Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:43 PM UTC

PDB ID	:	7E0J / pdb_00007e0j
EMDB ID	:	EMD-30934
Title	:	LHCII-1 in the state transition supercomplex PSI-LHCI-LHCII from the double phosphatase mutant pph1;pbcp of Chlamydomonas reinhardti.
Authors	:	Pan, X.W.; Li, A.J.; Liu, Z.F.; Li, M.
Deposited on	:	2021-01-28
Resolution	:	3.13 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:

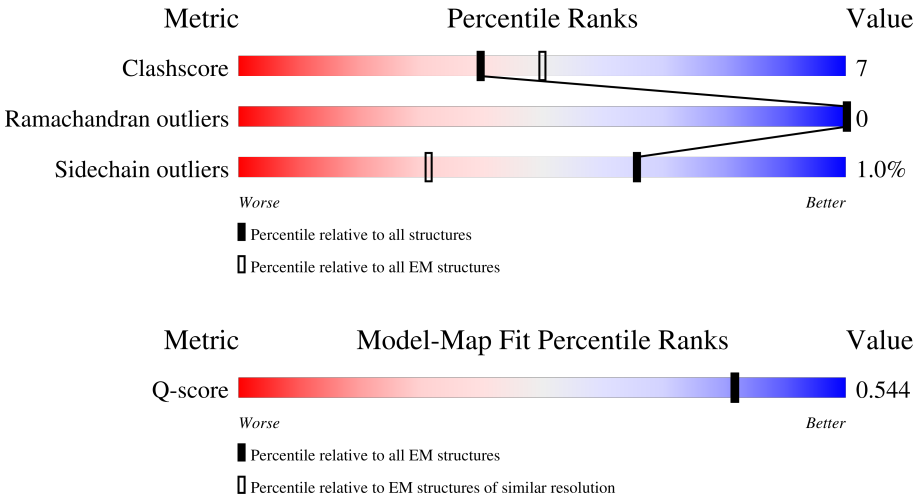
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.13 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14478 (2.63 - 3.63)

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	X	249	10% 78% 10% 12%
2	Y	257	7% 75% 9% 14%
3	Z	256	9% 85% 5% 9%

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
4	CHL	X	601	X	-	-	-
4	CHL	X	605	X	-	-	-
4	CHL	X	607	X	-	-	-
4	CHL	X	608	X	-	-	-
4	CHL	X	609	X	-	-	-
4	CHL	Y	601	X	-	-	-
4	CHL	Y	605	X	-	-	-
4	CHL	Y	606	X	-	-	-
4	CHL	Y	607	X	-	-	-
4	CHL	Y	608	X	-	-	-
4	CHL	Y	609	X	-	-	-
4	CHL	Z	601	X	-	-	-
4	CHL	Z	605	X	-	-	-
4	CHL	Z	606	X	-	-	-
4	CHL	Z	607	X	-	-	-
4	CHL	Z	608	X	-	-	-
4	CHL	Z	609	X	-	-	-
5	CLA	X	602	X	-	-	-
5	CLA	X	603	X	-	-	-
5	CLA	X	604	X	-	-	-
5	CLA	X	610	X	-	-	-
5	CLA	X	611	X	-	-	-
5	CLA	X	612	X	-	-	-
5	CLA	X	613	X	-	-	-
5	CLA	X	614	X	-	-	-
5	CLA	Y	602	X	-	-	-
5	CLA	Y	603	X	-	-	-
5	CLA	Y	604	X	-	-	-
5	CLA	Y	610	X	-	-	-
5	CLA	Y	611	X	-	-	-
5	CLA	Y	612	X	-	-	-
5	CLA	Y	613	X	-	-	-
5	CLA	Y	614	X	-	-	-
5	CLA	Z	602	X	-	-	-
5	CLA	Z	603	X	-	-	-
5	CLA	Z	604	X	-	-	-
5	CLA	Z	610	X	-	-	-
5	CLA	Z	611	X	-	-	-
5	CLA	Z	612	X	-	-	-
5	CLA	Z	613	X	-	-	-
5	CLA	Z	614	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8140 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	X	220	1675	1088	273	309	5	0	0

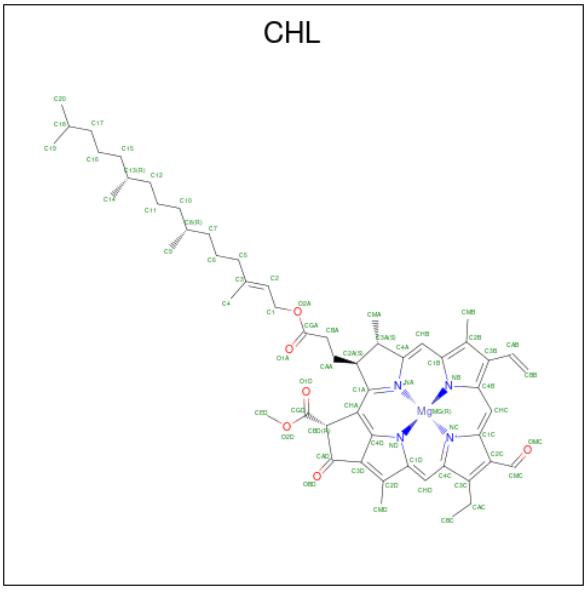
- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Y	220	1679	1086	273	315	5	0	0

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

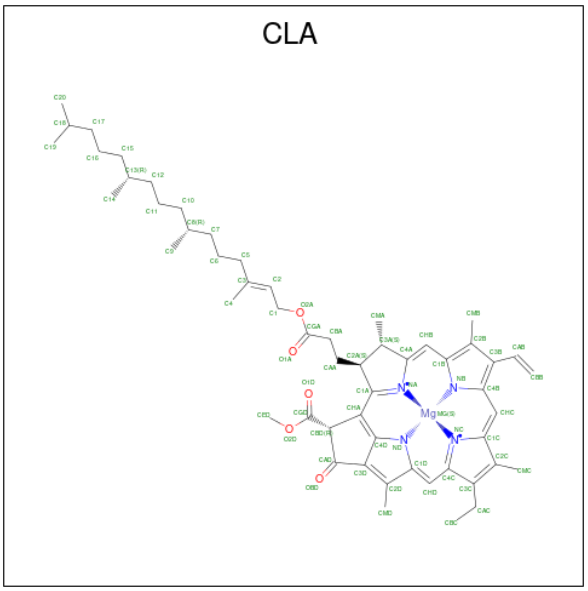
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
3	Z	232	1780	1154	291	329	1	5	0	0

- Molecule 4 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	Y	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
4	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	Y	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
4	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	Z	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
4	Z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	Z	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
4	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 5 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
5	X	1	Total 62	C 52	Mg 1	N 4	O 5	0
5	X	1	Total 49	C 39	Mg 1	N 4	O 5	0
5	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
5	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
5	X	1	Total 43	C 35	Mg 1	N 4	O 3	0
5	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
5	X	1	Total 42	C 34	Mg 1	N 4	O 3	0
5	Y	1	Total 58	C 48	Mg 1	N 4	O 5	0
5	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
5	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
5	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
5	Y	1	Total 43	C 35	Mg 1	N 4	O 3	0
5	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0

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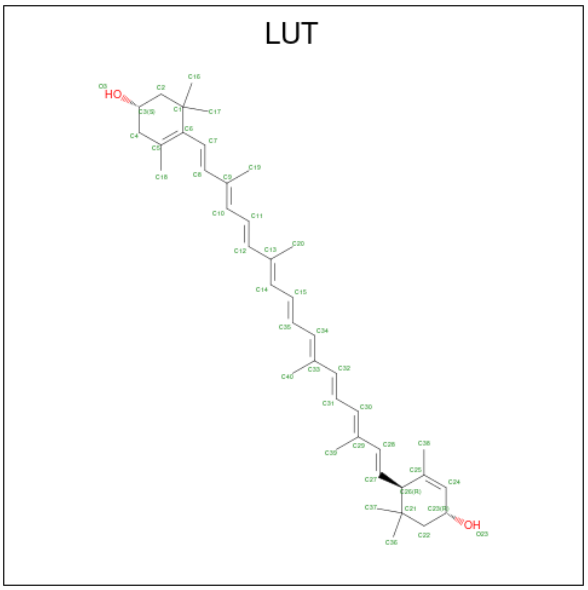
Mol	Chain	Residues	Atoms					AltConf
5	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	Y	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
5	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
5	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	Z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
5	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
5	Z	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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



Mol	Chain	Residues	Atoms			AltConf
6	X	1	Total	C	O	0
			42	40	2	

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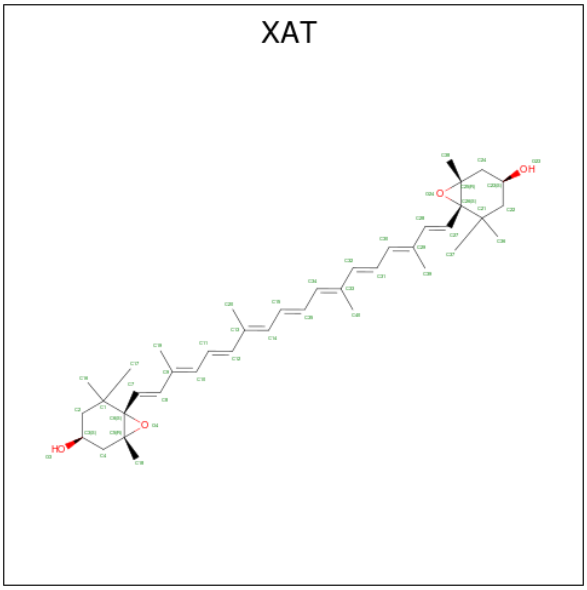
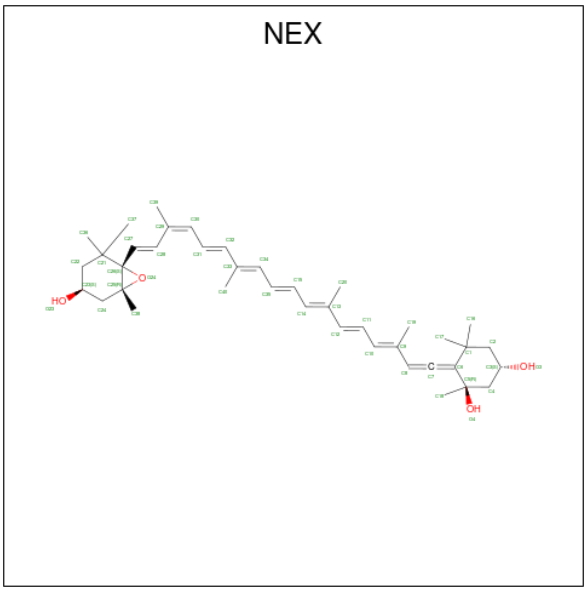
Mol	Chain	Residues	Atoms	AltConf
6	X	1	Total C O 42 40 2	0
6	Y	1	Total C O 42 40 2	0
6	Y	1	Total C O 42 40 2	0
6	Z	1	Total C O 42 40 2	0
6	Z	1	Total C O 42 40 2	0

- Molecule 7 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



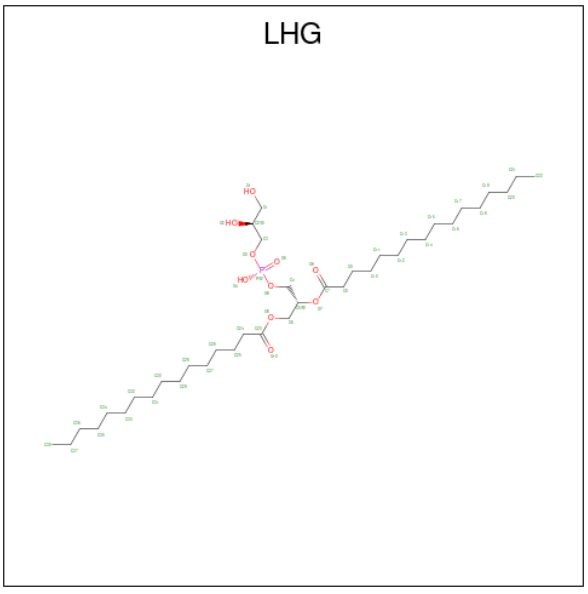
Mol	Chain	Residues	Atoms	AltConf
7	X	1	Total C O 44 40 4	0
7	Y	1	Total C O 44 40 4	0
7	Z	1	Total C O 44 40 4	0

- Molecule 8 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
8	X	1	Total	C	O	0
			44	40	4	
8	Y	1	Total	C	O	0
			43	40	3	
8	Z	1	Total	C	O	0
			44	40	4	

- Molecule 9 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).

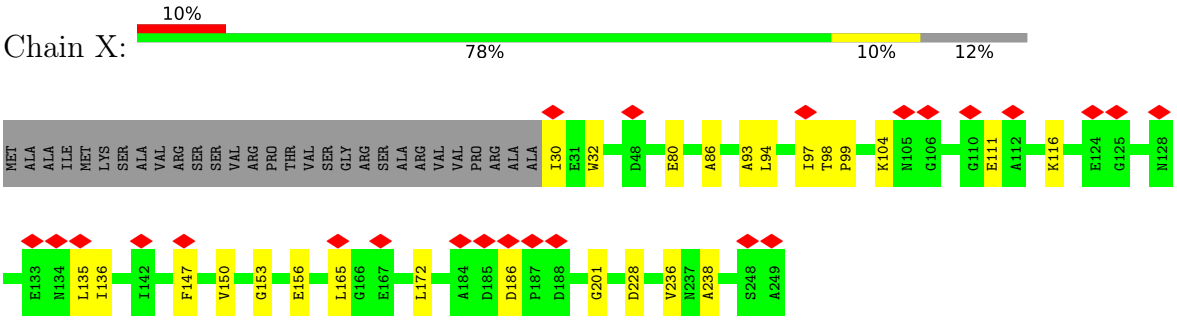


Mol	Chain	Residues	Atoms				AltConf
9	X	1	Total	C	O	P	0
			49	38	10	1	
9	Y	1	Total	C	O	P	0
			49	38	10	1	
9	Z	1	Total	C	O	P	0
			49	38	10	1	

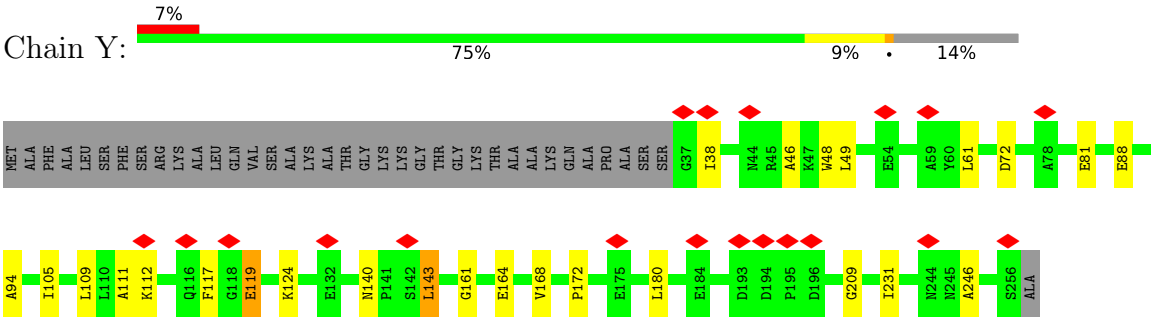
3 Residue-property plots (i)

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.

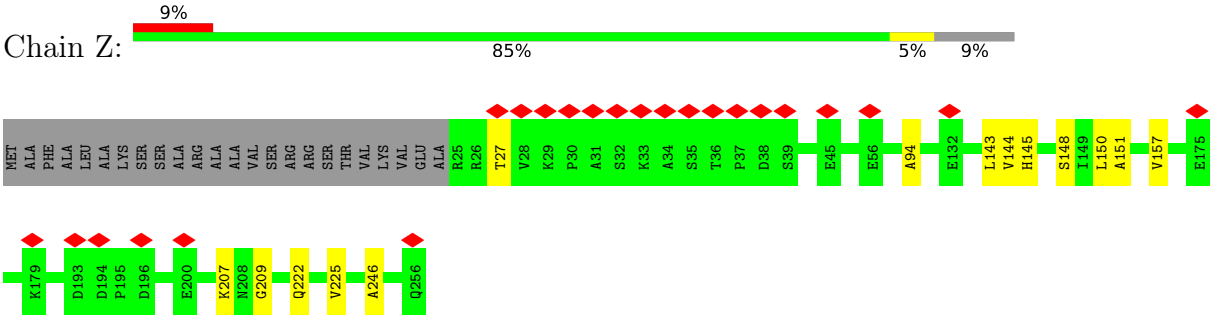
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic



• Molecule 2: Chlorophyll a-b binding protein, chloroplastic



• Molecule 3: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55601	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	1.5625	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.146	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	480.0, 480.0, 480.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CHL, XAT, LHG, CLA, NEX, LUT, TPO

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	X	0.23	0/1725	0.47	0/2348
2	Y	0.29	0/1727	0.48	0/2350
3	Z	0.13	0/1822	0.31	0/2474
All	All	0.22	0/5274	0.43	0/7172

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	X	1675	0	1617	26	0
2	Y	1679	0	1620	30	0
3	Z	1780	0	1723	11	0
4	X	310	0	311	13	0
4	Y	335	0	302	15	0
4	Z	338	0	309	14	0
5	X	436	0	415	6	0
5	Y	429	0	389	5	0
5	Z	496	0	520	2	0
6	X	84	0	112	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Y	84	0	112	3	0
6	Z	84	0	112	5	0
7	X	44	0	56	3	0
7	Y	44	0	56	3	0
7	Z	44	0	56	4	0
8	X	44	0	56	2	0
8	Y	43	0	55	2	0
8	Z	44	0	56	2	0
9	X	49	0	74	1	0
9	Y	49	0	74	1	0
9	Z	49	0	74	3	0
All	All	8140	0	8099	115	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 7.

All (115) 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)
2:Y:140:ASN:HD22	2:Y:143:LEU:HD13	1.20	1.03
2:Y:140:ASN:HD22	2:Y:143:LEU:CD1	1.72	1.01
1:X:135:LEU:CD2	1:X:136:ILE:HG12	1.91	1.00
1:X:135:LEU:HD23	1:X:136:ILE:HG12	1.54	0.86
1:X:135:LEU:HD22	1:X:136:ILE:HG12	1.59	0.82
2:Y:140:ASN:ND2	2:Y:143:LEU:HD13	1.97	0.78
1:X:111:GLU:OE2	1:X:116:LYS:HD2	1.88	0.73
4:Z:606:CHL:HBB2	4:Z:609:CHL:HBC1	1.72	0.72
2:Y:109:LEU:CD2	2:Y:231:ILE:HD12	2.21	0.70
4:Z:606:CHL:CBB	4:Z:609:CHL:HBC1	2.22	0.70
1:X:94:LEU:O	1:X:98:THR:HG23	1.96	0.66
1:X:98:THR:OG1	1:X:99:PRO:HD3	1.98	0.63
1:X:135:LEU:HD22	1:X:136:ILE:CG1	2.28	0.63
2:Y:109:LEU:HD21	2:Y:231:ILE:HD12	1.82	0.61
2:Y:105:ILE:HG23	2:Y:231:ILE:HD11	1.83	0.59
2:Y:109:LEU:HD23	2:Y:231:ILE:HD12	1.85	0.58
1:X:238:ALA:N	5:X:613:CLA:O1A	2.34	0.56
3:Z:222:GLN:NE2	6:Z:1620:LUT:O3	2.40	0.54
6:X:1620:LUT:H8	6:X:1620:LUT:H171	1.90	0.54
2:Y:172:PRO:HG2	4:Y:608:CHL:CBB	2.36	0.54
6:Y:1620:LUT:H8	6:Y:1620:LUT:H171	1.89	0.54
6:Z:1620:LUT:H181	6:Z:1620:LUT:C8	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:607:CHL:CBB	6:Z:1621:LUT:H193	2.38	0.53
2:Y:161:GLY:CA	4:Y:609:CHL:HAB	2.39	0.53
5:X:613:CLA:HMB1	6:X:1620:LUT:H7	1.91	0.53
1:X:153:GLY:CA	4:X:609:CHL:HAB	2.39	0.52
4:X:601:CHL:H41	9:X:2630:LHG:H161	1.91	0.52
5:Y:613:CLA:HMB1	6:Y:1620:LUT:H7	1.91	0.51
4:Z:606:CHL:HMB3	4:Z:606:CHL:HBB1	1.92	0.51
2:Y:46:ALA:HB1	4:Y:601:CHL:HBC1	1.92	0.51
1:X:153:GLY:HA2	4:X:609:CHL:HAB	1.92	0.50
1:X:86:ALA:HB1	1:X:201:GLY:HA3	1.94	0.50
1:X:135:LEU:CD2	1:X:136:ILE:CG1	2.78	0.50
2:Y:88:GLU:HA	2:Y:180:LEU:HD21	1.93	0.50
3:Z:94:ALA:HB1	3:Z:209:GLY:HA3	1.94	0.50
3:Z:246:ALA:N	5:Z:613:CLA:O1A	2.42	0.50
1:X:80:GLU:HA	1:X:172:LEU:HD21	1.93	0.50
2:Y:124:LYS:HA	4:Y:607:CHL:O1D	2.12	0.49
3:Z:222:GLN:HA	3:Z:225:VAL:HG22	1.94	0.49
2:Y:38:ILE:CD1	5:Y:611:CLA:HMA1	2.41	0.49
4:Z:607:CHL:HBB2	6:Z:1621:LUT:H193	1.93	0.49
4:Z:606:CHL:CBB	4:Z:609:CHL:CBC	2.91	0.49
1:X:98:THR:OG1	1:X:99:PRO:CD	2.60	0.48
2:Y:38:ILE:HD13	5:Y:611:CLA:CMA	2.43	0.48
4:Y:601:CHL:H41	9:Y:2630:LHG:H161	1.94	0.48
2:Y:94:ALA:HB1	2:Y:209:GLY:HA3	1.94	0.48
2:Y:140:ASN:ND2	2:Y:143:LEU:CD1	2.57	0.48
2:Y:161:GLY:HA2	4:Y:609:CHL:HAB	1.95	0.48
3:Z:207:LYS:NZ	9:Z:2630:LHG:O4	2.43	0.47
1:X:147:PHE:O	1:X:150:VAL:HG12	2.14	0.47
1:X:228:ASP:HB3	1:X:236:VAL:HG11	1.97	0.47
1:X:156:GLU:OE2	4:X:609:CHL:NC	2.48	0.47
4:X:609:CHL:HMB3	4:Y:601:CHL:HHB	1.97	0.47
4:Y:609:CHL:HBB1	4:Z:601:CHL:H51	1.97	0.46
8:Z:1623:NEX:H183	8:Z:1623:NEX:H192	1.97	0.46
4:Z:601:CHL:H61	4:Z:601:CHL:H102	1.71	0.46
1:X:30:ILE:HD13	5:X:611:CLA:CMA	2.46	0.45
2:Y:38:ILE:CD1	5:Y:611:CLA:CMA	2.94	0.45
1:X:111:GLU:HG2	1:X:116:LYS:HB2	1.98	0.45
4:X:608:CHL:H152	8:X:1623:NEX:H402	1.99	0.45
4:Y:601:CHL:H102	4:Y:601:CHL:H61	1.79	0.45
7:Y:1622:XAT:H31	7:Y:1622:XAT:H391	1.78	0.45
7:Z:1622:XAT:H35	7:Z:1622:XAT:H401	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:1623:NEX:H35	8:Y:1623:NEX:H401	1.80	0.45
2:Y:140:ASN:HB2	2:Y:143:LEU:HD13	1.98	0.44
2:Y:164:GLU:OE2	4:Y:609:CHL:NC	2.50	0.44
7:X:1622:XAT:H31	7:X:1622:XAT:H391	1.78	0.44
4:Z:601:CHL:H162	9:Z:2630:LHG:H212	2.00	0.44
1:X:116:LYS:HA	4:X:607:CHL:O1D	2.18	0.44
1:X:30:ILE:CD1	5:X:611:CLA:HMA1	2.47	0.44
8:X:1623:NEX:H35	8:X:1623:NEX:H401	1.80	0.44
2:Y:246:ALA:N	5:Y:613:CLA:O1A	2.42	0.44
4:Z:605:CHL:HBB1	4:Z:605:CHL:HHC	2.00	0.44
4:Z:609:CHL:H91	4:Z:609:CHL:H112	1.86	0.44
4:Y:606:CHL:HBB1	4:Y:606:CHL:HHC	1.98	0.44
4:Z:608:CHL:HHC	4:Z:608:CHL:HBB1	2.00	0.44
1:X:30:ILE:HG21	1:X:32:TRP:CZ2	2.53	0.43
7:X:1622:XAT:H15	7:X:1622:XAT:H201	1.68	0.43
3:Z:150:LEU:H	3:Z:150:LEU:HD23	1.84	0.43
4:X:601:CHL:H102	4:X:601:CHL:H61	1.79	0.43
2:Y:111:ALA:HB2	2:Y:117:PHE:HD2	1.84	0.43
7:Y:1622:XAT:H35	7:Y:1622:XAT:H401	1.86	0.43
1:X:30:ILE:CD1	5:X:611:CLA:CMA	2.96	0.43
3:Z:157:VAL:HG23	4:Z:609:CHL:HBB2	2.01	0.43
1:X:135:LEU:HD23	1:X:135:LEU:C	2.44	0.43
7:X:1622:XAT:H35	7:X:1622:XAT:H401	1.86	0.43
2:Y:112:LYS:HE3	2:Y:231:ILE:HG22	2.00	0.43
4:X:605:CHL:HHC	4:X:605:CHL:HBB1	2.01	0.43
4:Y:605:CHL:HBB1	4:Y:605:CHL:HHC	2.01	0.42
4:Y:606:CHL:CBB	4:Y:607:CHL:HHC	2.49	0.42
6:Y:1620:LUT:H8	6:Y:1620:LUT:C17	2.49	0.42
4:X:607:CHL:H142	4:X:607:CHL:H112	1.88	0.42
6:X:1620:LUT:H8	6:X:1620:LUT:C17	2.49	0.42
3:Z:148:SER:OG	3:Z:151:ALA:HB3	2.19	0.42
1:X:165:LEU:HG	4:X:608:CHL:HBB1	2.00	0.42
2:Y:119:GLU:HG3	2:Y:124:LYS:HB2	2.01	0.42
2:Y:48:TRP:HE3	4:Y:601:CHL:HAA1	1.84	0.42
5:X:603:CLA:H13	4:X:609:CHL:H93	2.02	0.42
8:Y:1623:NEX:H15	8:Y:1623:NEX:H201	1.75	0.42
7:Z:1622:XAT:H201	7:Z:1622:XAT:H15	1.71	0.42
4:Z:607:CHL:HAA2	7:Z:1622:XAT:H41	2.02	0.41
6:Z:1620:LUT:C8	6:Z:1620:LUT:C18	2.98	0.41
3:Z:143:LEU:O	3:Z:144:VAL:C	2.63	0.41
3:Z:144:VAL:HG23	3:Z:145:HIS:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:1622:XAT:H31	7:Z:1622:XAT:H391	1.82	0.41
1:X:93:ALA:O	1:X:97:ILE:HG13	2.21	0.40
2:Y:61:LEU:HD11	2:Y:72:ASP:HB2	2.03	0.40
2:Y:109:LEU:HD21	2:Y:231:ILE:CD1	2.50	0.40
3:Z:225:VAL:HG21	5:Z:613:CLA:HMD2	2.03	0.40
4:X:608:CHL:H143	4:X:608:CHL:H111	1.89	0.40
2:Y:109:LEU:CD2	2:Y:231:ILE:CD1	2.97	0.40
8:Z:1623:NEX:H15	8:Z:1623:NEX:H201	1.92	0.40
2:Y:49:LEU:O	4:Y:601:CHL:HBB1	2.22	0.40
7:Y:1622:XAT:H12	9:Z:2630:LHG:H192	2.02	0.40
2:Y:164:GLU:O	2:Y:168:VAL:HG23	2.22	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	X	218/249 (88%)	207 (95%)	11 (5%)	0	100	100
2	Y	218/257 (85%)	202 (93%)	16 (7%)	0	100	100
3	Z	229/256 (90%)	223 (97%)	6 (3%)	0	100	100
All	All	665/762 (87%)	632 (95%)	33 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	X	165/187 (88%)	163 (99%)	2 (1%)	63 74
2	Y	170/194 (88%)	167 (98%)	3 (2%)	51 69
3	Z	178/195 (91%)	178 (100%)	0	100 100
All	All	513/576 (89%)	508 (99%)	5 (1%)	65 76

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	104	LYS
1	X	186	ASP
2	Y	81	GLU
2	Y	119	GLU
2	Y	143	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	128	ASN
1	X	137	HIS
1	X	139	GLN
1	X	148	GLN
2	Y	140	ASN
2	Y	145	HIS
2	Y	147	GLN
3	Z	131	GLN
3	Z	169	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
3	TPO	Z	27	3	8,10,11	1.12	0	10,14,16	1.81	1 (10%)

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
3	TPO	Z	27	3	-	1/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	27	TPO	P-OG1-CB	-5.11	109.43	123.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Z	27	TPO	C-CA-CB-CG2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides 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	$\#\|Z\| > 2$
4	CHL	Z	606	-	40,54,74	4.17	19 (47%)	34,90,114	3.09	16 (47%)
5	CLA	X	602	1	69,73,73	1.19	7 (10%)	82,113,113	1.10	4 (4%)
5	CLA	X	604	-	53,57,73	1.33	7 (13%)	61,93,113	1.17	5 (8%)
4	CHL	Z	607	-	60,74,74	3.36	18 (30%)	58,114,114	2.48	18 (31%)
6	LUT	X	1621	-	42,43,43	0.80	1 (2%)	51,60,60	1.85	16 (31%)
5	CLA	Y	604	-	54,58,73	1.33	7 (12%)	64,95,113	1.17	6 (9%)
8	NEX	Y	1623	-	41,45,46	1.04	3 (7%)	50,67,70	2.35	18 (36%)
7	XAT	X	1622	-	41,47,47	0.93	2 (4%)	54,74,74	4.33	24 (44%)
5	CLA	X	612	1	47,51,73	1.40	7 (14%)	55,86,113	1.28	4 (7%)
5	CLA	Y	614	-	52,56,73	1.37	7 (13%)	61,92,113	1.21	5 (8%)
9	LHG	Y	2630	5	48,48,48	0.96	2 (4%)	51,54,54	0.98	2 (3%)
5	CLA	Z	614	-	58,62,73	1.29	6 (10%)	68,99,113	1.15	4 (5%)
4	CHL	X	605	1	40,54,74	4.21	19 (47%)	34,90,114	3.23	16 (47%)
5	CLA	Z	603	-	69,73,73	1.17	6 (8%)	82,113,113	1.22	4 (4%)
5	CLA	Y	602	2	62,66,73	1.25	7 (11%)	73,104,113	1.14	4 (5%)
4	CHL	Y	607	-	60,74,74	3.40	19 (31%)	58,114,114	2.22	19 (32%)
5	CLA	X	610	1	69,73,73	1.19	7 (10%)	82,113,113	1.11	6 (7%)
9	LHG	Z	2630	5	48,48,48	0.94	2 (4%)	51,54,54	0.86	2 (3%)
6	LUT	Y	1621	-	42,43,43	0.79	0	51,60,60	1.85	16 (31%)
7	XAT	Y	1622	-	41,47,47	0.94	2 (4%)	54,74,74	4.33	24 (44%)
7	XAT	Z	1622	-	41,47,47	0.92	2 (4%)	54,74,74	4.30	24 (44%)
5	CLA	Y	612	2	49,53,73	1.40	7 (14%)	58,89,113	1.29	4 (6%)
4	CHL	Y	609	2	60,74,74	3.36	20 (33%)	58,114,114	2.34	16 (27%)
8	NEX	X	1623	-	40,46,46	1.03	3 (7%)	50,70,70	2.33	17 (34%)
4	CHL	Z	608	-	44,58,74	3.99	19 (43%)	37,94,114	2.93	17 (45%)
5	CLA	Z	604	-	61,65,73	1.25	6 (9%)	72,103,113	1.17	4 (5%)
4	CHL	Y	606	-	40,54,74	4.14	18 (45%)	34,90,114	3.10	15 (44%)
5	CLA	Z	611	9	69,73,73	1.16	5 (7%)	82,113,113	1.12	4 (4%)
5	CLA	Y	610	2	69,73,73	1.20	7 (10%)	82,113,113	1.12	6 (7%)
9	LHG	X	2630	5	48,48,48	0.96	2 (4%)	51,54,54	0.98	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	CLA	Y	613	2	69,73,73	1.19	8 (11%)	82,113,113	1.14	6 (7%)
8	NEX	Z	1623	-	40,46,46	1.27	4 (10%)	50,70,70	2.24	17 (34%)
5	CLA	X	603	-	66,70,73	1.22	7 (10%)	78,109,113	1.18	5 (6%)
5	CLA	Z	602	3	64,68,73	1.23	6 (9%)	76,107,113	1.13	6 (7%)
4	CHL	Y	601	2	60,74,74	3.34	20 (33%)	58,114,114	2.55	15 (25%)
5	CLA	X	614	-	46,50,73	1.40	7 (15%)	53,85,113	1.24	4 (7%)
4	CHL	Y	605	2	36,50,74	4.37	18 (50%)	29,85,114	3.18	16 (55%)
4	CHL	X	607	-	60,74,74	3.41	19 (31%)	58,114,114	2.21	18 (31%)
6	LUT	Y	1620	-	42,43,43	0.80	1 (2%)	51,60,60	2.04	12 (23%)
5	CLA	Z	610	3	69,73,73	1.17	6 (8%)	82,113,113	1.15	7 (8%)
6	LUT	Z	1621	-	42,43,43	0.77	1 (2%)	51,60,60	1.89	16 (31%)
4	CHL	Z	601	3	60,74,74	3.33	19 (31%)	58,114,114	2.62	16 (27%)
5	CLA	X	611	9	49,53,73	1.40	7 (14%)	58,89,113	1.30	6 (10%)
6	LUT	Z	1620	-	42,43,43	0.74	1 (2%)	51,60,60	1.87	12 (23%)
5	CLA	Z	612	3	69,73,73	1.18	6 (8%)	82,113,113	1.11	3 (3%)
5	CLA	X	613	1	69,73,73	1.18	8 (11%)	82,113,113	1.15	6 (7%)
4	CHL	Z	609	3	60,74,74	3.42	20 (33%)	58,114,114	2.00	16 (27%)
4	CHL	X	601	1	60,74,74	3.34	20 (33%)	58,114,114	2.55	15 (25%)
4	CHL	X	609	1	60,74,74	3.36	20 (33%)	58,114,114	2.35	16 (27%)
4	CHL	X	608	-	60,74,74	3.34	19 (31%)	58,114,114	2.28	16 (27%)
5	CLA	Y	611	9	47,51,73	1.41	7 (14%)	55,86,113	1.27	4 (7%)
6	LUT	X	1620	-	42,43,43	0.80	1 (2%)	51,60,60	2.03	11 (21%)
4	CHL	Y	608	-	43,57,74	4.07	18 (41%)	37,93,114	2.89	16 (43%)
5	CLA	Z	613	3	69,73,73	1.17	8 (11%)	82,113,113	1.12	5 (6%)
5	CLA	Y	603	-	59,63,73	1.29	7 (11%)	70,101,113	1.23	5 (7%)
4	CHL	Z	605	3	38,52,74	4.26	18 (47%)	31,87,114	3.17	18 (58%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CHL	Z	606	-	3/3/16/26	4/15/113/137	-
5	CLA	X	602	1	1/1/15/20	9/39/115/115	-
5	CLA	X	604	-	1/1/11/20	6/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CHL	Z	607	-	3/3/20/26	17/39/137/137	-
6	LUT	X	1621	-	-	1/29/67/67	0/2/2/2
5	CLA	Y	604	-	1/1/12/20	4/21/97/115	-
8	NEX	Y	1623	-	-	3/27/80/83	0/3/3/3
7	XAT	X	1622	-	-	4/31/93/93	0/4/4/4
5	CLA	X	612	1	1/1/10/20	4/13/89/115	-
5	CLA	Y	614	-	1/1/11/20	8/19/95/115	-
9	LHG	Y	2630	5	-	11/53/53/53	-
5	CLA	Z	614	-	1/1/12/20	7/26/102/115	-
4	CHL	X	605	1	3/3/16/26	1/15/113/137	-
5	CLA	Z	603	-	1/1/15/20	20/39/115/115	-
5	CLA	Y	602	2	1/1/13/20	6/31/107/115	-
4	CHL	Y	607	-	3/3/20/26	21/39/137/137	-
5	CLA	X	610	1	1/1/15/20	9/39/115/115	-
9	LHG	Z	2630	5	-	17/53/53/53	-
6	LUT	Y	1621	-	-	1/29/67/67	0/2/2/2
7	XAT	Y	1622	-	-	4/31/93/93	0/4/4/4
7	XAT	Z	1622	-	-	4/31/93/93	0/4/4/4
5	CLA	Y	612	2	1/1/11/20	6/15/91/115	-
4	CHL	Y	609	2	3/3/20/26	16/39/137/137	-
8	NEX	X	1623	-	-	3/27/83/83	0/3/3/3
4	CHL	Z	608	-	3/3/16/26	5/20/118/137	-
5	CLA	Z	604	-	1/1/13/20	6/30/106/115	-
4	CHL	Y	606	-	3/3/16/26	2/15/113/137	-
5	CLA	Z	611	9	1/1/15/20	5/39/115/115	-
5	CLA	Y	610	2	1/1/15/20	9/39/115/115	-
9	LHG	X	2630	5	-	10/53/53/53	-
5	CLA	Y	613	2	1/1/15/20	14/39/115/115	-
8	NEX	Z	1623	-	-	3/27/83/83	0/3/3/3
5	CLA	X	603	-	1/1/14/20	11/36/112/115	-
5	CLA	Z	602	3	1/1/14/20	3/33/109/115	-
4	CHL	Y	601	2	3/3/20/26	18/39/137/137	-
5	CLA	X	614	-	1/1/10/20	5/12/88/115	-
4	CHL	Y	605	2	3/3/15/26	0/10/108/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CHL	X	607	-	3/3/20/26	21/39/137/137	-
6	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
5	CLA	Z	610	3	1/1/15/20	10/39/115/115	-
6	LUT	Z	1621	-	-	2/29/67/67	0/2/2/2
4	CHL	Z	601	3	3/3/20/26	16/39/137/137	-
5	CLA	X	611	9	1/1/11/20	8/15/91/115	-
6	LUT	Z	1620	-	-	0/29/67/67	0/2/2/2
5	CLA	Z	612	3	1/1/15/20	6/39/115/115	-
5	CLA	X	613	1	1/1/15/20	14/39/115/115	-
4	CHL	Z	609	3	3/3/20/26	23/39/137/137	-
4	CHL	X	601	1	3/3/20/26	18/39/137/137	-
4	CHL	X	609	1	3/3/20/26	16/39/137/137	-
4	CHL	X	608	-	3/3/20/26	20/39/137/137	-
5	CLA	Y	611	9	1/1/10/20	6/13/89/115	-
6	LUT	X	1620	-	-	2/29/67/67	0/2/2/2
4	CHL	Y	608	-	3/3/16/26	6/19/117/137	-
5	CLA	Z	613	3	1/1/15/20	16/39/115/115	-
5	CLA	Y	603	-	1/1/13/20	11/27/103/115	-
4	CHL	Z	605	3	3/3/15/26	1/13/111/137	-

