Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 01:03 PM UTC

PDB ID	:	6X80 / pdb_00006x80
EMDB ID	:	EMD-22088
Title	:	Structure of the Campylobacter jejuni G508A Flagellar Filament
Authors	:	Kreutzberger, M.A.B.; Wang, F.; Egelman, E.H.
Deposited on	:	2020-06-01
Resolution	:	3.50 Å(reported)

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

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

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

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

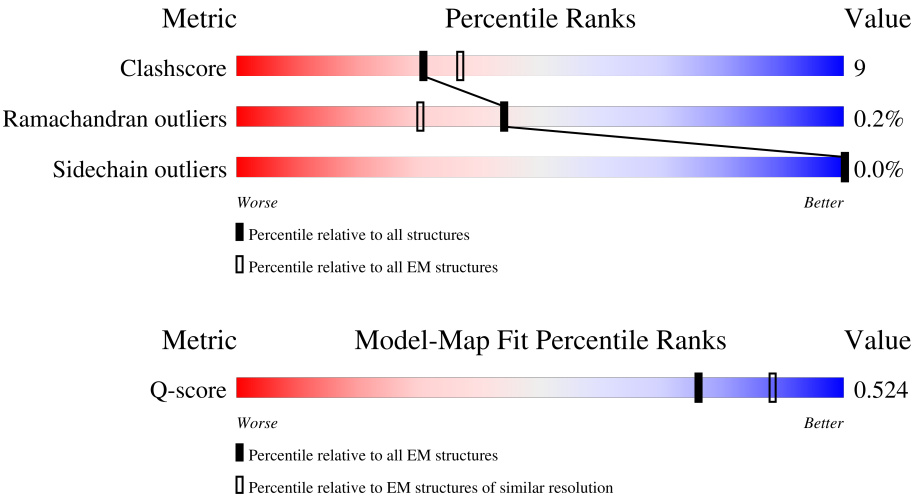
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	576	80% 20%
1	B	576	83% 16%
1	C	576	84% 15%
1	D	576	78% 22%

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Mol	Chain	Length	Quality of chain
1	E	576	81% 18%
1	F	576	82% 18%
1	G	576	83% 16%
1	H	576	79% 20%
1	I	576	82% 17%
1	J	576	83% 16%
1	K	576	81% 19%
1	L	576	84% 15%
1	M	576	83% 16%
1	N	576	82% 17%
1	O	576	83% 16%
1	P	576	81% 18%
1	Q	576	83% 17%
1	R	576	81% 19%
1	S	576	82% 18%
1	T	576	84% 16%
1	U	576	80% 19%
1	V	576	84% 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 97482 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 Flagellin A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	574	Total 4159	C 2533	N 731	O 883	S 12	0	0
1	B	574	Total 4159	C 2533	N 731	O 883	S 12	0	0
1	C	574	Total 4159	C 2533	N 731	O 883	S 12	0	0
1	D	574	Total 4159	C 2533	N 731	O 883	S 12	0	0
1	E	574	Total 4159	C 2533	N 731	O 883	S 12	0	0
1	F	574	Total 4159	C 2533	N 731	O 883	S 12	0	0
1	G	574	Total 4159	C 2533	N 731	O 883	S 12	0	0
1	H	574	Total 4159	C 2533	N 731	O 883	S 12	0	0
1	I	574	Total 4159	C 2533	N 731	O 883	S 12	0	0
1	J	574	Total 4159	C 2533	N 731	O 883	S 12	0	0
1	K	574	Total 4159	C 2533	N 731	O 883	S 12	0	0
1	L	574	Total 4159	C 2533	N 731	O 883	S 12	0	0
1	M	574	Total 4159	C 2533	N 731	O 883	S 12	0	0
1	N	574	Total 4159	C 2533	N 731	O 883	S 12	0	0
1	O	574	Total 4159	C 2533	N 731	O 883	S 12	0	0
1	P	574	Total 4159	C 2533	N 731	O 883	S 12	0	0
1	Q	574	Total 4159	C 2533	N 731	O 883	S 12	0	0

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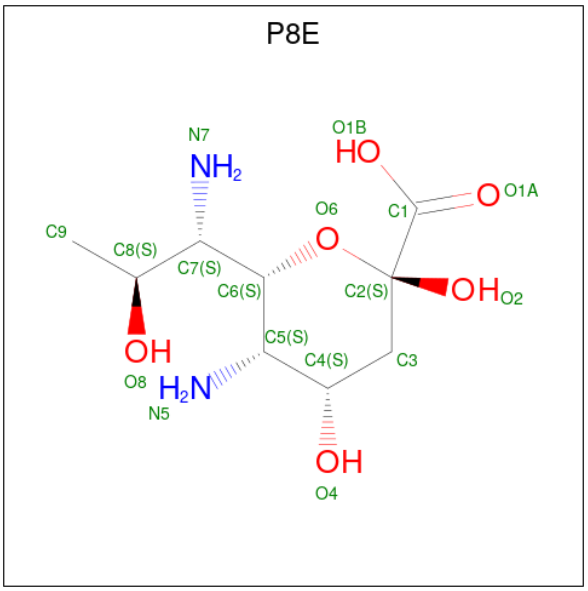
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	574	Total	C	N	O	S	0	0
			4159	2533	731	883	12		
1	S	574	Total	C	N	O	S	0	0
			4159	2533	731	883	12		
1	T	574	Total	C	N	O	S	0	0
			4159	2533	731	883	12		
1	U	574	Total	C	N	O	S	0	0
			4159	2533	731	883	12		
1	V	574	Total	C	N	O	S	0	0
			4159	2533	731	883	12		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	ALA	GLY	engineered mutation	UNP P22251
B	508	ALA	GLY	engineered mutation	UNP P22251
C	508	ALA	GLY	engineered mutation	UNP P22251
D	508	ALA	GLY	engineered mutation	UNP P22251
E	508	ALA	GLY	engineered mutation	UNP P22251
F	508	ALA	GLY	engineered mutation	UNP P22251
G	508	ALA	GLY	engineered mutation	UNP P22251
H	508	ALA	GLY	engineered mutation	UNP P22251
I	508	ALA	GLY	engineered mutation	UNP P22251
J	508	ALA	GLY	engineered mutation	UNP P22251
K	508	ALA	GLY	engineered mutation	UNP P22251
L	508	ALA	GLY	engineered mutation	UNP P22251
M	508	ALA	GLY	engineered mutation	UNP P22251
N	508	ALA	GLY	engineered mutation	UNP P22251
O	508	ALA	GLY	engineered mutation	UNP P22251
P	508	ALA	GLY	engineered mutation	UNP P22251
Q	508	ALA	GLY	engineered mutation	UNP P22251
R	508	ALA	GLY	engineered mutation	UNP P22251
S	508	ALA	GLY	engineered mutation	UNP P22251
T	508	ALA	GLY	engineered mutation	UNP P22251
U	508	ALA	GLY	engineered mutation	UNP P22251
V	508	ALA	GLY	engineered mutation	UNP P22251

- Molecule 2 is 5,7-diamino-3,5,7,9-tetradeoxy-L-glycero-alpha-L-manno-non-2-ulopyranosonic acid (CCD ID: P8E) (formula: $C_9H_{18}N_2O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			16	9	2	5	
2	A	1	Total	C	N	O	0
			16	9	2	5	
2	A	1	Total	C	N	O	0
			16	9	2	5	
2	A	1	Total	C	N	O	0
			16	9	2	5	
2	A	1	Total	C	N	O	0
			16	9	2	5	
2	A	1	Total	C	N	O	0
			16	9	2	5	
2	A	1	Total	C	N	O	0
			16	9	2	5	
2	A	1	Total	C	N	O	0
			16	9	2	5	
2	A	1	Total	C	N	O	0
			16	9	2	5	
2	A	1	Total	C	N	O	0
			16	9	2	5	
2	A	1	Total	C	N	O	0
			16	9	2	5	
2	A	1	Total	C	N	O	0
			16	9	2	5	
2	A	1	Total	C	N	O	0
			16	9	2	5	
2	A	1	Total	C	N	O	0
			16	9	2	5	
2	A	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			16	9	2	5	
2	A	1	Total	C	N	O	0
			16	9	2	5	
2	A	1	Total	C	N	O	0
			16	9	2	5	
2	B	1	Total	C	N	O	0
			16	9	2	5	
2	B	1	Total	C	N	O	0
			16	9	2	5	
2	B	1	Total	C	N	O	0
			16	9	2	5	
2	B	1	Total	C	N	O	0
			16	9	2	5	
2	B	1	Total	C	N	O	0
			16	9	2	5	
2	B	1	Total	C	N	O	0
			16	9	2	5	
2	B	1	Total	C	N	O	0
			16	9	2	5	
2	B	1	Total	C	N	O	0
			16	9	2	5	
2	B	1	Total	C	N	O	0
			16	9	2	5	
2	B	1	Total	C	N	O	0
			16	9	2	5	
2	B	1	Total	C	N	O	0
			16	9	2	5	
2	B	1	Total	C	N	O	0
			16	9	2	5	
2	B	1	Total	C	N	O	0
			16	9	2	5	
2	B	1	Total	C	N	O	0
			16	9	2	5	
2	B	1	Total	C	N	O	0
			16	9	2	5	
2	B	1	Total	C	N	O	0
			16	9	2	5	
2	B	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	C	1	Total	C	N	O	0
			16	9	2	5	
2	D	1	Total	C	N	O	0
			16	9	2	5	
2	D	1	Total	C	N	O	0
			16	9	2	5	
2	D	1	Total	C	N	O	0
			16	9	2	5	
2	D	1	Total	C	N	O	0
			16	9	2	5	
2	D	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
2	D	1	Total	C	N	O	0
			16	9	2	5	
2	D	1	Total	C	N	O	0
			16	9	2	5	
2	D	1	Total	C	N	O	0
			16	9	2	5	
2	D	1	Total	C	N	O	0
			16	9	2	5	
2	D	1	Total	C	N	O	0
			16	9	2	5	
2	D	1	Total	C	N	O	0
			16	9	2	5	
2	D	1	Total	C	N	O	0
			16	9	2	5	
2	D	1	Total	C	N	O	0
			16	9	2	5	
2	D	1	Total	C	N	O	0
			16	9	2	5	
2	D	1	Total	C	N	O	0
			16	9	2	5	
2	D	1	Total	C	N	O	0
			16	9	2	5	
2	D	1	Total	C	N	O	0
			16	9	2	5	
2	D	1	Total	C	N	O	0
			16	9	2	5	
2	E	1	Total	C	N	O	0
			16	9	2	5	
2	E	1	Total	C	N	O	0
			16	9	2	5	
2	E	1	Total	C	N	O	0
			16	9	2	5	
2	E	1	Total	C	N	O	0
			16	9	2	5	
2	E	1	Total	C	N	O	0
			16	9	2	5	
2	E	1	Total	C	N	O	0
			16	9	2	5	
2	E	1	Total	C	N	O	0
			16	9	2	5	
2	E	1	Total	C	N	O	0
			16	9	2	5	
2	E	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
2	E	1	Total	C	N	O	0
			16	9	2	5	
2	E	1	Total	C	N	O	0
			16	9	2	5	
2	E	1	Total	C	N	O	0
			16	9	2	5	
2	E	1	Total	C	N	O	0
			16	9	2	5	
2	E	1	Total	C	N	O	0
			16	9	2	5	
2	E	1	Total	C	N	O	0
			16	9	2	5	
2	E	1	Total	C	N	O	0
			16	9	2	5	
2	E	1	Total	C	N	O	0
			16	9	2	5	
2	F	1	Total	C	N	O	0
			16	9	2	5	
2	F	1	Total	C	N	O	0
			16	9	2	5	
2	F	1	Total	C	N	O	0
			16	9	2	5	
2	F	1	Total	C	N	O	0
			16	9	2	5	
2	F	1	Total	C	N	O	0
			16	9	2	5	
2	F	1	Total	C	N	O	0
			16	9	2	5	
2	F	1	Total	C	N	O	0
			16	9	2	5	
2	F	1	Total	C	N	O	0
			16	9	2	5	
2	F	1	Total	C	N	O	0
			16	9	2	5	
2	F	1	Total	C	N	O	0
			16	9	2	5	
2	F	1	Total	C	N	O	0
			16	9	2	5	
2	F	1	Total	C	N	O	0
			16	9	2	5	
2	F	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
2	F	1	Total	C	N	O	0
			16	9	2	5	
2	F	1	Total	C	N	O	0
			16	9	2	5	
2	F	1	Total	C	N	O	0
			16	9	2	5	
2	F	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	
2	G	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	H	1	Total	C	N	O	0
			16	9	2	5	
2	I	1	Total	C	N	O	0
			16	9	2	5	
2	I	1	Total	C	N	O	0
			16	9	2	5	
2	I	1	Total	C	N	O	0
			16	9	2	5	
2	I	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
2	I	1	Total	C	N	O	0
			16	9	2	5	
2	I	1	Total	C	N	O	0
			16	9	2	5	
2	I	1	Total	C	N	O	0
			16	9	2	5	
2	I	1	Total	C	N	O	0
			16	9	2	5	
2	I	1	Total	C	N	O	0
			16	9	2	5	
2	I	1	Total	C	N	O	0
			16	9	2	5	
2	I	1	Total	C	N	O	0
			16	9	2	5	
2	I	1	Total	C	N	O	0
			16	9	2	5	
2	I	1	Total	C	N	O	0
			16	9	2	5	
2	I	1	Total	C	N	O	0
			16	9	2	5	
2	I	1	Total	C	N	O	0
			16	9	2	5	
2	I	1	Total	C	N	O	0
			16	9	2	5	
2	I	1	Total	C	N	O	0
			16	9	2	5	
2	I	1	Total	C	N	O	0
			16	9	2	5	
2	J	1	Total	C	N	O	0
			16	9	2	5	
2	J	1	Total	C	N	O	0
			16	9	2	5	
2	J	1	Total	C	N	O	0
			16	9	2	5	
2	J	1	Total	C	N	O	0
			16	9	2	5	
2	J	1	Total	C	N	O	0
			16	9	2	5	
2	J	1	Total	C	N	O	0
			16	9	2	5	
2	J	1	Total	C	N	O	0
			16	9	2	5	
2	J	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
2	J	1	Total	C	N	O	0
			16	9	2	5	
2	J	1	Total	C	N	O	0
			16	9	2	5	
2	J	1	Total	C	N	O	0
			16	9	2	5	
2	J	1	Total	C	N	O	0
			16	9	2	5	
2	J	1	Total	C	N	O	0
			16	9	2	5	
2	J	1	Total	C	N	O	0
			16	9	2	5	
2	J	1	Total	C	N	O	0
			16	9	2	5	
2	J	1	Total	C	N	O	0
			16	9	2	5	
2	J	1	Total	C	N	O	0
			16	9	2	5	
2	K	1	Total	C	N	O	0
			16	9	2	5	
2	K	1	Total	C	N	O	0
			16	9	2	5	
2	K	1	Total	C	N	O	0
			16	9	2	5	
2	K	1	Total	C	N	O	0
			16	9	2	5	
2	K	1	Total	C	N	O	0
			16	9	2	5	
2	K	1	Total	C	N	O	0
			16	9	2	5	
2	K	1	Total	C	N	O	0
			16	9	2	5	
2	K	1	Total	C	N	O	0
			16	9	2	5	
2	K	1	Total	C	N	O	0
			16	9	2	5	
2	K	1	Total	C	N	O	0
			16	9	2	5	
2	K	1	Total	C	N	O	0
			16	9	2	5	
2	K	1	Total	C	N	O	0
			16	9	2	5	
2	K	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
2	K	1	Total	C	N	O	0
			16	9	2	5	
2	K	1	Total	C	N	O	0
			16	9	2	5	
2	K	1	Total	C	N	O	0
			16	9	2	5	
2	K	1	Total	C	N	O	0
			16	9	2	5	
2	K	1	Total	C	N	O	0
			16	9	2	5	
2	L	1	Total	C	N	O	0
			16	9	2	5	
2	L	1	Total	C	N	O	0
			16	9	2	5	
2	L	1	Total	C	N	O	0
			16	9	2	5	
2	L	1	Total	C	N	O	0
			16	9	2	5	
2	L	1	Total	C	N	O	0
			16	9	2	5	
2	L	1	Total	C	N	O	0
			16	9	2	5	
2	L	1	Total	C	N	O	0
			16	9	2	5	
2	L	1	Total	C	N	O	0
			16	9	2	5	
2	L	1	Total	C	N	O	0
			16	9	2	5	
2	L	1	Total	C	N	O	0
			16	9	2	5	
2	L	1	Total	C	N	O	0
			16	9	2	5	
2	L	1	Total	C	N	O	0
			16	9	2	5	
2	L	1	Total	C	N	O	0
			16	9	2	5	
2	L	1	Total	C	N	O	0
			16	9	2	5	
2	L	1	Total	C	N	O	0
			16	9	2	5	
2	L	1	Total	C	N	O	0
			16	9	2	5	
2	L	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
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2	M	1	Total	C	N	O	0
			16	9	2	5	
2	M	1	Total	C	N	O	0
			16	9	2	5	
2	M	1	Total	C	N	O	0
			16	9	2	5	
2	M	1	Total	C	N	O	0
			16	9	2	5	
2	M	1	Total	C	N	O	0
			16	9	2	5	
2	M	1	Total	C	N	O	0
			16	9	2	5	
2	M	1	Total	C	N	O	0
			16	9	2	5	
2	M	1	Total	C	N	O	0
			16	9	2	5	
2	M	1	Total	C	N	O	0
			16	9	2	5	
2	M	1	Total	C	N	O	0
			16	9	2	5	
2	M	1	Total	C	N	O	0
			16	9	2	5	
2	M	1	Total	C	N	O	0
			16	9	2	5	
2	M	1	Total	C	N	O	0
			16	9	2	5	
2	M	1	Total	C	N	O	0
			16	9	2	5	
2	M	1	Total	C	N	O	0
			16	9	2	5	
2	M	1	Total	C	N	O	0
			16	9	2	5	
2	M	1	Total	C	N	O	0
			16	9	2	5	
2	N	1	Total	C	N	O	0
			16	9	2	5	
2	N	1	Total	C	N	O	0
			16	9	2	5	
2	N	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
2	N	1	Total	C	N	O	0
			16	9	2	5	
2	N	1	Total	C	N	O	0
			16	9	2	5	
2	N	1	Total	C	N	O	0
			16	9	2	5	
2	N	1	Total	C	N	O	0
			16	9	2	5	
2	N	1	Total	C	N	O	0
			16	9	2	5	
2	N	1	Total	C	N	O	0
			16	9	2	5	
2	N	1	Total	C	N	O	0
			16	9	2	5	
2	N	1	Total	C	N	O	0
			16	9	2	5	
2	N	1	Total	C	N	O	0
			16	9	2	5	
2	N	1	Total	C	N	O	0
			16	9	2	5	
2	N	1	Total	C	N	O	0
			16	9	2	5	
2	N	1	Total	C	N	O	0
			16	9	2	5	
2	N	1	Total	C	N	O	0
			16	9	2	5	
2	N	1	Total	C	N	O	0
			16	9	2	5	
2	N	1	Total	C	N	O	0
			16	9	2	5	
2	O	1	Total	C	N	O	0
			16	9	2	5	
2	O	1	Total	C	N	O	0
			16	9	2	5	
2	O	1	Total	C	N	O	0
			16	9	2	5	
2	O	1	Total	C	N	O	0
			16	9	2	5	
2	O	1	Total	C	N	O	0
			16	9	2	5	
2	O	1	Total	C	N	O	0
			16	9	2	5	
2	O	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
2	O	1	Total	C	N	O	0
			16	9	2	5	
2	O	1	Total	C	N	O	0
			16	9	2	5	
2	O	1	Total	C	N	O	0
			16	9	2	5	
2	O	1	Total	C	N	O	0
			16	9	2	5	
2	O	1	Total	C	N	O	0
			16	9	2	5	
2	O	1	Total	C	N	O	0
			16	9	2	5	
2	O	1	Total	C	N	O	0
			16	9	2	5	
2	O	1	Total	C	N	O	0
			16	9	2	5	
2	O	1	Total	C	N	O	0
			16	9	2	5	
2	O	1	Total	C	N	O	0
			16	9	2	5	
2	P	1	Total	C	N	O	0
			16	9	2	5	
2	P	1	Total	C	N	O	0
			16	9	2	5	
2	P	1	Total	C	N	O	0
			16	9	2	5	
2	P	1	Total	C	N	O	0
			16	9	2	5	
2	P	1	Total	C	N	O	0
			16	9	2	5	
2	P	1	Total	C	N	O	0
			16	9	2	5	
2	P	1	Total	C	N	O	0
			16	9	2	5	
2	P	1	Total	C	N	O	0
			16	9	2	5	
2	P	1	Total	C	N	O	0
			16	9	2	5	
2	P	1	Total	C	N	O	0
			16	9	2	5	
2	P	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
2	P	1	Total	C	N	O	0
			16	9	2	5	
2	P	1	Total	C	N	O	0
			16	9	2	5	
2	P	1	Total	C	N	O	0
			16	9	2	5	
2	P	1	Total	C	N	O	0
			16	9	2	5	
2	P	1	Total	C	N	O	0
			16	9	2	5	
2	P	1	Total	C	N	O	0
			16	9	2	5	
2	Q	1	Total	C	N	O	0
			16	9	2	5	
2	Q	1	Total	C	N	O	0
			16	9	2	5	
2	Q	1	Total	C	N	O	0
			16	9	2	5	
2	Q	1	Total	C	N	O	0
			16	9	2	5	
2	Q	1	Total	C	N	O	0
			16	9	2	5	
2	Q	1	Total	C	N	O	0
			16	9	2	5	
2	Q	1	Total	C	N	O	0
			16	9	2	5	
2	Q	1	Total	C	N	O	0
			16	9	2	5	
2	Q	1	Total	C	N	O	0
			16	9	2	5	
2	Q	1	Total	C	N	O	0
			16	9	2	5	
2	Q	1	Total	C	N	O	0
			16	9	2	5	
2	Q	1	Total	C	N	O	0
			16	9	2	5	
2	Q	1	Total	C	N	O	0
			16	9	2	5	
2	Q	1	Total	C	N	O	0
			16	9	2	5	
2	Q	1	Total	C	N	O	0
			16	9	2	5	
2	Q	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
2	Q	1	Total	C	N	O	0
			16	9	2	5	
2	Q	1	Total	C	N	O	0
			16	9	2	5	
2	R	1	Total	C	N	O	0
			16	9	2	5	
2	R	1	Total	C	N	O	0
			16	9	2	5	
2	R	1	Total	C	N	O	0
			16	9	2	5	
2	R	1	Total	C	N	O	0
			16	9	2	5	
2	R	1	Total	C	N	O	0
			16	9	2	5	
2	R	1	Total	C	N	O	0
			16	9	2	5	
2	R	1	Total	C	N	O	0
			16	9	2	5	
2	R	1	Total	C	N	O	0
			16	9	2	5	
2	R	1	Total	C	N	O	0
			16	9	2	5	
2	R	1	Total	C	N	O	0
			16	9	2	5	
2	R	1	Total	C	N	O	0
			16	9	2	5	
2	R	1	Total	C	N	O	0
			16	9	2	5	
2	R	1	Total	C	N	O	0
			16	9	2	5	
2	R	1	Total	C	N	O	0
			16	9	2	5	
2	R	1	Total	C	N	O	0
			16	9	2	5	
2	R	1	Total	C	N	O	0
			16	9	2	5	
2	R	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	S	1	Total	C	N	O	0
			16	9	2	5	
2	T	1	Total	C	N	O	0
			16	9	2	5	
2	T	1	Total	C	N	O	0
			16	9	2	5	
2	T	1	Total	C	N	O	0
			16	9	2	5	
2	T	1	Total	C	N	O	0
			16	9	2	5	
2	T	1	Total	C	N	O	0
			16	9	2	5	
2	T	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
2	T	1	Total	C	N	O	0
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2	T	1	Total	C	N	O	0
			16	9	2	5	
2	T	1	Total	C	N	O	0
			16	9	2	5	
2	T	1	Total	C	N	O	0
			16	9	2	5	
2	T	1	Total	C	N	O	0
			16	9	2	5	
2	T	1	Total	C	N	O	0
			16	9	2	5	
2	T	1	Total	C	N	O	0
			16	9	2	5	
2	T	1	Total	C	N	O	0
			16	9	2	5	
2	T	1	Total	C	N	O	0
			16	9	2	5	
2	T	1	Total	C	N	O	0
			16	9	2	5	
2	T	1	Total	C	N	O	0
			16	9	2	5	
2	U	1	Total	C	N	O	0
			16	9	2	5	
2	U	1	Total	C	N	O	0
			16	9	2	5	
2	U	1	Total	C	N	O	0
			16	9	2	5	
2	U	1	Total	C	N	O	0
			16	9	2	5	
2	U	1	Total	C	N	O	0
			16	9	2	5	
2	U	1	Total	C	N	O	0
			16	9	2	5	
2	U	1	Total	C	N	O	0
			16	9	2	5	
2	U	1	Total	C	N	O	0
			16	9	2	5	
2	U	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
2	U	1	Total	C	N	O	0
			16	9	2	5	
2	U	1	Total	C	N	O	0
			16	9	2	5	
2	U	1	Total	C	N	O	0
			16	9	2	5	
2	U	1	Total	C	N	O	0
			16	9	2	5	
2	U	1	Total	C	N	O	0
			16	9	2	5	
2	U	1	Total	C	N	O	0
			16	9	2	5	
2	U	1	Total	C	N	O	0
			16	9	2	5	
2	V	1	Total	C	N	O	0
			16	9	2	5	
2	V	1	Total	C	N	O	0
			16	9	2	5	
2	V	1	Total	C	N	O	0
			16	9	2	5	
2	V	1	Total	C	N	O	0
			16	9	2	5	
2	V	1	Total	C	N	O	0
			16	9	2	5	
2	V	1	Total	C	N	O	0
			16	9	2	5	
2	V	1	Total	C	N	O	0
			16	9	2	5	
2	V	1	Total	C	N	O	0
			16	9	2	5	
2	V	1	Total	C	N	O	0
			16	9	2	5	
2	V	1	Total	C	N	O	0
			16	9	2	5	
2	V	1	Total	C	N	O	0
			16	9	2	5	
2	V	1	Total	C	N	O	0
			16	9	2	5	
2	V	1	Total	C	N	O	0
			16	9	2	5	
2	V	1	Total	C	N	O	0
			16	9	2	5	

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Mol	Chain	Residues	Atoms				AltConf
2	V	1	Total	C	N	O	0
			16	9	2	5	
2	V	1	Total	C	N	O	0
			16	9	2	5	
2	V	1	Total	C	N	O	0
			16	9	2	5	

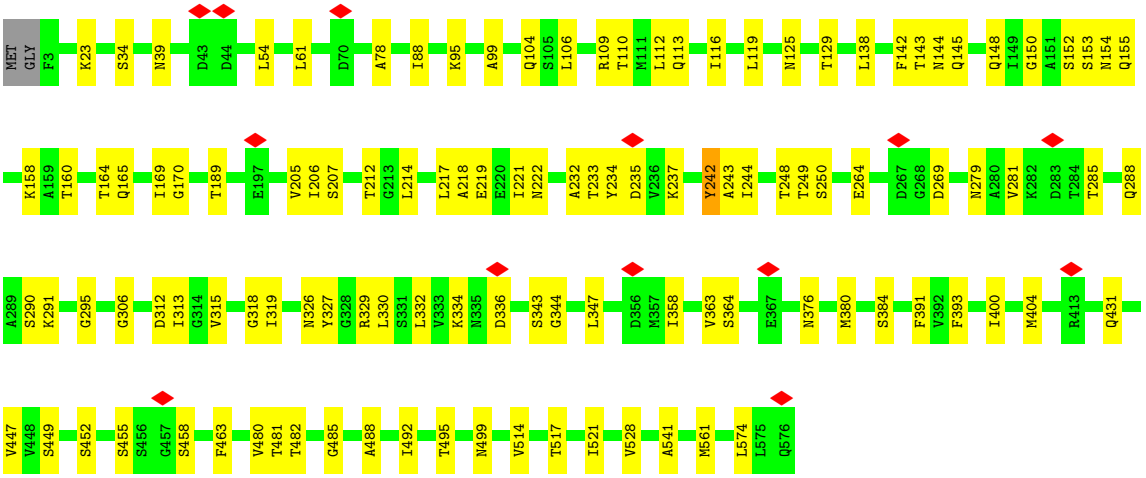
3 Residue-property plots (i)

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: Flagellin A

Chain A:

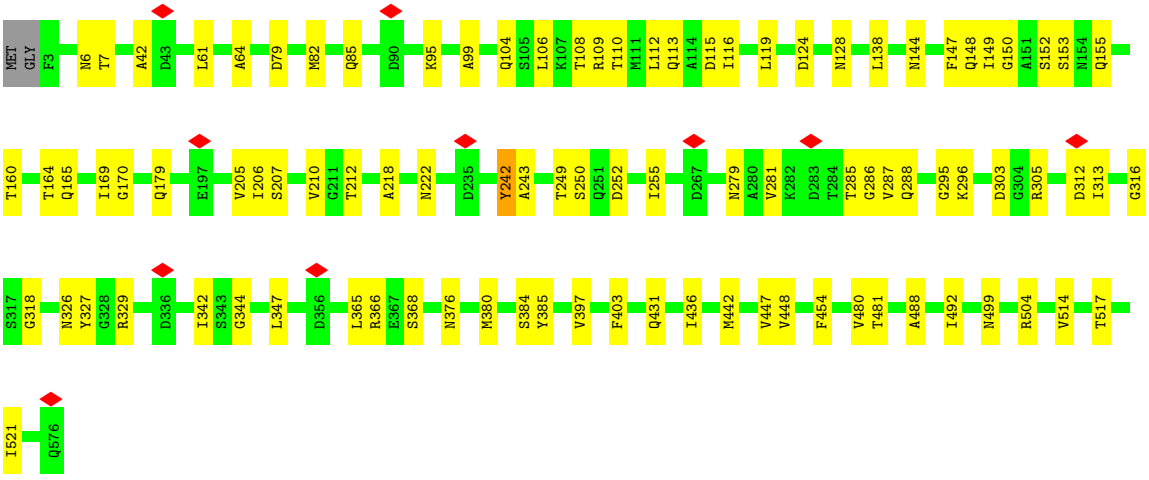




• Molecule 1: Flagellin A

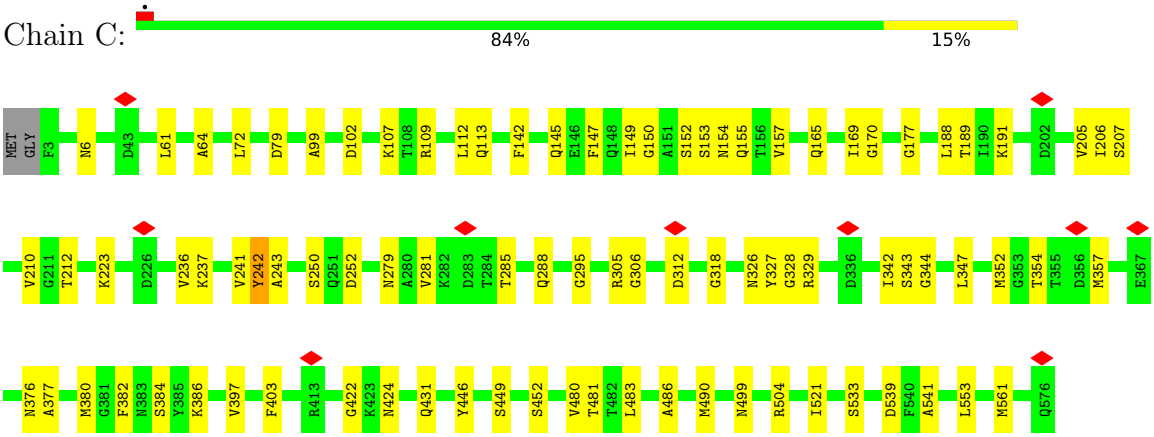
Chain B:





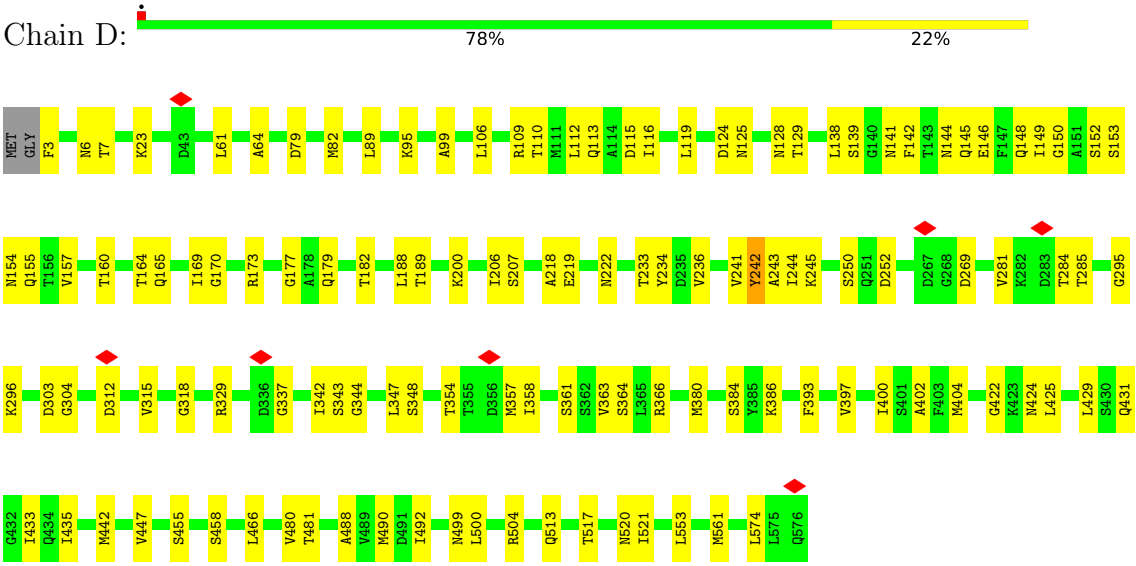
• Molecule 1: Flagellin A

Chain C:



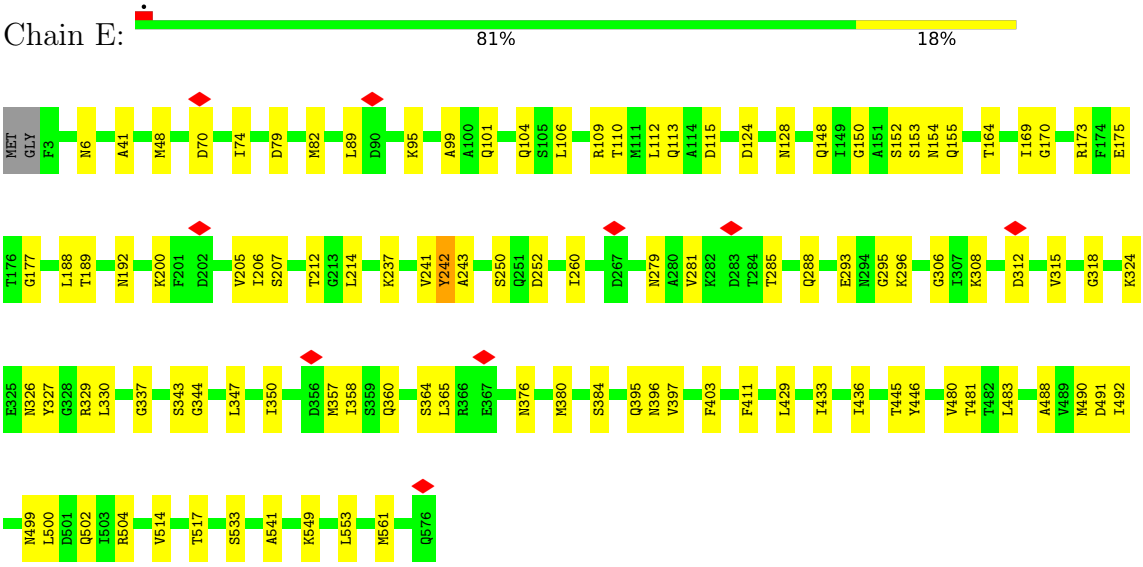
• Molecule 1: Flagellin A

Chain D:



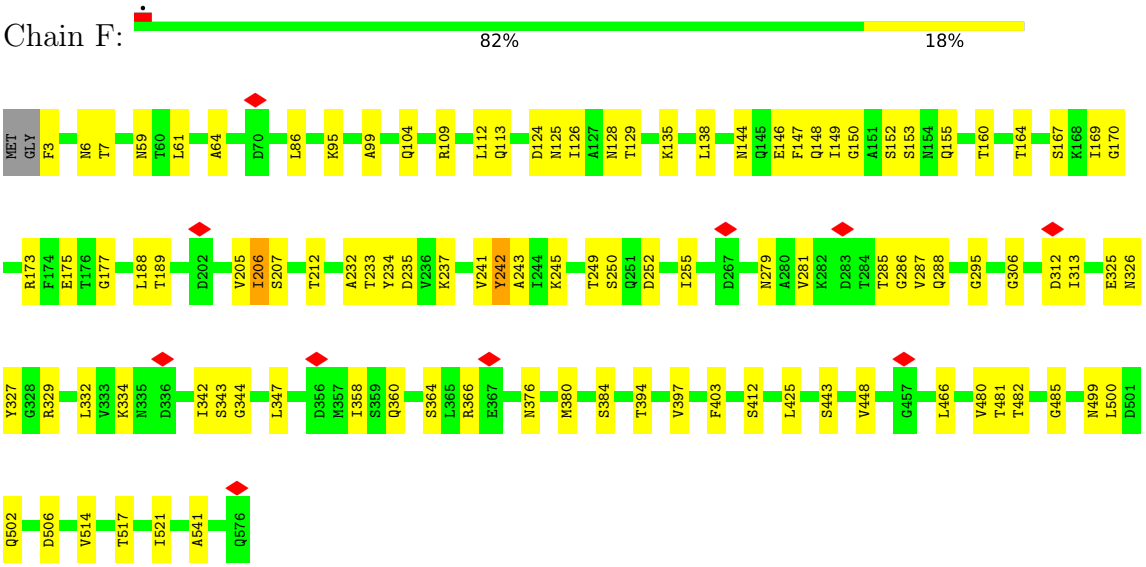
• Molecule 1: Flagellin A

Chain E:



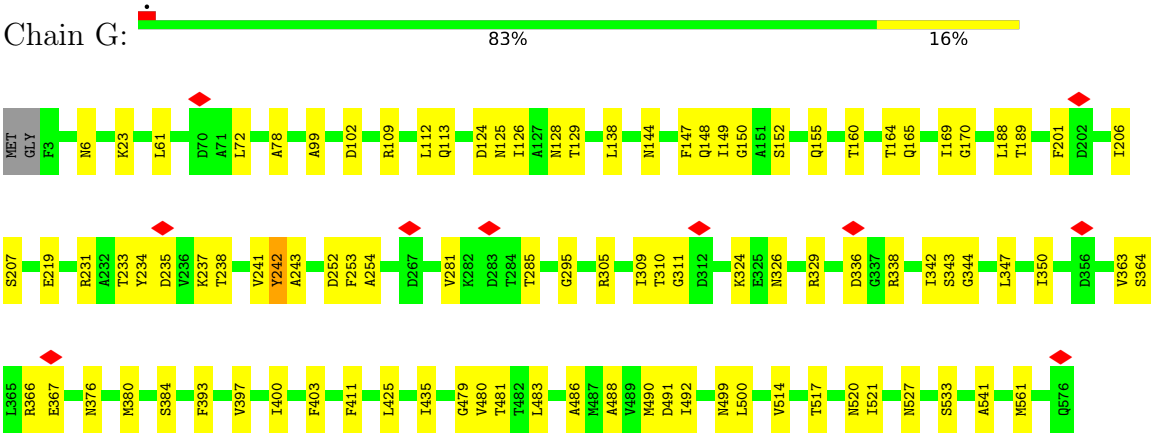
• Molecule 1: Flagellin A

Chain F:



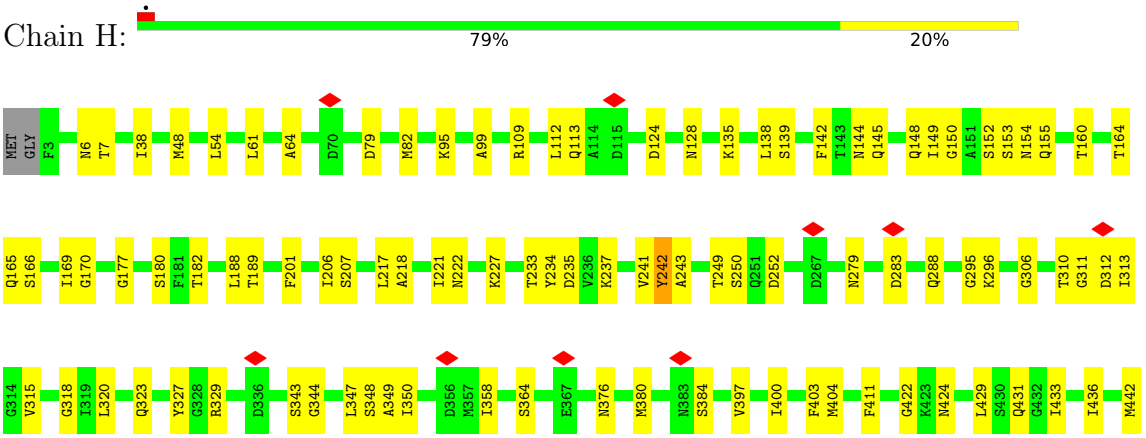
• Molecule 1: Flagellin A

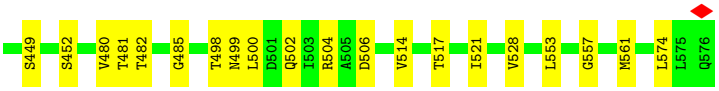
Chain G:



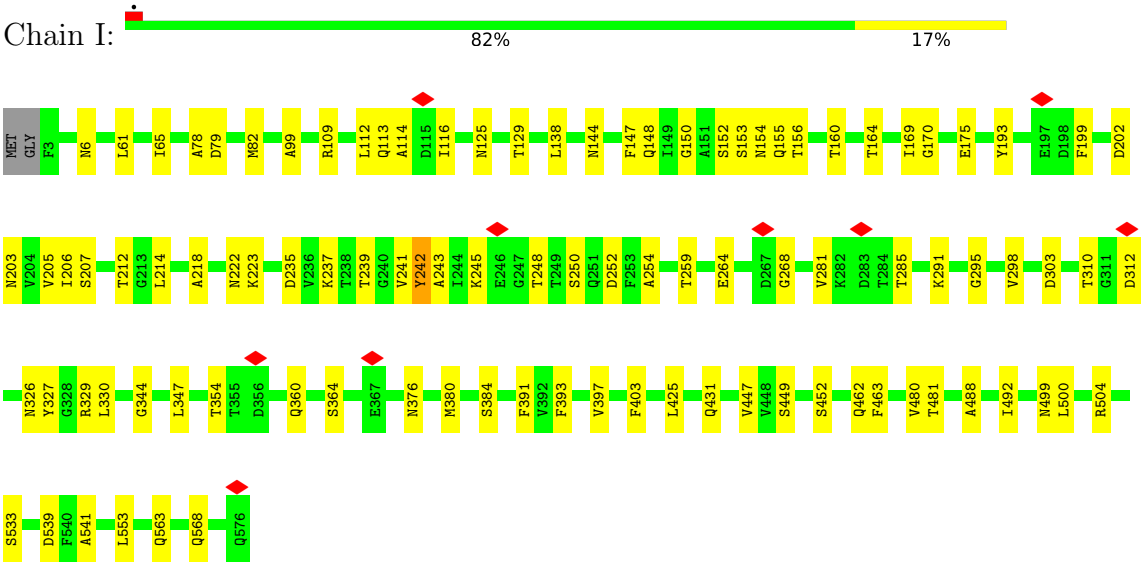
• Molecule 1: Flagellin A

Chain H:

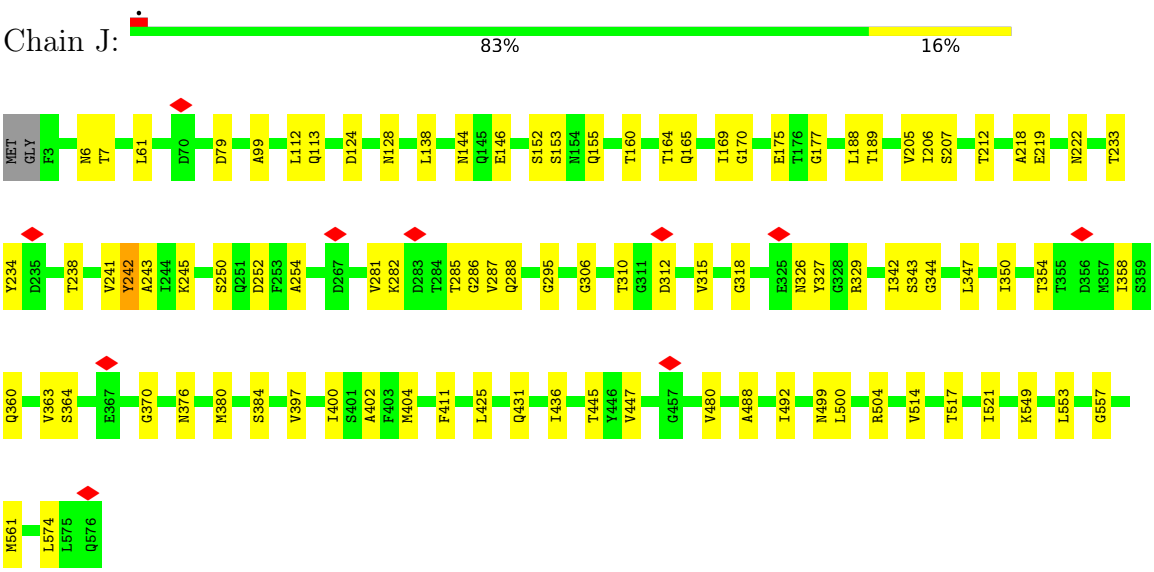




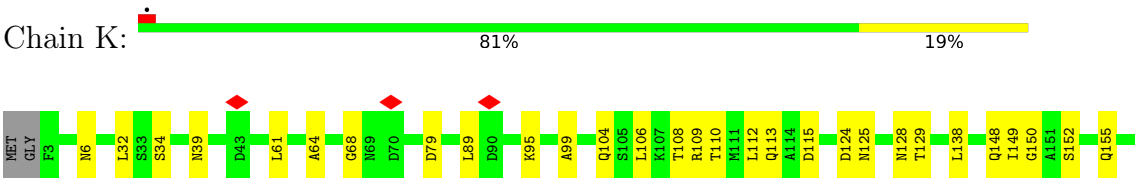
• Molecule 1: Flagellin A

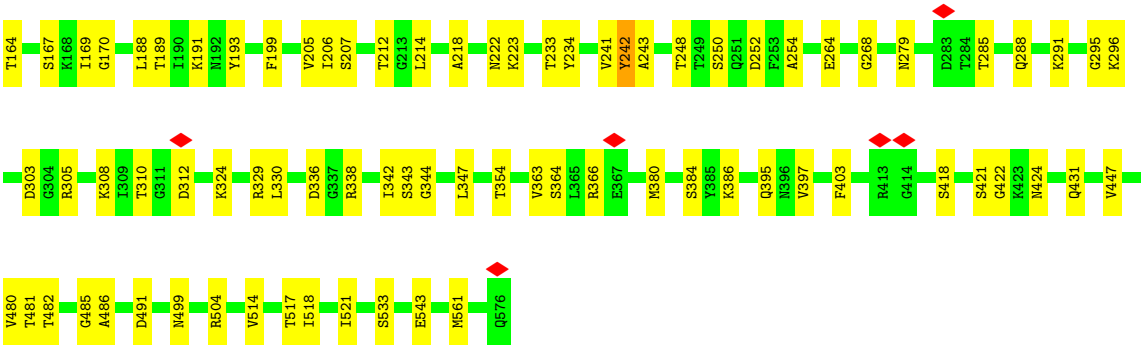


• Molecule 1: Flagellin A



• Molecule 1: Flagellin A

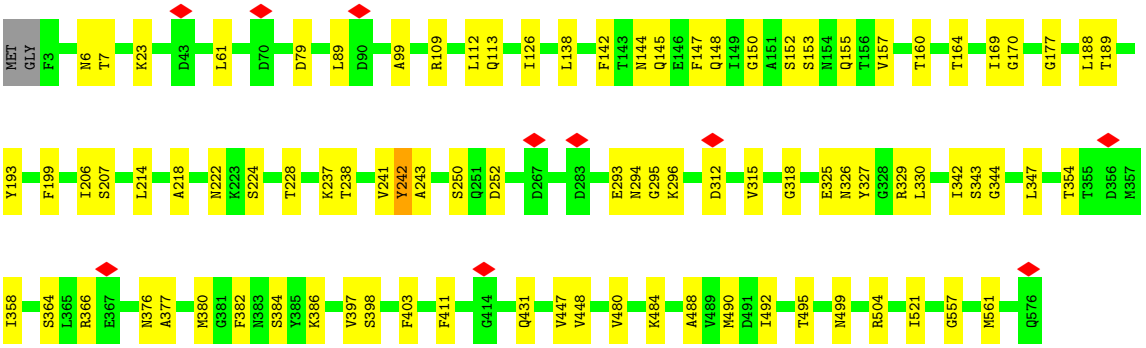




• Molecule 1: Flagellin A

Chain L:

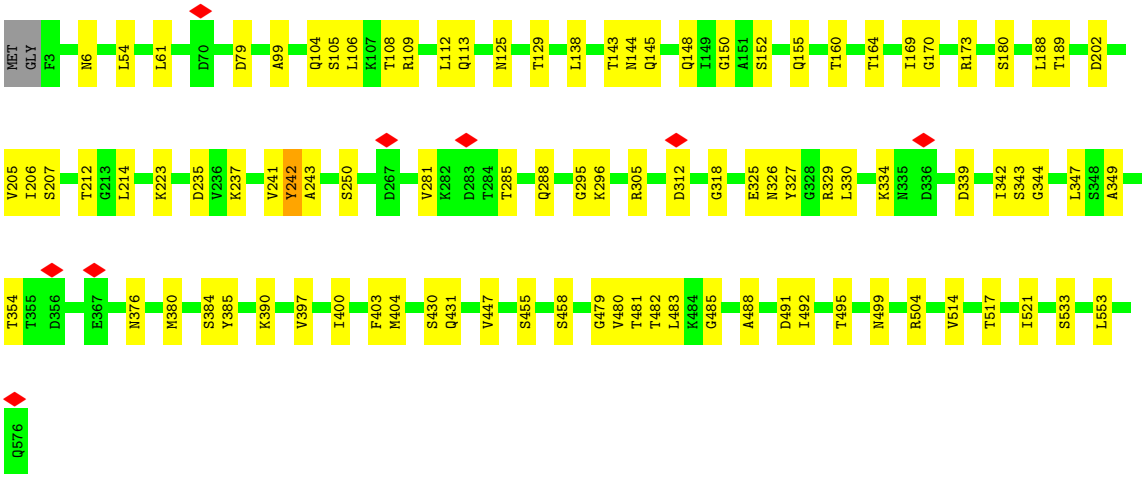




• Molecule 1: Flagellin A

Chain M:

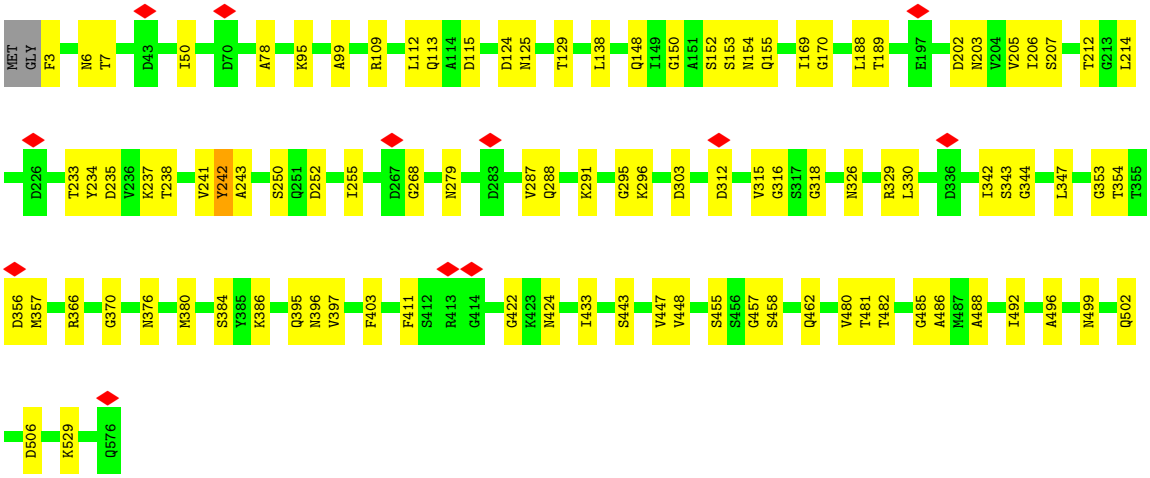




• Molecule 1: Flagellin A

Chain N:

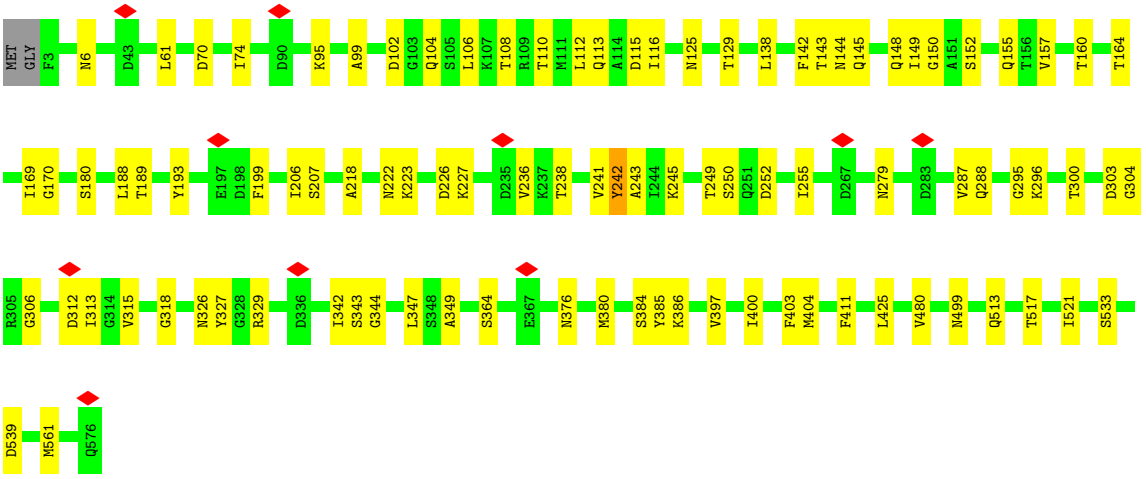




• Molecule 1: Flagellin A

Chain O:

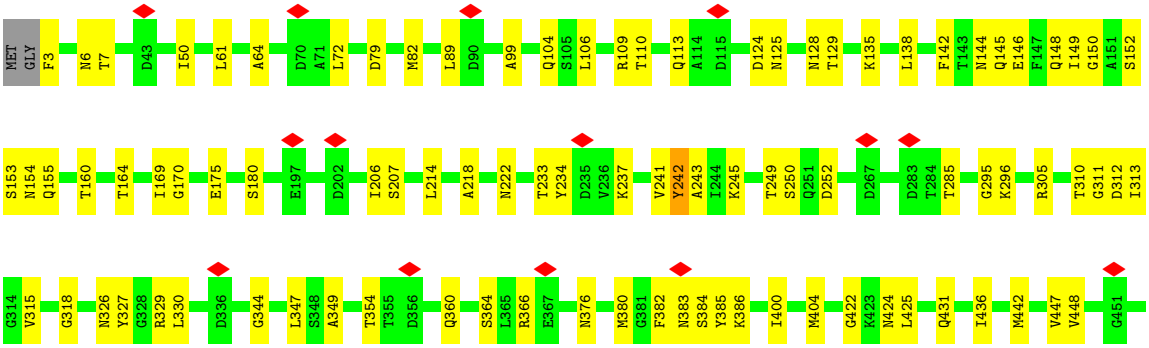


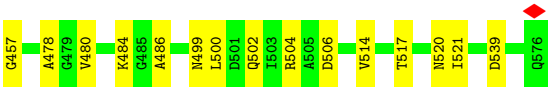


• Molecule 1: Flagellin A

Chain P:



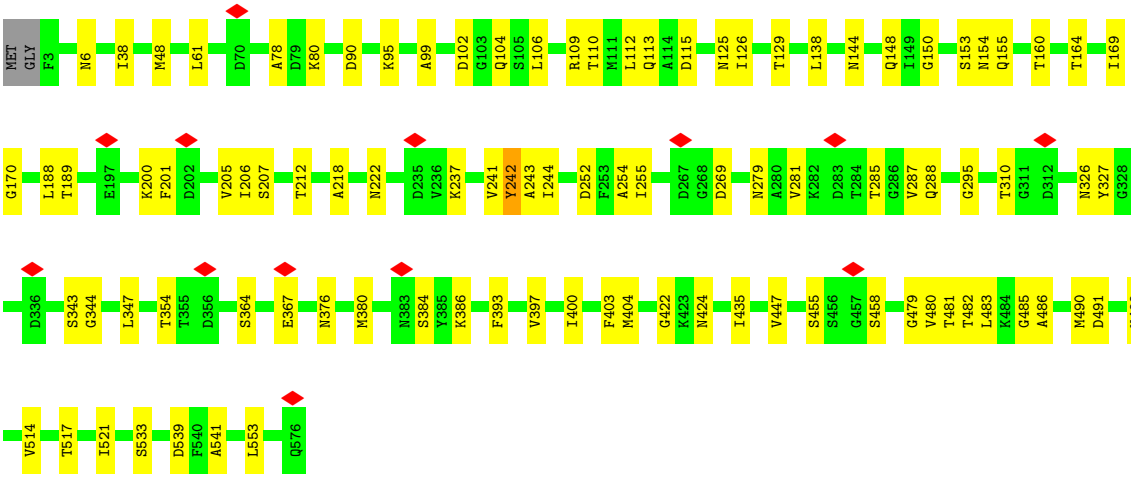




• Molecule 1: Flagellin A

Chain Q:

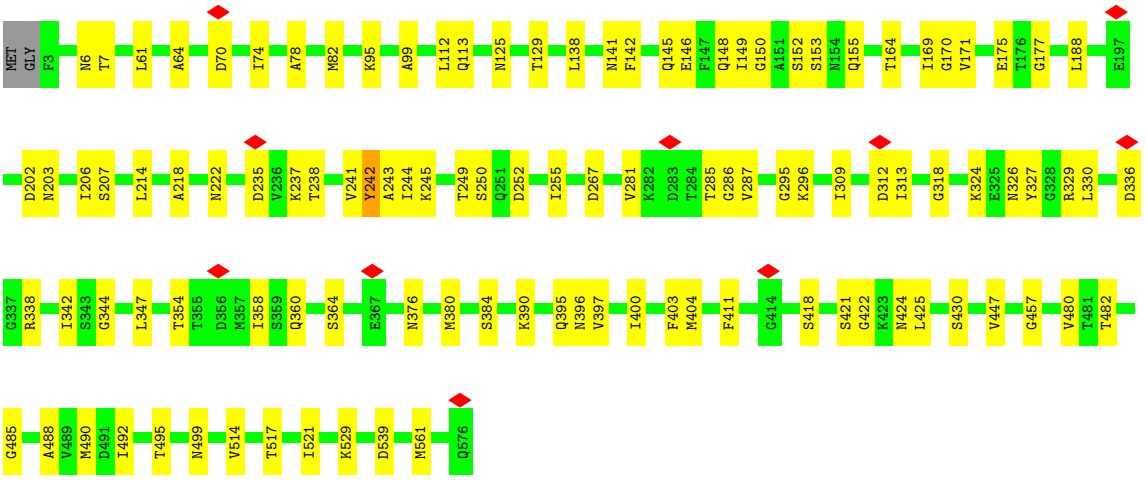




• Molecule 1: Flagellin A

Chain R:

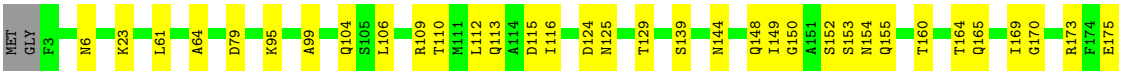


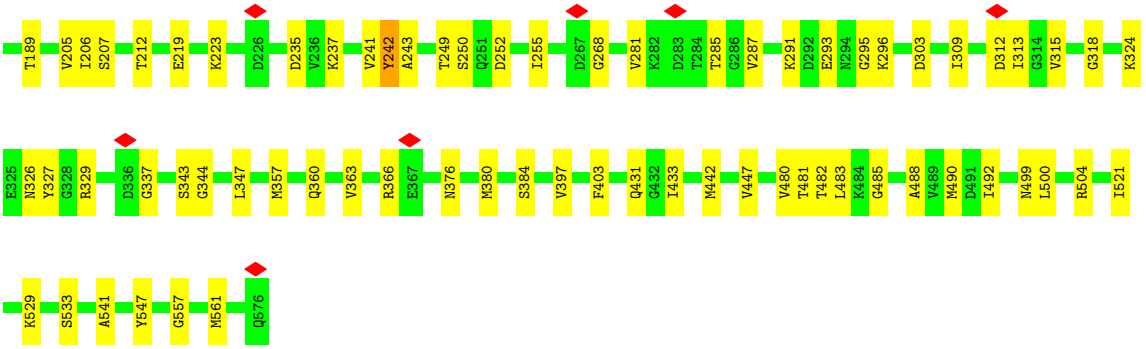


• Molecule 1: Flagellin A

Chain S:



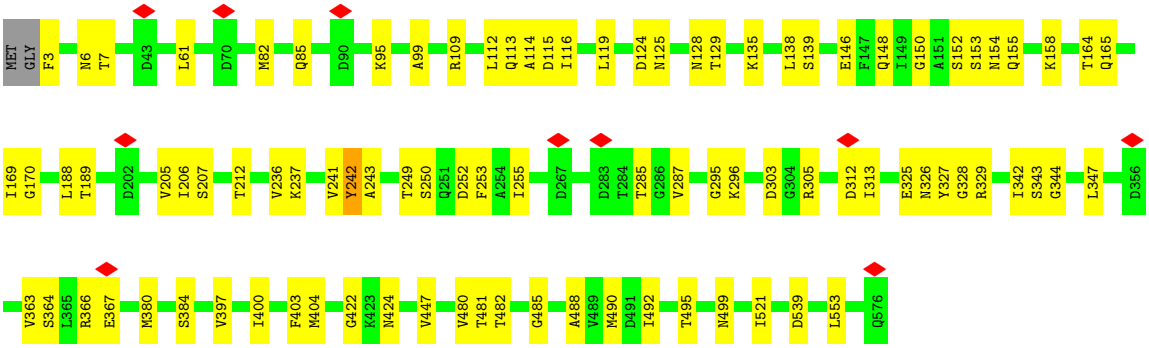




• Molecule 1: Flagellin A

Chain T:

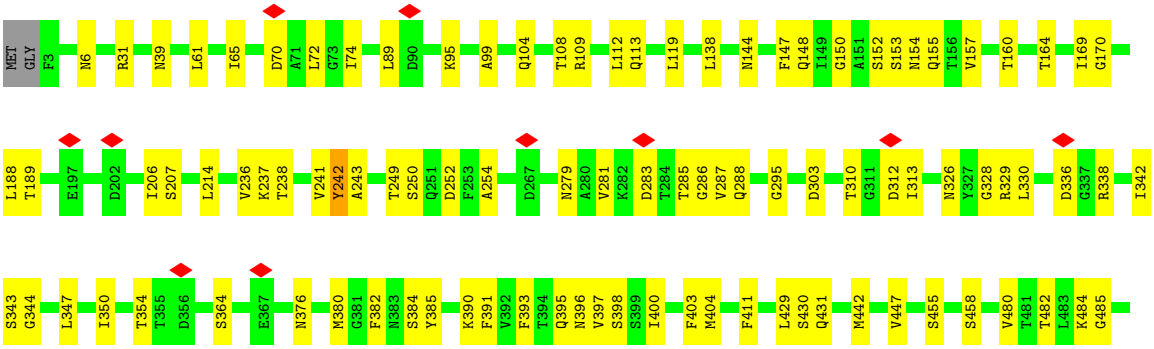




• Molecule 1: Flagellin A

Chain U:

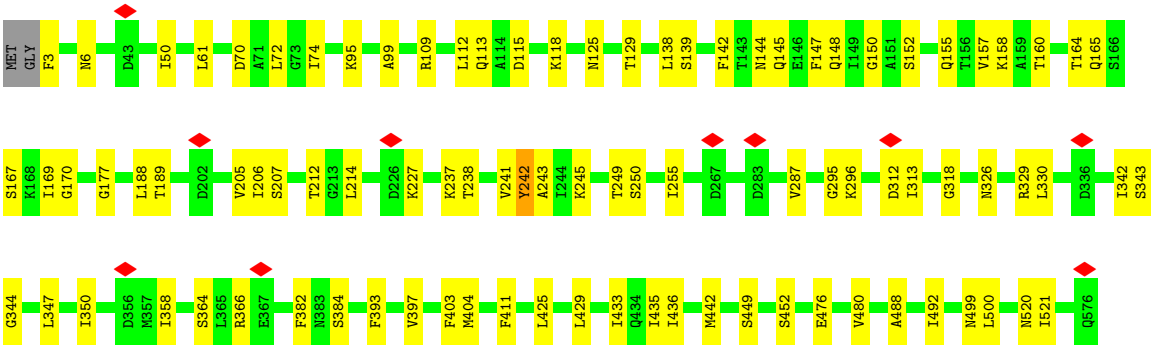




• Molecule 1: Flagellin A

Chain V:




MET GLY F3 N6 D43 I50 L61 D70 A71 L72 G73 I74 K95 A99 R109 L112 Q113 A114 D115 K118 N125 T129 L138 S139 F142 T143 N144 Q145 E146 F147 Q148 I149 G150 A151 S152 Q155 T156 V157 K158 A159 T160 T164 Q165 S166
S167 K168 I169 G170 G177 L188 T189 D202 V205 I206 S207 T212 G213 L214 D226 K227 K237 T238 V241 Y242 A243 I244 K245 T249 S250 I255 D267 D283 V287 G295 K296 D312 I313 G318 N326 R329 L330 D336 I342 S343
G344 L347 I350 D356 M357 I358 S364 L365 R366 E367 F382 N383 S384 F393 V397 F403 M404 F411 L425 L429 I433 Q434 I435 I436 M442 S449 S452 E476 V480 A488 I492 N499 L500 N520 I521 Q576

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=65.32°, rise=4.8 Å, axial sym=C1	Depositor
Number of segments used	116959	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.019	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0054	Depositor
Map size (Å)	414.72003, 414.72003, 453.6	wwPDB
Map dimensions	384, 384, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P8E

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.27	0/4185	0.38	0/5642
1	B	0.27	0/4185	0.38	1/5642 (0.0%)
1	C	0.28	0/4185	0.39	0/5642
1	D	0.27	0/4185	0.38	0/5642
1	E	0.28	0/4185	0.38	0/5642
1	F	0.28	0/4185	0.38	0/5642
1	G	0.27	0/4185	0.38	0/5642
1	H	0.27	0/4185	0.37	0/5642
1	I	0.27	0/4185	0.39	0/5642
1	J	0.28	0/4185	0.40	0/5642
1	K	0.27	0/4185	0.38	0/5642
1	L	0.28	0/4185	0.38	0/5642
1	M	0.27	0/4185	0.37	0/5642
1	N	0.27	0/4185	0.38	1/5642 (0.0%)
1	O	0.27	0/4185	0.39	0/5642
1	P	0.27	0/4185	0.39	0/5642
1	Q	0.28	0/4185	0.38	0/5642
1	R	0.27	0/4185	0.38	0/5642
1	S	0.27	0/4185	0.39	0/5642
1	T	0.27	0/4185	0.38	0/5642
1	U	0.27	0/4185	0.39	0/5642
1	V	0.27	0/4185	0.37	0/5642
All	All	0.27	0/92070	0.38	2/124124 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2
1	L	0	2
1	M	0	2
1	N	0	2
1	O	0	2
1	P	0	2
1	Q	0	2
1	R	0	2
1	S	0	2
1	T	0	2
1	U	0	2
1	V	0	2
All	All	0	44

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	316	GLY	N-CA-C	-5.48	107.96	114.48
1	B	316	GLY	N-CA-C	-5.14	108.08	113.58

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	ILE	Peptide
1	A	242	TYR	Peptide
1	B	206	ILE	Peptide
1	B	242	TYR	Peptide
1	C	206	ILE	Peptide
1	C	242	TYR	Peptide
1	D	206	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	D	242	TYR	Peptide
1	E	206	ILE	Peptide
1	E	242	TYR	Peptide
1	F	206	ILE	Peptide
1	F	242	TYR	Peptide
1	G	206	ILE	Peptide
1	G	242	TYR	Peptide
1	H	206	ILE	Peptide
1	H	242	TYR	Peptide
1	I	206	ILE	Peptide
1	I	242	TYR	Peptide
1	J	206	ILE	Peptide
1	J	242	TYR	Peptide
1	K	206	ILE	Peptide
1	K	242	TYR	Peptide
1	L	206	ILE	Peptide
1	L	242	TYR	Peptide
1	M	206	ILE	Peptide
1	M	242	TYR	Peptide
1	N	206	ILE	Peptide
1	N	242	TYR	Peptide
1	O	206	ILE	Peptide
1	O	242	TYR	Peptide
1	P	206	ILE	Peptide
1	P	242	TYR	Peptide
1	Q	206	ILE	Peptide
1	Q	242	TYR	Peptide
1	R	206	ILE	Peptide
1	R	242	TYR	Peptide
1	S	206	ILE	Peptide
1	S	242	TYR	Peptide
1	T	206	ILE	Peptide
1	T	242	TYR	Peptide
1	U	206	ILE	Peptide
1	U	242	TYR	Peptide
1	V	206	ILE	Peptide
1	V	242	TYR	Peptide

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	A	4159	0	4125	74	0
1	B	4159	0	4125	60	0
1	C	4159	0	4125	60	0
1	D	4159	0	4125	86	0
1	E	4159	0	4125	72	0
1	F	4159	0	4125	74	0
1	G	4159	0	4125	68	0
1	H	4159	0	4125	74	0
1	I	4159	0	4125	65	0
1	J	4159	0	4125	65	0
1	K	4159	0	4125	70	0
1	L	4159	0	4125	62	0
1	M	4159	0	4125	63	0
1	N	4159	0	4125	64	0
1	O	4159	0	4125	64	0
1	P	4159	0	4125	78	0
1	Q	4159	0	4125	68	0
1	R	4159	0	4125	73	0
1	S	4159	0	4125	68	0
1	T	4159	0	4125	61	0
1	U	4159	0	4125	78	0
1	V	4159	0	4125	60	0
2	A	272	0	0	13	0
2	B	272	0	0	11	0
2	C	272	0	0	16	0
2	D	272	0	0	13	0
2	E	272	0	0	10	0
2	F	272	0	0	14	0
2	G	272	0	0	13	0
2	H	272	0	0	14	0
2	I	272	0	0	14	0
2	J	272	0	0	13	0
2	K	272	0	0	14	0
2	L	272	0	0	14	0
2	M	272	0	0	14	0
2	N	272	0	0	13	0
2	O	272	0	0	13	0
2	P	272	0	0	16	0
2	Q	272	0	0	16	0
2	R	272	0	0	13	0
2	S	272	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	272	0	0	13	0
2	U	272	0	0	11	0
2	V	272	0	0	8	0
All	All	97482	0	90750	1675	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 9.

All (1675) 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:U:250:SER:HB3	1:U:312:ASP:HB3	1.62	0.81
1:R:250:SER:HB3	1:R:312:ASP:HB3	1.61	0.81
1:S:250:SER:HB3	1:S:312:ASP:HB3	1.63	0.81
1:D:344:GLY:H	1:D:347:LEU:HD11	1.47	0.79
1:O:144:ASN:H	1:O:160:THR:HG22	1.47	0.78
1:T:124:ASP:OD2	1:T:366:ARG:NH2	2.15	0.78
1:D:149:ILE:HD12	1:D:517:THR:HG21	1.64	0.78
1:L:144:ASN:H	1:L:160:THR:HG22	1.47	0.78
1:F:169:ILE:O	1:F:499:ASN:ND2	2.17	0.78
1:K:344:GLY:H	1:K:347:LEU:HD11	1.48	0.78
1:B:144:ASN:H	1:B:160:THR:HG22	1.50	0.77
1:E:169:ILE:O	1:E:499:ASN:ND2	2.17	0.77
1:A:344:GLY:H	1:A:347:LEU:HD11	1.50	0.76
1:H:344:GLY:H	1:H:347:LEU:HD11	1.50	0.76
1:P:169:ILE:O	1:P:499:ASN:ND2	2.19	0.76
1:G:344:GLY:H	1:G:347:LEU:HD11	1.48	0.76
1:F:344:GLY:H	1:F:347:LEU:HD11	1.49	0.76
1:E:344:GLY:H	1:E:347:LEU:HD11	1.50	0.76
1:V:152:SER:OG	1:V:155:GLN:NE2	2.18	0.75
1:E:152:SER:OG	1:E:155:GLN:NE2	2.18	0.75
1:Q:144:ASN:H	1:Q:160:THR:HG22	1.50	0.75
1:U:152:SER:OG	1:U:155:GLN:NE2	2.19	0.75
1:O:344:GLY:H	1:O:347:LEU:HD11	1.53	0.74
1:I:169:ILE:O	1:I:499:ASN:ND2	2.20	0.73
1:M:152:SER:OG	1:M:155:GLN:NE2	2.22	0.73
1:I:144:ASN:H	1:I:160:THR:HG22	1.54	0.73
1:T:152:SER:OG	1:T:155:GLN:NE2	2.21	0.73
1:O:99:ALA:HB2	1:O:112:LEU:HG	1.69	0.73
1:P:152:SER:OG	1:P:155:GLN:NE2	2.21	0.73
1:I:344:GLY:H	1:I:347:LEU:HD11	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:344:GLY:H	1:T:347:LEU:HD11	1.52	0.73
1:N:169:ILE:O	1:N:499:ASN:ND2	2.22	0.73
1:P:344:GLY:H	1:P:347:LEU:HD11	1.54	0.72
1:A:219:GLU:OE2	1:L:366:ARG:NH2	2.20	0.72
1:H:169:ILE:O	1:H:499:ASN:ND2	2.22	0.72
1:B:169:ILE:O	1:B:499:ASN:ND2	2.22	0.72
1:J:169:ILE:O	1:J:499:ASN:ND2	2.21	0.72
1:D:169:ILE:O	1:D:499:ASN:ND2	2.22	0.72
1:F:152:SER:OG	1:F:155:GLN:NE2	2.19	0.72
1:S:169:ILE:O	1:S:499:ASN:ND2	2.23	0.71
1:F:541:ALA:HB1	1:R:561:MET:HE1	1.72	0.71
1:J:329:ARG:NH1	1:J:384:SER:O	2.24	0.71
1:K:124:ASP:OD2	1:K:366:ARG:NH2	2.23	0.71
1:V:250:SER:HB2	1:V:312:ASP:HB3	1.71	0.71
1:A:144:ASN:H	1:A:160:THR:HG22	1.54	0.71
1:N:344:GLY:H	1:N:347:LEU:HD11	1.55	0.71
1:F:153:SER:OG	1:Q:491:ASP:OD1	2.08	0.71
1:V:344:GLY:H	1:V:347:LEU:HD11	1.56	0.71
1:E:561:MET:HE1	1:Q:541:ALA:HB1	1.73	0.70
1:S:144:ASN:H	1:S:160:THR:HG22	1.56	0.70
1:G:169:ILE:O	1:G:499:ASN:ND2	2.24	0.70
1:J:363:VAL:HG21	1:J:380:MET:HE1	1.72	0.70
1:B:431:GLN:NE2	2:B:610:P8E:O1B	2.24	0.70
1:J:344:GLY:H	1:J:347:LEU:HD11	1.55	0.70
1:K:152:SER:OG	1:K:155:GLN:NE2	2.20	0.70
1:A:495:THR:O	1:A:499:ASN:ND2	2.24	0.70
1:H:144:ASN:H	1:H:160:THR:HG22	1.56	0.69
1:U:344:GLY:H	1:U:347:LEU:HD11	1.56	0.69
1:O:279:ASN:ND2	1:O:288:GLN:OE1	2.26	0.69
1:U:279:ASN:ND2	1:U:288:GLN:OE1	2.25	0.69
1:P:329:ARG:NH1	1:P:384:SER:O	2.26	0.69
1:R:152:SER:OG	1:R:155:GLN:NE2	2.23	0.69
1:H:152:SER:OG	1:H:155:GLN:OE1	2.11	0.69
1:I:153:SER:OG	1:I:154:ASN:ND2	2.26	0.69
1:F:160:THR:OG1	1:Q:288:GLN:NE2	2.26	0.68
1:H:160:THR:OG1	1:O:288:GLN:NE2	2.26	0.68
1:P:124:ASP:OD2	1:P:366:ARG:NH2	2.24	0.68
1:F:99:ALA:HB2	1:F:112:LEU:HG	1.75	0.68
1:A:400:ILE:HG22	1:A:404:MET:HE2	1.74	0.68
1:C:152:SER:OG	1:C:155:GLN:NE2	2.18	0.68
1:K:491:ASP:OD2	1:L:153:SER:OG	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:149:ILE:HD12	1:O:517:THR:HG21	1.75	0.68
1:I:250:SER:HB2	1:I:312:ASP:HB3	1.75	0.68
1:V:169:ILE:O	1:V:499:ASN:ND2	2.27	0.68
1:K:279:ASN:ND2	1:K:288:GLN:OE1	2.27	0.67
1:F:279:ASN:ND2	1:F:288:GLN:OE1	2.28	0.67
1:L:152:SER:OG	1:L:155:GLN:NE2	2.23	0.67
1:S:153:SER:OG	1:S:154:ASN:ND2	2.28	0.67
1:C:431:GLN:NE2	2:C:610:P8E:O1B	2.28	0.67
1:I:79:ASP:OD2	1:I:504:ARG:NE	2.24	0.67
1:D:99:ALA:HB2	1:D:112:LEU:HG	1.76	0.66
1:K:288:GLN:NE2	1:L:160:THR:OG1	2.28	0.66
1:N:329:ARG:NH1	1:N:384:SER:O	2.27	0.66
1:F:188:LEU:HD22	1:F:342:ILE:HD11	1.78	0.66
1:M:329:ARG:NH1	1:M:384:SER:O	2.28	0.66
1:J:124:ASP:O	1:J:128:ASN:ND2	2.29	0.66
1:L:431:GLN:NE2	2:L:610:P8E:O1B	2.28	0.66
1:M:376:ASN:O	1:M:380:MET:HG2	1.96	0.66
1:B:344:GLY:H	1:B:347:LEU:HD11	1.59	0.66
1:P:144:ASN:H	1:P:160:THR:HG22	1.59	0.66
1:H:250:SER:HB3	1:H:312:ASP:HB3	1.78	0.66
1:O:152:SER:OG	1:O:155:GLN:NE2	2.27	0.66
1:P:153:SER:OG	1:P:154:ASN:ND2	2.28	0.66
1:B:99:ALA:O	1:B:109:ARG:NH1	2.28	0.66
1:B:124:ASP:OD2	1:B:366:ARG:NH2	2.28	0.66
1:G:231:ARG:HH12	1:P:153:SER:HB3	1.60	0.66
2:J:615:P8E:O6	2:J:615:P8E:O8	2.11	0.66
1:A:99:ALA:HB2	1:A:112:LEU:HG	1.78	0.66
1:H:431:GLN:NE2	2:H:610:P8E:O1B	2.29	0.66
1:S:344:GLY:H	1:S:347:LEU:HD11	1.60	0.66
1:H:400:ILE:HG22	1:H:404:MET:HE2	1.77	0.65
1:B:279:ASN:ND2	1:B:288:GLN:OE1	2.29	0.65
1:Q:169:ILE:O	1:Q:499:ASN:ND2	2.29	0.65
1:J:153:SER:OG	1:M:491:ASP:OD1	2.12	0.65
1:N:152:SER:OG	1:N:155:GLN:NE2	2.24	0.65
1:H:329:ARG:NH1	1:H:384:SER:O	2.22	0.65
1:F:124:ASP:OD2	1:F:366:ARG:NH2	2.27	0.65
1:U:376:ASN:O	1:U:380:MET:HG2	1.97	0.65
1:C:169:ILE:O	1:C:499:ASN:ND2	2.30	0.65
1:K:169:ILE:O	1:K:499:ASN:ND2	2.30	0.65
1:M:169:ILE:O	1:M:499:ASN:ND2	2.29	0.65
1:K:422:GLY:O	1:K:424:ASN:ND2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:SER:OG	1:A:155:GLN:NE2	2.28	0.65
1:O:169:ILE:O	1:O:499:ASN:ND2	2.30	0.65
1:P:241:VAL:HG23	1:P:242:TYR:HD2	1.62	0.64
1:Q:344:GLY:H	1:Q:347:LEU:HD11	1.60	0.64
1:B:160:THR:OG1	1:U:288:GLN:NE2	2.31	0.64
1:N:250:SER:HB2	1:N:312:ASP:HB3	1.79	0.64
1:S:109:ARG:HB3	1:S:481:THR:HA	1.79	0.64
1:J:144:ASN:H	1:J:160:THR:HG22	1.63	0.64
1:Q:148:GLN:NE2	1:Q:150:GLY:O	2.30	0.64
1:S:152:SER:OG	1:S:155:GLN:NE2	2.24	0.64
1:J:152:SER:OG	1:J:155:GLN:OE1	2.14	0.64
1:M:188:LEU:HD22	1:M:342:ILE:HD11	1.80	0.64
1:D:152:SER:OG	1:D:155:GLN:NE2	2.25	0.64
1:F:144:ASN:H	1:F:160:THR:HG22	1.62	0.64
1:P:50:ILE:HD11	1:Q:104:GLN:HG2	1.78	0.64
1:N:99:ALA:O	1:N:109:ARG:NH1	2.30	0.64
1:O:400:ILE:HG22	1:O:404:MET:HE2	1.79	0.64
1:F:146:GLU:HB2	1:Q:483:LEU:HD21	1.79	0.64
1:V:237:LYS:O	1:V:326:ASN:ND2	2.31	0.64
1:C:376:ASN:O	1:C:380:MET:HG2	1.98	0.64
1:C:483:LEU:HD21	1:T:146:GLU:HG3	1.80	0.63
2:G:615:P8E:O8	2:G:615:P8E:O6	2.15	0.63
1:E:79:ASP:OD1	1:E:504:ARG:NE	2.26	0.63
1:R:329:ARG:HD2	1:R:384:SER:O	1.98	0.63
1:V:144:ASN:H	1:V:160:THR:HG22	1.63	0.63
1:C:153:SER:OG	1:C:154:ASN:ND2	2.31	0.63
1:D:124:ASP:OD2	1:D:366:ARG:NH2	2.31	0.63
1:Q:153:SER:OG	1:Q:154:ASN:ND2	2.31	0.63
1:U:431:GLN:NE2	2:U:610:P8E:O1B	2.31	0.63
1:E:329:ARG:NH1	1:E:384:SER:O	2.26	0.63
1:L:148:GLN:NE2	1:L:150:GLY:O	2.32	0.63
1:E:113:GLN:HE21	1:E:480:VAL:H	1.46	0.63
1:I:99:ALA:HB2	1:I:112:LEU:HG	1.79	0.63
1:C:279:ASN:ND2	1:C:288:GLN:OE1	2.32	0.63
1:G:99:ALA:HB2	1:G:112:LEU:HG	1.80	0.63
1:B:152:SER:OG	1:B:155:GLN:OE1	2.16	0.62
1:J:241:VAL:HG23	1:J:242:TYR:HD2	1.63	0.62
1:P:431:GLN:NE2	2:P:610:P8E:O1B	2.33	0.62
1:S:148:GLN:NE2	1:S:150:GLY:O	2.32	0.62
1:F:329:ARG:NH1	1:F:384:SER:O	2.31	0.62
1:N:148:GLN:NE2	1:N:150:GLY:O	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:395:GLN:HG2	1:U:396:ASN:H	1.64	0.62
1:C:344:GLY:H	1:C:347:LEU:HD11	1.65	0.62
1:A:214:LEU:HD12	1:A:330:LEU:HD13	1.80	0.62
2:V:603:P8E:O6	2:V:603:P8E:O8	2.16	0.62
2:J:614:P8E:O8	2:J:614:P8E:O6	2.15	0.62
1:L:377:ALA:HB1	1:L:382:PHE:HD2	1.63	0.62
2:N:603:P8E:O8	2:N:603:P8E:O6	2.17	0.62
1:L:344:GLY:H	1:L:347:LEU:HD11	1.63	0.62
1:M:99:ALA:HB2	1:M:112:LEU:HG	1.80	0.62
1:O:241:VAL:HG23	1:O:242:TYR:HD2	1.64	0.62
1:E:99:ALA:HB2	1:E:112:LEU:HG	1.81	0.62
1:E:279:ASN:ND2	1:E:288:GLN:OE1	2.33	0.62
1:R:329:ARG:NH1	1:R:384:SER:O	2.32	0.62
1:S:150:GLY:HA3	1:S:155:GLN:HB2	1.81	0.62
1:R:142:PHE:HA	1:R:145:GLN:HE21	1.65	0.62
1:J:376:ASN:O	1:J:380:MET:HG2	2.00	0.61
1:U:495:THR:O	1:U:499:ASN:ND2	2.30	0.61
1:A:218:ALA:O	1:A:222:ASN:ND2	2.33	0.61
1:G:152:SER:OG	1:G:155:GLN:NE2	2.25	0.61
1:N:279:ASN:ND2	1:N:288:GLN:OE1	2.33	0.61
1:K:148:GLN:NE2	1:K:150:GLY:O	2.33	0.61
1:S:99:ALA:HB2	1:S:112:LEU:HG	1.81	0.61
1:C:237:LYS:O	1:C:326:ASN:ND2	2.33	0.61
1:V:214:LEU:HD12	1:V:330:LEU:HD13	1.81	0.61
1:B:148:GLN:NE2	1:B:150:GLY:O	2.33	0.61
2:S:615:P8E:O8	2:S:615:P8E:O6	2.18	0.61
1:S:116:ILE:HD12	1:S:480:VAL:HG21	1.82	0.61
1:A:237:LYS:O	1:A:326:ASN:ND2	2.34	0.61
2:G:601:P8E:O6	2:G:601:P8E:O8	2.15	0.61
2:H:617:P8E:O1A	2:H:617:P8E:O8	2.18	0.61
1:U:99:ALA:HB2	1:U:112:LEU:HG	1.82	0.61
1:B:329:ARG:NH1	1:B:384:SER:O	2.28	0.61
1:I:431:GLN:NE2	2:I:610:P8E:O1B	2.34	0.61
1:B:303:ASP:OD2	1:B:305:ARG:NH2	2.34	0.60
2:E:616:P8E:O6	2:E:616:P8E:O8	2.16	0.60
1:G:366:ARG:NH2	1:S:219:GLU:OE2	2.32	0.60
1:K:329:ARG:NH1	1:K:384:SER:O	2.34	0.60
1:R:376:ASN:O	1:R:380:MET:HG2	2.01	0.60
1:E:124:ASP:O	1:E:128:ASN:ND2	2.34	0.60
1:O:148:GLN:NE2	1:O:150:GLY:O	2.34	0.60
1:P:148:GLN:NE2	1:P:150:GLY:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ALA:O	1:A:109:ARG:NH1	2.34	0.60
1:H:436:ILE:HG21	1:H:442:MET:HE2	1.83	0.60
1:K:431:GLN:NE2	2:K:610:P8E:O1B	2.34	0.60
1:M:150:GLY:HA3	1:M:155:GLN:HB2	1.83	0.60
2:V:615:P8E:O8	2:V:615:P8E:O6	2.18	0.60
1:T:124:ASP:OD1	1:T:128:ASN:ND2	2.34	0.60
1:C:142:PHE:HA	1:C:145:GLN:HE21	1.66	0.60
1:Q:364:SER:HB3	1:Q:367:GLU:HG3	1.82	0.60
1:D:148:GLN:NE2	1:D:150:GLY:O	2.35	0.60
1:F:502:GLN:NE2	1:F:506:ASP:OD1	2.35	0.60
2:M:615:P8E:O6	2:M:615:P8E:O8	2.19	0.60
1:B:250:SER:HB2	1:B:312:ASP:HB3	1.83	0.60
1:C:99:ALA:HB2	1:C:112:LEU:HG	1.82	0.60
1:D:144:ASN:H	1:D:160:THR:HG22	1.66	0.60
1:O:329:ARG:NH1	1:O:384:SER:O	2.34	0.60
1:Q:354:THR:O	2:Q:616:P8E:O4	2.19	0.60
1:R:344:GLY:H	1:R:347:LEU:HD11	1.66	0.60
1:R:422:GLY:O	1:R:424:ASN:ND2	2.35	0.60
1:D:250:SER:OG	1:D:252:ASP:OD1	2.19	0.59
1:D:354:THR:O	2:D:616:P8E:O4	2.20	0.59
1:G:376:ASN:O	1:G:380:MET:HG2	2.02	0.59
1:H:153:SER:OG	1:H:154:ASN:ND2	2.26	0.59
1:G:237:LYS:O	1:G:326:ASN:ND2	2.34	0.59
1:P:113:GLN:NE2	1:P:480:VAL:H	2.00	0.59
1:Q:376:ASN:O	1:Q:380:MET:HG2	2.02	0.59
1:I:175:GLU:HG2	1:I:360:GLN:HB3	1.84	0.59
1:N:205:VAL:HB	1:N:212:THR:HG22	1.84	0.59
2:Q:603:P8E:O6	2:Q:603:P8E:O8	2.21	0.59
1:S:235:ASP:OD1	1:S:237:LYS:NZ	2.35	0.59
1:I:329:ARG:NH1	1:I:384:SER:O	2.33	0.59
1:G:148:GLN:NE2	1:G:150:GLY:O	2.35	0.59
1:P:436:ILE:HG21	1:P:442:MET:HE2	1.84	0.59
1:B:436:ILE:HG21	1:B:442:MET:HE2	1.84	0.59
1:L:241:VAL:HG23	1:L:242:TYR:HD2	1.67	0.59
1:H:148:GLN:NE2	1:H:150:GLY:O	2.35	0.59
1:M:109:ARG:HB3	1:M:481:THR:HA	1.85	0.59
1:T:241:VAL:HG23	1:T:242:TYR:HD2	1.67	0.59
1:T:329:ARG:HD2	1:T:384:SER:O	2.02	0.59
1:B:124:ASP:OD1	1:B:128:ASN:ND2	2.35	0.59
1:D:82:MET:HE1	1:D:500:LEU:HD22	1.84	0.59
2:G:608:P8E:O6	2:G:608:P8E:O8	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:376:ASN:O	1:H:380:MET:HG2	2.02	0.59
1:J:7:THR:HG21	1:M:533:SER:HB2	1.83	0.59
1:R:169:ILE:O	1:R:499:ASN:ND2	2.35	0.59
1:T:169:ILE:O	1:T:499:ASN:ND2	2.36	0.59
1:E:491:ASP:OD2	1:R:153:SER:OG	2.15	0.58
1:L:329:ARG:NH1	1:L:384:SER:O	2.36	0.58
2:Q:610:P8E:O8	2:Q:610:P8E:O6	2.21	0.58
2:R:617:P8E:O1A	2:R:617:P8E:O8	2.22	0.58
1:U:144:ASN:H	1:U:160:THR:HG22	1.67	0.58
1:V:167:SER:HB3	1:V:366:ARG:HD2	1.84	0.58
2:C:615:P8E:O6	2:C:615:P8E:O8	2.21	0.58
1:G:533:SER:HB2	1:P:7:THR:HG21	1.85	0.58
1:K:533:SER:HB2	1:L:7:THR:HG21	1.85	0.58
1:N:422:GLY:O	1:N:424:ASN:ND2	2.36	0.58
1:A:329:ARG:NH1	1:A:384:SER:O	2.29	0.58
2:B:615:P8E:O8	2:B:615:P8E:O6	2.20	0.58
1:H:99:ALA:HB2	1:H:112:LEU:HG	1.85	0.58
1:L:99:ALA:O	1:L:109:ARG:NH1	2.36	0.58
1:E:533:SER:HB2	1:R:7:THR:HG21	1.84	0.58
2:E:617:P8E:O1A	2:E:617:P8E:O8	2.20	0.58
1:I:152:SER:OG	1:I:155:GLN:NE2	2.27	0.58
1:T:252:ASP:OD1	1:T:252:ASP:N	2.37	0.58
1:M:354:THR:O	2:M:616:P8E:O4	2.21	0.58
1:E:113:GLN:NE2	1:E:480:VAL:H	2.01	0.58
1:H:422:GLY:O	1:H:424:ASN:ND2	2.37	0.58
1:I:109:ARG:HB3	1:I:481:THR:HA	1.86	0.58
1:I:329:ARG:HD2	1:I:384:SER:O	2.04	0.58
1:G:329:ARG:HD2	1:G:384:SER:O	2.04	0.58
2:O:615:P8E:O6	2:O:615:P8E:O8	2.22	0.58
1:U:404:MET:HG2	1:U:411:PHE:CD2	2.39	0.58
2:H:612:P8E:O8	2:H:612:P8E:N5	2.37	0.58
1:J:431:GLN:NE2	2:J:610:P8E:O1B	2.33	0.58
1:A:150:GLY:HA3	1:A:155:GLN:HB2	1.85	0.57
2:F:615:P8E:O6	2:F:615:P8E:O8	2.20	0.57
1:L:293:GLU:OE2	1:V:227:LYS:NZ	2.37	0.57
2:M:617:P8E:O1A	2:M:617:P8E:O8	2.22	0.57
1:N:169:ILE:HG13	1:N:170:GLY:H	1.68	0.57
1:T:329:ARG:NH1	1:T:384:SER:O	2.35	0.57
1:T:422:GLY:O	1:T:424:ASN:ND2	2.37	0.57
2:A:601:P8E:O8	2:A:601:P8E:O6	2.22	0.57
1:E:214:LEU:HD12	1:E:330:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:LEU:HD22	1:F:521:ILE:HG23	1.84	0.57
2:O:603:P8E:O6	2:O:603:P8E:O8	2.21	0.57
1:T:150:GLY:HA3	1:T:155:GLN:HB2	1.86	0.57
1:B:210:VAL:HA	1:B:305:ARG:HH12	1.69	0.57
1:C:533:SER:HB2	1:T:7:THR:HG21	1.86	0.57
1:E:241:VAL:HG23	1:E:242:TYR:HD2	1.68	0.57
1:G:491:ASP:OD1	1:P:153:SER:HB2	2.04	0.57
2:P:606:P8E:O6	2:P:606:P8E:O8	2.22	0.57
1:V:148:GLN:NE2	1:V:150:GLY:O	2.37	0.57
2:C:610:P8E:O8	2:C:610:P8E:O6	2.21	0.57
2:E:616:P8E:O8	2:E:616:P8E:O4	2.22	0.57
2:I:603:P8E:O8	2:I:603:P8E:O6	2.19	0.57
1:L:354:THR:O	2:L:616:P8E:O4	2.23	0.57
1:P:99:ALA:O	1:P:109:ARG:NH1	2.38	0.57
2:B:617:P8E:O1A	2:B:617:P8E:O8	2.23	0.57
1:E:150:GLY:HA3	1:E:155:GLN:HB2	1.85	0.57
1:G:241:VAL:HG23	1:G:242:TYR:HD2	1.69	0.57
2:J:617:P8E:O1A	2:J:617:P8E:O8	2.21	0.57
1:L:382:PHE:CE1	1:L:484:LYS:HB2	2.40	0.57
2:T:610:P8E:O8	2:T:610:P8E:O6	2.20	0.57
1:P:400:ILE:HG22	1:P:404:MET:HE2	1.86	0.57
1:E:109:ARG:HB3	1:E:481:THR:HA	1.87	0.57
2:H:615:P8E:O6	2:H:615:P8E:O8	2.21	0.57
2:N:616:P8E:O6	2:N:616:P8E:O8	2.23	0.57
2:T:614:P8E:O8	2:T:614:P8E:O6	2.22	0.57
2:A:603:P8E:O8	2:A:603:P8E:O6	2.23	0.56
1:F:113:GLN:NE2	1:F:480:VAL:H	2.02	0.56
1:K:354:THR:O	2:K:616:P8E:O4	2.23	0.56
1:P:422:GLY:O	1:P:424:ASN:ND2	2.38	0.56
1:A:431:GLN:NE2	2:A:610:P8E:O1B	2.36	0.56
1:B:7:THR:HG21	1:U:533:SER:HB2	1.88	0.56
2:B:614:P8E:O6	2:B:614:P8E:O8	2.24	0.56
2:D:601:P8E:O8	2:D:601:P8E:O6	2.21	0.56
1:E:148:GLN:NE2	1:E:150:GLY:O	2.38	0.56
1:I:82:MET:HE1	1:I:500:LEU:HD22	1.87	0.56
2:L:617:P8E:O1A	2:L:617:P8E:O8	2.23	0.56
1:M:61:LEU:HD22	1:M:521:ILE:HG23	1.88	0.56
1:M:79:ASP:OD2	1:M:504:ARG:NE	2.29	0.56
2:M:606:P8E:O8	2:M:606:P8E:O6	2.22	0.56
2:O:617:P8E:O1A	2:O:617:P8E:O8	2.22	0.56
1:P:142:PHE:HA	1:P:145:GLN:HE21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:188:LEU:HD22	1:V:342:ILE:HD11	1.87	0.56
2:D:610:P8E:O6	2:D:610:P8E:O8	2.21	0.56
1:M:237:LYS:O	1:M:326:ASN:ND2	2.37	0.56
1:N:235:ASP:OD1	1:N:237:LYS:NZ	2.38	0.56
1:U:148:GLN:NE2	1:U:150:GLY:O	2.38	0.56
1:C:354:THR:O	2:C:616:P8E:O4	2.23	0.56
1:F:170:GLY:O	1:F:364:SER:HA	2.06	0.56
1:H:99:ALA:O	1:H:109:ARG:NH1	2.38	0.56
1:H:241:VAL:HG23	1:H:242:TYR:HD2	1.69	0.56
1:J:61:LEU:HD22	1:J:521:ILE:HG23	1.88	0.56
1:J:99:ALA:HB2	1:J:112:LEU:HG	1.86	0.56
1:N:113:GLN:NE2	1:N:480:VAL:H	2.04	0.56
1:N:502:GLN:NE2	1:N:506:ASP:OD1	2.39	0.56
1:D:400:ILE:HG22	1:D:404:MET:HE2	1.88	0.56
1:E:153:SER:OG	1:E:154:ASN:ND2	2.31	0.56
1:G:150:GLY:HA3	1:G:155:GLN:HB2	1.88	0.56
2:O:612:P8E:O8	2:O:612:P8E:N5	2.39	0.56
1:U:236:VAL:HG22	1:U:328:GLY:HA3	1.88	0.56
1:V:329:ARG:HD2	1:V:384:SER:O	2.06	0.56
2:V:617:P8E:O1A	2:V:617:P8E:O8	2.24	0.56
2:B:601:P8E:O6	2:B:601:P8E:O8	2.24	0.56
1:G:285:THR:O	1:G:305:ARG:NH2	2.39	0.56
1:M:205:VAL:HB	1:M:212:THR:HG22	1.86	0.56
2:E:601:P8E:O6	2:E:601:P8E:O8	2.22	0.56
1:F:241:VAL:HG23	1:F:242:TYR:HD2	1.70	0.56
2:P:612:P8E:N5	2:P:612:P8E:O8	2.38	0.56
1:L:113:GLN:NE2	1:L:480:VAL:H	2.04	0.56
2:N:606:P8E:O8	2:N:606:P8E:O1B	2.24	0.56
1:O:376:ASN:O	1:O:380:MET:HG2	2.05	0.56
1:F:252:ASP:OD1	1:F:252:ASP:N	2.39	0.55
1:N:250:SER:OG	1:N:252:ASP:OD1	2.19	0.55
1:A:248:THR:HG22	1:A:264:GLU:HA	1.88	0.55
1:J:188:LEU:HD22	1:J:342:ILE:HD11	1.89	0.55
1:L:214:LEU:HD12	1:L:330:LEU:HD13	1.87	0.55
1:O:113:GLN:NE2	1:O:480:VAL:H	2.04	0.55
1:U:113:GLN:NE2	1:U:480:VAL:H	2.04	0.55
2:V:612:P8E:O8	2:V:612:P8E:N5	2.39	0.55
2:L:612:P8E:O8	2:L:612:P8E:N5	2.40	0.55
1:E:250:SER:HB3	1:E:312:ASP:HB3	1.88	0.55
1:F:235:ASP:OD1	1:F:237:LYS:NZ	2.39	0.55
1:M:281:VAL:O	1:M:285:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:615:P8E:O8	2:N:615:P8E:O6	2.23	0.55
1:C:250:SER:HB3	1:C:312:ASP:HB3	1.88	0.55
1:E:205:VAL:HB	1:E:212:THR:HG22	1.87	0.55
1:H:61:LEU:HD22	1:H:521:ILE:HG23	1.87	0.55
2:K:612:P8E:N5	2:K:612:P8E:O8	2.39	0.55
1:M:144:ASN:H	1:M:160:THR:HG22	1.71	0.55
1:Q:99:ALA:O	1:Q:109:ARG:NH1	2.39	0.55
1:U:99:ALA:O	1:U:109:ARG:NH1	2.40	0.55
2:V:606:P8E:O6	2:V:606:P8E:O8	2.25	0.55
1:H:218:ALA:O	1:H:222:ASN:ND2	2.40	0.55
2:L:606:P8E:O6	2:L:606:P8E:O8	2.25	0.55
1:U:400:ILE:HG22	1:U:404:MET:HE2	1.88	0.55
1:V:61:LEU:HD22	1:V:521:ILE:HG23	1.87	0.55
2:L:601:P8E:O6	2:L:601:P8E:O8	2.24	0.55
2:L:608:P8E:O6	2:L:608:P8E:O8	2.23	0.55
2:O:608:P8E:O8	2:O:608:P8E:O6	2.25	0.55
1:Q:329:ARG:HD2	1:Q:384:SER:O	2.07	0.55
1:Q:329:ARG:NH1	1:Q:384:SER:O	2.40	0.55
2:T:606:P8E:O8	2:T:606:P8E:O6	2.23	0.55
1:A:279:ASN:ND2	1:A:288:GLN:OE1	2.40	0.55
1:G:138:LEU:HB3	1:G:164:THR:HG21	1.87	0.55
1:J:400:ILE:HG22	1:J:404:MET:HE2	1.88	0.55
1:K:169:ILE:HG13	1:K:170:GLY:H	1.71	0.55
1:P:376:ASN:O	1:P:380:MET:HG2	2.07	0.55
1:D:182:THR:OG1	1:D:348:SER:O	2.25	0.55
1:M:344:GLY:H	1:M:347:LEU:HD11	1.72	0.55
2:P:617:P8E:O1A	2:P:617:P8E:O8	2.25	0.55
2:I:606:P8E:O8	2:I:606:P8E:O1B	2.25	0.54
2:K:606:P8E:O6	2:K:606:P8E:O8	2.24	0.54
1:D:329:ARG:NH1	1:D:384:SER:O	2.39	0.54
1:J:113:GLN:NE2	1:J:480:VAL:H	2.05	0.54
2:J:608:P8E:O8	2:J:608:P8E:O6	2.25	0.54
1:S:124:ASP:OD2	1:S:366:ARG:NH2	2.29	0.54
2:S:603:P8E:O8	2:S:603:P8E:O6	2.25	0.54
2:F:606:P8E:O8	2:F:606:P8E:O1B	2.25	0.54
2:I:612:P8E:O8	2:I:612:P8E:N5	2.41	0.54
2:N:612:P8E:O8	2:N:612:P8E:N5	2.40	0.54
1:P:457:GLY:N	2:P:616:P8E:O1A	2.28	0.54
2:T:615:P8E:O6	2:T:615:P8E:O8	2.25	0.54
2:U:617:P8E:O1A	2:U:617:P8E:O8	2.26	0.54
1:E:541:ALA:HB1	1:H:561:MET:HE1	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:238:THR:OG1	1:J:326:ASN:ND2	2.30	0.54
2:N:617:P8E:O1A	2:N:617:P8E:O8	2.25	0.54
1:P:61:LEU:HD22	1:P:521:ILE:HG23	1.89	0.54
1:A:574:LEU:HD11	1:K:561:MET:HE2	1.88	0.54
2:E:615:P8E:O8	2:E:615:P8E:O6	2.23	0.54
1:H:482:THR:HG23	1:H:485:GLY:H	1.73	0.54
1:I:354:THR:O	2:I:616:P8E:O4	2.24	0.54
2:O:614:P8E:O8	2:O:614:P8E:O6	2.24	0.54
1:P:245:LYS:HG3	1:P:425:LEU:HD11	1.89	0.54
1:P:329:ARG:HD2	1:P:384:SER:O	2.06	0.54
1:R:218:ALA:O	1:R:222:ASN:ND2	2.40	0.54
1:S:281:VAL:O	1:S:285:THR:HG23	2.07	0.54
1:B:205:VAL:HB	1:B:212:THR:HG22	1.88	0.54
1:B:250:SER:OG	1:B:252:ASP:OD1	2.24	0.54
1:K:61:LEU:HD22	1:K:521:ILE:HG23	1.89	0.54
1:Q:78:ALA:HB1	1:Q:138:LEU:HD21	1.90	0.54
1:U:329:ARG:NH1	1:U:384:SER:O	2.40	0.54
1:U:382:PHE:CE1	1:U:484:LYS:HB2	2.42	0.54
1:C:113:GLN:NE2	1:C:480:VAL:H	2.05	0.54
1:C:329:ARG:NH1	1:C:384:SER:O	2.40	0.54
1:D:113:GLN:NE2	1:D:480:VAL:H	2.06	0.54
1:I:376:ASN:O	1:I:380:MET:HG2	2.08	0.54
1:N:354:THR:O	2:N:616:P8E:O4	2.24	0.54
1:U:241:VAL:HG23	1:U:242:TYR:CD2	2.42	0.54
1:A:205:VAL:HB	1:A:212:THR:HG22	1.88	0.54
2:F:612:P8E:O1B	2:F:612:P8E:N5	2.41	0.54
1:L:61:LEU:HD22	1:L:521:ILE:HG23	1.89	0.54
1:C:165:GLN:HE22	1:O:223:LYS:NZ	2.05	0.54
2:C:601:P8E:O6	2:C:601:P8E:O8	2.26	0.54
1:E:124:ASP:OD2	1:E:128:ASN:ND2	2.40	0.54
1:G:188:LEU:HD22	1:G:342:ILE:HD11	1.89	0.54
2:I:606:P8E:O8	2:I:606:P8E:O6	2.24	0.54
1:J:250:SER:HB2	1:J:312:ASP:HB3	1.90	0.54
1:O:180:SER:OG	1:O:349:ALA:O	2.17	0.54
1:Q:99:ALA:HA	1:Q:104:GLN:HE22	1.72	0.54
1:Q:113:GLN:NE2	1:Q:480:VAL:H	2.06	0.54
1:R:125:ASN:O	1:R:129:THR:OG1	2.23	0.54
1:V:243:ALA:HB1	1:V:295:GLY:C	2.33	0.54
2:C:606:P8E:O8	2:C:606:P8E:O6	2.25	0.54
1:L:376:ASN:O	1:L:380:MET:HG2	2.06	0.54
1:O:243:ALA:HB1	1:O:295:GLY:C	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:218:ALA:O	1:Q:222:ASN:ND2	2.39	0.54
1:S:482:THR:HG23	1:S:485:GLY:H	1.73	0.54
1:D:61:LEU:HD22	1:D:521:ILE:HG23	1.89	0.53
2:G:612:P8E:O8	2:G:612:P8E:N5	2.41	0.53
1:I:239:THR:HG22	1:I:298:VAL:HG22	1.90	0.53
2:S:612:P8E:O8	2:S:612:P8E:N5	2.41	0.53
1:A:148:GLN:NE2	1:A:150:GLY:O	2.41	0.53
1:F:169:ILE:HG13	1:F:170:GLY:H	1.73	0.53
2:I:617:P8E:O1A	2:I:617:P8E:O8	2.26	0.53
1:N:488:ALA:O	1:N:492:ILE:HG13	2.08	0.53
1:R:188:LEU:HD22	1:R:342:ILE:HD11	1.90	0.53
2:A:616:P8E:O8	2:A:616:P8E:O6	2.26	0.53
2:E:612:P8E:O8	2:E:612:P8E:N5	2.41	0.53
1:G:125:ASN:O	1:G:129:THR:OG1	2.19	0.53
1:N:169:ILE:HG13	1:N:170:GLY:N	2.23	0.53
2:O:612:P8E:N5	2:O:612:P8E:O1B	2.42	0.53
2:P:611:P8E:O8	2:P:611:P8E:O6	2.27	0.53
1:N:376:ASN:O	1:N:380:MET:HG2	2.08	0.53
1:R:395:GLN:HG2	1:R:396:ASN:H	1.73	0.53
1:A:142:PHE:HA	1:A:145:GLN:HE21	1.72	0.53
1:D:393:PHE:HB2	1:D:435:ILE:HA	1.90	0.53
1:F:7:THR:HG21	1:Q:533:SER:HB2	1.91	0.53
2:U:614:P8E:O6	2:U:614:P8E:O8	2.27	0.53
1:E:237:LYS:O	1:E:326:ASN:ND2	2.42	0.53
1:F:150:GLY:HA3	1:F:155:GLN:HB2	1.90	0.53
2:F:601:P8E:O8	2:F:601:P8E:O6	2.23	0.53
2:H:606:P8E:O8	2:H:606:P8E:O6	2.25	0.53
1:I:533:SER:HB2	1:N:7:THR:HG21	1.90	0.53
1:U:188:LEU:HD22	1:U:342:ILE:HD11	1.89	0.53
1:I:147:PHE:H	1:I:156:THR:HG1	1.57	0.53
1:K:218:ALA:O	1:K:222:ASN:ND2	2.42	0.53
2:A:612:P8E:O8	2:A:612:P8E:N5	2.41	0.53
1:G:99:ALA:O	1:G:109:ARG:NH1	2.42	0.53
2:N:601:P8E:O6	2:N:601:P8E:O8	2.23	0.53
1:A:125:ASN:O	1:A:129:THR:OG1	2.17	0.53
2:B:612:P8E:O1B	2:B:612:P8E:N5	2.41	0.53
2:C:608:P8E:O8	2:C:608:P8E:O6	2.26	0.53
1:L:237:LYS:O	1:L:326:ASN:ND2	2.42	0.53
2:M:612:P8E:O1B	2:M:612:P8E:N5	2.42	0.53
1:N:214:LEU:HD12	1:N:330:LEU:HD13	1.90	0.53
1:P:180:SER:OG	1:P:349:ALA:O	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:601:P8E:O8	2:R:601:P8E:O6	2.27	0.53
2:V:601:P8E:O6	2:V:601:P8E:O8	2.24	0.53
2:D:617:P8E:O6	2:D:617:P8E:O8	2.26	0.53
1:E:488:ALA:O	1:E:492:ILE:HG13	2.09	0.53
1:F:250:SER:HB3	1:F:312:ASP:HB3	1.91	0.53
1:I:148:GLN:NE2	1:I:150:GLY:O	2.42	0.53
1:I:202:ASP:OD1	1:I:203:ASN:N	2.42	0.53
1:K:113:GLN:NE2	1:K:480:VAL:H	2.07	0.53
1:N:243:ALA:HA	1:N:296:LYS:HG2	1.91	0.53
1:P:354:THR:O	2:P:616:P8E:O4	2.28	0.53
1:R:214:LEU:HD12	1:R:330:LEU:HD13	1.90	0.53
1:C:61:LEU:HD22	1:C:521:ILE:HG23	1.91	0.52
1:I:116:ILE:HD12	1:I:480:VAL:HG21	1.90	0.52
1:J:160:THR:OG1	1:M:288:GLN:NE2	2.41	0.52
1:O:150:GLY:HA3	1:O:155:GLN:HB2	1.90	0.52
1:P:214:LEU:HD12	1:P:330:LEU:HD13	1.89	0.52
1:Q:189:THR:HG23	1:Q:200:LYS:HG2	1.91	0.52
1:R:169:ILE:HG13	1:R:170:GLY:H	1.73	0.52
1:T:363:VAL:HG11	1:T:380:MET:HE2	1.90	0.52
2:I:601:P8E:O6	2:I:601:P8E:O8	2.25	0.52
2:N:614:P8E:O6	2:N:614:P8E:O8	2.24	0.52
1:U:303:ASP:OD1	1:U:303:ASP:N	2.34	0.52
2:G:617:P8E:O1A	2:G:617:P8E:O8	2.26	0.52
1:H:124:ASP:OD2	1:H:166:SER:OG	2.27	0.52
1:L:99:ALA:HB2	1:L:112:LEU:HG	1.91	0.52
1:M:148:GLN:NE2	1:M:150:GLY:O	2.42	0.52
2:T:612:P8E:O1B	2:T:612:P8E:N5	2.42	0.52
2:U:601:P8E:O8	2:U:601:P8E:O6	2.23	0.52
1:B:113:GLN:NE2	1:B:480:VAL:H	2.07	0.52
1:G:336:ASP:OD1	1:G:338:ARG:NE	2.42	0.52
2:G:603:P8E:O6	2:G:603:P8E:O8	2.27	0.52
1:H:79:ASP:OD1	1:H:504:ARG:NE	2.29	0.52
2:L:603:P8E:O6	2:L:603:P8E:O8	2.27	0.52
1:D:250:SER:HB2	1:D:312:ASP:HB3	1.91	0.52
1:U:329:ARG:HD2	1:U:384:SER:O	2.08	0.52
1:U:336:ASP:OD2	1:U:338:ARG:NH1	2.43	0.52
1:C:281:VAL:O	1:C:285:THR:HG23	2.09	0.52
1:E:169:ILE:HG13	1:E:170:GLY:H	1.75	0.52
1:F:167:SER:HB3	1:F:366:ARG:HD2	1.90	0.52
2:K:603:P8E:O8	2:K:603:P8E:O6	2.25	0.52
1:P:250:SER:HB3	1:P:312:ASP:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:514:VAL:O	1:R:517:THR:OG1	2.27	0.52
1:D:245:LYS:HG3	1:D:425:LEU:HD11	1.91	0.52
1:F:329:ARG:HD2	1:F:384:SER:O	2.09	0.52
1:Q:241:VAL:HG23	1:Q:242:TYR:HD2	1.74	0.52
1:S:431:GLN:NE2	2:S:610:P8E:O1B	2.42	0.52
1:T:109:ARG:HB3	1:T:481:THR:HA	1.91	0.52
1:U:252:ASP:OD1	1:U:252:ASP:N	2.42	0.52
2:A:606:P8E:O8	2:A:606:P8E:O1B	2.28	0.52
1:L:79:ASP:OD1	1:L:504:ARG:NE	2.26	0.52
2:O:601:P8E:O6	2:O:601:P8E:O8	2.25	0.52
2:U:612:P8E:O1B	2:U:612:P8E:N5	2.42	0.52
1:D:455:SER:O	1:D:458:SER:OG	2.27	0.52
1:E:376:ASN:O	1:E:380:MET:HG2	2.10	0.52
2:L:616:P8E:O8	2:L:616:P8E:N5	2.43	0.52
1:O:400:ILE:HA	1:O:403:PHE:HB3	1.91	0.52
2:P:601:P8E:O8	2:P:601:P8E:O6	2.24	0.52
2:T:603:P8E:O6	2:T:603:P8E:O8	2.28	0.52
1:A:449:SER:O	1:A:452:SER:OG	2.28	0.52
2:C:613:P8E:O6	2:C:613:P8E:O8	2.26	0.52
1:D:363:VAL:HG21	1:D:380:MET:HE1	1.92	0.52
2:K:611:P8E:O8	2:K:611:P8E:O6	2.27	0.52
1:L:169:ILE:HG13	1:L:170:GLY:H	1.75	0.52
1:M:235:ASP:OD1	1:M:237:LYS:NZ	2.43	0.52
1:N:242:TYR:CE2	1:N:318:GLY:HA2	2.45	0.52
2:C:617:P8E:O1A	2:C:617:P8E:O8	2.26	0.51
1:T:99:ALA:HB2	1:T:112:LEU:HG	1.91	0.51
2:H:612:P8E:N5	2:H:612:P8E:O1B	2.43	0.51
1:P:169:ILE:HG13	1:P:170:GLY:H	1.76	0.51
1:Q:281:VAL:O	1:Q:285:THR:HG23	2.10	0.51
1:Q:400:ILE:HG22	1:Q:404:MET:HE2	1.92	0.51
1:R:99:ALA:HB2	1:R:112:LEU:HG	1.92	0.51
1:V:449:SER:O	1:V:452:SER:OG	2.28	0.51
1:B:106:LEU:O	1:B:110:THR:OG1	2.27	0.51
1:D:150:GLY:HA3	1:D:155:GLN:HB2	1.92	0.51
1:L:170:GLY:O	1:L:364:SER:HA	2.10	0.51
2:O:606:P8E:O8	2:O:606:P8E:O6	2.26	0.51
2:P:610:P8E:O6	2:P:610:P8E:O8	2.27	0.51
2:Q:612:P8E:O8	2:Q:612:P8E:N5	2.43	0.51
2:Q:617:P8E:O1A	2:Q:617:P8E:O8	2.28	0.51
2:R:603:P8E:O8	2:R:603:P8E:O6	2.28	0.51
2:A:615:P8E:O6	2:A:615:P8E:O8	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:603:P8E:O6	2:C:603:P8E:O8	2.27	0.51
2:E:611:P8E:O6	2:E:611:P8E:O8	2.28	0.51
2:G:606:P8E:O6	2:G:606:P8E:O8	2.26	0.51
1:M:495:THR:HG22	1:M:499:ASN:HD21	1.75	0.51
1:A:281:VAL:O	1:A:285:THR:HG23	2.11	0.51
2:C:612:P8E:O1B	2:C:612:P8E:N5	2.44	0.51
1:J:175:GLU:HG2	1:J:360:GLN:HB3	1.91	0.51
1:M:243:ALA:HB1	1:M:295:GLY:C	2.36	0.51
1:N:315:VAL:HG21	1:N:411:PHE:CZ	2.46	0.51
1:P:170:GLY:O	1:P:364:SER:HA	2.10	0.51
2:Q:611:P8E:O6	2:Q:611:P8E:O8	2.29	0.51
1:S:243:ALA:HB1	1:S:295:GLY:C	2.36	0.51
1:U:243:ALA:HB1	1:U:295:GLY:C	2.36	0.51
1:A:61:LEU:HD22	1:A:521:ILE:HG23	1.93	0.51
2:J:601:P8E:O6	2:J:601:P8E:O8	2.28	0.51
2:S:601:P8E:O6	2:S:601:P8E:O8	2.26	0.51
1:U:113:GLN:HE21	1:U:480:VAL:H	1.58	0.51
1:U:237:LYS:O	1:U:326:ASN:ND2	2.44	0.51
1:U:241:VAL:HG23	1:U:242:TYR:HD2	1.76	0.51
1:C:64:ALA:HB1	1:C:149:ILE:HA	1.93	0.51
1:G:113:GLN:NE2	1:G:480:VAL:H	2.08	0.51
1:G:243:ALA:HB1	1:G:295:GLY:C	2.36	0.51
1:I:281:VAL:O	1:I:285:THR:HG23	2.10	0.51
1:N:188:LEU:HD22	1:N:342:ILE:HD11	1.91	0.51
1:P:382:PHE:CE2	1:P:484:LYS:HB2	2.46	0.51
1:B:165:GLN:HE22	1:K:223:LYS:NZ	2.08	0.51
1:B:281:VAL:O	1:B:285:THR:HG23	2.11	0.51
2:E:612:P8E:N5	2:E:612:P8E:O1B	2.43	0.51
2:F:617:P8E:O8	2:F:617:P8E:O1A	2.29	0.51
2:H:606:P8E:O8	2:H:606:P8E:O1B	2.28	0.51
1:Q:422:GLY:O	1:Q:424:ASN:ND2	2.44	0.51
2:S:614:P8E:O6	2:S:614:P8E:O8	2.27	0.51
1:D:431:GLN:NE2	2:D:610:P8E:O1B	2.44	0.51
1:E:177:GLY:HA2	1:E:358:ILE:HG22	1.93	0.51
1:J:188:LEU:HD21	1:J:350:ILE:HD13	1.92	0.51
1:O:113:GLN:HE21	1:O:480:VAL:H	1.57	0.51
1:O:170:GLY:O	1:O:364:SER:HA	2.11	0.51
2:P:603:P8E:O8	2:P:603:P8E:O6	2.28	0.51
2:R:606:P8E:O8	2:R:606:P8E:O6	2.26	0.51
1:H:124:ASP:OD1	1:H:128:ASN:ND2	2.43	0.51
2:I:612:P8E:N5	2:I:612:P8E:O1B	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:252:ASP:OD1	1:L:252:ASP:N	2.43	0.51
2:P:614:P8E:O6	2:P:614:P8E:O8	2.28	0.51
2:Q:606:P8E:O6	2:Q:606:P8E:O8	2.27	0.51
1:S:241:VAL:HG23	1:S:242:TYR:HD2	1.76	0.51
1:U:169:ILE:HG13	1:U:170:GLY:H	1.75	0.51
1:B:255:ILE:HD11	1:B:287:VAL:HG21	1.92	0.50
1:G:188:LEU:HB2	1:G:201:PHE:HD1	1.76	0.50
1:J:354:THR:O	2:J:616:P8E:O4	2.28	0.50
1:B:243:ALA:HB1	1:B:295:GLY:C	2.37	0.50
1:B:365:LEU:O	1:B:368:SER:OG	2.27	0.50
1:D:243:ALA:HB1	1:D:295:GLY:C	2.37	0.50
1:E:170:GLY:O	1:E:364:SER:HA	2.11	0.50
1:I:218:ALA:O	1:I:222:ASN:ND2	2.38	0.50
1:K:104:GLN:HG2	1:V:50:ILE:HD11	1.93	0.50
1:N:238:THR:OG1	1:N:326:ASN:ND2	2.31	0.50
1:R:241:VAL:HG23	1:R:242:TYR:HD2	1.75	0.50
1:S:326:ASN:OD1	1:S:327:TYR:N	2.44	0.50
1:V:245:LYS:HG3	1:V:425:LEU:HD11	1.94	0.50
1:A:169:ILE:HG13	1:A:170:GLY:H	1.76	0.50
1:Q:189:THR:HB	1:Q:343:SER:O	2.11	0.50
1:R:148:GLN:NE2	1:R:150:GLY:O	2.44	0.50
1:H:139:SER:O	1:H:165:GLN:NE2	2.45	0.50
1:R:113:GLN:NE2	1:R:480:VAL:H	2.09	0.50
1:T:146:GLU:OE2	1:T:158:LYS:HG2	2.11	0.50
1:T:303:ASP:OD1	1:T:303:ASP:N	2.32	0.50
1:U:397:VAL:HG11	1:U:403:PHE:N	2.27	0.50
1:E:189:THR:HG23	1:E:200:LYS:HG2	1.94	0.50
1:E:502:GLN:O	1:E:502:GLN:NE2	2.43	0.50
2:F:606:P8E:O8	2:F:606:P8E:O6	2.30	0.50
1:H:252:ASP:OD1	1:H:252:ASP:N	2.42	0.50
1:J:243:ALA:HB1	1:J:295:GLY:C	2.37	0.50
1:J:245:LYS:HG3	1:J:425:LEU:HD11	1.94	0.50
2:K:601:P8E:O8	2:K:601:P8E:O6	2.29	0.50
1:R:326:ASN:OD1	1:R:327:TYR:N	2.44	0.50
1:R:336:ASP:OD1	1:R:338:ARG:NE	2.43	0.50
1:C:243:ALA:HB1	1:C:295:GLY:C	2.37	0.50
2:D:612:P8E:O8	2:D:612:P8E:N5	2.45	0.50
2:K:612:P8E:N5	2:K:612:P8E:O1B	2.44	0.50
1:R:397:VAL:HG11	1:R:403:PHE:N	2.27	0.50
1:U:354:THR:O	2:U:616:P8E:O4	2.29	0.50
2:D:606:P8E:O6	2:D:606:P8E:O8	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:113:GLN:NE2	1:I:480:VAL:H	2.09	0.50
1:K:363:VAL:HG21	1:K:380:MET:HE2	1.94	0.50
1:L:193:TYR:CD1	1:L:199:PHE:HB2	2.47	0.50
1:N:455:SER:O	1:N:458:SER:OG	2.30	0.50
1:O:329:ARG:HD2	1:O:384:SER:O	2.11	0.50
1:S:64:ALA:HB1	1:S:149:ILE:HA	1.93	0.50
2:S:606:P8E:O8	2:S:606:P8E:O1B	2.30	0.50
1:F:281:VAL:O	1:F:285:THR:HG23	2.12	0.50
2:K:615:P8E:O6	2:K:615:P8E:O8	2.28	0.50
1:Q:244:ILE:HD13	1:Q:269:ASP:HB2	1.93	0.50
1:R:354:THR:O	2:R:616:P8E:O4	2.29	0.50
1:E:169:ILE:HG13	1:E:170:GLY:N	2.27	0.50
2:G:612:P8E:N5	2:G:612:P8E:O1B	2.45	0.50
2:L:615:P8E:O8	2:L:615:P8E:O6	2.30	0.50
1:O:397:VAL:HG11	1:O:403:PHE:N	2.27	0.50
1:S:268:GLY:O	1:S:291:LYS:NZ	2.32	0.50
2:G:611:P8E:O8	2:G:611:P8E:O6	2.29	0.49
1:M:125:ASN:O	1:M:129:THR:OG1	2.22	0.49
2:R:610:P8E:O8	2:R:610:P8E:O6	2.28	0.49
2:A:612:P8E:N5	2:A:612:P8E:O1B	2.46	0.49
1:D:7:THR:HG21	1:S:533:SER:HB2	1.94	0.49
1:H:135:LYS:NZ	1:O:102:ASP:O	2.45	0.49
2:H:608:P8E:O8	2:H:608:P8E:O6	2.29	0.49
1:I:488:ALA:O	1:I:492:ILE:HG13	2.12	0.49
1:O:116:ILE:HD12	1:O:480:VAL:HG21	1.94	0.49
1:P:243:ALA:HB1	1:P:295:GLY:C	2.37	0.49
1:Q:169:ILE:HG13	1:Q:170:GLY:H	1.77	0.49
1:V:99:ALA:O	1:V:109:ARG:NH1	2.45	0.49
1:B:61:LEU:HD22	1:B:521:ILE:HG23	1.94	0.49
2:B:616:P8E:O6	2:B:616:P8E:O8	2.30	0.49
2:C:612:P8E:O8	2:C:612:P8E:O6	2.29	0.49
2:N:606:P8E:O8	2:N:606:P8E:O6	2.29	0.49
1:T:61:LEU:HD22	1:T:521:ILE:HG23	1.93	0.49
1:F:237:LYS:O	1:F:326:ASN:ND2	2.43	0.49
2:H:601:P8E:O8	2:H:601:P8E:O6	2.28	0.49
1:J:281:VAL:O	1:J:285:THR:HG23	2.13	0.49
1:V:142:PHE:HA	1:V:145:GLN:HE21	1.77	0.49
1:A:290:SER:OG	1:A:291:LYS:N	2.44	0.49
1:H:170:GLY:O	1:H:364:SER:HA	2.12	0.49
1:H:449:SER:O	1:H:452:SER:OG	2.30	0.49
2:J:606:P8E:O8	2:J:606:P8E:O6	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:188:LEU:HD22	1:L:342:ILE:HD11	1.94	0.49
1:L:238:THR:HG1	1:L:326:ASN:HD22	1.54	0.49
1:N:255:ILE:HD11	1:N:287:VAL:HG11	1.95	0.49
1:P:175:GLU:HG2	1:P:360:GLN:HB3	1.94	0.49
1:V:169:ILE:HG13	1:V:170:GLY:H	1.77	0.49
1:J:138:LEU:HB3	1:J:164:THR:HG21	1.93	0.49
1:M:514:VAL:O	1:M:517:THR:OG1	2.30	0.49
1:S:169:ILE:HG13	1:S:170:GLY:H	1.76	0.49
1:S:237:LYS:O	1:S:326:ASN:ND2	2.44	0.49
1:C:241:VAL:HG23	1:C:242:TYR:HD2	1.77	0.49
1:F:169:ILE:HG13	1:F:170:GLY:N	2.27	0.49
1:M:143:THR:O	1:M:145:GLN:NE2	2.46	0.49
1:N:241:VAL:HG23	1:N:242:TYR:HD2	1.78	0.49
1:P:150:GLY:HA3	1:P:155:GLN:HB2	1.93	0.49
1:P:252:ASP:OD1	1:P:252:ASP:N	2.41	0.49
1:S:95:LYS:HE3	1:S:115:ASP:OD2	2.13	0.49
1:D:64:ALA:HB1	1:D:149:ILE:HA	1.94	0.49
1:G:363:VAL:HG21	1:G:380:MET:HE1	1.94	0.49
1:H:113:GLN:NE2	1:H:480:VAL:H	2.11	0.49
1:R:175:GLU:HG2	1:R:360:GLN:HB3	1.94	0.49
1:A:34:SER:OG	1:A:39:ASN:ND2	2.44	0.49
1:F:285:THR:OG1	1:F:287:VAL:HG22	2.13	0.49
1:H:397:VAL:HG11	1:H:403:PHE:N	2.28	0.49
1:I:241:VAL:HG23	1:I:242:TYR:HD2	1.77	0.49
1:K:99:ALA:HB2	1:K:112:LEU:HG	1.93	0.49
1:K:241:VAL:HG23	1:K:242:TYR:HD2	1.78	0.49
1:L:142:PHE:HA	1:L:145:GLN:HE21	1.76	0.49
1:M:113:GLN:NE2	1:M:480:VAL:H	2.10	0.49
1:O:149:ILE:HD11	1:O:157:VAL:HG13	1.95	0.49
1:S:242:TYR:CE2	1:S:318:GLY:HA2	2.47	0.49
2:T:601:P8E:O6	2:T:601:P8E:O8	2.27	0.49
1:D:124:ASP:OD1	1:D:128:ASN:ND2	2.45	0.49
1:D:243:ALA:HA	1:D:296:LYS:HG2	1.94	0.49
1:F:125:ASN:O	1:F:129:THR:OG1	2.23	0.49
1:H:153:SER:OG	1:H:154:ASN:N	2.45	0.49
1:I:326:ASN:OD1	1:I:327:TYR:N	2.46	0.49
1:L:218:ALA:O	1:L:222:ASN:ND2	2.46	0.49
2:L:612:P8E:N5	2:L:612:P8E:O1B	2.45	0.49
2:O:616:P8E:O6	2:O:616:P8E:O8	2.30	0.49
1:T:113:GLN:NE2	1:T:480:VAL:H	2.10	0.49
1:V:404:MET:HG2	1:V:411:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:541:ALA:HB2	1:P:3:PHE:CD2	2.48	0.48
1:I:303:ASP:OD1	1:I:303:ASP:N	2.36	0.48
1:J:79:ASP:OD1	1:J:504:ARG:NE	2.26	0.48
1:M:180:SER:OG	1:M:349:ALA:O	2.21	0.48
1:P:242:TYR:CE2	1:P:318:GLY:HA2	2.49	0.48
1:S:329:ARG:HD2	1:S:384:SER:O	2.13	0.48
1:T:139:SER:O	1:T:165:GLN:NE2	2.45	0.48
2:T:612:P8E:N5	2:T:612:P8E:O8	2.45	0.48
1:U:188:LEU:HD21	1:U:350:ILE:HD13	1.95	0.48
1:E:243:ALA:HA	1:E:296:LYS:HG2	1.93	0.48
2:G:614:P8E:O6	2:G:614:P8E:O8	2.31	0.48
1:H:243:ALA:HB1	1:H:295:GLY:C	2.38	0.48
1:I:214:LEU:HD12	1:I:330:LEU:HD13	1.95	0.48
1:R:281:VAL:O	1:R:285:THR:HG23	2.13	0.48
1:S:169:ILE:HG13	1:S:170:GLY:N	2.27	0.48
1:A:106:LEU:O	1:A:110:THR:OG1	2.29	0.48
1:D:241:VAL:HG23	1:D:242:TYR:HD2	1.78	0.48
1:E:436:ILE:HG12	1:E:445:THR:HG21	1.95	0.48
1:F:366:ARG:NH2	1:G:219:GLU:OE2	2.45	0.48
2:J:612:P8E:N5	2:J:612:P8E:O1B	2.45	0.48
1:K:243:ALA:HB1	1:K:295:GLY:C	2.38	0.48
1:M:169:ILE:HG13	1:M:170:GLY:H	1.76	0.48
1:O:188:LEU:HD22	1:O:342:ILE:HD11	1.95	0.48
2:Q:601:P8E:O6	2:Q:601:P8E:O8	2.29	0.48
2:S:617:P8E:O8	2:S:617:P8E:O6	2.30	0.48
1:C:561:MET:HE2	1:H:574:LEU:HD11	1.95	0.48
1:D:244:ILE:HD13	1:D:269:ASP:HB2	1.95	0.48
1:F:135:LYS:NZ	1:Q:102:ASP:OD2	2.46	0.48
1:J:170:GLY:O	1:J:364:SER:HA	2.13	0.48
1:L:397:VAL:HG11	1:L:403:PHE:N	2.28	0.48
2:Q:608:P8E:O6	2:Q:608:P8E:O8	2.32	0.48
1:R:150:GLY:HA3	1:R:155:GLN:HB2	1.95	0.48
1:T:237:LYS:O	1:T:326:ASN:ND2	2.46	0.48
1:V:170:GLY:O	1:V:364:SER:HA	2.13	0.48
1:C:107:LYS:HZ2	1:H:498:THR:HG21	1.78	0.48
2:E:610:P8E:O8	2:E:610:P8E:O6	2.31	0.48
1:F:243:ALA:HB1	1:F:295:GLY:C	2.39	0.48
1:G:252:ASP:OD1	1:G:252:ASP:N	2.43	0.48
1:P:480:VAL:HG23	1:P:486:ALA:HA	1.94	0.48
1:R:495:THR:HG22	1:R:499:ASN:HD21	1.78	0.48
1:U:170:GLY:O	1:U:364:SER:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LYS:HB3	1:B:112:LEU:HD12	1.96	0.48
1:G:169:ILE:HG13	1:G:170:GLY:H	1.78	0.48
2:I:610:P8E:O6	2:I:610:P8E:O8	2.31	0.48
1:J:205:VAL:HB	1:J:212:THR:HG22	1.96	0.48
1:J:250:SER:OG	1:J:252:ASP:OD1	2.22	0.48
2:K:617:P8E:O6	2:K:617:P8E:O8	2.31	0.48
1:N:482:THR:HG23	1:N:485:GLY:H	1.77	0.48
1:R:404:MET:HG2	1:R:411:PHE:CG	2.49	0.48
1:B:64:ALA:HB1	1:B:149:ILE:HA	1.95	0.48
1:D:397:VAL:HG13	1:D:402:ALA:HB3	1.95	0.48
1:E:106:LEU:O	1:E:110:THR:OG1	2.25	0.48
1:G:235:ASP:OD1	1:G:237:LYS:NZ	2.43	0.48
2:K:615:P8E:O8	2:K:615:P8E:O1A	2.32	0.48
1:P:124:ASP:OD1	1:P:128:ASN:ND2	2.46	0.48
2:Q:612:P8E:N5	2:Q:612:P8E:O1B	2.46	0.48
1:A:541:ALA:HB1	1:L:561:MET:HE1	1.94	0.48
1:C:329:ARG:HD2	1:C:384:SER:O	2.13	0.48
1:G:109:ARG:HB3	1:G:481:THR:HA	1.94	0.48
1:H:279:ASN:HD21	1:H:288:GLN:NE2	2.10	0.48
2:J:609:P8E:O6	2:J:609:P8E:O8	2.32	0.48
1:K:95:LYS:HE3	1:K:115:ASP:OD2	2.13	0.48
1:N:237:LYS:O	1:N:326:ASN:ND2	2.46	0.48
2:N:610:P8E:O6	2:N:610:P8E:O8	2.28	0.48
1:O:164:THR:O	1:O:164:THR:OG1	2.31	0.48
1:Q:393:PHE:HB2	1:Q:435:ILE:HA	1.95	0.48
1:R:243:ALA:HB1	1:R:295:GLY:C	2.39	0.48
1:U:400:ILE:HA	1:U:403:PHE:HB3	1.96	0.48
1:A:109:ARG:HB3	1:A:481:THR:HA	1.96	0.48
1:B:99:ALA:HB2	1:B:112:LEU:HG	1.95	0.48
1:I:250:SER:OG	1:I:252:ASP:OD1	2.26	0.48
1:L:243:ALA:HB1	1:L:295:GLY:C	2.39	0.48
2:M:601:P8E:O8	2:M:601:P8E:O6	2.28	0.48
1:Q:205:VAL:HB	1:Q:212:THR:HG22	1.96	0.48
1:B:116:ILE:HD12	1:B:480:VAL:HG21	1.96	0.48
1:D:169:ILE:HG13	1:D:170:GLY:H	1.78	0.48
1:D:189:THR:HB	1:D:343:SER:O	2.13	0.48
1:O:189:THR:HB	1:O:343:SER:O	2.14	0.48
1:Q:153:SER:OG	1:Q:154:ASN:N	2.45	0.48
2:S:606:P8E:O8	2:S:606:P8E:O6	2.32	0.48
1:T:138:LEU:HB3	1:T:164:THR:HG21	1.96	0.48
1:U:150:GLY:HA3	1:U:155:GLN:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:THR:OG1	1:B:286:GLY:N	2.47	0.47
1:E:243:ALA:HB1	1:E:295:GLY:C	2.39	0.47
1:H:142:PHE:HA	1:H:145:GLN:HE21	1.79	0.47
1:J:238:THR:HG1	1:J:326:ASN:HD22	1.57	0.47
1:Q:326:ASN:OD1	1:Q:327:TYR:N	2.47	0.47
2:R:612:P8E:O1B	2:R:612:P8E:N5	2.47	0.47
1:T:250:SER:HB3	1:T:312:ASP:HB3	1.95	0.47
1:K:248:THR:HG22	1:K:264:GLU:HA	1.96	0.47
2:L:610:P8E:O6	2:L:610:P8E:O8	2.30	0.47
1:M:250:SER:HB3	1:M:312:ASP:HB3	1.96	0.47
1:R:235:ASP:OD2	1:R:237:LYS:NZ	2.48	0.47
1:R:488:ALA:O	1:R:492:ILE:HG13	2.13	0.47
1:S:173:ARG:HB2	1:S:337:GLY:HA2	1.95	0.47
1:T:326:ASN:OD1	1:T:327:TYR:N	2.47	0.47
1:V:238:THR:HG1	1:V:326:ASN:HD22	1.58	0.47
1:A:113:GLN:NE2	1:A:480:VAL:H	2.12	0.47
1:A:116:ILE:HD12	1:A:480:VAL:HG21	1.95	0.47
1:D:79:ASP:OD1	1:D:504:ARG:NE	2.36	0.47
1:H:64:ALA:HB1	1:H:149:ILE:HA	1.95	0.47
1:H:557:GLY:O	1:H:561:MET:HG3	2.14	0.47
1:M:285:THR:O	1:M:305:ARG:NH2	2.47	0.47
1:M:400:ILE:HG22	1:M:404:MET:HE2	1.96	0.47
1:N:243:ALA:HB1	1:N:295:GLY:C	2.39	0.47
1:O:242:TYR:CE2	1:O:318:GLY:HA2	2.48	0.47
1:Q:95:LYS:HB3	1:Q:112:LEU:HD12	1.95	0.47
1:S:125:ASN:O	1:S:129:THR:OG1	2.20	0.47
1:S:243:ALA:HA	1:S:296:LYS:HG2	1.96	0.47
1:U:249:THR:HG22	1:U:313:ILE:O	2.15	0.47
1:A:95:LYS:HB3	1:A:112:LEU:HD12	1.96	0.47
2:C:612:P8E:N5	2:C:612:P8E:O8	2.48	0.47
1:D:113:GLN:HE21	1:D:480:VAL:H	1.62	0.47
1:G:238:THR:OG1	1:G:326:ASN:ND2	2.36	0.47
1:I:235:ASP:OD1	1:I:237:LYS:NZ	2.47	0.47
1:K:124:ASP:OD1	1:K:128:ASN:ND2	2.48	0.47
1:K:138:LEU:HB3	1:K:164:THR:HG21	1.96	0.47
1:N:189:THR:HB	1:N:343:SER:O	2.14	0.47
1:R:482:THR:HG23	1:R:485:GLY:H	1.79	0.47
2:R:606:P8E:O8	2:R:606:P8E:O1B	2.33	0.47
1:S:61:LEU:HD22	1:S:521:ILE:HG23	1.95	0.47
1:B:243:ALA:HA	1:B:296:LYS:HG2	1.97	0.47
2:G:616:P8E:O8	2:G:616:P8E:N5	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:603:P8E:O6	2:H:603:P8E:O8	2.33	0.47
1:I:245:LYS:HG3	1:I:425:LEU:HD11	1.97	0.47
2:I:608:P8E:O6	2:I:608:P8E:O8	2.30	0.47
1:M:242:TYR:CE2	1:M:318:GLY:HA2	2.49	0.47
2:N:612:P8E:N5	2:N:612:P8E:O1B	2.48	0.47
1:O:143:THR:N	1:O:145:GLN:HE21	2.13	0.47
1:O:245:LYS:HG3	1:O:425:LEU:HD11	1.96	0.47
1:R:242:TYR:CE2	1:R:318:GLY:HA2	2.48	0.47
2:R:616:P8E:O8	2:R:616:P8E:N5	2.47	0.47
1:U:169:ILE:HG13	1:U:170:GLY:N	2.30	0.47
1:U:285:THR:OG1	1:U:287:VAL:HG22	2.15	0.47
1:D:422:GLY:O	1:D:424:ASN:ND2	2.48	0.47
2:D:606:P8E:O8	2:D:606:P8E:O1B	2.32	0.47
1:H:188:LEU:HB2	1:H:201:PHE:HD1	1.79	0.47
1:L:169:ILE:HG13	1:L:170:GLY:N	2.30	0.47
1:L:495:THR:O	1:L:499:ASN:ND2	2.41	0.47
1:M:431:GLN:NE2	2:M:610:P8E:O1B	2.44	0.47
2:U:610:P8E:O6	2:U:610:P8E:O8	2.29	0.47
1:A:78:ALA:HB1	1:A:138:LEU:HD21	1.97	0.47
1:A:306:GLY:HA3	1:A:327:TYR:HD1	1.80	0.47
1:A:363:VAL:HG21	1:A:380:MET:HE2	1.95	0.47
1:C:102:ASP:OD1	1:T:135:LYS:NZ	2.44	0.47
1:D:109:ARG:HB3	1:D:481:THR:HA	1.97	0.47
1:D:153:SER:OG	1:D:154:ASN:N	2.46	0.47
1:D:386:LYS:HE3	1:D:466:LEU:HD11	1.97	0.47
1:E:242:TYR:CE2	1:E:318:GLY:HA2	2.50	0.47
1:F:148:GLN:NE2	1:F:150:GLY:O	2.47	0.47
1:F:232:ALA:HB2	1:F:332:LEU:HD23	1.97	0.47
1:I:170:GLY:O	1:I:364:SER:HA	2.14	0.47
2:I:616:P8E:O6	2:I:616:P8E:O8	2.32	0.47
1:K:336:ASP:OD2	1:K:338:ARG:NE	2.48	0.47
1:O:252:ASP:OD1	1:O:252:ASP:N	2.42	0.47
1:O:315:VAL:HG21	1:O:411:PHE:CZ	2.50	0.47
2:P:612:P8E:N5	2:P:612:P8E:O1B	2.48	0.47
2:P:615:P8E:O6	2:P:615:P8E:O8	2.32	0.47
1:R:418:SER:O	1:R:421:SER:OG	2.23	0.47
1:S:139:SER:O	1:S:165:GLN:NE2	2.48	0.47
1:T:495:THR:HG22	1:T:499:ASN:HD21	1.80	0.47
1:U:285:THR:OG1	1:U:286:GLY:N	2.47	0.47
1:J:436:ILE:HG12	1:J:445:THR:HG21	1.96	0.47
1:L:329:ARG:HD2	1:L:384:SER:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:279:ASN:ND2	1:Q:288:GLN:OE1	2.47	0.47
1:S:309:ILE:HD11	1:S:324:LYS:HG2	1.97	0.47
2:C:606:P8E:O8	2:C:606:P8E:O1B	2.33	0.47
1:E:315:VAL:HG21	1:E:411:PHE:CZ	2.50	0.47
1:G:170:GLY:O	1:G:364:SER:HA	2.14	0.47
2:G:606:P8E:O8	2:G:606:P8E:O1B	2.33	0.47
1:K:169:ILE:HG13	1:K:170:GLY:N	2.30	0.47
1:M:202:ASP:OD1	1:M:202:ASP:N	2.48	0.47
1:M:214:LEU:HD12	1:M:330:LEU:HD13	1.96	0.47
1:M:243:ALA:HA	1:M:296:LYS:HG2	1.96	0.47
1:P:113:GLN:HE21	1:P:480:VAL:H	1.62	0.47
1:Q:106:LEU:O	1:Q:110:THR:OG1	2.31	0.47
1:S:500:LEU:HD23	1:S:500:LEU:HA	1.64	0.47
2:T:617:P8E:O6	2:T:617:P8E:O8	2.33	0.47
1:C:205:VAL:HB	1:C:212:THR:HG22	1.96	0.47
2:F:616:P8E:O8	2:F:616:P8E:O6	2.31	0.47
1:H:243:ALA:HA	1:H:296:LYS:HG2	1.97	0.47
1:I:449:SER:O	1:I:452:SER:OG	2.28	0.47
1:L:382:PHE:HE1	1:L:484:LYS:HB2	1.78	0.47
1:Q:514:VAL:O	1:Q:517:THR:OG1	2.29	0.47
1:R:78:ALA:HB1	1:R:138:LEU:HD21	1.97	0.47
2:R:612:P8E:N5	2:R:612:P8E:O8	2.48	0.47
2:S:612:P8E:N5	2:S:612:P8E:O1B	2.47	0.47
1:T:148:GLN:NE2	1:T:150:GLY:O	2.47	0.47
1:V:164:THR:O	1:V:164:THR:OG1	2.33	0.47
1:A:170:GLY:O	1:A:364:SER:HA	2.16	0.46
1:B:488:ALA:O	1:B:492:ILE:HG13	2.15	0.46
1:G:189:THR:HB	1:G:343:SER:O	2.15	0.46
1:I:205:VAL:HB	1:I:212:THR:HG22	1.97	0.46
1:L:326:ASN:OD1	1:L:327:TYR:N	2.47	0.46
1:M:105:SER:OG	1:M:106:LEU:N	2.48	0.46
1:M:189:THR:HB	1:M:343:SER:O	2.15	0.46
1:O:384:SER:O	1:O:386:LYS:N	2.46	0.46
1:Q:125:ASN:O	1:Q:129:THR:OG1	2.28	0.46
1:R:177:GLY:HA2	1:R:358:ILE:HG22	1.97	0.46
1:R:250:SER:OG	1:R:252:ASP:OD1	2.23	0.46
1:S:113:GLN:NE2	1:S:480:VAL:H	2.13	0.46
1:U:153:SER:HG	1:U:154:ASN:HD22	1.57	0.46
1:A:514:VAL:O	1:A:517:THR:OG1	2.31	0.46
1:D:219:GLU:OE2	1:P:366:ARG:NH2	2.48	0.46
1:G:488:ALA:O	1:G:492:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:390:LYS:NZ	1:M:430:SER:O	2.48	0.46
1:O:61:LEU:HD22	1:O:521:ILE:HG23	1.98	0.46
1:O:125:ASN:O	1:O:129:THR:OG1	2.33	0.46
1:E:514:VAL:O	1:E:517:THR:OG1	2.31	0.46
1:F:394:THR:O	2:F:603:P8E:O8	2.34	0.46
1:H:320:LEU:N	1:H:323:GLN:OE1	2.45	0.46
1:K:104:GLN:HB3	1:K:108:THR:OG1	2.16	0.46
1:N:353:GLY:N	1:N:356:ASP:OD2	2.45	0.46
1:P:242:TYR:OH	1:P:315:VAL:HG22	2.16	0.46
1:T:138:LEU:HB3	1:T:164:THR:CG2	2.44	0.46
1:T:397:VAL:HG11	1:T:403:PHE:N	2.30	0.46
1:V:177:GLY:HA2	1:V:358:ILE:HG22	1.96	0.46
1:V:241:VAL:HG23	1:V:242:TYR:CD2	2.50	0.46
1:A:235:ASP:OD1	1:A:237:LYS:NZ	2.44	0.46
1:C:252:ASP:OD1	1:C:252:ASP:N	2.48	0.46
1:D:284:THR:HG23	1:P:478:ALA:HB2	1.98	0.46
2:F:612:P8E:N5	2:F:612:P8E:O8	2.48	0.46
1:H:180:SER:OG	1:H:349:ALA:O	2.26	0.46
1:K:252:ASP:OD1	1:K:252:ASP:N	2.48	0.46
1:O:218:ALA:O	1:O:222:ASN:ND2	2.47	0.46
1:P:164:THR:O	1:P:164:THR:OG1	2.30	0.46
1:V:139:SER:O	1:V:165:GLN:NE2	2.46	0.46
1:D:125:ASN:O	1:D:129:THR:OG1	2.27	0.46
1:J:146:GLU:HB2	1:M:483:LEU:HD21	1.97	0.46
1:J:177:GLY:HA2	1:J:358:ILE:HG22	1.98	0.46
1:J:488:ALA:O	1:J:492:ILE:HG13	2.15	0.46
1:K:480:VAL:HG23	1:K:486:ALA:HA	1.98	0.46
1:R:285:THR:OG1	1:R:286:GLY:N	2.49	0.46
1:V:500:LEU:HD23	1:V:500:LEU:HA	1.77	0.46
1:E:41:ALA:HB2	1:E:48:MET:HE2	1.98	0.46
1:E:397:VAL:HG11	1:E:403:PHE:N	2.30	0.46
1:G:253:PHE:HA	1:G:311:GLY:HA3	1.97	0.46
1:K:268:GLY:O	1:K:291:LYS:NZ	2.31	0.46
1:R:495:THR:O	1:R:499:ASN:ND2	2.49	0.46
1:T:488:ALA:O	1:T:492:ILE:HG13	2.15	0.46
1:V:95:LYS:HB3	1:V:112:LEU:HD12	1.98	0.46
1:V:95:LYS:HE3	1:V:115:ASP:OD2	2.14	0.46
1:D:106:LEU:O	1:D:110:THR:OG1	2.28	0.46
1:F:99:ALA:O	1:F:109:ARG:NH1	2.49	0.46
2:J:610:P8E:O8	2:J:610:P8E:O6	2.32	0.46
1:K:34:SER:OG	1:K:39:ASN:ND2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:189:THR:HB	1:L:343:SER:O	2.16	0.46
2:Q:606:P8E:O8	2:Q:606:P8E:O1B	2.34	0.46
1:U:539:ASP:OD1	1:U:539:ASP:N	2.45	0.46
1:C:150:GLY:HA3	1:C:155:GLN:HB2	1.98	0.46
1:C:191:LYS:HB3	1:C:191:LYS:HE2	1.84	0.46
1:C:326:ASN:OD1	1:C:327:TYR:N	2.49	0.46
1:C:384:SER:O	1:C:386:LYS:N	2.45	0.46
2:C:616:P8E:O8	2:C:616:P8E:O6	2.34	0.46
2:D:612:P8E:N5	2:D:612:P8E:O1B	2.49	0.46
2:F:612:P8E:O8	2:F:612:P8E:O6	2.32	0.46
2:J:612:P8E:N5	2:J:612:P8E:O8	2.49	0.46
1:N:124:ASP:OD2	1:N:366:ARG:NH2	2.48	0.46
1:O:241:VAL:HG23	1:O:242:TYR:CD2	2.49	0.46
1:R:400:ILE:HG22	1:R:404:MET:HE2	1.97	0.46
1:S:175:GLU:HG2	1:S:360:GLN:HB3	1.97	0.46
2:S:610:P8E:O6	2:S:610:P8E:O8	2.30	0.46
1:T:169:ILE:HG13	1:T:170:GLY:H	1.79	0.46
1:T:400:ILE:HG22	1:T:404:MET:HE2	1.97	0.46
1:B:169:ILE:HG13	1:B:170:GLY:H	1.80	0.46
1:C:449:SER:O	1:C:452:SER:OG	2.34	0.46
2:D:612:P8E:O8	2:D:612:P8E:O6	2.30	0.46
2:D:614:P8E:O6	2:D:614:P8E:O8	2.32	0.46
1:G:144:ASN:H	1:G:160:THR:HG22	1.80	0.46
1:J:242:TYR:CE2	1:J:318:GLY:HA2	2.51	0.46
1:L:242:TYR:CE2	1:L:318:GLY:HA2	2.51	0.46
1:M:143:THR:N	1:M:145:GLN:HE21	2.14	0.46
1:N:50:ILE:HD11	1:S:104:GLN:HG2	1.97	0.46
2:Q:615:P8E:O8	2:Q:615:P8E:O6	2.34	0.46
2:Q:616:P8E:O6	2:Q:616:P8E:O8	2.34	0.46
1:V:113:GLN:NE2	1:V:480:VAL:H	2.14	0.46
1:A:488:ALA:O	1:A:492:ILE:HG13	2.16	0.46
1:C:539:ASP:OD1	1:C:539:ASP:N	2.39	0.46
1:G:483:LEU:HD21	1:P:146:GLU:HB2	1.98	0.46
1:K:170:GLY:O	1:K:364:SER:HA	2.16	0.46
1:Q:480:VAL:HG23	1:Q:486:ALA:HA	1.97	0.46
1:T:243:ALA:HB1	1:T:295:GLY:C	2.41	0.46
1:V:138:LEU:HB3	1:V:164:THR:HG21	1.98	0.46
1:A:138:LEU:HB3	1:A:164:THR:HG21	1.96	0.45
2:A:610:P8E:O6	2:A:610:P8E:O8	2.29	0.45
1:G:72:LEU:HD23	1:G:72:LEU:HA	1.81	0.45
2:I:614:P8E:O6	2:I:614:P8E:O8	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:602:P8E:O6	2:K:602:P8E:O8	2.34	0.45
2:M:616:P8E:O8	2:M:616:P8E:N5	2.49	0.45
1:O:169:ILE:HG13	1:O:170:GLY:H	1.81	0.45
2:O:606:P8E:O8	2:O:606:P8E:O1B	2.33	0.45
1:T:364:SER:HB3	1:T:367:GLU:HG3	1.96	0.45
2:H:614:P8E:O6	2:H:614:P8E:O8	2.34	0.45
1:K:395:GLN:HG2	1:K:397:VAL:HG23	1.98	0.45
1:K:397:VAL:HG11	1:K:403:PHE:N	2.31	0.45
1:V:242:TYR:CZ	1:V:318:GLY:HA2	2.51	0.45
2:B:612:P8E:N5	2:B:612:P8E:O8	2.49	0.45
1:C:188:LEU:HD22	1:C:342:ILE:HD11	1.97	0.45
1:D:157:VAL:HG12	1:D:513:GLN:NE2	2.31	0.45
1:D:553:LEU:HD11	1:P:6:ASN:HB2	1.98	0.45
1:G:393:PHE:HD2	1:G:435:ILE:HG12	1.81	0.45
1:L:177:GLY:HA2	1:L:358:ILE:HG22	1.97	0.45
2:M:612:P8E:N5	2:M:612:P8E:O8	2.49	0.45
1:O:250:SER:HB3	1:O:312:ASP:HB3	1.98	0.45
2:R:615:P8E:O6	2:R:615:P8E:O8	2.34	0.45
1:U:455:SER:O	1:U:458:SER:OG	2.33	0.45
1:B:397:VAL:HG11	1:B:403:PHE:N	2.31	0.45
2:B:603:P8E:O6	2:B:603:P8E:O8	2.34	0.45
1:K:482:THR:HG23	1:K:485:GLY:H	1.81	0.45
1:N:78:ALA:HB1	1:N:138:LEU:HD21	1.98	0.45
1:N:153:SER:OG	1:N:154:ASN:ND2	2.36	0.45
1:P:384:SER:OG	1:P:385:TYR:N	2.50	0.45
1:S:205:VAL:HB	1:S:212:THR:HG22	1.99	0.45
2:T:608:P8E:O8	2:T:608:P8E:O6	2.34	0.45
1:V:411:PHE:CE2	1:V:429:LEU:HD11	2.52	0.45
1:B:138:LEU:HB3	1:B:164:THR:HG21	1.99	0.45
1:G:514:VAL:O	1:G:517:THR:OG1	2.30	0.45
1:I:397:VAL:HG11	1:I:403:PHE:N	2.32	0.45
1:K:109:ARG:HB3	1:K:481:THR:HA	1.99	0.45
1:P:502:GLN:NE2	1:P:506:ASP:OD1	2.49	0.45
1:U:72:LEU:HD23	1:U:72:LEU:HA	1.80	0.45
1:U:281:VAL:O	1:U:285:THR:HG23	2.16	0.45
1:V:72:LEU:HD23	1:V:72:LEU:HA	1.80	0.45
1:A:482:THR:HG23	1:A:485:GLY:H	1.82	0.45
1:C:79:ASP:OD1	1:C:504:ARG:NE	2.29	0.45
1:C:242:TYR:CE2	1:C:318:GLY:HA2	2.51	0.45
2:F:606:P8E:O1B	2:F:606:P8E:N5	2.49	0.45
1:M:113:GLN:NE2	1:M:479:GLY:HA3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:397:VAL:HG11	1:N:403:PHE:N	2.32	0.45
1:P:326:ASN:OD1	1:P:327:TYR:N	2.49	0.45
1:Q:243:ALA:HB1	1:Q:295:GLY:C	2.41	0.45
1:T:188:LEU:HD22	1:T:342:ILE:HD11	1.99	0.45
1:U:488:ALA:O	1:U:492:ILE:HG13	2.17	0.45
1:H:182:THR:OG1	1:H:348:SER:O	2.34	0.45
1:I:248:THR:HG22	1:I:264:GLU:HA	1.98	0.45
1:J:169:ILE:HG13	1:J:170:GLY:H	1.82	0.45
1:J:252:ASP:OD1	1:J:252:ASP:N	2.49	0.45
1:K:514:VAL:O	1:K:517:THR:OG1	2.30	0.45
1:O:238:THR:OG1	1:O:326:ASN:ND2	2.33	0.45
1:S:106:LEU:O	1:S:110:THR:OG1	2.29	0.45
1:U:70:ASP:O	1:U:74:ILE:HG13	2.16	0.45
1:U:391:PHE:HD2	1:U:393:PHE:HE1	1.65	0.45
1:U:514:VAL:O	1:U:517:THR:OG1	2.32	0.45
1:A:242:TYR:OH	1:A:315:VAL:HG13	2.16	0.45
2:A:608:P8E:O8	2:A:608:P8E:O6	2.35	0.45
1:N:109:ARG:HB3	1:N:481:THR:HA	1.99	0.45
1:N:125:ASN:O	1:N:129:THR:OG1	2.23	0.45
1:Q:455:SER:O	1:Q:458:SER:OG	2.33	0.45
1:T:539:ASP:OD1	1:T:539:ASP:N	2.39	0.45
1:U:164:THR:O	1:U:164:THR:OG1	2.30	0.45
1:U:214:LEU:HD12	1:U:330:LEU:HD13	1.98	0.45
1:U:411:PHE:CE2	1:U:429:LEU:HD11	2.51	0.45
1:V:243:ALA:HA	1:V:296:LYS:HG2	1.99	0.45
1:E:281:VAL:O	1:E:285:THR:HG23	2.16	0.45
1:G:397:VAL:HG11	1:G:403:PHE:N	2.31	0.45
2:H:610:P8E:O8	2:H:610:P8E:O6	2.32	0.45
2:I:602:P8E:O6	2:I:602:P8E:O8	2.35	0.45
1:M:104:GLN:HB3	1:M:108:THR:OG1	2.17	0.45
1:M:325:GLU:OE2	1:M:327:TYR:OH	2.25	0.45
1:M:329:ARG:HD2	1:M:384:SER:O	2.17	0.45
1:N:252:ASP:OD1	1:N:252:ASP:N	2.49	0.45
1:P:106:LEU:O	1:P:110:THR:OG1	2.34	0.45
1:R:390:LYS:NZ	1:R:430:SER:O	2.50	0.45
1:T:153:SER:OG	1:T:154:ASN:N	2.49	0.45
1:A:138:LEU:HB3	1:A:164:THR:CG2	2.47	0.45
1:E:500:LEU:HA	1:E:500:LEU:HD23	1.77	0.45
1:F:113:GLN:HE21	1:F:480:VAL:H	1.65	0.45
1:F:138:LEU:HB3	1:F:164:THR:HG21	1.99	0.45
1:H:502:GLN:NE2	1:H:506:ASP:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:188:LEU:HD22	1:K:342:ILE:HD11	1.99	0.45
1:K:214:LEU:HD12	1:K:330:LEU:HD13	1.98	0.45
1:K:384:SER:O	1:K:386:LYS:N	2.43	0.45
2:K:616:P8E:O8	2:K:616:P8E:N5	2.50	0.45
1:S:249:THR:HG22	1:S:313:ILE:O	2.17	0.45
1:T:255:ILE:HD11	1:T:287:VAL:HG21	1.99	0.45
1:V:205:VAL:HB	1:V:212:THR:HG22	1.98	0.45
1:B:104:GLN:HB3	1:B:108:THR:OG1	2.17	0.44
1:H:7:THR:HG21	1:O:533:SER:HB2	1.99	0.44
1:M:488:ALA:O	1:M:492:ILE:HG13	2.17	0.44
1:N:303:ASP:OD1	1:N:303:ASP:N	2.31	0.44
1:R:138:LEU:HB3	1:R:164:THR:HG21	1.98	0.44
1:R:170:GLY:O	1:R:364:SER:HA	2.17	0.44
1:U:31:ARG:HG2	1:U:39:ASN:HD21	1.80	0.44
1:V:393:PHE:HD2	1:V:435:ILE:HG12	1.81	0.44
1:A:165:GLN:HE22	1:M:223:LYS:NZ	2.14	0.44
1:B:249:THR:HG22	1:B:313:ILE:O	2.17	0.44
1:C:169:ILE:HG13	1:C:170:GLY:H	1.81	0.44
1:D:281:VAL:O	1:D:285:THR:HG23	2.18	0.44
1:D:429:LEU:HD22	1:D:433:ILE:HG13	1.98	0.44
1:F:482:THR:HG23	1:F:485:GLY:H	1.82	0.44
1:I:114:ALA:HB2	1:U:283:ASP:OD2	2.17	0.44
1:L:250:SER:HB3	1:L:312:ASP:HB3	1.98	0.44
1:P:99:ALA:HA	1:P:104:GLN:HE22	1.82	0.44
1:P:539:ASP:OD1	1:P:539:ASP:N	2.39	0.44
1:Q:164:THR:O	1:Q:164:THR:OG1	2.35	0.44
1:Q:252:ASP:OD1	1:Q:252:ASP:N	2.47	0.44
1:Q:393:PHE:HD2	1:Q:435:ILE:HG12	1.81	0.44
1:S:79:ASP:OD1	1:S:504:ARG:NE	2.33	0.44
1:S:557:GLY:O	1:S:561:MET:HG3	2.16	0.44
2:U:612:P8E:N5	2:U:612:P8E:O8	2.51	0.44
2:A:617:P8E:O6	2:A:617:P8E:O8	2.35	0.44
1:B:153:SER:HB3	1:U:491:ASP:OD2	2.17	0.44
1:C:6:ASN:OD1	1:C:6:ASN:C	2.61	0.44
1:E:175:GLU:HG2	1:E:360:GLN:HB3	1.98	0.44
1:F:205:VAL:HB	1:F:212:THR:HG22	1.99	0.44
1:G:500:LEU:HD23	1:G:500:LEU:HA	1.71	0.44
2:R:606:P8E:O1B	2:R:606:P8E:N5	2.50	0.44
1:T:325:GLU:OE2	1:T:327:TYR:OH	2.23	0.44
1:U:411:PHE:HE2	1:U:429:LEU:HD11	1.82	0.44
1:A:250:SER:HB3	1:A:312:ASP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ILE:HD12	1:D:480:VAL:HG21	1.98	0.44
1:H:235:ASP:OD1	1:H:237:LYS:NZ	2.43	0.44
1:I:125:ASN:O	1:I:129:THR:OG1	2.21	0.44
1:O:6:ASN:OD1	1:O:6:ASN:C	2.60	0.44
1:R:447:VAL:O	1:R:447:VAL:HG13	2.17	0.44
2:T:606:P8E:O8	2:T:606:P8E:O1B	2.36	0.44
2:T:617:P8E:O8	2:T:617:P8E:O1A	2.35	0.44
1:V:147:PHE:HB2	1:V:157:VAL:HG22	1.99	0.44
1:A:233:THR:OG1	1:A:234:TYR:N	2.50	0.44
1:B:42:ALA:HA	1:U:508:ALA:HB1	2.00	0.44
1:D:329:ARG:HD2	1:D:384:SER:O	2.18	0.44
1:D:561:MET:HE1	1:I:541:ALA:HB1	2.00	0.44
1:G:411:PHE:HE2	1:G:425:LEU:HD23	1.82	0.44
2:M:606:P8E:O8	2:M:606:P8E:O1B	2.35	0.44
1:O:255:ILE:HD11	1:O:287:VAL:HG21	2.00	0.44
1:P:233:THR:OG1	1:P:234:TYR:N	2.50	0.44
1:T:116:ILE:HD12	1:T:480:VAL:HG21	1.98	0.44
1:V:70:ASP:O	1:V:74:ILE:HG13	2.18	0.44
2:V:612:P8E:N5	2:V:612:P8E:O1B	2.50	0.44
1:B:109:ARG:HB3	1:B:481:THR:HA	1.99	0.44
1:H:217:LEU:O	1:H:221:ILE:HG13	2.17	0.44
1:O:104:GLN:HB3	1:O:108:THR:OG1	2.18	0.44
1:Q:384:SER:O	1:Q:386:LYS:N	2.45	0.44
1:S:95:LYS:HB3	1:S:112:LEU:HD12	2.00	0.44
1:S:189:THR:HB	1:S:343:SER:O	2.18	0.44
1:V:397:VAL:HG11	1:V:403:PHE:N	2.33	0.44
1:B:514:VAL:O	1:B:517:THR:OG1	2.33	0.44
1:F:59:ASN:ND2	1:Q:90:ASP:OD2	2.51	0.44
1:K:79:ASP:OD1	1:K:504:ARG:NE	2.30	0.44
1:R:64:ALA:HB1	1:R:149:ILE:HA	1.98	0.44
1:C:223:LYS:NZ	1:J:165:GLN:HE22	2.15	0.44
1:E:82:MET:HB3	1:E:82:MET:HE3	1.85	0.44
2:F:614:P8E:O8	2:F:614:P8E:O6	2.34	0.44
1:H:188:LEU:HD21	1:H:350:ILE:HD13	2.00	0.44
1:O:236:VAL:HG21	1:O:304:GLY:HA2	2.00	0.44
1:P:500:LEU:HD23	1:P:500:LEU:HA	1.79	0.44
2:S:616:P8E:O8	2:S:616:P8E:N5	2.50	0.44
1:U:447:VAL:HG13	1:U:447:VAL:O	2.17	0.44
1:V:188:LEU:HD21	1:V:350:ILE:HD13	1.99	0.44
1:A:358:ILE:HD11	1:A:463:PHE:HE1	1.82	0.44
1:E:70:ASP:O	1:E:74:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:GLN:HE22	1:S:223:LYS:NZ	2.16	0.44
1:J:138:LEU:HB3	1:J:164:THR:CG2	2.48	0.44
1:K:243:ALA:HA	1:K:296:LYS:HG2	1.99	0.44
1:L:315:VAL:HG21	1:L:411:PHE:CZ	2.53	0.44
1:M:447:VAL:HG13	1:M:447:VAL:O	2.18	0.44
1:O:193:TYR:CD1	1:O:199:PHE:HB2	2.53	0.44
1:P:64:ALA:HB1	1:P:149:ILE:HA	1.99	0.44
1:Q:254:ALA:HB3	1:Q:310:THR:OG1	2.17	0.44
2:T:616:P8E:O8	2:T:616:P8E:O6	2.35	0.44
1:E:101:GLN:HE21	1:E:104:GLN:HG3	1.83	0.43
1:E:252:ASP:OD1	1:E:252:ASP:N	2.50	0.43
1:F:245:LYS:HG3	1:F:425:LEU:HD11	2.00	0.43
1:G:400:ILE:HA	1:G:403:PHE:HB3	2.00	0.43
1:I:6:ASN:OD1	1:I:6:ASN:C	2.61	0.43
1:K:447:VAL:O	1:K:447:VAL:HG13	2.18	0.43
2:O:610:P8E:O8	2:O:610:P8E:O6	2.35	0.43
1:T:6:ASN:OD1	1:T:6:ASN:C	2.61	0.43
1:C:189:THR:HB	1:C:343:SER:O	2.18	0.43
1:C:306:GLY:HA3	1:C:327:TYR:HD1	1.84	0.43
1:D:89:LEU:HD12	1:D:500:LEU:HD12	2.00	0.43
1:E:189:THR:HB	1:E:343:SER:O	2.17	0.43
1:H:189:THR:HB	1:H:343:SER:O	2.19	0.43
1:H:514:VAL:O	1:H:517:THR:OG1	2.32	0.43
1:K:191:LYS:HE2	1:K:191:LYS:HB3	1.85	0.43
1:M:6:ASN:C	1:M:6:ASN:OD1	2.61	0.43
2:M:608:P8E:O6	2:M:608:P8E:O8	2.37	0.43
1:O:306:GLY:HA3	1:O:327:TYR:HD1	1.81	0.43
1:Q:6:ASN:OD1	1:Q:6:ASN:C	2.61	0.43
1:R:6:ASN:OD1	1:R:6:ASN:C	2.62	0.43
1:R:78:ALA:O	1:R:82:MET:HG2	2.18	0.43
1:R:243:ALA:HA	1:R:296:LYS:HG2	1.98	0.43
1:S:363:VAL:HG21	1:S:380:MET:HE2	2.00	0.43
1:T:243:ALA:HA	1:T:296:LYS:HG2	2.00	0.43
1:U:89:LEU:HD12	1:U:500:LEU:HD12	2.00	0.43
1:A:242:TYR:CE2	1:A:318:GLY:HA2	2.53	0.43
1:A:243:ALA:HB1	1:A:295:GLY:C	2.43	0.43
1:B:179:GLN:HA	1:B:329:ARG:HG2	2.00	0.43
1:E:6:ASN:OD1	1:E:6:ASN:C	2.62	0.43
1:E:89:LEU:HD23	1:E:89:LEU:HA	1.88	0.43
1:G:61:LEU:HD22	1:G:521:ILE:HG23	2.00	0.43
1:G:281:VAL:O	1:G:285:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:490:MET:HE3	1:G:490:MET:HB2	1.74	0.43
1:H:561:MET:HE2	1:H:561:MET:HB3	1.81	0.43
1:L:126:ILE:HG12	1:V:520:ASN:ND2	2.32	0.43
1:M:173:ARG:HB3	1:M:334:LYS:HB3	2.00	0.43
1:R:245:LYS:HG3	1:R:425:LEU:HD11	1.99	0.43
1:R:285:THR:OG1	1:R:287:VAL:HG22	2.18	0.43
1:A:54:LEU:HD22	1:A:528:VAL:HG13	2.01	0.43
1:B:95:LYS:HE3	1:B:115:ASP:OD2	2.19	0.43
1:F:164:THR:O	1:F:164:THR:OG1	2.34	0.43
1:G:113:GLN:NE2	1:G:479:GLY:HA3	2.34	0.43
1:H:95:LYS:HB3	1:H:112:LEU:HD12	1.99	0.43
1:I:169:ILE:HG13	1:I:170:GLY:H	1.84	0.43
1:J:6:ASN:OD1	1:J:6:ASN:C	2.61	0.43
1:T:95:LYS:HE3	1:T:115:ASP:OD2	2.18	0.43
1:T:447:VAL:O	1:T:447:VAL:HG13	2.17	0.43
1:C:422:GLY:C	1:C:424:ASN:HD22	2.26	0.43
1:E:553:LEU:HD23	1:E:553:LEU:HA	1.85	0.43
1:G:188:LEU:HD21	1:G:350:ILE:HD13	2.00	0.43
1:I:138:LEU:HB3	1:I:164:THR:CG2	2.48	0.43
1:I:447:VAL:O	1:I:447:VAL:HG13	2.18	0.43
1:J:315:VAL:HG21	1:J:411:PHE:CZ	2.53	0.43
1:K:189:THR:HB	1:K:343:SER:O	2.18	0.43
1:K:250:SER:HB3	1:K:312:ASP:HB3	2.00	0.43
1:N:242:TYR:OH	1:N:315:VAL:HG22	2.18	0.43
1:O:539:ASP:OD1	1:O:539:ASP:N	2.40	0.43
1:R:61:LEU:HD22	1:R:521:ILE:HG23	1.98	0.43
1:S:255:ILE:HD11	1:S:287:VAL:HG21	2.00	0.43
1:U:147:PHE:HB2	1:U:157:VAL:HG22	2.00	0.43
1:B:6:ASN:OD1	1:B:6:ASN:C	2.62	0.43
1:E:173:ARG:HB2	1:E:337:GLY:HA2	2.00	0.43
2:E:603:P8E:O6	2:E:603:P8E:O8	2.37	0.43
1:F:6:ASN:OD1	1:F:6:ASN:C	2.61	0.43
1:F:124:ASP:OD1	1:F:128:ASN:ND2	2.52	0.43
1:G:364:SER:H	1:G:367:GLU:HB2	1.84	0.43
1:Q:99:ALA:HA	1:Q:104:GLN:NE2	2.33	0.43
1:Q:113:GLN:NE2	1:Q:479:GLY:HA3	2.33	0.43
1:Q:397:VAL:HG11	1:Q:403:PHE:N	2.33	0.43
1:S:447:VAL:O	1:S:447:VAL:HG13	2.17	0.43
1:A:313:ILE:HD13	1:A:319:ILE:HD12	2.01	0.43
1:B:242:TYR:CE2	1:B:318:GLY:HA2	2.54	0.43
1:C:210:VAL:HG21	1:J:370:GLY:HA3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:357:MET:HG2	1:E:446:TYR:CE2	2.53	0.43
1:H:315:VAL:HG21	1:H:411:PHE:CZ	2.54	0.43
1:I:254:ALA:HB3	1:I:310:THR:OG1	2.18	0.43
1:L:557:GLY:O	1:L:561:MET:HG3	2.19	0.43
1:M:384:SER:OG	1:M:385:TYR:N	2.52	0.43
1:O:303:ASP:OD1	1:O:303:ASP:N	2.36	0.43
1:P:6:ASN:OD1	1:P:6:ASN:C	2.62	0.43
1:Q:61:LEU:HD22	1:Q:521:ILE:HG23	2.01	0.43
1:Q:150:GLY:HA3	1:Q:155:GLN:HB2	1.99	0.43
2:Q:606:P8E:O1B	2:Q:606:P8E:N5	2.52	0.43
1:S:397:VAL:HG11	1:S:403:PHE:N	2.33	0.43
1:V:6:ASN:OD1	1:V:6:ASN:C	2.61	0.43
1:A:250:SER:OG	1:A:312:ASP:N	2.52	0.43
1:D:173:ARG:HB2	1:D:337:GLY:HA2	2.01	0.43
1:F:500:LEU:HD23	1:F:500:LEU:HA	1.74	0.43
1:H:138:LEU:HB3	1:H:164:THR:CG2	2.49	0.43
1:H:177:GLY:HA2	1:H:358:ILE:HG22	2.01	0.43
2:H:616:P8E:O8	2:H:616:P8E:N5	2.51	0.43
2:J:616:P8E:O8	2:J:616:P8E:N5	2.51	0.43
1:K:303:ASP:OD1	1:K:303:ASP:N	2.46	0.43
1:L:6:ASN:OD1	1:L:6:ASN:C	2.61	0.43
1:P:514:VAL:O	1:P:517:THR:OG1	2.32	0.43
1:R:255:ILE:HD11	1:R:287:VAL:HG11	2.01	0.43
1:T:205:VAL:HB	1:T:212:THR:HG22	2.00	0.43
1:U:482:THR:HG23	1:U:485:GLY:H	1.83	0.43
1:A:541:ALA:HB2	1:V:3:PHE:CD2	2.53	0.43
1:C:241:VAL:HG23	1:C:242:TYR:CD2	2.53	0.43
1:C:285:THR:O	1:C:305:ARG:NH2	2.52	0.43
1:D:95:LYS:HE3	1:D:115:ASP:OD2	2.19	0.43
1:H:429:LEU:HD22	1:H:433:ILE:HG13	2.00	0.43
1:K:167:SER:HB3	1:K:366:ARG:HD2	2.01	0.43
1:L:89:LEU:HD23	1:L:89:LEU:HA	1.86	0.43
1:L:325:GLU:OE2	1:L:327:TYR:OH	2.22	0.43
1:O:70:ASP:O	1:O:74:ILE:HG13	2.19	0.43
1:P:89:LEU:HD12	1:P:500:LEU:HD12	2.01	0.43
1:P:447:VAL:HG13	1:P:447:VAL:O	2.18	0.43
1:Q:95:LYS:HE3	1:Q:115:ASP:OD1	2.18	0.43
1:Q:482:THR:HG23	1:Q:485:GLY:H	1.83	0.43
1:R:70:ASP:O	1:R:74:ILE:HG13	2.18	0.43
1:R:202:ASP:OD1	1:R:203:ASN:N	2.52	0.43
1:R:309:ILE:HD11	1:R:324:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:THR:HG22	1:A:313:ILE:O	2.19	0.43
1:B:148:GLN:NE2	1:B:150:GLY:H	2.17	0.43
1:C:177:GLY:N	1:C:352:MET:HE2	2.34	0.43
1:D:6:ASN:OD1	1:D:6:ASN:C	2.62	0.43
1:F:95:LYS:HB3	1:F:112:LEU:HD12	2.01	0.43
1:F:177:GLY:HA2	1:F:358:ILE:HG22	1.99	0.43
1:H:306:GLY:HA3	1:H:327:TYR:HD1	1.83	0.43
1:H:310:THR:OG1	1:H:311:GLY:N	2.52	0.43
1:K:64:ALA:HB1	1:K:149:ILE:HA	1.99	0.43
2:P:616:P8E:O8	2:P:616:P8E:N5	2.52	0.43
1:Q:447:VAL:O	1:Q:447:VAL:HG13	2.18	0.43
1:Q:539:ASP:OD1	1:Q:539:ASP:N	2.51	0.43
1:U:6:ASN:OD1	1:U:6:ASN:C	2.62	0.43
1:U:189:THR:HB	1:U:343:SER:O	2.18	0.43
1:A:143:THR:HA	1:A:160:THR:HA	2.01	0.42
1:A:447:VAL:O	1:A:447:VAL:HG13	2.18	0.42
2:A:606:P8E:O8	2:A:606:P8E:O6	2.35	0.42
1:B:447:VAL:O	1:B:447:VAL:HG13	2.19	0.42
2:B:606:P8E:O8	2:B:606:P8E:O6	2.37	0.42
1:C:541:ALA:HB2	1:T:3:PHE:CD2	2.54	0.42
1:D:142:PHE:HA	1:D:145:GLN:HE21	1.83	0.42
1:F:126:ILE:HG12	1:P:520:ASN:ND2	2.34	0.42
1:G:78:ALA:HB1	1:G:138:LEU:HD21	2.01	0.42
1:H:144:ASN:OD1	1:O:300:THR:HG21	2.19	0.42
1:I:539:ASP:OD1	1:I:539:ASP:N	2.38	0.42
2:M:614:P8E:O6	2:M:614:P8E:O8	2.37	0.42
1:N:95:LYS:HB3	1:N:112:LEU:HD12	2.01	0.42
1:O:384:SER:OG	1:O:385:TYR:N	2.52	0.42
1:T:285:THR:O	1:T:305:ARG:NH2	2.52	0.42
1:U:398:SER:HA	2:U:611:P8E:O1A	2.18	0.42
1:V:382:PHE:CD1	1:V:382:PHE:N	2.86	0.42
2:A:617:P8E:O8	2:A:617:P8E:O1A	2.37	0.42
1:D:233:THR:OG1	1:D:234:TYR:N	2.52	0.42
1:D:490:MET:HE3	1:D:490:MET:HB2	1.76	0.42
2:D:616:P8E:O6	2:D:616:P8E:O8	2.37	0.42
1:G:329:ARG:NH1	1:G:384:SER:O	2.52	0.42
1:M:241:VAL:HG23	1:M:242:TYR:HD2	1.83	0.42
1:R:400:ILE:HA	1:R:403:PHE:HB3	2.01	0.42
1:R:457:GLY:N	2:R:616:P8E:O1A	2.39	0.42
1:V:150:GLY:HA3	1:V:155:GLN:HB2	2.00	0.42
1:A:232:ALA:HB2	1:A:332:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:HD23	1:B:119:LEU:HA	1.92	0.42
1:D:189:THR:HG23	1:D:200:LYS:HG2	2.00	0.42
1:L:488:ALA:O	1:L:492:ILE:HG13	2.20	0.42
2:M:610:P8E:O8	2:M:610:P8E:O6	2.36	0.42
1:O:226:ASP:OD1	1:O:227:LYS:HG3	2.19	0.42
1:R:95:LYS:HB3	1:R:112:LEU:HD12	2.01	0.42
1:A:189:THR:HB	1:A:343:SER:O	2.20	0.42
1:A:217:LEU:O	1:A:221:ILE:HG13	2.18	0.42
1:C:236:VAL:HG22	1:C:328:GLY:HA3	2.01	0.42
1:E:308:LYS:HA	1:E:324:LYS:O	2.19	0.42
1:H:38:ILE:HD12	1:H:48:MET:SD	2.59	0.42
1:H:553:LEU:HD11	1:T:6:ASN:HB2	2.01	0.42
1:J:189:THR:HB	1:J:343:SER:O	2.18	0.42
2:K:617:P8E:O8	2:K:617:P8E:O1A	2.36	0.42
1:O:106:LEU:O	1:O:110:THR:OG1	2.32	0.42
1:R:238:THR:OG1	1:R:326:ASN:ND2	2.50	0.42
1:V:189:THR:HB	1:V:343:SER:O	2.19	0.42
1:H:242:TYR:CE2	1:H:318:GLY:HA2	2.54	0.42
1:L:293:GLU:HG2	1:L:294:ASN:HD22	1.85	0.42
1:N:150:GLY:HA3	1:N:155:GLN:HB2	2.00	0.42
1:N:480:VAL:HG23	1:N:486:ALA:HA	2.00	0.42
2:P:615:P8E:O1A	2:P:615:P8E:N5	2.53	0.42
2:V:616:P8E:O8	2:V:616:P8E:N5	2.51	0.42
1:B:210:VAL:HG21	1:N:370:GLY:HA3	2.02	0.42
1:D:170:GLY:O	1:D:364:SER:HA	2.19	0.42
1:E:164:THR:O	1:E:164:THR:OG1	2.33	0.42
1:G:124:ASP:OD2	1:G:128:ASN:ND2	2.53	0.42
1:G:254:ALA:HB3	1:G:310:THR:OG1	2.19	0.42
1:I:541:ALA:HB2	1:N:3:PHE:CD2	2.55	0.42
1:I:553:LEU:HD23	1:I:553:LEU:HA	1.91	0.42
1:K:89:LEU:HA	1:K:89:LEU:HD23	1.85	0.42
1:M:99:ALA:O	1:M:109:ARG:NH1	2.53	0.42
1:P:218:ALA:O	1:P:222:ASN:ND2	2.52	0.42
1:P:310:THR:OG1	1:P:311:GLY:N	2.53	0.42
2:U:616:P8E:O8	2:U:616:P8E:N5	2.53	0.42
1:V:249:THR:HG22	1:V:313:ILE:O	2.20	0.42
1:B:79:ASP:OD1	1:B:504:ARG:NE	2.39	0.42
1:C:153:SER:OG	1:C:154:ASN:N	2.51	0.42
1:D:138:LEU:HB3	1:D:164:THR:HG21	2.02	0.42
1:D:173:ARG:HD2	1:D:361:SER:O	2.18	0.42
1:E:124:ASP:CG	1:E:128:ASN:HD21	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:364:SER:OG	1:E:365:LEU:N	2.53	0.42
1:F:99:ALA:HA	1:F:104:GLN:NE2	2.35	0.42
1:F:189:THR:HB	1:F:343:SER:O	2.20	0.42
1:G:6:ASN:OD1	1:G:6:ASN:C	2.63	0.42
1:G:102:ASP:O	1:P:135:LYS:NZ	2.53	0.42
1:G:233:THR:OG1	1:G:234:TYR:N	2.52	0.42
1:L:138:LEU:HB3	1:L:164:THR:CG2	2.50	0.42
1:L:243:ALA:HA	1:L:296:LYS:HG2	2.02	0.42
1:N:95:LYS:HE3	1:N:115:ASP:OD2	2.19	0.42
1:N:395:GLN:HG2	1:N:396:ASN:H	1.85	0.42
1:N:529:LYS:HE2	1:N:529:LYS:HB2	1.89	0.42
2:Q:616:P8E:O8	2:Q:616:P8E:N5	2.53	0.42
1:S:164:THR:OG1	1:S:500:LEU:HD21	2.19	0.42
1:S:376:ASN:O	1:S:380:MET:HG2	2.19	0.42
1:S:488:ALA:O	1:S:492:ILE:HG13	2.20	0.42
1:T:82:MET:HE2	1:T:82:MET:HB3	1.92	0.42
1:T:125:ASN:O	1:T:129:THR:OG1	2.29	0.42
1:D:179:GLN:HA	1:D:329:ARG:HG2	2.02	0.42
1:E:242:TYR:OH	1:E:315:VAL:HG22	2.20	0.42
1:F:173:ARG:HB3	1:F:334:LYS:HB3	2.02	0.42
2:F:616:P8E:O8	2:F:616:P8E:N5	2.53	0.42
1:H:249:THR:HG22	1:H:313:ILE:O	2.20	0.42
1:K:138:LEU:HB3	1:K:164:THR:CG2	2.50	0.42
1:K:150:GLY:HA3	1:K:155:GLN:HB2	2.02	0.42
1:K:254:ALA:HB3	1:K:310:THR:OG1	2.20	0.42
1:K:285:THR:O	1:K:305:ARG:NH2	2.52	0.42
1:K:329:ARG:HD2	1:K:384:SER:O	2.19	0.42
1:L:224:SER:O	1:L:228:THR:OG1	2.34	0.42
1:L:447:VAL:O	1:L:447:VAL:HG13	2.19	0.42
1:N:6:ASN:OD1	1:N:6:ASN:C	2.62	0.42
1:N:447:VAL:HG13	1:N:447:VAL:O	2.20	0.42
1:Q:237:LYS:O	1:Q:326:ASN:ND2	2.52	0.42
2:Q:617:P8E:O8	2:Q:617:P8E:O6	2.38	0.42
1:T:236:VAL:HG22	1:T:328:GLY:HA3	2.00	0.42
1:V:436:ILE:HG21	1:V:442:MET:HE2	2.01	0.42
1:A:376:ASN:O	1:A:380:MET:HG2	2.20	0.42
1:A:495:THR:HG22	1:A:499:ASN:HD21	1.84	0.42
1:D:141:ASN:ND2	1:S:293:GLU:HG2	2.35	0.42
1:D:241:VAL:HG23	1:D:242:TYR:CD2	2.54	0.42
1:F:325:GLU:OE2	1:F:327:TYR:OH	2.20	0.42
1:F:397:VAL:HG11	1:F:403:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6:ASN:OD1	1:H:6:ASN:C	2.62	0.42
1:J:561:MET:HE2	1:J:561:MET:HB3	1.82	0.42
1:L:398:SER:HA	2:L:611:P8E:O1A	2.19	0.42
1:Q:38:ILE:HD12	1:Q:48:MET:SD	2.60	0.42
1:Q:553:LEU:HD23	1:Q:553:LEU:HA	1.90	0.42
1:S:490:MET:HE3	1:S:490:MET:HB2	1.77	0.42
1:T:553:LEU:HD23	1:T:553:LEU:HA	1.89	0.42
1:U:95:LYS:HB3	1:U:112:LEU:HD12	2.02	0.42
1:U:104:GLN:HB3	1:U:108:THR:OG1	2.19	0.42
1:B:218:ALA:O	1:B:222:ASN:ND2	2.51	0.42
1:C:490:MET:HE3	1:C:490:MET:HB2	1.85	0.42
1:D:119:LEU:HD23	1:D:119:LEU:HA	1.83	0.42
1:D:165:GLN:HE22	1:I:223:LYS:NZ	2.18	0.42
1:E:188:LEU:HD21	1:E:350:ILE:HD13	2.01	0.42
1:F:138:LEU:HB3	1:F:164:THR:CG2	2.50	0.42
1:J:306:GLY:HA3	1:J:327:TYR:HD1	1.83	0.42
1:L:147:PHE:HB2	1:L:157:VAL:HG22	2.00	0.42
1:N:329:ARG:HD2	1:N:384:SER:O	2.19	0.42
1:N:384:SER:O	1:N:386:LYS:N	2.46	0.42
1:O:404:MET:HG2	1:O:411:PHE:CG	2.54	0.42
1:R:529:LYS:HE2	1:R:529:LYS:HB2	1.93	0.42
1:T:482:THR:HG23	1:T:485:GLY:H	1.85	0.42
1:A:23:LYS:HE3	1:A:23:LYS:HB2	1.88	0.41
1:B:448:VAL:HG13	1:B:454:PHE:O	2.20	0.41
1:C:72:LEU:HD23	1:C:72:LEU:HA	1.80	0.41
1:D:146:GLU:HB2	1:S:483:LEU:HD21	2.02	0.41
1:D:236:VAL:HG21	1:D:304:GLY:HA2	2.01	0.41
1:D:520:ASN:ND2	1:G:126:ILE:HG12	2.34	0.41
1:H:169:ILE:HG13	1:H:170:GLY:H	1.84	0.41
1:I:254:ALA:HB2	1:I:259:THR:HA	2.01	0.41
1:J:219:GLU:OE2	1:V:366:ARG:NH2	2.52	0.41
1:K:99:ALA:O	1:K:109:ARG:NH1	2.53	0.41
1:M:495:THR:O	1:M:499:ASN:ND2	2.53	0.41
1:O:95:LYS:HE3	1:O:115:ASP:OD2	2.19	0.41
2:P:616:P8E:O8	2:P:616:P8E:O6	2.37	0.41
1:S:561:MET:HE2	1:S:561:MET:HB3	1.86	0.41
1:A:88:ILE:HG23	1:A:119:LEU:HD22	2.02	0.41
1:A:99:ALA:HA	1:A:104:GLN:NE2	2.35	0.41
1:B:448:VAL:HG12	1:B:448:VAL:O	2.20	0.41
1:C:357:MET:HG2	1:C:446:TYR:CE2	2.55	0.41
2:C:611:P8E:O6	2:C:611:P8E:O8	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:ASP:OD1	1:D:303:ASP:N	2.43	0.41
1:E:95:LYS:HE3	1:E:115:ASP:OD2	2.20	0.41
1:E:483:LEU:HD21	1:R:146:GLU:HB2	2.02	0.41
1:F:64:ALA:HB1	1:F:149:ILE:HA	2.01	0.41
1:F:255:ILE:HD13	1:F:287:VAL:HG21	2.02	0.41
1:I:150:GLY:HA3	1:I:155:GLN:HB2	2.02	0.41
1:J:113:GLN:HE21	1:J:480:VAL:H	1.67	0.41
1:K:125:ASN:O	1:K:129:THR:OG1	2.24	0.41
1:U:61:LEU:HD22	1:U:521:ILE:HG23	2.01	0.41
2:U:603:P8E:O6	2:U:603:P8E:O8	2.38	0.41
1:V:145:GLN:O	1:V:158:LYS:HA	2.20	0.41
1:D:164:THR:O	1:D:164:THR:OG1	2.36	0.41
1:F:249:THR:HG22	1:F:313:ILE:O	2.20	0.41
1:F:285:THR:OG1	1:F:286:GLY:N	2.53	0.41
1:K:106:LEU:O	1:K:110:THR:OG1	2.31	0.41
1:K:233:THR:OG1	1:K:234:TYR:N	2.53	0.41
2:L:606:P8E:O8	2:L:606:P8E:O1B	2.38	0.41
1:N:268:GLY:O	1:N:291:LYS:NZ	2.38	0.41
1:R:539:ASP:OD1	1:R:539:ASP:N	2.37	0.41
1:T:249:THR:HG22	1:T:313:ILE:O	2.20	0.41
1:U:442:MET:O	1:U:442:MET:HG3	2.21	0.41
1:V:488:ALA:O	1:V:492:ILE:HG13	2.19	0.41
1:C:147:PHE:HB2	1:C:157:VAL:HG22	2.03	0.41
1:C:541:ALA:HB1	1:J:561:MET:HE1	2.01	0.41
1:D:488:ALA:O	1:D:492:ILE:HG13	2.20	0.41
1:E:429:LEU:O	1:E:433:ILE:HB	2.21	0.41
1:G:520:ASN:ND2	1:Q:126:ILE:HG12	2.35	0.41
1:I:243:ALA:HB1	1:I:295:GLY:C	2.46	0.41
1:J:282:LYS:HE3	1:J:288:GLN:HE22	1.85	0.41
1:K:6:ASN:OD1	1:K:6:ASN:C	2.62	0.41
1:N:169:ILE:HD12	1:N:496:ALA:HB1	2.03	0.41
1:N:357:MET:SD	1:N:462:GLN:HA	2.60	0.41
1:P:169:ILE:HG13	1:P:170:GLY:N	2.34	0.41
1:Q:188:LEU:HB2	1:Q:201:PHE:HD1	1.85	0.41
1:S:6:ASN:OD1	1:S:6:ASN:C	2.63	0.41
1:U:61:LEU:O	1:U:65:ILE:HG13	2.21	0.41
1:A:334:LYS:HD3	1:A:336:ASP:OD1	2.20	0.41
1:B:384:SER:OG	1:B:385:TYR:N	2.53	0.41
1:D:218:ALA:O	1:D:222:ASN:ND2	2.52	0.41
1:D:242:TYR:OH	1:D:315:VAL:HG22	2.20	0.41
1:F:175:GLU:HG2	1:F:360:GLN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:457:GLY:H	2:N:616:P8E:C1	2.33	0.41
1:P:82:MET:HE3	1:P:82:MET:HB3	1.98	0.41
1:T:253:PHE:CE1	1:T:313:ILE:HG13	2.55	0.41
1:A:153:SER:OG	1:A:154:ASN:ND2	2.47	0.41
1:C:397:VAL:HG11	1:C:403:PHE:N	2.36	0.41
1:D:3:PHE:CD2	1:S:541:ALA:HB2	2.55	0.41
1:D:447:VAL:O	1:D:447:VAL:HG13	2.20	0.41
1:D:500:LEU:HD23	1:D:500:LEU:HA	1.80	0.41
2:D:616:P8E:O8	2:D:616:P8E:N5	2.54	0.41
1:I:164:THR:O	1:I:164:THR:OG1	2.34	0.41
1:I:268:GLY:O	1:I:291:LYS:NZ	2.34	0.41
1:I:568:GLN:HE21	1:I:568:GLN:HB2	1.66	0.41
1:J:254:ALA:HB3	1:J:310:THR:OG1	2.20	0.41
1:M:173:ARG:NH2	1:M:339:ASP:OD1	2.53	0.41
1:M:397:VAL:HG11	1:M:403:PHE:N	2.35	0.41
1:M:553:LEU:HD23	1:M:553:LEU:HA	1.87	0.41
1:O:243:ALA:HA	1:O:296:LYS:HG2	2.01	0.41
1:P:72:LEU:HD23	1:P:72:LEU:HA	1.83	0.41
1:S:242:TYR:OH	1:S:315:VAL:HG22	2.20	0.41
1:A:561:MET:HE2	1:J:574:LEU:HD11	2.03	0.41
1:D:177:GLY:HA2	1:D:358:ILE:HG22	2.02	0.41
1:D:188:LEU:HD22	1:D:342:ILE:HD11	2.03	0.41
1:G:23:LYS:HE3	1:G:23:LYS:HB2	1.87	0.41
1:I:237:LYS:O	1:I:326:ASN:ND2	2.54	0.41
1:K:205:VAL:HB	1:K:212:THR:HG22	2.01	0.41
1:K:418:SER:O	1:K:421:SER:OG	2.28	0.41
1:L:138:LEU:HB3	1:L:164:THR:HG21	2.02	0.41
2:O:616:P8E:O8	2:O:616:P8E:N5	2.53	0.41
1:R:490:MET:HE3	1:R:490:MET:HB2	1.85	0.41
1:T:82:MET:HA	1:T:85:GLN:HE21	1.84	0.41
1:V:118:LYS:HA	1:V:118:LYS:HD3	1.92	0.41
1:C:109:ARG:HB3	1:C:481:THR:HA	2.03	0.41
1:C:553:LEU:HD11	1:J:6:ASN:HB2	2.03	0.41
1:D:139:SER:O	1:D:165:GLN:NE2	2.53	0.41
1:E:153:SER:OG	1:E:154:ASN:N	2.52	0.41
1:H:233:THR:OG1	1:H:234:TYR:N	2.54	0.41
1:J:218:ALA:O	1:J:222:ASN:ND2	2.39	0.41
1:K:193:TYR:CD1	1:K:199:PHE:HB2	2.55	0.41
1:L:384:SER:O	1:L:386:LYS:N	2.46	0.41
1:O:561:MET:HE2	1:O:561:MET:HB3	1.84	0.41
1:P:138:LEU:HB3	1:P:164:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:243:ALA:HA	1:P:296:LYS:HG2	2.01	0.41
1:Q:255:ILE:HD11	1:Q:287:VAL:HG21	2.02	0.41
1:A:455:SER:O	1:A:458:SER:OG	2.25	0.41
1:B:326:ASN:OD1	1:B:327:TYR:N	2.53	0.41
1:C:480:VAL:HG23	1:C:486:ALA:HA	2.03	0.41
1:D:219:GLU:CD	1:P:366:ARG:HH22	2.29	0.41
1:D:574:LEU:HD11	1:G:561:MET:HE2	2.02	0.41
1:E:192:ASN:ND2	1:E:192:ASN:O	2.54	0.41
1:E:260:ILE:O	1:R:338:ARG:NH1	2.54	0.41
1:E:293:GLU:HG2	1:R:141:ASN:ND2	2.36	0.41
1:E:549:LYS:HD2	1:H:6:ASN:C	2.46	0.41
1:F:3:PHE:CD2	1:Q:541:ALA:HB2	2.55	0.41
1:F:206:ILE:HD13	1:F:206:ILE:HA	1.95	0.41
1:F:376:ASN:O	1:F:380:MET:HG2	2.20	0.41
1:F:443:SER:HA	1:F:448:VAL:HG12	2.02	0.41
1:F:514:VAL:O	1:F:517:THR:OG1	2.35	0.41
1:G:147:PHE:O	1:G:149:ILE:HG23	2.21	0.41
1:G:169:ILE:HG13	1:G:170:GLY:N	2.36	0.41
1:I:500:LEU:HD23	1:I:500:LEU:HA	1.79	0.41
1:J:285:THR:OG1	1:J:287:VAL:HG22	2.21	0.41
1:J:549:LYS:HD2	1:V:6:ASN:C	2.46	0.41
1:N:233:THR:OG1	1:N:234:TYR:N	2.54	0.41
1:O:157:VAL:HG12	1:O:513:GLN:NE2	2.36	0.41
1:O:249:THR:HG22	1:O:313:ILE:O	2.21	0.41
1:P:382:PHE:HB2	1:P:383:ASN:ND2	2.34	0.41
1:P:448:VAL:O	1:P:448:VAL:HG12	2.20	0.41
1:R:171:VAL:HG13	1:R:171:VAL:O	2.21	0.41
1:R:244:ILE:HG23	1:R:267:ASP:O	2.21	0.41
1:S:303:ASP:OD1	1:S:303:ASP:N	2.54	0.41
1:S:529:LYS:HE2	1:S:529:LYS:HB2	1.90	0.41
1:T:490:MET:HE3	1:T:490:MET:HB2	1.85	0.41
1:V:382:PHE:CD2	1:V:476:GLU:HG3	2.56	0.41
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.95	0.41
1:D:242:TYR:CE2	1:D:318:GLY:HA2	2.56	0.41
1:E:95:LYS:HB3	1:E:112:LEU:HD12	2.02	0.41
1:E:395:GLN:HG2	1:E:396:ASN:H	1.86	0.41
1:F:109:ARG:HB3	1:F:481:THR:HA	2.03	0.41
1:G:480:VAL:HG23	1:G:486:ALA:HA	2.02	0.41
1:H:54:LEU:HD22	1:H:528:VAL:HG13	2.03	0.41
1:H:283:ASP:OD2	1:T:114:ALA:HB2	2.21	0.41
1:H:500:LEU:HD23	1:H:500:LEU:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:61:LEU:O	1:I:65:ILE:HG13	2.20	0.41
1:J:447:VAL:O	1:J:447:VAL:HG13	2.21	0.41
1:M:138:LEU:HB3	1:M:164:THR:CG2	2.51	0.41
1:S:357:MET:HE3	1:S:442:MET:HE3	2.03	0.41
1:U:238:THR:OG1	1:U:326:ASN:ND2	2.34	0.41
1:V:255:ILE:HD11	1:V:287:VAL:HG11	2.02	0.41
1:B:376:ASN:O	1:B:380:MET:HG3	2.21	0.40
1:C:377:ALA:O	1:C:382:PHE:HD1	2.04	0.40
1:F:147:PHE:O	1:F:149:ILE:HG23	2.21	0.40
1:H:227:LYS:HB3	1:H:227:LYS:HE2	1.86	0.40
2:H:611:P8E:O8	2:H:611:P8E:O6	2.39	0.40
1:I:193:TYR:CD1	1:I:199:PHE:HB2	2.56	0.40
1:I:241:VAL:HG23	1:I:242:TYR:CD2	2.55	0.40
1:M:482:THR:HG23	1:M:485:GLY:H	1.86	0.40
1:S:250:SER:OG	1:S:252:ASP:OD1	2.24	0.40
1:U:384:SER:OG	1:U:385:TYR:N	2.53	0.40
1:U:390:LYS:NZ	1:U:430:SER:O	2.54	0.40
1:A:391:PHE:CD2	1:A:393:PHE:HE1	2.39	0.40
1:D:149:ILE:HD11	1:D:157:VAL:HG13	2.02	0.40
1:E:490:MET:HE3	1:E:490:MET:HB2	1.76	0.40
1:G:138:LEU:HB3	1:G:164:THR:CG2	2.51	0.40
1:G:527:ASN:HD21	1:Q:80:LYS:HB2	1.87	0.40
1:J:514:VAL:O	1:J:517:THR:OG1	2.34	0.40
1:J:557:GLY:O	1:J:561:MET:HG3	2.22	0.40
1:L:23:LYS:HE3	1:L:23:LYS:HB2	1.90	0.40
1:M:54:LEU:HD23	1:M:54:LEU:HA	1.87	0.40
1:M:164:THR:O	1:M:164:THR:OG1	2.30	0.40
1:M:455:SER:O	1:M:458:SER:OG	2.30	0.40
2:M:612:P8E:O8	2:M:612:P8E:O6	2.39	0.40
1:P:79:ASP:OD1	1:P:504:ARG:NE	2.33	0.40
1:P:249:THR:HG22	1:P:313:ILE:O	2.22	0.40
1:S:23:LYS:HB2	1:S:23:LYS:HE3	1.87	0.40
1:A:244:ILE:HD13	1:A:269:ASP:HB2	2.03	0.40
1:B:147:PHE:O	1:B:149:ILE:HG23	2.21	0.40
1:F:306:GLY:HA3	1:F:327:TYR:HD1	1.85	0.40
1:G:309:ILE:HD11	1:G:324:LYS:HG2	2.04	0.40
2:G:606:P8E:O1B	2:G:606:P8E:N5	2.54	0.40
1:H:82:MET:HE2	1:H:82:MET:HB3	1.86	0.40
1:I:78:ALA:O	1:I:82:MET:HG2	2.22	0.40
1:I:462:GLN:HG3	1:I:463:PHE:CE1	2.56	0.40
1:J:553:LEU:HD11	1:V:6:ASN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:32:LEU:HD13	1:K:543:GLU:HG3	2.04	0.40
1:L:448:VAL:HG12	1:L:448:VAL:O	2.22	0.40
1:N:202:ASP:OD1	1:N:203:ASN:N	2.52	0.40
1:P:125:ASN:O	1:P:129:THR:OG1	2.27	0.40
1:P:384:SER:O	1:P:386:LYS:N	2.49	0.40
1:U:500:LEU:HA	1:U:500:LEU:HD23	1.80	0.40
1:U:575:LEU:HD23	1:U:575:LEU:HA	1.87	0.40
1:V:433:ILE:HD13	1:V:433:ILE:HA	1.91	0.40
1:A:145:GLN:O	1:A:158:LYS:HA	2.22	0.40
1:A:169:ILE:HG13	1:A:170:GLY:N	2.36	0.40
1:B:82:MET:HA	1:B:85:GLN:HE21	1.86	0.40
2:B:616:P8E:O8	2:B:616:P8E:N5	2.54	0.40
1:D:23:LYS:HB2	1:D:23:LYS:HE3	1.89	0.40
1:D:357:MET:HE3	1:D:442:MET:HE3	2.04	0.40
1:F:412:SER:HB3	2:F:607:P8E:O1B	2.19	0.40
1:J:397:VAL:HG13	1:J:402:ALA:HB3	2.02	0.40
1:J:500:LEU:HD23	1:J:500:LEU:HA	1.85	0.40
1:K:308:LYS:HA	1:K:324:LYS:O	2.21	0.40
1:L:490:MET:HB2	1:L:490:MET:HE3	1.74	0.40
1:N:433:ILE:HD13	1:N:433:ILE:HA	1.92	0.40
1:O:138:LEU:HB3	1:O:164:THR:HG21	2.02	0.40
1:O:142:PHE:C	1:O:145:GLN:HE21	2.29	0.40
1:Q:490:MET:HE3	1:Q:490:MET:HB2	1.87	0.40
1:T:189:THR:HB	1:T:343:SER:O	2.21	0.40
1:U:119:LEU:HD23	1:U:119:LEU:HA	1.93	0.40
1:U:254:ALA:HB3	1:U:310:THR:OG1	2.22	0.40
1:E:306:GLY:HA3	1:E:327:TYR:HD1	1.87	0.40
1:F:86:LEU:HD13	1:F:86:LEU:HA	1.96	0.40
1:F:233:THR:OG1	1:F:234:TYR:N	2.52	0.40
1:F:466:LEU:HD12	1:F:466:LEU:HA	1.85	0.40
1:H:109:ARG:HB3	1:H:481:THR:HA	2.03	0.40
1:I:391:PHE:CD2	1:I:393:PHE:HE1	2.39	0.40
1:I:563:GLN:OE1	1:S:547:TYR:OH	2.34	0.40
1:J:233:THR:OG1	1:J:234:TYR:N	2.54	0.40
1:J:285:THR:OG1	1:J:286:GLY:N	2.54	0.40
1:K:68:GLY:C	1:K:518:ILE:HD11	2.46	0.40
1:N:443:SER:HA	1:N:448:VAL:HG12	2.03	0.40
1:P:237:LYS:O	1:P:326:ASN:ND2	2.54	0.40
1:P:285:THR:O	1:P:305:ARG:NH1	2.54	0.40
1:Q:109:ARG:HB3	1:Q:481:THR:HA	2.03	0.40
1:R:249:THR:HG22	1:R:313:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:309:ILE:HD12	1:R:313:ILE:HB	2.04	0.40
1:S:433:ILE:HD13	1:S:433:ILE:HA	1.96	0.40
1:T:119:LEU:HD23	1:T:119:LEU:HA	1.87	0.40
1:U:138:LEU:HB3	1:U:164:THR:HG21	2.04	0.40
1:V:125:ASN:O	1:V:129:THR:OG1	2.28	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	572/576 (99%)	524 (92%)	47 (8%)	1 (0%)	43	74
1	B	572/576 (99%)	526 (92%)	45 (8%)	1 (0%)	43	74
1	C	572/576 (99%)	524 (92%)	47 (8%)	1 (0%)	43	74
1	D	572/576 (99%)	522 (91%)	49 (9%)	1 (0%)	43	74
1	E	572/576 (99%)	522 (91%)	49 (9%)	1 (0%)	43	74
1	F	572/576 (99%)	517 (90%)	54 (9%)	1 (0%)	43	74
1	G	572/576 (99%)	528 (92%)	43 (8%)	1 (0%)	43	74
1	H	572/576 (99%)	521 (91%)	50 (9%)	1 (0%)	43	74
1	I	572/576 (99%)	523 (91%)	48 (8%)	1 (0%)	43	74
1	J	572/576 (99%)	526 (92%)	45 (8%)	1 (0%)	43	74
1	K	572/576 (99%)	519 (91%)	52 (9%)	1 (0%)	43	74
1	L	572/576 (99%)	523 (91%)	48 (8%)	1 (0%)	43	74
1	M	572/576 (99%)	526 (92%)	45 (8%)	1 (0%)	43	74
1	N	572/576 (99%)	527 (92%)	44 (8%)	1 (0%)	43	74
1	O	572/576 (99%)	517 (90%)	54 (9%)	1 (0%)	43	74
1	P	572/576 (99%)	521 (91%)	50 (9%)	1 (0%)	43	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	572/576 (99%)	518 (91%)	53 (9%)	1 (0%)	43	74
1	R	572/576 (99%)	522 (91%)	49 (9%)	1 (0%)	43	74
1	S	572/576 (99%)	521 (91%)	50 (9%)	1 (0%)	43	74
1	T	572/576 (99%)	519 (91%)	52 (9%)	1 (0%)	43	74
1	U	572/576 (99%)	524 (92%)	47 (8%)	1 (0%)	43	74
1	V	572/576 (99%)	523 (91%)	48 (8%)	1 (0%)	43	74
All	All	12584/12672 (99%)	11493 (91%)	1069 (8%)	22 (0%)	44	74

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	207	SER
1	F	207	SER
1	G	207	SER
1	H	207	SER
1	J	207	SER
1	K	207	SER
1	L	207	SER
1	M	207	SER
1	N	207	SER
1	P	207	SER
1	Q	207	SER
1	R	207	SER
1	S	207	SER
1	T	207	SER
1	U	207	SER
1	A	207	SER
1	B	207	SER
1	D	207	SER
1	E	207	SER
1	I	207	SER
1	O	207	SER
1	V	207	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	450/451 (100%)	450 (100%)	0	100	100
1	B	450/451 (100%)	449 (100%)	1 (0%)	87	85
1	C	450/451 (100%)	450 (100%)	0	100	100
1	D	450/451 (100%)	450 (100%)	0	100	100
1	E	450/451 (100%)	450 (100%)	0	100	100
1	F	450/451 (100%)	450 (100%)	0	100	100
1	G	450/451 (100%)	450 (100%)	0	100	100
1	H	450/451 (100%)	450 (100%)	0	100	100
1	I	450/451 (100%)	450 (100%)	0	100	100
1	J	450/451 (100%)	450 (100%)	0	100	100
1	K	450/451 (100%)	450 (100%)	0	100	100
1	L	450/451 (100%)	450 (100%)	0	100	100
1	M	450/451 (100%)	450 (100%)	0	100	100
1	N	450/451 (100%)	450 (100%)	0	100	100
1	O	450/451 (100%)	450 (100%)	0	100	100
1	P	450/451 (100%)	450 (100%)	0	100	100
1	Q	450/451 (100%)	450 (100%)	0	100	100
1	R	450/451 (100%)	450 (100%)	0	100	100
1	S	450/451 (100%)	450 (100%)	0	100	100
1	T	450/451 (100%)	450 (100%)	0	100	100
1	U	450/451 (100%)	450 (100%)	0	100	100
1	V	450/451 (100%)	450 (100%)	0	100	100
All	All	9900/9922 (100%)	9899 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	B	342	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (277) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	39	ASN
1	A	98	GLN
1	A	104	GLN
1	A	113	GLN
1	A	128	ASN
1	A	141	ASN
1	A	148	GLN
1	A	154	ASN
1	A	155	GLN
1	A	165	GLN
1	A	383	ASN
1	A	511	GLN
1	A	519	ASN
1	A	568	GLN
1	B	63	GLN
1	B	85	GLN
1	B	98	GLN
1	B	104	GLN
1	B	113	GLN
1	B	125	ASN
1	B	165	GLN
1	B	294	ASN
1	B	511	GLN
1	B	519	ASN
1	B	534	GLN
1	B	568	GLN
1	C	63	GLN
1	C	85	GLN
1	C	98	GLN
1	C	113	GLN
1	C	154	ASN
1	C	155	GLN
1	C	165	GLN
1	C	279	ASN
1	C	322	ASN
1	C	383	ASN
1	C	396	ASN
1	C	424	ASN
1	C	431	GLN
1	C	511	GLN
1	C	519	ASN
1	C	568	GLN

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Mol	Chain	Res	Type
1	D	13	ASN
1	D	98	GLN
1	D	104	GLN
1	D	113	GLN
1	D	141	ASN
1	D	154	ASN
1	D	155	GLN
1	D	165	GLN
1	D	396	ASN
1	D	431	GLN
1	D	511	GLN
1	D	519	ASN
1	D	520	ASN
1	E	13	ASN
1	E	63	GLN
1	E	85	GLN
1	E	98	GLN
1	E	101	GLN
1	E	104	GLN
1	E	113	GLN
1	E	128	ASN
1	E	141	ASN
1	E	154	ASN
1	E	155	GLN
1	E	279	ASN
1	E	288	GLN
1	E	294	ASN
1	E	376	ASN
1	E	396	ASN
1	E	424	ASN
1	E	511	GLN
1	E	519	ASN
1	F	13	ASN
1	F	98	GLN
1	F	104	GLN
1	F	113	GLN
1	F	128	ASN
1	F	155	GLN
1	F	294	ASN
1	F	519	ASN
1	F	568	GLN
1	G	13	ASN

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Mol	Chain	Res	Type
1	G	98	GLN
1	G	104	GLN
1	G	113	GLN
1	G	128	ASN
1	G	165	GLN
1	G	511	GLN
1	G	519	ASN
1	G	520	ASN
1	G	534	GLN
1	H	85	GLN
1	H	98	GLN
1	H	104	GLN
1	H	113	GLN
1	H	154	ASN
1	H	279	ASN
1	H	294	ASN
1	H	519	ASN
1	H	520	ASN
1	I	13	ASN
1	I	98	GLN
1	I	113	GLN
1	I	154	ASN
1	I	155	GLN
1	I	511	GLN
1	I	519	ASN
1	I	568	GLN
1	J	63	GLN
1	J	98	GLN
1	J	113	GLN
1	J	128	ASN
1	J	154	ASN
1	J	165	GLN
1	J	294	ASN
1	J	383	ASN
1	J	444	ASN
1	J	511	GLN
1	J	519	ASN
1	J	520	ASN
1	J	568	GLN
1	K	39	ASN
1	K	63	GLN
1	K	98	GLN

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Mol	Chain	Res	Type
1	K	113	GLN
1	K	136	GLN
1	K	155	GLN
1	K	279	ASN
1	K	288	GLN
1	K	424	ASN
1	K	444	ASN
1	K	511	GLN
1	K	519	ASN
1	K	520	ASN
1	K	527	ASN
1	L	63	GLN
1	L	98	GLN
1	L	104	GLN
1	L	113	GLN
1	L	125	ASN
1	L	128	ASN
1	L	145	GLN
1	L	155	GLN
1	L	294	ASN
1	L	376	ASN
1	L	383	ASN
1	L	511	GLN
1	L	519	ASN
1	L	568	GLN
1	M	63	GLN
1	M	98	GLN
1	M	104	GLN
1	M	113	GLN
1	M	125	ASN
1	M	128	ASN
1	M	145	GLN
1	M	155	GLN
1	M	294	ASN
1	M	499	ASN
1	M	511	GLN
1	M	519	ASN
1	M	568	GLN
1	N	85	GLN
1	N	98	GLN
1	N	113	GLN
1	N	128	ASN

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Mol	Chain	Res	Type
1	N	154	ASN
1	N	155	GLN
1	N	511	GLN
1	N	519	ASN
1	O	63	GLN
1	O	98	GLN
1	O	113	GLN
1	O	128	ASN
1	O	136	GLN
1	O	141	ASN
1	O	145	GLN
1	O	155	GLN
1	O	179	GLN
1	O	294	ASN
1	O	499	ASN
1	O	511	GLN
1	O	519	ASN
1	P	63	GLN
1	P	98	GLN
1	P	104	GLN
1	P	113	GLN
1	P	128	ASN
1	P	136	GLN
1	P	154	ASN
1	P	155	GLN
1	P	251	GLN
1	P	383	ASN
1	P	424	ASN
1	P	511	GLN
1	P	519	ASN
1	P	520	ASN
1	P	568	GLN
1	Q	63	GLN
1	Q	98	GLN
1	Q	104	GLN
1	Q	113	GLN
1	Q	128	ASN
1	Q	141	ASN
1	Q	154	ASN
1	Q	179	GLN
1	Q	279	ASN
1	Q	294	ASN

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Mol	Chain	Res	Type
1	Q	444	ASN
1	Q	511	GLN
1	Q	519	ASN
1	Q	568	GLN
1	R	98	GLN
1	R	104	GLN
1	R	113	GLN
1	R	128	ASN
1	R	141	ASN
1	R	155	GLN
1	R	179	GLN
1	R	251	GLN
1	R	294	ASN
1	R	499	ASN
1	R	511	GLN
1	R	519	ASN
1	S	98	GLN
1	S	104	GLN
1	S	128	ASN
1	S	141	ASN
1	S	145	GLN
1	S	154	ASN
1	S	155	GLN
1	S	294	ASN
1	S	511	GLN
1	S	519	ASN
1	S	568	GLN
1	T	63	GLN
1	T	85	GLN
1	T	98	GLN
1	T	104	GLN
1	T	113	GLN
1	T	141	ASN
1	T	154	ASN
1	T	155	GLN
1	T	271	ASN
1	T	499	ASN
1	T	511	GLN
1	T	519	ASN
1	T	568	GLN
1	U	63	GLN
1	U	98	GLN

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Mol	Chain	Res	Type
1	U	104	GLN
1	U	113	GLN
1	U	128	ASN
1	U	145	GLN
1	U	154	ASN
1	U	155	GLN
1	U	431	GLN
1	U	511	GLN
1	U	519	ASN
1	U	568	GLN
1	V	63	GLN
1	V	98	GLN
1	V	104	GLN
1	V	113	GLN
1	V	128	ASN
1	V	136	GLN
1	V	141	ASN
1	V	155	GLN
1	V	288	GLN
1	V	383	ASN
1	V	511	GLN
1	V	519	ASN
1	V	520	ASN
1	V	568	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

374 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	P8E	A	613	-	15,16,17	1.56	2 (13%)	17,23,26	1.26	2 (11%)
2	P8E	O	602	-	15,16,17	1.58	2 (13%)	17,23,26	1.31	2 (11%)
2	P8E	F	608	-	15,16,17	1.51	2 (13%)	17,23,26	1.39	2 (11%)
2	P8E	H	603	-	15,16,17	1.55	2 (13%)	17,23,26	1.39	3 (17%)
2	P8E	I	601	-	15,16,17	1.53	2 (13%)	17,23,26	1.27	2 (11%)
2	P8E	K	605	-	15,16,17	1.55	2 (13%)	17,23,26	1.36	3 (17%)
2	P8E	S	606	-	15,16,17	1.54	2 (13%)	17,23,26	1.40	4 (23%)
2	P8E	E	610	-	15,16,17	1.57	2 (13%)	17,23,26	1.26	2 (11%)
2	P8E	J	607	-	15,16,17	1.59	2 (13%)	17,23,26	1.49	2 (11%)
2	P8E	P	608	-	15,16,17	1.55	2 (13%)	17,23,26	1.41	3 (17%)
2	P8E	V	616	-	15,16,17	1.49	2 (13%)	17,23,26	1.42	4 (23%)
2	P8E	A	603	-	15,16,17	1.53	2 (13%)	17,23,26	1.41	3 (17%)
2	P8E	S	602	-	15,16,17	1.57	2 (13%)	17,23,26	1.29	2 (11%)
2	P8E	A	604	-	15,16,17	1.55	2 (13%)	17,23,26	1.40	3 (17%)
2	P8E	H	615	-	15,16,17	1.52	2 (13%)	17,23,26	1.36	3 (17%)
2	P8E	V	601	-	15,16,17	1.57	2 (13%)	17,23,26	1.30	2 (11%)
2	P8E	U	610	-	15,16,17	1.58	2 (13%)	17,23,26	1.29	3 (17%)
2	P8E	K	609	-	15,16,17	1.58	2 (13%)	17,23,26	1.32	3 (17%)
2	P8E	O	607	-	15,16,17	1.59	2 (13%)	17,23,26	1.40	3 (17%)
2	P8E	L	615	-	15,16,17	1.56	2 (13%)	17,23,26	1.44	4 (23%)
2	P8E	A	616	-	15,16,17	1.48	2 (13%)	17,23,26	1.57	5 (29%)
2	P8E	D	613	-	15,16,17	1.57	2 (13%)	17,23,26	1.27	2 (11%)
2	P8E	J	613	-	15,16,17	1.56	2 (13%)	17,23,26	1.25	2 (11%)
2	P8E	A	605	-	15,16,17	1.55	2 (13%)	17,23,26	1.34	3 (17%)
2	P8E	S	607	-	15,16,17	1.59	2 (13%)	17,23,26	1.49	3 (17%)
2	P8E	V	617	-	15,16,17	1.65	2 (13%)	17,23,26	1.58	4 (23%)
2	P8E	S	611	-	15,16,17	1.58	2 (13%)	17,23,26	1.33	3 (17%)
2	P8E	R	616	-	15,16,17	1.51	2 (13%)	17,23,26	1.49	4 (23%)
2	P8E	H	610	-	15,16,17	1.58	2 (13%)	17,23,26	1.34	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	P8E	E	617	-	15,16,17	1.66	2 (13%)	17,23,26	1.66	4 (23%)
2	P8E	P	616	-	15,16,17	1.51	2 (13%)	17,23,26	1.47	4 (23%)
2	P8E	V	602	-	15,16,17	1.58	2 (13%)	17,23,26	1.40	3 (17%)
2	P8E	N	604	-	15,16,17	1.54	2 (13%)	17,23,26	1.35	2 (11%)
2	P8E	N	613	-	15,16,17	1.57	2 (13%)	17,23,26	1.29	2 (11%)
2	P8E	T	615	-	15,16,17	1.54	2 (13%)	17,23,26	1.40	2 (11%)
2	P8E	K	610	-	15,16,17	1.56	2 (13%)	17,23,26	1.26	2 (11%)
2	P8E	H	611	-	15,16,17	1.60	2 (13%)	17,23,26	1.33	3 (17%)
2	P8E	K	615	-	15,16,17	1.54	2 (13%)	17,23,26	1.48	4 (23%)
2	P8E	U	607	-	15,16,17	1.63	2 (13%)	17,23,26	1.51	3 (17%)
2	P8E	C	610	-	15,16,17	1.59	2 (13%)	17,23,26	1.35	3 (17%)
2	P8E	F	613	-	15,16,17	1.55	2 (13%)	17,23,26	1.20	1 (5%)
2	P8E	U	608	-	15,16,17	1.53	2 (13%)	17,23,26	1.41	3 (17%)
2	P8E	V	607	-	15,16,17	1.60	2 (13%)	17,23,26	1.59	3 (17%)
2	P8E	E	607	-	15,16,17	1.60	2 (13%)	17,23,26	1.46	3 (17%)
2	P8E	F	610	-	15,16,17	1.57	2 (13%)	17,23,26	1.27	3 (17%)
2	P8E	R	604	-	15,16,17	1.54	2 (13%)	17,23,26	1.37	2 (11%)
2	P8E	L	601	-	15,16,17	1.55	2 (13%)	17,23,26	1.34	3 (17%)
2	P8E	O	605	-	15,16,17	1.53	2 (13%)	17,23,26	1.33	3 (17%)
2	P8E	U	612	-	15,16,17	1.54	2 (13%)	17,23,26	1.38	3 (17%)
2	P8E	A	602	-	15,16,17	1.55	2 (13%)	17,23,26	1.37	3 (17%)
2	P8E	E	612	-	15,16,17	1.53	2 (13%)	17,23,26	1.44	4 (23%)
2	P8E	L	609	-	15,16,17	1.59	2 (13%)	17,23,26	1.36	2 (11%)
2	P8E	M	608	-	15,16,17	1.51	2 (13%)	17,23,26	1.38	2 (11%)
2	P8E	G	601	-	15,16,17	1.53	2 (13%)	17,23,26	1.30	2 (11%)
2	P8E	A	615	-	15,16,17	1.54	2 (13%)	17,23,26	1.34	3 (17%)
2	P8E	F	609	-	15,16,17	1.59	2 (13%)	17,23,26	1.39	2 (11%)
2	P8E	U	613	-	15,16,17	1.56	2 (13%)	17,23,26	1.34	3 (17%)
2	P8E	T	614	-	15,16,17	1.57	2 (13%)	17,23,26	1.31	2 (11%)
2	P8E	P	610	-	15,16,17	1.56	2 (13%)	17,23,26	1.28	3 (17%)
2	P8E	T	617	-	15,16,17	1.63	2 (13%)	17,23,26	1.56	4 (23%)
2	P8E	T	613	-	15,16,17	1.57	2 (13%)	17,23,26	1.27	2 (11%)
2	P8E	P	611	-	15,16,17	1.57	2 (13%)	17,23,26	1.29	2 (11%)
2	P8E	U	601	-	15,16,17	1.54	2 (13%)	17,23,26	1.25	2 (11%)
2	P8E	G	602	-	15,16,17	1.55	2 (13%)	17,23,26	1.33	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	P8E	T	605	-	15,16,17	1.55	2 (13%)	17,23,26	1.40	3 (17%)
2	P8E	E	613	-	15,16,17	1.57	2 (13%)	17,23,26	1.29	3 (17%)
2	P8E	S	604	-	15,16,17	1.54	2 (13%)	17,23,26	1.35	2 (11%)
2	P8E	U	611	-	15,16,17	1.58	2 (13%)	17,23,26	1.43	3 (17%)
2	P8E	A	610	-	15,16,17	1.58	2 (13%)	17,23,26	1.26	2 (11%)
2	P8E	N	616	-	15,16,17	1.53	2 (13%)	17,23,26	1.44	4 (23%)
2	P8E	R	602	-	15,16,17	1.56	2 (13%)	17,23,26	1.29	2 (11%)
2	P8E	D	608	-	15,16,17	1.54	2 (13%)	17,23,26	1.37	3 (17%)
2	P8E	H	613	-	15,16,17	1.59	2 (13%)	17,23,26	1.29	2 (11%)
2	P8E	G	607	-	15,16,17	1.60	2 (13%)	17,23,26	1.53	3 (17%)
2	P8E	R	607	-	15,16,17	1.59	2 (13%)	17,23,26	1.47	3 (17%)
2	P8E	U	603	-	15,16,17	1.53	2 (13%)	17,23,26	1.35	3 (17%)
2	P8E	N	609	-	15,16,17	1.56	2 (13%)	17,23,26	1.30	2 (11%)
2	P8E	M	601	-	15,16,17	1.54	2 (13%)	17,23,26	1.26	2 (11%)
2	P8E	H	606	-	15,16,17	1.52	2 (13%)	17,23,26	1.43	4 (23%)
2	P8E	O	612	-	15,16,17	1.53	2 (13%)	17,23,26	1.44	3 (17%)
2	P8E	R	601	-	15,16,17	1.60	2 (13%)	17,23,26	1.28	3 (17%)
2	P8E	S	603	-	15,16,17	1.53	2 (13%)	17,23,26	1.39	3 (17%)
2	P8E	I	604	-	15,16,17	1.56	2 (13%)	17,23,26	1.38	3 (17%)
2	P8E	K	606	-	15,16,17	1.55	2 (13%)	17,23,26	1.47	4 (23%)
2	P8E	K	612	-	15,16,17	1.51	2 (13%)	17,23,26	1.41	3 (17%)
2	P8E	L	616	-	15,16,17	1.50	2 (13%)	17,23,26	1.45	4 (23%)
2	P8E	C	606	-	15,16,17	1.52	2 (13%)	17,23,26	1.42	4 (23%)
2	P8E	L	602	-	15,16,17	1.55	2 (13%)	17,23,26	1.32	2 (11%)
2	P8E	E	616	-	15,16,17	1.52	2 (13%)	17,23,26	1.32	2 (11%)
2	P8E	Q	605	-	15,16,17	1.56	2 (13%)	17,23,26	1.41	3 (17%)
2	P8E	Q	614	-	15,16,17	1.55	2 (13%)	17,23,26	1.21	2 (11%)
2	P8E	A	607	-	15,16,17	1.61	2 (13%)	17,23,26	1.48	3 (17%)
2	P8E	L	610	-	15,16,17	1.58	2 (13%)	17,23,26	1.32	3 (17%)
2	P8E	F	602	-	15,16,17	1.55	2 (13%)	17,23,26	1.29	2 (11%)
2	P8E	E	604	-	15,16,17	1.56	2 (13%)	17,23,26	1.38	3 (17%)
2	P8E	I	616	-	15,16,17	1.51	2 (13%)	17,23,26	1.47	4 (23%)
2	P8E	Q	617	-	15,16,17	1.64	2 (13%)	17,23,26	1.60	4 (23%)
2	P8E	B	614	-	15,16,17	1.57	2 (13%)	17,23,26	1.34	2 (11%)
2	P8E	L	607	-	15,16,17	1.61	2 (13%)	17,23,26	1.46	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	P8E	H	604	-	15,16,17	1.54	2 (13%)	17,23,26	1.34	2 (11%)
2	P8E	N	601	-	15,16,17	1.57	2 (13%)	17,23,26	1.28	2 (11%)
2	P8E	T	608	-	15,16,17	1.53	2 (13%)	17,23,26	1.30	1 (5%)
2	P8E	M	610	-	15,16,17	1.58	2 (13%)	17,23,26	1.30	2 (11%)
2	P8E	N	615	-	15,16,17	1.56	2 (13%)	17,23,26	1.29	2 (11%)
2	P8E	C	604	-	15,16,17	1.55	2 (13%)	17,23,26	1.35	2 (11%)
2	P8E	S	612	-	15,16,17	1.53	2 (13%)	17,23,26	1.41	3 (17%)
2	P8E	O	614	-	15,16,17	1.58	2 (13%)	17,23,26	1.26	2 (11%)
2	P8E	S	614	-	15,16,17	1.59	2 (13%)	17,23,26	1.28	2 (11%)
2	P8E	G	615	-	15,16,17	1.52	2 (13%)	17,23,26	1.48	4 (23%)
2	P8E	Q	609	-	15,16,17	1.57	2 (13%)	17,23,26	1.28	2 (11%)
2	P8E	B	616	-	15,16,17	1.49	2 (13%)	17,23,26	1.57	5 (29%)
2	P8E	P	606	-	15,16,17	1.53	2 (13%)	17,23,26	1.49	4 (23%)
2	P8E	E	602	-	15,16,17	1.60	2 (13%)	17,23,26	1.38	3 (17%)
2	P8E	J	605	-	15,16,17	1.55	2 (13%)	17,23,26	1.44	4 (23%)
2	P8E	E	605	-	15,16,17	1.55	2 (13%)	17,23,26	1.42	4 (23%)
2	P8E	A	606	-	15,16,17	1.57	2 (13%)	17,23,26	1.46	3 (17%)
2	P8E	I	610	-	15,16,17	1.59	2 (13%)	17,23,26	1.32	3 (17%)
2	P8E	Q	608	-	15,16,17	1.54	2 (13%)	17,23,26	1.30	2 (11%)
2	P8E	C	614	-	15,16,17	1.59	2 (13%)	17,23,26	1.32	3 (17%)
2	P8E	Q	610	-	15,16,17	1.55	2 (13%)	17,23,26	1.24	2 (11%)
2	P8E	L	614	-	15,16,17	1.57	2 (13%)	17,23,26	1.29	2 (11%)
2	P8E	P	604	-	15,16,17	1.54	2 (13%)	17,23,26	1.37	3 (17%)
2	P8E	H	602	-	15,16,17	1.54	2 (13%)	17,23,26	1.28	2 (11%)
2	P8E	M	611	-	15,16,17	1.57	2 (13%)	17,23,26	1.31	3 (17%)
2	P8E	V	614	-	15,16,17	1.57	2 (13%)	17,23,26	1.27	2 (11%)
2	P8E	N	603	-	15,16,17	1.51	2 (13%)	17,23,26	1.36	3 (17%)
2	P8E	B	611	-	15,16,17	1.61	2 (13%)	17,23,26	1.38	3 (17%)
2	P8E	O	617	-	15,16,17	1.65	2 (13%)	17,23,26	1.60	4 (23%)
2	P8E	S	617	-	15,16,17	1.63	2 (13%)	17,23,26	1.59	4 (23%)
2	P8E	N	602	-	15,16,17	1.55	2 (13%)	17,23,26	1.29	2 (11%)
2	P8E	L	608	-	15,16,17	1.52	2 (13%)	17,23,26	1.24	1 (5%)
2	P8E	L	604	-	15,16,17	1.55	2 (13%)	17,23,26	1.38	3 (17%)
2	P8E	H	616	-	15,16,17	1.53	2 (13%)	17,23,26	1.46	4 (23%)
2	P8E	R	615	-	15,16,17	1.53	2 (13%)	17,23,26	1.33	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	P8E	H	607	-	15,16,17	1.59	2 (13%)	17,23,26	1.51	3 (17%)
2	P8E	I	614	-	15,16,17	1.59	2 (13%)	17,23,26	1.31	2 (11%)
2	P8E	D	605	-	15,16,17	1.54	2 (13%)	17,23,26	1.37	3 (17%)
2	P8E	F	604	-	15,16,17	1.55	2 (13%)	17,23,26	1.40	2 (11%)
2	P8E	G	614	-	15,16,17	1.58	2 (13%)	17,23,26	1.29	2 (11%)
2	P8E	H	612	-	15,16,17	1.53	2 (13%)	17,23,26	1.45	3 (17%)
2	P8E	H	608	-	15,16,17	1.52	2 (13%)	17,23,26	1.36	2 (11%)
2	P8E	I	602	-	15,16,17	1.56	2 (13%)	17,23,26	1.33	3 (17%)
2	P8E	J	609	-	15,16,17	1.56	2 (13%)	17,23,26	1.23	1 (5%)
2	P8E	U	604	-	15,16,17	1.55	2 (13%)	17,23,26	1.39	2 (11%)
2	P8E	N	607	-	15,16,17	1.58	2 (13%)	17,23,26	1.40	3 (17%)
2	P8E	U	606	-	15,16,17	1.54	2 (13%)	17,23,26	1.47	4 (23%)
2	P8E	C	616	-	15,16,17	1.52	2 (13%)	17,23,26	1.47	4 (23%)
2	P8E	L	606	-	15,16,17	1.54	2 (13%)	17,23,26	1.45	4 (23%)
2	P8E	C	602	-	15,16,17	1.53	2 (13%)	17,23,26	1.26	1 (5%)
2	P8E	C	607	-	15,16,17	1.60	2 (13%)	17,23,26	1.50	3 (17%)
2	P8E	S	608	-	15,16,17	1.53	2 (13%)	17,23,26	1.37	3 (17%)
2	P8E	C	615	-	15,16,17	1.54	2 (13%)	17,23,26	1.33	1 (5%)
2	P8E	D	602	-	15,16,17	1.54	2 (13%)	17,23,26	1.24	2 (11%)
2	P8E	B	617	-	15,16,17	1.65	2 (13%)	17,23,26	1.63	4 (23%)
2	P8E	I	611	-	15,16,17	1.59	2 (13%)	17,23,26	1.37	3 (17%)
2	P8E	J	610	-	15,16,17	1.57	2 (13%)	17,23,26	1.31	3 (17%)
2	P8E	V	605	-	15,16,17	1.55	2 (13%)	17,23,26	1.33	2 (11%)
2	P8E	T	601	-	15,16,17	1.55	2 (13%)	17,23,26	1.29	2 (11%)
2	P8E	Q	606	-	15,16,17	1.52	2 (13%)	17,23,26	1.45	4 (23%)
2	P8E	G	606	-	15,16,17	1.52	2 (13%)	17,23,26	1.45	4 (23%)
2	P8E	E	601	-	15,16,17	1.57	2 (13%)	17,23,26	1.30	3 (17%)
2	P8E	G	616	-	15,16,17	1.52	2 (13%)	17,23,26	1.46	4 (23%)
2	P8E	A	612	-	15,16,17	1.51	2 (13%)	17,23,26	1.45	3 (17%)
2	P8E	M	606	-	15,16,17	1.56	2 (13%)	17,23,26	1.47	4 (23%)
2	P8E	J	615	-	15,16,17	1.52	2 (13%)	17,23,26	1.39	3 (17%)
2	P8E	P	602	-	15,16,17	1.58	2 (13%)	17,23,26	1.48	4 (23%)
2	P8E	D	609	-	15,16,17	1.58	2 (13%)	17,23,26	1.36	3 (17%)
2	P8E	R	612	-	15,16,17	1.54	2 (13%)	17,23,26	1.38	3 (17%)
2	P8E	T	603	-	15,16,17	1.53	2 (13%)	17,23,26	1.38	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	P8E	C	611	-	15,16,17	1.56	2 (13%)	17,23,26	1.28	2 (11%)
2	P8E	S	613	-	15,16,17	1.56	2 (13%)	17,23,26	1.20	1 (5%)
2	P8E	B	609	-	15,16,17	1.59	2 (13%)	17,23,26	1.43	3 (17%)
2	P8E	H	601	-	15,16,17	1.55	2 (13%)	17,23,26	1.19	2 (11%)
2	P8E	F	606	-	15,16,17	1.53	2 (13%)	17,23,26	1.48	4 (23%)
2	P8E	P	607	-	15,16,17	1.58	2 (13%)	17,23,26	1.45	3 (17%)
2	P8E	I	607	-	15,16,17	1.59	2 (13%)	17,23,26	1.44	3 (17%)
2	P8E	P	615	-	15,16,17	1.56	2 (13%)	17,23,26	1.43	3 (17%)
2	P8E	P	612	-	15,16,17	1.51	2 (13%)	17,23,26	1.45	3 (17%)
2	P8E	V	612	-	15,16,17	1.53	2 (13%)	17,23,26	1.42	3 (17%)
2	P8E	F	616	-	15,16,17	1.50	2 (13%)	17,23,26	1.56	5 (29%)
2	P8E	P	601	-	15,16,17	1.59	2 (13%)	17,23,26	1.28	3 (17%)
2	P8E	U	616	-	15,16,17	1.53	2 (13%)	17,23,26	1.46	4 (23%)
2	P8E	E	606	-	15,16,17	1.57	2 (13%)	17,23,26	1.50	4 (23%)
2	P8E	C	601	-	15,16,17	1.63	2 (13%)	17,23,26	1.50	3 (17%)
2	P8E	L	603	-	15,16,17	1.55	2 (13%)	17,23,26	1.37	3 (17%)
2	P8E	I	606	-	15,16,17	1.56	2 (13%)	17,23,26	1.49	4 (23%)
2	P8E	P	609	-	15,16,17	1.58	2 (13%)	17,23,26	1.36	2 (11%)
2	P8E	A	601	-	15,16,17	1.59	2 (13%)	17,23,26	1.31	3 (17%)
2	P8E	C	617	-	15,16,17	1.66	2 (13%)	17,23,26	1.56	4 (23%)
2	P8E	F	615	-	15,16,17	1.54	2 (13%)	17,23,26	1.33	3 (17%)
2	P8E	G	609	-	15,16,17	1.59	2 (13%)	17,23,26	1.35	2 (11%)
2	P8E	L	617	-	15,16,17	1.63	2 (13%)	17,23,26	1.59	4 (23%)
2	P8E	R	614	-	15,16,17	1.58	2 (13%)	17,23,26	1.31	2 (11%)
2	P8E	G	617	-	15,16,17	1.65	2 (13%)	17,23,26	1.61	4 (23%)
2	P8E	N	608	-	15,16,17	1.53	2 (13%)	17,23,26	1.42	3 (17%)
2	P8E	P	617	-	15,16,17	1.62	2 (13%)	17,23,26	1.62	4 (23%)
2	P8E	D	610	-	15,16,17	1.57	2 (13%)	17,23,26	1.24	2 (11%)
2	P8E	T	616	-	15,16,17	1.51	2 (13%)	17,23,26	1.45	4 (23%)
2	P8E	B	603	-	15,16,17	1.52	2 (13%)	17,23,26	1.36	3 (17%)
2	P8E	O	613	-	15,16,17	1.57	2 (13%)	17,23,26	1.33	3 (17%)
2	P8E	J	608	-	15,16,17	1.52	2 (13%)	17,23,26	1.31	1 (5%)
2	P8E	F	601	-	15,16,17	1.58	2 (13%)	17,23,26	1.33	3 (17%)
2	P8E	K	614	-	15,16,17	1.58	2 (13%)	17,23,26	1.25	1 (5%)
2	P8E	Q	602	-	15,16,17	1.60	2 (13%)	17,23,26	1.49	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	P8E	M	604	-	15,16,17	1.54	2 (13%)	17,23,26	1.37	2 (11%)
2	P8E	D	604	-	15,16,17	1.52	2 (13%)	17,23,26	1.34	2 (11%)
2	P8E	L	611	-	15,16,17	1.58	2 (13%)	17,23,26	1.29	2 (11%)
2	P8E	J	606	-	15,16,17	1.55	2 (13%)	17,23,26	1.44	4 (23%)
2	P8E	D	616	-	15,16,17	1.51	2 (13%)	17,23,26	1.45	4 (23%)
2	P8E	E	603	-	15,16,17	1.54	2 (13%)	17,23,26	1.36	3 (17%)
2	P8E	F	617	-	15,16,17	1.65	2 (13%)	17,23,26	1.55	4 (23%)
2	P8E	K	604	-	15,16,17	1.54	2 (13%)	17,23,26	1.36	2 (11%)
2	P8E	A	611	-	15,16,17	1.55	2 (13%)	17,23,26	1.25	2 (11%)
2	P8E	N	612	-	15,16,17	1.52	2 (13%)	17,23,26	1.40	3 (17%)
2	P8E	I	603	-	15,16,17	1.53	2 (13%)	17,23,26	1.40	3 (17%)
2	P8E	O	615	-	15,16,17	1.53	2 (13%)	17,23,26	1.35	3 (17%)
2	P8E	Q	611	-	15,16,17	1.60	2 (13%)	17,23,26	1.36	3 (17%)
2	P8E	R	610	-	15,16,17	1.57	2 (13%)	17,23,26	1.27	2 (11%)
2	P8E	G	611	-	15,16,17	1.57	2 (13%)	17,23,26	1.27	2 (11%)
2	P8E	M	602	-	15,16,17	1.53	2 (13%)	17,23,26	1.31	1 (5%)
2	P8E	F	614	-	15,16,17	1.59	2 (13%)	17,23,26	1.31	2 (11%)
2	P8E	O	603	-	15,16,17	1.53	2 (13%)	17,23,26	1.34	3 (17%)
2	P8E	J	612	-	15,16,17	1.53	2 (13%)	17,23,26	1.40	4 (23%)
2	P8E	M	614	-	15,16,17	1.59	2 (13%)	17,23,26	1.33	3 (17%)
2	P8E	Q	616	-	15,16,17	1.54	2 (13%)	17,23,26	1.50	4 (23%)
2	P8E	F	607	-	15,16,17	1.61	2 (13%)	17,23,26	1.53	4 (23%)
2	P8E	D	606	-	15,16,17	1.53	2 (13%)	17,23,26	1.45	4 (23%)
2	P8E	N	606	-	15,16,17	1.55	2 (13%)	17,23,26	1.49	4 (23%)
2	P8E	O	610	-	15,16,17	1.56	2 (13%)	17,23,26	1.27	2 (11%)
2	P8E	L	612	-	15,16,17	1.53	2 (13%)	17,23,26	1.41	3 (17%)
2	P8E	T	610	-	15,16,17	1.55	2 (13%)	17,23,26	1.25	2 (11%)
2	P8E	Q	607	-	15,16,17	1.63	2 (13%)	17,23,26	1.47	3 (17%)
2	P8E	O	611	-	15,16,17	1.58	2 (13%)	17,23,26	1.30	2 (11%)
2	P8E	C	603	-	15,16,17	1.55	2 (13%)	17,23,26	1.38	3 (17%)
2	P8E	M	616	-	15,16,17	1.51	2 (13%)	17,23,26	1.45	4 (23%)
2	P8E	I	612	-	15,16,17	1.53	2 (13%)	17,23,26	1.40	3 (17%)
2	P8E	N	614	-	15,16,17	1.59	2 (13%)	17,23,26	1.29	2 (11%)
2	P8E	B	610	-	15,16,17	1.57	2 (13%)	17,23,26	1.29	3 (17%)
2	P8E	D	615	-	15,16,17	1.53	2 (13%)	17,23,26	1.40	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	P8E	L	613	-	15,16,17	1.58	2 (13%)	17,23,26	1.30	3 (17%)
2	P8E	Q	603	-	15,16,17	1.54	2 (13%)	17,23,26	1.38	3 (17%)
2	P8E	E	614	-	15,16,17	1.59	2 (13%)	17,23,26	1.32	3 (17%)
2	P8E	G	603	-	15,16,17	1.53	2 (13%)	17,23,26	1.37	3 (17%)
2	P8E	R	617	-	15,16,17	1.65	2 (13%)	17,23,26	1.59	4 (23%)
2	P8E	T	604	-	15,16,17	1.55	2 (13%)	17,23,26	1.37	2 (11%)
2	P8E	K	603	-	15,16,17	1.54	2 (13%)	17,23,26	1.38	3 (17%)
2	P8E	J	611	-	15,16,17	1.56	2 (13%)	17,23,26	1.24	2 (11%)
2	P8E	S	601	-	15,16,17	1.56	2 (13%)	17,23,26	1.32	3 (17%)
2	P8E	K	617	-	15,16,17	1.65	2 (13%)	17,23,26	1.57	3 (17%)
2	P8E	Q	604	-	15,16,17	1.56	2 (13%)	17,23,26	1.39	2 (11%)
2	P8E	V	603	-	15,16,17	1.53	2 (13%)	17,23,26	1.34	3 (17%)
2	P8E	H	605	-	15,16,17	1.53	2 (13%)	17,23,26	1.34	2 (11%)
2	P8E	J	616	-	15,16,17	1.53	2 (13%)	17,23,26	1.47	4 (23%)
2	P8E	J	602	-	15,16,17	1.58	2 (13%)	17,23,26	1.32	2 (11%)
2	P8E	N	611	-	15,16,17	1.60	2 (13%)	17,23,26	1.38	3 (17%)
2	P8E	D	611	-	15,16,17	1.58	2 (13%)	17,23,26	1.29	2 (11%)
2	P8E	V	608	-	15,16,17	1.52	2 (13%)	17,23,26	1.30	2 (11%)
2	P8E	R	608	-	15,16,17	1.54	2 (13%)	17,23,26	1.22	1 (5%)
2	P8E	I	617	-	15,16,17	1.64	2 (13%)	17,23,26	1.57	4 (23%)
2	P8E	N	617	-	15,16,17	1.66	2 (13%)	17,23,26	1.57	4 (23%)
2	P8E	K	602	-	15,16,17	1.58	2 (13%)	17,23,26	1.33	3 (17%)
2	P8E	K	613	-	15,16,17	1.56	2 (13%)	17,23,26	1.32	2 (11%)
2	P8E	R	609	-	15,16,17	1.58	2 (13%)	17,23,26	1.33	2 (11%)
2	P8E	M	617	-	15,16,17	1.66	2 (13%)	17,23,26	1.54	4 (23%)
2	P8E	F	605	-	15,16,17	1.55	2 (13%)	17,23,26	1.42	3 (17%)
2	P8E	V	611	-	15,16,17	1.57	2 (13%)	17,23,26	1.25	2 (11%)
2	P8E	H	614	-	15,16,17	1.54	2 (13%)	17,23,26	1.31	2 (11%)
2	P8E	O	606	-	15,16,17	1.54	2 (13%)	17,23,26	1.43	4 (23%)
2	P8E	D	607	-	15,16,17	1.62	2 (13%)	17,23,26	1.51	3 (17%)
2	P8E	M	613	-	15,16,17	1.55	2 (13%)	17,23,26	1.20	1 (5%)
2	P8E	E	611	-	15,16,17	1.57	2 (13%)	17,23,26	1.28	2 (11%)
2	P8E	R	613	-	15,16,17	1.58	2 (13%)	17,23,26	1.29	3 (17%)
2	P8E	T	606	-	15,16,17	1.54	2 (13%)	17,23,26	1.47	4 (23%)
2	P8E	B	613	-	15,16,17	1.58	2 (13%)	17,23,26	1.37	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	P8E	G	610	-	15,16,17	1.57	2 (13%)	17,23,26	1.29	3 (17%)
2	P8E	G	605	-	15,16,17	1.53	2 (13%)	17,23,26	1.38	3 (17%)
2	P8E	C	612	-	15,16,17	1.52	2 (13%)	17,23,26	1.45	3 (17%)
2	P8E	M	607	-	15,16,17	1.61	2 (13%)	17,23,26	1.44	3 (17%)
2	P8E	P	605	-	15,16,17	1.54	2 (13%)	17,23,26	1.42	3 (17%)
2	P8E	R	606	-	15,16,17	1.53	2 (13%)	17,23,26	1.43	4 (23%)
2	P8E	I	613	-	15,16,17	1.56	2 (13%)	17,23,26	1.31	2 (11%)
2	P8E	N	605	-	15,16,17	1.53	2 (13%)	17,23,26	1.32	2 (11%)
2	P8E	K	607	-	15,16,17	1.58	2 (13%)	17,23,26	1.49	3 (17%)
2	P8E	B	606	-	15,16,17	1.54	2 (13%)	17,23,26	1.41	4 (23%)
2	P8E	S	605	-	15,16,17	1.56	2 (13%)	17,23,26	1.35	3 (17%)
2	P8E	A	614	-	15,16,17	1.58	2 (13%)	17,23,26	1.30	3 (17%)
2	P8E	T	609	-	15,16,17	1.60	2 (13%)	17,23,26	1.44	3 (17%)
2	P8E	Q	615	-	15,16,17	1.53	2 (13%)	17,23,26	1.43	3 (17%)
2	P8E	S	609	-	15,16,17	1.60	2 (13%)	17,23,26	1.36	3 (17%)
2	P8E	O	604	-	15,16,17	1.55	2 (13%)	17,23,26	1.34	2 (11%)
2	P8E	Q	612	-	15,16,17	1.52	2 (13%)	17,23,26	1.42	3 (17%)
2	P8E	R	603	-	15,16,17	1.53	2 (13%)	17,23,26	1.36	3 (17%)
2	P8E	G	612	-	15,16,17	1.53	2 (13%)	17,23,26	1.44	3 (17%)
2	P8E	U	602	-	15,16,17	1.56	2 (13%)	17,23,26	1.35	3 (17%)
2	P8E	J	614	-	15,16,17	1.58	2 (13%)	17,23,26	1.28	2 (11%)
2	P8E	M	609	-	15,16,17	1.59	2 (13%)	17,23,26	1.38	2 (11%)
2	P8E	E	608	-	15,16,17	1.54	2 (13%)	17,23,26	1.27	1 (5%)
2	P8E	G	608	-	15,16,17	1.53	2 (13%)	17,23,26	1.40	4 (23%)
2	P8E	J	604	-	15,16,17	1.54	2 (13%)	17,23,26	1.37	2 (11%)
2	P8E	B	604	-	15,16,17	1.54	2 (13%)	17,23,26	1.39	2 (11%)
2	P8E	F	612	-	15,16,17	1.54	2 (13%)	17,23,26	1.44	3 (17%)
2	P8E	K	608	-	15,16,17	1.53	2 (13%)	17,23,26	1.32	1 (5%)
2	P8E	T	611	-	15,16,17	1.60	2 (13%)	17,23,26	1.42	3 (17%)
2	P8E	R	611	-	15,16,17	1.56	2 (13%)	17,23,26	1.29	2 (11%)
2	P8E	U	609	-	15,16,17	1.59	2 (13%)	17,23,26	1.33	2 (11%)
2	P8E	V	610	-	15,16,17	1.57	2 (13%)	17,23,26	1.24	2 (11%)
2	P8E	S	615	-	15,16,17	1.54	2 (13%)	17,23,26	1.34	3 (17%)
2	P8E	C	613	-	15,16,17	1.56	2 (13%)	17,23,26	1.24	2 (11%)
2	P8E	E	609	-	15,16,17	1.58	2 (13%)	17,23,26	1.33	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	P8E	Q	601	-	15,16,17	1.54	2 (13%)	17,23,26	1.26	2 (11%)
2	P8E	F	603	-	15,16,17	1.54	2 (13%)	17,23,26	1.33	3 (17%)
2	P8E	D	614	-	15,16,17	1.56	2 (13%)	17,23,26	1.26	2 (11%)
2	P8E	I	609	-	15,16,17	1.61	2 (13%)	17,23,26	1.38	3 (17%)
2	P8E	U	605	-	15,16,17	1.53	2 (13%)	17,23,26	1.39	3 (17%)
2	P8E	M	603	-	15,16,17	1.52	2 (13%)	17,23,26	1.36	3 (17%)
2	P8E	H	609	-	15,16,17	1.56	2 (13%)	17,23,26	1.32	2 (11%)
2	P8E	P	603	-	15,16,17	1.53	2 (13%)	17,23,26	1.38	3 (17%)
2	P8E	H	617	-	15,16,17	1.63	2 (13%)	17,23,26	1.59	4 (23%)
2	P8E	T	602	-	15,16,17	1.56	2 (13%)	17,23,26	1.34	2 (11%)
2	P8E	S	610	-	15,16,17	1.59	2 (13%)	17,23,26	1.30	3 (17%)
2	P8E	U	615	-	15,16,17	1.55	2 (13%)	17,23,26	1.35	3 (17%)
2	P8E	M	605	-	15,16,17	1.56	2 (13%)	17,23,26	1.42	3 (17%)
2	P8E	O	616	-	15,16,17	1.51	2 (13%)	17,23,26	1.55	5 (29%)
2	P8E	C	609	-	15,16,17	1.57	2 (13%)	17,23,26	1.32	1 (5%)
2	P8E	E	615	-	15,16,17	1.51	2 (13%)	17,23,26	1.37	3 (17%)
2	P8E	P	614	-	15,16,17	1.57	2 (13%)	17,23,26	1.33	2 (11%)
2	P8E	O	608	-	15,16,17	1.53	2 (13%)	17,23,26	1.26	2 (11%)
2	P8E	R	605	-	15,16,17	1.55	2 (13%)	17,23,26	1.35	3 (17%)
2	P8E	B	605	-	15,16,17	1.53	2 (13%)	17,23,26	1.39	3 (17%)
2	P8E	K	616	-	15,16,17	1.51	2 (13%)	17,23,26	1.45	4 (23%)
2	P8E	O	609	-	15,16,17	1.61	2 (13%)	17,23,26	1.39	2 (11%)
2	P8E	B	608	-	15,16,17	1.52	2 (13%)	17,23,26	1.45	3 (17%)
2	P8E	D	612	-	15,16,17	1.52	2 (13%)	17,23,26	1.45	3 (17%)
2	P8E	V	604	-	15,16,17	1.54	2 (13%)	17,23,26	1.39	3 (17%)
2	P8E	J	603	-	15,16,17	1.54	2 (13%)	17,23,26	1.41	3 (17%)
2	P8E	M	615	-	15,16,17	1.53	2 (13%)	17,23,26	1.35	2 (11%)
2	P8E	J	601	-	15,16,17	1.59	2 (13%)	17,23,26	1.24	2 (11%)
2	P8E	A	617	-	15,16,17	1.63	2 (13%)	17,23,26	1.56	4 (23%)
2	P8E	L	605	-	15,16,17	1.53	2 (13%)	17,23,26	1.39	3 (17%)
2	P8E	B	615	-	15,16,17	1.54	2 (13%)	17,23,26	1.38	3 (17%)
2	P8E	B	612	-	15,16,17	1.54	2 (13%)	17,23,26	1.41	3 (17%)
2	P8E	N	610	-	15,16,17	1.57	2 (13%)	17,23,26	1.24	2 (11%)
2	P8E	G	604	-	15,16,17	1.54	2 (13%)	17,23,26	1.37	2 (11%)
2	P8E	I	608	-	15,16,17	1.53	2 (13%)	17,23,26	1.43	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	P8E	I	605	-	15,16,17	1.53	2 (13%)	17,23,26	1.33	2 (11%)
2	P8E	K	601	-	15,16,17	1.58	2 (13%)	17,23,26	1.29	3 (17%)
2	P8E	Q	613	-	15,16,17	1.56	2 (13%)	17,23,26	1.26	2 (11%)
2	P8E	G	613	-	15,16,17	1.57	2 (13%)	17,23,26	1.29	2 (11%)
2	P8E	C	608	-	15,16,17	1.53	2 (13%)	17,23,26	1.26	1 (5%)
2	P8E	V	615	-	15,16,17	1.52	2 (13%)	17,23,26	1.33	3 (17%)
2	P8E	A	608	-	15,16,17	1.51	2 (13%)	17,23,26	1.27	1 (5%)
2	P8E	P	613	-	15,16,17	1.61	2 (13%)	17,23,26	1.37	3 (17%)
2	P8E	S	616	-	15,16,17	1.50	2 (13%)	17,23,26	1.60	5 (29%)
2	P8E	T	607	-	15,16,17	1.61	2 (13%)	17,23,26	1.50	3 (17%)
2	P8E	K	611	-	15,16,17	1.59	2 (13%)	17,23,26	1.42	3 (17%)
2	P8E	F	611	-	15,16,17	1.58	2 (13%)	17,23,26	1.32	3 (17%)
2	P8E	B	602	-	15,16,17	1.55	2 (13%)	17,23,26	1.29	2 (11%)
2	P8E	O	601	-	15,16,17	1.63	2 (13%)	17,23,26	1.58	3 (17%)
2	P8E	V	609	-	15,16,17	1.58	2 (13%)	17,23,26	1.31	2 (11%)
2	P8E	A	609	-	15,16,17	1.58	2 (13%)	17,23,26	1.34	2 (11%)
2	P8E	U	614	-	15,16,17	1.59	2 (13%)	17,23,26	1.26	2 (11%)
2	P8E	D	603	-	15,16,17	1.54	2 (13%)	17,23,26	1.43	2 (11%)
2	P8E	D	601	-	15,16,17	1.58	2 (13%)	17,23,26	1.25	3 (17%)
2	P8E	I	615	-	15,16,17	1.55	2 (13%)	17,23,26	1.37	3 (17%)
2	P8E	V	613	-	15,16,17	1.58	2 (13%)	17,23,26	1.29	3 (17%)
2	P8E	V	606	-	15,16,17	1.56	2 (13%)	17,23,26	1.45	4 (23%)
2	P8E	T	612	-	15,16,17	1.54	2 (13%)	17,23,26	1.36	3 (17%)
2	P8E	C	605	-	15,16,17	1.52	2 (13%)	17,23,26	1.39	3 (17%)
2	P8E	B	607	-	15,16,17	1.61	2 (13%)	17,23,26	1.45	3 (17%)
2	P8E	B	601	-	15,16,17	1.57	2 (13%)	17,23,26	1.27	3 (17%)
2	P8E	D	617	-	15,16,17	1.64	2 (13%)	17,23,26	1.61	3 (17%)
2	P8E	M	612	-	15,16,17	1.54	2 (13%)	17,23,26	1.38	3 (17%)
2	P8E	J	617	-	15,16,17	1.64	2 (13%)	17,23,26	1.59	4 (23%)
2	P8E	U	617	-	15,16,17	1.64	2 (13%)	17,23,26	1.53	4 (23%)

