Full wwPDB EM Validation Report ⓘ

Apr 9, 2024 – 12:25 PM EDT

PDB ID	:	8CUE
EMDB ID	:	EMD-26999
Title	:	CryoEM structure of the T-pilus from Agrobacterium tumefaciens
Authors	:	Bui, K.H.; Black, C.S.
Deposited on	:	2022-05-17
Resolution	:	3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

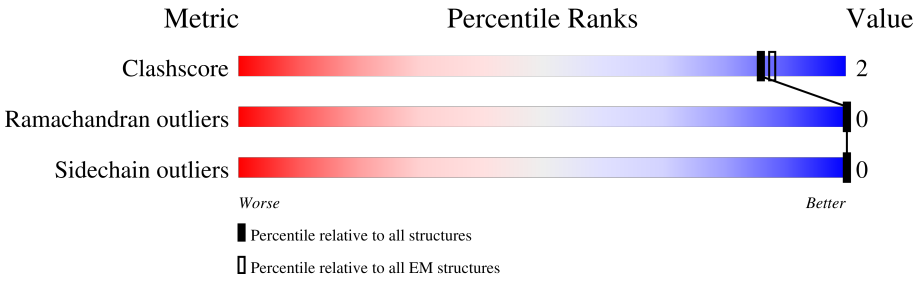
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1A	121	7% 57% · 42%
1	1B	121	· 57% · 42%
1	1C	121	· 57% · 42%
1	1D	121	· 57% · 42%
1	1E	121	· 57% · 42%
1	1F	121	· 57% · 42%
1	1G	121	· 57% · 42%
1	1H	121	· 56% · 42%

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Mol	Chain	Length	Quality of chain
1	1I	121	57% 42%
1	1J	121	57% 42%
1	1K	121	57% 42%
1	1L	121	57% 42%
1	1M	121	57% 42%
1	1N	121	57% 42%
1	2A	121	7% 57% 42%
1	2B	121	57% 42%
1	2C	121	57% 42%
1	2D	121	57% 42%
1	2E	121	57% 42%
1	2F	121	57% 42%
1	2G	121	57% 42%
1	2H	121	56% 42%
1	2I	121	57% 42%
1	2J	121	57% 42%
1	2K	121	57% 42%
1	2L	121	57% 42%
1	2M	121	57% 42%
1	2N	121	57% 42%
1	3A	121	7% 57% 42%
1	3B	121	57% 42%
1	3C	121	57% 42%
1	3D	121	57% 42%
1	3E	121	57% 42%

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Mol	Chain	Length	Quality of chain
1	3F	121	57% 42%
1	3G	121	57% 42%
1	3H	121	57% 42%
1	3I	121	57% 42%
1	3J	121	57% 42%
1	3K	121	57% 42%
1	3L	121	57% 42%
1	3M	121	57% 42%
1	3N	121	57% 42%
1	4A	121	7% 57% 42%
1	4B	121	57% 42%
1	4C	121	57% 42%
1	4D	121	57% 42%
1	4E	121	57% 42%
1	4F	121	57% 42%
1	4G	121	57% 42%
1	4H	121	57% 42%
1	4I	121	57% 42%
1	4J	121	57% 42%
1	4K	121	57% 42%
1	4L	121	57% 42%
1	4M	121	57% 42%
1	4N	121	57% 42%
1	5A	121	7% 57% 42%
1	5B	121	57% 42%

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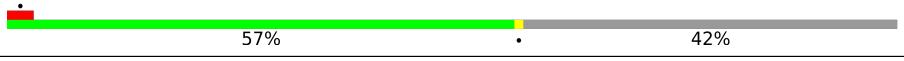
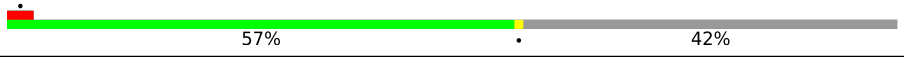
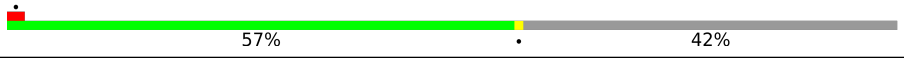
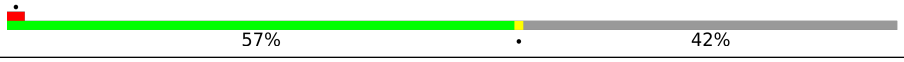
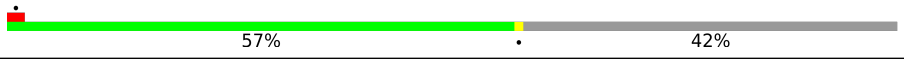
Mol	Chain	Length	Quality of chain
1	5C	121	
1	5D	121	
1	5E	121	
1	5F	121	
1	5G	121	
1	5H	121	
1	5I	121	
1	5J	121	
1	5K	121	
1	5L	121	
1	5M	121	
1	5N	121	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 37240 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 Protein virB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	1B	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	1C	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	1D	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	1E	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	1F	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	1G	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	1H	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	1I	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	1J	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	1K	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	1L	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	1M	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	1N	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	2A	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	2B	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	2C	70	Total	C	N	O	S	0	0
			480	314	78	84	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	2D	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	2E	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	2F	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	2G	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	2H	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	2I	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	2J	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	2K	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	2L	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	2M	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	2N	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	3A	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	3B	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	3C	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	3D	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	3E	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	3F	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	3G	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	3H	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	3I	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	3J	70	Total	C	N	O	S	0	0
			480	314	78	84	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	3K	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	3L	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	3M	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	3N	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	4A	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	4B	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	4C	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	4D	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	4E	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	4F	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	4G	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	4H	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	4I	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	4J	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	4K	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	4L	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	4M	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	4N	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	5A	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	5B	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	5C	70	Total	C	N	O	S	0	0
			480	314	78	84	4		

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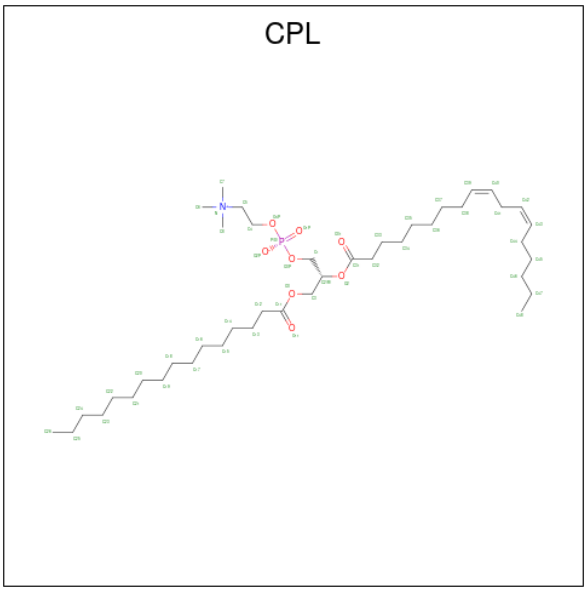
Mol	Chain	Residues	Atoms					AltConf	Trace
1	5D	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	5E	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	5F	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	5G	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	5H	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	5I	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	5J	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	5K	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	5L	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	5M	70	Total	C	N	O	S	0	0
			480	314	78	84	4		
1	5N	70	Total	C	N	O	S	0	0
			480	314	78	84	4		

- Molecule 2 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: CPL) (formula: $C_{42}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	1A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	1B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	1C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	1D	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	1E	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	1F	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	1G	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	1H	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	1I	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	1J	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	1K	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	1L	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	1M	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	1N	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	2A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	2B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	2C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	2D	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	2E	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	2F	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	2G	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	2H	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
2	2I	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	2J	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	2K	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	2L	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	2M	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	2N	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	3A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	3B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	3C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	3D	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	3E	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	3F	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	3G	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	3H	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	3I	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	3J	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	3K	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	3L	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	3M	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	3N	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	4A	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
2	4B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	4C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	4D	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	4E	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	4F	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	4G	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	4H	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	4I	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	4J	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	4K	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	4L	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	4M	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	4N	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	5A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	5B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	5C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	5D	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	5E	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	5F	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	5G	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	5H	1	Total	C	N	O	P	0
			52	42	1	8	1	

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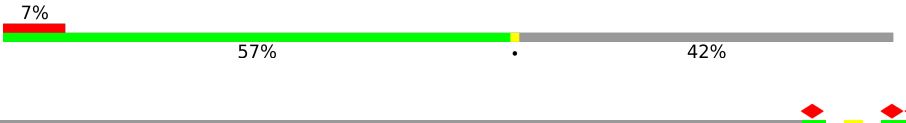
Mol	Chain	Residues	Atoms					AltConf
2	5I	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	5J	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	5K	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	5L	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	5M	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	5N	1	Total	C	N	O	P	0
			52	42	1	8	1	

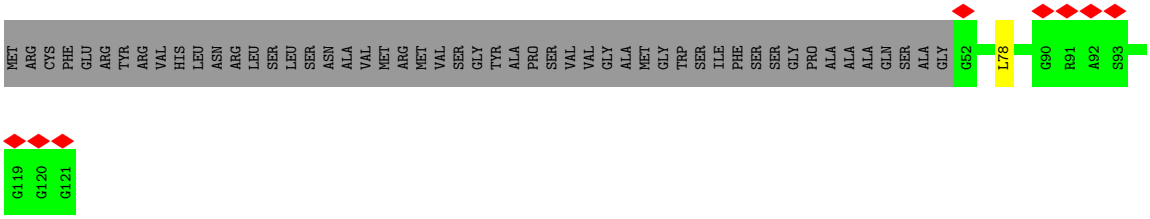
3 Residue-property plots (i)

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

• Molecule 1: Protein virB2

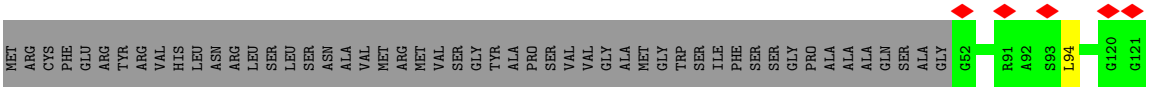
Chain 1A:





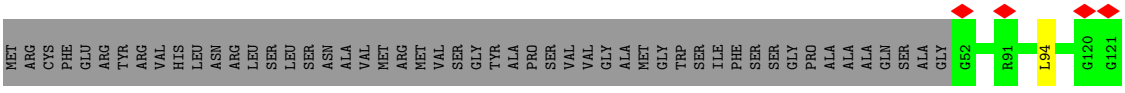
• Molecule 1: Protein virB2

Chain 1B:



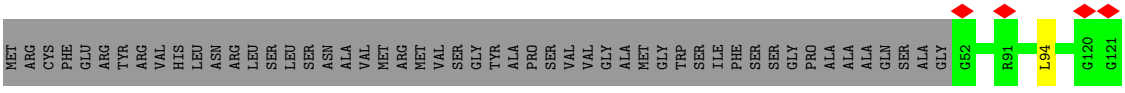
• Molecule 1: Protein virB2

Chain 1C:



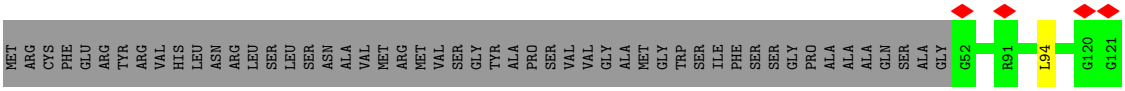
• Molecule 1: Protein virB2

Chain 1D:

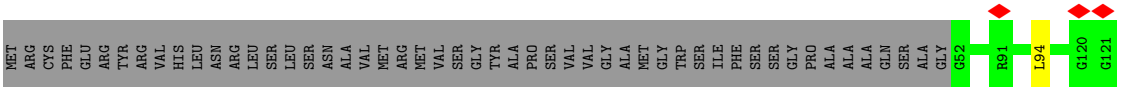


• Molecule 1: Protein virB2

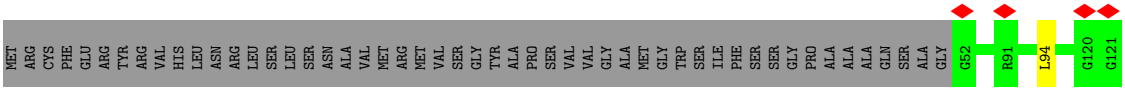
Chain 1E:



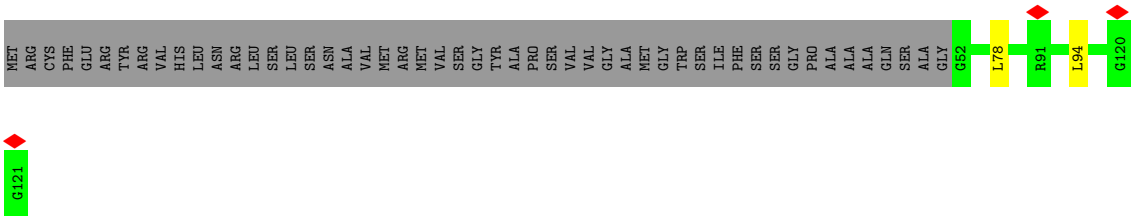
• Molecule 1: Protein virB2



• Molecule 1: Protein virB2



• Molecule 1: Protein virB2



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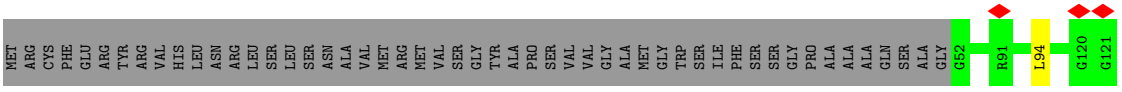

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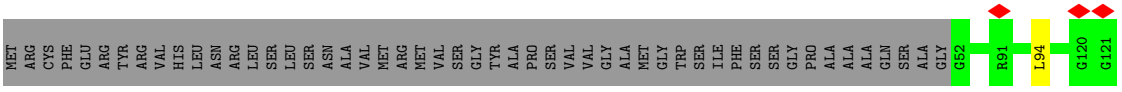

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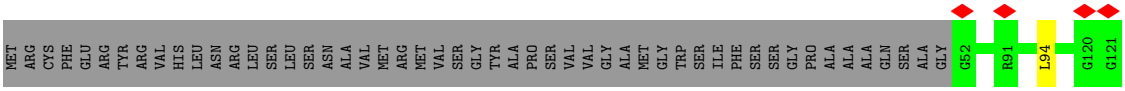
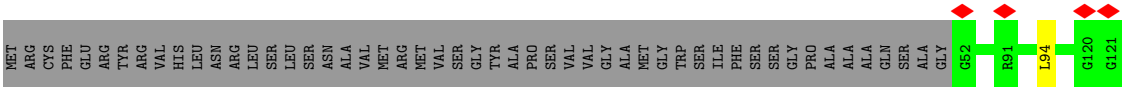
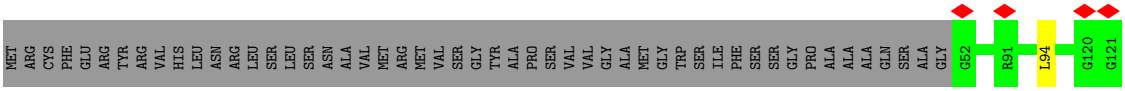


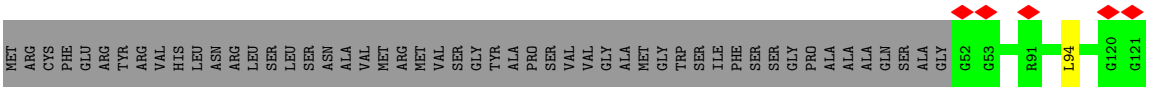
• Molecule 1: Protein virB2



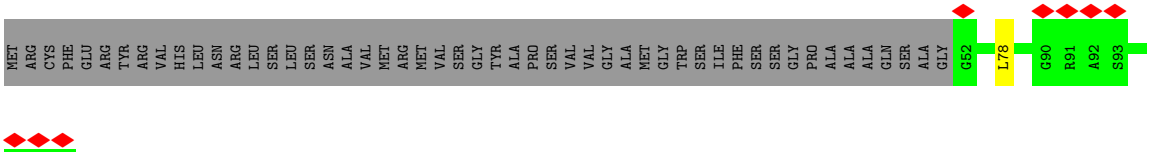
• Molecule 1: Protein virB2



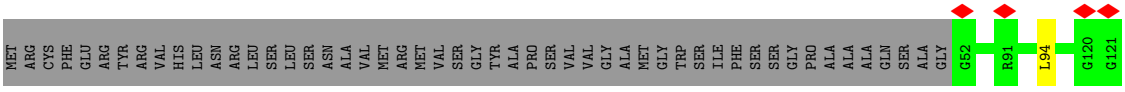
• Molecule 1: Protein virB2



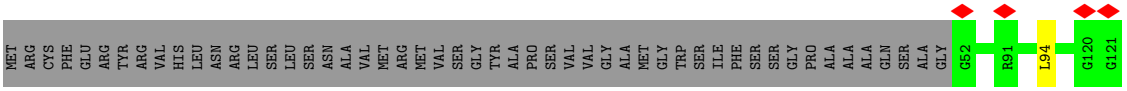
• Molecule 1: Protein virB2



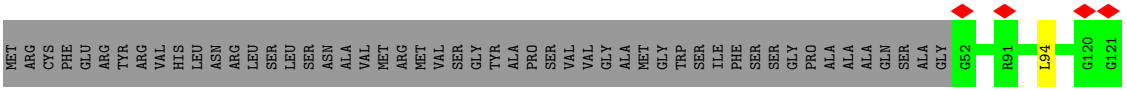
• Molecule 1: Protein virB2



• Molecule 1: Protein virB2



• Molecule 1: Protein virB2



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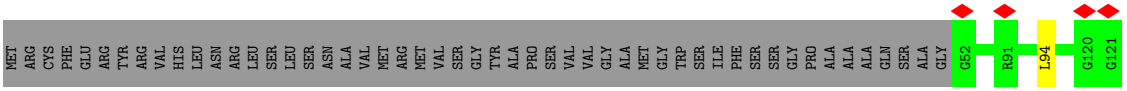
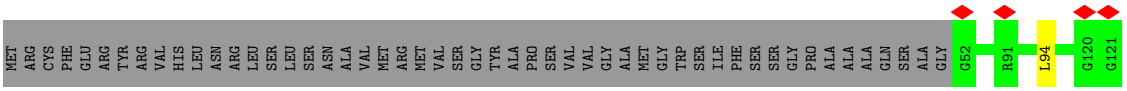


• Molecule 1: Protein virB2



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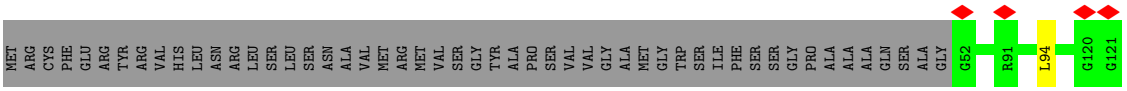
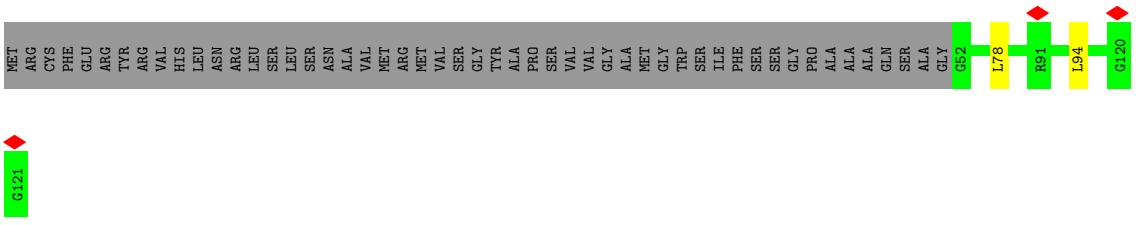
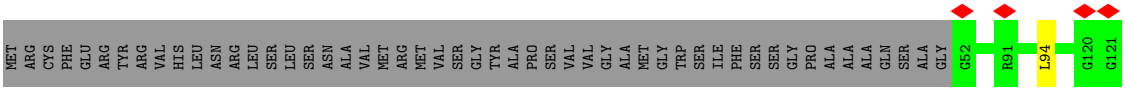


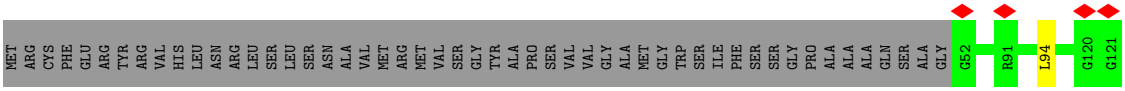
• Molecule 1: Protein virB2



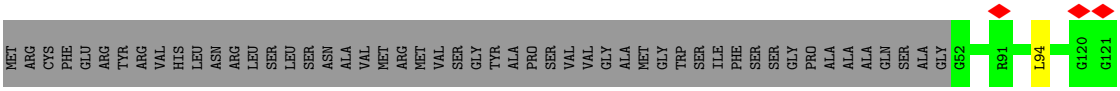
• Molecule 1: Protein virB2



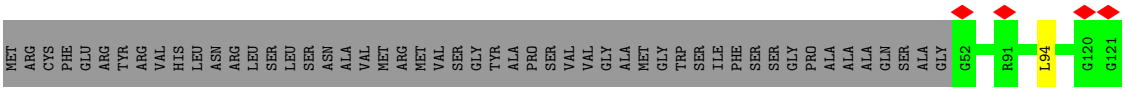
• Molecule 1: Protein virB2



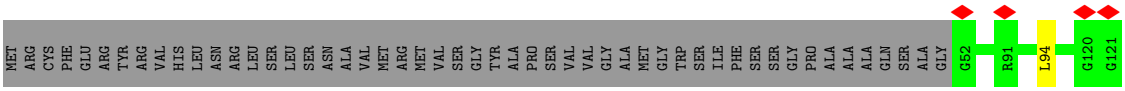
• Molecule 1: Protein virB2



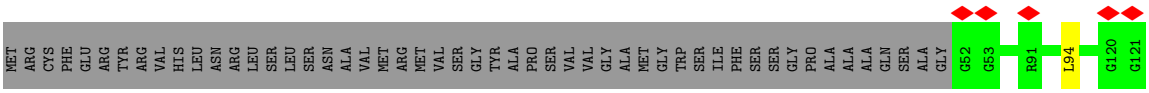
• Molecule 1: Protein virB2



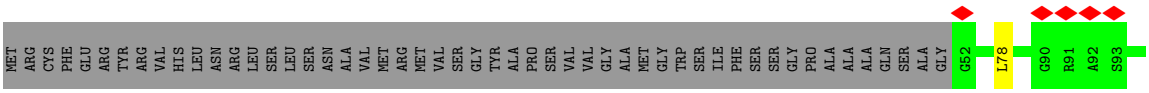
• Molecule 1: Protein virB2



• Molecule 1: Protein virB2

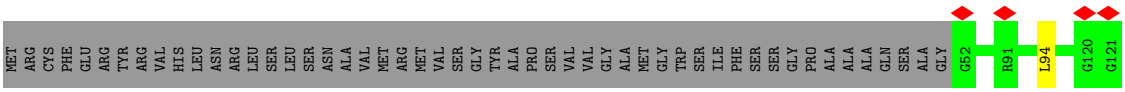


• Molecule 1: Protein virB2



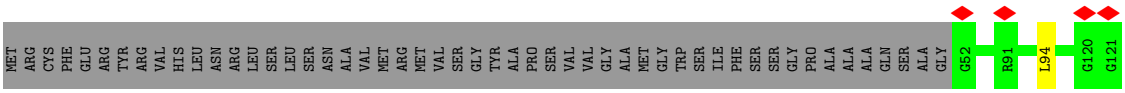
• Molecule 1: Protein virB2

Chain 3B:



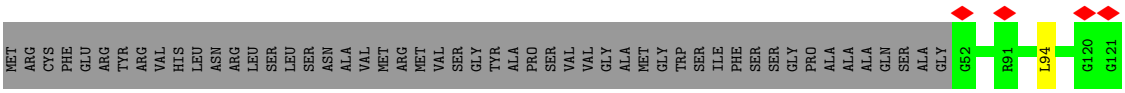
• Molecule 1: Protein virB2

Chain 3C:



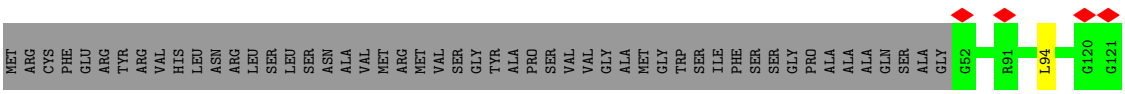
• Molecule 1: Protein virB2

Chain 3D:



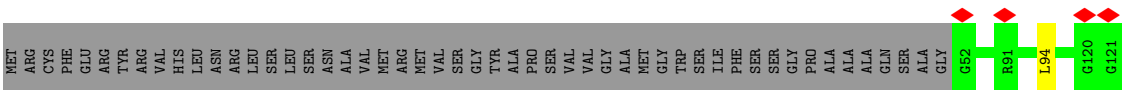
• Molecule 1: Protein virB2

Chain 3E:



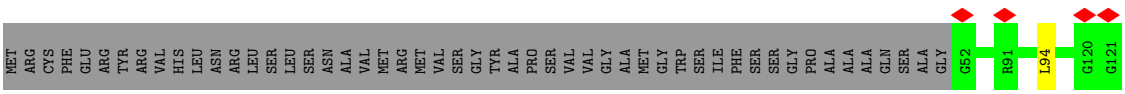
• Molecule 1: Protein virB2

Chain 3F:



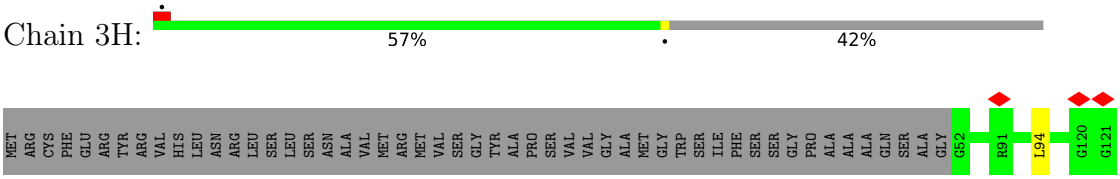
• Molecule 1: Protein virB2

Chain 3G:



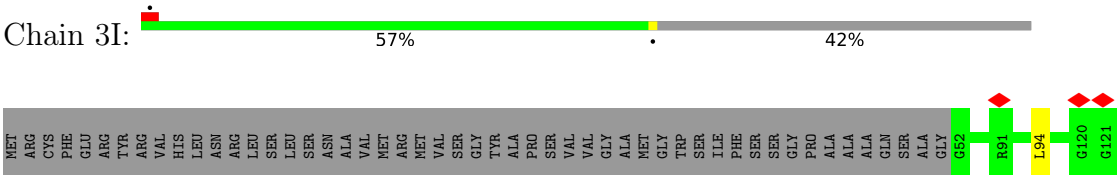
• Molecule 1: Protein virB2

Chain 3H:



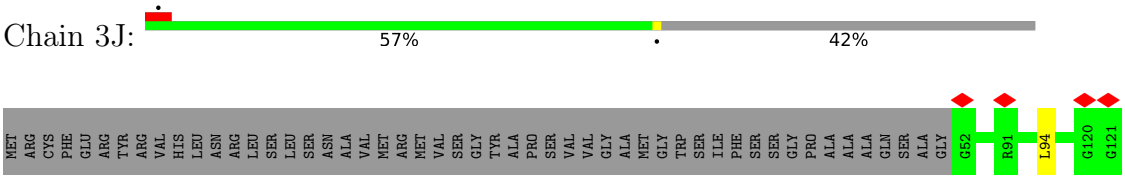
• Molecule 1: Protein virB2

Chain 3I:



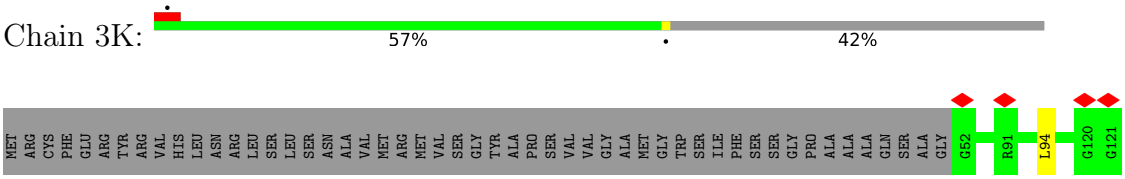
• Molecule 1: Protein virB2

Chain 3J:



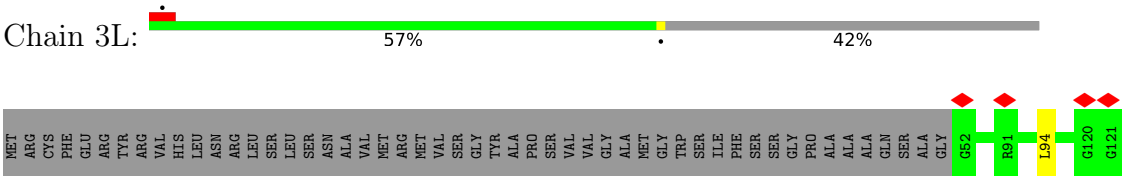
• Molecule 1: Protein virB2

Chain 3K:



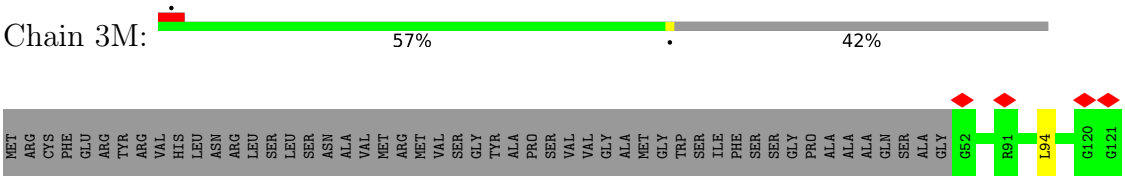
• Molecule 1: Protein virB2

Chain 3L:



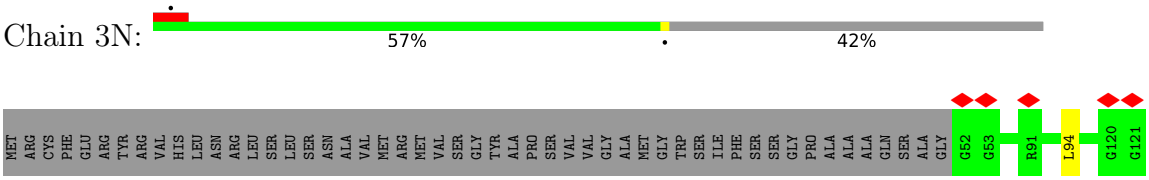
• Molecule 1: Protein virB2

Chain 3M:



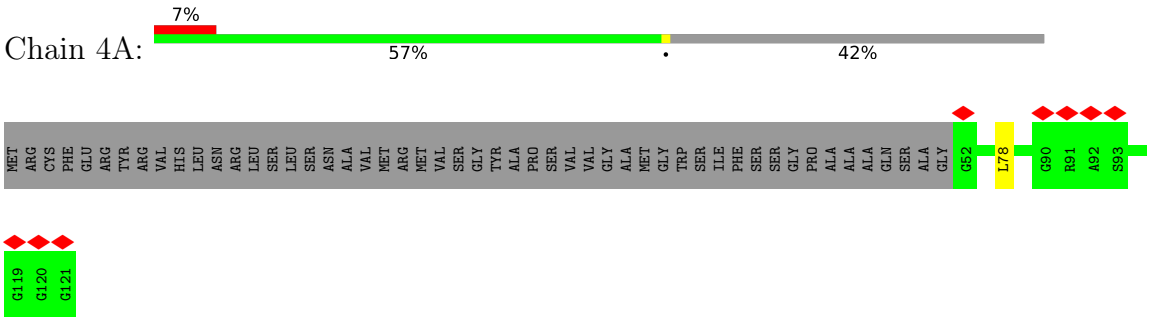
• Molecule 1: Protein virB2

Chain 3N:



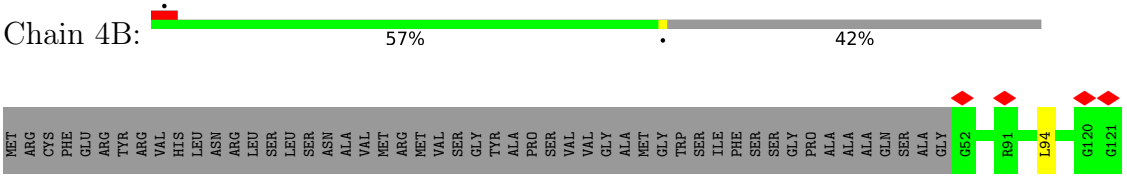
• Molecule 1: Protein virB2

Chain 4A:



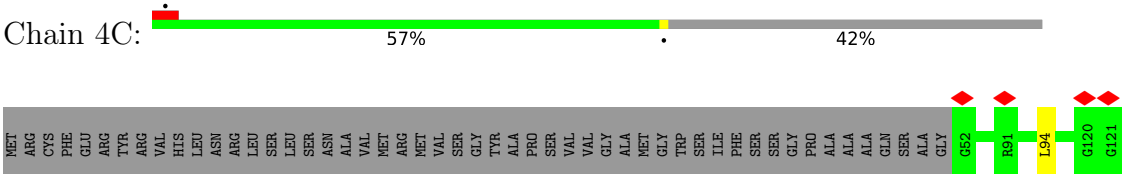
• Molecule 1: Protein virB2

Chain 4B:



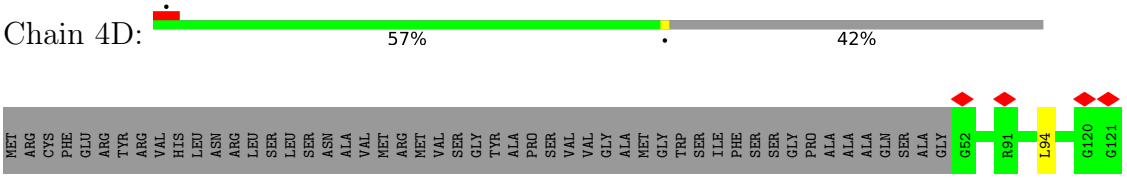
• Molecule 1: Protein virB2

Chain 4C:



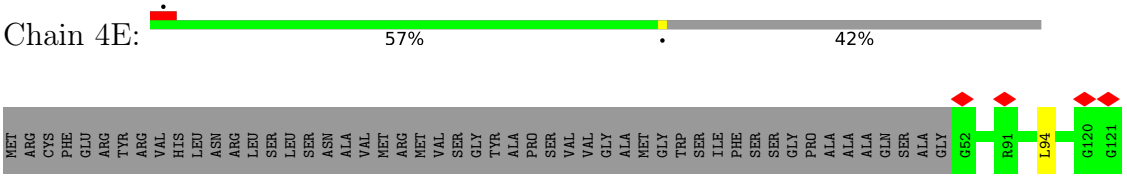
• Molecule 1: Protein virB2

Chain 4D:



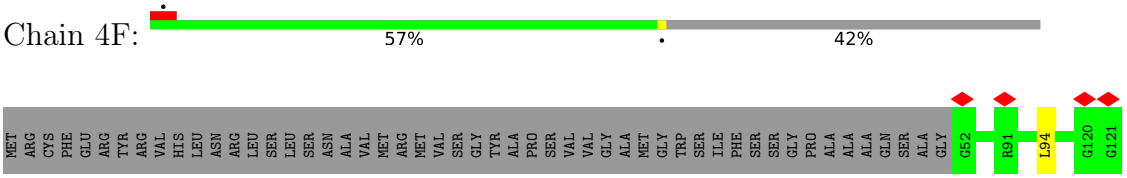
• Molecule 1: Protein virB2

Chain 4E:



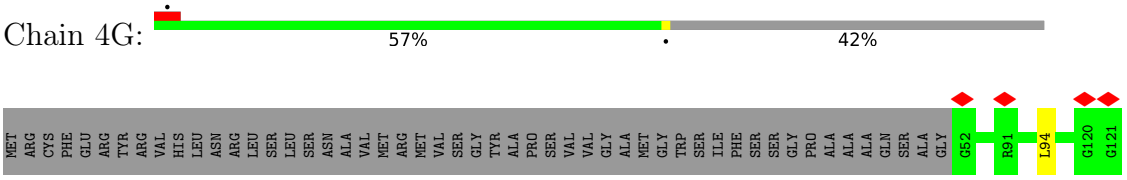
• Molecule 1: Protein virB2

Chain 4F:



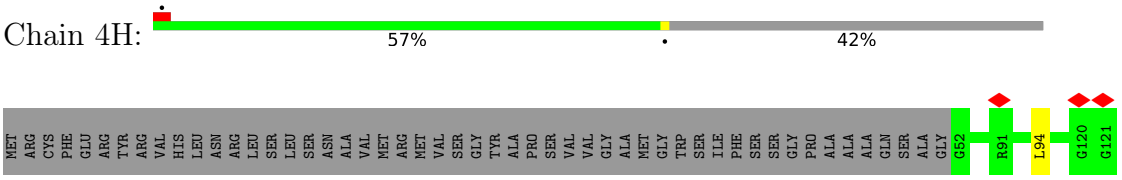
• Molecule 1: Protein virB2

Chain 4G:



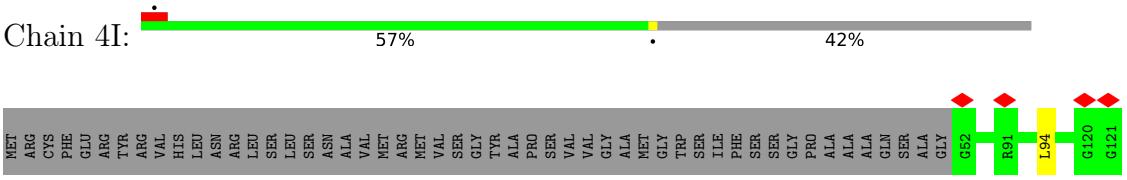
• Molecule 1: Protein virB2

Chain 4H:



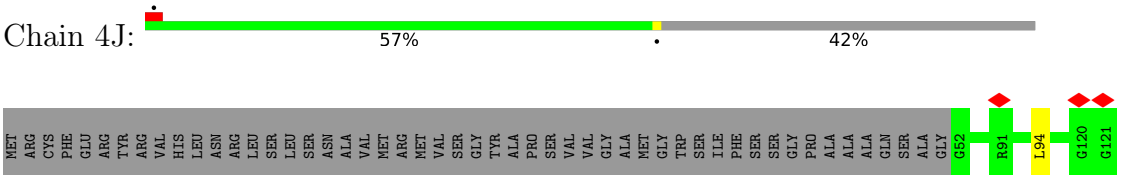
• Molecule 1: Protein virB2

Chain 4I:



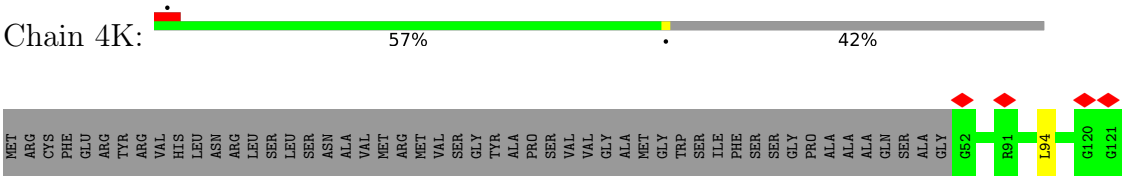
• Molecule 1: Protein virB2

Chain 4J:



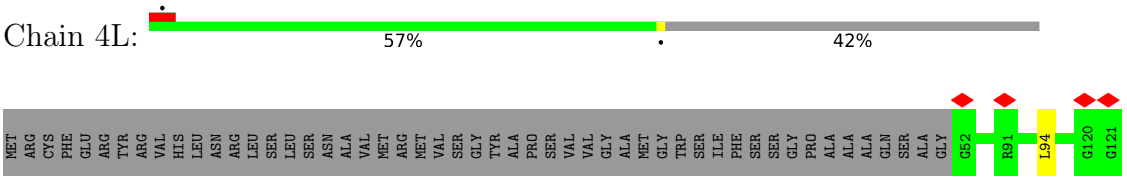
• Molecule 1: Protein virB2

Chain 4K:



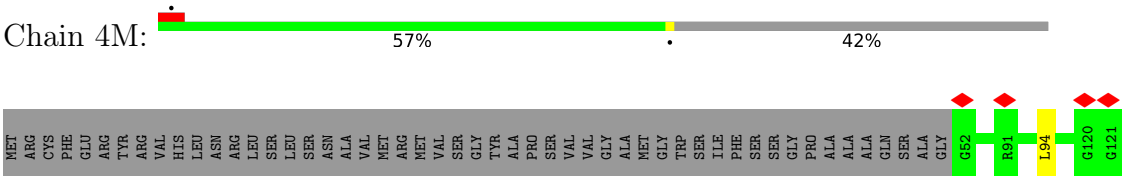
• Molecule 1: Protein virB2

Chain 4L:



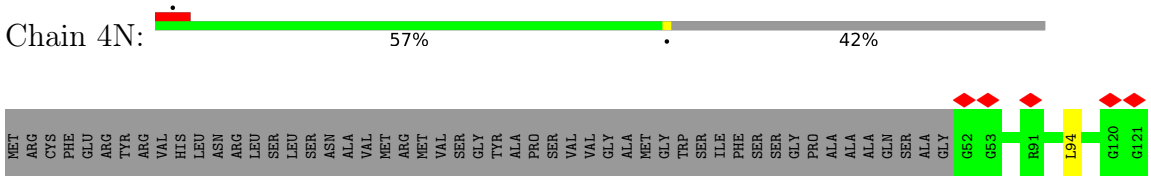
• Molecule 1: Protein virB2

Chain 4M:



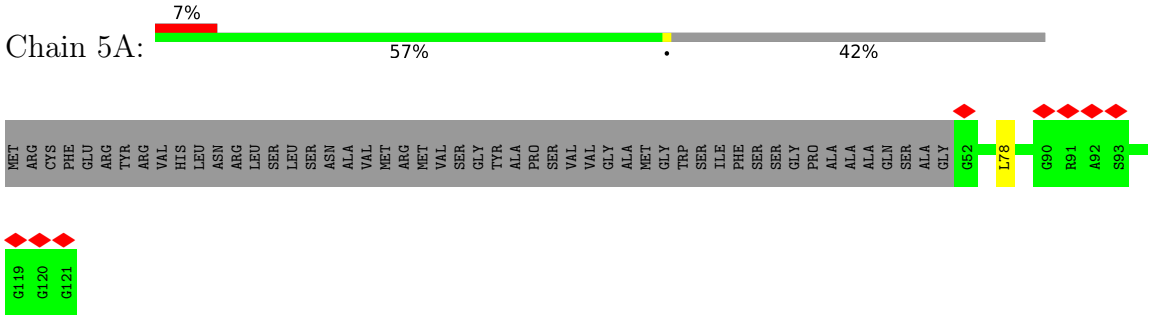
• Molecule 1: Protein virB2

Chain 4N:



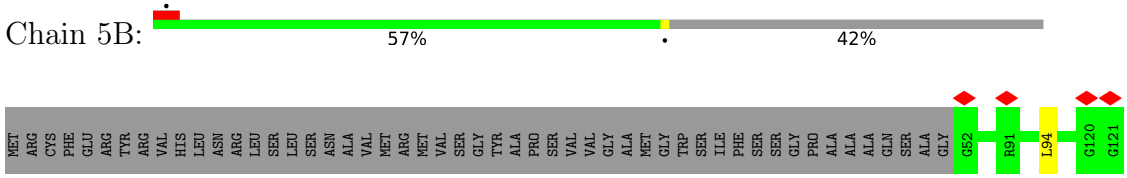
• Molecule 1: Protein virB2

Chain 5A:



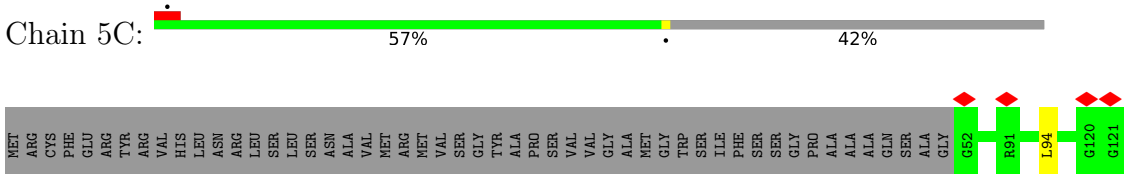
• Molecule 1: Protein virB2

Chain 5B:



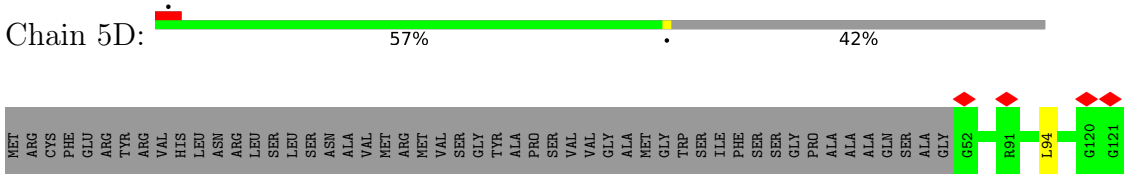
• Molecule 1: Protein virB2

Chain 5C:



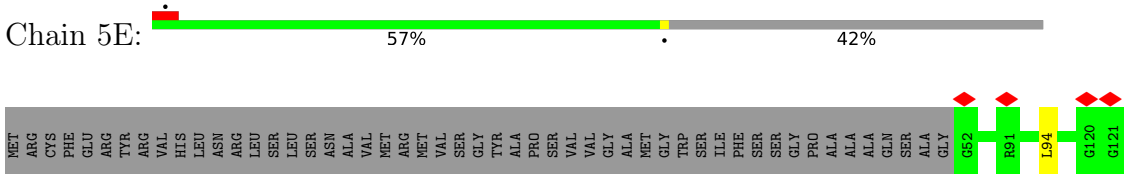
• Molecule 1: Protein virB2

Chain 5D:



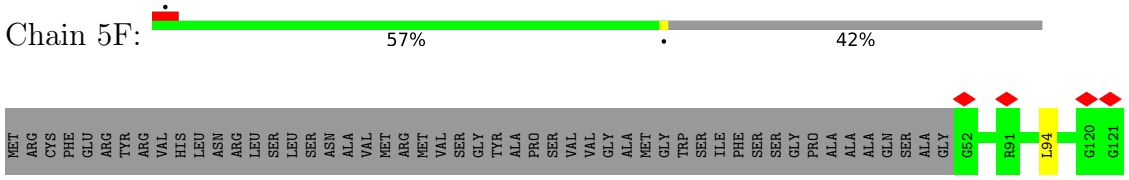
• Molecule 1: Protein virB2

Chain 5E:



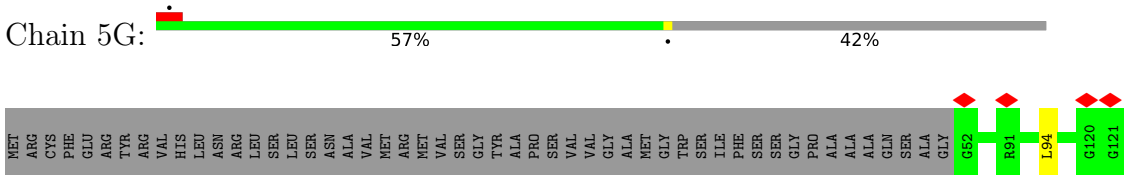
• Molecule 1: Protein virB2

Chain 5F:



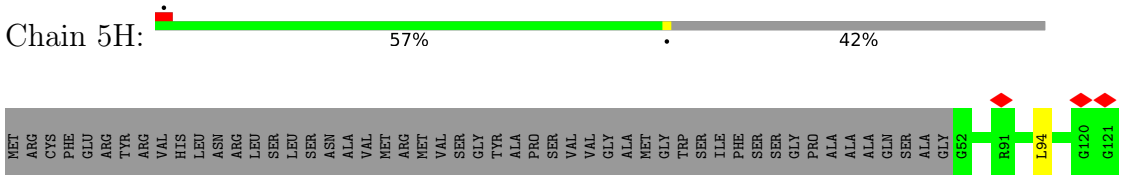
• Molecule 1: Protein virB2

Chain 5G:



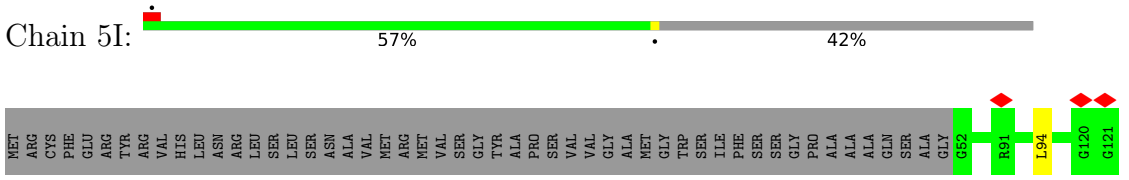
• Molecule 1: Protein virB2

Chain 5H:



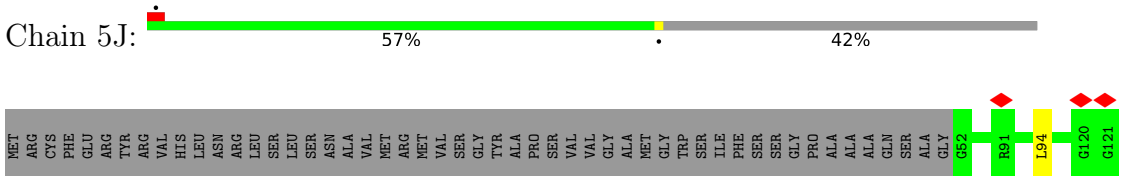
• Molecule 1: Protein virB2

Chain 5I:



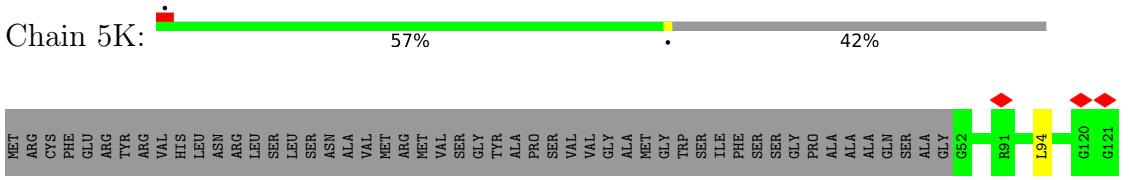
• Molecule 1: Protein virB2

Chain 5J:



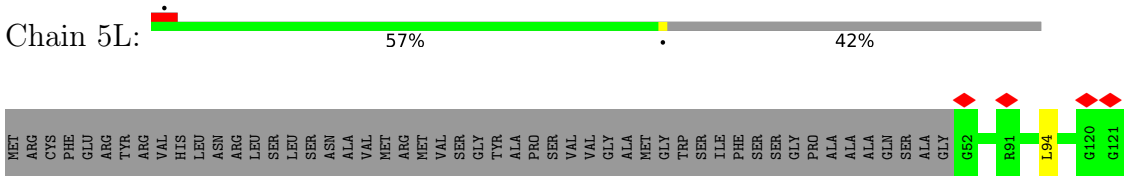
• Molecule 1: Protein virB2

Chain 5K:



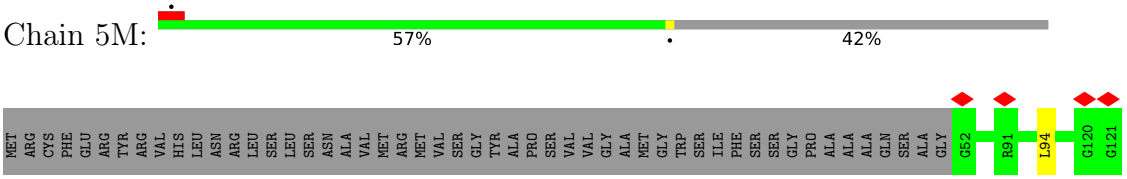
• Molecule 1: Protein virB2

Chain 5L:



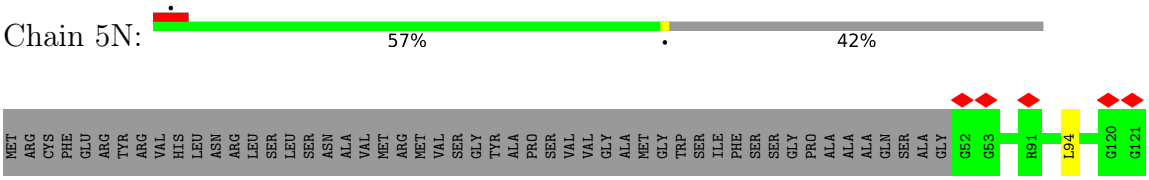
• Molecule 1: Protein virB2

Chain 5M:



• Molecule 1: Protein virB2

Chain 5N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	615500	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.891	Depositor
Minimum map value	-1.349	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.135	Depositor
Recommended contour level	0.593	Depositor
Map size (Å)	279.04, 279.04, 279.04	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CPL

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	1A	0.24	0/488	0.40	0/660
1	1B	0.24	0/488	0.41	0/660
1	1C	0.24	0/488	0.41	0/660
1	1D	0.24	0/488	0.40	0/660
1	1E	0.24	0/488	0.40	0/660
1	1F	0.24	0/488	0.40	0/660
1	1G	0.24	0/488	0.40	0/660
1	1H	0.24	0/488	0.40	0/660
1	1I	0.24	0/488	0.40	0/660
1	1J	0.24	0/488	0.40	0/660
1	1K	0.24	0/488	0.40	0/660
1	1L	0.24	0/488	0.41	0/660
1	1M	0.24	0/488	0.40	0/660
1	1N	0.24	0/488	0.40	0/660
1	2A	0.24	0/488	0.40	0/660
1	2B	0.24	0/488	0.40	0/660
1	2C	0.24	0/488	0.40	0/660
1	2D	0.24	0/488	0.41	0/660
1	2E	0.24	0/488	0.40	0/660
1	2F	0.24	0/488	0.41	0/660
1	2G	0.24	0/488	0.41	0/660
1	2H	0.24	0/488	0.40	0/660
1	2I	0.24	0/488	0.40	0/660
1	2J	0.24	0/488	0.41	0/660
1	2K	0.24	0/488	0.40	0/660
1	2L	0.24	0/488	0.40	0/660
1	2M	0.24	0/488	0.41	0/660
1	2N	0.24	0/488	0.41	0/660
1	3A	0.24	0/488	0.40	0/660
1	3B	0.25	0/488	0.40	0/660
1	3C	0.24	0/488	0.40	0/660
1	3D	0.24	0/488	0.40	0/660

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	3E	0.24	0/488	0.40	0/660
1	3F	0.24	0/488	0.40	0/660
1	3G	0.24	0/488	0.41	0/660
1	3H	0.24	0/488	0.40	0/660
1	3I	0.24	0/488	0.40	0/660
1	3J	0.24	0/488	0.40	0/660
1	3K	0.24	0/488	0.40	0/660
1	3L	0.24	0/488	0.40	0/660
1	3M	0.24	0/488	0.40	0/660
1	3N	0.24	0/488	0.40	0/660
1	4A	0.24	0/488	0.40	0/660
1	4B	0.24	0/488	0.40	0/660
1	4C	0.24	0/488	0.41	0/660
1	4D	0.24	0/488	0.41	0/660
1	4E	0.24	0/488	0.40	0/660
1	4F	0.24	0/488	0.40	0/660
1	4G	0.24	0/488	0.40	0/660
1	4H	0.24	0/488	0.40	0/660
1	4I	0.24	0/488	0.40	0/660
1	4J	0.24	0/488	0.40	0/660
1	4K	0.24	0/488	0.40	0/660
1	4L	0.24	0/488	0.41	0/660
1	4M	0.24	0/488	0.40	0/660
1	4N	0.24	0/488	0.41	0/660
1	5A	0.24	0/488	0.40	0/660
1	5B	0.24	0/488	0.40	0/660
1	5C	0.24	0/488	0.40	0/660
1	5D	0.24	0/488	0.40	0/660
1	5E	0.24	0/488	0.40	0/660
1	5F	0.24	0/488	0.40	0/660
1	5G	0.24	0/488	0.40	0/660
1	5H	0.25	0/488	0.40	0/660
1	5I	0.24	0/488	0.40	0/660
1	5J	0.24	0/488	0.40	0/660
1	5K	0.24	0/488	0.40	0/660
1	5L	0.24	0/488	0.41	0/660
1	5M	0.24	0/488	0.41	0/660
1	5N	0.24	0/488	0.40	0/660
All	All	0.24	0/34160	0.40	0/46200

