Full wwPDB EM Validation Report ⓘ

Oct 26, 2021 – 06:23 am BST

PDB ID	:	7PIL
EMDB ID	:	EMD-13441
Title	:	Cryo-EM structure of the Rhodobacter sphaeroides RC-LH1-PufXY monomer complex at 2.5 A
Authors	:	Qian, P.; Hunter, C.N.
Deposited on	:	2021-08-20
Resolution	:	2.50 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 following versions of software and data (see references ⓘ) were used in the production of this report:

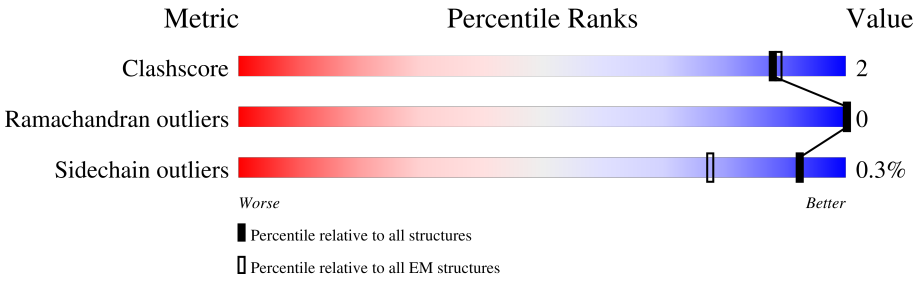
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	AA	55	82% · 16%
1	AB	55	98% ·
1	AC	55	96% ·
1	AD	55	93% 7%
1	AE	55	96% ·
1	AF	55	98% ·
1	AG	55	98% ·
1	AH	55	98% ·

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Mol	Chain	Length	Quality of chain
1	AI	55	96%
1	AJ	55	96%
1	AK	55	98%
1	AL	55	95% 5%
1	AM	55	5% 98%
1	AN	55	15% 91% 7%
2	BA	43	93% 7%
2	BB	43	95% 5%
2	BC	43	93% 5%
2	BD	43	95% 5%
2	BE	43	98%
2	BF	43	95% 5%
2	BG	43	100%
2	BH	43	98%
2	BI	43	5% 95% 5%
2	BJ	43	5% 100%
2	BK	43	12% 98%
2	BL	43	5% 100%
2	BM	43	16% 95% 5%
2	BN	43	26% 88% 12%
3	H	246	99%
4	L	281	98%
5	M	307	98%
6	UU	49	100%
7	X	55	98%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 22480 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 Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	46	Total	C	N	O	S	0	0
			392	271	60	58	3		
1	AB	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AC	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
1	AD	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AE	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AF	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AG	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AH	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AI	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AJ	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AK	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AL	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AM	55	Total	C	N	O	S	0	0
			461	313	74	71	3		
1	AN	51	Total	C	N	O	S	0	0
			432	296	69	65	2		

- Molecule 2 is a protein called Light-harvesting protein B-875 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BA	43	Total	C	N	O	S	0	0
			352	236	55	60	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BB	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BC	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
2	BD	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BE	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BF	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BG	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BH	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BI	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BJ	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BK	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BL	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BM	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
2	BN	38	Total	C	N	O	S	0	0
			317	213	50	53	1		

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	246	Total	C	N	O	S	0	0
			1867	1196	316	345	10		

- Molecule 4 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	281	Total	C	N	O	S	0	0
			2232	1507	355	362	8		

- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	307	Total	C	N	O	S	0	0
			2445	1630	400	404	11		

- Molecule 6 is a protein called RC-Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	UU	49	Total	C	N	O	S	0	0
			363	247	56	57	3		

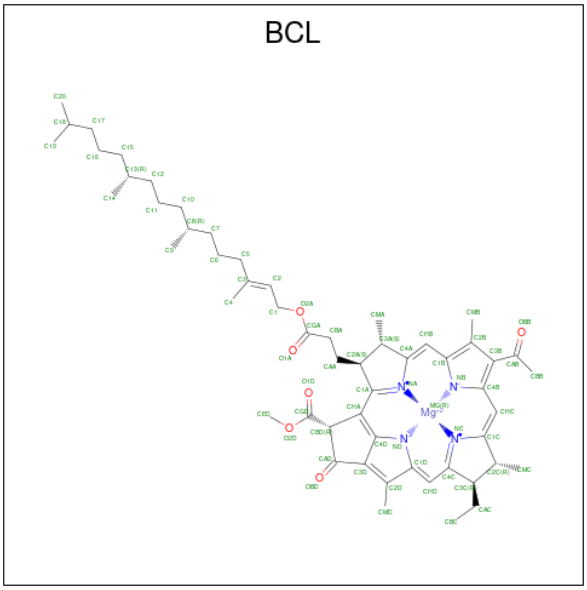
- Molecule 7 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	55	Total	C	N	O	S	0	0
			422	281	71	67	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	53	LEU	ARG	conflict	UNP P13402

- Molecule 8 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	AA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
8	AB	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	AC	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	AD	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	AE	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	AE	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	AF	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	AG	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	AH	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	AI	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	AJ	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	AK	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	AK	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	AL	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	AM	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	AM	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	AN	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	BA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	BB	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	BC	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	BD	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	BF	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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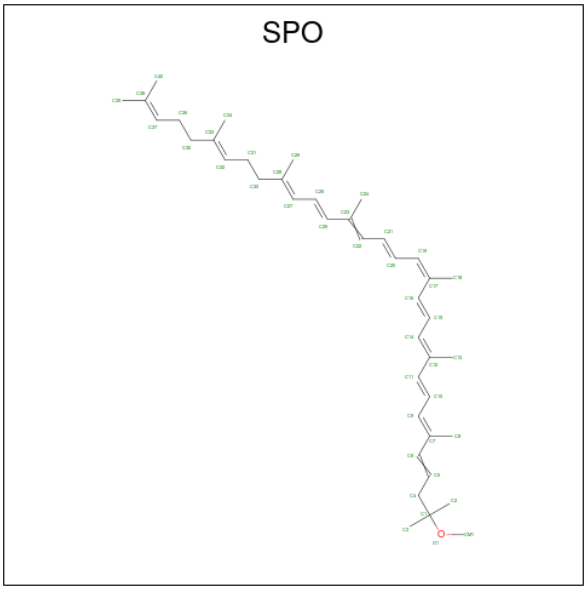
Mol	Chain	Residues	Atoms					AltConf
8	BG	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	BH	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	BI	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	BJ	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	BL	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	BN	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	L	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	L	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	M	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	M	1	Total	C	Mg	N	O	0
			132	110	2	8	12	

- Molecule 9 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms			AltConf
9	AA	1	Total	C	O	0
			42	41	1	

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Mol	Chain	Residues	Atoms	AltConf
9	AB	1	Total C O 42 41 1	0
9	AC	1	Total C O 84 82 2	0
9	AC	1	Total C O 84 82 2	0
9	AD	1	Total C O 84 82 2	0
9	AD	1	Total C O 84 82 2	0
9	AE	1	Total C O 42 41 1	0
9	AF	1	Total C O 84 82 2	0
9	AF	1	Total C O 84 82 2	0
9	AG	1	Total C O 84 82 2	0
9	AG	1	Total C O 84 82 2	0
9	AH	1	Total C O 84 82 2	0
9	AH	1	Total C O 84 82 2	0
9	AI	1	Total C O 84 82 2	0
9	AI	1	Total C O 84 82 2	0
9	AJ	1	Total C O 84 82 2	0
9	AJ	1	Total C O 84 82 2	0
9	AK	1	Total C O 84 82 2	0
9	AK	1	Total C O 84 82 2	0
9	AL	1	Total C O 42 41 1	0
9	AM	1	Total C O 84 82 2	0
9	AM	1	Total C O 84 82 2	0

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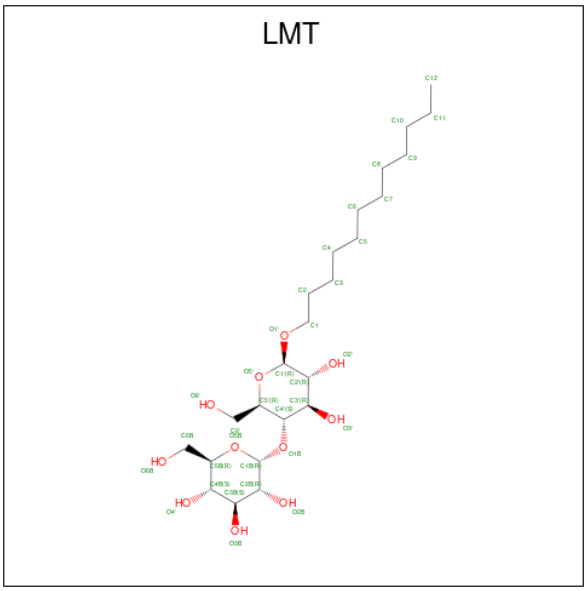
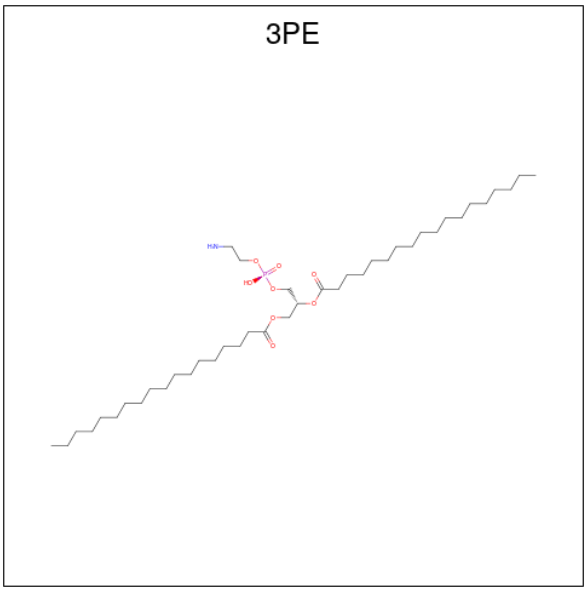
Mol	Chain	Residues	Atoms	AltConf
9	BA	1	Total C O 42 41 1	0
9	BE	1	Total C O 42 41 1	0
9	BL	1	Total C O 42 41 1	0
9	M	1	Total C O 42 41 1	0

- Molecule 10 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



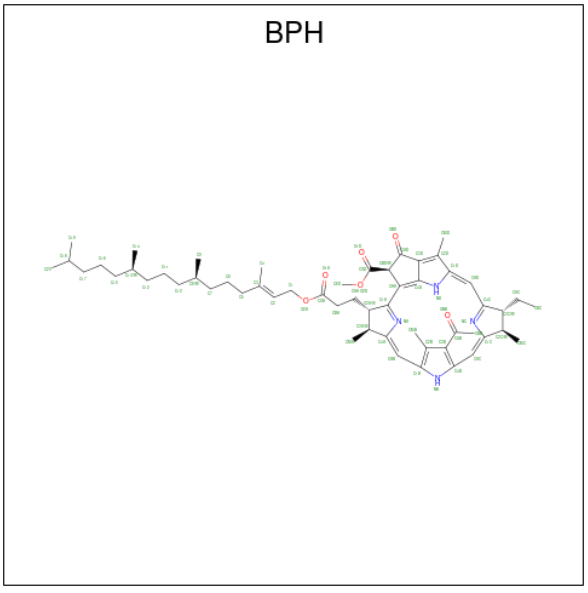
Mol	Chain	Residues	Atoms	AltConf
10	AA	1	Total C O 35 24 11	0
10	AB	1	Total C O 35 24 11	0
10	M	1	Total C O 35 24 11	0
10	X	1	Total C O 35 24 11	0

- Molecule 11 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



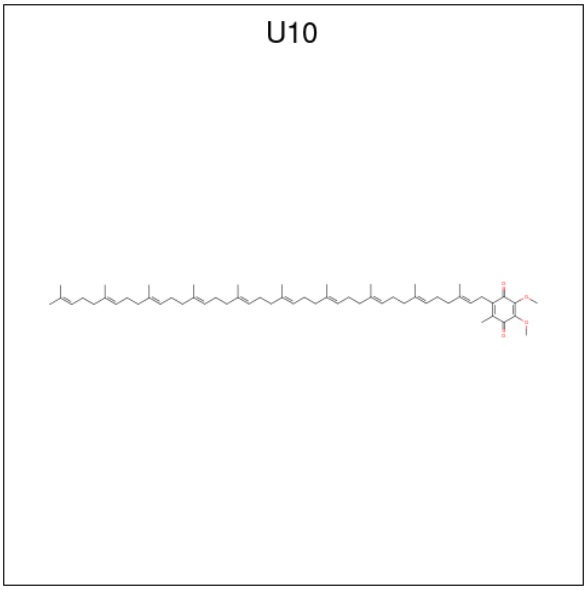
Mol	Chain	Residues	Atoms					AltConf
11	AB	1	Total	C	N	O	P	0
			51	41	1	8	1	
11	AC	1	Total	C	N	O	P	0
			51	41	1	8	1	
11	H	1	Total	C	N	O	P	0
			102	82	2	16	2	
11	H	1	Total	C	N	O	P	0
			102	82	2	16	2	

- Molecule 12 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



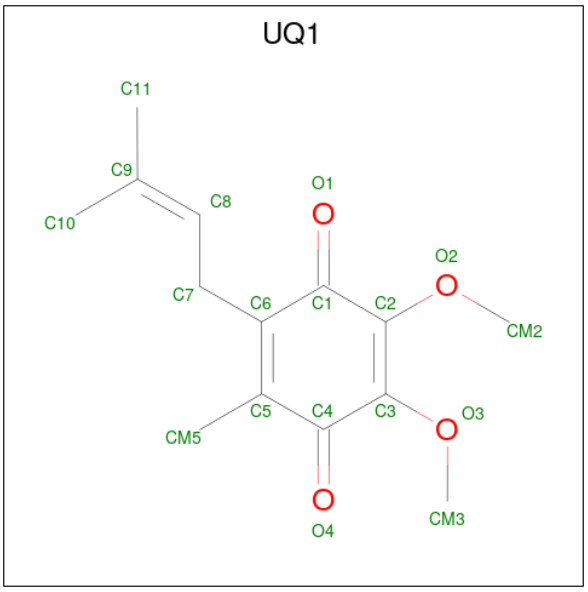
Mol	Chain	Residues	Atoms				AltConf
12	L	1	Total	C	N	O	0
			65	55	4	6	
12	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 13 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



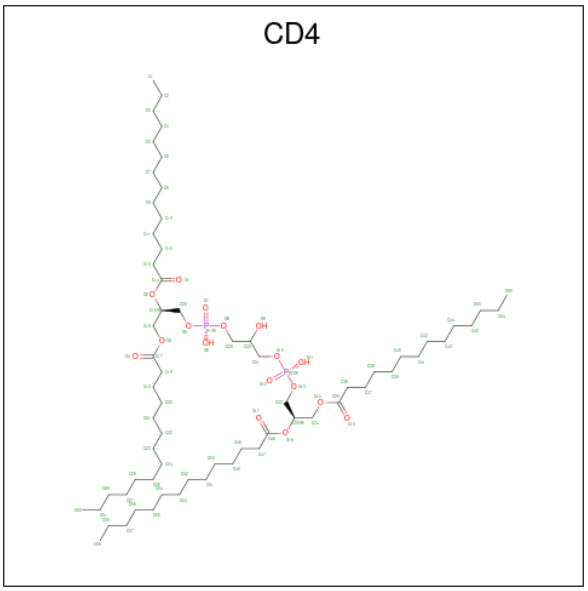
Mol	Chain	Residues	Atoms			AltConf
13	L	1	Total	C	O	0
			63	59	4	
13	M	1	Total	C	O	0
			63	59	4	

- Molecule 14 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
14	L	1	18	14	4	0

- Molecule 15 is (2R,5R,11R,14R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-2,14-bis(tetradecanoyloxy)-4,6,10,12,16-pentaoxa-5,11-diphosphatriacont-1-yl tetradecanoate (three-letter code: CD4) (formula: $C_{65}H_{126}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
15	M	1	84	65	17	2	0

- Molecule 16 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	AltConf
16	M	1	Total Fe 1 1	0

- Molecule 17 is water.

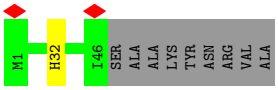
Mol	Chain	Residues	Atoms	AltConf
17	AB	1	Total O 1 1	0
17	H	2	Total O 2 2	0
17	X	1	Total O 1 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

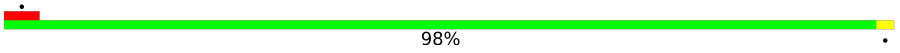
• Molecule 1: Light-harvesting protein B-875 alpha chain

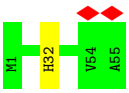
Chain AA:



• Molecule 1: Light-harvesting protein B-875 alpha chain

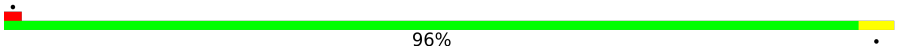
Chain AB:

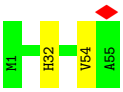




• Molecule 1: Light-harvesting protein B-875 alpha chain

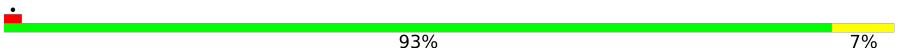
Chain AC:

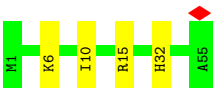




• Molecule 1: Light-harvesting protein B-875 alpha chain

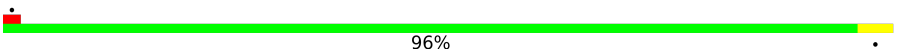
Chain AD:

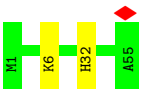




• Molecule 1: Light-harvesting protein B-875 alpha chain

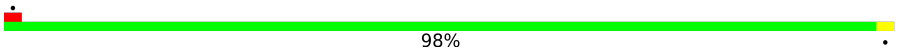
Chain AE:

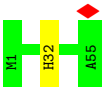




• Molecule 1: Light-harvesting protein B-875 alpha chain

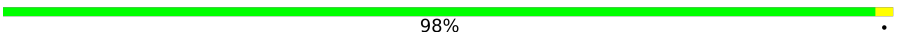
Chain AF:





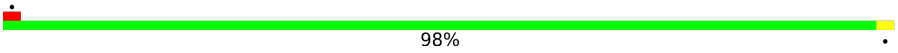
• Molecule 1: Light-harvesting protein B-875 alpha chain

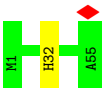
Chain AG:



• Molecule 1: Light-harvesting protein B-875 alpha chain

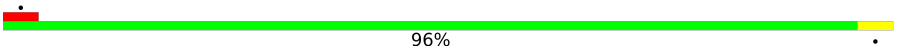
Chain AH:

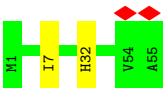




• Molecule 1: Light-harvesting protein B-875 alpha chain

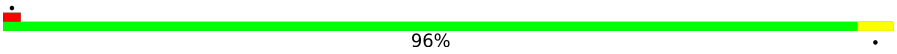
Chain AI:

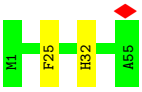




• Molecule 1: Light-harvesting protein B-875 alpha chain

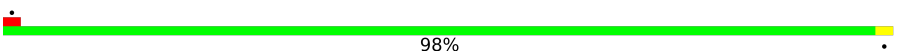
Chain AJ:

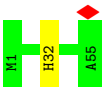




• Molecule 1: Light-harvesting protein B-875 alpha chain

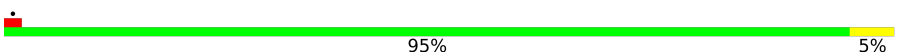
Chain AK:

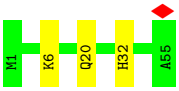




• Molecule 1: Light-harvesting protein B-875 alpha chain

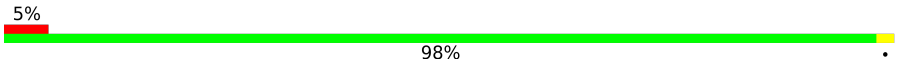
Chain AL:





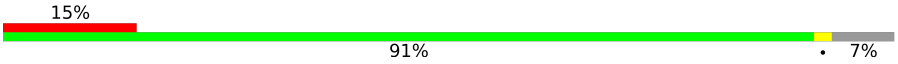
• Molecule 1: Light-harvesting protein B-875 alpha chain

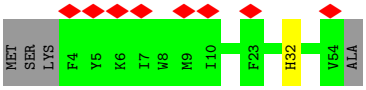
Chain AM:



• Molecule 1: Light-harvesting protein B-875 alpha chain

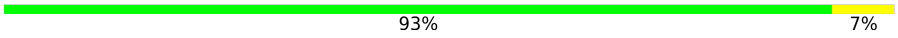
Chain AN:





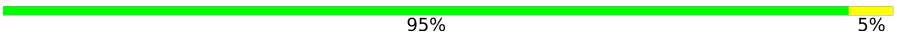
• Molecule 2: Light-harvesting protein B-875 beta chain

Chain BA:



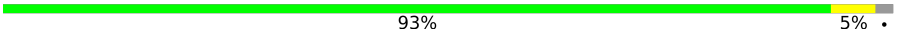
• Molecule 2: Light-harvesting protein B-875 beta chain

Chain BB:



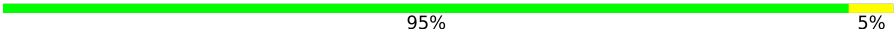
• Molecule 2: Light-harvesting protein B-875 beta chain

Chain BC:



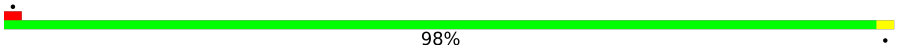
• Molecule 2: Light-harvesting protein B-875 beta chain

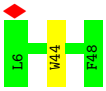
Chain BD:



• Molecule 2: Light-harvesting protein B-875 beta chain

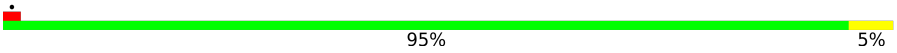
Chain BE:

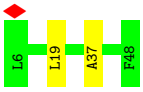




• Molecule 2: Light-harvesting protein B-875 beta chain

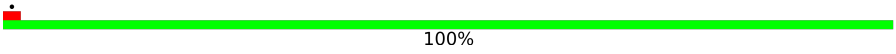
Chain BF:





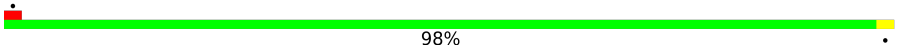
• Molecule 2: Light-harvesting protein B-875 beta chain

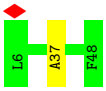
Chain BG:



• Molecule 2: Light-harvesting protein B-875 beta chain

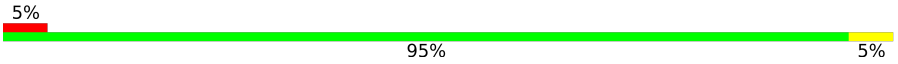
Chain BH:

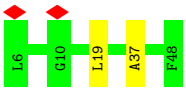




• Molecule 2: Light-harvesting protein B-875 beta chain

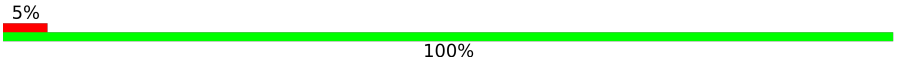
Chain BI:





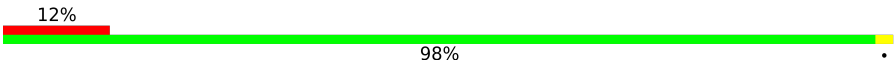
• Molecule 2: Light-harvesting protein B-875 beta chain

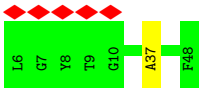
Chain BJ:



• Molecule 2: Light-harvesting protein B-875 beta chain

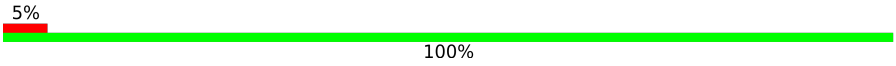
Chain BK:





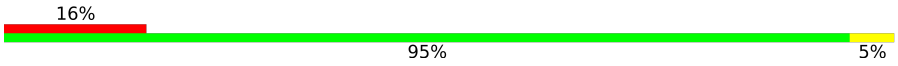
• Molecule 2: Light-harvesting protein B-875 beta chain

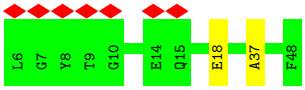
Chain BL:



• Molecule 2: Light-harvesting protein B-875 beta chain

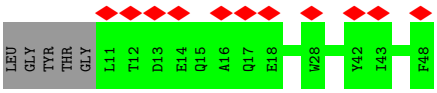
Chain BM:





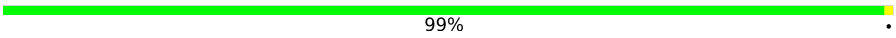
• Molecule 2: Light-harvesting protein B-875 beta chain

Chain BN:



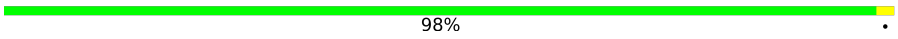
• Molecule 3: Reaction center protein H chain

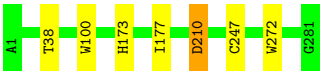
Chain H:



• Molecule 4: Reaction center protein L chain

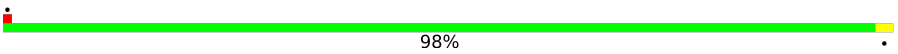
Chain L:





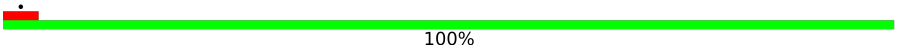
• Molecule 5: Reaction center protein M chain

Chain M:



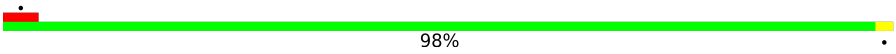
• Molecule 6: RC-Y

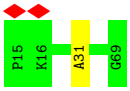
Chain UU:



• Molecule 7: Intrinsic membrane protein PufX

Chain X:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	250613	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44.94	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.172	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0187	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CD4, BCL, LMT, UQ1, BPH, 3PE, U10, FE, SPO

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	AA	0.26	0/405	0.49	0/549
1	AB	0.27	0/475	0.50	0/642
1	AC	0.28	0/474	0.51	0/642
1	AD	0.26	0/475	0.48	0/642
1	AE	0.27	0/475	0.52	0/642
1	AF	0.27	0/475	0.52	0/642
1	AG	0.27	0/475	0.52	0/642
1	AH	0.26	0/475	0.53	0/642
1	AI	0.27	0/475	0.51	0/642
1	AJ	0.27	0/475	0.51	0/642
1	AK	0.26	0/475	0.53	0/642
1	AL	0.26	0/475	0.51	0/642
1	AM	0.28	0/475	0.53	0/642
1	AN	0.27	0/446	0.48	0/606
2	BA	0.23	0/365	0.45	0/499
2	BB	0.26	0/365	0.48	0/499
2	BC	0.24	0/357	0.44	0/488
2	BD	0.24	0/365	0.43	0/499
2	BE	0.24	0/365	0.46	0/499
2	BF	0.25	0/365	0.48	0/499
2	BG	0.24	0/365	0.45	0/499
2	BH	0.24	0/365	0.47	0/499
2	BI	0.24	0/365	0.47	0/499
2	BJ	0.23	0/365	0.45	0/499
2	BK	0.24	0/365	0.50	0/499
2	BL	0.25	0/365	0.48	0/499
2	BM	0.24	0/365	0.45	0/499
2	BN	0.24	0/329	0.45	0/450
3	H	0.25	0/1917	0.53	0/2609
4	L	0.25	0/2320	0.49	0/3175
5	M	0.25	0/2538	0.50	0/3464
6	UU	0.27	0/374	0.44	0/505

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
7	X	0.26	0/434	0.46	0/586
All	All	0.25	0/19199	0.49	0/26124

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AD	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AD	15	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	392	0	412	1	0
1	AB	461	0	482	1	0
1	AC	460	0	482	3	0
1	AD	461	0	482	3	0
1	AE	461	0	482	2	0
1	AF	461	0	482	1	0
1	AG	461	0	482	1	0
1	AH	461	0	482	1	0
1	AI	461	0	482	2	0
1	AJ	461	0	482	2	0
1	AK	461	0	482	1	0
1	AL	461	0	482	4	0
1	AM	461	0	482	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AN	432	0	447	2	0
2	BA	352	0	336	3	0
2	BB	352	0	336	2	0
2	BC	344	0	325	2	0
2	BD	352	0	336	2	0
2	BE	352	0	336	1	0
2	BF	352	0	336	2	0
2	BG	352	0	336	0	0
2	BH	352	0	336	1	0
2	BI	352	0	336	2	0
2	BJ	352	0	336	0	0
2	BK	352	0	336	1	0
2	BL	352	0	336	0	0
2	BM	352	0	336	2	0
2	BN	317	0	303	0	0
3	H	1867	0	1864	2	0
4	L	2232	0	2187	3	0
5	M	2445	0	2359	4	0
6	UU	363	0	358	0	0
7	X	422	0	436	1	0
8	AA	66	0	74	1	0
8	AB	66	0	74	3	0
8	AC	66	0	74	2	0
8	AD	66	0	74	0	0
8	AE	132	0	148	3	0
8	AF	66	0	74	1	0
8	AG	66	0	74	1	0
8	AH	66	0	74	0	0
8	AI	66	0	74	2	0
8	AJ	66	0	74	4	0
8	AK	132	0	148	1	0
8	AL	66	0	74	0	0
8	AM	132	0	148	3	0
8	AN	66	0	74	1	0
8	BA	66	0	74	1	0
8	BB	66	0	74	1	0
8	BC	66	0	74	2	0
8	BD	66	0	74	1	0
8	BF	66	0	74	1	0
8	BG	66	0	74	1	0
8	BH	66	0	74	1	0
8	BI	66	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	BJ	66	0	74	1	0
8	BL	66	0	74	1	0
8	BN	66	0	74	1	0
8	L	132	0	148	1	0
8	M	132	0	148	0	0
9	AA	42	0	60	3	0
9	AB	42	0	60	3	0
9	AC	84	0	120	2	0
9	AD	84	0	120	3	0
9	AE	42	0	60	3	0
9	AF	84	0	120	6	0
9	AG	84	0	120	0	0
9	AH	84	0	120	3	0
9	AI	84	0	120	5	0
9	AJ	84	0	120	3	0
9	AK	84	0	120	2	0
9	AL	42	0	60	3	0
9	AM	84	0	120	5	0
9	BA	42	0	60	3	0
9	BE	42	0	60	2	0
9	BL	42	0	60	0	0
9	M	42	0	60	1	0
10	AA	35	0	45	0	0
10	AB	35	0	45	0	0
10	M	35	0	46	0	0
10	X	35	0	46	0	0
11	AB	51	0	82	0	0
11	AC	51	0	82	0	0
11	H	102	0	164	1	0
12	L	65	0	76	0	0
12	M	65	0	76	1	0
13	L	63	0	90	1	0
13	M	63	0	90	1	0
14	L	18	0	18	1	0
15	M	84	0	124	1	0
16	M	1	0	0	0	0
17	AB	1	0	0	0	0
17	H	2	0	0	0	0
17	X	1	0	0	0	0
All	All	22480	0	23419	86	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 2.

All (86) 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)
9:AI:102:SPO:H132	8:AJ:101:BCL:H42	1.70	0.73
2:BD:48:PHE:HB3	9:BE:1000:SPO:H343	1.72	0.72
1:AC:54:VAL:O	1:AC:54:VAL:HG23	1.97	0.64
2:BE:44:TRP:CD1	9:BE:1000:SPO:H342	2.32	0.64
13:M:404:U10:H371	13:M:404:U10:H502	1.80	0.63
1:AA:32:HIS:CE1	8:BA:102:BCL:HMD1	2.33	0.63
1:AD:6:LYS:HB3	9:AE:102:SPO:H402	1.81	0.63
1:AC:32:HIS:CE1	8:BC:101:BCL:HMD1	2.35	0.61
1:AD:32:HIS:CE1	8:BD:101:BCL:HMD1	2.35	0.61
1:AL:32:HIS:CE1	8:BL:102:BCL:HMD1	2.36	0.61
1:AK:32:HIS:CE1	8:AK:103:BCL:HMD1	2.37	0.59
1:AB:32:HIS:CE1	8:BB:1001:BCL:HMD1	2.38	0.59
9:AE:102:SPO:H6	8:AF:102:BCL:HMB2	1.86	0.57
9:AH:101:SPO:H132	8:AI:101:BCL:H42	1.86	0.57
9:AB:103:SPO:H242	2:BB:37:ALA:HB1	1.87	0.57
1:AM:32:HIS:CE1	8:AM:1003:BCL:HMD1	2.40	0.57
1:AF:32:HIS:CE1	8:BF:101:BCL:HMD1	2.40	0.57
9:AI:102:SPO:H402	2:BI:19:LEU:HA	1.87	0.56
1:AE:32:HIS:CE1	8:AE:103:BCL:HMD1	2.41	0.56
1:AJ:32:HIS:CE1	8:BJ:101:BCL:HMD1	2.41	0.56
9:AL:1002:SPO:H6	8:AM:1001:BCL:HMB2	1.86	0.56
8:AA:1001:BCL:H41	7:X:31:ALA:HB2	1.87	0.56
4:L:38:THR:HG21	4:L:100:TRP:HE3	1.71	0.55
1:AL:6:LYS:HB3	9:AM:1002:SPO:H402	1.89	0.54
9:AF:101:SPO:H6	8:AG:102:BCL:HMB2	1.90	0.54
1:AH:32:HIS:CE1	8:BH:101:BCL:HMD1	2.43	0.53
9:AD:103:SPO:H242	2:BD:37:ALA:HB1	1.92	0.52
8:AB:101:BCL:H72	8:AB:101:BCL:H41	1.92	0.51
8:AB:101:BCL:HED2	9:AB:103:SPO:H16	1.91	0.51
9:AH:103:SPO:H242	2:BH:37:ALA:HB1	1.92	0.51
9:AF:103:SPO:H242	2:BF:37:ALA:HB1	1.92	0.50
1:AI:32:HIS:CE1	8:BI:101:BCL:HMD1	2.47	0.50
1:AJ:25:PHE:HB2	8:AJ:101:BCL:H43	1.95	0.49
9:AA:1002:SPO:H402	2:BB:19:LEU:HA	1.94	0.49
5:M:157:TRP:CE2	9:M:407:SPO:H293	2.48	0.49
1:AE:6:LYS:HD3	9:AF:101:SPO:H393	1.95	0.48
1:AG:32:HIS:CE1	8:BG:101:BCL:HMD1	2.48	0.48
9:AK:104:SPO:H242	2:BK:37:ALA:HB1	1.95	0.48
1:AN:32:HIS:CE1	8:BN:101:BCL:HMD1	2.49	0.48
13:L:302:U10:H402	13:L:302:U10:H33	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AH:101:SPO:H6	8:AI:101:BCL:HMB2	1.97	0.47
5:M:229:PHE:HB2	5:M:244:ALA:HB2	1.96	0.47
9:AI:103:SPO:H242	2:BI:37:ALA:HB1	1.96	0.47
9:AD:101:SPO:H6	8:AE:101:BCL:HMB2	1.97	0.46
2:BA:27:LEU:HD13	9:BA:101:SPO:C20	2.45	0.46
9:AJ:103:SPO:H341	9:AJ:103:SPO:C37	2.46	0.46
3:H:40:TYR:CE2	11:H:302:3PE:H112	2.51	0.46
9:AM:1004:SPO:H242	2:BM:37:ALA:HB1	1.98	0.45
5:M:202:HIS:CE1	5:M:206:ILE:HD11	2.51	0.45
4:L:173:HIS:CE1	4:L:177:ILE:HD11	2.51	0.45
9:AI:102:SPO:H6	8:AJ:101:BCL:HMB2	1.99	0.44
9:AA:1002:SPO:H6	8:AC:102:BCL:HMB2	2.00	0.43
9:BA:101:SPO:H291	9:BA:101:SPO:H311	1.66	0.43
5:M:145:HIS:CD2	15:M:405:CD4:H30	2.53	0.43
9:AC:103:SPO:H26	9:AC:103:SPO:H241	1.90	0.43
9:AD:103:SPO:H341	9:AD:103:SPO:C37	2.48	0.43
9:AA:1002:SPO:H393	2:BA:6:LEU:HD23	2.00	0.43
9:AF:103:SPO:H26	9:AF:103:SPO:H241	1.90	0.43
9:AF:101:SPO:H26	9:AF:101:SPO:H241	1.89	0.43
1:AI:7:ILE:HB	9:AJ:102:SPO:H343	2.01	0.42
1:AC:54:VAL:O	1:AC:54:VAL:CG2	2.67	0.42
9:AC:103:SPO:H242	2:BC:37:ALA:HB1	2.00	0.42
2:BA:26:GLY:HA3	9:BA:101:SPO:C27	2.50	0.42
1:AL:6:LYS:NZ	2:BM:18:GLU:OE2	2.40	0.42
9:AL:1002:SPO:H26	9:AL:1002:SPO:H241	1.93	0.42
9:AM:1002:SPO:H6	8:AN:101:BCL:HMB2	2.02	0.42
2:BC:41:VAL:HG11	8:BC:101:BCL:HBC1	2.02	0.42
8:AB:101:BCL:OBB	8:AB:101:BCL:HHC	2.19	0.41
9:AI:102:SPO:H341	9:AI:102:SPO:H361	1.83	0.41
1:AL:20:GLN:HE21	9:AL:1002:SPO:C20	2.33	0.41
8:AC:102:BCL:OBB	8:AC:102:BCL:HHC	2.21	0.41
1:AD:10:ILE:HD11	9:AE:102:SPO:H403	2.03	0.41
9:AJ:102:SPO:H241	9:AJ:102:SPO:H26	1.84	0.41
9:AM:1002:SPO:H41	1:AN:32:HIS:CG	2.56	0.41
8:AJ:101:BCL:H61	8:AJ:101:BCL:H41	1.93	0.41
12:M:402:BPH:HHD	12:M:402:BPH:HBC3	2.03	0.41
9:AM:1004:SPO:H26	9:AM:1004:SPO:H241	1.90	0.41
3:H:157:ASP:OD1	3:H:157:ASP:N	2.54	0.41
8:L:305:BCL:HBB2	8:L:305:BCL:HMB1	2.03	0.40
9:AF:101:SPO:H403	2:BF:19:LEU:HD12	2.02	0.40
9:AB:103:SPO:H26	9:AB:103:SPO:H241	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AK:104:SPO:H26	9:AK:104:SPO:H241	1.84	0.40
8:AM:1001:BCL:HHC	8:AM:1001:BCL:OBB	2.21	0.40
8:AE:101:BCL:OBB	8:AE:101:BCL:HHC	2.22	0.40
4:L:210:ASP:OD1	4:L:210:ASP:N	2.54	0.40
14:L:303:UQ1:HM51	14:L:303:UQ1:H71	1.81	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	AA	44/55 (80%)	43 (98%)	1 (2%)	0	100	100
1	AB	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AC	53/55 (96%)	53 (100%)	0	0	100	100
1	AD	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AE	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AF	53/55 (96%)	53 (100%)	0	0	100	100
1	AG	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AH	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AI	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
1	AJ	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AK	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
1	AL	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AM	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AN	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
2	BA	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
2	BB	41/43 (95%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BC	40/43 (93%)	40 (100%)	0	0	100	100
2	BD	41/43 (95%)	41 (100%)	0	0	100	100
2	BE	41/43 (95%)	41 (100%)	0	0	100	100
2	BF	41/43 (95%)	41 (100%)	0	0	100	100
2	BG	41/43 (95%)	41 (100%)	0	0	100	100
2	BH	41/43 (95%)	41 (100%)	0	0	100	100
2	BI	41/43 (95%)	41 (100%)	0	0	100	100
2	BJ	41/43 (95%)	41 (100%)	0	0	100	100
2	BK	41/43 (95%)	41 (100%)	0	0	100	100
2	BL	41/43 (95%)	41 (100%)	0	0	100	100
2	BM	41/43 (95%)	41 (100%)	0	0	100	100
2	BN	36/43 (84%)	35 (97%)	1 (3%)	0	100	100
3	H	244/246 (99%)	240 (98%)	4 (2%)	0	100	100
4	L	279/281 (99%)	273 (98%)	6 (2%)	0	100	100
5	M	305/307 (99%)	297 (97%)	8 (3%)	0	100	100
6	UU	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
7	X	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
All	All	2225/2310 (96%)	2188 (98%)	37 (2%)	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	AA	43/49 (88%)	43 (100%)	0	100	100
1	AB	49/49 (100%)	49 (100%)	0	100	100
1	AC	49/49 (100%)	49 (100%)	0	100	100
1	AD	49/49 (100%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AE	49/49 (100%)	49 (100%)	0	100	100
1	AF	49/49 (100%)	49 (100%)	0	100	100
1	AG	49/49 (100%)	49 (100%)	0	100	100
1	AH	49/49 (100%)	49 (100%)	0	100	100
1	AI	49/49 (100%)	49 (100%)	0	100	100
1	AJ	49/49 (100%)	49 (100%)	0	100	100
1	AK	49/49 (100%)	49 (100%)	0	100	100
1	AL	49/49 (100%)	49 (100%)	0	100	100
1	AM	49/49 (100%)	49 (100%)	0	100	100
1	AN	46/49 (94%)	46 (100%)	0	100	100
2	BA	35/35 (100%)	35 (100%)	0	100	100
2	BB	35/35 (100%)	35 (100%)	0	100	100
2	BC	34/35 (97%)	34 (100%)	0	100	100
2	BD	35/35 (100%)	35 (100%)	0	100	100
2	BE	35/35 (100%)	35 (100%)	0	100	100
2	BF	35/35 (100%)	35 (100%)	0	100	100
2	BG	35/35 (100%)	35 (100%)	0	100	100
2	BH	35/35 (100%)	35 (100%)	0	100	100
2	BI	35/35 (100%)	35 (100%)	0	100	100
2	BJ	35/35 (100%)	35 (100%)	0	100	100
2	BK	35/35 (100%)	35 (100%)	0	100	100
2	BL	35/35 (100%)	35 (100%)	0	100	100
2	BM	35/35 (100%)	35 (100%)	0	100	100
2	BN	32/35 (91%)	32 (100%)	0	100	100
3	H	198/198 (100%)	197 (100%)	1 (0%)	88	96
4	L	220/220 (100%)	217 (99%)	3 (1%)	67	86
5	M	240/240 (100%)	239 (100%)	1 (0%)	91	97
6	UU	33/33 (100%)	33 (100%)	0	100	100
7	X	42/42 (100%)	42 (100%)	0	100	100
All	All	1896/1909 (99%)	1891 (100%)	5 (0%)	92	97