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	P8E	A	613	-	-	2/11/28/32	0/1/1/1
2	P8E	O	602	-	-	4/11/28/32	0/1/1/1
2	P8E	F	608	-	-	4/11/28/32	0/1/1/1
2	P8E	H	603	-	-	3/11/28/32	0/1/1/1
2	P8E	I	601	-	-	4/11/28/32	0/1/1/1
2	P8E	K	605	-	-	6/11/28/32	0/1/1/1
2	P8E	S	606	-	-	3/11/28/32	0/1/1/1
2	P8E	E	610	-	-	4/11/28/32	0/1/1/1
2	P8E	J	607	-	-	7/11/28/32	0/1/1/1
2	P8E	P	608	-	-	4/11/28/32	0/1/1/1
2	P8E	V	616	-	-	5/11/28/32	0/1/1/1
2	P8E	A	603	-	-	0/11/28/32	0/1/1/1
2	P8E	S	602	-	-	4/11/28/32	0/1/1/1
2	P8E	A	604	-	-	7/11/28/32	0/1/1/1
2	P8E	H	615	-	-	4/11/28/32	0/1/1/1
2	P8E	V	601	-	-	4/11/28/32	0/1/1/1
2	P8E	U	610	-	-	5/11/28/32	0/1/1/1
2	P8E	K	609	-	-	1/11/28/32	0/1/1/1
2	P8E	O	607	-	-	4/11/28/32	0/1/1/1
2	P8E	L	615	-	-	3/11/28/32	0/1/1/1
2	P8E	A	616	-	-	6/11/28/32	0/1/1/1
2	P8E	D	613	-	-	2/11/28/32	0/1/1/1
2	P8E	J	613	-	-	4/11/28/32	0/1/1/1
2	P8E	A	605	-	-	5/11/28/32	0/1/1/1
2	P8E	S	607	-	-	4/11/28/32	0/1/1/1
2	P8E	V	617	-	-	3/11/28/32	0/1/1/1
2	P8E	S	611	-	-	1/11/28/32	0/1/1/1
2	P8E	R	616	-	-	5/11/28/32	0/1/1/1
2	P8E	H	610	-	-	4/11/28/32	0/1/1/1
2	P8E	E	617	-	-	1/11/28/32	0/1/1/1
2	P8E	P	616	-	-	5/11/28/32	0/1/1/1
2	P8E	V	602	-	-	4/11/28/32	0/1/1/1
2	P8E	N	604	-	-	4/11/28/32	0/1/1/1
2	P8E	N	613	-	-	0/11/28/32	0/1/1/1
2	P8E	T	615	-	-	3/11/28/32	0/1/1/1
2	P8E	K	610	-	-	4/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	H	611	-	-	1/11/28/32	0/1/1/1
2	P8E	K	615	-	-	3/11/28/32	0/1/1/1
2	P8E	U	607	-	-	4/11/28/32	0/1/1/1
2	P8E	C	610	-	-	4/11/28/32	0/1/1/1
2	P8E	F	613	-	-	0/11/28/32	0/1/1/1
2	P8E	U	608	-	-	4/11/28/32	0/1/1/1
2	P8E	V	607	-	-	4/11/28/32	0/1/1/1
2	P8E	E	607	-	-	4/11/28/32	0/1/1/1
2	P8E	F	610	-	-	4/11/28/32	0/1/1/1
2	P8E	R	604	-	-	4/11/28/32	0/1/1/1
2	P8E	L	601	-	-	3/11/28/32	0/1/1/1
2	P8E	O	605	-	-	4/11/28/32	0/1/1/1
2	P8E	U	612	-	-	4/11/28/32	0/1/1/1
2	P8E	A	602	-	-	4/11/28/32	0/1/1/1
2	P8E	E	612	-	-	3/11/28/32	0/1/1/1
2	P8E	L	609	-	-	1/11/28/32	0/1/1/1
2	P8E	M	608	-	-	4/11/28/32	0/1/1/1
2	P8E	G	601	-	-	7/11/28/32	0/1/1/1
2	P8E	A	615	-	-	3/11/28/32	0/1/1/1
2	P8E	F	609	-	-	5/11/28/32	0/1/1/1
2	P8E	U	613	-	-	3/11/28/32	0/1/1/1
2	P8E	T	614	-	-	6/11/28/32	0/1/1/1
2	P8E	P	610	-	-	4/11/28/32	0/1/1/1
2	P8E	T	617	-	-	3/11/28/32	0/1/1/1
2	P8E	T	613	-	-	7/11/28/32	0/1/1/1
2	P8E	P	611	-	-	1/11/28/32	0/1/1/1
2	P8E	U	601	-	-	6/11/28/32	0/1/1/1
2	P8E	G	602	-	-	4/11/28/32	0/1/1/1
2	P8E	T	605	-	-	7/11/28/32	0/1/1/1
2	P8E	E	613	-	-	7/11/28/32	0/1/1/1
2	P8E	S	604	-	-	6/11/28/32	0/1/1/1
2	P8E	U	611	-	-	3/11/28/32	0/1/1/1
2	P8E	A	610	-	-	4/11/28/32	0/1/1/1
2	P8E	N	616	-	-	6/11/28/32	0/1/1/1
2	P8E	R	602	-	-	4/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	D	608	-	-	4/11/28/32	0/1/1/1
2	P8E	H	613	-	-	0/11/28/32	0/1/1/1
2	P8E	G	607	-	-	5/11/28/32	0/1/1/1
2	P8E	R	607	-	-	1/11/28/32	0/1/1/1
2	P8E	U	603	-	-	3/11/28/32	0/1/1/1
2	P8E	N	609	-	-	2/11/28/32	0/1/1/1
2	P8E	M	601	-	-	3/11/28/32	0/1/1/1
2	P8E	H	606	-	-	6/11/28/32	0/1/1/1
2	P8E	O	612	-	-	4/11/28/32	0/1/1/1
2	P8E	R	601	-	-	4/11/28/32	0/1/1/1
2	P8E	S	603	-	-	0/11/28/32	0/1/1/1
2	P8E	I	604	-	-	3/11/28/32	0/1/1/1
2	P8E	K	606	-	-	6/11/28/32	0/1/1/1
2	P8E	K	612	-	-	3/11/28/32	0/1/1/1
2	P8E	L	616	-	-	4/11/28/32	0/1/1/1
2	P8E	C	606	-	-	6/11/28/32	0/1/1/1
2	P8E	L	602	-	-	4/11/28/32	0/1/1/1
2	P8E	E	616	-	-	8/11/28/32	0/1/1/1
2	P8E	Q	605	-	-	4/11/28/32	0/1/1/1
2	P8E	Q	614	-	-	7/11/28/32	0/1/1/1
2	P8E	A	607	-	-	5/11/28/32	0/1/1/1
2	P8E	L	610	-	-	4/11/28/32	0/1/1/1
2	P8E	F	602	-	-	4/11/28/32	0/1/1/1
2	P8E	E	604	-	-	6/11/28/32	0/1/1/1
2	P8E	I	616	-	-	5/11/28/32	0/1/1/1
2	P8E	Q	617	-	-	3/11/28/32	0/1/1/1
2	P8E	B	614	-	-	5/11/28/32	0/1/1/1
2	P8E	L	607	-	-	0/11/28/32	0/1/1/1
2	P8E	H	604	-	-	6/11/28/32	0/1/1/1
2	P8E	N	601	-	-	3/11/28/32	0/1/1/1
2	P8E	T	608	-	-	4/11/28/32	0/1/1/1
2	P8E	M	610	-	-	4/11/28/32	0/1/1/1
2	P8E	N	615	-	-	2/11/28/32	0/1/1/1
2	P8E	C	604	-	-	7/11/28/32	0/1/1/1
2	P8E	S	612	-	-	3/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	O	614	-	-	3/11/28/32	0/1/1/1
2	P8E	S	614	-	-	4/11/28/32	0/1/1/1
2	P8E	G	615	-	-	3/11/28/32	0/1/1/1
2	P8E	Q	609	-	-	6/11/28/32	0/1/1/1
2	P8E	B	616	-	-	6/11/28/32	0/1/1/1
2	P8E	P	606	-	-	7/11/28/32	0/1/1/1
2	P8E	E	602	-	-	4/11/28/32	0/1/1/1
2	P8E	J	605	-	-	4/11/28/32	0/1/1/1
2	P8E	E	605	-	-	4/11/28/32	0/1/1/1
2	P8E	A	606	-	-	3/11/28/32	0/1/1/1
2	P8E	I	610	-	-	4/11/28/32	0/1/1/1
2	P8E	Q	608	-	-	4/11/28/32	0/1/1/1
2	P8E	C	614	-	-	6/11/28/32	0/1/1/1
2	P8E	Q	610	-	-	4/11/28/32	0/1/1/1
2	P8E	L	614	-	-	0/11/28/32	0/1/1/1
2	P8E	P	604	-	-	6/11/28/32	0/1/1/1
2	P8E	H	602	-	-	4/11/28/32	0/1/1/1
2	P8E	M	611	-	-	3/11/28/32	0/1/1/1
2	P8E	V	614	-	-	5/11/28/32	0/1/1/1
2	P8E	N	603	-	-	0/11/28/32	0/1/1/1
2	P8E	B	611	-	-	2/11/28/32	0/1/1/1
2	P8E	O	617	-	-	1/11/28/32	0/1/1/1
2	P8E	S	617	-	-	0/11/28/32	0/1/1/1
2	P8E	N	602	-	-	4/11/28/32	0/1/1/1
2	P8E	L	608	-	-	3/11/28/32	0/1/1/1
2	P8E	L	604	-	-	6/11/28/32	0/1/1/1
2	P8E	H	616	-	-	5/11/28/32	0/1/1/1
2	P8E	R	615	-	-	4/11/28/32	0/1/1/1
2	P8E	H	607	-	-	1/11/28/32	0/1/1/1
2	P8E	I	614	-	-	6/11/28/32	0/1/1/1
2	P8E	D	605	-	-	4/11/28/32	0/1/1/1
2	P8E	F	604	-	-	6/11/28/32	0/1/1/1
2	P8E	G	614	-	-	0/11/28/32	0/1/1/1
2	P8E	H	612	-	-	5/11/28/32	0/1/1/1
2	P8E	H	608	-	-	4/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	I	602	-	-	4/11/28/32	0/1/1/1
2	P8E	J	609	-	-	3/11/28/32	0/1/1/1
2	P8E	U	604	-	-	4/11/28/32	0/1/1/1
2	P8E	N	607	-	-	4/11/28/32	0/1/1/1
2	P8E	U	606	-	-	3/11/28/32	0/1/1/1
2	P8E	C	616	-	-	5/11/28/32	0/1/1/1
2	P8E	L	606	-	-	6/11/28/32	0/1/1/1
2	P8E	C	602	-	-	5/11/28/32	0/1/1/1
2	P8E	C	607	-	-	4/11/28/32	0/1/1/1
2	P8E	S	608	-	-	4/11/28/32	0/1/1/1
2	P8E	C	615	-	-	3/11/28/32	0/1/1/1
2	P8E	D	602	-	-	4/11/28/32	0/1/1/1
2	P8E	B	617	-	-	1/11/28/32	0/1/1/1
2	P8E	I	611	-	-	5/11/28/32	0/1/1/1
2	P8E	J	610	-	-	4/11/28/32	0/1/1/1
2	P8E	V	605	-	-	4/11/28/32	0/1/1/1
2	P8E	T	601	-	-	3/11/28/32	0/1/1/1
2	P8E	Q	606	-	-	6/11/28/32	0/1/1/1
2	P8E	G	606	-	-	7/11/28/32	0/1/1/1
2	P8E	E	601	-	-	3/11/28/32	0/1/1/1
2	P8E	G	616	-	-	4/11/28/32	0/1/1/1
2	P8E	A	612	-	-	5/11/28/32	0/1/1/1
2	P8E	M	606	-	-	6/11/28/32	0/1/1/1
2	P8E	J	615	-	-	3/11/28/32	0/1/1/1
2	P8E	P	602	-	-	4/11/28/32	0/1/1/1
2	P8E	D	609	-	-	4/11/28/32	0/1/1/1
2	P8E	R	612	-	-	3/11/28/32	0/1/1/1
2	P8E	T	603	-	-	3/11/28/32	0/1/1/1
2	P8E	C	611	-	-	1/11/28/32	0/1/1/1
2	P8E	S	613	-	-	0/11/28/32	0/1/1/1
2	P8E	B	609	-	-	3/11/28/32	0/1/1/1
2	P8E	H	601	-	-	3/11/28/32	0/1/1/1
2	P8E	F	606	-	-	3/11/28/32	0/1/1/1
2	P8E	P	607	-	-	5/11/28/32	0/1/1/1
2	P8E	I	607	-	-	3/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	P	615	-	-	3/11/28/32	0/1/1/1
2	P8E	P	612	-	-	4/11/28/32	0/1/1/1
2	P8E	V	612	-	-	5/11/28/32	0/1/1/1
2	P8E	F	616	-	-	6/11/28/32	0/1/1/1
2	P8E	P	601	-	-	4/11/28/32	0/1/1/1
2	P8E	U	616	-	-	5/11/28/32	0/1/1/1
2	P8E	E	606	-	-	4/11/28/32	0/1/1/1
2	P8E	C	601	-	-	4/11/28/32	0/1/1/1
2	P8E	L	603	-	-	3/11/28/32	0/1/1/1
2	P8E	I	606	-	-	6/11/28/32	0/1/1/1
2	P8E	P	609	-	-	1/11/28/32	0/1/1/1
2	P8E	A	601	-	-	4/11/28/32	0/1/1/1
2	P8E	C	617	-	-	2/11/28/32	0/1/1/1
2	P8E	F	615	-	-	4/11/28/32	0/1/1/1
2	P8E	G	609	-	-	4/11/28/32	0/1/1/1
2	P8E	L	617	-	-	1/11/28/32	0/1/1/1
2	P8E	R	614	-	-	1/11/28/32	0/1/1/1
2	P8E	G	617	-	-	3/11/28/32	0/1/1/1
2	P8E	N	608	-	-	4/11/28/32	0/1/1/1
2	P8E	P	617	-	-	3/11/28/32	0/1/1/1
2	P8E	D	610	-	-	6/11/28/32	0/1/1/1
2	P8E	T	616	-	-	5/11/28/32	0/1/1/1
2	P8E	B	603	-	-	4/11/28/32	0/1/1/1
2	P8E	O	613	-	-	2/11/28/32	0/1/1/1
2	P8E	J	608	-	-	4/11/28/32	0/1/1/1
2	P8E	F	601	-	-	3/11/28/32	0/1/1/1
2	P8E	K	614	-	-	4/11/28/32	0/1/1/1
2	P8E	Q	602	-	-	4/11/28/32	0/1/1/1
2	P8E	M	604	-	-	7/11/28/32	0/1/1/1
2	P8E	D	604	-	-	6/11/28/32	0/1/1/1
2	P8E	L	611	-	-	0/11/28/32	0/1/1/1
2	P8E	J	606	-	-	6/11/28/32	0/1/1/1
2	P8E	D	616	-	-	5/11/28/32	0/1/1/1
2	P8E	E	603	-	-	0/11/28/32	0/1/1/1
2	P8E	F	617	-	-	3/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	K	604	-	-	3/11/28/32	0/1/1/1
2	P8E	A	611	-	-	7/11/28/32	0/1/1/1
2	P8E	N	612	-	-	5/11/28/32	0/1/1/1
2	P8E	I	603	-	-	4/11/28/32	0/1/1/1
2	P8E	O	615	-	-	3/11/28/32	0/1/1/1
2	P8E	Q	611	-	-	1/11/28/32	0/1/1/1
2	P8E	R	610	-	-	4/11/28/32	0/1/1/1
2	P8E	G	611	-	-	0/11/28/32	0/1/1/1
2	P8E	M	602	-	-	4/11/28/32	0/1/1/1
2	P8E	F	614	-	-	5/11/28/32	0/1/1/1
2	P8E	O	603	-	-	0/11/28/32	0/1/1/1
2	P8E	J	612	-	-	3/11/28/32	0/1/1/1
2	P8E	M	614	-	-	5/11/28/32	0/1/1/1
2	P8E	Q	616	-	-	6/11/28/32	0/1/1/1
2	P8E	F	607	-	-	4/11/28/32	0/1/1/1
2	P8E	D	606	-	-	4/11/28/32	0/1/1/1
2	P8E	N	606	-	-	5/11/28/32	0/1/1/1
2	P8E	O	610	-	-	4/11/28/32	0/1/1/1
2	P8E	L	612	-	-	5/11/28/32	0/1/1/1
2	P8E	T	610	-	-	6/11/28/32	0/1/1/1
2	P8E	Q	607	-	-	5/11/28/32	0/1/1/1
2	P8E	O	611	-	-	1/11/28/32	0/1/1/1
2	P8E	C	603	-	-	3/11/28/32	0/1/1/1
2	P8E	M	616	-	-	5/11/28/32	0/1/1/1
2	P8E	I	612	-	-	5/11/28/32	0/1/1/1
2	P8E	N	614	-	-	9/11/28/32	0/1/1/1
2	P8E	B	610	-	-	4/11/28/32	0/1/1/1
2	P8E	D	615	-	-	6/11/28/32	0/1/1/1
2	P8E	L	613	-	-	3/11/28/32	0/1/1/1
2	P8E	Q	603	-	-	4/11/28/32	0/1/1/1
2	P8E	E	614	-	-	4/11/28/32	0/1/1/1
2	P8E	G	603	-	-	3/11/28/32	0/1/1/1
2	P8E	R	617	-	-	3/11/28/32	0/1/1/1
2	P8E	T	604	-	-	7/11/28/32	0/1/1/1
2	P8E	K	603	-	-	3/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	J	611	-	-	3/11/28/32	0/1/1/1
2	P8E	S	601	-	-	4/11/28/32	0/1/1/1
2	P8E	K	617	-	-	0/11/28/32	0/1/1/1
2	P8E	Q	604	-	-	6/11/28/32	0/1/1/1
2	P8E	V	603	-	-	0/11/28/32	0/1/1/1
2	P8E	H	605	-	-	4/11/28/32	0/1/1/1
2	P8E	J	616	-	-	5/11/28/32	0/1/1/1
2	P8E	J	602	-	-	4/11/28/32	0/1/1/1
2	P8E	N	611	-	-	0/11/28/32	0/1/1/1
2	P8E	D	611	-	-	3/11/28/32	0/1/1/1
2	P8E	V	608	-	-	4/11/28/32	0/1/1/1
2	P8E	R	608	-	-	4/11/28/32	0/1/1/1
2	P8E	I	617	-	-	3/11/28/32	0/1/1/1
2	P8E	N	617	-	-	3/11/28/32	0/1/1/1
2	P8E	K	602	-	-	4/11/28/32	0/1/1/1
2	P8E	K	613	-	-	3/11/28/32	0/1/1/1
2	P8E	R	609	-	-	2/11/28/32	0/1/1/1
2	P8E	M	617	-	-	4/11/28/32	0/1/1/1
2	P8E	F	605	-	-	4/11/28/32	0/1/1/1
2	P8E	V	611	-	-	1/11/28/32	0/1/1/1
2	P8E	H	614	-	-	5/11/28/32	0/1/1/1
2	P8E	O	606	-	-	6/11/28/32	0/1/1/1
2	P8E	D	607	-	-	4/11/28/32	0/1/1/1
2	P8E	M	613	-	-	3/11/28/32	0/1/1/1
2	P8E	E	611	-	-	7/11/28/32	0/1/1/1
2	P8E	R	613	-	-	5/11/28/32	0/1/1/1
2	P8E	T	606	-	-	7/11/28/32	0/1/1/1
2	P8E	B	613	-	-	2/11/28/32	0/1/1/1
2	P8E	G	610	-	-	4/11/28/32	0/1/1/1
2	P8E	G	605	-	-	7/11/28/32	0/1/1/1
2	P8E	C	612	-	-	9/11/28/32	0/1/1/1
2	P8E	M	607	-	-	5/11/28/32	0/1/1/1
2	P8E	P	605	-	-	6/11/28/32	0/1/1/1
2	P8E	R	606	-	-	5/11/28/32	0/1/1/1
2	P8E	I	613	-	-	6/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	N	605	-	-	4/11/28/32	0/1/1/1
2	P8E	K	607	-	-	0/11/28/32	0/1/1/1
2	P8E	B	606	-	-	3/11/28/32	0/1/1/1
2	P8E	S	605	-	-	6/11/28/32	0/1/1/1
2	P8E	A	614	-	-	0/11/28/32	0/1/1/1
2	P8E	T	609	-	-	8/11/28/32	0/1/1/1
2	P8E	Q	615	-	-	3/11/28/32	0/1/1/1
2	P8E	S	609	-	-	1/11/28/32	0/1/1/1
2	P8E	O	604	-	-	7/11/28/32	0/1/1/1
2	P8E	Q	612	-	-	7/11/28/32	0/1/1/1
2	P8E	R	603	-	-	0/11/28/32	0/1/1/1
2	P8E	G	612	-	-	6/11/28/32	0/1/1/1
2	P8E	U	602	-	-	4/11/28/32	0/1/1/1
2	P8E	J	614	-	-	7/11/28/32	0/1/1/1
2	P8E	M	609	-	-	5/11/28/32	0/1/1/1
2	P8E	E	608	-	-	4/11/28/32	0/1/1/1
2	P8E	G	608	-	-	4/11/28/32	0/1/1/1
2	P8E	J	604	-	-	6/11/28/32	0/1/1/1
2	P8E	B	604	-	-	6/11/28/32	0/1/1/1
2	P8E	F	612	-	-	9/11/28/32	0/1/1/1
2	P8E	K	608	-	-	4/11/28/32	0/1/1/1
2	P8E	T	611	-	-	5/11/28/32	0/1/1/1
2	P8E	R	611	-	-	1/11/28/32	0/1/1/1
2	P8E	U	609	-	-	6/11/28/32	0/1/1/1
2	P8E	V	610	-	-	4/11/28/32	0/1/1/1
2	P8E	S	615	-	-	0/11/28/32	0/1/1/1
2	P8E	C	613	-	-	4/11/28/32	0/1/1/1
2	P8E	E	609	-	-	3/11/28/32	0/1/1/1
2	P8E	Q	601	-	-	3/11/28/32	0/1/1/1
2	P8E	F	603	-	-	3/11/28/32	0/1/1/1
2	P8E	D	614	-	-	4/11/28/32	0/1/1/1
2	P8E	I	609	-	-	6/11/28/32	0/1/1/1
2	P8E	U	605	-	-	5/11/28/32	0/1/1/1
2	P8E	M	603	-	-	3/11/28/32	0/1/1/1
2	P8E	H	609	-	-	4/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	P	603	-	-	4/11/28/32	0/1/1/1
2	P8E	H	617	-	-	4/11/28/32	0/1/1/1
2	P8E	T	602	-	-	4/11/28/32	0/1/1/1
2	P8E	S	610	-	-	4/11/28/32	0/1/1/1
2	P8E	U	615	-	-	3/11/28/32	0/1/1/1
2	P8E	M	605	-	-	4/11/28/32	0/1/1/1
2	P8E	O	616	-	-	6/11/28/32	0/1/1/1
2	P8E	C	609	-	-	5/11/28/32	0/1/1/1
2	P8E	E	615	-	-	4/11/28/32	0/1/1/1
2	P8E	P	614	-	-	4/11/28/32	0/1/1/1
2	P8E	O	608	-	-	4/11/28/32	0/1/1/1
2	P8E	R	605	-	-	5/11/28/32	0/1/1/1
2	P8E	B	605	-	-	7/11/28/32	0/1/1/1
2	P8E	K	616	-	-	5/11/28/32	0/1/1/1
2	P8E	O	609	-	-	2/11/28/32	0/1/1/1
2	P8E	B	608	-	-	4/11/28/32	0/1/1/1
2	P8E	D	612	-	-	7/11/28/32	0/1/1/1
2	P8E	V	604	-	-	7/11/28/32	0/1/1/1
2	P8E	J	603	-	-	3/11/28/32	0/1/1/1
2	P8E	M	615	-	-	3/11/28/32	0/1/1/1
2	P8E	J	601	-	-	4/11/28/32	0/1/1/1
2	P8E	A	617	-	-	1/11/28/32	0/1/1/1
2	P8E	L	605	-	-	6/11/28/32	0/1/1/1
2	P8E	B	615	-	-	3/11/28/32	0/1/1/1
2	P8E	B	612	-	-	4/11/28/32	0/1/1/1
2	P8E	N	610	-	-	4/11/28/32	0/1/1/1
2	P8E	G	604	-	-	6/11/28/32	0/1/1/1
2	P8E	I	608	-	-	4/11/28/32	0/1/1/1
2	P8E	I	605	-	-	4/11/28/32	0/1/1/1
2	P8E	K	601	-	-	4/11/28/32	0/1/1/1
2	P8E	Q	613	-	-	0/11/28/32	0/1/1/1
2	P8E	G	613	-	-	3/11/28/32	0/1/1/1
2	P8E	C	608	-	-	4/11/28/32	0/1/1/1
2	P8E	V	615	-	-	0/11/28/32	0/1/1/1
2	P8E	A	608	-	-	4/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	P	613	-	-	3/11/28/32	0/1/1/1
2	P8E	S	616	-	-	6/11/28/32	0/1/1/1
2	P8E	T	607	-	-	3/11/28/32	0/1/1/1
2	P8E	K	611	-	-	3/11/28/32	0/1/1/1
2	P8E	F	611	-	-	4/11/28/32	0/1/1/1
2	P8E	B	602	-	-	4/11/28/32	0/1/1/1
2	P8E	O	601	-	-	4/11/28/32	0/1/1/1
2	P8E	V	609	-	-	2/11/28/32	0/1/1/1
2	P8E	A	609	-	-	1/11/28/32	0/1/1/1
2	P8E	U	614	-	-	5/11/28/32	0/1/1/1
2	P8E	D	603	-	-	3/11/28/32	0/1/1/1
2	P8E	D	601	-	-	4/11/28/32	0/1/1/1
2	P8E	I	615	-	-	3/11/28/32	0/1/1/1
2	P8E	V	613	-	-	2/11/28/32	0/1/1/1
2	P8E	V	606	-	-	6/11/28/32	0/1/1/1
2	P8E	T	612	-	-	3/11/28/32	0/1/1/1
2	P8E	C	605	-	-	6/11/28/32	0/1/1/1
2	P8E	B	607	-	-	5/11/28/32	0/1/1/1
2	P8E	B	601	-	-	4/11/28/32	0/1/1/1
2	P8E	D	617	-	-	0/11/28/32	0/1/1/1
2	P8E	M	612	-	-	3/11/28/32	0/1/1/1
2	P8E	J	617	-	-	3/11/28/32	0/1/1/1
2	P8E	U	617	-	-	4/11/28/32	0/1/1/1

All (748) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	617	P8E	O6-C2	3.80	1.50	1.43
2	U	617	P8E	O6-C2	3.75	1.50	1.43
2	Q	617	P8E	O6-C2	3.74	1.50	1.43
2	M	617	P8E	O6-C2	3.74	1.50	1.43
2	B	617	P8E	O6-C2	3.73	1.50	1.43
2	C	617	P8E	O6-C2	3.73	1.50	1.43
2	N	617	P8E	O6-C2	3.72	1.50	1.43
2	G	617	P8E	O6-C2	3.70	1.50	1.43
2	J	617	P8E	O6-C2	3.69	1.50	1.43
2	Q	607	P8E	O6-C2	3.69	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	617	P8E	O6-C2	3.69	1.50	1.43
2	I	617	P8E	O6-C2	3.68	1.50	1.43
2	T	617	P8E	O6-C2	3.68	1.50	1.43
2	O	617	P8E	O6-C2	3.68	1.50	1.43
2	E	617	P8E	O6-C2	3.68	1.50	1.43
2	F	617	P8E	O6-C2	3.67	1.50	1.43
2	U	607	P8E	O6-C2	3.67	1.50	1.43
2	F	607	P8E	O6-C2	3.66	1.50	1.43
2	O	601	P8E	O6-C2	3.66	1.50	1.43
2	S	617	P8E	O6-C2	3.65	1.50	1.43
2	A	617	P8E	O6-C2	3.65	1.50	1.43
2	D	607	P8E	O6-C2	3.64	1.50	1.43
2	H	604	P8E	O6-C2	3.64	1.50	1.43
2	O	604	P8E	O6-C2	3.64	1.50	1.43
2	A	607	P8E	O6-C2	3.64	1.50	1.43
2	E	602	P8E	C3-C4	-3.64	1.45	1.52
2	M	607	P8E	O6-C2	3.64	1.50	1.43
2	L	617	P8E	O6-C2	3.64	1.50	1.43
2	C	604	P8E	O6-C2	3.63	1.50	1.43
2	K	617	P8E	O6-C2	3.63	1.50	1.43
2	D	617	P8E	O6-C2	3.63	1.50	1.43
2	M	604	P8E	O6-C2	3.63	1.50	1.43
2	C	601	P8E	O6-C2	3.62	1.50	1.43
2	Q	604	P8E	O6-C2	3.61	1.50	1.43
2	O	607	P8E	O6-C2	3.61	1.50	1.43
2	L	604	P8E	O6-C2	3.60	1.50	1.43
2	V	607	P8E	O6-C2	3.60	1.50	1.43
2	P	617	P8E	O6-C2	3.60	1.50	1.43
2	B	607	P8E	O6-C2	3.60	1.50	1.43
2	J	604	P8E	O6-C2	3.60	1.50	1.43
2	U	604	P8E	O6-C2	3.60	1.50	1.43
2	B	604	P8E	O6-C2	3.60	1.50	1.43
2	I	609	P8E	O6-C2	3.59	1.50	1.43
2	T	607	P8E	O6-C2	3.59	1.50	1.43
2	Q	602	P8E	C3-C4	-3.59	1.45	1.52
2	S	604	P8E	O6-C2	3.59	1.50	1.43
2	E	604	P8E	O6-C2	3.59	1.50	1.43
2	C	607	P8E	O6-C2	3.59	1.50	1.43
2	H	617	P8E	O6-C2	3.59	1.50	1.43
2	T	604	P8E	O6-C2	3.58	1.50	1.43
2	P	602	P8E	C3-C4	-3.58	1.45	1.52
2	K	617	P8E	C3-C4	-3.58	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	607	P8E	O6-C2	3.58	1.50	1.43
2	N	604	P8E	O6-C2	3.58	1.50	1.43
2	R	617	P8E	C3-C4	-3.58	1.45	1.52
2	B	612	P8E	O6-C2	3.58	1.50	1.43
2	E	607	P8E	O6-C2	3.58	1.50	1.43
2	N	611	P8E	O6-C2	3.58	1.50	1.43
2	E	617	P8E	C3-C4	-3.57	1.45	1.52
2	U	612	P8E	O6-C2	3.57	1.50	1.43
2	D	604	P8E	O6-C2	3.57	1.50	1.43
2	G	607	P8E	O6-C2	3.57	1.50	1.43
2	B	611	P8E	C3-C4	-3.57	1.46	1.52
2	I	606	P8E	O6-C2	3.56	1.50	1.43
2	V	604	P8E	O6-C2	3.56	1.50	1.43
2	P	604	P8E	O6-C2	3.56	1.50	1.43
2	Q	611	P8E	C3-C4	-3.55	1.46	1.52
2	R	604	P8E	O6-C2	3.55	1.50	1.43
2	I	604	P8E	O6-C2	3.55	1.50	1.43
2	O	609	P8E	O6-C2	3.55	1.50	1.43
2	O	617	P8E	C3-C4	-3.54	1.46	1.52
2	R	607	P8E	O6-C2	3.54	1.50	1.43
2	S	602	P8E	C3-C4	-3.54	1.46	1.52
2	I	611	P8E	O6-C2	3.54	1.50	1.43
2	L	607	P8E	O6-C2	3.54	1.50	1.43
2	N	617	P8E	C3-C4	-3.54	1.46	1.52
2	K	604	P8E	O6-C2	3.54	1.50	1.43
2	J	607	P8E	O6-C2	3.54	1.50	1.43
2	T	609	P8E	O6-C2	3.54	1.50	1.43
2	M	617	P8E	C3-C4	-3.54	1.46	1.52
2	A	601	P8E	O6-C2	3.54	1.50	1.43
2	G	604	P8E	O6-C2	3.53	1.50	1.43
2	O	616	P8E	O6-C2	3.53	1.50	1.43
2	H	603	P8E	O6-C2	3.53	1.50	1.43
2	J	603	P8E	O6-C2	3.53	1.50	1.43
2	T	612	P8E	O6-C2	3.53	1.50	1.43
2	A	604	P8E	O6-C2	3.53	1.50	1.43
2	P	613	P8E	O6-C2	3.53	1.50	1.43
2	S	607	P8E	O6-C2	3.53	1.50	1.43
2	J	601	P8E	O6-C2	3.52	1.50	1.43
2	G	617	P8E	C3-C4	-3.52	1.46	1.52
2	R	601	P8E	O6-C2	3.52	1.50	1.43
2	B	611	P8E	O6-C2	3.52	1.50	1.43
2	K	601	P8E	O6-C2	3.52	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	602	P8E	C3-C4	-3.52	1.46	1.52
2	F	611	P8E	O6-C2	3.52	1.50	1.43
2	M	605	P8E	O6-C2	3.52	1.50	1.43
2	U	615	P8E	O6-C2	3.52	1.50	1.43
2	F	604	P8E	O6-C2	3.52	1.50	1.43
2	L	611	P8E	C3-C4	-3.52	1.46	1.52
2	F	617	P8E	C3-C4	-3.51	1.46	1.52
2	G	605	P8E	O6-C2	3.51	1.50	1.43
2	P	607	P8E	O6-C2	3.51	1.50	1.43
2	U	606	P8E	O6-C2	3.51	1.50	1.43
2	J	617	P8E	C3-C4	-3.51	1.46	1.52
2	K	606	P8E	O6-C2	3.51	1.50	1.43
2	U	605	P8E	O6-C2	3.51	1.50	1.43
2	V	605	P8E	O6-C2	3.51	1.50	1.43
2	O	601	P8E	C3-C4	-3.50	1.46	1.52
2	O	602	P8E	C3-C4	-3.50	1.46	1.52
2	U	611	P8E	C3-C4	-3.50	1.46	1.52
2	F	601	P8E	O6-C2	3.50	1.50	1.43
2	C	617	P8E	C3-C4	-3.50	1.46	1.52
2	K	605	P8E	O6-C2	3.50	1.50	1.43
2	H	617	P8E	C3-C4	-3.50	1.46	1.52
2	H	611	P8E	O6-C2	3.50	1.50	1.43
2	E	614	P8E	C3-C4	-3.50	1.46	1.52
2	P	615	P8E	O6-C2	3.50	1.50	1.43
2	R	605	P8E	O6-C2	3.50	1.50	1.43
2	D	605	P8E	O6-C2	3.50	1.50	1.43
2	S	605	P8E	O6-C2	3.50	1.50	1.43
2	K	602	P8E	C3-C4	-3.50	1.46	1.52
2	L	605	P8E	O6-C2	3.50	1.50	1.43
2	S	616	P8E	O6-C2	3.50	1.50	1.43
2	I	607	P8E	O6-C2	3.50	1.50	1.43
2	L	606	P8E	O6-C2	3.49	1.50	1.43
2	I	610	P8E	O6-C2	3.49	1.50	1.43
2	V	612	P8E	O6-C2	3.49	1.50	1.43
2	F	612	P8E	O6-C2	3.49	1.50	1.43
2	F	609	P8E	O6-C2	3.49	1.50	1.43
2	M	606	P8E	O6-C2	3.49	1.50	1.43
2	M	609	P8E	O6-C2	3.49	1.50	1.43
2	F	616	P8E	O6-C2	3.49	1.50	1.43
2	R	603	P8E	O6-C2	3.49	1.50	1.43
2	B	617	P8E	C3-C4	-3.49	1.46	1.52
2	C	605	P8E	O6-C2	3.49	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	611	P8E	O6-C2	3.49	1.50	1.43
2	L	603	P8E	O6-C2	3.49	1.50	1.43
2	H	612	P8E	O6-C2	3.49	1.50	1.43
2	Q	605	P8E	O6-C2	3.49	1.50	1.43
2	T	611	P8E	O6-C2	3.49	1.50	1.43
2	S	614	P8E	C3-C4	-3.49	1.46	1.52
2	G	603	P8E	O6-C2	3.48	1.50	1.43
2	C	603	P8E	O6-C2	3.48	1.50	1.43
2	L	612	P8E	O6-C2	3.48	1.50	1.43
2	C	601	P8E	C3-C4	-3.48	1.46	1.52
2	A	605	P8E	O6-C2	3.48	1.50	1.43
2	Q	608	P8E	O6-C2	3.48	1.50	1.43
2	R	613	P8E	O6-C2	3.48	1.50	1.43
2	P	605	P8E	O6-C2	3.48	1.50	1.43
2	T	605	P8E	O6-C2	3.48	1.50	1.43
2	L	607	P8E	C3-C4	-3.48	1.46	1.52
2	A	614	P8E	C3-C4	-3.48	1.46	1.52
2	M	610	P8E	O6-C2	3.48	1.50	1.43
2	E	609	P8E	C3-C4	-3.48	1.46	1.52
2	V	606	P8E	O6-C2	3.48	1.50	1.43
2	C	612	P8E	O6-C2	3.48	1.50	1.43
2	B	605	P8E	O6-C2	3.48	1.50	1.43
2	A	615	P8E	O6-C2	3.47	1.50	1.43
2	J	606	P8E	O6-C2	3.47	1.50	1.43
2	I	609	P8E	C3-C4	-3.47	1.46	1.52
2	J	610	P8E	O6-C2	3.47	1.50	1.43
2	L	613	P8E	O6-C2	3.47	1.50	1.43
2	R	606	P8E	O6-C2	3.47	1.50	1.43
2	U	602	P8E	C3-C4	-3.47	1.46	1.52
2	K	611	P8E	C3-C4	-3.47	1.46	1.52
2	Q	617	P8E	C3-C4	-3.47	1.46	1.52
2	C	606	P8E	O6-C2	3.47	1.50	1.43
2	P	606	P8E	O6-C2	3.47	1.50	1.43
2	K	603	P8E	O6-C2	3.47	1.50	1.43
2	R	612	P8E	O6-C2	3.47	1.50	1.43
2	N	606	P8E	O6-C2	3.47	1.50	1.43
2	C	610	P8E	C3-C4	-3.47	1.46	1.52
2	L	617	P8E	C3-C4	-3.47	1.46	1.52
2	N	614	P8E	C3-C4	-3.47	1.46	1.52
2	U	610	P8E	C3-C4	-3.47	1.46	1.52
2	H	611	P8E	C3-C4	-3.47	1.46	1.52
2	R	614	P8E	C3-C4	-3.47	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	603	P8E	O6-C2	3.47	1.50	1.43
2	I	605	P8E	O6-C2	3.47	1.50	1.43
2	O	606	P8E	O6-C2	3.47	1.50	1.43
2	T	617	P8E	C3-C4	-3.47	1.46	1.52
2	K	614	P8E	C3-C4	-3.46	1.46	1.52
2	V	602	P8E	C3-C4	-3.46	1.46	1.52
2	O	605	P8E	O6-C2	3.46	1.50	1.43
2	N	607	P8E	O6-C2	3.46	1.50	1.43
2	U	614	P8E	C3-C4	-3.46	1.46	1.52
2	O	603	P8E	O6-C2	3.46	1.50	1.43
2	Q	607	P8E	C3-C4	-3.46	1.46	1.52
2	U	611	P8E	O6-C2	3.46	1.50	1.43
2	L	615	P8E	O6-C2	3.46	1.50	1.43
2	O	614	P8E	C3-C4	-3.46	1.46	1.52
2	U	608	P8E	O6-C2	3.46	1.50	1.43
2	K	609	P8E	C3-C4	-3.46	1.46	1.52
2	A	606	P8E	O6-C2	3.46	1.50	1.43
2	B	606	P8E	O6-C2	3.46	1.50	1.43
2	P	613	P8E	C3-C4	-3.46	1.46	1.52
2	N	615	P8E	O6-C2	3.46	1.50	1.43
2	F	605	P8E	O6-C2	3.45	1.50	1.43
2	A	609	P8E	C3-C4	-3.45	1.46	1.52
2	R	601	P8E	C3-C4	-3.45	1.46	1.52
2	D	603	P8E	O6-C2	3.45	1.50	1.43
2	E	605	P8E	O6-C2	3.45	1.50	1.43
2	S	601	P8E	O6-C2	3.45	1.50	1.43
2	L	609	P8E	C3-C4	-3.45	1.46	1.52
2	C	610	P8E	O6-C2	3.45	1.50	1.43
2	K	607	P8E	O6-C2	3.45	1.50	1.43
2	D	612	P8E	O6-C2	3.45	1.50	1.43
2	T	606	P8E	O6-C2	3.45	1.50	1.43
2	S	610	P8E	O6-C2	3.45	1.50	1.43
2	E	603	P8E	O6-C2	3.45	1.50	1.43
2	A	603	P8E	O6-C2	3.45	1.50	1.43
2	A	616	P8E	O6-C2	3.45	1.50	1.43
2	H	613	P8E	C3-C4	-3.45	1.46	1.52
2	J	616	P8E	O6-C2	3.45	1.50	1.43
2	N	610	P8E	O6-C2	3.45	1.50	1.43
2	S	609	P8E	C3-C4	-3.45	1.46	1.52
2	B	603	P8E	O6-C2	3.45	1.50	1.43
2	C	609	P8E	O6-C2	3.45	1.50	1.43
2	E	606	P8E	O6-C2	3.45	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	614	P8E	C3-C4	-3.45	1.46	1.52
2	T	602	P8E	C3-C4	-3.45	1.46	1.52
2	I	617	P8E	C3-C4	-3.45	1.46	1.52
2	S	609	P8E	O6-C2	3.45	1.50	1.43
2	E	612	P8E	O6-C2	3.45	1.50	1.43
2	G	606	P8E	O6-C2	3.45	1.50	1.43
2	B	601	P8E	O6-C2	3.45	1.50	1.43
2	N	605	P8E	O6-C2	3.45	1.50	1.43
2	R	610	P8E	O6-C2	3.45	1.50	1.43
2	H	610	P8E	C3-C4	-3.45	1.46	1.52
2	G	609	P8E	O6-C2	3.44	1.50	1.43
2	L	610	P8E	O6-C2	3.44	1.50	1.43
2	U	603	P8E	O6-C2	3.44	1.50	1.43
2	S	617	P8E	C3-C4	-3.44	1.46	1.52
2	M	614	P8E	O6-C2	3.44	1.50	1.43
2	P	603	P8E	O6-C2	3.44	1.50	1.43
2	Q	611	P8E	O6-C2	3.44	1.50	1.43
2	J	614	P8E	C3-C4	-3.44	1.46	1.52
2	T	611	P8E	C3-C4	-3.44	1.46	1.52
2	J	605	P8E	O6-C2	3.44	1.50	1.43
2	I	607	P8E	C3-C4	-3.44	1.46	1.52
2	D	609	P8E	O6-C2	3.44	1.50	1.43
2	K	607	P8E	C3-C4	-3.44	1.46	1.52
2	S	611	P8E	C3-C4	-3.44	1.46	1.52
2	D	608	P8E	O6-C2	3.44	1.50	1.43
2	M	612	P8E	O6-C2	3.44	1.50	1.43
2	F	606	P8E	O6-C2	3.44	1.50	1.43
2	P	617	P8E	C3-C4	-3.44	1.46	1.52
2	E	610	P8E	O6-C2	3.44	1.50	1.43
2	I	614	P8E	O6-C2	3.44	1.50	1.43
2	P	601	P8E	O6-C2	3.44	1.50	1.43
2	T	609	P8E	C3-C4	-3.44	1.46	1.52
2	O	612	P8E	O6-C2	3.44	1.50	1.43
2	E	611	P8E	C3-C4	-3.44	1.46	1.52
2	F	602	P8E	C3-C4	-3.44	1.46	1.52
2	R	609	P8E	O6-C2	3.44	1.50	1.43
2	B	613	P8E	C3-C4	-3.44	1.46	1.52
2	Q	616	P8E	C3-C4	-3.44	1.46	1.52
2	B	616	P8E	O6-C2	3.44	1.50	1.43
2	E	601	P8E	C3-C4	-3.44	1.46	1.52
2	M	609	P8E	C3-C4	-3.44	1.46	1.52
2	G	612	P8E	O6-C2	3.44	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	606	P8E	O6-C2	3.43	1.50	1.43
2	S	611	P8E	O6-C2	3.43	1.50	1.43
2	B	610	P8E	O6-C2	3.43	1.50	1.43
2	F	615	P8E	O6-C2	3.43	1.50	1.43
2	T	615	P8E	O6-C2	3.43	1.50	1.43
2	I	614	P8E	C3-C4	-3.43	1.46	1.52
2	A	610	P8E	O6-C2	3.43	1.50	1.43
2	I	615	P8E	O6-C2	3.43	1.50	1.43
2	B	602	P8E	C3-C4	-3.43	1.46	1.52
2	O	610	P8E	O6-C2	3.43	1.50	1.43
2	M	614	P8E	C3-C4	-3.43	1.46	1.52
2	B	609	P8E	O6-C2	3.43	1.50	1.43
2	R	611	P8E	O6-C2	3.43	1.50	1.43
2	P	601	P8E	C3-C4	-3.43	1.46	1.52
2	E	613	P8E	O6-C2	3.43	1.50	1.43
2	C	615	P8E	O6-C2	3.43	1.50	1.43
2	L	601	P8E	O6-C2	3.43	1.50	1.43
2	F	601	P8E	C3-C4	-3.43	1.46	1.52
2	H	605	P8E	O6-C2	3.43	1.50	1.43
2	A	601	P8E	C3-C4	-3.43	1.46	1.52
2	P	609	P8E	O6-C2	3.43	1.50	1.43
2	A	617	P8E	C3-C4	-3.43	1.46	1.52
2	G	613	P8E	O6-C2	3.43	1.50	1.43
2	M	611	P8E	O6-C2	3.43	1.50	1.43
2	D	601	P8E	C3-C4	-3.43	1.46	1.52
2	V	609	P8E	C3-C4	-3.43	1.46	1.52
2	E	608	P8E	O6-C2	3.43	1.50	1.43
2	G	614	P8E	O6-C2	3.43	1.50	1.43
2	H	606	P8E	O6-C2	3.43	1.50	1.43
2	H	610	P8E	O6-C2	3.43	1.50	1.43
2	U	609	P8E	O6-C2	3.43	1.50	1.43
2	Q	615	P8E	O6-C2	3.43	1.50	1.43
2	F	614	P8E	C3-C4	-3.43	1.46	1.52
2	B	613	P8E	O6-C2	3.43	1.50	1.43
2	D	617	P8E	C3-C4	-3.43	1.46	1.52
2	L	610	P8E	C3-C4	-3.42	1.46	1.52
2	P	611	P8E	C3-C4	-3.42	1.46	1.52
2	V	601	P8E	O6-C2	3.42	1.50	1.43
2	V	613	P8E	O6-C2	3.42	1.50	1.43
2	U	609	P8E	C3-C4	-3.42	1.46	1.52
2	G	608	P8E	O6-C2	3.42	1.50	1.43
2	Q	616	P8E	O6-C2	3.42	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	606	P8E	O6-C2	3.42	1.50	1.43
2	B	607	P8E	C3-C4	-3.42	1.46	1.52
2	U	607	P8E	C3-C4	-3.42	1.46	1.52
2	N	608	P8E	O6-C2	3.42	1.50	1.43
2	N	612	P8E	O6-C2	3.42	1.50	1.43
2	D	601	P8E	O6-C2	3.42	1.50	1.43
2	L	609	P8E	O6-C2	3.42	1.50	1.43
2	Q	609	P8E	C3-C4	-3.42	1.46	1.52
2	O	615	P8E	O6-C2	3.42	1.50	1.43
2	K	610	P8E	O6-C2	3.42	1.50	1.43
2	M	603	P8E	O6-C2	3.42	1.50	1.43
2	Q	603	P8E	O6-C2	3.42	1.50	1.43
2	D	607	P8E	C3-C4	-3.42	1.46	1.52
2	S	612	P8E	O6-C2	3.42	1.50	1.43
2	Q	613	P8E	O6-C2	3.42	1.50	1.43
2	U	610	P8E	O6-C2	3.42	1.50	1.43
2	V	610	P8E	O6-C2	3.42	1.50	1.43
2	M	607	P8E	C3-C4	-3.41	1.46	1.52
2	L	602	P8E	C3-C4	-3.41	1.46	1.52
2	N	614	P8E	O6-C2	3.41	1.50	1.43
2	V	613	P8E	C3-C4	-3.41	1.46	1.52
2	E	601	P8E	O6-C2	3.41	1.50	1.43
2	V	609	P8E	O6-C2	3.41	1.50	1.43
2	I	610	P8E	C3-C4	-3.41	1.46	1.52
2	J	607	P8E	C3-C4	-3.41	1.46	1.52
2	F	614	P8E	O6-C2	3.41	1.50	1.43
2	I	613	P8E	C3-C4	-3.41	1.46	1.52
2	B	615	P8E	O6-C2	3.41	1.50	1.43
2	U	613	P8E	O6-C2	3.41	1.50	1.43
2	G	611	P8E	O6-C2	3.41	1.50	1.43
2	V	603	P8E	O6-C2	3.41	1.50	1.43
2	G	610	P8E	O6-C2	3.41	1.50	1.43
2	S	603	P8E	O6-C2	3.41	1.50	1.43
2	E	616	P8E	C3-C4	-3.41	1.46	1.52
2	N	602	P8E	C3-C4	-3.41	1.46	1.52
2	D	611	P8E	C3-C4	-3.41	1.46	1.52
2	J	601	P8E	C3-C4	-3.41	1.46	1.52
2	A	609	P8E	O6-C2	3.41	1.50	1.43
2	J	615	P8E	O6-C2	3.40	1.50	1.43
2	S	608	P8E	O6-C2	3.40	1.50	1.43
2	T	603	P8E	O6-C2	3.40	1.50	1.43
2	A	602	P8E	C3-C4	-3.40	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	610	P8E	C3-C4	-3.40	1.46	1.52
2	C	614	P8E	O6-C2	3.40	1.50	1.43
2	J	614	P8E	O6-C2	3.40	1.50	1.43
2	K	613	P8E	O6-C2	3.40	1.50	1.43
2	U	614	P8E	O6-C2	3.40	1.50	1.43
2	O	613	P8E	O6-C2	3.40	1.50	1.43
2	M	615	P8E	O6-C2	3.40	1.50	1.43
2	P	610	P8E	O6-C2	3.40	1.50	1.43
2	C	614	P8E	C3-C4	-3.40	1.46	1.52
2	P	608	P8E	O6-C2	3.40	1.50	1.43
2	F	610	P8E	O6-C2	3.40	1.50	1.43
2	J	609	P8E	O6-C2	3.40	1.50	1.43
2	F	611	P8E	C3-C4	-3.40	1.46	1.52
2	S	610	P8E	C3-C4	-3.40	1.46	1.52
2	D	611	P8E	O6-C2	3.40	1.50	1.43
2	O	611	P8E	C3-C4	-3.40	1.46	1.52
2	D	606	P8E	O6-C2	3.40	1.50	1.43
2	O	611	P8E	O6-C2	3.40	1.50	1.43
2	F	609	P8E	C3-C4	-3.40	1.46	1.52
2	G	602	P8E	C3-C4	-3.40	1.46	1.52
2	P	607	P8E	C3-C4	-3.40	1.46	1.52
2	K	608	P8E	O6-C2	3.40	1.50	1.43
2	T	613	P8E	C3-C4	-3.40	1.46	1.52
2	C	616	P8E	O6-C2	3.40	1.50	1.43
2	D	613	P8E	O6-C2	3.39	1.50	1.43
2	G	609	P8E	C3-C4	-3.39	1.46	1.52
2	S	601	P8E	C3-C4	-3.39	1.46	1.52
2	K	612	P8E	O6-C2	3.39	1.50	1.43
2	T	614	P8E	C3-C4	-3.39	1.46	1.52
2	V	617	P8E	C3-C4	-3.39	1.46	1.52
2	G	616	P8E	O6-C2	3.39	1.50	1.43
2	R	609	P8E	C3-C4	-3.39	1.46	1.52
2	T	610	P8E	O6-C2	3.39	1.50	1.43
2	N	609	P8E	O6-C2	3.39	1.50	1.43
2	J	612	P8E	O6-C2	3.39	1.50	1.43
2	T	613	P8E	O6-C2	3.39	1.50	1.43
2	F	607	P8E	C3-C4	-3.39	1.46	1.52
2	T	601	P8E	C3-C4	-3.39	1.46	1.52
2	E	609	P8E	O6-C2	3.39	1.50	1.43
2	P	611	P8E	O6-C2	3.39	1.50	1.43
2	B	614	P8E	O6-C2	3.39	1.50	1.43
2	A	612	P8E	O6-C2	3.39	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	610	P8E	O6-C2	3.39	1.50	1.43
2	N	601	P8E	C3-C4	-3.39	1.46	1.52
2	A	607	P8E	C3-C4	-3.39	1.46	1.52
2	I	602	P8E	O6-C2	3.39	1.50	1.43
2	L	611	P8E	O6-C2	3.39	1.50	1.43
2	C	607	P8E	C3-C4	-3.39	1.46	1.52
2	G	614	P8E	C3-C4	-3.39	1.46	1.52
2	H	613	P8E	O6-C2	3.39	1.50	1.43
2	H	616	P8E	O6-C2	3.38	1.50	1.43
2	J	611	P8E	O6-C2	3.38	1.50	1.43
2	H	607	P8E	C3-C4	-3.38	1.46	1.52
2	N	616	P8E	C3-C4	-3.38	1.46	1.52
2	V	601	P8E	C3-C4	-3.38	1.46	1.52
2	R	608	P8E	O6-C2	3.38	1.50	1.43
2	R	602	P8E	C3-C4	-3.38	1.46	1.52
2	T	608	P8E	O6-C2	3.38	1.50	1.43
2	G	610	P8E	C3-C4	-3.38	1.46	1.52
2	L	613	P8E	C3-C4	-3.38	1.46	1.52
2	V	611	P8E	O6-C2	3.38	1.50	1.43
2	A	611	P8E	C3-C4	-3.38	1.46	1.52
2	N	613	P8E	C3-C4	-3.38	1.46	1.52
2	N	616	P8E	O6-C2	3.38	1.50	1.43
2	K	609	P8E	O6-C2	3.38	1.50	1.43
2	T	601	P8E	O6-C2	3.38	1.50	1.43
2	V	614	P8E	C3-C4	-3.38	1.46	1.52
2	D	615	P8E	O6-C2	3.38	1.50	1.43
2	D	613	P8E	C3-C4	-3.38	1.46	1.52
2	N	609	P8E	C3-C4	-3.38	1.46	1.52
2	U	617	P8E	C3-C4	-3.38	1.46	1.52
2	C	613	P8E	C3-C4	-3.38	1.46	1.52
2	U	616	P8E	O6-C2	3.38	1.50	1.43
2	H	609	P8E	C3-C4	-3.38	1.46	1.52
2	I	603	P8E	O6-C2	3.38	1.50	1.43
2	I	602	P8E	C3-C4	-3.37	1.46	1.52
2	I	608	P8E	O6-C2	3.37	1.50	1.43
2	M	610	P8E	C3-C4	-3.37	1.46	1.52
2	D	616	P8E	O6-C2	3.37	1.50	1.43
2	F	610	P8E	C3-C4	-3.37	1.46	1.52
2	H	608	P8E	O6-C2	3.37	1.50	1.43
2	V	608	P8E	O6-C2	3.37	1.50	1.43
2	O	609	P8E	C3-C4	-3.37	1.46	1.52
2	J	610	P8E	C3-C4	-3.37	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	613	P8E	C3-C4	-3.37	1.46	1.52
2	S	607	P8E	C3-C4	-3.37	1.46	1.52
2	D	609	P8E	C3-C4	-3.37	1.46	1.52
2	B	609	P8E	C3-C4	-3.37	1.46	1.52
2	K	601	P8E	C3-C4	-3.37	1.46	1.52
2	N	613	P8E	O6-C2	3.37	1.50	1.43
2	J	613	P8E	C3-C4	-3.37	1.46	1.52
2	L	601	P8E	C3-C4	-3.37	1.46	1.52
2	N	601	P8E	O6-C2	3.37	1.50	1.43
2	P	609	P8E	C3-C4	-3.37	1.46	1.52
2	Q	602	P8E	O6-C2	3.37	1.50	1.43
2	T	607	P8E	C3-C4	-3.37	1.46	1.52
2	J	609	P8E	C3-C4	-3.37	1.46	1.52
2	B	610	P8E	C3-C4	-3.37	1.46	1.52
2	K	614	P8E	O6-C2	3.36	1.50	1.43
2	V	611	P8E	C3-C4	-3.36	1.46	1.52
2	A	602	P8E	O6-C2	3.36	1.50	1.43
2	R	613	P8E	C3-C4	-3.36	1.46	1.52
2	I	616	P8E	O6-C2	3.36	1.50	1.43
2	H	614	P8E	C3-C4	-3.36	1.46	1.52
2	Q	610	P8E	O6-C2	3.36	1.50	1.43
2	T	616	P8E	O6-C2	3.36	1.50	1.43
2	V	615	P8E	O6-C2	3.36	1.50	1.43
2	E	607	P8E	C3-C4	-3.36	1.46	1.52
2	C	611	P8E	O6-C2	3.36	1.50	1.43
2	E	615	P8E	O6-C2	3.36	1.50	1.43
2	J	613	P8E	O6-C2	3.36	1.50	1.43
2	R	602	P8E	O6-C2	3.36	1.50	1.43
2	T	614	P8E	O6-C2	3.36	1.50	1.43
2	M	602	P8E	C3-C4	-3.36	1.46	1.52
2	F	613	P8E	O6-C2	3.36	1.50	1.43
2	G	611	P8E	C3-C4	-3.36	1.46	1.52
2	I	612	P8E	O6-C2	3.36	1.50	1.43
2	P	616	P8E	C3-C4	-3.36	1.46	1.52
2	H	609	P8E	O6-C2	3.35	1.50	1.43
2	P	614	P8E	O6-C2	3.35	1.50	1.43
2	B	614	P8E	C3-C4	-3.35	1.46	1.52
2	N	611	P8E	C3-C4	-3.35	1.46	1.52
2	R	607	P8E	C3-C4	-3.35	1.46	1.52
2	S	613	P8E	C3-C4	-3.35	1.46	1.52
2	E	611	P8E	O6-C2	3.35	1.50	1.43
2	B	601	P8E	C3-C4	-3.35	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	613	P8E	C3-C4	-3.35	1.46	1.52
2	E	602	P8E	O6-C2	3.35	1.50	1.43
2	C	602	P8E	C3-C4	-3.35	1.46	1.52
2	H	615	P8E	O6-C2	3.35	1.50	1.43
2	R	615	P8E	O6-C2	3.35	1.50	1.43
2	G	601	P8E	O6-C2	3.35	1.50	1.43
2	C	609	P8E	C3-C4	-3.35	1.46	1.52
2	E	613	P8E	C3-C4	-3.35	1.46	1.52
2	O	613	P8E	C3-C4	-3.35	1.46	1.52
2	D	610	P8E	C3-C4	-3.35	1.46	1.52
2	P	610	P8E	C3-C4	-3.35	1.46	1.52
2	Q	601	P8E	O6-C2	3.35	1.50	1.43
2	K	615	P8E	O6-C2	3.35	1.50	1.43
2	M	611	P8E	C3-C4	-3.35	1.46	1.52
2	I	613	P8E	O6-C2	3.35	1.50	1.43
2	P	602	P8E	O6-C2	3.35	1.50	1.43
2	C	616	P8E	C3-C4	-3.34	1.46	1.52
2	H	602	P8E	C3-C4	-3.34	1.46	1.52
2	J	608	P8E	O6-C2	3.34	1.50	1.43
2	V	610	P8E	C3-C4	-3.34	1.46	1.52
2	C	608	P8E	O6-C2	3.34	1.50	1.43
2	O	602	P8E	O6-C2	3.34	1.50	1.43
2	E	614	P8E	O6-C2	3.34	1.50	1.43
2	V	614	P8E	O6-C2	3.34	1.50	1.43
2	A	613	P8E	O6-C2	3.34	1.50	1.43
2	L	608	P8E	O6-C2	3.34	1.50	1.43
2	N	603	P8E	O6-C2	3.34	1.50	1.43
2	S	614	P8E	O6-C2	3.34	1.50	1.43
2	U	613	P8E	C3-C4	-3.34	1.46	1.52
2	K	602	P8E	O6-C2	3.34	1.50	1.43
2	P	616	P8E	O6-C2	3.34	1.50	1.43
2	L	614	P8E	C3-C4	-3.34	1.46	1.52
2	S	615	P8E	O6-C2	3.34	1.50	1.43
2	M	608	P8E	O6-C2	3.34	1.50	1.43
2	C	613	P8E	O6-C2	3.34	1.50	1.43
2	A	614	P8E	O6-C2	3.34	1.50	1.43
2	J	616	P8E	C3-C4	-3.34	1.46	1.52
2	O	608	P8E	O6-C2	3.34	1.50	1.43
2	A	608	P8E	O6-C2	3.34	1.50	1.43
2	R	616	P8E	O6-C2	3.34	1.50	1.43
2	I	611	P8E	C3-C4	-3.34	1.46	1.52
2	K	610	P8E	C3-C4	-3.34	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	616	P8E	C3-C4	-3.34	1.46	1.52
2	P	614	P8E	C3-C4	-3.34	1.46	1.52
2	K	616	P8E	C3-C4	-3.34	1.46	1.52
2	R	611	P8E	C3-C4	-3.34	1.46	1.52
2	U	616	P8E	C3-C4	-3.34	1.46	1.52
2	E	610	P8E	C3-C4	-3.33	1.46	1.52
2	H	601	P8E	C3-C4	-3.33	1.46	1.52
2	D	602	P8E	C3-C4	-3.33	1.46	1.52
2	M	613	P8E	O6-C2	3.33	1.50	1.43
2	G	607	P8E	C3-C4	-3.33	1.46	1.52
2	N	607	P8E	C3-C4	-3.33	1.46	1.52
2	L	614	P8E	O6-C2	3.33	1.50	1.43
2	K	616	P8E	O6-C2	3.33	1.50	1.43
2	S	613	P8E	O6-C2	3.33	1.50	1.43
2	U	601	P8E	O6-C2	3.33	1.50	1.43
2	N	610	P8E	C3-C4	-3.33	1.46	1.52
2	T	610	P8E	C3-C4	-3.33	1.46	1.52
2	P	612	P8E	O6-C2	3.33	1.50	1.43
2	M	616	P8E	O6-C2	3.33	1.50	1.43
2	Q	613	P8E	C3-C4	-3.33	1.46	1.52
2	V	602	P8E	O6-C2	3.32	1.50	1.43
2	O	614	P8E	O6-C2	3.32	1.50	1.43
2	A	613	P8E	C3-C4	-3.32	1.46	1.52
2	L	616	P8E	C3-C4	-3.32	1.46	1.52
2	J	611	P8E	C3-C4	-3.32	1.46	1.52
2	H	616	P8E	C3-C4	-3.32	1.46	1.52
2	G	616	P8E	C3-C4	-3.32	1.46	1.52
2	L	616	P8E	O6-C2	3.32	1.50	1.43
2	S	602	P8E	O6-C2	3.32	1.50	1.43
2	G	601	P8E	C3-C4	-3.32	1.46	1.52
2	L	602	P8E	O6-C2	3.32	1.50	1.43
2	O	607	P8E	C3-C4	-3.32	1.46	1.52
2	B	608	P8E	O6-C2	3.32	1.50	1.43
2	Q	614	P8E	O6-C2	3.31	1.50	1.43
2	D	616	P8E	C3-C4	-3.31	1.46	1.52
2	T	616	P8E	C3-C4	-3.31	1.46	1.52
2	R	610	P8E	C3-C4	-3.31	1.46	1.52
2	U	601	P8E	C3-C4	-3.31	1.46	1.52
2	F	608	P8E	O6-C2	3.31	1.50	1.43
2	T	602	P8E	O6-C2	3.31	1.50	1.43
2	I	616	P8E	C3-C4	-3.31	1.46	1.52
2	Q	612	P8E	O6-C2	3.31	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	601	P8E	O6-C2	3.31	1.49	1.43
2	R	616	P8E	C3-C4	-3.31	1.46	1.52
2	O	610	P8E	C3-C4	-3.31	1.46	1.52
2	Q	601	P8E	C3-C4	-3.31	1.46	1.52
2	C	611	P8E	C3-C4	-3.30	1.46	1.52
2	U	602	P8E	O6-C2	3.30	1.49	1.43
2	I	601	P8E	C3-C4	-3.30	1.46	1.52
2	Q	610	P8E	C3-C4	-3.30	1.46	1.52
2	R	614	P8E	O6-C2	3.30	1.49	1.43
2	M	601	P8E	C3-C4	-3.29	1.46	1.52
2	Q	614	P8E	C3-C4	-3.29	1.46	1.52
2	M	613	P8E	C3-C4	-3.29	1.46	1.52
2	D	614	P8E	O6-C2	3.29	1.49	1.43
2	N	602	P8E	O6-C2	3.29	1.49	1.43
2	G	602	P8E	O6-C2	3.29	1.49	1.43
2	J	602	P8E	O6-C2	3.29	1.49	1.43
2	H	602	P8E	O6-C2	3.28	1.49	1.43
2	M	602	P8E	O6-C2	3.28	1.49	1.43
2	F	613	P8E	C3-C4	-3.28	1.46	1.52
2	V	616	P8E	C3-C4	-3.28	1.46	1.52
2	A	611	P8E	O6-C2	3.28	1.49	1.43
2	I	601	P8E	O6-C2	3.28	1.49	1.43
2	C	602	P8E	O6-C2	3.28	1.49	1.43
2	F	602	P8E	O6-C2	3.28	1.49	1.43
2	H	601	P8E	O6-C2	3.28	1.49	1.43
2	Q	609	P8E	O6-C2	3.28	1.49	1.43
2	D	602	P8E	O6-C2	3.27	1.49	1.43
2	B	602	P8E	O6-C2	3.26	1.49	1.43
2	G	615	P8E	O6-C2	3.26	1.49	1.43
2	V	607	P8E	C3-C4	-3.25	1.46	1.52
2	H	614	P8E	O6-C2	3.25	1.49	1.43
2	E	616	P8E	O6-C2	3.24	1.49	1.43
2	V	616	P8E	O6-C2	3.24	1.49	1.43
2	Q	612	P8E	C3-C4	-3.20	1.46	1.52
2	Q	605	P8E	C3-C4	-3.16	1.46	1.52
2	J	605	P8E	C3-C4	-3.15	1.46	1.52
2	R	608	P8E	C3-C4	-3.14	1.46	1.52
2	I	603	P8E	C3-C4	-3.14	1.46	1.52
2	P	608	P8E	C3-C4	-3.14	1.46	1.52
2	S	605	P8E	C3-C4	-3.13	1.46	1.52
2	F	605	P8E	C3-C4	-3.13	1.46	1.52
2	P	603	P8E	C3-C4	-3.12	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	612	P8E	C3-C4	-3.12	1.46	1.52
2	S	612	P8E	C3-C4	-3.12	1.46	1.52
2	D	605	P8E	C3-C4	-3.12	1.46	1.52
2	Q	603	P8E	C3-C4	-3.12	1.46	1.52
2	V	605	P8E	C3-C4	-3.12	1.46	1.52
2	S	615	P8E	C3-C4	-3.11	1.46	1.52
2	I	608	P8E	C3-C4	-3.11	1.46	1.52
2	M	605	P8E	C3-C4	-3.11	1.46	1.52
2	G	615	P8E	C3-C4	-3.11	1.46	1.52
2	I	612	P8E	C3-C4	-3.11	1.46	1.52
2	O	612	P8E	C3-C4	-3.10	1.46	1.52
2	C	608	P8E	C3-C4	-3.10	1.46	1.52
2	E	605	P8E	C3-C4	-3.10	1.46	1.52
2	L	603	P8E	C3-C4	-3.10	1.46	1.52
2	A	605	P8E	C3-C4	-3.10	1.46	1.52
2	L	615	P8E	C3-C4	-3.10	1.46	1.52
2	P	612	P8E	C3-C4	-3.10	1.46	1.52
2	D	603	P8E	C3-C4	-3.10	1.46	1.52
2	K	615	P8E	C3-C4	-3.10	1.46	1.52
2	R	612	P8E	C3-C4	-3.10	1.46	1.52
2	A	606	P8E	C3-C4	-3.09	1.46	1.52
2	R	605	P8E	C3-C4	-3.09	1.46	1.52
2	B	615	P8E	C3-C4	-3.09	1.46	1.52
2	V	603	P8E	C3-C4	-3.09	1.46	1.52
2	H	605	P8E	C3-C4	-3.09	1.46	1.52
2	G	612	P8E	C3-C4	-3.09	1.46	1.52
2	E	608	P8E	C3-C4	-3.09	1.46	1.52
2	C	603	P8E	C3-C4	-3.09	1.46	1.52
2	M	612	P8E	C3-C4	-3.08	1.46	1.52
2	A	612	P8E	C3-C4	-3.08	1.46	1.52
2	D	612	P8E	C3-C4	-3.08	1.46	1.52
2	S	603	P8E	C3-C4	-3.08	1.46	1.52
2	N	615	P8E	C3-C4	-3.08	1.46	1.52
2	O	608	P8E	C3-C4	-3.08	1.46	1.52
2	K	603	P8E	C3-C4	-3.08	1.46	1.52
2	A	603	P8E	C3-C4	-3.07	1.46	1.52
2	N	612	P8E	C3-C4	-3.07	1.46	1.52
2	A	608	P8E	C3-C4	-3.07	1.46	1.52
2	J	612	P8E	C3-C4	-3.07	1.46	1.52
2	P	605	P8E	C3-C4	-3.07	1.46	1.52
2	H	608	P8E	C3-C4	-3.07	1.46	1.52
2	D	615	P8E	C3-C4	-3.07	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	605	P8E	C3-C4	-3.07	1.46	1.52
2	E	606	P8E	C3-C4	-3.06	1.46	1.52
2	H	603	P8E	C3-C4	-3.06	1.46	1.52
2	N	605	P8E	C3-C4	-3.06	1.46	1.52
2	T	608	P8E	C3-C4	-3.06	1.46	1.52
2	E	612	P8E	C3-C4	-3.06	1.46	1.52
2	E	603	P8E	C3-C4	-3.06	1.46	1.52
2	B	605	P8E	C3-C4	-3.06	1.46	1.52
2	M	603	P8E	C3-C4	-3.06	1.46	1.52
2	I	605	P8E	C3-C4	-3.06	1.46	1.52
2	F	603	P8E	C3-C4	-3.05	1.46	1.52
2	V	612	P8E	C3-C4	-3.05	1.46	1.52
2	J	603	P8E	C3-C4	-3.05	1.46	1.52
2	G	608	P8E	C3-C4	-3.05	1.46	1.52
2	G	603	P8E	C3-C4	-3.05	1.46	1.52
2	L	608	P8E	C3-C4	-3.05	1.46	1.52
2	F	615	P8E	C3-C4	-3.05	1.46	1.52
2	H	615	P8E	C3-C4	-3.04	1.46	1.52
2	H	612	P8E	C3-C4	-3.04	1.46	1.52
2	T	612	P8E	C3-C4	-3.04	1.46	1.52
2	T	605	P8E	C3-C4	-3.04	1.46	1.52
2	T	606	P8E	C3-C4	-3.04	1.46	1.52
2	U	612	P8E	C3-C4	-3.04	1.46	1.52
2	J	608	P8E	C3-C4	-3.04	1.47	1.52
2	K	606	P8E	C3-C4	-3.04	1.47	1.52
2	O	603	P8E	C3-C4	-3.04	1.47	1.52
2	U	615	P8E	C3-C4	-3.04	1.47	1.52
2	I	615	P8E	C3-C4	-3.03	1.47	1.52
2	S	616	P8E	C3-C4	-3.03	1.47	1.52
2	Q	606	P8E	C3-C4	-3.03	1.47	1.52
2	B	608	P8E	C3-C4	-3.03	1.47	1.52
2	V	606	P8E	C3-C4	-3.03	1.47	1.52
2	S	606	P8E	C3-C4	-3.03	1.47	1.52
2	F	606	P8E	C3-C4	-3.03	1.47	1.52
2	O	615	P8E	C3-C4	-3.03	1.47	1.52
2	U	608	P8E	C3-C4	-3.03	1.47	1.52
2	V	615	P8E	C3-C4	-3.03	1.47	1.52
2	U	603	P8E	C3-C4	-3.03	1.47	1.52
2	G	606	P8E	C3-C4	-3.03	1.47	1.52
2	N	603	P8E	C3-C4	-3.02	1.47	1.52
2	A	615	P8E	C3-C4	-3.02	1.47	1.52
2	O	616	P8E	C3-C4	-3.02	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	608	P8E	C3-C4	-3.02	1.47	1.52
2	T	603	P8E	C3-C4	-3.02	1.47	1.52
2	O	606	P8E	C3-C4	-3.02	1.47	1.52
2	S	608	P8E	C3-C4	-3.02	1.47	1.52
2	U	606	P8E	C3-C4	-3.02	1.47	1.52
2	L	612	P8E	C3-C4	-3.02	1.47	1.52
2	I	606	P8E	C3-C4	-3.02	1.47	1.52
2	T	615	P8E	C3-C4	-3.01	1.47	1.52
2	B	606	P8E	C3-C4	-3.01	1.47	1.52
2	N	606	P8E	C3-C4	-3.01	1.47	1.52
2	V	608	P8E	C3-C4	-3.01	1.47	1.52
2	E	615	P8E	C3-C4	-3.01	1.47	1.52
2	Q	608	P8E	C3-C4	-3.01	1.47	1.52
2	O	605	P8E	C3-C4	-3.01	1.47	1.52
2	R	615	P8E	C3-C4	-3.01	1.47	1.52
2	L	606	P8E	C3-C4	-3.01	1.47	1.52
2	N	608	P8E	C3-C4	-3.01	1.47	1.52
2	A	604	P8E	C3-C4	-3.00	1.47	1.52
2	M	608	P8E	C3-C4	-3.00	1.47	1.52
2	L	605	P8E	C3-C4	-3.00	1.47	1.52
2	D	606	P8E	C3-C4	-3.00	1.47	1.52
2	Q	615	P8E	C3-C4	-3.00	1.47	1.52
2	B	603	P8E	C3-C4	-3.00	1.47	1.52
2	C	615	P8E	C3-C4	-3.00	1.47	1.52
2	J	615	P8E	C3-C4	-3.00	1.47	1.52
2	Q	604	P8E	C3-C4	-3.00	1.47	1.52
2	C	612	P8E	C3-C4	-3.00	1.47	1.52
2	M	606	P8E	C3-C4	-2.99	1.47	1.52
2	A	616	P8E	C3-C4	-2.99	1.47	1.52
2	J	604	P8E	C3-C4	-2.99	1.47	1.52
2	P	604	P8E	C3-C4	-2.99	1.47	1.52
2	E	604	P8E	C3-C4	-2.99	1.47	1.52
2	R	606	P8E	C3-C4	-2.99	1.47	1.52
2	H	606	P8E	C3-C4	-2.98	1.47	1.52
2	K	612	P8E	C3-C4	-2.98	1.47	1.52
2	C	605	P8E	C3-C4	-2.98	1.47	1.52
2	R	603	P8E	C3-C4	-2.98	1.47	1.52
2	I	604	P8E	C3-C4	-2.98	1.47	1.52
2	F	604	P8E	C3-C4	-2.98	1.47	1.52
2	C	606	P8E	C3-C4	-2.98	1.47	1.52
2	M	615	P8E	C3-C4	-2.97	1.47	1.52
2	K	608	P8E	C3-C4	-2.97	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	612	P8E	C3-C4	-2.97	1.47	1.52
2	P	615	P8E	C3-C4	-2.97	1.47	1.52
2	J	606	P8E	C3-C4	-2.97	1.47	1.52
2	F	616	P8E	C3-C4	-2.97	1.47	1.52
2	M	604	P8E	C3-C4	-2.97	1.47	1.52
2	V	604	P8E	C3-C4	-2.96	1.47	1.52
2	F	608	P8E	C3-C4	-2.96	1.47	1.52
2	T	604	P8E	C3-C4	-2.96	1.47	1.52
2	G	605	P8E	C3-C4	-2.96	1.47	1.52
2	U	604	P8E	C3-C4	-2.95	1.47	1.52
2	B	616	P8E	C3-C4	-2.95	1.47	1.52
2	P	606	P8E	C3-C4	-2.95	1.47	1.52
2	N	604	P8E	C3-C4	-2.95	1.47	1.52
2	C	604	P8E	C3-C4	-2.95	1.47	1.52
2	R	604	P8E	C3-C4	-2.94	1.47	1.52
2	K	604	P8E	C3-C4	-2.94	1.47	1.52
2	B	604	P8E	C3-C4	-2.94	1.47	1.52
2	G	604	P8E	C3-C4	-2.94	1.47	1.52
2	L	604	P8E	C3-C4	-2.93	1.47	1.52
2	O	604	P8E	C3-C4	-2.93	1.47	1.52
2	U	605	P8E	C3-C4	-2.92	1.47	1.52
2	S	604	P8E	C3-C4	-2.91	1.47	1.52
2	D	604	P8E	C3-C4	-2.90	1.47	1.52
2	H	604	P8E	C3-C4	-2.89	1.47	1.52

All (1049) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	601	P8E	O6-C2-C3	4.42	116.50	110.56
2	C	601	P8E	O6-C2-C3	3.89	115.79	110.56
2	V	607	P8E	O6-C2-C3	3.77	115.62	110.56
2	O	617	P8E	O6-C2-C3	3.61	115.41	110.56
2	D	617	P8E	O6-C2-C3	3.59	115.38	110.56
2	E	617	P8E	O6-C2-C3	3.56	115.34	110.56
2	G	607	P8E	O6-C2-C3	3.52	115.28	110.56
2	K	617	P8E	O6-C2-C3	3.49	115.25	110.56
2	H	617	P8E	O6-C2-C3	3.45	115.20	110.56
2	R	617	P8E	O6-C2-C3	3.40	115.13	110.56
2	S	617	P8E	O6-C2-C3	3.39	115.11	110.56
2	K	607	P8E	O1B-C1-C2	3.38	121.50	112.71
2	F	607	P8E	O1B-C1-C2	3.37	121.49	112.71
2	B	617	P8E	O6-C2-C3	3.36	115.08	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	607	P8E	O1B-C1-C2	3.36	121.45	112.71
2	J	617	P8E	O6-C2-C3	3.36	115.07	110.56
2	P	617	P8E	O6-C2-C3	3.35	115.06	110.56
2	N	617	P8E	O6-C2-C3	3.33	115.03	110.56
2	Q	607	P8E	O1B-C1-C2	3.31	121.32	112.71
2	H	607	P8E	O6-C2-C3	3.31	115.00	110.56
2	T	607	P8E	O1B-C1-C2	3.31	121.31	112.71
2	M	607	P8E	O1B-C1-C2	3.31	121.31	112.71
2	G	617	P8E	O6-C2-C3	3.30	115.00	110.56
2	A	617	P8E	O6-C2-C3	3.30	115.00	110.56
2	A	607	P8E	O1B-C1-C2	3.30	121.29	112.71
2	C	607	P8E	O1B-C1-C2	3.29	121.27	112.71
2	L	617	P8E	O6-C2-C3	3.29	114.98	110.56
2	D	607	P8E	O1B-C1-C2	3.29	121.26	112.71
2	U	607	P8E	O1B-C1-C2	3.28	121.25	112.71
2	I	617	P8E	O6-C2-C3	3.28	114.96	110.56
2	R	607	P8E	O1B-C1-C2	3.28	121.24	112.71
2	B	607	P8E	O1B-C1-C2	3.26	121.19	112.71
2	E	607	P8E	O1B-C1-C2	3.26	121.19	112.71
2	F	617	P8E	O6-C2-C3	3.25	114.92	110.56
2	M	609	P8E	O1B-C1-C2	3.24	121.13	112.71
2	J	607	P8E	O1B-C1-C2	3.23	121.12	112.71
2	T	617	P8E	O6-C2-C3	3.23	114.90	110.56
2	S	607	P8E	O1B-C1-C2	3.23	121.10	112.71
2	G	607	P8E	O1B-C1-C2	3.23	121.10	112.71
2	H	607	P8E	O1B-C1-C2	3.22	121.10	112.71
2	J	607	P8E	O6-C2-C3	3.22	114.89	110.56
2	L	607	P8E	O1B-C1-C2	3.22	121.08	112.71
2	O	607	P8E	O1B-C1-C2	3.22	121.08	112.71
2	I	607	P8E	O1B-C1-C2	3.21	121.06	112.71
2	O	609	P8E	O1B-C1-C2	3.20	121.04	112.71
2	F	609	P8E	O1B-C1-C2	3.20	121.04	112.71
2	Q	617	P8E	O6-C2-C3	3.20	114.86	110.56
2	P	602	P8E	O1B-C1-C2	3.19	121.02	112.71
2	S	609	P8E	O1B-C1-C2	3.19	121.00	112.71
2	N	607	P8E	O1B-C1-C2	3.19	121.00	112.71
2	D	607	P8E	O6-C2-C3	3.18	114.83	110.56
2	B	609	P8E	O1B-C1-C2	3.17	120.96	112.71
2	T	609	P8E	O1B-C1-C2	3.17	120.95	112.71
2	V	617	P8E	O6-C2-C3	3.16	114.81	110.56
2	U	617	P8E	O6-C2-C3	3.16	114.81	110.56
2	P	607	P8E	O1B-C1-C2	3.16	120.94	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	609	P8E	O1B-C1-C2	3.14	120.88	112.71
2	S	607	P8E	O6-C2-C3	3.13	114.77	110.56
2	D	617	P8E	O6-C6-C5	3.13	114.57	108.94
2	R	609	P8E	O1B-C1-C2	3.12	120.83	112.71
2	C	617	P8E	O6-C2-C3	3.12	114.75	110.56
2	M	617	P8E	O6-C2-C3	3.12	114.75	110.56
2	P	609	P8E	O1B-C1-C2	3.11	120.81	112.71
2	I	609	P8E	O1B-C1-C2	3.11	120.80	112.71
2	G	609	P8E	O1B-C1-C2	3.10	120.77	112.71
2	A	609	P8E	O1B-C1-C2	3.09	120.75	112.71
2	L	602	P8E	O1B-C1-C2	3.08	120.72	112.71
2	Q	602	P8E	O1B-C1-C2	3.08	120.71	112.71
2	U	609	P8E	O1B-C1-C2	3.07	120.69	112.71
2	H	609	P8E	O1B-C1-C2	3.06	120.68	112.71
2	D	609	P8E	O1B-C1-C2	3.06	120.67	112.71
2	B	602	P8E	O1B-C1-C2	3.06	120.66	112.71
2	E	617	P8E	O6-C6-C5	3.05	114.43	108.94
2	U	607	P8E	O6-C2-C3	3.05	114.65	110.56
2	C	609	P8E	O1B-C1-C2	3.04	120.62	112.71
2	F	607	P8E	O6-C2-C3	3.04	114.65	110.56
2	E	606	P8E	O6-C6-C5	3.04	114.39	108.94
2	E	616	P8E	O1B-C1-C2	3.03	120.59	112.71
2	K	609	P8E	O1B-C1-C2	3.03	120.58	112.71
2	V	609	P8E	O1B-C1-C2	3.02	120.57	112.71
2	F	608	P8E	O1B-C1-C2	3.02	120.56	112.71
2	E	609	P8E	O1B-C1-C2	3.01	120.54	112.71
2	N	609	P8E	O1B-C1-C2	3.01	120.53	112.71
2	U	602	P8E	O1B-C1-C2	3.00	120.53	112.71
2	V	602	P8E	O1B-C1-C2	2.99	120.48	112.71
2	S	616	P8E	O6-C2-C3	2.98	114.56	110.56
2	N	616	P8E	O1B-C1-C2	2.98	120.46	112.71
2	R	602	P8E	O1B-C1-C2	2.98	120.45	112.71
2	U	611	P8E	O6-C2-C3	2.97	114.55	110.56
2	E	602	P8E	O1B-C1-C2	2.97	120.44	112.71
2	M	602	P8E	O1B-C1-C2	2.97	120.43	112.71
2	T	602	P8E	O1B-C1-C2	2.97	120.43	112.71
2	P	615	P8E	O1B-C1-C2	2.96	120.42	112.71
2	Q	616	P8E	O1B-C1-C2	2.94	120.37	112.71
2	U	611	P8E	O1B-C1-C2	2.94	120.36	112.71
2	F	604	P8E	O1B-C1-C2	2.94	120.36	112.71
2	K	617	P8E	O6-C6-C5	2.94	114.22	108.94
2	S	617	P8E	O6-C6-C5	2.94	114.22	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	615	P8E	O1B-C1-C2	2.93	120.34	112.71
2	T	611	P8E	O6-C2-C3	2.93	114.50	110.56
2	U	608	P8E	O1B-C1-C2	2.93	120.33	112.71
2	A	604	P8E	O1B-C1-C2	2.93	120.32	112.71
2	O	602	P8E	O1B-C1-C2	2.93	120.32	112.71
2	B	604	P8E	O1B-C1-C2	2.93	120.32	112.71
2	J	602	P8E	O1B-C1-C2	2.93	120.32	112.71
2	U	604	P8E	O1B-C1-C2	2.93	120.32	112.71
2	L	615	P8E	O1B-C1-C2	2.92	120.31	112.71
2	O	616	P8E	O6-C2-C3	2.92	114.48	110.56
2	K	608	P8E	O1B-C1-C2	2.92	120.30	112.71
2	Q	615	P8E	O1B-C1-C2	2.92	120.30	112.71
2	F	602	P8E	O1B-C1-C2	2.92	120.29	112.71
2	C	607	P8E	O6-C2-C3	2.92	114.48	110.56
2	T	607	P8E	O6-C2-C3	2.91	114.47	110.56
2	Q	604	P8E	O1B-C1-C2	2.91	120.28	112.71
2	G	615	P8E	O6-C6-C5	2.91	114.17	108.94
2	N	611	P8E	O1B-C1-C2	2.91	120.27	112.71
2	I	604	P8E	O1B-C1-C2	2.90	120.26	112.71
2	P	617	P8E	O6-C6-C5	2.90	114.16	108.94
2	A	607	P8E	O6-C2-C3	2.90	114.46	110.56
2	B	616	P8E	O1B-C1-C2	2.90	120.24	112.71
2	I	608	P8E	O6-C6-C5	2.89	114.14	108.94
2	N	602	P8E	O1B-C1-C2	2.89	120.24	112.71
2	V	604	P8E	O1B-C1-C2	2.89	120.23	112.71
2	K	611	P8E	O1B-C1-C2	2.89	120.23	112.71
2	M	605	P8E	O1B-C1-C2	2.89	120.23	112.71
2	O	617	P8E	O6-C6-C5	2.89	114.13	108.94
2	A	612	P8E	O6-C2-C3	2.89	114.44	110.56
2	K	615	P8E	O1B-C1-C2	2.89	120.22	112.71
2	S	614	P8E	O1B-C1-C2	2.89	120.22	112.71
2	L	614	P8E	O1B-C1-C2	2.89	120.21	112.71
2	B	617	P8E	O6-C6-C5	2.88	114.12	108.94
2	T	604	P8E	O1B-C1-C2	2.88	120.21	112.71
2	E	604	P8E	O1B-C1-C2	2.88	120.21	112.71
2	F	616	P8E	O6-C2-C3	2.88	114.43	110.56
2	T	608	P8E	O1B-C1-C2	2.88	120.20	112.71
2	A	617	P8E	O6-C6-C5	2.88	114.11	108.94
2	A	602	P8E	O1B-C1-C2	2.88	120.20	112.71
2	L	604	P8E	O1B-C1-C2	2.87	120.19	112.71
2	R	604	P8E	O1B-C1-C2	2.87	120.18	112.71
2	P	614	P8E	O1B-C1-C2	2.87	120.18	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	609	P8E	O1B-C1-C2	2.87	120.17	112.71
2	H	617	P8E	O6-C6-C5	2.87	114.10	108.94
2	N	608	P8E	O1B-C1-C2	2.87	120.17	112.71
2	M	608	P8E	O1B-C1-C2	2.87	120.16	112.71
2	M	615	P8E	O1B-C1-C2	2.87	120.16	112.71
2	I	602	P8E	O1B-C1-C2	2.87	120.16	112.71
2	R	611	P8E	O1B-C1-C2	2.86	120.15	112.71
2	U	613	P8E	O1B-C1-C2	2.86	120.15	112.71
2	K	604	P8E	O1B-C1-C2	2.86	120.15	112.71
2	P	612	P8E	O6-C2-C3	2.86	114.40	110.56
2	P	608	P8E	O1B-C1-C2	2.86	120.14	112.71
2	D	611	P8E	O1B-C1-C2	2.86	120.14	112.71
2	O	604	P8E	O1B-C1-C2	2.86	120.14	112.71
2	G	602	P8E	O1B-C1-C2	2.85	120.13	112.71
2	I	613	P8E	O1B-C1-C2	2.85	120.13	112.71
2	E	611	P8E	O1B-C1-C2	2.85	120.12	112.71
2	N	604	P8E	O1B-C1-C2	2.85	120.11	112.71
2	H	611	P8E	O1B-C1-C2	2.84	120.11	112.71
2	Q	617	P8E	O6-C6-C5	2.84	114.05	108.94
2	D	614	P8E	O1B-C1-C2	2.84	120.10	112.71
2	G	604	P8E	O1B-C1-C2	2.84	120.09	112.71
2	H	610	P8E	O1B-C1-C2	2.84	120.09	112.71
2	L	611	P8E	O1B-C1-C2	2.84	120.09	112.71
2	B	611	P8E	O1B-C1-C2	2.84	120.09	112.71
2	O	611	P8E	O1B-C1-C2	2.83	120.08	112.71
2	K	602	P8E	O1B-C1-C2	2.83	120.08	112.71
2	P	605	P8E	O1B-C1-C2	2.83	120.08	112.71
2	H	612	P8E	O6-C2-C3	2.83	114.36	110.56
2	S	602	P8E	O1B-C1-C2	2.83	120.08	112.71
2	H	604	P8E	O1B-C1-C2	2.83	120.07	112.71
2	T	615	P8E	O1B-C1-C2	2.83	120.07	112.71
2	S	611	P8E	O1B-C1-C2	2.83	120.06	112.71
2	E	614	P8E	O1B-C1-C2	2.83	120.06	112.71
2	T	605	P8E	O1B-C1-C2	2.83	120.06	112.71
2	J	604	P8E	O1B-C1-C2	2.82	120.06	112.71
2	O	614	P8E	O1B-C1-C2	2.82	120.05	112.71
2	C	610	P8E	O1B-C1-C2	2.82	120.05	112.71
2	A	616	P8E	O6-C2-C3	2.82	114.35	110.56
2	P	616	P8E	O1B-C1-C2	2.82	120.05	112.71
2	G	611	P8E	O1B-C1-C2	2.82	120.05	112.71
2	N	617	P8E	O1B-C1-C2	2.82	120.04	112.71
2	B	615	P8E	O1B-C1-C2	2.82	120.04	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	612	P8E	O6-C2-C3	2.82	114.34	110.56
2	J	613	P8E	O1B-C1-C2	2.82	120.03	112.71
2	S	608	P8E	O1B-C1-C2	2.82	120.03	112.71
2	K	613	P8E	O1B-C1-C2	2.81	120.02	112.71
2	L	601	P8E	O1B-C1-C2	2.81	120.02	112.71
2	Q	611	P8E	O1B-C1-C2	2.81	120.02	112.71
2	D	605	P8E	O1B-C1-C2	2.81	120.02	112.71
2	S	616	P8E	O1B-C1-C2	2.81	120.02	112.71
2	U	617	P8E	O6-C6-C5	2.81	113.99	108.94
2	A	615	P8E	O1B-C1-C2	2.81	120.02	112.71
2	B	605	P8E	O1B-C1-C2	2.81	120.01	112.71
2	C	604	P8E	O1B-C1-C2	2.81	120.01	112.71
2	G	617	P8E	O6-C6-C5	2.81	113.99	108.94
2	M	610	P8E	O1B-C1-C2	2.81	120.01	112.71
2	B	613	P8E	O1B-C1-C2	2.81	120.01	112.71
2	H	614	P8E	O1B-C1-C2	2.80	120.00	112.71
2	I	617	P8E	O6-C6-C5	2.80	113.98	108.94
2	G	614	P8E	O1B-C1-C2	2.80	120.00	112.71
2	R	616	P8E	O1B-C1-C2	2.80	120.00	112.71
2	N	606	P8E	O6-C6-C5	2.80	113.97	108.94
2	D	604	P8E	O1B-C1-C2	2.80	119.99	112.71
2	P	607	P8E	O6-C2-C3	2.80	114.32	110.56
2	G	617	P8E	O1B-C1-C2	2.80	119.99	112.71
2	S	615	P8E	O1B-C1-C2	2.80	119.99	112.71
2	L	610	P8E	O1B-C1-C2	2.80	119.98	112.71
2	P	610	P8E	O1B-C1-C2	2.79	119.98	112.71
2	T	601	P8E	O1B-C1-C2	2.79	119.98	112.71
2	D	608	P8E	O1B-C1-C2	2.79	119.97	112.71
2	P	604	P8E	O1B-C1-C2	2.79	119.97	112.71
2	B	614	P8E	O1B-C1-C2	2.79	119.97	112.71
2	Q	605	P8E	O1B-C1-C2	2.79	119.97	112.71
2	T	613	P8E	O1B-C1-C2	2.79	119.97	112.71
2	O	615	P8E	O1B-C1-C2	2.79	119.97	112.71
2	A	603	P8E	O6-C2-C3	2.79	114.31	110.56
2	E	617	P8E	O1B-C1-C2	2.79	119.96	112.71
2	S	604	P8E	O1B-C1-C2	2.79	119.96	112.71
2	R	614	P8E	O1B-C1-C2	2.79	119.96	112.71
2	F	610	P8E	O1B-C1-C2	2.79	119.96	112.71
2	A	611	P8E	O1B-C1-C2	2.79	119.96	112.71
2	E	607	P8E	O6-C2-C3	2.78	114.30	110.56
2	L	617	P8E	O6-C6-C5	2.78	113.94	108.94
2	N	605	P8E	O1B-C1-C2	2.78	119.95	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	605	P8E	O1B-C1-C2	2.78	119.95	112.71
2	M	611	P8E	O1B-C1-C2	2.78	119.95	112.71
2	L	608	P8E	O1B-C1-C2	2.78	119.95	112.71
2	O	610	P8E	O1B-C1-C2	2.78	119.95	112.71
2	F	614	P8E	O1B-C1-C2	2.78	119.94	112.71
2	V	617	P8E	O1B-C1-C2	2.78	119.94	112.71
2	I	611	P8E	O6-C2-C3	2.78	114.29	110.56
2	E	605	P8E	O1B-C1-C2	2.78	119.94	112.71
2	H	602	P8E	O1B-C1-C2	2.78	119.94	112.71
2	J	610	P8E	O1B-C1-C2	2.78	119.94	112.71
2	J	611	P8E	O1B-C1-C2	2.78	119.93	112.71
2	P	611	P8E	O1B-C1-C2	2.78	119.93	112.71
2	C	611	P8E	O1B-C1-C2	2.78	119.93	112.71
2	V	611	P8E	O1B-C1-C2	2.78	119.93	112.71
2	R	617	P8E	O6-C6-C5	2.77	113.93	108.94
2	R	617	P8E	O1B-C1-C2	2.77	119.92	112.71
2	C	616	P8E	O1B-C1-C2	2.77	119.92	112.71
2	M	614	P8E	O1B-C1-C2	2.77	119.92	112.71
2	F	617	P8E	O1B-C1-C2	2.77	119.92	112.71
2	M	617	P8E	O1B-C1-C2	2.77	119.92	112.71
2	J	605	P8E	O1B-C1-C2	2.77	119.92	112.71
2	D	612	P8E	O6-C2-C3	2.77	114.28	110.56
2	J	617	P8E	O1B-C1-C2	2.77	119.92	112.71
2	M	601	P8E	O1B-C1-C2	2.77	119.91	112.71
2	K	614	P8E	O1B-C1-C2	2.77	119.90	112.71
2	E	615	P8E	O1B-C1-C2	2.76	119.90	112.71
2	M	604	P8E	O1B-C1-C2	2.76	119.90	112.71
2	J	603	P8E	O1B-C1-C2	2.76	119.89	112.71
2	A	613	P8E	O1B-C1-C2	2.76	119.89	112.71
2	T	614	P8E	O1B-C1-C2	2.76	119.89	112.71
2	A	614	P8E	O1B-C1-C2	2.76	119.89	112.71
2	J	615	P8E	O1B-C1-C2	2.76	119.89	112.71
2	B	617	P8E	O1B-C1-C2	2.76	119.89	112.71
2	F	605	P8E	O1B-C1-C2	2.76	119.89	112.71
2	S	610	P8E	O1B-C1-C2	2.76	119.89	112.71
2	I	605	P8E	O1B-C1-C2	2.76	119.88	112.71
2	G	610	P8E	O1B-C1-C2	2.76	119.88	112.71
2	N	601	P8E	O1B-C1-C2	2.76	119.88	112.71
2	F	606	P8E	O6-C6-C5	2.76	113.89	108.94
2	C	617	P8E	O1B-C1-C2	2.75	119.88	112.71
2	H	608	P8E	O1B-C1-C2	2.75	119.87	112.71
2	F	616	P8E	O1B-C1-C2	2.75	119.87	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	616	P8E	O1B-C1-C2	2.75	119.87	112.71
2	G	612	P8E	O6-C2-C3	2.75	114.26	110.56
2	N	610	P8E	O1B-C1-C2	2.75	119.87	112.71
2	A	616	P8E	O1B-C1-C2	2.75	119.87	112.71
2	V	617	P8E	O6-C6-C5	2.75	113.88	108.94
2	S	605	P8E	O1B-C1-C2	2.75	119.86	112.71
2	D	603	P8E	O6-C2-C3	2.75	114.25	110.56
2	K	605	P8E	O1B-C1-C2	2.75	119.86	112.71
2	Q	601	P8E	O1B-C1-C2	2.75	119.86	112.71
2	O	616	P8E	O1B-C1-C2	2.75	119.86	112.71
2	V	608	P8E	O1B-C1-C2	2.75	119.86	112.71
2	E	610	P8E	O1B-C1-C2	2.75	119.86	112.71
2	E	608	P8E	O1B-C1-C2	2.74	119.85	112.71
2	U	605	P8E	O1B-C1-C2	2.74	119.85	112.71
2	T	617	P8E	O6-C6-C5	2.74	113.87	108.94
2	U	610	P8E	O1B-C1-C2	2.74	119.84	112.71
2	A	608	P8E	O1B-C1-C2	2.74	119.84	112.71
2	I	617	P8E	O1B-C1-C2	2.74	119.84	112.71
2	U	601	P8E	O1B-C1-C2	2.74	119.84	112.71
2	T	611	P8E	O1B-C1-C2	2.74	119.83	112.71
2	B	610	P8E	O1B-C1-C2	2.74	119.83	112.71
2	G	615	P8E	O1B-C1-C2	2.74	119.83	112.71
2	A	610	P8E	O1B-C1-C2	2.74	119.83	112.71
2	F	611	P8E	O1B-C1-C2	2.74	119.82	112.71
2	R	610	P8E	O1B-C1-C2	2.74	119.82	112.71
2	A	606	P8E	O6-C6-C5	2.73	113.86	108.94
2	I	611	P8E	O1B-C1-C2	2.73	119.82	112.71
2	G	601	P8E	O1B-C1-C2	2.73	119.81	112.71
2	I	610	P8E	O1B-C1-C2	2.73	119.81	112.71
2	J	614	P8E	O1B-C1-C2	2.73	119.80	112.71
2	C	617	P8E	O6-C6-C5	2.73	113.84	108.94
2	Q	617	P8E	O1B-C1-C2	2.73	119.80	112.71
2	N	613	P8E	O1B-C1-C2	2.72	119.79	112.71
2	F	613	P8E	O1B-C1-C2	2.72	119.79	112.71
2	C	602	P8E	O1B-C1-C2	2.72	119.79	112.71
2	K	610	P8E	O1B-C1-C2	2.72	119.79	112.71
2	T	616	P8E	O1B-C1-C2	2.72	119.78	112.71
2	K	616	P8E	O1B-C1-C2	2.72	119.78	112.71
2	C	615	P8E	O1B-C1-C2	2.72	119.78	112.71
2	I	601	P8E	O1B-C1-C2	2.72	119.78	112.71
2	P	612	P8E	O1B-C1-C2	2.72	119.78	112.71
2	A	617	P8E	O1B-C1-C2	2.72	119.78	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	605	P8E	O1B-C1-C2	2.72	119.77	112.71
2	T	617	P8E	O1B-C1-C2	2.72	119.77	112.71
2	T	610	P8E	O1B-C1-C2	2.72	119.77	112.71
2	O	617	P8E	O1B-C1-C2	2.71	119.77	112.71
2	A	603	P8E	O1B-C1-C2	2.71	119.77	112.71
2	D	602	P8E	O1B-C1-C2	2.71	119.76	112.71
2	B	603	P8E	O1B-C1-C2	2.71	119.76	112.71
2	P	613	P8E	O1B-C1-C2	2.71	119.76	112.71
2	S	617	P8E	O1B-C1-C2	2.71	119.76	112.71
2	V	605	P8E	O1B-C1-C2	2.71	119.76	112.71
2	U	614	P8E	O1B-C1-C2	2.71	119.75	112.71
2	L	617	P8E	O1B-C1-C2	2.70	119.74	112.71
2	E	601	P8E	O1B-C1-C2	2.70	119.74	112.71
2	D	616	P8E	O1B-C1-C2	2.70	119.74	112.71
2	H	613	P8E	O1B-C1-C2	2.70	119.73	112.71
2	L	607	P8E	O6-C2-C3	2.70	114.19	110.56
2	G	613	P8E	O1B-C1-C2	2.70	119.73	112.71
2	I	614	P8E	O1B-C1-C2	2.70	119.73	112.71
2	K	606	P8E	O1B-C1-C2	2.70	119.73	112.71
2	V	614	P8E	O1B-C1-C2	2.70	119.73	112.71
2	F	612	P8E	O1B-C1-C2	2.70	119.73	112.71
2	Q	614	P8E	O1B-C1-C2	2.70	119.72	112.71
2	H	605	P8E	O1B-C1-C2	2.70	119.72	112.71
2	V	613	P8E	O1B-C1-C2	2.70	119.72	112.71
2	Q	612	P8E	O6-C2-C3	2.70	114.18	110.56
2	O	613	P8E	O1B-C1-C2	2.70	119.72	112.71
2	B	608	P8E	O6-C6-C5	2.70	113.78	108.94
2	P	617	P8E	O1B-C1-C2	2.69	119.72	112.71
2	J	617	P8E	O6-C6-C5	2.69	113.78	108.94
2	B	614	P8E	C9-C8-C7	-2.69	108.41	112.66
2	O	612	P8E	O6-C2-C3	2.69	114.18	110.56
2	L	613	P8E	O1B-C1-C2	2.69	119.71	112.71
2	Q	613	P8E	O1B-C1-C2	2.69	119.71	112.71
2	K	611	P8E	O6-C2-C3	2.69	114.17	110.56
2	U	615	P8E	O1B-C1-C2	2.69	119.71	112.71
2	H	601	P8E	O1B-C1-C2	2.69	119.71	112.71
2	J	608	P8E	O1B-C1-C2	2.69	119.70	112.71
2	R	605	P8E	O1B-C1-C2	2.69	119.70	112.71
2	C	605	P8E	O1B-C1-C2	2.69	119.70	112.71
2	N	614	P8E	O1B-C1-C2	2.69	119.70	112.71
2	D	603	P8E	O1B-C1-C2	2.69	119.70	112.71
2	T	603	P8E	O6-C2-C3	2.68	114.17	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	616	P8E	O1B-C1-C2	2.68	119.69	112.71
2	C	612	P8E	O6-C2-C3	2.68	114.16	110.56
2	U	616	P8E	O1B-C1-C2	2.68	119.69	112.71
2	N	617	P8E	O6-C6-C5	2.68	113.76	108.94
2	M	613	P8E	O1B-C1-C2	2.68	119.69	112.71
2	Q	606	P8E	O1B-C1-C2	2.68	119.68	112.71
2	V	612	P8E	C9-C8-C7	-2.68	108.43	112.66
2	Q	602	P8E	O6-C6-C5	2.68	113.75	108.94
2	M	616	P8E	O1B-C1-C2	2.68	119.67	112.71
2	Q	608	P8E	O1B-C1-C2	2.68	119.67	112.71
2	H	615	P8E	O1B-C1-C2	2.68	119.67	112.71
2	F	617	P8E	O6-C6-C5	2.68	113.75	108.94
2	D	606	P8E	O1B-C1-C2	2.67	119.66	112.71
2	K	617	P8E	O1B-C1-C2	2.67	119.66	112.71
2	P	606	P8E	O1B-C1-C2	2.67	119.66	112.71
2	A	606	P8E	O1B-C1-C2	2.67	119.66	112.71
2	B	608	P8E	O1B-C1-C2	2.67	119.66	112.71
2	F	615	P8E	O1B-C1-C2	2.67	119.66	112.71
2	V	610	P8E	O1B-C1-C2	2.67	119.65	112.71
2	C	613	P8E	O1B-C1-C2	2.67	119.65	112.71
2	I	615	P8E	O1B-C1-C2	2.67	119.64	112.71
2	N	606	P8E	O1B-C1-C2	2.67	119.64	112.71
2	O	608	P8E	O1B-C1-C2	2.67	119.64	112.71
2	H	617	P8E	O1B-C1-C2	2.66	119.64	112.71
2	J	606	P8E	O1B-C1-C2	2.66	119.64	112.71
2	E	613	P8E	O1B-C1-C2	2.66	119.64	112.71
2	L	616	P8E	O1B-C1-C2	2.66	119.63	112.71
2	I	612	P8E	O6-C2-C3	2.66	114.13	110.56
2	F	601	P8E	O1B-C1-C2	2.66	119.63	112.71
2	L	612	P8E	O6-C2-C3	2.66	114.13	110.56
2	O	606	P8E	O1B-C1-C2	2.66	119.63	112.71
2	G	612	P8E	O1B-C1-C2	2.66	119.63	112.71
2	D	613	P8E	O1B-C1-C2	2.66	119.62	112.71
2	B	613	P8E	O6-C2-C3	2.66	114.13	110.56
2	I	616	P8E	O1B-C1-C2	2.66	119.62	112.71
2	Q	610	P8E	O1B-C1-C2	2.66	119.62	112.71
2	A	605	P8E	O1B-C1-C2	2.66	119.62	112.71
2	M	606	P8E	O1B-C1-C2	2.66	119.62	112.71
2	P	603	P8E	O1B-C1-C2	2.66	119.62	112.71
2	I	606	P8E	O1B-C1-C2	2.65	119.61	112.71
2	T	603	P8E	O1B-C1-C2	2.65	119.61	112.71
2	V	606	P8E	O1B-C1-C2	2.65	119.61	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	616	P8E	C4-C5-N5	-2.65	105.63	111.11
2	M	603	P8E	O6-C2-C3	2.65	114.12	110.56
2	D	610	P8E	O1B-C1-C2	2.65	119.60	112.71
2	I	612	P8E	O1B-C1-C2	2.65	119.60	112.71
2	M	617	P8E	O6-C6-C5	2.65	113.70	108.94
2	G	616	P8E	O1B-C1-C2	2.65	119.60	112.71
2	R	613	P8E	O1B-C1-C2	2.65	119.60	112.71
2	V	615	P8E	O1B-C1-C2	2.65	119.60	112.71
2	D	612	P8E	C9-C8-C7	-2.65	108.48	112.66
2	Q	607	P8E	O6-C2-C3	2.64	114.11	110.56
2	E	612	P8E	O6-C2-C3	2.64	114.11	110.56
2	S	606	P8E	O1B-C1-C2	2.64	119.57	112.71
2	C	614	P8E	O1B-C1-C2	2.64	119.57	112.71
2	B	607	P8E	O6-C2-C3	2.64	114.10	110.56
2	K	612	P8E	O6-C2-C3	2.64	114.10	110.56
2	D	617	P8E	O1B-C1-C2	2.64	119.57	112.71
2	R	606	P8E	O1B-C1-C2	2.64	119.57	112.71
2	C	612	P8E	O1B-C1-C2	2.63	119.56	112.71
2	L	603	P8E	O1B-C1-C2	2.63	119.56	112.71
2	E	606	P8E	O1B-C1-C2	2.63	119.56	112.71
2	D	612	P8E	O1B-C1-C2	2.63	119.56	112.71
2	B	616	P8E	O6-C2-C3	2.63	114.09	110.56
2	U	612	P8E	O6-C2-C3	2.63	114.09	110.56
2	J	616	P8E	O6-C6-C7	2.63	112.04	105.79
2	E	603	P8E	O1B-C1-C2	2.63	119.55	112.71
2	I	603	P8E	O1B-C1-C2	2.63	119.55	112.71
2	O	605	P8E	O1B-C1-C2	2.63	119.54	112.71
2	B	606	P8E	O1B-C1-C2	2.63	119.54	112.71
2	H	610	P8E	O6-C6-C5	2.63	113.66	108.94
2	S	612	P8E	O6-C2-C3	2.62	114.08	110.56
2	T	606	P8E	O1B-C1-C2	2.62	119.54	112.71
2	U	617	P8E	O1B-C1-C2	2.62	119.53	112.71
2	H	606	P8E	O1B-C1-C2	2.62	119.53	112.71
2	L	606	P8E	O1B-C1-C2	2.62	119.53	112.71
2	C	606	P8E	O1B-C1-C2	2.62	119.52	112.71
2	F	606	P8E	O1B-C1-C2	2.62	119.52	112.71
2	S	613	P8E	O1B-C1-C2	2.62	119.52	112.71
2	V	601	P8E	C9-C8-C7	-2.62	108.53	112.66
2	N	603	P8E	O1B-C1-C2	2.62	119.51	112.71
2	J	603	P8E	O6-C2-C3	2.62	114.07	110.56
2	G	608	P8E	O1B-C1-C2	2.61	119.51	112.71
2	R	603	P8E	O1B-C1-C2	2.61	119.51	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	608	P8E	O1B-C1-C2	2.61	119.50	112.71
2	I	603	P8E	O6-C2-C3	2.61	114.07	110.56
2	H	603	P8E	O1B-C1-C2	2.61	119.50	112.71
2	P	613	P8E	O6-C2-C3	2.61	114.06	110.56
2	I	606	P8E	O6-C6-C5	2.61	113.62	108.94
2	G	603	P8E	O1B-C1-C2	2.61	119.49	112.71
2	C	612	P8E	C9-C8-C7	-2.60	108.55	112.66
2	G	606	P8E	O1B-C1-C2	2.60	119.48	112.71
2	I	608	P8E	O1B-C1-C2	2.60	119.48	112.71
2	O	603	P8E	O1B-C1-C2	2.60	119.48	112.71
2	Q	603	P8E	O1B-C1-C2	2.60	119.48	112.71
2	R	615	P8E	O1B-C1-C2	2.60	119.48	112.71
2	K	607	P8E	O6-C2-C3	2.60	114.05	110.56
2	R	608	P8E	O1B-C1-C2	2.60	119.48	112.71
2	M	616	P8E	O6-C6-C7	2.60	111.97	105.79
2	N	612	P8E	O6-C2-C3	2.60	114.05	110.56
2	H	612	P8E	O1B-C1-C2	2.60	119.47	112.71
2	J	609	P8E	O1B-C1-C2	2.60	119.47	112.71
2	K	603	P8E	O1B-C1-C2	2.60	119.47	112.71
2	Q	612	P8E	O1B-C1-C2	2.60	119.47	112.71
2	J	606	P8E	O6-C6-C5	2.60	113.61	108.94
2	E	603	P8E	O6-C2-C3	2.60	114.05	110.56
2	D	606	P8E	O6-C6-C5	2.60	113.61	108.94
2	C	603	P8E	O1B-C1-C2	2.60	119.46	112.71
2	L	612	P8E	O1B-C1-C2	2.60	119.46	112.71
2	U	606	P8E	O6-C6-C5	2.59	113.60	108.94
2	S	603	P8E	O6-C2-C3	2.59	114.04	110.56
2	M	606	P8E	O6-C6-C5	2.59	113.59	108.94
2	N	615	P8E	O1B-C1-C2	2.59	119.44	112.71
2	O	612	P8E	O1B-C1-C2	2.59	119.44	112.71
2	H	616	P8E	O1B-C1-C2	2.59	119.44	112.71
2	N	612	P8E	O1B-C1-C2	2.59	119.44	112.71
2	V	612	P8E	O1B-C1-C2	2.59	119.44	112.71
2	A	612	P8E	O1B-C1-C2	2.58	119.43	112.71
2	H	616	P8E	C4-C5-N5	-2.58	105.77	111.11
2	S	616	P8E	C4-C5-N5	-2.58	105.78	111.11
2	B	606	P8E	O6-C6-C5	2.58	113.58	108.94
2	T	606	P8E	O6-C6-C5	2.58	113.58	108.94
2	A	601	P8E	O1B-C1-C2	2.58	119.42	112.71
2	E	612	P8E	O1B-C1-C2	2.58	119.41	112.71
2	P	601	P8E	O1B-C1-C2	2.58	119.41	112.71
2	P	603	P8E	O6-C2-C3	2.58	114.02	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	612	P8E	O1B-C1-C2	2.57	119.40	112.71
2	H	614	P8E	C9-C8-C7	-2.57	108.60	112.66
2	F	601	P8E	O6-C2-C3	2.57	114.01	110.56
2	G	616	P8E	O6-C6-C7	2.56	111.88	105.79
2	K	612	P8E	O1B-C1-C2	2.56	119.38	112.71
2	J	601	P8E	O1B-C1-C2	2.56	119.36	112.71
2	V	601	P8E	O1B-C1-C2	2.56	119.36	112.71
2	I	616	P8E	C9-C8-C7	-2.56	108.62	112.66
2	A	616	P8E	C4-C5-N5	-2.55	105.83	111.11
2	U	603	P8E	O1B-C1-C2	2.55	119.35	112.71
2	B	603	P8E	O6-C2-C3	2.55	113.99	110.56
2	H	616	P8E	O6-C6-C7	2.55	111.85	105.79
2	S	603	P8E	O1B-C1-C2	2.55	119.35	112.71
2	M	603	P8E	O1B-C1-C2	2.55	119.33	112.71
2	L	616	P8E	O6-C6-C7	2.55	111.84	105.79
2	V	603	P8E	O1B-C1-C2	2.54	119.33	112.71
2	R	612	P8E	O1B-C1-C2	2.54	119.32	112.71
2	C	605	P8E	O6-C2-C3	2.54	113.97	110.56
2	B	608	P8E	O6-C2-C3	2.54	113.97	110.56
2	F	603	P8E	O1B-C1-C2	2.54	119.31	112.71
2	G	606	P8E	O6-C2-C3	2.54	113.97	110.56
2	R	607	P8E	O6-C2-C3	2.54	113.97	110.56
2	K	615	P8E	O6-C6-C5	2.54	113.50	108.94
2	U	616	P8E	O6-C6-C7	2.53	111.81	105.79
2	A	614	P8E	C9-C8-C7	-2.53	108.66	112.66
2	F	612	P8E	C9-C8-C7	-2.53	108.66	112.66
2	I	616	P8E	O6-C6-C7	2.53	111.80	105.79
2	H	603	P8E	O6-C2-C3	2.53	113.96	110.56
2	Q	612	P8E	C9-C8-C7	-2.53	108.67	112.66
2	F	612	P8E	O6-C2-C3	2.53	113.95	110.56
2	G	612	P8E	C9-C8-C7	-2.53	108.67	112.66
2	U	603	P8E	O6-C2-C3	2.52	113.95	110.56
2	S	612	P8E	O1B-C1-C2	2.52	119.26	112.71
2	T	616	P8E	O6-C6-C7	2.52	111.78	105.79
2	S	601	P8E	O1B-C1-C2	2.52	119.26	112.71
2	T	612	P8E	C9-C8-C7	-2.52	108.68	112.66
2	G	605	P8E	O6-C2-C3	2.52	113.94	110.56
2	B	612	P8E	O1B-C1-C2	2.52	119.25	112.71
2	U	606	P8E	O1B-C1-C2	2.52	119.25	112.71
2	H	613	P8E	C9-C8-C7	-2.51	108.69	112.66
2	R	601	P8E	O6-C2-C3	2.51	113.93	110.56
2	U	612	P8E	O1B-C1-C2	2.51	119.23	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	616	P8E	C4-C5-N5	-2.51	105.93	111.11
2	B	609	P8E	C9-C8-C7	-2.51	108.70	112.66
2	N	603	P8E	O6-C2-C3	2.50	113.92	110.56
2	R	616	P8E	C4-C5-N5	-2.50	105.94	111.11
2	V	602	P8E	O6-C6-C5	2.50	113.44	108.94
2	V	612	P8E	O6-C2-C3	2.50	113.92	110.56
2	T	609	P8E	O6-C2-C3	2.50	113.92	110.56
2	L	616	P8E	C4-C5-N5	-2.50	105.94	111.11
2	L	606	P8E	O6-C6-C5	2.50	113.43	108.94
2	J	612	P8E	O1B-C1-C2	2.50	119.21	112.71
2	U	613	P8E	O6-C2-C3	2.50	113.91	110.56
2	Q	616	P8E	C4-C5-N5	-2.49	105.95	111.11
2	T	612	P8E	O1B-C1-C2	2.49	119.20	112.71
2	D	616	P8E	O6-C6-C7	2.49	111.72	105.79
2	E	616	P8E	C9-C8-C7	-2.49	108.72	112.66
2	P	606	P8E	C9-C8-C7	-2.49	108.73	112.66
2	O	603	P8E	O6-C2-C3	2.49	113.90	110.56
2	I	607	P8E	O6-C2-C3	2.49	113.90	110.56
2	D	605	P8E	O6-C2-C3	2.49	113.90	110.56
2	R	614	P8E	C9-C8-C7	-2.49	108.73	112.66
2	M	604	P8E	O6-C2-C3	2.49	113.90	110.56
2	N	607	P8E	O6-C2-C3	2.49	113.90	110.56
2	B	616	P8E	C4-C5-N5	-2.49	105.97	111.11
2	K	601	P8E	O1B-C1-C2	2.48	119.17	112.71
2	Q	616	P8E	O6-C6-C7	2.48	111.69	105.79
2	K	616	P8E	O6-C6-C7	2.48	111.69	105.79
2	K	606	P8E	O6-C6-C5	2.48	113.40	108.94
2	P	612	P8E	C9-C8-C7	-2.48	108.74	112.66
2	V	606	P8E	O6-C6-C5	2.48	113.39	108.94
2	U	606	P8E	O6-C2-C3	2.48	113.89	110.56
2	F	616	P8E	C4-C5-N5	-2.48	105.99	111.11
2	M	616	P8E	C9-C8-C7	-2.47	108.75	112.66
2	F	605	P8E	O6-C2-C3	2.47	113.88	110.56
2	L	610	P8E	O6-C6-C5	2.47	113.38	108.94
2	R	606	P8E	O6-C6-C5	2.47	113.38	108.94
2	P	613	P8E	C9-C8-C7	-2.47	108.76	112.66
2	S	612	P8E	C9-C8-C7	-2.47	108.76	112.66
2	C	606	P8E	O6-C2-C3	2.47	113.87	110.56
2	I	614	P8E	C9-C8-C7	-2.47	108.76	112.66
2	L	614	P8E	C9-C8-C7	-2.46	108.78	112.66
2	K	601	P8E	O6-C2-C3	2.46	113.86	110.56
2	P	616	P8E	C4-C5-N5	-2.46	106.03	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	612	P8E	C9-C8-C7	-2.46	108.78	112.66
2	T	614	P8E	C9-C8-C7	-2.46	108.78	112.66
2	B	601	P8E	O1B-C1-C2	2.45	119.09	112.71
2	L	603	P8E	O6-C2-C3	2.45	113.85	110.56
2	C	605	P8E	C9-C8-C7	-2.45	108.79	112.66
2	H	612	P8E	C9-C8-C7	-2.45	108.79	112.66
2	L	605	P8E	O6-C2-C3	2.45	113.85	110.56
2	G	603	P8E	O6-C2-C3	2.45	113.85	110.56
2	B	617	P8E	C9-C8-C7	-2.45	108.79	112.66
2	F	603	P8E	O6-C2-C3	2.45	113.85	110.56
2	Q	616	P8E	C9-C8-C7	-2.45	108.80	112.66
2	E	605	P8E	C9-C8-C7	-2.45	108.80	112.66
2	L	606	P8E	C9-C8-C7	-2.44	108.80	112.66
2	O	606	P8E	O6-C6-C5	2.44	113.33	108.94
2	O	612	P8E	C9-C8-C7	-2.44	108.80	112.66
2	R	612	P8E	O6-C2-C3	2.44	113.84	110.56
2	U	616	P8E	C4-C5-N5	-2.44	106.06	111.11
2	I	616	P8E	C4-C5-N5	-2.44	106.07	111.11
2	M	607	P8E	O6-C2-C3	2.44	113.83	110.56
2	Q	603	P8E	O6-C2-C3	2.44	113.83	110.56
2	R	616	P8E	O6-C6-C7	2.44	111.58	105.79
2	B	605	P8E	O6-C2-C3	2.44	113.83	110.56
2	C	616	P8E	O6-C6-C7	2.44	111.58	105.79
2	L	612	P8E	C9-C8-C7	-2.43	108.81	112.66
2	P	606	P8E	O6-C2-C3	2.43	113.83	110.56
2	F	616	P8E	C9-C8-C7	-2.43	108.82	112.66
2	M	612	P8E	C9-C8-C7	-2.43	108.82	112.66
2	K	613	P8E	C9-C8-C7	-2.43	108.82	112.66
2	G	614	P8E	C9-C8-C7	-2.43	108.82	112.66
2	O	605	P8E	O6-C2-C3	2.43	113.82	110.56
2	J	604	P8E	O6-C2-C3	2.43	113.82	110.56
2	S	606	P8E	O6-C6-C5	2.43	113.31	108.94
2	D	601	P8E	O1B-C1-C2	2.43	119.03	112.71
2	Q	606	P8E	O6-C2-C3	2.43	113.82	110.56
2	H	608	P8E	O6-C2-C3	2.42	113.82	110.56
2	J	612	P8E	O6-C2-C3	2.42	113.81	110.56
2	C	614	P8E	C9-C8-C7	-2.42	108.83	112.66
2	H	605	P8E	O6-C2-C3	2.42	113.81	110.56
2	V	616	P8E	C4-C5-N5	-2.42	106.11	111.11
2	K	603	P8E	O6-C2-C3	2.42	113.81	110.56
2	N	613	P8E	C9-C8-C7	-2.42	108.84	112.66
2	T	616	P8E	C4-C5-N5	-2.42	106.11	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	615	P8E	O6-C2-C3	2.42	113.81	110.56
2	B	611	P8E	O6-C2-C3	2.42	113.80	110.56
2	G	613	P8E	C9-C8-C7	-2.41	108.85	112.66
2	O	601	P8E	O1B-C1-C2	2.41	118.98	112.71
2	B	616	P8E	C9-C8-C7	-2.41	108.85	112.66
2	M	614	P8E	C9-C8-C7	-2.41	108.86	112.66
2	R	601	P8E	O1B-C1-C2	2.41	118.97	112.71
2	N	616	P8E	C9-C8-C7	-2.41	108.86	112.66
2	V	613	P8E	C9-C8-C7	-2.41	108.86	112.66
2	K	616	P8E	C9-C8-C7	-2.41	108.86	112.66
2	G	608	P8E	O6-C2-C3	2.41	113.79	110.56
2	V	605	P8E	O6-C2-C3	2.41	113.79	110.56
2	A	601	P8E	O6-C2-C3	2.40	113.79	110.56
2	D	616	P8E	C9-C8-C7	-2.40	108.87	112.66
2	S	616	P8E	C9-C8-C7	-2.40	108.87	112.66
2	N	612	P8E	C9-C8-C7	-2.40	108.87	112.66
2	F	611	P8E	O6-C2-C3	2.40	113.78	110.56
2	O	613	P8E	C9-C8-C7	-2.40	108.87	112.66
2	L	613	P8E	C9-C8-C7	-2.40	108.87	112.66
2	Q	609	P8E	C9-C8-C7	-2.40	108.87	112.66
2	T	611	P8E	C9-C8-C7	-2.40	108.87	112.66
2	C	601	P8E	O1B-C1-C2	2.40	118.94	112.71
2	K	612	P8E	C9-C8-C7	-2.39	108.88	112.66
2	J	616	P8E	C4-C5-N5	-2.39	106.16	111.11
2	P	616	P8E	O6-C6-C7	2.39	111.48	105.79
2	P	617	P8E	C9-C8-C7	-2.39	108.88	112.66
2	A	602	P8E	C9-C8-C7	-2.39	108.88	112.66
2	U	605	P8E	O6-C2-C3	2.39	113.77	110.56
2	O	616	P8E	C9-C8-C7	-2.39	108.89	112.66
2	N	614	P8E	C9-C8-C7	-2.39	108.89	112.66
2	P	608	P8E	O6-C2-C3	2.38	113.76	110.56
2	U	605	P8E	C9-C8-C7	-2.38	108.90	112.66
2	M	606	P8E	C9-C8-C7	-2.38	108.91	112.66
2	R	616	P8E	C9-C8-C7	-2.38	108.91	112.66
2	F	605	P8E	C9-C8-C7	-2.38	108.91	112.66
2	J	612	P8E	C9-C8-C7	-2.38	108.91	112.66
2	S	601	P8E	O6-C2-C3	2.38	113.75	110.56
2	I	601	P8E	C9-C8-C7	-2.37	108.91	112.66
2	V	616	P8E	C9-C8-C7	-2.37	108.91	112.66
2	Q	611	P8E	O6-C2-C3	2.37	113.75	110.56
2	V	606	P8E	C9-C8-C7	-2.37	108.91	112.66
2	A	604	P8E	O6-C2-C3	2.37	113.74	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	605	P8E	O6-C2-C3	2.37	113.74	110.56
2	F	604	P8E	O6-C2-C3	2.37	113.74	110.56
2	C	603	P8E	O6-C2-C3	2.37	113.74	110.56
2	K	616	P8E	C4-C5-N5	-2.36	106.22	111.11
2	P	605	P8E	O6-C2-C3	2.36	113.73	110.56
2	G	601	P8E	C9-C8-C7	-2.36	108.93	112.66
2	V	604	P8E	O6-C2-C3	2.36	113.73	110.56
2	L	601	P8E	C9-C8-C7	-2.36	108.93	112.66
2	O	613	P8E	O6-C2-C3	2.36	113.73	110.56
2	I	606	P8E	C9-C8-C7	-2.36	108.93	112.66
2	P	616	P8E	C9-C8-C7	-2.36	108.93	112.66
2	T	606	P8E	C9-C8-C7	-2.36	108.93	112.66
2	T	604	P8E	O6-C2-C3	2.36	113.73	110.56
2	J	616	P8E	C9-C8-C7	-2.36	108.94	112.66
2	F	608	P8E	O6-C2-C3	2.36	113.72	110.56
2	E	602	P8E	O6-C6-C5	2.35	113.17	108.94
2	S	610	P8E	O6-C6-C5	2.35	113.17	108.94
2	G	608	P8E	C9-C8-C7	-2.35	108.94	112.66
2	B	604	P8E	O6-C2-C3	2.35	113.71	110.56
2	E	613	P8E	O6-C2-C3	2.35	113.71	110.56
2	U	616	P8E	C9-C8-C7	-2.35	108.95	112.66
2	V	603	P8E	O6-C2-C3	2.35	113.71	110.56
2	N	608	P8E	O6-C2-C3	2.35	113.71	110.56
2	E	614	P8E	O6-C6-C5	2.35	113.16	108.94
2	G	606	P8E	C9-C8-C7	-2.35	108.95	112.66
2	H	606	P8E	C9-C8-C7	-2.34	108.96	112.66
2	Q	606	P8E	C9-C8-C7	-2.34	108.96	112.66
2	M	601	P8E	C9-C8-C7	-2.34	108.97	112.66
2	F	614	P8E	C9-C8-C7	-2.34	108.97	112.66
2	D	613	P8E	C9-C8-C7	-2.33	108.98	112.66
2	U	608	P8E	O6-C2-C3	2.33	113.69	110.56
2	S	601	P8E	C9-C8-C7	-2.33	108.99	112.66
2	J	602	P8E	C9-C8-C7	-2.33	108.99	112.66
2	R	612	P8E	C9-C8-C7	-2.32	108.99	112.66
2	A	616	P8E	C9-C8-C7	-2.32	108.99	112.66
2	H	615	P8E	O6-C2-C3	2.32	113.68	110.56
2	T	616	P8E	C9-C8-C7	-2.32	108.99	112.66
2	A	605	P8E	O6-C2-C3	2.32	113.68	110.56
2	E	609	P8E	C9-C8-C7	-2.32	108.99	112.66
2	E	611	P8E	C9-C8-C7	-2.32	108.99	112.66
2	D	616	P8E	C4-C5-N5	-2.32	106.31	111.11
2	P	605	P8E	C9-C8-C7	-2.32	109.00	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	616	P8E	C4-C5-N5	-2.32	106.32	111.11
2	U	601	P8E	C9-C8-C7	-2.32	109.00	112.66
2	H	606	P8E	O6-C6-C5	2.31	113.10	108.94
2	K	605	P8E	O6-C2-C3	2.31	113.67	110.56
2	O	606	P8E	C9-C8-C7	-2.31	109.00	112.66
2	M	616	P8E	C4-C5-N5	-2.31	106.33	111.11
2	G	605	P8E	C9-C8-C7	-2.31	109.00	112.66
2	C	610	P8E	O6-C6-C5	2.31	113.10	108.94
2	L	617	P8E	C9-C8-C7	-2.31	109.01	112.66
2	N	611	P8E	O6-C2-C3	2.31	113.66	110.56
2	P	602	P8E	O6-C6-C5	2.31	113.09	108.94
2	N	602	P8E	C9-C8-C7	-2.31	109.01	112.66
2	N	616	P8E	C4-C5-N5	-2.31	106.34	111.11
2	U	606	P8E	C9-C8-C7	-2.31	109.02	112.66
2	C	606	P8E	C9-C8-C7	-2.31	109.02	112.66
2	G	617	P8E	C9-C8-C7	-2.31	109.02	112.66
2	T	606	P8E	O6-C2-C3	2.30	113.65	110.56
2	P	602	P8E	O6-C2-C3	2.30	113.65	110.56
2	Q	617	P8E	C9-C8-C7	-2.30	109.02	112.66
2	I	613	P8E	C9-C8-C7	-2.30	109.03	112.66
2	B	601	P8E	C9-C8-C7	-2.30	109.03	112.66
2	H	606	P8E	O6-C2-C3	2.30	113.65	110.56
2	O	607	P8E	O6-C2-C3	2.30	113.64	110.56
2	U	614	P8E	C9-C8-C7	-2.30	109.03	112.66
2	B	613	P8E	C9-C8-C7	-2.30	109.03	112.66
2	J	611	P8E	C9-C8-C7	-2.30	109.03	112.66
2	R	603	P8E	O6-C2-C3	2.30	113.64	110.56
2	M	612	P8E	O6-C2-C3	2.29	113.64	110.56
2	P	614	P8E	C9-C8-C7	-2.29	109.04	112.66
2	R	604	P8E	O6-C2-C3	2.29	113.64	110.56
2	H	616	P8E	C9-C8-C7	-2.29	109.04	112.66
2	N	605	P8E	O6-C2-C3	2.29	113.64	110.56
2	B	612	P8E	C9-C8-C7	-2.29	109.04	112.66
2	N	604	P8E	O6-C2-C3	2.29	113.64	110.56
2	F	606	P8E	O6-C2-C3	2.29	113.63	110.56
2	P	606	P8E	O6-C6-C5	2.29	113.05	108.94
2	U	612	P8E	C9-C8-C7	-2.29	109.05	112.66
2	P	604	P8E	O6-C2-C3	2.29	113.63	110.56
2	Q	606	P8E	O6-C6-C5	2.28	113.05	108.94
2	A	616	P8E	O6-C6-C7	2.28	111.22	105.79
2	G	602	P8E	O6-C2-C3	2.28	113.63	110.56
2	K	605	P8E	C9-C8-C7	-2.28	109.05	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	601	P8E	O6-C2-C3	2.28	113.62	110.56
2	N	601	P8E	C9-C8-C7	-2.28	109.06	112.66
2	K	606	P8E	C9-C8-C7	-2.28	109.06	112.66
2	N	611	P8E	C9-C8-C7	-2.28	109.06	112.66
2	G	616	P8E	C9-C8-C7	-2.28	109.06	112.66
2	R	613	P8E	C9-C8-C7	-2.28	109.06	112.66
2	I	607	P8E	C9-C8-C7	-2.28	109.06	112.66
2	R	606	P8E	C9-C8-C7	-2.28	109.06	112.66
2	U	604	P8E	O6-C2-C3	2.28	113.61	110.56
2	L	605	P8E	C9-C8-C7	-2.27	109.07	112.66
2	I	608	P8E	O6-C2-C3	2.27	113.61	110.56
2	S	602	P8E	C9-C8-C7	-2.27	109.07	112.66
2	E	612	P8E	C9-C8-C7	-2.27	109.08	112.66
2	G	604	P8E	O6-C2-C3	2.27	113.61	110.56
2	T	615	P8E	C9-C8-C7	-2.27	109.08	112.66
2	E	606	P8E	C9-C8-C7	-2.27	109.08	112.66
2	T	612	P8E	O6-C2-C3	2.27	113.60	110.56
2	Q	605	P8E	O6-C2-C3	2.26	113.60	110.56
2	E	602	P8E	C9-C8-C7	-2.26	109.09	112.66
2	A	606	P8E	C9-C8-C7	-2.26	109.09	112.66
2	K	602	P8E	C9-C8-C7	-2.26	109.09	112.66
2	A	613	P8E	C9-C8-C7	-2.26	109.09	112.66
2	I	615	P8E	O6-C2-C3	2.26	113.59	110.56
2	Q	601	P8E	C9-C8-C7	-2.26	109.09	112.66
2	J	605	P8E	O6-C6-C5	2.26	112.99	108.94
2	E	601	P8E	C9-C8-C7	-2.26	109.10	112.66
2	V	617	P8E	C9-C8-C7	-2.26	109.10	112.66
2	Q	615	P8E	O6-C2-C3	2.26	113.59	110.56
2	V	616	P8E	O6-C6-C7	2.26	111.15	105.79
2	D	602	P8E	C9-C8-C7	-2.25	109.10	112.66
2	F	607	P8E	C9-C8-C7	-2.25	109.10	112.66
2	S	604	P8E	O6-C2-C3	2.25	113.59	110.56
2	K	611	P8E	C9-C8-C7	-2.25	109.10	112.66
2	N	606	P8E	C9-C8-C7	-2.25	109.10	112.66
2	G	610	P8E	O6-C6-C5	2.25	112.98	108.94
2	O	602	P8E	C9-C8-C7	-2.25	109.11	112.66
2	T	605	P8E	O6-C2-C3	2.25	113.58	110.56
2	E	612	P8E	O6-C6-C5	2.25	112.98	108.94
2	C	616	P8E	C9-C8-C7	-2.25	109.11	112.66
2	D	606	P8E	C9-C8-C7	-2.25	109.11	112.66
2	R	615	P8E	C9-C8-C7	-2.25	109.11	112.66
2	T	609	P8E	C9-C8-C7	-2.25	109.11	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	609	P8E	C9-C8-C7	-2.25	109.11	112.66
2	A	601	P8E	C9-C8-C7	-2.24	109.12	112.66
2	S	611	P8E	C9-C8-C7	-2.24	109.12	112.66
2	Q	604	P8E	O6-C2-C3	2.24	113.57	110.56
2	A	611	P8E	C9-C8-C7	-2.24	109.12	112.66
2	S	608	P8E	O6-C2-C3	2.24	113.57	110.56
2	K	607	P8E	C9-C8-C7	-2.24	109.12	112.66
2	D	608	P8E	O6-C2-C3	2.24	113.57	110.56
2	L	615	P8E	O6-C6-C5	2.24	112.96	108.94
2	C	614	P8E	O6-C2-C3	2.24	113.56	110.56
2	S	616	P8E	O6-C6-C7	2.24	111.11	105.79
2	K	606	P8E	O6-C2-C3	2.24	113.56	110.56
2	R	607	P8E	C9-C8-C7	-2.23	109.13	112.66
2	K	615	P8E	C9-C8-C7	-2.23	109.13	112.66
2	H	611	P8E	C9-C8-C7	-2.23	109.14	112.66
2	T	607	P8E	C9-C8-C7	-2.23	109.14	112.66
2	I	602	P8E	C9-C8-C7	-2.23	109.14	112.66
2	J	601	P8E	C9-C8-C7	-2.23	109.14	112.66
2	Q	602	P8E	C9-C8-C7	-2.23	109.14	112.66
2	S	606	P8E	C9-C8-C7	-2.23	109.14	112.66
2	P	610	P8E	C9-C8-C7	-2.23	109.14	112.66
2	Q	610	P8E	C9-C8-C7	-2.23	109.14	112.66
2	L	615	P8E	C9-C8-C7	-2.22	109.15	112.66
2	M	611	P8E	C9-C8-C7	-2.22	109.15	112.66
2	D	604	P8E	O6-C2-C3	2.22	113.55	110.56
2	J	605	P8E	C9-C8-C7	-2.22	109.15	112.66
2	R	605	P8E	C9-C8-C7	-2.22	109.15	112.66
2	S	609	P8E	O6-C6-C5	2.22	112.94	108.94
2	V	615	P8E	O6-C2-C3	2.22	113.54	110.56
2	D	606	P8E	O6-C2-C3	2.22	113.54	110.56
2	V	614	P8E	C9-C8-C7	-2.22	109.15	112.66
2	R	610	P8E	C9-C8-C7	-2.22	109.15	112.66
2	K	604	P8E	O6-C2-C3	2.22	113.54	110.56
2	D	609	P8E	C9-C8-C7	-2.22	109.16	112.66
2	P	609	P8E	C9-C8-C7	-2.22	109.16	112.66
2	L	607	P8E	C9-C8-C7	-2.22	109.16	112.66
2	F	602	P8E	C9-C8-C7	-2.21	109.16	112.66
2	I	612	P8E	C9-C8-C7	-2.21	109.16	112.66
2	F	601	P8E	C9-C8-C7	-2.21	109.16	112.66
2	M	605	P8E	C9-C8-C7	-2.21	109.16	112.66
2	S	611	P8E	O6-C2-C3	2.21	113.53	110.56
2	T	617	P8E	C9-C8-C7	-2.21	109.17	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	608	P8E	O6-C2-C3	2.21	113.53	110.56
2	S	615	P8E	O6-C2-C3	2.21	113.53	110.56
2	S	610	P8E	C9-C8-C7	-2.21	109.17	112.66
2	Q	602	P8E	O6-C2-C3	2.21	113.53	110.56
2	J	614	P8E	C9-C8-C7	-2.21	109.17	112.66
2	J	612	P8E	O6-C6-C5	2.21	112.91	108.94
2	P	611	P8E	C9-C8-C7	-2.21	109.17	112.66
2	C	617	P8E	C9-C8-C7	-2.21	109.18	112.66
2	P	601	P8E	C9-C8-C7	-2.21	109.18	112.66
2	N	606	P8E	O6-C2-C3	2.21	113.52	110.56
2	M	603	P8E	C9-C8-C7	-2.20	109.18	112.66
2	C	604	P8E	O6-C2-C3	2.20	113.52	110.56
2	P	610	P8E	O6-C6-C5	2.20	112.90	108.94
2	K	615	P8E	O6-C2-C3	2.20	113.52	110.56
2	G	609	P8E	C9-C8-C7	-2.20	109.18	112.66
2	R	605	P8E	O6-C2-C3	2.20	113.51	110.56
2	L	616	P8E	C9-C8-C7	-2.20	109.19	112.66
2	L	604	P8E	O6-C2-C3	2.20	113.51	110.56
2	Q	607	P8E	C9-C8-C7	-2.20	109.19	112.66
2	T	601	P8E	C9-C8-C7	-2.20	109.19	112.66
2	J	606	P8E	O6-C2-C3	2.20	113.51	110.56
2	E	610	P8E	C9-C8-C7	-2.20	109.19	112.66
2	O	611	P8E	C9-C8-C7	-2.20	109.19	112.66
2	B	616	P8E	O6-C6-C7	2.19	111.00	105.79
2	Q	613	P8E	O6-C2-C3	2.19	113.51	110.56
2	I	604	P8E	O6-C2-C3	2.19	113.50	110.56
2	I	606	P8E	O6-C2-C3	2.19	113.50	110.56
2	D	611	P8E	C9-C8-C7	-2.19	109.20	112.66
2	G	606	P8E	O6-C6-C5	2.19	112.88	108.94
2	D	610	P8E	C9-C8-C7	-2.19	109.20	112.66
2	J	615	P8E	C9-C8-C7	-2.19	109.20	112.66
2	S	614	P8E	C9-C8-C7	-2.19	109.20	112.66
2	C	603	P8E	C9-C8-C7	-2.19	109.21	112.66
2	T	605	P8E	C9-C8-C7	-2.19	109.21	112.66
2	B	611	P8E	C9-C8-C7	-2.19	109.21	112.66
2	U	617	P8E	C9-C8-C7	-2.18	109.21	112.66
2	E	604	P8E	O6-C2-C3	2.18	113.49	110.56
2	B	605	P8E	C9-C8-C7	-2.18	109.21	112.66
2	G	603	P8E	C9-C8-C7	-2.18	109.21	112.66
2	D	601	P8E	C9-C8-C7	-2.18	109.21	112.66
2	L	609	P8E	C9-C8-C7	-2.18	109.21	112.66
2	C	607	P8E	C9-C8-C7	-2.18	109.22	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	605	P8E	O6-C2-C3	2.18	113.49	110.56
2	I	609	P8E	C9-C8-C7	-2.18	109.22	112.66
2	H	604	P8E	O6-C2-C3	2.18	113.49	110.56
2	H	611	P8E	O6-C2-C3	2.18	113.48	110.56
2	D	614	P8E	C9-C8-C7	-2.18	109.22	112.66
2	L	606	P8E	O6-C2-C3	2.18	113.48	110.56
2	G	602	P8E	C9-C8-C7	-2.18	109.22	112.66
2	E	605	P8E	O6-C2-C3	2.17	113.48	110.56
2	O	616	P8E	O6-C6-C7	2.17	110.96	105.79
2	K	602	P8E	O6-C2-C3	2.17	113.48	110.56
2	R	615	P8E	O6-C2-C3	2.17	113.48	110.56
2	B	601	P8E	O6-C2-C3	2.17	113.48	110.56
2	I	610	P8E	C9-C8-C7	-2.17	109.23	112.66
2	F	606	P8E	C9-C8-C7	-2.17	109.23	112.66
2	I	611	P8E	C9-C8-C7	-2.17	109.23	112.66
2	V	610	P8E	C9-C8-C7	-2.17	109.23	112.66
2	E	607	P8E	C9-C8-C7	-2.17	109.24	112.66
2	I	615	P8E	C9-C8-C7	-2.17	109.24	112.66
2	C	611	P8E	C9-C8-C7	-2.17	109.24	112.66
2	M	611	P8E	O6-C2-C3	2.16	113.47	110.56
2	Q	615	P8E	C9-C8-C7	-2.16	109.24	112.66
2	A	610	P8E	C9-C8-C7	-2.16	109.25	112.66
2	A	603	P8E	C9-C8-C7	-2.16	109.25	112.66
2	O	609	P8E	C9-C8-C7	-2.16	109.25	112.66
2	K	601	P8E	C9-C8-C7	-2.16	109.25	112.66
2	R	613	P8E	O6-C2-C3	2.16	113.46	110.56
2	E	615	P8E	C9-C8-C7	-2.16	109.25	112.66
2	J	605	P8E	O6-C2-C3	2.16	113.46	110.56
2	U	615	P8E	O6-C2-C3	2.16	113.46	110.56
2	O	606	P8E	O6-C2-C3	2.16	113.45	110.56
2	L	611	P8E	C9-C8-C7	-2.16	109.25	112.66
2	R	606	P8E	O6-C2-C3	2.15	113.45	110.56
2	B	607	P8E	C9-C8-C7	-2.15	109.26	112.66
2	T	610	P8E	C9-C8-C7	-2.15	109.26	112.66
2	S	609	P8E	C9-C8-C7	-2.15	109.26	112.66
2	S	605	P8E	C9-C8-C7	-2.15	109.26	112.66
2	T	613	P8E	C9-C8-C7	-2.15	109.26	112.66
2	B	615	P8E	C9-C8-C7	-2.15	109.26	112.66
2	J	610	P8E	C9-C8-C7	-2.15	109.26	112.66
2	E	617	P8E	C9-C8-C7	-2.15	109.27	112.66
2	R	603	P8E	C9-C8-C7	-2.15	109.27	112.66
2	C	606	P8E	O6-C6-C5	2.15	112.80	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	610	P8E	C9-C8-C7	-2.15	109.27	112.66
2	V	611	P8E	C9-C8-C7	-2.15	109.27	112.66
2	U	607	P8E	C9-C8-C7	-2.15	109.27	112.66
2	Q	611	P8E	C9-C8-C7	-2.14	109.27	112.66
2	I	603	P8E	C9-C8-C7	-2.14	109.28	112.66
2	J	603	P8E	C9-C8-C7	-2.14	109.28	112.66
2	R	601	P8E	C9-C8-C7	-2.14	109.28	112.66
2	U	610	P8E	C9-C8-C7	-2.14	109.28	112.66
2	F	615	P8E	C9-C8-C7	-2.14	109.28	112.66
2	H	610	P8E	C9-C8-C7	-2.14	109.28	112.66
2	O	610	P8E	C9-C8-C7	-2.14	109.28	112.66
2	D	615	P8E	O6-C2-C3	2.14	113.43	110.56
2	C	610	P8E	C9-C8-C7	-2.14	109.29	112.66
2	B	603	P8E	C9-C8-C7	-2.13	109.29	112.66
2	M	609	P8E	O6-C6-C5	2.13	112.77	108.94
2	A	609	P8E	C9-C8-C7	-2.13	109.29	112.66
2	O	614	P8E	C9-C8-C7	-2.13	109.30	112.66
2	E	613	P8E	C9-C8-C7	-2.13	109.30	112.66
2	Q	605	P8E	C9-C8-C7	-2.13	109.30	112.66
2	O	604	P8E	O6-C2-C3	2.13	113.42	110.56
2	G	611	P8E	C9-C8-C7	-2.13	109.30	112.66
2	H	602	P8E	C9-C8-C7	-2.13	109.30	112.66
2	H	615	P8E	C9-C8-C7	-2.13	109.30	112.66
2	P	607	P8E	C9-C8-C7	-2.12	109.30	112.66
2	D	615	P8E	C9-C8-C7	-2.12	109.31	112.66
2	J	615	P8E	O6-C6-C5	2.12	112.75	108.94
2	P	603	P8E	C9-C8-C7	-2.12	109.31	112.66
2	I	617	P8E	C9-C8-C7	-2.12	109.31	112.66
2	L	603	P8E	C9-C8-C7	-2.12	109.31	112.66
2	N	617	P8E	C9-C8-C7	-2.12	109.31	112.66
2	K	603	P8E	C9-C8-C7	-2.12	109.31	112.66
2	I	609	P8E	O6-C2-C3	2.11	113.40	110.56
2	G	610	P8E	C9-C8-C7	-2.11	109.32	112.66
2	J	606	P8E	C9-C8-C7	-2.11	109.32	112.66
2	S	607	P8E	C9-C8-C7	-2.11	109.32	112.66
2	G	608	P8E	O6-C6-C5	2.11	112.73	108.94
2	O	615	P8E	O6-C2-C3	2.11	113.39	110.56
2	N	616	P8E	O6-C6-C7	2.11	110.81	105.79
2	J	617	P8E	C9-C8-C7	-2.11	109.33	112.66
2	R	609	P8E	C9-C8-C7	-2.11	109.33	112.66
2	F	617	P8E	C9-C8-C7	-2.11	109.33	112.66
2	N	603	P8E	C9-C8-C7	-2.11	109.33	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	606	P8E	O6-C2-C3	2.11	113.39	110.56
2	S	606	P8E	O6-C2-C3	2.11	113.39	110.56
2	H	617	P8E	C9-C8-C7	-2.11	109.33	112.66
2	M	607	P8E	C9-C8-C7	-2.11	109.33	112.66
2	V	602	P8E	C9-C8-C7	-2.11	109.33	112.66
2	N	610	P8E	C9-C8-C7	-2.11	109.33	112.66
2	F	603	P8E	C9-C8-C7	-2.10	109.34	112.66
2	A	602	P8E	O6-C2-C3	2.10	113.39	110.56
2	O	603	P8E	C9-C8-C7	-2.10	109.34	112.66
2	Q	608	P8E	C9-C8-C7	-2.10	109.34	112.66
2	U	611	P8E	C9-C8-C7	-2.10	109.34	112.66
2	H	607	P8E	C9-C8-C7	-2.10	109.34	112.66
2	P	608	P8E	C9-C8-C7	-2.10	109.34	112.66
2	T	603	P8E	C9-C8-C7	-2.10	109.34	112.66
2	M	606	P8E	O6-C2-C3	2.10	113.38	110.56
2	B	610	P8E	O6-C6-C5	2.10	112.71	108.94
2	E	614	P8E	C9-C8-C7	-2.10	109.34	112.66
2	R	611	P8E	C9-C8-C7	-2.10	109.35	112.66
2	D	605	P8E	C9-C8-C7	-2.09	109.35	112.66
2	E	605	P8E	O6-C6-C5	2.09	112.70	108.94
2	B	609	P8E	O6-C2-C3	2.09	113.37	110.56
2	U	610	P8E	O6-C6-C5	2.09	112.70	108.94
2	S	605	P8E	O6-C2-C3	2.09	113.37	110.56
2	O	605	P8E	C9-C8-C7	-2.09	109.36	112.66
2	U	603	P8E	C9-C8-C7	-2.09	109.36	112.66
2	O	601	P8E	C9-C8-C7	-2.09	109.36	112.66
2	R	602	P8E	C9-C8-C7	-2.09	109.36	112.66
2	Q	614	P8E	C9-C8-C7	-2.09	109.36	112.66
2	B	602	P8E	C9-C8-C7	-2.09	109.37	112.66
2	B	610	P8E	C9-C8-C7	-2.08	109.37	112.66
2	F	611	P8E	C9-C8-C7	-2.08	109.37	112.66
2	R	617	P8E	C9-C8-C7	-2.08	109.37	112.66
2	B	615	P8E	O6-C2-C3	2.08	113.36	110.56
2	J	610	P8E	O6-C6-C5	2.08	112.68	108.94
2	H	603	P8E	C9-C8-C7	-2.08	109.38	112.66
2	C	601	P8E	C9-C8-C7	-2.08	109.38	112.66
2	S	603	P8E	C9-C8-C7	-2.08	109.38	112.66
2	L	613	P8E	O6-C2-C3	2.08	113.35	110.56
2	A	605	P8E	C9-C8-C7	-2.08	109.38	112.66
2	D	607	P8E	C9-C8-C7	-2.07	109.38	112.66
2	Q	603	P8E	C9-C8-C7	-2.07	109.39	112.66
2	U	615	P8E	C9-C8-C7	-2.07	109.39	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	615	P8E	O6-C2-C3	2.07	113.34	110.56
2	V	606	P8E	O6-C2-C3	2.07	113.34	110.56
2	E	604	P8E	C9-C8-C7	-2.07	109.39	112.66
2	V	603	P8E	C9-C8-C7	-2.07	109.39	112.66
2	N	615	P8E	C9-C8-C7	-2.07	109.39	112.66
2	O	617	P8E	C9-C8-C7	-2.07	109.39	112.66
2	D	608	P8E	O6-C6-C5	2.07	112.65	108.94
2	D	609	P8E	O6-C2-C3	2.07	113.33	110.56
2	S	617	P8E	C9-C8-C7	-2.07	109.40	112.66
2	S	608	P8E	O6-C6-C5	2.07	112.65	108.94
2	F	609	P8E	C9-C8-C7	-2.06	109.40	112.66
2	U	609	P8E	C9-C8-C7	-2.06	109.40	112.66
2	K	609	P8E	C9-C8-C7	-2.06	109.40	112.66
2	U	602	P8E	O6-C6-C5	2.06	112.64	108.94
2	F	615	P8E	O6-C2-C3	2.06	113.33	110.56
2	I	610	P8E	O6-C6-C5	2.06	112.64	108.94
2	L	615	P8E	O6-C2-C3	2.06	113.32	110.56
2	C	613	P8E	C9-C8-C7	-2.05	109.42	112.66
2	K	609	P8E	O6-C6-C5	2.05	112.63	108.94
2	E	603	P8E	C9-C8-C7	-2.05	109.42	112.66
2	O	607	P8E	C9-C8-C7	-2.05	109.42	112.66
2	H	601	P8E	C9-C8-C7	-2.05	109.42	112.66
2	F	616	P8E	O6-C6-C7	2.05	110.67	105.79
2	G	607	P8E	C9-C8-C7	-2.05	109.42	112.66
2	K	610	P8E	C9-C8-C7	-2.05	109.42	112.66
2	L	604	P8E	C9-C8-C7	-2.05	109.42	112.66
2	L	610	P8E	C9-C8-C7	-2.05	109.42	112.66
2	O	615	P8E	C9-C8-C7	-2.05	109.43	112.66
2	I	602	P8E	O6-C2-C3	2.05	113.31	110.56
2	G	615	P8E	C9-C8-C7	-2.05	109.43	112.66
2	P	602	P8E	C9-C8-C7	-2.04	109.43	112.66
2	E	606	P8E	O6-C2-C3	2.04	113.31	110.56
2	G	615	P8E	O6-C2-C3	2.04	113.31	110.56
2	A	604	P8E	C9-C8-C7	-2.04	109.43	112.66
2	A	617	P8E	C9-C8-C7	-2.04	109.43	112.66
2	L	602	P8E	C9-C8-C7	-2.04	109.43	112.66
2	M	617	P8E	C9-C8-C7	-2.04	109.43	112.66
2	V	615	P8E	C9-C8-C7	-2.04	109.44	112.66
2	P	615	P8E	O6-C6-C5	2.04	112.60	108.94
2	D	601	P8E	O6-C2-C3	2.04	113.30	110.56
2	U	602	P8E	C9-C8-C7	-2.04	109.44	112.66
2	N	608	P8E	C9-C8-C7	-2.04	109.44	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	614	P8E	O6-C6-C5	2.03	112.59	108.94
2	A	615	P8E	C9-C8-C7	-2.03	109.45	112.66
2	N	609	P8E	C9-C8-C7	-2.03	109.45	112.66
2	B	606	P8E	C9-C8-C7	-2.03	109.45	112.66
2	U	613	P8E	C9-C8-C7	-2.03	109.46	112.66
2	E	601	P8E	O6-C2-C3	2.03	113.28	110.56
2	F	610	P8E	C9-C8-C7	-2.03	109.46	112.66
2	O	608	P8E	C9-C8-C7	-2.03	109.46	112.66
2	P	604	P8E	C9-C8-C7	-2.03	109.46	112.66
2	L	601	P8E	O6-C2-C3	2.02	113.28	110.56
2	V	604	P8E	C9-C8-C7	-2.02	109.47	112.66
2	V	609	P8E	C9-C8-C7	-2.02	109.47	112.66
2	A	607	P8E	C9-C8-C7	-2.02	109.48	112.66
2	F	610	P8E	O6-C6-C5	2.01	112.56	108.94
2	N	607	P8E	C9-C8-C7	-2.01	109.48	112.66
2	M	614	P8E	O6-C2-C3	2.01	113.26	110.56
2	V	607	P8E	C9-C8-C7	-2.01	109.48	112.66
2	T	602	P8E	C9-C8-C7	-2.01	109.49	112.66
2	V	608	P8E	C9-C8-C7	-2.01	109.49	112.66
2	A	615	P8E	O6-C2-C3	2.01	113.25	110.56
2	I	604	P8E	C9-C8-C7	-2.01	109.49	112.66
2	U	608	P8E	C9-C8-C7	-2.01	109.49	112.66
2	M	615	P8E	O6-C2-C3	2.01	113.25	110.56
2	F	607	P8E	O1B-C1-O1A	-2.00	119.53	124.08
2	J	613	P8E	C9-C8-C7	-2.00	109.50	112.66
2	S	615	P8E	C9-C8-C7	-2.00	109.50	112.66
2	V	613	P8E	O6-C2-C3	2.00	113.25	110.56

There are no chirality outliers.

All (1456) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	P8E	O6-C6-C7-N7
2	A	602	P8E	C6-C7-C8-C9
2	A	602	P8E	N7-C7-C8-C9
2	A	602	P8E	C6-C7-C8-O8
2	A	602	P8E	N7-C7-C8-O8
2	A	604	P8E	N7-C7-C8-C9
2	A	604	P8E	C6-C7-C8-O8
2	A	604	P8E	O6-C6-C7-N7
2	A	605	P8E	C6-C7-C8-O8
2	A	607	P8E	O6-C6-C7-N7

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Mol	Chain	Res	Type	Atoms
2	A	608	P8E	N7-C7-C8-C9
2	A	608	P8E	C6-C7-C8-O8
2	A	608	P8E	N7-C7-C8-O8
2	A	609	P8E	O1A-C1-C2-O6
2	A	610	P8E	C6-C7-C8-C9
2	A	610	P8E	N7-C7-C8-C9
2	A	610	P8E	C6-C7-C8-O8
2	A	610	P8E	N7-C7-C8-O8
2	A	611	P8E	N7-C7-C8-C9
2	A	611	P8E	C6-C7-C8-O8
2	A	611	P8E	O1A-C1-C2-O6
2	A	612	P8E	C5-C6-C7-C8
2	A	612	P8E	O6-C6-C7-C8
2	A	612	P8E	O6-C6-C7-N7
2	A	615	P8E	O6-C6-C7-N7
2	A	616	P8E	C6-C7-C8-C9
2	A	616	P8E	N7-C7-C8-C9
2	A	616	P8E	C6-C7-C8-O8
2	A	616	P8E	N7-C7-C8-O8
2	B	602	P8E	N7-C7-C8-C9
2	B	602	P8E	C6-C7-C8-O8
2	B	602	P8E	N7-C7-C8-O8
2	B	603	P8E	N7-C7-C8-C9
2	B	603	P8E	C6-C7-C8-O8
2	B	604	P8E	N7-C7-C8-C9
2	B	604	P8E	O6-C6-C7-N7
2	B	605	P8E	C6-C7-C8-O8
2	B	605	P8E	O6-C6-C7-N7
2	B	607	P8E	O6-C6-C7-N7
2	B	608	P8E	C6-C7-C8-C9
2	B	608	P8E	N7-C7-C8-C9
2	B	608	P8E	C6-C7-C8-O8
2	B	608	P8E	N7-C7-C8-O8
2	B	610	P8E	C6-C7-C8-C9
2	B	610	P8E	N7-C7-C8-C9
2	B	610	P8E	C6-C7-C8-O8
2	B	610	P8E	N7-C7-C8-O8
2	B	612	P8E	C5-C6-C7-C8
2	B	612	P8E	O6-C6-C7-C8
2	B	612	P8E	O6-C6-C7-N7
2	B	614	P8E	C6-C7-C8-C9
2	B	614	P8E	N7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	B	614	P8E	C6-C7-C8-O8
2	B	614	P8E	N7-C7-C8-O8
2	B	615	P8E	N7-C7-C8-C9
2	B	615	P8E	C6-C7-C8-O8
2	B	615	P8E	N7-C7-C8-O8
2	B	616	P8E	C6-C7-C8-C9
2	B	616	P8E	N7-C7-C8-C9
2	B	616	P8E	C6-C7-C8-O8
2	B	616	P8E	N7-C7-C8-O8
2	C	602	P8E	N7-C7-C8-C9
2	C	602	P8E	C6-C7-C8-O8
2	C	603	P8E	N7-C7-C8-C9
2	C	603	P8E	C6-C7-C8-O8
2	C	604	P8E	N7-C7-C8-C9
2	C	604	P8E	C6-C7-C8-O8
2	C	604	P8E	C5-C6-C7-C8
2	C	604	P8E	O6-C6-C7-N7
2	C	605	P8E	C6-C7-C8-O8
2	C	605	P8E	O6-C6-C7-N7
2	C	606	P8E	N7-C7-C8-C9
2	C	606	P8E	C6-C7-C8-O8
2	C	607	P8E	O6-C6-C7-N7
2	C	608	P8E	N7-C7-C8-C9
2	C	608	P8E	C6-C7-C8-O8
2	C	608	P8E	N7-C7-C8-O8
2	C	609	P8E	O6-C6-C7-N7
2	C	610	P8E	C6-C7-C8-C9
2	C	610	P8E	N7-C7-C8-C9
2	C	610	P8E	C6-C7-C8-O8
2	C	610	P8E	N7-C7-C8-O8
2	C	612	P8E	N7-C7-C8-C9
2	C	612	P8E	C6-C7-C8-O8
2	C	612	P8E	C5-C6-C7-C8
2	C	612	P8E	O6-C6-C7-C8
2	C	612	P8E	O6-C6-C7-N7
2	C	613	P8E	N7-C7-C8-C9
2	C	613	P8E	C6-C7-C8-O8
2	C	613	P8E	N7-C7-C8-O8
2	C	614	P8E	N7-C7-C8-C9
2	C	614	P8E	O1A-C1-C2-C3
2	C	614	P8E	O1A-C1-C2-O6
2	C	615	P8E	O6-C6-C7-N7

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Mol	Chain	Res	Type	Atoms
2	C	616	P8E	C6-C7-C8-C9
2	C	616	P8E	N7-C7-C8-C9
2	C	616	P8E	C6-C7-C8-O8
2	C	616	P8E	N7-C7-C8-O8
2	D	602	P8E	C6-C7-C8-C9
2	D	602	P8E	N7-C7-C8-C9
2	D	602	P8E	C6-C7-C8-O8
2	D	602	P8E	N7-C7-C8-O8
2	D	603	P8E	N7-C7-C8-C9
2	D	603	P8E	C6-C7-C8-O8
2	D	604	P8E	N7-C7-C8-C9
2	D	604	P8E	C6-C7-C8-O8
2	D	604	P8E	O6-C6-C7-N7
2	D	605	P8E	C6-C7-C8-O8
2	D	605	P8E	O6-C6-C7-N7
2	D	607	P8E	O6-C6-C7-N7
2	D	608	P8E	C6-C7-C8-C9
2	D	608	P8E	N7-C7-C8-C9
2	D	608	P8E	C6-C7-C8-O8
2	D	608	P8E	N7-C7-C8-O8
2	D	610	P8E	C6-C7-C8-C9
2	D	610	P8E	N7-C7-C8-C9
2	D	610	P8E	C6-C7-C8-O8
2	D	610	P8E	N7-C7-C8-O8
2	D	611	P8E	O1A-C1-C2-O6
2	D	612	P8E	N7-C7-C8-C9
2	D	612	P8E	C6-C7-C8-O8
2	D	612	P8E	N7-C7-C8-O8
2	D	612	P8E	O6-C6-C7-C8
2	D	612	P8E	O6-C6-C7-N7
2	D	614	P8E	C6-C7-C8-C9
2	D	614	P8E	N7-C7-C8-C9
2	D	614	P8E	C6-C7-C8-O8
2	D	614	P8E	N7-C7-C8-O8
2	D	615	P8E	N7-C7-C8-C9
2	D	615	P8E	C6-C7-C8-O8
2	D	615	P8E	N7-C7-C8-O8
2	D	616	P8E	C6-C7-C8-C9
2	D	616	P8E	N7-C7-C8-C9
2	D	616	P8E	C6-C7-C8-O8
2	D	616	P8E	N7-C7-C8-O8
2	E	602	P8E	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	E	602	P8E	N7-C7-C8-C9
2	E	602	P8E	C6-C7-C8-O8
2	E	602	P8E	N7-C7-C8-O8
2	E	604	P8E	N7-C7-C8-C9
2	E	604	P8E	C6-C7-C8-O8
2	E	604	P8E	O6-C6-C7-N7
2	E	605	P8E	C6-C7-C8-C9
2	E	605	P8E	N7-C7-C8-C9
2	E	605	P8E	C6-C7-C8-O8
2	E	605	P8E	N7-C7-C8-O8
2	E	608	P8E	C6-C7-C8-C9
2	E	608	P8E	N7-C7-C8-C9
2	E	608	P8E	C6-C7-C8-O8
2	E	608	P8E	N7-C7-C8-O8
2	E	610	P8E	C6-C7-C8-C9
2	E	610	P8E	N7-C7-C8-C9
2	E	610	P8E	C6-C7-C8-O8
2	E	610	P8E	N7-C7-C8-O8
2	E	611	P8E	N7-C7-C8-C9
2	E	611	P8E	C6-C7-C8-O8
2	E	611	P8E	O1A-C1-C2-O6
2	E	612	P8E	C5-C6-C7-C8
2	E	612	P8E	O6-C6-C7-C8
2	E	612	P8E	O6-C6-C7-N7
2	E	613	P8E	N7-C7-C8-C9
2	E	613	P8E	O6-C6-C7-N7
2	E	614	P8E	C6-C7-C8-C9
2	E	614	P8E	N7-C7-C8-C9
2	E	614	P8E	C6-C7-C8-O8
2	E	614	P8E	N7-C7-C8-O8
2	E	615	P8E	C6-C7-C8-C9
2	E	615	P8E	N7-C7-C8-C9
2	E	615	P8E	C6-C7-C8-O8
2	E	615	P8E	N7-C7-C8-O8
2	E	616	P8E	N7-C7-C8-C9
2	E	616	P8E	C6-C7-C8-O8
2	E	616	P8E	N7-C7-C8-O8
2	E	616	P8E	O6-C6-C7-N7
2	F	602	P8E	C6-C7-C8-C9
2	F	602	P8E	N7-C7-C8-C9
2	F	602	P8E	C6-C7-C8-O8
2	F	602	P8E	N7-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
2	F	603	P8E	N7-C7-C8-C9
2	F	604	P8E	O6-C6-C7-N7
2	F	605	P8E	C6-C7-C8-C9
2	F	605	P8E	N7-C7-C8-C9
2	F	605	P8E	C6-C7-C8-O8
2	F	605	P8E	N7-C7-C8-O8
2	F	607	P8E	O6-C6-C7-N7
2	F	608	P8E	C6-C7-C8-C9
2	F	608	P8E	N7-C7-C8-C9
2	F	608	P8E	C6-C7-C8-O8
2	F	608	P8E	N7-C7-C8-O8
2	F	609	P8E	N7-C7-C8-C9
2	F	609	P8E	C6-C7-C8-O8
2	F	609	P8E	O1A-C1-C2-O6
2	F	610	P8E	C6-C7-C8-C9
2	F	610	P8E	N7-C7-C8-C9
2	F	610	P8E	C6-C7-C8-O8
2	F	610	P8E	N7-C7-C8-O8
2	F	611	P8E	N7-C7-C8-C9
2	F	611	P8E	C6-C7-C8-O8
2	F	612	P8E	N7-C7-C8-C9
2	F	612	P8E	C5-C6-C7-C8
2	F	612	P8E	O6-C6-C7-C8
2	F	612	P8E	O6-C6-C7-N7
2	F	614	P8E	N7-C7-C8-C9
2	F	614	P8E	C6-C7-C8-O8
2	F	615	P8E	N7-C7-C8-C9
2	F	615	P8E	C6-C7-C8-O8
2	F	615	P8E	N7-C7-C8-O8
2	F	616	P8E	C6-C7-C8-C9
2	F	616	P8E	N7-C7-C8-C9
2	F	616	P8E	C6-C7-C8-O8
2	F	616	P8E	N7-C7-C8-O8
2	G	601	P8E	N7-C7-C8-C9
2	G	601	P8E	C6-C7-C8-O8
2	G	602	P8E	C6-C7-C8-C9
2	G	602	P8E	N7-C7-C8-C9
2	G	602	P8E	C6-C7-C8-O8
2	G	602	P8E	N7-C7-C8-O8
2	G	603	P8E	N7-C7-C8-C9
2	G	604	P8E	N7-C7-C8-C9
2	G	604	P8E	O6-C6-C7-N7

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Mol	Chain	Res	Type	Atoms
2	G	605	P8E	N7-C7-C8-C9
2	G	605	P8E	C6-C7-C8-O8
2	G	606	P8E	N7-C7-C8-C9
2	G	606	P8E	C6-C7-C8-O8
2	G	606	P8E	O6-C6-C7-C8
2	G	606	P8E	O6-C6-C7-N7
2	G	607	P8E	O6-C6-C7-N7
2	G	608	P8E	N7-C7-C8-C9
2	G	608	P8E	C6-C7-C8-O8
2	G	610	P8E	C6-C7-C8-C9
2	G	610	P8E	N7-C7-C8-C9
2	G	610	P8E	C6-C7-C8-O8
2	G	610	P8E	N7-C7-C8-O8
2	G	612	P8E	C5-C6-C7-C8
2	G	612	P8E	O6-C6-C7-C8
2	G	612	P8E	O6-C6-C7-N7
2	G	613	P8E	O6-C6-C7-N7
2	G	615	P8E	O6-C6-C7-N7
2	G	616	P8E	C6-C7-C8-C9
2	G	616	P8E	N7-C7-C8-C9
2	G	616	P8E	C6-C7-C8-O8
2	G	616	P8E	N7-C7-C8-O8
2	H	602	P8E	C6-C7-C8-C9
2	H	602	P8E	N7-C7-C8-C9
2	H	602	P8E	C6-C7-C8-O8
2	H	602	P8E	N7-C7-C8-O8
2	H	603	P8E	N7-C7-C8-C9
2	H	604	P8E	N7-C7-C8-C9
2	H	604	P8E	O6-C6-C7-N7
2	H	605	P8E	C6-C7-C8-O8
2	H	605	P8E	O6-C6-C7-N7
2	H	606	P8E	N7-C7-C8-C9
2	H	606	P8E	C6-C7-C8-O8
2	H	608	P8E	N7-C7-C8-C9
2	H	608	P8E	C6-C7-C8-O8
2	H	608	P8E	N7-C7-C8-O8
2	H	609	P8E	O1A-C1-C2-O6
2	H	610	P8E	C6-C7-C8-C9
2	H	610	P8E	N7-C7-C8-C9
2	H	610	P8E	C6-C7-C8-O8
2	H	610	P8E	N7-C7-C8-O8
2	H	612	P8E	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	H	612	P8E	O6-C6-C7-C8
2	H	612	P8E	O6-C6-C7-N7
2	H	614	P8E	N7-C7-C8-C9
2	H	614	P8E	C6-C7-C8-O8
2	H	614	P8E	N7-C7-C8-O8
2	H	615	P8E	N7-C7-C8-C9
2	H	615	P8E	C6-C7-C8-O8
2	H	615	P8E	N7-C7-C8-O8
2	H	616	P8E	C6-C7-C8-C9
2	H	616	P8E	N7-C7-C8-C9
2	H	616	P8E	C6-C7-C8-O8
2	H	616	P8E	N7-C7-C8-O8
2	I	602	P8E	N7-C7-C8-C9
2	I	602	P8E	C6-C7-C8-O8
2	I	602	P8E	N7-C7-C8-O8
2	I	603	P8E	N7-C7-C8-C9
2	I	603	P8E	C6-C7-C8-O8
2	I	603	P8E	N7-C7-C8-O8
2	I	605	P8E	O6-C6-C7-N7
2	I	606	P8E	N7-C7-C8-C9
2	I	606	P8E	C6-C7-C8-O8
2	I	608	P8E	N7-C7-C8-C9
2	I	608	P8E	C6-C7-C8-O8
2	I	608	P8E	N7-C7-C8-O8
2	I	609	P8E	N7-C7-C8-C9
2	I	609	P8E	O6-C6-C7-N7
2	I	609	P8E	O1A-C1-C2-O6
2	I	610	P8E	C6-C7-C8-C9
2	I	610	P8E	N7-C7-C8-C9
2	I	610	P8E	C6-C7-C8-O8
2	I	610	P8E	N7-C7-C8-O8
2	I	611	P8E	N7-C7-C8-C9
2	I	612	P8E	C5-C6-C7-C8
2	I	612	P8E	O6-C6-C7-C8
2	I	612	P8E	O6-C6-C7-N7
2	I	613	P8E	N7-C7-C8-C9
2	I	613	P8E	C6-C7-C8-O8
2	I	614	P8E	N7-C7-C8-C9
2	I	614	P8E	C6-C7-C8-O8
2	I	614	P8E	N7-C7-C8-O8
2	I	615	P8E	O6-C6-C7-N7
2	I	616	P8E	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	I	616	P8E	N7-C7-C8-C9
2	I	616	P8E	C6-C7-C8-O8
2	I	616	P8E	N7-C7-C8-O8
2	J	601	P8E	O1A-C1-C2-O6
2	J	602	P8E	C6-C7-C8-C9
2	J	602	P8E	N7-C7-C8-C9
2	J	602	P8E	C6-C7-C8-O8
2	J	602	P8E	N7-C7-C8-O8
2	J	603	P8E	N7-C7-C8-C9
2	J	603	P8E	C6-C7-C8-O8
2	J	604	P8E	N7-C7-C8-C9
2	J	604	P8E	C6-C7-C8-O8
2	J	604	P8E	O6-C6-C7-N7
2	J	605	P8E	C6-C7-C8-C9
2	J	605	P8E	N7-C7-C8-C9
2	J	605	P8E	C6-C7-C8-O8
2	J	605	P8E	N7-C7-C8-O8
2	J	606	P8E	N7-C7-C8-C9
2	J	607	P8E	N7-C7-C8-C9
2	J	607	P8E	O6-C6-C7-N7
2	J	608	P8E	N7-C7-C8-C9
2	J	608	P8E	C6-C7-C8-O8
2	J	608	P8E	N7-C7-C8-O8
2	J	609	P8E	N7-C7-C8-C9
2	J	610	P8E	C6-C7-C8-C9
2	J	610	P8E	N7-C7-C8-C9
2	J	610	P8E	C6-C7-C8-O8
2	J	610	P8E	N7-C7-C8-O8
2	J	611	P8E	O1A-C1-C2-O6
2	J	613	P8E	N7-C7-C8-C9
2	J	613	P8E	C6-C7-C8-O8
2	J	613	P8E	N7-C7-C8-O8
2	J	614	P8E	C6-C7-C8-C9
2	J	614	P8E	N7-C7-C8-C9
2	J	614	P8E	C6-C7-C8-O8
2	J	614	P8E	N7-C7-C8-O8
2	J	614	P8E	O6-C6-C7-C8
2	J	614	P8E	O6-C6-C7-N7
2	J	615	P8E	O6-C6-C7-C8
2	J	615	P8E	O6-C6-C7-N7
2	J	616	P8E	C6-C7-C8-C9
2	J	616	P8E	N7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	J	616	P8E	C6-C7-C8-O8
2	J	616	P8E	N7-C7-C8-O8
2	K	601	P8E	O1A-C1-C2-O6
2	K	602	P8E	C6-C7-C8-C9
2	K	602	P8E	N7-C7-C8-C9
2	K	602	P8E	C6-C7-C8-O8
2	K	602	P8E	N7-C7-C8-O8
2	K	603	P8E	N7-C7-C8-C9
2	K	604	P8E	O6-C6-C7-N7
2	K	605	P8E	N7-C7-C8-C9
2	K	605	P8E	C6-C7-C8-O8
2	K	606	P8E	N7-C7-C8-C9
2	K	608	P8E	C6-C7-C8-C9
2	K	608	P8E	N7-C7-C8-C9
2	K	608	P8E	C6-C7-C8-O8
2	K	608	P8E	N7-C7-C8-O8
2	K	609	P8E	O1A-C1-C2-O6
2	K	610	P8E	C6-C7-C8-C9
2	K	610	P8E	N7-C7-C8-C9
2	K	610	P8E	C6-C7-C8-O8
2	K	610	P8E	N7-C7-C8-O8
2	K	611	P8E	O1A-C1-C2-O6
2	K	612	P8E	C5-C6-C7-C8
2	K	612	P8E	O6-C6-C7-C8
2	K	612	P8E	O6-C6-C7-N7
2	K	613	P8E	O6-C6-C7-N7
2	K	614	P8E	C6-C7-C8-C9
2	K	614	P8E	N7-C7-C8-C9
2	K	614	P8E	C6-C7-C8-O8
2	K	614	P8E	N7-C7-C8-O8
2	K	616	P8E	C6-C7-C8-C9
2	K	616	P8E	N7-C7-C8-C9
2	K	616	P8E	C6-C7-C8-O8
2	K	616	P8E	N7-C7-C8-O8
2	L	602	P8E	C6-C7-C8-C9
2	L	602	P8E	N7-C7-C8-C9
2	L	602	P8E	C6-C7-C8-O8
2	L	602	P8E	N7-C7-C8-O8
2	L	603	P8E	N7-C7-C8-C9
2	L	603	P8E	C6-C7-C8-O8
2	L	604	P8E	N7-C7-C8-C9
2	L	604	P8E	O6-C6-C7-N7

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Mol	Chain	Res	Type	Atoms
2	L	605	P8E	N7-C7-C8-C9
2	L	605	P8E	C6-C7-C8-O8
2	L	606	P8E	N7-C7-C8-C9
2	L	606	P8E	C6-C7-C8-O8
2	L	608	P8E	N7-C7-C8-C9
2	L	608	P8E	C6-C7-C8-O8
2	L	610	P8E	C6-C7-C8-C9
2	L	610	P8E	N7-C7-C8-C9
2	L	610	P8E	C6-C7-C8-O8
2	L	610	P8E	N7-C7-C8-O8
2	L	612	P8E	C5-C6-C7-C8
2	L	612	P8E	O6-C6-C7-C8
2	L	612	P8E	O6-C6-C7-N7
2	L	613	P8E	O6-C6-C7-N7
2	L	615	P8E	O6-C6-C7-N7
2	L	616	P8E	C6-C7-C8-C9
2	L	616	P8E	N7-C7-C8-C9
2	L	616	P8E	C6-C7-C8-O8
2	L	616	P8E	N7-C7-C8-O8
2	M	602	P8E	C6-C7-C8-C9
2	M	602	P8E	N7-C7-C8-C9
2	M	602	P8E	C6-C7-C8-O8
2	M	602	P8E	N7-C7-C8-O8
2	M	603	P8E	N7-C7-C8-C9
2	M	604	P8E	N7-C7-C8-C9
2	M	604	P8E	C6-C7-C8-O8
2	M	604	P8E	O6-C6-C7-N7
2	M	605	P8E	C6-C7-C8-C9
2	M	605	P8E	N7-C7-C8-C9
2	M	605	P8E	C6-C7-C8-O8
2	M	605	P8E	N7-C7-C8-O8
2	M	606	P8E	N7-C7-C8-C9
2	M	606	P8E	C6-C7-C8-O8
2	M	606	P8E	O6-C6-C7-C8
2	M	606	P8E	O6-C6-C7-N7
2	M	608	P8E	N7-C7-C8-C9
2	M	608	P8E	C6-C7-C8-O8
2	M	609	P8E	N7-C7-C8-C9
2	M	609	P8E	C6-C7-C8-O8
2	M	609	P8E	N7-C7-C8-O8
2	M	610	P8E	C6-C7-C8-C9
2	M	610	P8E	N7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	M	610	P8E	C6-C7-C8-O8
2	M	610	P8E	N7-C7-C8-O8
2	M	614	P8E	C6-C7-C8-C9
2	M	614	P8E	N7-C7-C8-C9
2	M	614	P8E	C6-C7-C8-O8
2	M	614	P8E	N7-C7-C8-O8
2	M	615	P8E	C5-C6-C7-C8
2	M	615	P8E	O6-C6-C7-N7
2	M	616	P8E	C6-C7-C8-C9
2	M	616	P8E	N7-C7-C8-C9
2	M	616	P8E	C6-C7-C8-O8
2	M	616	P8E	N7-C7-C8-O8
2	N	602	P8E	N7-C7-C8-C9
2	N	602	P8E	C6-C7-C8-O8
2	N	602	P8E	N7-C7-C8-O8
2	N	604	P8E	O6-C6-C7-N7
2	N	605	P8E	O6-C6-C7-N7
2	N	608	P8E	C6-C7-C8-C9
2	N	608	P8E	N7-C7-C8-C9
2	N	608	P8E	C6-C7-C8-O8
2	N	608	P8E	N7-C7-C8-O8
2	N	610	P8E	C6-C7-C8-C9
2	N	610	P8E	N7-C7-C8-C9
2	N	610	P8E	C6-C7-C8-O8
2	N	610	P8E	N7-C7-C8-O8
2	N	612	P8E	C5-C6-C7-C8
2	N	612	P8E	O6-C6-C7-C8
2	N	612	P8E	O6-C6-C7-N7
2	N	614	P8E	C6-C7-C8-C9
2	N	614	P8E	N7-C7-C8-C9
2	N	614	P8E	C6-C7-C8-O8
2	N	614	P8E	N7-C7-C8-O8
2	N	614	P8E	O1A-C1-C2-O6
2	N	616	P8E	C6-C7-C8-C9
2	N	616	P8E	N7-C7-C8-C9
2	N	616	P8E	C6-C7-C8-O8
2	N	616	P8E	N7-C7-C8-O8
2	N	616	P8E	O6-C6-C7-N7
2	O	602	P8E	C6-C7-C8-C9
2	O	602	P8E	N7-C7-C8-C9
2	O	602	P8E	C6-C7-C8-O8
2	O	602	P8E	N7-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
2	O	604	P8E	N7-C7-C8-C9
2	O	604	P8E	C6-C7-C8-O8
2	O	604	P8E	O6-C6-C7-N7
2	O	605	P8E	C6-C7-C8-O8
2	O	605	P8E	O6-C6-C7-N7
2	O	606	P8E	N7-C7-C8-C9
2	O	608	P8E	N7-C7-C8-C9
2	O	608	P8E	C6-C7-C8-O8
2	O	608	P8E	N7-C7-C8-O8
2	O	610	P8E	C6-C7-C8-C9
2	O	610	P8E	N7-C7-C8-C9
2	O	610	P8E	C6-C7-C8-O8
2	O	610	P8E	N7-C7-C8-O8
2	O	612	P8E	C5-C6-C7-C8
2	O	612	P8E	O6-C6-C7-C8
2	O	612	P8E	O6-C6-C7-N7
2	O	615	P8E	N7-C7-C8-C9
2	O	615	P8E	C6-C7-C8-O8
2	O	615	P8E	N7-C7-C8-O8
2	O	616	P8E	C6-C7-C8-C9
2	O	616	P8E	N7-C7-C8-C9
2	O	616	P8E	C6-C7-C8-O8
2	O	616	P8E	N7-C7-C8-O8
2	P	601	P8E	O1A-C1-C2-O6
2	P	602	P8E	C6-C7-C8-C9
2	P	602	P8E	N7-C7-C8-C9
2	P	602	P8E	C6-C7-C8-O8
2	P	602	P8E	N7-C7-C8-O8
2	P	603	P8E	N7-C7-C8-C9
2	P	603	P8E	C6-C7-C8-O8
2	P	603	P8E	N7-C7-C8-O8
2	P	604	P8E	N7-C7-C8-C9
2	P	604	P8E	C6-C7-C8-O8
2	P	605	P8E	N7-C7-C8-C9
2	P	605	P8E	C6-C7-C8-O8
2	P	605	P8E	N7-C7-C8-O8
2	P	606	P8E	N7-C7-C8-C9
2	P	606	P8E	C6-C7-C8-O8
2	P	606	P8E	N7-C7-C8-O8
2	P	606	P8E	C5-C6-C7-C8
2	P	606	P8E	O6-C6-C7-C8
2	P	606	P8E	O6-C6-C7-N7

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Mol	Chain	Res	Type	Atoms
2	P	607	P8E	O6-C6-C7-N7
2	P	608	P8E	C6-C7-C8-C9
2	P	608	P8E	N7-C7-C8-C9
2	P	608	P8E	C6-C7-C8-O8
2	P	608	P8E	N7-C7-C8-O8
2	P	610	P8E	C6-C7-C8-C9
2	P	610	P8E	N7-C7-C8-C9
2	P	610	P8E	C6-C7-C8-O8
2	P	610	P8E	N7-C7-C8-O8
2	P	612	P8E	C5-C6-C7-C8
2	P	612	P8E	O6-C6-C7-C8
2	P	612	P8E	O6-C6-C7-N7
2	P	613	P8E	O6-C6-C7-N7
2	P	614	P8E	N7-C7-C8-C9
2	P	614	P8E	C6-C7-C8-O8
2	P	615	P8E	C5-C6-C7-C8
2	P	615	P8E	O6-C6-C7-N7
2	P	616	P8E	C6-C7-C8-C9
2	P	616	P8E	N7-C7-C8-C9
2	P	616	P8E	C6-C7-C8-O8
2	P	616	P8E	N7-C7-C8-O8
2	Q	602	P8E	C6-C7-C8-C9
2	Q	602	P8E	N7-C7-C8-C9
2	Q	602	P8E	C6-C7-C8-O8
2	Q	602	P8E	N7-C7-C8-O8
2	Q	603	P8E	N7-C7-C8-C9
2	Q	603	P8E	C6-C7-C8-O8
2	Q	604	P8E	N7-C7-C8-C9
2	Q	604	P8E	C6-C7-C8-O8
2	Q	604	P8E	N7-C7-C8-O8
2	Q	604	P8E	O6-C6-C7-N7
2	Q	605	P8E	C6-C7-C8-C9
2	Q	605	P8E	N7-C7-C8-C9
2	Q	605	P8E	C6-C7-C8-O8
2	Q	605	P8E	N7-C7-C8-O8
2	Q	606	P8E	N7-C7-C8-C9
2	Q	606	P8E	C6-C7-C8-O8
2	Q	606	P8E	O6-C6-C7-C8
2	Q	606	P8E	O6-C6-C7-N7
2	Q	608	P8E	C6-C7-C8-C9
2	Q	608	P8E	N7-C7-C8-C9
2	Q	608	P8E	C6-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
2	Q	608	P8E	N7-C7-C8-O8
2	Q	609	P8E	N7-C7-C8-C9
2	Q	609	P8E	C6-C7-C8-O8
2	Q	609	P8E	N7-C7-C8-O8
2	Q	610	P8E	N7-C7-C8-C9
2	Q	610	P8E	C6-C7-C8-O8
2	Q	610	P8E	N7-C7-C8-O8
2	Q	612	P8E	C5-C6-C7-C8
2	Q	612	P8E	O6-C6-C7-C8
2	Q	612	P8E	O6-C6-C7-N7
2	Q	614	P8E	C6-C7-C8-C9
2	Q	614	P8E	N7-C7-C8-C9
2	Q	614	P8E	C6-C7-C8-O8
2	Q	614	P8E	N7-C7-C8-O8
2	Q	614	P8E	O1A-C1-C2-O6
2	Q	615	P8E	C5-C6-C7-C8
2	Q	615	P8E	O6-C6-C7-N7
2	Q	616	P8E	C6-C7-C8-C9
2	Q	616	P8E	N7-C7-C8-C9
2	Q	616	P8E	C6-C7-C8-O8
2	Q	616	P8E	N7-C7-C8-O8
2	R	601	P8E	O1A-C1-C2-O6
2	R	602	P8E	C6-C7-C8-C9
2	R	602	P8E	N7-C7-C8-C9
2	R	602	P8E	C6-C7-C8-O8
2	R	602	P8E	N7-C7-C8-O8
2	R	604	P8E	O6-C6-C7-N7
2	R	605	P8E	N7-C7-C8-C9
2	R	605	P8E	C6-C7-C8-O8
2	R	608	P8E	C6-C7-C8-C9
2	R	608	P8E	N7-C7-C8-C9
2	R	608	P8E	C6-C7-C8-O8
2	R	608	P8E	N7-C7-C8-O8
2	R	610	P8E	C6-C7-C8-C9
2	R	610	P8E	N7-C7-C8-C9
2	R	610	P8E	C6-C7-C8-O8
2	R	610	P8E	N7-C7-C8-O8
2	R	613	P8E	N7-C7-C8-C9
2	R	613	P8E	O6-C6-C7-N7
2	R	615	P8E	N7-C7-C8-C9
2	R	615	P8E	C6-C7-C8-O8
2	R	615	P8E	N7-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
2	R	616	P8E	C6-C7-C8-C9
2	R	616	P8E	N7-C7-C8-C9
2	R	616	P8E	C6-C7-C8-O8
2	R	616	P8E	N7-C7-C8-O8
2	S	602	P8E	C6-C7-C8-C9
2	S	602	P8E	N7-C7-C8-C9
2	S	602	P8E	C6-C7-C8-O8
2	S	602	P8E	N7-C7-C8-O8
2	S	604	P8E	N7-C7-C8-C9
2	S	604	P8E	C6-C7-C8-O8
2	S	604	P8E	O6-C6-C7-N7
2	S	605	P8E	C6-C7-C8-O8
2	S	605	P8E	O6-C6-C7-N7
2	S	607	P8E	O6-C6-C7-N7
2	S	608	P8E	C6-C7-C8-C9
2	S	608	P8E	N7-C7-C8-C9
2	S	608	P8E	C6-C7-C8-O8
2	S	608	P8E	N7-C7-C8-O8
2	S	610	P8E	C6-C7-C8-C9
2	S	610	P8E	N7-C7-C8-C9
2	S	610	P8E	C6-C7-C8-O8
2	S	610	P8E	N7-C7-C8-O8
2	S	612	P8E	C5-C6-C7-C8
2	S	612	P8E	O6-C6-C7-C8
2	S	612	P8E	O6-C6-C7-N7
2	S	614	P8E	C6-C7-C8-C9
2	S	614	P8E	N7-C7-C8-C9
2	S	614	P8E	C6-C7-C8-O8
2	S	614	P8E	N7-C7-C8-O8
2	S	616	P8E	C6-C7-C8-C9
2	S	616	P8E	N7-C7-C8-C9
2	S	616	P8E	C6-C7-C8-O8
2	S	616	P8E	N7-C7-C8-O8
2	S	616	P8E	O1A-C1-C2-O6
2	T	602	P8E	C6-C7-C8-C9
2	T	602	P8E	N7-C7-C8-C9
2	T	602	P8E	C6-C7-C8-O8
2	T	602	P8E	N7-C7-C8-O8
2	T	603	P8E	N7-C7-C8-C9
2	T	603	P8E	C6-C7-C8-O8
2	T	604	P8E	N7-C7-C8-C9
2	T	604	P8E	C6-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
2	T	604	P8E	O6-C6-C7-N7
2	T	605	P8E	C6-C7-C8-O8
2	T	606	P8E	N7-C7-C8-C9
2	T	606	P8E	C6-C7-C8-O8
2	T	606	P8E	O6-C6-C7-C8
2	T	606	P8E	O6-C6-C7-N7
2	T	608	P8E	N7-C7-C8-C9
2	T	608	P8E	C6-C7-C8-O8
2	T	608	P8E	N7-C7-C8-O8
2	T	609	P8E	N7-C7-C8-C9
2	T	609	P8E	O6-C6-C7-N7
2	T	610	P8E	C6-C7-C8-C9
2	T	610	P8E	N7-C7-C8-C9
2	T	610	P8E	C6-C7-C8-O8
2	T	610	P8E	N7-C7-C8-O8
2	T	611	P8E	O1A-C1-C2-O6
2	T	613	P8E	N7-C7-C8-C9
2	T	614	P8E	C6-C7-C8-C9
2	T	614	P8E	N7-C7-C8-C9
2	T	614	P8E	C6-C7-C8-O8
2	T	614	P8E	N7-C7-C8-O8
2	T	615	P8E	O6-C6-C7-N7
2	T	616	P8E	C6-C7-C8-C9
2	T	616	P8E	N7-C7-C8-C9
2	T	616	P8E	C6-C7-C8-O8
2	T	616	P8E	N7-C7-C8-O8
2	U	601	P8E	N7-C7-C8-C9
2	U	602	P8E	C6-C7-C8-C9
2	U	602	P8E	N7-C7-C8-C9
2	U	602	P8E	C6-C7-C8-O8
2	U	602	P8E	N7-C7-C8-O8
2	U	603	P8E	N7-C7-C8-C9
2	U	603	P8E	C6-C7-C8-O8
2	U	604	P8E	O6-C6-C7-N7
2	U	605	P8E	N7-C7-C8-C9
2	U	605	P8E	C6-C7-C8-O8
2	U	607	P8E	O1A-C1-C2-O6
2	U	608	P8E	C6-C7-C8-C9
2	U	608	P8E	N7-C7-C8-C9
2	U	608	P8E	C6-C7-C8-O8
2	U	608	P8E	N7-C7-C8-O8
2	U	609	P8E	N7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	U	610	P8E	C6-C7-C8-C9
2	U	610	P8E	N7-C7-C8-C9
2	U	610	P8E	C6-C7-C8-O8
2	U	610	P8E	N7-C7-C8-O8
2	U	611	P8E	O1A-C1-C2-O6
2	U	612	P8E	C5-C6-C7-C8
2	U	612	P8E	O6-C6-C7-C8
2	U	612	P8E	O6-C6-C7-N7
2	U	614	P8E	C6-C7-C8-C9
2	U	614	P8E	N7-C7-C8-C9
2	U	614	P8E	C6-C7-C8-O8
2	U	614	P8E	N7-C7-C8-O8
2	U	615	P8E	O6-C6-C7-N7
2	U	616	P8E	C6-C7-C8-C9
2	U	616	P8E	N7-C7-C8-C9
2	U	616	P8E	C6-C7-C8-O8
2	U	616	P8E	N7-C7-C8-O8
2	V	602	P8E	C6-C7-C8-C9
2	V	602	P8E	N7-C7-C8-C9
2	V	602	P8E	C6-C7-C8-O8
2	V	602	P8E	N7-C7-C8-O8
2	V	604	P8E	N7-C7-C8-C9
2	V	604	P8E	C6-C7-C8-O8
2	V	604	P8E	O6-C6-C7-N7
2	V	605	P8E	O6-C6-C7-N7
2	V	606	P8E	N7-C7-C8-C9
2	V	608	P8E	C6-C7-C8-C9
2	V	608	P8E	N7-C7-C8-C9
2	V	608	P8E	C6-C7-C8-O8
2	V	608	P8E	N7-C7-C8-O8
2	V	610	P8E	C6-C7-C8-C9
2	V	610	P8E	N7-C7-C8-C9
2	V	610	P8E	C6-C7-C8-O8
2	V	610	P8E	N7-C7-C8-O8
2	V	612	P8E	C5-C6-C7-C8
2	V	612	P8E	O6-C6-C7-C8
2	V	612	P8E	O6-C6-C7-N7
2	V	614	P8E	C6-C7-C8-C9
2	V	614	P8E	N7-C7-C8-C9
2	V	614	P8E	C6-C7-C8-O8
2	V	614	P8E	N7-C7-C8-O8
2	V	616	P8E	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	V	616	P8E	N7-C7-C8-C9
2	V	616	P8E	C6-C7-C8-O8
2	V	616	P8E	N7-C7-C8-O8
2	A	601	P8E	O6-C6-C7-C8
2	A	606	P8E	O6-C6-C7-C8
2	A	615	P8E	O6-C6-C7-C8
2	B	601	P8E	O6-C6-C7-C8
2	B	606	P8E	O6-C6-C7-C8
2	C	601	P8E	O6-C6-C7-C8
2	C	604	P8E	O6-C6-C7-C8
2	C	606	P8E	O6-C6-C7-C8
2	C	615	P8E	O6-C6-C7-C8
2	D	601	P8E	O6-C6-C7-C8
2	D	606	P8E	O6-C6-C7-C8
2	E	601	P8E	O6-C6-C7-C8
2	E	606	P8E	O6-C6-C7-C8
2	F	601	P8E	O6-C6-C7-C8
2	F	606	P8E	O6-C6-C7-C8
2	G	601	P8E	O6-C6-C7-C8
2	G	615	P8E	O6-C6-C7-C8
2	H	601	P8E	O6-C6-C7-C8
2	H	606	P8E	O6-C6-C7-C8
2	I	601	P8E	O6-C6-C7-C8
2	I	606	P8E	O6-C6-C7-C8
2	J	601	P8E	O6-C6-C7-C8
2	J	606	P8E	O6-C6-C7-C8
2	J	612	P8E	O6-C6-C7-C8
2	K	601	P8E	O6-C6-C7-C8
2	K	606	P8E	O6-C6-C7-C8
2	K	615	P8E	O6-C6-C7-C8
2	L	601	P8E	O6-C6-C7-C8
2	L	606	P8E	O6-C6-C7-C8
2	M	601	P8E	O6-C6-C7-C8
2	M	612	P8E	O6-C6-C7-C8
2	M	615	P8E	O6-C6-C7-C8
2	N	601	P8E	O6-C6-C7-C8
2	N	606	P8E	O6-C6-C7-C8
2	O	601	P8E	O6-C6-C7-C8
2	O	606	P8E	O6-C6-C7-C8
2	P	601	P8E	O6-C6-C7-C8
2	P	615	P8E	O6-C6-C7-C8
2	Q	601	P8E	O6-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	Q	615	P8E	O6-C6-C7-C8
2	R	601	P8E	O6-C6-C7-C8
2	R	606	P8E	O6-C6-C7-C8
2	R	612	P8E	O6-C6-C7-C8
2	S	601	P8E	O6-C6-C7-C8
2	S	606	P8E	O6-C6-C7-C8
2	T	601	P8E	O6-C6-C7-C8
2	T	612	P8E	O6-C6-C7-C8
2	T	615	P8E	O6-C6-C7-C8
2	U	601	P8E	O6-C6-C7-C8
2	U	606	P8E	O6-C6-C7-C8
2	U	615	P8E	O6-C6-C7-C8
2	V	601	P8E	O6-C6-C7-C8
2	V	606	P8E	O6-C6-C7-C8
2	A	616	P8E	O1A-C1-C2-O6
2	B	601	P8E	O1A-C1-C2-O6
2	B	609	P8E	O1A-C1-C2-O6
2	B	611	P8E	O1A-C1-C2-O6
2	C	609	P8E	O1A-C1-C2-O6
2	D	609	P8E	O1A-C1-C2-O6
2	E	616	P8E	O1A-C1-C2-O6
2	F	616	P8E	O1A-C1-C2-O6
2	G	609	P8E	O1A-C1-C2-O6
2	H	607	P8E	O1A-C1-C2-O6
2	I	614	P8E	O1A-C1-C2-O6
2	L	609	P8E	O1A-C1-C2-O6
2	M	611	P8E	O1A-C1-C2-O6
2	O	609	P8E	O1A-C1-C2-O6
2	O	616	P8E	O1A-C1-C2-O6
2	P	609	P8E	O1A-C1-C2-O6
2	S	609	P8E	O1A-C1-C2-O6
2	T	609	P8E	O1A-C1-C2-O6
2	U	609	P8E	O1A-C1-C2-O6
2	V	617	P8E	O1A-C1-C2-O6
2	E	616	P8E	O6-C6-C7-C8
2	I	615	P8E	O6-C6-C7-C8
2	A	604	P8E	O6-C6-C7-C8
2	A	607	P8E	O6-C6-C7-C8
2	B	604	P8E	O6-C6-C7-C8
2	B	605	P8E	O6-C6-C7-C8
2	B	607	P8E	O6-C6-C7-C8
2	C	605	P8E	O6-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	C	607	P8E	O6-C6-C7-C8
2	C	609	P8E	O6-C6-C7-C8
2	D	604	P8E	O6-C6-C7-C8
2	D	605	P8E	O6-C6-C7-C8
2	E	604	P8E	O6-C6-C7-C8
2	E	613	P8E	O6-C6-C7-C8
2	F	604	P8E	O6-C6-C7-C8
2	F	607	P8E	O6-C6-C7-C8
2	G	604	P8E	O6-C6-C7-C8
2	G	607	P8E	O6-C6-C7-C8
2	G	613	P8E	O6-C6-C7-C8
2	H	604	P8E	O6-C6-C7-C8
2	H	605	P8E	O6-C6-C7-C8
2	I	605	P8E	O6-C6-C7-C8
2	I	609	P8E	O6-C6-C7-C8
2	J	604	P8E	O6-C6-C7-C8
2	J	607	P8E	O6-C6-C7-C8
2	K	604	P8E	O6-C6-C7-C8
2	K	613	P8E	O6-C6-C7-C8
2	L	604	P8E	O6-C6-C7-C8
2	L	613	P8E	O6-C6-C7-C8
2	L	615	P8E	O6-C6-C7-C8
2	M	604	P8E	O6-C6-C7-C8
2	N	604	P8E	O6-C6-C7-C8
2	N	605	P8E	O6-C6-C7-C8
2	O	604	P8E	O6-C6-C7-C8
2	O	605	P8E	O6-C6-C7-C8
2	P	607	P8E	O6-C6-C7-C8
2	P	613	P8E	O6-C6-C7-C8
2	Q	604	P8E	O6-C6-C7-C8
2	R	604	P8E	O6-C6-C7-C8
2	R	613	P8E	O6-C6-C7-C8
2	S	604	P8E	O6-C6-C7-C8
2	S	605	P8E	O6-C6-C7-C8
2	S	607	P8E	O6-C6-C7-C8
2	T	604	P8E	O6-C6-C7-C8
2	T	609	P8E	O6-C6-C7-C8
2	U	604	P8E	O6-C6-C7-C8
2	V	604	P8E	O6-C6-C7-C8
2	V	605	P8E	O6-C6-C7-C8
2	A	601	P8E	C5-C6-C7-C8
2	A	604	P8E	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	A	606	P8E	C5-C6-C7-C8
2	A	607	P8E	C5-C6-C7-C8
2	A	615	P8E	C5-C6-C7-C8
2	A	616	P8E	C5-C6-C7-C8
2	B	601	P8E	C5-C6-C7-C8
2	B	604	P8E	C5-C6-C7-C8
2	B	605	P8E	C5-C6-C7-C8
2	B	606	P8E	C5-C6-C7-C8
2	B	607	P8E	C5-C6-C7-C8
2	B	616	P8E	C5-C6-C7-C8
2	C	601	P8E	C5-C6-C7-C8
2	C	606	P8E	C5-C6-C7-C8
2	C	615	P8E	C5-C6-C7-C8
2	D	601	P8E	C5-C6-C7-C8
2	D	604	P8E	C5-C6-C7-C8
2	D	606	P8E	C5-C6-C7-C8
2	D	612	P8E	C5-C6-C7-C8
2	E	601	P8E	C5-C6-C7-C8
2	E	604	P8E	C5-C6-C7-C8
2	E	606	P8E	C5-C6-C7-C8
2	E	613	P8E	C5-C6-C7-C8
2	E	616	P8E	C5-C6-C7-C8
2	F	601	P8E	C5-C6-C7-C8
2	F	604	P8E	C5-C6-C7-C8
2	F	606	P8E	C5-C6-C7-C8
2	F	616	P8E	C5-C6-C7-C8
2	G	601	P8E	C5-C6-C7-C8
2	G	604	P8E	C5-C6-C7-C8
2	G	606	P8E	C5-C6-C7-C8
2	G	607	P8E	C5-C6-C7-C8
2	G	615	P8E	C5-C6-C7-C8
2	H	601	P8E	C5-C6-C7-C8
2	H	604	P8E	C5-C6-C7-C8
2	H	606	P8E	C5-C6-C7-C8
2	I	601	P8E	C5-C6-C7-C8
2	I	605	P8E	C5-C6-C7-C8
2	I	606	P8E	C5-C6-C7-C8
2	I	609	P8E	C5-C6-C7-C8
2	I	616	P8E	C5-C6-C7-C8
2	J	601	P8E	C5-C6-C7-C8
2	J	604	P8E	C5-C6-C7-C8
2	J	606	P8E	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	J	612	P8E	C5-C6-C7-C8
2	J	614	P8E	C5-C6-C7-C8
2	J	615	P8E	C5-C6-C7-C8
2	J	616	P8E	C5-C6-C7-C8
2	K	601	P8E	C5-C6-C7-C8
2	K	604	P8E	C5-C6-C7-C8
2	K	606	P8E	C5-C6-C7-C8
2	K	613	P8E	C5-C6-C7-C8
2	K	615	P8E	C5-C6-C7-C8
2	K	616	P8E	C5-C6-C7-C8
2	L	601	P8E	C5-C6-C7-C8
2	L	604	P8E	C5-C6-C7-C8
2	L	606	P8E	C5-C6-C7-C8
2	L	613	P8E	C5-C6-C7-C8
2	M	601	P8E	C5-C6-C7-C8
2	M	604	P8E	C5-C6-C7-C8
2	M	606	P8E	C5-C6-C7-C8
2	M	612	P8E	C5-C6-C7-C8
2	N	601	P8E	C5-C6-C7-C8
2	N	604	P8E	C5-C6-C7-C8
2	N	605	P8E	C5-C6-C7-C8
2	N	606	P8E	C5-C6-C7-C8
2	N	616	P8E	C5-C6-C7-C8
2	O	601	P8E	C5-C6-C7-C8
2	O	604	P8E	C5-C6-C7-C8
2	O	605	P8E	C5-C6-C7-C8
2	O	606	P8E	C5-C6-C7-C8
2	O	616	P8E	C5-C6-C7-C8
2	P	601	P8E	C5-C6-C7-C8
2	P	607	P8E	C5-C6-C7-C8
2	P	613	P8E	C5-C6-C7-C8
2	Q	601	P8E	C5-C6-C7-C8
2	Q	604	P8E	C5-C6-C7-C8
2	Q	606	P8E	C5-C6-C7-C8
2	Q	616	P8E	C5-C6-C7-C8
2	R	601	P8E	C5-C6-C7-C8
2	R	604	P8E	C5-C6-C7-C8
2	R	606	P8E	C5-C6-C7-C8
2	R	612	P8E	C5-C6-C7-C8
2	R	613	P8E	C5-C6-C7-C8
2	S	601	P8E	C5-C6-C7-C8
2	S	604	P8E	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	S	606	P8E	C5-C6-C7-C8
2	T	601	P8E	C5-C6-C7-C8
2	T	604	P8E	C5-C6-C7-C8
2	T	606	P8E	C5-C6-C7-C8
2	T	609	P8E	C5-C6-C7-C8
2	T	612	P8E	C5-C6-C7-C8
2	T	615	P8E	C5-C6-C7-C8
2	U	601	P8E	C5-C6-C7-C8
2	U	604	P8E	C5-C6-C7-C8
2	U	606	P8E	C5-C6-C7-C8
2	U	615	P8E	C5-C6-C7-C8
2	V	601	P8E	C5-C6-C7-C8
2	V	604	P8E	C5-C6-C7-C8
2	V	605	P8E	C5-C6-C7-C8
2	V	606	P8E	C5-C6-C7-C8
2	V	616	P8E	C5-C6-C7-C8
2	B	604	P8E	C6-C7-C8-O8
2	F	603	P8E	C6-C7-C8-O8
2	F	612	P8E	C6-C7-C8-O8
2	G	603	P8E	C6-C7-C8-O8
2	G	604	P8E	C6-C7-C8-O8
2	H	603	P8E	C6-C7-C8-O8
2	H	604	P8E	C6-C7-C8-O8
2	J	607	P8E	C6-C7-C8-O8
2	J	609	P8E	C6-C7-C8-O8
2	K	603	P8E	C6-C7-C8-O8
2	K	606	P8E	C6-C7-C8-O8
2	L	604	P8E	C6-C7-C8-O8
2	M	603	P8E	C6-C7-C8-O8
2	N	605	P8E	C6-C7-C8-O8
2	O	606	P8E	C6-C7-C8-O8
2	U	609	P8E	C6-C7-C8-O8
2	V	605	P8E	C6-C7-C8-O8
2	V	606	P8E	C6-C7-C8-O8
2	A	611	P8E	O1A-C1-C2-C3
2	A	611	P8E	O1B-C1-C2-C3
2	C	614	P8E	O1B-C1-C2-C3
2	D	611	P8E	O1B-C1-C2-C3
2	E	611	P8E	O1A-C1-C2-C3
2	E	611	P8E	O1B-C1-C2-C3
2	F	617	P8E	O1A-C1-C2-C3
2	F	617	P8E	O1B-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	G	617	P8E	O1A-C1-C2-C3
2	G	617	P8E	O1B-C1-C2-C3
2	H	617	P8E	N7-C7-C8-C9
2	I	617	P8E	O1B-C1-C2-C3
2	J	611	P8E	O1B-C1-C2-C3
2	K	611	P8E	O1B-C1-C2-C3
2	M	611	P8E	O1B-C1-C2-C3
2	M	613	P8E	N7-C7-C8-C9
2	M	617	P8E	N7-C7-C8-C9
2	M	617	P8E	O1A-C1-C2-C3
2	M	617	P8E	O1B-C1-C2-C3
2	N	614	P8E	O1A-C1-C2-C3
2	N	614	P8E	O1B-C1-C2-C3
2	N	617	P8E	O1B-C1-C2-C3
2	O	614	P8E	N7-C7-C8-C9
2	O	617	P8E	N7-C7-C8-C9
2	P	617	P8E	O1B-C1-C2-C3
2	Q	612	P8E	N7-C7-C8-C9
2	Q	614	P8E	O1A-C1-C2-C3
2	Q	614	P8E	O1B-C1-C2-C3
2	Q	617	P8E	O1A-C1-C2-C3
2	Q	617	P8E	O1B-C1-C2-C3
2	R	617	P8E	O1A-C1-C2-C3
2	R	617	P8E	O1B-C1-C2-C3
2	T	611	P8E	O1A-C1-C2-C3
2	T	611	P8E	O1B-C1-C2-C3
2	T	617	P8E	O1A-C1-C2-C3
2	T	617	P8E	O1B-C1-C2-C3
2	U	611	P8E	O1A-C1-C2-C3
2	U	611	P8E	O1B-C1-C2-C3
2	U	617	P8E	O1A-C1-C2-C3
2	U	617	P8E	O1B-C1-C2-C3
2	V	617	P8E	O1A-C1-C2-C3
2	V	617	P8E	O1B-C1-C2-C3
2	A	608	P8E	C6-C7-C8-C9
2	B	602	P8E	C6-C7-C8-C9
2	B	605	P8E	C6-C7-C8-C9
2	C	602	P8E	C6-C7-C8-C9
2	C	605	P8E	C6-C7-C8-C9
2	E	616	P8E	C6-C7-C8-C9
2	G	605	P8E	C6-C7-C8-C9
2	H	608	P8E	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	K	605	P8E	C6-C7-C8-C9
2	L	605	P8E	C6-C7-C8-C9
2	P	605	P8E	C6-C7-C8-C9
2	R	605	P8E	C6-C7-C8-C9
2	S	605	P8E	C6-C7-C8-C9
2	T	605	P8E	C6-C7-C8-C9
2	U	605	P8E	C6-C7-C8-C9
2	A	604	P8E	N7-C7-C8-O8
2	A	611	P8E	N7-C7-C8-O8
2	B	603	P8E	N7-C7-C8-O8
2	C	602	P8E	N7-C7-C8-O8
2	C	603	P8E	N7-C7-C8-O8
2	C	604	P8E	N7-C7-C8-O8
2	C	612	P8E	N7-C7-C8-O8
2	D	604	P8E	N7-C7-C8-O8
2	E	604	P8E	N7-C7-C8-O8
2	E	611	P8E	N7-C7-C8-O8
2	E	613	P8E	N7-C7-C8-O8
2	F	609	P8E	N7-C7-C8-O8
2	F	614	P8E	N7-C7-C8-O8
2	G	601	P8E	N7-C7-C8-O8
2	G	606	P8E	N7-C7-C8-O8
2	G	608	P8E	N7-C7-C8-O8
2	I	606	P8E	N7-C7-C8-O8
2	J	604	P8E	N7-C7-C8-O8
2	L	608	P8E	N7-C7-C8-O8
2	M	604	P8E	N7-C7-C8-O8
2	M	606	P8E	N7-C7-C8-O8
2	M	608	P8E	N7-C7-C8-O8
2	O	604	P8E	N7-C7-C8-O8
2	P	614	P8E	N7-C7-C8-O8
2	Q	603	P8E	N7-C7-C8-O8
2	Q	606	P8E	N7-C7-C8-O8
2	S	604	P8E	N7-C7-C8-O8
2	T	604	P8E	N7-C7-C8-O8
2	T	606	P8E	N7-C7-C8-O8
2	T	609	P8E	N7-C7-C8-O8
2	V	604	P8E	N7-C7-C8-O8
2	D	607	P8E	O6-C6-C7-C8
2	D	609	P8E	O6-C6-C7-C8
2	E	607	P8E	O6-C6-C7-C8
2	G	605	P8E	O6-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	G	609	P8E	O6-C6-C7-C8
2	I	607	P8E	O6-C6-C7-C8
2	I	611	P8E	O6-C6-C7-C8
2	K	605	P8E	O6-C6-C7-C8
2	M	607	P8E	O6-C6-C7-C8
2	N	614	P8E	O6-C6-C7-C8
2	N	615	P8E	O6-C6-C7-C8
2	T	605	P8E	O6-C6-C7-C8
2	A	607	P8E	O1A-C1-C2-O6
2	A	617	P8E	O1A-C1-C2-O6
2	B	605	P8E	O1A-C1-C2-O6
2	B	607	P8E	O1A-C1-C2-O6
2	B	614	P8E	O1A-C1-C2-O6
2	B	616	P8E	O1A-C1-C2-O6
2	B	617	P8E	O1A-C1-C2-O6
2	C	601	P8E	O1A-C1-C2-O6
2	C	611	P8E	O1A-C1-C2-O6
2	C	617	P8E	O1A-C1-C2-O6
2	D	607	P8E	O1A-C1-C2-O6
2	D	610	P8E	O1A-C1-C2-O6
2	E	609	P8E	O1A-C1-C2-O6
2	E	617	P8E	O1A-C1-C2-O6
2	F	607	P8E	O1A-C1-C2-O6
2	F	611	P8E	O1A-C1-C2-O6
2	F	614	P8E	O1A-C1-C2-O6
2	F	617	P8E	O1A-C1-C2-O6
2	G	607	P8E	O1A-C1-C2-O6
2	G	617	P8E	O1A-C1-C2-O6
2	H	611	P8E	O1A-C1-C2-O6
2	H	614	P8E	O1A-C1-C2-O6
2	H	617	P8E	O1A-C1-C2-O6
2	I	611	P8E	O1A-C1-C2-O6
2	I	617	P8E	O1A-C1-C2-O6
2	J	617	P8E	O1A-C1-C2-O6
2	L	617	P8E	O1A-C1-C2-O6
2	M	607	P8E	O1A-C1-C2-O6
2	M	609	P8E	O1A-C1-C2-O6
2	M	614	P8E	O1A-C1-C2-O6
2	M	617	P8E	O1A-C1-C2-O6
2	N	607	P8E	O1A-C1-C2-O6
2	N	617	P8E	O1A-C1-C2-O6
2	O	601	P8E	O1A-C1-C2-O6

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Mol	Chain	Res	Type	Atoms
2	O	611	P8E	O1A-C1-C2-O6
2	P	605	P8E	O1A-C1-C2-O6
2	P	611	P8E	O1A-C1-C2-O6
2	P	617	P8E	O1A-C1-C2-O6
2	Q	607	P8E	O1A-C1-C2-O6
2	Q	609	P8E	O1A-C1-C2-O6
2	Q	611	P8E	O1A-C1-C2-O6
2	Q	616	P8E	O1A-C1-C2-O6
2	Q	617	P8E	O1A-C1-C2-O6
2	R	609	P8E	O1A-C1-C2-O6
2	R	611	P8E	O1A-C1-C2-O6
2	R	614	P8E	O1A-C1-C2-O6
2	R	617	P8E	O1A-C1-C2-O6
2	S	611	P8E	O1A-C1-C2-O6
2	T	607	P8E	O1A-C1-C2-O6
2	T	614	P8E	O1A-C1-C2-O6
2	T	617	P8E	O1A-C1-C2-O6
2	U	610	P8E	O1A-C1-C2-O6
2	U	614	P8E	O1A-C1-C2-O6
2	U	617	P8E	O1A-C1-C2-O6
2	V	601	P8E	O1A-C1-C2-O6
2	V	607	P8E	O1A-C1-C2-O6
2	V	609	P8E	O1A-C1-C2-O6
2	V	611	P8E	O1A-C1-C2-O6
2	V	614	P8E	O1A-C1-C2-O6
2	B	609	P8E	O6-C6-C7-C8
2	E	609	P8E	O6-C6-C7-C8
2	H	609	P8E	O6-C6-C7-C8
2	I	604	P8E	O6-C6-C7-C8
2	N	607	P8E	O6-C6-C7-C8
2	O	607	P8E	O6-C6-C7-C8
2	P	604	P8E	O6-C6-C7-C8
2	Q	607	P8E	O6-C6-C7-C8
2	T	610	P8E	O6-C6-C7-C8
2	T	613	P8E	O6-C6-C7-C8
2	U	607	P8E	O6-C6-C7-C8
2	U	609	P8E	O6-C6-C7-C8
2	U	613	P8E	O6-C6-C7-C8
2	V	607	P8E	O6-C6-C7-C8
2	A	605	P8E	O6-C6-C7-C8
2	I	613	P8E	O6-C6-C7-C8
2	O	609	P8E	O6-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	O	613	P8E	O6-C6-C7-C8
2	P	605	P8E	O6-C6-C7-C8
2	R	605	P8E	O6-C6-C7-C8
2	T	607	P8E	O6-C6-C7-C8
2	U	605	P8E	O6-C6-C7-C8
2	V	613	P8E	O6-C6-C7-C8
2	A	601	P8E	O1A-C1-C2-O6
2	A	612	P8E	O1A-C1-C2-O6
2	C	607	P8E	O1A-C1-C2-O6
2	C	612	P8E	O1A-C1-C2-O6
2	D	601	P8E	O1A-C1-C2-O6
2	D	612	P8E	O1A-C1-C2-O6
2	E	606	P8E	O1A-C1-C2-O6
2	E	607	P8E	O1A-C1-C2-O6
2	F	612	P8E	O1A-C1-C2-O6
2	G	612	P8E	O1A-C1-C2-O6
2	H	612	P8E	O1A-C1-C2-O6
2	I	607	P8E	O1A-C1-C2-O6
2	I	612	P8E	O1A-C1-C2-O6
2	J	607	P8E	O1A-C1-C2-O6
2	L	612	P8E	O1A-C1-C2-O6
2	N	612	P8E	O1A-C1-C2-O6
2	O	607	P8E	O1A-C1-C2-O6
2	O	612	P8E	O1A-C1-C2-O6
2	P	612	P8E	O1A-C1-C2-O6
2	Q	612	P8E	O1A-C1-C2-O6
2	S	601	P8E	O1A-C1-C2-O6
2	S	607	P8E	O1A-C1-C2-O6
2	V	612	P8E	O1A-C1-C2-O6
2	A	613	P8E	O6-C6-C7-C8
2	B	613	P8E	O6-C6-C7-C8
2	C	602	P8E	O6-C6-C7-C8
2	D	613	P8E	O6-C6-C7-C8
2	L	605	P8E	O6-C6-C7-C8
2	R	609	P8E	O6-C6-C7-C8
2	T	611	P8E	O6-C6-C7-C8
2	V	609	P8E	O6-C6-C7-C8
2	A	605	P8E	C5-C6-C7-C8
2	C	605	P8E	C5-C6-C7-C8
2	C	607	P8E	C5-C6-C7-C8
2	C	609	P8E	C5-C6-C7-C8
2	C	616	P8E	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	D	605	P8E	C5-C6-C7-C8
2	D	607	P8E	C5-C6-C7-C8
2	D	609	P8E	C5-C6-C7-C8
2	D	616	P8E	C5-C6-C7-C8
2	E	607	P8E	C5-C6-C7-C8
2	F	607	P8E	C5-C6-C7-C8
2	G	605	P8E	C5-C6-C7-C8
2	G	609	P8E	C5-C6-C7-C8
2	G	613	P8E	C5-C6-C7-C8
2	H	605	P8E	C5-C6-C7-C8
2	H	609	P8E	C5-C6-C7-C8
2	H	616	P8E	C5-C6-C7-C8
2	I	604	P8E	C5-C6-C7-C8
2	I	613	P8E	C5-C6-C7-C8
2	I	615	P8E	C5-C6-C7-C8
2	J	607	P8E	C5-C6-C7-C8
2	L	615	P8E	C5-C6-C7-C8
2	M	607	P8E	C5-C6-C7-C8
2	M	616	P8E	C5-C6-C7-C8
2	N	607	P8E	C5-C6-C7-C8
2	O	607	P8E	C5-C6-C7-C8
2	P	604	P8E	C5-C6-C7-C8
2	P	616	P8E	C5-C6-C7-C8
2	Q	607	P8E	C5-C6-C7-C8
2	R	616	P8E	C5-C6-C7-C8
2	S	605	P8E	C5-C6-C7-C8
2	S	607	P8E	C5-C6-C7-C8
2	S	616	P8E	C5-C6-C7-C8
2	T	605	P8E	C5-C6-C7-C8
2	T	613	P8E	C5-C6-C7-C8
2	T	616	P8E	C5-C6-C7-C8
2	U	607	P8E	C5-C6-C7-C8
2	U	613	P8E	C5-C6-C7-C8
2	U	616	P8E	C5-C6-C7-C8
2	C	614	P8E	C6-C7-C8-O8
2	D	606	P8E	C6-C7-C8-O8
2	E	613	P8E	C6-C7-C8-O8
2	F	604	P8E	C6-C7-C8-O8
2	I	605	P8E	C6-C7-C8-O8
2	J	606	P8E	C6-C7-C8-O8
2	M	613	P8E	C6-C7-C8-O8
2	N	604	P8E	C6-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
2	N	606	P8E	C6-C7-C8-O8
2	O	614	P8E	C6-C7-C8-O8
2	P	607	P8E	C6-C7-C8-O8
2	Q	612	P8E	C6-C7-C8-O8
2	R	604	P8E	C6-C7-C8-O8
2	R	606	P8E	C6-C7-C8-O8
2	T	609	P8E	C6-C7-C8-O8
2	T	613	P8E	C6-C7-C8-O8
2	U	601	P8E	C6-C7-C8-O8
2	U	604	P8E	C6-C7-C8-O8
2	A	607	P8E	O1A-C1-C2-C3
2	A	612	P8E	O1A-C1-C2-C3
2	B	607	P8E	O1A-C1-C2-C3
2	B	611	P8E	O1A-C1-C2-C3
2	B	612	P8E	N7-C7-C8-C9
2	C	609	P8E	O1A-C1-C2-C3
2	C	612	P8E	O1A-C1-C2-C3
2	C	617	P8E	O1A-C1-C2-C3
2	D	611	P8E	O1A-C1-C2-C3
2	D	615	P8E	O1A-C1-C2-C3
2	D	615	P8E	O1B-C1-C2-C3
2	F	604	P8E	N7-C7-C8-C9
2	F	612	P8E	O1A-C1-C2-C3
2	F	612	P8E	O1B-C1-C2-C3
2	G	607	P8E	O1A-C1-C2-C3
2	G	612	P8E	O1A-C1-C2-C3
2	G	612	P8E	O1B-C1-C2-C3
2	H	612	P8E	O1A-C1-C2-C3
2	H	617	P8E	O1A-C1-C2-C3
2	H	617	P8E	O1B-C1-C2-C3
2	I	601	P8E	N7-C7-C8-C9
2	I	612	P8E	O1A-C1-C2-C3
2	I	614	P8E	O1A-C1-C2-C3
2	I	617	P8E	O1A-C1-C2-C3
2	J	611	P8E	O1A-C1-C2-C3
2	J	617	P8E	O1A-C1-C2-C3
2	J	617	P8E	O1B-C1-C2-C3
2	K	611	P8E	O1A-C1-C2-C3
2	L	612	P8E	O1A-C1-C2-C3
2	M	607	P8E	O1A-C1-C2-C3
2	M	611	P8E	O1A-C1-C2-C3
2	N	606	P8E	N7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	N	609	P8E	O1A-C1-C2-C3
2	N	609	P8E	O1B-C1-C2-C3
2	N	612	P8E	O1A-C1-C2-C3
2	N	617	P8E	O1A-C1-C2-C3
2	P	607	P8E	N7-C7-C8-C9
2	P	617	P8E	O1A-C1-C2-C3
2	Q	607	P8E	O1A-C1-C2-C3
2	Q	609	P8E	O1A-C1-C2-C3
2	R	606	P8E	N7-C7-C8-C9
2	T	605	P8E	N7-C7-C8-C9
2	T	607	P8E	O1A-C1-C2-C3
2	U	612	P8E	N7-C7-C8-C9
2	U	617	P8E	N7-C7-C8-C9
2	V	607	P8E	O1A-C1-C2-C3
2	V	612	P8E	O1A-C1-C2-C3
2	A	604	P8E	C6-C7-C8-C9
2	A	611	P8E	C6-C7-C8-C9
2	B	603	P8E	C6-C7-C8-C9
2	C	604	P8E	C6-C7-C8-C9
2	C	608	P8E	C6-C7-C8-C9
2	C	612	P8E	C6-C7-C8-C9
2	C	613	P8E	C6-C7-C8-C9
2	D	615	P8E	C6-C7-C8-C9
2	E	611	P8E	C6-C7-C8-C9
2	E	613	P8E	C6-C7-C8-C9
2	F	609	P8E	C6-C7-C8-C9
2	F	614	P8E	C6-C7-C8-C9
2	F	615	P8E	C6-C7-C8-C9
2	G	601	P8E	C6-C7-C8-C9
2	G	606	P8E	C6-C7-C8-C9
2	G	608	P8E	C6-C7-C8-C9
2	H	614	P8E	C6-C7-C8-C9
2	H	615	P8E	C6-C7-C8-C9
2	I	602	P8E	C6-C7-C8-C9
2	I	603	P8E	C6-C7-C8-C9
2	I	608	P8E	C6-C7-C8-C9
2	I	614	P8E	C6-C7-C8-C9
2	J	608	P8E	C6-C7-C8-C9
2	J	613	P8E	C6-C7-C8-C9
2	M	604	P8E	C6-C7-C8-C9
2	M	608	P8E	C6-C7-C8-C9
2	M	609	P8E	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	N	602	P8E	C6-C7-C8-C9
2	O	604	P8E	C6-C7-C8-C9
2	O	608	P8E	C6-C7-C8-C9
2	P	603	P8E	C6-C7-C8-C9
2	P	606	P8E	C6-C7-C8-C9
2	P	614	P8E	C6-C7-C8-C9
2	Q	603	P8E	C6-C7-C8-C9
2	Q	609	P8E	C6-C7-C8-C9
2	Q	610	P8E	C6-C7-C8-C9
2	R	615	P8E	C6-C7-C8-C9
2	T	604	P8E	C6-C7-C8-C9
2	T	606	P8E	C6-C7-C8-C9
2	T	608	P8E	C6-C7-C8-C9
2	T	609	P8E	C6-C7-C8-C9
2	T	613	P8E	C6-C7-C8-C9
2	V	604	P8E	C6-C7-C8-C9
2	A	605	P8E	N7-C7-C8-O8
2	B	604	P8E	N7-C7-C8-O8
2	B	605	P8E	N7-C7-C8-O8
2	C	605	P8E	N7-C7-C8-O8
2	C	606	P8E	N7-C7-C8-O8
2	C	614	P8E	N7-C7-C8-O8
2	D	603	P8E	N7-C7-C8-O8
2	F	603	P8E	N7-C7-C8-O8
2	F	604	P8E	N7-C7-C8-O8
2	F	611	P8E	N7-C7-C8-O8
2	F	612	P8E	N7-C7-C8-O8
2	G	603	P8E	N7-C7-C8-O8
2	G	604	P8E	N7-C7-C8-O8
2	G	605	P8E	N7-C7-C8-O8
2	H	603	P8E	N7-C7-C8-O8
2	H	604	P8E	N7-C7-C8-O8
2	H	606	P8E	N7-C7-C8-O8
2	I	609	P8E	N7-C7-C8-O8
2	I	611	P8E	N7-C7-C8-O8
2	I	613	P8E	N7-C7-C8-O8
2	J	603	P8E	N7-C7-C8-O8
2	J	606	P8E	N7-C7-C8-O8
2	J	607	P8E	N7-C7-C8-O8
2	J	609	P8E	N7-C7-C8-O8
2	K	603	P8E	N7-C7-C8-O8
2	K	605	P8E	N7-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
2	K	606	P8E	N7-C7-C8-O8
2	L	603	P8E	N7-C7-C8-O8
2	L	604	P8E	N7-C7-C8-O8
2	L	605	P8E	N7-C7-C8-O8
2	L	606	P8E	N7-C7-C8-O8
2	M	603	P8E	N7-C7-C8-O8
2	M	613	P8E	N7-C7-C8-O8
2	O	606	P8E	N7-C7-C8-O8
2	O	614	P8E	N7-C7-C8-O8
2	P	604	P8E	N7-C7-C8-O8
2	Q	612	P8E	N7-C7-C8-O8
2	R	605	P8E	N7-C7-C8-O8
2	R	613	P8E	N7-C7-C8-O8
2	S	605	P8E	N7-C7-C8-O8
2	T	603	P8E	N7-C7-C8-O8
2	T	605	P8E	N7-C7-C8-O8
2	T	613	P8E	N7-C7-C8-O8
2	U	601	P8E	N7-C7-C8-O8
2	U	603	P8E	N7-C7-C8-O8
2	U	605	P8E	N7-C7-C8-O8
2	U	609	P8E	N7-C7-C8-O8
2	V	606	P8E	N7-C7-C8-O8
2	A	605	P8E	O6-C6-C7-N7
2	A	606	P8E	O6-C6-C7-N7
2	A	613	P8E	O6-C6-C7-N7
2	B	601	P8E	O6-C6-C7-N7
2	B	606	P8E	O6-C6-C7-N7
2	B	609	P8E	O6-C6-C7-N7
2	B	613	P8E	O6-C6-C7-N7
2	C	601	P8E	O6-C6-C7-N7
2	C	606	P8E	O6-C6-C7-N7
2	D	601	P8E	O6-C6-C7-N7
2	D	606	P8E	O6-C6-C7-N7
2	D	609	P8E	O6-C6-C7-N7
2	D	613	P8E	O6-C6-C7-N7
2	E	601	P8E	O6-C6-C7-N7
2	E	606	P8E	O6-C6-C7-N7
2	E	607	P8E	O6-C6-C7-N7
2	E	609	P8E	O6-C6-C7-N7
2	F	601	P8E	O6-C6-C7-N7
2	F	606	P8E	O6-C6-C7-N7
2	G	601	P8E	O6-C6-C7-N7

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Mol	Chain	Res	Type	Atoms
2	G	605	P8E	O6-C6-C7-N7
2	G	609	P8E	O6-C6-C7-N7
2	H	601	P8E	O6-C6-C7-N7
2	H	606	P8E	O6-C6-C7-N7
2	H	609	P8E	O6-C6-C7-N7
2	I	601	P8E	O6-C6-C7-N7
2	I	604	P8E	O6-C6-C7-N7
2	I	606	P8E	O6-C6-C7-N7
2	I	607	P8E	O6-C6-C7-N7
2	I	611	P8E	O6-C6-C7-N7
2	I	613	P8E	O6-C6-C7-N7
2	J	601	P8E	O6-C6-C7-N7
2	J	606	P8E	O6-C6-C7-N7
2	J	612	P8E	O6-C6-C7-N7
2	K	601	P8E	O6-C6-C7-N7
2	K	605	P8E	O6-C6-C7-N7
2	K	606	P8E	O6-C6-C7-N7
2	K	615	P8E	O6-C6-C7-N7
2	L	601	P8E	O6-C6-C7-N7
2	L	605	P8E	O6-C6-C7-N7
2	L	606	P8E	O6-C6-C7-N7
2	M	601	P8E	O6-C6-C7-N7
2	M	607	P8E	O6-C6-C7-N7
2	M	612	P8E	O6-C6-C7-N7
2	N	601	P8E	O6-C6-C7-N7
2	N	606	P8E	O6-C6-C7-N7
2	N	607	P8E	O6-C6-C7-N7
2	N	614	P8E	O6-C6-C7-N7
2	N	615	P8E	O6-C6-C7-N7
2	O	601	P8E	O6-C6-C7-N7
2	O	606	P8E	O6-C6-C7-N7
2	O	607	P8E	O6-C6-C7-N7
2	O	613	P8E	O6-C6-C7-N7
2	P	601	P8E	O6-C6-C7-N7
2	P	604	P8E	O6-C6-C7-N7
2	Q	601	P8E	O6-C6-C7-N7
2	Q	607	P8E	O6-C6-C7-N7
2	R	601	P8E	O6-C6-C7-N7
2	R	606	P8E	O6-C6-C7-N7
2	R	612	P8E	O6-C6-C7-N7
2	S	601	P8E	O6-C6-C7-N7
2	S	606	P8E	O6-C6-C7-N7

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Mol	Chain	Res	Type	Atoms
2	T	601	P8E	O6-C6-C7-N7
2	T	605	P8E	O6-C6-C7-N7
2	T	610	P8E	O6-C6-C7-N7
2	T	611	P8E	O6-C6-C7-N7
2	T	612	P8E	O6-C6-C7-N7
2	T	613	P8E	O6-C6-C7-N7
2	U	601	P8E	O6-C6-C7-N7
2	U	606	P8E	O6-C6-C7-N7
2	U	607	P8E	O6-C6-C7-N7
2	U	609	P8E	O6-C6-C7-N7
2	U	613	P8E	O6-C6-C7-N7
2	V	601	P8E	O6-C6-C7-N7
2	V	606	P8E	O6-C6-C7-N7
2	V	607	P8E	O6-C6-C7-N7
2	V	613	P8E	O6-C6-C7-N7
2	D	610	P8E	O6-C6-C7-C8
2	R	607	P8E	O6-C6-C7-C8
2	T	614	P8E	O6-C6-C7-C8

There are no ring outliers.