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	1A	480	0	500	1	0
1	1B	480	0	500	1	0
1	1C	480	0	500	1	0
1	1D	480	0	500	1	0
1	1E	480	0	500	1	0
1	1F	480	0	500	1	0
1	1G	480	0	500	1	0
1	1H	480	0	500	2	0
1	1I	480	0	500	1	0
1	1J	480	0	500	1	0
1	1K	480	0	500	1	0
1	1L	480	0	500	1	0
1	1M	480	0	500	1	0
1	1N	480	0	500	1	0
1	2A	480	0	500	1	0
1	2B	480	0	500	1	0
1	2C	480	0	500	1	0
1	2D	480	0	500	1	0
1	2E	480	0	500	1	0
1	2F	480	0	500	1	0
1	2G	480	0	500	1	0
1	2H	480	0	500	2	0
1	2I	480	0	500	1	0
1	2J	480	0	500	1	0
1	2K	480	0	500	1	0
1	2L	480	0	500	1	0
1	2M	480	0	500	1	0
1	2N	480	0	500	1	0
1	3A	480	0	500	1	0
1	3B	480	0	500	1	0
1	3C	480	0	500	1	0
1	3D	480	0	500	1	0
1	3E	480	0	500	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3F	480	0	500	1	0
1	3G	480	0	500	1	0
1	3H	480	0	500	1	0
1	3I	480	0	500	1	0
1	3J	480	0	500	1	0
1	3K	480	0	500	1	0
1	3L	480	0	500	1	0
1	3M	480	0	500	1	0
1	3N	480	0	500	1	0
1	4A	480	0	500	1	0
1	4B	480	0	500	1	0
1	4C	480	0	500	1	0
1	4D	480	0	500	1	0
1	4E	480	0	500	1	0
1	4F	480	0	500	1	0
1	4G	480	0	500	1	0
1	4H	480	0	500	1	0
1	4I	480	0	500	1	0
1	4J	480	0	500	1	0
1	4K	480	0	500	1	0
1	4L	480	0	500	1	0
1	4M	480	0	500	1	0
1	4N	480	0	500	1	0
1	5A	480	0	500	1	0
1	5B	480	0	500	1	0
1	5C	480	0	500	1	0
1	5D	480	0	500	1	0
1	5E	480	0	500	1	0
1	5F	480	0	500	1	0
1	5G	480	0	500	1	0
1	5H	480	0	500	1	0
1	5I	480	0	500	1	0
1	5J	480	0	500	1	0
1	5K	480	0	500	1	0
1	5L	480	0	500	1	0
1	5M	480	0	500	1	0
1	5N	480	0	500	1	0
2	1A	52	0	80	3	0
2	1B	52	0	80	2	0
2	1C	52	0	80	2	0
2	1D	52	0	80	2	0
2	1E	52	0	80	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1F	52	0	80	2	0
2	1G	52	0	80	2	0
2	1H	52	0	80	3	0
2	1I	52	0	80	2	0
2	1J	52	0	80	1	0
2	1K	52	0	80	3	0
2	1L	52	0	80	3	0
2	1M	52	0	80	4	0
2	1N	52	0	80	2	0
2	2A	52	0	80	4	0
2	2B	52	0	80	3	0
2	2C	52	0	80	1	0
2	2D	52	0	80	2	0
2	2E	52	0	80	2	0
2	2F	52	0	80	2	0
2	2G	52	0	80	3	0
2	2H	52	0	80	3	0
2	2I	52	0	80	3	0
2	2J	52	0	80	3	0
2	2K	52	0	80	3	0
2	2L	52	0	80	2	0
2	2M	52	0	80	3	0
2	2N	52	0	80	0	0
2	3A	52	0	80	4	0
2	3B	52	0	80	1	0
2	3C	52	0	80	2	0
2	3D	52	0	80	2	0
2	3E	52	0	80	3	0
2	3F	52	0	80	2	0
2	3G	52	0	80	2	0
2	3H	52	0	80	3	0
2	3I	52	0	80	5	0
2	3J	52	0	80	4	0
2	3K	52	0	80	3	0
2	3L	52	0	80	2	0
2	3M	52	0	80	2	0
2	3N	52	0	80	2	0
2	4A	52	0	80	3	0
2	4B	52	0	80	2	0
2	4C	52	0	80	3	0
2	4D	52	0	80	1	0
2	4E	52	0	80	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	4F	52	0	80	2	0
2	4G	52	0	80	3	0
2	4H	52	0	80	4	0
2	4I	52	0	80	2	0
2	4J	52	0	80	1	0
2	4K	52	0	80	2	0
2	4L	52	0	80	2	0
2	4M	52	0	80	3	0
2	4N	52	0	80	0	0
2	5A	52	0	80	3	0
2	5B	52	0	80	3	0
2	5C	52	0	80	2	0
2	5D	52	0	80	4	0
2	5E	52	0	80	4	0
2	5F	52	0	80	5	0
2	5G	52	0	80	1	0
2	5H	52	0	80	2	0
2	5I	52	0	80	3	0
2	5J	52	0	80	3	0
2	5K	52	0	80	3	0
2	5L	52	0	80	3	0
2	5M	52	0	80	3	0
2	5N	52	0	80	1	0
All	All	37240	0	40600	166	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 (166) 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)
1:3H:94:LEU:HD13	2:4G:201:CPL:H131	1.92	0.52
1:2J:94:LEU:HD13	2:3I:201:CPL:H131	1.92	0.52
1:4H:94:LEU:HD13	2:5G:201:CPL:H131	1.93	0.51
1:4L:94:LEU:HD13	2:5K:201:CPL:H131	1.93	0.50
2:1D:201:CPL:H131	1:5E:94:LEU:HD13	1.93	0.50
1:2L:94:LEU:HD13	2:3K:201:CPL:H131	1.94	0.50
2:1G:201:CPL:H131	1:5H:94:LEU:HD13	1.93	0.50
2:1K:201:CPL:H131	1:5L:94:LEU:HD13	1.94	0.50
1:4J:94:LEU:HD13	2:5I:201:CPL:H131	1.93	0.50
2:1I:201:CPL:H131	1:5J:94:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1F:94:LEU:HD13	2:2E:201:CPL:H131	1.94	0.50
1:2F:94:LEU:HD13	2:3E:201:CPL:H131	1.94	0.50
1:1H:94:LEU:HD13	2:2G:201:CPL:H131	1.94	0.49
1:4F:94:LEU:HD13	2:5E:201:CPL:H131	1.95	0.49
1:1K:94:LEU:HD13	2:2J:201:CPL:H131	1.95	0.49
1:1L:94:LEU:HD13	2:2K:201:CPL:H131	1.95	0.49
1:2K:94:LEU:HD13	2:3J:201:CPL:H131	1.94	0.49
1:1N:94:LEU:HD13	2:2M:201:CPL:H131	1.95	0.49
1:1J:94:LEU:HD13	2:2I:201:CPL:H131	1.95	0.49
1:4E:94:LEU:HD13	2:5D:201:CPL:H131	1.95	0.49
1:3L:94:LEU:HD13	2:4K:201:CPL:H131	1.95	0.49
1:3J:94:LEU:HD13	2:4I:201:CPL:H131	1.95	0.48
1:3K:94:LEU:HD13	2:4J:201:CPL:H131	1.95	0.48
1:4G:94:LEU:HD13	2:5F:201:CPL:H131	1.95	0.48
2:1E:201:CPL:H131	1:5F:94:LEU:HD13	1.95	0.48
2:1J:201:CPL:H131	1:5K:94:LEU:HD13	1.96	0.48
1:3G:94:LEU:HD13	2:4F:201:CPL:H131	1.96	0.48
1:2E:94:LEU:HD13	2:3D:201:CPL:H131	1.95	0.48
1:3E:94:LEU:HD13	2:4D:201:CPL:H131	1.96	0.48
1:2G:94:LEU:HD13	2:3F:201:CPL:H131	1.96	0.48
1:2I:94:LEU:HD13	2:3H:201:CPL:H131	1.96	0.48
2:4H:201:CPL:H232	2:4H:201:CPL:H202	1.71	0.48
2:5F:201:CPL:H232	2:5F:201:CPL:H202	1.71	0.48
1:4M:94:LEU:HD13	2:5L:201:CPL:H131	1.96	0.48
2:3A:201:CPL:H232	2:3A:201:CPL:H202	1.71	0.47
1:1E:94:LEU:HD13	2:2D:201:CPL:H131	1.96	0.47
1:1M:94:LEU:HD13	2:2L:201:CPL:H131	1.96	0.47
1:3D:94:LEU:HD13	2:4C:201:CPL:H131	1.96	0.47
1:2H:94:LEU:HD13	2:3G:201:CPL:H131	1.97	0.47
1:3I:94:LEU:HD13	2:4H:201:CPL:H131	1.97	0.47
1:1B:94:LEU:HD13	2:2A:201:CPL:H131	1.97	0.47
1:3F:94:LEU:HD13	2:4E:201:CPL:H131	1.97	0.47
2:1A:201:CPL:H131	1:5B:94:LEU:HD13	1.97	0.47
2:1L:201:CPL:H131	1:5M:94:LEU:HD13	1.97	0.47
2:1M:201:CPL:H131	1:5N:94:LEU:HD13	1.97	0.47
1:2D:94:LEU:HD13	2:3C:201:CPL:H131	1.97	0.47
2:1F:201:CPL:H131	1:5G:94:LEU:HD13	1.97	0.46
1:2N:94:LEU:HD13	2:3M:201:CPL:H131	1.97	0.46
1:1I:94:LEU:HD13	2:2H:201:CPL:H131	1.98	0.46
1:1G:94:LEU:HD13	2:2F:201:CPL:H131	1.97	0.46
1:4N:94:LEU:HD13	2:5M:201:CPL:H131	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1D:94:LEU:HD13	2:2C:201:CPL:H131	1.98	0.46
1:3N:94:LEU:HD13	2:4M:201:CPL:H131	1.97	0.46
1:4K:94:LEU:HD13	2:5J:201:CPL:H131	1.97	0.46
2:1H:201:CPL:H131	1:5I:94:LEU:HD13	1.98	0.46
1:2B:94:LEU:HD13	2:3A:201:CPL:H131	1.97	0.46
1:4B:94:LEU:HD13	2:5A:201:CPL:H131	1.98	0.46
2:1C:201:CPL:H131	1:5D:94:LEU:HD13	1.99	0.46
1:3M:94:LEU:HD13	2:4L:201:CPL:H131	1.98	0.46
2:1B:201:CPL:H131	1:5C:94:LEU:HD13	1.99	0.45
1:4I:94:LEU:HD13	2:5H:201:CPL:H131	1.98	0.45
1:5A:78:LEU:HD13	2:5A:201:CPL:H231	1.99	0.45
2:2A:201:CPL:H39	2:2A:201:CPL:H362	1.75	0.44
1:3B:94:LEU:HD13	2:4A:201:CPL:H131	1.98	0.44
1:2M:94:LEU:HD13	2:3L:201:CPL:H131	2.00	0.44
2:3D:201:CPL:H39	2:3D:201:CPL:H362	1.75	0.44
1:4C:94:LEU:HD13	2:5B:201:CPL:H131	2.00	0.44
1:4D:94:LEU:HD13	2:5C:201:CPL:H131	2.00	0.44
1:3A:78:LEU:HD13	2:3A:201:CPL:H231	2.00	0.44
1:1C:94:LEU:HD13	2:2B:201:CPL:H131	2.00	0.43
2:1B:201:CPL:H201	2:1B:201:CPL:H171	1.86	0.43
1:4A:78:LEU:HD13	2:4A:201:CPL:H231	2.00	0.43
2:1M:201:CPL:H201	2:1M:201:CPL:H171	1.86	0.43
1:2A:78:LEU:HD13	2:2A:201:CPL:H231	2.01	0.43
2:2K:201:CPL:H201	2:2K:201:CPL:H171	1.86	0.43
1:1A:78:LEU:HD13	2:1A:201:CPL:H231	2.01	0.43
2:4G:201:CPL:H201	2:4G:201:CPL:H171	1.86	0.43
2:1M:201:CPL:HC41	2:1M:201:CPL:HC72	1.84	0.43
2:2L:201:CPL:H171	2:2L:201:CPL:H201	1.86	0.43
2:3H:201:CPL:H201	2:3H:201:CPL:H171	1.86	0.43
2:4M:201:CPL:HC41	2:4M:201:CPL:HC72	1.84	0.43
2:2A:201:CPL:H201	2:2A:201:CPL:H171	1.86	0.43
2:5E:201:CPL:H201	2:5E:201:CPL:H171	1.86	0.43
2:5E:201:CPL:H39	2:5E:201:CPL:H362	1.75	0.43
2:1C:201:CPL:H201	2:1C:201:CPL:H171	1.86	0.43
2:1N:201:CPL:H171	2:1N:201:CPL:H201	1.86	0.43
2:5H:201:CPL:HC72	2:5H:201:CPL:HC41	1.84	0.43
2:2J:201:CPL:H171	2:2J:201:CPL:H201	1.86	0.43
2:4F:201:CPL:H201	2:4F:201:CPL:H171	1.86	0.43
2:4K:201:CPL:HC72	2:4K:201:CPL:HC41	1.84	0.43
2:5D:201:CPL:H201	2:5D:201:CPL:H171	1.86	0.43
2:3I:201:CPL:H201	2:3I:201:CPL:H171	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3J:201:CPL:H171	2:3J:201:CPL:H201	1.86	0.42
2:4E:201:CPL:HC72	2:4E:201:CPL:HC41	1.84	0.42
2:2E:201:CPL:H251	2:2F:201:CPL:H372	2.01	0.42
2:4H:201:CPL:H171	2:4H:201:CPL:H201	1.86	0.42
2:5K:201:CPL:H39	2:5K:201:CPL:H362	1.75	0.42
1:2C:94:LEU:HD13	2:3B:201:CPL:H131	2.00	0.42
2:2M:201:CPL:HC72	2:2M:201:CPL:HC41	1.84	0.42
2:4I:201:CPL:HC72	2:4I:201:CPL:HC41	1.84	0.42
2:1H:201:CPL:HC41	2:1H:201:CPL:HC72	1.84	0.42
2:2D:201:CPL:HC72	2:2D:201:CPL:HC41	1.84	0.42
2:3N:201:CPL:HC72	2:3N:201:CPL:HC41	1.84	0.42
2:4L:201:CPL:HC41	2:4L:201:CPL:HC72	1.84	0.42
2:1A:201:CPL:H171	2:1A:201:CPL:H201	1.86	0.42
2:4A:201:CPL:HC41	2:4A:201:CPL:HC72	1.84	0.42
2:1E:201:CPL:H251	2:1F:201:CPL:H372	2.02	0.42
2:1E:201:CPL:HC72	2:1E:201:CPL:HC41	1.84	0.42
2:2I:201:CPL:HC72	2:2I:201:CPL:HC41	1.84	0.42
2:3A:201:CPL:HC72	2:3A:201:CPL:HC41	1.84	0.42
2:4E:201:CPL:H171	2:4E:201:CPL:H201	1.86	0.42
2:5N:201:CPL:H171	2:5N:201:CPL:H201	1.86	0.42
2:2J:201:CPL:HC41	2:2J:201:CPL:HC72	1.84	0.42
2:3I:201:CPL:H39	2:3I:201:CPL:H362	1.75	0.42
2:5C:201:CPL:H171	2:5C:201:CPL:H201	1.86	0.42
2:1G:201:CPL:HC72	2:1G:201:CPL:HC41	1.84	0.42
2:1L:201:CPL:H171	2:1L:201:CPL:H201	1.86	0.42
1:3C:94:LEU:HD13	2:4B:201:CPL:H131	2.02	0.41
2:5I:201:CPL:H251	2:5J:201:CPL:H372	2.02	0.41
2:5F:201:CPL:H171	2:5F:201:CPL:H201	1.86	0.41
2:1I:201:CPL:H39	2:1I:201:CPL:H362	1.75	0.41
2:2B:201:CPL:H171	2:2B:201:CPL:H201	1.86	0.41
2:2K:201:CPL:H39	2:2K:201:CPL:H362	1.75	0.41
2:3C:201:CPL:HC72	2:3C:201:CPL:HC41	1.84	0.41
2:5M:201:CPL:HC72	2:5M:201:CPL:HC41	1.84	0.41
2:2M:201:CPL:H171	2:2M:201:CPL:H201	1.86	0.41
2:3G:201:CPL:H171	2:3G:201:CPL:H201	1.86	0.41
2:4B:201:CPL:H39	2:4B:201:CPL:H362	1.75	0.41
2:4H:201:CPL:HC41	2:4H:201:CPL:HC72	1.84	0.41
2:1D:201:CPL:H171	2:1D:201:CPL:H201	1.86	0.41
2:2G:201:CPL:H39	2:2G:201:CPL:H362	1.75	0.41
2:4G:201:CPL:HC41	2:4G:201:CPL:HC72	1.84	0.41
2:5F:201:CPL:HC72	2:5F:201:CPL:HC41	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:201:CPL:HC72	2:2B:201:CPL:HC41	1.84	0.41
2:3I:201:CPL:HC72	2:3I:201:CPL:HC41	1.84	0.41
2:5D:201:CPL:H39	2:5D:201:CPL:H362	1.75	0.41
2:3I:201:CPL:H251	2:3J:201:CPL:H372	2.02	0.41
2:1K:201:CPL:H171	2:1K:201:CPL:H201	1.86	0.41
2:1N:201:CPL:HC72	2:1N:201:CPL:HC41	1.84	0.41
2:3E:201:CPL:H39	2:3E:201:CPL:H362	1.75	0.41
2:3J:201:CPL:HC72	2:3J:201:CPL:HC41	1.84	0.41
2:3K:201:CPL:H171	2:3K:201:CPL:H201	1.86	0.41
2:4C:201:CPL:HC41	2:4C:201:CPL:HC72	1.84	0.41
2:5E:201:CPL:H251	2:5F:201:CPL:H372	2.02	0.41
2:5J:201:CPL:HC72	2:5J:201:CPL:HC41	1.84	0.41
2:1K:201:CPL:H251	2:1L:201:CPL:H372	2.02	0.40
2:2G:201:CPL:H201	2:2G:201:CPL:H171	1.86	0.40
2:5B:201:CPL:H171	2:5B:201:CPL:H201	1.86	0.40
2:5D:201:CPL:HC41	2:5D:201:CPL:HC72	1.84	0.40
2:5K:201:CPL:H251	2:5L:201:CPL:H372	2.02	0.40
2:2I:201:CPL:H171	2:2I:201:CPL:H201	1.86	0.40
2:3E:201:CPL:H251	2:3F:201:CPL:H372	2.02	0.40
2:3M:201:CPL:H251	2:3N:201:CPL:H372	2.04	0.40
2:5B:201:CPL:HC41	2:5B:201:CPL:HC72	1.84	0.40
2:5I:201:CPL:HC41	2:5I:201:CPL:HC72	1.84	0.40
2:1M:201:CPL:H39	2:1M:201:CPL:H362	1.75	0.40
1:2H:78:LEU:HD13	2:2H:201:CPL:H231	2.04	0.40
2:4C:201:CPL:H39	2:4C:201:CPL:H362	1.75	0.40
2:5M:201:CPL:H171	2:5M:201:CPL:H201	1.86	0.40
2:2H:201:CPL:HC41	2:2H:201:CPL:HC72	1.84	0.40
2:3K:201:CPL:H251	2:3L:201:CPL:H372	2.04	0.40
2:4M:201:CPL:H39	2:4M:201:CPL:H362	1.75	0.40
2:5L:201:CPL:H39	2:5L:201:CPL:H362	1.75	0.40
1:1H:78:LEU:HD13	2:1H:201:CPL:H231	2.04	0.40
2:3H:201:CPL:H39	2:3H:201:CPL:H362	1.75	0.40
2:5A:201:CPL:H39	2:5A:201:CPL:H362	1.75	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	1A	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	1B	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	1C	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	1D	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	1E	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	1F	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	1G	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	1H	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	1I	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	1J	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	1K	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	1L	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	1M	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	1N	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	2A	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	2B	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	2C	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	2D	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	2E	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	2F	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	2G	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	2H	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	2I	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	2J	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	2K	68/121 (56%)	67 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2L	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	2M	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	2N	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	3A	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	3B	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	3C	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	3D	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	3E	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	3F	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	3G	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	3H	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	3I	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	3J	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	3K	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	3L	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	3M	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	3N	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	4A	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	4B	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	4C	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	4D	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	4E	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	4F	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	4G	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	4H	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	4I	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	4J	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	4K	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	4L	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	4M	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	4N	68/121 (56%)	67 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5A	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	5B	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	5C	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	5D	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	5E	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	5F	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	5G	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	5H	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	5I	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	5J	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	5K	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	5L	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	5M	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
1	5N	68/121 (56%)	67 (98%)	1 (2%)	0	100	100
All	All	4760/8470 (56%)	4690 (98%)	70 (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	1A	48/87 (55%)	48 (100%)	0	100	100
1	1B	48/87 (55%)	48 (100%)	0	100	100
1	1C	48/87 (55%)	48 (100%)	0	100	100
1	1D	48/87 (55%)	48 (100%)	0	100	100
1	1E	48/87 (55%)	48 (100%)	0	100	100
1	1F	48/87 (55%)	48 (100%)	0	100	100
1	1G	48/87 (55%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1H	48/87 (55%)	48 (100%)	0	100	100
1	1I	48/87 (55%)	48 (100%)	0	100	100
1	1J	48/87 (55%)	48 (100%)	0	100	100
1	1K	48/87 (55%)	48 (100%)	0	100	100
1	1L	48/87 (55%)	48 (100%)	0	100	100
1	1M	48/87 (55%)	48 (100%)	0	100	100
1	1N	48/87 (55%)	48 (100%)	0	100	100
1	2A	48/87 (55%)	48 (100%)	0	100	100
1	2B	48/87 (55%)	48 (100%)	0	100	100
1	2C	48/87 (55%)	48 (100%)	0	100	100
1	2D	48/87 (55%)	48 (100%)	0	100	100
1	2E	48/87 (55%)	48 (100%)	0	100	100
1	2F	48/87 (55%)	48 (100%)	0	100	100
1	2G	48/87 (55%)	48 (100%)	0	100	100
1	2H	48/87 (55%)	48 (100%)	0	100	100
1	2I	48/87 (55%)	48 (100%)	0	100	100
1	2J	48/87 (55%)	48 (100%)	0	100	100
1	2K	48/87 (55%)	48 (100%)	0	100	100
1	2L	48/87 (55%)	48 (100%)	0	100	100
1	2M	48/87 (55%)	48 (100%)	0	100	100
1	2N	48/87 (55%)	48 (100%)	0	100	100
1	3A	48/87 (55%)	48 (100%)	0	100	100
1	3B	48/87 (55%)	48 (100%)	0	100	100
1	3C	48/87 (55%)	48 (100%)	0	100	100
1	3D	48/87 (55%)	48 (100%)	0	100	100
1	3E	48/87 (55%)	48 (100%)	0	100	100
1	3F	48/87 (55%)	48 (100%)	0	100	100
1	3G	48/87 (55%)	48 (100%)	0	100	100
1	3H	48/87 (55%)	48 (100%)	0	100	100
1	3I	48/87 (55%)	48 (100%)	0	100	100
1	3J	48/87 (55%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3K	48/87 (55%)	48 (100%)	0	100	100
1	3L	48/87 (55%)	48 (100%)	0	100	100
1	3M	48/87 (55%)	48 (100%)	0	100	100
1	3N	48/87 (55%)	48 (100%)	0	100	100
1	4A	48/87 (55%)	48 (100%)	0	100	100
1	4B	48/87 (55%)	48 (100%)	0	100	100
1	4C	48/87 (55%)	48 (100%)	0	100	100
1	4D	48/87 (55%)	48 (100%)	0	100	100
1	4E	48/87 (55%)	48 (100%)	0	100	100
1	4F	48/87 (55%)	48 (100%)	0	100	100
1	4G	48/87 (55%)	48 (100%)	0	100	100
1	4H	48/87 (55%)	48 (100%)	0	100	100
1	4I	48/87 (55%)	48 (100%)	0	100	100
1	4J	48/87 (55%)	48 (100%)	0	100	100
1	4K	48/87 (55%)	48 (100%)	0	100	100
1	4L	48/87 (55%)	48 (100%)	0	100	100
1	4M	48/87 (55%)	48 (100%)	0	100	100
1	4N	48/87 (55%)	48 (100%)	0	100	100
1	5A	48/87 (55%)	48 (100%)	0	100	100
1	5B	48/87 (55%)	48 (100%)	0	100	100
1	5C	48/87 (55%)	48 (100%)	0	100	100
1	5D	48/87 (55%)	48 (100%)	0	100	100
1	5E	48/87 (55%)	48 (100%)	0	100	100
1	5F	48/87 (55%)	48 (100%)	0	100	100
1	5G	48/87 (55%)	48 (100%)	0	100	100
1	5H	48/87 (55%)	48 (100%)	0	100	100
1	5I	48/87 (55%)	48 (100%)	0	100	100
1	5J	48/87 (55%)	48 (100%)	0	100	100
1	5K	48/87 (55%)	48 (100%)	0	100	100
1	5L	48/87 (55%)	48 (100%)	0	100	100
1	5M	48/87 (55%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5N	48/87 (55%)	48 (100%)	0	100	100
All	All	3360/6090 (55%)	3360 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

70 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CPL	1C	201	-	51,51,51	1.12	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	1J	201	-	51,51,51	1.12	3 (5%)	57,59,59	1.11	4 (7%)
2	CPL	2G	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	3G	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	4M	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.11	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CPL	4C	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	4E	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	1D	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	3A	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	5E	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	4A	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	3H	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	2C	201	-	51,51,51	1.12	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	2M	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.11	4 (7%)
2	CPL	2K	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	5B	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	5K	201	-	51,51,51	1.12	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	1G	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	5N	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	1N	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	3D	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.11	4 (7%)
2	CPL	1L	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	3L	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	4F	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	1A	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	4I	201	-	51,51,51	1.12	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	5J	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	1K	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	3E	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.11	4 (7%)
2	CPL	2I	201	-	51,51,51	1.12	3 (5%)	57,59,59	1.11	4 (7%)
2	CPL	1F	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.11	4 (7%)
2	CPL	5H	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	2J	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	3I	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	3N	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	5I	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	2N	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.11	4 (7%)
2	CPL	1H	201	-	51,51,51	1.12	3 (5%)	57,59,59	1.11	4 (7%)
2	CPL	4J	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	1I	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.11	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CPL	3K	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	3B	201	-	51,51,51	1.12	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	3J	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	5D	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	2H	201	-	51,51,51	1.12	3 (5%)	57,59,59	1.11	4 (7%)
2	CPL	4H	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.11	4 (7%)
2	CPL	4G	201	-	51,51,51	1.12	3 (5%)	57,59,59	1.11	4 (7%)
2	CPL	2B	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	3M	201	-	51,51,51	1.12	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	5M	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	2D	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	2A	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	1E	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	2L	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	3C	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	4D	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	4L	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.11	4 (7%)
2	CPL	4B	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.11	4 (7%)
2	CPL	5G	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.11	4 (7%)
2	CPL	5L	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	1M	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	4K	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	5C	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	4N	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	5A	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	2F	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	2E	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	5F	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	3F	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.10	4 (7%)
2	CPL	1B	201	-	51,51,51	1.12	3 (5%)	57,59,59	1.10	4 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPL	1C	201	-	-	29/55/55/55	-
2	CPL	1J	201	-	-	29/55/55/55	-
2	CPL	2G	201	-	-	28/55/55/55	-
2	CPL	3G	201	-	-	29/55/55/55	-
2	CPL	4M	201	-	-	29/55/55/55	-
2	CPL	4C	201	-	-	29/55/55/55	-
2	CPL	4E	201	-	-	29/55/55/55	-
2	CPL	1D	201	-	-	29/55/55/55	-
2	CPL	3A	201	-	-	29/55/55/55	-
2	CPL	5E	201	-	-	29/55/55/55	-
2	CPL	4A	201	-	-	28/55/55/55	-
2	CPL	3H	201	-	-	29/55/55/55	-
2	CPL	2C	201	-	-	29/55/55/55	-
2	CPL	2M	201	-	-	29/55/55/55	-
2	CPL	2K	201	-	-	28/55/55/55	-
2	CPL	5B	201	-	-	28/55/55/55	-
2	CPL	5K	201	-	-	29/55/55/55	-
2	CPL	1G	201	-	-	29/55/55/55	-
2	CPL	5N	201	-	-	29/55/55/55	-
2	CPL	1N	201	-	-	29/55/55/55	-
2	CPL	3D	201	-	-	29/55/55/55	-
2	CPL	1L	201	-	-	29/55/55/55	-
2	CPL	3L	201	-	-	29/55/55/55	-
2	CPL	4F	201	-	-	29/55/55/55	-
2	CPL	1A	201	-	-	29/55/55/55	-
2	CPL	4I	201	-	-	29/55/55/55	-
2	CPL	5J	201	-	-	29/55/55/55	-
2	CPL	1K	201	-	-	28/55/55/55	-
2	CPL	3E	201	-	-	29/55/55/55	-
2	CPL	2I	201	-	-	29/55/55/55	-
2	CPL	1F	201	-	-	28/55/55/55	-
2	CPL	5H	201	-	-	29/55/55/55	-
2	CPL	2J	201	-	-	29/55/55/55	-
2	CPL	3I	201	-	-	29/55/55/55	-
2	CPL	3N	201	-	-	29/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPL	5I	201	-	-	28/55/55/55	-
2	CPL	2N	201	-	-	29/55/55/55	-
2	CPL	1H	201	-	-	29/55/55/55	-
2	CPL	4J	201	-	-	29/55/55/55	-
2	CPL	1I	201	-	-	28/55/55/55	-
2	CPL	3K	201	-	-	29/55/55/55	-
2	CPL	3B	201	-	-	29/55/55/55	-
2	CPL	3J	201	-	-	29/55/55/55	-
2	CPL	5D	201	-	-	28/55/55/55	-
2	CPL	2H	201	-	-	29/55/55/55	-
2	CPL	4H	201	-	-	29/55/55/55	-
2	CPL	4G	201	-	-	29/55/55/55	-
2	CPL	2B	201	-	-	29/55/55/55	-
2	CPL	3M	201	-	-	29/55/55/55	-
2	CPL	5M	201	-	-	28/55/55/55	-
2	CPL	2D	201	-	-	29/55/55/55	-
2	CPL	2A	201	-	-	29/55/55/55	-
2	CPL	1E	201	-	-	29/55/55/55	-
2	CPL	2L	201	-	-	29/55/55/55	-
2	CPL	3C	201	-	-	29/55/55/55	-
2	CPL	4D	201	-	-	29/55/55/55	-
2	CPL	4L	201	-	-	28/55/55/55	-
2	CPL	4B	201	-	-	29/55/55/55	-
2	CPL	5G	201	-	-	29/55/55/55	-
2	CPL	5L	201	-	-	29/55/55/55	-
2	CPL	1M	201	-	-	29/55/55/55	-
2	CPL	4K	201	-	-	28/55/55/55	-
2	CPL	5C	201	-	-	28/55/55/55	-
2	CPL	4N	201	-	-	29/55/55/55	-
2	CPL	5A	201	-	-	28/55/55/55	-
2	CPL	2F	201	-	-	29/55/55/55	-
2	CPL	2E	201	-	-	29/55/55/55	-
2	CPL	5F	201	-	-	28/55/55/55	-
2	CPL	3F	201	-	-	29/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPL	1B	201	-	-	29/55/55/55	-

All (210) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3A	201	CPL	O3-C11	3.27	1.42	1.33
2	5F	201	CPL	O3-C11	3.27	1.42	1.33
2	1M	201	CPL	O3-C11	3.26	1.42	1.33
2	5G	201	CPL	O3-C11	3.25	1.42	1.33
2	1A	201	CPL	O3-C11	3.25	1.42	1.33
2	4D	201	CPL	O3-C11	3.25	1.42	1.33
2	5N	201	CPL	O3-C11	3.25	1.42	1.33
2	1I	201	CPL	O3-C11	3.25	1.42	1.33
2	2D	201	CPL	O3-C11	3.25	1.42	1.33
2	5B	201	CPL	O3-C11	3.25	1.42	1.33
2	5C	201	CPL	O3-C11	3.25	1.42	1.33
2	2J	201	CPL	O3-C11	3.25	1.42	1.33
2	4H	201	CPL	O3-C11	3.25	1.42	1.33
2	5H	201	CPL	O3-C11	3.25	1.42	1.33
2	3K	201	CPL	O3-C11	3.25	1.42	1.33
2	3I	201	CPL	O3-C11	3.25	1.42	1.33
2	4K	201	CPL	O3-C11	3.25	1.42	1.33
2	1D	201	CPL	O3-C11	3.25	1.42	1.33
2	1L	201	CPL	O3-C11	3.24	1.42	1.33
2	5A	201	CPL	O3-C11	3.24	1.42	1.33
2	4B	201	CPL	O3-C11	3.24	1.42	1.33
2	3F	201	CPL	O3-C11	3.24	1.42	1.33
2	2B	201	CPL	O3-C11	3.24	1.42	1.33
2	4G	201	CPL	O3-C11	3.24	1.42	1.33
2	2A	201	CPL	O3-C11	3.24	1.42	1.33
2	4A	201	CPL	O3-C11	3.24	1.42	1.33
2	2M	201	CPL	O3-C11	3.24	1.42	1.33
2	4E	201	CPL	O3-C11	3.24	1.42	1.33
2	4L	201	CPL	O3-C11	3.24	1.42	1.33
2	5L	201	CPL	O3-C11	3.24	1.42	1.33
2	1F	201	CPL	O3-C11	3.24	1.42	1.33
2	1N	201	CPL	O3-C11	3.24	1.42	1.33
2	3C	201	CPL	O3-C11	3.24	1.42	1.33
2	1G	201	CPL	O3-C11	3.24	1.42	1.33
2	4C	201	CPL	O3-C11	3.24	1.42	1.33
2	2N	201	CPL	O3-C11	3.23	1.42	1.33
2	2L	201	CPL	O3-C11	3.23	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2K	201	CPL	O3-C11	3.23	1.42	1.33
2	3H	201	CPL	O3-C11	3.23	1.42	1.33
2	4N	201	CPL	O3-C11	3.23	1.42	1.33
2	4M	201	CPL	O3-C11	3.23	1.42	1.33
2	1K	201	CPL	O3-C11	3.23	1.42	1.33
2	2F	201	CPL	O3-C11	3.23	1.42	1.33
2	1E	201	CPL	O3-C11	3.23	1.42	1.33
2	3M	201	CPL	O3-C11	3.23	1.42	1.33
2	4J	201	CPL	O3-C11	3.23	1.42	1.33
2	4F	201	CPL	O3-C11	3.23	1.42	1.33
2	2G	201	CPL	O3-C11	3.23	1.42	1.33
2	3D	201	CPL	O3-C11	3.23	1.42	1.33
2	3N	201	CPL	O3-C11	3.22	1.42	1.33
2	3J	201	CPL	O3-C11	3.22	1.42	1.33
2	5D	201	CPL	O3-C11	3.22	1.42	1.33
2	1C	201	CPL	O3-C11	3.22	1.42	1.33
2	2C	201	CPL	O3-C11	3.22	1.42	1.33
2	3B	201	CPL	O3-C11	3.22	1.42	1.33
2	3L	201	CPL	O3-C11	3.22	1.42	1.33
2	5M	201	CPL	O3-C11	3.22	1.42	1.33
2	4I	201	CPL	O3-C11	3.22	1.42	1.33
2	5I	201	CPL	O3-C11	3.22	1.42	1.33
2	1B	201	CPL	O3-C11	3.22	1.42	1.33
2	1J	201	CPL	O3-C11	3.22	1.42	1.33
2	2E	201	CPL	O3-C11	3.22	1.42	1.33
2	3E	201	CPL	O3-C11	3.21	1.42	1.33
2	5J	201	CPL	O3-C11	3.21	1.42	1.33
2	5K	201	CPL	O3-C11	3.21	1.42	1.33
2	2H	201	CPL	O3-C11	3.21	1.42	1.33
2	5E	201	CPL	O3-C11	3.21	1.42	1.33
2	2I	201	CPL	O3-C11	3.21	1.42	1.33
2	1H	201	CPL	O3-C11	3.21	1.42	1.33
2	3G	201	CPL	O3-C11	3.20	1.42	1.33
2	2K	201	CPL	O2-C31	3.04	1.42	1.34
2	4L	201	CPL	O2-C31	3.03	1.42	1.34
2	4C	201	CPL	O2-C31	3.03	1.42	1.34
2	1K	201	CPL	O2-C31	3.03	1.42	1.34
2	5C	201	CPL	O2-C31	3.03	1.42	1.34
2	2I	201	CPL	O2-C31	3.03	1.42	1.34
2	1L	201	CPL	O2-C31	3.02	1.42	1.34
2	2E	201	CPL	O2-C31	3.02	1.42	1.34
2	4E	201	CPL	O2-C31	3.02	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4J	201	CPL	O2-C31	3.02	1.42	1.34
2	5I	201	CPL	O2-C31	3.02	1.42	1.34
2	5J	201	CPL	O2-C31	3.02	1.42	1.34
2	2D	201	CPL	O2-C31	3.02	1.42	1.34
2	5F	201	CPL	O2-C31	3.02	1.42	1.34
2	1F	201	CPL	O2-C31	3.02	1.42	1.34
2	2G	201	CPL	O2-C31	3.02	1.42	1.34
2	5G	201	CPL	O2-C31	3.02	1.42	1.34
2	5N	201	CPL	O2-C31	3.02	1.42	1.34
2	1G	201	CPL	O2-C31	3.02	1.42	1.34
2	3J	201	CPL	O2-C31	3.02	1.42	1.34
2	5B	201	CPL	O2-C31	3.02	1.42	1.34
2	2F	201	CPL	O2-C31	3.01	1.42	1.34
2	3F	201	CPL	O2-C31	3.01	1.42	1.34
2	3A	201	CPL	O2-C31	3.01	1.42	1.34
2	3D	201	CPL	O2-C31	3.01	1.42	1.34
2	3G	201	CPL	O2-C31	3.01	1.42	1.34
2	1E	201	CPL	O2-C31	3.01	1.42	1.34
2	4M	201	CPL	O2-C31	3.01	1.42	1.34
2	3M	201	CPL	O2-C31	3.01	1.42	1.34
2	4F	201	CPL	O2-C31	3.01	1.42	1.34
2	3N	201	CPL	O2-C31	3.01	1.42	1.34
2	1J	201	CPL	O2-C31	3.01	1.42	1.34
2	4N	201	CPL	O2-C31	3.01	1.42	1.34
2	1A	201	CPL	O2-C31	3.01	1.42	1.34
2	5E	201	CPL	O2-C31	3.01	1.42	1.34
2	1N	201	CPL	O2-C31	3.01	1.42	1.34
2	4B	201	CPL	O2-C31	3.00	1.42	1.34
2	5M	201	CPL	O2-C31	3.00	1.42	1.34
2	2C	201	CPL	O2-C31	3.00	1.42	1.34
2	2B	201	CPL	O2-C31	3.00	1.42	1.34
2	3C	201	CPL	O2-C31	3.00	1.42	1.34
2	3K	201	CPL	O2-C31	3.00	1.42	1.34
2	2M	201	CPL	O2-C31	3.00	1.42	1.34
2	1C	201	CPL	O2-C31	3.00	1.42	1.34
2	5L	201	CPL	O2-C31	3.00	1.42	1.34
2	4K	201	CPL	O2-C31	3.00	1.42	1.34
2	2A	201	CPL	O2-C31	3.00	1.42	1.34
2	4H	201	CPL	O2-C31	3.00	1.42	1.34
2	5K	201	CPL	O2-C31	3.00	1.42	1.34
2	3H	201	CPL	O2-C31	3.00	1.42	1.34
2	2N	201	CPL	O2-C31	2.99	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3E	201	CPL	O2-C31	2.99	1.42	1.34
2	1D	201	CPL	O2-C31	2.99	1.42	1.34
2	3L	201	CPL	O2-C31	2.99	1.42	1.34
2	4A	201	CPL	O2-C31	2.99	1.42	1.34
2	1H	201	CPL	O2-C31	2.99	1.42	1.34
2	2H	201	CPL	O2-C31	2.99	1.42	1.34
2	5A	201	CPL	O2-C31	2.99	1.42	1.34
2	2J	201	CPL	O2-C31	2.99	1.42	1.34
2	4D	201	CPL	O2-C31	2.99	1.42	1.34
2	5D	201	CPL	O2-C31	2.99	1.42	1.34
2	4I	201	CPL	O2-C31	2.98	1.42	1.34
2	3B	201	CPL	O2-C31	2.98	1.42	1.34
2	1I	201	CPL	O2-C31	2.98	1.42	1.34
2	2L	201	CPL	O2-C31	2.98	1.42	1.34
2	5H	201	CPL	O2-C31	2.98	1.42	1.34
2	3I	201	CPL	O2-C31	2.98	1.42	1.34
2	4G	201	CPL	O2-C31	2.97	1.42	1.34
2	1M	201	CPL	O2-C31	2.97	1.42	1.34
2	1B	201	CPL	O2-C31	2.97	1.42	1.34
2	5C	201	CPL	O2-C2	-2.34	1.40	1.46
2	2K	201	CPL	O2-C2	-2.34	1.40	1.46
2	3E	201	CPL	O2-C2	-2.34	1.40	1.46
2	2D	201	CPL	O2-C2	-2.33	1.40	1.46
2	5D	201	CPL	O2-C2	-2.33	1.40	1.46
2	2B	201	CPL	O2-C2	-2.33	1.40	1.46
2	3D	201	CPL	O2-C2	-2.32	1.40	1.46
2	2E	201	CPL	O2-C2	-2.32	1.40	1.46
2	2G	201	CPL	O2-C2	-2.32	1.40	1.46
2	3H	201	CPL	O2-C2	-2.32	1.40	1.46
2	3J	201	CPL	O2-C2	-2.32	1.40	1.46
2	5J	201	CPL	O2-C2	-2.32	1.40	1.46
2	4E	201	CPL	O2-C2	-2.32	1.40	1.46
2	5B	201	CPL	O2-C2	-2.32	1.40	1.46
2	4B	201	CPL	O2-C2	-2.31	1.40	1.46
2	3L	201	CPL	O2-C2	-2.31	1.40	1.46
2	1I	201	CPL	O2-C2	-2.31	1.40	1.46
2	5F	201	CPL	O2-C2	-2.31	1.40	1.46
2	3C	201	CPL	O2-C2	-2.31	1.40	1.46
2	5I	201	CPL	O2-C2	-2.31	1.40	1.46
2	4M	201	CPL	O2-C2	-2.31	1.40	1.46
2	3A	201	CPL	O2-C2	-2.31	1.40	1.46
2	5M	201	CPL	O2-C2	-2.31	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1H	201	CPL	O2-C2	-2.31	1.40	1.46
2	4J	201	CPL	O2-C2	-2.31	1.40	1.46
2	2F	201	CPL	O2-C2	-2.31	1.40	1.46
2	3I	201	CPL	O2-C2	-2.31	1.40	1.46
2	2N	201	CPL	O2-C2	-2.31	1.40	1.46
2	1N	201	CPL	O2-C2	-2.31	1.40	1.46
2	5E	201	CPL	O2-C2	-2.31	1.40	1.46
2	3G	201	CPL	O2-C2	-2.30	1.40	1.46
2	2L	201	CPL	O2-C2	-2.30	1.40	1.46
2	3K	201	CPL	O2-C2	-2.30	1.40	1.46
2	1E	201	CPL	O2-C2	-2.30	1.40	1.46
2	1G	201	CPL	O2-C2	-2.30	1.40	1.46
2	1L	201	CPL	O2-C2	-2.30	1.40	1.46
2	1B	201	CPL	O2-C2	-2.30	1.40	1.46
2	2I	201	CPL	O2-C2	-2.30	1.40	1.46
2	4F	201	CPL	O2-C2	-2.30	1.40	1.46
2	5N	201	CPL	O2-C2	-2.30	1.40	1.46
2	1F	201	CPL	O2-C2	-2.30	1.40	1.46
2	2J	201	CPL	O2-C2	-2.30	1.40	1.46
2	2M	201	CPL	O2-C2	-2.30	1.40	1.46
2	4L	201	CPL	O2-C2	-2.30	1.40	1.46
2	4K	201	CPL	O2-C2	-2.29	1.40	1.46
2	1M	201	CPL	O2-C2	-2.29	1.40	1.46
2	3B	201	CPL	O2-C2	-2.29	1.40	1.46
2	2A	201	CPL	O2-C2	-2.29	1.40	1.46
2	2H	201	CPL	O2-C2	-2.29	1.40	1.46
2	4H	201	CPL	O2-C2	-2.29	1.40	1.46
2	4N	201	CPL	O2-C2	-2.29	1.40	1.46
2	1C	201	CPL	O2-C2	-2.29	1.40	1.46
2	5A	201	CPL	O2-C2	-2.29	1.40	1.46
2	1J	201	CPL	O2-C2	-2.29	1.40	1.46
2	4C	201	CPL	O2-C2	-2.29	1.40	1.46
2	1K	201	CPL	O2-C2	-2.29	1.40	1.46
2	5K	201	CPL	O2-C2	-2.29	1.40	1.46
2	4A	201	CPL	O2-C2	-2.29	1.40	1.46
2	5H	201	CPL	O2-C2	-2.29	1.40	1.46
2	1A	201	CPL	O2-C2	-2.28	1.40	1.46
2	3F	201	CPL	O2-C2	-2.28	1.40	1.46
2	3N	201	CPL	O2-C2	-2.28	1.40	1.46
2	2C	201	CPL	O2-C2	-2.28	1.40	1.46
2	5G	201	CPL	O2-C2	-2.28	1.40	1.46
2	1D	201	CPL	O2-C2	-2.28	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4I	201	CPL	O2-C2	-2.27	1.40	1.46
2	4D	201	CPL	O2-C2	-2.27	1.40	1.46
2	4G	201	CPL	O2-C2	-2.27	1.40	1.46
2	5L	201	CPL	O2-C2	-2.27	1.40	1.46
2	3M	201	CPL	O2-C2	-2.26	1.40	1.46

All (280) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1J	201	CPL	O2-C31-C32	4.11	120.36	111.50
2	2N	201	CPL	O2-C31-C32	4.10	120.34	111.50
2	4G	201	CPL	O2-C31-C32	4.10	120.34	111.50
2	4M	201	CPL	O2-C31-C32	4.10	120.33	111.50
2	1I	201	CPL	O2-C31-C32	4.09	120.33	111.50
2	2M	201	CPL	O2-C31-C32	4.09	120.32	111.50
2	4H	201	CPL	O2-C31-C32	4.09	120.32	111.50
2	3H	201	CPL	O2-C31-C32	4.09	120.31	111.50
2	2H	201	CPL	O2-C31-C32	4.09	120.31	111.50
2	3D	201	CPL	O2-C31-C32	4.09	120.31	111.50
2	5B	201	CPL	O2-C31-C32	4.09	120.31	111.50
2	5A	201	CPL	O2-C31-C32	4.09	120.31	111.50
2	1F	201	CPL	O2-C31-C32	4.09	120.31	111.50
2	5I	201	CPL	O2-C31-C32	4.08	120.30	111.50
2	1H	201	CPL	O2-C31-C32	4.08	120.30	111.50
2	5M	201	CPL	O2-C31-C32	4.08	120.30	111.50
2	2J	201	CPL	O2-C31-C32	4.08	120.30	111.50
2	1D	201	CPL	O2-C31-C32	4.08	120.29	111.50
2	1C	201	CPL	O2-C31-C32	4.08	120.29	111.50
2	4B	201	CPL	O2-C31-C32	4.08	120.29	111.50
2	3B	201	CPL	O2-C31-C32	4.08	120.29	111.50
2	3E	201	CPL	O2-C31-C32	4.08	120.29	111.50
2	4I	201	CPL	O2-C31-C32	4.08	120.29	111.50
2	1B	201	CPL	O2-C31-C32	4.08	120.29	111.50
2	2E	201	CPL	O2-C31-C32	4.08	120.29	111.50
2	2I	201	CPL	O2-C31-C32	4.08	120.29	111.50
2	2K	201	CPL	O2-C31-C32	4.08	120.29	111.50
2	4E	201	CPL	O2-C31-C32	4.08	120.29	111.50
2	1A	201	CPL	O2-C31-C32	4.08	120.29	111.50
2	3G	201	CPL	O2-C31-C32	4.08	120.29	111.50
2	5H	201	CPL	O2-C31-C32	4.08	120.29	111.50
2	5L	201	CPL	O2-C31-C32	4.08	120.29	111.50
2	2L	201	CPL	O2-C31-C32	4.08	120.28	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	3A	201	CPL	O2-C31-C32	4.08	120.28	111.50
2	3I	201	CPL	O2-C31-C32	4.08	120.28	111.50
2	4C	201	CPL	O2-C31-C32	4.08	120.28	111.50
2	4L	201	CPL	O2-C31-C32	4.08	120.28	111.50
2	5N	201	CPL	O2-C31-C32	4.07	120.28	111.50
2	3J	201	CPL	O2-C31-C32	4.07	120.28	111.50
2	5K	201	CPL	O2-C31-C32	4.07	120.28	111.50
2	5G	201	CPL	O2-C31-C32	4.07	120.28	111.50
2	3M	201	CPL	O2-C31-C32	4.07	120.28	111.50
2	3L	201	CPL	O2-C31-C32	4.07	120.28	111.50
2	4D	201	CPL	O2-C31-C32	4.07	120.28	111.50
2	5D	201	CPL	O2-C31-C32	4.07	120.28	111.50
2	1N	201	CPL	O2-C31-C32	4.07	120.28	111.50
2	2B	201	CPL	O2-C31-C32	4.07	120.28	111.50
2	4A	201	CPL	O2-C31-C32	4.07	120.27	111.50
2	1M	201	CPL	O2-C31-C32	4.07	120.27	111.50
2	4J	201	CPL	O2-C31-C32	4.07	120.27	111.50
2	4K	201	CPL	O2-C31-C32	4.07	120.27	111.50
2	3C	201	CPL	O2-C31-C32	4.07	120.27	111.50
2	3K	201	CPL	O2-C31-C32	4.07	120.27	111.50
2	1G	201	CPL	O2-C31-C32	4.07	120.27	111.50
2	2A	201	CPL	O2-C31-C32	4.07	120.27	111.50
2	4F	201	CPL	O2-C31-C32	4.07	120.26	111.50
2	1L	201	CPL	O2-C31-C32	4.06	120.26	111.50
2	3F	201	CPL	O2-C31-C32	4.06	120.26	111.50
2	1E	201	CPL	O2-C31-C32	4.06	120.25	111.50
2	2G	201	CPL	O2-C31-C32	4.06	120.25	111.50
2	5J	201	CPL	O2-C31-C32	4.06	120.25	111.50
2	1K	201	CPL	O2-C31-C32	4.06	120.25	111.50
2	4N	201	CPL	O2-C31-C32	4.06	120.25	111.50
2	5E	201	CPL	O2-C31-C32	4.06	120.25	111.50
2	5F	201	CPL	O2-C31-C32	4.06	120.25	111.50
2	2C	201	CPL	O2-C31-C32	4.06	120.24	111.50
2	2D	201	CPL	O2-C31-C32	4.05	120.24	111.50
2	5C	201	CPL	O2-C31-C32	4.05	120.23	111.50
2	3N	201	CPL	O2-C31-C32	4.05	120.23	111.50
2	2F	201	CPL	O2-C31-C32	4.05	120.22	111.50
2	1C	201	CPL	C38-C39-C40	3.80	153.91	124.73
2	4I	201	CPL	C38-C39-C40	3.80	153.88	124.73
2	3F	201	CPL	C38-C39-C40	3.80	153.88	124.73
2	1J	201	CPL	C38-C39-C40	3.80	153.88	124.73
2	4M	201	CPL	C38-C39-C40	3.80	153.88	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1N	201	CPL	C38-C39-C40	3.80	153.87	124.73
2	3I	201	CPL	C38-C39-C40	3.80	153.87	124.73
2	4F	201	CPL	C38-C39-C40	3.80	153.87	124.73
2	5J	201	CPL	C38-C39-C40	3.80	153.87	124.73
2	5G	201	CPL	C38-C39-C40	3.80	153.86	124.73
2	2N	201	CPL	C38-C39-C40	3.80	153.86	124.73
2	3N	201	CPL	C38-C39-C40	3.80	153.86	124.73
2	2E	201	CPL	C38-C39-C40	3.80	153.85	124.73
2	5A	201	CPL	C38-C39-C40	3.80	153.85	124.73
2	2D	201	CPL	C38-C39-C40	3.80	153.85	124.73
2	3H	201	CPL	C38-C39-C40	3.80	153.85	124.73
2	4E	201	CPL	C38-C39-C40	3.79	153.85	124.73
2	1B	201	CPL	C38-C39-C40	3.79	153.84	124.73
2	2I	201	CPL	C38-C39-C40	3.79	153.84	124.73
2	5L	201	CPL	C38-C39-C40	3.79	153.84	124.73
2	5N	201	CPL	C38-C39-C40	3.79	153.84	124.73
2	1I	201	CPL	C38-C39-C40	3.79	153.84	124.73
2	3M	201	CPL	C38-C39-C40	3.79	153.84	124.73
2	1M	201	CPL	C38-C39-C40	3.79	153.84	124.73
2	4K	201	CPL	C38-C39-C40	3.79	153.84	124.73
2	4C	201	CPL	C38-C39-C40	3.79	153.84	124.73
2	3C	201	CPL	C38-C39-C40	3.79	153.84	124.73
2	1E	201	CPL	C38-C39-C40	3.79	153.84	124.73
2	4G	201	CPL	C38-C39-C40	3.79	153.84	124.73
2	5M	201	CPL	C38-C39-C40	3.79	153.84	124.73
2	4D	201	CPL	C38-C39-C40	3.79	153.84	124.73
2	5K	201	CPL	C38-C39-C40	3.79	153.84	124.73
2	3J	201	CPL	C38-C39-C40	3.79	153.83	124.73
2	4L	201	CPL	C38-C39-C40	3.79	153.83	124.73
2	2B	201	CPL	C38-C39-C40	3.79	153.83	124.73
2	2K	201	CPL	C38-C39-C40	3.79	153.83	124.73
2	1D	201	CPL	C38-C39-C40	3.79	153.83	124.73
2	2G	201	CPL	C38-C39-C40	3.79	153.83	124.73
2	2M	201	CPL	C38-C39-C40	3.79	153.83	124.73
2	1A	201	CPL	C38-C39-C40	3.79	153.82	124.73
2	1H	201	CPL	C38-C39-C40	3.79	153.82	124.73
2	3K	201	CPL	C38-C39-C40	3.79	153.82	124.73
2	3E	201	CPL	C38-C39-C40	3.79	153.82	124.73
2	5D	201	CPL	C38-C39-C40	3.79	153.82	124.73
2	1K	201	CPL	C38-C39-C40	3.79	153.82	124.73
2	2A	201	CPL	C38-C39-C40	3.79	153.82	124.73
2	5I	201	CPL	C38-C39-C40	3.79	153.82	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2F	201	CPL	C38-C39-C40	3.79	153.82	124.73
2	2J	201	CPL	C38-C39-C40	3.79	153.82	124.73
2	5E	201	CPL	C38-C39-C40	3.79	153.82	124.73
2	3G	201	CPL	C38-C39-C40	3.79	153.82	124.73
2	3L	201	CPL	C38-C39-C40	3.79	153.81	124.73
2	2L	201	CPL	C38-C39-C40	3.79	153.81	124.73
2	4A	201	CPL	C38-C39-C40	3.79	153.81	124.73
2	5F	201	CPL	C38-C39-C40	3.79	153.81	124.73
2	2C	201	CPL	C38-C39-C40	3.79	153.81	124.73
2	3B	201	CPL	C38-C39-C40	3.79	153.81	124.73
2	5H	201	CPL	C38-C39-C40	3.79	153.81	124.73
2	2H	201	CPL	C38-C39-C40	3.79	153.81	124.73
2	1F	201	CPL	C38-C39-C40	3.79	153.81	124.73
2	4H	201	CPL	C38-C39-C40	3.79	153.81	124.73
2	1G	201	CPL	C38-C39-C40	3.79	153.81	124.73
2	5C	201	CPL	C38-C39-C40	3.79	153.80	124.73
2	3A	201	CPL	C38-C39-C40	3.79	153.80	124.73
2	3D	201	CPL	C38-C39-C40	3.79	153.80	124.73
2	1L	201	CPL	C38-C39-C40	3.79	153.80	124.73
2	4N	201	CPL	C38-C39-C40	3.79	153.79	124.73
2	4B	201	CPL	C38-C39-C40	3.79	153.79	124.73
2	5B	201	CPL	C38-C39-C40	3.79	153.79	124.73
2	4J	201	CPL	C38-C39-C40	3.78	153.76	124.73
2	5B	201	CPL	C41-C40-C39	3.58	153.76	123.57
2	1L	201	CPL	C41-C40-C39	3.58	153.75	123.57
2	3B	201	CPL	C41-C40-C39	3.58	153.75	123.57
2	5D	201	CPL	C41-C40-C39	3.58	153.75	123.57
2	1K	201	CPL	C41-C40-C39	3.58	153.74	123.57
2	5F	201	CPL	C41-C40-C39	3.58	153.74	123.57
2	4B	201	CPL	C41-C40-C39	3.57	153.74	123.57
2	4J	201	CPL	C41-C40-C39	3.57	153.74	123.57
2	5C	201	CPL	C41-C40-C39	3.57	153.74	123.57
2	1F	201	CPL	C41-C40-C39	3.57	153.74	123.57
2	2C	201	CPL	C41-C40-C39	3.57	153.74	123.57
2	4E	201	CPL	C41-C40-C39	3.57	153.74	123.57
2	3L	201	CPL	C41-C40-C39	3.57	153.73	123.57
2	2H	201	CPL	C41-C40-C39	3.57	153.73	123.57
2	4A	201	CPL	C41-C40-C39	3.57	153.73	123.57
2	4N	201	CPL	C41-C40-C39	3.57	153.73	123.57
2	5J	201	CPL	C41-C40-C39	3.57	153.73	123.57
2	2J	201	CPL	C41-C40-C39	3.57	153.73	123.57
2	3D	201	CPL	C41-C40-C39	3.57	153.73	123.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	4G	201	CPL	C41-C40-C39	3.57	153.73	123.57
2	1G	201	CPL	C41-C40-C39	3.57	153.72	123.57
2	2G	201	CPL	C41-C40-C39	3.57	153.72	123.57
2	2M	201	CPL	C41-C40-C39	3.57	153.72	123.57
2	5H	201	CPL	C41-C40-C39	3.57	153.72	123.57
2	3A	201	CPL	C41-C40-C39	3.57	153.72	123.57
2	2E	201	CPL	C41-C40-C39	3.57	153.72	123.57
2	3I	201	CPL	C41-C40-C39	3.57	153.72	123.57
2	5L	201	CPL	C41-C40-C39	3.57	153.72	123.57
2	3H	201	CPL	C41-C40-C39	3.57	153.72	123.57
2	1D	201	CPL	C41-C40-C39	3.57	153.72	123.57
2	4L	201	CPL	C41-C40-C39	3.57	153.71	123.57
2	1I	201	CPL	C41-C40-C39	3.57	153.71	123.57
2	4H	201	CPL	C41-C40-C39	3.57	153.71	123.57
2	5M	201	CPL	C41-C40-C39	3.57	153.71	123.57
2	1A	201	CPL	C41-C40-C39	3.57	153.71	123.57
2	2F	201	CPL	C41-C40-C39	3.57	153.71	123.57
2	1H	201	CPL	C41-C40-C39	3.57	153.71	123.57
2	2A	201	CPL	C41-C40-C39	3.57	153.71	123.57
2	5G	201	CPL	C41-C40-C39	3.57	153.71	123.57
2	1M	201	CPL	C41-C40-C39	3.57	153.70	123.57
2	1B	201	CPL	C41-C40-C39	3.57	153.70	123.57
2	5N	201	CPL	C41-C40-C39	3.57	153.70	123.57
2	5E	201	CPL	C41-C40-C39	3.57	153.70	123.57
2	5K	201	CPL	C41-C40-C39	3.57	153.70	123.57
2	2I	201	CPL	C41-C40-C39	3.57	153.70	123.57
2	3G	201	CPL	C41-C40-C39	3.57	153.70	123.57
2	3M	201	CPL	C41-C40-C39	3.57	153.70	123.57
2	3C	201	CPL	C41-C40-C39	3.57	153.70	123.57
2	3N	201	CPL	C41-C40-C39	3.57	153.70	123.57
2	5I	201	CPL	C41-C40-C39	3.57	153.70	123.57
2	3J	201	CPL	C41-C40-C39	3.57	153.69	123.57
2	2K	201	CPL	C41-C40-C39	3.57	153.69	123.57
2	3E	201	CPL	C41-C40-C39	3.57	153.69	123.57
2	2B	201	CPL	C41-C40-C39	3.57	153.69	123.57
2	2L	201	CPL	C41-C40-C39	3.57	153.69	123.57
2	3K	201	CPL	C41-C40-C39	3.57	153.69	123.57
2	2D	201	CPL	C41-C40-C39	3.57	153.69	123.57
2	1N	201	CPL	C41-C40-C39	3.57	153.68	123.57
2	1E	201	CPL	C41-C40-C39	3.57	153.68	123.57
2	4F	201	CPL	C41-C40-C39	3.57	153.68	123.57
2	4D	201	CPL	C41-C40-C39	3.57	153.68	123.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	4C	201	CPL	C41-C40-C39	3.57	153.67	123.57
2	2N	201	CPL	C41-C40-C39	3.57	153.67	123.57
2	3F	201	CPL	C41-C40-C39	3.57	153.67	123.57
2	4K	201	CPL	C41-C40-C39	3.57	153.67	123.57
2	5A	201	CPL	C41-C40-C39	3.57	153.67	123.57
2	1J	201	CPL	C41-C40-C39	3.57	153.66	123.57
2	4M	201	CPL	C41-C40-C39	3.56	153.65	123.57
2	4I	201	CPL	C41-C40-C39	3.56	153.64	123.57
2	1C	201	CPL	C41-C40-C39	3.56	153.63	123.57
2	2I	201	CPL	O3-C11-C12	2.67	120.28	111.91
2	5K	201	CPL	O3-C11-C12	2.66	120.26	111.91
2	4H	201	CPL	O3-C11-C12	2.65	120.24	111.91
2	3E	201	CPL	O3-C11-C12	2.65	120.23	111.91
2	1H	201	CPL	O3-C11-C12	2.65	120.23	111.91
2	3D	201	CPL	O3-C11-C12	2.65	120.23	111.91
2	4J	201	CPL	O3-C11-C12	2.65	120.23	111.91
2	3N	201	CPL	O3-C11-C12	2.65	120.23	111.91
2	5M	201	CPL	O3-C11-C12	2.65	120.23	111.91
2	4I	201	CPL	O3-C11-C12	2.65	120.23	111.91
2	3C	201	CPL	O3-C11-C12	2.65	120.22	111.91
2	4C	201	CPL	O3-C11-C12	2.65	120.22	111.91
2	5G	201	CPL	O3-C11-C12	2.65	120.22	111.91
2	2L	201	CPL	O3-C11-C12	2.65	120.22	111.91
2	4K	201	CPL	O3-C11-C12	2.65	120.22	111.91
2	5A	201	CPL	O3-C11-C12	2.65	120.22	111.91
2	2A	201	CPL	O3-C11-C12	2.65	120.22	111.91
2	1F	201	CPL	O3-C11-C12	2.65	120.22	111.91
2	3J	201	CPL	O3-C11-C12	2.65	120.22	111.91
2	3B	201	CPL	O3-C11-C12	2.65	120.22	111.91
2	2F	201	CPL	O3-C11-C12	2.65	120.21	111.91
2	3M	201	CPL	O3-C11-C12	2.65	120.21	111.91
2	2H	201	CPL	O3-C11-C12	2.65	120.21	111.91
2	3F	201	CPL	O3-C11-C12	2.65	120.21	111.91
2	4N	201	CPL	O3-C11-C12	2.65	120.21	111.91
2	1I	201	CPL	O3-C11-C12	2.65	120.21	111.91
2	2K	201	CPL	O3-C11-C12	2.65	120.21	111.91
2	5J	201	CPL	O3-C11-C12	2.65	120.21	111.91
2	1B	201	CPL	O3-C11-C12	2.65	120.21	111.91
2	2B	201	CPL	O3-C11-C12	2.65	120.21	111.91
2	2E	201	CPL	O3-C11-C12	2.65	120.21	111.91
2	1J	201	CPL	O3-C11-C12	2.64	120.21	111.91
2	4F	201	CPL	O3-C11-C12	2.64	120.21	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	4M	201	CPL	O3-C11-C12	2.64	120.21	111.91
2	1L	201	CPL	O3-C11-C12	2.64	120.21	111.91
2	2D	201	CPL	O3-C11-C12	2.64	120.21	111.91
2	5L	201	CPL	O3-C11-C12	2.64	120.21	111.91
2	2G	201	CPL	O3-C11-C12	2.64	120.20	111.91
2	1G	201	CPL	O3-C11-C12	2.64	120.20	111.91
2	2C	201	CPL	O3-C11-C12	2.64	120.20	111.91
2	4A	201	CPL	O3-C11-C12	2.64	120.20	111.91
2	5E	201	CPL	O3-C11-C12	2.64	120.20	111.91
2	1M	201	CPL	O3-C11-C12	2.64	120.20	111.91
2	4B	201	CPL	O3-C11-C12	2.64	120.20	111.91
2	2N	201	CPL	O3-C11-C12	2.64	120.20	111.91
2	3G	201	CPL	O3-C11-C12	2.64	120.19	111.91
2	2J	201	CPL	O3-C11-C12	2.64	120.19	111.91
2	4L	201	CPL	O3-C11-C12	2.64	120.19	111.91
2	5B	201	CPL	O3-C11-C12	2.64	120.19	111.91
2	5F	201	CPL	O3-C11-C12	2.64	120.19	111.91
2	1N	201	CPL	O3-C11-C12	2.64	120.19	111.91
2	1D	201	CPL	O3-C11-C12	2.64	120.19	111.91
2	1E	201	CPL	O3-C11-C12	2.64	120.18	111.91
2	4D	201	CPL	O3-C11-C12	2.64	120.18	111.91
2	4E	201	CPL	O3-C11-C12	2.64	120.18	111.91
2	5D	201	CPL	O3-C11-C12	2.64	120.18	111.91
2	3H	201	CPL	O3-C11-C12	2.64	120.18	111.91
2	1A	201	CPL	O3-C11-C12	2.64	120.18	111.91
2	3K	201	CPL	O3-C11-C12	2.64	120.18	111.91
2	5C	201	CPL	O3-C11-C12	2.64	120.18	111.91
2	1K	201	CPL	O3-C11-C12	2.64	120.18	111.91
2	4G	201	CPL	O3-C11-C12	2.63	120.17	111.91
2	2M	201	CPL	O3-C11-C12	2.63	120.17	111.91
2	5N	201	CPL	O3-C11-C12	2.63	120.17	111.91
2	5I	201	CPL	O3-C11-C12	2.63	120.17	111.91
2	1C	201	CPL	O3-C11-C12	2.63	120.16	111.91
2	3L	201	CPL	O3-C11-C12	2.63	120.16	111.91
2	3A	201	CPL	O3-C11-C12	2.63	120.16	111.91
2	3I	201	CPL	O3-C11-C12	2.63	120.15	111.91
2	5H	201	CPL	O3-C11-C12	2.63	120.15	111.91

There are no chirality outliers.