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

Mol	Chain	Res	Type
3	H	231	ASP
4	L	210	ASP
4	L	247	CYS
4	L	272	TRP
5	M	216	PHE

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

Mol	Chain	Res	Type
1	AI	20	GLN
2	BJ	17	GLN
5	M	300	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 73 ligands modelled in this entry, 1 is monoatomic - leaving 72 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	SPO	AK	102	-	40,41,41	0.23	0	47,50,50	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	3PE	H	302	-	50,50,50	0.51	0	53,55,55	0.66	2 (3%)
12	BPH	L	301	-	64,70,70	0.84	3 (4%)	76,101,101	1.08	6 (7%)
10	LMT	AA	1003	-	36,36,36	1.08	4 (11%)	47,47,47	0.94	2 (4%)
10	LMT	AB	104	-	36,36,36	1.12	4 (11%)	47,47,47	0.83	0
9	SPO	AA	1002	-	40,41,41	0.17	0	47,50,50	0.71	2 (4%)
13	U10	L	302	-	63,63,63	2.68	17 (26%)	76,79,79	1.56	18 (23%)
8	BCL	AM	1003	-	58,74,74	1.28	4 (6%)	69,115,115	1.33	9 (13%)
9	SPO	AF	101	-	40,41,41	0.39	0	47,50,50	0.58	1 (2%)
11	3PE	H	301	-	50,50,50	0.53	0	53,55,55	0.51	1 (1%)
8	BCL	AJ	101	-	58,74,74	1.31	5 (8%)	69,115,115	1.53	10 (14%)
8	BCL	AC	102	-	58,74,74	1.28	4 (6%)	69,115,115	1.33	9 (13%)
11	3PE	AC	104	-	50,50,50	0.53	0	53,55,55	0.58	1 (1%)
8	BCL	BC	101	-	58,74,74	1.25	3 (5%)	69,115,115	1.33	9 (13%)
11	3PE	AB	102	-	50,50,50	0.53	0	53,55,55	0.54	1 (1%)
8	BCL	AE	101	-	58,74,74	1.26	4 (6%)	69,115,115	1.37	9 (13%)
8	BCL	L	305	-	58,74,74	1.26	4 (6%)	69,115,115	1.32	11 (15%)
8	BCL	BD	101	-	58,74,74	1.26	3 (5%)	69,115,115	1.41	11 (15%)
8	BCL	AK	101	-	58,74,74	1.32	5 (8%)	69,115,115	1.40	11 (15%)
9	SPO	AF	103	-	40,41,41	0.31	0	47,50,50	0.34	0
10	LMT	M	401	-	36,36,36	1.06	5 (13%)	47,47,47	0.97	2 (4%)
8	BCL	M	406	-	58,74,74	1.24	3 (5%)	69,115,115	1.41	12 (17%)
8	BCL	BF	101	-	58,74,74	1.28	3 (5%)	69,115,115	1.31	10 (14%)
8	BCL	AM	1001	-	58,74,74	1.30	4 (6%)	69,115,115	1.43	11 (15%)
8	BCL	AN	101	-	58,74,74	1.30	4 (6%)	69,115,115	1.33	9 (13%)
9	SPO	AC	101	-	40,41,41	0.19	0	47,50,50	0.45	0
8	BCL	AI	101	-	58,74,74	1.32	3 (5%)	69,115,115	1.39	11 (15%)
8	BCL	BH	101	-	58,74,74	1.27	4 (6%)	69,115,115	1.38	10 (14%)
9	SPO	AC	103	-	40,41,41	0.23	0	47,50,50	0.25	0
8	BCL	AE	103	-	58,74,74	1.28	3 (5%)	69,115,115	1.41	11 (15%)
9	SPO	AH	103	-	40,41,41	0.28	0	47,50,50	0.54	0
8	BCL	BL	102	-	58,74,74	1.27	3 (5%)	69,115,115	1.35	12 (17%)
8	BCL	AA	1001	-	58,74,74	1.35	4 (6%)	69,115,115	1.32	9 (13%)
8	BCL	BA	102	-	58,74,74	1.28	4 (6%)	69,115,115	1.43	12 (17%)
9	SPO	BE	1000	-	40,41,41	0.38	0	47,50,50	0.49	0
9	SPO	BL	101	-	40,41,41	0.35	0	47,50,50	0.35	0
13	U10	M	404	-	63,63,63	2.65	17 (26%)	76,79,79	1.67	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	SPO	AJ	102	-	40,41,41	0.22	0	47,50,50	0.51	0
9	SPO	AD	103	-	40,41,41	0.20	0	47,50,50	0.40	0
8	BCL	AD	102	-	58,74,74	1.29	4 (6%)	69,115,115	1.52	11 (15%)
8	BCL	BI	101	-	58,74,74	1.27	3 (5%)	69,115,115	1.36	12 (17%)
8	BCL	BN	101	-	58,74,74	1.31	5 (8%)	69,115,115	1.43	12 (17%)
8	BCL	M	403	-	58,74,74	1.31	4 (6%)	69,115,115	1.36	9 (13%)
9	SPO	AE	102	-	40,41,41	0.32	0	47,50,50	0.51	0
9	SPO	AJ	103	-	40,41,41	0.35	0	47,50,50	0.68	2 (4%)
9	SPO	AM	1002	-	40,41,41	0.24	0	47,50,50	0.41	0
8	BCL	AB	101	-	58,74,74	1.32	3 (5%)	69,115,115	1.49	12 (17%)
9	SPO	AM	1004	-	40,41,41	0.38	0	47,50,50	0.39	0
14	UQ1	L	303	-	18,18,18	0.78	0	22,25,25	1.85	6 (27%)
8	BCL	AG	102	-	58,74,74	1.27	4 (6%)	69,115,115	1.36	9 (13%)
9	SPO	AD	101	-	40,41,41	0.16	0	47,50,50	0.44	0
9	SPO	AI	102	-	40,41,41	0.37	0	47,50,50	0.79	2 (4%)
9	SPO	AI	103	-	40,41,41	0.33	0	47,50,50	0.86	2 (4%)
9	SPO	AH	101	-	40,41,41	0.19	0	47,50,50	0.46	1 (2%)
9	SPO	AK	104	-	40,41,41	0.19	0	47,50,50	0.40	0
9	SPO	BA	101	-	40,41,41	0.18	0	47,50,50	0.66	1 (2%)
8	BCL	BJ	101	-	58,74,74	1.28	4 (6%)	69,115,115	1.34	9 (13%)
15	CD4	M	405	-	83,83,83	0.50	0	89,95,95	0.97	4 (4%)
8	BCL	BB	1001	-	58,74,74	1.26	3 (5%)	69,115,115	1.36	10 (14%)
8	BCL	AF	102	-	58,74,74	1.32	4 (6%)	69,115,115	1.43	10 (14%)
8	BCL	AL	1001	-	58,74,74	1.31	4 (6%)	69,115,115	1.46	14 (20%)
12	BPH	M	402	-	64,70,70	0.88	3 (4%)	76,101,101	1.15	7 (9%)
9	SPO	AB	103	-	40,41,41	0.39	0	47,50,50	0.71	2 (4%)
8	BCL	L	304	-	58,74,74	1.28	4 (6%)	69,115,115	1.28	9 (13%)
9	SPO	M	407	-	40,41,41	0.20	0	47,50,50	0.51	0
8	BCL	AH	102	-	58,74,74	1.31	4 (6%)	69,115,115	1.37	10 (14%)
9	SPO	AG	101	-	40,41,41	0.29	0	47,50,50	0.41	0
9	SPO	AG	103	-	40,41,41	0.30	0	47,50,50	0.51	0
8	BCL	AK	103	-	58,74,74	1.27	3 (5%)	69,115,115	1.36	10 (14%)
9	SPO	AL	1002	-	40,41,41	0.37	0	47,50,50	0.68	2 (4%)
10	LMT	X	101	-	36,36,36	1.11	5 (13%)	47,47,47	0.89	2 (4%)
8	BCL	BG	101	-	58,74,74	1.29	3 (5%)	69,115,115	1.35	11 (15%)

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
9	SPO	AK	102	-	-	4/47/47/47	-
11	3PE	H	302	-	-	14/54/54/54	-
12	BPH	L	301	-	-	5/54/105/105	0/5/6/6
10	LMT	AA	1003	-	-	3/21/61/61	0/2/2/2
10	LMT	AB	104	-	-	4/21/61/61	0/2/2/2
9	SPO	AA	1002	-	-	8/47/47/47	-
13	U10	L	302	-	-	13/63/87/87	0/1/1/1
8	BCL	AM	1003	-	-	6/37/137/137	-
9	SPO	AF	101	-	-	4/47/47/47	-
11	3PE	H	301	-	-	16/54/54/54	-
8	BCL	AJ	101	-	-	7/37/137/137	-
8	BCL	AC	102	-	-	10/37/137/137	-
11	3PE	AC	104	-	-	12/54/54/54	-
8	BCL	BC	101	-	-	7/37/137/137	-
11	3PE	AB	102	-	-	10/54/54/54	-
8	BCL	AE	101	-	-	3/37/137/137	-
8	BCL	L	305	-	-	4/37/137/137	-
8	BCL	BD	101	-	-	2/37/137/137	-
8	BCL	AK	101	-	-	5/37/137/137	-
9	SPO	AF	103	-	-	2/47/47/47	-
10	LMT	M	401	-	-	4/21/61/61	0/2/2/2
8	BCL	M	406	-	-	7/37/137/137	-
8	BCL	BF	101	-	-	8/37/137/137	-
8	BCL	AM	1001	-	-	4/37/137/137	-
8	BCL	AN	101	-	-	5/37/137/137	-
9	SPO	AC	101	-	-	2/47/47/47	-
8	BCL	AI	101	-	-	11/37/137/137	-
8	BCL	BH	101	-	-	7/37/137/137	-
9	SPO	AC	103	-	-	3/47/47/47	-
8	BCL	AE	103	-	-	5/37/137/137	-
9	SPO	AH	103	-	-	3/47/47/47	-
8	BCL	BL	102	-	-	11/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	AA	1001	-	-	6/37/137/137	-
8	BCL	BA	102	-	-	4/37/137/137	-
9	SPO	BE	1000	-	-	7/47/47/47	-
9	SPO	BL	101	-	-	5/47/47/47	-
13	U10	M	404	-	-	8/63/87/87	0/1/1/1
9	SPO	AJ	102	-	-	6/47/47/47	-
9	SPO	AD	103	-	-	4/47/47/47	-
8	BCL	AD	102	-	-	4/37/137/137	-
8	BCL	BI	101	-	-	3/37/137/137	-
8	BCL	BN	101	-	-	6/37/137/137	-
8	BCL	M	403	-	-	1/37/137/137	-
9	SPO	AE	102	-	-	3/47/47/47	-
9	SPO	AJ	103	-	-	4/47/47/47	-
9	SPO	AM	1002	-	-	2/47/47/47	-
8	BCL	AB	101	-	-	7/37/137/137	-
9	SPO	AM	1004	-	-	3/47/47/47	-
14	UQ1	L	303	-	-	4/9/33/33	0/1/1/1
8	BCL	AG	102	-	-	1/37/137/137	-
9	SPO	AD	101	-	-	5/47/47/47	-
9	SPO	AI	102	-	-	4/47/47/47	-
9	SPO	AI	103	-	-	4/47/47/47	-
9	SPO	AH	101	-	-	2/47/47/47	-
9	SPO	AK	104	-	-	8/47/47/47	-
9	SPO	BA	101	-	-	3/47/47/47	-
8	BCL	BJ	101	-	-	6/37/137/137	-
15	CD4	M	405	-	-	12/94/94/94	-
8	BCL	BB	1001	-	-	7/37/137/137	-
8	BCL	AF	102	-	-	3/37/137/137	-
8	BCL	AL	1001	-	-	5/37/137/137	-
12	BPH	M	402	-	-	7/54/105/105	0/5/6/6
9	SPO	AB	103	-	-	9/47/47/47	-
8	BCL	L	304	-	-	1/37/137/137	-
9	SPO	M	407	-	-	2/47/47/47	-
8	BCL	AH	102	-	-	1/37/137/137	-
9	SPO	AG	101	-	-	2/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SPO	AG	103	-	-	2/47/47/47	-
8	BCL	AK	103	-	-	5/37/137/137	-
9	SPO	AL	1002	-	-	2/47/47/47	-
10	LMT	X	101	-	-	1/21/61/61	0/2/2/2
8	BCL	BG	101	-	-	7/37/137/137	-

All (177) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	302	U10	C43-C44	6.14	1.47	1.33
13	M	404	U10	C43-C44	6.11	1.47	1.33
13	L	302	U10	C48-C49	6.11	1.47	1.33
13	L	302	U10	C18-C19	6.10	1.47	1.33
13	M	404	U10	C18-C19	6.08	1.47	1.33
13	L	302	U10	C23-C24	6.07	1.47	1.33
13	M	404	U10	C28-C29	6.06	1.47	1.33
13	L	302	U10	C38-C39	6.06	1.47	1.33
13	M	404	U10	C8-C9	6.05	1.47	1.33
13	M	404	U10	C48-C49	6.04	1.47	1.33
13	L	302	U10	C8-C9	6.03	1.47	1.33
13	M	404	U10	C33-C34	6.03	1.47	1.33
13	L	302	U10	C33-C34	6.03	1.47	1.33
13	L	302	U10	C28-C29	6.02	1.47	1.33
13	M	404	U10	C38-C39	6.01	1.47	1.33
13	L	302	U10	C13-C14	6.00	1.47	1.33
13	M	404	U10	C13-C14	5.97	1.47	1.33
13	M	404	U10	C23-C24	5.97	1.47	1.33
8	AA	1001	BCL	MG-NA	5.63	2.19	2.06
8	M	403	BCL	MG-NA	5.56	2.19	2.06
8	AB	101	BCL	MG-NA	5.45	2.19	2.06
8	AL	1001	BCL	MG-NA	5.43	2.19	2.06
13	M	404	U10	C53-C54	5.42	1.48	1.32
8	AM	1001	BCL	MG-NA	5.42	2.19	2.06
8	BN	101	BCL	MG-NA	5.41	2.19	2.06
13	L	302	U10	O4-C4	-5.38	1.23	1.36
8	AJ	101	BCL	MG-NA	5.38	2.19	2.06
8	AF	102	BCL	MG-NA	5.37	2.19	2.06
8	AH	102	BCL	MG-NA	5.34	2.19	2.06
13	L	302	U10	C53-C54	5.32	1.47	1.32
8	AD	102	BCL	MG-NA	5.32	2.18	2.06
8	AI	101	BCL	MG-NA	5.31	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	AC	102	BCL	MG-NA	5.27	2.18	2.06
8	AN	101	BCL	MG-NA	5.26	2.18	2.06
8	AK	101	BCL	MG-NA	5.25	2.18	2.06
8	BH	101	BCL	MG-NA	5.23	2.18	2.06
8	AE	103	BCL	MG-NA	5.16	2.18	2.06
8	AG	102	BCL	MG-NA	5.16	2.18	2.06
8	AE	101	BCL	MG-NA	5.14	2.18	2.06
8	AM	1003	BCL	MG-NA	5.07	2.18	2.06
8	BI	101	BCL	MG-NA	5.06	2.18	2.06
8	BD	101	BCL	MG-NA	5.06	2.18	2.06
8	BG	101	BCL	C1B-NB	5.05	1.39	1.35
8	BC	101	BCL	MG-NA	5.05	2.18	2.06
8	BJ	101	BCL	MG-NA	5.05	2.18	2.06
8	L	304	BCL	MG-NA	5.05	2.18	2.06
8	BL	102	BCL	MG-NA	5.04	2.18	2.06
8	BF	101	BCL	MG-NA	5.02	2.18	2.06
8	BB	1001	BCL	MG-NA	5.02	2.18	2.06
8	BG	101	BCL	MG-NA	5.02	2.18	2.06
8	AN	101	BCL	C1B-NB	5.01	1.39	1.35
8	BA	102	BCL	MG-NA	5.01	2.18	2.06
8	AL	1001	BCL	C1B-NB	4.98	1.39	1.35
8	AK	103	BCL	MG-NA	4.97	2.18	2.06
8	AH	102	BCL	C1B-NB	4.96	1.39	1.35
8	BJ	101	BCL	C1B-NB	4.96	1.39	1.35
8	L	305	BCL	MG-NA	4.95	2.18	2.06
8	M	406	BCL	MG-NA	4.94	2.18	2.06
8	AK	101	BCL	C1B-NB	4.93	1.39	1.35
8	L	305	BCL	C1B-NB	4.93	1.39	1.35
8	BL	102	BCL	C1B-NB	4.92	1.39	1.35
8	BN	101	BCL	C1B-NB	4.91	1.39	1.35
8	AI	101	BCL	C1B-NB	4.91	1.39	1.35
8	BI	101	BCL	C1B-NB	4.91	1.39	1.35
8	AM	1003	BCL	C1B-NB	4.90	1.39	1.35
8	AM	1001	BCL	C1B-NB	4.90	1.39	1.35
8	AK	103	BCL	C1B-NB	4.89	1.39	1.35
8	BF	101	BCL	C1B-NB	4.89	1.39	1.35
8	AD	102	BCL	C1B-NB	4.88	1.39	1.35
8	AA	1001	BCL	C1B-NB	4.86	1.39	1.35
8	BB	1001	BCL	C1B-NB	4.84	1.39	1.35
8	AJ	101	BCL	C1B-NB	4.84	1.39	1.35
8	AC	102	BCL	C1B-NB	4.84	1.39	1.35
13	L	302	U10	O3-C3	-4.83	1.25	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	AG	102	BCL	C1B-NB	4.81	1.39	1.35
8	AB	101	BCL	C1B-NB	4.81	1.39	1.35
8	M	406	BCL	C1B-NB	4.81	1.39	1.35
13	M	404	U10	O3-C3	-4.79	1.25	1.36
8	AF	102	BCL	C1B-NB	4.78	1.39	1.35
8	BC	101	BCL	C1B-NB	4.77	1.39	1.35
8	BA	102	BCL	C1B-NB	4.75	1.39	1.35
8	AE	103	BCL	C1B-NB	4.75	1.39	1.35
13	M	404	U10	O4-C4	-4.73	1.25	1.36
8	BH	101	BCL	C1B-NB	4.70	1.39	1.35
8	M	403	BCL	C1B-NB	4.68	1.39	1.35
8	L	304	BCL	C1B-NB	4.65	1.39	1.35
8	AE	101	BCL	C1B-NB	4.63	1.39	1.35
8	BD	101	BCL	C1B-NB	4.58	1.39	1.35
8	AA	1001	BCL	MG-NC	4.16	2.16	2.06
8	AI	101	BCL	MG-NC	3.93	2.15	2.06
8	AJ	101	BCL	MG-NC	3.93	2.15	2.06
8	BF	101	BCL	MG-NC	3.91	2.15	2.06
8	BJ	101	BCL	MG-NC	3.91	2.15	2.06
8	AB	101	BCL	MG-NC	3.91	2.15	2.06
8	BH	101	BCL	MG-NC	3.90	2.15	2.06
8	AH	102	BCL	MG-NC	3.87	2.15	2.06
8	AD	102	BCL	MG-NC	3.86	2.15	2.06
8	AL	1001	BCL	MG-NC	3.85	2.15	2.06
8	L	304	BCL	MG-NC	3.85	2.15	2.06
8	AM	1001	BCL	MG-NC	3.82	2.15	2.06
8	AF	102	BCL	MG-NC	3.80	2.15	2.06
8	AK	101	BCL	MG-NC	3.79	2.15	2.06
8	BG	101	BCL	MG-NC	3.79	2.15	2.06
8	AN	101	BCL	MG-NC	3.77	2.15	2.06
8	AE	103	BCL	MG-NC	3.77	2.15	2.06
8	AC	102	BCL	MG-NC	3.77	2.15	2.06
8	AM	1003	BCL	MG-NC	3.76	2.15	2.06
8	BB	1001	BCL	MG-NC	3.74	2.15	2.06
8	BD	101	BCL	MG-NC	3.74	2.15	2.06
8	BA	102	BCL	MG-NC	3.73	2.15	2.06
8	BI	101	BCL	MG-NC	3.72	2.15	2.06
8	BL	102	BCL	MG-NC	3.72	2.15	2.06
8	BC	101	BCL	MG-NC	3.71	2.15	2.06
8	BN	101	BCL	MG-NC	3.70	2.15	2.06
8	AG	102	BCL	MG-NC	3.69	2.15	2.06
8	AK	103	BCL	MG-NC	3.69	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	AE	101	BCL	MG-NC	3.62	2.14	2.06
8	M	403	BCL	MG-NC	3.61	2.14	2.06
8	M	406	BCL	MG-NC	3.55	2.14	2.06
8	L	305	BCL	MG-NC	3.43	2.14	2.06
13	L	302	U10	C4-C5	-3.19	1.39	1.48
13	M	404	U10	C4-C5	-3.15	1.39	1.48
12	M	402	BPH	C3D-CAD	-2.82	1.41	1.47
12	L	301	BPH	C3D-CAD	-2.78	1.41	1.47
13	M	404	U10	C6-C5	-2.71	1.39	1.46
13	L	302	U10	C6-C5	-2.68	1.39	1.46
10	AA	1003	LMT	O3'-C3'	-2.67	1.36	1.43
13	L	302	U10	C3-C2	-2.66	1.41	1.48
10	AB	104	LMT	O3'-C3'	-2.63	1.36	1.43
10	AB	104	LMT	O2'-C2'	-2.56	1.36	1.43
10	M	401	LMT	O3'-C3'	-2.56	1.36	1.43
10	X	101	LMT	O3'-C3'	-2.55	1.37	1.43
13	M	404	U10	C3-C2	-2.40	1.42	1.48
8	AA	1001	BCL	C4B-NB	2.39	1.37	1.35
13	L	302	U10	C6-C1	2.37	1.39	1.35
10	AA	1003	LMT	O2B-C2B	-2.37	1.37	1.43
12	L	301	BPH	C1B-C2B	-2.36	1.40	1.45
13	M	404	U10	C6-C1	2.33	1.39	1.35
12	M	402	BPH	CHC-C1C	2.29	1.41	1.36
10	M	401	LMT	O3B-C3B	-2.28	1.37	1.43
10	AA	1003	LMT	O3B-C3B	-2.27	1.37	1.43
10	X	101	LMT	O3B-C3B	-2.27	1.37	1.43
10	X	101	LMT	O2B-C2B	-2.26	1.37	1.43
8	BN	101	BCL	C4B-NB	2.26	1.37	1.35
10	AA	1003	LMT	O2'-C2'	-2.25	1.37	1.43
8	M	403	BCL	C4B-NB	2.25	1.37	1.35
12	L	301	BPH	CHC-C1C	2.25	1.41	1.36
8	AF	102	BCL	C4B-NB	2.24	1.37	1.35
10	AB	104	LMT	O2B-C2B	-2.24	1.37	1.43
8	AM	1003	BCL	C4B-NB	2.23	1.37	1.35
12	M	402	BPH	C1B-C2B	-2.23	1.41	1.45
10	M	401	LMT	O2'-C2'	-2.22	1.37	1.43
8	AD	102	BCL	C4B-NB	2.20	1.37	1.35
10	M	401	LMT	O2B-C2B	-2.19	1.37	1.43
8	AM	1001	BCL	C4B-NB	2.18	1.37	1.35
8	AL	1001	BCL	C4B-NB	2.18	1.37	1.35
10	AB	104	LMT	O3B-C3B	-2.18	1.37	1.43
8	AJ	101	BCL	C4B-NB	2.18	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	X	101	LMT	O2'-C2'	-2.16	1.37	1.43
8	AK	101	BCL	C4B-NB	2.13	1.37	1.35
8	BN	101	BCL	OBD-CAD	2.13	1.25	1.22
13	M	404	U10	C1-C2	-2.11	1.39	1.47
8	L	305	BCL	C4B-NB	2.10	1.37	1.35
8	AE	101	BCL	C4B-NB	2.09	1.37	1.35
10	X	101	LMT	O4'-C4B	-2.09	1.38	1.43
13	L	302	U10	C1-C2	-2.09	1.39	1.47
8	BA	102	BCL	OBD-CAD	2.08	1.25	1.22
8	L	304	BCL	C4B-NB	2.08	1.37	1.35
10	M	401	LMT	O4'-C4B	-2.06	1.38	1.43
8	AH	102	BCL	C4B-NB	2.05	1.37	1.35
8	AG	102	BCL	C4B-NB	2.05	1.37	1.35
8	BH	101	BCL	C4B-NB	2.05	1.37	1.35
8	AN	101	BCL	C4B-NB	2.04	1.37	1.35
8	BJ	101	BCL	C4B-NB	2.04	1.37	1.35
8	AC	102	BCL	C4B-NB	2.01	1.37	1.35
8	AJ	101	BCL	OBD-CAD	2.01	1.25	1.22
8	AK	101	BCL	OBD-CAD	2.01	1.25	1.22

