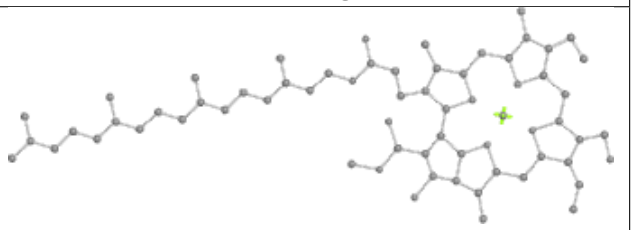
Bond lengths



Bond angles

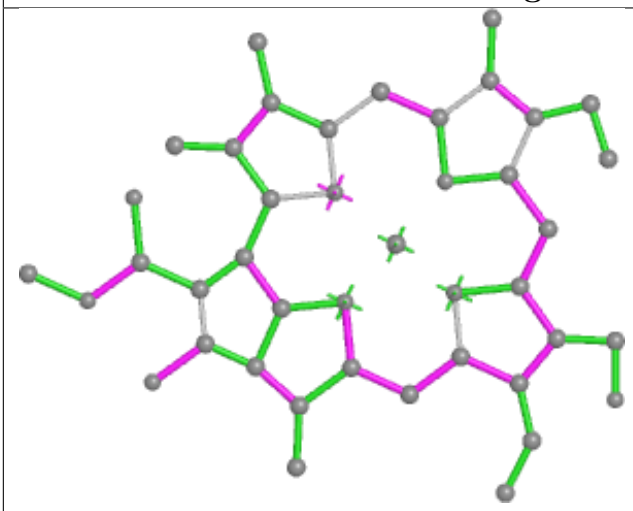


Torsions

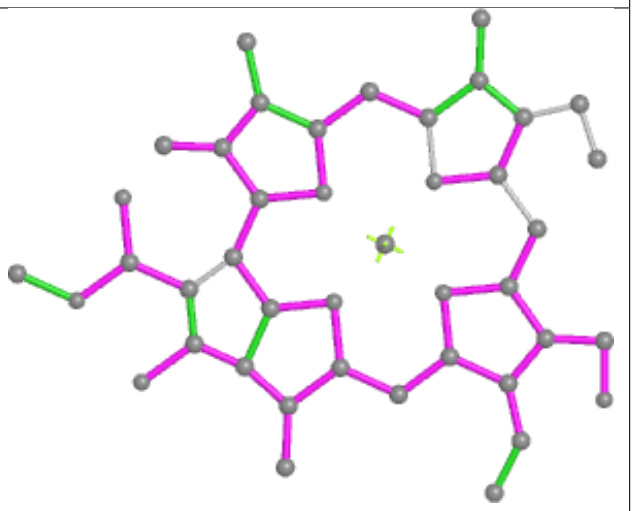


Rings

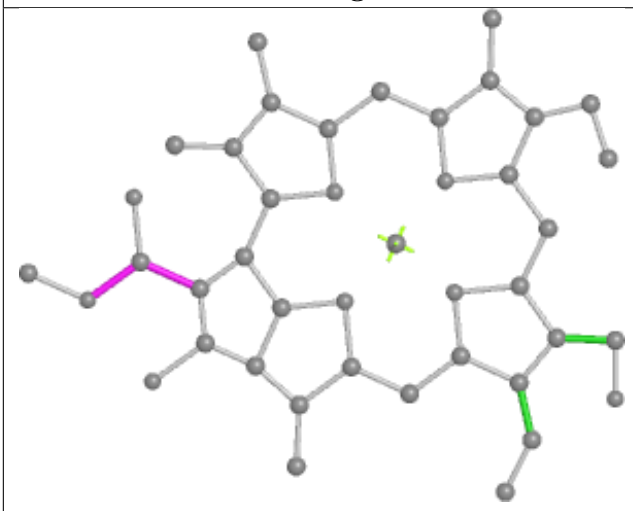
Ligand CHL B 318



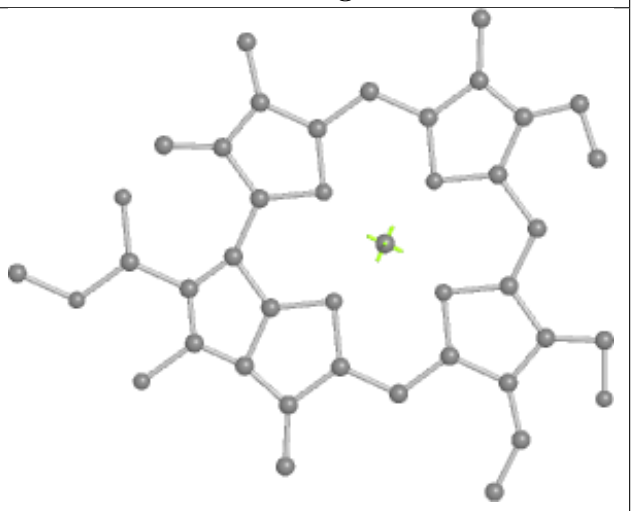
Bond lengths



Bond angles

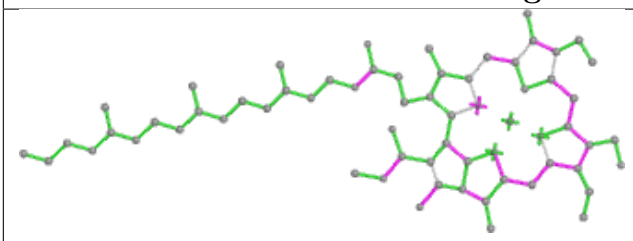


Torsions

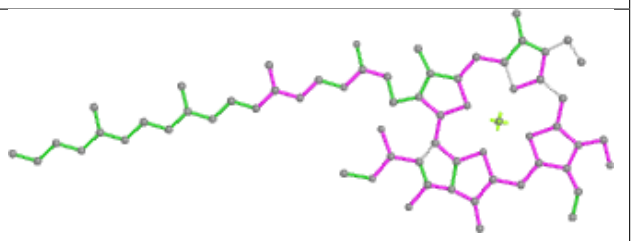


Rings

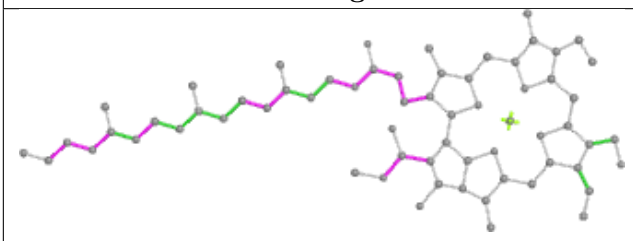
Ligand CHL C 306



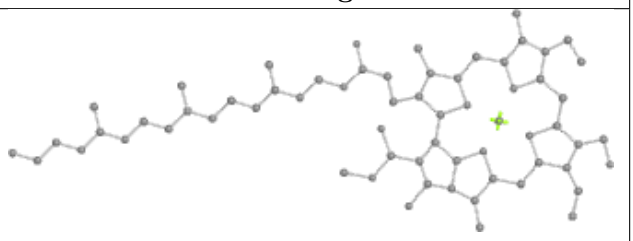
Bond lengths



Bond angles

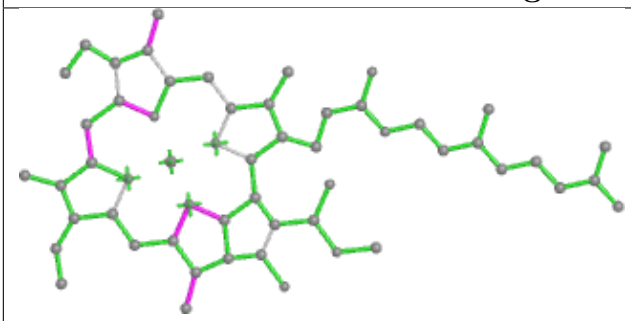


Torsions

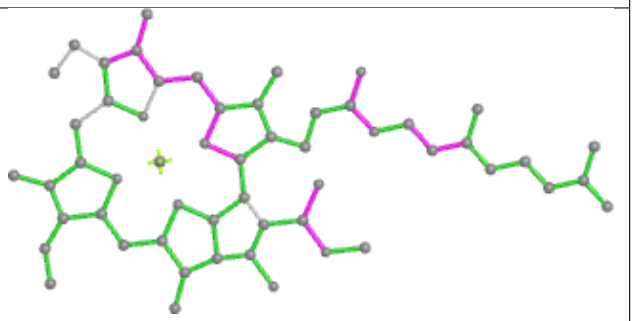


Rings

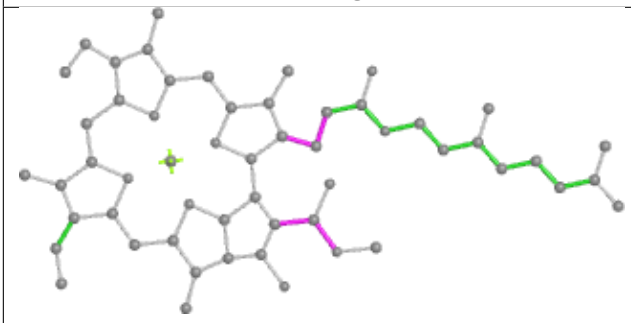
Ligand CLA A 313



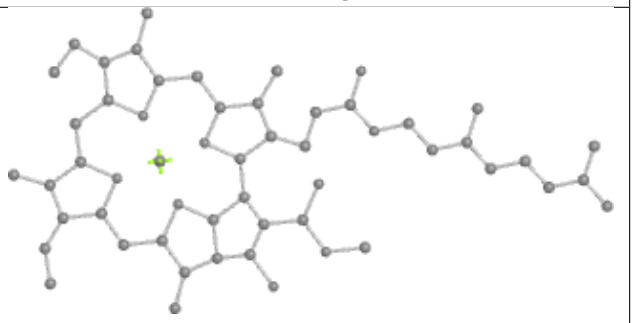
Bond lengths



Bond angles

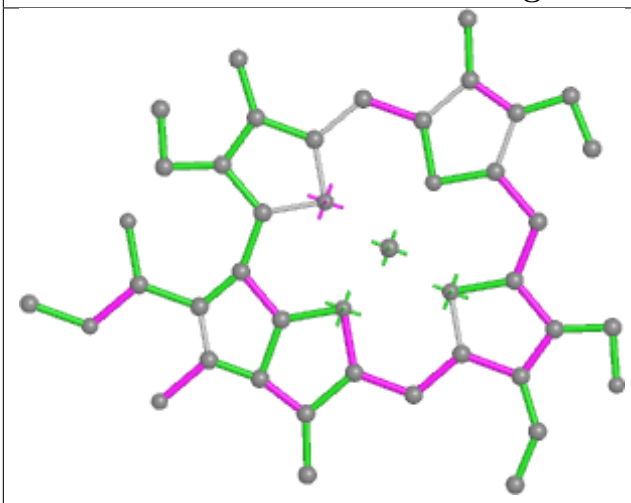


Torsions

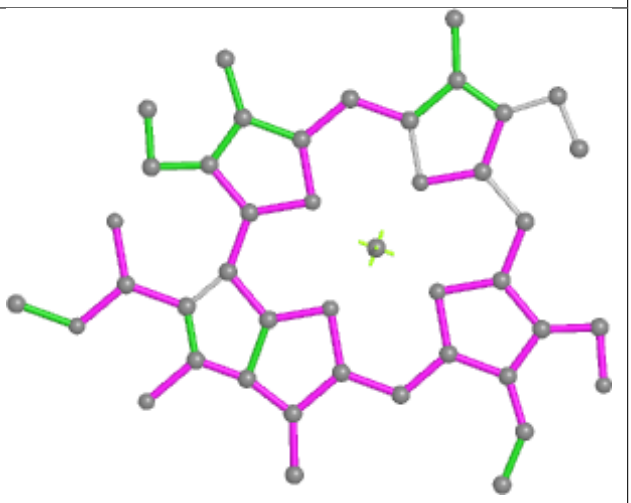


Rings

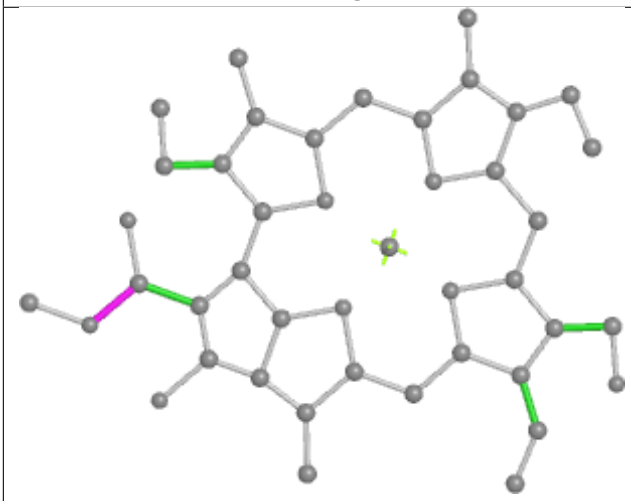
Ligand CHL A 308