All (2015) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1A	201	CPL	O4P-C4-C5-N
2	1A	201	CPL	C32-C31-O2-C2
2	1B	201	CPL	O4P-C4-C5-N
2	1B	201	CPL	C32-C31-O2-C2
2	1C	201	CPL	O4P-C4-C5-N
2	1C	201	CPL	C32-C31-O2-C2
2	1D	201	CPL	O4P-C4-C5-N
2	1D	201	CPL	C32-C31-O2-C2
2	1E	201	CPL	O4P-C4-C5-N
2	1E	201	CPL	C32-C31-O2-C2
2	1F	201	CPL	O4P-C4-C5-N
2	1F	201	CPL	C32-C31-O2-C2
2	1G	201	CPL	O4P-C4-C5-N
2	1G	201	CPL	C32-C31-O2-C2
2	1H	201	CPL	O4P-C4-C5-N
2	1H	201	CPL	C32-C31-O2-C2
2	1I	201	CPL	O4P-C4-C5-N
2	1I	201	CPL	C32-C31-O2-C2
2	1J	201	CPL	O4P-C4-C5-N
2	1J	201	CPL	C32-C31-O2-C2
2	1K	201	CPL	O4P-C4-C5-N
2	1K	201	CPL	C32-C31-O2-C2
2	1L	201	CPL	O4P-C4-C5-N
2	1L	201	CPL	C32-C31-O2-C2
2	1M	201	CPL	O4P-C4-C5-N
2	1M	201	CPL	C32-C31-O2-C2
2	1N	201	CPL	O4P-C4-C5-N
2	1N	201	CPL	C32-C31-O2-C2
2	2A	201	CPL	O4P-C4-C5-N
2	2A	201	CPL	C32-C31-O2-C2
2	2B	201	CPL	O4P-C4-C5-N
2	2B	201	CPL	C32-C31-O2-C2
2	2C	201	CPL	O4P-C4-C5-N
2	2C	201	CPL	C32-C31-O2-C2
2	2D	201	CPL	O4P-C4-C5-N
2	2D	201	CPL	C32-C31-O2-C2
2	2E	201	CPL	O4P-C4-C5-N
2	2E	201	CPL	C32-C31-O2-C2
2	2F	201	CPL	O4P-C4-C5-N
2	2F	201	CPL	C32-C31-O2-C2
2	2G	201	CPL	O4P-C4-C5-N
2	2G	201	CPL	C32-C31-O2-C2
2	2H	201	CPL	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
2	2H	201	CPL	C32-C31-O2-C2
2	2I	201	CPL	O4P-C4-C5-N
2	2I	201	CPL	C32-C31-O2-C2
2	2J	201	CPL	O4P-C4-C5-N
2	2J	201	CPL	C32-C31-O2-C2
2	2K	201	CPL	O4P-C4-C5-N
2	2K	201	CPL	C32-C31-O2-C2
2	2L	201	CPL	O4P-C4-C5-N
2	2L	201	CPL	C32-C31-O2-C2
2	2M	201	CPL	O4P-C4-C5-N
2	2M	201	CPL	C32-C31-O2-C2
2	2N	201	CPL	O4P-C4-C5-N
2	2N	201	CPL	C32-C31-O2-C2
2	3A	201	CPL	O4P-C4-C5-N
2	3A	201	CPL	C32-C31-O2-C2
2	3B	201	CPL	O4P-C4-C5-N
2	3B	201	CPL	C32-C31-O2-C2
2	3C	201	CPL	O4P-C4-C5-N
2	3C	201	CPL	C32-C31-O2-C2
2	3D	201	CPL	O4P-C4-C5-N
2	3D	201	CPL	C32-C31-O2-C2
2	3E	201	CPL	O4P-C4-C5-N
2	3E	201	CPL	C32-C31-O2-C2
2	3F	201	CPL	O4P-C4-C5-N
2	3F	201	CPL	C32-C31-O2-C2
2	3G	201	CPL	O4P-C4-C5-N
2	3G	201	CPL	C32-C31-O2-C2
2	3H	201	CPL	O4P-C4-C5-N
2	3H	201	CPL	C32-C31-O2-C2
2	3I	201	CPL	O4P-C4-C5-N
2	3I	201	CPL	C32-C31-O2-C2
2	3J	201	CPL	O4P-C4-C5-N
2	3J	201	CPL	C32-C31-O2-C2
2	3K	201	CPL	O4P-C4-C5-N
2	3K	201	CPL	C32-C31-O2-C2
2	3L	201	CPL	O4P-C4-C5-N
2	3L	201	CPL	C32-C31-O2-C2
2	3M	201	CPL	O4P-C4-C5-N
2	3M	201	CPL	C32-C31-O2-C2
2	3N	201	CPL	O4P-C4-C5-N
2	3N	201	CPL	C32-C31-O2-C2
2	4A	201	CPL	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
2	4A	201	CPL	C32-C31-O2-C2
2	4B	201	CPL	O4P-C4-C5-N
2	4B	201	CPL	C32-C31-O2-C2
2	4C	201	CPL	O4P-C4-C5-N
2	4C	201	CPL	C32-C31-O2-C2
2	4D	201	CPL	O4P-C4-C5-N
2	4D	201	CPL	C32-C31-O2-C2
2	4E	201	CPL	O4P-C4-C5-N
2	4E	201	CPL	C32-C31-O2-C2
2	4F	201	CPL	O4P-C4-C5-N
2	4F	201	CPL	C32-C31-O2-C2
2	4G	201	CPL	O4P-C4-C5-N
2	4G	201	CPL	C32-C31-O2-C2
2	4H	201	CPL	O4P-C4-C5-N
2	4H	201	CPL	C32-C31-O2-C2
2	4I	201	CPL	O4P-C4-C5-N
2	4I	201	CPL	C32-C31-O2-C2
2	4J	201	CPL	O4P-C4-C5-N
2	4J	201	CPL	C32-C31-O2-C2
2	4K	201	CPL	O4P-C4-C5-N
2	4K	201	CPL	C32-C31-O2-C2
2	4L	201	CPL	O4P-C4-C5-N
2	4L	201	CPL	C32-C31-O2-C2
2	4M	201	CPL	O4P-C4-C5-N
2	4M	201	CPL	C32-C31-O2-C2
2	4N	201	CPL	O4P-C4-C5-N
2	4N	201	CPL	C32-C31-O2-C2
2	5A	201	CPL	O4P-C4-C5-N
2	5A	201	CPL	C32-C31-O2-C2
2	5B	201	CPL	O4P-C4-C5-N
2	5B	201	CPL	C32-C31-O2-C2
2	5C	201	CPL	O4P-C4-C5-N
2	5C	201	CPL	C32-C31-O2-C2
2	5D	201	CPL	O4P-C4-C5-N
2	5D	201	CPL	C32-C31-O2-C2
2	5E	201	CPL	O4P-C4-C5-N
2	5E	201	CPL	C32-C31-O2-C2
2	5F	201	CPL	O4P-C4-C5-N
2	5F	201	CPL	C32-C31-O2-C2
2	5G	201	CPL	O4P-C4-C5-N
2	5G	201	CPL	C32-C31-O2-C2
2	5H	201	CPL	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
2	5H	201	CPL	C32-C31-O2-C2
2	5I	201	CPL	O4P-C4-C5-N
2	5I	201	CPL	C32-C31-O2-C2
2	5J	201	CPL	O4P-C4-C5-N
2	5J	201	CPL	C32-C31-O2-C2
2	5K	201	CPL	O4P-C4-C5-N
2	5K	201	CPL	C32-C31-O2-C2
2	5L	201	CPL	O4P-C4-C5-N
2	5L	201	CPL	C32-C31-O2-C2
2	5M	201	CPL	O4P-C4-C5-N
2	5M	201	CPL	C32-C31-O2-C2
2	5N	201	CPL	O4P-C4-C5-N
2	5N	201	CPL	C32-C31-O2-C2
2	1A	201	CPL	O31-C31-O2-C2
2	1B	201	CPL	O31-C31-O2-C2
2	1C	201	CPL	O31-C31-O2-C2
2	1D	201	CPL	O31-C31-O2-C2
2	1E	201	CPL	O31-C31-O2-C2
2	1F	201	CPL	O31-C31-O2-C2
2	1G	201	CPL	O31-C31-O2-C2
2	1H	201	CPL	O31-C31-O2-C2
2	1I	201	CPL	O31-C31-O2-C2
2	1J	201	CPL	O31-C31-O2-C2
2	1K	201	CPL	O31-C31-O2-C2
2	1L	201	CPL	O31-C31-O2-C2
2	1M	201	CPL	O31-C31-O2-C2
2	1N	201	CPL	O31-C31-O2-C2
2	2A	201	CPL	O31-C31-O2-C2
2	2B	201	CPL	O31-C31-O2-C2
2	2C	201	CPL	O31-C31-O2-C2
2	2D	201	CPL	O31-C31-O2-C2
2	2E	201	CPL	O31-C31-O2-C2
2	2F	201	CPL	O31-C31-O2-C2
2	2G	201	CPL	O31-C31-O2-C2
2	2H	201	CPL	O31-C31-O2-C2
2	2I	201	CPL	O31-C31-O2-C2
2	2J	201	CPL	O31-C31-O2-C2
2	2K	201	CPL	O31-C31-O2-C2
2	2L	201	CPL	O31-C31-O2-C2
2	2M	201	CPL	O31-C31-O2-C2
2	2N	201	CPL	O31-C31-O2-C2
2	3A	201	CPL	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
2	3B	201	CPL	O31-C31-O2-C2
2	3C	201	CPL	O31-C31-O2-C2
2	3D	201	CPL	O31-C31-O2-C2
2	3E	201	CPL	O31-C31-O2-C2
2	3F	201	CPL	O31-C31-O2-C2
2	3G	201	CPL	O31-C31-O2-C2
2	3H	201	CPL	O31-C31-O2-C2
2	3I	201	CPL	O31-C31-O2-C2
2	3J	201	CPL	O31-C31-O2-C2
2	3K	201	CPL	O31-C31-O2-C2
2	3L	201	CPL	O31-C31-O2-C2
2	3M	201	CPL	O31-C31-O2-C2
2	3N	201	CPL	O31-C31-O2-C2
2	4A	201	CPL	O31-C31-O2-C2
2	4B	201	CPL	O31-C31-O2-C2
2	4C	201	CPL	O31-C31-O2-C2
2	4D	201	CPL	O31-C31-O2-C2
2	4E	201	CPL	O31-C31-O2-C2
2	4F	201	CPL	O31-C31-O2-C2
2	4G	201	CPL	O31-C31-O2-C2
2	4H	201	CPL	O31-C31-O2-C2
2	4I	201	CPL	O31-C31-O2-C2
2	4J	201	CPL	O31-C31-O2-C2
2	4K	201	CPL	O31-C31-O2-C2
2	4L	201	CPL	O31-C31-O2-C2
2	4M	201	CPL	O31-C31-O2-C2
2	4N	201	CPL	O31-C31-O2-C2
2	5A	201	CPL	O31-C31-O2-C2
2	5B	201	CPL	O31-C31-O2-C2
2	5C	201	CPL	O31-C31-O2-C2
2	5D	201	CPL	O31-C31-O2-C2
2	5E	201	CPL	O31-C31-O2-C2
2	5F	201	CPL	O31-C31-O2-C2
2	5G	201	CPL	O31-C31-O2-C2
2	5H	201	CPL	O31-C31-O2-C2
2	5I	201	CPL	O31-C31-O2-C2
2	5J	201	CPL	O31-C31-O2-C2
2	5K	201	CPL	O31-C31-O2-C2
2	5L	201	CPL	O31-C31-O2-C2
2	5M	201	CPL	O31-C31-O2-C2
2	5N	201	CPL	O31-C31-O2-C2
2	1A	201	CPL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
2	1B	201	CPL	C20-C21-C22-C23
2	1C	201	CPL	C20-C21-C22-C23
2	1D	201	CPL	C20-C21-C22-C23
2	1E	201	CPL	C20-C21-C22-C23
2	1F	201	CPL	C20-C21-C22-C23
2	1G	201	CPL	C20-C21-C22-C23
2	1H	201	CPL	C20-C21-C22-C23
2	1I	201	CPL	C20-C21-C22-C23
2	1J	201	CPL	C20-C21-C22-C23
2	1K	201	CPL	C20-C21-C22-C23
2	1L	201	CPL	C20-C21-C22-C23
2	1M	201	CPL	C20-C21-C22-C23
2	1N	201	CPL	C20-C21-C22-C23
2	2A	201	CPL	C20-C21-C22-C23
2	2B	201	CPL	C20-C21-C22-C23
2	2C	201	CPL	C20-C21-C22-C23
2	2D	201	CPL	C20-C21-C22-C23
2	2E	201	CPL	C20-C21-C22-C23
2	2F	201	CPL	C20-C21-C22-C23
2	2G	201	CPL	C20-C21-C22-C23
2	2H	201	CPL	C20-C21-C22-C23
2	2I	201	CPL	C20-C21-C22-C23
2	2J	201	CPL	C20-C21-C22-C23
2	2K	201	CPL	C20-C21-C22-C23
2	2L	201	CPL	C20-C21-C22-C23
2	2M	201	CPL	C20-C21-C22-C23
2	2N	201	CPL	C20-C21-C22-C23
2	3A	201	CPL	C20-C21-C22-C23
2	3B	201	CPL	C20-C21-C22-C23
2	3C	201	CPL	C20-C21-C22-C23
2	3D	201	CPL	C20-C21-C22-C23
2	3E	201	CPL	C20-C21-C22-C23
2	3F	201	CPL	C20-C21-C22-C23
2	3G	201	CPL	C20-C21-C22-C23
2	3H	201	CPL	C20-C21-C22-C23
2	3I	201	CPL	C20-C21-C22-C23
2	3J	201	CPL	C20-C21-C22-C23
2	3K	201	CPL	C20-C21-C22-C23
2	3L	201	CPL	C20-C21-C22-C23
2	3M	201	CPL	C20-C21-C22-C23
2	3N	201	CPL	C20-C21-C22-C23
2	4A	201	CPL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
2	4B	201	CPL	C20-C21-C22-C23
2	4C	201	CPL	C20-C21-C22-C23
2	4D	201	CPL	C20-C21-C22-C23
2	4E	201	CPL	C20-C21-C22-C23
2	4F	201	CPL	C20-C21-C22-C23
2	4G	201	CPL	C20-C21-C22-C23
2	4H	201	CPL	C20-C21-C22-C23
2	4I	201	CPL	C20-C21-C22-C23
2	4J	201	CPL	C20-C21-C22-C23
2	4K	201	CPL	C20-C21-C22-C23
2	4L	201	CPL	C20-C21-C22-C23
2	4M	201	CPL	C20-C21-C22-C23
2	4N	201	CPL	C20-C21-C22-C23
2	5A	201	CPL	C20-C21-C22-C23
2	5B	201	CPL	C20-C21-C22-C23
2	5C	201	CPL	C20-C21-C22-C23
2	5D	201	CPL	C20-C21-C22-C23
2	5E	201	CPL	C20-C21-C22-C23
2	5F	201	CPL	C20-C21-C22-C23
2	5G	201	CPL	C20-C21-C22-C23
2	5H	201	CPL	C20-C21-C22-C23
2	5I	201	CPL	C20-C21-C22-C23
2	5J	201	CPL	C20-C21-C22-C23
2	5K	201	CPL	C20-C21-C22-C23
2	5L	201	CPL	C20-C21-C22-C23
2	5M	201	CPL	C20-C21-C22-C23
2	5N	201	CPL	C20-C21-C22-C23
2	1A	201	CPL	C34-C35-C36-C37
2	1B	201	CPL	C34-C35-C36-C37
2	1C	201	CPL	C34-C35-C36-C37
2	1D	201	CPL	C34-C35-C36-C37
2	1E	201	CPL	C34-C35-C36-C37
2	1F	201	CPL	C34-C35-C36-C37
2	1G	201	CPL	C34-C35-C36-C37
2	1H	201	CPL	C34-C35-C36-C37
2	1I	201	CPL	C34-C35-C36-C37
2	1J	201	CPL	C34-C35-C36-C37
2	1K	201	CPL	C34-C35-C36-C37
2	1L	201	CPL	C34-C35-C36-C37
2	1M	201	CPL	C34-C35-C36-C37
2	1N	201	CPL	C34-C35-C36-C37
2	2A	201	CPL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
2	2B	201	CPL	C34-C35-C36-C37
2	2C	201	CPL	C34-C35-C36-C37
2	2D	201	CPL	C34-C35-C36-C37
2	2E	201	CPL	C34-C35-C36-C37
2	2F	201	CPL	C34-C35-C36-C37
2	2G	201	CPL	C34-C35-C36-C37
2	2H	201	CPL	C34-C35-C36-C37
2	2I	201	CPL	C34-C35-C36-C37
2	2J	201	CPL	C34-C35-C36-C37
2	2K	201	CPL	C34-C35-C36-C37
2	2L	201	CPL	C34-C35-C36-C37
2	2M	201	CPL	C34-C35-C36-C37
2	2N	201	CPL	C34-C35-C36-C37
2	3A	201	CPL	C34-C35-C36-C37
2	3B	201	CPL	C34-C35-C36-C37
2	3C	201	CPL	C34-C35-C36-C37
2	3D	201	CPL	C34-C35-C36-C37
2	3E	201	CPL	C34-C35-C36-C37
2	3F	201	CPL	C34-C35-C36-C37
2	3G	201	CPL	C34-C35-C36-C37
2	3H	201	CPL	C34-C35-C36-C37
2	3I	201	CPL	C34-C35-C36-C37
2	3J	201	CPL	C34-C35-C36-C37
2	3K	201	CPL	C34-C35-C36-C37
2	3L	201	CPL	C34-C35-C36-C37
2	3M	201	CPL	C34-C35-C36-C37
2	3N	201	CPL	C34-C35-C36-C37
2	4A	201	CPL	C34-C35-C36-C37
2	4B	201	CPL	C34-C35-C36-C37
2	4C	201	CPL	C34-C35-C36-C37
2	4D	201	CPL	C34-C35-C36-C37
2	4E	201	CPL	C34-C35-C36-C37
2	4F	201	CPL	C34-C35-C36-C37
2	4G	201	CPL	C34-C35-C36-C37
2	4H	201	CPL	C34-C35-C36-C37
2	4I	201	CPL	C34-C35-C36-C37
2	4J	201	CPL	C34-C35-C36-C37
2	4K	201	CPL	C34-C35-C36-C37
2	4L	201	CPL	C34-C35-C36-C37
2	4M	201	CPL	C34-C35-C36-C37
2	4N	201	CPL	C34-C35-C36-C37
2	5A	201	CPL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
2	5B	201	CPL	C34-C35-C36-C37
2	5C	201	CPL	C34-C35-C36-C37
2	5D	201	CPL	C34-C35-C36-C37
2	5E	201	CPL	C34-C35-C36-C37
2	5F	201	CPL	C34-C35-C36-C37
2	5G	201	CPL	C34-C35-C36-C37
2	5H	201	CPL	C34-C35-C36-C37
2	5I	201	CPL	C34-C35-C36-C37
2	5J	201	CPL	C34-C35-C36-C37
2	5K	201	CPL	C34-C35-C36-C37
2	5L	201	CPL	C34-C35-C36-C37
2	5M	201	CPL	C34-C35-C36-C37
2	5N	201	CPL	C34-C35-C36-C37
2	1A	201	CPL	C11-C12-C13-C14
2	1B	201	CPL	C11-C12-C13-C14
2	1C	201	CPL	C11-C12-C13-C14
2	1D	201	CPL	C11-C12-C13-C14
2	1E	201	CPL	C11-C12-C13-C14
2	1F	201	CPL	C11-C12-C13-C14
2	1G	201	CPL	C11-C12-C13-C14
2	1H	201	CPL	C11-C12-C13-C14
2	1I	201	CPL	C11-C12-C13-C14
2	1J	201	CPL	C11-C12-C13-C14
2	1K	201	CPL	C11-C12-C13-C14
2	1L	201	CPL	C11-C12-C13-C14
2	1M	201	CPL	C11-C12-C13-C14
2	1N	201	CPL	C11-C12-C13-C14
2	2A	201	CPL	C11-C12-C13-C14
2	2B	201	CPL	C11-C12-C13-C14
2	2C	201	CPL	C11-C12-C13-C14
2	2D	201	CPL	C11-C12-C13-C14
2	2E	201	CPL	C11-C12-C13-C14
2	2F	201	CPL	C11-C12-C13-C14
2	2G	201	CPL	C11-C12-C13-C14
2	2H	201	CPL	C11-C12-C13-C14
2	2I	201	CPL	C11-C12-C13-C14
2	2J	201	CPL	C11-C12-C13-C14
2	2K	201	CPL	C11-C12-C13-C14
2	2L	201	CPL	C11-C12-C13-C14
2	2M	201	CPL	C11-C12-C13-C14
2	2N	201	CPL	C11-C12-C13-C14
2	3A	201	CPL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
2	3B	201	CPL	C11-C12-C13-C14
2	3C	201	CPL	C11-C12-C13-C14
2	3D	201	CPL	C11-C12-C13-C14
2	3E	201	CPL	C11-C12-C13-C14
2	3F	201	CPL	C11-C12-C13-C14
2	3G	201	CPL	C11-C12-C13-C14
2	3H	201	CPL	C11-C12-C13-C14
2	3I	201	CPL	C11-C12-C13-C14
2	3J	201	CPL	C11-C12-C13-C14
2	3K	201	CPL	C11-C12-C13-C14
2	3L	201	CPL	C11-C12-C13-C14
2	3M	201	CPL	C11-C12-C13-C14
2	3N	201	CPL	C11-C12-C13-C14
2	4A	201	CPL	C11-C12-C13-C14
2	4B	201	CPL	C11-C12-C13-C14
2	4C	201	CPL	C11-C12-C13-C14
2	4D	201	CPL	C11-C12-C13-C14
2	4E	201	CPL	C11-C12-C13-C14
2	4F	201	CPL	C11-C12-C13-C14
2	4G	201	CPL	C11-C12-C13-C14
2	4H	201	CPL	C11-C12-C13-C14
2	4I	201	CPL	C11-C12-C13-C14
2	4J	201	CPL	C11-C12-C13-C14
2	4K	201	CPL	C11-C12-C13-C14
2	4L	201	CPL	C11-C12-C13-C14
2	4M	201	CPL	C11-C12-C13-C14
2	4N	201	CPL	C11-C12-C13-C14
2	5A	201	CPL	C11-C12-C13-C14
2	5B	201	CPL	C11-C12-C13-C14
2	5C	201	CPL	C11-C12-C13-C14
2	5D	201	CPL	C11-C12-C13-C14
2	5E	201	CPL	C11-C12-C13-C14
2	5F	201	CPL	C11-C12-C13-C14
2	5G	201	CPL	C11-C12-C13-C14
2	5H	201	CPL	C11-C12-C13-C14
2	5I	201	CPL	C11-C12-C13-C14
2	5J	201	CPL	C11-C12-C13-C14
2	5K	201	CPL	C11-C12-C13-C14
2	5L	201	CPL	C11-C12-C13-C14
2	5M	201	CPL	C11-C12-C13-C14
2	5N	201	CPL	C11-C12-C13-C14
2	1A	201	CPL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
2	1B	201	CPL	C36-C37-C38-C39
2	1C	201	CPL	C36-C37-C38-C39
2	1D	201	CPL	C36-C37-C38-C39
2	1E	201	CPL	C36-C37-C38-C39
2	1F	201	CPL	C36-C37-C38-C39
2	1G	201	CPL	C36-C37-C38-C39
2	1H	201	CPL	C36-C37-C38-C39
2	1I	201	CPL	C36-C37-C38-C39
2	1J	201	CPL	C36-C37-C38-C39
2	1K	201	CPL	C36-C37-C38-C39
2	1L	201	CPL	C36-C37-C38-C39
2	1M	201	CPL	C36-C37-C38-C39
2	1N	201	CPL	C36-C37-C38-C39
2	2A	201	CPL	C36-C37-C38-C39
2	2B	201	CPL	C36-C37-C38-C39
2	2C	201	CPL	C36-C37-C38-C39
2	2D	201	CPL	C36-C37-C38-C39
2	2E	201	CPL	C36-C37-C38-C39
2	2F	201	CPL	C36-C37-C38-C39
2	2G	201	CPL	C36-C37-C38-C39
2	2H	201	CPL	C36-C37-C38-C39
2	2I	201	CPL	C36-C37-C38-C39
2	2J	201	CPL	C36-C37-C38-C39
2	2K	201	CPL	C36-C37-C38-C39
2	2L	201	CPL	C36-C37-C38-C39
2	2M	201	CPL	C36-C37-C38-C39
2	2N	201	CPL	C36-C37-C38-C39
2	3A	201	CPL	C36-C37-C38-C39
2	3B	201	CPL	C36-C37-C38-C39
2	3C	201	CPL	C36-C37-C38-C39
2	3D	201	CPL	C36-C37-C38-C39
2	3E	201	CPL	C36-C37-C38-C39
2	3F	201	CPL	C36-C37-C38-C39
2	3G	201	CPL	C36-C37-C38-C39
2	3H	201	CPL	C36-C37-C38-C39
2	3I	201	CPL	C36-C37-C38-C39
2	3J	201	CPL	C36-C37-C38-C39
2	3K	201	CPL	C36-C37-C38-C39
2	3L	201	CPL	C36-C37-C38-C39
2	3M	201	CPL	C36-C37-C38-C39
2	3N	201	CPL	C36-C37-C38-C39
2	4A	201	CPL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
2	4B	201	CPL	C36-C37-C38-C39
2	4C	201	CPL	C36-C37-C38-C39
2	4D	201	CPL	C36-C37-C38-C39
2	4E	201	CPL	C36-C37-C38-C39
2	4F	201	CPL	C36-C37-C38-C39
2	4G	201	CPL	C36-C37-C38-C39
2	4H	201	CPL	C36-C37-C38-C39
2	4I	201	CPL	C36-C37-C38-C39
2	4J	201	CPL	C36-C37-C38-C39
2	4K	201	CPL	C36-C37-C38-C39
2	4L	201	CPL	C36-C37-C38-C39
2	4M	201	CPL	C36-C37-C38-C39
2	4N	201	CPL	C36-C37-C38-C39
2	5A	201	CPL	C36-C37-C38-C39
2	5B	201	CPL	C36-C37-C38-C39
2	5C	201	CPL	C36-C37-C38-C39
2	5D	201	CPL	C36-C37-C38-C39
2	5E	201	CPL	C36-C37-C38-C39
2	5F	201	CPL	C36-C37-C38-C39
2	5G	201	CPL	C36-C37-C38-C39
2	5H	201	CPL	C36-C37-C38-C39
2	5I	201	CPL	C36-C37-C38-C39
2	5J	201	CPL	C36-C37-C38-C39
2	5K	201	CPL	C36-C37-C38-C39
2	5L	201	CPL	C36-C37-C38-C39
2	5M	201	CPL	C36-C37-C38-C39
2	5N	201	CPL	C36-C37-C38-C39
2	1A	201	CPL	C4-O4P-P-O3P
2	1B	201	CPL	C4-O4P-P-O3P
2	1C	201	CPL	C4-O4P-P-O3P
2	1D	201	CPL	C4-O4P-P-O3P
2	1E	201	CPL	C4-O4P-P-O3P
2	1F	201	CPL	C4-O4P-P-O3P
2	1G	201	CPL	C4-O4P-P-O3P
2	1H	201	CPL	C4-O4P-P-O3P
2	1I	201	CPL	C4-O4P-P-O3P
2	1J	201	CPL	C4-O4P-P-O3P
2	1K	201	CPL	C4-O4P-P-O3P
2	1L	201	CPL	C4-O4P-P-O3P
2	1M	201	CPL	C4-O4P-P-O3P
2	1N	201	CPL	C4-O4P-P-O3P
2	2A	201	CPL	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
2	2B	201	CPL	C4-O4P-P-O3P
2	2C	201	CPL	C4-O4P-P-O3P
2	2D	201	CPL	C4-O4P-P-O3P
2	2E	201	CPL	C4-O4P-P-O3P
2	2F	201	CPL	C4-O4P-P-O3P
2	2G	201	CPL	C4-O4P-P-O3P
2	2H	201	CPL	C4-O4P-P-O3P
2	2I	201	CPL	C4-O4P-P-O3P
2	2J	201	CPL	C4-O4P-P-O3P
2	2K	201	CPL	C4-O4P-P-O3P
2	2L	201	CPL	C4-O4P-P-O3P
2	2M	201	CPL	C4-O4P-P-O3P
2	2N	201	CPL	C4-O4P-P-O3P
2	3A	201	CPL	C4-O4P-P-O3P
2	3B	201	CPL	C4-O4P-P-O3P
2	3C	201	CPL	C4-O4P-P-O3P
2	3D	201	CPL	C4-O4P-P-O3P
2	3E	201	CPL	C4-O4P-P-O3P
2	3F	201	CPL	C4-O4P-P-O3P
2	3G	201	CPL	C4-O4P-P-O3P
2	3H	201	CPL	C4-O4P-P-O3P
2	3I	201	CPL	C4-O4P-P-O3P
2	3J	201	CPL	C4-O4P-P-O3P
2	3K	201	CPL	C4-O4P-P-O3P
2	3L	201	CPL	C4-O4P-P-O3P
2	3M	201	CPL	C4-O4P-P-O3P
2	3N	201	CPL	C4-O4P-P-O3P
2	4A	201	CPL	C4-O4P-P-O3P
2	4B	201	CPL	C4-O4P-P-O3P
2	4C	201	CPL	C4-O4P-P-O3P
2	4D	201	CPL	C4-O4P-P-O3P
2	4E	201	CPL	C4-O4P-P-O3P
2	4F	201	CPL	C4-O4P-P-O3P
2	4G	201	CPL	C4-O4P-P-O3P
2	4H	201	CPL	C4-O4P-P-O3P
2	4I	201	CPL	C4-O4P-P-O3P
2	4J	201	CPL	C4-O4P-P-O3P
2	4K	201	CPL	C4-O4P-P-O3P
2	4L	201	CPL	C4-O4P-P-O3P
2	4M	201	CPL	C4-O4P-P-O3P
2	4N	201	CPL	C4-O4P-P-O3P
2	5A	201	CPL	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
2	5B	201	CPL	C4-O4P-P-O3P
2	5C	201	CPL	C4-O4P-P-O3P
2	5D	201	CPL	C4-O4P-P-O3P
2	5E	201	CPL	C4-O4P-P-O3P
2	5F	201	CPL	C4-O4P-P-O3P
2	5G	201	CPL	C4-O4P-P-O3P
2	5H	201	CPL	C4-O4P-P-O3P
2	5I	201	CPL	C4-O4P-P-O3P
2	5J	201	CPL	C4-O4P-P-O3P
2	5K	201	CPL	C4-O4P-P-O3P
2	5L	201	CPL	C4-O4P-P-O3P
2	5M	201	CPL	C4-O4P-P-O3P
2	5N	201	CPL	C4-O4P-P-O3P
2	1A	201	CPL	C13-C14-C15-C16
2	1B	201	CPL	C13-C14-C15-C16
2	1C	201	CPL	C13-C14-C15-C16
2	1D	201	CPL	C13-C14-C15-C16
2	1E	201	CPL	C13-C14-C15-C16
2	1F	201	CPL	C13-C14-C15-C16
2	1G	201	CPL	C13-C14-C15-C16
2	1H	201	CPL	C13-C14-C15-C16
2	1I	201	CPL	C13-C14-C15-C16
2	1K	201	CPL	C13-C14-C15-C16
2	1L	201	CPL	C13-C14-C15-C16
2	1M	201	CPL	C13-C14-C15-C16
2	1N	201	CPL	C13-C14-C15-C16
2	2A	201	CPL	C13-C14-C15-C16
2	2B	201	CPL	C13-C14-C15-C16
2	2C	201	CPL	C13-C14-C15-C16
2	2E	201	CPL	C13-C14-C15-C16
2	2F	201	CPL	C13-C14-C15-C16
2	2G	201	CPL	C13-C14-C15-C16
2	2H	201	CPL	C13-C14-C15-C16
2	2I	201	CPL	C13-C14-C15-C16
2	2J	201	CPL	C13-C14-C15-C16
2	2K	201	CPL	C13-C14-C15-C16
2	2M	201	CPL	C13-C14-C15-C16
2	2N	201	CPL	C13-C14-C15-C16
2	3A	201	CPL	C13-C14-C15-C16
2	3B	201	CPL	C13-C14-C15-C16
2	3C	201	CPL	C13-C14-C15-C16
2	3D	201	CPL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
2	3E	201	CPL	C13-C14-C15-C16
2	3F	201	CPL	C13-C14-C15-C16
2	3G	201	CPL	C13-C14-C15-C16
2	3H	201	CPL	C13-C14-C15-C16
2	3I	201	CPL	C13-C14-C15-C16
2	3J	201	CPL	C13-C14-C15-C16
2	3K	201	CPL	C13-C14-C15-C16
2	3L	201	CPL	C13-C14-C15-C16
2	3M	201	CPL	C13-C14-C15-C16
2	3N	201	CPL	C13-C14-C15-C16
2	4A	201	CPL	C13-C14-C15-C16
2	4B	201	CPL	C13-C14-C15-C16
2	4C	201	CPL	C13-C14-C15-C16
2	4D	201	CPL	C13-C14-C15-C16
2	4E	201	CPL	C13-C14-C15-C16
2	4F	201	CPL	C13-C14-C15-C16
2	4G	201	CPL	C13-C14-C15-C16
2	4H	201	CPL	C13-C14-C15-C16
2	4I	201	CPL	C13-C14-C15-C16
2	4J	201	CPL	C13-C14-C15-C16
2	4L	201	CPL	C13-C14-C15-C16
2	4M	201	CPL	C13-C14-C15-C16
2	4N	201	CPL	C13-C14-C15-C16
2	5A	201	CPL	C13-C14-C15-C16
2	5B	201	CPL	C13-C14-C15-C16
2	5C	201	CPL	C13-C14-C15-C16
2	5D	201	CPL	C13-C14-C15-C16
2	5E	201	CPL	C13-C14-C15-C16
2	5F	201	CPL	C13-C14-C15-C16
2	5G	201	CPL	C13-C14-C15-C16
2	5H	201	CPL	C13-C14-C15-C16
2	5I	201	CPL	C13-C14-C15-C16
2	5J	201	CPL	C13-C14-C15-C16
2	5K	201	CPL	C13-C14-C15-C16
2	5L	201	CPL	C13-C14-C15-C16
2	5M	201	CPL	C13-C14-C15-C16
2	5N	201	CPL	C13-C14-C15-C16
2	1J	201	CPL	C13-C14-C15-C16
2	2D	201	CPL	C13-C14-C15-C16
2	2L	201	CPL	C13-C14-C15-C16
2	4K	201	CPL	C13-C14-C15-C16
2	1A	201	CPL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
2	1B	201	CPL	C35-C36-C37-C38
2	1C	201	CPL	C35-C36-C37-C38
2	1D	201	CPL	C35-C36-C37-C38
2	1E	201	CPL	C35-C36-C37-C38
2	1F	201	CPL	C35-C36-C37-C38
2	1G	201	CPL	C35-C36-C37-C38
2	1H	201	CPL	C35-C36-C37-C38
2	1I	201	CPL	C35-C36-C37-C38
2	1J	201	CPL	C35-C36-C37-C38
2	1K	201	CPL	C35-C36-C37-C38
2	1L	201	CPL	C35-C36-C37-C38
2	1M	201	CPL	C35-C36-C37-C38
2	1N	201	CPL	C35-C36-C37-C38
2	2A	201	CPL	C35-C36-C37-C38
2	2B	201	CPL	C35-C36-C37-C38
2	2C	201	CPL	C35-C36-C37-C38
2	2D	201	CPL	C35-C36-C37-C38
2	2E	201	CPL	C35-C36-C37-C38
2	2F	201	CPL	C35-C36-C37-C38
2	2G	201	CPL	C35-C36-C37-C38
2	2H	201	CPL	C35-C36-C37-C38
2	2I	201	CPL	C35-C36-C37-C38
2	2J	201	CPL	C35-C36-C37-C38
2	2K	201	CPL	C35-C36-C37-C38
2	2L	201	CPL	C35-C36-C37-C38
2	2M	201	CPL	C35-C36-C37-C38
2	2N	201	CPL	C35-C36-C37-C38
2	3A	201	CPL	C35-C36-C37-C38
2	3B	201	CPL	C35-C36-C37-C38
2	3C	201	CPL	C35-C36-C37-C38
2	3D	201	CPL	C35-C36-C37-C38
2	3E	201	CPL	C35-C36-C37-C38
2	3F	201	CPL	C35-C36-C37-C38
2	3G	201	CPL	C35-C36-C37-C38
2	3H	201	CPL	C35-C36-C37-C38
2	3I	201	CPL	C35-C36-C37-C38
2	3J	201	CPL	C35-C36-C37-C38
2	3K	201	CPL	C35-C36-C37-C38
2	3L	201	CPL	C35-C36-C37-C38
2	3M	201	CPL	C35-C36-C37-C38
2	3N	201	CPL	C35-C36-C37-C38
2	4A	201	CPL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
2	4B	201	CPL	C35-C36-C37-C38
2	4C	201	CPL	C35-C36-C37-C38
2	4D	201	CPL	C35-C36-C37-C38
2	4E	201	CPL	C35-C36-C37-C38
2	4F	201	CPL	C35-C36-C37-C38
2	4G	201	CPL	C35-C36-C37-C38
2	4H	201	CPL	C35-C36-C37-C38
2	4I	201	CPL	C35-C36-C37-C38
2	4J	201	CPL	C35-C36-C37-C38
2	4K	201	CPL	C35-C36-C37-C38
2	4L	201	CPL	C35-C36-C37-C38
2	4M	201	CPL	C35-C36-C37-C38
2	4N	201	CPL	C35-C36-C37-C38
2	5A	201	CPL	C35-C36-C37-C38
2	5B	201	CPL	C35-C36-C37-C38
2	5C	201	CPL	C35-C36-C37-C38
2	5D	201	CPL	C35-C36-C37-C38
2	5E	201	CPL	C35-C36-C37-C38
2	5F	201	CPL	C35-C36-C37-C38
2	5G	201	CPL	C35-C36-C37-C38
2	5H	201	CPL	C35-C36-C37-C38
2	5I	201	CPL	C35-C36-C37-C38
2	5J	201	CPL	C35-C36-C37-C38
2	5K	201	CPL	C35-C36-C37-C38
2	5L	201	CPL	C35-C36-C37-C38
2	5M	201	CPL	C35-C36-C37-C38
2	5N	201	CPL	C35-C36-C37-C38
2	1D	201	CPL	C19-C20-C21-C22
2	1F	201	CPL	C19-C20-C21-C22
2	1H	201	CPL	C19-C20-C21-C22
2	1I	201	CPL	C19-C20-C21-C22
2	1L	201	CPL	C19-C20-C21-C22
2	1N	201	CPL	C19-C20-C21-C22
2	2A	201	CPL	C19-C20-C21-C22
2	2B	201	CPL	C19-C20-C21-C22
2	2D	201	CPL	C19-C20-C21-C22
2	2I	201	CPL	C19-C20-C21-C22
2	2J	201	CPL	C19-C20-C21-C22
2	2L	201	CPL	C19-C20-C21-C22
2	2M	201	CPL	C19-C20-C21-C22
2	2N	201	CPL	C19-C20-C21-C22
2	3C	201	CPL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
2	3D	201	CPL	C19-C20-C21-C22
2	3E	201	CPL	C19-C20-C21-C22
2	3F	201	CPL	C19-C20-C21-C22
2	3M	201	CPL	C19-C20-C21-C22
2	3N	201	CPL	C19-C20-C21-C22
2	4A	201	CPL	C19-C20-C21-C22
2	4H	201	CPL	C19-C20-C21-C22
2	4I	201	CPL	C19-C20-C21-C22
2	4K	201	CPL	C19-C20-C21-C22
2	4L	201	CPL	C19-C20-C21-C22
2	4N	201	CPL	C19-C20-C21-C22
2	5I	201	CPL	C19-C20-C21-C22
2	5J	201	CPL	C19-C20-C21-C22
2	5M	201	CPL	C19-C20-C21-C22
2	5N	201	CPL	C19-C20-C21-C22
2	1A	201	CPL	C19-C20-C21-C22
2	1B	201	CPL	C19-C20-C21-C22
2	1C	201	CPL	C19-C20-C21-C22
2	1E	201	CPL	C19-C20-C21-C22
2	1G	201	CPL	C19-C20-C21-C22
2	1J	201	CPL	C19-C20-C21-C22
2	1K	201	CPL	C19-C20-C21-C22
2	1M	201	CPL	C19-C20-C21-C22
2	2C	201	CPL	C19-C20-C21-C22
2	2E	201	CPL	C19-C20-C21-C22
2	2F	201	CPL	C19-C20-C21-C22
2	2G	201	CPL	C19-C20-C21-C22
2	2H	201	CPL	C19-C20-C21-C22
2	2K	201	CPL	C19-C20-C21-C22
2	3A	201	CPL	C19-C20-C21-C22
2	3B	201	CPL	C19-C20-C21-C22
2	3G	201	CPL	C19-C20-C21-C22
2	3H	201	CPL	C19-C20-C21-C22
2	3I	201	CPL	C19-C20-C21-C22
2	3J	201	CPL	C19-C20-C21-C22
2	3K	201	CPL	C19-C20-C21-C22
2	3L	201	CPL	C19-C20-C21-C22
2	4B	201	CPL	C19-C20-C21-C22
2	4C	201	CPL	C19-C20-C21-C22
2	4D	201	CPL	C19-C20-C21-C22
2	4E	201	CPL	C19-C20-C21-C22
2	4F	201	CPL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
2	4G	201	CPL	C19-C20-C21-C22
2	4J	201	CPL	C19-C20-C21-C22
2	4M	201	CPL	C19-C20-C21-C22
2	5A	201	CPL	C19-C20-C21-C22
2	5B	201	CPL	C19-C20-C21-C22
2	5C	201	CPL	C19-C20-C21-C22
2	5D	201	CPL	C19-C20-C21-C22
2	5E	201	CPL	C19-C20-C21-C22
2	5F	201	CPL	C19-C20-C21-C22
2	5G	201	CPL	C19-C20-C21-C22
2	5H	201	CPL	C19-C20-C21-C22
2	5K	201	CPL	C19-C20-C21-C22
2	5L	201	CPL	C19-C20-C21-C22
2	1D	201	CPL	C14-C15-C16-C17
2	1H	201	CPL	C14-C15-C16-C17
2	1I	201	CPL	C14-C15-C16-C17
2	1J	201	CPL	C14-C15-C16-C17
2	1M	201	CPL	C14-C15-C16-C17
2	2E	201	CPL	C14-C15-C16-C17
2	2F	201	CPL	C14-C15-C16-C17
2	2G	201	CPL	C14-C15-C16-C17
2	2I	201	CPL	C14-C15-C16-C17
2	3B	201	CPL	C14-C15-C16-C17
2	3G	201	CPL	C14-C15-C16-C17
2	3H	201	CPL	C14-C15-C16-C17
2	3I	201	CPL	C14-C15-C16-C17
2	3K	201	CPL	C14-C15-C16-C17
2	4A	201	CPL	C14-C15-C16-C17
2	4B	201	CPL	C14-C15-C16-C17
2	4E	201	CPL	C14-C15-C16-C17
2	4F	201	CPL	C14-C15-C16-C17
2	4J	201	CPL	C14-C15-C16-C17
2	5E	201	CPL	C14-C15-C16-C17
2	5F	201	CPL	C14-C15-C16-C17
2	5H	201	CPL	C14-C15-C16-C17
2	5J	201	CPL	C14-C15-C16-C17
2	1A	201	CPL	C1-O3P-P-O4P
2	1B	201	CPL	C1-O3P-P-O4P
2	1C	201	CPL	C1-O3P-P-O4P
2	1D	201	CPL	C1-O3P-P-O4P
2	1E	201	CPL	C1-O3P-P-O4P
2	1F	201	CPL	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
2	1G	201	CPL	C1-O3P-P-O4P
2	1H	201	CPL	C1-O3P-P-O4P
2	1I	201	CPL	C1-O3P-P-O4P
2	1J	201	CPL	C1-O3P-P-O4P
2	1K	201	CPL	C1-O3P-P-O4P
2	1L	201	CPL	C1-O3P-P-O4P
2	1M	201	CPL	C1-O3P-P-O4P
2	1N	201	CPL	C1-O3P-P-O4P
2	2A	201	CPL	C1-O3P-P-O4P
2	2B	201	CPL	C1-O3P-P-O4P
2	2C	201	CPL	C1-O3P-P-O4P
2	2D	201	CPL	C1-O3P-P-O4P
2	2E	201	CPL	C1-O3P-P-O4P
2	2F	201	CPL	C1-O3P-P-O4P
2	2G	201	CPL	C1-O3P-P-O4P
2	2H	201	CPL	C1-O3P-P-O4P
2	2I	201	CPL	C1-O3P-P-O4P
2	2J	201	CPL	C1-O3P-P-O4P
2	2K	201	CPL	C1-O3P-P-O4P
2	2L	201	CPL	C1-O3P-P-O4P
2	2M	201	CPL	C1-O3P-P-O4P
2	2N	201	CPL	C1-O3P-P-O4P
2	3A	201	CPL	C1-O3P-P-O4P
2	3B	201	CPL	C1-O3P-P-O4P
2	3C	201	CPL	C1-O3P-P-O4P
2	3D	201	CPL	C1-O3P-P-O4P
2	3E	201	CPL	C1-O3P-P-O4P
2	3F	201	CPL	C1-O3P-P-O4P
2	3G	201	CPL	C1-O3P-P-O4P
2	3H	201	CPL	C1-O3P-P-O4P
2	3I	201	CPL	C1-O3P-P-O4P
2	3J	201	CPL	C1-O3P-P-O4P
2	3K	201	CPL	C1-O3P-P-O4P
2	3L	201	CPL	C1-O3P-P-O4P
2	3M	201	CPL	C1-O3P-P-O4P
2	3N	201	CPL	C1-O3P-P-O4P
2	4A	201	CPL	C1-O3P-P-O4P
2	4B	201	CPL	C1-O3P-P-O4P
2	4C	201	CPL	C1-O3P-P-O4P
2	4D	201	CPL	C1-O3P-P-O4P
2	4E	201	CPL	C1-O3P-P-O4P
2	4F	201	CPL	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
2	4G	201	CPL	C1-O3P-P-O4P
2	4H	201	CPL	C1-O3P-P-O4P
2	4I	201	CPL	C1-O3P-P-O4P
2	4J	201	CPL	C1-O3P-P-O4P
2	4K	201	CPL	C1-O3P-P-O4P
2	4L	201	CPL	C1-O3P-P-O4P
2	4M	201	CPL	C1-O3P-P-O4P
2	4N	201	CPL	C1-O3P-P-O4P
2	5A	201	CPL	C1-O3P-P-O4P
2	5B	201	CPL	C1-O3P-P-O4P
2	5C	201	CPL	C1-O3P-P-O4P
2	5D	201	CPL	C1-O3P-P-O4P
2	5E	201	CPL	C1-O3P-P-O4P
2	5F	201	CPL	C1-O3P-P-O4P
2	5G	201	CPL	C1-O3P-P-O4P
2	5H	201	CPL	C1-O3P-P-O4P
2	5I	201	CPL	C1-O3P-P-O4P
2	5J	201	CPL	C1-O3P-P-O4P
2	5K	201	CPL	C1-O3P-P-O4P
2	5L	201	CPL	C1-O3P-P-O4P
2	5M	201	CPL	C1-O3P-P-O4P
2	5N	201	CPL	C1-O3P-P-O4P
2	1A	201	CPL	C14-C15-C16-C17
2	1B	201	CPL	C14-C15-C16-C17
2	1C	201	CPL	C14-C15-C16-C17
2	1E	201	CPL	C14-C15-C16-C17
2	1F	201	CPL	C14-C15-C16-C17
2	1G	201	CPL	C14-C15-C16-C17
2	1K	201	CPL	C14-C15-C16-C17
2	1L	201	CPL	C14-C15-C16-C17
2	1N	201	CPL	C14-C15-C16-C17
2	2A	201	CPL	C14-C15-C16-C17
2	2B	201	CPL	C14-C15-C16-C17
2	2C	201	CPL	C14-C15-C16-C17
2	2D	201	CPL	C14-C15-C16-C17
2	2H	201	CPL	C14-C15-C16-C17
2	2J	201	CPL	C14-C15-C16-C17
2	2K	201	CPL	C14-C15-C16-C17
2	2L	201	CPL	C14-C15-C16-C17
2	2M	201	CPL	C14-C15-C16-C17
2	2N	201	CPL	C14-C15-C16-C17
2	3A	201	CPL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
2	3C	201	CPL	C14-C15-C16-C17
2	3D	201	CPL	C14-C15-C16-C17
2	3E	201	CPL	C14-C15-C16-C17
2	3F	201	CPL	C14-C15-C16-C17
2	3J	201	CPL	C14-C15-C16-C17
2	3L	201	CPL	C14-C15-C16-C17
2	3M	201	CPL	C14-C15-C16-C17
2	3N	201	CPL	C14-C15-C16-C17
2	4C	201	CPL	C14-C15-C16-C17
2	4D	201	CPL	C14-C15-C16-C17
2	4G	201	CPL	C14-C15-C16-C17
2	4H	201	CPL	C14-C15-C16-C17
2	4I	201	CPL	C14-C15-C16-C17
2	4K	201	CPL	C14-C15-C16-C17
2	4L	201	CPL	C14-C15-C16-C17
2	4M	201	CPL	C14-C15-C16-C17
2	4N	201	CPL	C14-C15-C16-C17
2	5A	201	CPL	C14-C15-C16-C17
2	5B	201	CPL	C14-C15-C16-C17
2	5C	201	CPL	C14-C15-C16-C17
2	5D	201	CPL	C14-C15-C16-C17
2	5G	201	CPL	C14-C15-C16-C17
2	5I	201	CPL	C14-C15-C16-C17
2	5K	201	CPL	C14-C15-C16-C17
2	5L	201	CPL	C14-C15-C16-C17
2	5M	201	CPL	C14-C15-C16-C17
2	5N	201	CPL	C14-C15-C16-C17
2	2F	201	CPL	C22-C23-C24-C25
2	3H	201	CPL	C22-C23-C24-C25
2	3J	201	CPL	C22-C23-C24-C25
2	4C	201	CPL	C22-C23-C24-C25
2	4L	201	CPL	C22-C23-C24-C25
2	5B	201	CPL	C22-C23-C24-C25
2	5F	201	CPL	C22-C23-C24-C25
2	1A	201	CPL	C22-C23-C24-C25
2	1D	201	CPL	C22-C23-C24-C25
2	1G	201	CPL	C22-C23-C24-C25
2	1H	201	CPL	C22-C23-C24-C25
2	1J	201	CPL	C22-C23-C24-C25
2	1K	201	CPL	C22-C23-C24-C25
2	1N	201	CPL	C22-C23-C24-C25
2	2A	201	CPL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
2	2B	201	CPL	C22-C23-C24-C25
2	2C	201	CPL	C22-C23-C24-C25
2	2D	201	CPL	C22-C23-C24-C25
2	2E	201	CPL	C22-C23-C24-C25
2	2H	201	CPL	C22-C23-C24-C25
2	2J	201	CPL	C22-C23-C24-C25
2	2K	201	CPL	C22-C23-C24-C25
2	3B	201	CPL	C22-C23-C24-C25
2	3C	201	CPL	C22-C23-C24-C25
2	3F	201	CPL	C22-C23-C24-C25
2	3G	201	CPL	C22-C23-C24-C25
2	3I	201	CPL	C22-C23-C24-C25
2	3K	201	CPL	C22-C23-C24-C25
2	3M	201	CPL	C22-C23-C24-C25
2	3N	201	CPL	C22-C23-C24-C25
2	4A	201	CPL	C22-C23-C24-C25
2	4B	201	CPL	C22-C23-C24-C25
2	4E	201	CPL	C22-C23-C24-C25
2	4F	201	CPL	C22-C23-C24-C25
2	4G	201	CPL	C22-C23-C24-C25
2	4N	201	CPL	C22-C23-C24-C25
2	5C	201	CPL	C22-C23-C24-C25
2	5K	201	CPL	C22-C23-C24-C25
2	5M	201	CPL	C22-C23-C24-C25
2	5N	201	CPL	C22-C23-C24-C25
2	1B	201	CPL	C22-C23-C24-C25
2	1C	201	CPL	C22-C23-C24-C25
2	1E	201	CPL	C22-C23-C24-C25
2	1F	201	CPL	C22-C23-C24-C25
2	1I	201	CPL	C22-C23-C24-C25
2	1L	201	CPL	C22-C23-C24-C25
2	1M	201	CPL	C22-C23-C24-C25
2	2G	201	CPL	C22-C23-C24-C25
2	2I	201	CPL	C22-C23-C24-C25
2	2L	201	CPL	C22-C23-C24-C25
2	2M	201	CPL	C22-C23-C24-C25
2	2N	201	CPL	C22-C23-C24-C25
2	3A	201	CPL	C22-C23-C24-C25
2	3E	201	CPL	C22-C23-C24-C25
2	3L	201	CPL	C22-C23-C24-C25
2	4D	201	CPL	C22-C23-C24-C25
2	4H	201	CPL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
2	4I	201	CPL	C22-C23-C24-C25
2	4J	201	CPL	C22-C23-C24-C25
2	4K	201	CPL	C22-C23-C24-C25
2	4M	201	CPL	C22-C23-C24-C25
2	5A	201	CPL	C22-C23-C24-C25
2	5E	201	CPL	C22-C23-C24-C25
2	5G	201	CPL	C22-C23-C24-C25
2	5H	201	CPL	C22-C23-C24-C25
2	5I	201	CPL	C22-C23-C24-C25
2	5J	201	CPL	C22-C23-C24-C25
2	5L	201	CPL	C22-C23-C24-C25
2	3D	201	CPL	C22-C23-C24-C25
2	5D	201	CPL	C22-C23-C24-C25
2	1D	201	CPL	C12-C11-O3-C3
2	1E	201	CPL	C12-C11-O3-C3
2	1F	201	CPL	C12-C11-O3-C3
2	1G	201	CPL	C12-C11-O3-C3
2	1H	201	CPL	C12-C11-O3-C3
2	1J	201	CPL	C12-C11-O3-C3
2	1K	201	CPL	C12-C11-O3-C3
2	1M	201	CPL	C12-C11-O3-C3
2	1N	201	CPL	C12-C11-O3-C3
2	2A	201	CPL	C12-C11-O3-C3
2	2B	201	CPL	C12-C11-O3-C3
2	2C	201	CPL	C12-C11-O3-C3
2	2E	201	CPL	C12-C11-O3-C3
2	2F	201	CPL	C12-C11-O3-C3
2	2G	201	CPL	C12-C11-O3-C3
2	2I	201	CPL	C12-C11-O3-C3
2	2J	201	CPL	C12-C11-O3-C3
2	2K	201	CPL	C12-C11-O3-C3
2	2L	201	CPL	C12-C11-O3-C3
2	2M	201	CPL	C12-C11-O3-C3
2	3A	201	CPL	C12-C11-O3-C3
2	3B	201	CPL	C12-C11-O3-C3
2	3C	201	CPL	C12-C11-O3-C3
2	3E	201	CPL	C12-C11-O3-C3
2	3I	201	CPL	C12-C11-O3-C3
2	3J	201	CPL	C12-C11-O3-C3
2	3K	201	CPL	C12-C11-O3-C3
2	3L	201	CPL	C12-C11-O3-C3
2	3M	201	CPL	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
2	3N	201	CPL	C12-C11-O3-C3
2	4A	201	CPL	C12-C11-O3-C3
2	4D	201	CPL	C12-C11-O3-C3
2	4E	201	CPL	C12-C11-O3-C3
2	4G	201	CPL	C12-C11-O3-C3
2	4I	201	CPL	C12-C11-O3-C3
2	4J	201	CPL	C12-C11-O3-C3
2	4K	201	CPL	C12-C11-O3-C3
2	5B	201	CPL	C12-C11-O3-C3
2	5C	201	CPL	C12-C11-O3-C3
2	5I	201	CPL	C12-C11-O3-C3
2	5J	201	CPL	C12-C11-O3-C3
2	5K	201	CPL	C12-C11-O3-C3
2	5L	201	CPL	C12-C11-O3-C3
2	5N	201	CPL	C12-C11-O3-C3
2	1A	201	CPL	C18-C19-C20-C21
2	3F	201	CPL	C18-C19-C20-C21
2	5G	201	CPL	C18-C19-C20-C21
2	1C	201	CPL	C18-C19-C20-C21
2	1D	201	CPL	C18-C19-C20-C21
2	1E	201	CPL	C18-C19-C20-C21
2	1F	201	CPL	C18-C19-C20-C21
2	1G	201	CPL	C18-C19-C20-C21
2	1H	201	CPL	C18-C19-C20-C21
2	1I	201	CPL	C18-C19-C20-C21
2	1J	201	CPL	C18-C19-C20-C21
2	1K	201	CPL	C18-C19-C20-C21
2	1L	201	CPL	C18-C19-C20-C21
2	1M	201	CPL	C18-C19-C20-C21
2	1N	201	CPL	C18-C19-C20-C21
2	2A	201	CPL	C18-C19-C20-C21
2	2C	201	CPL	C18-C19-C20-C21
2	2D	201	CPL	C18-C19-C20-C21
2	2E	201	CPL	C18-C19-C20-C21
2	2F	201	CPL	C18-C19-C20-C21
2	2I	201	CPL	C18-C19-C20-C21
2	2J	201	CPL	C18-C19-C20-C21
2	2L	201	CPL	C18-C19-C20-C21
2	2M	201	CPL	C18-C19-C20-C21
2	2N	201	CPL	C18-C19-C20-C21
2	3A	201	CPL	C18-C19-C20-C21
2	3B	201	CPL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
2	3C	201	CPL	C18-C19-C20-C21
2	3D	201	CPL	C18-C19-C20-C21
2	3E	201	CPL	C18-C19-C20-C21
2	3H	201	CPL	C18-C19-C20-C21
2	3I	201	CPL	C18-C19-C20-C21
2	3J	201	CPL	C18-C19-C20-C21
2	3K	201	CPL	C18-C19-C20-C21
2	3L	201	CPL	C18-C19-C20-C21
2	3M	201	CPL	C18-C19-C20-C21
2	3N	201	CPL	C18-C19-C20-C21
2	4A	201	CPL	C18-C19-C20-C21
2	4B	201	CPL	C18-C19-C20-C21
2	4D	201	CPL	C18-C19-C20-C21
2	4E	201	CPL	C18-C19-C20-C21
2	4G	201	CPL	C18-C19-C20-C21
2	4H	201	CPL	C18-C19-C20-C21
2	4I	201	CPL	C18-C19-C20-C21
2	4J	201	CPL	C18-C19-C20-C21
2	4K	201	CPL	C18-C19-C20-C21
2	4L	201	CPL	C18-C19-C20-C21
2	4N	201	CPL	C18-C19-C20-C21
2	5A	201	CPL	C18-C19-C20-C21
2	5B	201	CPL	C18-C19-C20-C21
2	5C	201	CPL	C18-C19-C20-C21
2	5D	201	CPL	C18-C19-C20-C21
2	5E	201	CPL	C18-C19-C20-C21
2	5F	201	CPL	C18-C19-C20-C21
2	5H	201	CPL	C18-C19-C20-C21
2	5I	201	CPL	C18-C19-C20-C21
2	5K	201	CPL	C18-C19-C20-C21
2	5L	201	CPL	C18-C19-C20-C21
2	5M	201	CPL	C18-C19-C20-C21
2	5N	201	CPL	C18-C19-C20-C21
2	1B	201	CPL	C18-C19-C20-C21
2	2B	201	CPL	C18-C19-C20-C21
2	2G	201	CPL	C18-C19-C20-C21
2	2H	201	CPL	C18-C19-C20-C21
2	2K	201	CPL	C18-C19-C20-C21
2	3G	201	CPL	C18-C19-C20-C21
2	4C	201	CPL	C18-C19-C20-C21
2	4F	201	CPL	C18-C19-C20-C21
2	4M	201	CPL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
2	5J	201	CPL	C18-C19-C20-C21
2	2C	201	CPL	C15-C16-C17-C18
2	3A	201	CPL	C15-C16-C17-C18
2	3J	201	CPL	C15-C16-C17-C18
2	4H	201	CPL	C15-C16-C17-C18
2	4L	201	CPL	C15-C16-C17-C18
2	5N	201	CPL	C15-C16-C17-C18
2	1A	201	CPL	C15-C16-C17-C18
2	1E	201	CPL	C15-C16-C17-C18
2	2B	201	CPL	C15-C16-C17-C18
2	2K	201	CPL	C15-C16-C17-C18
2	2M	201	CPL	C15-C16-C17-C18
2	2N	201	CPL	C15-C16-C17-C18
2	3C	201	CPL	C15-C16-C17-C18
2	3G	201	CPL	C15-C16-C17-C18
2	3H	201	CPL	C15-C16-C17-C18
2	3L	201	CPL	C15-C16-C17-C18
2	4G	201	CPL	C15-C16-C17-C18
2	4I	201	CPL	C15-C16-C17-C18
2	4M	201	CPL	C15-C16-C17-C18
2	5C	201	CPL	C15-C16-C17-C18
2	5F	201	CPL	C15-C16-C17-C18
2	5G	201	CPL	C15-C16-C17-C18
2	5I	201	CPL	C15-C16-C17-C18
2	1A	201	CPL	C12-C11-O3-C3
2	1B	201	CPL	C12-C11-O3-C3
2	1C	201	CPL	C12-C11-O3-C3
2	1I	201	CPL	C12-C11-O3-C3
2	1L	201	CPL	C12-C11-O3-C3
2	2D	201	CPL	C12-C11-O3-C3
2	2H	201	CPL	C12-C11-O3-C3
2	2N	201	CPL	C12-C11-O3-C3
2	3D	201	CPL	C12-C11-O3-C3
2	3F	201	CPL	C12-C11-O3-C3
2	3G	201	CPL	C12-C11-O3-C3
2	3H	201	CPL	C12-C11-O3-C3
2	4B	201	CPL	C12-C11-O3-C3
2	4C	201	CPL	C12-C11-O3-C3
2	4F	201	CPL	C12-C11-O3-C3
2	4H	201	CPL	C12-C11-O3-C3
2	4L	201	CPL	C12-C11-O3-C3
2	4M	201	CPL	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
2	4N	201	CPL	C12-C11-O3-C3
2	5A	201	CPL	C12-C11-O3-C3
2	5D	201	CPL	C12-C11-O3-C3
2	5E	201	CPL	C12-C11-O3-C3
2	5F	201	CPL	C12-C11-O3-C3
2	5G	201	CPL	C12-C11-O3-C3
2	5H	201	CPL	C12-C11-O3-C3
2	5M	201	CPL	C12-C11-O3-C3
2	1B	201	CPL	C15-C16-C17-C18
2	1D	201	CPL	C15-C16-C17-C18
2	1F	201	CPL	C15-C16-C17-C18
2	1H	201	CPL	C15-C16-C17-C18
2	1I	201	CPL	C15-C16-C17-C18
2	1J	201	CPL	C15-C16-C17-C18
2	1K	201	CPL	C15-C16-C17-C18
2	1N	201	CPL	C15-C16-C17-C18
2	2A	201	CPL	C15-C16-C17-C18
2	2D	201	CPL	C15-C16-C17-C18
2	2F	201	CPL	C15-C16-C17-C18
2	2H	201	CPL	C15-C16-C17-C18
2	2J	201	CPL	C15-C16-C17-C18
2	2L	201	CPL	C15-C16-C17-C18
2	3B	201	CPL	C15-C16-C17-C18
2	3E	201	CPL	C15-C16-C17-C18
2	3M	201	CPL	C15-C16-C17-C18
2	3N	201	CPL	C15-C16-C17-C18
2	4A	201	CPL	C15-C16-C17-C18
2	4C	201	CPL	C15-C16-C17-C18
2	4E	201	CPL	C15-C16-C17-C18
2	4F	201	CPL	C15-C16-C17-C18
2	4J	201	CPL	C15-C16-C17-C18
2	4K	201	CPL	C15-C16-C17-C18
2	4N	201	CPL	C15-C16-C17-C18
2	5A	201	CPL	C15-C16-C17-C18
2	5B	201	CPL	C15-C16-C17-C18
2	5E	201	CPL	C15-C16-C17-C18
2	5J	201	CPL	C15-C16-C17-C18
2	5K	201	CPL	C15-C16-C17-C18
2	5L	201	CPL	C15-C16-C17-C18
2	5M	201	CPL	C15-C16-C17-C18
2	1G	201	CPL	C15-C16-C17-C18
2	1L	201	CPL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
2	2E	201	CPL	C15-C16-C17-C18
2	2I	201	CPL	C15-C16-C17-C18
2	3D	201	CPL	C15-C16-C17-C18
2	3F	201	CPL	C15-C16-C17-C18
2	3I	201	CPL	C15-C16-C17-C18
2	3K	201	CPL	C15-C16-C17-C18
2	4B	201	CPL	C15-C16-C17-C18
2	5D	201	CPL	C15-C16-C17-C18
2	5H	201	CPL	C15-C16-C17-C18
2	1A	201	CPL	C1-C2-C3-O3
2	1B	201	CPL	C1-C2-C3-O3
2	1C	201	CPL	C1-C2-C3-O3
2	1D	201	CPL	C1-C2-C3-O3
2	1E	201	CPL	C1-C2-C3-O3
2	1F	201	CPL	C1-C2-C3-O3
2	1G	201	CPL	C1-C2-C3-O3
2	1H	201	CPL	C1-C2-C3-O3
2	1I	201	CPL	C1-C2-C3-O3
2	1J	201	CPL	C1-C2-C3-O3
2	1K	201	CPL	C1-C2-C3-O3
2	1L	201	CPL	C1-C2-C3-O3
2	1M	201	CPL	C1-C2-C3-O3
2	1N	201	CPL	C1-C2-C3-O3
2	2A	201	CPL	C1-C2-C3-O3
2	2B	201	CPL	C1-C2-C3-O3
2	2C	201	CPL	C1-C2-C3-O3
2	2D	201	CPL	C1-C2-C3-O3
2	2E	201	CPL	C1-C2-C3-O3
2	2F	201	CPL	C1-C2-C3-O3
2	2G	201	CPL	C1-C2-C3-O3
2	2H	201	CPL	C1-C2-C3-O3
2	2I	201	CPL	C1-C2-C3-O3
2	2J	201	CPL	C1-C2-C3-O3
2	2K	201	CPL	C1-C2-C3-O3
2	2L	201	CPL	C1-C2-C3-O3
2	2M	201	CPL	C1-C2-C3-O3
2	2N	201	CPL	C1-C2-C3-O3
2	3A	201	CPL	C1-C2-C3-O3
2	3B	201	CPL	C1-C2-C3-O3
2	3C	201	CPL	C1-C2-C3-O3
2	3D	201	CPL	C1-C2-C3-O3
2	3E	201	CPL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	3F	201	CPL	C1-C2-C3-O3
2	3G	201	CPL	C1-C2-C3-O3
2	3H	201	CPL	C1-C2-C3-O3
2	3I	201	CPL	C1-C2-C3-O3
2	3J	201	CPL	C1-C2-C3-O3
2	3K	201	CPL	C1-C2-C3-O3
2	3L	201	CPL	C1-C2-C3-O3
2	3M	201	CPL	C1-C2-C3-O3
2	3N	201	CPL	C1-C2-C3-O3
2	4A	201	CPL	C1-C2-C3-O3
2	4B	201	CPL	C1-C2-C3-O3
2	4C	201	CPL	C1-C2-C3-O3
2	4D	201	CPL	C1-C2-C3-O3
2	4E	201	CPL	C1-C2-C3-O3
2	4F	201	CPL	C1-C2-C3-O3
2	4G	201	CPL	C1-C2-C3-O3
2	4H	201	CPL	C1-C2-C3-O3
2	4I	201	CPL	C1-C2-C3-O3
2	4J	201	CPL	C1-C2-C3-O3
2	4K	201	CPL	C1-C2-C3-O3
2	4L	201	CPL	C1-C2-C3-O3
2	4M	201	CPL	C1-C2-C3-O3
2	4N	201	CPL	C1-C2-C3-O3
2	5A	201	CPL	C1-C2-C3-O3
2	5B	201	CPL	C1-C2-C3-O3
2	5C	201	CPL	C1-C2-C3-O3
2	5D	201	CPL	C1-C2-C3-O3
2	5E	201	CPL	C1-C2-C3-O3
2	5F	201	CPL	C1-C2-C3-O3
2	5G	201	CPL	C1-C2-C3-O3
2	5H	201	CPL	C1-C2-C3-O3
2	5I	201	CPL	C1-C2-C3-O3
2	5J	201	CPL	C1-C2-C3-O3
2	5K	201	CPL	C1-C2-C3-O3
2	5L	201	CPL	C1-C2-C3-O3
2	5M	201	CPL	C1-C2-C3-O3
2	5N	201	CPL	C1-C2-C3-O3
2	1C	201	CPL	C15-C16-C17-C18
2	1M	201	CPL	C15-C16-C17-C18
2	2G	201	CPL	C15-C16-C17-C18
2	4D	201	CPL	C15-C16-C17-C18
2	1A	201	CPL	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
2	1B	201	CPL	O11-C11-O3-C3
2	1C	201	CPL	O11-C11-O3-C3
2	1D	201	CPL	O11-C11-O3-C3
2	1E	201	CPL	O11-C11-O3-C3
2	1F	201	CPL	O11-C11-O3-C3
2	1G	201	CPL	O11-C11-O3-C3
2	1H	201	CPL	O11-C11-O3-C3
2	1I	201	CPL	O11-C11-O3-C3
2	1J	201	CPL	O11-C11-O3-C3
2	1K	201	CPL	O11-C11-O3-C3
2	1L	201	CPL	O11-C11-O3-C3
2	1M	201	CPL	O11-C11-O3-C3
2	1N	201	CPL	O11-C11-O3-C3
2	2A	201	CPL	O11-C11-O3-C3
2	2B	201	CPL	O11-C11-O3-C3
2	2C	201	CPL	O11-C11-O3-C3
2	2D	201	CPL	O11-C11-O3-C3
2	2E	201	CPL	O11-C11-O3-C3
2	2F	201	CPL	O11-C11-O3-C3
2	2G	201	CPL	O11-C11-O3-C3
2	2H	201	CPL	O11-C11-O3-C3
2	2I	201	CPL	O11-C11-O3-C3
2	2J	201	CPL	O11-C11-O3-C3
2	2K	201	CPL	O11-C11-O3-C3
2	2L	201	CPL	O11-C11-O3-C3
2	2M	201	CPL	O11-C11-O3-C3
2	2N	201	CPL	O11-C11-O3-C3
2	3A	201	CPL	O11-C11-O3-C3
2	3B	201	CPL	O11-C11-O3-C3
2	3C	201	CPL	O11-C11-O3-C3
2	3D	201	CPL	O11-C11-O3-C3
2	3E	201	CPL	O11-C11-O3-C3
2	3F	201	CPL	O11-C11-O3-C3
2	3G	201	CPL	O11-C11-O3-C3
2	3H	201	CPL	O11-C11-O3-C3
2	3I	201	CPL	O11-C11-O3-C3
2	3J	201	CPL	O11-C11-O3-C3
2	3K	201	CPL	O11-C11-O3-C3
2	3L	201	CPL	O11-C11-O3-C3
2	3M	201	CPL	O11-C11-O3-C3
2	3N	201	CPL	O11-C11-O3-C3
2	4A	201	CPL	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
2	4B	201	CPL	O11-C11-O3-C3
2	4C	201	CPL	O11-C11-O3-C3
2	4D	201	CPL	O11-C11-O3-C3
2	4E	201	CPL	O11-C11-O3-C3
2	4F	201	CPL	O11-C11-O3-C3
2	4G	201	CPL	O11-C11-O3-C3
2	4H	201	CPL	O11-C11-O3-C3
2	4I	201	CPL	O11-C11-O3-C3
2	4J	201	CPL	O11-C11-O3-C3
2	4K	201	CPL	O11-C11-O3-C3
2	4L	201	CPL	O11-C11-O3-C3
2	4M	201	CPL	O11-C11-O3-C3
2	4N	201	CPL	O11-C11-O3-C3
2	5A	201	CPL	O11-C11-O3-C3
2	5B	201	CPL	O11-C11-O3-C3
2	5C	201	CPL	O11-C11-O3-C3
2	5D	201	CPL	O11-C11-O3-C3
2	5E	201	CPL	O11-C11-O3-C3
2	5F	201	CPL	O11-C11-O3-C3
2	5G	201	CPL	O11-C11-O3-C3
2	5H	201	CPL	O11-C11-O3-C3
2	5I	201	CPL	O11-C11-O3-C3
2	5J	201	CPL	O11-C11-O3-C3
2	5K	201	CPL	O11-C11-O3-C3
2	5L	201	CPL	O11-C11-O3-C3
2	5M	201	CPL	O11-C11-O3-C3
2	5N	201	CPL	O11-C11-O3-C3
2	1A	201	CPL	C1-O3P-P-O2P
2	1A	201	CPL	C4-O4P-P-O1P
2	1B	201	CPL	C1-O3P-P-O2P
2	1B	201	CPL	C4-O4P-P-O1P
2	1C	201	CPL	C1-O3P-P-O2P
2	1C	201	CPL	C4-O4P-P-O1P
2	1D	201	CPL	C1-O3P-P-O2P
2	1D	201	CPL	C4-O4P-P-O1P
2	1E	201	CPL	C1-O3P-P-O2P
2	1E	201	CPL	C4-O4P-P-O1P
2	1F	201	CPL	C1-O3P-P-O2P
2	1F	201	CPL	C4-O4P-P-O1P
2	1G	201	CPL	C1-O3P-P-O2P
2	1G	201	CPL	C4-O4P-P-O1P
2	1H	201	CPL	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
2	1H	201	CPL	C4-O4P-P-O1P
2	1I	201	CPL	C1-O3P-P-O2P
2	1I	201	CPL	C4-O4P-P-O1P
2	1J	201	CPL	C1-O3P-P-O2P
2	1J	201	CPL	C4-O4P-P-O1P
2	1K	201	CPL	C1-O3P-P-O2P
2	1K	201	CPL	C4-O4P-P-O1P
2	1L	201	CPL	C1-O3P-P-O2P
2	1L	201	CPL	C4-O4P-P-O1P
2	1M	201	CPL	C1-O3P-P-O2P
2	1M	201	CPL	C4-O4P-P-O1P
2	1N	201	CPL	C1-O3P-P-O2P
2	1N	201	CPL	C4-O4P-P-O1P
2	2A	201	CPL	C1-O3P-P-O2P
2	2A	201	CPL	C4-O4P-P-O1P
2	2B	201	CPL	C1-O3P-P-O2P
2	2B	201	CPL	C4-O4P-P-O1P
2	2C	201	CPL	C1-O3P-P-O2P
2	2C	201	CPL	C4-O4P-P-O1P
2	2D	201	CPL	C1-O3P-P-O2P
2	2D	201	CPL	C4-O4P-P-O1P
2	2E	201	CPL	C1-O3P-P-O2P
2	2E	201	CPL	C4-O4P-P-O1P
2	2F	201	CPL	C1-O3P-P-O2P
2	2F	201	CPL	C4-O4P-P-O1P
2	2G	201	CPL	C1-O3P-P-O2P
2	2G	201	CPL	C4-O4P-P-O1P
2	2H	201	CPL	C1-O3P-P-O2P
2	2H	201	CPL	C4-O4P-P-O1P
2	2I	201	CPL	C1-O3P-P-O2P
2	2I	201	CPL	C4-O4P-P-O1P
2	2J	201	CPL	C1-O3P-P-O2P
2	2J	201	CPL	C4-O4P-P-O1P
2	2K	201	CPL	C1-O3P-P-O2P
2	2K	201	CPL	C4-O4P-P-O1P
2	2L	201	CPL	C1-O3P-P-O2P
2	2L	201	CPL	C4-O4P-P-O1P
2	2M	201	CPL	C1-O3P-P-O2P
2	2M	201	CPL	C4-O4P-P-O1P
2	2N	201	CPL	C1-O3P-P-O2P
2	2N	201	CPL	C4-O4P-P-O1P
2	3A	201	CPL	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
2	3A	201	CPL	C4-O4P-P-O1P
2	3B	201	CPL	C1-O3P-P-O2P
2	3B	201	CPL	C4-O4P-P-O1P
2	3C	201	CPL	C1-O3P-P-O2P
2	3C	201	CPL	C4-O4P-P-O1P
2	3D	201	CPL	C1-O3P-P-O2P
2	3D	201	CPL	C4-O4P-P-O1P
2	3E	201	CPL	C1-O3P-P-O2P
2	3E	201	CPL	C4-O4P-P-O1P
2	3F	201	CPL	C1-O3P-P-O2P
2	3F	201	CPL	C4-O4P-P-O1P
2	3G	201	CPL	C1-O3P-P-O2P
2	3G	201	CPL	C4-O4P-P-O1P
2	3H	201	CPL	C1-O3P-P-O2P
2	3H	201	CPL	C4-O4P-P-O1P
2	3I	201	CPL	C1-O3P-P-O2P
2	3I	201	CPL	C4-O4P-P-O1P
2	3J	201	CPL	C1-O3P-P-O2P
2	3J	201	CPL	C4-O4P-P-O1P
2	3K	201	CPL	C1-O3P-P-O2P
2	3K	201	CPL	C4-O4P-P-O1P
2	3L	201	CPL	C1-O3P-P-O2P
2	3L	201	CPL	C4-O4P-P-O1P
2	3M	201	CPL	C1-O3P-P-O2P
2	3M	201	CPL	C4-O4P-P-O1P
2	3N	201	CPL	C1-O3P-P-O2P
2	3N	201	CPL	C4-O4P-P-O1P
2	4A	201	CPL	C1-O3P-P-O2P
2	4A	201	CPL	C4-O4P-P-O1P
2	4B	201	CPL	C1-O3P-P-O2P
2	4B	201	CPL	C4-O4P-P-O1P
2	4C	201	CPL	C1-O3P-P-O2P
2	4C	201	CPL	C4-O4P-P-O1P
2	4D	201	CPL	C1-O3P-P-O2P
2	4D	201	CPL	C4-O4P-P-O1P
2	4E	201	CPL	C1-O3P-P-O2P
2	4E	201	CPL	C4-O4P-P-O1P
2	4F	201	CPL	C1-O3P-P-O2P
2	4F	201	CPL	C4-O4P-P-O1P
2	4G	201	CPL	C1-O3P-P-O2P
2	4G	201	CPL	C4-O4P-P-O1P
2	4H	201	CPL	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
2	4H	201	CPL	C4-O4P-P-O1P
2	4I	201	CPL	C1-O3P-P-O2P
2	4I	201	CPL	C4-O4P-P-O1P
2	4J	201	CPL	C1-O3P-P-O2P
2	4J	201	CPL	C4-O4P-P-O1P
2	4K	201	CPL	C1-O3P-P-O2P
2	4K	201	CPL	C4-O4P-P-O1P
2	4L	201	CPL	C1-O3P-P-O2P
2	4L	201	CPL	C4-O4P-P-O1P
2	4M	201	CPL	C1-O3P-P-O2P
2	4M	201	CPL	C4-O4P-P-O1P
2	4N	201	CPL	C1-O3P-P-O2P
2	4N	201	CPL	C4-O4P-P-O1P
2	5A	201	CPL	C1-O3P-P-O2P
2	5A	201	CPL	C4-O4P-P-O1P
2	5B	201	CPL	C1-O3P-P-O2P
2	5B	201	CPL	C4-O4P-P-O1P
2	5C	201	CPL	C1-O3P-P-O2P
2	5C	201	CPL	C4-O4P-P-O1P
2	5D	201	CPL	C1-O3P-P-O2P
2	5D	201	CPL	C4-O4P-P-O1P
2	5E	201	CPL	C1-O3P-P-O2P
2	5E	201	CPL	C4-O4P-P-O1P
2	5F	201	CPL	C1-O3P-P-O2P
2	5F	201	CPL	C4-O4P-P-O1P
2	5G	201	CPL	C1-O3P-P-O2P
2	5G	201	CPL	C4-O4P-P-O1P
2	5H	201	CPL	C1-O3P-P-O2P
2	5H	201	CPL	C4-O4P-P-O1P
2	5I	201	CPL	C1-O3P-P-O2P
2	5I	201	CPL	C4-O4P-P-O1P
2	5J	201	CPL	C1-O3P-P-O2P
2	5J	201	CPL	C4-O4P-P-O1P
2	5K	201	CPL	C1-O3P-P-O2P
2	5K	201	CPL	C4-O4P-P-O1P
2	5L	201	CPL	C1-O3P-P-O2P
2	5L	201	CPL	C4-O4P-P-O1P
2	5M	201	CPL	C1-O3P-P-O2P
2	5M	201	CPL	C4-O4P-P-O1P
2	5N	201	CPL	C1-O3P-P-O2P
2	5N	201	CPL	C4-O4P-P-O1P
2	1A	201	CPL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
2	1B	201	CPL	C31-C32-C33-C34
2	1C	201	CPL	C31-C32-C33-C34
2	1D	201	CPL	C31-C32-C33-C34
2	1E	201	CPL	C31-C32-C33-C34
2	1F	201	CPL	C31-C32-C33-C34
2	1G	201	CPL	C31-C32-C33-C34
2	1H	201	CPL	C31-C32-C33-C34
2	1I	201	CPL	C31-C32-C33-C34
2	1J	201	CPL	C31-C32-C33-C34
2	1K	201	CPL	C31-C32-C33-C34
2	1L	201	CPL	C31-C32-C33-C34
2	1M	201	CPL	C31-C32-C33-C34
2	1N	201	CPL	C31-C32-C33-C34
2	2A	201	CPL	C31-C32-C33-C34
2	2B	201	CPL	C31-C32-C33-C34
2	2C	201	CPL	C31-C32-C33-C34
2	2D	201	CPL	C31-C32-C33-C34
2	2E	201	CPL	C31-C32-C33-C34
2	2F	201	CPL	C31-C32-C33-C34
2	2G	201	CPL	C31-C32-C33-C34
2	2H	201	CPL	C31-C32-C33-C34
2	2I	201	CPL	C31-C32-C33-C34
2	2J	201	CPL	C31-C32-C33-C34
2	2K	201	CPL	C31-C32-C33-C34
2	2L	201	CPL	C31-C32-C33-C34
2	2M	201	CPL	C31-C32-C33-C34
2	2N	201	CPL	C31-C32-C33-C34
2	3A	201	CPL	C31-C32-C33-C34
2	3B	201	CPL	C31-C32-C33-C34
2	3C	201	CPL	C31-C32-C33-C34
2	3D	201	CPL	C31-C32-C33-C34
2	3E	201	CPL	C31-C32-C33-C34
2	3F	201	CPL	C31-C32-C33-C34
2	3G	201	CPL	C31-C32-C33-C34
2	3H	201	CPL	C31-C32-C33-C34
2	3I	201	CPL	C31-C32-C33-C34
2	3J	201	CPL	C31-C32-C33-C34
2	3K	201	CPL	C31-C32-C33-C34
2	3L	201	CPL	C31-C32-C33-C34
2	3M	201	CPL	C31-C32-C33-C34
2	3N	201	CPL	C31-C32-C33-C34
2	4A	201	CPL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
2	4B	201	CPL	C31-C32-C33-C34
2	4C	201	CPL	C31-C32-C33-C34
2	4D	201	CPL	C31-C32-C33-C34
2	4E	201	CPL	C31-C32-C33-C34
2	4F	201	CPL	C31-C32-C33-C34
2	4G	201	CPL	C31-C32-C33-C34
2	4H	201	CPL	C31-C32-C33-C34
2	4I	201	CPL	C31-C32-C33-C34
2	4J	201	CPL	C31-C32-C33-C34
2	4K	201	CPL	C31-C32-C33-C34
2	4L	201	CPL	C31-C32-C33-C34
2	4M	201	CPL	C31-C32-C33-C34
2	4N	201	CPL	C31-C32-C33-C34
2	5A	201	CPL	C31-C32-C33-C34
2	5B	201	CPL	C31-C32-C33-C34
2	5C	201	CPL	C31-C32-C33-C34
2	5D	201	CPL	C31-C32-C33-C34
2	5E	201	CPL	C31-C32-C33-C34
2	5F	201	CPL	C31-C32-C33-C34
2	5G	201	CPL	C31-C32-C33-C34
2	5H	201	CPL	C31-C32-C33-C34
2	5I	201	CPL	C31-C32-C33-C34
2	5J	201	CPL	C31-C32-C33-C34
2	5K	201	CPL	C31-C32-C33-C34
2	5L	201	CPL	C31-C32-C33-C34
2	5M	201	CPL	C31-C32-C33-C34
2	5N	201	CPL	C31-C32-C33-C34
2	1A	201	CPL	O2-C31-C32-C33
2	1B	201	CPL	O2-C31-C32-C33
2	1C	201	CPL	O2-C31-C32-C33
2	1D	201	CPL	O2-C31-C32-C33
2	1E	201	CPL	O2-C31-C32-C33
2	1F	201	CPL	O2-C31-C32-C33
2	1G	201	CPL	O2-C31-C32-C33
2	1H	201	CPL	O2-C31-C32-C33
2	1I	201	CPL	O2-C31-C32-C33
2	1J	201	CPL	O2-C31-C32-C33
2	1K	201	CPL	O2-C31-C32-C33
2	1L	201	CPL	O2-C31-C32-C33
2	1M	201	CPL	O2-C31-C32-C33
2	1N	201	CPL	O2-C31-C32-C33
2	2A	201	CPL	O2-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
2	2B	201	CPL	O2-C31-C32-C33
2	2E	201	CPL	O2-C31-C32-C33
2	2F	201	CPL	O2-C31-C32-C33
2	2G	201	CPL	O2-C31-C32-C33
2	2H	201	CPL	O2-C31-C32-C33
2	2I	201	CPL	O2-C31-C32-C33
2	2J	201	CPL	O2-C31-C32-C33
2	2K	201	CPL	O2-C31-C32-C33
2	2L	201	CPL	O2-C31-C32-C33
2	2N	201	CPL	O2-C31-C32-C33
2	3A	201	CPL	O2-C31-C32-C33
2	3B	201	CPL	O2-C31-C32-C33
2	3C	201	CPL	O2-C31-C32-C33
2	3E	201	CPL	O2-C31-C32-C33
2	3F	201	CPL	O2-C31-C32-C33
2	3G	201	CPL	O2-C31-C32-C33
2	3I	201	CPL	O2-C31-C32-C33
2	3J	201	CPL	O2-C31-C32-C33
2	3K	201	CPL	O2-C31-C32-C33
2	3M	201	CPL	O2-C31-C32-C33
2	3N	201	CPL	O2-C31-C32-C33
2	4A	201	CPL	O2-C31-C32-C33
2	4B	201	CPL	O2-C31-C32-C33
2	4C	201	CPL	O2-C31-C32-C33
2	4D	201	CPL	O2-C31-C32-C33
2	4E	201	CPL	O2-C31-C32-C33
2	4F	201	CPL	O2-C31-C32-C33
2	4G	201	CPL	O2-C31-C32-C33
2	4H	201	CPL	O2-C31-C32-C33
2	4I	201	CPL	O2-C31-C32-C33
2	4J	201	CPL	O2-C31-C32-C33
2	4L	201	CPL	O2-C31-C32-C33
2	4M	201	CPL	O2-C31-C32-C33
2	4N	201	CPL	O2-C31-C32-C33
2	5A	201	CPL	O2-C31-C32-C33
2	5D	201	CPL	O2-C31-C32-C33
2	5E	201	CPL	O2-C31-C32-C33
2	5F	201	CPL	O2-C31-C32-C33
2	5G	201	CPL	O2-C31-C32-C33
2	5H	201	CPL	O2-C31-C32-C33
2	5I	201	CPL	O2-C31-C32-C33
2	5J	201	CPL	O2-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
2	5K	201	CPL	O2-C31-C32-C33
2	5L	201	CPL	O2-C31-C32-C33
2	5M	201	CPL	O2-C31-C32-C33
2	5N	201	CPL	O2-C31-C32-C33
2	2C	201	CPL	O2-C31-C32-C33
2	2D	201	CPL	O2-C31-C32-C33
2	2M	201	CPL	O2-C31-C32-C33
2	3L	201	CPL	O2-C31-C32-C33
2	5B	201	CPL	O2-C31-C32-C33
2	1A	201	CPL	O2-C2-C3-O3
2	1B	201	CPL	O2-C2-C3-O3
2	1C	201	CPL	O2-C2-C3-O3
2	1D	201	CPL	O2-C2-C3-O3
2	1E	201	CPL	O2-C2-C3-O3
2	1F	201	CPL	O2-C2-C3-O3
2	1G	201	CPL	O2-C2-C3-O3
2	1H	201	CPL	O2-C2-C3-O3
2	1I	201	CPL	O2-C2-C3-O3
2	1J	201	CPL	O2-C2-C3-O3
2	1K	201	CPL	O2-C2-C3-O3
2	1L	201	CPL	O2-C2-C3-O3
2	1M	201	CPL	O2-C2-C3-O3
2	1N	201	CPL	O2-C2-C3-O3
2	2A	201	CPL	O2-C2-C3-O3
2	2B	201	CPL	O2-C2-C3-O3
2	2C	201	CPL	O2-C2-C3-O3
2	2D	201	CPL	O2-C2-C3-O3
2	2E	201	CPL	O2-C2-C3-O3
2	2F	201	CPL	O2-C2-C3-O3
2	2G	201	CPL	O2-C2-C3-O3
2	2H	201	CPL	O2-C2-C3-O3
2	2I	201	CPL	O2-C2-C3-O3
2	2J	201	CPL	O2-C2-C3-O3
2	2K	201	CPL	O2-C2-C3-O3
2	2L	201	CPL	O2-C2-C3-O3
2	2M	201	CPL	O2-C2-C3-O3
2	2N	201	CPL	O2-C2-C3-O3
2	3A	201	CPL	O2-C2-C3-O3
2	3B	201	CPL	O2-C2-C3-O3
2	3C	201	CPL	O2-C2-C3-O3
2	3D	201	CPL	O2-C2-C3-O3
2	3E	201	CPL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	3F	201	CPL	O2-C2-C3-O3
2	3G	201	CPL	O2-C2-C3-O3
2	3H	201	CPL	O2-C2-C3-O3
2	3I	201	CPL	O2-C2-C3-O3
2	3J	201	CPL	O2-C2-C3-O3
2	3K	201	CPL	O2-C2-C3-O3
2	3L	201	CPL	O2-C2-C3-O3
2	3M	201	CPL	O2-C2-C3-O3
2	3N	201	CPL	O2-C2-C3-O3
2	4A	201	CPL	O2-C2-C3-O3
2	4B	201	CPL	O2-C2-C3-O3
2	4C	201	CPL	O2-C2-C3-O3
2	4D	201	CPL	O2-C2-C3-O3
2	4E	201	CPL	O2-C2-C3-O3
2	4F	201	CPL	O2-C2-C3-O3
2	4G	201	CPL	O2-C2-C3-O3
2	4H	201	CPL	O2-C2-C3-O3
2	4I	201	CPL	O2-C2-C3-O3
2	4J	201	CPL	O2-C2-C3-O3
2	4K	201	CPL	O2-C2-C3-O3
2	4L	201	CPL	O2-C2-C3-O3
2	4M	201	CPL	O2-C2-C3-O3
2	4N	201	CPL	O2-C2-C3-O3
2	5A	201	CPL	O2-C2-C3-O3
2	5B	201	CPL	O2-C2-C3-O3
2	5C	201	CPL	O2-C2-C3-O3
2	5D	201	CPL	O2-C2-C3-O3
2	5E	201	CPL	O2-C2-C3-O3
2	5F	201	CPL	O2-C2-C3-O3
2	5G	201	CPL	O2-C2-C3-O3
2	5H	201	CPL	O2-C2-C3-O3
2	5I	201	CPL	O2-C2-C3-O3
2	5J	201	CPL	O2-C2-C3-O3
2	5K	201	CPL	O2-C2-C3-O3
2	5L	201	CPL	O2-C2-C3-O3
2	5M	201	CPL	O2-C2-C3-O3
2	5N	201	CPL	O2-C2-C3-O3
2	3D	201	CPL	O2-C31-C32-C33
2	3H	201	CPL	O2-C31-C32-C33
2	4K	201	CPL	O2-C31-C32-C33
2	5C	201	CPL	O2-C31-C32-C33
2	1A	201	CPL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
2	1B	201	CPL	C39-C40-C41-C42
2	1C	201	CPL	C39-C40-C41-C42
2	1D	201	CPL	C39-C40-C41-C42
2	1E	201	CPL	C39-C40-C41-C42
2	1F	201	CPL	C39-C40-C41-C42
2	1G	201	CPL	C39-C40-C41-C42
2	1H	201	CPL	C39-C40-C41-C42
2	1I	201	CPL	C39-C40-C41-C42
2	1J	201	CPL	C39-C40-C41-C42
2	1K	201	CPL	C39-C40-C41-C42
2	1L	201	CPL	C39-C40-C41-C42
2	1M	201	CPL	C39-C40-C41-C42
2	1N	201	CPL	C39-C40-C41-C42
2	2A	201	CPL	C39-C40-C41-C42
2	2B	201	CPL	C39-C40-C41-C42
2	2C	201	CPL	C39-C40-C41-C42
2	2D	201	CPL	C39-C40-C41-C42
2	2E	201	CPL	C39-C40-C41-C42
2	2F	201	CPL	C39-C40-C41-C42
2	2G	201	CPL	C39-C40-C41-C42
2	2H	201	CPL	C39-C40-C41-C42
2	2I	201	CPL	C39-C40-C41-C42
2	2J	201	CPL	C39-C40-C41-C42
2	2K	201	CPL	C39-C40-C41-C42
2	2L	201	CPL	C39-C40-C41-C42
2	2M	201	CPL	C39-C40-C41-C42
2	2N	201	CPL	C39-C40-C41-C42
2	3A	201	CPL	C39-C40-C41-C42
2	3B	201	CPL	C39-C40-C41-C42
2	3C	201	CPL	C39-C40-C41-C42
2	3D	201	CPL	C39-C40-C41-C42
2	3E	201	CPL	C39-C40-C41-C42
2	3F	201	CPL	C39-C40-C41-C42
2	3G	201	CPL	C39-C40-C41-C42
2	3H	201	CPL	C39-C40-C41-C42
2	3I	201	CPL	C39-C40-C41-C42
2	3J	201	CPL	C39-C40-C41-C42
2	3K	201	CPL	C39-C40-C41-C42
2	3L	201	CPL	C39-C40-C41-C42
2	3M	201	CPL	C39-C40-C41-C42
2	3N	201	CPL	C39-C40-C41-C42
2	4A	201	CPL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
2	4B	201	CPL	C39-C40-C41-C42
2	4C	201	CPL	C39-C40-C41-C42
2	4D	201	CPL	C39-C40-C41-C42
2	4E	201	CPL	C39-C40-C41-C42
2	4F	201	CPL	C39-C40-C41-C42
2	4G	201	CPL	C39-C40-C41-C42
2	4H	201	CPL	C39-C40-C41-C42
2	4I	201	CPL	C39-C40-C41-C42
2	4J	201	CPL	C39-C40-C41-C42
2	4K	201	CPL	C39-C40-C41-C42
2	4L	201	CPL	C39-C40-C41-C42
2	4M	201	CPL	C39-C40-C41-C42
2	4N	201	CPL	C39-C40-C41-C42
2	5A	201	CPL	C39-C40-C41-C42
2	5B	201	CPL	C39-C40-C41-C42
2	5C	201	CPL	C39-C40-C41-C42
2	5D	201	CPL	C39-C40-C41-C42
2	5E	201	CPL	C39-C40-C41-C42
2	5F	201	CPL	C39-C40-C41-C42
2	5G	201	CPL	C39-C40-C41-C42
2	5H	201	CPL	C39-C40-C41-C42
2	5I	201	CPL	C39-C40-C41-C42
2	5J	201	CPL	C39-C40-C41-C42
2	5K	201	CPL	C39-C40-C41-C42
2	5L	201	CPL	C39-C40-C41-C42
2	5M	201	CPL	C39-C40-C41-C42
2	5N	201	CPL	C39-C40-C41-C42
2	2B	201	CPL	C17-C18-C19-C20
2	4L	201	CPL	C17-C18-C19-C20
2	5H	201	CPL	C17-C18-C19-C20
2	1B	201	CPL	C17-C18-C19-C20
2	1J	201	CPL	C17-C18-C19-C20
2	3I	201	CPL	C17-C18-C19-C20
2	4D	201	CPL	C17-C18-C19-C20
2	4M	201	CPL	C17-C18-C19-C20
2	1C	201	CPL	C17-C18-C19-C20
2	3B	201	CPL	C17-C18-C19-C20
2	3E	201	CPL	C17-C18-C19-C20
2	4I	201	CPL	C17-C18-C19-C20
2	5E	201	CPL	C17-C18-C19-C20
2	1G	201	CPL	C17-C18-C19-C20
2	1N	201	CPL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
2	2E	201	CPL	C17-C18-C19-C20
2	2F	201	CPL	C17-C18-C19-C20
2	2M	201	CPL	C17-C18-C19-C20
2	3M	201	CPL	C17-C18-C19-C20
2	4G	201	CPL	C17-C18-C19-C20
2	4H	201	CPL	C17-C18-C19-C20
2	4J	201	CPL	C17-C18-C19-C20
2	5A	201	CPL	C17-C18-C19-C20
2	5F	201	CPL	C17-C18-C19-C20
2	5G	201	CPL	C17-C18-C19-C20
2	1A	201	CPL	C17-C18-C19-C20
2	1D	201	CPL	C17-C18-C19-C20
2	1L	201	CPL	C17-C18-C19-C20
2	1M	201	CPL	C17-C18-C19-C20
2	2D	201	CPL	C17-C18-C19-C20
2	2H	201	CPL	C17-C18-C19-C20
2	2I	201	CPL	C17-C18-C19-C20
2	2N	201	CPL	C17-C18-C19-C20
2	3A	201	CPL	C17-C18-C19-C20
2	3D	201	CPL	C17-C18-C19-C20
2	3F	201	CPL	C17-C18-C19-C20
2	3G	201	CPL	C17-C18-C19-C20
2	3J	201	CPL	C17-C18-C19-C20
2	3K	201	CPL	C17-C18-C19-C20
2	3L	201	CPL	C17-C18-C19-C20
2	4C	201	CPL	C17-C18-C19-C20
2	5C	201	CPL	C17-C18-C19-C20
2	5J	201	CPL	C17-C18-C19-C20
2	5M	201	CPL	C17-C18-C19-C20
2	1E	201	CPL	C17-C18-C19-C20
2	1H	201	CPL	C17-C18-C19-C20
2	1I	201	CPL	C17-C18-C19-C20
2	1K	201	CPL	C17-C18-C19-C20
2	2A	201	CPL	C17-C18-C19-C20
2	2C	201	CPL	C17-C18-C19-C20
2	2G	201	CPL	C17-C18-C19-C20
2	2K	201	CPL	C17-C18-C19-C20
2	2L	201	CPL	C17-C18-C19-C20
2	3H	201	CPL	C17-C18-C19-C20
2	3N	201	CPL	C17-C18-C19-C20
2	4B	201	CPL	C17-C18-C19-C20
2	4E	201	CPL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
2	4N	201	CPL	C17-C18-C19-C20
2	5B	201	CPL	C17-C18-C19-C20
2	5K	201	CPL	C17-C18-C19-C20
2	1F	201	CPL	C17-C18-C19-C20
2	2J	201	CPL	C17-C18-C19-C20
2	3C	201	CPL	C17-C18-C19-C20
2	4A	201	CPL	C17-C18-C19-C20
2	5I	201	CPL	C17-C18-C19-C20
2	5N	201	CPL	C17-C18-C19-C20
2	4F	201	CPL	C17-C18-C19-C20
2	4K	201	CPL	C17-C18-C19-C20
2	5L	201	CPL	C17-C18-C19-C20
2	5D	201	CPL	C17-C18-C19-C20
2	1A	201	CPL	C42-C43-C44-C45
2	1B	201	CPL	C42-C43-C44-C45
2	1C	201	CPL	C42-C43-C44-C45
2	1D	201	CPL	C42-C43-C44-C45
2	1E	201	CPL	C42-C43-C44-C45
2	1F	201	CPL	C42-C43-C44-C45
2	1G	201	CPL	C42-C43-C44-C45
2	1H	201	CPL	C42-C43-C44-C45
2	1I	201	CPL	C42-C43-C44-C45
2	1J	201	CPL	C42-C43-C44-C45
2	1K	201	CPL	C42-C43-C44-C45
2	1L	201	CPL	C42-C43-C44-C45
2	1M	201	CPL	C42-C43-C44-C45
2	1N	201	CPL	C42-C43-C44-C45
2	2A	201	CPL	C42-C43-C44-C45
2	2B	201	CPL	C42-C43-C44-C45
2	2C	201	CPL	C42-C43-C44-C45
2	2D	201	CPL	C42-C43-C44-C45
2	2E	201	CPL	C42-C43-C44-C45
2	2F	201	CPL	C42-C43-C44-C45
2	2G	201	CPL	C42-C43-C44-C45
2	2H	201	CPL	C42-C43-C44-C45
2	2I	201	CPL	C42-C43-C44-C45
2	2J	201	CPL	C42-C43-C44-C45
2	2K	201	CPL	C42-C43-C44-C45
2	2L	201	CPL	C42-C43-C44-C45
2	2M	201	CPL	C42-C43-C44-C45
2	2N	201	CPL	C42-C43-C44-C45
2	3B	201	CPL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
2	3C	201	CPL	C42-C43-C44-C45
2	3D	201	CPL	C42-C43-C44-C45
2	3E	201	CPL	C42-C43-C44-C45
2	3F	201	CPL	C42-C43-C44-C45
2	3G	201	CPL	C42-C43-C44-C45
2	3H	201	CPL	C42-C43-C44-C45
2	3I	201	CPL	C42-C43-C44-C45
2	3J	201	CPL	C42-C43-C44-C45
2	3K	201	CPL	C42-C43-C44-C45
2	3L	201	CPL	C42-C43-C44-C45
2	3M	201	CPL	C42-C43-C44-C45
2	3N	201	CPL	C42-C43-C44-C45
2	4A	201	CPL	C42-C43-C44-C45
2	4B	201	CPL	C42-C43-C44-C45
2	4C	201	CPL	C42-C43-C44-C45
2	4D	201	CPL	C42-C43-C44-C45
2	4E	201	CPL	C42-C43-C44-C45
2	4F	201	CPL	C42-C43-C44-C45
2	4G	201	CPL	C42-C43-C44-C45
2	4H	201	CPL	C42-C43-C44-C45
2	4I	201	CPL	C42-C43-C44-C45
2	4J	201	CPL	C42-C43-C44-C45
2	4K	201	CPL	C42-C43-C44-C45
2	4L	201	CPL	C42-C43-C44-C45
2	4M	201	CPL	C42-C43-C44-C45
2	4N	201	CPL	C42-C43-C44-C45
2	5A	201	CPL	C42-C43-C44-C45
2	5B	201	CPL	C42-C43-C44-C45
2	5C	201	CPL	C42-C43-C44-C45
2	5D	201	CPL	C42-C43-C44-C45
2	5E	201	CPL	C42-C43-C44-C45
2	5F	201	CPL	C42-C43-C44-C45
2	5G	201	CPL	C42-C43-C44-C45
2	5H	201	CPL	C42-C43-C44-C45
2	5I	201	CPL	C42-C43-C44-C45
2	5J	201	CPL	C42-C43-C44-C45
2	5K	201	CPL	C42-C43-C44-C45
2	5L	201	CPL	C42-C43-C44-C45
2	5M	201	CPL	C42-C43-C44-C45
2	5N	201	CPL	C42-C43-C44-C45
2	3A	201	CPL	C42-C43-C44-C45
2	4F	201	CPL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
2	1H	201	CPL	C23-C24-C25-C26
2	1J	201	CPL	C23-C24-C25-C26
2	2A	201	CPL	C23-C24-C25-C26
2	2H	201	CPL	C23-C24-C25-C26
2	3A	201	CPL	C23-C24-C25-C26
2	3B	201	CPL	C23-C24-C25-C26
2	3L	201	CPL	C23-C24-C25-C26
2	3M	201	CPL	C23-C24-C25-C26
2	4E	201	CPL	C23-C24-C25-C26
2	4G	201	CPL	C23-C24-C25-C26
2	4N	201	CPL	C23-C24-C25-C26
2	5B	201	CPL	C23-C24-C25-C26
2	5C	201	CPL	C23-C24-C25-C26
2	1B	201	CPL	C23-C24-C25-C26
2	1D	201	CPL	C23-C24-C25-C26
2	1N	201	CPL	C23-C24-C25-C26
2	2B	201	CPL	C23-C24-C25-C26
2	2C	201	CPL	C23-C24-C25-C26
2	2D	201	CPL	C23-C24-C25-C26
2	2J	201	CPL	C23-C24-C25-C26
2	2K	201	CPL	C23-C24-C25-C26
2	2L	201	CPL	C23-C24-C25-C26
2	3H	201	CPL	C23-C24-C25-C26
2	3K	201	CPL	C23-C24-C25-C26
2	3N	201	CPL	C23-C24-C25-C26
2	4C	201	CPL	C23-C24-C25-C26
2	4D	201	CPL	C23-C24-C25-C26
2	4H	201	CPL	C23-C24-C25-C26
2	4I	201	CPL	C23-C24-C25-C26
2	4K	201	CPL	C23-C24-C25-C26
2	4L	201	CPL	C23-C24-C25-C26
2	5K	201	CPL	C23-C24-C25-C26
2	1A	201	CPL	C23-C24-C25-C26
2	1C	201	CPL	C23-C24-C25-C26
2	1E	201	CPL	C23-C24-C25-C26
2	1F	201	CPL	C23-C24-C25-C26
2	1G	201	CPL	C23-C24-C25-C26
2	1I	201	CPL	C23-C24-C25-C26
2	1K	201	CPL	C23-C24-C25-C26
2	1L	201	CPL	C23-C24-C25-C26
2	1M	201	CPL	C23-C24-C25-C26
2	2E	201	CPL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
2	2F	201	CPL	C23-C24-C25-C26
2	2G	201	CPL	C23-C24-C25-C26
2	2I	201	CPL	C23-C24-C25-C26
2	2M	201	CPL	C23-C24-C25-C26
2	2N	201	CPL	C23-C24-C25-C26
2	3D	201	CPL	C23-C24-C25-C26
2	3F	201	CPL	C23-C24-C25-C26
2	3G	201	CPL	C23-C24-C25-C26
2	3I	201	CPL	C23-C24-C25-C26
2	3J	201	CPL	C23-C24-C25-C26
2	4A	201	CPL	C23-C24-C25-C26
2	4B	201	CPL	C23-C24-C25-C26
2	4J	201	CPL	C23-C24-C25-C26
2	4M	201	CPL	C23-C24-C25-C26
2	5A	201	CPL	C23-C24-C25-C26
2	5E	201	CPL	C23-C24-C25-C26
2	5F	201	CPL	C23-C24-C25-C26
2	5G	201	CPL	C23-C24-C25-C26
2	5H	201	CPL	C23-C24-C25-C26
2	5I	201	CPL	C23-C24-C25-C26
2	5J	201	CPL	C23-C24-C25-C26
2	5L	201	CPL	C23-C24-C25-C26
2	5M	201	CPL	C23-C24-C25-C26
2	5N	201	CPL	C23-C24-C25-C26
2	3C	201	CPL	C23-C24-C25-C26
2	3E	201	CPL	C23-C24-C25-C26
2	5D	201	CPL	C23-C24-C25-C26
2	1A	201	CPL	C2-C1-O3P-P
2	1B	201	CPL	C2-C1-O3P-P
2	1C	201	CPL	C2-C1-O3P-P
2	1D	201	CPL	C2-C1-O3P-P
2	1E	201	CPL	C2-C1-O3P-P
2	1G	201	CPL	C2-C1-O3P-P
2	1H	201	CPL	C2-C1-O3P-P
2	1J	201	CPL	C2-C1-O3P-P
2	1L	201	CPL	C2-C1-O3P-P
2	1M	201	CPL	C2-C1-O3P-P
2	1N	201	CPL	C2-C1-O3P-P
2	2A	201	CPL	C2-C1-O3P-P
2	2B	201	CPL	C2-C1-O3P-P
2	2C	201	CPL	C2-C1-O3P-P
2	2D	201	CPL	C2-C1-O3P-P