All (513) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	608	CHL	C2C-C3C	11.44	1.47	1.36
4	Z	606	CHL	C2C-C3C	11.30	1.47	1.36
4	Y	606	CHL	C2C-C3C	11.14	1.47	1.36
4	X	605	CHL	C2C-C3C	11.04	1.47	1.36
4	Z	605	CHL	C2C-C3C	11.04	1.47	1.36
4	Z	608	CHL	C2C-C3C	10.96	1.47	1.36
4	Y	605	CHL	C2C-C3C	10.94	1.47	1.36
4	Z	609	CHL	C2C-C3C	10.76	1.46	1.36
4	X	608	CHL	C2C-C3C	10.37	1.46	1.36
4	X	609	CHL	C2C-C3C	10.36	1.46	1.36
4	Y	609	CHL	C2C-C3C	10.34	1.46	1.36
4	X	609	CHL	C1D-C2D	10.26	1.51	1.39
4	X	607	CHL	C2C-C3C	10.24	1.46	1.36
4	Y	609	CHL	C1D-C2D	10.24	1.51	1.39
4	Z	607	CHL	C2C-C3C	10.23	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	609	CHL	C1D-C2D	10.20	1.51	1.39
4	Y	601	CHL	C2C-C3C	10.18	1.46	1.36
4	Y	607	CHL	C2C-C3C	10.11	1.46	1.36
4	X	601	CHL	C2C-C3C	10.09	1.46	1.36
4	Z	601	CHL	C2C-C3C	10.07	1.46	1.36
4	Z	601	CHL	C1D-C2D	9.90	1.50	1.39
4	X	601	CHL	C1D-C2D	9.78	1.50	1.39
4	Y	601	CHL	C1D-C2D	9.78	1.50	1.39
4	Y	607	CHL	C1A-CHA	9.74	1.51	1.40
4	X	607	CHL	C1A-CHA	9.71	1.51	1.40
4	Y	608	CHL	C3B-C4B	9.65	1.50	1.41
4	Z	608	CHL	C3B-C4B	9.61	1.50	1.41
4	Z	605	CHL	C3B-C4B	9.61	1.50	1.41
4	Y	606	CHL	C3B-C4B	9.60	1.50	1.41
4	X	608	CHL	C1D-C2D	9.59	1.50	1.39
4	X	605	CHL	C3B-C4B	9.57	1.50	1.41
4	Y	605	CHL	C3B-C4B	9.54	1.50	1.41
4	Y	607	CHL	C1D-C2D	9.45	1.50	1.39
4	X	607	CHL	C1D-C2D	9.38	1.50	1.39
4	Z	607	CHL	C1D-C2D	9.26	1.50	1.39
4	Z	607	CHL	C1A-CHA	8.88	1.50	1.40
4	X	608	CHL	C1A-CHA	8.56	1.49	1.40
4	Z	606	CHL	C1B-C2B	8.52	1.49	1.39
4	Z	605	CHL	C1D-C2D	8.41	1.49	1.39
4	Z	606	CHL	C1D-C2D	8.40	1.49	1.39
4	Y	601	CHL	C1A-CHA	8.37	1.49	1.40
4	X	601	CHL	C1A-CHA	8.34	1.49	1.40
4	Z	608	CHL	C1D-C2D	8.30	1.49	1.39
4	Y	605	CHL	C1A-CHA	8.24	1.49	1.40
4	X	605	CHL	C1A-CHA	8.19	1.49	1.40
4	Z	601	CHL	C1A-CHA	8.17	1.49	1.40
4	X	609	CHL	C1A-CHA	8.16	1.49	1.40
4	X	605	CHL	C1D-C2D	8.15	1.48	1.39
4	Z	609	CHL	C1B-C2B	8.15	1.48	1.39
4	Y	609	CHL	C1A-CHA	8.13	1.49	1.40
4	Z	601	CHL	C1B-C2B	8.13	1.48	1.39
4	Z	605	CHL	C1B-C2B	8.12	1.48	1.39
4	Y	601	CHL	C1B-C2B	8.11	1.48	1.39
4	X	601	CHL	C1B-C2B	8.10	1.48	1.39
4	Y	605	CHL	C1D-C2D	8.10	1.48	1.39
4	Y	605	CHL	C1B-C2B	8.07	1.48	1.39
4	Y	608	CHL	C1D-C2D	8.05	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	605	CHL	C1B-C2B	8.05	1.48	1.39
4	Y	606	CHL	C1D-C2D	8.00	1.48	1.39
4	Z	609	CHL	C1A-CHA	8.00	1.49	1.40
4	Z	608	CHL	C1A-CHA	7.99	1.49	1.40
4	X	608	CHL	C1B-C2B	7.92	1.48	1.39
4	Z	607	CHL	C1B-C2B	7.85	1.48	1.39
4	Z	606	CHL	C3B-C4B	7.82	1.49	1.41
4	X	609	CHL	C1B-C2B	7.76	1.48	1.39
4	Y	609	CHL	C1B-C2B	7.75	1.48	1.39
4	Z	605	CHL	C1A-CHA	7.67	1.48	1.40
4	Y	608	CHL	C1A-CHA	7.64	1.48	1.40
4	Z	608	CHL	C1B-C2B	7.60	1.48	1.39
4	Y	607	CHL	C1B-C2B	7.60	1.48	1.39
4	X	607	CHL	C1B-C2B	7.58	1.48	1.39
4	X	607	CHL	C3B-C4B	7.57	1.48	1.41
4	Y	608	CHL	C1B-C2B	7.53	1.48	1.39
4	Y	606	CHL	C1B-C2B	7.47	1.48	1.39
4	Z	607	CHL	C3B-C4B	7.47	1.48	1.41
4	Z	606	CHL	C1A-CHA	7.46	1.48	1.40
4	Y	607	CHL	C3B-C4B	7.43	1.48	1.41
4	Y	601	CHL	C3B-C4B	7.37	1.48	1.41
4	X	601	CHL	C3B-C4B	7.37	1.48	1.41
4	X	608	CHL	C3B-C4B	7.34	1.48	1.41
4	Z	601	CHL	C3B-C4B	7.27	1.48	1.41
4	Y	606	CHL	C1A-CHA	7.24	1.48	1.40
4	Z	609	CHL	C3B-C4B	6.82	1.48	1.41
4	Y	609	CHL	C3B-C4B	6.66	1.47	1.41
4	X	609	CHL	C3B-C4B	6.61	1.47	1.41
4	Z	606	CHL	C3B-C2B	5.83	1.48	1.40
4	Z	609	CHL	C3D-C4D	-5.72	1.32	1.41
4	Z	605	CHL	C3B-C2B	5.70	1.48	1.40
4	X	605	CHL	C3B-C2B	5.61	1.48	1.40
4	Y	609	CHL	C3D-C4D	-5.57	1.33	1.41
4	X	609	CHL	C3D-C4D	-5.56	1.33	1.41
4	Y	605	CHL	C3B-C2B	5.53	1.47	1.40
4	Z	606	CHL	C3D-C2D	5.51	1.49	1.39
4	X	608	CHL	C3D-C4D	-5.51	1.33	1.41
4	Y	605	CHL	C2A-C3A	-5.51	1.50	1.54
4	Z	601	CHL	C3D-C4D	-5.51	1.33	1.41
4	Y	601	CHL	C3D-C4D	-5.48	1.33	1.41
4	X	601	CHL	C3D-C4D	-5.47	1.33	1.41
4	Y	608	CHL	C3D-C2D	5.44	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	607	CHL	C3A-C2A	-5.43	1.50	1.54
4	Z	608	CHL	C3D-C2D	5.43	1.48	1.39
4	Y	605	CHL	C3D-C2D	5.41	1.48	1.39
4	X	605	CHL	C3D-C2D	5.41	1.48	1.39
4	X	607	CHL	CHB-C4A	-5.37	1.32	1.38
4	Z	605	CHL	C3D-C2D	5.37	1.48	1.39
4	Y	607	CHL	C3D-C4D	-5.36	1.33	1.41
4	Y	607	CHL	CHB-C4A	-5.34	1.32	1.38
4	Y	606	CHL	CHC-C4B	5.34	1.48	1.39
4	Z	607	CHL	C3D-C4D	-5.32	1.33	1.41
4	X	607	CHL	C3D-C4D	-5.31	1.33	1.41
4	Y	606	CHL	C3D-C2D	5.26	1.48	1.39
4	Z	608	CHL	C3B-C2B	5.24	1.47	1.40
4	Y	608	CHL	C3A-C2A	-5.20	1.50	1.54
4	Y	606	CHL	O2D-CGD	5.19	1.46	1.33
4	Y	608	CHL	C3B-C2B	5.17	1.47	1.40
4	Z	606	CHL	C3A-C2A	-5.15	1.50	1.54
4	Z	606	CHL	O2D-CGD	5.14	1.45	1.33
4	Y	608	CHL	CHC-C4B	5.14	1.47	1.39
4	Y	608	CHL	OBD-CAD	5.12	1.29	1.22
4	Z	605	CHL	O2D-CGD	5.12	1.45	1.33
4	Y	608	CHL	O2D-CGD	5.10	1.45	1.33
4	X	605	CHL	C3A-C2A	-5.10	1.50	1.54
4	Z	608	CHL	O2D-CGD	5.10	1.45	1.33
4	Z	608	CHL	C3A-C2A	-5.08	1.50	1.54
4	X	605	CHL	O2D-CGD	5.08	1.45	1.33
4	X	605	CHL	OBD-CAD	5.07	1.28	1.22
4	Z	607	CHL	O2D-CGD	5.05	1.45	1.33
4	Y	605	CHL	OBD-CAD	5.04	1.28	1.22
4	Z	609	CHL	C3B-C2B	5.04	1.47	1.40
4	Z	608	CHL	OBD-CAD	5.04	1.28	1.22
4	Y	605	CHL	O2D-CGD	5.03	1.45	1.33
4	Y	609	CHL	O2D-CGD	5.03	1.45	1.33
4	Y	606	CHL	C3B-C2B	5.02	1.47	1.40
4	Z	601	CHL	O2D-CGD	5.01	1.45	1.33
4	Z	609	CHL	O2D-CGD	5.01	1.45	1.33
4	X	609	CHL	O2D-CGD	5.01	1.45	1.33
4	X	601	CHL	O2D-CGD	5.01	1.45	1.33
4	Y	601	CHL	O2D-CGD	5.00	1.45	1.33
4	X	607	CHL	O2D-CGD	4.97	1.45	1.33
4	Z	605	CHL	CHC-C4B	4.97	1.47	1.39
4	Y	607	CHL	O2D-CGD	4.96	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	605	CHL	OBD-CAD	4.94	1.28	1.22
4	X	608	CHL	O2D-CGD	4.93	1.45	1.33
4	Y	606	CHL	CHB-C4A	-4.90	1.32	1.38
4	Y	605	CHL	CHC-C4B	4.89	1.47	1.39
4	Z	606	CHL	OBD-CAD	4.89	1.28	1.22
4	Y	607	CHL	OBD-CAD	4.89	1.28	1.22
4	X	605	CHL	CHC-C4B	4.88	1.47	1.39
4	X	609	CHL	C3B-C2B	4.88	1.47	1.40
4	Y	606	CHL	C3A-C2A	-4.87	1.50	1.54
4	Y	609	CHL	OBD-CAD	4.87	1.28	1.22
4	X	609	CHL	OBD-CAD	4.86	1.28	1.22
4	Y	601	CHL	OBD-CAD	4.85	1.28	1.22
4	Y	608	CHL	CHB-C4A	-4.84	1.32	1.38
4	X	601	CHL	OBD-CAD	4.84	1.28	1.22
4	Z	607	CHL	OBD-CAD	4.83	1.28	1.22
4	X	607	CHL	OBD-CAD	4.82	1.28	1.22
4	Z	609	CHL	CHD-C1D	4.82	1.47	1.39
4	Z	609	CHL	CHB-C1B	4.81	1.47	1.39
4	Z	608	CHL	CHC-C4B	4.80	1.47	1.39
4	Y	609	CHL	C3B-C2B	4.80	1.46	1.40
4	X	607	CHL	C3A-C2A	-4.77	1.50	1.54
4	Z	605	CHL	C3A-C2A	-4.77	1.50	1.54
4	Z	607	CHL	CHB-C4A	-4.75	1.32	1.38
4	X	607	CHL	C3B-C2B	4.74	1.46	1.40
4	Y	607	CHL	C3A-C2A	-4.74	1.50	1.54
4	Z	609	CHL	CHD-C4C	4.74	1.48	1.39
4	Y	607	CHL	C3B-C2B	4.74	1.46	1.40
4	Y	606	CHL	OBD-CAD	4.71	1.28	1.22
4	Z	606	CHL	CHD-C1D	4.71	1.47	1.39
4	X	608	CHL	CHC-C4B	4.70	1.47	1.39
4	Z	609	CHL	OBD-CAD	4.69	1.28	1.22
4	Z	608	CHL	CHB-C4A	-4.69	1.33	1.38
4	X	601	CHL	C3A-C2A	-4.68	1.50	1.54
4	Z	607	CHL	CHC-C4B	4.67	1.47	1.39
4	Z	601	CHL	OBD-CAD	4.65	1.28	1.22
4	Y	601	CHL	C3A-C2A	-4.65	1.50	1.54
4	Y	601	CHL	CHB-C4A	-4.64	1.33	1.38
4	X	608	CHL	C3A-C2A	-4.62	1.50	1.54
4	X	601	CHL	CHB-C4A	-4.60	1.33	1.38
4	X	609	CHL	CHB-C1B	4.60	1.47	1.39
4	X	608	CHL	CHB-C4A	-4.59	1.33	1.38
4	Z	601	CHL	CHB-C4A	-4.58	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	609	CHL	C3A-C2A	-4.57	1.50	1.54
4	Y	606	CHL	O2A-CGA	4.57	1.45	1.30
4	X	605	CHL	O2A-CGA	4.57	1.45	1.30
4	Z	606	CHL	CHC-C4B	4.56	1.47	1.39
4	Z	605	CHL	CHD-C1D	4.56	1.47	1.39
4	Y	609	CHL	CHB-C1B	4.55	1.47	1.39
4	Z	608	CHL	CHD-C4C	4.55	1.48	1.39
4	Z	608	CHL	CHD-C1D	4.55	1.47	1.39
4	Z	607	CHL	CHC-C1C	4.55	1.48	1.39
4	Z	606	CHL	O2A-CGA	4.55	1.45	1.30
4	Z	601	CHL	C3B-C2B	4.55	1.46	1.40
4	Y	601	CHL	CHC-C4B	4.54	1.47	1.39
4	Y	607	CHL	CHC-C4B	4.53	1.47	1.39
4	X	609	CHL	C3A-C2A	-4.53	1.50	1.54
4	Z	605	CHL	CHB-C1B	4.53	1.47	1.39
4	Y	609	CHL	CHB-C4A	-4.53	1.33	1.38
4	Y	605	CHL	CHB-C1B	4.52	1.46	1.39
4	Y	609	CHL	CHD-C1D	4.52	1.46	1.39
4	Z	606	CHL	CHD-C4C	4.51	1.48	1.39
4	Y	608	CHL	CHD-C4C	4.51	1.48	1.39
4	X	609	CHL	CHB-C4A	-4.51	1.33	1.38
4	X	609	CHL	CHD-C1D	4.50	1.46	1.39
4	Z	606	CHL	CHB-C1B	4.49	1.46	1.39
4	X	607	CHL	CHC-C4B	4.49	1.46	1.39
4	X	609	CHL	CHD-C4C	4.49	1.48	1.39
4	Y	609	CHL	CHD-C4C	4.48	1.48	1.39
4	X	605	CHL	CHB-C1B	4.48	1.46	1.39
4	X	601	CHL	CHC-C4B	4.48	1.46	1.39
4	X	608	CHL	OBD-CAD	4.47	1.28	1.22
4	X	608	CHL	CHC-C1C	4.45	1.47	1.39
4	Y	606	CHL	CHD-C4C	4.45	1.47	1.39
4	Z	605	CHL	CHD-C4C	4.45	1.47	1.39
4	Z	601	CHL	CHD-C4C	4.45	1.47	1.39
4	Z	609	CHL	CHC-C4B	4.44	1.46	1.39
4	Z	609	CHL	CHB-C4A	-4.43	1.33	1.38
4	Z	607	CHL	C3B-C2B	4.42	1.46	1.40
4	Z	606	CHL	CHB-C4A	-4.42	1.33	1.38
4	X	608	CHL	C3B-C2B	4.40	1.46	1.40
4	Y	608	CHL	CHC-C1C	4.40	1.47	1.39
4	Y	605	CHL	CHD-C1D	4.40	1.46	1.39
4	Y	609	CHL	CHC-C4B	4.38	1.46	1.39
4	X	605	CHL	CHB-C4A	-4.38	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	609	CHL	CHC-C1C	4.38	1.47	1.39
4	Z	601	CHL	C3A-C2A	-4.38	1.50	1.54
4	X	608	CHL	CHB-C1B	4.38	1.46	1.39
4	Y	608	CHL	O2A-CGA	4.37	1.46	1.33
4	Z	605	CHL	CHB-C4A	-4.37	1.33	1.38
4	Y	601	CHL	C3B-C2B	4.37	1.46	1.40
4	X	605	CHL	CHD-C1D	4.37	1.46	1.39
4	Z	608	CHL	O2A-CGA	4.37	1.46	1.33
4	X	609	CHL	CHC-C4B	4.36	1.46	1.39
4	Y	605	CHL	CHB-C4A	-4.35	1.33	1.38
4	Y	607	CHL	CHD-C1D	4.35	1.46	1.39
4	X	601	CHL	C3B-C2B	4.34	1.46	1.40
4	Z	601	CHL	CHD-C1D	4.34	1.46	1.39
9	Z	2630	LHG	O8-C23	4.34	1.46	1.33
4	Y	601	CHL	CHD-C4C	4.33	1.47	1.39
4	Y	606	CHL	CHC-C1C	4.33	1.47	1.39
9	X	2630	LHG	O8-C23	4.32	1.45	1.33
4	Y	605	CHL	CHD-C4C	4.32	1.47	1.39
4	X	601	CHL	CHD-C4C	4.31	1.47	1.39
4	X	605	CHL	CHD-C4C	4.31	1.47	1.39
9	Y	2630	LHG	O8-C23	4.31	1.45	1.33
4	X	607	CHL	CHD-C1D	4.30	1.46	1.39
4	Y	608	CHL	CHD-C1D	4.30	1.46	1.39
4	X	607	CHL	CHD-C4C	4.29	1.47	1.39
9	Y	2630	LHG	O7-C7	4.28	1.46	1.34
9	X	2630	LHG	O7-C7	4.28	1.46	1.34
4	X	608	CHL	CHD-C4C	4.27	1.47	1.39
8	Z	1623	NEX	C7-C8	-4.27	1.25	1.31
4	Y	607	CHL	CHC-C1C	4.26	1.47	1.39
4	X	601	CHL	CHD-C1D	4.26	1.46	1.39
4	Z	609	CHL	C3A-C2A	-4.26	1.51	1.54
4	Z	601	CHL	CHC-C4B	4.26	1.46	1.39
4	Z	608	CHL	CHB-C1B	4.26	1.46	1.39
4	Y	607	CHL	CHD-C4C	4.25	1.47	1.39
4	X	601	CHL	CHC-C1C	4.23	1.47	1.39
4	X	609	CHL	O2A-CGA	4.23	1.45	1.33
4	Y	609	CHL	O2A-CGA	4.23	1.45	1.33
4	Z	601	CHL	O2A-CGA	4.22	1.45	1.33
4	Y	606	CHL	CHD-C1D	4.21	1.46	1.39
4	X	607	CHL	O2A-CGA	4.21	1.45	1.33
4	X	607	CHL	CHC-C1C	4.21	1.47	1.39
4	X	605	CHL	CHC-C1C	4.20	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	608	CHL	CHB-C1B	4.20	1.46	1.39
4	Y	601	CHL	CHD-C1D	4.19	1.46	1.39
4	Y	607	CHL	O2A-CGA	4.19	1.45	1.33
4	Y	601	CHL	CHC-C1C	4.19	1.47	1.39
4	Z	607	CHL	CHD-C4C	4.18	1.47	1.39
4	X	609	CHL	CHC-C1C	4.17	1.47	1.39
4	Y	601	CHL	CHB-C1B	4.17	1.46	1.39
4	X	601	CHL	CHB-C1B	4.17	1.46	1.39
4	X	608	CHL	O2A-CGA	4.16	1.45	1.33
4	Y	605	CHL	CHC-C1C	4.14	1.47	1.39
4	X	601	CHL	O2A-CGA	4.12	1.45	1.33
4	Z	609	CHL	O2A-CGA	4.12	1.45	1.33
4	Z	607	CHL	O2A-CGA	4.12	1.45	1.33
4	Y	609	CHL	CHC-C1C	4.11	1.47	1.39
4	Z	605	CHL	CHC-C1C	4.10	1.47	1.39
4	Z	608	CHL	CHC-C1C	4.10	1.47	1.39
4	Y	601	CHL	O2A-CGA	4.09	1.45	1.33
4	Y	606	CHL	CHB-C1B	4.09	1.46	1.39
4	Z	601	CHL	CHB-C1B	4.08	1.46	1.39
4	X	608	CHL	CHD-C1D	4.07	1.46	1.39
9	Z	2630	LHG	O7-C7	4.03	1.45	1.34
4	Z	607	CHL	CHD-C1D	4.01	1.46	1.39
4	Z	606	CHL	CHC-C1C	4.01	1.47	1.39
4	Z	607	CHL	CHB-C1B	3.98	1.46	1.39
4	Z	601	CHL	CHC-C1C	3.98	1.47	1.39
4	Z	609	CHL	C3D-C2D	3.88	1.46	1.39
4	X	607	CHL	CHB-C1B	3.84	1.45	1.39
4	Y	607	CHL	CHB-C1B	3.83	1.45	1.39
8	Z	1623	NEX	C7-C6	-3.80	1.26	1.30
4	Z	607	CHL	C3D-C2D	3.75	1.46	1.39
4	X	609	CHL	C3D-C2D	3.74	1.46	1.39
4	Z	601	CHL	C3D-C2D	3.73	1.46	1.39
5	Z	604	CLA	C1D-ND	3.73	1.42	1.37
5	Z	614	CLA	C1D-ND	3.72	1.42	1.37
4	Y	607	CHL	C3D-C2D	3.69	1.45	1.39
4	Y	609	CHL	C3D-C2D	3.68	1.45	1.39
4	X	607	CHL	C3D-C2D	3.67	1.45	1.39
5	Y	614	CLA	C1D-ND	3.66	1.42	1.37
5	Y	613	CLA	C1D-ND	3.66	1.42	1.37
5	Z	612	CLA	C1D-ND	3.65	1.42	1.37
5	X	610	CLA	C4B-NB	3.61	1.42	1.37
5	X	611	CLA	C1D-ND	3.60	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	X	610	CLA	C1D-ND	3.59	1.42	1.37
5	Z	610	CLA	C1D-ND	3.59	1.42	1.37
4	X	601	CHL	C3D-C2D	3.59	1.45	1.39
5	X	612	CLA	C1D-ND	3.59	1.42	1.37
5	Y	611	CLA	C1D-ND	3.58	1.42	1.37
5	Y	612	CLA	C1D-ND	3.58	1.42	1.37
4	Y	601	CHL	C3D-C2D	3.58	1.45	1.39
5	X	602	CLA	C4B-NB	3.58	1.42	1.37
5	Y	610	CLA	C1D-ND	3.57	1.42	1.37
5	X	603	CLA	C1D-ND	3.56	1.42	1.37
5	Y	610	CLA	C4B-NB	3.56	1.42	1.37
5	Y	604	CLA	C1D-ND	3.54	1.42	1.37
5	Y	603	CLA	C1D-ND	3.54	1.42	1.37
5	Z	603	CLA	C1D-ND	3.51	1.42	1.37
5	X	604	CLA	C1D-ND	3.50	1.42	1.37
5	X	614	CLA	C1D-ND	3.50	1.42	1.37
4	X	608	CHL	C3D-C2D	3.50	1.45	1.39
5	X	613	CLA	C1D-ND	3.48	1.42	1.37
5	Z	602	CLA	C4B-NB	3.48	1.42	1.37
5	X	613	CLA	C4B-NB	3.47	1.42	1.37
5	Y	602	CLA	C4B-NB	3.47	1.42	1.37
5	Y	604	CLA	C4B-NB	3.47	1.42	1.37
5	Y	613	CLA	C4B-NB	3.45	1.42	1.37
5	Z	613	CLA	C1D-ND	3.44	1.42	1.37
5	X	604	CLA	C4B-NB	3.42	1.42	1.37
5	Z	611	CLA	C1D-ND	3.40	1.42	1.37
5	Z	613	CLA	C4B-NB	3.39	1.42	1.37
5	Y	611	CLA	C4B-NB	3.37	1.42	1.37
5	Y	614	CLA	C4B-NB	3.36	1.42	1.37
5	Y	602	CLA	C1D-ND	3.34	1.42	1.37
5	X	612	CLA	C4B-NB	3.34	1.42	1.37
5	Y	603	CLA	C4B-NB	3.33	1.42	1.37
5	X	614	CLA	C4B-NB	3.32	1.42	1.37
5	Z	610	CLA	C4B-NB	3.31	1.42	1.37
5	X	611	CLA	C4B-NB	3.31	1.42	1.37
5	X	603	CLA	C4B-NB	3.30	1.42	1.37
5	Y	612	CLA	C4B-NB	3.30	1.42	1.37
5	Z	602	CLA	C1D-ND	3.26	1.42	1.37
5	X	602	CLA	C1D-ND	3.25	1.42	1.37
5	Z	604	CLA	C4B-NB	3.23	1.42	1.37
5	Z	611	CLA	C4B-NB	3.21	1.42	1.37
5	Z	614	CLA	C4B-NB	3.18	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Z	612	CLA	C4B-NB	3.17	1.42	1.37
8	Y	1623	NEX	C7-C6	-3.17	1.27	1.30
4	Y	608	CHL	CHA-CBD	-3.11	1.48	1.51
4	Z	606	CHL	CHA-CBD	-3.08	1.48	1.51
4	Y	606	CHL	CHA-CBD	-3.03	1.48	1.51
5	Z	603	CLA	C1B-C2B	2.98	1.50	1.43
5	X	613	CLA	C1B-C2B	2.93	1.50	1.43
8	X	1623	NEX	C7-C6	-2.91	1.27	1.30
5	Z	612	CLA	C1B-C2B	2.91	1.50	1.43
5	Z	603	CLA	C4B-NB	2.89	1.41	1.37
5	Y	613	CLA	C1B-C2B	2.89	1.49	1.43
4	Z	605	CHL	CHA-CBD	-2.88	1.48	1.51
5	Z	611	CLA	C1B-C2B	2.85	1.49	1.43
8	Z	1623	NEX	C1-C6	-2.84	1.49	1.54
5	Z	613	CLA	C1B-C2B	2.81	1.49	1.43
5	Y	604	CLA	C1B-C2B	2.80	1.49	1.43
4	Z	608	CHL	CHA-CBD	-2.79	1.48	1.51
5	X	604	CLA	C1B-C2B	2.79	1.49	1.43
5	Z	604	CLA	C1B-C2B	2.75	1.49	1.43
5	X	611	CLA	C1B-C2B	2.74	1.49	1.43
5	X	603	CLA	C1B-C2B	2.73	1.49	1.43
5	Y	614	CLA	C1B-C2B	2.73	1.49	1.43
8	Y	1623	NEX	C7-C8	-2.73	1.27	1.31
5	Y	603	CLA	C1B-C2B	2.73	1.49	1.43
8	X	1623	NEX	C7-C8	-2.71	1.27	1.31
5	X	614	CLA	C1B-C2B	2.69	1.49	1.43
5	Z	610	CLA	C1B-C2B	2.68	1.49	1.43
5	Y	611	CLA	C1B-C2B	2.67	1.49	1.43
5	Z	614	CLA	C1B-C2B	2.65	1.49	1.43
5	Y	602	CLA	C1B-C2B	2.64	1.49	1.43
5	X	612	CLA	C1B-C2B	2.64	1.49	1.43
5	Y	612	CLA	C1B-C2B	2.64	1.49	1.43
5	Y	610	CLA	C1B-C2B	2.63	1.49	1.43
5	Z	602	CLA	C1B-C2B	2.62	1.49	1.43
5	Z	610	CLA	C3B-C4B	2.60	1.50	1.42
4	X	607	CHL	CBD-CGD	-2.59	1.49	1.52
5	X	602	CLA	C1B-C2B	2.58	1.49	1.43
5	X	610	CLA	C1B-C2B	2.57	1.49	1.43
5	Z	602	CLA	C3B-C4B	2.51	1.50	1.42
4	Y	607	CHL	CBD-CGD	-2.50	1.49	1.52
5	Y	610	CLA	C3B-C4B	2.48	1.49	1.42
5	Y	602	CLA	C3B-C4B	2.47	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	X	602	CLA	C3B-C4B	2.46	1.49	1.42
5	X	610	CLA	C3B-C4B	2.46	1.49	1.42
5	Y	602	CLA	CHC-C1C	2.44	1.43	1.38
5	Z	602	CLA	CHC-C1C	2.44	1.43	1.38
7	Y	1622	XAT	O24-C25	-2.43	1.43	1.46
7	X	1622	XAT	O24-C25	-2.42	1.43	1.46
5	X	602	CLA	CHC-C1C	2.39	1.43	1.38
5	Y	610	CLA	CHC-C1C	2.39	1.43	1.38
5	X	610	CLA	CHC-C1C	2.37	1.43	1.38
5	Z	614	CLA	C3B-C4B	2.36	1.49	1.42
5	Z	604	CLA	C3B-C4B	2.36	1.49	1.42
7	Z	1622	XAT	O24-C25	-2.34	1.43	1.46
5	Y	612	CLA	C3B-C4B	2.34	1.49	1.42
5	Y	611	CLA	C3B-C4B	2.33	1.49	1.42
5	X	612	CLA	C3B-C4B	2.33	1.49	1.42
5	X	611	CLA	C3B-C4B	2.31	1.49	1.42
5	Y	614	CLA	C3B-C4B	2.31	1.49	1.42
5	X	614	CLA	C3B-C4B	2.30	1.49	1.42
5	Y	604	CLA	C3B-C4B	2.30	1.49	1.42
5	X	613	CLA	C3B-C4B	2.30	1.49	1.42
5	X	603	CLA	CMB-C2B	-2.30	1.46	1.50
5	Z	611	CLA	C3B-C4B	2.30	1.49	1.42
5	Z	603	CLA	CMD-C2D	-2.29	1.46	1.50
7	Y	1622	XAT	O4-C5	-2.29	1.43	1.46
5	Y	603	CLA	C3B-C4B	2.28	1.49	1.42
5	Y	612	CLA	CHC-C1C	2.27	1.43	1.38
5	Z	612	CLA	C3B-C4B	2.27	1.49	1.42
5	X	603	CLA	C3B-C4B	2.27	1.49	1.42
7	Z	1622	XAT	O4-C5	-2.26	1.43	1.46
4	Z	609	CHL	CBD-CGD	-2.26	1.49	1.52
5	Y	613	CLA	C3B-C4B	2.26	1.49	1.42
5	X	604	CLA	C3B-C4B	2.26	1.49	1.42
5	Z	613	CLA	C3B-C4B	2.24	1.49	1.42
5	Z	610	CLA	CMD-C2D	-2.24	1.46	1.50
5	Z	602	CLA	CMD-C2D	-2.23	1.46	1.50
5	Y	614	CLA	CHC-C1C	2.23	1.43	1.38
5	Y	603	CLA	CMB-C2B	-2.23	1.46	1.50
7	X	1622	XAT	O4-C5	-2.22	1.43	1.46
4	Y	605	CHL	CHA-CBD	-2.22	1.49	1.51
4	Z	601	CHL	CMC-C2C	2.22	1.49	1.44
5	X	612	CLA	CHC-C1C	2.20	1.42	1.38
5	X	603	CLA	CMD-C2D	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	614	CLA	CMD-C2D	-2.20	1.46	1.50
5	Z	610	CLA	CHC-C1C	2.18	1.42	1.38
4	X	609	CHL	CMC-C2C	2.18	1.49	1.44
6	X	1621	LUT	C22-C21	-2.18	1.52	1.54
5	Y	603	CLA	CMD-C2D	-2.18	1.46	1.50
4	X	605	CHL	CHA-CBD	-2.18	1.49	1.51
6	Z	1620	LUT	C22-C21	-2.17	1.52	1.54
5	Z	614	CLA	CMD-C2D	-2.17	1.46	1.50
5	X	610	CLA	CMD-C2D	-2.17	1.46	1.50
4	Y	609	CHL	CMC-C2C	2.16	1.49	1.44
8	Y	1623	NEX	O24-C25	-2.16	1.43	1.46
5	Z	613	CLA	CMD-C2D	-2.16	1.46	1.50
5	Y	611	CLA	CHC-C1C	2.16	1.42	1.38
5	X	614	CLA	CHC-C1C	2.15	1.42	1.38
5	Y	602	CLA	CMD-C2D	-2.15	1.46	1.50
5	Y	610	CLA	CMD-C2D	-2.15	1.46	1.50
4	Y	609	CHL	CBD-CGD	-2.15	1.49	1.52
5	Z	614	CLA	CHC-C1C	2.14	1.42	1.38
8	X	1623	NEX	O24-C25	-2.12	1.43	1.46
6	Z	1621	LUT	C22-C21	-2.12	1.52	1.54
5	X	604	CLA	CHC-C1C	2.12	1.42	1.38
5	Y	604	CLA	CHC-C1C	2.11	1.42	1.38
5	Y	610	CLA	CMB-C2B	-2.11	1.46	1.50
5	Y	611	CLA	CMD-C2D	-2.11	1.46	1.50
4	X	609	CHL	CBD-CGD	-2.11	1.49	1.52
5	Y	613	CLA	CMD-C2D	-2.11	1.46	1.50
5	Z	604	CLA	CHC-C1C	2.11	1.42	1.38
4	Z	606	CHL	CMC-C2C	2.10	1.49	1.44
5	X	614	CLA	CMD-C2D	-2.10	1.46	1.50
5	Y	612	CLA	CMD-C2D	-2.10	1.46	1.50
5	X	612	CLA	CMB-C2B	-2.10	1.46	1.50
5	X	604	CLA	CMD-C2D	-2.09	1.46	1.50
5	X	602	CLA	CMC-C2C	-2.09	1.46	1.50
4	Y	601	CHL	CBD-CGD	-2.09	1.49	1.52
5	X	604	CLA	CMB-C2B	-2.09	1.46	1.50
6	Y	1620	LUT	C22-C21	-2.09	1.52	1.54
5	Y	604	CLA	CMB-C2B	-2.09	1.46	1.50
4	X	601	CHL	CMC-C2C	2.08	1.49	1.44
5	X	613	CLA	CMD-C2D	-2.08	1.46	1.50
4	X	605	CHL	CMC-C2C	2.08	1.49	1.44
5	Y	613	CLA	CMB-C2B	-2.08	1.46	1.50
5	Y	604	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	609	CHL	CMC-C2C	2.08	1.49	1.44
5	X	611	CLA	CHC-C1C	2.07	1.42	1.38
6	X	1620	LUT	C22-C21	-2.07	1.52	1.54
5	X	613	CLA	CMB-C2B	-2.07	1.46	1.50
4	Y	601	CHL	CMC-C2C	2.07	1.49	1.44
5	X	602	CLA	CMD-C2D	-2.07	1.46	1.50
4	X	608	CHL	CBD-CGD	-2.06	1.49	1.52
4	Z	608	CHL	CMC-C2C	2.06	1.49	1.44
5	Y	613	CLA	CHC-C1C	2.06	1.42	1.38
8	Z	1623	NEX	O24-C25	-2.06	1.43	1.46
5	Y	613	CLA	CMC-C2C	-2.06	1.46	1.50
5	X	603	CLA	CHC-C1C	2.05	1.42	1.38
5	X	613	CLA	CHC-C1C	2.05	1.42	1.38
5	Z	612	CLA	CMD-C2D	-2.05	1.46	1.50
5	X	611	CLA	CMD-C2D	-2.05	1.46	1.50
4	X	601	CHL	CBD-CGD	-2.05	1.49	1.52
5	Y	612	CLA	CMB-C2B	-2.05	1.46	1.50
5	X	613	CLA	CMC-C2C	-2.04	1.46	1.50
5	X	612	CLA	CMD-C2D	-2.04	1.46	1.50
5	Y	614	CLA	CMB-C2B	-2.04	1.46	1.50
5	X	614	CLA	CMB-C2B	-2.04	1.46	1.50
5	Z	612	CLA	CHC-C1C	2.04	1.42	1.38
5	Y	611	CLA	CMB-C2B	-2.04	1.46	1.50
5	X	610	CLA	CMB-C2B	-2.04	1.46	1.50
5	Z	611	CLA	CMD-C2D	-2.03	1.46	1.50
5	Z	603	CLA	C3B-C4B	2.03	1.48	1.42
5	Z	613	CLA	CMC-C2C	-2.02	1.46	1.50
5	X	611	CLA	CMB-C2B	-2.02	1.46	1.50
5	Z	604	CLA	CMD-C2D	-2.02	1.46	1.50
5	Z	603	CLA	CMB-C2B	-2.02	1.46	1.50
4	Y	605	CHL	CMC-C2C	2.02	1.49	1.44
4	Z	605	CHL	CMC-C2C	2.02	1.49	1.44
5	Z	613	CLA	CHC-C1C	2.01	1.42	1.38
5	Z	613	CLA	CMB-C2B	-2.01	1.46	1.50
5	Y	602	CLA	CMC-C2C	-2.01	1.46	1.50
5	Y	603	CLA	CHC-C1C	2.01	1.42	1.38