All (417) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	AD	102	BCL	C1-C2-C3	5.15	134.95	126.04
8	AJ	101	BCL	C1-C2-C3	5.11	134.88	126.04
14	L	303	UQ1	C6-C5-C4	4.86	123.03	119.18
8	AG	102	BCL	CMB-C2B-C1B	-4.43	121.65	128.46
8	AE	103	BCL	CMB-C2B-C1B	-4.41	121.68	128.46
8	AD	102	BCL	CMB-C2B-C1B	-4.36	121.76	128.46
8	AM	1001	BCL	CMB-C2B-C1B	-4.36	121.76	128.46
8	AF	102	BCL	CMB-C2B-C1B	-4.35	121.78	128.46
8	AK	103	BCL	CMB-C2B-C1B	-4.33	121.81	128.46
8	AN	101	BCL	CMB-C2B-C1B	-4.31	121.84	128.46
8	AI	101	BCL	CMB-C2B-C1B	-4.31	121.84	128.46
8	L	304	BCL	CMB-C2B-C1B	-4.31	121.84	128.46
8	AJ	101	BCL	CMB-C2B-C1B	-4.31	121.84	128.46
8	AK	101	BCL	CMB-C2B-C1B	-4.29	121.87	128.46
8	BN	101	BCL	CMB-C2B-C1B	-4.29	121.87	128.46
8	M	403	BCL	CMB-C2B-C1B	-4.27	121.89	128.46
8	BL	102	BCL	CMB-C2B-C1B	-4.27	121.91	128.46
8	AA	1001	BCL	CMB-C2B-C1B	-4.26	121.91	128.46
8	BD	101	BCL	CMB-C2B-C1B	-4.26	121.91	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	AM	1003	BCL	CMB-C2B-C1B	-4.25	121.93	128.46
8	BH	101	BCL	CMB-C2B-C1B	-4.25	121.94	128.46
8	AL	1001	BCL	CMB-C2B-C1B	-4.23	121.95	128.46
8	BI	101	BCL	CMB-C2B-C1B	-4.23	121.96	128.46
8	BC	101	BCL	CMB-C2B-C1B	-4.23	121.96	128.46
8	AH	102	BCL	CMB-C2B-C1B	-4.23	121.97	128.46
8	BJ	101	BCL	CMB-C2B-C1B	-4.22	121.98	128.46
8	AE	101	BCL	CMB-C2B-C1B	-4.22	121.98	128.46
8	BA	102	BCL	CMB-C2B-C1B	-4.19	122.03	128.46
8	AB	101	BCL	CMB-C2B-C1B	-4.18	122.03	128.46
8	BG	101	BCL	CMB-C2B-C1B	-4.17	122.06	128.46
8	AC	102	BCL	CMB-C2B-C1B	-4.17	122.06	128.46
8	BF	101	BCL	CMB-C2B-C1B	-4.14	122.09	128.46
8	BB	1001	BCL	CMB-C2B-C1B	-4.14	122.10	128.46
8	M	406	BCL	CMB-C2B-C1B	-4.13	122.12	128.46
8	L	305	BCL	CMB-C2B-C1B	-4.05	122.24	128.46
13	M	404	U10	C4M-O4-C4	3.92	130.35	116.47
13	M	404	U10	C3M-O3-C3	3.87	130.17	116.47
14	L	303	UQ1	CM3-O3-C3	3.77	129.84	116.47
8	M	406	BCL	C4D-C3D-CAD	-3.74	106.39	108.47
8	AL	1001	BCL	C1-C2-C3	3.74	132.51	126.04
8	AB	101	BCL	C1-C2-C3	3.74	132.50	126.04
8	AG	102	BCL	C4A-NA-C1A	3.68	108.36	106.71
8	AF	102	BCL	C4A-NA-C1A	3.67	108.36	106.71
13	L	302	U10	C25-C24-C26	3.67	121.45	115.27
8	AE	101	BCL	C4A-NA-C1A	3.61	108.33	106.71
8	AM	1001	BCL	C4A-NA-C1A	3.59	108.32	106.71
14	L	303	UQ1	C8-C7-C6	3.58	121.69	112.05
8	AI	101	BCL	C4D-C3D-CAD	-3.54	106.50	108.47
8	AB	101	BCL	C4A-NA-C1A	3.47	108.27	106.71
8	M	403	BCL	C4D-C3D-CAD	-3.46	106.54	108.47
8	AK	103	BCL	OBD-CAD-CBD	-3.43	121.00	125.89
8	AB	101	BCL	OBD-CAD-CBD	-3.41	121.02	125.89
8	AA	1001	BCL	C4A-NA-C1A	3.41	108.24	106.71
8	BN	101	BCL	C4A-NA-C1A	3.40	108.23	106.71
8	L	305	BCL	C4D-C3D-CAD	-3.38	106.58	108.47
8	M	403	BCL	CHA-C1A-NA	-3.38	118.65	126.40
8	AD	102	BCL	C4A-NA-C1A	3.38	108.23	106.71
8	AK	101	BCL	OBD-CAD-CBD	-3.37	121.08	125.89
8	AJ	101	BCL	C4A-NA-C1A	3.37	108.22	106.71
8	AM	1001	BCL	OBD-CAD-CBD	-3.37	121.08	125.89
8	AE	103	BCL	OBD-CAD-CBD	-3.36	121.09	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	BA	102	BCL	OBD-CAD-CBD	-3.36	121.09	125.89
8	M	406	BCL	OBD-CAD-CBD	-3.36	121.10	125.89
8	AF	102	BCL	OBD-CAD-CBD	-3.35	121.10	125.89
8	BL	102	BCL	OBD-CAD-CBD	-3.35	121.11	125.89
8	AI	101	BCL	OBD-CAD-CBD	-3.35	121.11	125.89
8	AL	1001	BCL	C4A-NA-C1A	3.34	108.21	106.71
8	AC	102	BCL	OBD-CAD-CBD	-3.34	121.12	125.89
8	AH	102	BCL	OBD-CAD-CBD	-3.34	121.12	125.89
8	AJ	101	BCL	OBD-CAD-CBD	-3.34	121.12	125.89
8	BH	101	BCL	OBD-CAD-CBD	-3.34	121.12	125.89
8	AA	1001	BCL	OBD-CAD-CBD	-3.34	121.12	125.89
8	AL	1001	BCL	OBD-CAD-CBD	-3.34	121.13	125.89
8	BF	101	BCL	OBD-CAD-CBD	-3.33	121.13	125.89
8	M	403	BCL	C4A-NA-C1A	3.33	108.20	106.71
8	BG	101	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
8	BN	101	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
8	BJ	101	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
8	AD	102	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
8	AG	102	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
8	AM	1003	BCL	OBD-CAD-CBD	-3.31	121.17	125.89
12	M	402	BPH	OBD-CAD-CBD	-3.31	121.17	125.89
8	AN	101	BCL	C4A-NA-C1A	3.30	108.19	106.71
8	AN	101	BCL	OBD-CAD-CBD	-3.30	121.18	125.89
8	BB	1001	BCL	OBD-CAD-CBD	-3.30	121.18	125.89
8	AH	102	BCL	C4A-NA-C1A	3.30	108.19	106.71
15	M	405	CD4	O2-C14-C13	3.29	118.60	111.50
8	AE	101	BCL	OBD-CAD-CBD	-3.29	121.19	125.89
8	BD	101	BCL	OBD-CAD-CBD	-3.28	121.21	125.89
8	AC	102	BCL	C4D-C3D-CAD	-3.28	106.64	108.47
8	BI	101	BCL	OBD-CAD-CBD	-3.28	121.21	125.89
8	BC	101	BCL	OBD-CAD-CBD	-3.28	121.21	125.89
8	AK	101	BCL	C4A-NA-C1A	3.27	108.18	106.71
8	M	403	BCL	OBD-CAD-CBD	-3.26	121.24	125.89
12	L	301	BPH	OBD-CAD-CBD	-3.26	121.24	125.89
8	L	305	BCL	OBD-CAD-CBD	-3.25	121.25	125.89
8	L	304	BCL	OBD-CAD-CBD	-3.23	121.28	125.89
8	AE	103	BCL	C4A-NA-C1A	3.20	108.14	106.71
8	BA	102	BCL	C4A-NA-C1A	3.20	108.14	106.71
8	AI	101	BCL	CHA-C1A-NA	-3.19	119.09	126.40
8	AG	102	BCL	C4D-C3D-CAD	-3.17	106.70	108.47
8	AG	102	BCL	CMB-C2B-C3B	3.16	130.60	124.68
8	AE	103	BCL	CMB-C2B-C3B	3.16	130.59	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	BF	101	BCL	CHA-C1A-NA	-3.12	119.25	126.40
8	AN	101	BCL	CMB-C2B-C3B	3.11	130.50	124.68
8	AF	102	BCL	CMB-C2B-C3B	3.11	130.50	124.68
8	AI	101	BCL	CMB-C2B-C3B	3.11	130.49	124.68
8	BN	101	BCL	CMB-C2B-C3B	3.11	130.49	124.68
8	AN	101	BCL	C4D-C3D-CAD	-3.11	106.74	108.47
8	BF	101	BCL	C4D-C3D-CAD	-3.11	106.74	108.47
8	AC	102	BCL	CHA-C1A-NA	-3.10	119.30	126.40
11	H	302	3PE	C2-O21-C21	3.10	125.42	117.79
8	AJ	101	BCL	CMB-C2B-C3B	3.10	130.48	124.68
8	AM	1001	BCL	CMB-C2B-C3B	3.09	130.47	124.68
8	AK	103	BCL	CMB-C2B-C3B	3.09	130.46	124.68
8	BL	102	BCL	CMB-C2B-C3B	3.09	130.45	124.68
8	AB	101	BCL	CHA-C1A-NA	-3.08	119.34	126.40
8	AD	102	BCL	CMB-C2B-C3B	3.08	130.44	124.68
13	M	404	U10	C35-C34-C36	3.08	120.45	115.27
8	BL	102	BCL	CHA-C1A-NA	-3.07	119.36	126.40
8	AE	101	BCL	CMB-C2B-C3B	3.07	130.42	124.68
8	AH	102	BCL	CMB-C2B-C3B	3.07	130.42	124.68
8	L	304	BCL	CMB-C2B-C3B	3.07	130.42	124.68
8	AB	101	BCL	C4D-C3D-CAD	-3.06	106.76	108.47
8	AE	103	BCL	CHA-C1A-NA	-3.06	119.39	126.40
8	BH	101	BCL	C4A-NA-C1A	3.06	108.08	106.71
8	M	403	BCL	CMB-C2B-C3B	3.06	130.40	124.68
8	BH	101	BCL	CHA-C1A-NA	-3.06	119.40	126.40
8	AM	1003	BCL	CMB-C2B-C3B	3.05	130.39	124.68
8	AK	101	BCL	CMB-C2B-C3B	3.05	130.39	124.68
8	BJ	101	BCL	C4D-C3D-CAD	-3.05	106.77	108.47
8	BD	101	BCL	CHA-C1A-NA	-3.05	119.41	126.40
13	L	302	U10	C12-C13-C14	-3.05	120.32	127.66
8	M	406	BCL	CMB-C2B-C3B	3.05	130.38	124.68
8	AB	101	BCL	CMB-C2B-C3B	3.05	130.38	124.68
8	BH	101	BCL	CMB-C2B-C3B	3.04	130.37	124.68
8	BI	101	BCL	CHA-C1A-NA	-3.04	119.43	126.40
13	L	302	U10	C30-C29-C31	3.04	120.39	115.27
8	AJ	101	BCL	CHA-C1A-NA	-3.04	119.44	126.40
8	BC	101	BCL	CMB-C2B-C3B	3.04	130.36	124.68
13	M	404	U10	C40-C39-C41	3.03	120.37	115.27
8	AC	102	BCL	CMB-C2B-C3B	3.03	130.34	124.68
13	M	404	U10	C17-C18-C19	-3.02	120.38	127.66
8	BA	102	BCL	CMB-C2B-C3B	3.02	130.33	124.68
8	M	406	BCL	C4A-NA-C1A	3.02	108.06	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	AH	102	BCL	CHA-C1A-NA	-3.02	119.49	126.40
8	BB	1001	BCL	CHA-C1A-NA	-3.01	119.50	126.40
8	BD	101	BCL	CMB-C2B-C3B	3.01	130.31	124.68
8	BN	101	BCL	CHA-C1A-NA	-3.01	119.50	126.40
8	BI	101	BCL	CMB-C2B-C3B	3.01	130.31	124.68
13	M	404	U10	C25-C24-C26	3.01	120.34	115.27
8	AN	101	BCL	CHA-C1A-NA	-3.01	119.50	126.40
8	AA	1001	BCL	CMB-C2B-C3B	3.01	130.31	124.68
8	BF	101	BCL	CMB-C2B-C3B	3.01	130.31	124.68
8	AF	102	BCL	C1-C2-C3	-3.01	120.84	126.04
8	BG	101	BCL	CMB-C2B-C3B	3.01	130.30	124.68
8	AK	103	BCL	CHA-C1A-NA	-3.01	119.52	126.40
13	M	404	U10	C50-C49-C51	3.00	120.33	115.27
8	AK	103	BCL	C4D-C3D-CAD	-3.00	106.80	108.47
8	BJ	101	BCL	CMB-C2B-C3B	3.00	130.29	124.68
8	AM	1003	BCL	CHA-C1A-NA	-2.99	119.54	126.40
8	BC	101	BCL	CHA-C1A-NA	-2.99	119.55	126.40
8	BJ	101	BCL	CHA-C1A-NA	-2.99	119.55	126.40
8	BA	102	BCL	CHA-C1A-NA	-2.99	119.56	126.40
8	AL	1001	BCL	CMB-C2B-C3B	2.98	130.26	124.68
8	AF	102	BCL	CHA-C1A-NA	-2.98	119.58	126.40
8	BB	1001	BCL	CMB-C2B-C3B	2.98	130.25	124.68
8	BG	101	BCL	C4D-C3D-CAD	-2.98	106.81	108.47
8	BI	101	BCL	C4D-C3D-CAD	-2.97	106.81	108.47
8	AM	1003	BCL	C4A-NA-C1A	2.97	108.04	106.71
8	BD	101	BCL	C4A-NA-C1A	2.97	108.04	106.71
8	AC	102	BCL	C4A-NA-C1A	2.96	108.04	106.71
9	AI	103	SPO	C20-C21-C22	2.96	129.53	123.47
8	AE	101	BCL	CHA-C1A-NA	-2.96	119.62	126.40
8	AK	101	BCL	CHA-C1A-NA	-2.95	119.63	126.40
8	L	305	BCL	CHA-C1A-NA	-2.95	119.64	126.40
8	AG	102	BCL	CHA-C1A-NA	-2.94	119.66	126.40
8	BG	101	BCL	CHA-C1A-NA	-2.94	119.66	126.40
8	BA	102	BCL	C4D-C3D-CAD	-2.94	106.83	108.47
8	L	305	BCL	CMB-C2B-C3B	2.93	130.17	124.68
8	AA	1001	BCL	CHA-C1A-NA	-2.93	119.69	126.40
8	BL	102	BCL	C4D-C3D-CAD	-2.93	106.84	108.47
8	AM	1001	BCL	CHA-C1A-NA	-2.92	119.70	126.40
8	M	406	BCL	CHA-C1A-NA	-2.91	119.72	126.40
12	L	301	BPH	C1C-NC-C4C	-2.91	107.98	110.54
8	AM	1003	BCL	C4D-C3D-CAD	-2.91	106.85	108.47
8	AD	102	BCL	CHA-C1A-NA	-2.90	119.75	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	AF	102	BCL	C4D-C3D-CAD	-2.89	106.86	108.47
8	L	305	BCL	C2A-C1A-CHA	2.89	128.90	123.86
8	AE	101	BCL	C4D-C3D-CAD	-2.88	106.86	108.47
8	AA	1001	BCL	C4D-C3D-CAD	-2.87	106.87	108.47
8	BB	1001	BCL	C4D-C3D-CAD	-2.87	106.87	108.47
8	BC	101	BCL	C4A-NA-C1A	2.87	108.00	106.71
8	AH	102	BCL	C4D-C3D-CAD	-2.87	106.87	108.47
8	AL	1001	BCL	CHA-C1A-NA	-2.87	119.83	126.40
8	AL	1001	BCL	C4D-C3D-CAD	-2.86	106.88	108.47
13	L	302	U10	C45-C44-C46	2.85	120.07	115.27
8	BB	1001	BCL	C4A-NA-C1A	2.85	107.99	106.71
13	M	404	U10	C10-C9-C11	2.84	120.06	115.27
13	L	302	U10	C3M-O3-C3	2.84	126.54	116.47
8	AK	101	BCL	C4D-C3D-CAD	-2.82	106.90	108.47
15	M	405	CD4	O3-C17-C18	2.82	120.76	111.91
9	AB	103	SPO	C1-C4-C5	2.81	120.51	113.06
8	AJ	101	BCL	C4D-C3D-CAD	-2.78	106.92	108.47
8	AE	103	BCL	CBA-CAA-C2A	2.78	122.07	113.86
8	BG	101	BCL	C4A-NA-C1A	2.78	107.95	106.71
8	BC	101	BCL	C4D-C3D-CAD	-2.78	106.92	108.47
8	L	304	BCL	CHA-C1A-NA	-2.76	120.07	126.40
8	L	304	BCL	C4D-C3D-CAD	-2.76	106.93	108.47
13	M	404	U10	C30-C29-C31	2.76	119.91	115.27
9	AI	102	SPO	C1-C4-C5	2.75	120.34	113.06
13	M	404	U10	C20-C19-C21	2.74	119.88	115.27
8	AE	103	BCL	C4D-C3D-CAD	-2.74	106.94	108.47
13	L	302	U10	C47-C48-C49	-2.73	121.09	127.66
8	BH	101	BCL	C4D-C3D-CAD	-2.73	106.95	108.47
8	AD	102	BCL	C4D-C3D-CAD	-2.72	106.95	108.47
13	M	404	U10	C15-C14-C16	2.72	119.85	115.27
8	BB	1001	BCL	C1-O2A-CGA	2.72	123.58	116.44
13	L	302	U10	C7-C8-C9	-2.72	122.27	126.79
8	BD	101	BCL	C4D-C3D-CAD	-2.72	106.96	108.47
8	BD	101	BCL	C2A-C1A-CHA	2.71	128.59	123.86
8	AM	1001	BCL	C4D-C3D-CAD	-2.70	106.97	108.47
13	M	404	U10	C45-C44-C46	2.70	119.81	115.27
8	BA	102	BCL	CBA-CAA-C2A	2.69	121.79	113.86
10	AA	1003	LMT	C3'-C4'-C5'	-2.68	104.78	110.93
10	M	401	LMT	C3'-C4'-C5'	-2.68	104.78	110.93
10	M	401	LMT	C1-O1'-C1'	2.67	118.27	113.84
8	BH	101	BCL	C2A-C1A-CHA	2.67	128.53	123.86
8	AJ	101	BCL	C2A-C1A-CHA	2.67	128.53	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	L	302	U10	C32-C33-C34	-2.66	121.25	127.66
13	L	302	U10	C1M-C1-C6	-2.66	120.06	124.40
8	M	403	BCL	C2A-C1A-CHA	2.63	128.47	123.86
8	BN	101	BCL	C4D-C3D-CAD	-2.63	107.00	108.47
8	M	406	BCL	C2A-C1A-CHA	2.62	128.44	123.86
13	L	302	U10	C10-C9-C11	2.62	119.68	115.27
9	AA	1002	SPO	C2-C1-C4	-2.62	106.83	110.86
9	AI	102	SPO	C2-C1-C4	-2.62	106.84	110.86
13	L	302	U10	C40-C39-C41	2.60	119.65	115.27
8	BL	102	BCL	CMD-C2D-C3D	2.60	129.54	124.68
8	AF	102	BCL	C2A-C1A-CHA	2.60	128.40	123.86
13	M	404	U10	C22-C23-C24	-2.59	121.43	127.66
9	AL	1002	SPO	C1-C4-C5	2.59	119.91	113.06
8	BA	102	BCL	CMD-C2D-C3D	2.58	129.51	124.68
8	BL	102	BCL	C1-O2A-CGA	2.57	123.19	116.44
8	AK	103	BCL	C4A-NA-C1A	2.57	107.86	106.71
8	BI	101	BCL	C4A-NA-C1A	2.55	107.85	106.71
12	M	402	BPH	C1C-NC-C4C	-2.55	108.30	110.54
8	AK	101	BCL	OBB-CAB-CBB	-2.54	114.44	120.17
8	AK	101	BCL	C1-C2-C3	2.54	130.44	126.04
8	AK	103	BCL	CMD-C2D-C3D	2.54	129.43	124.68
8	L	304	BCL	C4A-NA-C1A	2.54	107.85	106.71
8	AE	101	BCL	OBB-CAB-CBB	-2.53	114.47	120.17
8	AM	1001	BCL	OBB-CAB-CBB	-2.53	114.47	120.17
8	AD	102	BCL	OBB-CAB-CBB	-2.53	114.47	120.17
13	M	404	U10	C47-C48-C49	-2.53	121.57	127.66
8	BF	101	BCL	CMD-C2D-C3D	2.52	129.40	124.68
8	AI	101	BCL	C2A-C1A-CHA	2.52	128.26	123.86
8	AL	1001	BCL	OBB-CAB-CBB	-2.52	114.50	120.17
8	AE	101	BCL	C2A-C1A-CHA	2.52	128.26	123.86
8	M	403	BCL	OBB-CAB-CBB	-2.52	114.51	120.17
8	AI	101	BCL	OBB-CAB-CBB	-2.51	114.53	120.17
8	BG	101	BCL	C1-C2-C3	-2.51	121.71	126.04
8	AF	102	BCL	OBB-CAB-CBB	-2.51	114.53	120.17
8	BA	102	BCL	OBB-CAB-CBB	-2.50	114.54	120.17
8	BD	101	BCL	C1-O2A-CGA	2.50	123.00	116.44
8	L	304	BCL	C2A-C1A-CHA	2.49	128.22	123.86
8	AC	102	BCL	OBB-CAB-CBB	-2.49	114.56	120.17
8	AJ	101	BCL	OBB-CAB-CBB	-2.49	114.56	120.17
8	BN	101	BCL	OBB-CAB-CBB	-2.49	114.57	120.17
8	BJ	101	BCL	C4A-NA-C1A	2.48	107.82	106.71
8	AH	102	BCL	OBB-CAB-CBB	-2.48	114.58	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	AE	103	BCL	OBB-CAB-CBB	-2.48	114.59	120.17
8	BB	1001	BCL	CMD-C2D-C3D	2.48	129.32	124.68
9	AA	1002	SPO	C1-C4-C5	2.48	119.62	113.06
8	BC	101	BCL	CMD-C2D-C3D	2.48	129.31	124.68
8	AB	101	BCL	OBB-CAB-CBB	-2.48	114.60	120.17
8	BI	101	BCL	C1-C2-C3	-2.48	121.76	126.04
8	AN	101	BCL	OBB-CAB-CBB	-2.47	114.61	120.17
8	BL	102	BCL	OBB-CAB-CBB	-2.47	114.61	120.17
8	AM	1001	BCL	C1-C2-C3	2.47	130.31	126.04
8	M	406	BCL	OBB-CAB-CBB	-2.46	114.63	120.17
14	L	303	UQ1	O4-C4-C3	2.46	126.16	120.93
13	M	404	U10	C12-C13-C14	-2.46	121.74	127.66
8	BD	101	BCL	CMD-C2D-C3D	2.46	129.27	124.68
15	M	405	CD4	O16-C46-C47	2.45	116.78	111.50
8	AH	102	BCL	C2A-C1A-CHA	2.45	128.14	123.86
8	AG	102	BCL	OBB-CAB-CBB	-2.45	114.67	120.17
8	BD	101	BCL	OBB-CAB-CBB	-2.45	114.67	120.17
8	L	305	BCL	C4A-NA-C1A	2.44	107.80	106.71
8	AE	103	BCL	CMD-C2D-C3D	2.44	129.24	124.68
8	L	304	BCL	OBB-CAB-CBB	-2.44	114.68	120.17
8	BB	1001	BCL	OBB-CAB-CBB	-2.43	114.69	120.17
8	AB	101	BCL	C2A-C1A-CHA	2.43	128.10	123.86
8	AM	1003	BCL	CMD-C2D-C3D	2.42	129.22	124.68
8	AK	101	BCL	C2A-C1A-CHA	2.42	128.09	123.86
8	AK	103	BCL	OBB-CAB-CBB	-2.42	114.73	120.17
8	BF	101	BCL	C2A-C1A-CHA	2.42	128.08	123.86
8	AM	1003	BCL	OBB-CAB-CBB	-2.42	114.73	120.17
12	L	301	BPH	CHC-C1C-NC	-2.41	122.34	125.20
8	BJ	101	BCL	CMD-C2D-C3D	2.40	129.17	124.68
8	BB	1001	BCL	C2A-C1A-CHA	2.40	128.06	123.86
15	M	405	CD4	O14-C35-C36	2.40	119.43	111.91
8	AM	1003	BCL	C2A-C1A-CHA	2.40	128.05	123.86
9	AB	103	SPO	C31-C30-C28	2.40	120.86	112.98
8	AD	102	BCL	C6-C5-C3	2.39	119.73	113.45
8	BI	101	BCL	CMD-C2D-C3D	2.39	129.15	124.68
8	AK	103	BCL	C1-C2-C3	-2.39	121.91	126.04
8	BG	101	BCL	CMD-C2D-C3D	2.39	129.14	124.68
8	BH	101	BCL	OBB-CAB-CBB	-2.38	114.81	120.17
8	BI	101	BCL	OBB-CAB-CBB	-2.38	114.82	120.17
8	M	406	BCL	CMD-C2D-C3D	2.37	129.12	124.68
9	AI	103	SPO	C25-C23-C22	2.37	122.58	118.94
8	AC	102	BCL	CMD-C2D-C3D	2.37	129.11	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	BC	101	BCL	OBB-CAB-CBB	-2.36	114.85	120.17
8	AA	1001	BCL	OBB-CAB-CBB	-2.36	114.85	120.17
8	BA	102	BCL	C2A-C1A-CHA	2.36	127.99	123.86
8	BJ	101	BCL	OBB-CAB-CBB	-2.35	114.88	120.17
8	M	406	BCL	C1C-NC-C4C	2.35	107.76	106.71
8	M	406	BCL	C1-O2A-CGA	2.34	122.60	116.44
8	L	305	BCL	CMD-C2D-C3D	2.34	129.06	124.68
8	BH	101	BCL	CMD-C2D-C3D	2.34	129.06	124.68
8	L	305	BCL	C1-O2A-CGA	2.34	122.59	116.44
8	BC	101	BCL	C2A-C1A-CHA	2.32	127.92	123.86
12	M	402	BPH	CHC-C1C-NC	-2.32	122.44	125.20
12	L	301	BPH	CMD-C2D-C3D	2.32	129.02	124.68
8	AF	102	BCL	CMD-C2D-C3D	2.32	129.01	124.68
8	AH	102	BCL	CMD-C2D-C3D	2.31	129.01	124.68
8	BA	102	BCL	C1-O2A-CGA	2.31	122.50	116.44
8	AI	101	BCL	CMD-C2D-C3D	2.31	129.00	124.68
8	L	305	BCL	OBB-CAB-CBB	-2.31	114.98	120.17
8	BJ	101	BCL	C1-C2-C3	-2.31	122.05	126.04
8	BN	101	BCL	CMD-C2D-C3D	2.31	128.99	124.68
12	M	402	BPH	CMD-C2D-C3D	2.29	128.97	124.68
8	BN	101	BCL	C1-O2A-CGA	2.29	122.45	116.44
8	BF	101	BCL	OBB-CAB-CBB	-2.29	115.02	120.17
8	AD	102	BCL	CMD-C2D-C3D	2.29	128.96	124.68
8	BN	101	BCL	C2A-C1A-CHA	2.29	127.86	123.86
8	AE	101	BCL	CMD-C2D-C3D	2.28	128.95	124.68
8	M	403	BCL	CMD-C2D-C3D	2.27	128.93	124.68
10	X	101	LMT	C1'-O5'-C5'	-2.27	109.23	113.69
8	BL	102	BCL	C2A-C1A-CHA	2.27	127.83	123.86
8	AL	1001	BCL	CMD-C2D-C3D	2.27	128.92	124.68
8	AJ	101	BCL	CMD-C2D-C3D	2.26	128.91	124.68
8	AM	1001	BCL	CMD-C2D-C3D	2.26	128.91	124.68
8	AA	1001	BCL	C2A-C1A-CHA	2.26	127.82	123.86
8	BG	101	BCL	OBB-CAB-CBB	-2.26	115.08	120.17
11	AB	102	3PE	O12-P-O14	2.26	123.41	112.24
11	H	302	3PE	O12-P-O14	2.26	123.41	112.24
8	AG	102	BCL	CMD-C2D-C3D	2.26	128.90	124.68
8	AI	101	BCL	CAA-CBA-CGA	2.25	119.83	113.25
8	AH	102	BCL	C1-C2-C3	-2.24	122.17	126.04
8	AA	1001	BCL	CMD-C2D-C3D	2.23	128.85	124.68
8	AN	101	BCL	CMD-C2D-C3D	2.23	128.85	124.68
10	X	101	LMT	O1'-C1'-C2'	2.22	111.78	108.30
8	AK	101	BCL	CMD-C2D-C3D	2.22	128.84	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AF	101	SPO	C36-C35-C33	-2.21	105.69	112.98
8	BL	102	BCL	C4A-NA-C1A	2.21	107.70	106.71
8	AC	102	BCL	C2A-C1A-CHA	2.20	127.71	123.86
8	L	304	BCL	CMD-C2D-C3D	2.20	128.80	124.68
8	AG	102	BCL	C2A-C1A-CHA	2.20	127.71	123.86
8	AN	101	BCL	C2A-C1A-CHA	2.20	127.71	123.86
8	BI	101	BCL	C2A-C1A-CHA	2.19	127.70	123.86
11	H	301	3PE	O12-P-O14	2.19	123.09	112.24
13	L	302	U10	C56-C54-C55	2.19	119.45	114.60
8	AM	1001	BCL	C6-C5-C3	2.19	119.19	113.45
8	AK	101	BCL	C6-C5-C3	2.18	119.16	113.45
8	AD	102	BCL	C2A-C1A-CHA	2.17	127.66	123.86
8	AE	103	BCL	C2A-C1A-CHA	2.17	127.64	123.86
8	AB	101	BCL	CMD-C2D-C3D	2.16	128.73	124.68
13	L	302	U10	O3-C3-C2	2.16	123.88	116.56
8	M	406	BCL	C4B-C3B-CAB	-2.16	122.95	127.13
9	AJ	103	SPO	C1-C4-C5	2.16	118.77	113.06
13	L	302	U10	C20-C19-C21	2.15	118.89	115.27
8	BH	101	BCL	C1-O2A-CGA	2.15	122.09	116.44
8	L	305	BCL	C4B-C3B-CAB	-2.15	122.98	127.13
9	BA	101	SPO	C36-C35-C33	-2.15	105.92	112.98
8	BD	101	BCL	CAA-CBA-CGA	2.14	119.51	113.25
13	L	302	U10	C6-C1-C2	2.14	120.88	119.18
8	AK	103	BCL	C2A-C1A-CHA	2.14	127.59	123.86
12	L	301	BPH	C1-C2-C3	-2.14	122.35	126.04
8	AI	101	BCL	C4A-NA-C1A	2.13	107.66	106.71
8	BN	101	BCL	O2A-C1-C2	-2.13	103.04	108.64
8	BG	101	BCL	C2A-C1A-CHA	2.12	127.57	123.86
8	BL	102	BCL	C4B-C3B-CAB	-2.12	123.03	127.13
12	M	402	BPH	C1-O2A-CGA	2.11	121.97	116.44
11	AC	104	3PE	O12-P-O14	2.10	122.63	112.24
8	AL	1001	BCL	C1-O2A-CGA	2.10	121.95	116.44
8	AM	1001	BCL	C2A-C1A-CHA	2.10	127.53	123.86
9	AJ	103	SPO	C3-C1-C4	-2.10	107.64	110.86
12	L	301	BPH	OBB-CAB-CBB	-2.10	115.09	119.73
13	L	302	U10	O3-C3-C4	-2.09	115.76	123.64
8	BG	101	BCL	C1-O2A-CGA	2.08	121.91	116.44
13	L	302	U10	C50-C49-C51	2.08	118.77	115.27
8	BF	101	BCL	C4B-C3B-CAB	-2.08	123.11	127.13
13	L	302	U10	C15-C14-C16	2.08	118.77	115.27
8	AL	1001	BCL	O2A-C1-C2	-2.08	103.17	108.64
8	AB	101	BCL	C4B-C3B-CAB	-2.07	123.13	127.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	L	303	UQ1	C7-C6-C1	-2.07	115.99	118.48
12	M	402	BPH	OBB-CAB-CBB	-2.07	115.15	119.73
8	AL	1001	BCL	C4B-C3B-CAB	-2.06	123.16	127.13
9	AL	1002	SPO	C2-C1-C4	-2.06	107.70	110.86
14	L	303	UQ1	CM2-O2-C2	2.05	123.75	116.47
8	BL	102	BCL	CAA-CBA-CGA	2.05	119.25	113.25
10	AA	1003	LMT	O5B-C5B-C4B	2.05	113.41	109.69
8	BA	102	BCL	C4B-C3B-CAB	-2.04	123.20	127.13
8	BI	101	BCL	C4B-C3B-CAB	-2.03	123.20	127.13
13	M	404	U10	O2-C2-C1	-2.03	114.75	120.73
8	AE	103	BCL	C4B-C3B-CAB	-2.03	123.21	127.13
8	BN	101	BCL	C4B-C3B-CAB	-2.03	123.21	127.13
12	M	402	BPH	CHD-C4C-NC	-2.03	122.79	125.20
8	AL	1001	BCL	C6-C5-C3	2.02	118.76	113.45
8	BF	101	BCL	C4A-NA-C1A	2.02	107.61	106.71
8	BI	101	BCL	C1C-NC-C4C	2.02	107.61	106.71
8	AB	101	BCL	O2A-CGA-O1A	-2.02	118.50	123.59
9	AH	101	SPO	C2-C1-C4	-2.00	107.78	110.86
8	AL	1001	BCL	C2A-C1A-CHA	2.00	127.36	123.86
8	AI	101	BCL	C4B-C3B-CAB	-2.00	123.26	127.13

There are no chirality outliers.

All (385) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	AK	101	BCL	C2-C3-C5-C6
8	AK	101	BCL	C4-C3-C5-C6
8	AN	101	BCL	C4-C3-C5-C6
8	BA	102	BCL	C3A-C2A-CAA-CBA
8	BB	1001	BCL	C1A-C2A-CAA-CBA
8	BC	101	BCL	C1A-C2A-CAA-CBA
8	BF	101	BCL	C3A-C2A-CAA-CBA
8	BI	101	BCL	C1A-C2A-CAA-CBA
8	BJ	101	BCL	C1A-C2A-CAA-CBA
8	BL	102	BCL	C1A-C2A-CAA-CBA
9	AB	103	SPO	C2-C1-C4-C5
9	AI	103	SPO	C1-C4-C5-C6
9	AI	103	SPO	C22-C23-C25-C26
9	AI	103	SPO	C24-C23-C25-C26
9	AJ	102	SPO	C28-C30-C31-C32
9	AJ	103	SPO	C28-C30-C31-C32
9	BA	101	SPO	C28-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
9	BE	1000	SPO	C2-C1-C4-C5
9	BE	1000	SPO	C3-C1-C4-C5
9	BL	101	SPO	C27-C28-C30-C31
9	BL	101	SPO	C29-C28-C30-C31
11	AB	102	3PE	C1-O11-P-O12
11	AB	102	3PE	C1-O11-P-O13
11	AB	102	3PE	C1-O11-P-O14
11	AB	102	3PE	C11-O13-P-O12
11	AB	102	3PE	C2-C1-O11-P
11	AC	104	3PE	C1-O11-P-O12
11	AC	104	3PE	C11-O13-P-O11
11	AC	104	3PE	C11-O13-P-O14
11	AC	104	3PE	C12-C11-O13-P
11	H	302	3PE	C1-O11-P-O12
11	H	302	3PE	C11-O13-P-O11
11	H	302	3PE	C11-O13-P-O14
13	L	302	U10	C4-C3-O3-C3M
15	M	405	CD4	O16-C33-C34-O14
10	AB	104	LMT	O5'-C5'-C6'-O6'
10	AB	104	LMT	C4'-C5'-C6'-O6'
8	AI	101	BCL	C4-C3-C5-C6
8	AI	101	BCL	C2-C3-C5-C6
8	AN	101	BCL	C2-C3-C5-C6
9	AC	103	SPO	C28-C30-C31-C32
8	AI	101	BCL	C11-C10-C8-C9
8	AM	1003	BCL	C11-C10-C8-C9
9	AF	103	SPO	C15-C16-C17-C18
9	AG	103	SPO	C15-C16-C17-C18
9	AJ	103	SPO	C5-C6-C7-C8
9	AK	104	SPO	C10-C11-C12-C13
9	AK	104	SPO	C15-C16-C17-C18
9	AM	1004	SPO	C15-C16-C17-C18
9	BE	1000	SPO	C15-C16-C17-C18
9	M	407	SPO	C15-C16-C17-C18
8	AD	102	BCL	C3-C5-C6-C7
8	BH	101	BCL	C3-C5-C6-C7
13	M	404	U10	C4-C3-O3-C3M
14	L	303	UQ1	C2-C3-O3-CM3
9	AD	103	SPO	C28-C30-C31-C32
9	AI	102	SPO	C33-C35-C36-C37
9	AJ	102	SPO	C33-C35-C36-C37
13	L	302	U10	C24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
13	L	302	U10	C29-C31-C32-C33
11	AC	104	3PE	C1-O11-P-O13
11	H	302	3PE	C1-O11-P-O13
15	M	405	CD4	C32-O13-P2-O10
10	X	101	LMT	O5'-C5'-C6'-O6'
9	AA	1002	SPO	C34-C33-C35-C36
9	AD	101	SPO	C34-C33-C35-C36
8	BA	102	BCL	C2A-CAA-CBA-CGA
8	BC	101	BCL	C5-C6-C7-C8
8	BB	1001	BCL	C5-C6-C7-C8
8	BN	101	BCL	C13-C15-C16-C17
11	H	302	3PE	C26-C27-C28-C29
11	H	301	3PE	C22-C23-C24-C25
10	AA	1003	LMT	C2'-C1'-O1'-C1
9	AB	103	SPO	C34-C33-C35-C36
12	L	301	BPH	C4-C3-C5-C6
8	BF	101	BCL	C14-C13-C15-C16
12	M	402	BPH	C6-C7-C8-C9
11	H	301	3PE	C21-C22-C23-C24
8	AE	103	BCL	C2A-CAA-CBA-CGA
8	BJ	101	BCL	C5-C6-C7-C8
10	AA	1003	LMT	O5'-C1'-O1'-C1
8	AF	102	BCL	C15-C16-C17-C18
8	AK	103	BCL	C13-C15-C16-C17
11	H	302	3PE	C34-C35-C36-C37
8	AC	102	BCL	C3A-C2A-CAA-CBA
8	AI	101	BCL	C3A-C2A-CAA-CBA
8	AK	103	BCL	C3A-C2A-CAA-CBA
8	BB	1001	BCL	C3A-C2A-CAA-CBA
8	BC	101	BCL	C3A-C2A-CAA-CBA
8	BI	101	BCL	C3A-C2A-CAA-CBA
8	BJ	101	BCL	C3A-C2A-CAA-CBA
8	BL	102	BCL	C3A-C2A-CAA-CBA
11	H	301	3PE	C39-C3A-C3B-C3C
8	BN	101	BCL	C4-C3-C5-C6
9	AI	102	SPO	C34-C33-C35-C36
9	AA	1002	SPO	C32-C33-C35-C36
13	L	302	U10	C33-C34-C36-C37
13	L	302	U10	C48-C49-C51-C52
8	BB	1001	BCL	C2-C1-O2A-CGA
8	BL	102	BCL	C2-C1-O2A-CGA
11	AB	102	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
8	BB	1001	BCL	C8-C10-C11-C12
9	AB	103	SPO	C29-C28-C30-C31
13	L	302	U10	C50-C49-C51-C52
8	AI	101	BCL	C11-C10-C8-C7
8	AM	1003	BCL	C11-C10-C8-C7
8	BF	101	BCL	C12-C13-C15-C16
8	BJ	101	BCL	C12-C13-C15-C16
8	BN	101	BCL	C2-C3-C5-C6
9	AB	103	SPO	C27-C28-C30-C31
12	L	301	BPH	C2-C3-C5-C6
12	M	402	BPH	C6-C7-C8-C10
8	BH	101	BCL	C10-C11-C12-C13
8	AC	102	BCL	C2A-CAA-CBA-CGA
8	BL	102	BCL	C5-C6-C7-C8
8	AB	101	BCL	C3-C5-C6-C7
13	L	302	U10	C35-C34-C36-C37
8	AI	101	BCL	C11-C12-C13-C14
8	BJ	101	BCL	C14-C13-C15-C16
8	BN	101	BCL	C6-C7-C8-C9
12	M	402	BPH	C14-C13-C15-C16
8	AK	103	BCL	C3-C5-C6-C7
8	AI	101	BCL	C2A-CAA-CBA-CGA
8	AC	102	BCL	C1A-C2A-CAA-CBA
8	AI	101	BCL	C1A-C2A-CAA-CBA
8	AK	103	BCL	C1A-C2A-CAA-CBA
8	BA	102	BCL	C1A-C2A-CAA-CBA
8	BF	101	BCL	C1A-C2A-CAA-CBA
8	AM	1003	BCL	C5-C6-C7-C8
14	L	303	UQ1	C6-C7-C8-C9
8	BD	101	BCL	C8-C10-C11-C12
11	AC	104	3PE	C38-C39-C3A-C3B
13	L	302	U10	C15-C14-C16-C17
9	AI	102	SPO	C32-C33-C35-C36
15	M	405	CD4	C32-C33-C34-O14
9	AA	1002	SPO	C33-C35-C36-C37
8	BH	101	BCL	C5-C6-C7-C8
9	AF	101	SPO	C29-C28-C30-C31
9	AF	101	SPO	C27-C28-C30-C31
8	AB	101	BCL	C10-C11-C12-C13
9	AA	1002	SPO	C3-C1-C4-C5
9	AB	103	SPO	C3-C1-C4-C5
9	AL	1002	SPO	C2-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
9	AL	1002	SPO	C3-C1-C4-C5
8	AF	102	BCL	C6-C7-C8-C10
8	AI	101	BCL	C11-C12-C13-C15
8	AK	101	BCL	C11-C10-C8-C7
8	AL	1001	BCL	C11-C12-C13-C15
8	BC	101	BCL	C12-C13-C15-C16
8	L	305	BCL	C12-C13-C15-C16
12	M	402	BPH	C12-C13-C15-C16
13	L	302	U10	C13-C14-C16-C17
8	AF	102	BCL	C6-C7-C8-C9
8	AK	101	BCL	C11-C10-C8-C9
8	AN	101	BCL	C11-C10-C8-C9
8	BC	101	BCL	C14-C13-C15-C16
8	BD	101	BCL	C2A-CAA-CBA-CGA
11	H	302	3PE	C2C-C2D-C2E-C2F
9	BE	1000	SPO	O1-C1-C4-C5
9	AH	103	SPO	C15-C16-C17-C18
9	AK	102	SPO	C5-C6-C7-C8
8	AA	1001	BCL	C16-C17-C18-C20
15	M	405	CD4	C27-C60-C61-C62
11	H	302	3PE	C31-C32-C33-C34
8	AA	1001	BCL	C16-C17-C18-C19
8	AI	101	BCL	C5-C6-C7-C8
11	H	301	3PE	O11-C1-C2-C3
10	AA	1003	LMT	O5B-C5B-C6B-O6B
8	AE	103	BCL	C4-C3-C5-C6
9	AB	103	SPO	C32-C33-C35-C36
9	AD	101	SPO	C32-C33-C35-C36
8	AE	103	BCL	C3A-C2A-CAA-CBA
8	AM	1001	BCL	C13-C15-C16-C17
11	AC	104	3PE	C1-C2-C3-O31
15	M	405	CD4	C28-C15-C16-O3
11	H	301	3PE	C2A-C2B-C2C-C2D
8	BA	102	BCL	C3-C5-C6-C7
9	AC	103	SPO	C29-C28-C30-C31
8	AE	103	BCL	C2-C3-C5-C6
8	AC	102	BCL	C15-C16-C17-C18
9	AC	103	SPO	C27-C28-C30-C31
8	AB	101	BCL	C11-C12-C13-C14
10	M	401	LMT	O5B-C5B-C6B-O6B
8	AB	101	BCL	C4C-C3C-CAC-CBC
8	BC	101	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
9	AG	103	SPO	C15-C16-C17-C19
9	AK	104	SPO	C10-C11-C12-C14
9	AK	104	SPO	C15-C16-C17-C19
11	AC	104	3PE	O11-C1-C2-C3
8	AE	101	BCL	C11-C10-C8-C7
8	AL	1001	BCL	C6-C7-C8-C10
12	M	402	BPH	CAD-CBD-CGD-O2D
8	L	305	BCL	C15-C16-C17-C18
8	BL	102	BCL	C4-C3-C5-C6
9	BA	101	SPO	C29-C28-C30-C31
10	AB	104	LMT	C4B-C5B-C6B-O6B
14	L	303	UQ1	C4-C3-O3-CM3
11	H	301	3PE	C2-C1-O11-P
11	H	301	3PE	O11-C1-C2-O21
11	H	302	3PE	C28-C29-C2A-C2B
8	AL	1001	BCL	C6-C7-C8-C9
15	M	405	CD4	C41-C42-C43-C44
8	BJ	101	BCL	C2-C1-O2A-CGA
8	AD	102	BCL	C4-C3-C5-C6
11	AC	104	3PE	C2-C1-O11-P
15	M	405	CD4	C32-O13-P2-O11
8	AC	102	BCL	C16-C17-C18-C20
11	AB	102	3PE	C12-C11-O13-P
15	M	405	CD4	O3-C17-C18-C19
9	BL	101	SPO	C1-C4-C5-C6
11	H	301	3PE	C29-C2A-C2B-C2C
8	AB	101	BCL	C2C-C3C-CAC-CBC
8	AC	102	BCL	C11-C12-C13-C15
8	AJ	101	BCL	C11-C10-C8-C7
8	AM	1001	BCL	C6-C7-C8-C10
8	BL	102	BCL	C11-C12-C13-C15
11	AC	104	3PE	O11-C1-C2-O21
10	M	401	LMT	C2-C1-O1'-C1'
11	AC	104	3PE	O21-C2-C3-O31
8	AC	102	BCL	C16-C17-C18-C19
15	M	405	CD4	C33-C32-O13-P2
8	AD	102	BCL	C11-C12-C13-C14
8	AE	101	BCL	C11-C10-C8-C9
8	AL	1001	BCL	C11-C12-C13-C14
8	AM	1001	BCL	C6-C7-C8-C9
8	L	305	BCL	C14-C13-C15-C16
13	M	404	U10	C44-C46-C47-C48