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Mol	Chain	Res	Type	Atoms
2	2E	201	CPL	C2-C1-O3P-P
2	2F	201	CPL	C2-C1-O3P-P
2	2H	201	CPL	C2-C1-O3P-P
2	2I	201	CPL	C2-C1-O3P-P
2	2J	201	CPL	C2-C1-O3P-P
2	2L	201	CPL	C2-C1-O3P-P
2	2M	201	CPL	C2-C1-O3P-P
2	2N	201	CPL	C2-C1-O3P-P
2	3A	201	CPL	C2-C1-O3P-P
2	3B	201	CPL	C2-C1-O3P-P
2	3C	201	CPL	C2-C1-O3P-P
2	3D	201	CPL	C2-C1-O3P-P
2	3E	201	CPL	C2-C1-O3P-P
2	3F	201	CPL	C2-C1-O3P-P
2	3G	201	CPL	C2-C1-O3P-P
2	3H	201	CPL	C2-C1-O3P-P
2	3I	201	CPL	C2-C1-O3P-P
2	3J	201	CPL	C2-C1-O3P-P
2	3K	201	CPL	C2-C1-O3P-P
2	3L	201	CPL	C2-C1-O3P-P
2	3M	201	CPL	C2-C1-O3P-P
2	3N	201	CPL	C2-C1-O3P-P
2	4B	201	CPL	C2-C1-O3P-P
2	4C	201	CPL	C2-C1-O3P-P
2	4D	201	CPL	C2-C1-O3P-P
2	4E	201	CPL	C2-C1-O3P-P
2	4F	201	CPL	C2-C1-O3P-P
2	4G	201	CPL	C2-C1-O3P-P
2	4H	201	CPL	C2-C1-O3P-P
2	4I	201	CPL	C2-C1-O3P-P
2	4J	201	CPL	C2-C1-O3P-P
2	4M	201	CPL	C2-C1-O3P-P
2	4N	201	CPL	C2-C1-O3P-P
2	5E	201	CPL	C2-C1-O3P-P
2	5G	201	CPL	C2-C1-O3P-P
2	5H	201	CPL	C2-C1-O3P-P
2	5J	201	CPL	C2-C1-O3P-P
2	5K	201	CPL	C2-C1-O3P-P
2	5L	201	CPL	C2-C1-O3P-P
2	5N	201	CPL	C2-C1-O3P-P

There are no ring outliers.

68 monomers are involved in 166 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1C	201	CPL	2	0
2	1J	201	CPL	1	0
2	2G	201	CPL	3	0
2	3G	201	CPL	2	0
2	4M	201	CPL	3	0
2	4C	201	CPL	3	0
2	4E	201	CPL	3	0
2	1D	201	CPL	2	0
2	3A	201	CPL	4	0
2	5E	201	CPL	4	0
2	4A	201	CPL	3	0
2	3H	201	CPL	3	0
2	2C	201	CPL	1	0
2	2M	201	CPL	3	0
2	2K	201	CPL	3	0
2	5B	201	CPL	3	0
2	5K	201	CPL	3	0
2	1G	201	CPL	2	0
2	5N	201	CPL	1	0
2	1N	201	CPL	2	0
2	3D	201	CPL	2	0
2	1L	201	CPL	3	0
2	3L	201	CPL	2	0
2	4F	201	CPL	2	0
2	1A	201	CPL	3	0
2	4I	201	CPL	2	0
2	5J	201	CPL	3	0
2	1K	201	CPL	3	0
2	3E	201	CPL	3	0
2	2I	201	CPL	3	0
2	1F	201	CPL	2	0
2	5H	201	CPL	2	0
2	2J	201	CPL	3	0
2	3I	201	CPL	5	0
2	3N	201	CPL	2	0
2	5I	201	CPL	3	0
2	1H	201	CPL	3	0
2	4J	201	CPL	1	0
2	1I	201	CPL	2	0
2	3K	201	CPL	3	0
2	3B	201	CPL	1	0
2	3J	201	CPL	4	0

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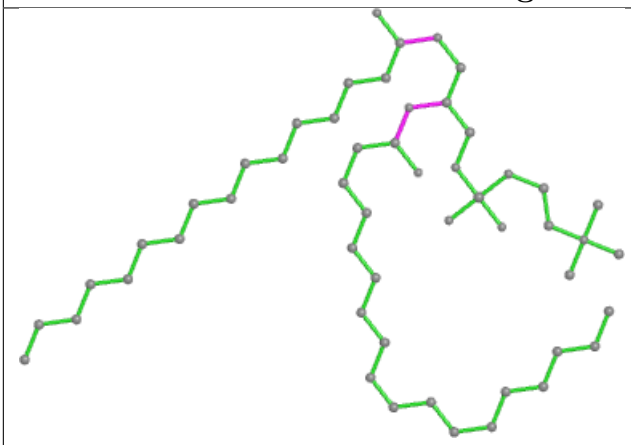
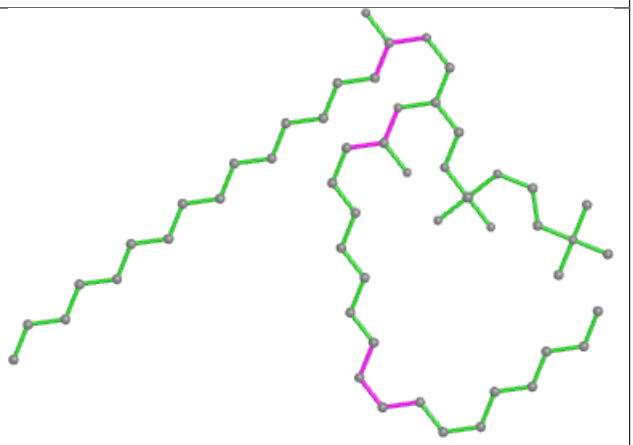
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	5D	201	CPL	4	0
2	2H	201	CPL	3	0
2	4H	201	CPL	4	0
2	4G	201	CPL	3	0
2	2B	201	CPL	3	0
2	3M	201	CPL	2	0
2	5M	201	CPL	3	0
2	2D	201	CPL	2	0
2	2A	201	CPL	4	0
2	1E	201	CPL	3	0
2	2L	201	CPL	2	0
2	3C	201	CPL	2	0
2	4D	201	CPL	1	0
2	4L	201	CPL	2	0
2	4B	201	CPL	2	0
2	5G	201	CPL	1	0
2	5L	201	CPL	3	0
2	1M	201	CPL	4	0
2	4K	201	CPL	2	0
2	5C	201	CPL	2	0
2	5A	201	CPL	3	0
2	2F	201	CPL	2	0
2	2E	201	CPL	2	0
2	5F	201	CPL	5	0
2	3F	201	CPL	2	0
2	1B	201	CPL	2	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.

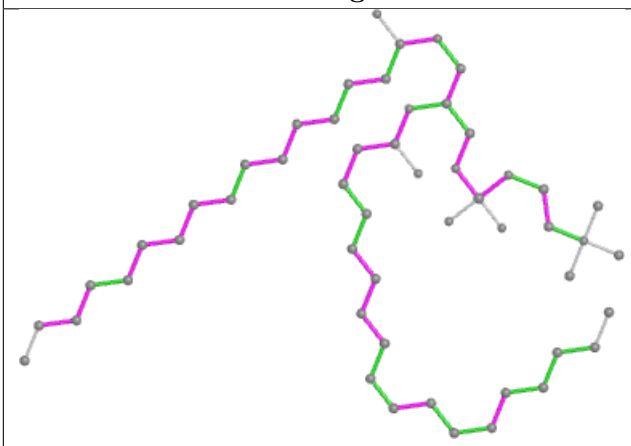
Ligand CPL 1C 201



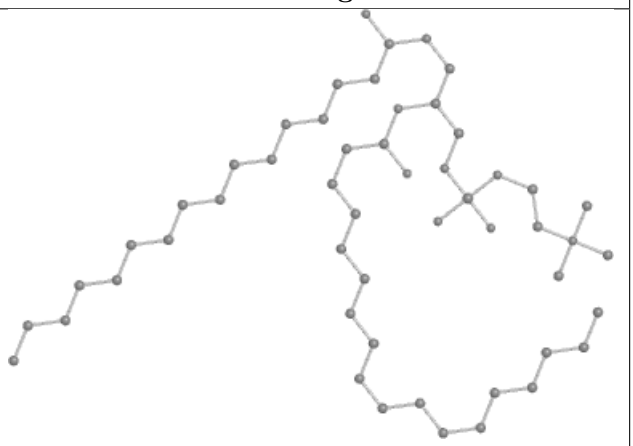
Bond lengths



Bond angles

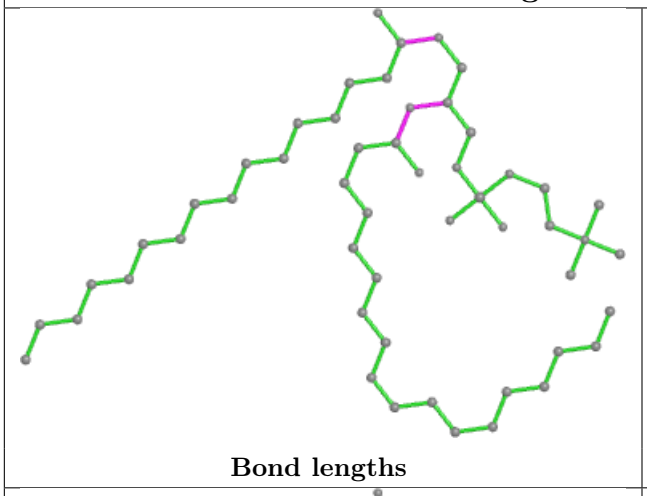


Torsions

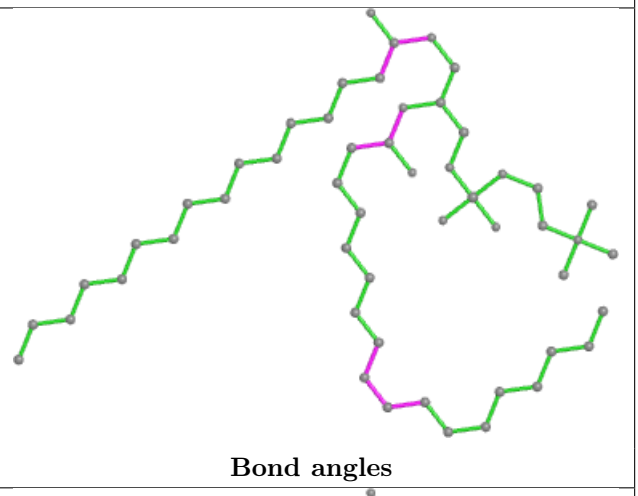


Rings

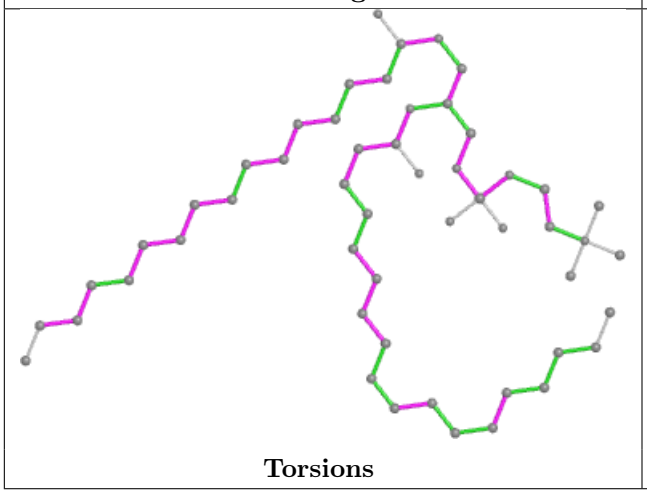
Ligand CPL 1J 201



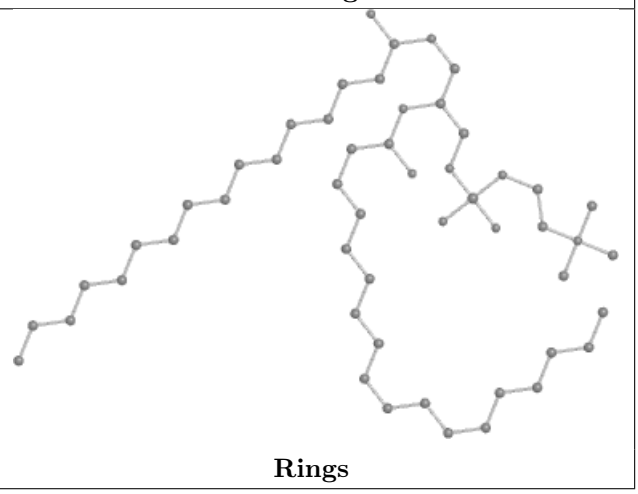
Bond lengths



Bond angles

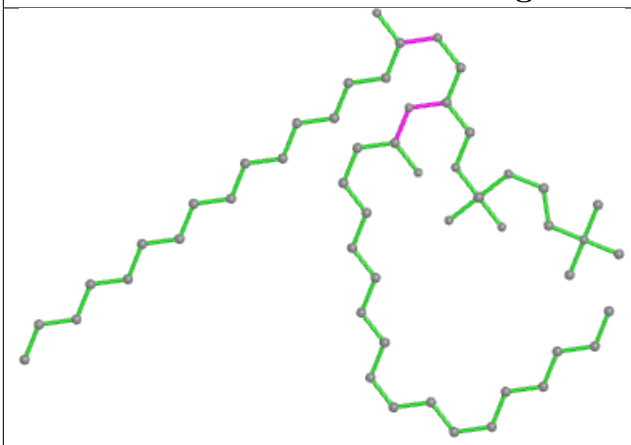


Torsions

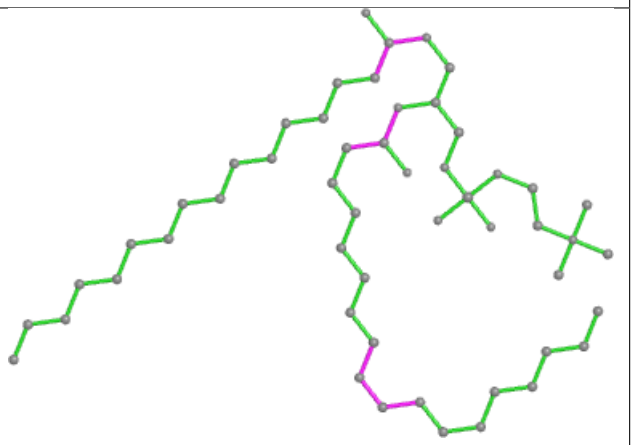


Rings

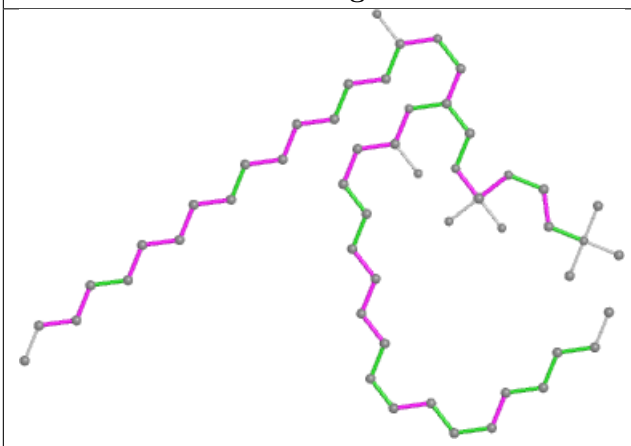
Ligand CPL 2G 201



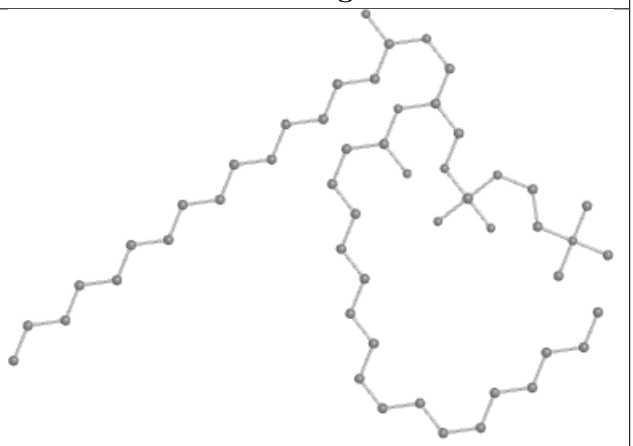
Bond lengths



Bond angles

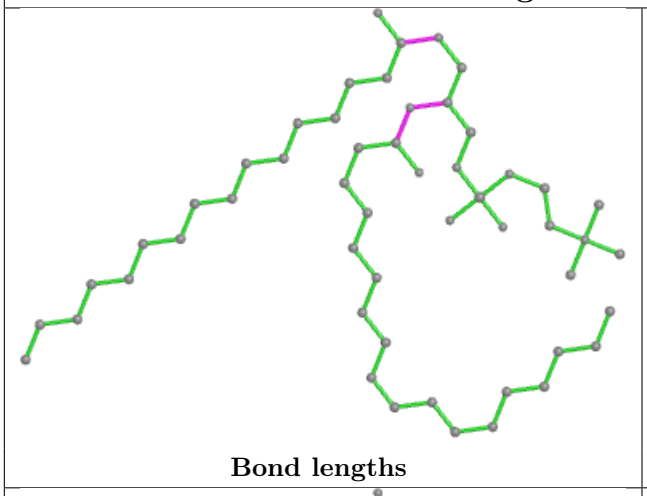


Torsions

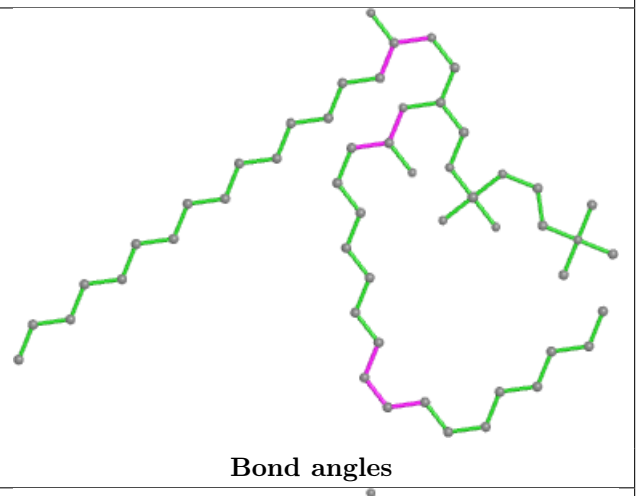


Rings

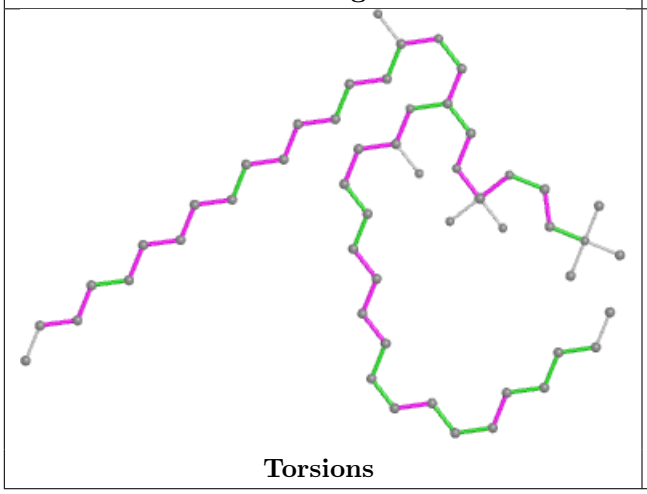
Ligand CPL 3G 201



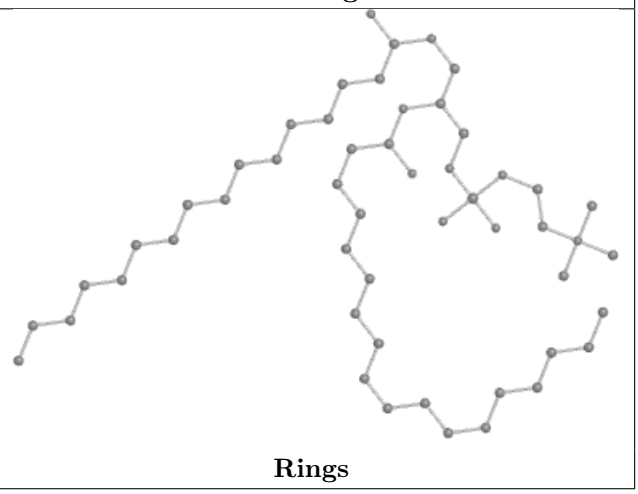
Bond lengths



Bond angles

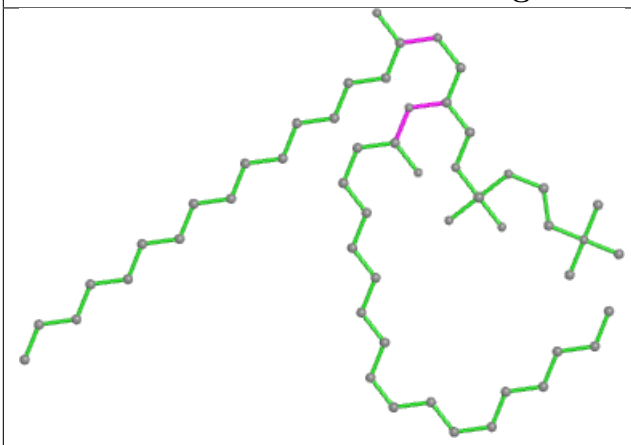


Torsions

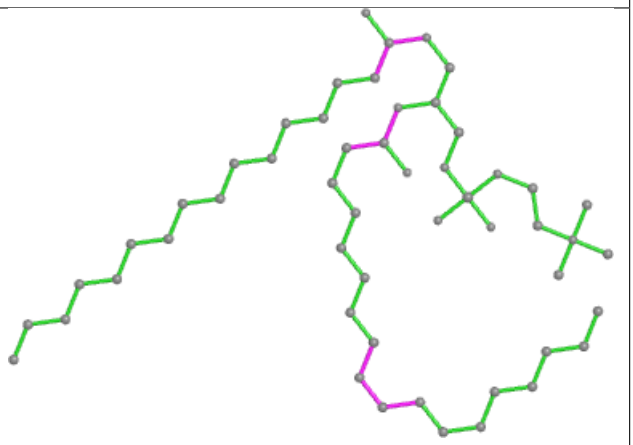


Rings

Ligand CPL 4M 201



Bond lengths



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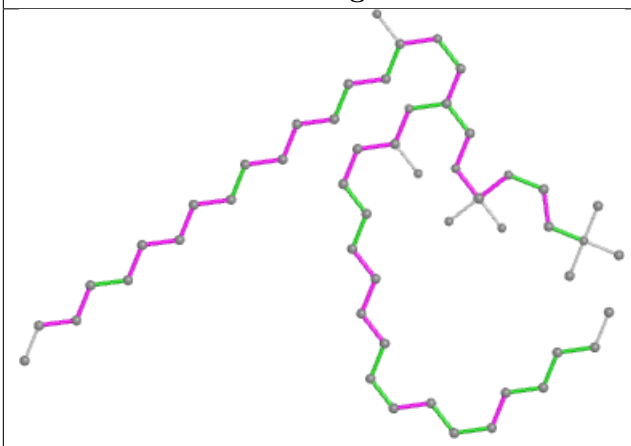

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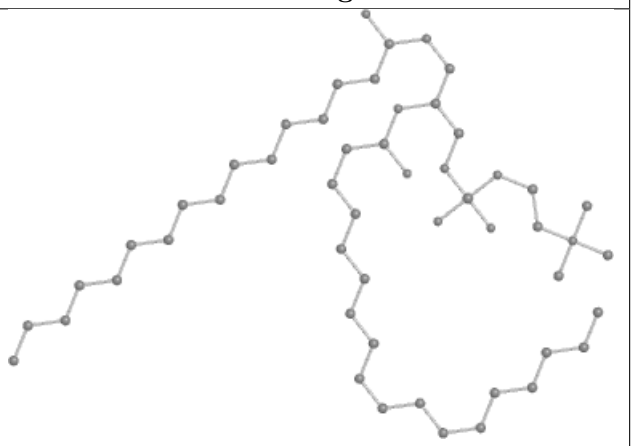
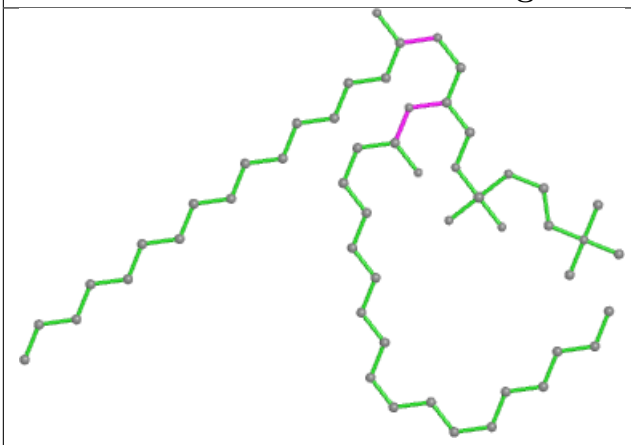


Rings

Ligand CPL 4C 201



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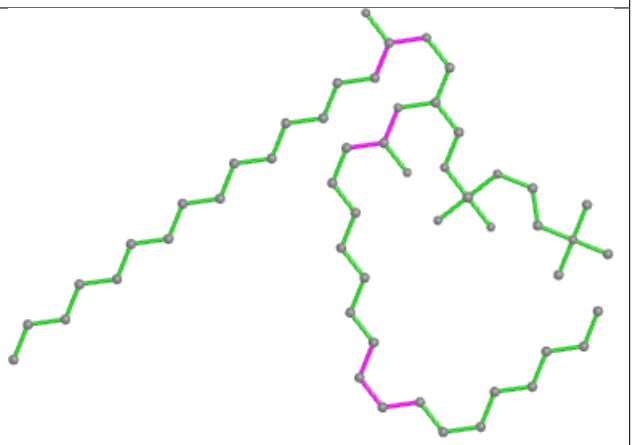
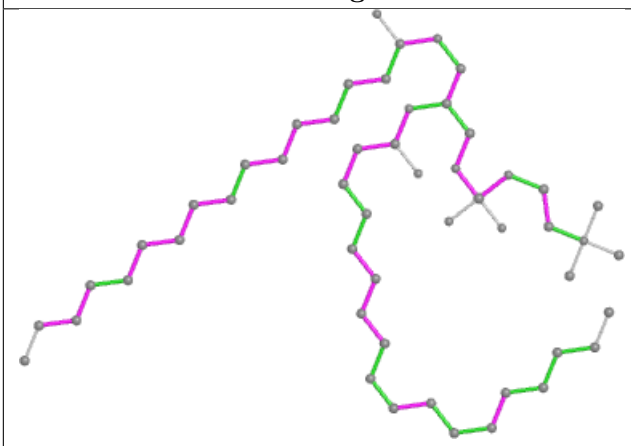


Bond angles



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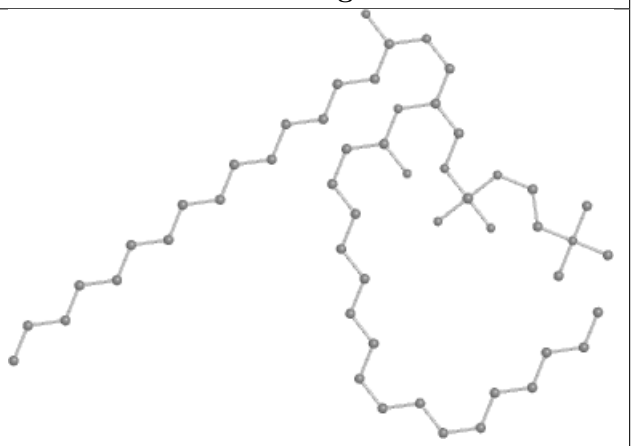

Rings

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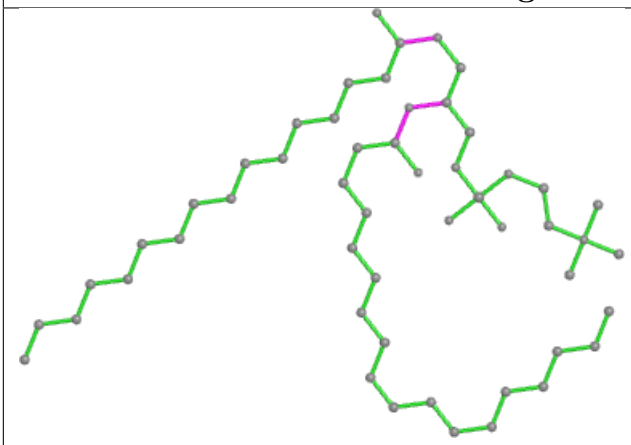

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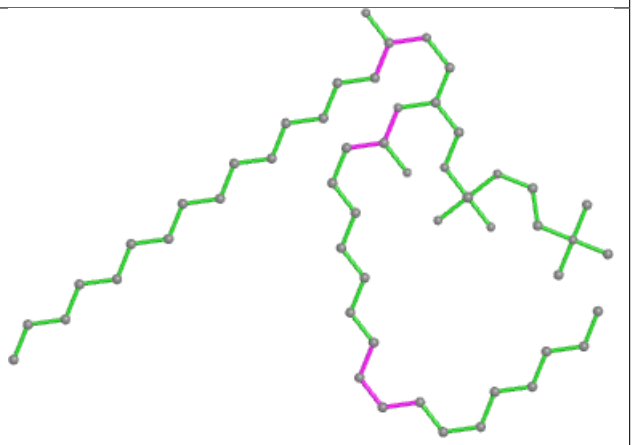
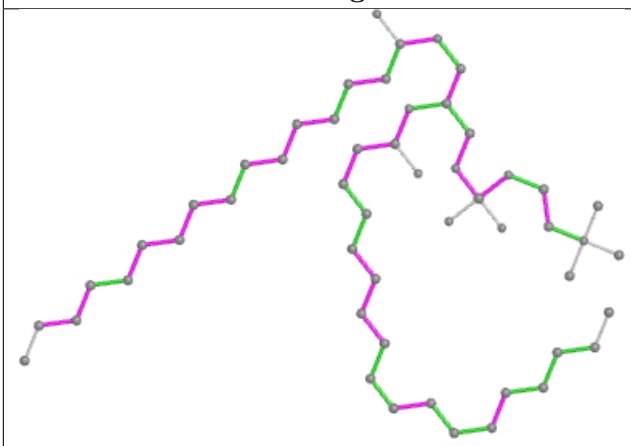
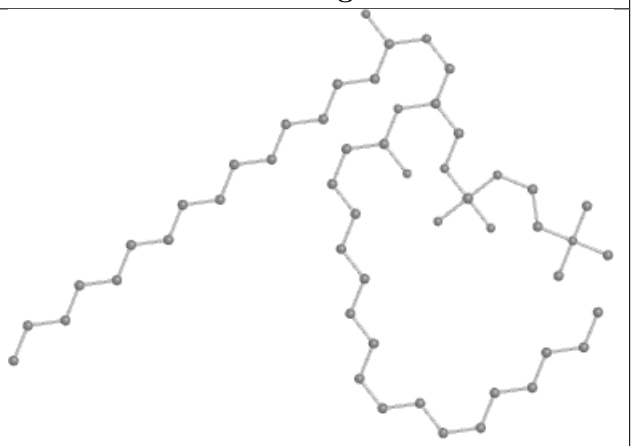


Bond angles

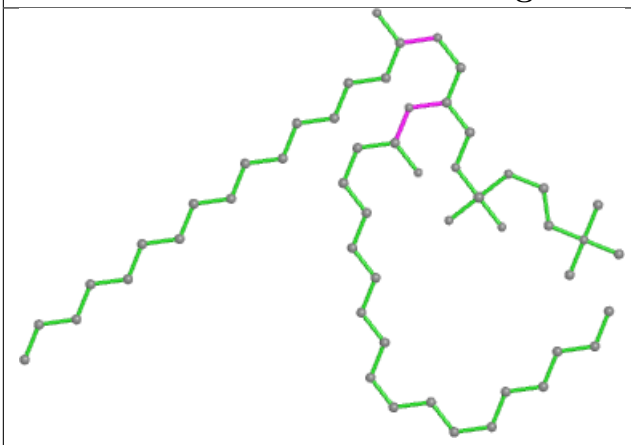


Torsions



Rings

Ligand CPL 1D 201



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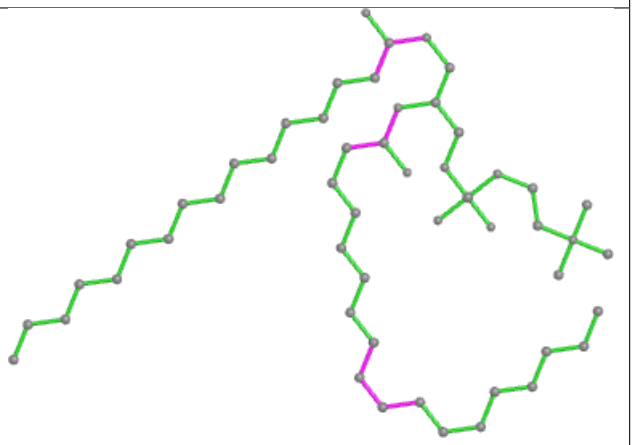
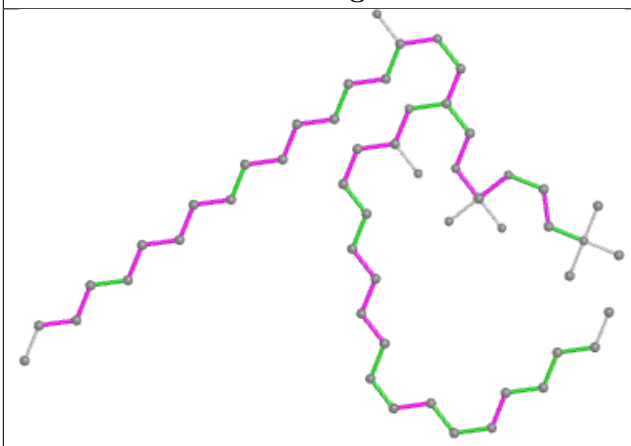


Bond angles



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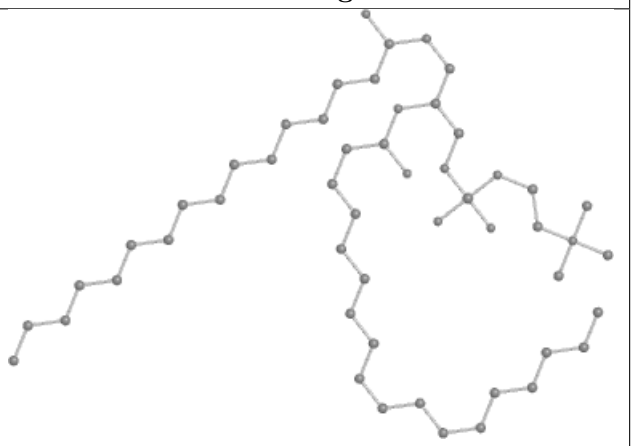
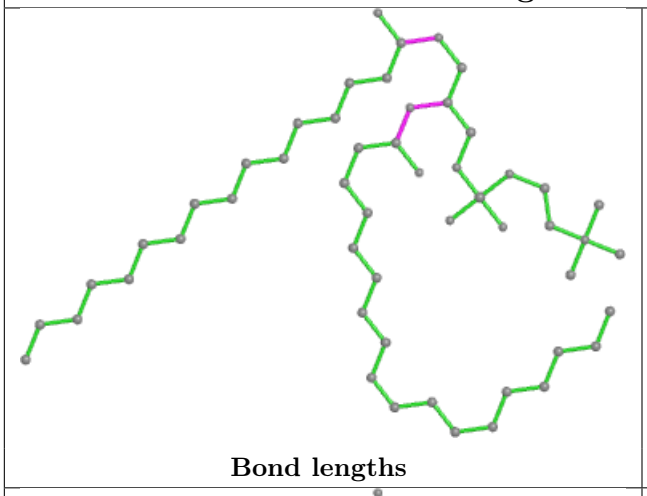


Rings

Ligand CPL 3A 201



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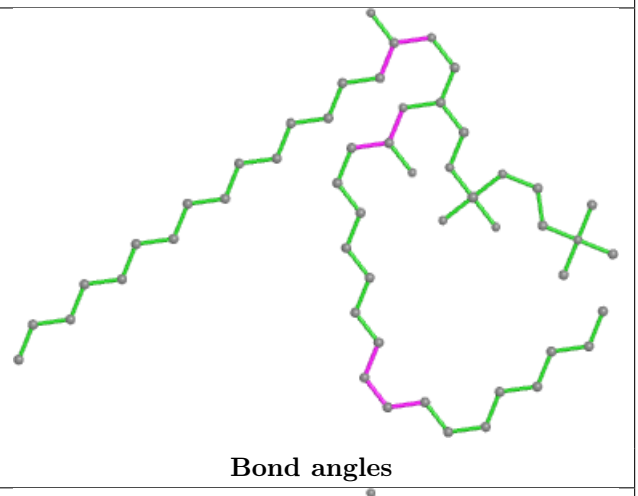
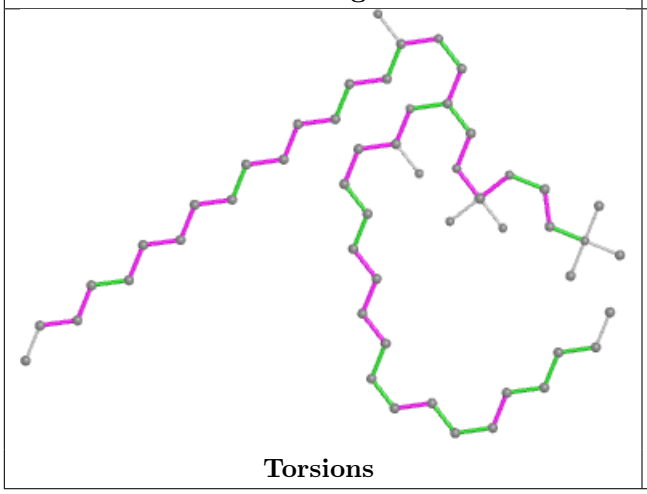