204 monomers are involved in 288 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	603	P8E	1	0
2	I	601	P8E	1	0
2	S	606	P8E	2	0
2	E	610	P8E	1	0
2	V	616	P8E	1	0
2	A	603	P8E	1	0
2	H	615	P8E	1	0
2	V	601	P8E	1	0
2	U	610	P8E	2	0
2	L	615	P8E	1	0
2	A	616	P8E	1	0
2	V	617	P8E	1	0
2	R	616	P8E	3	0
2	H	610	P8E	2	0
2	E	617	P8E	1	0
2	P	616	P8E	4	0
2	T	615	P8E	1	0
2	K	610	P8E	1	0
2	H	611	P8E	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	615	P8E	2	0
2	C	610	P8E	2	0
2	L	601	P8E	1	0
2	U	612	P8E	2	0
2	E	612	P8E	2	0
2	M	608	P8E	1	0
2	G	601	P8E	1	0
2	A	615	P8E	1	0
2	T	614	P8E	1	0
2	P	610	P8E	2	0
2	T	617	P8E	2	0
2	P	611	P8E	1	0
2	U	601	P8E	1	0
2	U	611	P8E	1	0
2	A	610	P8E	2	0
2	N	616	P8E	3	0
2	U	603	P8E	1	0
2	M	601	P8E	1	0
2	H	606	P8E	2	0
2	O	612	P8E	2	0
2	R	601	P8E	1	0
2	S	603	P8E	1	0
2	K	606	P8E	1	0
2	K	612	P8E	2	0
2	L	616	P8E	2	0
2	C	606	P8E	2	0
2	E	616	P8E	2	0
2	L	610	P8E	2	0
2	I	616	P8E	2	0
2	Q	617	P8E	2	0
2	B	614	P8E	1	0
2	N	601	P8E	1	0
2	T	608	P8E	1	0
2	M	610	P8E	2	0
2	N	615	P8E	1	0
2	S	612	P8E	2	0
2	O	614	P8E	1	0
2	S	614	P8E	1	0
2	G	615	P8E	1	0
2	B	616	P8E	2	0
2	P	606	P8E	1	0
2	A	606	P8E	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	610	P8E	2	0
2	Q	608	P8E	1	0
2	Q	610	P8E	1	0
2	N	603	P8E	1	0
2	O	617	P8E	1	0
2	S	617	P8E	1	0
2	L	608	P8E	1	0
2	H	616	P8E	1	0
2	R	615	P8E	1	0
2	I	614	P8E	1	0
2	G	614	P8E	1	0
2	H	612	P8E	2	0
2	H	608	P8E	1	0
2	I	602	P8E	1	0
2	J	609	P8E	1	0
2	C	616	P8E	2	0
2	L	606	P8E	2	0
2	C	615	P8E	1	0
2	B	617	P8E	1	0
2	J	610	P8E	2	0
2	T	601	P8E	1	0
2	Q	606	P8E	3	0
2	G	606	P8E	3	0
2	E	601	P8E	1	0
2	G	616	P8E	1	0
2	A	612	P8E	2	0
2	M	606	P8E	2	0
2	J	615	P8E	1	0
2	R	612	P8E	2	0
2	T	603	P8E	1	0
2	C	611	P8E	1	0
2	H	601	P8E	1	0
2	F	606	P8E	3	0
2	P	615	P8E	2	0
2	P	612	P8E	2	0
2	V	612	P8E	2	0
2	F	616	P8E	2	0
2	P	601	P8E	1	0
2	U	616	P8E	2	0
2	C	601	P8E	1	0
2	L	603	P8E	1	0
2	I	606	P8E	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	P8E	1	0
2	C	617	P8E	1	0
2	F	615	P8E	1	0
2	L	617	P8E	1	0
2	G	617	P8E	1	0
2	P	617	P8E	1	0
2	D	610	P8E	2	0
2	T	616	P8E	1	0
2	B	603	P8E	1	0
2	J	608	P8E	1	0
2	F	601	P8E	1	0
2	L	611	P8E	1	0
2	J	606	P8E	1	0
2	D	616	P8E	3	0
2	E	603	P8E	1	0
2	F	617	P8E	1	0
2	N	612	P8E	2	0
2	I	603	P8E	1	0
2	O	615	P8E	1	0
2	Q	611	P8E	1	0
2	R	610	P8E	1	0
2	G	611	P8E	1	0
2	F	614	P8E	1	0
2	O	603	P8E	1	0
2	J	612	P8E	2	0
2	M	614	P8E	1	0
2	Q	616	P8E	3	0
2	F	607	P8E	1	0
2	D	606	P8E	2	0
2	N	606	P8E	2	0
2	O	610	P8E	1	0
2	L	612	P8E	2	0
2	T	610	P8E	1	0
2	C	603	P8E	1	0
2	M	616	P8E	2	0
2	I	612	P8E	2	0
2	N	614	P8E	1	0
2	B	610	P8E	1	0
2	Q	603	P8E	1	0
2	G	603	P8E	1	0
2	R	617	P8E	1	0
2	K	603	P8E	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	601	P8E	1	0
2	K	617	P8E	2	0
2	V	603	P8E	1	0
2	J	616	P8E	2	0
2	I	617	P8E	1	0
2	N	617	P8E	1	0
2	K	602	P8E	1	0
2	M	617	P8E	1	0
2	H	614	P8E	1	0
2	O	606	P8E	2	0
2	E	611	P8E	1	0
2	T	606	P8E	2	0
2	C	612	P8E	3	0
2	R	606	P8E	3	0
2	B	606	P8E	1	0
2	Q	615	P8E	1	0
2	Q	612	P8E	2	0
2	R	603	P8E	1	0
2	G	612	P8E	2	0
2	J	614	P8E	1	0
2	G	608	P8E	1	0
2	F	612	P8E	3	0
2	S	615	P8E	1	0
2	C	613	P8E	1	0
2	Q	601	P8E	1	0
2	F	603	P8E	1	0
2	D	614	P8E	1	0
2	P	603	P8E	1	0
2	H	617	P8E	1	0
2	S	610	P8E	2	0
2	O	616	P8E	2	0
2	E	615	P8E	1	0
2	P	614	P8E	1	0
2	O	608	P8E	1	0
2	K	616	P8E	2	0
2	D	612	P8E	3	0
2	M	615	P8E	1	0
2	J	601	P8E	1	0
2	A	617	P8E	2	0
2	B	615	P8E	1	0
2	B	612	P8E	2	0
2	N	610	P8E	1	0

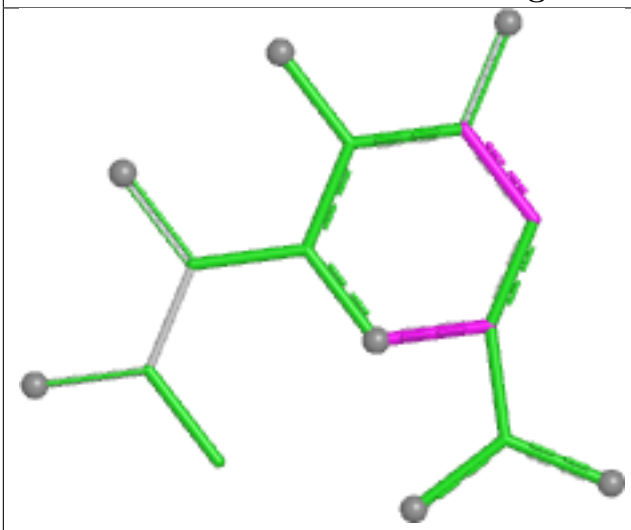
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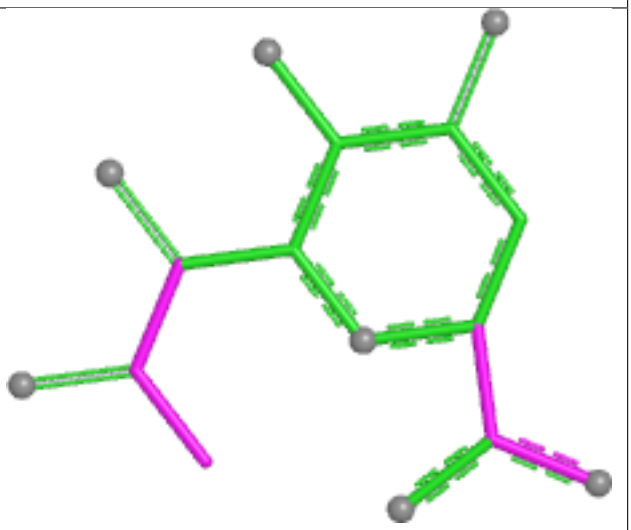
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	608	P8E	1	0
2	K	601	P8E	1	0
2	C	608	P8E	1	0
2	V	615	P8E	1	0
2	A	608	P8E	1	0
2	S	616	P8E	1	0
2	K	611	P8E	1	0
2	O	601	P8E	1	0
2	U	614	P8E	1	0
2	D	601	P8E	1	0
2	V	606	P8E	1	0
2	T	612	P8E	2	0
2	B	601	P8E	1	0
2	D	617	P8E	1	0
2	M	612	P8E	3	0
2	J	617	P8E	1	0
2	U	617	P8E	1	0

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

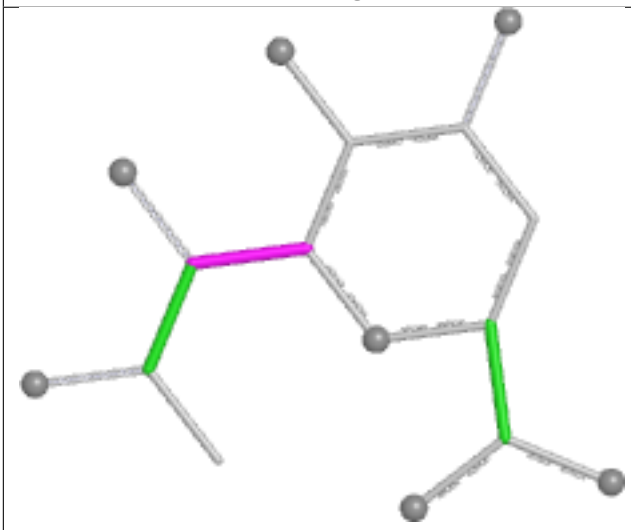
Ligand P8E A 613



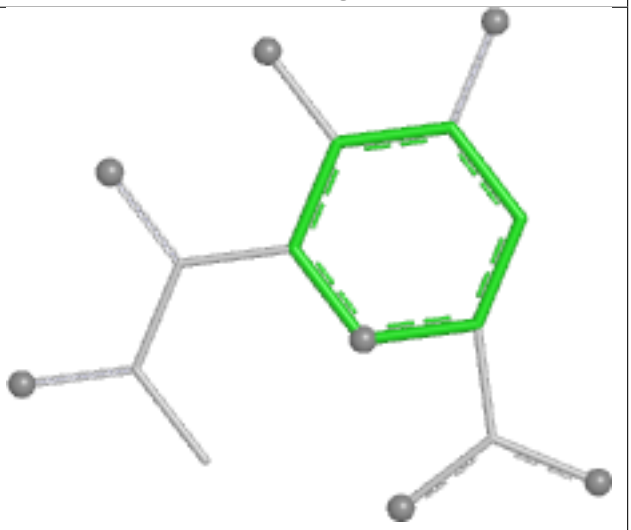
Bond lengths



Bond angles

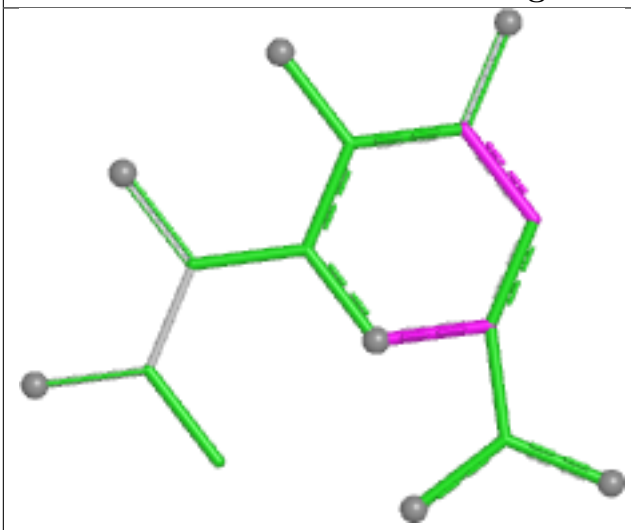


Torsions

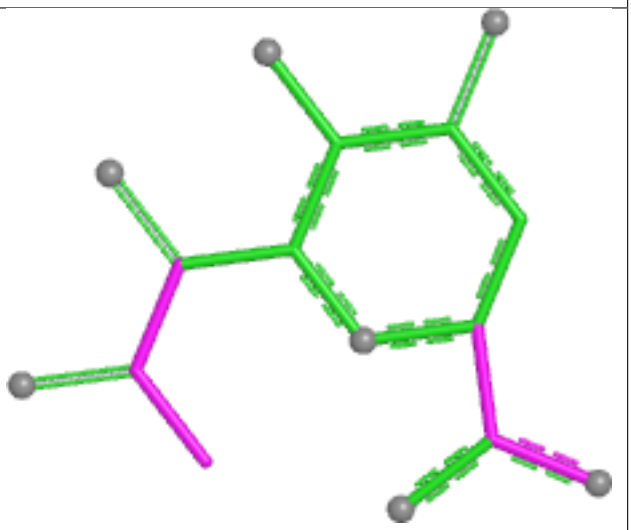


Rings

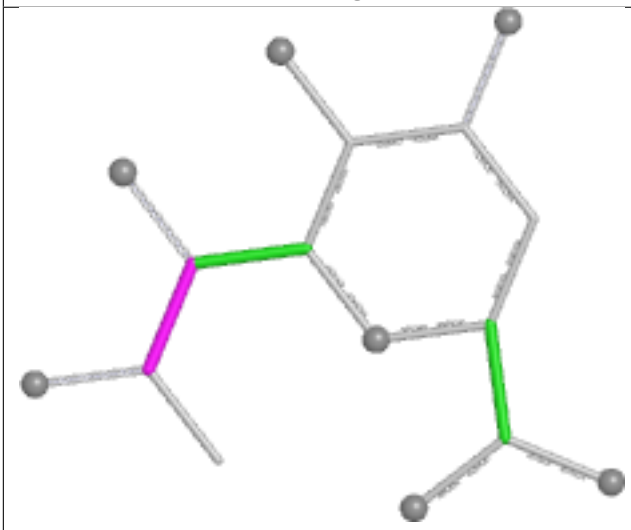
Ligand P8E O 602



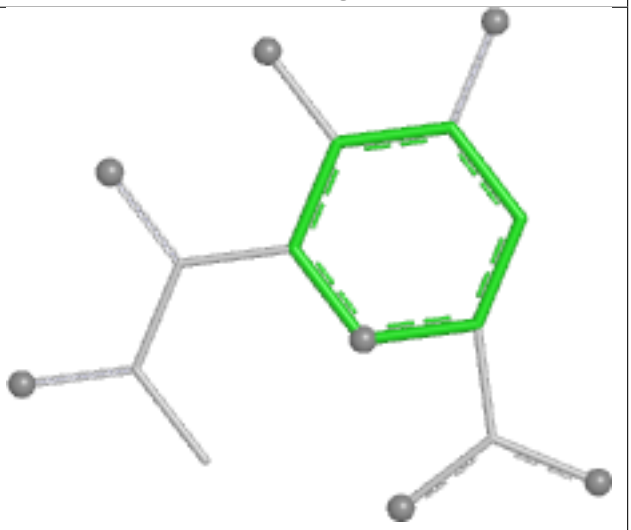
Bond lengths



Bond angles

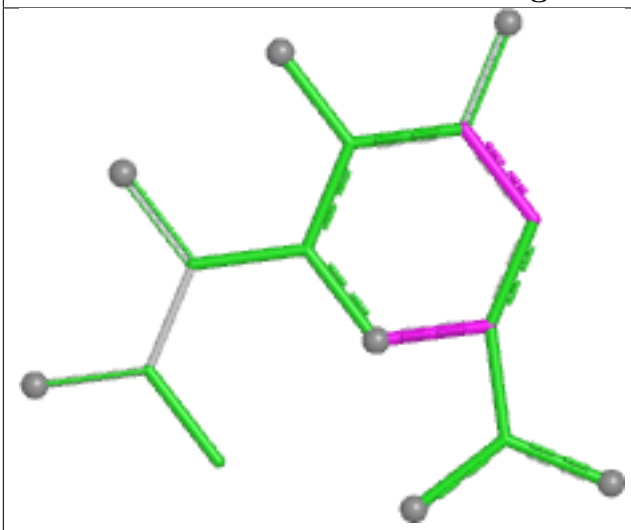


Torsions

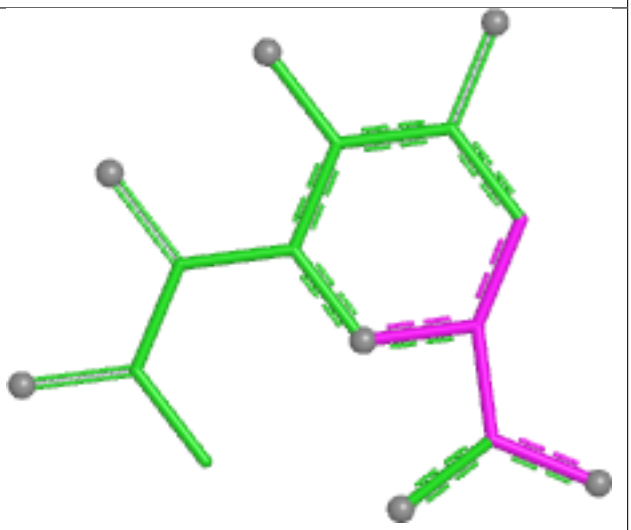


Rings

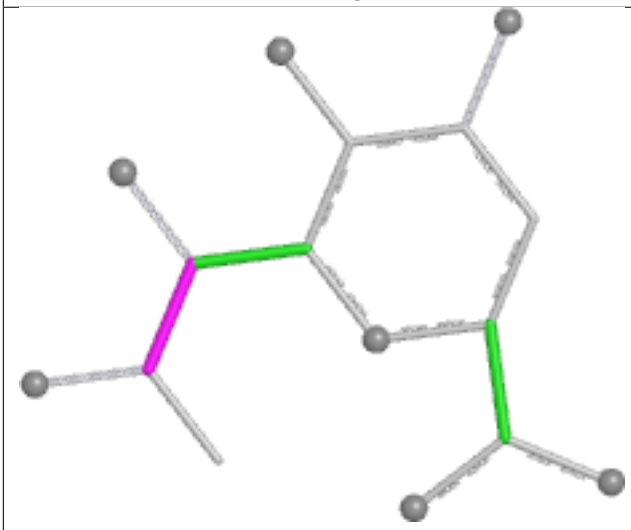
Ligand P8E F 608



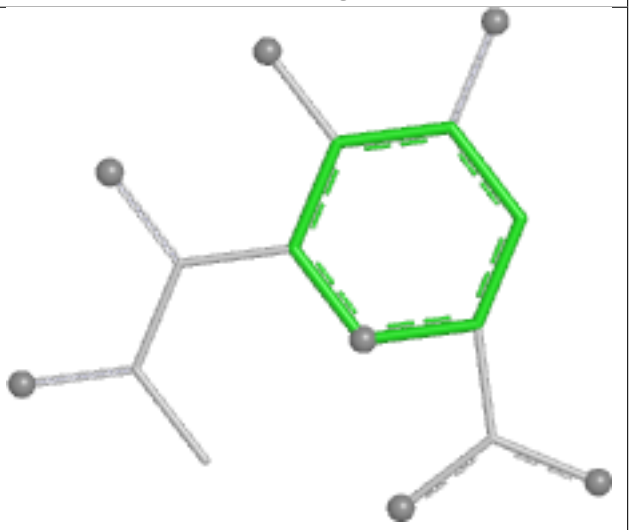
Bond lengths



Bond angles

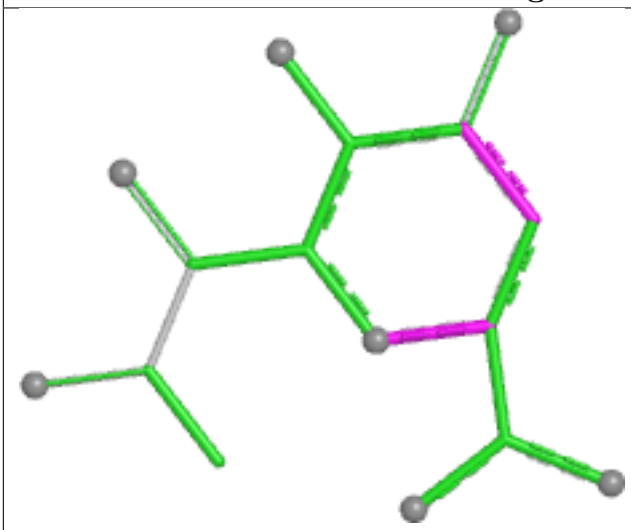


Torsions

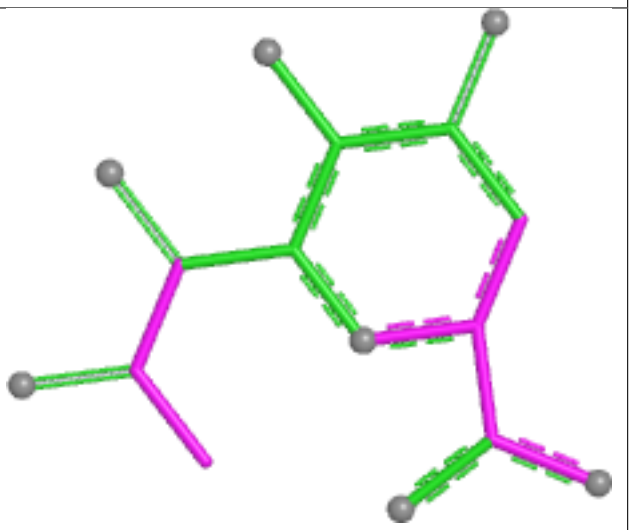


Rings

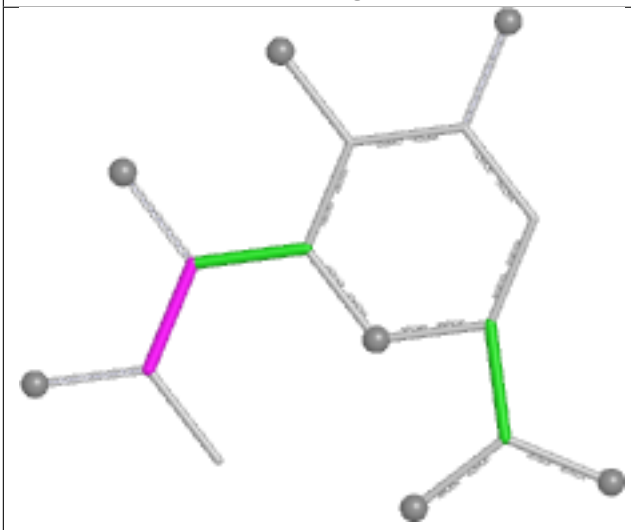
Ligand P8E H 603



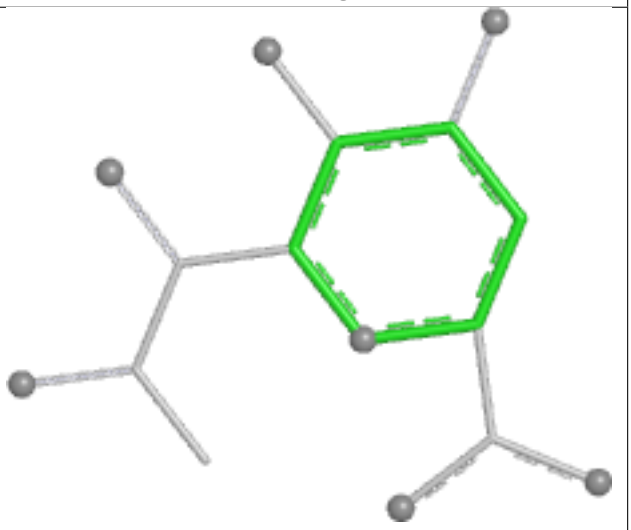
Bond lengths



Bond angles

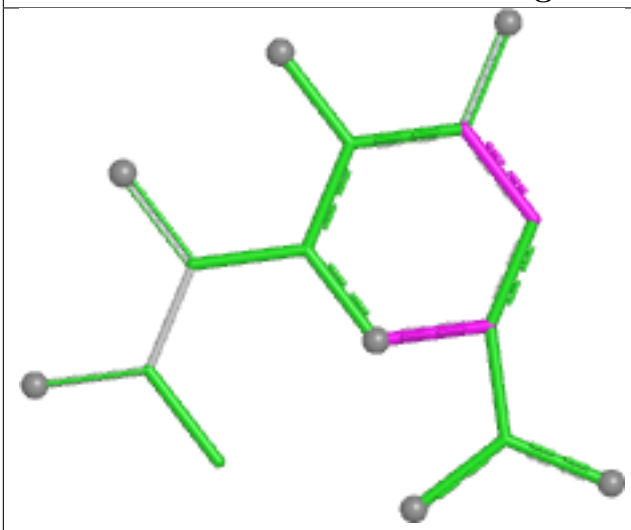


Torsions

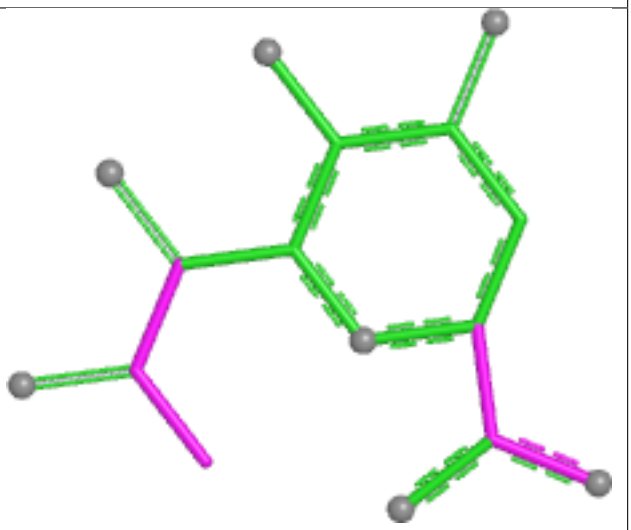


Rings

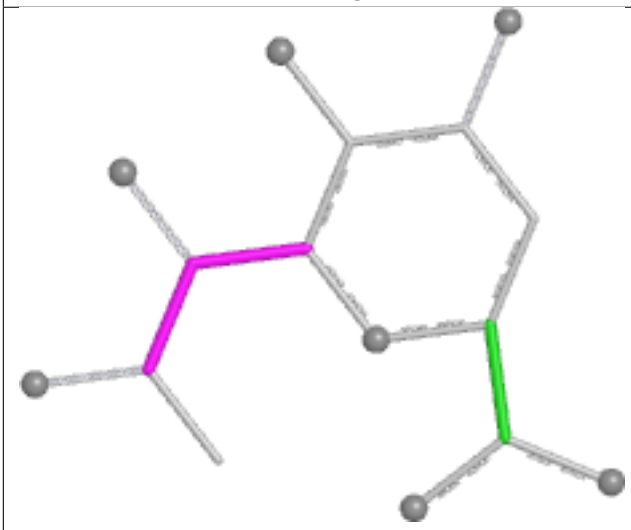
Ligand P8E I 601



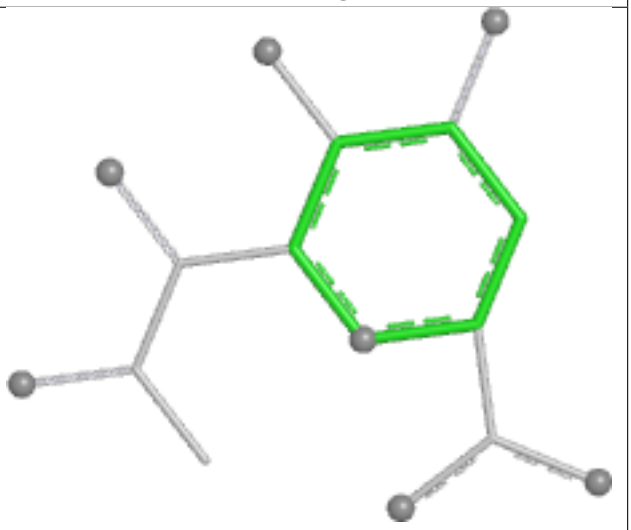
Bond lengths



Bond angles

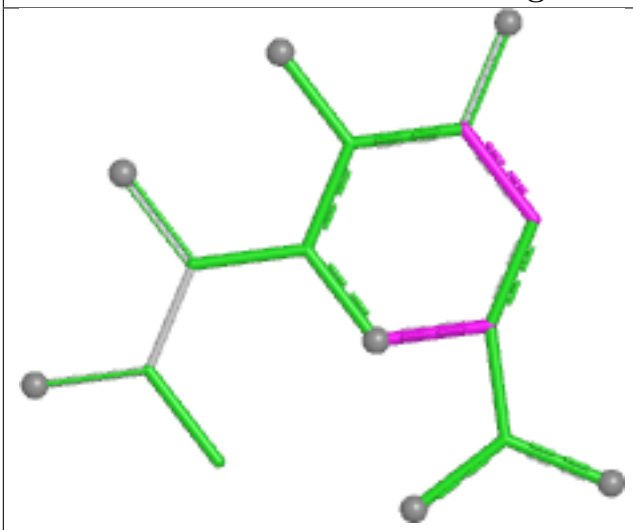


Torsions

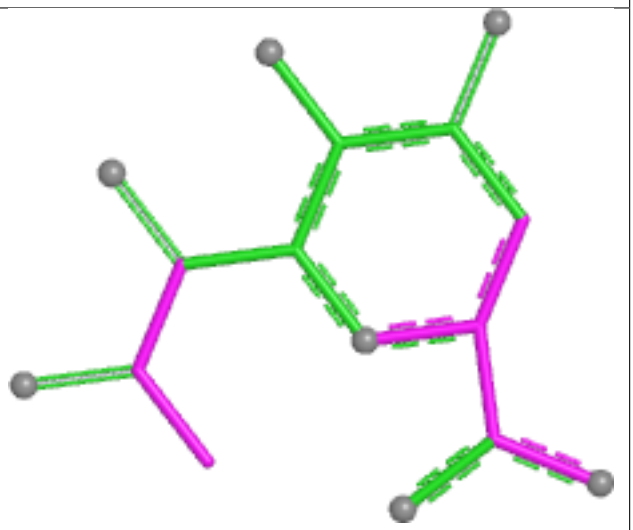


Rings

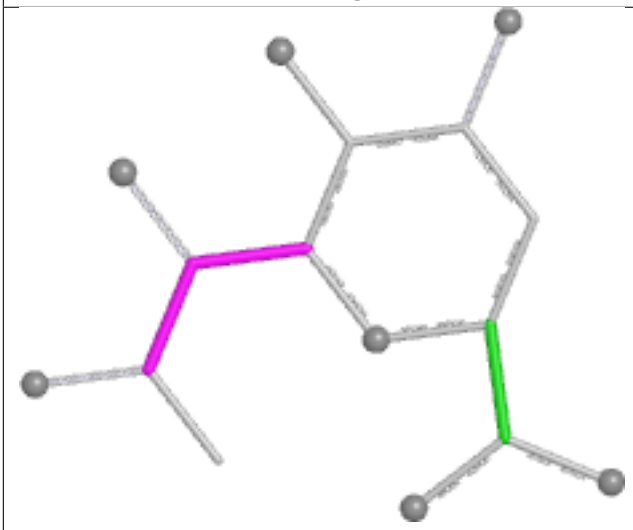
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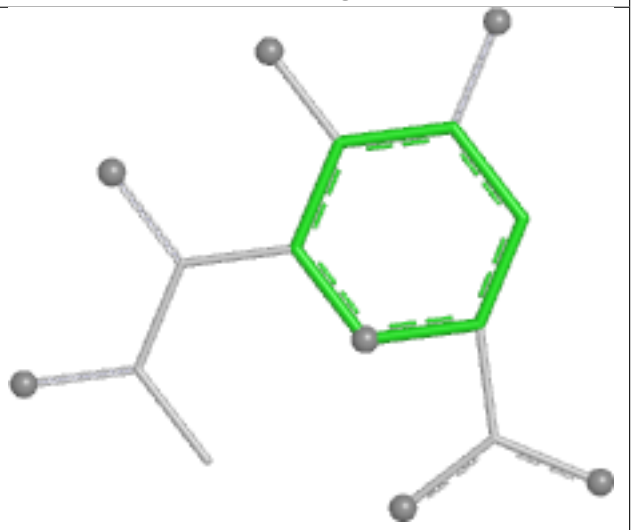
Bond lengths



Bond angles

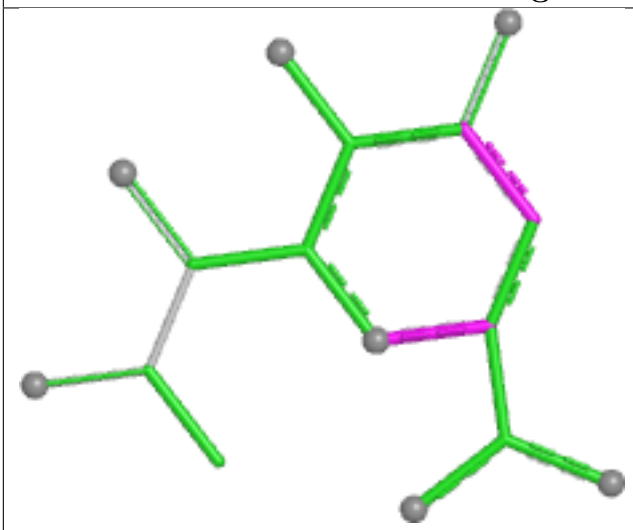


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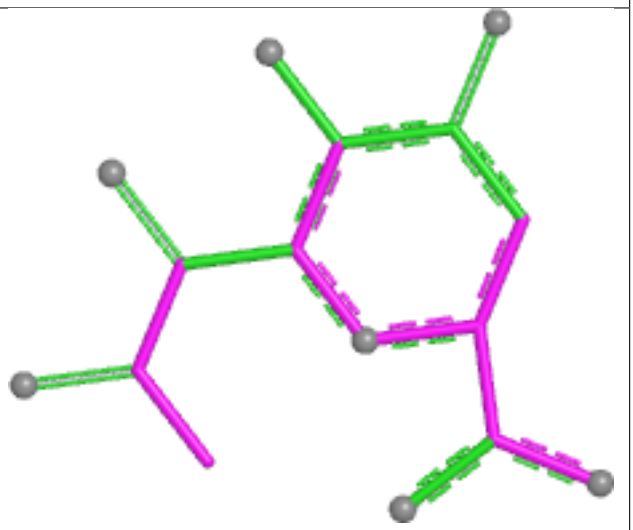


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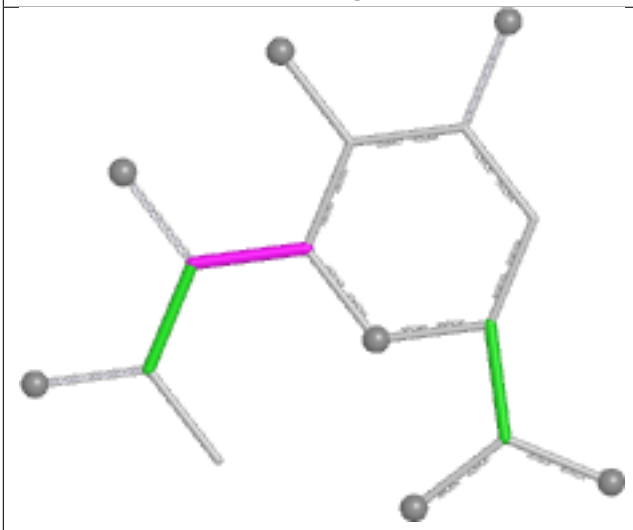
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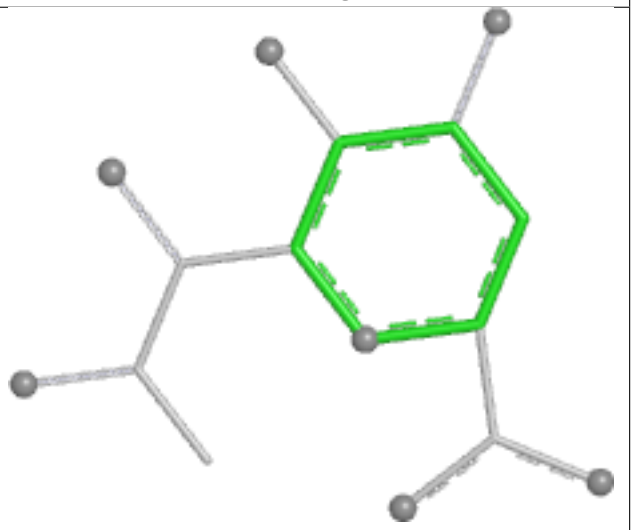
Bond lengths



Bond angles

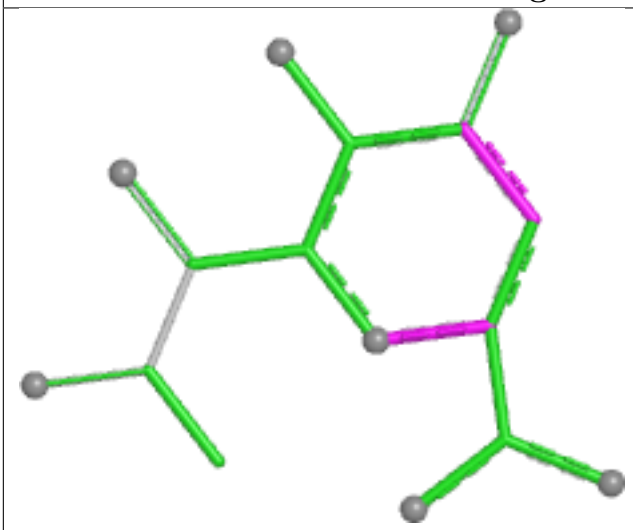


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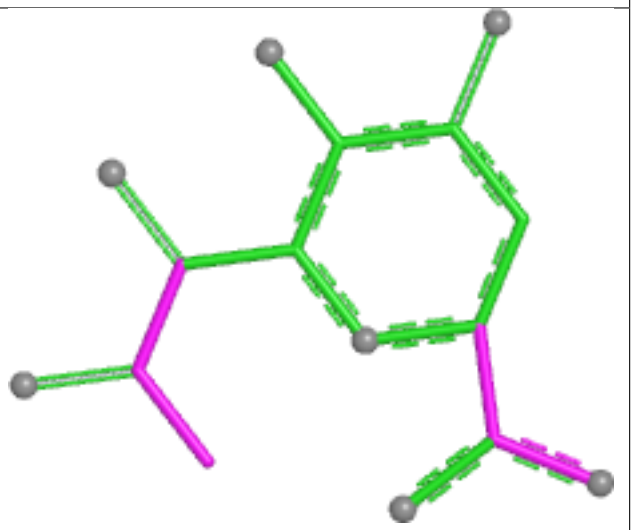


Rings

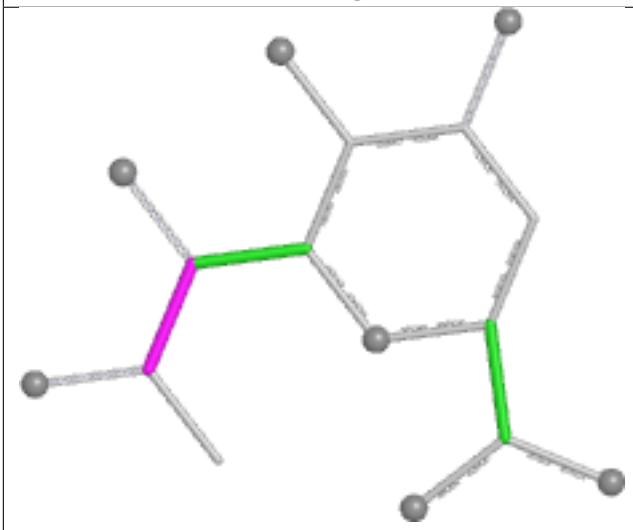
Ligand P8E E 610



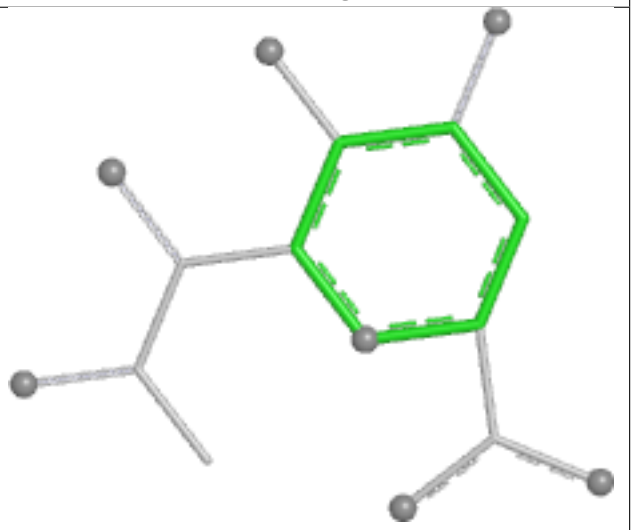
Bond lengths



Bond angles

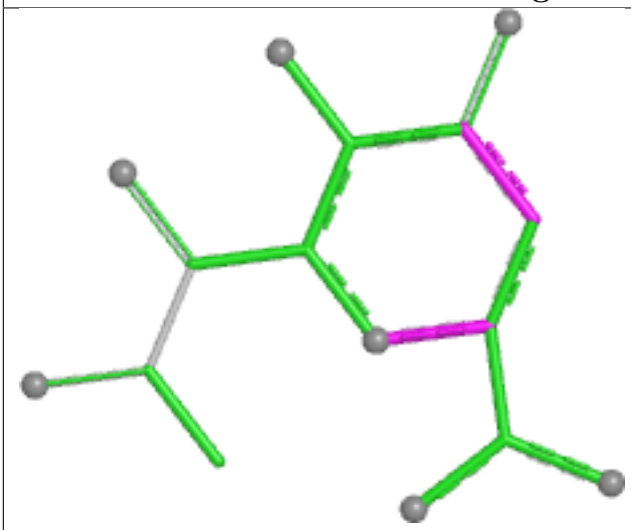


Torsions

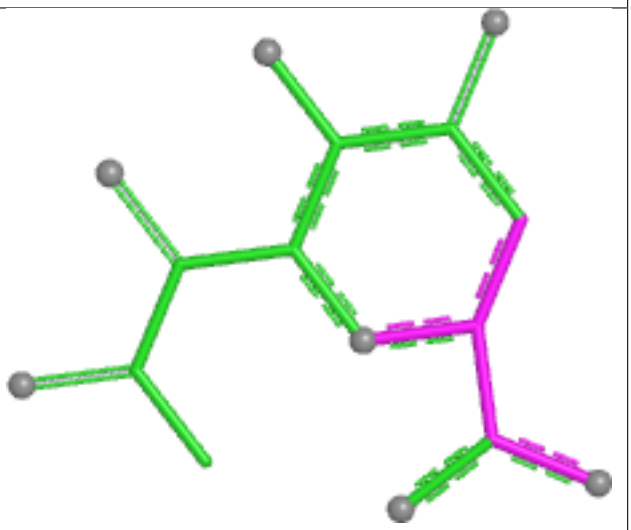


Rings

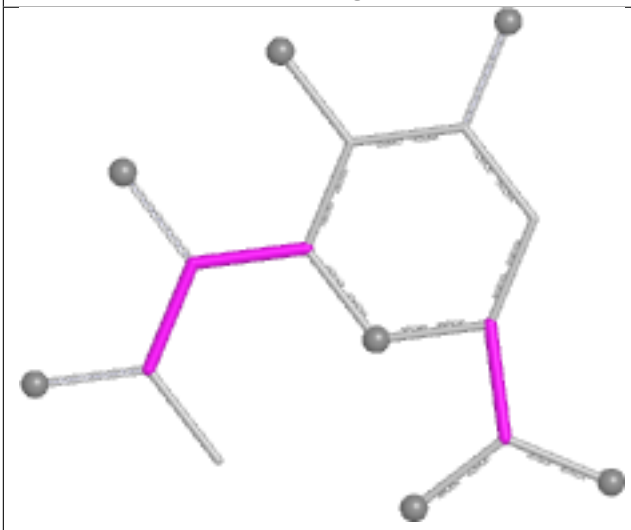
Ligand P8E J 607



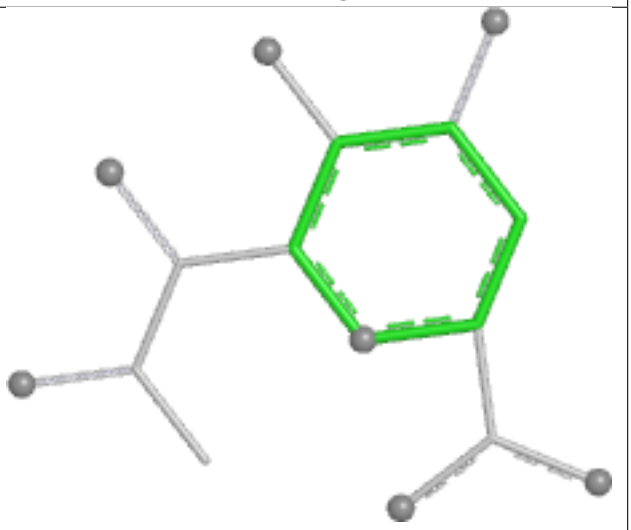
Bond lengths



Bond angles

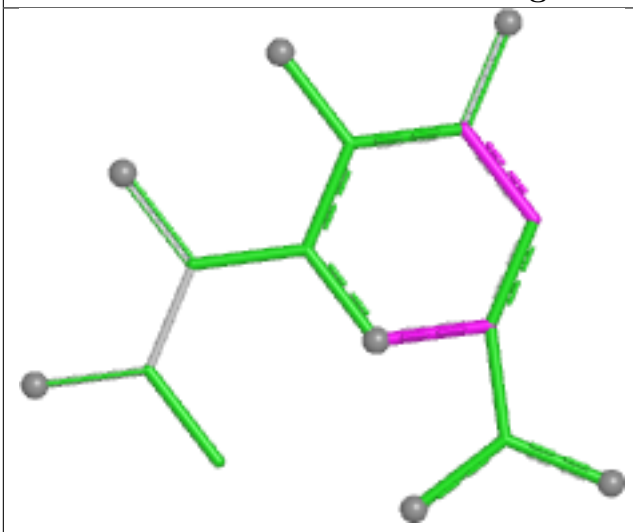


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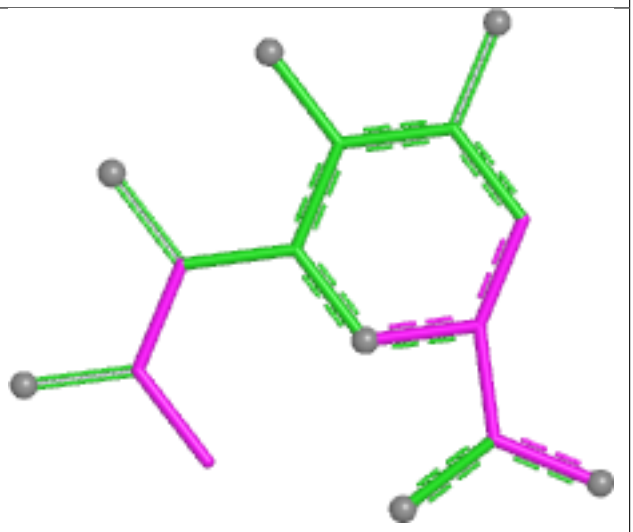


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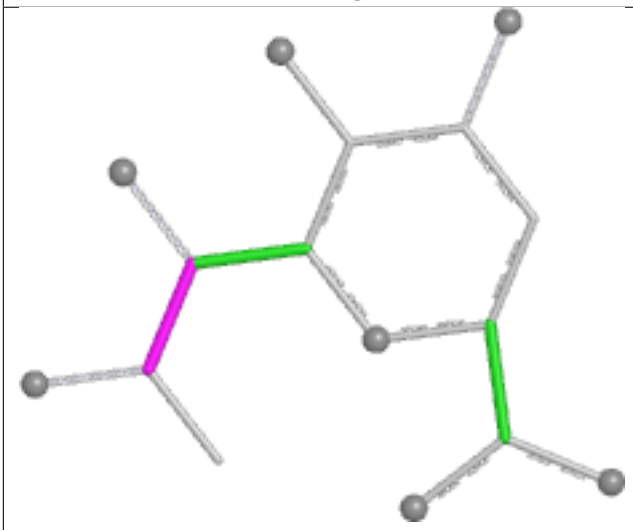
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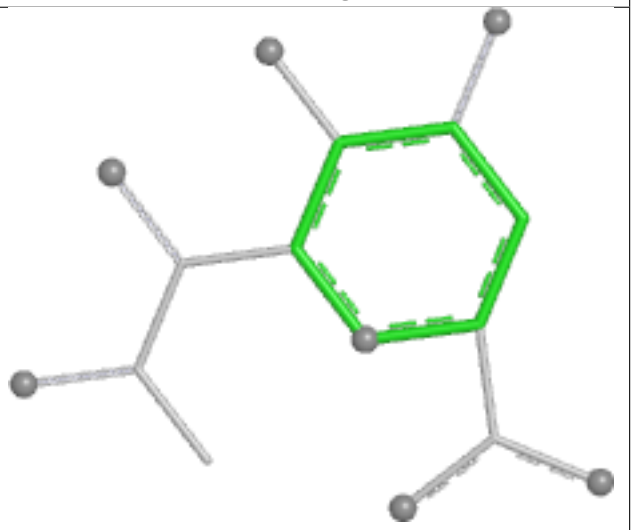
Bond lengths



Bond angles

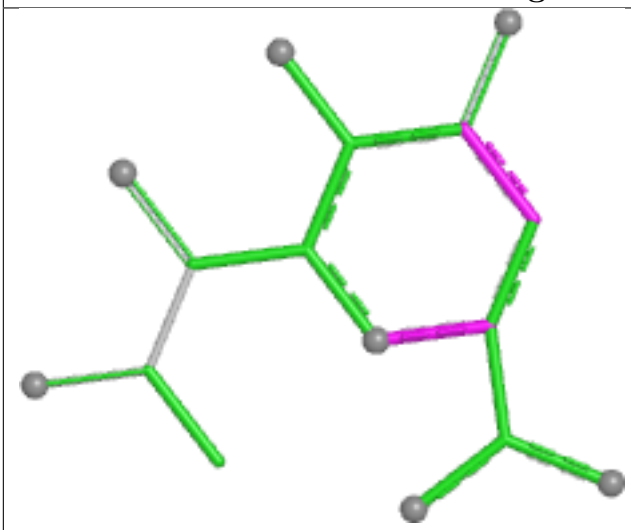


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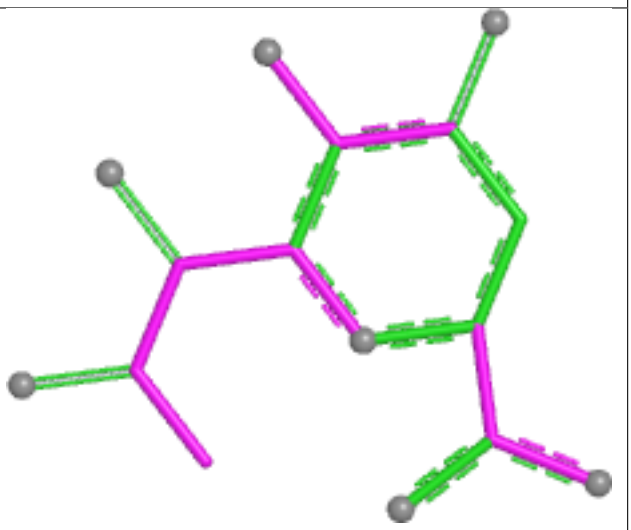


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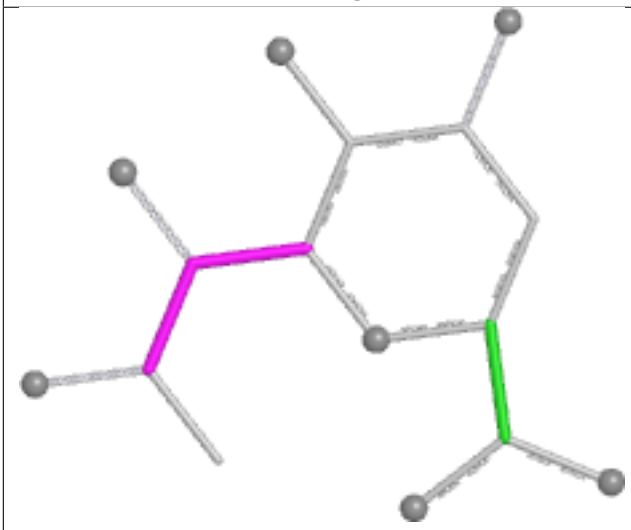
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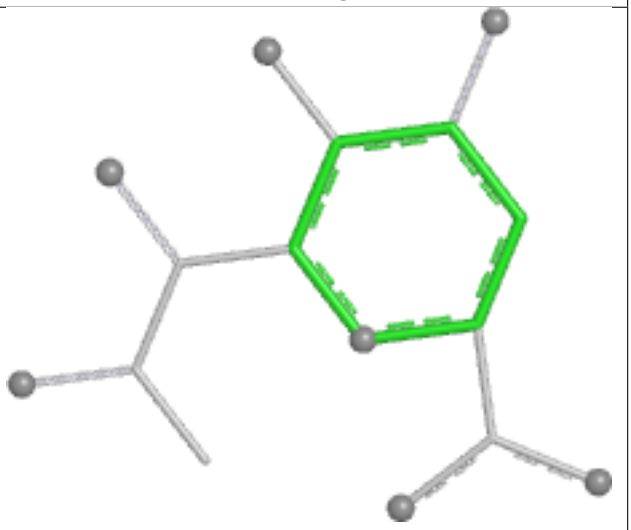
Bond lengths



Bond angles

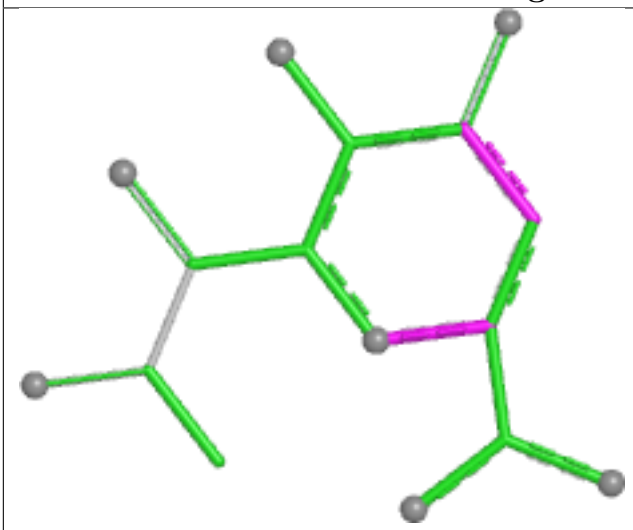


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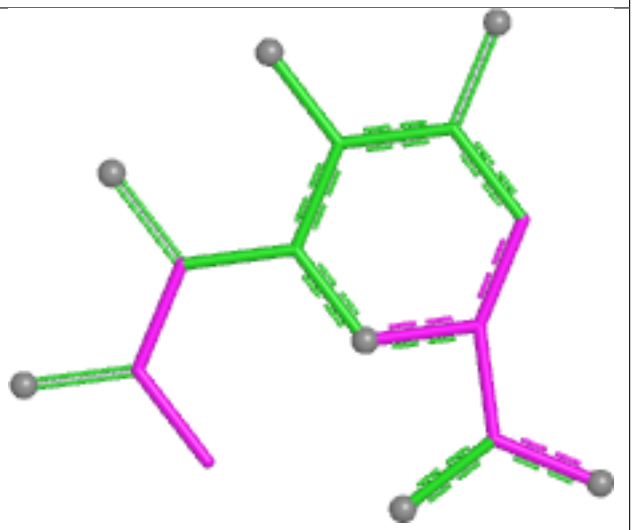


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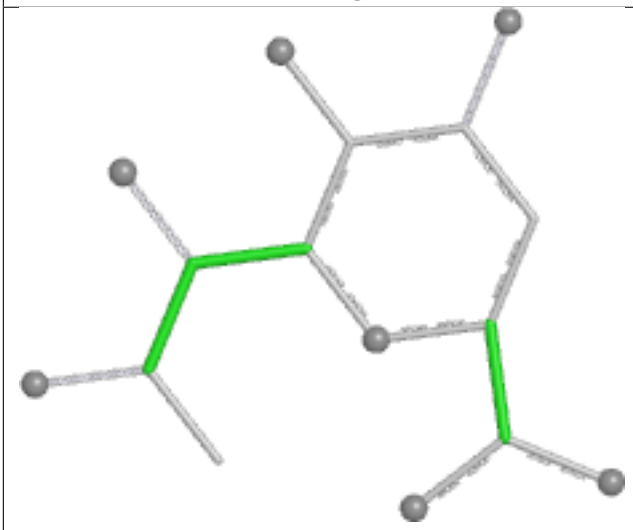
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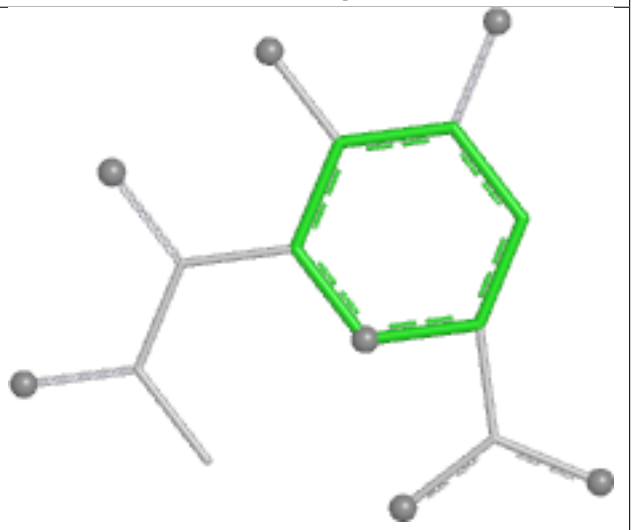
Bond lengths



Bond angles

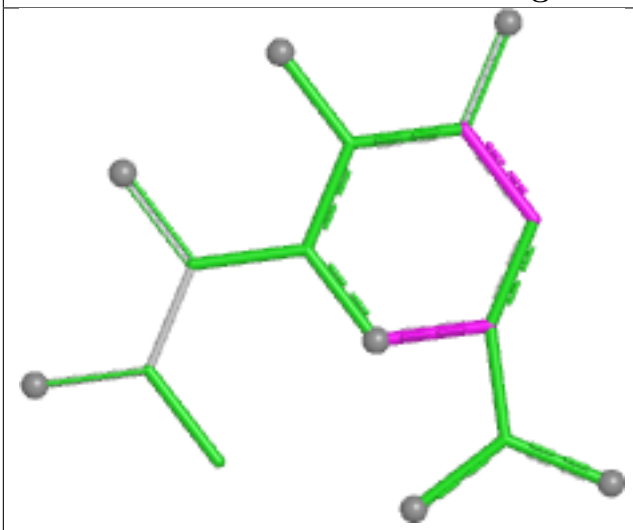


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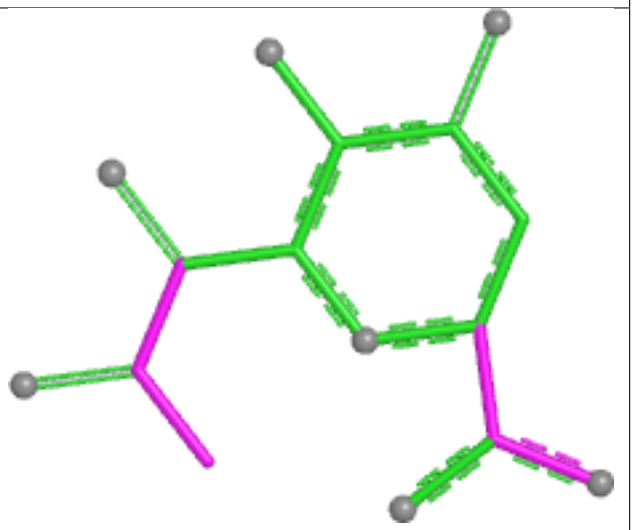


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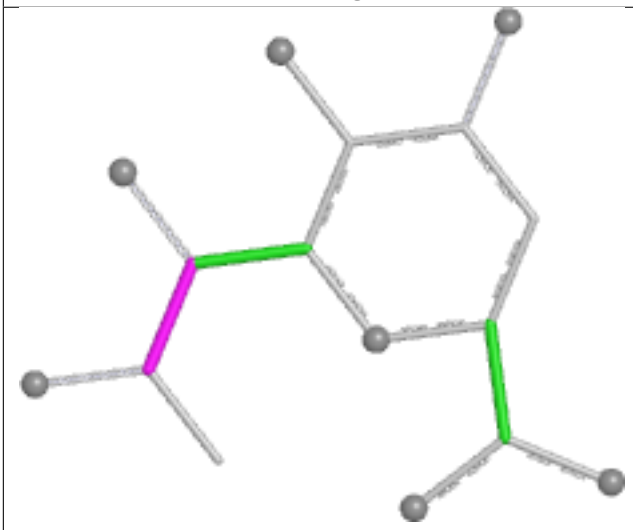
Ligand P8E S 602



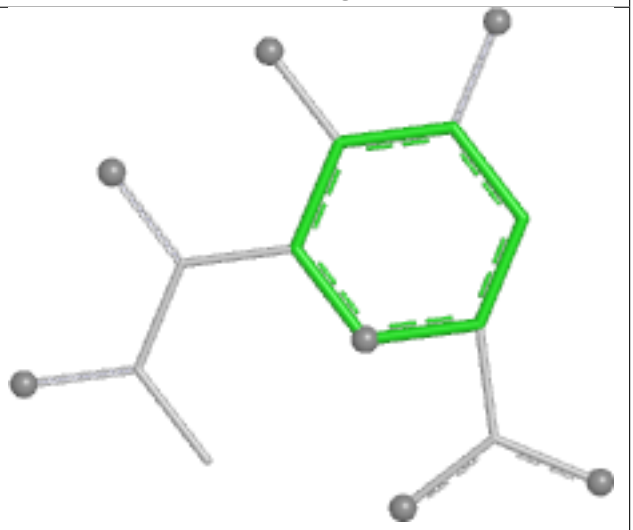
Bond lengths



Bond angles

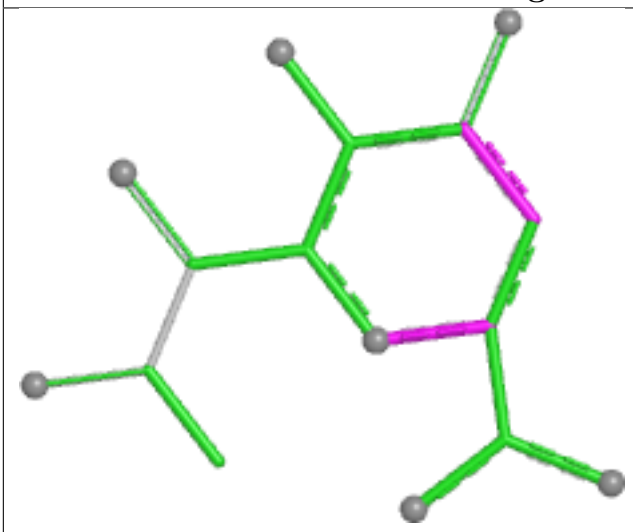


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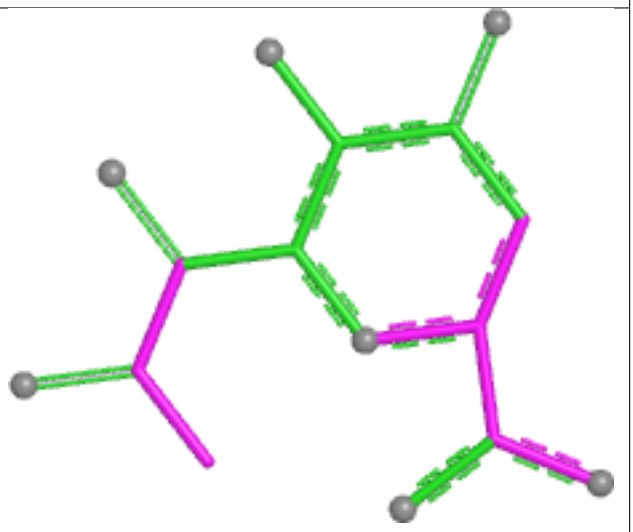


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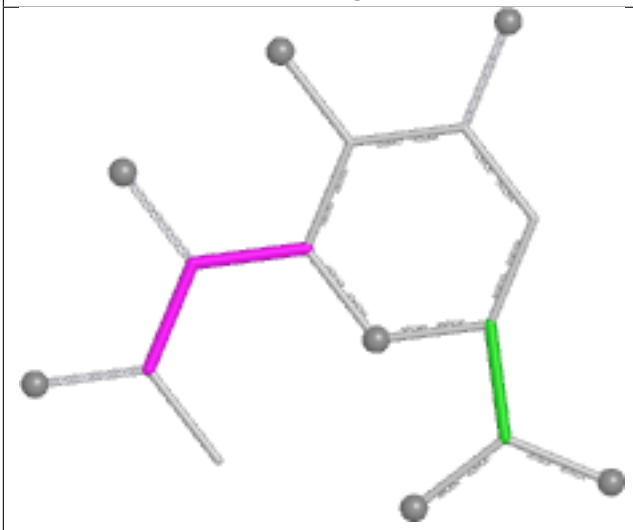
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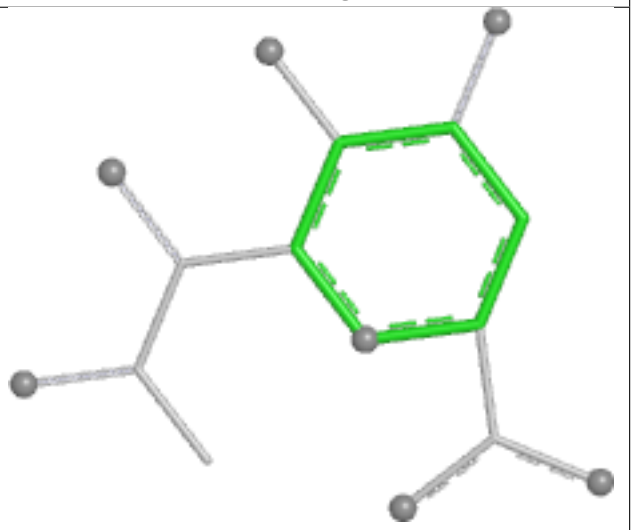
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Bond angles

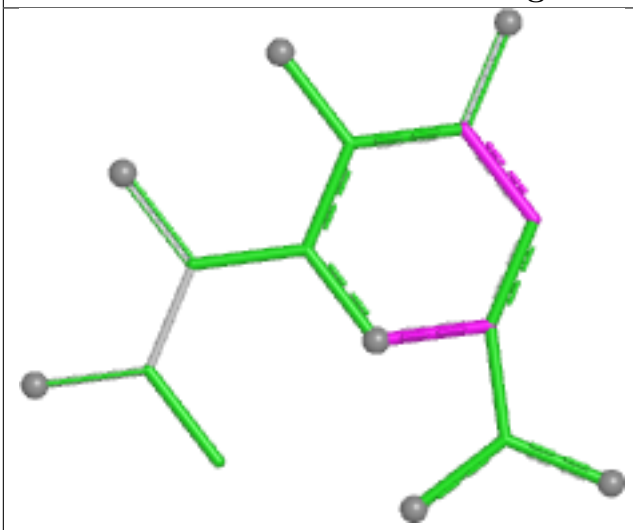


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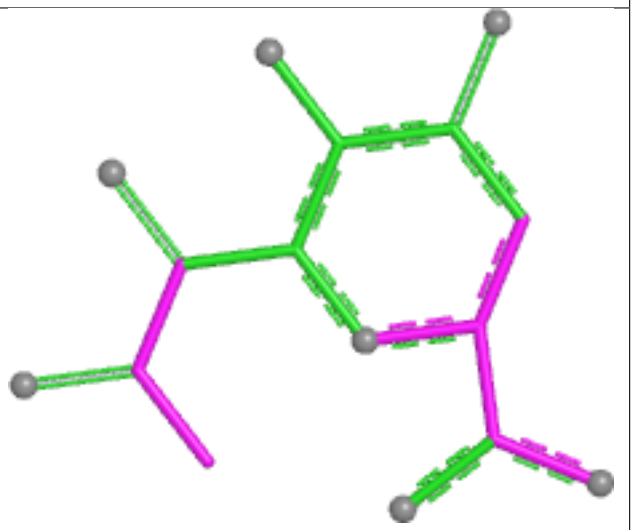


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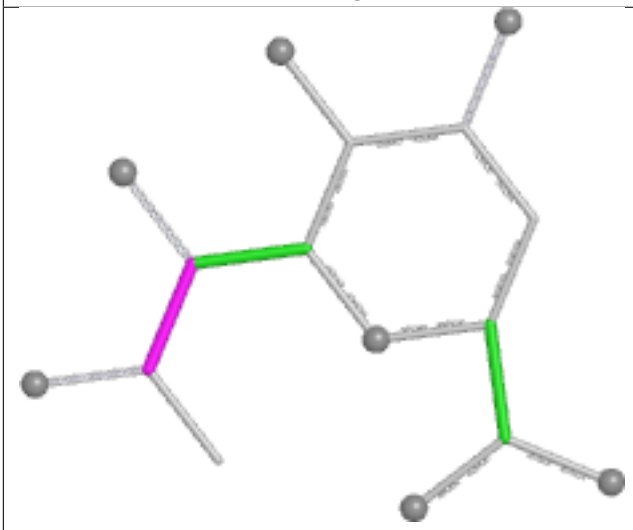
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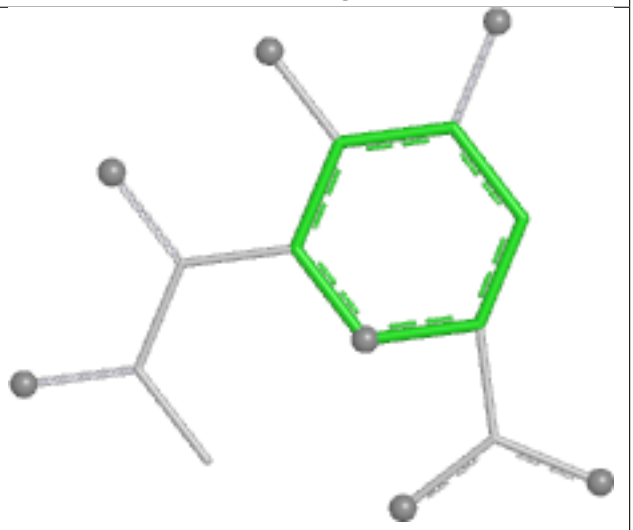
Bond lengths



Bond angles

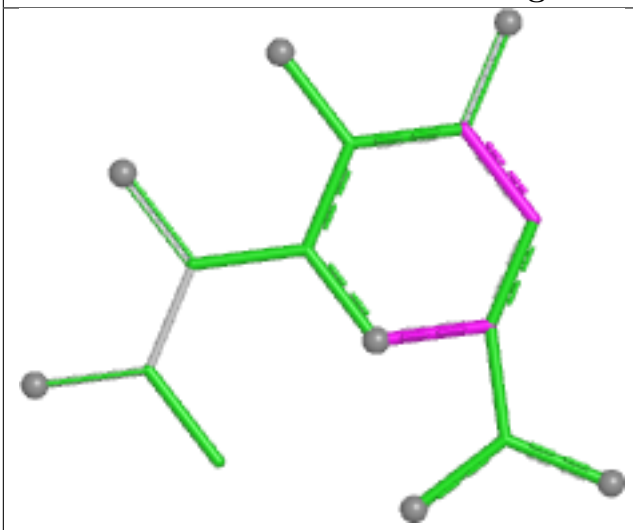


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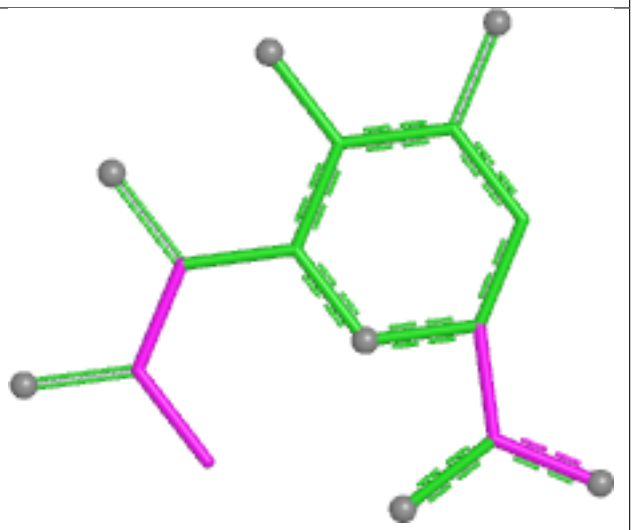


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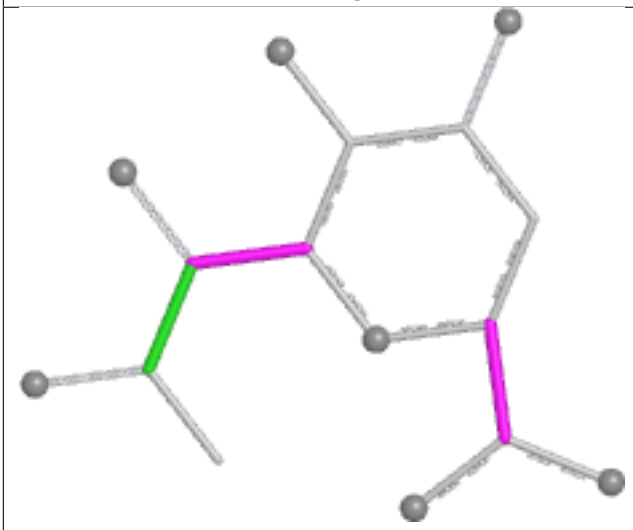
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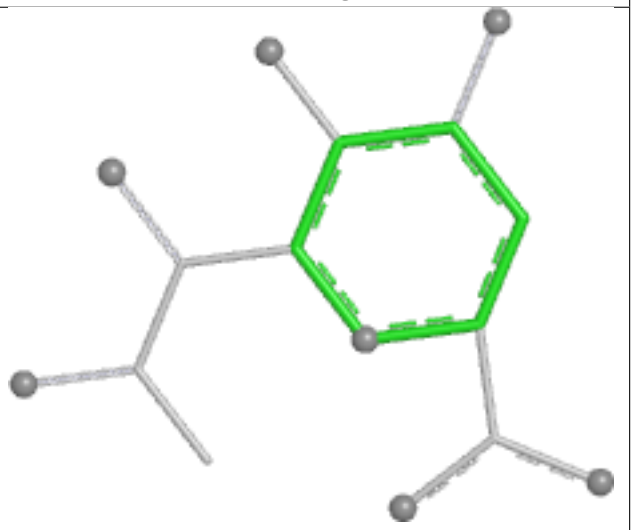
Bond lengths



Bond angles

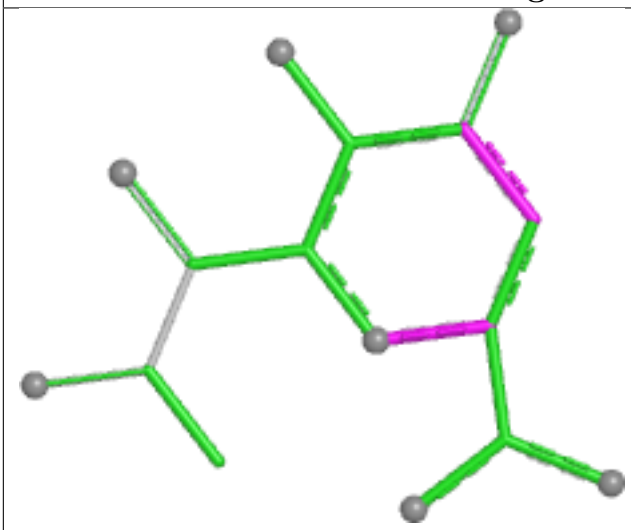


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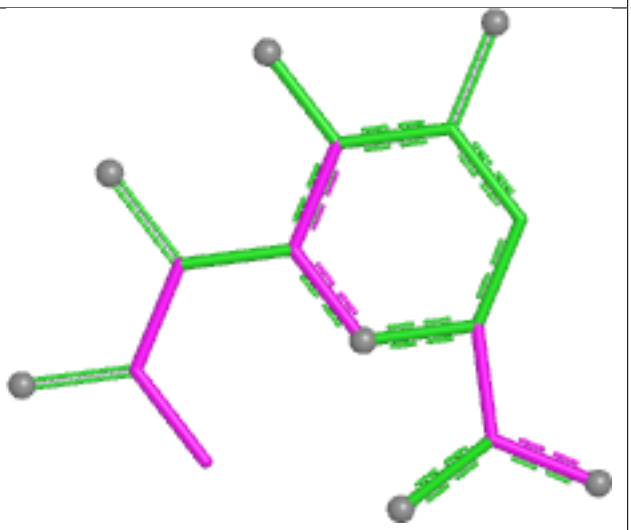


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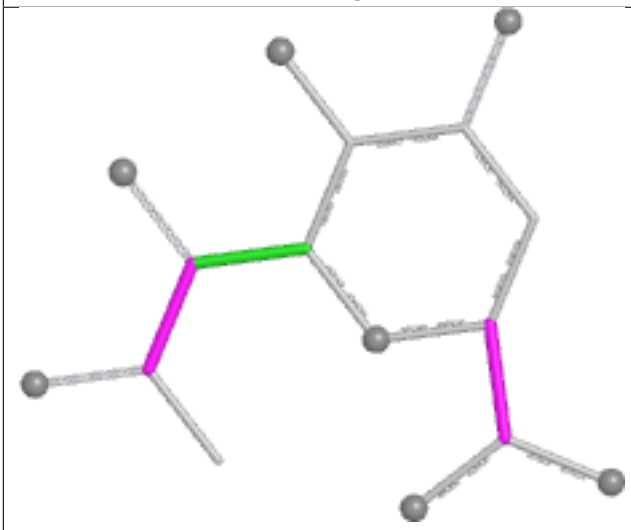
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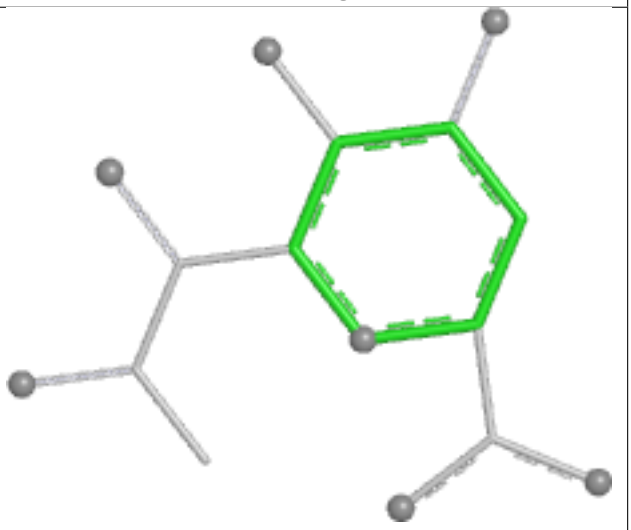
Bond lengths



Bond angles

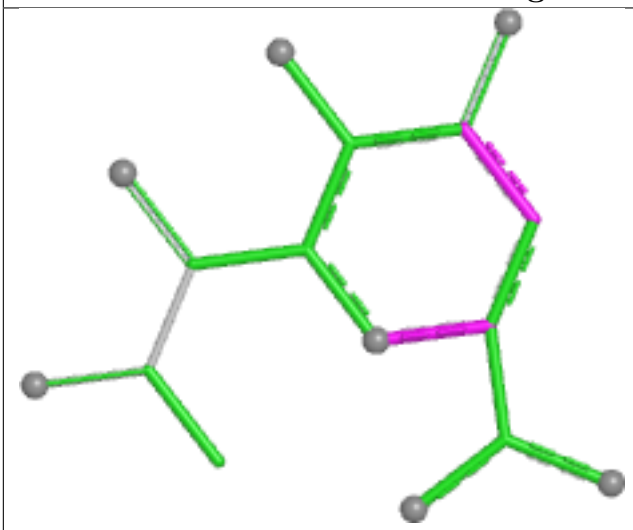


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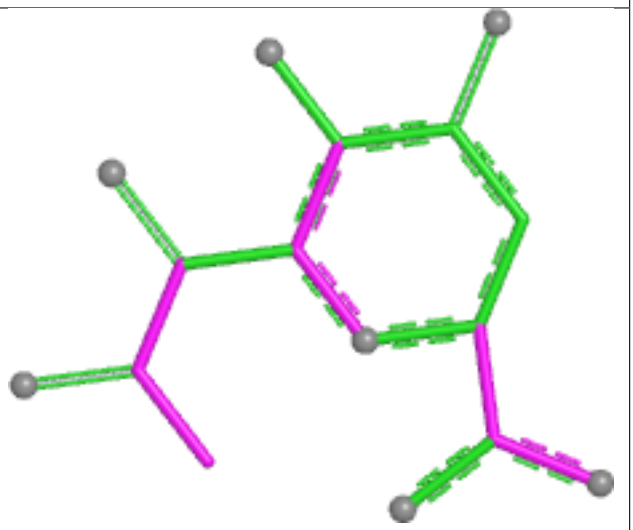


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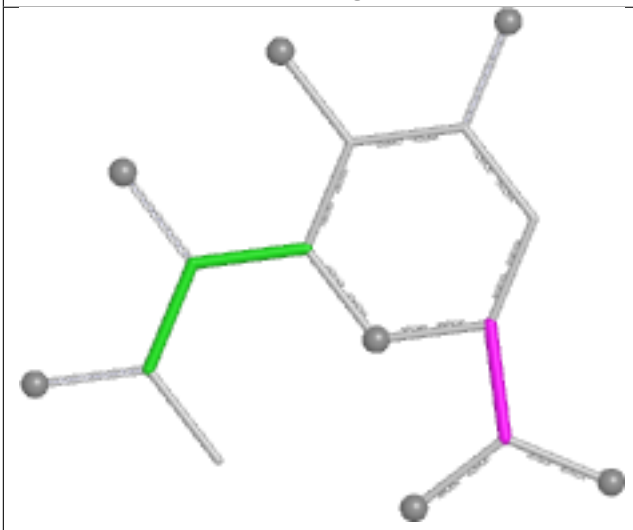
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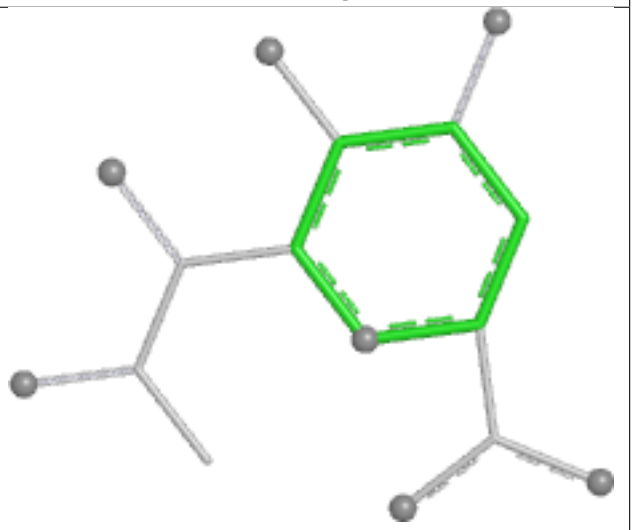
Bond lengths



Bond angles

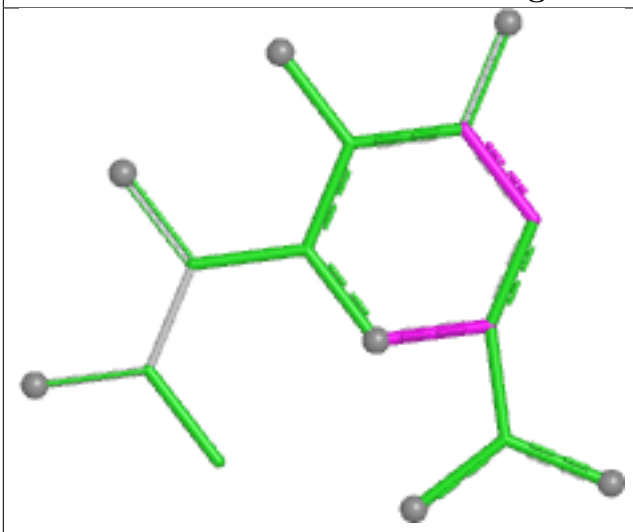


Torsions

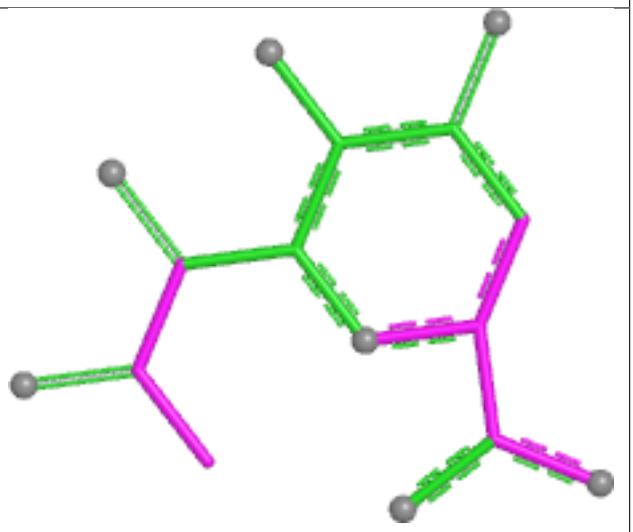


Rings

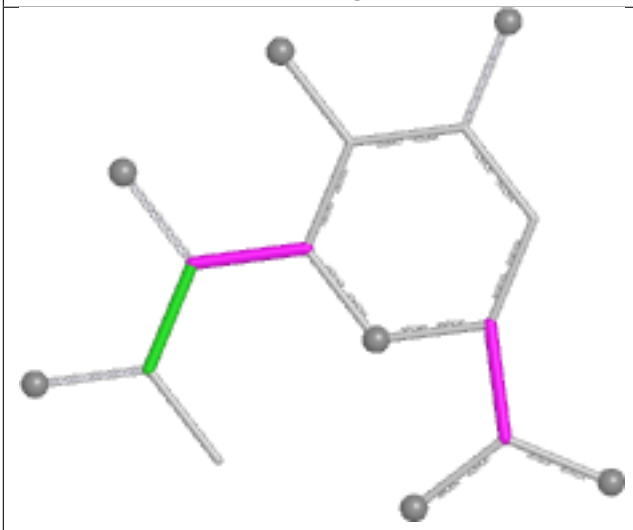
Ligand P8E O 607



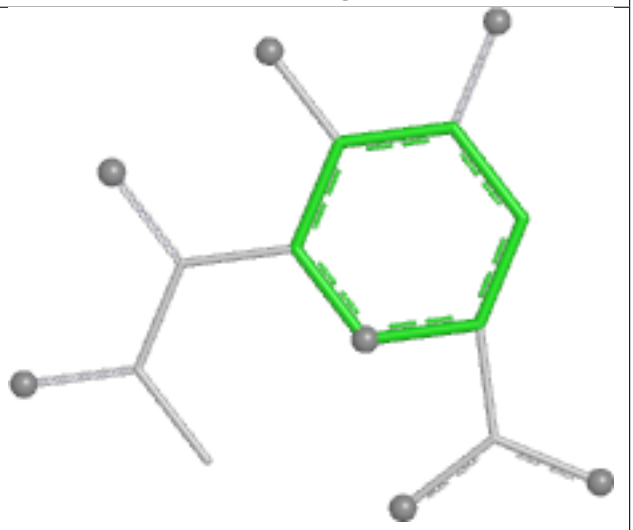
Bond lengths



Bond angles

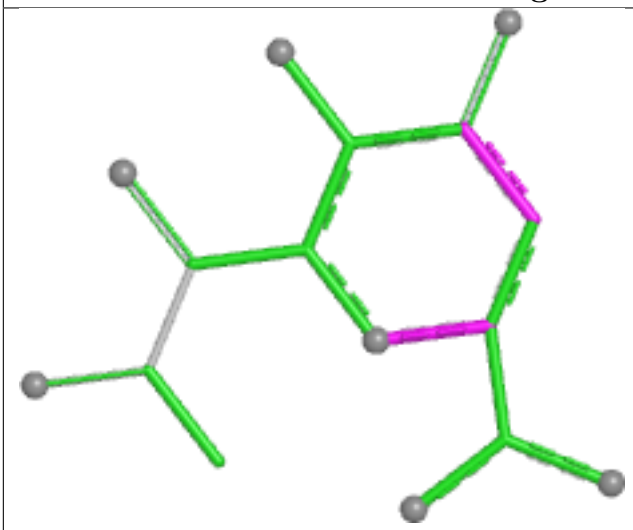


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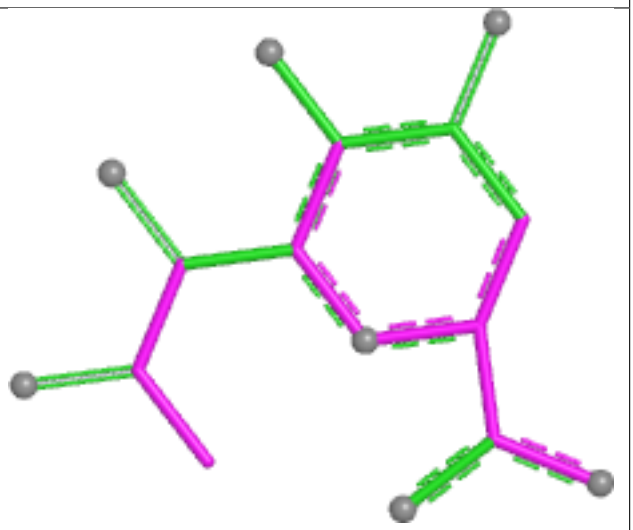


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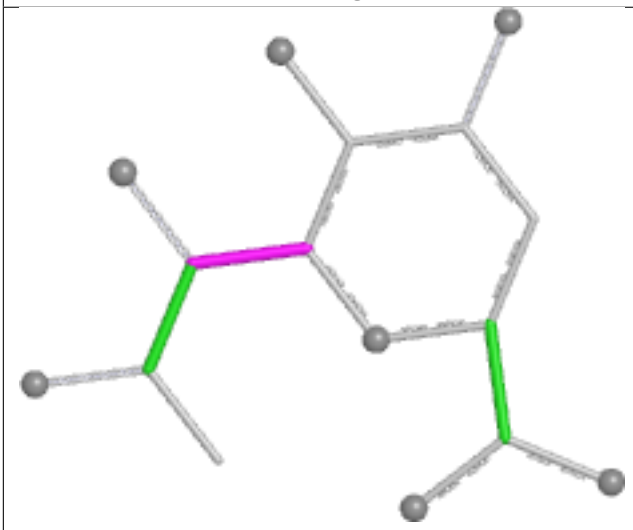
Ligand P8E L 615



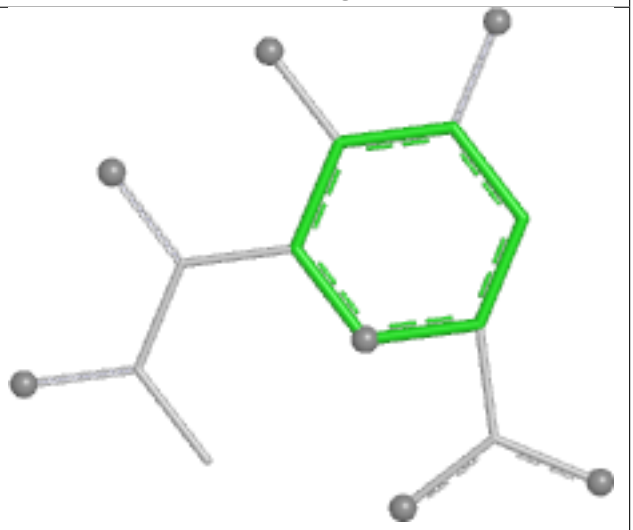
Bond lengths



Bond angles

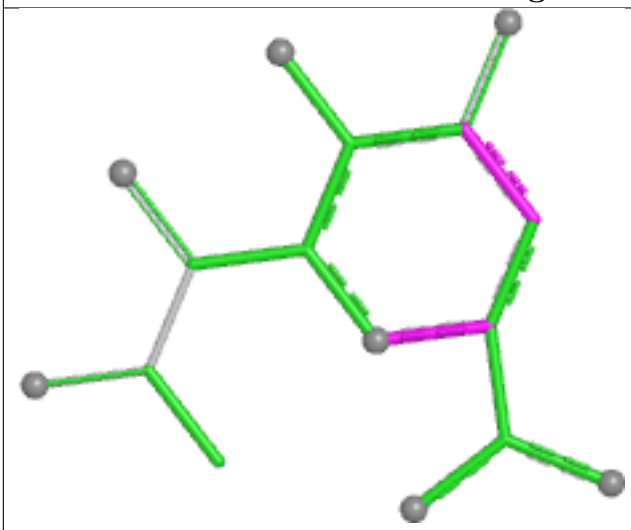


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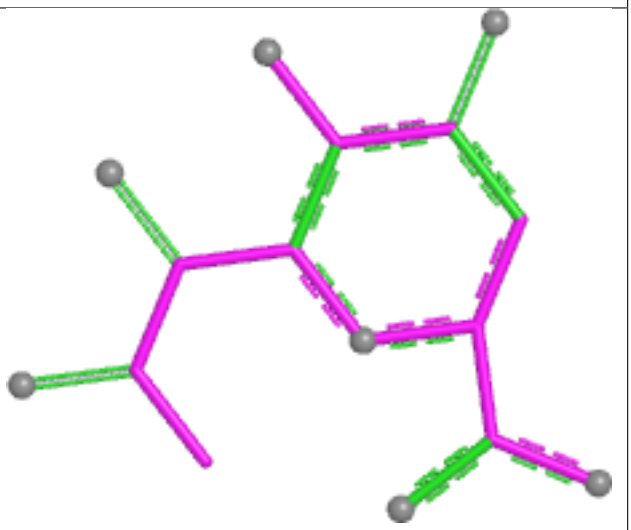


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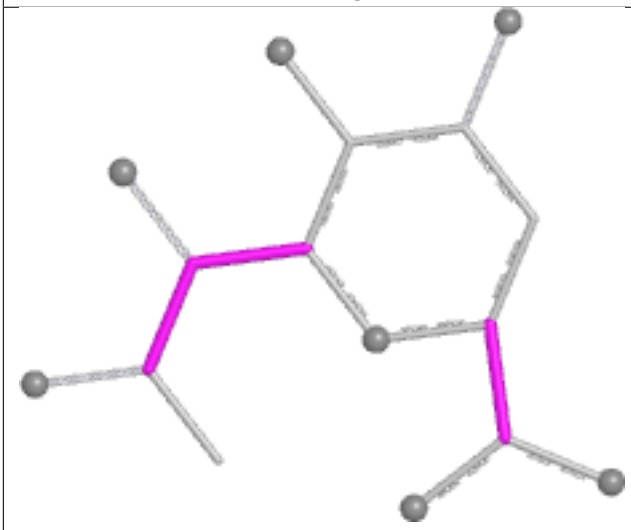
Ligand P8E A 616



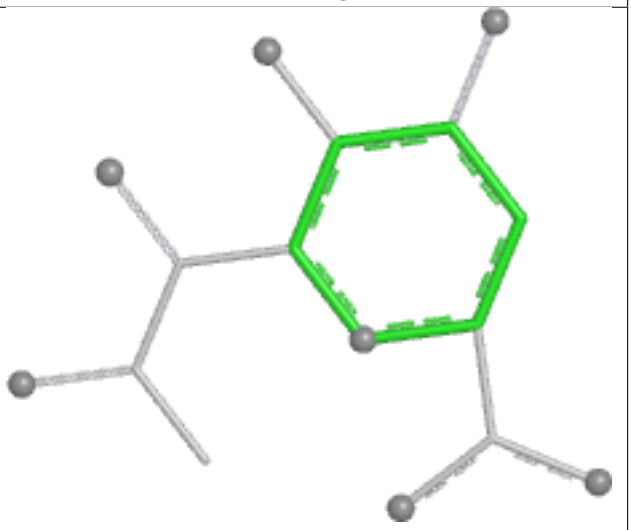
Bond lengths



Bond angles

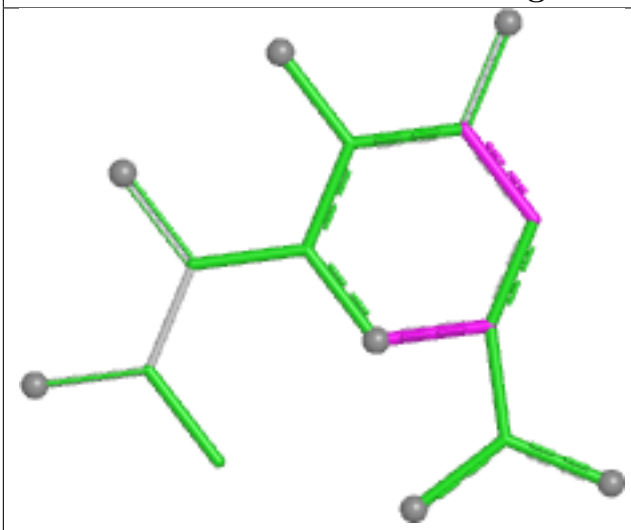


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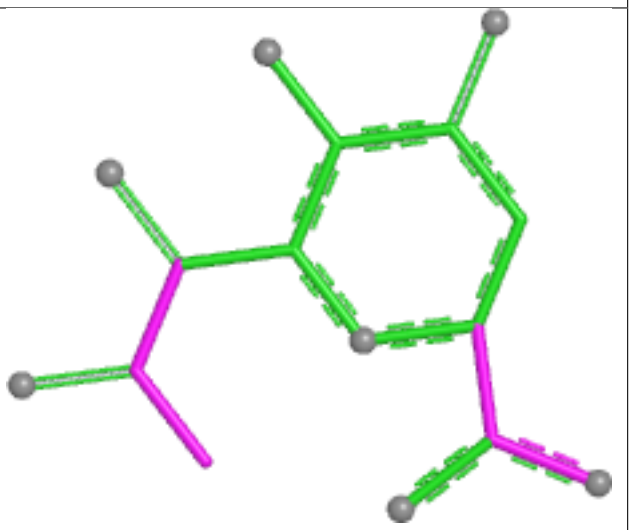


Rings

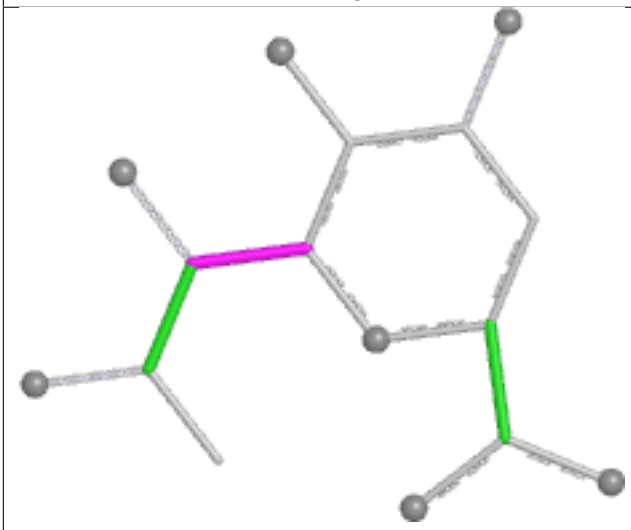
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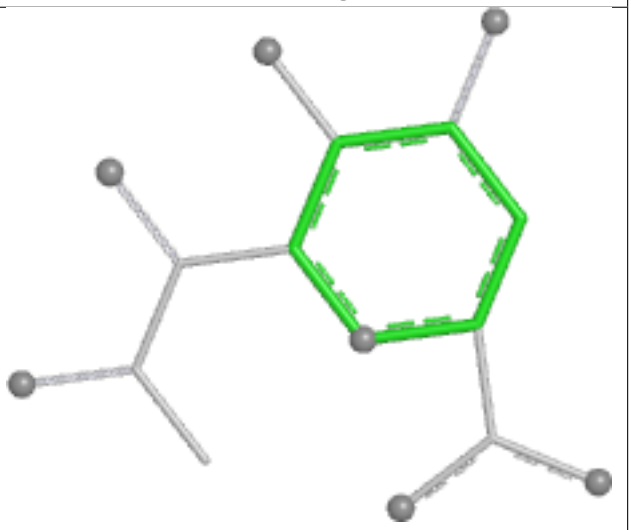
Bond lengths



Bond angles

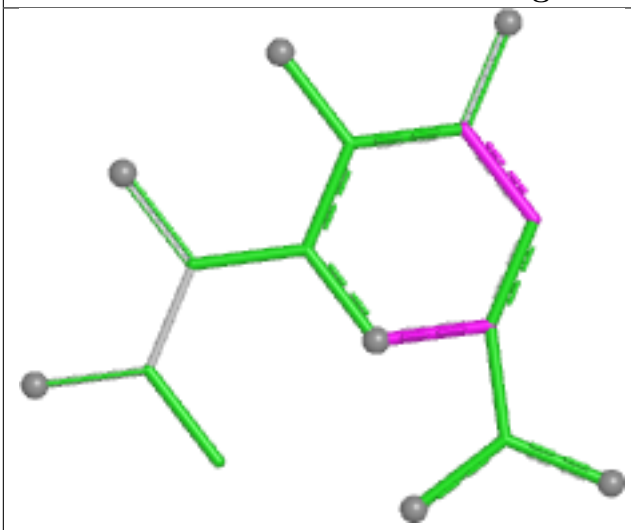


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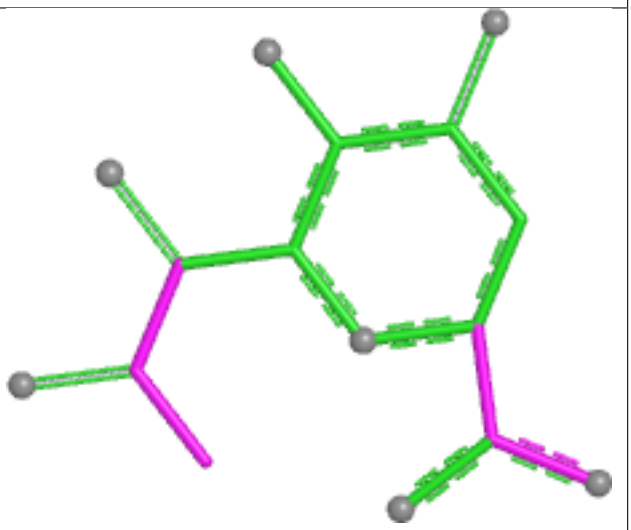


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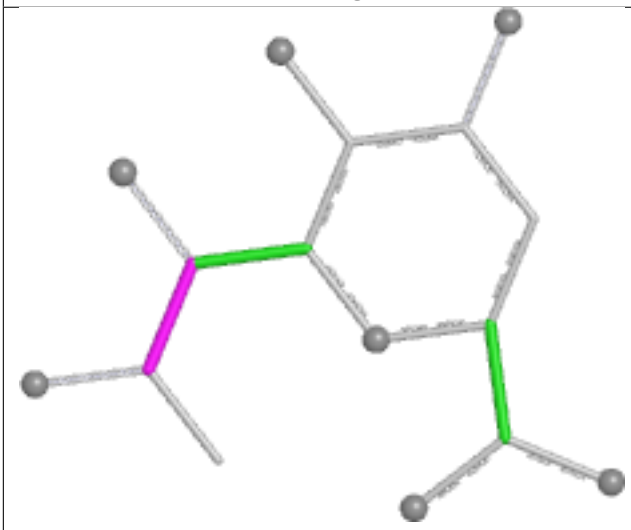
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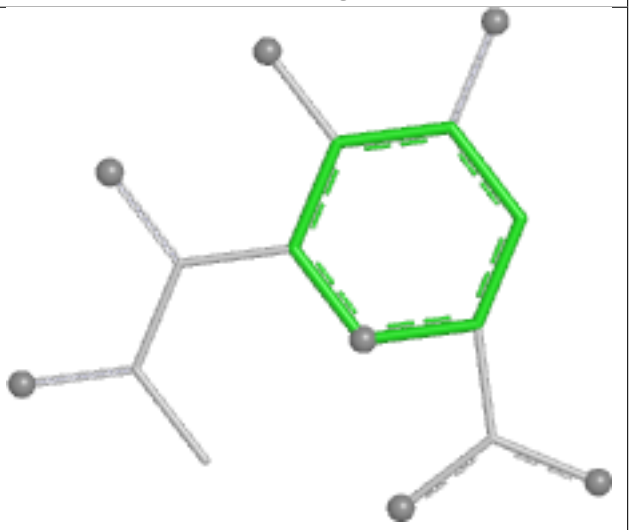
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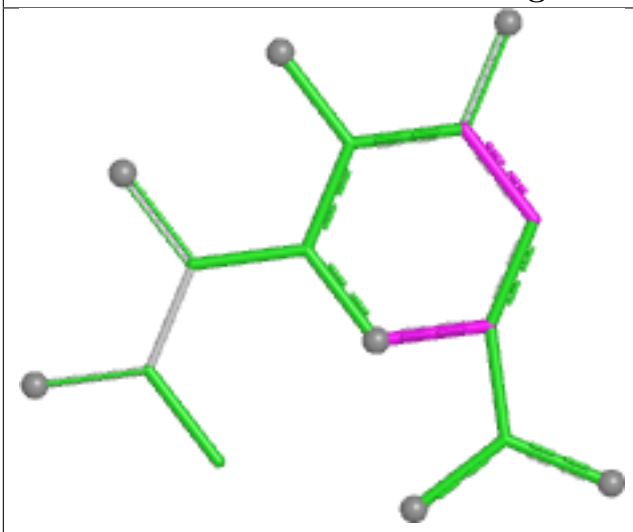


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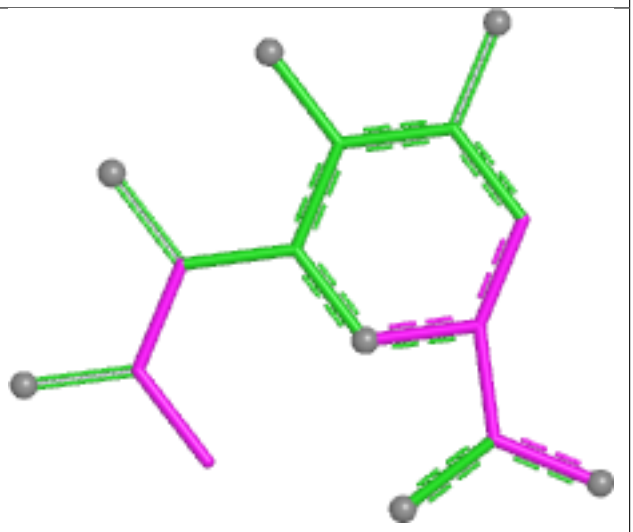


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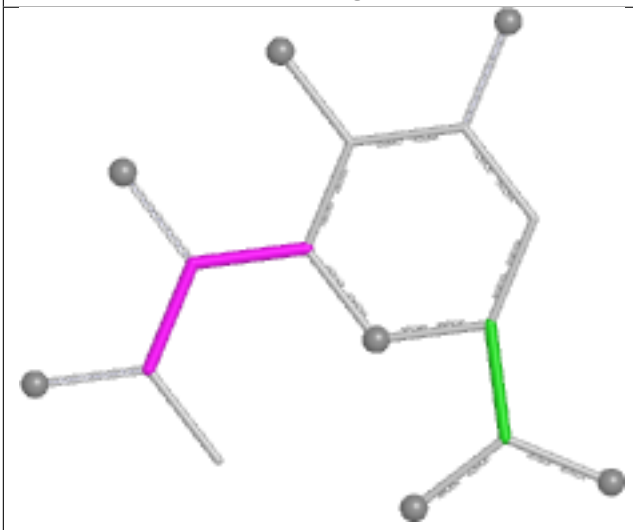
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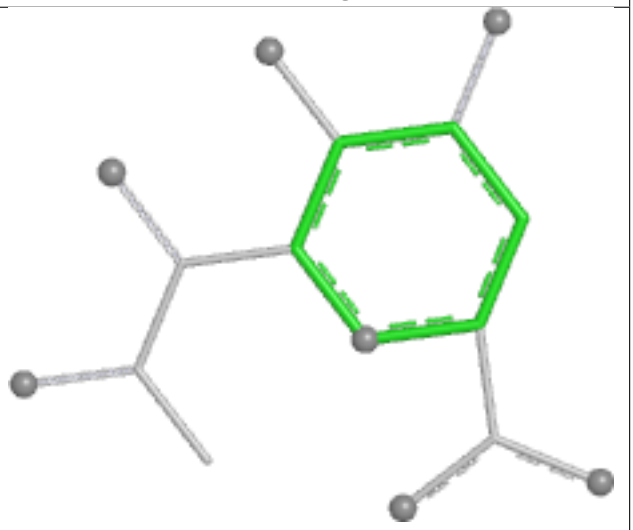
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Bond angles

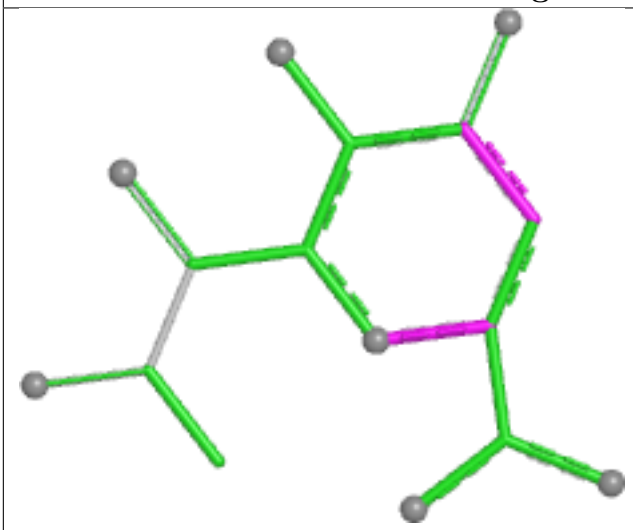


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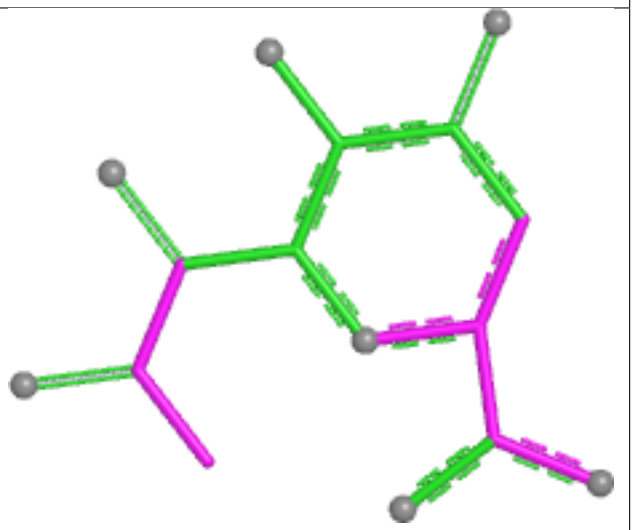


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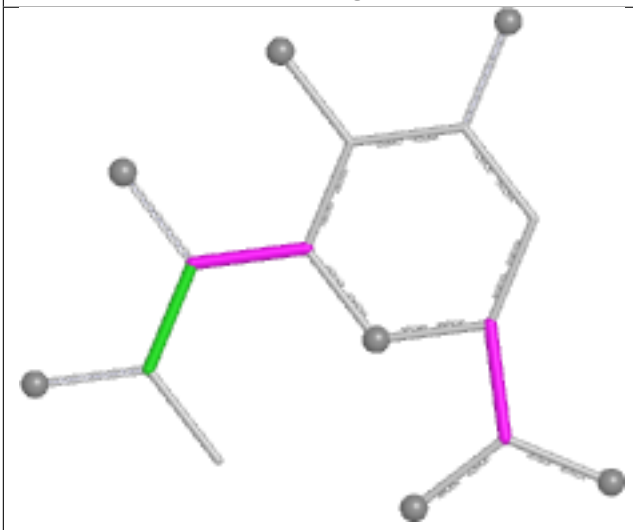
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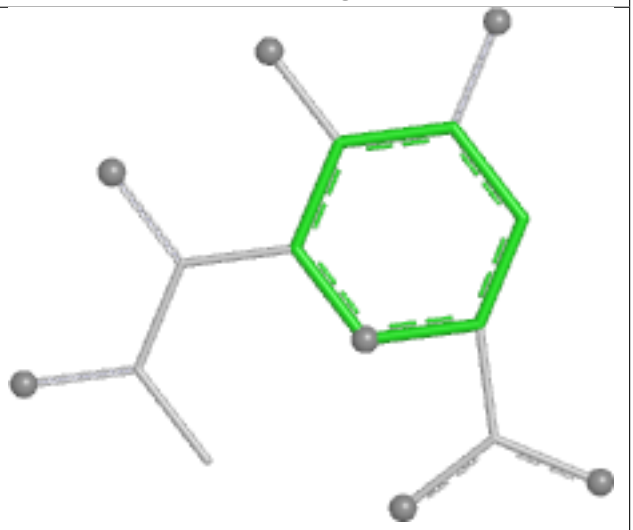
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Bond angles

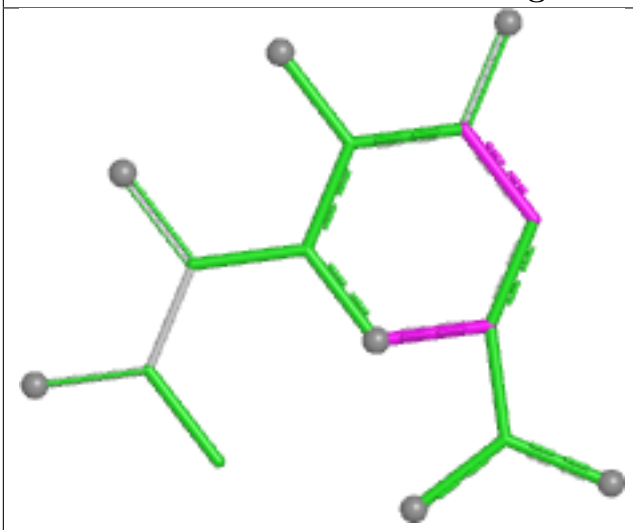


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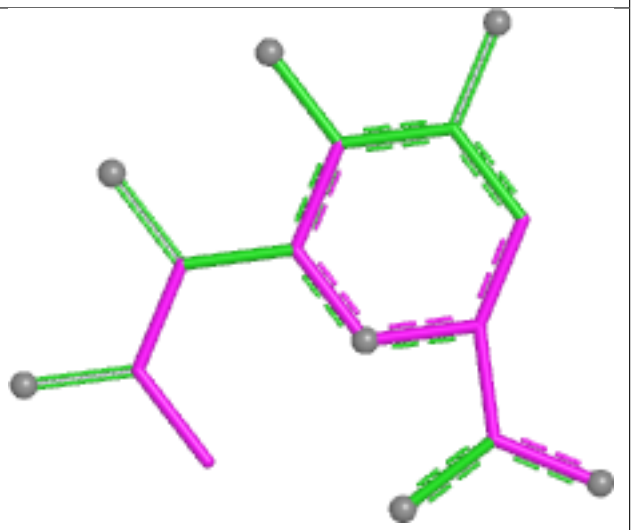


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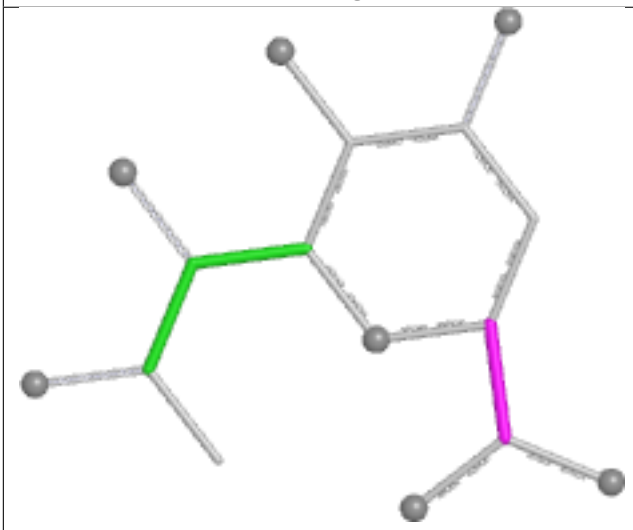
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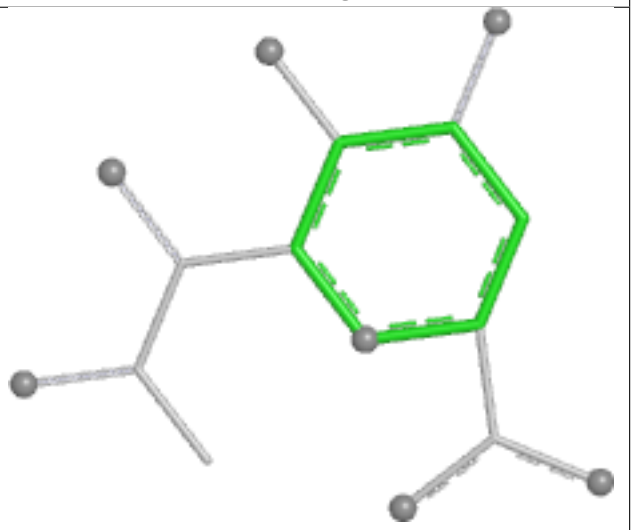
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Bond angles

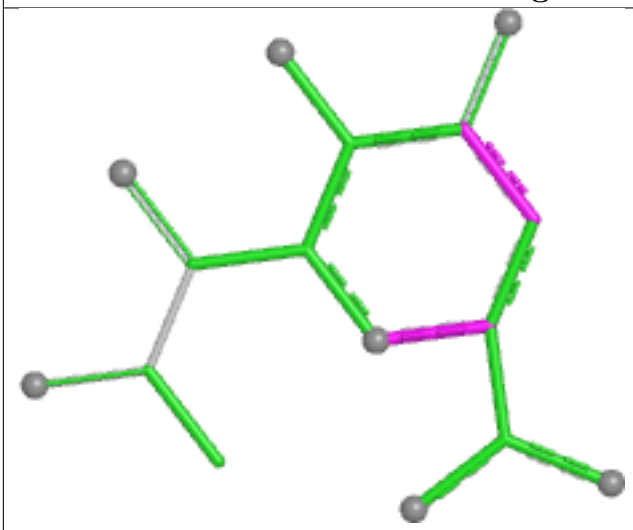


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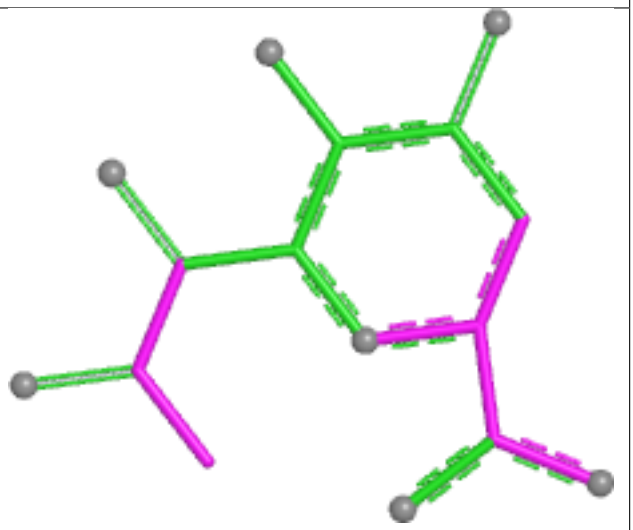


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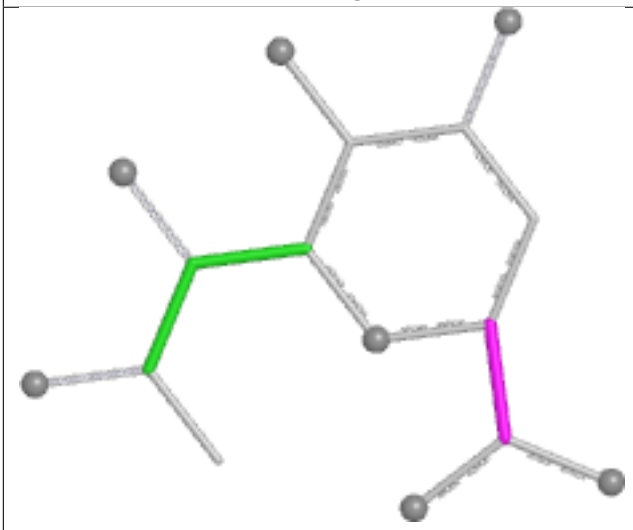
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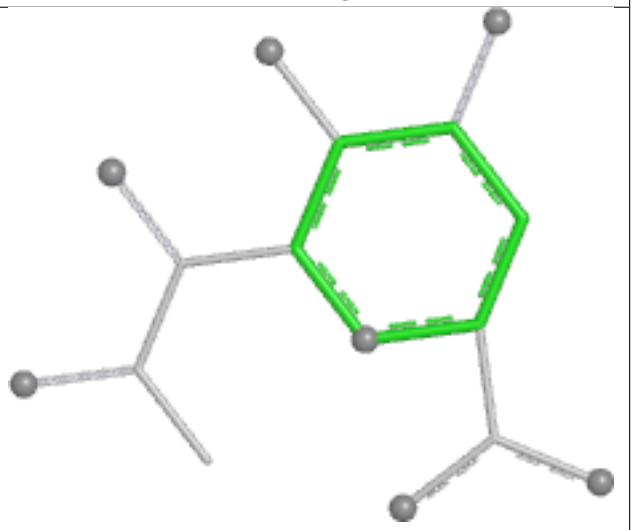
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Bond angles

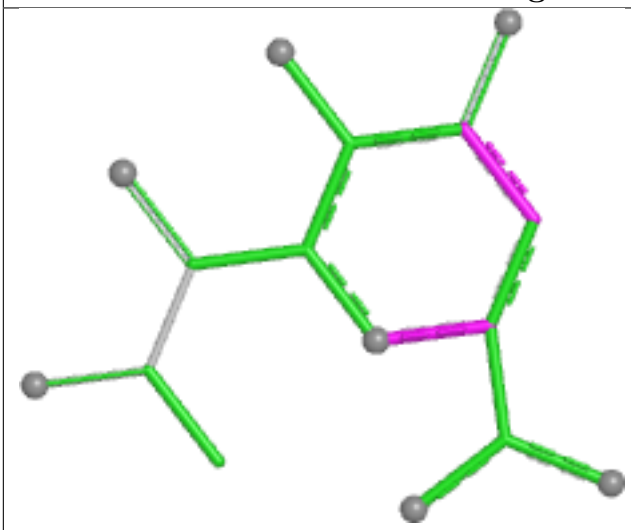


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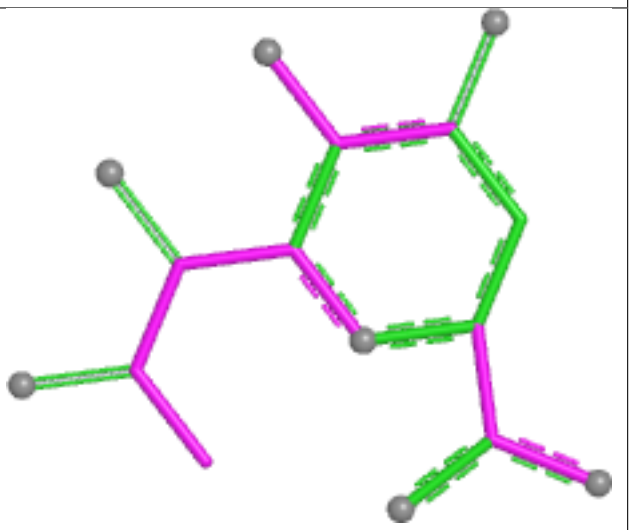


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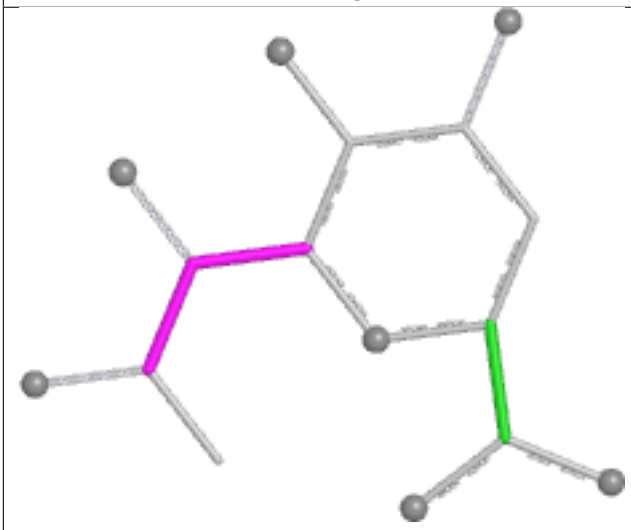
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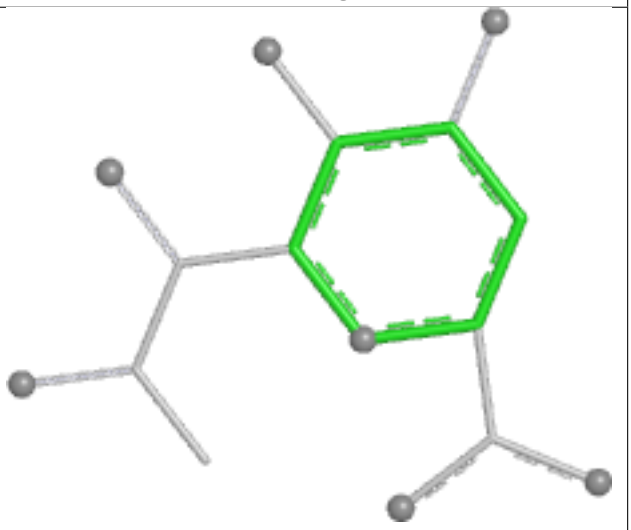
Bond lengths



Bond angles

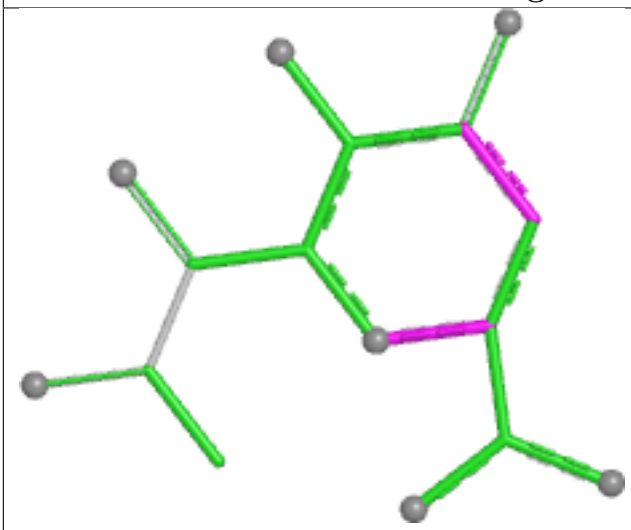


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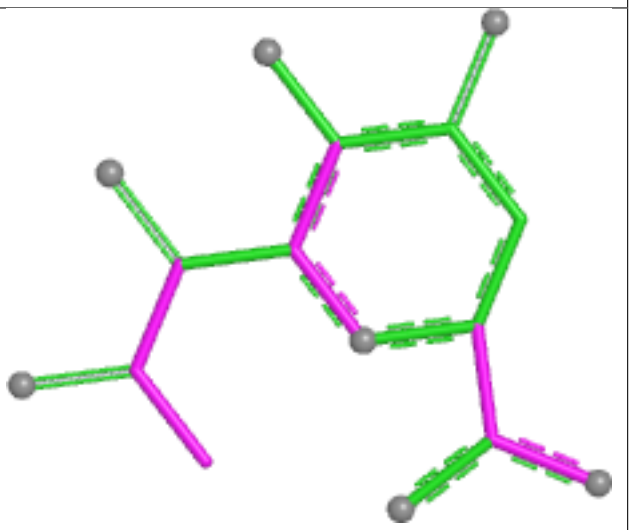


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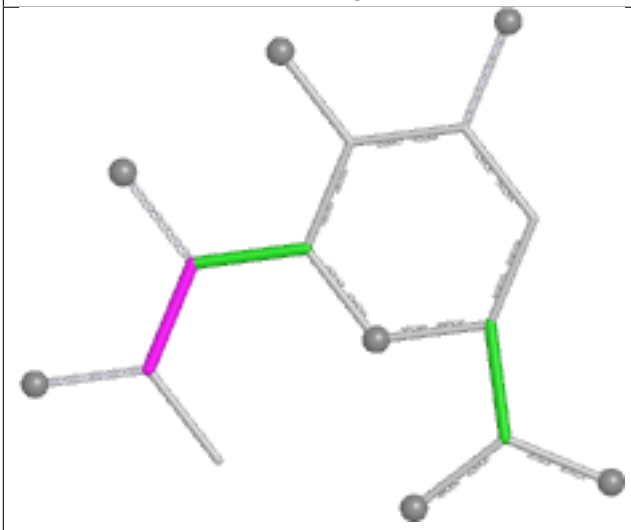
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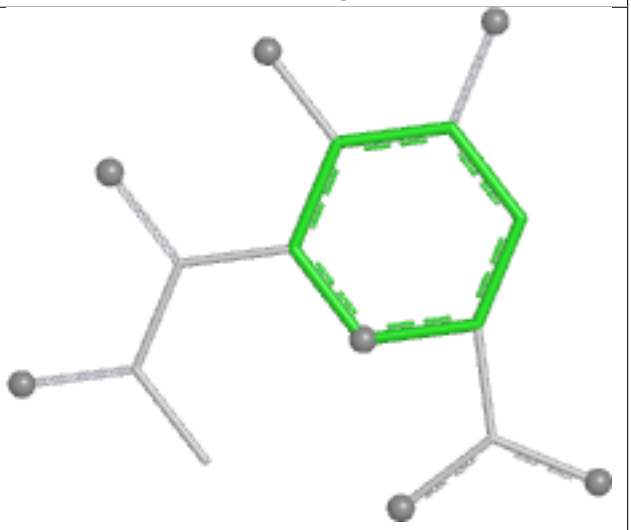
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Bond angles

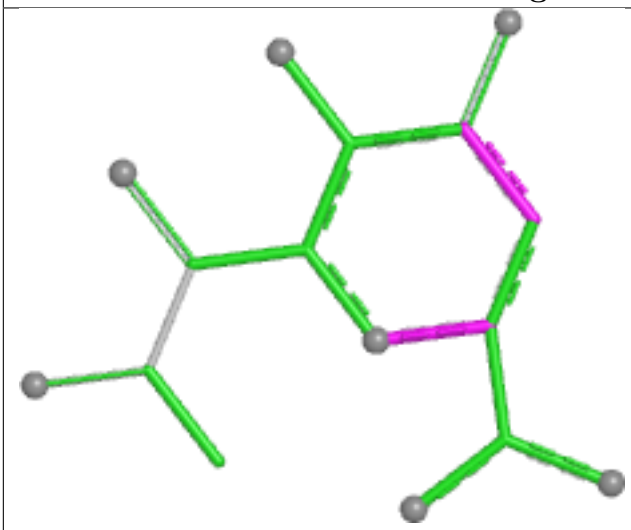


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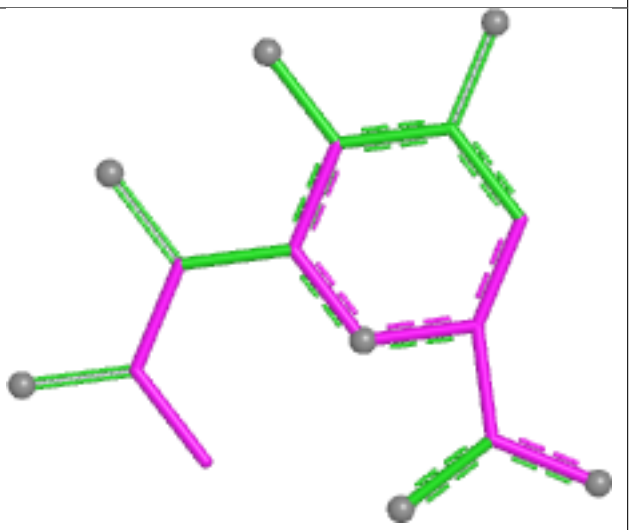


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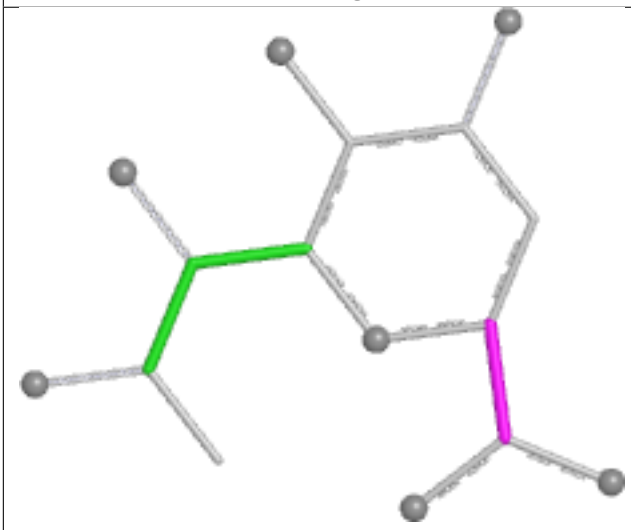
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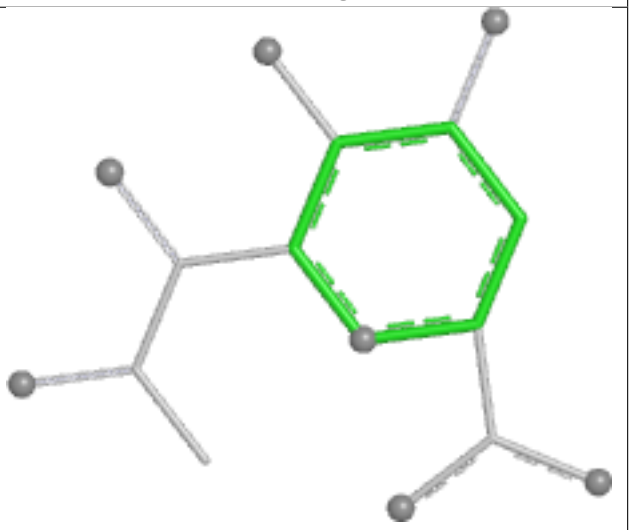
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Bond angles

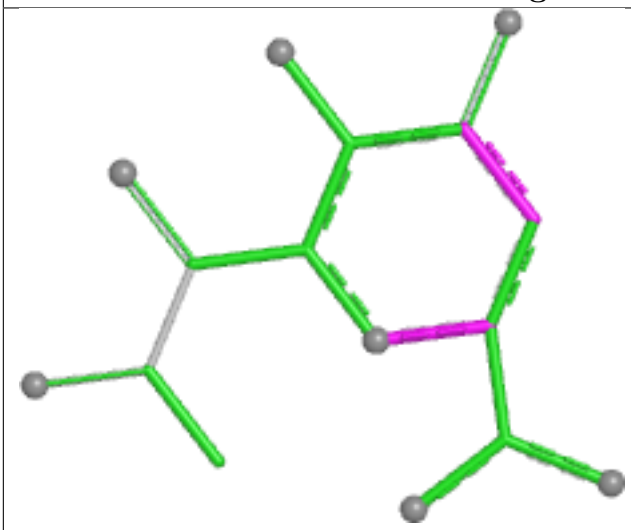


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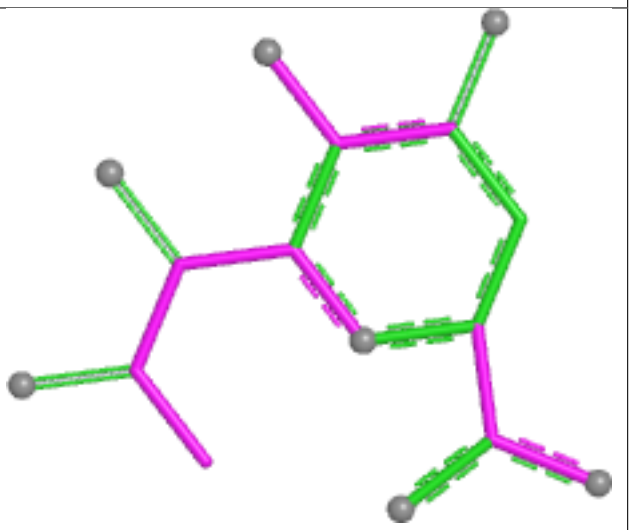


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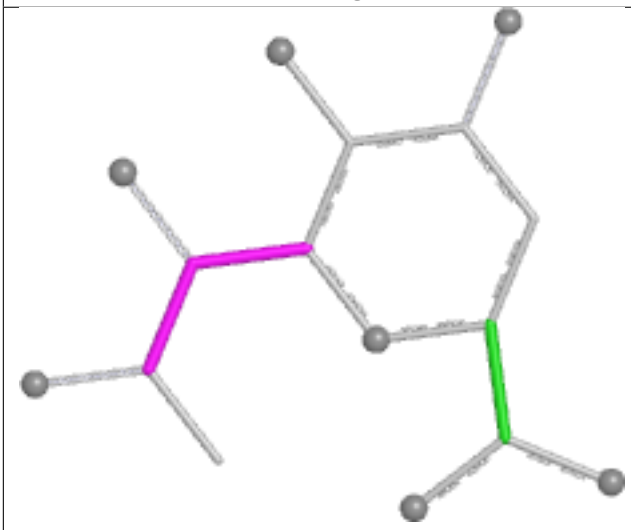
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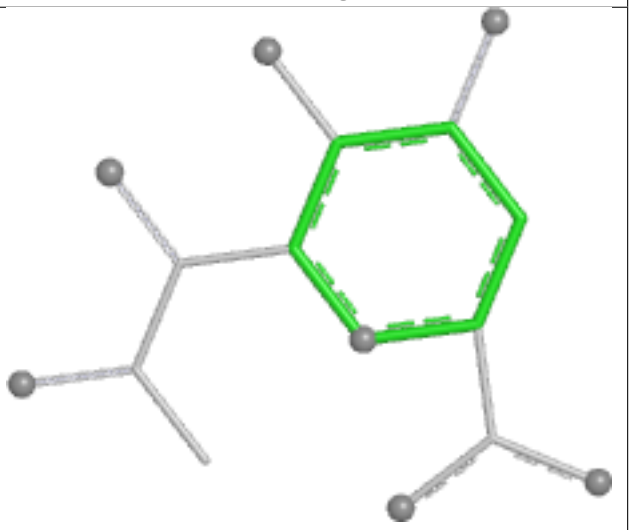
Bond lengths



Bond angles

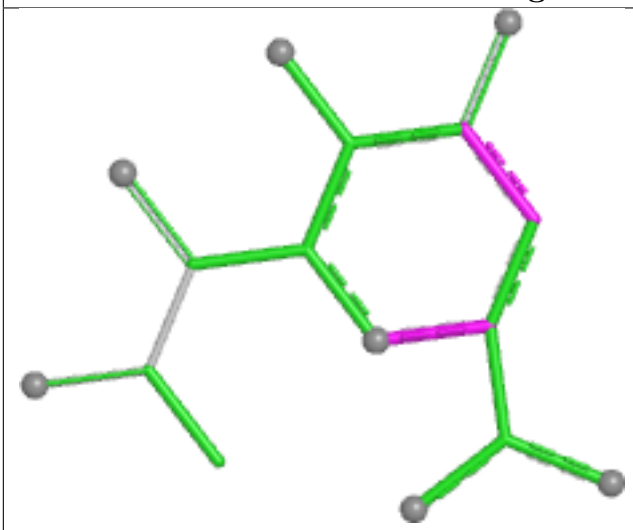


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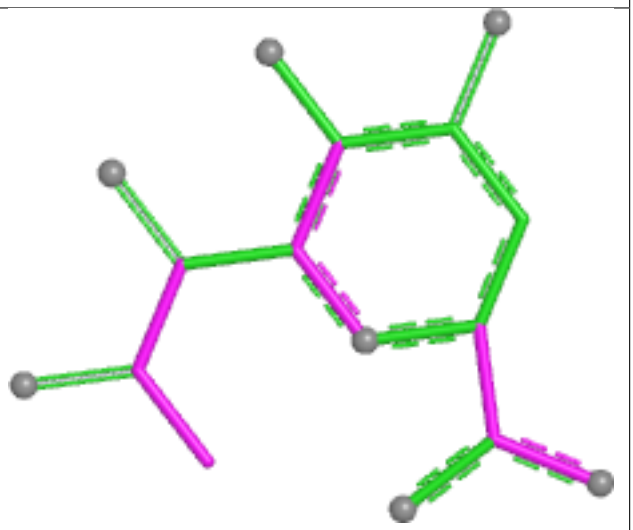


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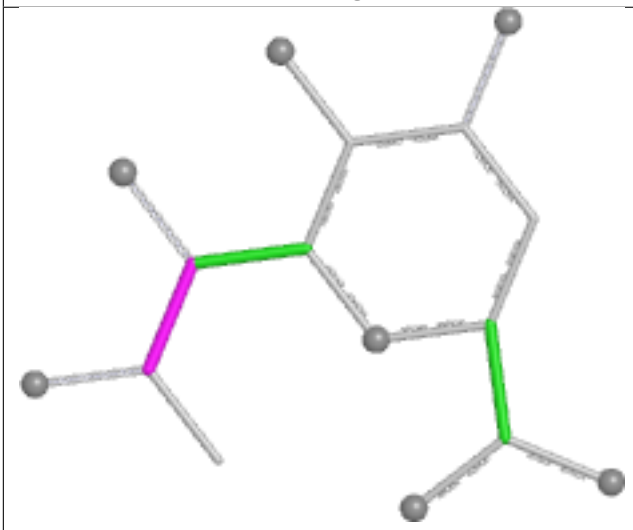
Ligand P8E V 602



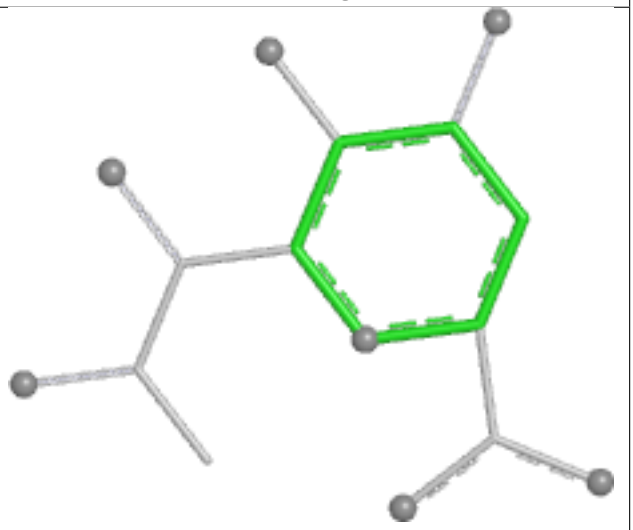
Bond lengths



Bond angles

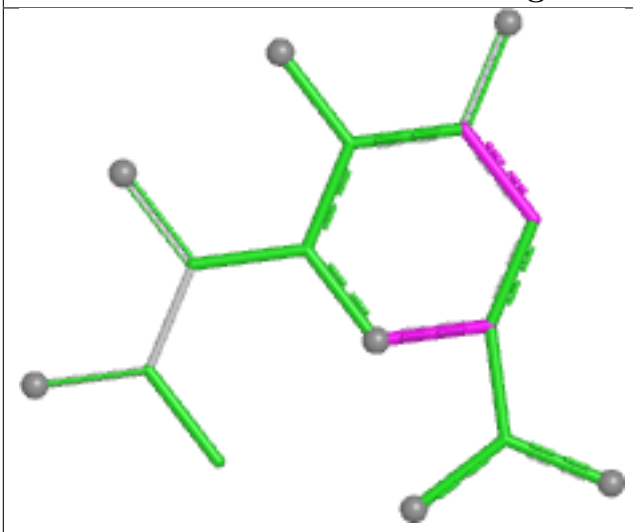


Torsions

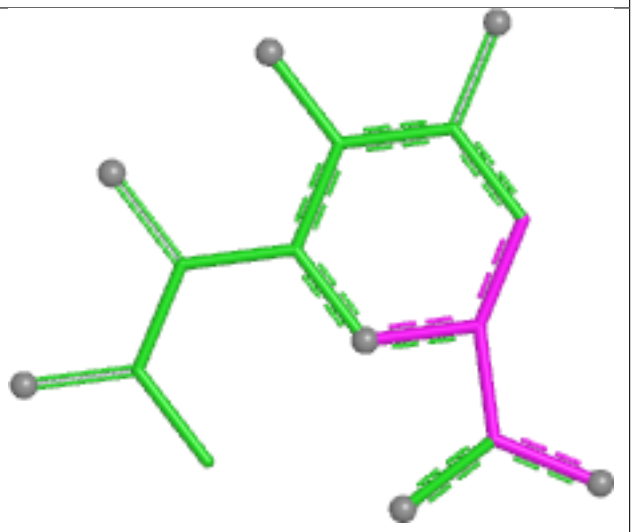


Rings

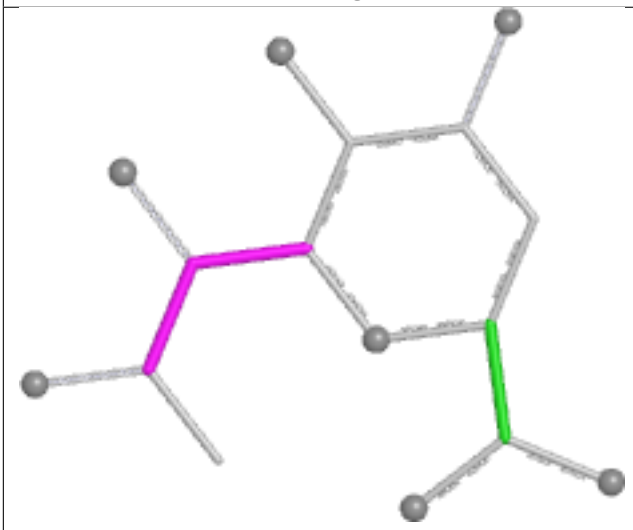
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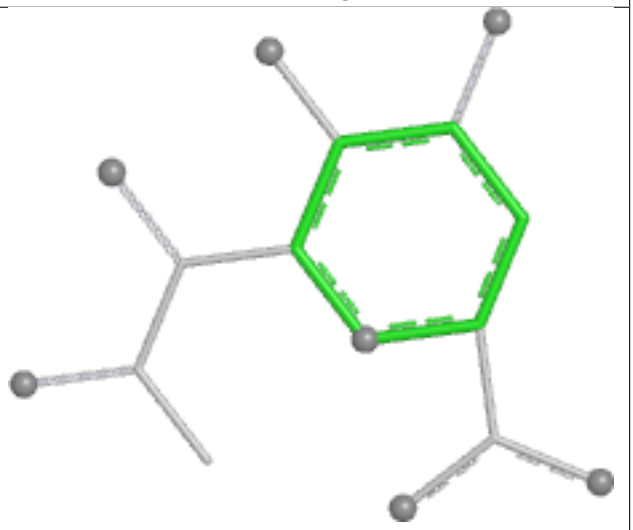
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Bond angles

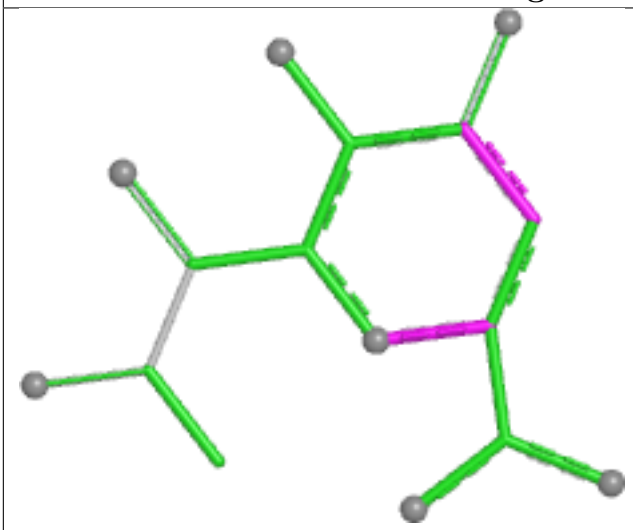


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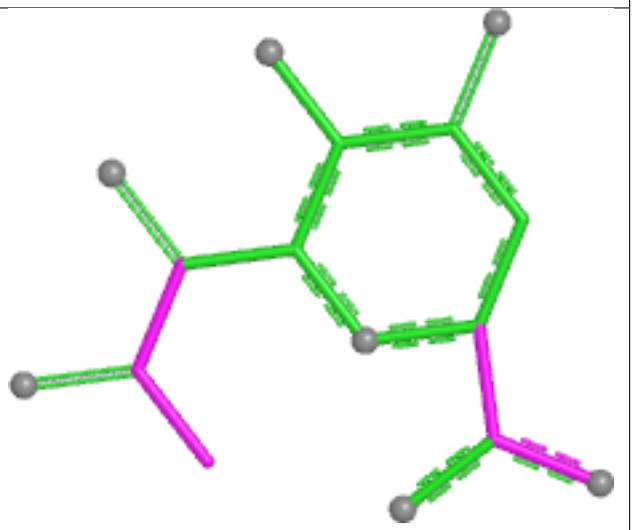


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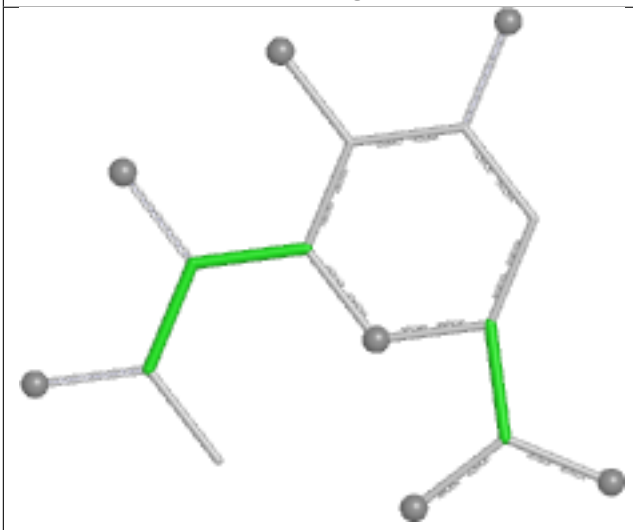
Ligand P8E N 613



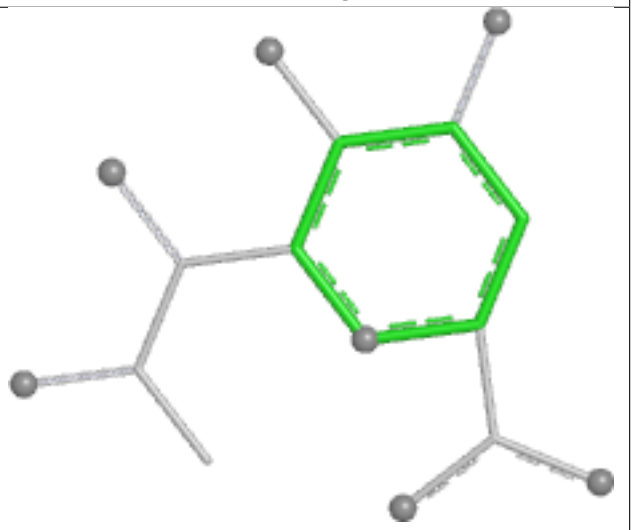
Bond lengths



Bond angles

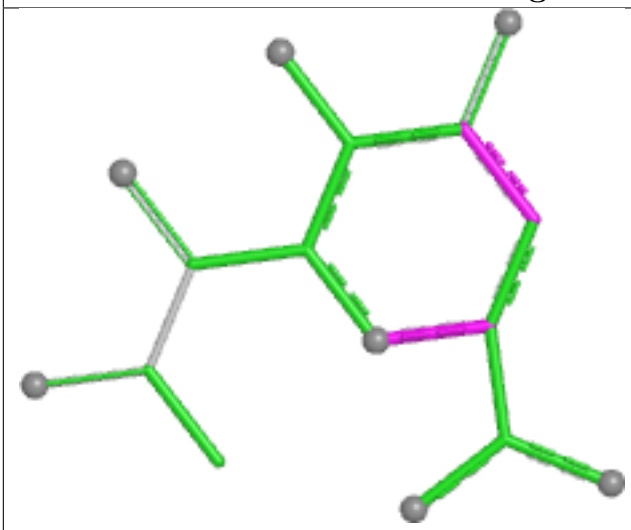


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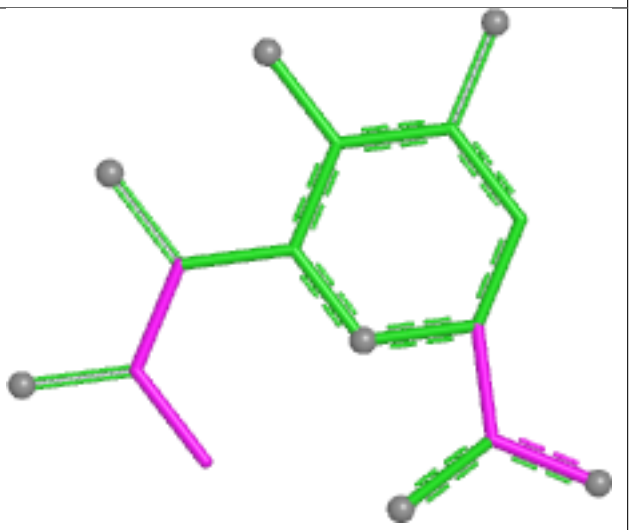


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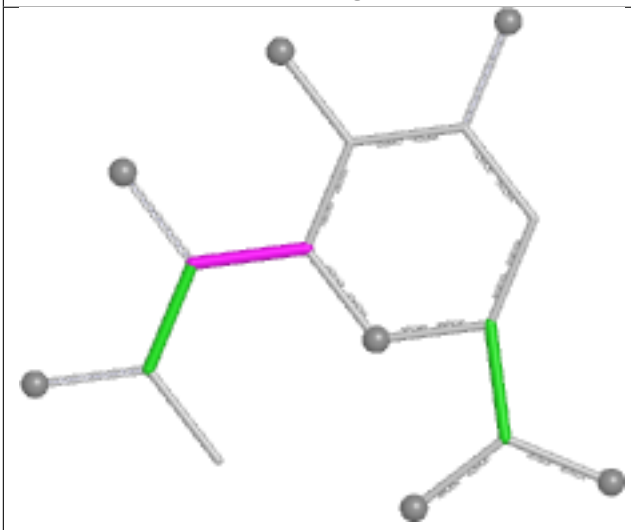
Ligand P8E T 615



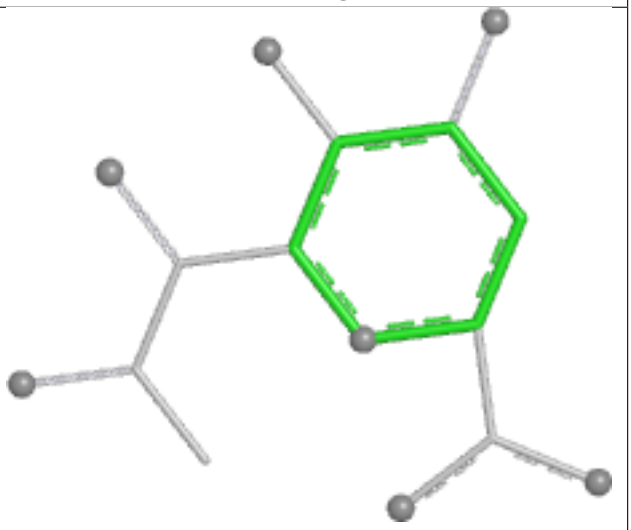
Bond lengths



Bond angles

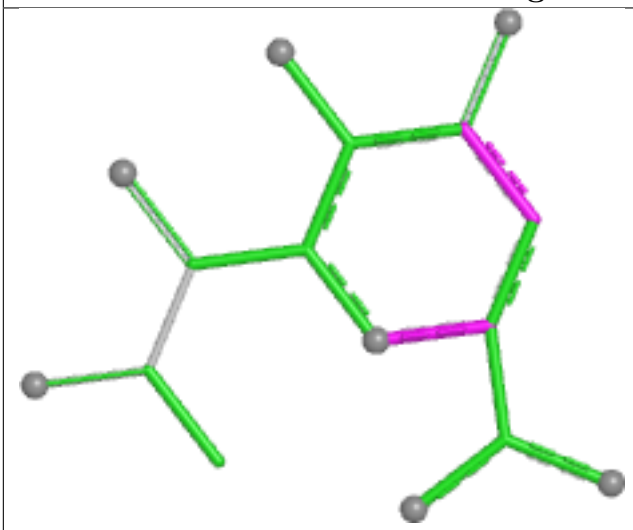


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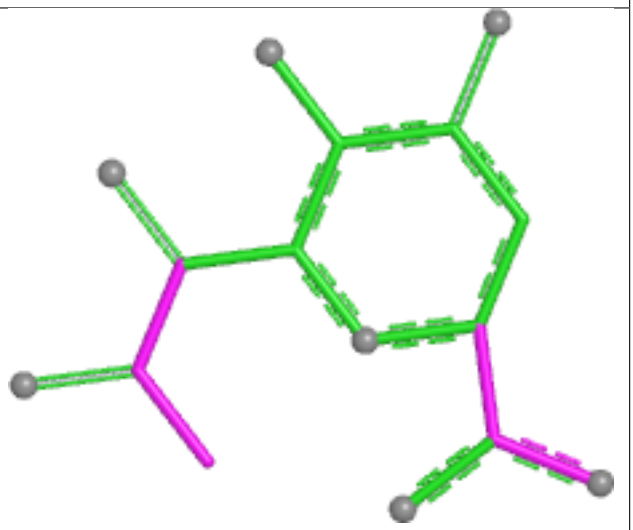


Rings

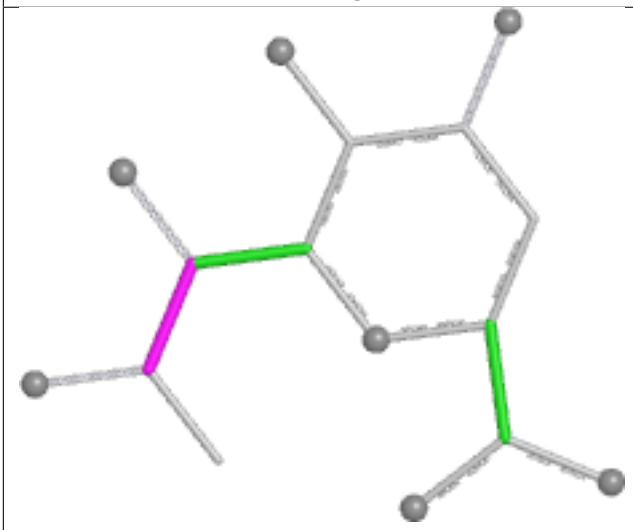
Ligand P8E K 610



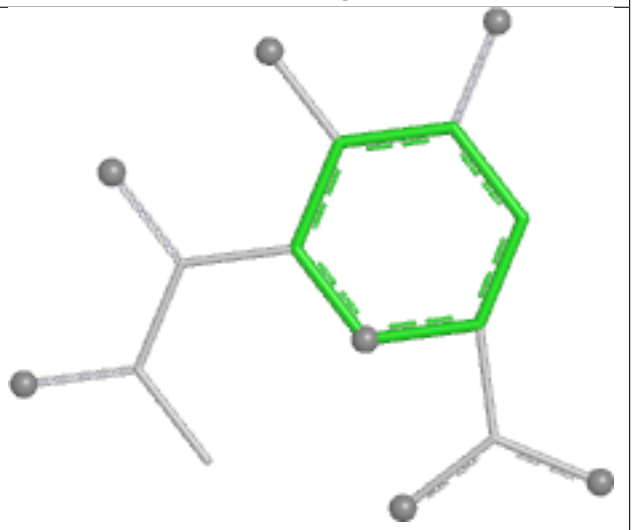
Bond lengths



Bond angles

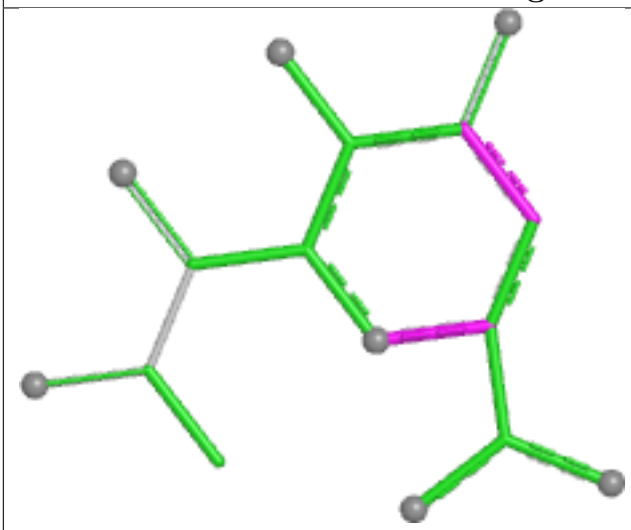


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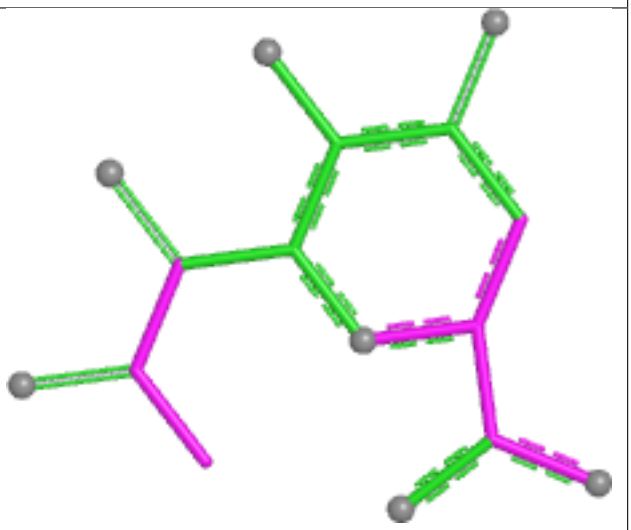


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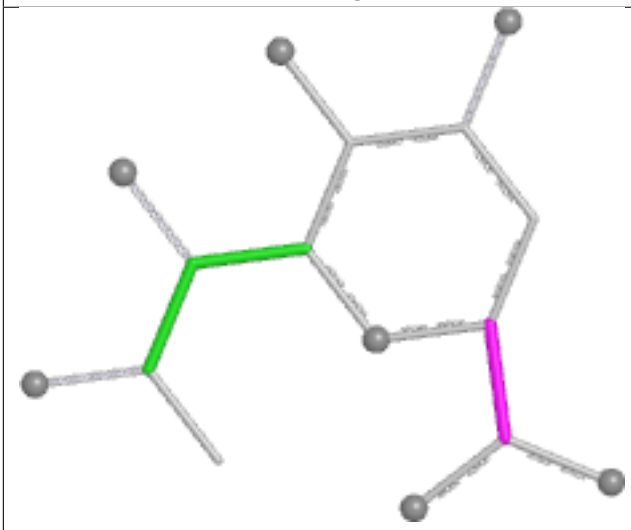
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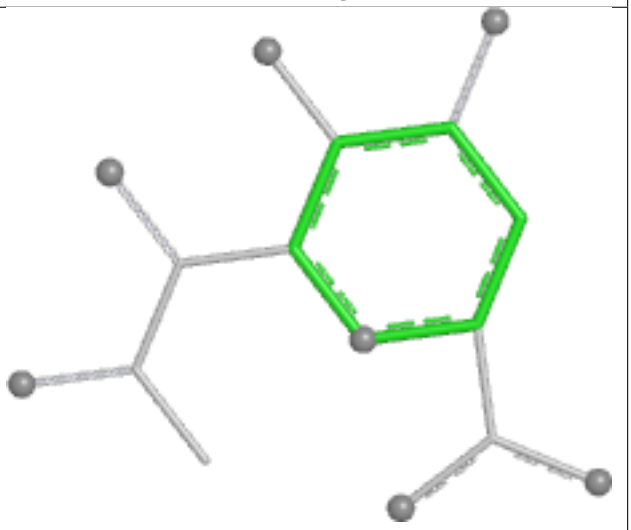
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Bond angles

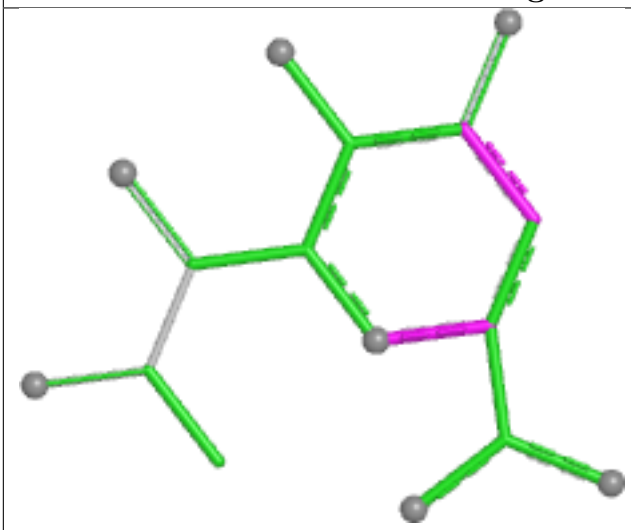


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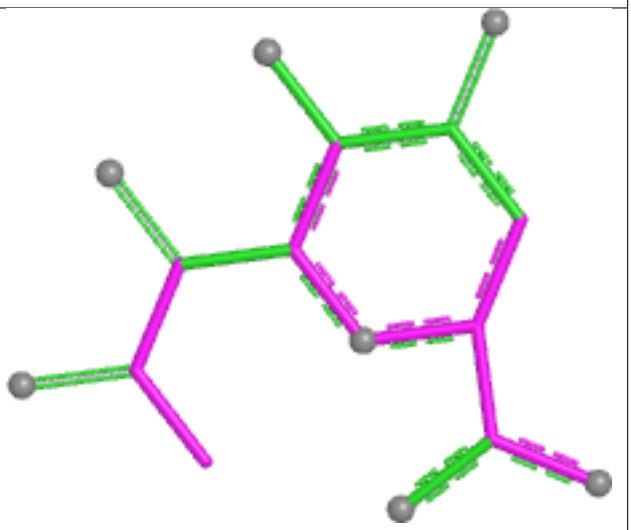


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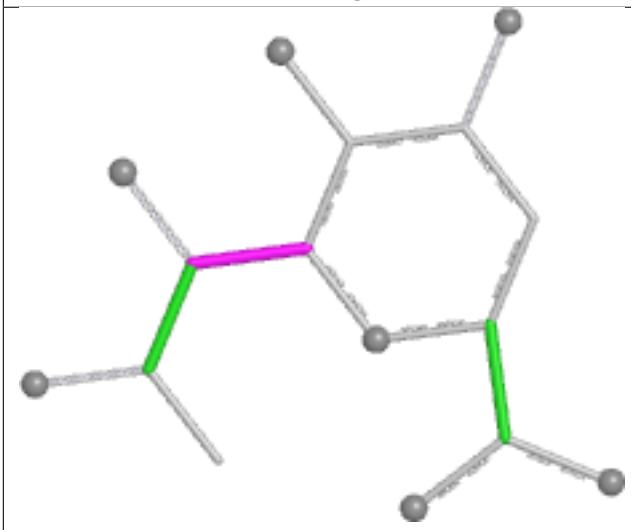
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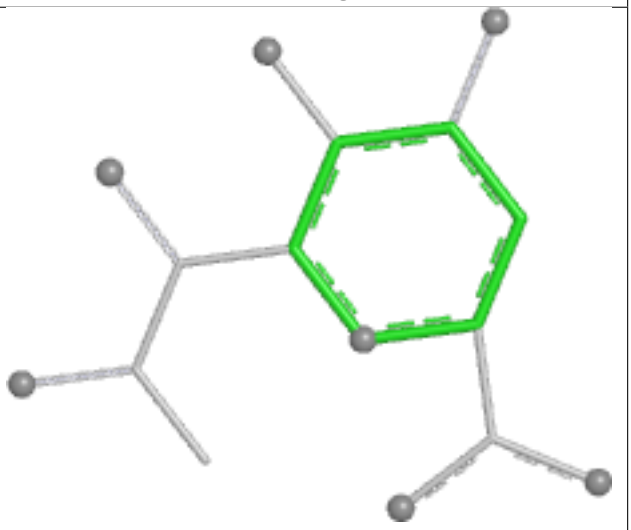
Bond lengths



Bond angles

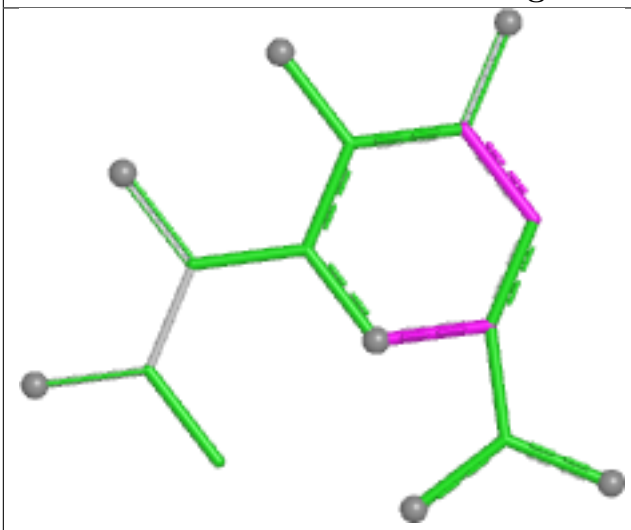


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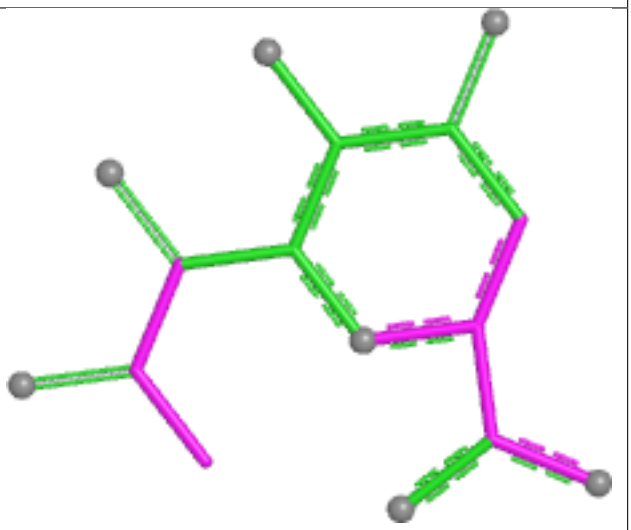


Rings

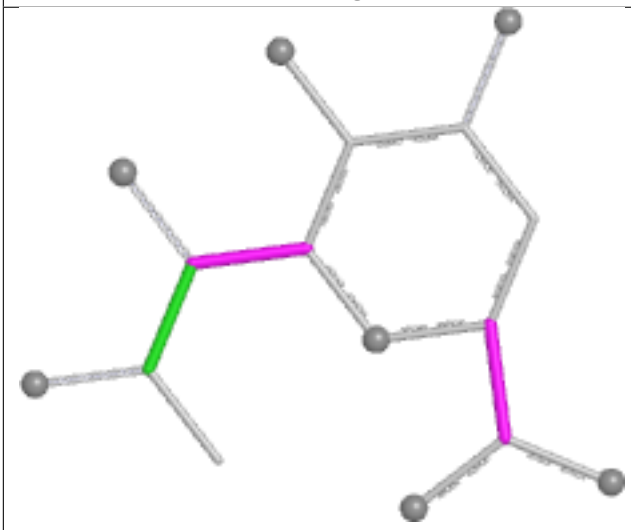
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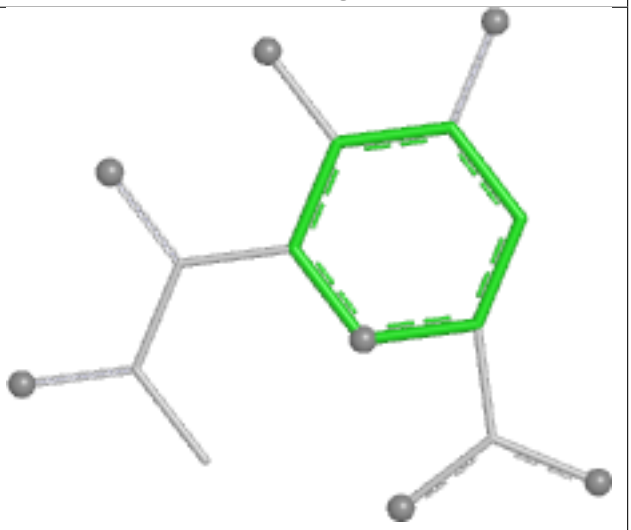
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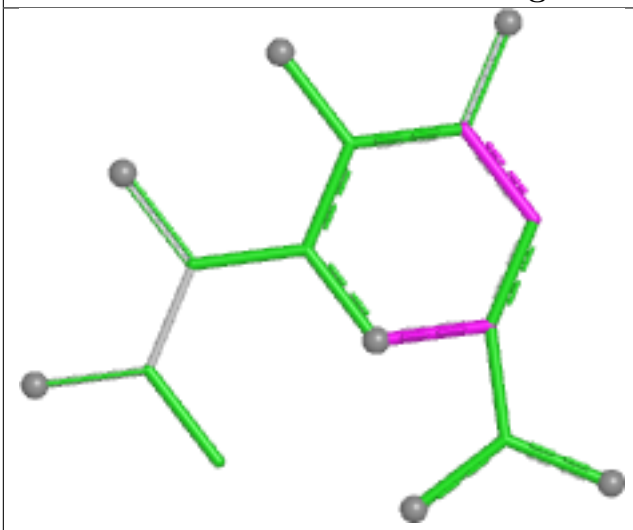


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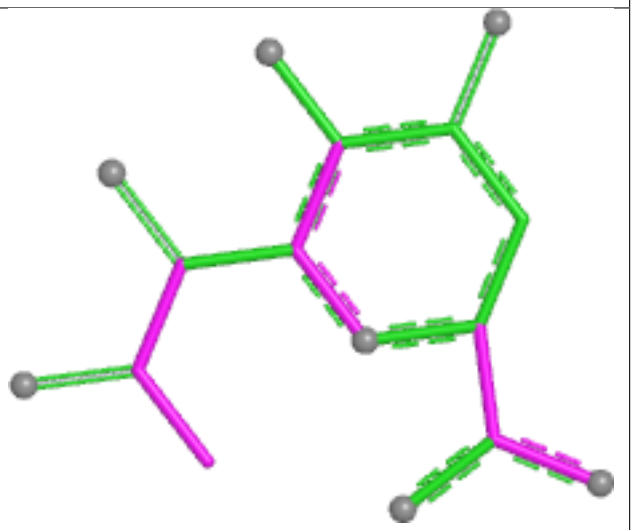


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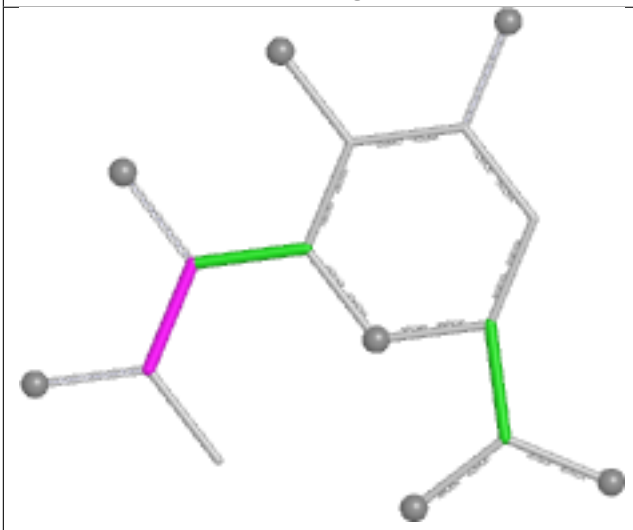
Ligand P8E C 610



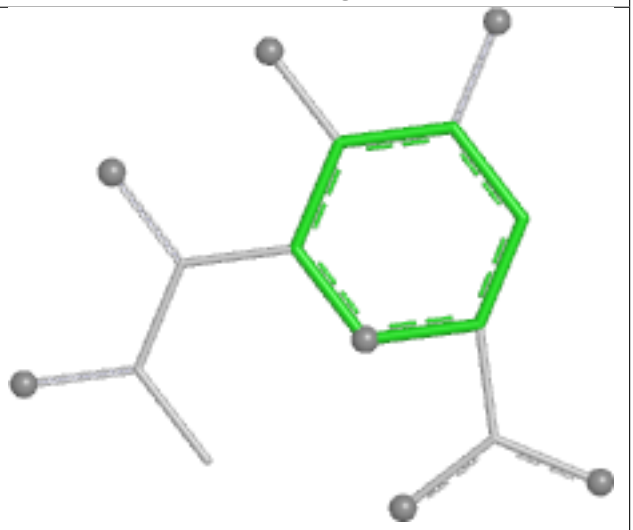
Bond lengths



Bond angles

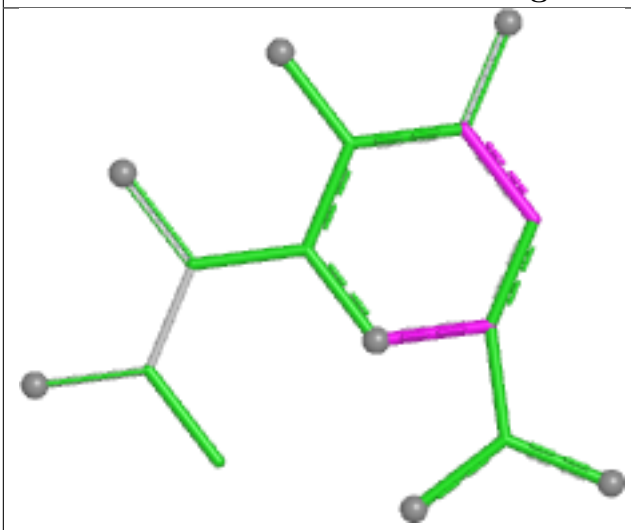


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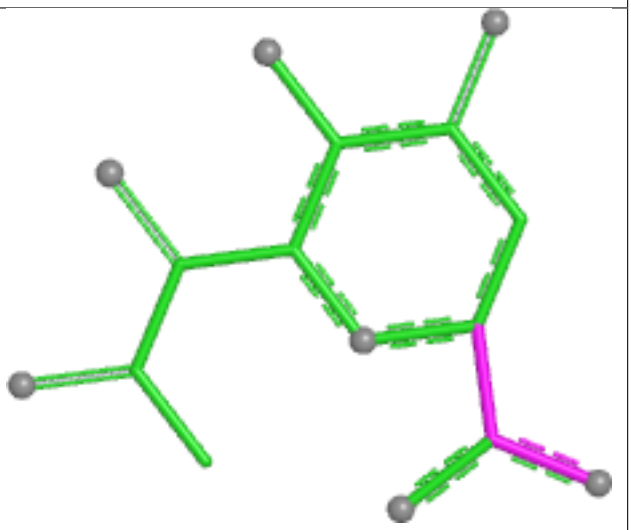


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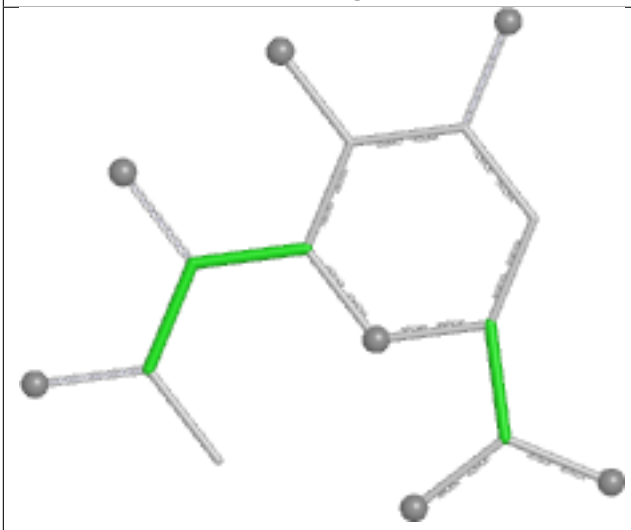
Ligand P8E F 613



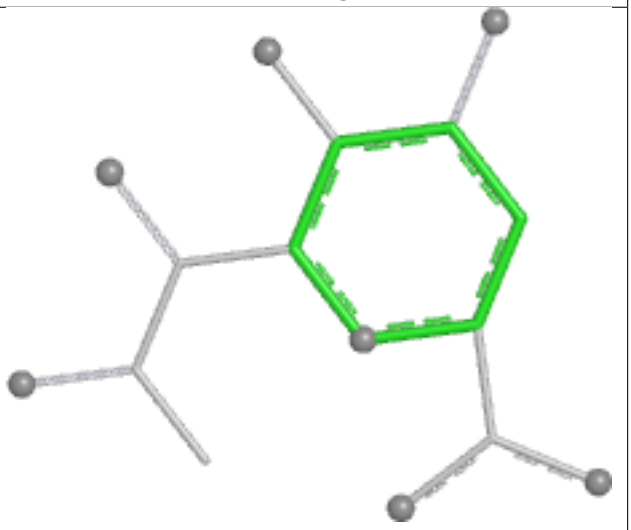
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Bond angles

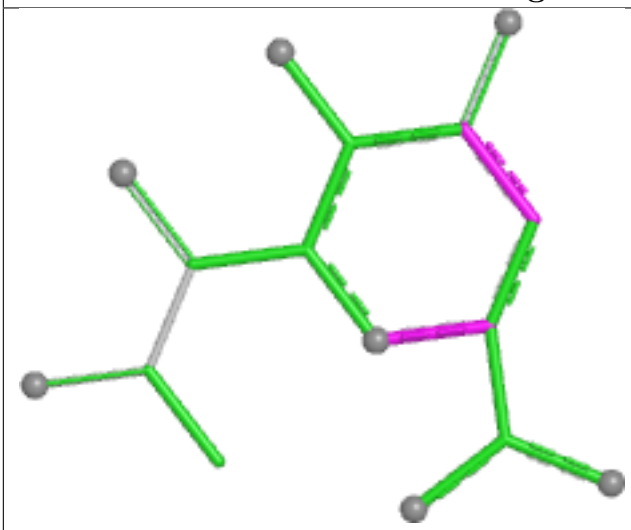


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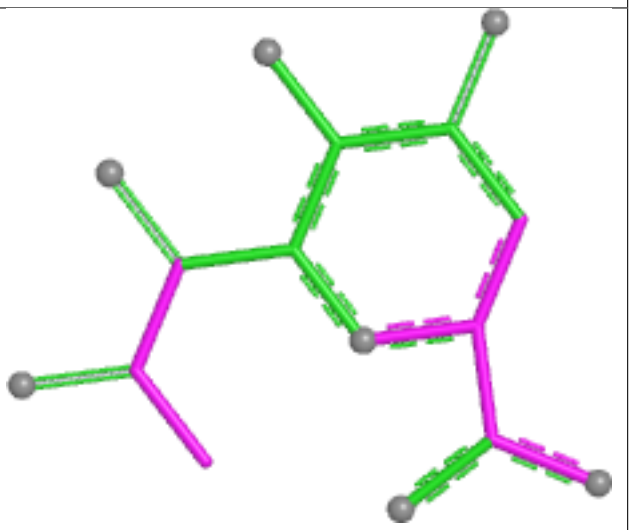


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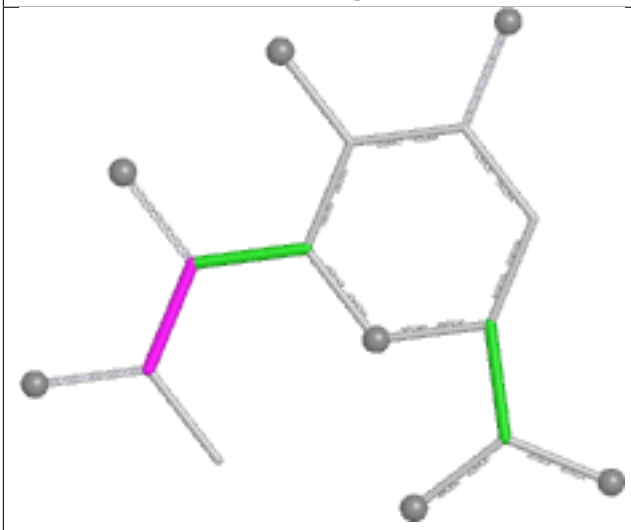
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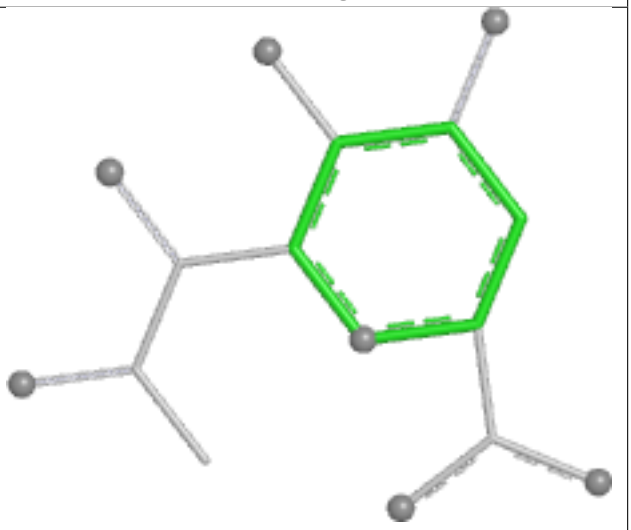
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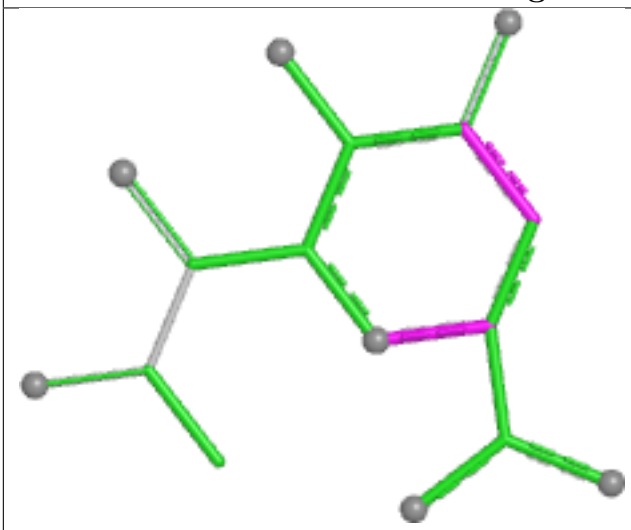


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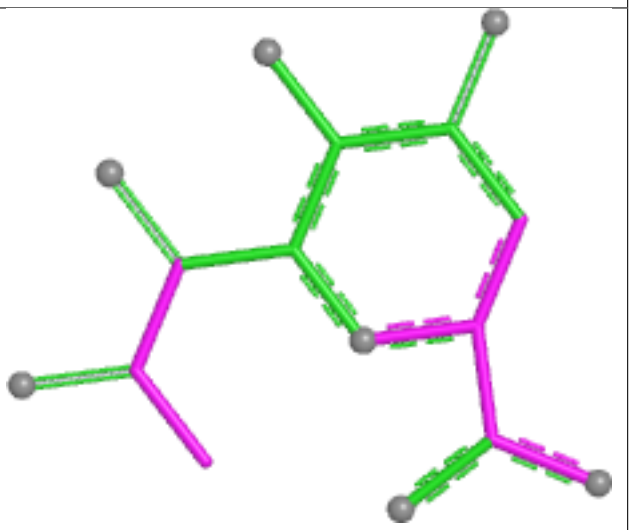


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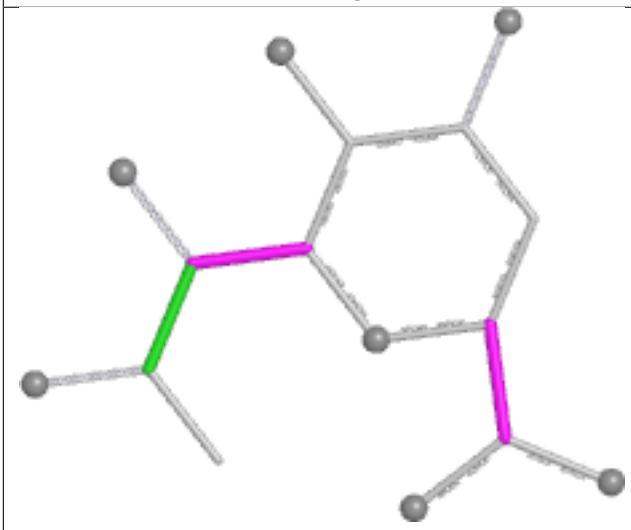
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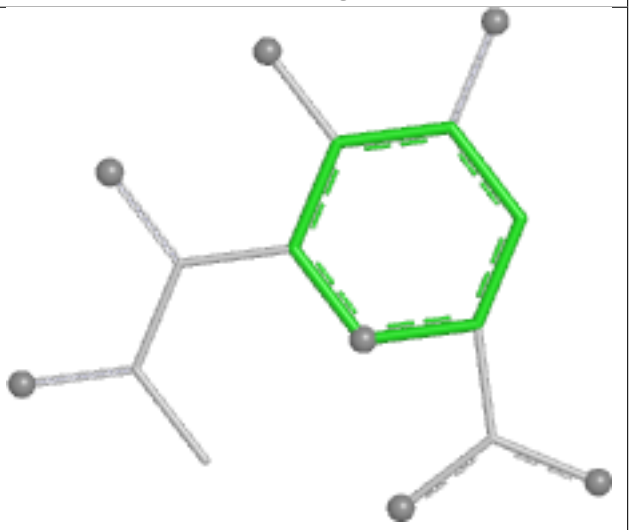
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Bond angles

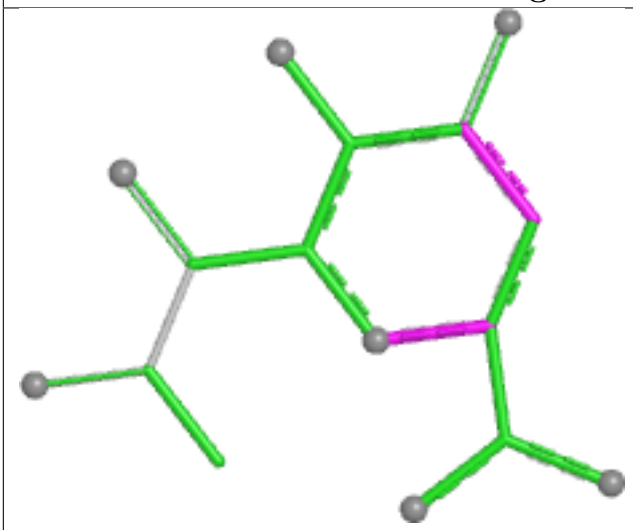


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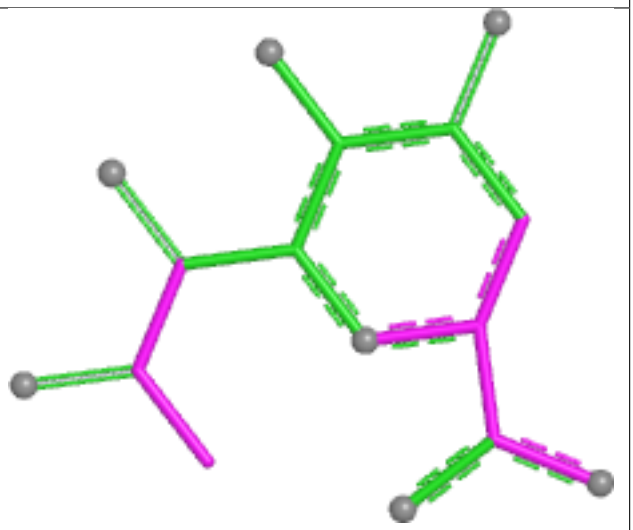


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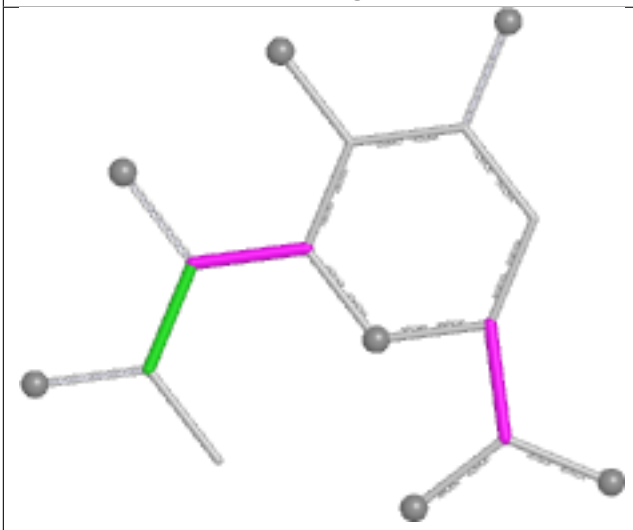
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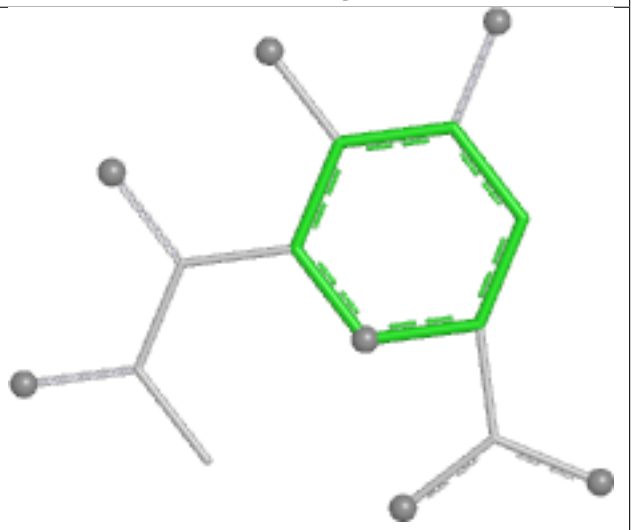
Bond lengths



Bond angles

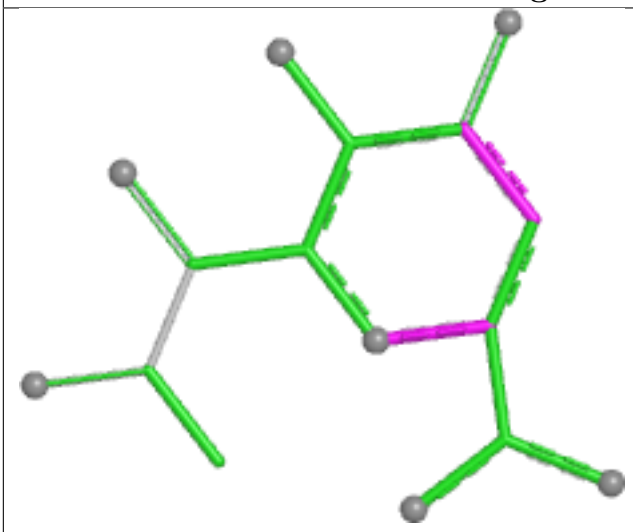


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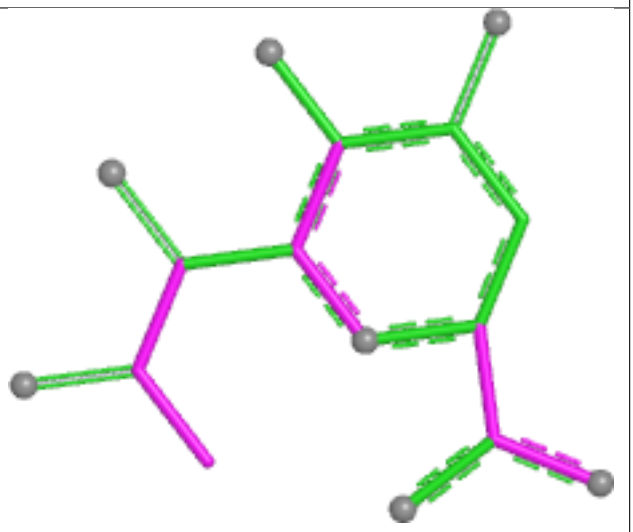


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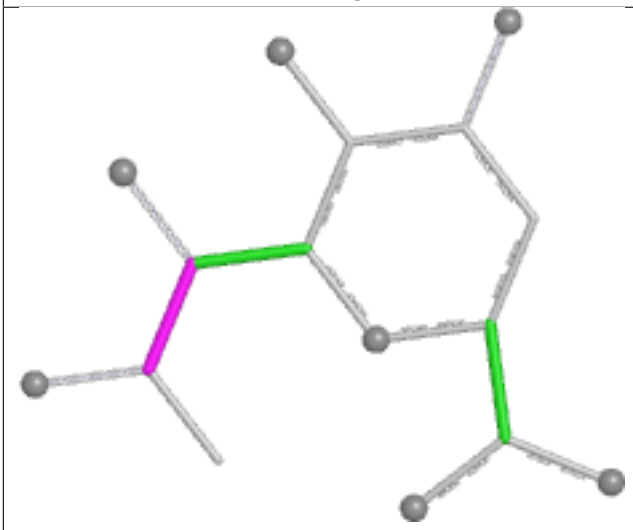
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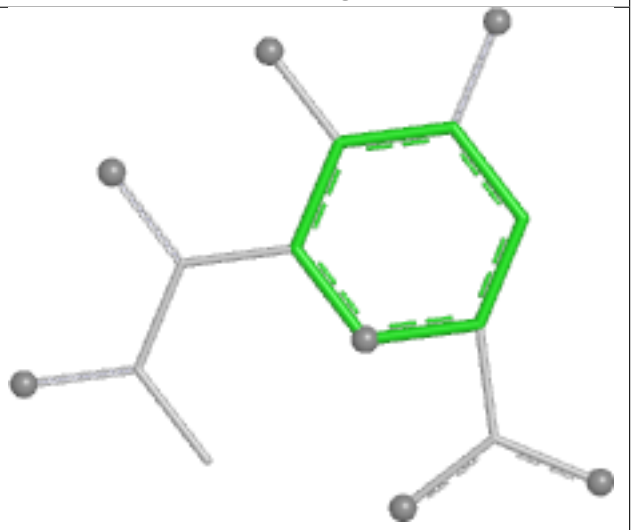
Bond lengths



Bond angles

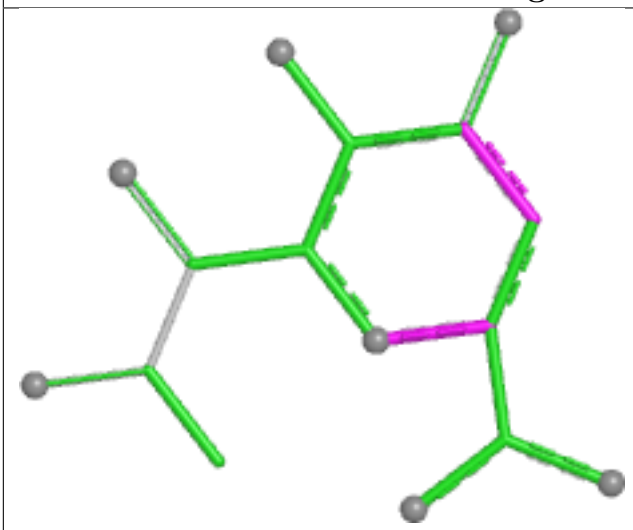


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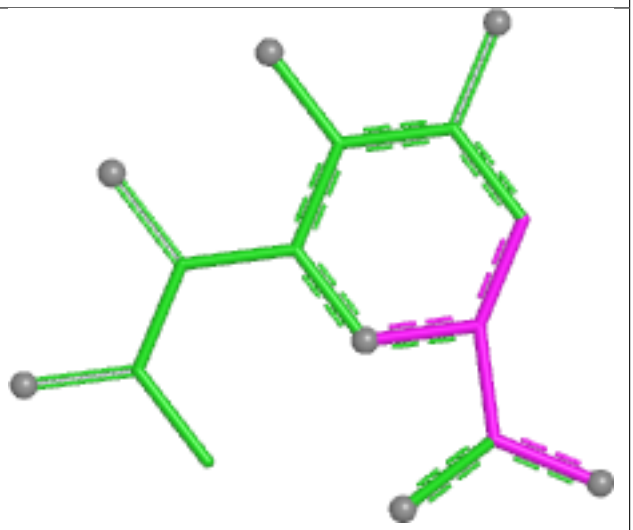


Rings

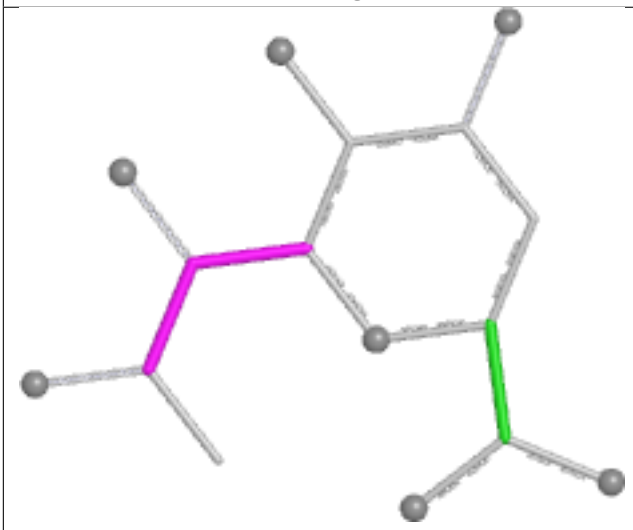
Ligand P8E R 604



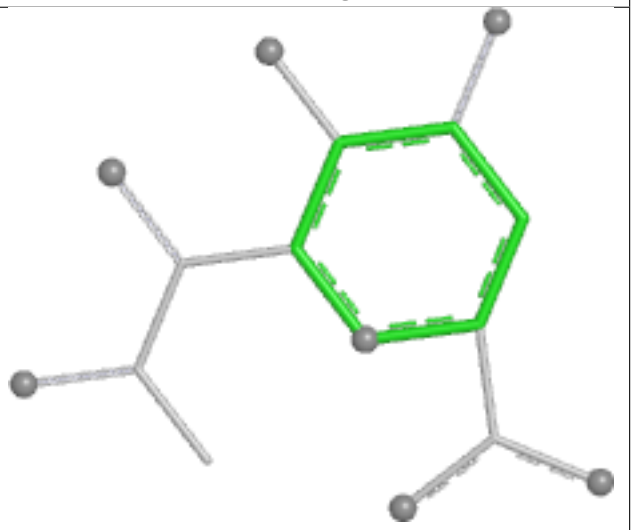
Bond lengths



Bond angles

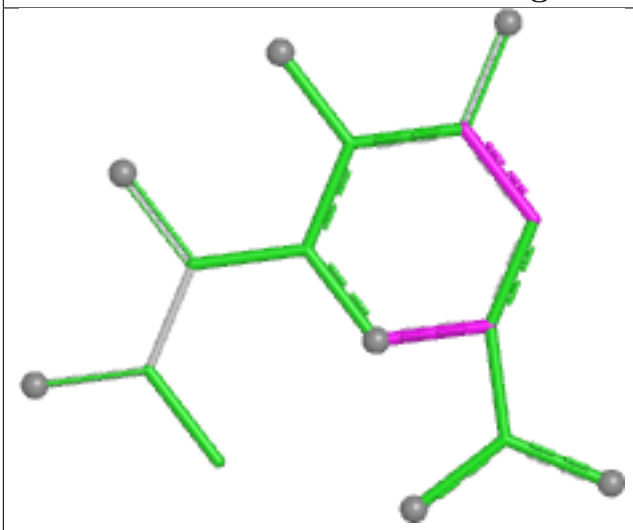


Torsions

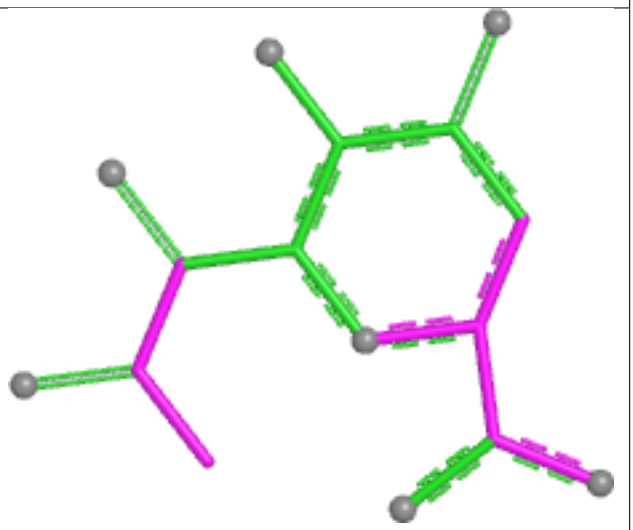


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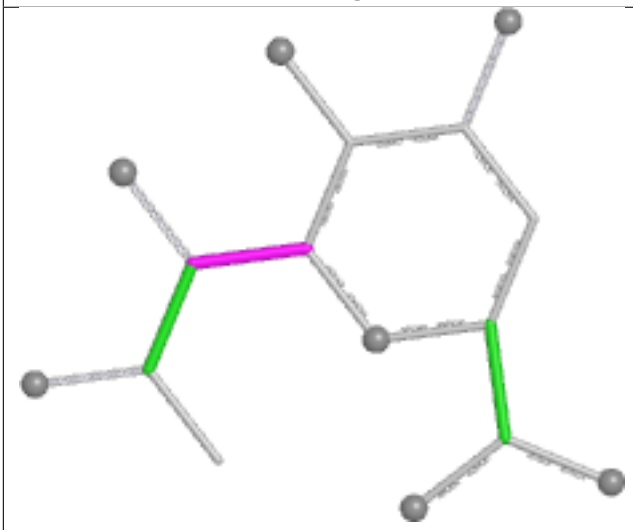
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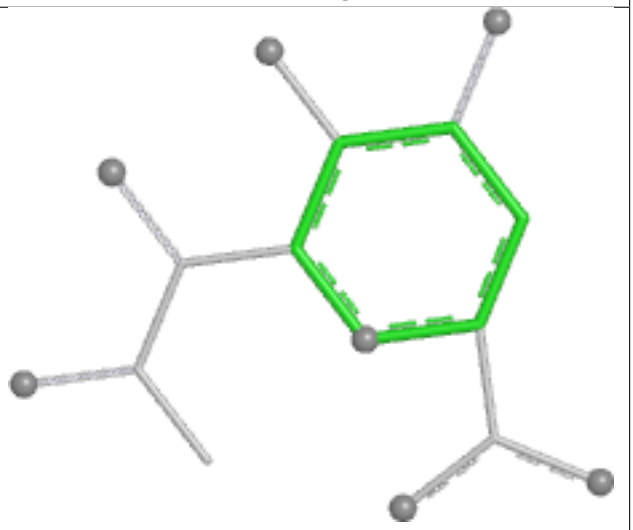
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Bond angles

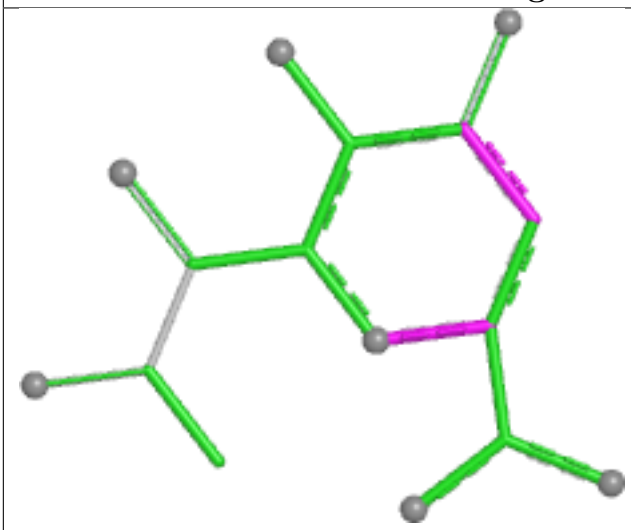


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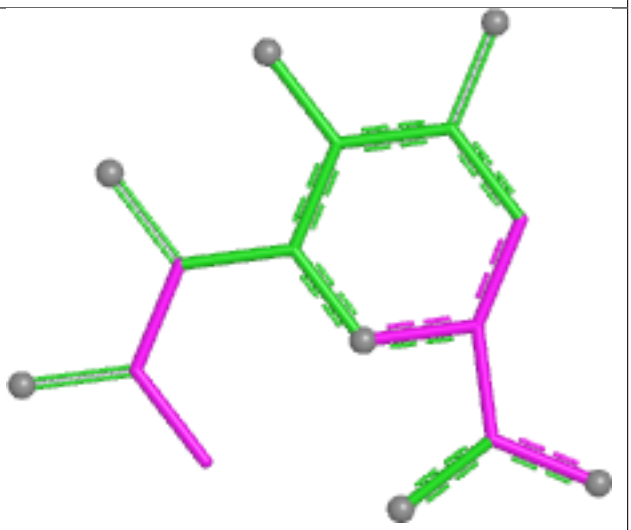


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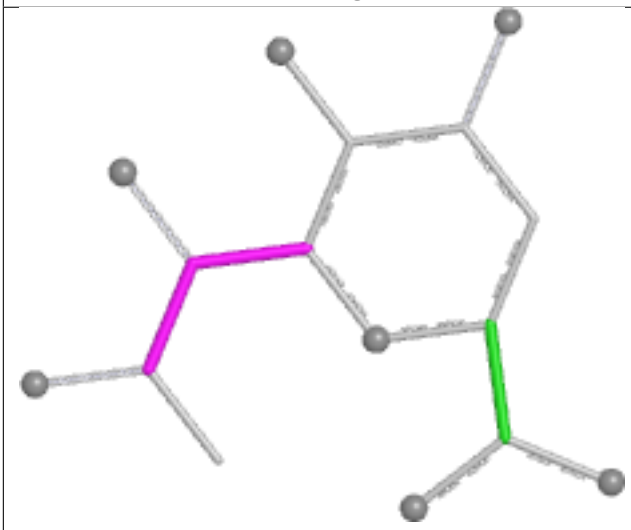
Ligand P8E O 605



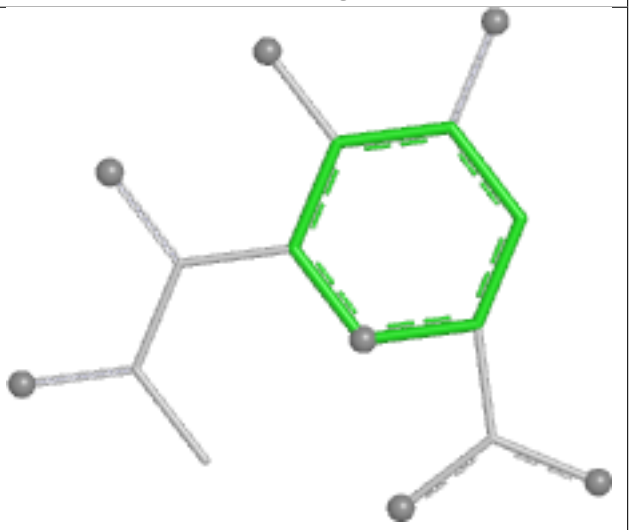
Bond lengths



Bond angles

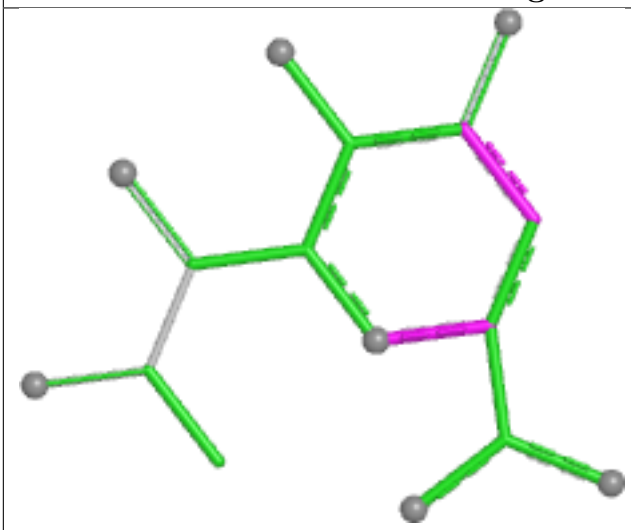


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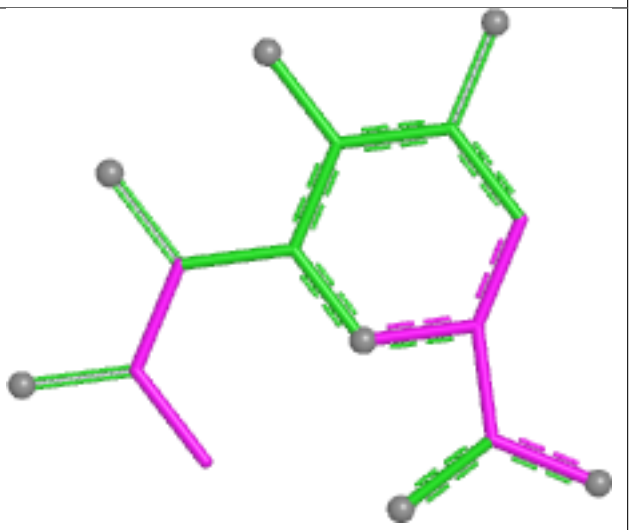


Rings

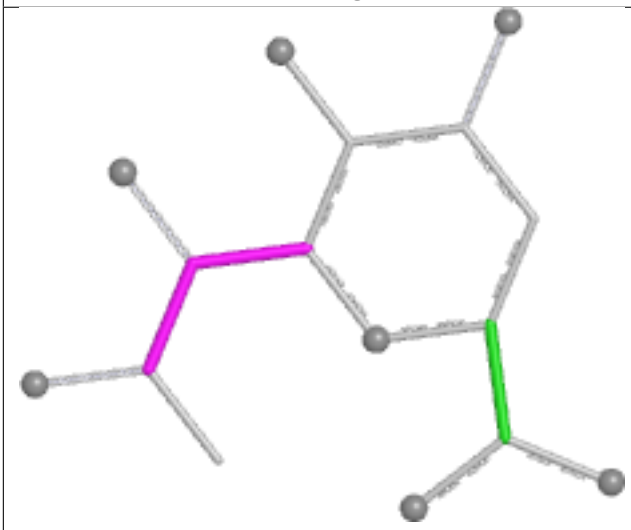
Ligand P8E U 612



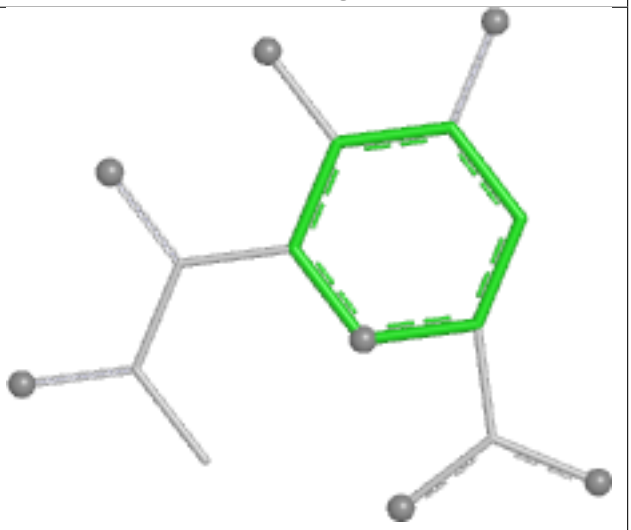
Bond lengths



Bond angles

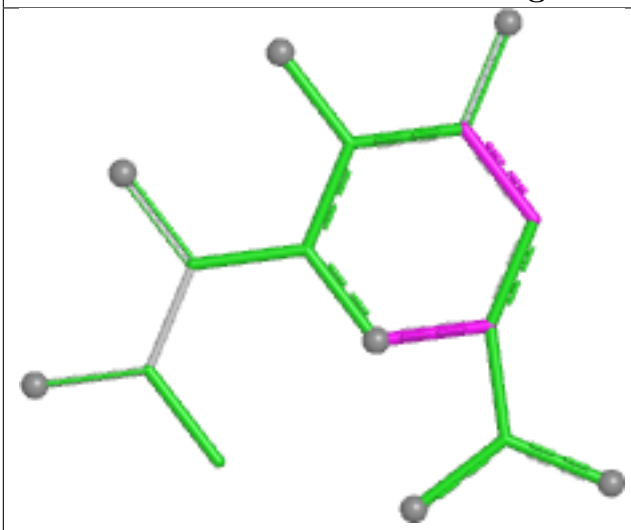


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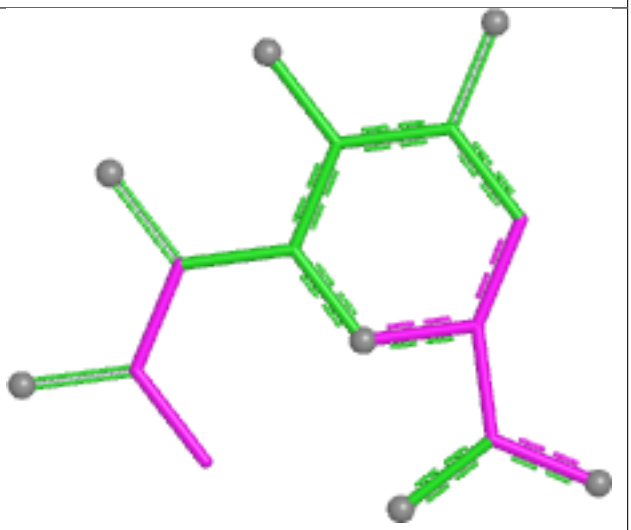


Rings

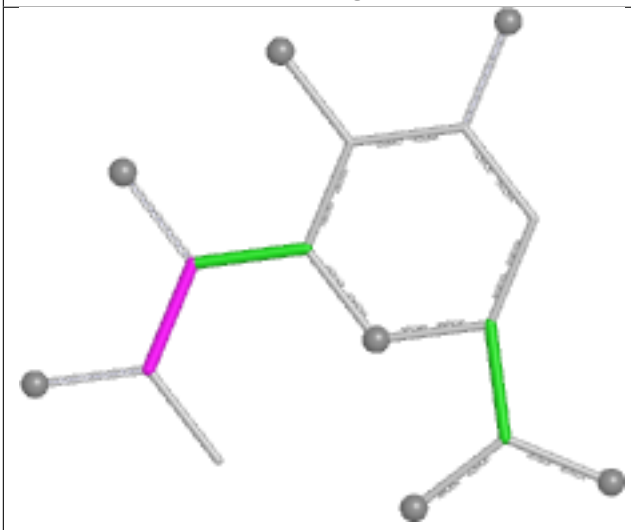
Ligand P8E A 602



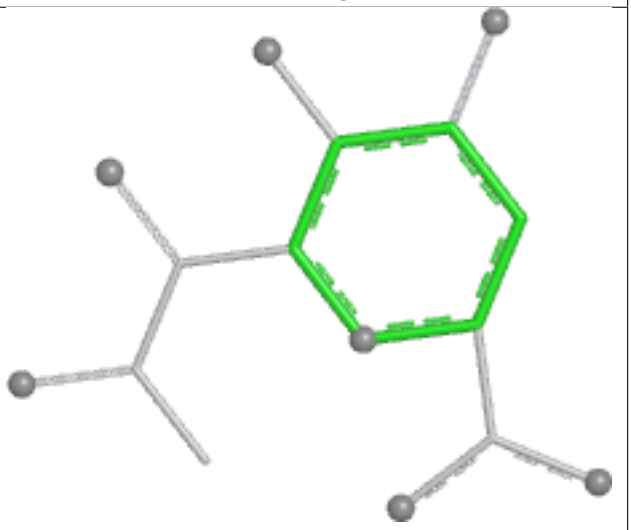
Bond lengths



Bond angles

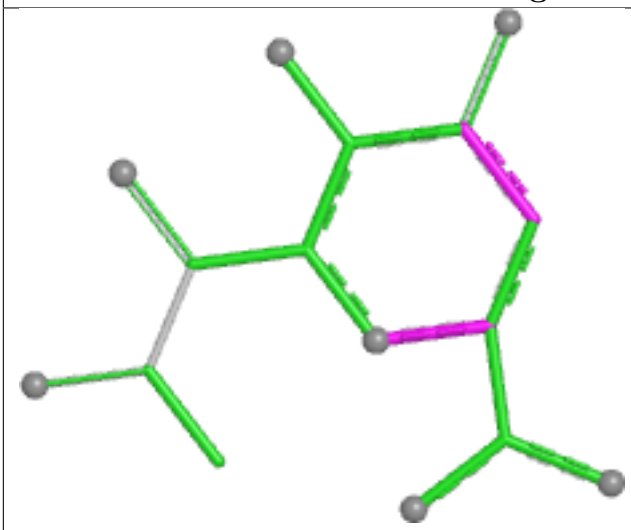


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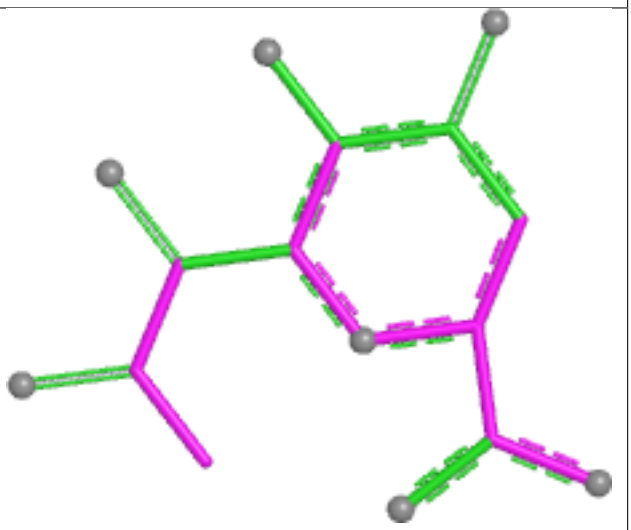


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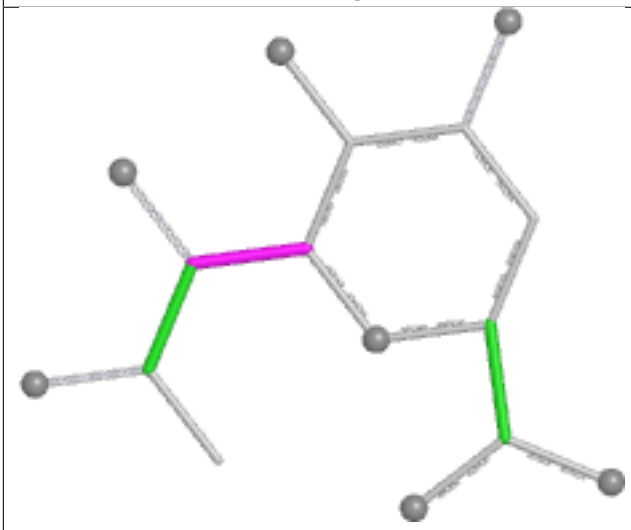
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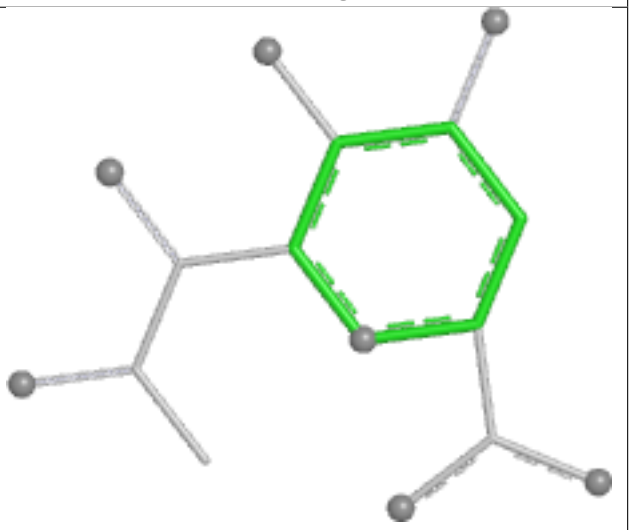
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Bond angles

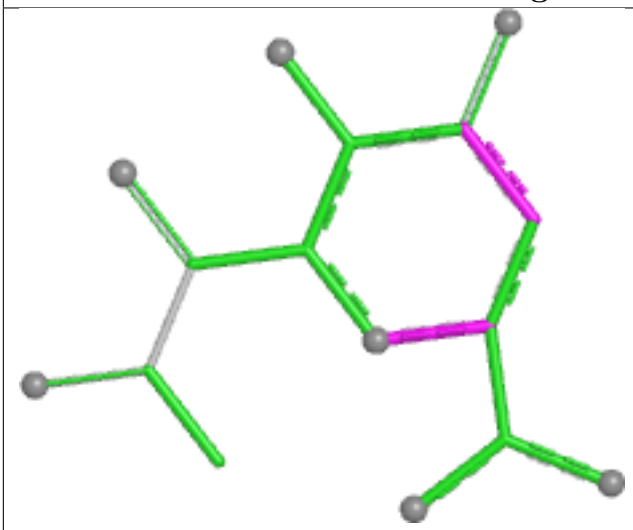


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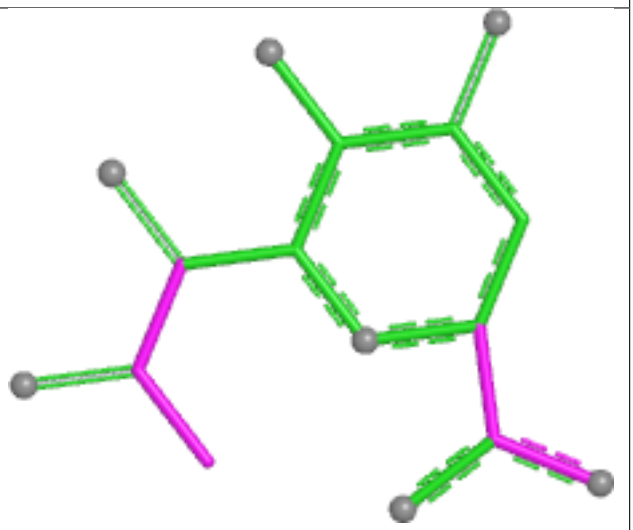


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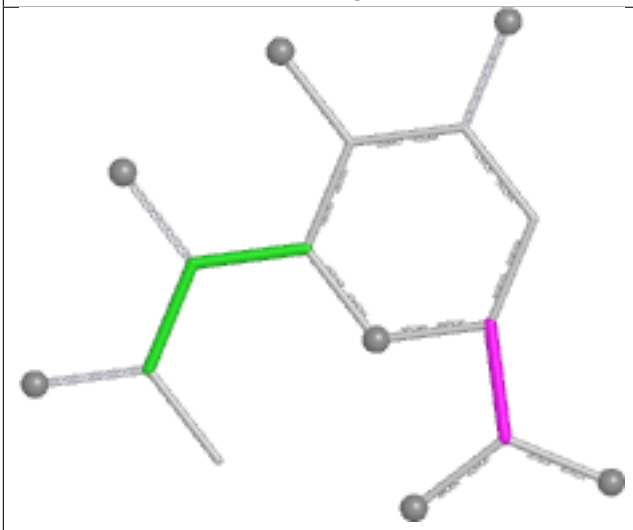
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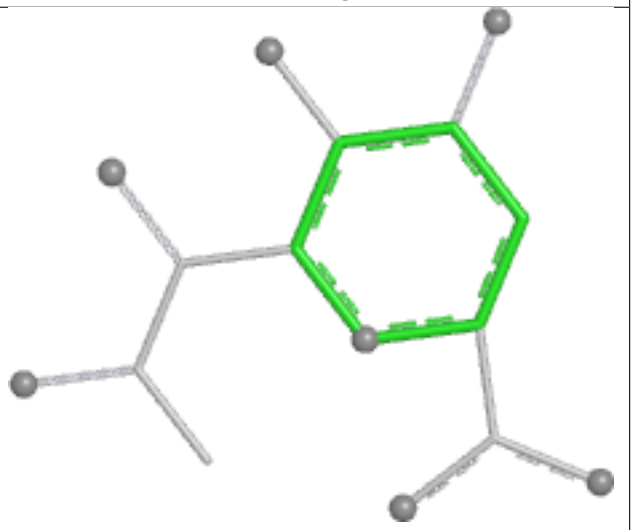
Bond lengths



Bond angles

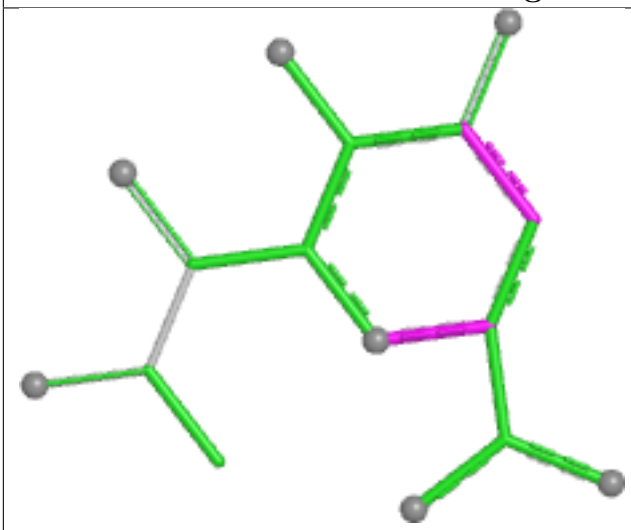


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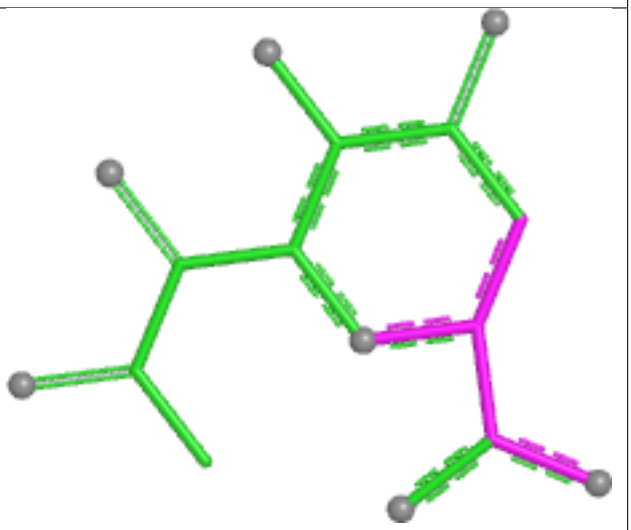


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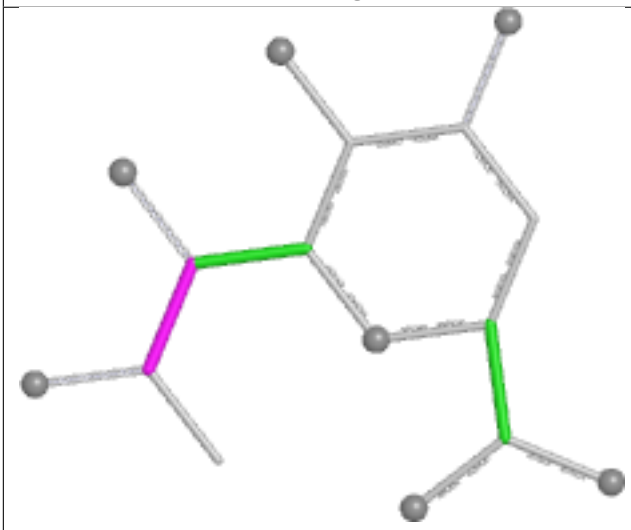
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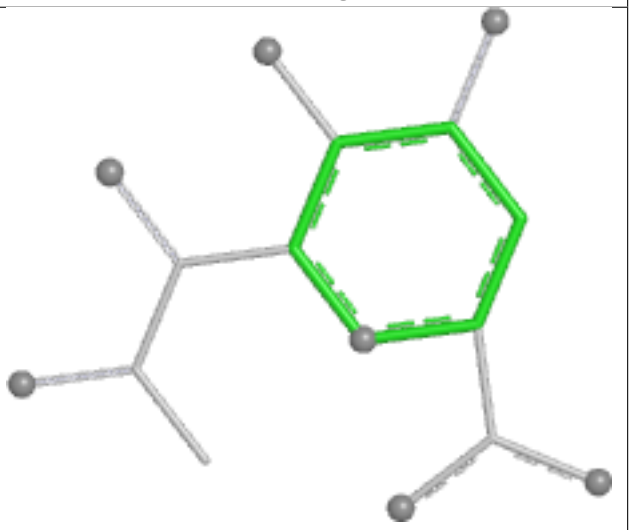
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Bond angles

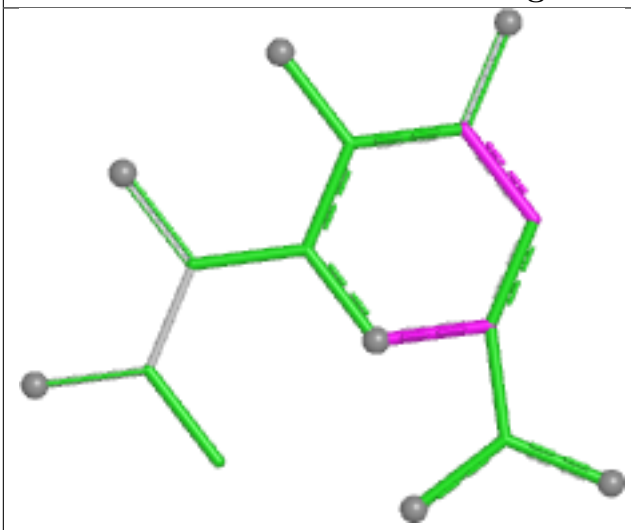


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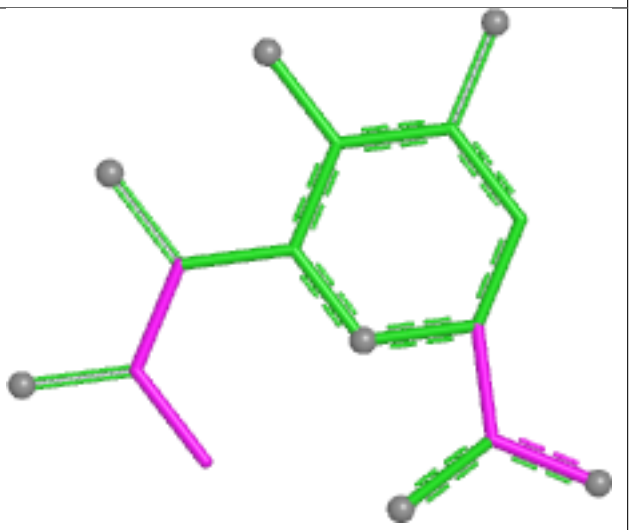


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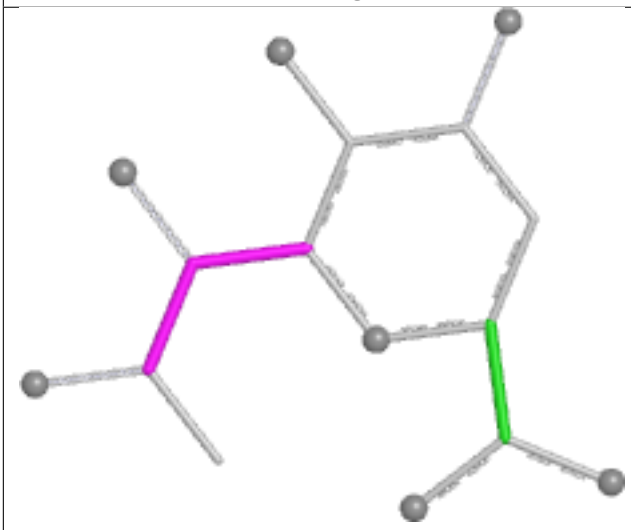
Ligand P8E G 601



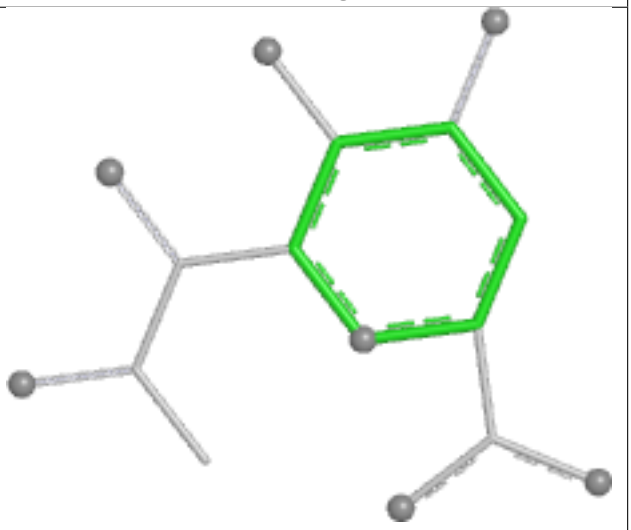
Bond lengths



Bond angles

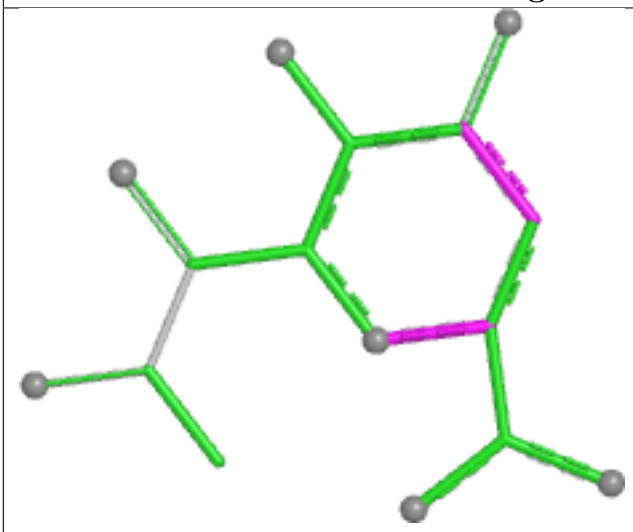


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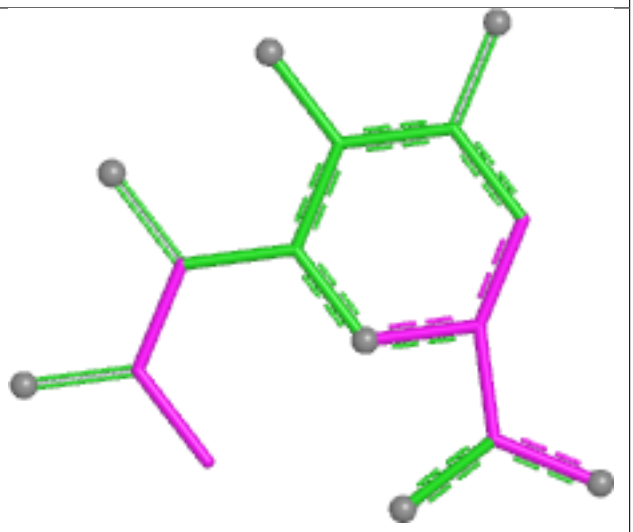


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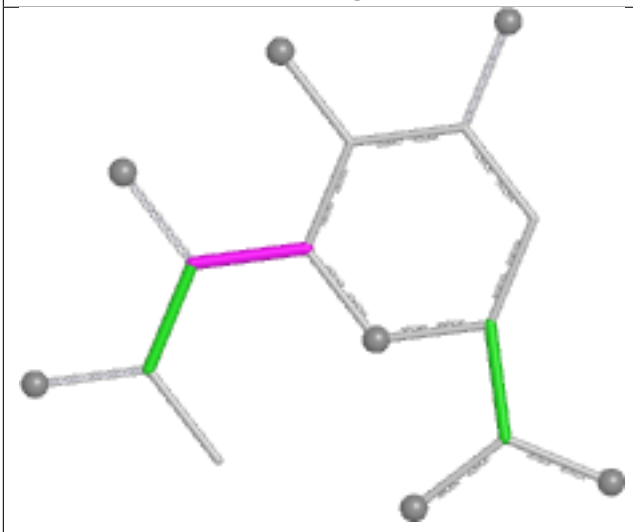
Ligand P8E A 615



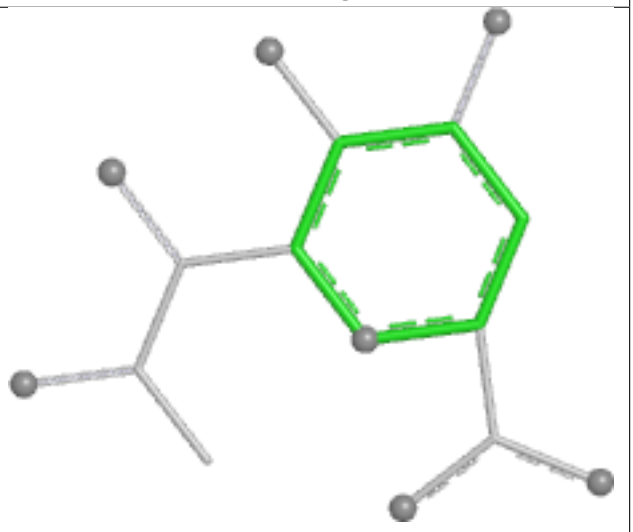
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Bond angles

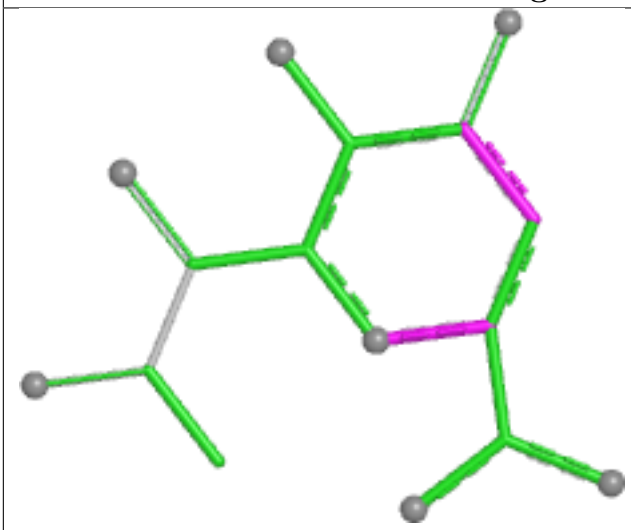


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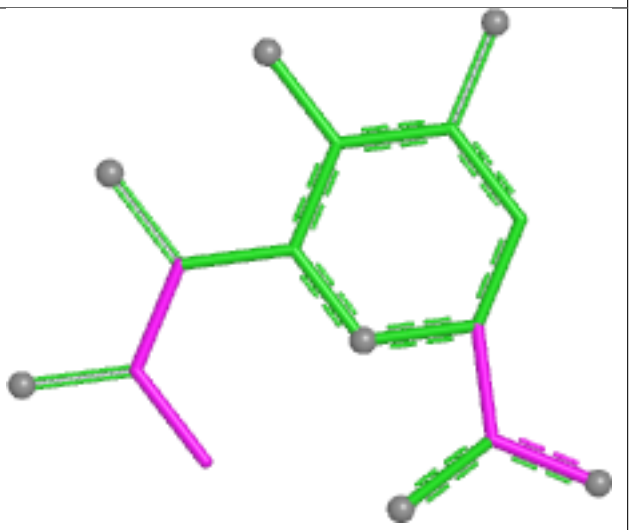


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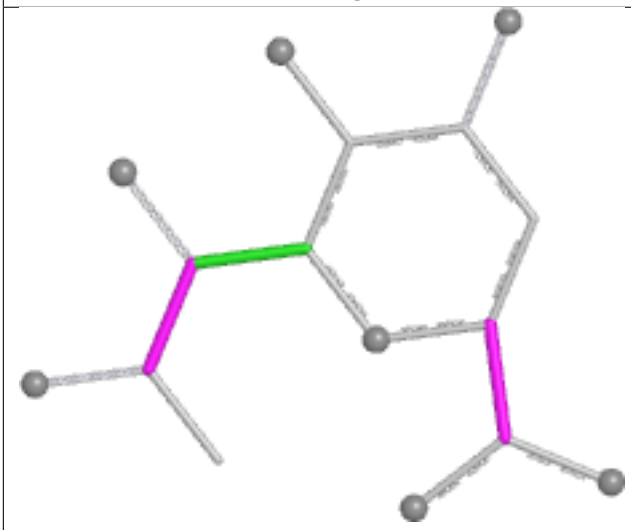
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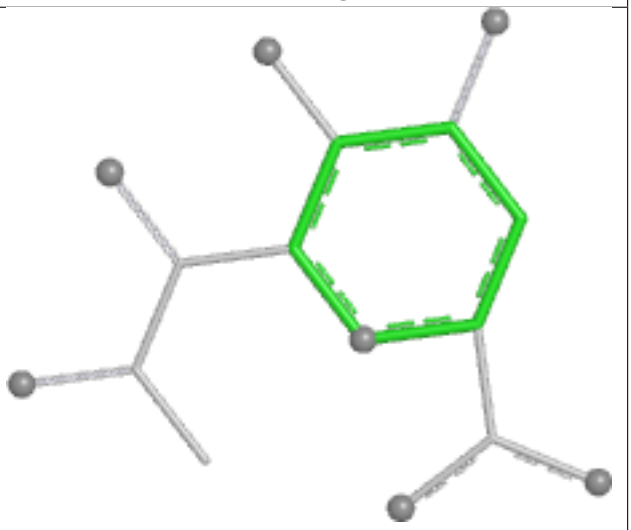
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Bond angles

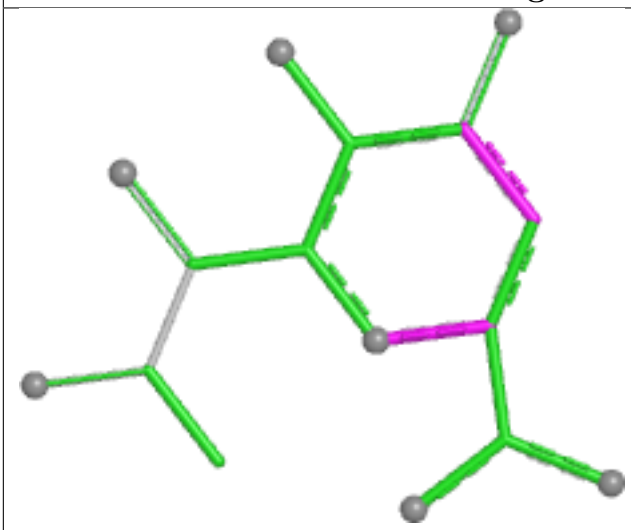


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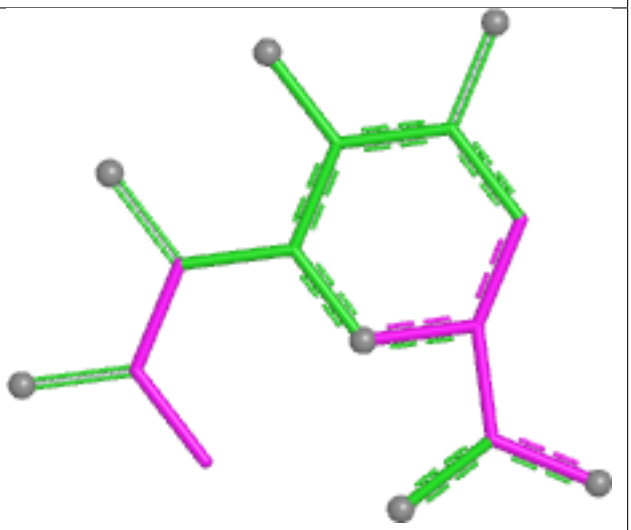


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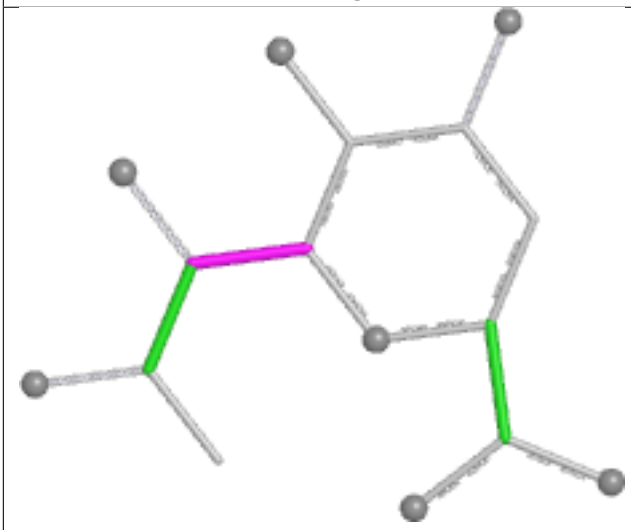
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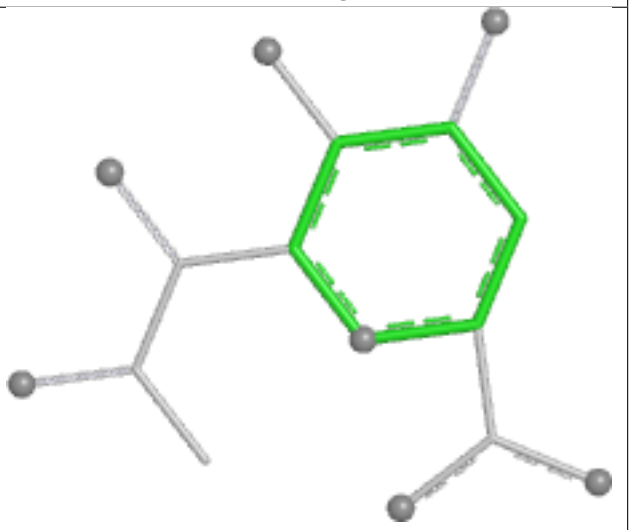
Bond lengths



Bond angles

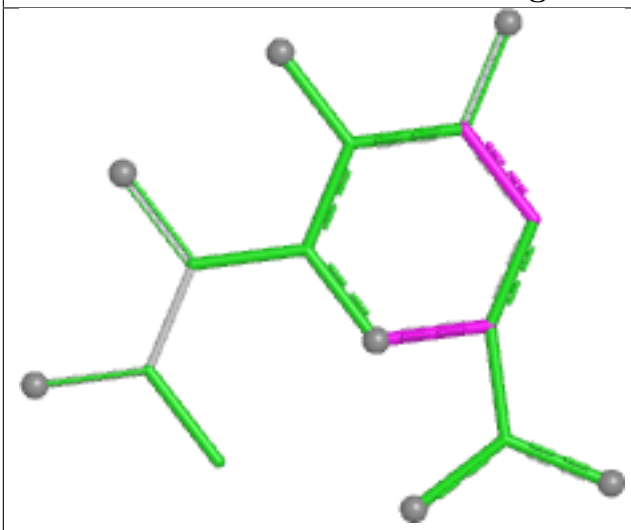


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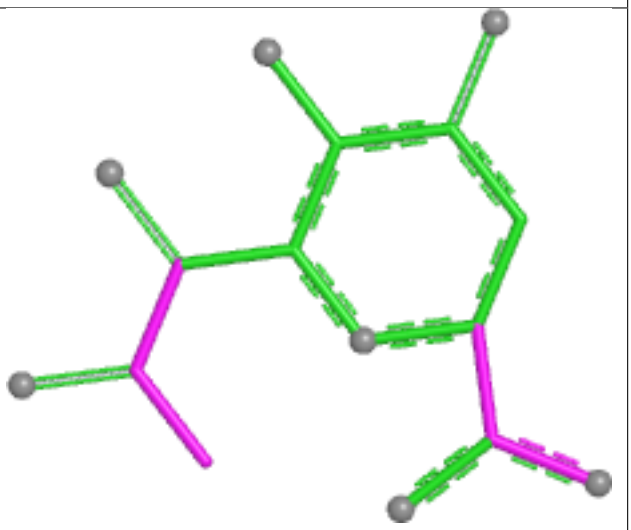


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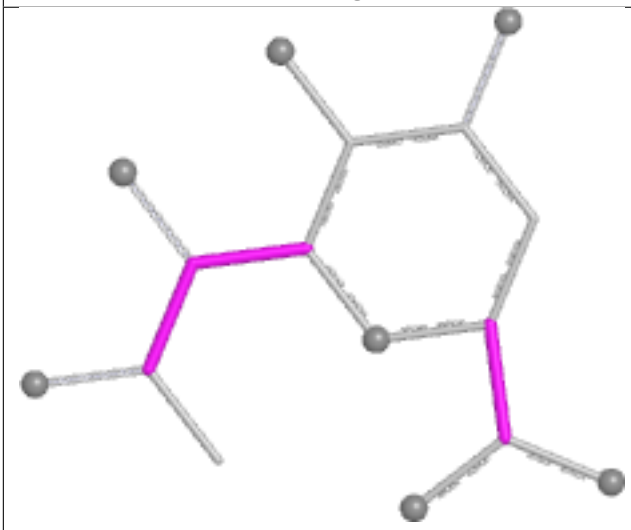
Ligand P8E T 614



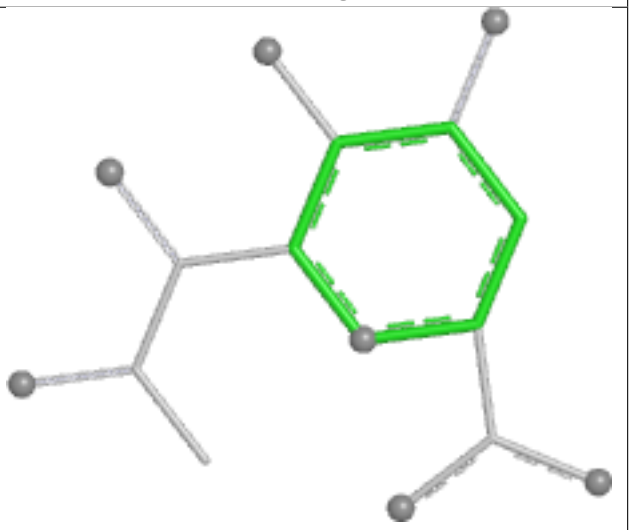
Bond lengths



Bond angles

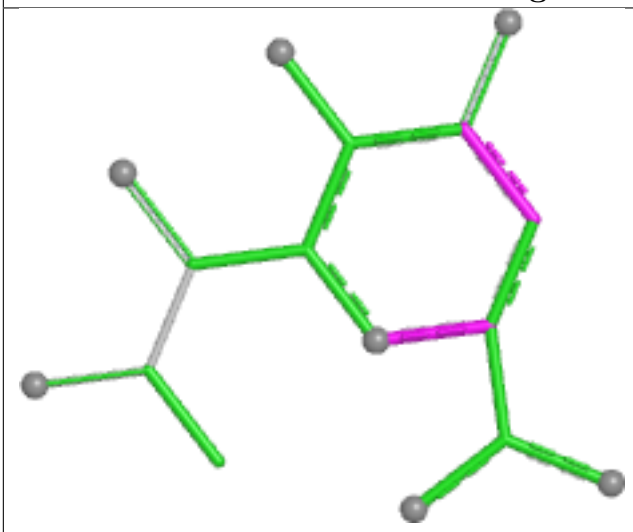


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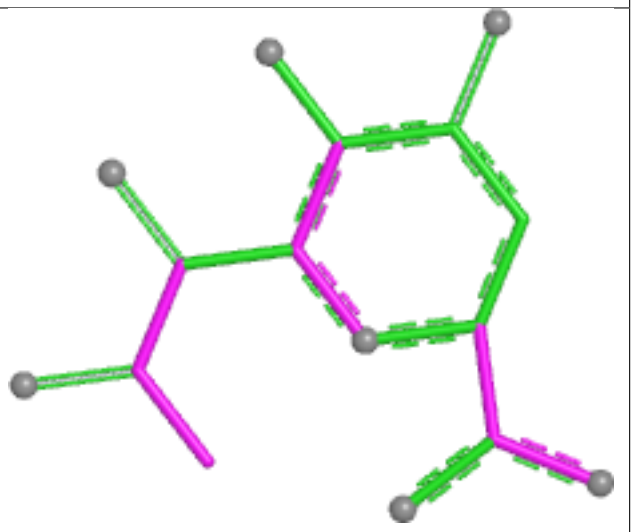


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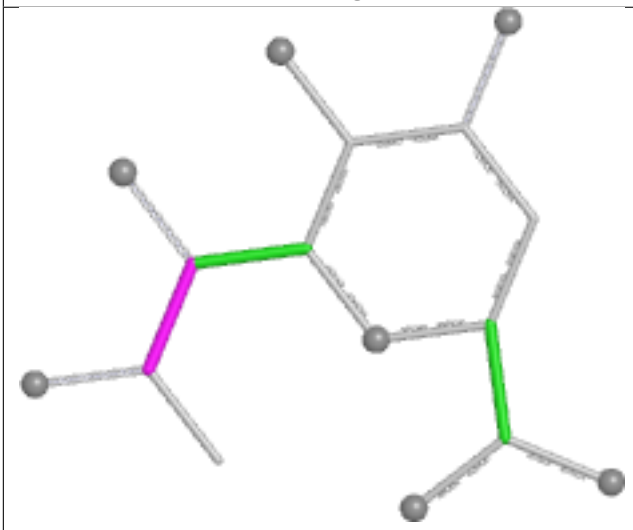
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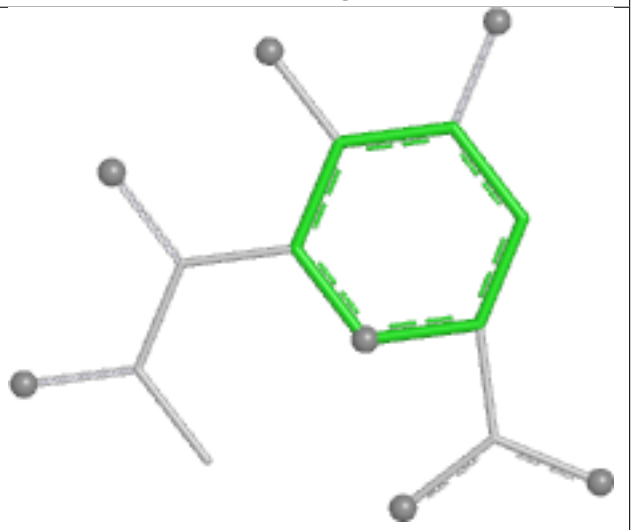
Bond lengths



Bond angles

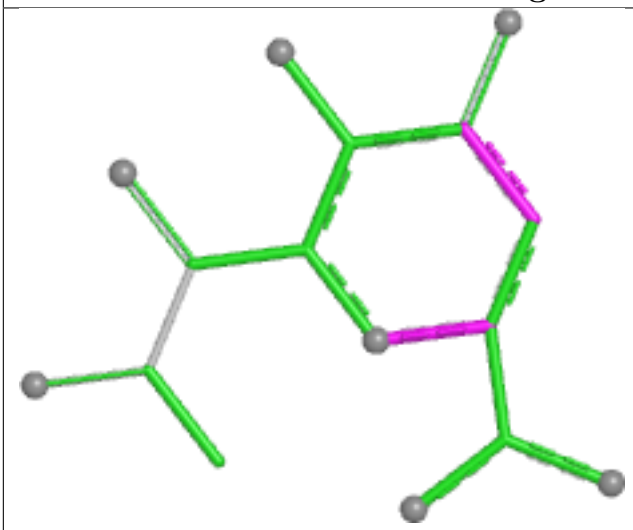


Torsions

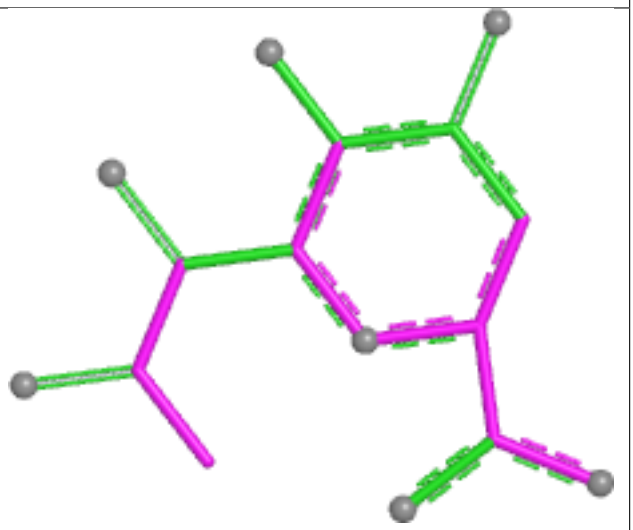


Rings

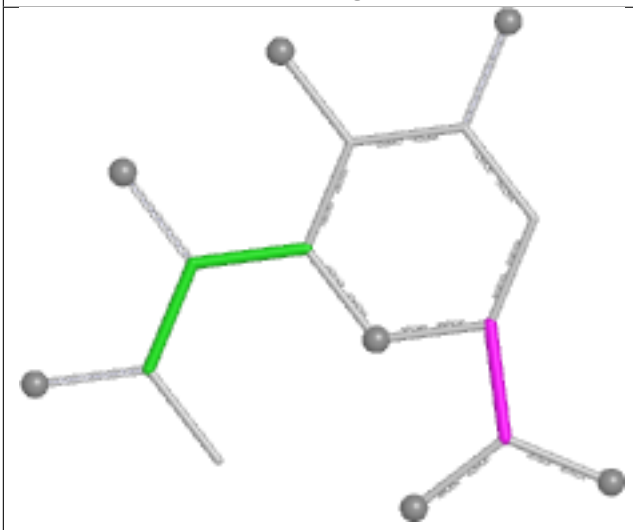
Ligand P8E T 617



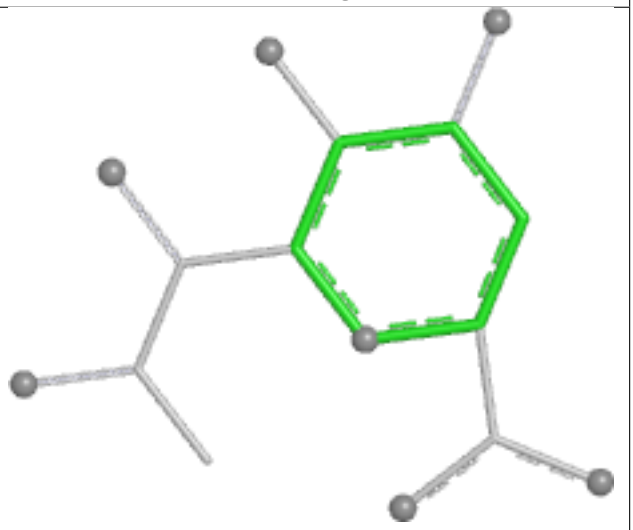
Bond lengths



Bond angles

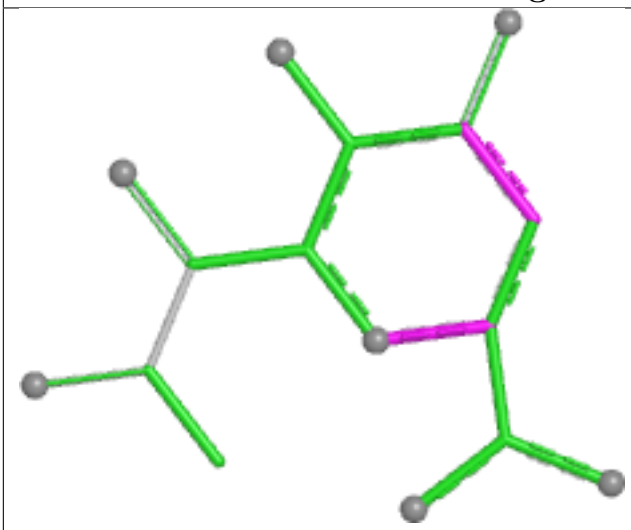


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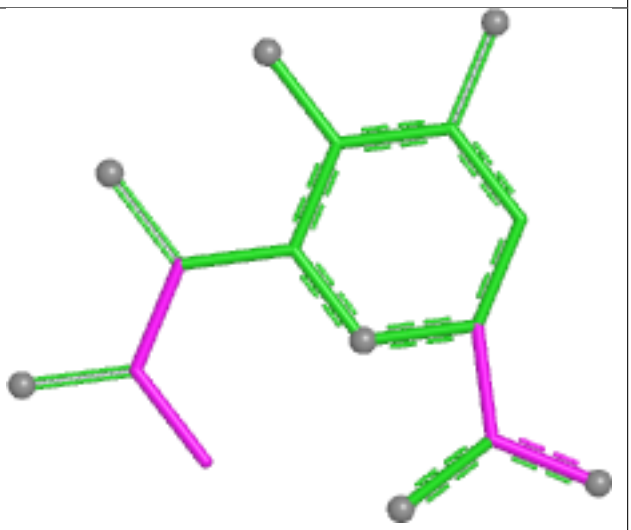


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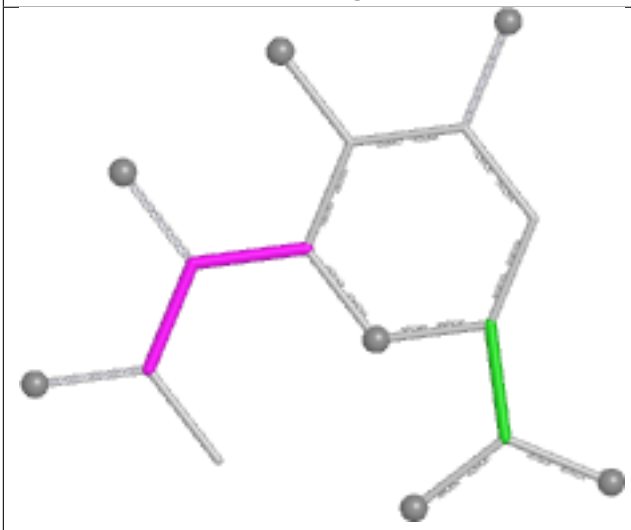
Ligand P8E T 613