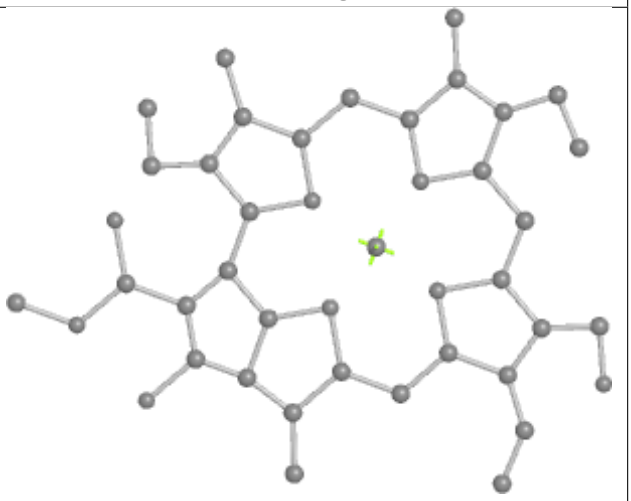
Bond lengths



Bond angles

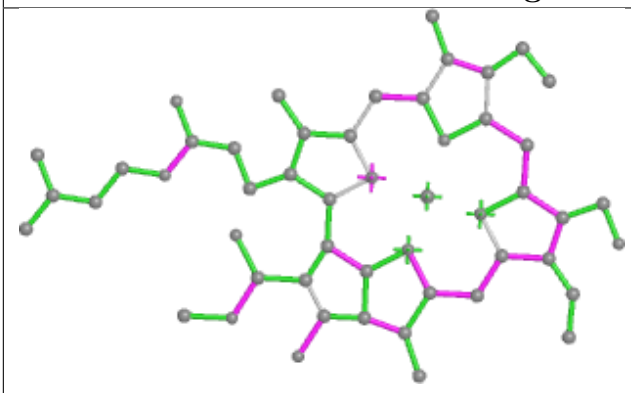


Torsions

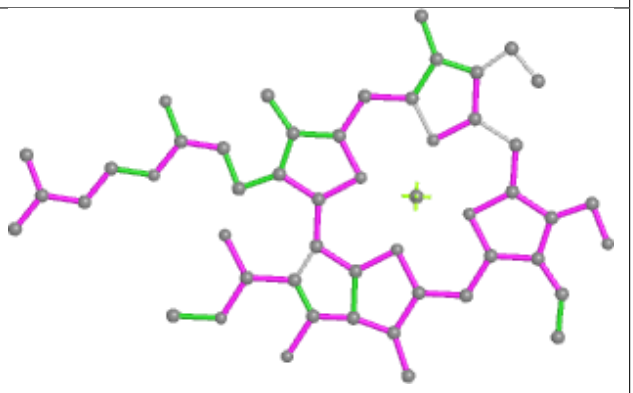


Rings

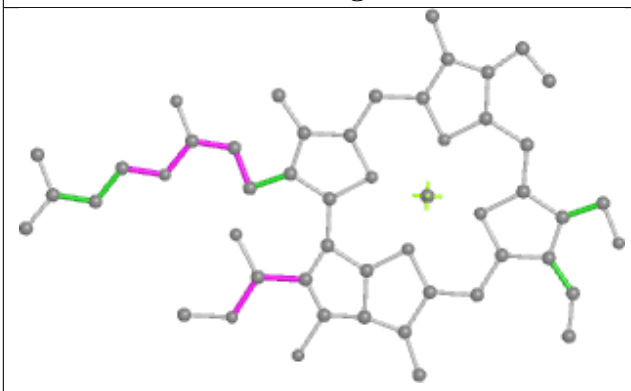
Ligand CHL B 310



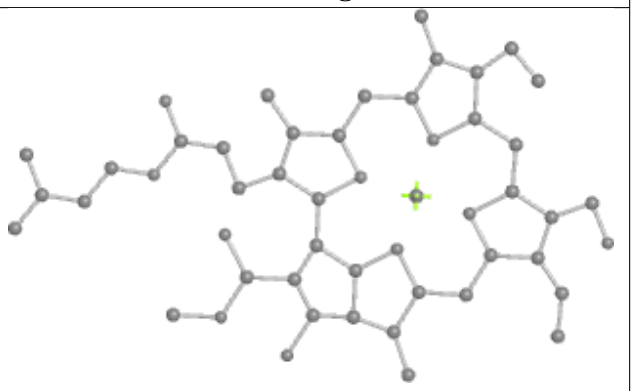
Bond lengths



Bond angles

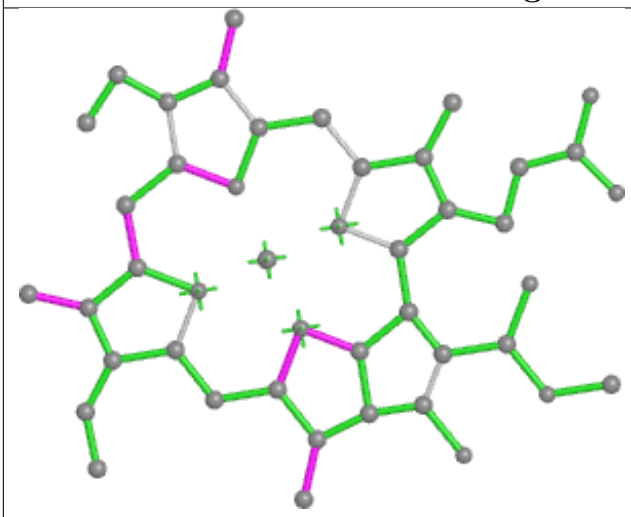


Torsions

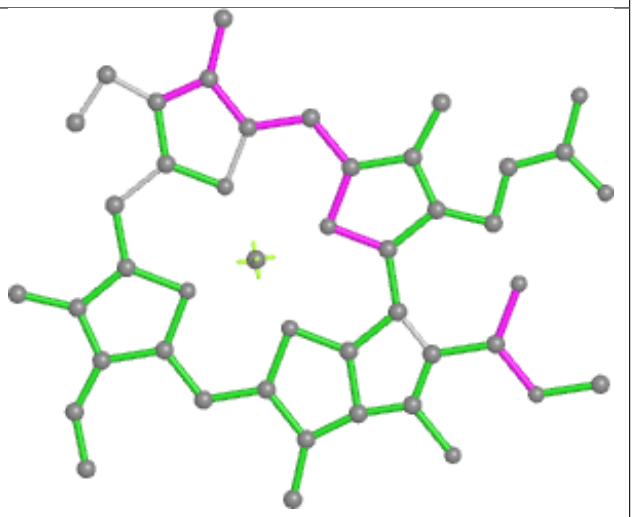


Rings

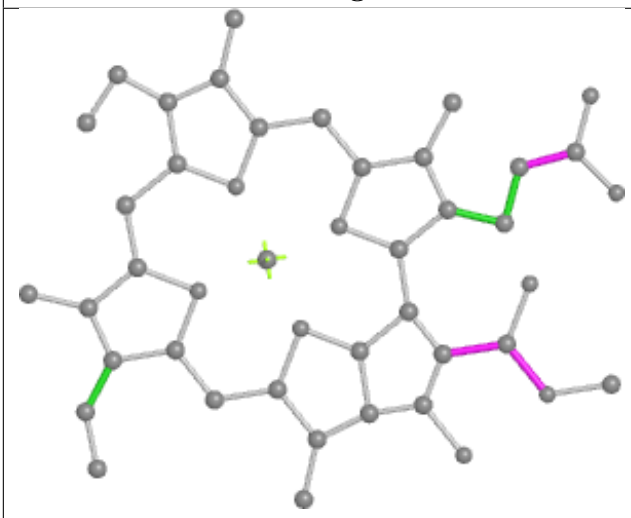
Ligand CLA A 315



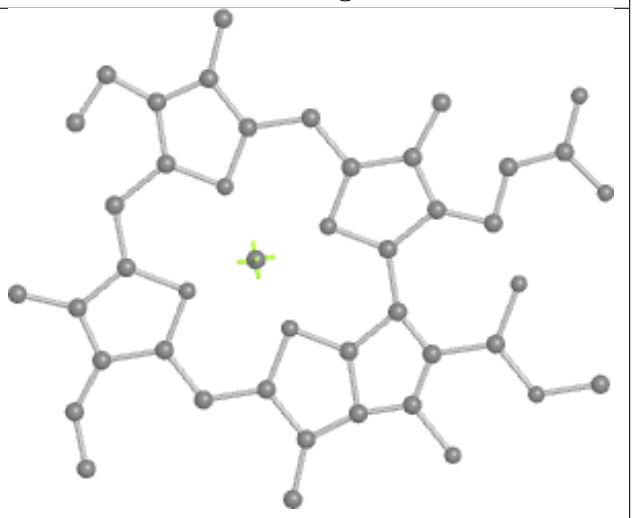
Bond lengths



Bond angles

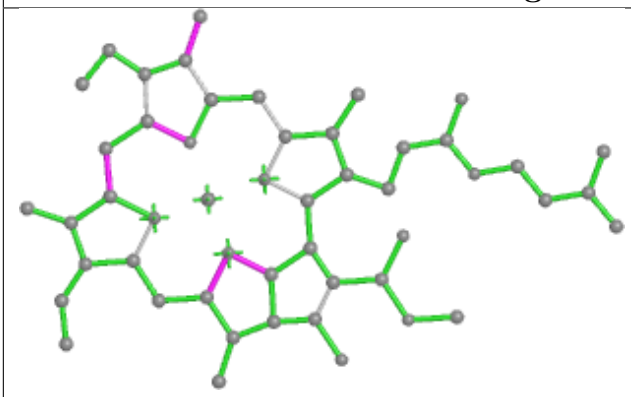


Torsions

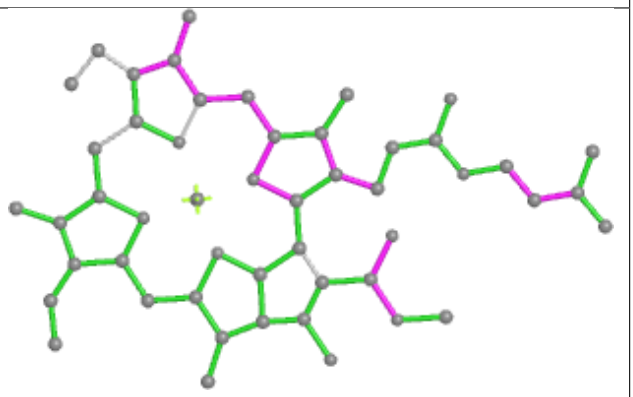


Rings

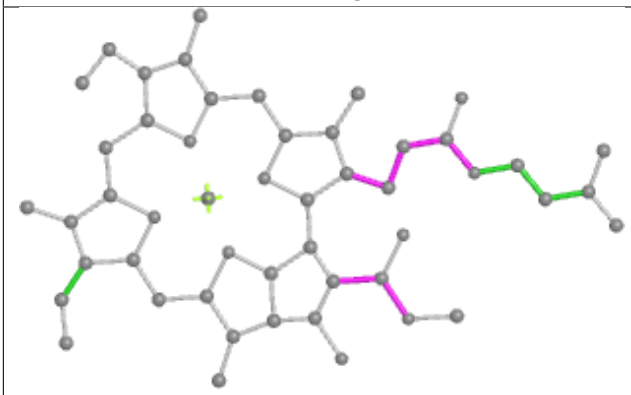
Ligand CLA B 308



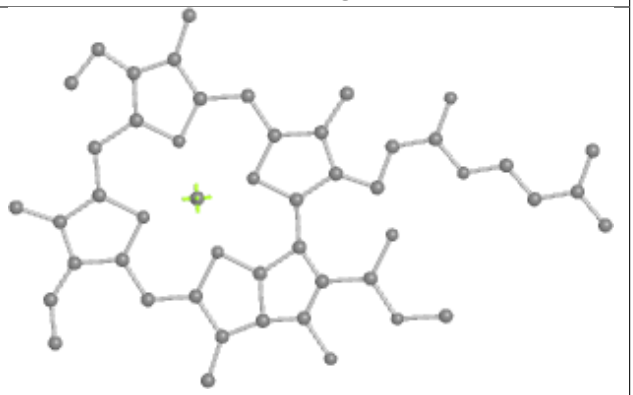
Bond lengths



Bond angles

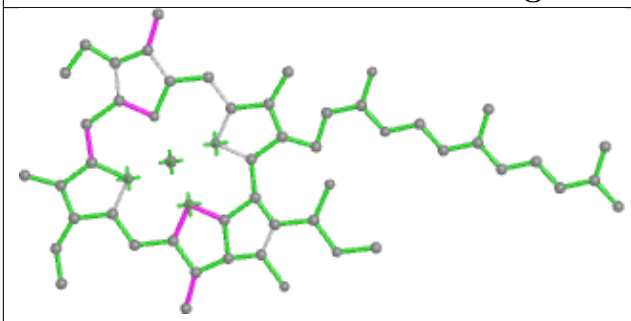


Torsions

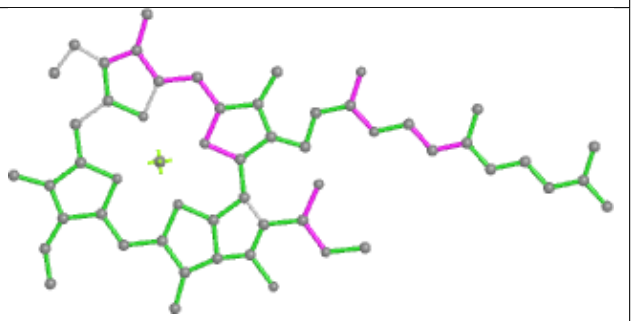


Rings

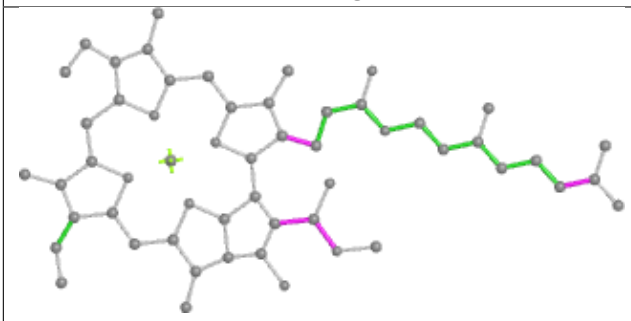
Ligand CLA B 314