All (609) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Z	1622	XAT	C37-C21-C36	-18.25	80.85	107.37
7	Y	1622	XAT	C37-C21-C36	-17.94	81.31	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	X	1622	XAT	C37-C21-C36	-17.94	81.31	107.37
7	Y	1622	XAT	C37-C21-C22	-14.95	82.70	108.97
7	X	1622	XAT	C37-C21-C22	-14.94	82.72	108.97
7	Z	1622	XAT	C37-C21-C22	-14.44	83.60	108.97
4	Z	601	CHL	C1B-CHB-C4A	10.96	128.37	121.32
4	Z	607	CHL	C1B-CHB-C4A	10.50	128.07	121.32
4	X	601	CHL	C1B-CHB-C4A	10.44	128.04	121.32
4	Y	601	CHL	C1B-CHB-C4A	10.35	127.98	121.32
4	X	605	CHL	O2D-CGD-CBD	9.43	121.31	110.95
4	Y	605	CHL	O2D-CGD-CBD	9.39	121.27	110.95
4	Y	609	CHL	O2D-CGD-CBD	8.76	120.57	110.95
4	X	609	CHL	O2D-CGD-CBD	8.75	120.56	110.95
4	Y	601	CHL	O2D-CGD-CBD	8.49	120.27	110.95
4	X	601	CHL	O2D-CGD-CBD	8.46	120.24	110.95
4	Z	609	CHL	O2D-CGD-CBD	8.43	120.21	110.95
4	Z	601	CHL	O2D-CGD-CBD	8.38	120.16	110.95
4	X	608	CHL	C1B-CHB-C4A	8.22	126.61	121.32
7	Z	1622	XAT	C36-C21-C22	8.14	123.28	108.97
4	Y	606	CHL	O2D-CGD-CBD	8.12	119.87	110.95
4	Y	607	CHL	O2D-CGD-CBD	7.91	119.64	110.95
4	X	607	CHL	O2D-CGD-CBD	7.90	119.63	110.95
4	Z	606	CHL	O2D-CGD-CBD	7.90	119.63	110.95
7	Y	1622	XAT	C36-C21-C22	7.89	122.84	108.97
7	X	1622	XAT	C36-C21-C22	7.89	122.83	108.97
4	Z	605	CHL	O2D-CGD-CBD	7.74	119.45	110.95
4	Z	606	CHL	CHA-C1A-C2A	-7.66	115.33	133.31
4	Y	606	CHL	CHA-C1A-C2A	-7.63	115.39	133.31
4	X	608	CHL	O2D-CGD-CBD	7.58	119.28	110.95
4	X	605	CHL	CHA-C1A-C2A	-7.48	115.74	133.31
4	Y	608	CHL	CHA-C1A-C2A	-7.45	115.82	133.31
4	Y	607	CHL	C1B-CHB-C4A	7.44	126.11	121.32
4	Z	608	CHL	O2D-CGD-CBD	7.41	119.09	110.95
4	Z	605	CHL	CHA-C1A-C2A	-7.41	115.91	133.31
4	X	607	CHL	C1B-CHB-C4A	7.38	126.07	121.32
4	Z	608	CHL	CHA-C1A-C2A	-7.36	116.04	133.31
4	Y	606	CHL	OBD-CAD-C3D	-7.28	116.53	127.89
4	Y	608	CHL	O2D-CGD-CBD	7.23	118.89	110.95
4	Z	607	CHL	O2D-CGD-CBD	7.22	118.88	110.95
6	Y	1620	LUT	C8-C7-C6	-7.21	107.75	127.00
6	X	1620	LUT	C8-C7-C6	-7.19	107.80	127.00
4	Z	605	CHL	OBD-CAD-C3D	-7.17	116.70	127.89
8	X	1623	NEX	O24-C25-C24	7.17	120.21	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	Y	1623	NEX	O24-C25-C24	7.12	120.17	113.49
4	Z	606	CHL	OBD-CAD-C3D	-7.08	116.85	127.89
4	X	605	CHL	OBD-CAD-C3D	-6.99	116.99	127.89
4	Y	605	CHL	OBD-CAD-C3D	-6.98	117.00	127.89
8	Z	1623	NEX	O24-C25-C24	6.91	119.97	113.49
4	Y	608	CHL	OBD-CAD-C3D	-6.88	117.16	127.89
4	Z	608	CHL	OBD-CAD-C3D	-6.84	117.22	127.89
4	Y	609	CHL	C1B-CHB-C4A	6.73	125.65	121.32
4	X	609	CHL	C1B-CHB-C4A	6.70	125.63	121.32
7	Y	1622	XAT	O24-C25-C24	6.52	119.60	113.49
7	X	1622	XAT	O24-C25-C24	6.51	119.59	113.49
4	X	601	CHL	C4D-ND-C1D	-6.38	100.37	105.22
4	Y	601	CHL	C4D-ND-C1D	-6.35	100.40	105.22
4	Z	601	CHL	C4D-ND-C1D	-6.32	100.42	105.22
4	Z	607	CHL	C4D-ND-C1D	-6.31	100.43	105.22
5	Z	603	CLA	C4A-NA-C1A	6.29	109.55	106.68
4	X	608	CHL	C4D-ND-C1D	-6.27	100.46	105.22
6	Y	1620	LUT	C21-C26-C27	-6.13	105.78	112.83
6	X	1620	LUT	C21-C26-C27	-6.02	105.90	112.83
7	Y	1622	XAT	C15-C14-C13	-6.01	118.85	127.28
7	X	1622	XAT	C15-C14-C13	-5.99	118.87	127.28
8	Y	1623	NEX	C11-C10-C9	-5.99	118.88	127.28
8	X	1623	NEX	C11-C10-C9	-5.98	118.89	127.28
7	Z	1622	XAT	C15-C14-C13	-5.87	119.04	127.28
4	Z	601	CHL	CBC-CAC-C3C	-5.84	104.51	112.87
4	X	609	CHL	C4D-ND-C1D	-5.83	100.80	105.22
4	Y	609	CHL	C4D-ND-C1D	-5.81	100.81	105.22
7	Z	1622	XAT	O24-C25-C24	5.66	118.80	113.49
4	Z	601	CHL	CHA-C1A-C2A	-5.64	120.06	133.31
7	Z	1622	XAT	C38-C25-C26	-5.56	113.15	122.30
4	Y	601	CHL	CHA-C1A-C2A	-5.56	120.25	133.31
4	X	601	CHL	CHA-C1A-C2A	-5.55	120.27	133.31
5	Z	611	CLA	C4A-NA-C1A	5.54	109.21	106.68
4	Z	606	CHL	C4D-ND-C1D	5.49	109.38	105.22
4	Y	609	CHL	CHA-C1A-C2A	-5.40	120.62	133.31
4	X	609	CHL	CHA-C1A-C2A	-5.40	120.62	133.31
4	Z	605	CHL	C4D-ND-C1D	5.37	109.29	105.22
7	Y	1622	XAT	O4-C5-C4	5.36	118.52	113.49
7	Z	1622	XAT	O4-C5-C4	5.35	118.51	113.49
4	Z	608	CHL	C4D-ND-C1D	5.34	109.27	105.22
7	X	1622	XAT	O4-C5-C4	5.31	118.47	113.49
4	X	608	CHL	CHA-C1A-C2A	-5.28	120.90	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	X	1621	LUT	C7-C8-C9	-5.27	118.43	126.23
6	Y	1621	LUT	C7-C8-C9	-5.25	118.46	126.23
4	Z	607	CHL	CHA-C1A-C2A	-5.23	121.03	133.31
4	Y	608	CHL	C4D-ND-C1D	5.19	109.16	105.22
5	Z	612	CLA	C4A-NA-C1A	5.18	109.04	106.68
5	X	603	CLA	C4A-NA-C1A	5.16	109.03	106.68
8	Z	1623	NEX	C38-C25-C26	-5.12	113.87	122.30
4	X	605	CHL	C4D-ND-C1D	5.08	109.07	105.22
5	Z	613	CLA	C4A-NA-C1A	5.08	109.00	106.68
5	Y	603	CLA	C4A-NA-C1A	5.05	108.98	106.68
4	Y	605	CHL	C4D-ND-C1D	5.05	109.05	105.22
7	X	1622	XAT	C38-C25-C26	-5.04	114.01	122.30
7	Y	1622	XAT	C38-C25-C26	-5.03	114.02	122.30
4	Y	606	CHL	C4D-ND-C1D	5.01	109.02	105.22
5	Y	612	CLA	C4A-NA-C1A	5.01	108.96	106.68
5	X	612	CLA	C4A-NA-C1A	4.96	108.94	106.68
6	Z	1621	LUT	C7-C8-C9	-4.93	118.95	126.23
7	X	1622	XAT	C6-C7-C8	-4.92	115.58	125.99
7	Y	1622	XAT	C6-C7-C8	-4.92	115.59	125.99
5	X	613	CLA	C4A-NA-C1A	4.92	108.92	106.68
7	Z	1622	XAT	C18-C5-C6	-4.91	114.23	122.30
4	Z	609	CHL	CHA-C1A-C2A	-4.88	121.84	133.31
4	Y	606	CHL	OBD-CAD-CBD	4.88	132.99	125.82
6	Z	1620	LUT	C26-C27-C28	-4.86	117.02	124.58
5	Y	613	CLA	C4A-NA-C1A	4.82	108.88	106.68
4	X	607	CHL	C4D-ND-C1D	-4.81	101.57	105.22
8	Y	1623	NEX	C38-C25-C26	-4.80	114.40	122.30
7	Y	1622	XAT	C18-C5-C6	-4.80	114.41	122.30
7	X	1622	XAT	C18-C5-C6	-4.80	114.41	122.30
8	X	1623	NEX	C38-C25-C26	-4.79	114.41	122.30
4	Y	607	CHL	C4D-ND-C1D	-4.79	101.58	105.22
7	Z	1622	XAT	C37-C21-C26	-4.74	97.26	110.05
4	Z	605	CHL	OBD-CAD-CBD	4.72	132.75	125.82
4	Y	608	CHL	OBD-CAD-CBD	4.71	132.74	125.82
7	Y	1622	XAT	C37-C21-C26	-4.71	97.34	110.05
7	X	1622	XAT	C37-C21-C26	-4.70	97.36	110.05
5	Y	614	CLA	C4A-NA-C1A	4.68	108.81	106.68
8	X	1623	NEX	C15-C14-C13	-4.68	120.72	127.28
7	Z	1622	XAT	O4-C5-C18	4.67	120.26	115.05
5	X	611	CLA	C4A-NA-C1A	4.66	108.80	106.68
8	Y	1623	NEX	C15-C14-C13	-4.65	120.75	127.28
7	X	1622	XAT	O4-C5-C18	4.64	120.23	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Y	1622	XAT	O4-C5-C18	4.62	120.22	115.05
5	X	614	CLA	C4A-NA-C1A	4.62	108.79	106.68
5	Z	604	CLA	C4A-NA-C1A	4.60	108.78	106.68
4	Z	608	CHL	OBD-CAD-CBD	4.59	132.56	125.82
4	X	605	CHL	OBD-CAD-CBD	4.59	132.56	125.82
4	Z	606	CHL	OBD-CAD-CBD	4.59	132.56	125.82
4	Y	605	CHL	OBD-CAD-CBD	4.59	132.56	125.82
4	Z	609	CHL	C4D-ND-C1D	-4.56	101.76	105.22
6	Z	1620	LUT	C8-C7-C6	-4.56	114.82	127.00
7	X	1622	XAT	C31-C30-C29	-4.53	120.93	127.28
8	Z	1623	NEX	C11-C10-C9	-4.52	120.93	127.28
7	Y	1622	XAT	C31-C30-C29	-4.52	120.94	127.28
5	Y	602	CLA	C4A-NA-C1A	4.52	108.74	106.68
4	X	609	CHL	CBC-CAC-C3C	-4.50	106.42	112.87
8	Y	1623	NEX	C35-C34-C33	-4.50	120.96	127.28
5	Y	611	CLA	C4A-NA-C1A	4.50	108.73	106.68
6	Z	1620	LUT	C21-C26-C27	-4.47	107.69	112.83
8	X	1623	NEX	C35-C34-C33	-4.46	121.02	127.28
4	Y	609	CHL	CBC-CAC-C3C	-4.44	106.52	112.87
7	Y	1622	XAT	C27-C28-C29	-4.39	118.72	125.53
5	X	604	CLA	C4A-NA-C1A	4.38	108.68	106.68
6	Z	1621	LUT	C17-C1-C6	-4.37	103.38	110.24
7	X	1622	XAT	C27-C28-C29	-4.37	118.75	125.53
5	X	602	CLA	C4A-NA-C1A	4.32	108.65	106.68
5	Y	604	CLA	C4A-NA-C1A	4.31	108.65	106.68
8	X	1623	NEX	C27-C28-C29	-4.25	118.93	125.53
5	Z	602	CLA	C4A-NA-C1A	4.23	108.61	106.68
8	Y	1623	NEX	C27-C28-C29	-4.22	118.98	125.53
7	X	1622	XAT	C15-C35-C34	-4.18	114.97	123.52
7	Y	1622	XAT	C15-C35-C34	-4.16	115.01	123.52
4	X	605	CHL	C1A-CHA-C4D	-4.15	112.06	118.98
7	Z	1622	XAT	C31-C30-C29	-4.15	121.46	127.28
4	Y	605	CHL	C1A-CHA-C4D	-4.14	112.07	118.98
7	Z	1622	XAT	O24-C25-C38	4.12	119.65	115.05
7	Z	1622	XAT	C6-C7-C8	-4.09	117.34	125.99
5	Z	614	CLA	C4A-NA-C1A	4.02	108.52	106.68
6	Z	1621	LUT	C21-C26-C27	-4.00	108.23	112.83
6	X	1620	LUT	C17-C1-C6	3.93	116.41	110.24
6	Y	1620	LUT	C17-C1-C6	3.89	116.35	110.24
7	Z	1622	XAT	C11-C10-C9	-3.87	121.86	127.28
4	Y	606	CHL	C1A-CHA-C4D	-3.83	112.59	118.98
7	Z	1622	XAT	C35-C34-C33	-3.82	121.92	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Z	1621	LUT	C26-C27-C28	-3.82	118.63	124.58
7	Y	1622	XAT	C35-C34-C33	-3.78	121.98	127.28
7	X	1622	XAT	C35-C34-C33	-3.77	121.99	127.28
4	Z	605	CHL	C1A-CHA-C4D	-3.73	112.76	118.98
4	Z	606	CHL	C1A-CHA-C4D	-3.72	112.77	118.98
6	Y	1620	LUT	C26-C27-C28	-3.72	118.78	124.58
6	X	1620	LUT	C26-C27-C28	-3.70	118.83	124.58
8	Z	1623	NEX	C15-C14-C13	-3.68	122.11	127.28
4	Y	607	CHL	CHA-C1A-C2A	-3.67	124.69	133.31
4	X	607	CHL	CHA-C1A-C2A	-3.66	124.72	133.31
7	Y	1622	XAT	O24-C25-C38	3.66	119.13	115.05
8	Z	1623	NEX	C15-C35-C34	-3.65	116.06	123.52
8	Z	1623	NEX	C26-C27-C28	-3.64	118.29	125.99
9	X	2630	LHG	O7-C7-C8	3.63	119.33	111.48
7	X	1622	XAT	O24-C25-C38	3.62	119.10	115.05
7	X	1622	XAT	C11-C10-C9	-3.62	122.21	127.28
8	Y	1623	NEX	O24-C25-C38	3.62	119.09	115.05
7	Y	1622	XAT	C11-C10-C9	-3.61	122.21	127.28
4	Z	606	CHL	CMB-C2B-C3B	3.61	131.90	124.68
6	Z	1620	LUT	C7-C8-C9	-3.61	120.90	126.23
9	Y	2630	LHG	O7-C7-C8	3.60	119.26	111.48
8	X	1623	NEX	O24-C25-C38	3.58	119.05	115.05
4	Z	608	CHL	C1A-CHA-C4D	-3.56	113.04	118.98
4	Y	608	CHL	C1A-CHA-C4D	-3.56	113.05	118.98
7	Z	1622	XAT	C27-C28-C29	-3.53	120.05	125.53
6	X	1621	LUT	C26-C27-C28	-3.51	119.11	124.58
6	Y	1621	LUT	C26-C27-C28	-3.50	119.12	124.58
5	X	610	CLA	C4A-NA-C1A	3.50	108.28	106.68
5	Y	610	CLA	C4A-NA-C1A	3.49	108.27	106.68
5	Z	610	CLA	C4A-NA-C1A	3.49	108.27	106.68
7	Y	1622	XAT	C4-C3-C2	-3.48	104.28	110.79
4	Z	605	CHL	C1C-C2C-CMC	3.47	133.05	126.80
7	X	1622	XAT	C4-C3-C2	-3.46	104.31	110.79
4	X	605	CHL	C1C-C2C-CMC	3.46	133.04	126.80
7	Z	1622	XAT	C15-C35-C34	-3.46	116.44	123.52
8	Y	1623	NEX	C4-C3-C2	-3.44	106.32	111.03
6	Z	1621	LUT	C8-C7-C6	-3.43	117.83	127.00
4	Y	605	CHL	C1C-C2C-CMC	3.43	132.98	126.80
4	Z	608	CHL	C1C-C2C-CMC	3.37	132.88	126.80
7	Y	1622	XAT	C10-C11-C12	-3.34	113.51	123.20
4	X	601	CHL	CBC-CAC-C3C	-3.33	108.11	112.87
6	X	1621	LUT	C17-C1-C6	-3.33	105.02	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	X	1622	XAT	C10-C11-C12	-3.33	113.56	123.20
4	Y	601	CHL	C4-C3-C5	3.32	120.99	115.23
4	Y	601	CHL	CBC-CAC-C3C	-3.30	108.14	112.87
4	X	601	CHL	C4-C3-C5	3.30	120.95	115.23
6	Y	1621	LUT	C17-C1-C6	-3.30	105.07	110.24
7	Z	1622	XAT	C4-C3-C2	-3.30	104.62	110.79
4	Z	601	CHL	C3D-C4D-ND	3.27	118.19	112.94
7	Z	1622	XAT	C26-C27-C28	-3.26	119.09	125.99
4	X	601	CHL	C3D-C4D-ND	3.24	118.14	112.94
4	X	609	CHL	C3D-C4D-ND	3.23	118.13	112.94
4	Y	601	CHL	C3D-C4D-ND	3.23	118.12	112.94
4	Y	607	CHL	CMB-C2B-C3B	3.22	131.12	124.68
4	Y	609	CHL	C1C-CHC-C4B	3.22	127.58	116.07
4	X	609	CHL	C1C-CHC-C4B	3.21	127.56	116.07
4	Y	609	CHL	C3D-C4D-ND	3.21	118.09	112.94
4	Z	606	CHL	OMC-CMC-C2C	-3.20	119.57	125.12
4	Y	608	CHL	C1C-C2C-CMC	3.19	132.55	126.80
6	Y	1621	LUT	C21-C26-C27	-3.19	109.16	112.83
4	X	607	CHL	CMB-C2B-C3B	3.19	131.05	124.68
4	X	601	CHL	C1C-CHC-C4B	3.17	127.42	116.07
8	Z	1623	NEX	C31-C30-C29	-3.17	122.83	127.28
4	Y	601	CHL	C1C-CHC-C4B	3.17	127.40	116.07
4	Y	607	CHL	O1D-CGD-CBD	-3.16	119.93	124.72
4	Y	606	CHL	CMD-C2D-C3D	3.15	130.98	124.68
9	Y	2630	LHG	O8-C23-C24	3.15	121.44	111.83
6	X	1621	LUT	C21-C26-C27	-3.13	109.22	112.83
4	Y	608	CHL	CMD-C2D-C3D	3.13	130.95	124.68
9	X	2630	LHG	O8-C23-C24	3.13	121.38	111.83
4	Z	601	CHL	C1C-CHC-C4B	3.13	127.27	116.07
4	X	607	CHL	O1D-CGD-CBD	-3.13	119.98	124.72
4	X	605	CHL	O1D-CGD-CBD	-3.13	119.98	124.72
7	Z	1622	XAT	C10-C11-C12	-3.13	114.14	123.20
4	Z	607	CHL	C1C-CHC-C4B	3.13	127.25	116.07
8	Z	1623	NEX	C27-C28-C29	-3.12	120.69	125.53
4	Y	605	CHL	O1D-CGD-CBD	-3.12	120.00	124.72
4	Z	607	CHL	C4-C3-C5	3.11	120.63	115.23
4	X	608	CHL	C1C-CHC-C4B	3.10	127.17	116.07
4	Y	606	CHL	OMC-CMC-C2C	-3.09	119.75	125.12
4	Z	609	CHL	C1C-CHC-C4B	3.06	127.02	116.07
4	Y	607	CHL	CMA-C3A-C4A	-3.05	108.05	114.61
8	Z	1623	NEX	O24-C25-C38	3.05	118.45	115.05
4	X	605	CHL	CMD-C2D-C3D	3.04	130.76	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Y	1622	XAT	C36-C21-C26	3.04	118.25	110.05
7	X	1622	XAT	C36-C21-C26	3.03	118.22	110.05
6	Z	1620	LUT	C35-C15-C14	-3.03	117.32	123.52
8	X	1623	NEX	C24-C23-C22	-3.03	105.13	110.79
4	X	607	CHL	CMA-C3A-C4A	-3.02	108.10	114.61
6	Z	1620	LUT	C28-C29-C30	-3.02	114.26	119.01
8	Y	1623	NEX	C24-C23-C22	-3.02	105.14	110.79
4	Z	606	CHL	CMD-C2D-C3D	3.02	130.71	124.68
5	Y	603	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
5	X	611	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
4	Y	605	CHL	CMD-C2D-C3D	2.99	130.66	124.68
5	Y	611	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
4	Z	607	CHL	C3D-C4D-ND	2.99	117.73	112.94
5	X	603	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
6	Z	1620	LUT	C11-C10-C9	-2.97	123.11	127.28
4	X	601	CHL	C1-C2-C3	-2.97	121.33	126.20
5	X	610	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
4	Z	601	CHL	C1-C2-C3	-2.97	121.34	126.20
5	Y	610	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
6	X	1620	LUT	C35-C15-C14	-2.96	117.47	123.52
4	Y	601	CHL	C1-C2-C3	-2.95	121.36	126.20
4	X	608	CHL	C3D-C4D-ND	2.95	117.66	112.94
6	Y	1621	LUT	C8-C7-C6	-2.94	119.14	127.00
4	Y	607	CHL	O2A-CGA-CBA	2.94	120.79	111.83
4	Z	608	CHL	OMC-CMC-C2C	-2.94	120.02	125.12
4	Y	607	CHL	C1C-CHC-C4B	2.93	126.57	116.07
4	X	607	CHL	O2A-CGA-CBA	2.93	120.77	111.83
7	Z	1622	XAT	C36-C21-C26	2.93	117.95	110.05
6	Y	1620	LUT	C35-C15-C14	-2.93	117.53	123.52
4	X	609	CHL	O1D-CGD-CBD	-2.93	120.28	124.72
4	X	607	CHL	C1C-CHC-C4B	2.92	126.52	116.07
4	Y	609	CHL	O1D-CGD-CBD	-2.92	120.30	124.72
6	X	1621	LUT	C8-C7-C6	-2.91	119.23	127.00
6	X	1621	LUT	C1-C6-C5	-2.91	118.66	122.64
4	Z	608	CHL	CMD-C2D-C3D	2.91	130.49	124.68
8	Z	1623	NEX	C39-C29-C30	-2.91	118.11	122.82
6	Y	1621	LUT	C1-C6-C5	-2.90	118.67	122.64
6	Z	1620	LUT	C3-C4-C5	-2.90	104.96	112.18
8	Z	1623	NEX	C11-C12-C13	-2.90	118.42	126.36
5	X	613	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
5	Y	613	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
4	Z	608	CHL	O2A-CGA-CBA	2.89	120.64	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Z	605	CHL	OMC-CMC-C2C	-2.87	120.14	125.12
6	Z	1621	LUT	C11-C10-C9	-2.86	123.26	127.28
4	X	609	CHL	CMB-C2B-C3B	2.86	130.40	124.68
9	Z	2630	LHG	O7-C7-C8	2.86	117.67	111.48
4	Z	607	CHL	O2A-CGA-CBA	2.86	120.55	111.83
4	X	605	CHL	OMC-CMC-C2C	-2.86	120.16	125.12
4	Y	609	CHL	CMB-C2B-C3B	2.85	130.37	124.68
4	Z	608	CHL	CMB-C2B-C3B	2.84	130.37	124.68
4	X	608	CHL	C1-C2-C3	-2.84	121.54	126.20
5	X	602	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
6	Y	1621	LUT	C11-C10-C9	-2.84	123.30	127.28
5	Y	614	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
6	X	1621	LUT	C11-C10-C9	-2.83	123.31	127.28
4	Y	605	CHL	OMC-CMC-C2C	-2.83	120.21	125.12
5	Z	603	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
4	Y	609	CHL	O2A-CGA-CBA	2.83	120.45	111.83
5	Y	602	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
4	X	609	CHL	O2A-CGA-CBA	2.82	120.44	111.83
5	X	614	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
4	Y	608	CHL	OMC-CMC-C2C	-2.82	120.22	125.12
4	Z	609	CHL	C3D-C4D-ND	2.82	117.46	112.94
5	Z	602	CLA	C3B-C4B-NB	-2.82	108.01	110.53
4	Z	605	CHL	CMD-C2D-C3D	2.80	130.28	124.68
7	Z	1622	XAT	C31-C32-C33	-2.80	118.68	126.36
4	X	608	CHL	C4-C3-C5	2.80	120.08	115.23
5	Z	610	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
5	Z	614	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
5	X	604	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
5	Y	604	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
8	Z	1623	NEX	C8-C7-C6	-2.77	174.40	177.66
4	Z	609	CHL	O1D-CGD-CBD	-2.76	120.54	124.72
4	Y	606	CHL	CMB-C2B-C3B	2.75	130.18	124.68
5	X	602	CLA	C3B-C4B-NB	-2.74	108.08	110.53
4	Z	609	CHL	CMB-C2B-C3B	2.73	130.13	124.68
4	Z	607	CHL	CAA-C2A-C3A	-2.72	105.64	113.00
4	Y	608	CHL	O2A-CGA-CBA	2.72	120.13	111.83
5	Z	613	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
5	Y	612	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
6	Z	1621	LUT	C3-C4-C5	-2.70	105.46	112.18
5	X	612	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
4	X	605	CHL	C1A-CHA-CBD	2.69	139.26	132.36
8	Y	1623	NEX	C11-C12-C13	-2.69	118.98	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	X	1623	NEX	C11-C12-C13	-2.69	119.00	126.36
5	Z	604	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
4	Y	605	CHL	C1A-CHA-CBD	2.68	139.24	132.36
6	Z	1620	LUT	C17-C1-C6	-2.67	106.05	110.24
4	Y	609	CHL	CMA-C3A-C4A	-2.67	108.86	114.61
5	Z	610	CLA	CMB-C2B-C1B	-2.66	121.36	125.42
5	Y	602	CLA	C3B-C4B-NB	-2.66	108.15	110.53
4	X	609	CHL	CMA-C3A-C4A	-2.66	108.89	114.61
4	Z	609	CHL	C4-C3-C5	2.66	119.84	115.23
4	X	605	CHL	O2D-CGD-O1D	-2.65	118.68	123.85
5	Z	611	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
5	Y	610	CLA	C3B-C4B-NB	-2.64	108.17	110.53
4	Y	605	CHL	O2D-CGD-O1D	-2.64	118.71	123.85
4	Y	606	CHL	C1C-C2C-CMC	2.64	131.56	126.80
5	Z	602	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
7	Y	1622	XAT	C31-C32-C33	-2.62	119.17	126.36
8	X	1623	NEX	C26-C27-C28	-2.62	120.45	125.99
4	Y	608	CHL	CMB-C2B-C3B	2.62	129.91	124.68
4	Y	607	CHL	CBC-CAC-C3C	-2.61	109.14	112.87
7	X	1622	XAT	C31-C32-C33	-2.61	119.21	126.36
4	Z	607	CHL	CMB-C2B-C3B	2.60	129.89	124.68
5	Y	610	CLA	C1-C2-C3	-2.60	121.93	126.20
8	Y	1623	NEX	C26-C27-C28	-2.60	120.49	125.99
4	X	607	CHL	CBC-CAC-C3C	-2.60	109.15	112.87
4	Z	608	CHL	CBC-CAC-C3C	-2.59	109.16	112.87
4	Z	606	CHL	O1D-CGD-CBD	-2.59	120.80	124.72
4	Z	607	CHL	C6-C5-C3	-2.59	107.16	113.47
5	X	610	CLA	C3B-C4B-NB	-2.59	108.22	110.53
4	X	601	CHL	O1D-CGD-CBD	-2.58	120.81	124.72
5	X	610	CLA	C1-C2-C3	-2.58	121.97	126.20
4	Y	601	CHL	O1D-CGD-CBD	-2.58	120.81	124.72
6	Z	1620	LUT	C35-C34-C33	-2.57	123.68	127.28
4	Y	606	CHL	C1B-CHB-C4A	-2.56	119.67	121.32
5	X	611	CLA	CHB-C4A-NA	2.56	128.10	124.40
6	Y	1620	LUT	C38-C25-C24	-2.55	117.31	123.36
4	Y	606	CHL	O1D-CGD-CBD	-2.55	120.86	124.72
5	Y	611	CLA	CHB-C4A-NA	2.55	128.07	124.40
4	Z	601	CHL	O1D-CGD-CBD	-2.54	120.87	124.72
4	Y	601	CHL	O2D-CGD-O1D	-2.53	118.92	123.85
4	X	608	CHL	O2A-CGA-CBA	2.53	119.55	111.83
4	X	601	CHL	O2A-CGA-CBA	2.52	119.52	111.83
4	X	601	CHL	O2D-CGD-O1D	-2.51	118.95	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Y	605	CHL	CMB-C2B-C3B	2.51	129.70	124.68
9	Z	2630	LHG	O8-C23-C24	2.51	119.48	111.83
6	Y	1620	LUT	C28-C29-C30	-2.51	115.06	119.01
4	Y	601	CHL	O2A-CGA-CBA	2.51	119.48	111.83
4	Z	601	CHL	O2D-CGD-O1D	-2.51	118.97	123.85
4	Z	609	CHL	O2A-CGA-CBA	2.50	119.47	111.83
4	X	607	CHL	OMC-CMC-C2C	-2.50	120.78	125.12
4	Z	605	CHL	O1D-CGD-CBD	-2.50	120.93	124.72
7	Z	1622	XAT	C7-C8-C9	-2.50	121.65	125.53
8	Z	1623	NEX	C24-C23-C22	-2.50	106.12	110.79
4	Z	608	CHL	C1B-CHB-C4A	-2.50	119.72	121.32
6	X	1620	LUT	C38-C25-C24	-2.49	117.46	123.36
4	Y	607	CHL	OMC-CMC-C2C	-2.49	120.80	125.12
4	Z	607	CHL	CMA-C3A-C4A	-2.48	109.27	114.61
5	Z	612	CLA	CHB-C4A-NA	2.48	127.97	124.40
5	Z	614	CLA	C3B-C4B-NB	-2.47	108.32	110.53
5	Z	603	CLA	CHB-C4A-NA	2.47	127.97	124.40
4	X	605	CHL	CMB-C2B-C3B	2.47	129.61	124.68
6	X	1620	LUT	C28-C29-C30	-2.46	115.13	119.01
8	X	1623	NEX	C39-C29-C30	-2.46	118.83	122.82
5	Z	612	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
4	Z	605	CHL	CMB-C2B-C3B	2.45	129.58	124.68
5	Y	612	CLA	C3B-C4B-NB	-2.45	108.34	110.53
8	Y	1623	NEX	C39-C29-C30	-2.45	118.85	122.82
5	X	612	CLA	C3B-C4B-NB	-2.44	108.35	110.53
8	Z	1623	NEX	C32-C33-C34	-2.44	115.17	119.01
4	Z	609	CHL	C1-C2-C3	-2.44	122.20	126.20
8	X	1623	NEX	C31-C30-C29	-2.43	123.86	127.28
4	X	609	CHL	C1-C2-C3	-2.42	122.22	126.20
4	Y	609	CHL	O2D-CGD-O1D	-2.42	119.13	123.85
6	X	1621	LUT	C18-C5-C4	2.41	118.86	114.42
4	Y	605	CHL	CMA-C3A-C4A	-2.41	109.42	114.61
7	Y	1622	XAT	C26-C27-C28	-2.41	120.90	125.99
4	X	609	CHL	O2D-CGD-O1D	-2.41	119.16	123.85
6	X	1620	LUT	C11-C10-C9	-2.41	123.90	127.28
7	X	1622	XAT	C26-C27-C28	-2.41	120.90	125.99
6	Y	1620	LUT	C11-C10-C9	-2.41	123.90	127.28
4	Y	609	CHL	C1-C2-C3	-2.41	122.25	126.20
4	X	605	CHL	CMA-C3A-C4A	-2.41	109.43	114.61
8	X	1623	NEX	C4-C3-C2	-2.40	106.29	110.79
8	Y	1623	NEX	C31-C30-C29	-2.40	123.91	127.28
6	Z	1621	LUT	C31-C30-C29	-2.40	123.91	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	612	CLA	CHB-C4A-NA	2.40	127.86	124.40
5	X	603	CLA	CHB-C4A-NA	2.40	127.86	124.40
5	X	612	CLA	CHB-C4A-NA	2.39	127.85	124.40
5	Z	610	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
5	Z	610	CLA	CMB-C2B-C3B	2.39	132.16	126.55
5	Z	613	CLA	C1-C2-C3	-2.38	122.30	126.20
4	Y	609	CHL	C4-C3-C5	2.38	119.35	115.23
5	Z	610	CLA	CHB-C4A-NA	2.38	127.83	124.40
5	X	614	CLA	C3B-C4B-NB	-2.37	108.41	110.53
4	X	609	CHL	C4-C3-C5	2.37	119.34	115.23
5	X	613	CLA	C1-C2-C3	-2.36	122.32	126.20
5	Y	602	CLA	CHB-C4A-NA	2.36	127.81	124.40
6	Y	1621	LUT	C18-C5-C4	2.36	118.77	114.42
5	Z	611	CLA	CHB-C4A-NA	2.36	127.81	124.40
4	Z	609	CHL	O2D-CGD-O1D	-2.36	119.26	123.85
4	Y	606	CHL	O2D-CGD-O1D	-2.35	119.27	123.85
6	Y	1621	LUT	C15-C35-C34	-2.34	118.72	123.52
5	Y	614	CLA	C3B-C4B-NB	-2.34	108.44	110.53
5	Y	603	CLA	C3B-C4B-NB	-2.33	108.45	110.53
5	X	602	CLA	CHB-C4A-NA	2.33	127.77	124.40
5	Y	603	CLA	CHB-C4A-NA	2.33	127.76	124.40
5	Y	610	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
4	Y	601	CHL	C1C-C2C-CMC	2.33	131.00	126.80
4	X	607	CHL	C3D-C4D-ND	2.33	116.67	112.94
8	Z	1623	NEX	C17-C1-C6	-2.32	108.39	110.47
4	X	608	CHL	CMB-C2B-C3B	2.32	129.32	124.68
5	X	610	CLA	CHB-C4A-NA	2.32	127.75	124.40
8	Y	1623	NEX	C15-C35-C34	-2.32	118.78	123.52
5	Y	613	CLA	C1-C2-C3	-2.31	122.41	126.20
4	Z	605	CHL	C1A-CHA-CBD	2.31	138.28	132.36
4	Z	608	CHL	C1A-CHA-CBD	2.31	138.28	132.36
4	Y	607	CHL	C3D-C4D-ND	2.31	116.64	112.94
4	X	601	CHL	C1C-C2C-CMC	2.31	130.96	126.80
5	X	603	CLA	C3B-C4B-NB	-2.31	108.47	110.53
6	Z	1620	LUT	C38-C25-C24	-2.31	117.90	123.36
8	X	1623	NEX	C15-C35-C34	-2.31	118.80	123.52
4	X	607	CHL	C4-C3-C5	2.30	119.22	115.23
5	Y	610	CLA	CHB-C4A-NA	2.30	127.72	124.40
4	Y	608	CHL	C1A-CHA-CBD	2.30	138.25	132.36
4	Y	608	CHL	C1B-CHB-C4A	-2.30	119.85	121.32
5	X	610	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
5	Z	610	CLA	C1-C2-C3	-2.29	122.44	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Z	606	CHL	C1C-C2C-CMC	2.29	130.93	126.80
4	Y	607	CHL	C4-C3-C5	2.29	119.20	115.23
4	X	608	CHL	O1D-CGD-CBD	-2.29	121.25	124.72
6	X	1621	LUT	C15-C35-C34	-2.28	118.84	123.52
4	X	607	CHL	C1-C2-C3	-2.28	122.45	126.20
6	X	1621	LUT	C15-C14-C13	-2.28	124.08	127.28
4	Y	608	CHL	O1D-CGD-CBD	-2.28	121.26	124.72
4	Y	607	CHL	C1-C2-C3	-2.28	122.46	126.20
5	Z	604	CLA	C3B-C4B-NB	-2.28	108.50	110.53
5	X	614	CLA	CHB-C4A-NA	2.28	127.68	124.40
5	Z	602	CLA	CHB-C4A-NA	2.27	127.68	124.40
4	Z	601	CHL	CMB-C2B-C3B	2.27	129.21	124.68
4	Z	606	CHL	C3D-CAD-CBD	2.27	110.59	107.61
5	X	613	CLA	C6-C5-C3	2.26	118.97	113.47
4	Y	606	CHL	C1A-CHA-CBD	2.25	138.13	132.36
5	Y	611	CLA	C3B-C4B-NB	-2.25	108.52	110.53
4	Z	608	CHL	O1D-CGD-CBD	-2.25	121.31	124.72
5	X	603	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
4	X	608	CHL	O2D-CGD-O1D	-2.25	119.47	123.85
5	Y	613	CLA	C6-C5-C3	2.25	118.94	113.47
6	Y	1621	LUT	C31-C30-C29	-2.24	124.13	127.28
5	Y	614	CLA	CHB-C4A-NA	2.24	127.63	124.40
6	X	1621	LUT	C3-C4-C5	-2.24	106.61	112.18
4	Y	605	CHL	CAC-C3C-C4C	2.24	129.78	124.03
5	X	604	CLA	CHB-C4A-NA	2.24	127.63	124.40
4	Z	607	CHL	C1-C2-C3	-2.23	122.54	126.20
4	Z	605	CHL	C3D-CAD-CBD	2.23	110.54	107.61
5	Y	604	CLA	C1-C2-C3	-2.23	123.15	126.76
4	X	605	CHL	CAC-C3C-C4C	2.23	129.76	124.03
4	Z	601	CHL	O2A-CGA-CBA	2.23	118.63	111.83
5	Z	604	CLA	CHB-C4A-NA	2.23	127.61	124.40
4	Z	601	CHL	C4C-CHD-C1D	2.22	124.03	116.07
5	Z	602	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
6	X	1621	LUT	C31-C30-C29	-2.22	124.16	127.28
5	Y	603	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
7	Y	1622	XAT	C40-C33-C32	2.22	121.47	118.09
4	Z	607	CHL	O1D-CGD-CBD	-2.22	121.36	124.72
4	Z	605	CHL	CAC-C3C-C4C	2.21	129.72	124.03
6	Y	1621	LUT	C15-C14-C13	-2.21	124.17	127.28
4	Z	607	CHL	CAC-C3C-C4C	2.21	129.72	124.03
6	Y	1621	LUT	O23-C23-C22	-2.21	106.14	110.06
6	Y	1621	LUT	C3-C4-C5	-2.21	106.68	112.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Z	606	CHL	O2D-CGD-O1D	-2.20	119.57	123.85
5	Z	611	CLA	C3B-C4B-NB	-2.19	108.58	110.53
6	Z	1621	LUT	O23-C23-C22	-2.19	106.18	110.06
4	Z	606	CHL	C1A-CHA-CBD	2.18	137.96	132.36
4	Y	606	CHL	C3D-CAD-CBD	2.18	110.48	107.61
4	Z	608	CHL	O2D-CGD-O1D	-2.18	119.60	123.85
7	X	1622	XAT	C40-C33-C32	2.18	121.42	118.09
5	Y	613	CLA	CHB-C4A-NA	2.18	127.54	124.40
4	Z	605	CHL	O2D-CGD-O1D	-2.18	119.61	123.85
6	X	1621	LUT	C18-C5-C6	-2.18	122.11	124.48
6	Z	1620	LUT	C30-C31-C32	-2.17	116.90	123.20
4	Y	601	CHL	C4C-CHD-C1D	2.17	123.84	116.07
5	X	613	CLA	CHB-C4A-NA	2.17	127.53	124.40
4	Z	606	CHL	C1B-CHB-C4A	-2.16	119.93	121.32
5	Z	613	CLA	CHB-C4A-NA	2.16	127.52	124.40
4	X	608	CHL	CBC-CAC-C3C	-2.16	109.78	112.87
4	X	607	CHL	CAA-C2A-C3A	-2.16	107.16	113.00
4	Z	608	CHL	CAC-C3C-C4C	2.16	129.58	124.03
5	Y	604	CLA	C3B-C4B-NB	-2.16	108.60	110.53
4	Z	609	CHL	CMD-C2D-C3D	-2.16	120.37	124.68
4	Y	607	CHL	CAA-C2A-C3A	-2.16	107.16	113.00
4	X	601	CHL	C4C-CHD-C1D	2.16	123.79	116.07
4	X	605	CHL	C3D-CAD-CBD	2.16	110.45	107.61
4	Y	605	CHL	C3D-CAD-CBD	2.16	110.45	107.61
4	Z	609	CHL	CBC-CAC-C3C	-2.15	109.79	112.87
4	X	609	CHL	CMD-C2D-C3D	-2.15	120.39	124.68
5	Y	604	CLA	CHB-C4A-NA	2.15	127.50	124.40
8	Z	1623	NEX	C40-C33-C32	2.15	121.37	118.09
6	X	1621	LUT	O23-C23-C22	-2.14	106.26	110.06
5	X	611	CLA	O1A-CGA-CBA	2.14	129.89	123.09
6	Z	1621	LUT	C35-C34-C33	-2.14	124.27	127.28
5	X	611	CLA	C3B-C4B-NB	-2.14	108.62	110.53
4	Y	609	CHL	CMD-C2D-C3D	-2.14	120.40	124.68
4	Z	607	CHL	C4C-CHD-C1D	2.14	123.72	116.07
4	Z	607	CHL	CED-O2D-CGD	2.14	120.77	115.92
5	X	604	CLA	C3B-C4B-NB	-2.14	108.62	110.53
8	Y	1623	NEX	C18-C5-C4	-2.13	108.08	111.51
6	Y	1621	LUT	C18-C5-C6	-2.13	122.16	124.48
4	X	608	CHL	OBD-CAD-C3D	-2.13	124.57	127.89
4	X	601	CHL	CMB-C2B-C3B	2.13	128.94	124.68
4	X	608	CHL	C1-O2A-CGA	2.13	121.80	116.65
4	Z	601	CHL	C1-O2A-CGA	2.13	121.80	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Y	601	CHL	CMB-C2B-C3B	2.12	128.93	124.68
6	Z	1621	LUT	C27-C28-C29	-2.12	121.76	126.32
6	Y	1620	LUT	C12-C13-C14	-2.12	115.68	119.01
4	Z	607	CHL	O2D-CGD-O1D	-2.11	119.73	123.85
4	Z	609	CHL	C1B-CHB-C4A	2.11	122.68	121.32
5	Z	614	CLA	CHB-C4A-NA	2.11	127.45	124.40
6	X	1620	LUT	C12-C13-C14	-2.10	115.71	119.01
4	Y	607	CHL	O2A-CGA-O1A	-2.10	118.38	123.63
6	Z	1621	LUT	C35-C15-C14	-2.10	119.23	123.52
5	Y	604	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
5	X	604	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
4	X	607	CHL	CAC-C3C-C4C	2.09	129.40	124.03
4	Y	607	CHL	CAC-C3C-C4C	2.09	129.40	124.03
4	Z	605	CHL	C1B-CHB-C4A	-2.09	119.98	121.32
5	Z	613	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
6	Z	1621	LUT	C36-C21-C26	2.08	112.70	109.55
4	Z	609	CHL	CAC-C3C-C4C	2.08	129.38	124.03
4	X	607	CHL	O2A-CGA-O1A	-2.08	118.42	123.63
6	Z	1621	LUT	C15-C14-C13	-2.08	124.36	127.28
6	Y	1620	LUT	C15-C35-C34	-2.08	119.27	123.52
5	Y	614	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
4	X	609	CHL	C1C-C2C-CMC	2.07	130.54	126.80
5	Z	603	CLA	C3B-C4B-NB	-2.07	108.68	110.53
4	Z	605	CHL	CBC-CAC-C3C	-2.07	109.91	112.87
5	Z	602	CLA	C1-C2-C3	-2.07	122.81	126.20
4	X	607	CHL	C6-C5-C3	-2.06	108.44	113.47
8	X	1623	NEX	O24-C25-C26	-2.06	57.29	58.93
6	X	1620	LUT	C15-C35-C34	-2.06	119.30	123.52
6	Z	1621	LUT	C38-C25-C24	-2.06	118.48	123.36
4	Y	607	CHL	C6-C5-C3	-2.06	108.45	113.47
7	Y	1622	XAT	O4-C5-C6	-2.06	57.30	58.93
8	Y	1623	NEX	C17-C1-C6	-2.06	108.63	110.47
7	X	1622	XAT	O4-C5-C6	-2.06	57.30	58.93
4	Y	608	CHL	O2D-CGD-O1D	-2.06	119.84	123.85
6	Y	1620	LUT	C35-C34-C33	-2.06	124.39	127.28
4	Y	608	CHL	CAC-C3C-C4C	2.06	129.32	124.03
5	X	613	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
4	Z	606	CHL	CED-O2D-CGD	2.05	120.56	115.92
5	Y	613	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
6	Y	1621	LUT	C38-C25-C24	-2.05	118.52	123.36
4	X	608	CHL	C4C-CHD-C1D	2.04	123.38	116.07
6	X	1621	LUT	C27-C28-C29	-2.04	121.94	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Y	609	CHL	C1C-C2C-CMC	2.04	130.47	126.80
6	Z	1621	LUT	C15-C35-C34	-2.04	119.35	123.52
4	Y	605	CHL	C1B-CHB-C4A	-2.04	120.01	121.32
4	Z	601	CHL	C1C-C2C-CMC	2.03	130.47	126.80
8	X	1623	NEX	C17-C1-C6	-2.03	108.65	110.47
6	Y	1621	LUT	C27-C28-C29	-2.03	121.96	126.32
5	X	611	CLA	O2A-CGA-O1A	-2.03	118.11	123.33
4	Z	605	CHL	CED-O2D-CGD	2.03	120.52	115.92
8	Y	1623	NEX	O24-C25-C26	-2.03	57.32	58.93
6	X	1621	LUT	C38-C25-C24	-2.03	118.57	123.36
4	Y	607	CHL	C4D-CHA-CBD	-2.02	106.93	108.97
7	Z	1622	XAT	O24-C25-C26	-2.01	57.33	58.93
4	Z	601	CHL	C4-C3-C5	2.01	118.72	115.23
8	X	1623	NEX	C30-C31-C32	-2.01	117.37	123.20
4	Z	609	CHL	C4C-CHD-C1D	2.01	123.26	116.07
8	Z	1623	NEX	C38-C25-C24	2.01	116.50	114.24
8	Y	1623	NEX	C30-C31-C32	-2.01	117.39	123.20
6	Y	1620	LUT	C11-C12-C13	-2.01	120.86	126.36
6	X	1620	LUT	C11-C12-C13	-2.00	120.87	126.36