Bond angles



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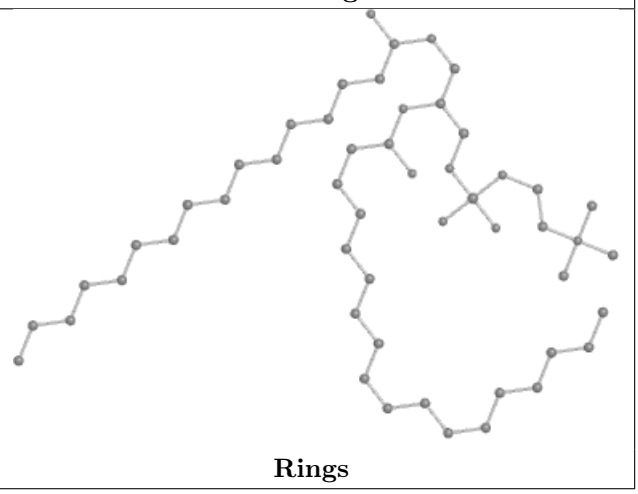
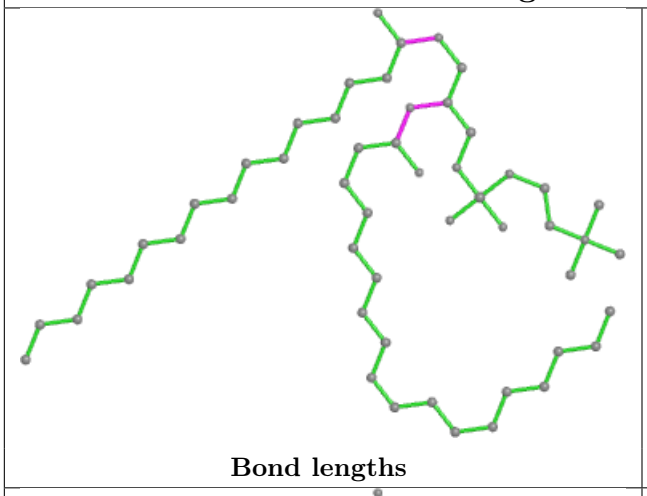


Rings

Ligand CPL 5E 201



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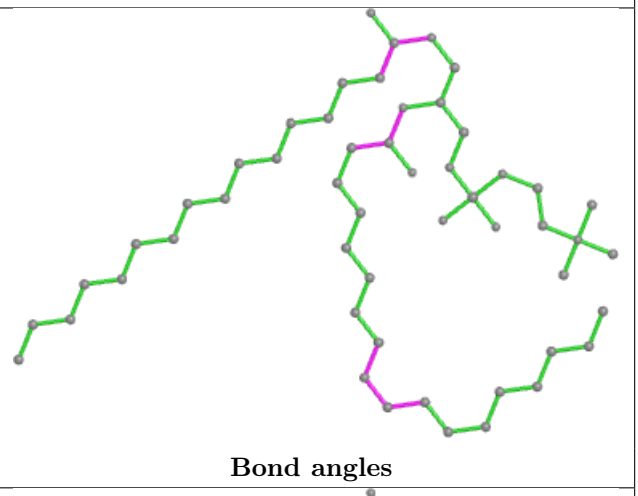
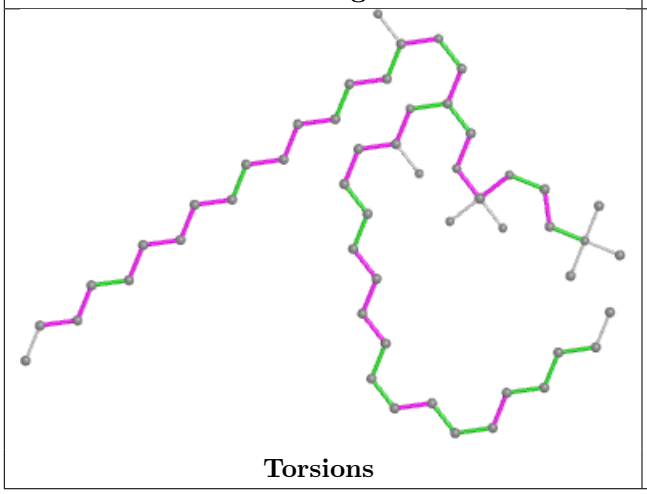


Bond angles



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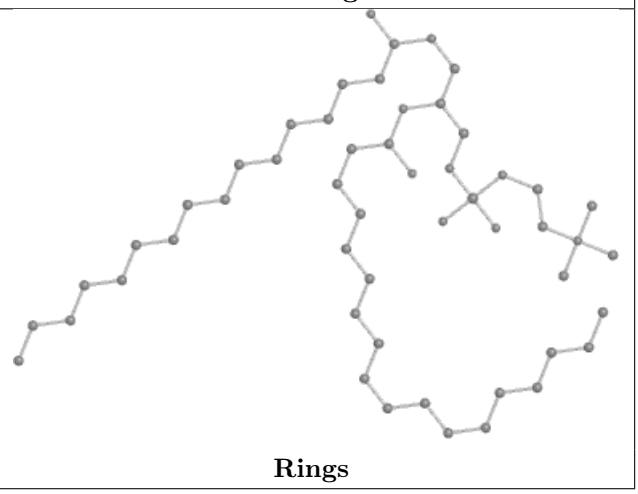
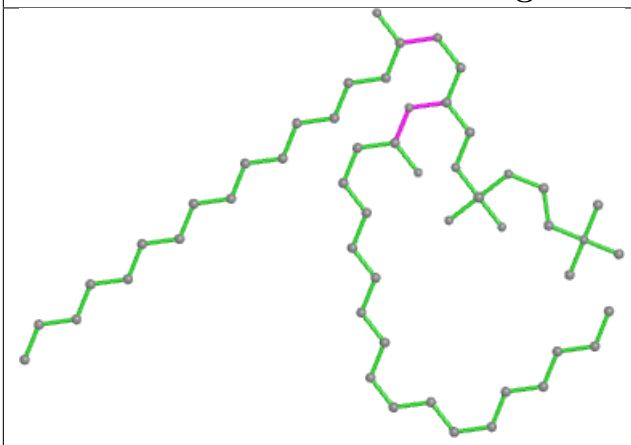


Rings

Ligand CPL 4A 201



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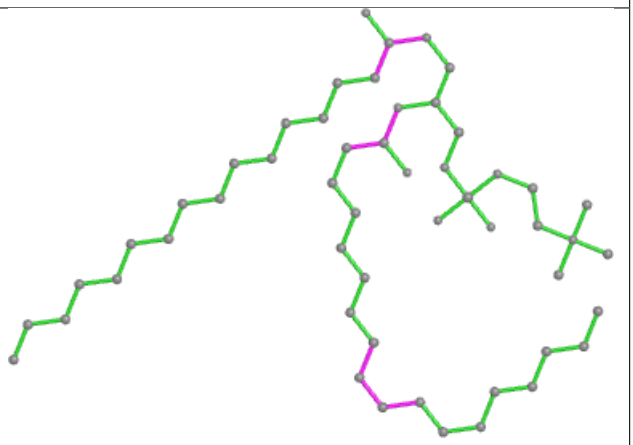
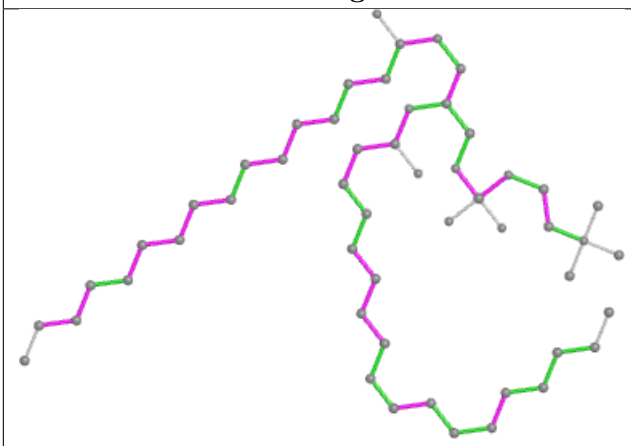


Bond angles



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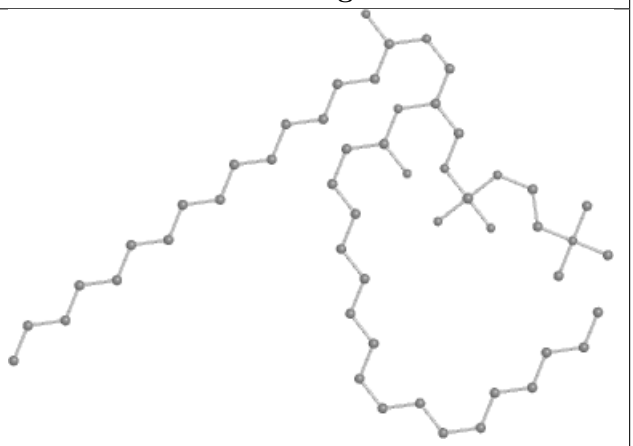
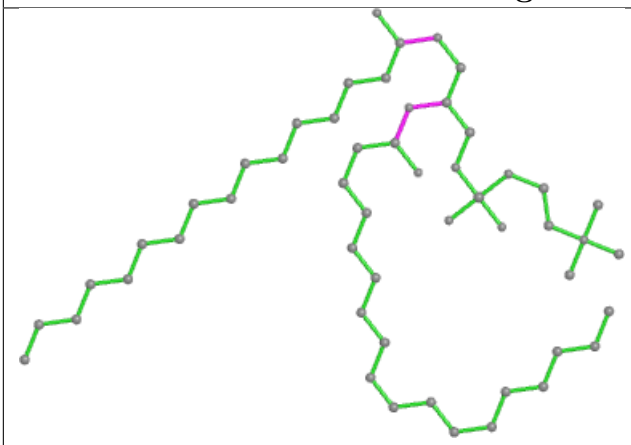


Rings

Ligand CPL 3H 201



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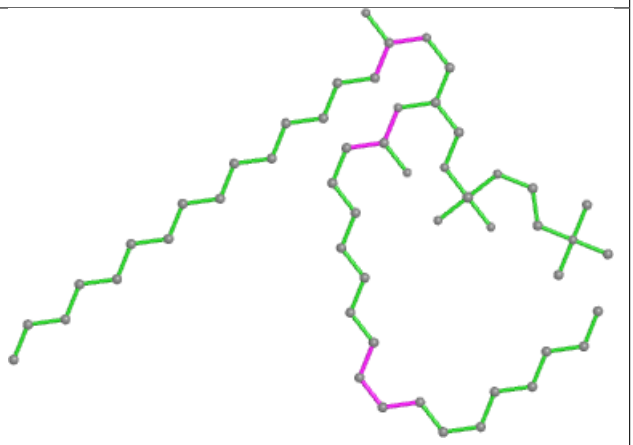
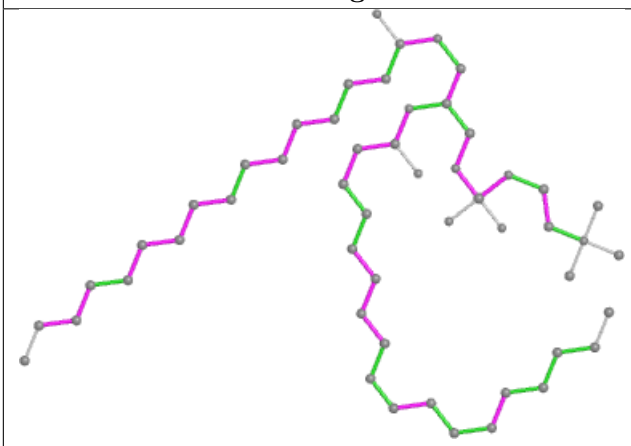


Bond angles



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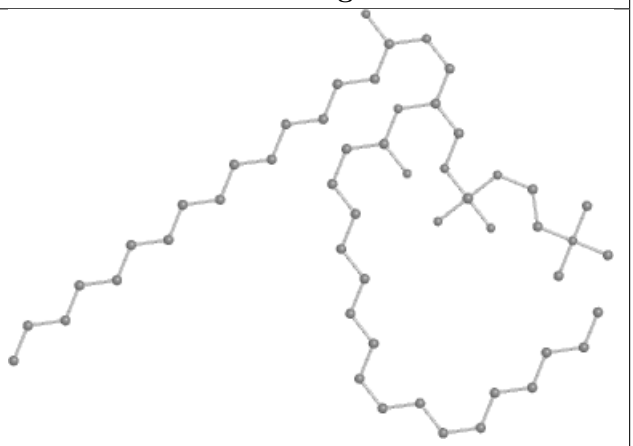
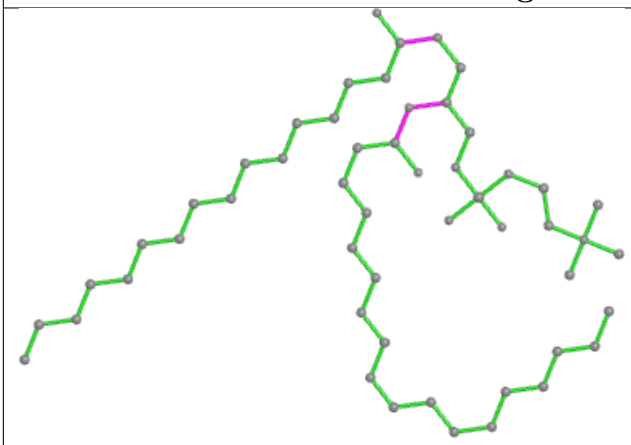


Rings

Ligand CPL 2C 201



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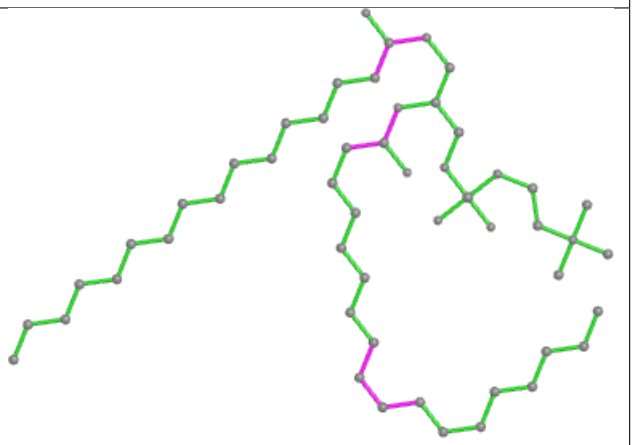
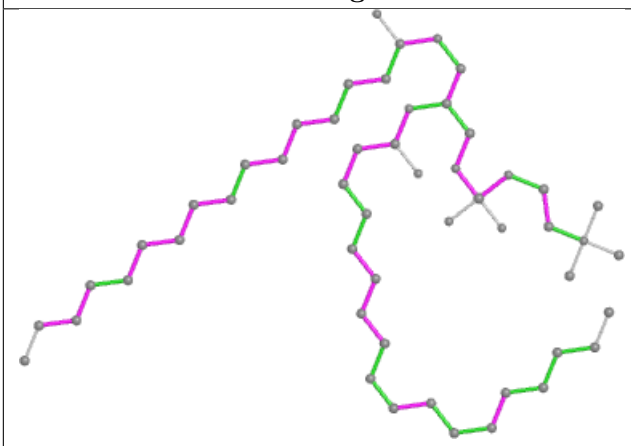
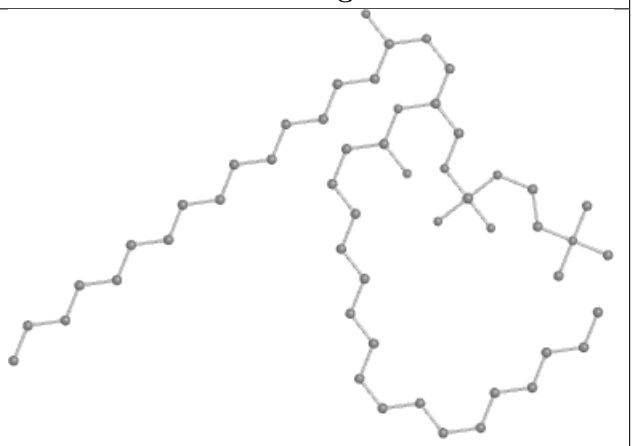


Bond angles

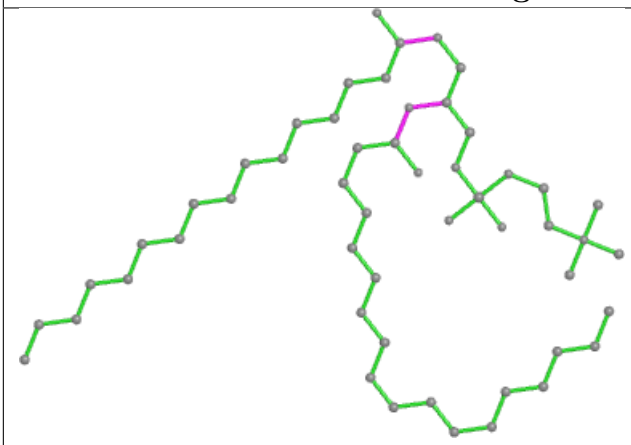


Torsions

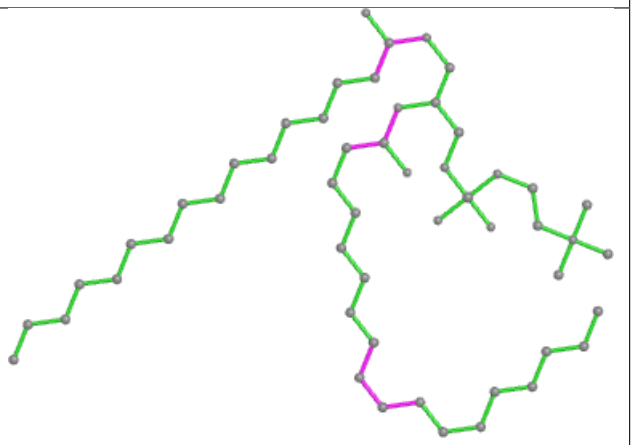


Rings

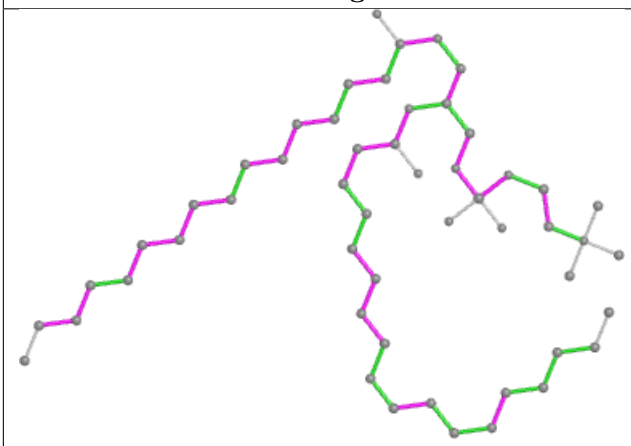
Ligand CPL 2M 201



Bond lengths



Bond angles



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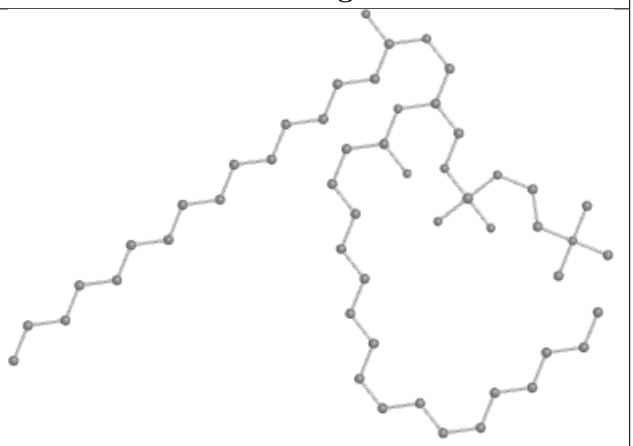
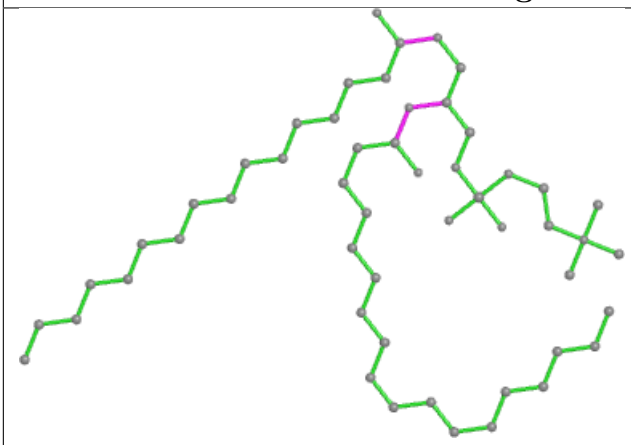


Rings

Ligand CPL 2K 201



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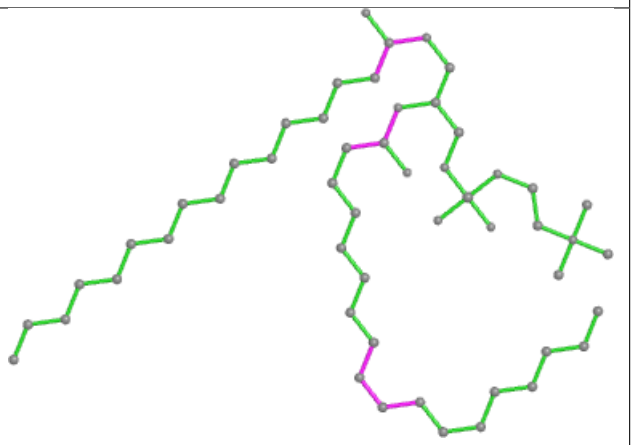
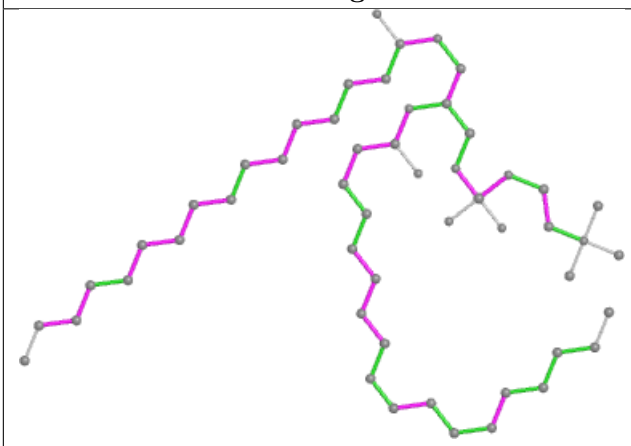


Bond angles



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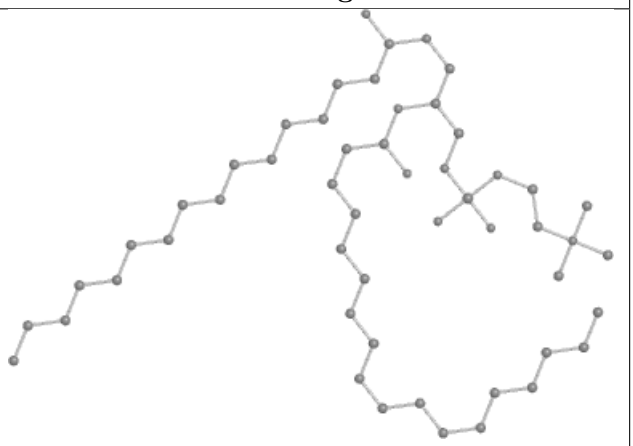
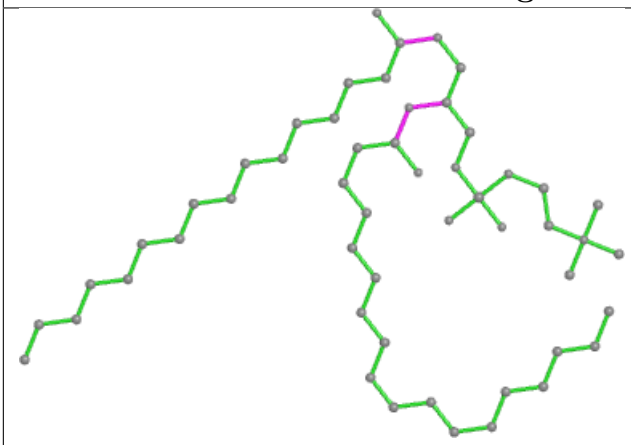
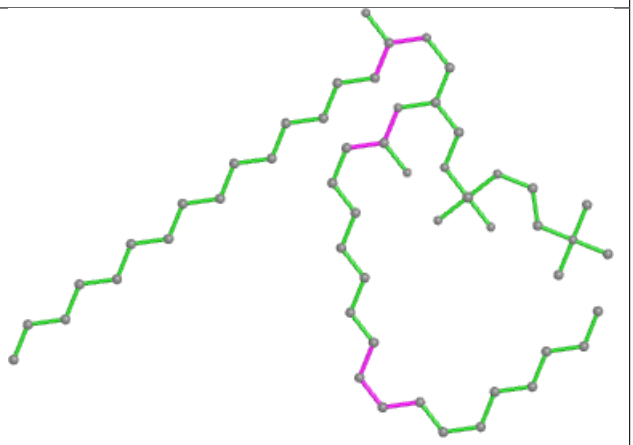


Rings

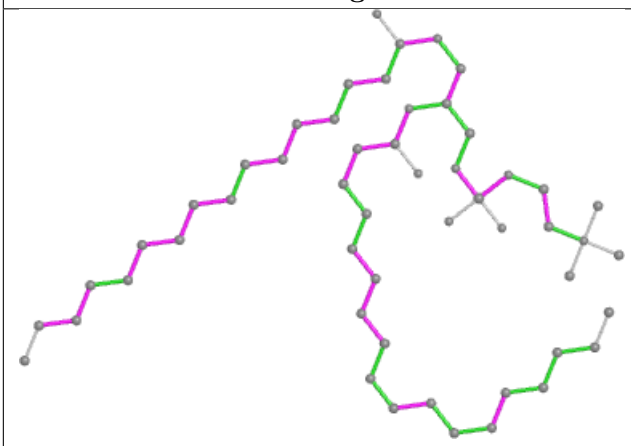
Ligand CPL 5B 201



Bond lengths



Bond angles



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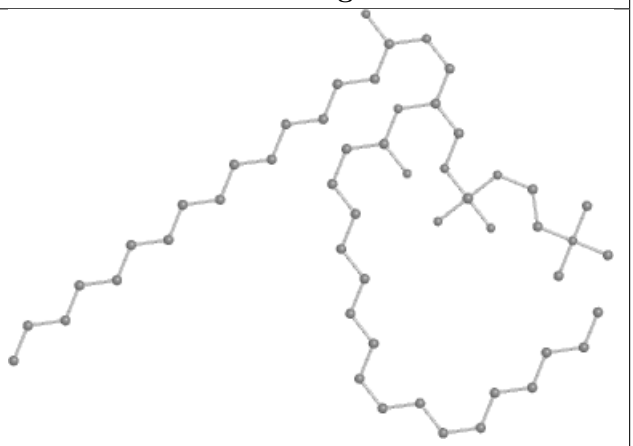
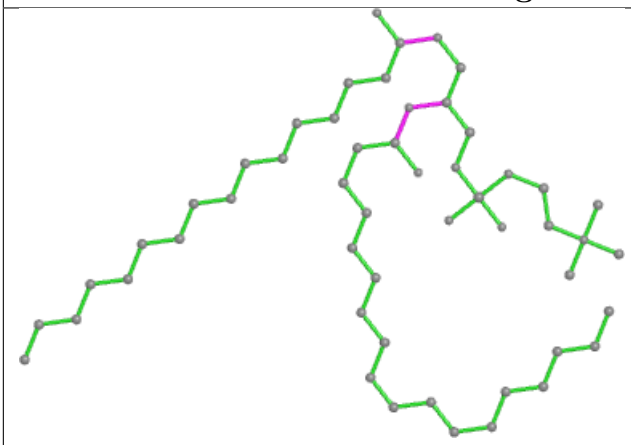


Rings

Ligand CPL 5K 201



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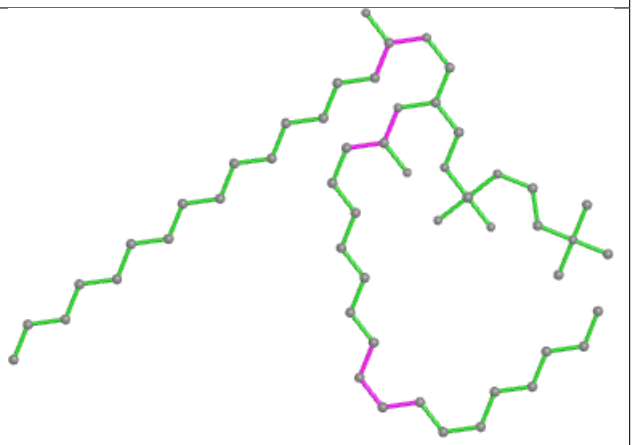
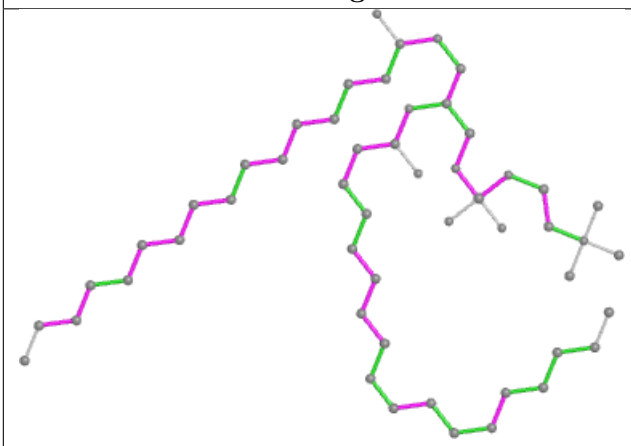


Bond angles



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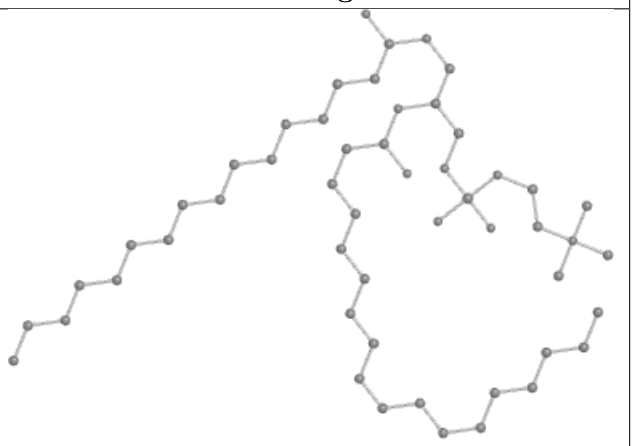
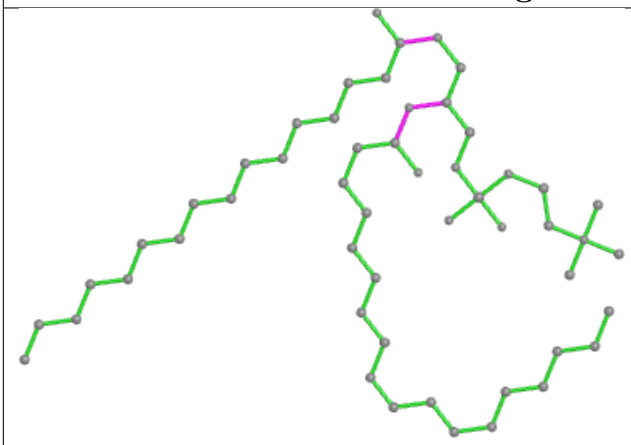
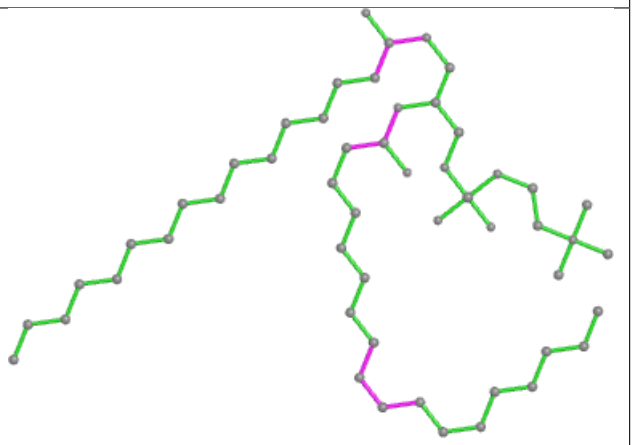


Rings

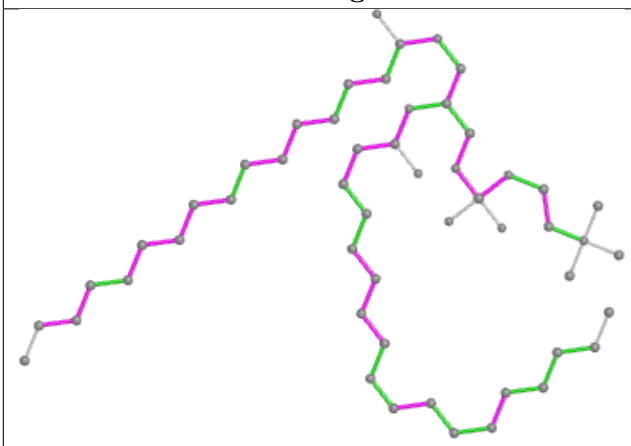
Ligand CPL 1G 201



Bond lengths



Bond angles



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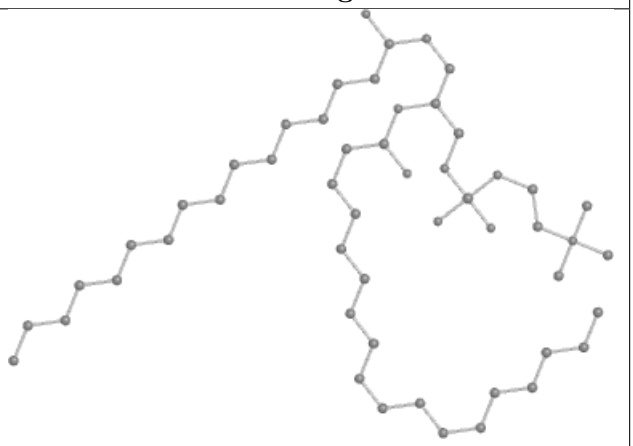
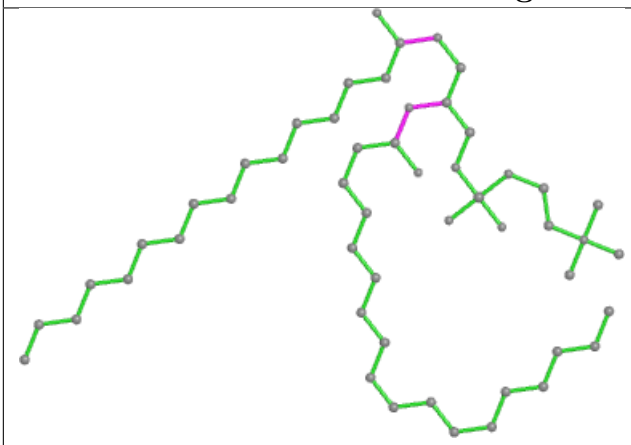
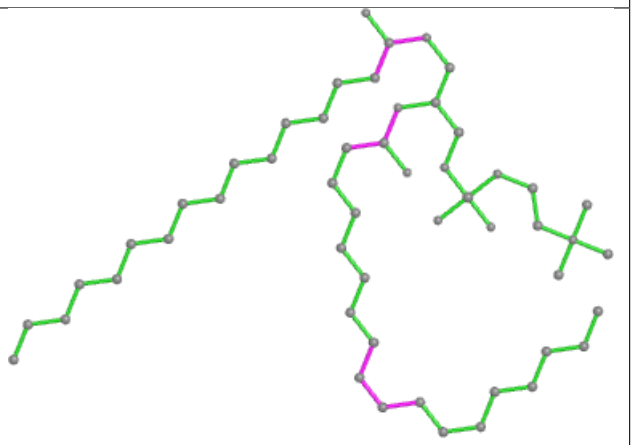


Rings

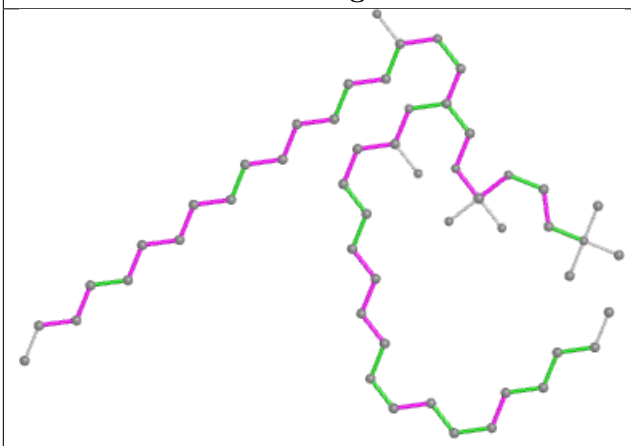
Ligand CPL 5N 201



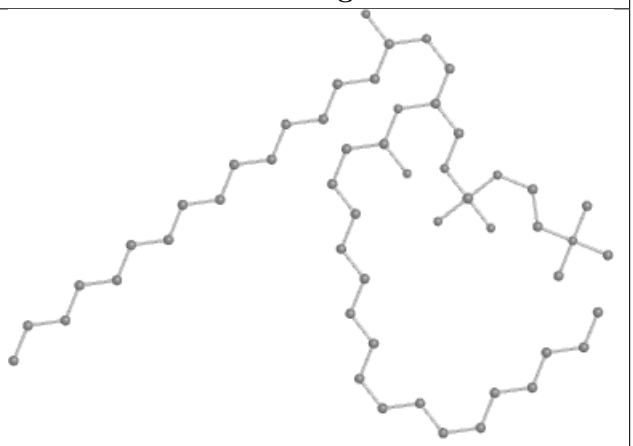
Bond lengths



Bond angles

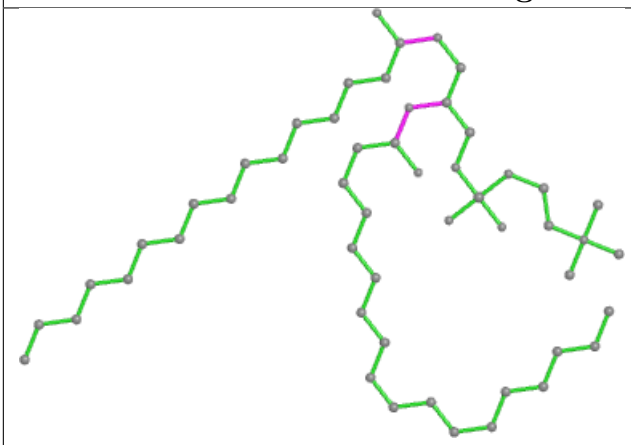


Torsions



Rings

Ligand CPL 1N 201



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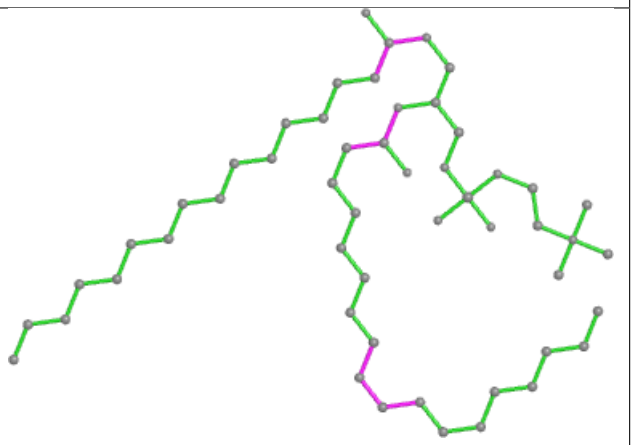

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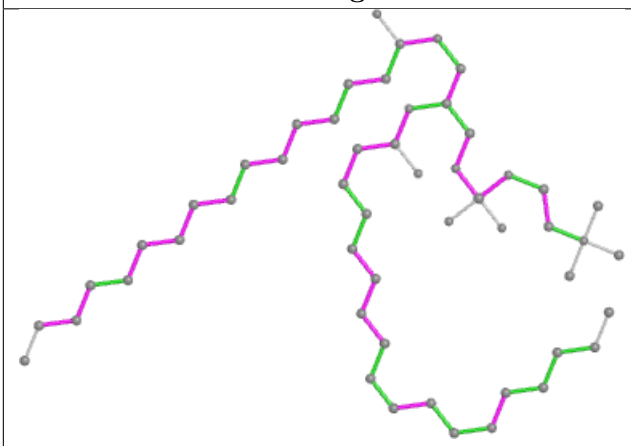

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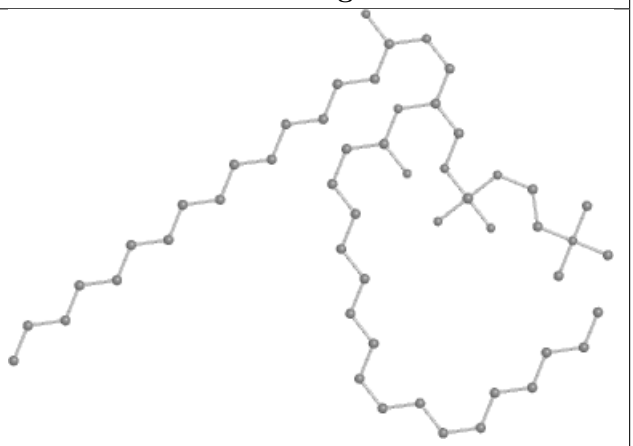
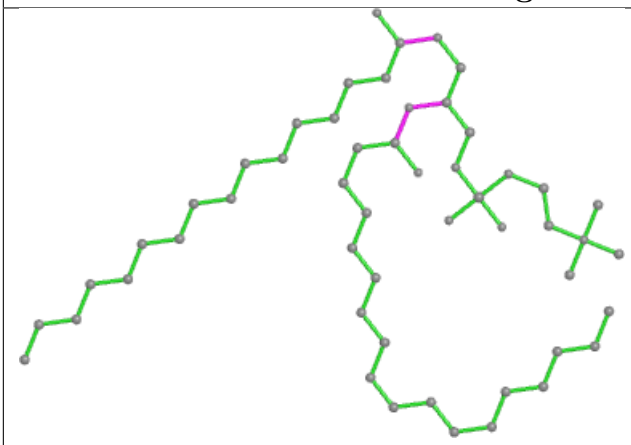


Rings

Ligand CPL 3D 201



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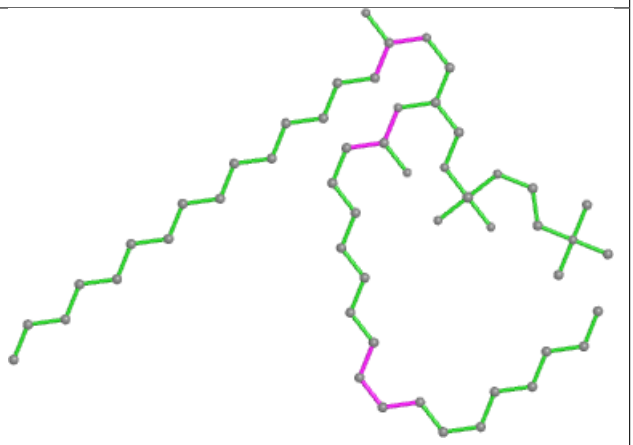
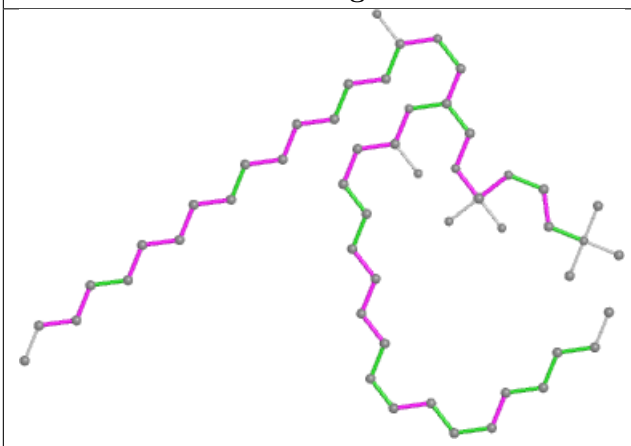


Bond angles



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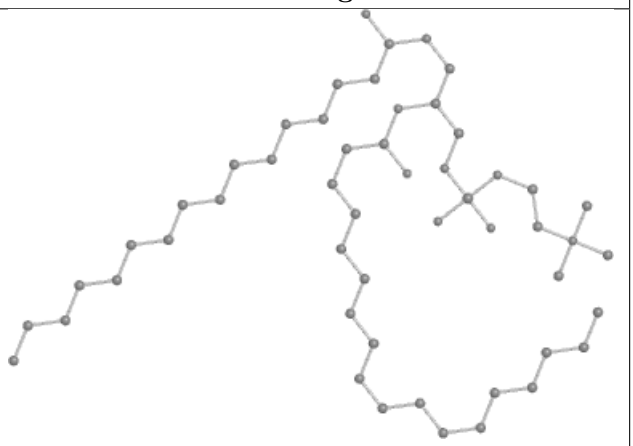
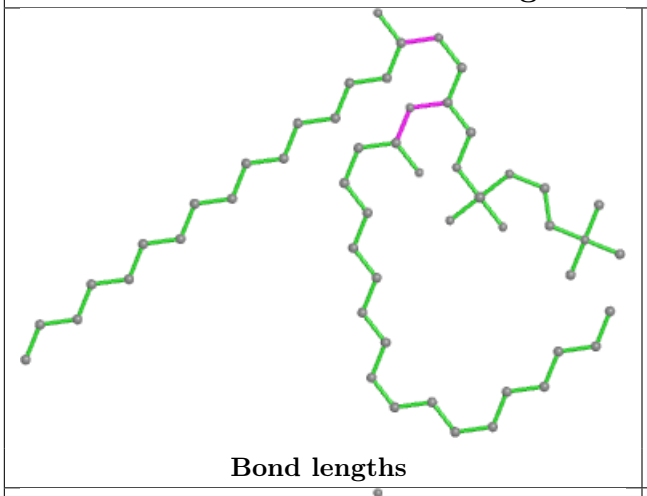


Rings

Ligand CPL 1L 201



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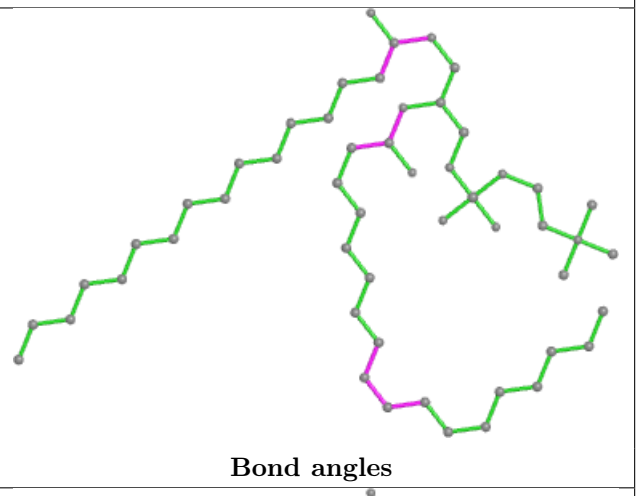

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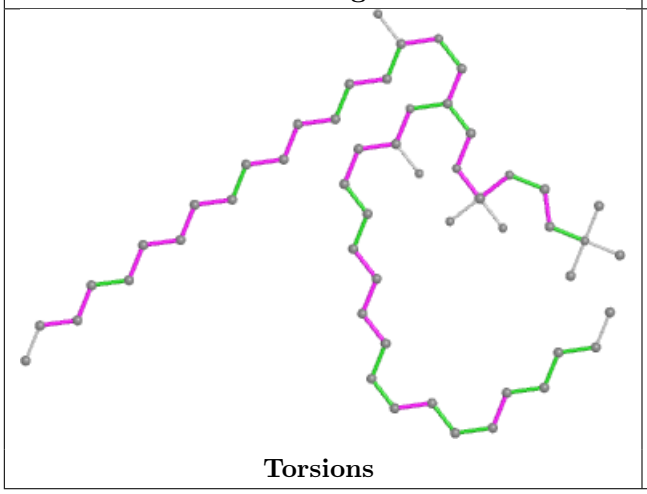

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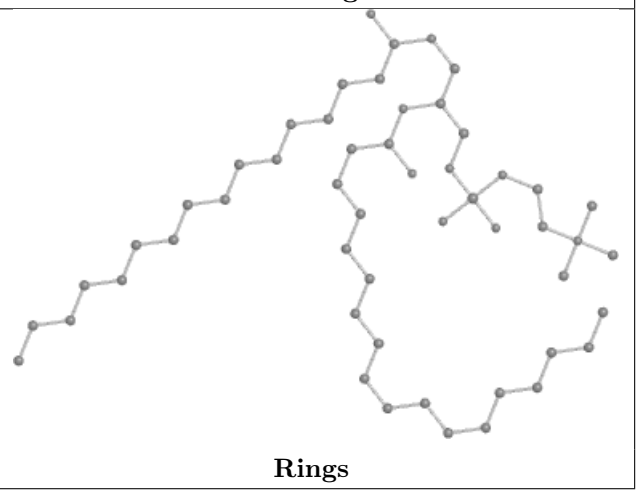
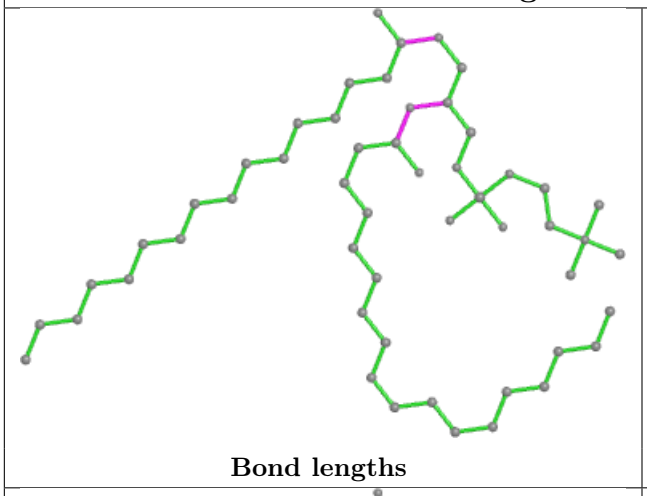


Rings

Ligand CPL 3L 201



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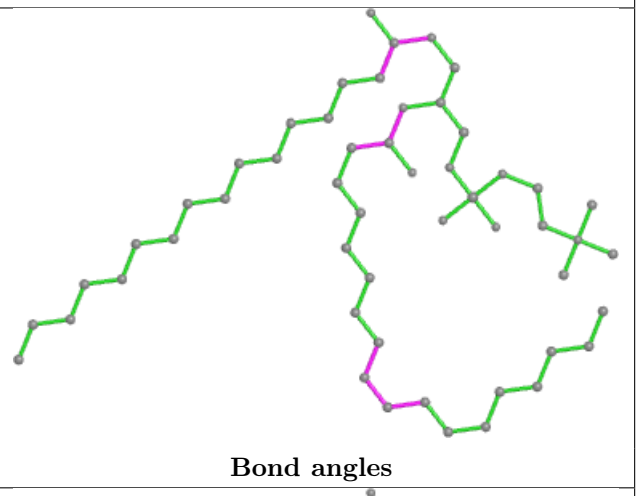

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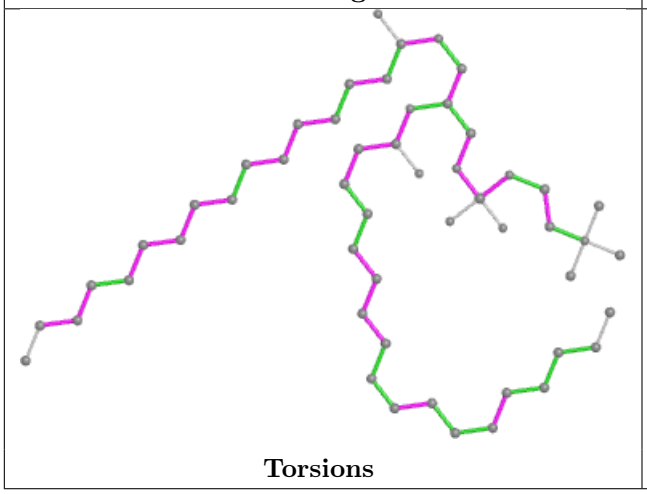

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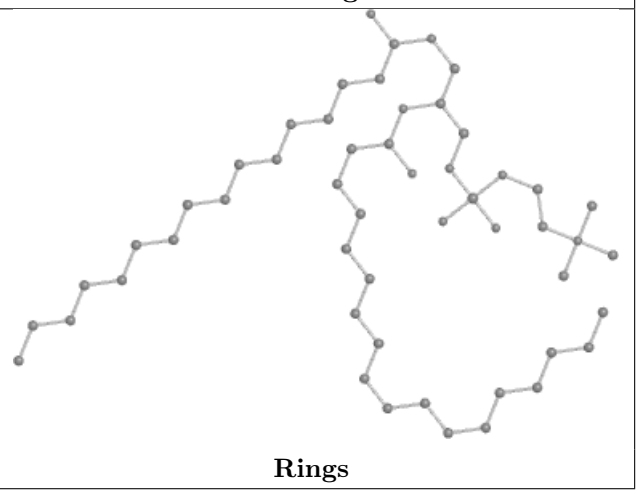
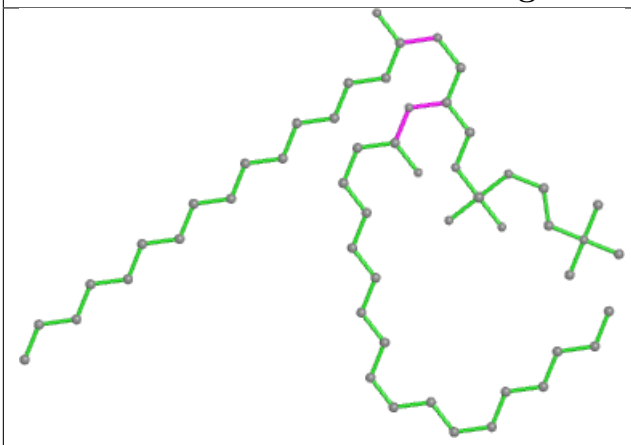


Rings

Ligand CPL 4F 201



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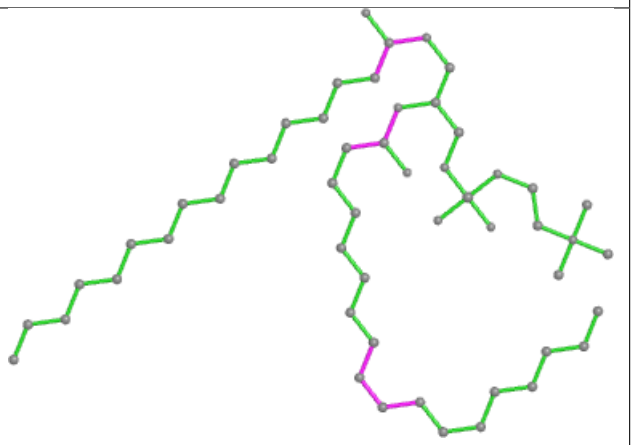
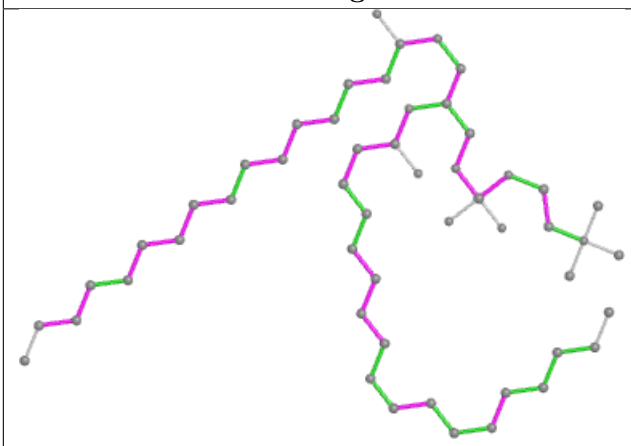


Bond angles



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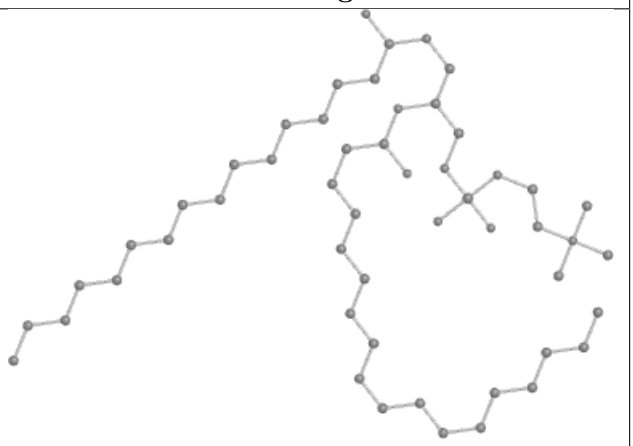
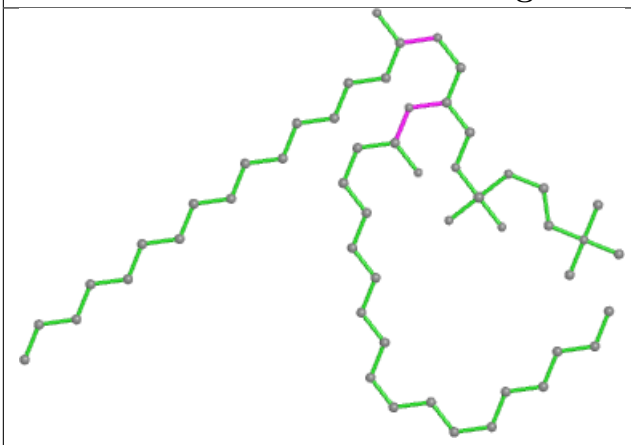


Rings

Ligand CPL 1A 201



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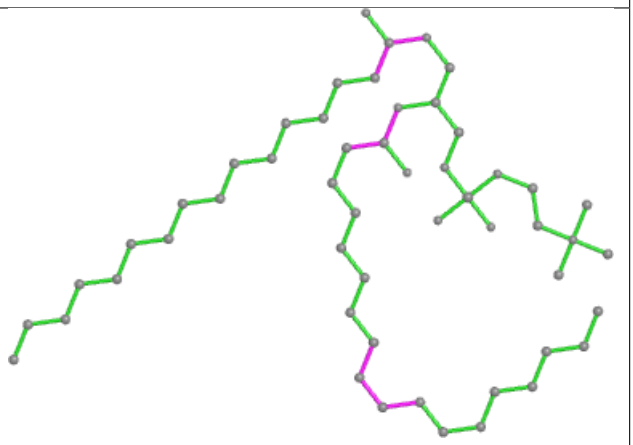
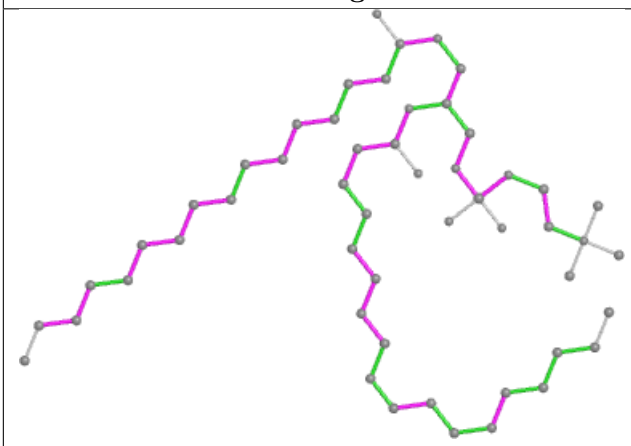


Bond angles



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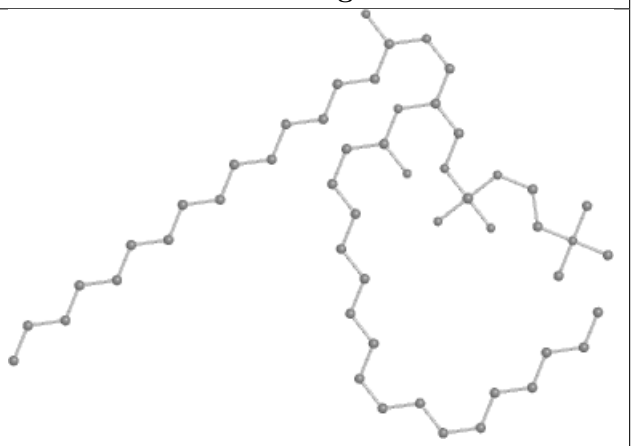
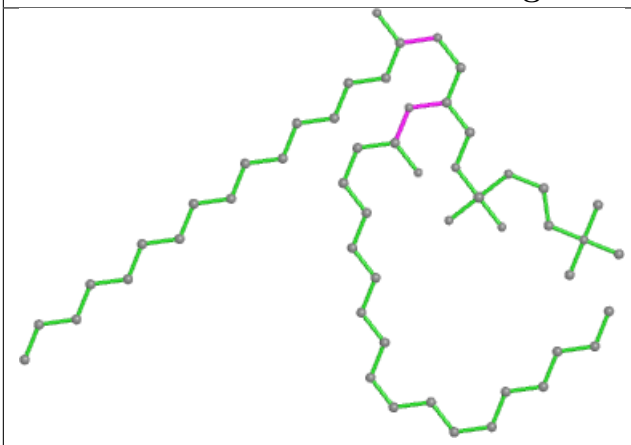


Rings

Ligand CPL 4I 201



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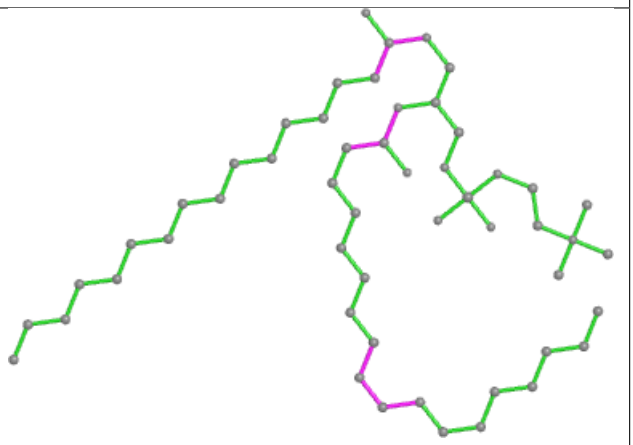

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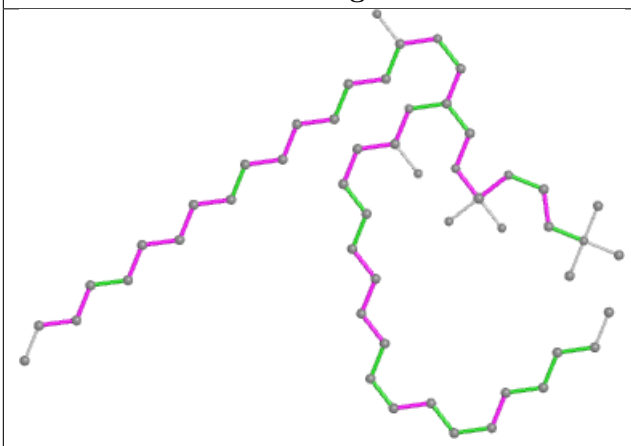

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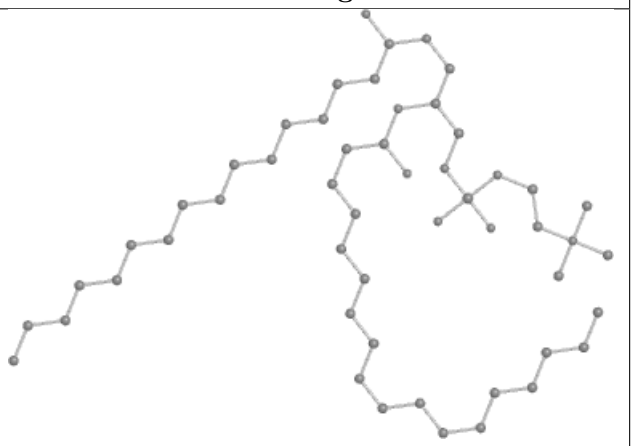
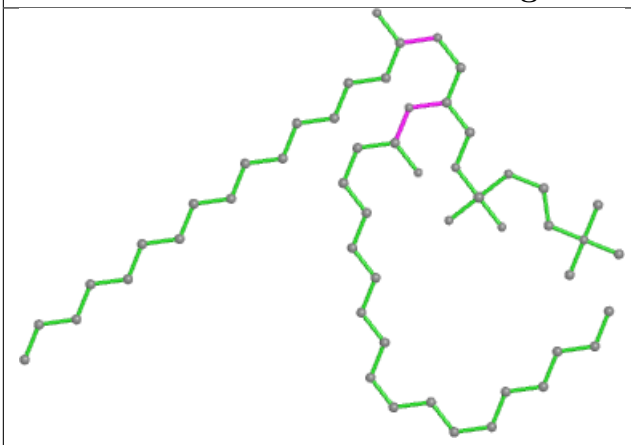


Rings

Ligand CPL 5J 201



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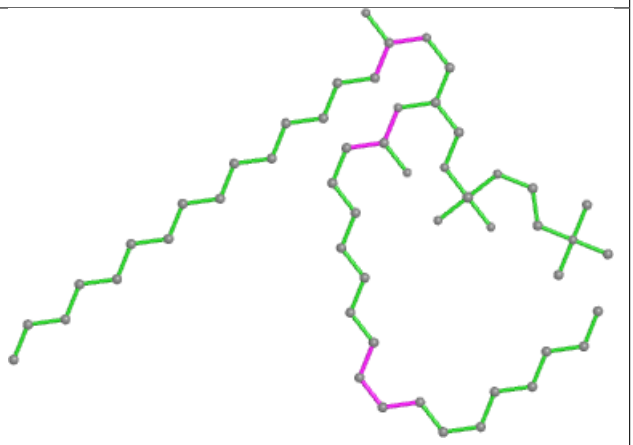

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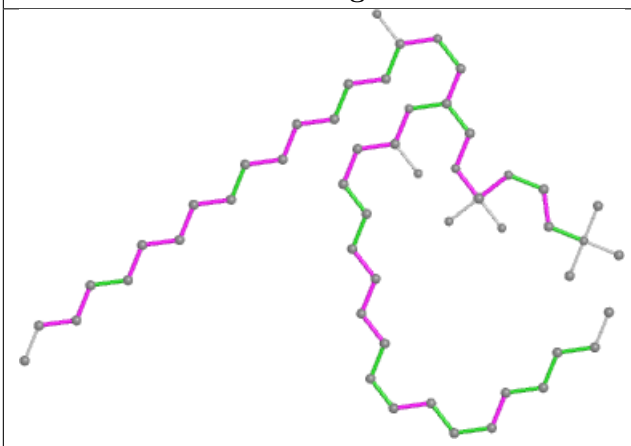

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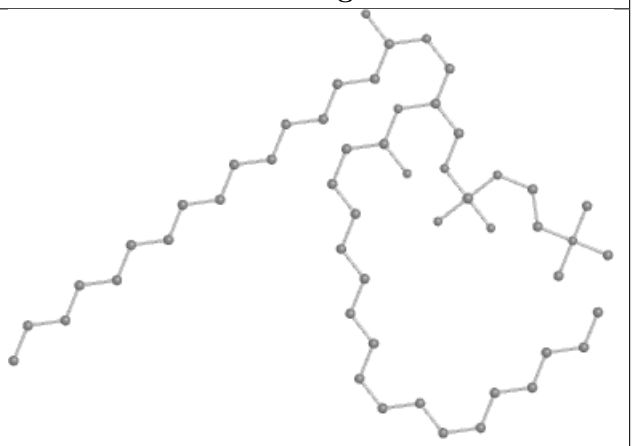
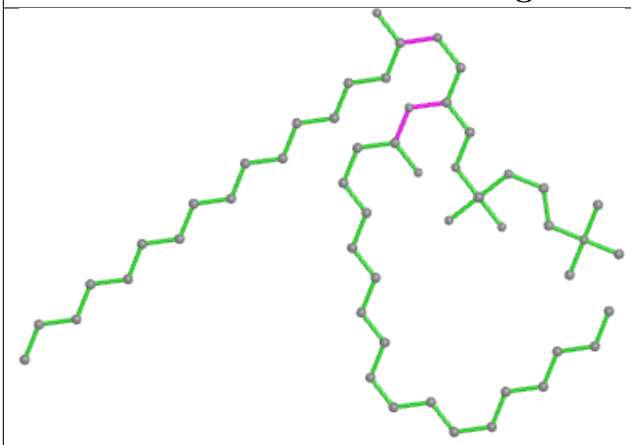