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Mol	Chain	Res	Type	Atoms
15	M	405	CD4	C39-C40-C41-C42
13	L	302	U10	C5-C4-O4-C4M
11	H	302	3PE	C1-C2-O21-C21
8	BL	102	BCL	C2A-CAA-CBA-CGA
8	AM	1003	BCL	C2-C1-O2A-CGA
8	BH	101	BCL	C4-C3-C5-C6
8	BL	102	BCL	C2-C3-C5-C6
8	BG	101	BCL	C2A-CAA-CBA-CGA
15	M	405	CD4	O2-C15-C16-O3
9	AA	1002	SPO	C2-C1-C4-C5
9	AI	102	SPO	C3-C1-C4-C5
9	AK	104	SPO	C3-C1-C4-C5
8	AN	101	BCL	C11-C10-C8-C7
8	BN	101	BCL	C6-C7-C8-C10
8	AC	102	BCL	C11-C12-C13-C14
9	AB	103	SPO	O1-C1-C4-C5
9	AF	101	SPO	O1-C1-C4-C5
9	AJ	102	SPO	O1-C1-C4-C5
9	BE	1000	SPO	C15-C16-C17-C19
8	AA	1001	BCL	C15-C16-C17-C18
8	BI	101	BCL	C2A-CAA-CBA-CGA
9	AD	101	SPO	C33-C35-C36-C37
10	M	401	LMT	C9-C10-C11-C12
9	AK	104	SPO	C34-C33-C35-C36
13	M	404	U10	C35-C34-C36-C37
9	AK	104	SPO	C32-C33-C35-C36
9	BL	101	SPO	C32-C33-C35-C36
11	H	301	3PE	C2B-C2C-C2D-C2E
11	H	301	3PE	C2D-C2E-C2F-C2G
15	M	405	CD4	C43-C44-C45-C63
8	AM	1003	BCL	C2A-CAA-CBA-CGA
9	AC	101	SPO	C29-C28-C30-C31
9	AH	101	SPO	C29-C28-C30-C31
9	BL	101	SPO	C34-C33-C35-C36
13	L	302	U10	C12-C11-C9-C10
8	AA	1001	BCL	C11-C12-C13-C14
8	BF	101	BCL	O2A-C1-C2-C3
8	BN	101	BCL	O2A-C1-C2-C3
12	L	301	BPH	O2A-C1-C2-C3
9	AB	103	SPO	C15-C16-C17-C18
11	H	301	3PE	C26-C27-C28-C29
9	AA	1002	SPO	C29-C28-C30-C31

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Mol	Chain	Res	Type	Atoms
9	AG	101	SPO	C29-C28-C30-C31
9	AM	1002	SPO	C29-C28-C30-C31
8	AE	103	BCL	C1A-C2A-CAA-CBA
8	BG	101	BCL	C1A-C2A-CAA-CBA
8	BB	1001	BCL	C15-C16-C17-C18
12	L	301	BPH	C8-C10-C11-C12
11	H	301	3PE	C32-C33-C34-C35
11	H	302	3PE	C2A-C2B-C2C-C2D
8	AD	102	BCL	C2-C3-C5-C6
8	BH	101	BCL	C2-C3-C5-C6
9	AJ	103	SPO	C35-C36-C37-C38
11	H	301	3PE	C37-C38-C39-C3A
11	AB	102	3PE	C29-C2A-C2B-C2C
9	AK	102	SPO	C29-C28-C30-C31
9	BE	1000	SPO	C34-C33-C35-C36
8	BG	101	BCL	C2-C1-O2A-CGA
9	AA	1002	SPO	C27-C28-C30-C31
9	AH	101	SPO	C27-C28-C30-C31
13	L	302	U10	C12-C11-C9-C8
8	AL	1001	BCL	C10-C11-C12-C13
9	AE	102	SPO	C29-C28-C30-C31
8	AJ	101	BCL	C4C-C3C-CAC-CBC
9	AF	103	SPO	C15-C16-C17-C19
9	AM	1004	SPO	C15-C16-C17-C19
9	AC	101	SPO	C27-C28-C30-C31
9	AM	1002	SPO	C27-C28-C30-C31
13	M	404	U10	C33-C34-C36-C37
11	H	302	3PE	C2E-C2F-C2G-C2H
11	H	302	3PE	C3B-C3C-C3D-C3E
8	M	406	BCL	C4-C3-C5-C6
9	AJ	102	SPO	C29-C28-C30-C31
9	AM	1004	SPO	C29-C28-C30-C31
9	AF	101	SPO	C33-C35-C36-C37
8	AB	101	BCL	C11-C12-C13-C15
9	AE	102	SPO	C27-C28-C30-C31
9	AG	101	SPO	C27-C28-C30-C31
9	AK	102	SPO	C27-C28-C30-C31
9	AH	103	SPO	C11-C10-C9-C7
8	AC	102	BCL	CAA-CBA-CGA-O2A
8	BF	101	BCL	C4-C3-C5-C6
9	AD	101	SPO	C29-C28-C30-C31
9	AJ	102	SPO	C34-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
9	BA	101	SPO	C27-C28-C30-C31
8	BL	102	BCL	C11-C12-C13-C14
8	M	406	BCL	C8-C10-C11-C12
8	AB	101	BCL	CAD-CBD-CGD-O2D
8	L	304	BCL	CAD-CBD-CGD-O2D
8	L	305	BCL	CAD-CBD-CGD-O2D
8	M	406	BCL	CAD-CBD-CGD-O2D
12	L	301	BPH	CAD-CBD-CGD-O2D
10	AB	104	LMT	O5B-C5B-C6B-O6B
11	AC	104	3PE	C3A-C3B-C3C-C3D
11	H	301	3PE	O31-C31-C32-C33
13	M	404	U10	C50-C49-C51-C52
9	AD	101	SPO	C27-C28-C30-C31
9	AJ	102	SPO	C27-C28-C30-C31
13	M	404	U10	C48-C49-C51-C52
9	AH	103	SPO	C15-C16-C17-C19
9	AJ	103	SPO	C5-C6-C7-C9
9	AK	102	SPO	C5-C6-C7-C9
9	M	407	SPO	C15-C16-C17-C19
13	M	404	U10	C5-C4-O4-C4M
14	L	303	UQ1	C1-C2-O2-CM2
10	M	401	LMT	C5'-C4'-O1B-C1B
8	AN	101	BCL	C5-C6-C7-C8
8	AJ	101	BCL	O2A-C1-C2-C3
8	BL	102	BCL	O2A-C1-C2-C3
12	M	402	BPH	O2A-C1-C2-C3
8	AG	102	BCL	CHA-CBD-CGD-O2D
8	AH	102	BCL	CHA-CBD-CGD-O2D
8	BG	101	BCL	CHA-CBD-CGD-O1D
8	BG	101	BCL	CHA-CBD-CGD-O2D
8	M	406	BCL	CHA-CBD-CGD-O2D
12	M	402	BPH	CHA-CBD-CGD-O2D
11	AB	102	3PE	C27-C28-C29-C2A
8	M	406	BCL	C2-C3-C5-C6
8	BG	101	BCL	CAA-CBA-CGA-O2A
8	BL	102	BCL	CAA-CBA-CGA-O2A
9	AD	103	SPO	C30-C31-C32-C33
9	AK	104	SPO	C29-C28-C30-C31
8	M	406	BCL	C11-C10-C8-C7
8	AJ	101	BCL	C11-C10-C8-C9
9	AD	103	SPO	C33-C35-C36-C37
9	AE	102	SPO	C28-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
11	H	302	3PE	C27-C28-C29-C2A
13	L	302	U10	C3-C4-O4-C4M
8	BF	101	BCL	CAA-CBA-CGA-O2A
8	AK	103	BCL	C2A-CAA-CBA-CGA
8	BB	1001	BCL	C2A-CAA-CBA-CGA
8	BC	101	BCL	C2A-CAA-CBA-CGA
9	AD	103	SPO	C15-C16-C17-C18
9	BE	1000	SPO	C32-C33-C35-C36
8	AM	1003	BCL	C1A-C2A-CAA-CBA
11	H	301	3PE	O32-C31-C32-C33
8	AC	102	BCL	CAA-CBA-CGA-O1A
11	H	301	3PE	C3D-C3E-C3F-C3G
8	M	403	BCL	CAA-CBA-CGA-O2A
11	AB	102	3PE	C11-O13-P-O14
8	AE	101	BCL	C8-C10-C11-C12
8	AM	1001	BCL	C11-C12-C13-C14
8	BH	101	BCL	C14-C13-C15-C16
8	M	406	BCL	C11-C10-C8-C9
8	BF	101	BCL	C13-C15-C16-C17
8	AJ	101	BCL	C4-C3-C5-C6
8	AA	1001	BCL	C11-C12-C13-C15
8	AJ	101	BCL	C2-C3-C5-C6
8	BG	101	BCL	C3A-C2A-CAA-CBA
8	BH	101	BCL	C12-C13-C15-C16
9	AB	103	SPO	C15-C16-C17-C19
8	AA	1001	BCL	C8-C10-C11-C12
9	AI	103	SPO	C33-C35-C36-C37
8	AJ	101	BCL	C8-C10-C11-C12
8	AK	101	BCL	C15-C16-C17-C18
9	AA	1002	SPO	C30-C31-C32-C33
13	M	404	U10	C41-C42-C43-C44
8	AI	101	BCL	CAA-CBA-CGA-O1A

There are no ring outliers.

52 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	H	302	3PE	1	0
9	AA	1002	SPO	3	0
13	L	302	U10	1	0
8	AM	1003	BCL	1	0
9	AF	101	SPO	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	AJ	101	BCL	4	0
8	AC	102	BCL	2	0
8	BC	101	BCL	2	0
8	AE	101	BCL	2	0
8	L	305	BCL	1	0
8	BD	101	BCL	1	0
9	AF	103	SPO	2	0
8	BF	101	BCL	1	0
8	AM	1001	BCL	2	0
8	AN	101	BCL	1	0
8	AI	101	BCL	2	0
8	BH	101	BCL	1	0
9	AC	103	SPO	2	0
8	AE	103	BCL	1	0
9	AH	103	SPO	1	0
8	BL	102	BCL	1	0
8	AA	1001	BCL	1	0
8	BA	102	BCL	1	0
9	BE	1000	SPO	2	0
13	M	404	U10	1	0
9	AJ	102	SPO	2	0
9	AD	103	SPO	2	0
8	BI	101	BCL	1	0
8	BN	101	BCL	1	0
9	AE	102	SPO	3	0
9	AJ	103	SPO	1	0
9	AM	1002	SPO	3	0
8	AB	101	BCL	3	0
9	AM	1004	SPO	2	0
14	L	303	UQ1	1	0
8	AG	102	BCL	1	0
9	AD	101	SPO	1	0
9	AI	102	SPO	4	0
9	AI	103	SPO	1	0
9	AH	101	SPO	2	0
9	AK	104	SPO	2	0
9	BA	101	SPO	3	0
8	BJ	101	BCL	1	0
15	M	405	CD4	1	0
8	BB	1001	BCL	1	0
8	AF	102	BCL	1	0
12	M	402	BPH	1	0

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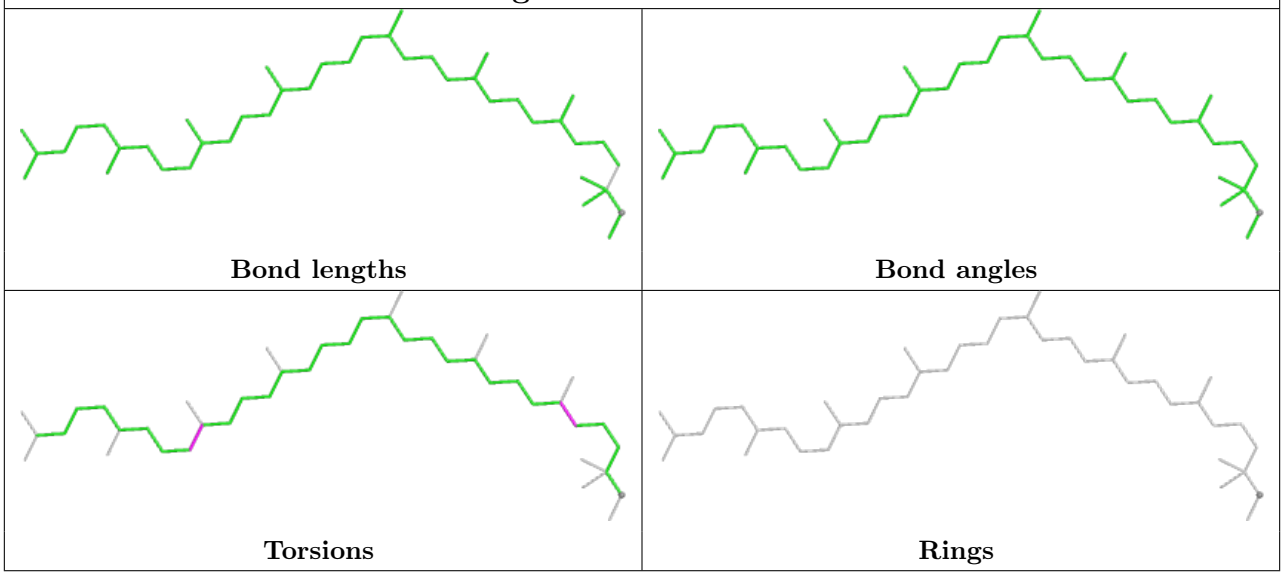
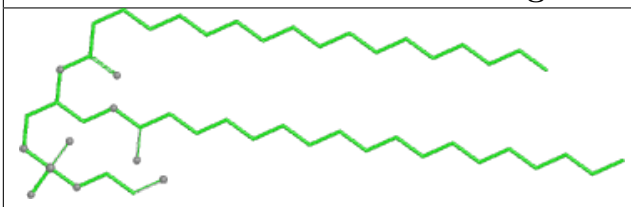
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	AB	103	SPO	3	0
9	M	407	SPO	1	0
8	AK	103	BCL	1	0
9	AL	1002	SPO	3	0
8	BG	101	BCL	1	0

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.

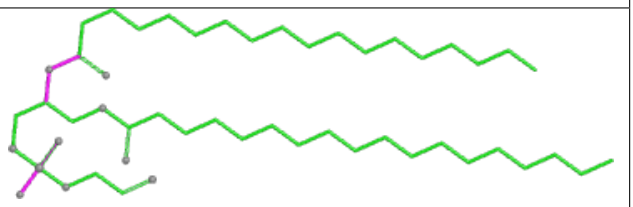
Ligand SPO AK 102



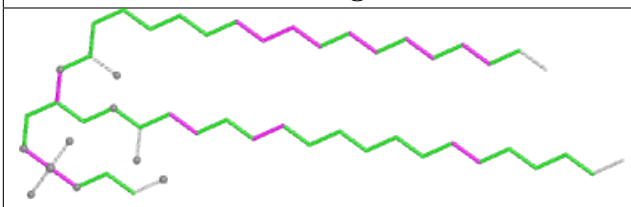
Ligand 3PE H 302



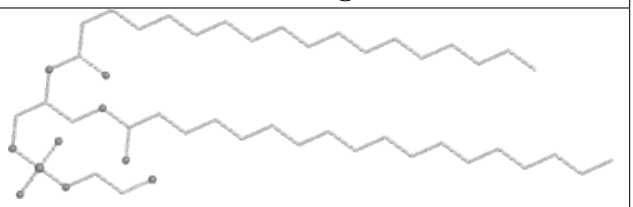
Bond lengths



Bond angles

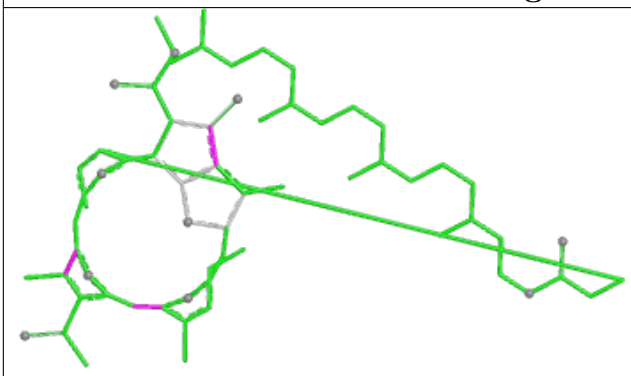


Torsions

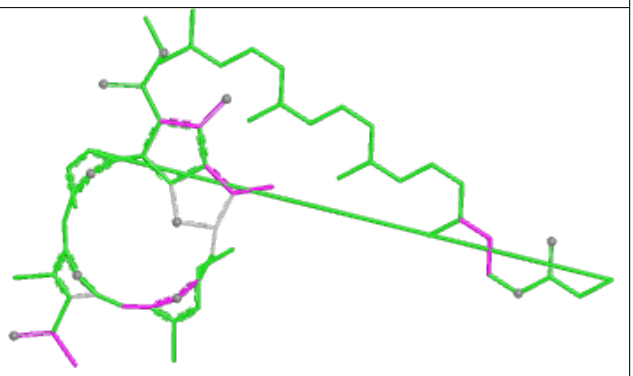


Rings

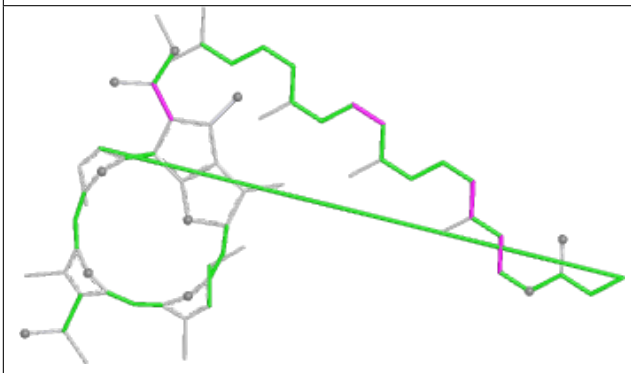
Ligand BPH L 301



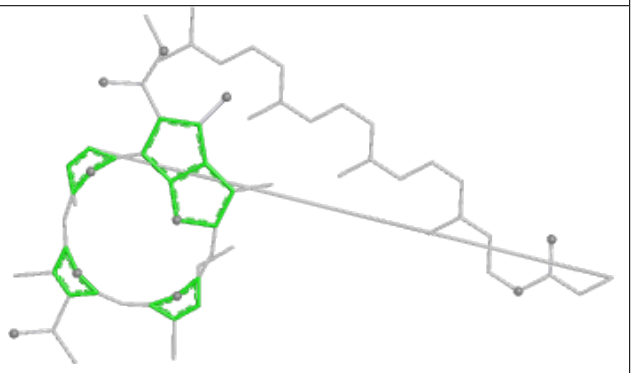
Bond lengths



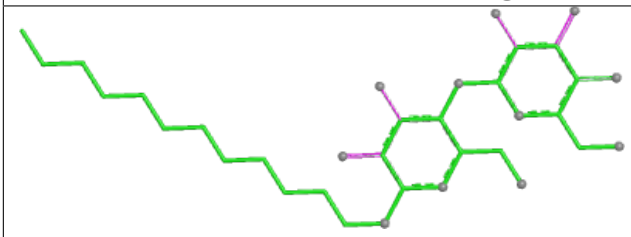
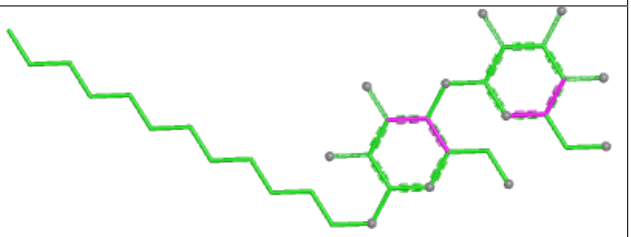
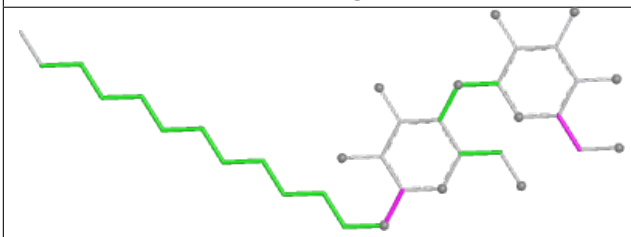
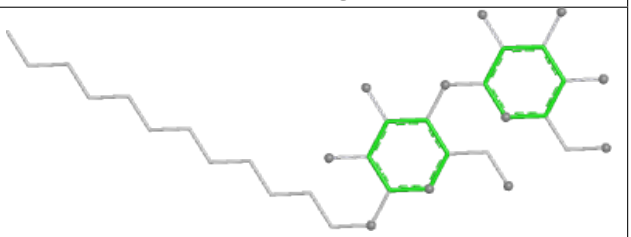
Bond angles

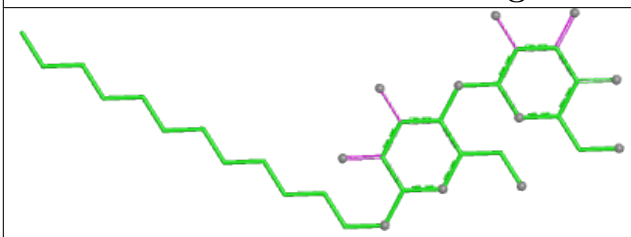
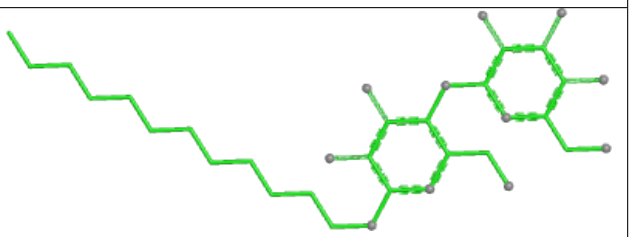
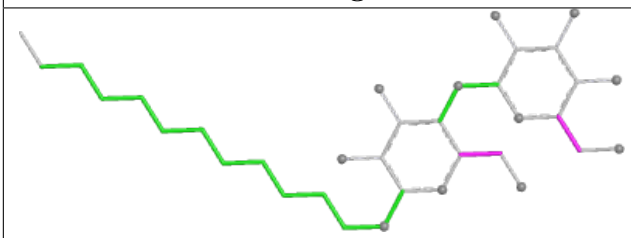
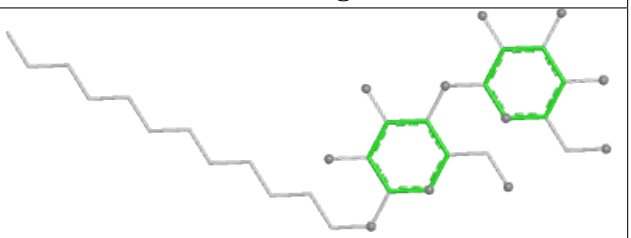


Torsions

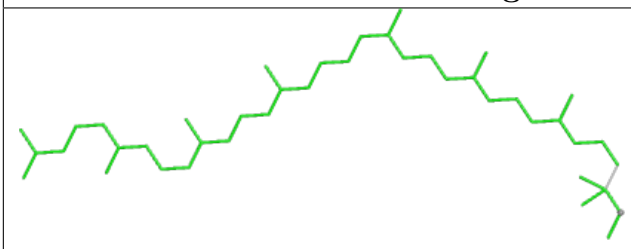


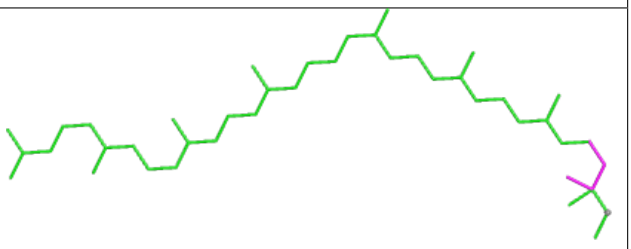
Rings

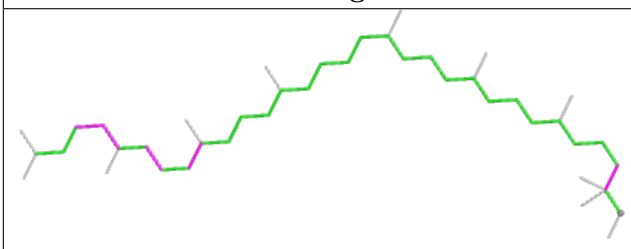
Ligand LMT AA 1003	
 Bond lengths	 Bond angles
 Torsions	 Rings

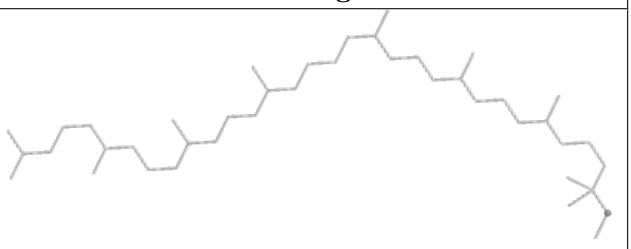
Ligand LMT AB 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPO AA 1002

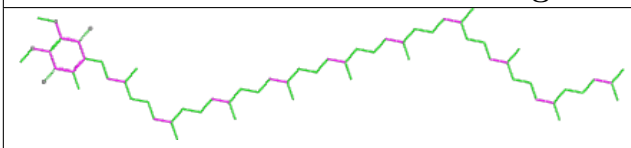

Bond lengths


Bond angles


Torsions


Rings

Ligand U10 L 302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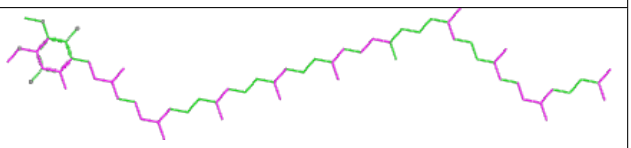
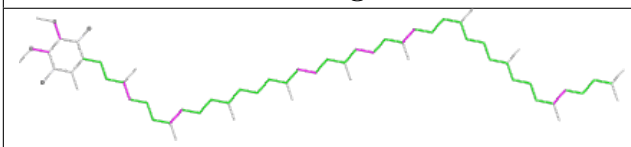
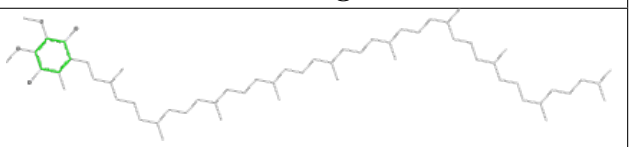
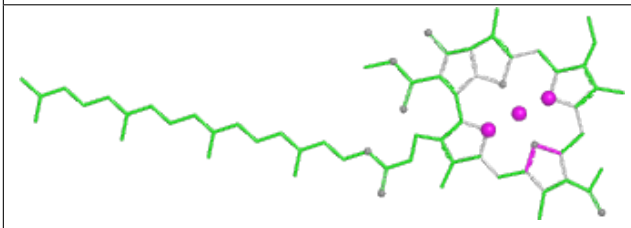

Bond angles


Torsions


Rings

Ligand BCL AM 1003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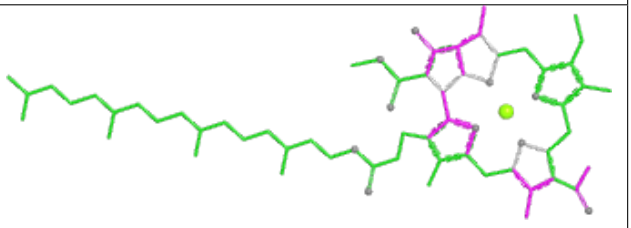
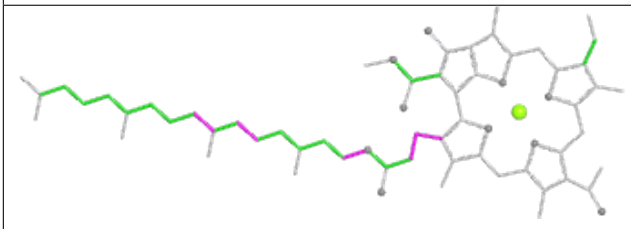

Bond angles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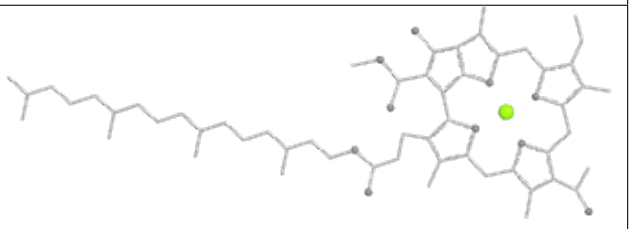
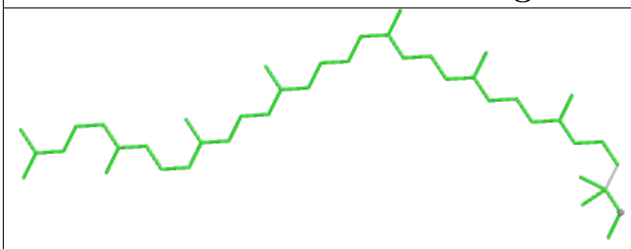

Rings

Ligand SPO AF 101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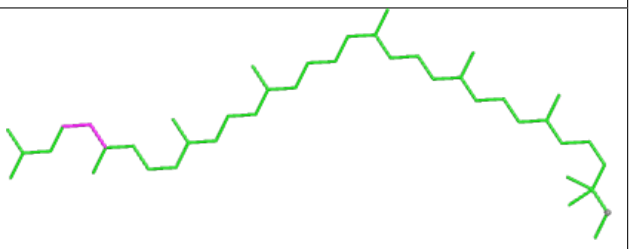
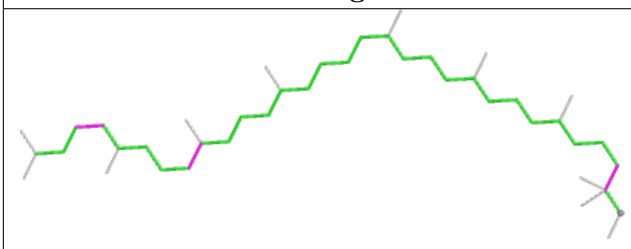
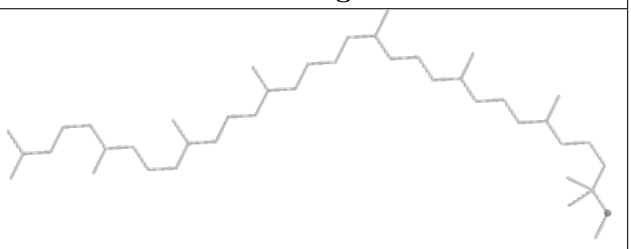
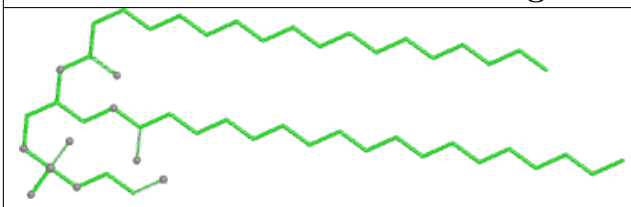
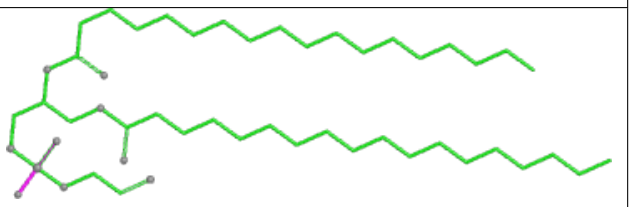

Bond angles

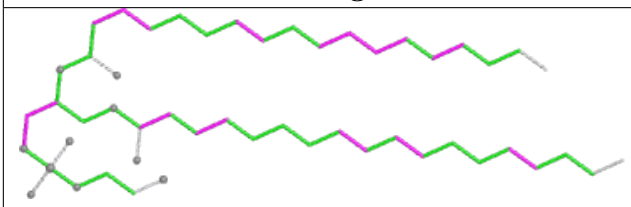

Torsions

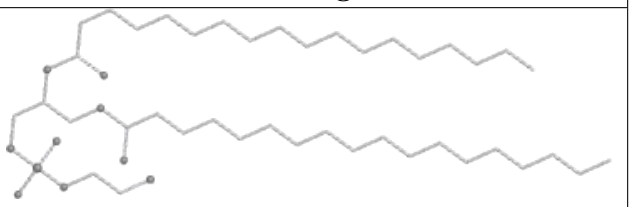

Rings

Ligand 3PE H 301

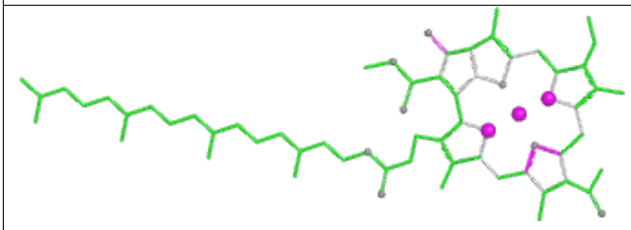

Bond lengths

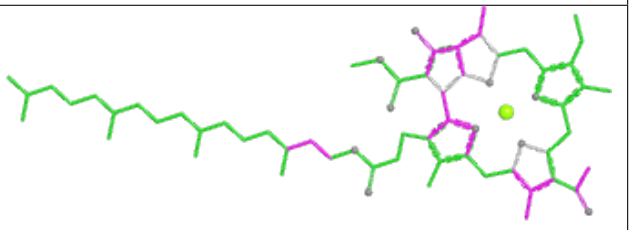

Bond angles

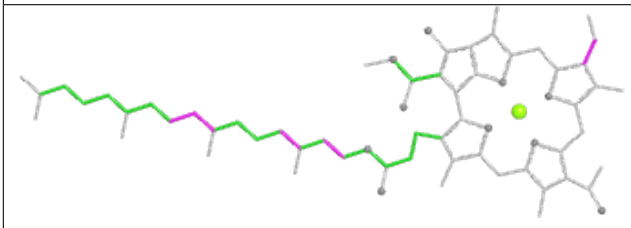

Torsions

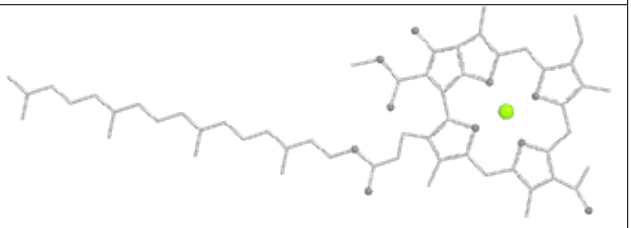

Rings

Ligand BCL AJ 101

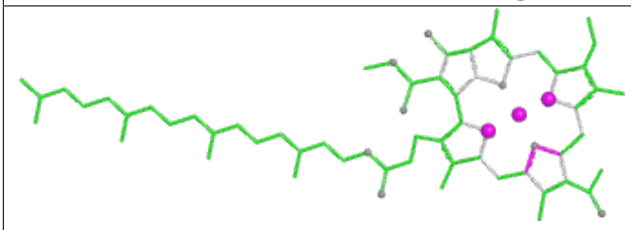

Bond lengths


Bond angles


Torsions


Rings

Ligand BCL AC 102



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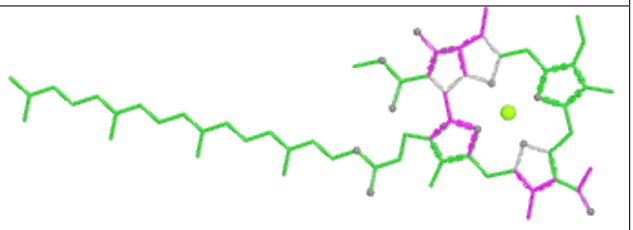
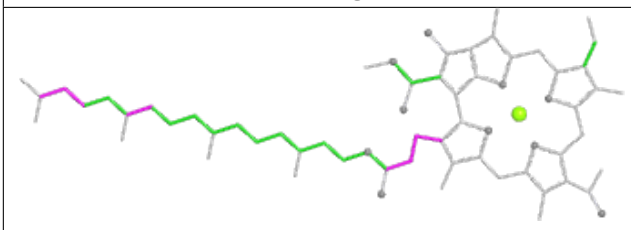


Bond angles



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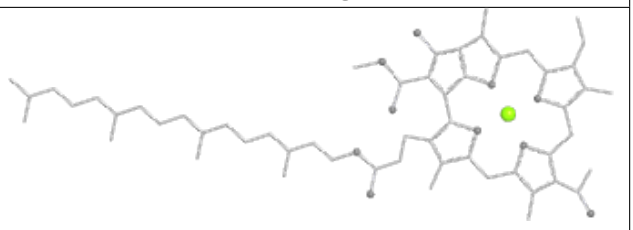
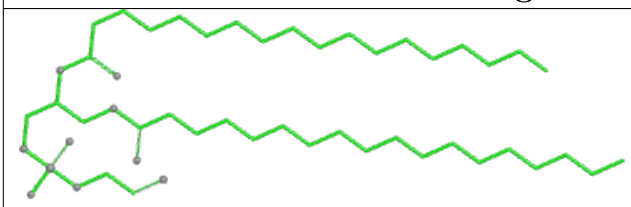