All (75) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	X	601	CHL	NC
4	X	601	CHL	NA
4	X	601	CHL	ND
4	X	605	CHL	NC
4	X	605	CHL	NA
4	X	605	CHL	ND
4	X	607	CHL	NC
4	X	607	CHL	NA
4	X	607	CHL	ND
4	X	608	CHL	NC
4	X	608	CHL	NA
4	X	608	CHL	ND
4	X	609	CHL	NC
4	X	609	CHL	NA
4	X	609	CHL	ND
4	Y	601	CHL	NC
4	Y	601	CHL	NA
4	Y	601	CHL	ND
4	Y	605	CHL	NC

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Mol	Chain	Res	Type	Atom
4	Y	605	CHL	NA
4	Y	605	CHL	ND
4	Y	606	CHL	NC
4	Y	606	CHL	NA
4	Y	606	CHL	ND
4	Y	607	CHL	NC
4	Y	607	CHL	NA
4	Y	607	CHL	ND
4	Y	608	CHL	NC
4	Y	608	CHL	NA
4	Y	608	CHL	ND
4	Y	609	CHL	NC
4	Y	609	CHL	NA
4	Y	609	CHL	ND
4	Z	601	CHL	NC
4	Z	601	CHL	NA
4	Z	601	CHL	ND
4	Z	605	CHL	NC
4	Z	605	CHL	NA
4	Z	605	CHL	ND
4	Z	606	CHL	NC
4	Z	606	CHL	NA
4	Z	606	CHL	ND
4	Z	607	CHL	NC
4	Z	607	CHL	NA
4	Z	607	CHL	ND
4	Z	608	CHL	NC
4	Z	608	CHL	NA
4	Z	608	CHL	ND
4	Z	609	CHL	NC
4	Z	609	CHL	NA
4	Z	609	CHL	ND
5	X	602	CLA	ND
5	X	603	CLA	ND
5	X	604	CLA	ND
5	X	610	CLA	ND
5	X	611	CLA	ND
5	X	612	CLA	ND
5	X	613	CLA	ND
5	X	614	CLA	ND
5	Y	602	CLA	ND
5	Y	603	CLA	ND

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Mol	Chain	Res	Type	Atom
5	Y	604	CLA	ND
5	Y	610	CLA	ND
5	Y	611	CLA	ND
5	Y	612	CLA	ND
5	Y	613	CLA	ND
5	Y	614	CLA	ND
5	Z	602	CLA	ND
5	Z	603	CLA	ND
5	Z	604	CLA	ND
5	Z	610	CLA	ND
5	Z	611	CLA	ND
5	Z	612	CLA	ND
5	Z	613	CLA	ND
5	Z	614	CLA	ND

All (475) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	607	CHL	C1C-C2C-CMC-OMC
4	X	607	CHL	C3C-C2C-CMC-OMC
4	X	607	CHL	C6-C7-C8-C9
4	X	608	CHL	C1C-C2C-CMC-OMC
4	X	608	CHL	C3C-C2C-CMC-OMC
4	X	609	CHL	C3A-C2A-CAA-CBA
4	Y	607	CHL	C1C-C2C-CMC-OMC
4	Y	607	CHL	C3C-C2C-CMC-OMC
4	Y	607	CHL	C6-C7-C8-C9
4	Y	609	CHL	C3A-C2A-CAA-CBA
4	Z	607	CHL	C1C-C2C-CMC-OMC
4	Z	607	CHL	C3C-C2C-CMC-OMC
4	Z	609	CHL	C1C-C2C-CMC-OMC
4	Z	609	CHL	C3C-C2C-CMC-OMC
5	X	603	CLA	CHA-CBD-CGD-O2D
5	X	610	CLA	CBD-CGD-O2D-CED
5	X	611	CLA	C1A-C2A-CAA-CBA
5	X	611	CLA	C3A-C2A-CAA-CBA
5	X	611	CLA	C2B-C3B-CAB-CBB
5	X	611	CLA	C4B-C3B-CAB-CBB
5	X	612	CLA	CHA-CBD-CGD-O1D
5	X	612	CLA	CHA-CBD-CGD-O2D
5	X	614	CLA	CBD-CGD-O2D-CED
5	Y	603	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
5	Y	610	CLA	CBD-CGD-O2D-CED
5	Y	611	CLA	C1A-C2A-CAA-CBA
5	Y	611	CLA	C3A-C2A-CAA-CBA
5	Y	611	CLA	C2B-C3B-CAB-CBB
5	Y	611	CLA	C4B-C3B-CAB-CBB
5	Y	612	CLA	CHA-CBD-CGD-O2D
5	Y	614	CLA	CBD-CGD-O2D-CED
7	X	1622	XAT	C11-C12-C13-C14
7	Y	1622	XAT	C11-C12-C13-C14
7	Z	1622	XAT	C11-C12-C13-C14
7	Z	1622	XAT	C31-C32-C33-C34
8	Z	1623	NEX	O24-C26-C27-C28
9	X	2630	LHG	C3-O3-P-O4
9	X	2630	LHG	C3-O3-P-O6
9	X	2630	LHG	C4-O6-P-O3
9	X	2630	LHG	C4-O6-P-O5
9	Y	2630	LHG	C3-O3-P-O4
9	Y	2630	LHG	C3-O3-P-O6
9	Y	2630	LHG	C4-O6-P-O3
9	Y	2630	LHG	C4-O6-P-O5
9	Z	2630	LHG	C3-O3-P-O4
9	Z	2630	LHG	C3-O3-P-O6
9	Z	2630	LHG	C4-O6-P-O3
9	Z	2630	LHG	C4-O6-P-O4
9	Z	2630	LHG	C4-O6-P-O5
4	X	607	CHL	O1D-CGD-O2D-CED
4	Y	607	CHL	O1D-CGD-O2D-CED
4	X	607	CHL	CBD-CGD-O2D-CED
4	X	608	CHL	CBD-CGD-O2D-CED
4	Y	607	CHL	CBD-CGD-O2D-CED
4	Y	608	CHL	CBD-CGD-O2D-CED
4	Z	608	CHL	CBD-CGD-O2D-CED
5	X	602	CLA	CBD-CGD-O2D-CED
5	Y	602	CLA	CBD-CGD-O2D-CED
5	Z	610	CLA	CBD-CGD-O2D-CED
4	Z	608	CHL	O1D-CGD-O2D-CED
5	X	614	CLA	O1D-CGD-O2D-CED
5	Y	614	CLA	O1D-CGD-O2D-CED
5	X	610	CLA	O1D-CGD-O2D-CED
5	Y	610	CLA	O1D-CGD-O2D-CED
4	Z	601	CHL	C3-C5-C6-C7
5	Z	603	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
5	Z	613	CLA	C3-C5-C6-C7
4	Z	606	CHL	CBD-CGD-O2D-CED
5	X	611	CLA	CBD-CGD-O2D-CED
5	Y	611	CLA	CBD-CGD-O2D-CED
5	Z	614	CLA	CBD-CGD-O2D-CED
4	X	601	CHL	C4-C3-C5-C6
4	Y	601	CHL	C4-C3-C5-C6
4	X	601	CHL	C2-C3-C5-C6
4	Y	601	CHL	C2-C3-C5-C6
4	X	608	CHL	O1D-CGD-O2D-CED
4	Y	608	CHL	O1D-CGD-O2D-CED
5	X	613	CLA	C3-C5-C6-C7
5	Y	613	CLA	C3-C5-C6-C7
5	Z	603	CLA	CBD-CGD-O2D-CED
5	X	602	CLA	O1D-CGD-O2D-CED
5	Z	610	CLA	O1D-CGD-O2D-CED
5	Y	602	CLA	O1D-CGD-O2D-CED
5	Y	614	CLA	CBA-CGA-O2A-C1
4	X	601	CHL	CBA-CGA-O2A-C1
4	Y	601	CHL	CBA-CGA-O2A-C1
5	Y	614	CLA	O1A-CGA-O2A-C1
5	X	604	CLA	CBA-CGA-O2A-C1
5	Y	604	CLA	CBA-CGA-O2A-C1
4	X	609	CHL	C11-C12-C13-C14
4	Y	609	CHL	C11-C12-C13-C14
4	Z	607	CHL	C6-C7-C8-C9
4	Z	609	CHL	C14-C13-C15-C16
5	Z	614	CLA	O1D-CGD-O2D-CED
4	X	601	CHL	CBD-CGD-O2D-CED
4	Y	601	CHL	CBD-CGD-O2D-CED
4	Z	609	CHL	CBD-CGD-O2D-CED
7	X	1622	XAT	C11-C12-C13-C20
7	Y	1622	XAT	C11-C12-C13-C20
7	Z	1622	XAT	C11-C12-C13-C20
7	Z	1622	XAT	C31-C32-C33-C40
4	Z	608	CHL	C2A-CAA-CBA-CGA
5	X	611	CLA	O1D-CGD-O2D-CED
5	Y	611	CLA	O1D-CGD-O2D-CED
4	X	601	CHL	C13-C15-C16-C17
4	Y	601	CHL	C13-C15-C16-C17
5	X	604	CLA	O1A-CGA-O2A-C1
5	Y	604	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
4	X	601	CHL	C6-C7-C8-C10
4	X	608	CHL	C11-C10-C8-C7
4	Y	601	CHL	C6-C7-C8-C10
5	X	602	CLA	C8-C10-C11-C12
5	Y	602	CLA	C8-C10-C11-C12
5	Z	604	CLA	C5-C6-C7-C8
5	Z	611	CLA	C8-C10-C11-C12
4	X	607	CHL	C2A-CAA-CBA-CGA
4	Y	607	CHL	C2A-CAA-CBA-CGA
4	Y	608	CHL	C2A-CAA-CBA-CGA
4	X	608	CHL	C15-C16-C17-C18
4	Z	601	CHL	C5-C6-C7-C8
4	Z	609	CHL	C15-C16-C17-C18
4	X	601	CHL	O1A-CGA-O2A-C1
4	Y	601	CHL	O1A-CGA-O2A-C1
4	Z	606	CHL	O1D-CGD-O2D-CED
4	X	601	CHL	C5-C6-C7-C8
4	X	608	CHL	C13-C15-C16-C17
4	X	609	CHL	C13-C15-C16-C17
4	Y	601	CHL	C5-C6-C7-C8
4	Y	609	CHL	C13-C15-C16-C17
4	Z	601	CHL	C13-C15-C16-C17
4	Z	607	CHL	C8-C10-C11-C12
5	X	602	CLA	C13-C15-C16-C17
5	X	610	CLA	C8-C10-C11-C12
5	Y	610	CLA	C8-C10-C11-C12
4	Z	609	CHL	C13-C15-C16-C17
5	Z	603	CLA	O1D-CGD-O2D-CED
4	X	601	CHL	C8-C10-C11-C12
4	Y	601	CHL	C8-C10-C11-C12
4	X	608	CHL	C5-C6-C7-C8
5	Z	610	CLA	C5-C6-C7-C8
4	X	608	CHL	C2A-CAA-CBA-CGA
4	Z	607	CHL	C2A-CAA-CBA-CGA
5	Z	610	CLA	C13-C15-C16-C17
5	Z	604	CLA	CBD-CGD-O2D-CED
4	X	608	CHL	C8-C10-C11-C12
5	Z	613	CLA	C15-C16-C17-C18
4	X	607	CHL	C8-C10-C11-C12
4	Y	607	CHL	C8-C10-C11-C12
5	X	602	CLA	C10-C11-C12-C13
4	X	609	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
4	Y	609	CHL	C11-C10-C8-C9
4	X	607	CHL	C16-C17-C18-C20
4	Y	607	CHL	C16-C17-C18-C20
7	X	1622	XAT	C31-C32-C33-C40
7	Y	1622	XAT	C31-C32-C33-C40
4	Z	605	CHL	C2A-CAA-CBA-CGA
6	Z	1621	LUT	C7-C8-C9-C10
4	X	609	CHL	C16-C17-C18-C19
4	Y	609	CHL	C16-C17-C18-C19
4	Y	608	CHL	O2A-C1-C2-C3
4	X	607	CHL	C16-C17-C18-C19
4	X	608	CHL	C16-C17-C18-C19
4	Y	607	CHL	C16-C17-C18-C19
4	Z	609	CHL	C16-C17-C18-C19
5	Z	610	CLA	C16-C17-C18-C20
5	Z	613	CLA	C16-C17-C18-C20
5	X	603	CLA	C4B-C3B-CAB-CBB
5	X	612	CLA	C4B-C3B-CAB-CBB
5	X	614	CLA	C4B-C3B-CAB-CBB
5	Y	603	CLA	C4B-C3B-CAB-CBB
5	Y	612	CLA	C4B-C3B-CAB-CBB
5	Y	614	CLA	C4B-C3B-CAB-CBB
4	X	608	CHL	C16-C17-C18-C20
4	X	609	CHL	C16-C17-C18-C20
4	Y	609	CHL	C16-C17-C18-C20
4	X	601	CHL	C10-C11-C12-C13
4	X	607	CHL	C13-C15-C16-C17
4	Y	601	CHL	C10-C11-C12-C13
4	Y	607	CHL	C13-C15-C16-C17
5	Z	612	CLA	C10-C11-C12-C13
5	Z	603	CLA	C3A-C2A-CAA-CBA
5	X	610	CLA	C5-C6-C7-C8
5	Y	610	CLA	C5-C6-C7-C8
4	Z	607	CHL	C16-C17-C18-C19
4	Z	607	CHL	C16-C17-C18-C20
5	Y	614	CLA	O2A-C1-C2-C3
9	Z	2630	LHG	C27-C28-C29-C30
5	Z	610	CLA	C16-C17-C18-C19
5	Z	613	CLA	C16-C17-C18-C19
5	X	603	CLA	C2B-C3B-CAB-CBB
5	X	612	CLA	C2B-C3B-CAB-CBB
5	Y	603	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
5	Y	612	CLA	C2B-C3B-CAB-CBB
6	X	1620	LUT	C1-C6-C7-C8
6	Y	1620	LUT	C1-C6-C7-C8
4	X	609	CHL	CBD-CGD-O2D-CED
4	Y	609	CHL	CBD-CGD-O2D-CED
5	Z	613	CLA	C2A-CAA-CBA-CGA
9	Z	2630	LHG	C28-C29-C30-C31
9	X	2630	LHG	C26-C27-C28-C29
9	Y	2630	LHG	C26-C27-C28-C29
5	X	613	CLA	CBA-CGA-O2A-C1
5	Y	613	CLA	CBA-CGA-O2A-C1
4	Z	609	CHL	C6-C7-C8-C9
4	X	601	CHL	C16-C17-C18-C19
4	Y	601	CHL	C16-C17-C18-C19
4	Z	601	CHL	C15-C16-C17-C18
4	X	607	CHL	C15-C16-C17-C18
4	Y	607	CHL	C15-C16-C17-C18
5	Z	613	CLA	C10-C11-C12-C13
9	X	2630	LHG	C16-C17-C18-C19
9	Y	2630	LHG	C16-C17-C18-C19
5	Z	611	CLA	C2-C3-C5-C6
5	X	613	CLA	C2A-CAA-CBA-CGA
5	Y	613	CLA	C2A-CAA-CBA-CGA
4	Z	609	CHL	C8-C10-C11-C12
4	X	601	CHL	O1D-CGD-O2D-CED
4	Y	601	CHL	O1D-CGD-O2D-CED
5	Z	603	CLA	C1A-C2A-CAA-CBA
4	Z	601	CHL	C8-C10-C11-C12
5	X	613	CLA	O1A-CGA-O2A-C1
5	Y	613	CLA	O1A-CGA-O2A-C1
4	Z	601	CHL	C6-C7-C8-C10
4	Z	601	CHL	C11-C10-C8-C7
4	Z	607	CHL	C11-C12-C13-C15
4	Z	609	CHL	C12-C13-C15-C16
5	X	602	CLA	C6-C7-C8-C10
5	X	613	CLA	C11-C10-C8-C7
5	X	613	CLA	C12-C13-C15-C16
5	Y	602	CLA	C6-C7-C8-C10
5	Y	613	CLA	C11-C10-C8-C7
5	Y	613	CLA	C12-C13-C15-C16
4	X	609	CHL	C15-C16-C17-C18
4	Y	609	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
5	Z	604	CLA	C4-C3-C5-C6
5	Z	604	CLA	C2-C3-C5-C6
5	Z	613	CLA	C2-C3-C5-C6
4	Z	609	CHL	O1D-CGD-O2D-CED
5	X	602	CLA	C6-C7-C8-C9
5	Y	602	CLA	C6-C7-C8-C9
9	X	2630	LHG	C17-C18-C19-C20
9	Y	2630	LHG	C17-C18-C19-C20
4	X	608	CHL	CBA-CGA-O2A-C1
5	Z	613	CLA	CBA-CGA-O2A-C1
5	Z	612	CLA	CBA-CGA-O2A-C1
4	X	601	CHL	C16-C17-C18-C20
4	Y	601	CHL	C16-C17-C18-C20
4	Z	607	CHL	CHA-CBD-CGD-O1D
4	Z	609	CHL	CHA-CBD-CGD-O1D
5	Z	611	CLA	C4-C3-C5-C6
5	Z	613	CLA	O1A-CGA-O2A-C1
4	Z	607	CHL	C10-C11-C12-C13
4	Y	608	CHL	CBA-CGA-O2A-C1
5	Y	602	CLA	C10-C11-C12-C13
5	X	603	CLA	CAA-CBA-CGA-O2A
5	Y	603	CLA	CAA-CBA-CGA-O2A
5	Z	604	CLA	O1D-CGD-O2D-CED
4	Z	601	CHL	C11-C10-C8-C9
4	Z	607	CHL	C11-C12-C13-C14
5	X	613	CLA	C11-C10-C8-C9
5	Y	613	CLA	C11-C10-C8-C9
5	Z	602	CLA	C6-C7-C8-C9
5	Z	613	CLA	C14-C13-C15-C16
5	Z	612	CLA	O1A-CGA-O2A-C1
5	X	610	CLA	C4B-C3B-CAB-CBB
5	X	613	CLA	C4B-C3B-CAB-CBB
5	Y	610	CLA	C4B-C3B-CAB-CBB
5	Y	613	CLA	C4B-C3B-CAB-CBB
5	Z	603	CLA	C16-C17-C18-C20
9	Z	2630	LHG	C19-C20-C21-C22
4	X	607	CHL	C12-C13-C15-C16
4	Y	607	CHL	C12-C13-C15-C16
5	Z	602	CLA	C6-C7-C8-C10
5	Z	603	CLA	C11-C10-C8-C7
5	Z	603	CLA	C11-C12-C13-C15
5	Z	613	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
5	Z	603	CLA	C15-C16-C17-C18
4	X	608	CHL	O1A-CGA-O2A-C1
5	Z	613	CLA	C4-C3-C5-C6
4	Z	609	CHL	C5-C6-C7-C8
7	X	1622	XAT	C31-C32-C33-C34
7	Y	1622	XAT	C31-C32-C33-C34
4	X	608	CHL	C4-C3-C5-C6
4	X	608	CHL	C2-C3-C5-C6
5	Z	614	CLA	C6-C7-C8-C9
4	X	607	CHL	C5-C6-C7-C8
4	Y	607	CHL	C5-C6-C7-C8
4	X	608	CHL	C11-C10-C8-C9
4	X	608	CHL	C11-C12-C13-C14
5	X	613	CLA	C14-C13-C15-C16
5	Y	613	CLA	C14-C13-C15-C16
4	Z	609	CHL	C16-C17-C18-C20
5	X	614	CLA	C1A-C2A-CAA-CBA
4	Z	609	CHL	CBA-CGA-O2A-C1
5	X	613	CLA	C5-C6-C7-C8
5	Y	613	CLA	C5-C6-C7-C8
4	Z	601	CHL	C11-C12-C13-C15
6	X	1621	LUT	C7-C8-C9-C10
6	Y	1621	LUT	C7-C8-C9-C10
5	X	610	CLA	CBA-CGA-O2A-C1
5	Y	610	CLA	CBA-CGA-O2A-C1
4	Y	608	CHL	O1A-CGA-O2A-C1
5	Y	603	CLA	C4-C3-C5-C6
5	X	610	CLA	C13-C15-C16-C17
5	Y	610	CLA	C13-C15-C16-C17
4	X	608	CHL	C10-C11-C12-C13
4	Y	609	CHL	O1D-CGD-O2D-CED
5	X	604	CLA	O2A-C1-C2-C3
4	X	609	CHL	O1D-CGD-O2D-CED
4	X	607	CHL	C4-C3-C5-C6
4	Y	607	CHL	C4-C3-C5-C6
5	X	603	CLA	C4-C3-C5-C6
4	Z	601	CHL	C11-C12-C13-C14
4	Z	601	CHL	C16-C17-C18-C20
5	Z	603	CLA	C16-C17-C18-C19
9	Z	2630	LHG	C11-C10-C9-C8
5	X	613	CLA	CBD-CGD-O2D-CED
4	Z	609	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
5	Z	614	CLA	C4B-C3B-CAB-CBB
9	Y	2630	LHG	C29-C30-C31-C32
9	X	2630	LHG	C29-C30-C31-C32
4	X	607	CHL	C2-C3-C5-C6
4	Y	607	CHL	C2-C3-C5-C6
5	Y	614	CLA	C2A-CAA-CBA-CGA
5	Y	613	CLA	CBD-CGD-O2D-CED
4	X	601	CHL	C12-C13-C15-C16
4	X	608	CHL	C12-C13-C15-C16
4	Y	601	CHL	C12-C13-C15-C16
4	Z	609	CHL	C11-C12-C13-C15
5	X	602	CLA	C11-C12-C13-C15
5	Z	610	CLA	C11-C12-C13-C15
4	Z	609	CHL	O1A-CGA-O2A-C1
4	Z	607	CHL	C3A-C2A-CAA-CBA
5	Y	603	CLA	C2-C3-C5-C6
4	X	607	CHL	C14-C13-C15-C16
4	Y	607	CHL	C14-C13-C15-C16
5	X	610	CLA	O1A-CGA-O2A-C1
4	X	607	CHL	CAA-CBA-CGA-O2A
4	Y	607	CHL	CAA-CBA-CGA-O2A
5	X	604	CLA	C1-C2-C3-C4
5	Y	610	CLA	O1A-CGA-O2A-C1
4	Z	608	CHL	O2A-C1-C2-C3
4	X	609	CHL	C4-C3-C5-C6
4	Y	609	CHL	C4-C3-C5-C6
5	X	603	CLA	C2-C3-C5-C6
9	Y	2630	LHG	C27-C28-C29-C30
9	X	2630	LHG	C27-C28-C29-C30
4	X	609	CHL	CHA-CBD-CGD-O1D
4	X	609	CHL	CHA-CBD-CGD-O2D
4	Y	609	CHL	CHA-CBD-CGD-O1D
4	Y	609	CHL	CHA-CBD-CGD-O2D
4	Z	607	CHL	CHA-CBD-CGD-O2D
4	Z	609	CHL	CHA-CBD-CGD-O2D
5	X	603	CLA	CHA-CBD-CGD-O1D
5	Y	603	CLA	CHA-CBD-CGD-O1D
5	Y	612	CLA	CHA-CBD-CGD-O1D
9	X	2630	LHG	C4-O6-P-O4
9	Y	2630	LHG	C4-O6-P-O4
5	Z	603	CLA	C4-C3-C5-C6
5	X	610	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
5	X	614	CLA	C2B-C3B-CAB-CBB
5	Y	610	CLA	C2B-C3B-CAB-CBB
5	Y	614	CLA	C2B-C3B-CAB-CBB
4	X	601	CHL	C15-C16-C17-C18
4	Y	601	CHL	C15-C16-C17-C18
6	Z	1621	LUT	C7-C8-C9-C19
5	Y	613	CLA	O1D-CGD-O2D-CED
5	Z	603	CLA	C11-C10-C8-C9
5	Z	603	CLA	C11-C12-C13-C14
5	Z	613	CLA	C6-C7-C8-C9
4	X	609	CHL	C11-C12-C13-C15
4	Y	609	CHL	C11-C12-C13-C15
4	Z	601	CHL	C12-C13-C15-C16
5	X	613	CLA	O1D-CGD-O2D-CED
9	Z	2630	LHG	C26-C27-C28-C29
9	Z	2630	LHG	C34-C35-C36-C37
4	X	605	CHL	C2A-CAA-CBA-CGA
5	Z	603	CLA	C5-C6-C7-C8
5	X	603	CLA	CAA-CBA-CGA-O1A
5	Y	603	CLA	CAA-CBA-CGA-O1A
4	X	601	CHL	C14-C13-C15-C16
4	Y	601	CHL	C14-C13-C15-C16
5	X	603	CLA	CBA-CGA-O2A-C1
5	Y	603	CLA	CBA-CGA-O2A-C1
9	Z	2630	LHG	C24-C23-O8-C6
4	X	609	CHL	C2-C3-C5-C6
4	Y	609	CHL	C2-C3-C5-C6
5	Z	603	CLA	C2-C3-C5-C6
9	Z	2630	LHG	O6-C4-C5-O7
5	Y	603	CLA	O1A-CGA-O2A-C1
5	X	603	CLA	O1A-CGA-O2A-C1
4	X	601	CHL	C3A-C2A-CAA-CBA
4	Y	601	CHL	C3A-C2A-CAA-CBA
8	X	1623	NEX	C39-C29-C30-C31
8	Y	1623	NEX	C39-C29-C30-C31
8	Z	1623	NEX	C39-C29-C30-C31
5	Z	603	CLA	C8-C10-C11-C12
5	Y	612	CLA	CAA-CBA-CGA-O1A
5	X	611	CLA	CAA-CBA-CGA-O2A
5	Z	613	CLA	C11-C10-C8-C9
5	X	611	CLA	CAA-CBA-CGA-O1A
4	X	609	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
4	Y	609	CHL	C1A-C2A-CAA-CBA
8	X	1623	NEX	C28-C29-C30-C31
8	Y	1623	NEX	C28-C29-C30-C31
8	Z	1623	NEX	C28-C29-C30-C31
5	X	613	CLA	C2B-C3B-CAB-CBB
5	Y	613	CLA	C2B-C3B-CAB-CBB
5	Z	614	CLA	C2B-C3B-CAB-CBB
6	X	1620	LUT	C5-C6-C7-C8
6	Y	1620	LUT	C5-C6-C7-C8
5	Y	612	CLA	CAA-CBA-CGA-O2A
5	Z	610	CLA	C12-C13-C15-C16
5	X	603	CLA	C3-C5-C6-C7
5	Z	602	CLA	C8-C10-C11-C12
4	Z	607	CHL	C4-C3-C5-C6
4	Z	609	CHL	C4-C3-C5-C6
4	Z	607	CHL	C2-C3-C5-C6
5	Z	611	CLA	C10-C11-C12-C13
5	Y	603	CLA	C3-C5-C6-C7
5	Y	604	CLA	C4B-C3B-CAB-CBB
9	Z	2630	LHG	O10-C23-O8-C6
5	X	613	CLA	C8-C10-C11-C12
5	Y	613	CLA	C8-C10-C11-C12
9	Z	2630	LHG	O6-C4-C5-C6
4	X	601	CHL	C6-C7-C8-C9
4	Y	601	CHL	C6-C7-C8-C9
5	Z	612	CLA	C11-C12-C13-C14
4	Z	608	CHL	C2-C1-O2A-CGA
4	Z	601	CHL	C3A-C2A-CAA-CBA
4	Y	606	CHL	CAA-CBA-CGA-O2A
8	X	1623	NEX	O24-C26-C27-C28
8	Y	1623	NEX	O24-C26-C27-C28
4	X	607	CHL	CBA-CGA-O2A-C1
4	Y	607	CHL	CBA-CGA-O2A-C1
9	Z	2630	LHG	O7-C5-C6-O8
4	Z	601	CHL	C14-C13-C15-C16
5	X	602	CLA	C11-C12-C13-C14
5	Z	611	CLA	C11-C12-C13-C14
4	Y	606	CHL	CAA-CBA-CGA-O1A
5	Z	613	CLA	C11-C10-C8-C7
5	X	604	CLA	C2B-C3B-CAB-CBB
5	Y	604	CLA	C2B-C3B-CAB-CBB
5	Z	612	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
5	Z	614	CLA	CBA-CGA-O2A-C1
5	Z	614	CLA	O1A-CGA-O2A-C1
4	Z	601	CHL	C16-C17-C18-C19
5	Z	604	CLA	C2A-CAA-CBA-CGA
5	Z	610	CLA	C11-C12-C13-C14
5	X	604	CLA	C4B-C3B-CAB-CBB
5	Z	603	CLA	C4B-C3B-CAB-CBB
5	Z	613	CLA	C4B-C3B-CAB-CBB
9	Y	2630	LHG	O7-C5-C6-O8
5	Z	603	CLA	CAA-CBA-CGA-O2A
9	Z	2630	LHG	C24-C25-C26-C27
4	Z	606	CHL	CAA-CBA-CGA-O2A
4	X	607	CHL	C6-C7-C8-C10
4	Y	607	CHL	C6-C7-C8-C10
5	Z	612	CLA	C11-C12-C13-C15
4	X	607	CHL	CAA-CBA-CGA-O1A
4	Y	607	CHL	CAA-CBA-CGA-O1A
4	Z	607	CHL	C5-C6-C7-C8
5	Z	603	CLA	C2A-CAA-CBA-CGA
4	Z	601	CHL	C6-C7-C8-C9
4	Z	609	CHL	C11-C12-C13-C14
5	Z	610	CLA	C14-C13-C15-C16
4	Z	609	CHL	C2C-C3C-CAC-CBC
4	Y	607	CHL	O1A-CGA-O2A-C1
5	Z	603	CLA	CAA-CBA-CGA-O1A
4	Z	606	CHL	CAA-CBA-CGA-O1A
4	X	607	CHL	O1A-CGA-O2A-C1
4	Z	609	CHL	C10-C11-C12-C13
4	X	609	CHL	C2-C1-O2A-CGA
4	Y	609	CHL	C2-C1-O2A-CGA
4	Z	607	CHL	C1A-C2A-CAA-CBA

There are no ring outliers.

36 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Z	606	CHL	4	0
4	Z	607	CHL	3	0
8	Y	1623	NEX	2	0
7	X	1622	XAT	3	0
9	Y	2630	LHG	1	0
4	X	605	CHL	1	0

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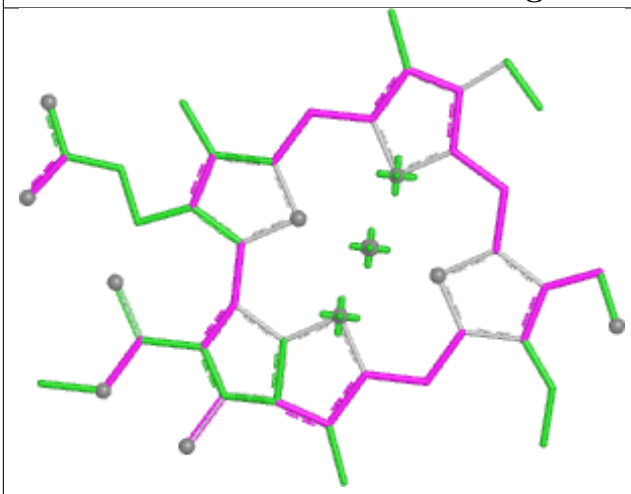
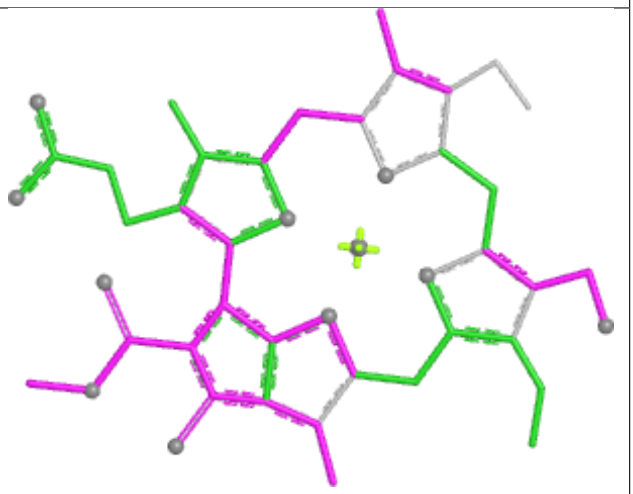
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	607	CHL	2	0
9	Z	2630	LHG	3	0
7	Y	1622	XAT	3	0
7	Z	1622	XAT	4	0
4	Y	609	CHL	4	0
8	X	1623	NEX	2	0
4	Z	608	CHL	1	0
4	Y	606	CHL	2	0
9	X	2630	LHG	1	0
5	Y	613	CLA	2	0
8	Z	1623	NEX	2	0
5	X	603	CLA	1	0
4	Y	601	CHL	6	0
4	Y	605	CHL	1	0
4	X	607	CHL	2	0
6	Y	1620	LUT	3	0
6	Z	1621	LUT	2	0
4	Z	601	CHL	3	0
5	X	611	CLA	3	0
6	Z	1620	LUT	3	0
5	X	613	CLA	2	0
4	Z	609	CHL	5	0
4	X	601	CHL	2	0
4	X	609	CHL	5	0
4	X	608	CHL	3	0
5	Y	611	CLA	3	0
6	X	1620	LUT	3	0
4	Y	608	CHL	1	0
5	Z	613	CLA	2	0
4	Z	605	CHL	1	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.