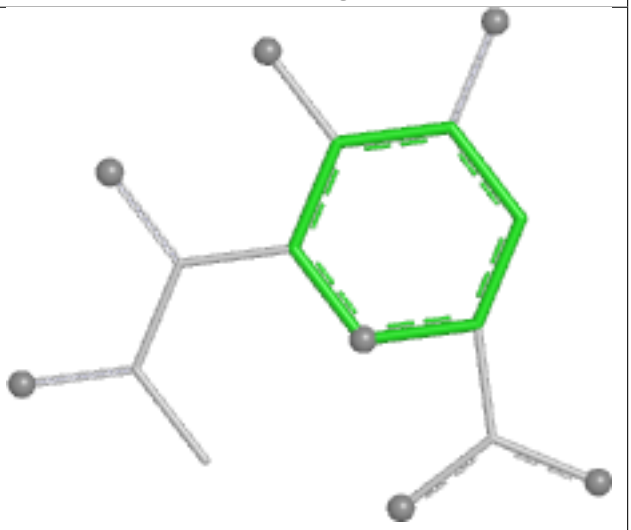
Bond lengths



Bond angles

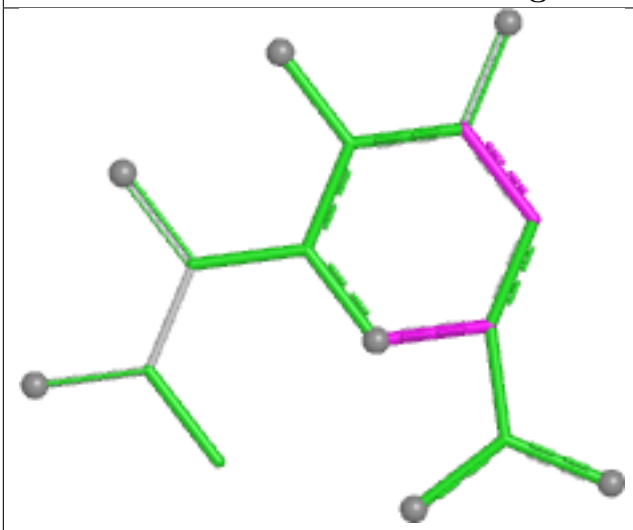


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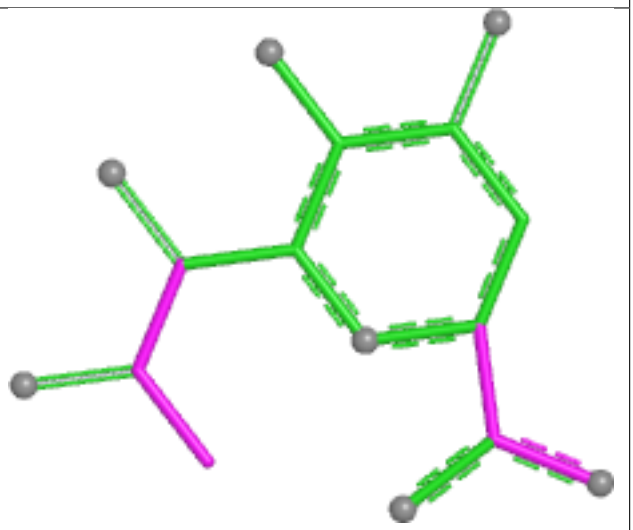


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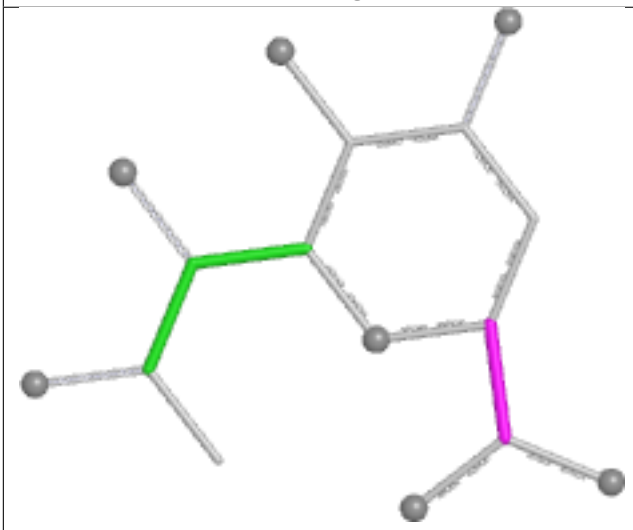
Ligand P8E P 611



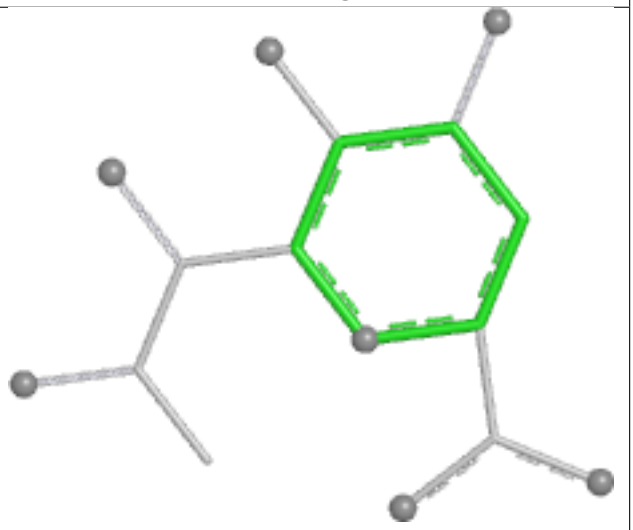
Bond lengths



Bond angles

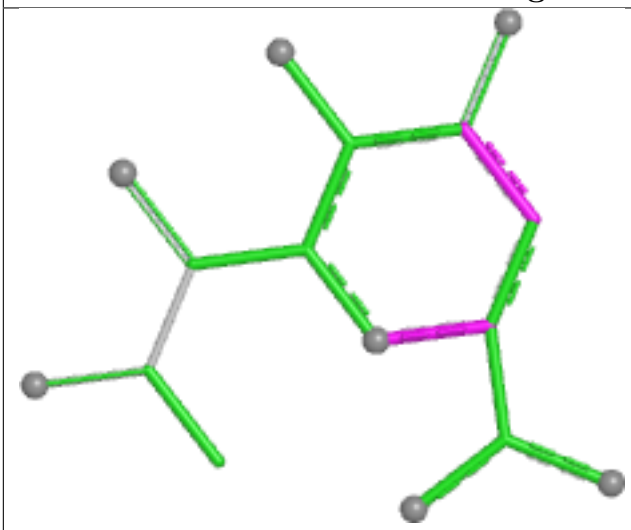


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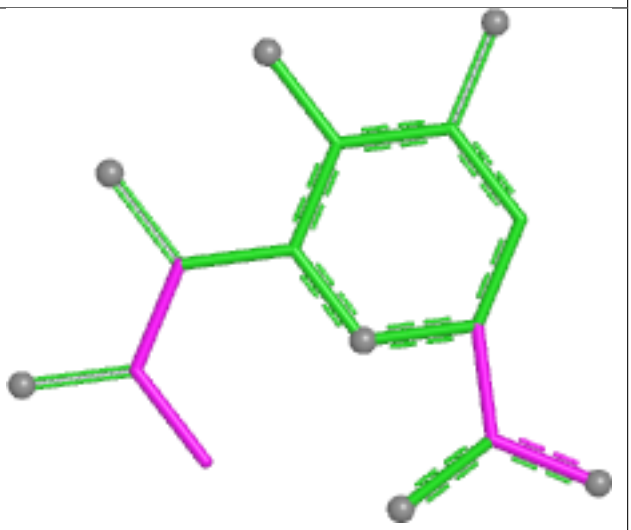


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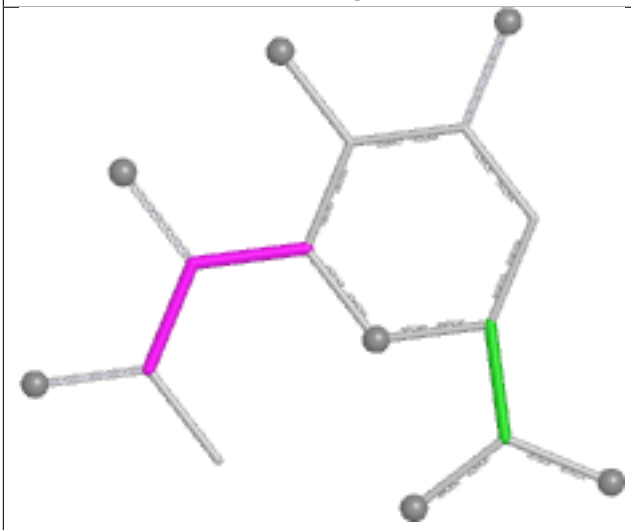
Ligand P8E U 601



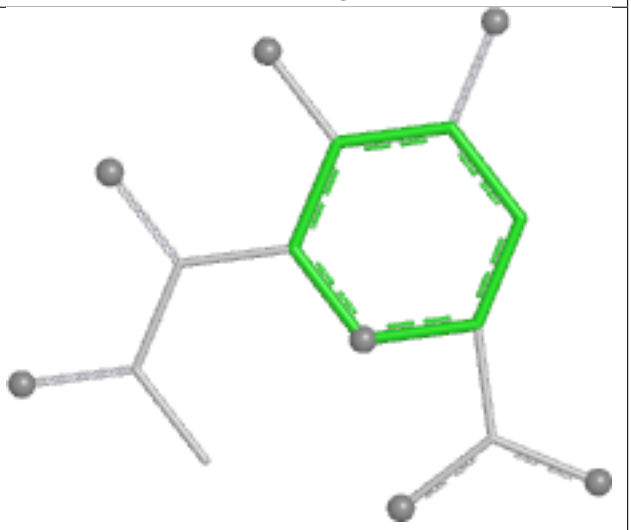
Bond lengths



Bond angles

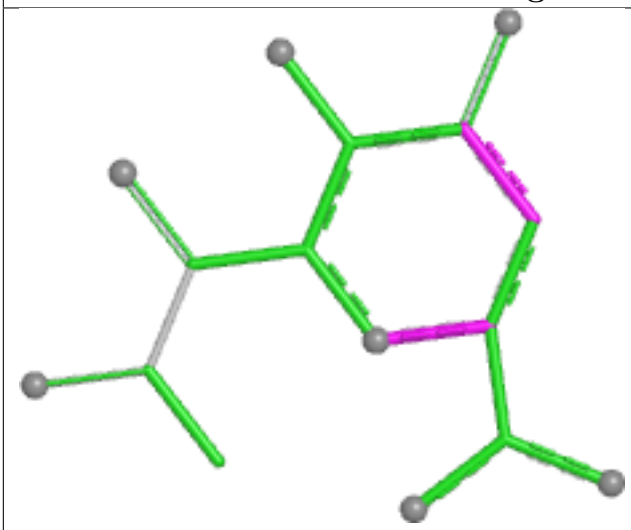


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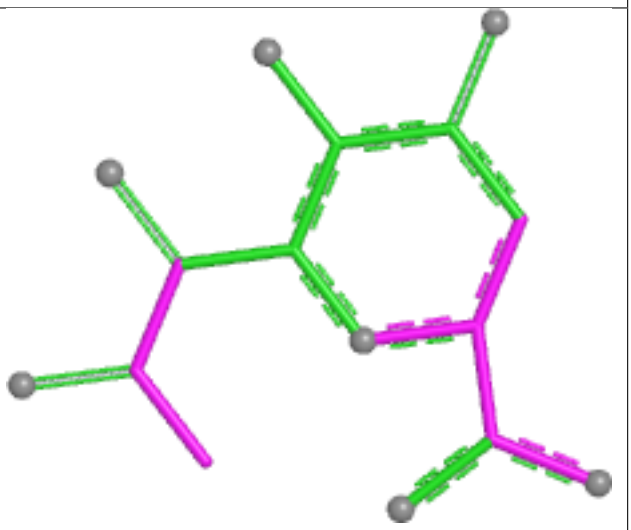


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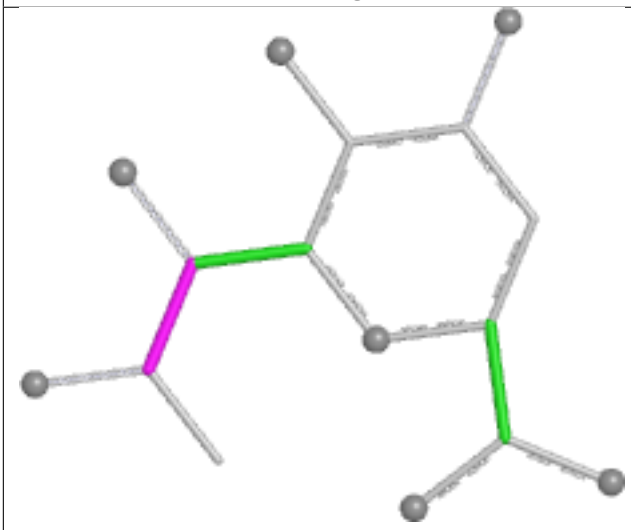
Ligand P8E G 602



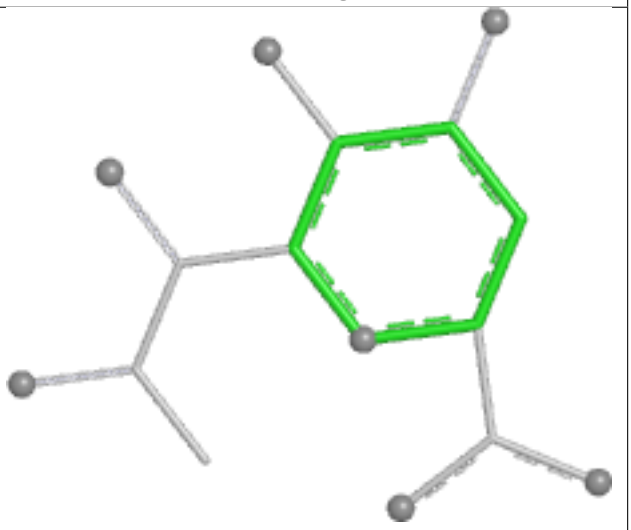
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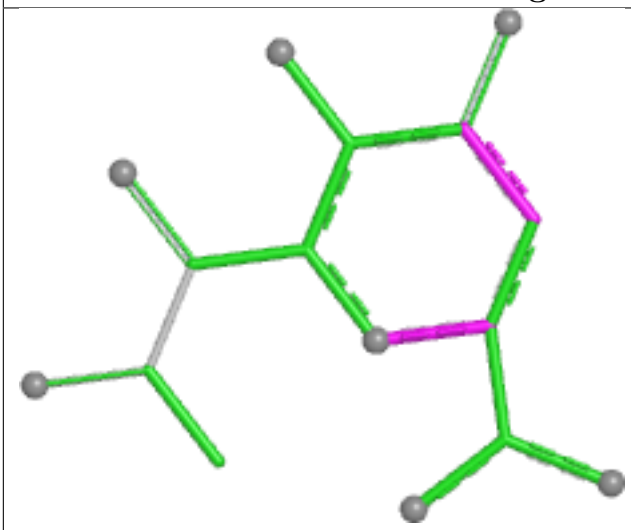


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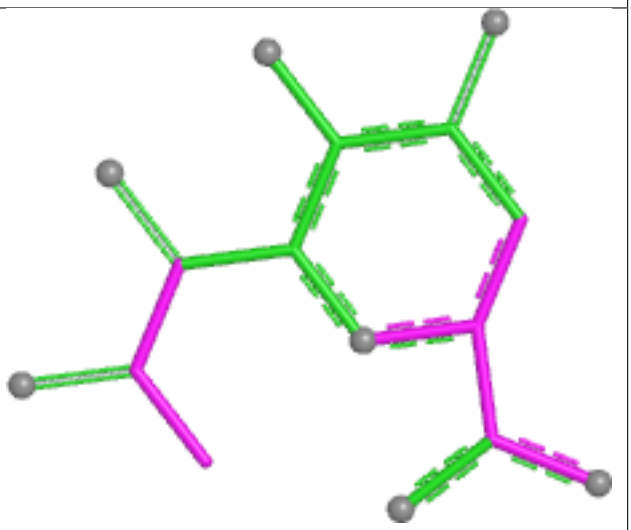


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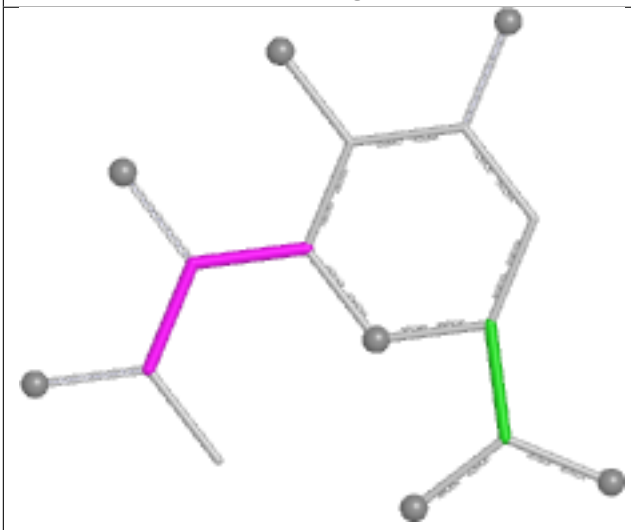
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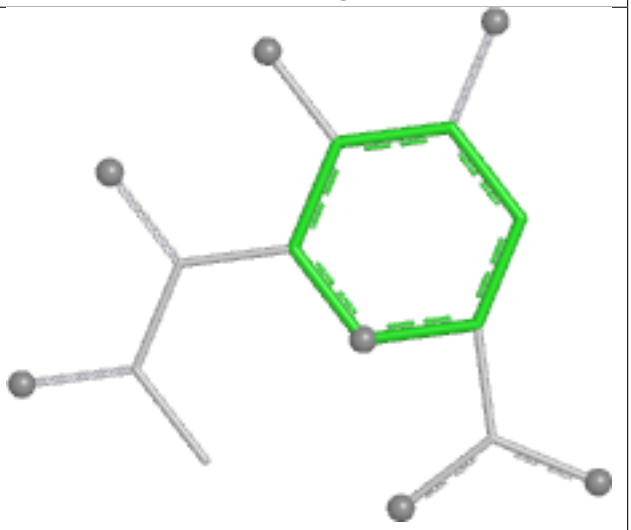
Bond lengths



Bond angles

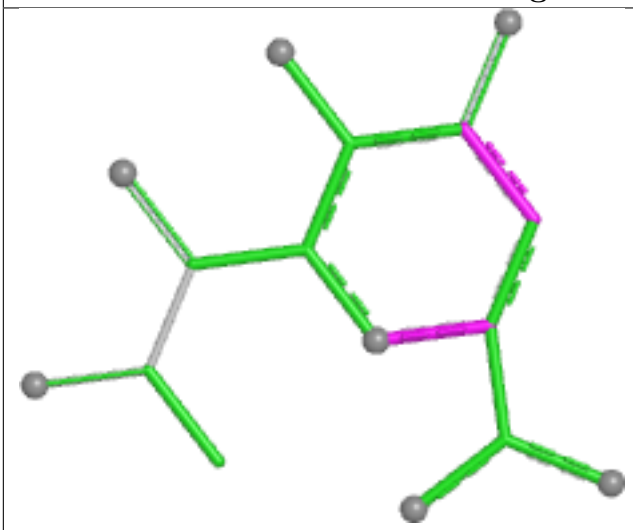


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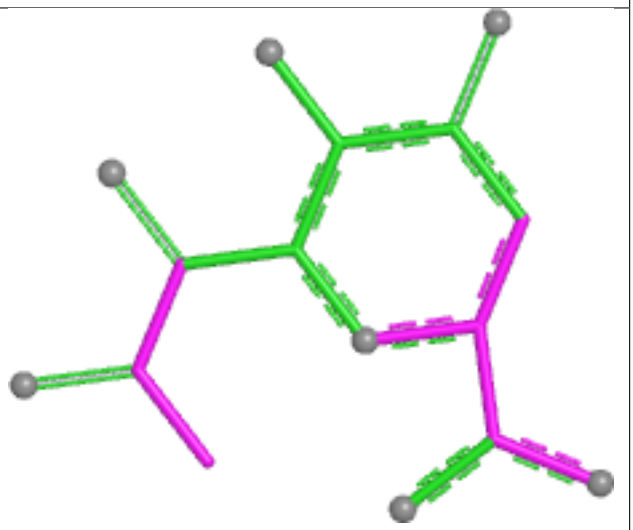


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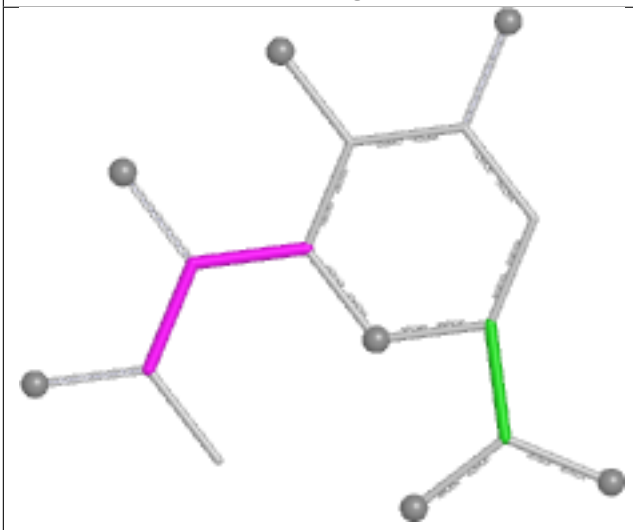
Ligand P8E E 613



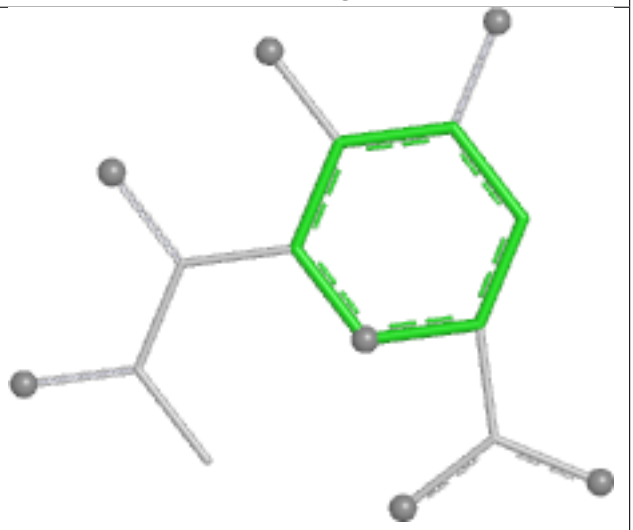
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Bond angles

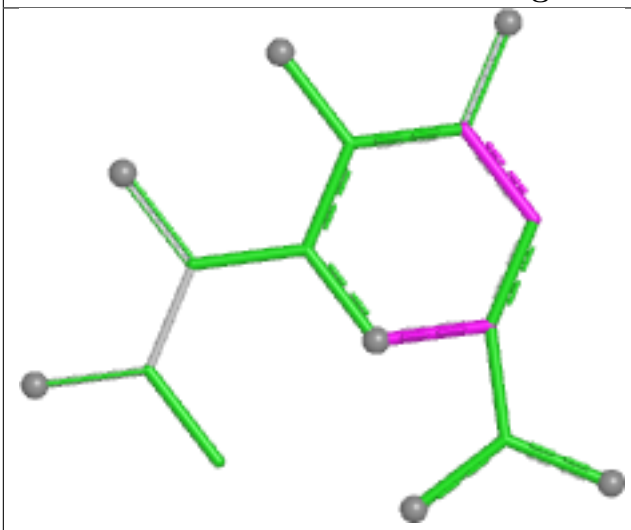


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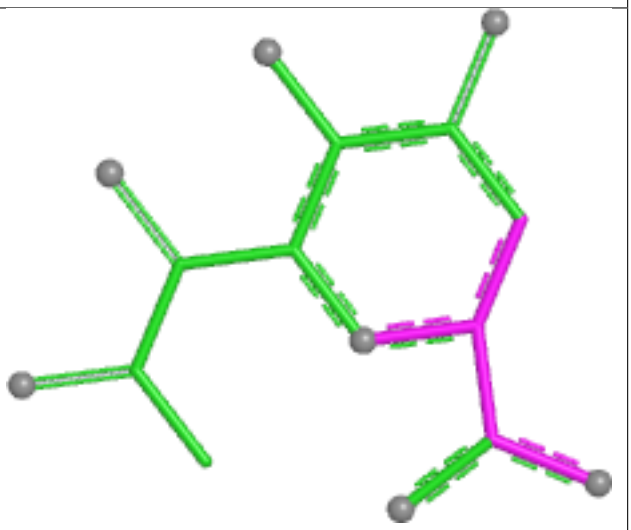


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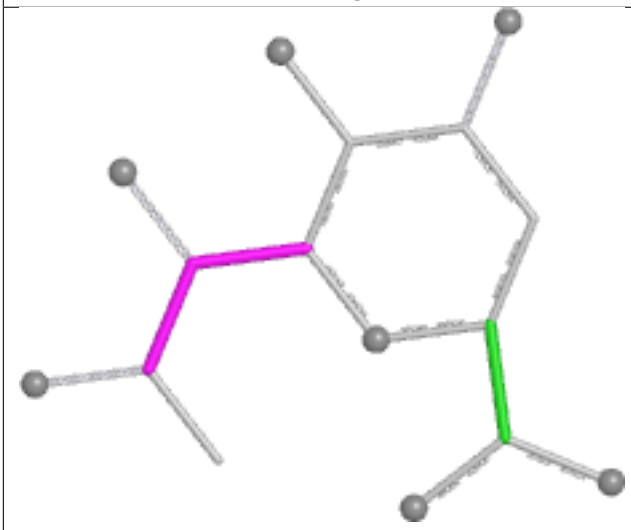
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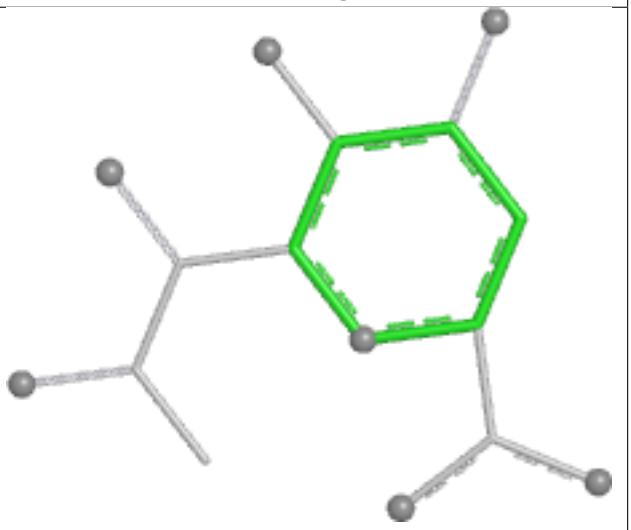
Bond lengths



Bond angles

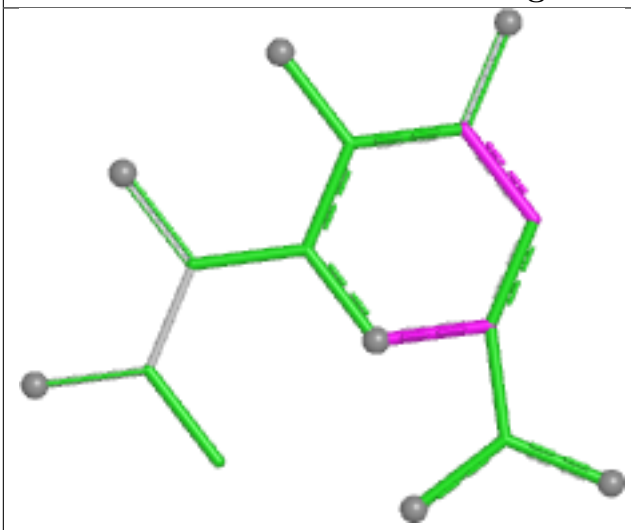


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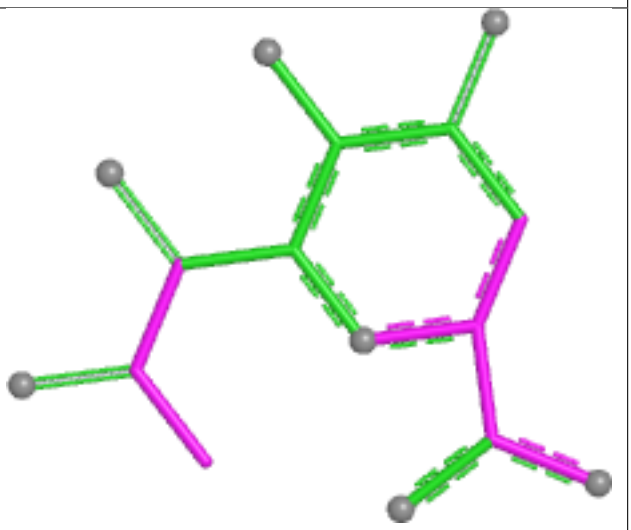


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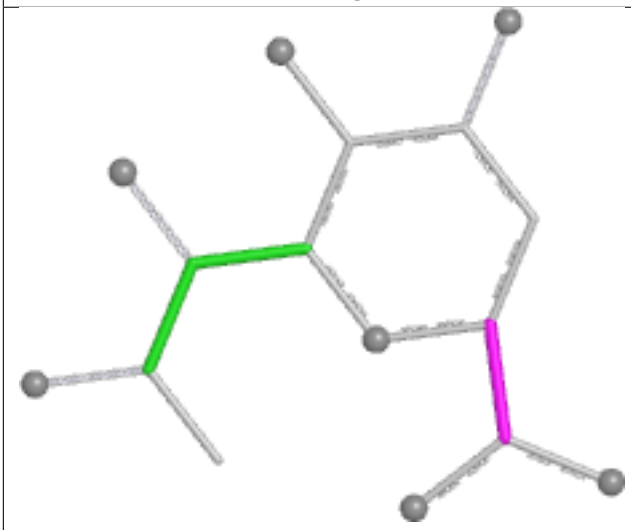
Ligand P8E U 611



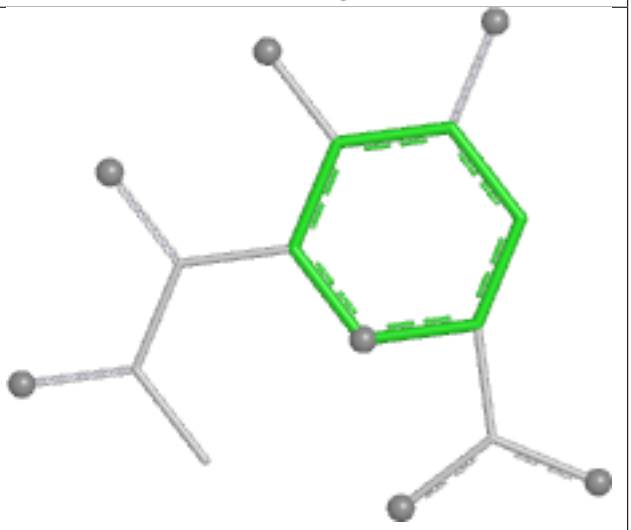
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Bond angles

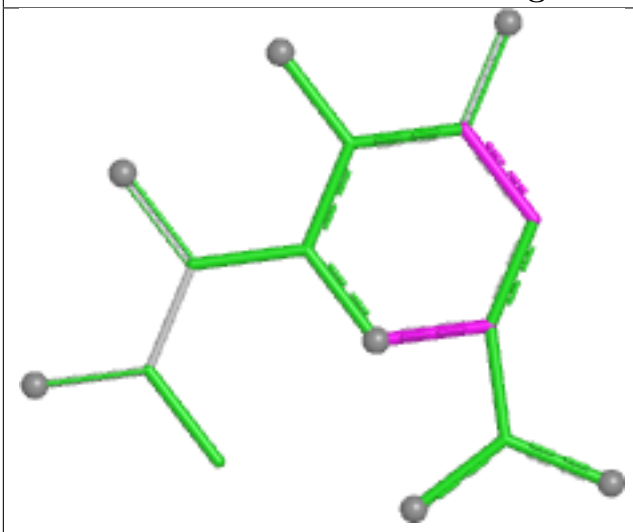


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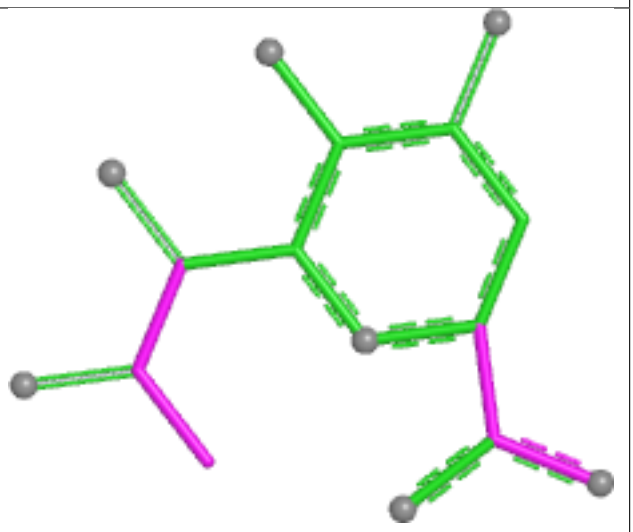


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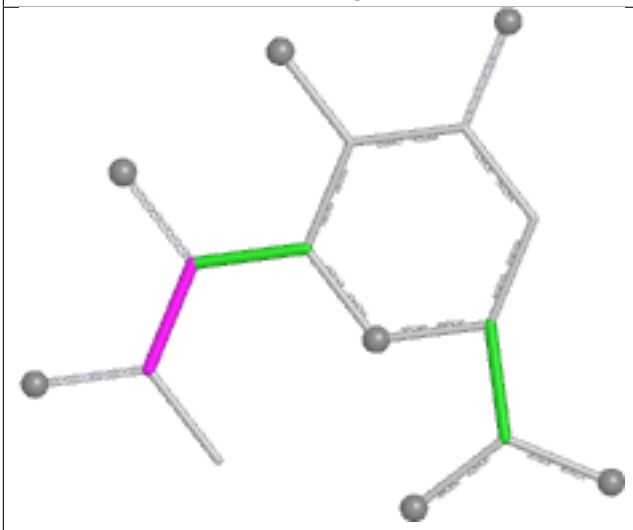
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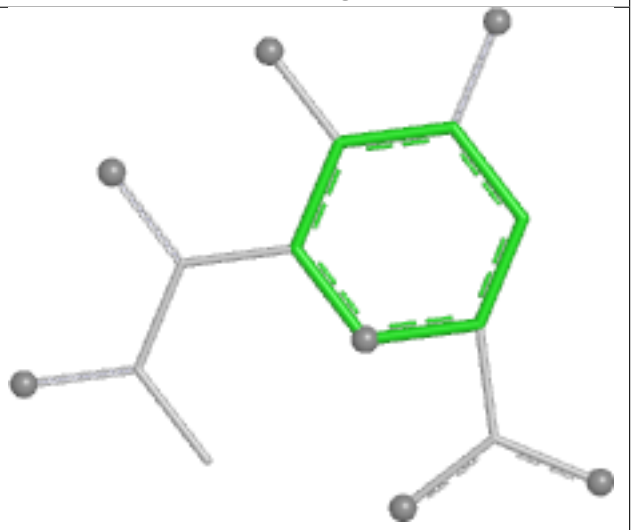
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Bond angles

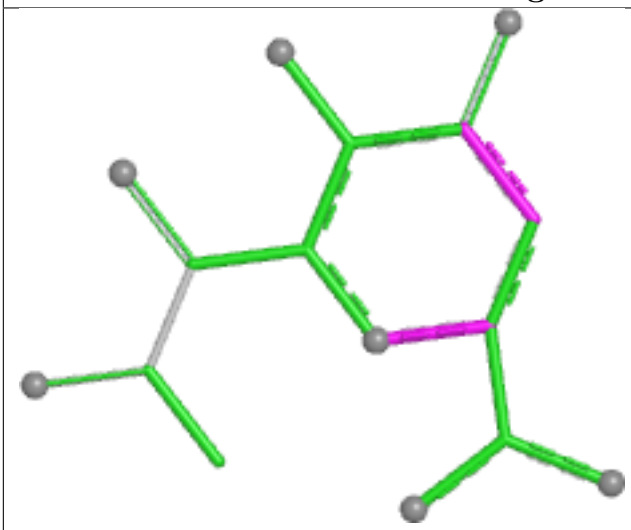


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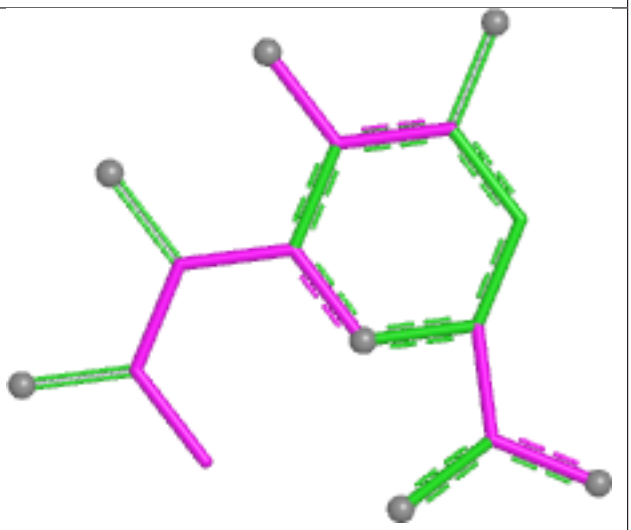


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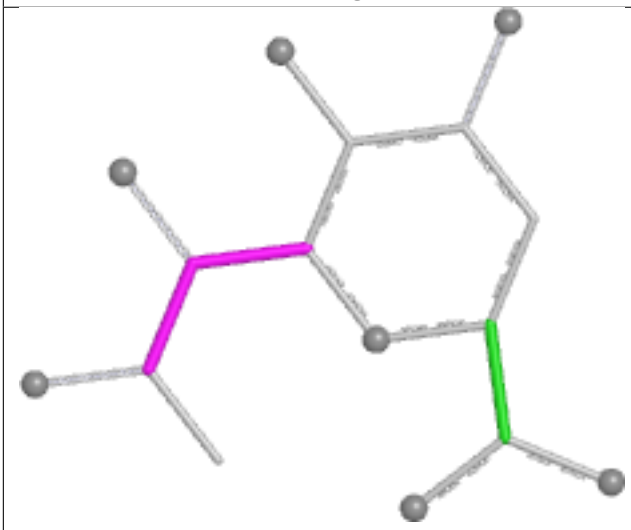
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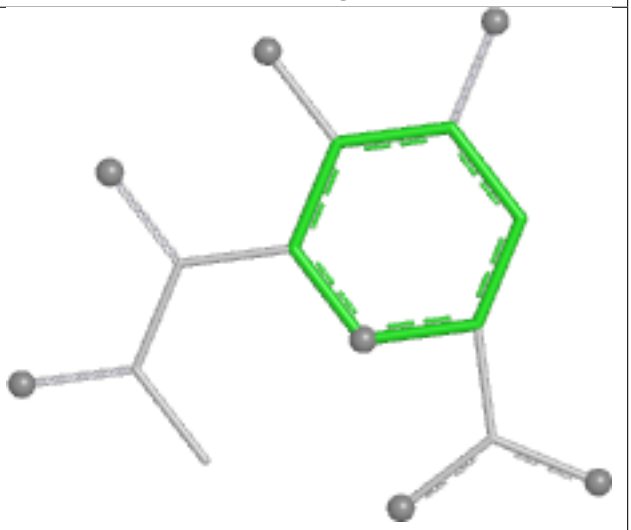
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Bond angles

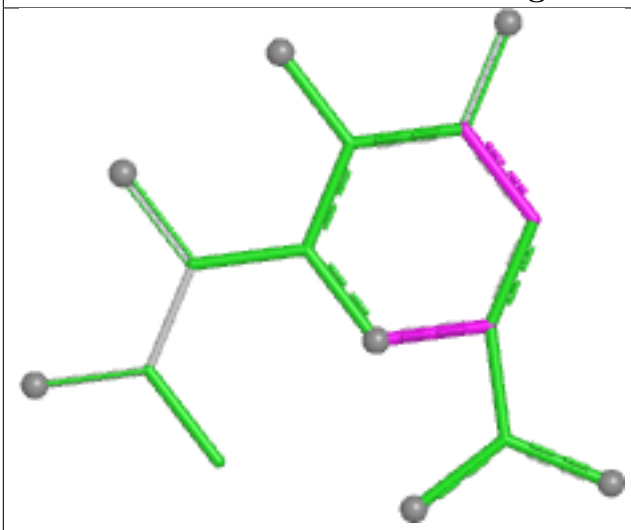


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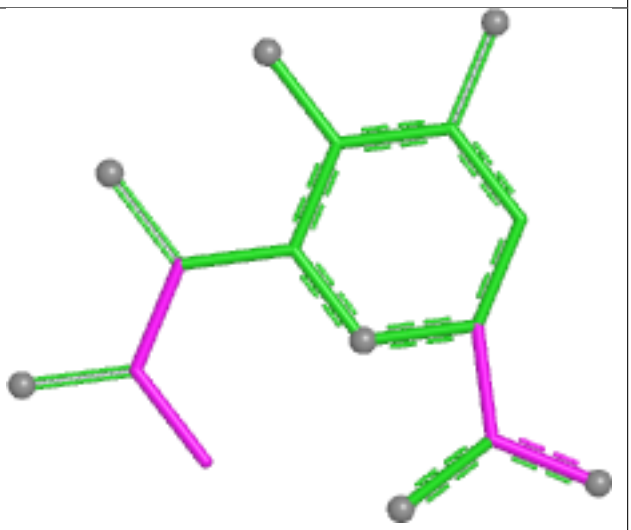


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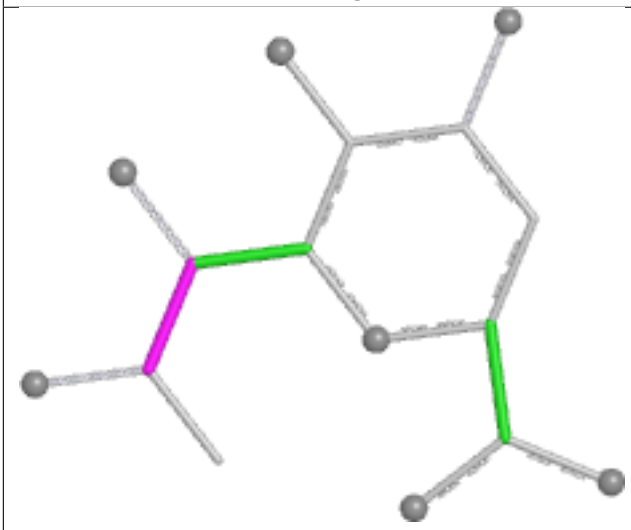
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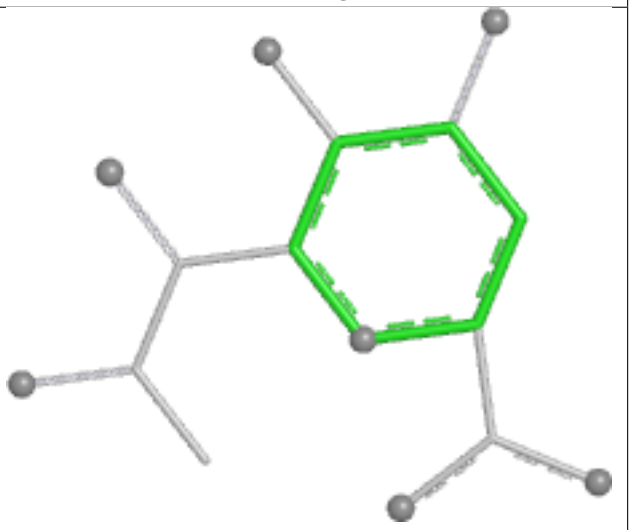
Bond lengths



Bond angles

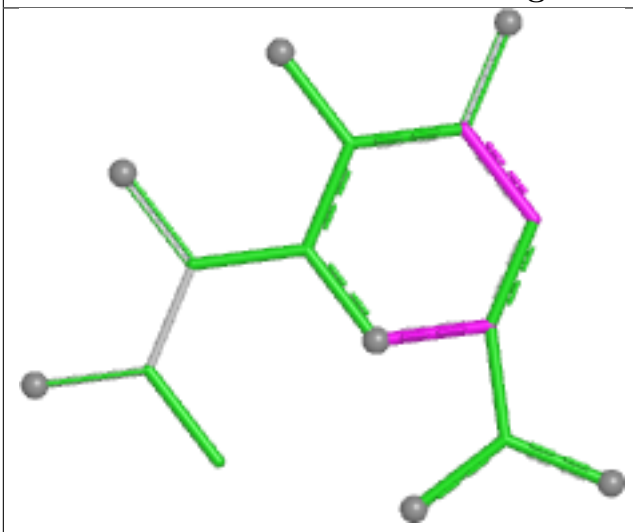


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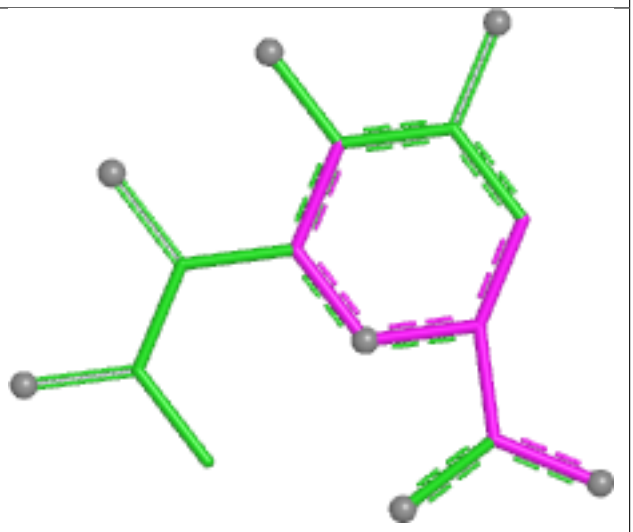


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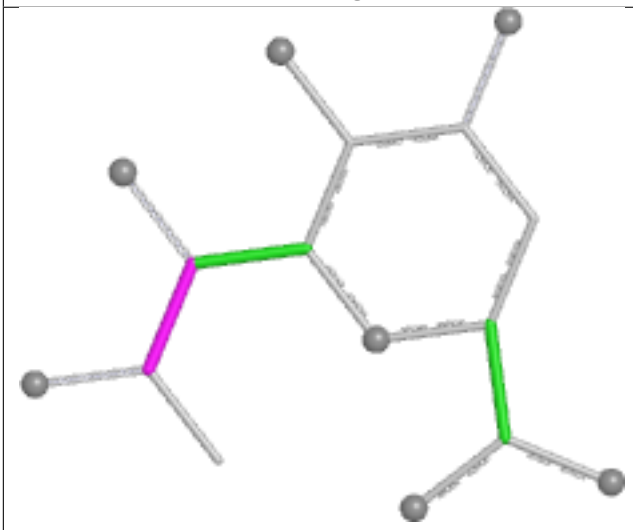
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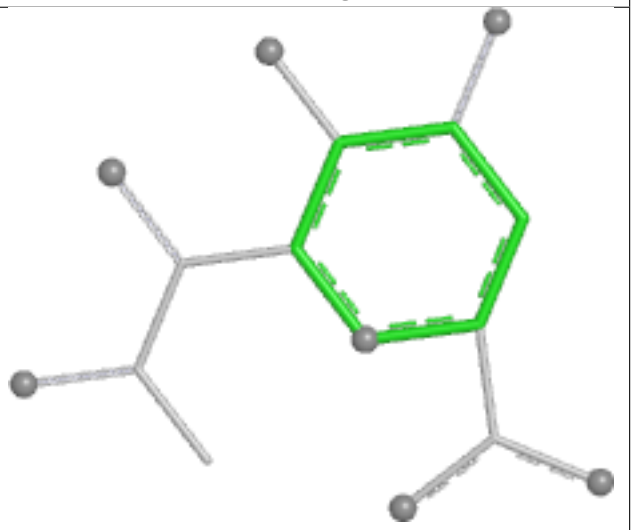
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Bond angles

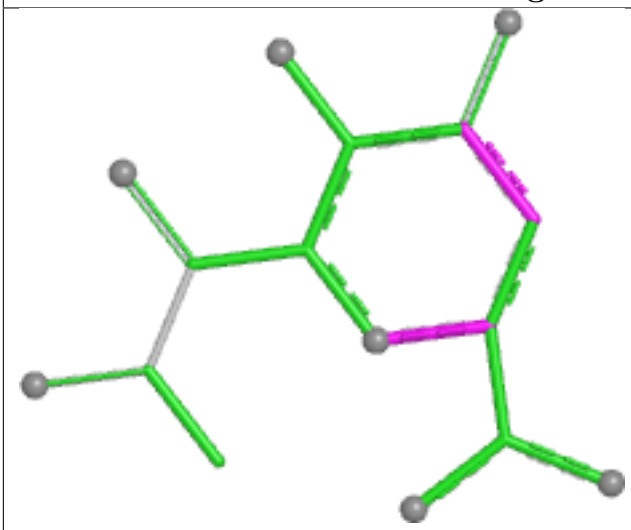


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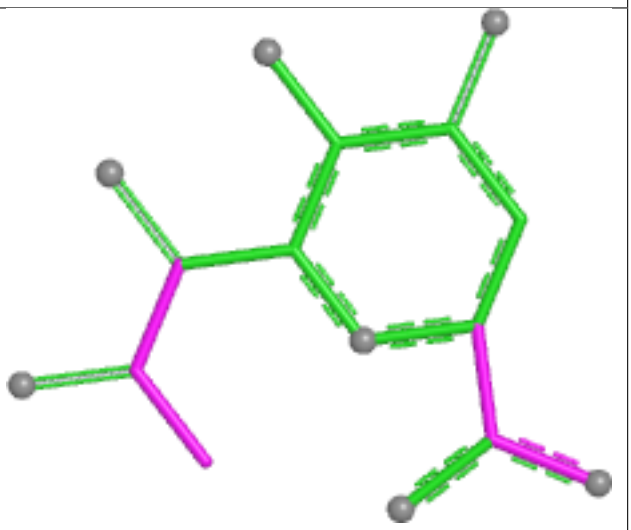


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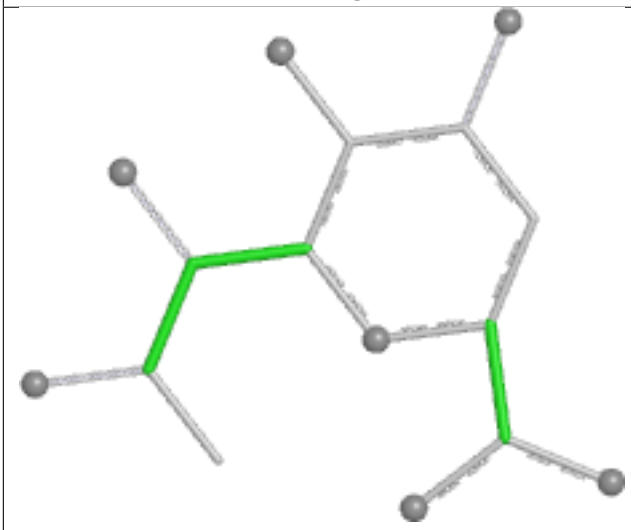
Ligand P8E H 613



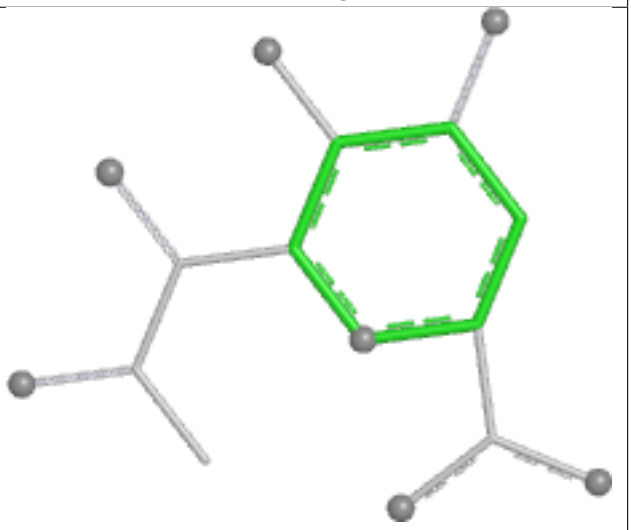
Bond lengths



Bond angles

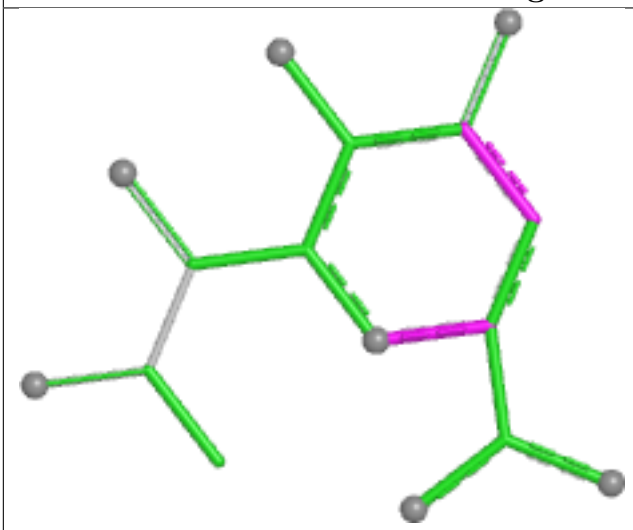


Torsions

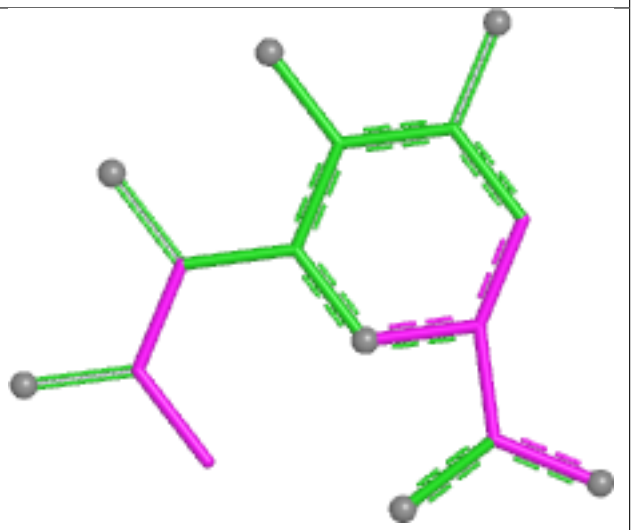


Rings

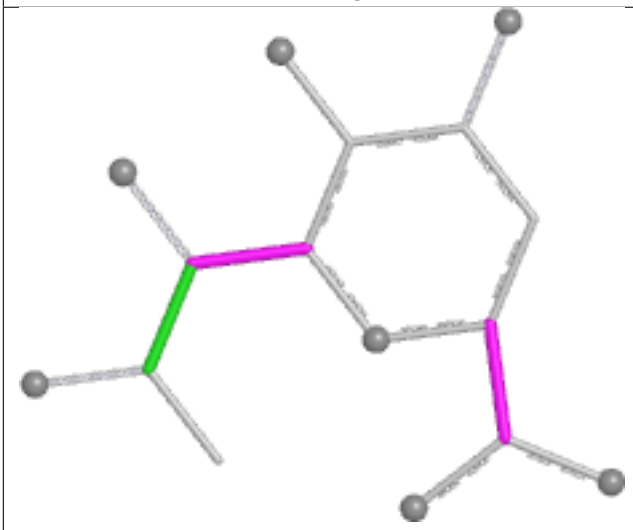
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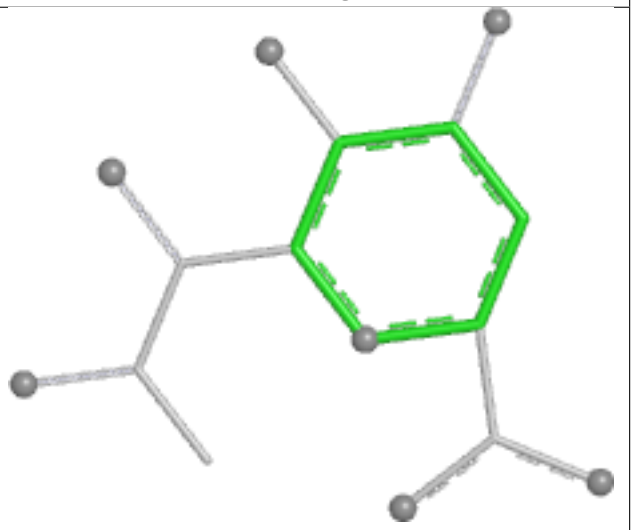
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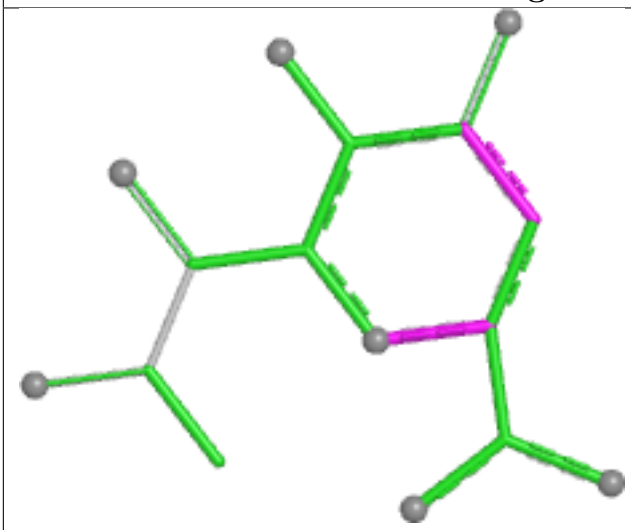


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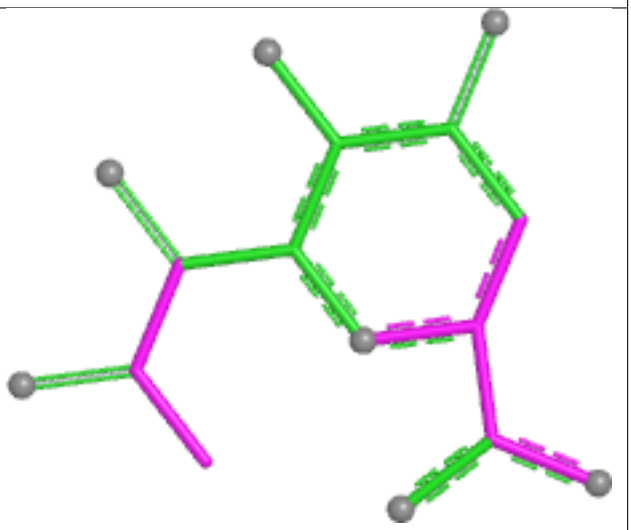


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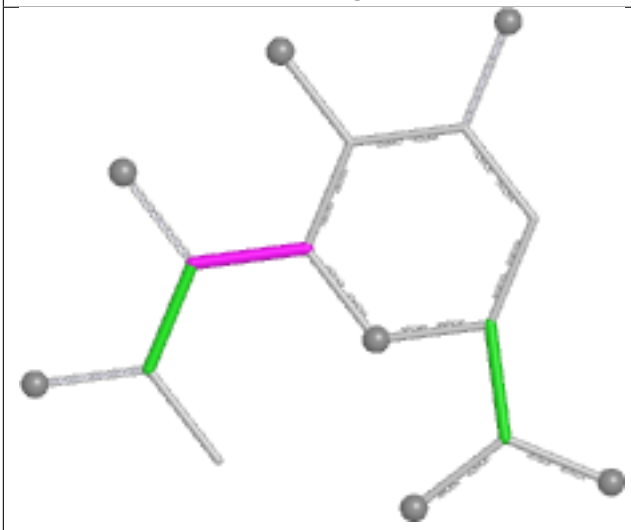
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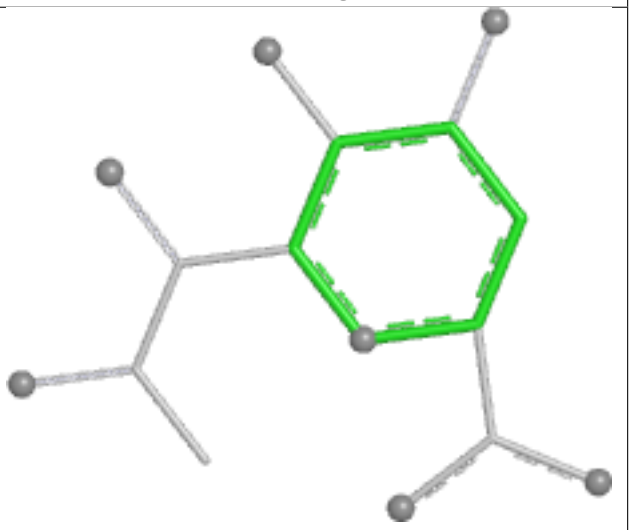
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Bond angles

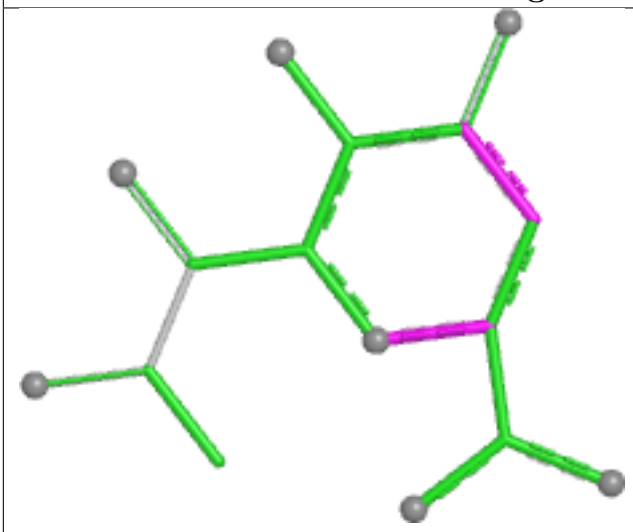


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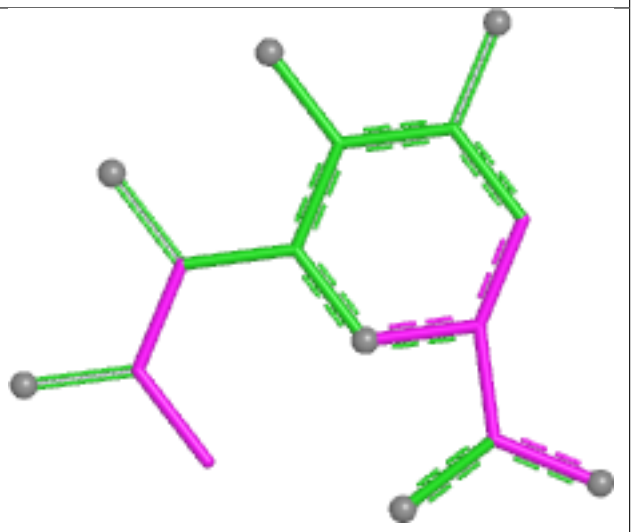


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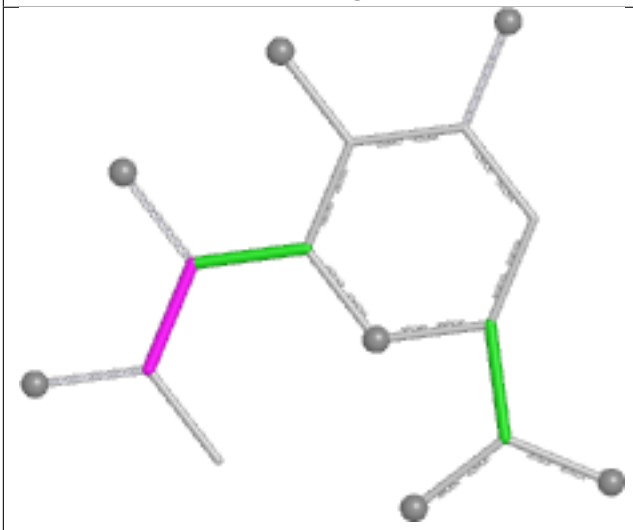
Ligand P8E U 603



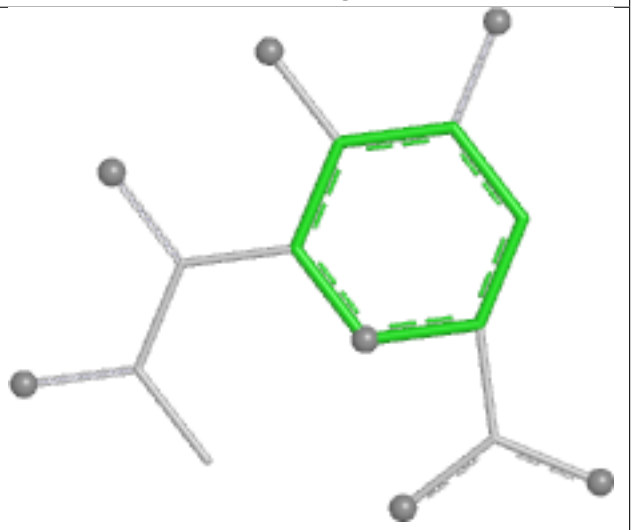
Bond lengths



Bond angles

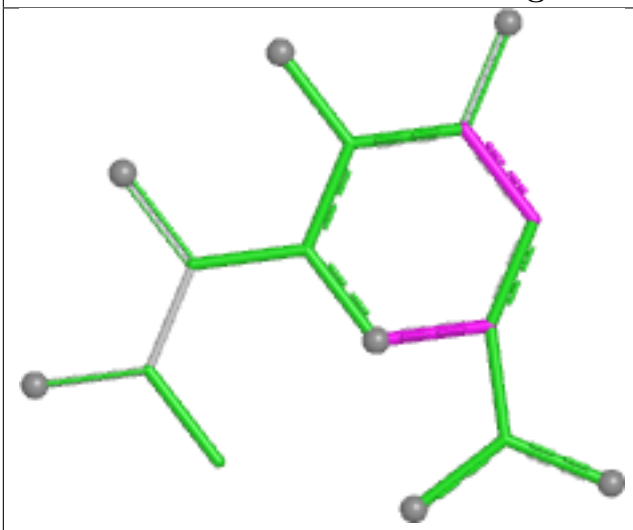


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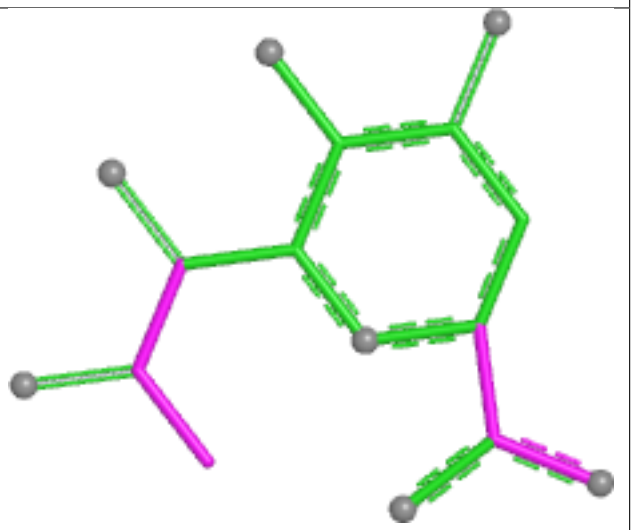


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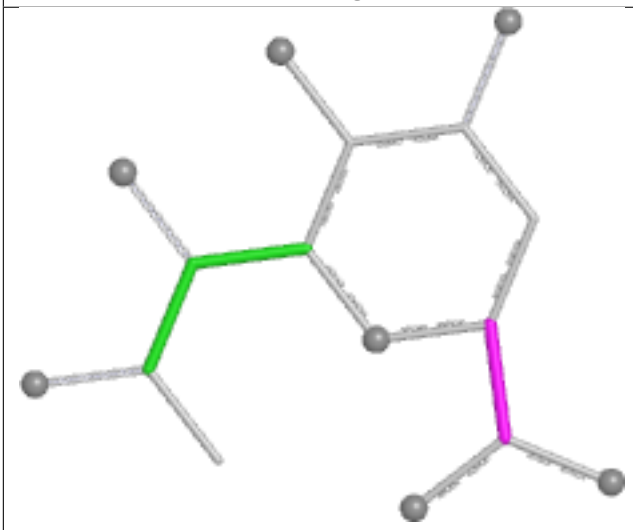
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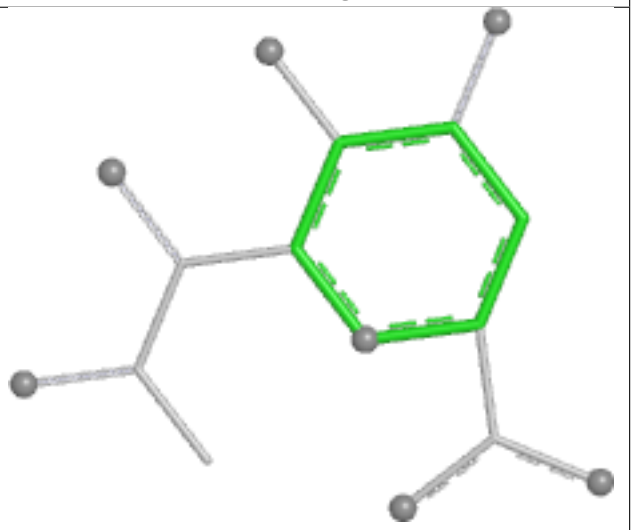
Bond lengths



Bond angles

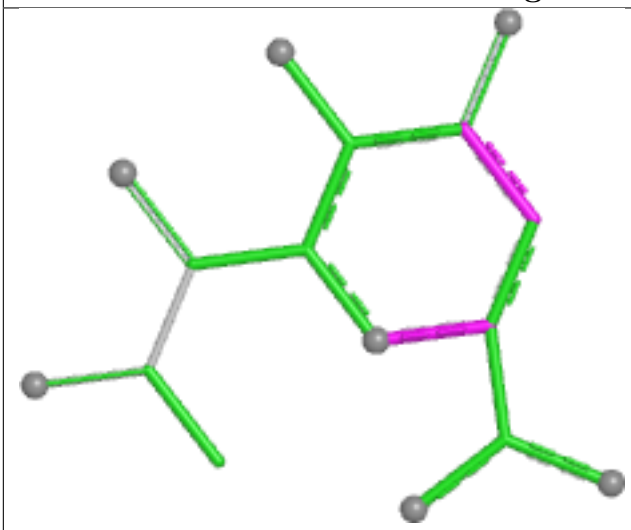


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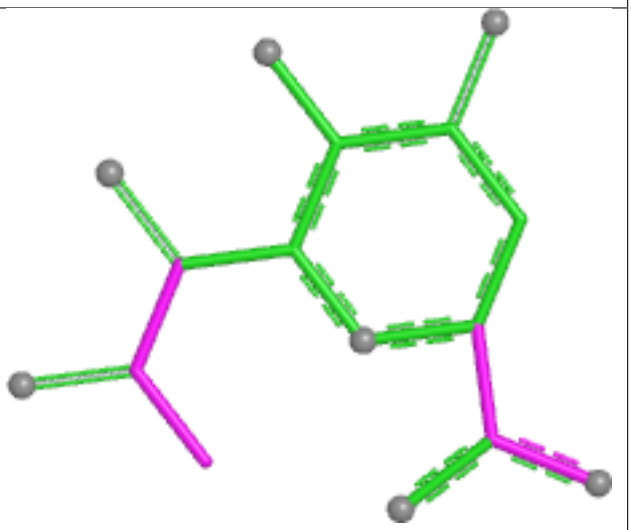


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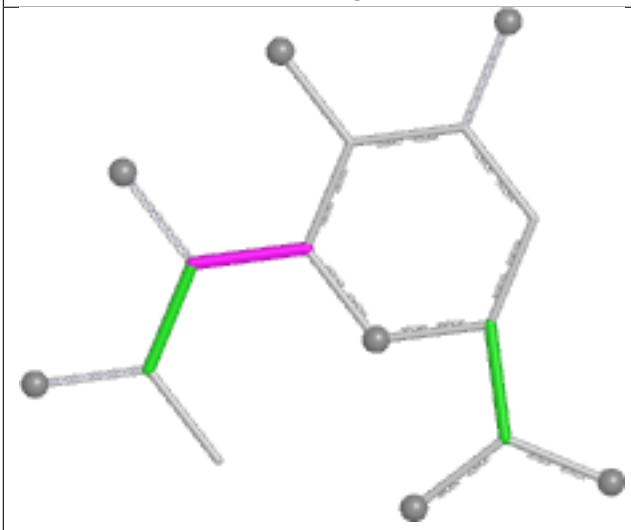
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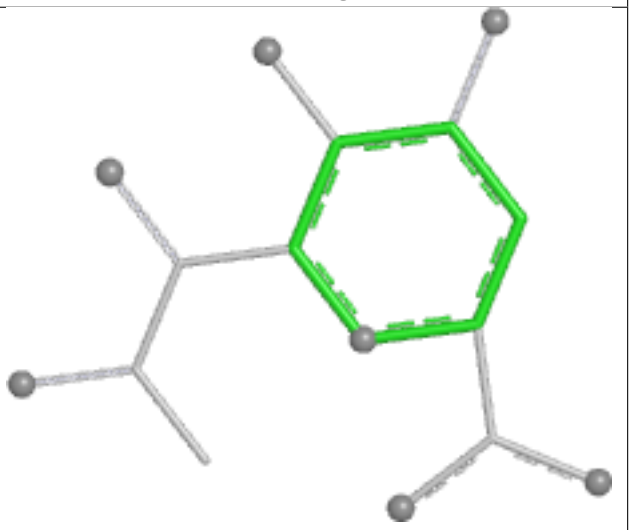
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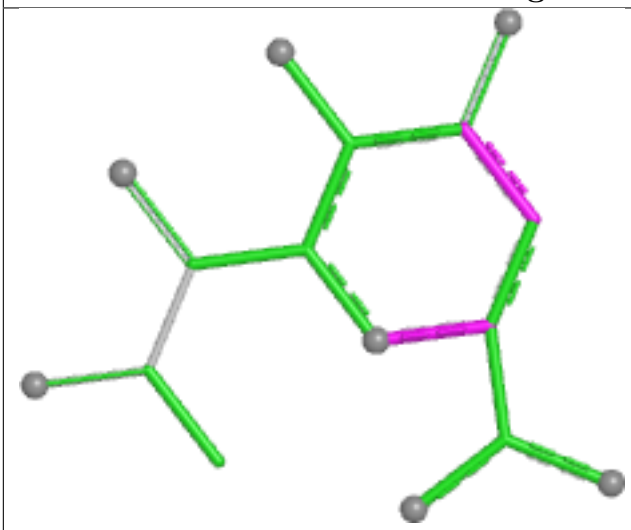


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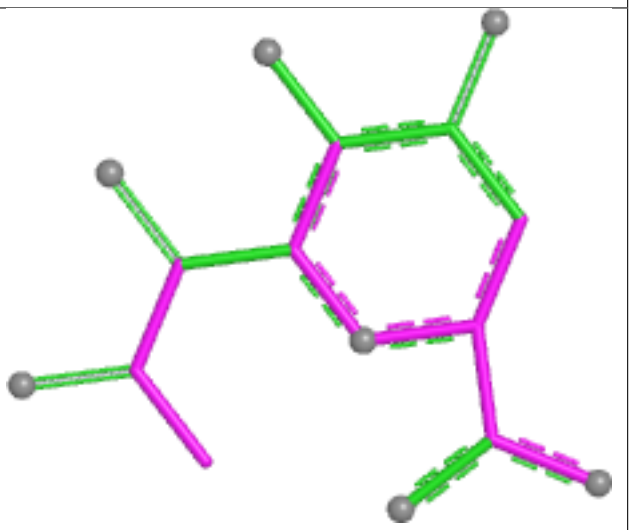


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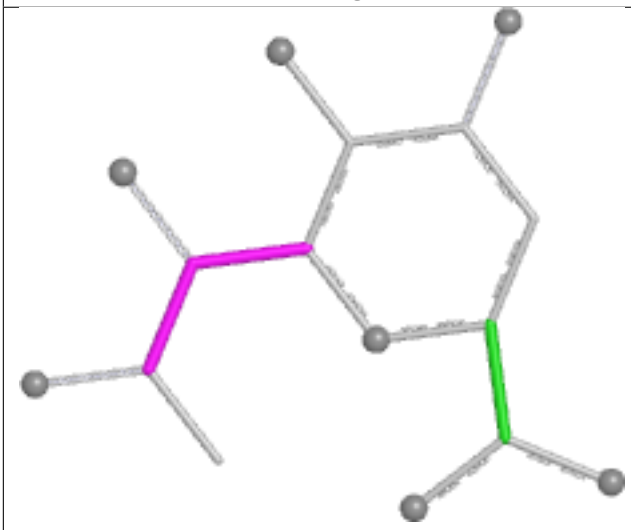
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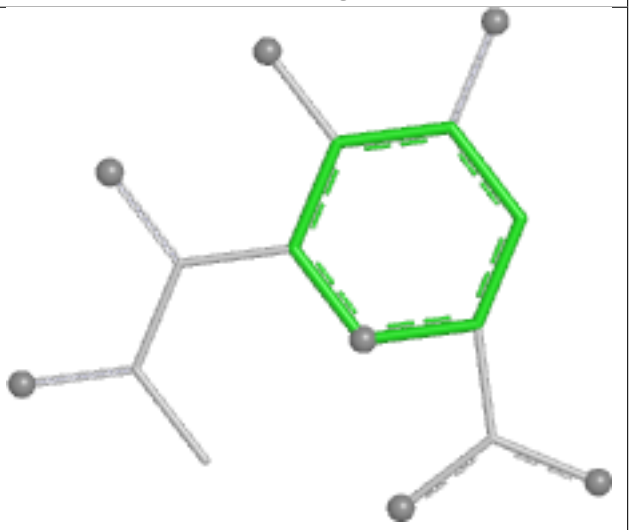
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Bond angles

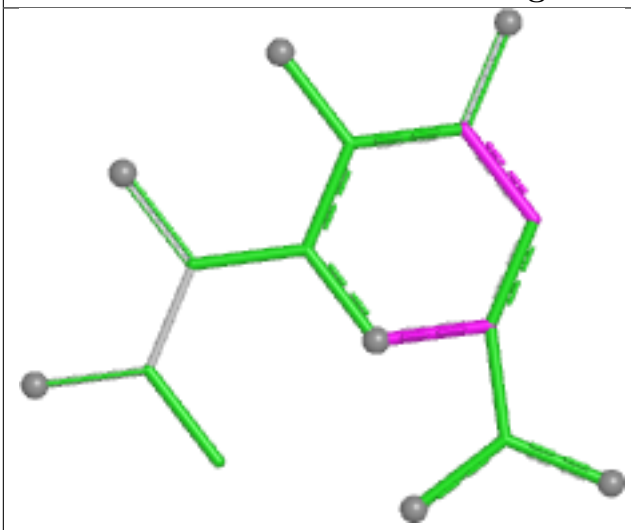


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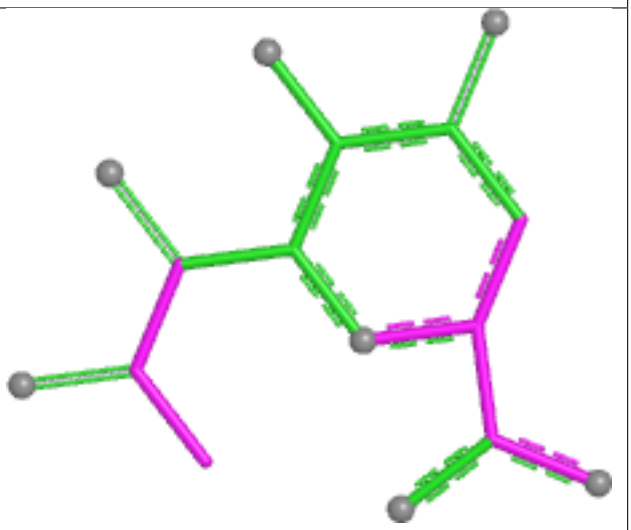


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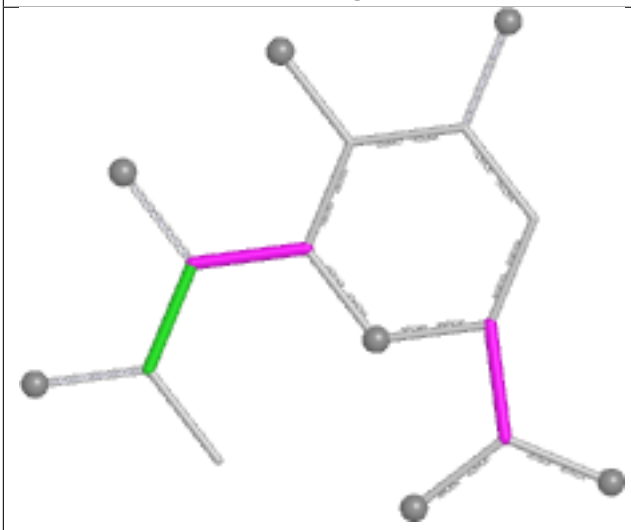
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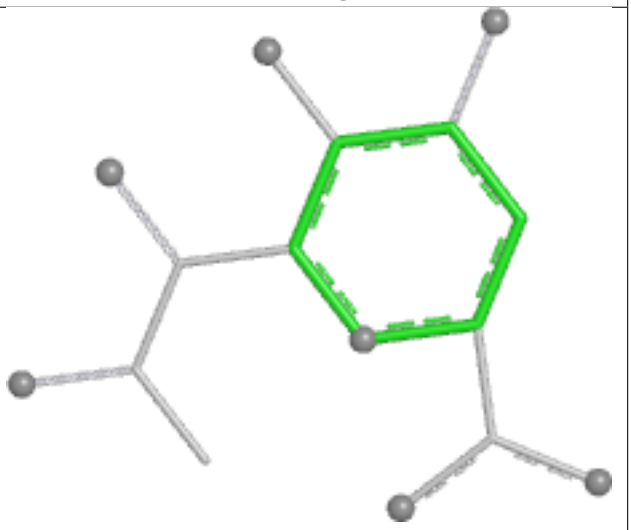
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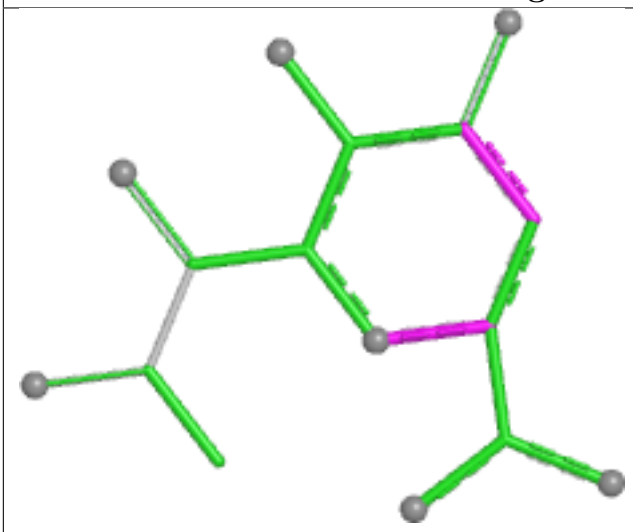


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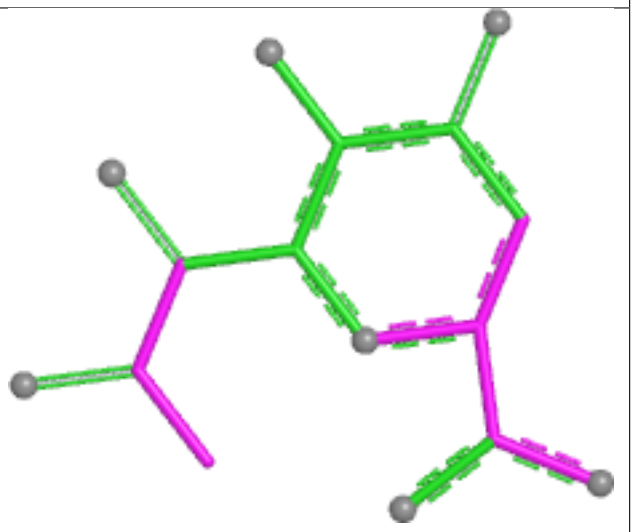


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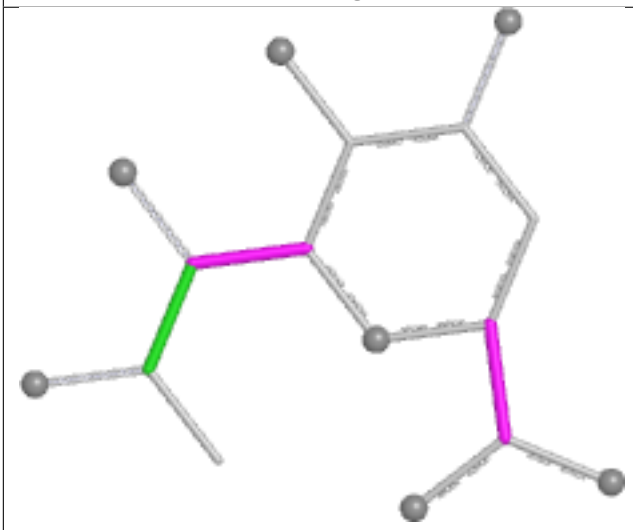
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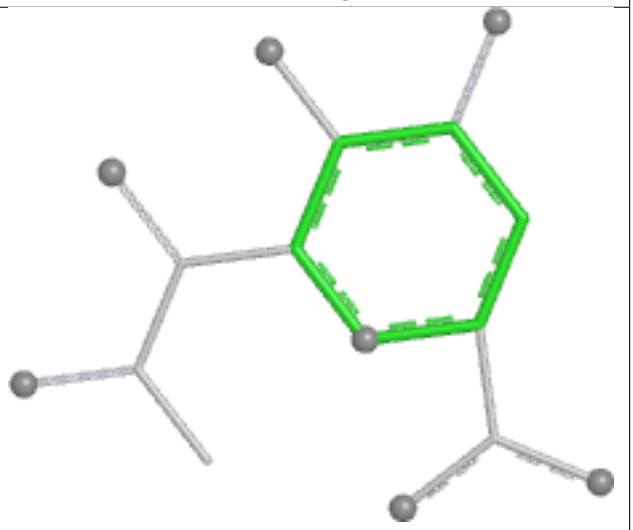
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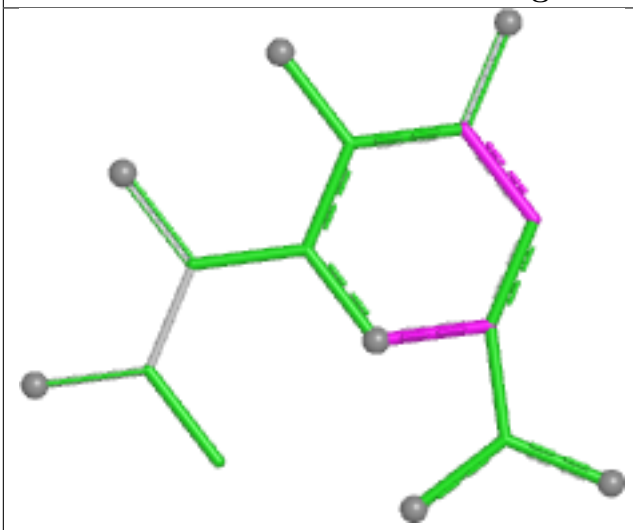


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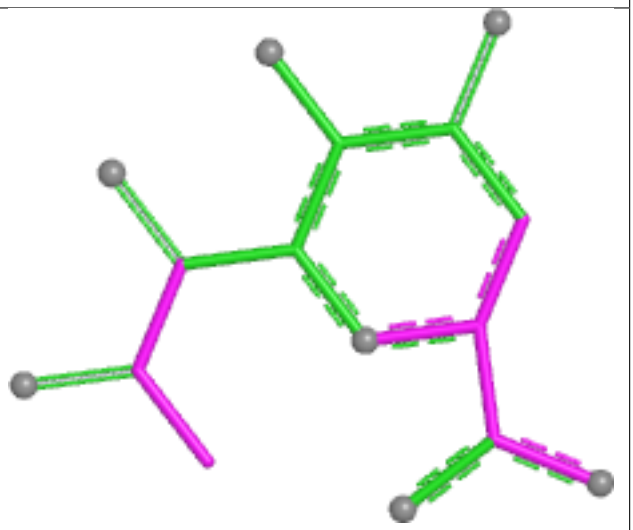


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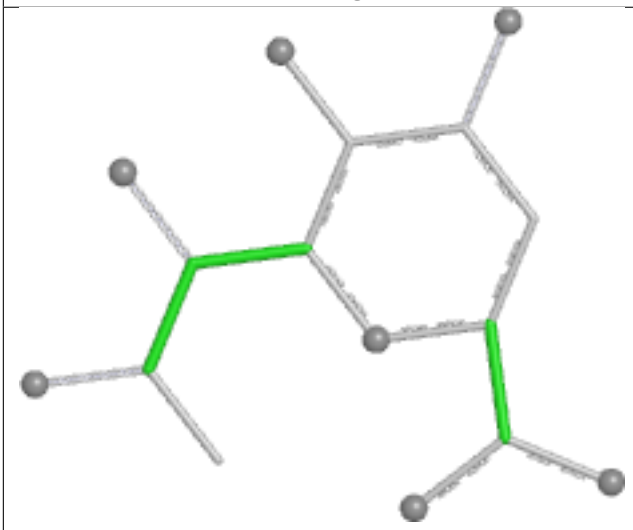
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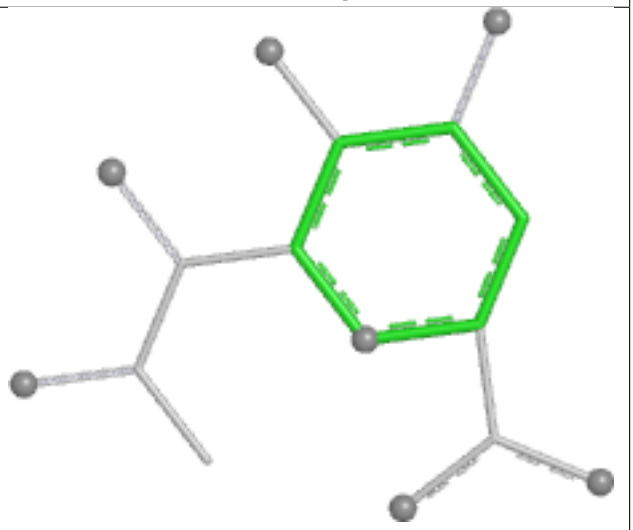
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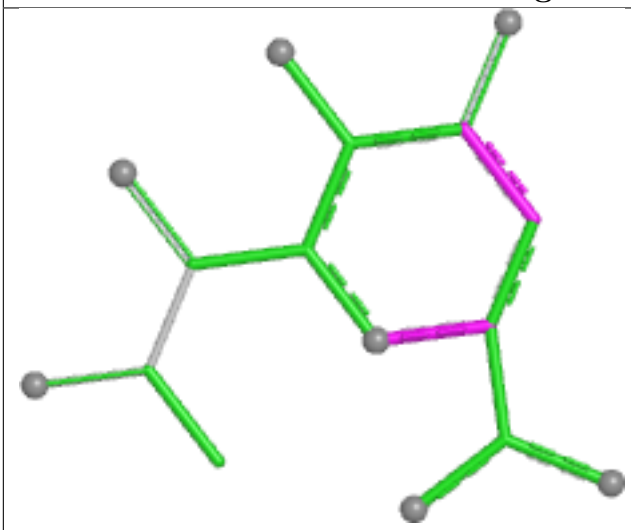


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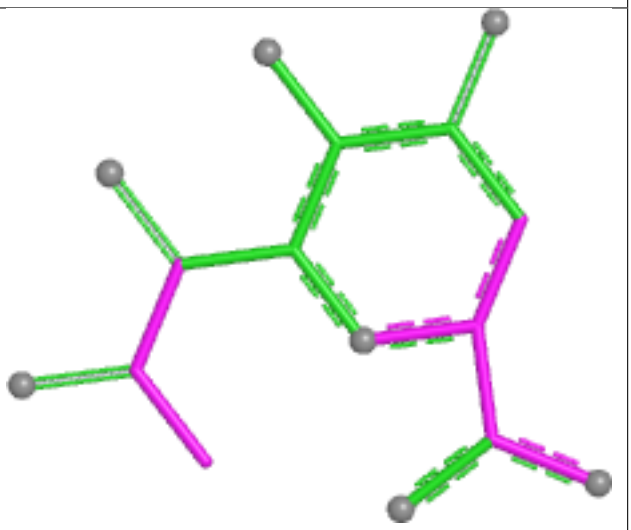


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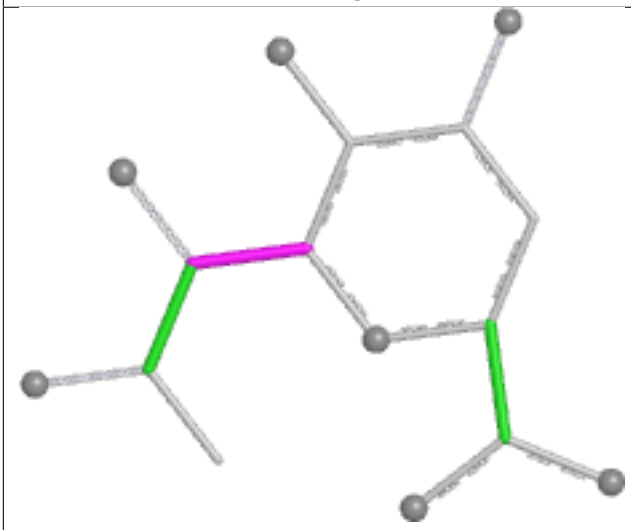
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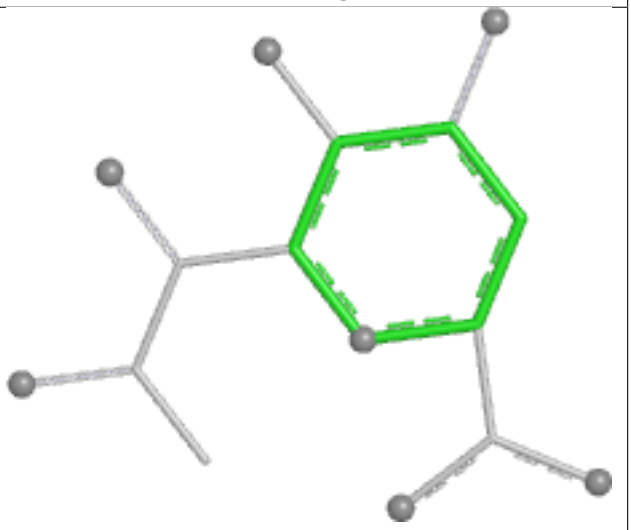
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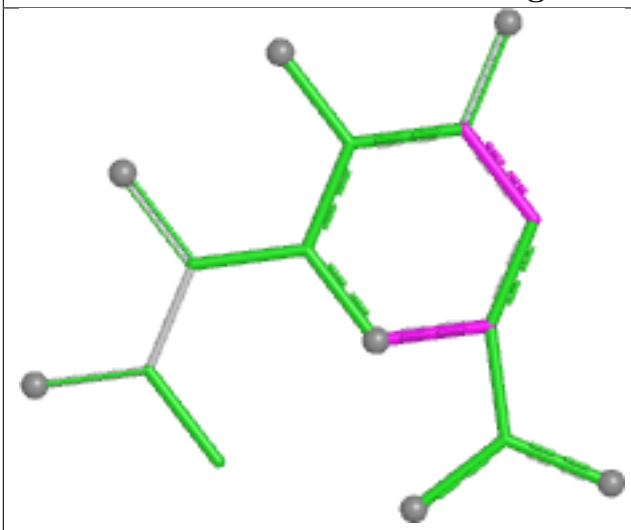


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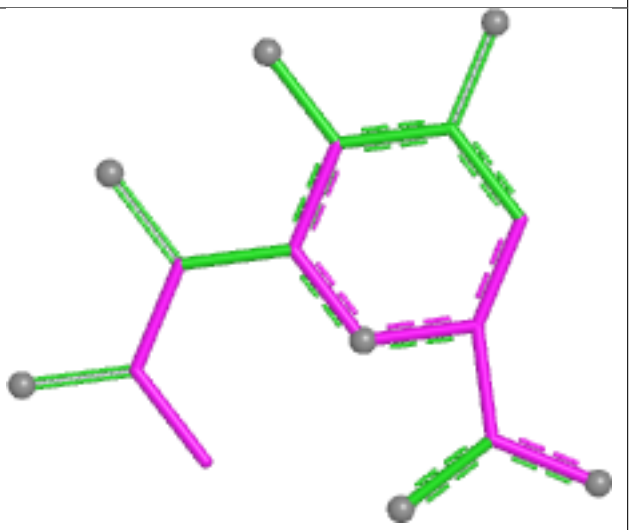


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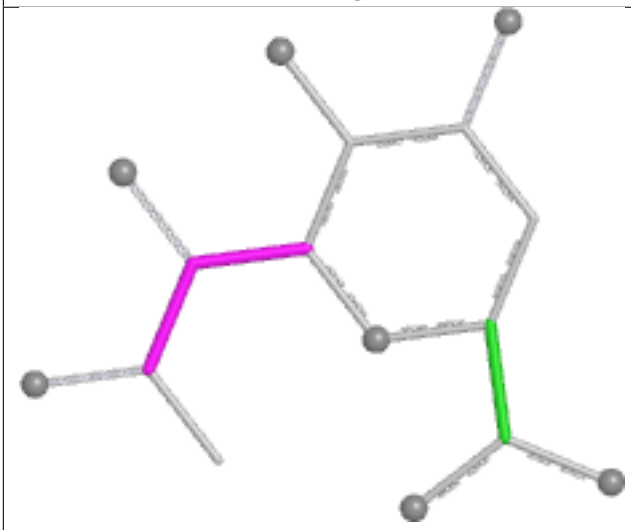
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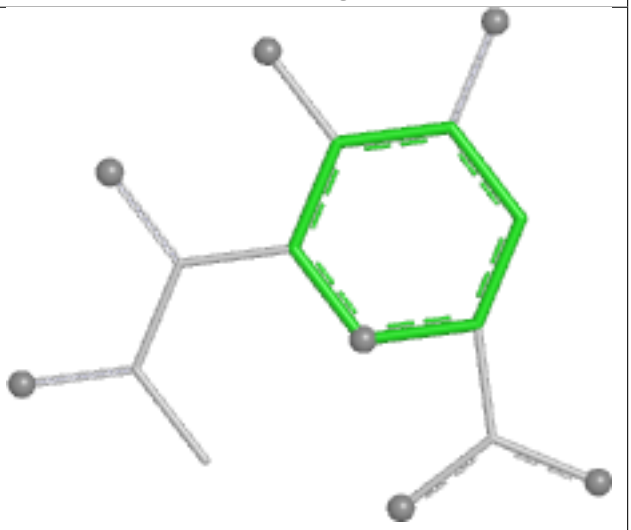
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Bond angles

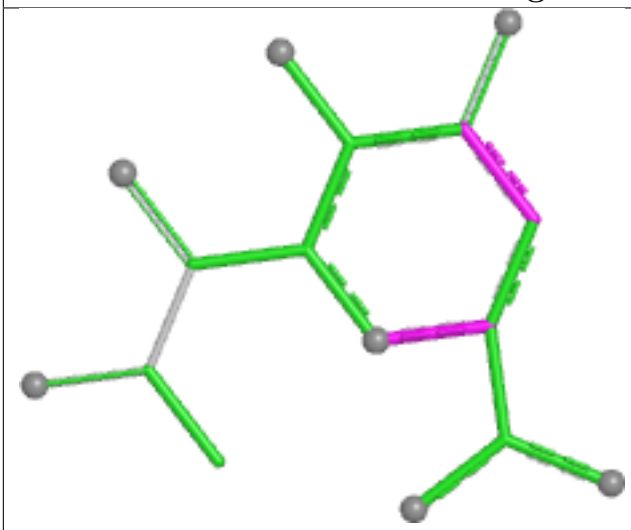


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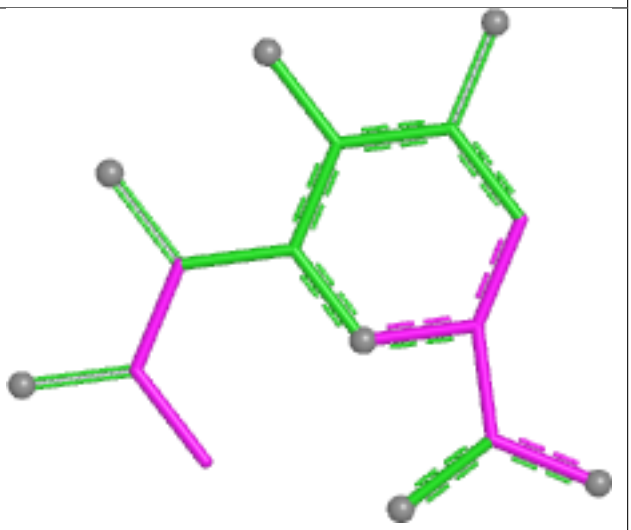


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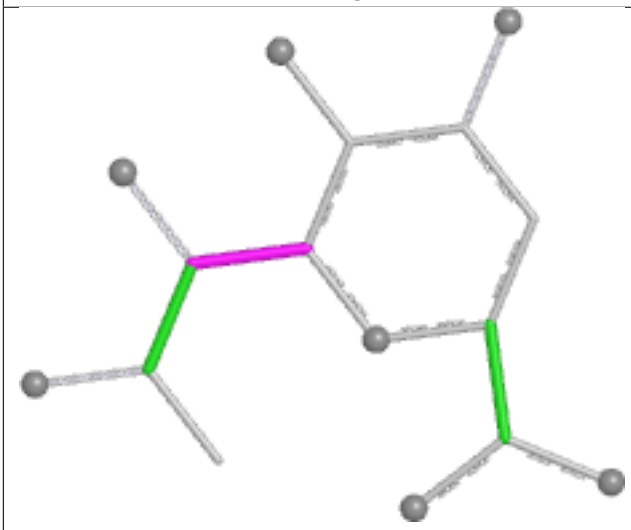
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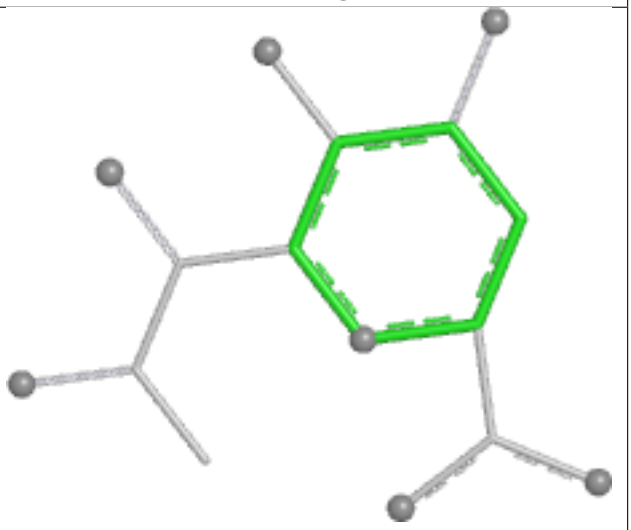
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Bond angles

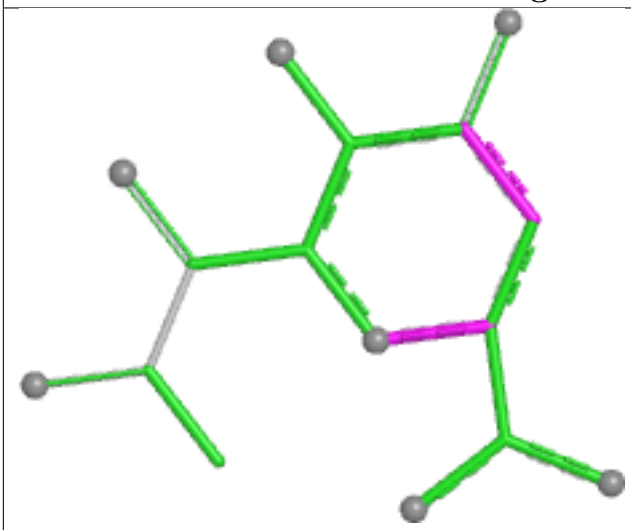


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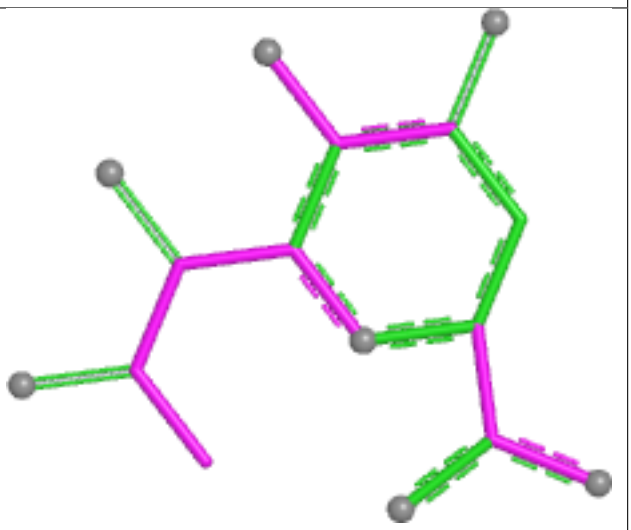


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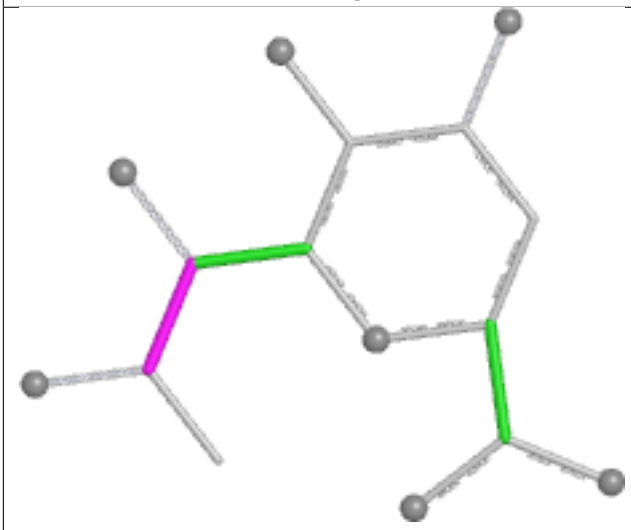
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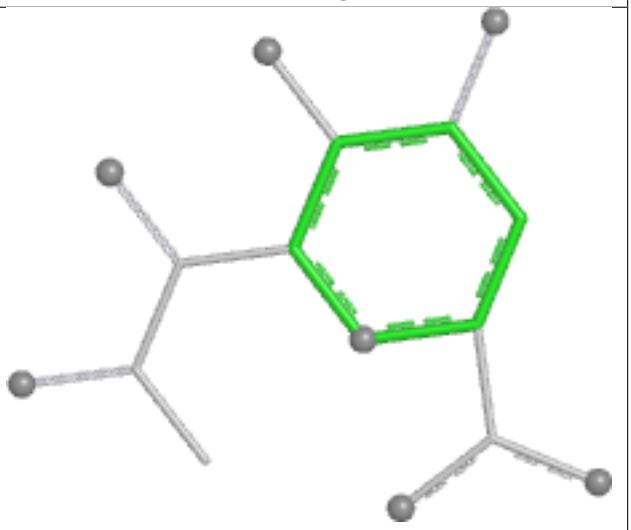
Bond lengths



Bond angles

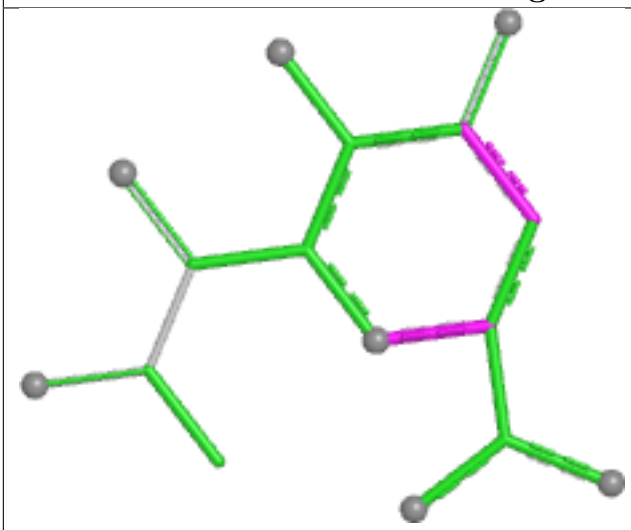


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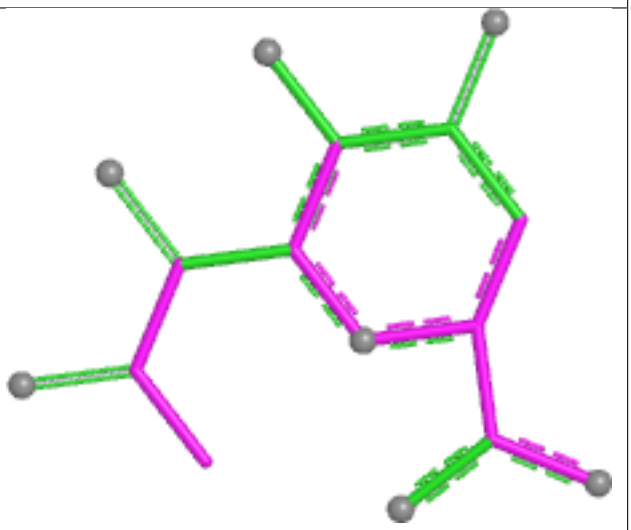


Rings

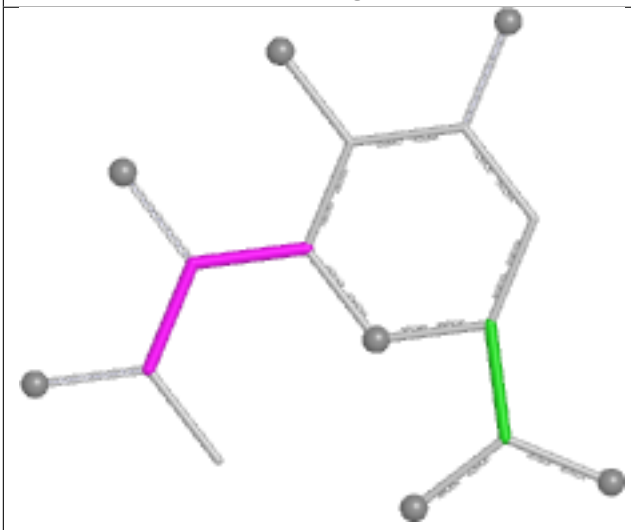
Ligand P8E C 606



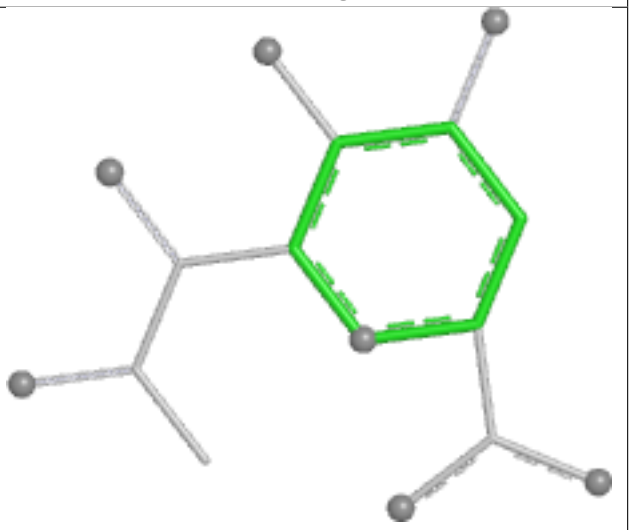
Bond lengths



Bond angles

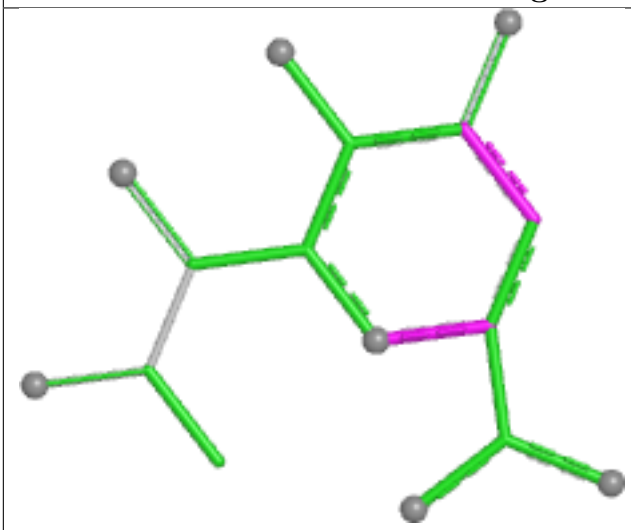


Torsions

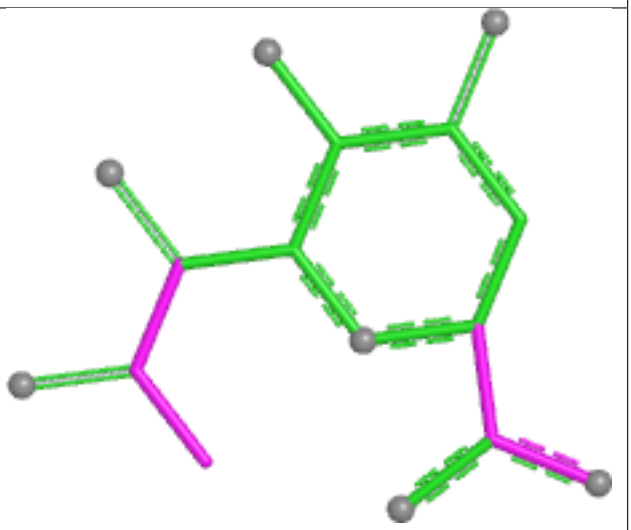


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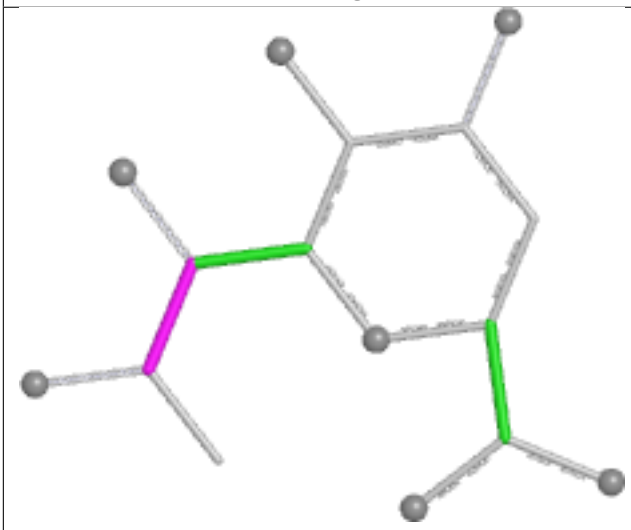
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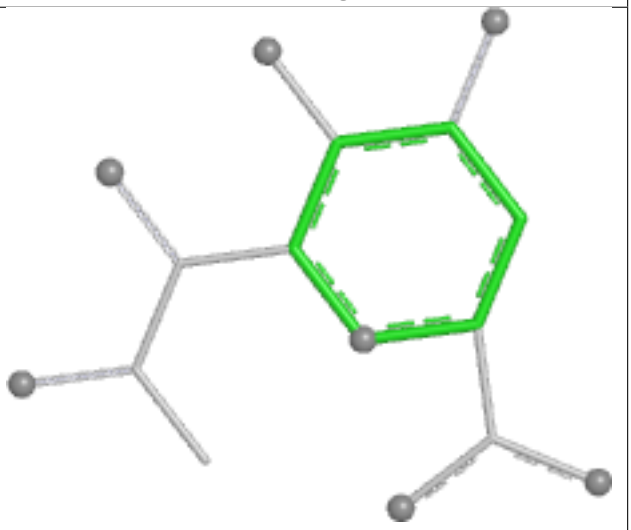
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Bond angles

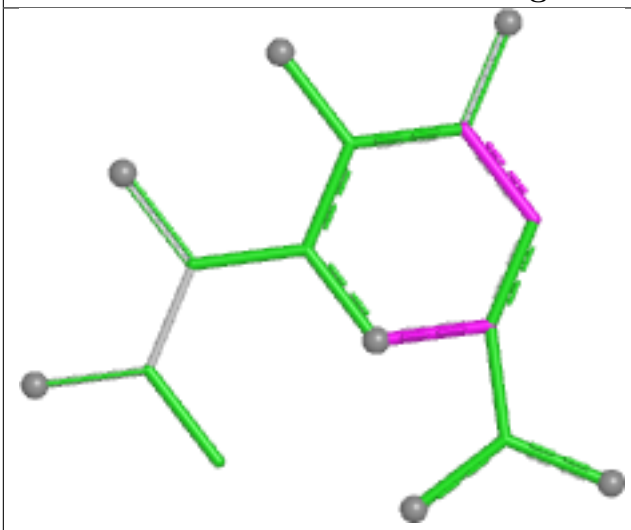


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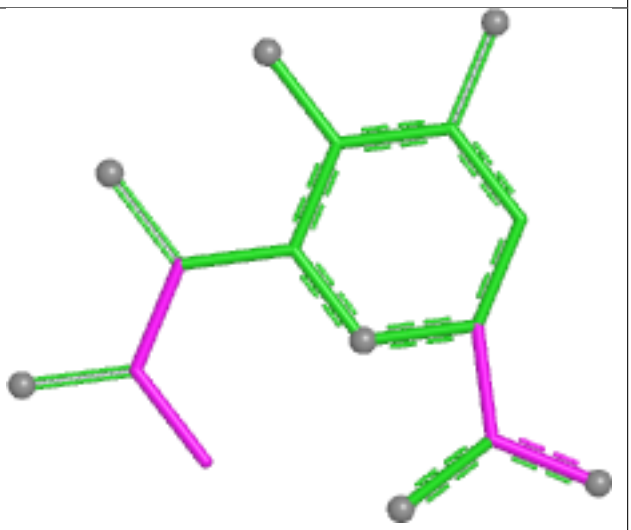


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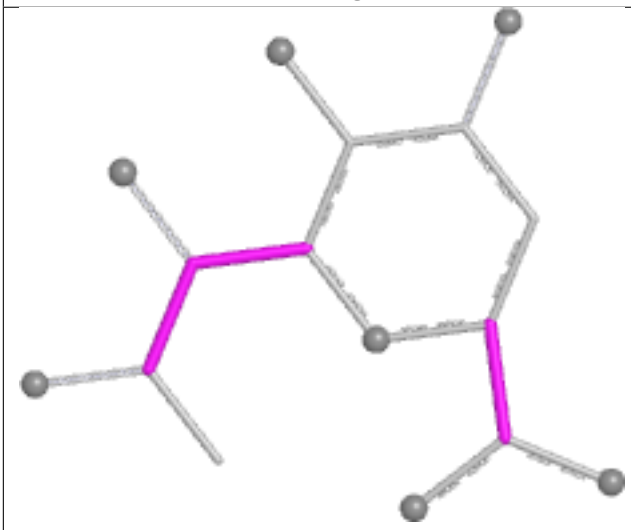
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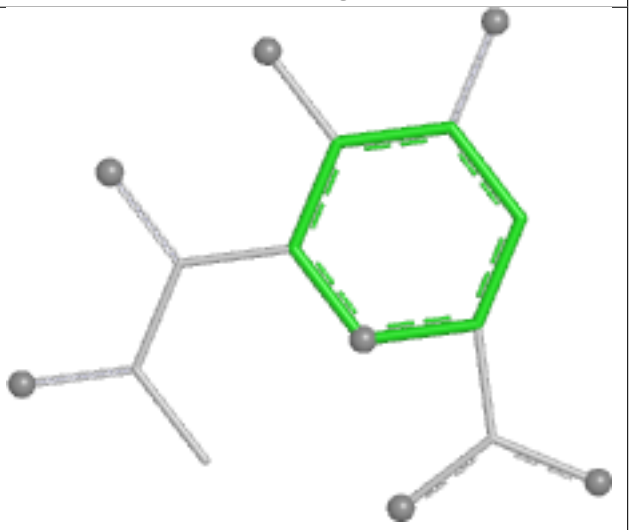
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Bond angles

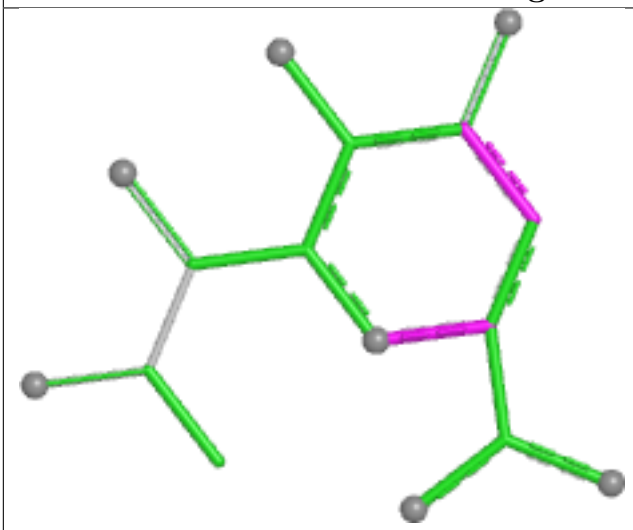


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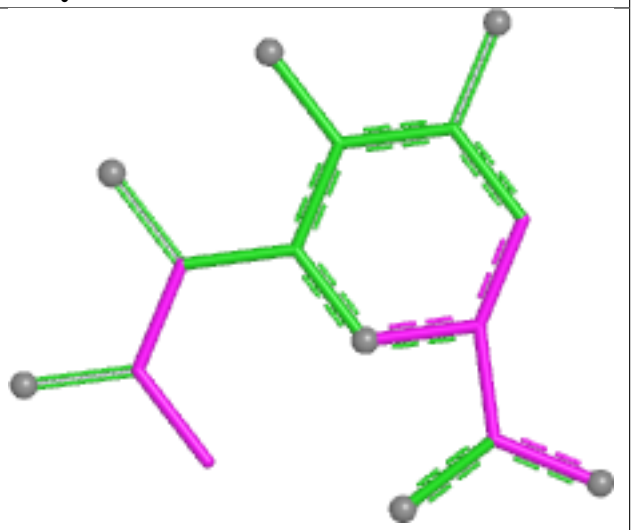


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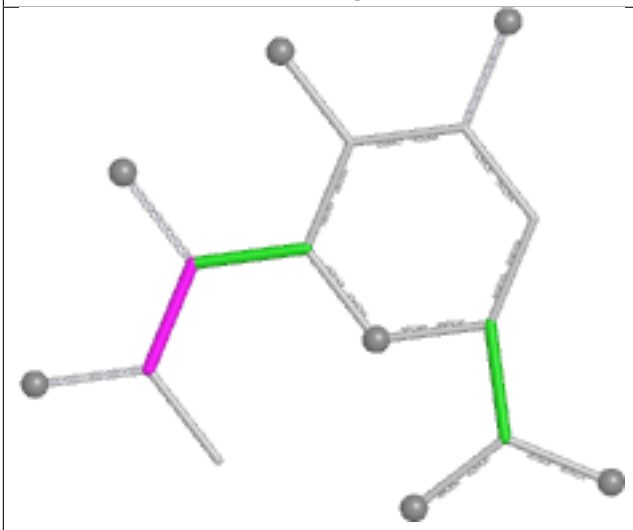
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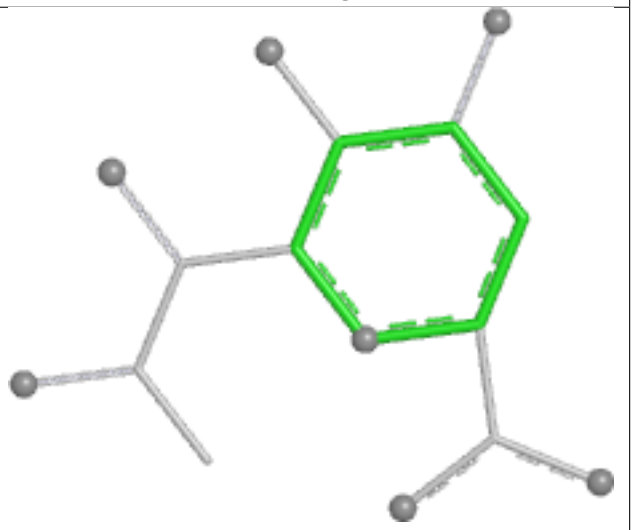
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Bond angles

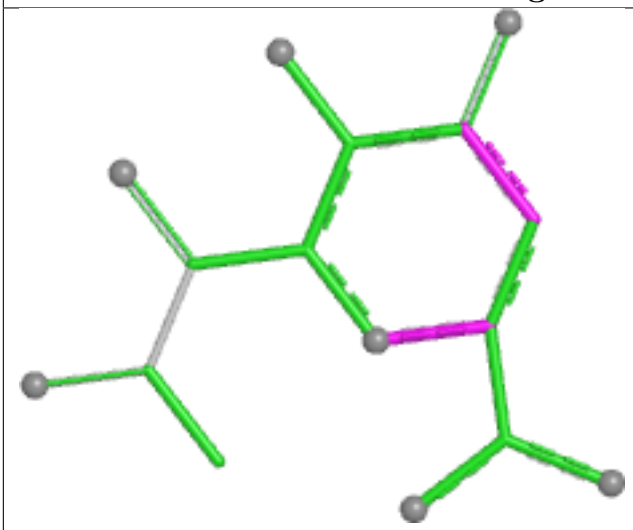


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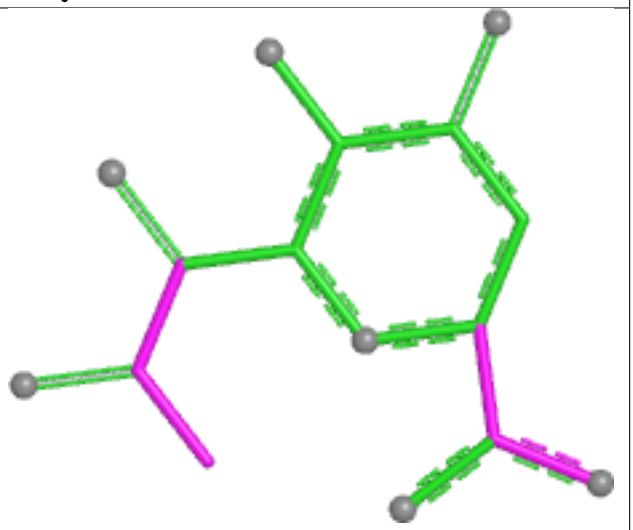


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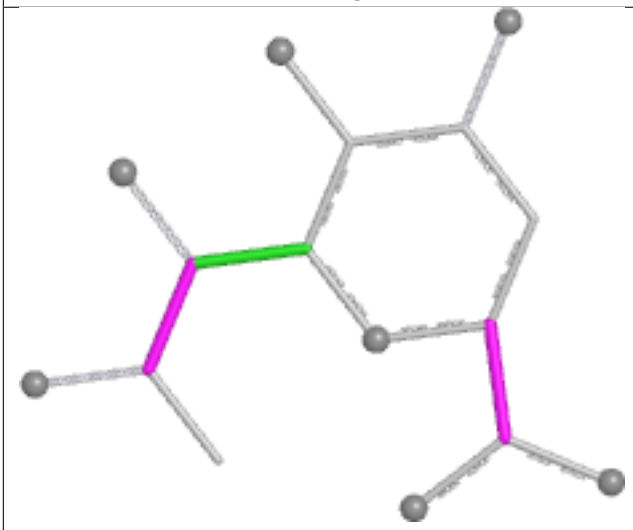
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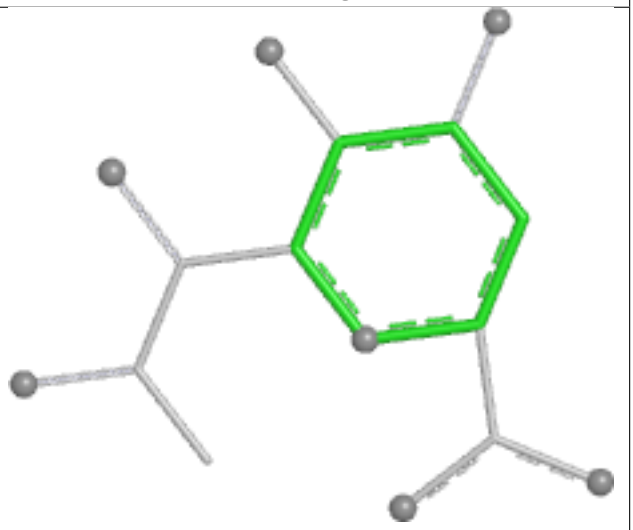
Bond lengths



Bond angles

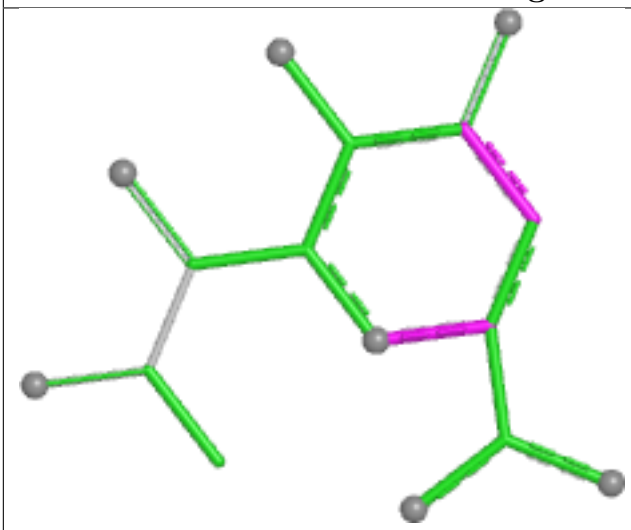


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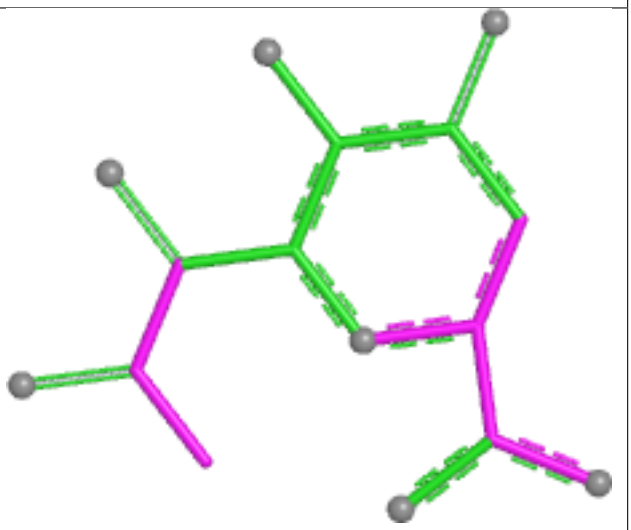


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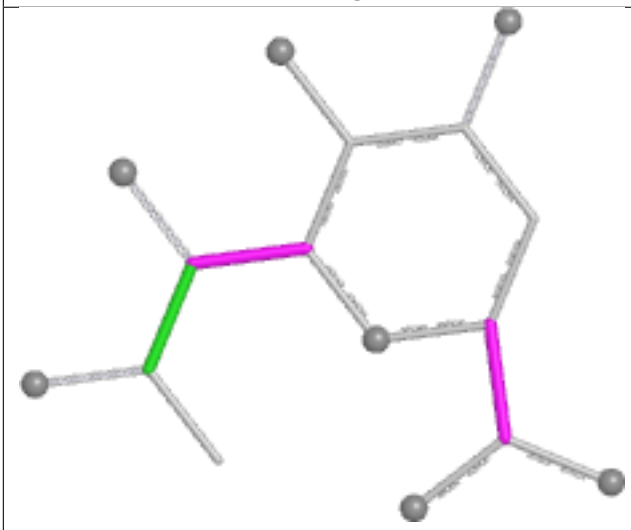
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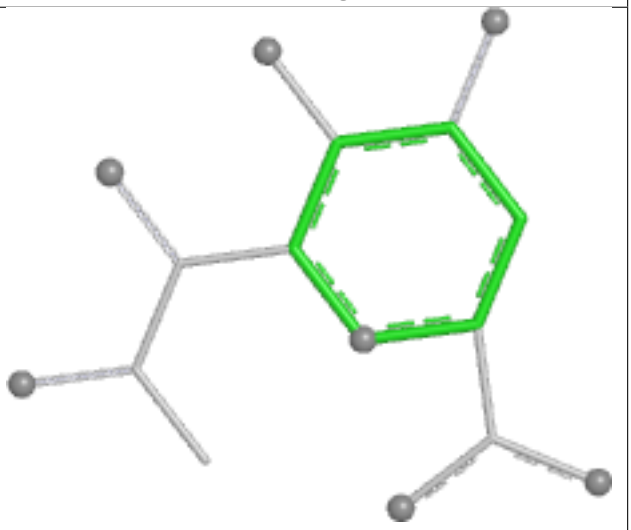
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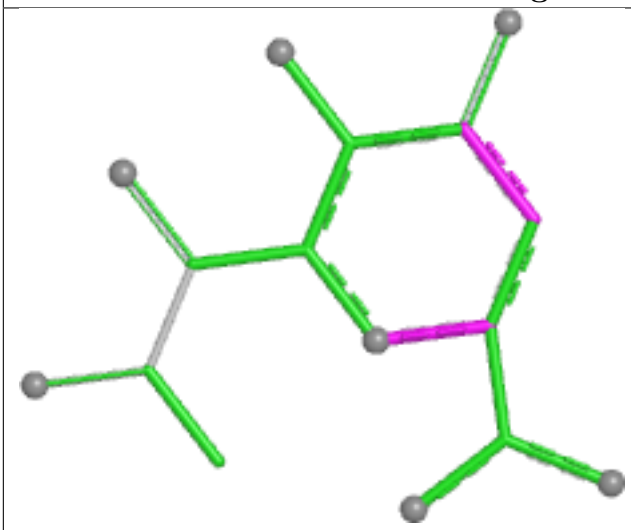


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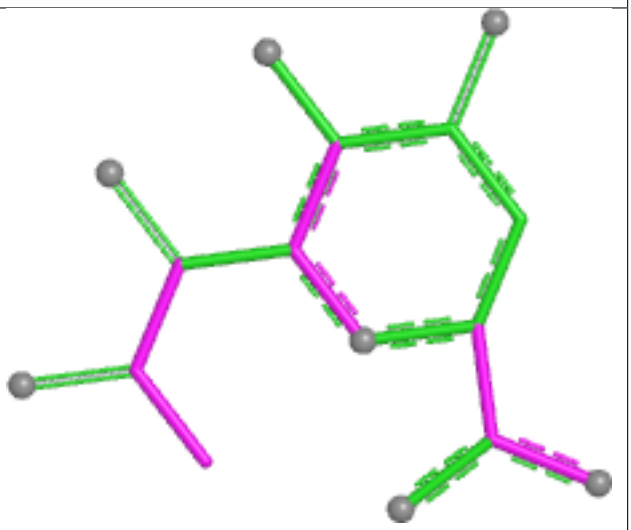


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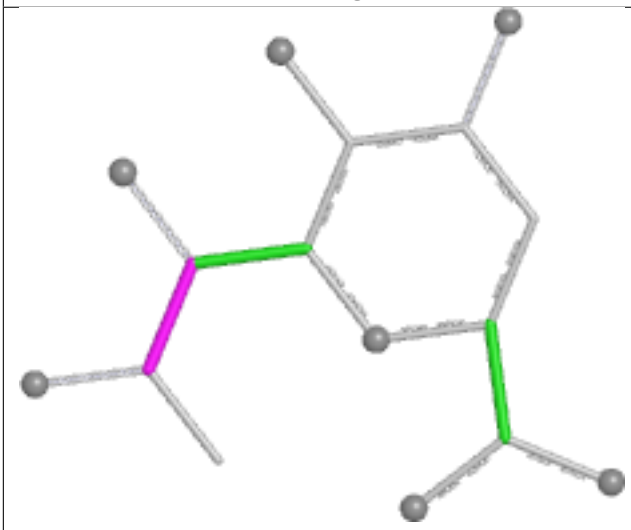
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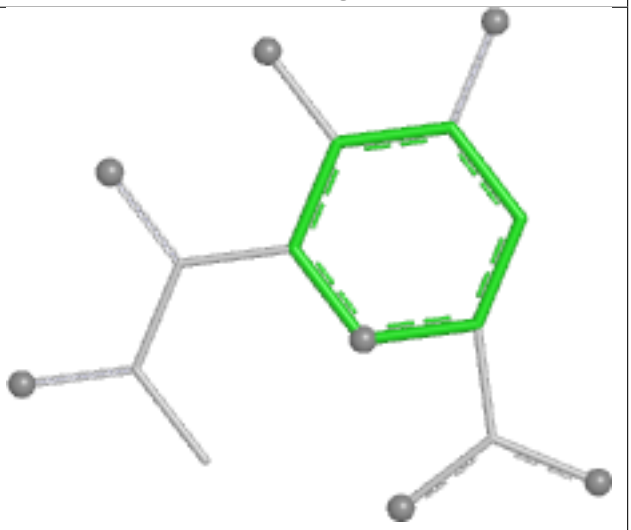
Bond lengths



Bond angles

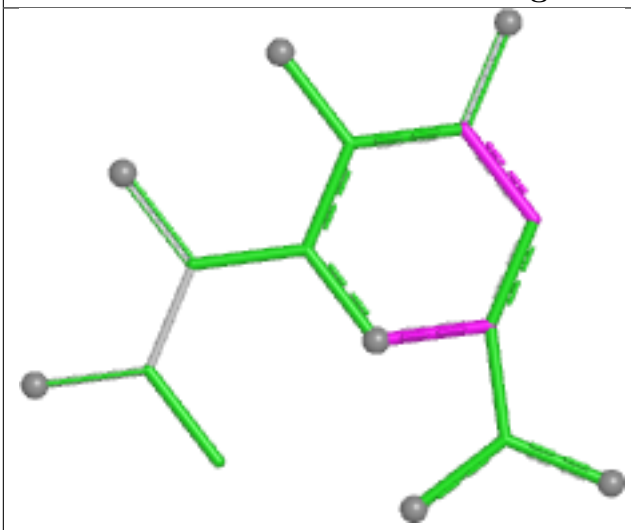


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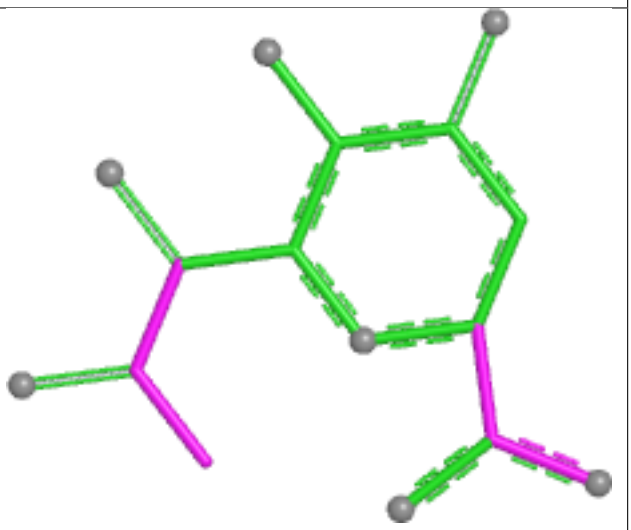


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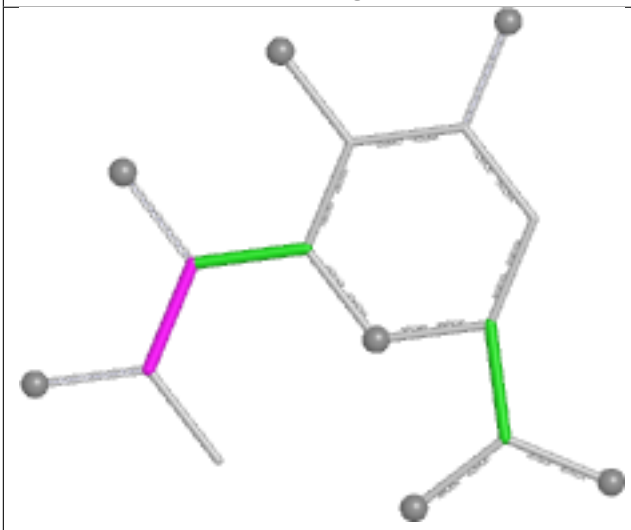
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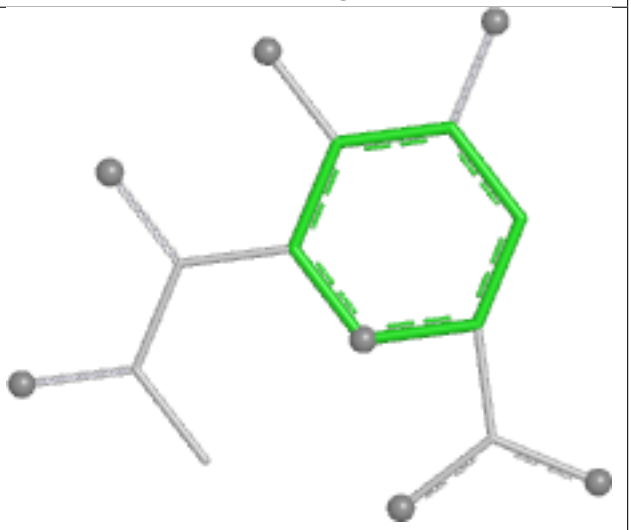
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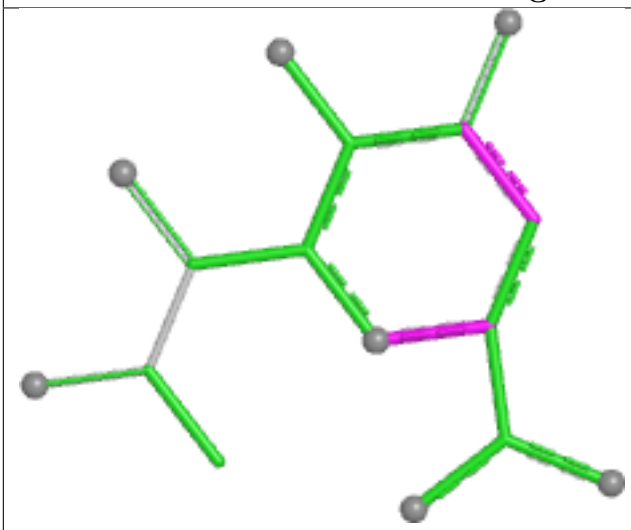


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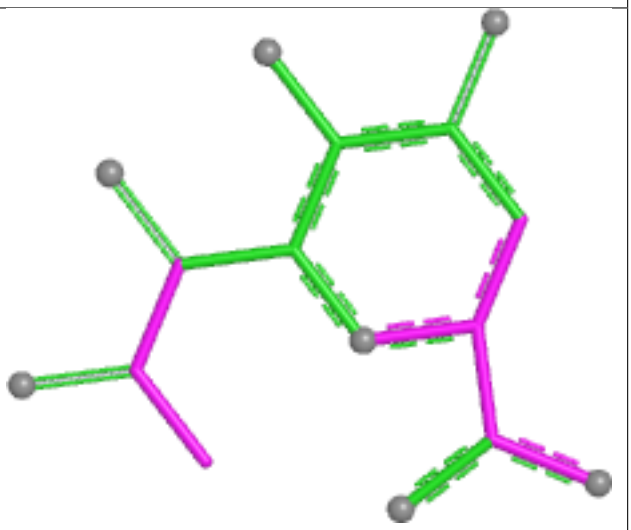


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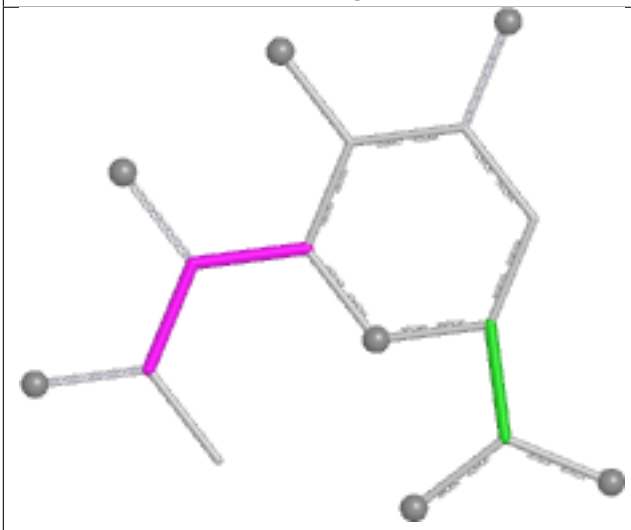
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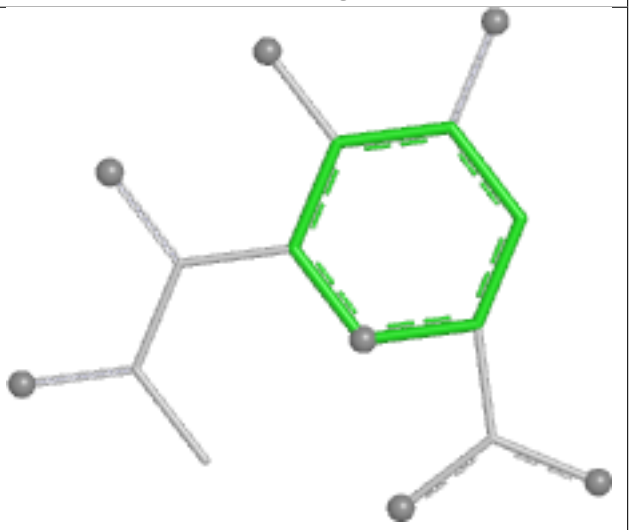
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Bond angles

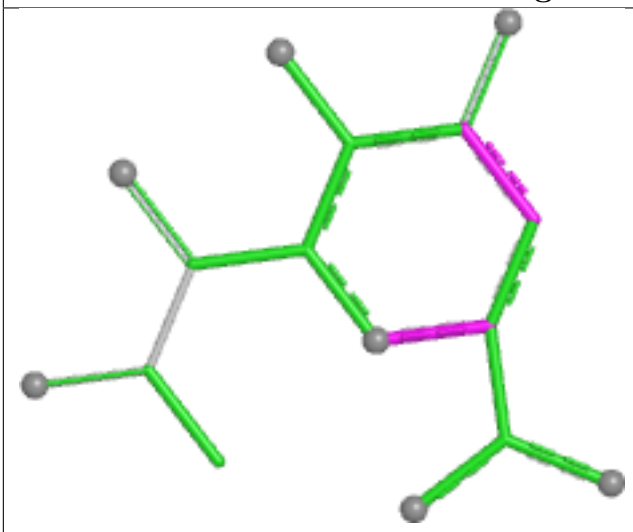


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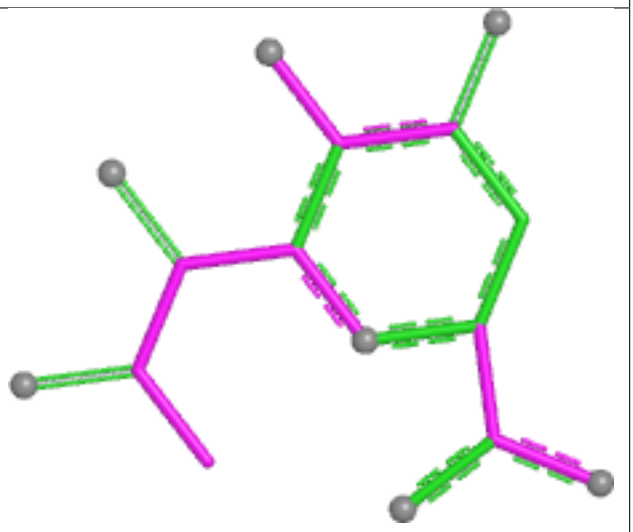


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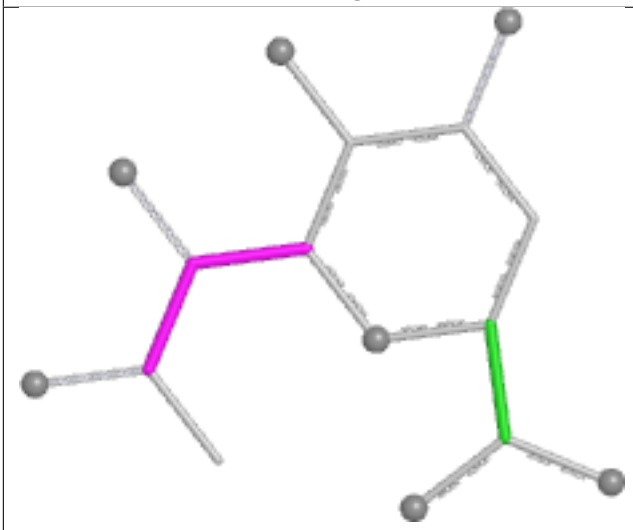
Ligand P8E I 616



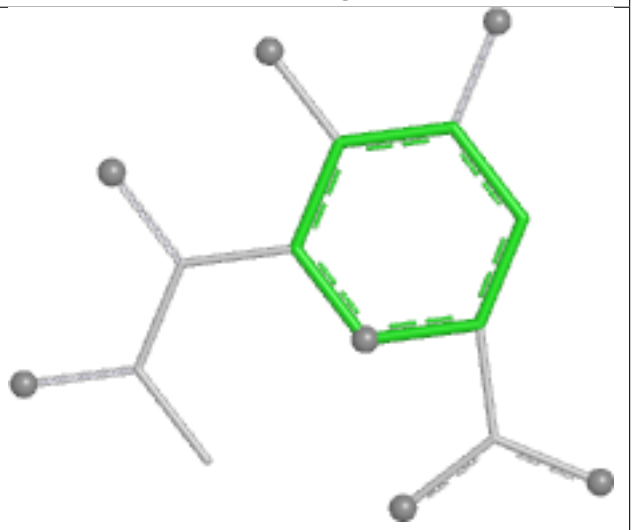
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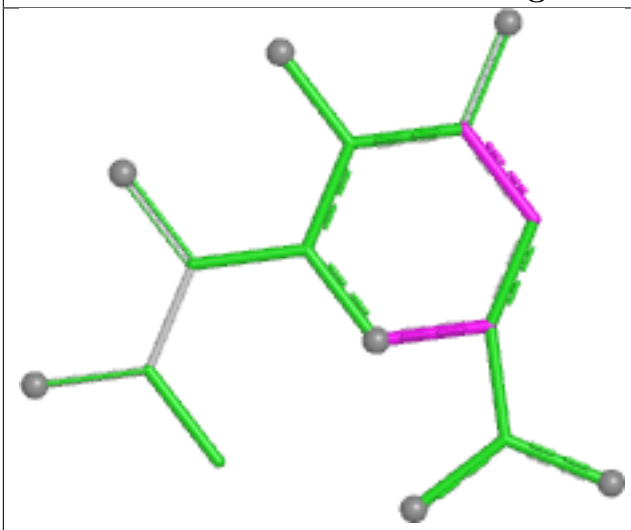


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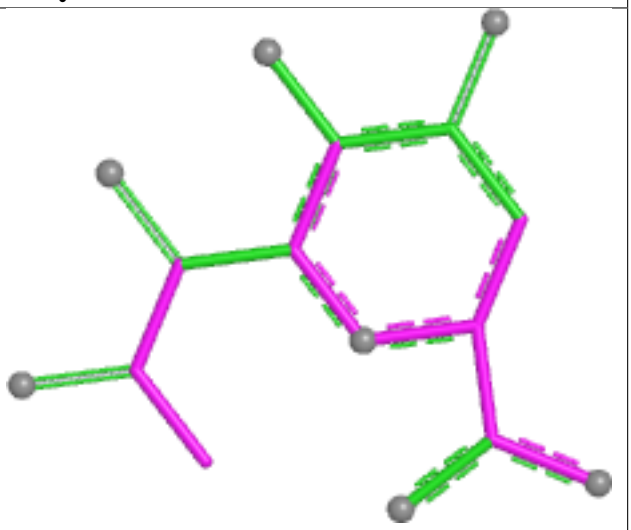


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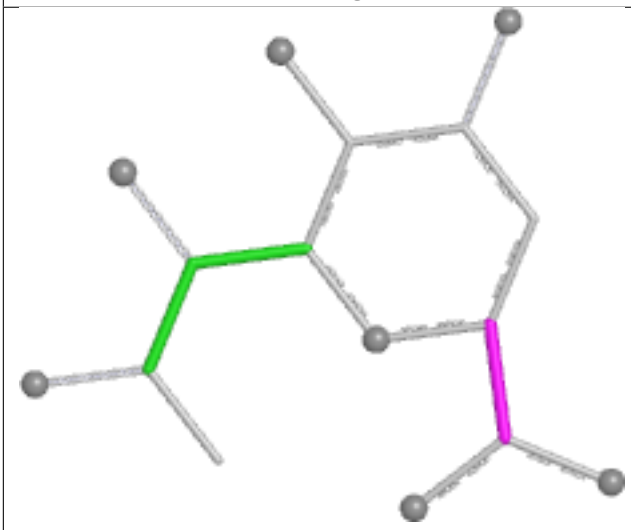
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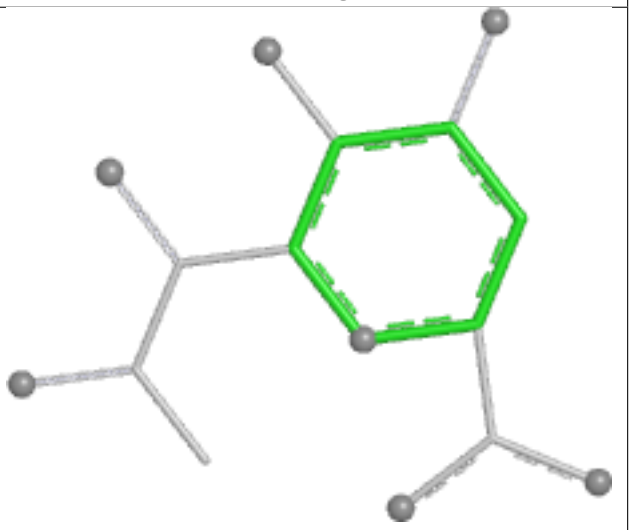
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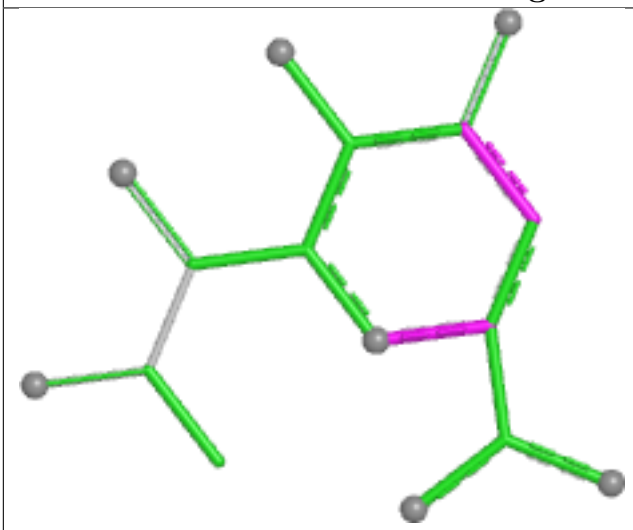


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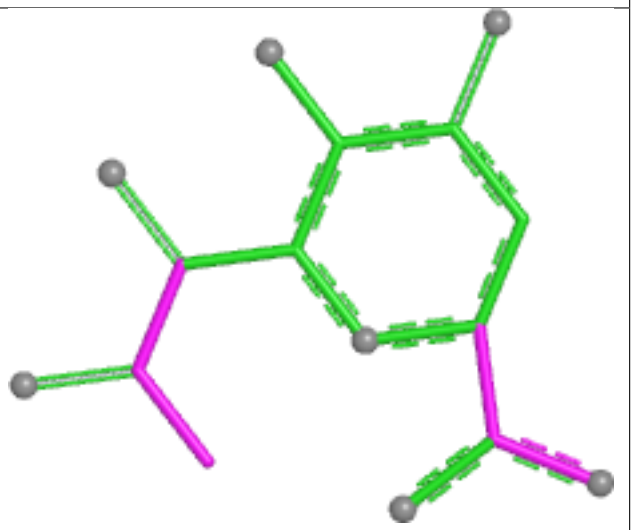


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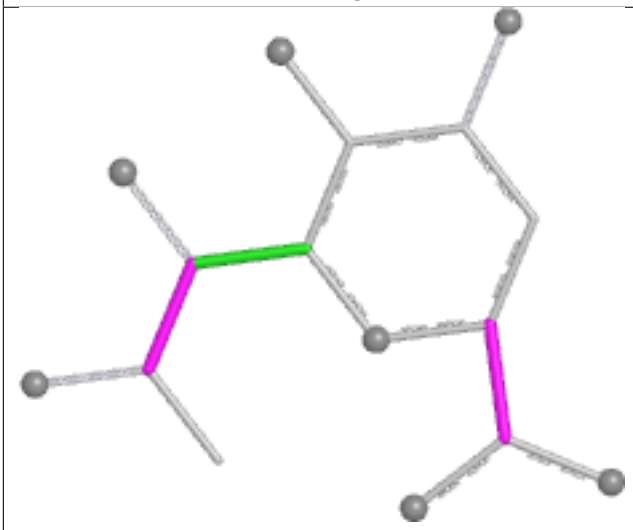
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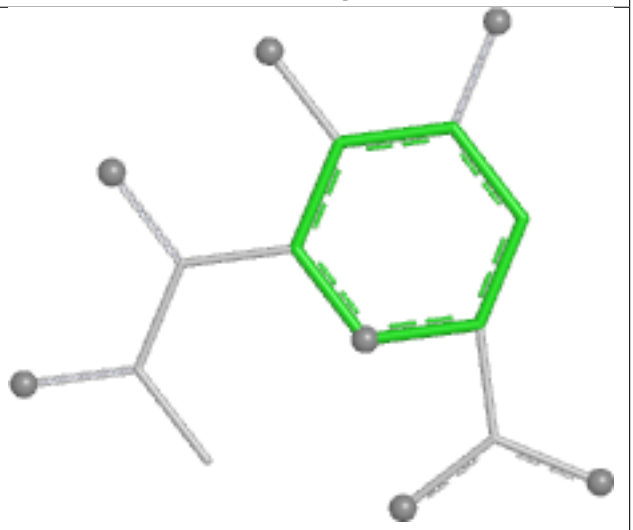
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Bond angles

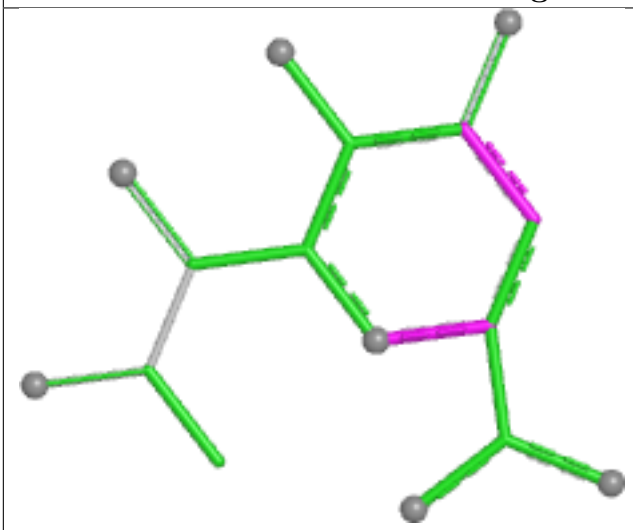


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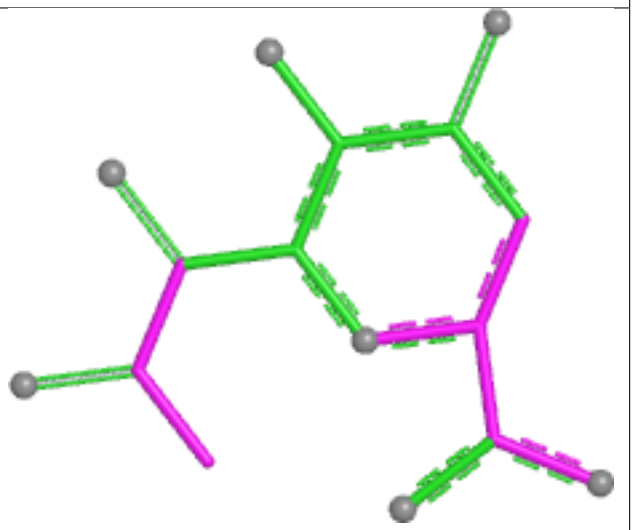


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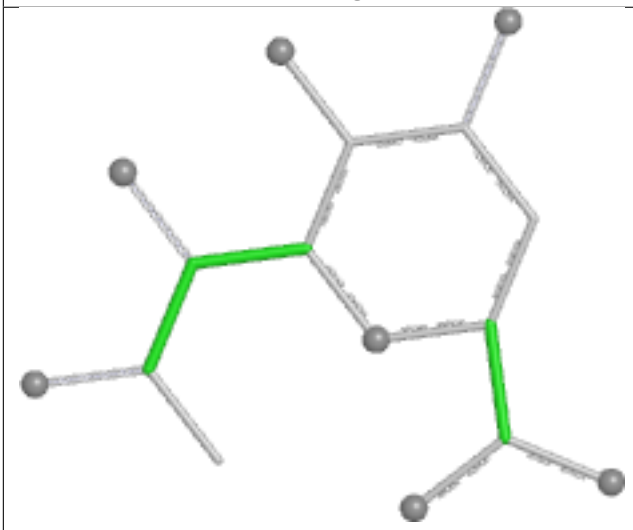
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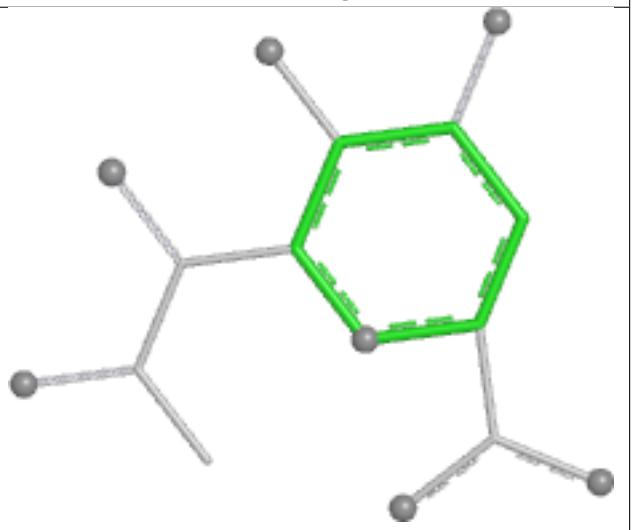
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Bond angles

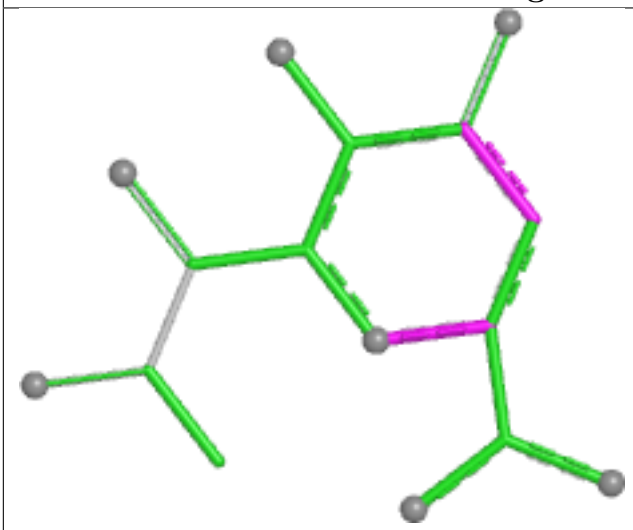


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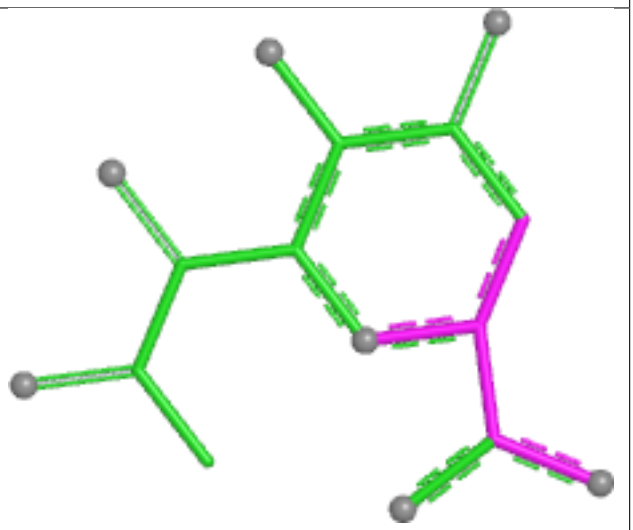


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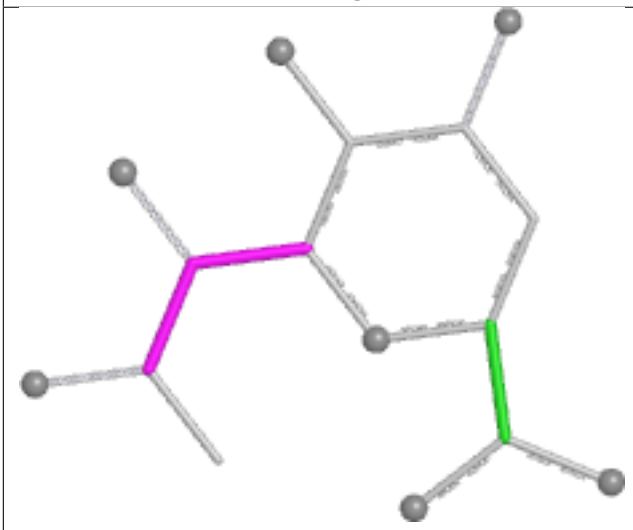
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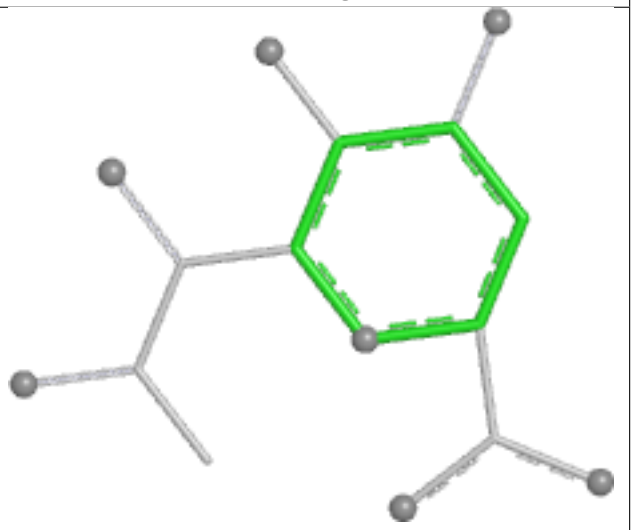
Bond lengths



Bond angles

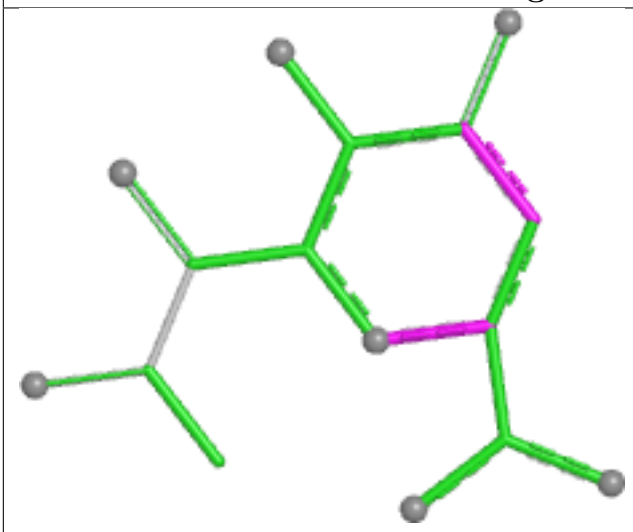


Torsions

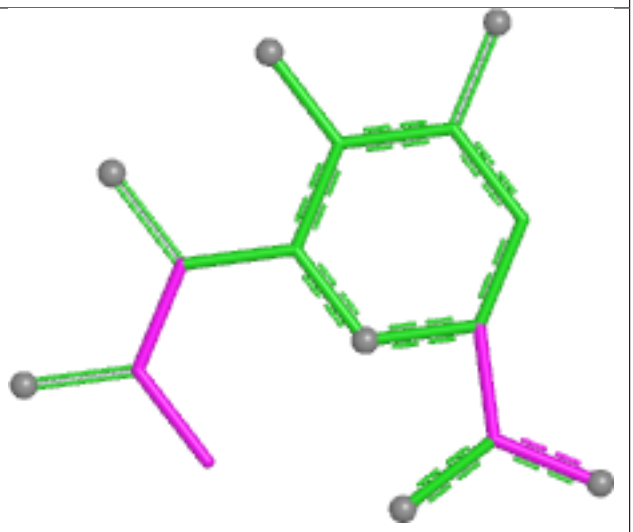


Rings

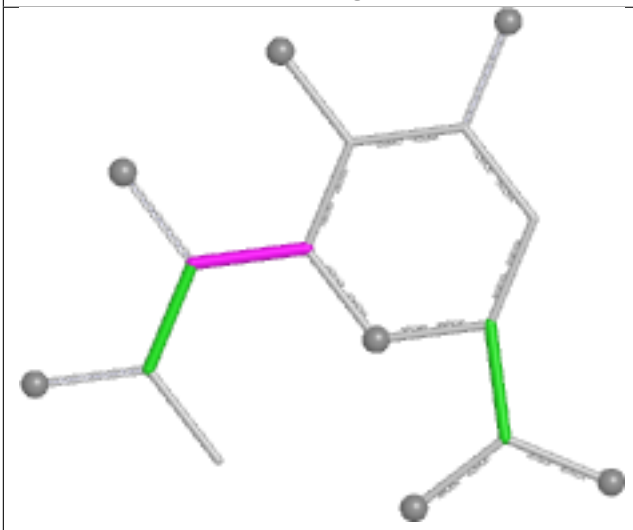
Ligand P8E N 601



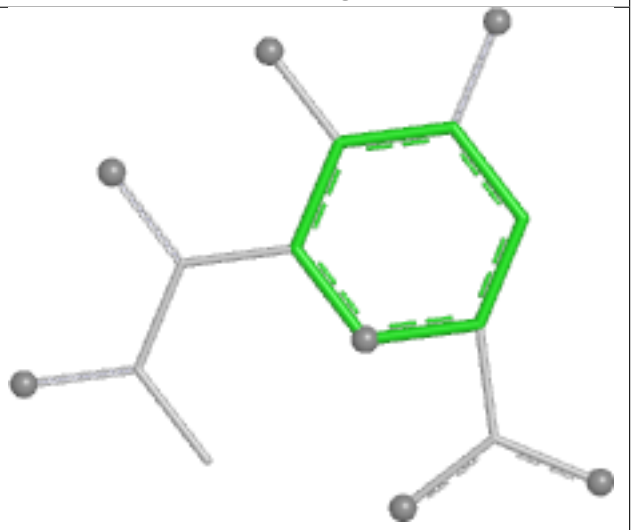
Bond lengths



Bond angles

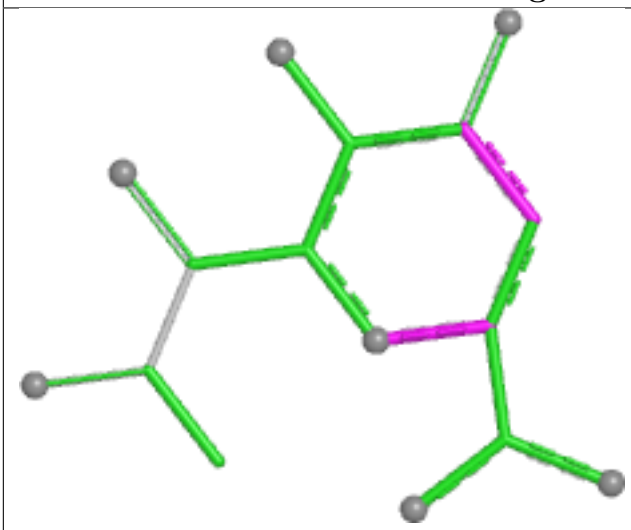


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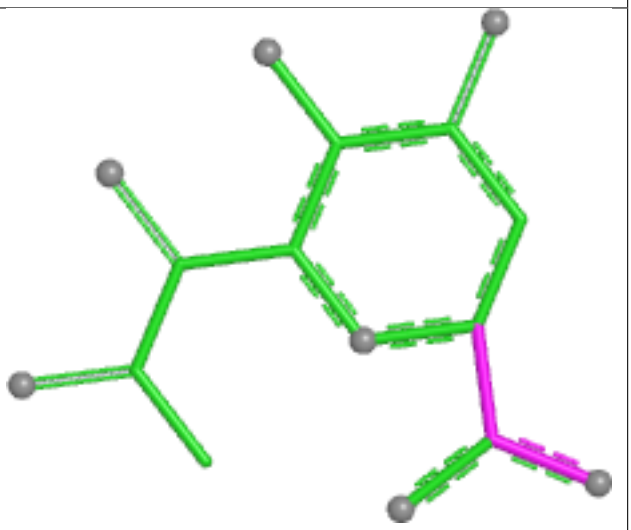


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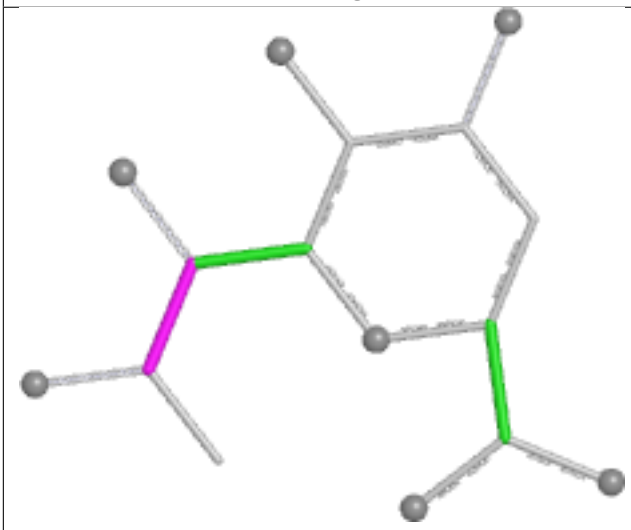
Ligand P8E T 608



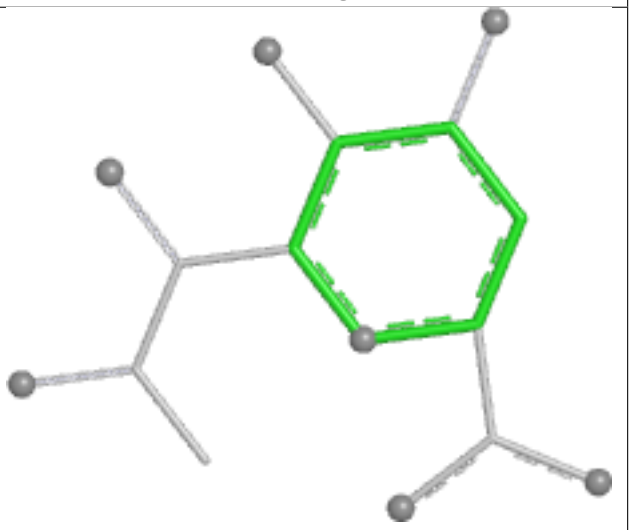
Bond lengths



Bond angles

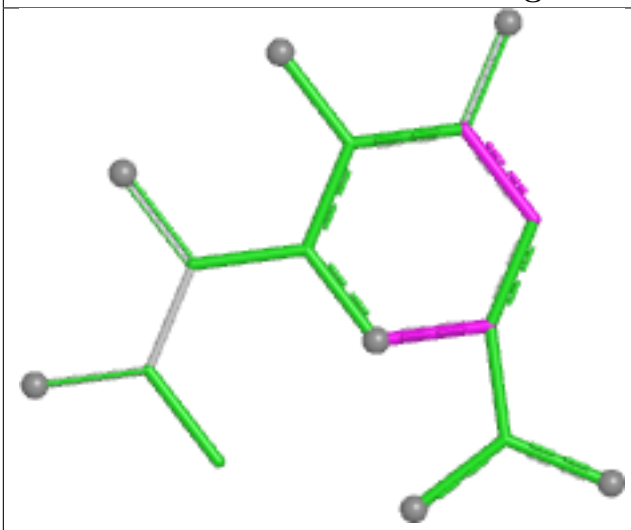


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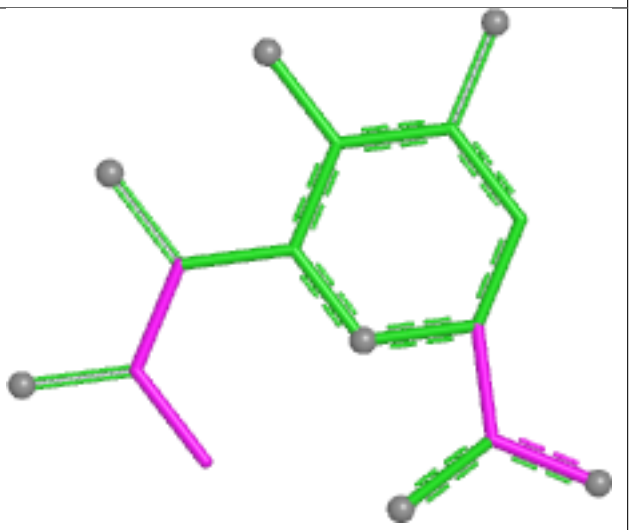


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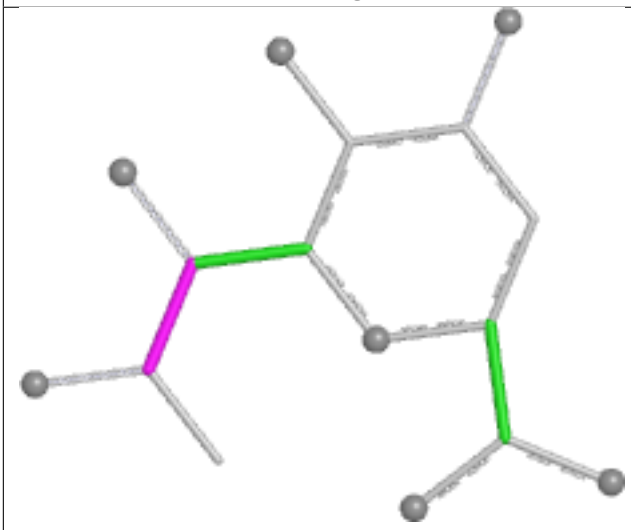
Ligand P8E M 610



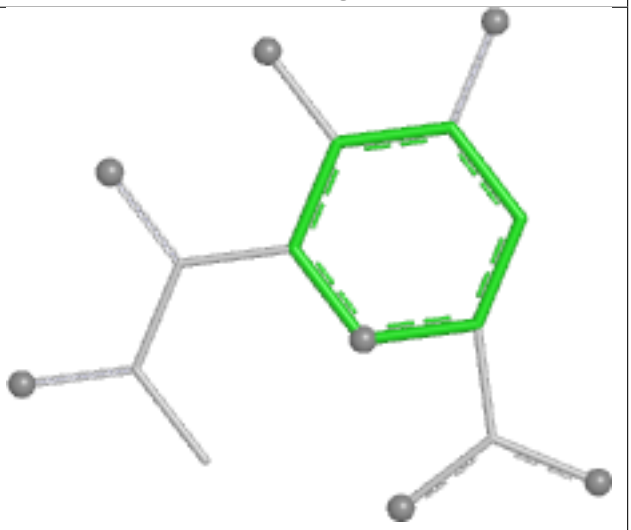
Bond lengths



Bond angles

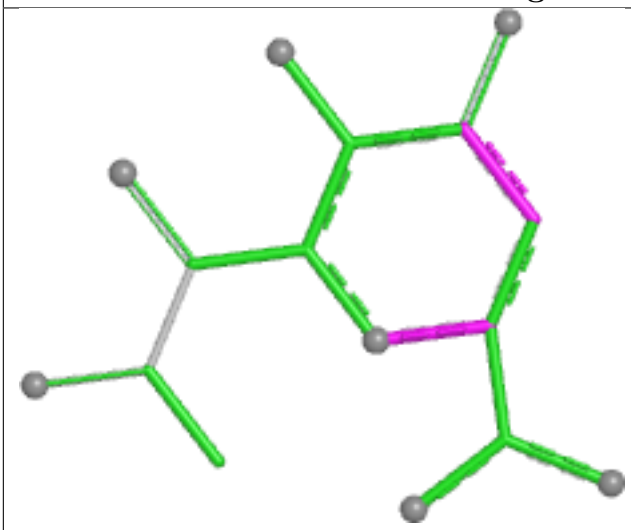


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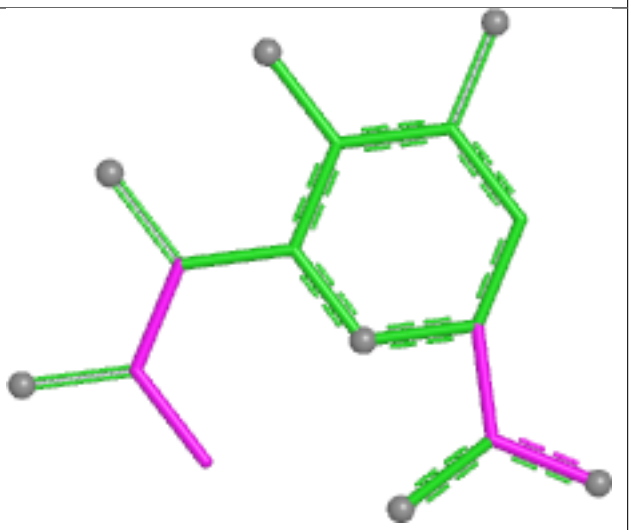


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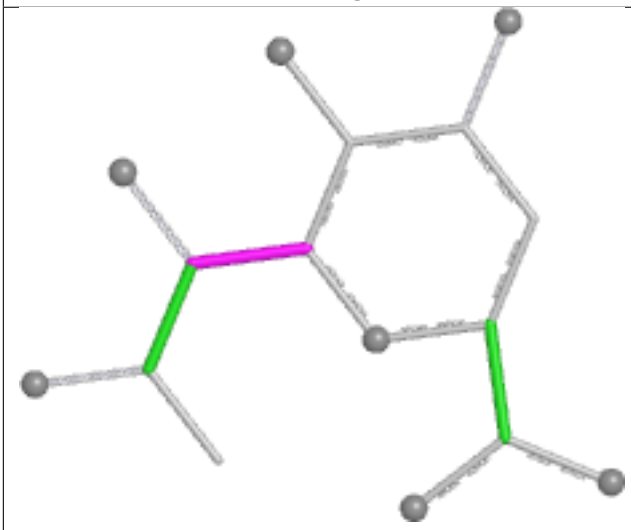
Ligand P8E N 615



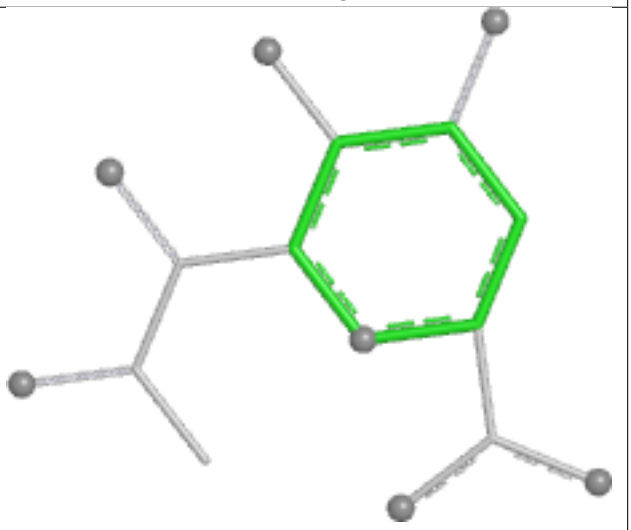
Bond lengths



Bond angles

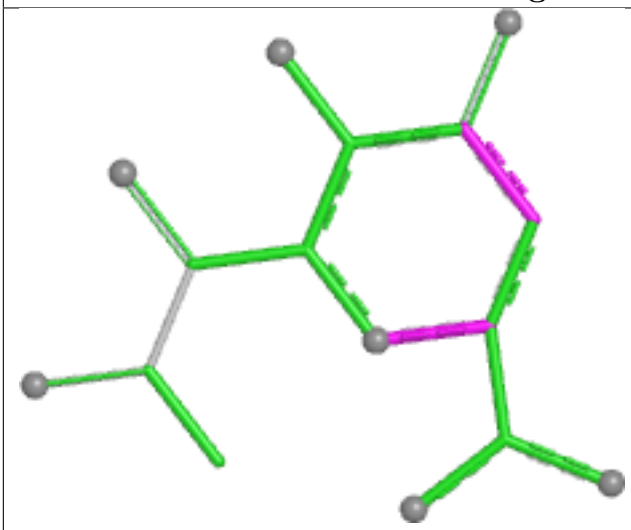


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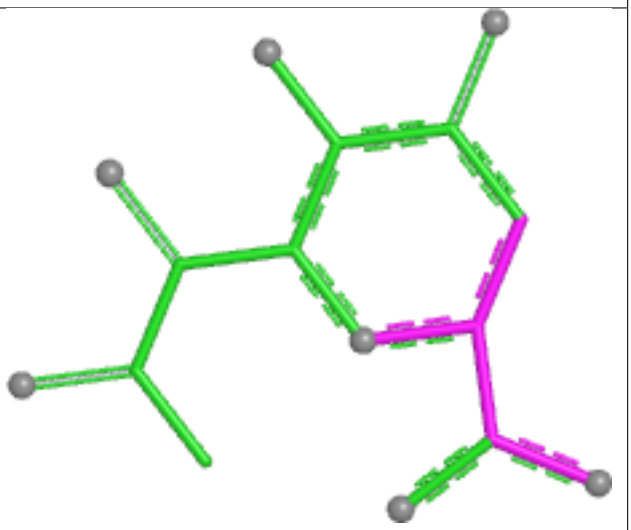


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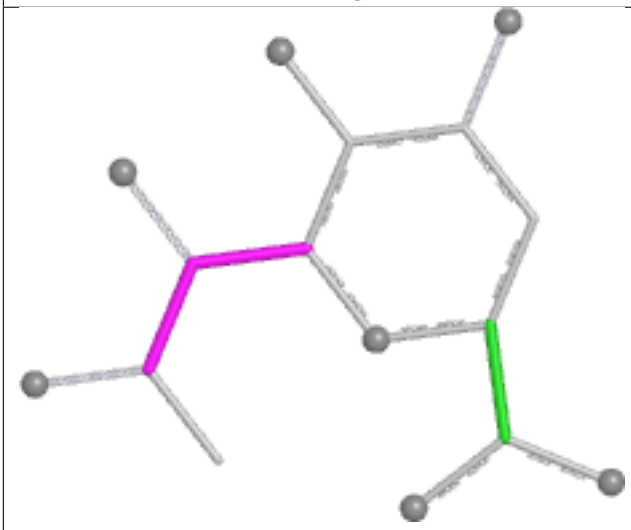
Ligand P8E C 604



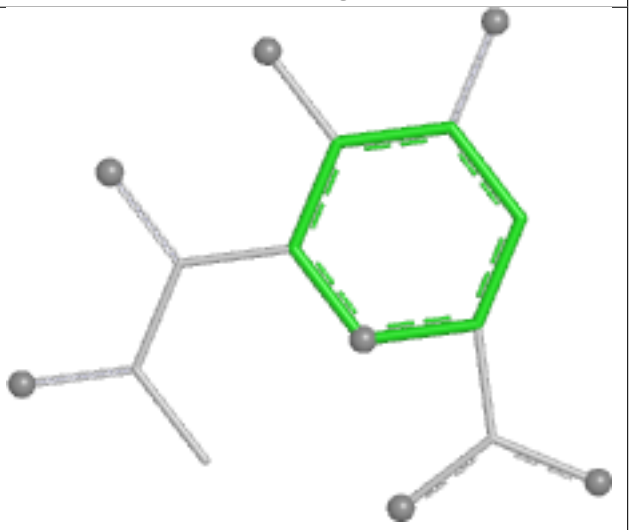
Bond lengths



Bond angles

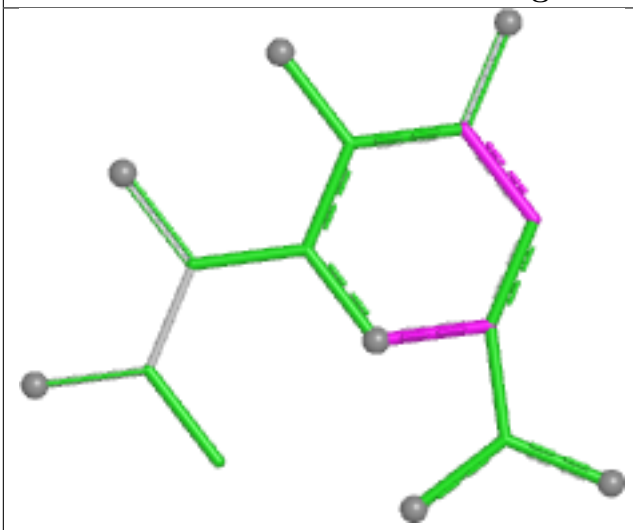


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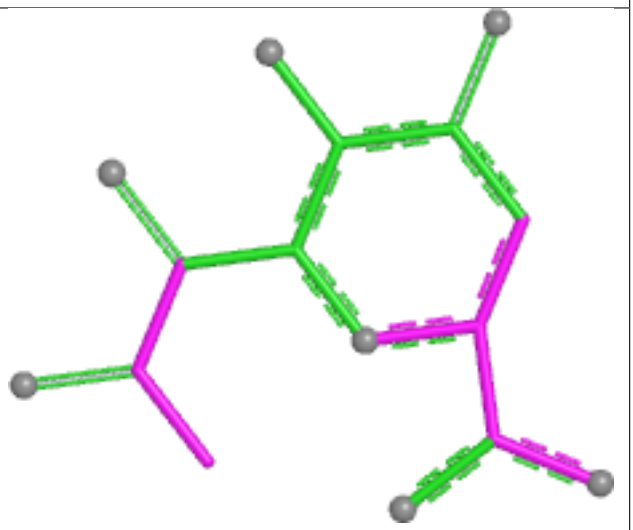


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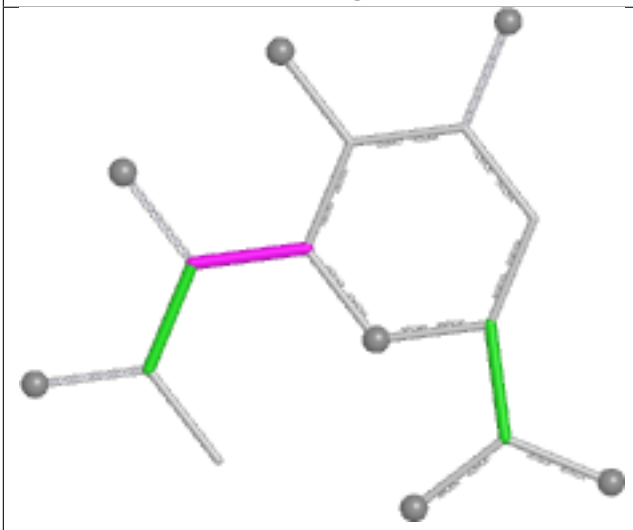
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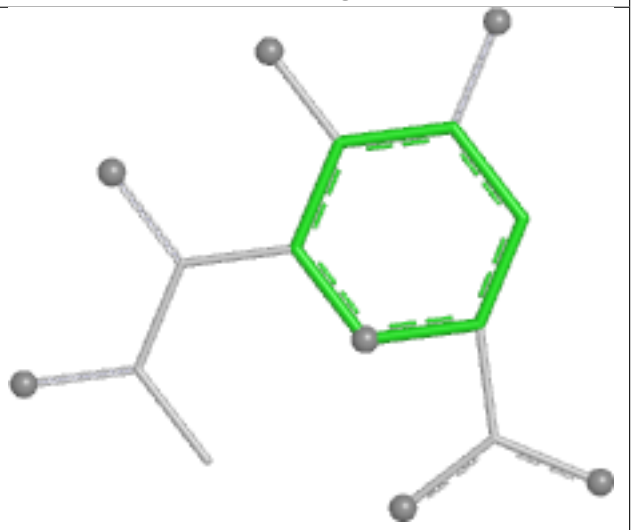
Bond lengths



Bond angles

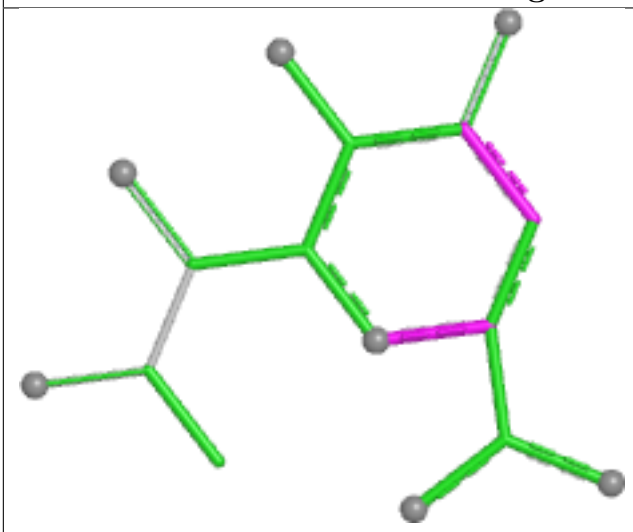


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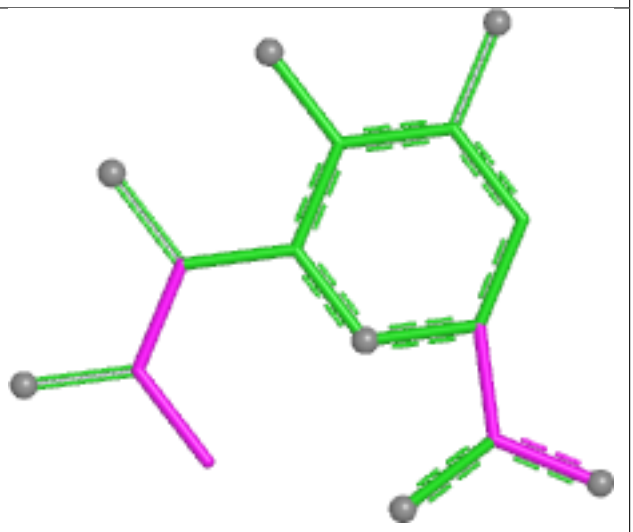


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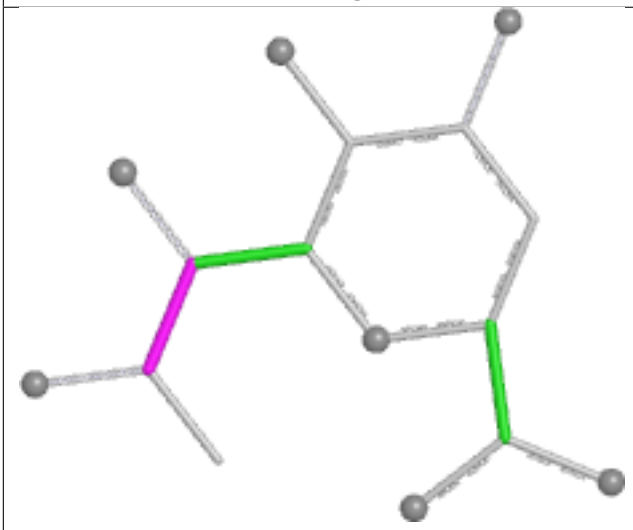
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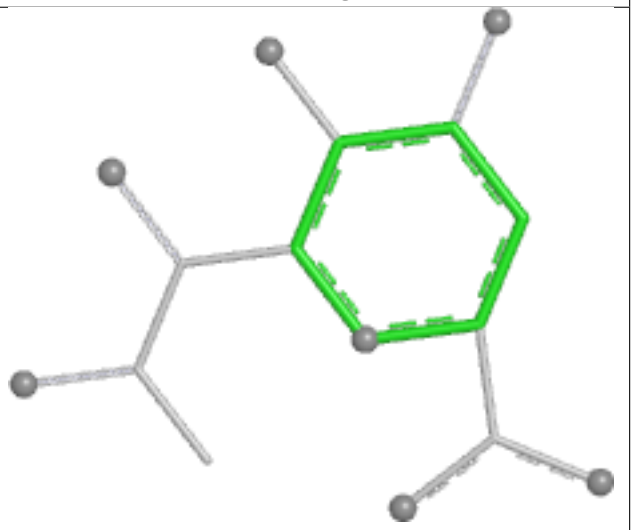
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Bond angles

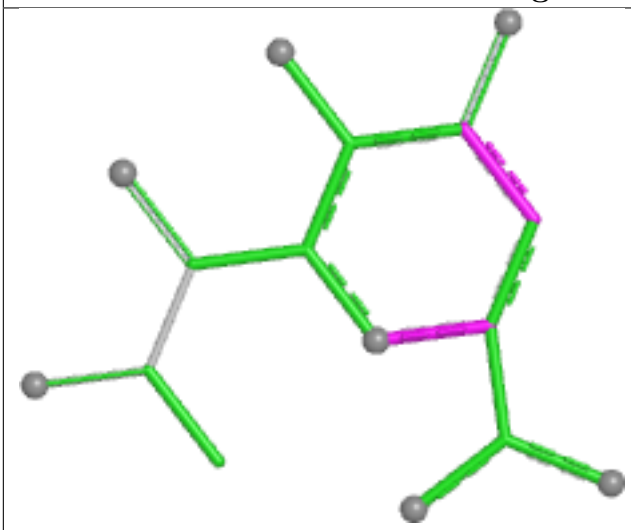


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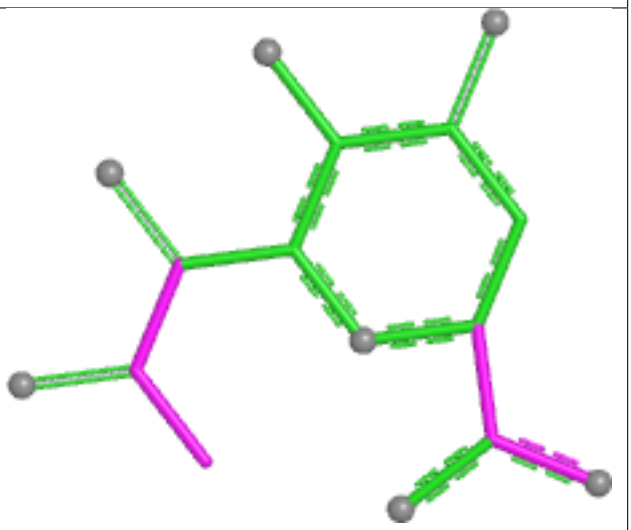


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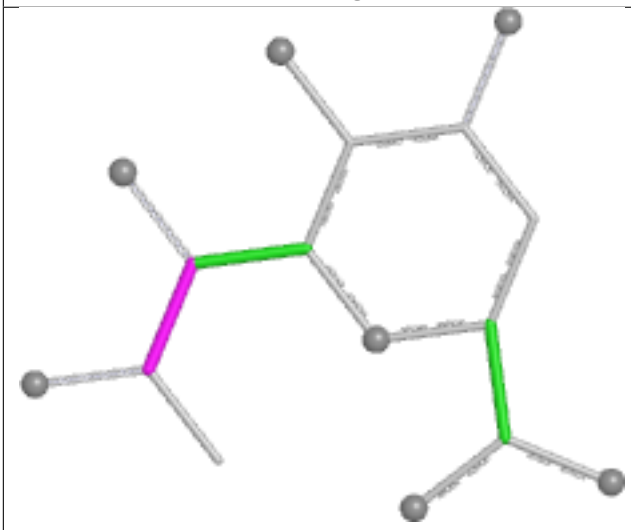
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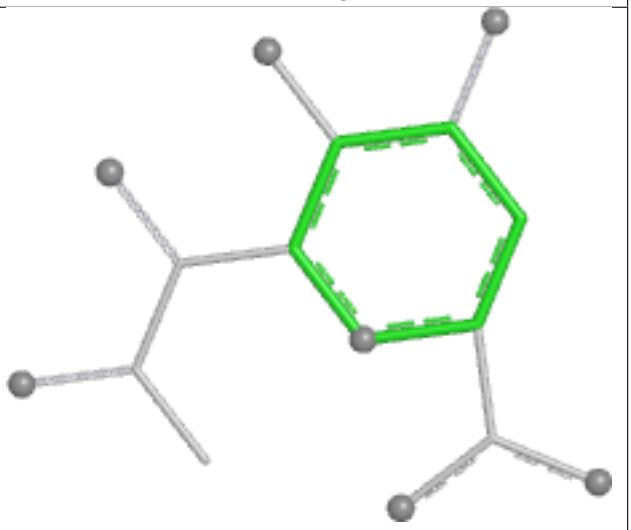
Bond lengths



Bond angles

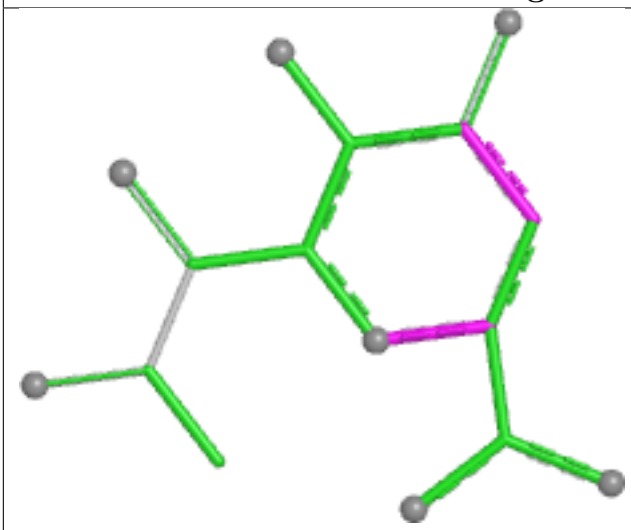


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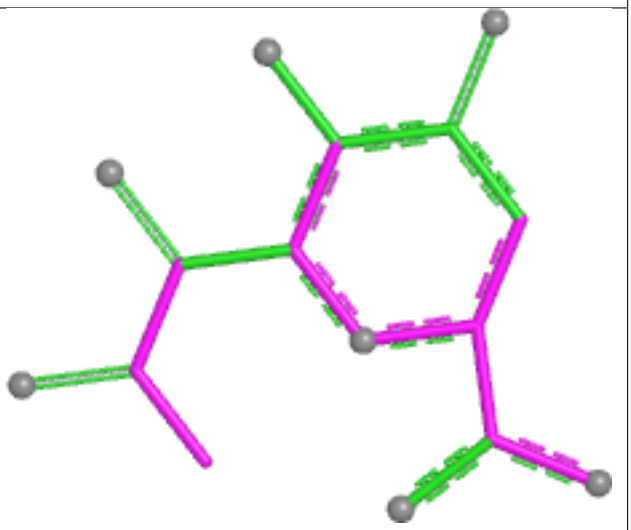


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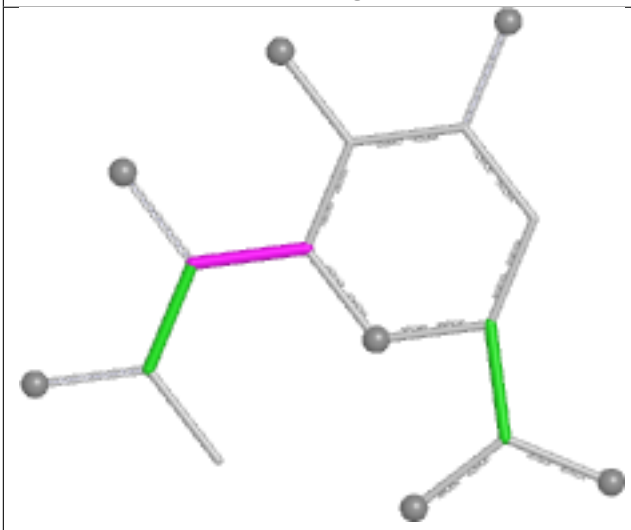
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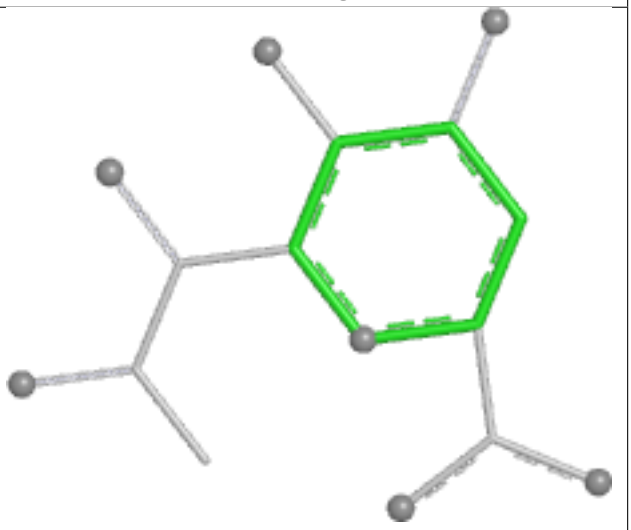
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Bond angles

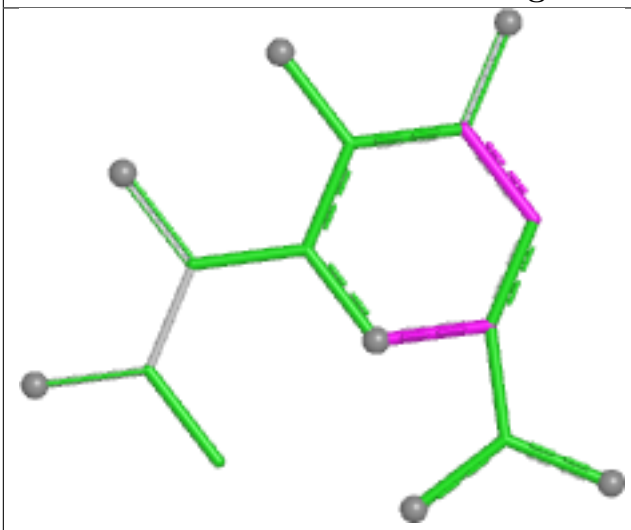


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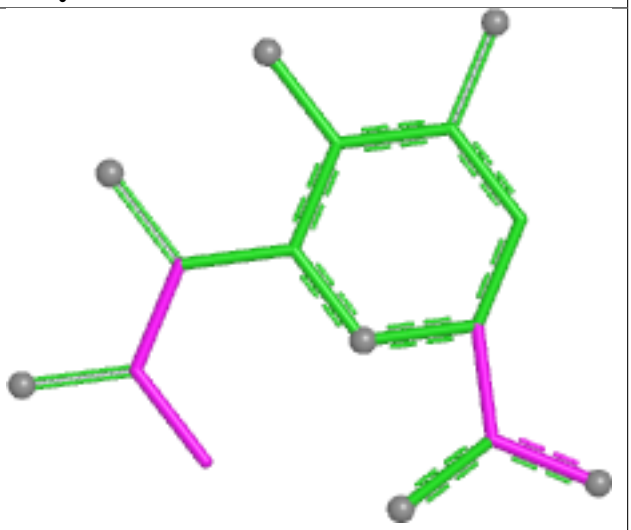


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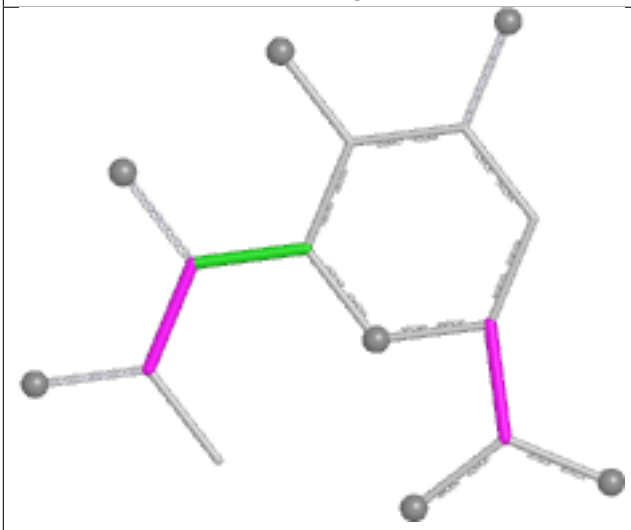
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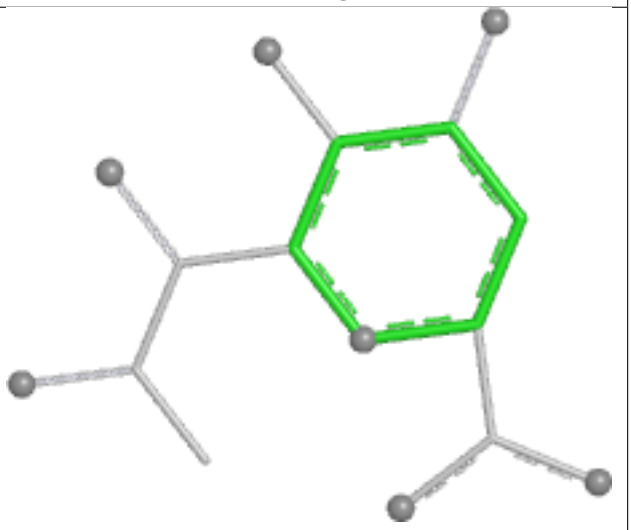
Bond lengths



Bond angles

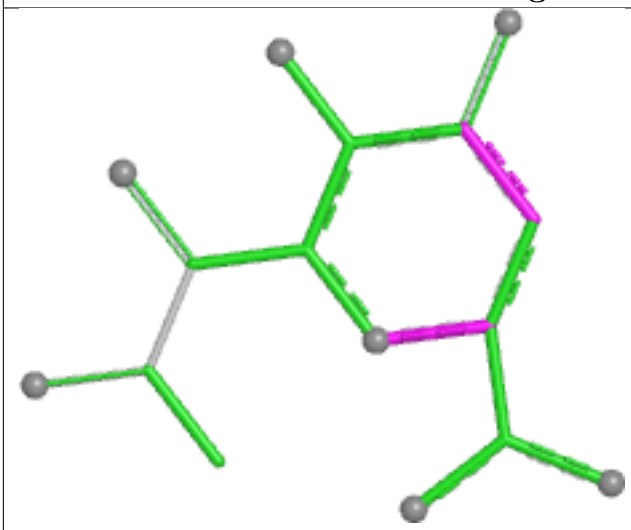


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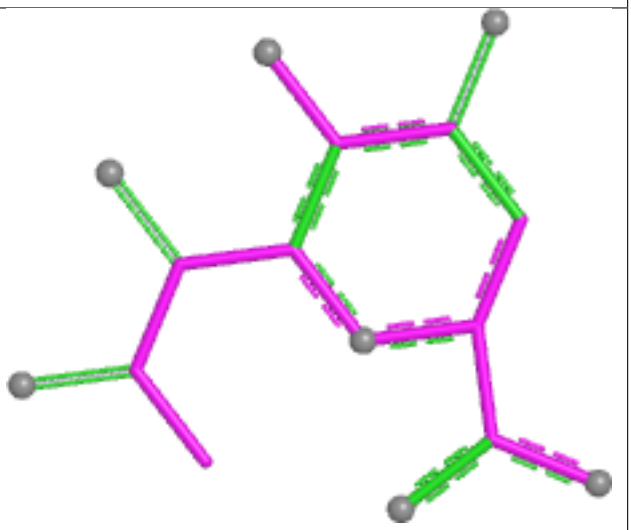


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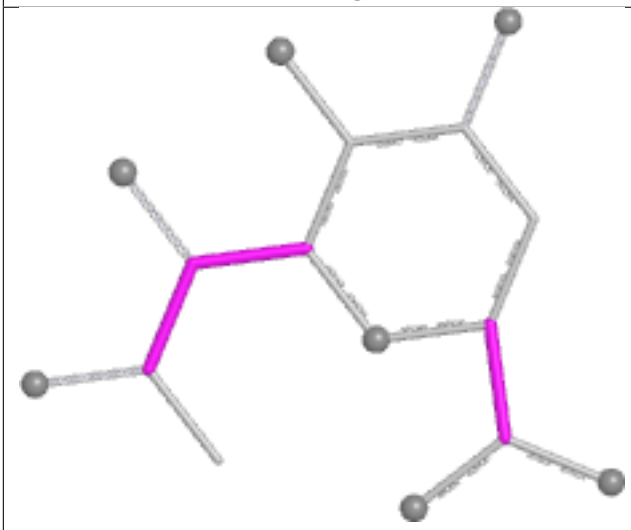
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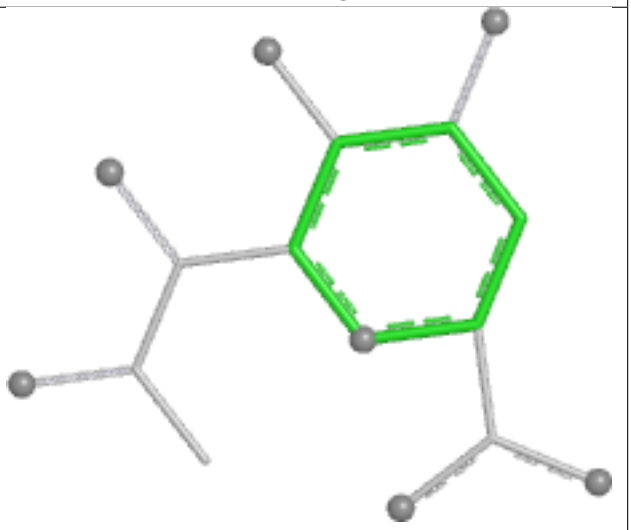
Bond lengths



Bond angles

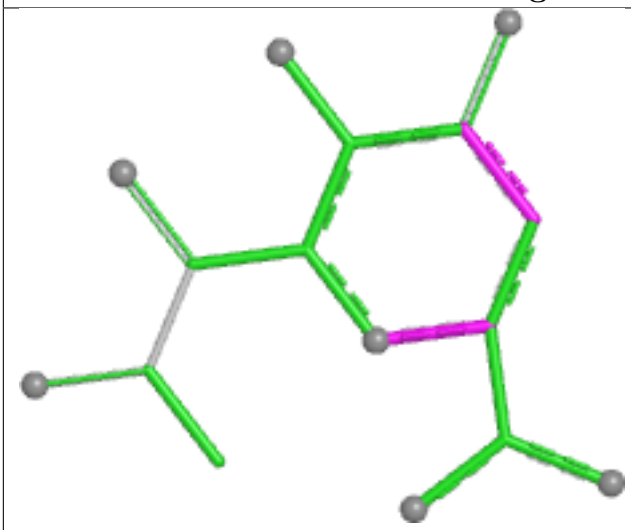


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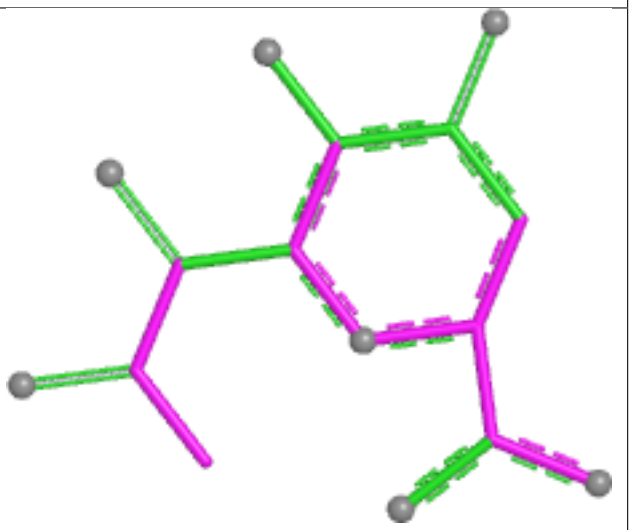


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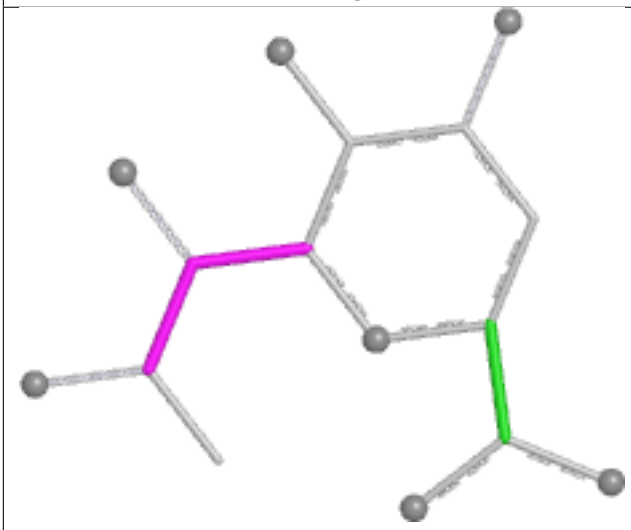
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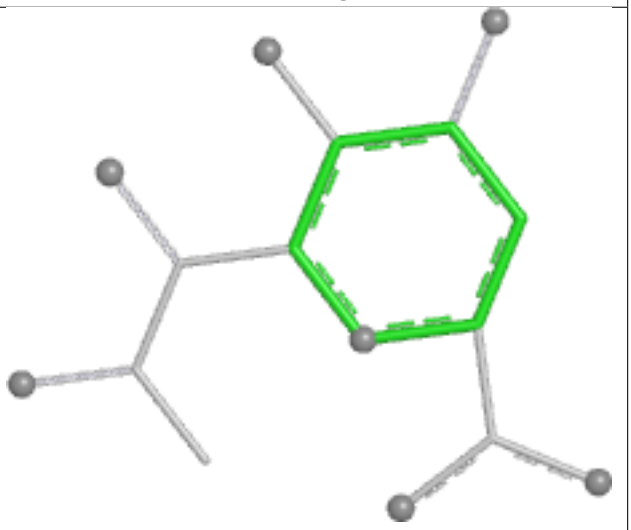
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Bond angles

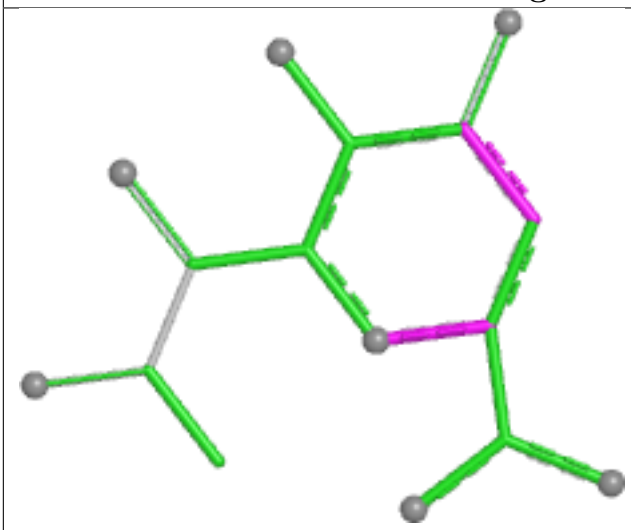


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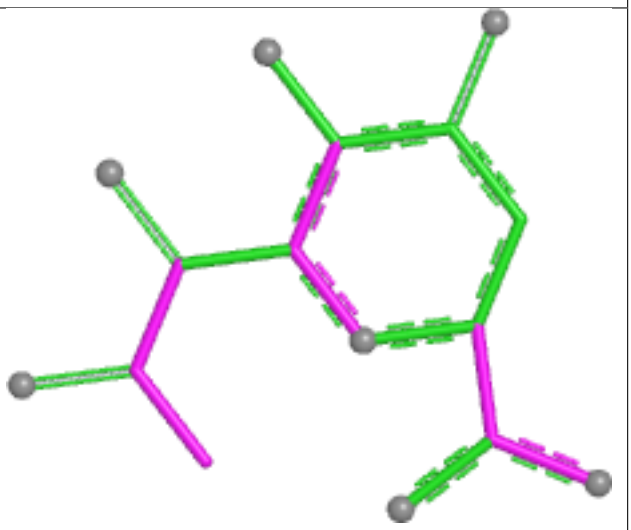


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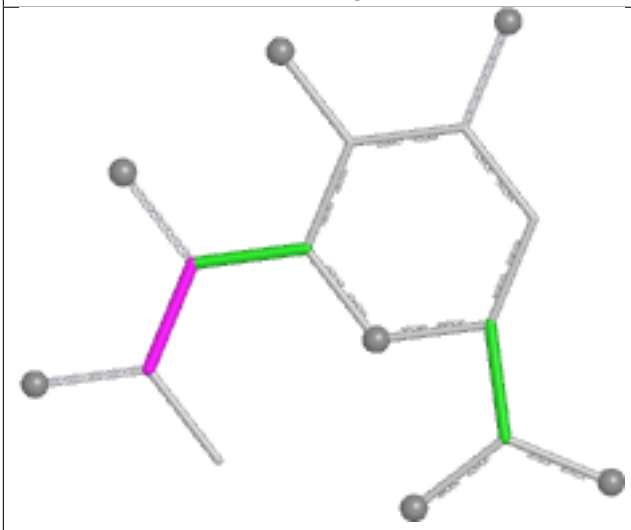
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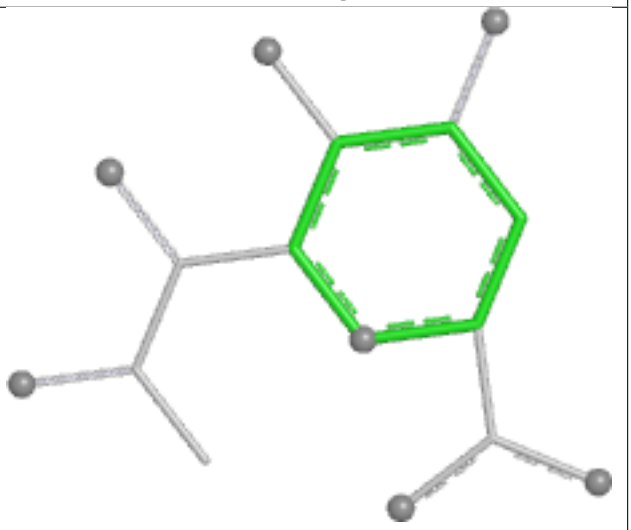
Bond lengths



Bond angles

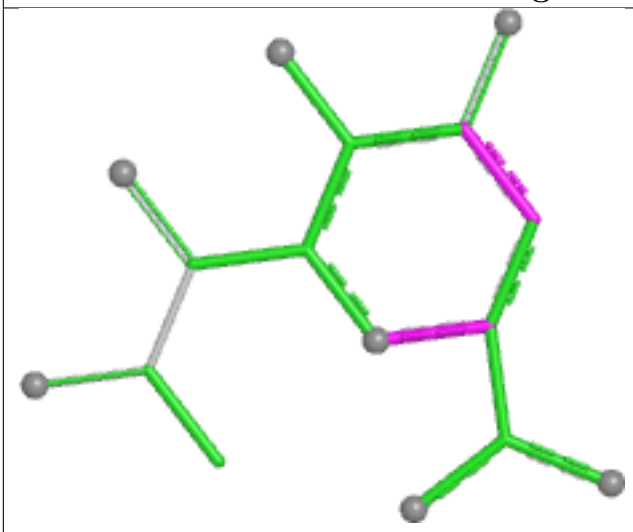


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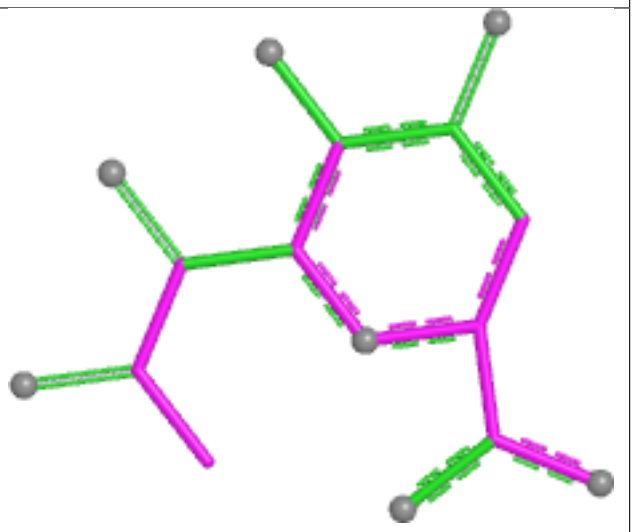


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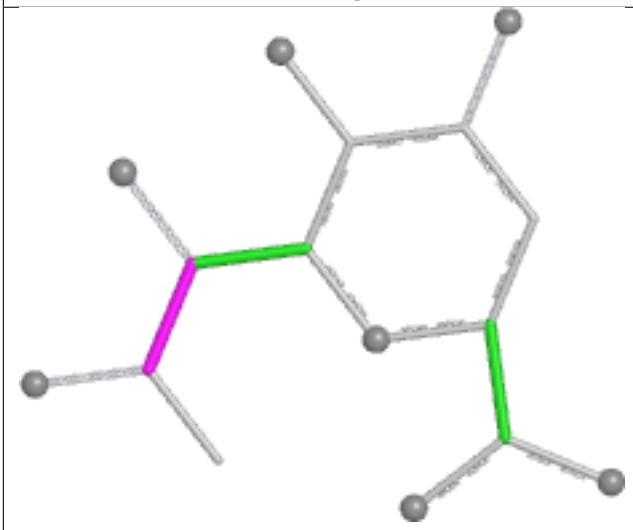
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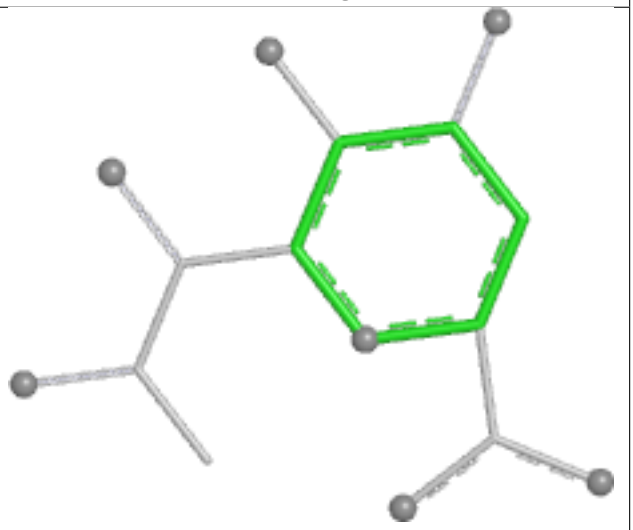
Bond lengths



Bond angles

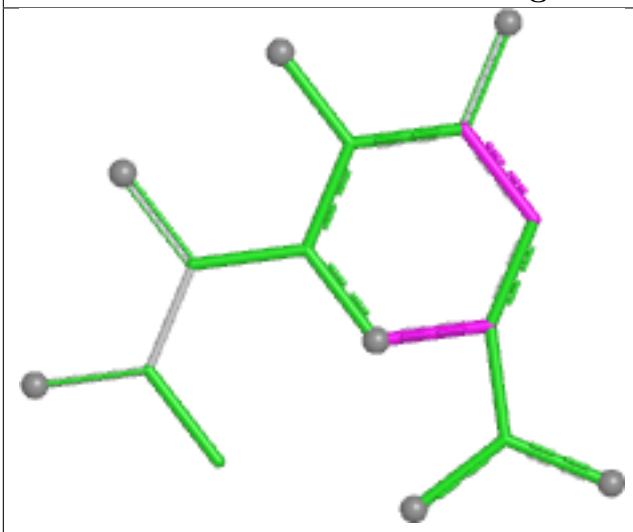


Torsions

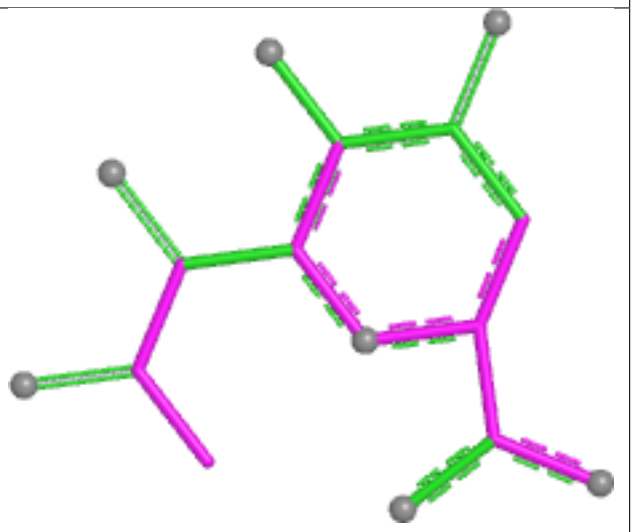


Rings

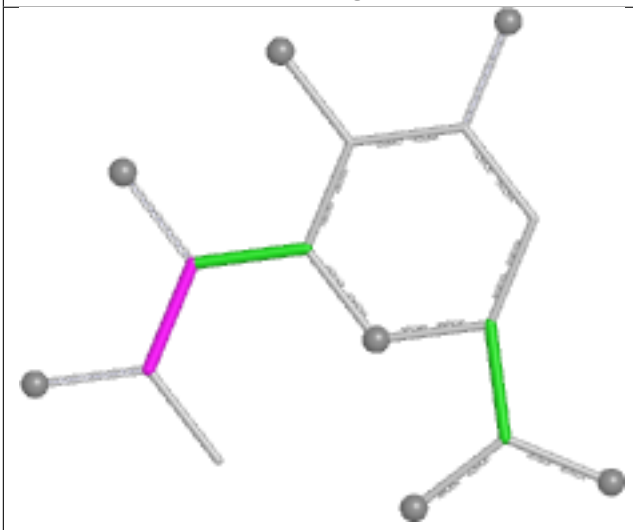
Ligand P8E E 605



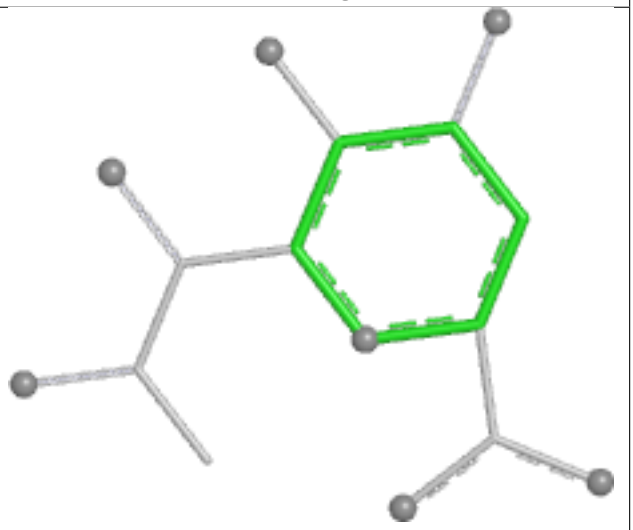
Bond lengths



Bond angles

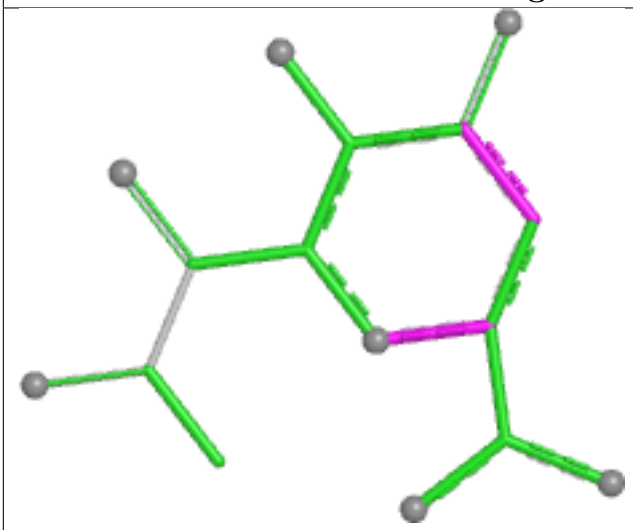


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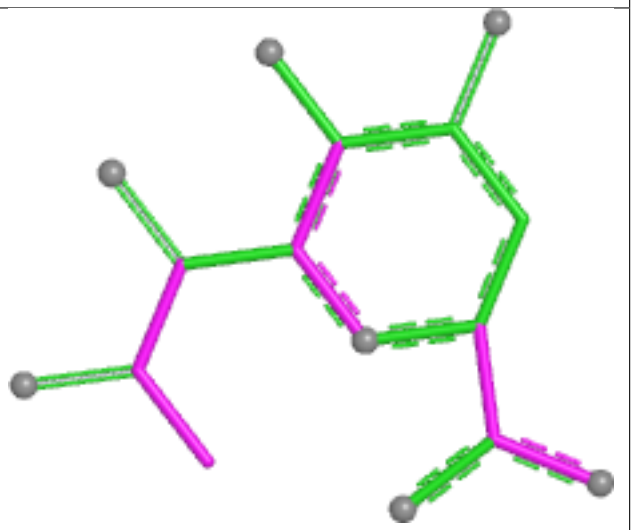


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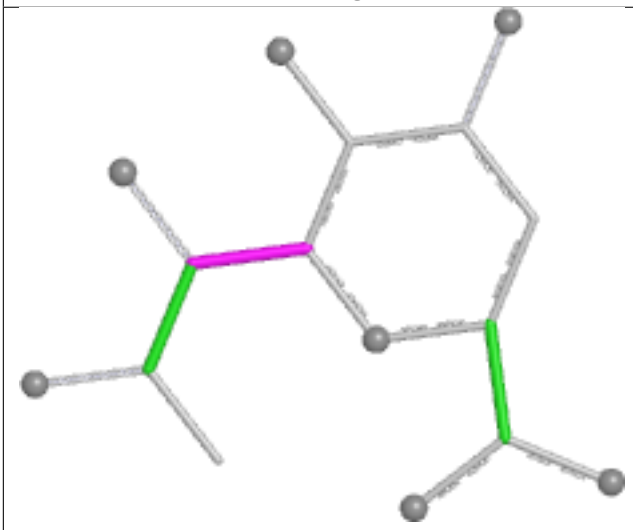
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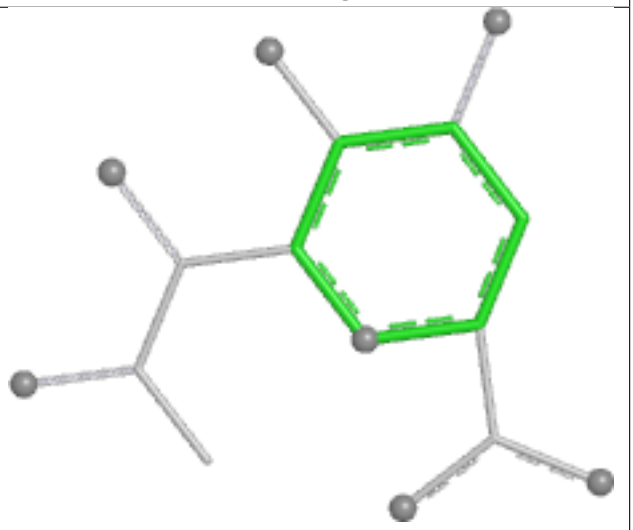
Bond lengths



Bond angles

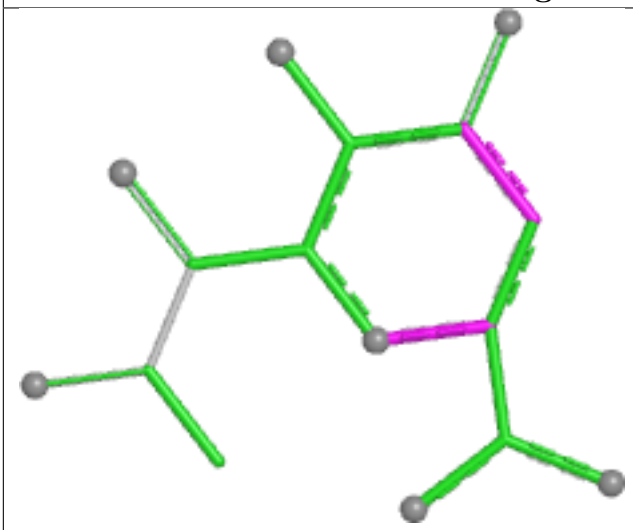


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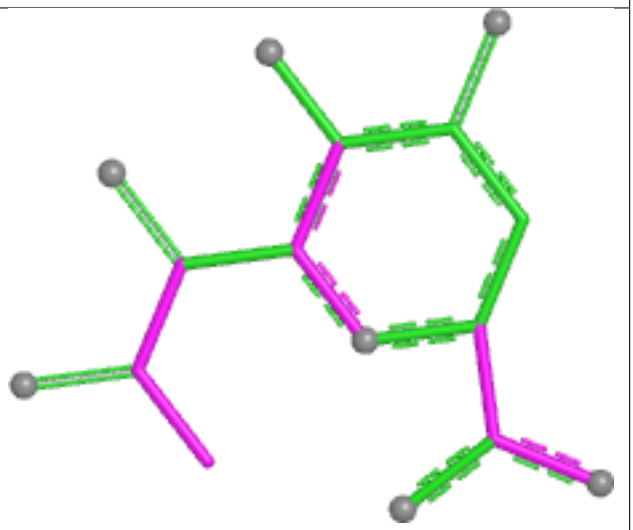


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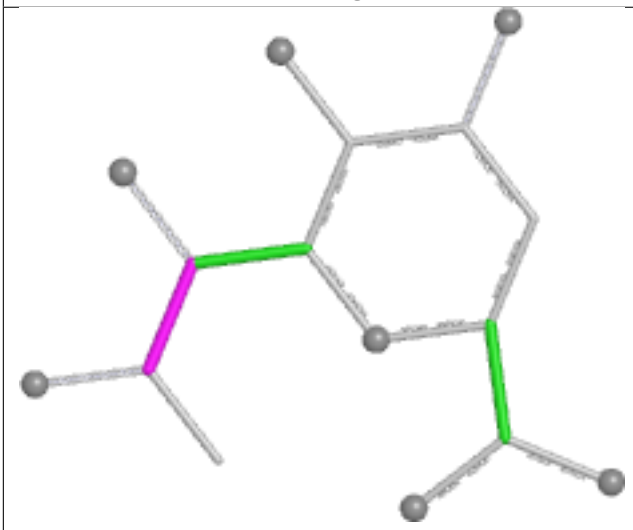
Ligand P8E I 610



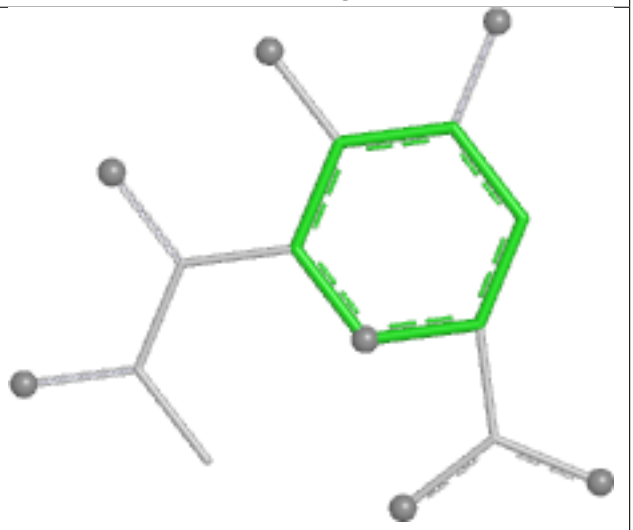
Bond lengths



Bond angles

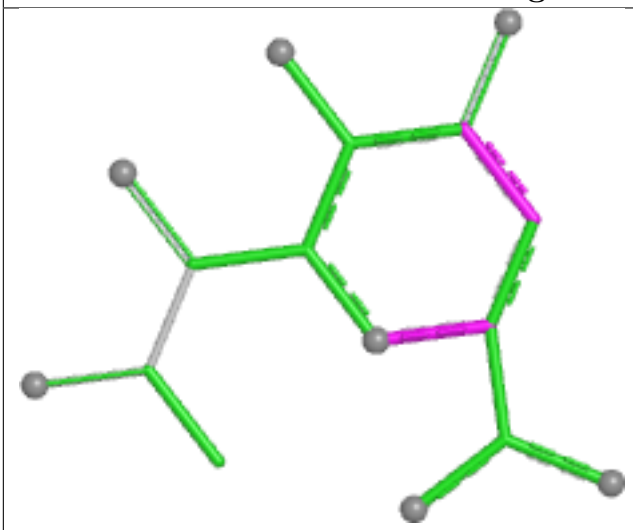


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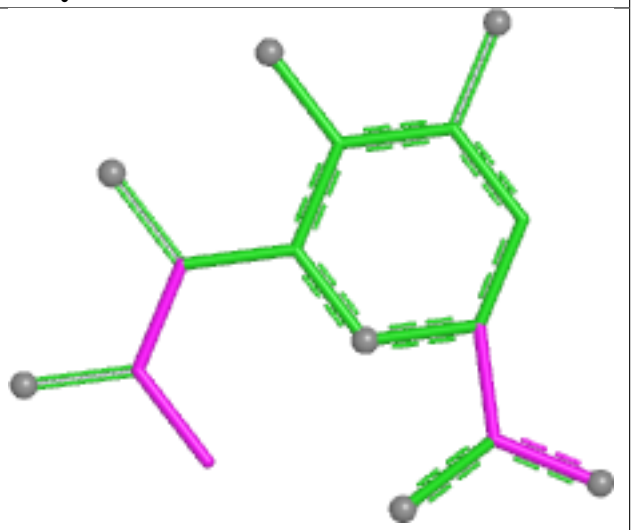


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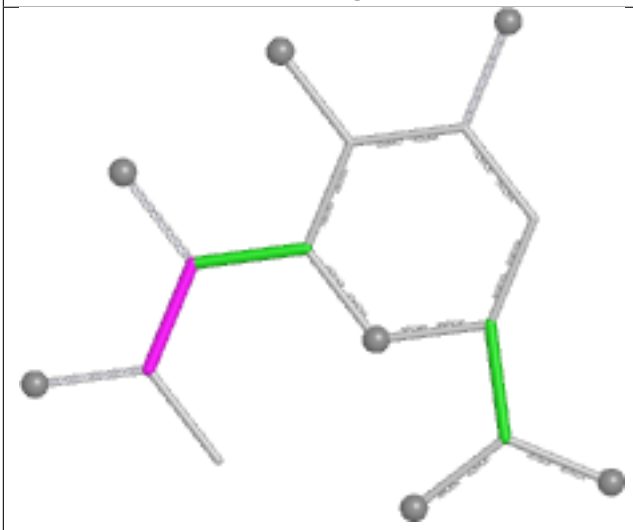
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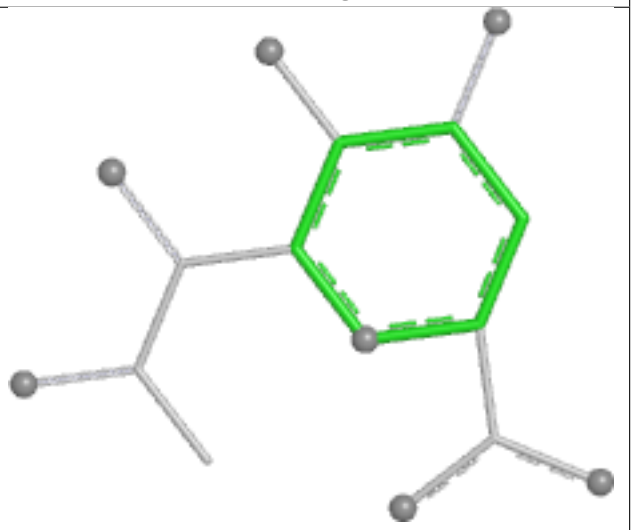
Bond lengths



Bond angles

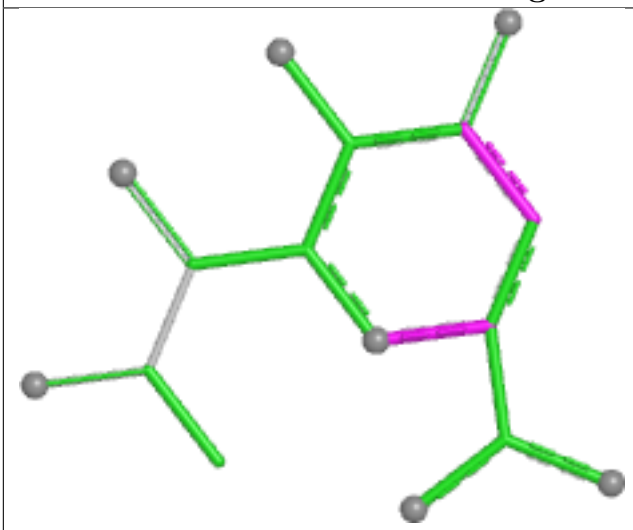


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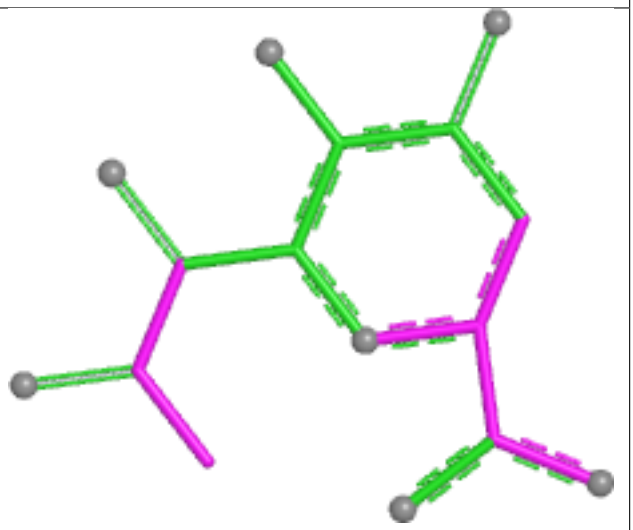


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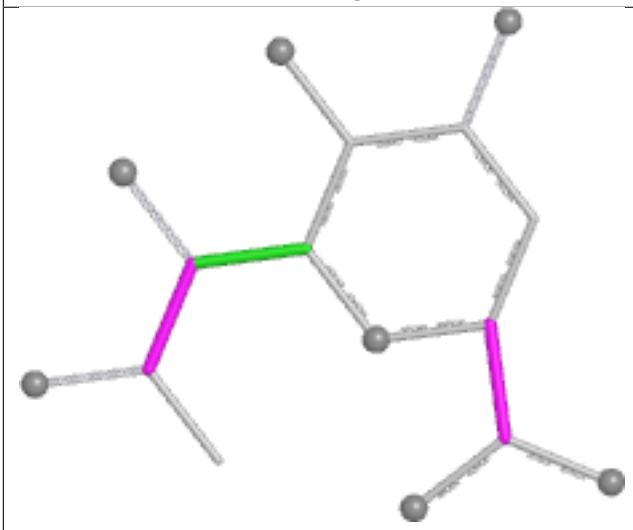
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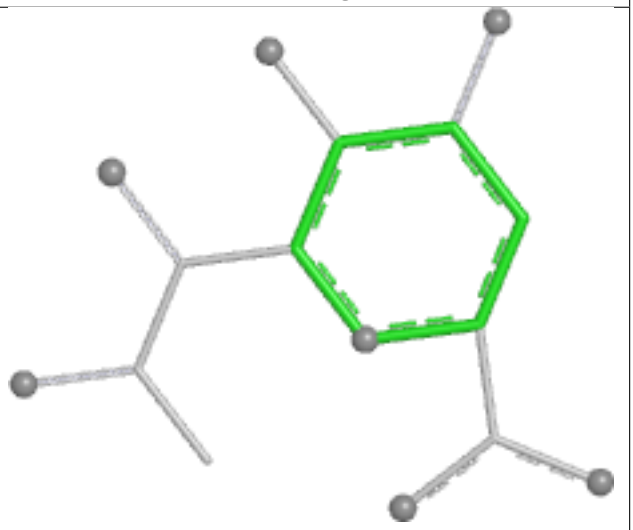
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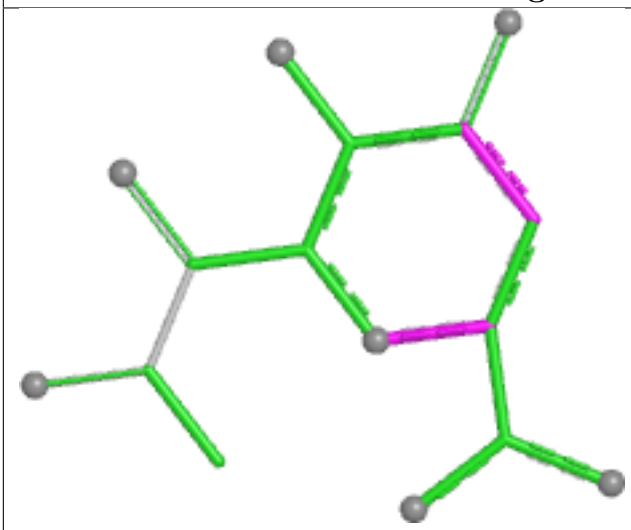


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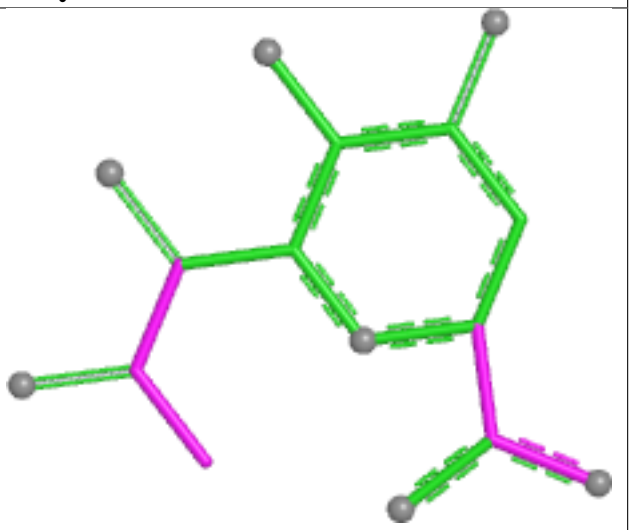


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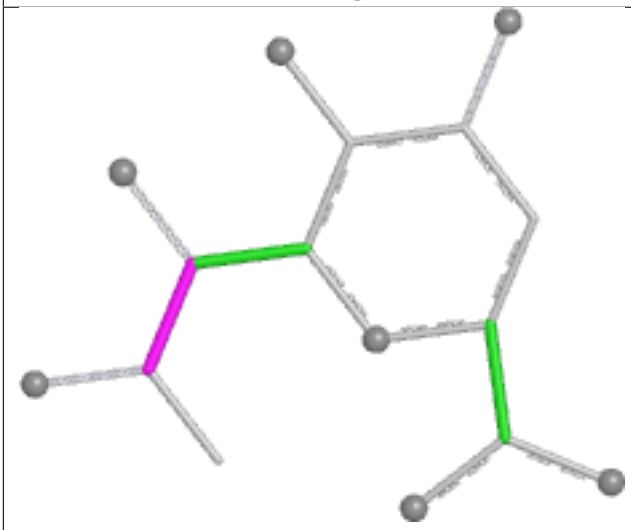
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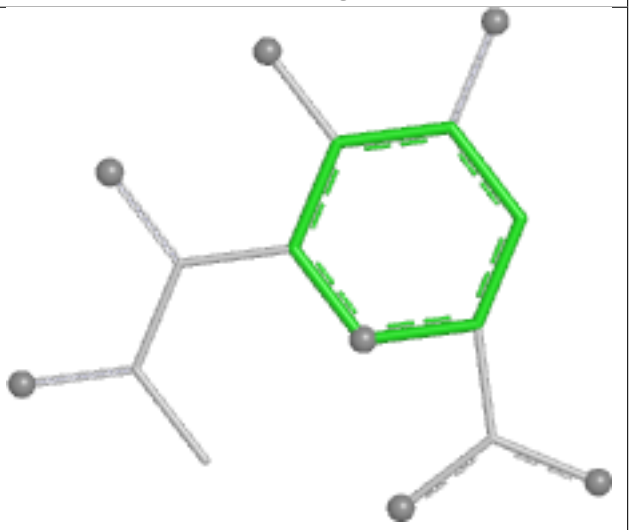
Bond lengths