Rings

Ligand 3PE AC 104



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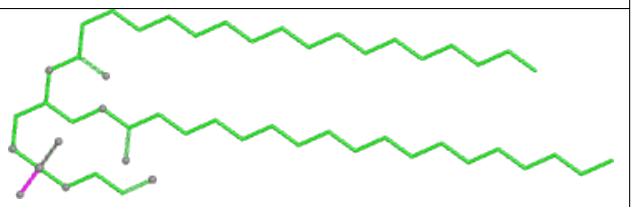
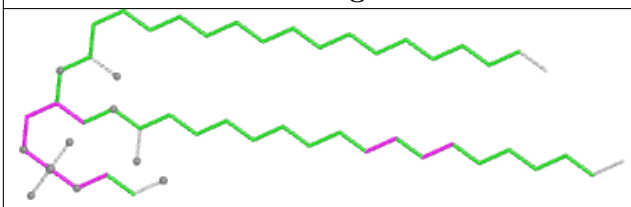
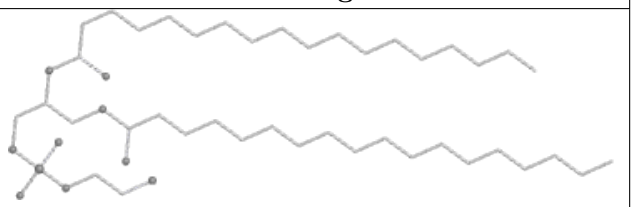


Bond angles

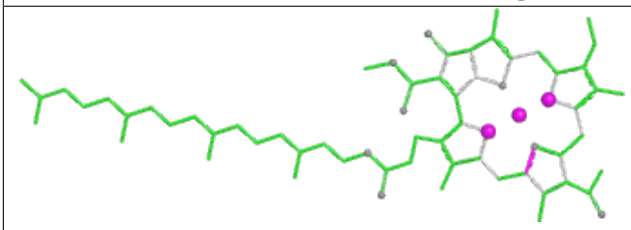


Torsions



Rings

Ligand BCL BC 101



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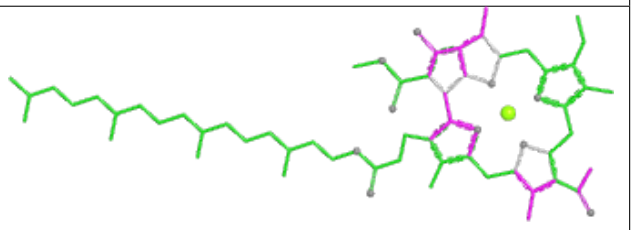
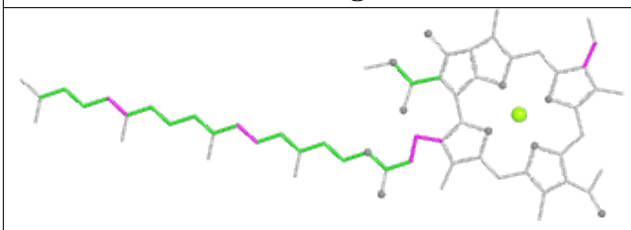
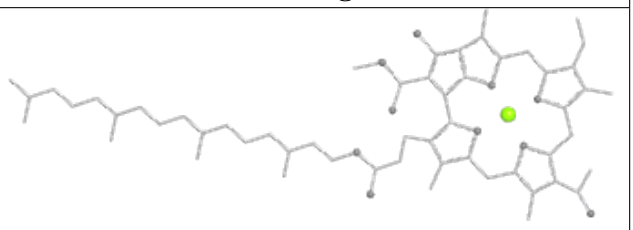


Bond angles

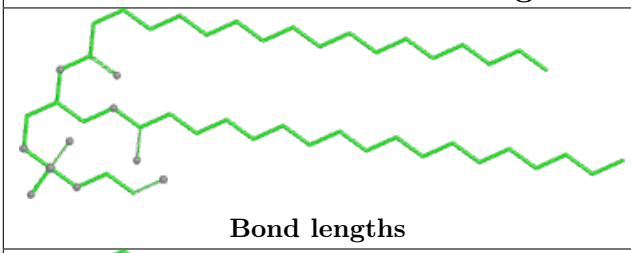


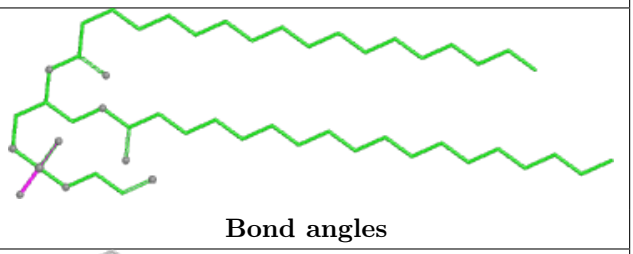
Torsions

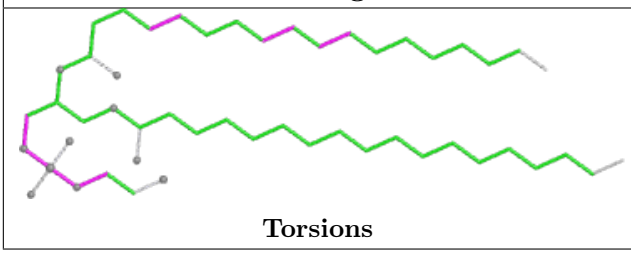


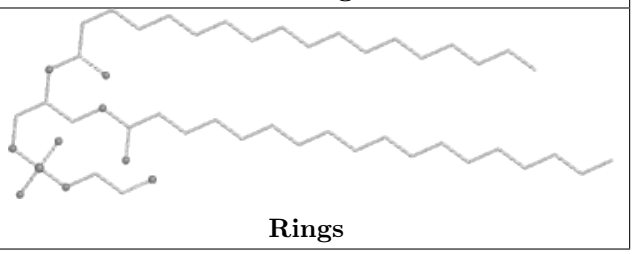
Rings

Ligand 3PE AB 102

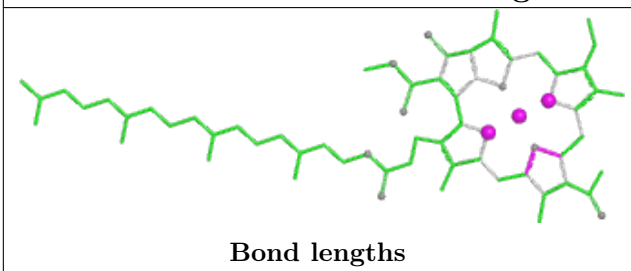

Bond lengths

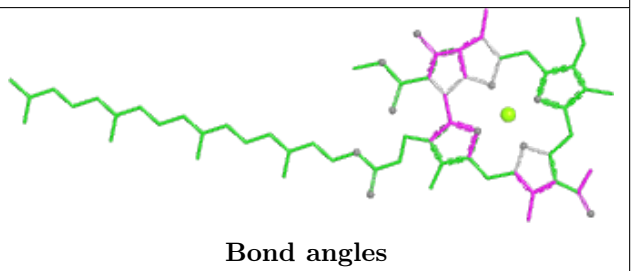

Bond angles

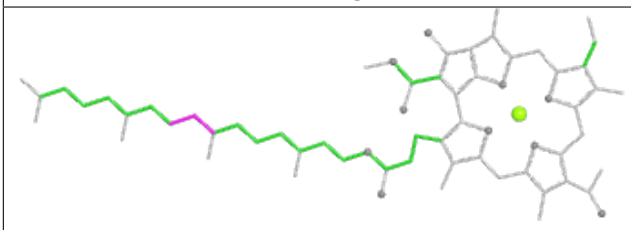

Torsions

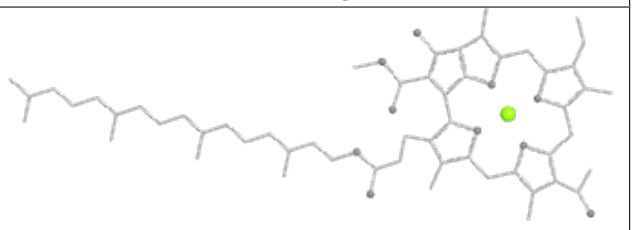

Rings

Ligand BCL AE 101

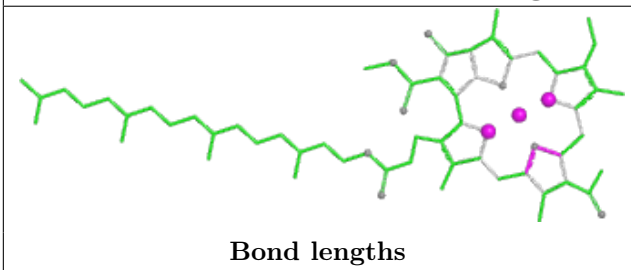

Bond lengths


Bond angles


Torsions


Rings

Ligand BCL L 305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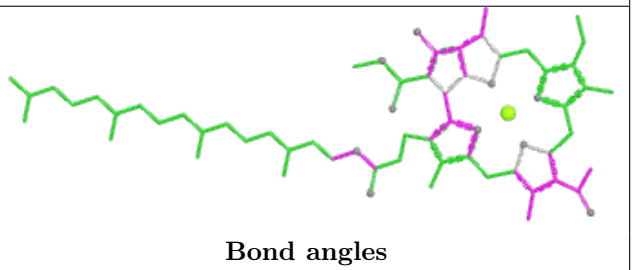
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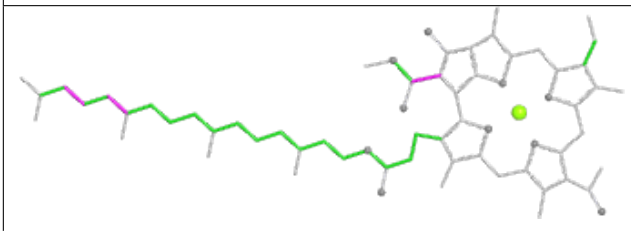
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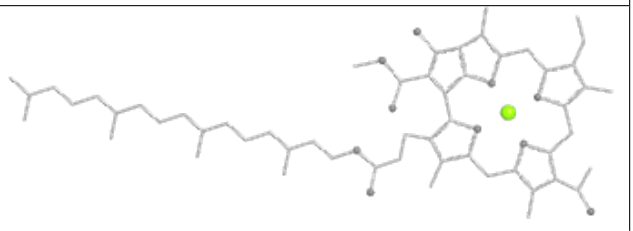
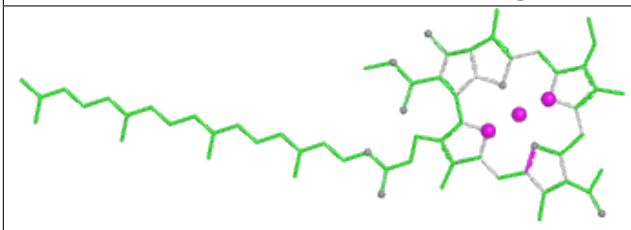

Rings

Ligand BCL BD 101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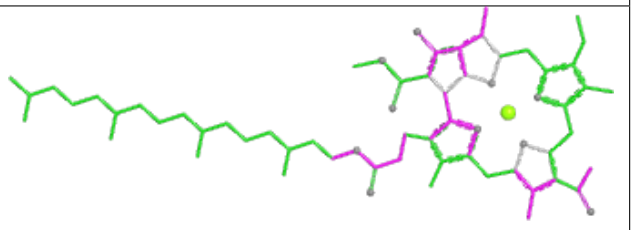
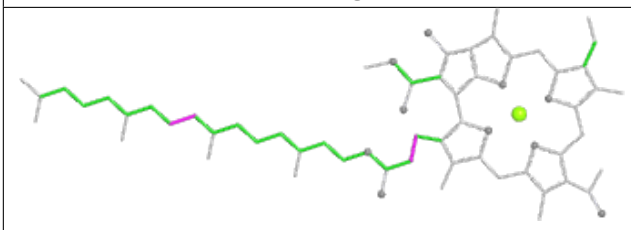

Bond angles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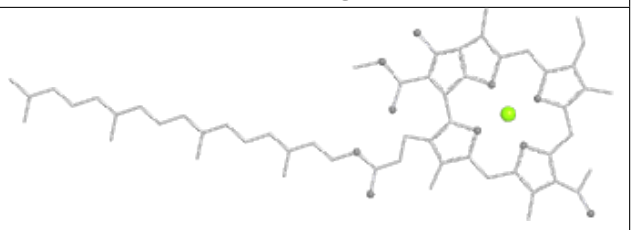
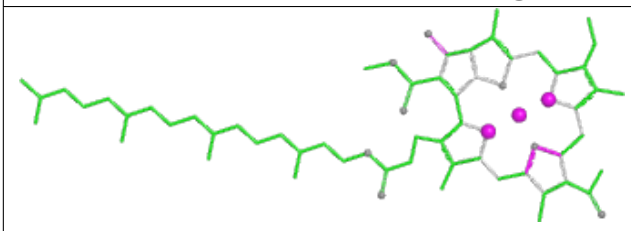

Rings

Ligand BCL AK 101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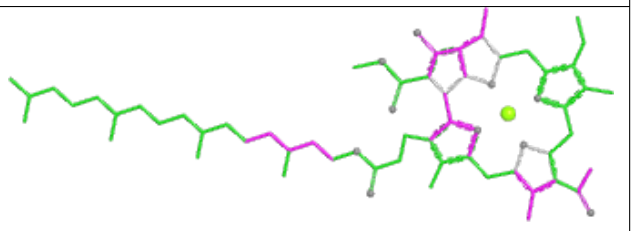
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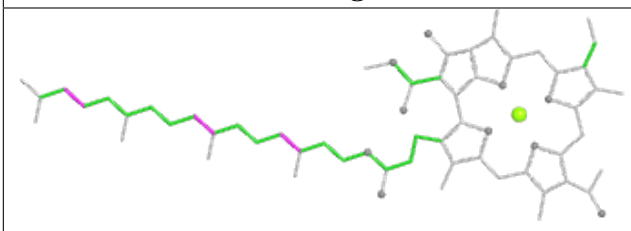
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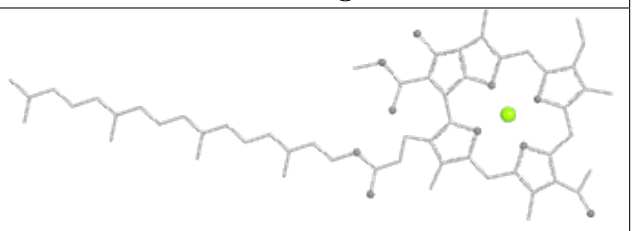
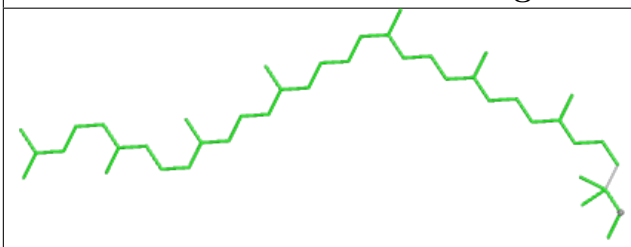

Rings

Ligand SPO AF 103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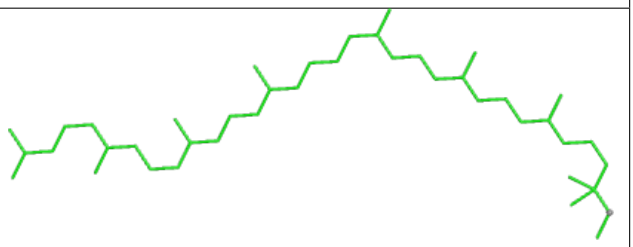
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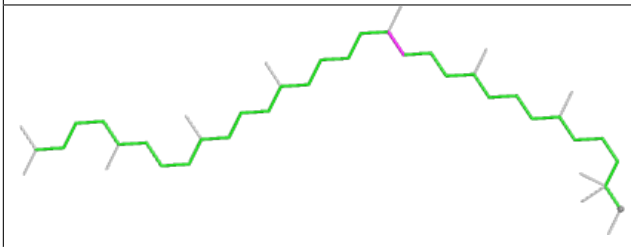
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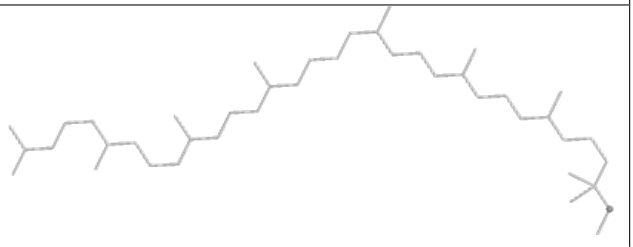
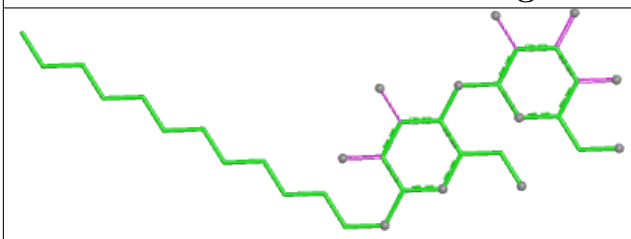

Rings

Ligand LMT M 401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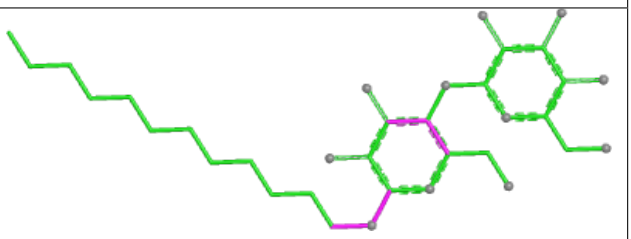
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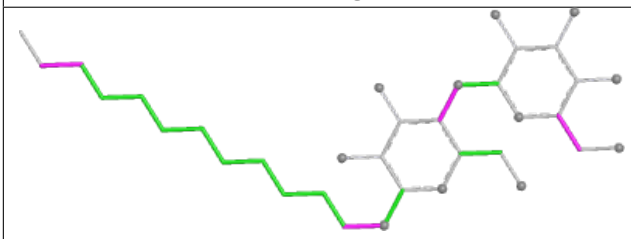
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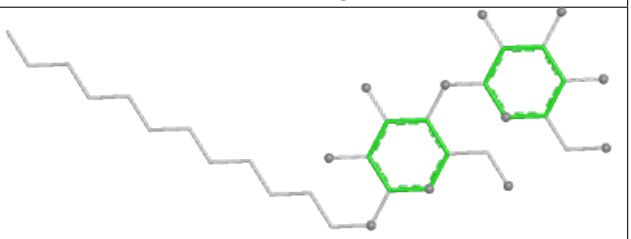
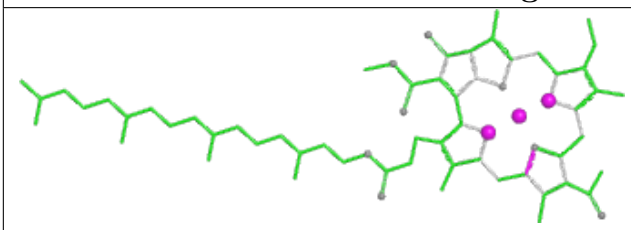

Rings

Ligand BCL M 406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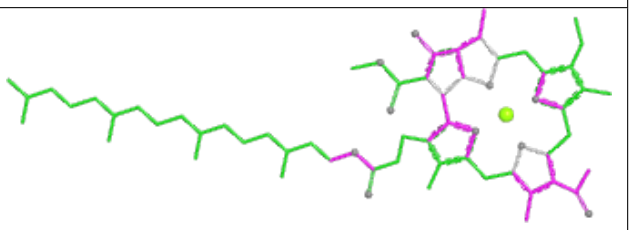
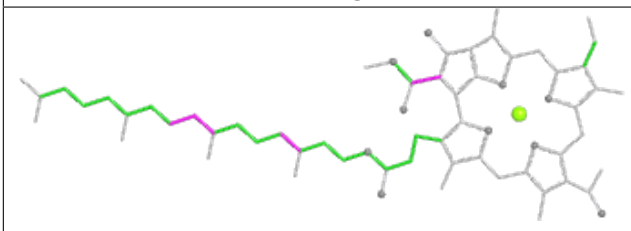

Bond angles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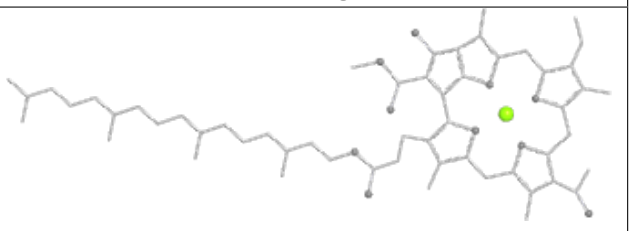
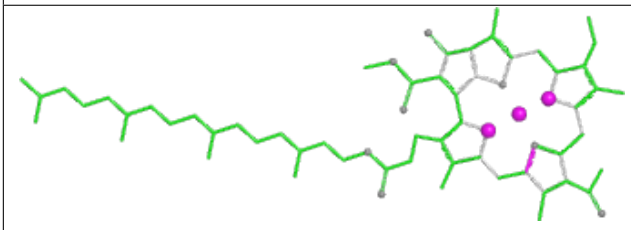

Rings

Ligand BCL BF 101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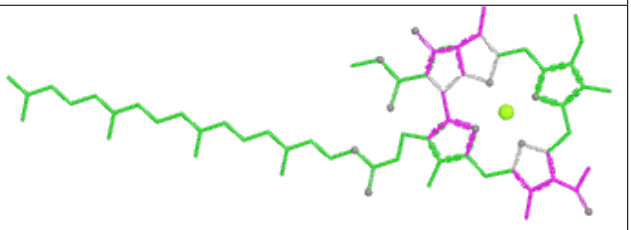
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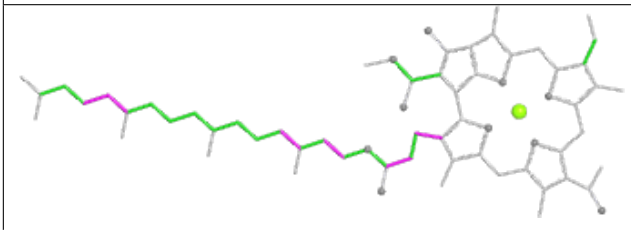
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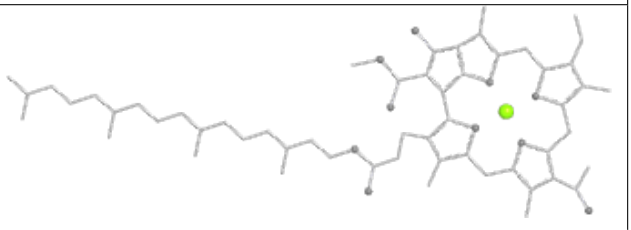
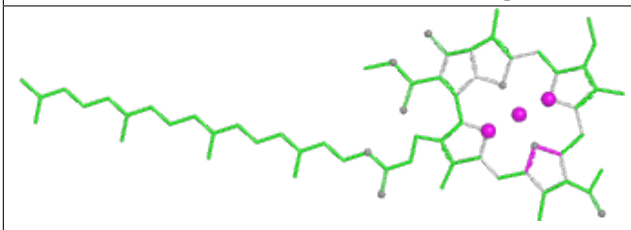
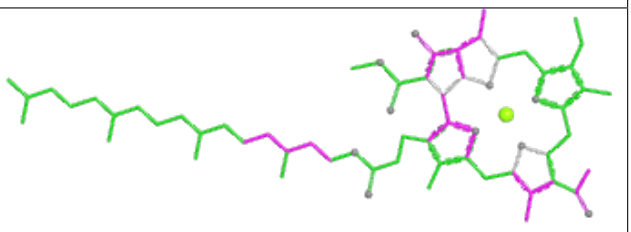
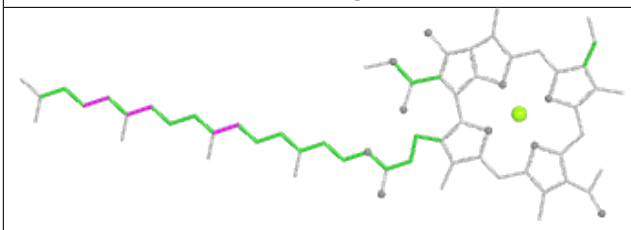
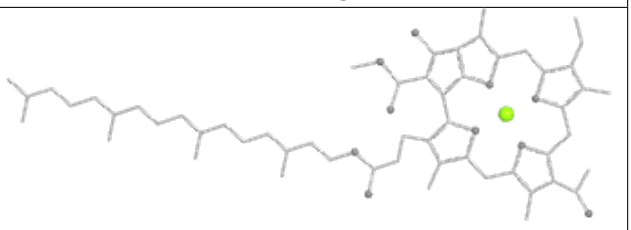
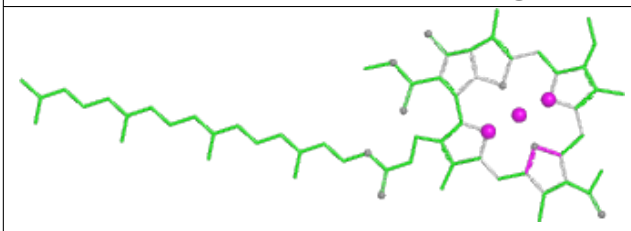
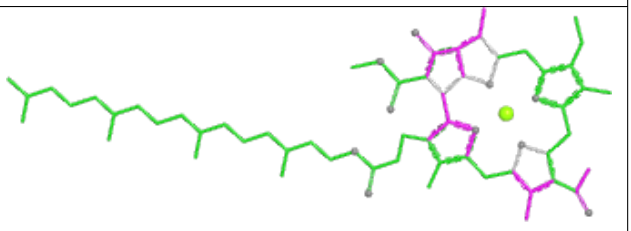
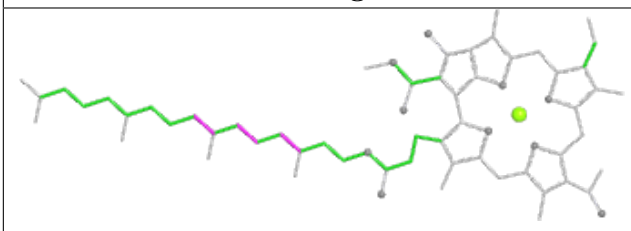
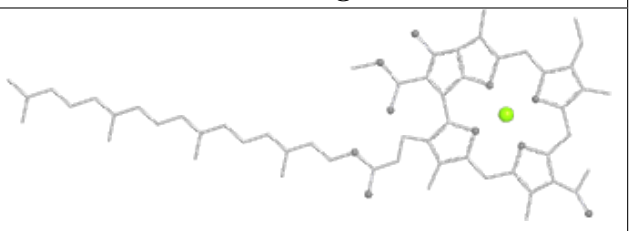
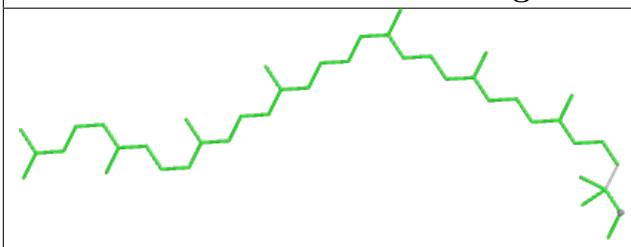
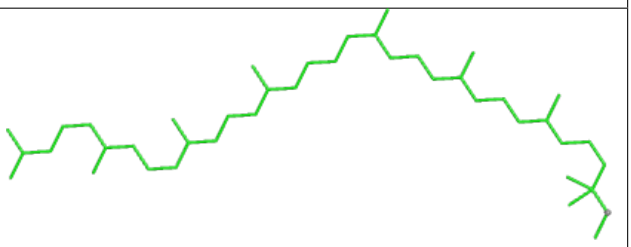
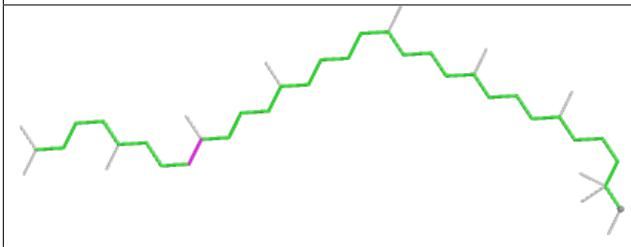
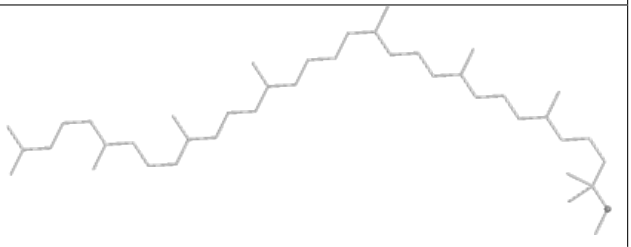
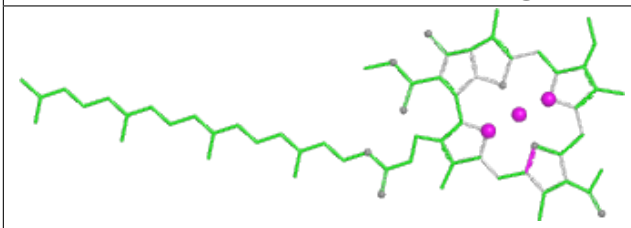

Rings

Ligand BCL AM 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

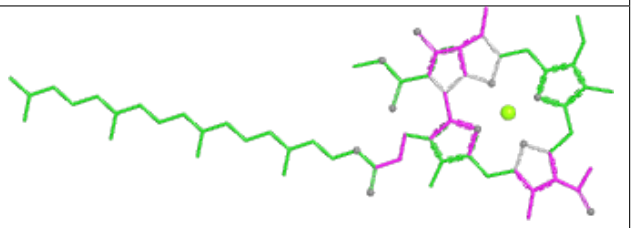
Ligand BCL AN 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPO AC 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

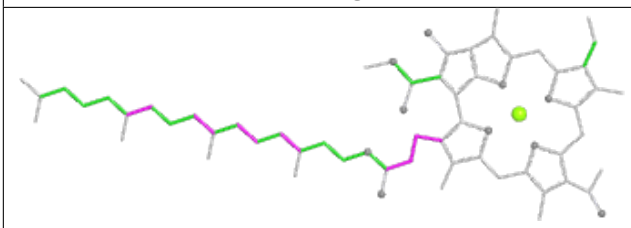
Ligand BCL AI 101



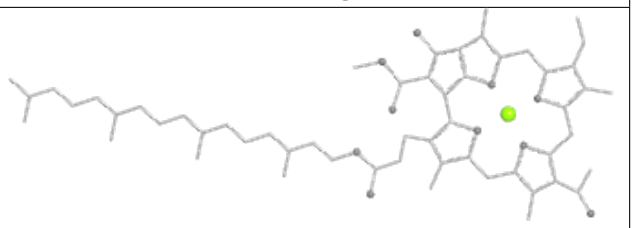
Bond lengths



Bond angles

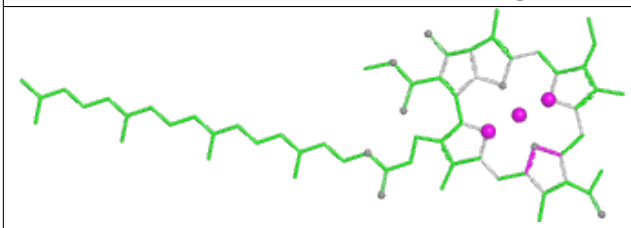


Torsions

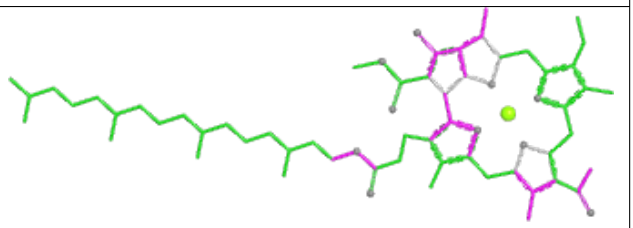


Rings

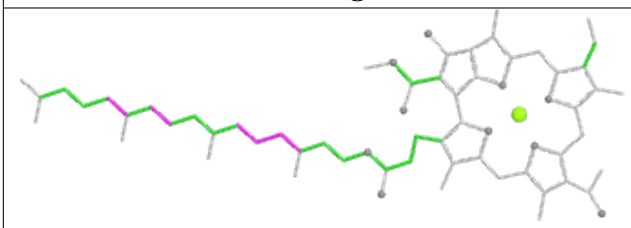
Ligand BCL BH 101



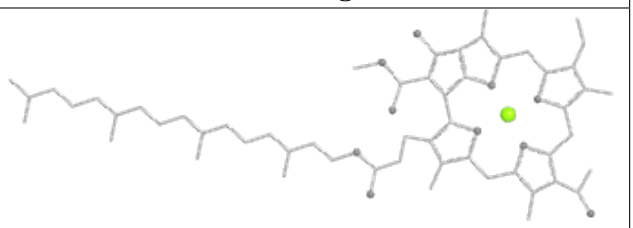
Bond lengths



Bond angles

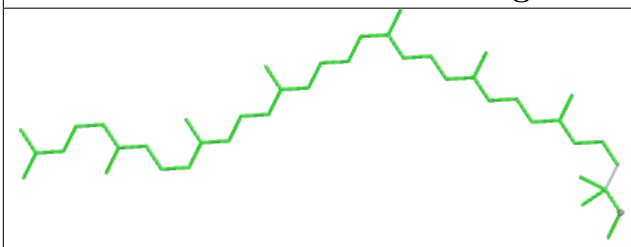


Torsions

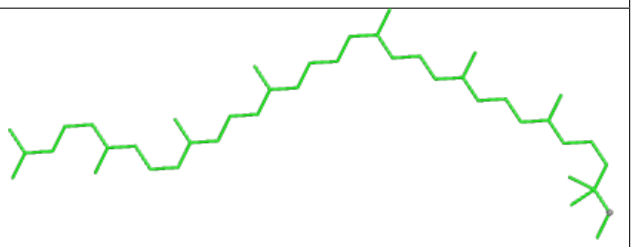


Rings

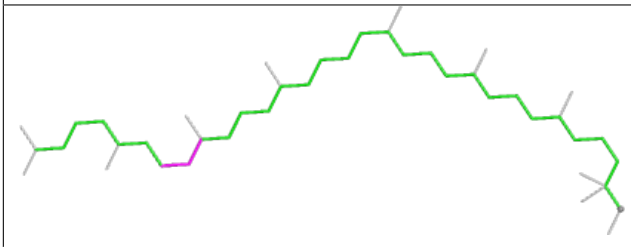
Ligand SPO AC 103



Bond lengths



Bond angles



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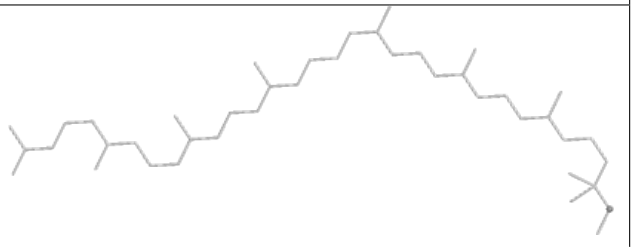
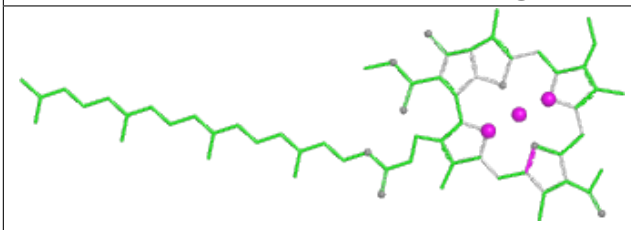
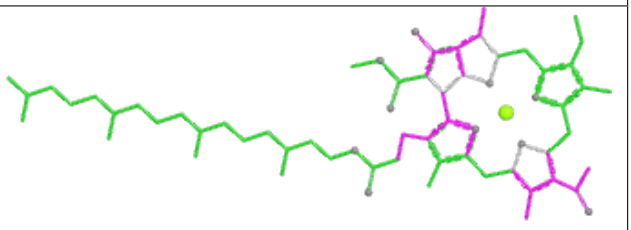
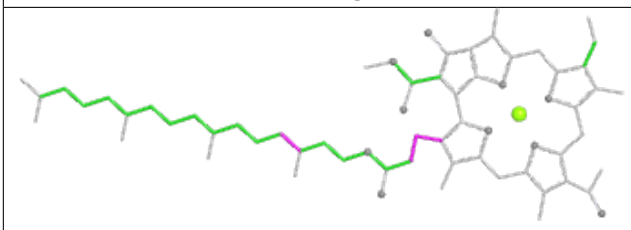
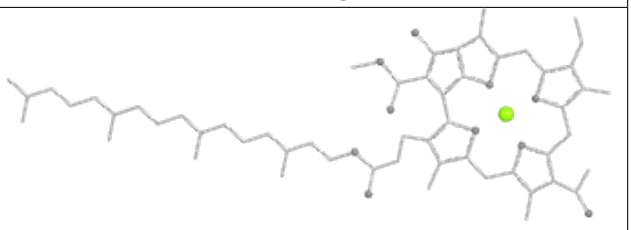
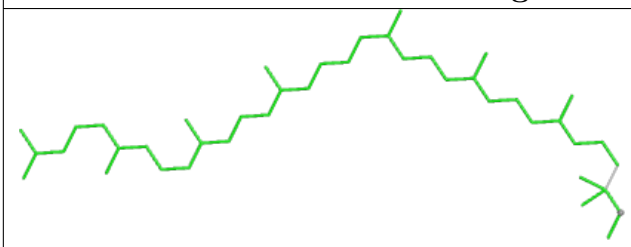
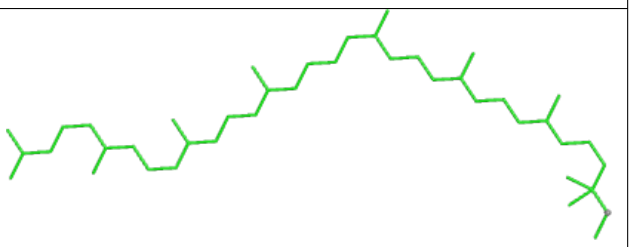
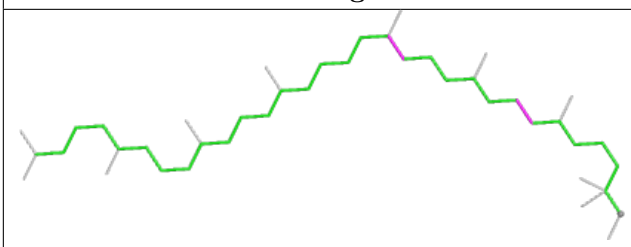
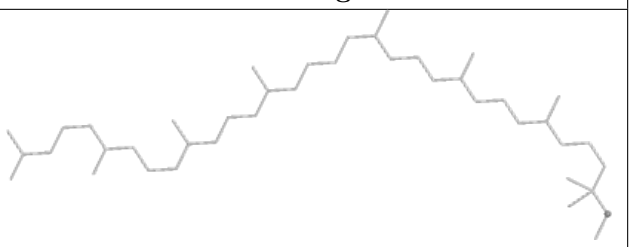
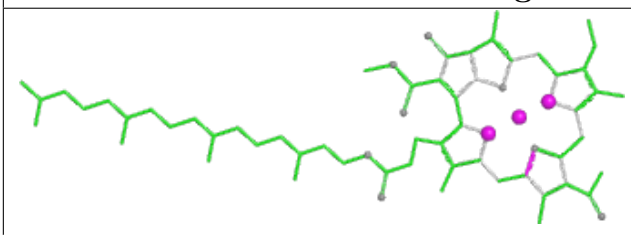
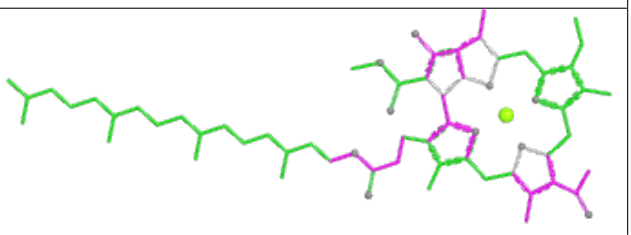
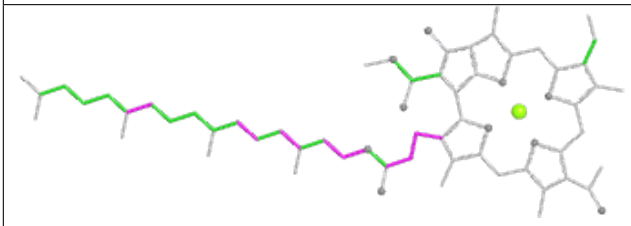
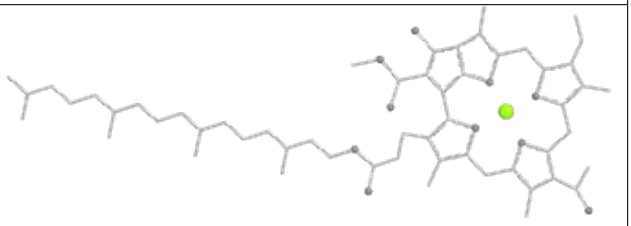