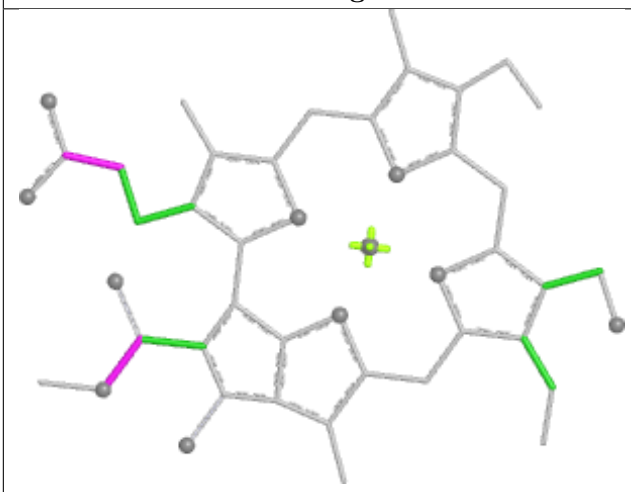
Ligand CHL Z 606



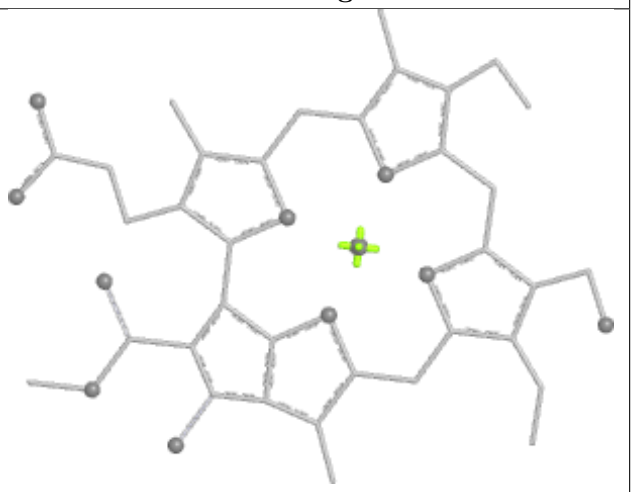
Bond lengths



Bond angles

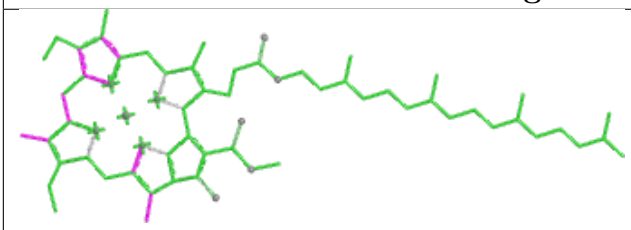


Torsions

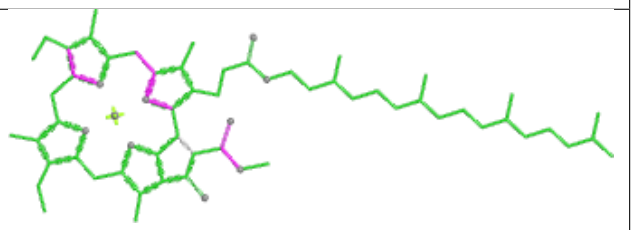


Rings

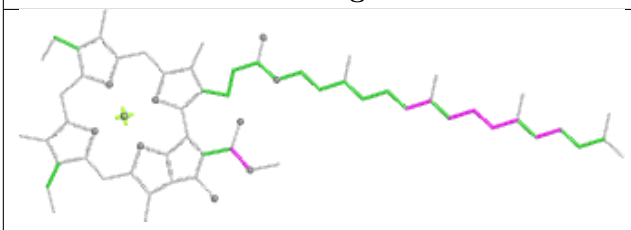
Ligand CLA X 602



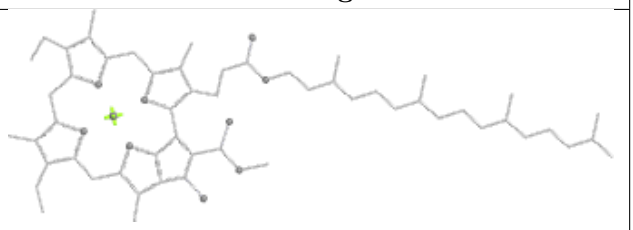
Bond lengths



Bond angles

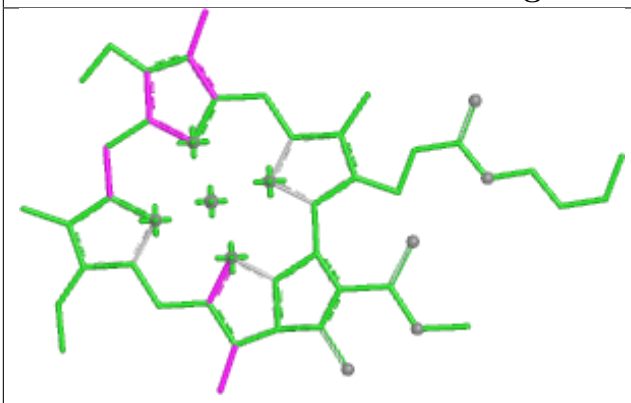


Torsions

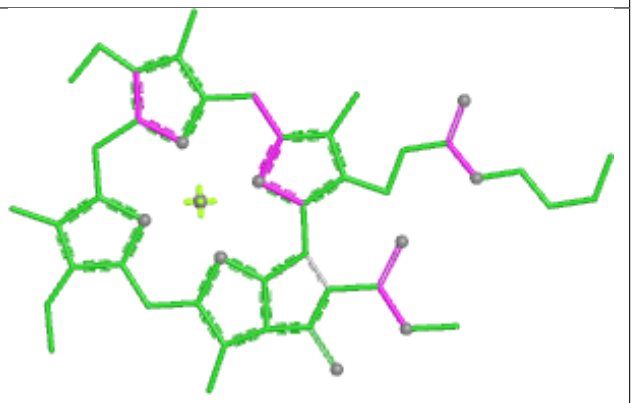


Rings

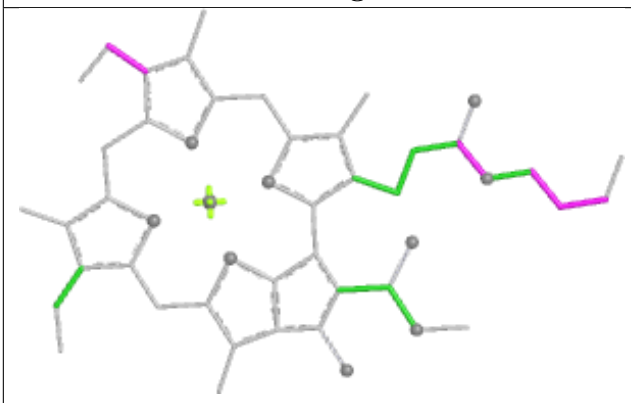
Ligand CLA X 604



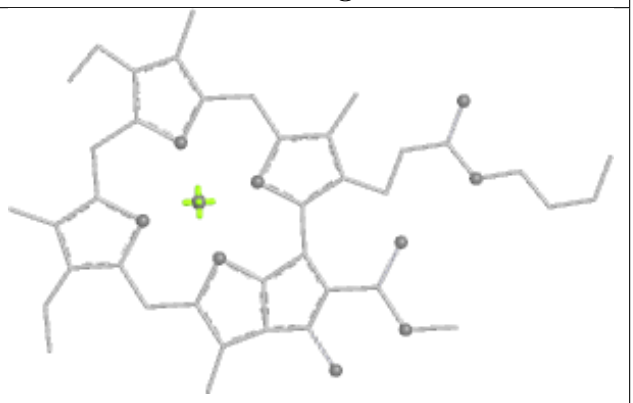
Bond lengths



Bond angles

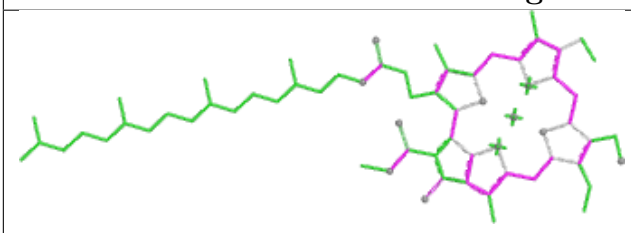


Torsions

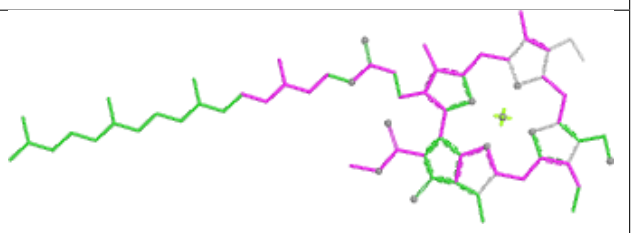


Rings

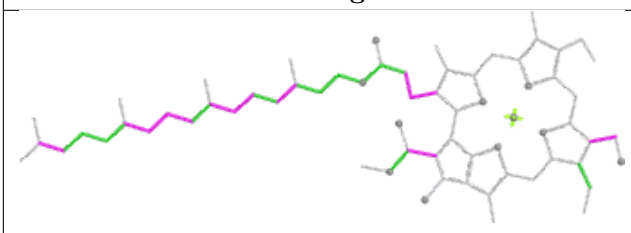
Ligand CHL Z 607



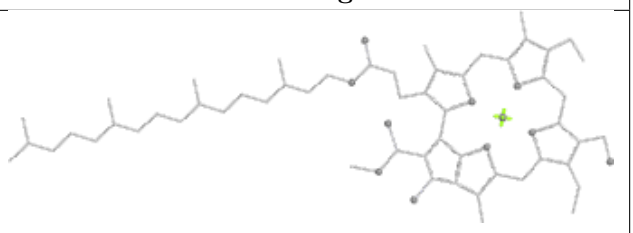
Bond lengths



Bond angles

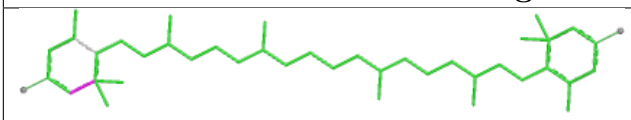


Torsions

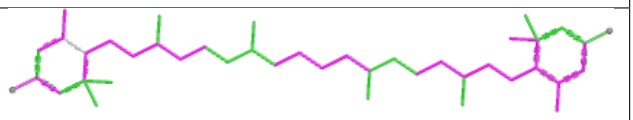


Rings

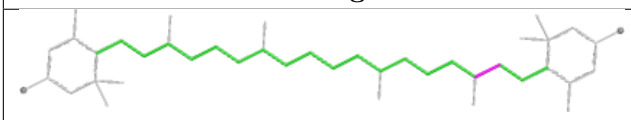
Ligand LUT X 1621



Bond lengths



Bond angles



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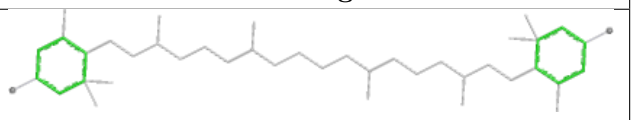
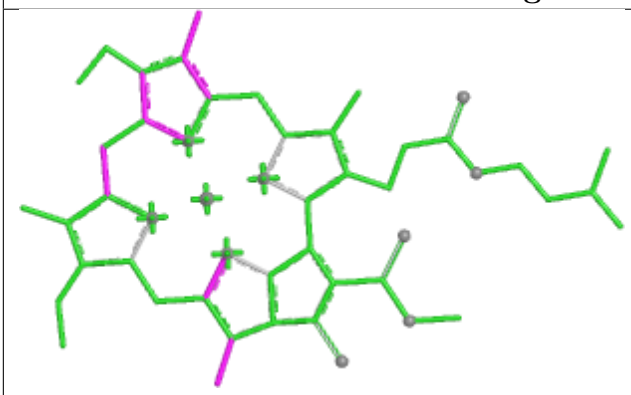


Rings

Ligand CLA Y 604



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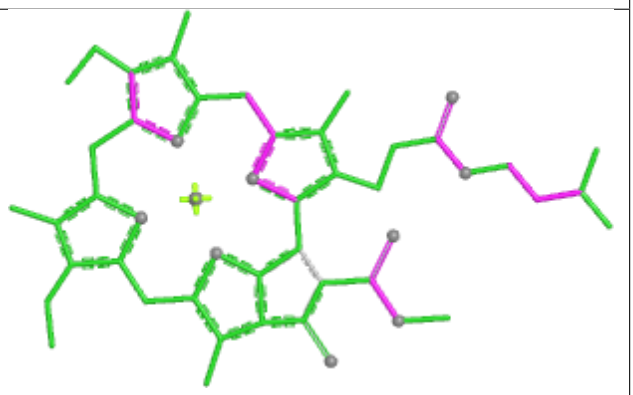
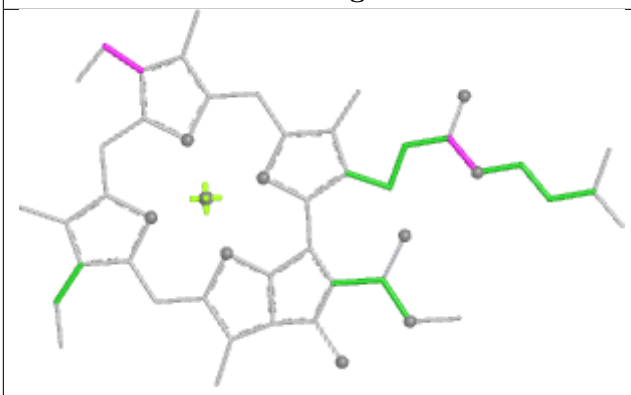


Bond angles



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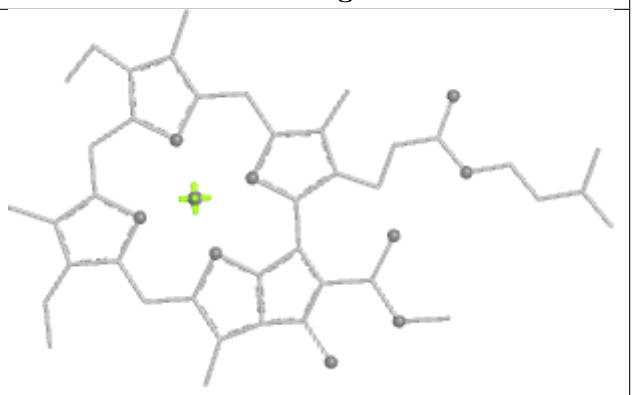
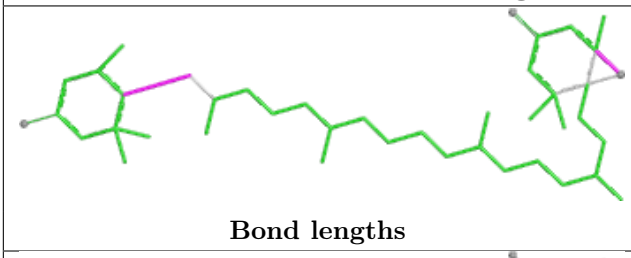


Rings

Ligand NEX Y 1623



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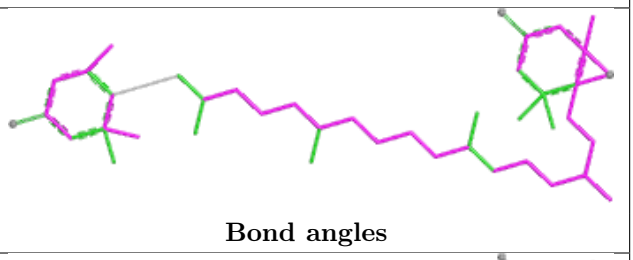
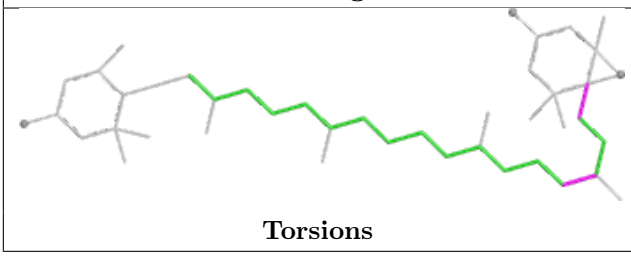


Bond angles



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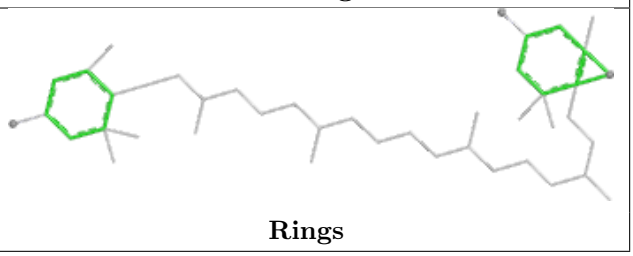
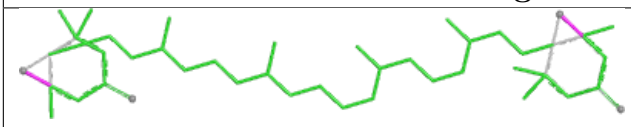


Rings

Ligand XAT X 1622



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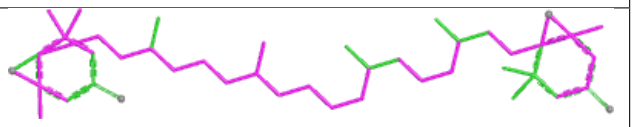
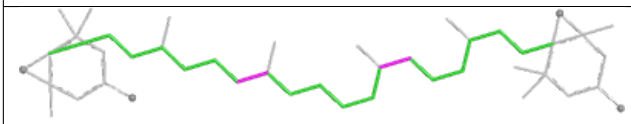
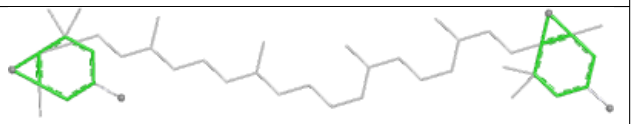


Bond angles

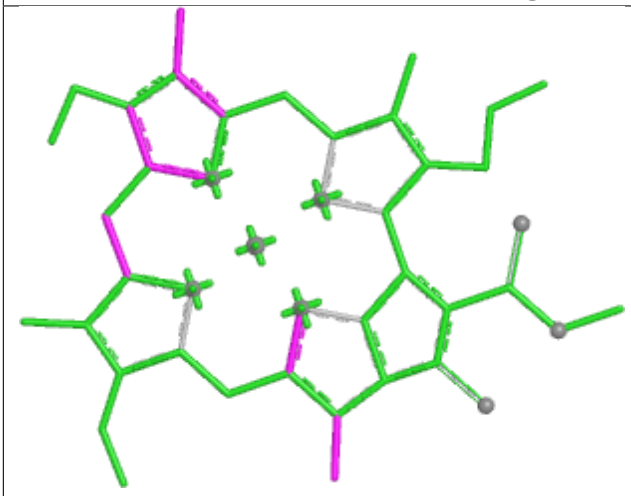


Torsions



Rings

Ligand CLA X 612



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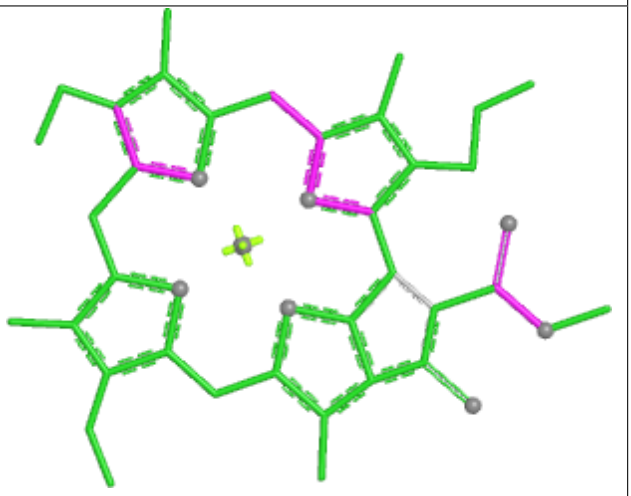
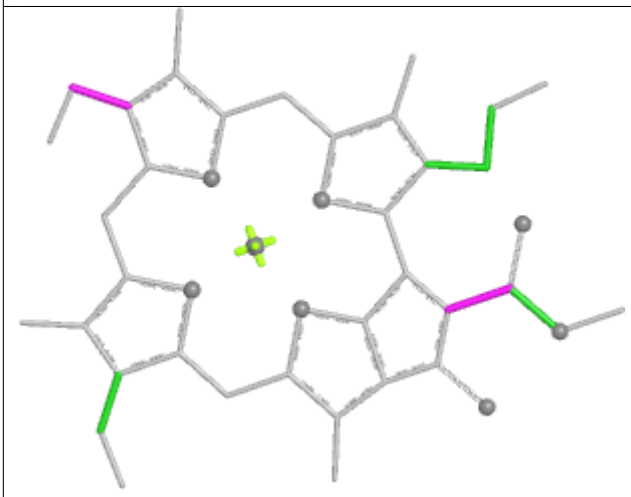
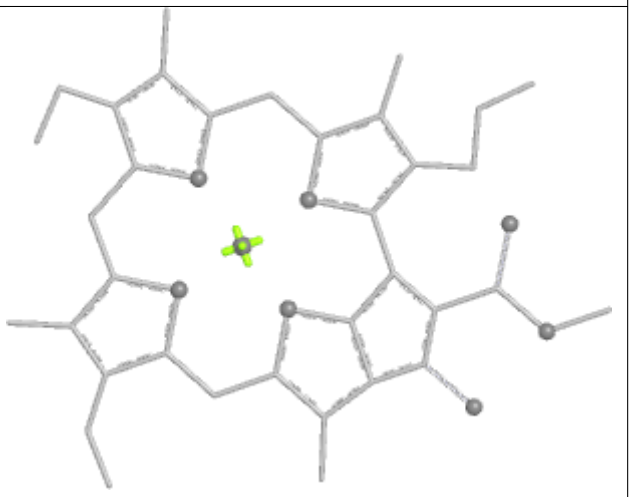


Bond angles

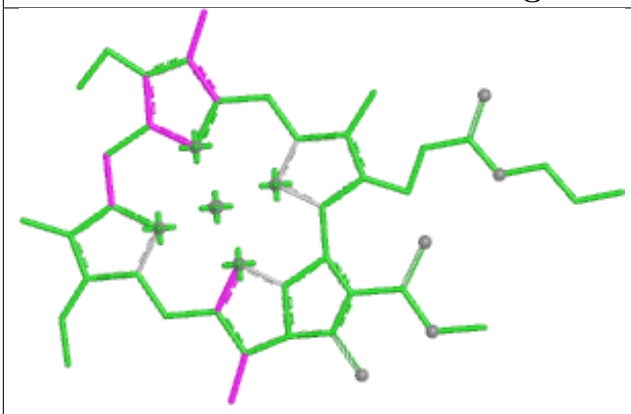


Torsions



Rings

Ligand CLA Y 614



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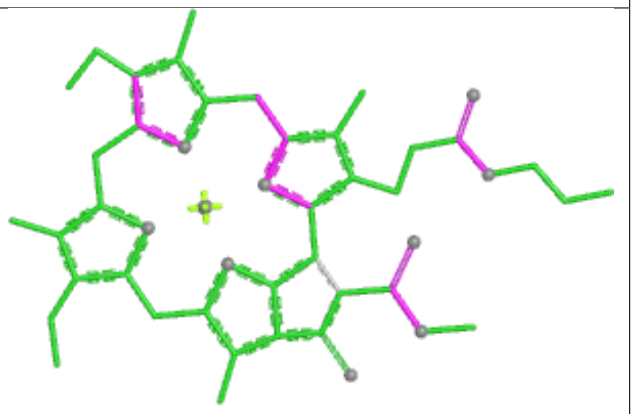
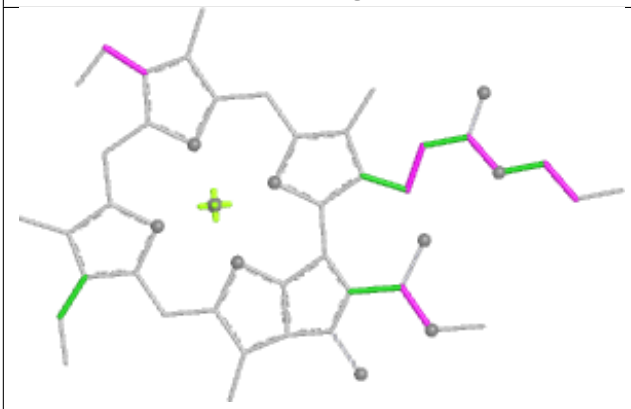


Bond angles



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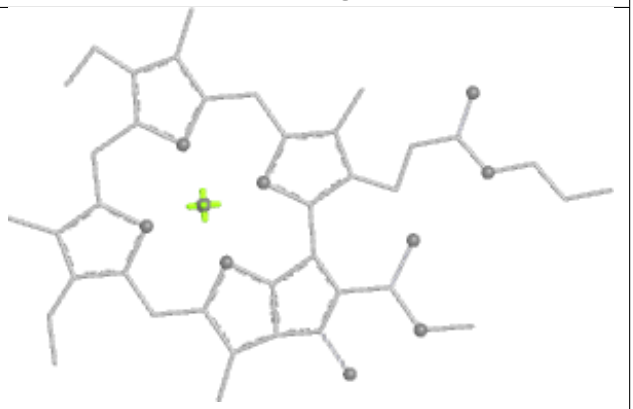
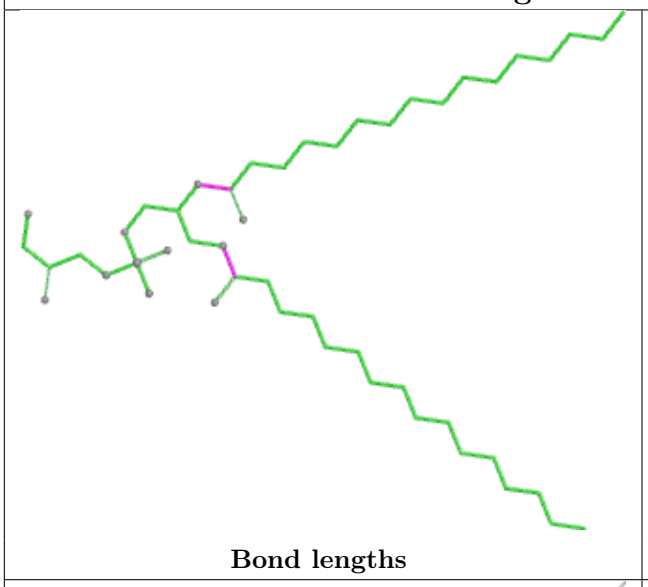


Rings

Ligand LHG Y 2630



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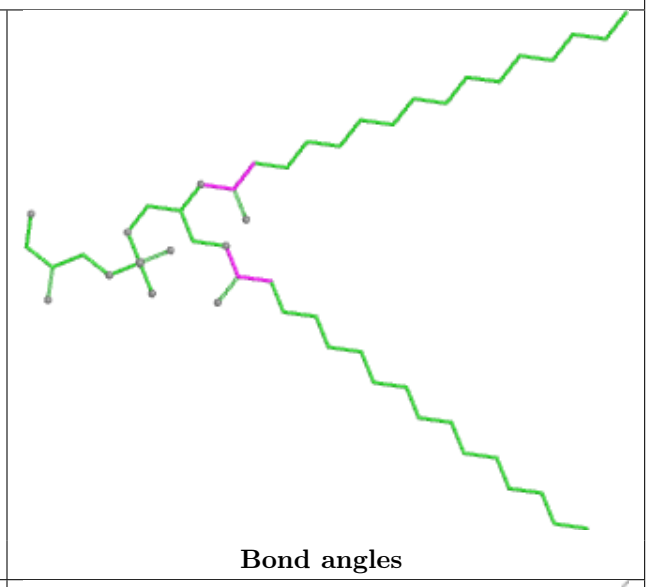
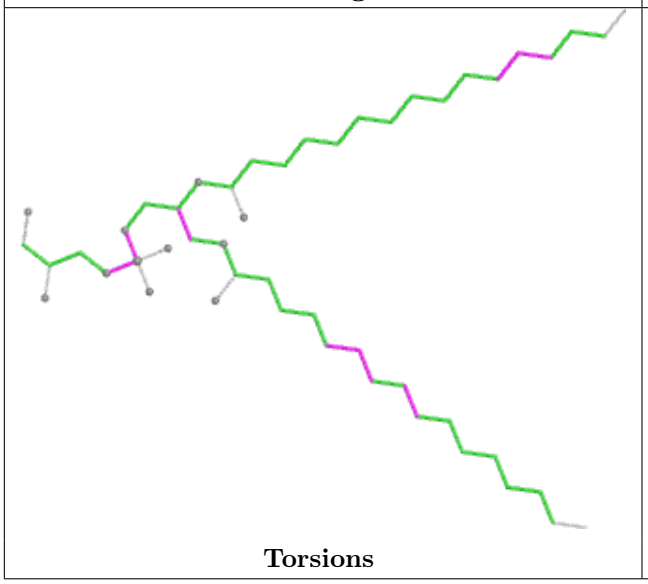


Bond angles



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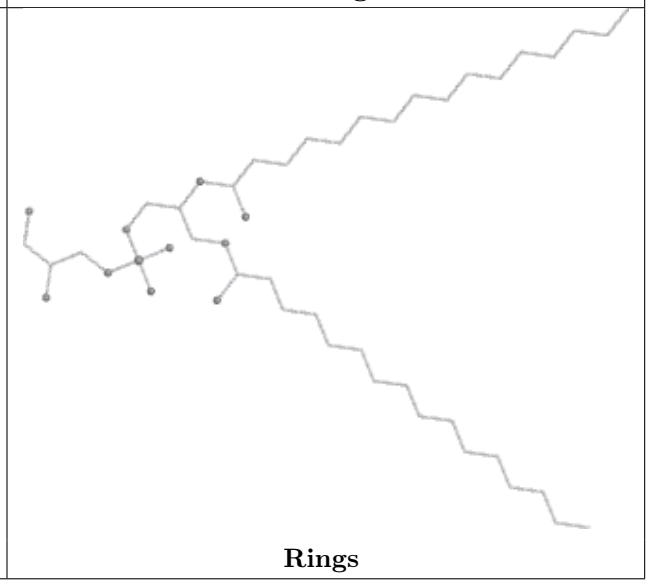
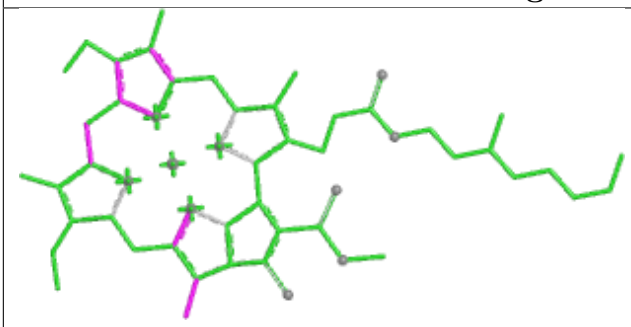


Rings

Ligand CLA Z 614



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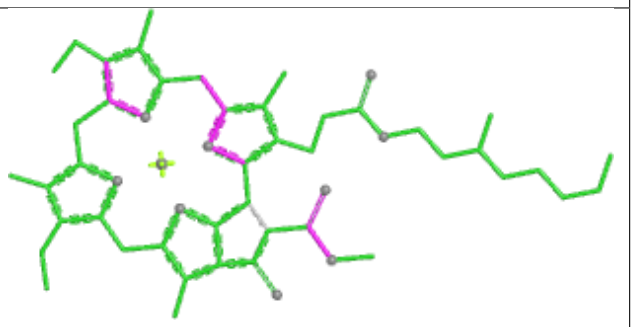
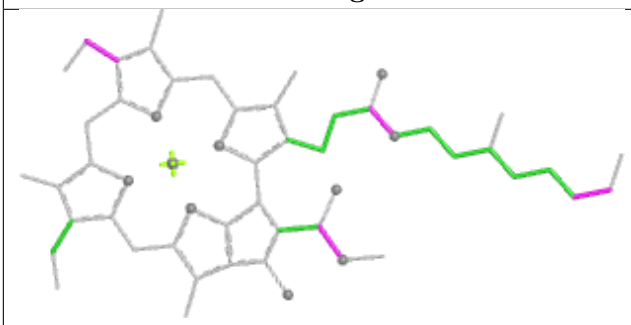
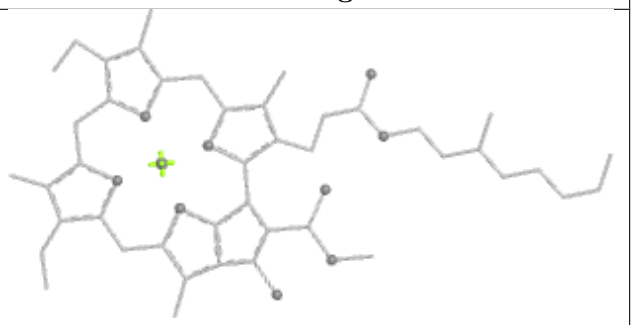


Bond angles

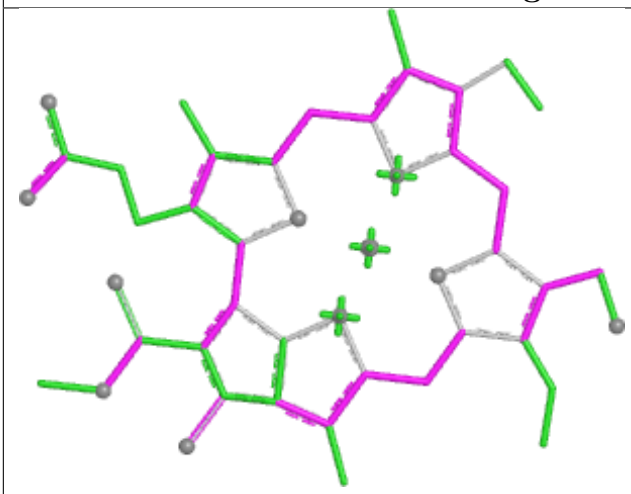


Torsions

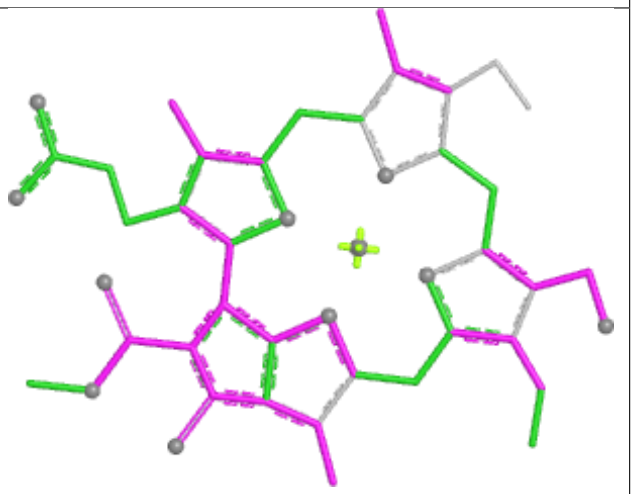


Rings

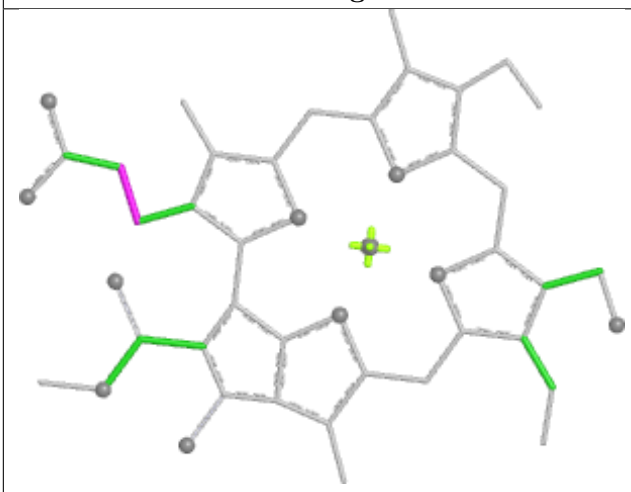
Ligand CHL X 605



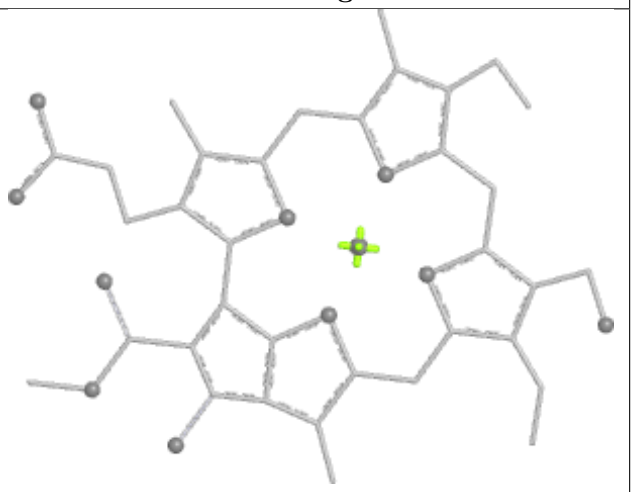
Bond lengths



Bond angles

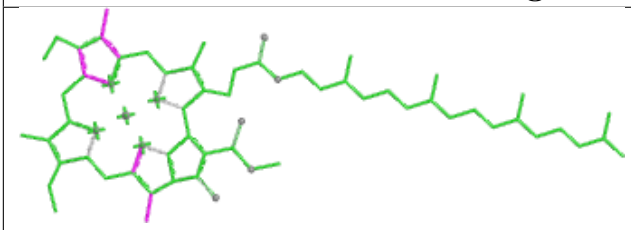


Torsions

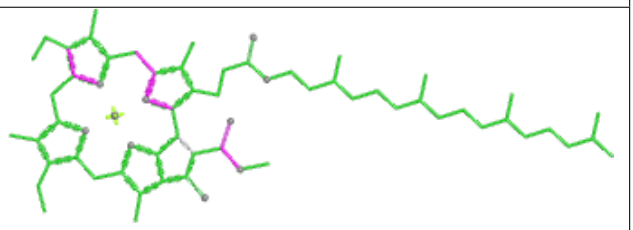


Rings

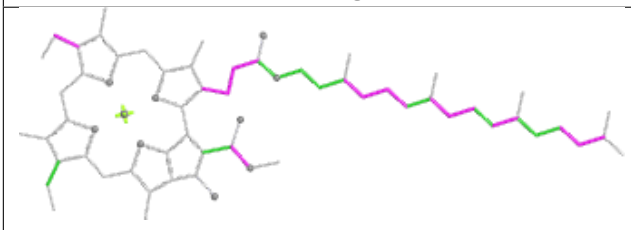
Ligand CLA Z 603



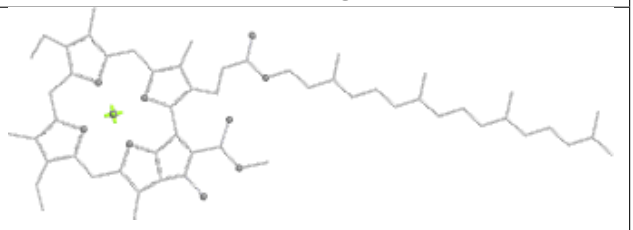
Bond lengths



Bond angles

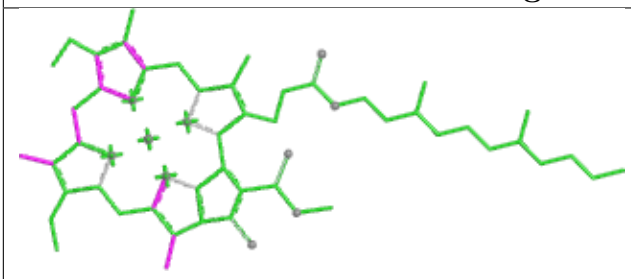


Torsions



Rings

Ligand CLA Y 602



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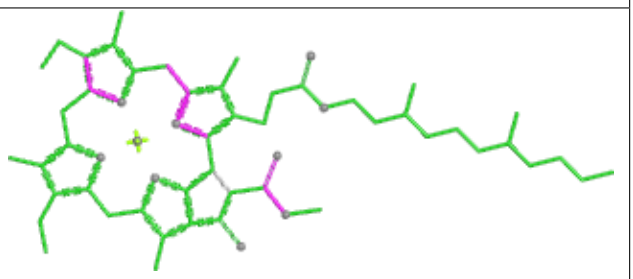
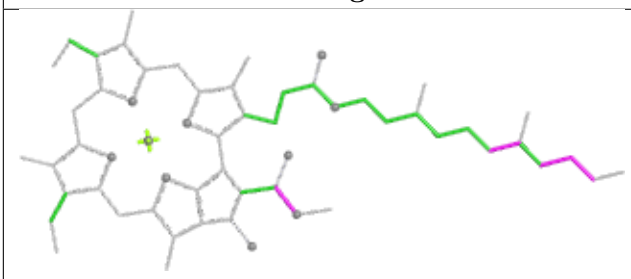
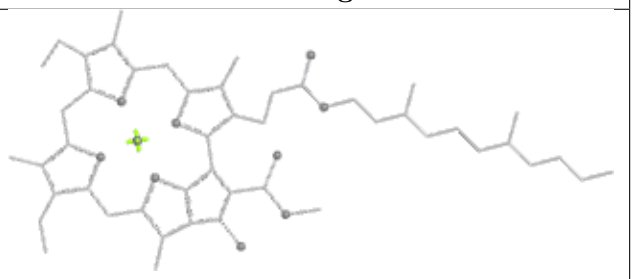


Bond angles

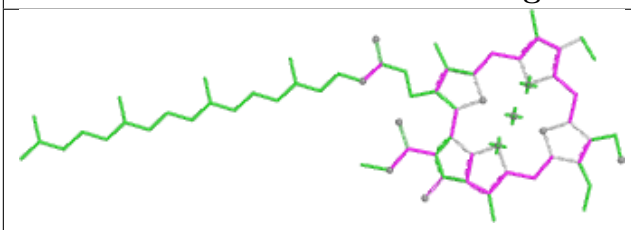


Torsions



Rings

Ligand CHL Y 607



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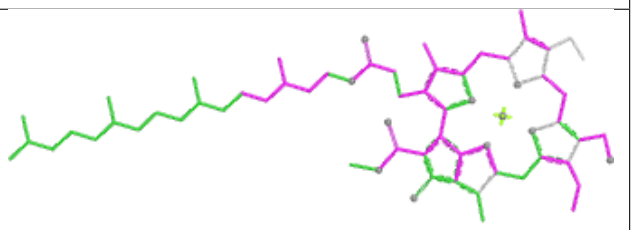
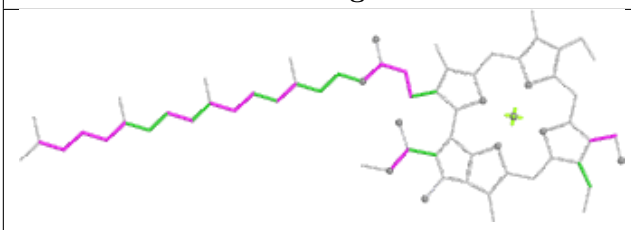


Bond angles



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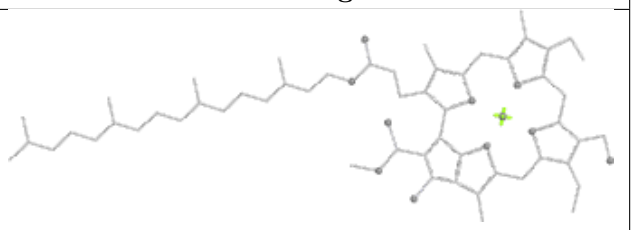
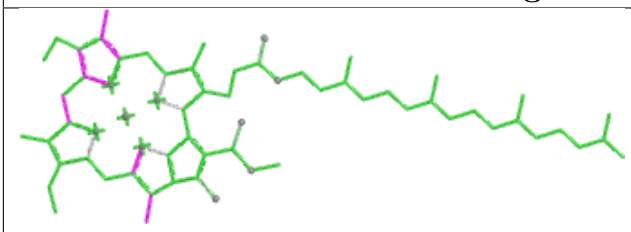


Rings

Ligand CLA X 610



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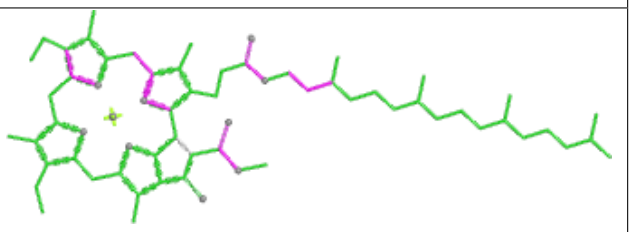
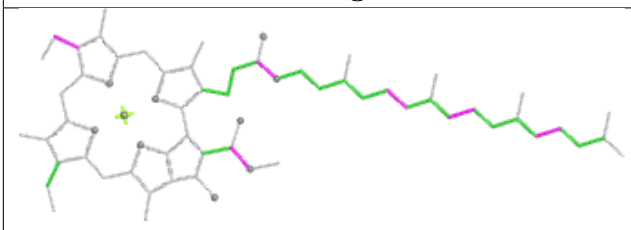