Rings

Ligand CPL 1K 201



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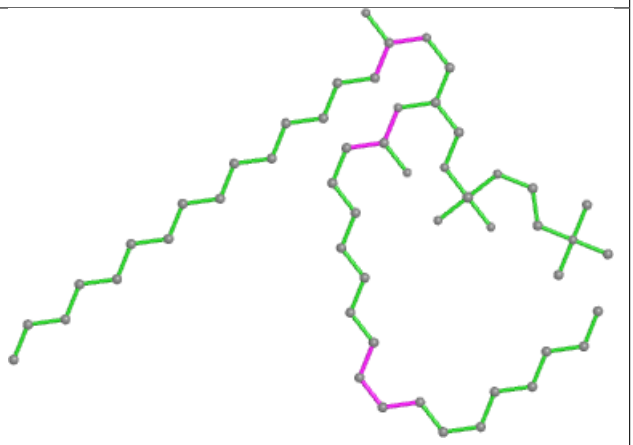
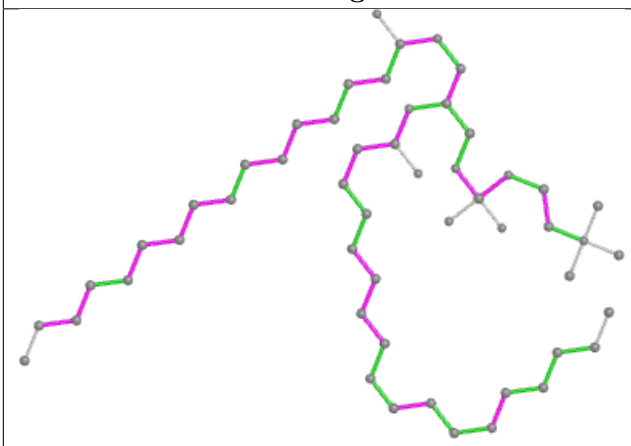


Bond angles



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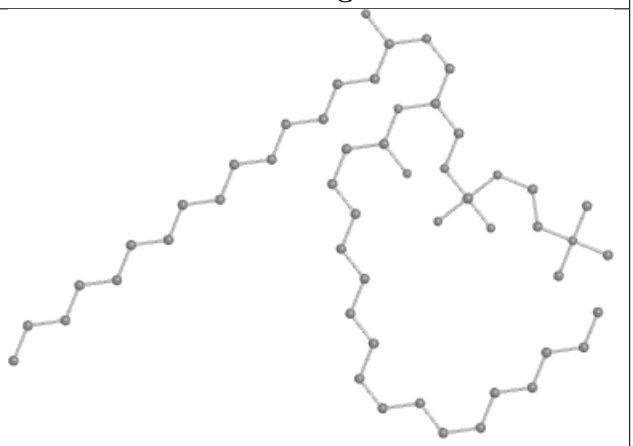
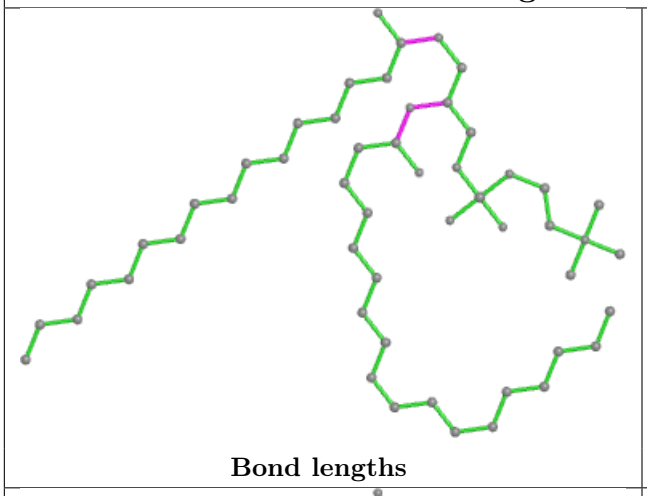


Rings

Ligand CPL 3E 201



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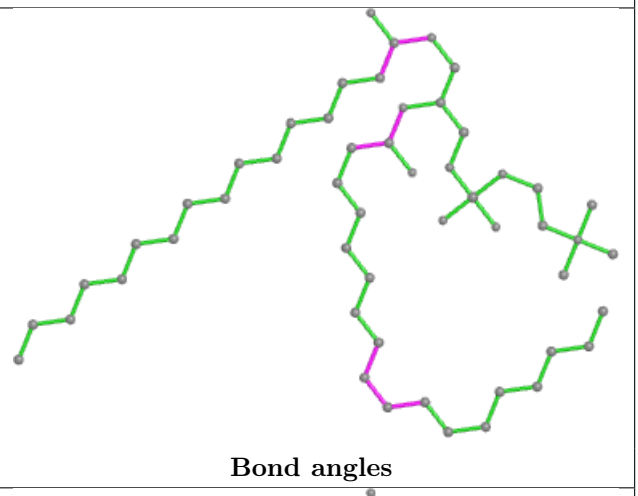
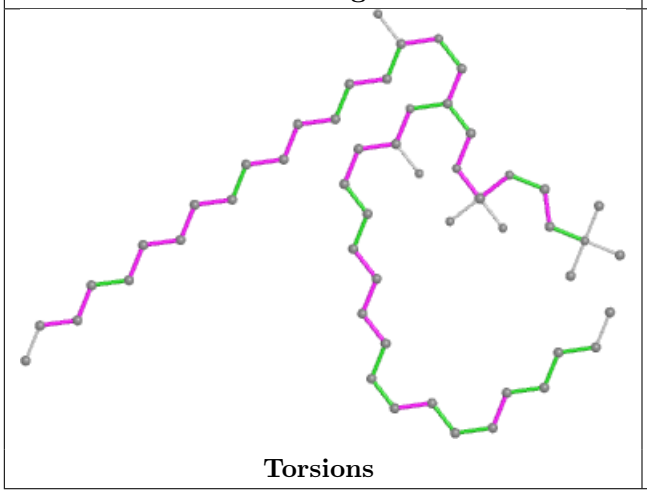
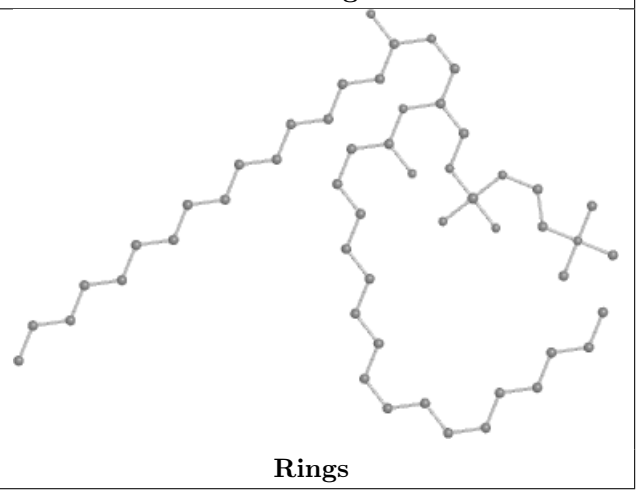


Bond angles

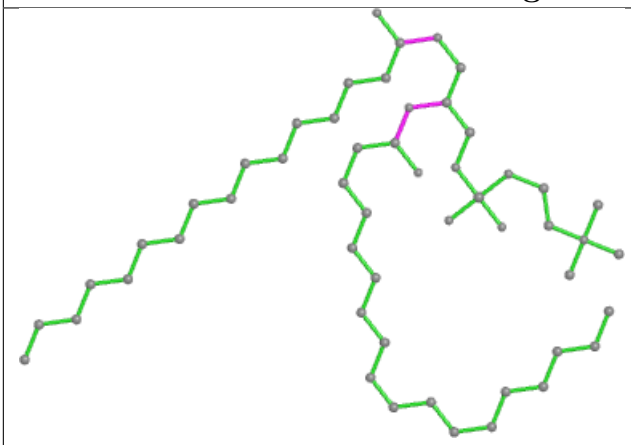


Torsions



Rings

Ligand CPL 2I 201



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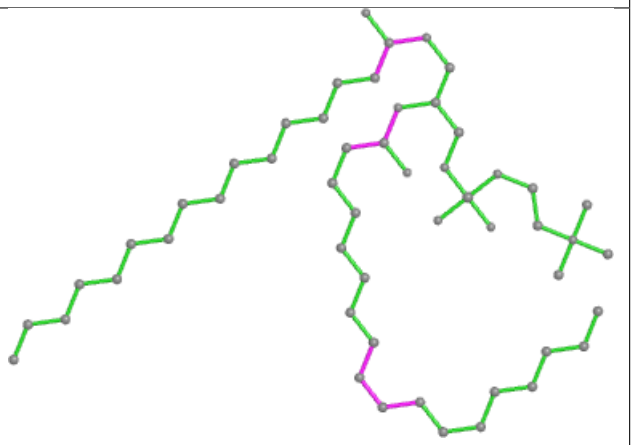
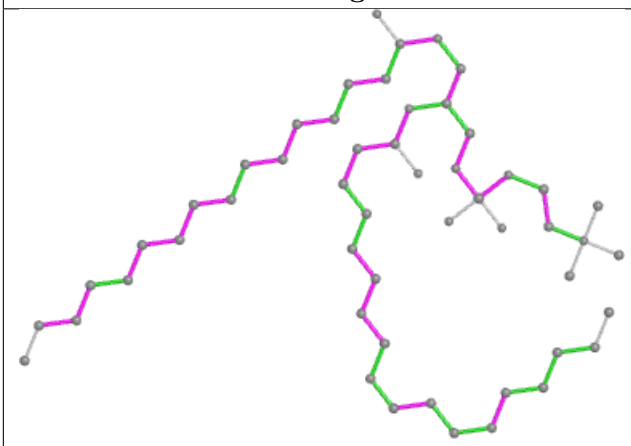


Bond angles



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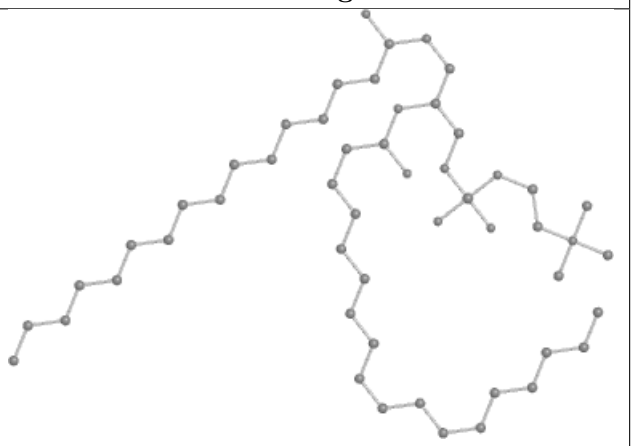
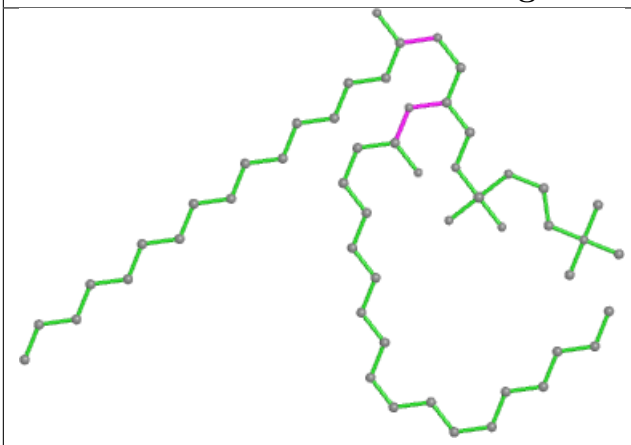
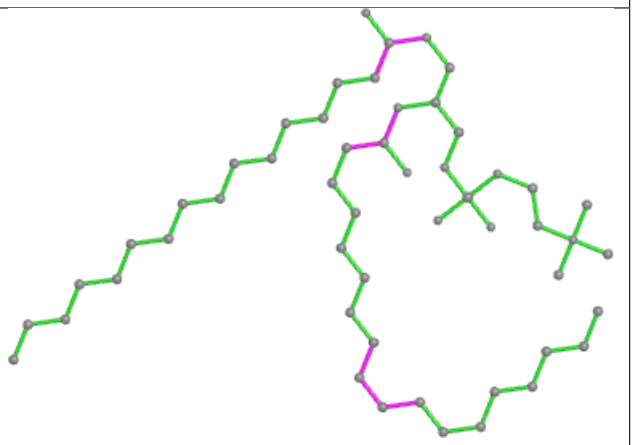


Rings

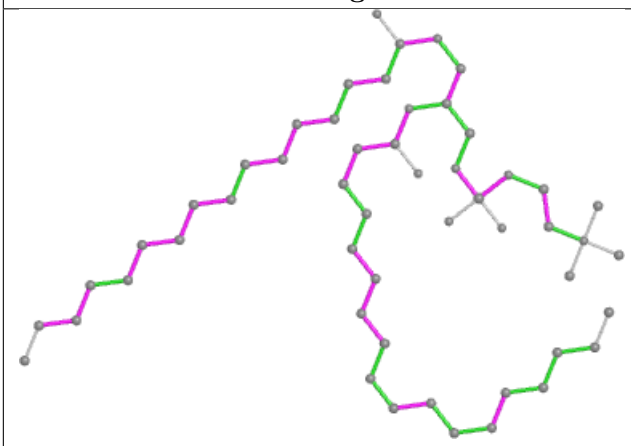
Ligand CPL 1F 201



Bond lengths



Bond angles



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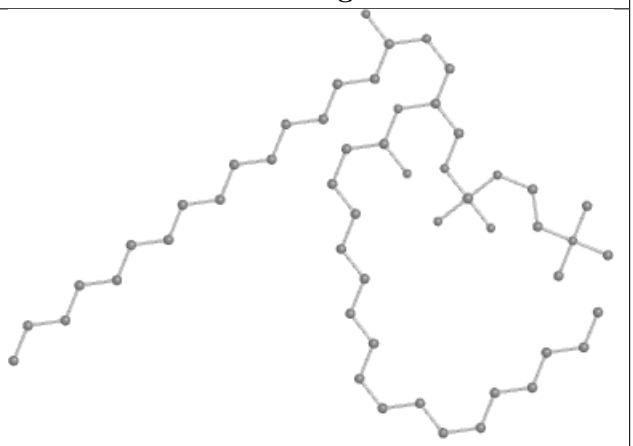
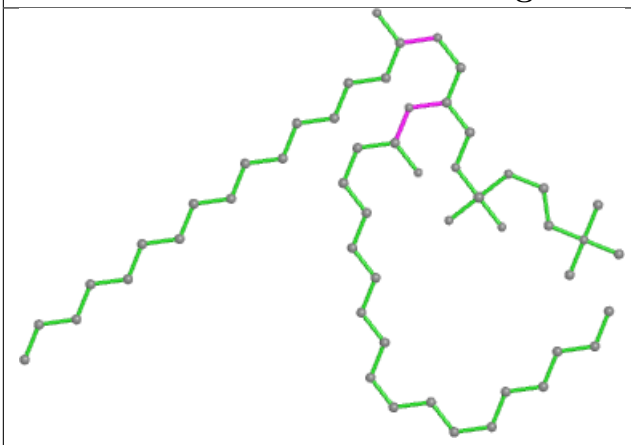
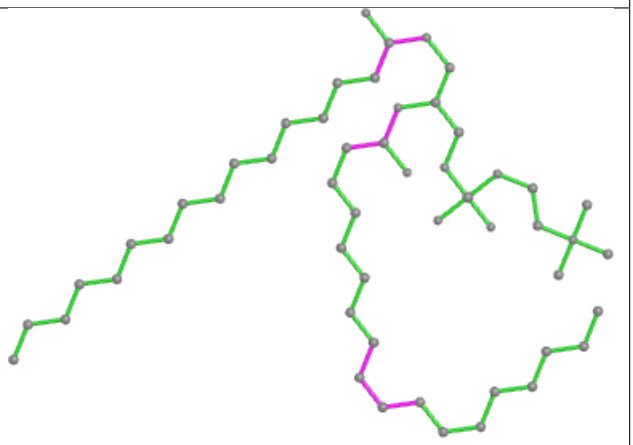


Rings

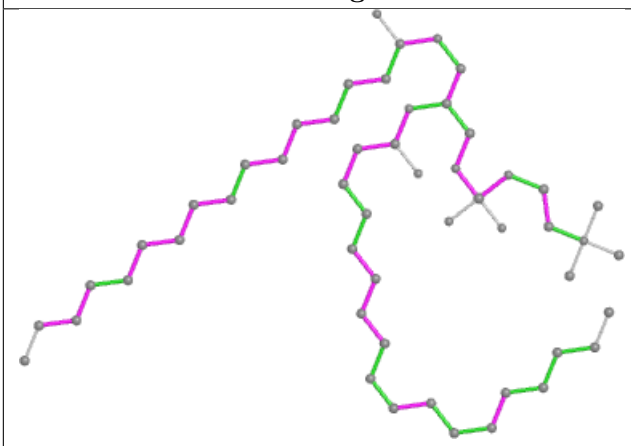
Ligand CPL 5H 201



Bond lengths



Bond angles



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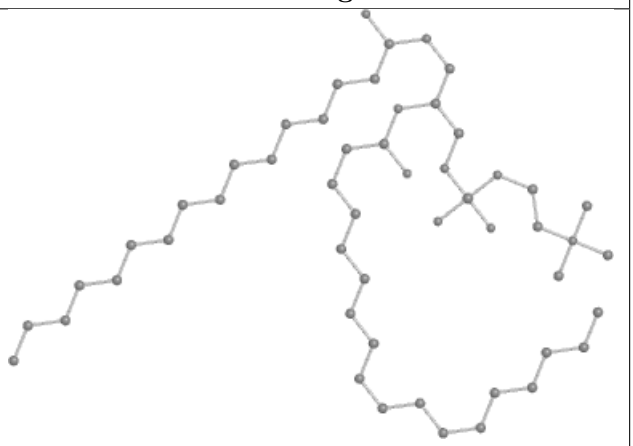
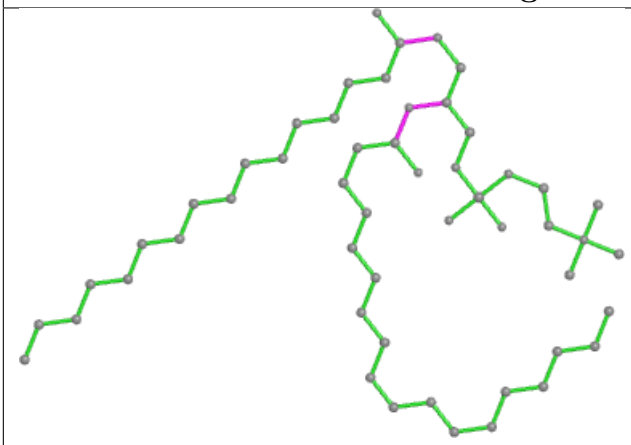


Rings

Ligand CPL 2J 201



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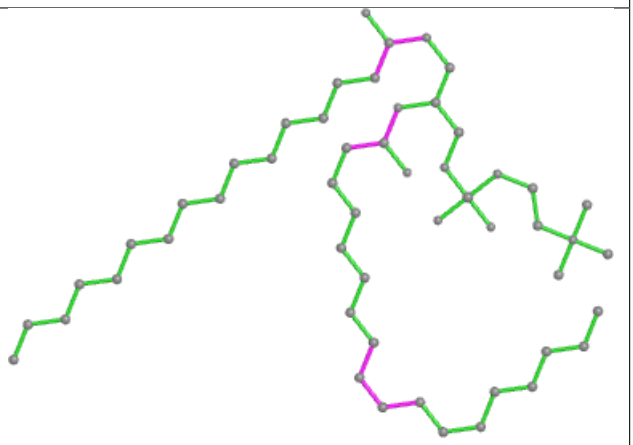
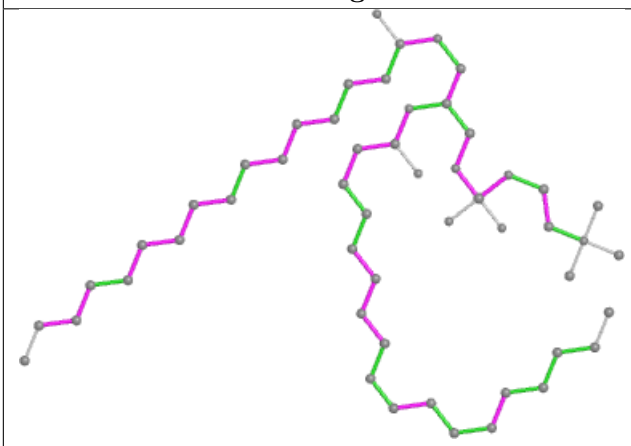


Bond angles



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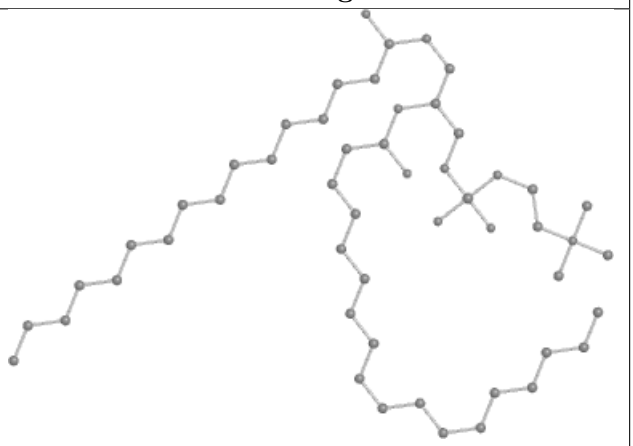
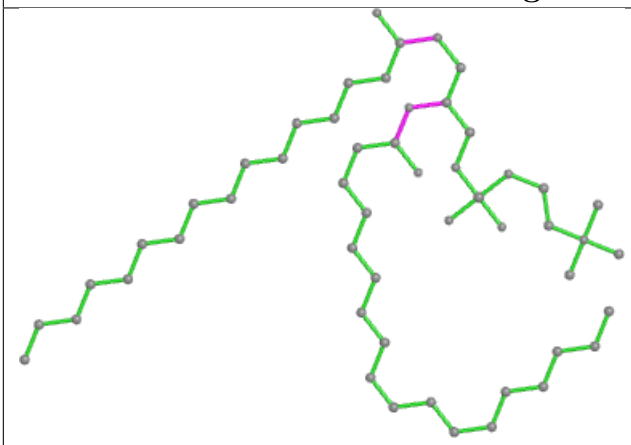
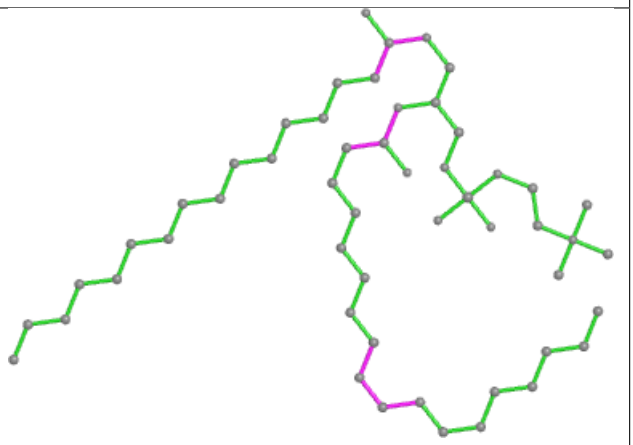


Rings

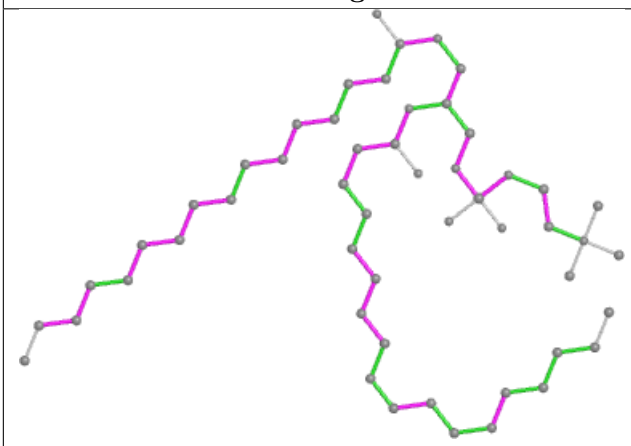
Ligand CPL 3I 201



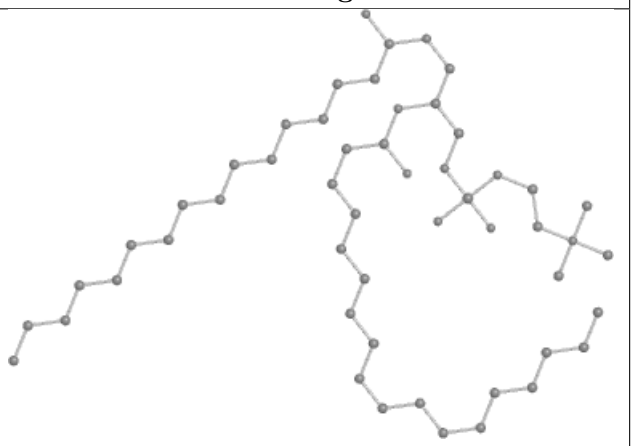
Bond lengths



Bond angles



Torsions



Rings

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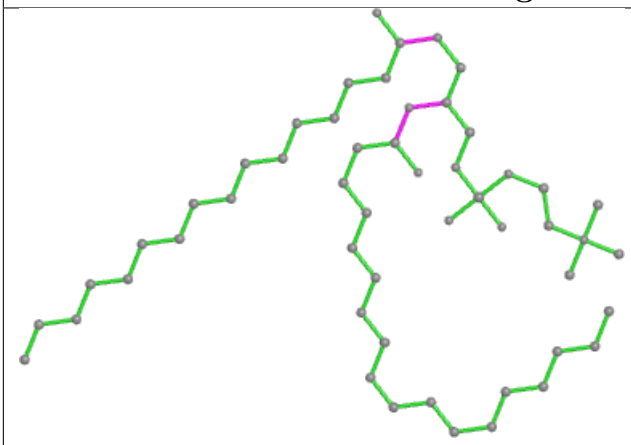

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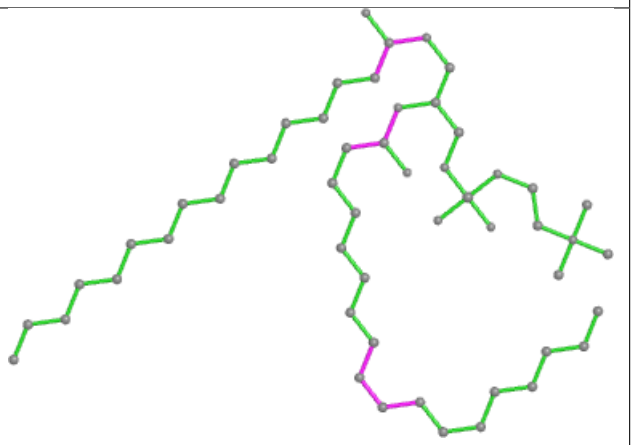

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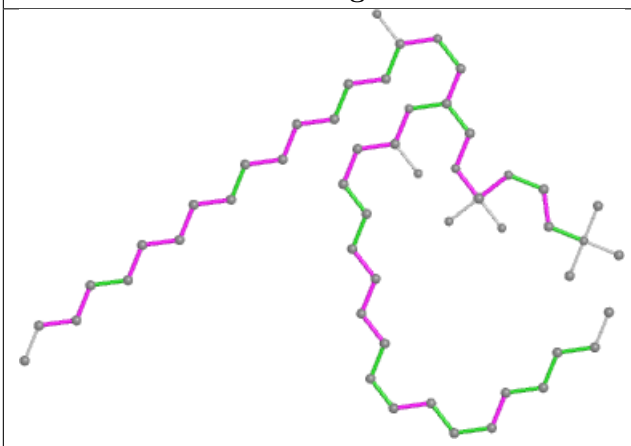

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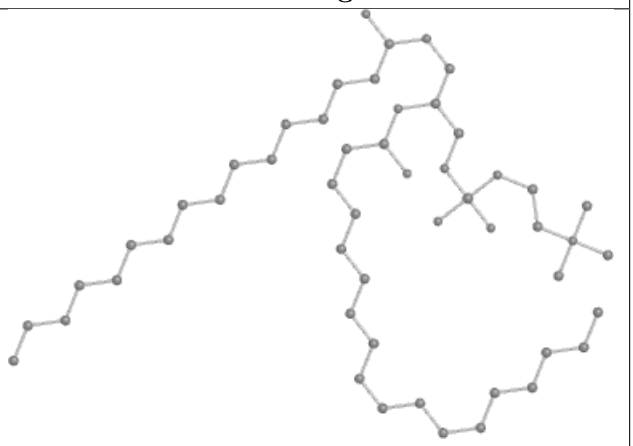

Rings

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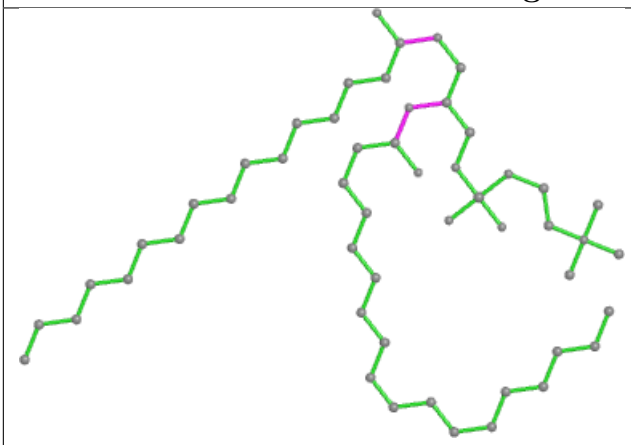

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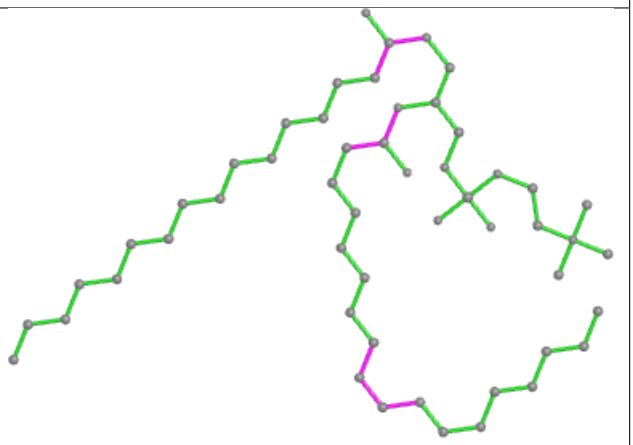

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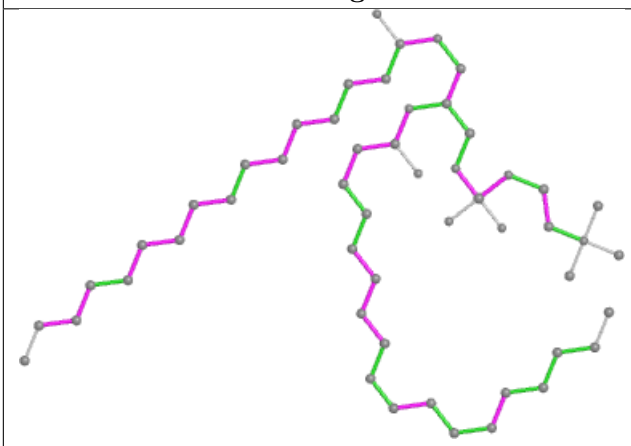

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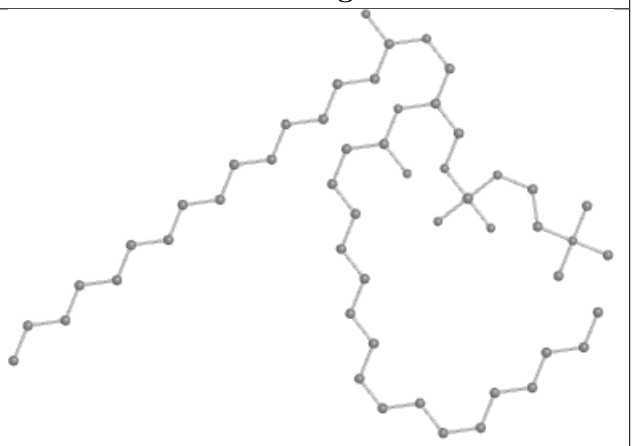

Rings

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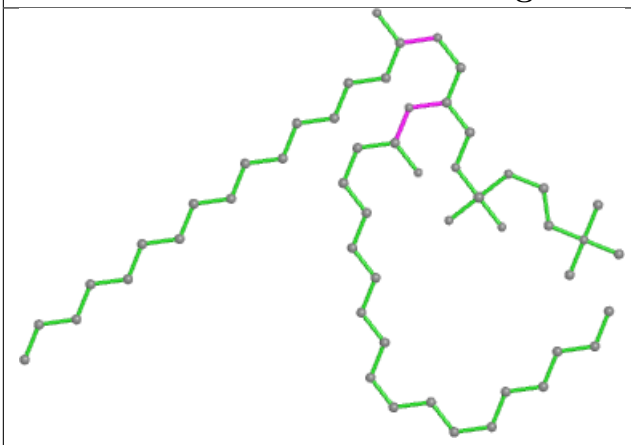

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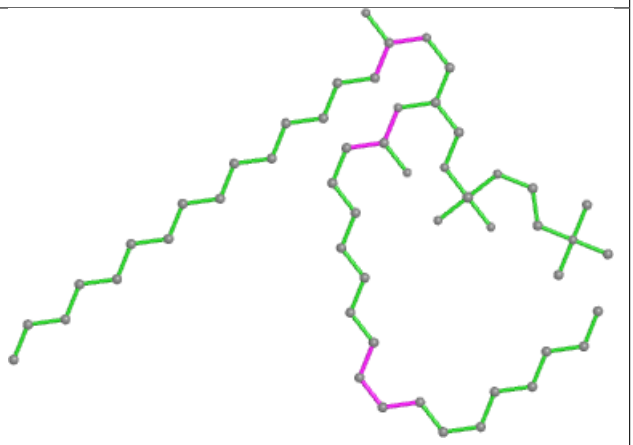
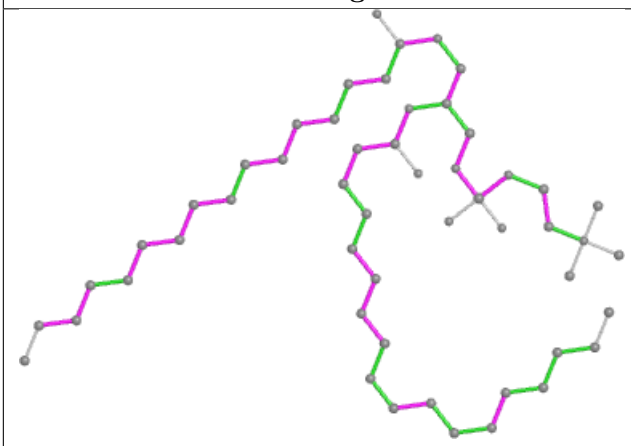


Bond angles



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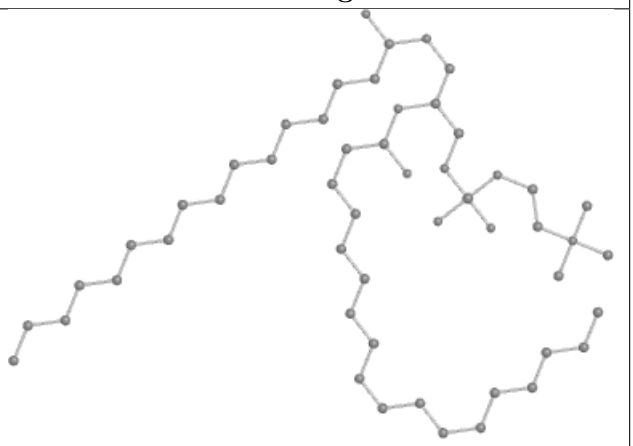
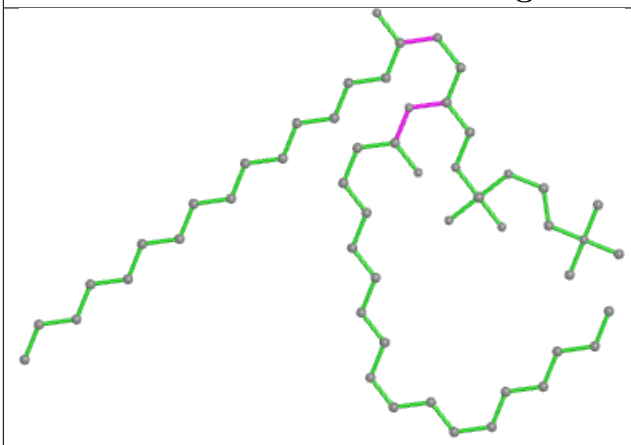


Rings

Ligand CPL 1H 201



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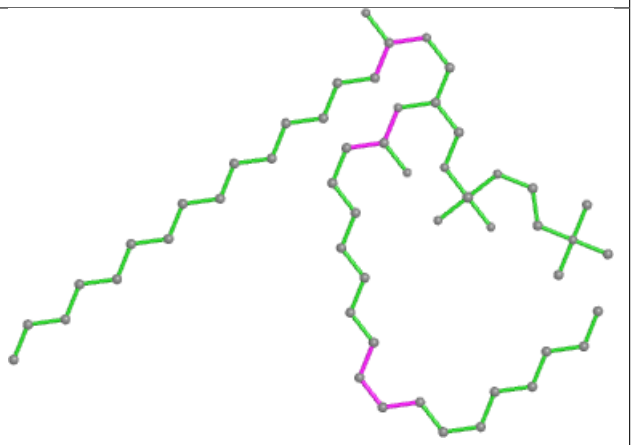

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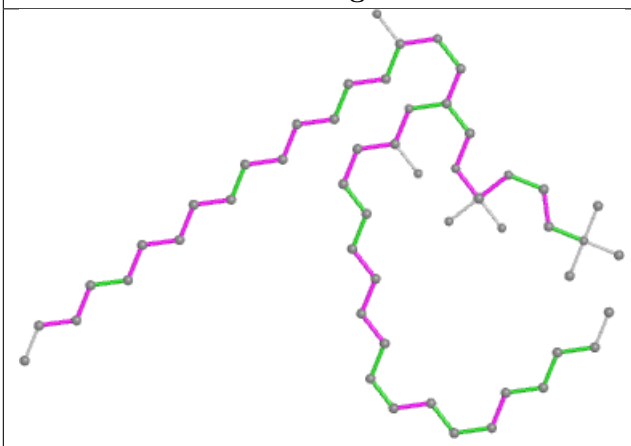

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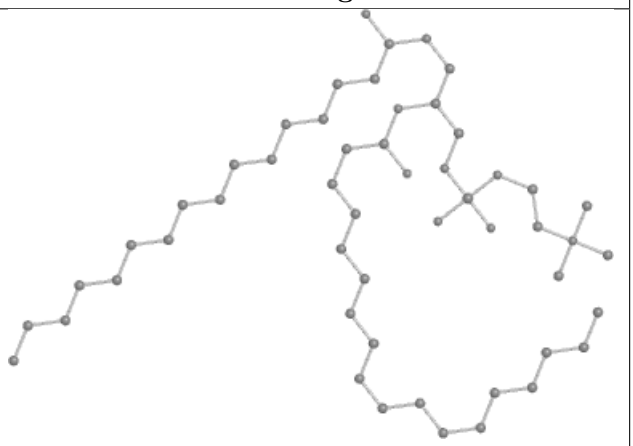
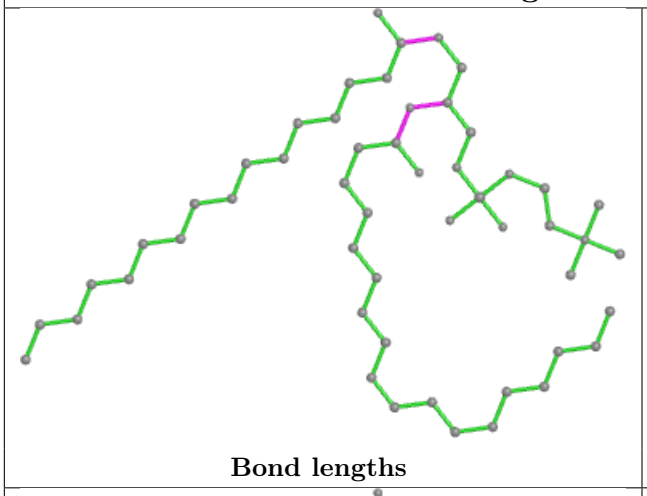


Rings

Ligand CPL 4J 201



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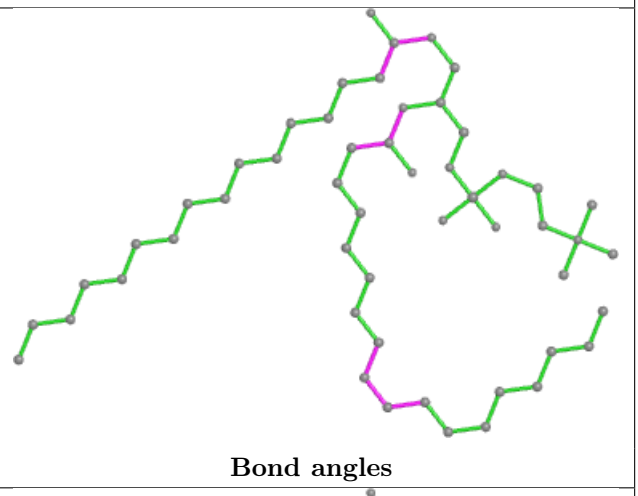

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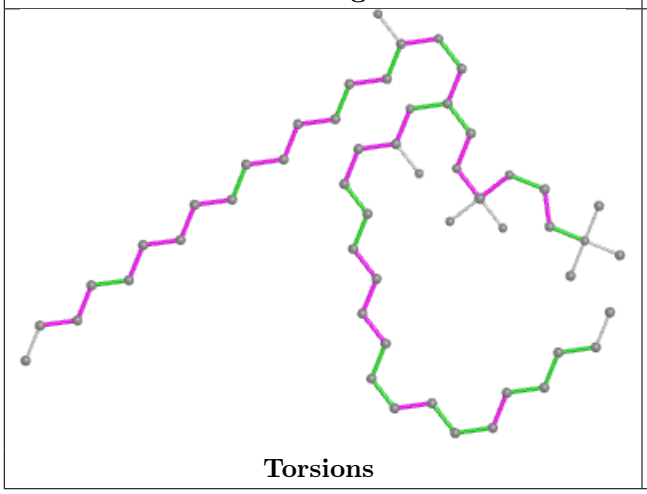

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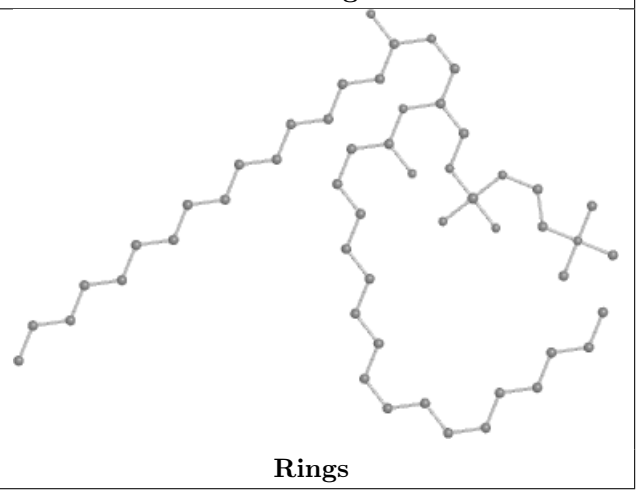

Rings

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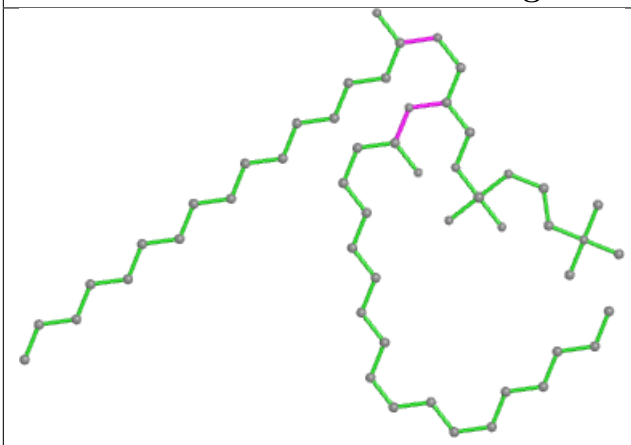

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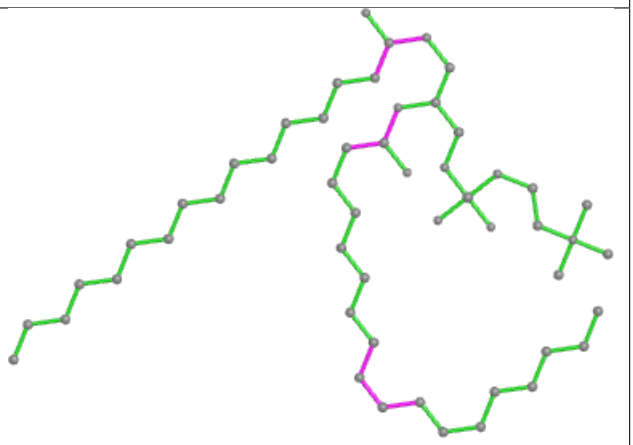

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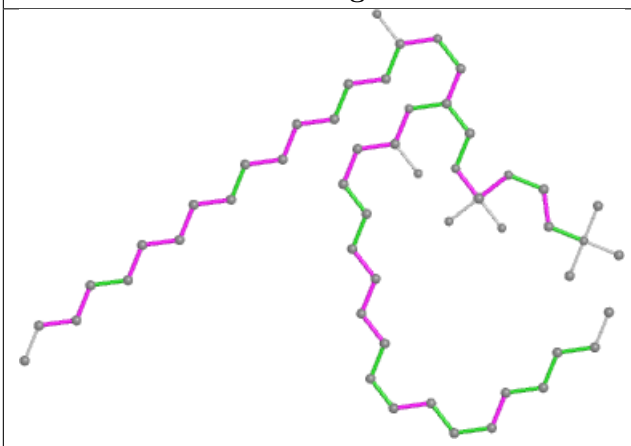

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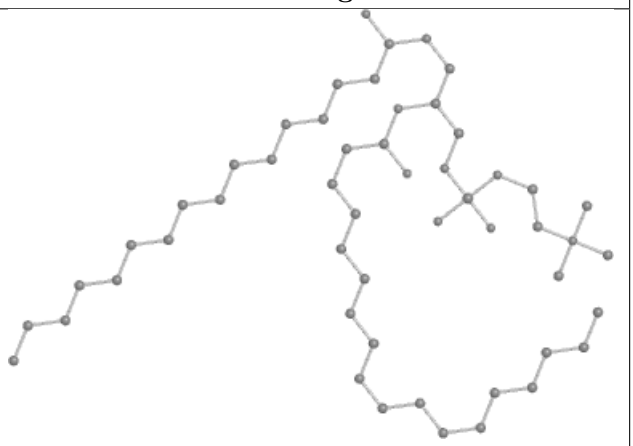
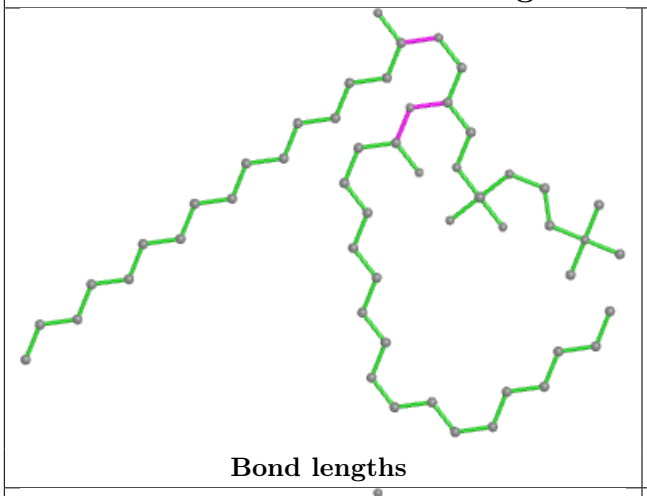


Rings

Ligand CPL 3K 201



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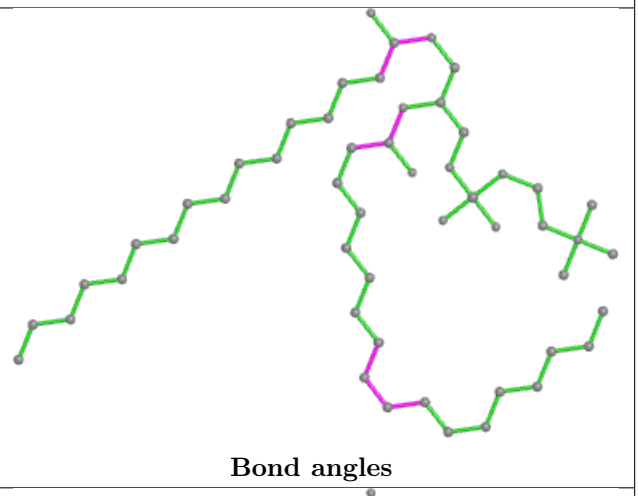
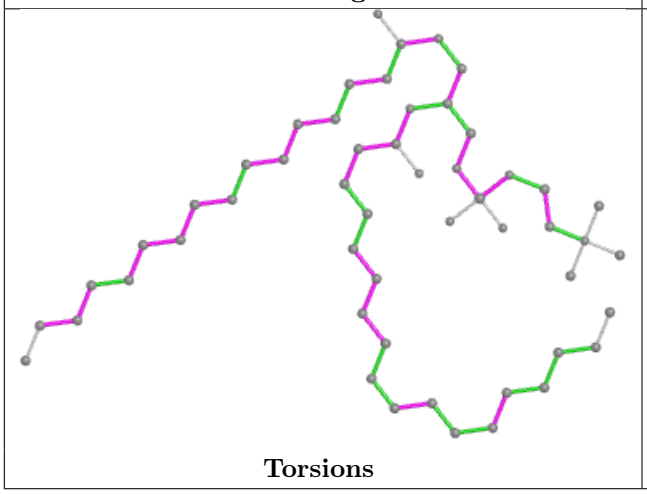


Bond angles



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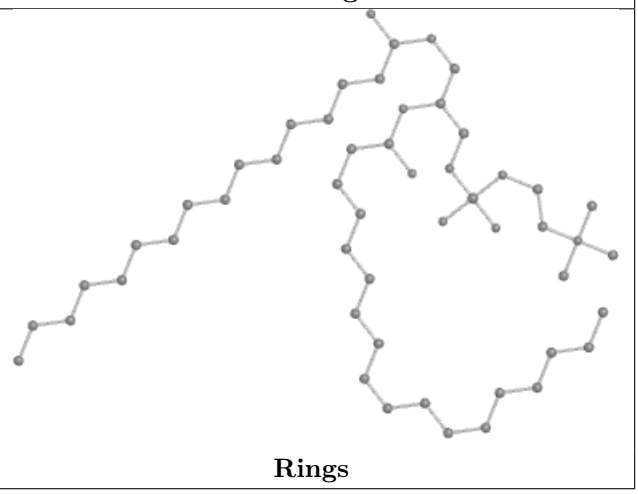
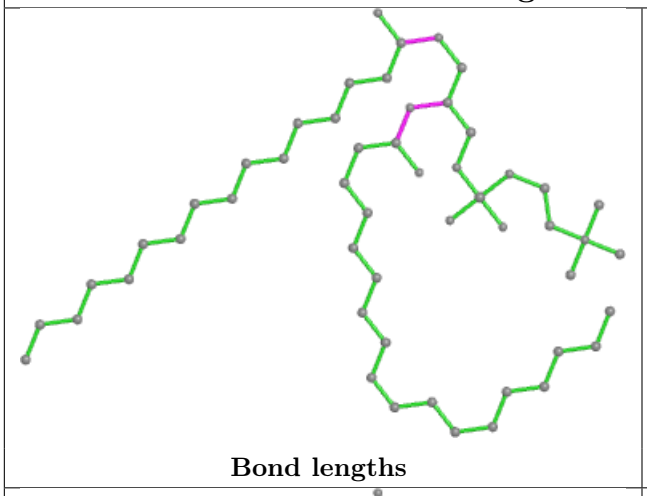


Rings

Ligand CPL 3B 201



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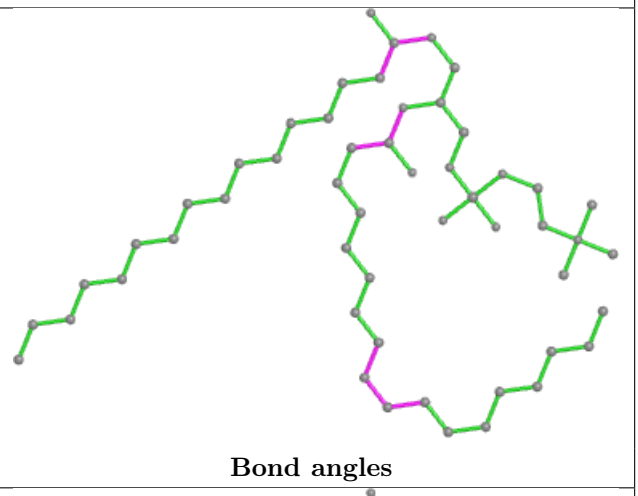
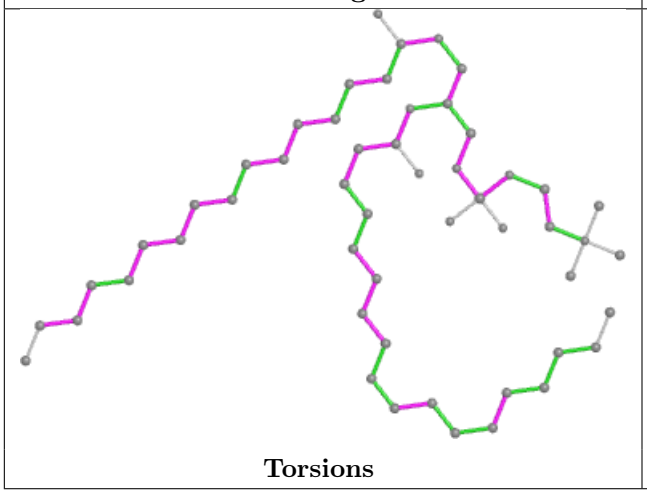


Bond angles



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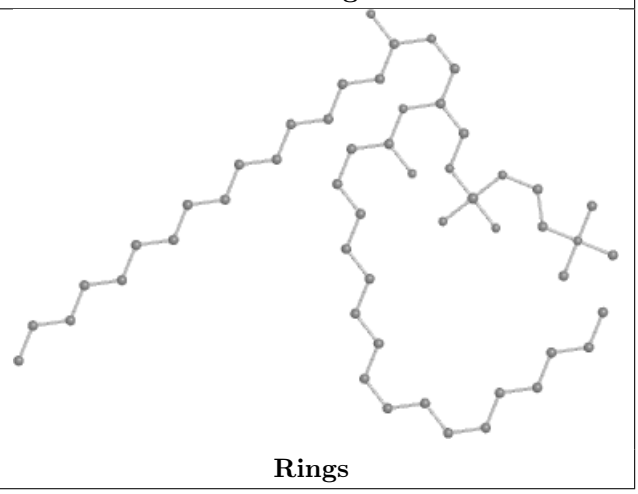
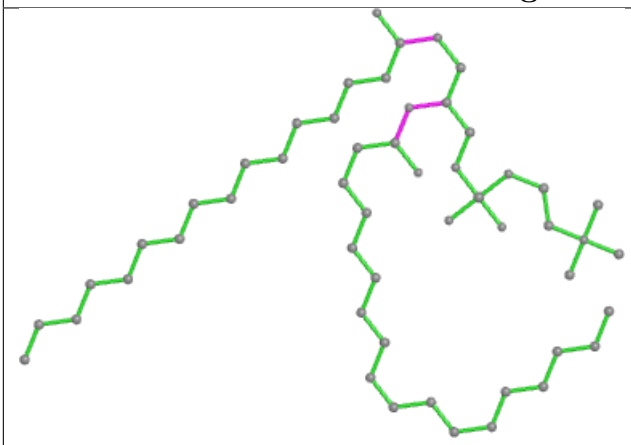


Rings

Ligand CPL 3J 201



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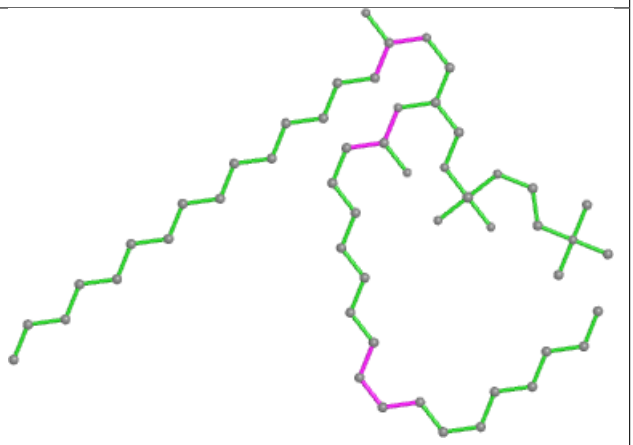
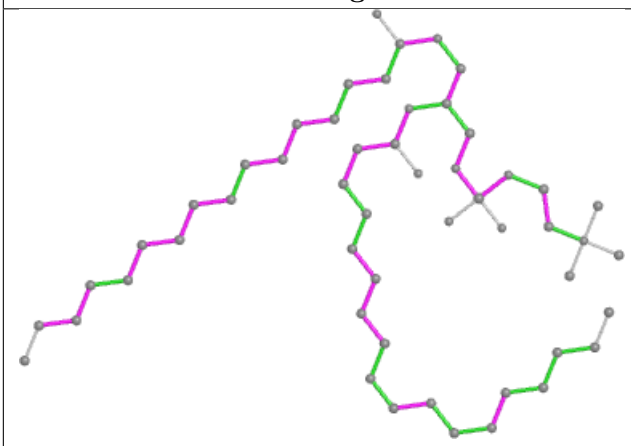


Bond angles



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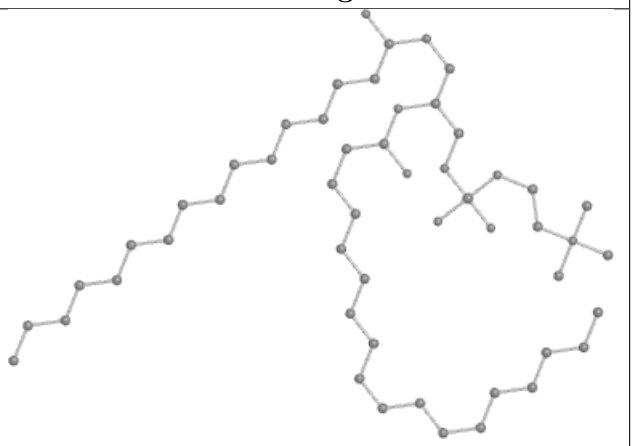
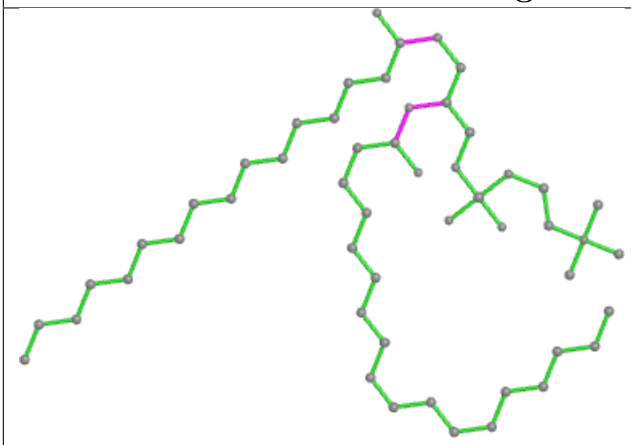


Rings

Ligand CPL 5D 201



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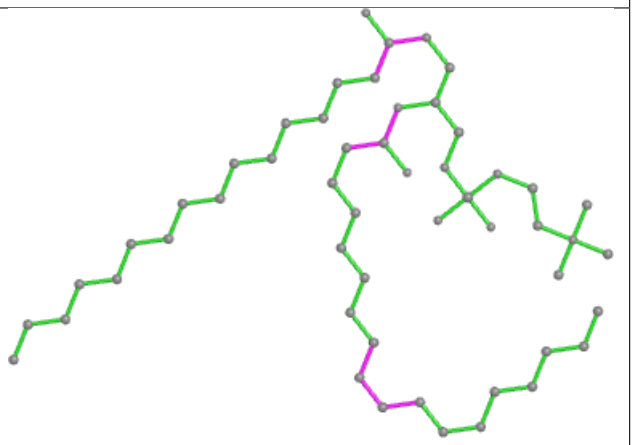
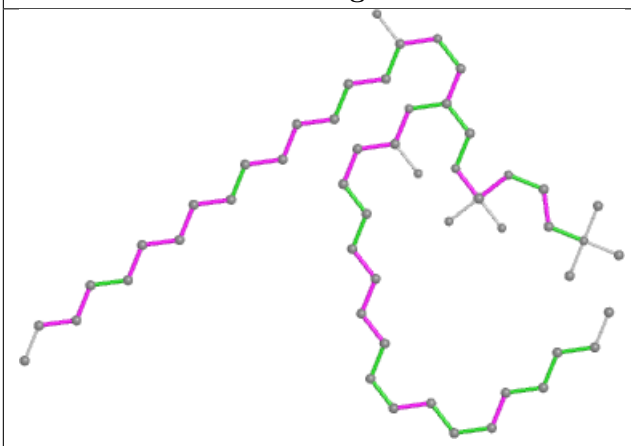


Bond angles



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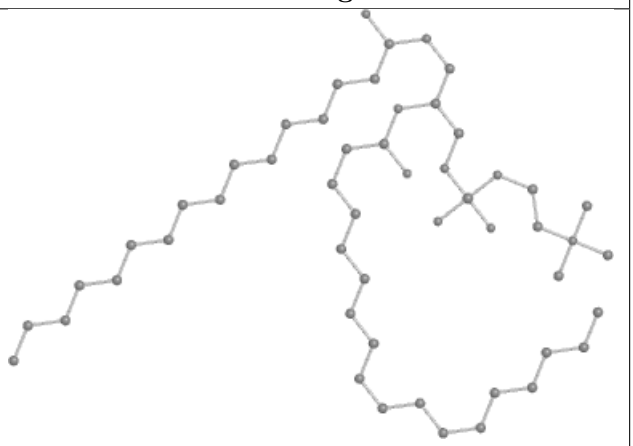
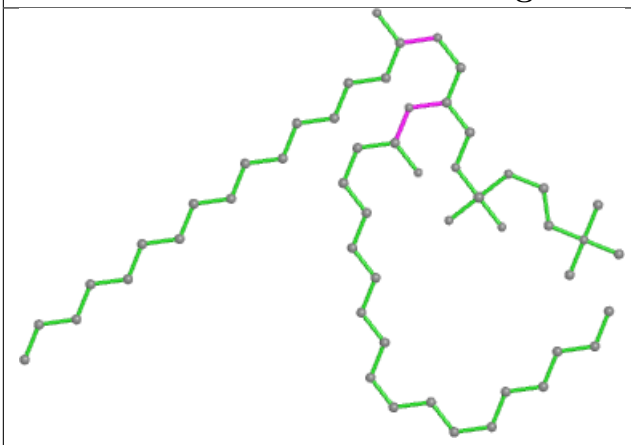


Rings

Ligand CPL 2H 201



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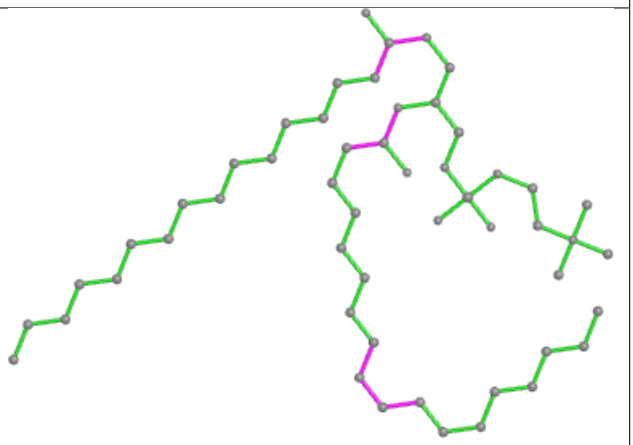

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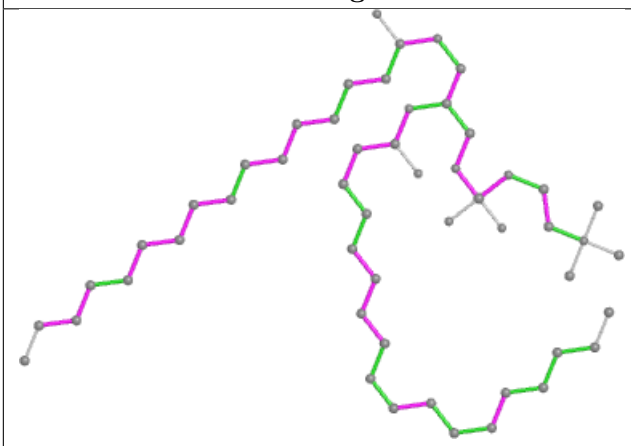

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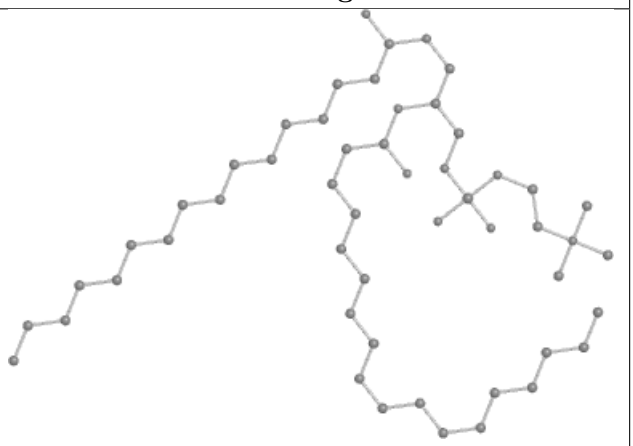

Rings

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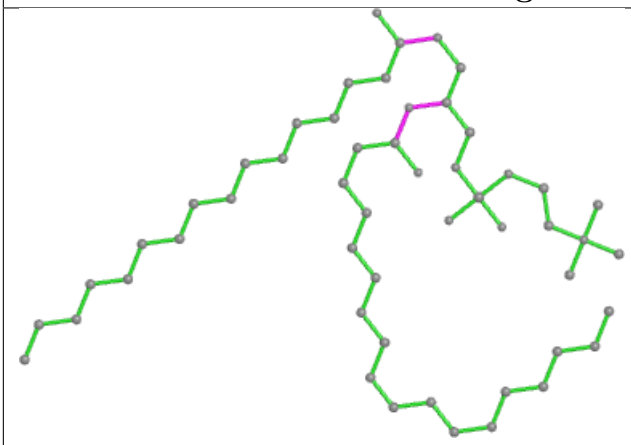
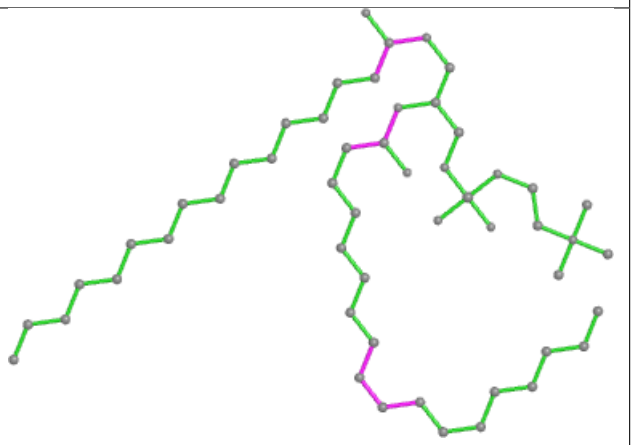