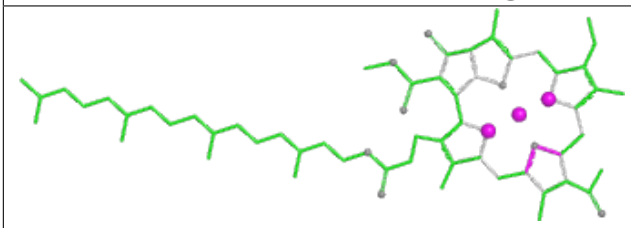
Rings

Ligand BCL AE 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

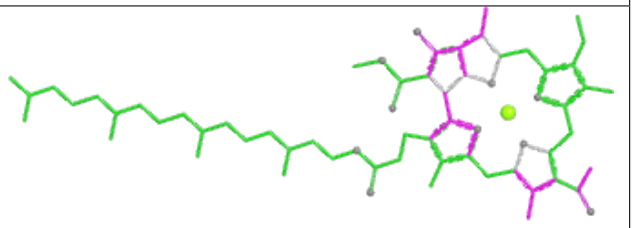
Ligand SPO AH 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL BL 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

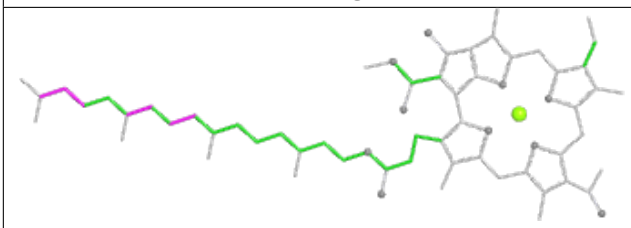
Ligand BCL AA 1001



Bond lengths



Bond angles



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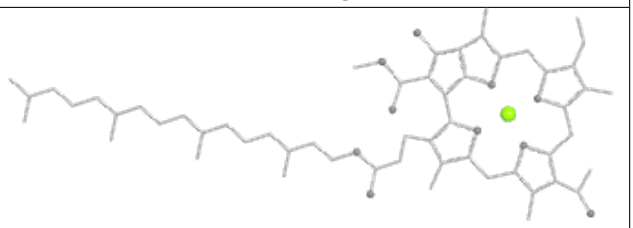
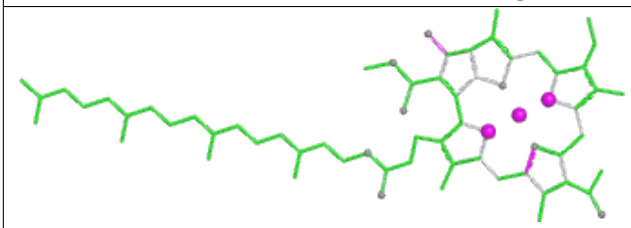


Rings

Ligand BCL BA 102



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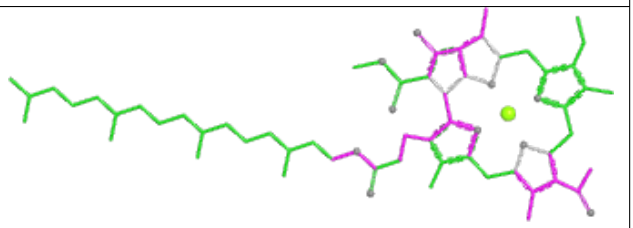
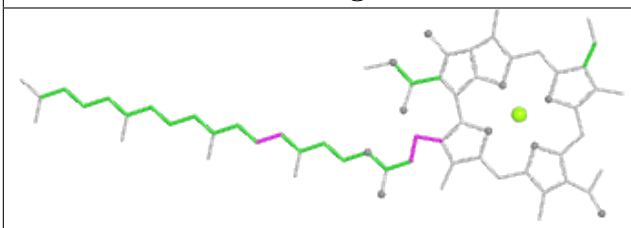


Bond angles



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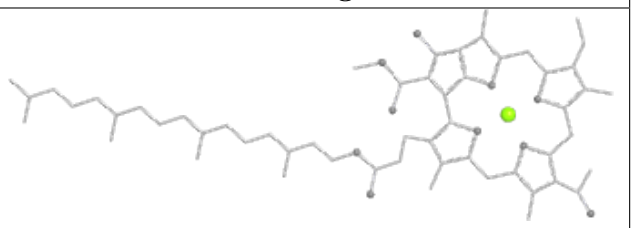
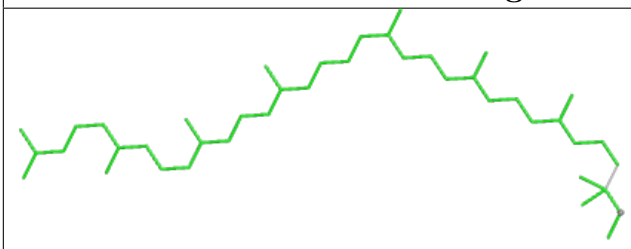


Rings

Ligand SPO BE 1000



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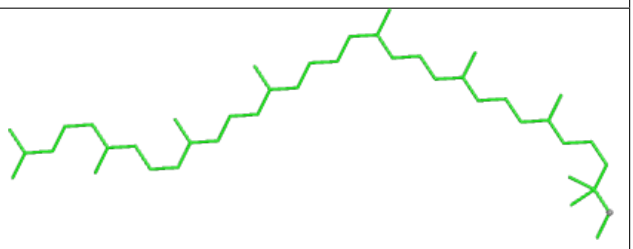
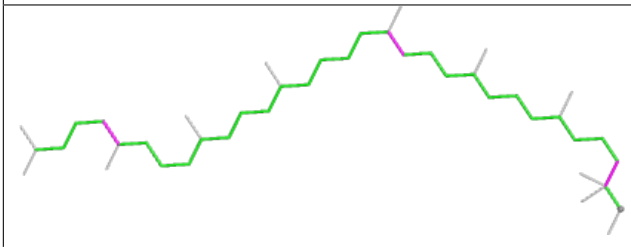


Bond angles



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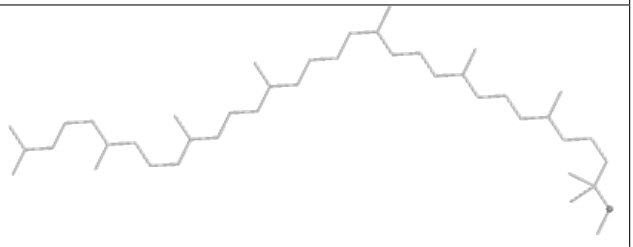
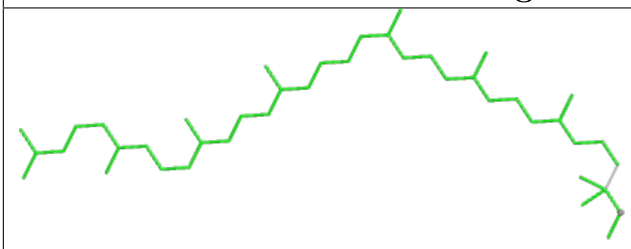


Rings

Ligand SPO BL 101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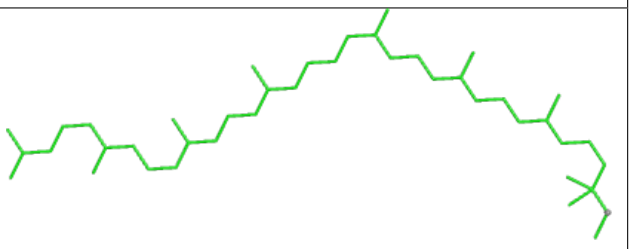
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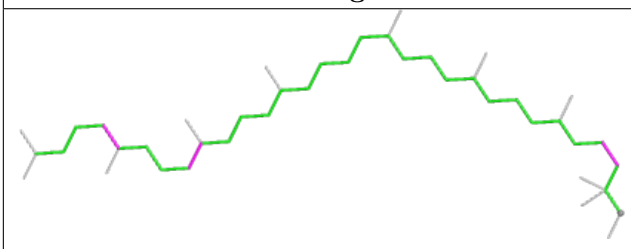
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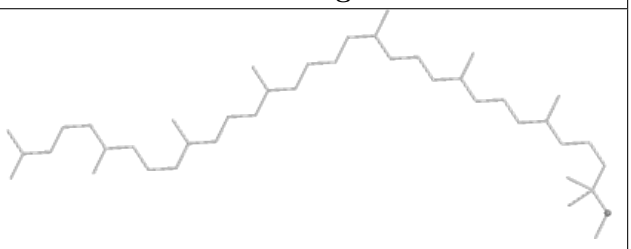
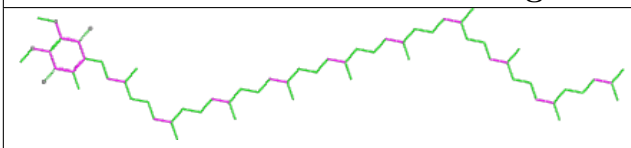

Rings

Ligand U10 M 404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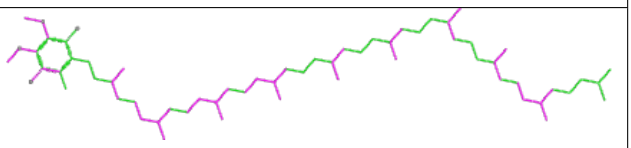
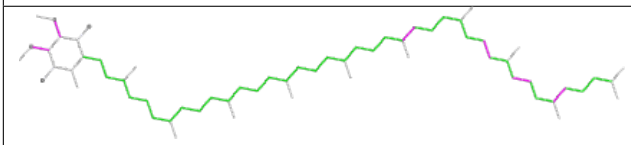

Bond angles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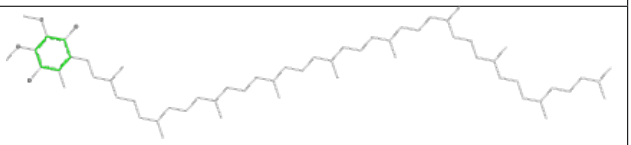
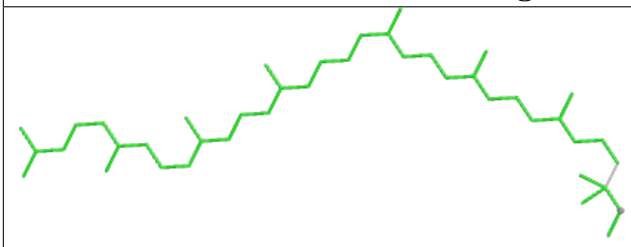

Rings

Ligand SPO AJ 102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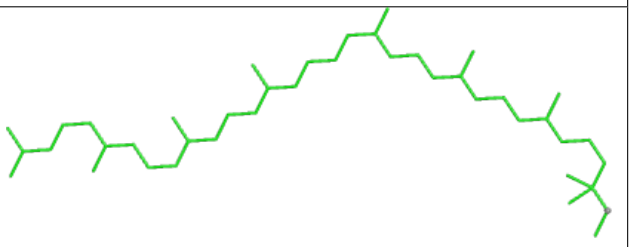
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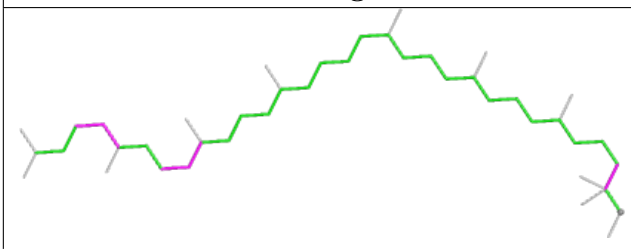
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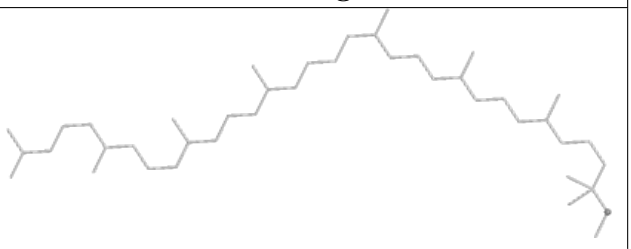
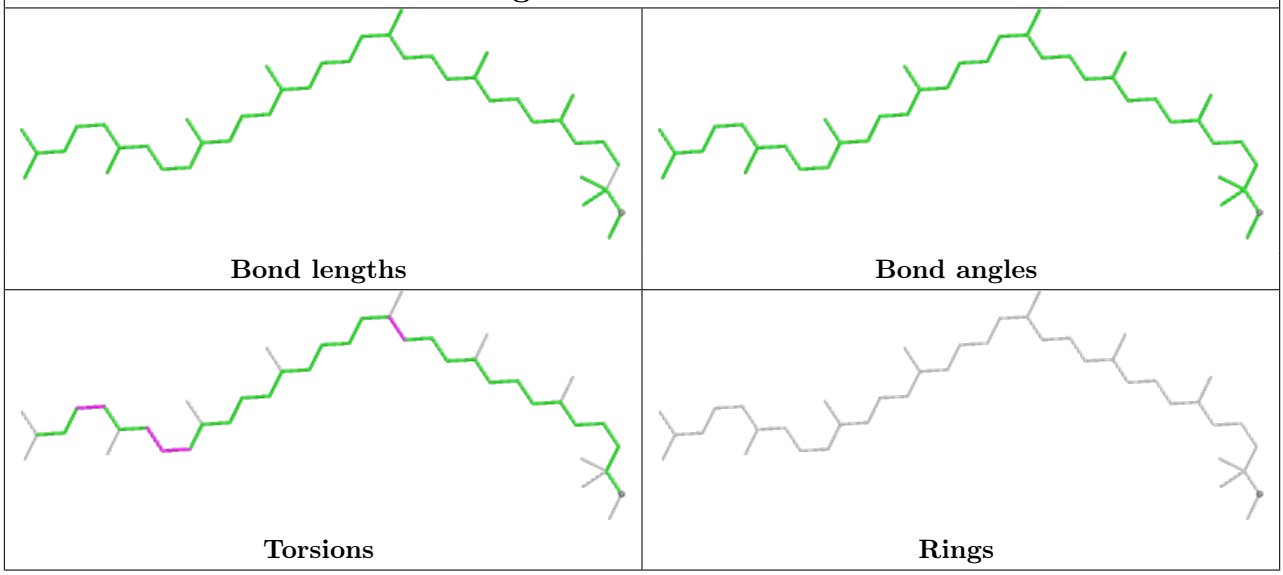
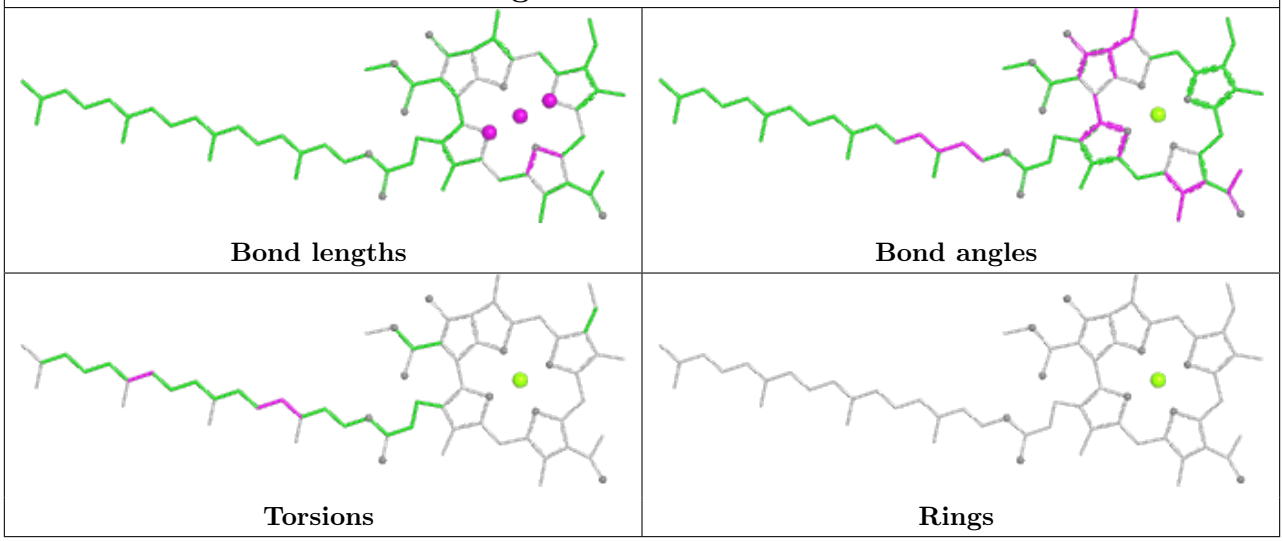

Rings

Ligand SPO AD 103



Ligand BCL AD 102



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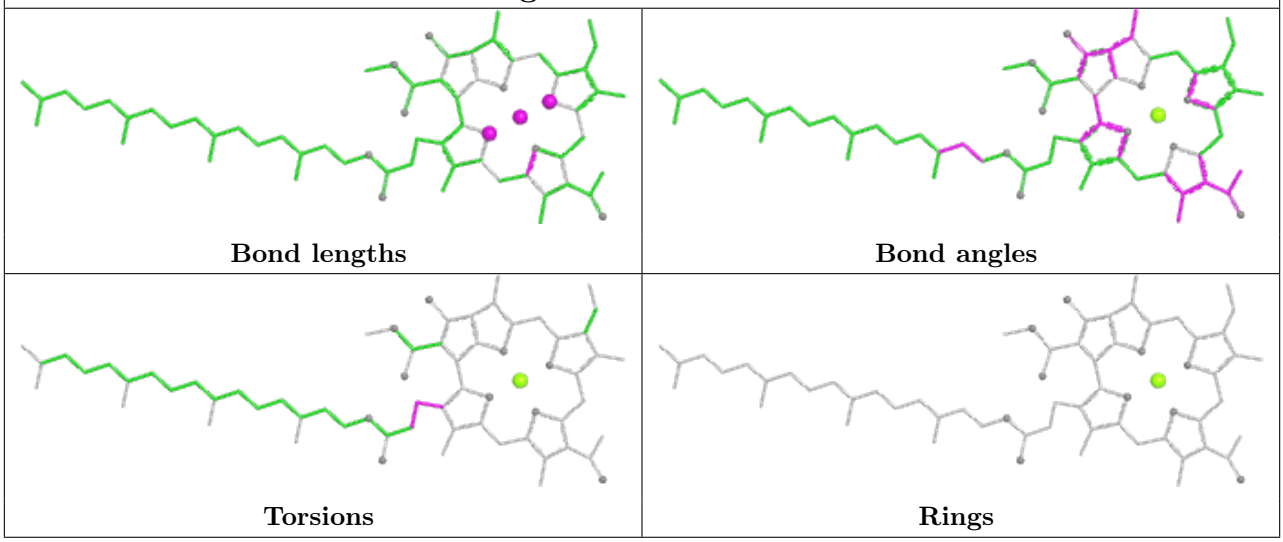

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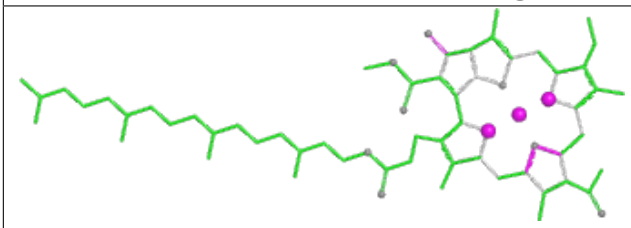
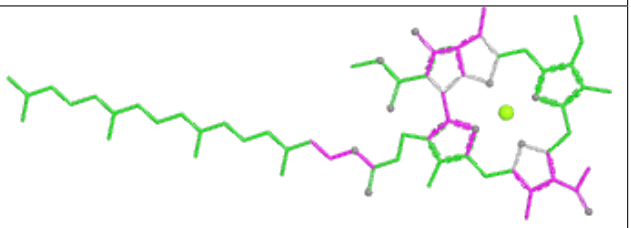
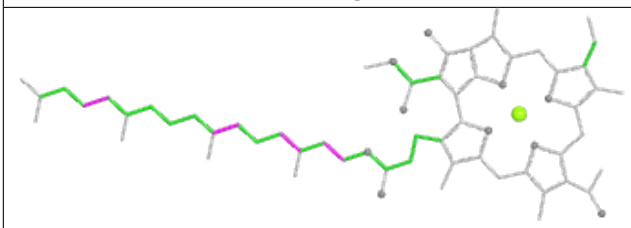


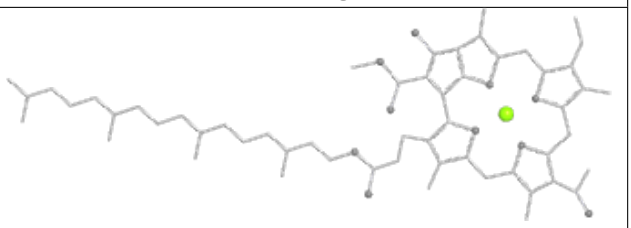
Bond lengths



Bond angles

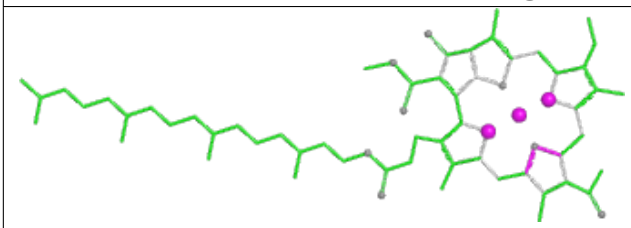


Torsions



Rings

Ligand BCL M 403



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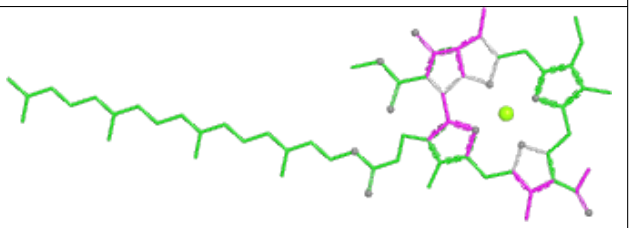
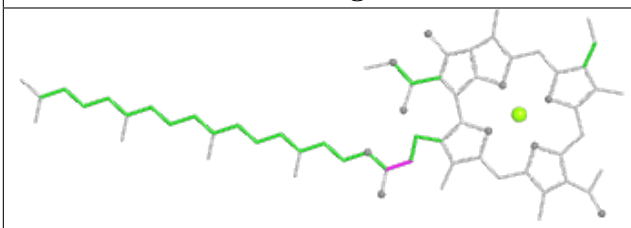


Bond angles



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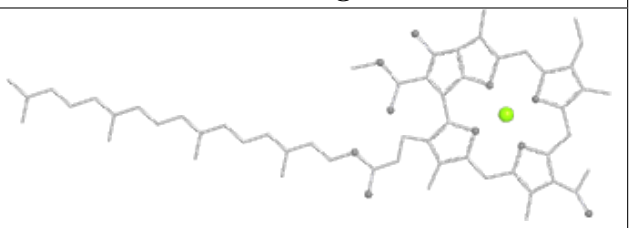
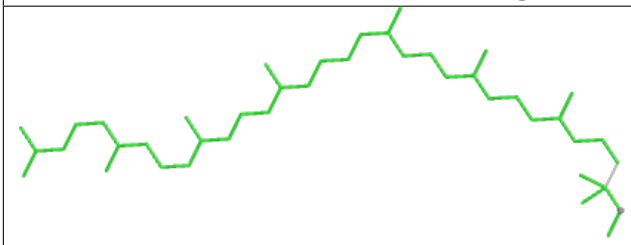
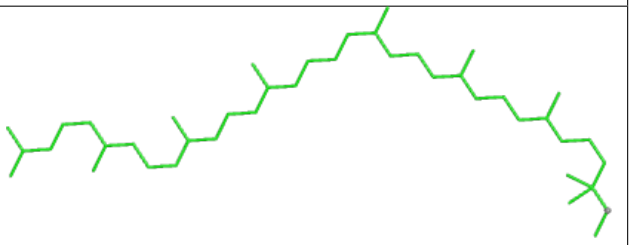


Rings

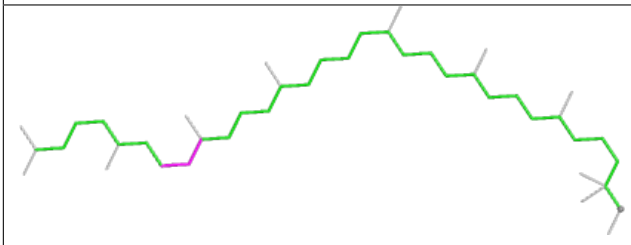
Ligand SPO AE 102



Bond lengths



Bond angles



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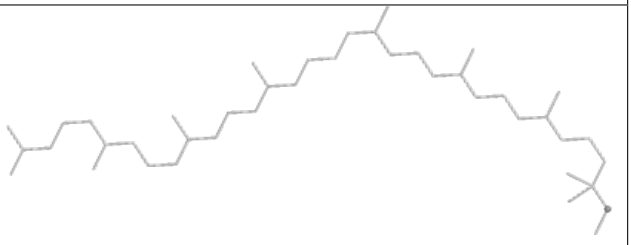
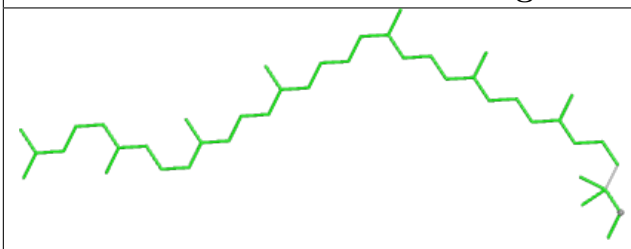
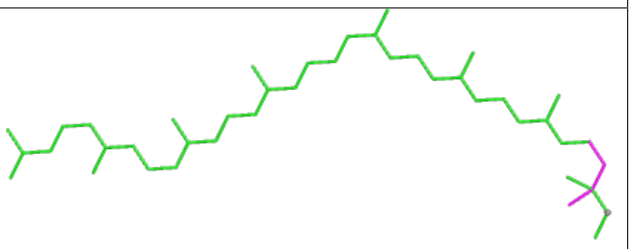
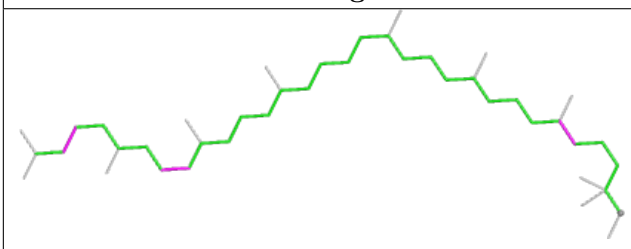
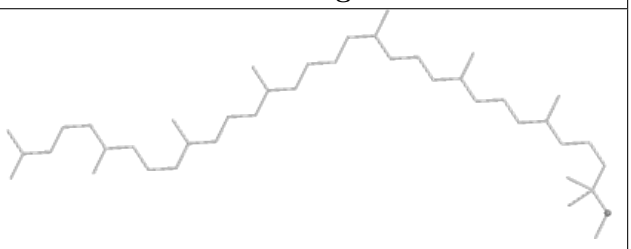
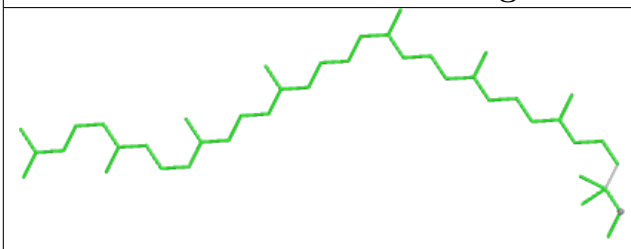
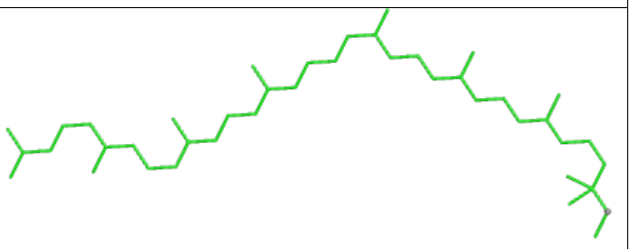
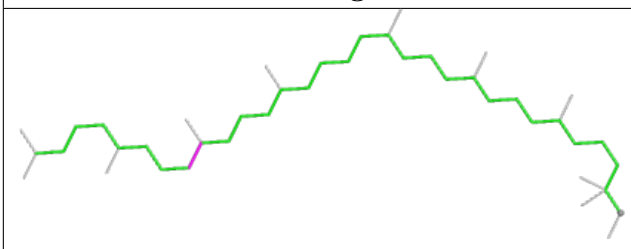
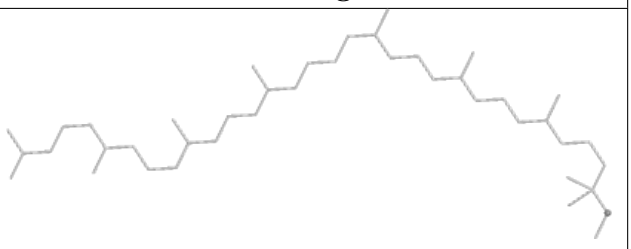
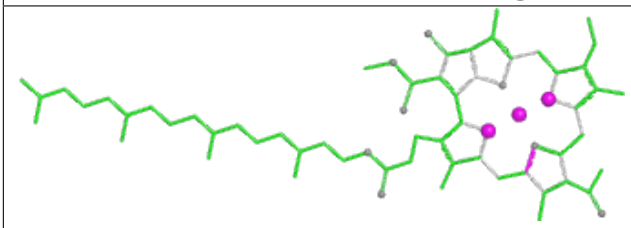
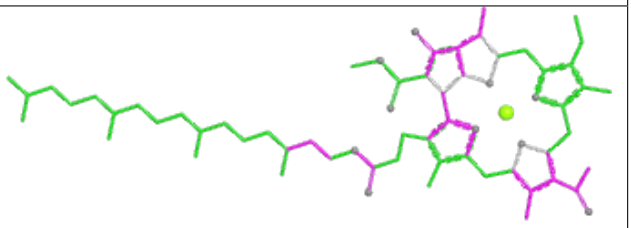
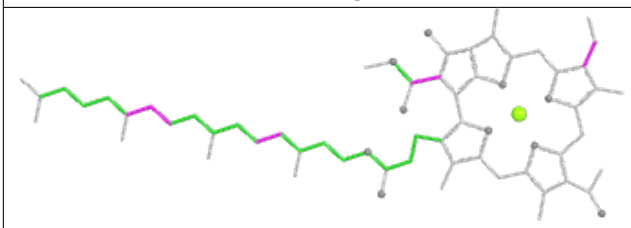
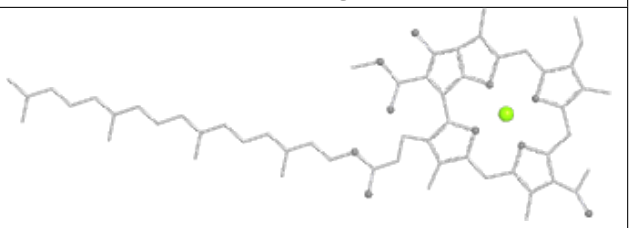


Rings

Ligand SPO AJ 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPO AM 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL AB 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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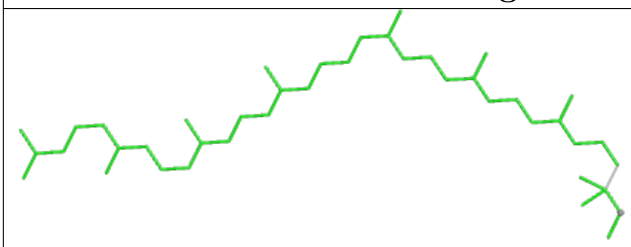
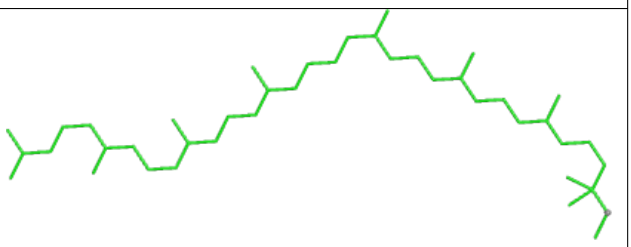
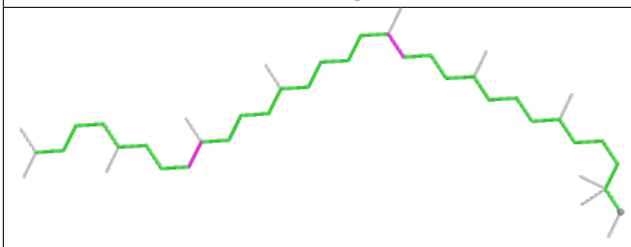
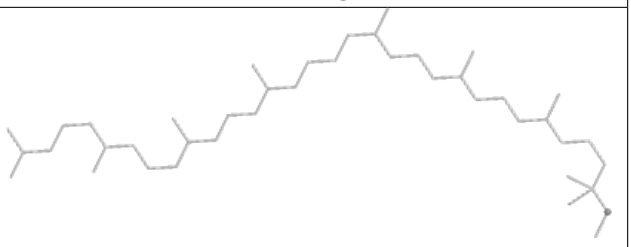
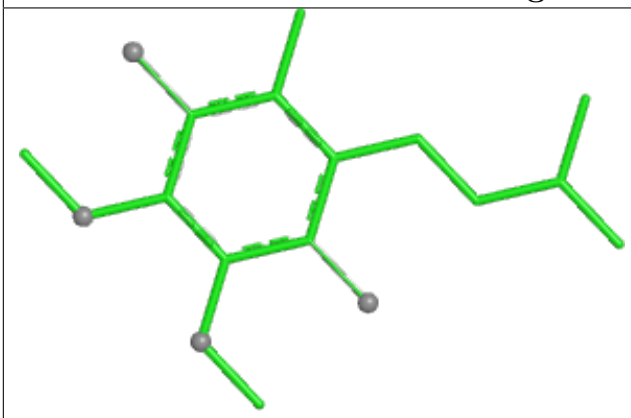
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UQ1 L 303



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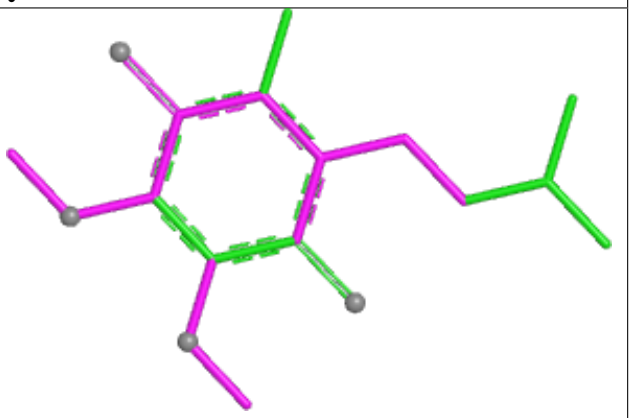

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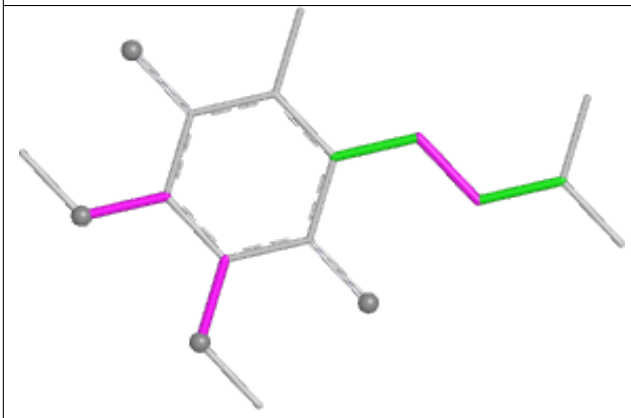