Bond angles



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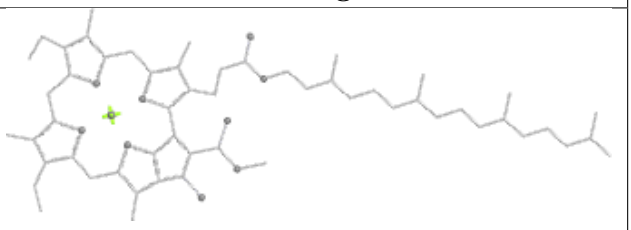
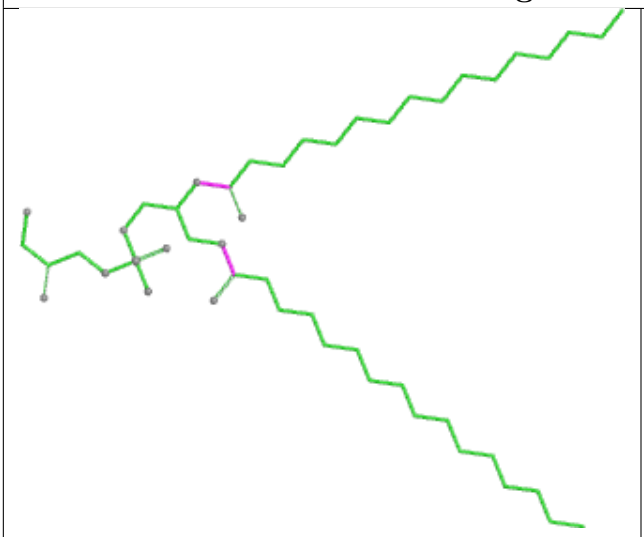


Rings

Ligand LHG Z 2630



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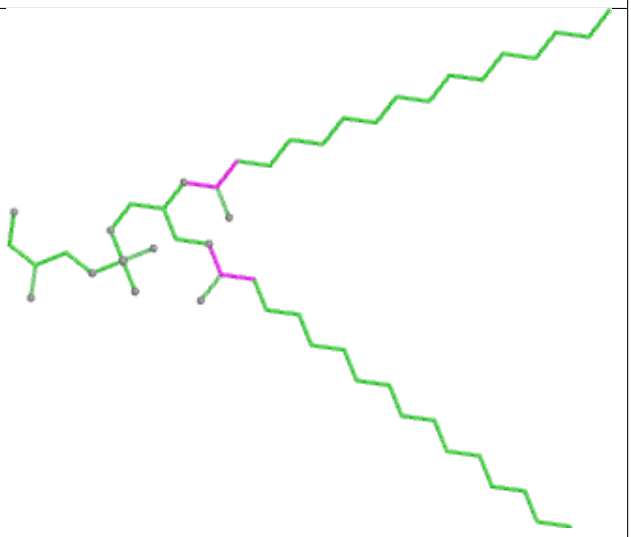
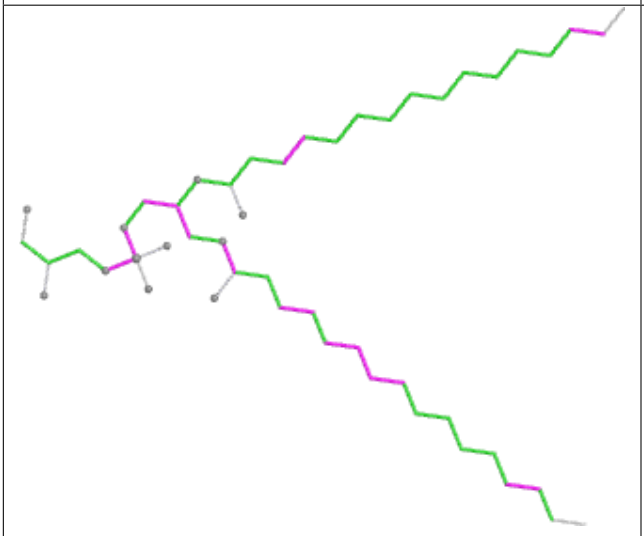


Bond angles



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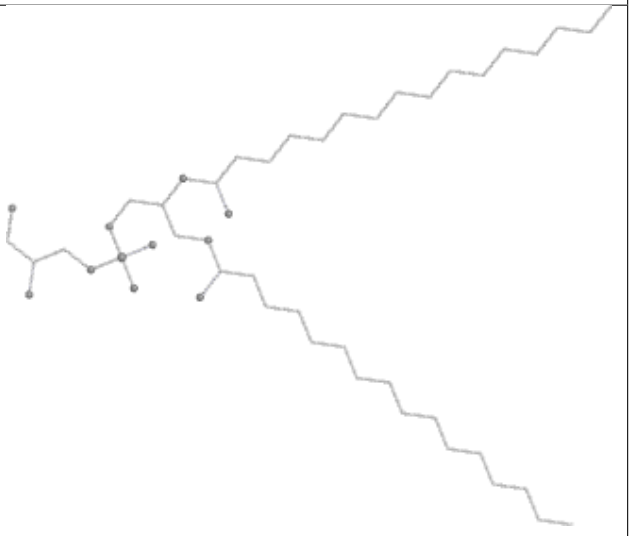
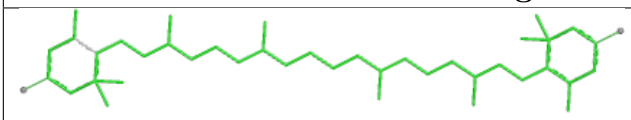


Rings

Ligand LUT Y 1621



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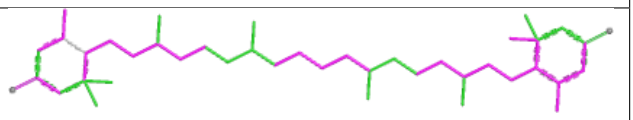
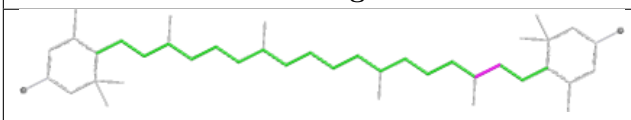


Bond angles



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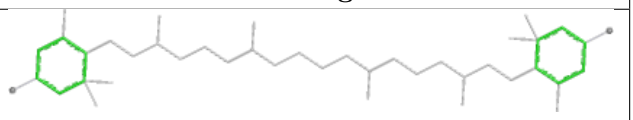
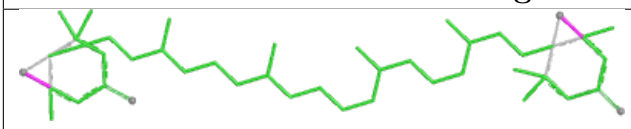
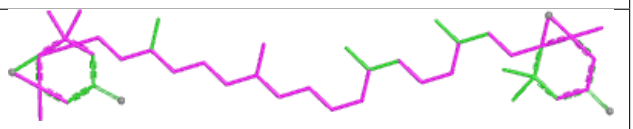


Rings

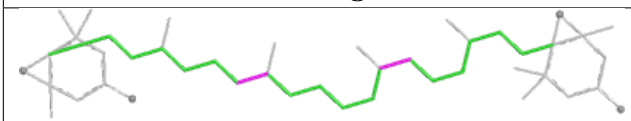
Ligand XAT Y 1622



Bond lengths



Bond angles



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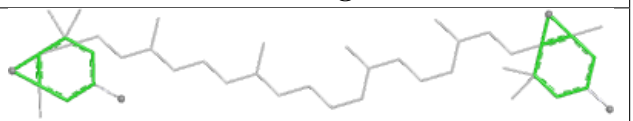
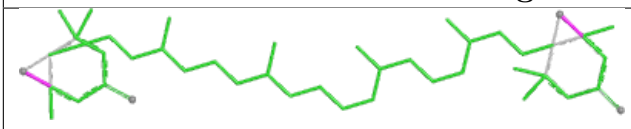


Rings

Ligand XAT Z 1622



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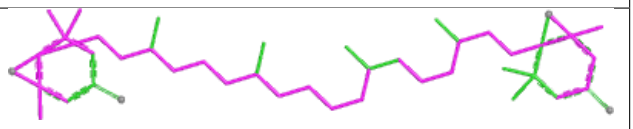
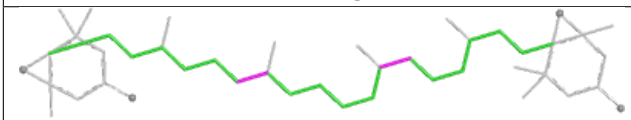


Bond angles



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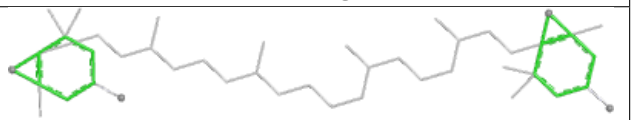
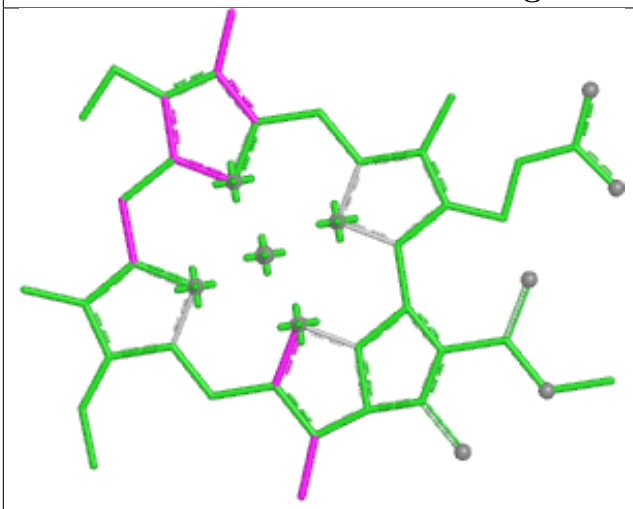
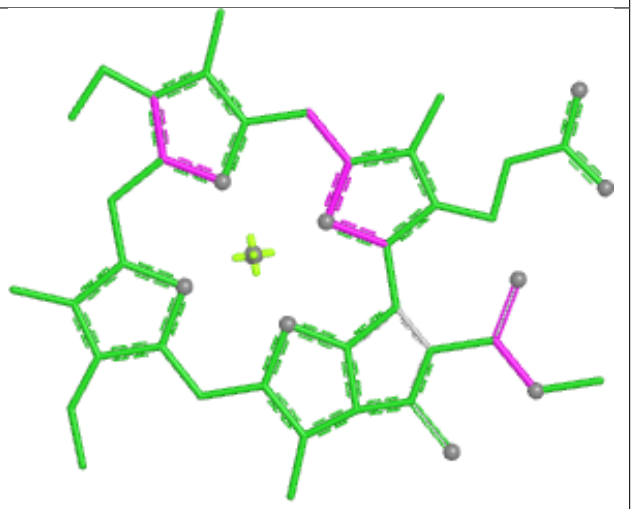


Rings

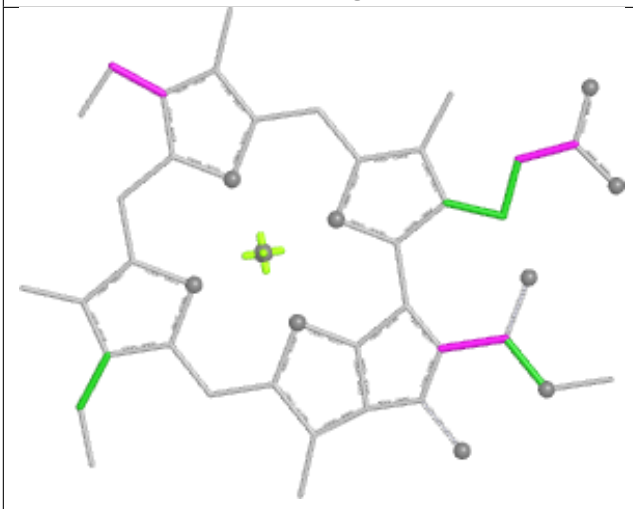
Ligand CLA Y 612



Bond lengths



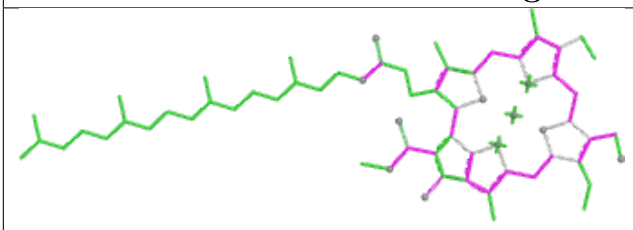
Bond angles



Torsions

Rings

Ligand CHL Y 609



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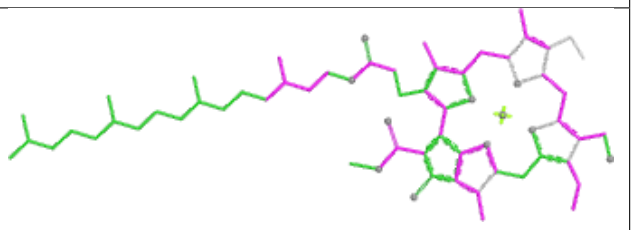
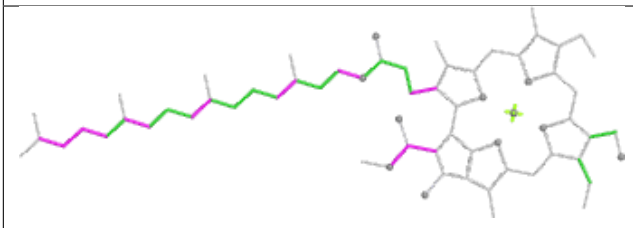
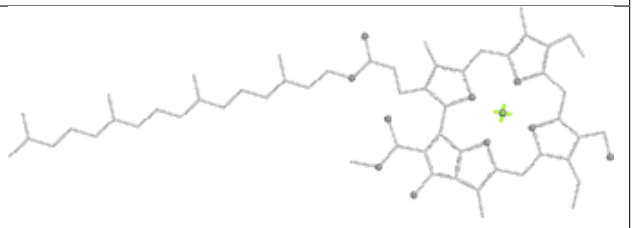


Bond angles

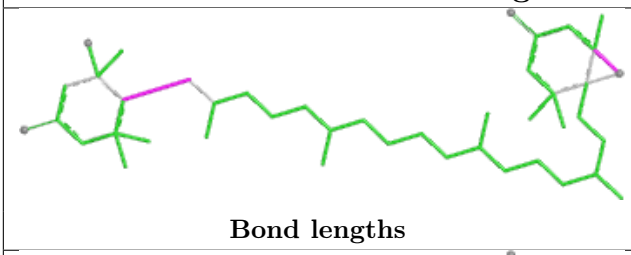


Torsions



Rings

Ligand NEX X 1623



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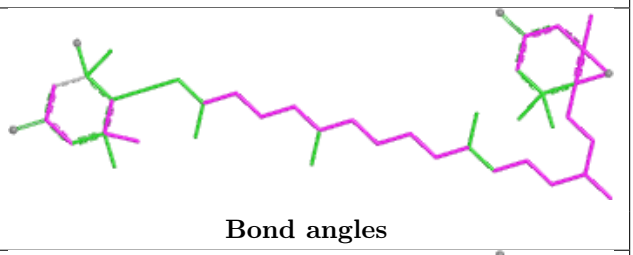
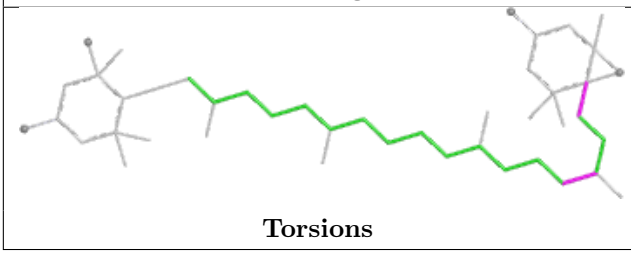
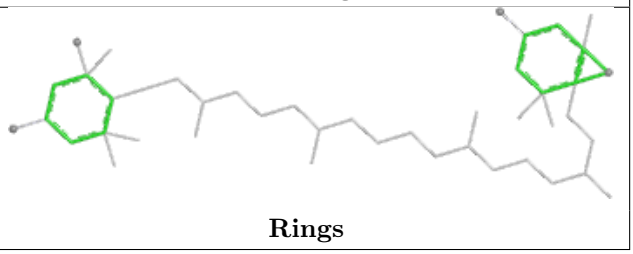


Bond angles

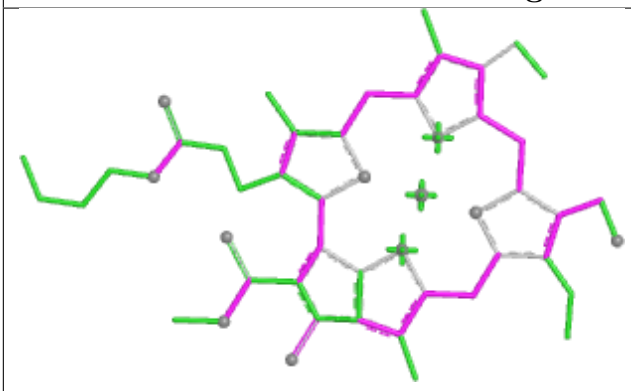


Torsions



Rings

Ligand CHL Z 608



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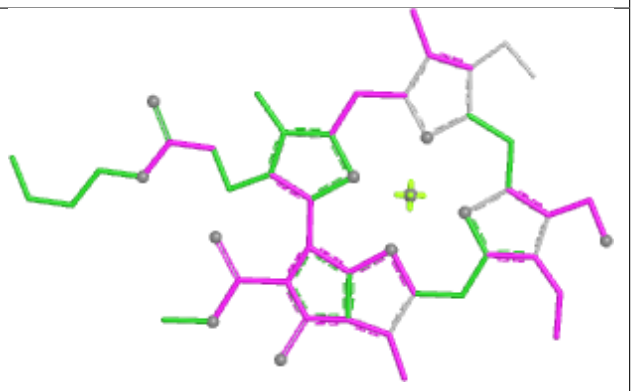
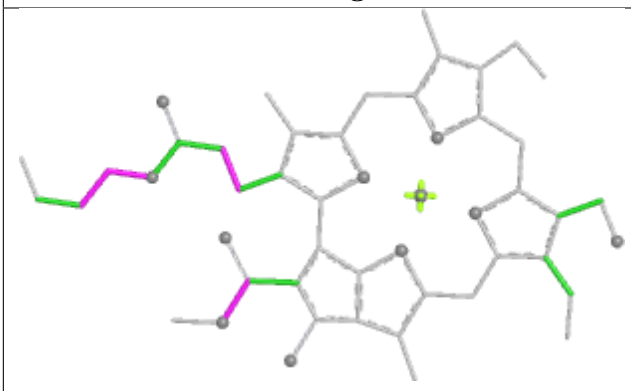
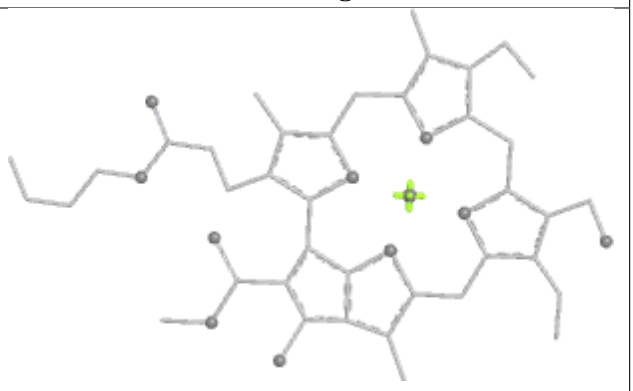


Bond angles

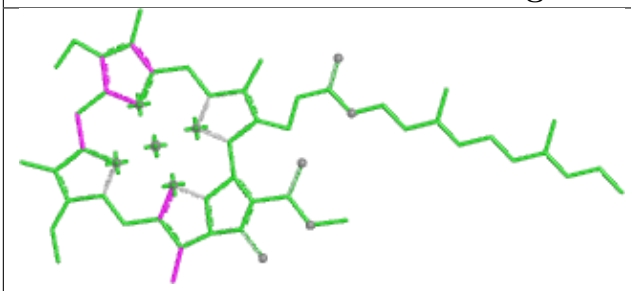


Torsions



Rings

Ligand CLA Z 604



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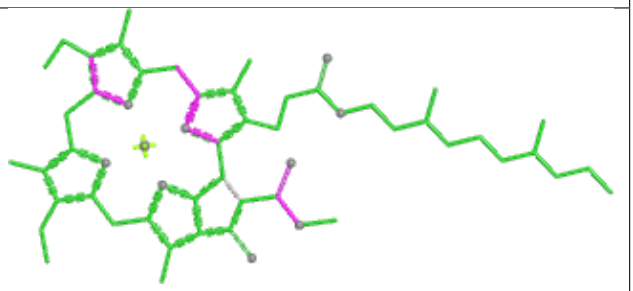
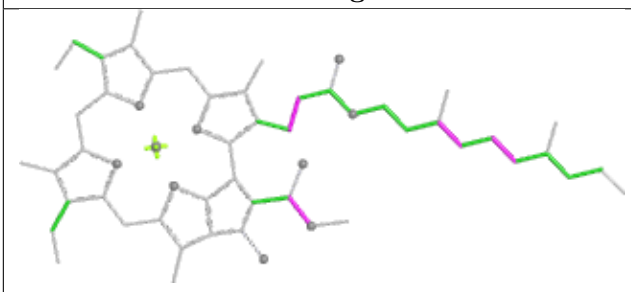
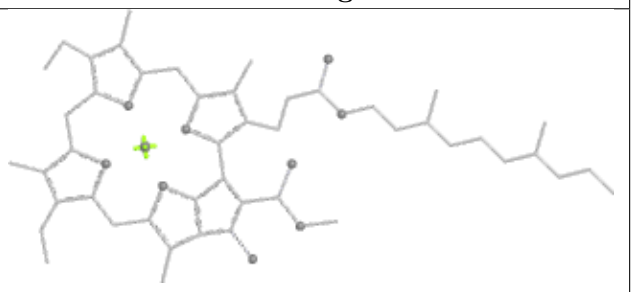


Bond angles

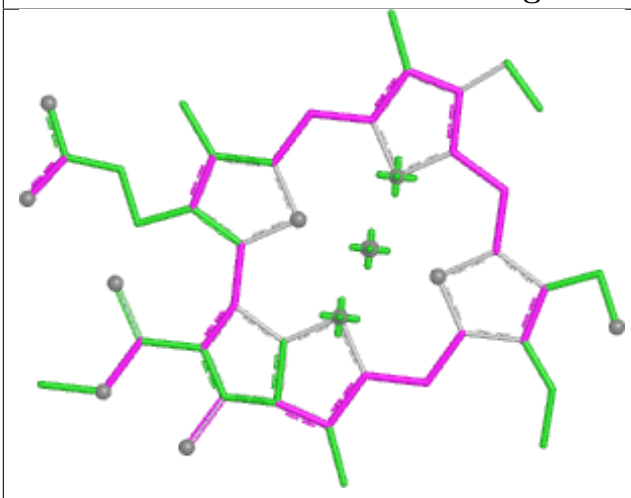


Torsions



Rings

Ligand CHL Y 606



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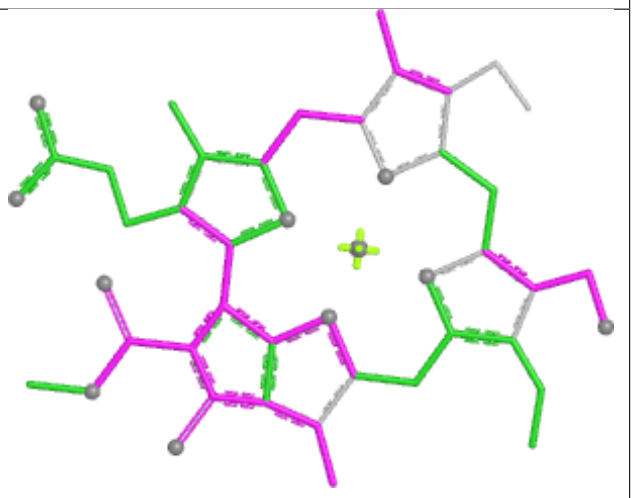
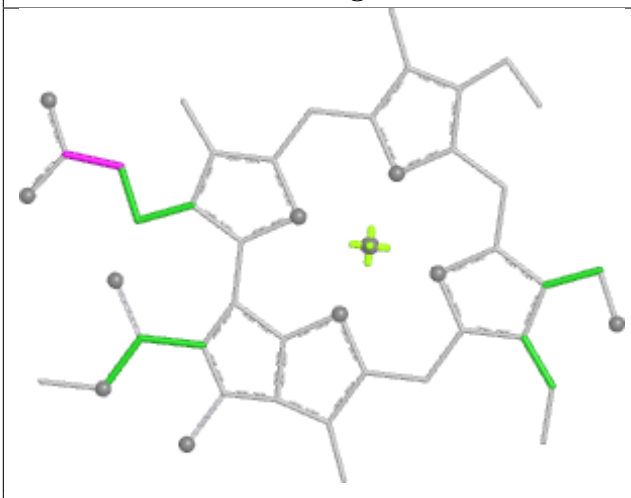


Bond angles



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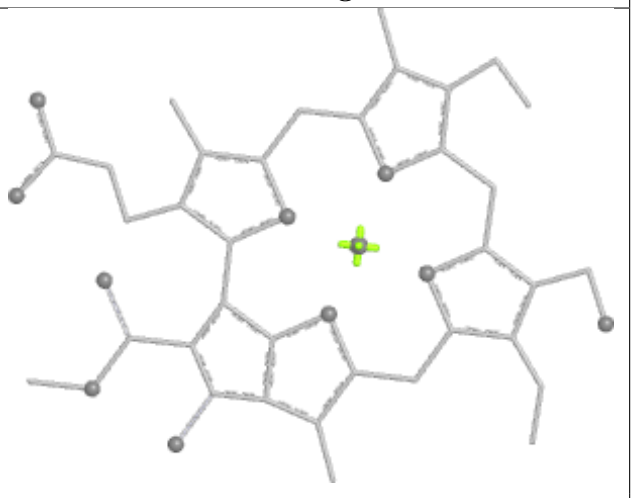
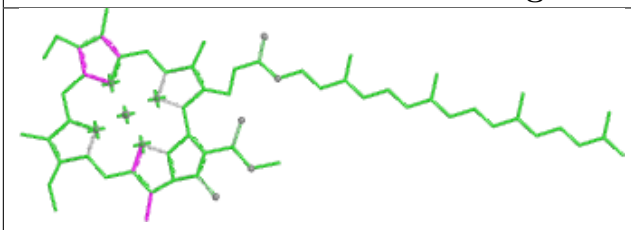
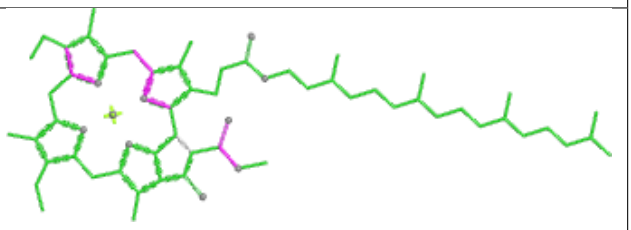
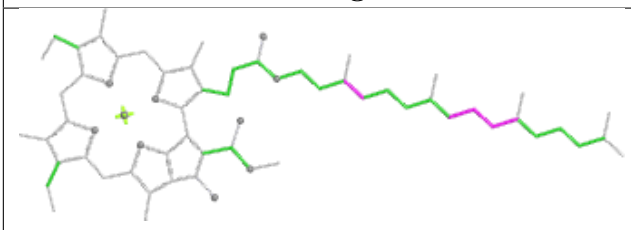
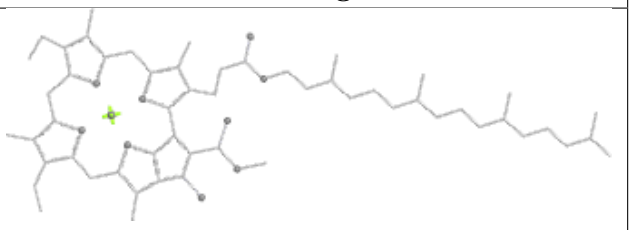
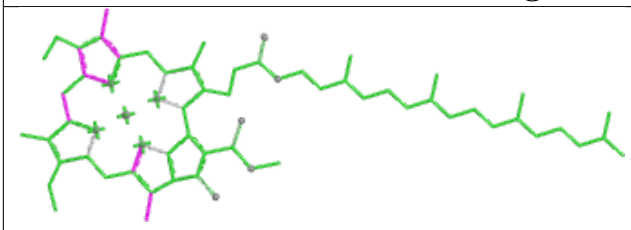
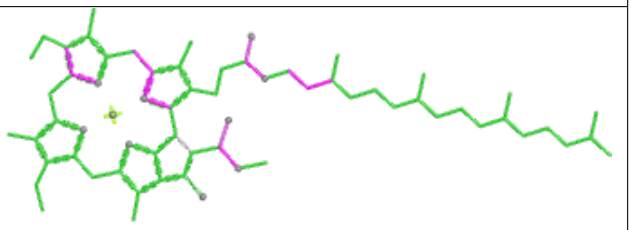
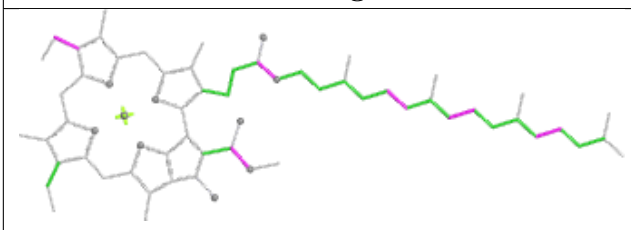
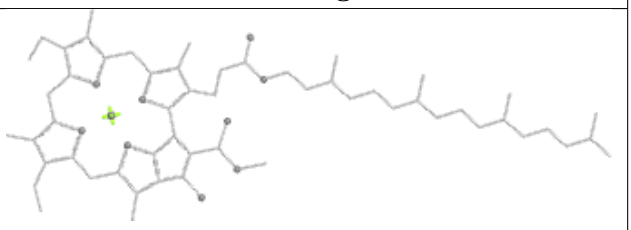
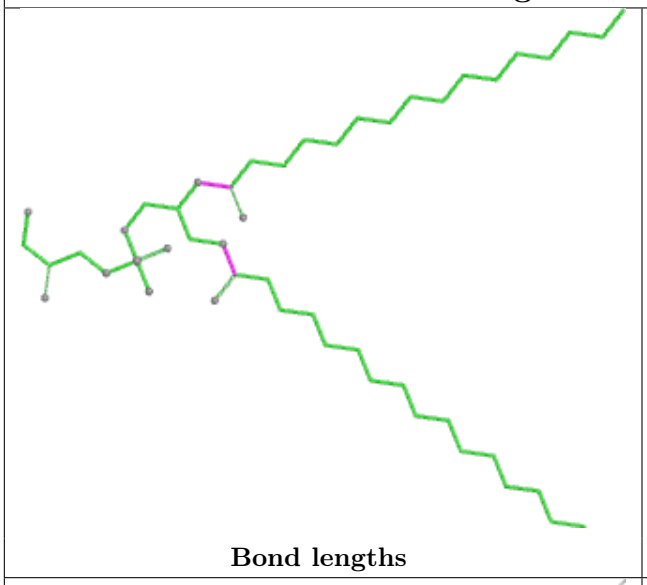


Rings

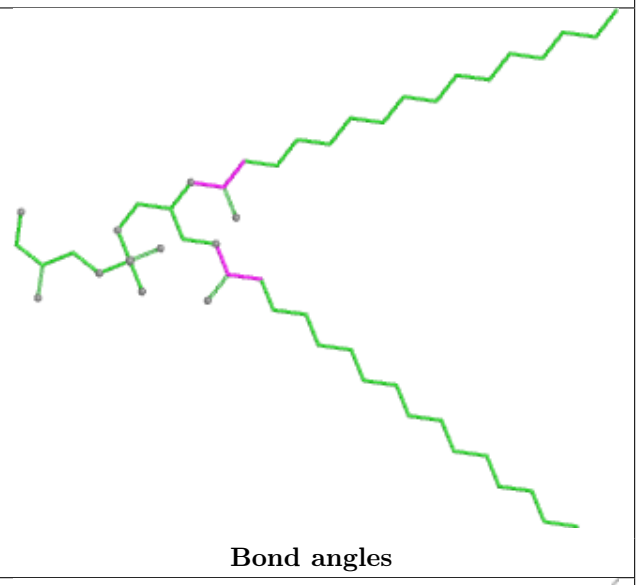
Ligand CLA Z 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Y 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

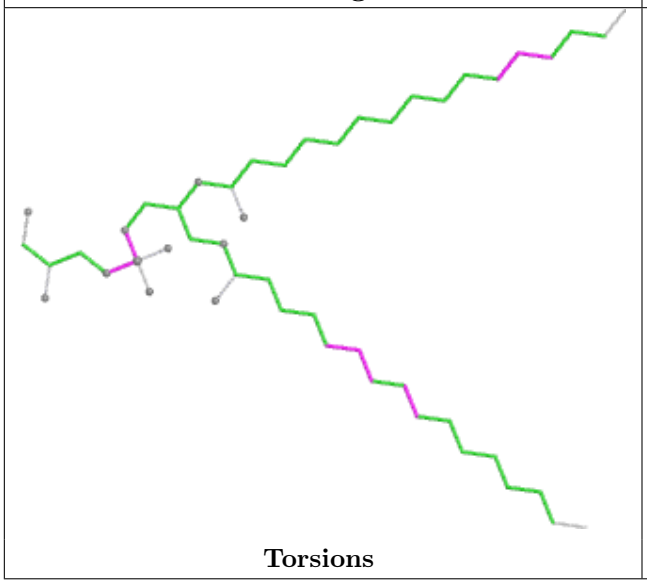
Ligand LHG X 2630



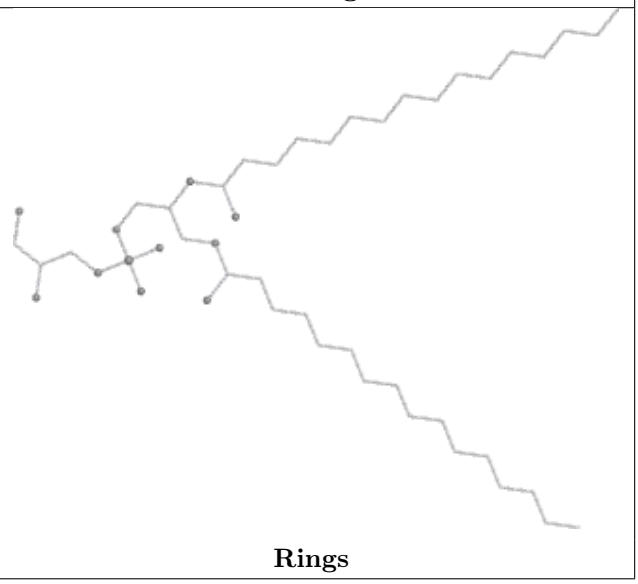
Bond lengths



Bond angles

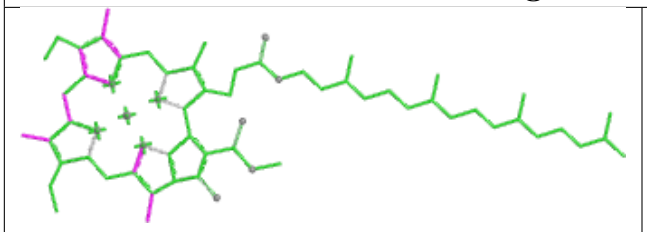


Torsions

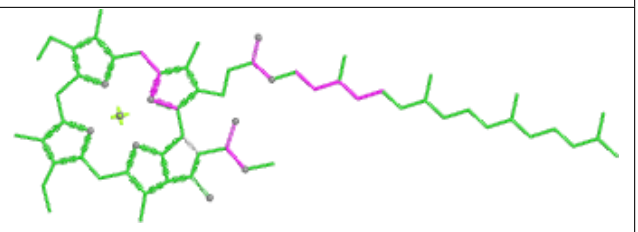


Rings

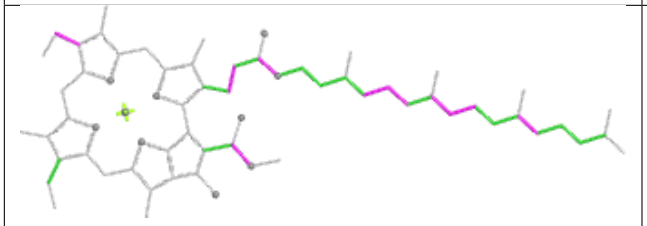
Ligand CLA Y 613



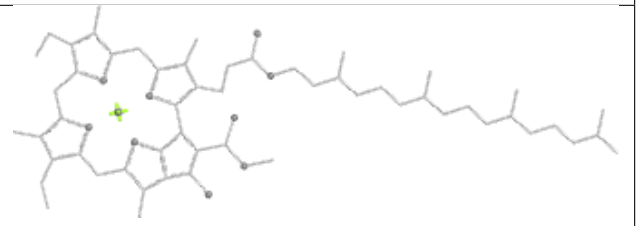
Bond lengths



Bond angles

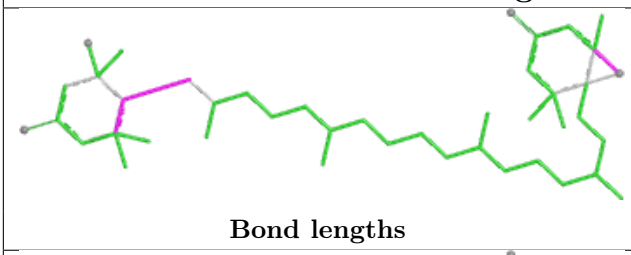


Torsions

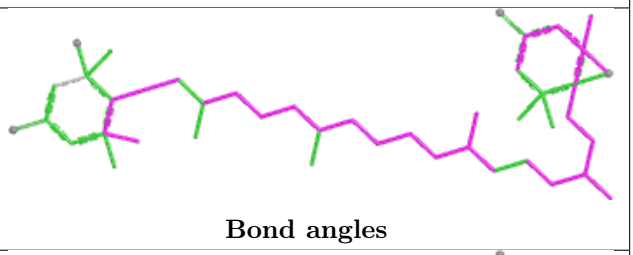


Rings

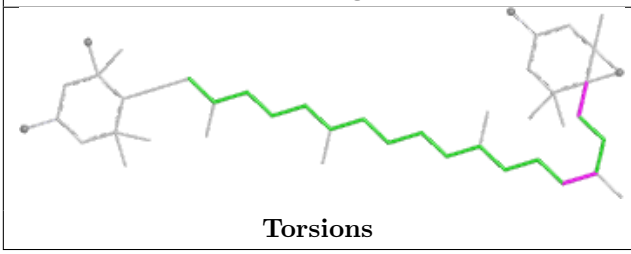
Ligand NEX Z 1623



Bond lengths



Bond angles



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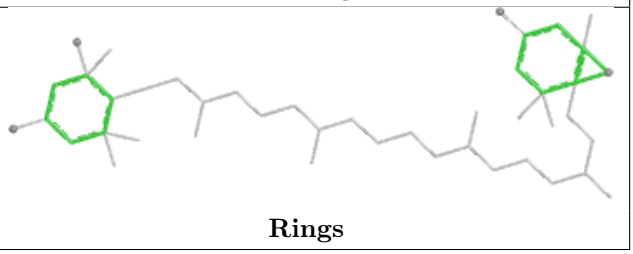
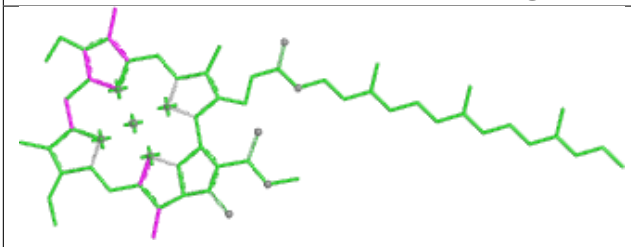
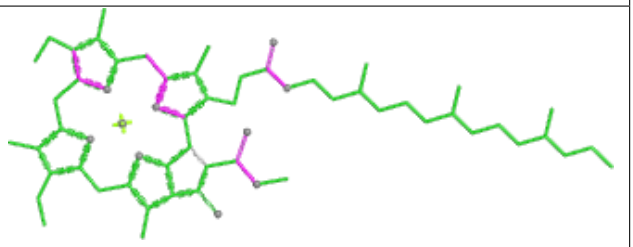