Bond angles

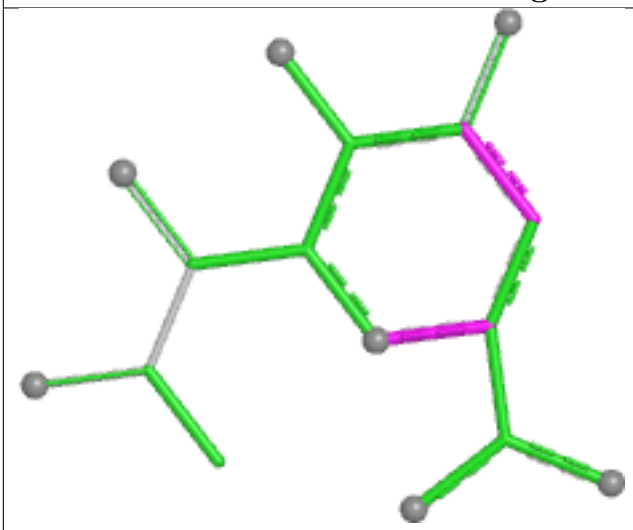


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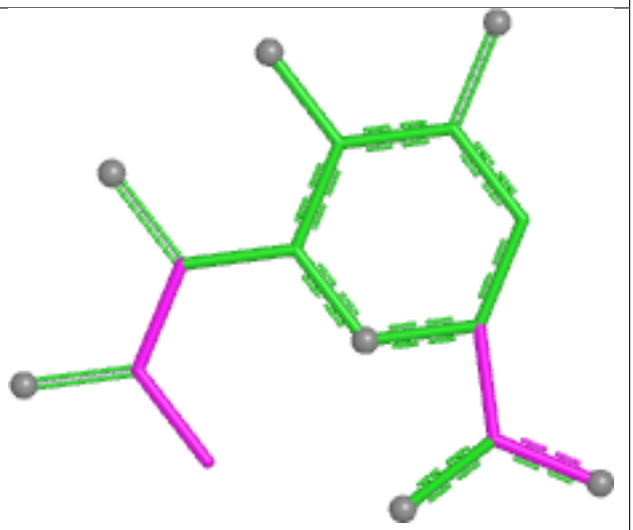


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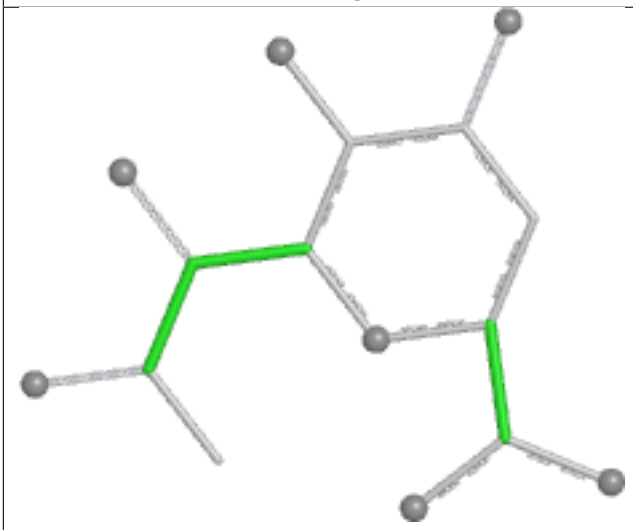
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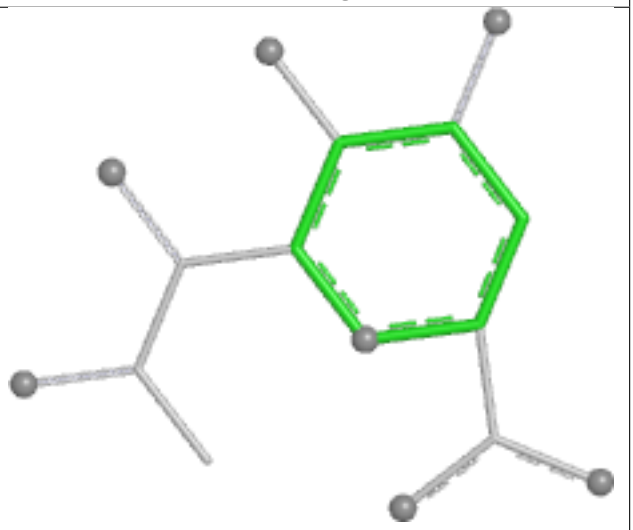
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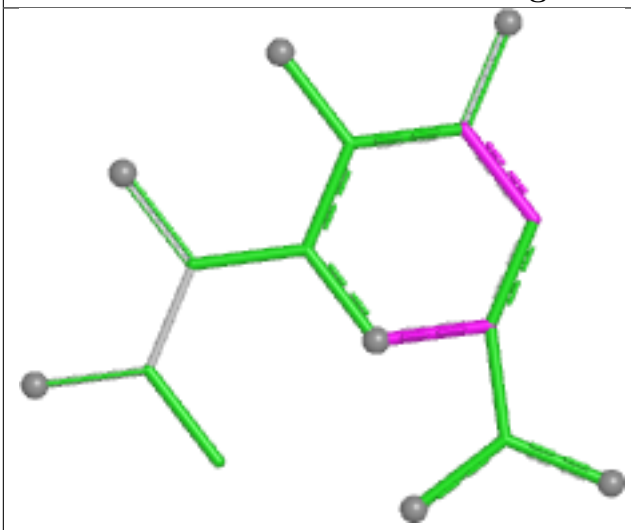


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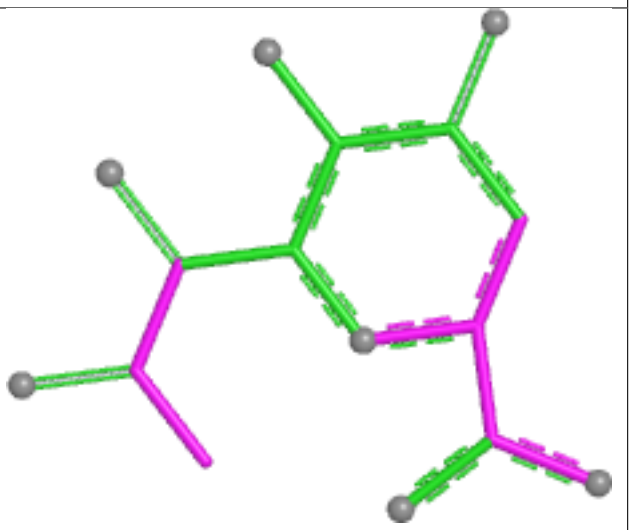


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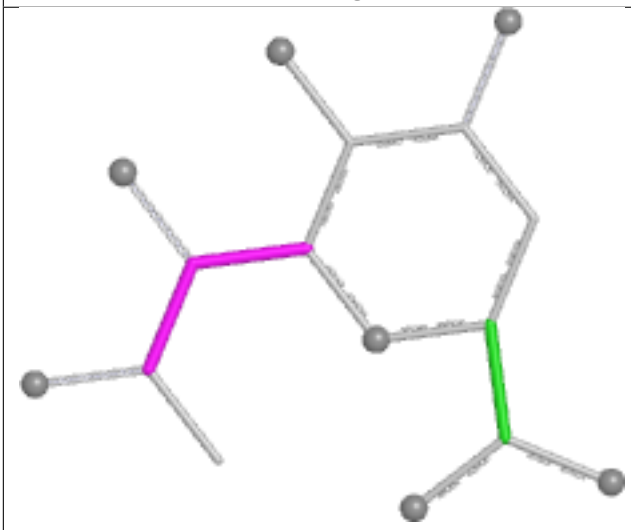
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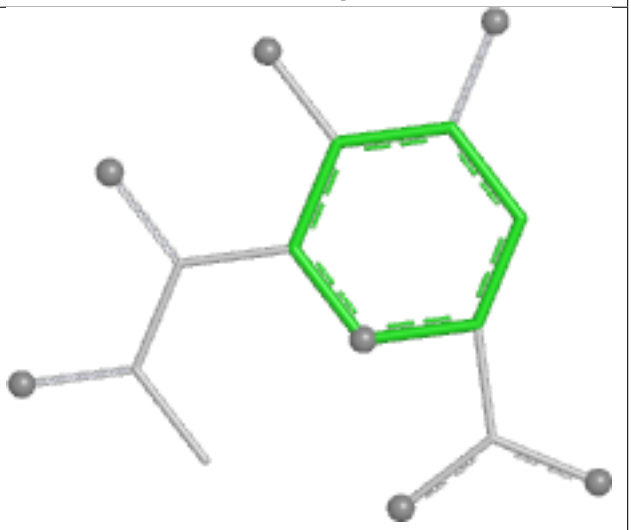
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Bond angles

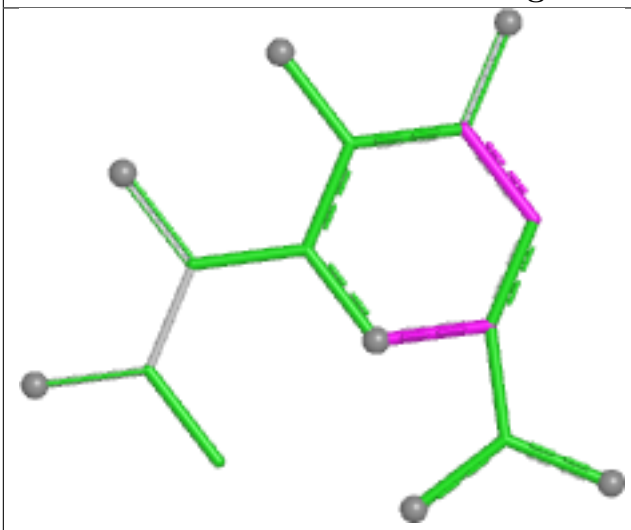


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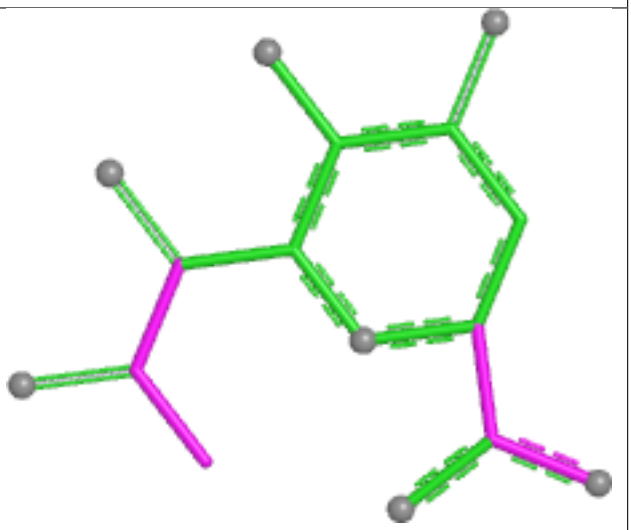


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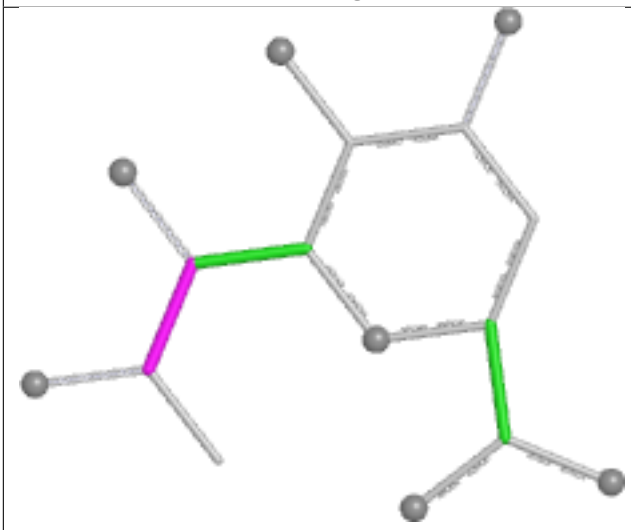
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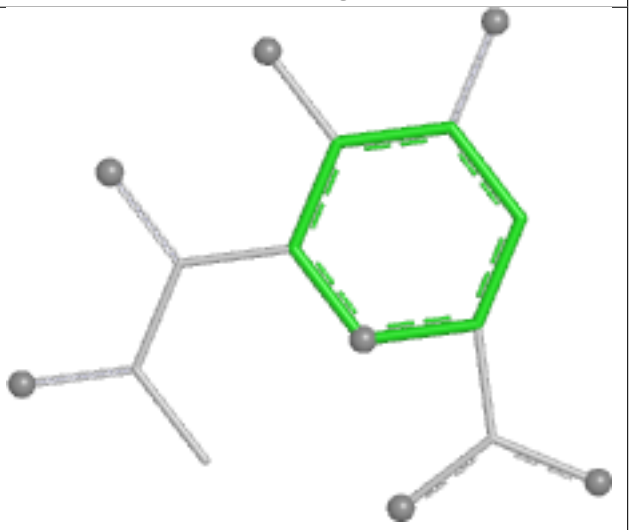
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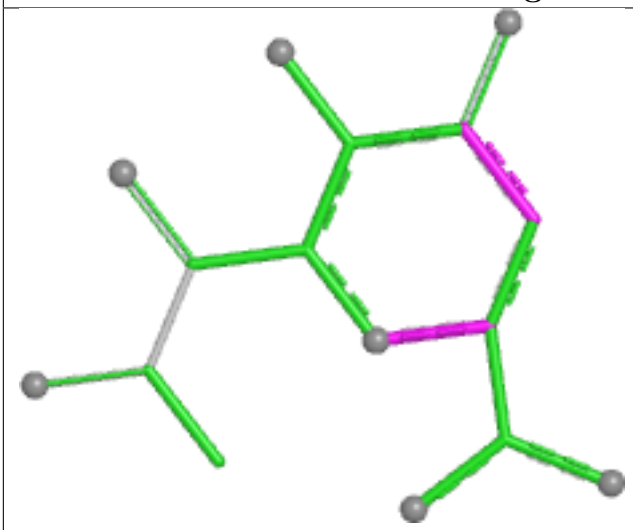


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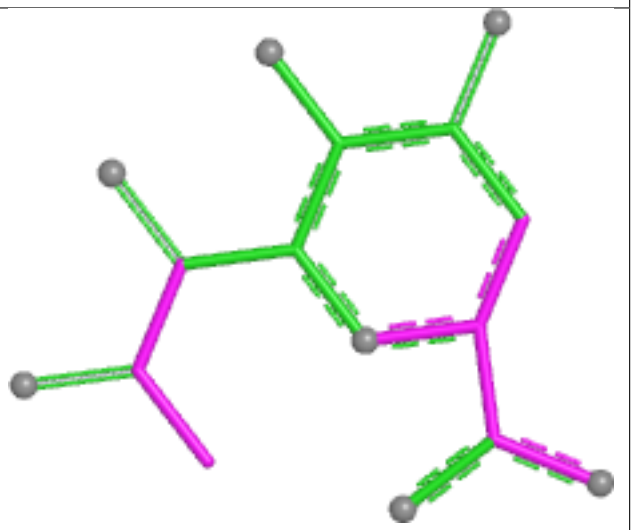


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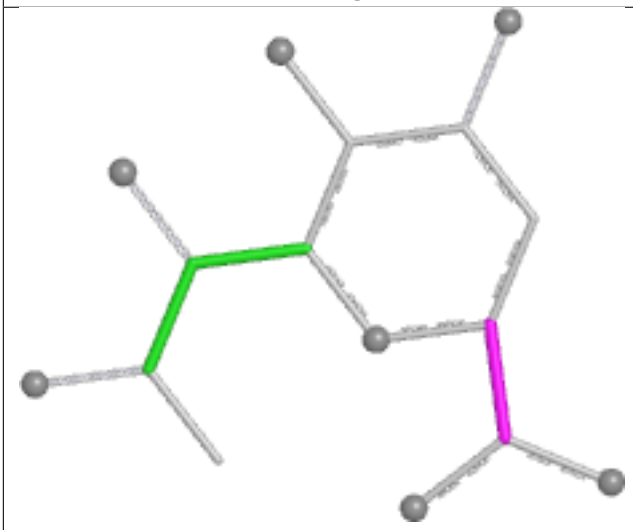
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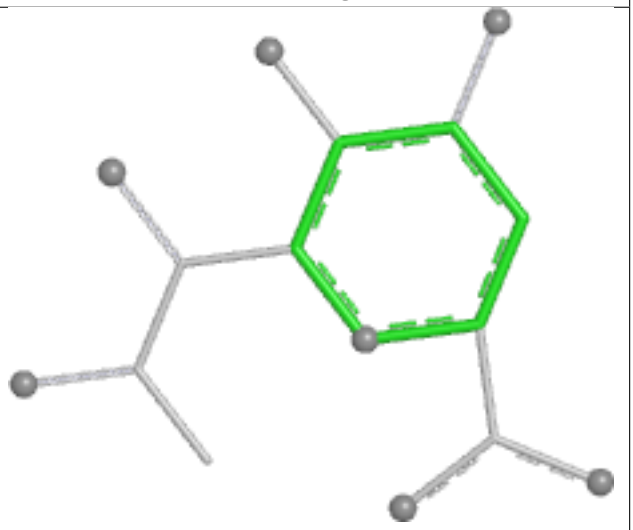
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Bond angles

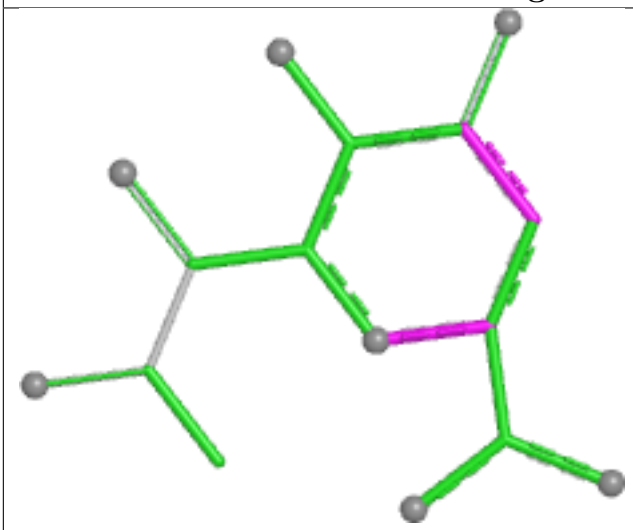


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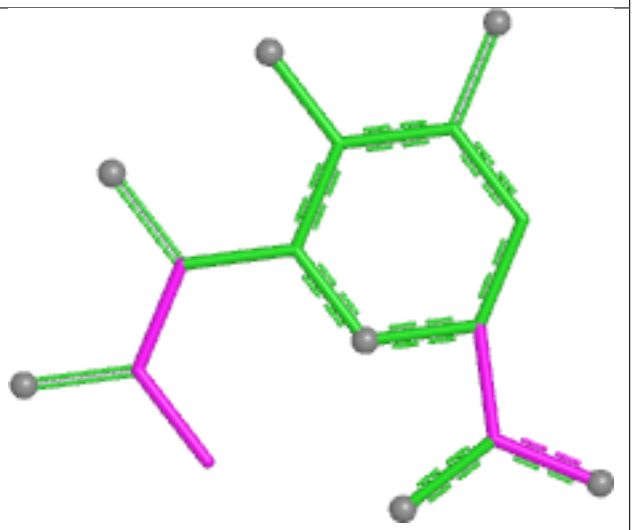


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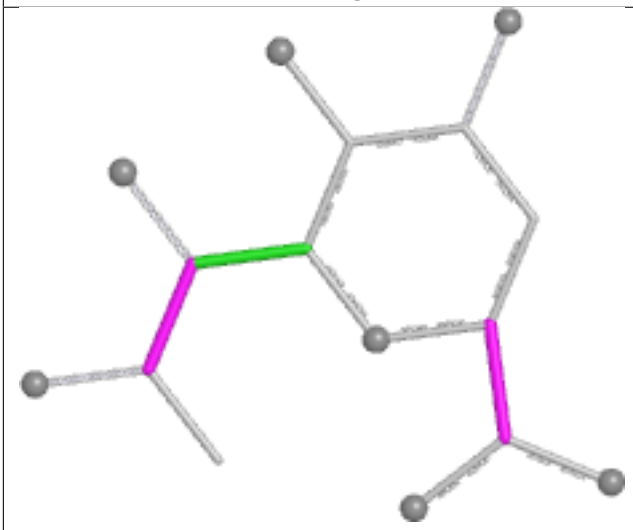
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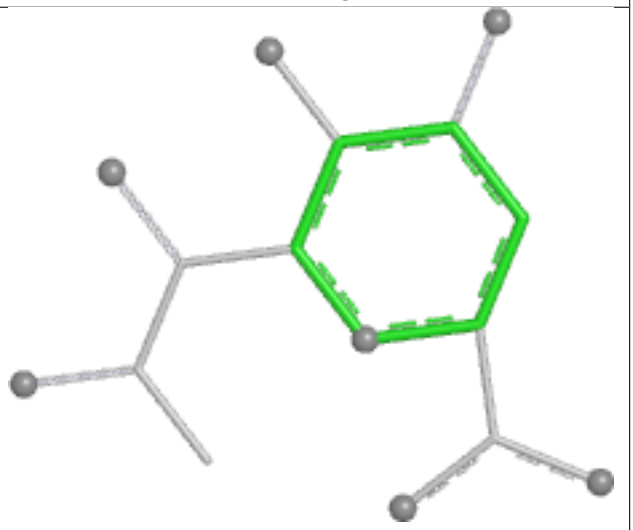
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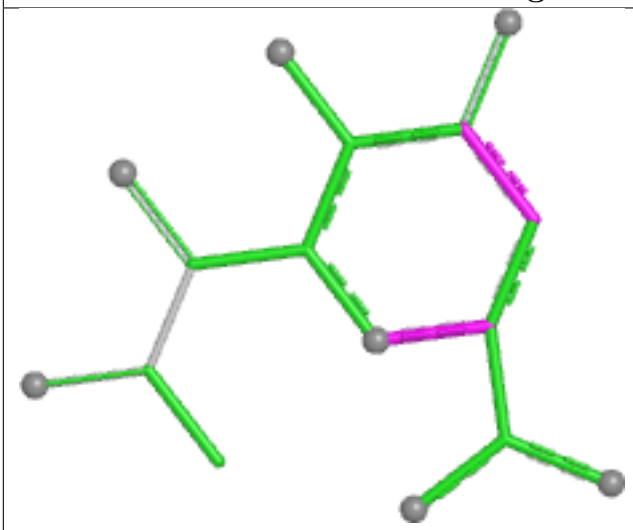


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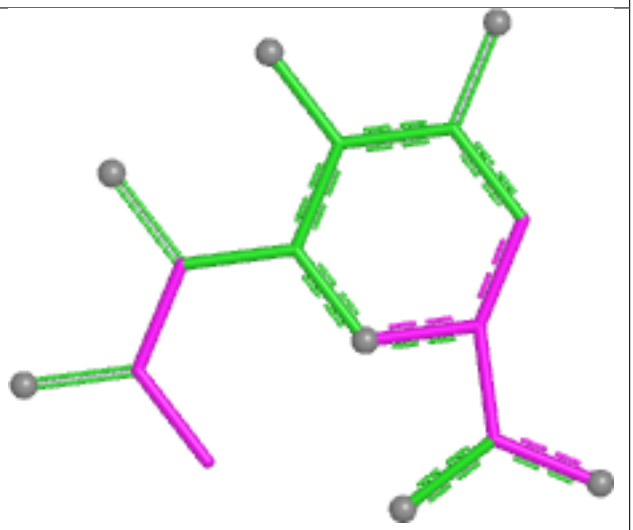


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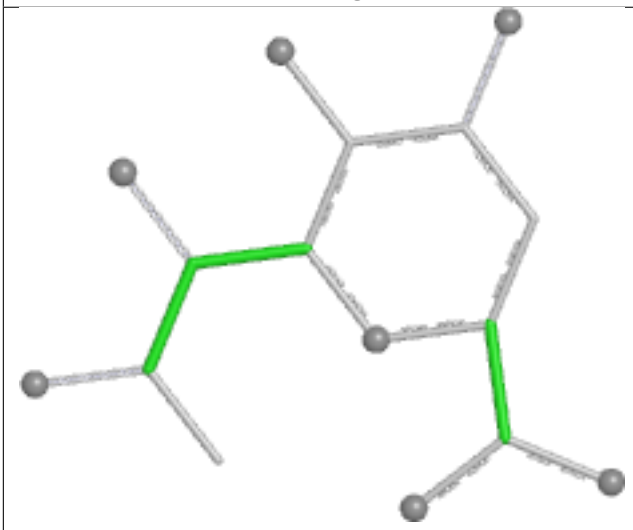
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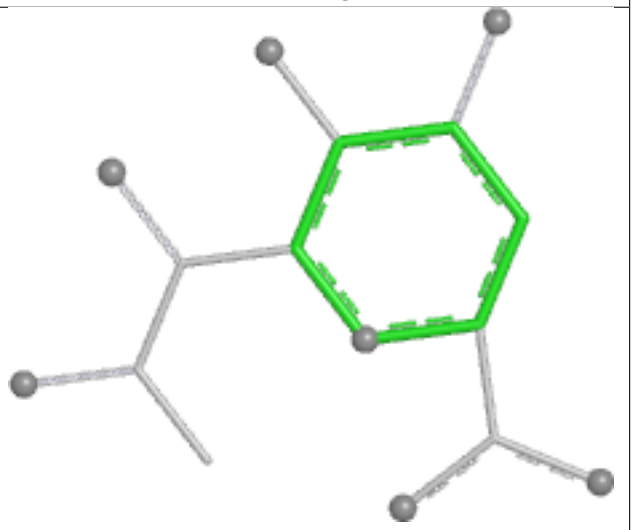
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Bond angles

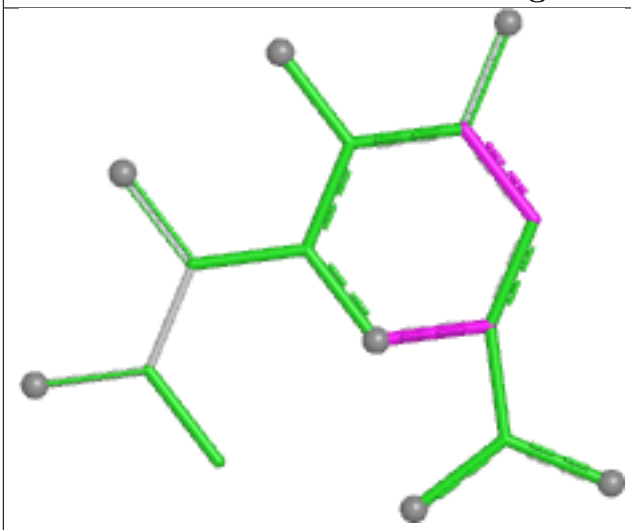


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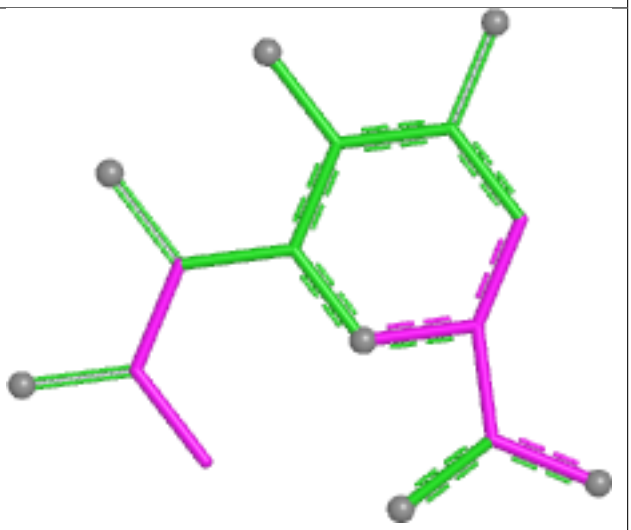


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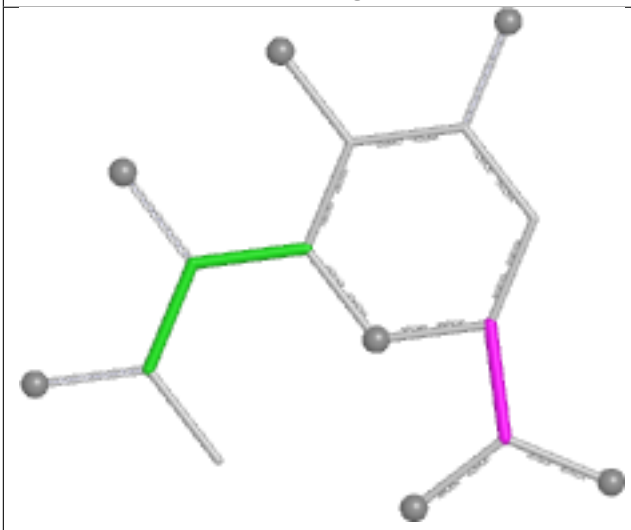
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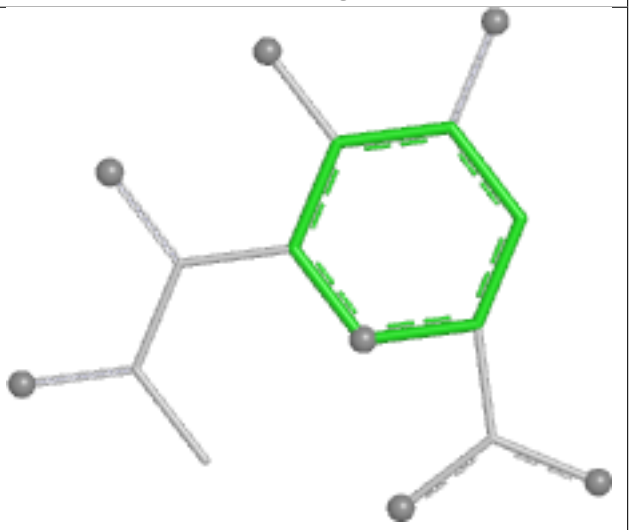
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Bond angles

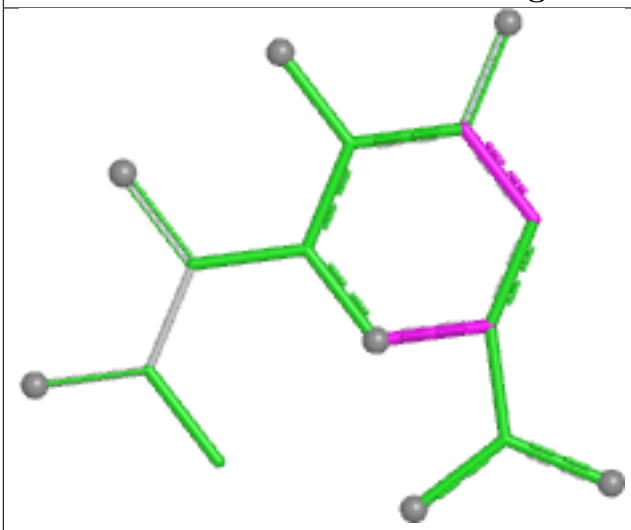


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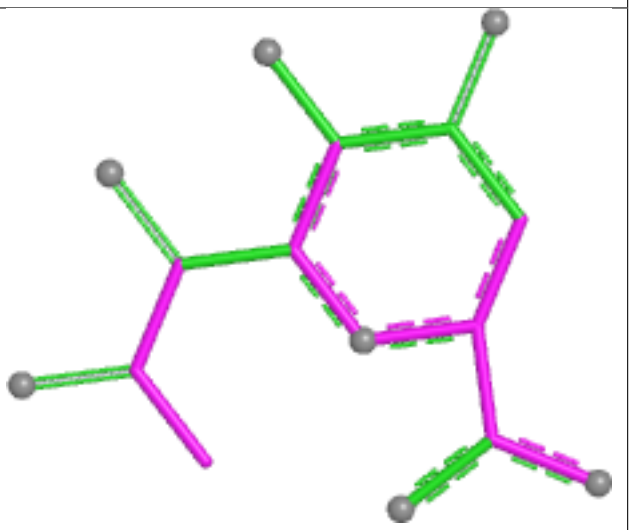


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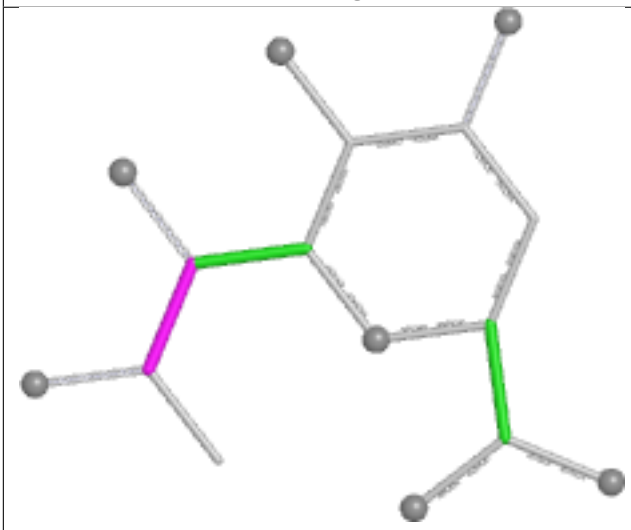
Ligand P8E O 617



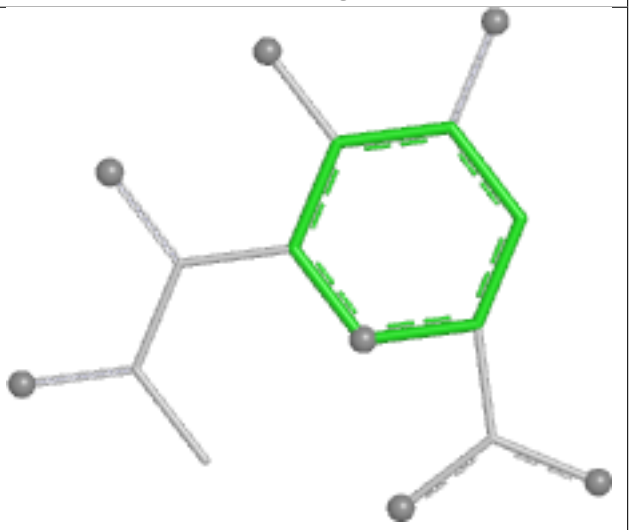
Bond lengths



Bond angles

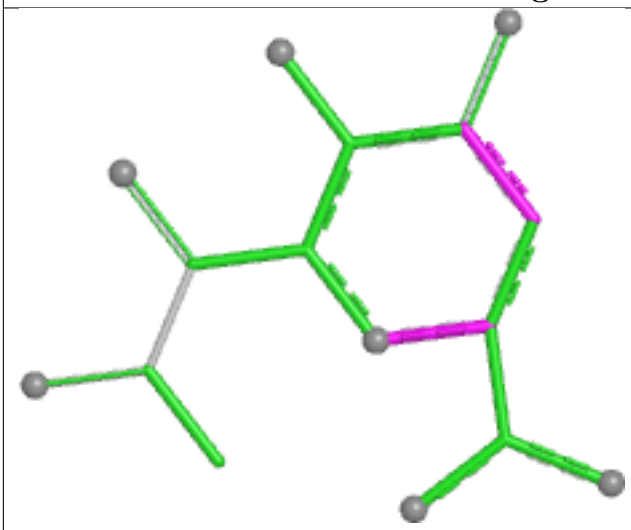


Torsions

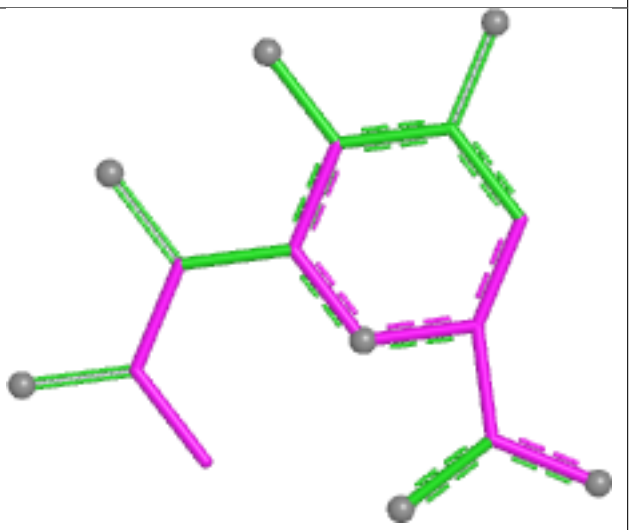


Rings

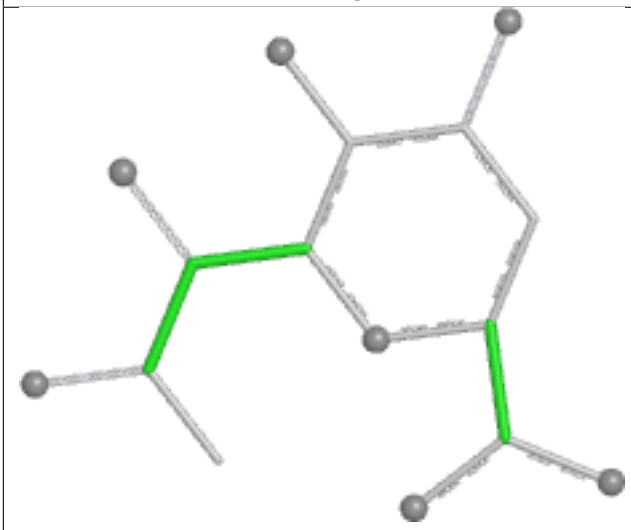
Ligand P8E S 617



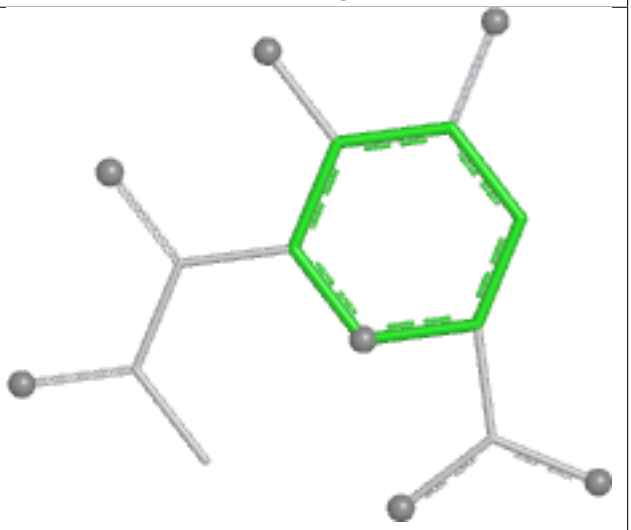
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Bond angles

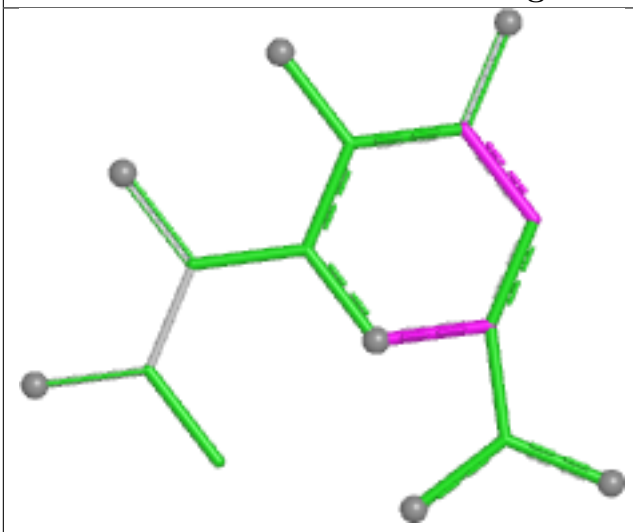


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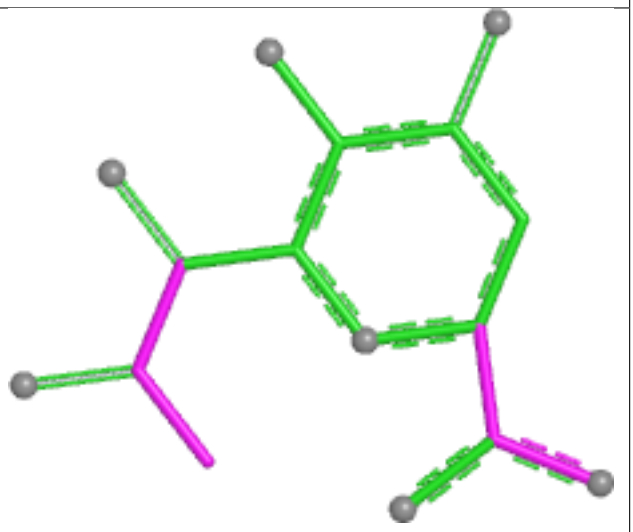


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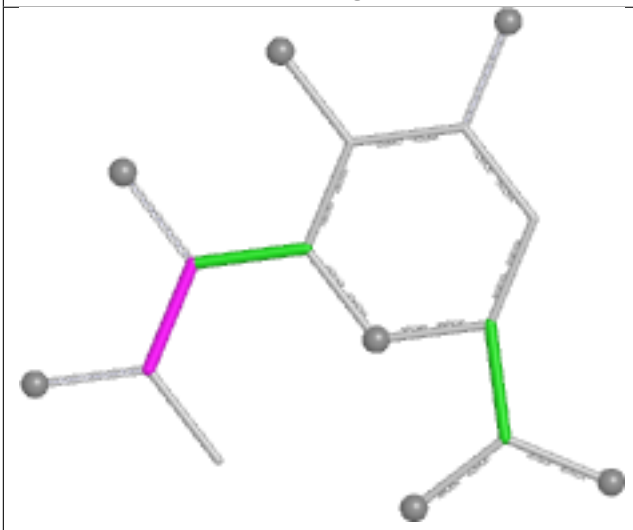
Ligand P8E N 602



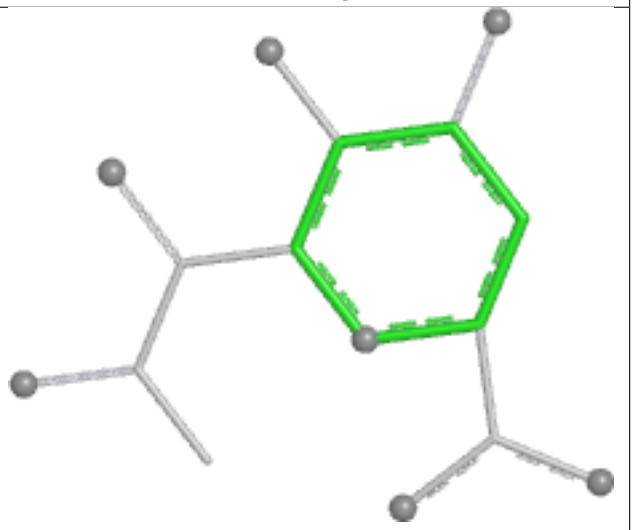
Bond lengths



Bond angles

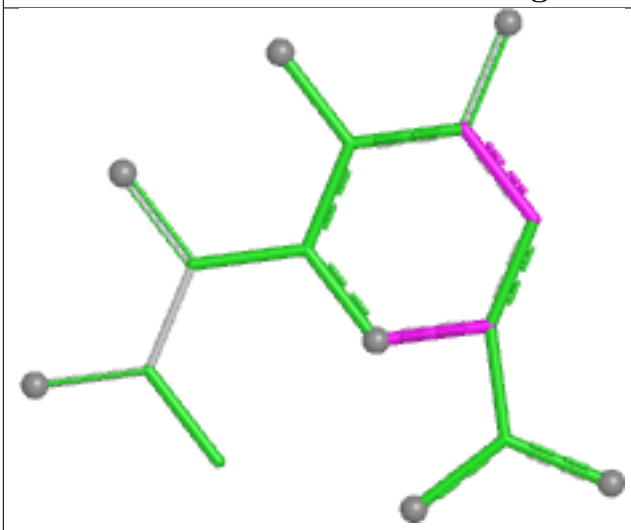


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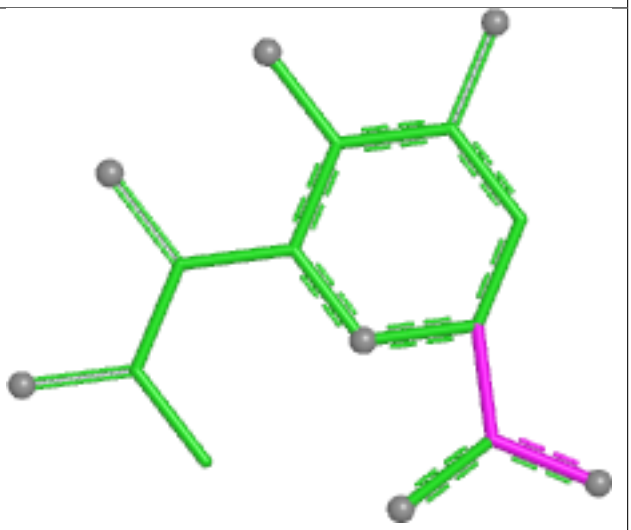


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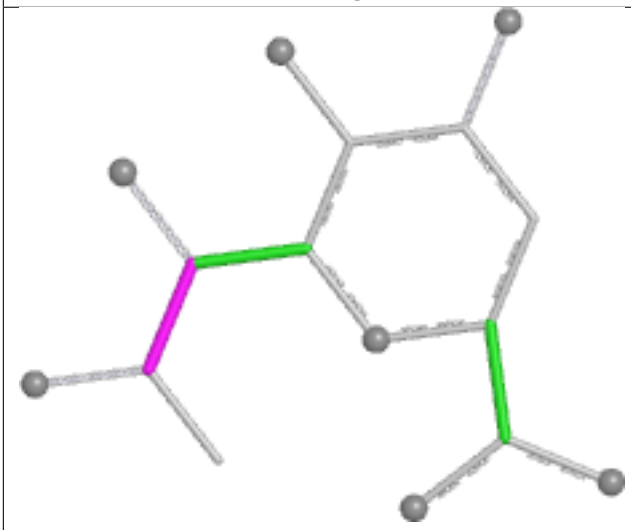
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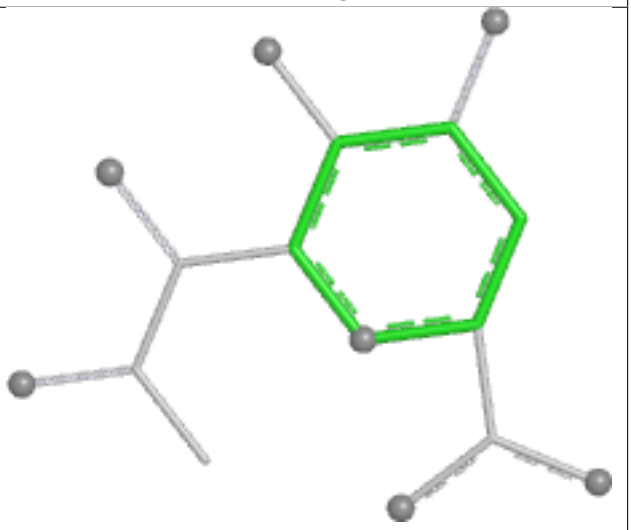
Bond lengths



Bond angles

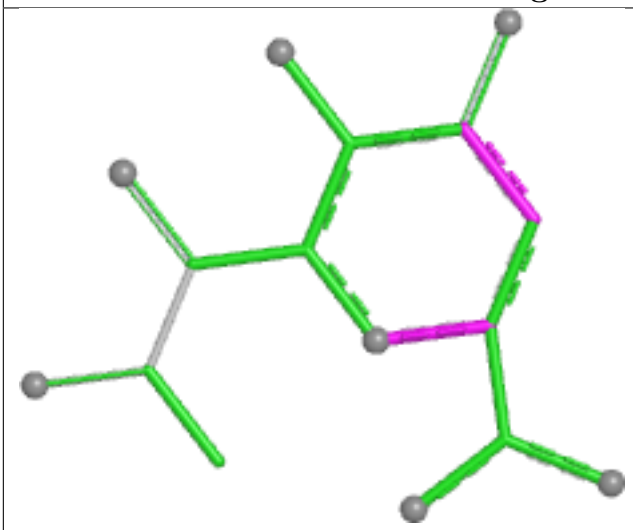


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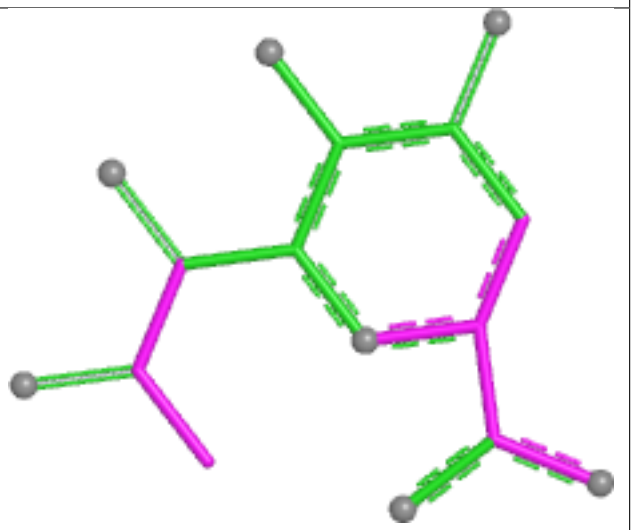


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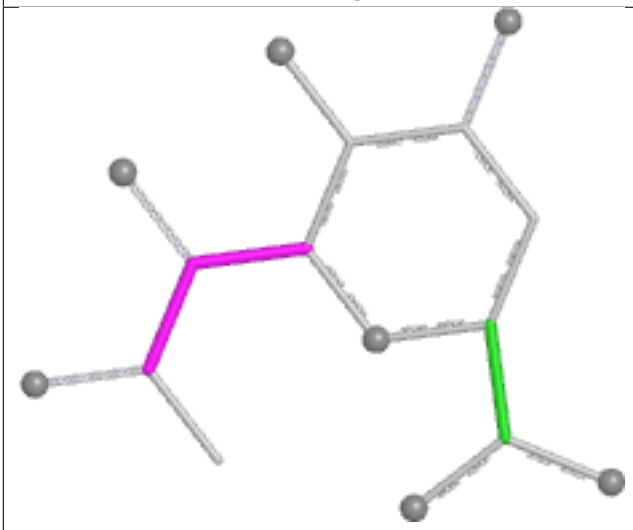
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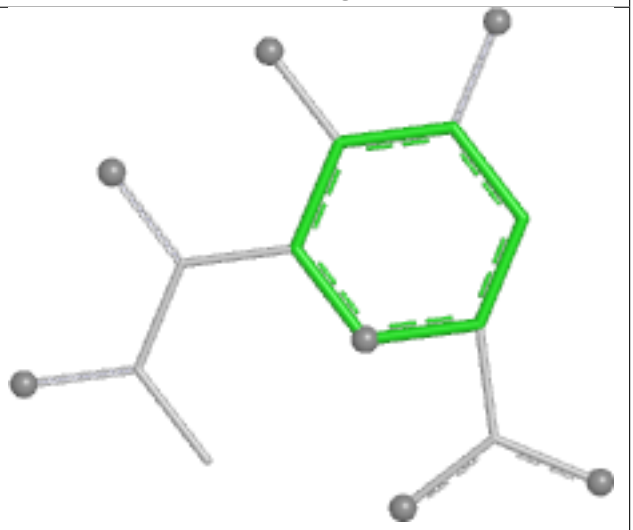
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Bond angles

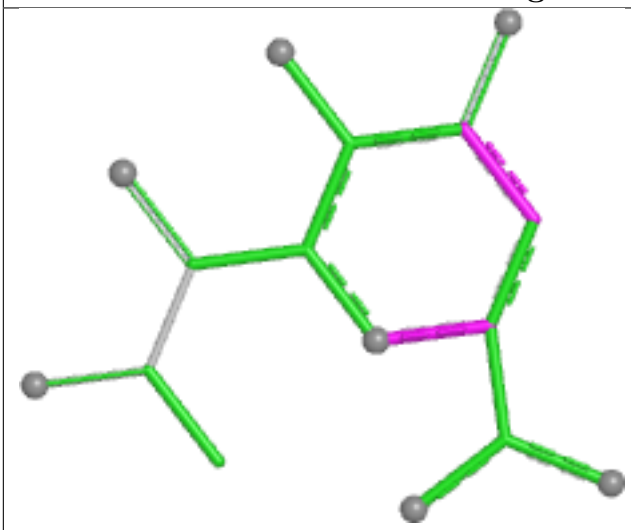


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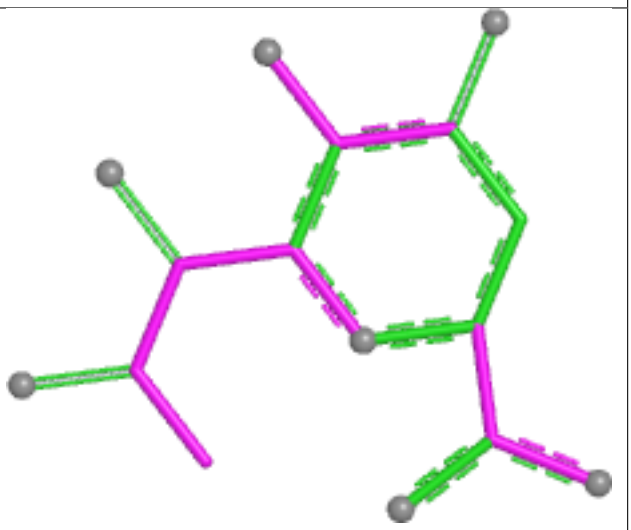


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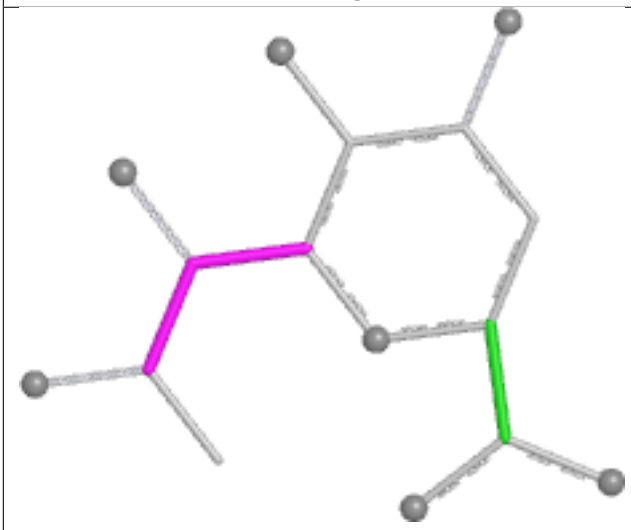
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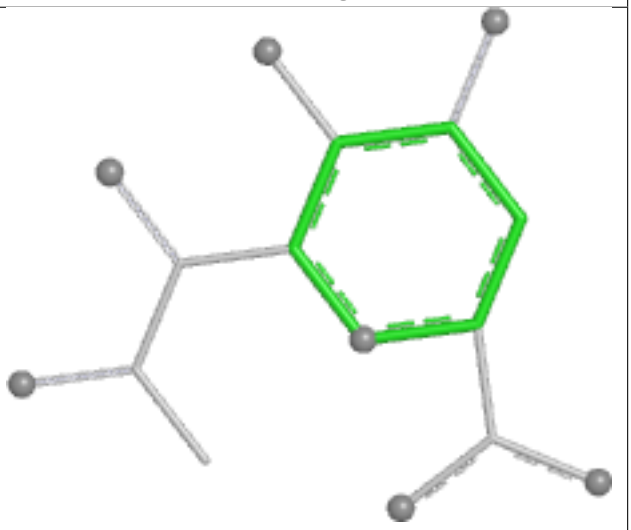
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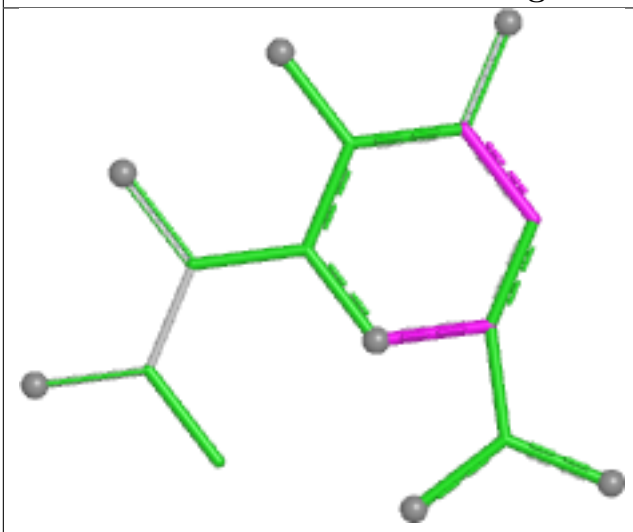


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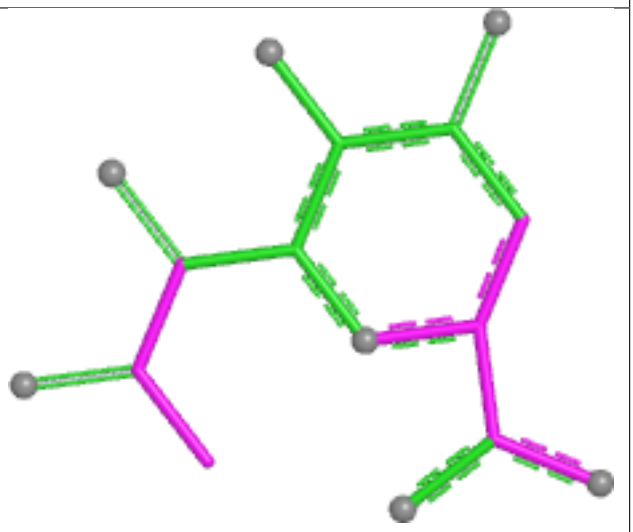


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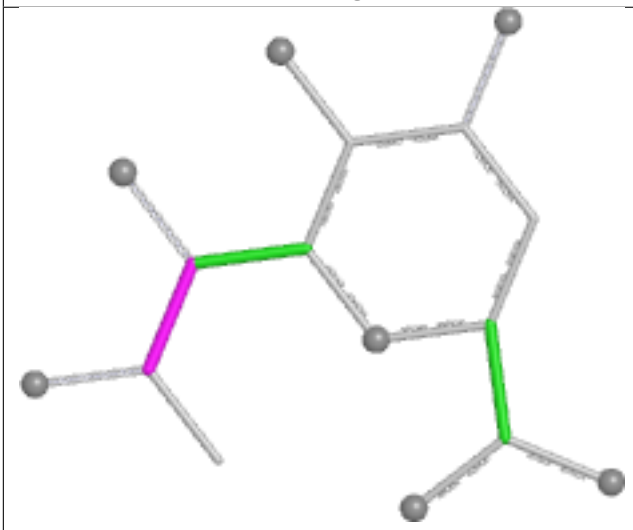
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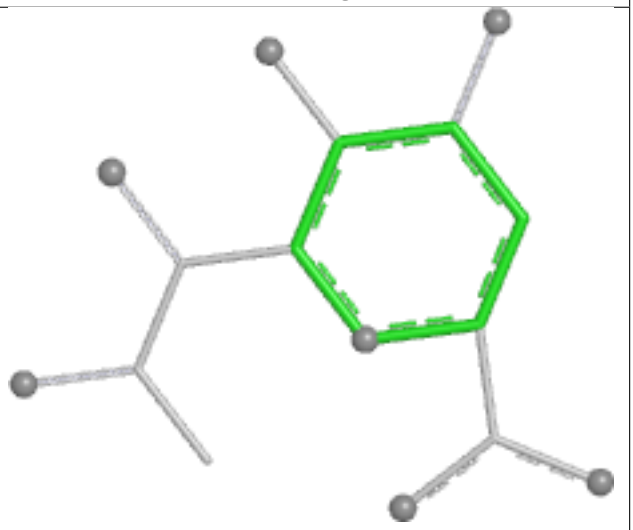
Bond lengths



Bond angles

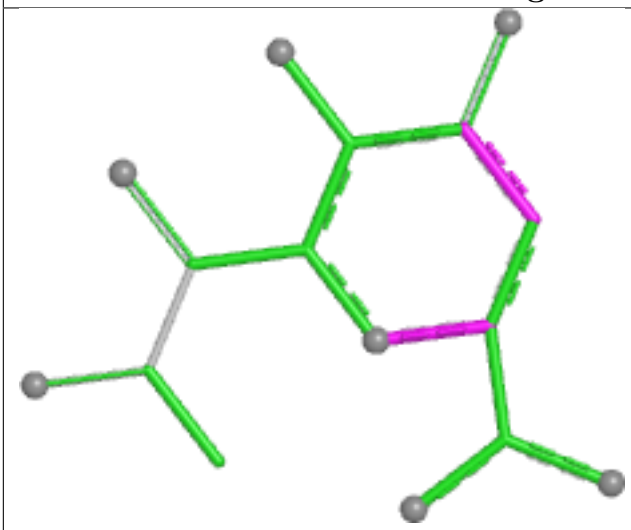


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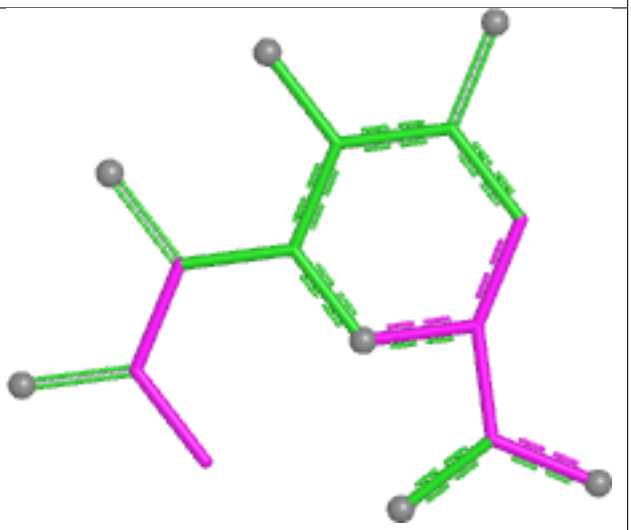


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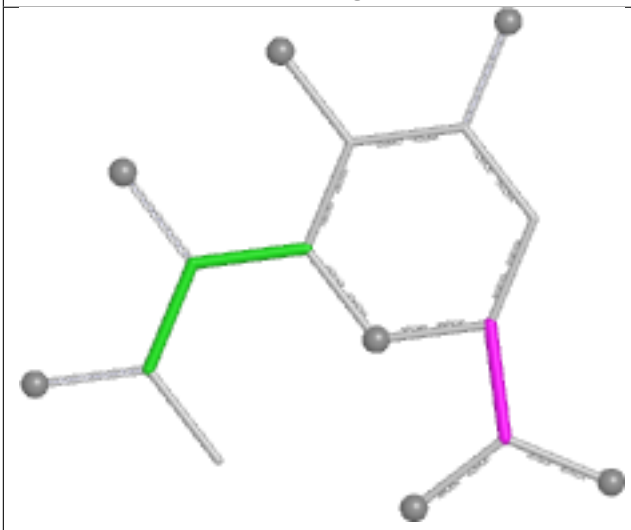
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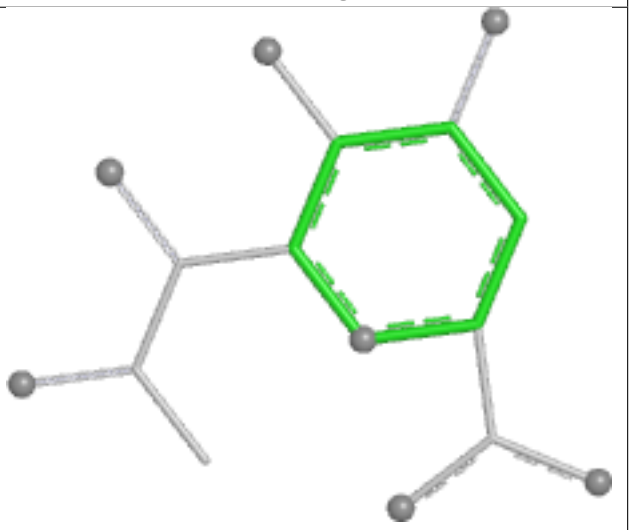
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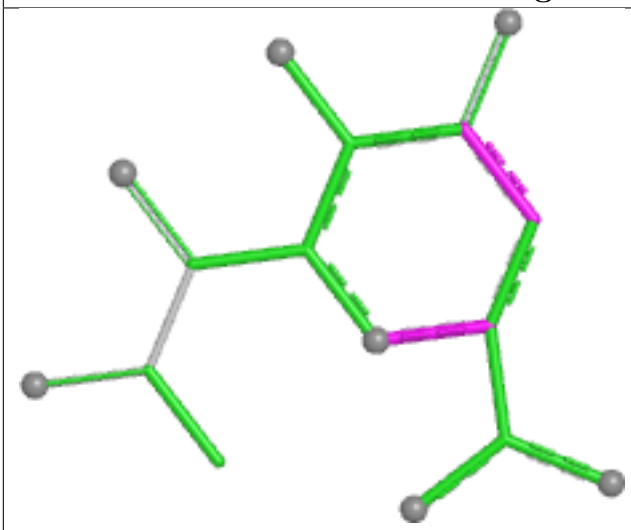


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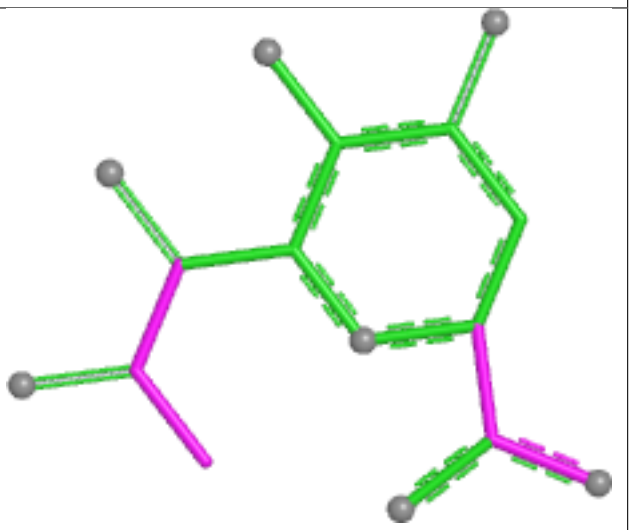


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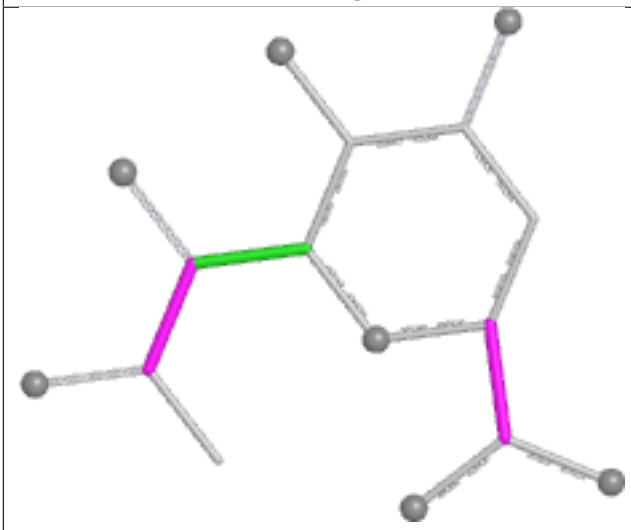
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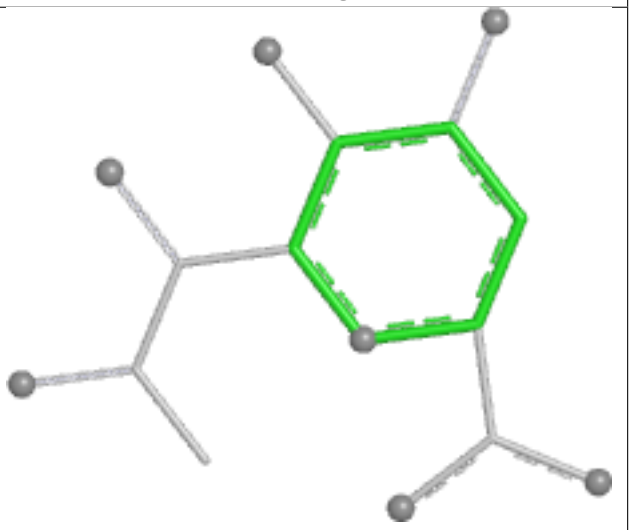
Bond lengths



Bond angles

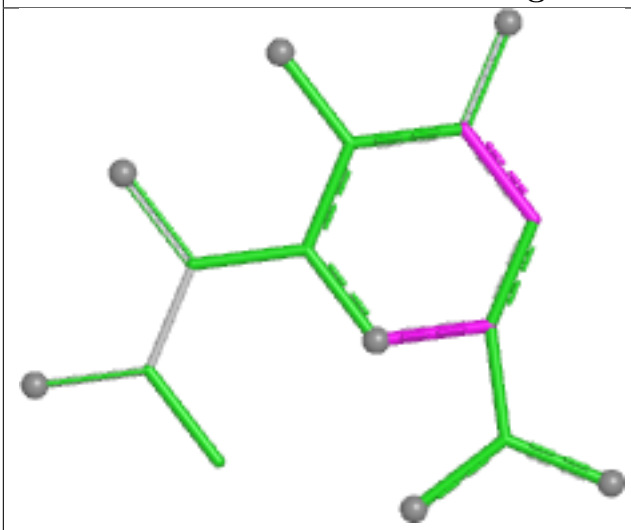


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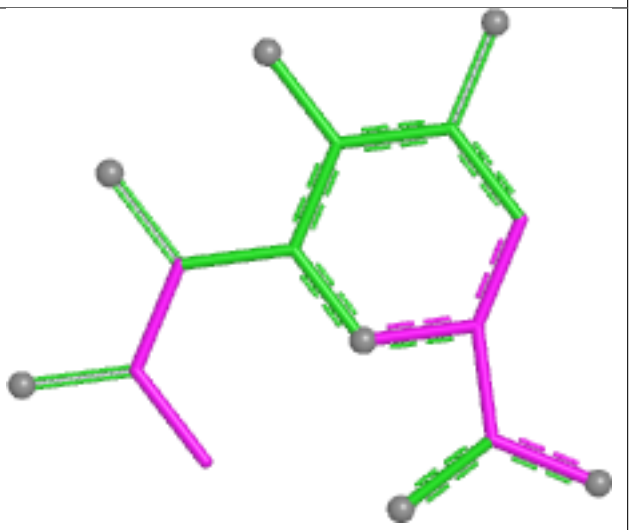


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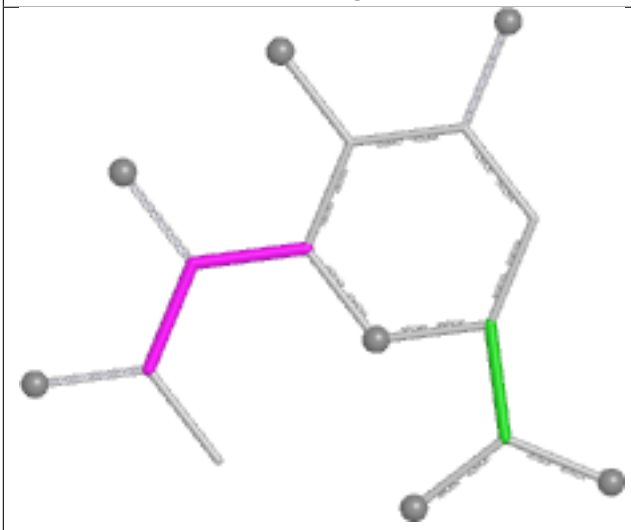
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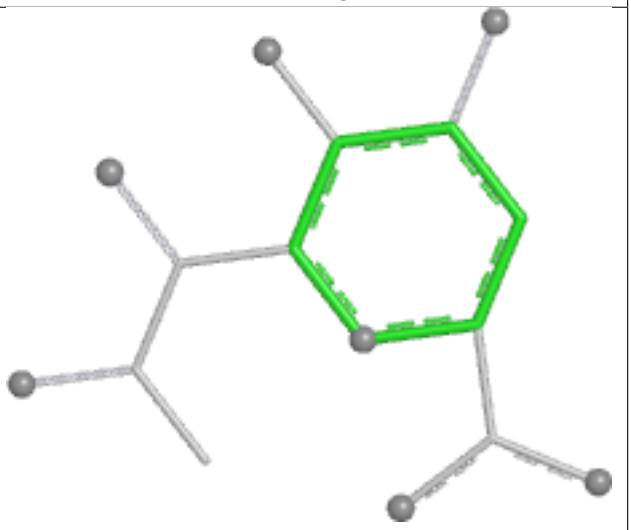
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Bond angles

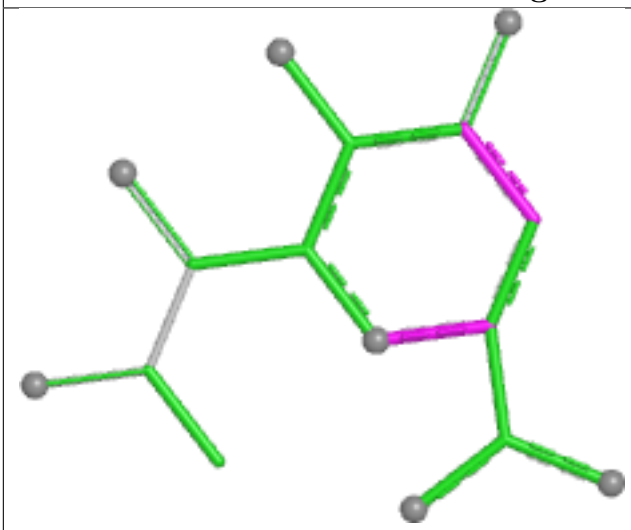


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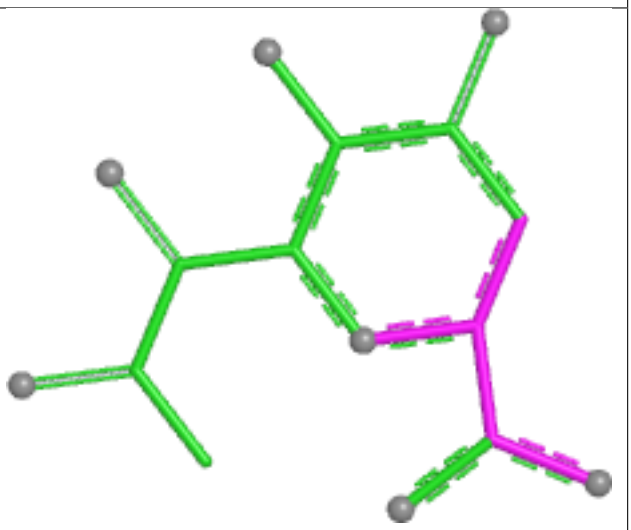


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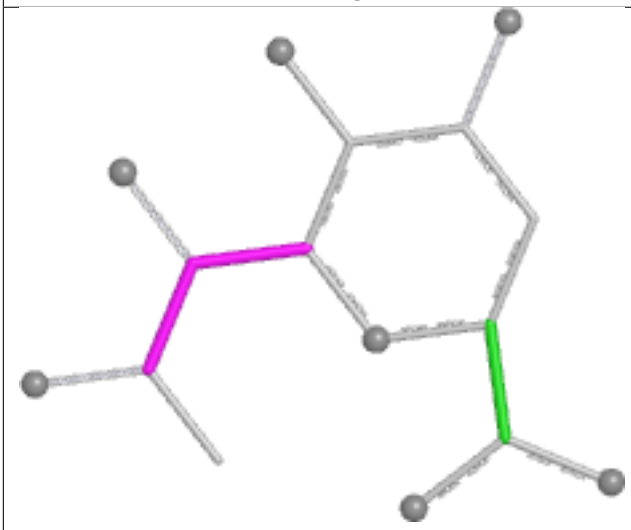
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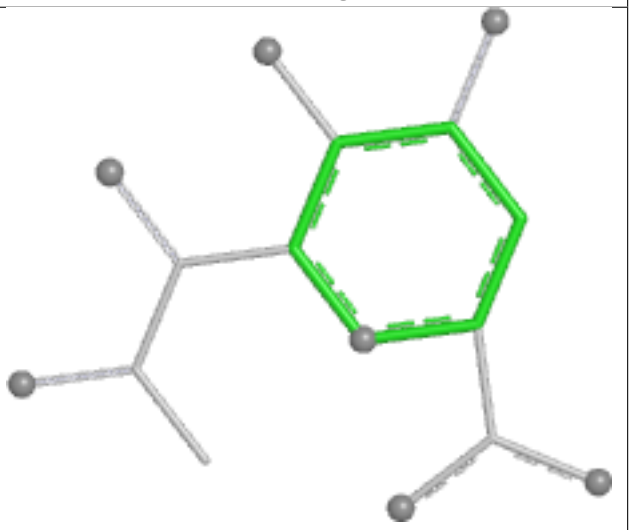
Bond lengths



Bond angles

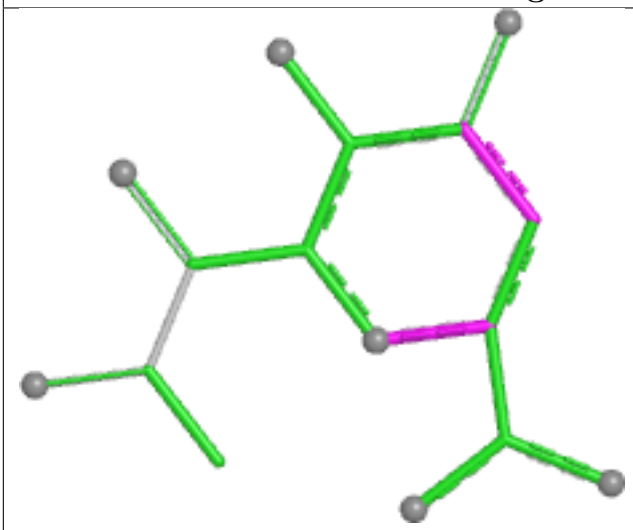


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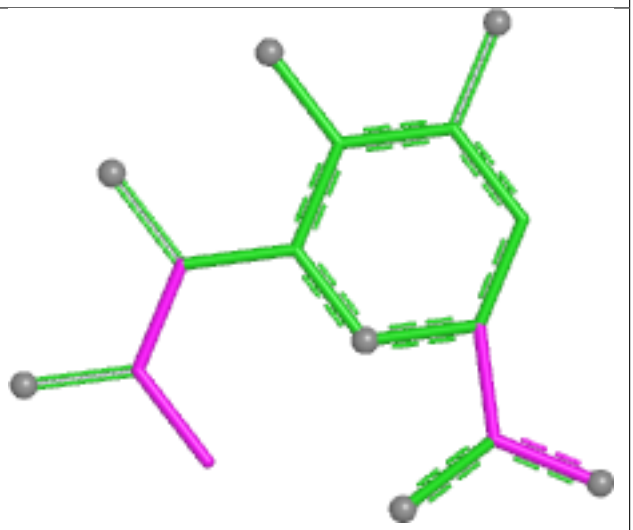


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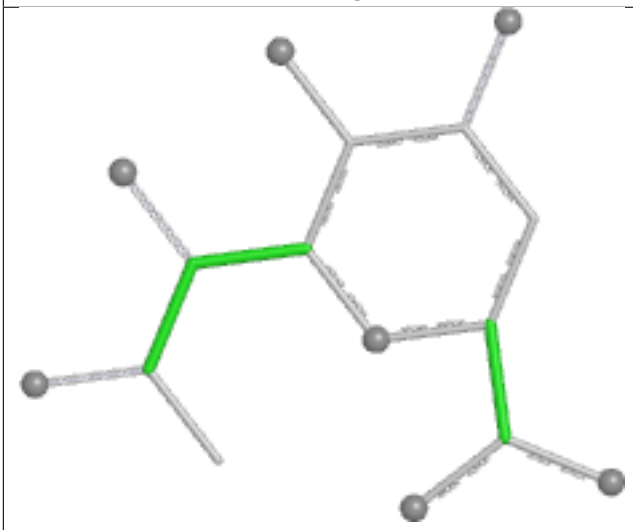
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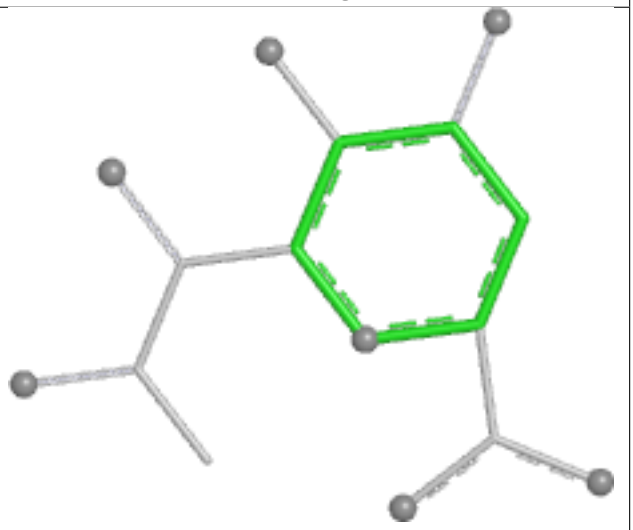
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Bond angles

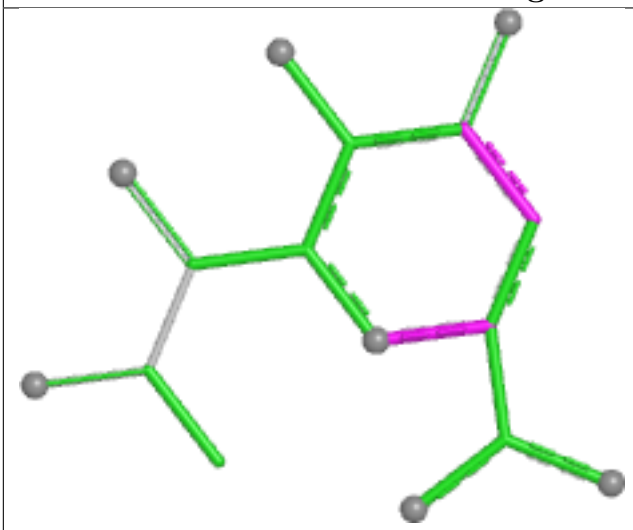


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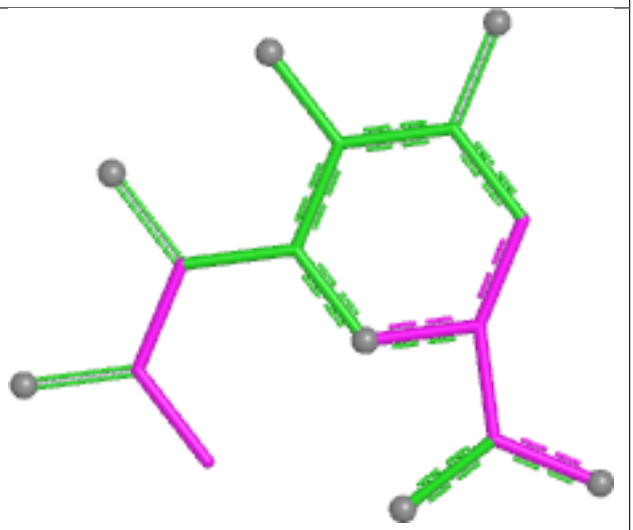


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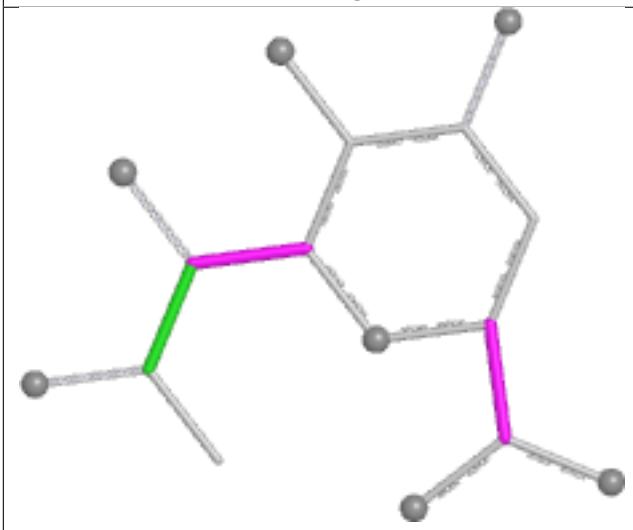
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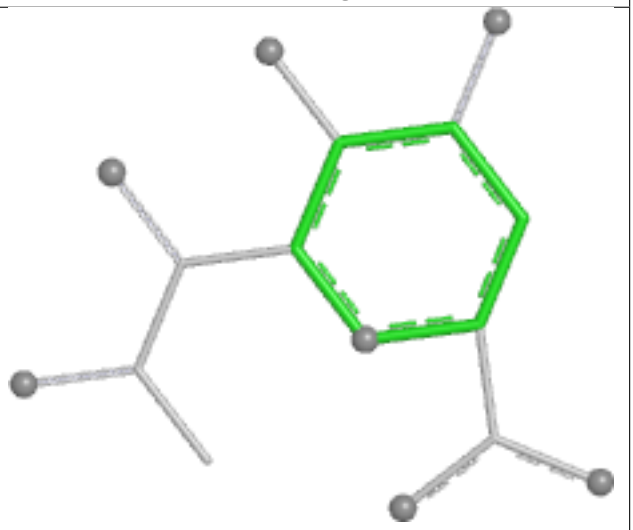
Bond lengths



Bond angles

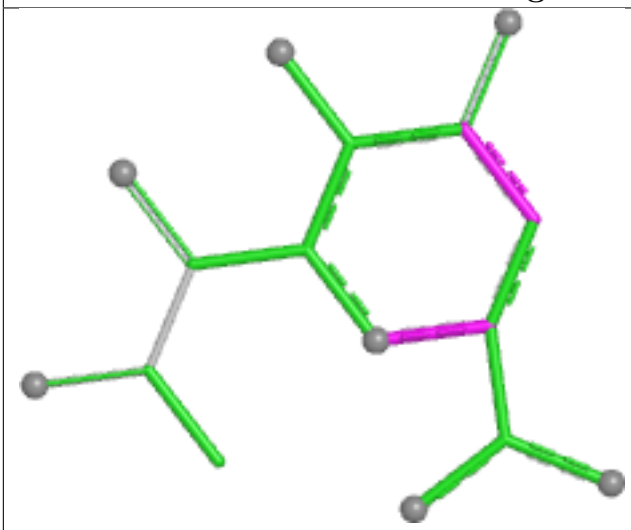


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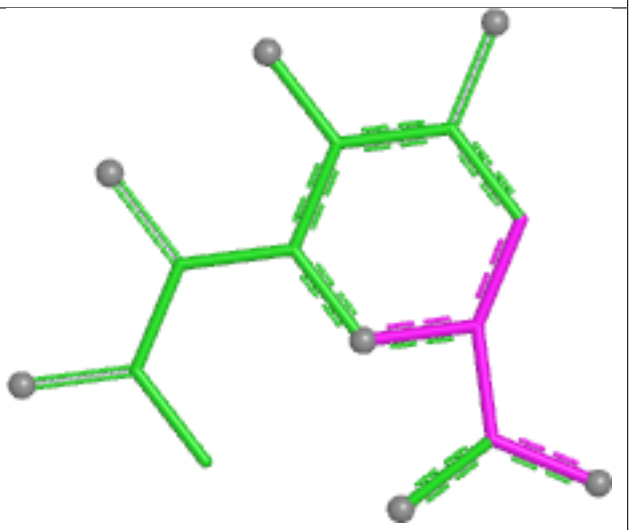


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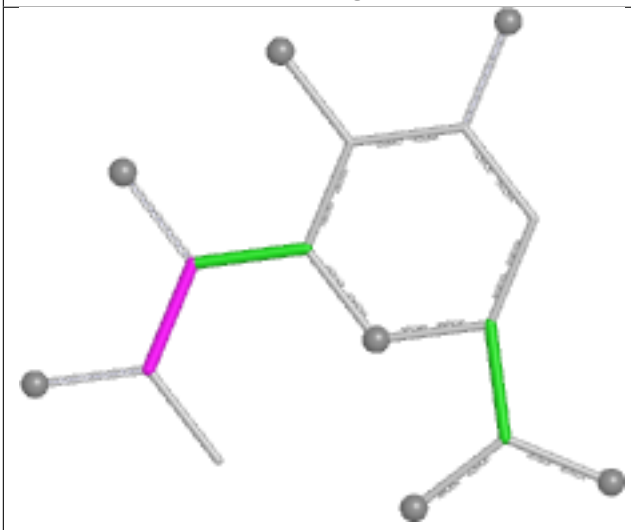
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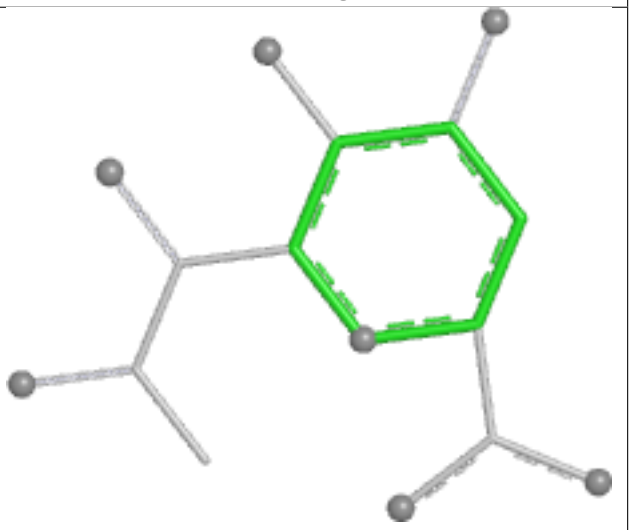
Bond lengths



Bond angles

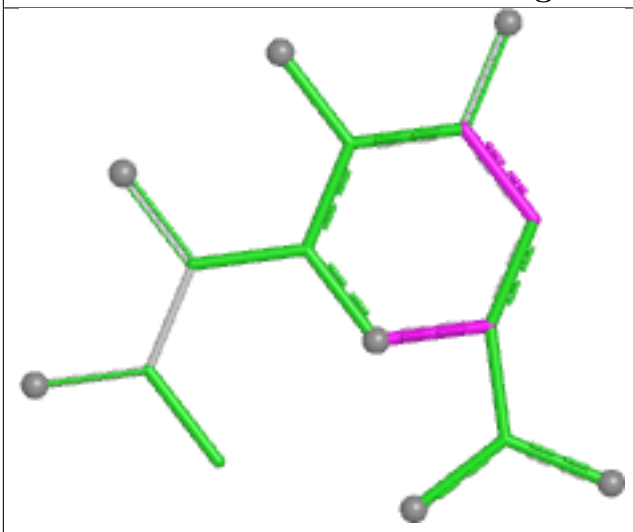


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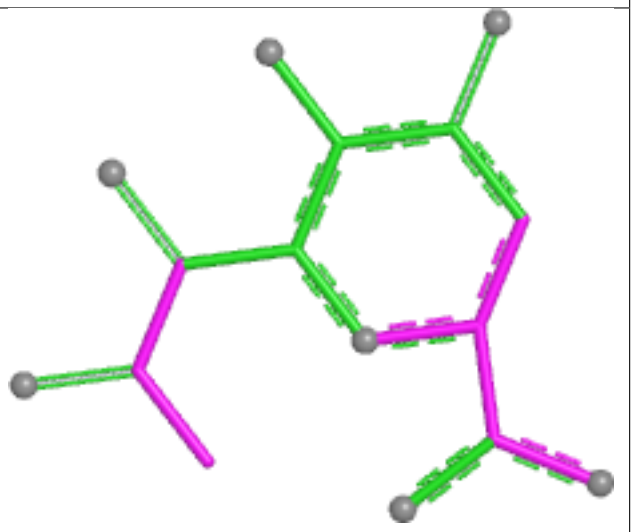


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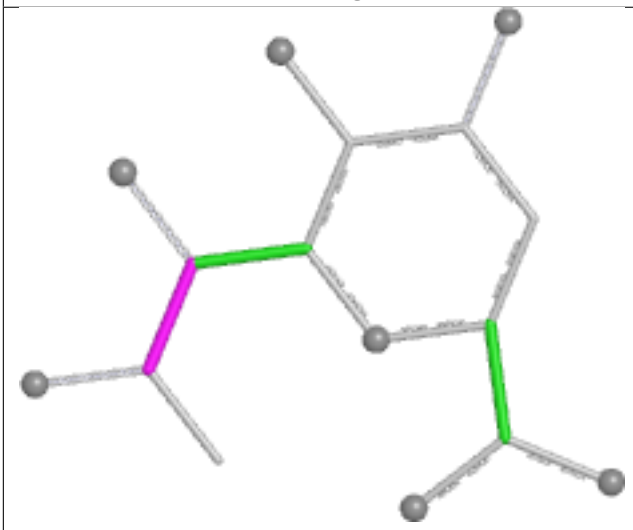
Ligand P8E I 602



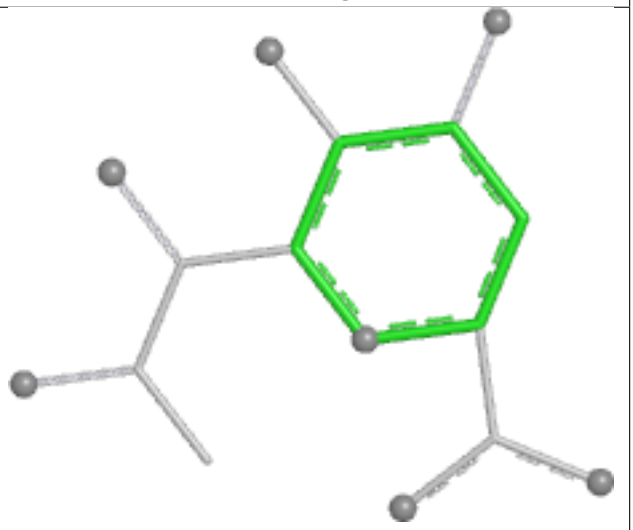
Bond lengths



Bond angles

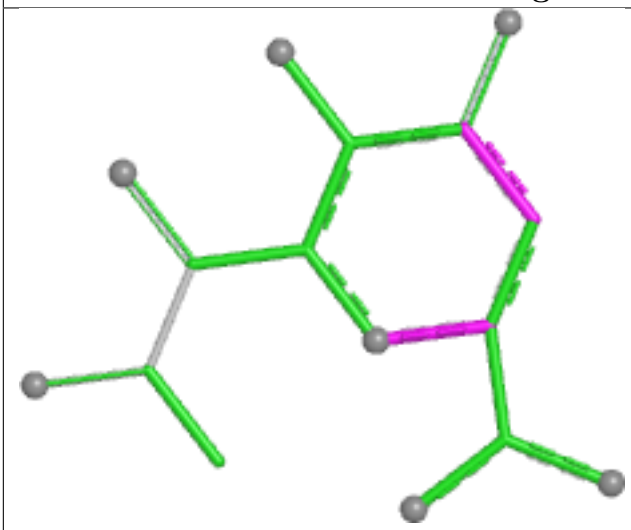


Torsions

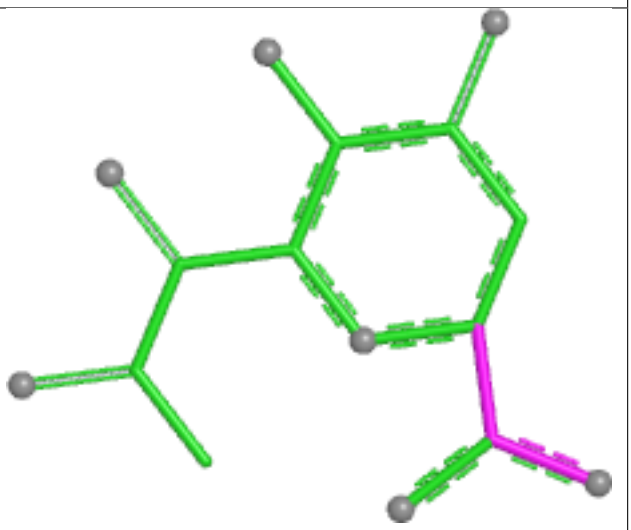


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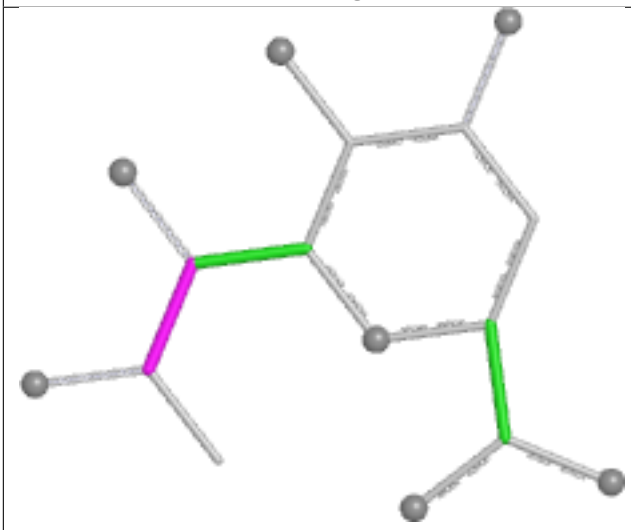
Ligand P8E J 609



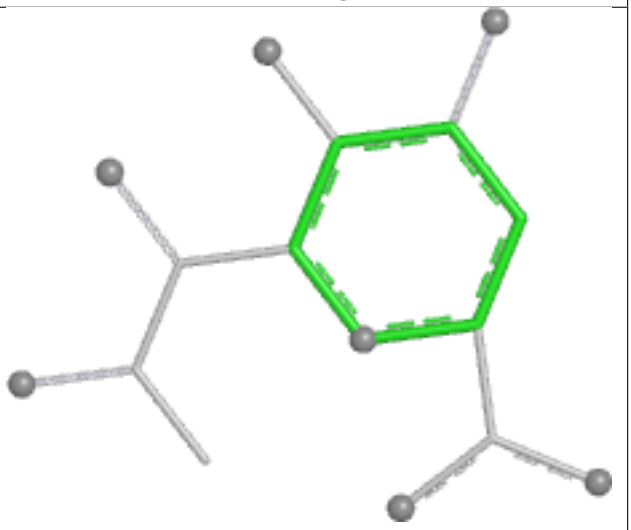
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Bond angles

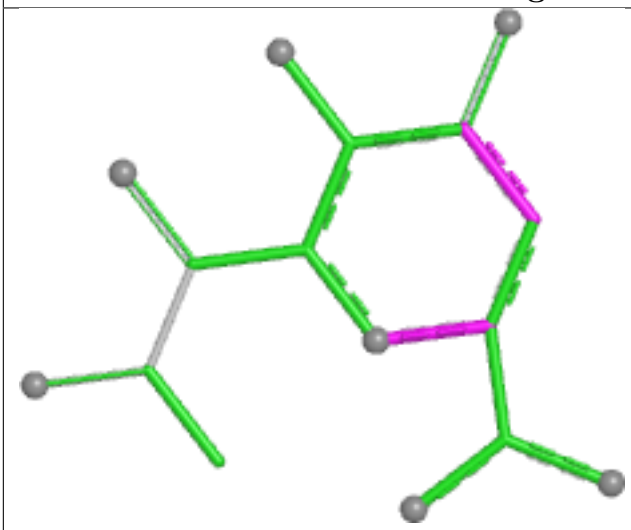


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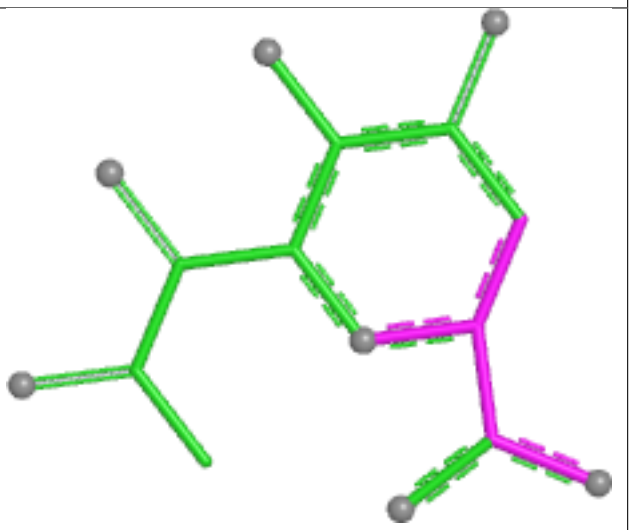


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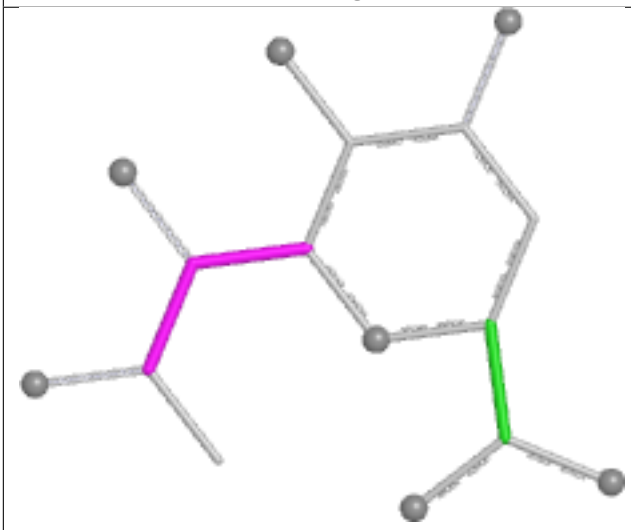
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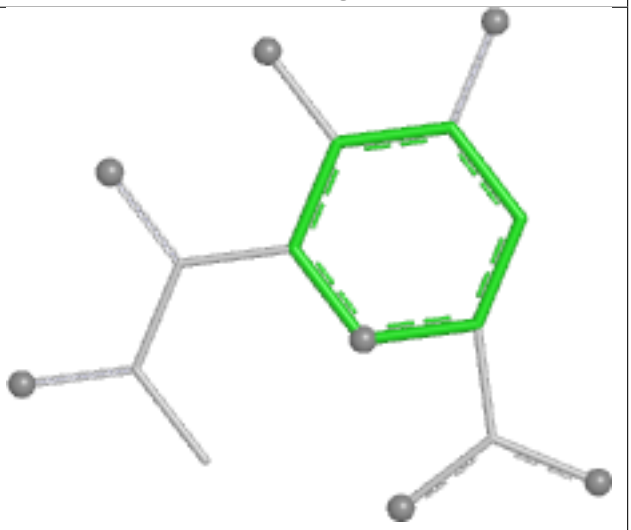
Bond lengths



Bond angles

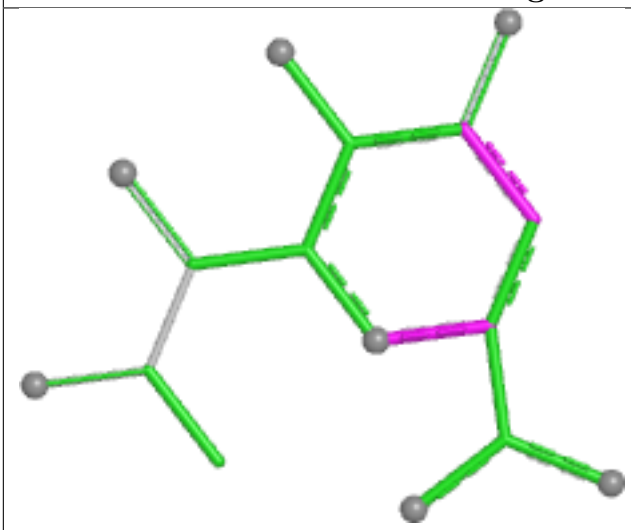


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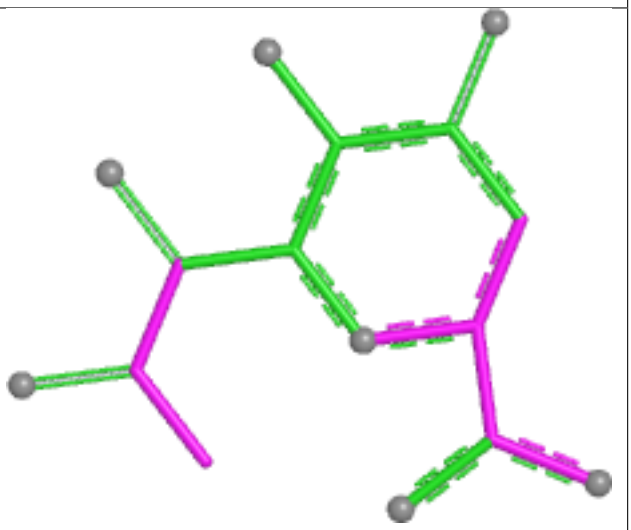


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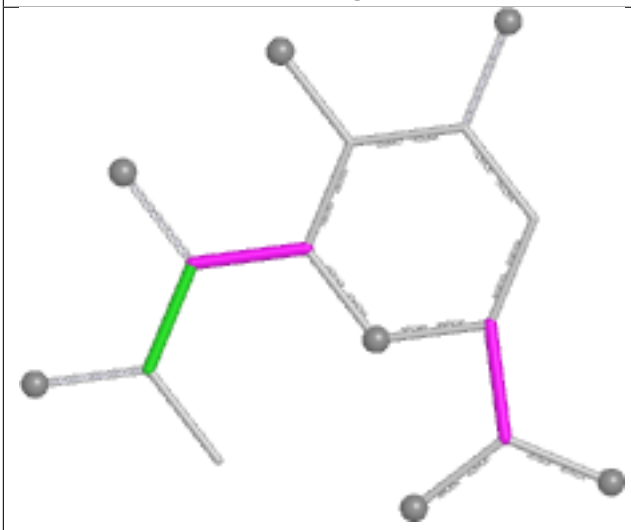
Ligand P8E N 607



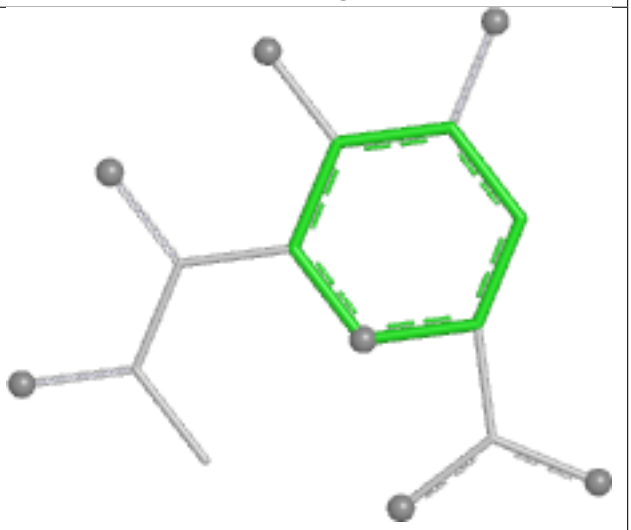
Bond lengths



Bond angles

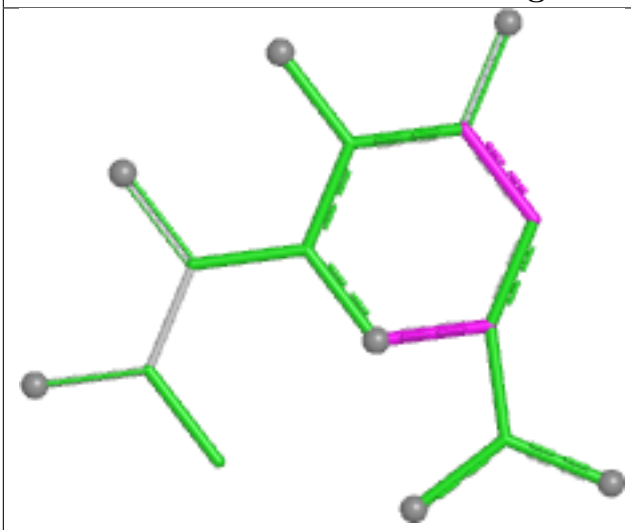


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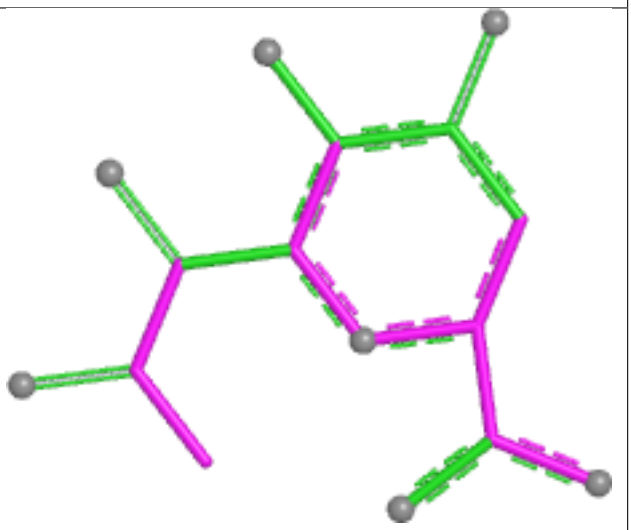


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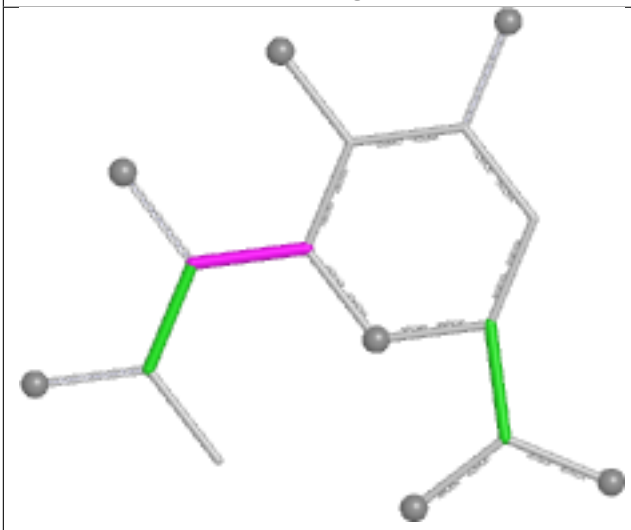
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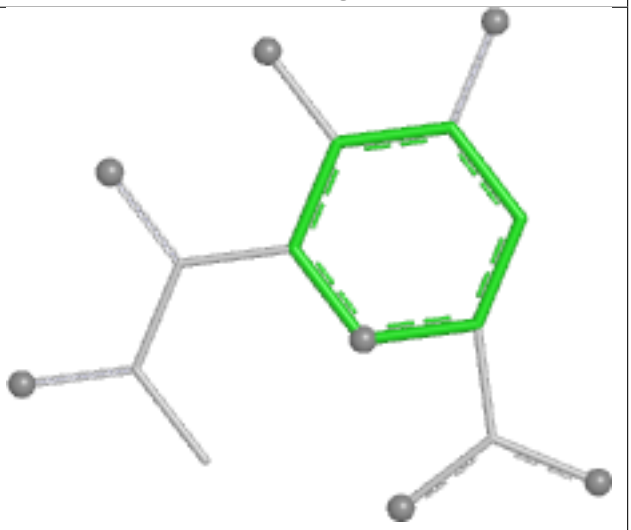
Bond lengths



Bond angles

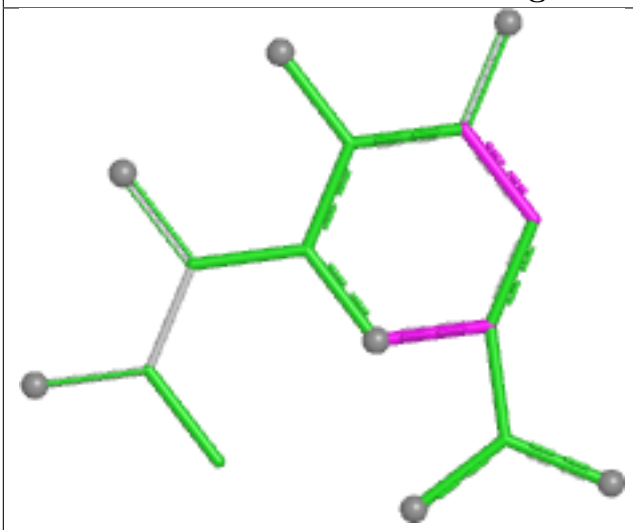


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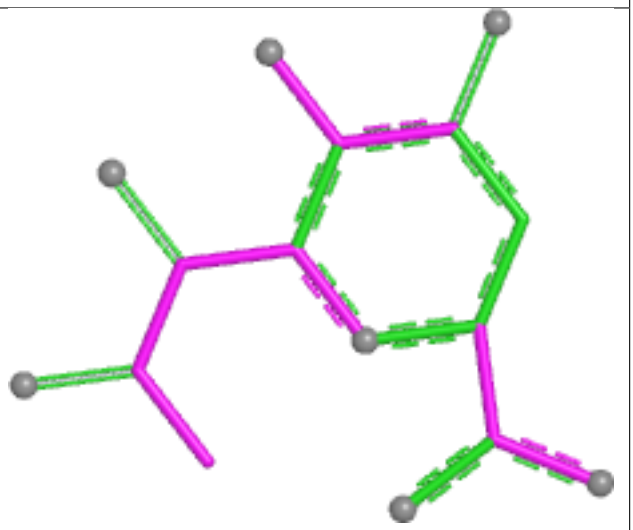


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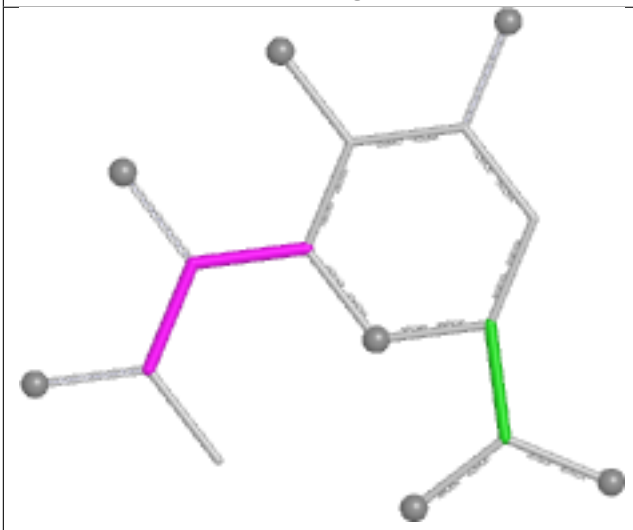
Ligand P8E C 616



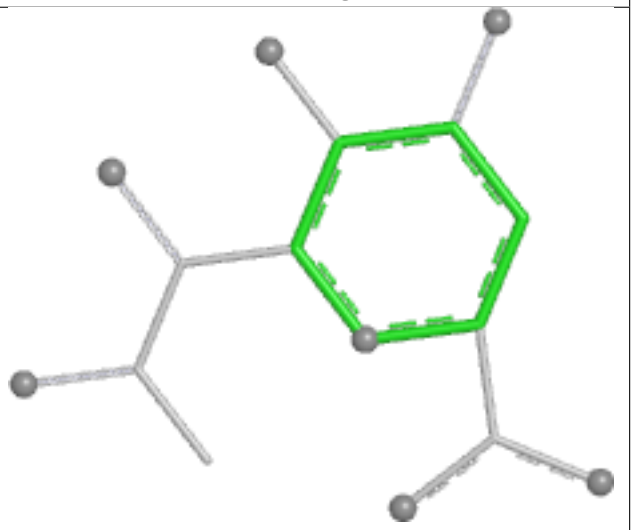
Bond lengths



Bond angles

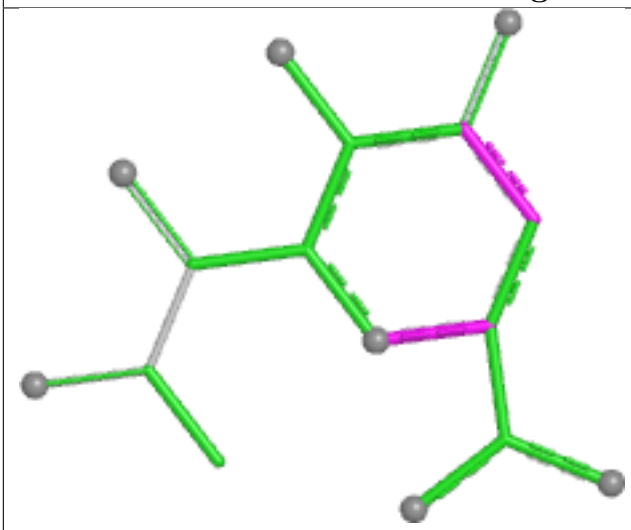


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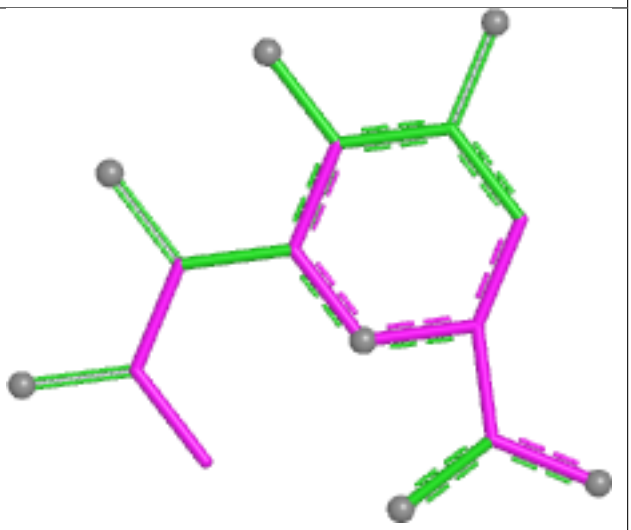


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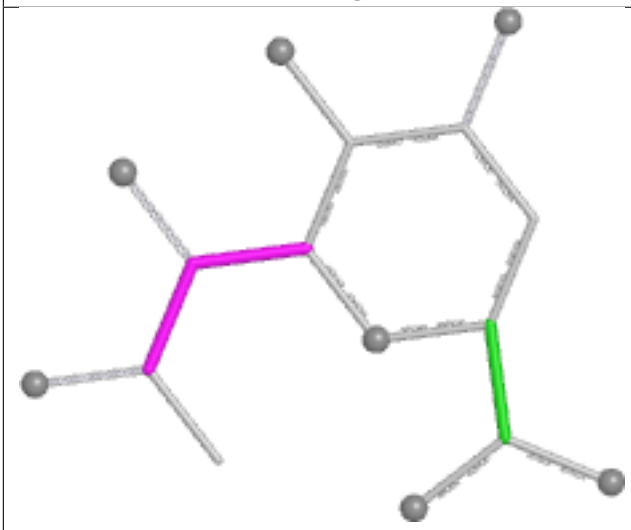
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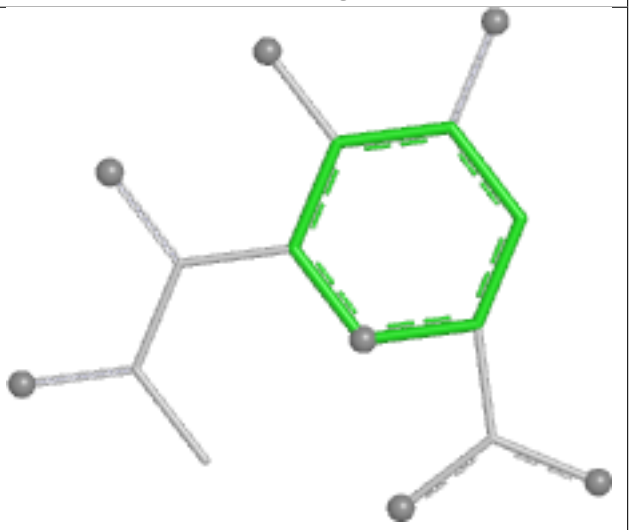
Bond lengths



Bond angles

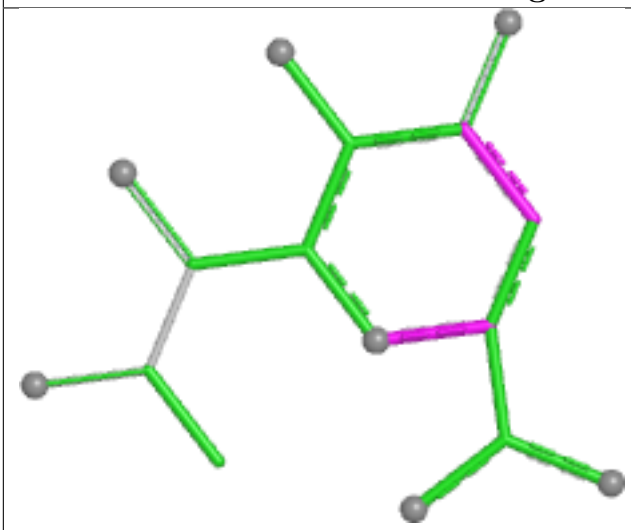


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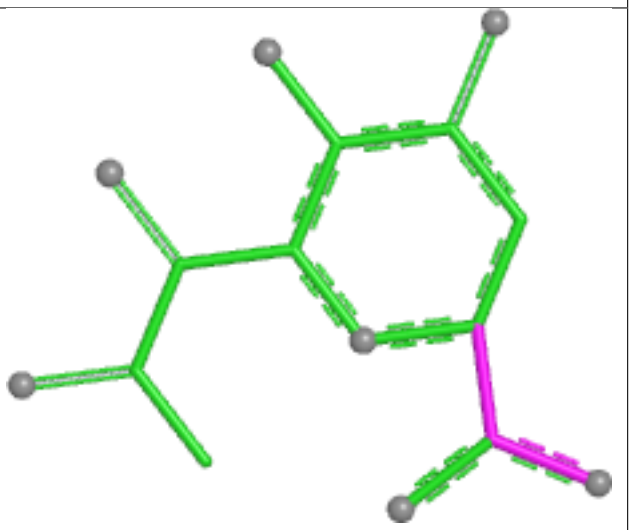


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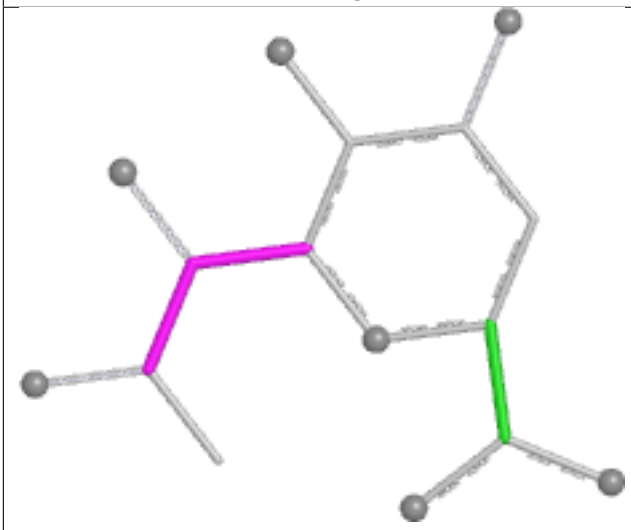
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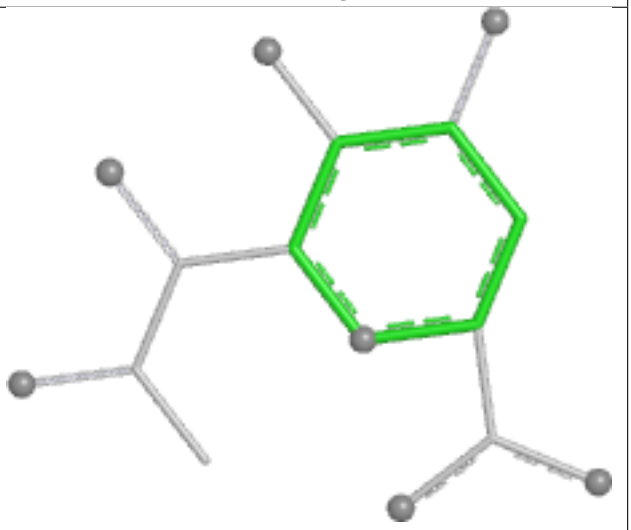
Bond lengths



Bond angles

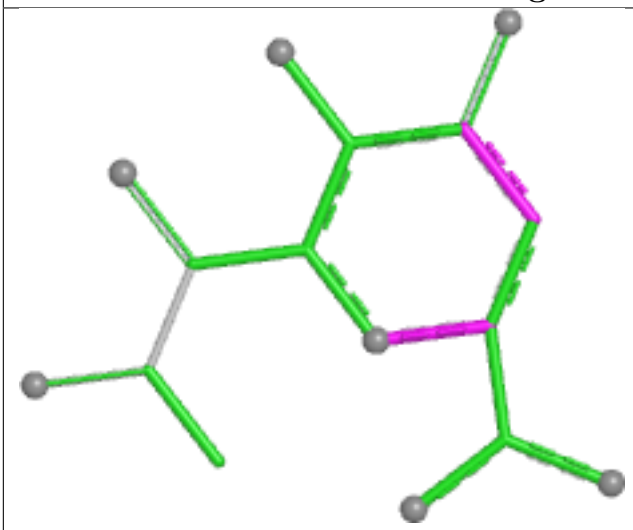


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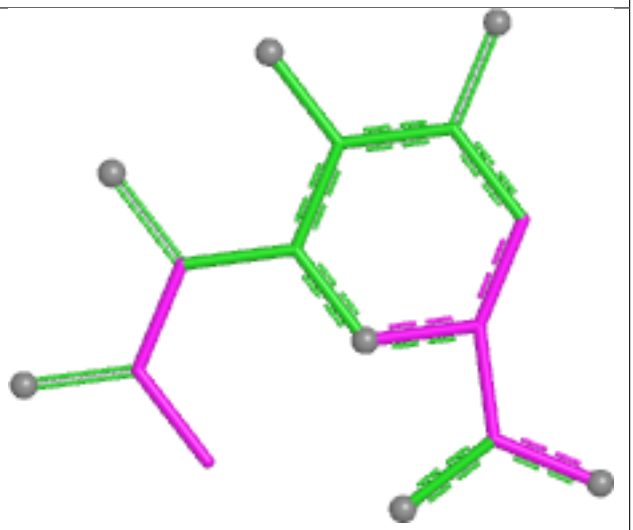


Rings

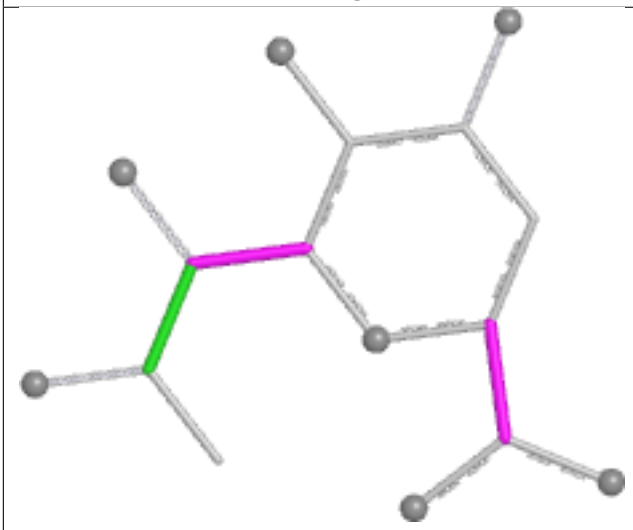
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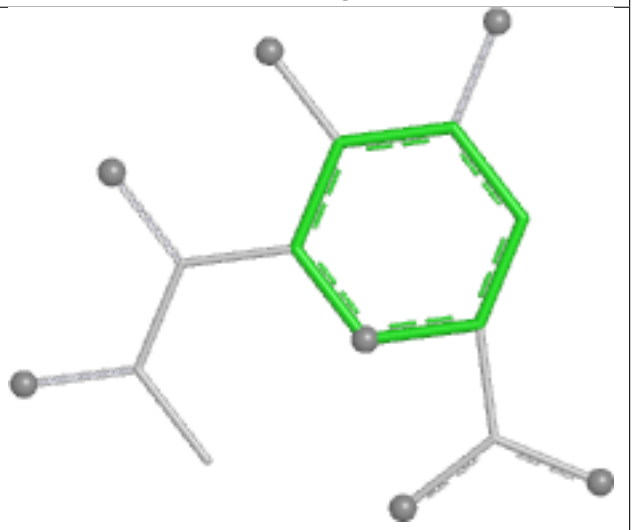
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Bond angles

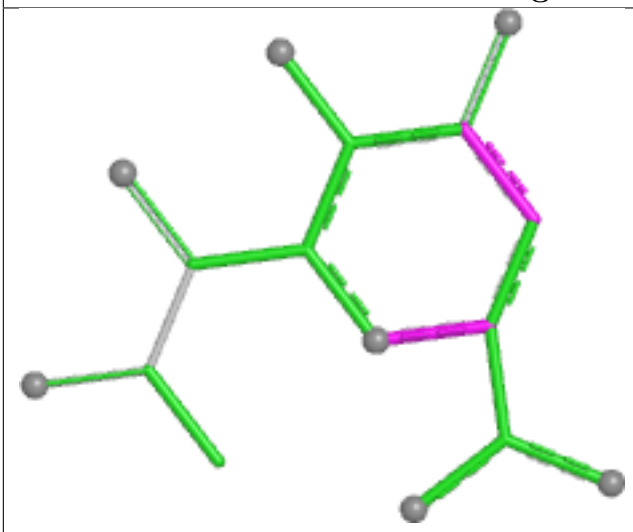


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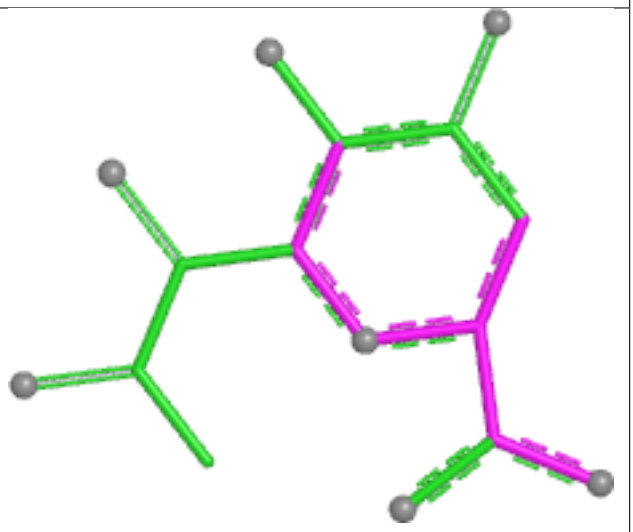


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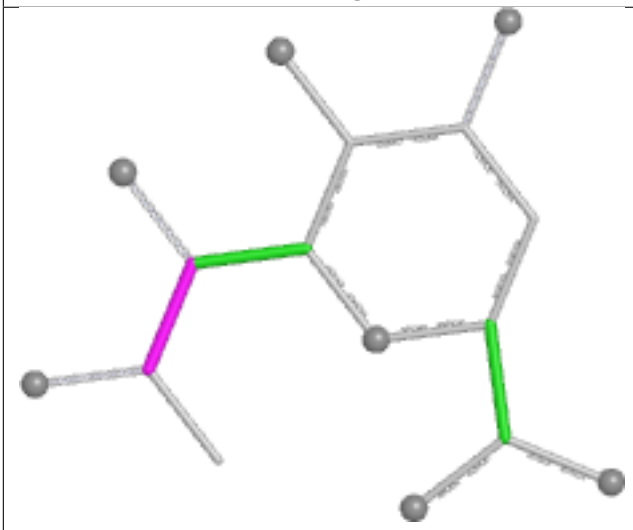
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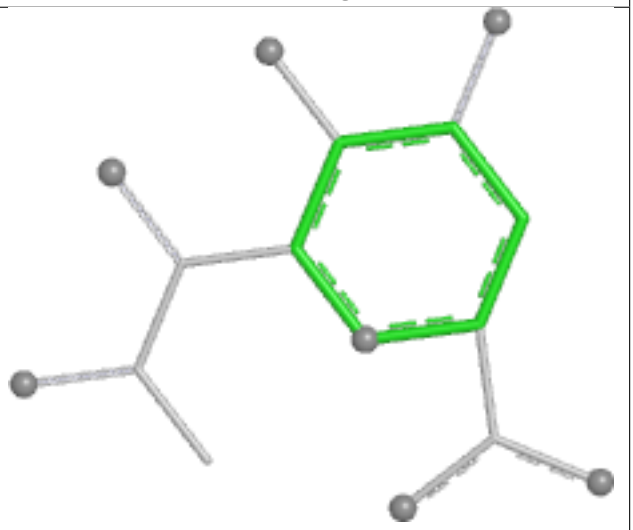
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Bond angles

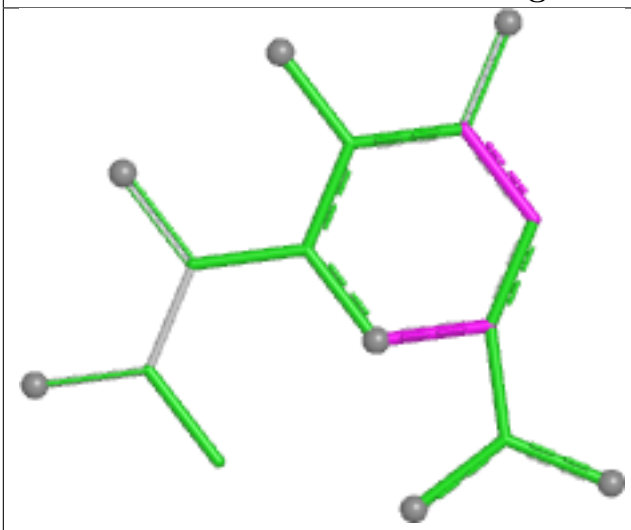


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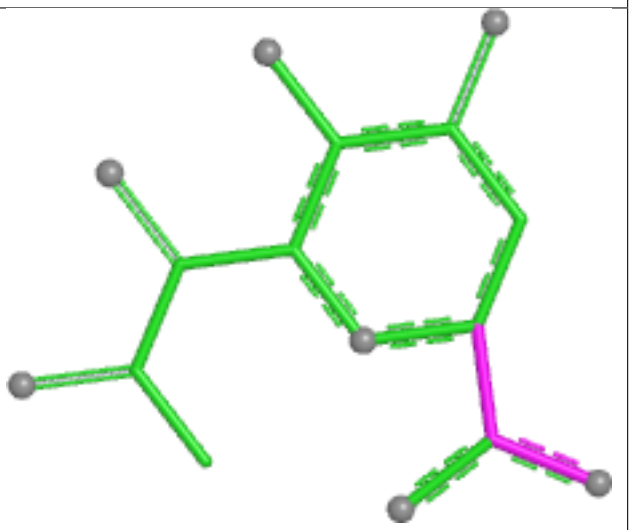


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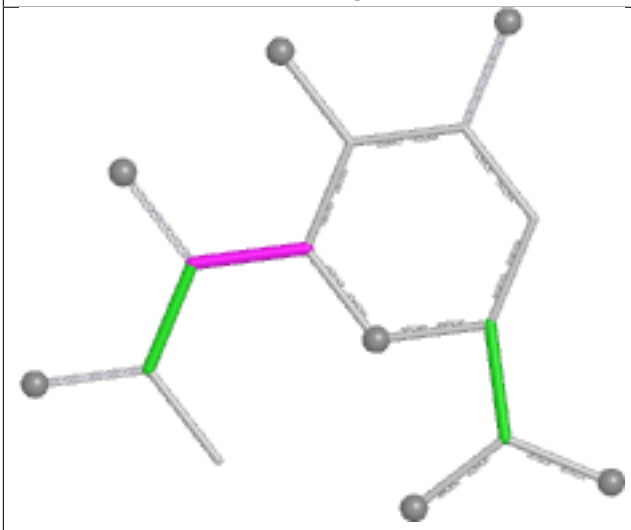
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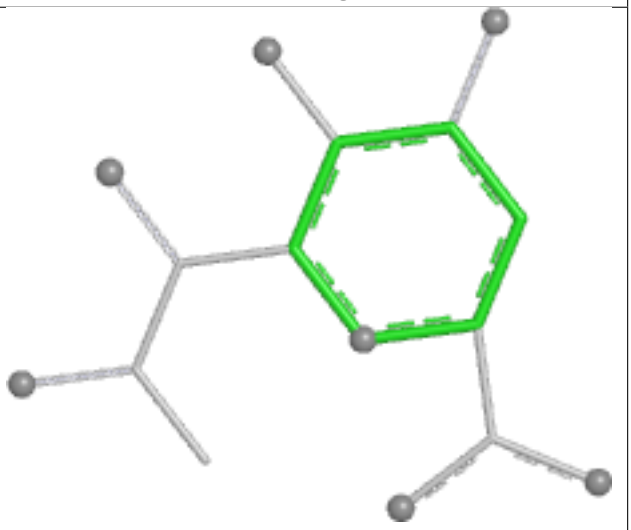
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Bond angles

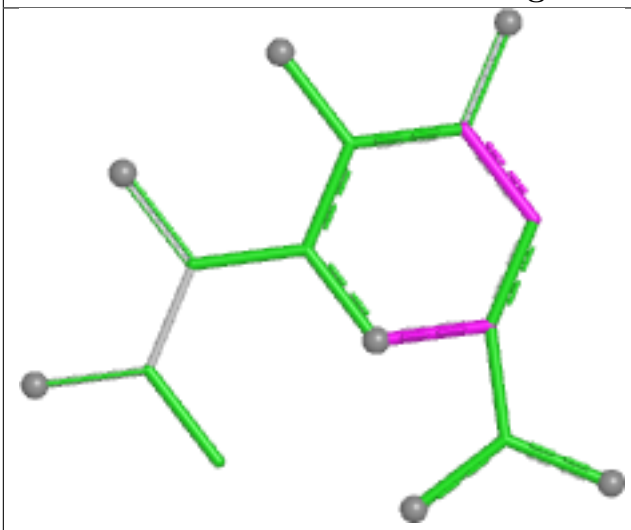


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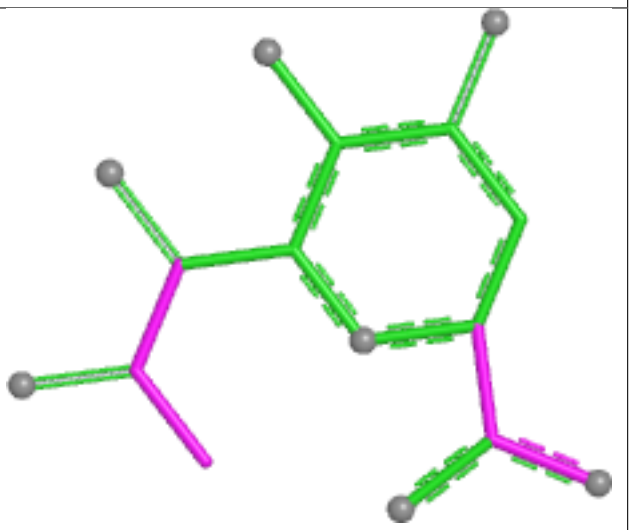


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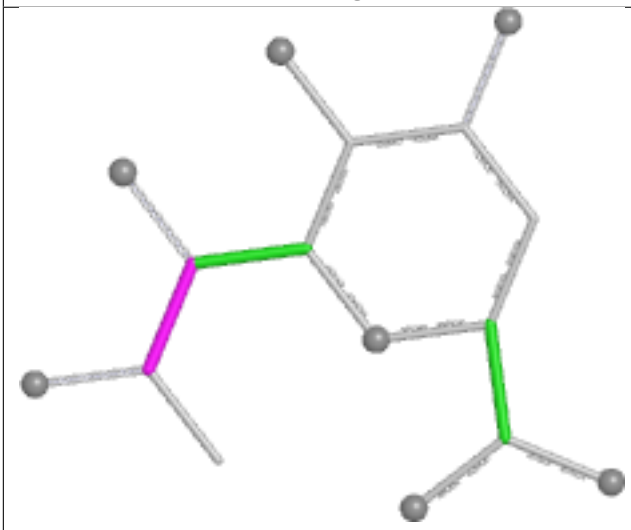
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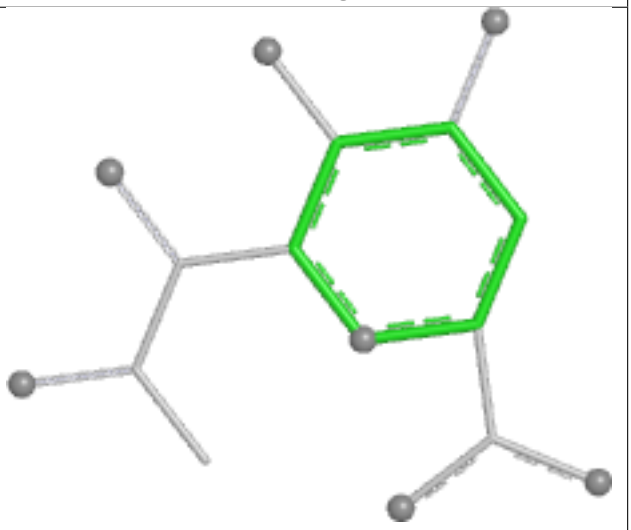
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Bond angles

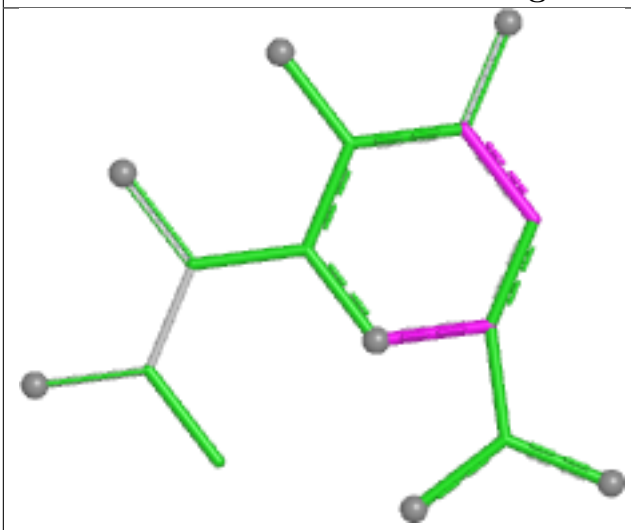


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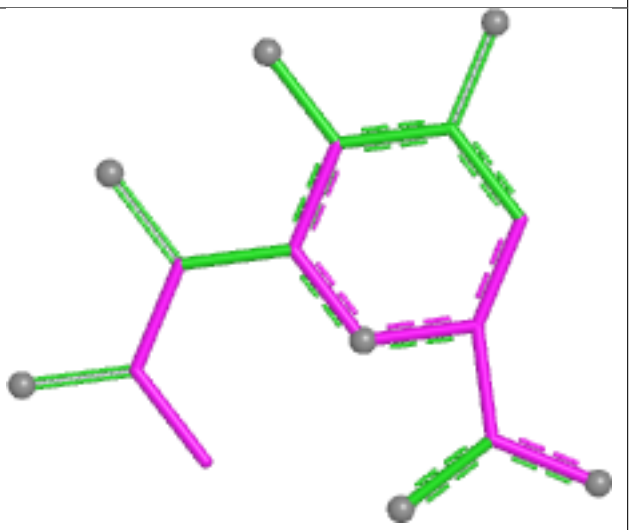


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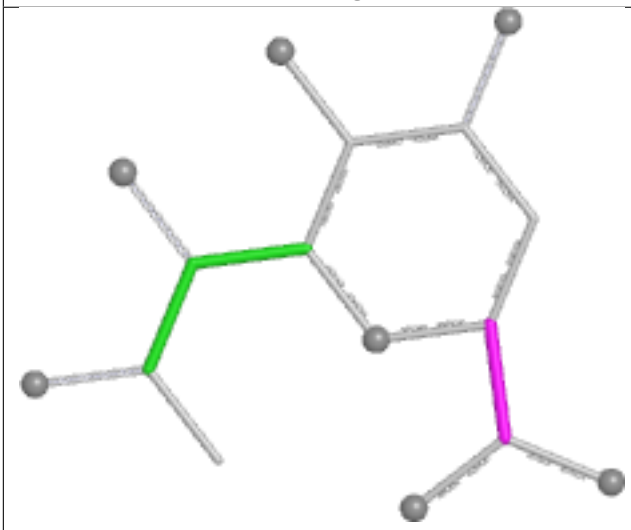
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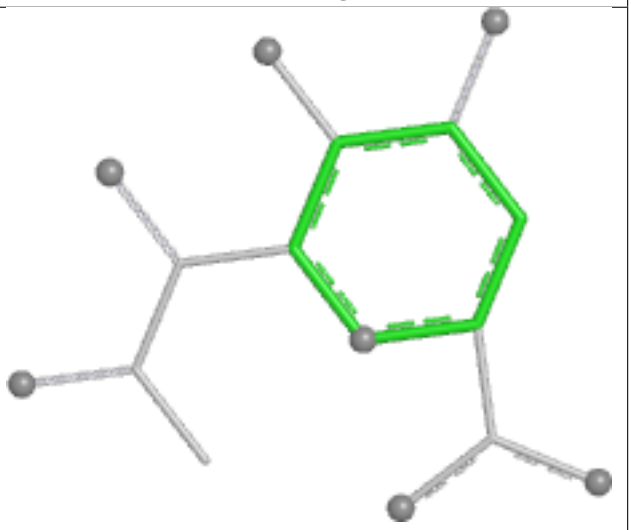
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Bond angles

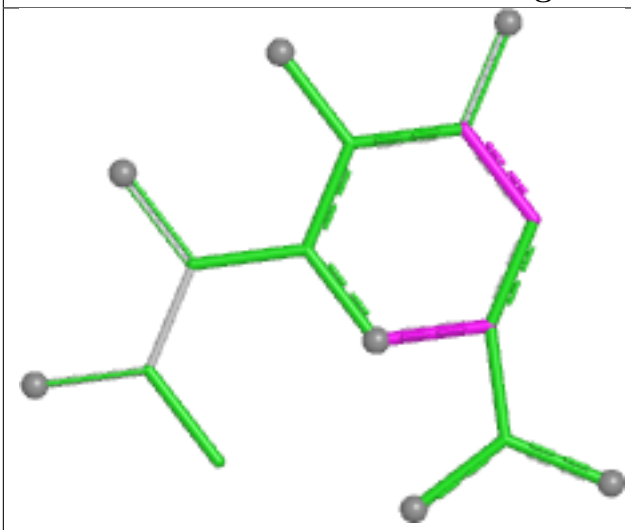


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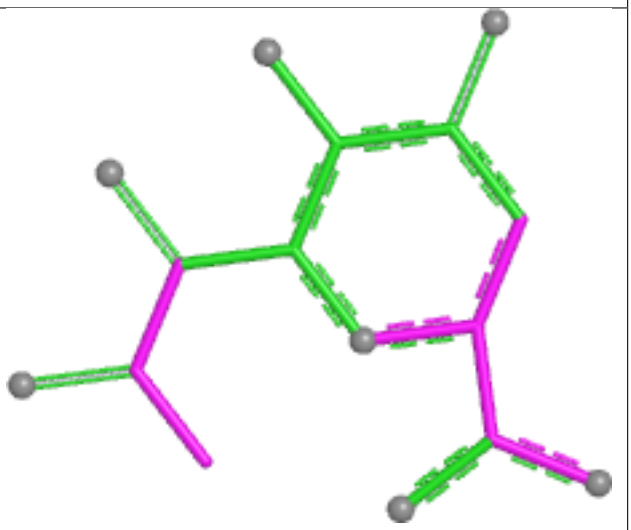


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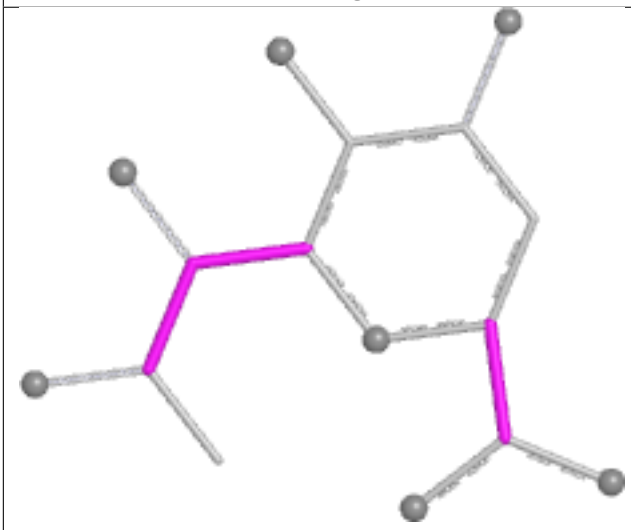
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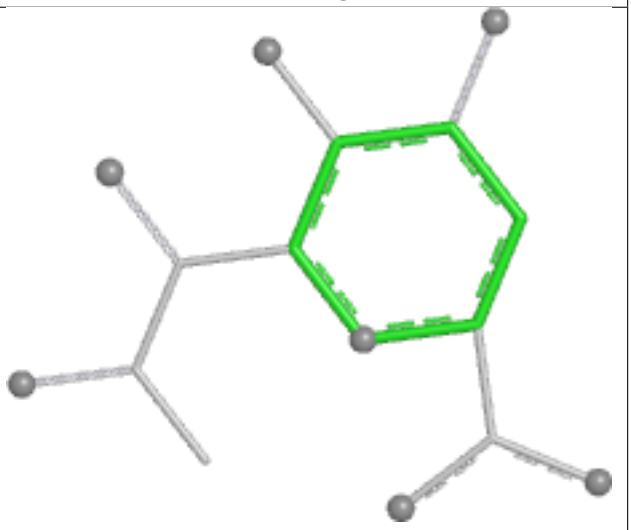
Bond lengths



Bond angles

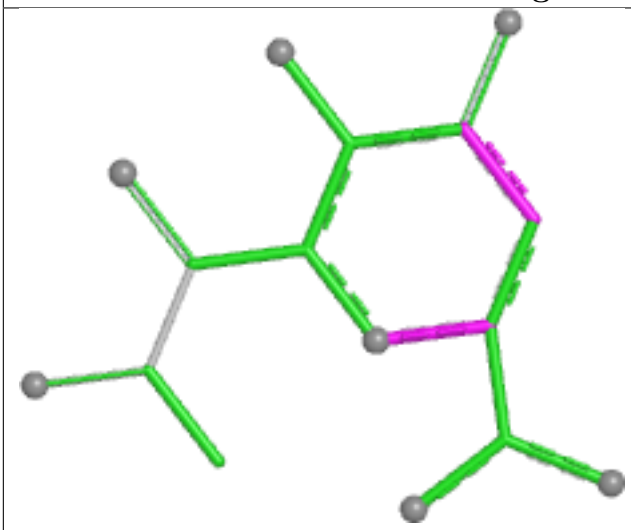


Torsions

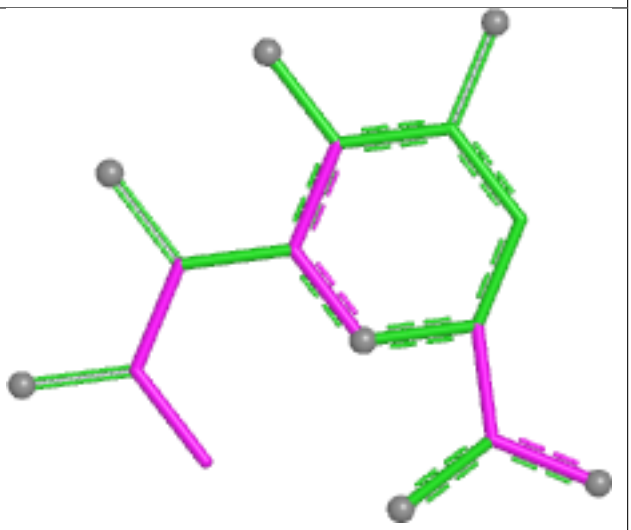


Rings

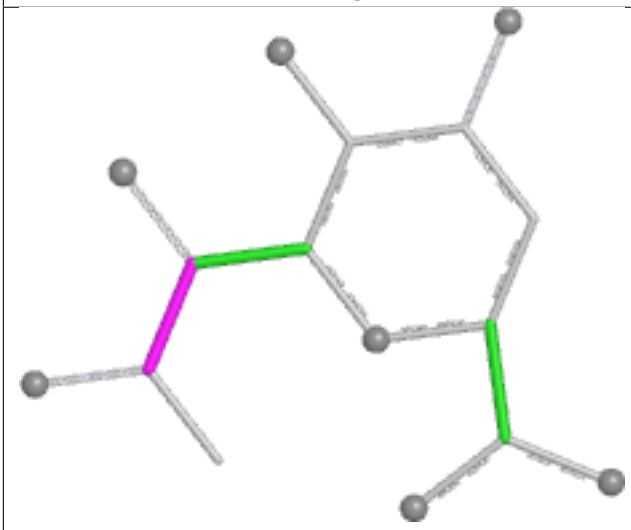
Ligand P8E J 610



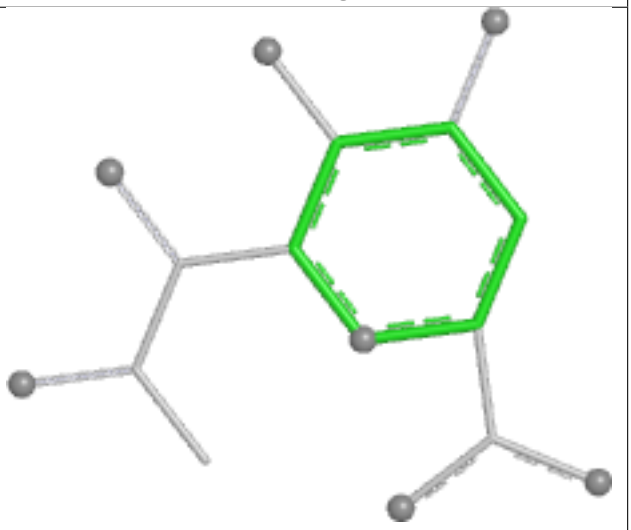
Bond lengths



Bond angles

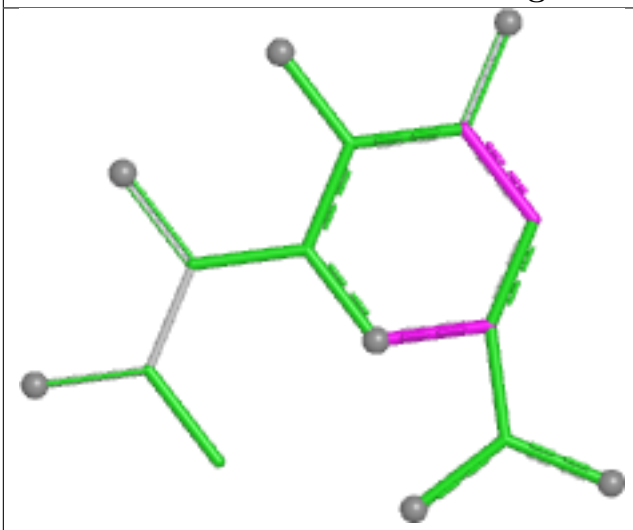


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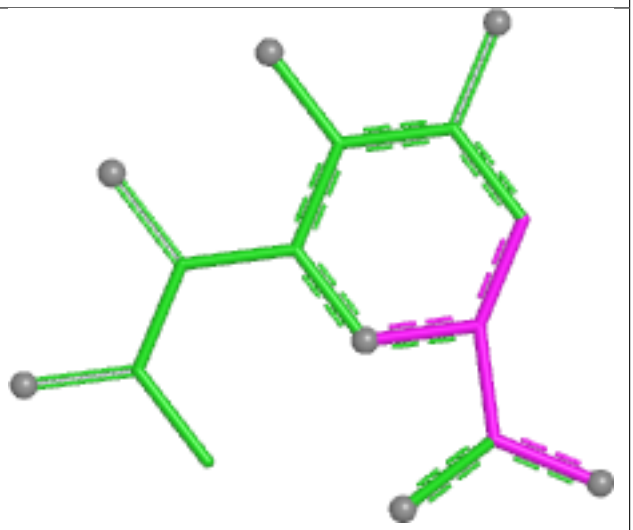


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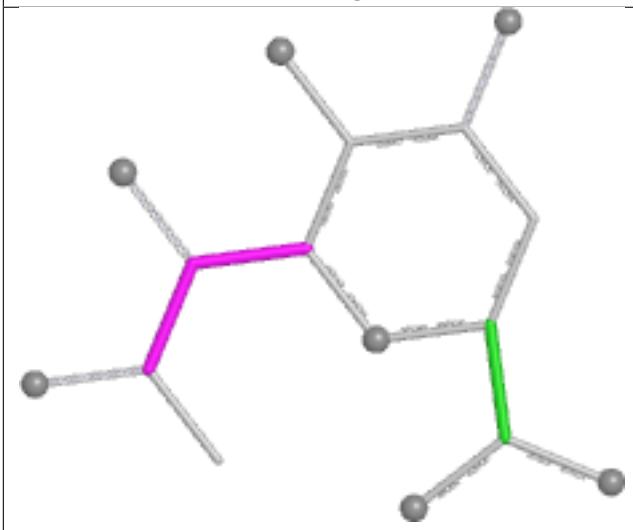
Ligand P8E V 605



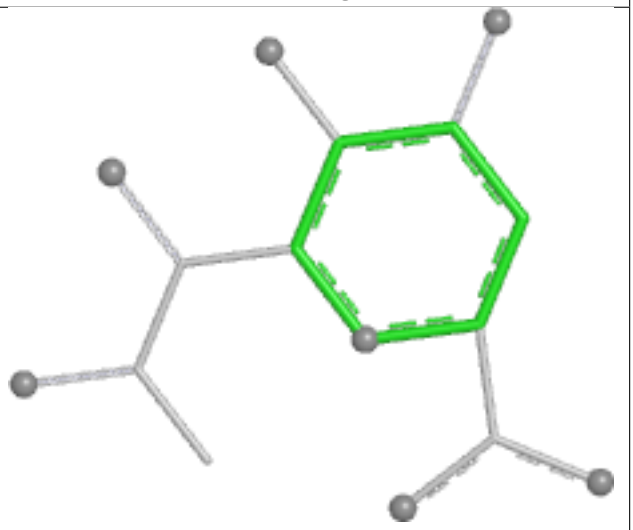
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Bond angles

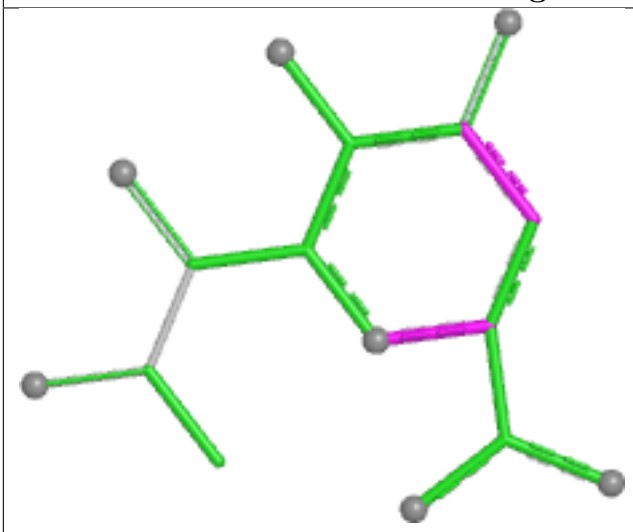


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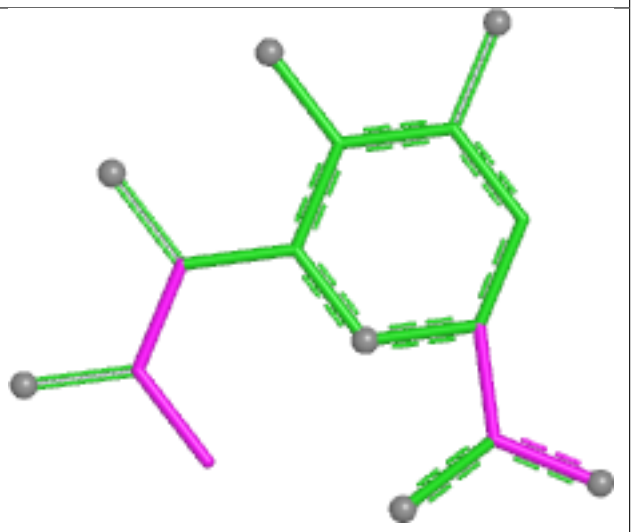


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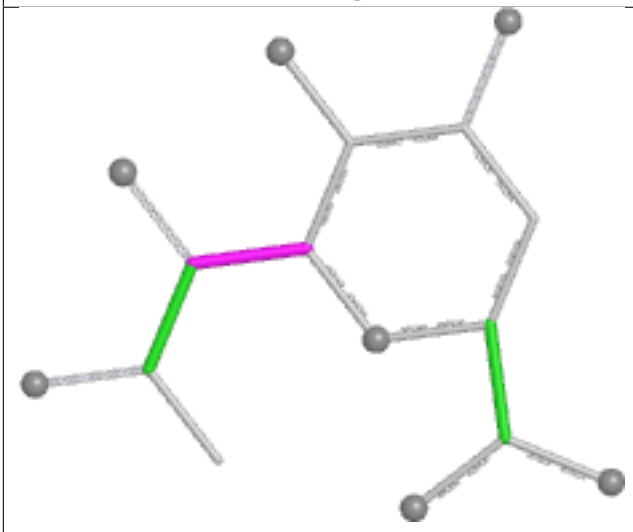
Ligand P8E T 601



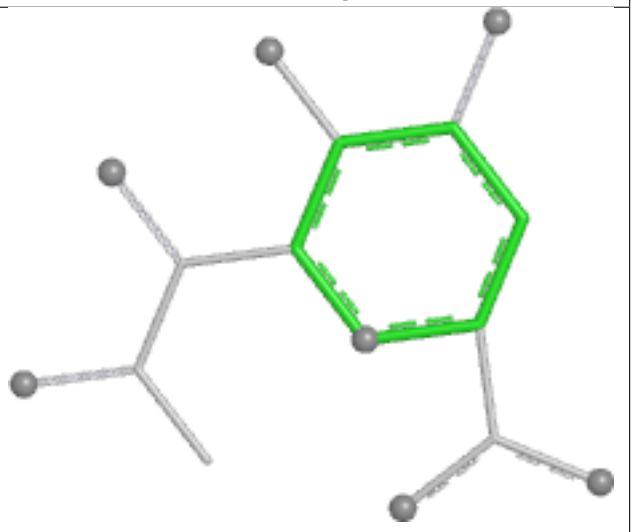
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Bond angles

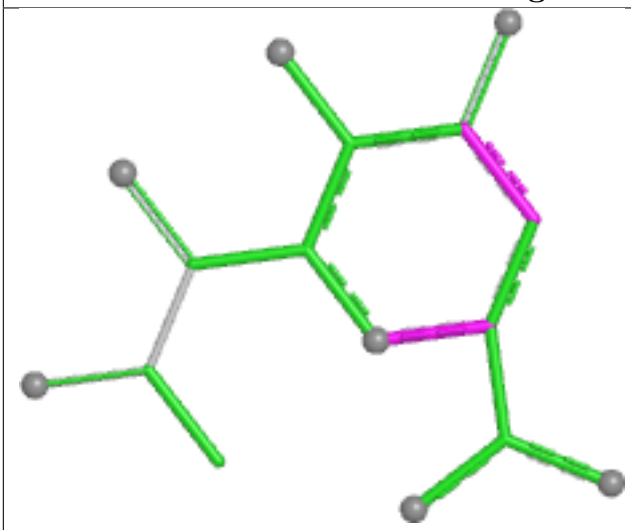


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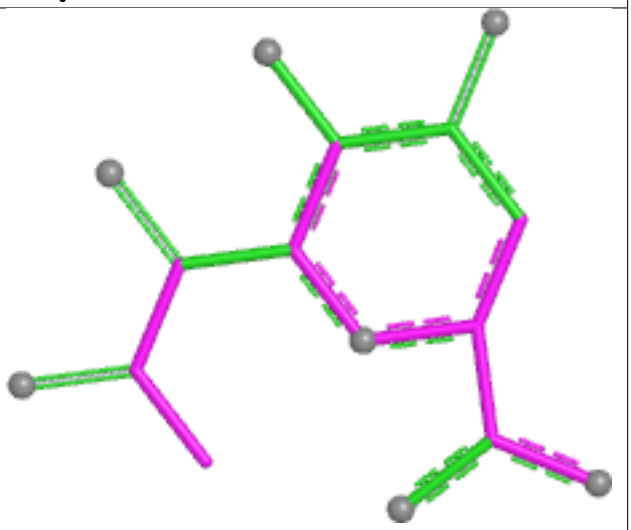


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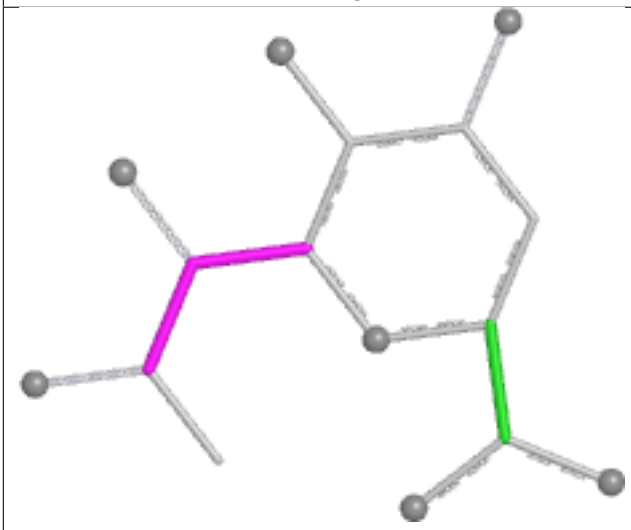
Ligand P8E Q 606



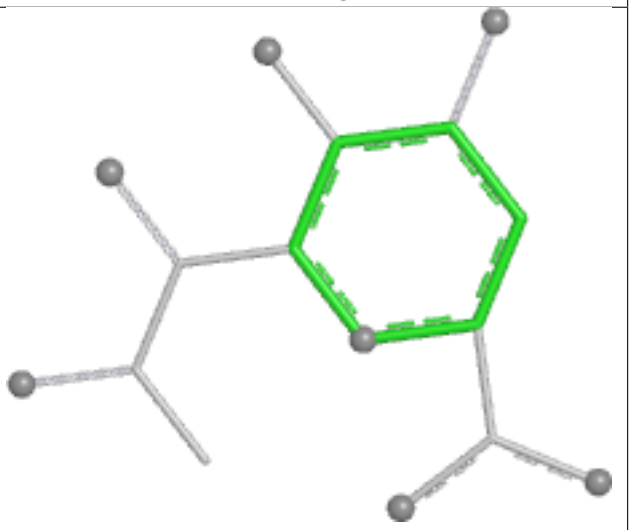
Bond lengths



Bond angles

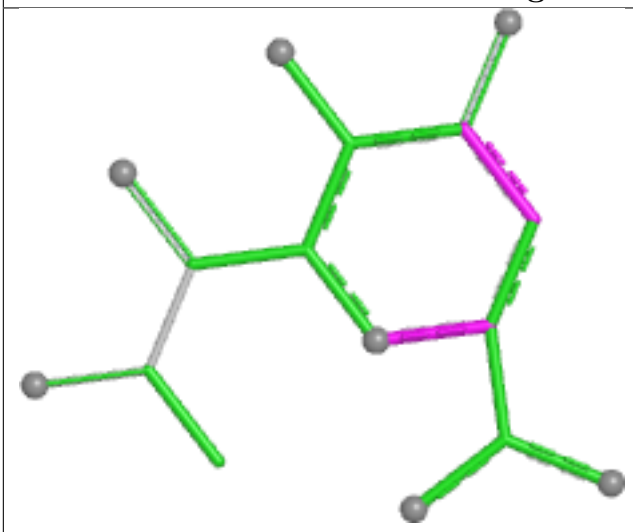


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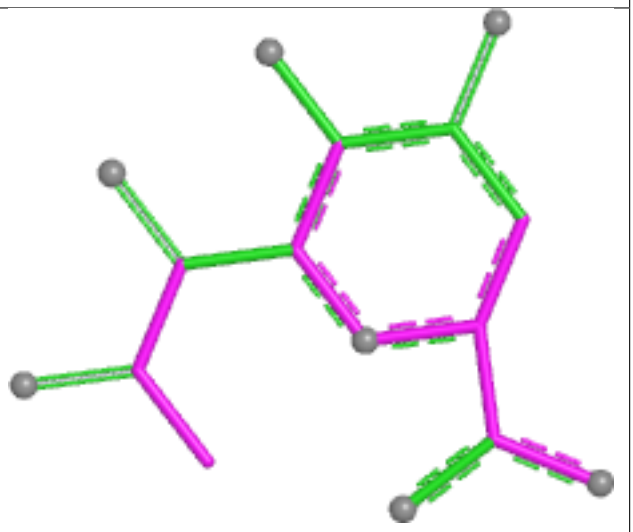


Rings

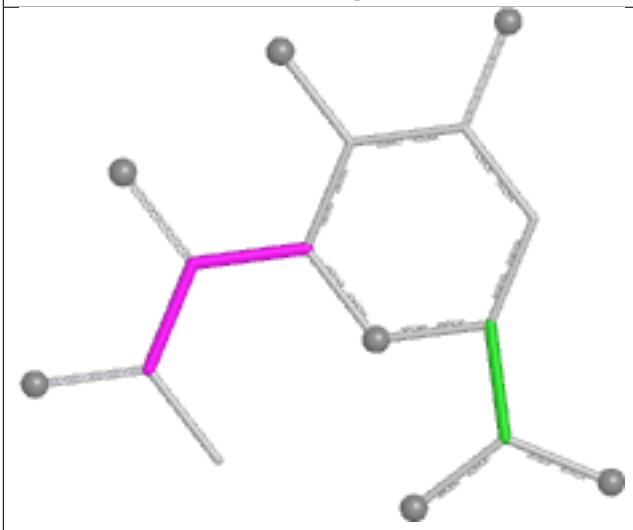
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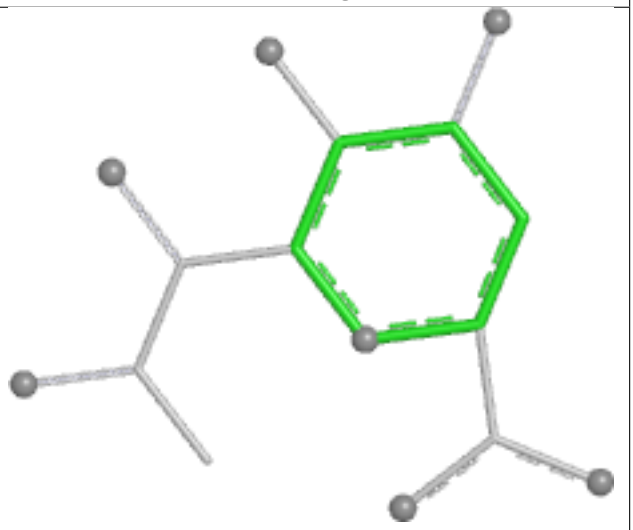
Bond lengths



Bond angles

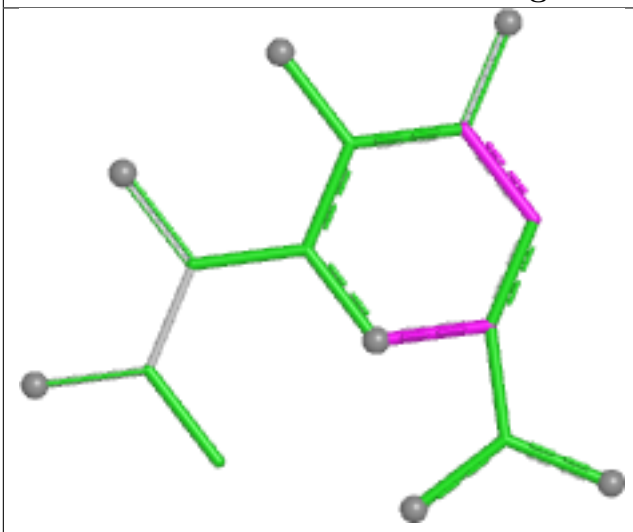


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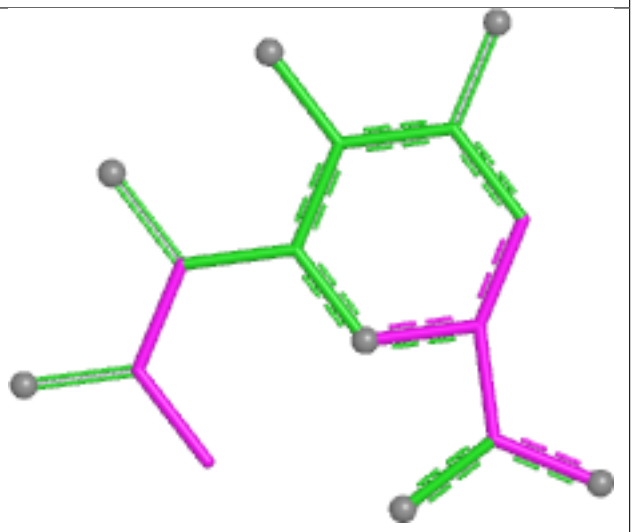


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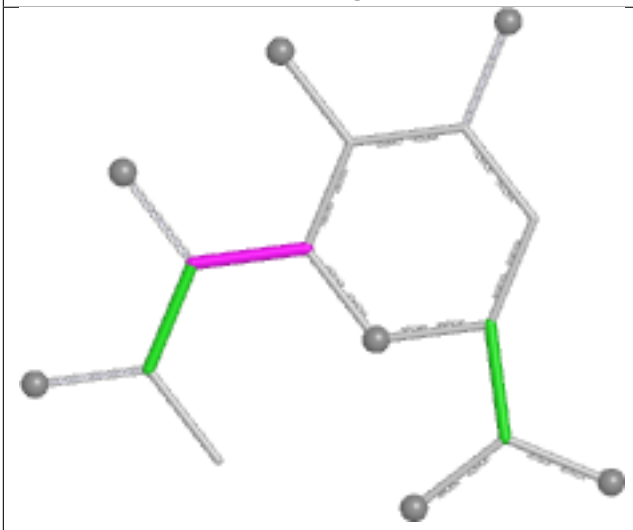
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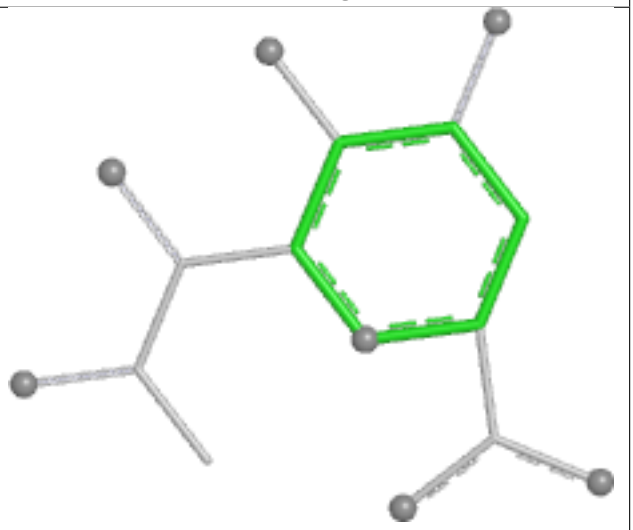
Bond lengths



Bond angles

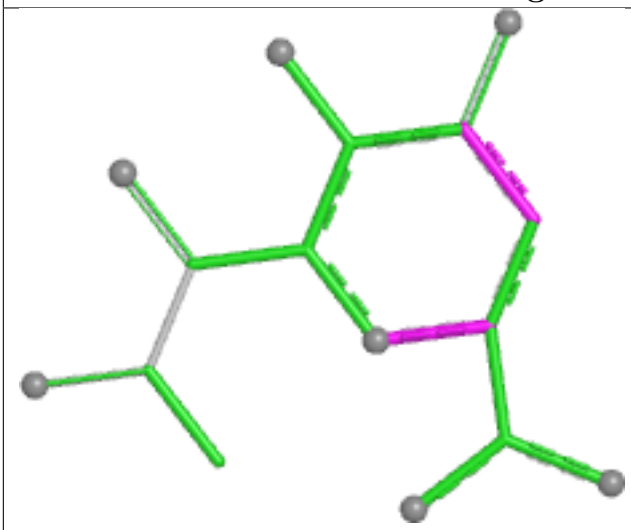


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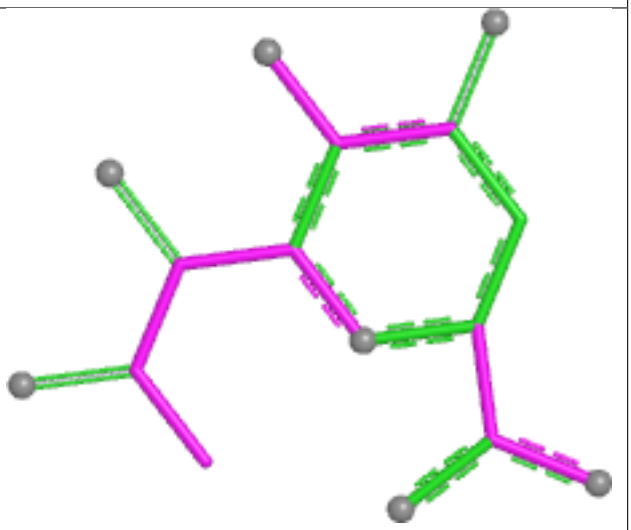


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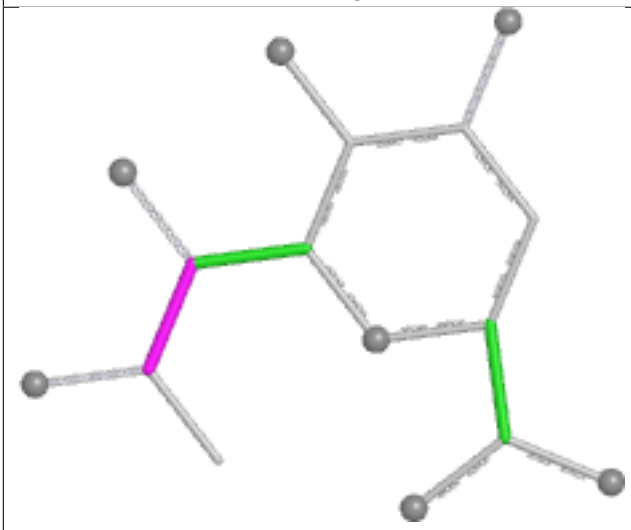
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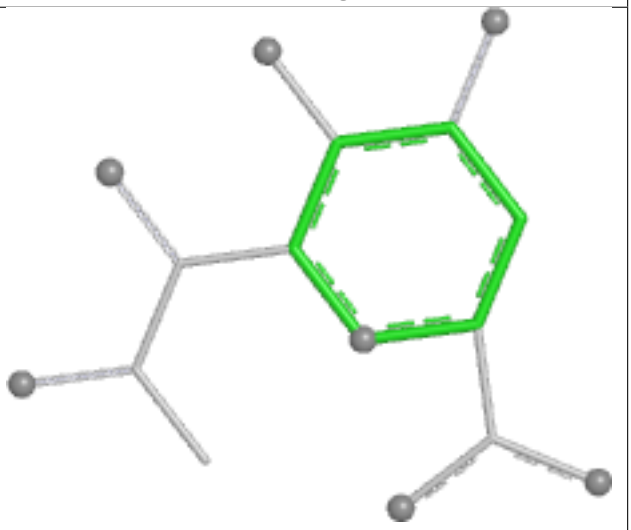
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Bond angles

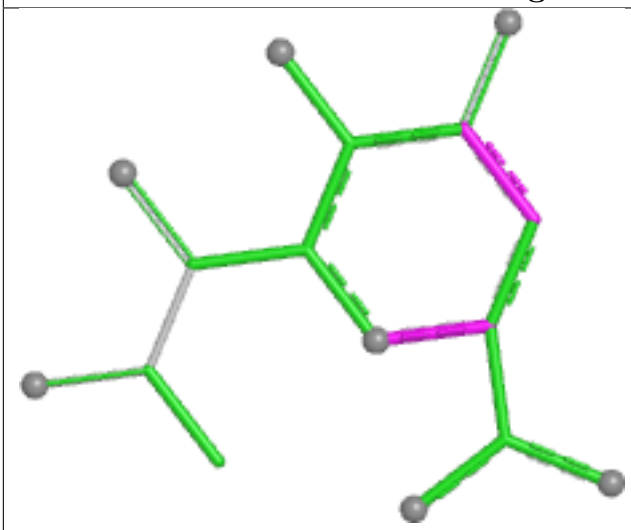


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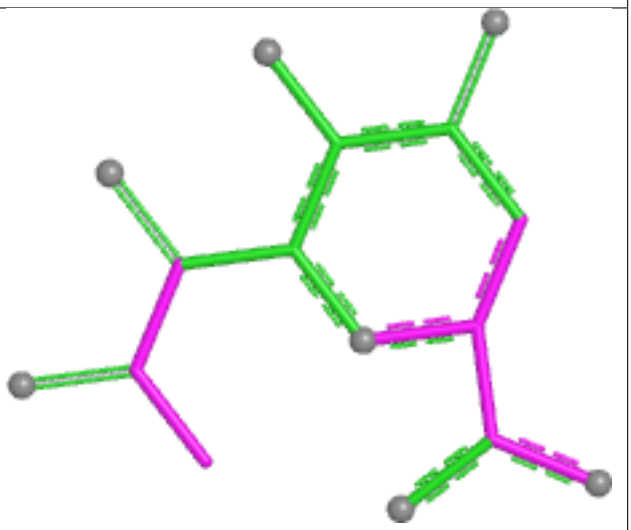


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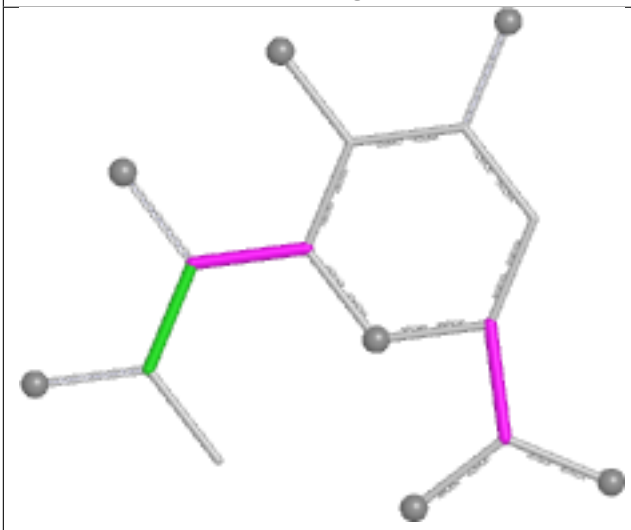
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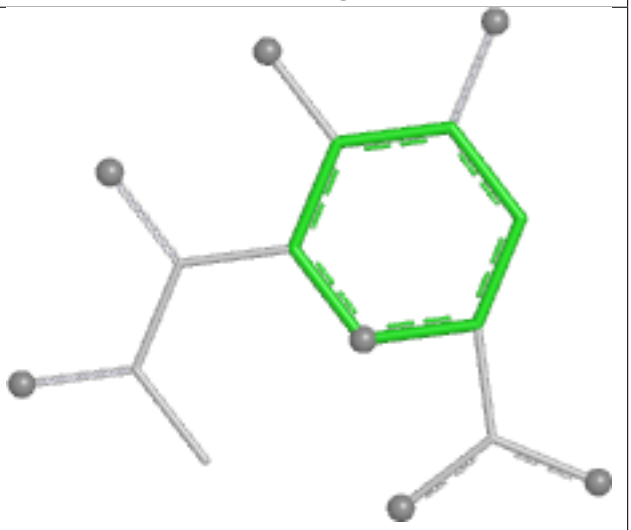
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Bond angles

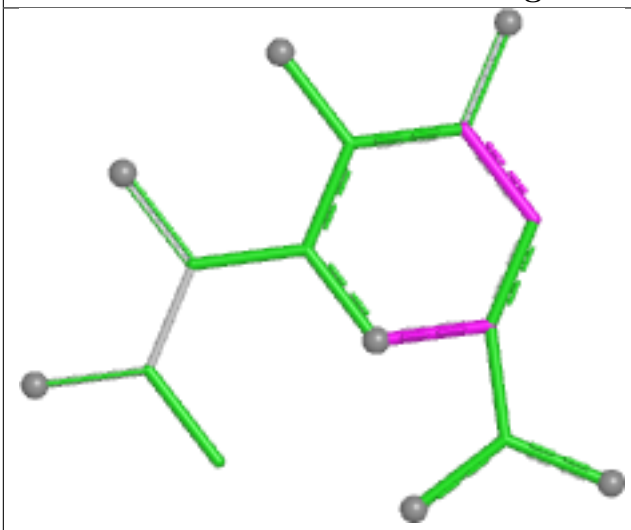


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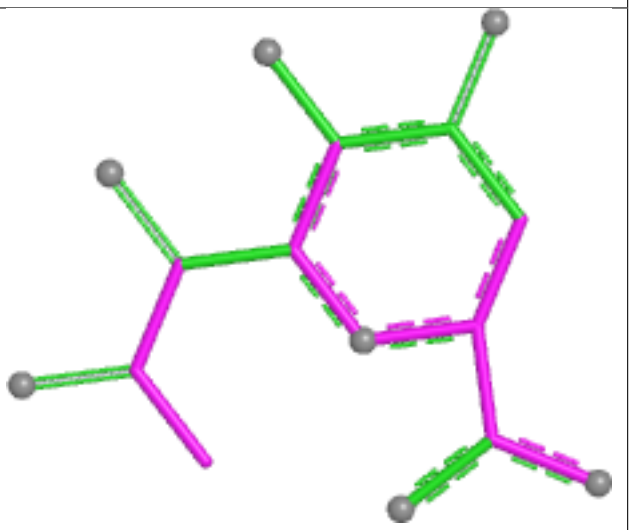


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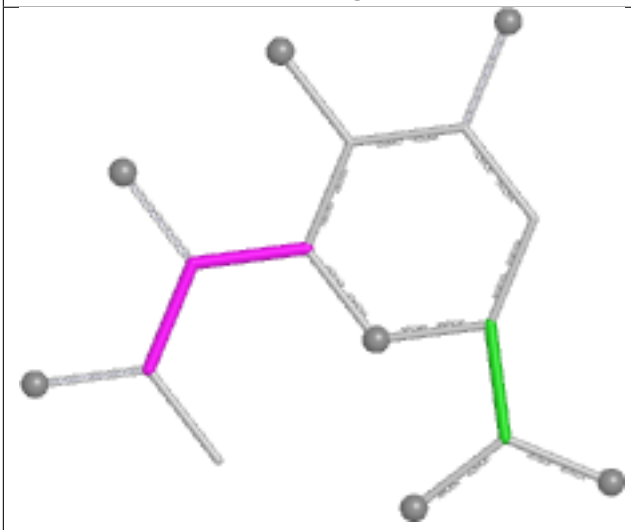
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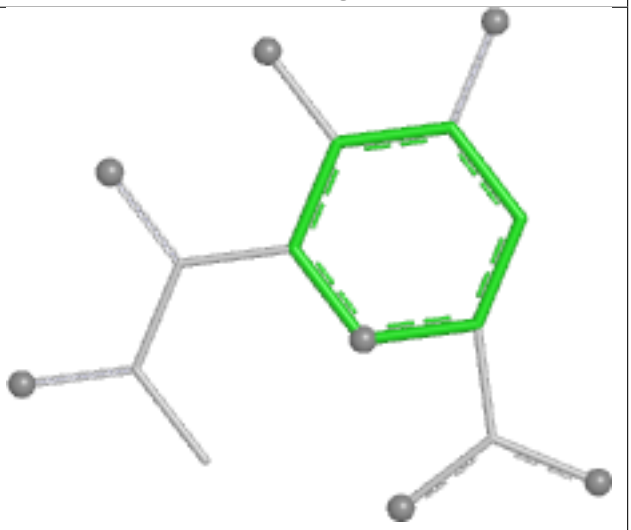
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Bond angles

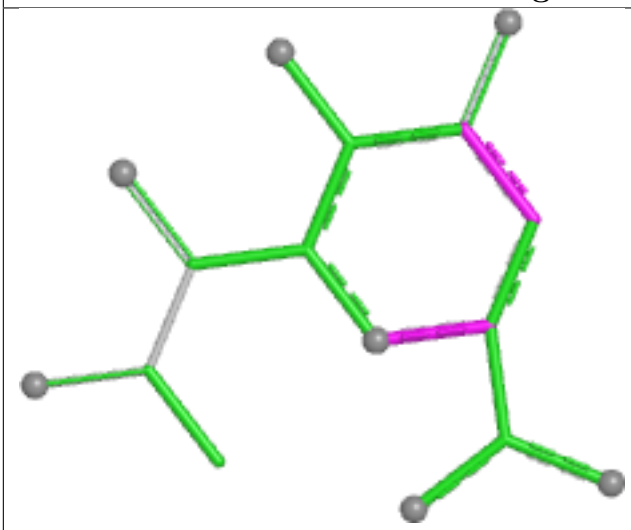


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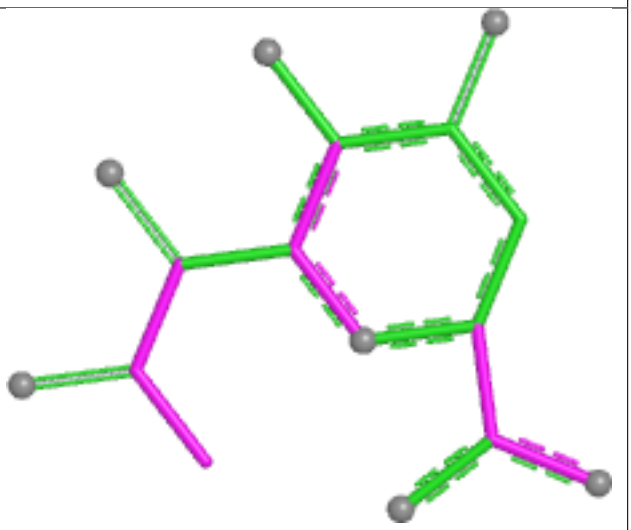


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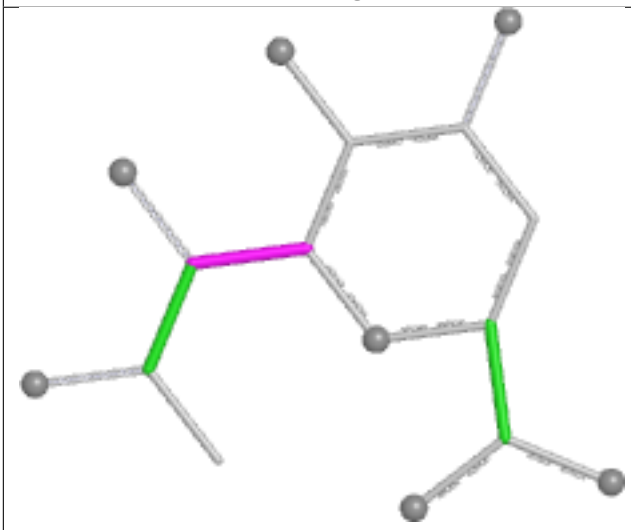
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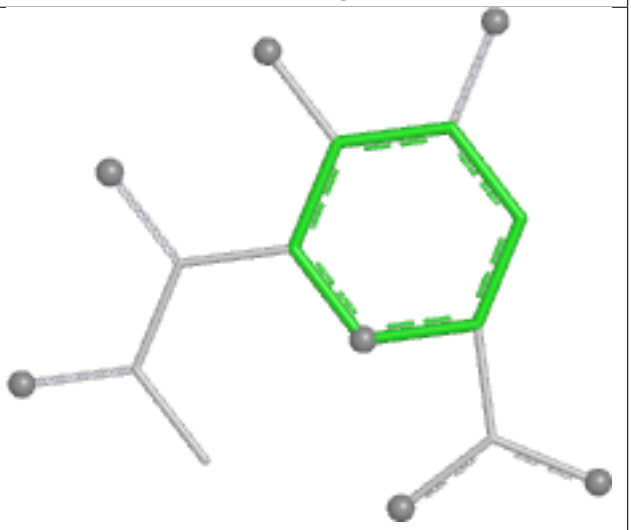
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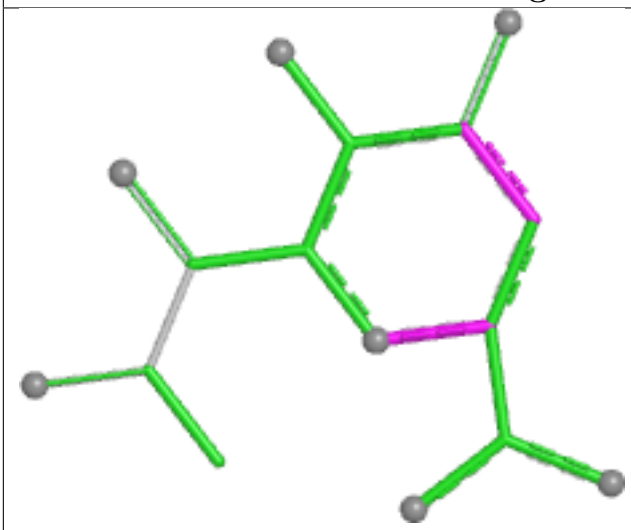


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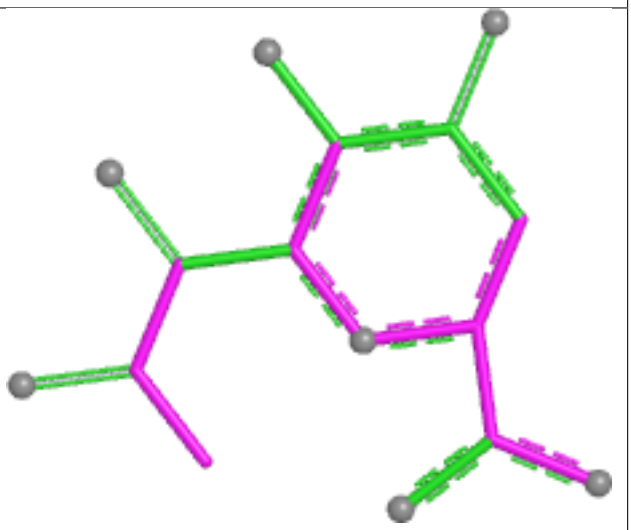


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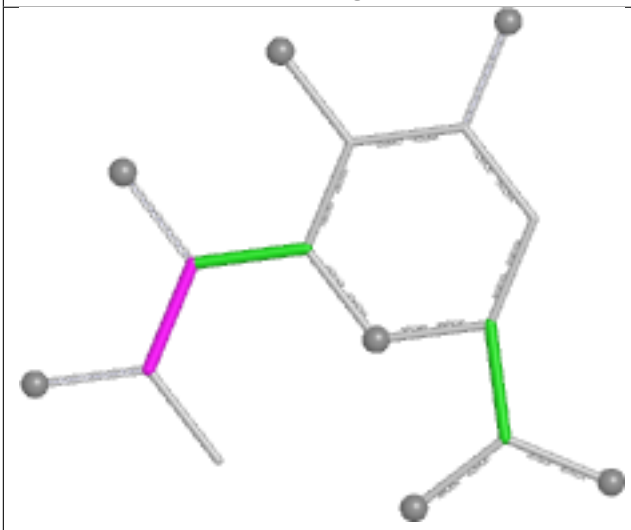
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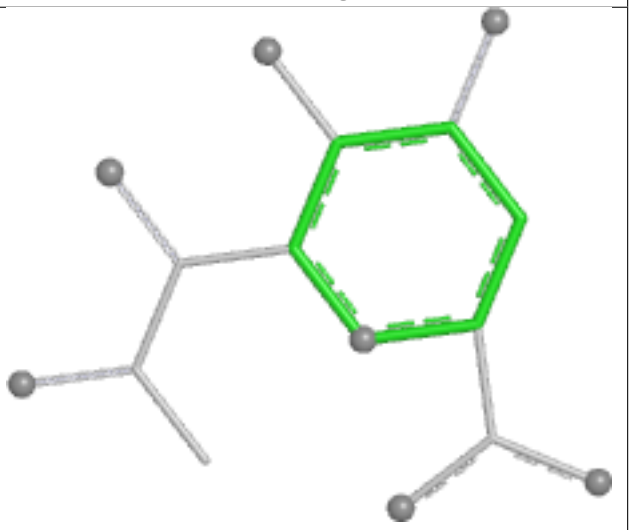
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Bond angles

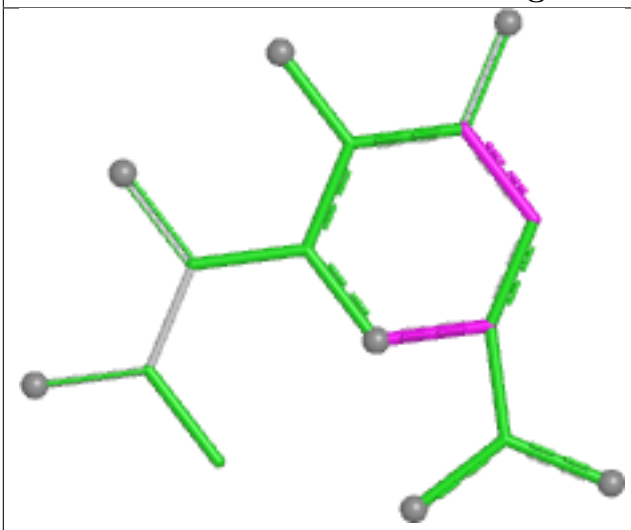


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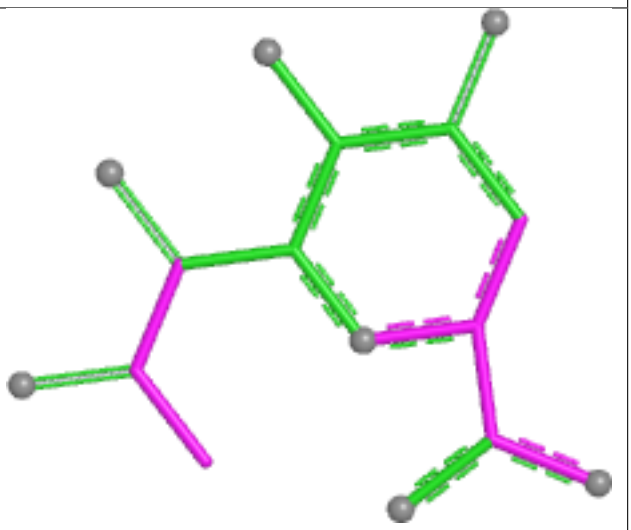


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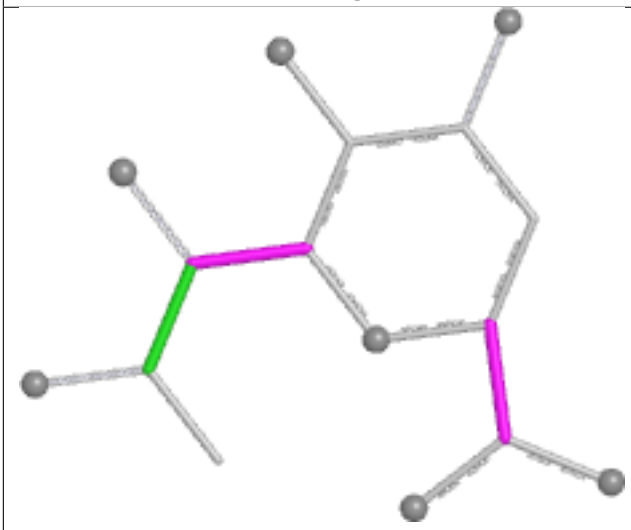
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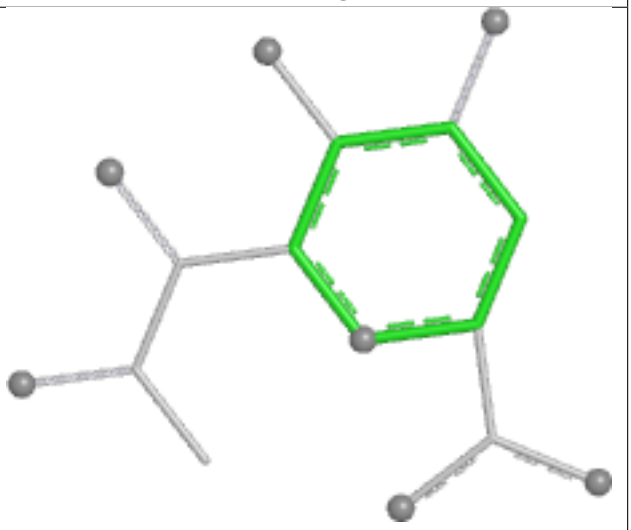
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Bond angles

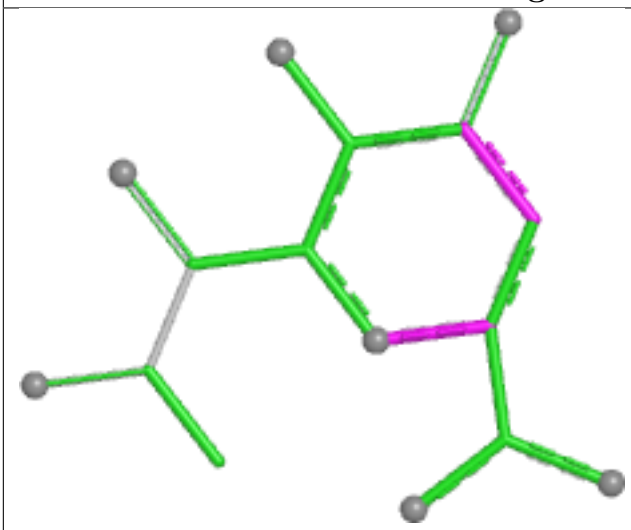


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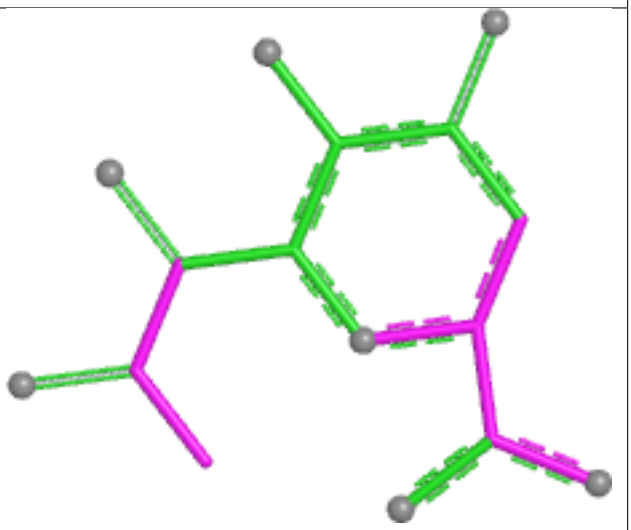


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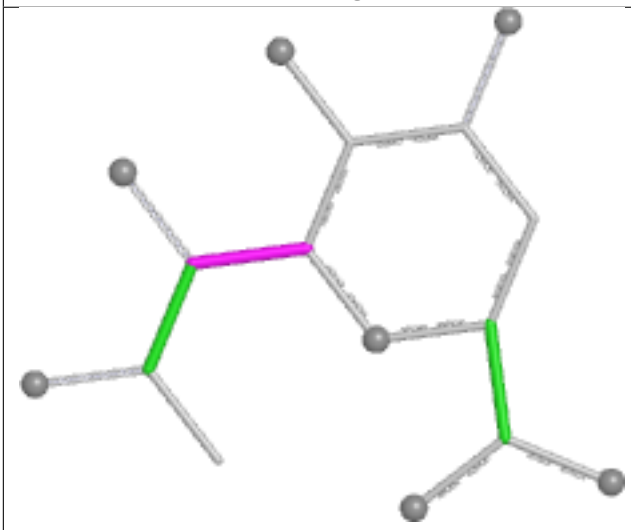
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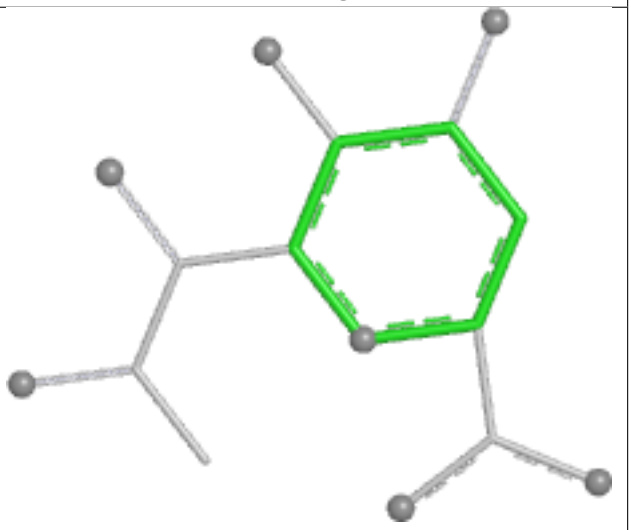
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Bond angles

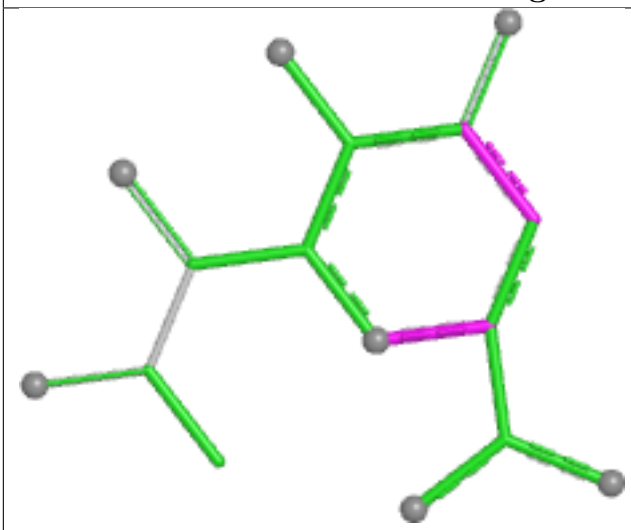


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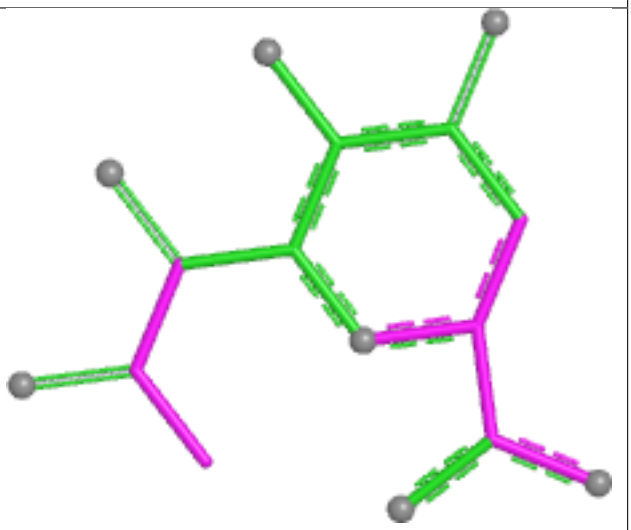


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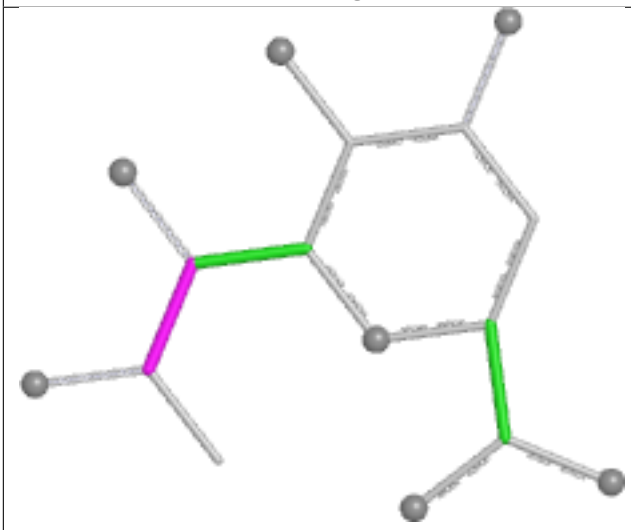
Ligand P8E T 603



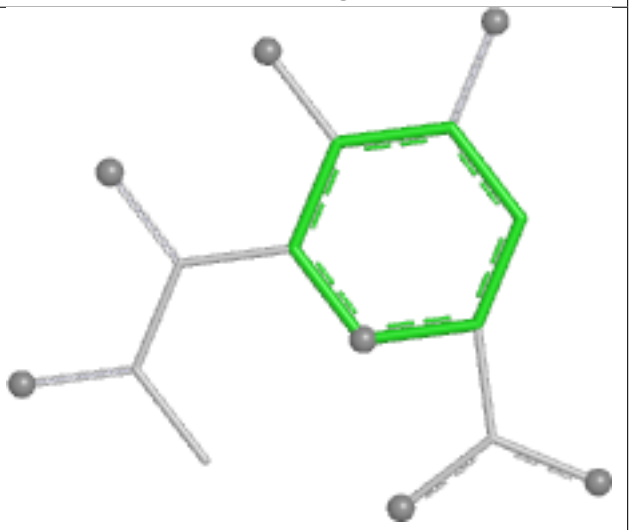
Bond lengths



Bond angles

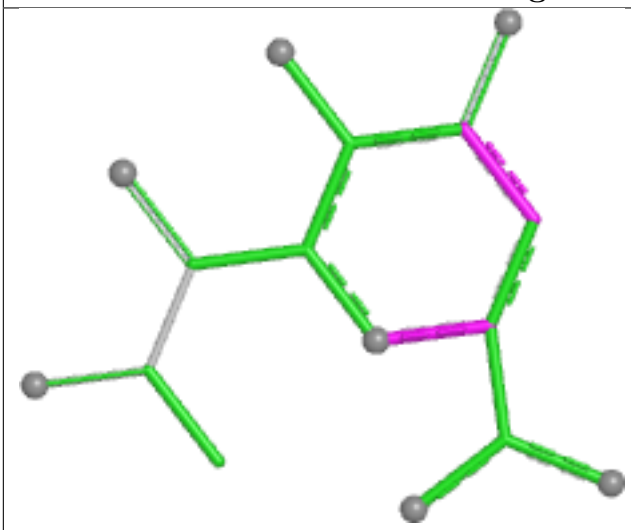


Torsions

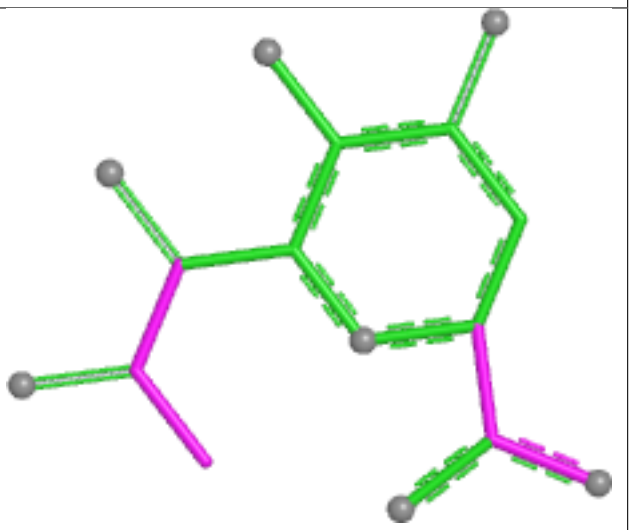


Rings

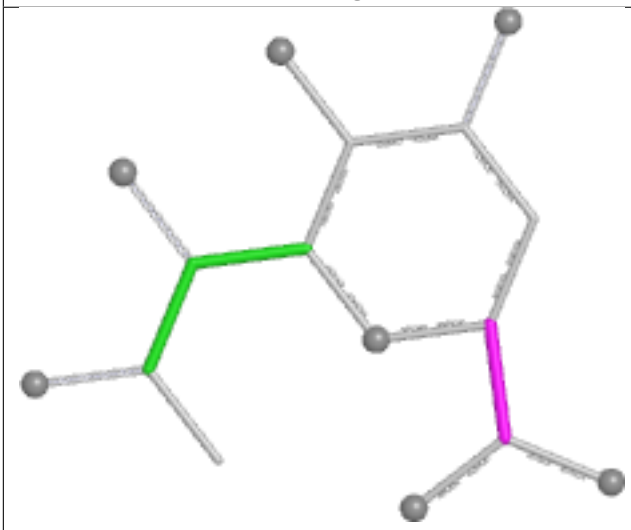
Ligand P8E C 611



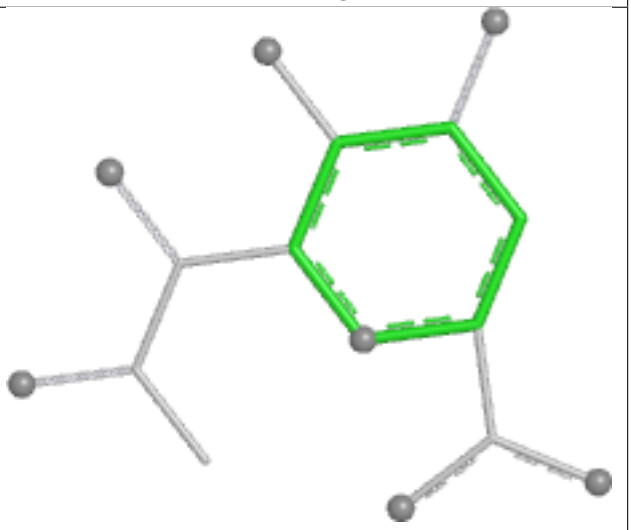
Bond lengths



Bond angles

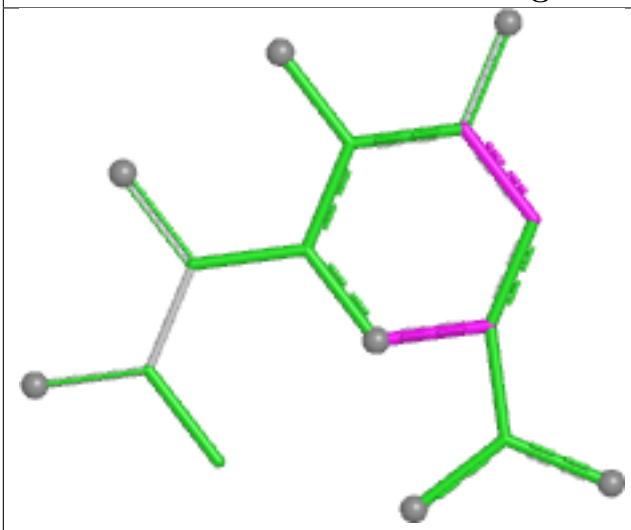


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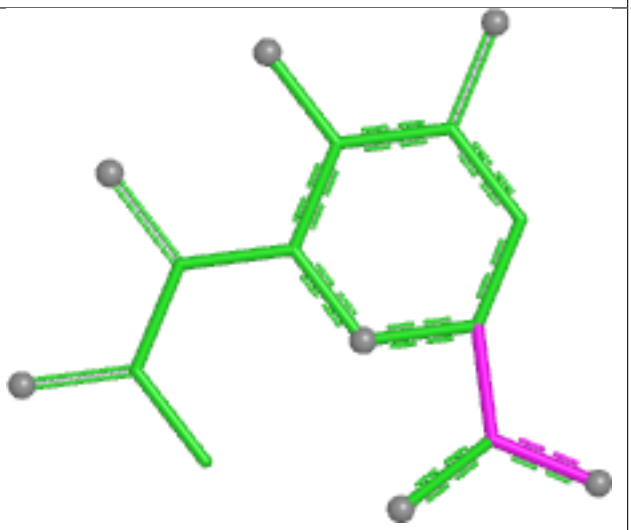


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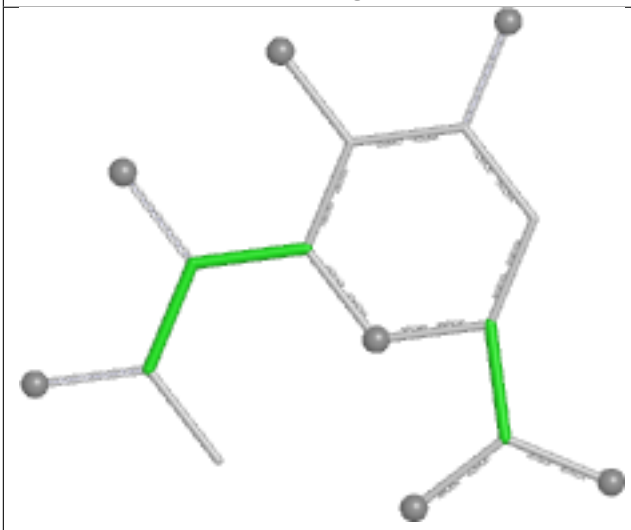
Ligand P8E S 613



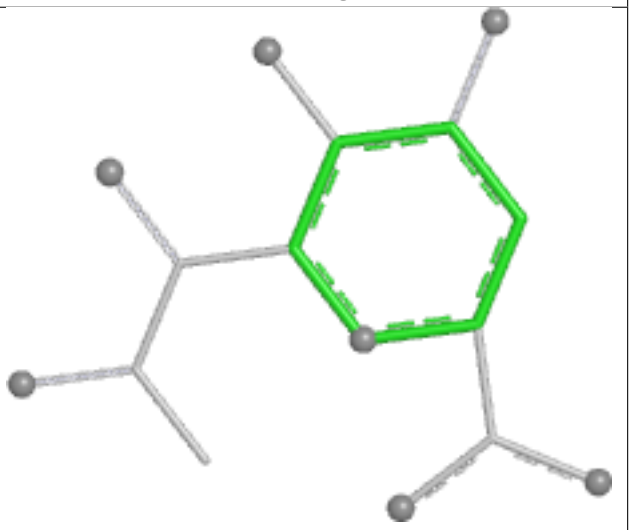
Bond lengths



Bond angles

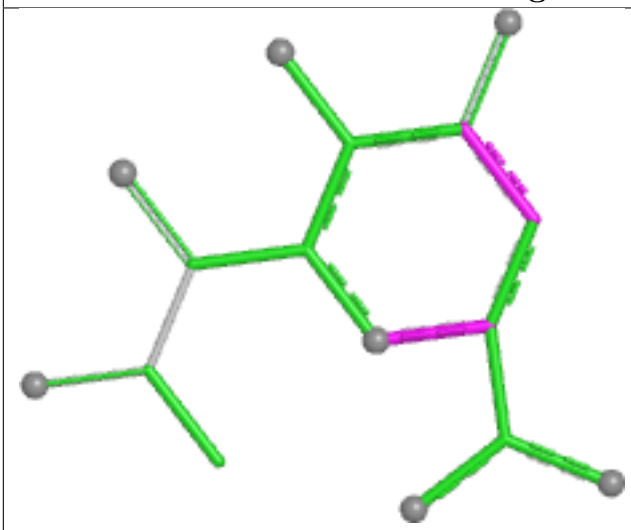


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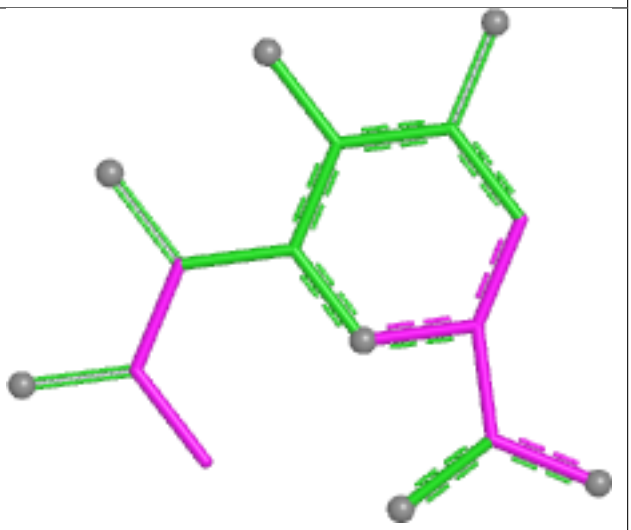


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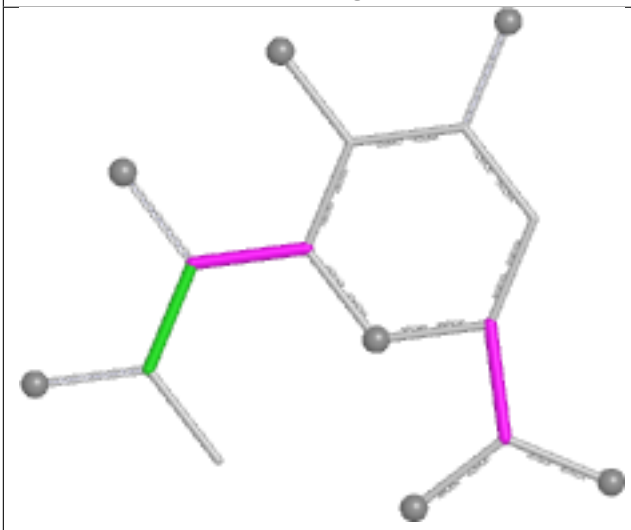
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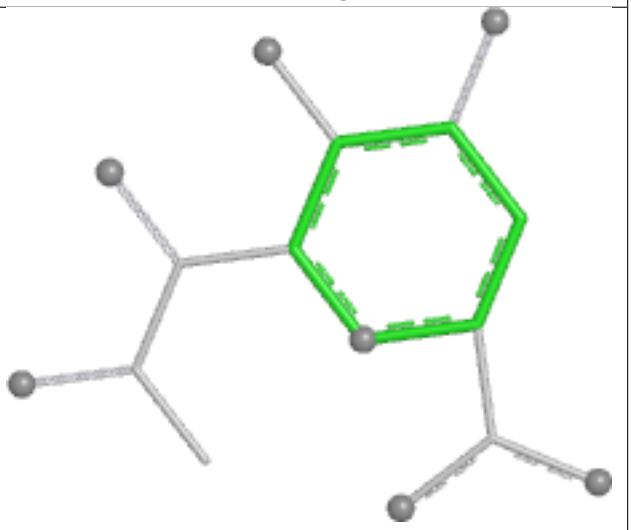
Bond lengths



Bond angles

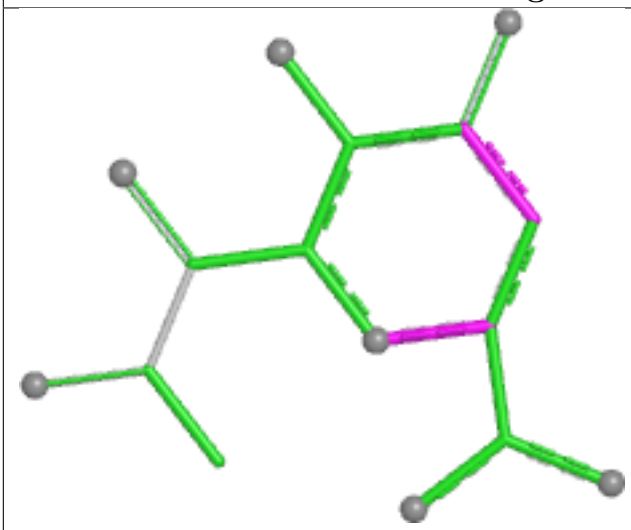


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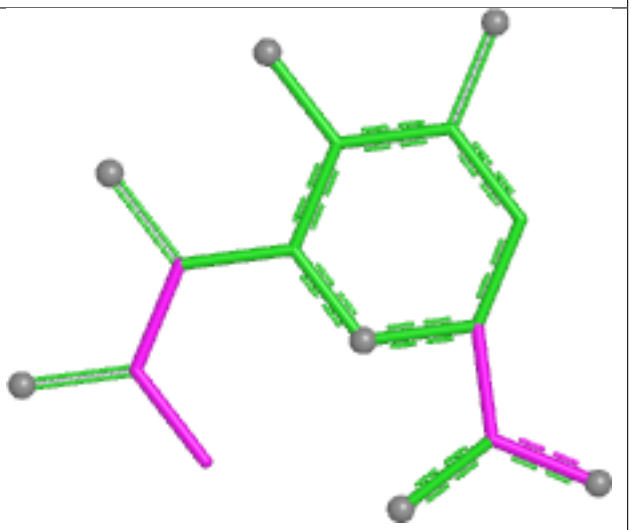


Rings

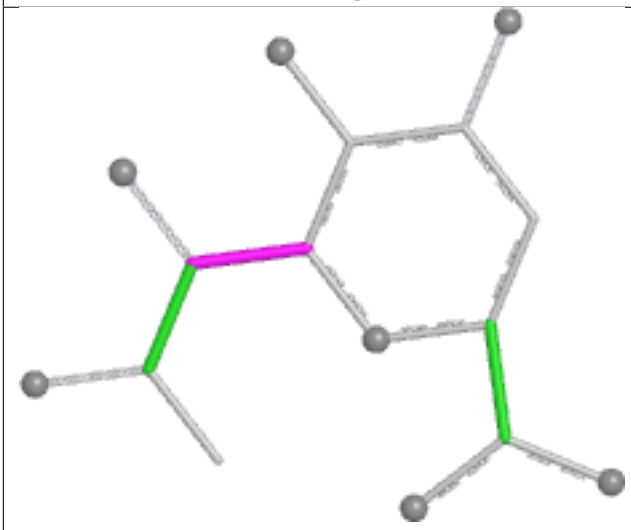
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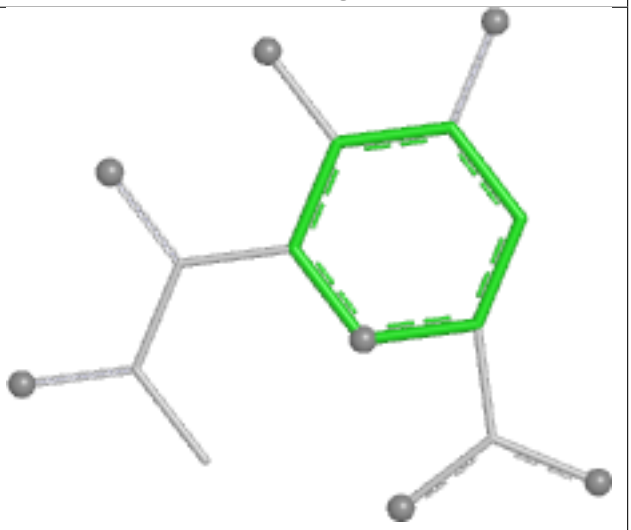
Bond lengths



Bond angles

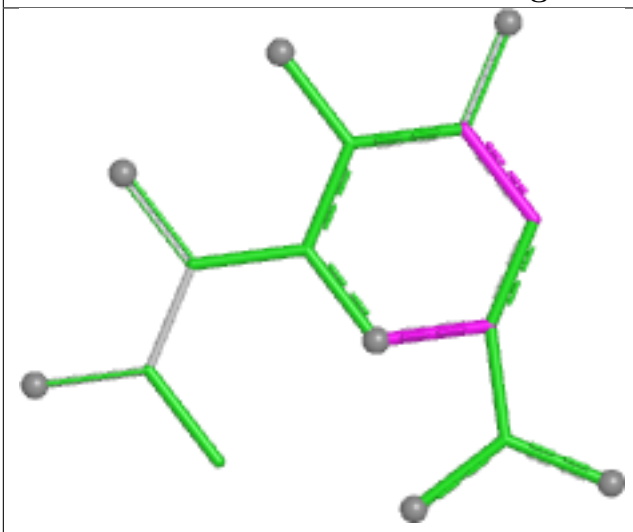


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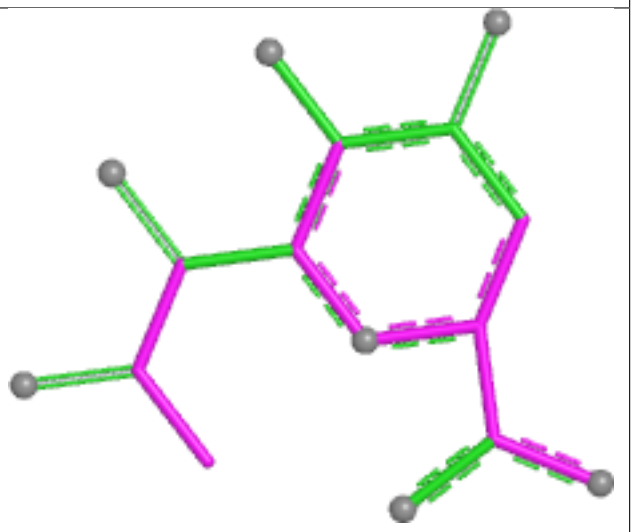


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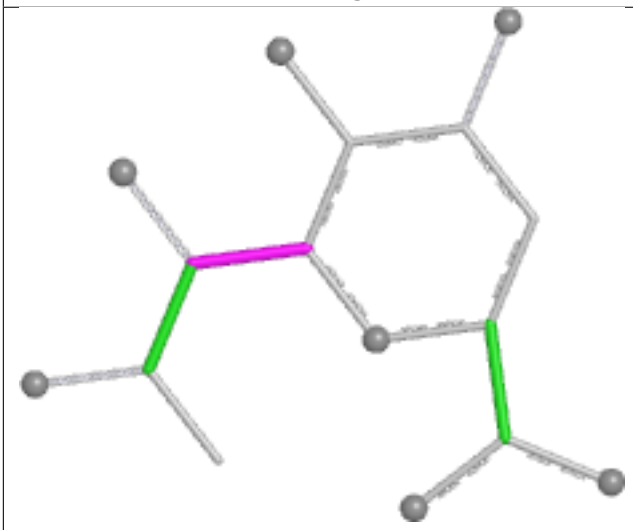
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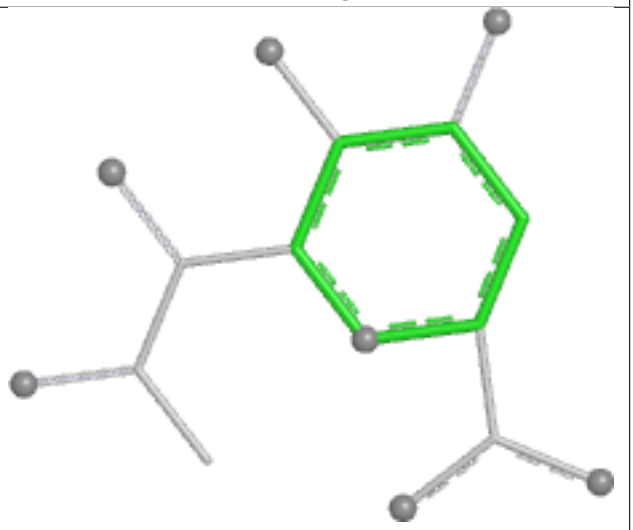
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Bond angles

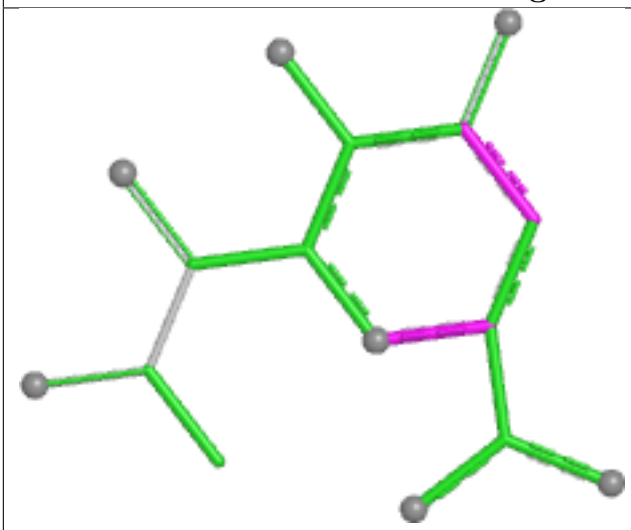


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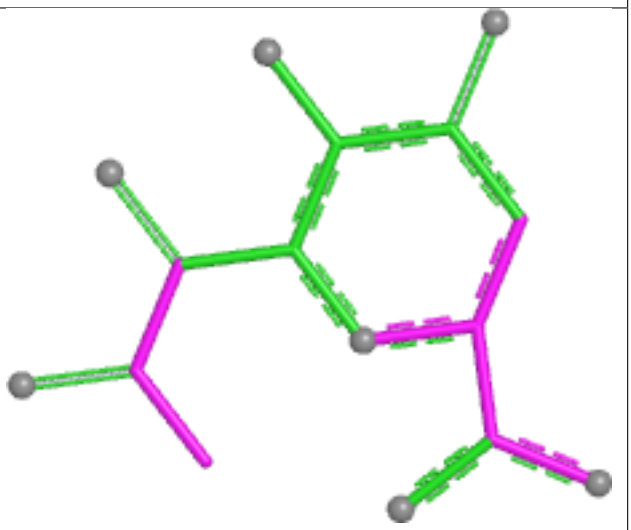


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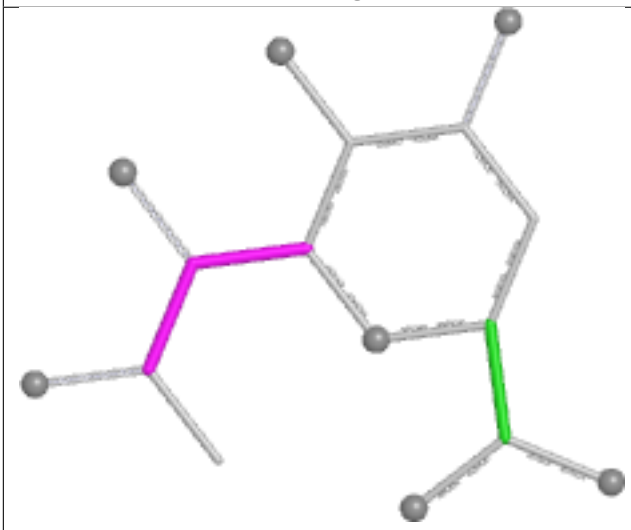
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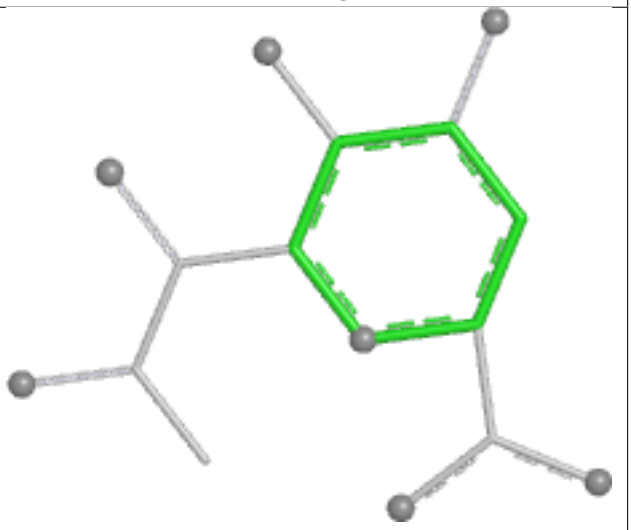
Bond lengths



Bond angles

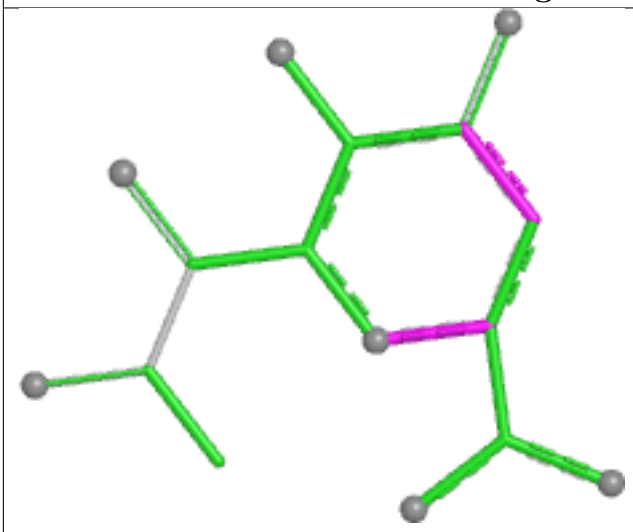


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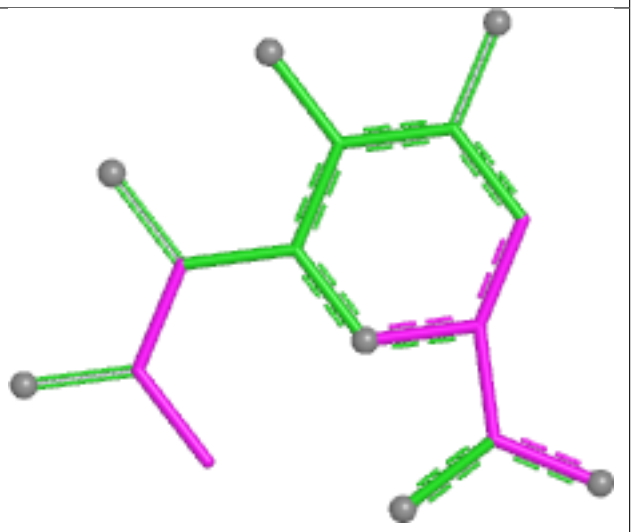


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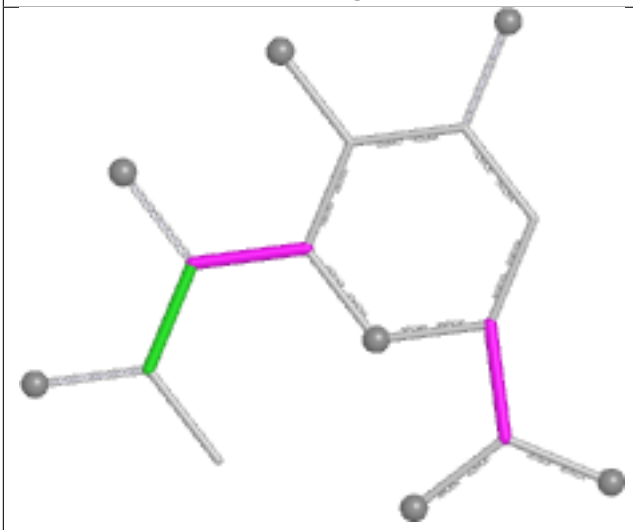
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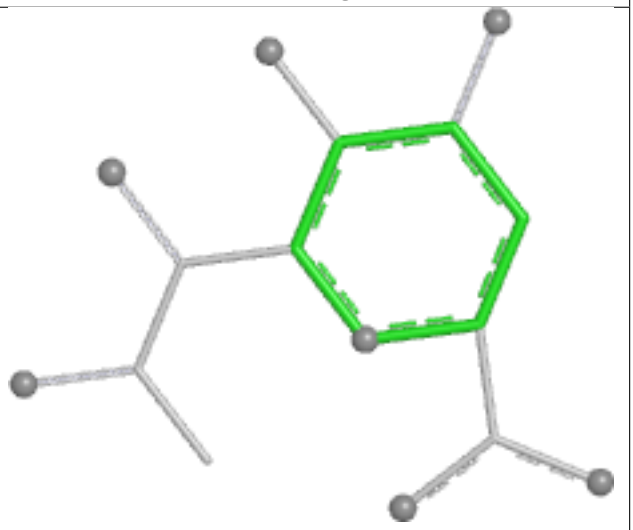
Bond lengths



Bond angles

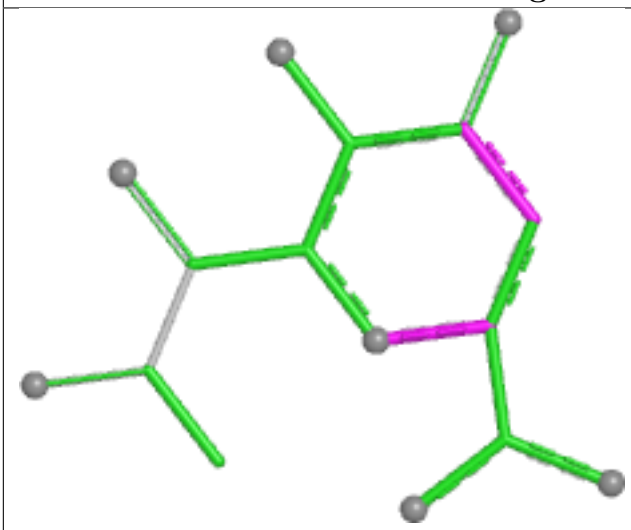


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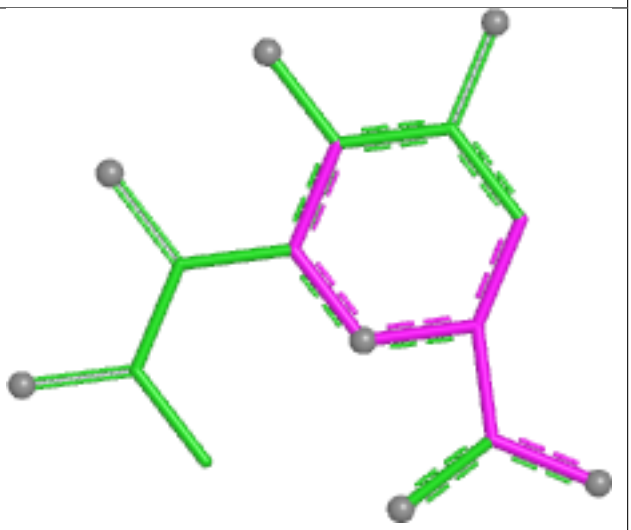


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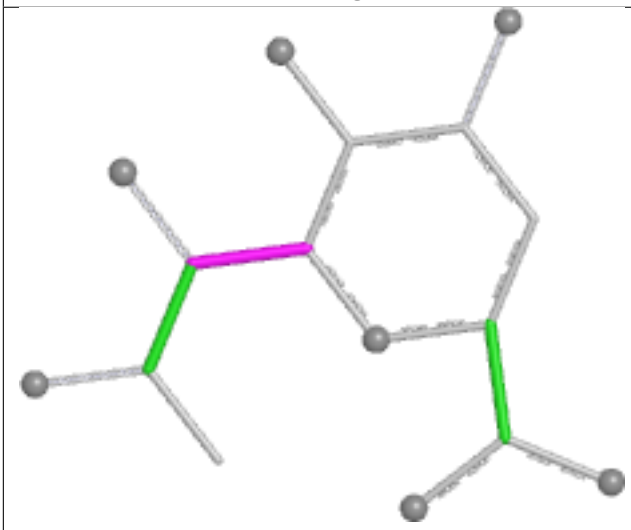
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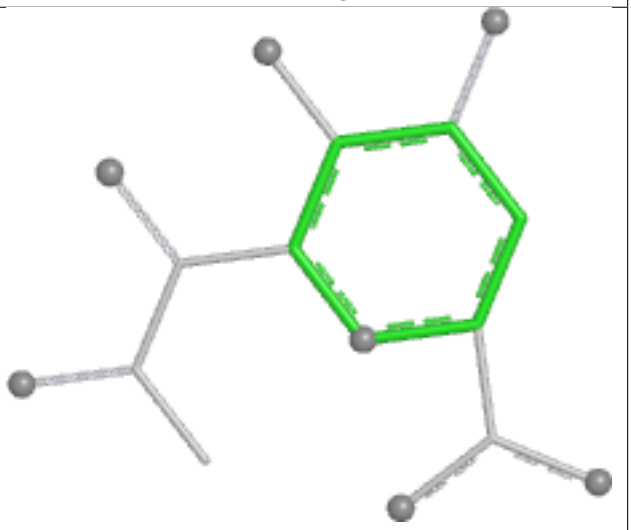
Bond lengths



Bond angles

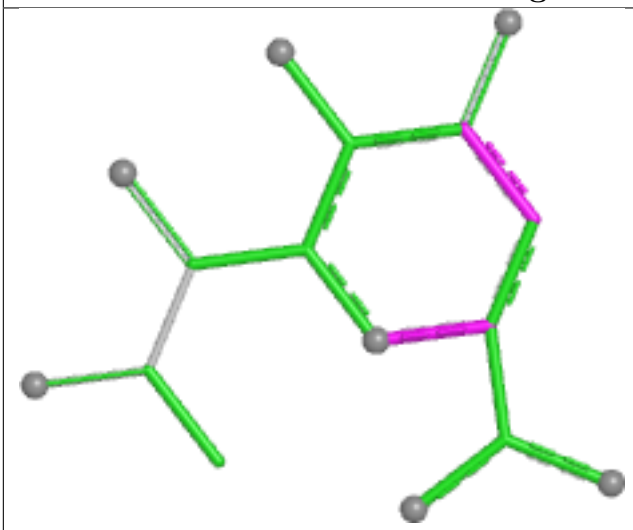


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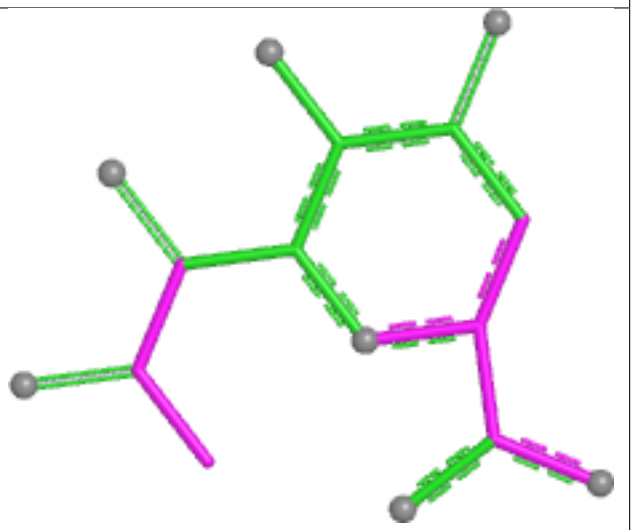


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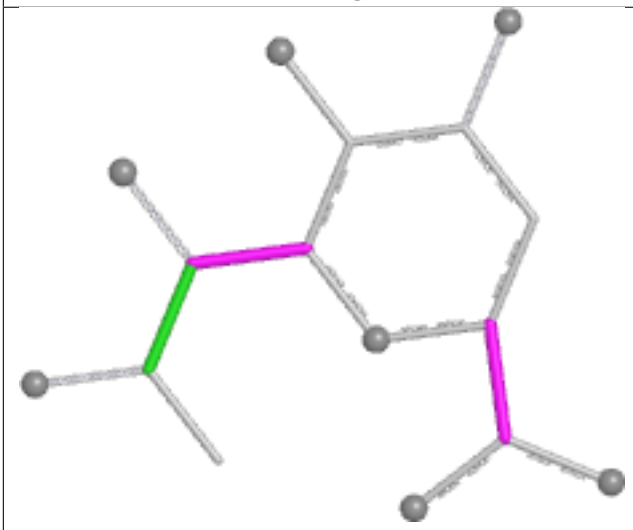
Ligand P8E P 612



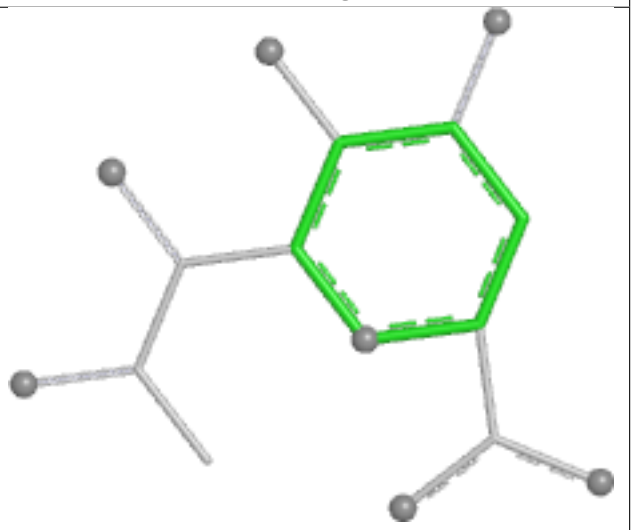
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Bond angles

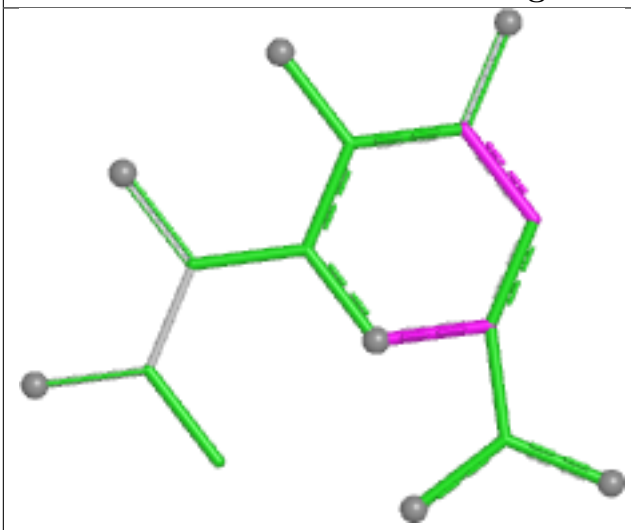


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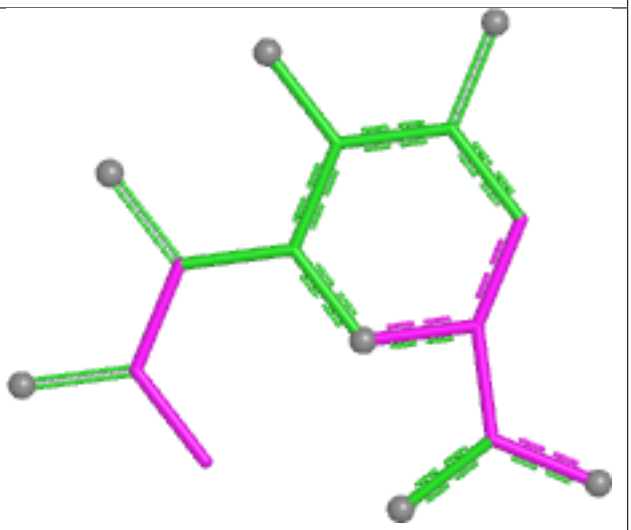


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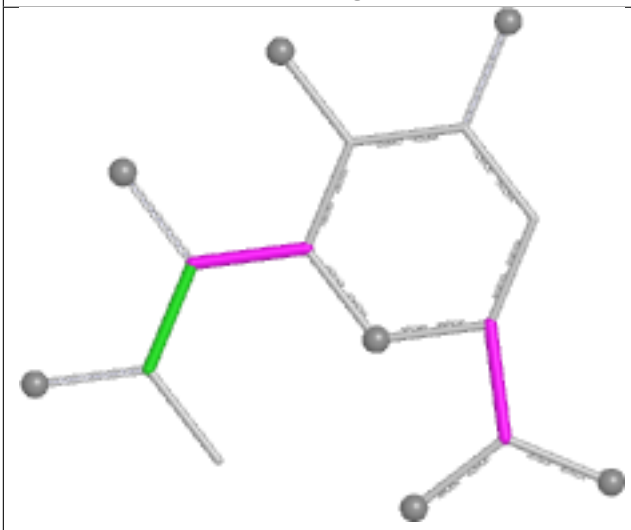
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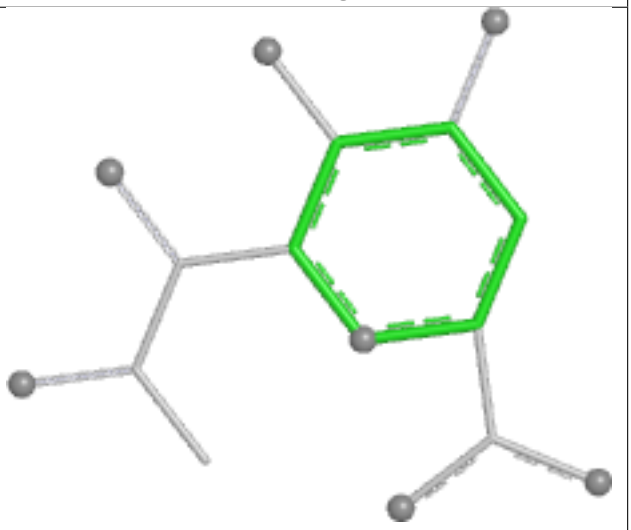
Bond lengths



Bond angles

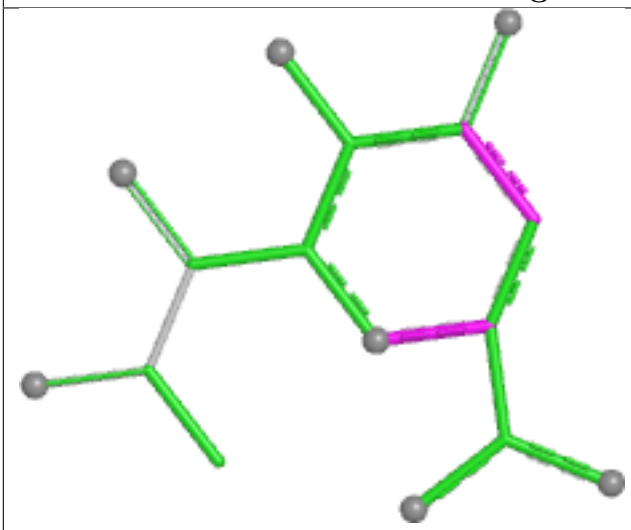


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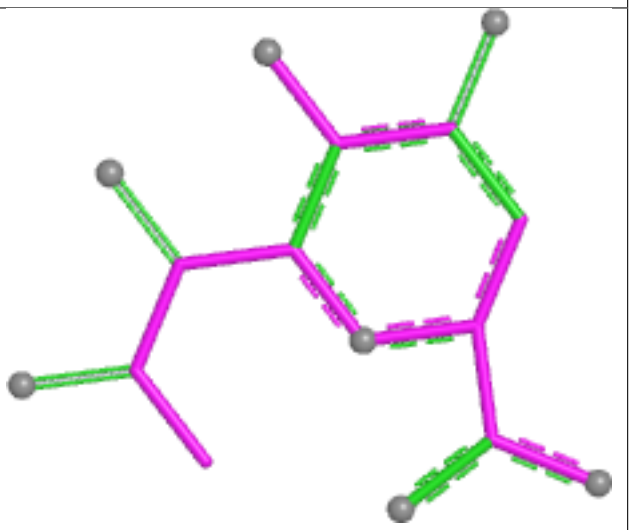


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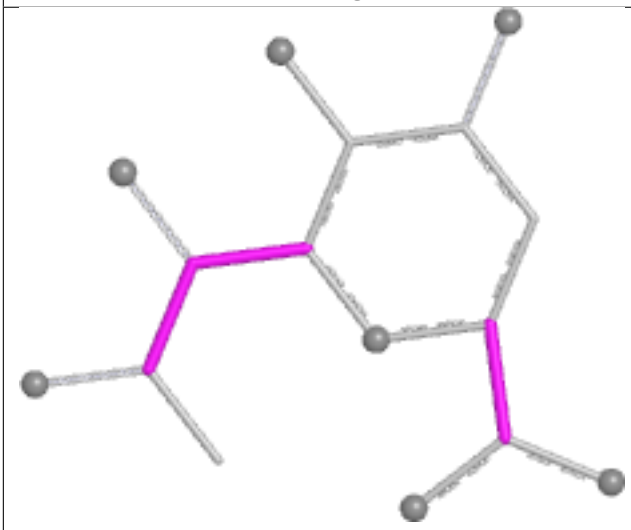
Ligand P8E F 616