Bond lengths



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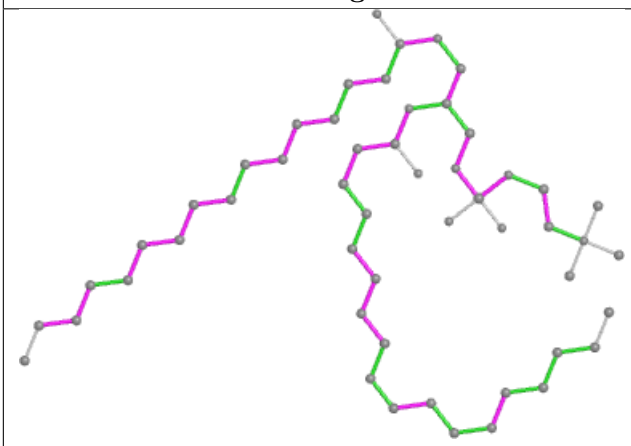

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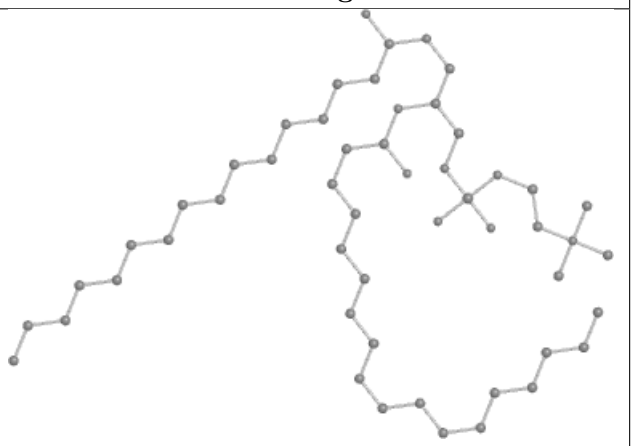
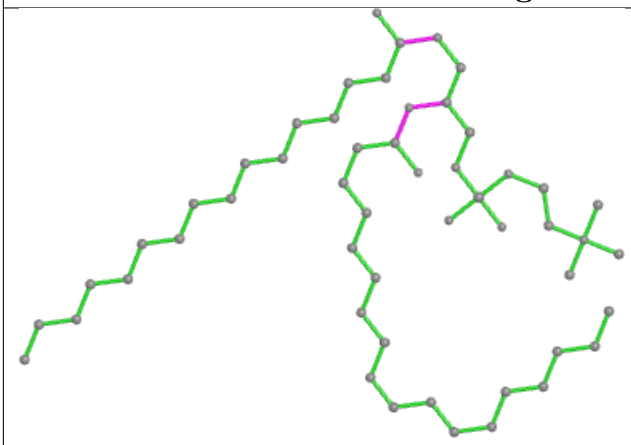
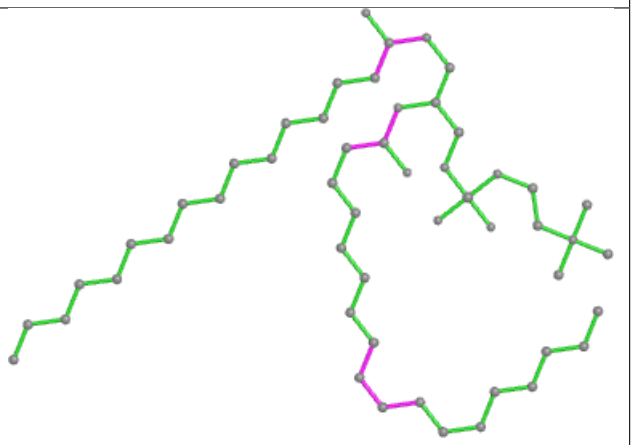


Rings

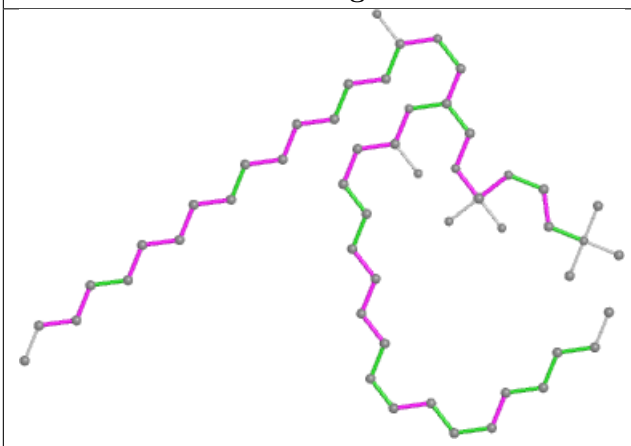
Ligand CPL 4G 201



Bond lengths



Bond angles



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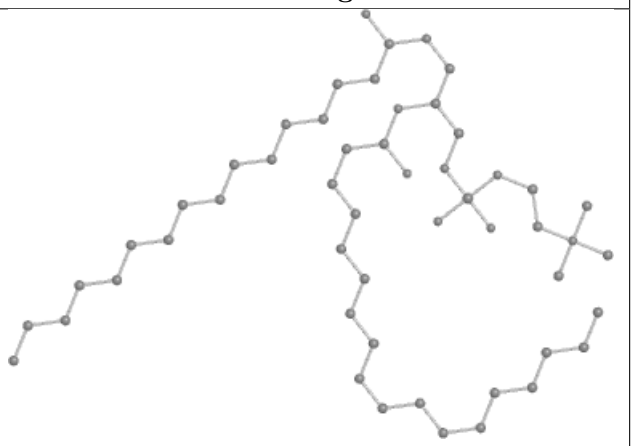
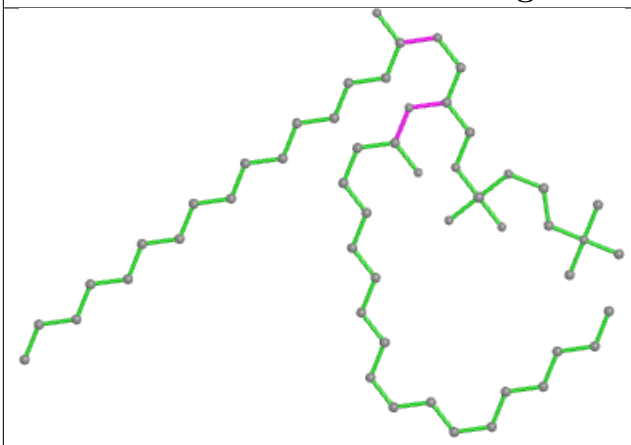
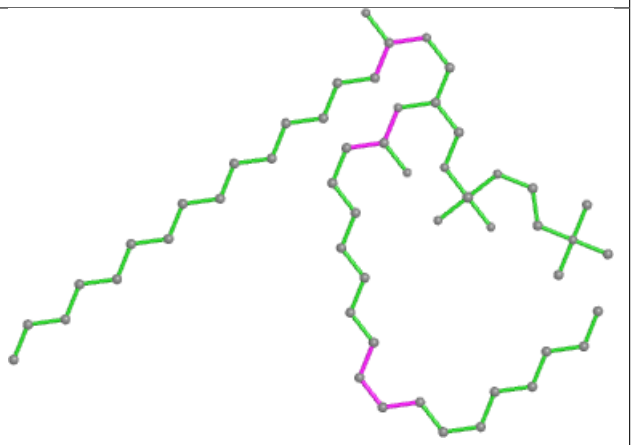


Rings

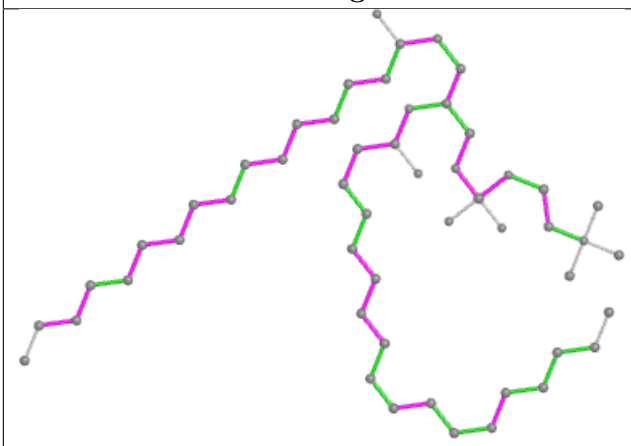
Ligand CPL 2B 201



Bond lengths



Bond angles



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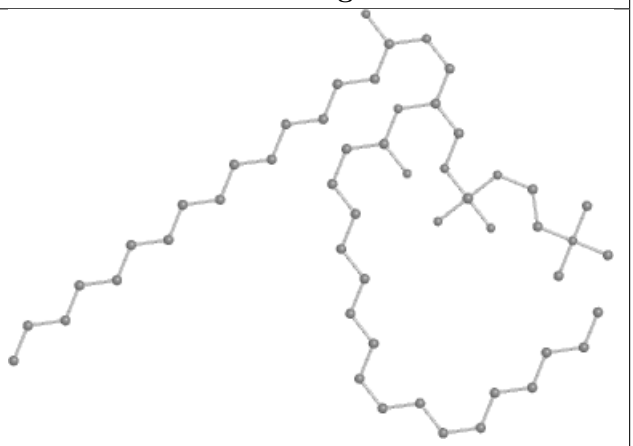
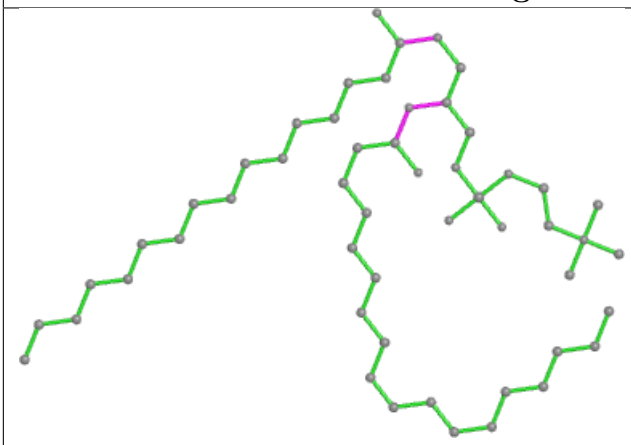
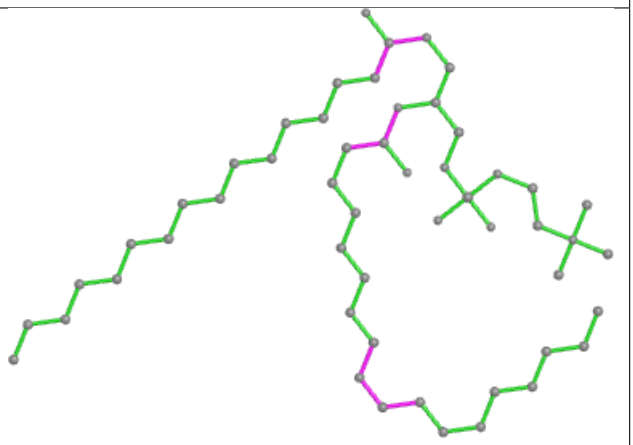


Rings

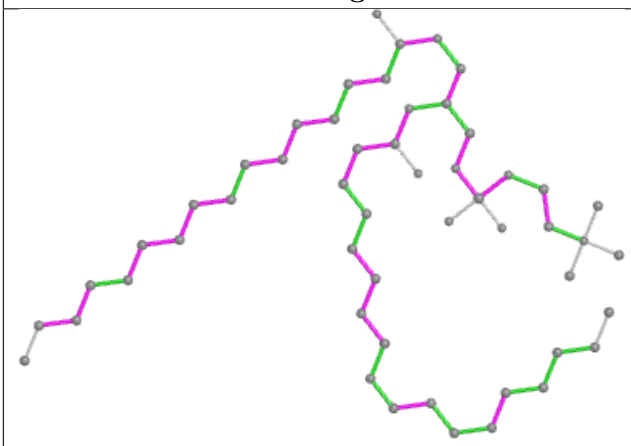
Ligand CPL 3M 201



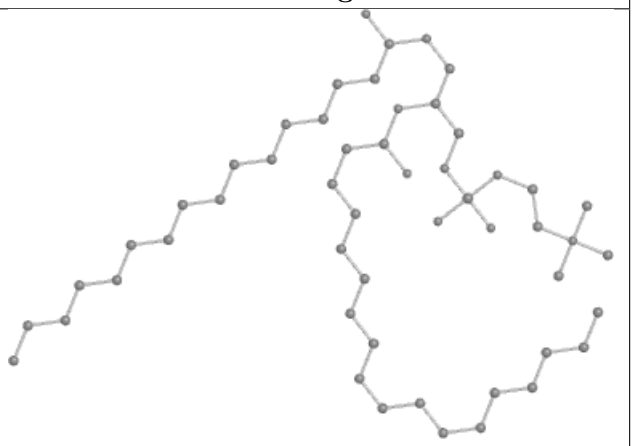
Bond lengths



Bond angles

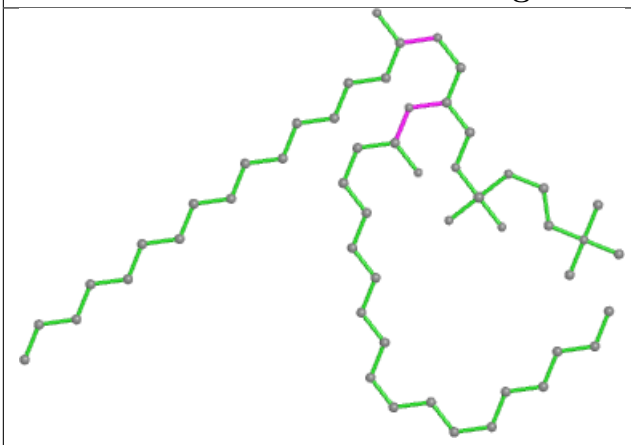


Torsions



Rings

Ligand CPL 5M 201



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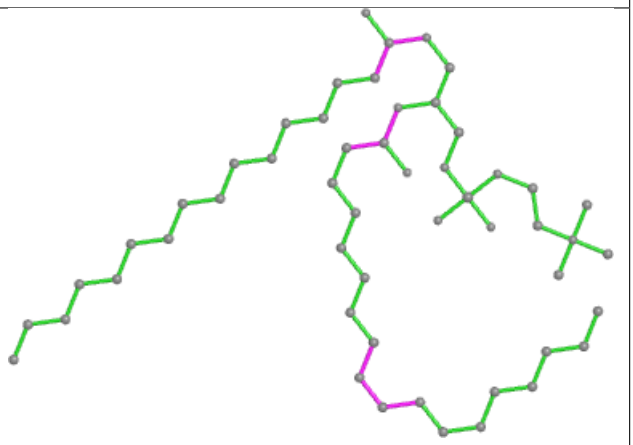

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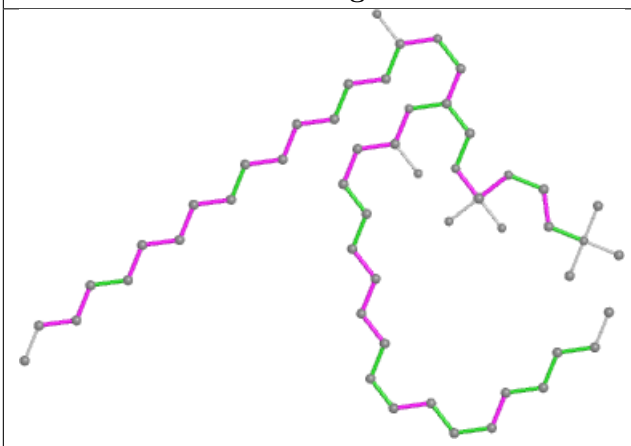

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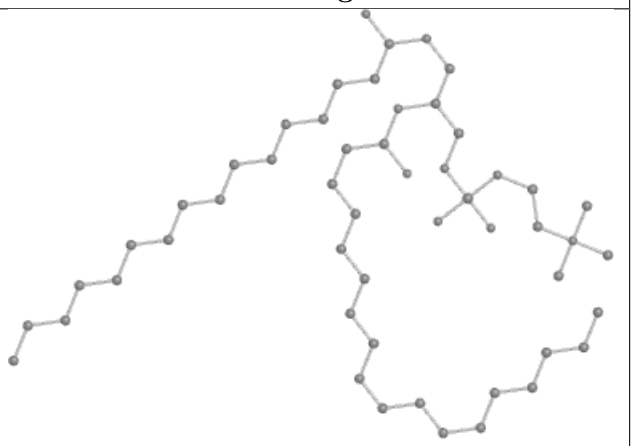

Rings

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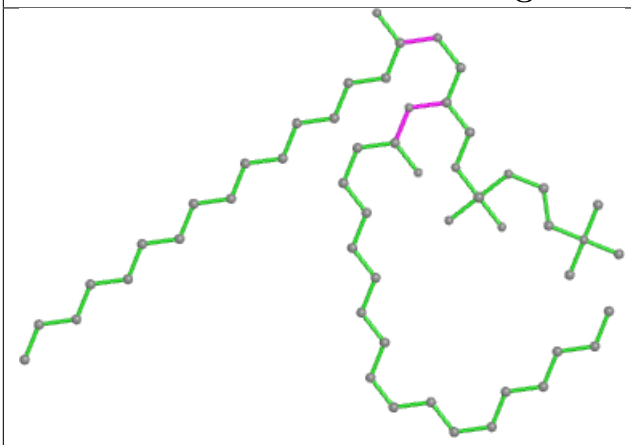

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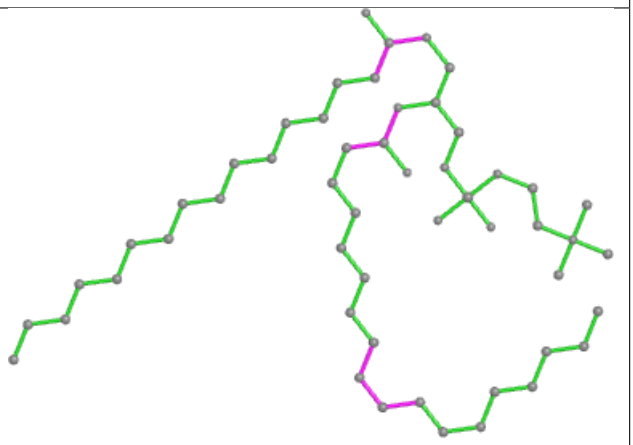

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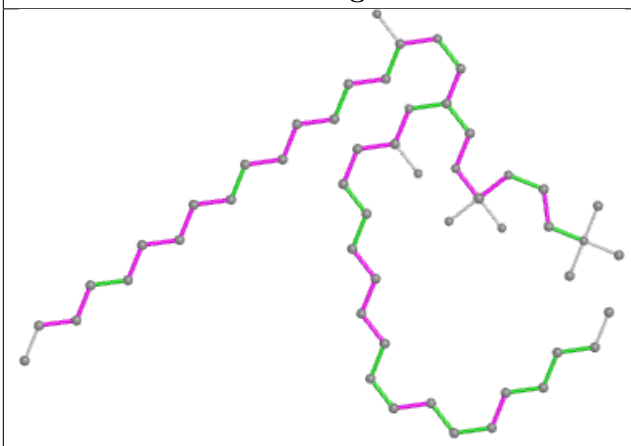

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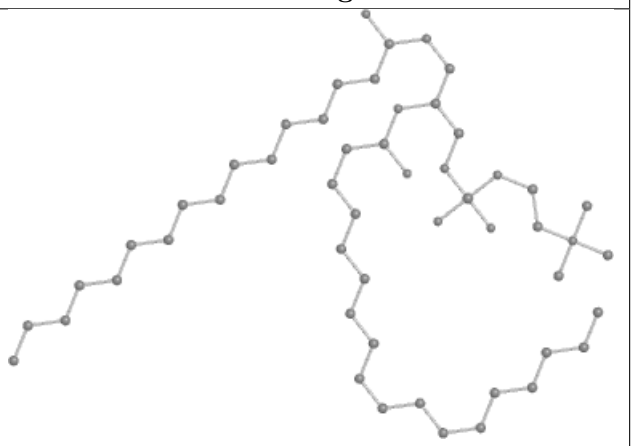

Rings

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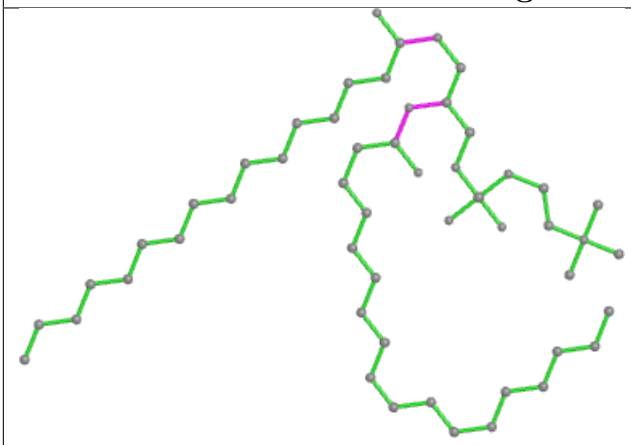

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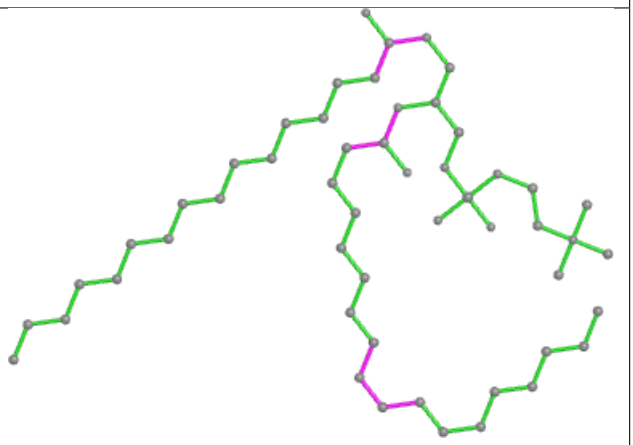
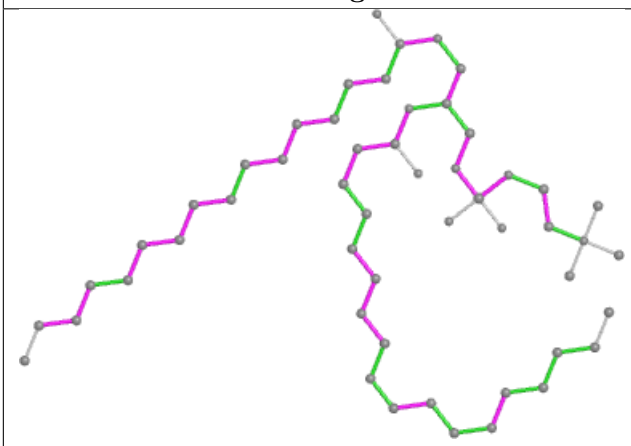


Bond angles



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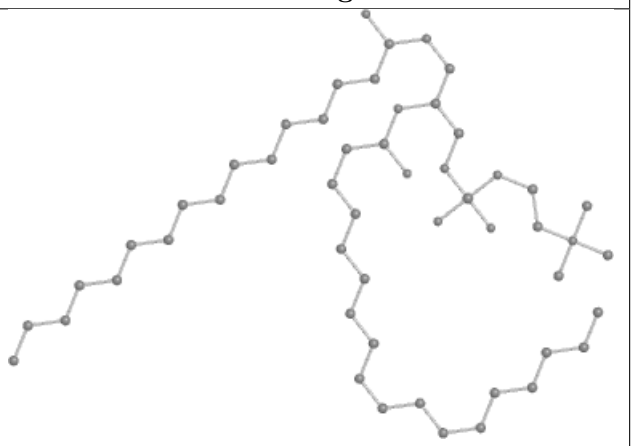
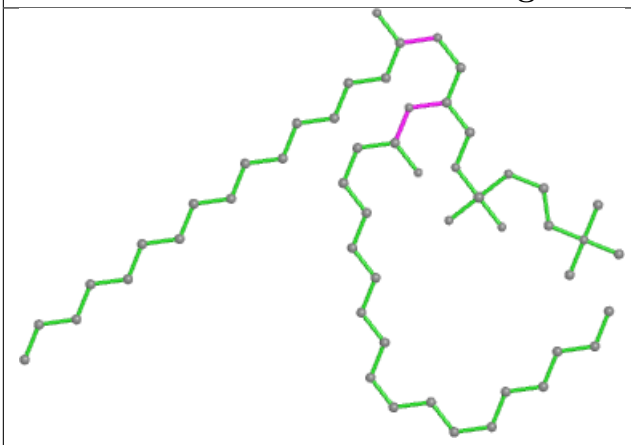


Rings

Ligand CPL 1E 201



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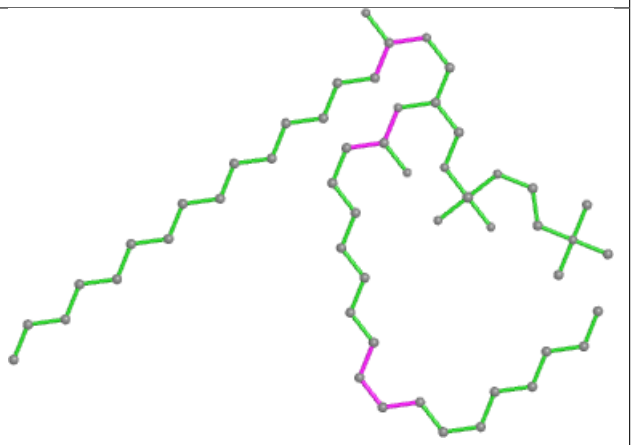
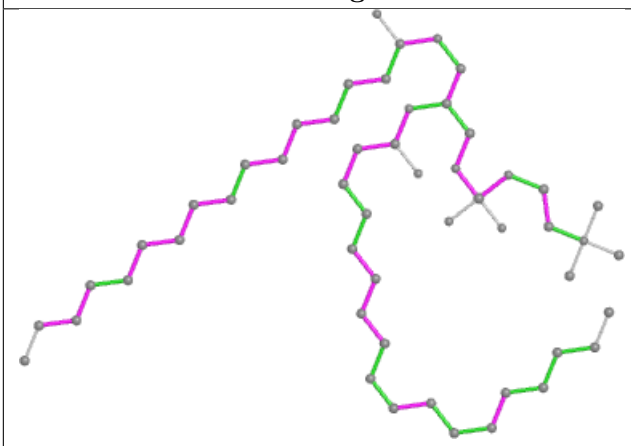


Bond angles



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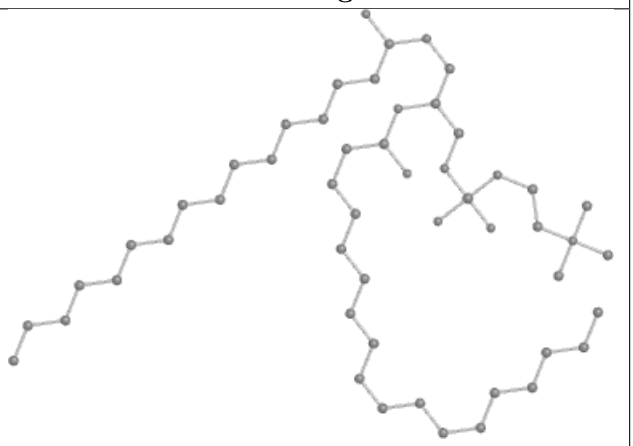

Rings

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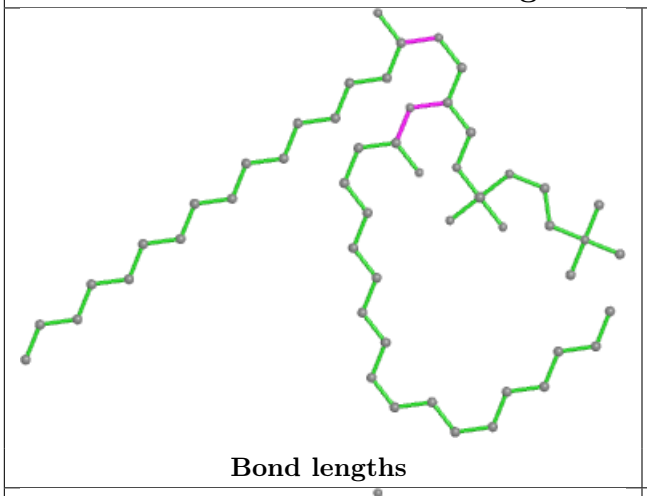

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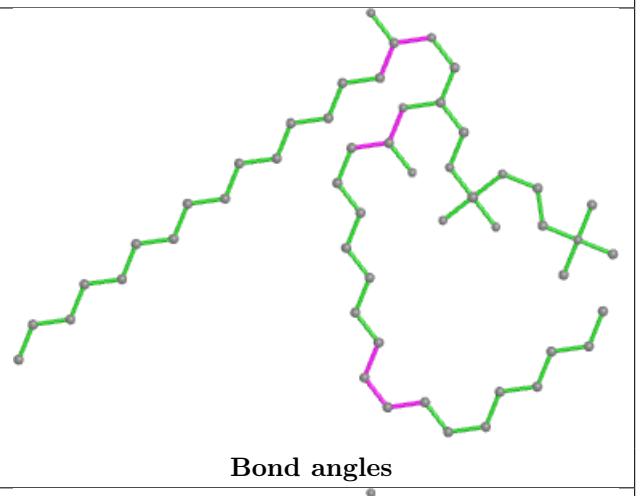

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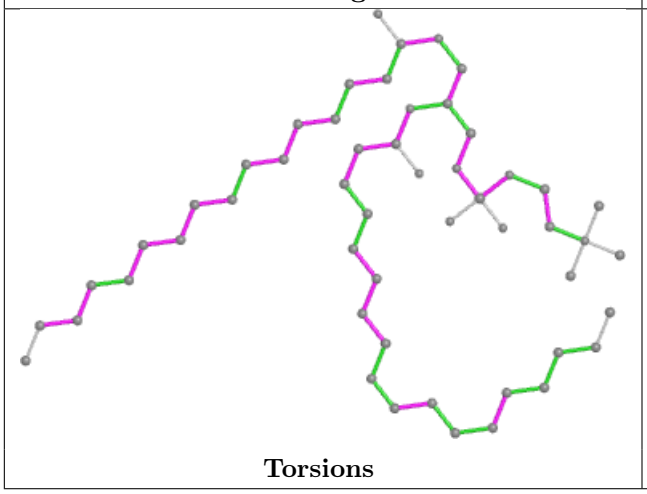

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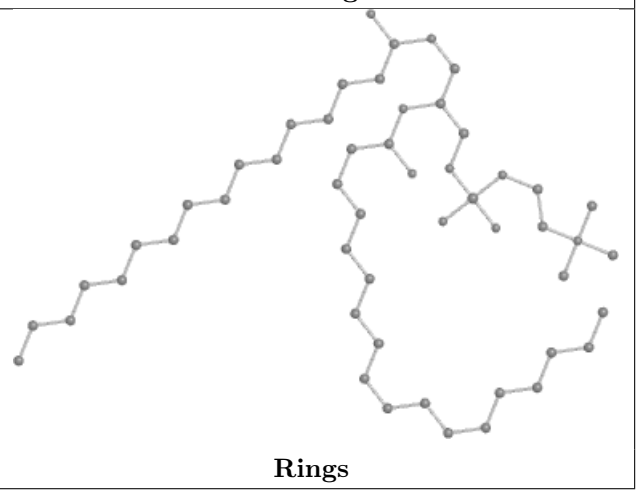
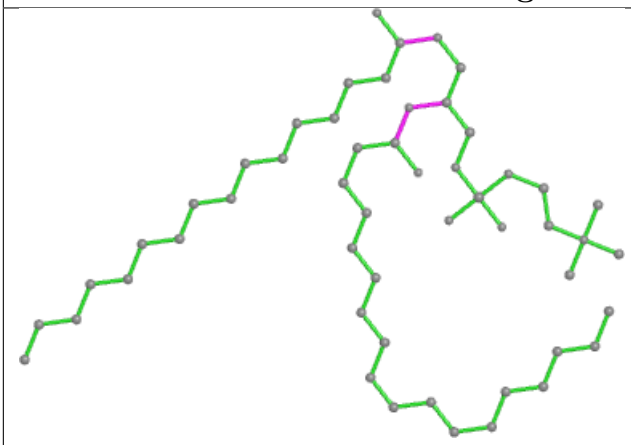


Rings

Ligand CPL 3C 201



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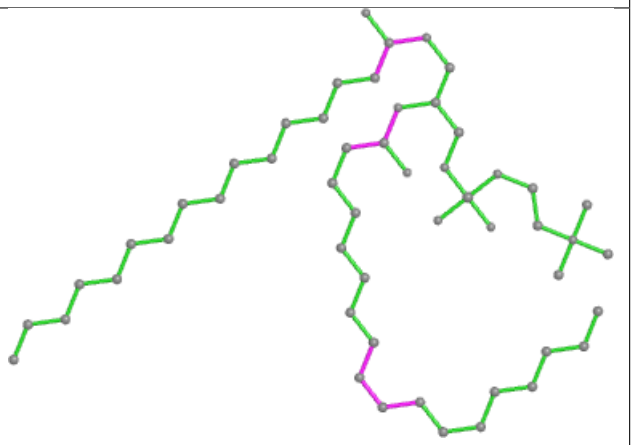
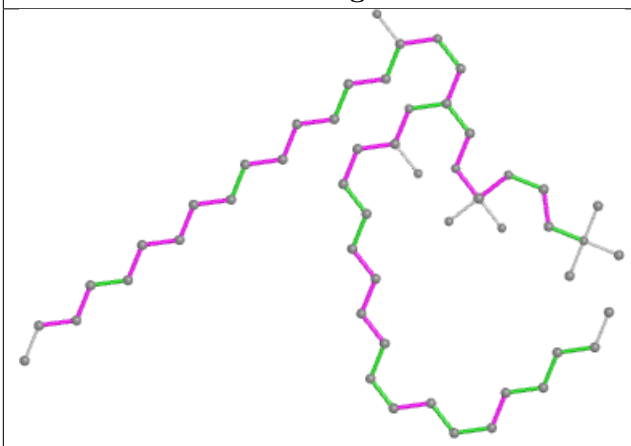


Bond angles



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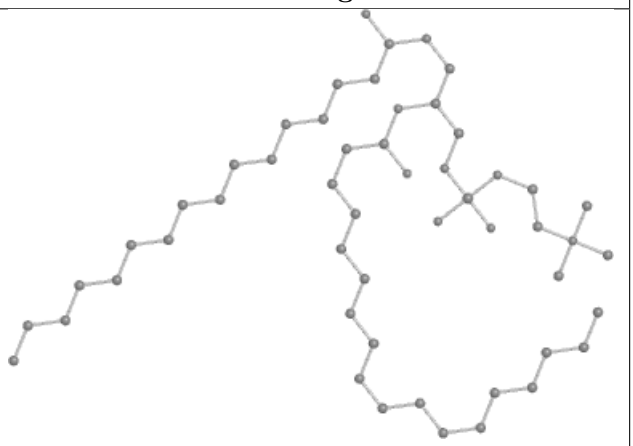
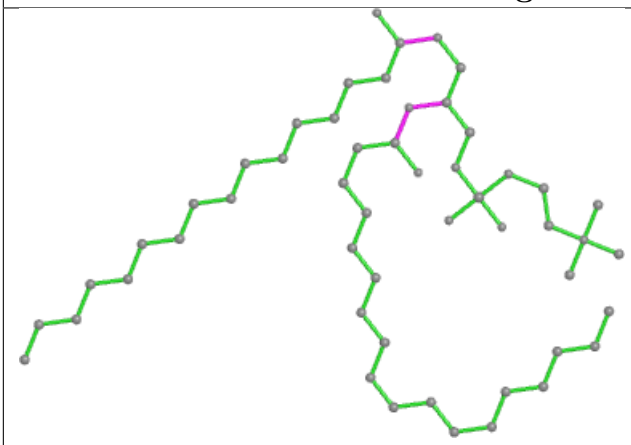


Rings

Ligand CPL 4D 201



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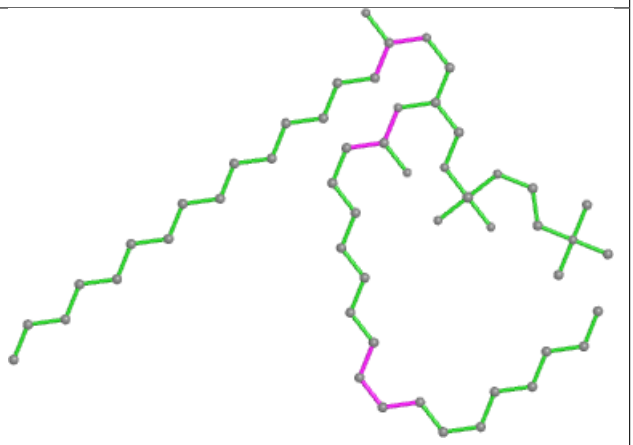

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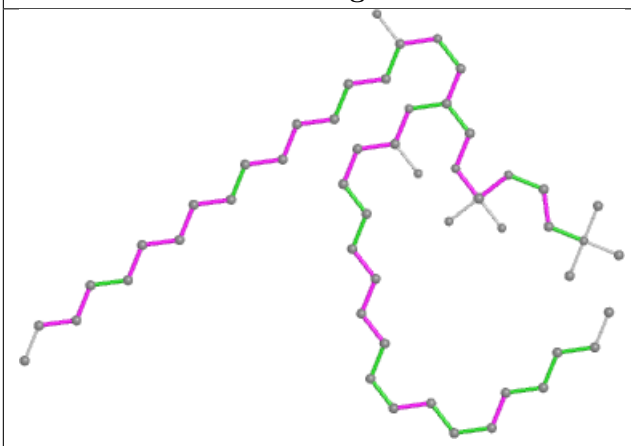

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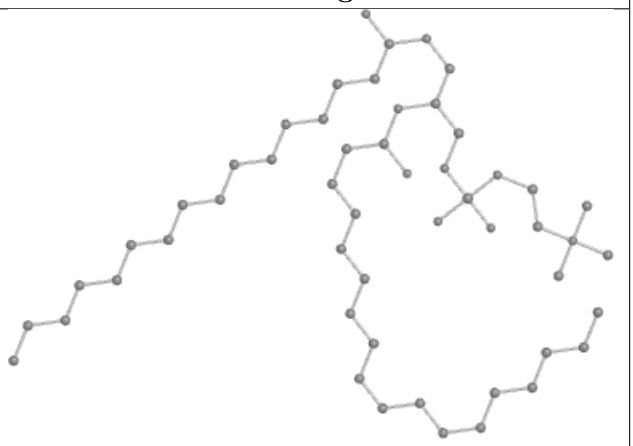

Rings

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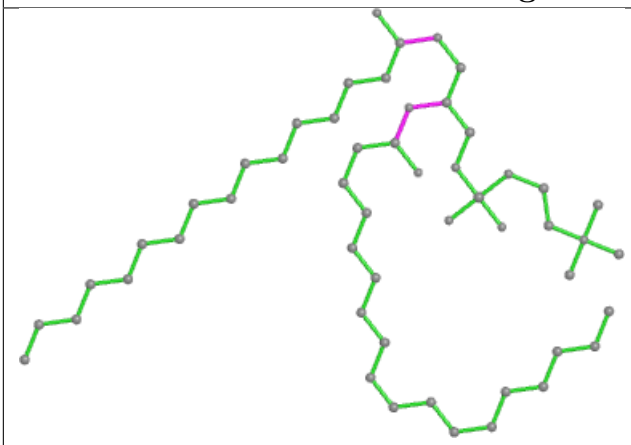

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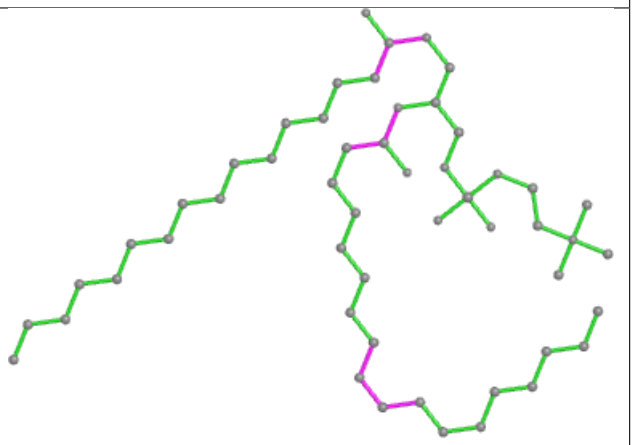

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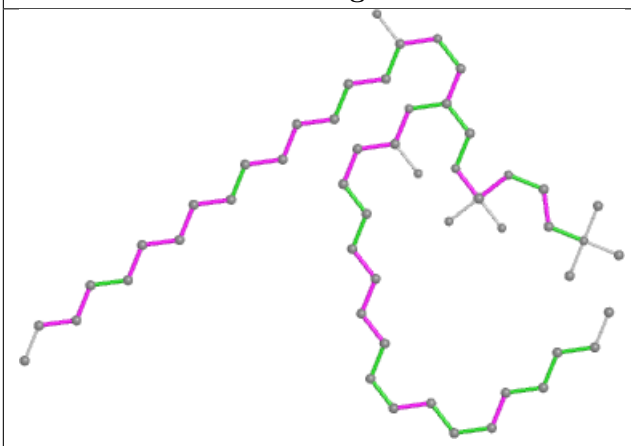

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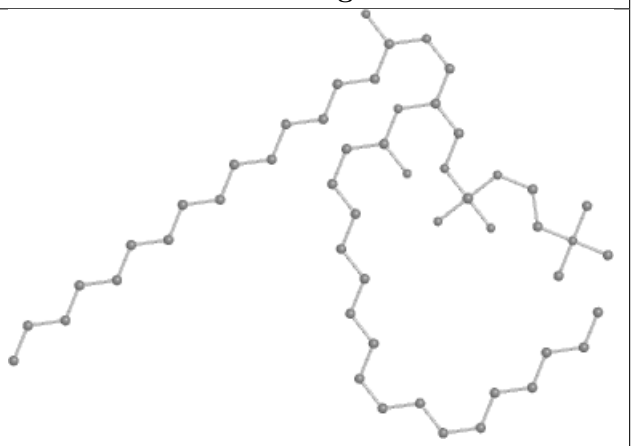
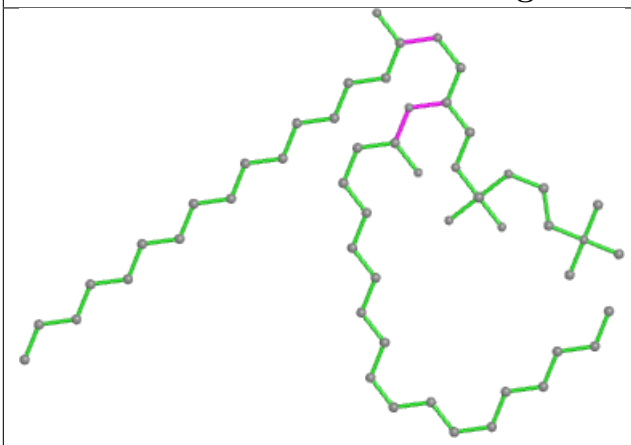


Rings

Ligand CPL 4B 201



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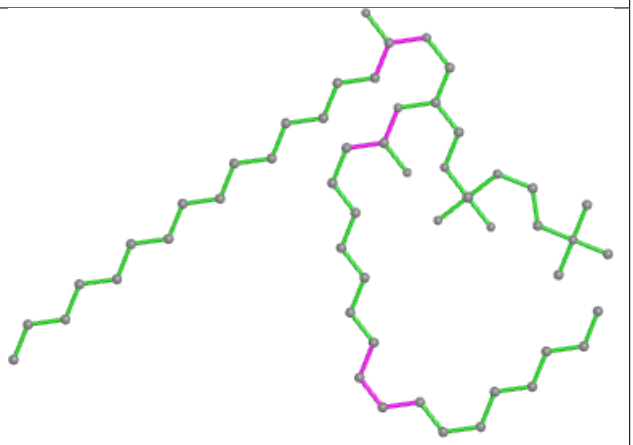
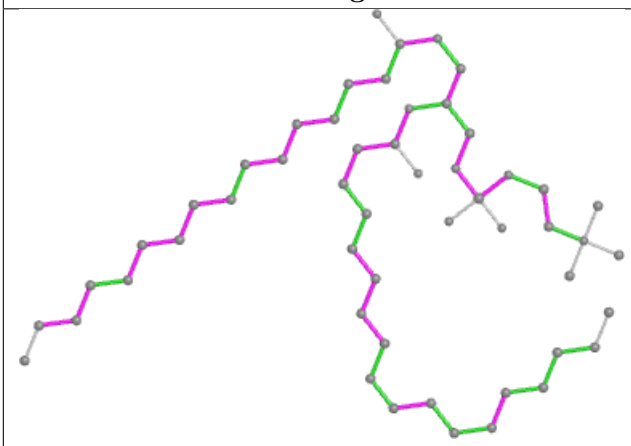


Bond angles



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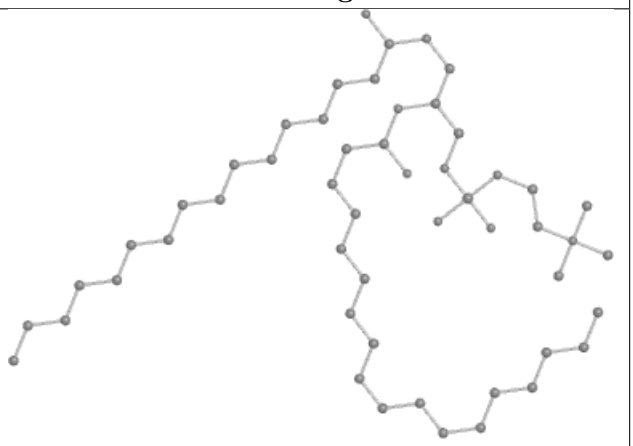
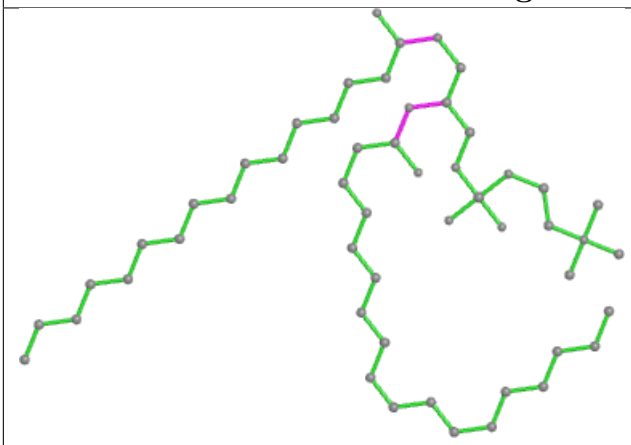


Rings

Ligand CPL 5G 201



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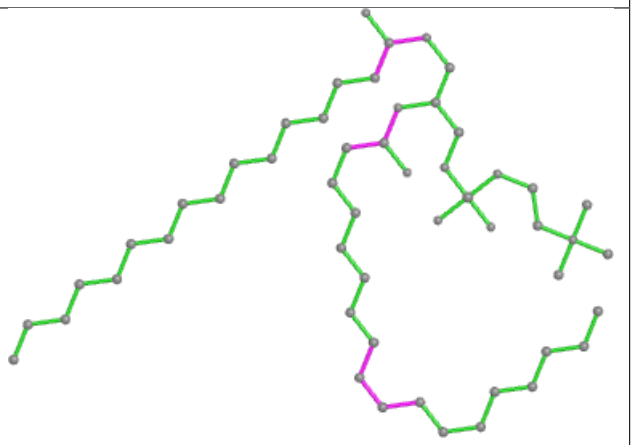

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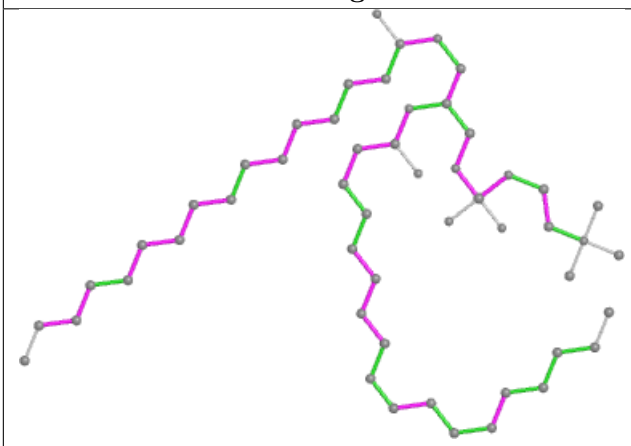

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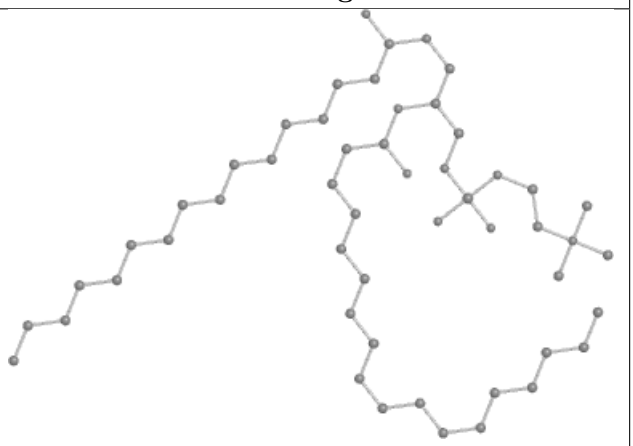
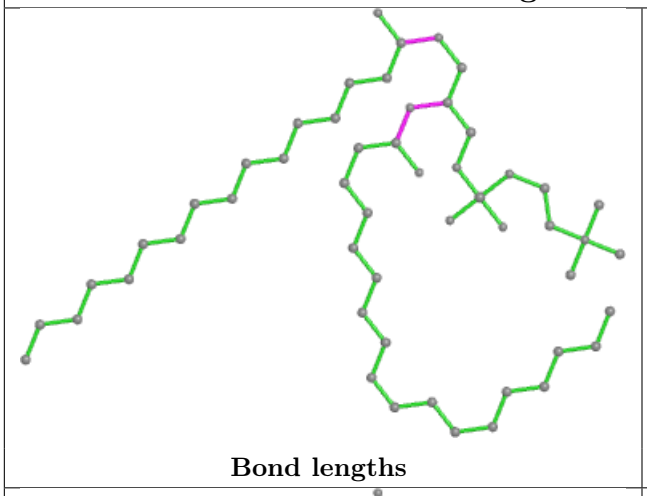


Rings

Ligand CPL 5L 201



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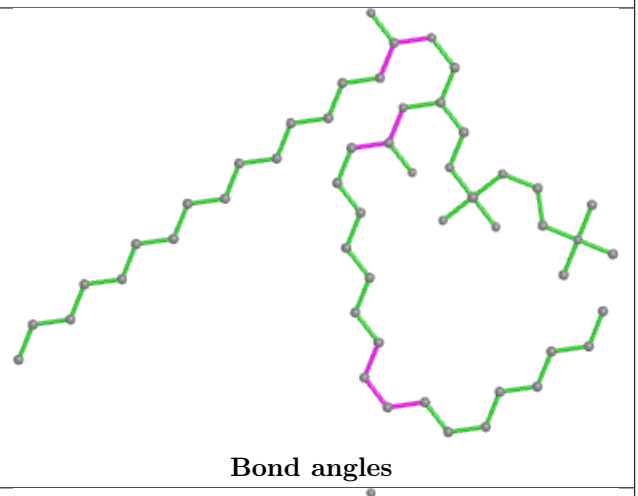

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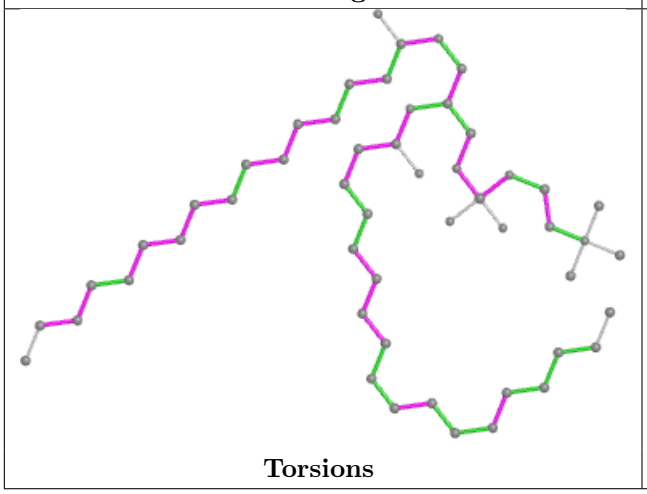

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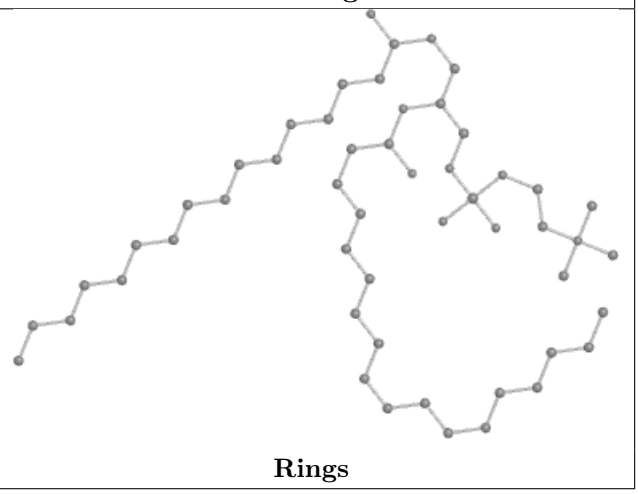

Rings

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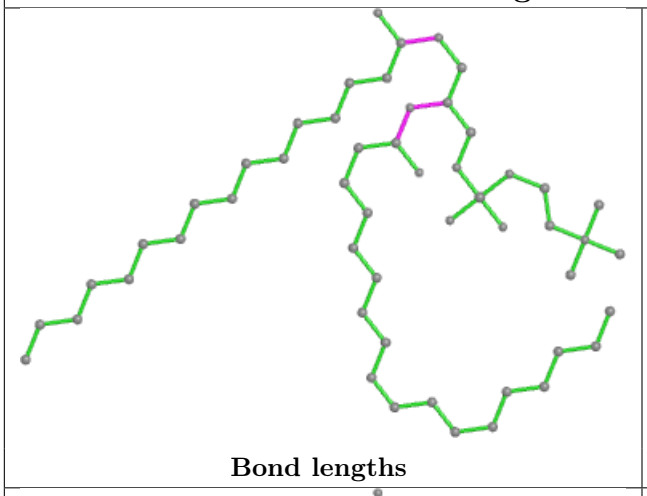

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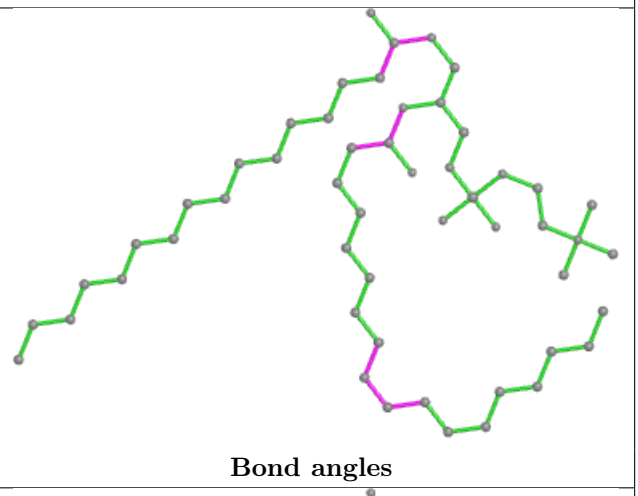

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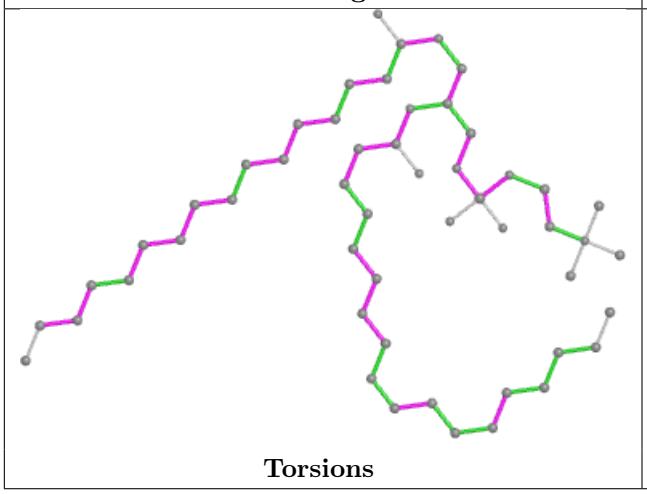

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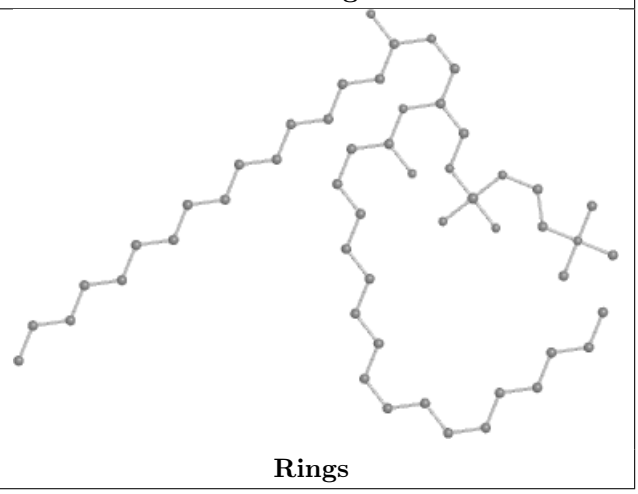
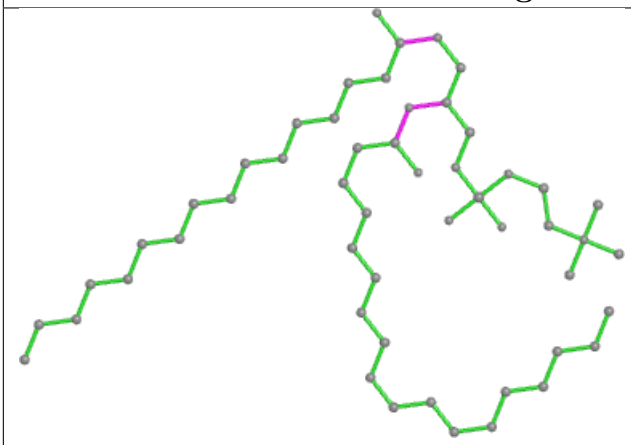
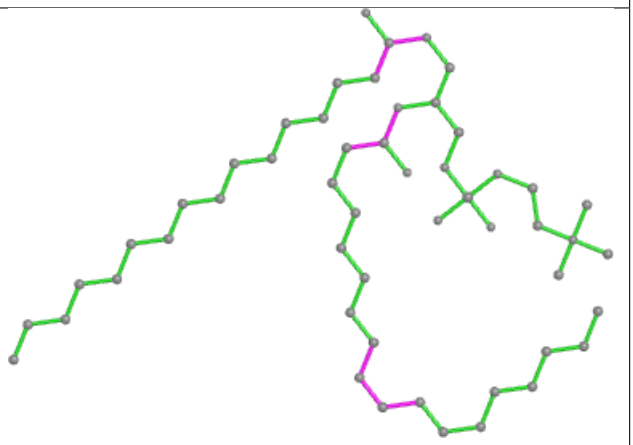


Rings

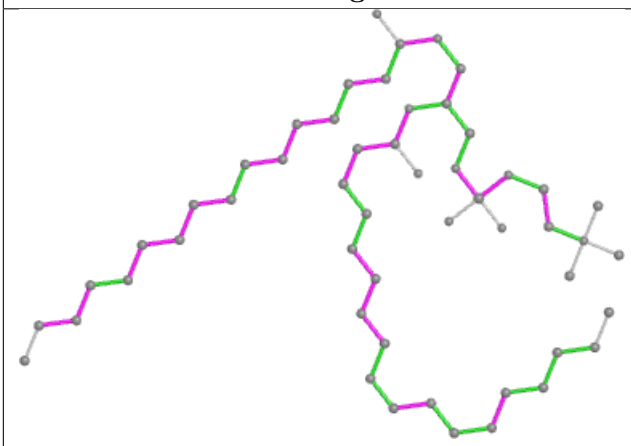
Ligand CPL 4K 201



Bond lengths



Bond angles



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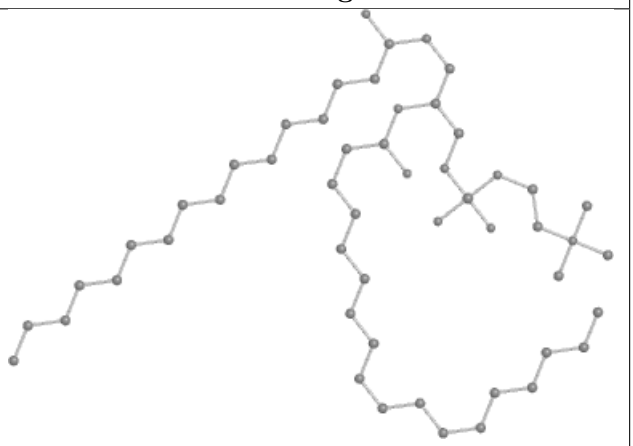
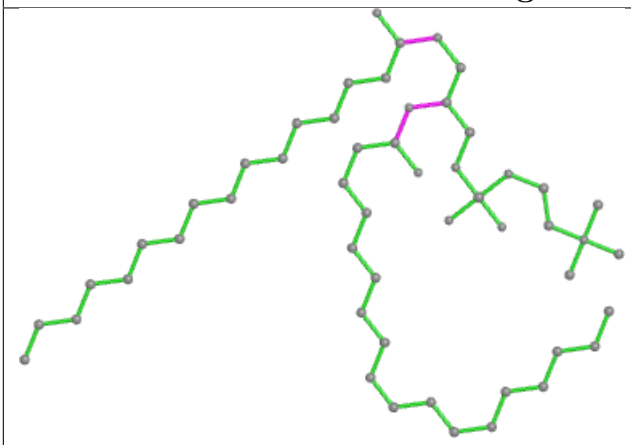
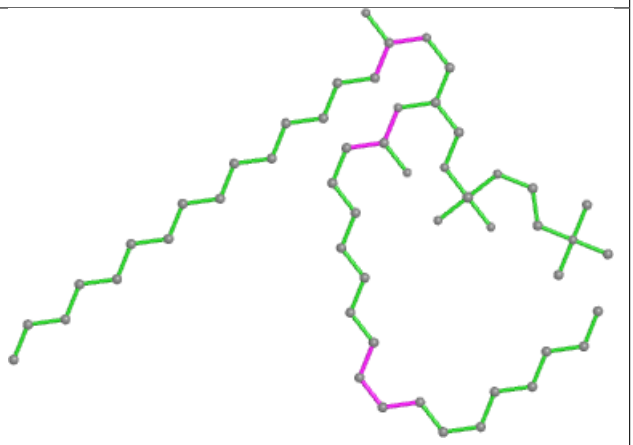


Rings

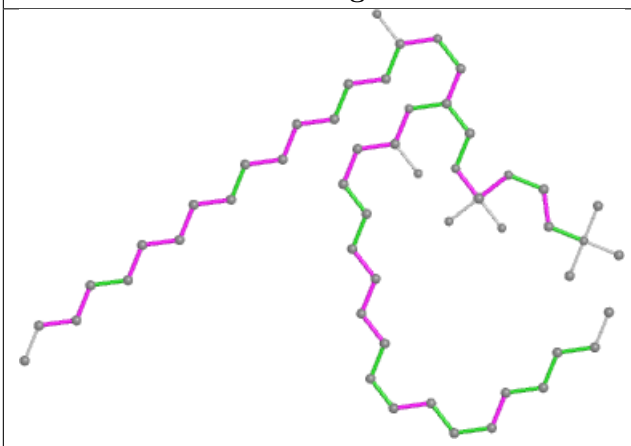
Ligand CPL 5C 201



Bond lengths



Bond angles



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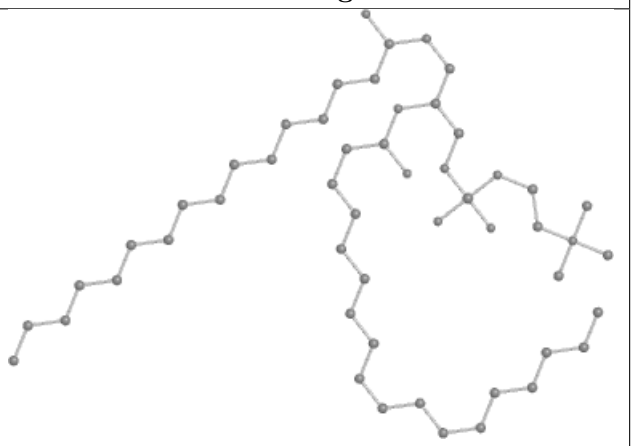
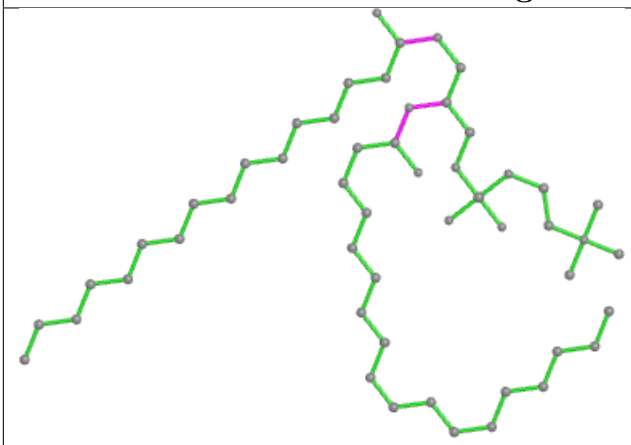
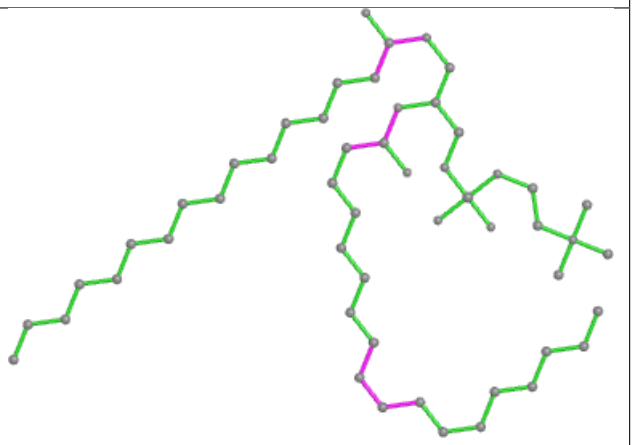