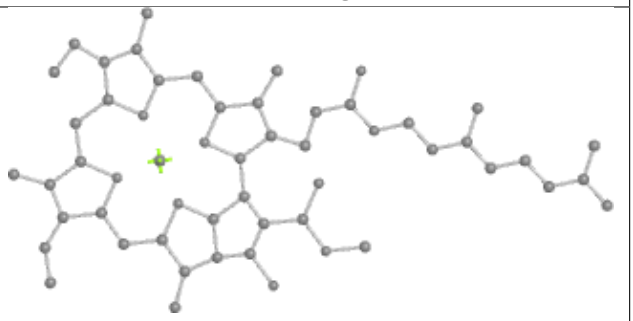
Bond lengths



Bond angles

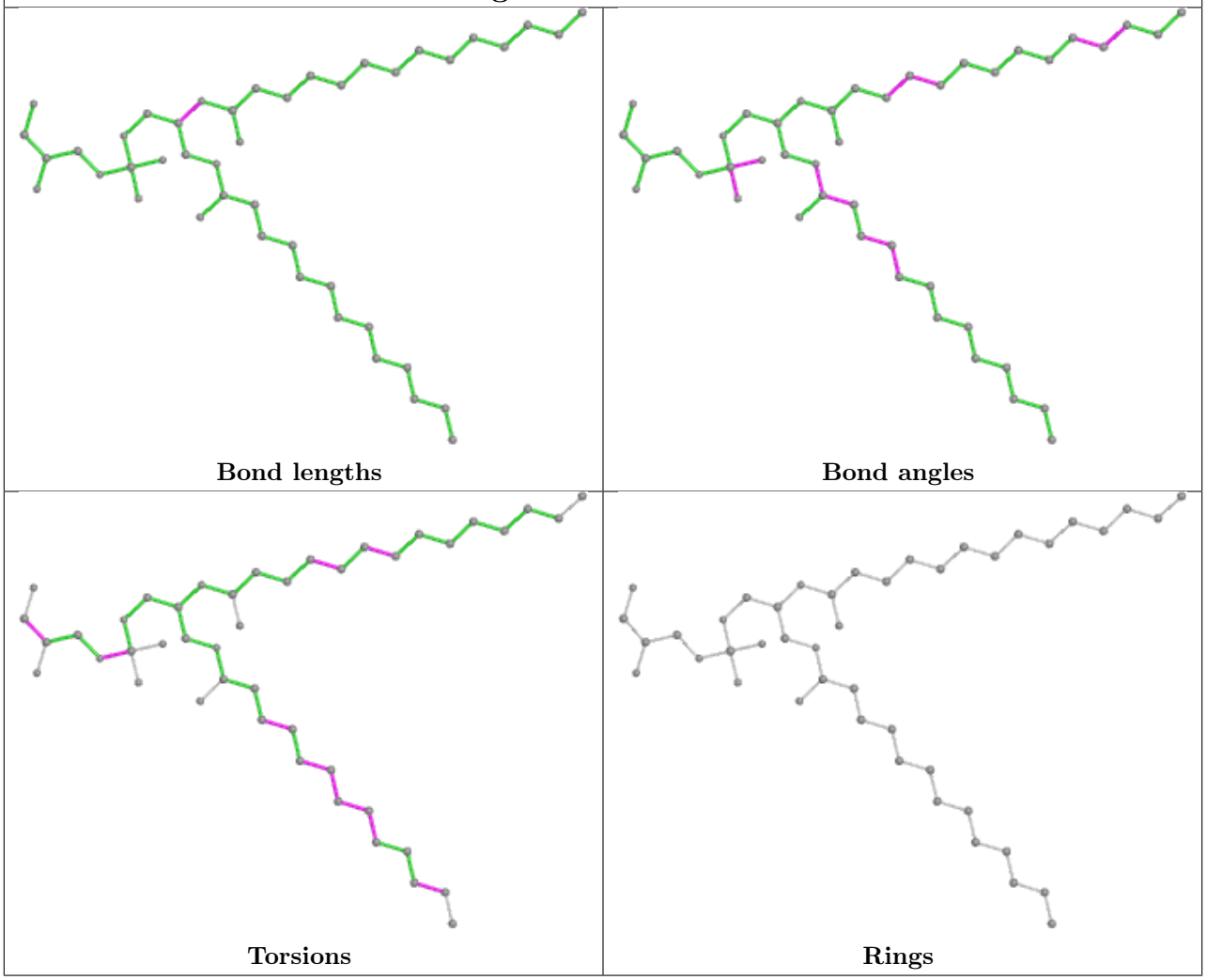


Torsions

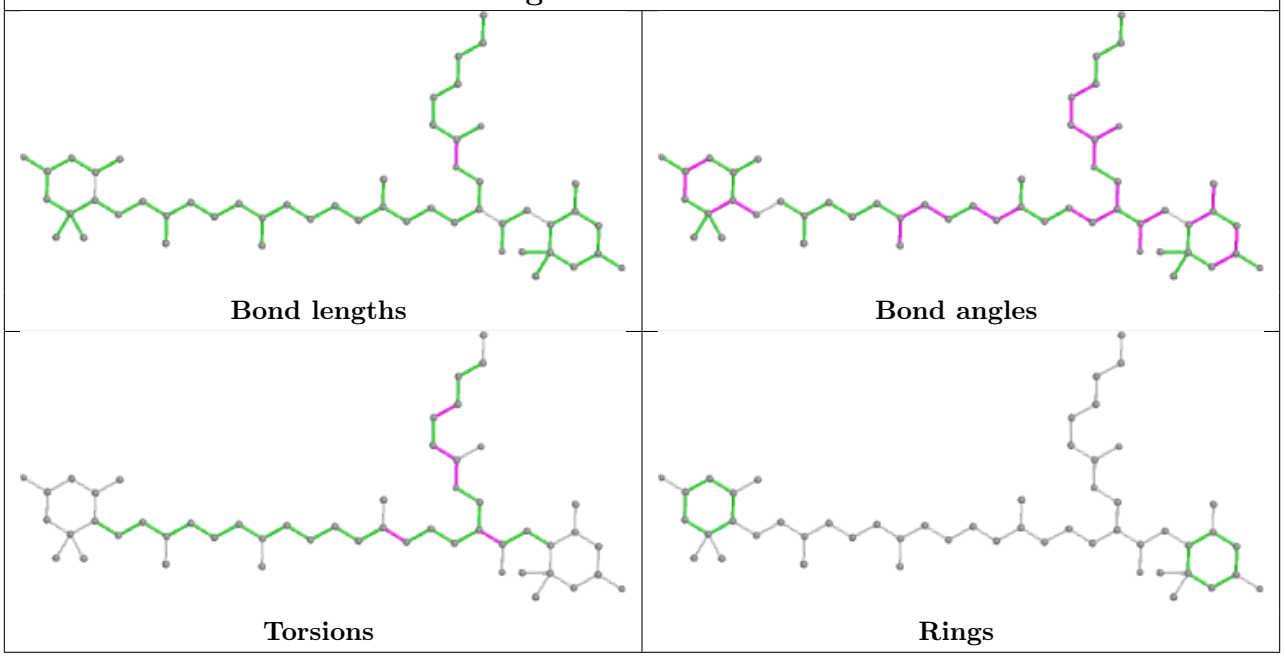


Rings

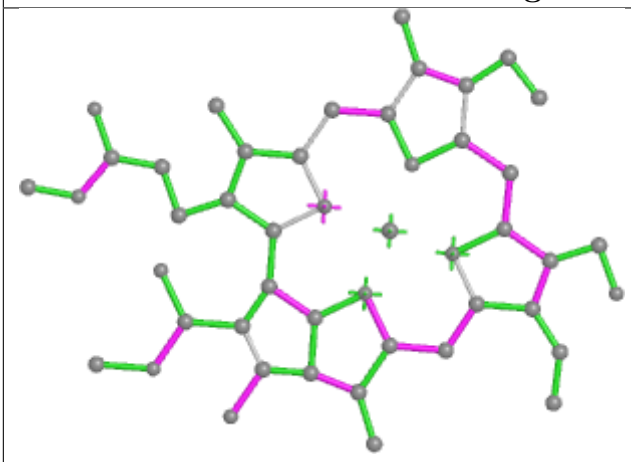
Ligand LHG B 319



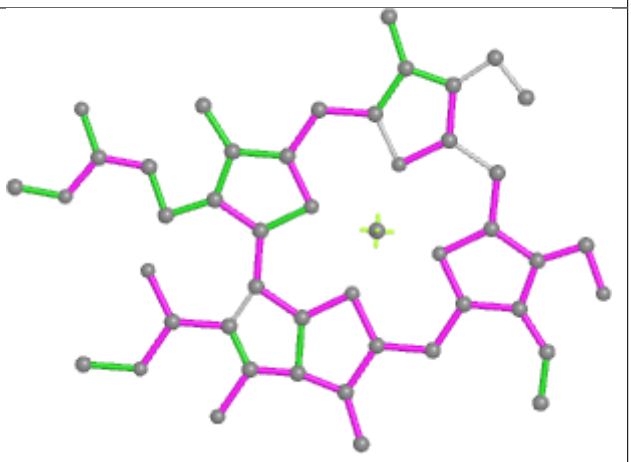
Ligand 0UR A 301



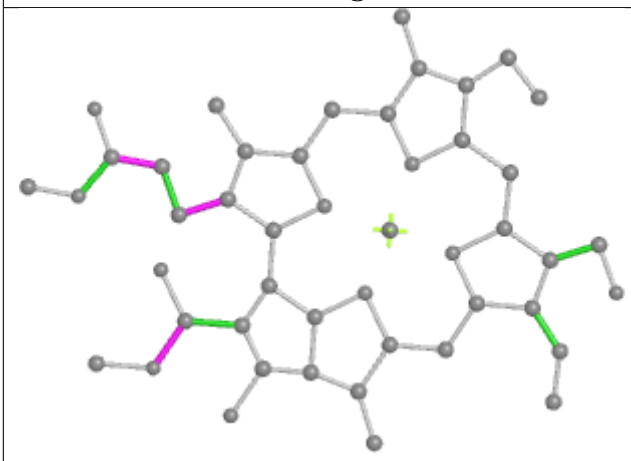
Ligand CHL B 311



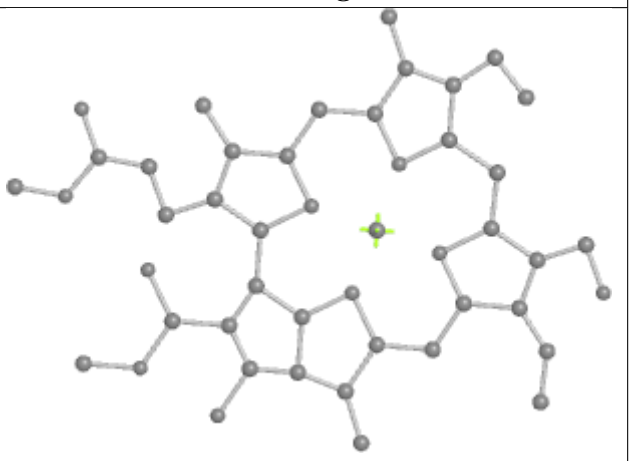
Bond lengths



Bond angles

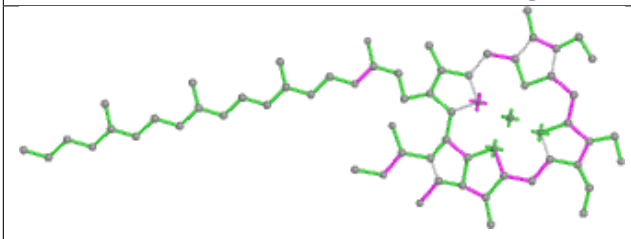


Torsions

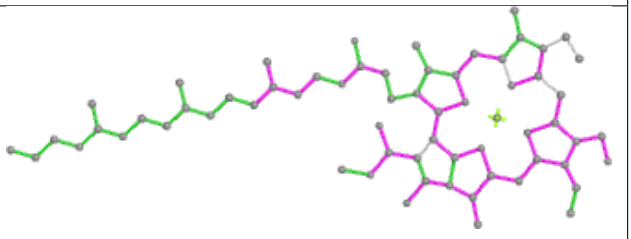


Rings

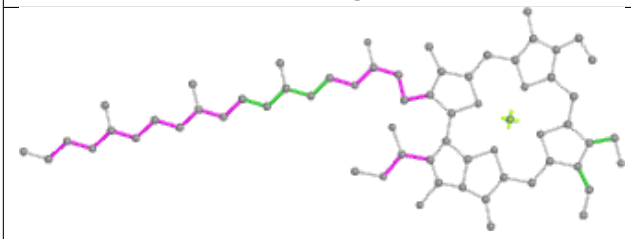
Ligand CHL A 305



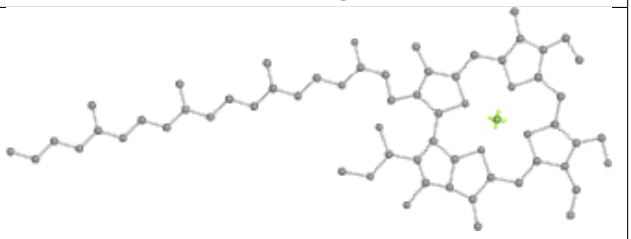
Bond lengths



Bond angles

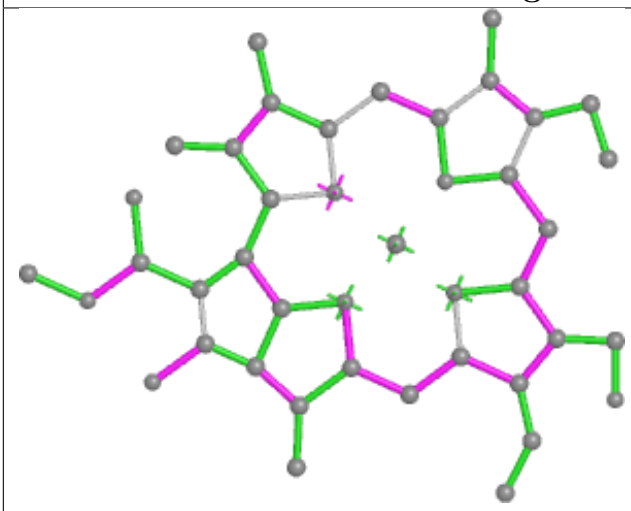


Torsions

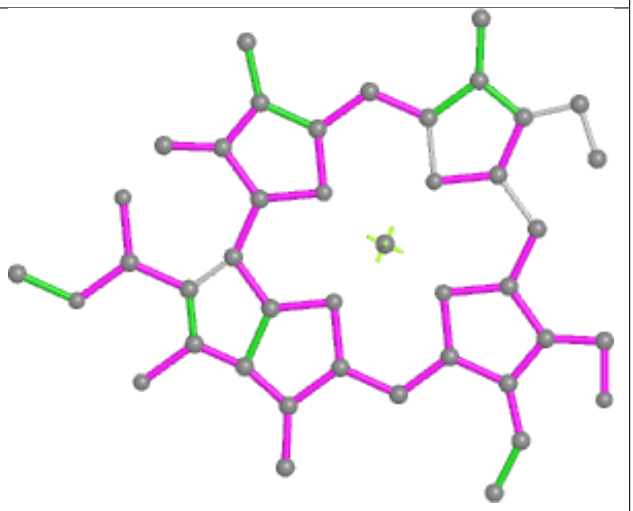


Rings

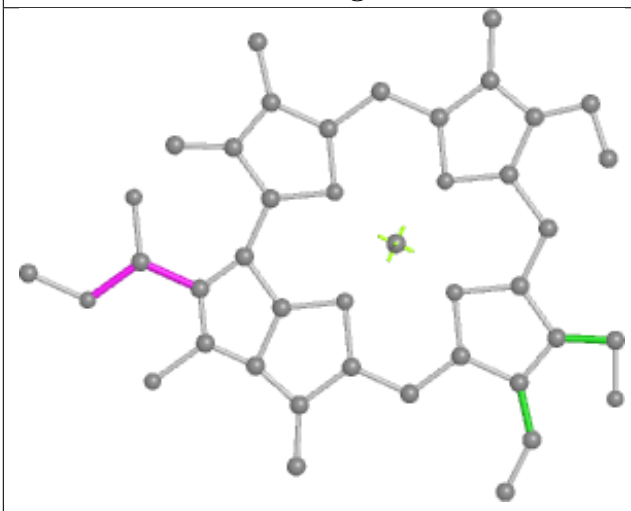
Ligand CHL A 317



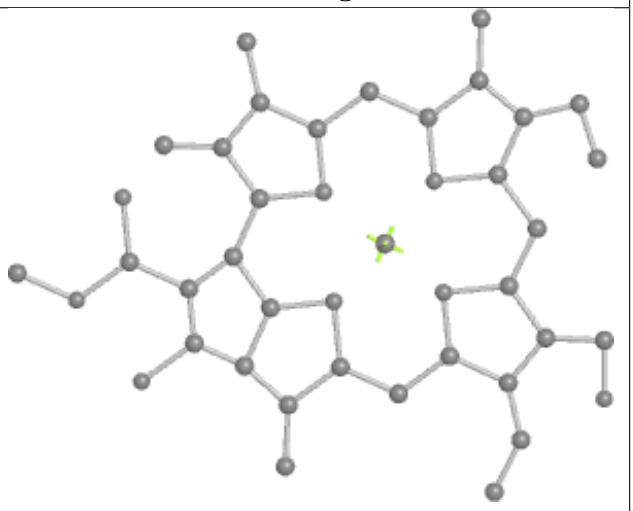
Bond lengths



Bond angles

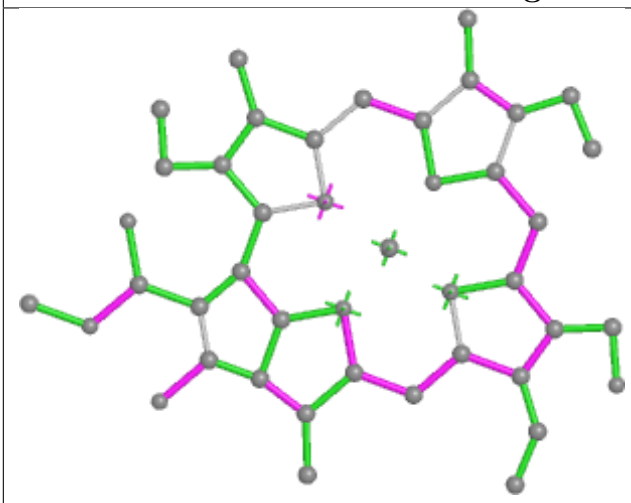