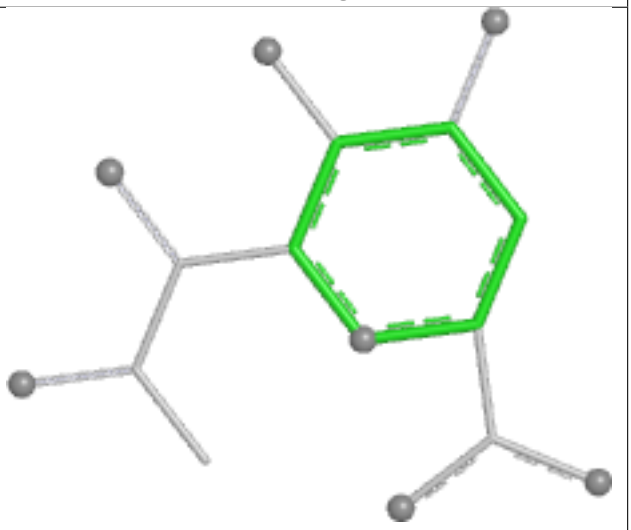
Bond lengths



Bond angles

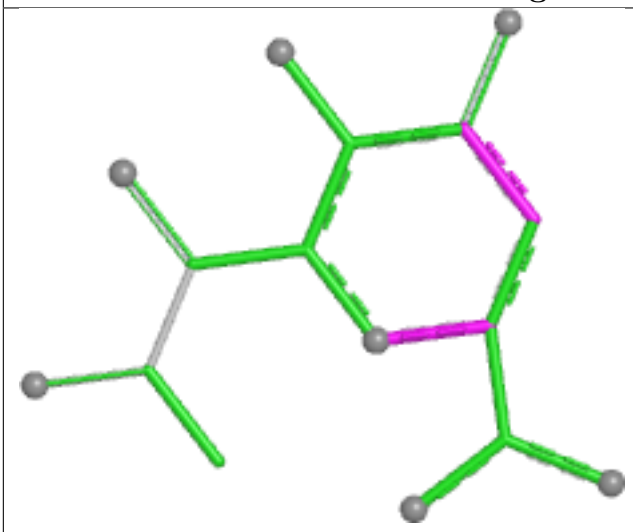


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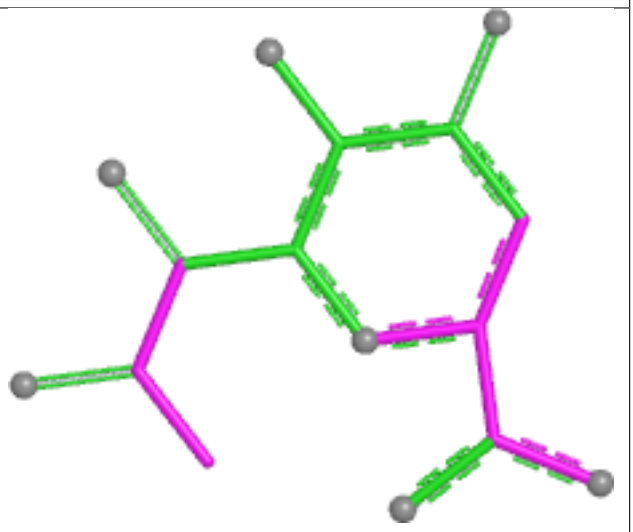


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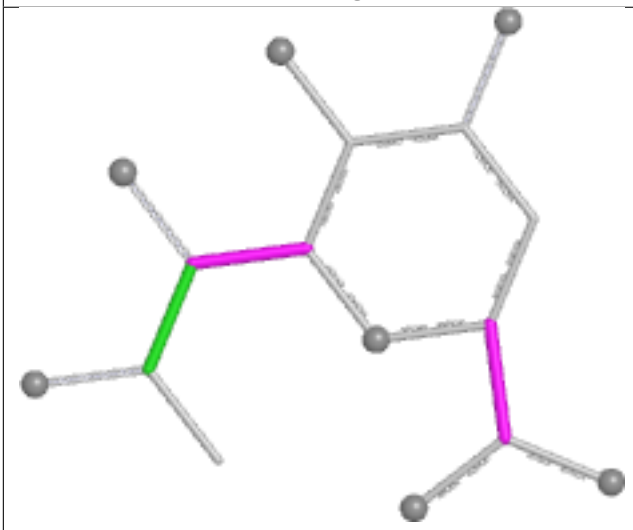
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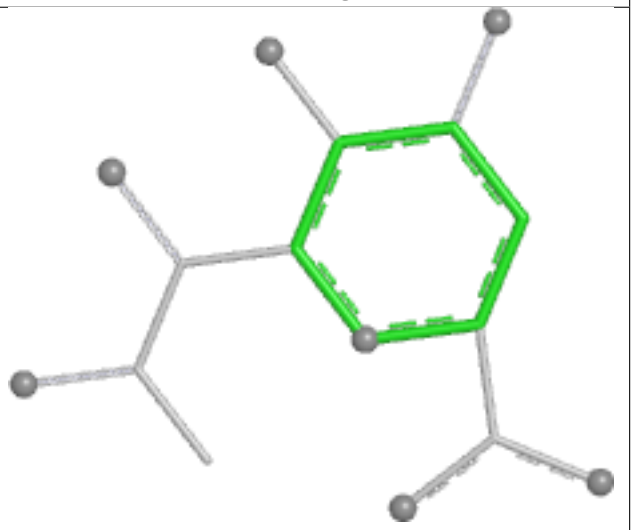
Bond lengths



Bond angles

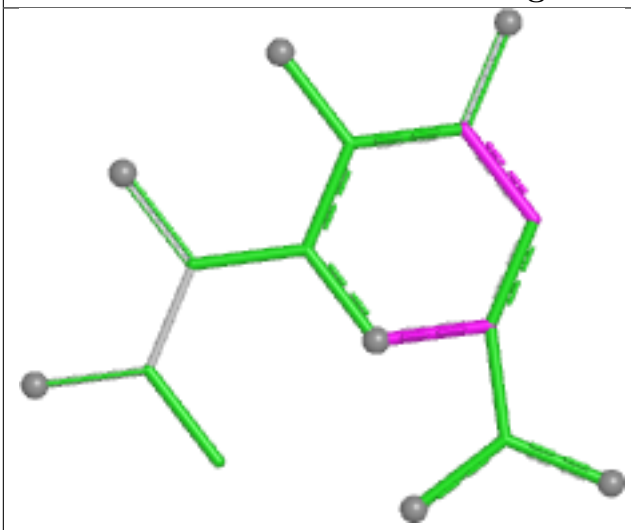


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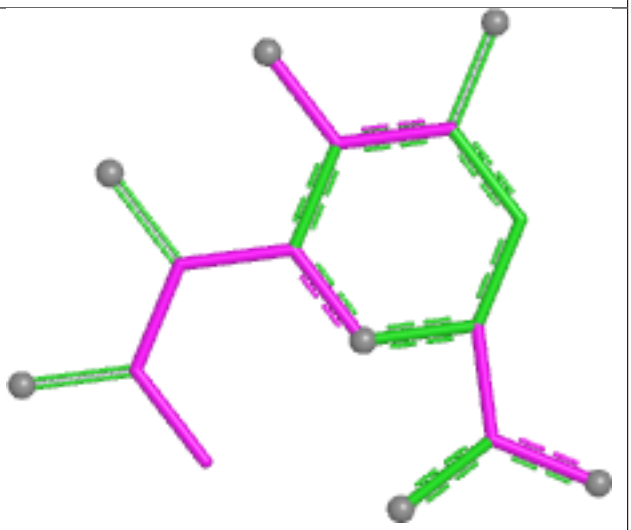


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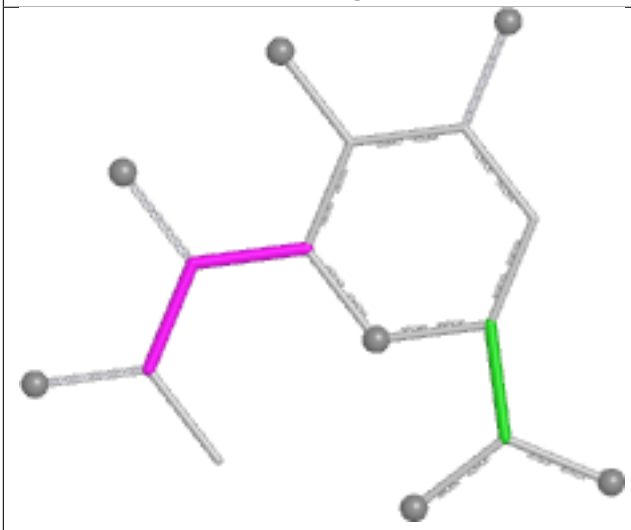
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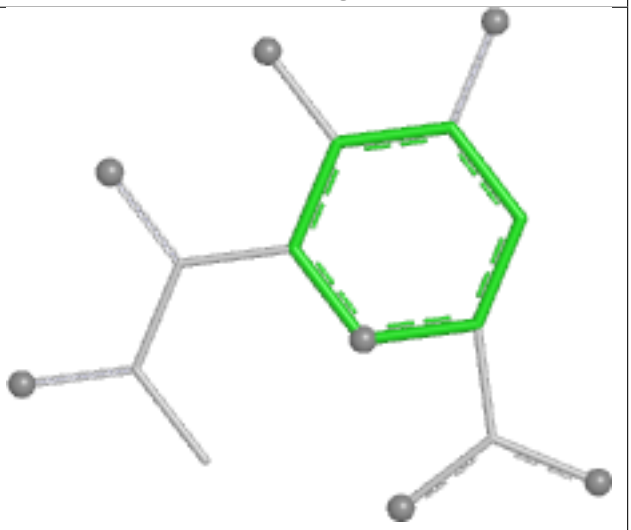
Bond lengths



Bond angles

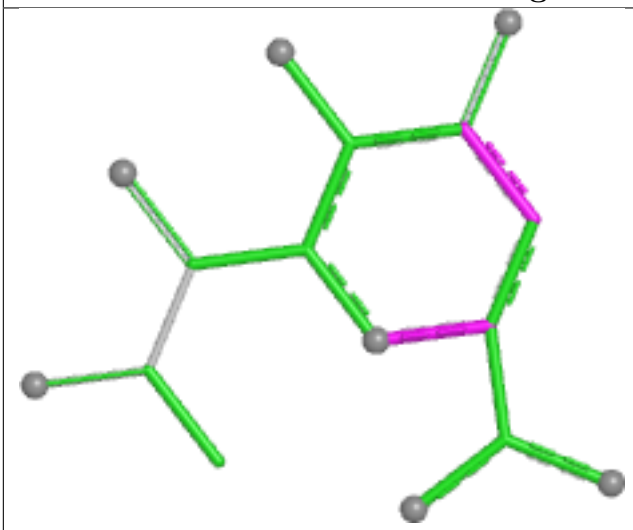


Torsions

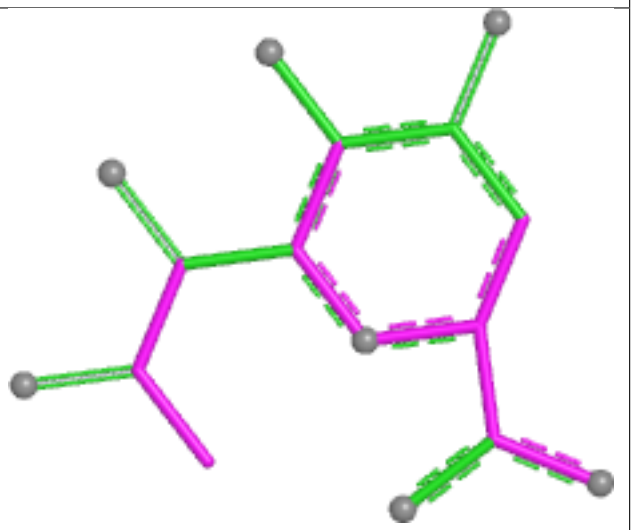


Rings

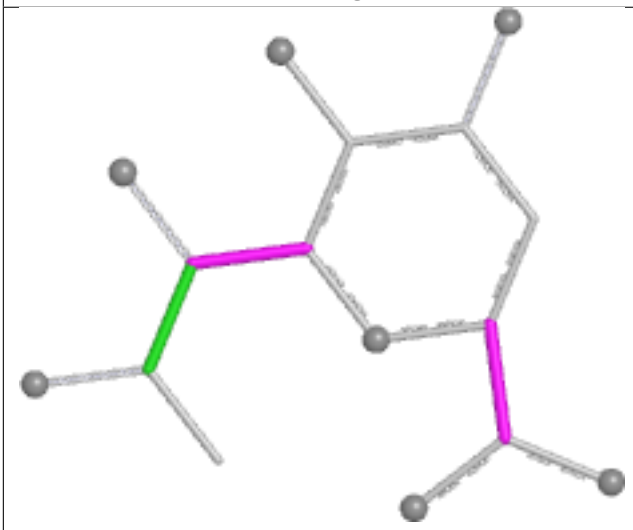
Ligand P8E E 606



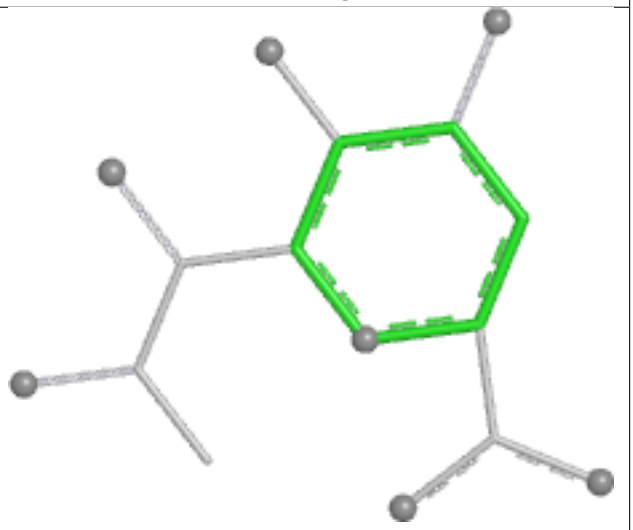
Bond lengths



Bond angles

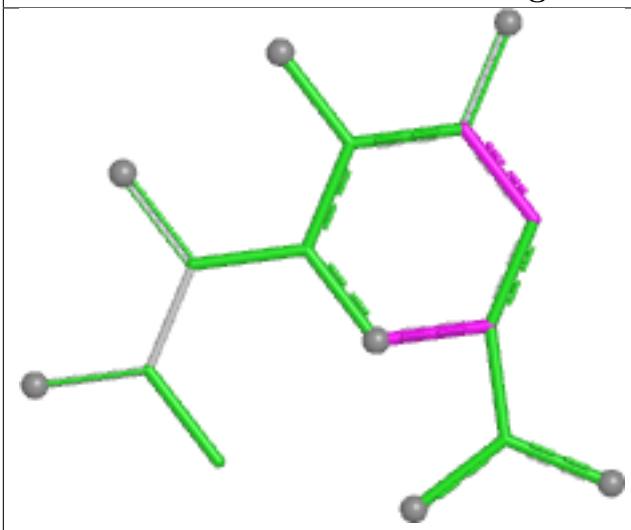


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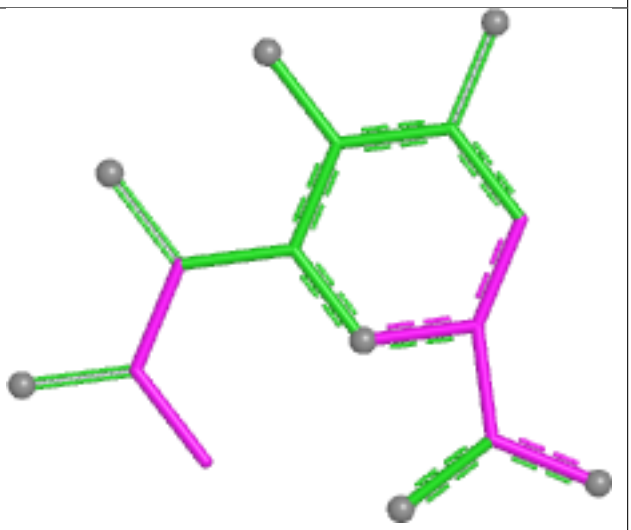


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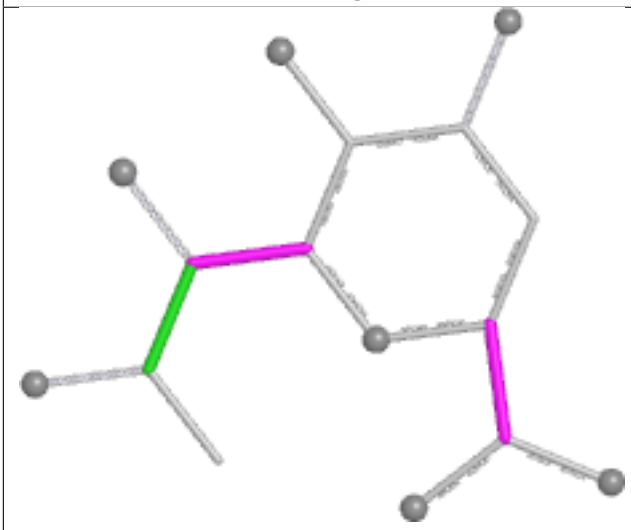
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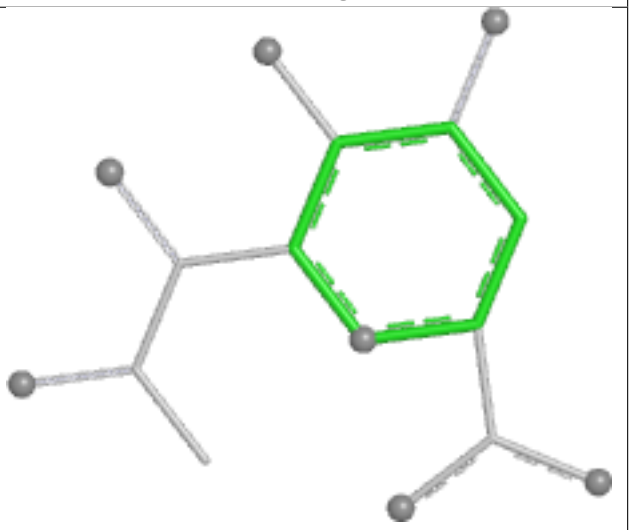
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Bond angles

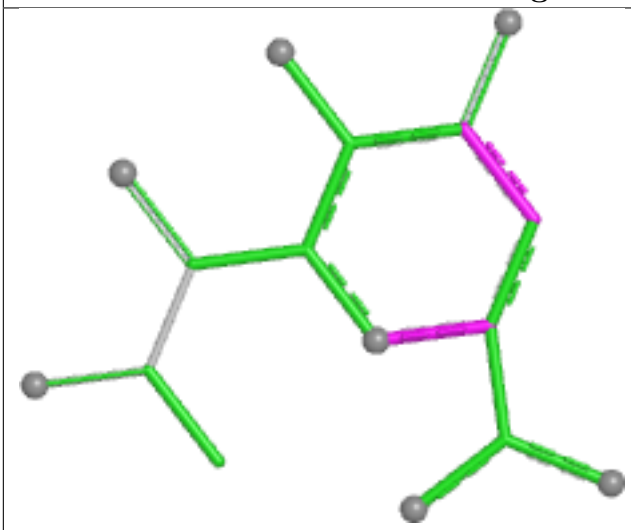


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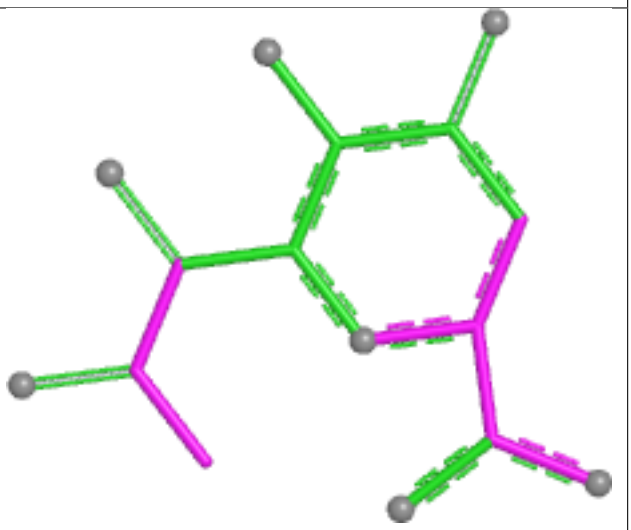


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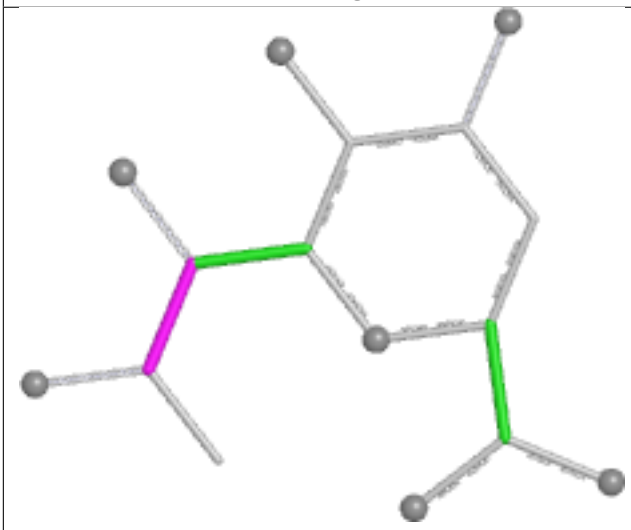
Ligand P8E L 603



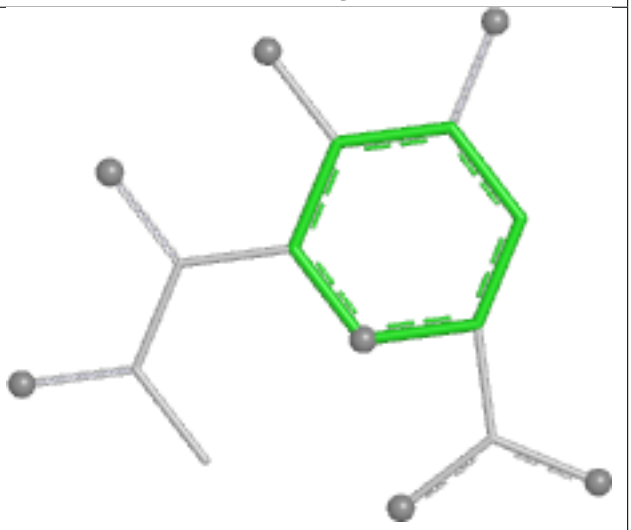
Bond lengths



Bond angles

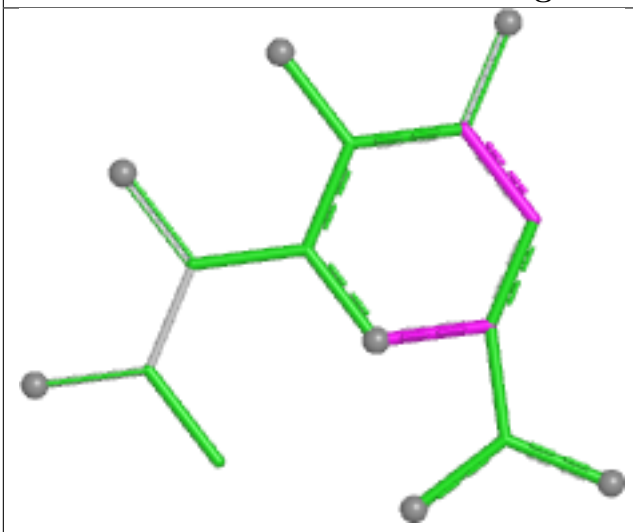


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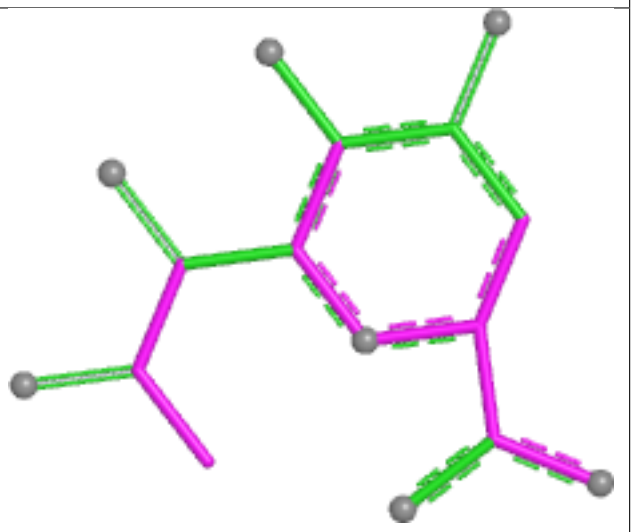


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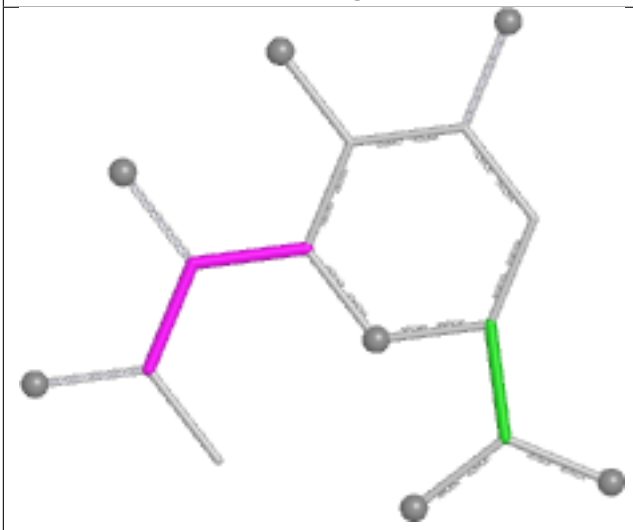
Ligand P8E I 606



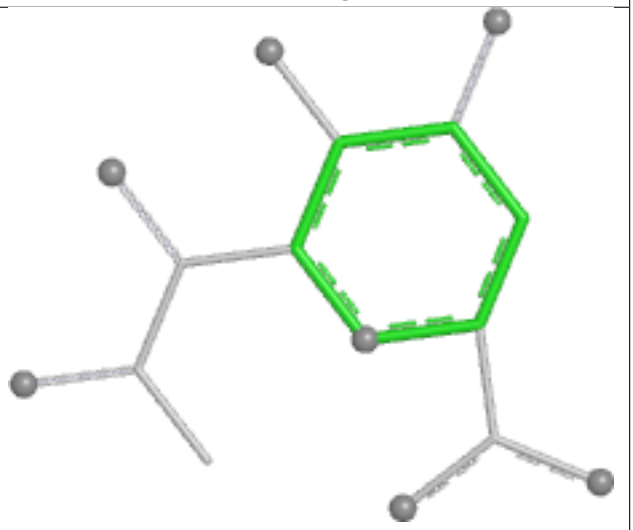
Bond lengths



Bond angles

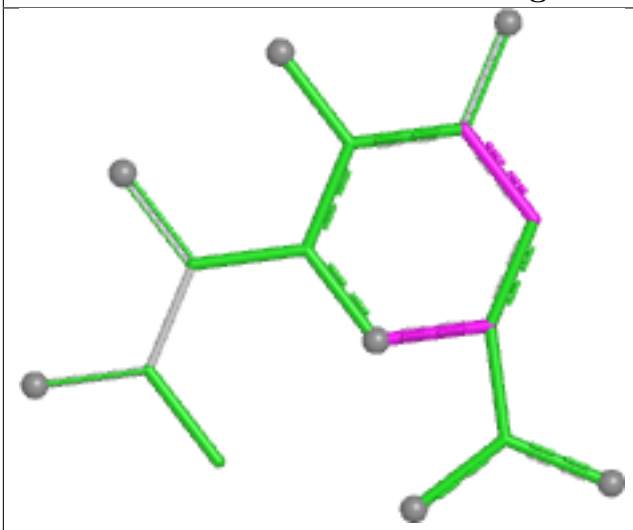


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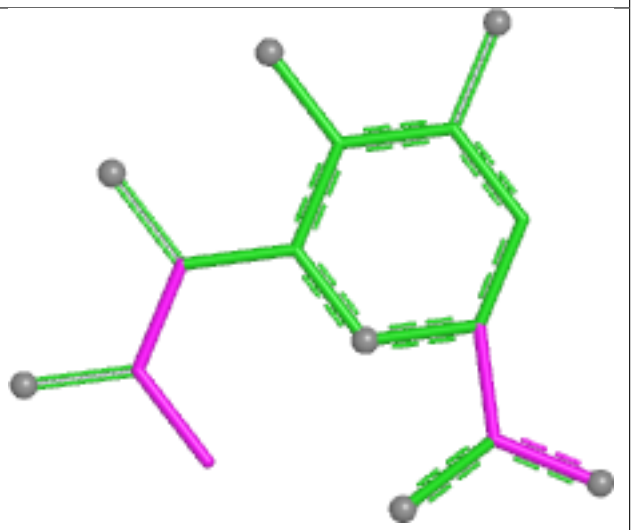


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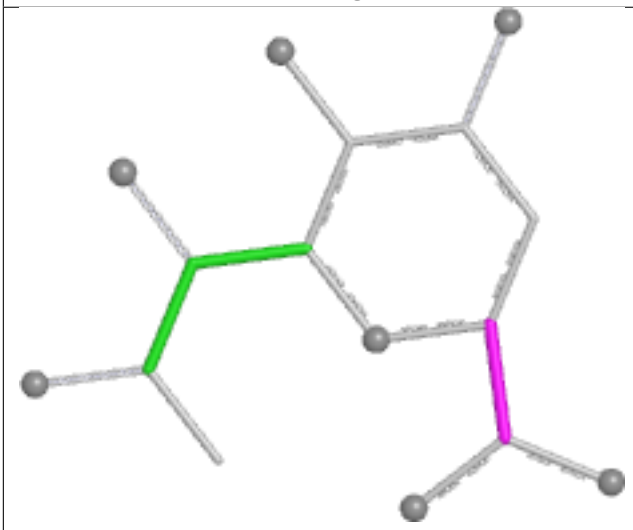
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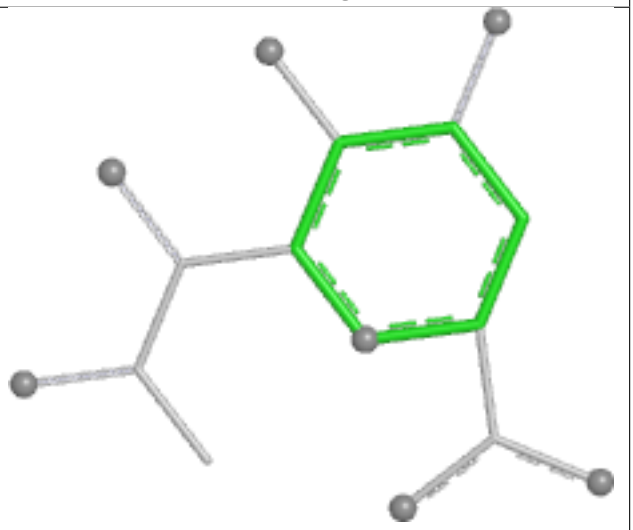
Bond lengths



Bond angles

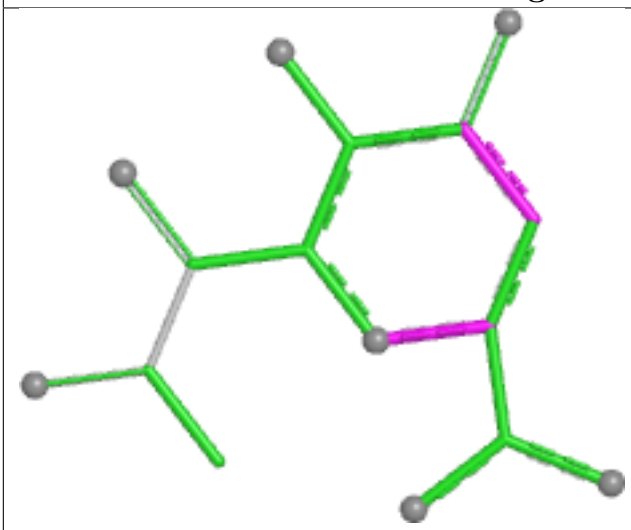


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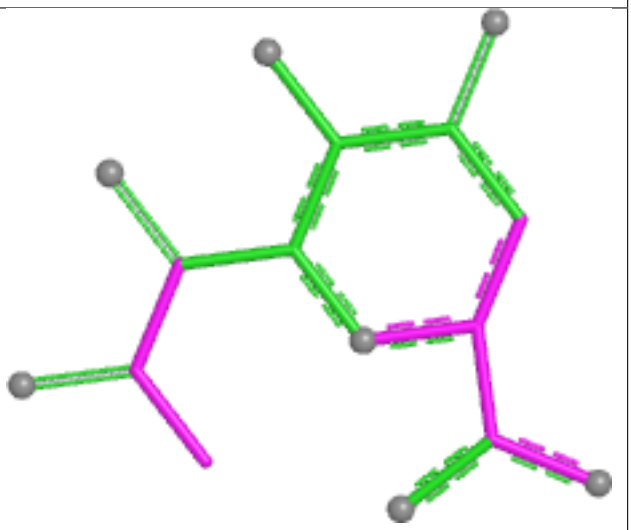


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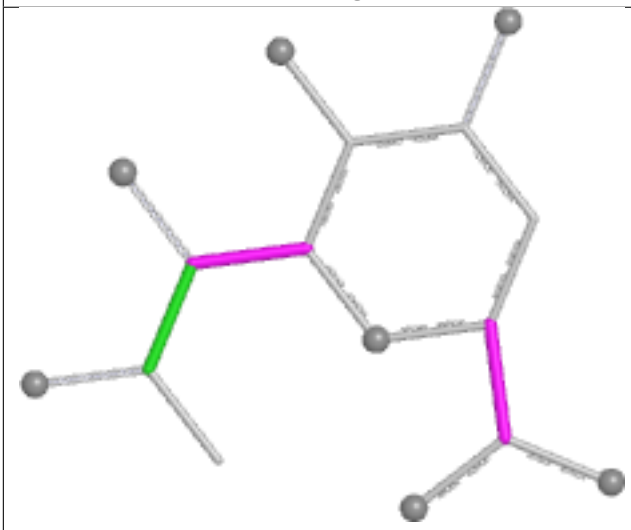
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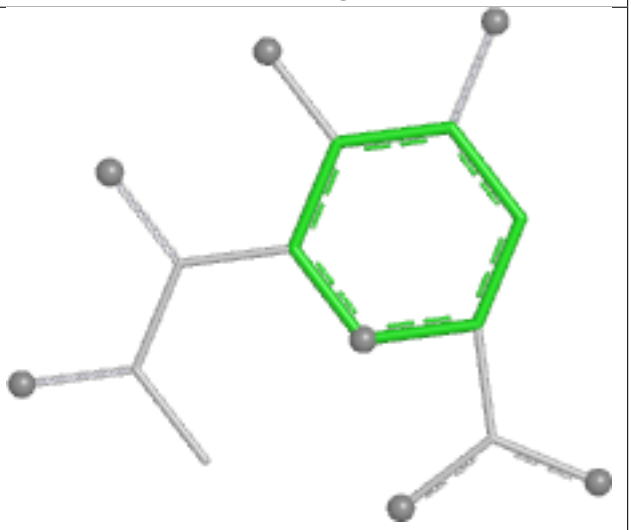
Bond lengths



Bond angles

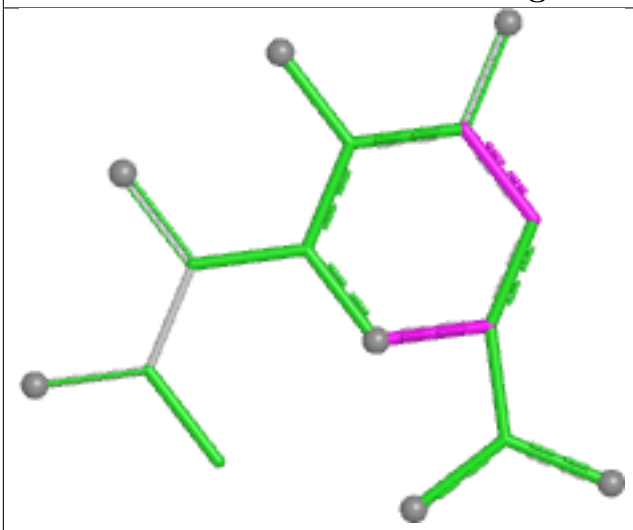


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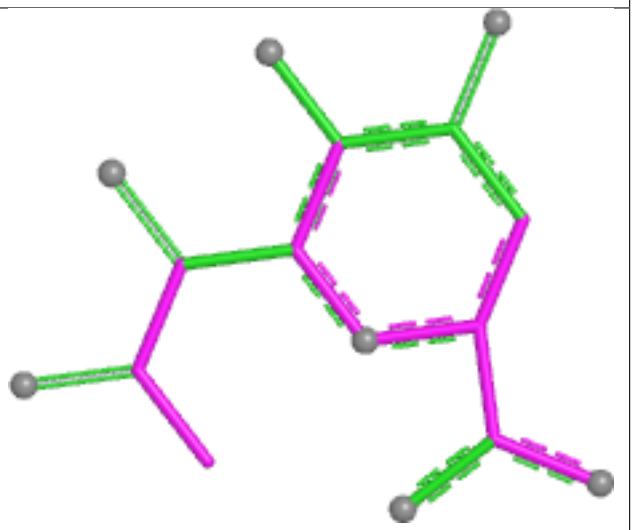


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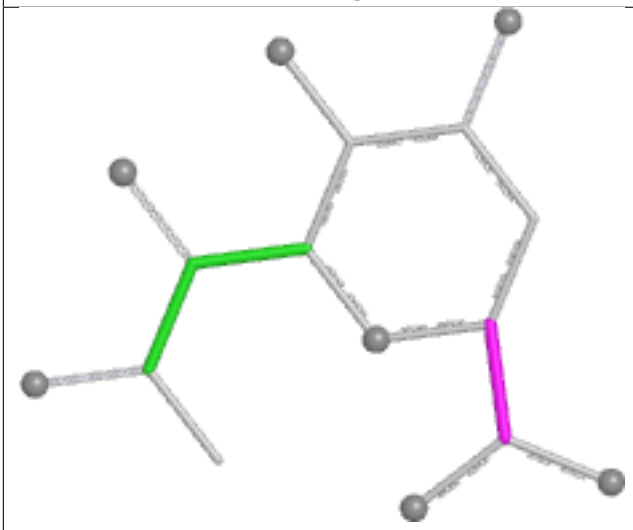
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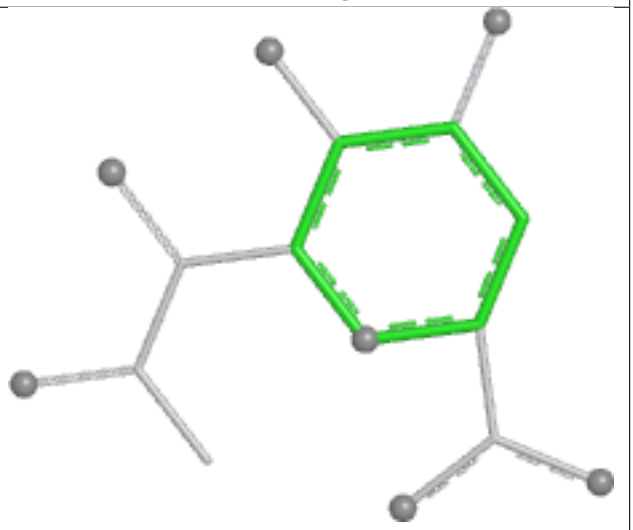
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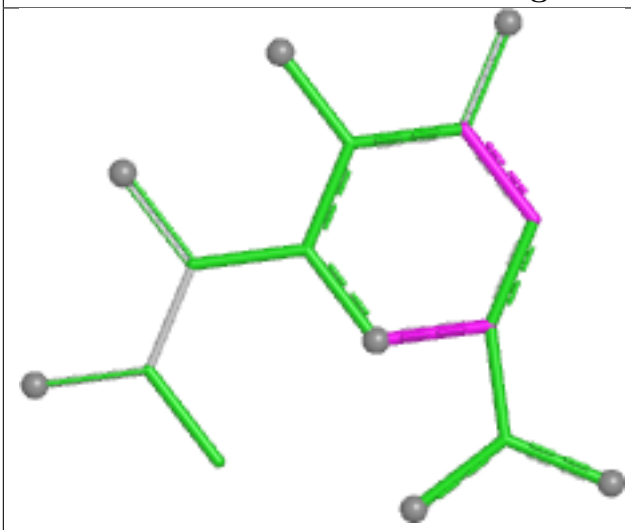


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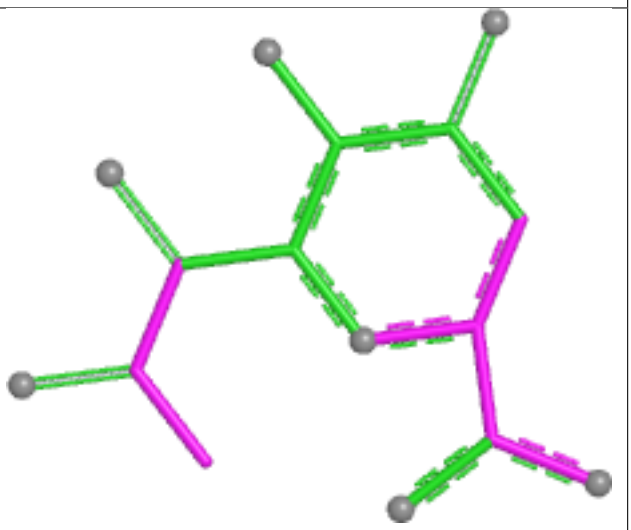


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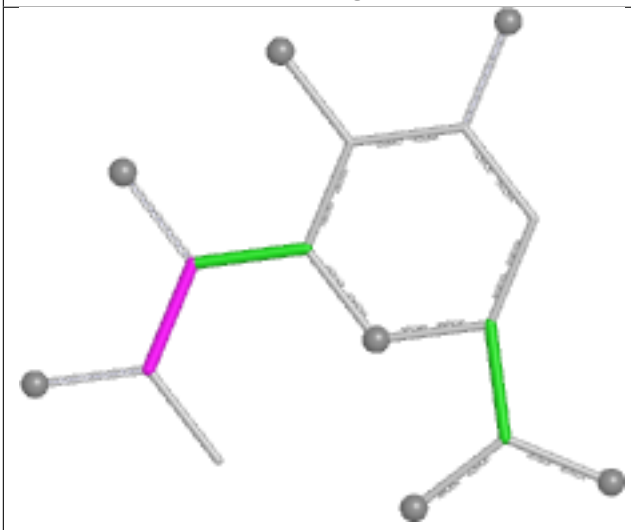
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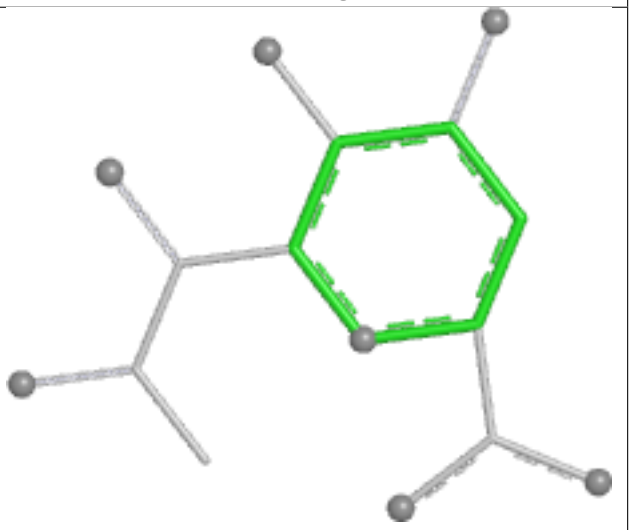
Bond lengths



Bond angles

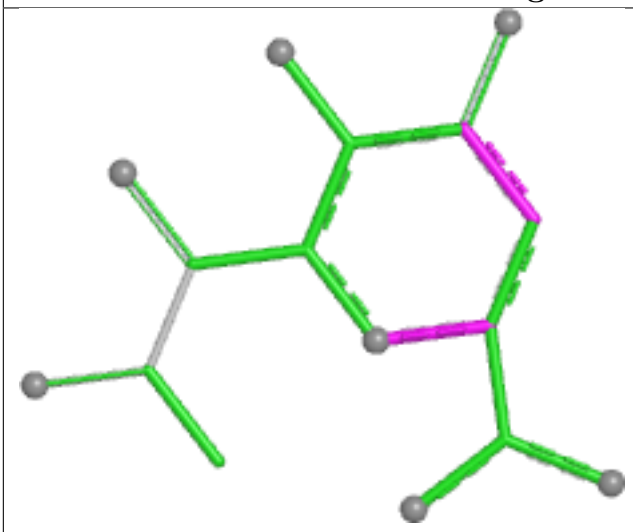


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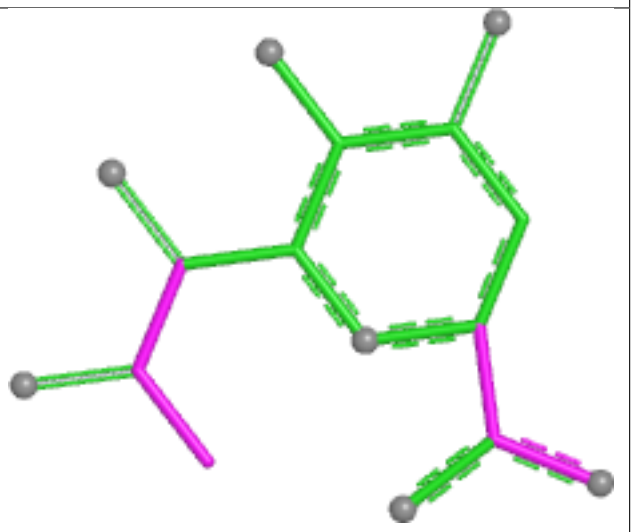


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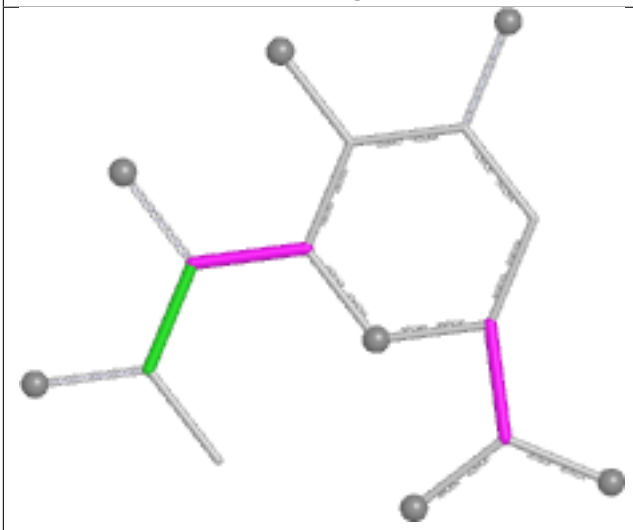
Ligand P8E G 609



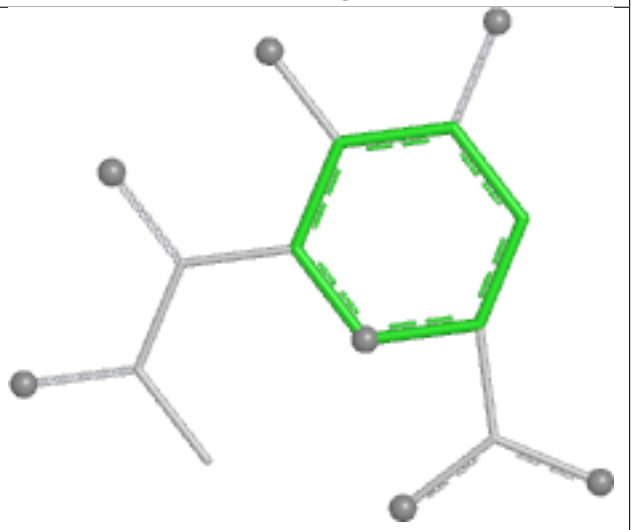
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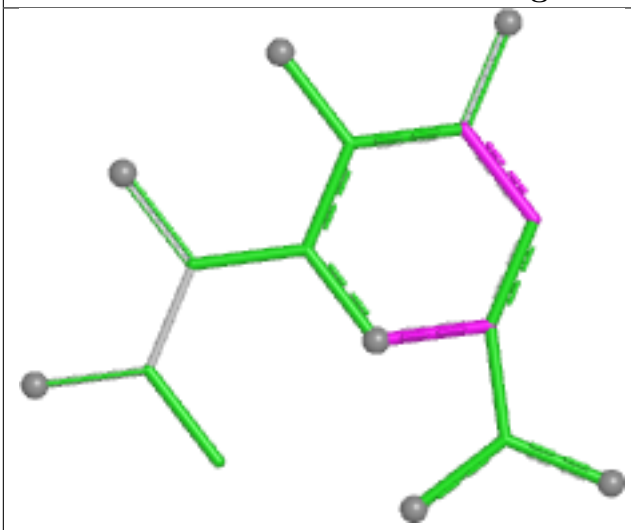


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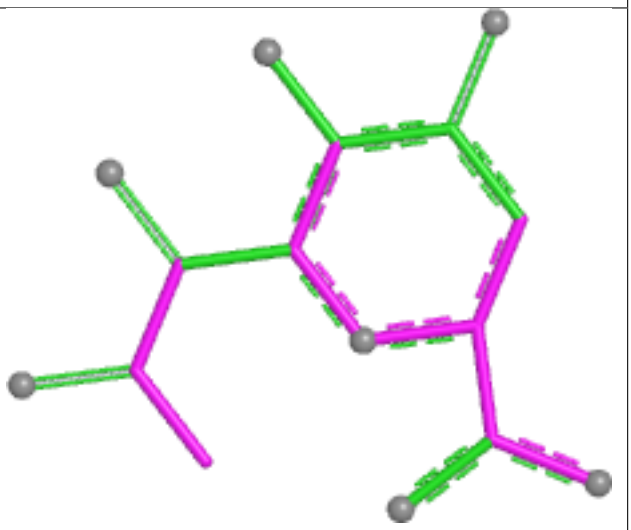


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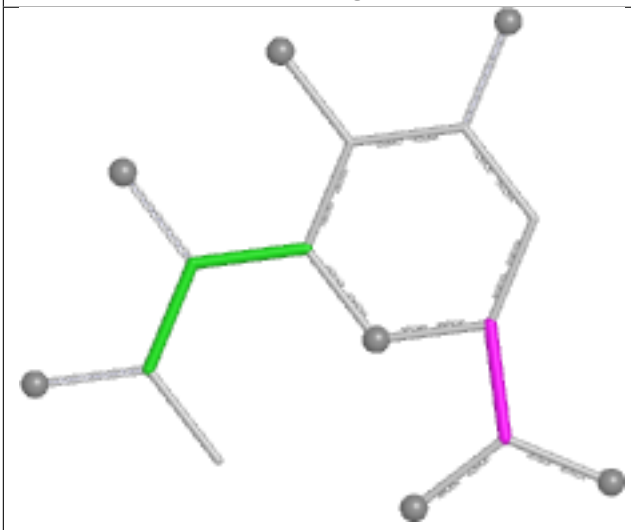
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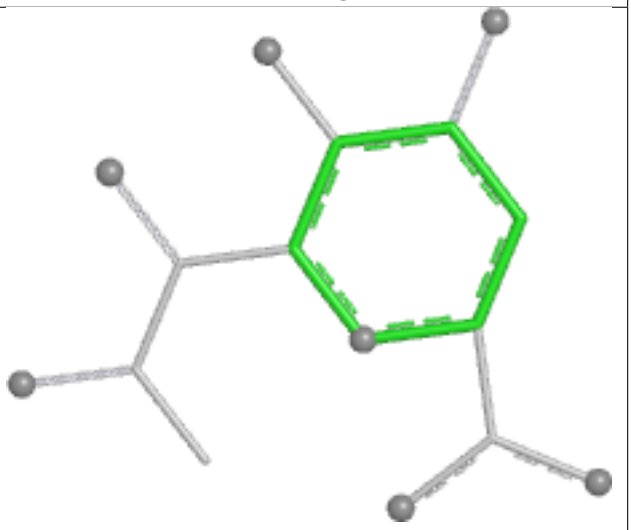
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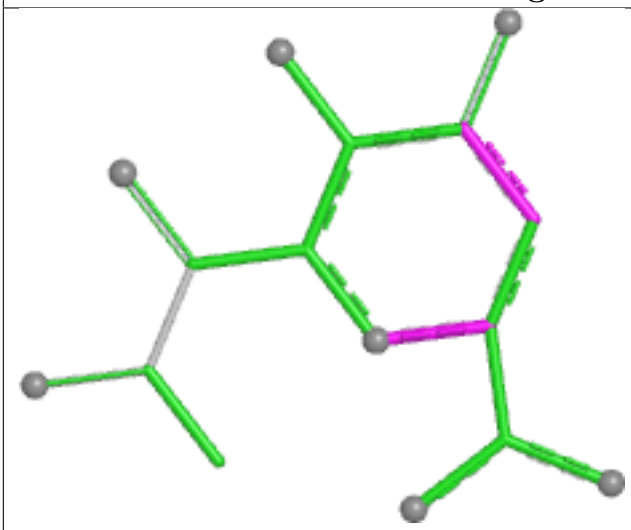


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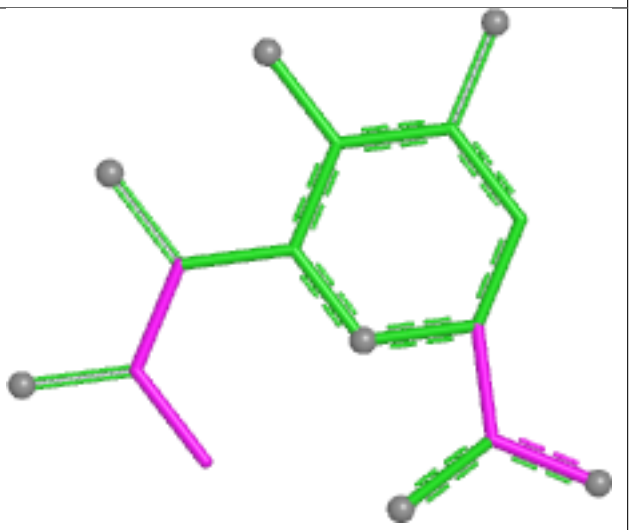


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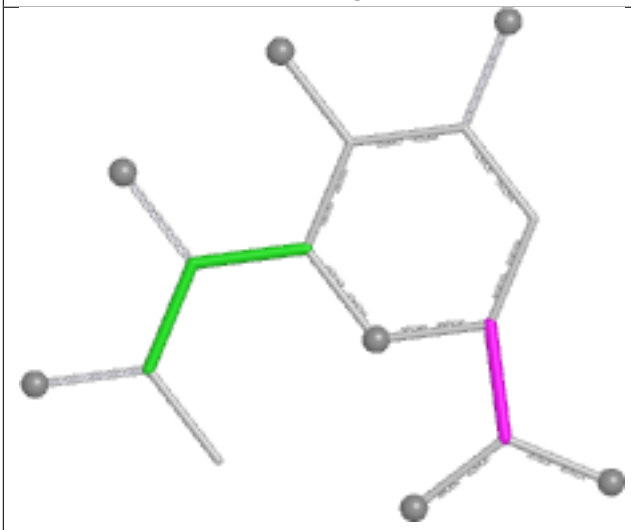
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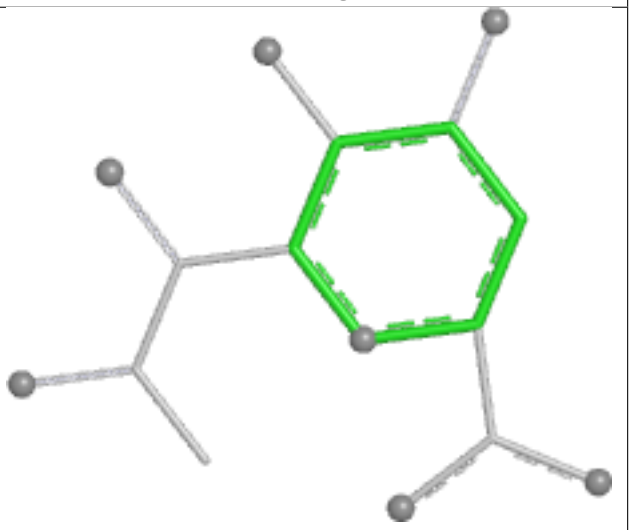
Bond lengths



Bond angles

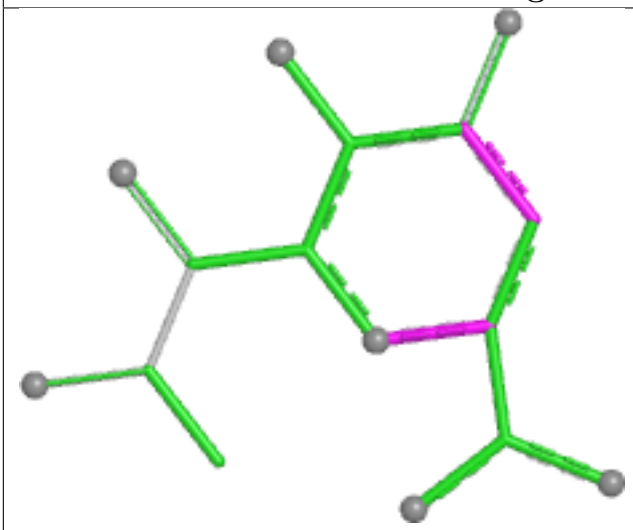


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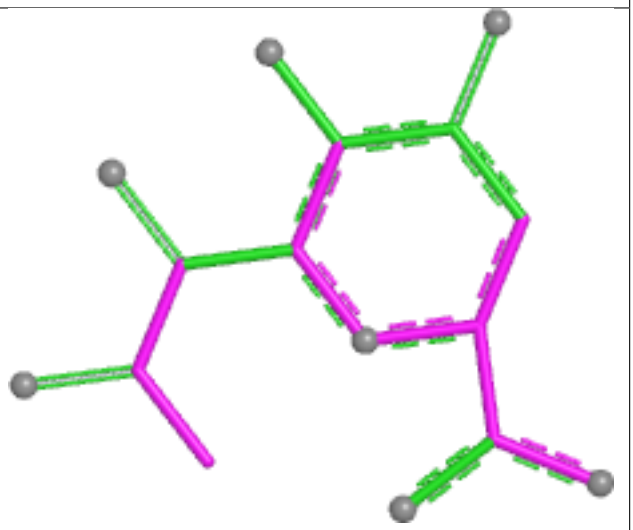


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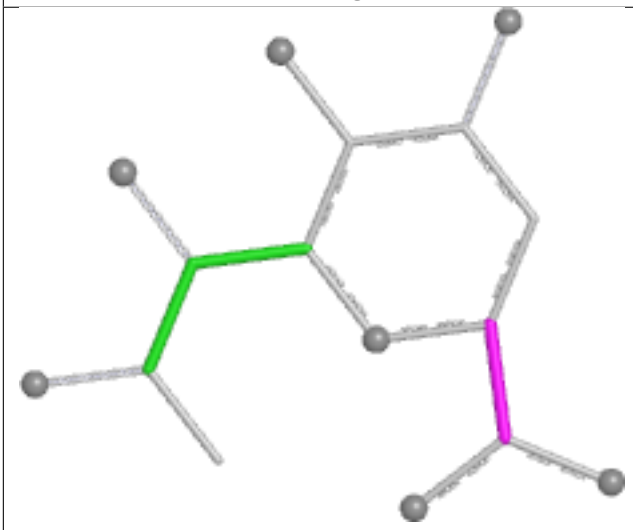
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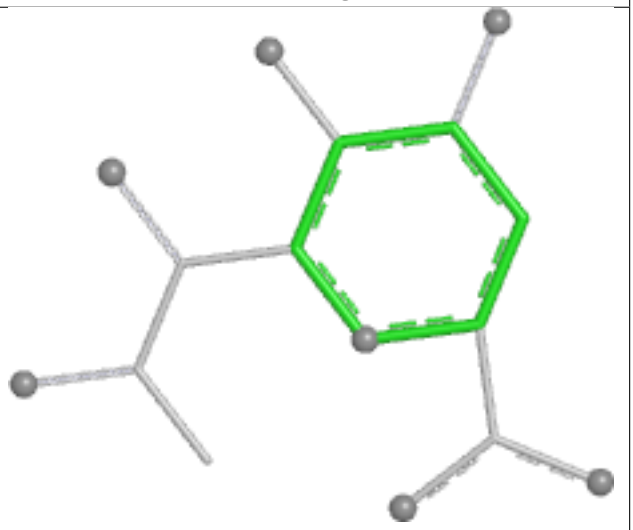
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Bond angles

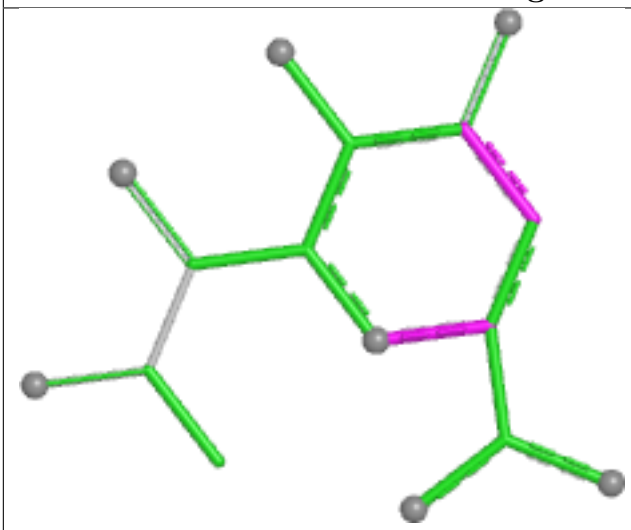


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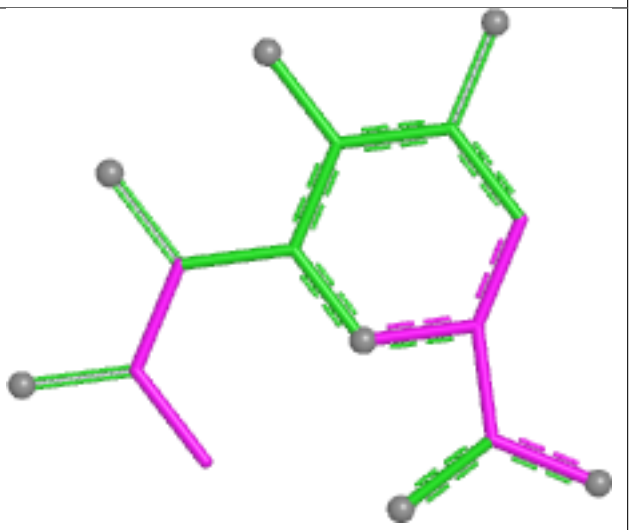


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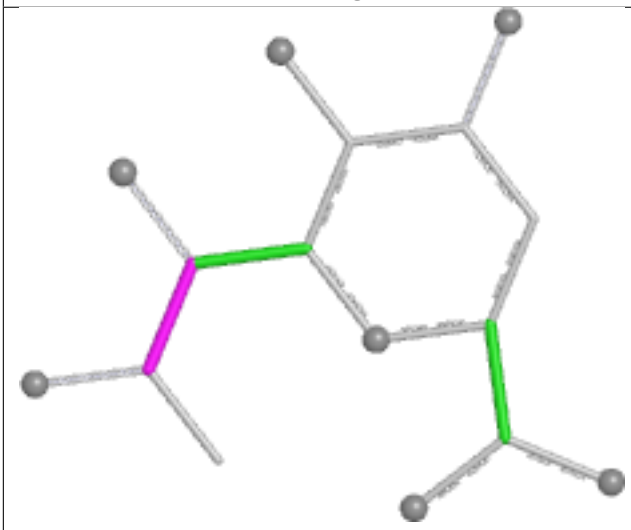
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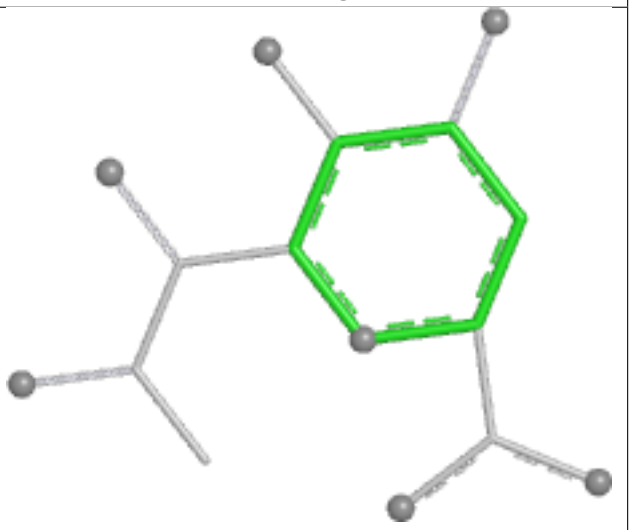
Bond lengths



Bond angles

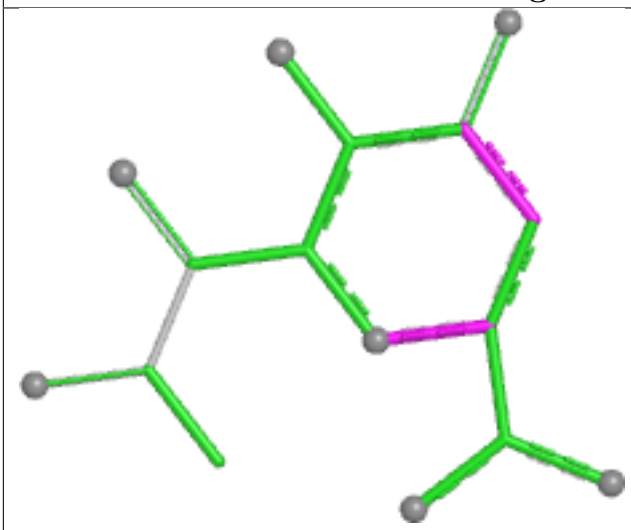


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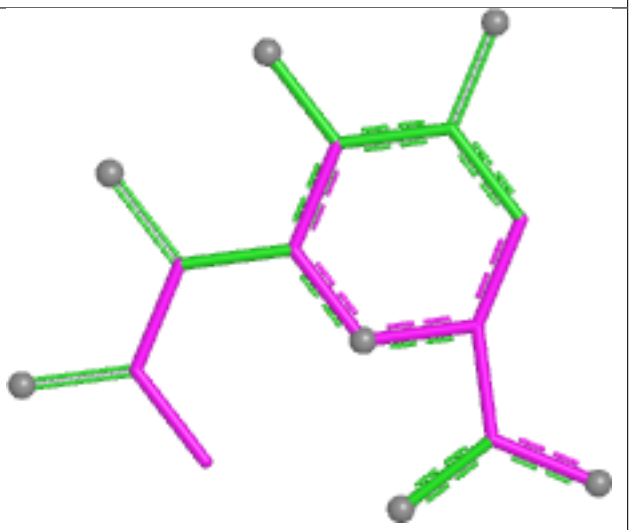


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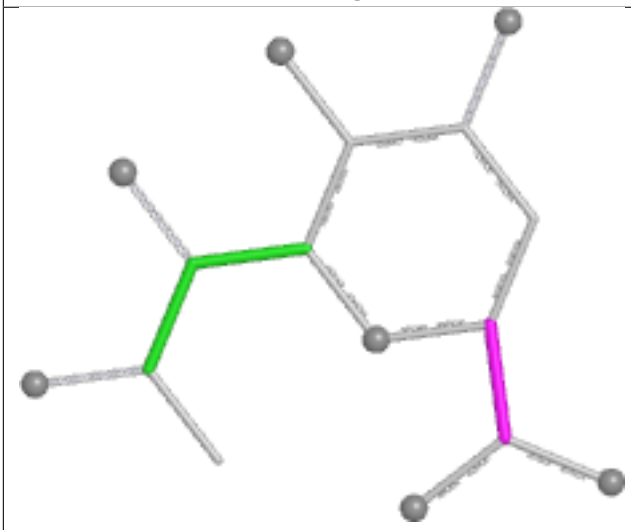
Ligand P8E P 617



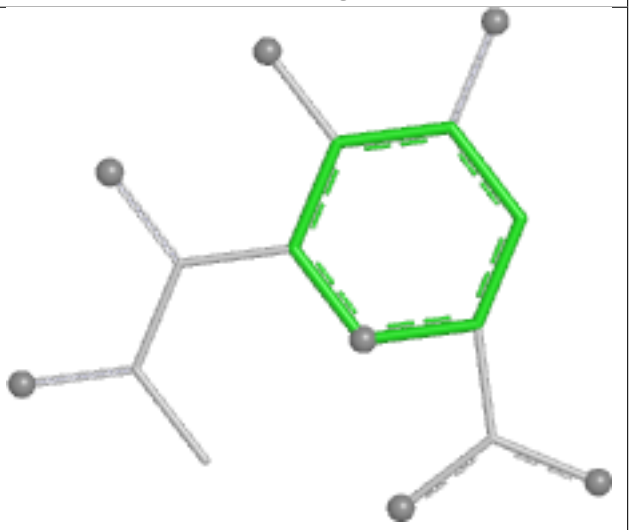
Bond lengths



Bond angles

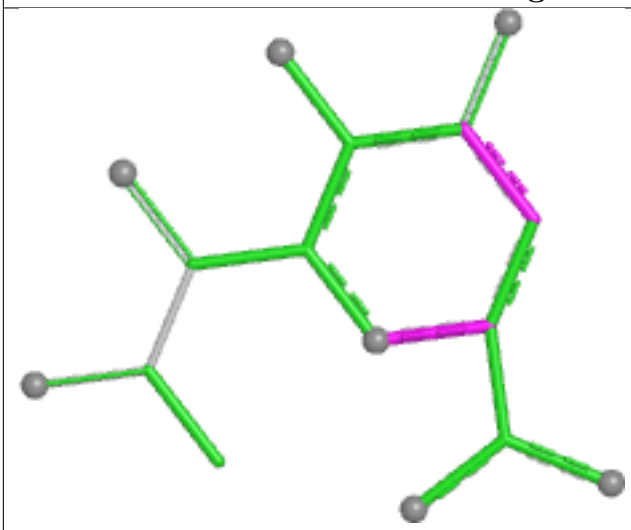


Torsions

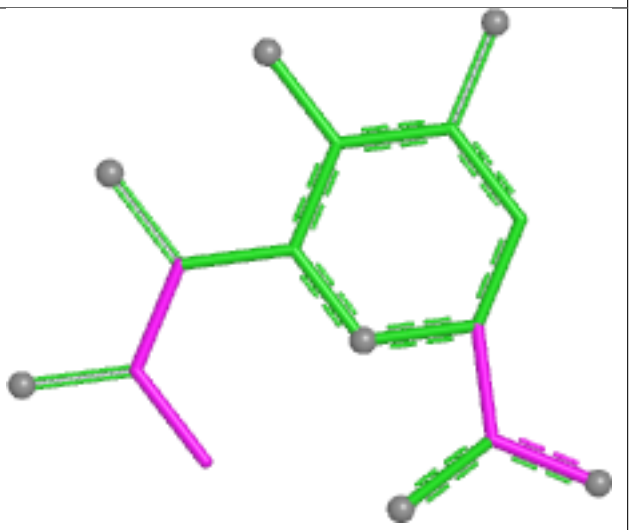


Rings

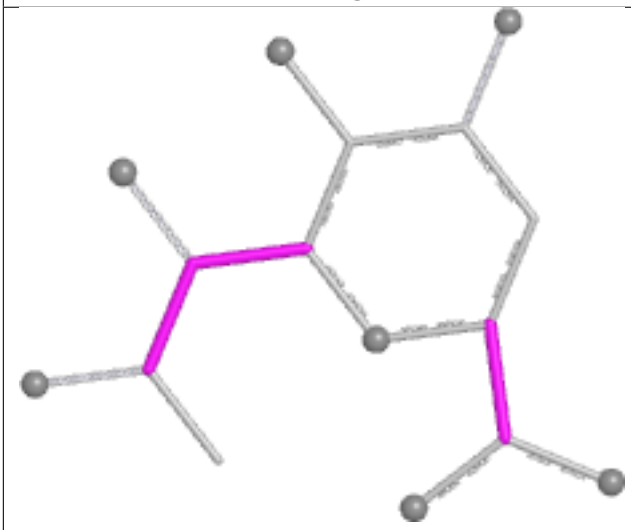
Ligand P8E D 610



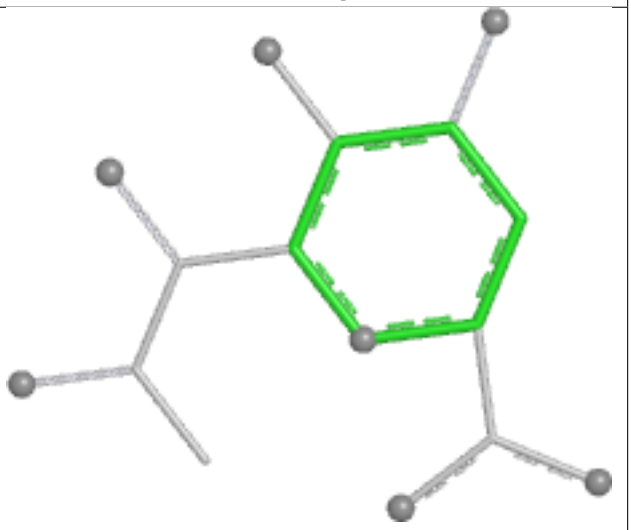
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Bond angles

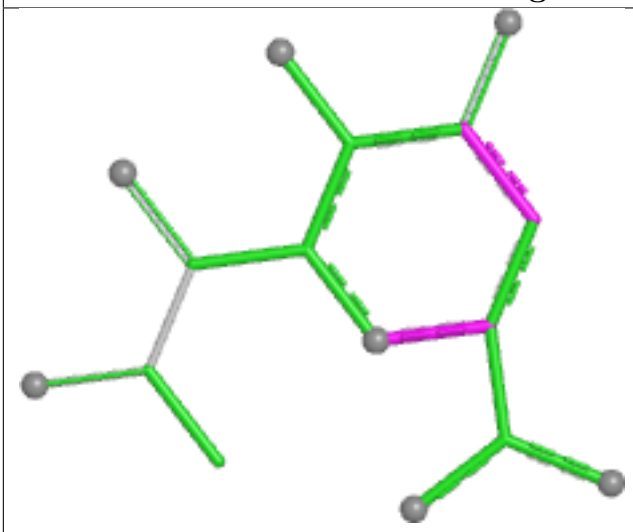


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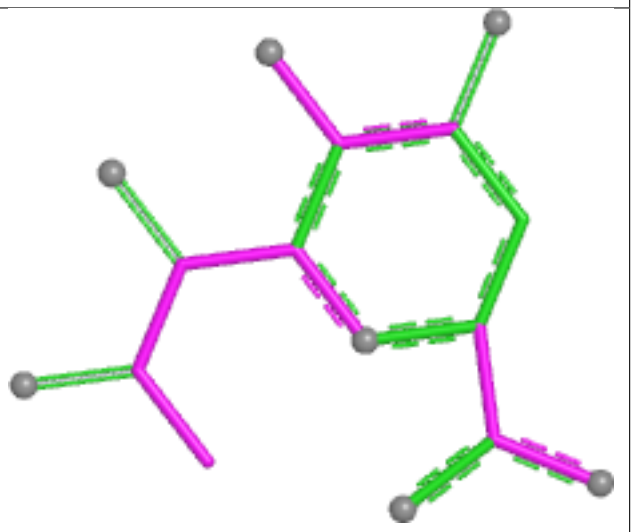


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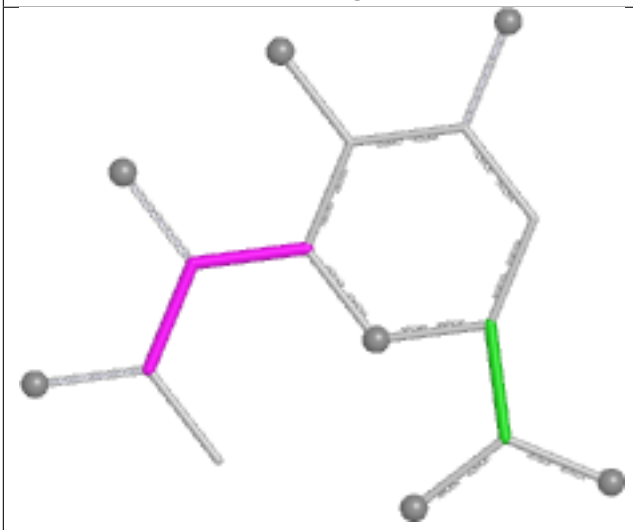
Ligand P8E T 616



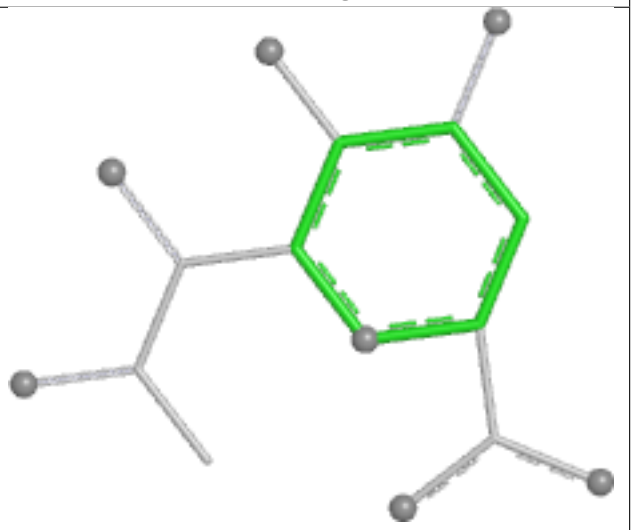
Bond lengths



Bond angles

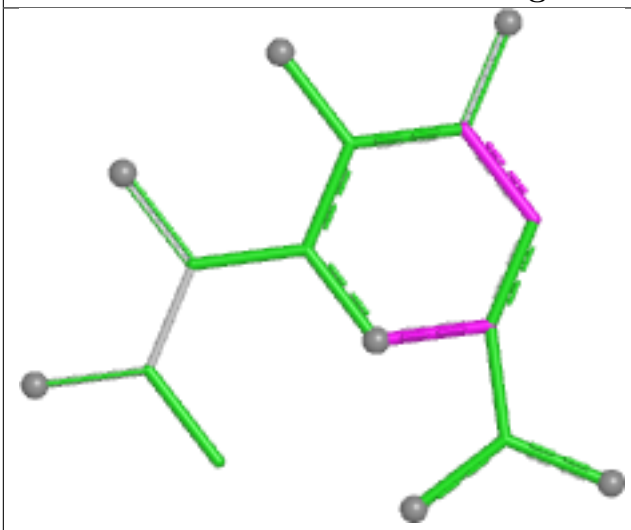


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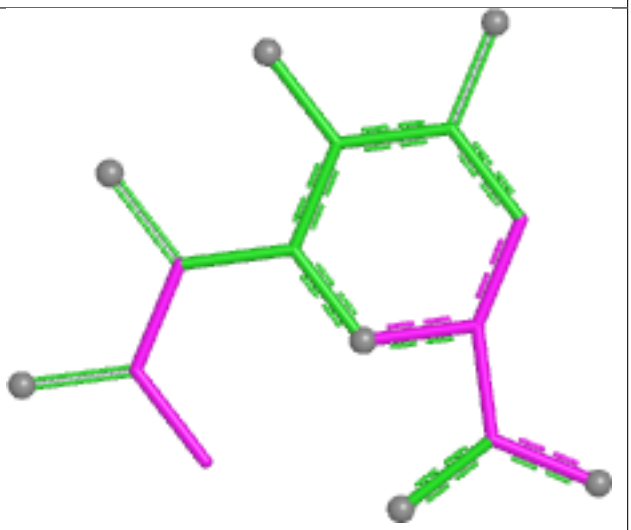


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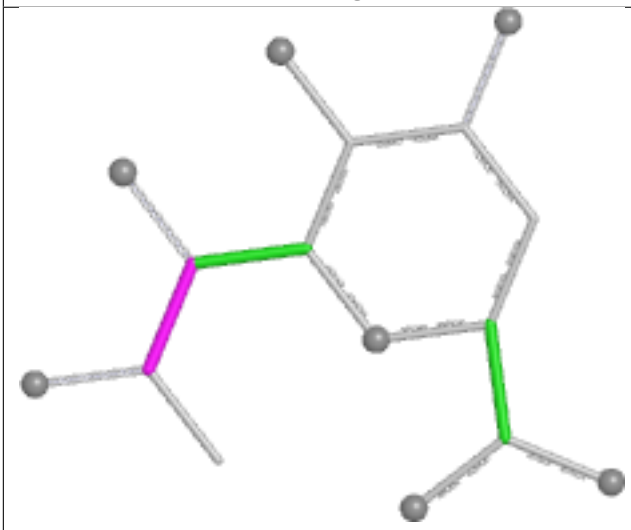
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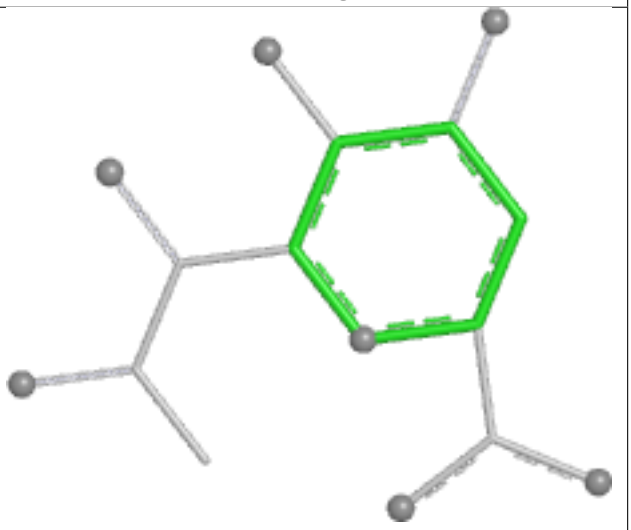
Bond lengths



Bond angles

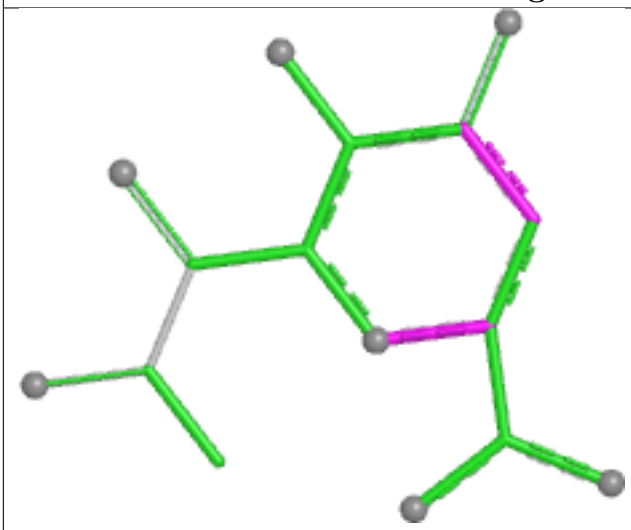


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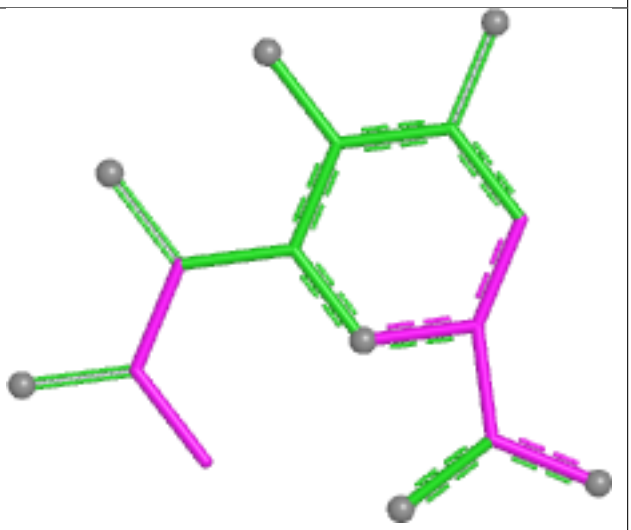


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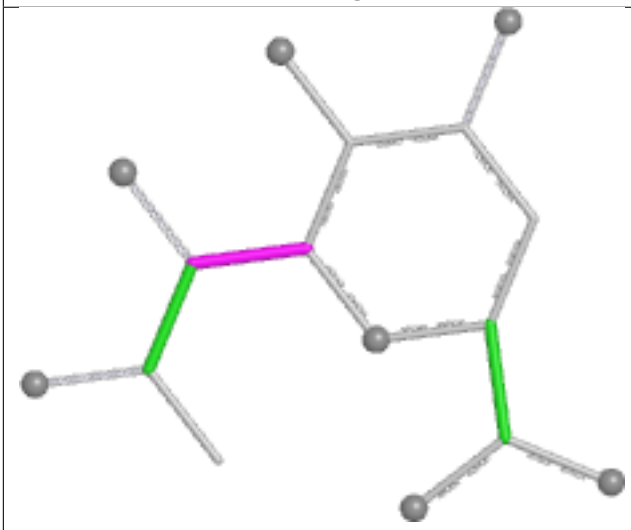
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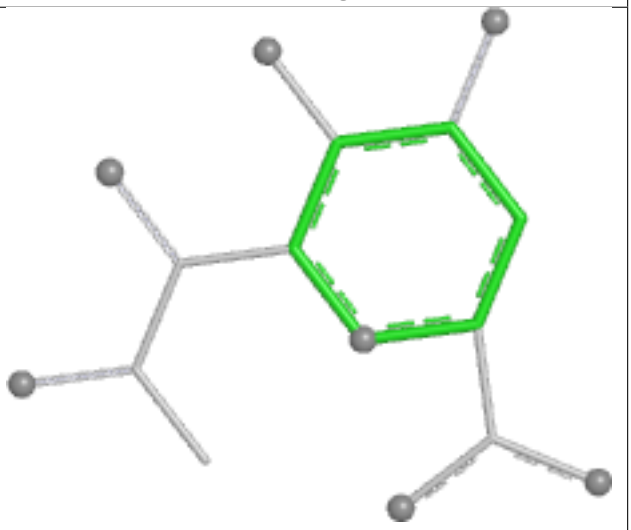
Bond lengths



Bond angles

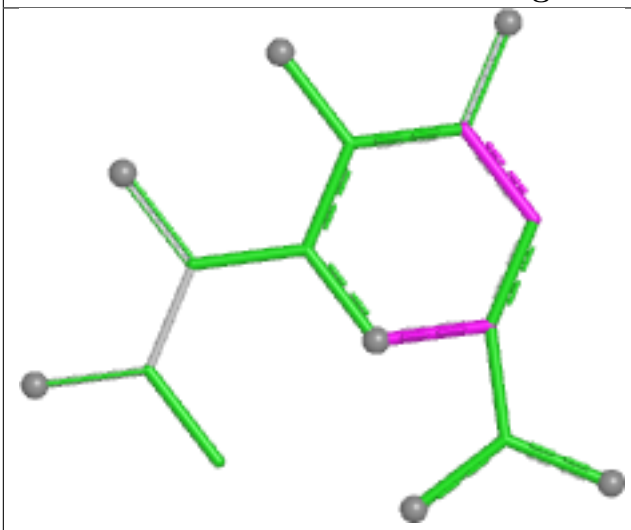


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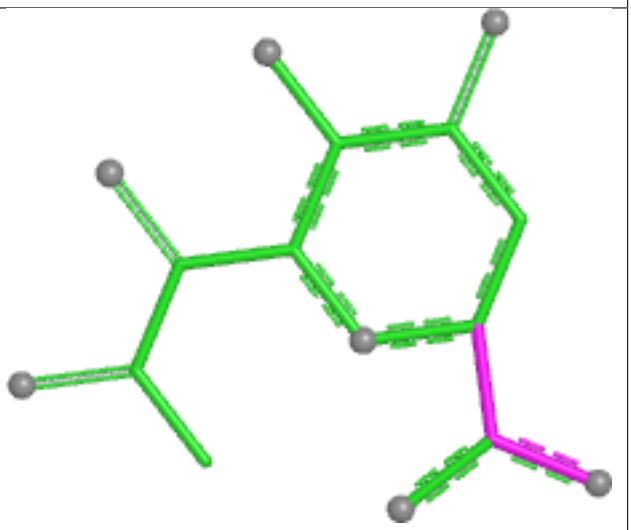


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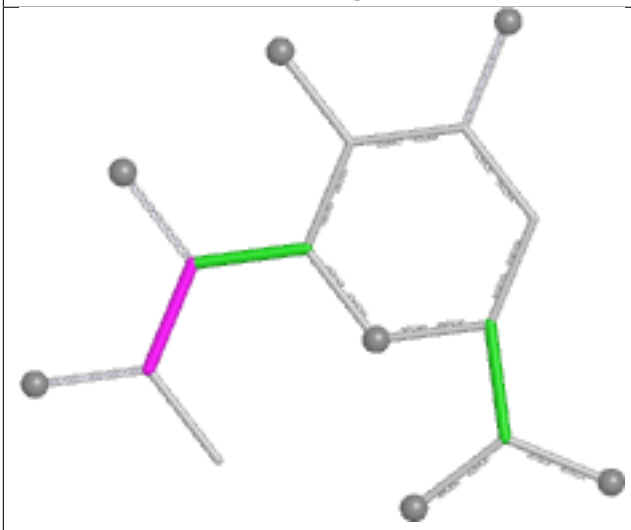
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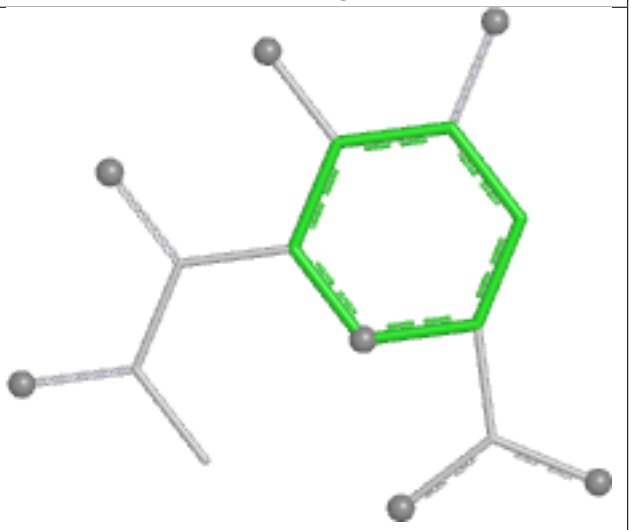
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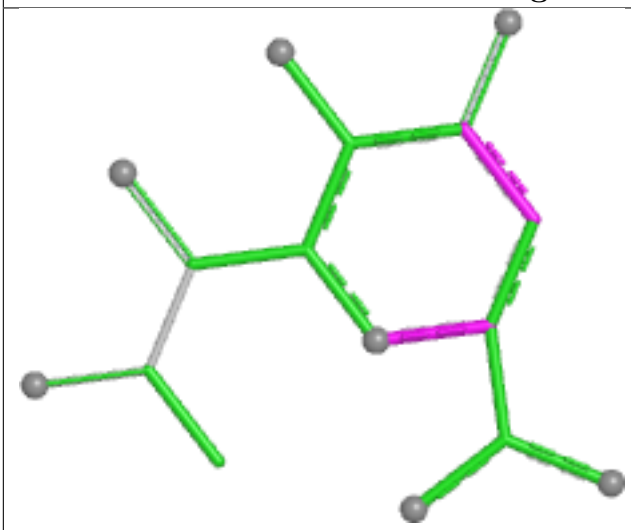


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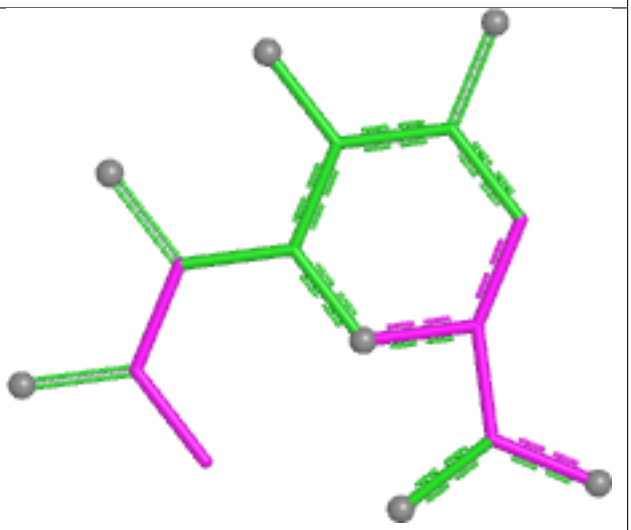


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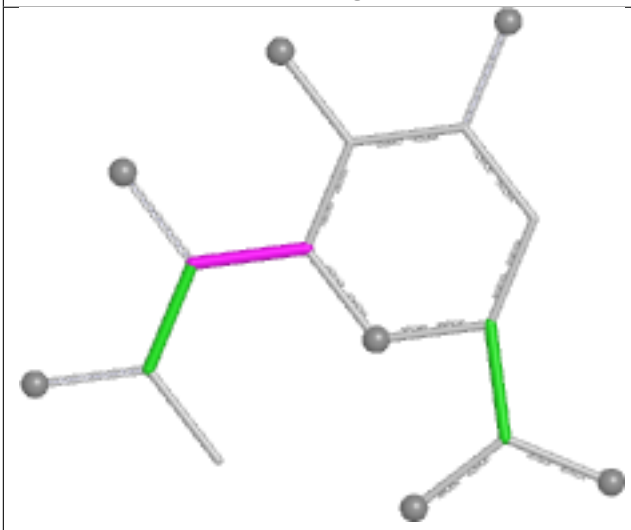
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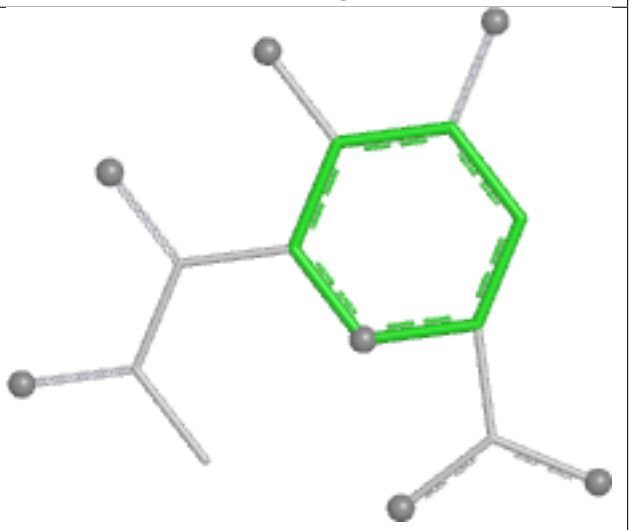
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Bond angles

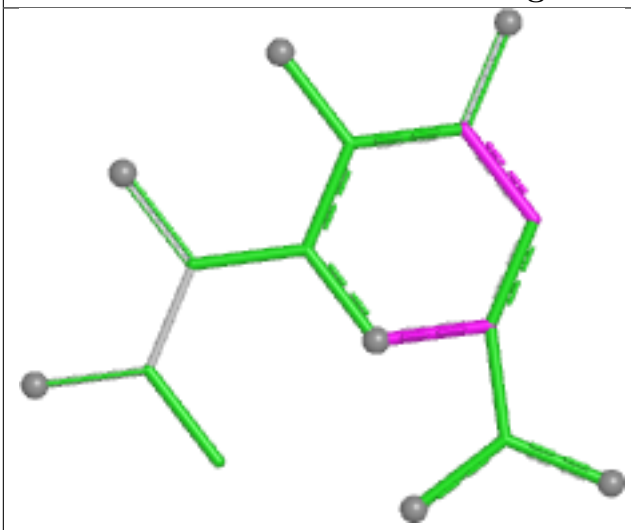


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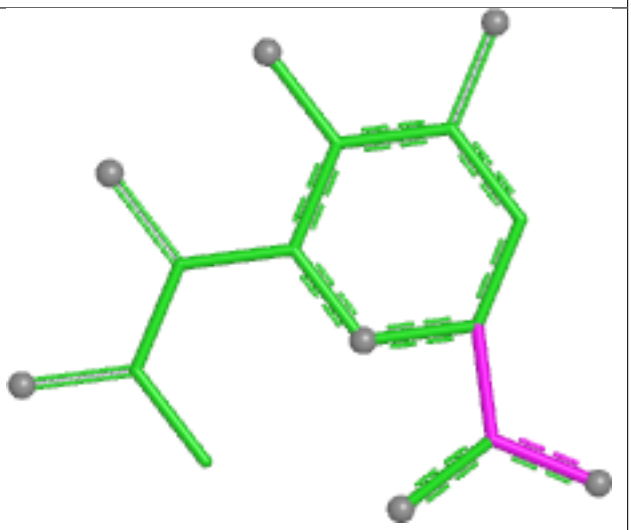


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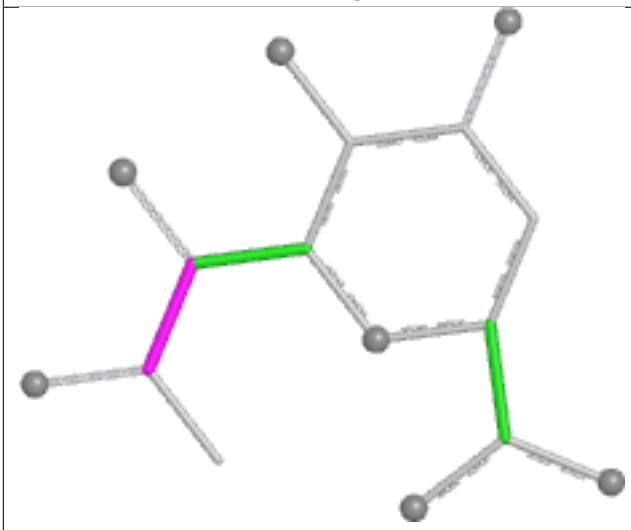
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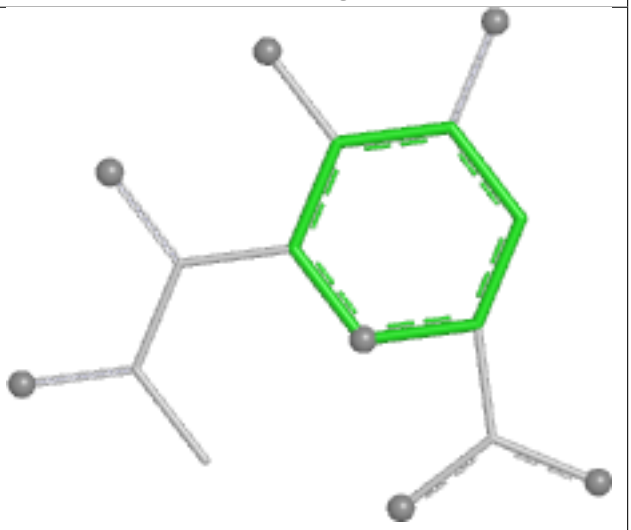
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Bond angles

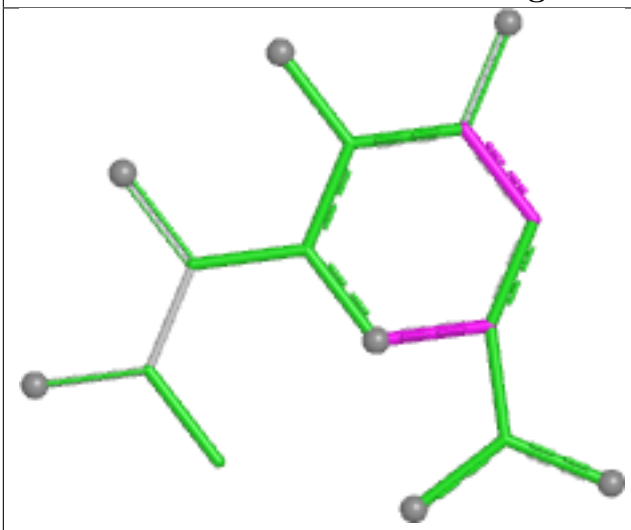


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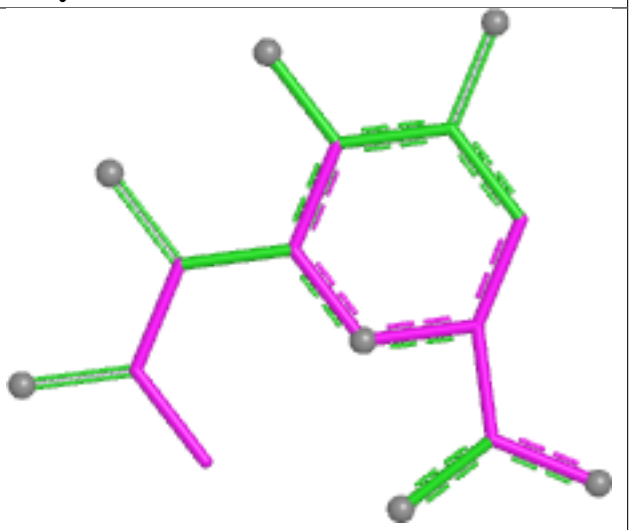


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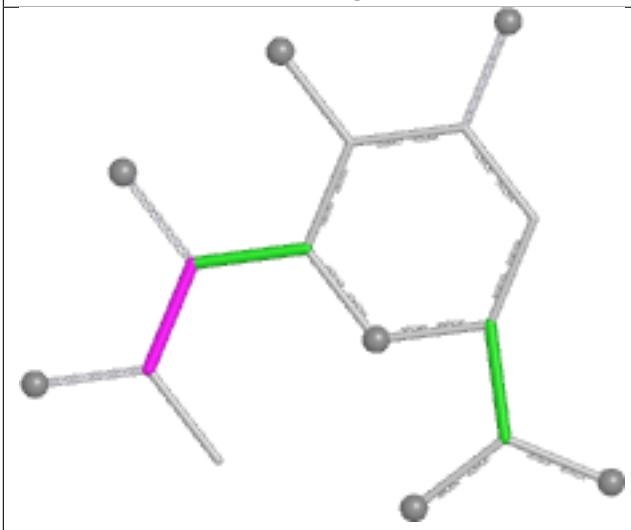
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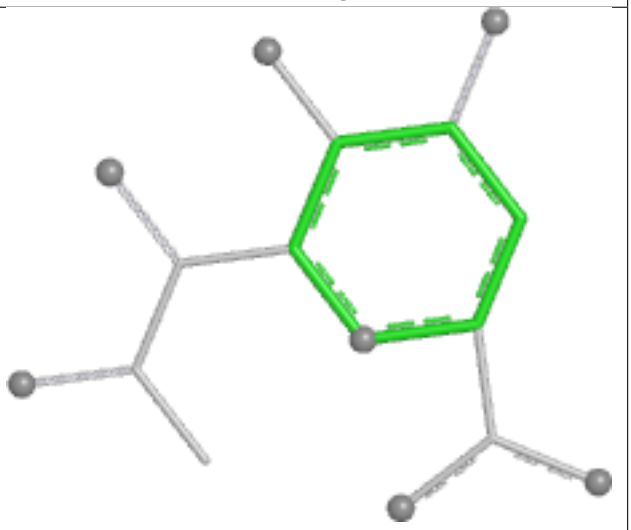
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Bond angles

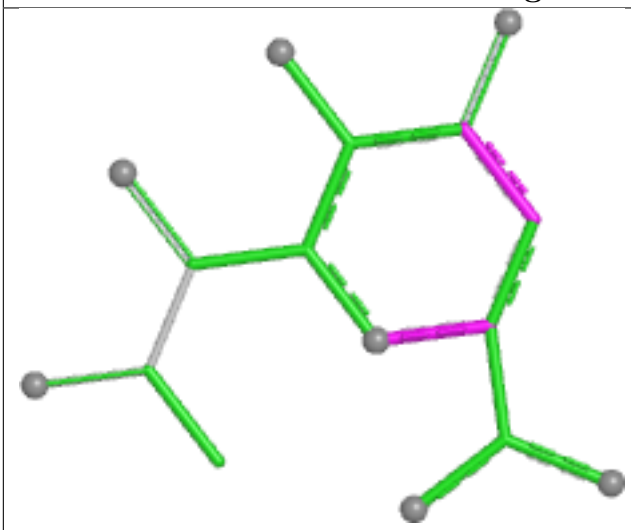


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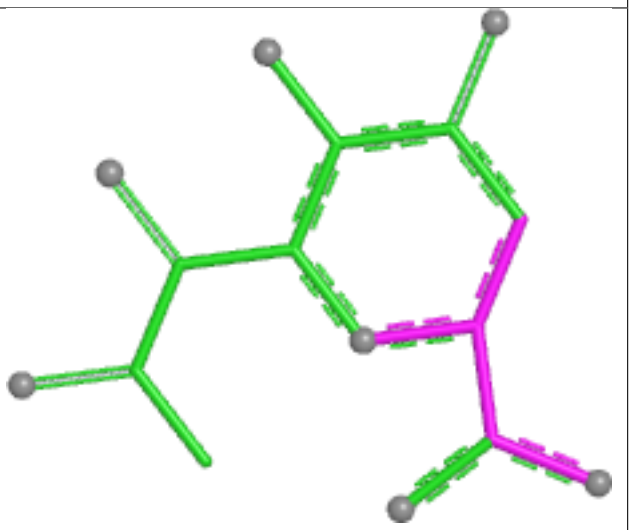


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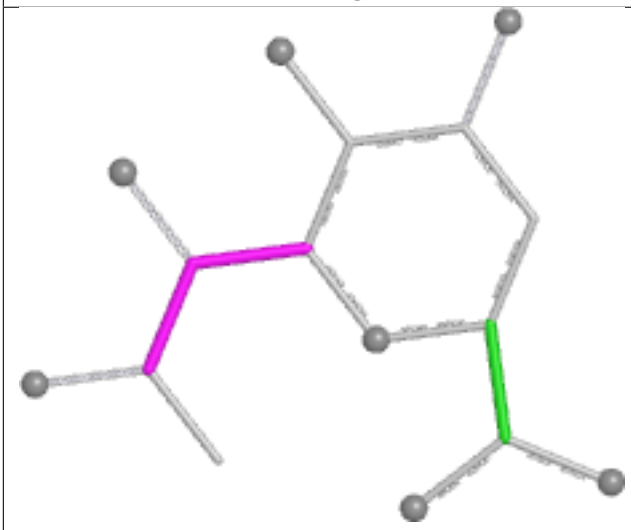
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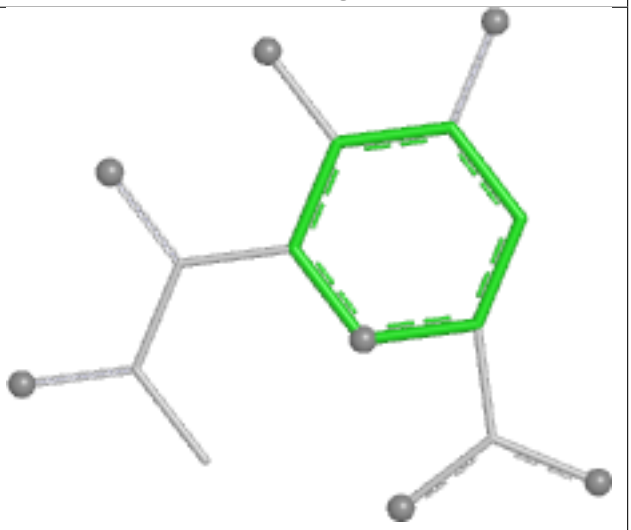
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Bond angles

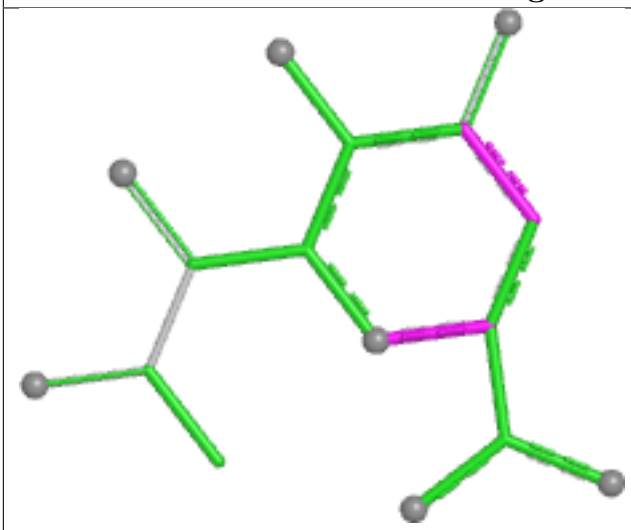


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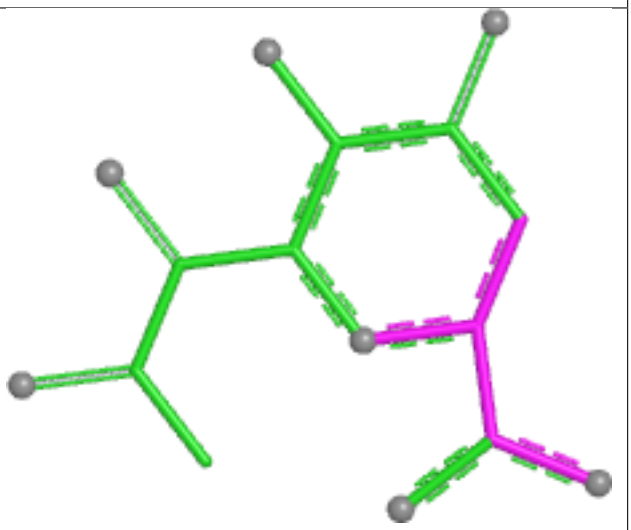


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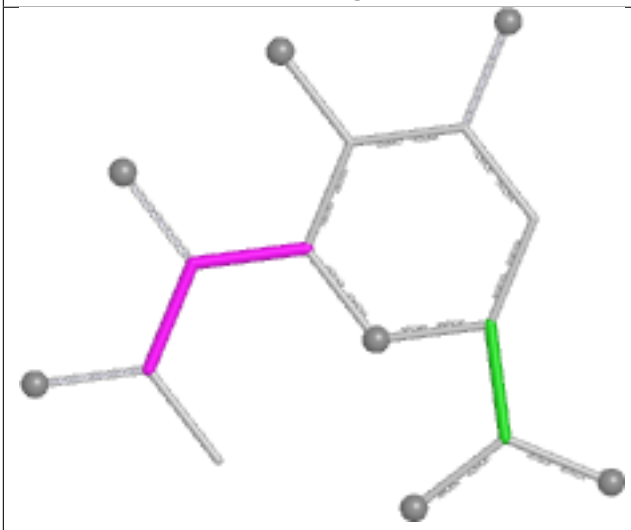
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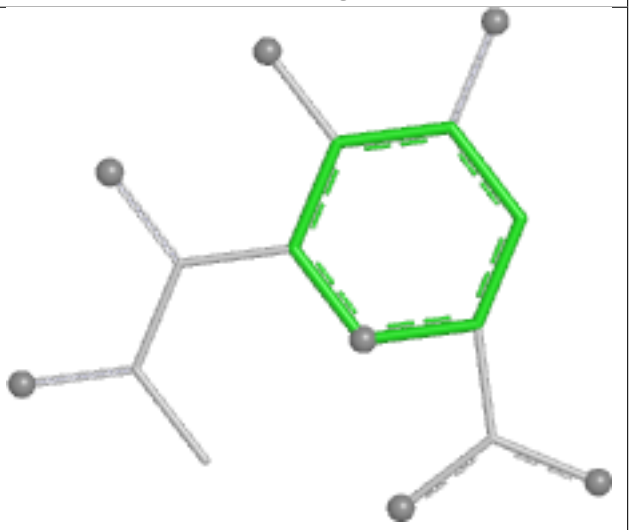
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Bond angles

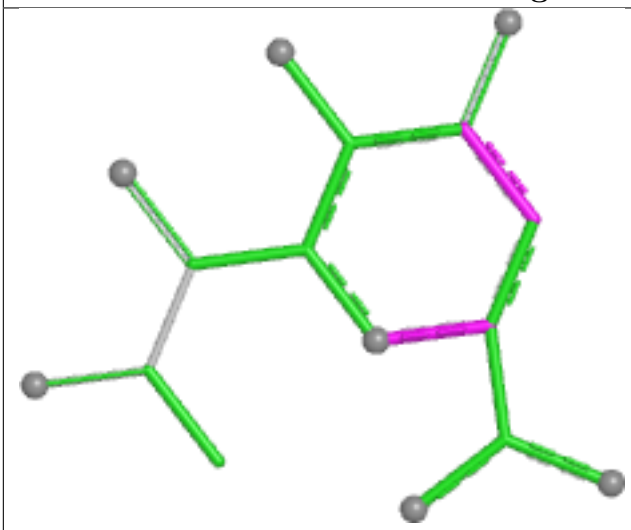


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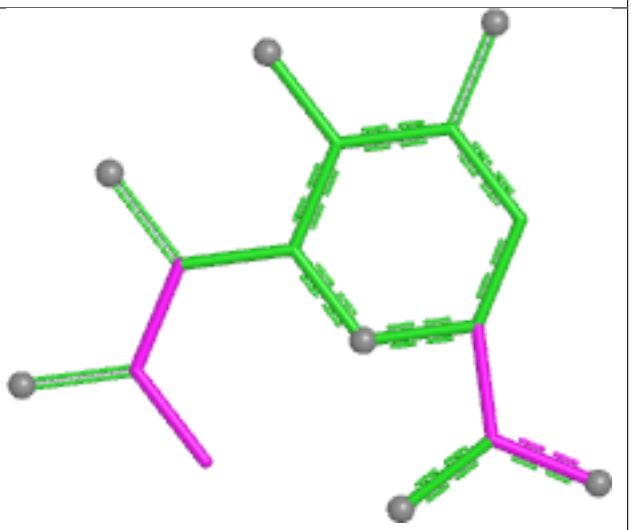


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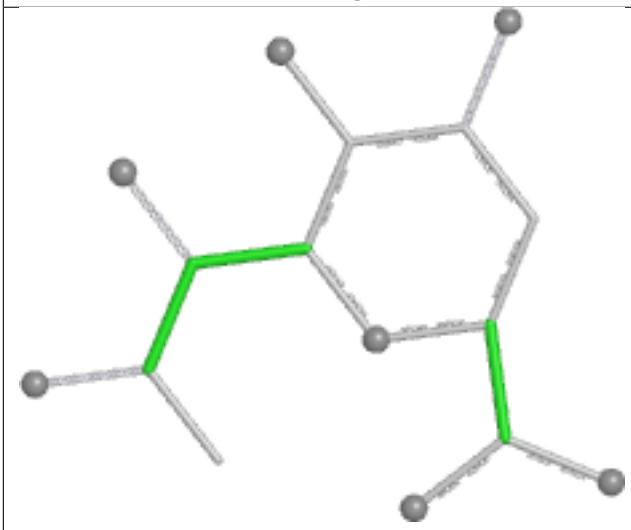
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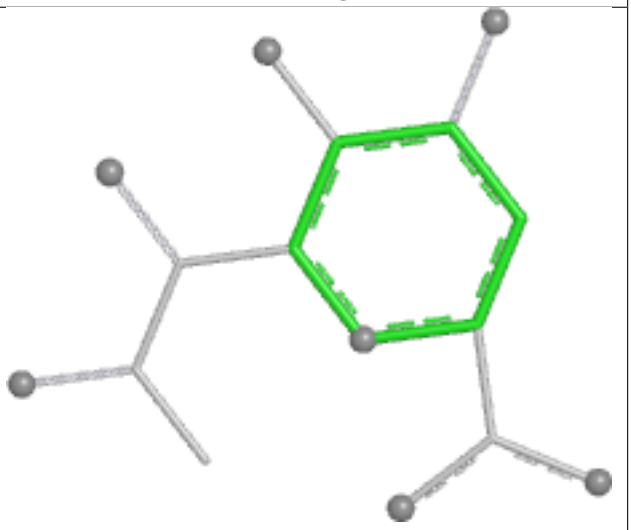
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Bond angles

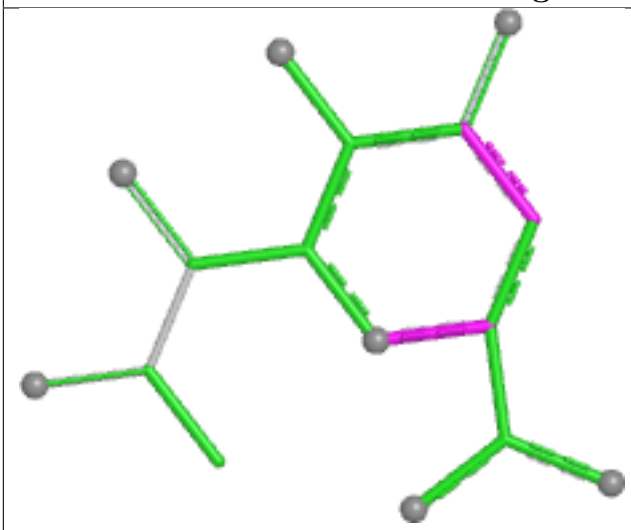


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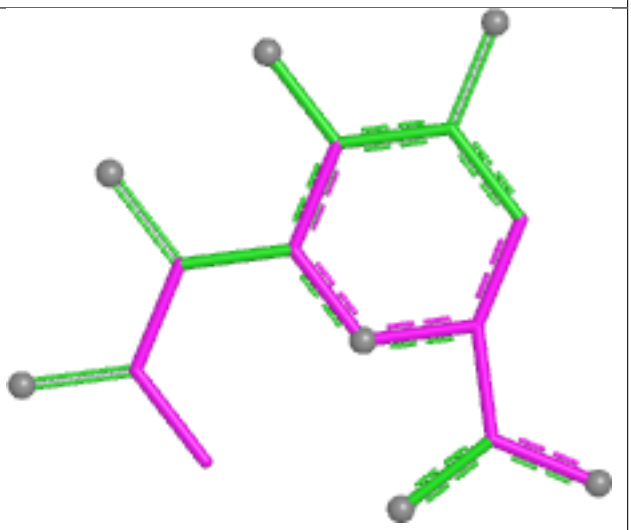


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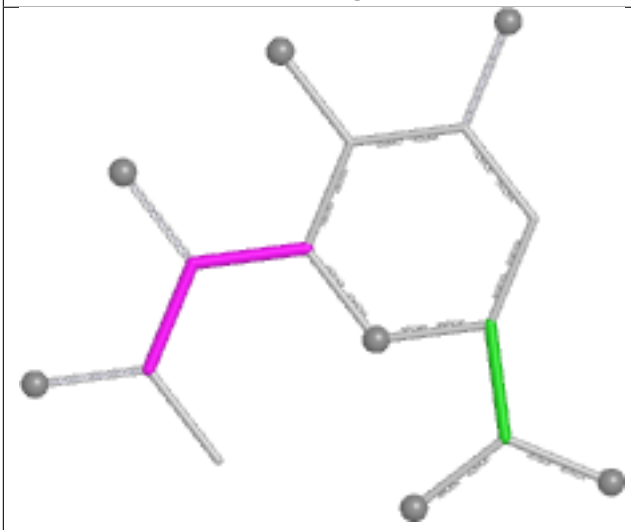
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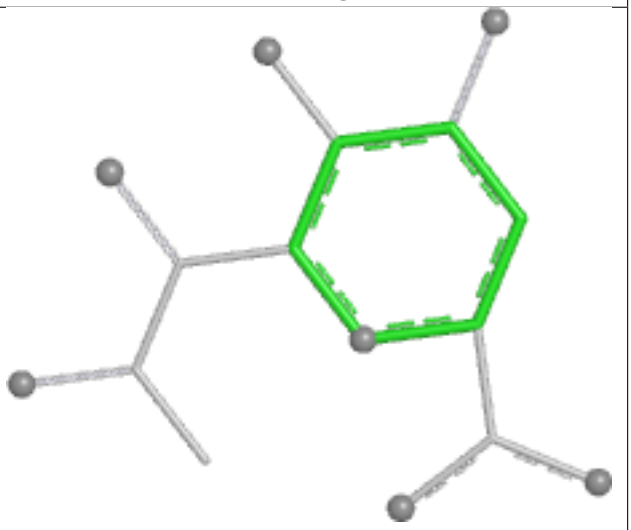
Bond lengths



Bond angles

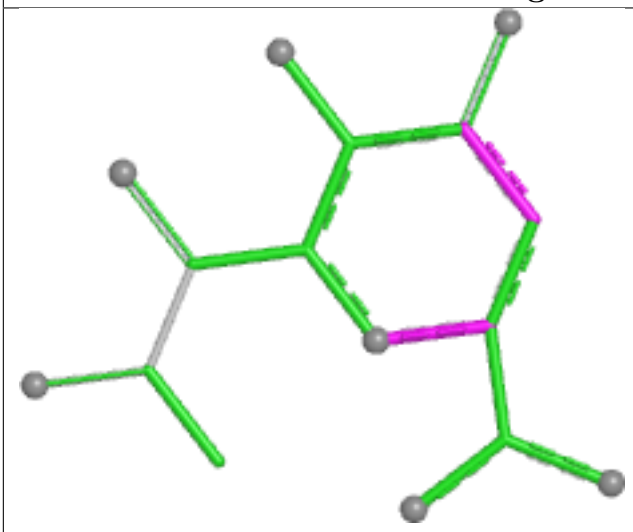


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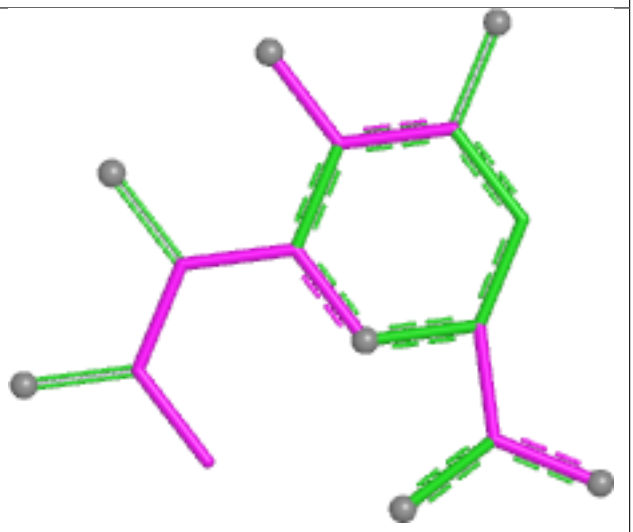


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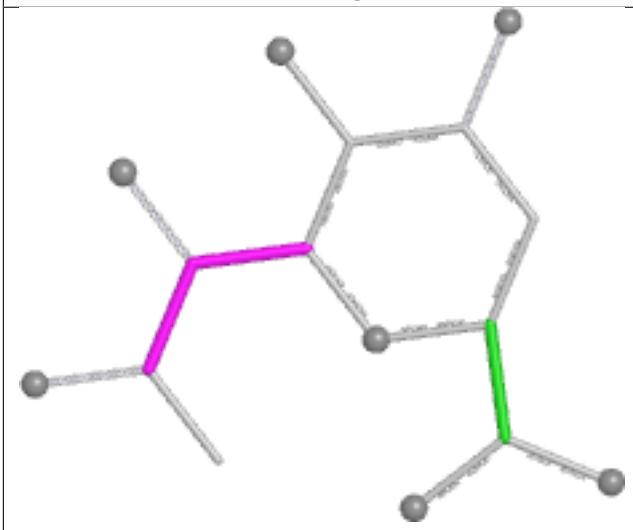
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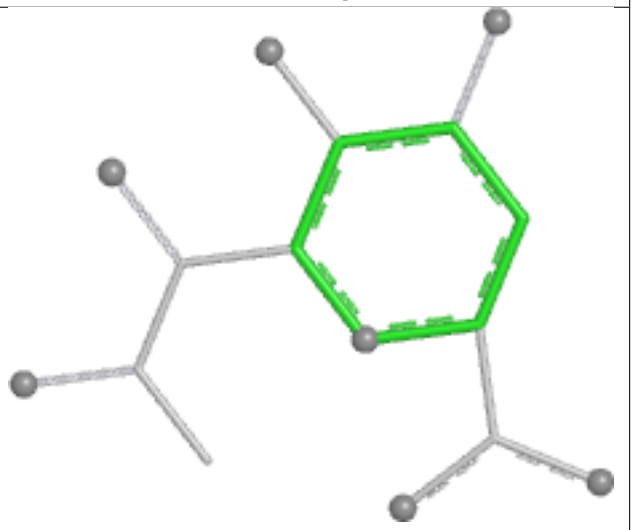
Bond lengths



Bond angles

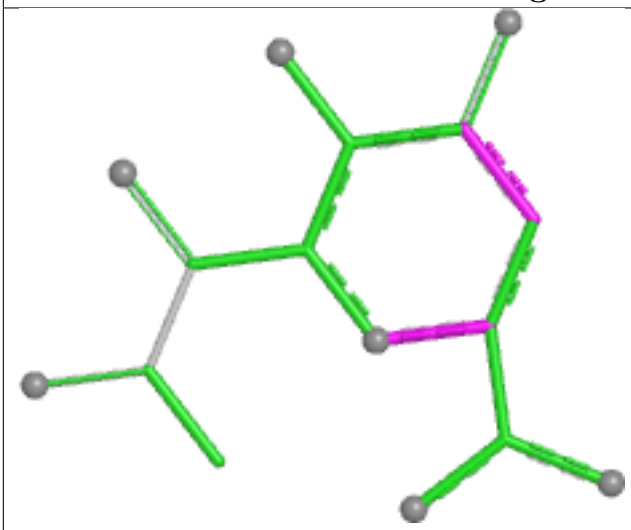


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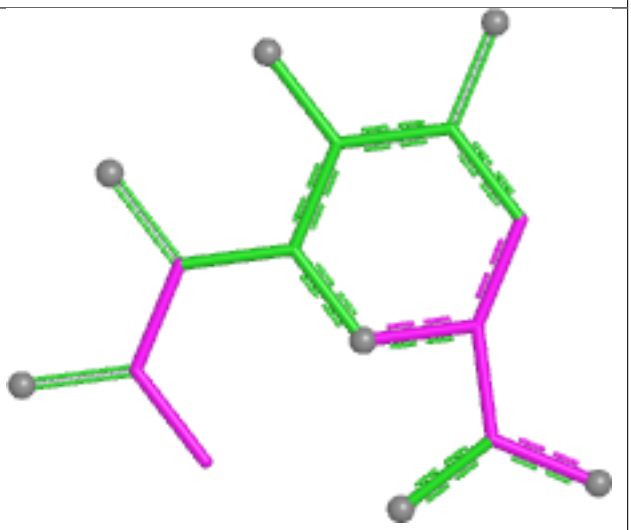


Rings

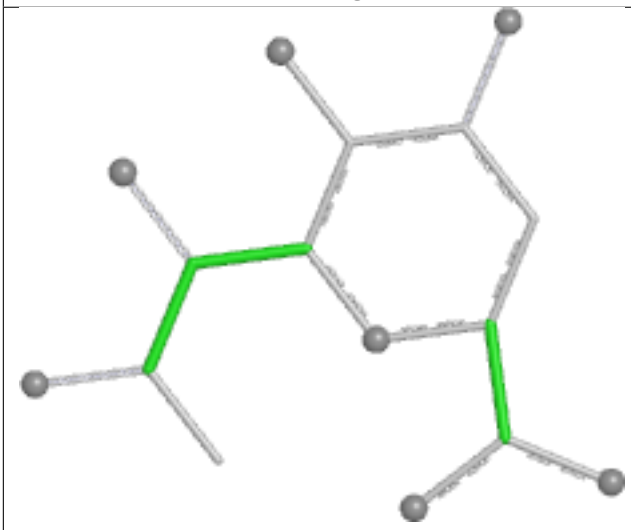
Ligand P8E E 603



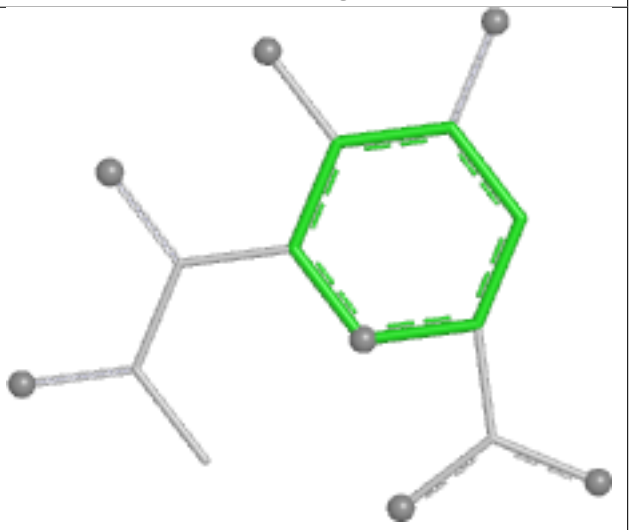
Bond lengths



Bond angles

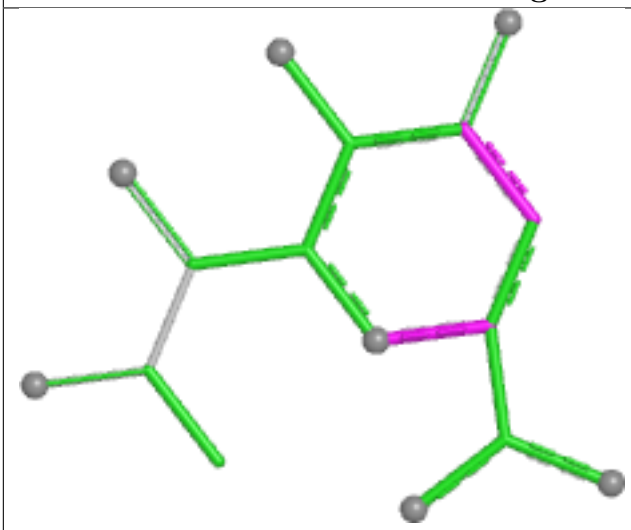


Torsions

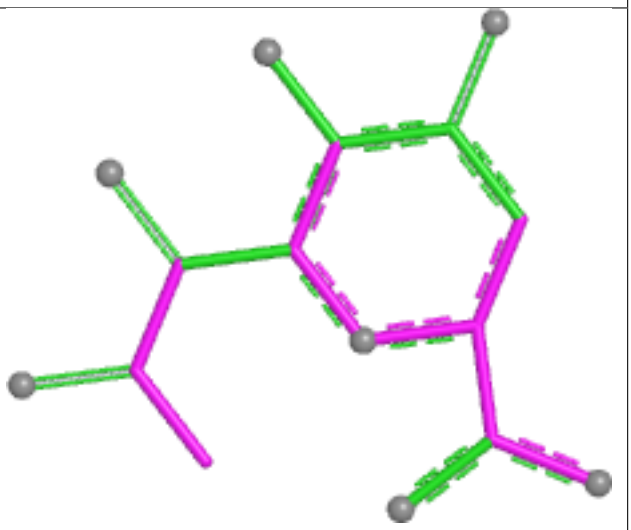


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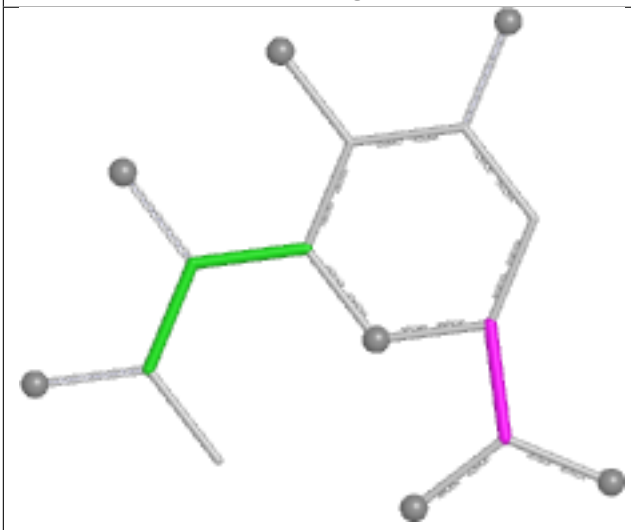
Ligand P8E F 617



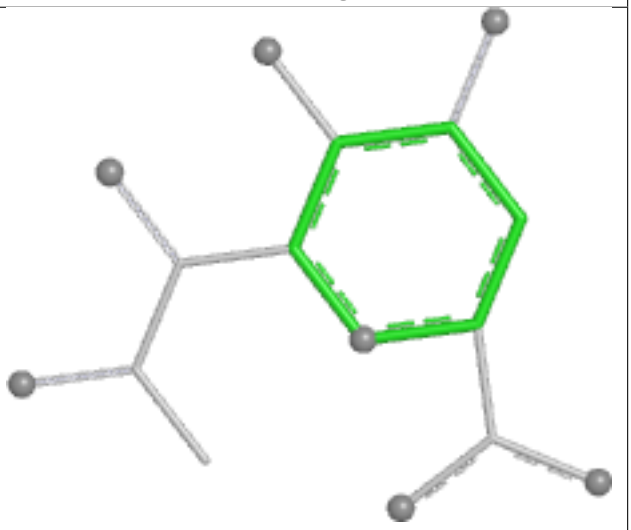
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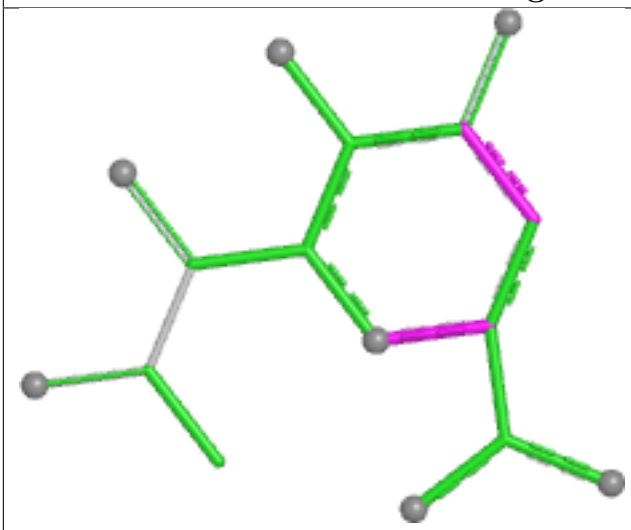


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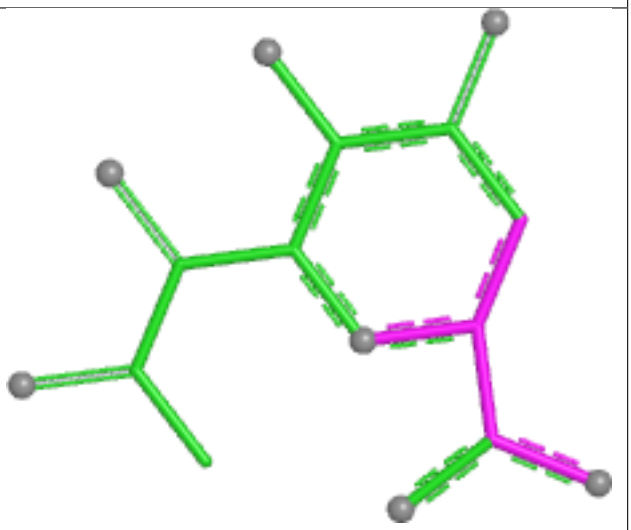


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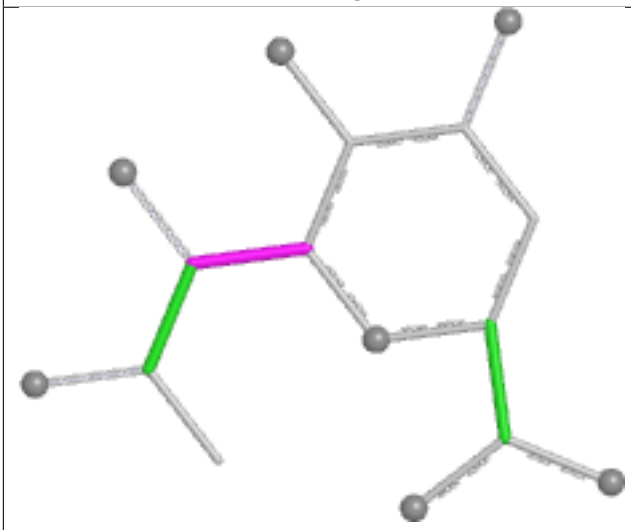
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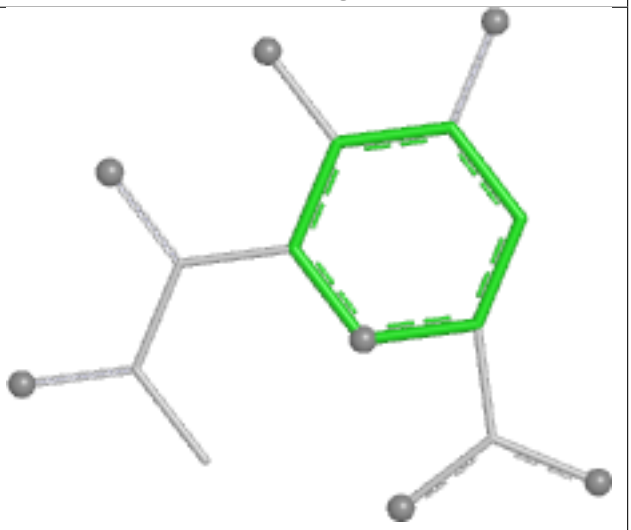
Bond lengths



Bond angles

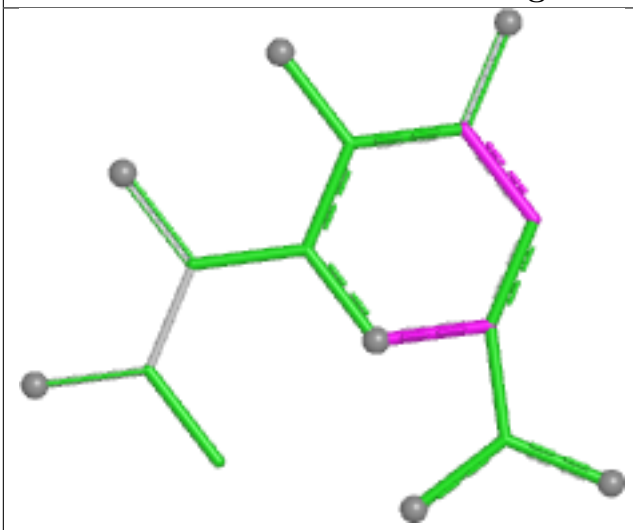


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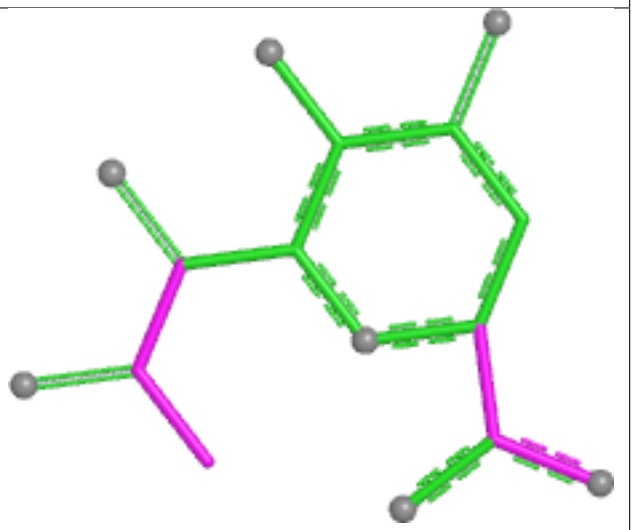


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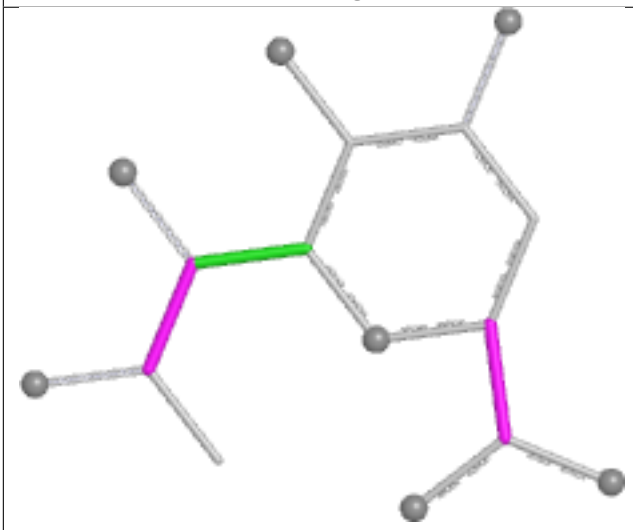
Ligand P8E A 611



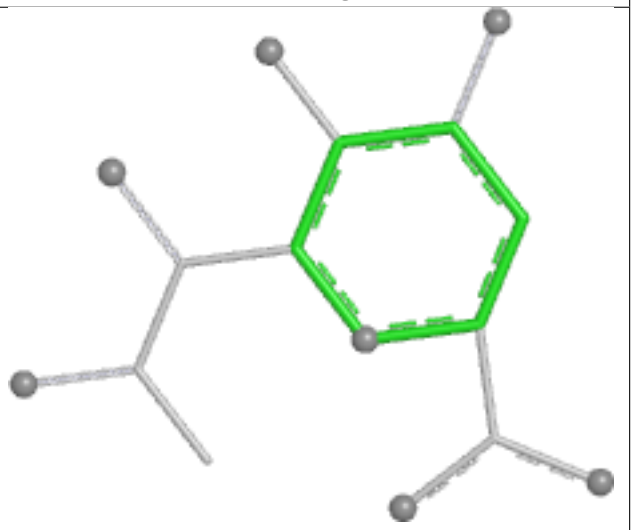
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Bond angles

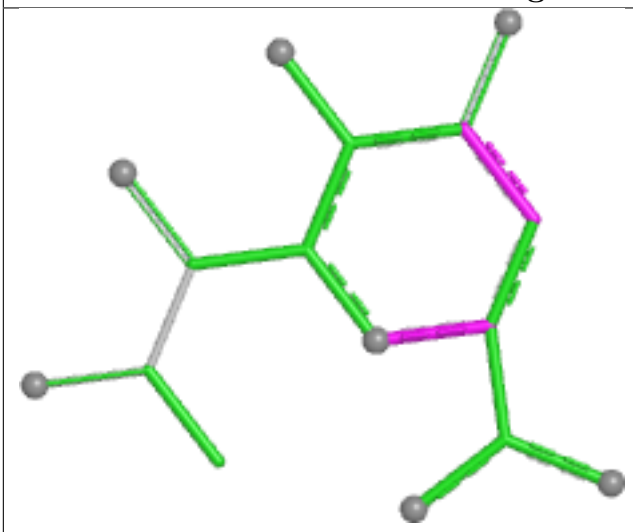


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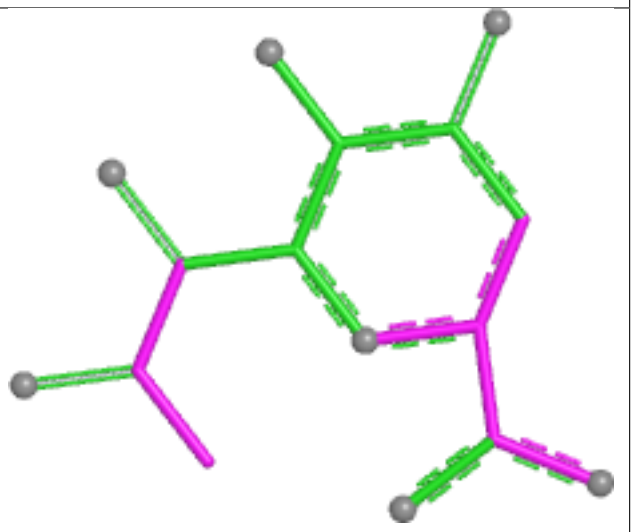


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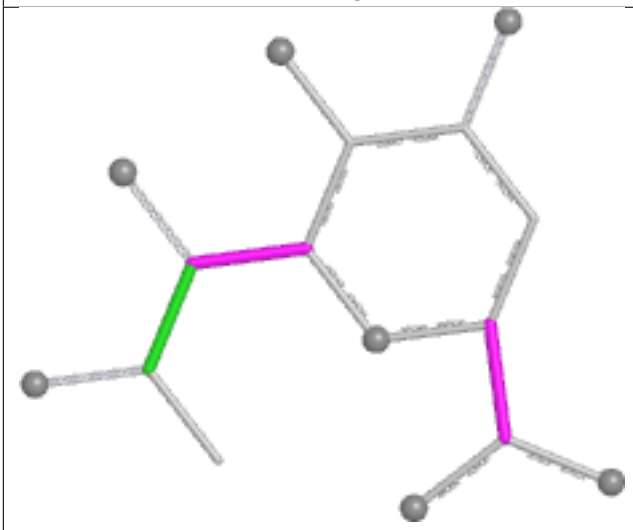
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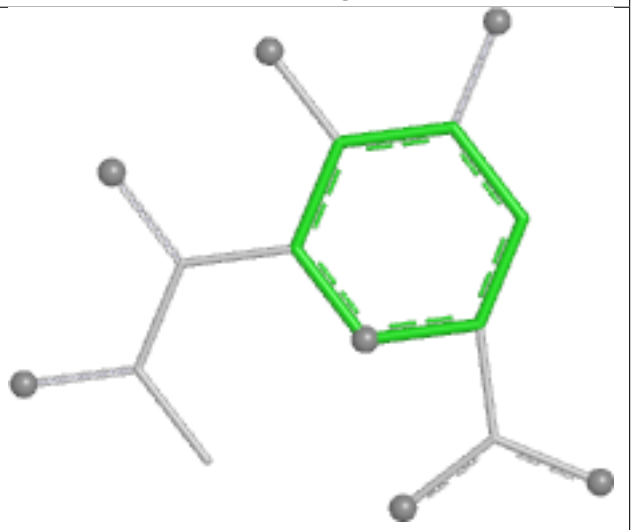
Bond lengths



Bond angles

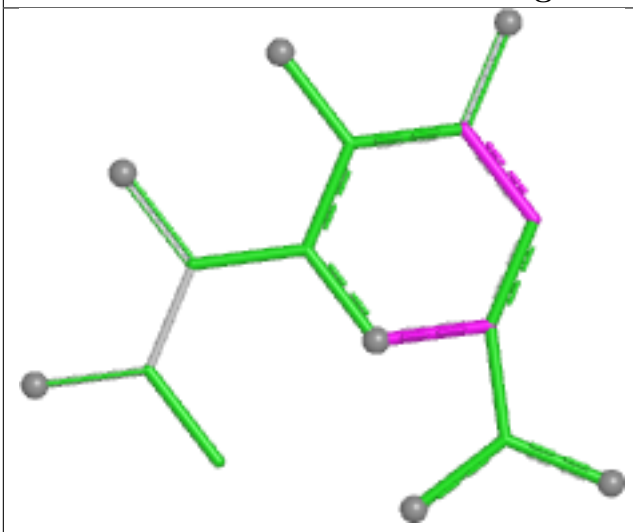


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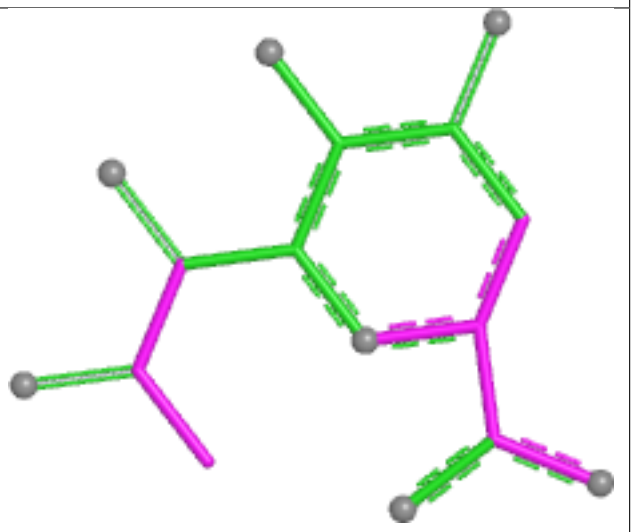


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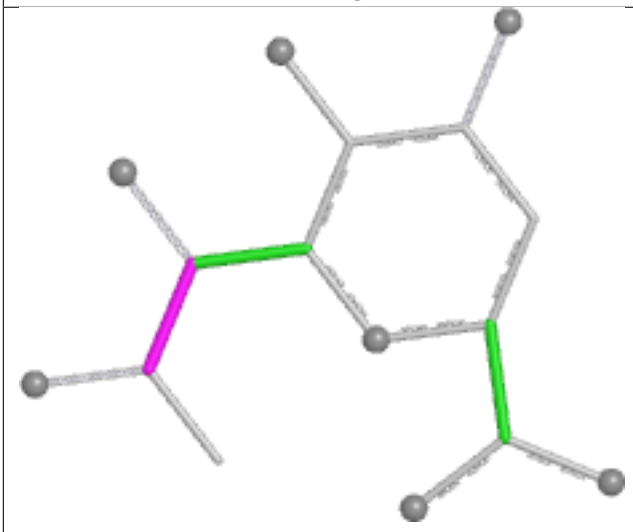
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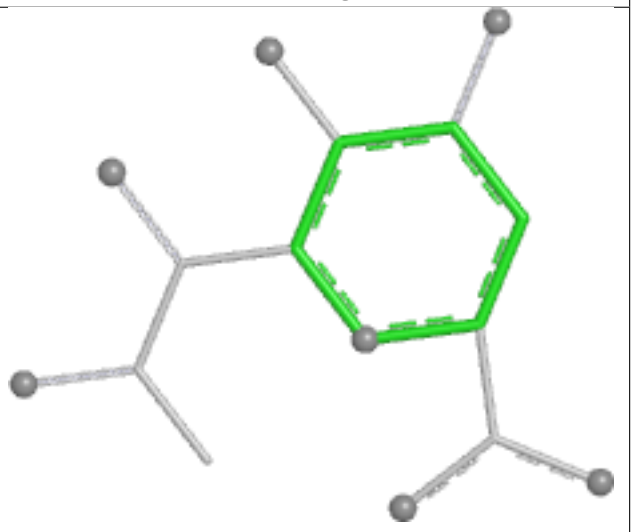
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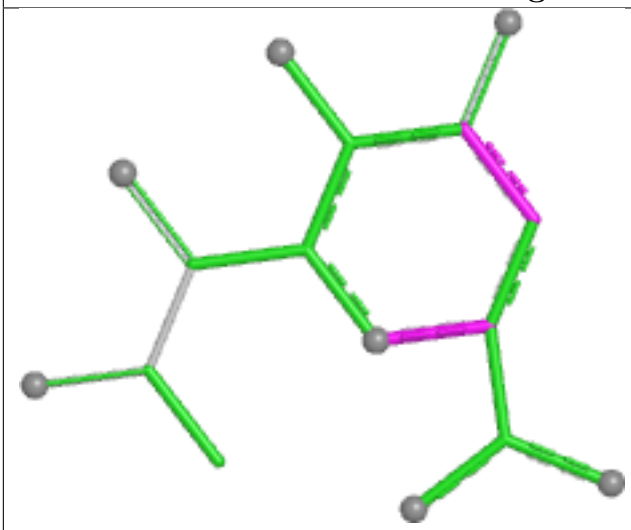


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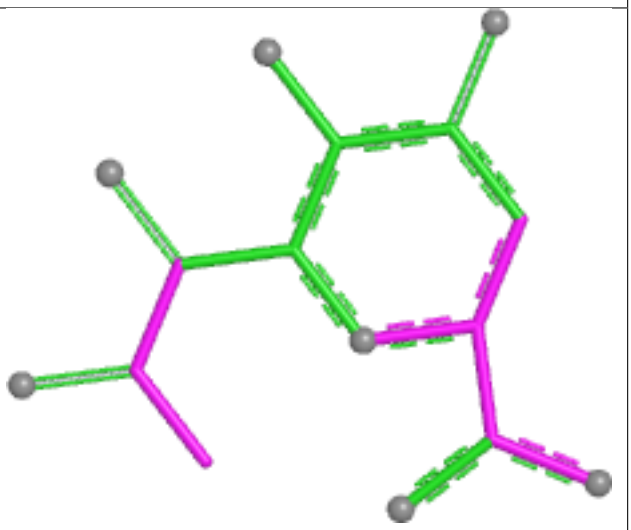


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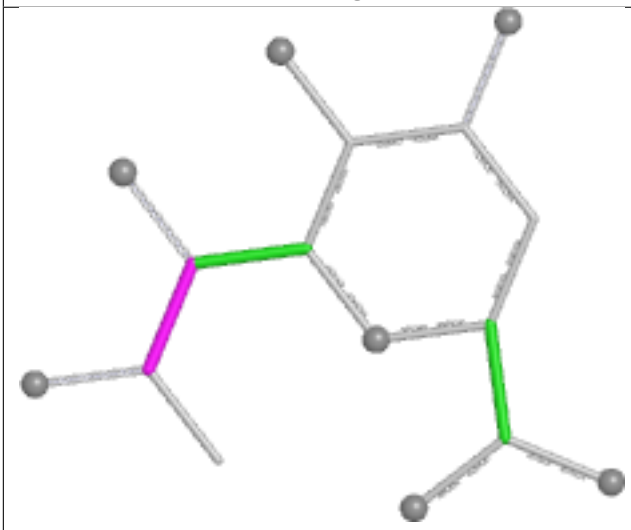
Ligand P8E O 615



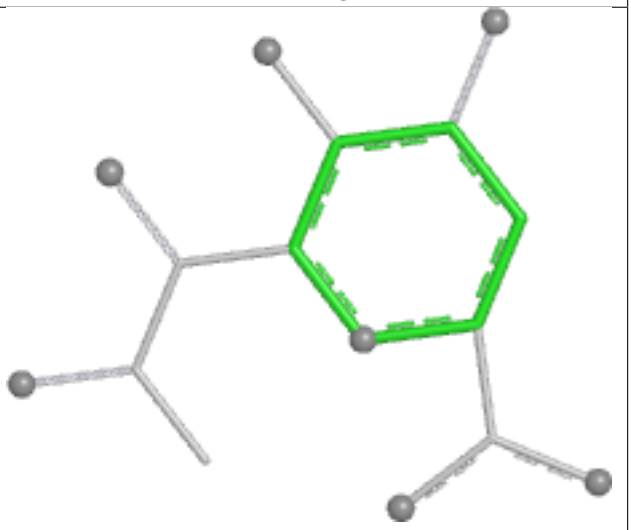
Bond lengths



Bond angles

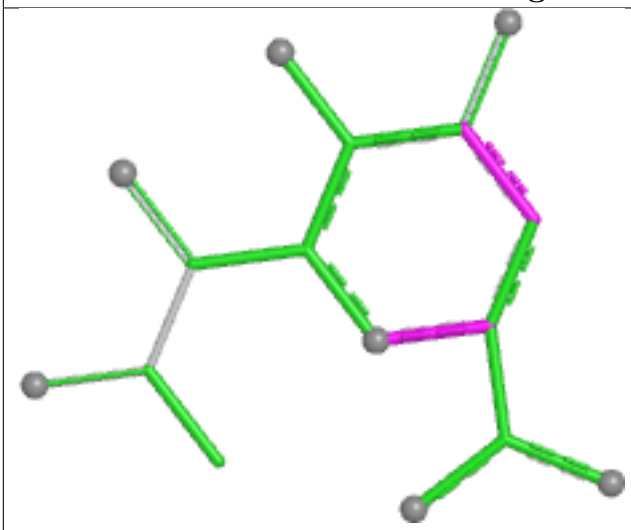


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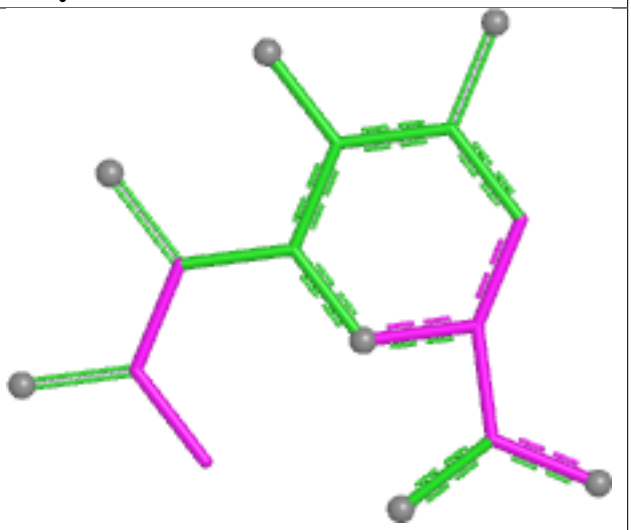


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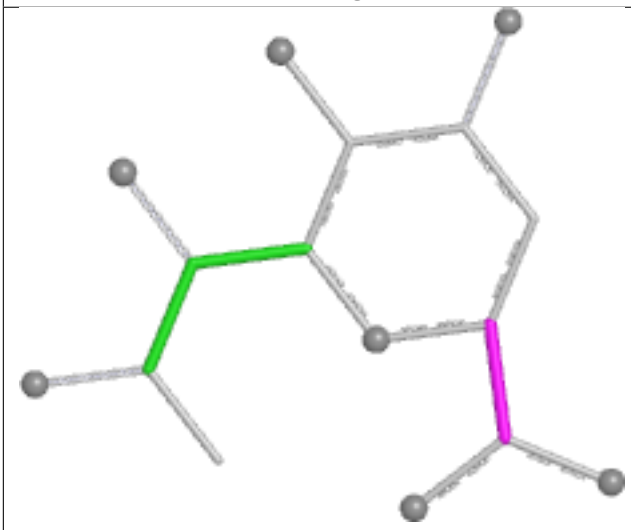
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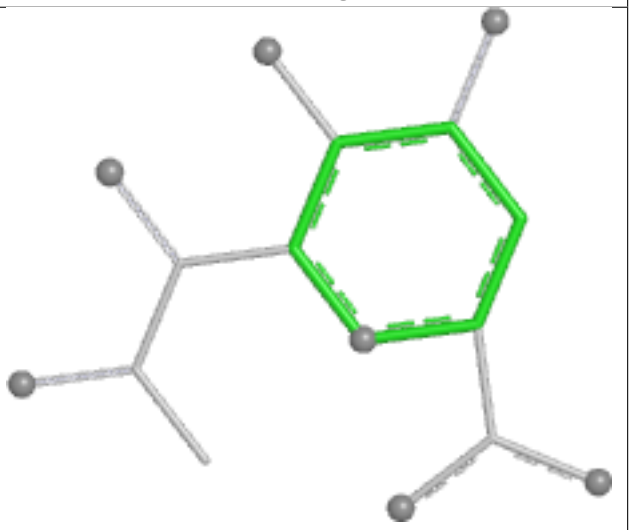
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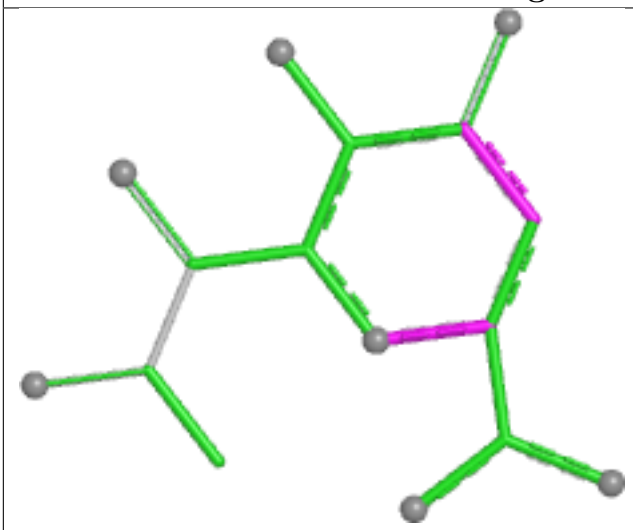


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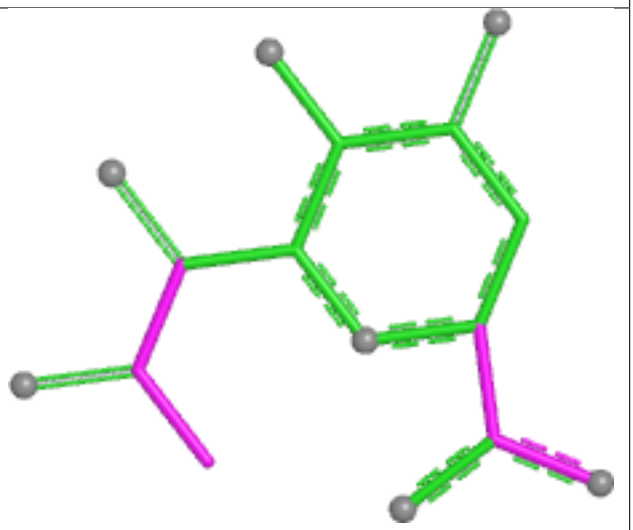


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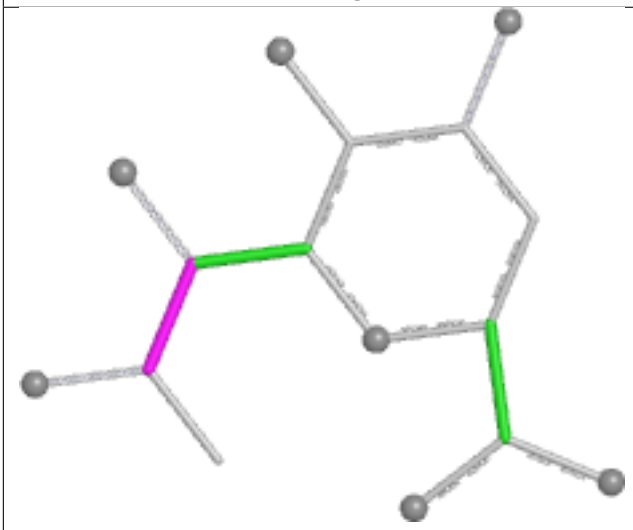
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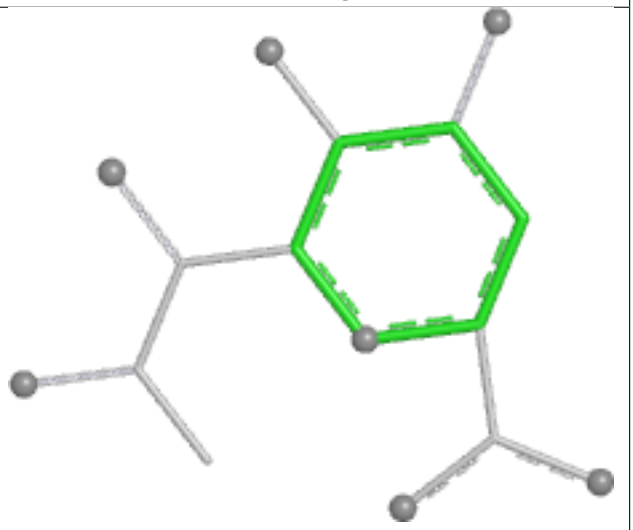
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Bond angles

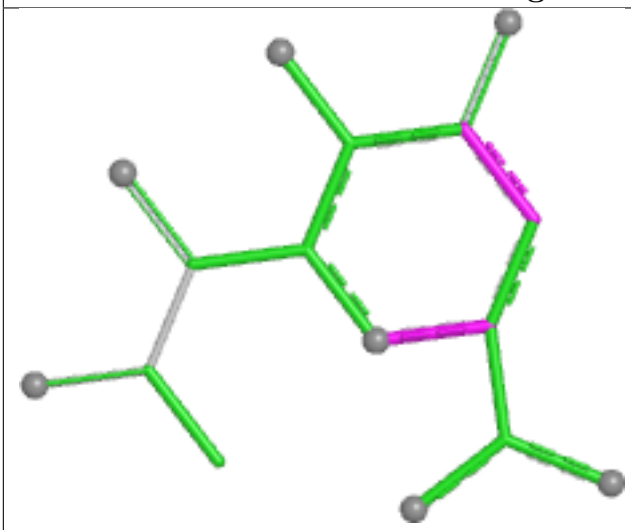


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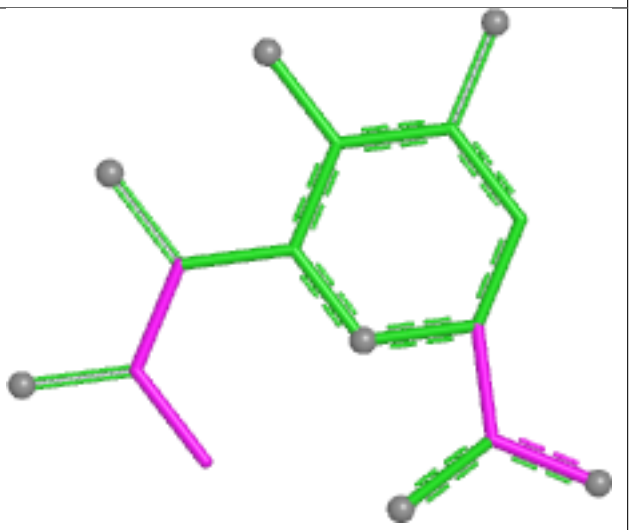


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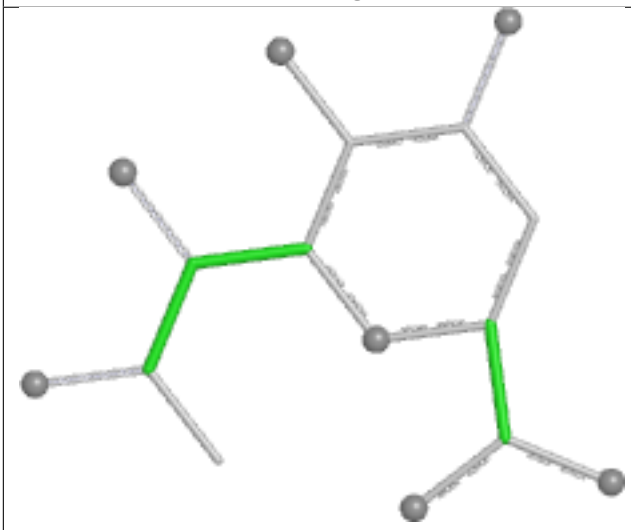
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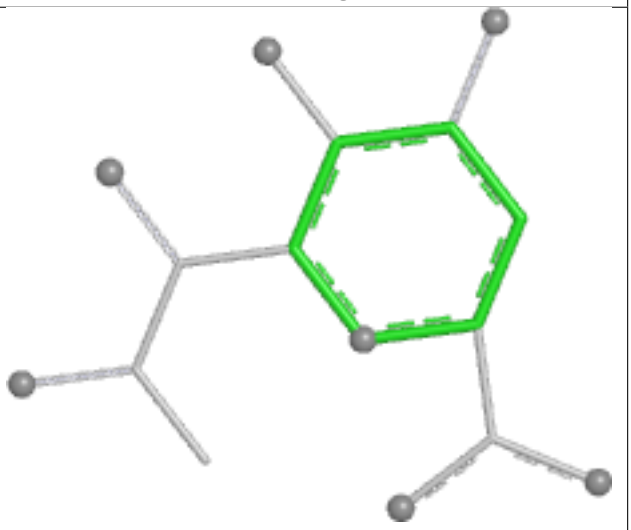
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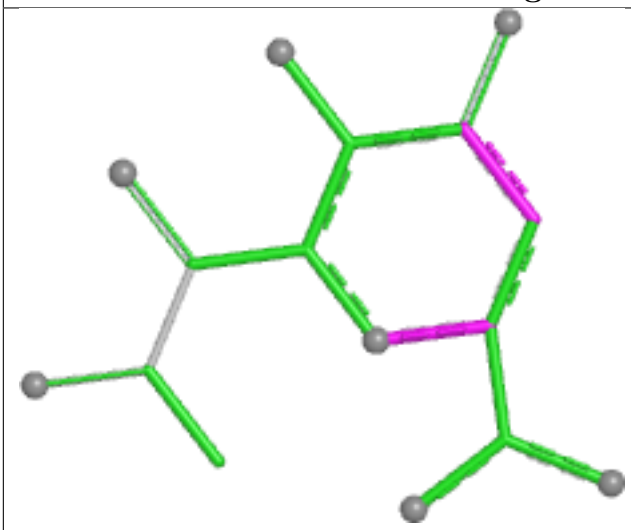


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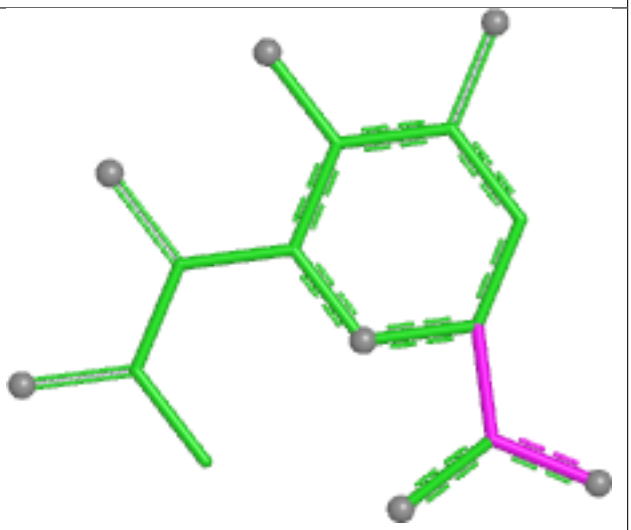


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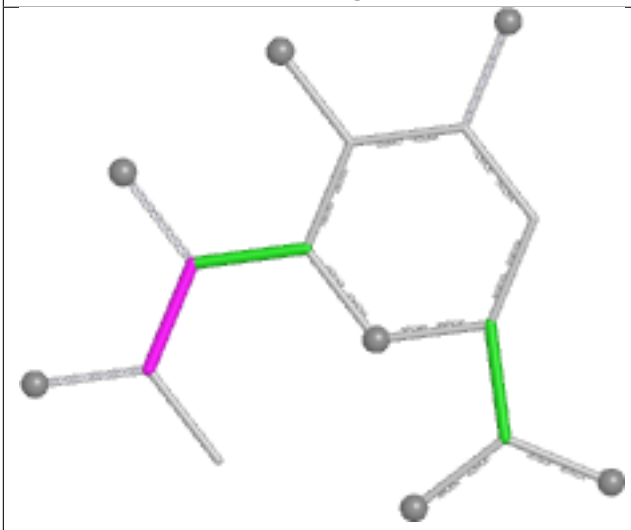
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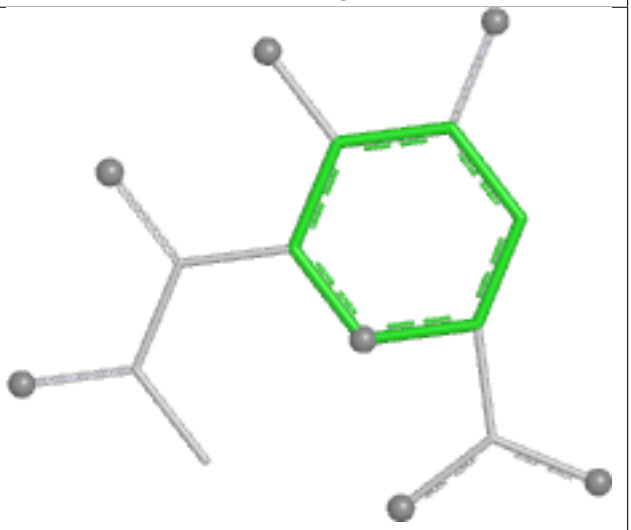
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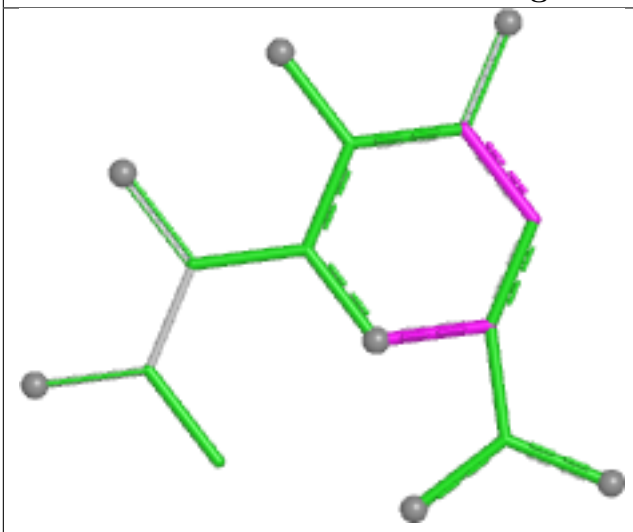


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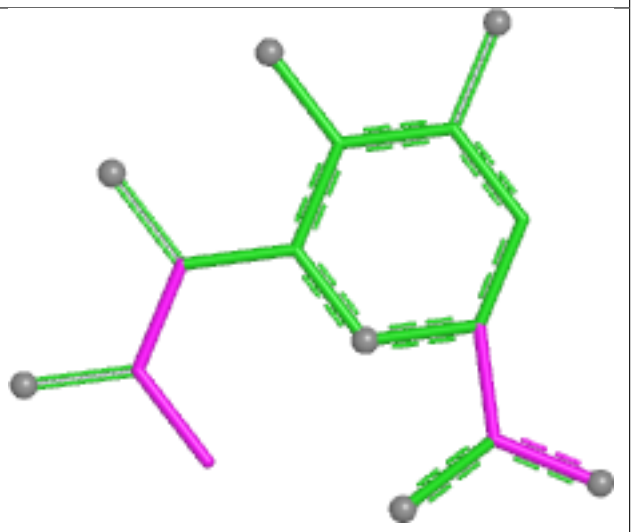


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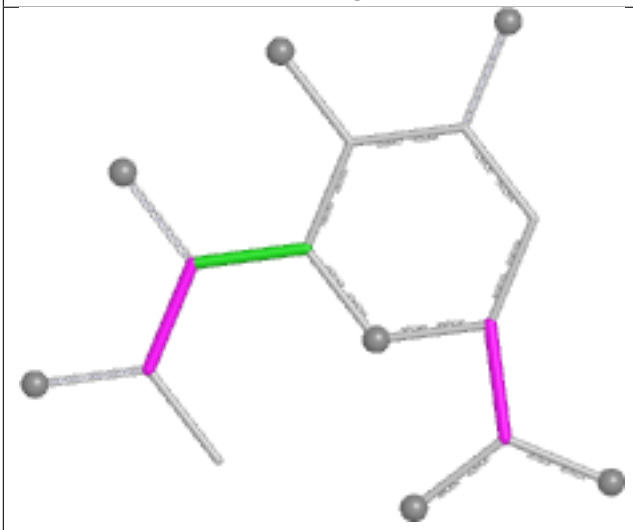
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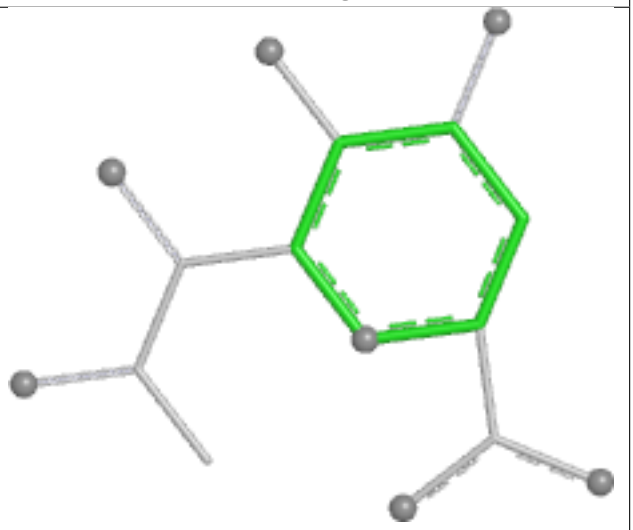
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Bond angles

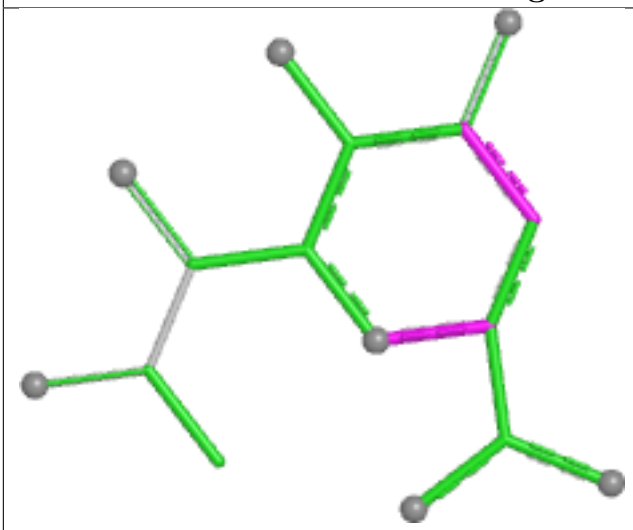


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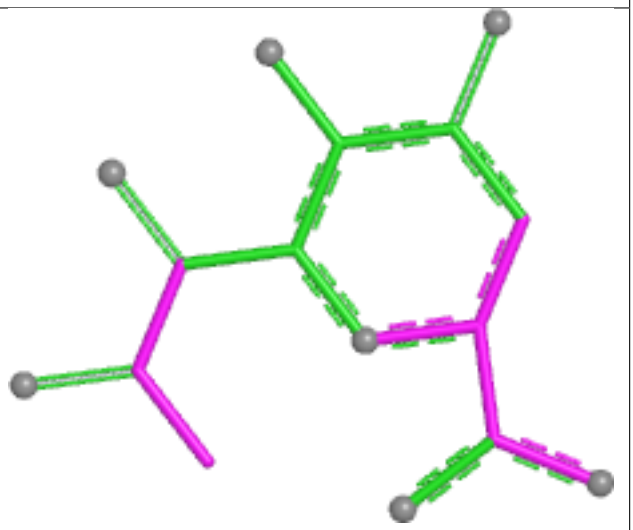


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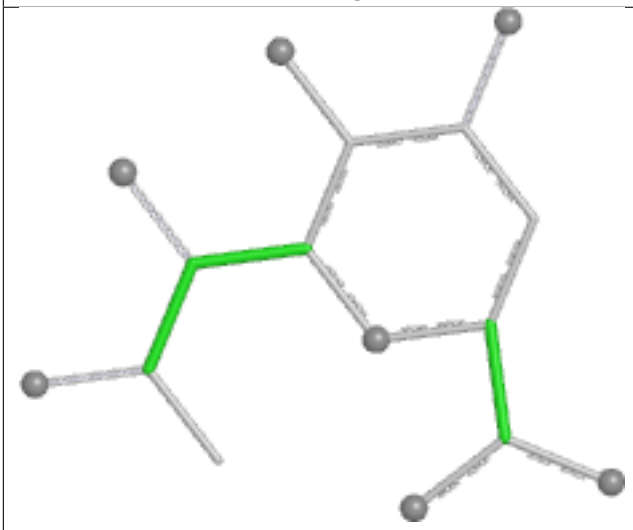
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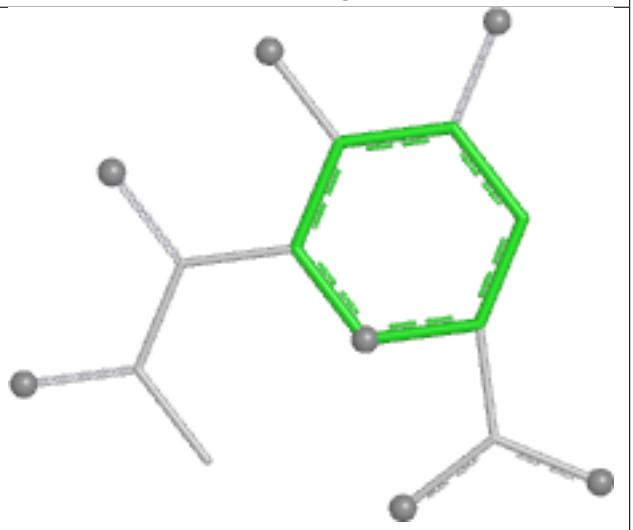
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Bond angles

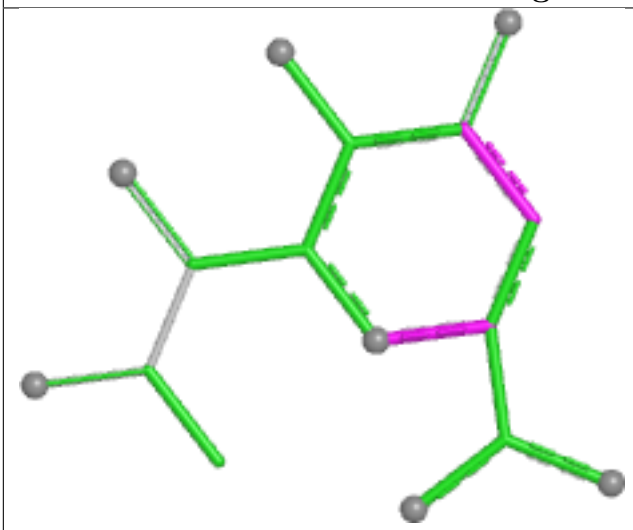


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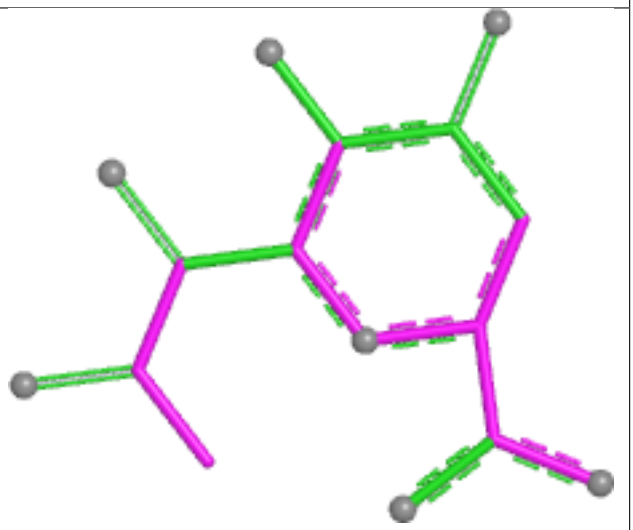


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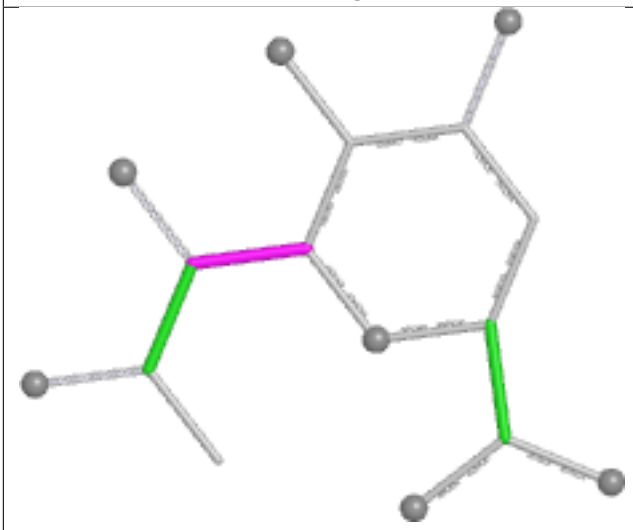
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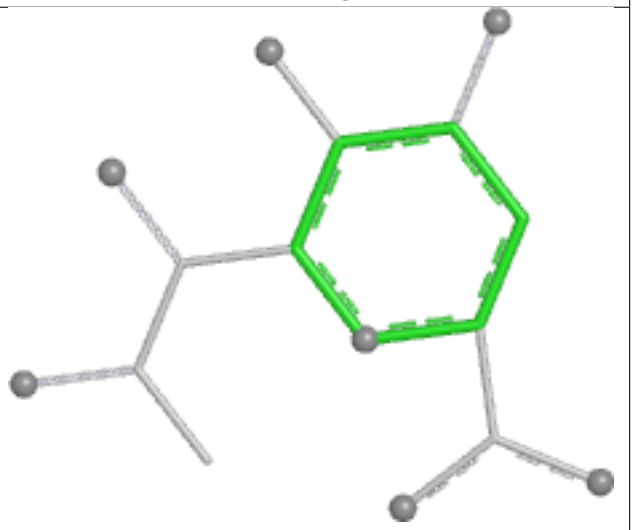
Bond lengths



Bond angles

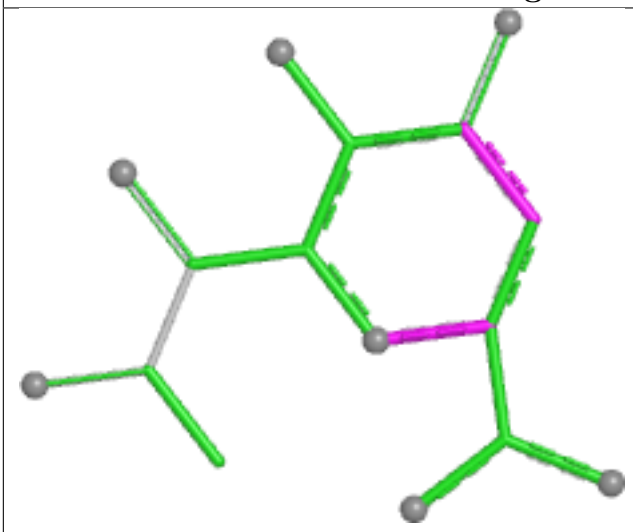


Torsions

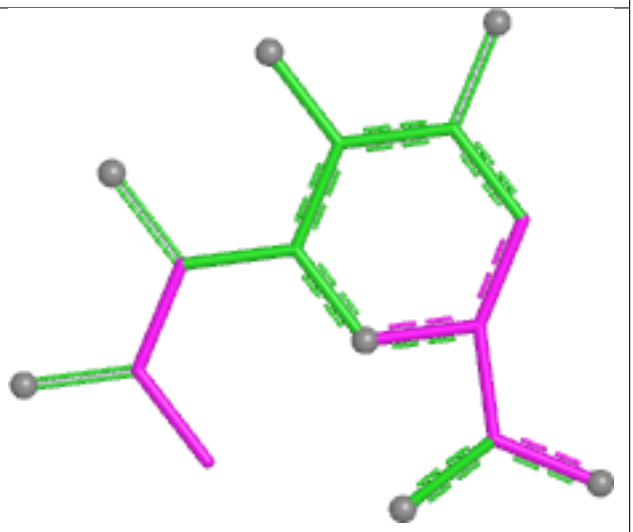


Rings

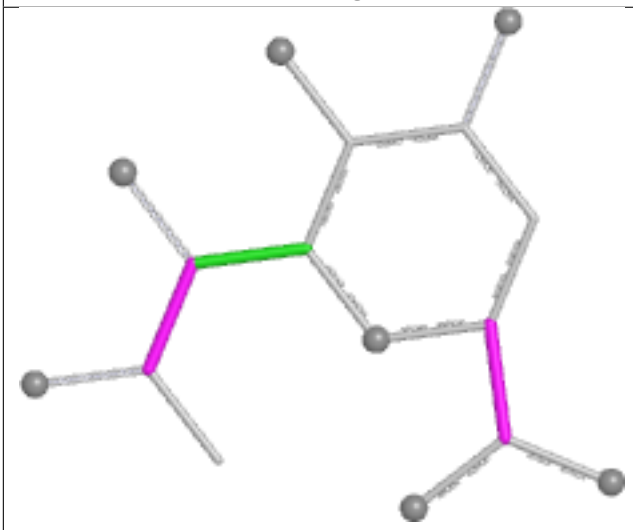
Ligand P8E M 614



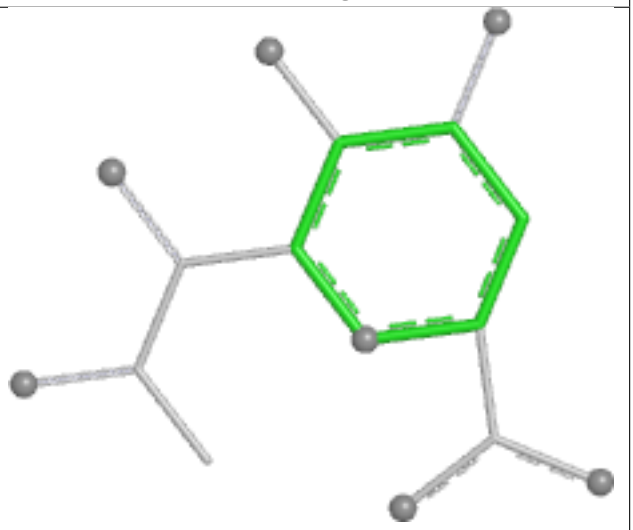
Bond lengths



Bond angles

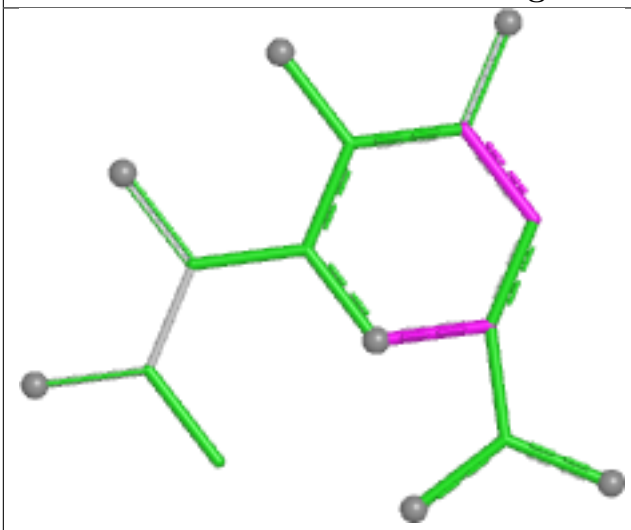


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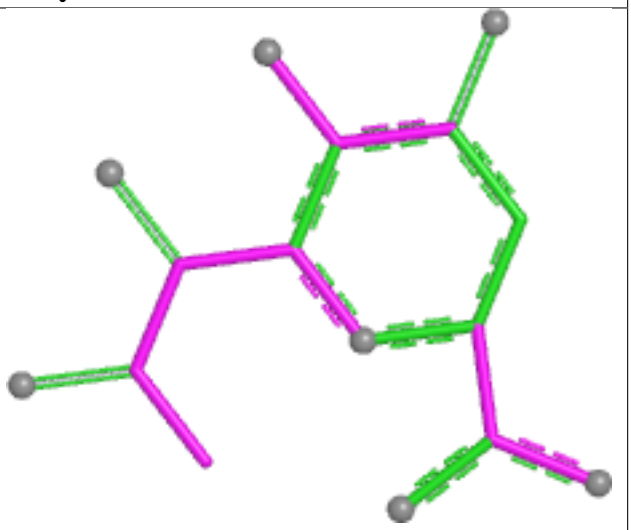


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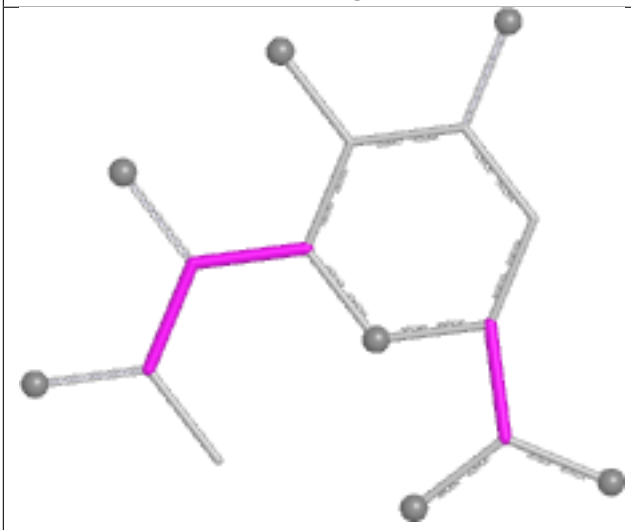
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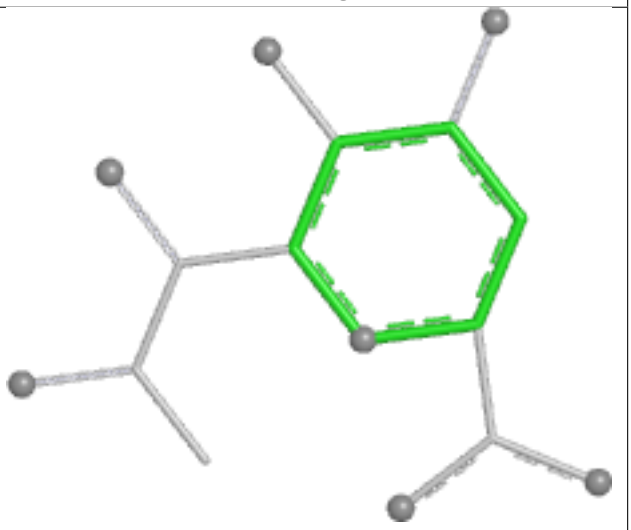
Bond lengths



Bond angles

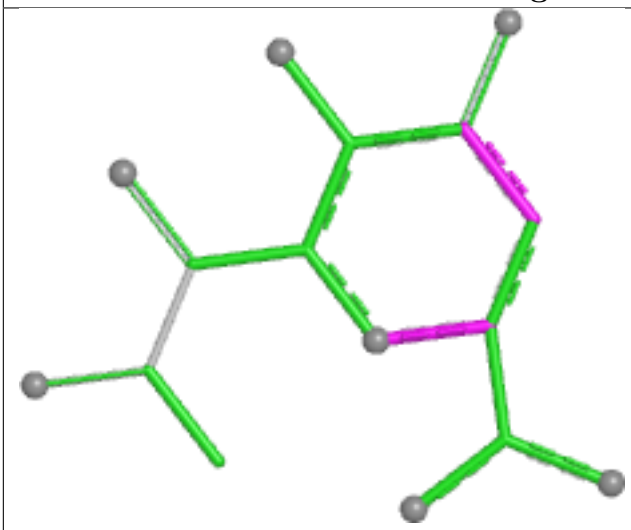


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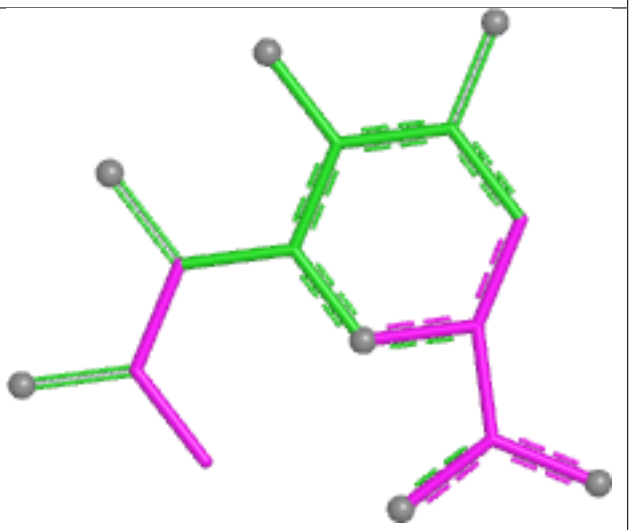


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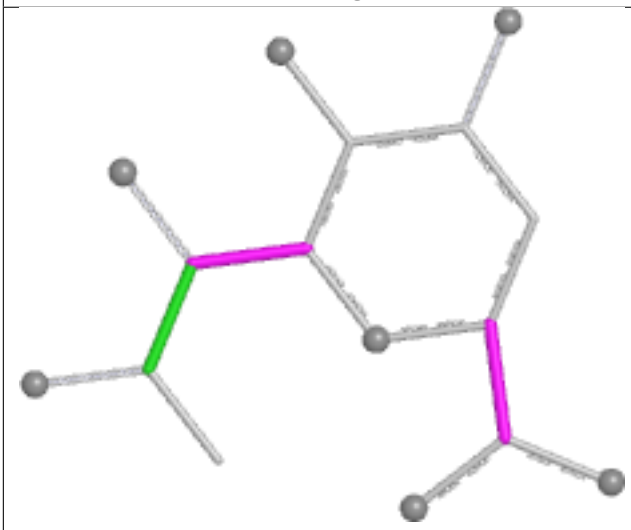
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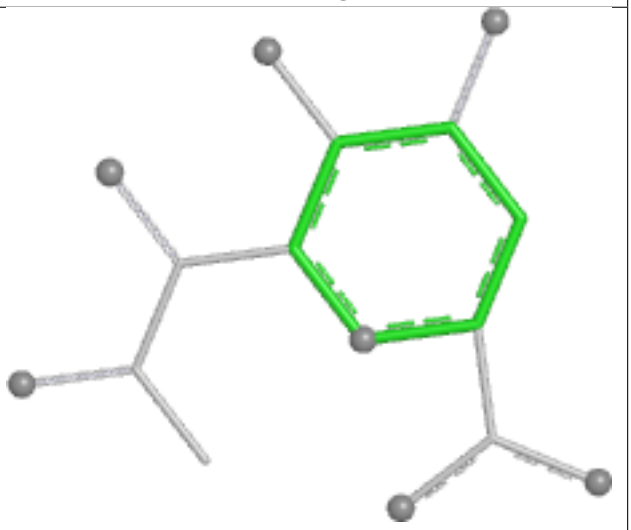
Bond lengths



Bond angles

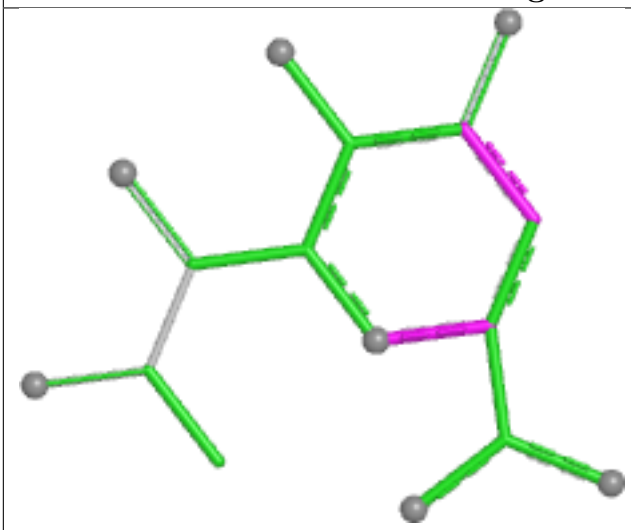


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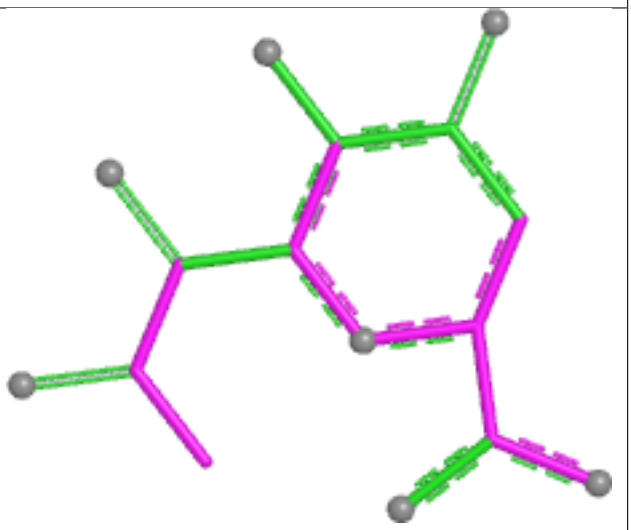


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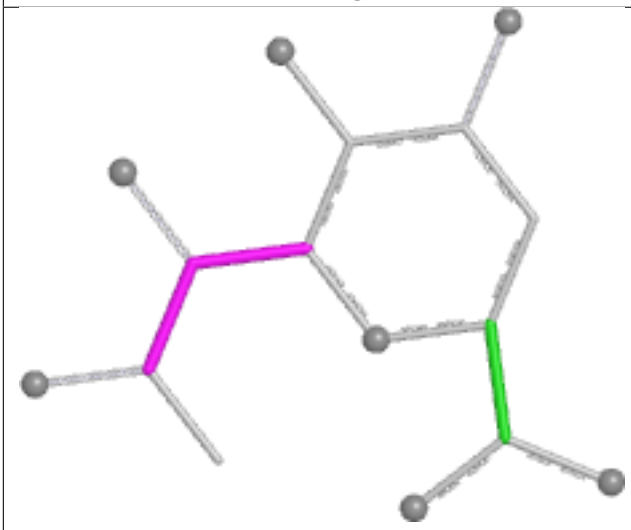
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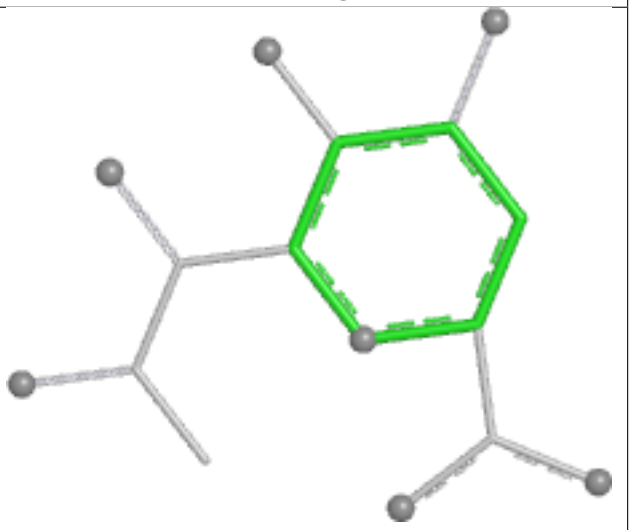
Bond lengths



Bond angles

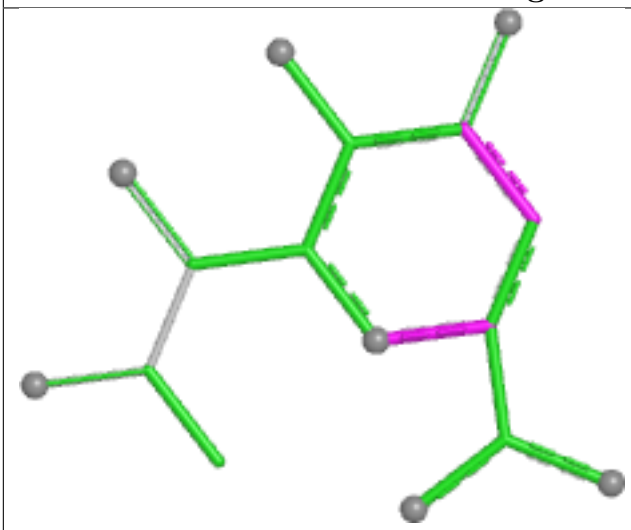


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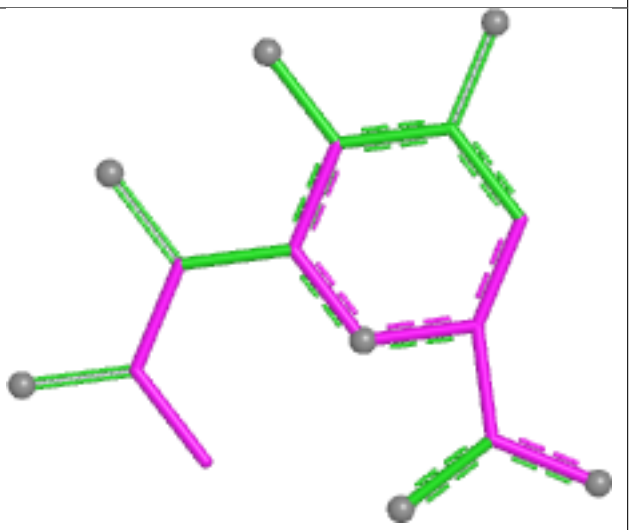


Rings

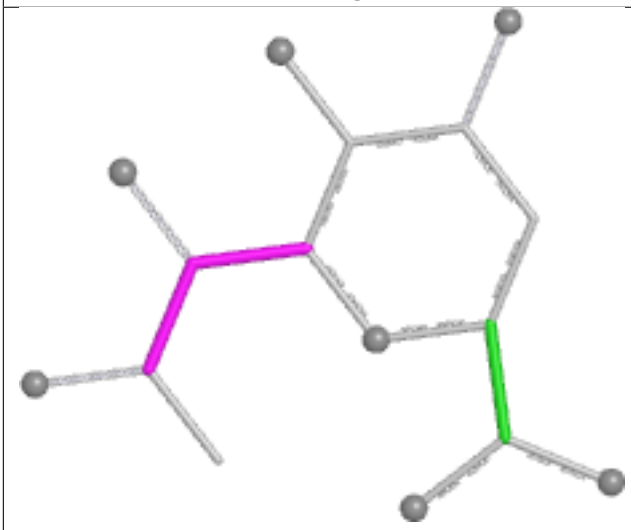
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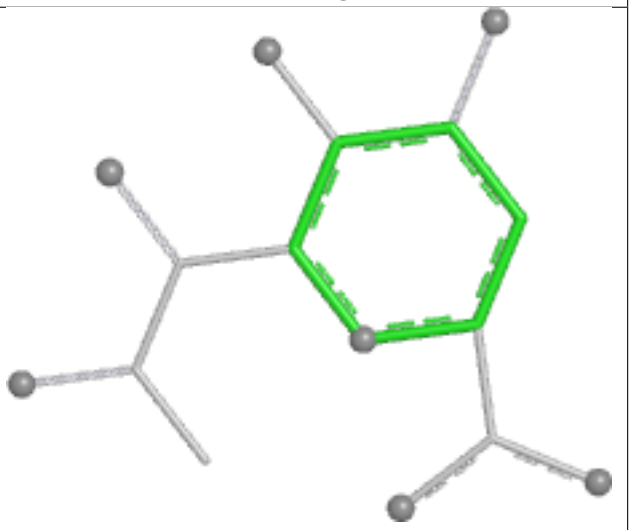
Bond lengths



Bond angles

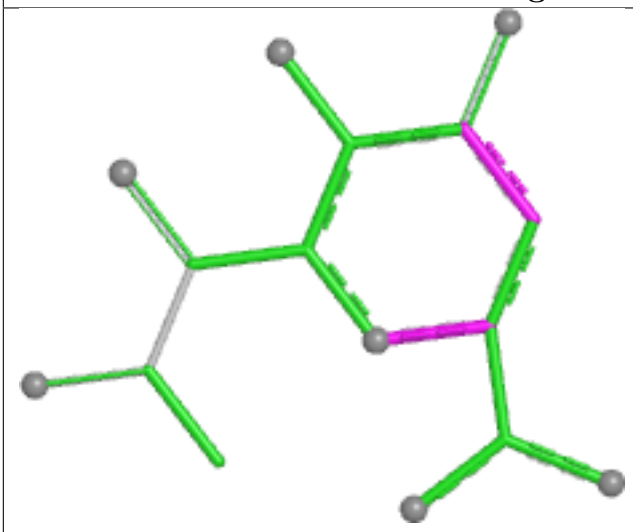


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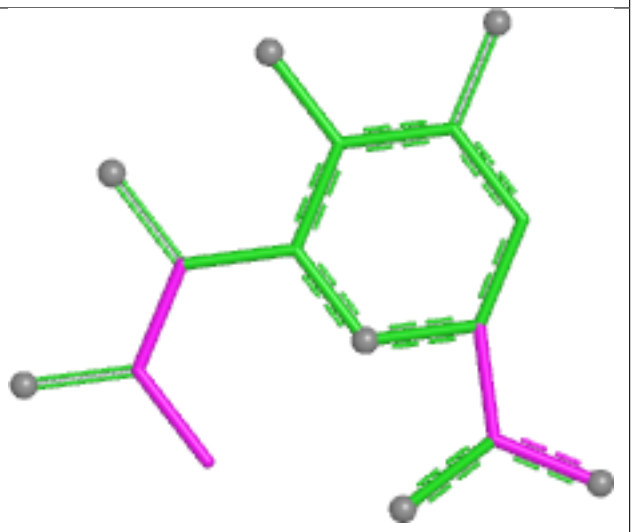


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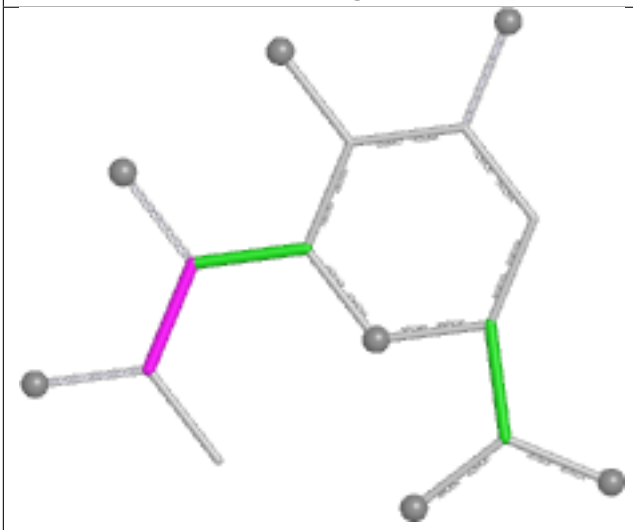
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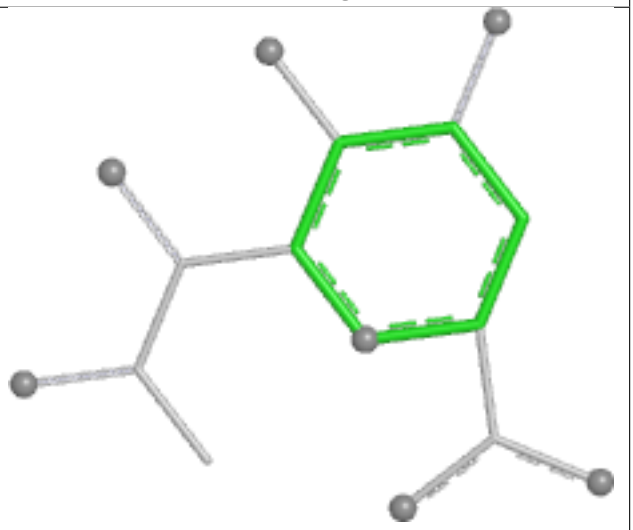
Bond lengths



Bond angles

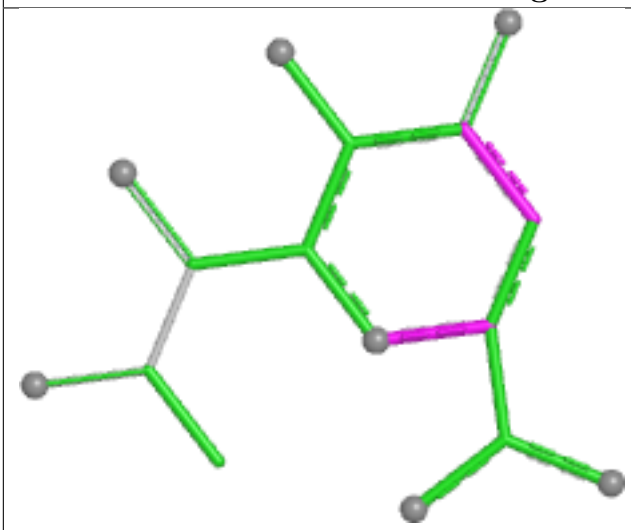


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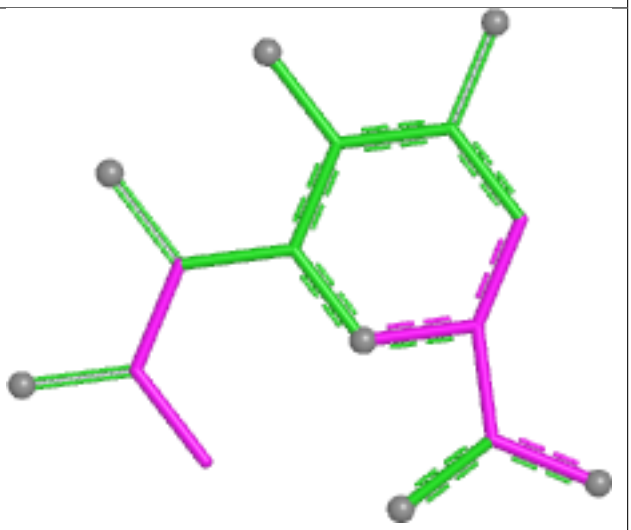


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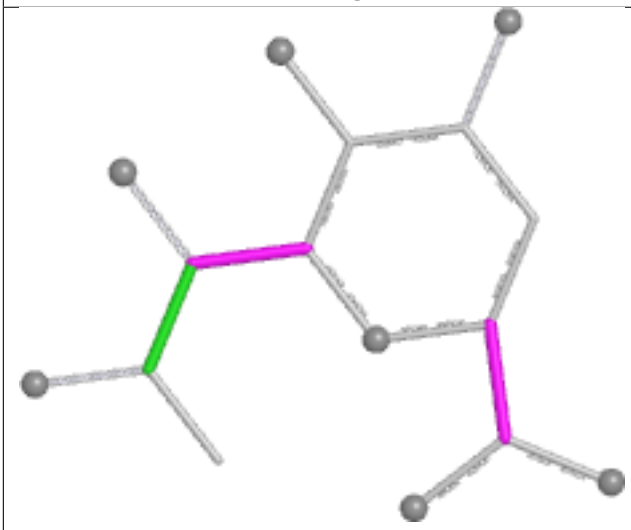
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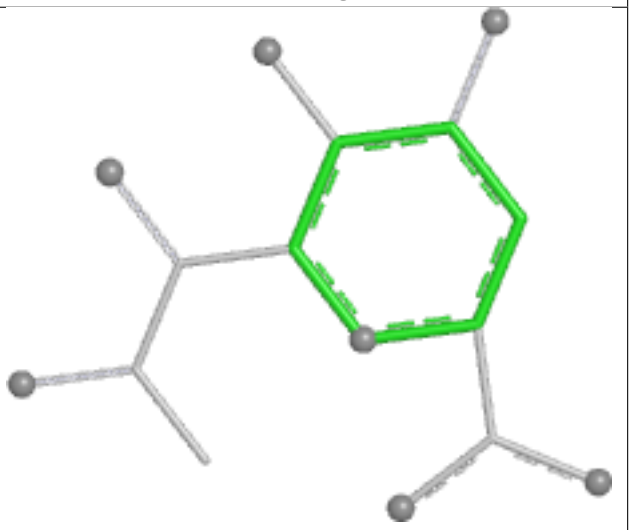
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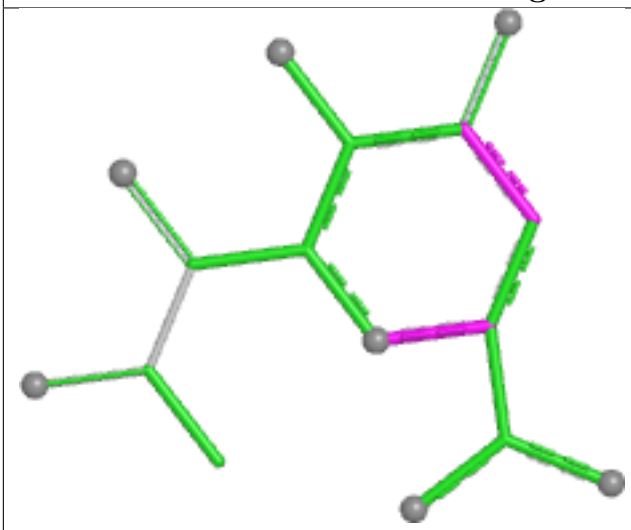


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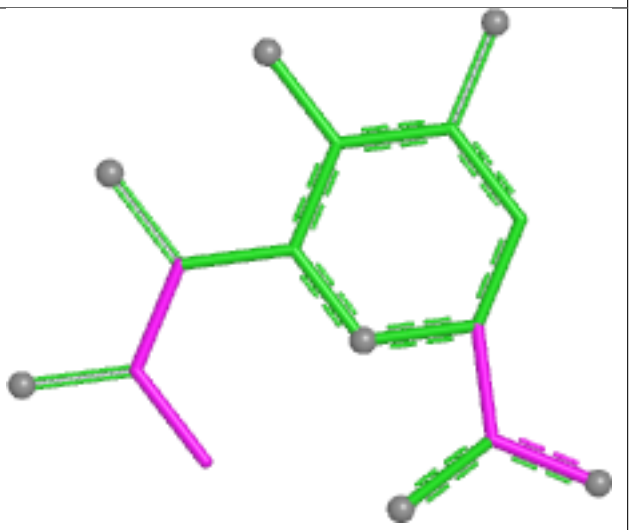


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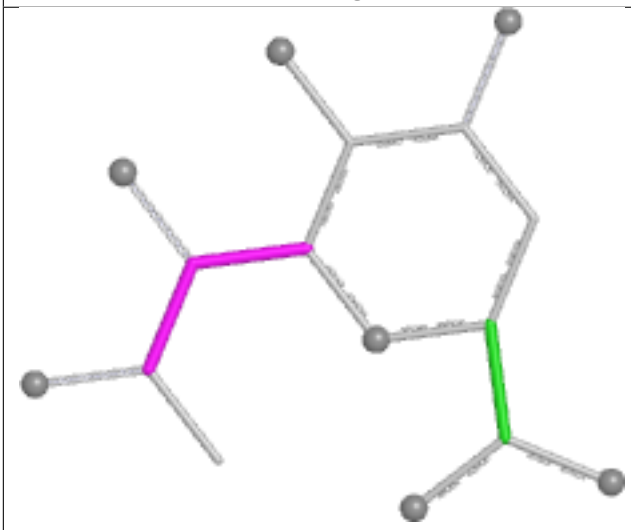
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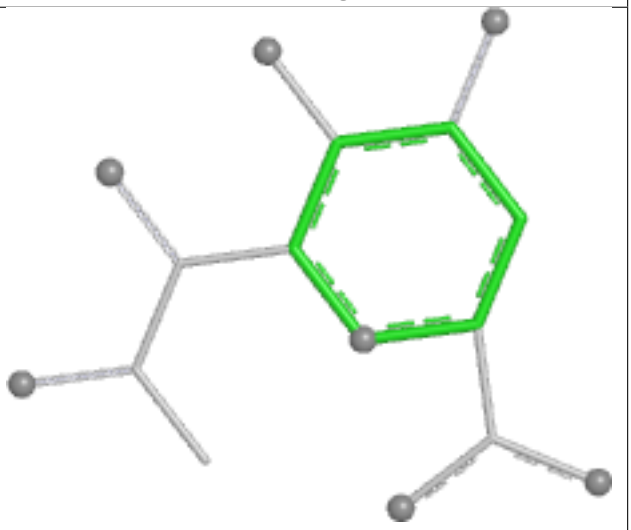
Bond lengths



Bond angles

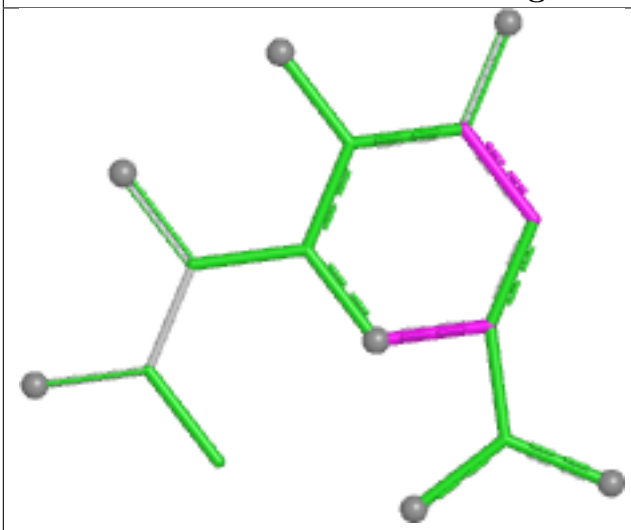


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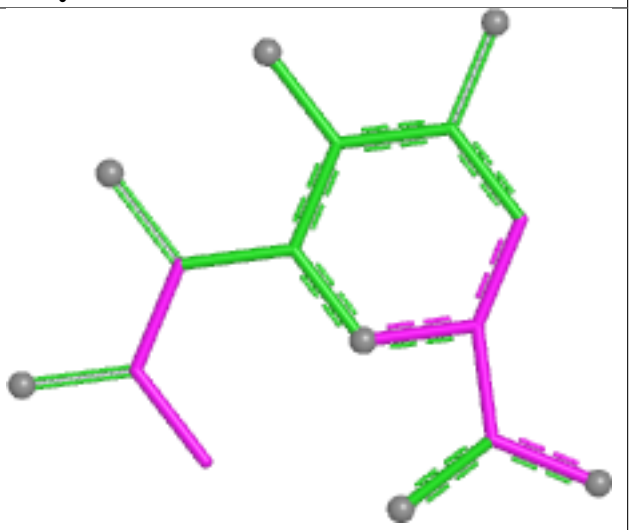


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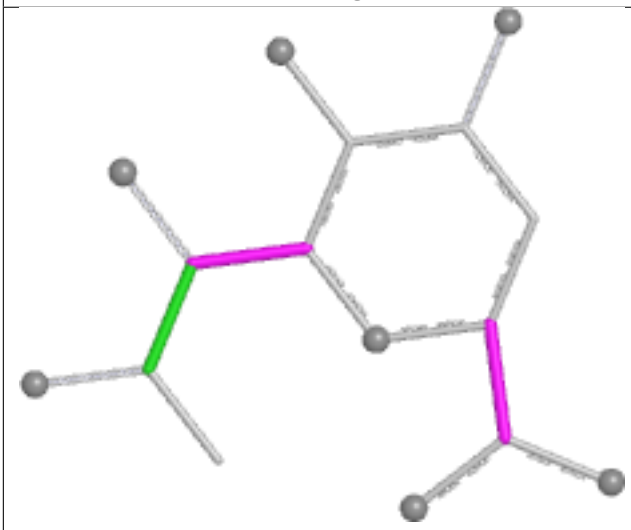
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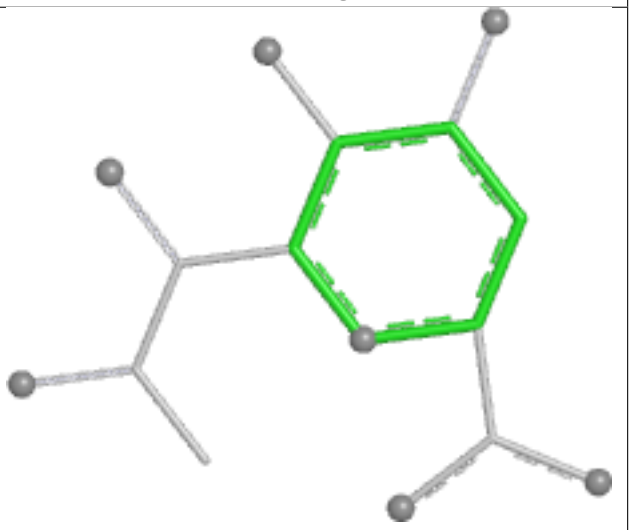
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Bond angles

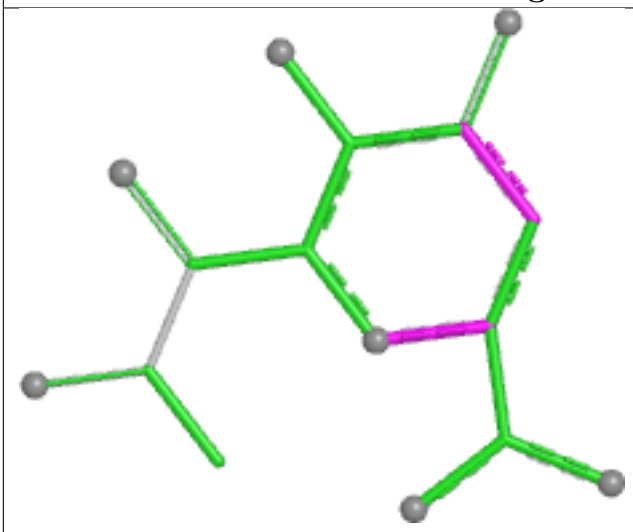


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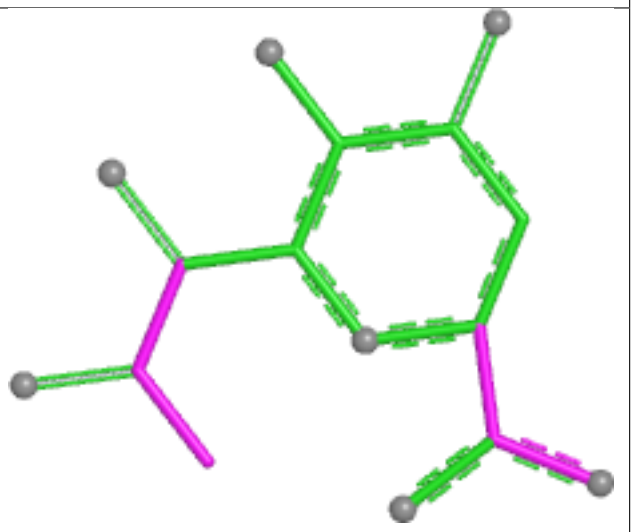


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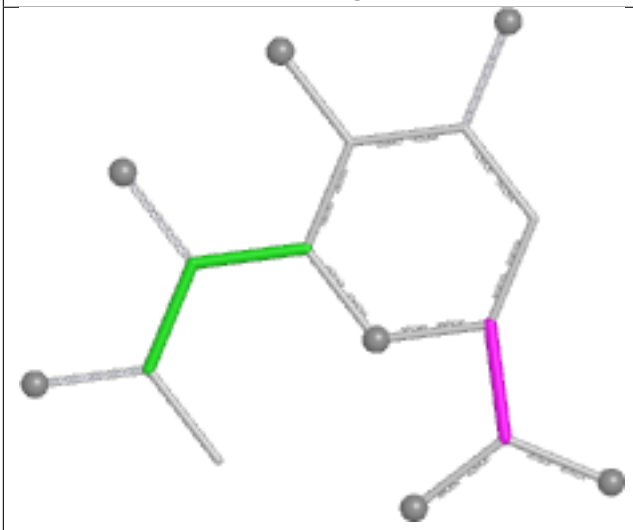
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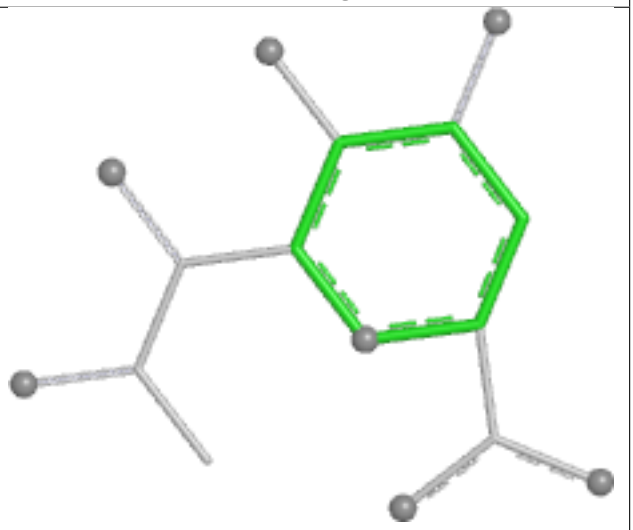
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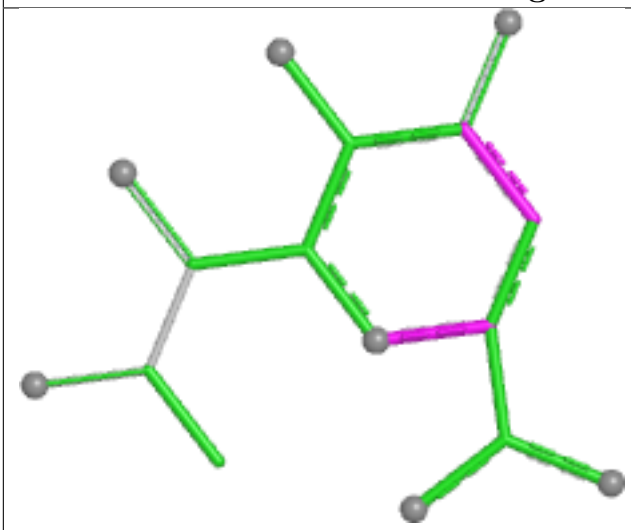


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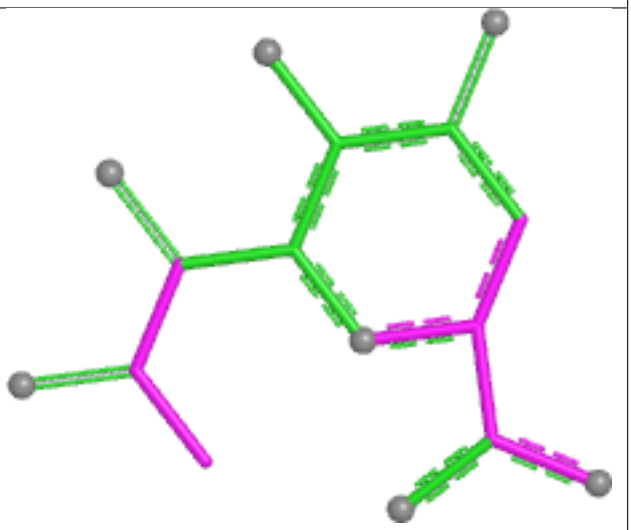


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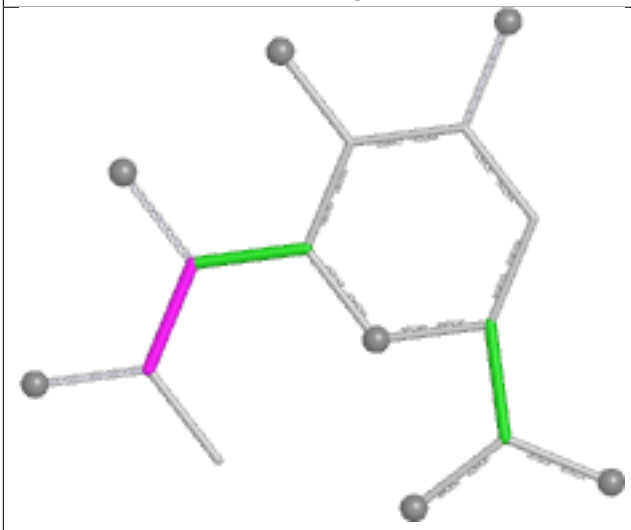
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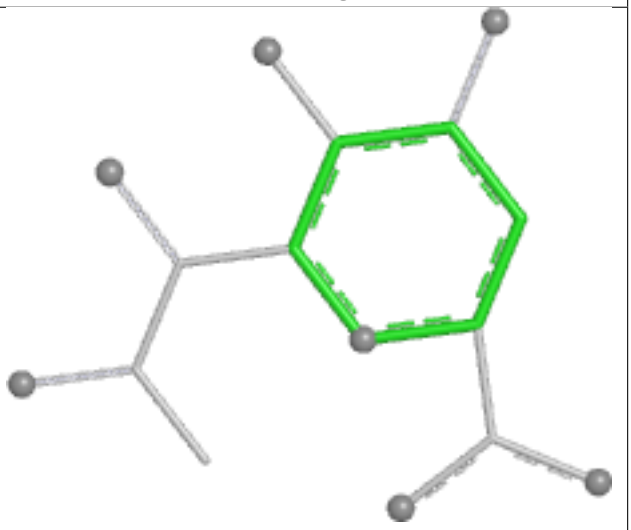
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Bond angles

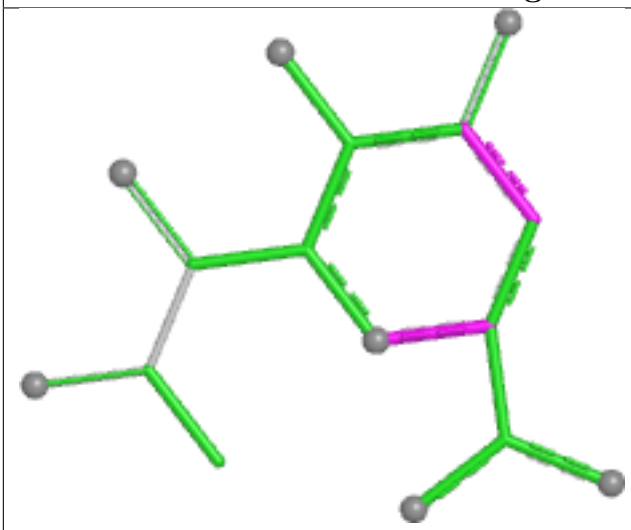


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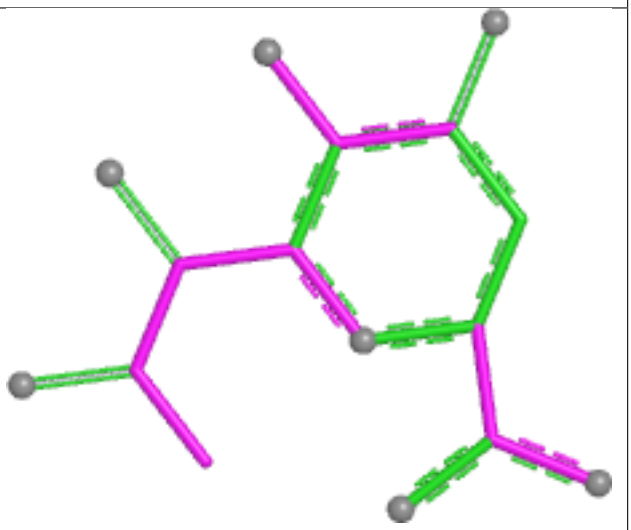


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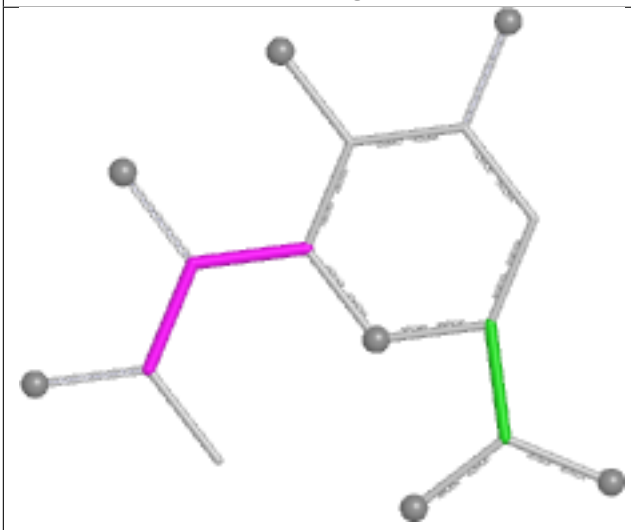
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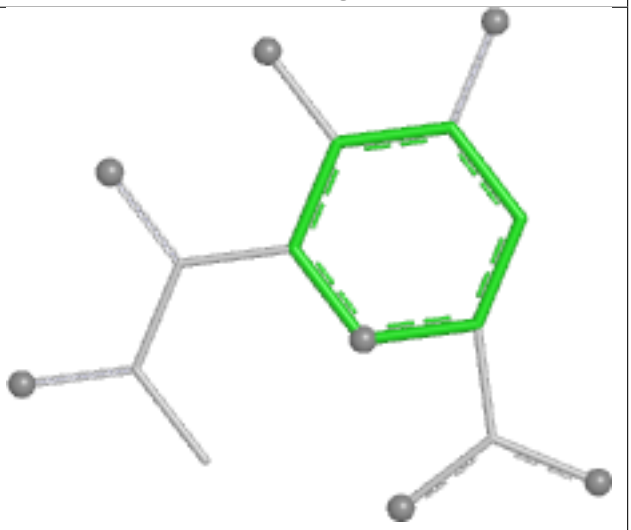
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Bond angles

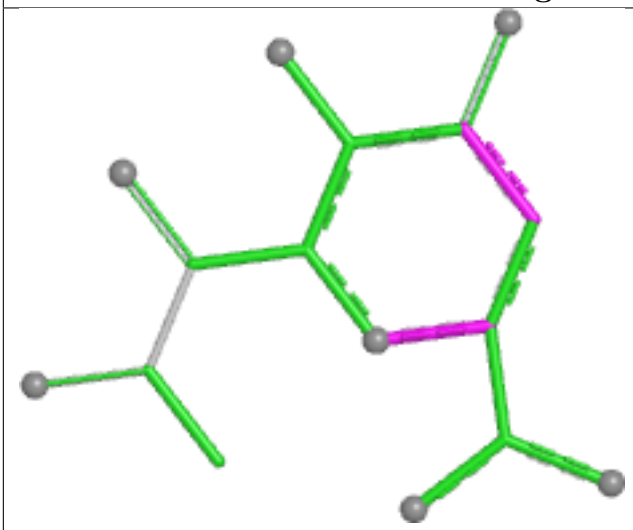


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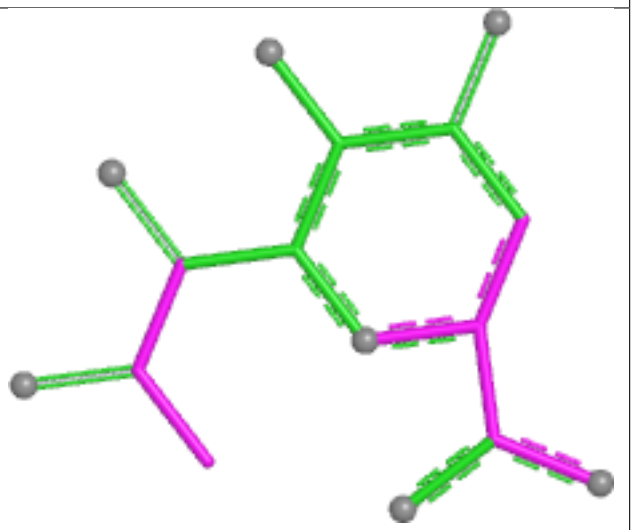


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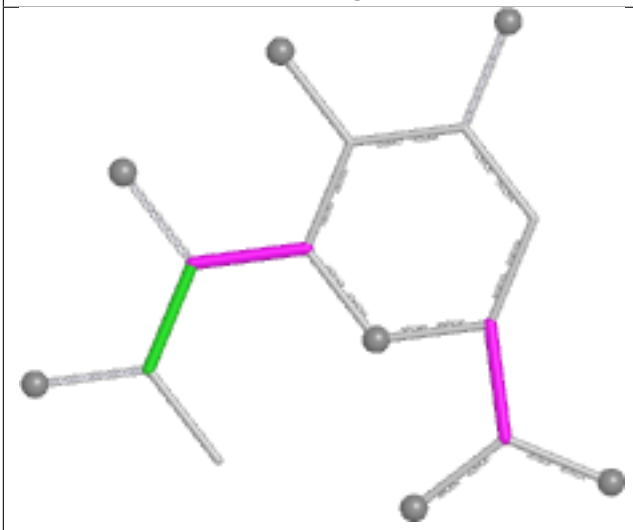
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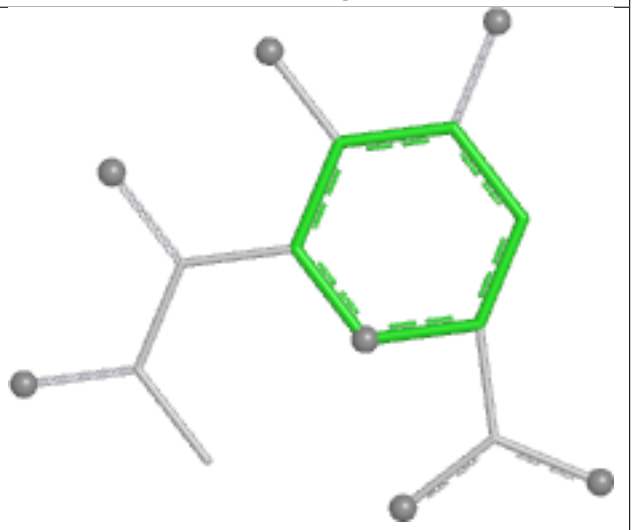
Bond lengths



Bond angles

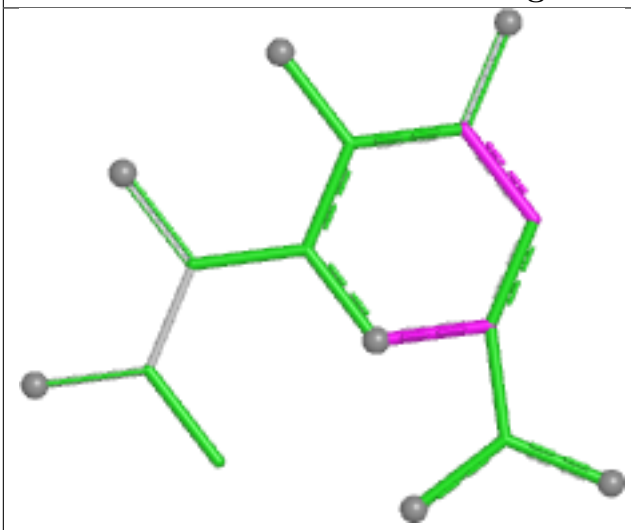


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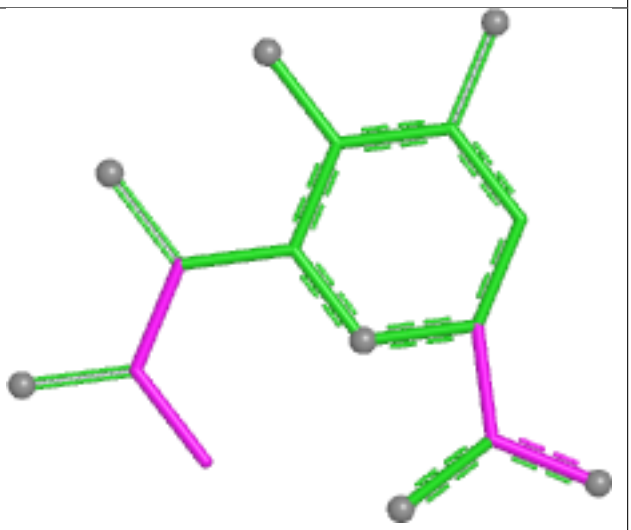


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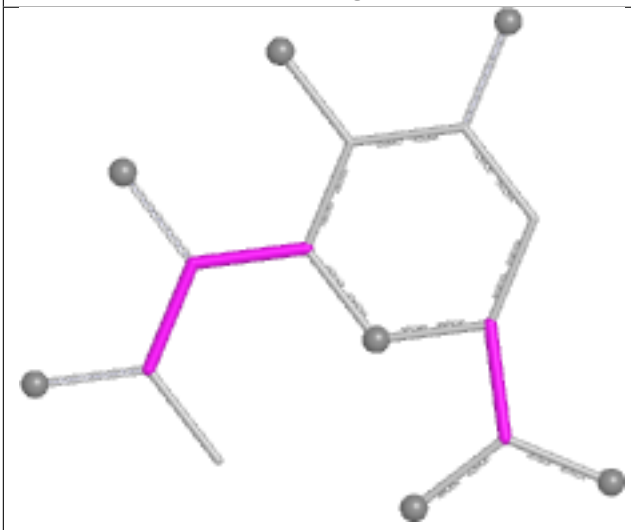
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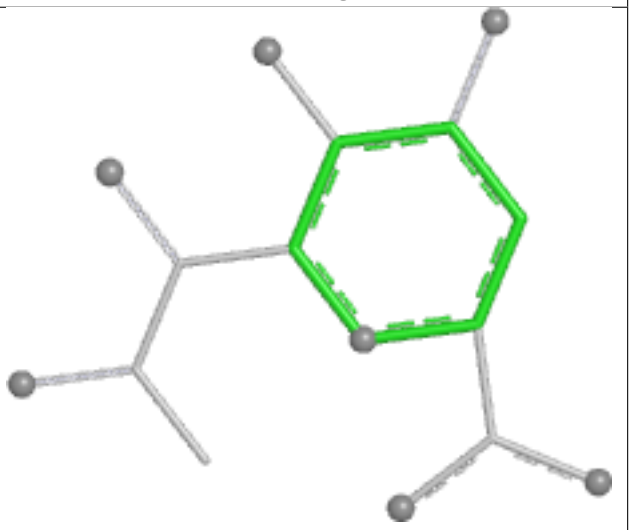
Bond lengths



Bond angles

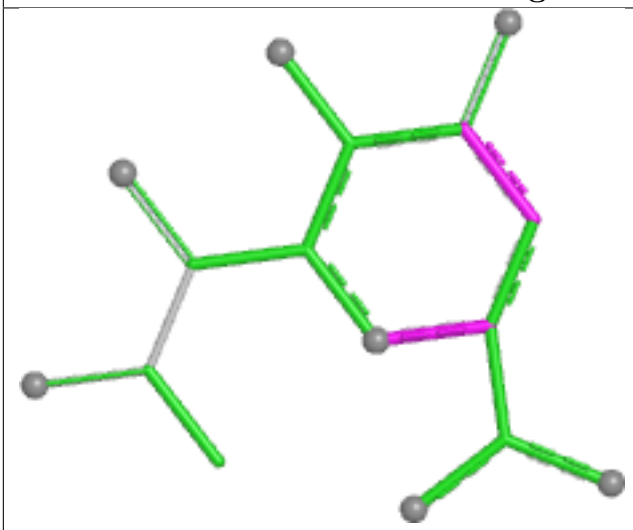


Torsions

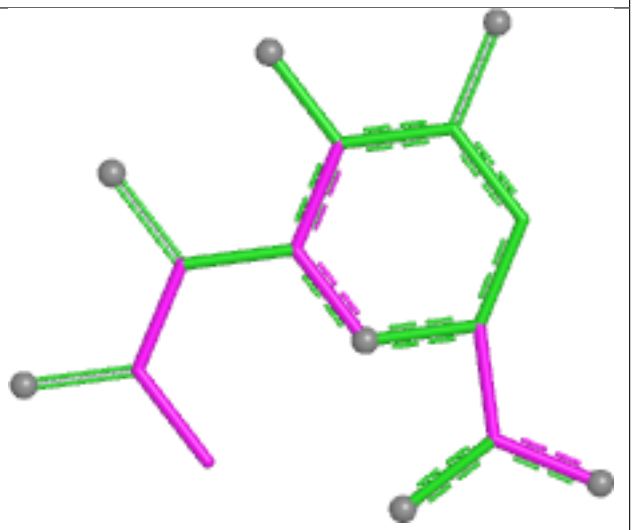


Rings

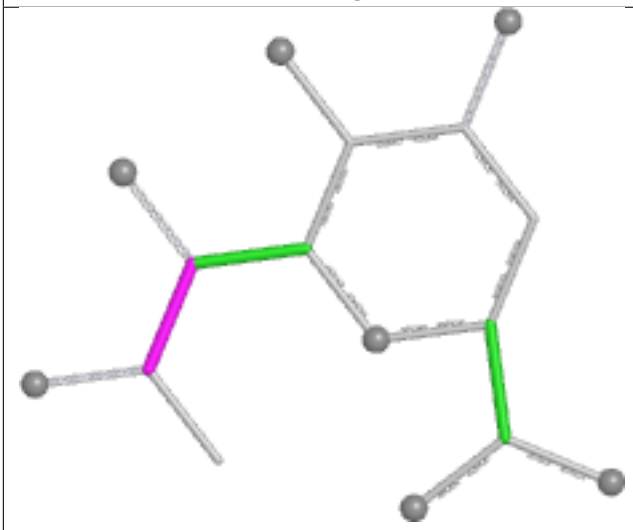
Ligand P8E B 610



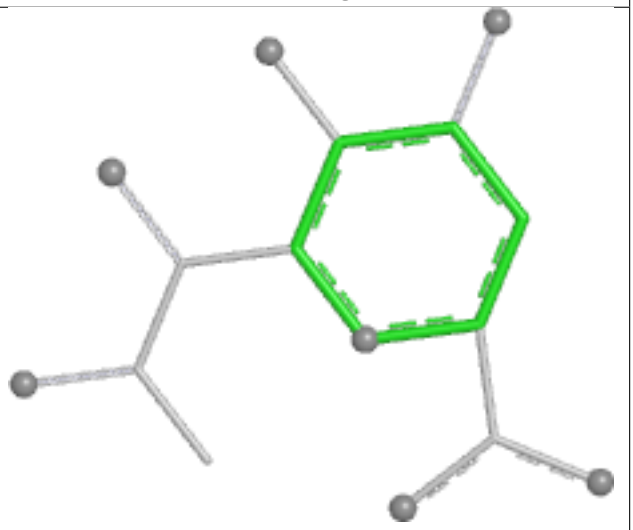
Bond lengths



Bond angles

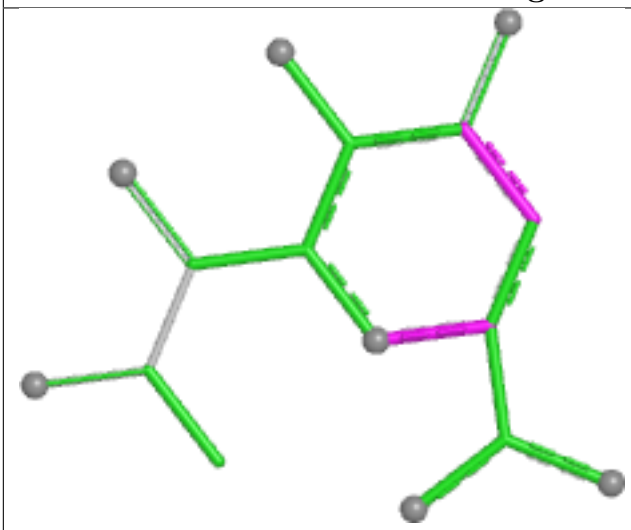


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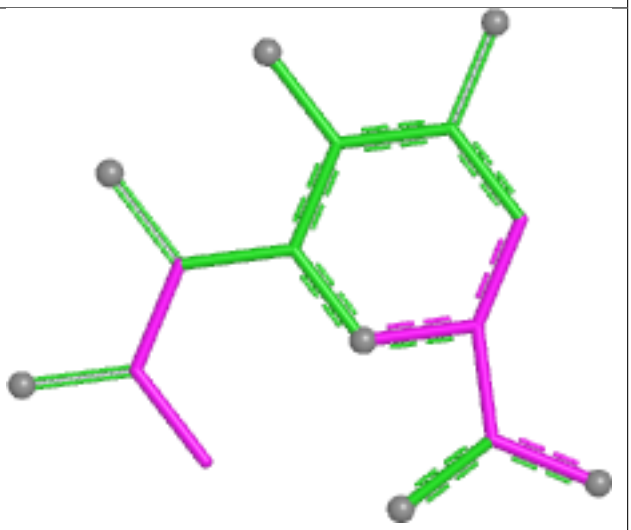


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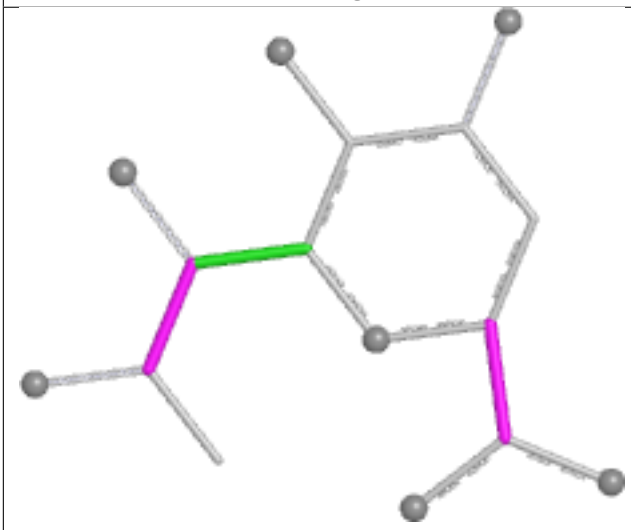
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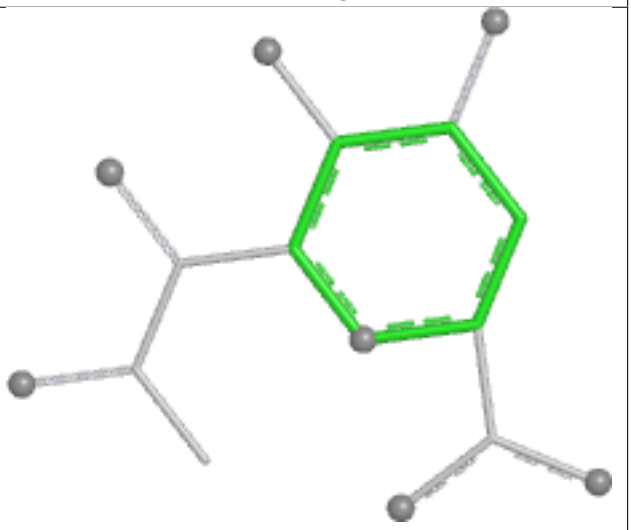
Bond lengths



Bond angles

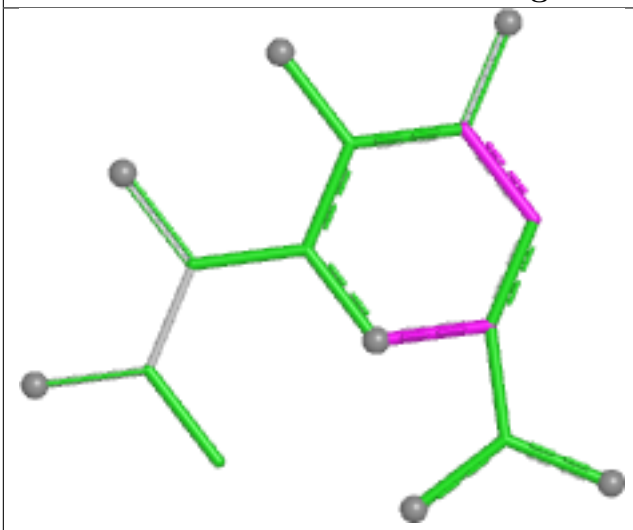


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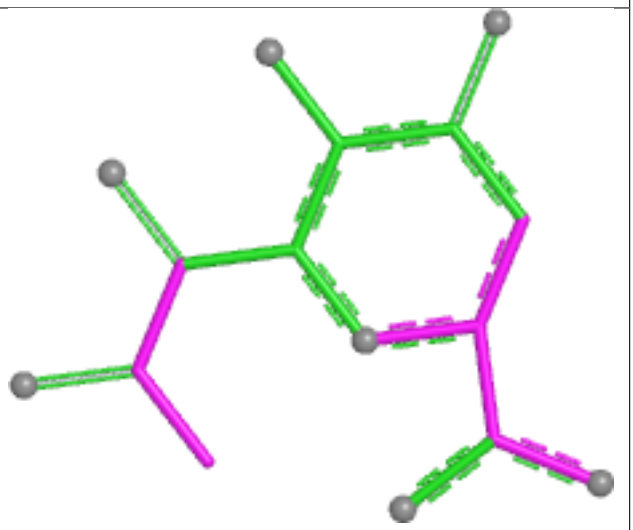