Rings

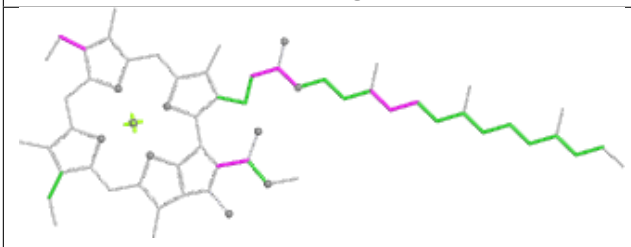
Ligand CLA X 603



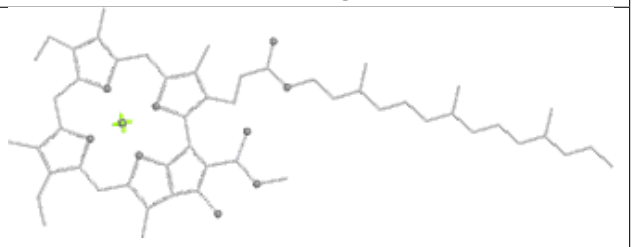
Bond lengths



Bond angles

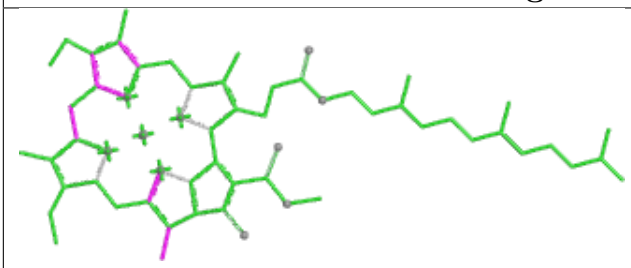


Torsions

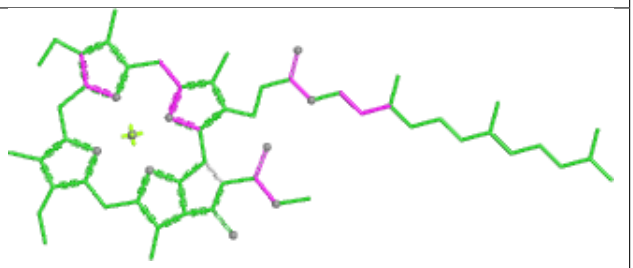


Rings

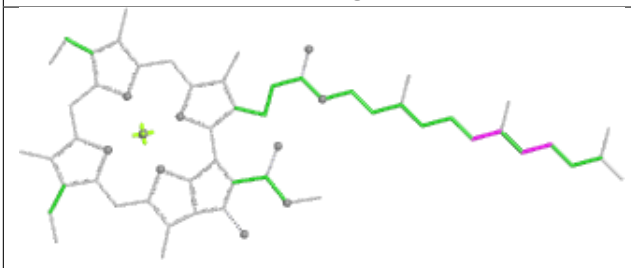
Ligand CLA Z 602



Bond lengths



Bond angles



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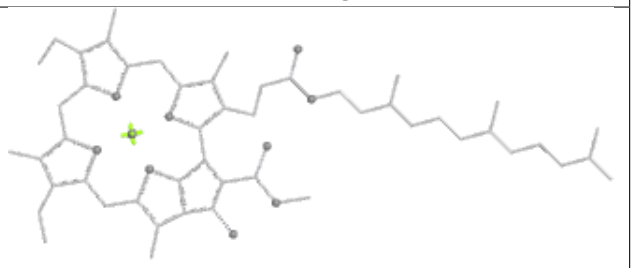
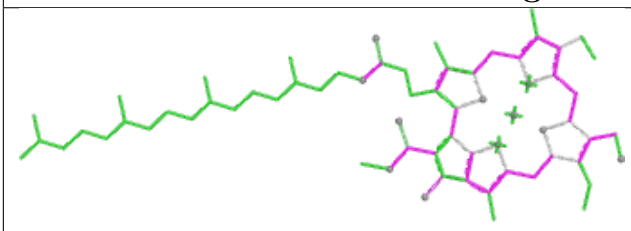
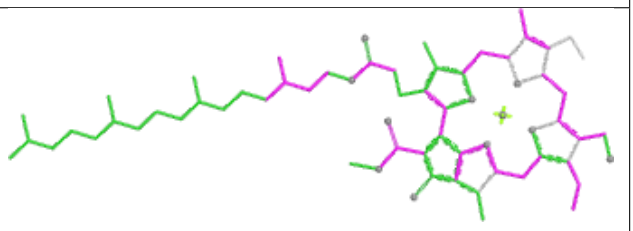


Rings

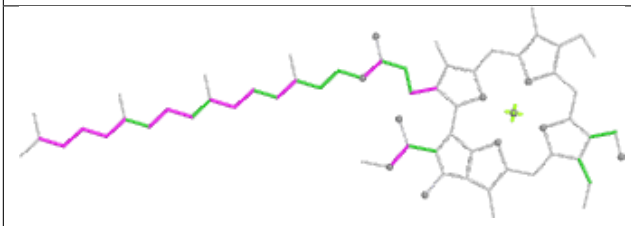
Ligand CHL Y 601



Bond lengths



Bond angles



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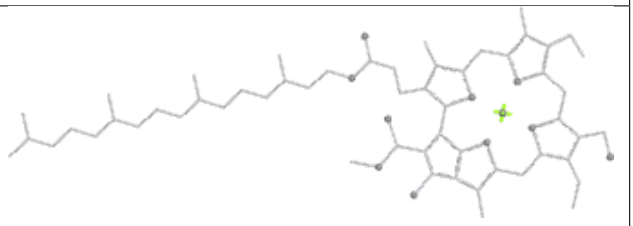
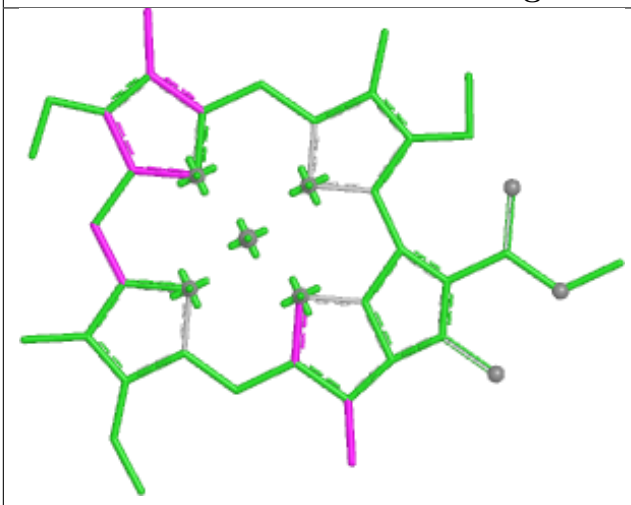
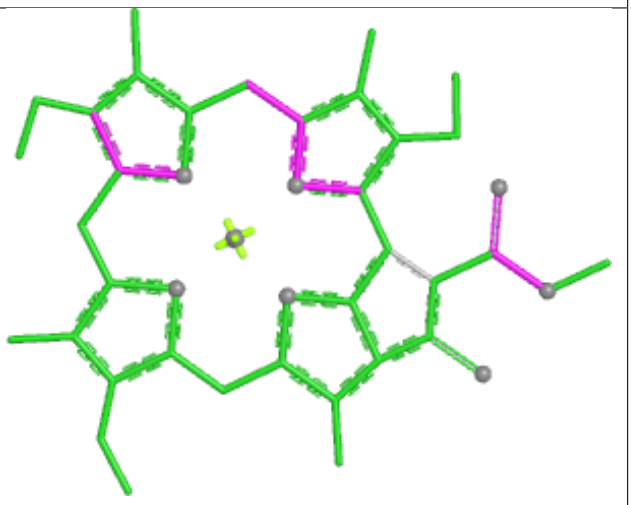


Rings

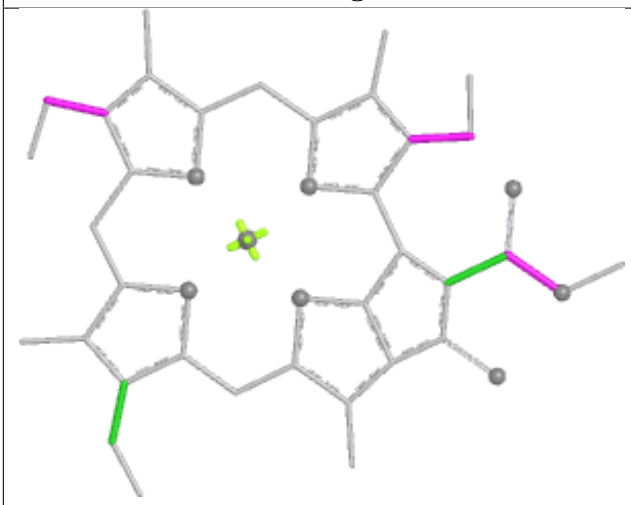
Ligand CLA X 614



Bond lengths



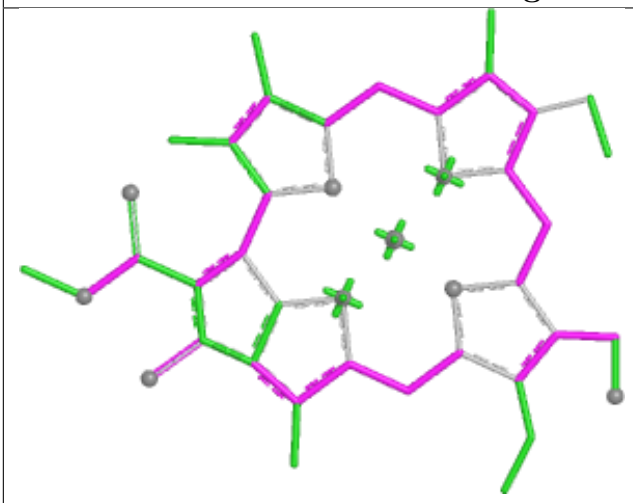
Bond angles



Torsions

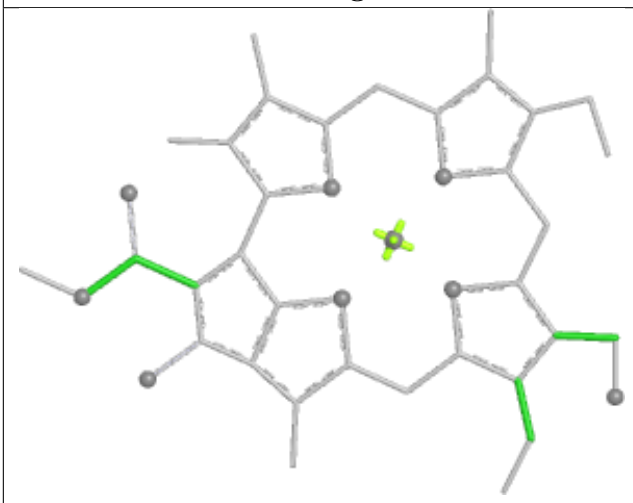
Rings

Ligand CHL Y 605

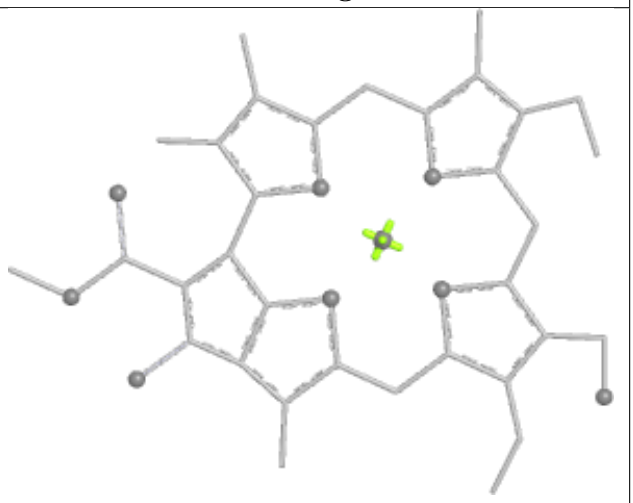


Bond lengths

Bond angles

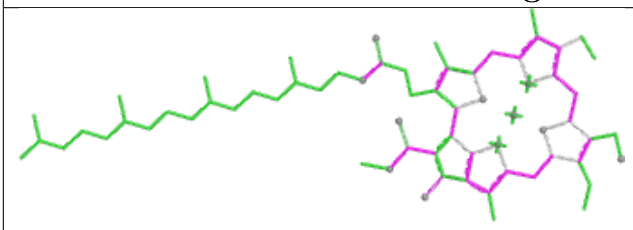


Torsions



Rings

Ligand CHL X 607



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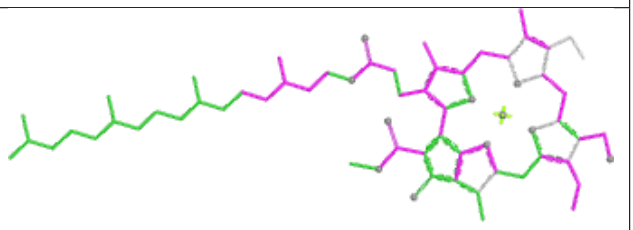
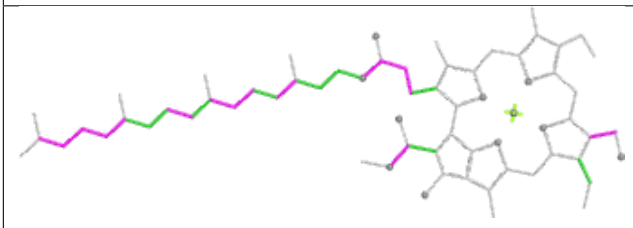
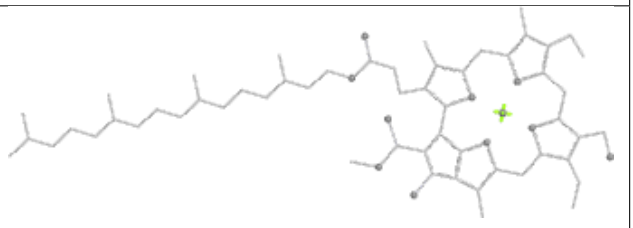


Bond angles

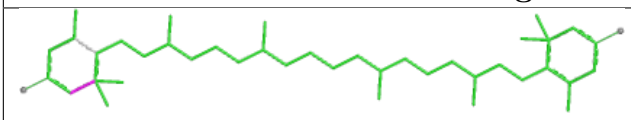


Torsions

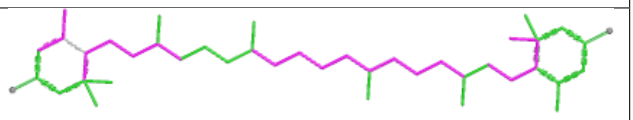


Rings

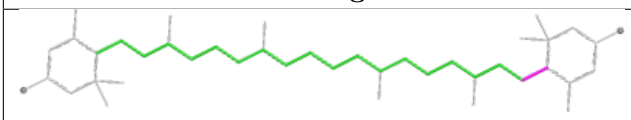
Ligand LUT Y 1620



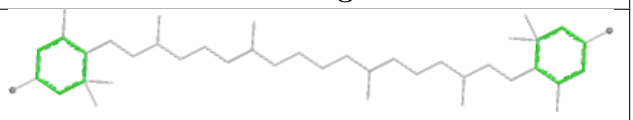
Bond lengths



Bond angles

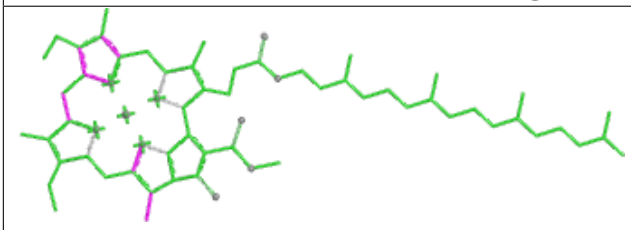


Torsions



Rings

Ligand CLA Z 610



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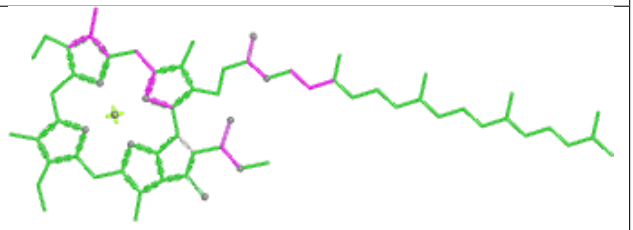
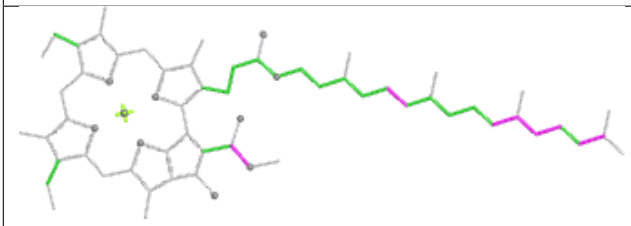
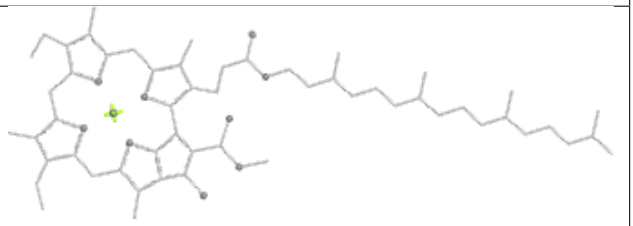


Bond angles

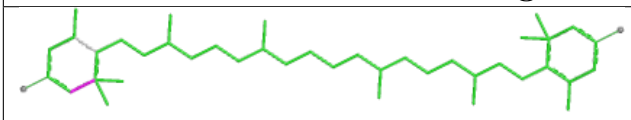


Torsions

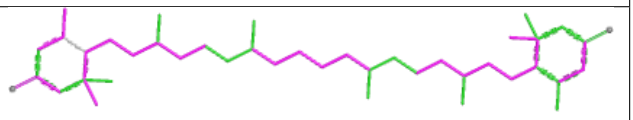


Rings

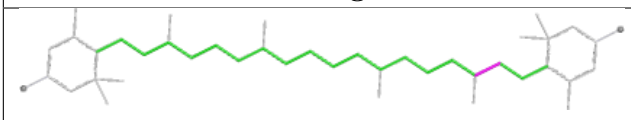
Ligand LUT Z 1621



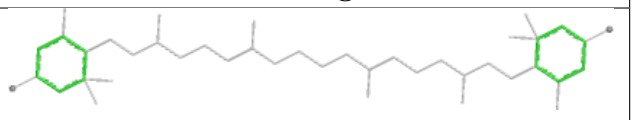
Bond lengths



Bond angles

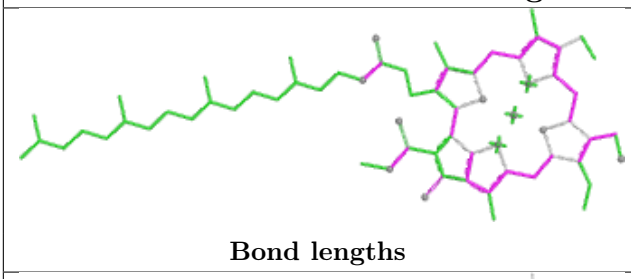


Torsions

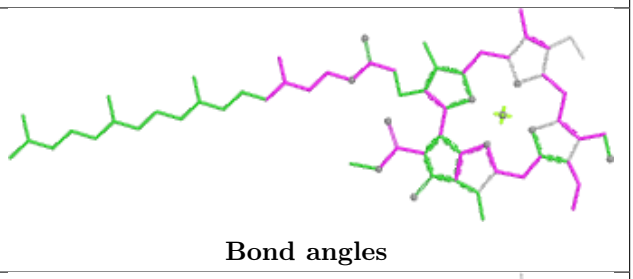


Rings

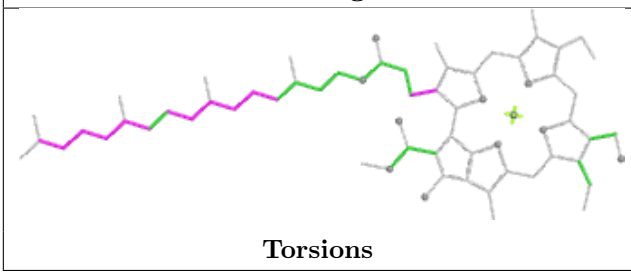
Ligand CHL Z 601



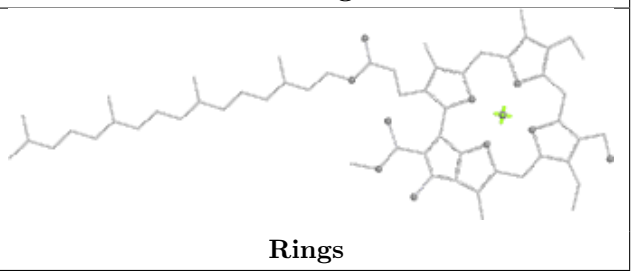
Bond lengths



Bond angles

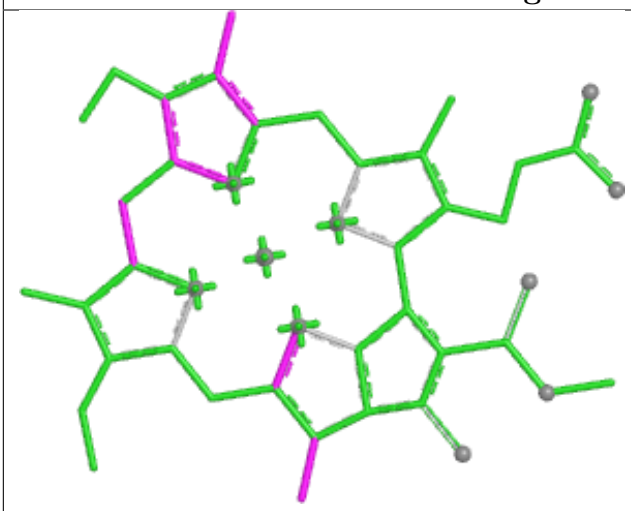


Torsions



Rings

Ligand CLA X 611



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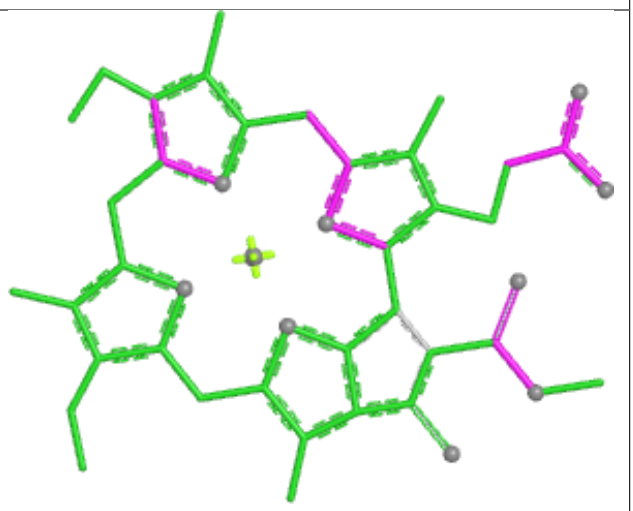

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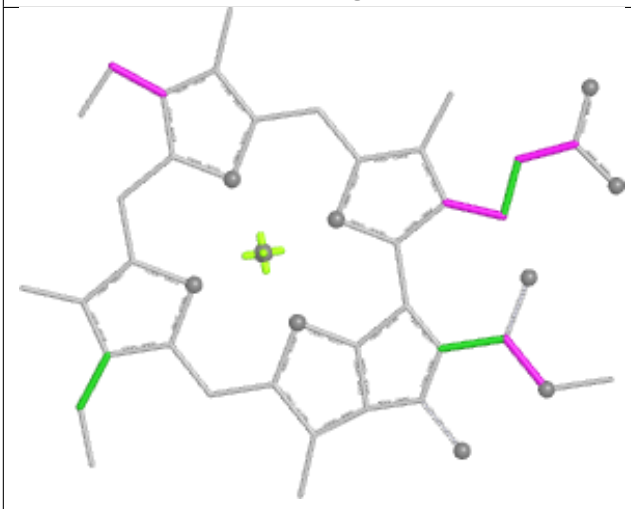
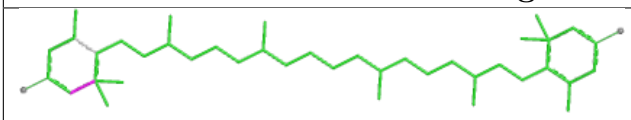


Torsions

Rings

Ligand LUT Z 1620



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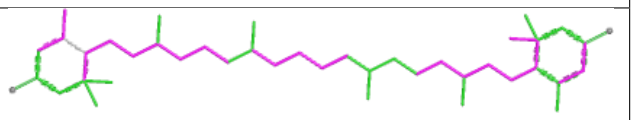
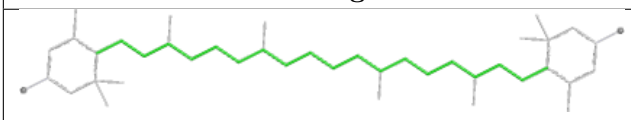


Bond angles



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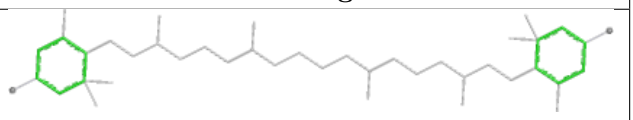
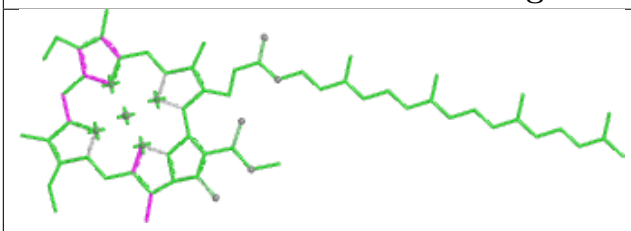
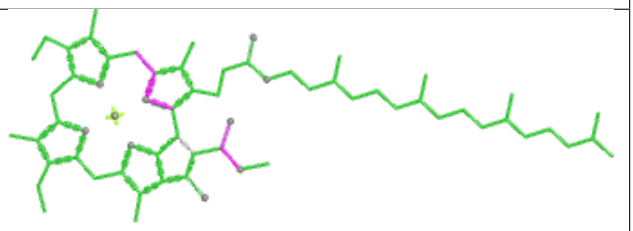


Rings

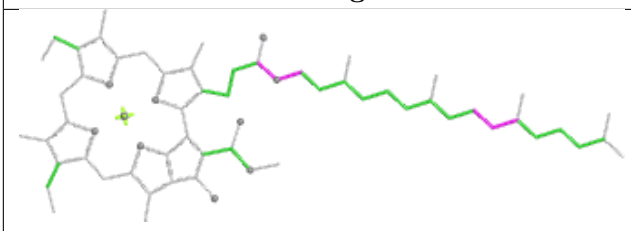
Ligand CLA Z 612



Bond lengths



Bond angles



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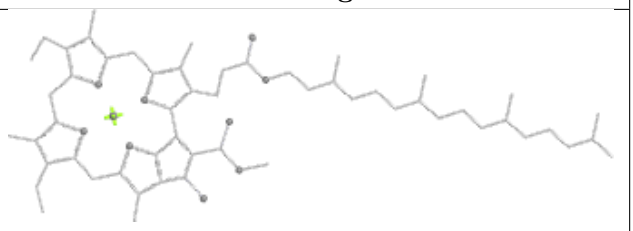
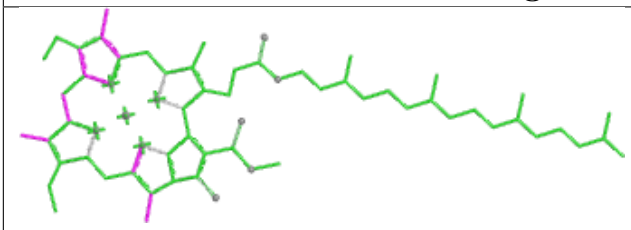
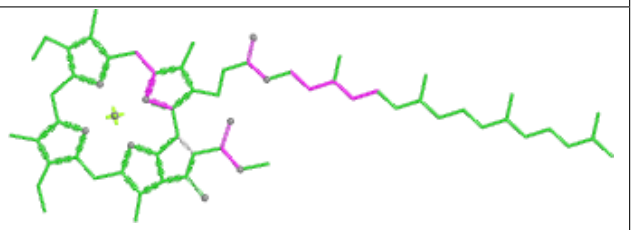


Rings

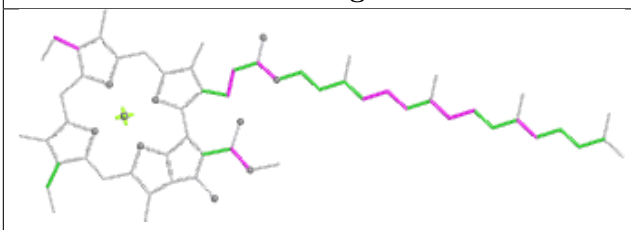
Ligand CLA X 613



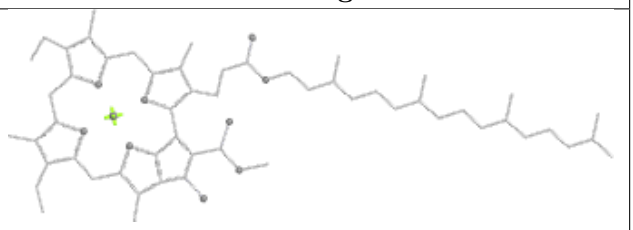
Bond lengths



Bond angles

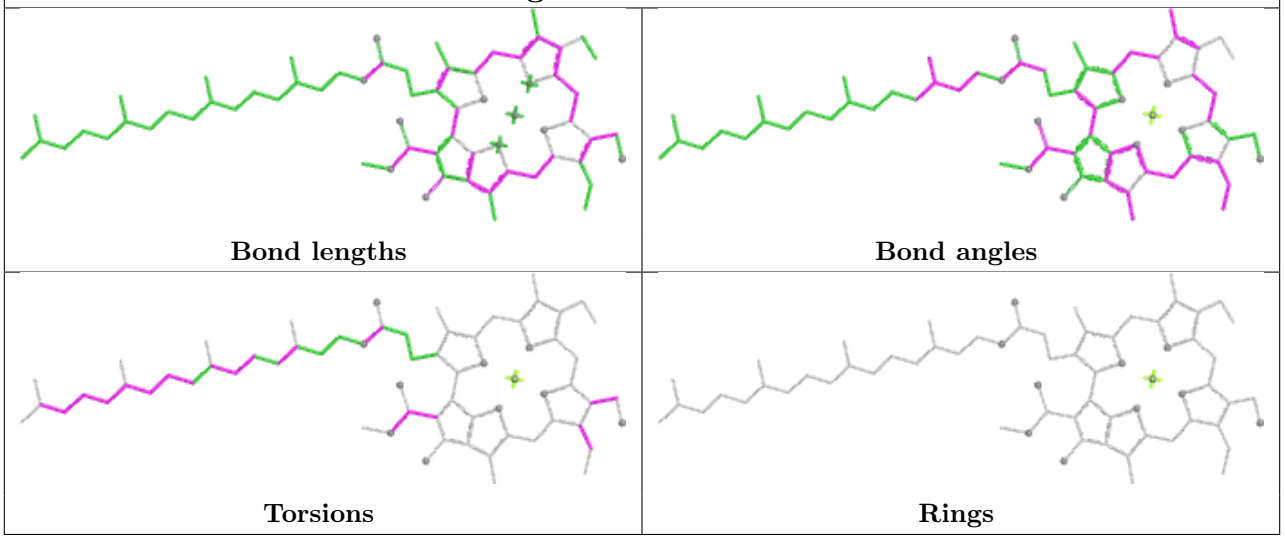


Torsions



Rings

Ligand CHL Z 609



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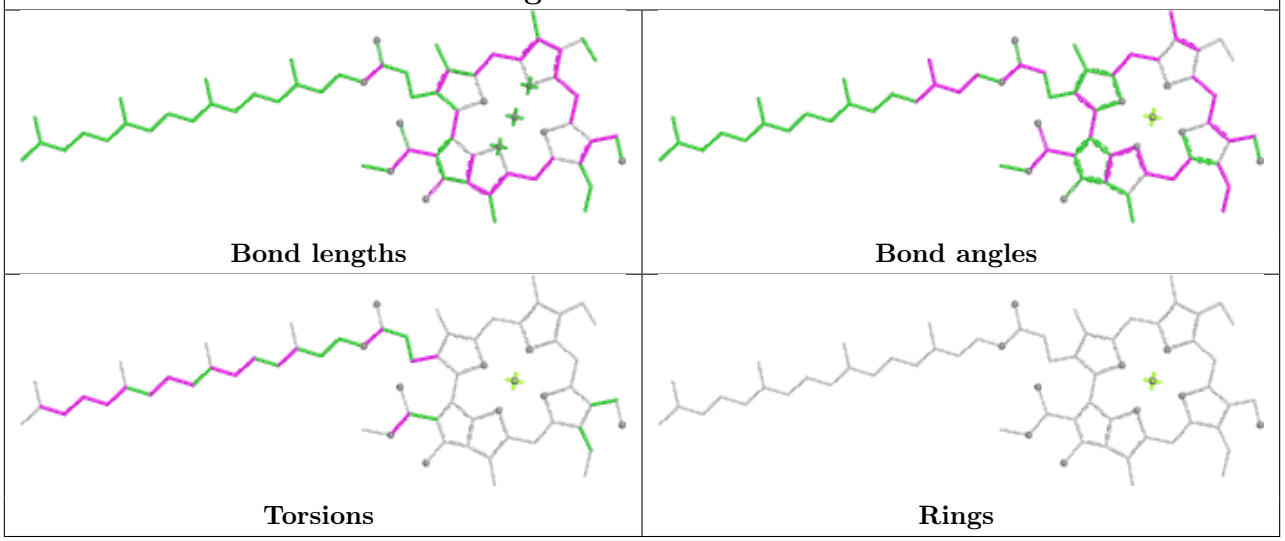

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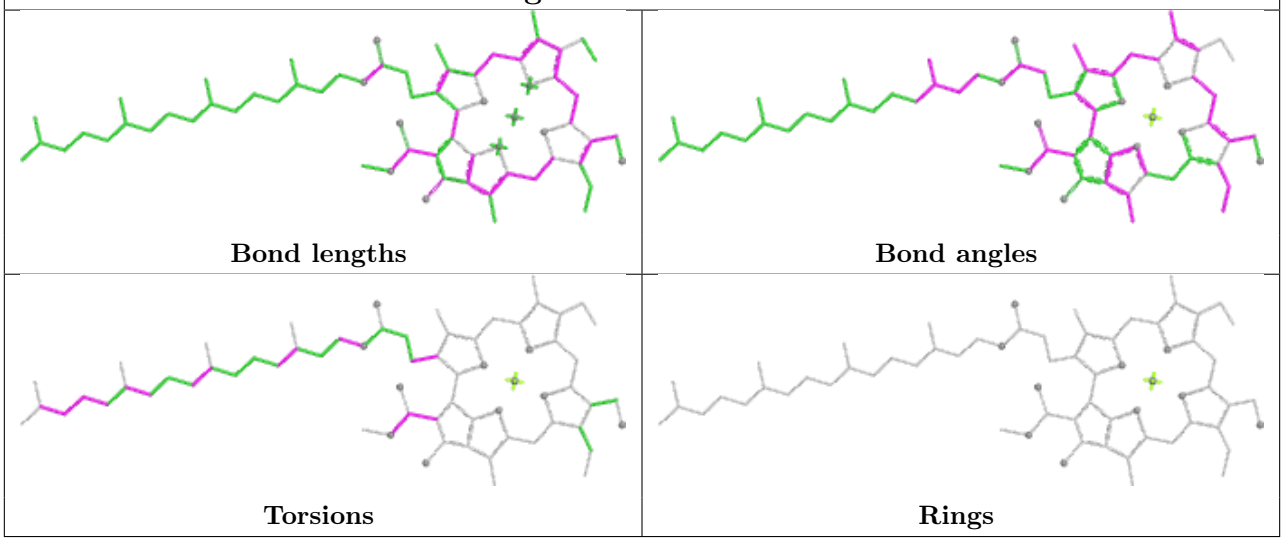

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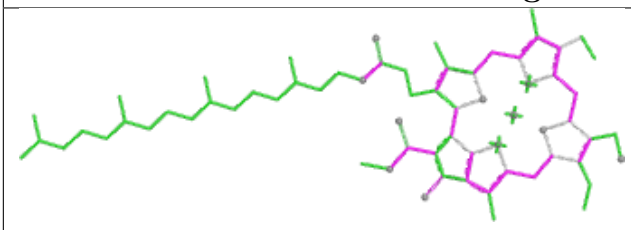
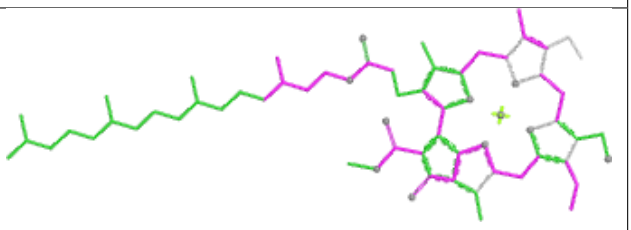
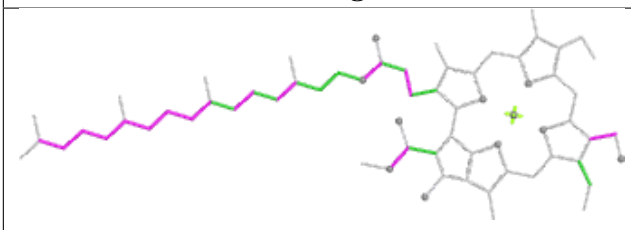