Torsions

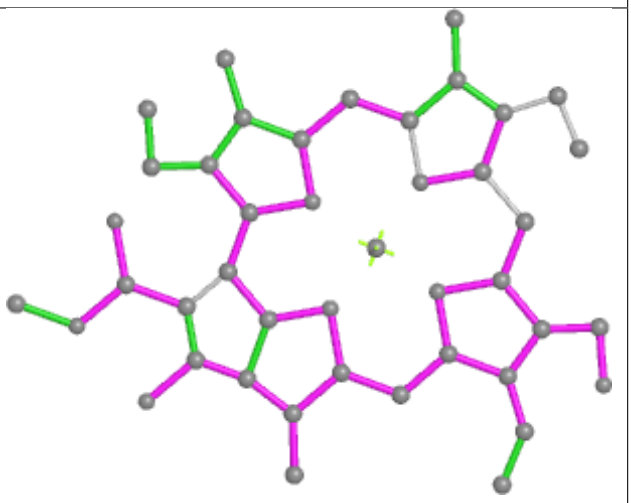


Rings

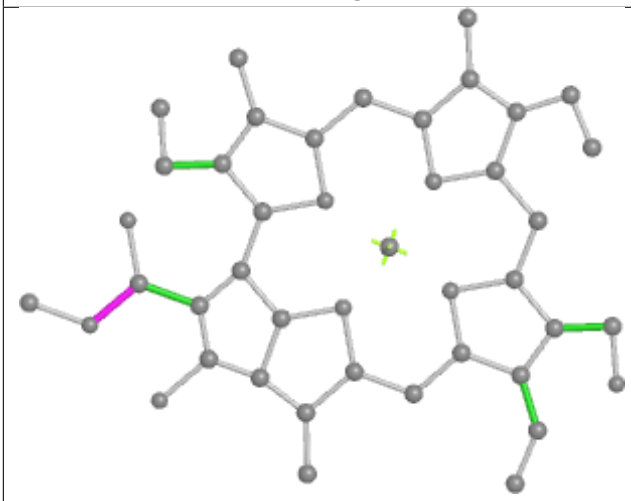
Ligand CHL C 309



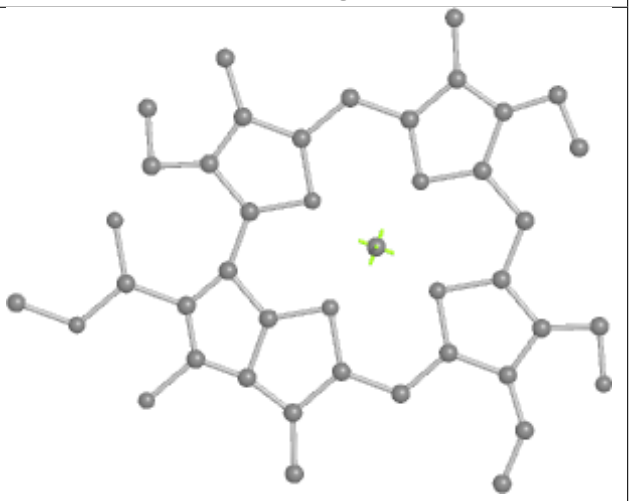
Bond lengths



Bond angles

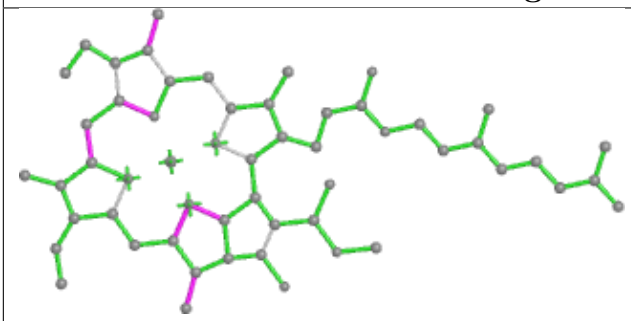


Torsions

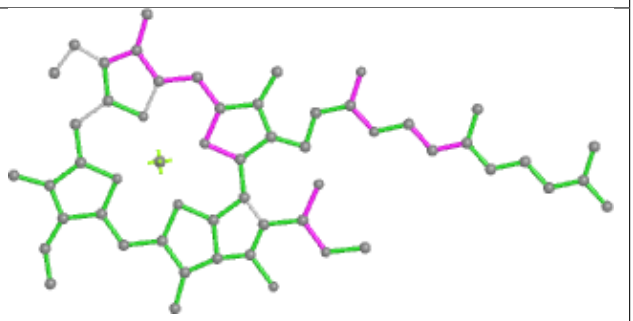


Rings

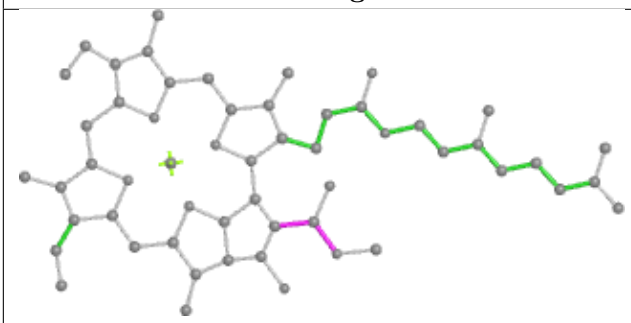
Ligand CLA C 314



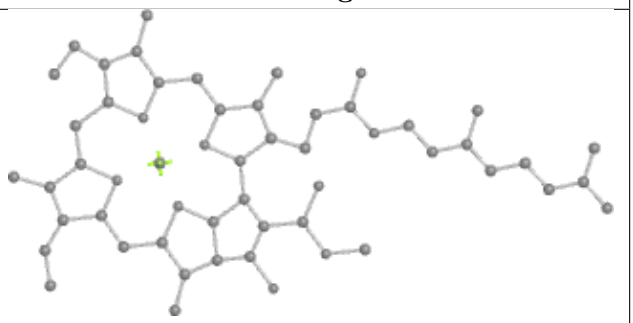
Bond lengths



Bond angles

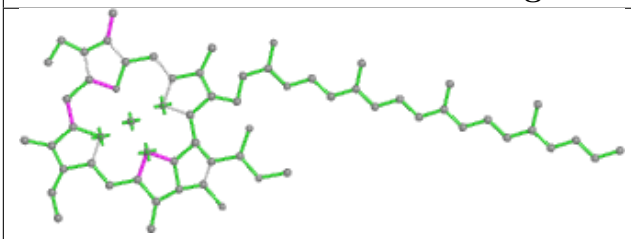


Torsions

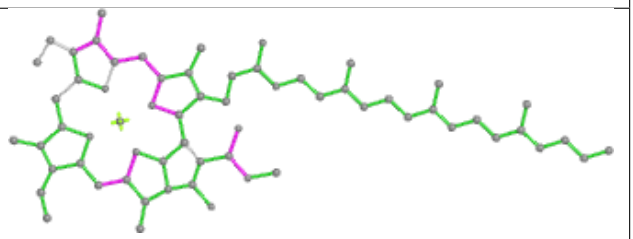


Rings

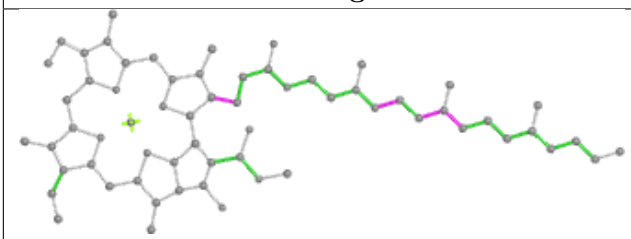
Ligand CLA C 315



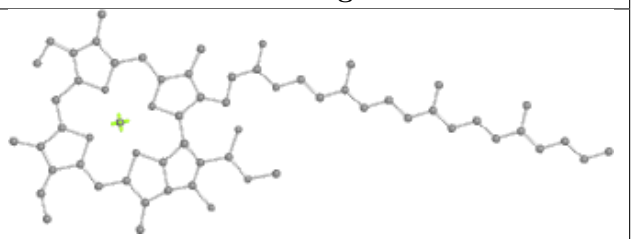
Bond lengths



Bond angles

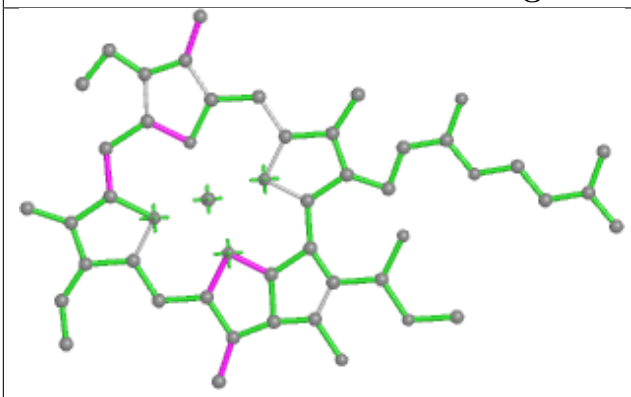


Torsions



Rings

Ligand CLA A 307



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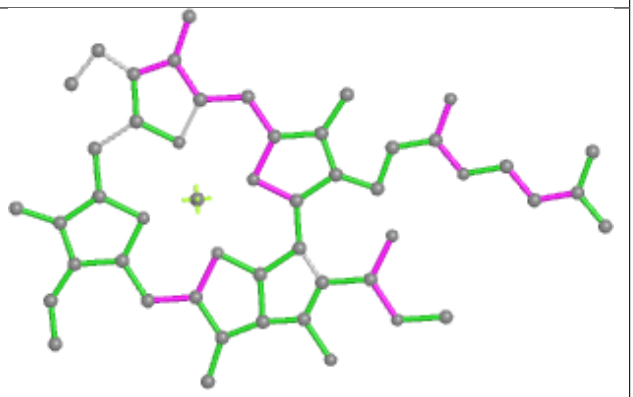
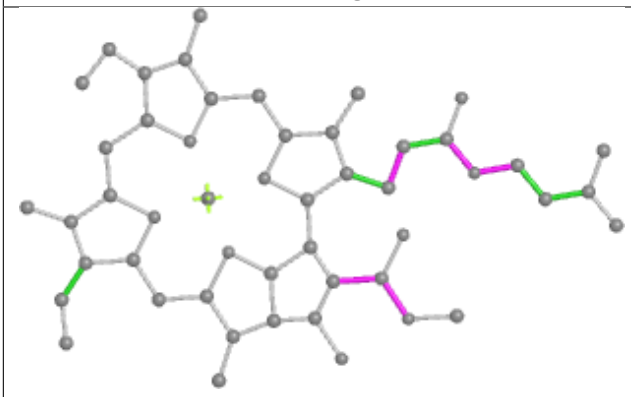
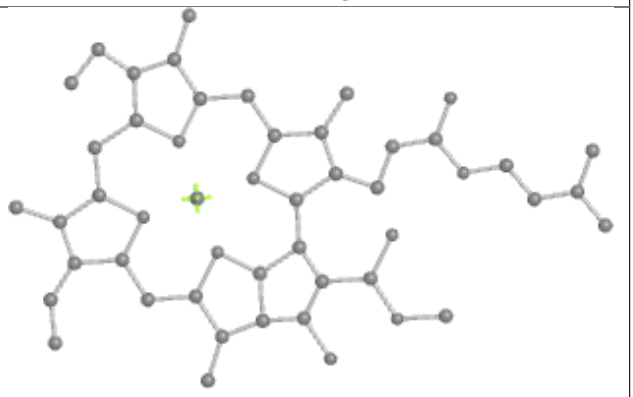