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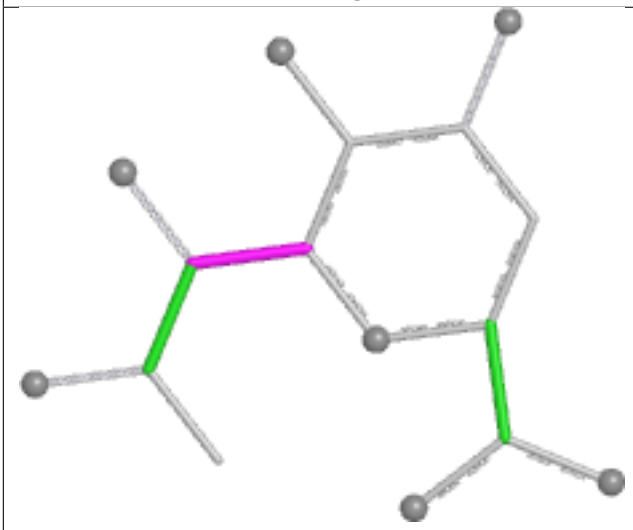
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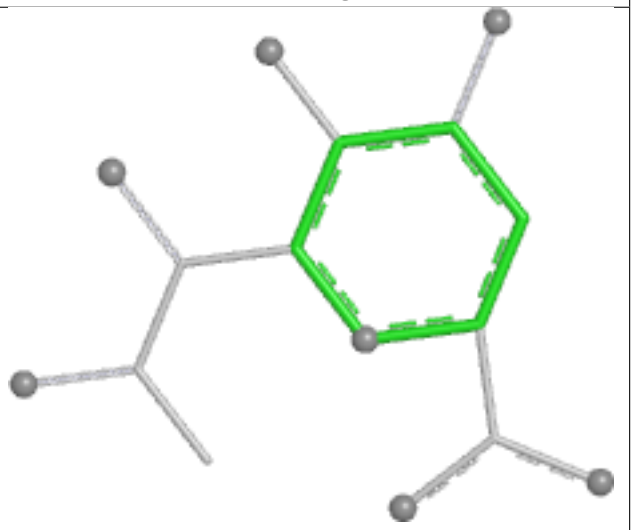
Bond lengths



Bond angles

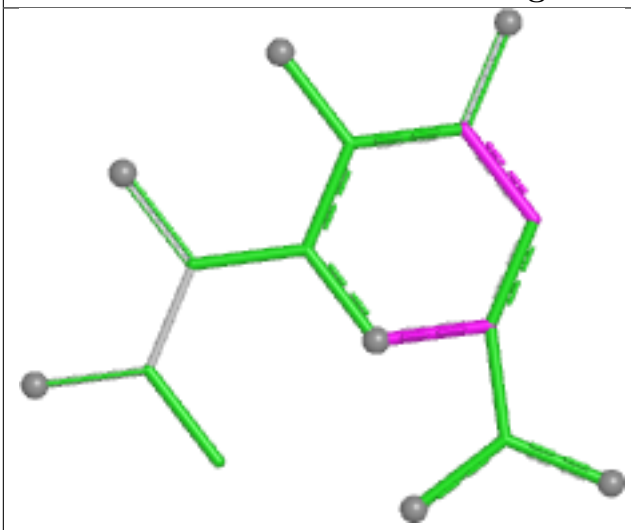


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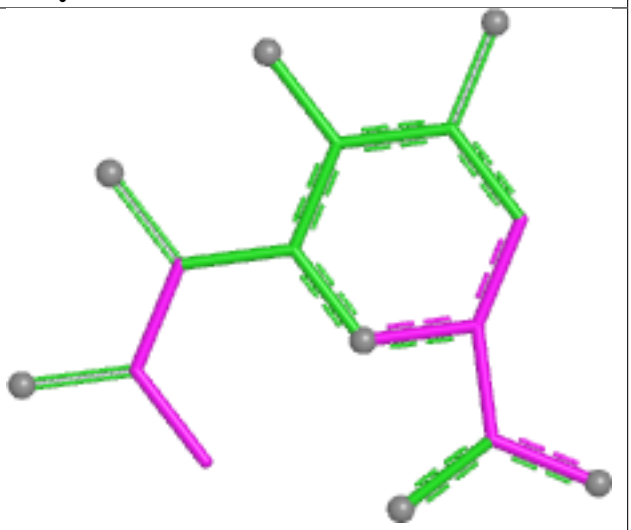


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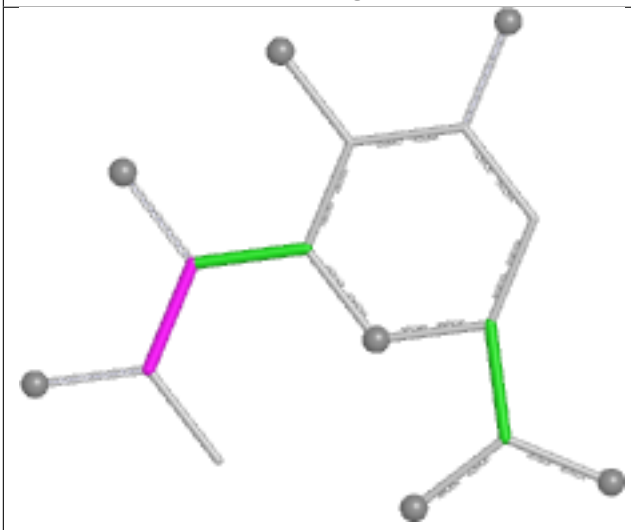
Ligand P8E Q 603



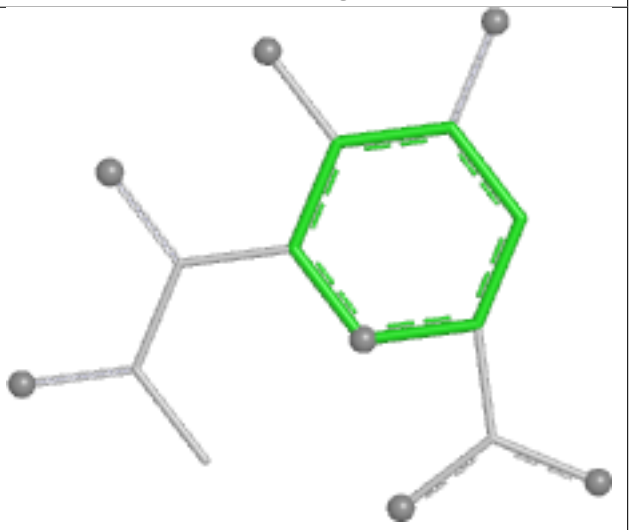
Bond lengths



Bond angles

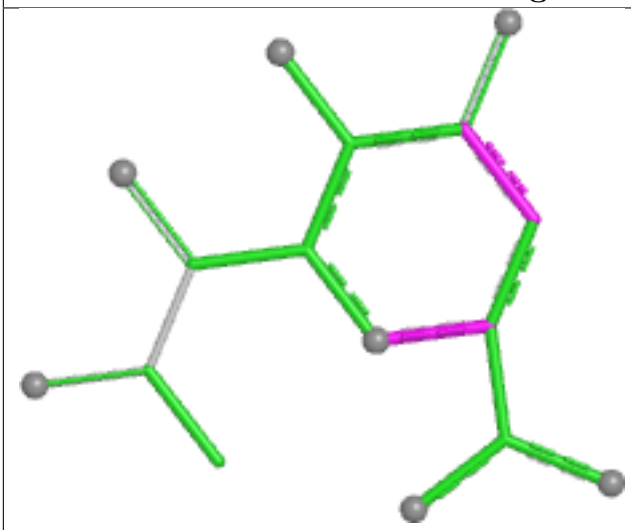


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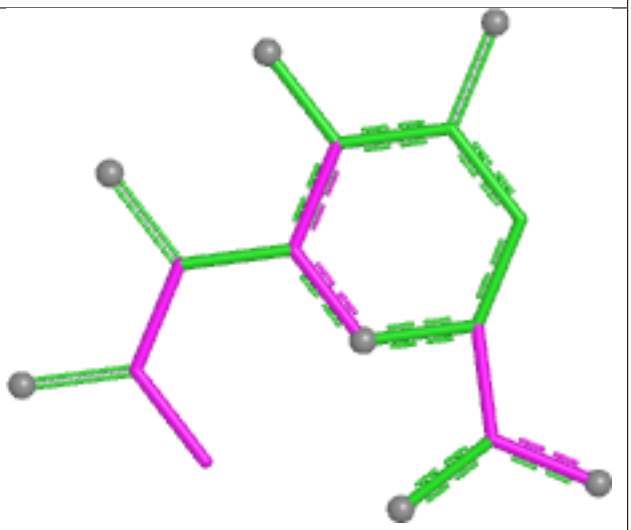


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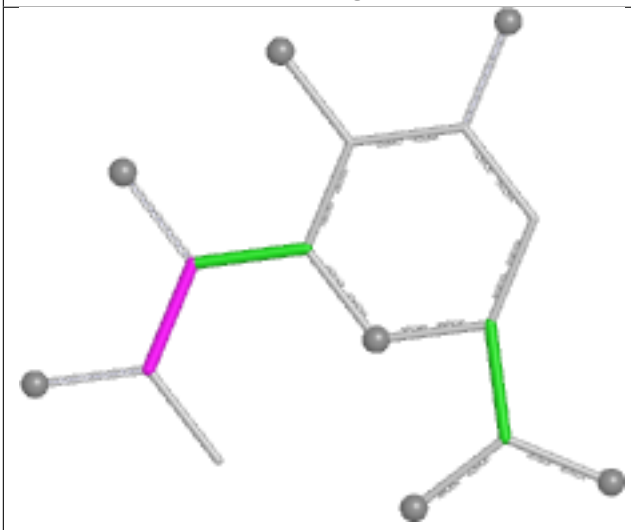
Ligand P8E E 614



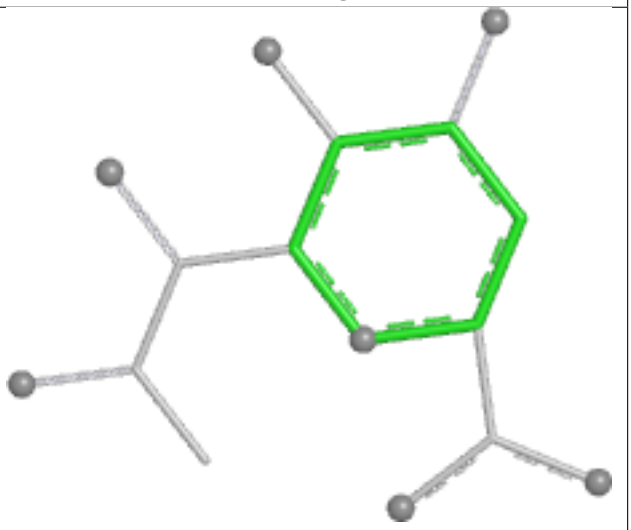
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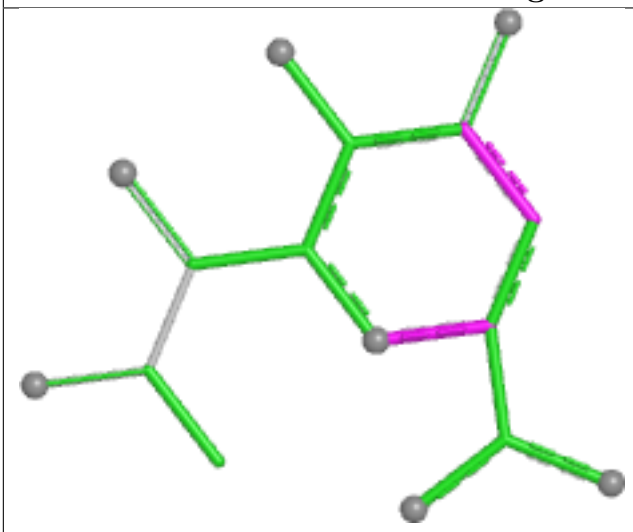


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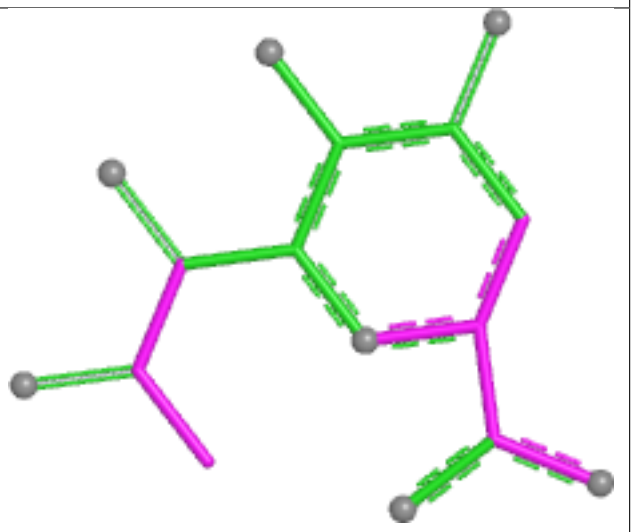


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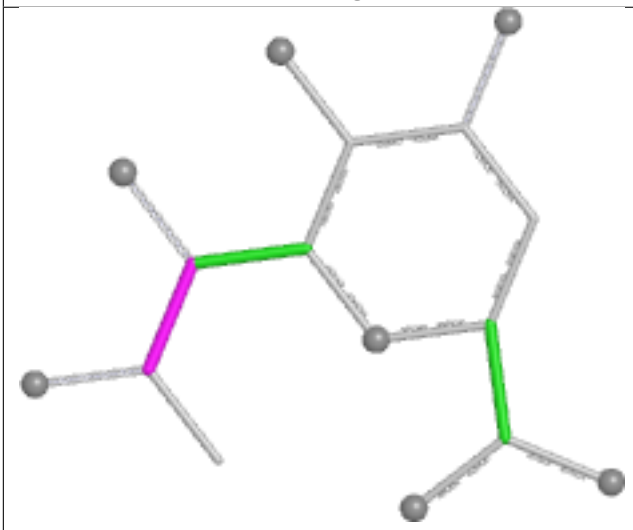
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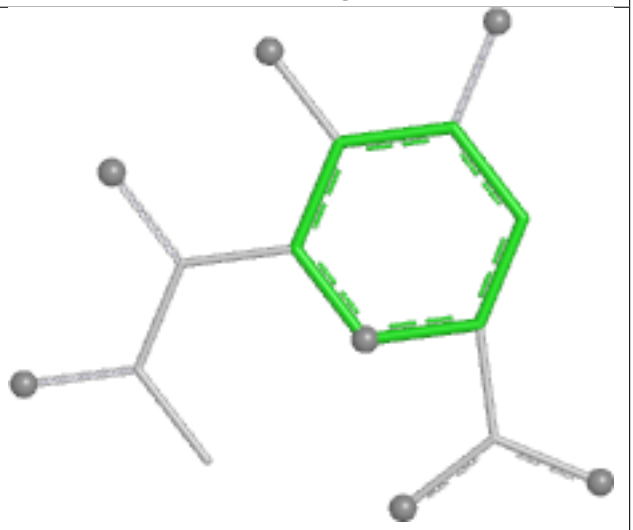
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Bond angles

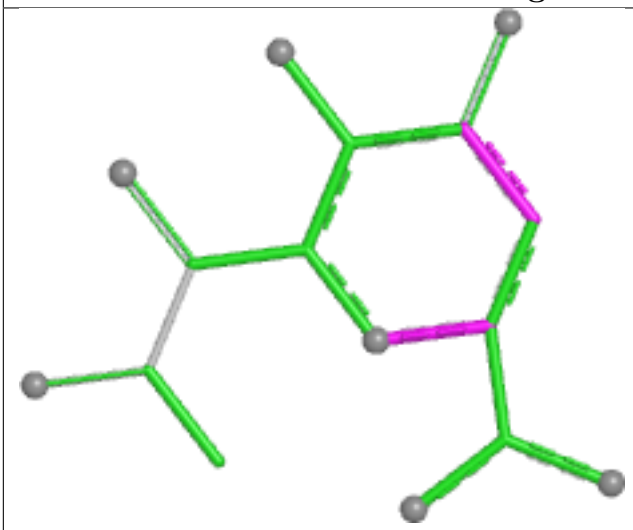


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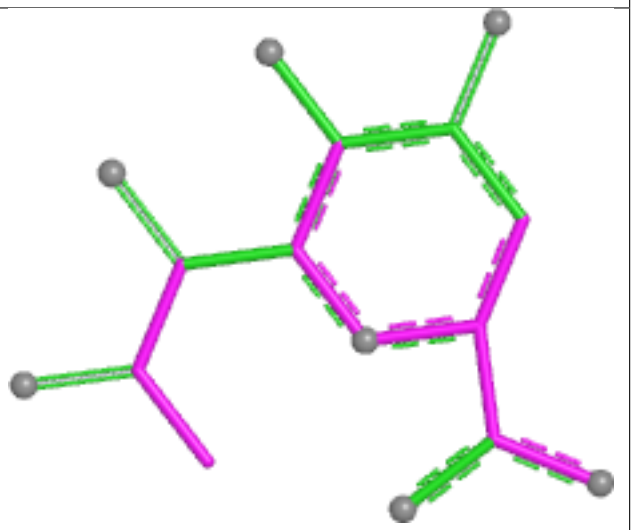


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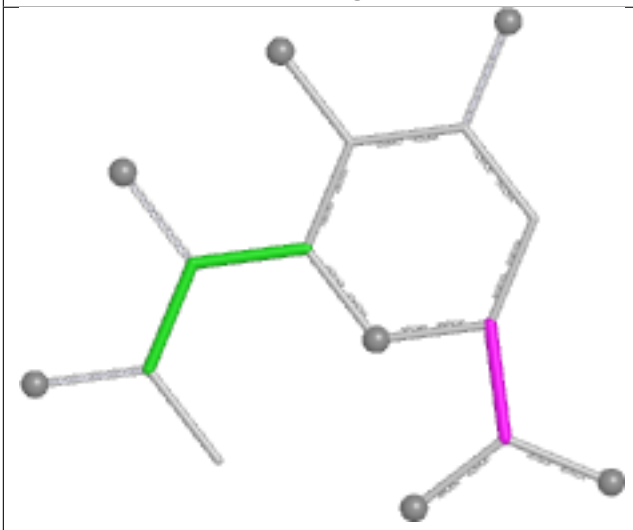
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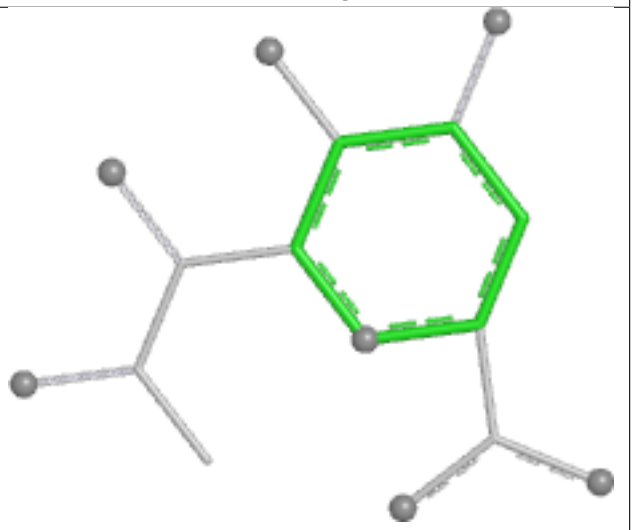
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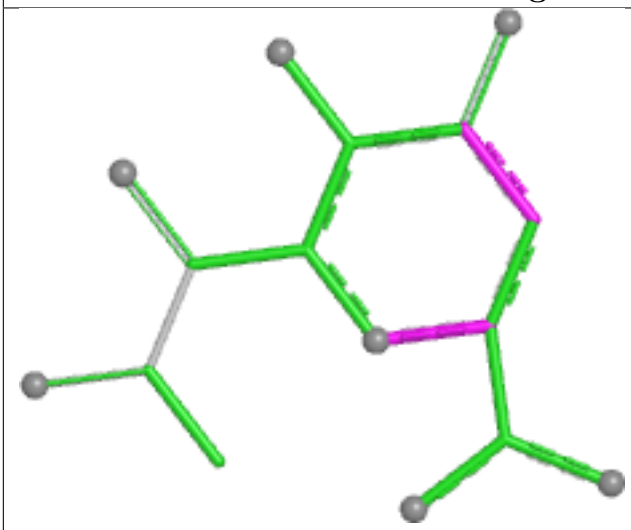


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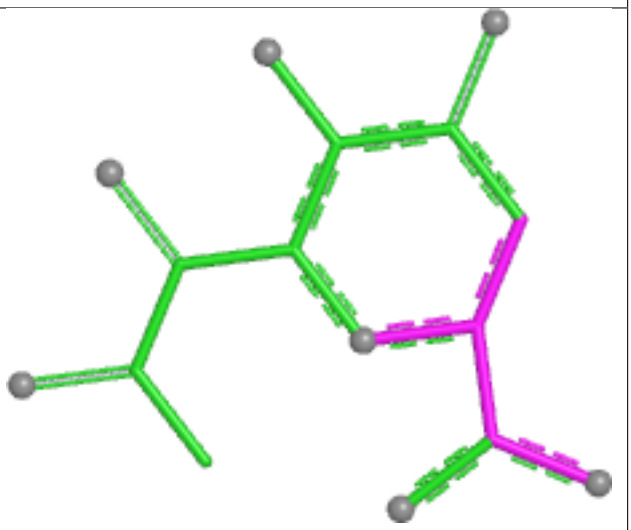


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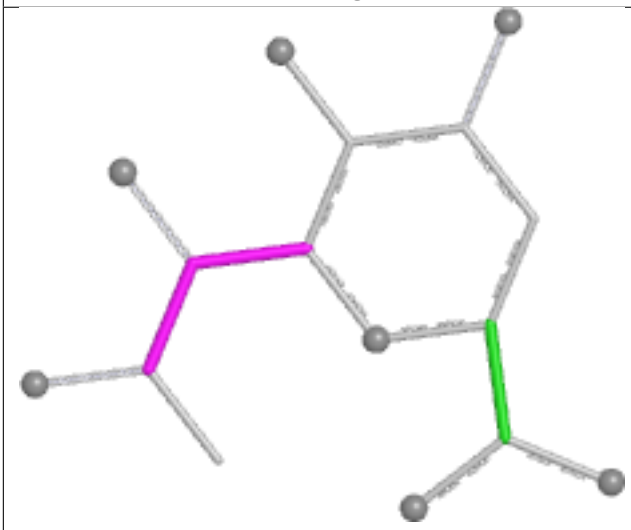
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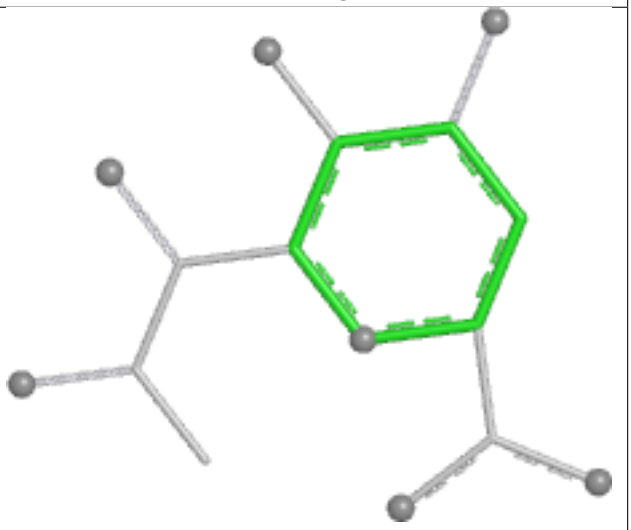
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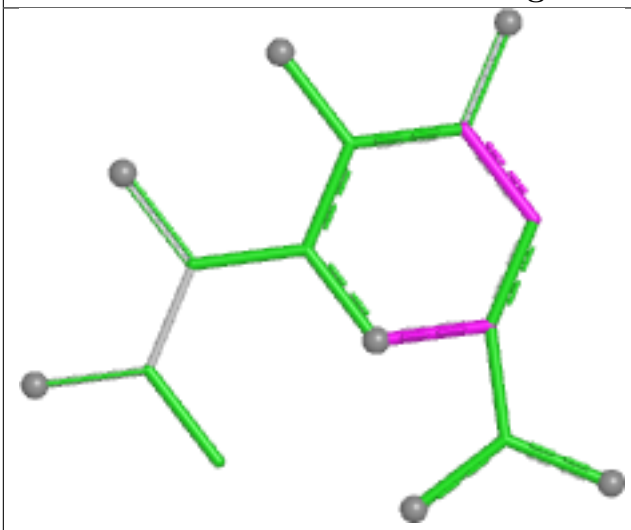


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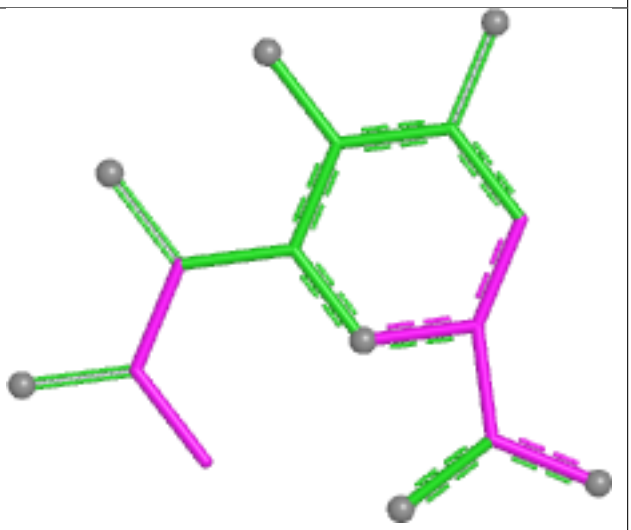


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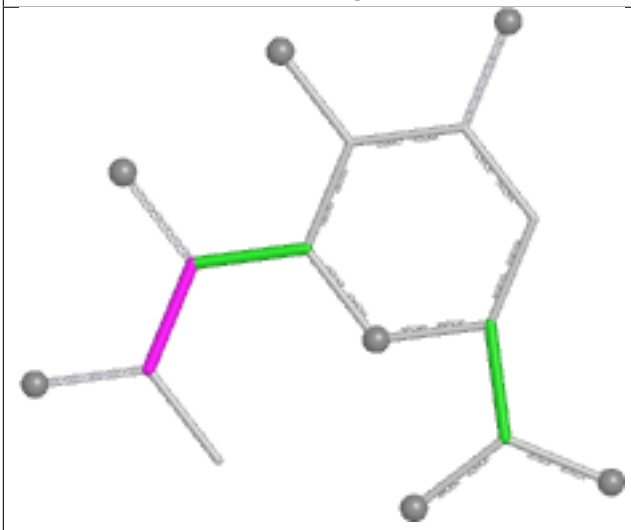
Ligand P8E K 603



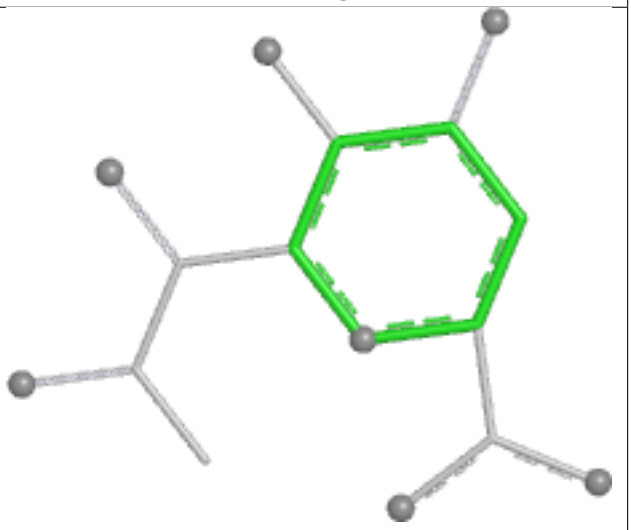
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Bond angles

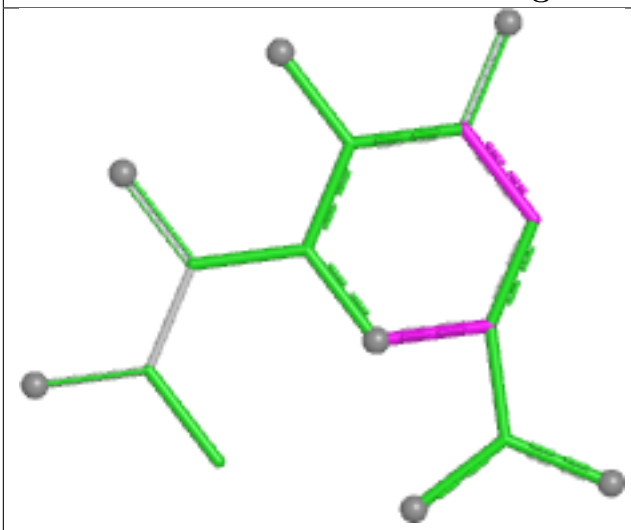


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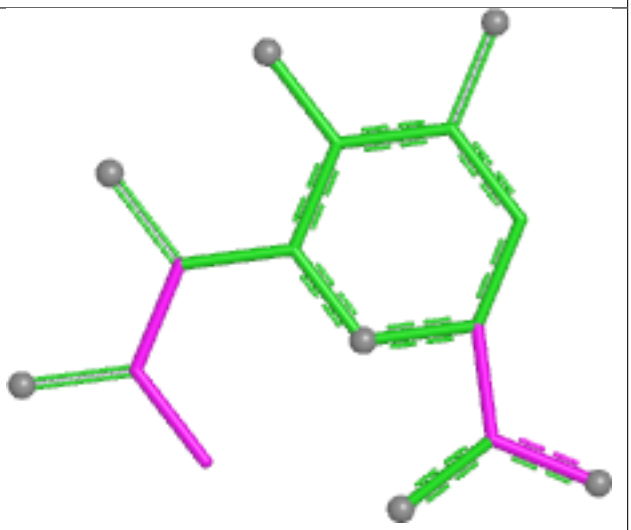


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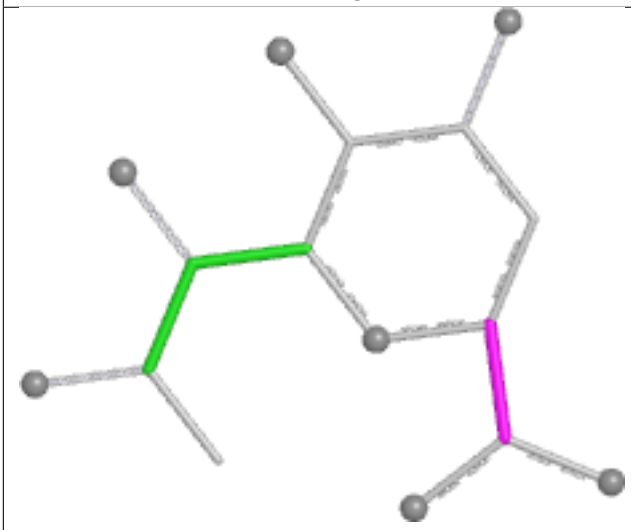
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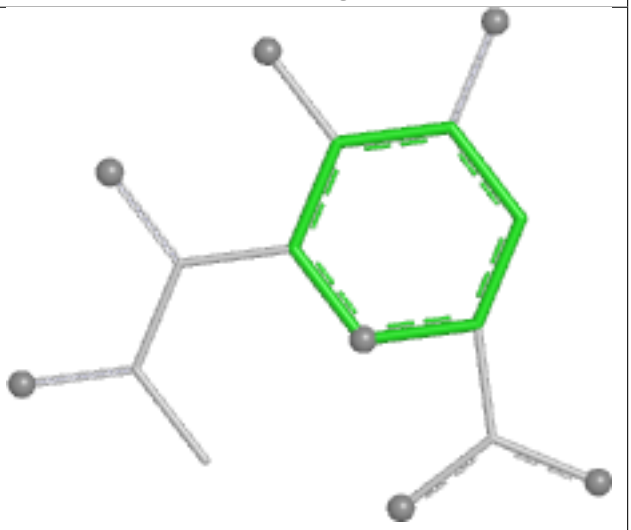
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Bond angles

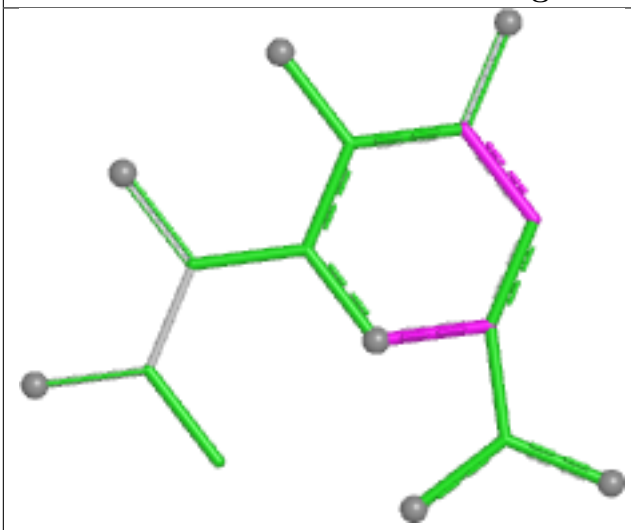


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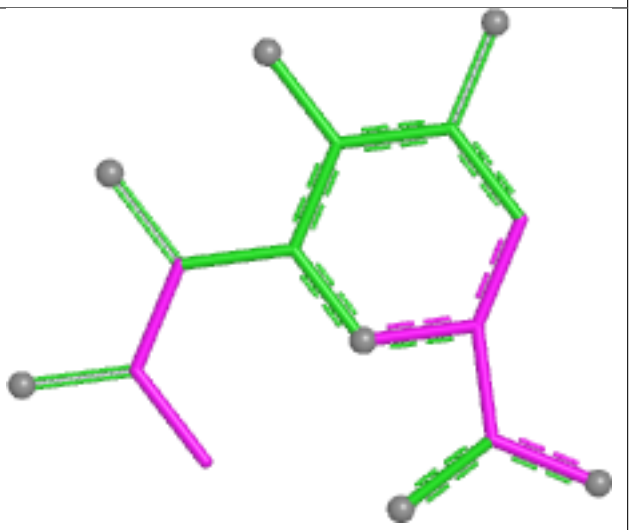


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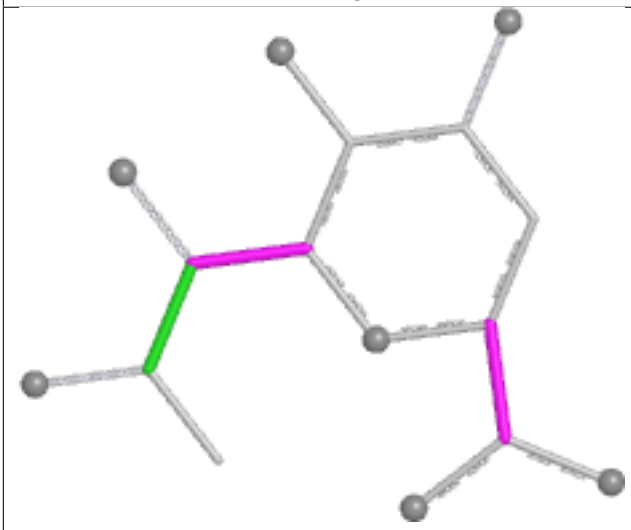
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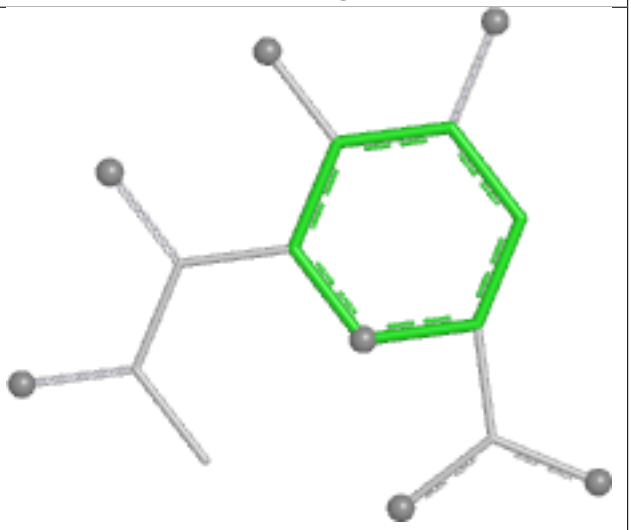
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Bond angles

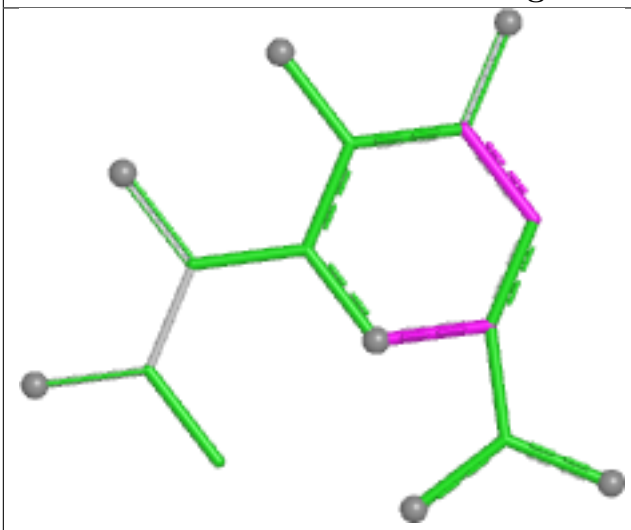


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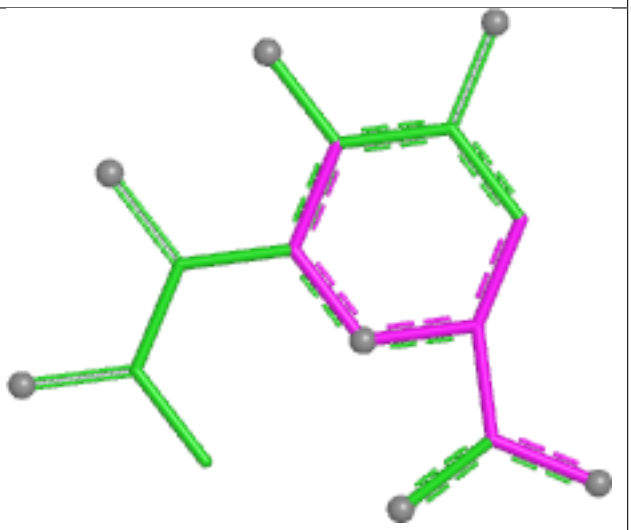


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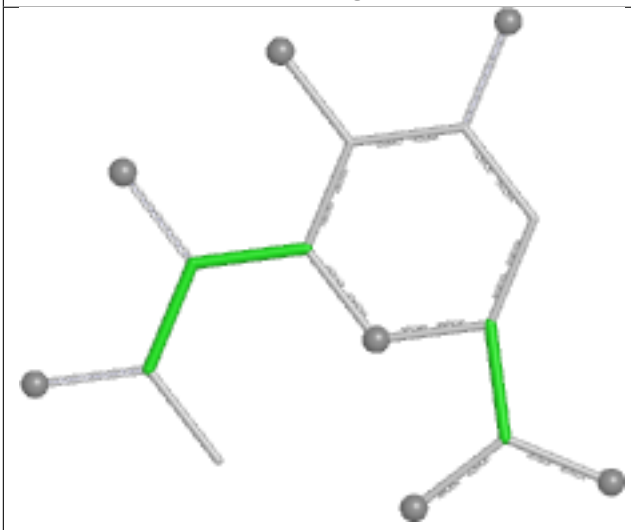
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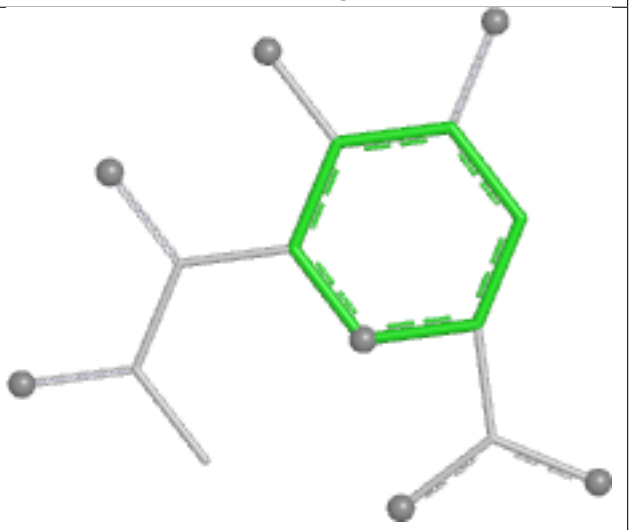
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Bond angles

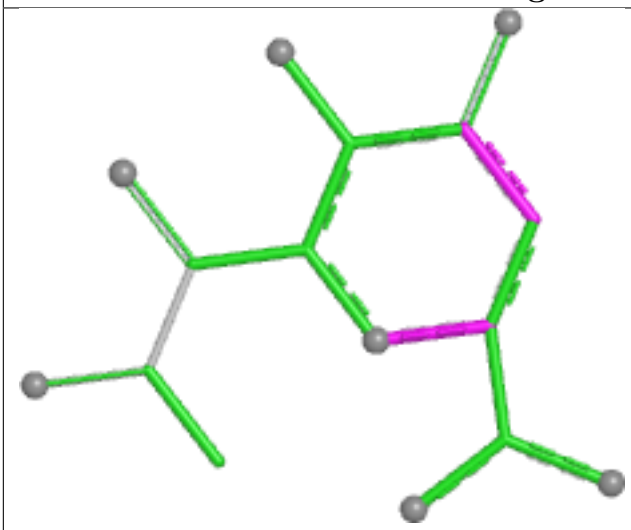


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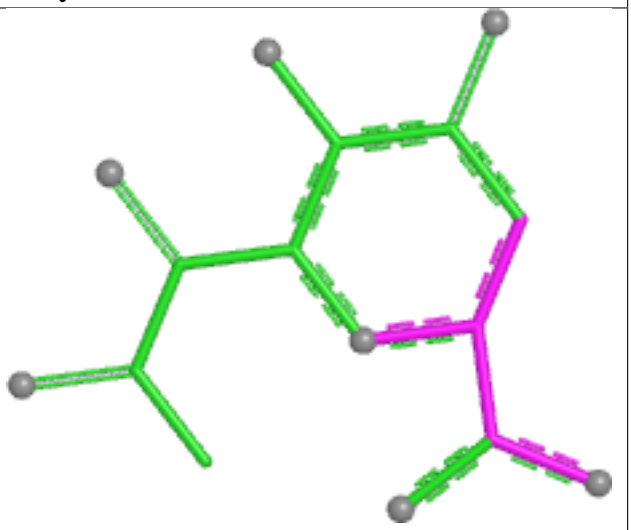


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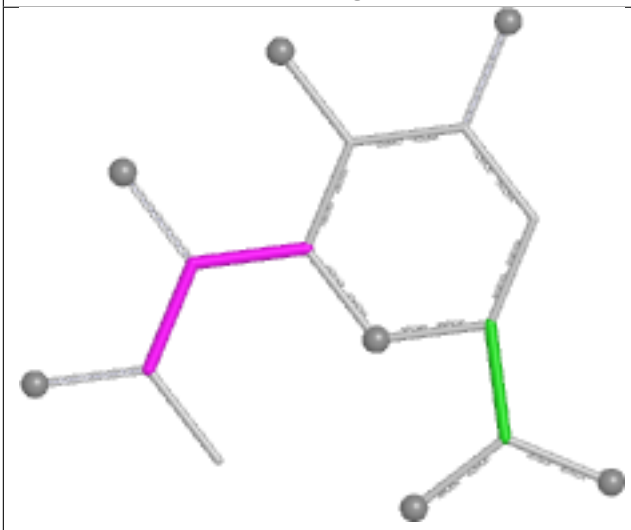
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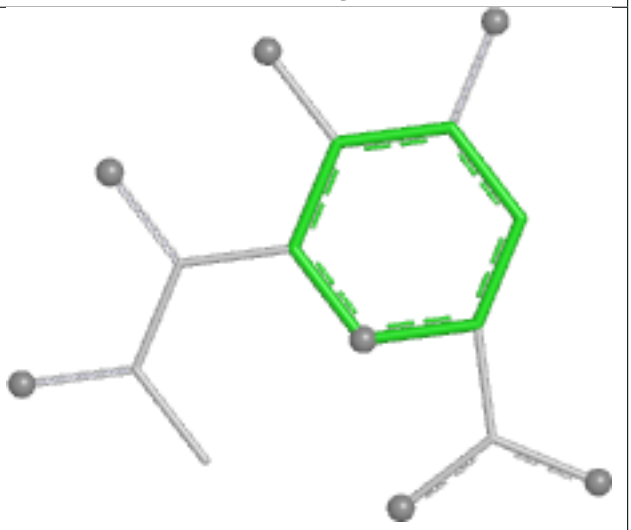
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Bond angles

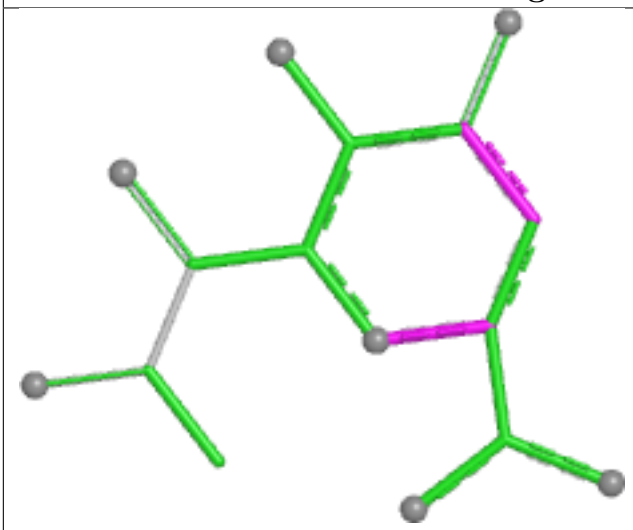


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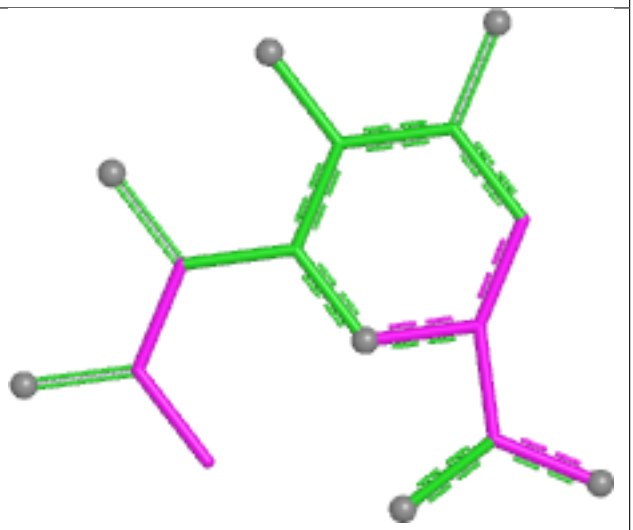


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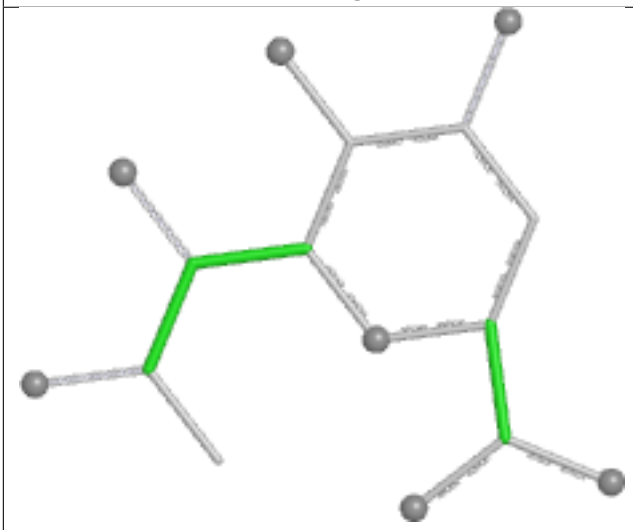
Ligand P8E V 603



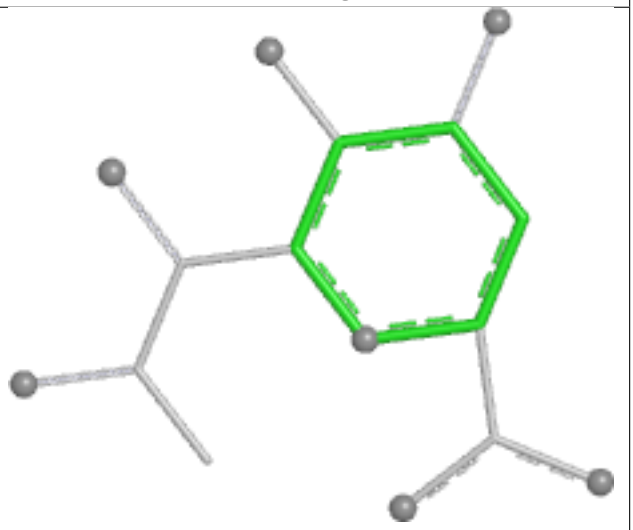
Bond lengths



Bond angles

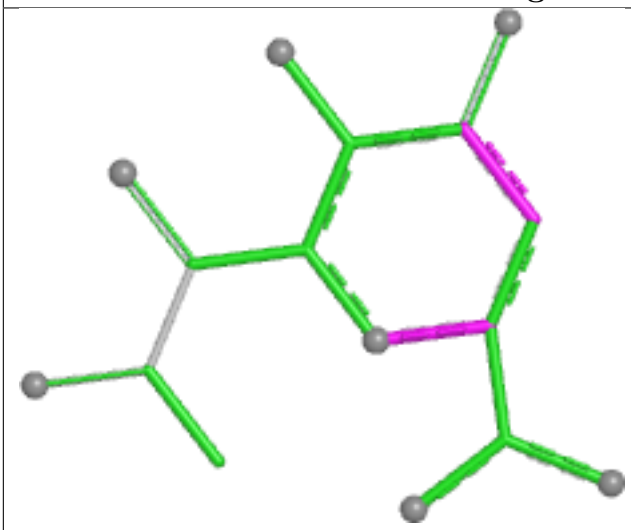


Torsions

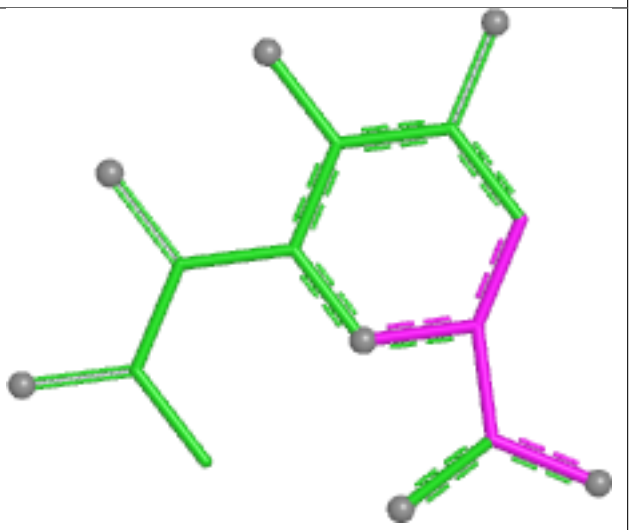


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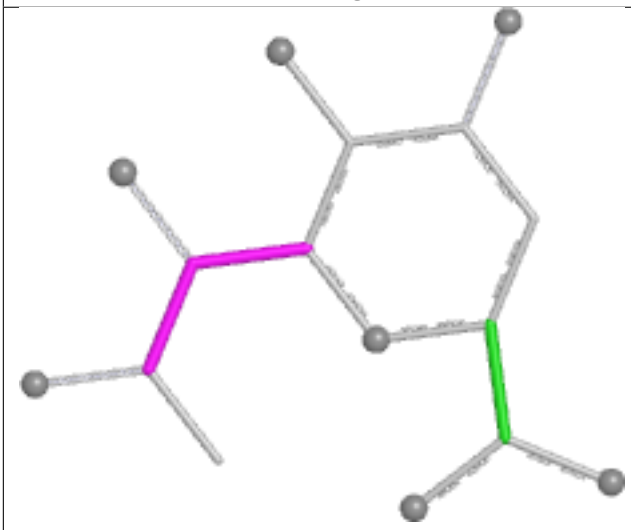
Ligand P8E H 605



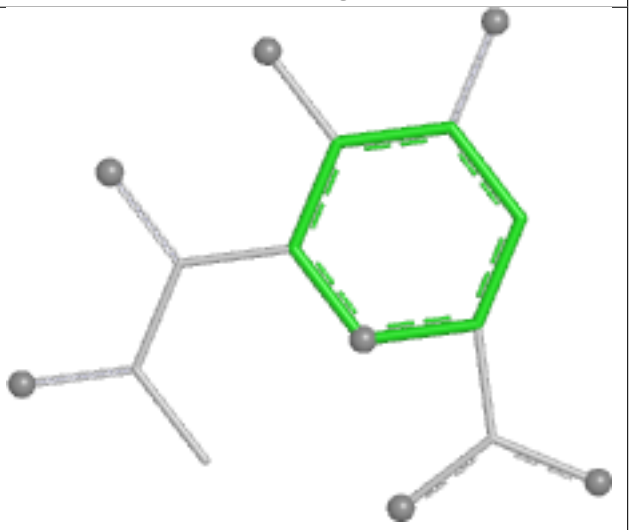
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Bond angles

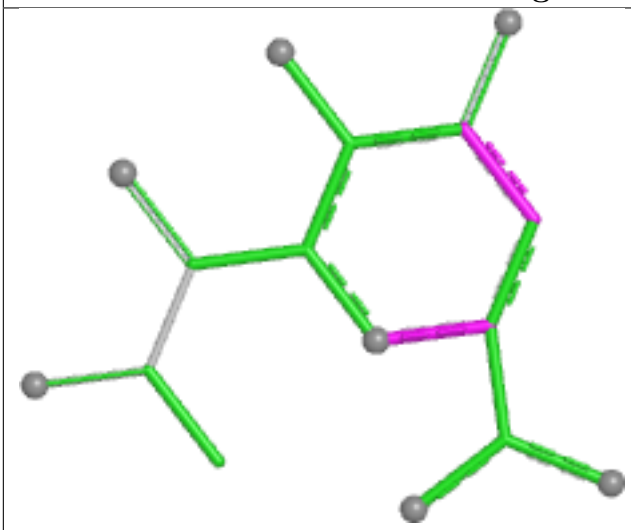


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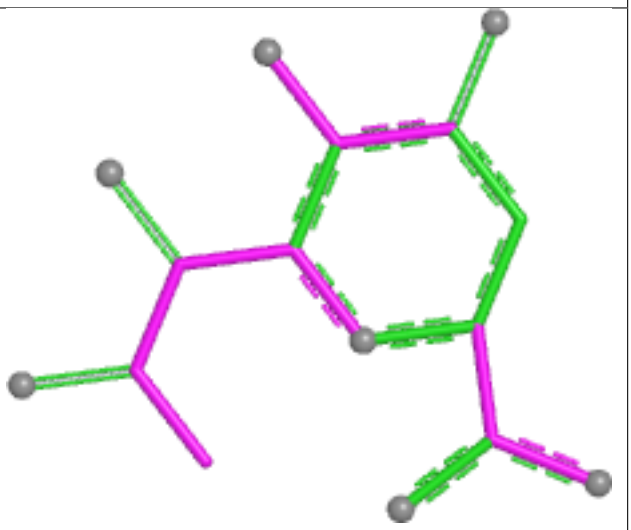


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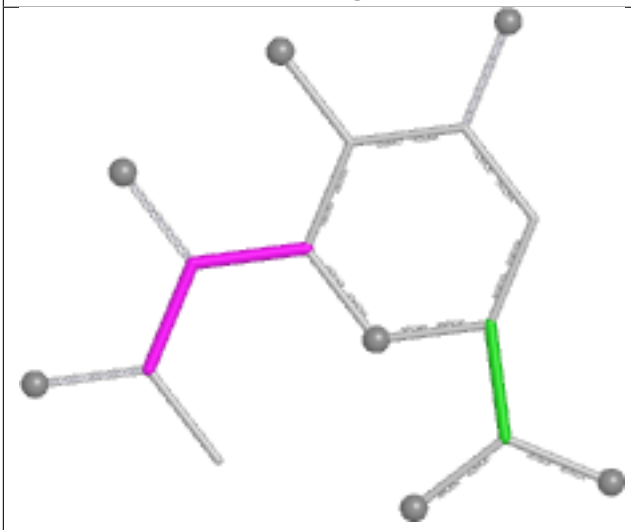
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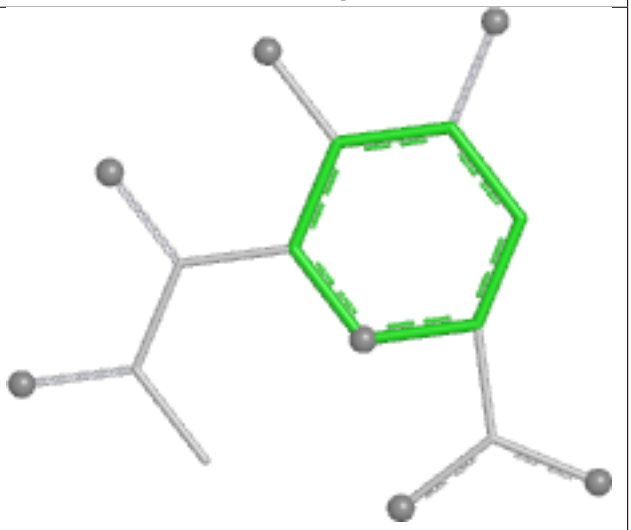
Bond lengths



Bond angles

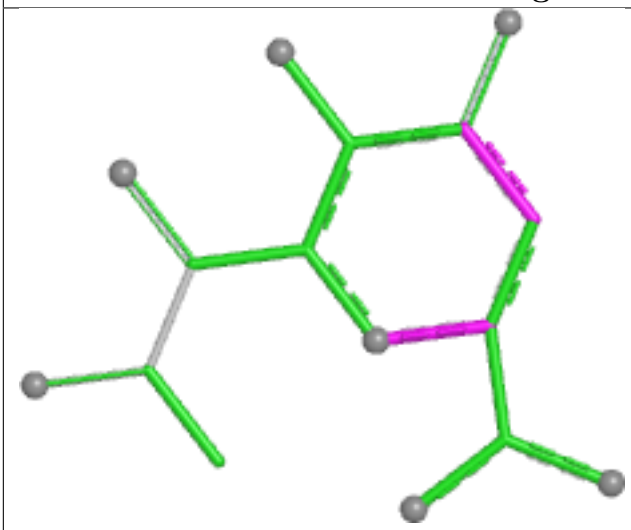


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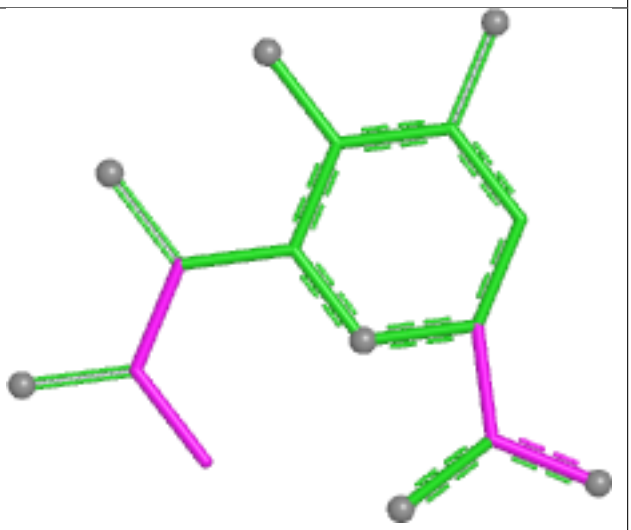


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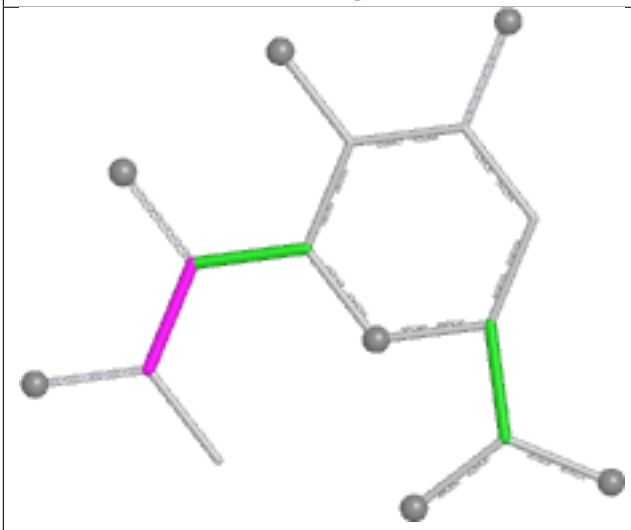
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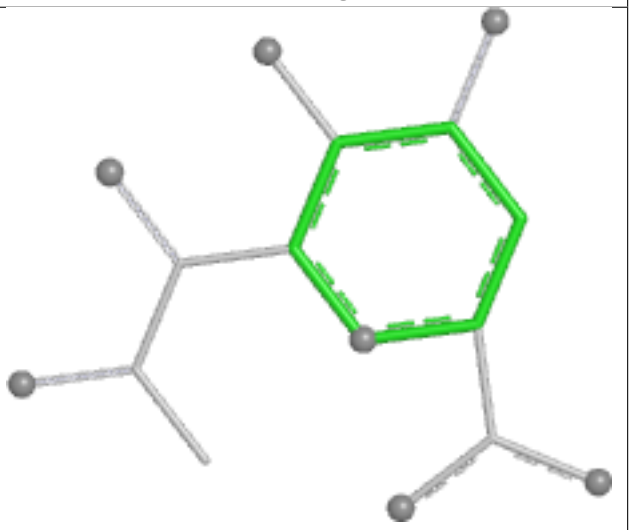
Bond lengths



Bond angles

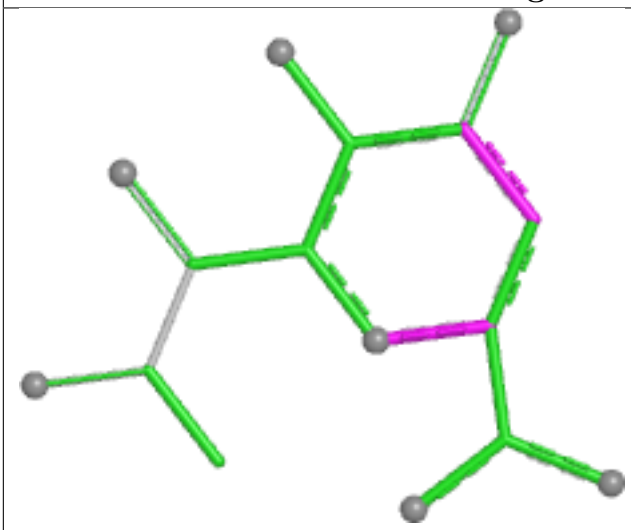


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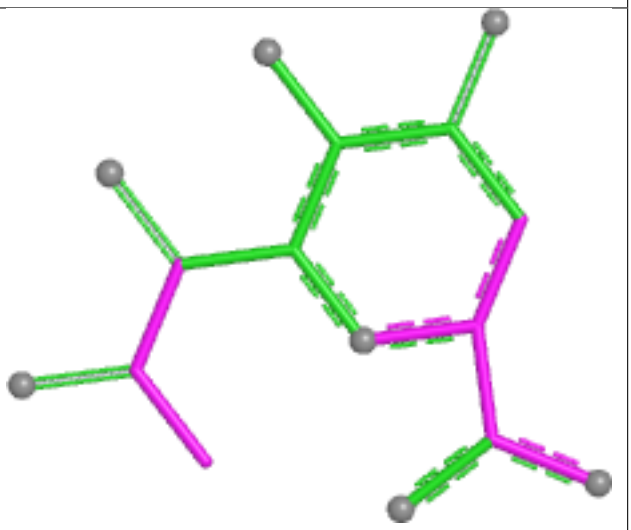


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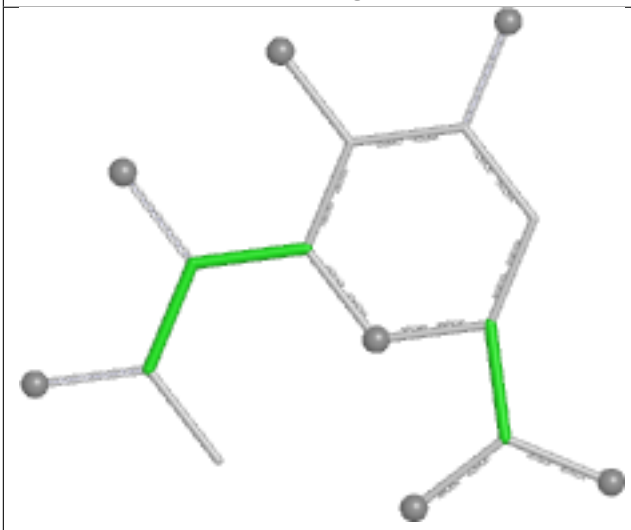
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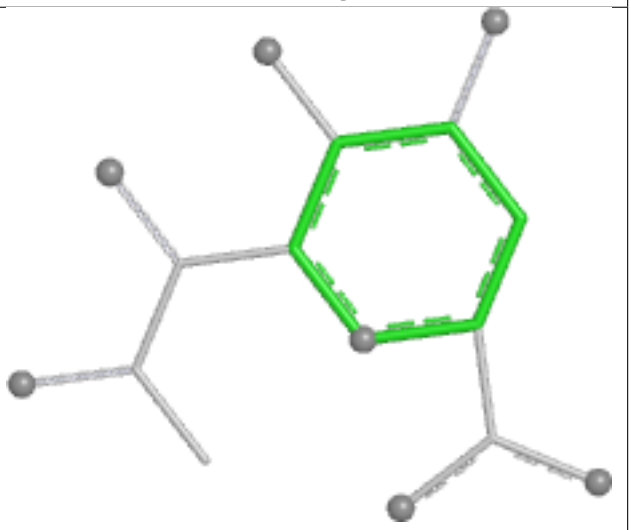
Bond lengths



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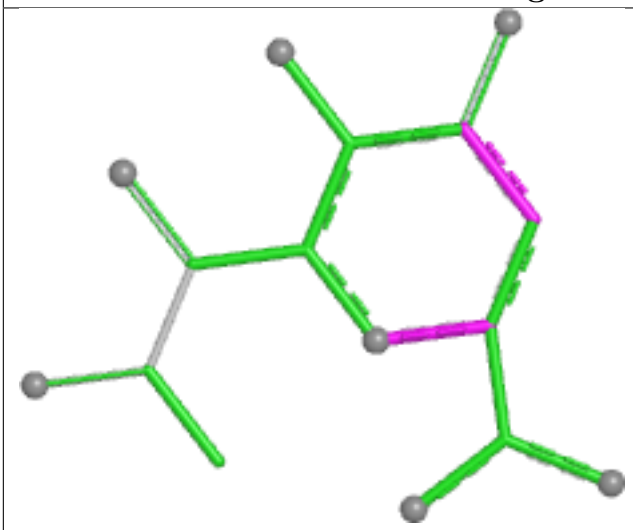


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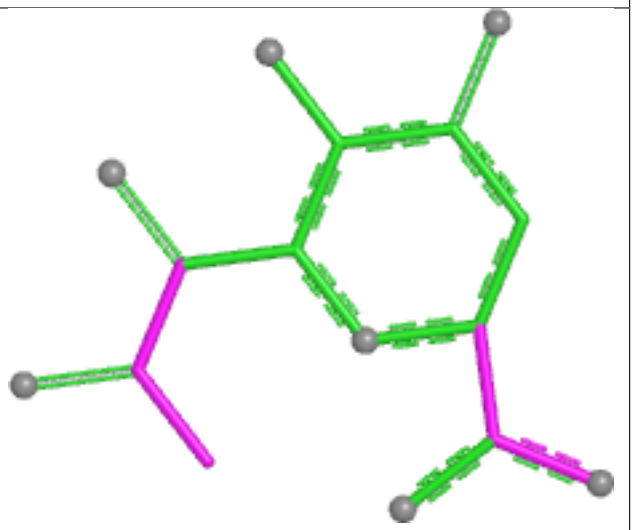


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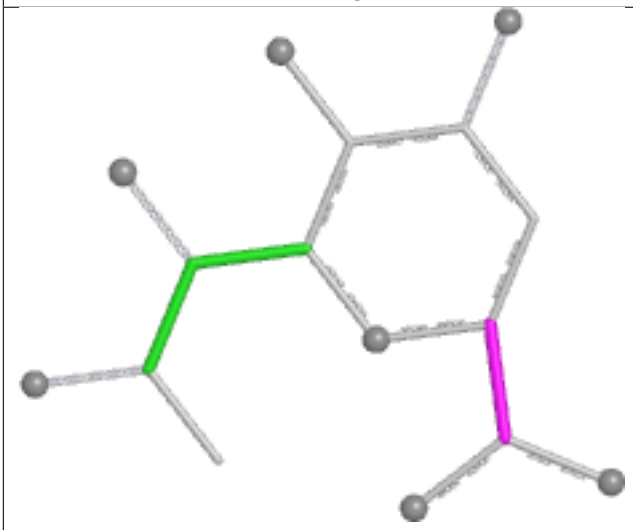
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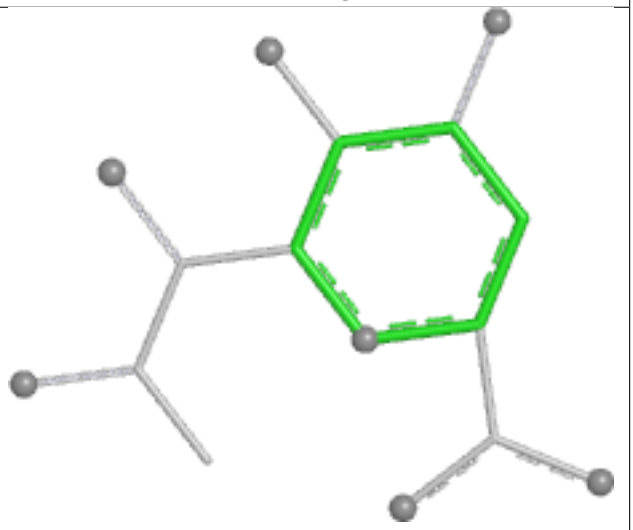
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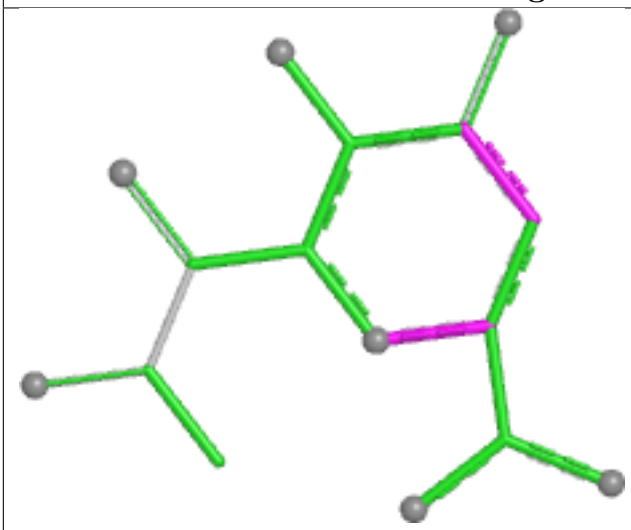


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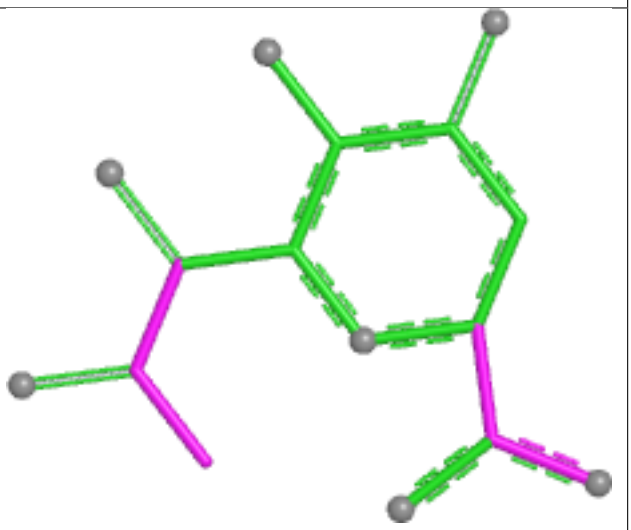


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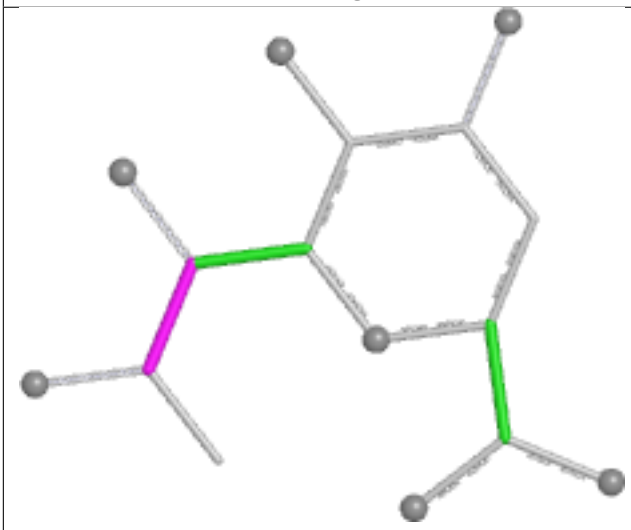
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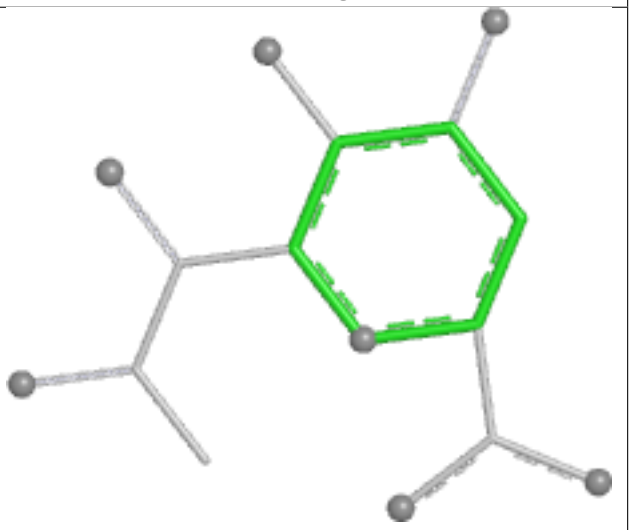
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Bond angles

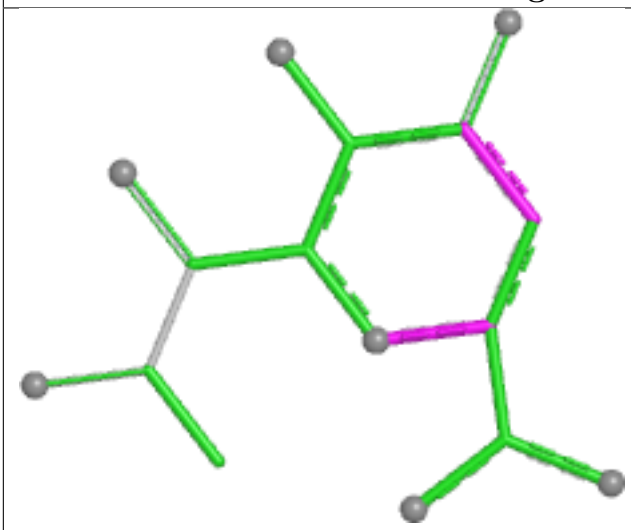


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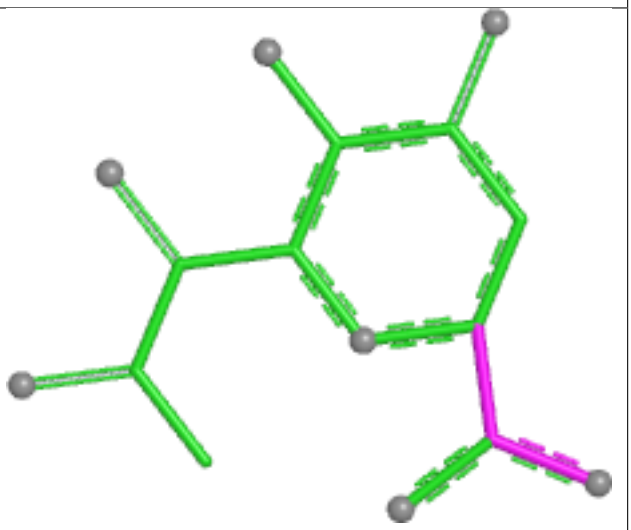


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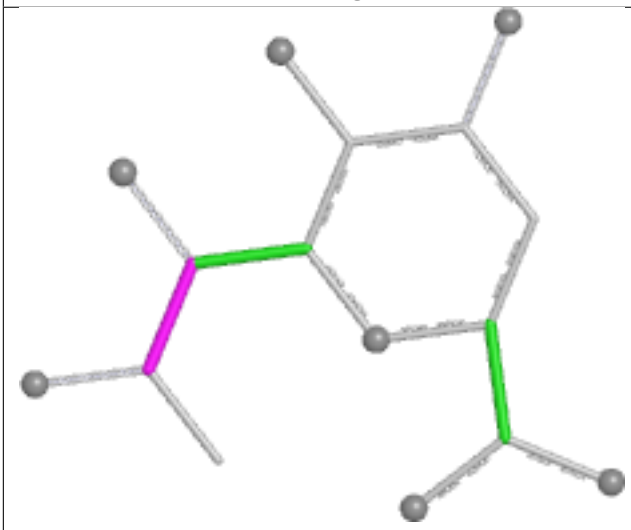
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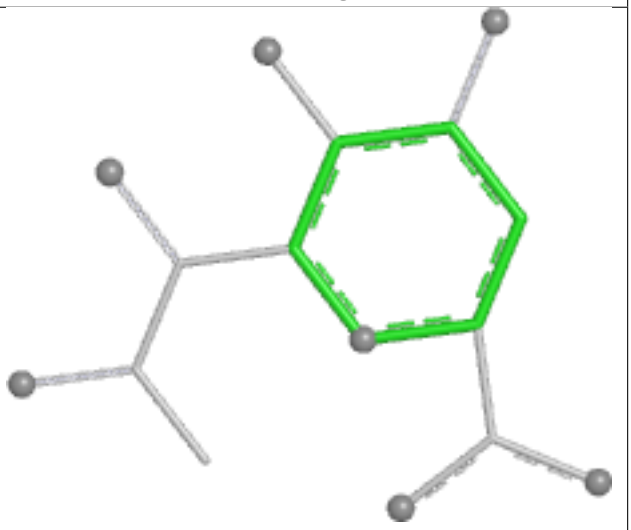
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Bond angles

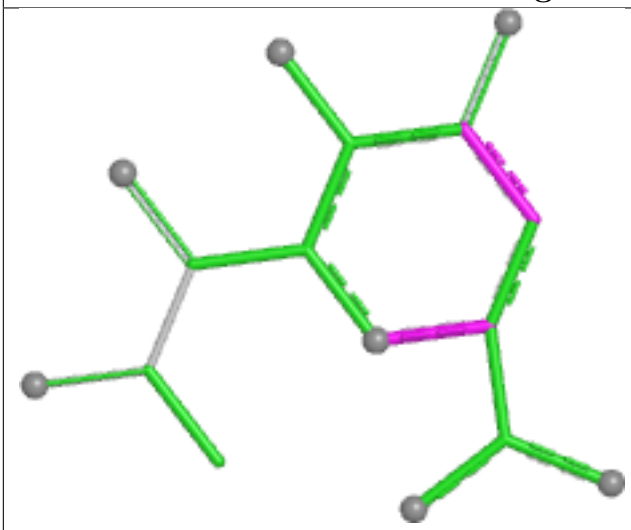


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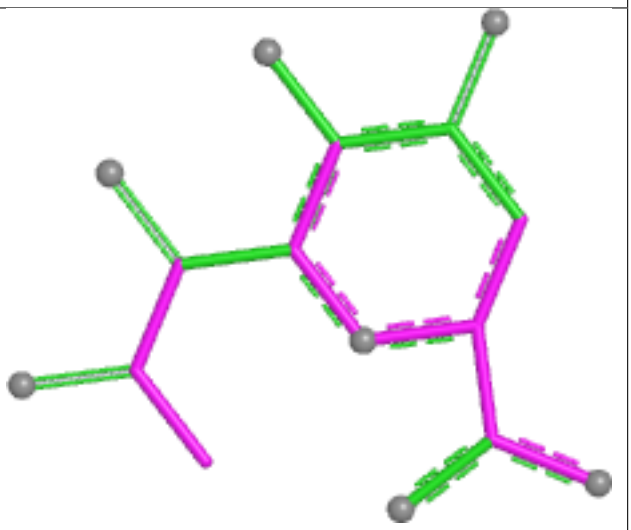


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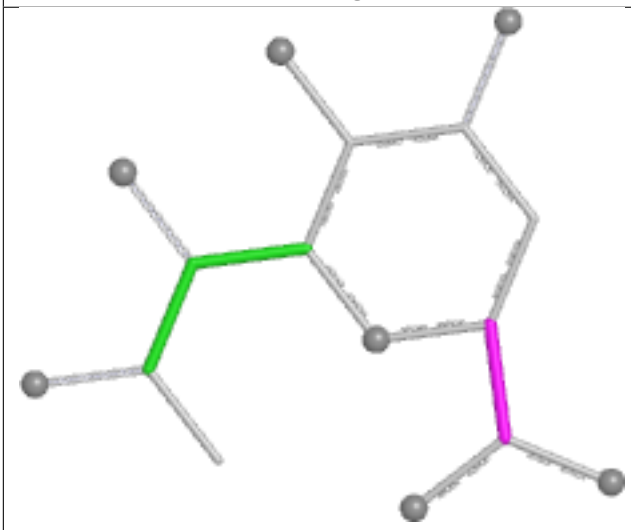
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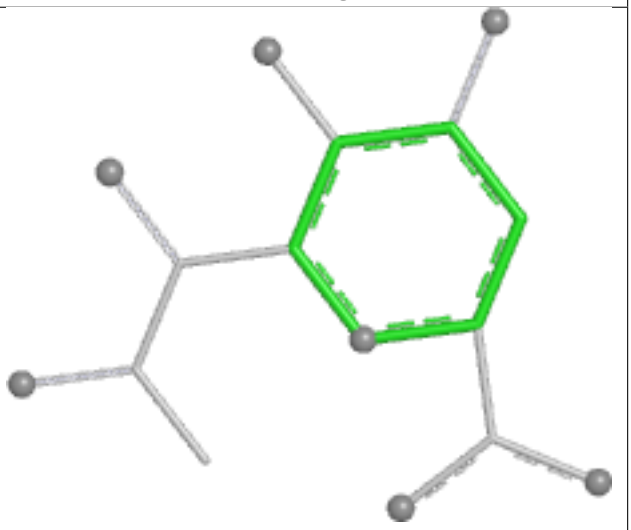
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Bond angles

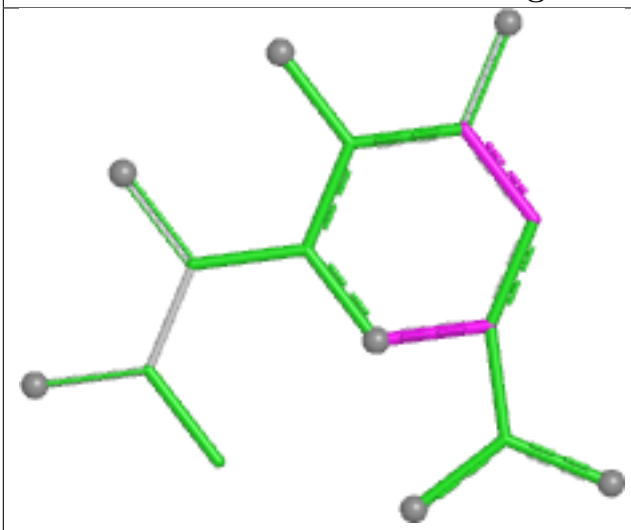


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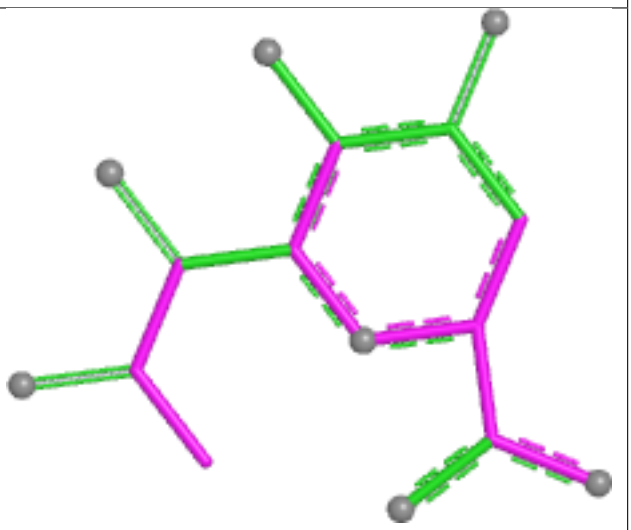


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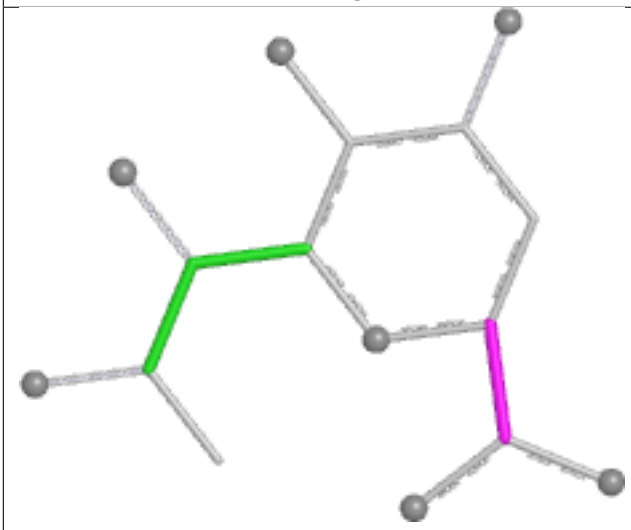
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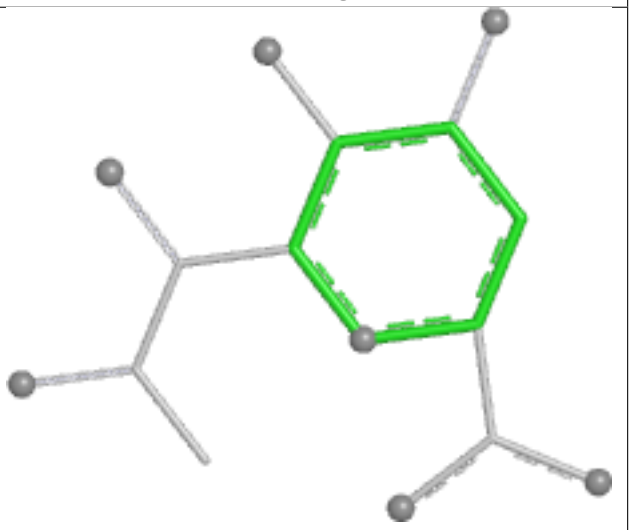
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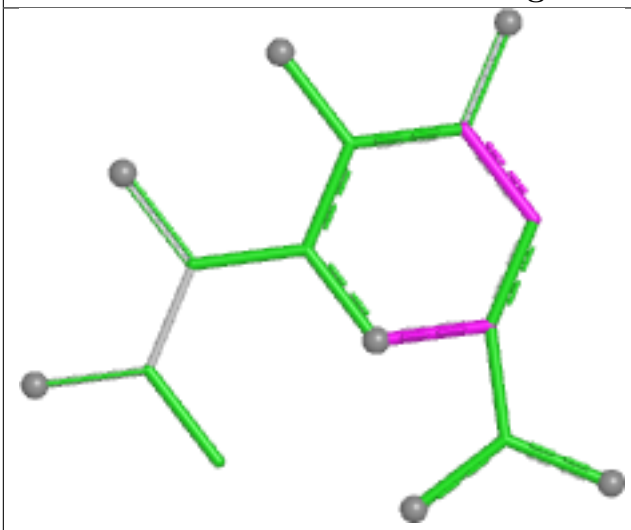


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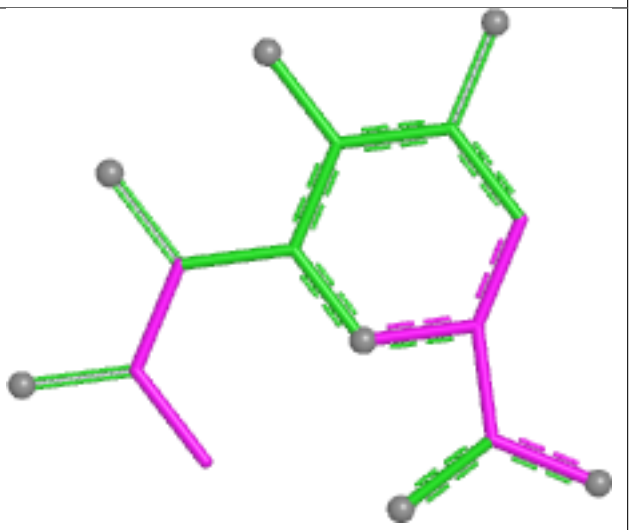


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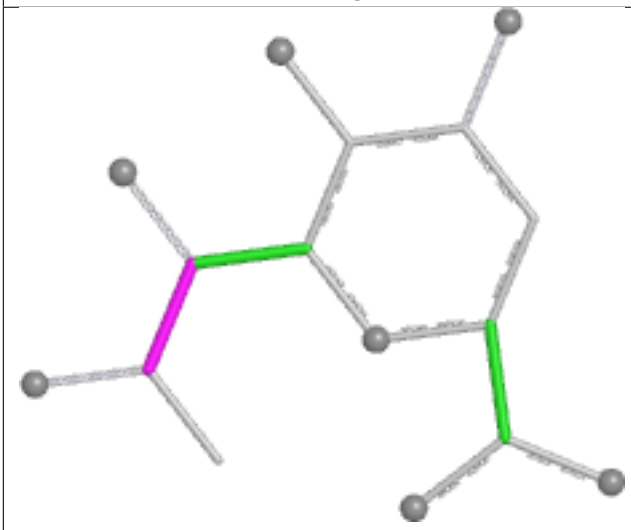
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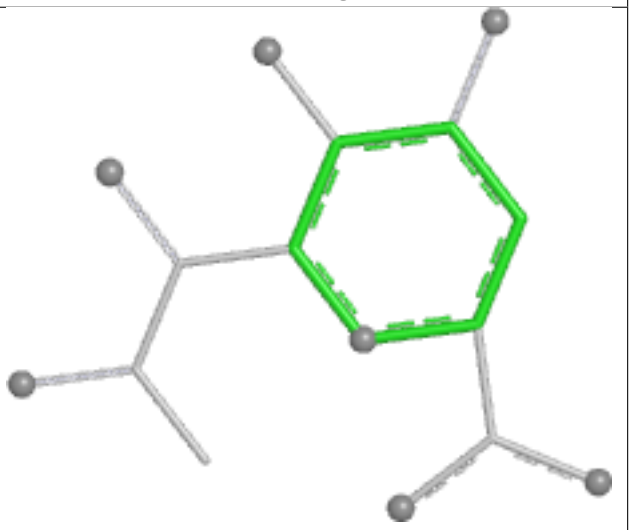
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Bond angles

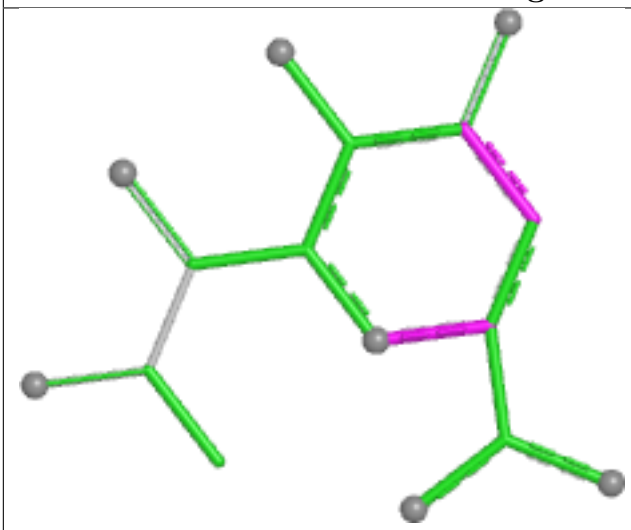


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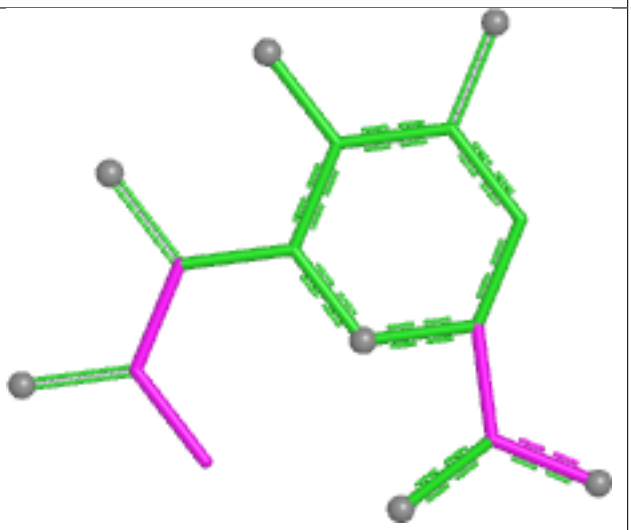


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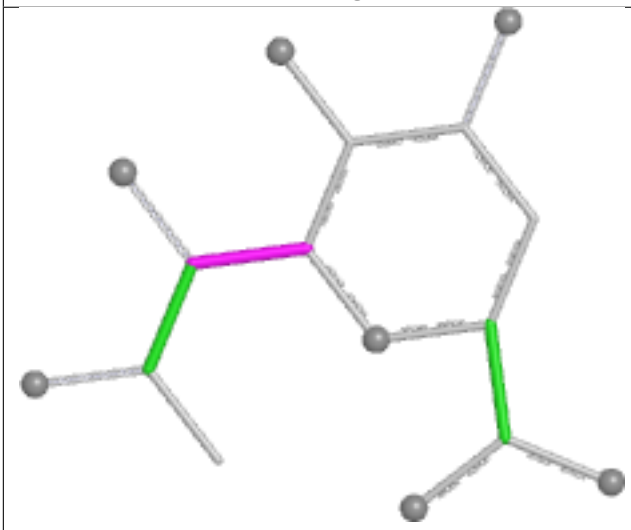
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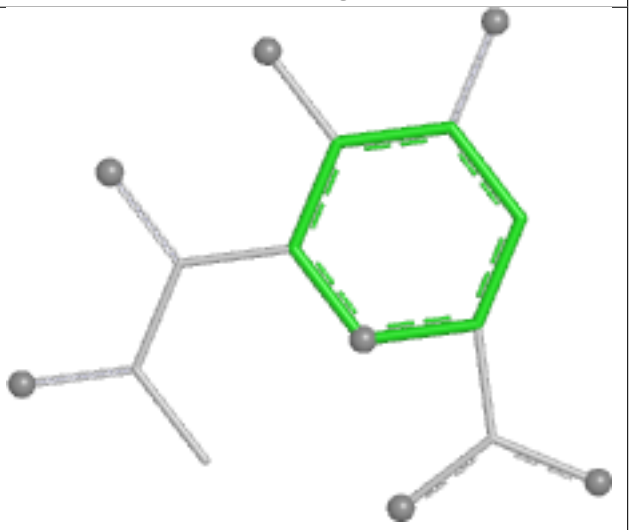
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Bond angles

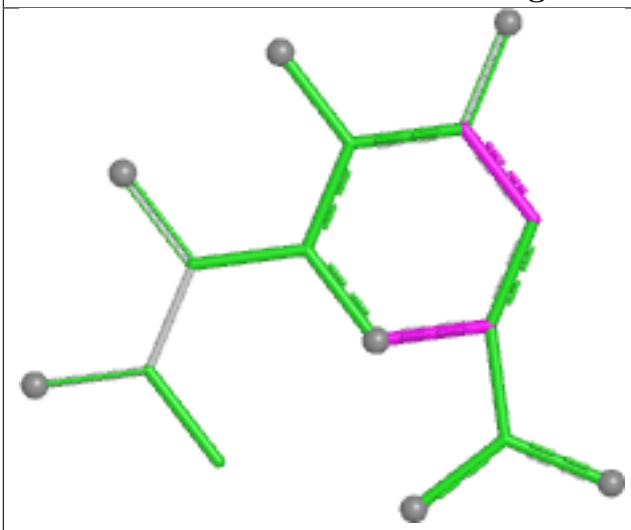


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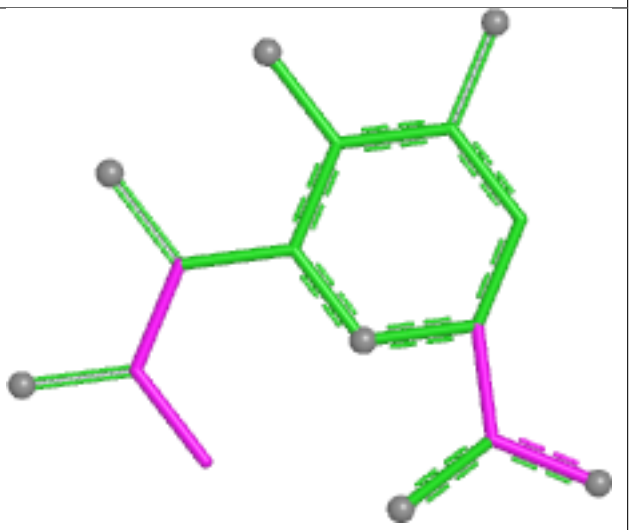


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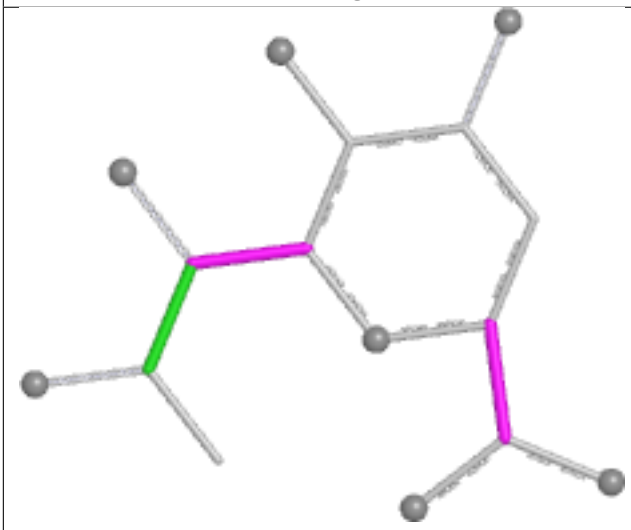
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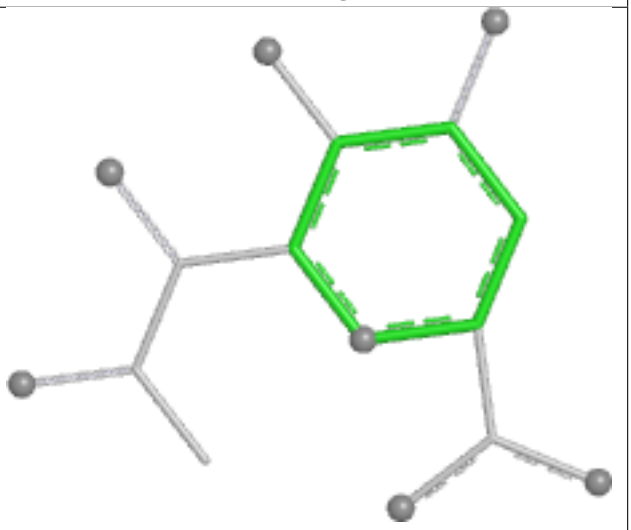
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Bond angles

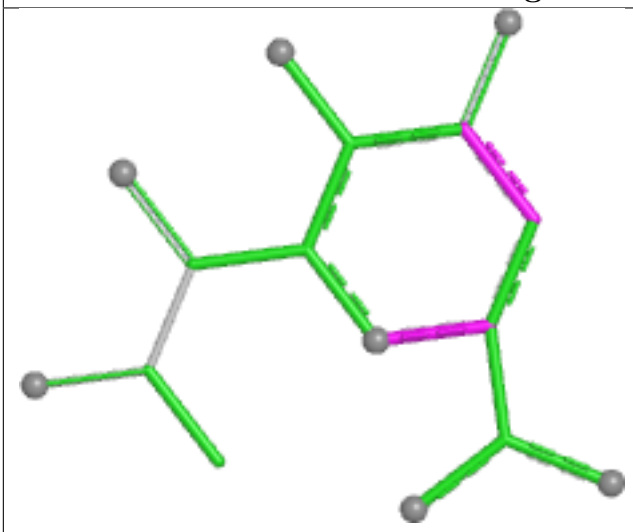


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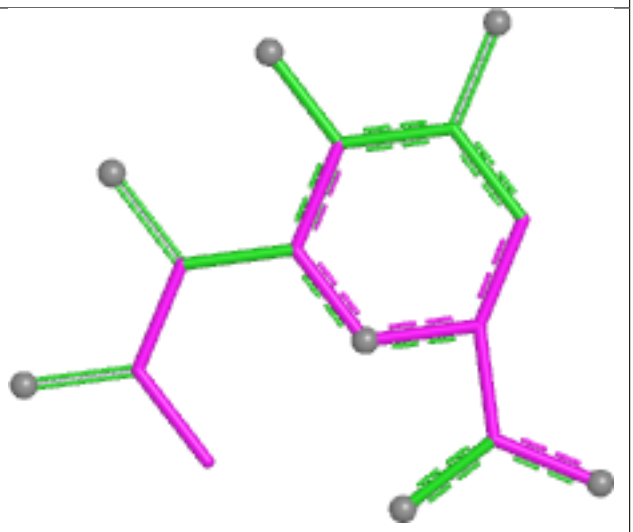


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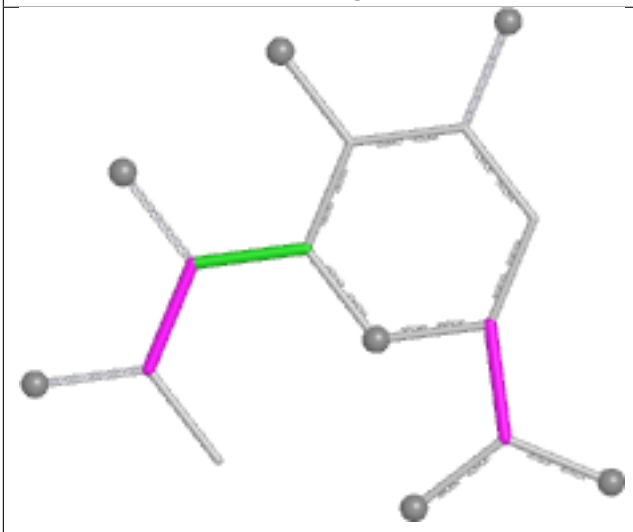
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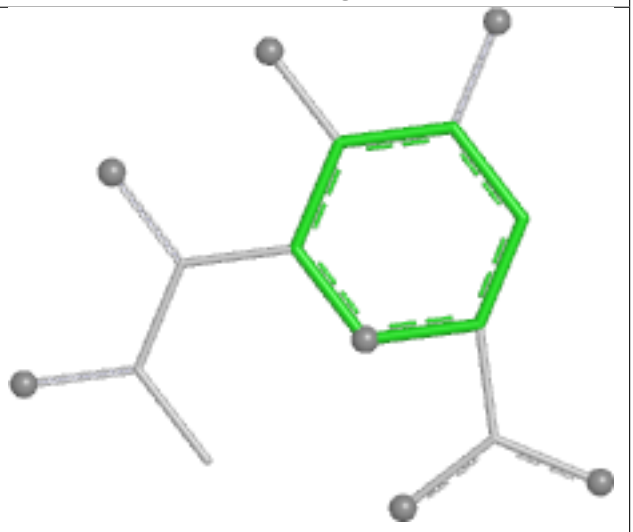
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Bond angles

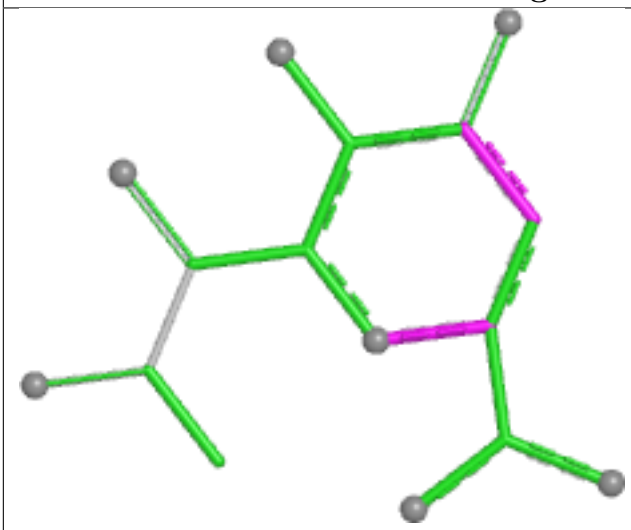


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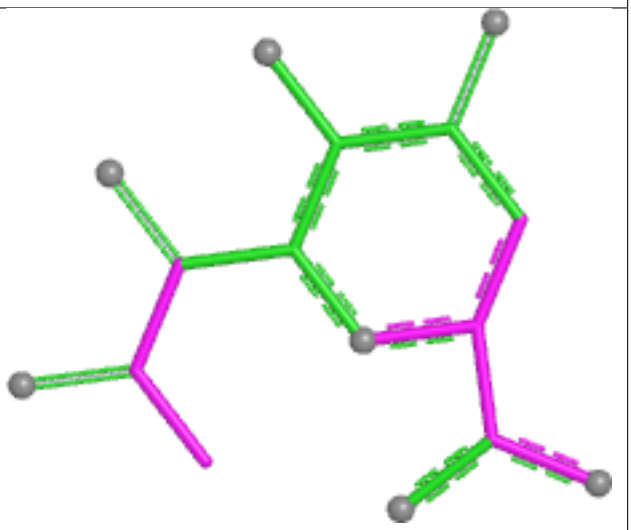


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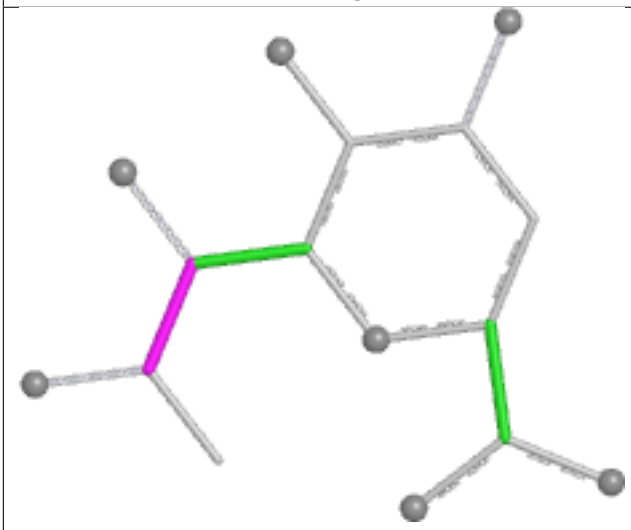
Ligand P8E F 605



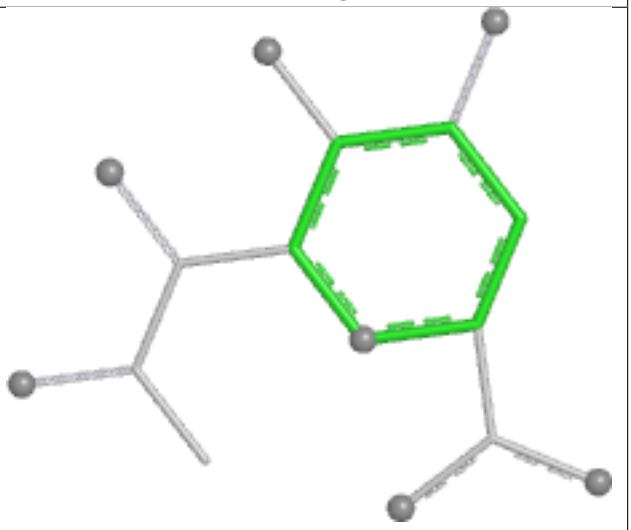
Bond lengths



Bond angles

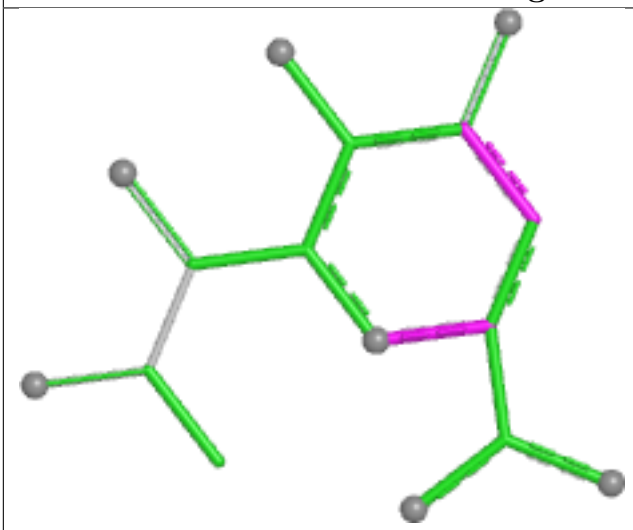


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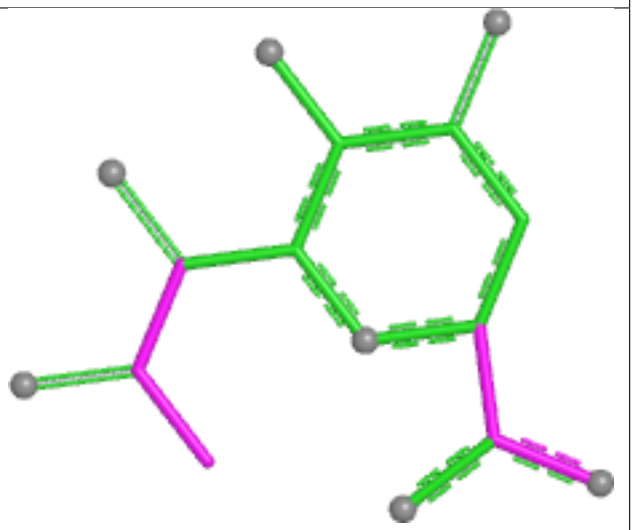


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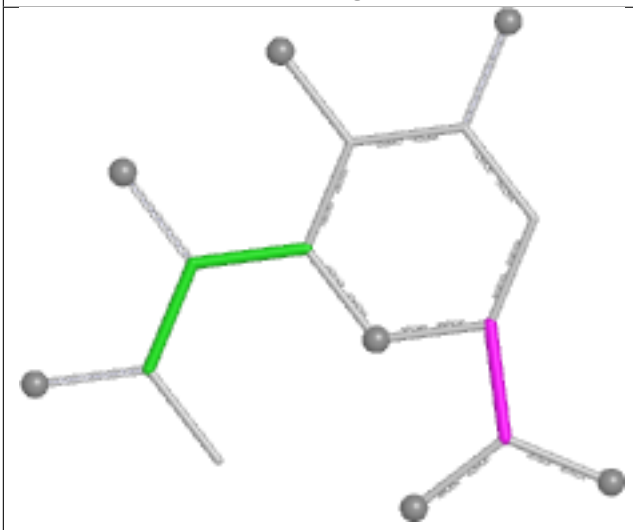
Ligand P8E V 611



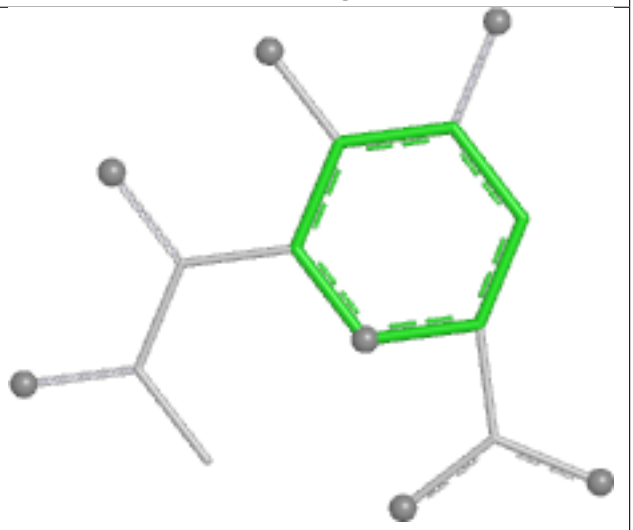
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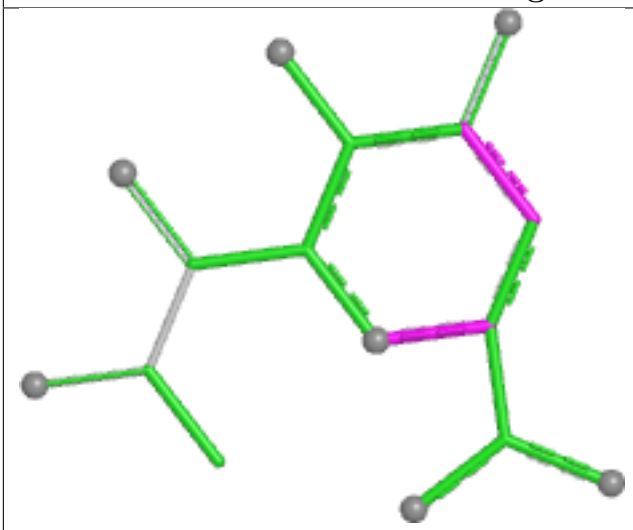


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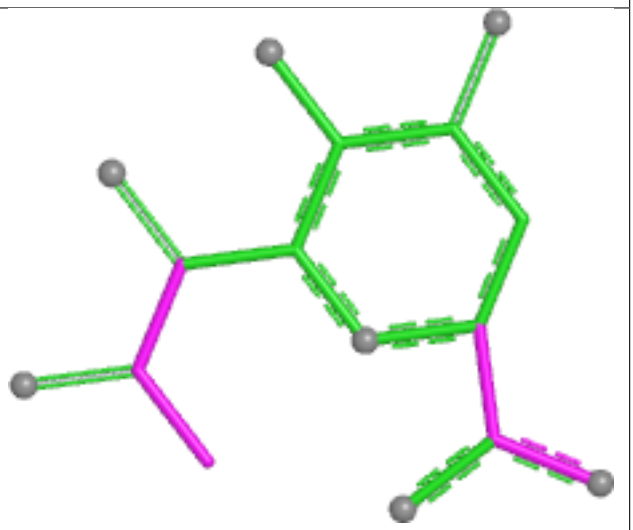


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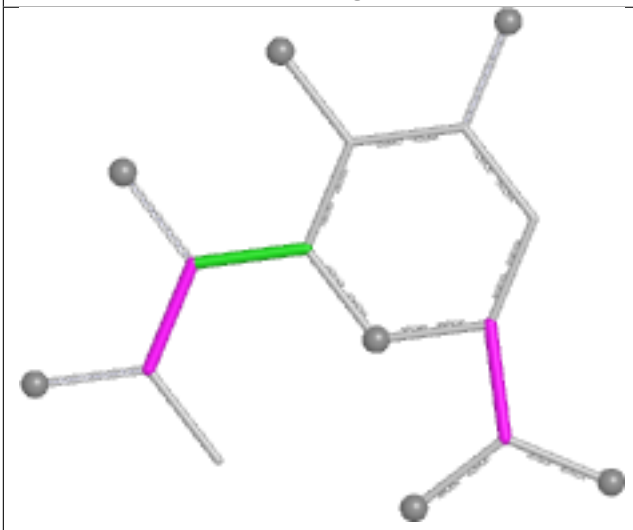
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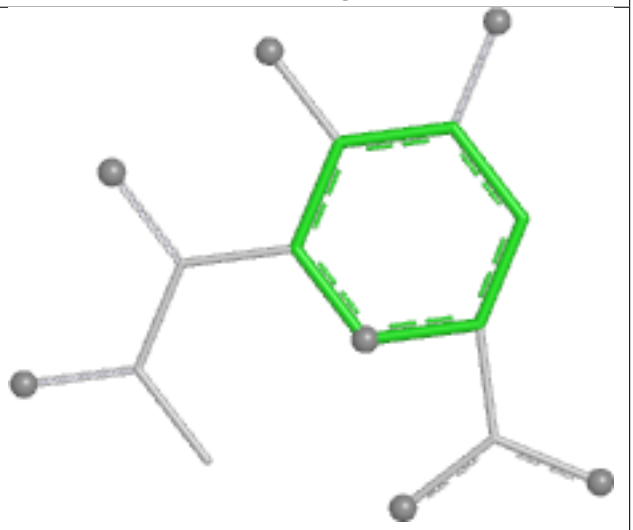
Bond lengths



Bond angles

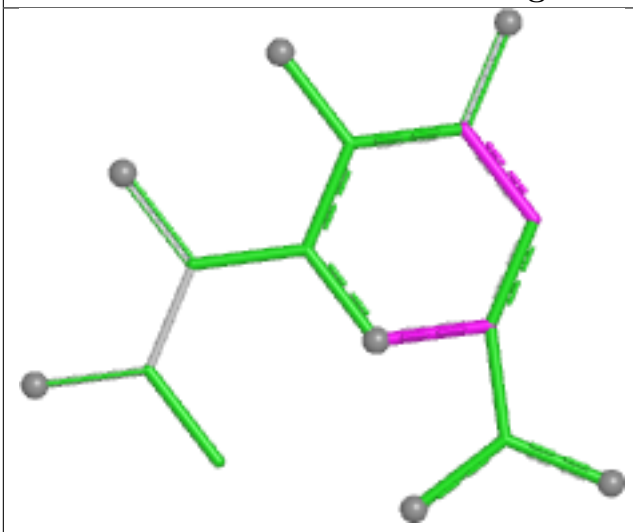


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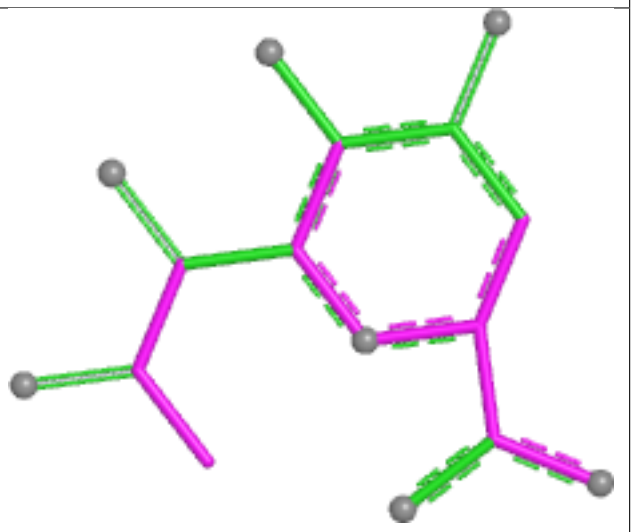


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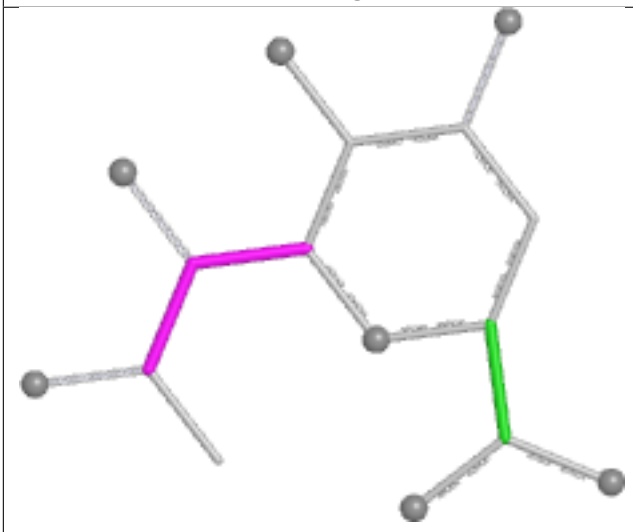
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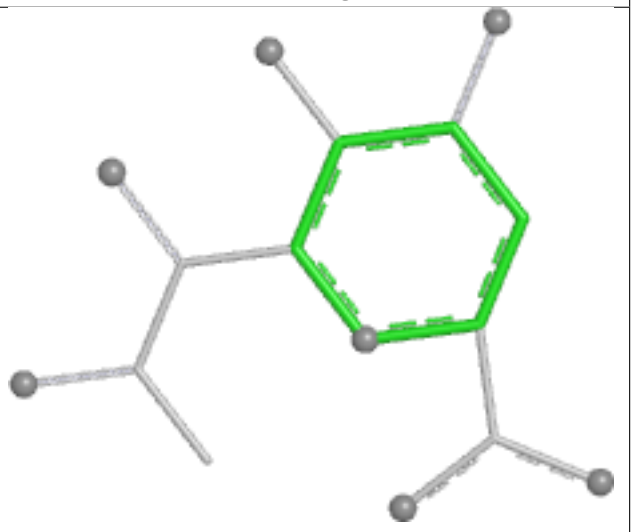
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Bond angles

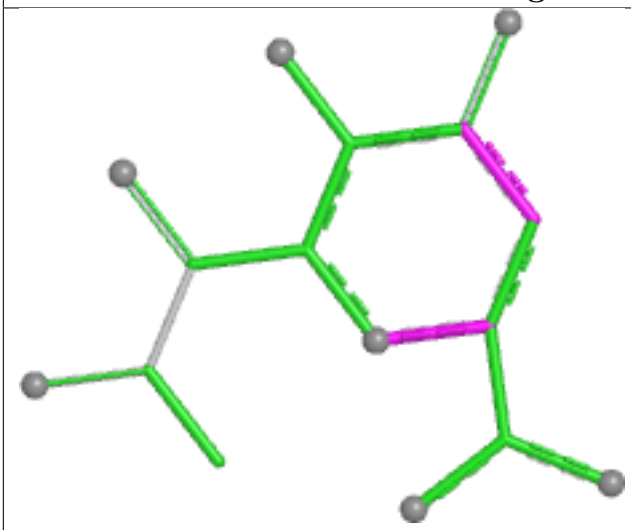


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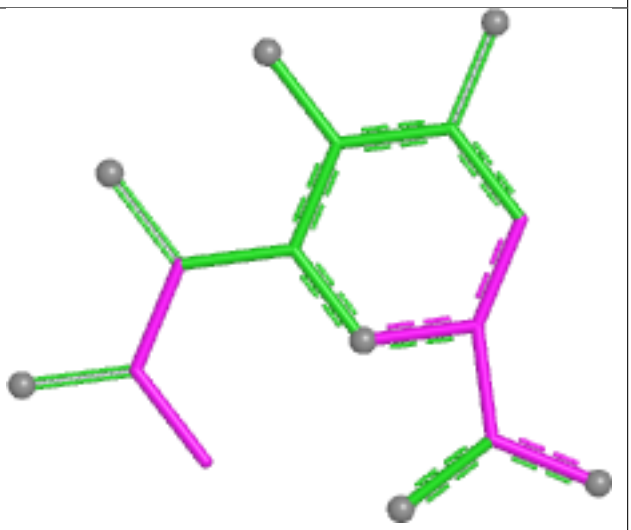


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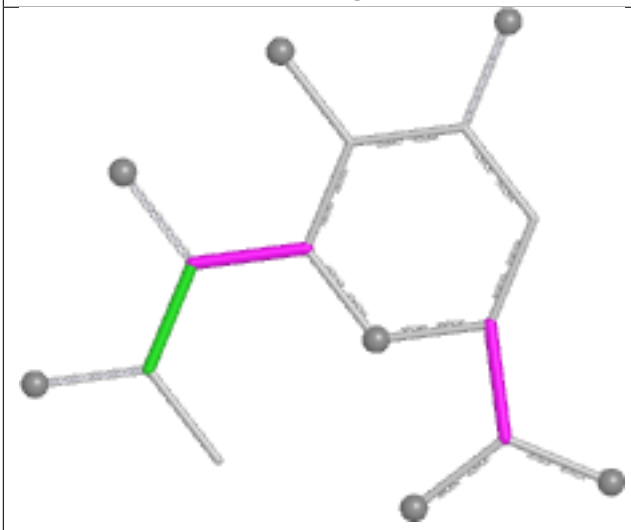
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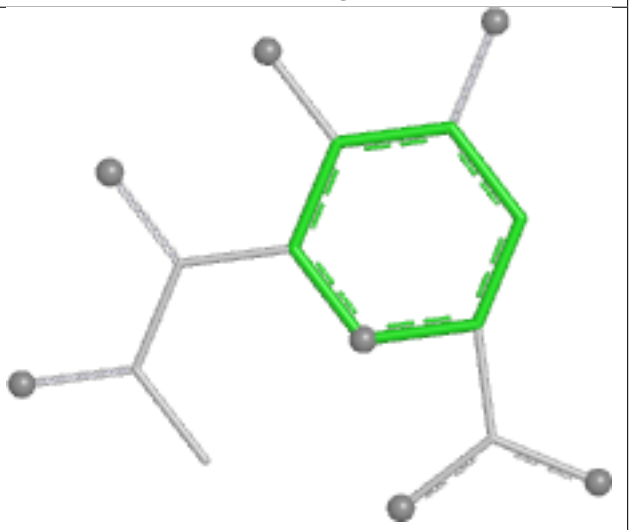
Bond lengths



Bond angles

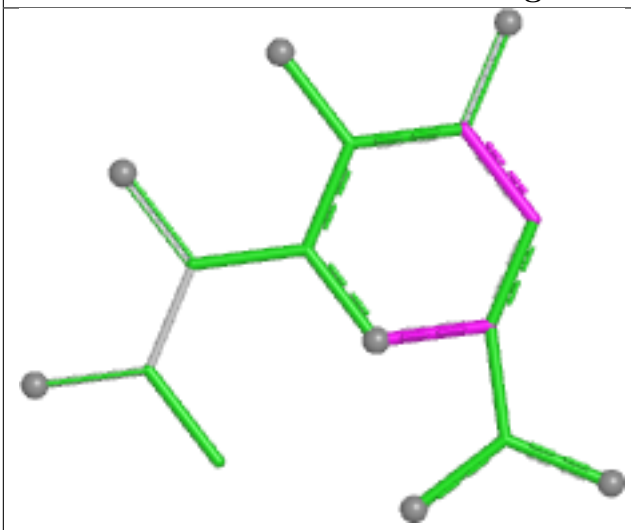


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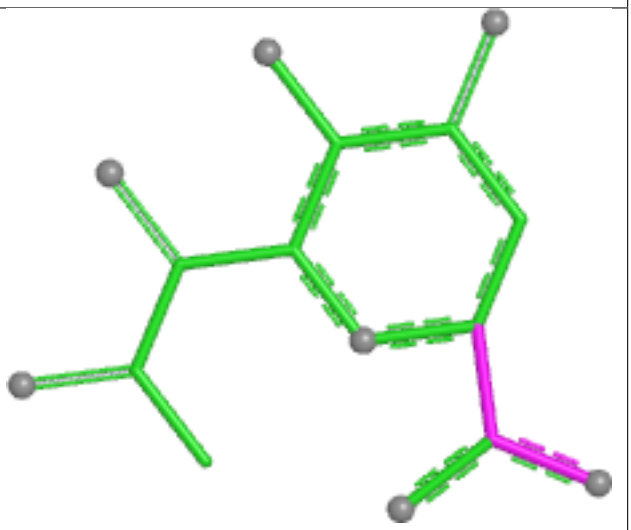


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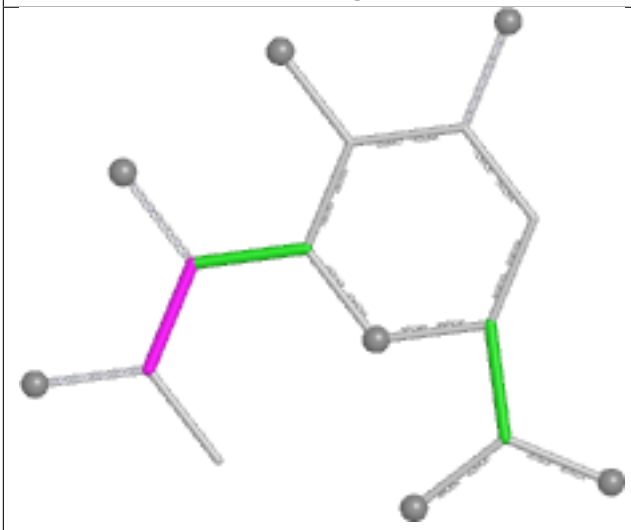
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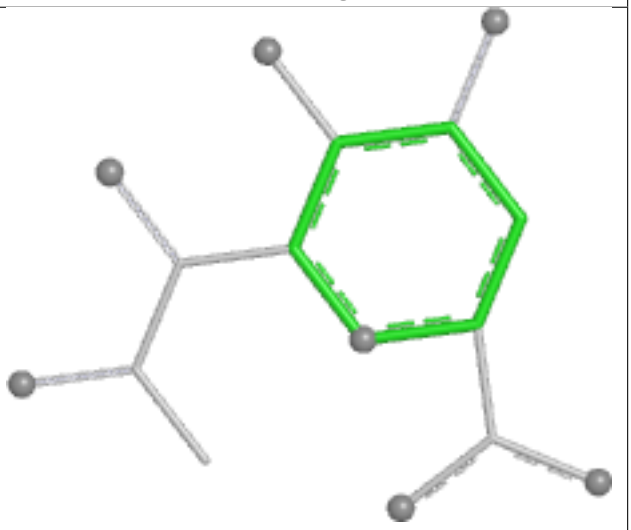
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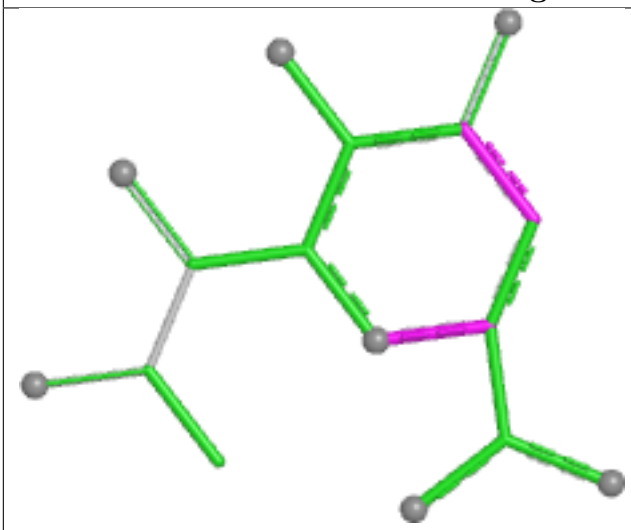


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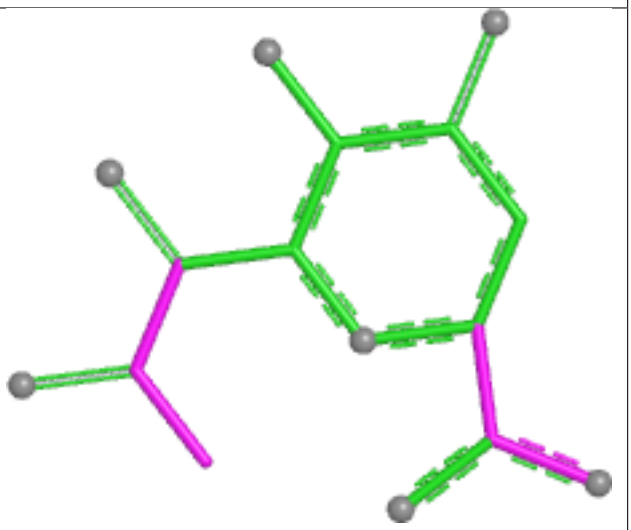


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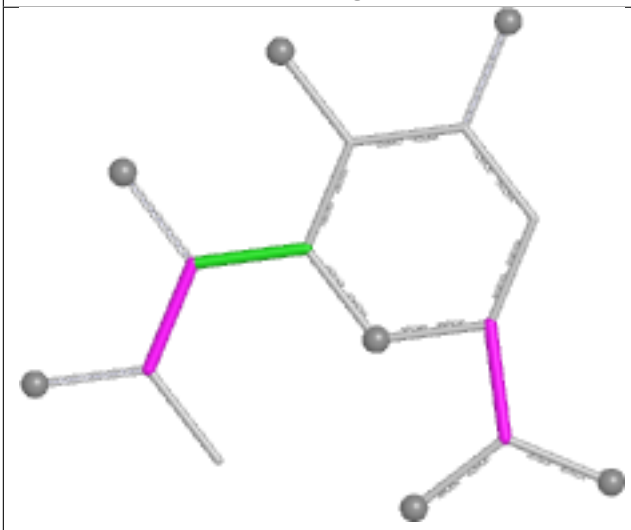
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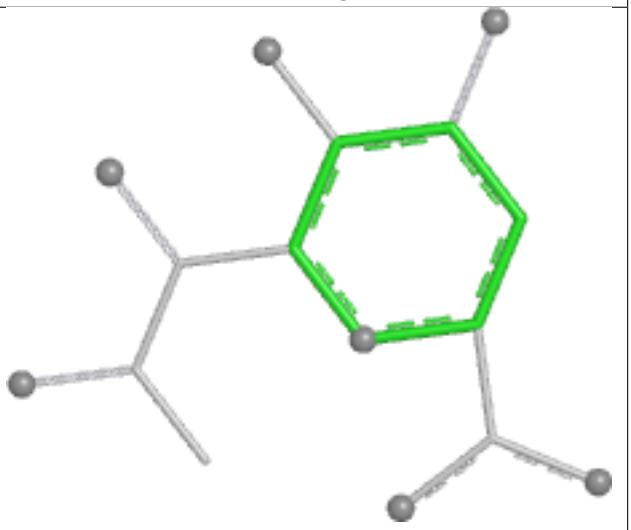
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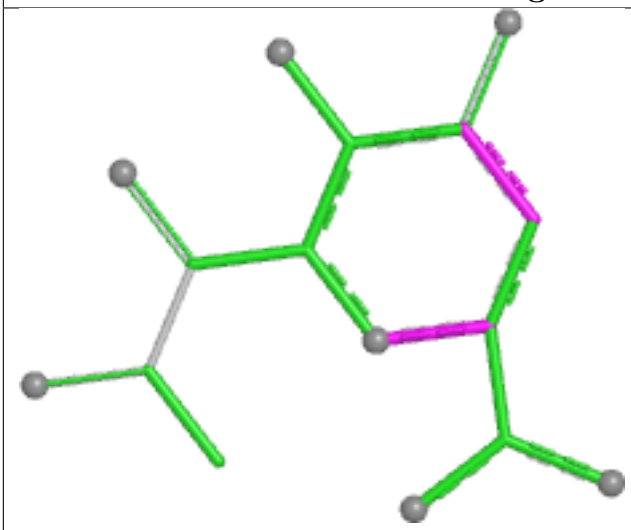


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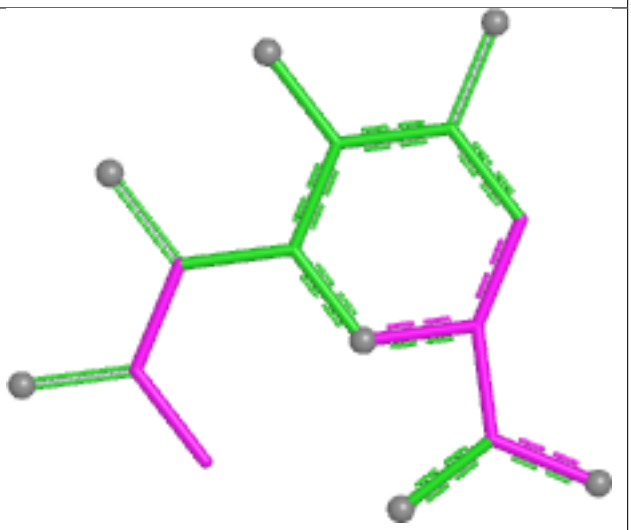


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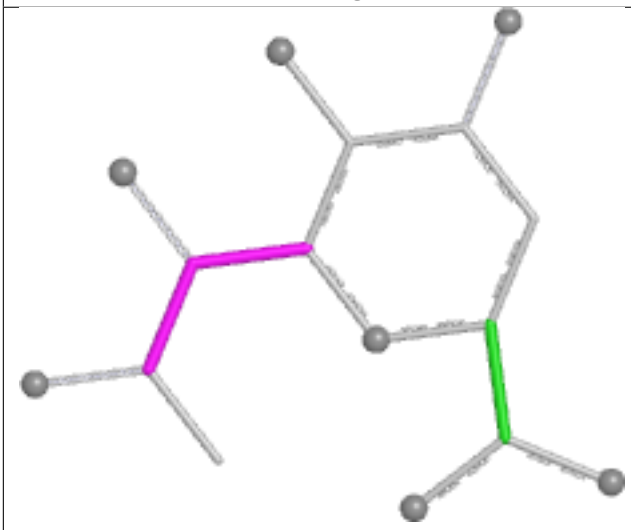
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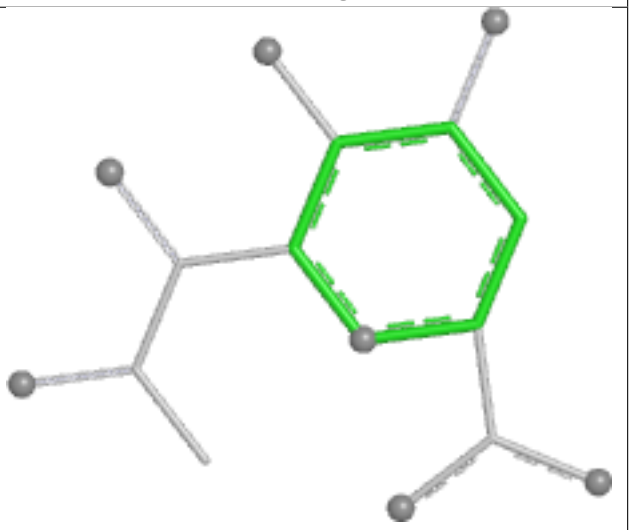
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Bond angles

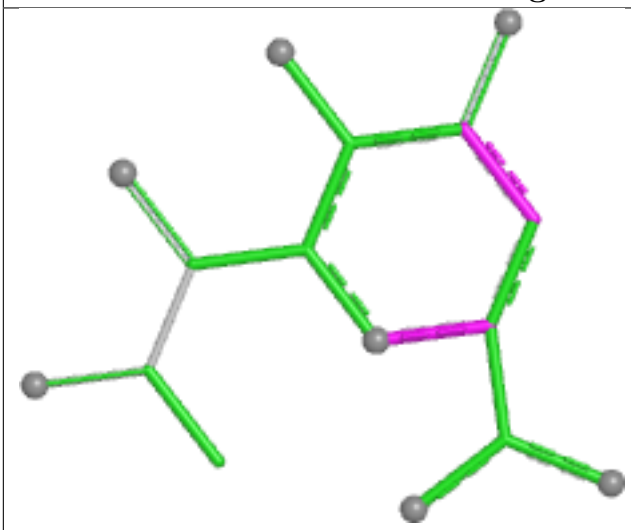


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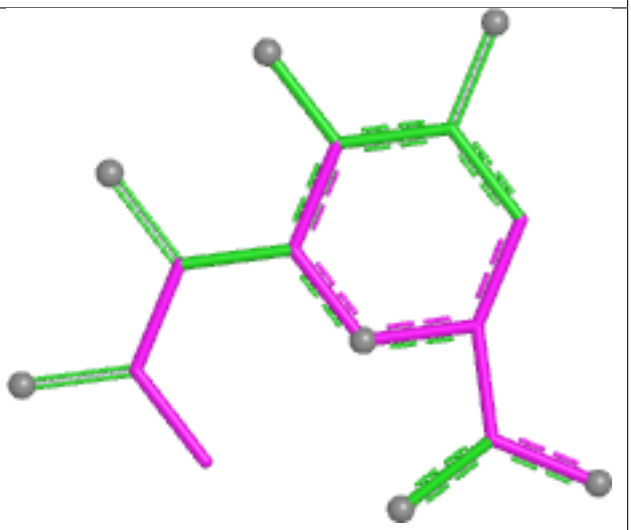


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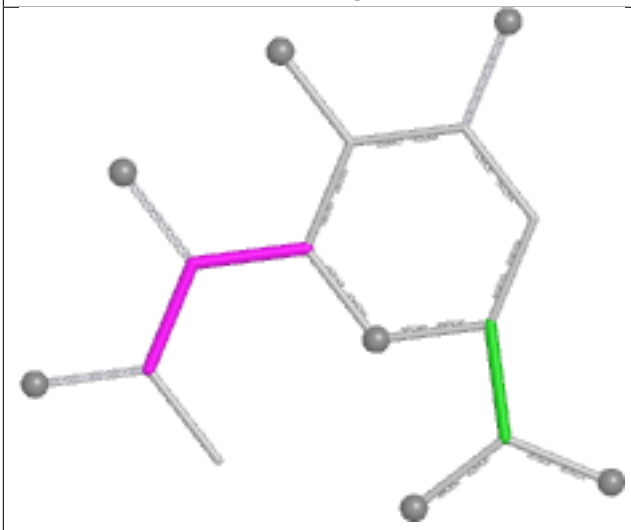
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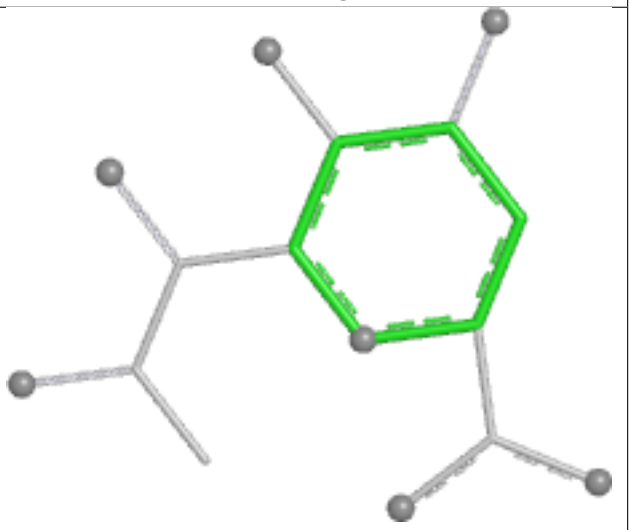
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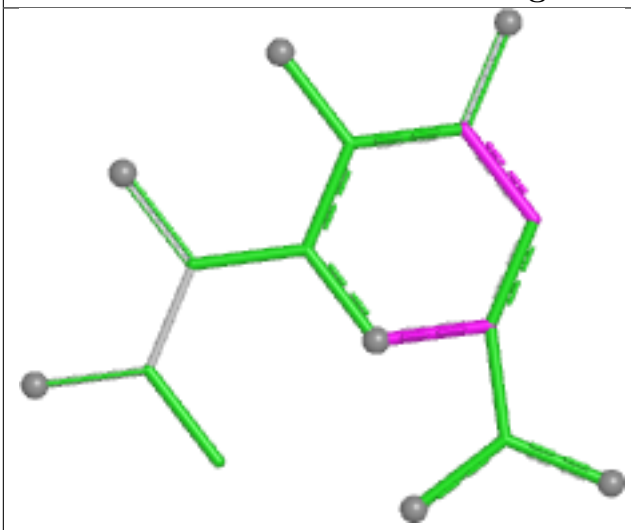


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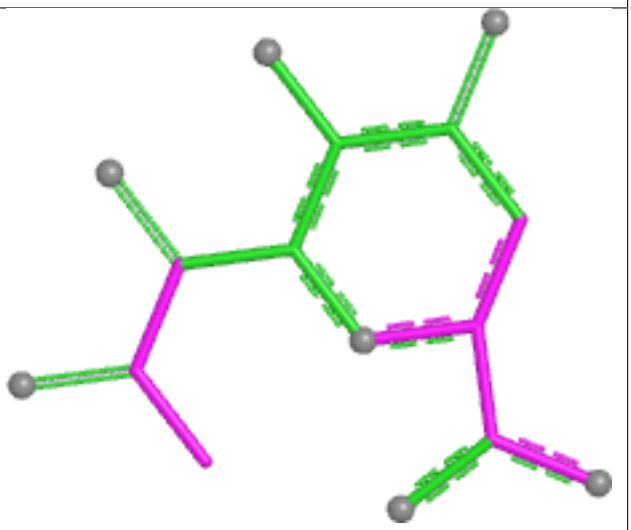


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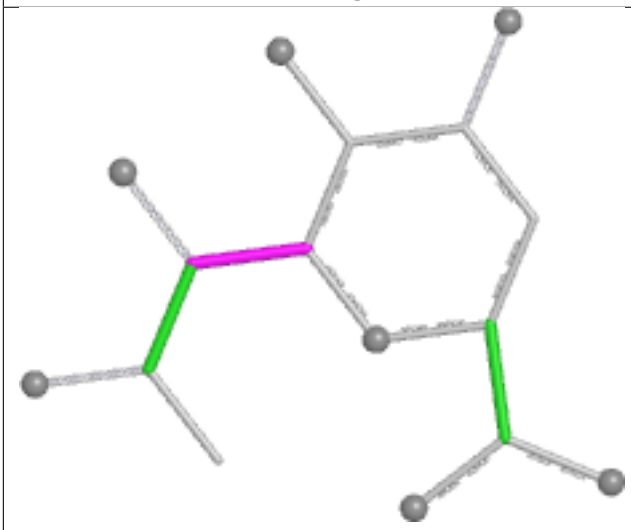
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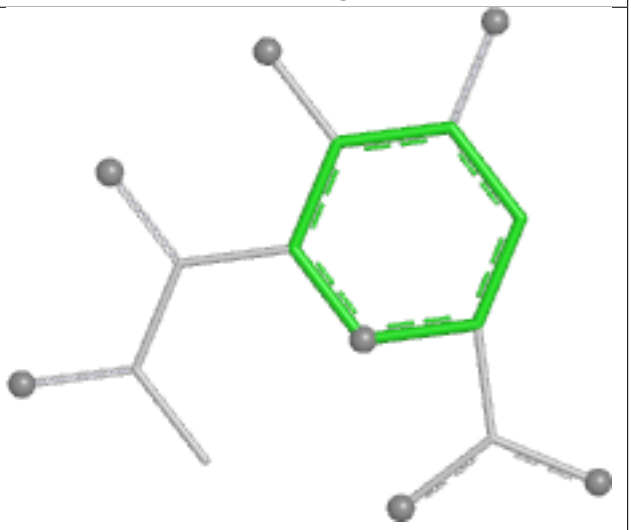
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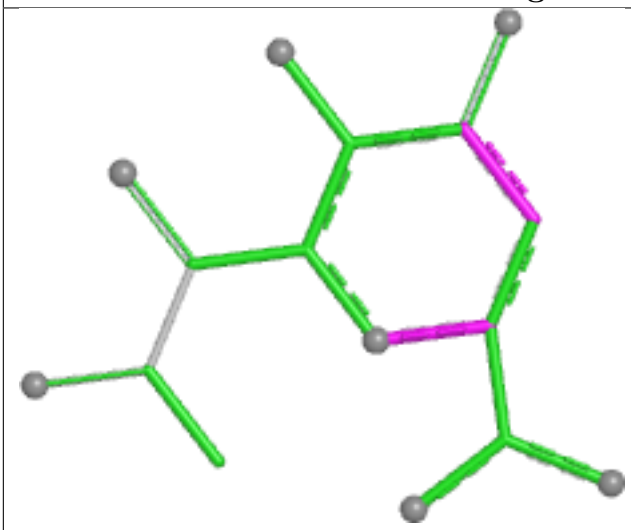


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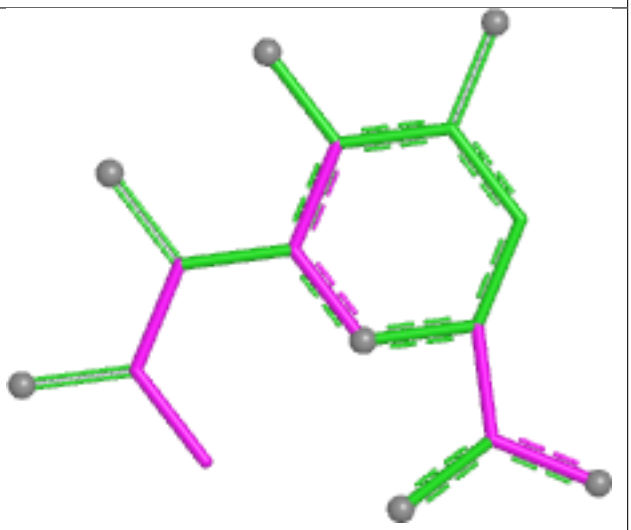


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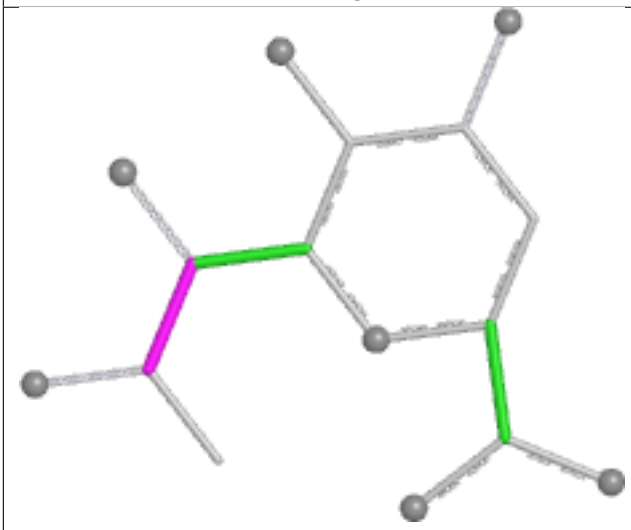
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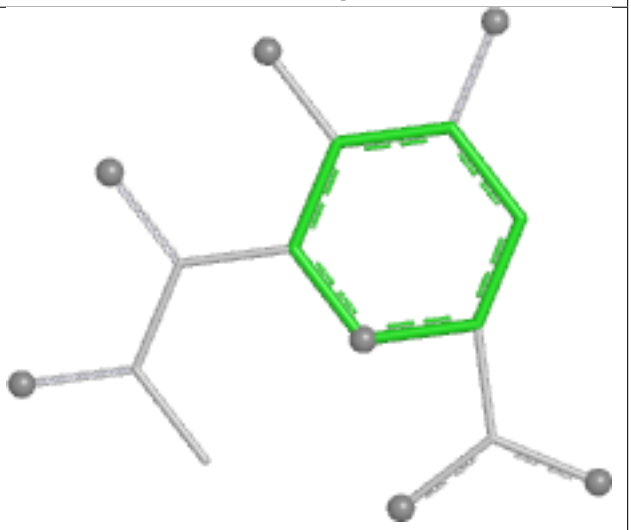
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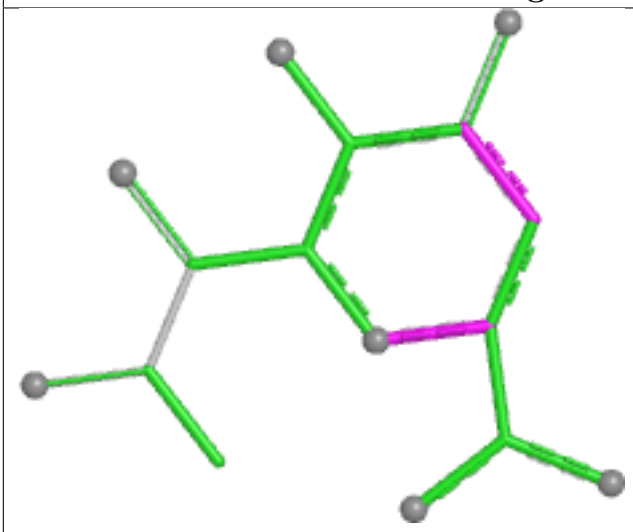


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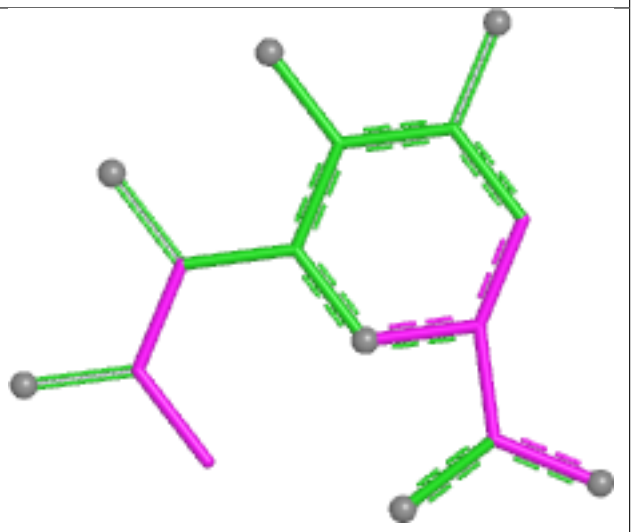


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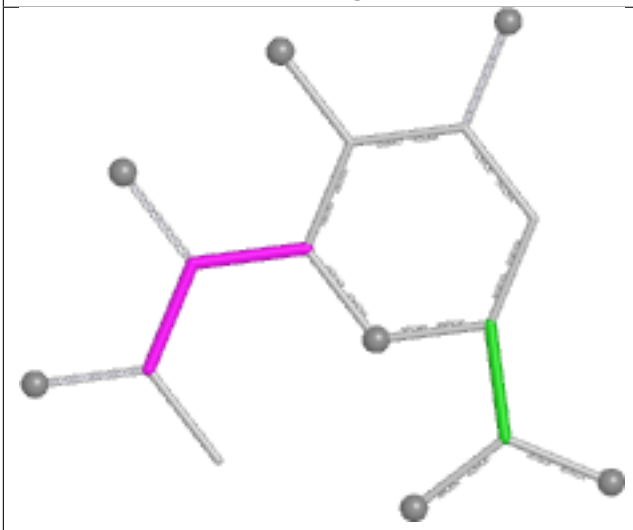
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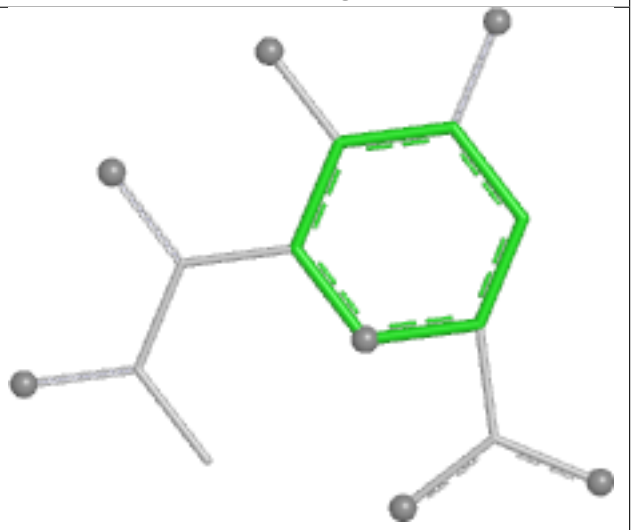
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Bond angles

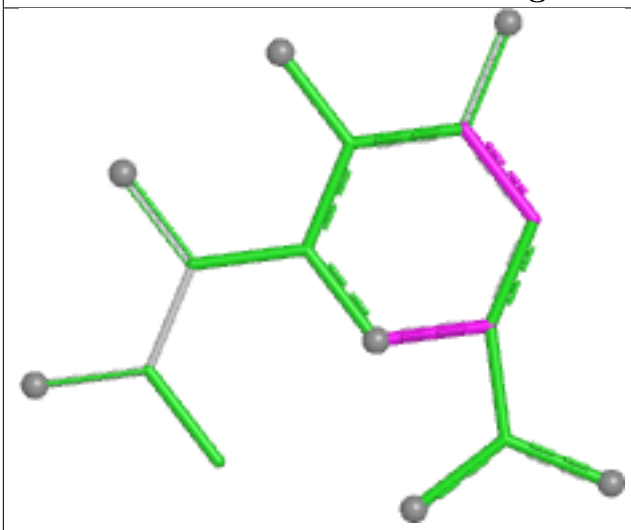


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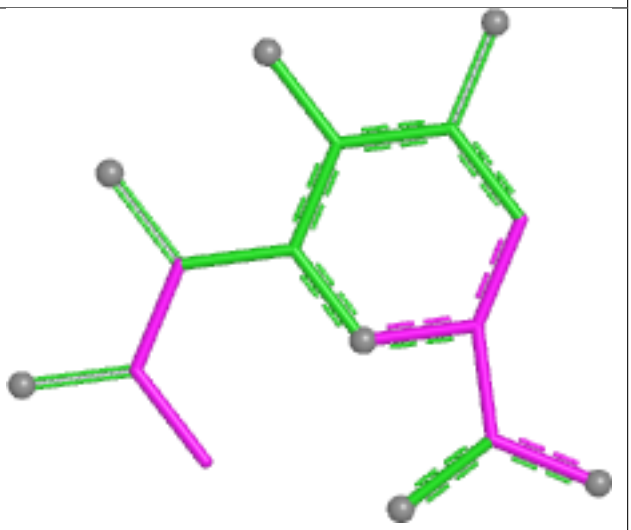


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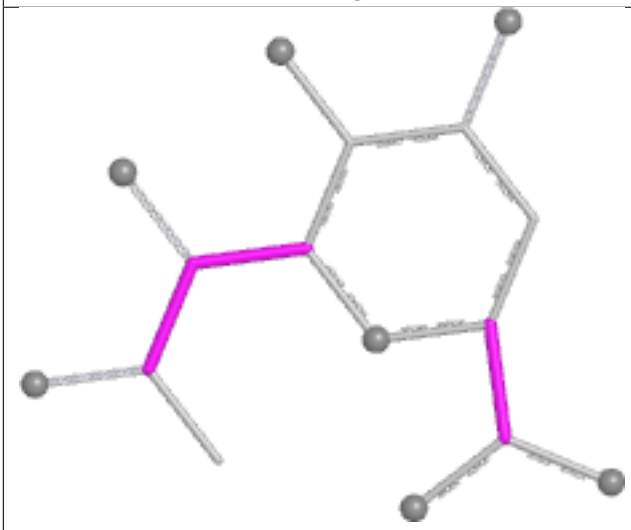
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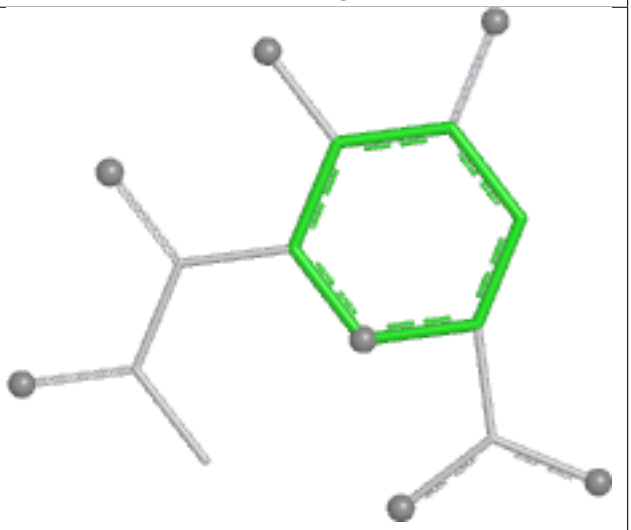
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Bond angles

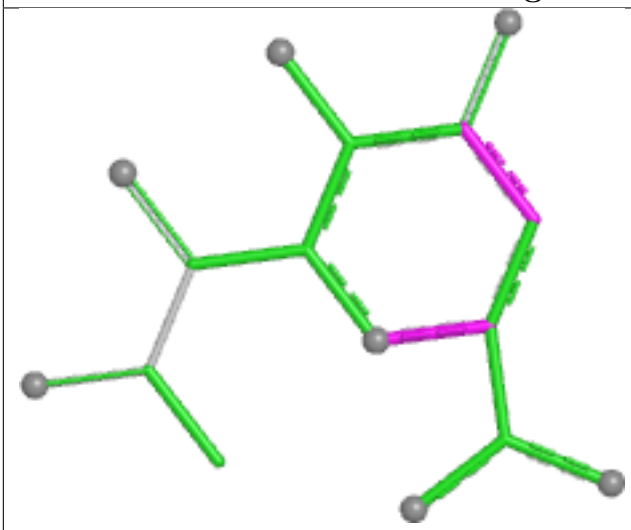


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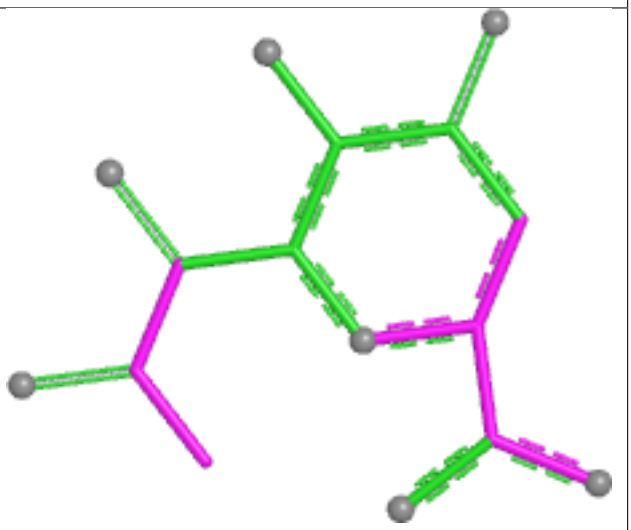


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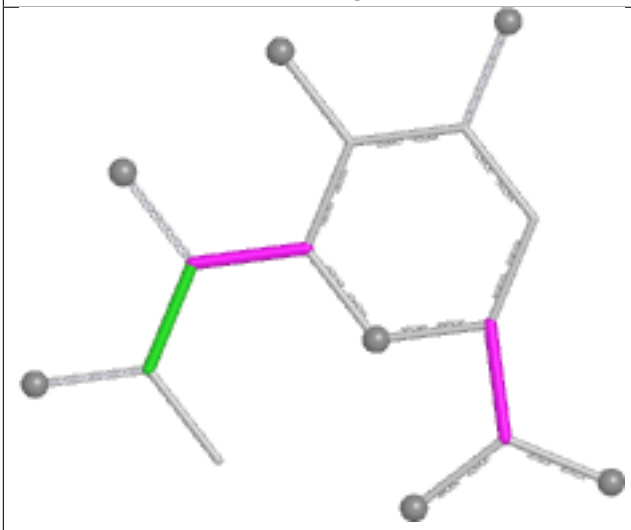
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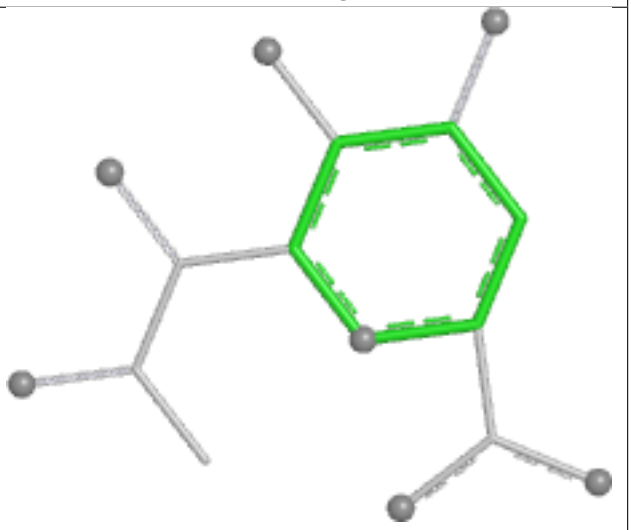
Bond lengths



Bond angles

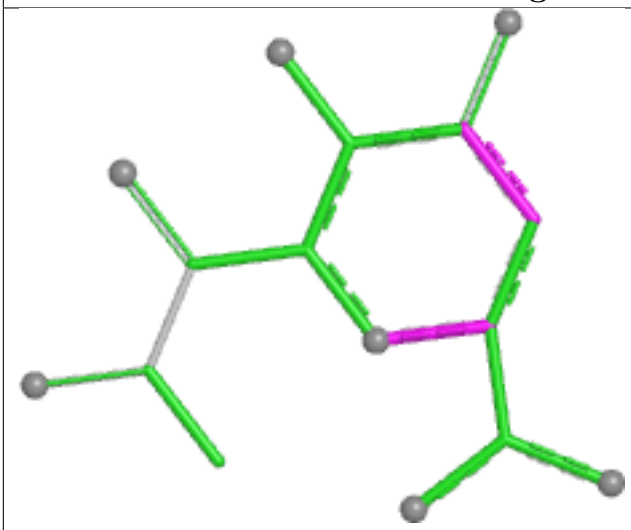


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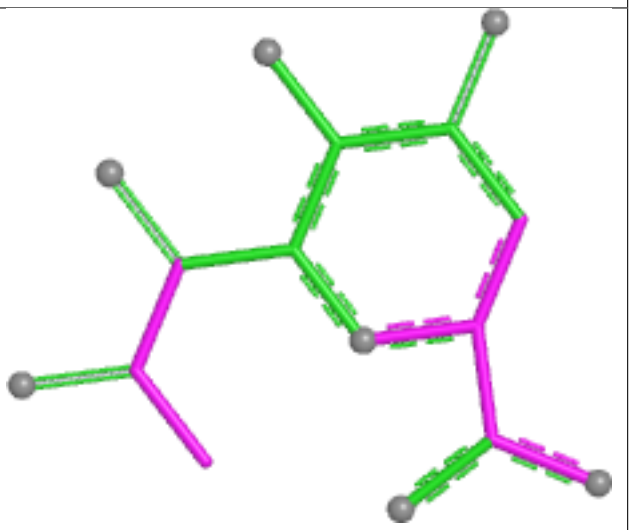


Rings

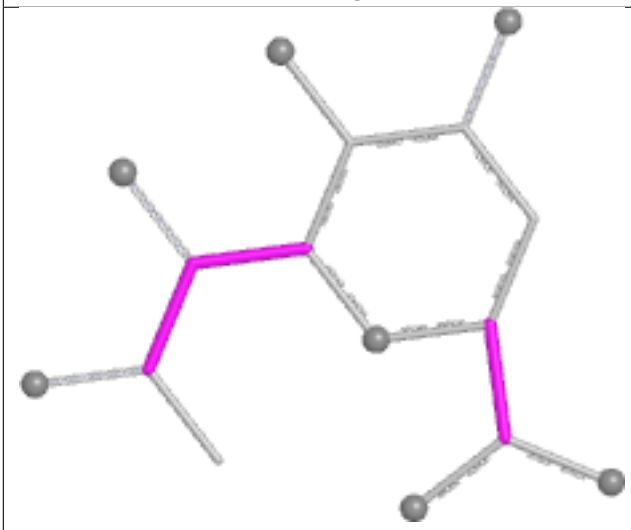
Ligand P8E P 605



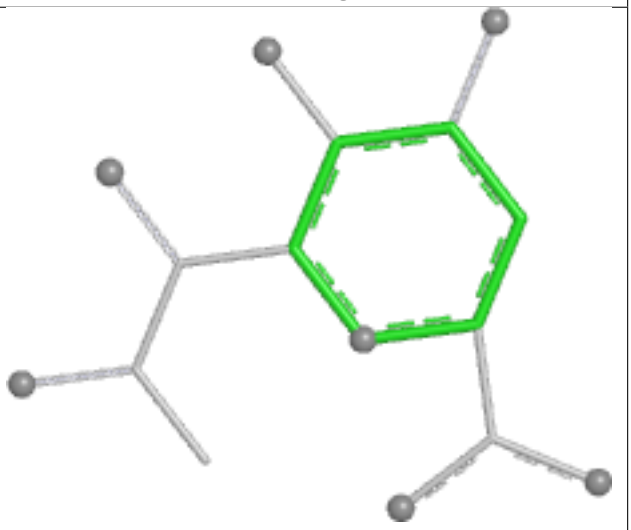
Bond lengths



Bond angles

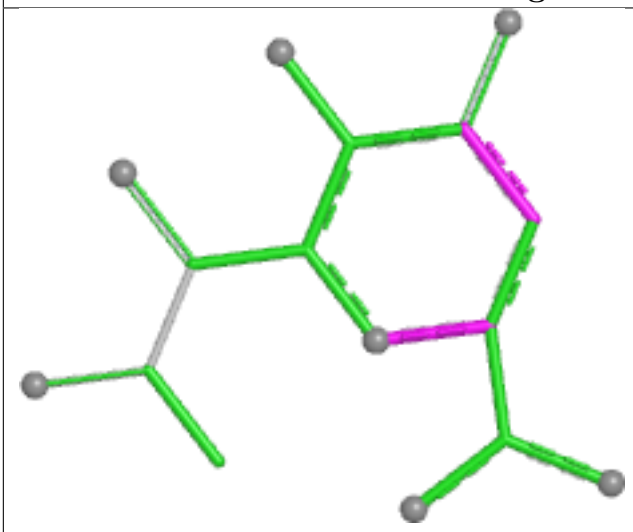


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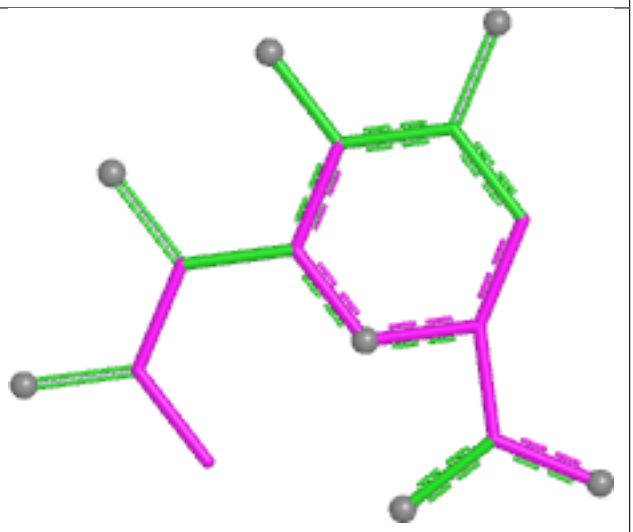


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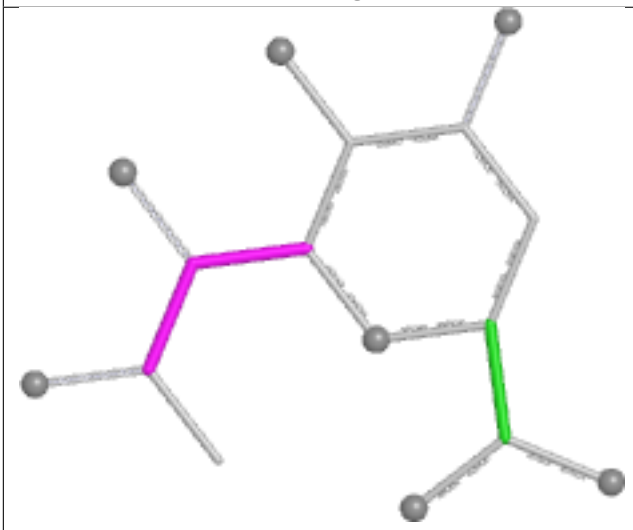
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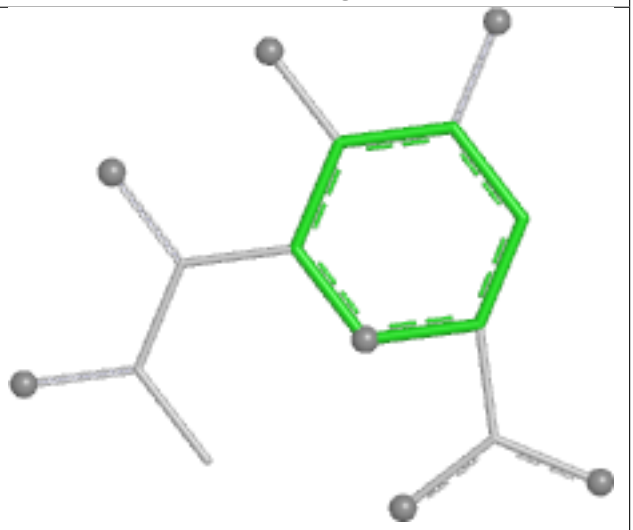
Bond lengths



Bond angles

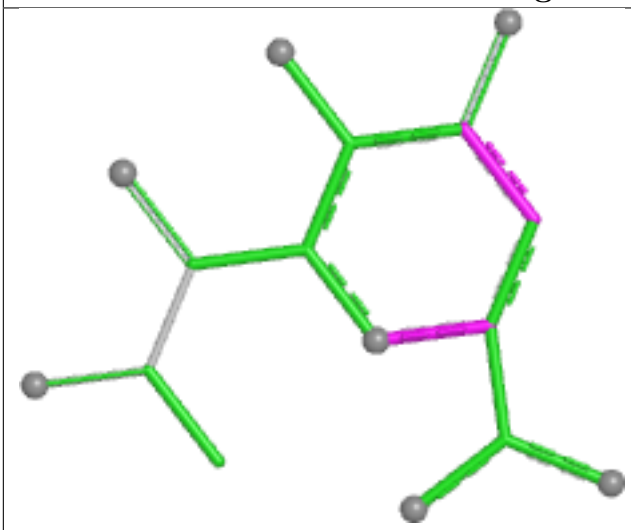


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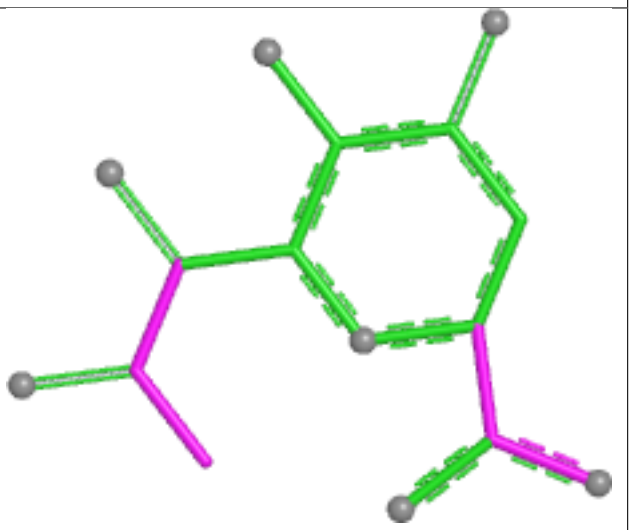


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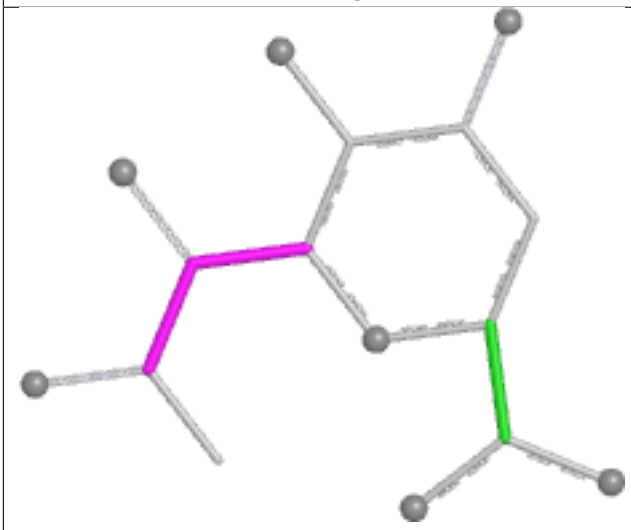
Ligand P8E I 613



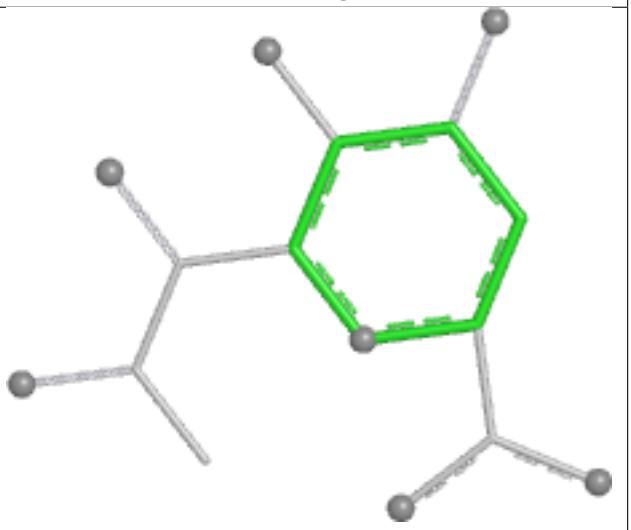
Bond lengths



Bond angles

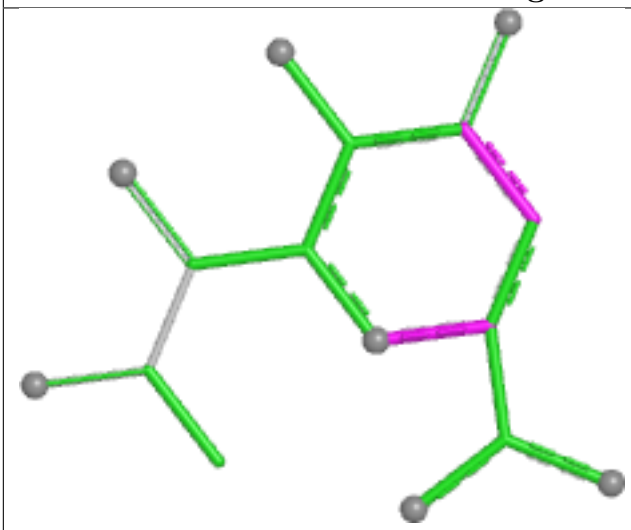


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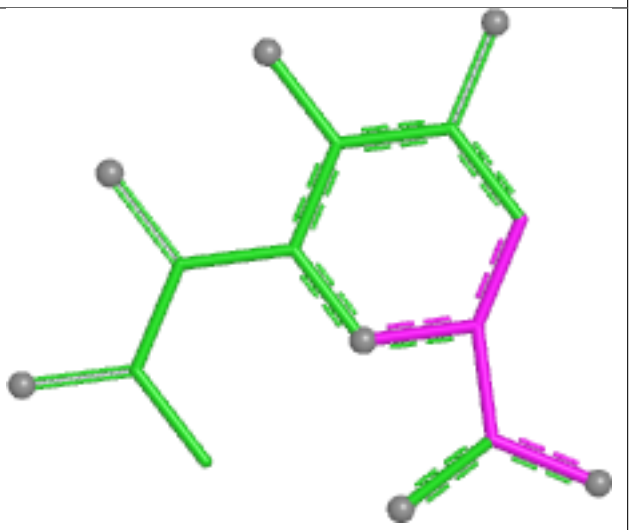


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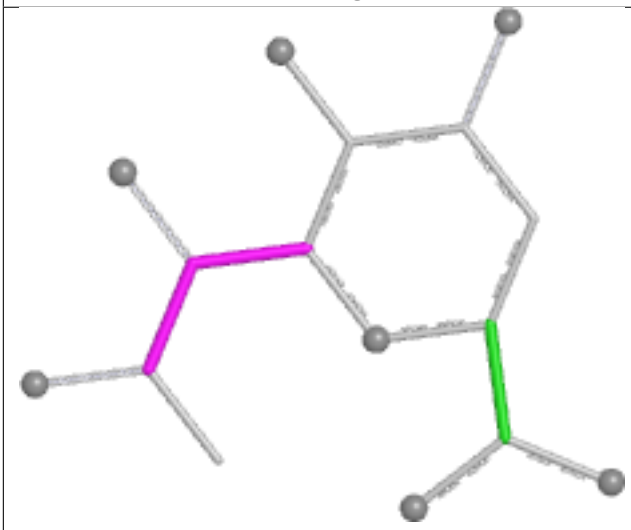
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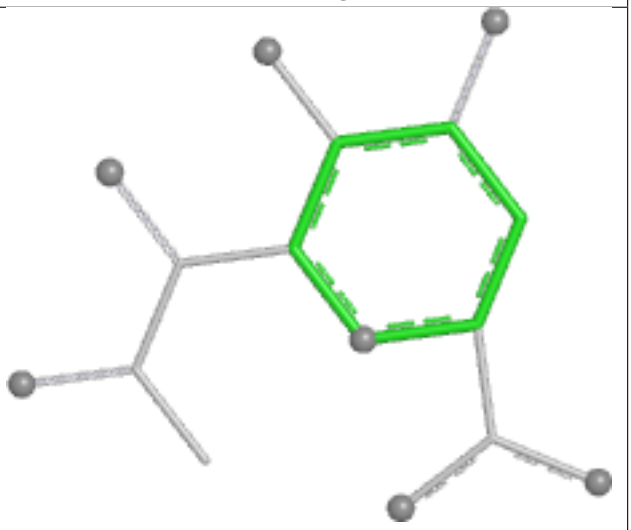
Bond lengths



Bond angles

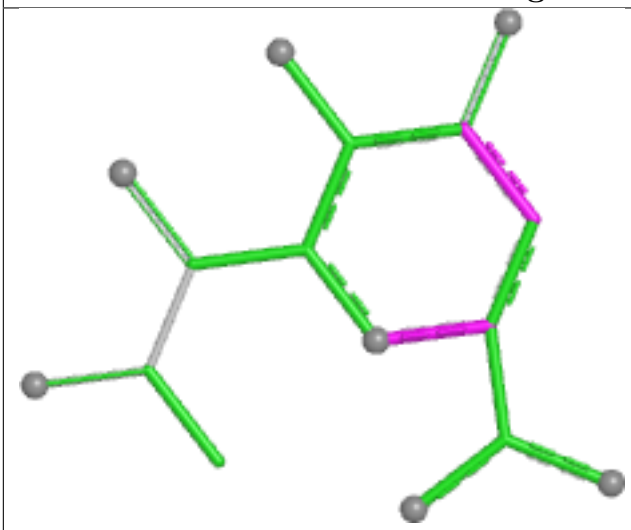


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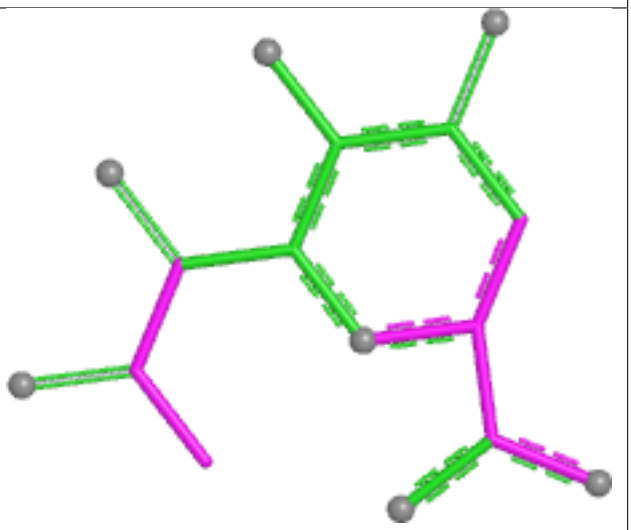


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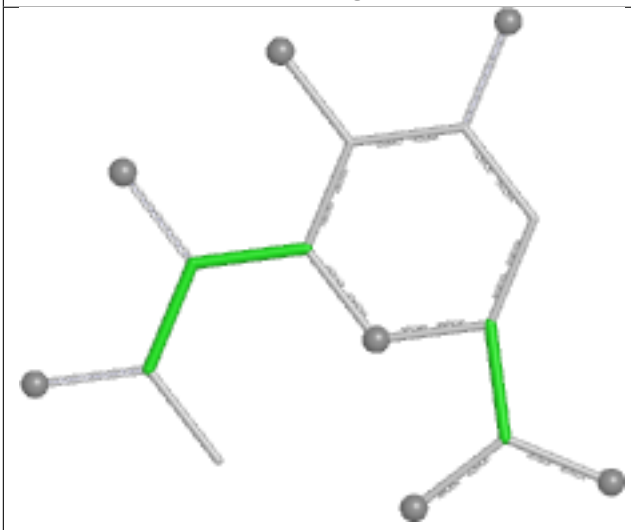
Ligand P8E K 607



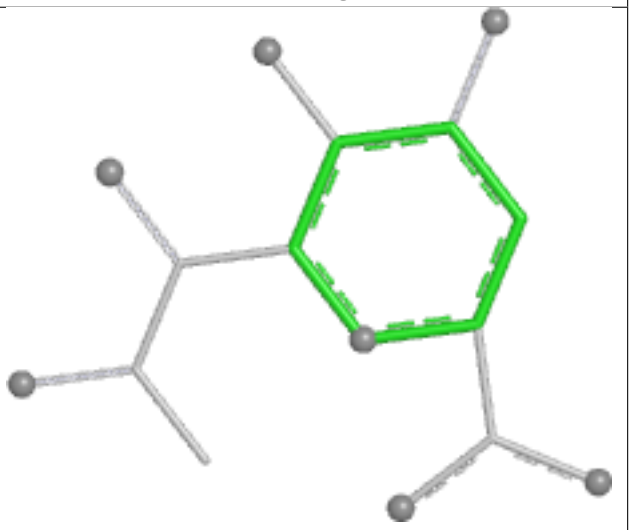
Bond lengths



Bond angles

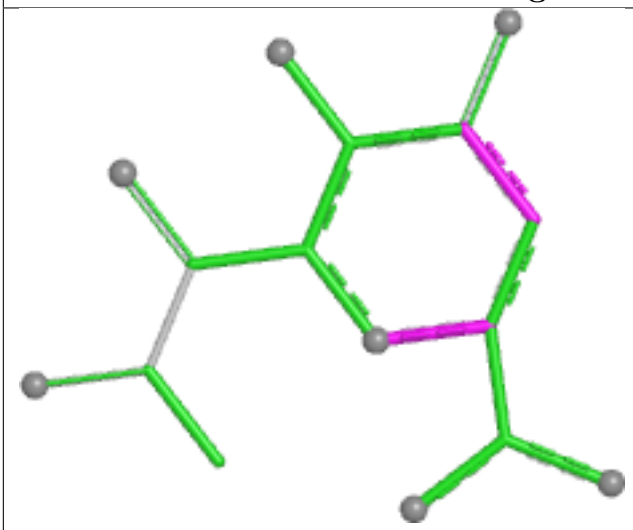


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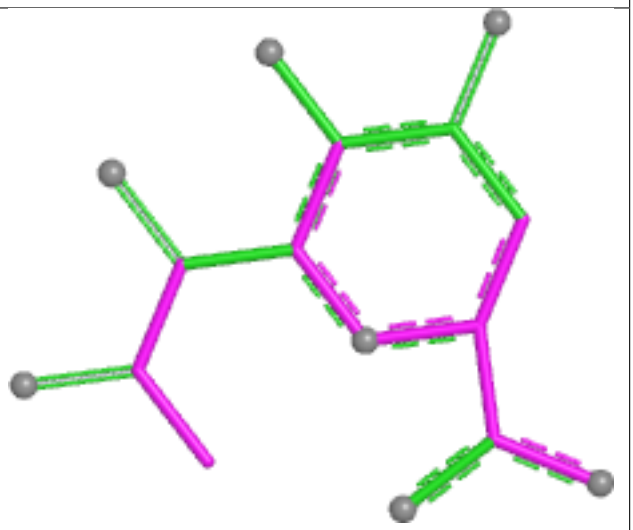


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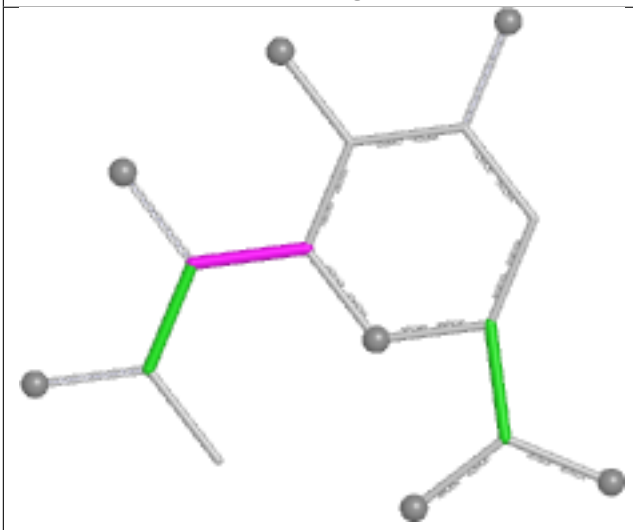
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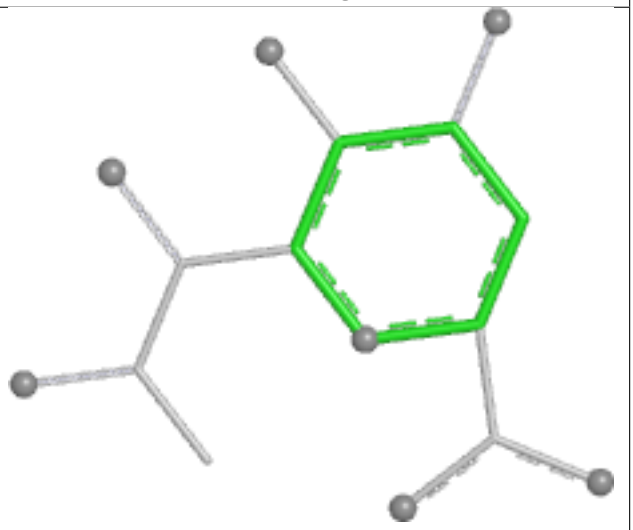
Bond lengths



Bond angles

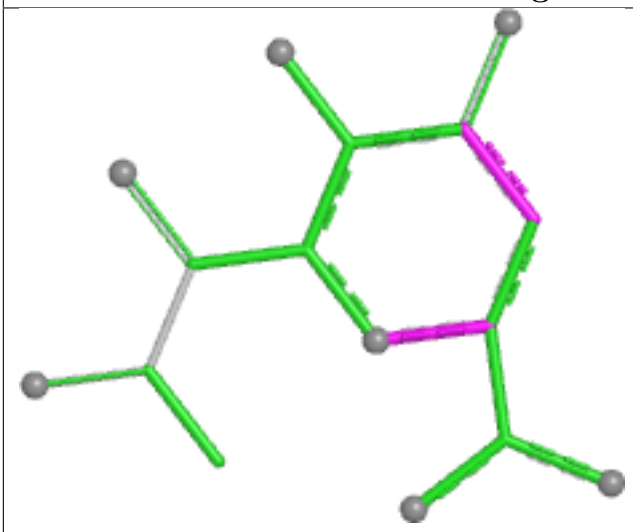


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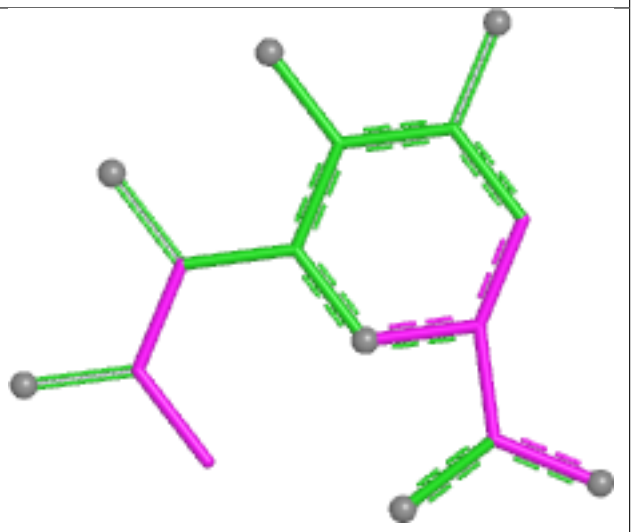


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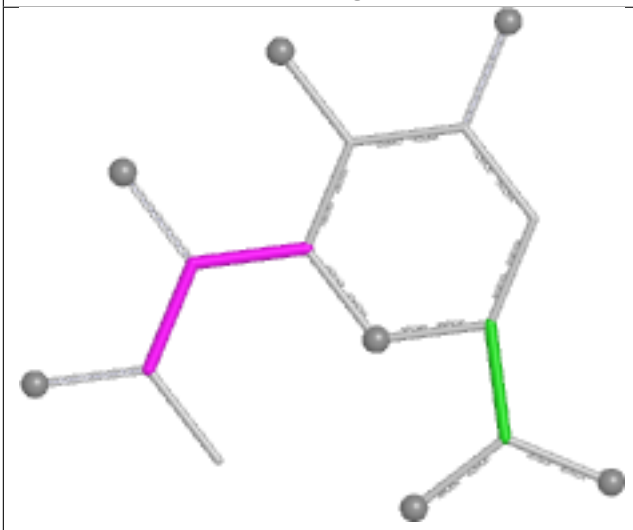
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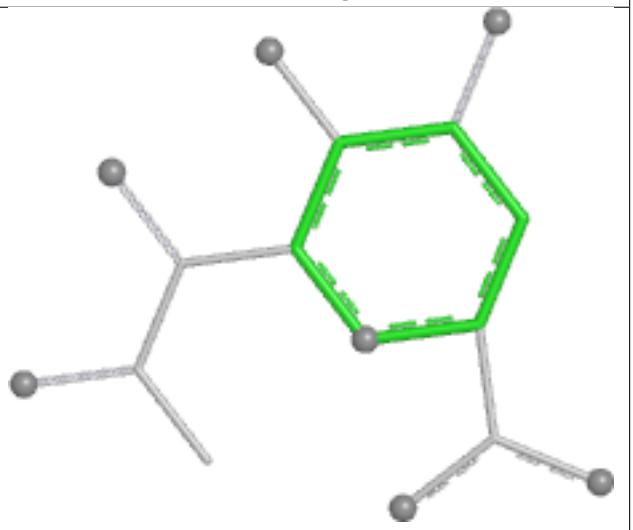
Bond lengths



Bond angles

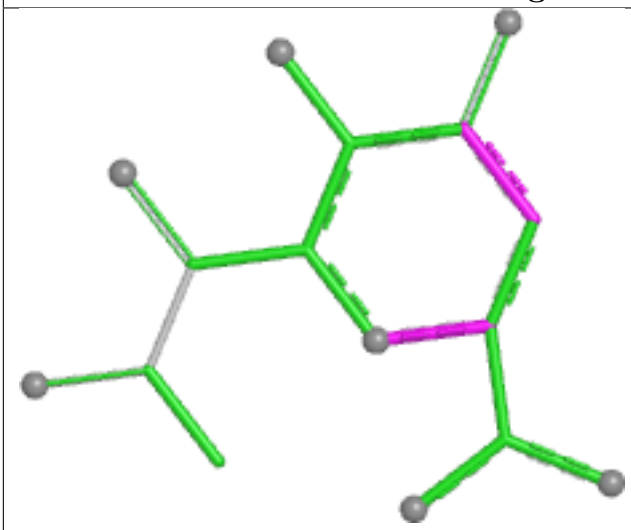


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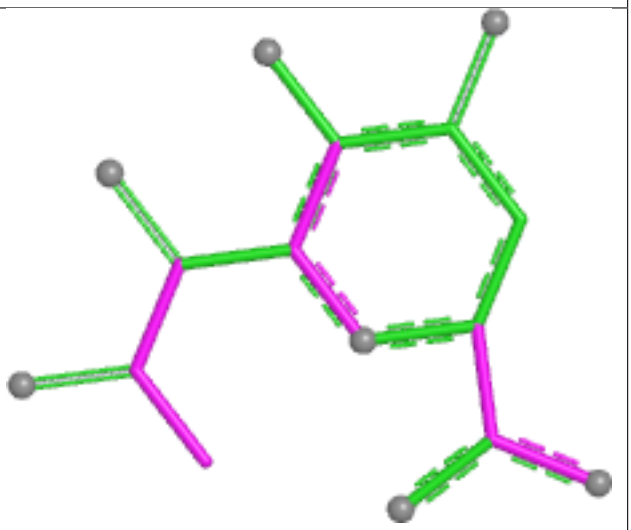


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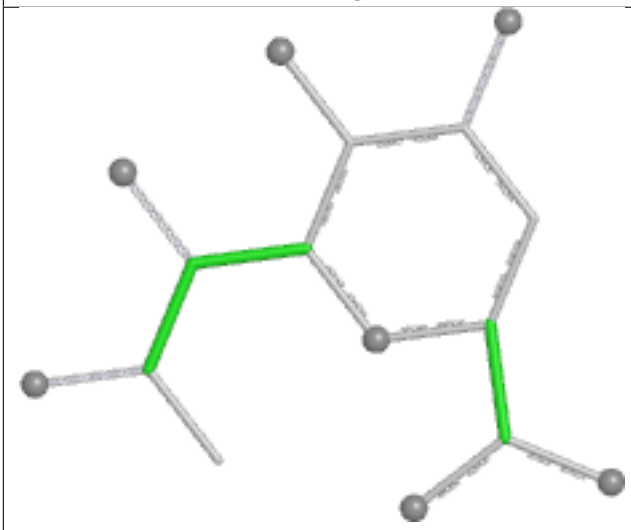
Ligand P8E A 614



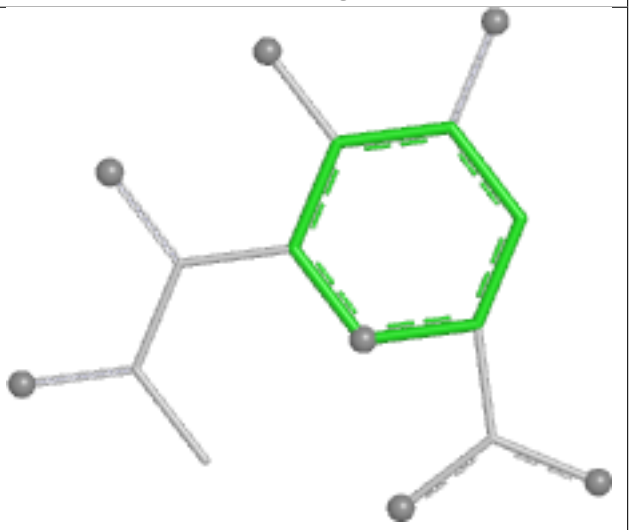
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Bond angles

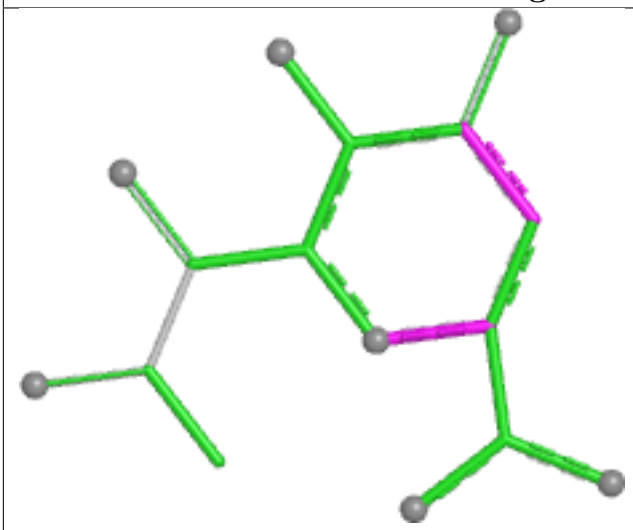


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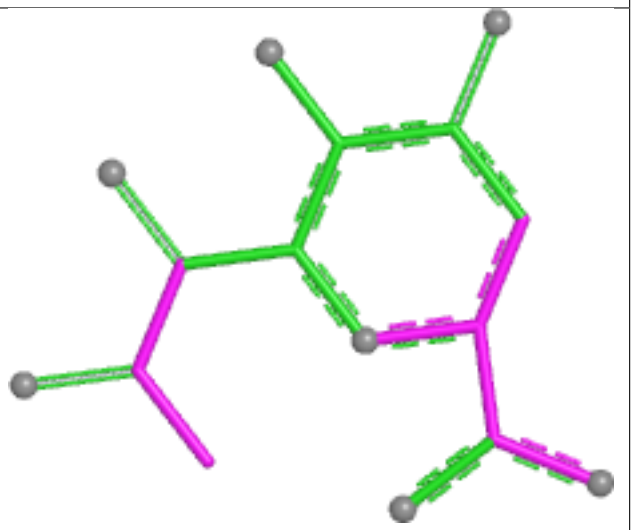


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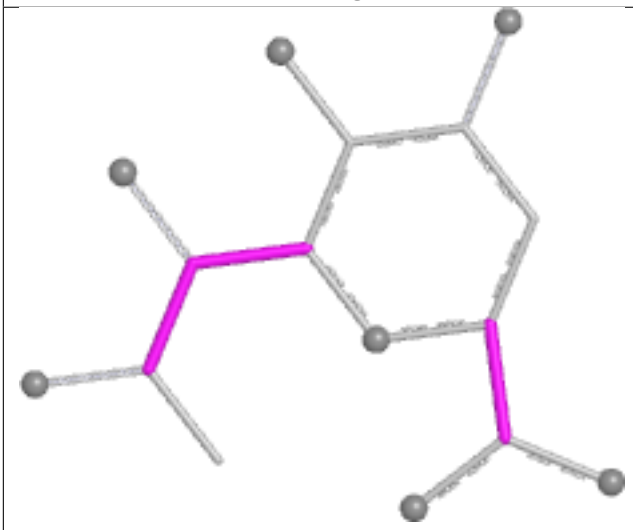
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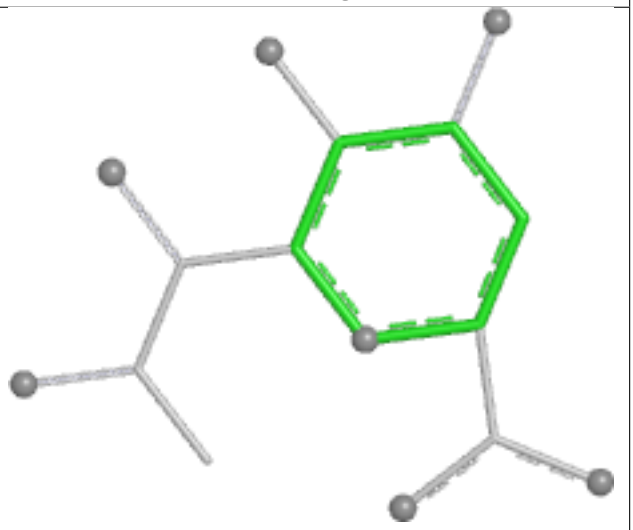
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Bond angles

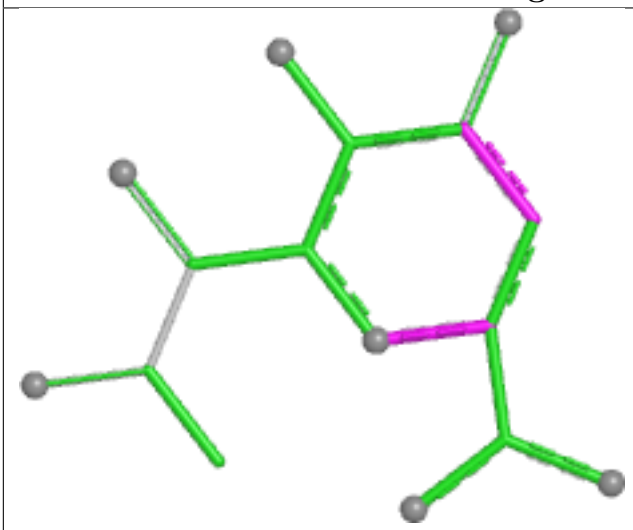


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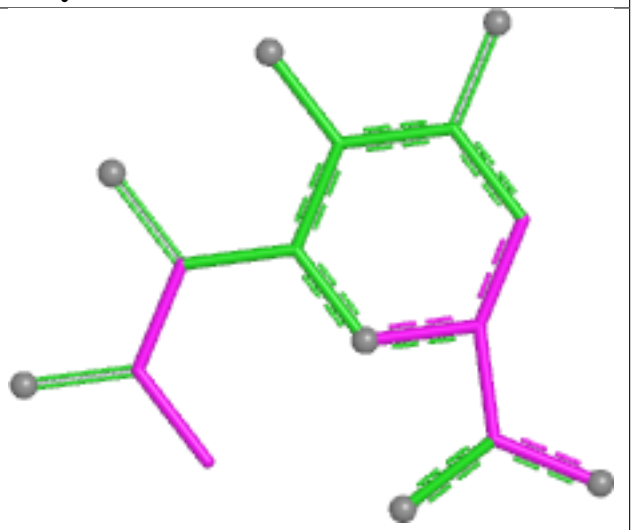


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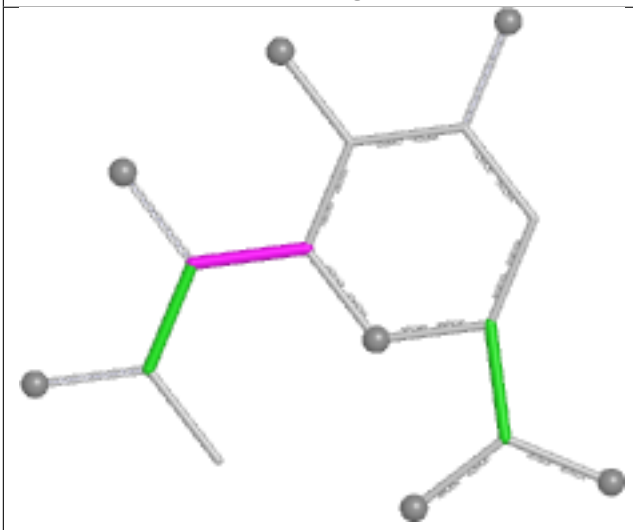
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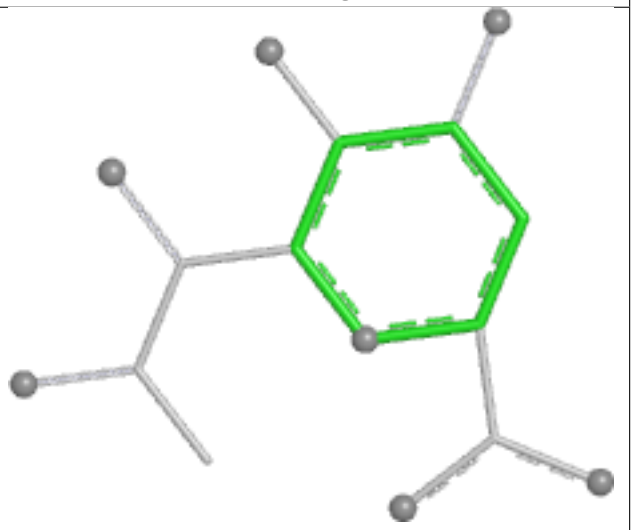
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Bond angles

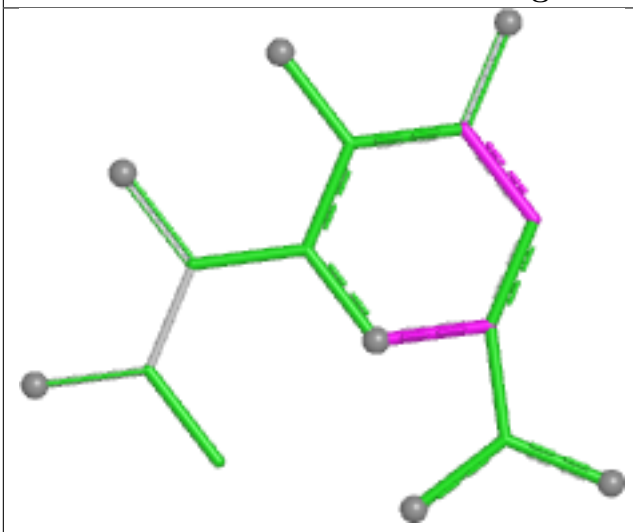


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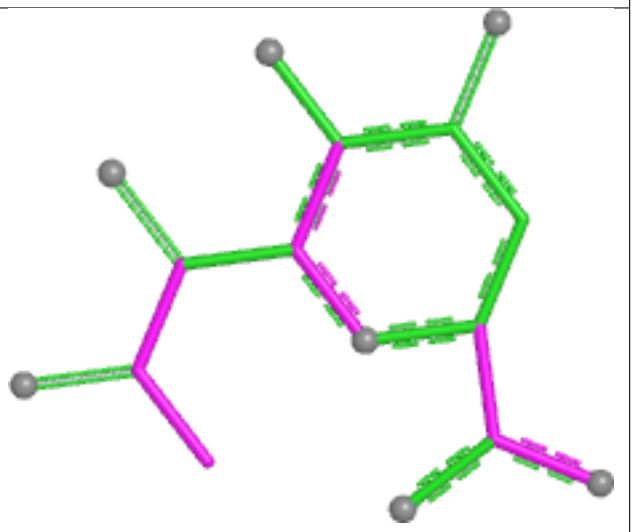


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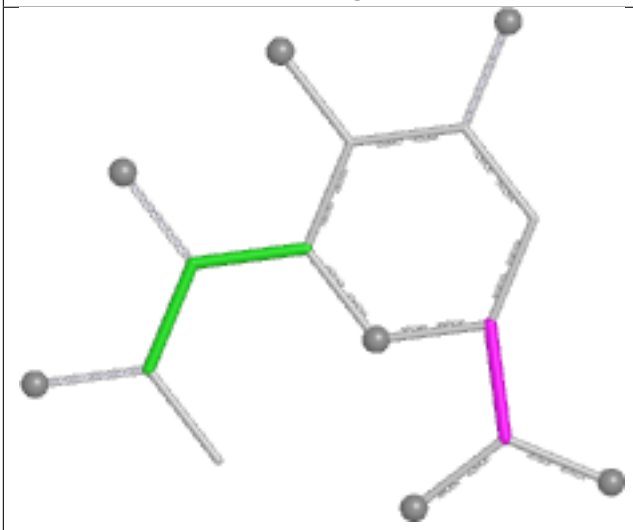
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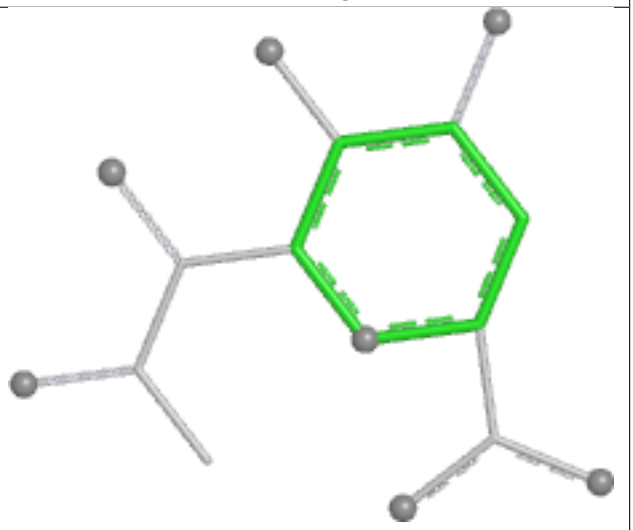
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Bond angles

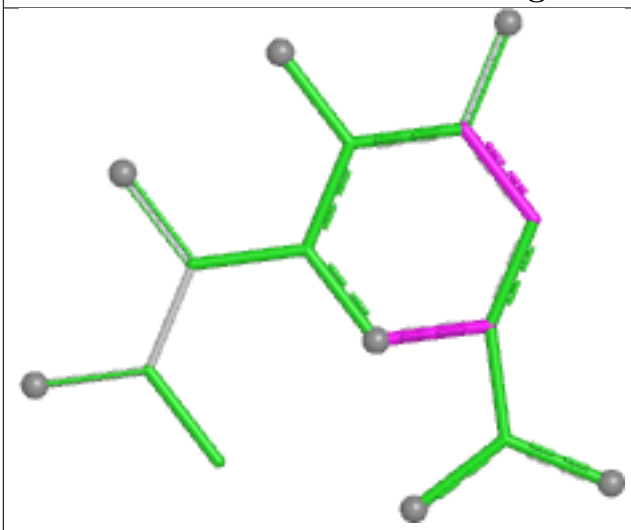


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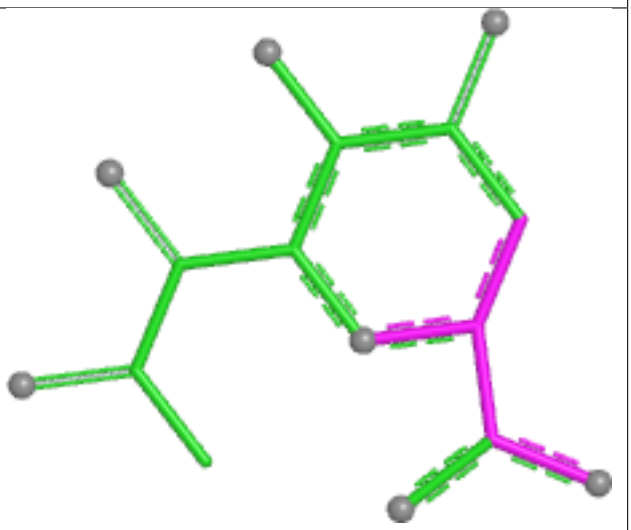


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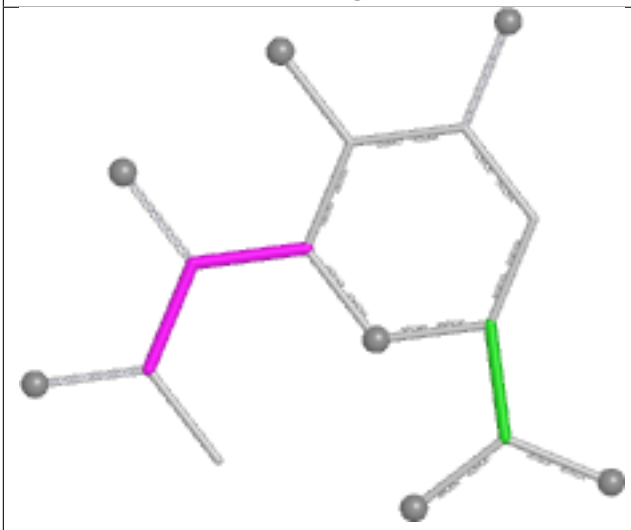
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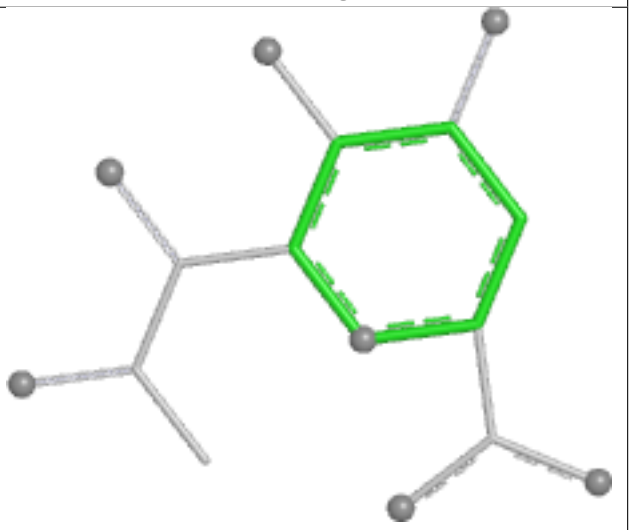
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Bond angles

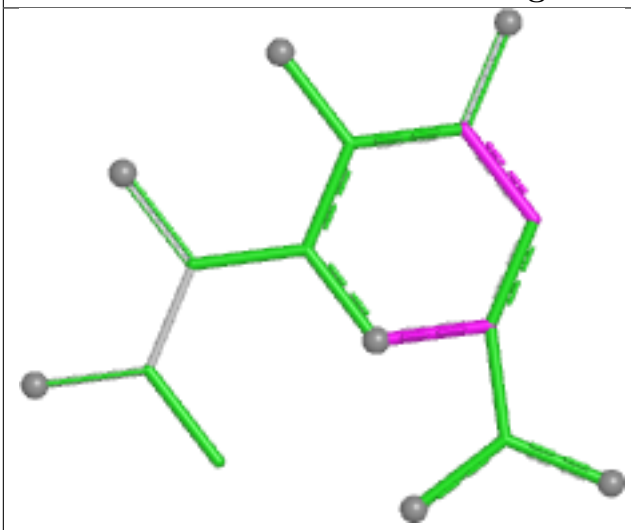


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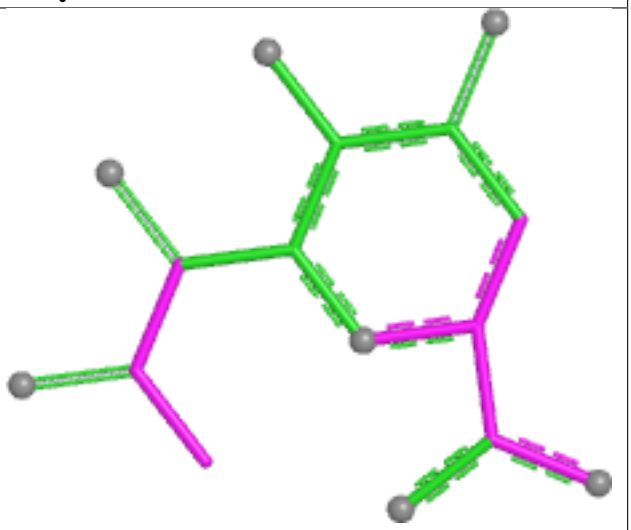


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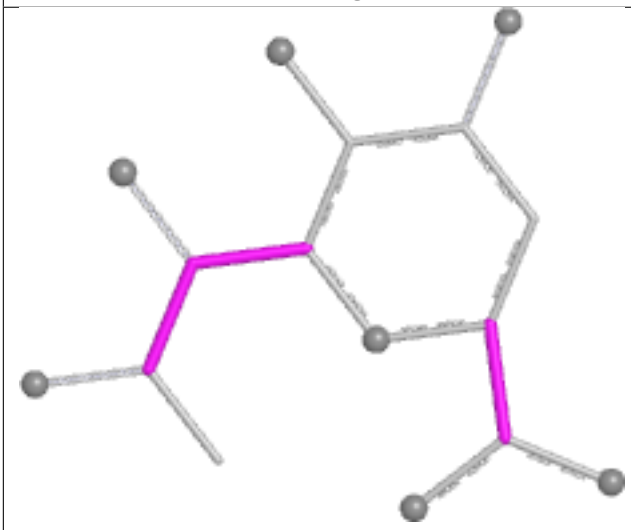
Ligand P8E Q 612



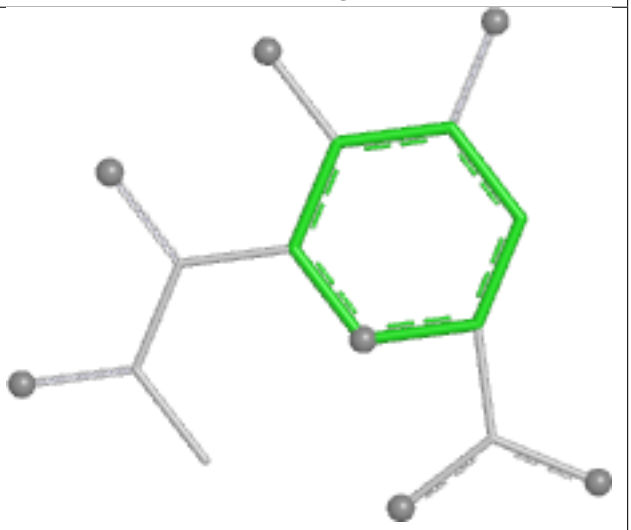
Bond lengths



Bond angles

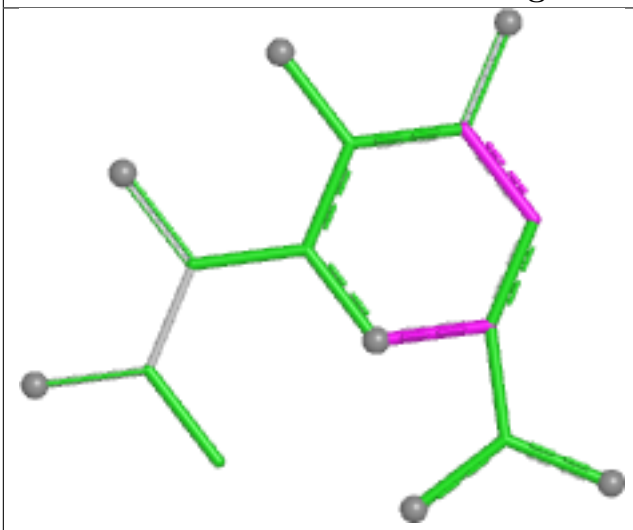


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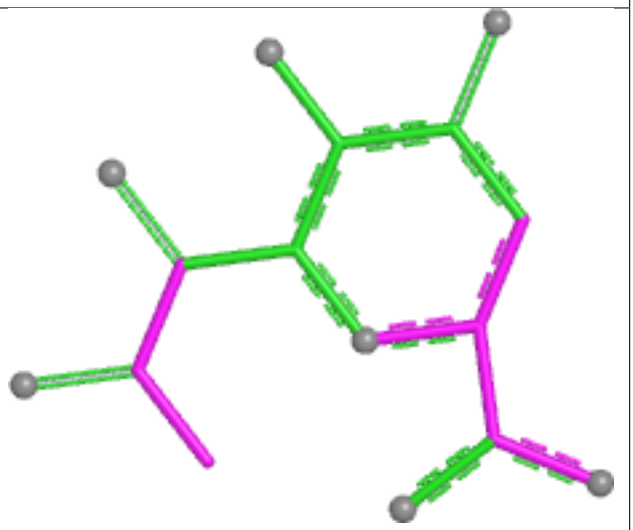


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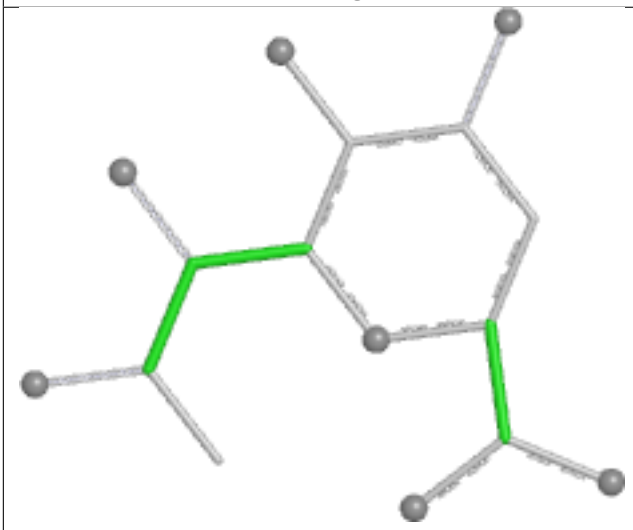
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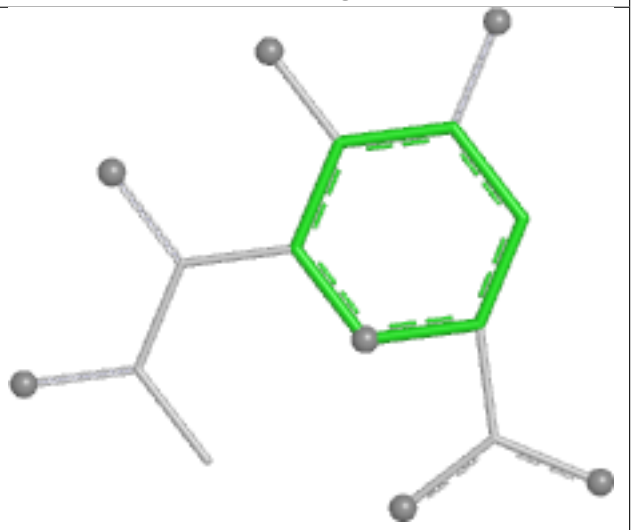
Bond lengths



Bond angles

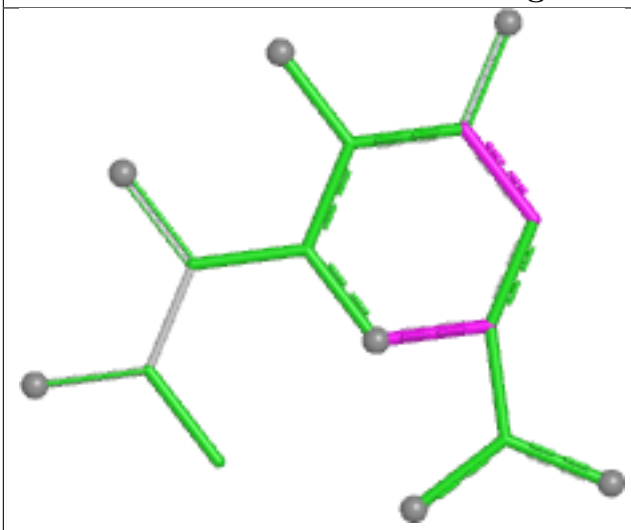


Torsions

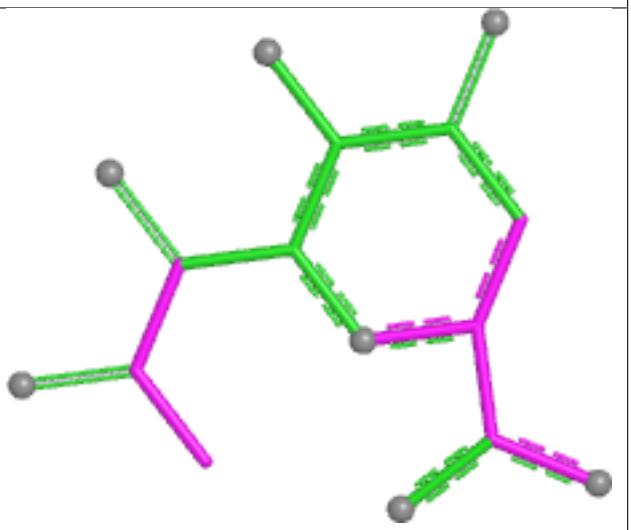


Rings

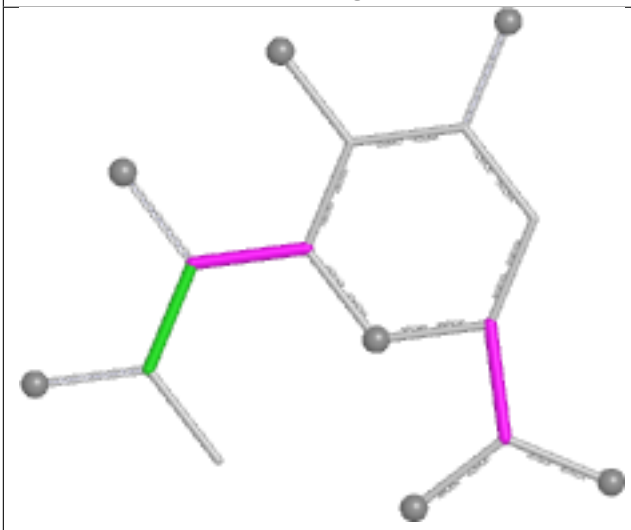
Ligand P8E G 612



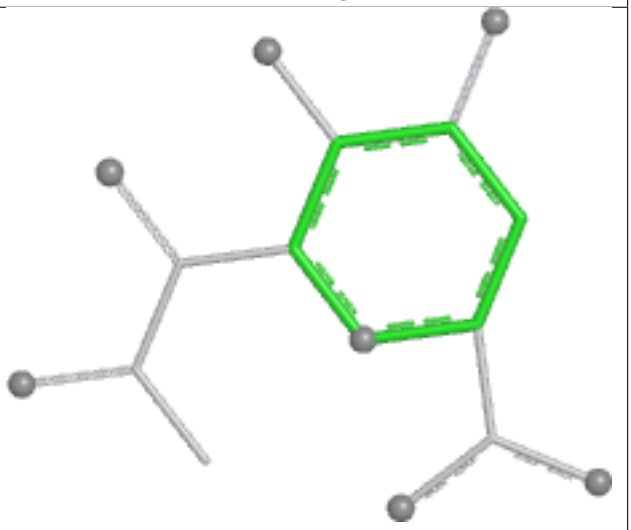
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Bond angles

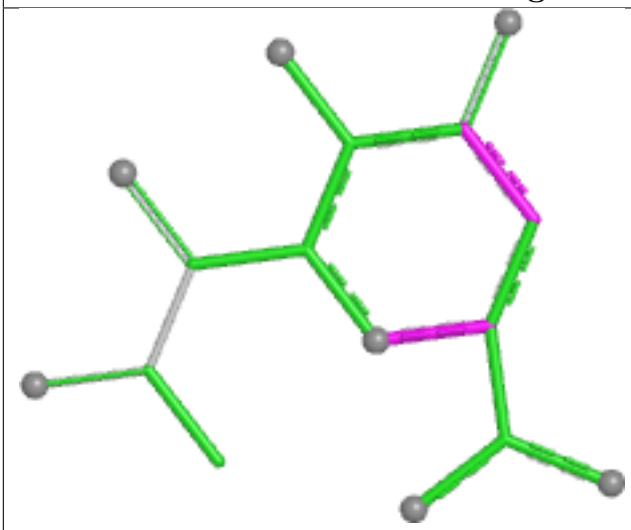


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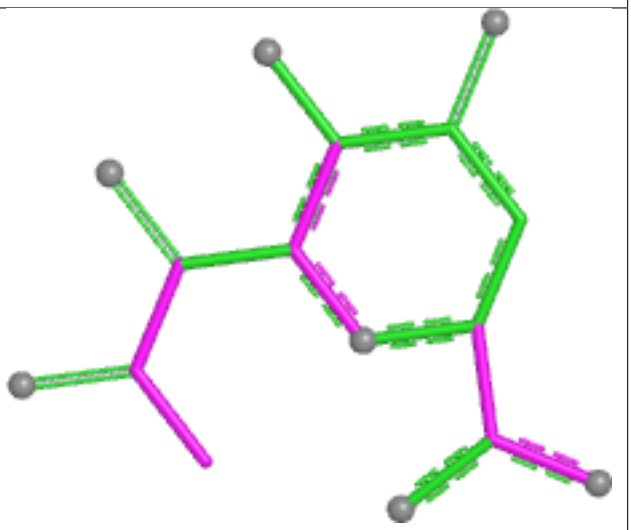


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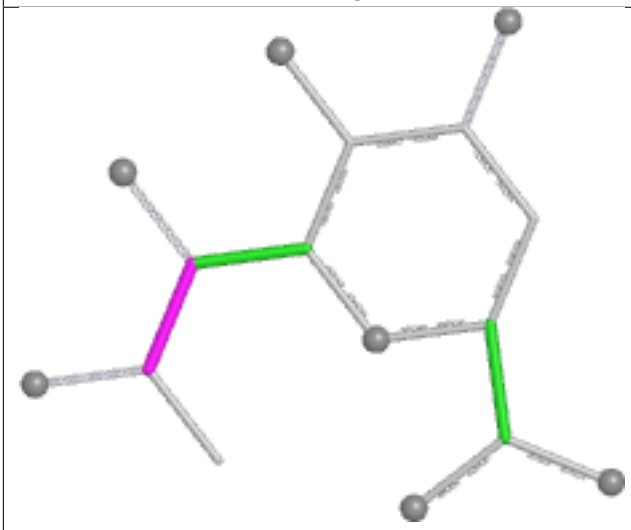
Ligand P8E U 602



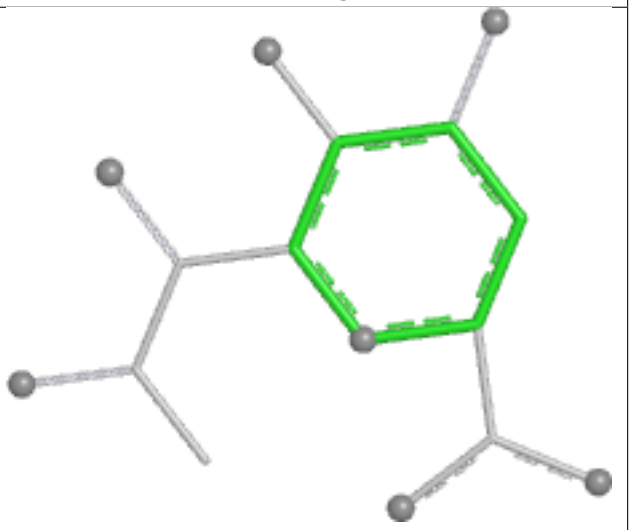
Bond lengths



Bond angles

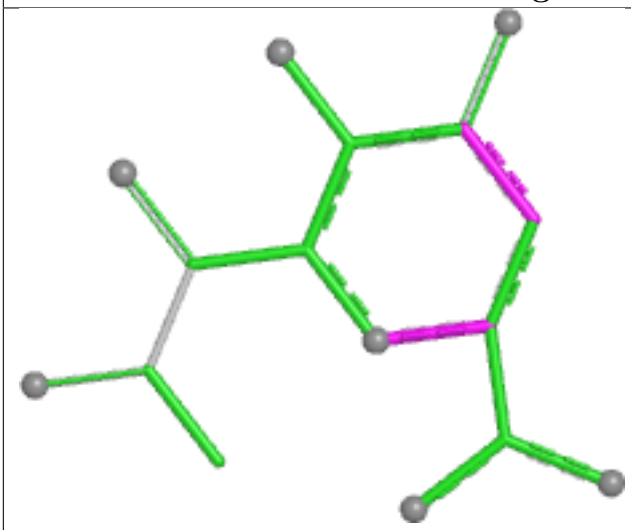


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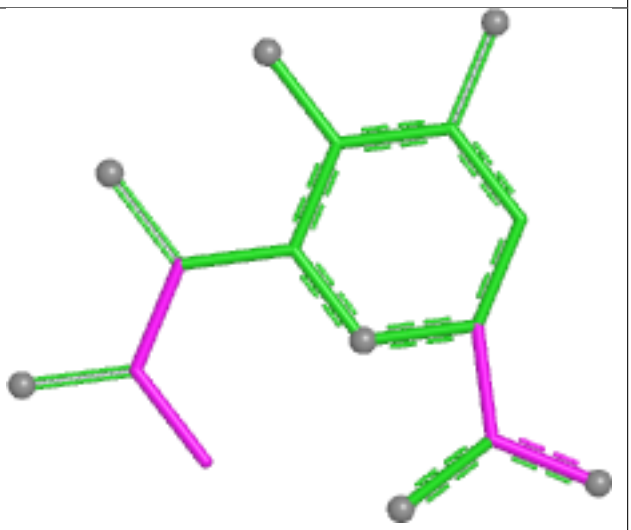


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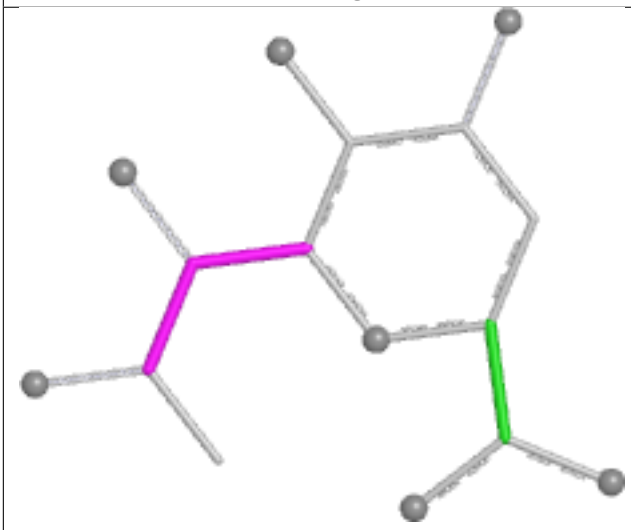
Ligand P8E J 614



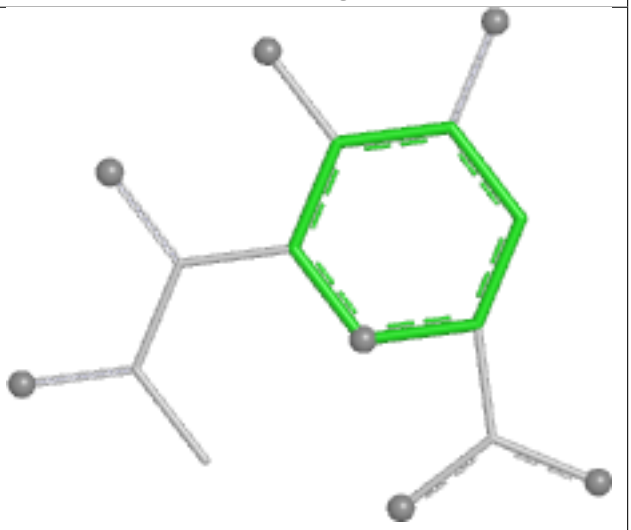
Bond lengths



Bond angles

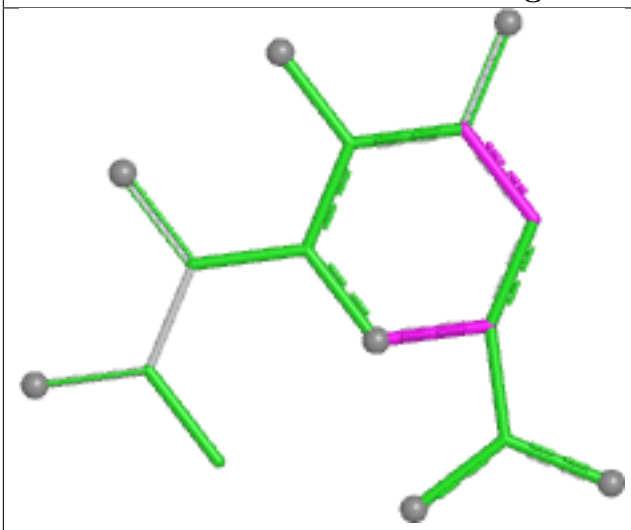


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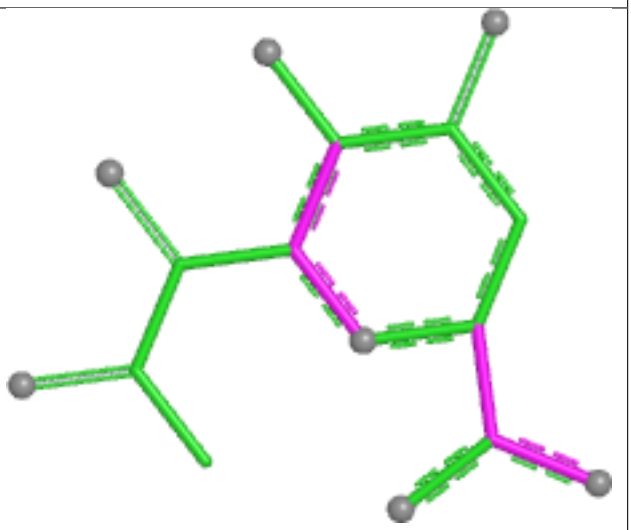


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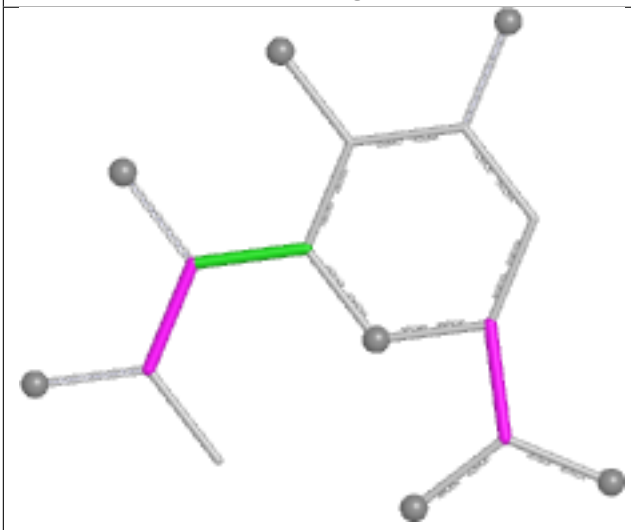
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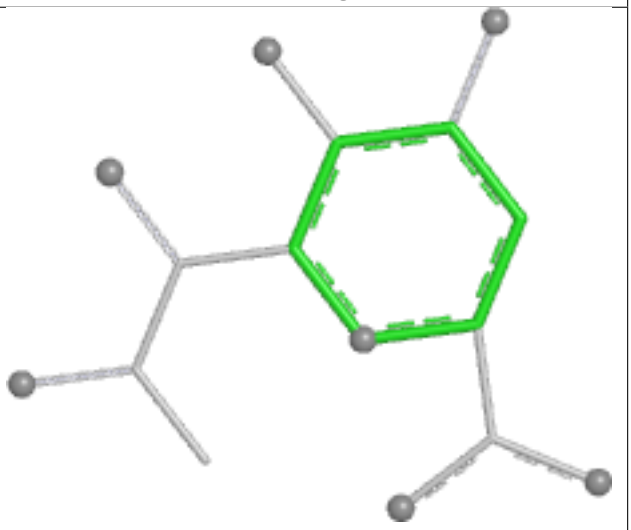
Bond lengths



Bond angles

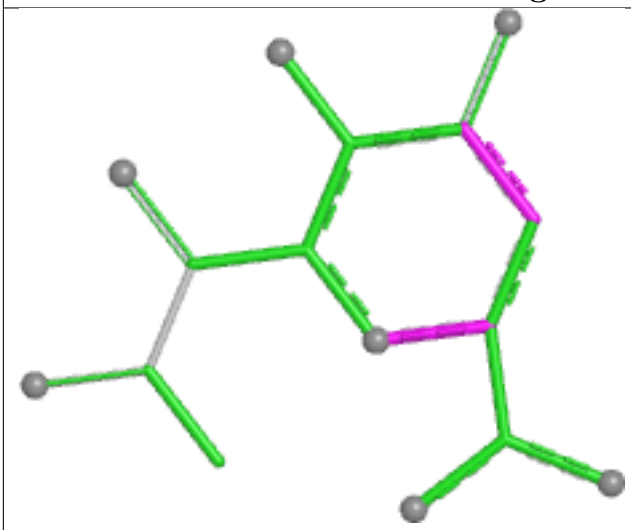


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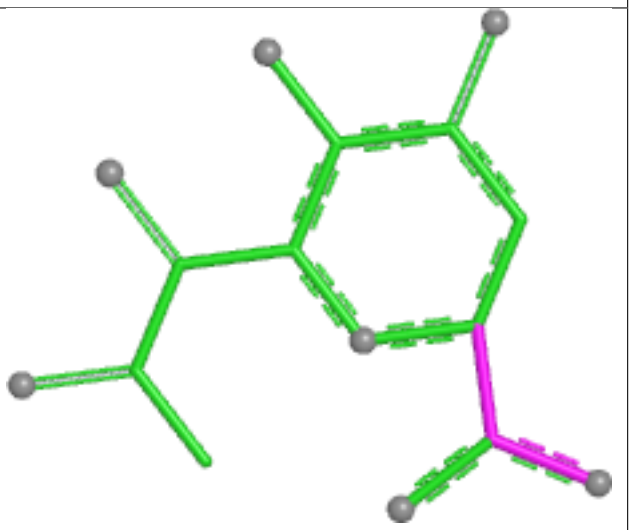


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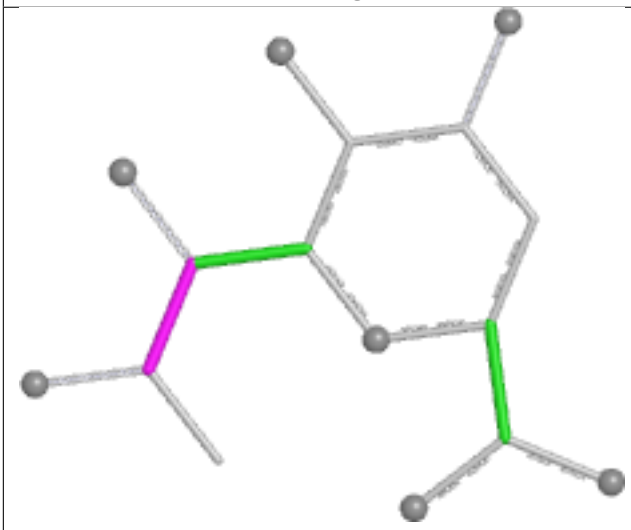
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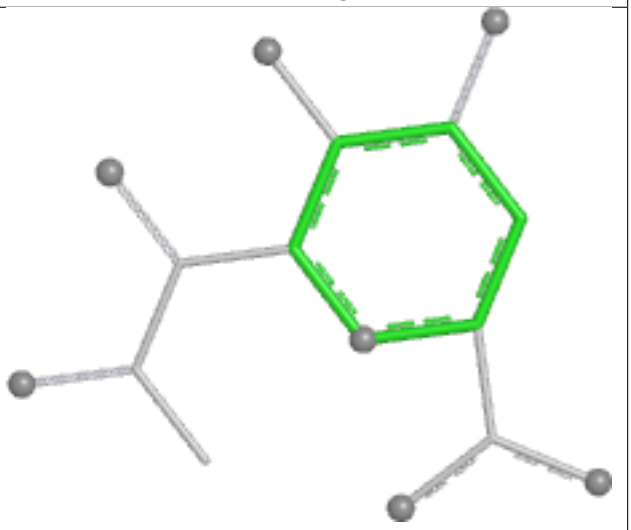
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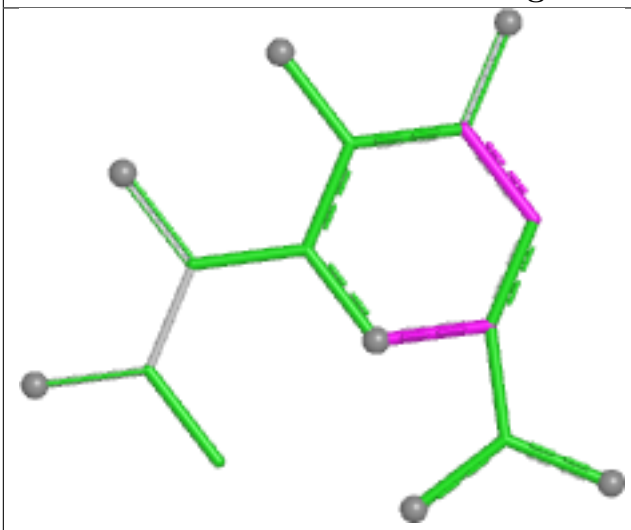


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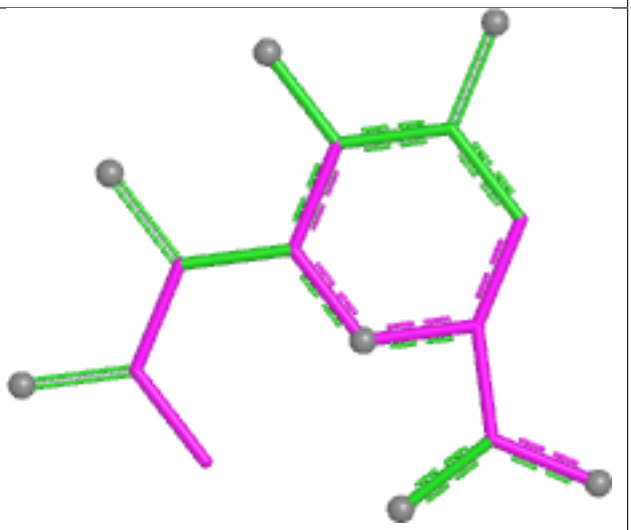


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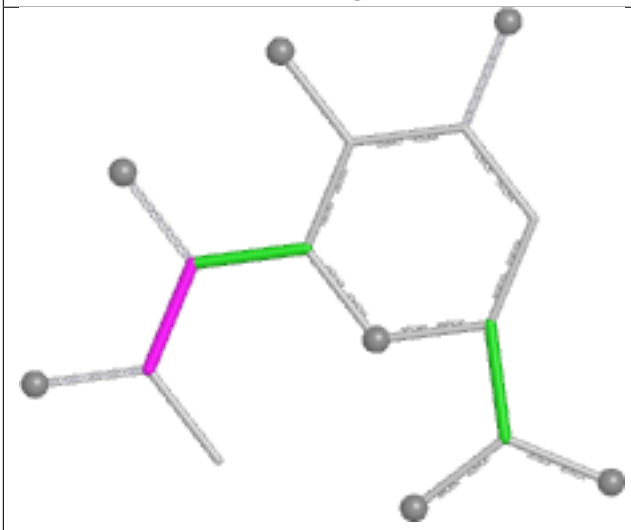
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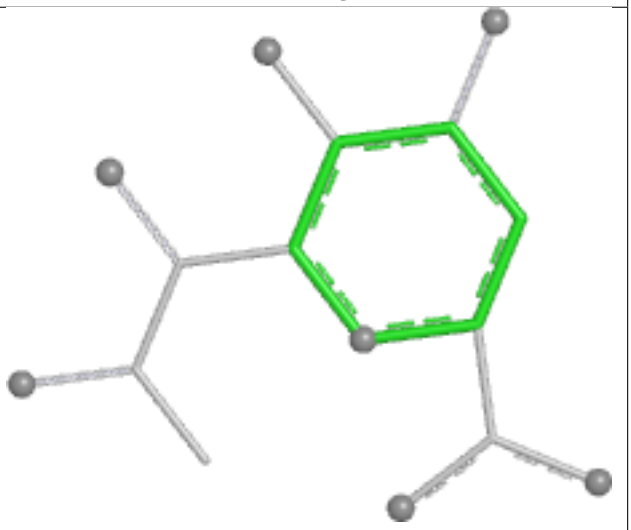
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Bond angles

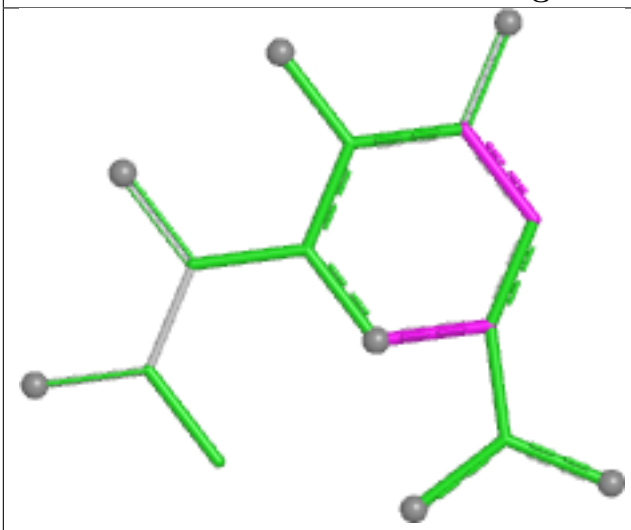


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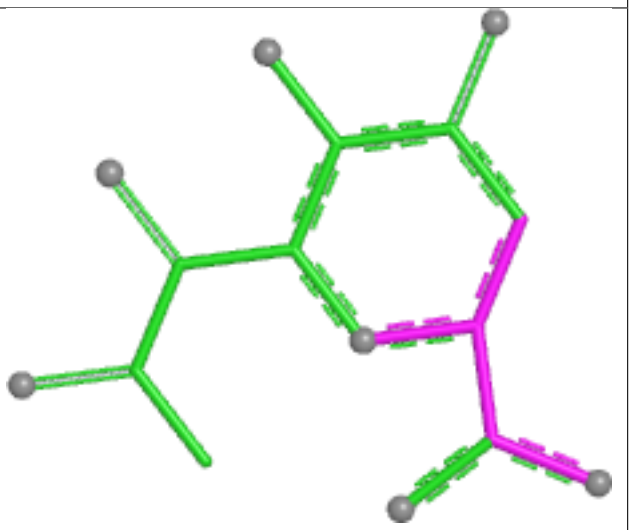


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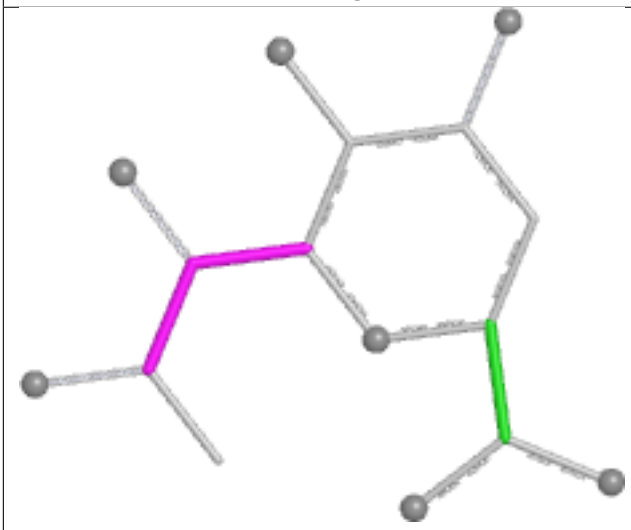
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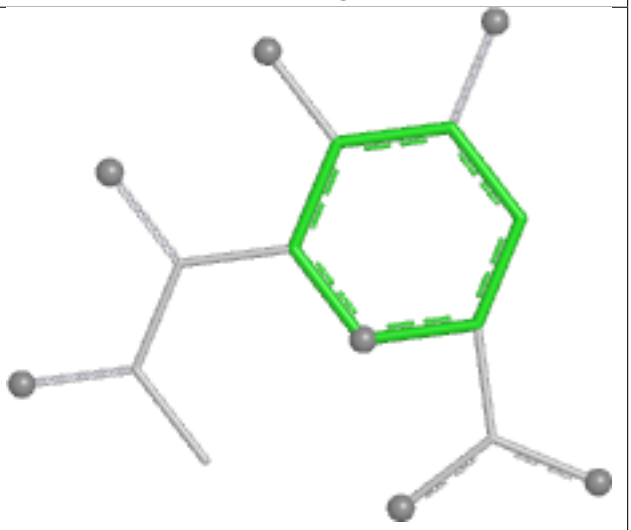
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Bond angles