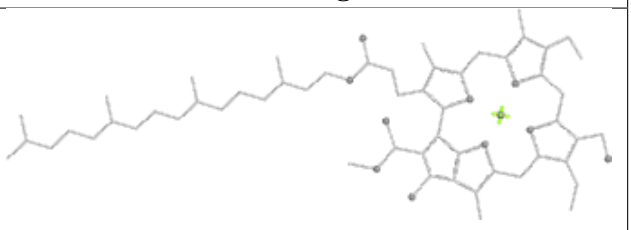
Bond lengths



Bond angles

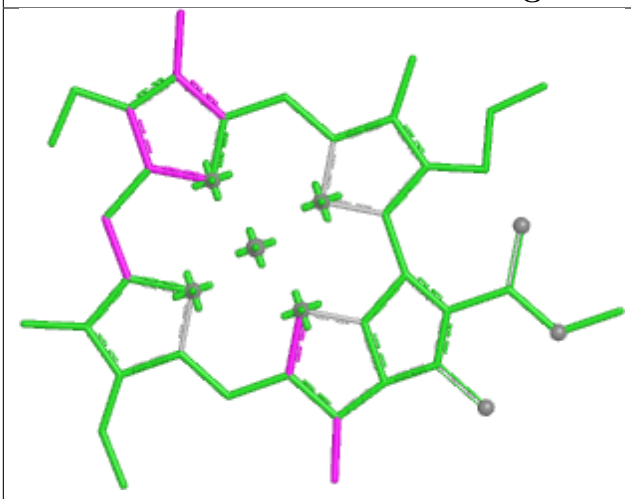


Torsions

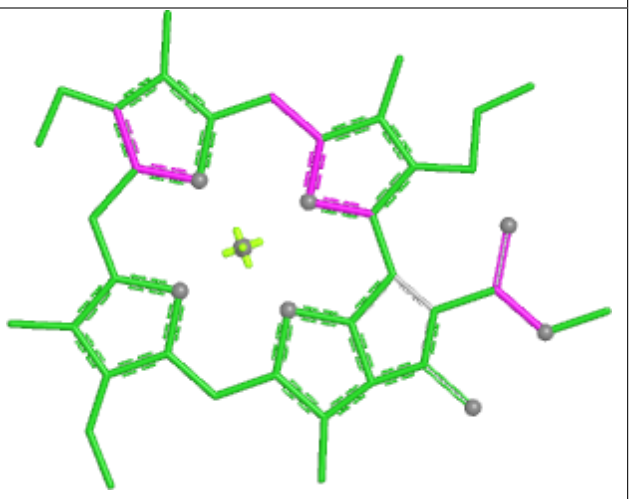


Rings

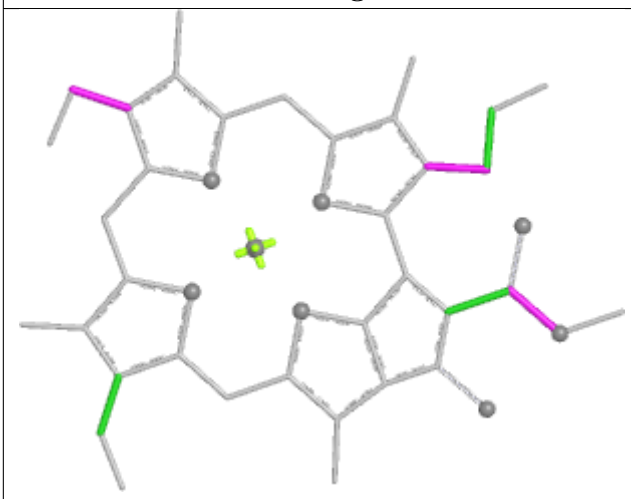
Ligand CLA Y 611



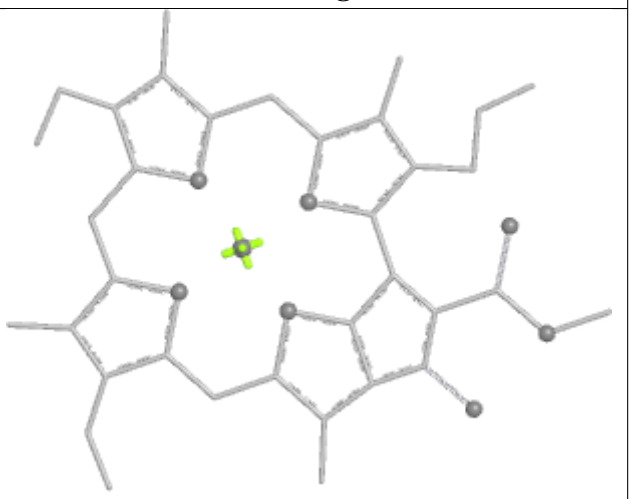
Bond lengths



Bond angles

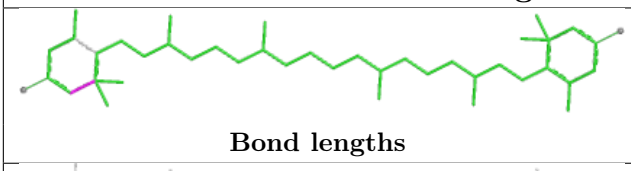


Torsions

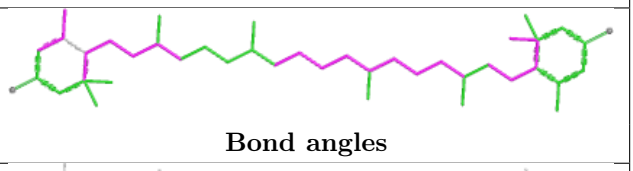


Rings

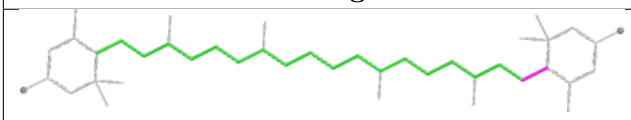
Ligand LUT X 1620



Bond lengths



Bond angles



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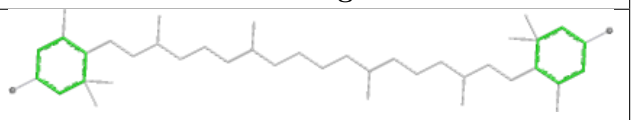
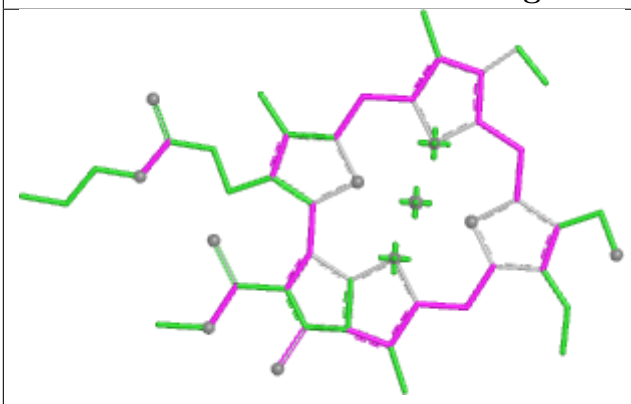
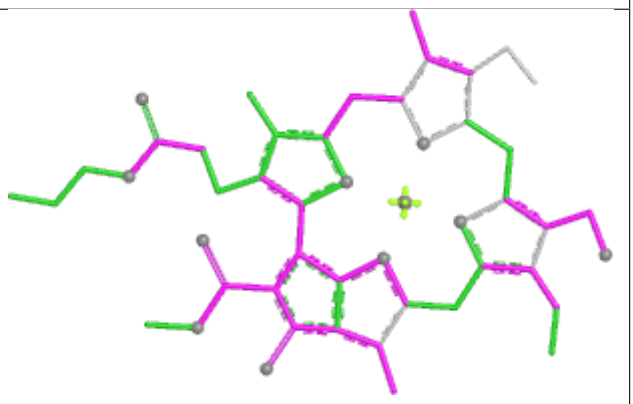


Rings

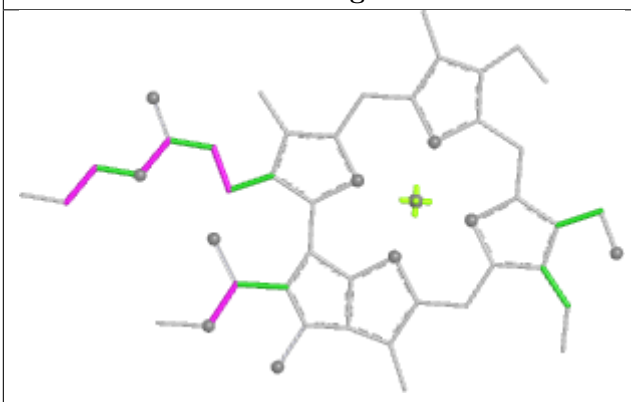
Ligand CHL Y 608



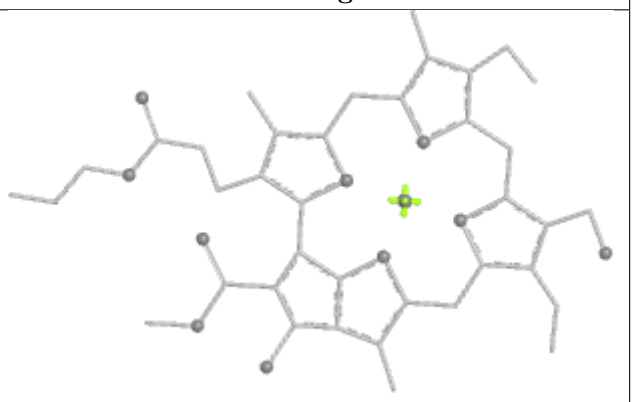
Bond lengths



Bond angles

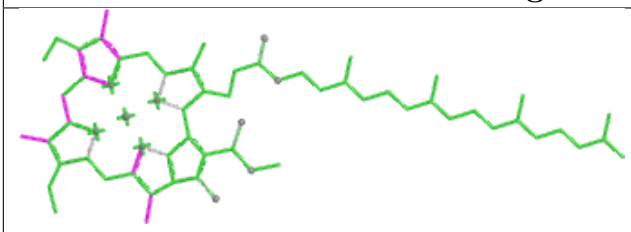


Torsions



Rings

Ligand CLA Z 613



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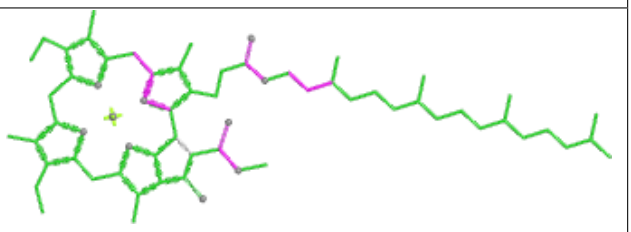
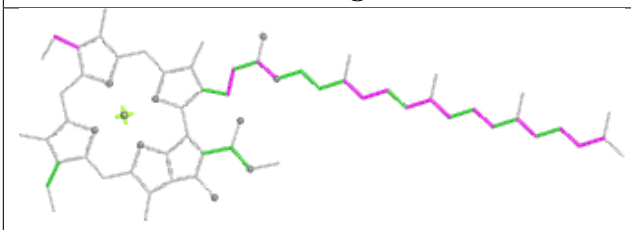
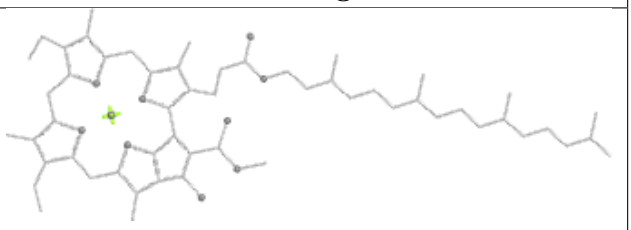


Bond angles

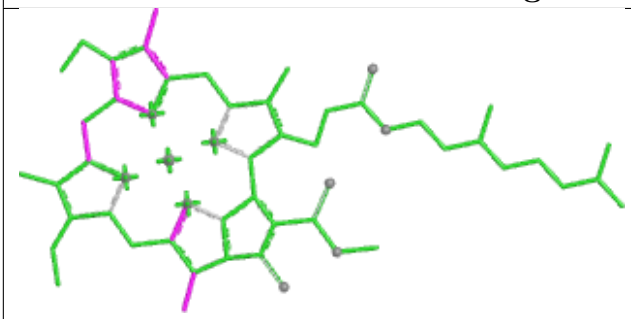


Torsions

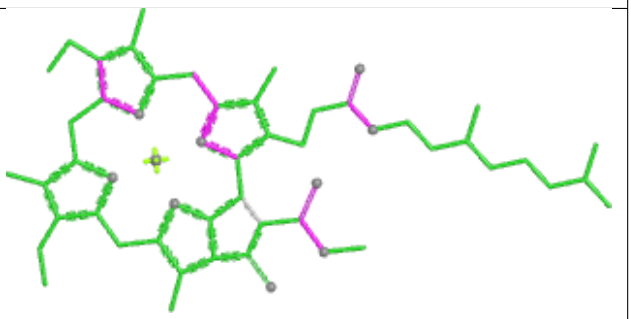


Rings

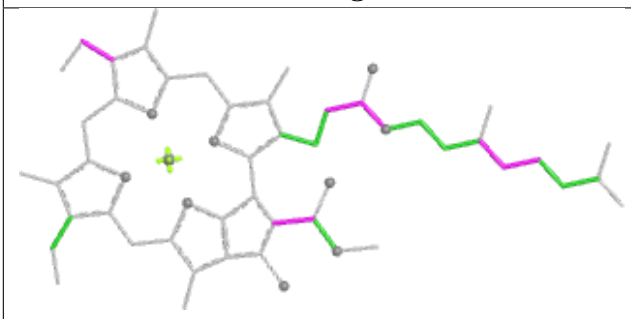
Ligand CLA Y 603



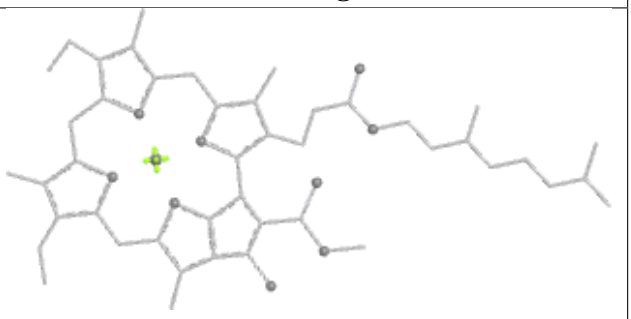
Bond lengths



Bond angles

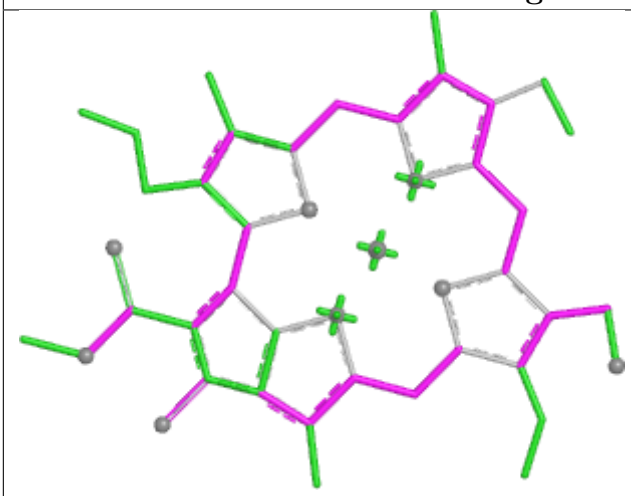


Torsions

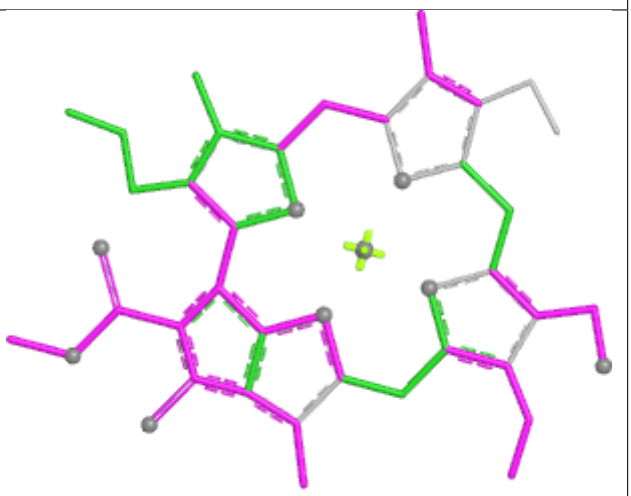


Rings

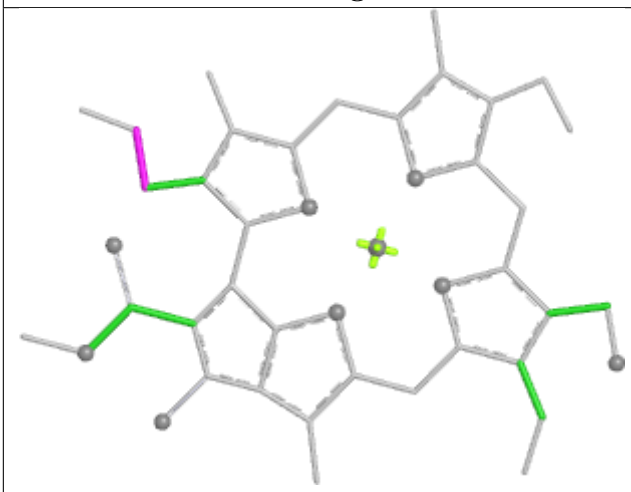
Ligand CHL Z 605



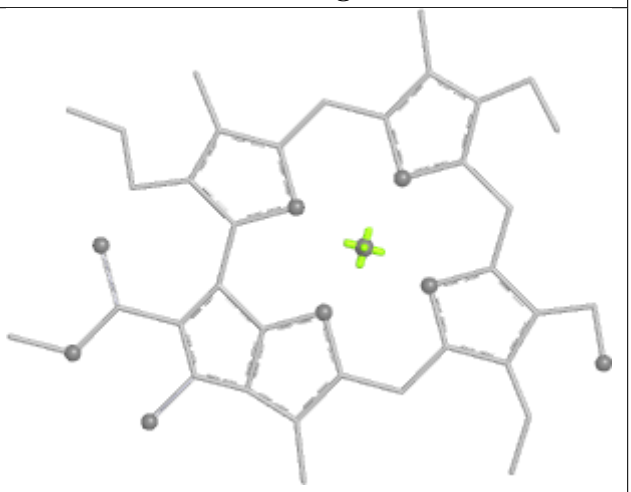
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

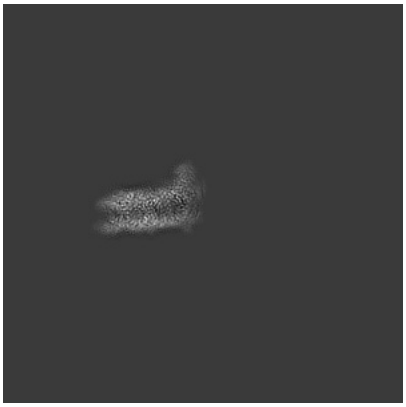
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30934. These allow visual inspection of the internal detail of the map and identification of artifacts.

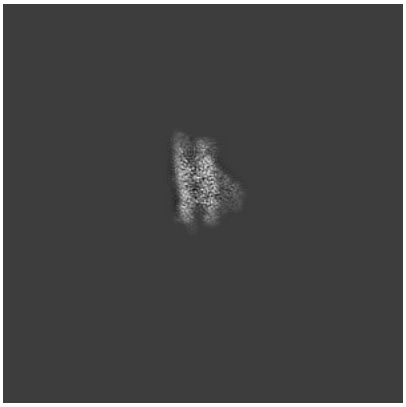
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

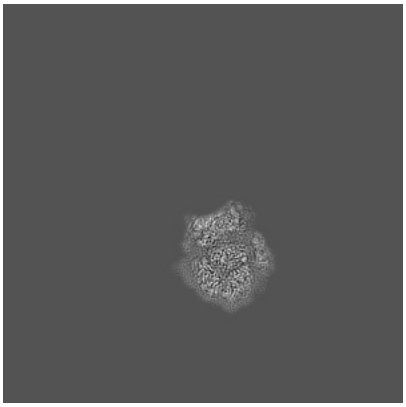
6.1.1 Primary map



X



Y

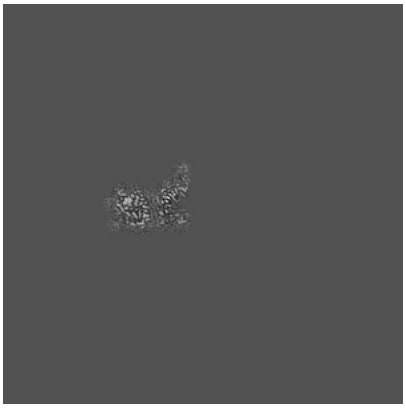


Z

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

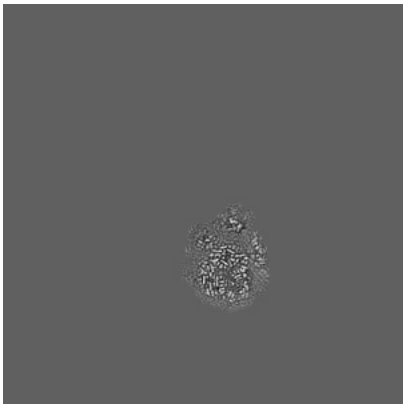
6.2 Central slices

6.2.1 Primary map



X Index: 240

Y Index: 240

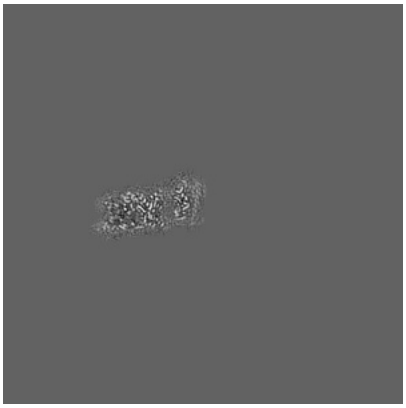


Z Index: 240

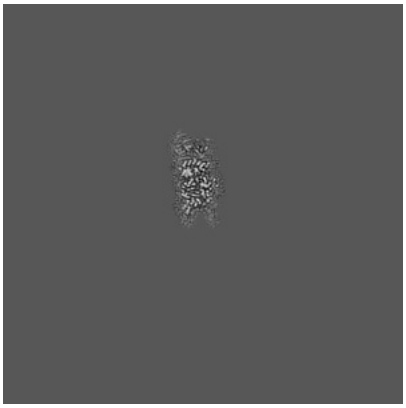
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

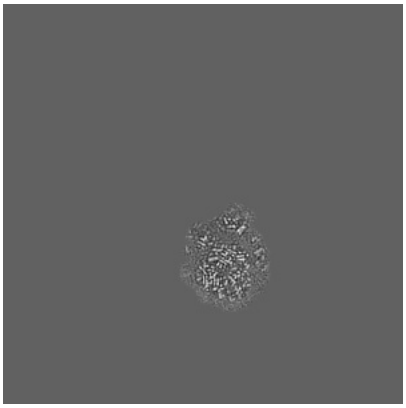
6.3.1 Primary map



X Index: 274



Y Index: 171

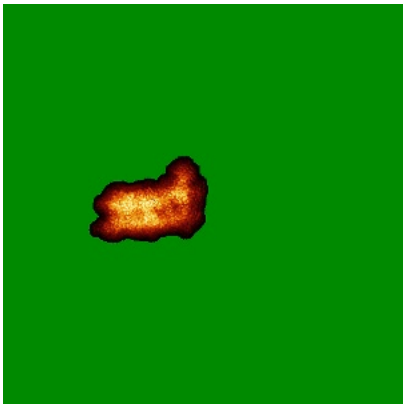


Z Index: 242

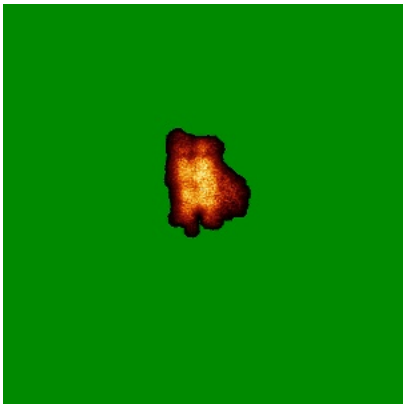
The images above show the largest variance slices of the map in three orthogonal directions.

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

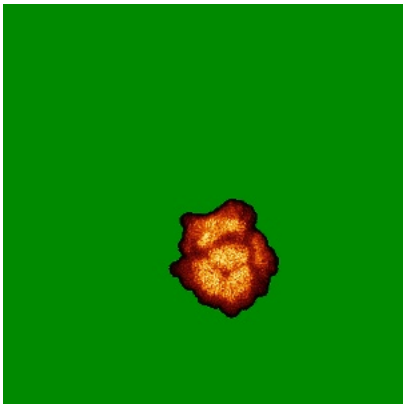
6.4.1 Primary map



X



Y



Z

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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

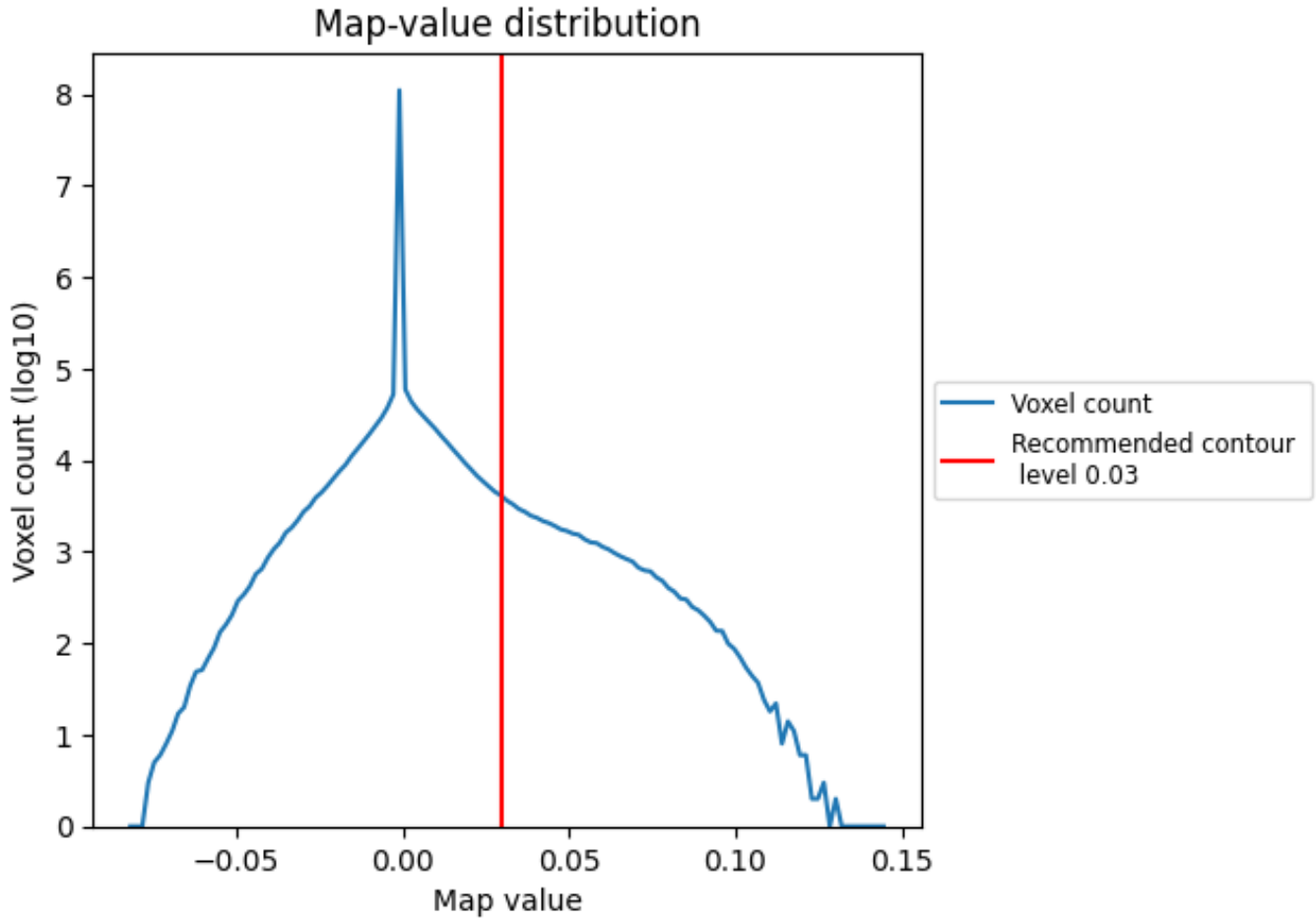
6.6 Mask visualisation (i)

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

7 Map analysis

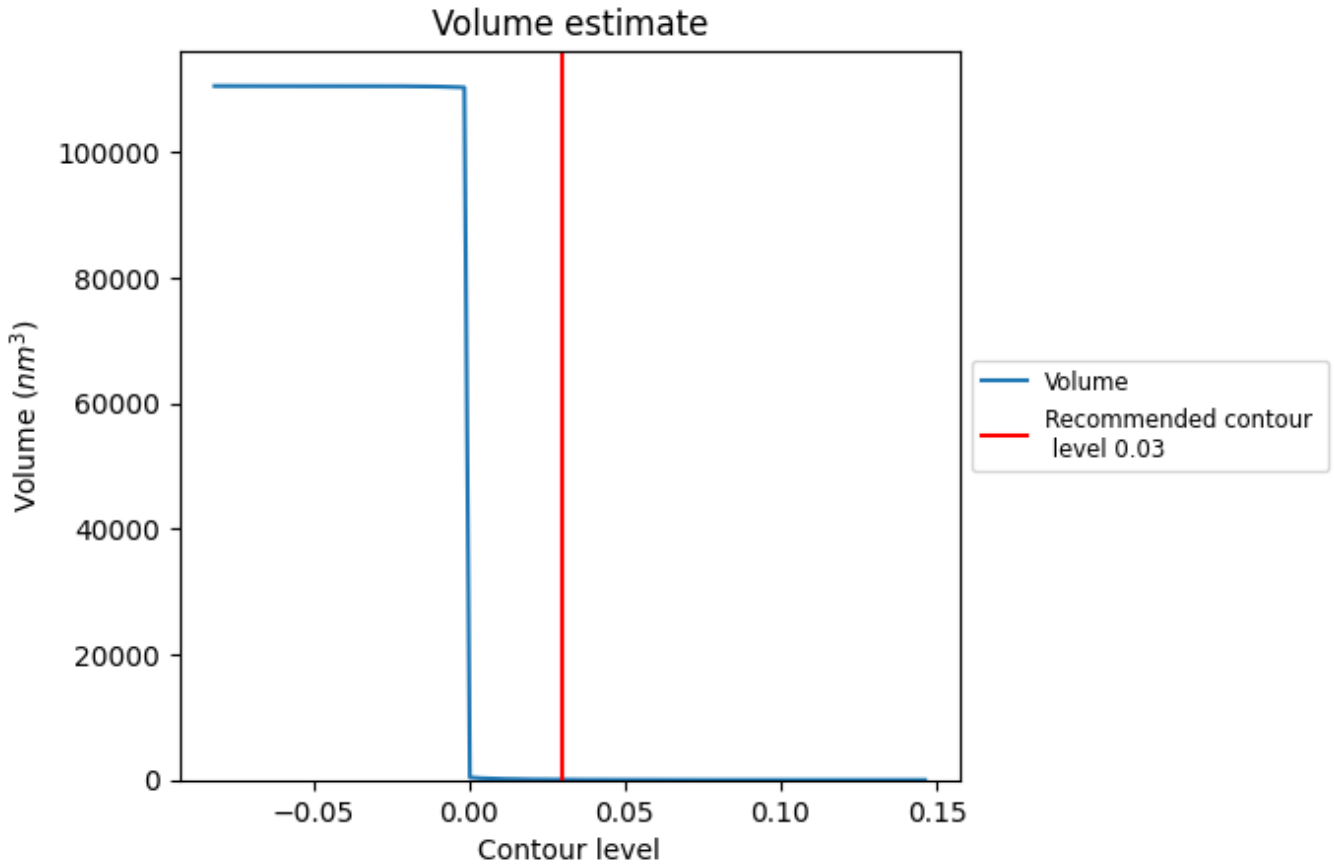
This section contains the results of statistical analysis of the map.

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.

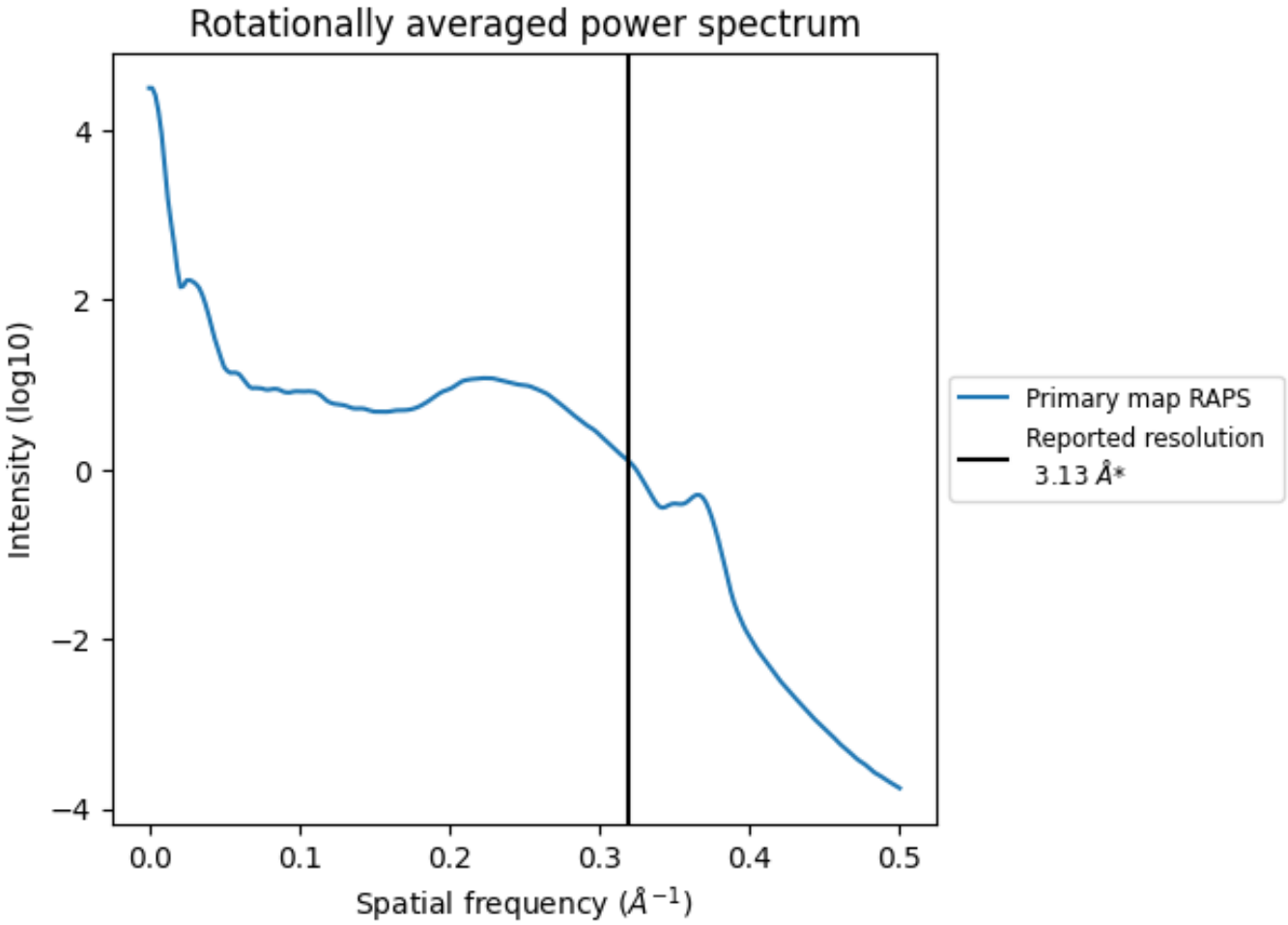
7.2 Volume estimate



The volume at the recommended contour level is 49 nm^3; this corresponds to an approximate mass of 44 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 0.319 Å^{-1}

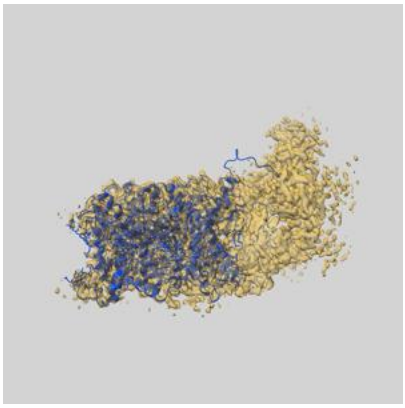
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

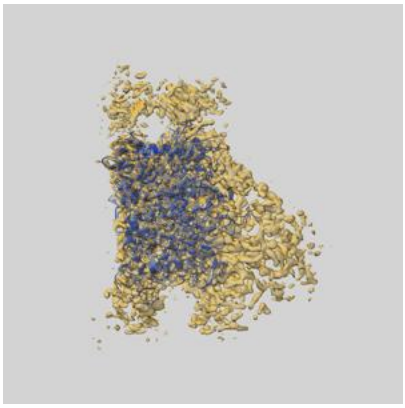
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30934 and PDB model 7E0J. Per-residue inclusion information can be found in section 3 on page 11.

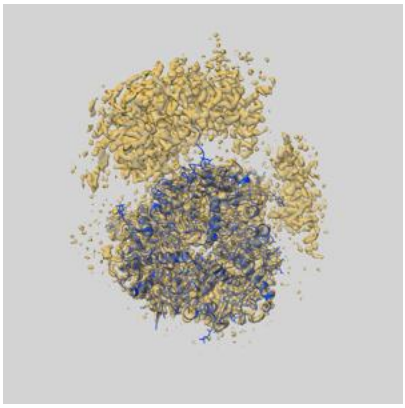
9.1 Map-model overlay



X



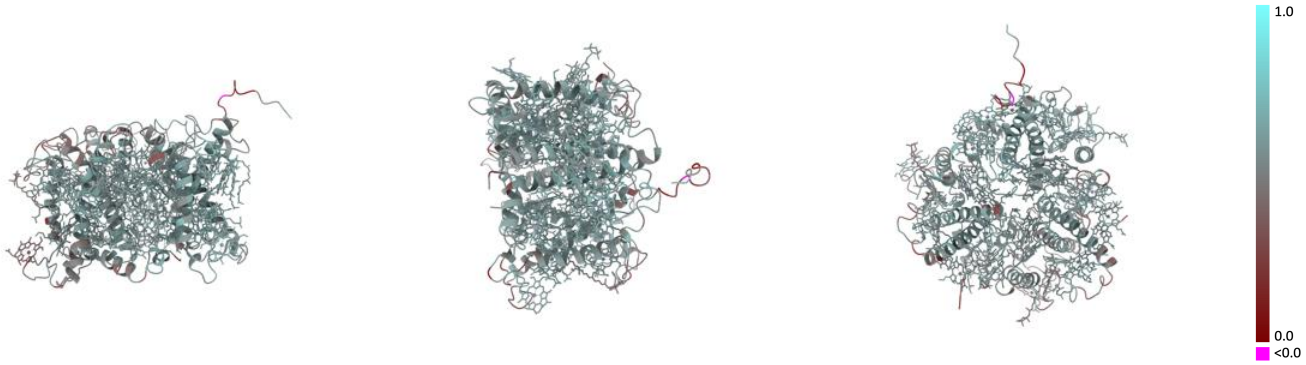
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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



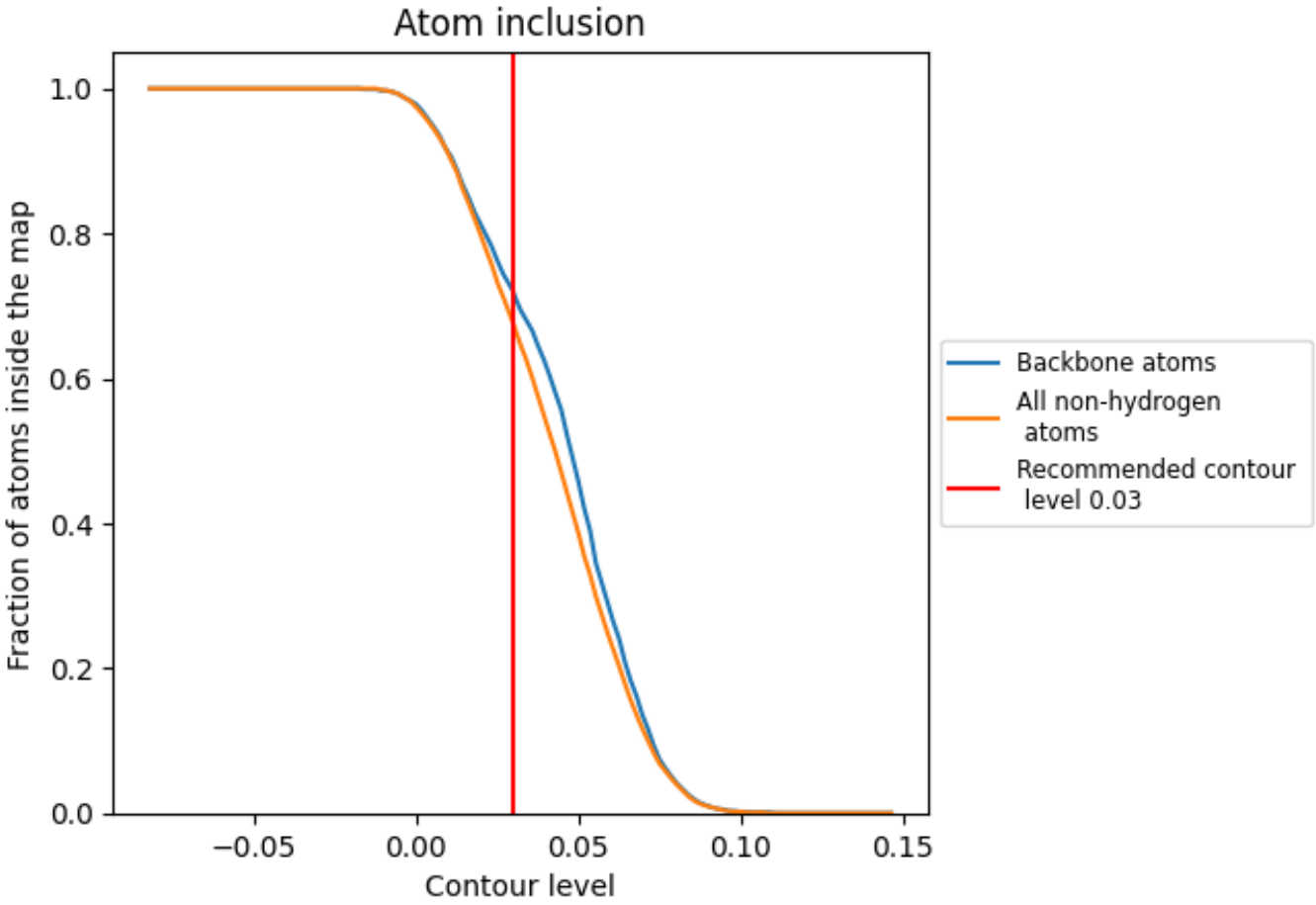
X Y Z

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

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 68% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6760	0.5440
X	0.6510	0.5290
Y	0.6790	0.5350
Z	0.6960	0.5660