Bond angles

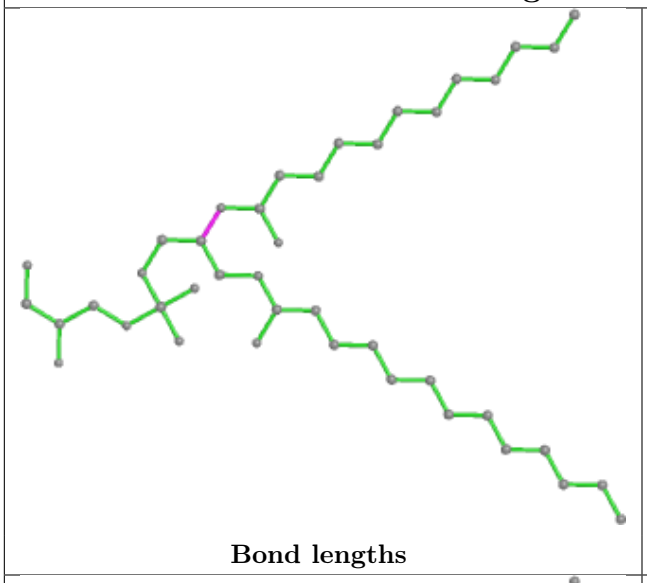


Torsions

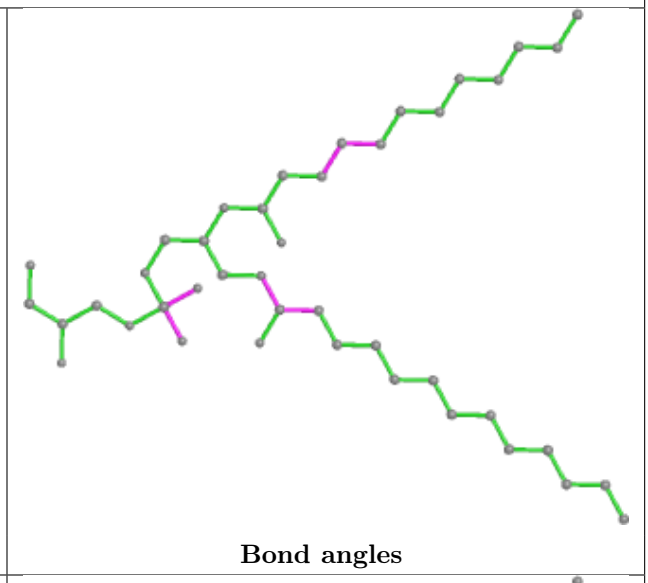


Rings

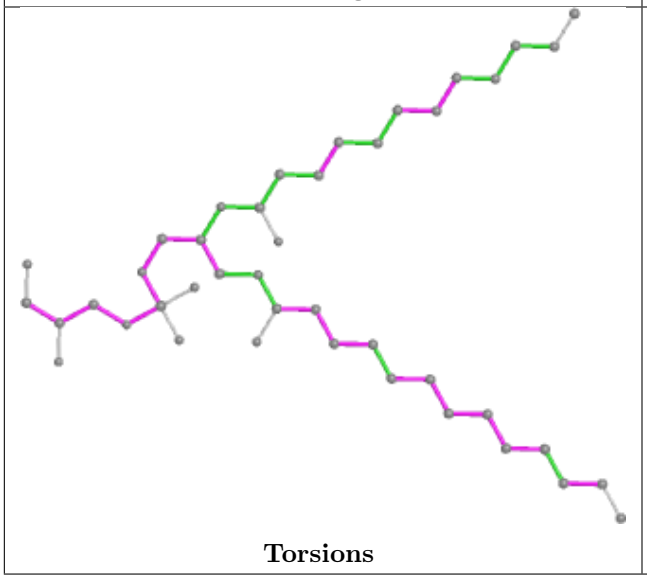
Ligand LHG A 318



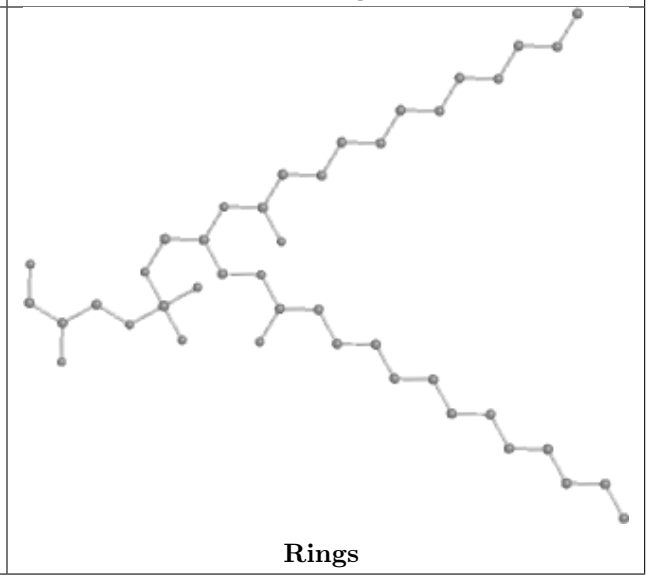
Bond lengths



Bond angles

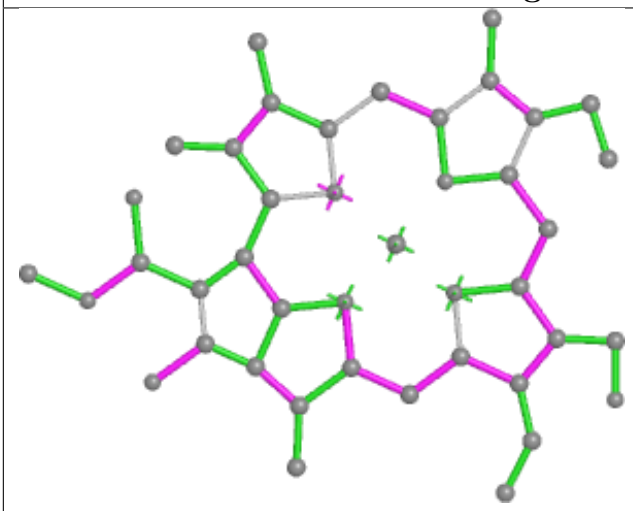


Torsions

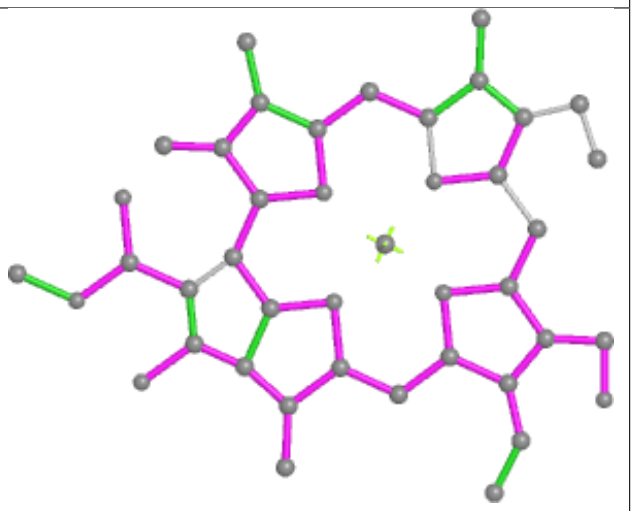


Rings

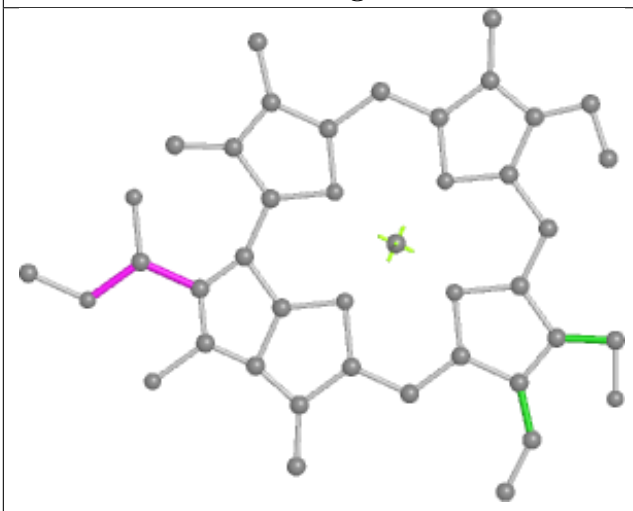
Ligand CHL C 318



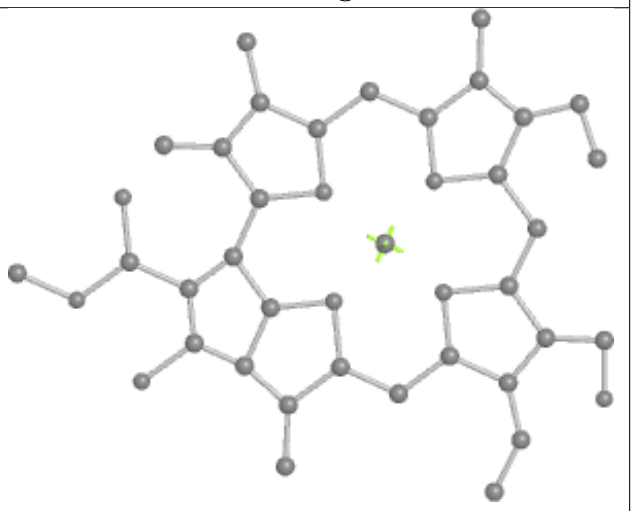
Bond lengths



Bond angles

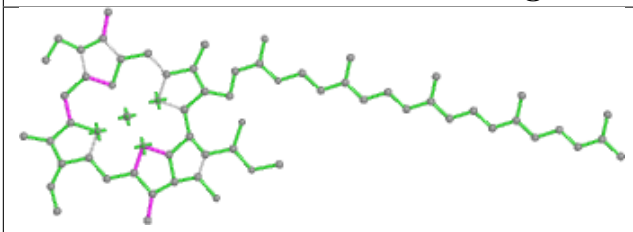


Torsions

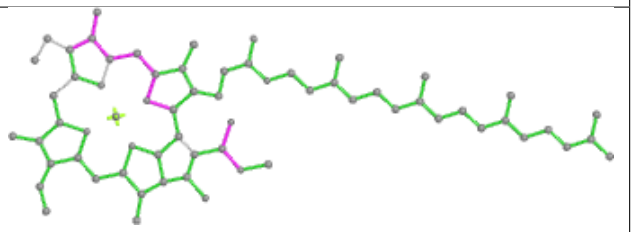


Rings

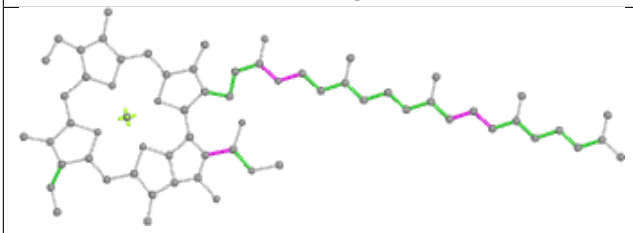
Ligand CLA C 307



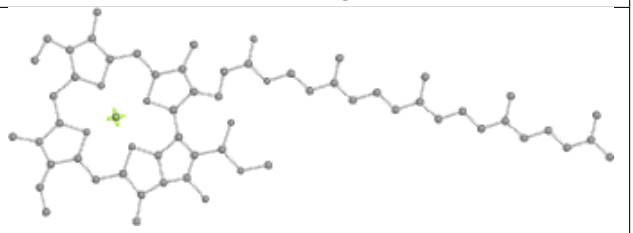
Bond lengths



Bond angles

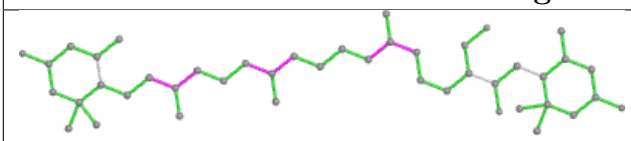


Torsions

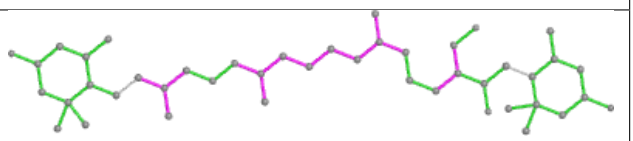


Rings

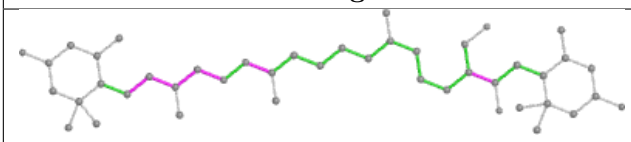
Ligand 0IE A 302



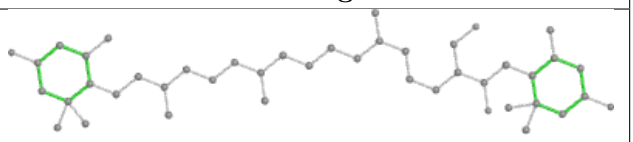
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

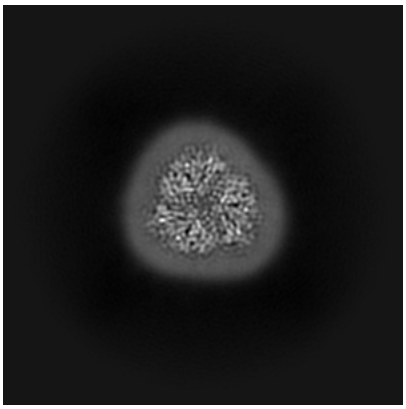
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34930. These allow visual inspection of the internal detail of the map and identification of artifacts.