Rings

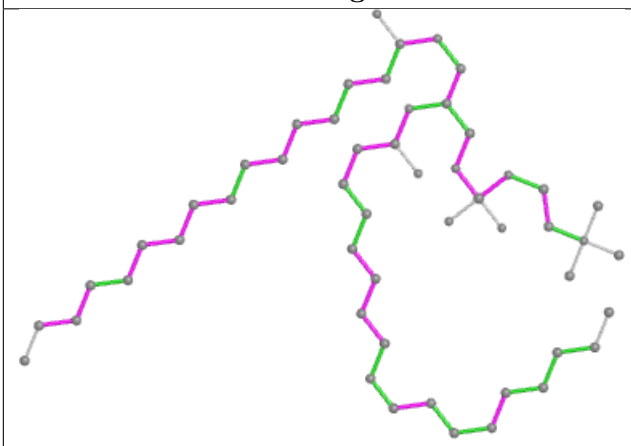
Ligand CPL 4N 201



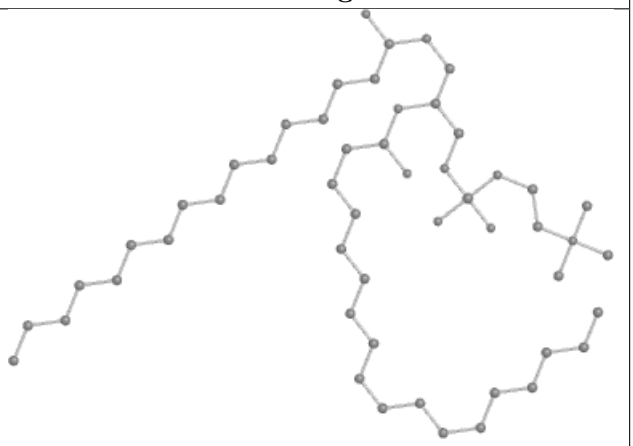
Bond lengths



Bond angles

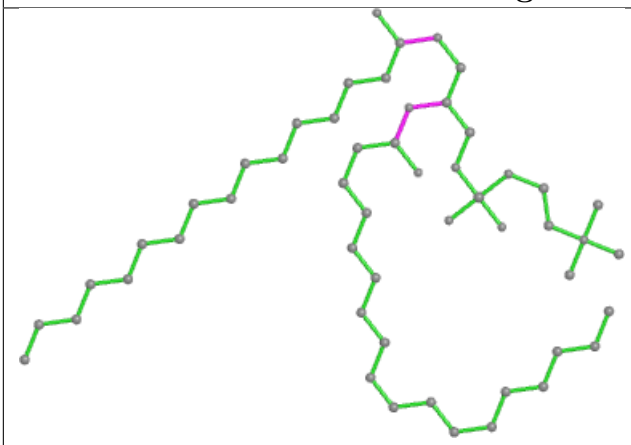


Torsions

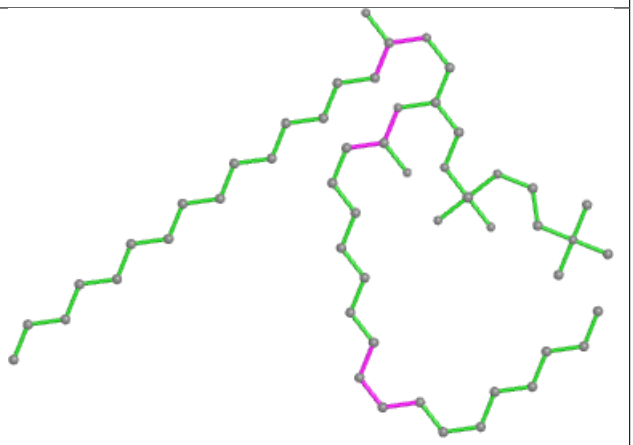


Rings

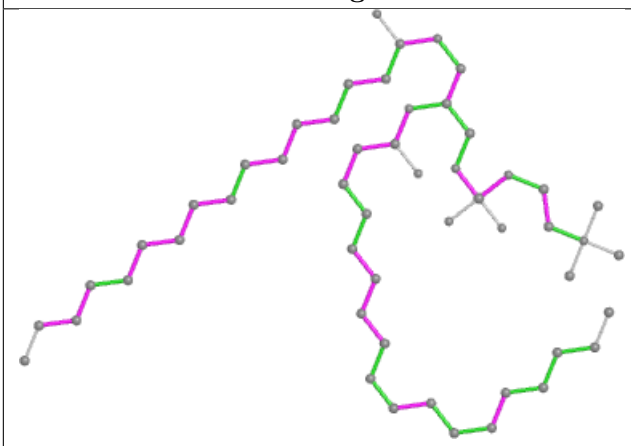
Ligand CPL 5A 201



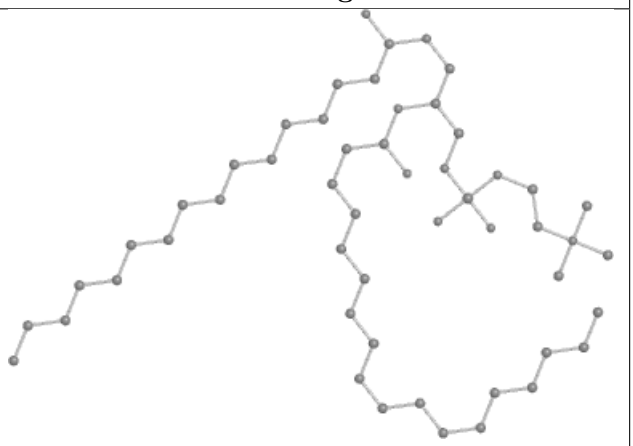
Bond lengths



Bond angles

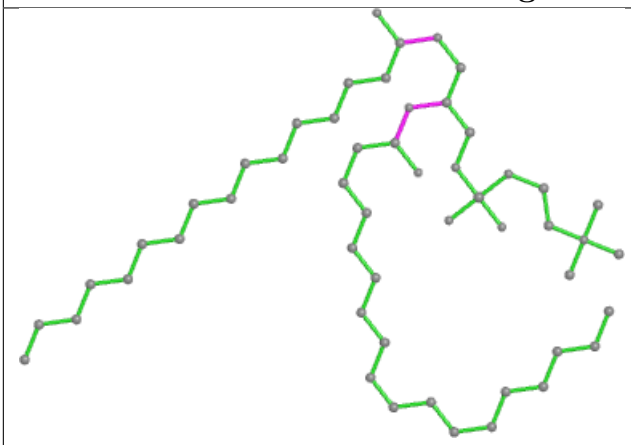


Torsions

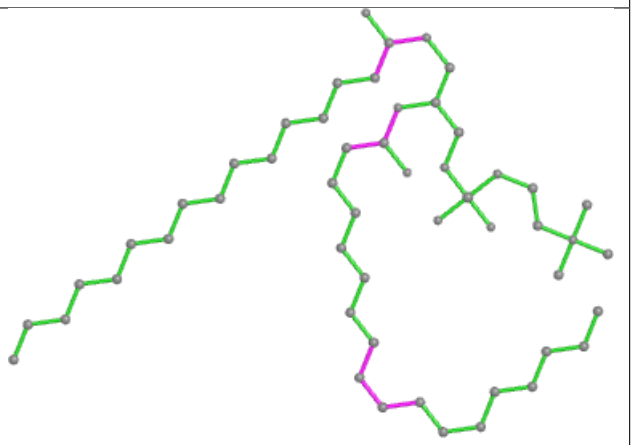


Rings

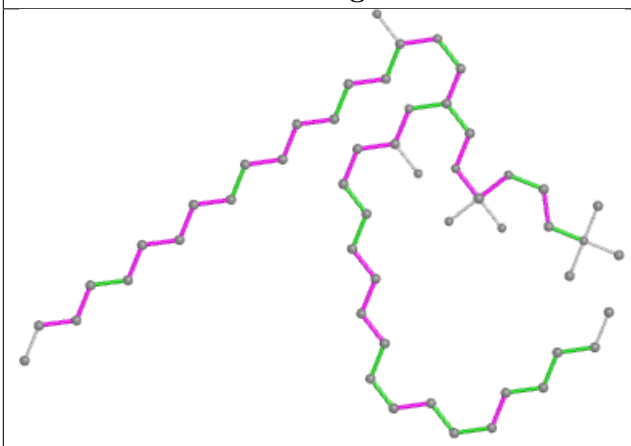
Ligand CPL 2F 201



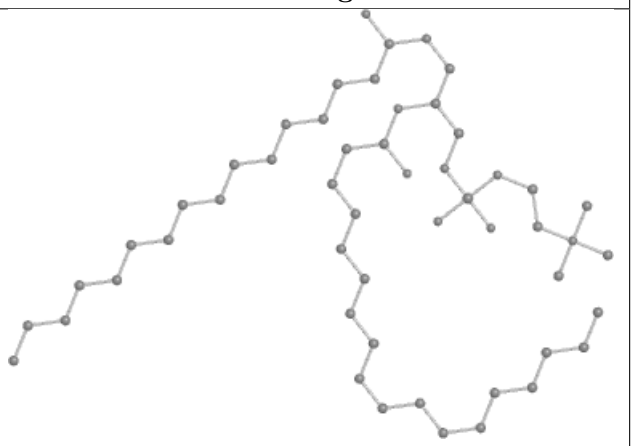
Bond lengths



Bond angles

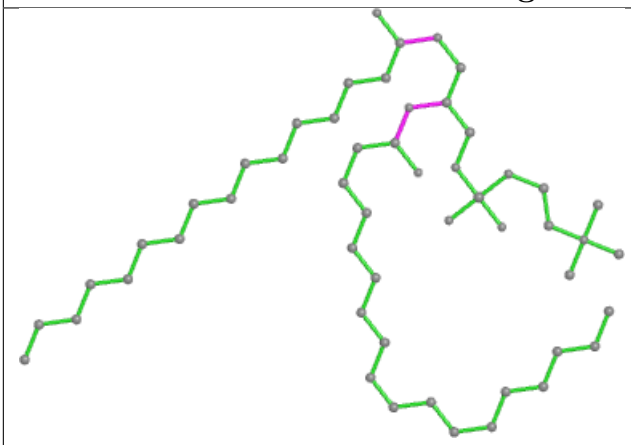


Torsions

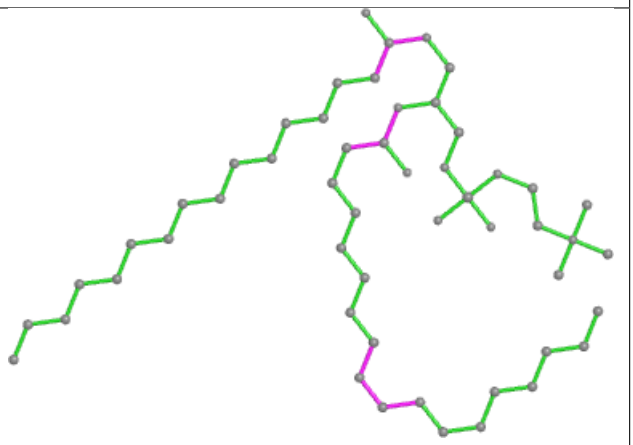


Rings

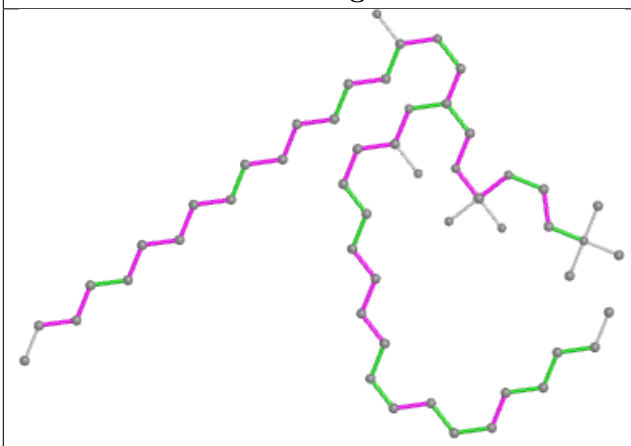
Ligand CPL 2E 201



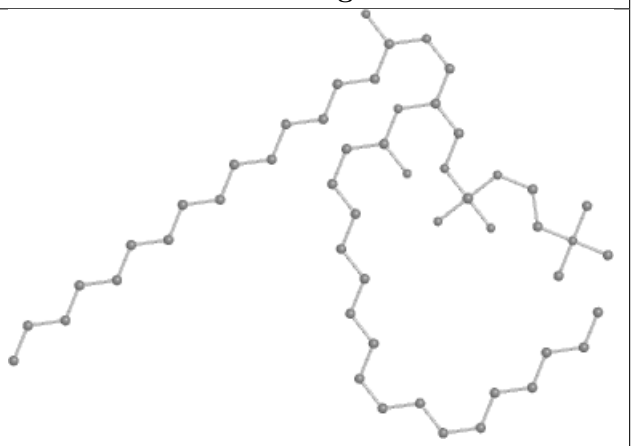
Bond lengths



Bond angles

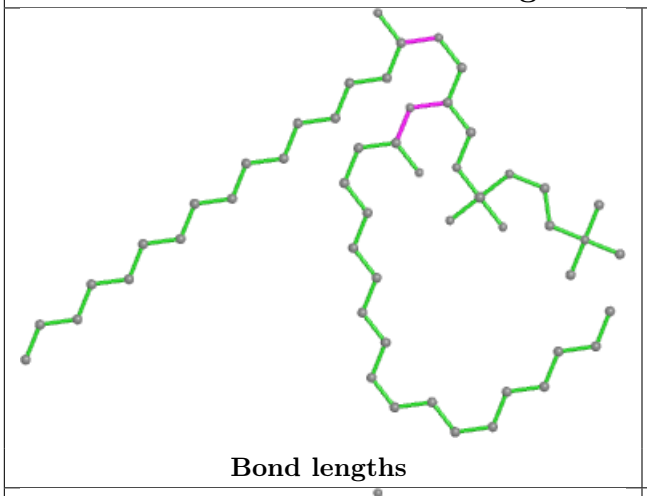


Torsions

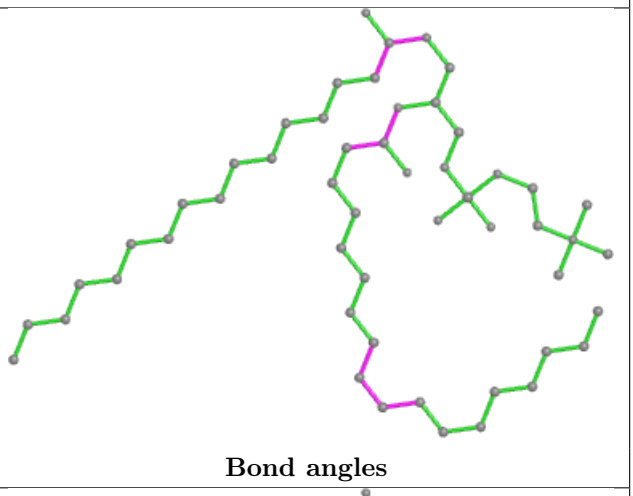


Rings

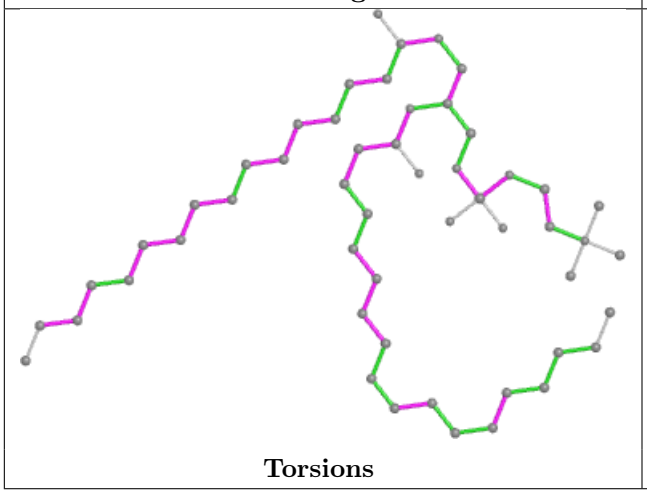
Ligand CPL 5F 201



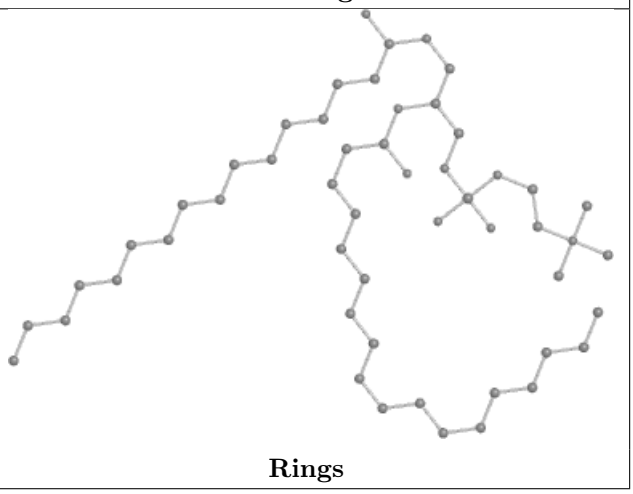
Bond lengths



Bond angles

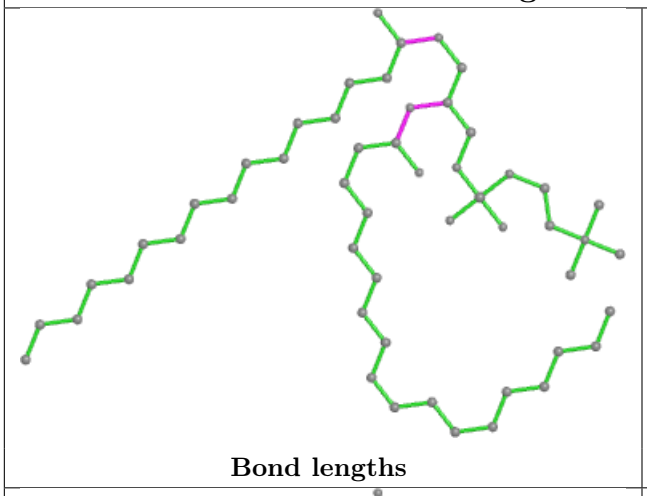


Torsions

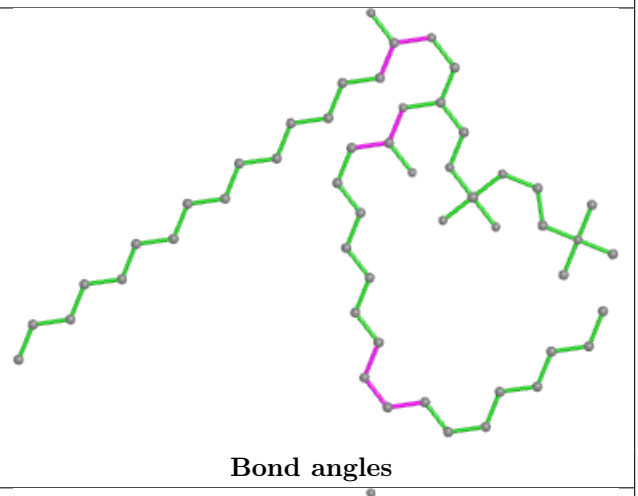


Rings

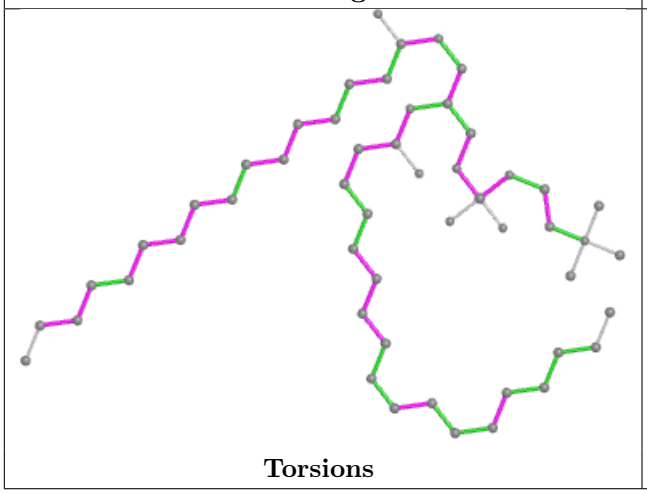
Ligand CPL 3F 201



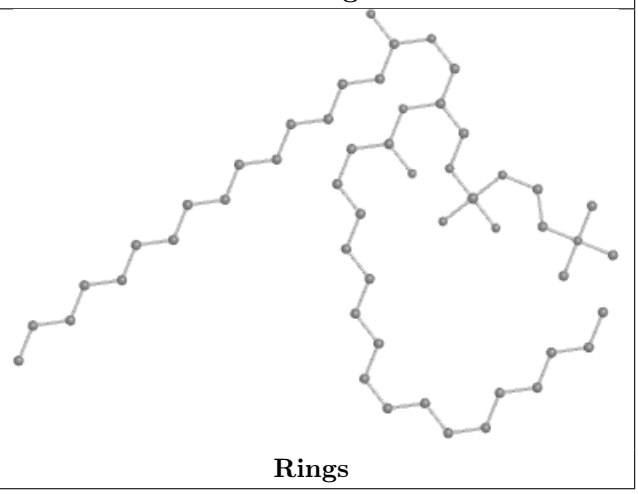
Bond lengths



Bond angles

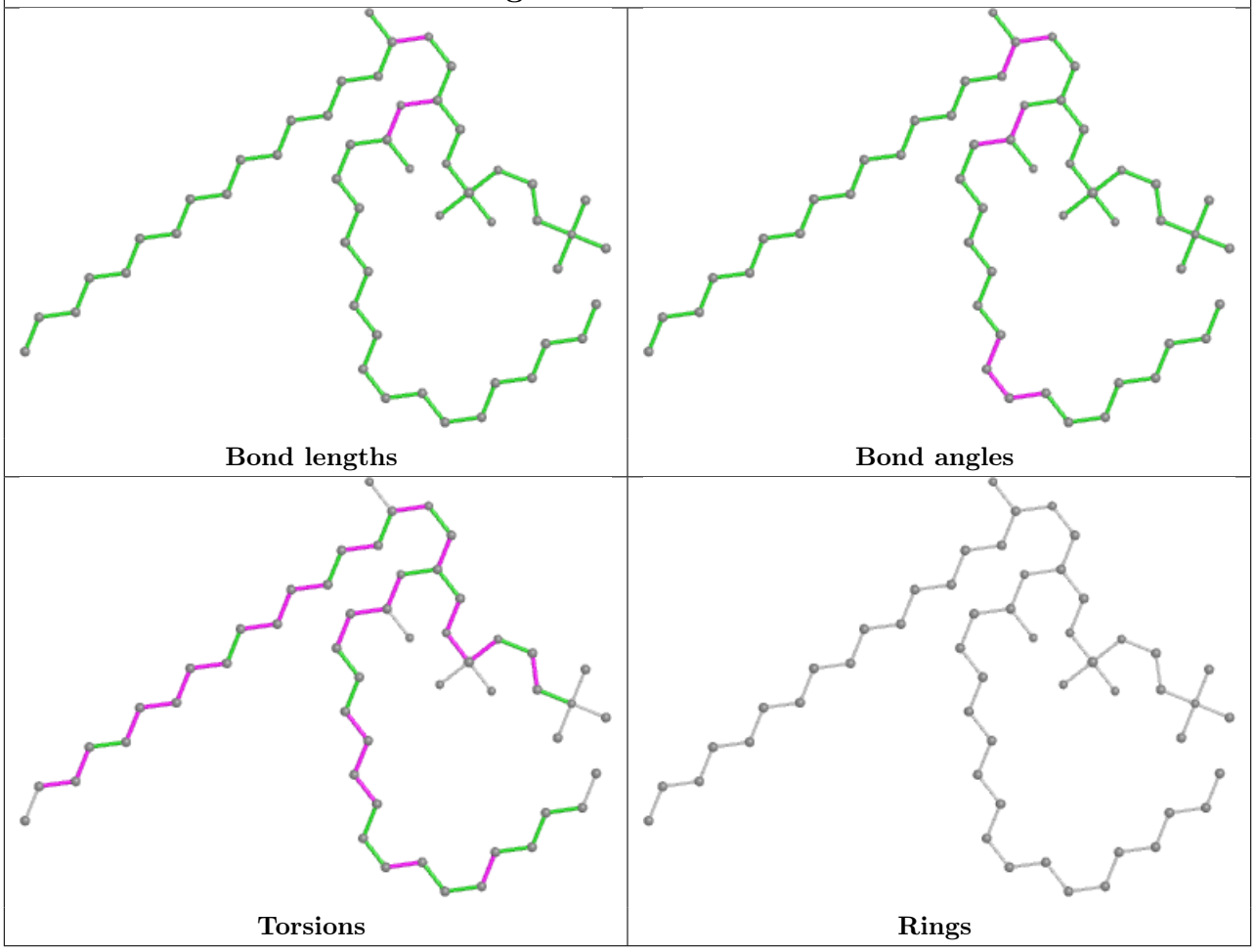


Torsions



Rings

Ligand CPL 1B 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

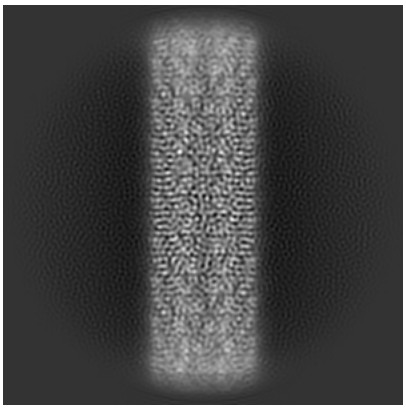
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26999. These allow visual inspection of the internal detail of the map and identification of artifacts.

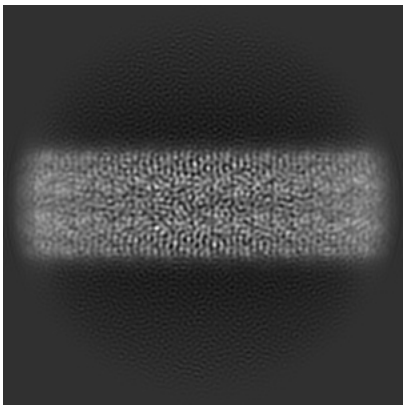
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

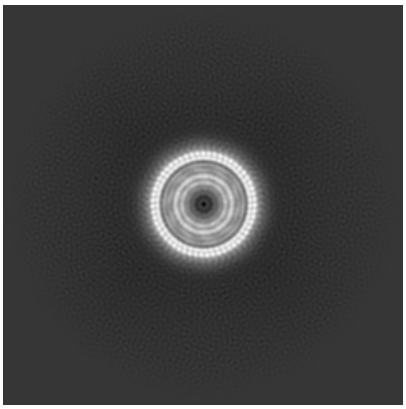
6.1.1 Primary map



X

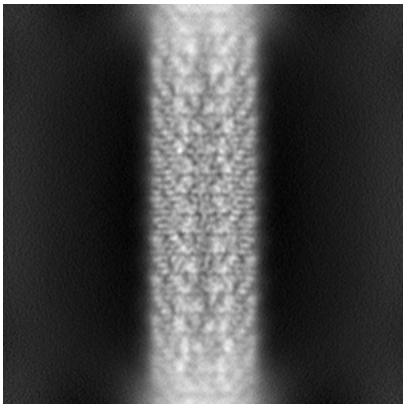


Y

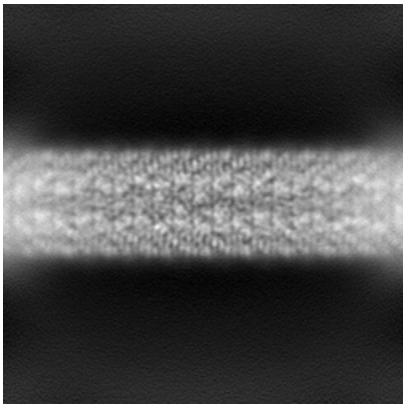


Z

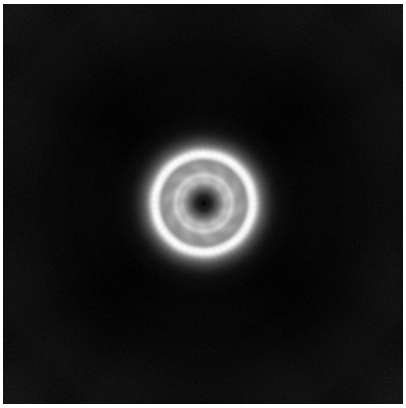
6.1.2 Raw map



X



Y

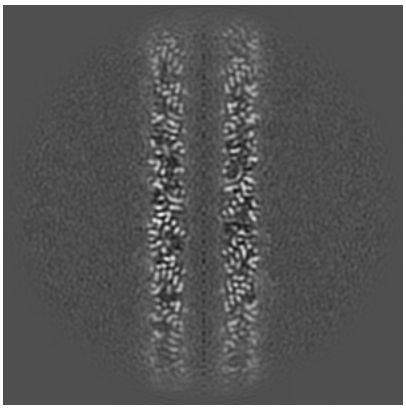


Z

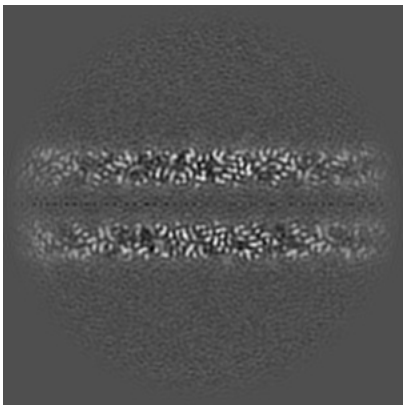
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

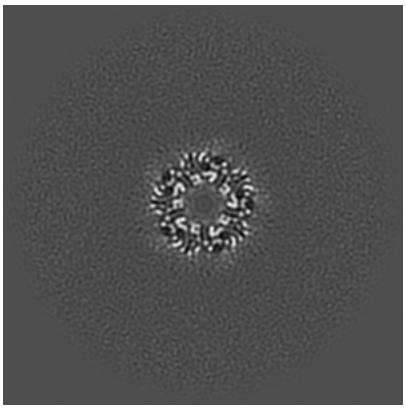
6.2.1 Primary map



X Index: 128

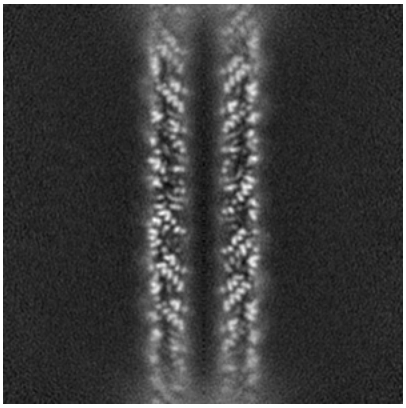


Y Index: 128

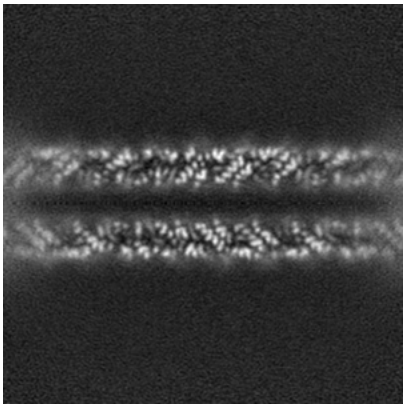


Z Index: 128

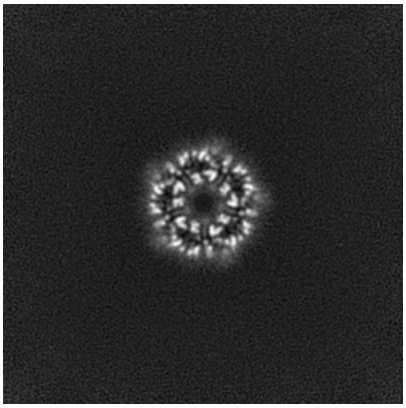
6.2.2 Raw map



X Index: 128



Y Index: 128

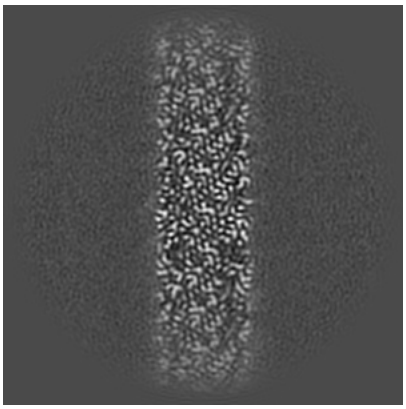


Z Index: 128

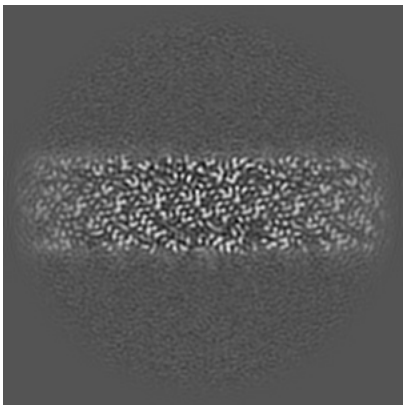
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

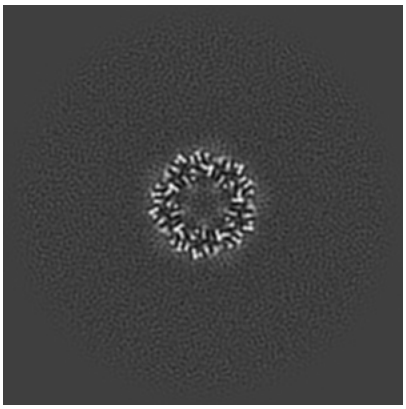
6.3.1 Primary map



X Index: 145

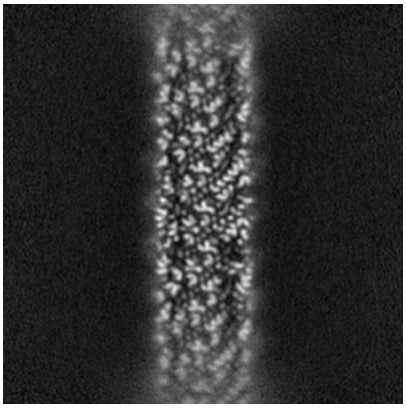


Y Index: 145

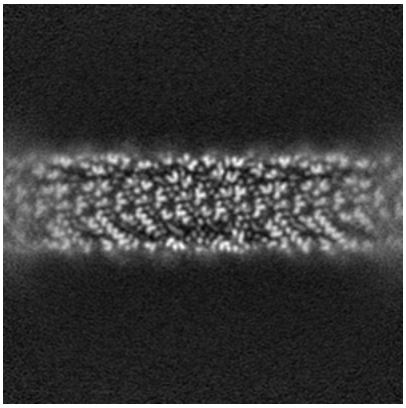


Z Index: 131

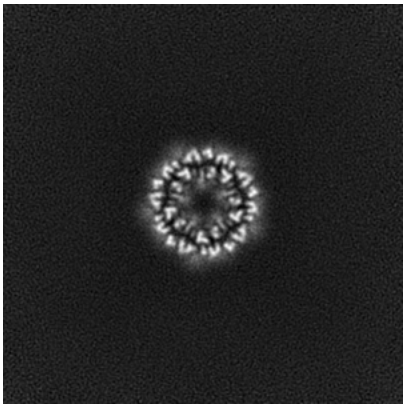
6.3.2 Raw map



X Index: 145



Y Index: 144

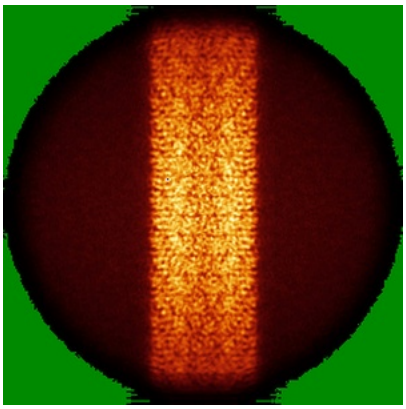


Z Index: 118

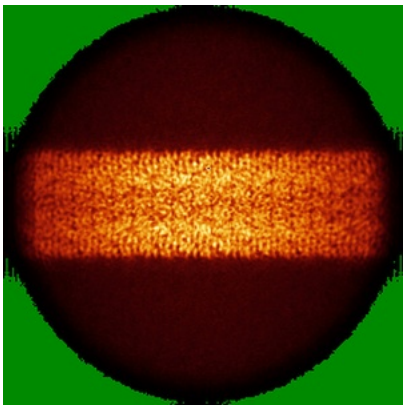
The images above show the largest variance slices of the map in three orthogonal directions.

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

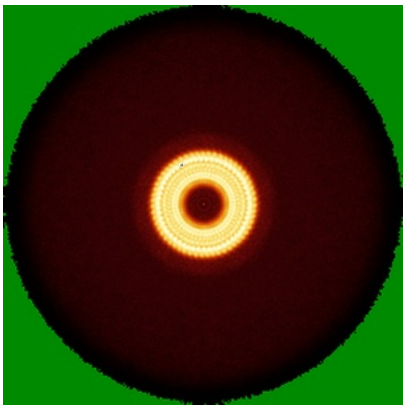
6.4.1 Primary map



X

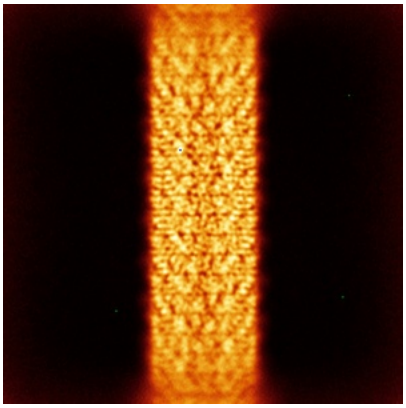


Y

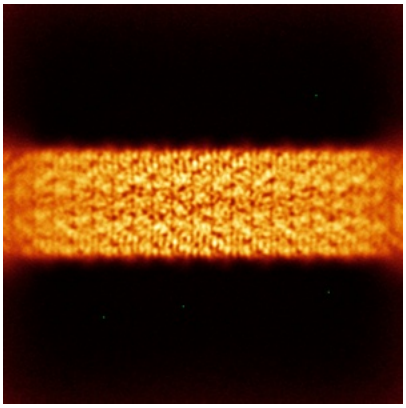


Z

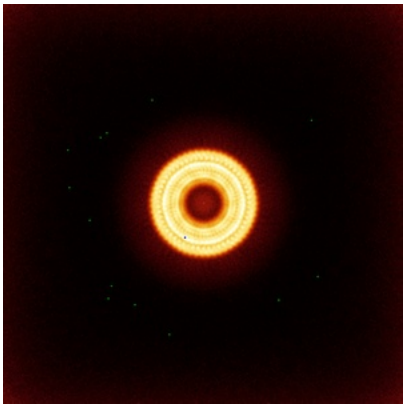
6.4.2 Raw map



X



Y

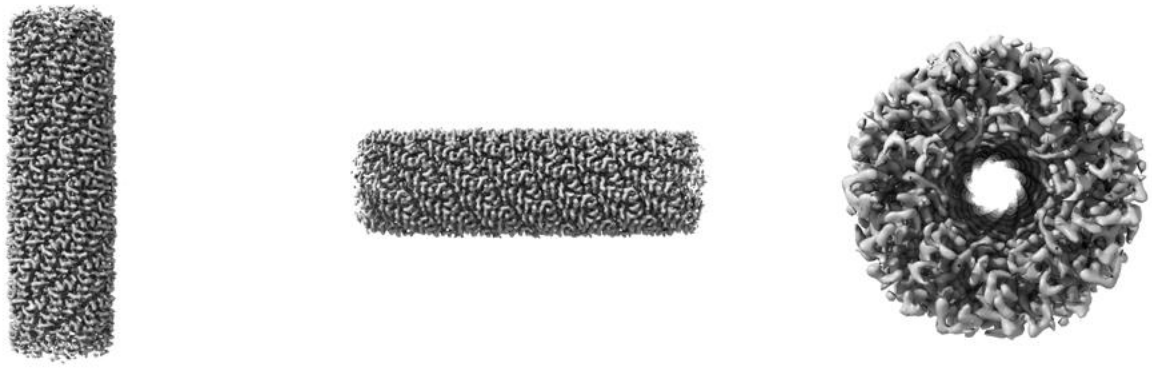


Z

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

6.5 Orthogonal surface views (i)

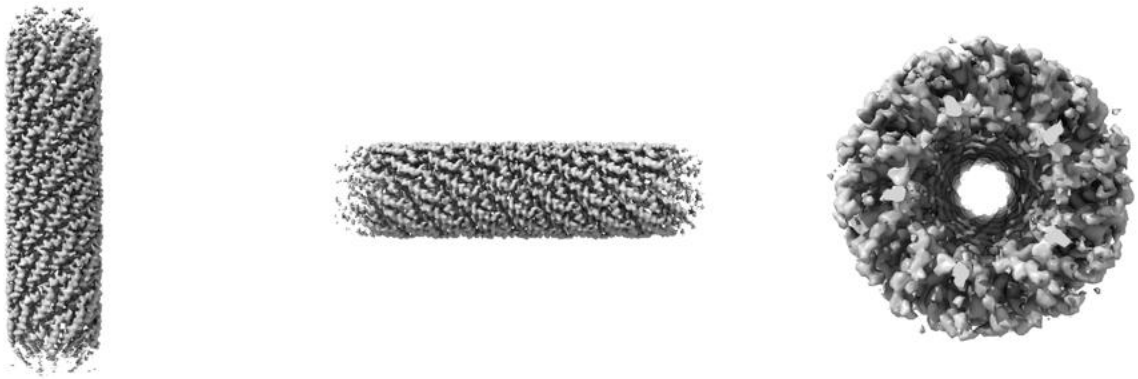
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.593. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

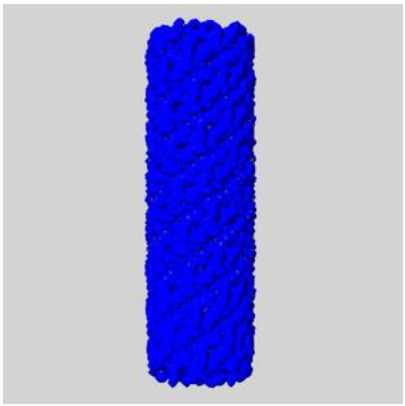
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

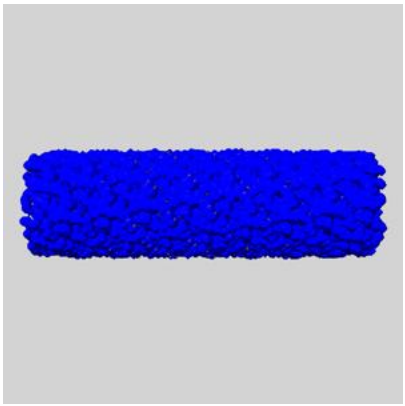
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

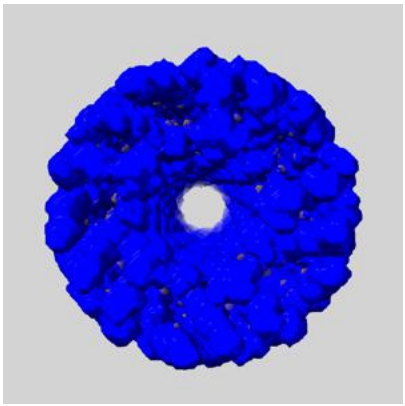
6.6.1 emd_26999_msk_1.map (i)



X



Y

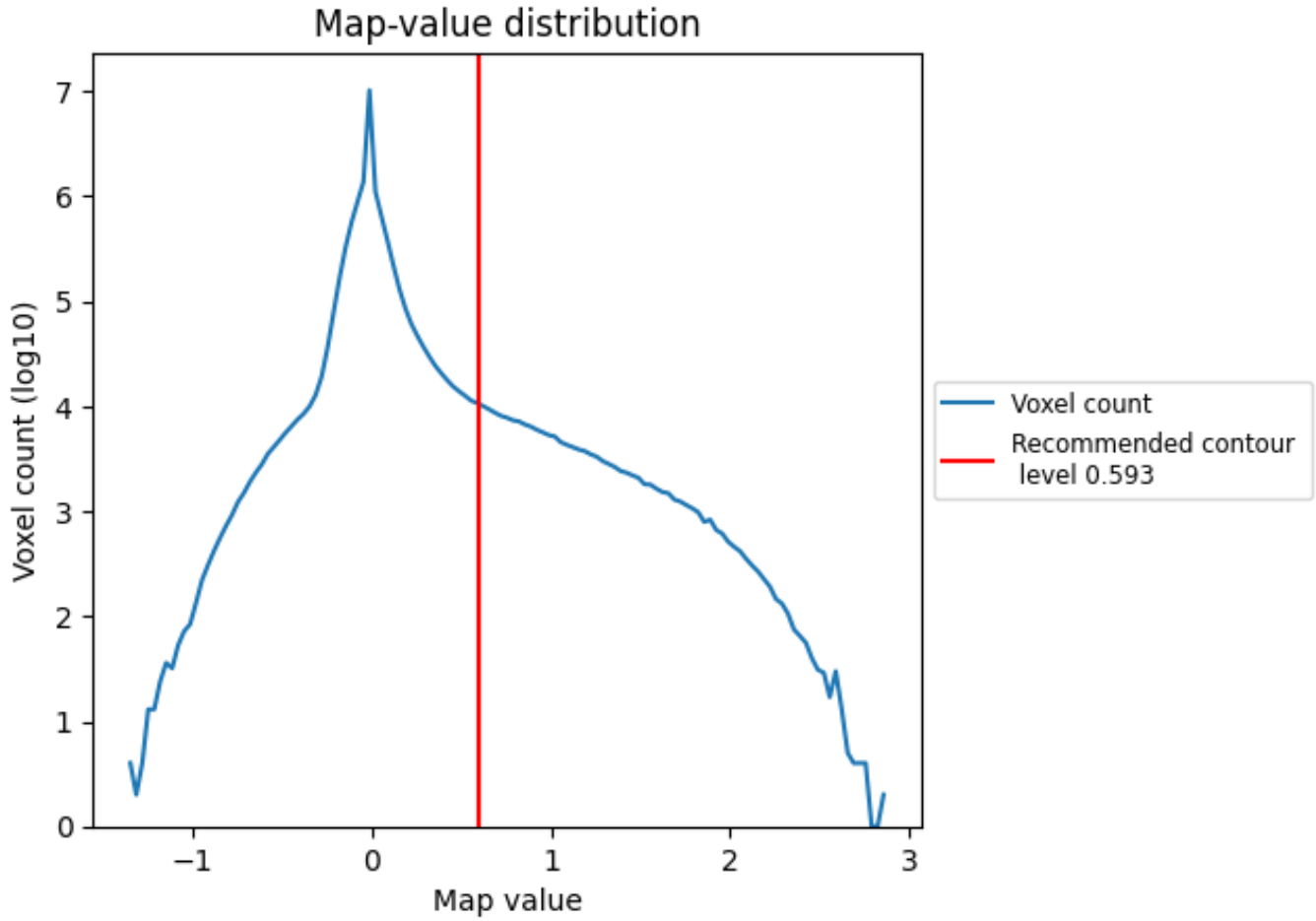


Z

7 Map analysis

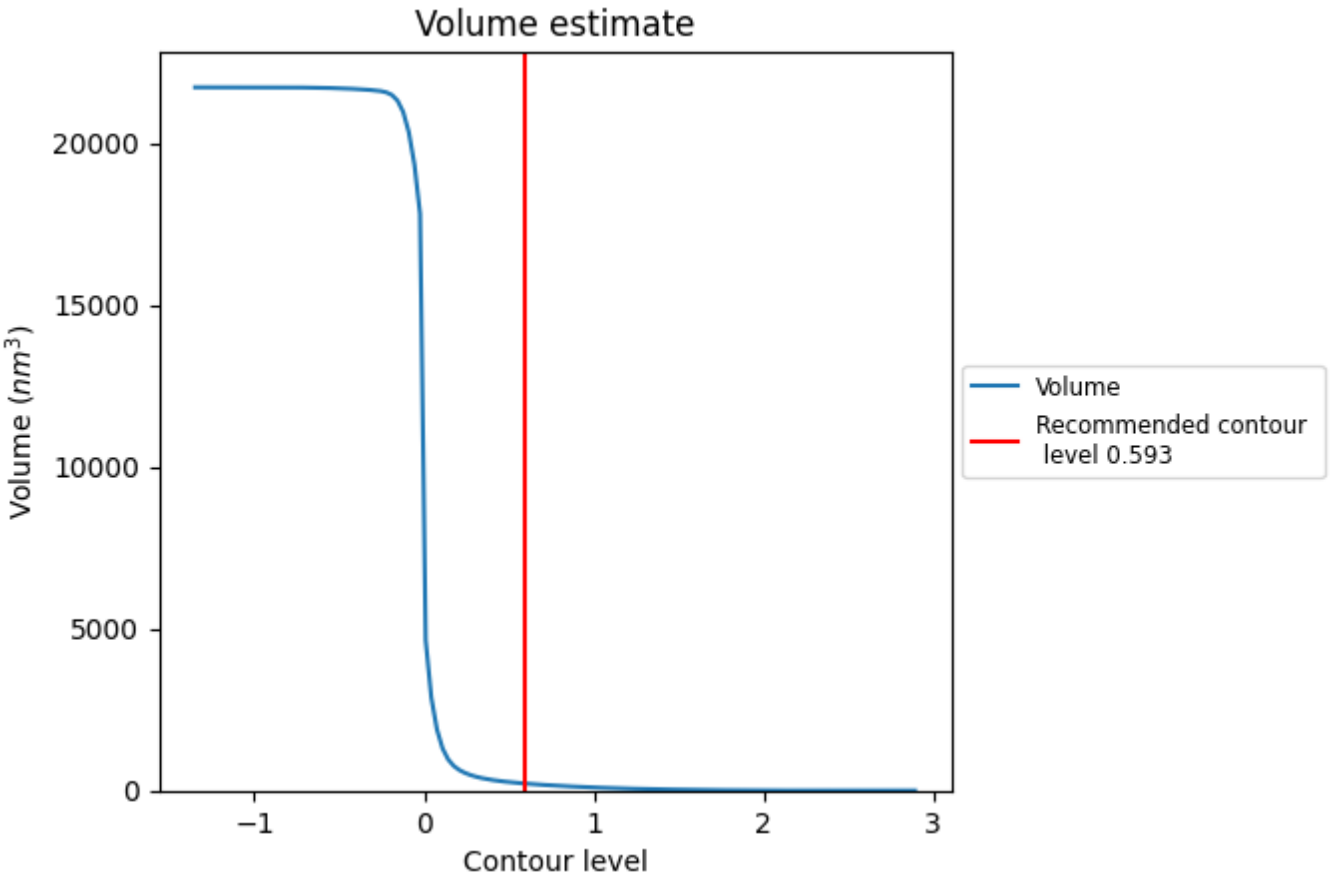
This section contains the results of statistical analysis of the map.

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.

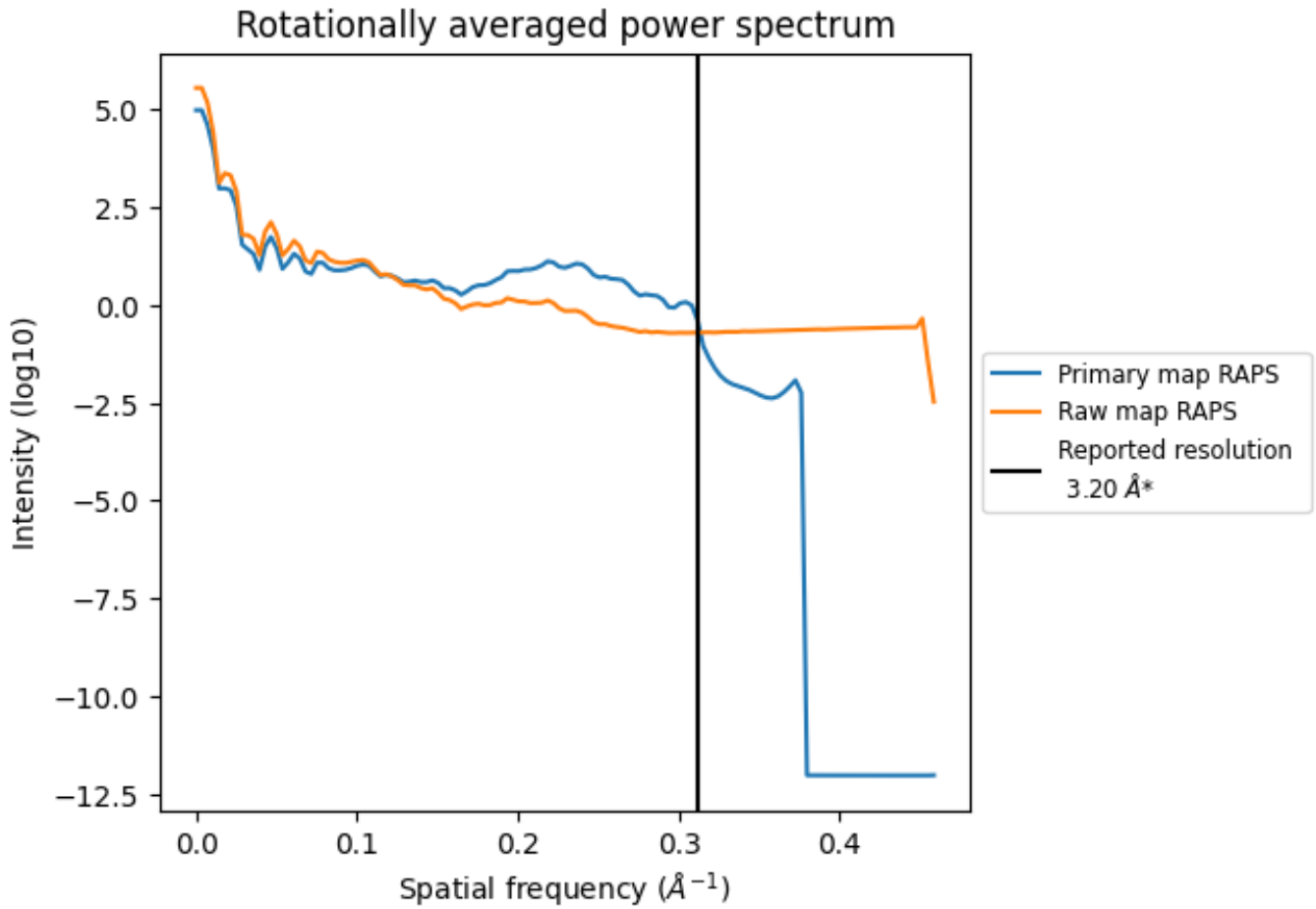
7.2 Volume estimate



The volume at the recommended contour level is 217 nm^3; this corresponds to an approximate mass of 196 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)

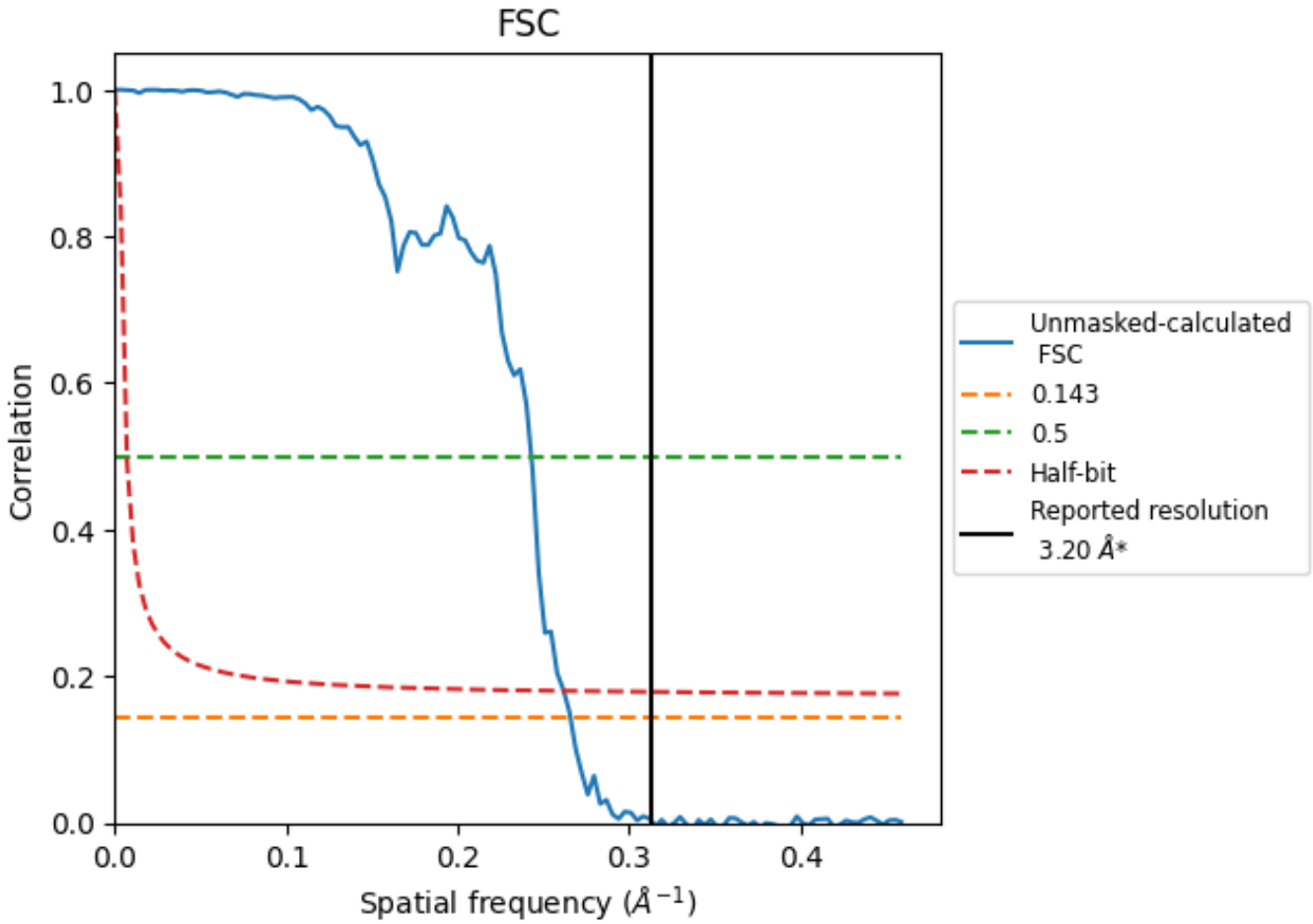


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

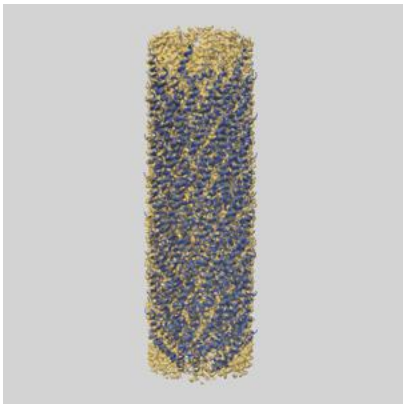
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.76	4.12	3.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.76 differs from the reported value 3.2 by more than 10 %

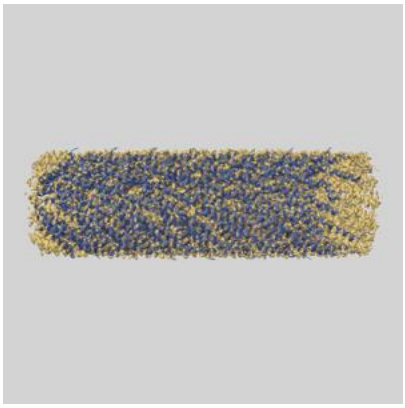
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26999 and PDB model 8CUE. Per-residue inclusion information can be found in section 3 on page 14.

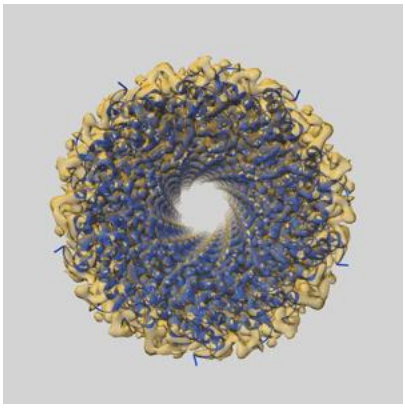
9.1 Map-model overlay



X



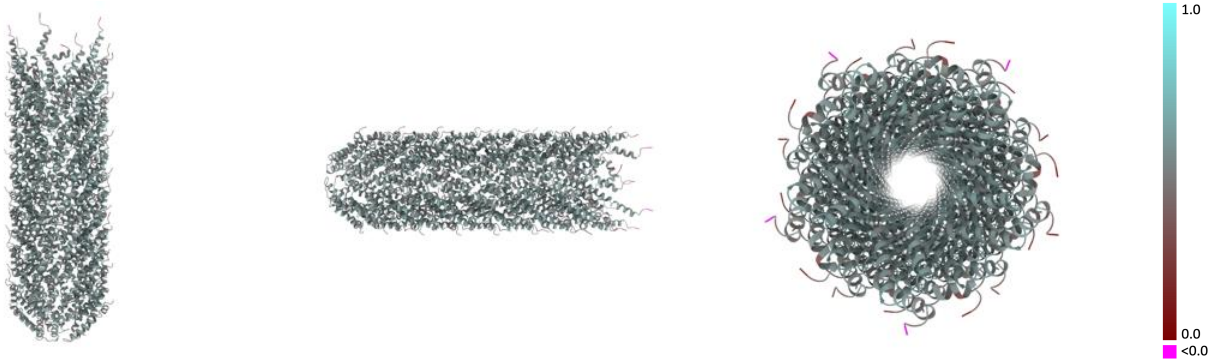
Y



Z

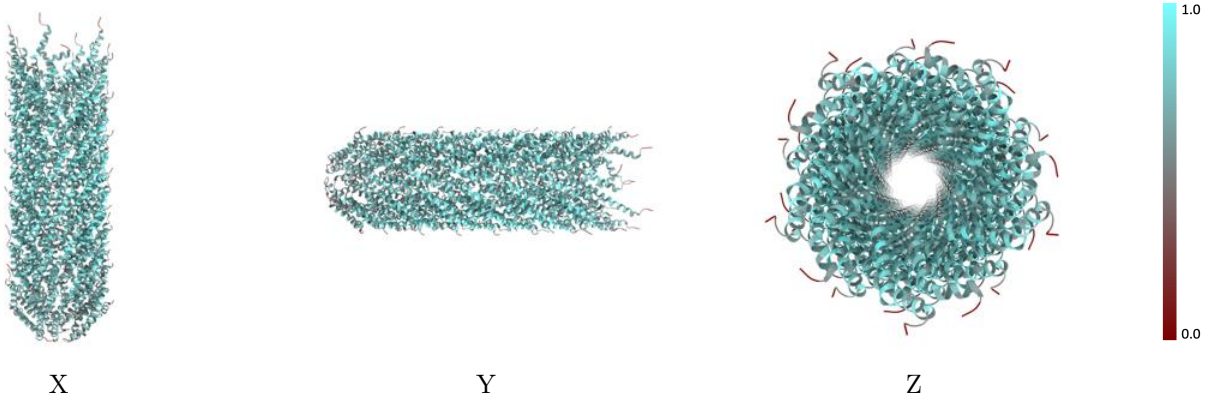
The images above show the 3D surface view of the map at the recommended contour level 0.593 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



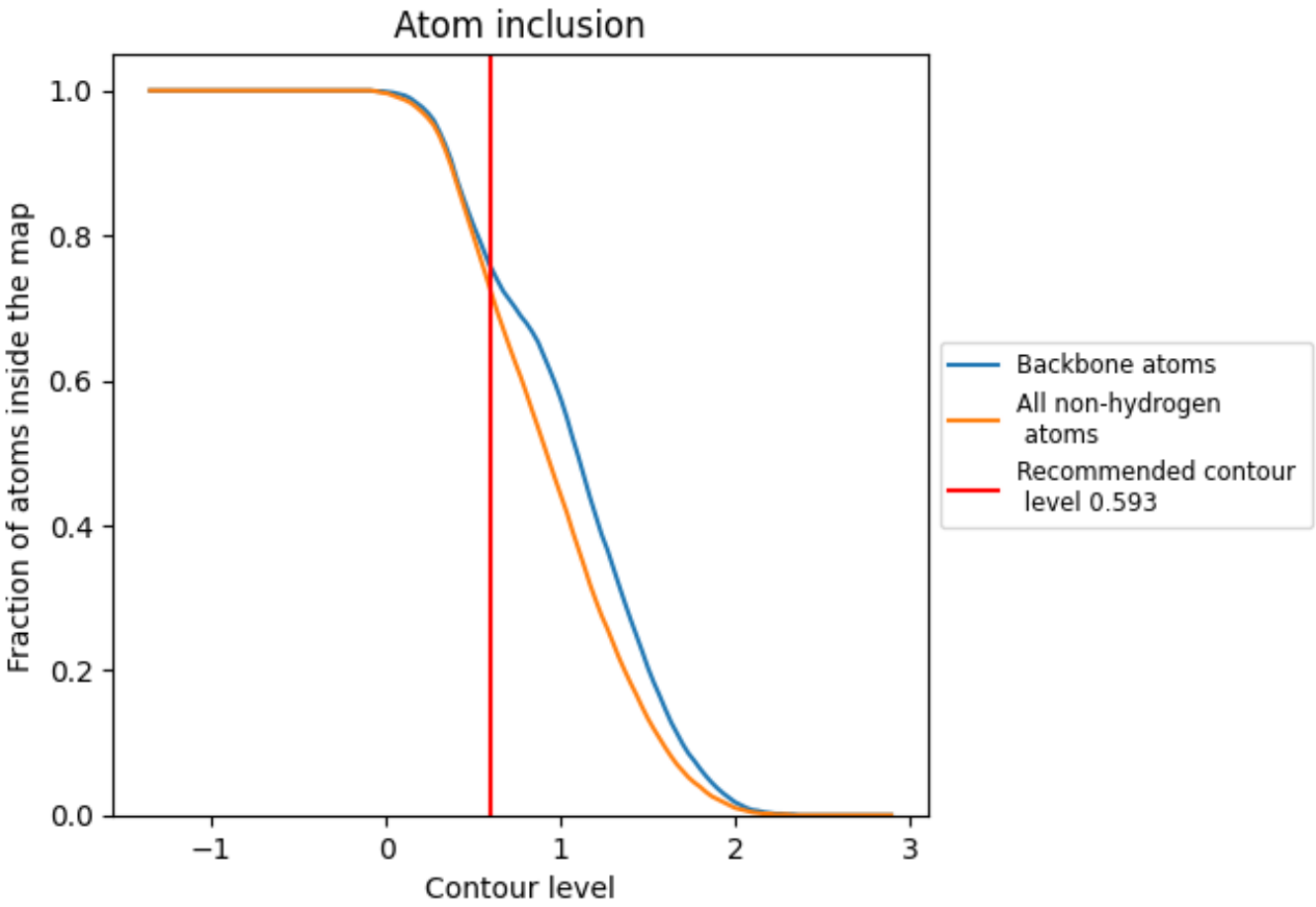
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.593).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.593) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7280	0.5290
1A	0.5520	0.5040
1B	0.6220	0.5210
1C	0.6990	0.5280
1D	0.7280	0.5310
1E	0.7660	0.5380
1F	0.7840	0.5330
1G	0.7810	0.5380
1H	0.7880	0.5410
1I	0.7840	0.5380
1J	0.7790	0.5380
1K	0.7730	0.5390
1L	0.7450	0.5320
1M	0.7160	0.5220
1N	0.6750	0.5120
2A	0.5590	0.5060
2B	0.6240	0.5250
2C	0.6980	0.5240
2D	0.7240	0.5340
2E	0.7660	0.5370
2F	0.7730	0.5340
2G	0.7790	0.5340
2H	0.7900	0.5400
2I	0.7860	0.5390
2J	0.7770	0.5360
2K	0.7730	0.5360
2L	0.7410	0.5330
2M	0.7130	0.5240
2N	0.6670	0.5140
3A	0.5350	0.5040
3B	0.6290	0.5240
3C	0.7050	0.5260
3D	0.7350	0.5370
3E	0.7690	0.5370
3F	0.7790	0.5350

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Chain	Atom inclusion	Q-score
3G	0.7840	0.5350
3H	0.7880	0.5400
3I	0.7830	0.5380
3J	0.7750	0.5350
3K	0.7750	0.5370
3L	0.7520	0.5340
3M	0.7160	0.5230
3N	0.6690	0.5130
4A	0.5480	0.5060
4B	0.6310	0.5250
4C	0.6940	0.5250
4D	0.7350	0.5340
4E	0.7660	0.5330
4F	0.7750	0.5330
4G	0.7790	0.5320
4H	0.7900	0.5360
4I	0.7810	0.5350
4J	0.7830	0.5360
4K	0.7750	0.5390
4L	0.7470	0.5340
4M	0.7180	0.5250
4N	0.6690	0.5090
5A	0.5590	0.5040
5B	0.6290	0.5230
5C	0.6940	0.5210
5D	0.7280	0.5330
5E	0.7600	0.5370
5F	0.7810	0.5310
5G	0.7860	0.5340
5H	0.7940	0.5380
5I	0.7840	0.5390
5J	0.7830	0.5380
5K	0.7620	0.5360
5L	0.7490	0.5320
5M	0.7090	0.5240
5N	0.6710	0.5110