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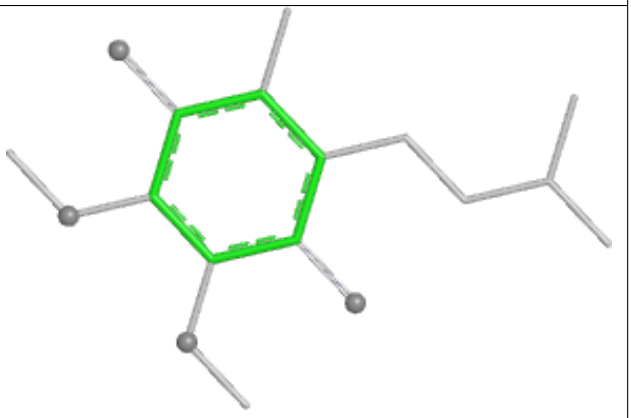
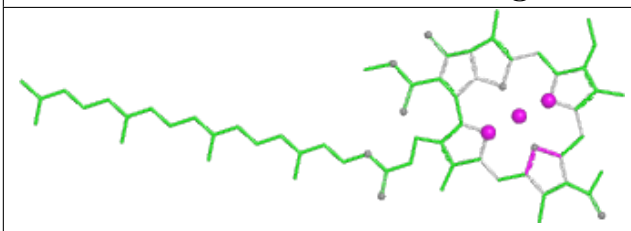


Rings

Ligand BCL AG 102



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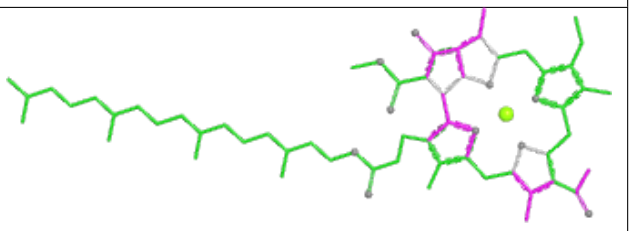

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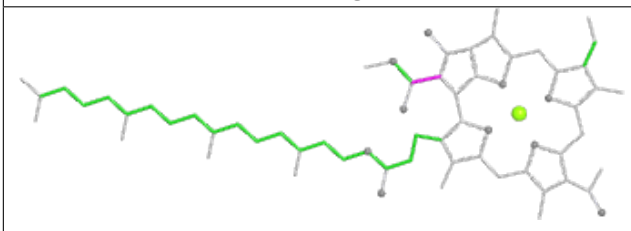

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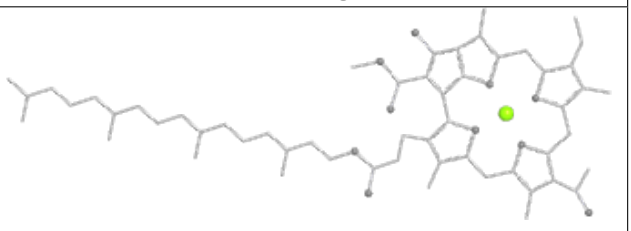

Rings

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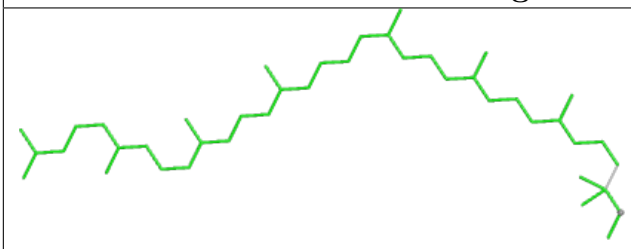
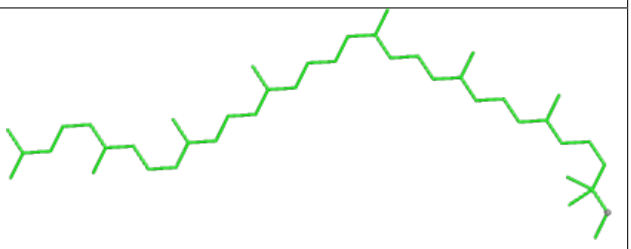
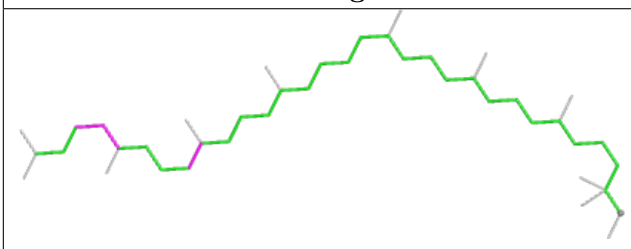
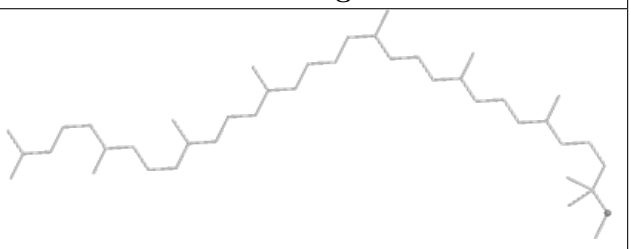
 Bond lengths	 Bond angles
 Torsions	 Rings

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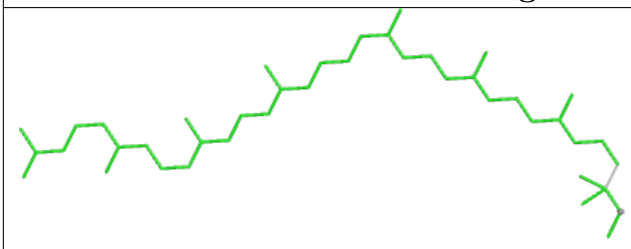
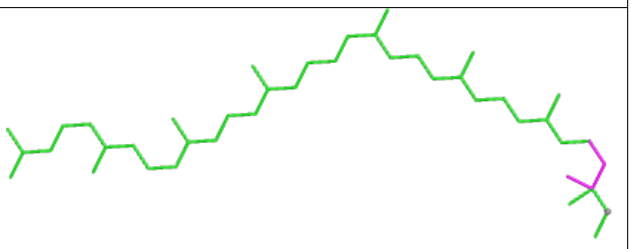
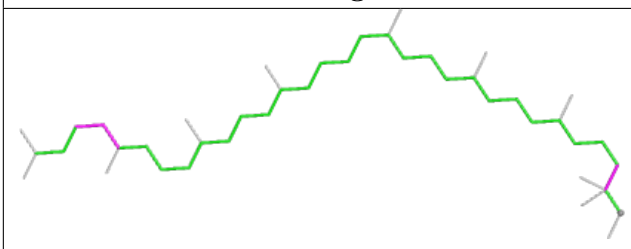
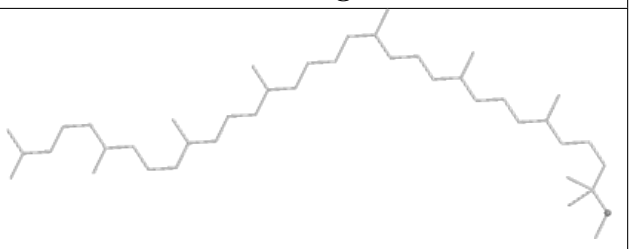
 Bond lengths	 Bond angles
 Torsions	 Rings

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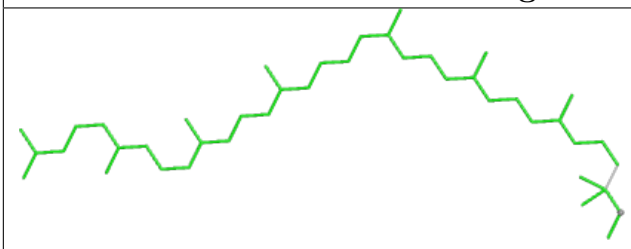
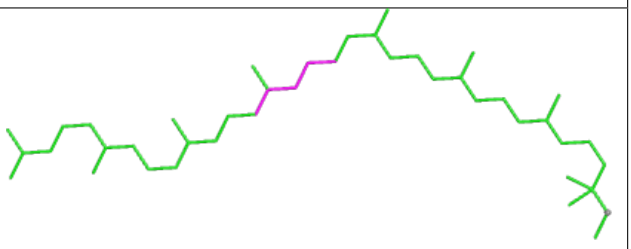
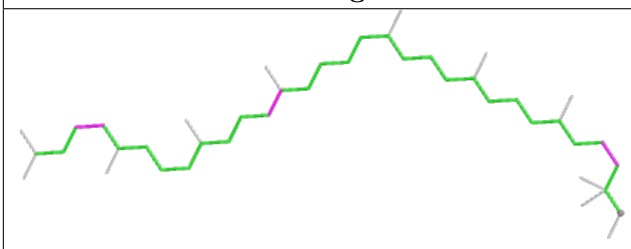
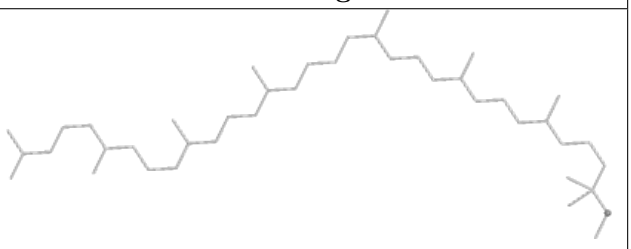
 Bond lengths	 Bond angles
 Torsions	 Rings

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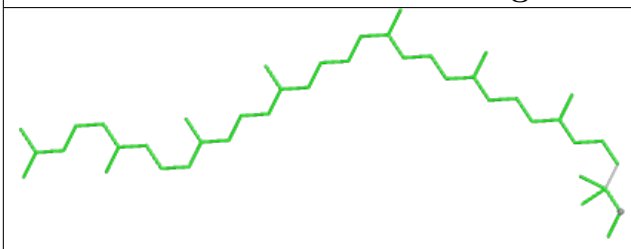
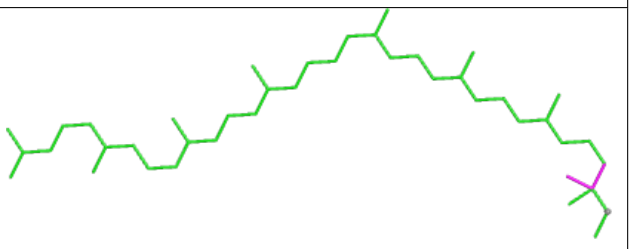
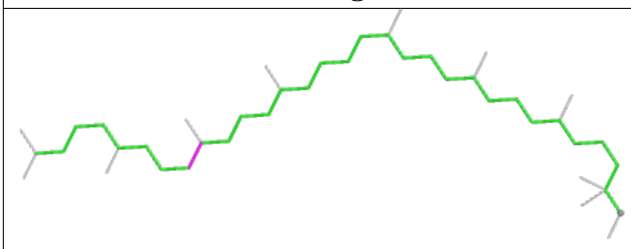
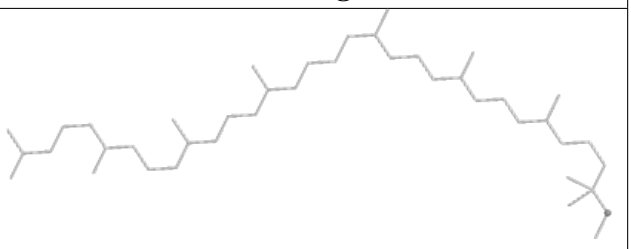
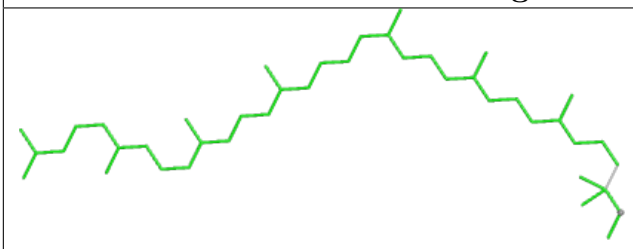
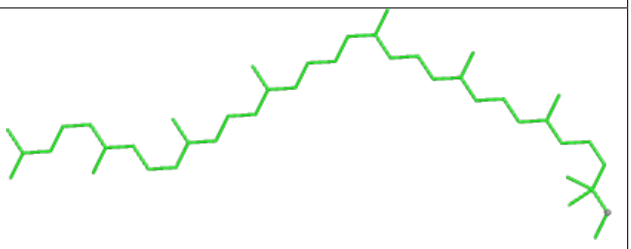
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPO AK 104



Bond lengths



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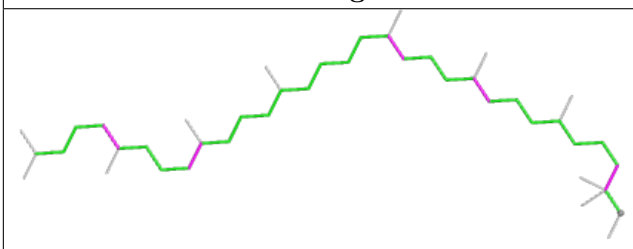

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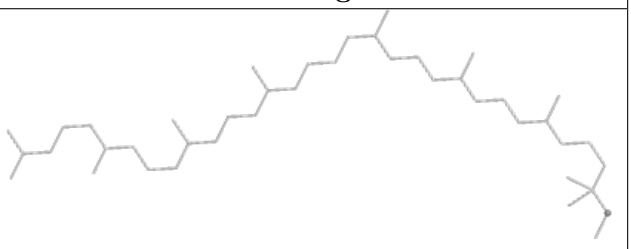
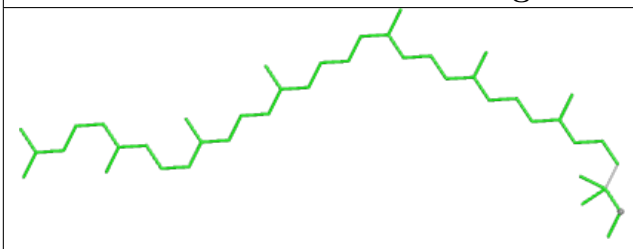


Rings

Ligand SPO BA 101



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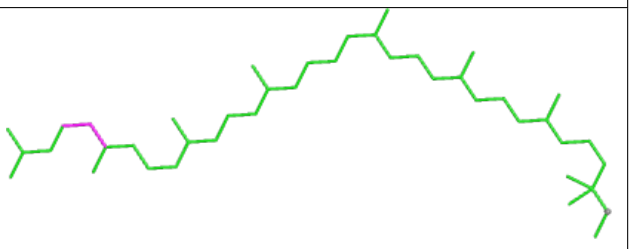

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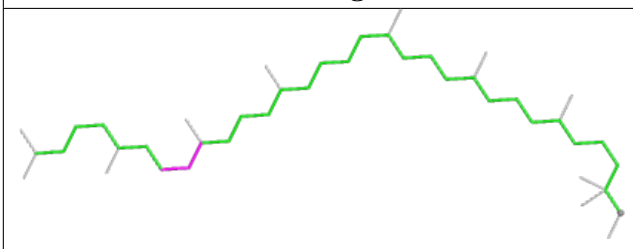

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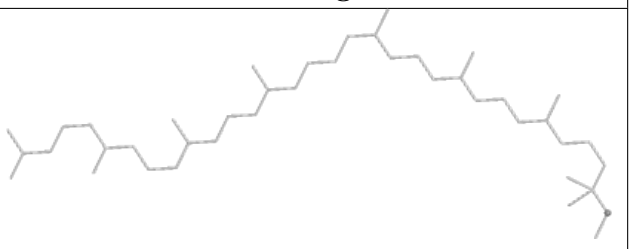

Rings

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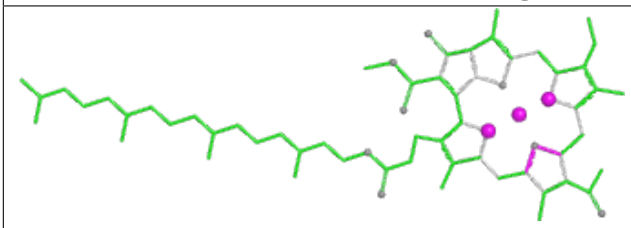
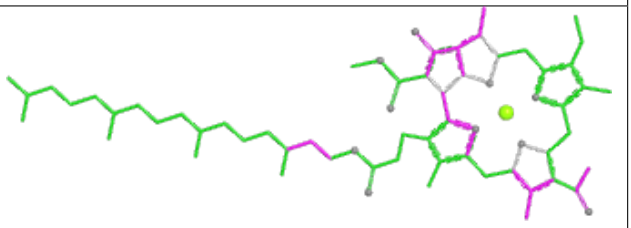
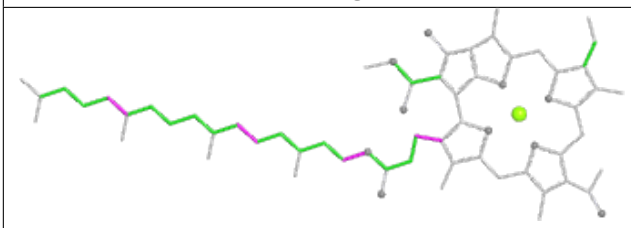
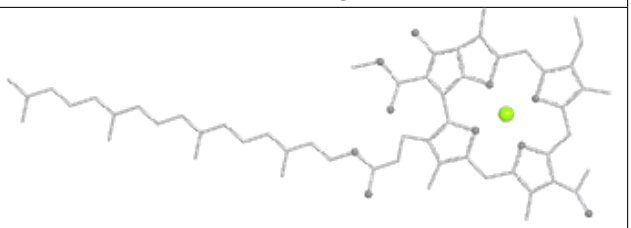
 Bond lengths	 Bond angles
 Torsions	 Rings

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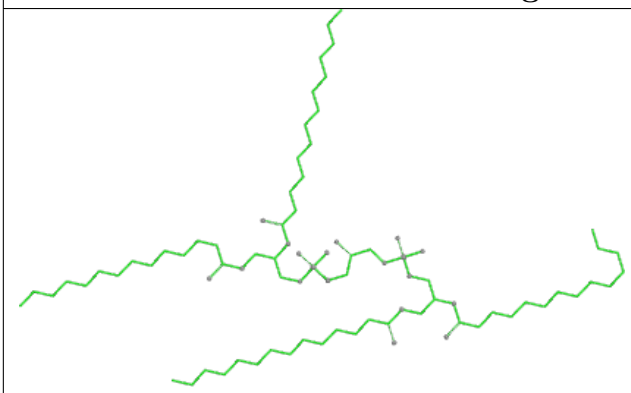
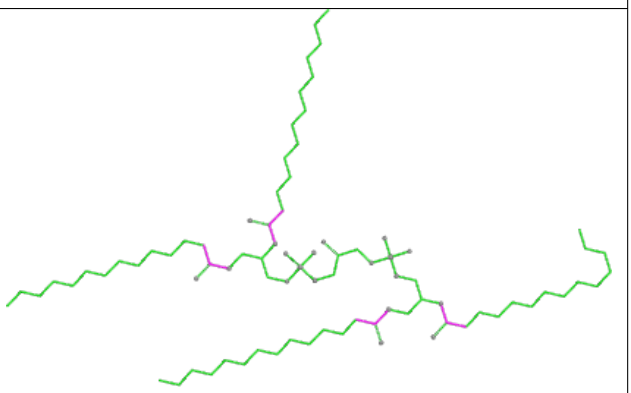
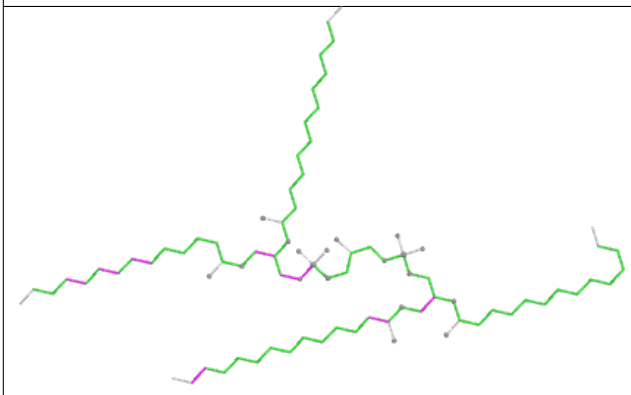
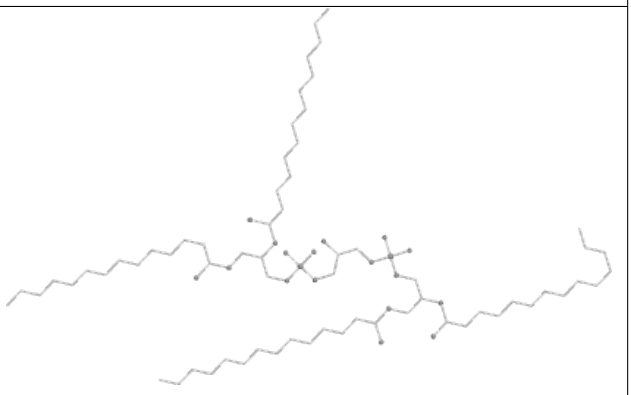
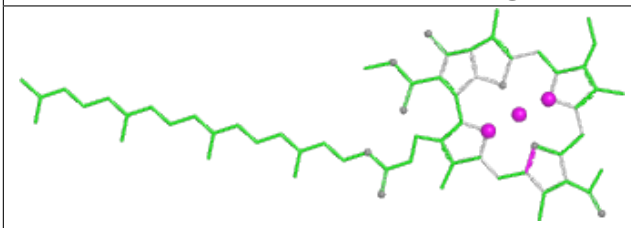
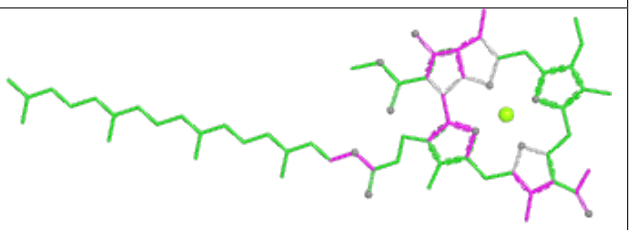
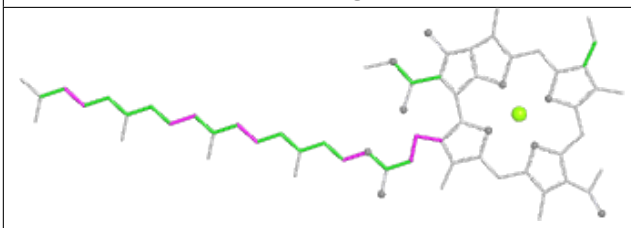
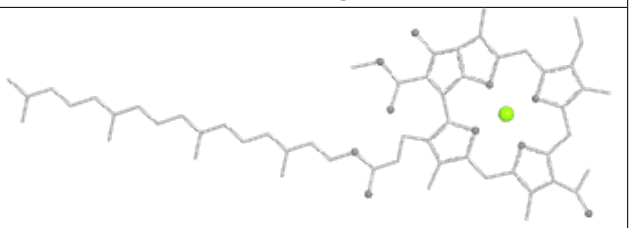
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL BB 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

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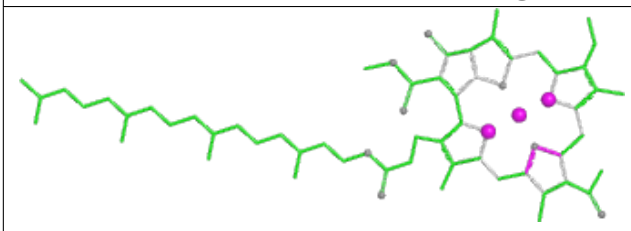
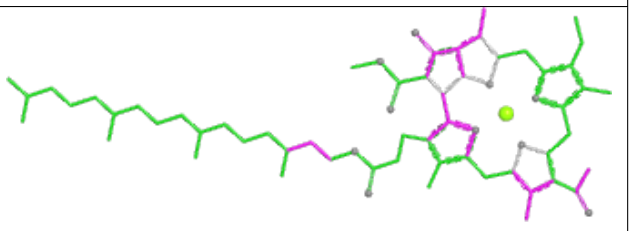
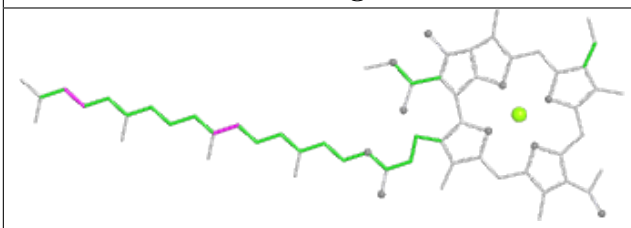
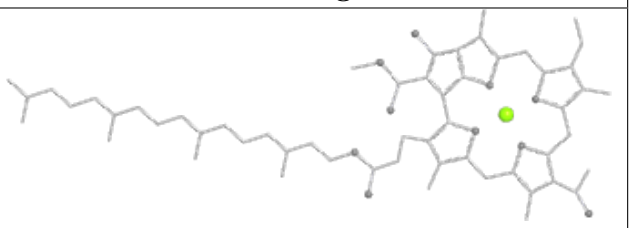
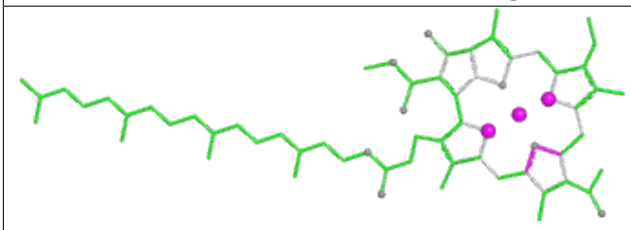
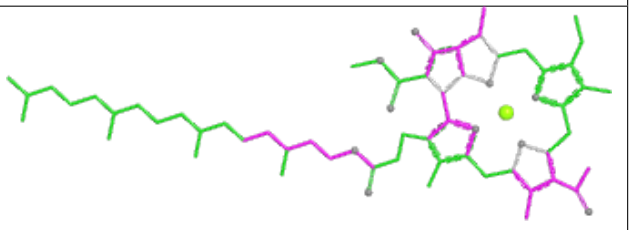
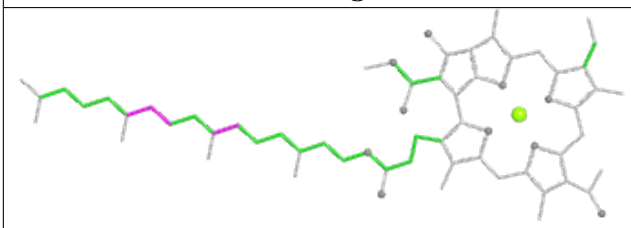
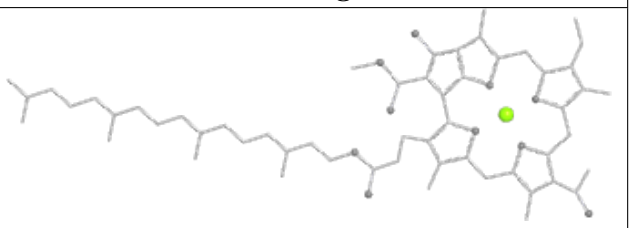
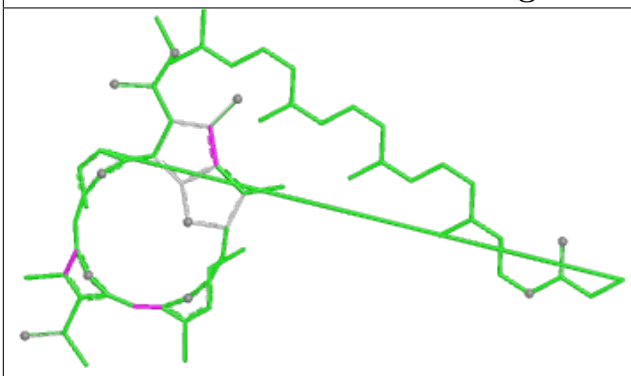
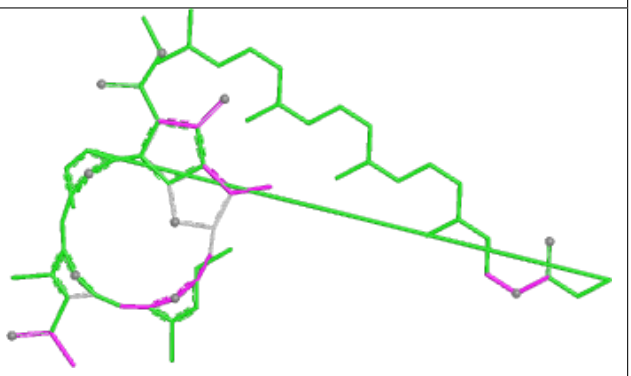
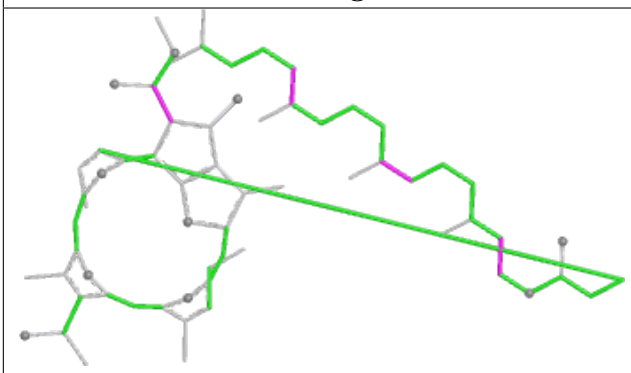
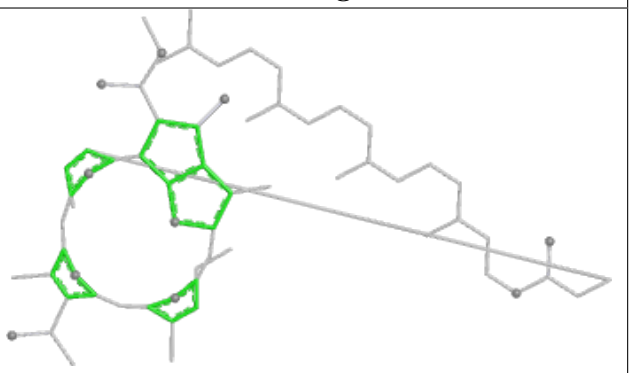
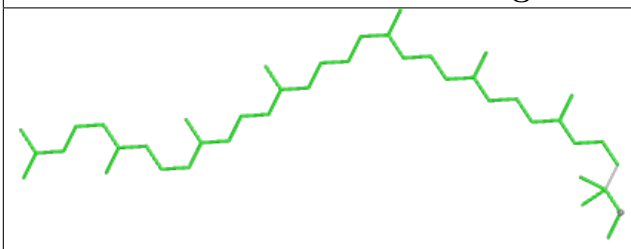
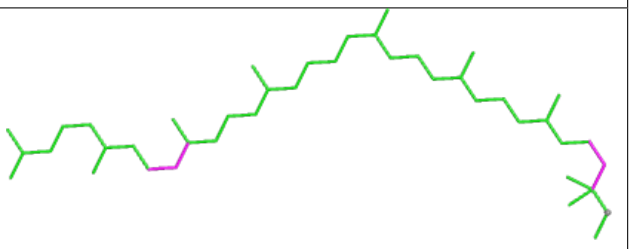
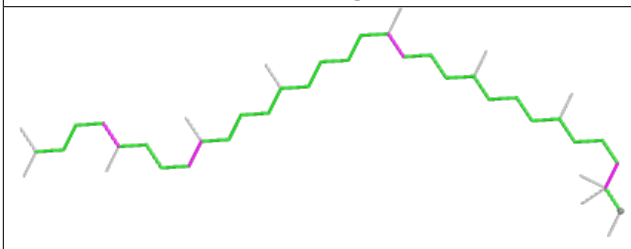
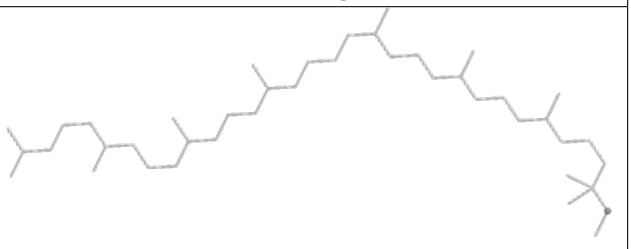
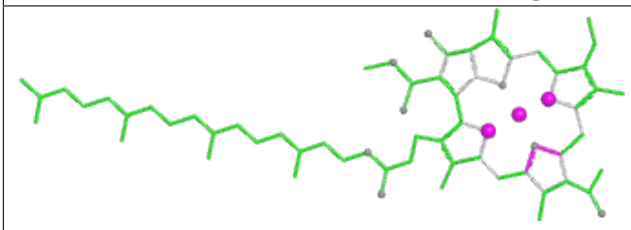
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL AL 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

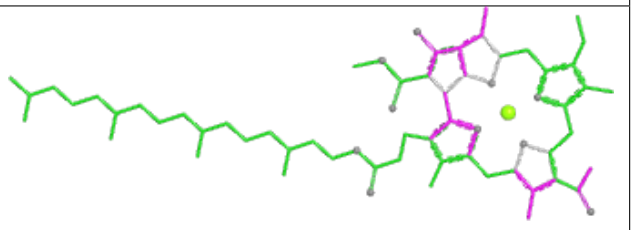
Ligand BPH M 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPO AB 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

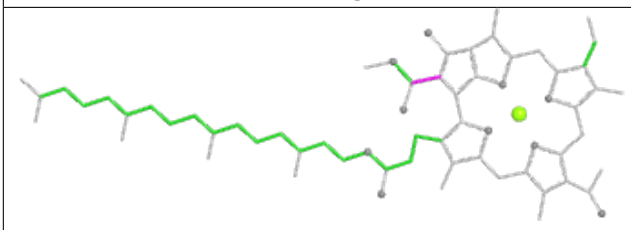
Ligand BCL L 304



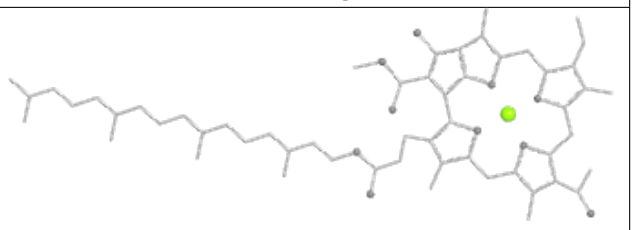
Bond lengths



Bond angles

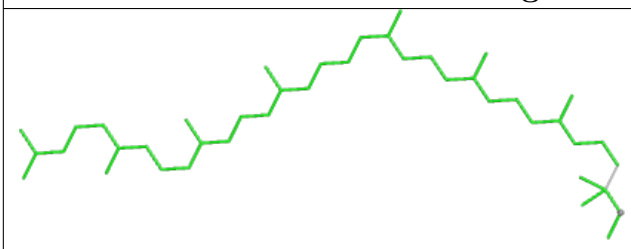


Torsions

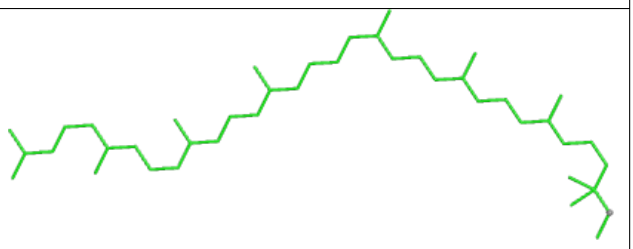


Rings

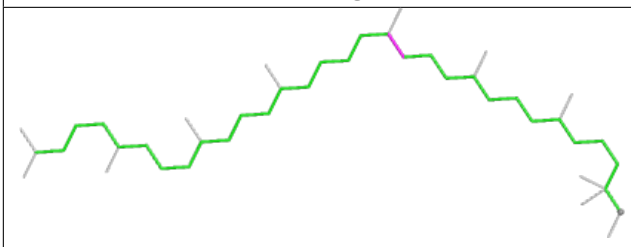
Ligand SPO M 407



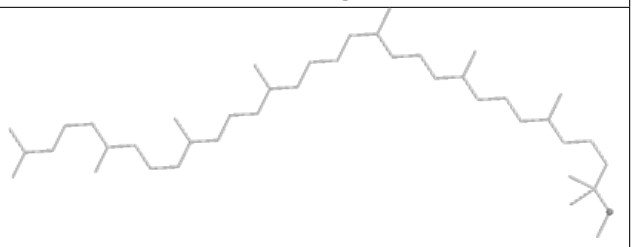
Bond lengths



Bond angles

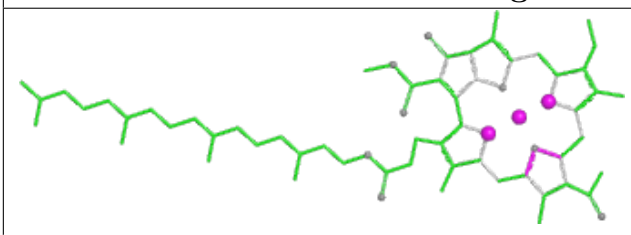


Torsions

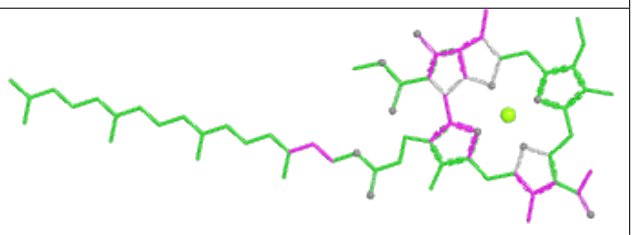


Rings

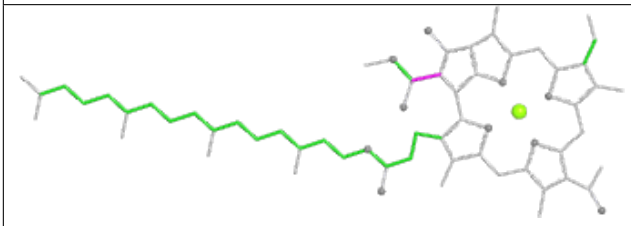
Ligand BCL AH 102



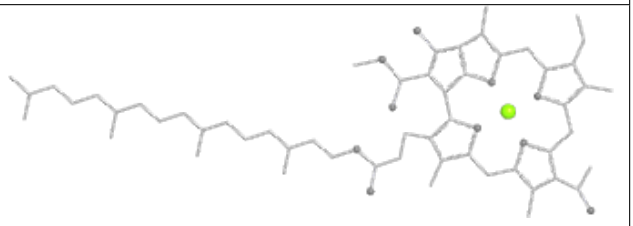
Bond lengths



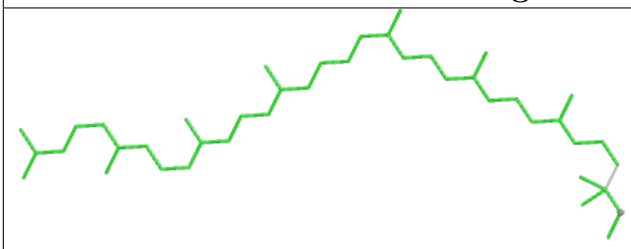
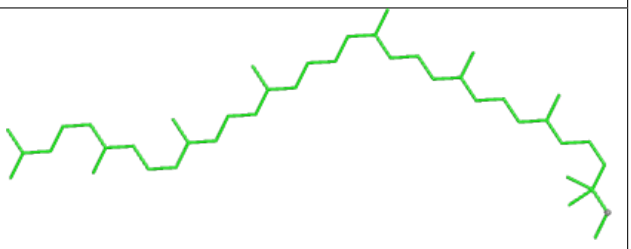
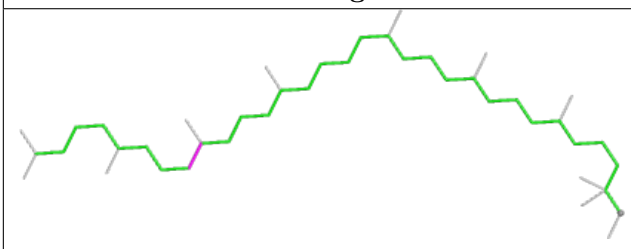
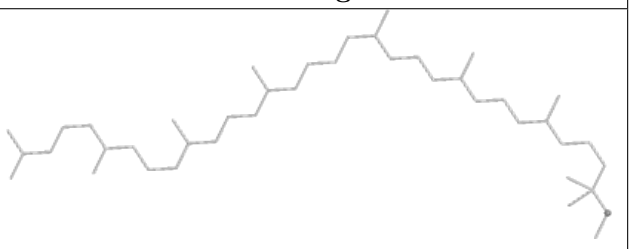
Bond angles