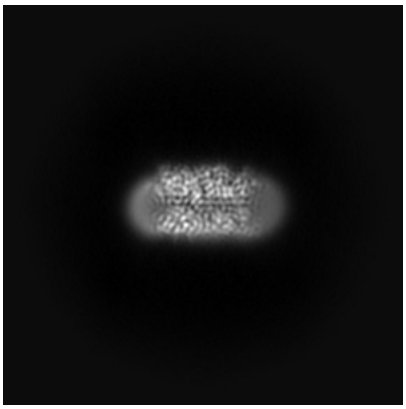
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

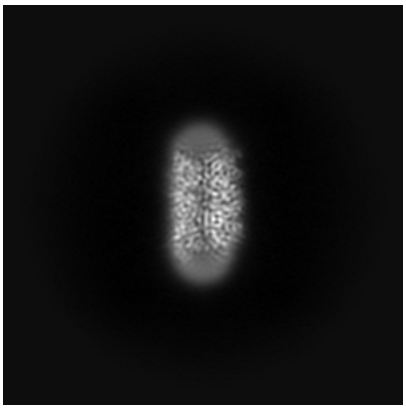
6.1.1 Primary map



X

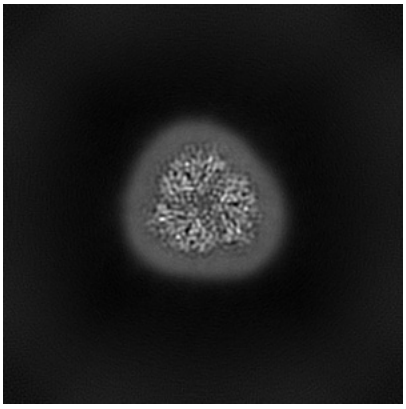


Y

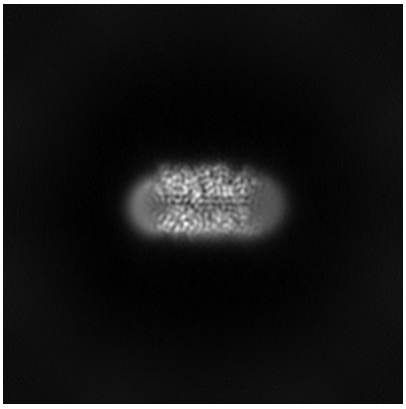


Z

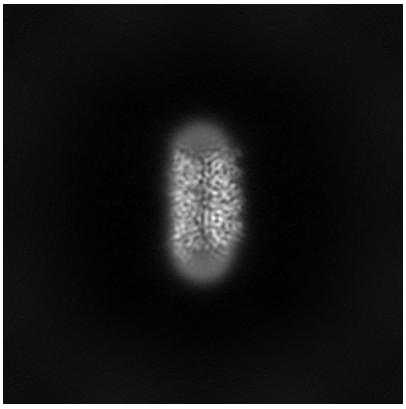
6.1.2 Raw map



X



Y

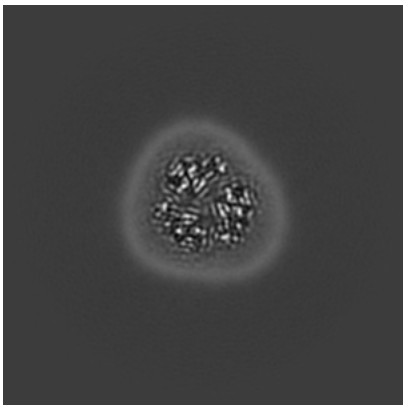


Z

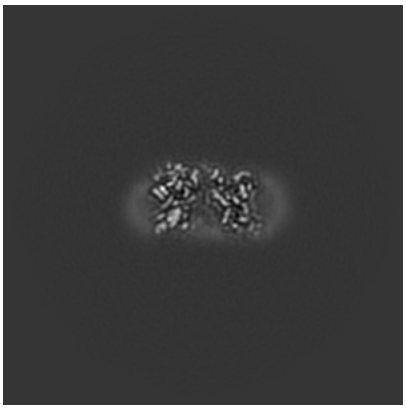
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

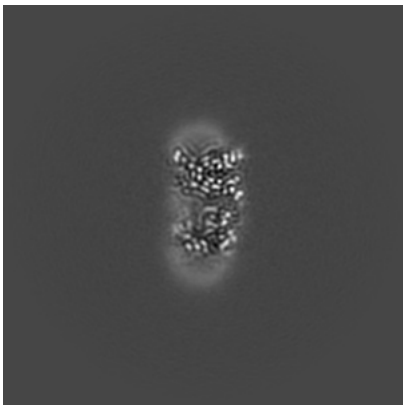
6.2.1 Primary map



X Index: 128

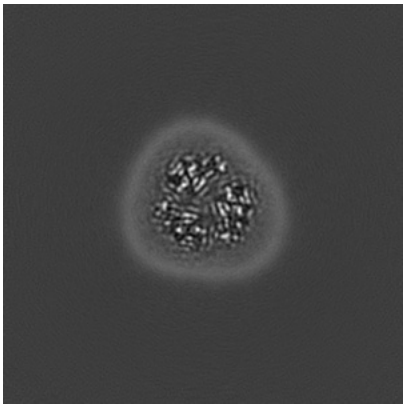


Y Index: 128

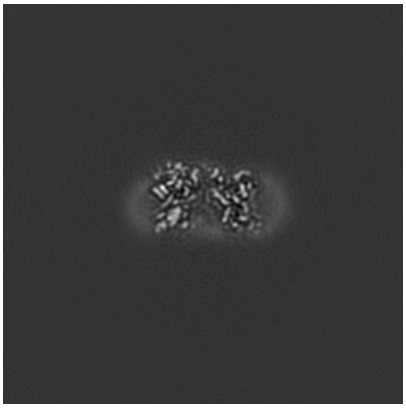


Z Index: 128

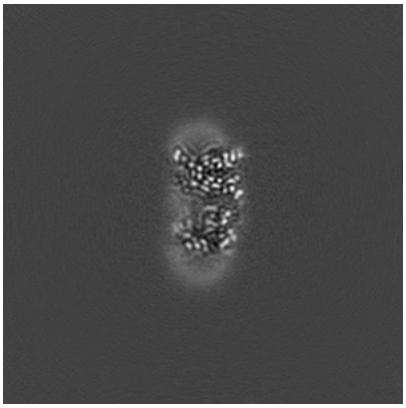
6.2.2 Raw map



X Index: 128



Y Index: 128

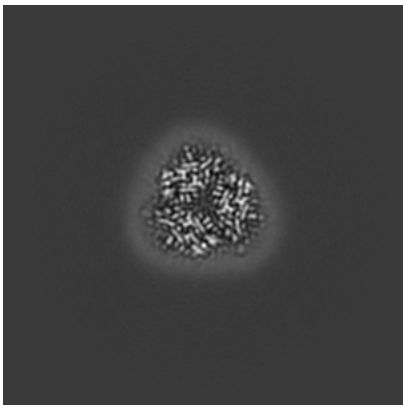


Z Index: 128

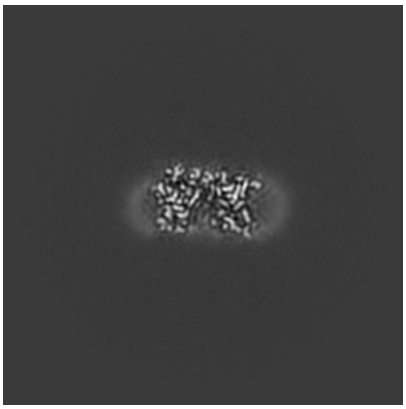
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

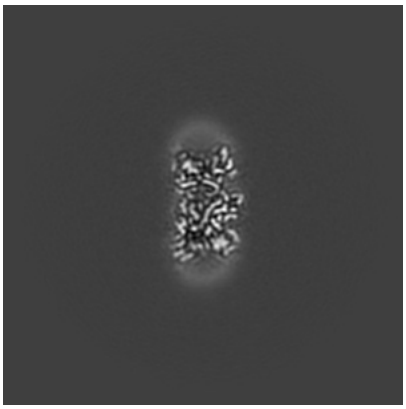
6.3.1 Primary map



X Index: 138

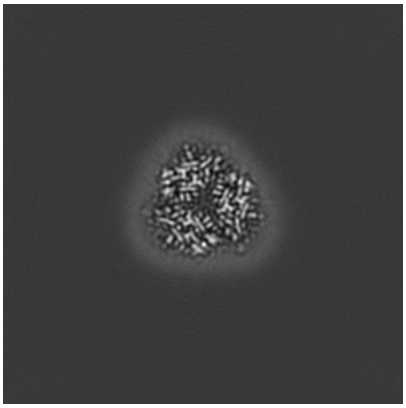


Y Index: 122

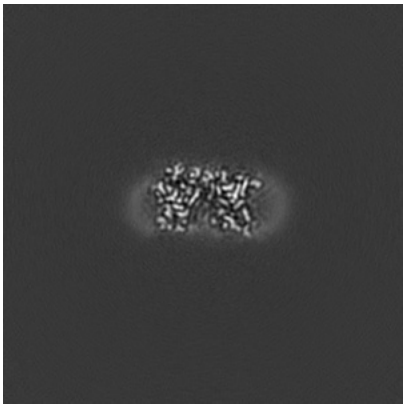


Z Index: 117

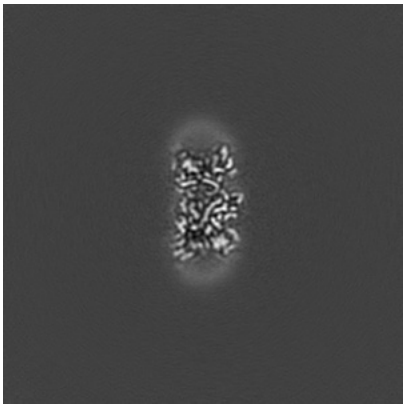
6.3.2 Raw map



X Index: 138



Y Index: 122

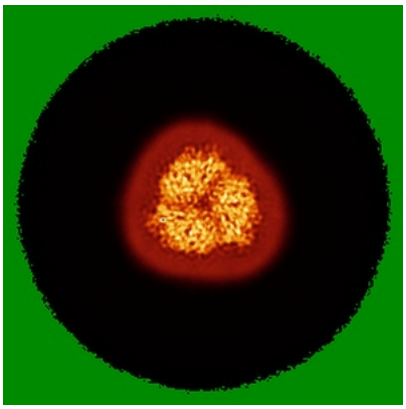


Z Index: 117

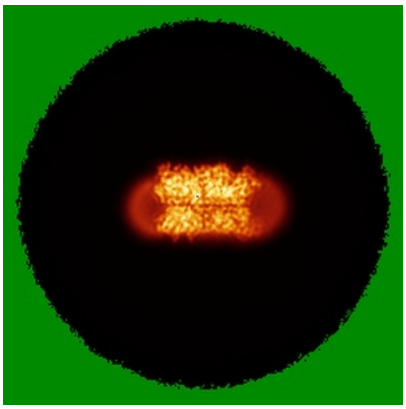
The images above show the largest variance slices of the map in three orthogonal directions.

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

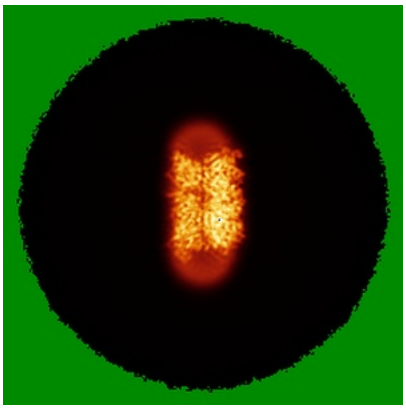
6.4.1 Primary map



X

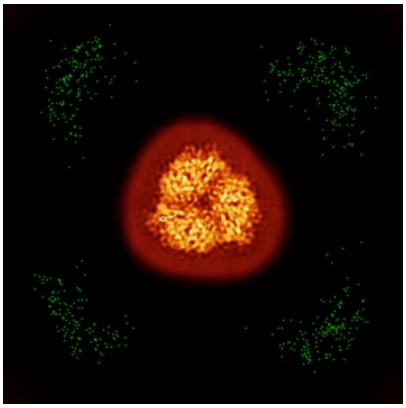


Y

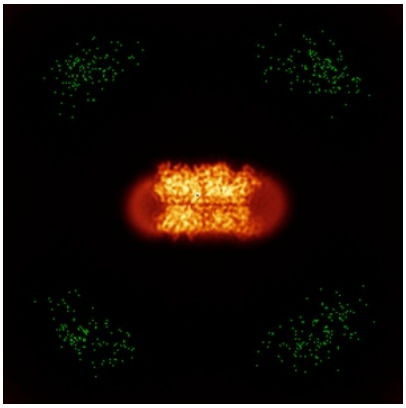


Z

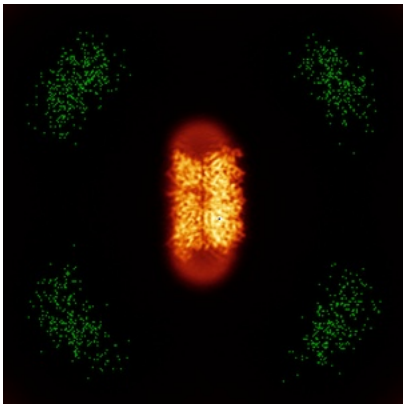
6.4.2 Raw map



X



Y

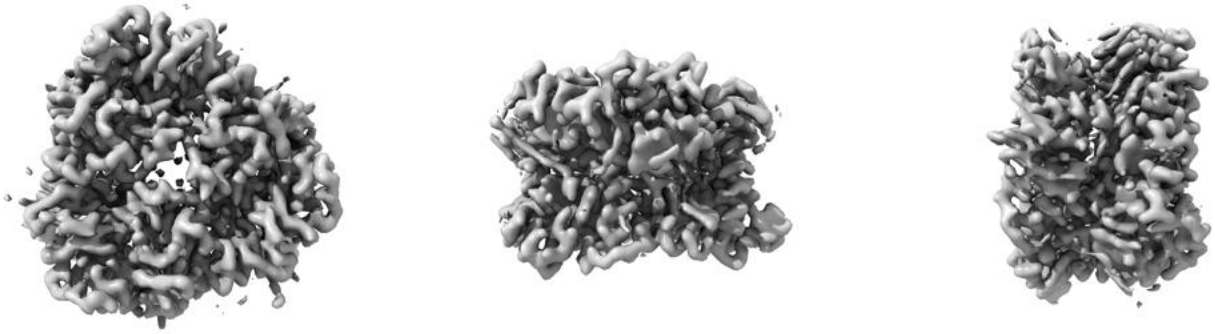


Z

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.

6.5 Orthogonal surface views (i)

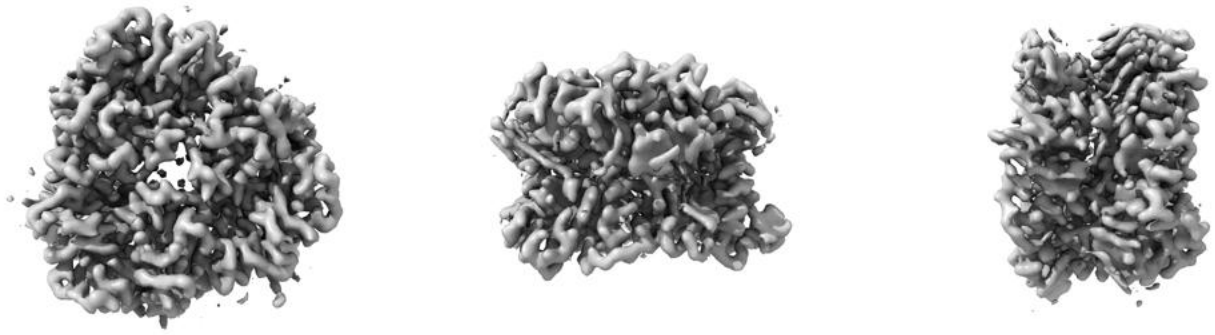
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.228. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

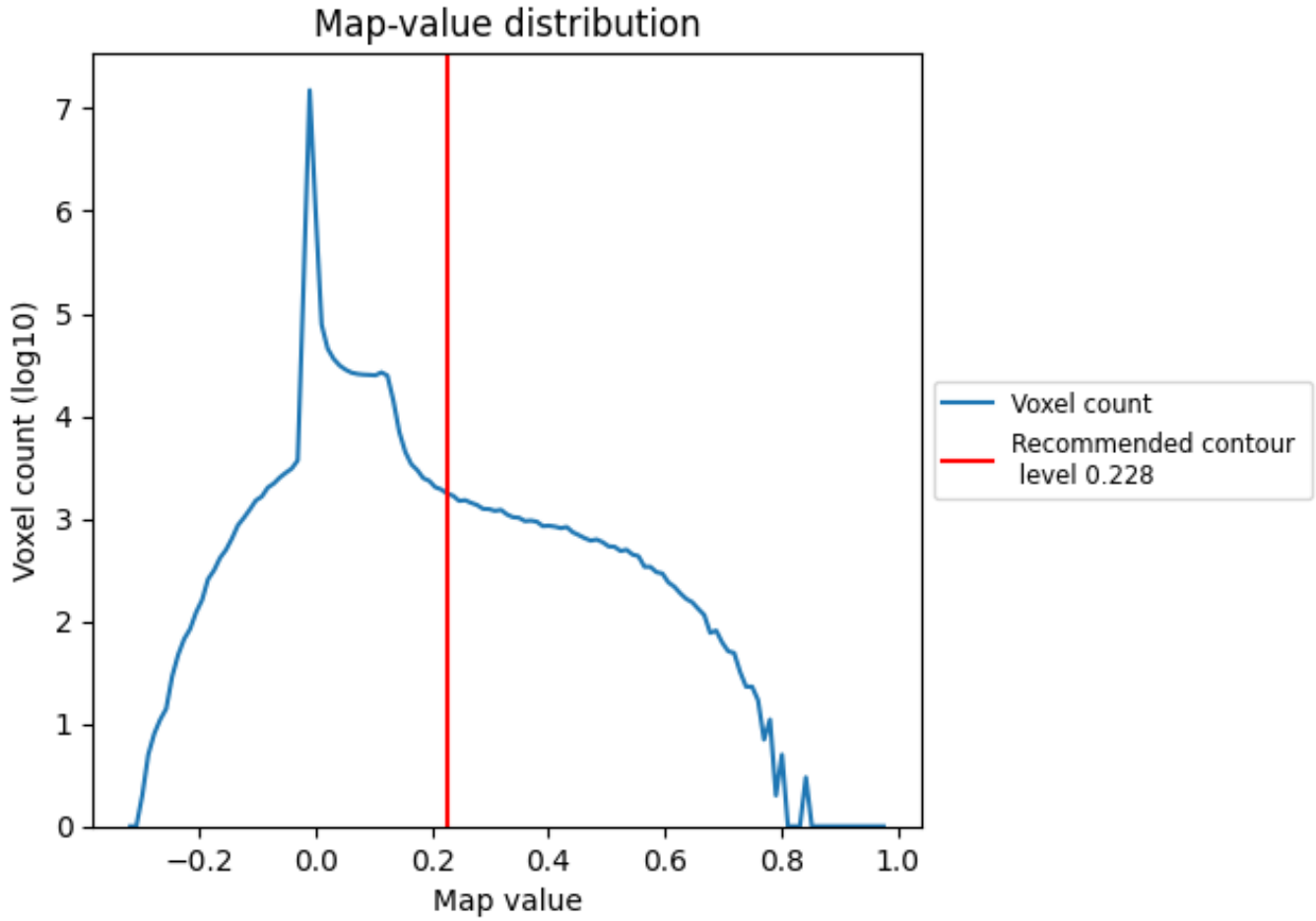
6.6 Mask visualisation (i)

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

7 Map analysis

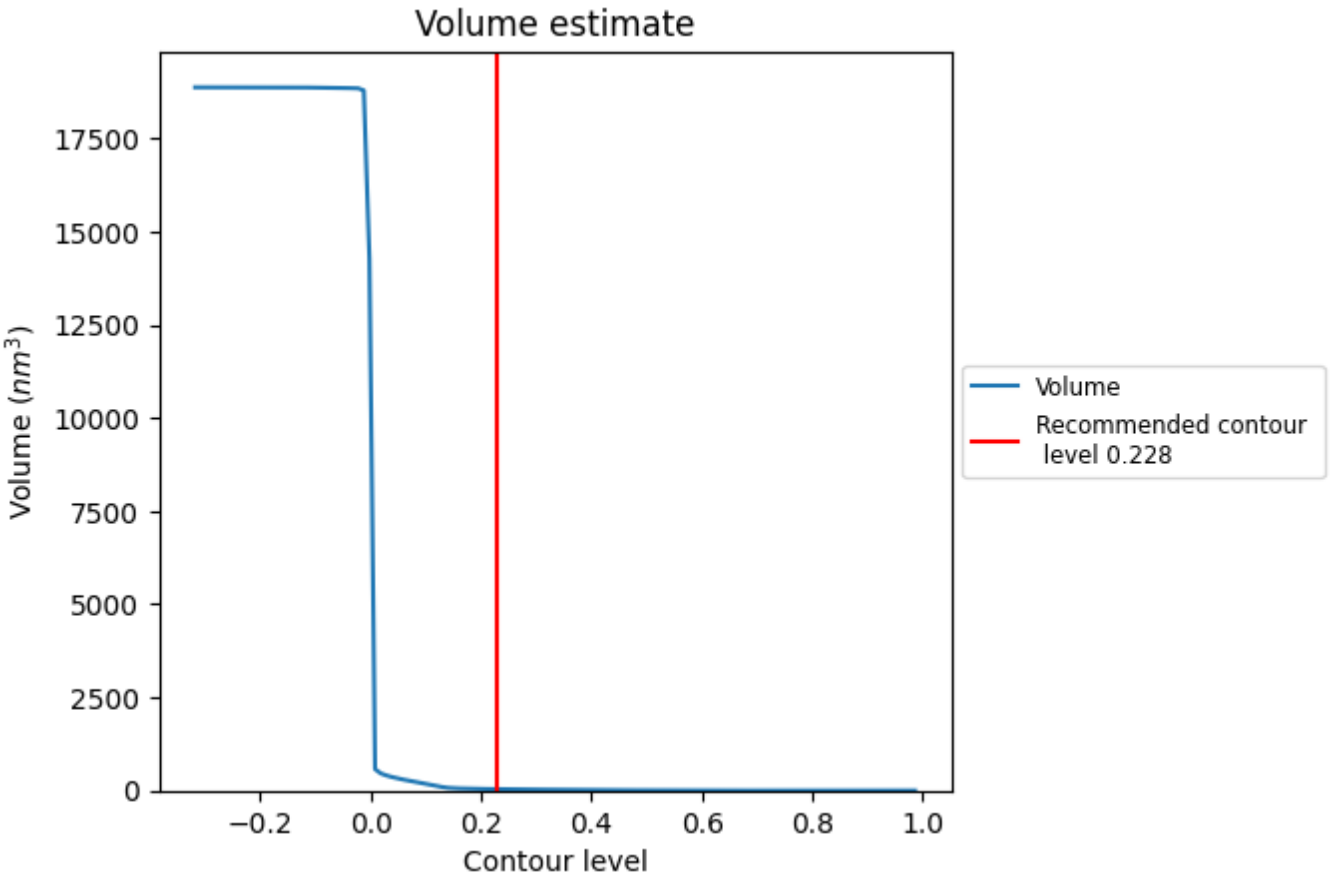
This section contains the results of statistical analysis of the map.

7.1 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.

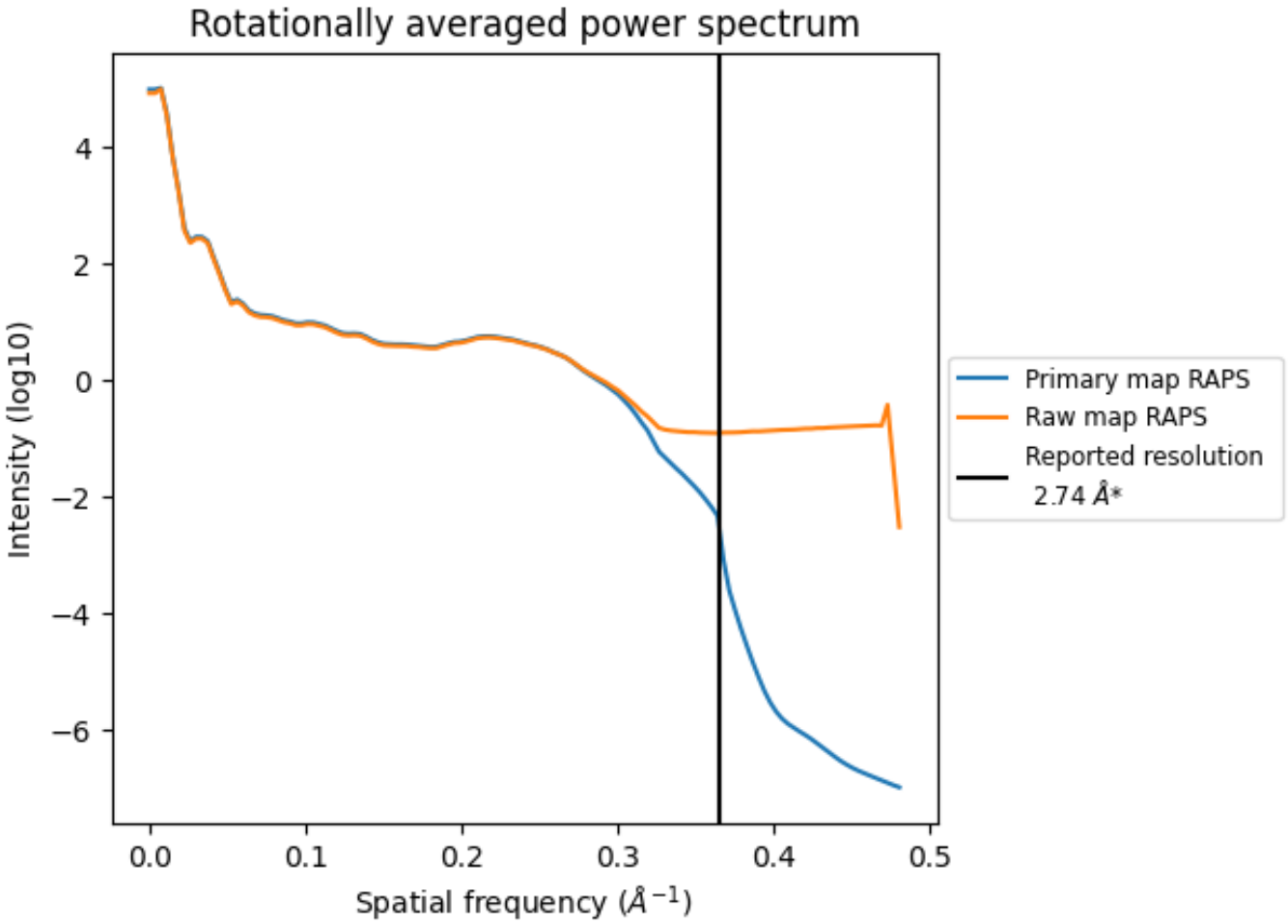
7.2 Volume estimate



The volume at the recommended contour level is 38 nm^3; this corresponds to an approximate mass of 34 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.