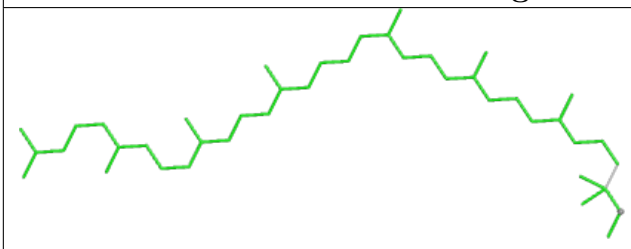
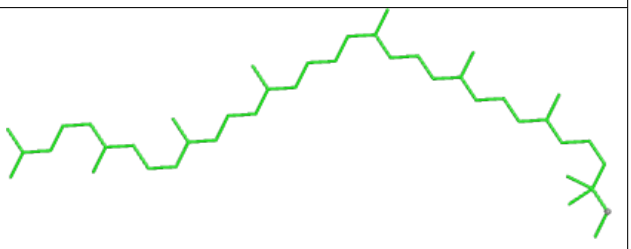
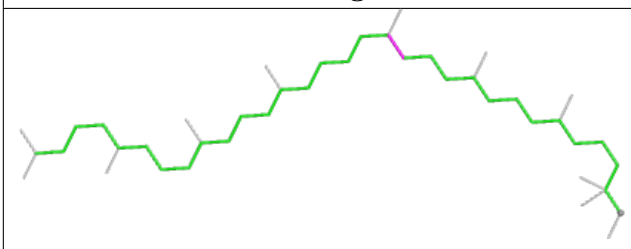
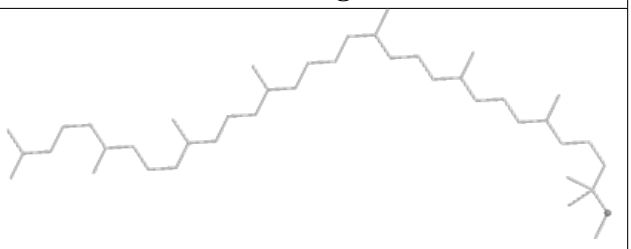


Torsions

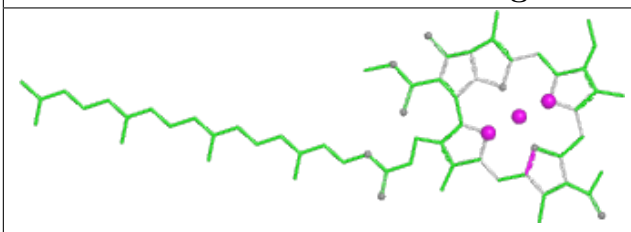


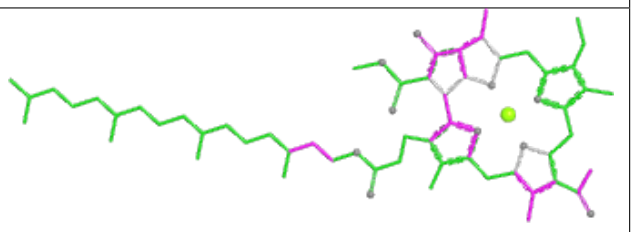
Rings

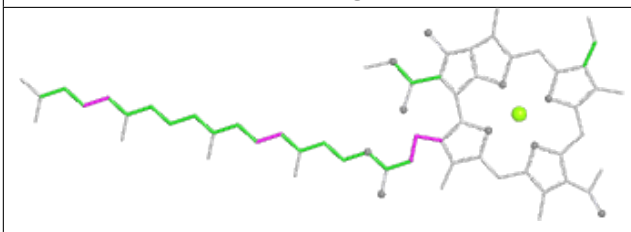
Ligand SPO AG 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

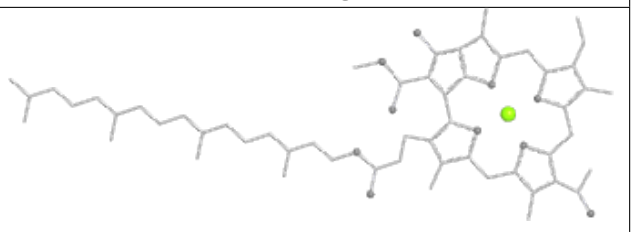
Ligand SPO AG 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL AK 103

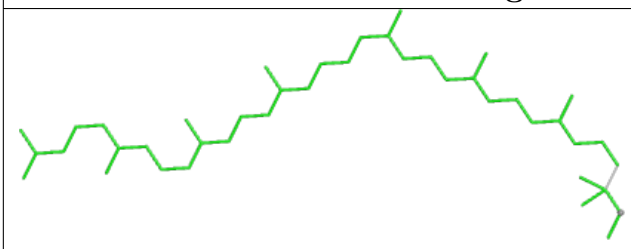

Bond lengths

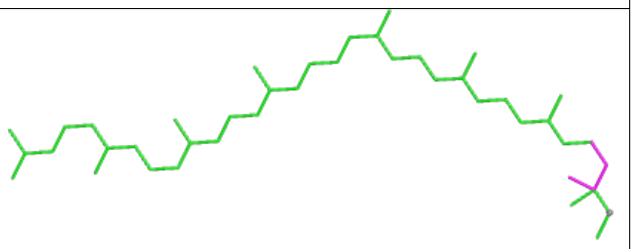

Bond angles

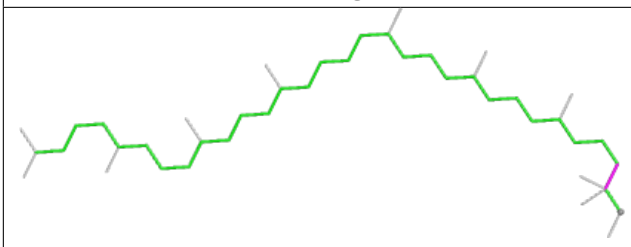

Torsions

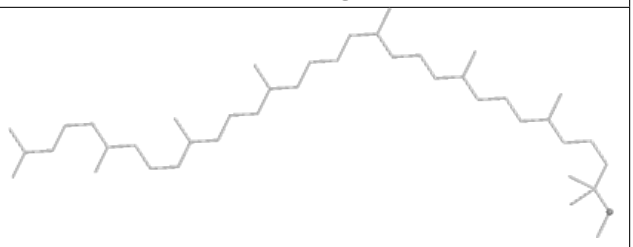

Rings

Ligand SPO AL 1002

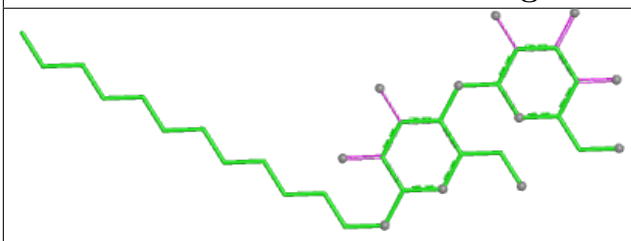

Bond lengths

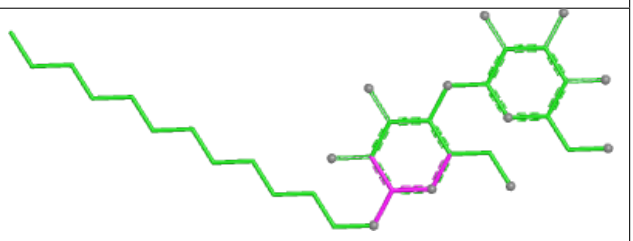

Bond angles

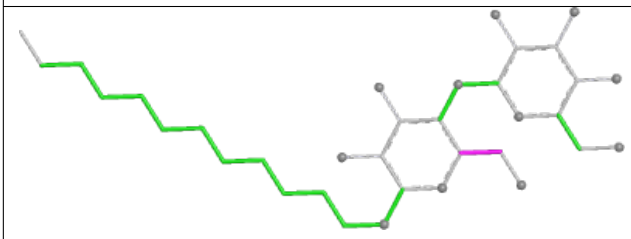

Torsions

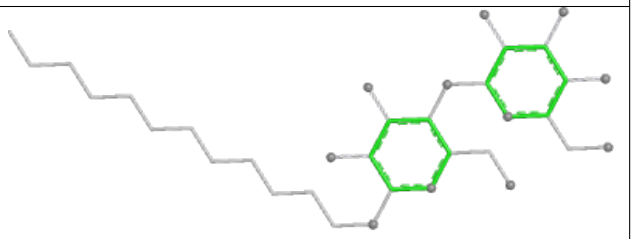

Rings

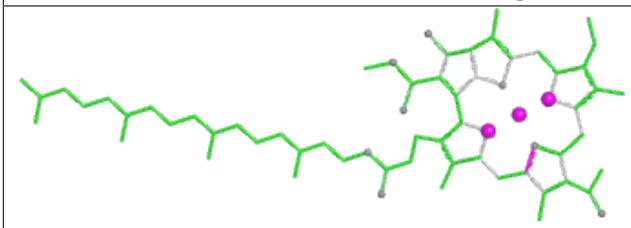
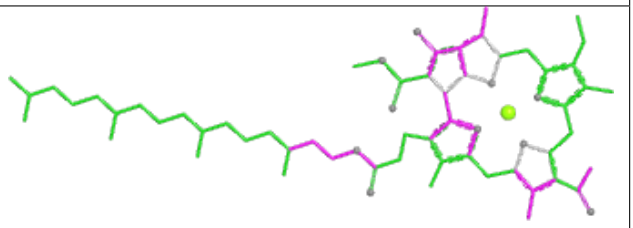
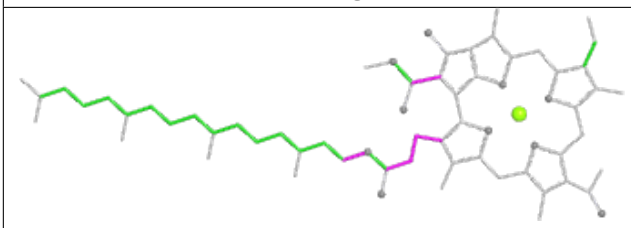
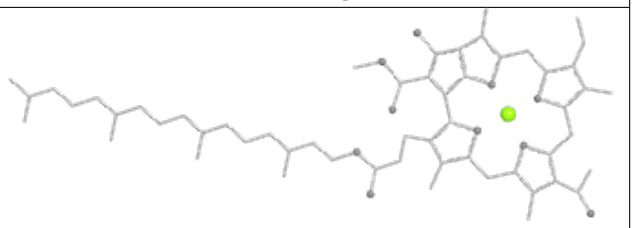
Ligand LMT X 101


Bond lengths


Bond angles


Torsions


Rings

Ligand BCL BG 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

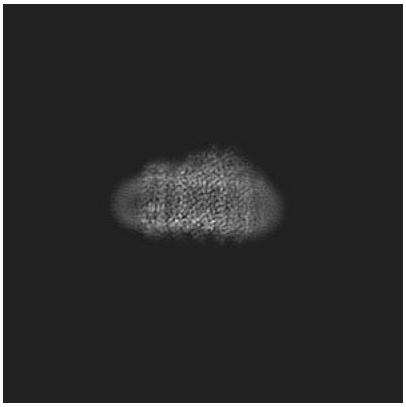
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13441. These allow visual inspection of the internal detail of the map and identification of artifacts.

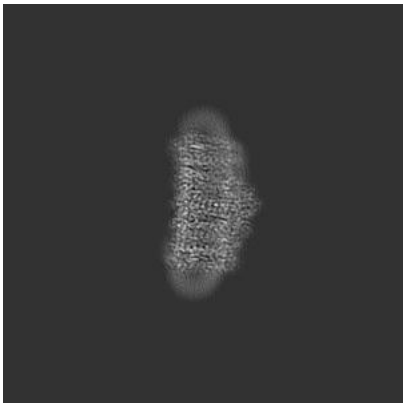
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

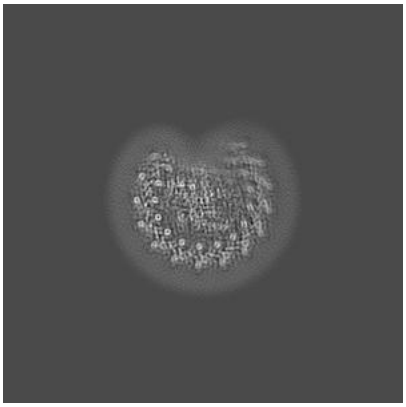
6.1.1 Primary map



X



Y

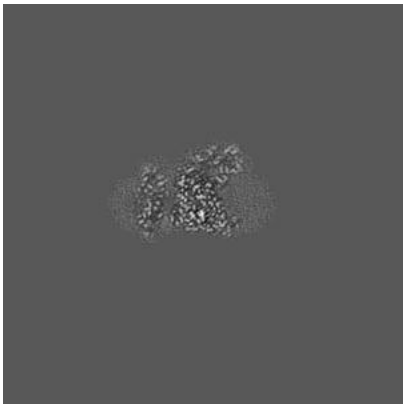


Z

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

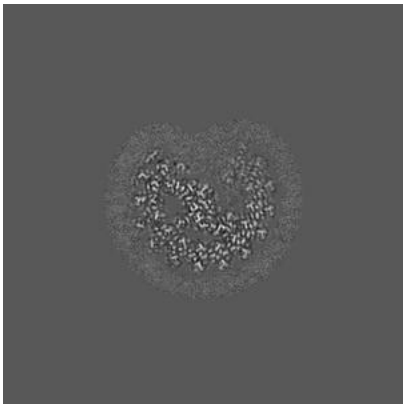
6.2 Central slices

6.2.1 Primary map



X Index: 256

Y Index: 256

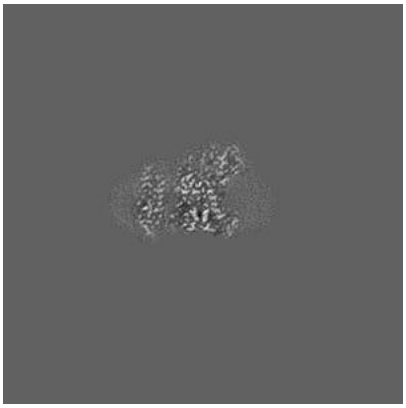


Z Index: 256

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

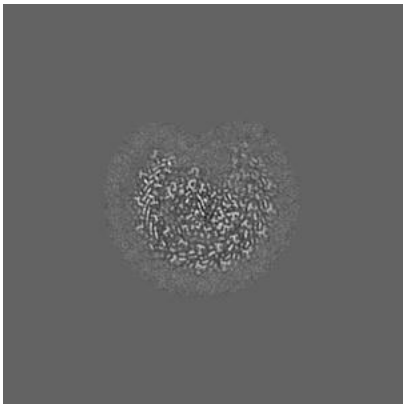
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 254

Y Index: 279



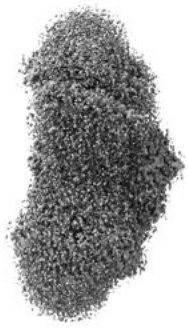
Z Index: 240

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

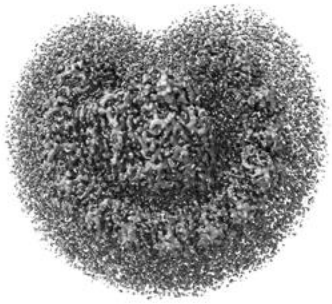
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0187. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

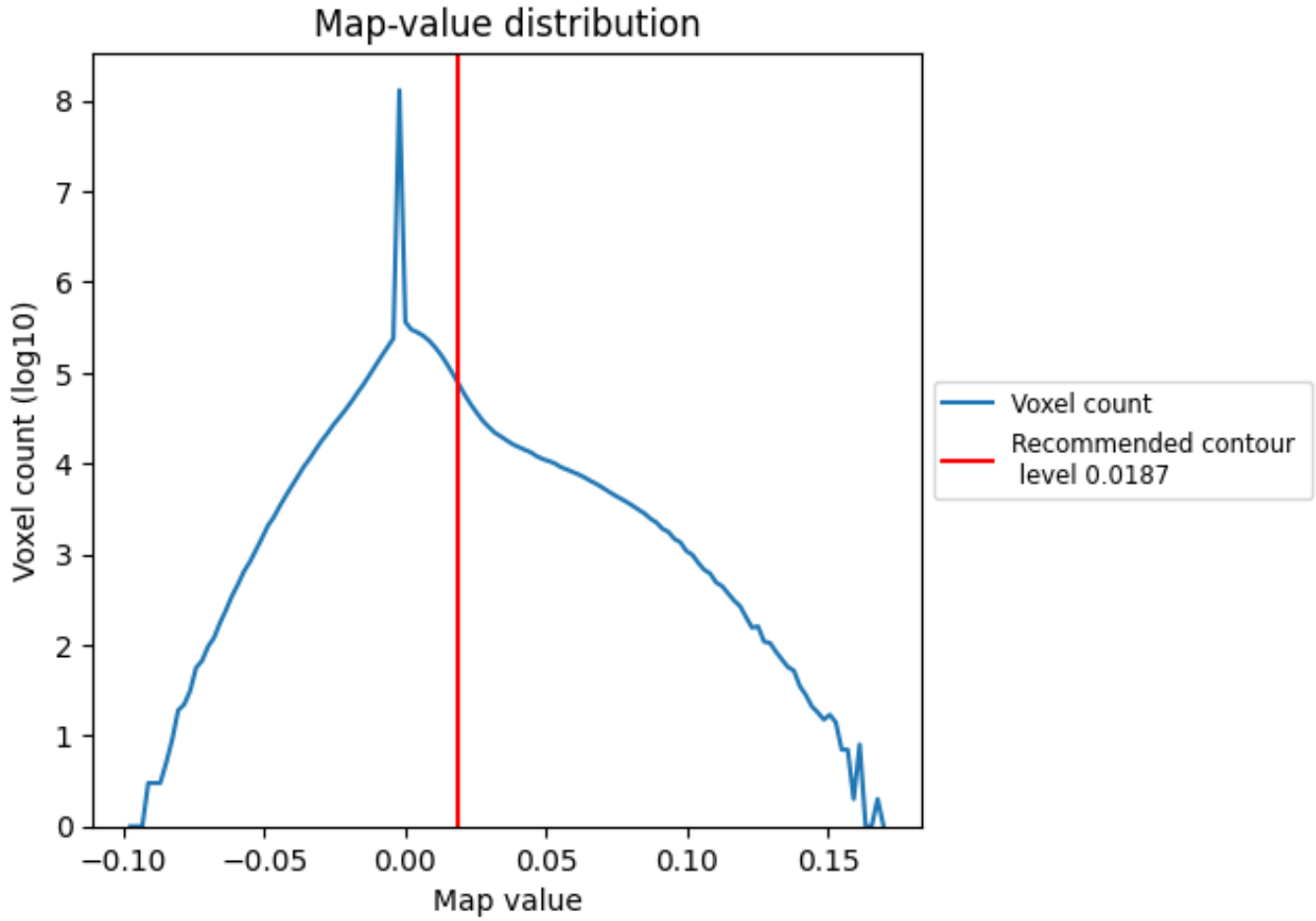
6.5 Mask visualisation (i)

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

7 Map analysis

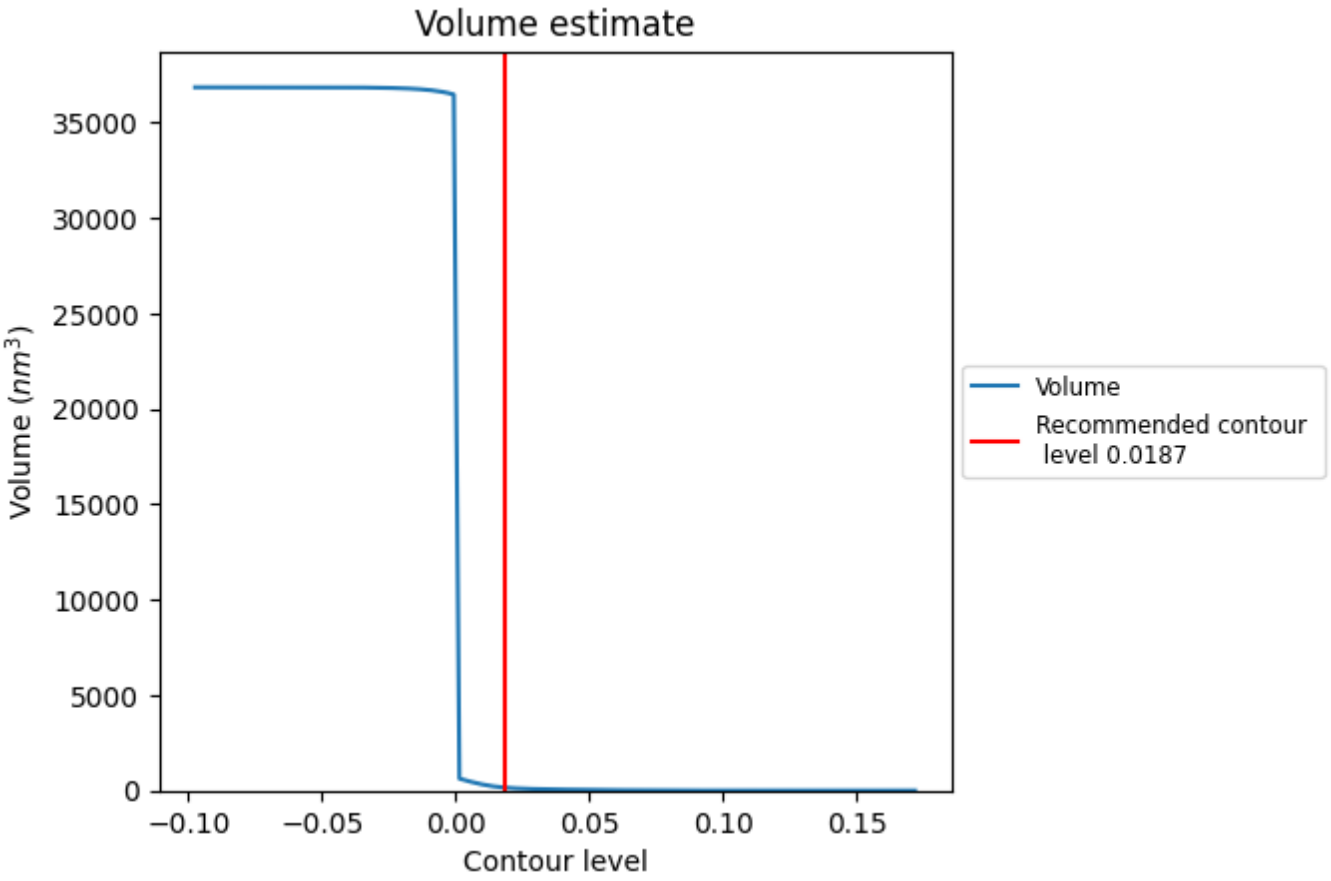
This section contains the results of statistical analysis of the map.

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.

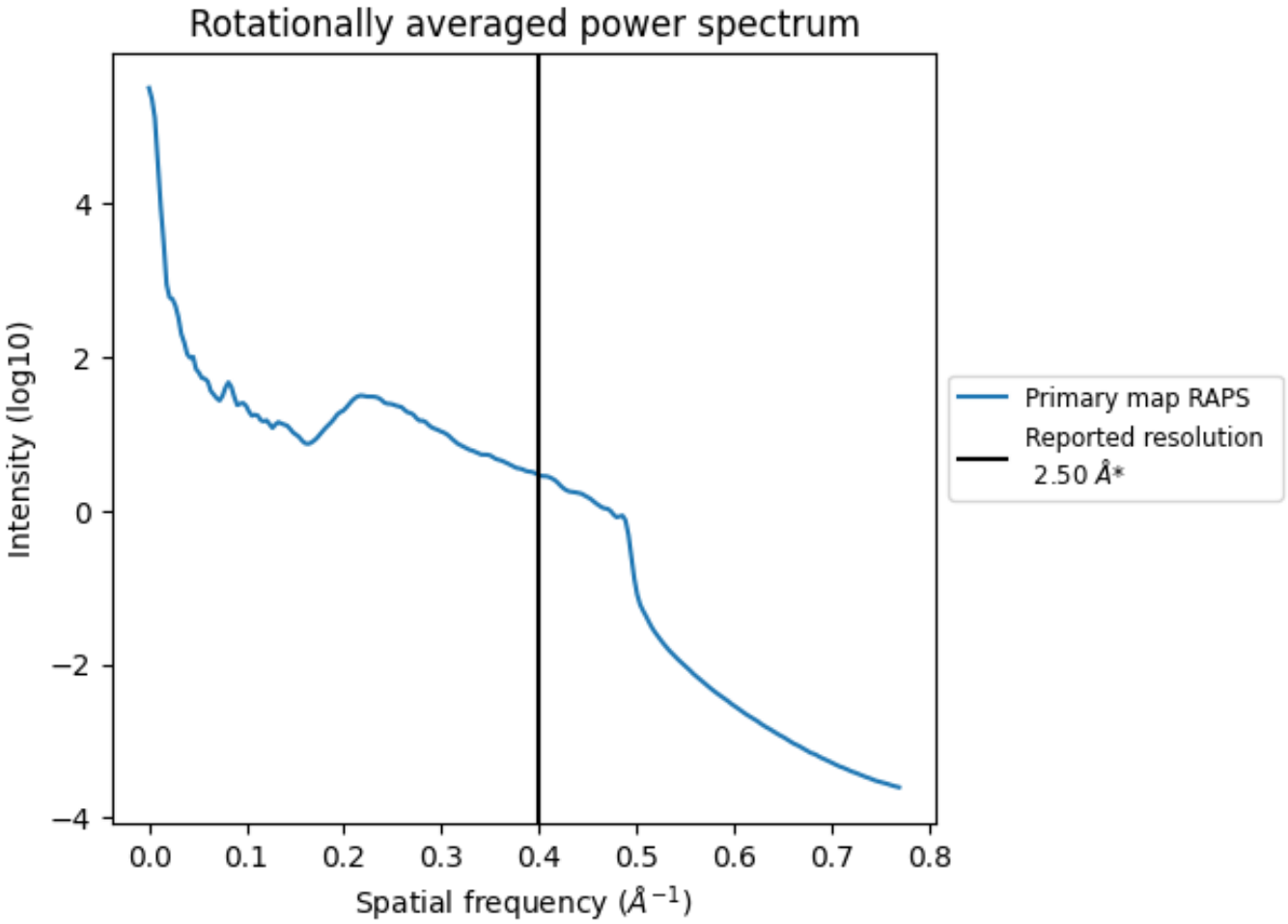
7.2 Volume estimate



The volume at the recommended contour level is 151 nm^3; this corresponds to an approximate mass of 136 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)

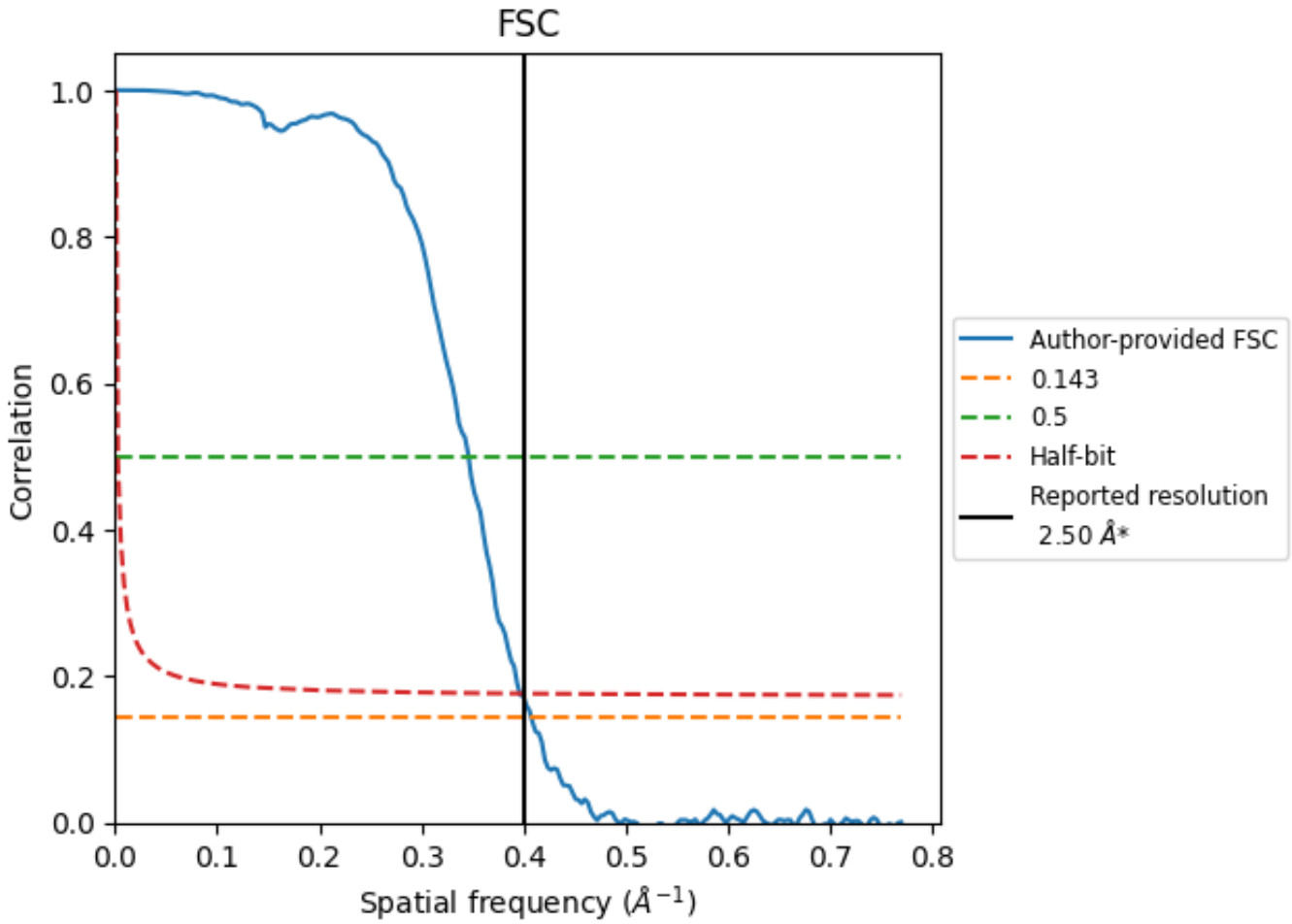


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates (i)

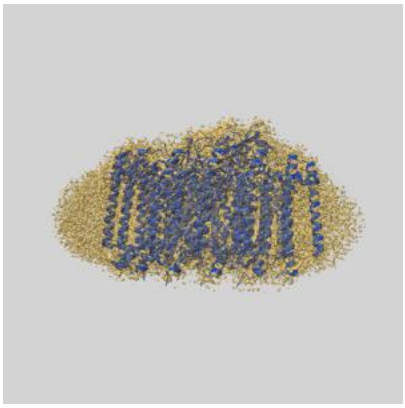
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.45	2.89	2.52
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

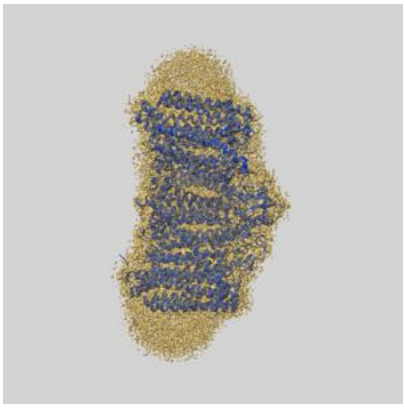
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13441 and PDB model 7PIL. Per-residue inclusion information can be found in section 3 on page 15.

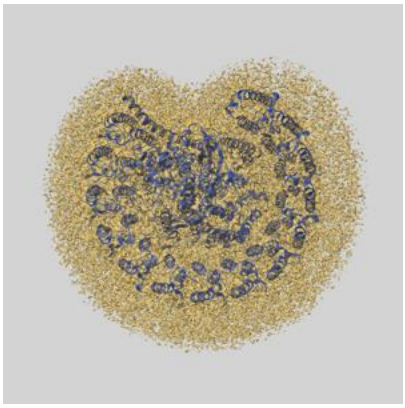
9.1 Map-model overlay



X



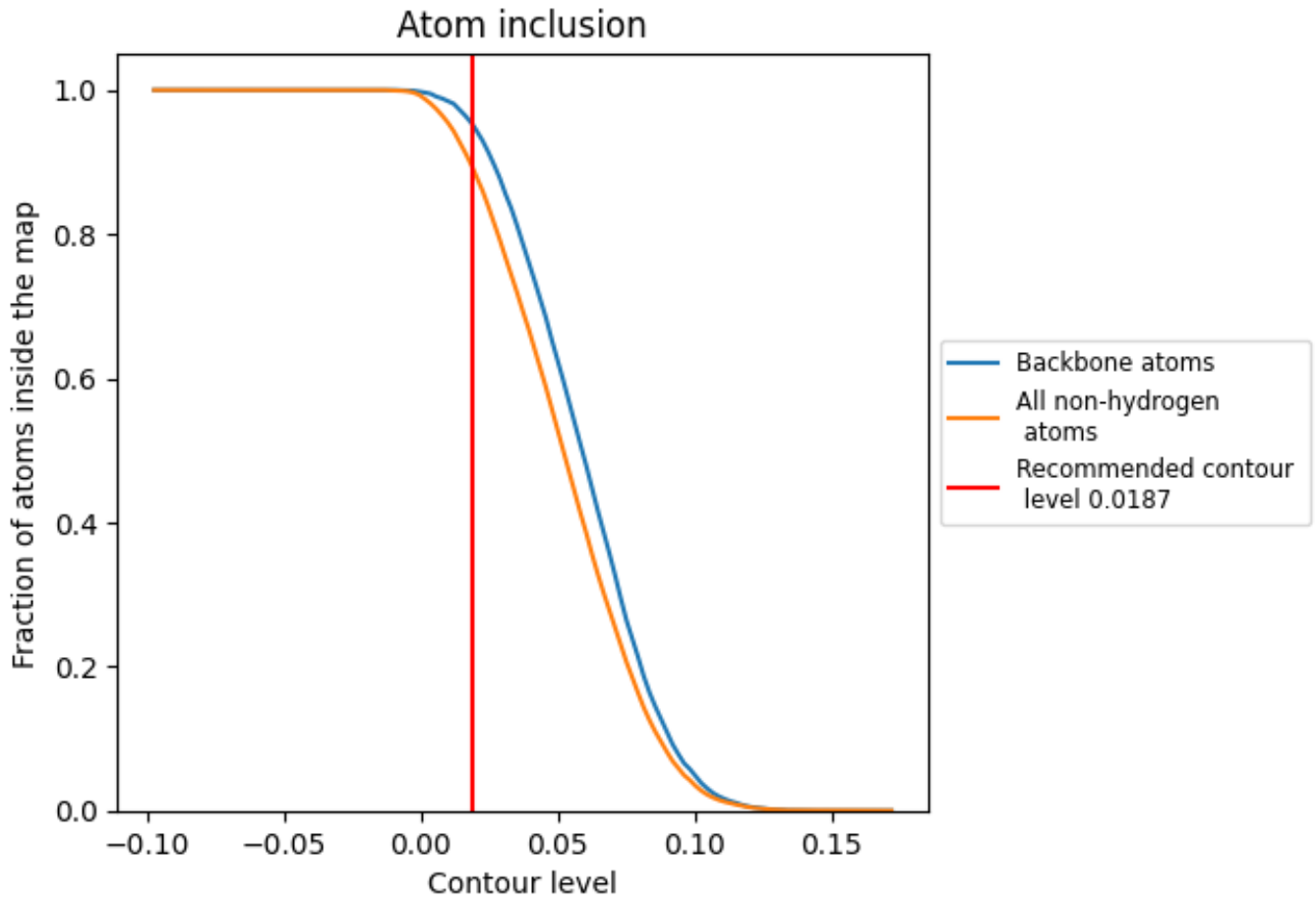
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0187 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 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.