7.3 Rotationally averaged power spectrum (i)

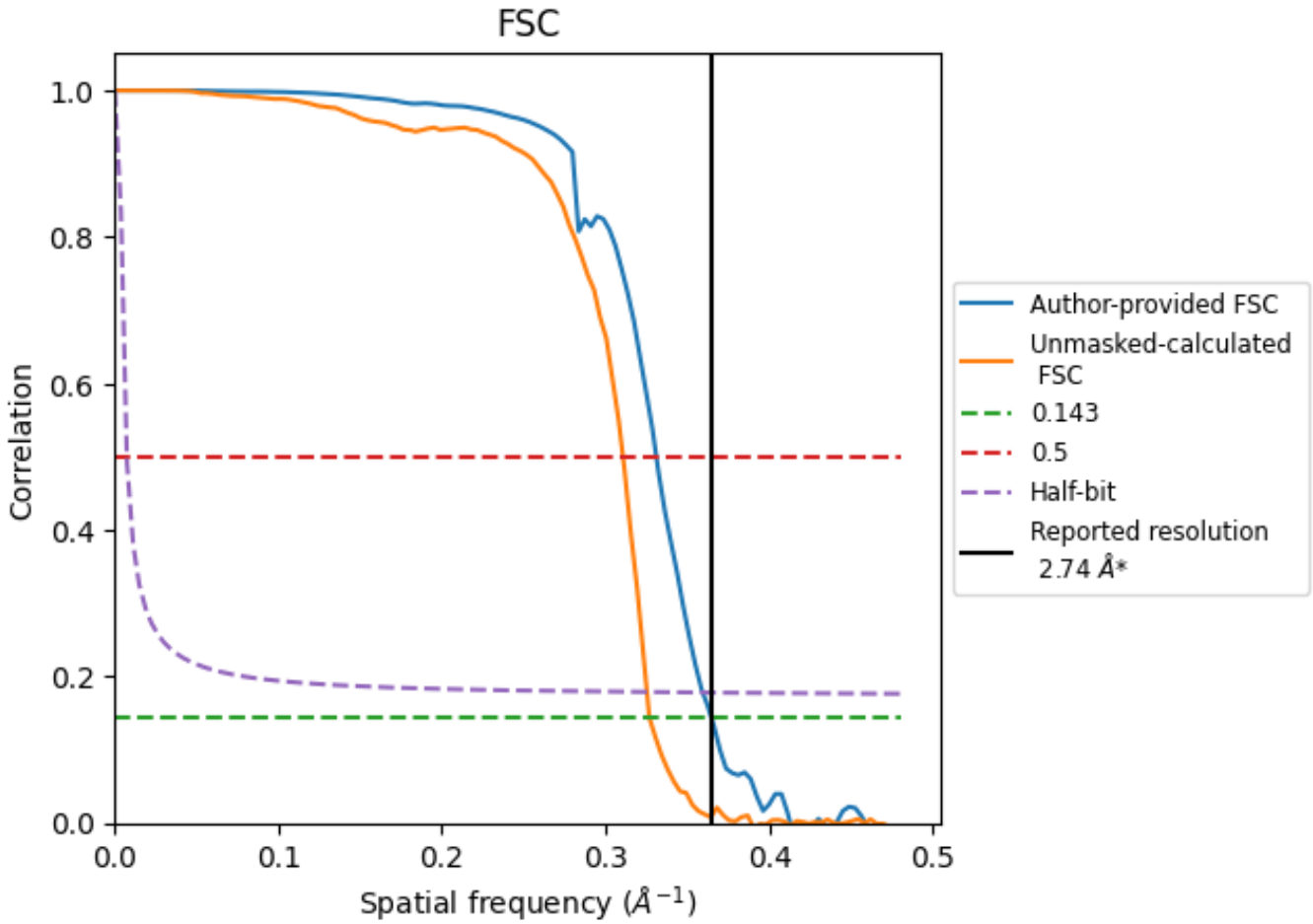


*Reported resolution corresponds to spatial frequency of 0.365 Å^{-1}

8 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.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.365 $Å^{-1}$

8.2 Resolution estimates (i)

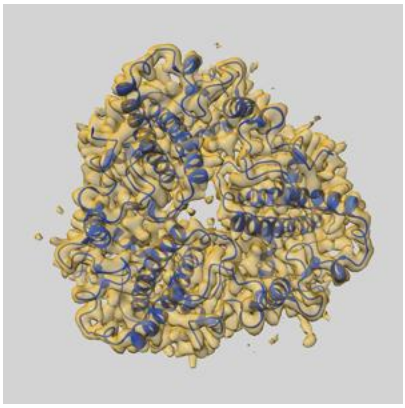
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.74	3.02	2.78
Unmasked-calculated*	3.06	3.22	3.07

*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 3.06 differs from the reported value 2.74 by more than 10 %

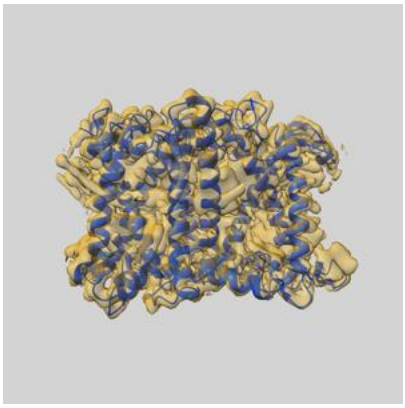
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34930 and PDB model 8HPD. Per-residue inclusion information can be found in section 3 on page 11.

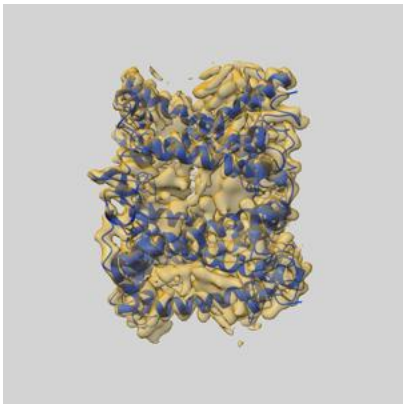
9.1 Map-model overlay



X



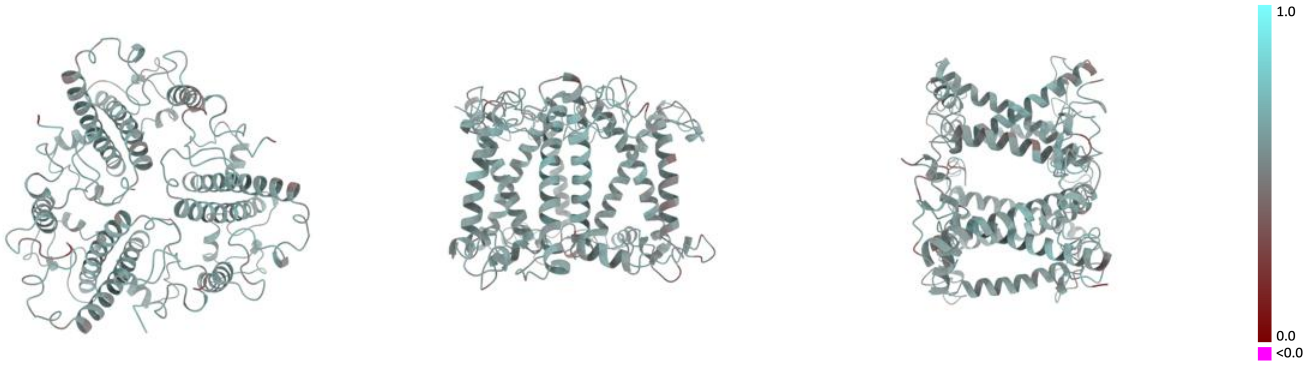
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.228 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.

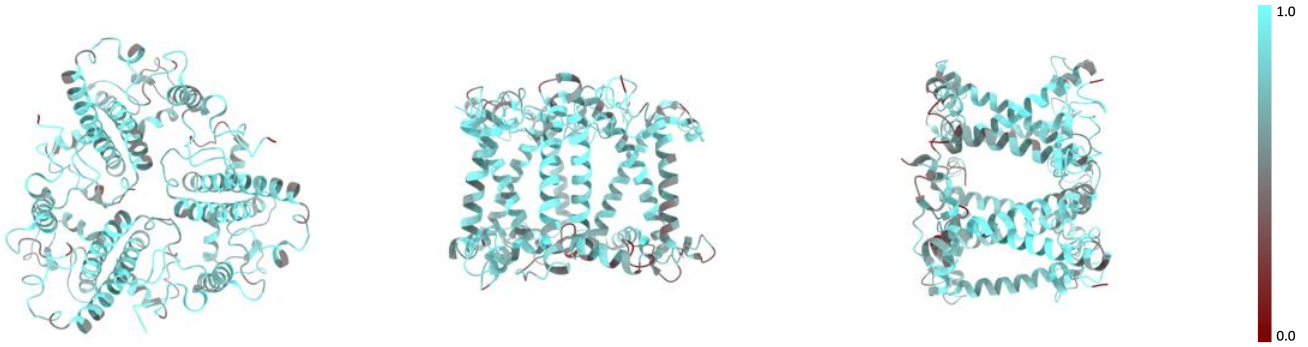
9.2 Q-score mapped to coordinate model (i)



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.

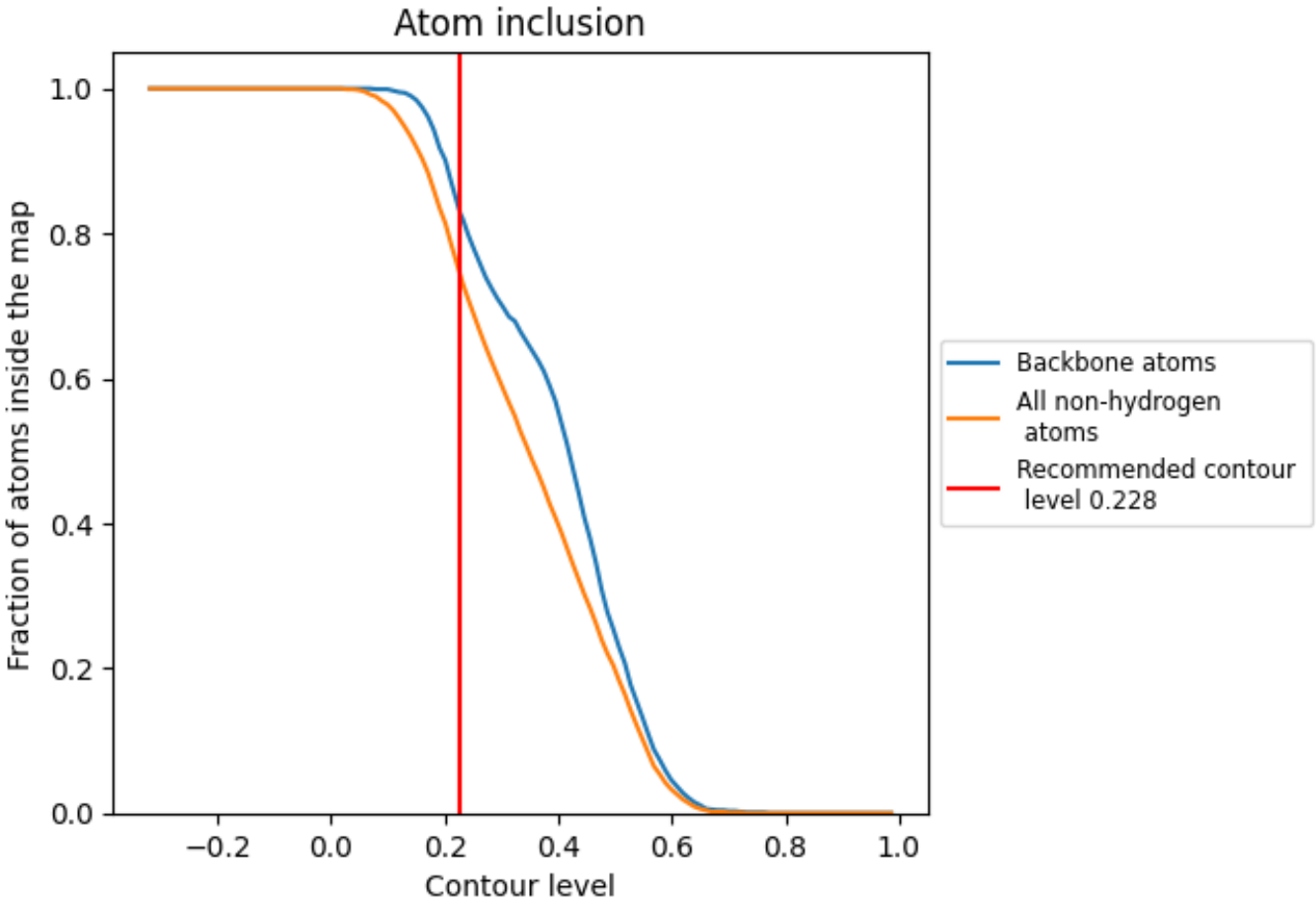
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.228).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.228) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7430	0.5710
A	0.7510	0.5760
B	0.7540	0.5710
C	0.7250	0.5650