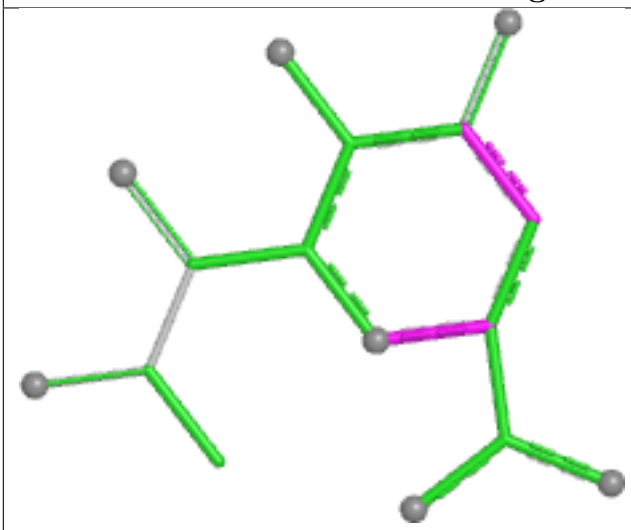


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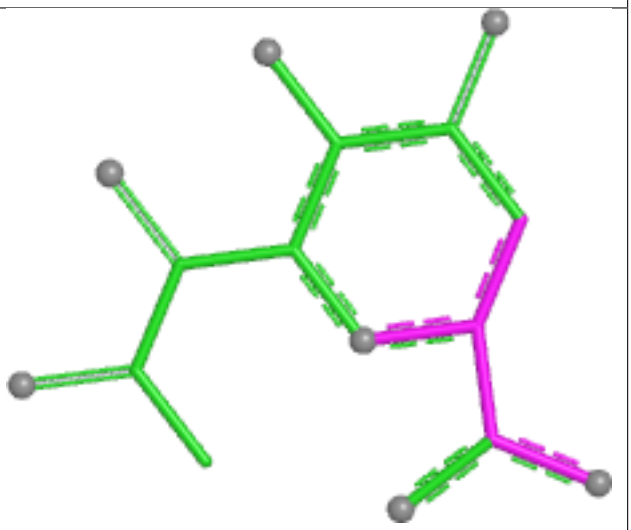


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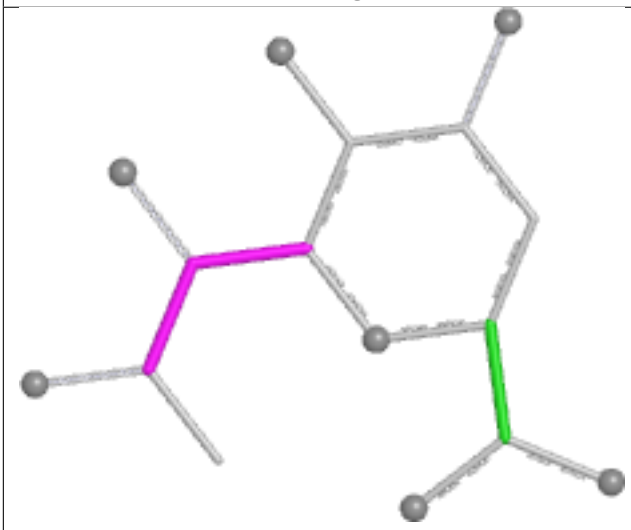
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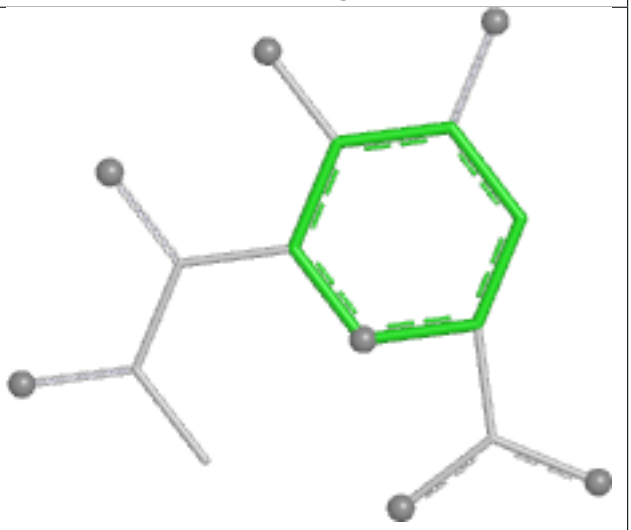
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Bond angles

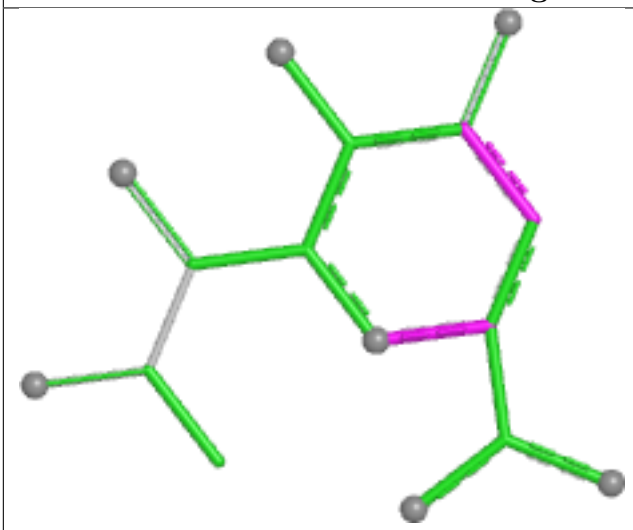


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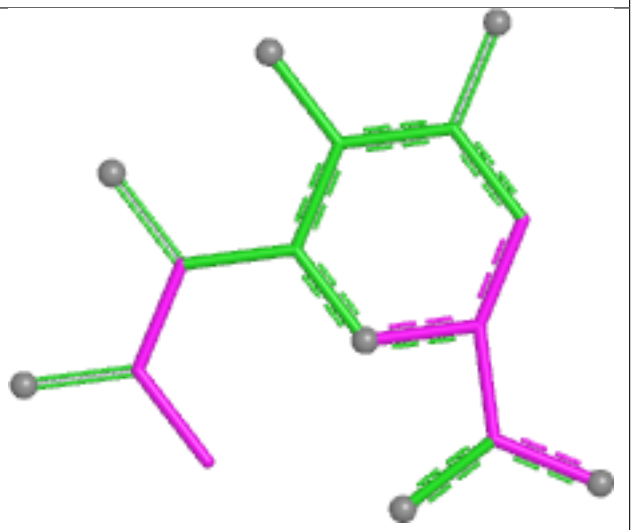


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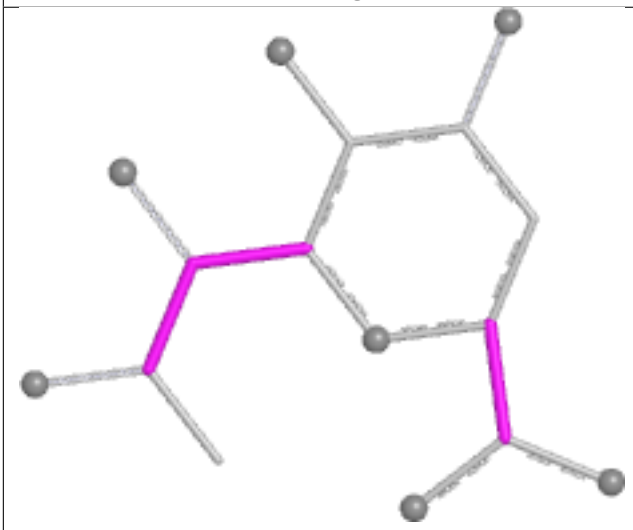
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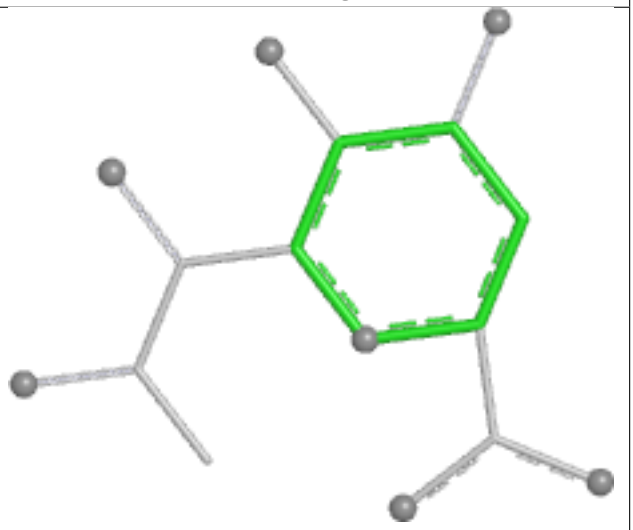
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Bond angles

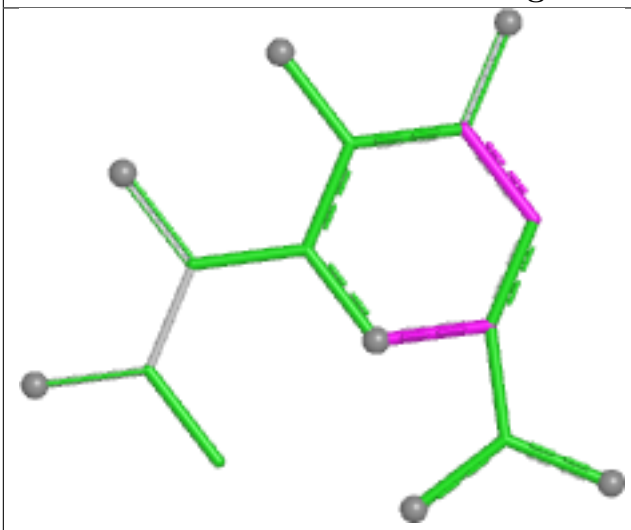


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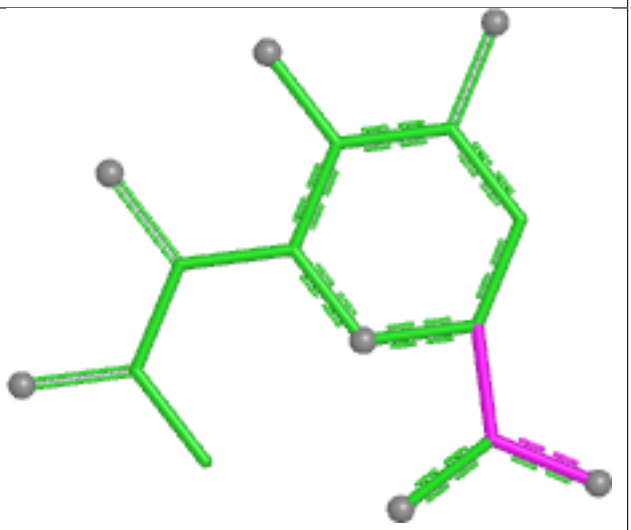


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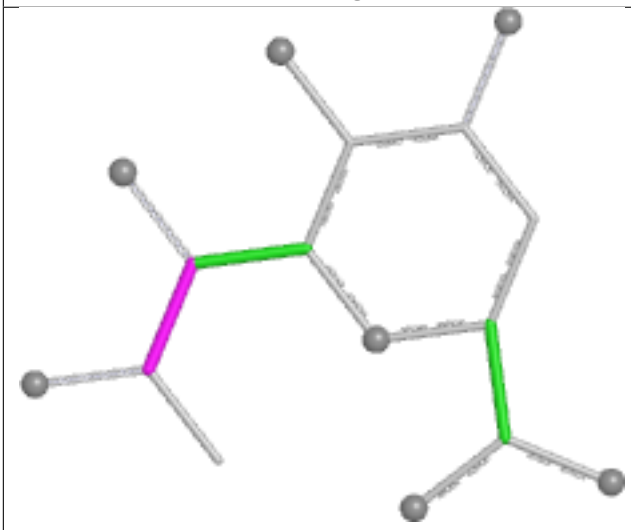
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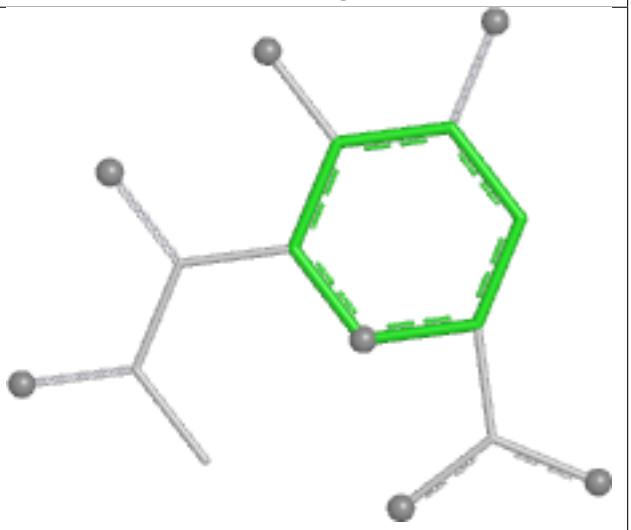
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Bond angles

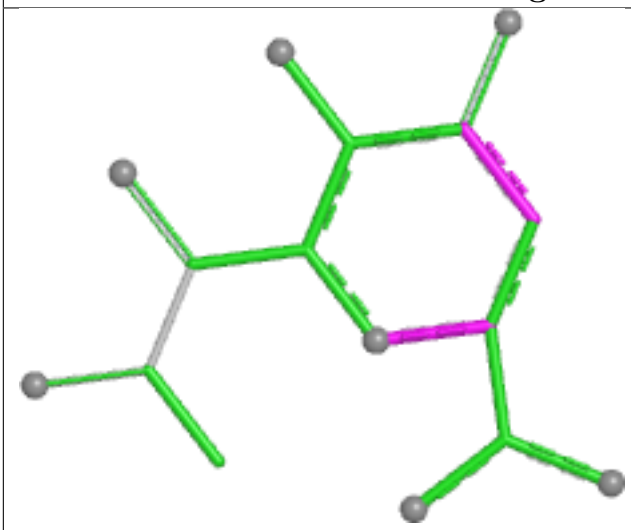


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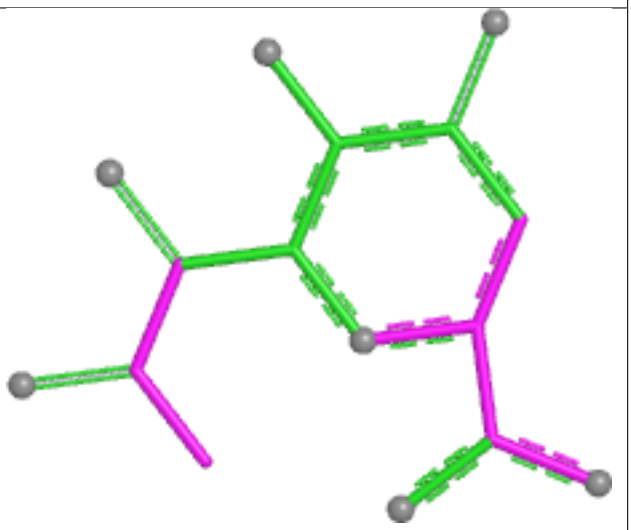


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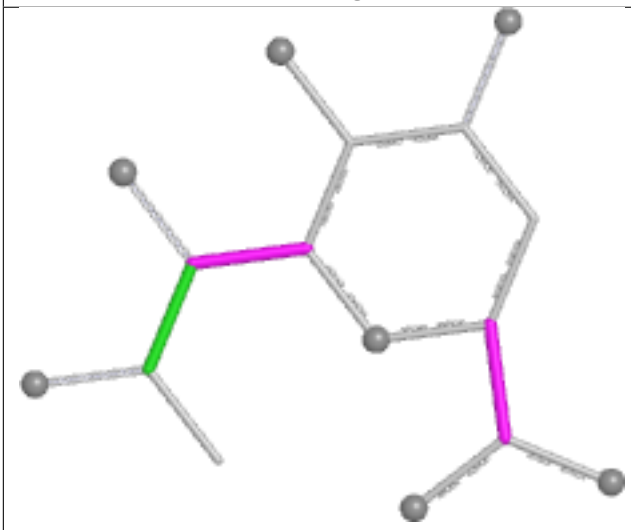
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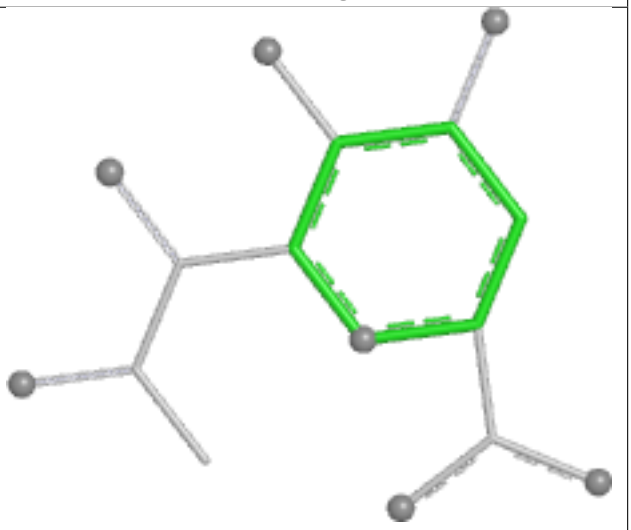
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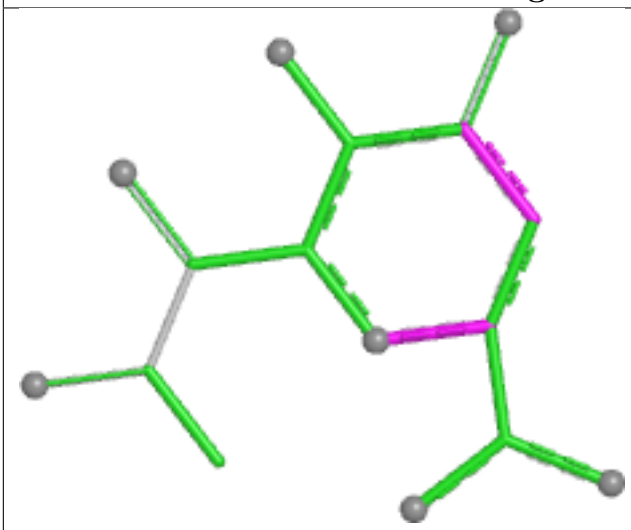


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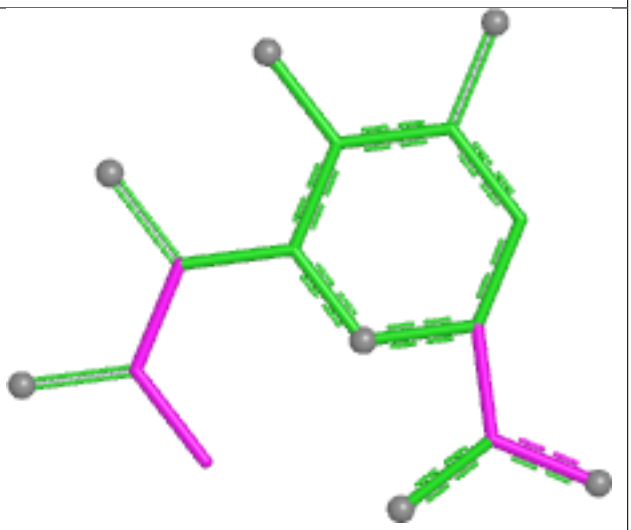


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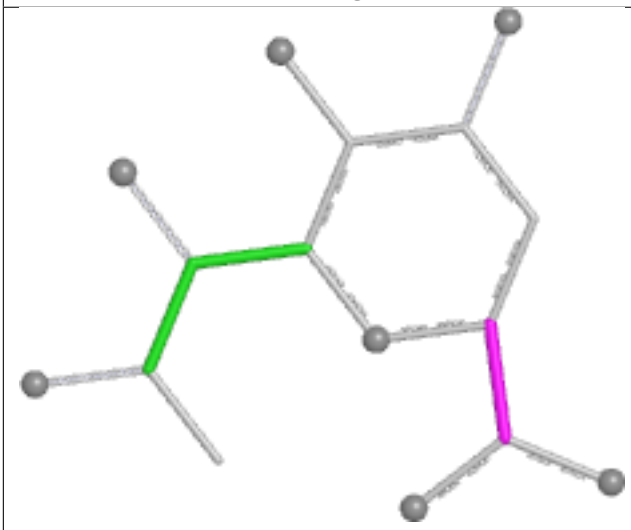
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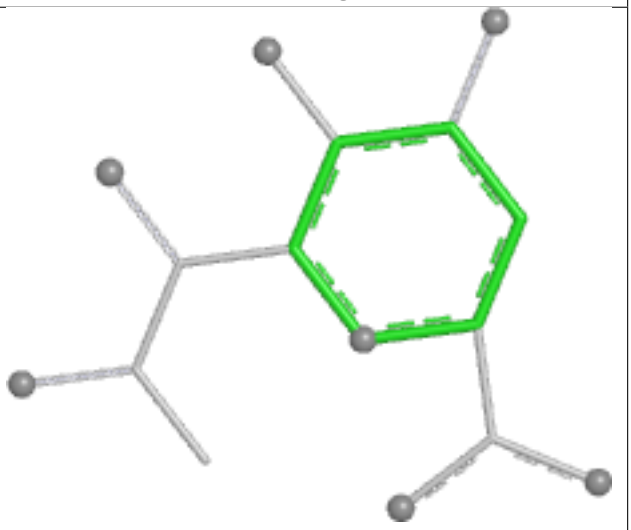
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Bond angles

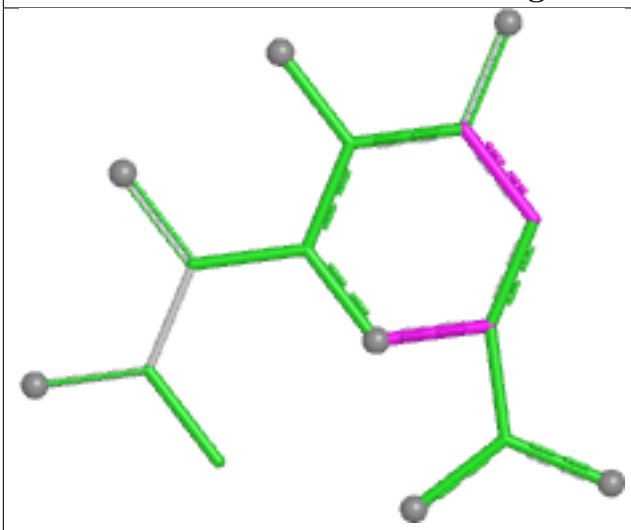


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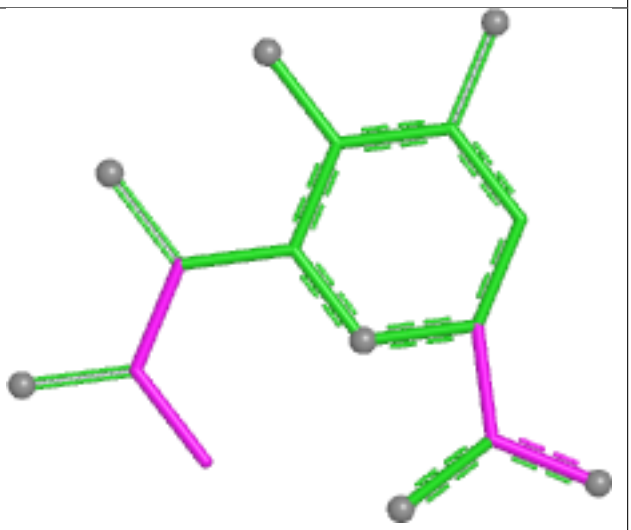


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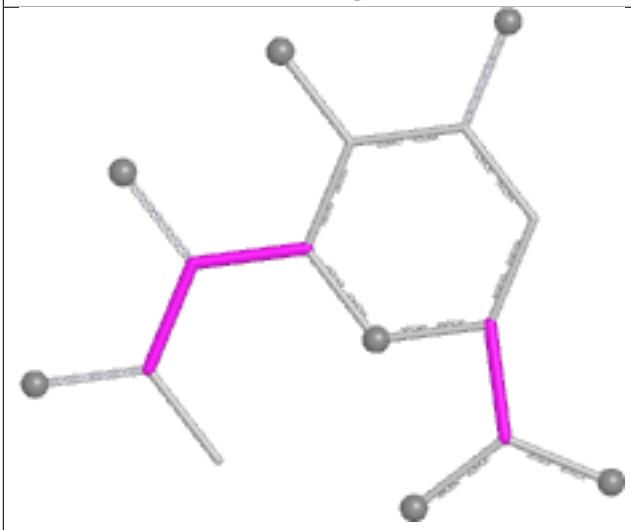
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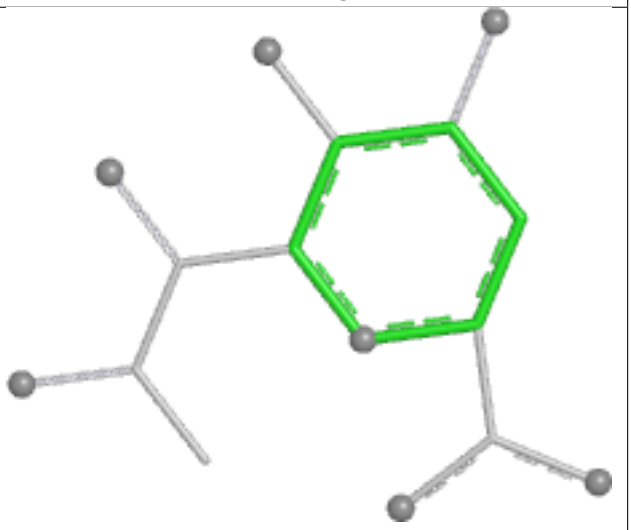
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Bond angles

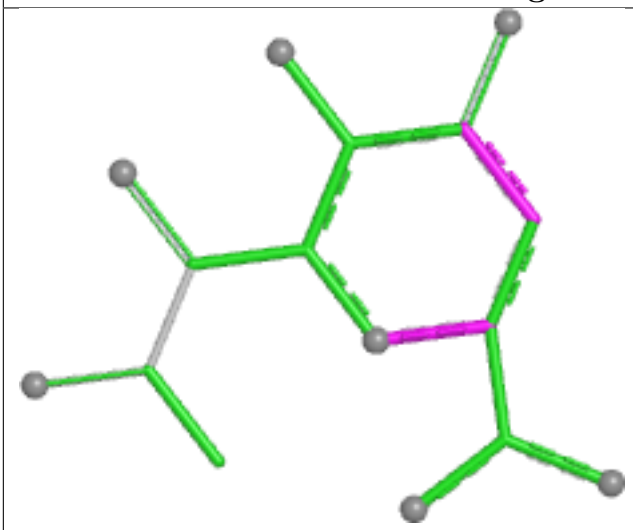


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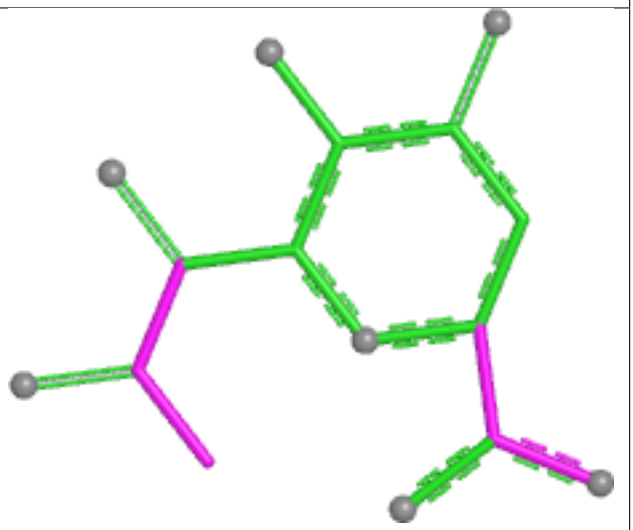


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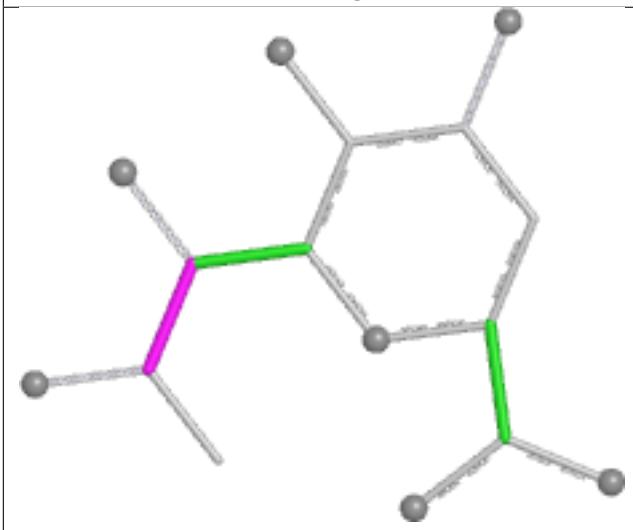
Ligand P8E V 610



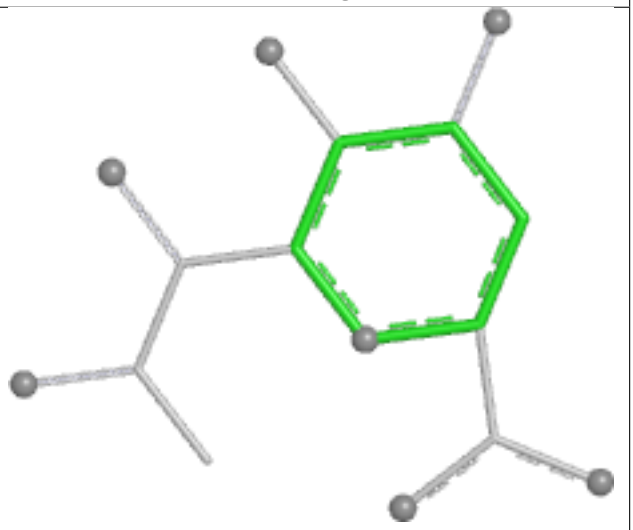
Bond lengths



Bond angles

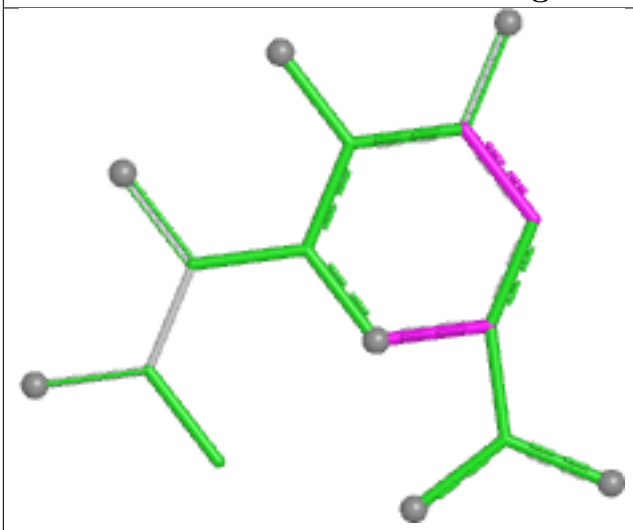


Torsions

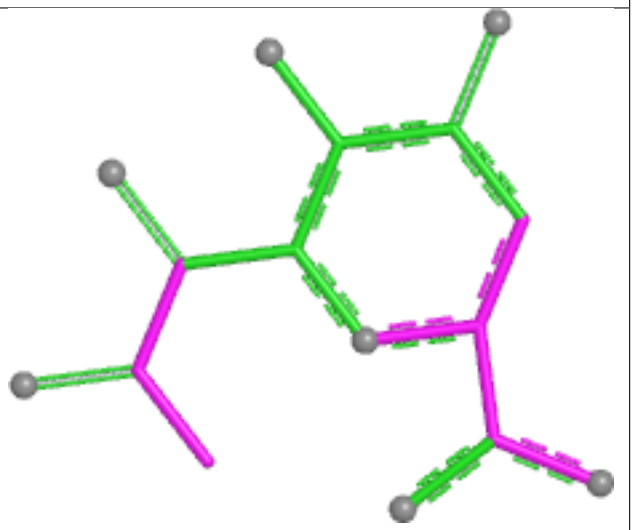


Rings

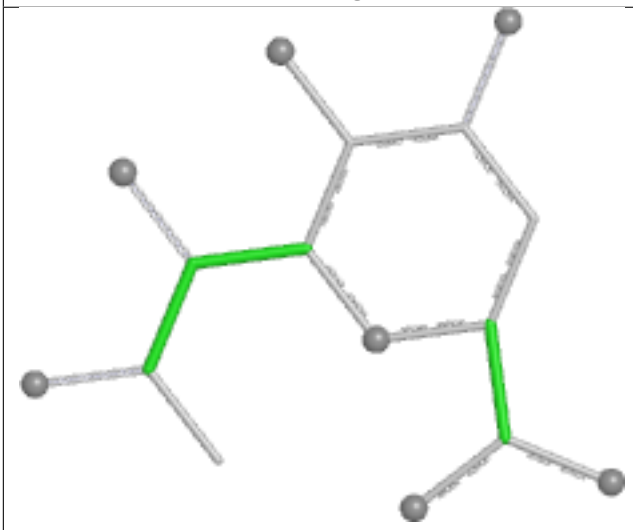
Ligand P8E S 615



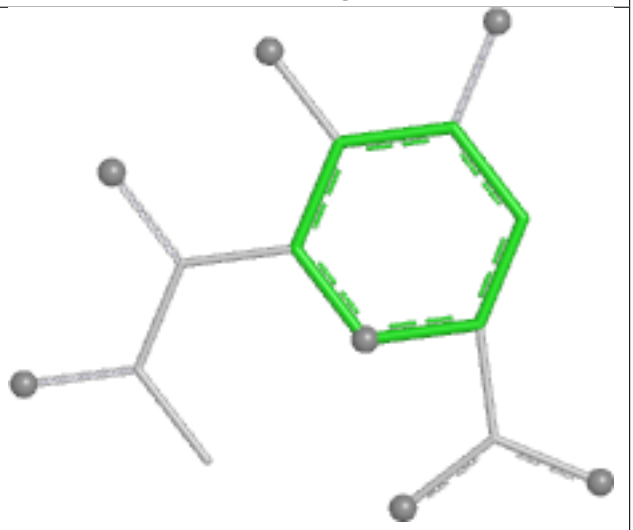
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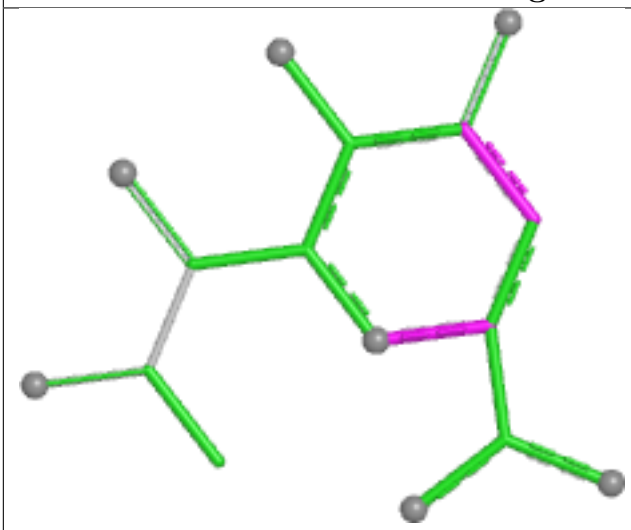


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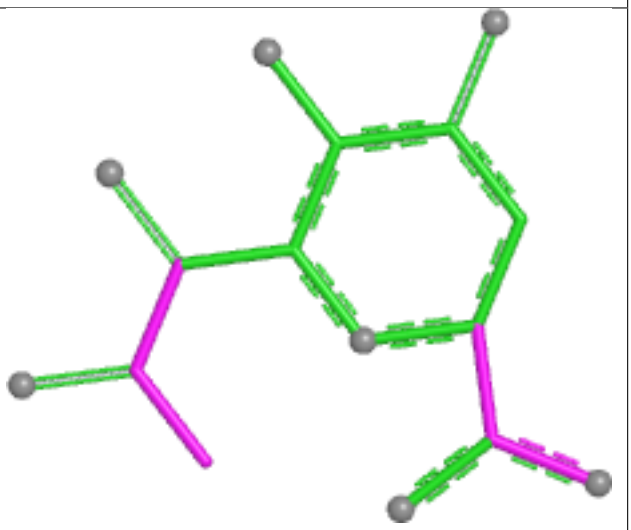


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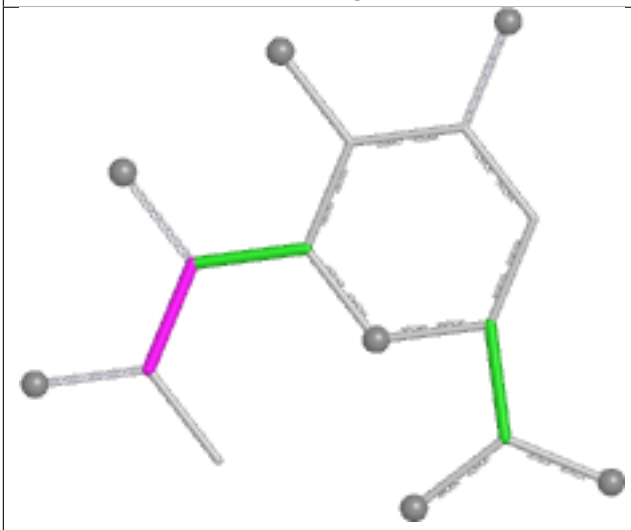
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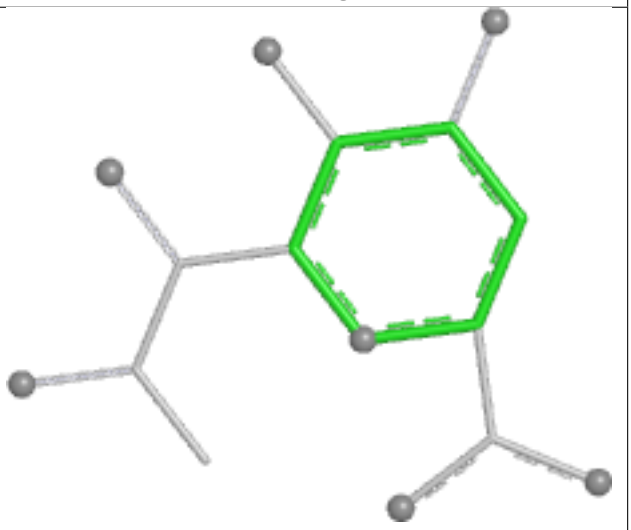
Bond lengths



Bond angles

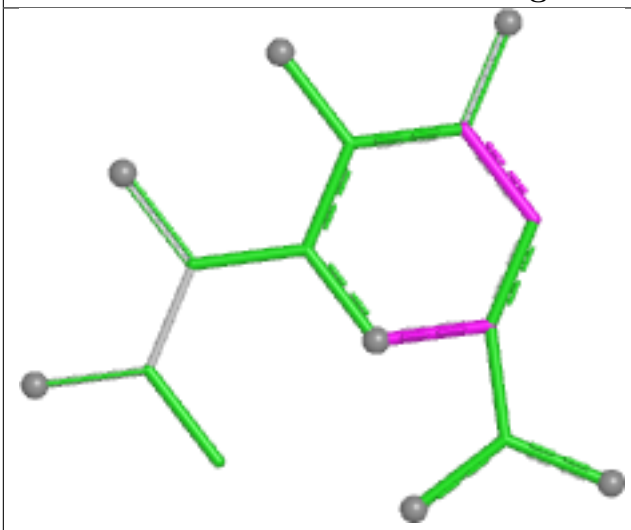


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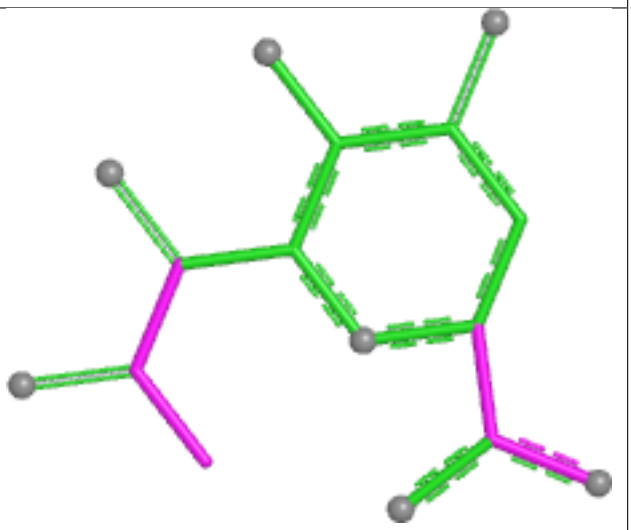


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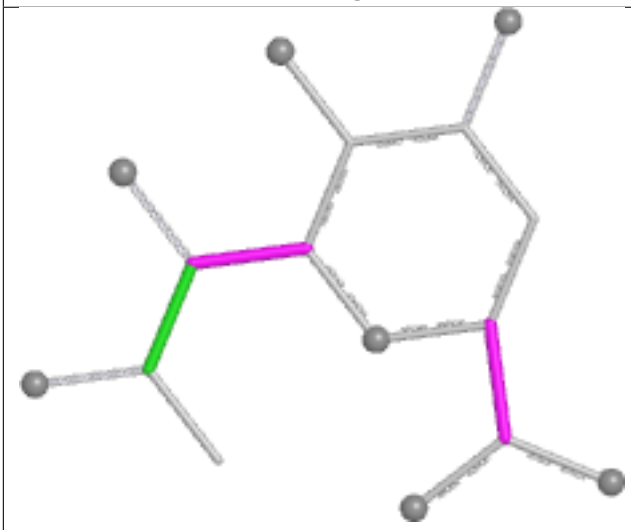
Ligand P8E E 609



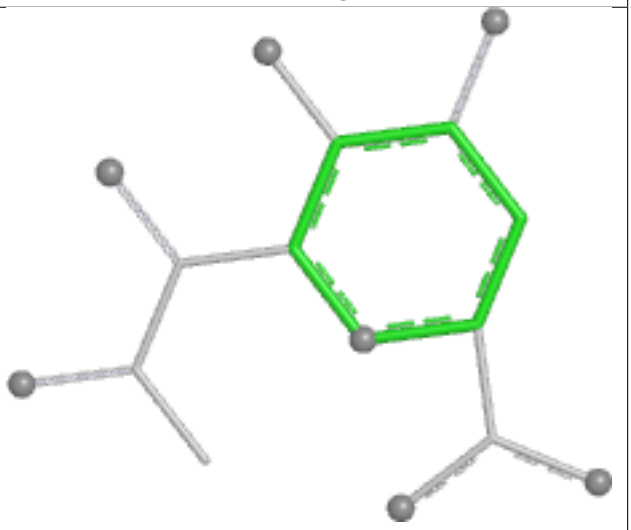
Bond lengths



Bond angles

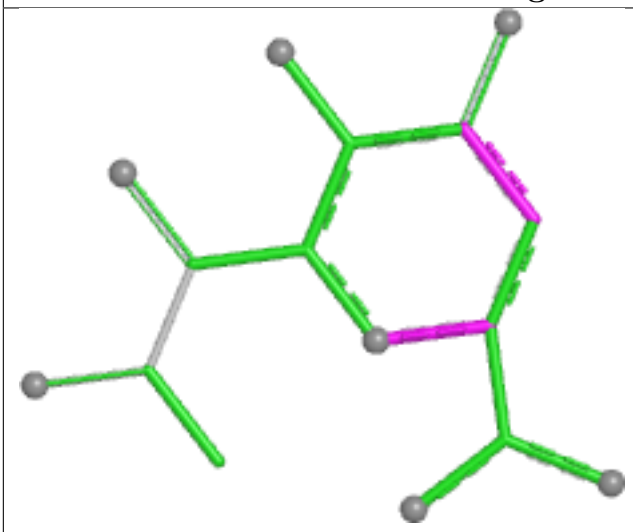


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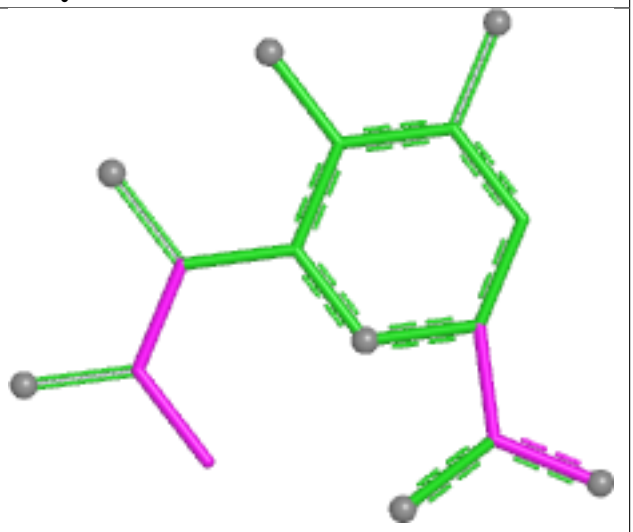


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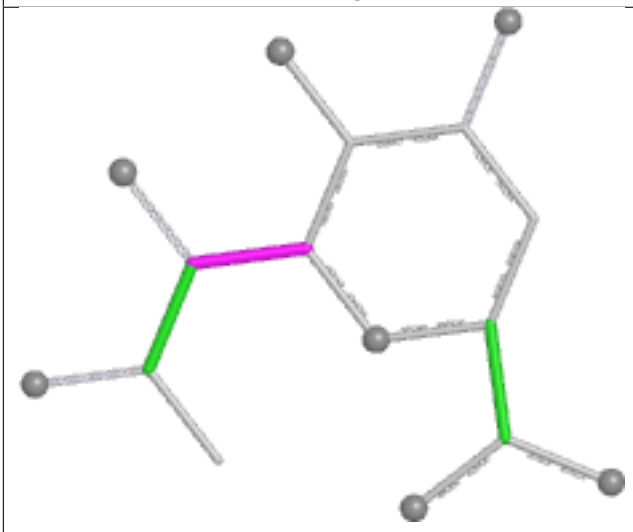
Ligand P8E Q 601



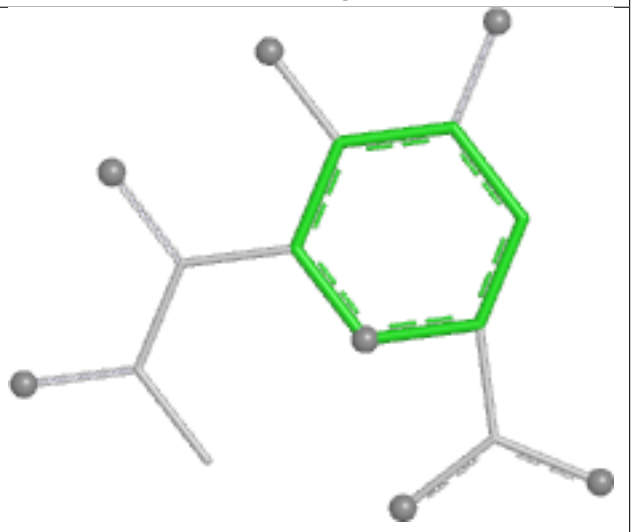
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Bond angles

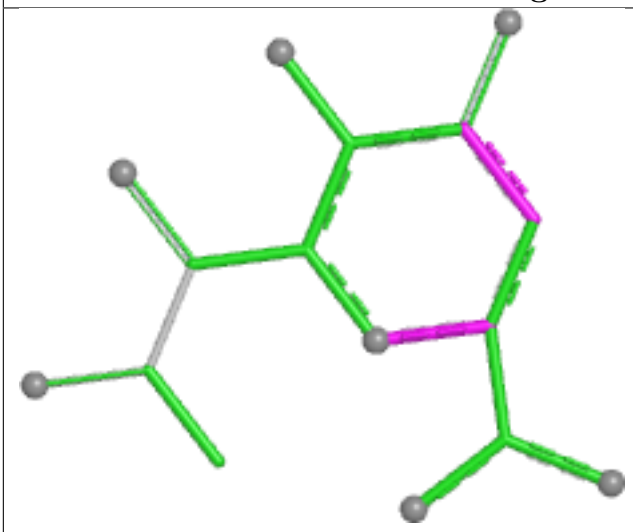


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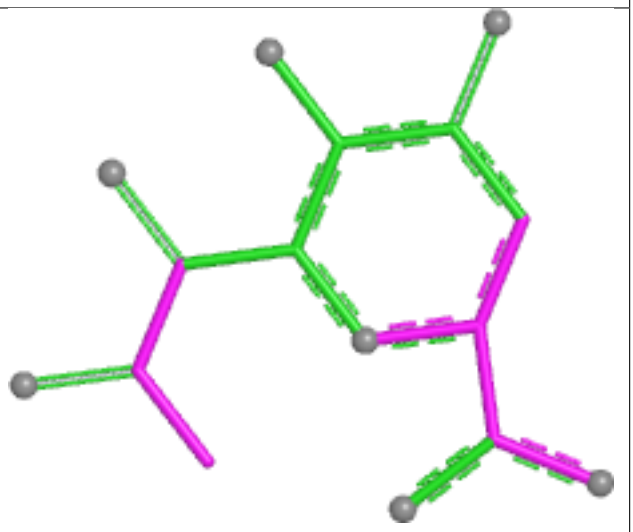


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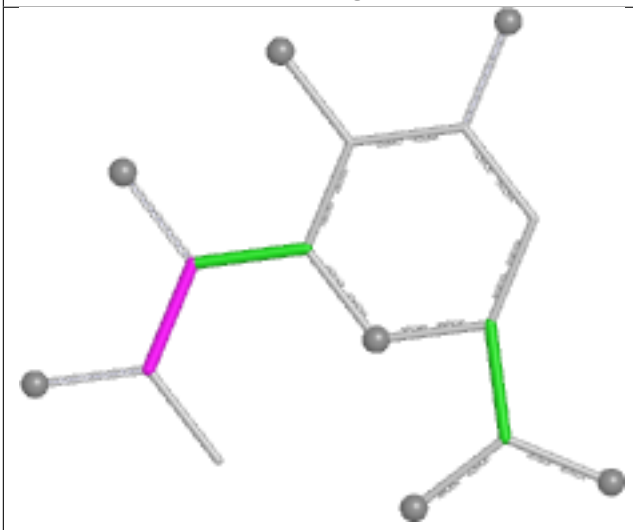
Ligand P8E F 603



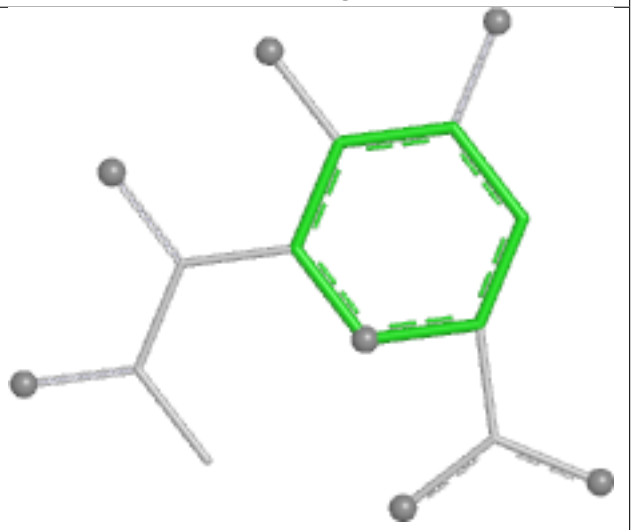
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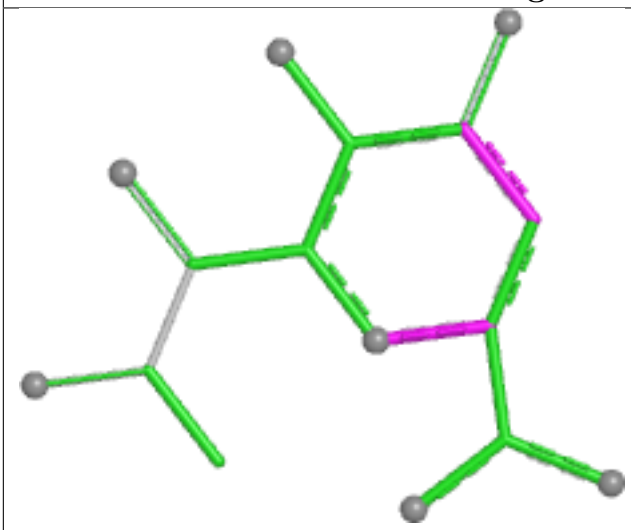


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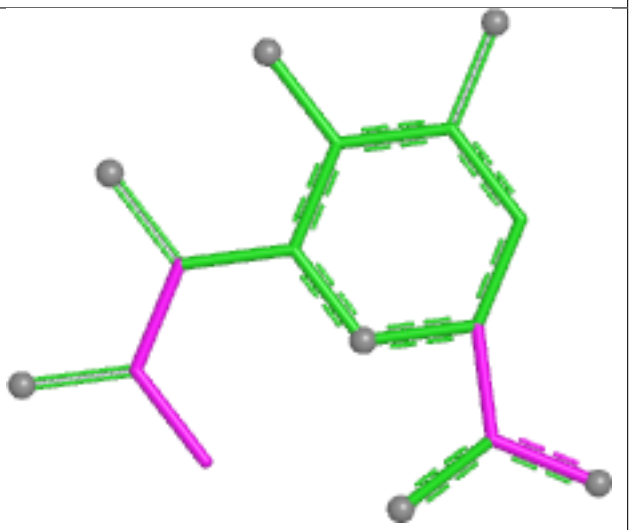


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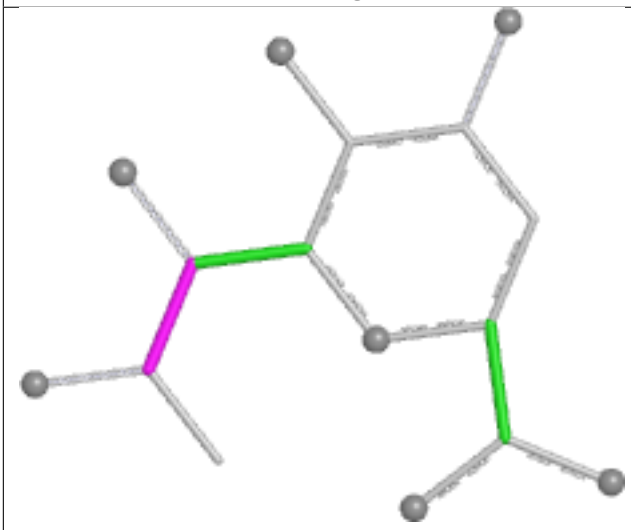
Ligand P8E D 614



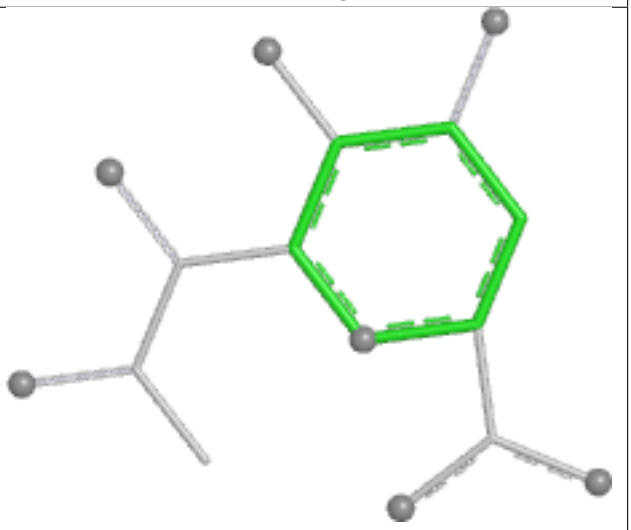
Bond lengths



Bond angles

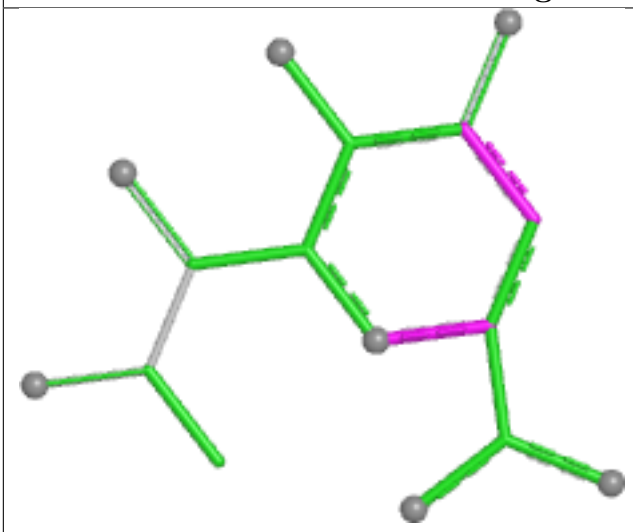


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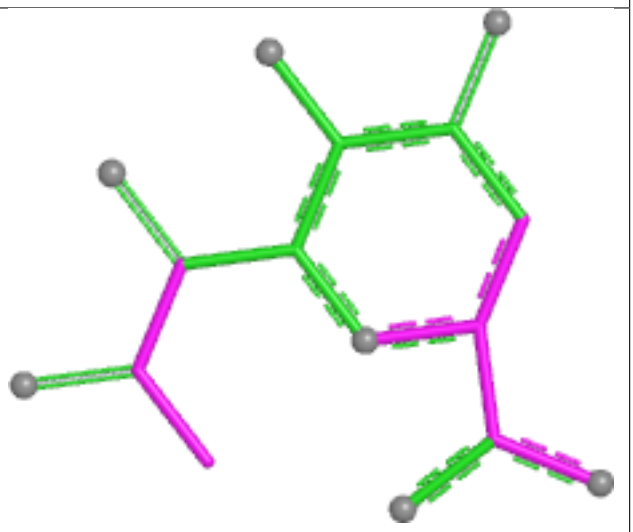


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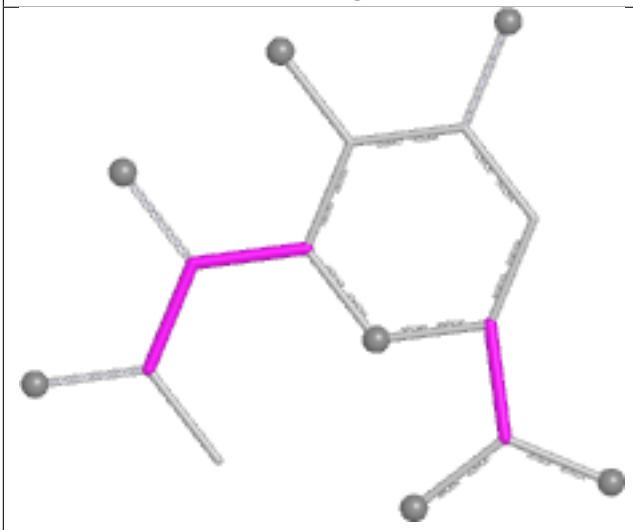
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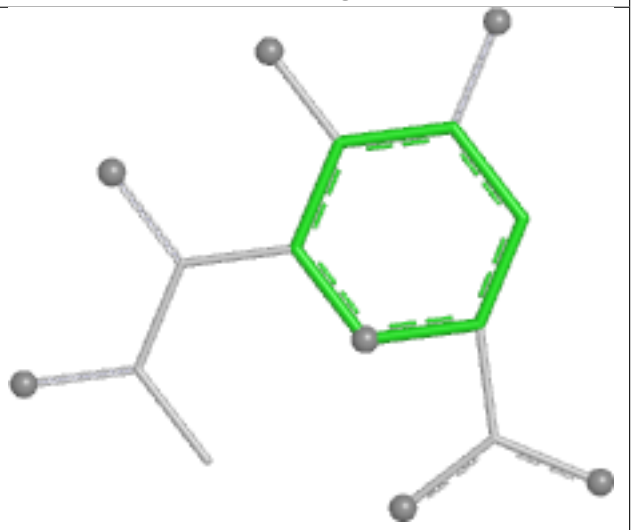
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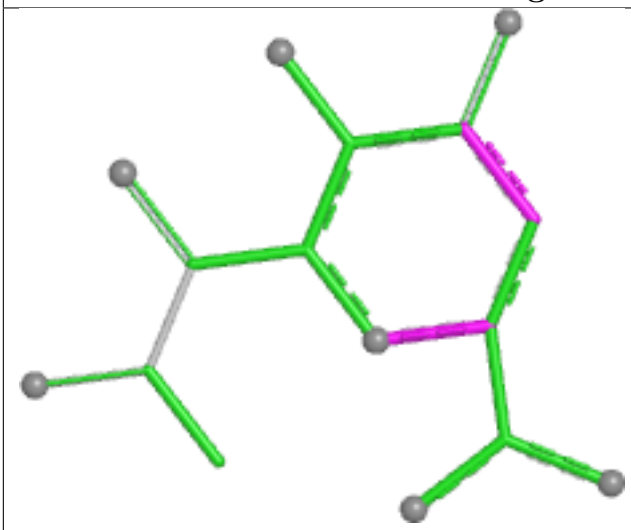


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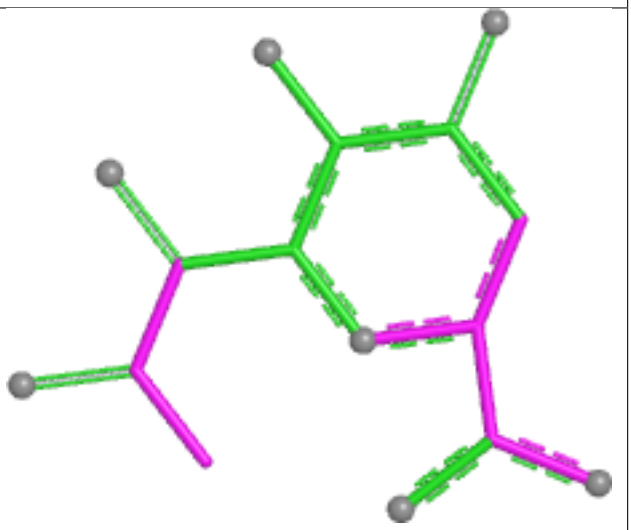


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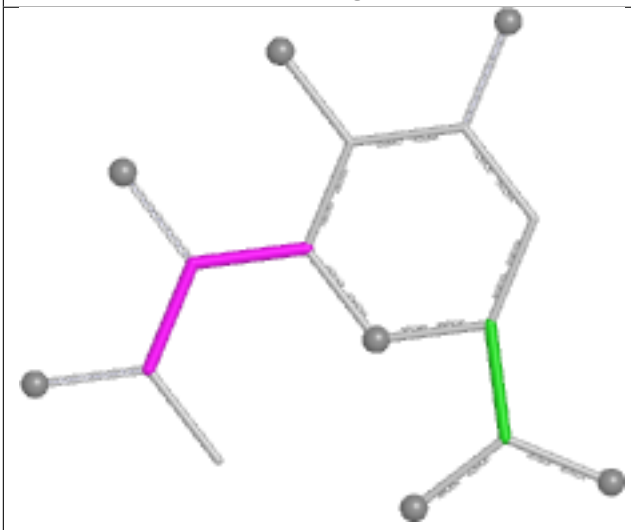
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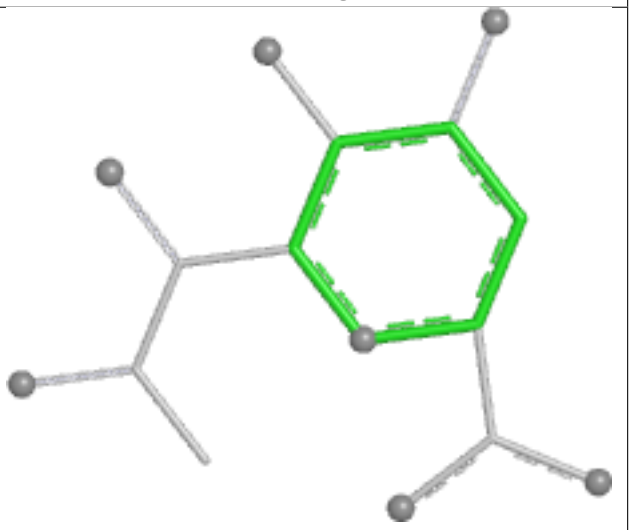
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Bond angles

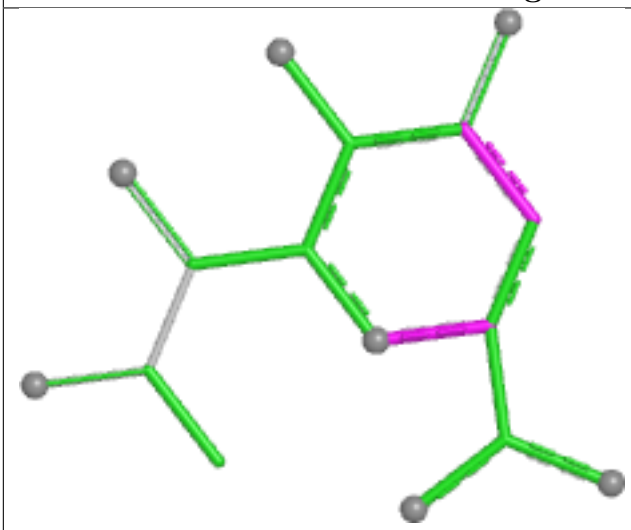


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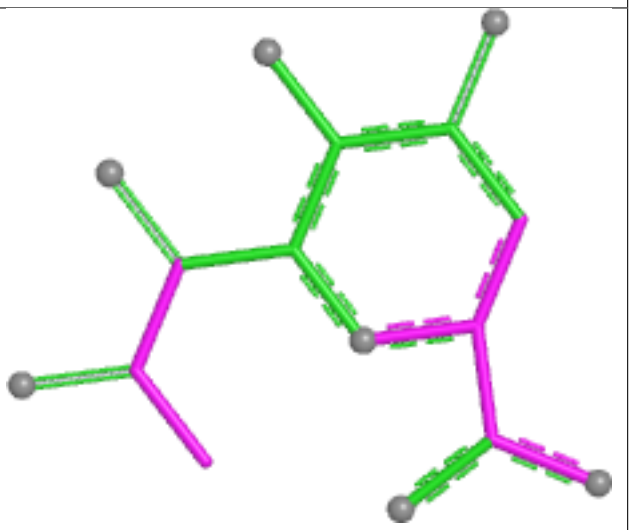


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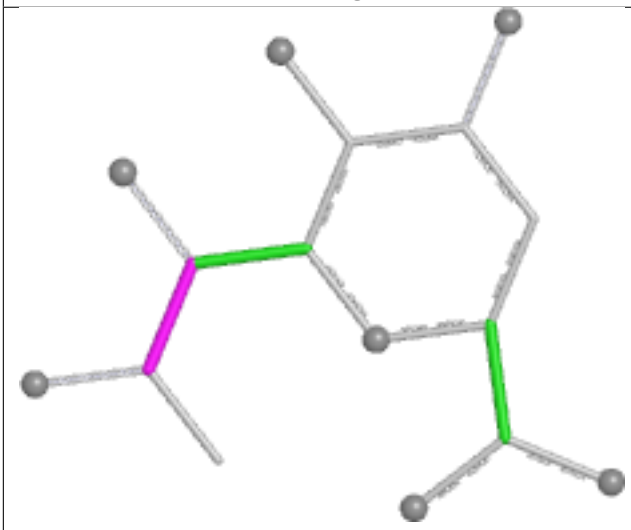
Ligand P8E M 603



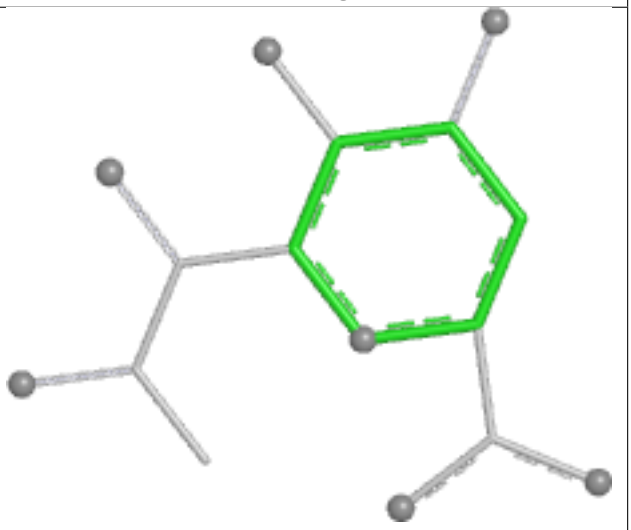
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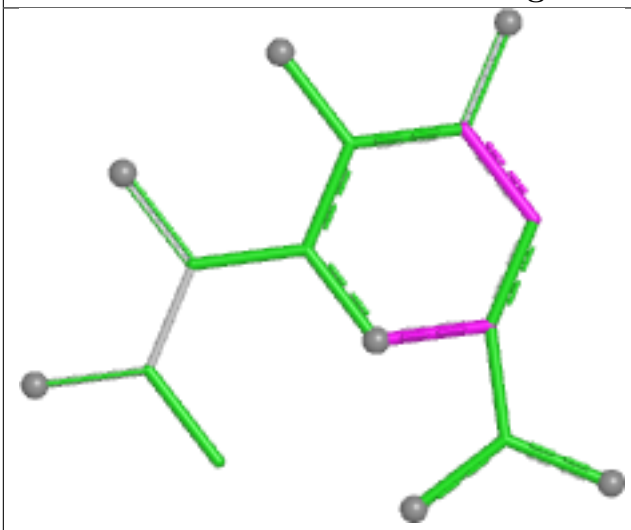


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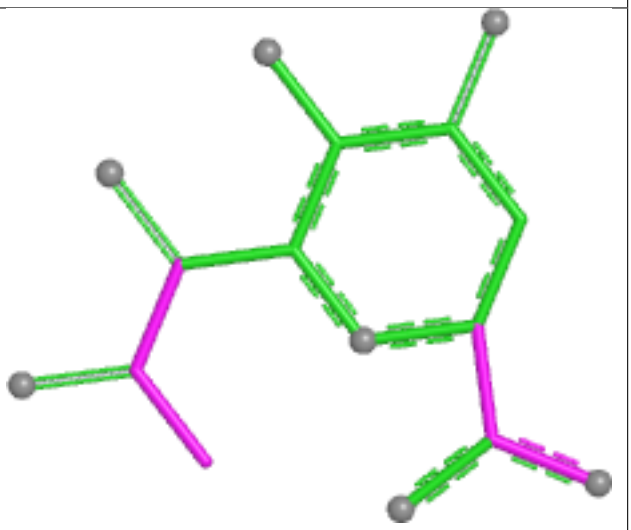


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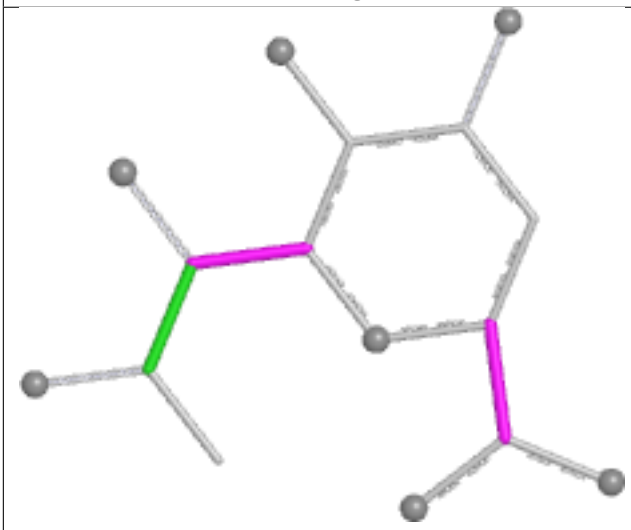
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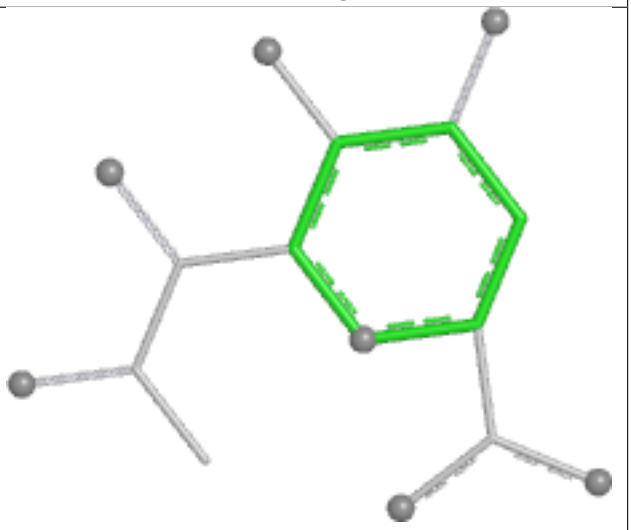
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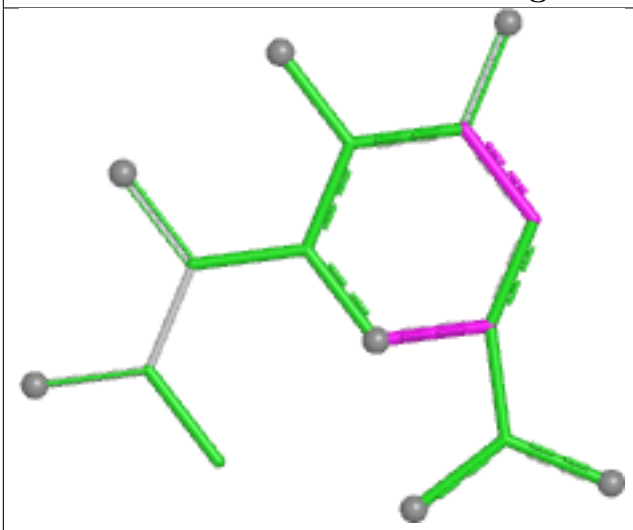


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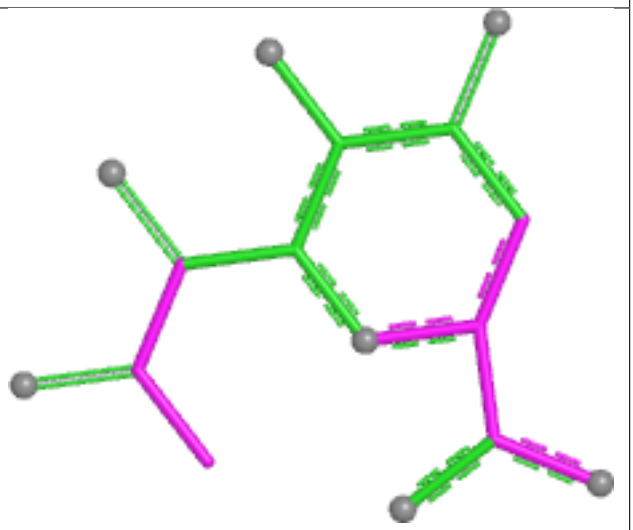


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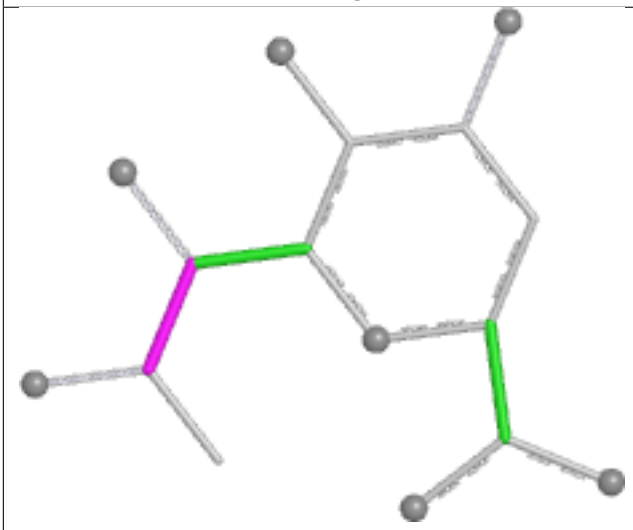
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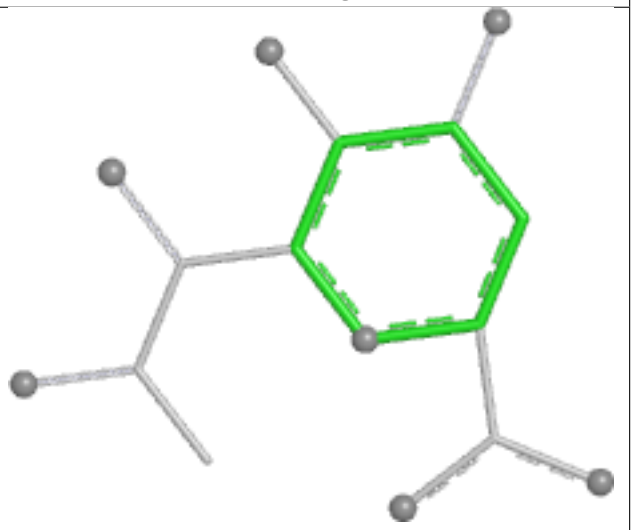
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Bond angles

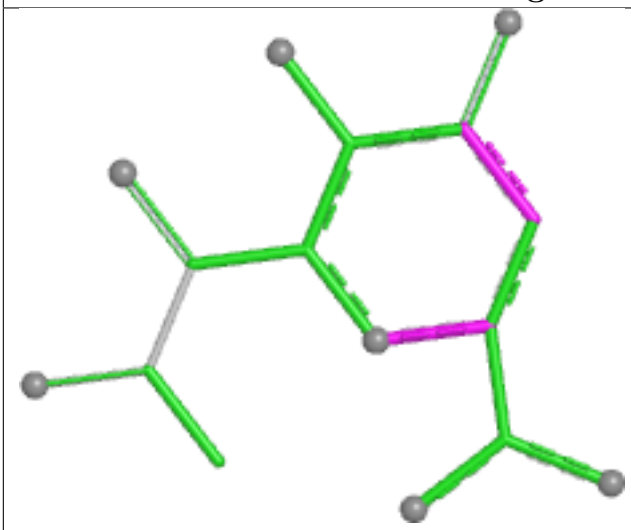


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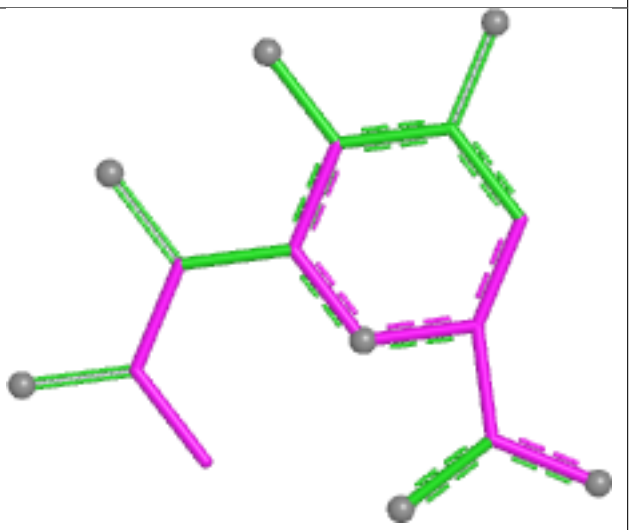


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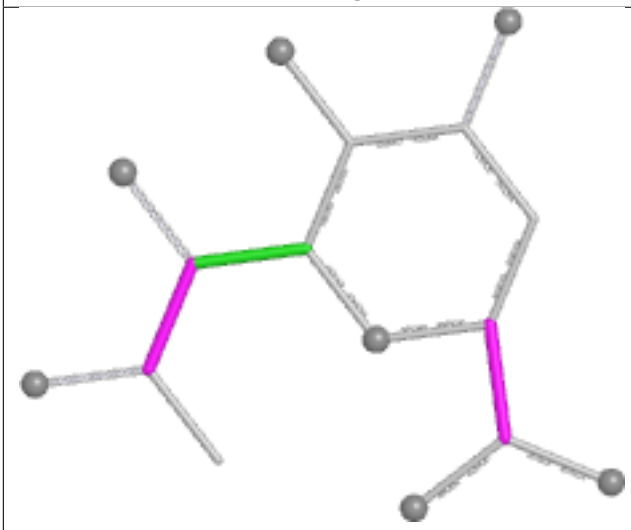
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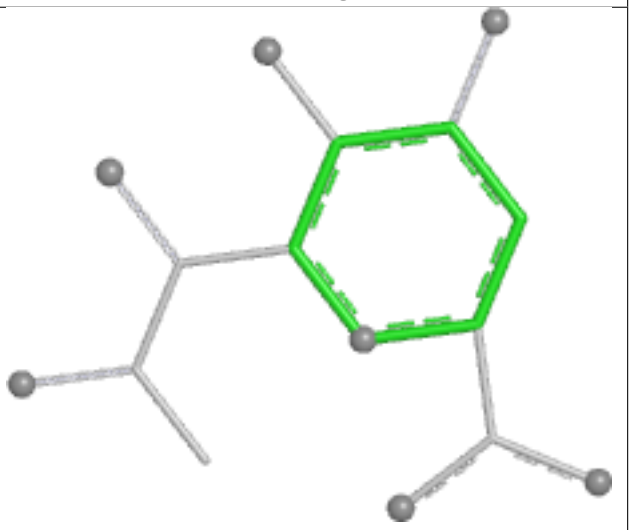
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Bond angles

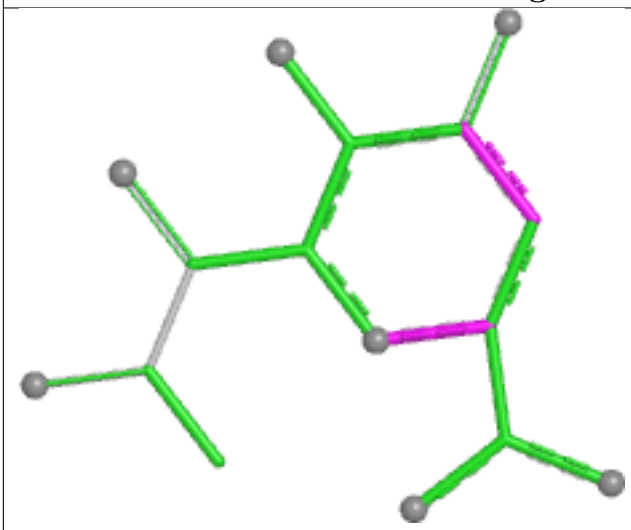


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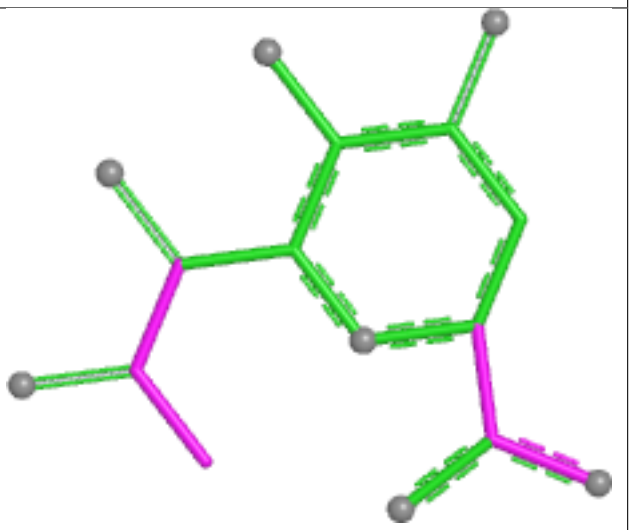


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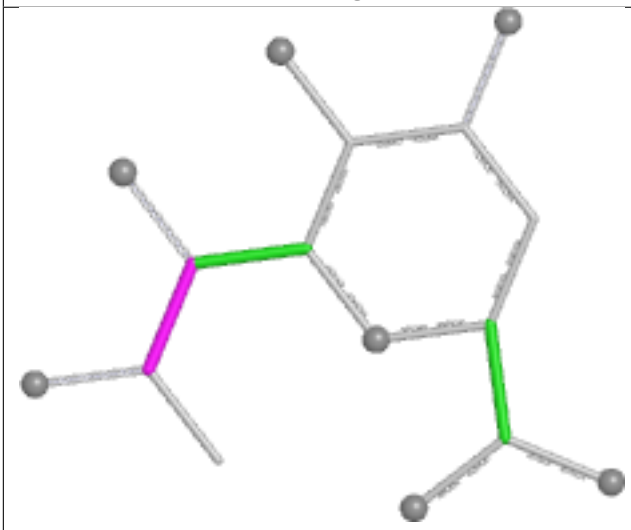
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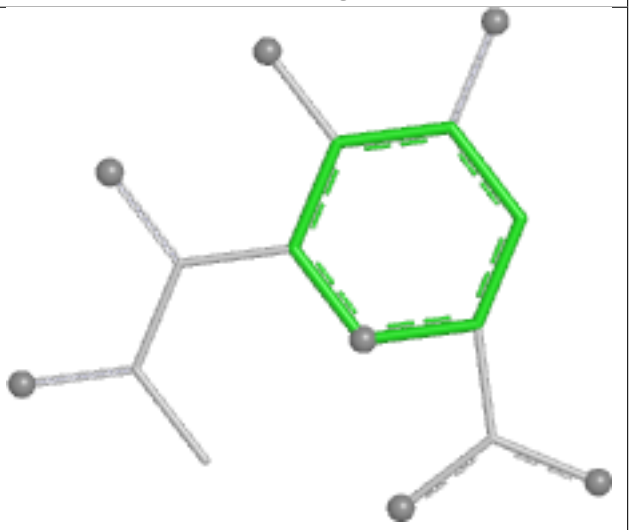
Bond lengths



Bond angles

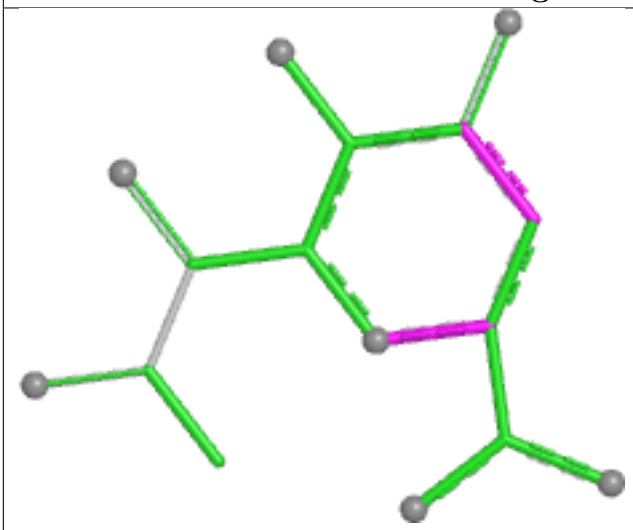


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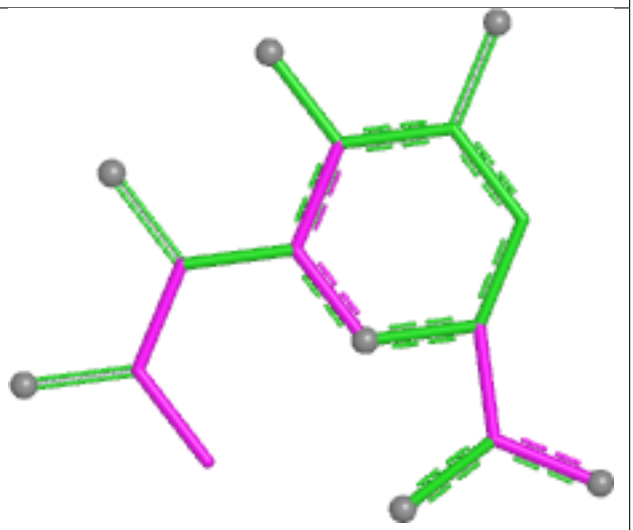


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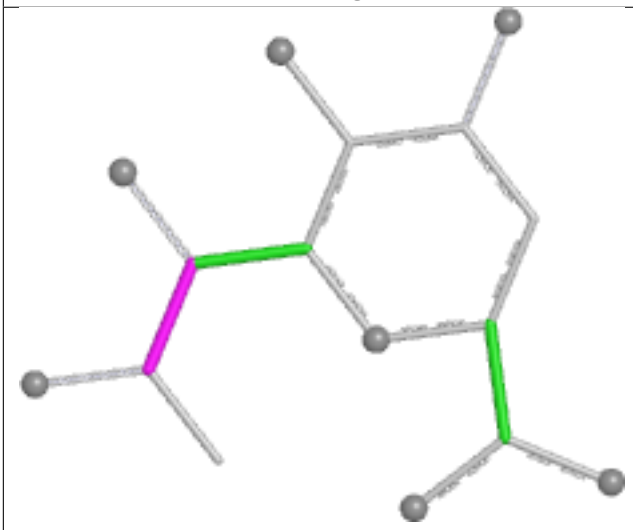
Ligand P8E S 610



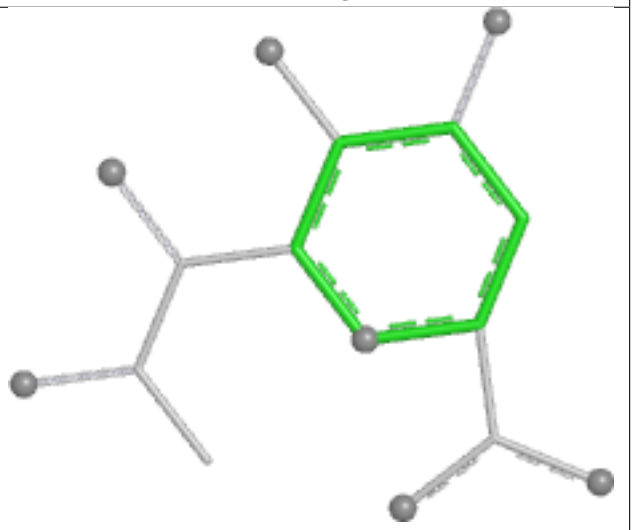
Bond lengths



Bond angles

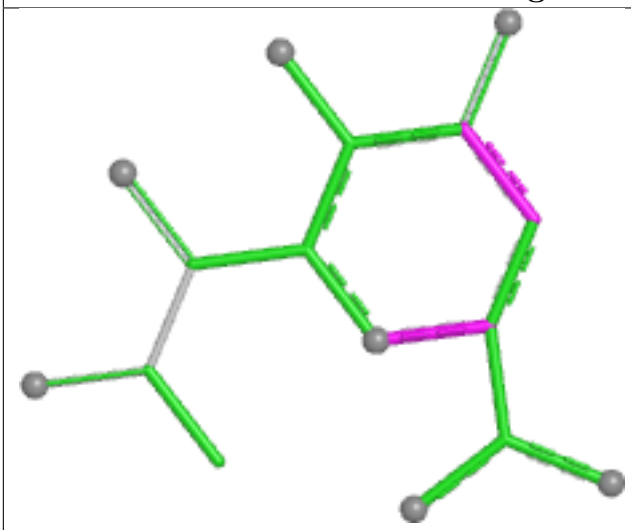


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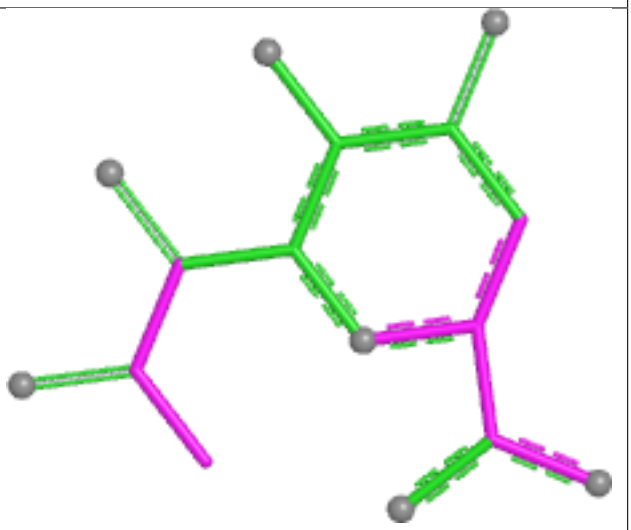


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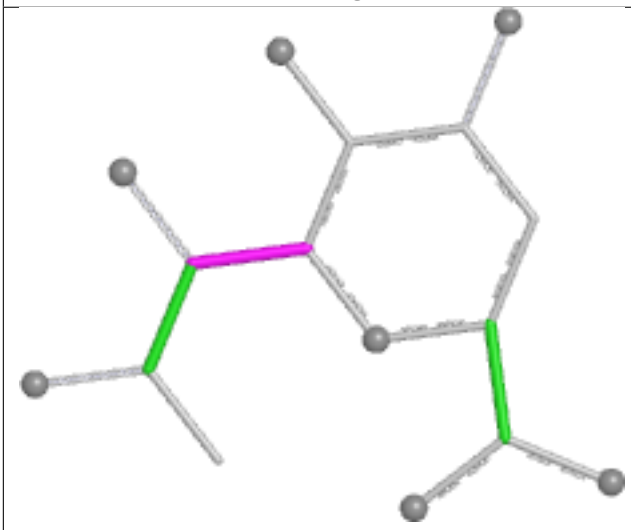
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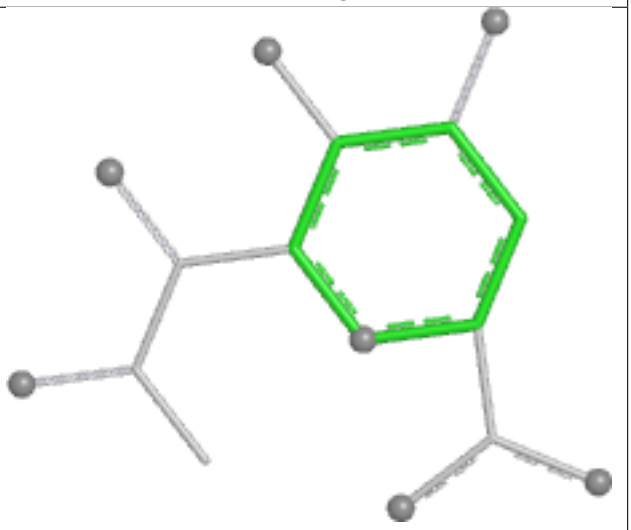
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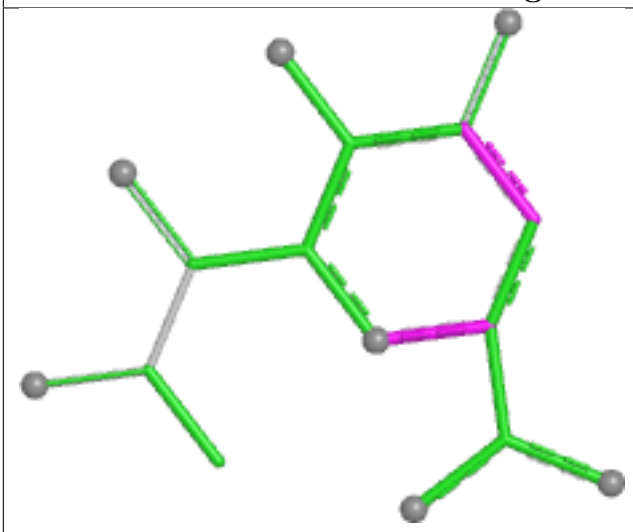


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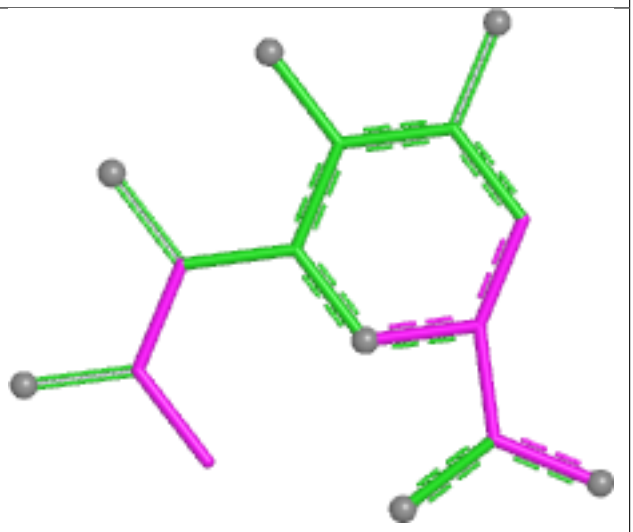


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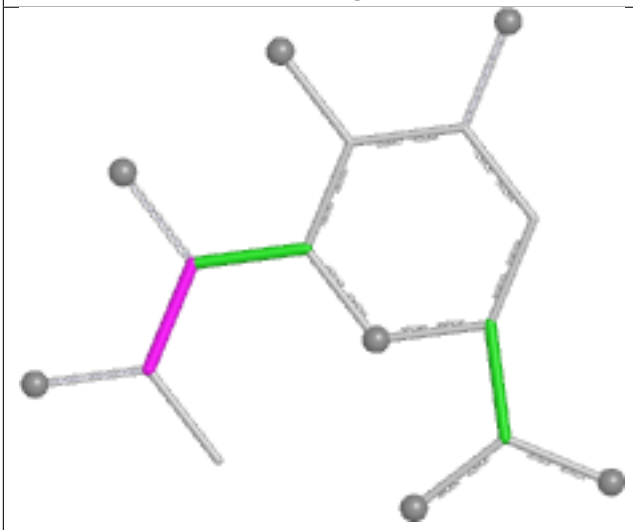
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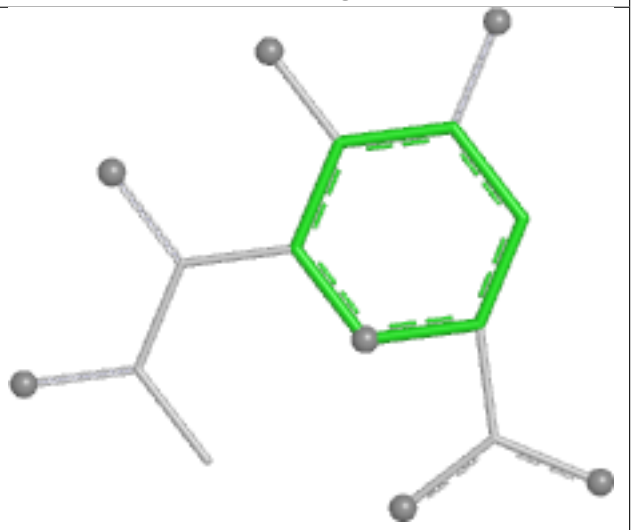
Bond lengths



Bond angles

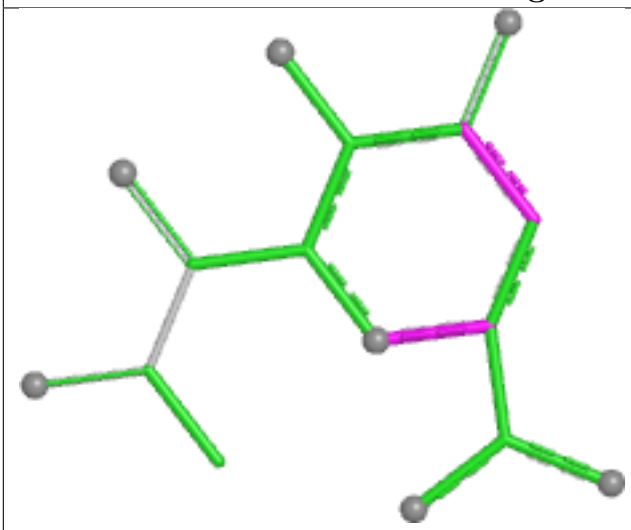


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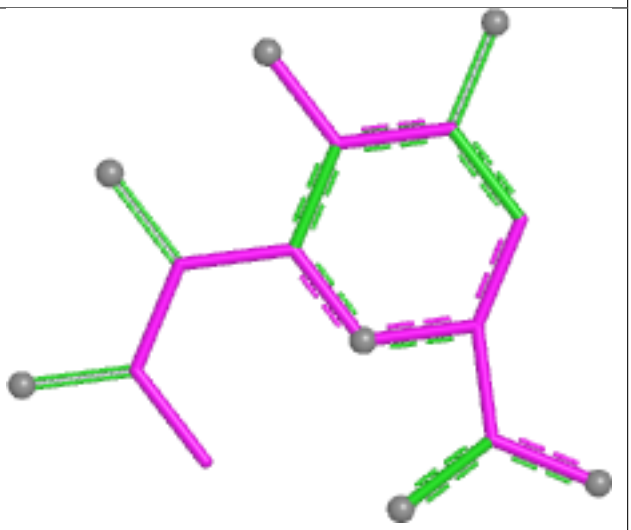


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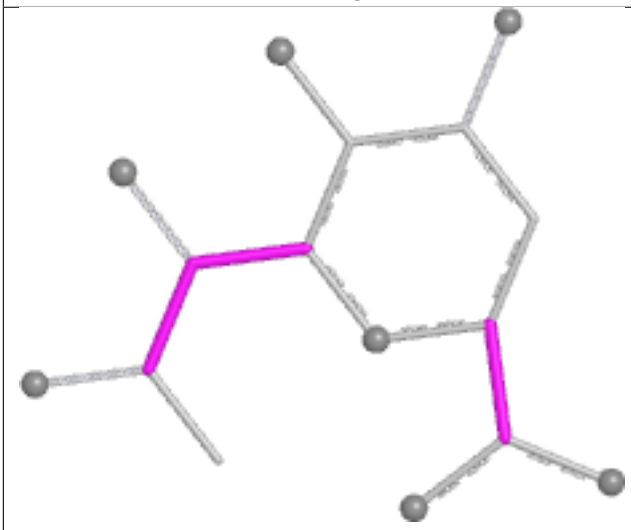
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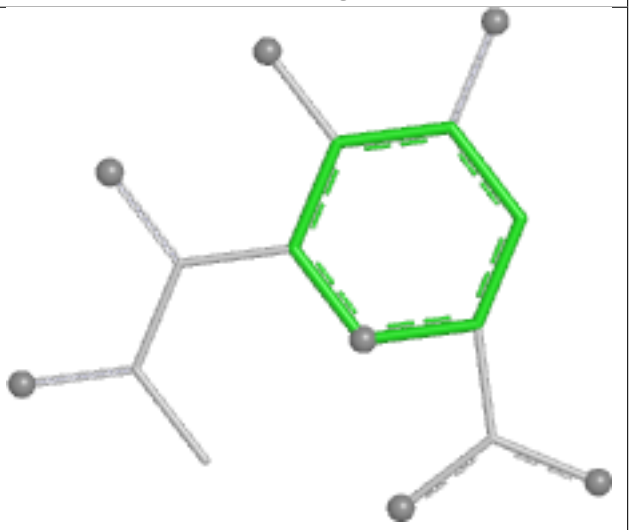
Bond lengths



Bond angles

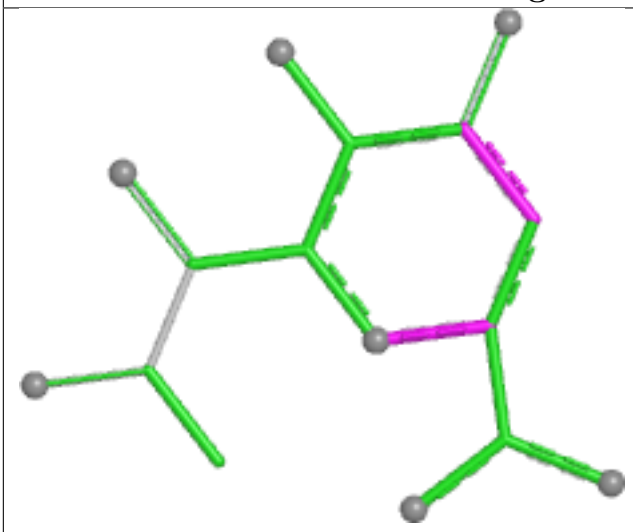


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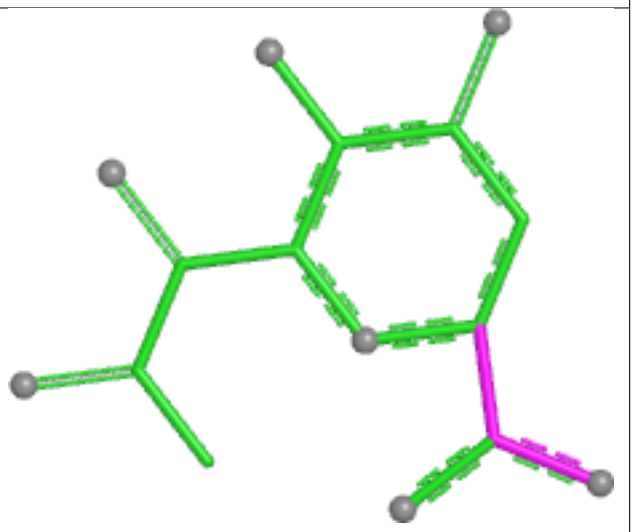


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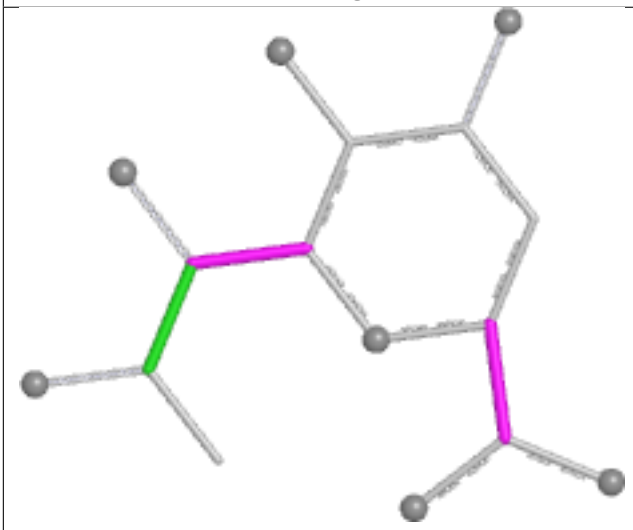
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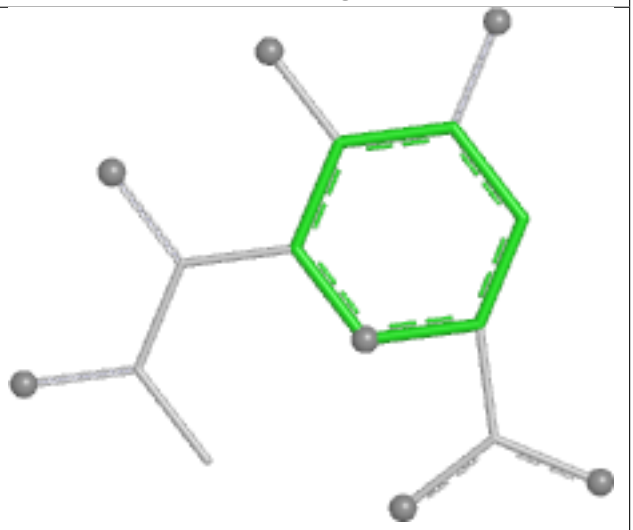
Bond lengths



Bond angles

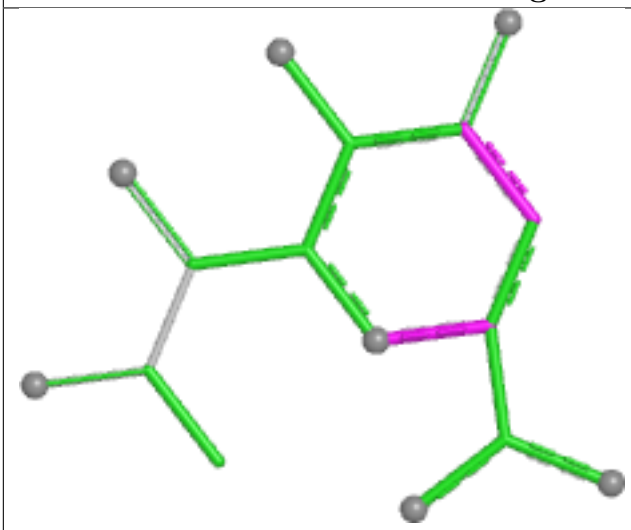


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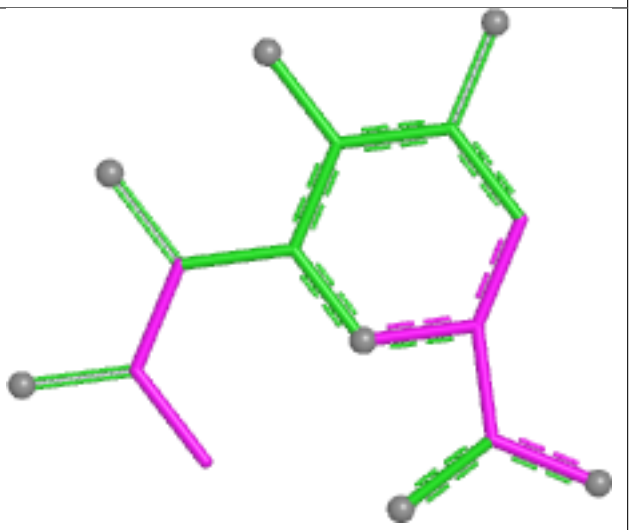


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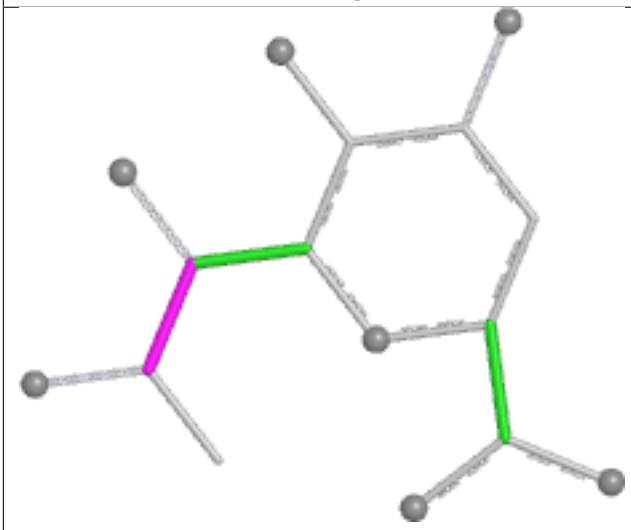
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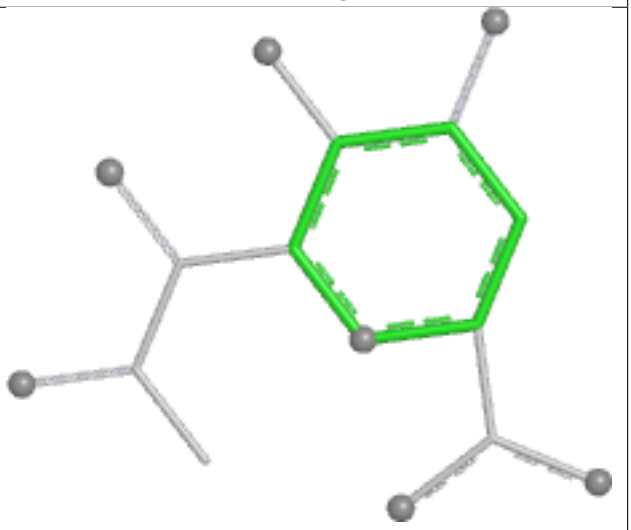
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Bond angles

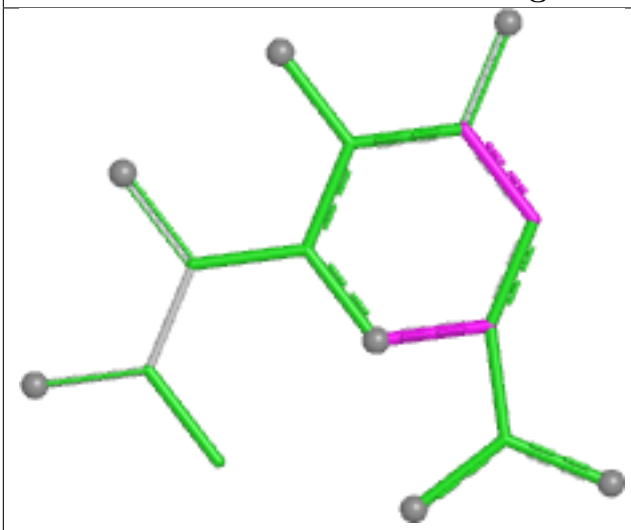


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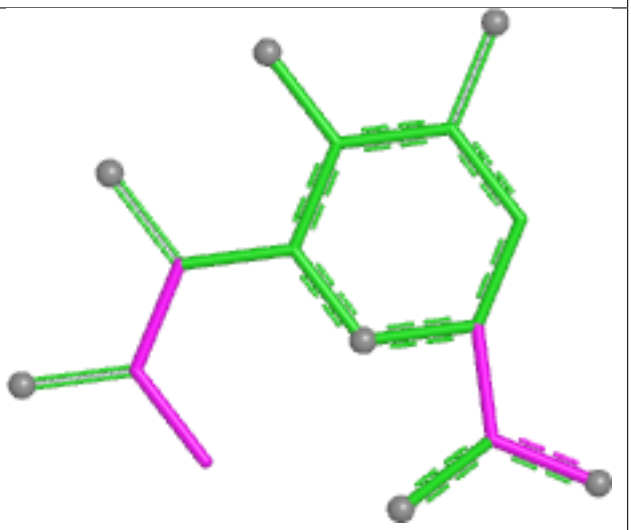


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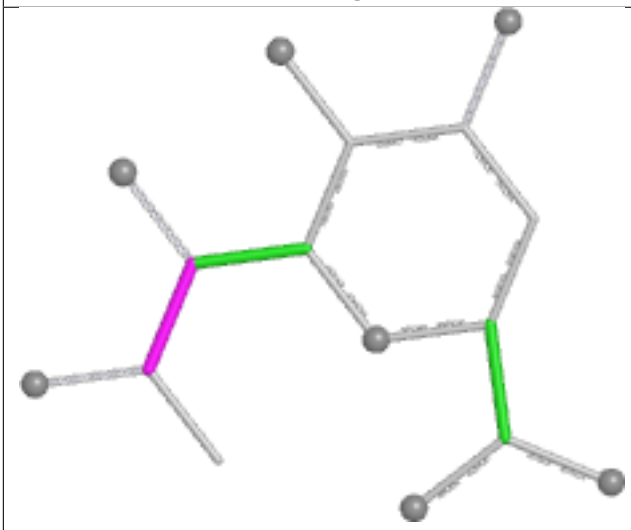
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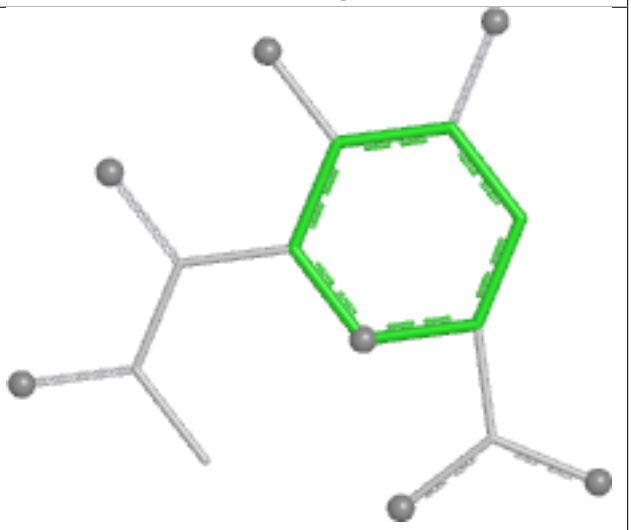
Bond lengths



Bond angles

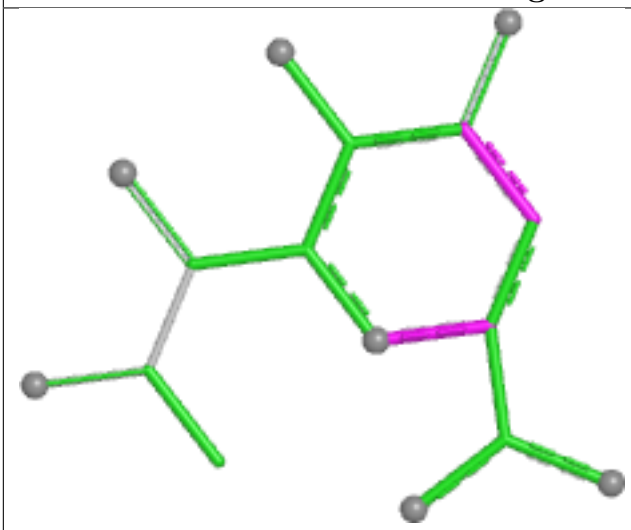


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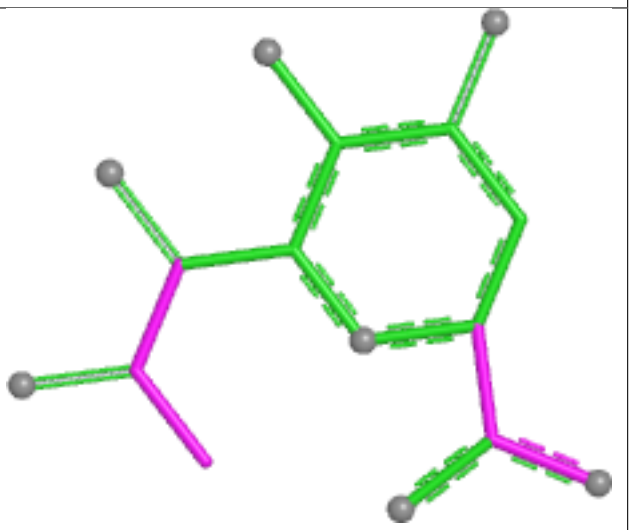


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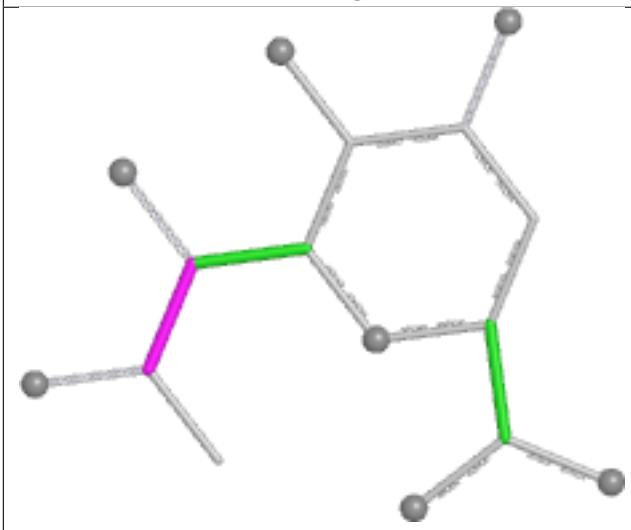
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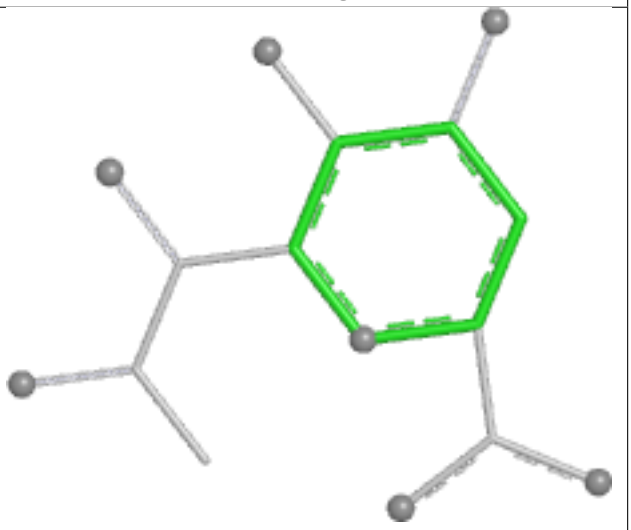
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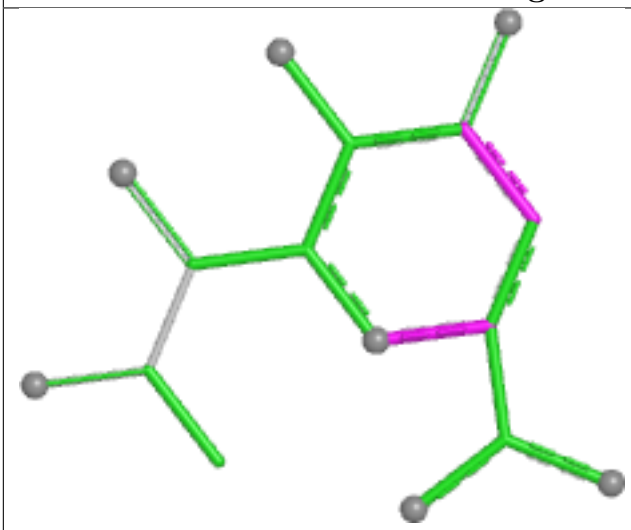


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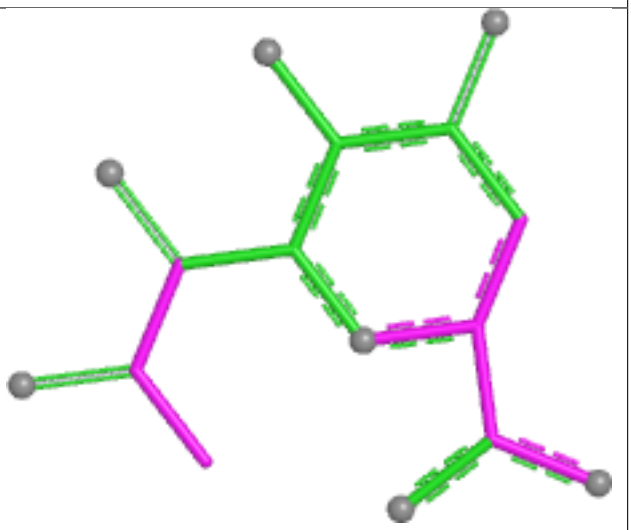


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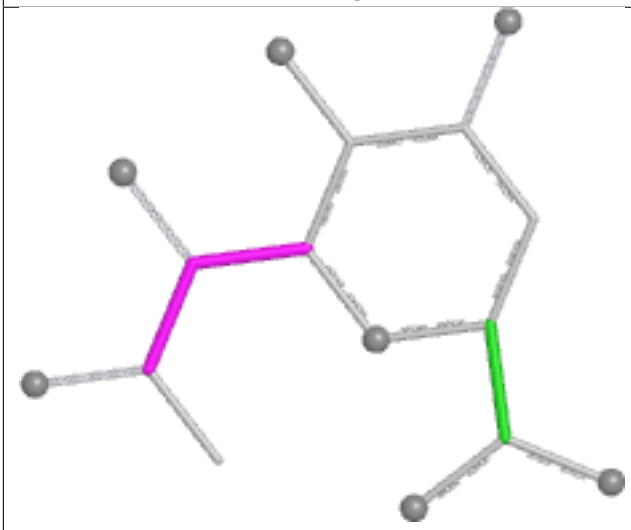
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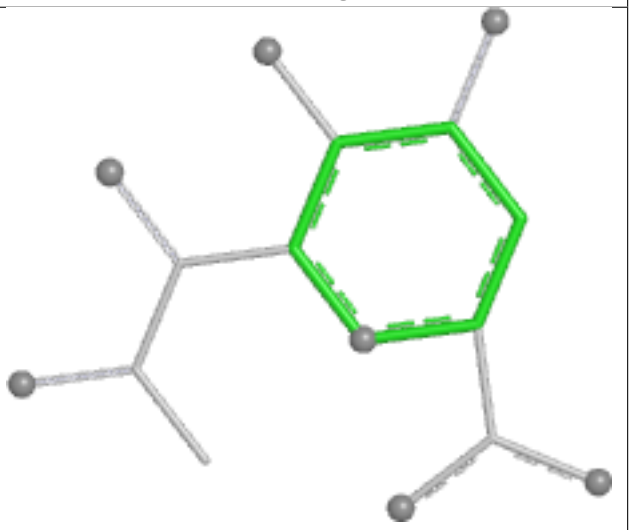
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Bond angles

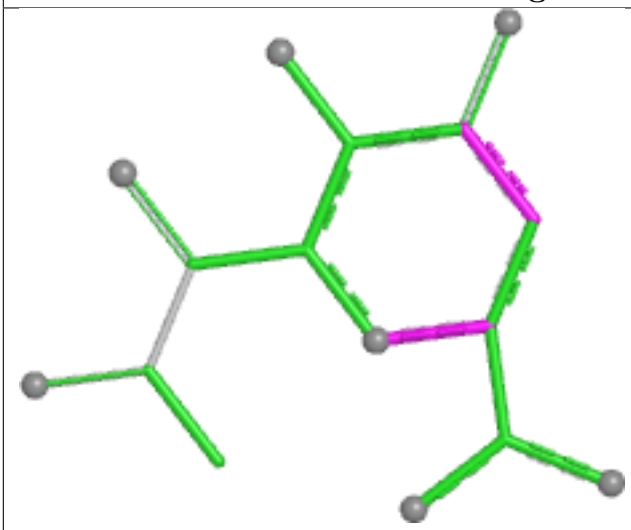


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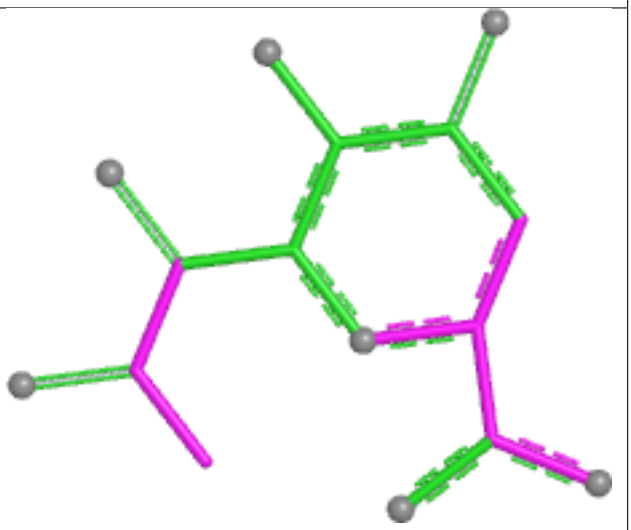


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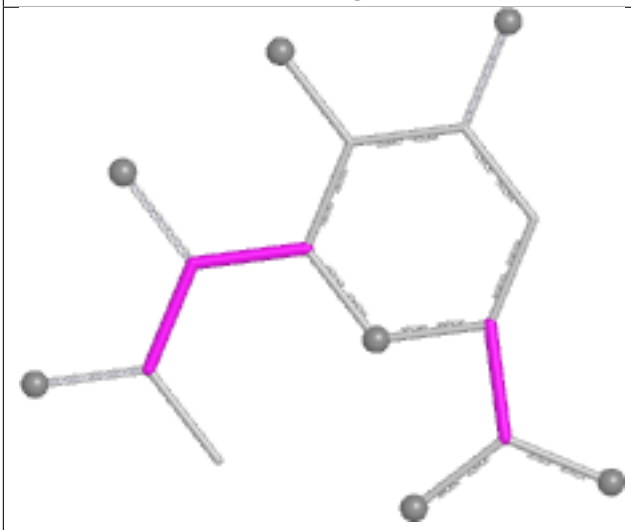
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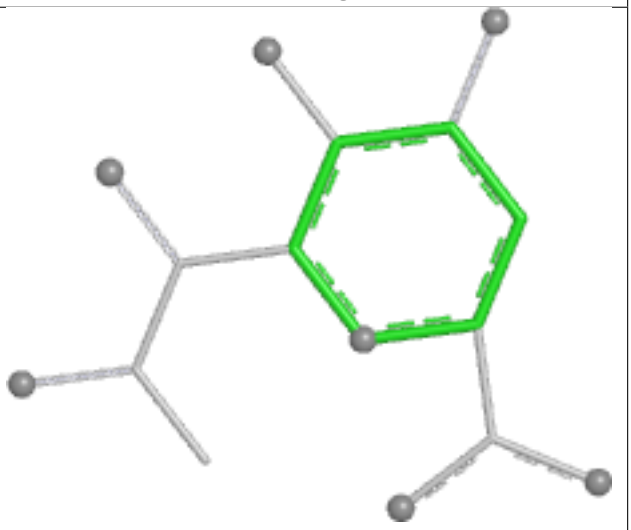
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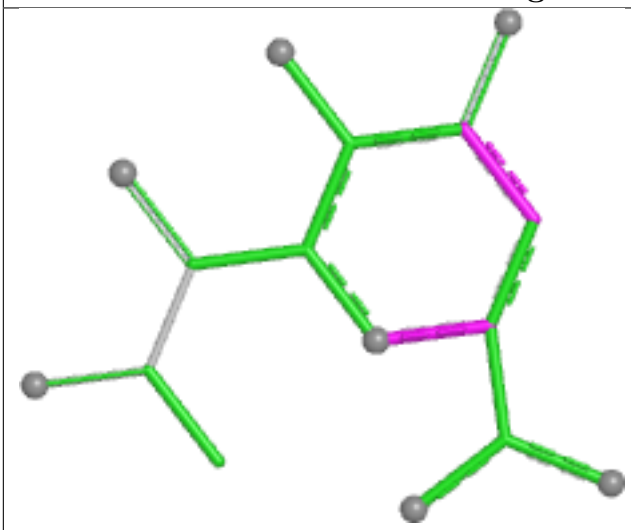


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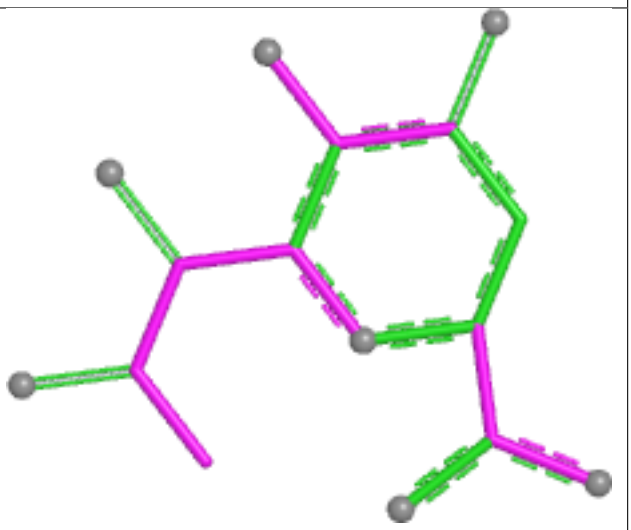


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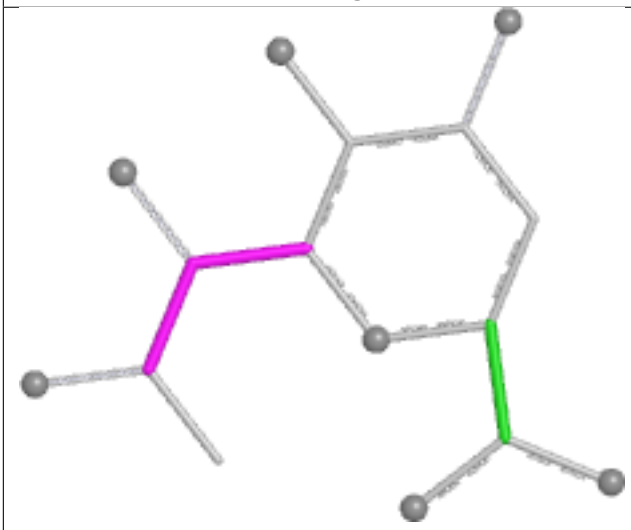
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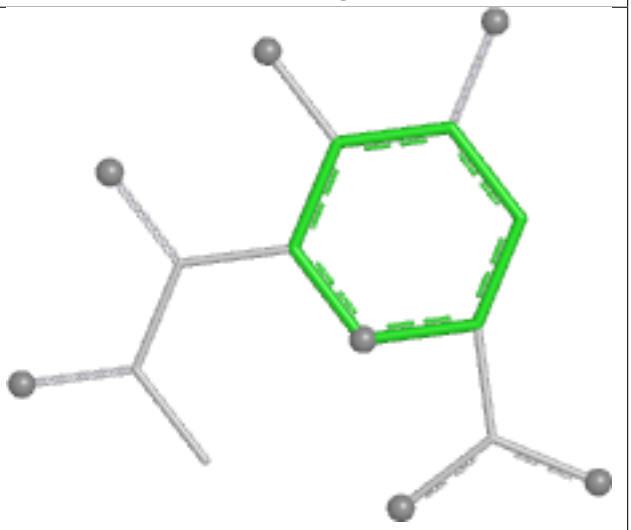
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Bond angles

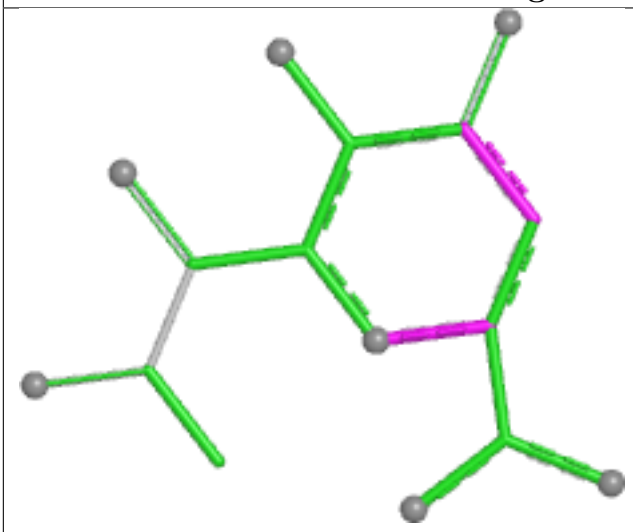


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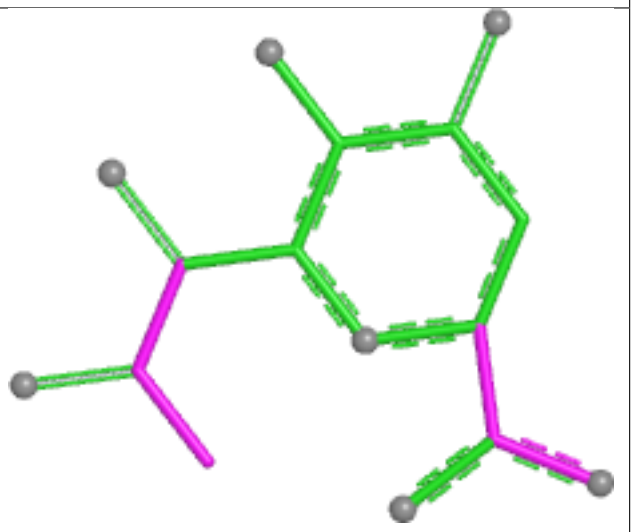


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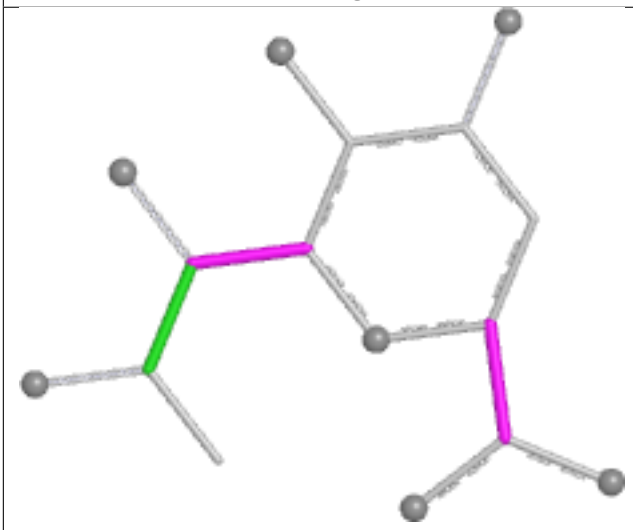
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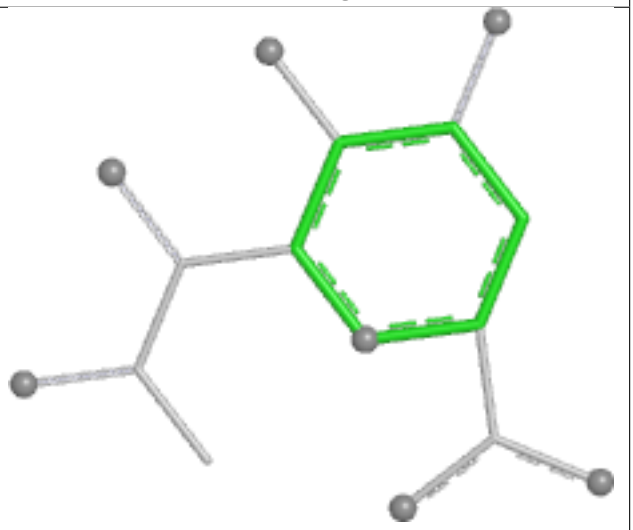
Bond lengths



Bond angles

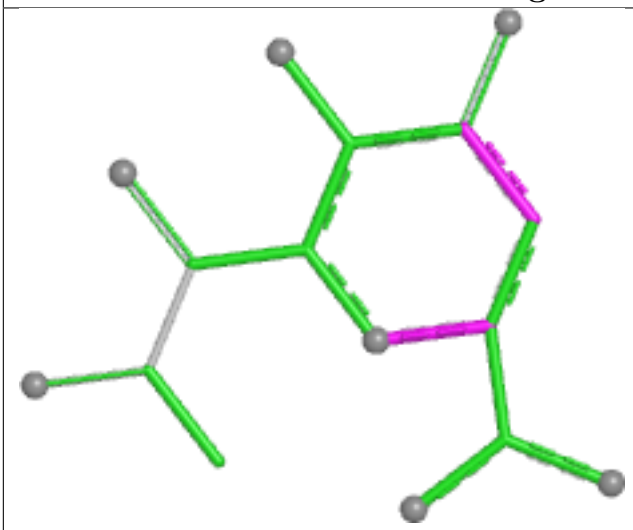


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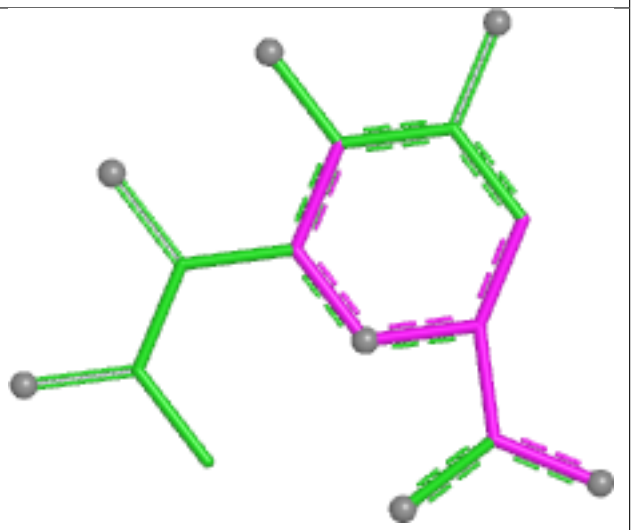


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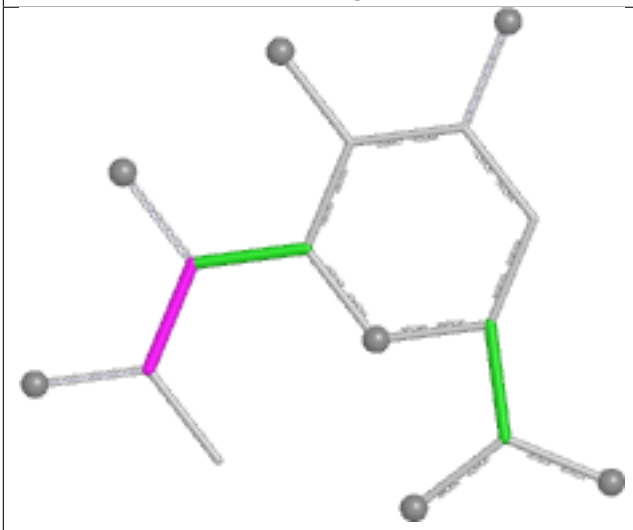
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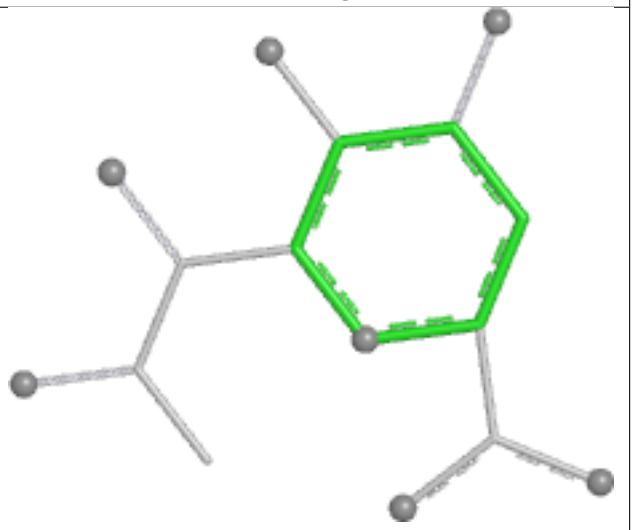
Bond lengths



Bond angles

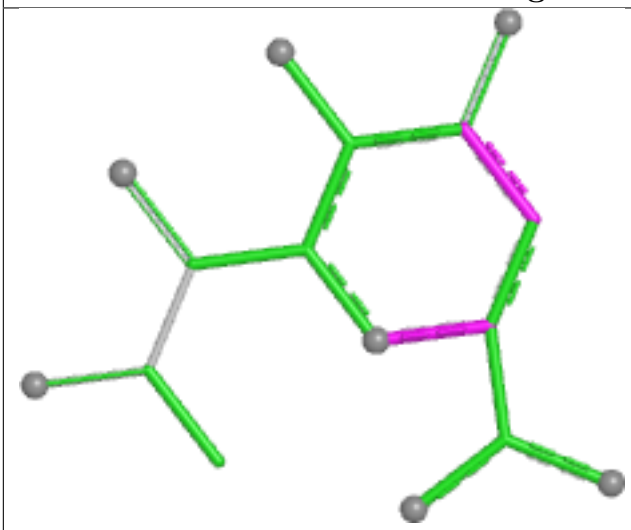


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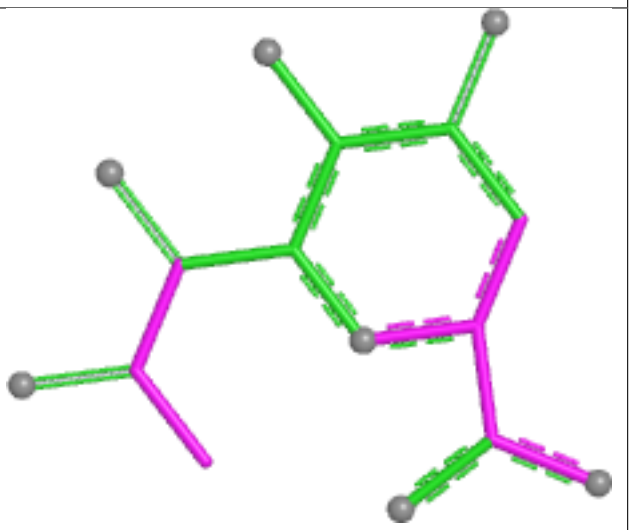


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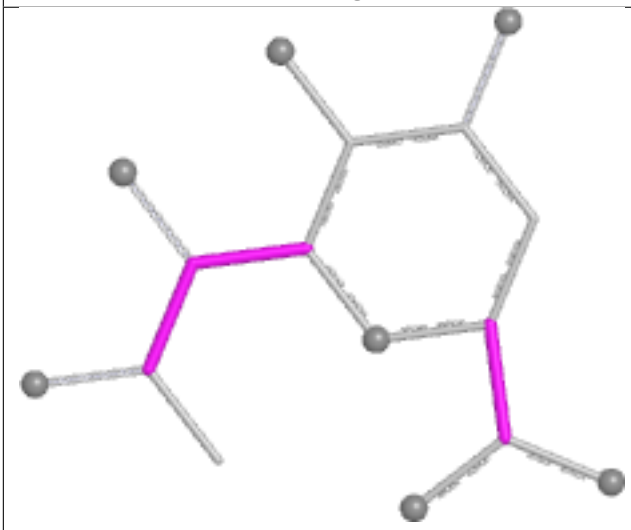
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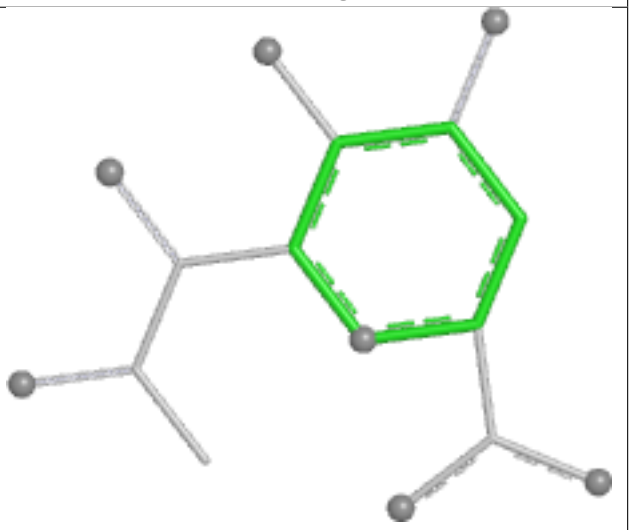
Bond lengths



Bond angles

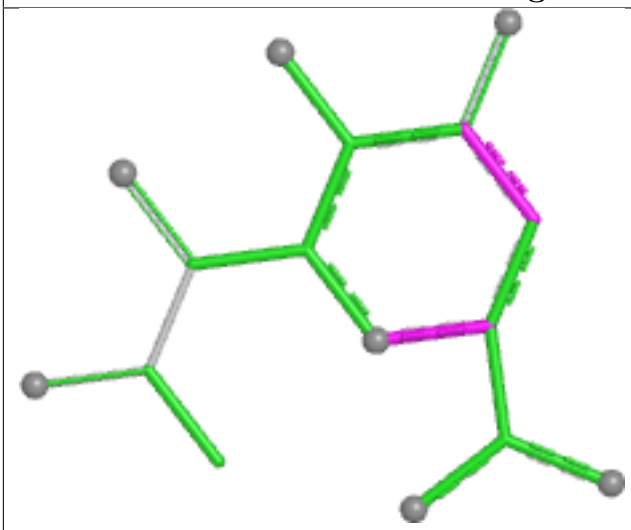


Torsions

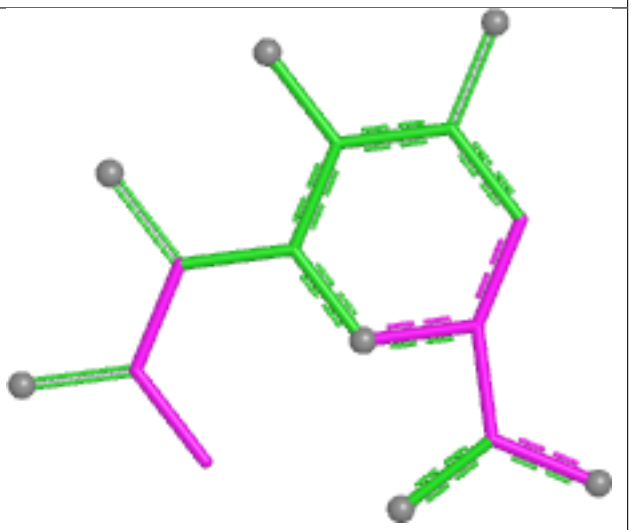


Rings

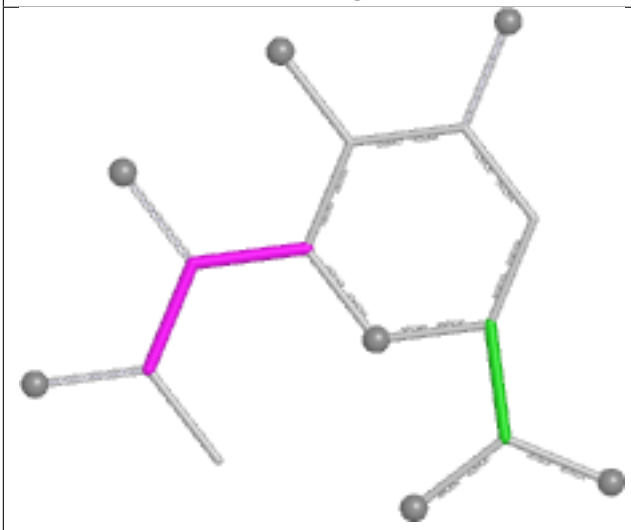
Ligand P8E V 604



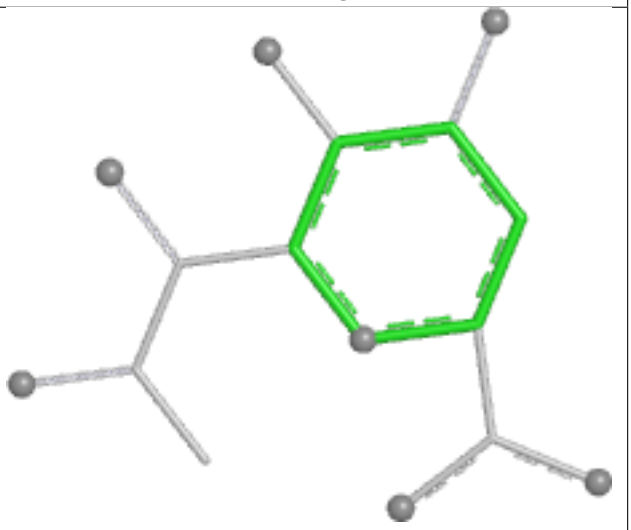
Bond lengths



Bond angles

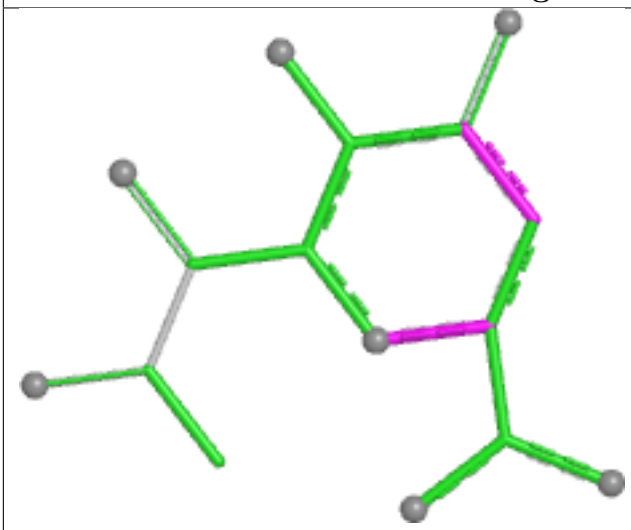


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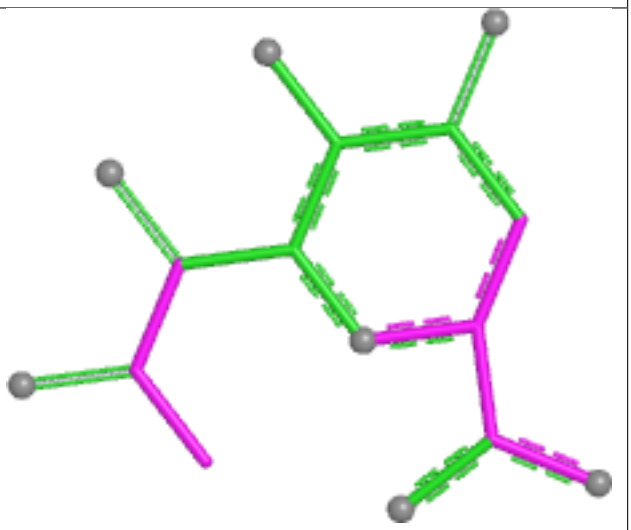


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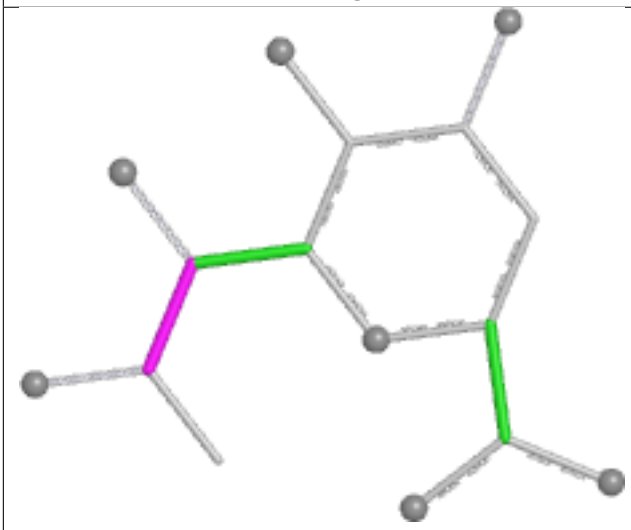
Ligand P8E J 603



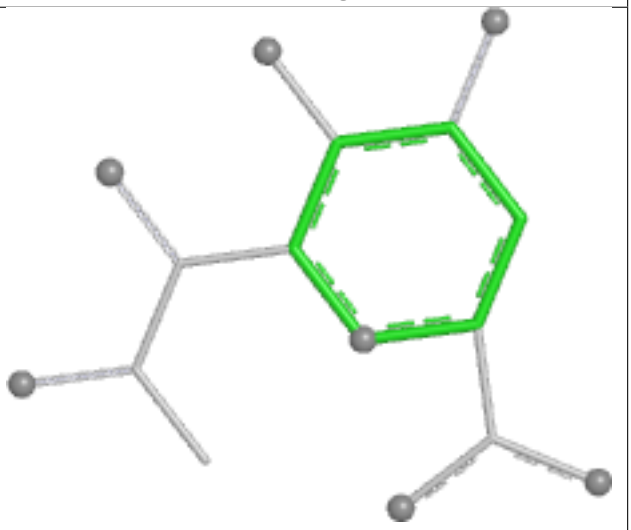
Bond lengths



Bond angles

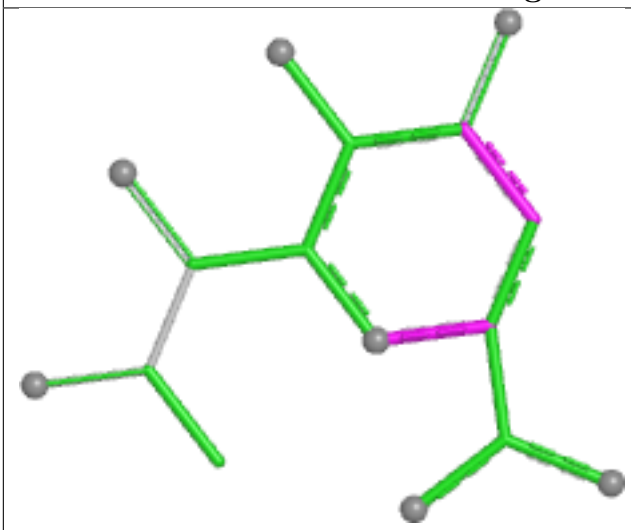


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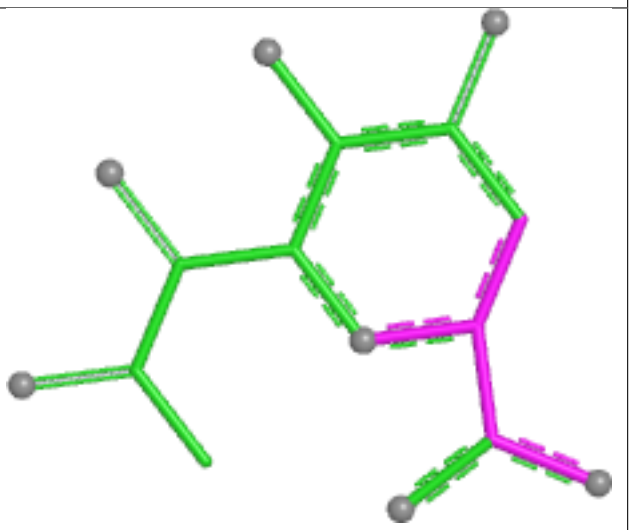


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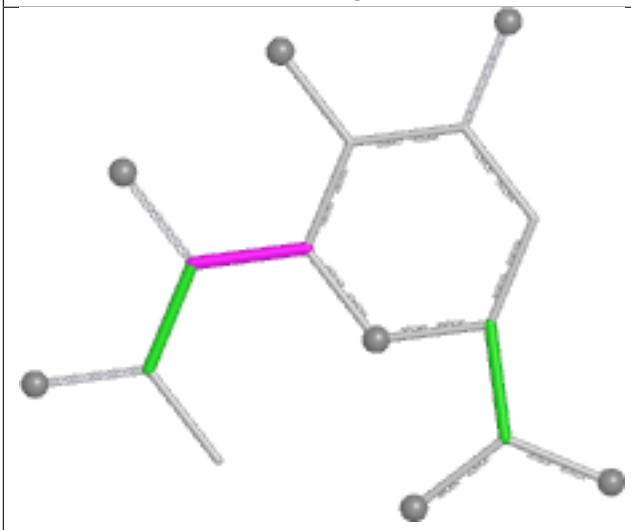
Ligand P8E M 615



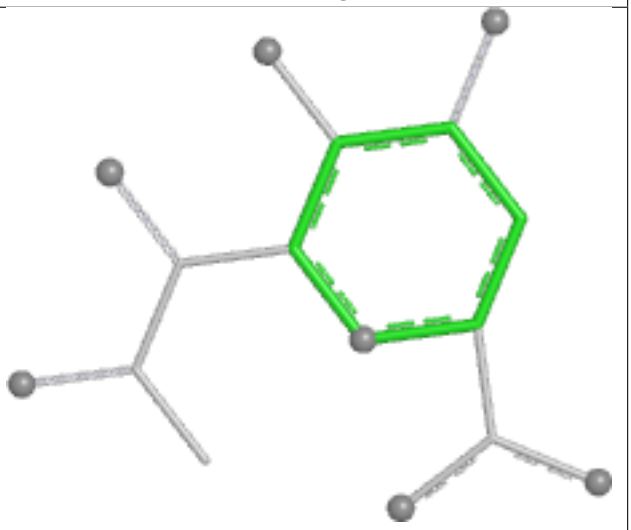
Bond lengths



Bond angles

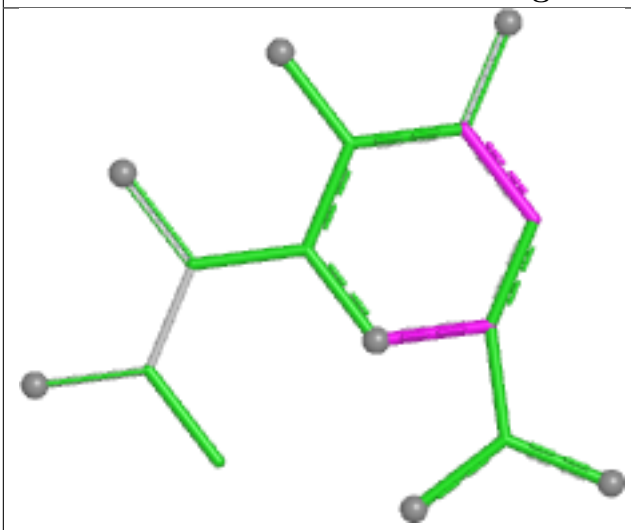


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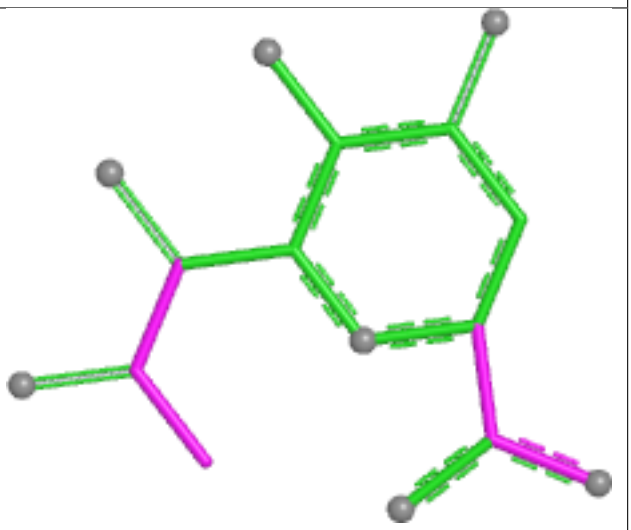


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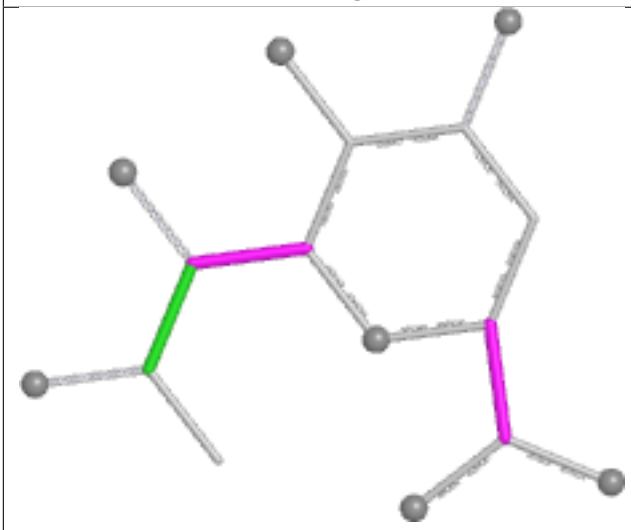
Ligand P8E J 601



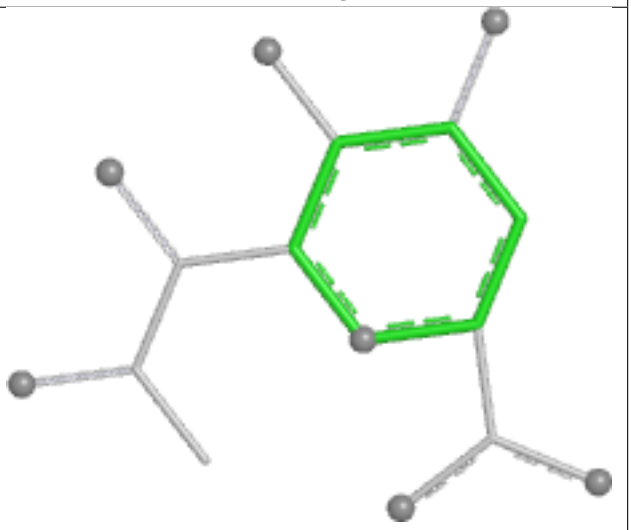
Bond lengths



Bond angles

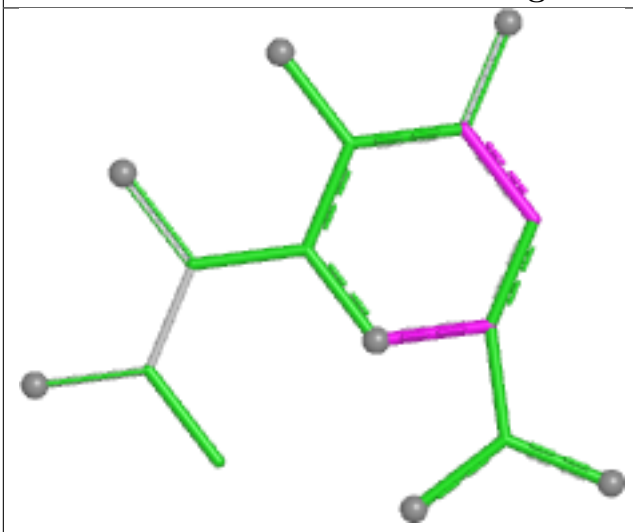


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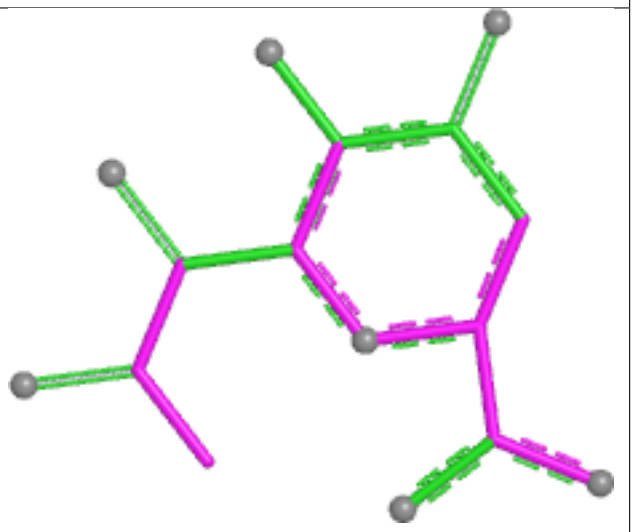


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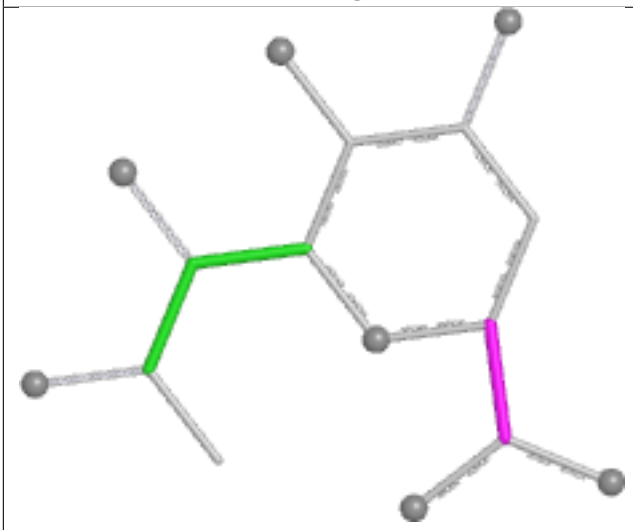
Ligand P8E A 617



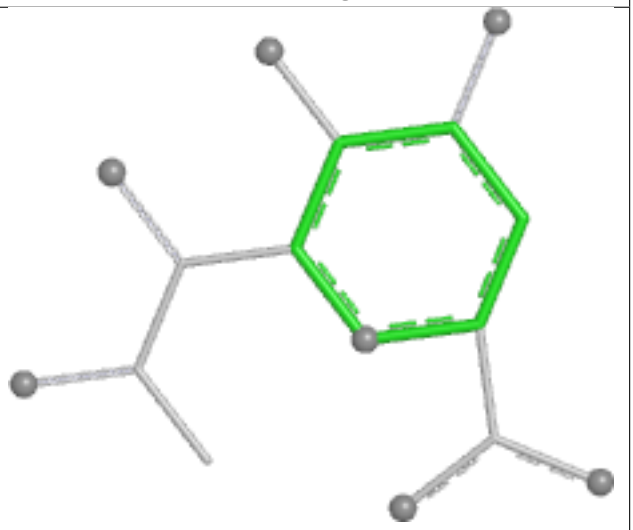
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Bond angles

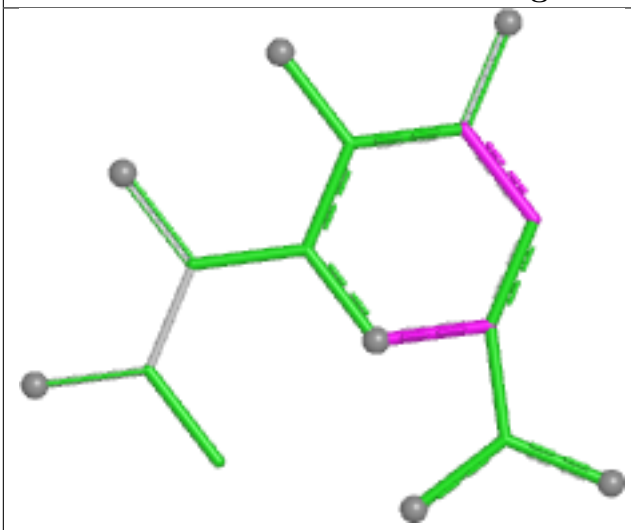


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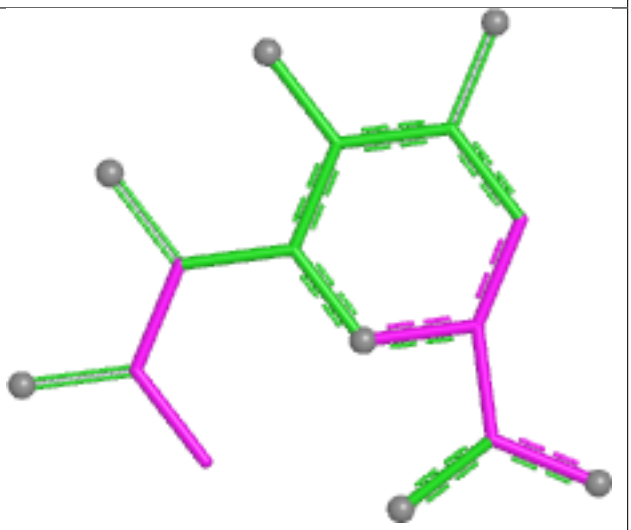


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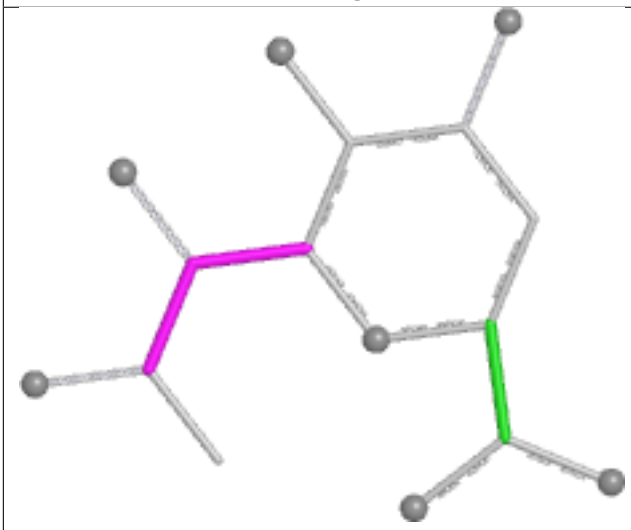
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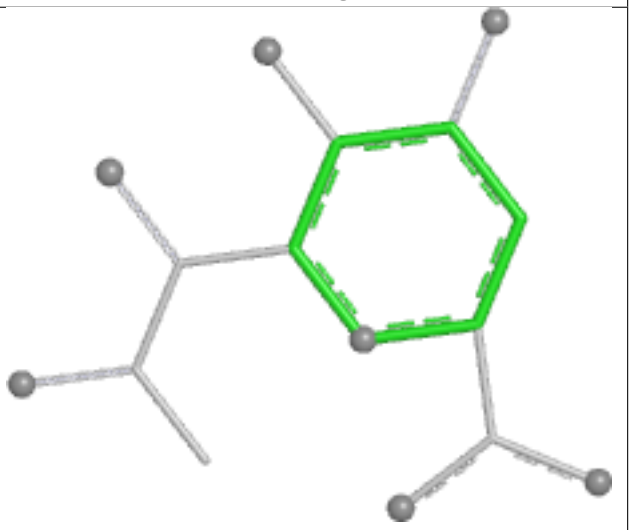
Bond lengths



Bond angles

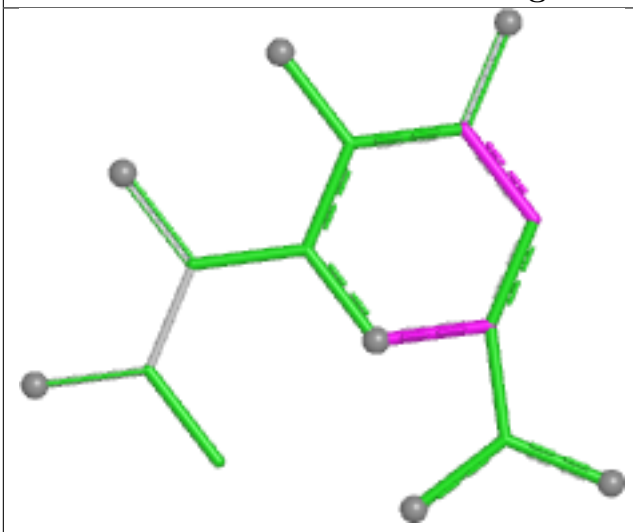


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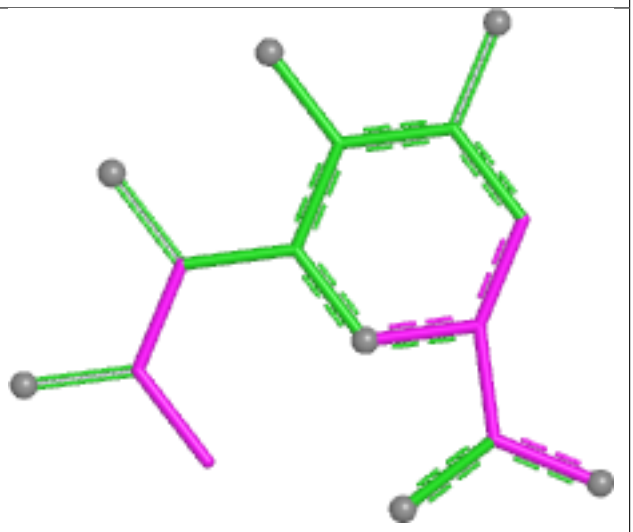


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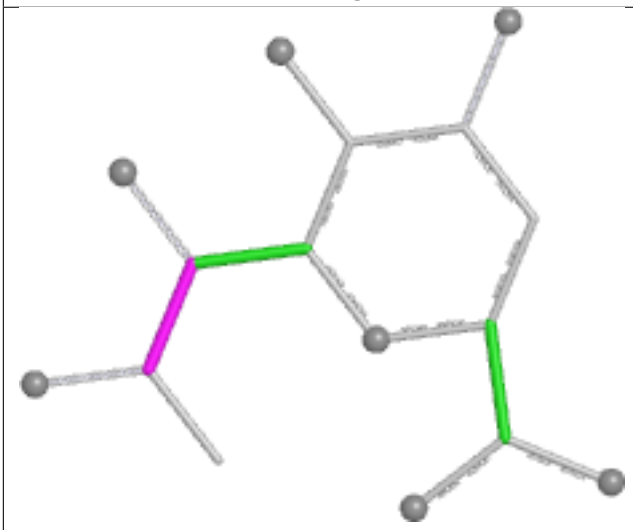
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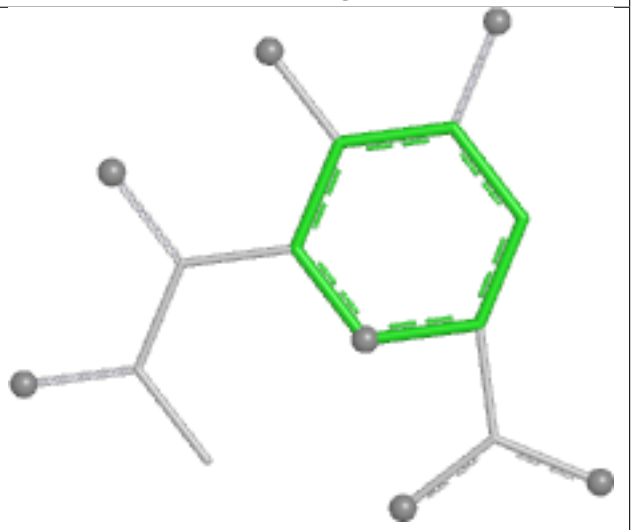
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Bond angles

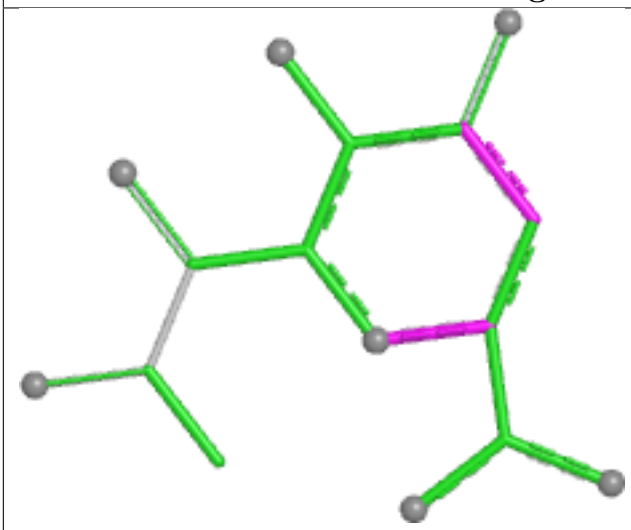


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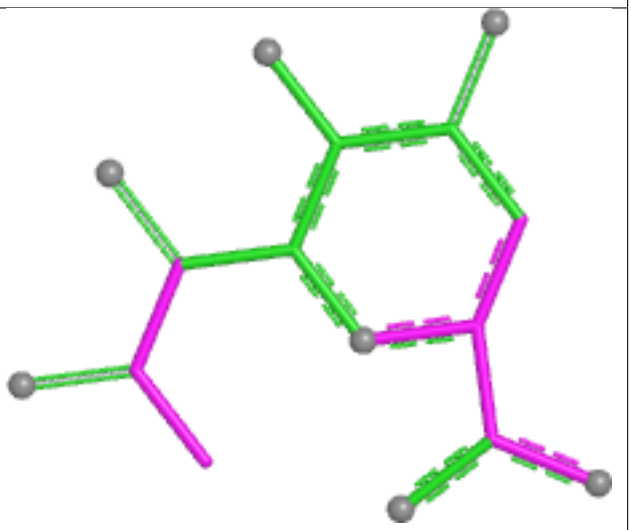


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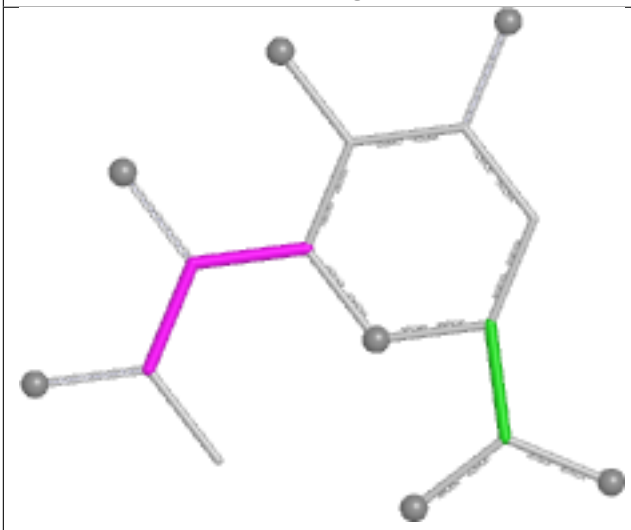
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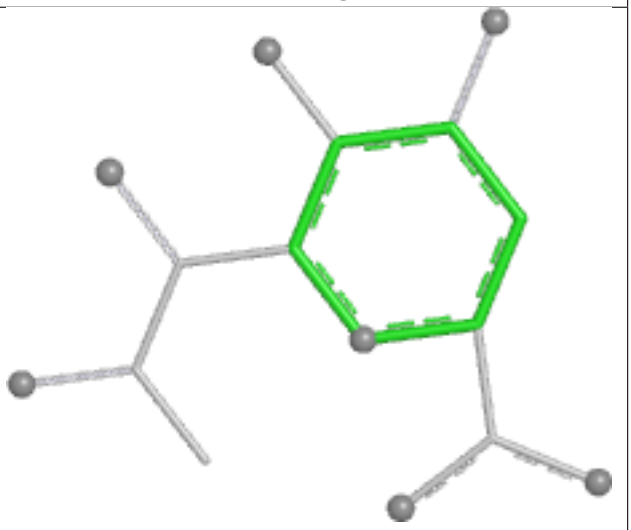
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Bond angles

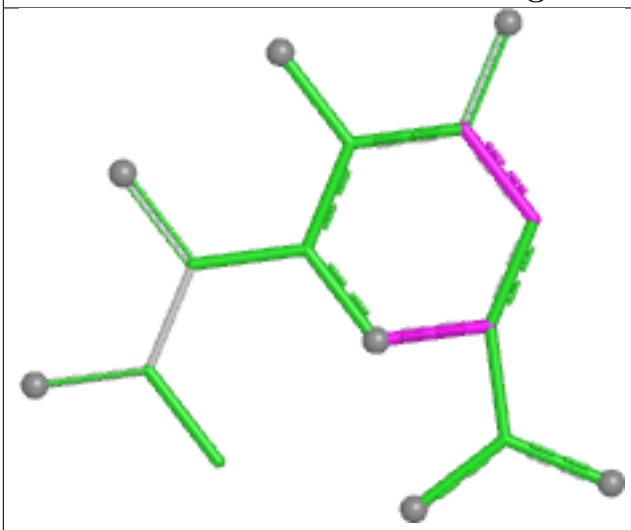


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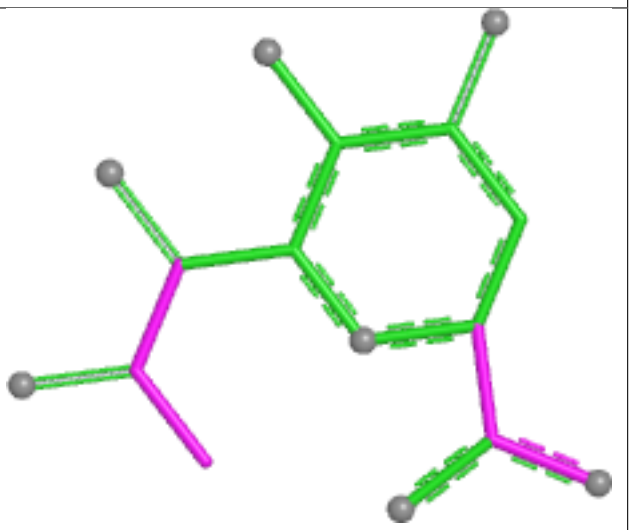


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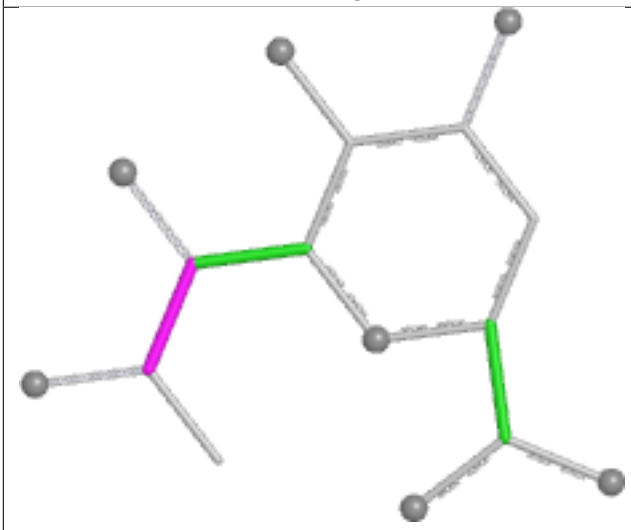
Ligand P8E N 610



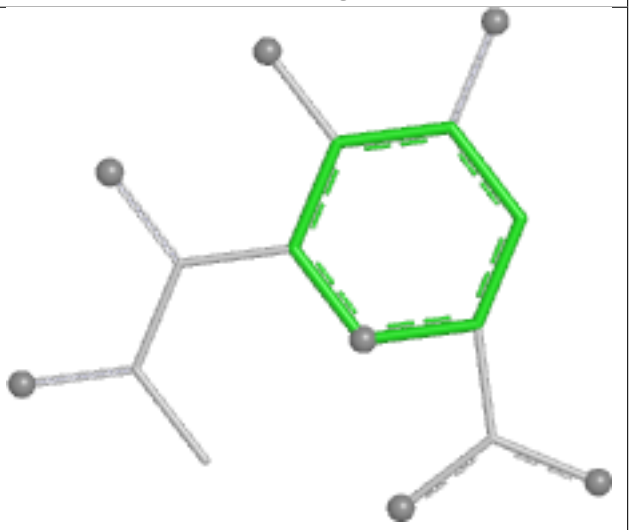
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Bond angles

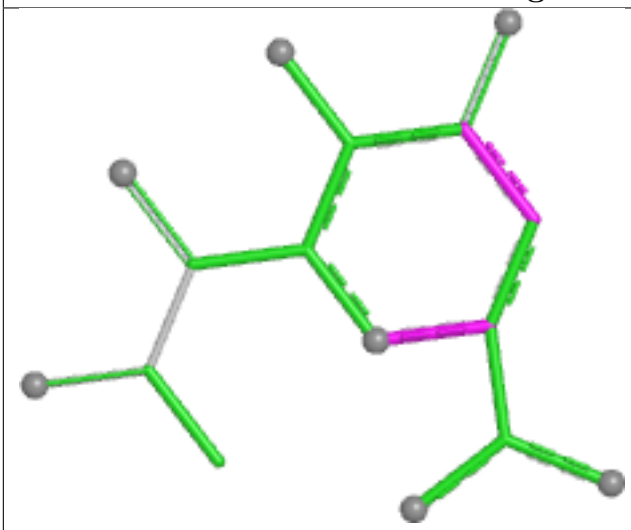


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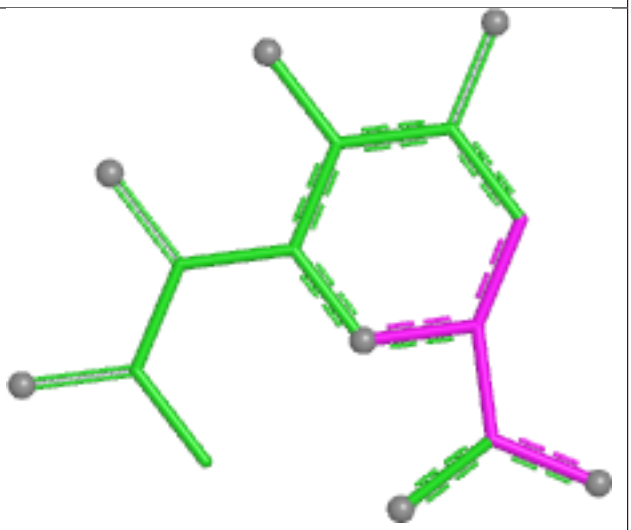


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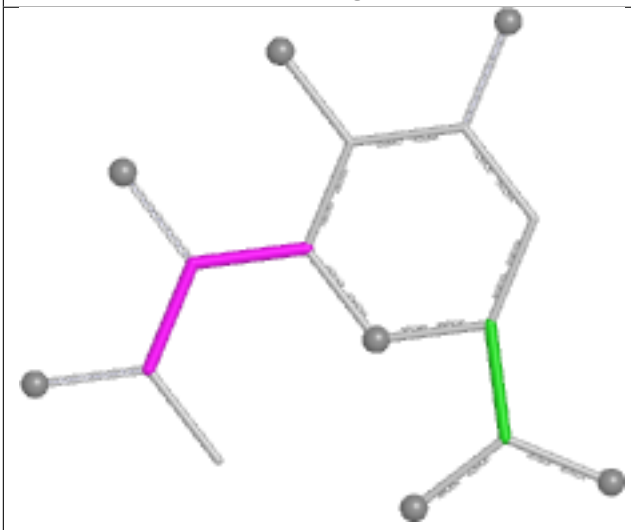
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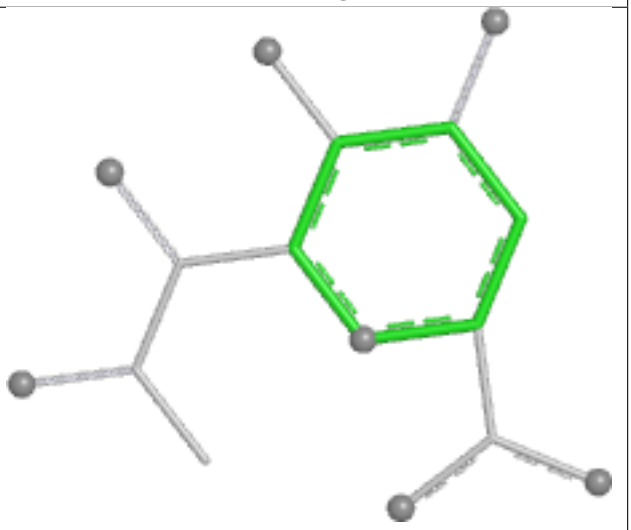
Bond lengths



Bond angles

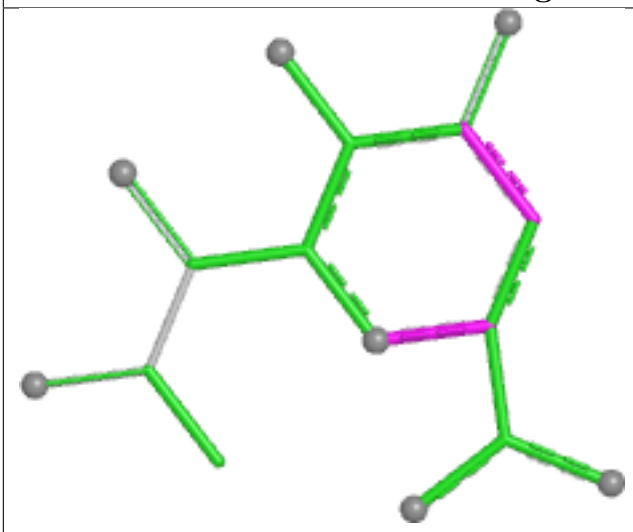


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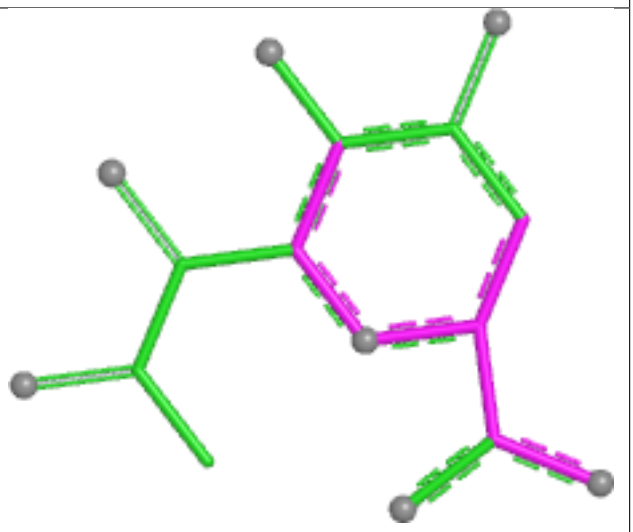


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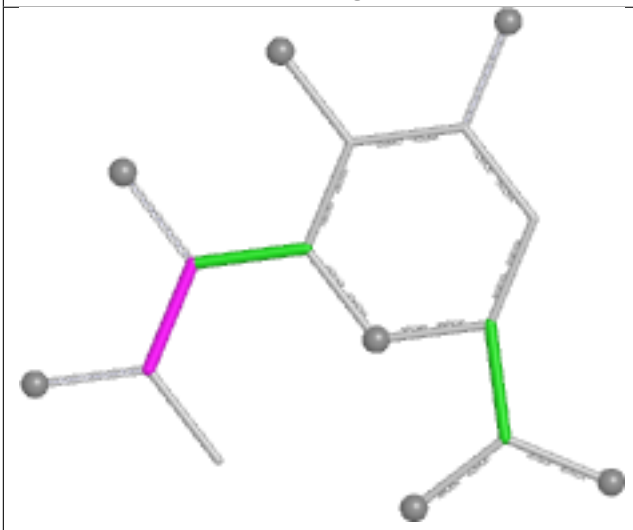
Ligand P8E I 608



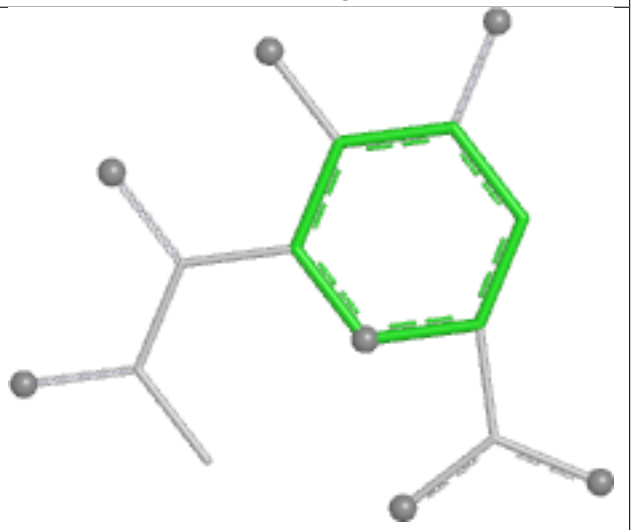
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Bond angles

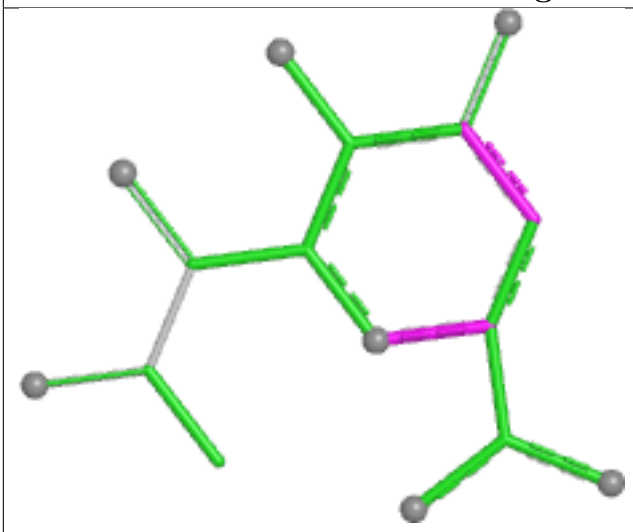


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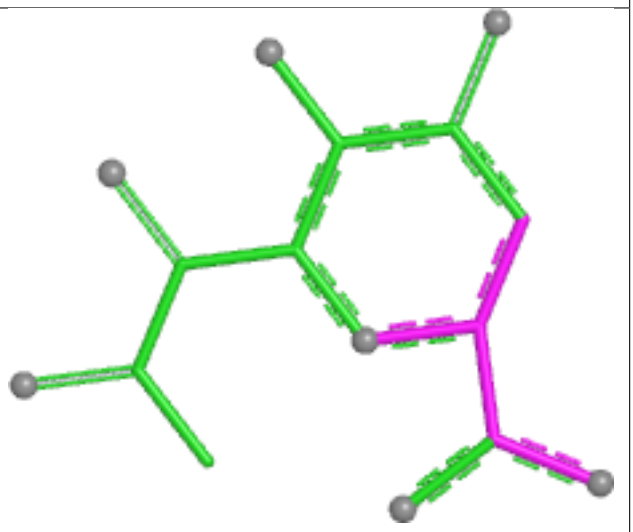


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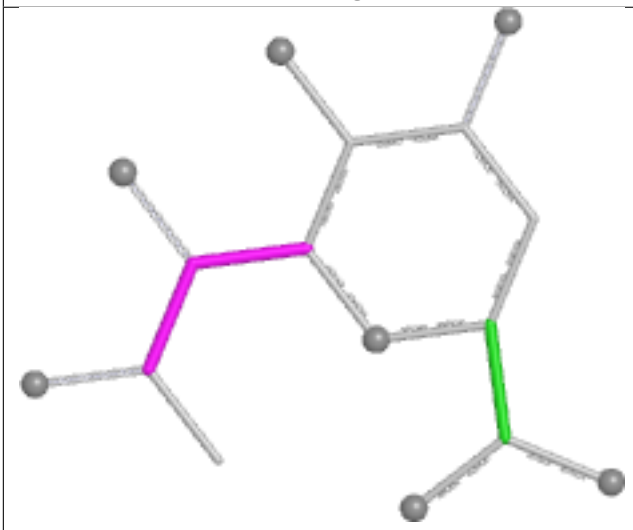
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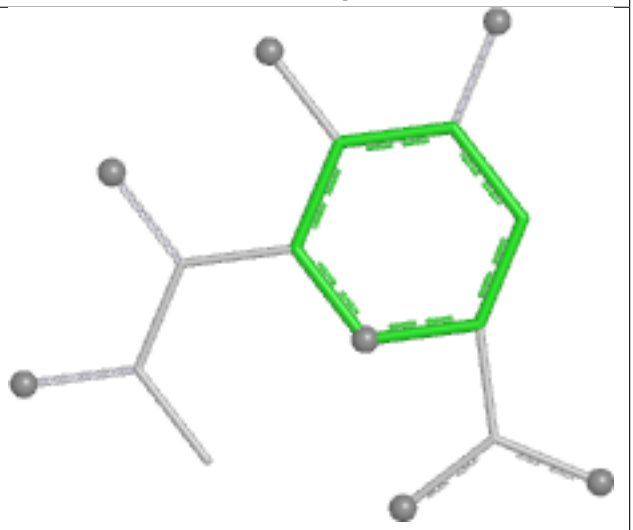
Bond lengths



Bond angles

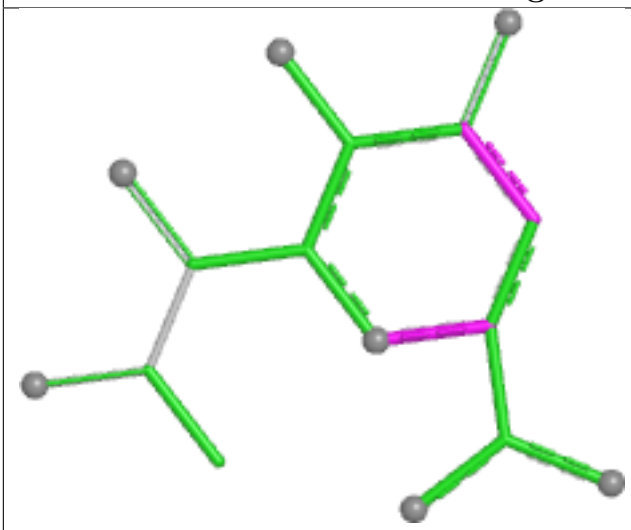


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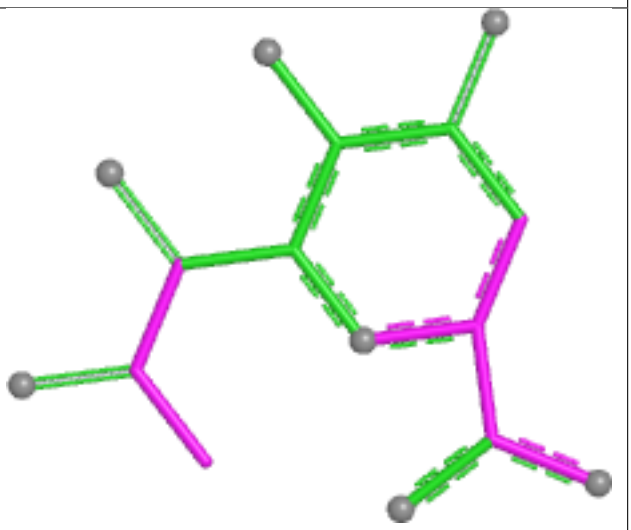


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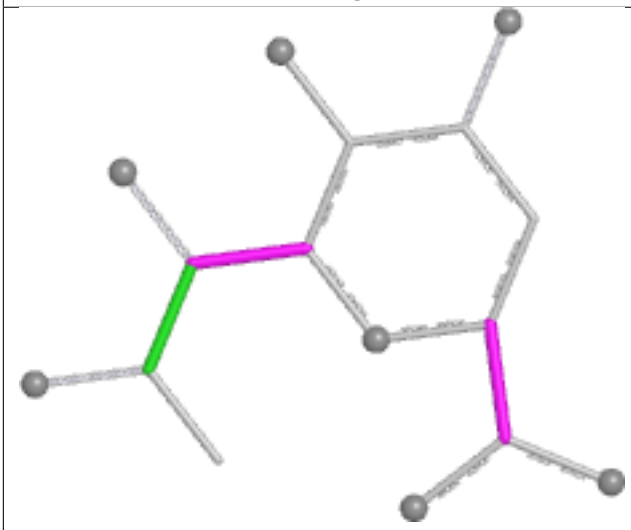
Ligand P8E K 601



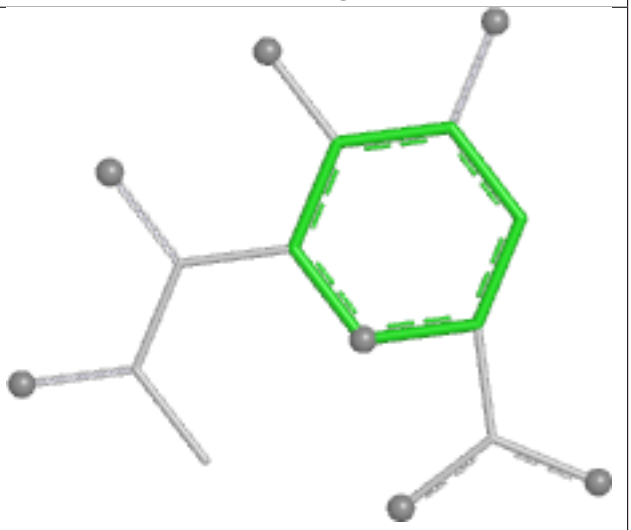
Bond lengths



Bond angles

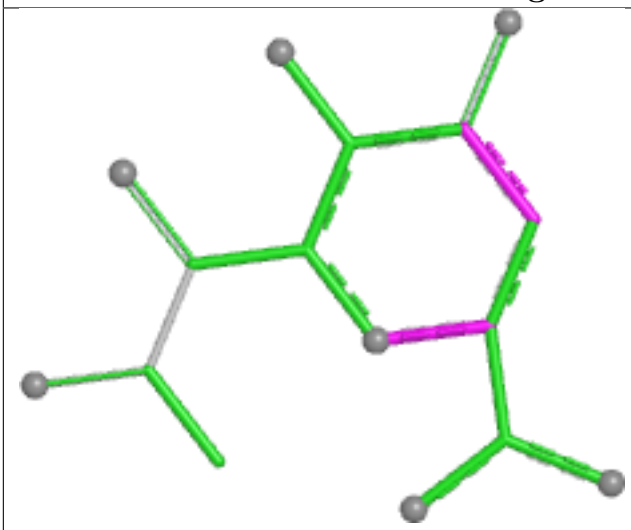


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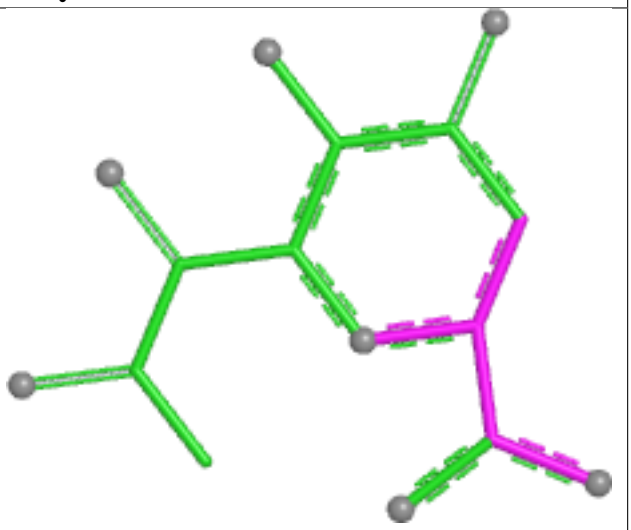


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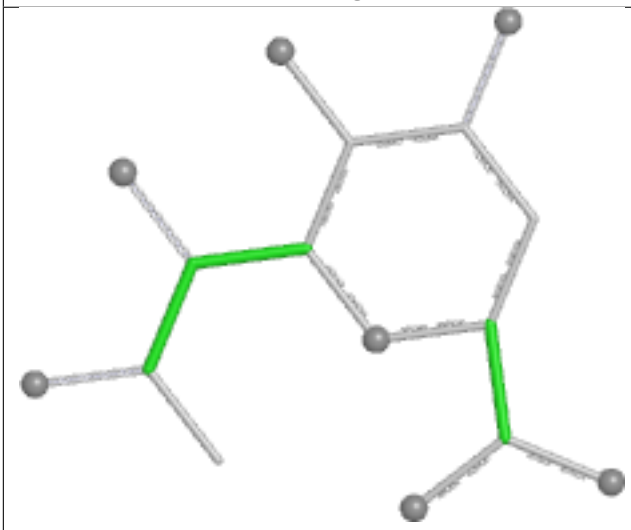
Ligand P8E Q 613



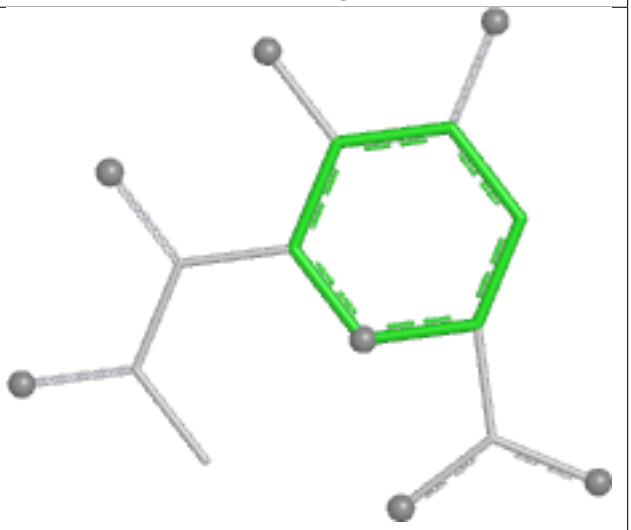
Bond lengths



Bond angles

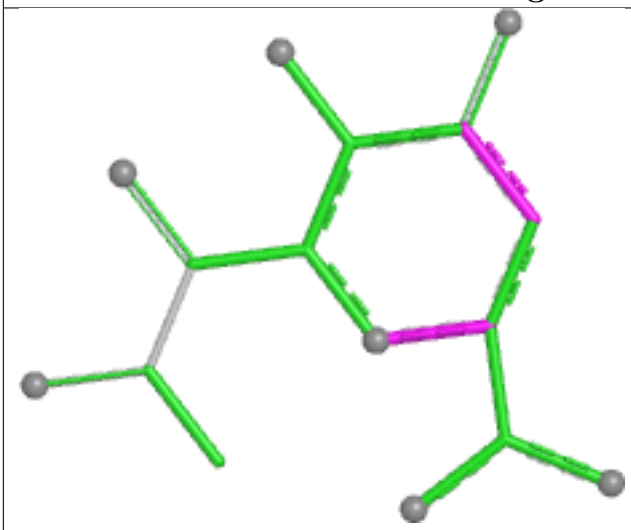


Torsions

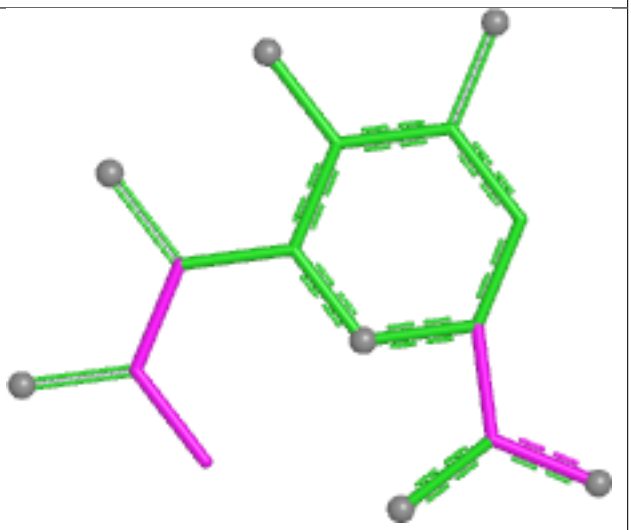


Rings

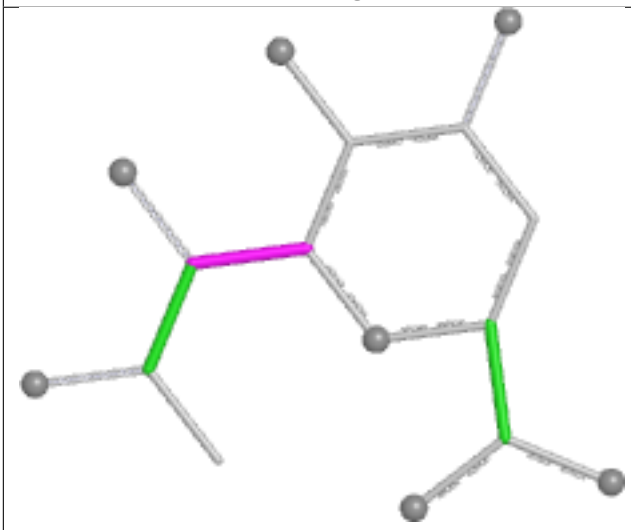
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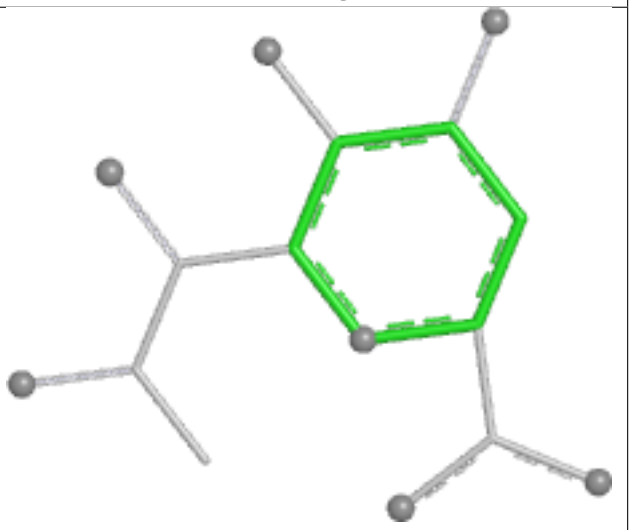
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Bond angles

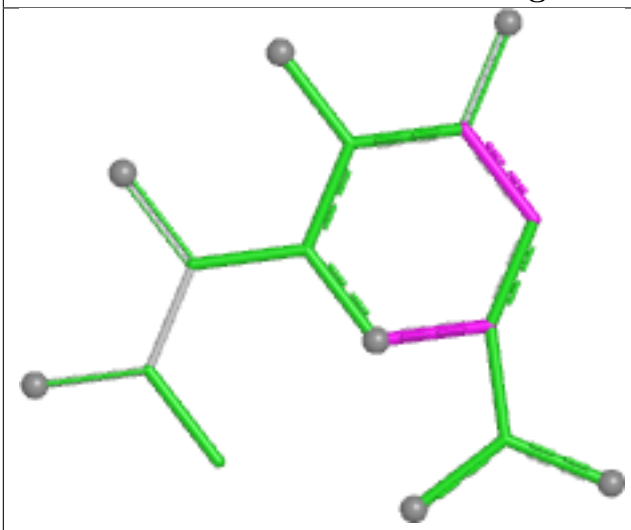


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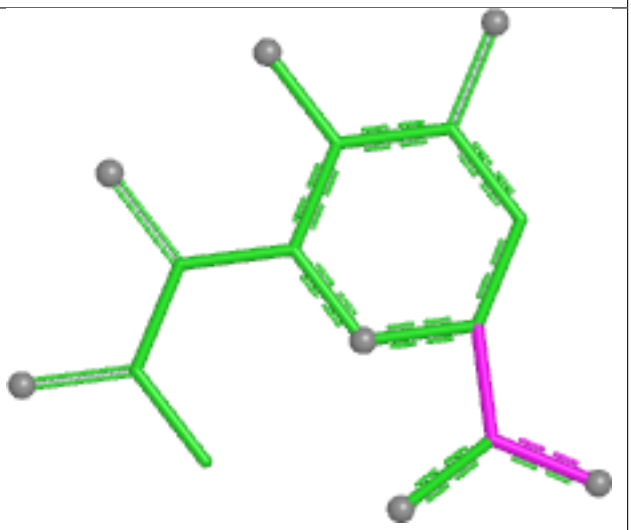


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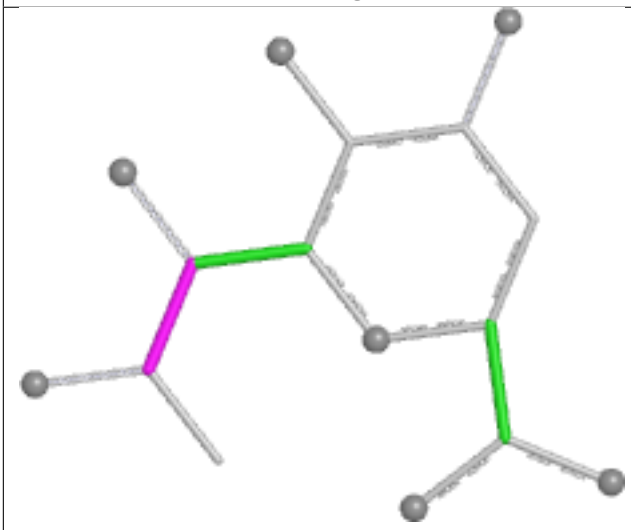
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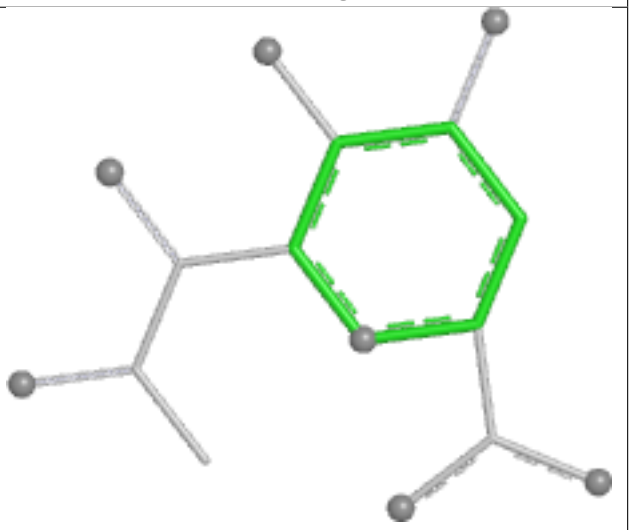
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Bond angles

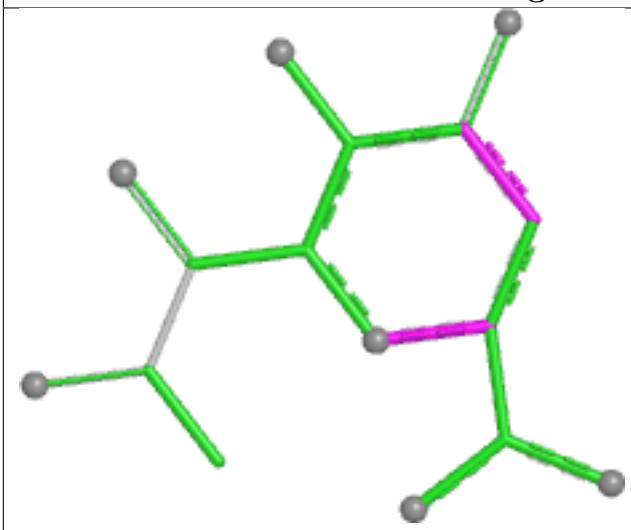


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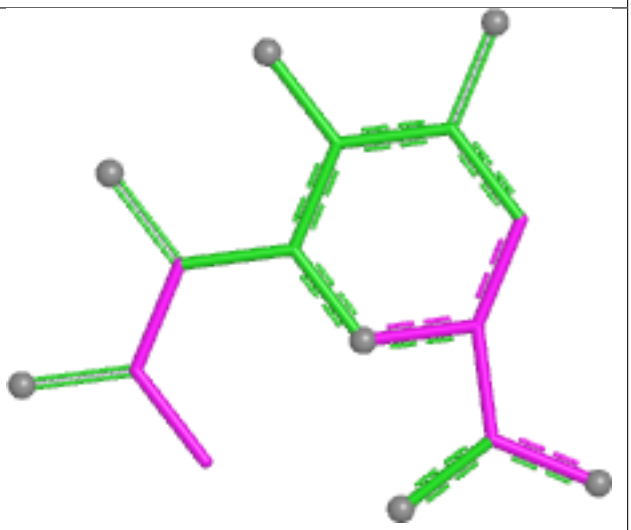


Rings

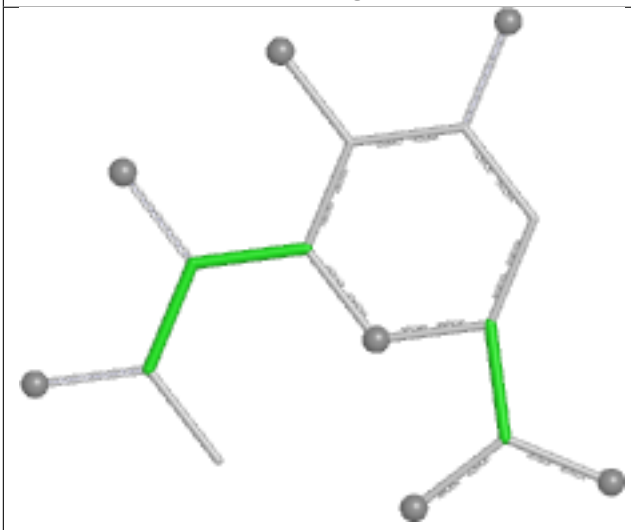
Ligand P8E V 615



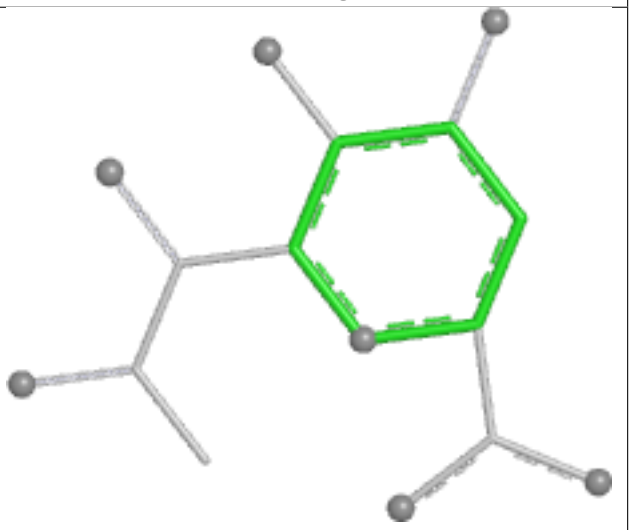
Bond lengths



Bond angles

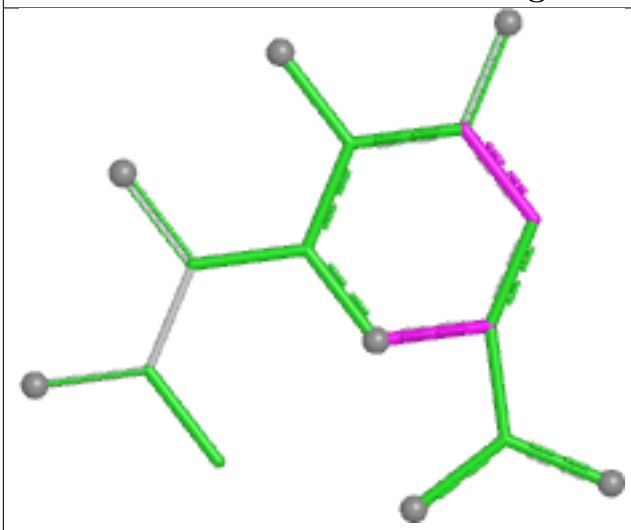


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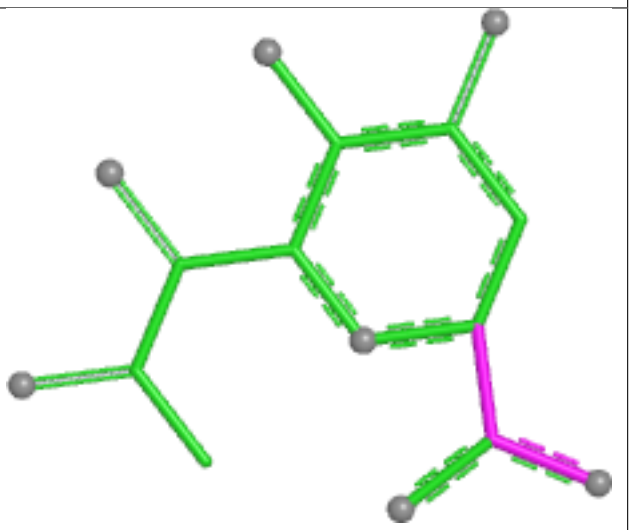


Rings

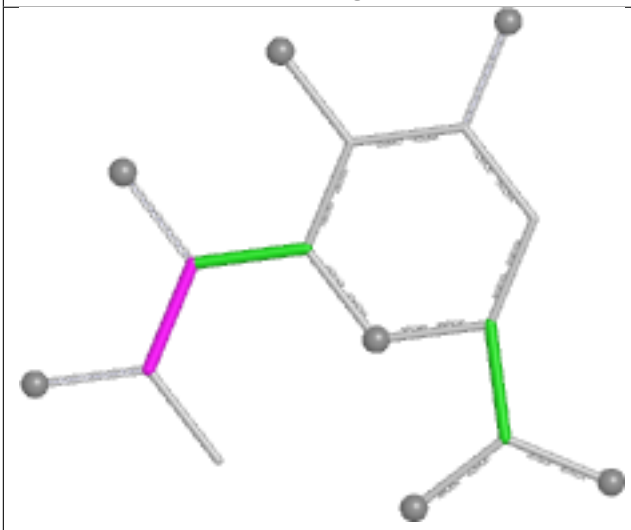
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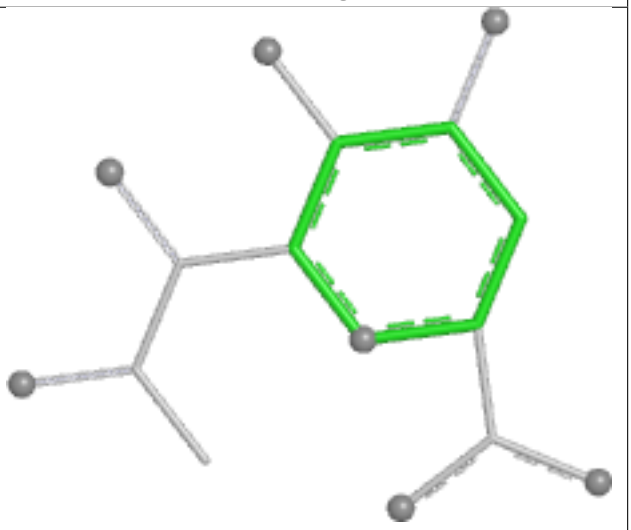
Bond lengths



Bond angles

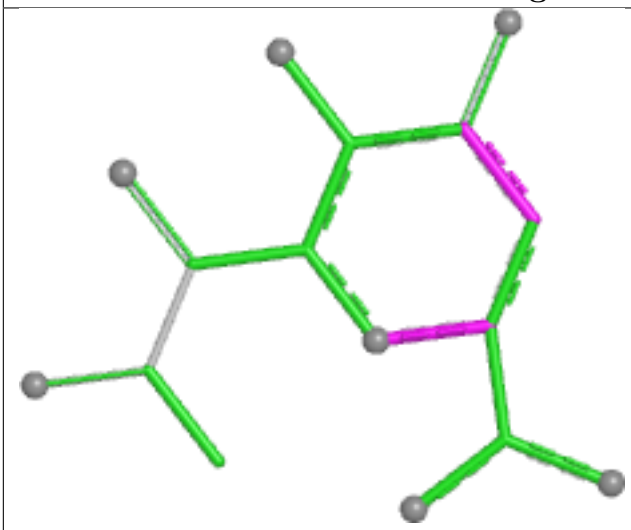


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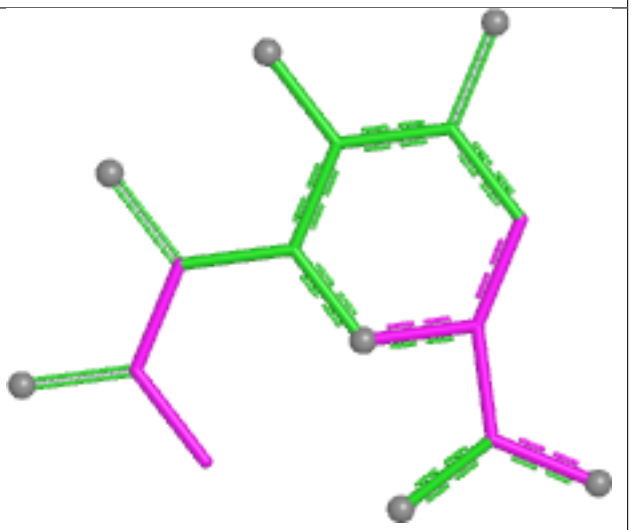


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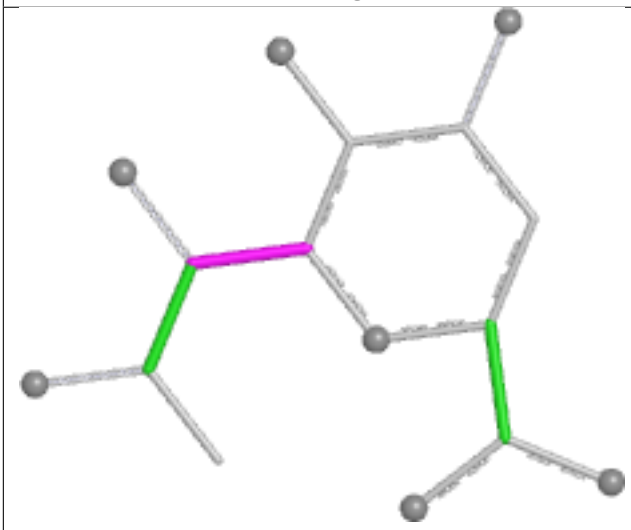
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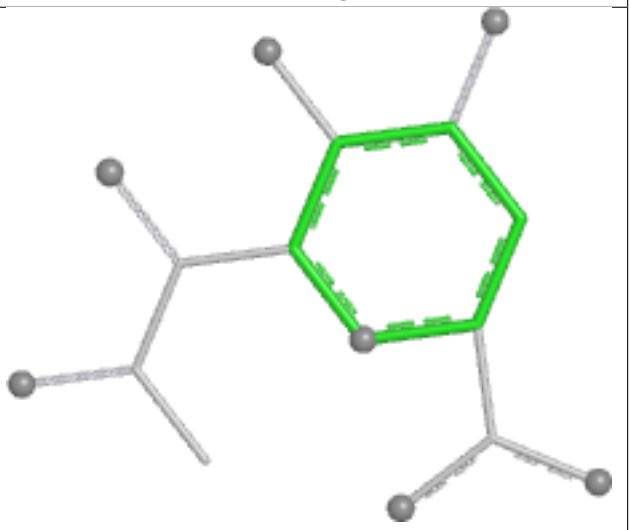
Bond lengths



Bond angles

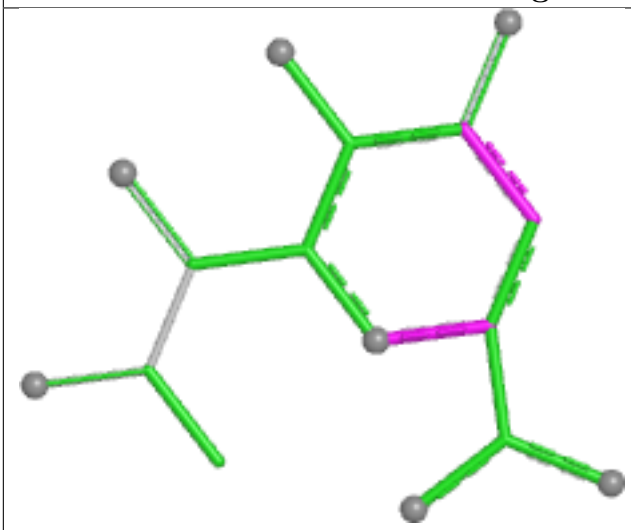


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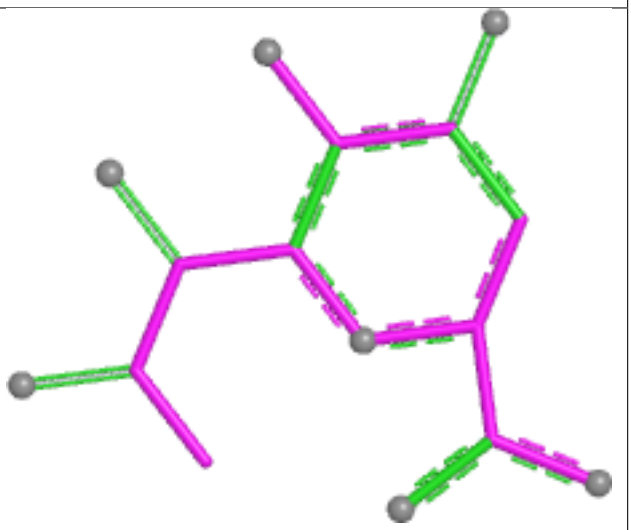


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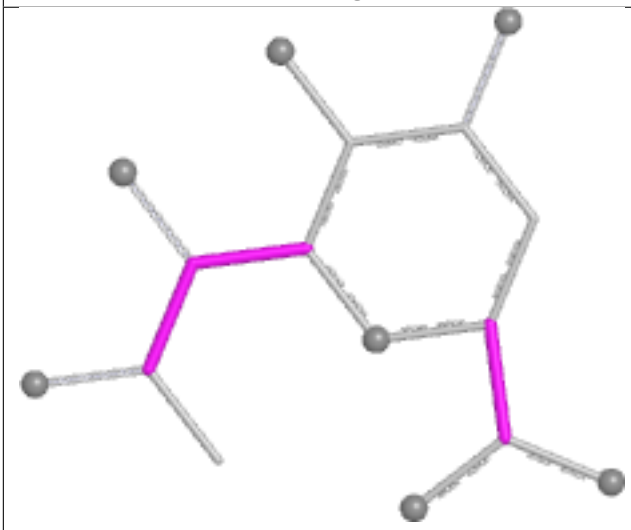
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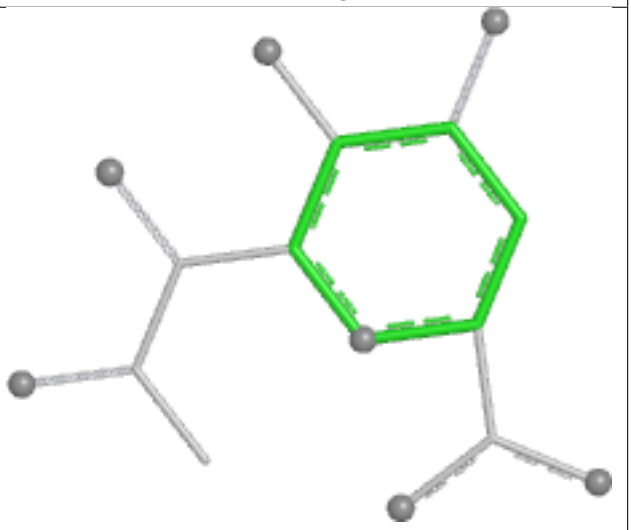
Bond lengths



Bond angles

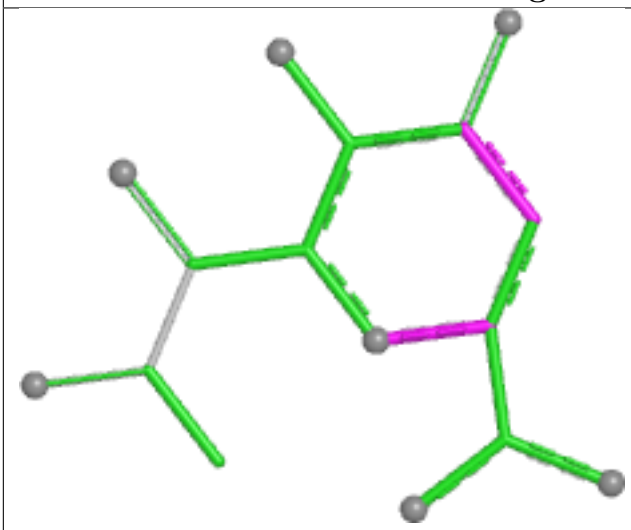


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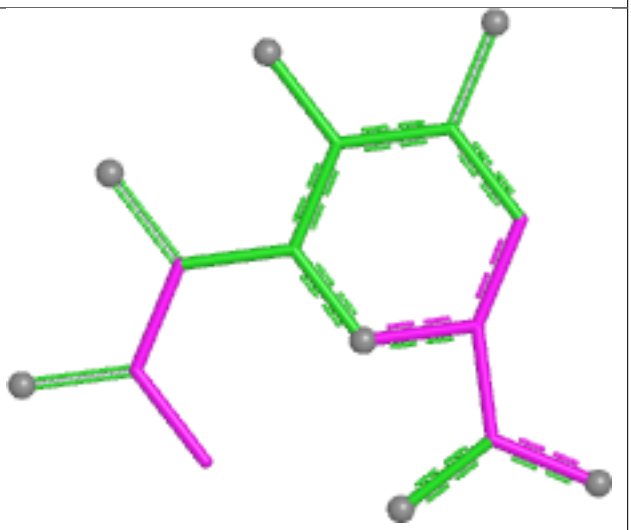


Rings

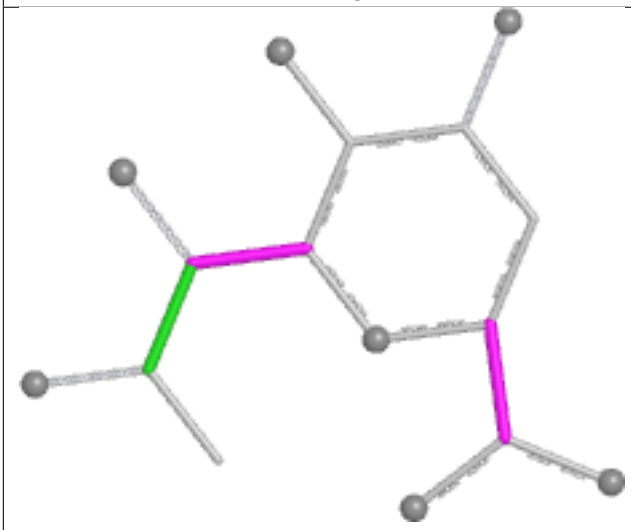
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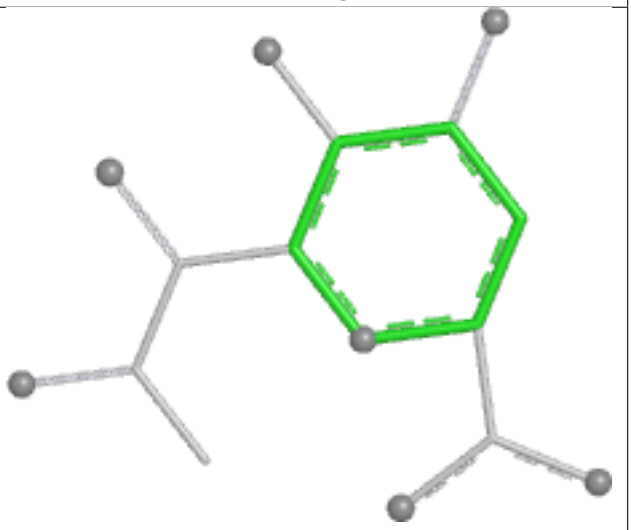
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Bond angles

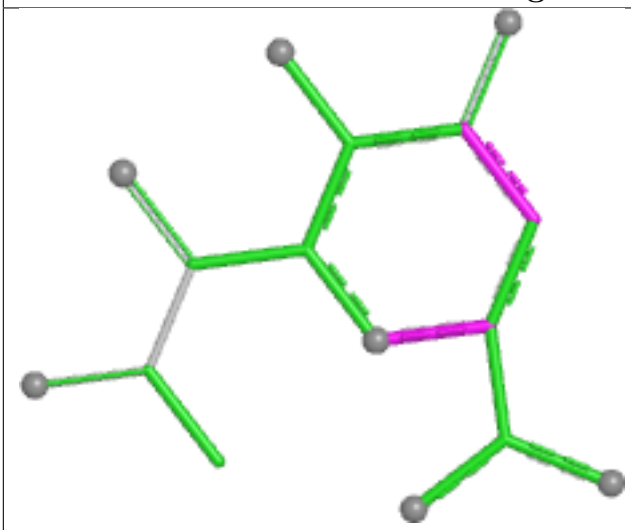


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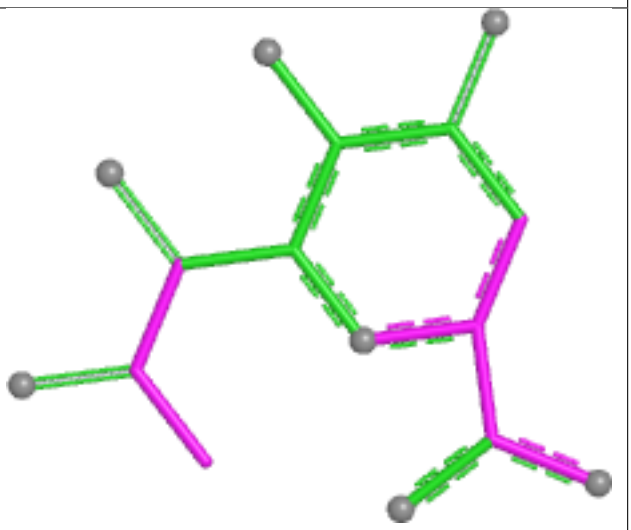


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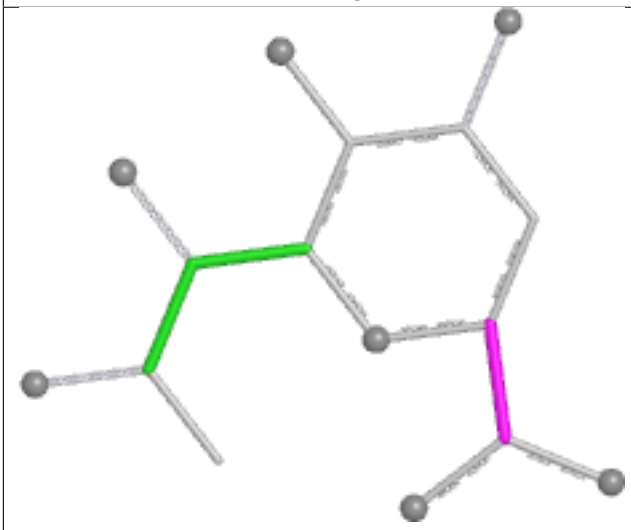
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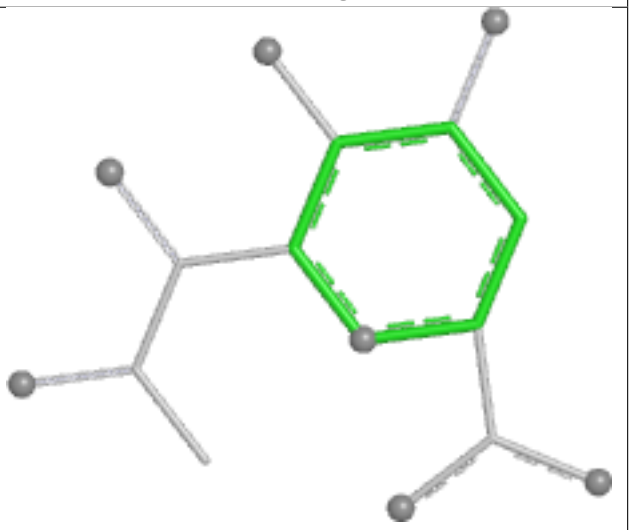
Bond lengths



Bond angles

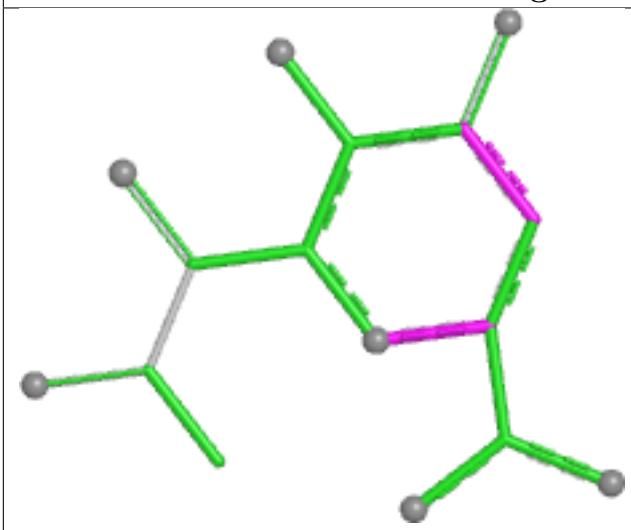


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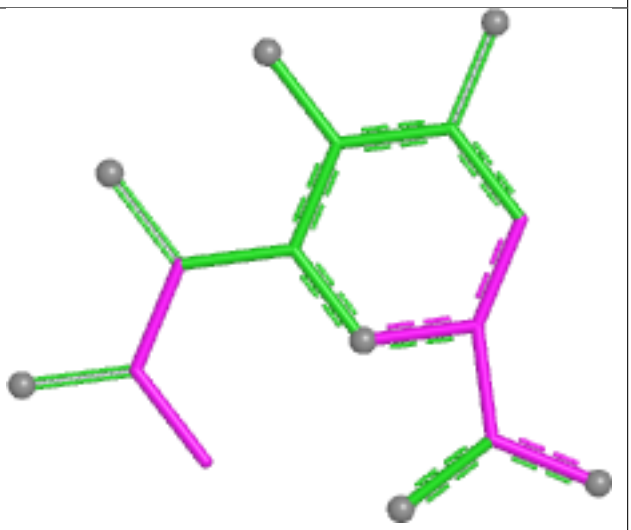


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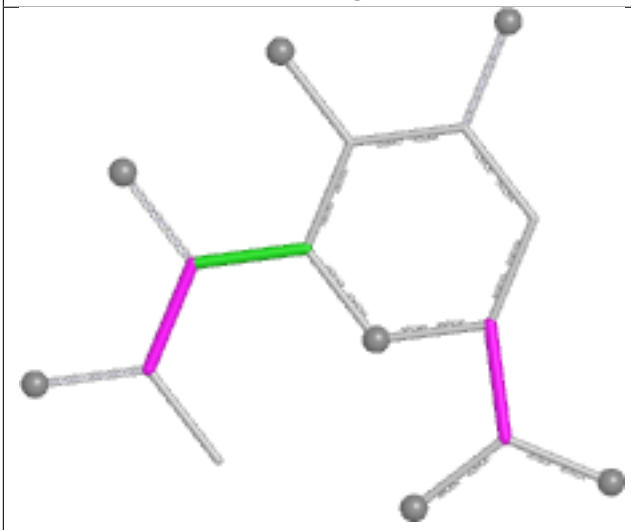
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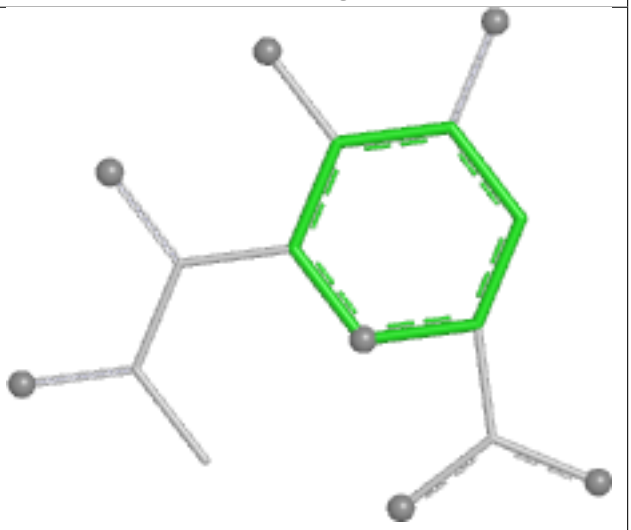
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Bond angles

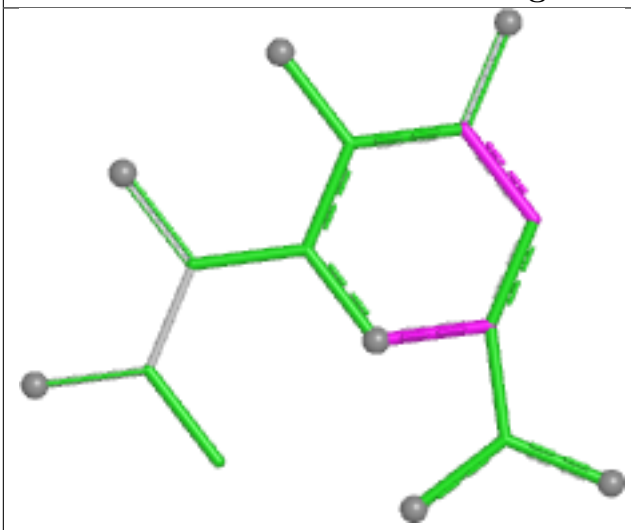


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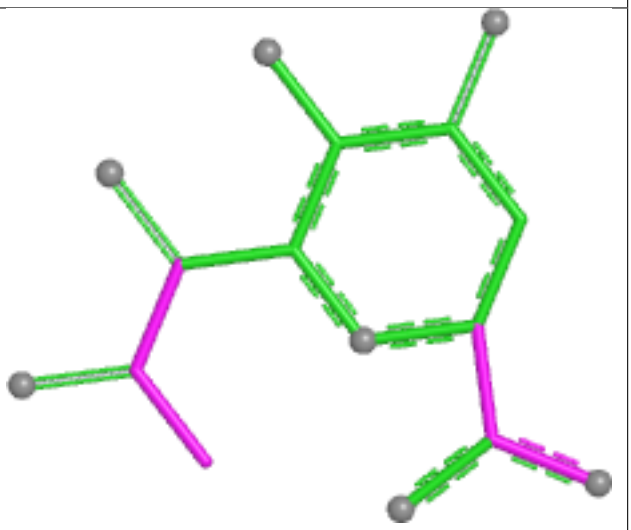


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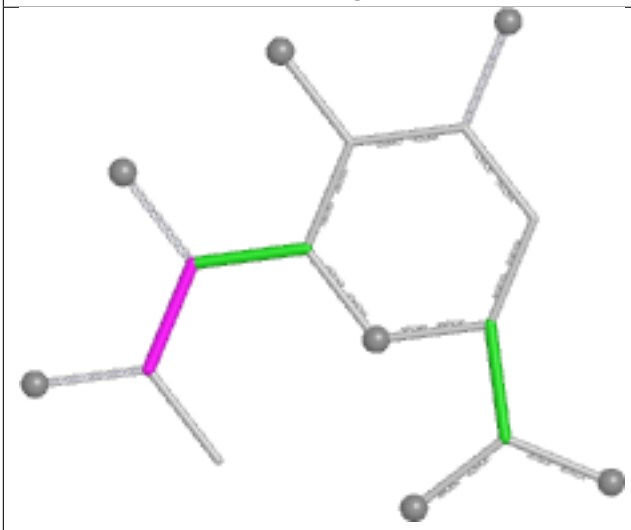
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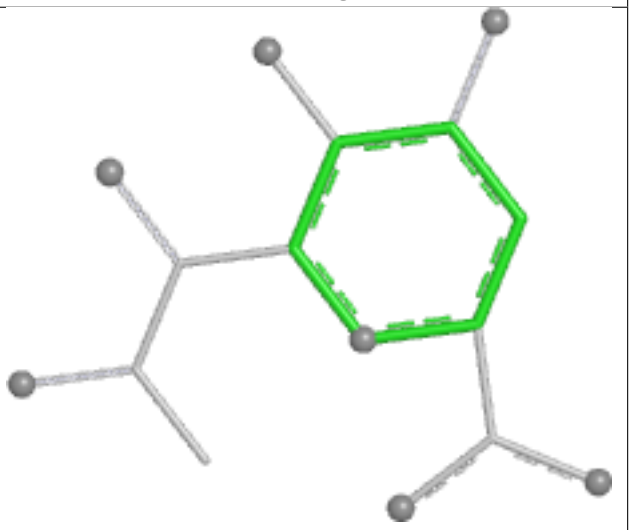
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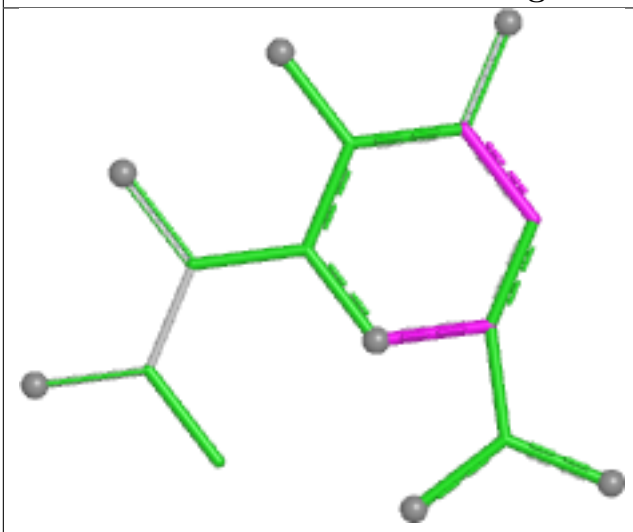


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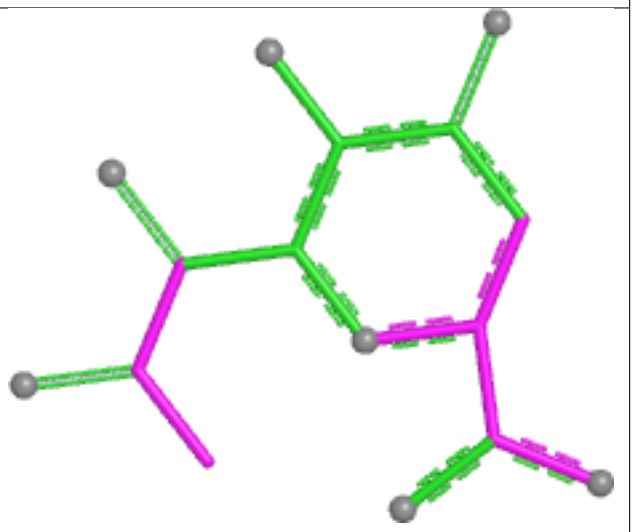


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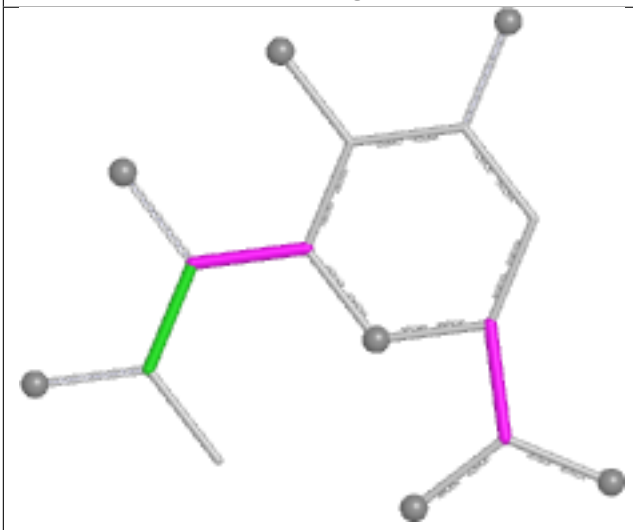
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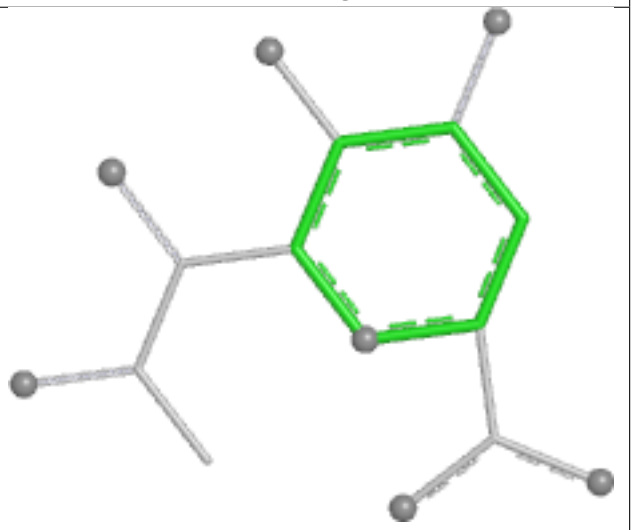
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Bond angles

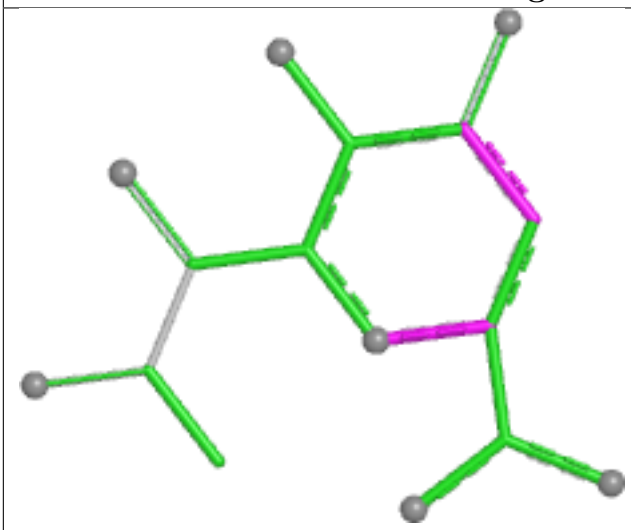


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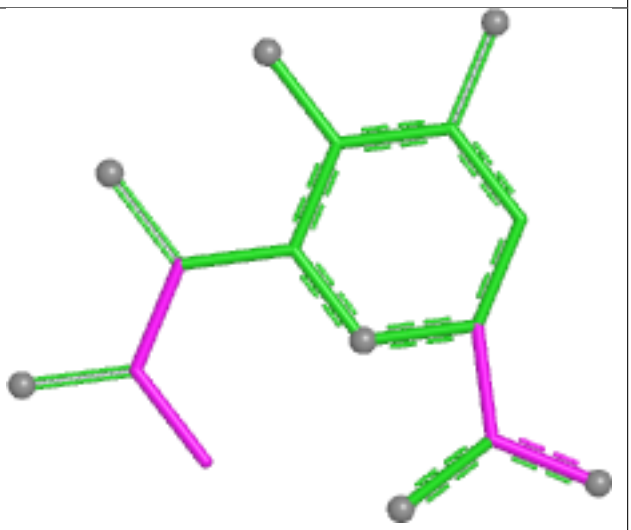


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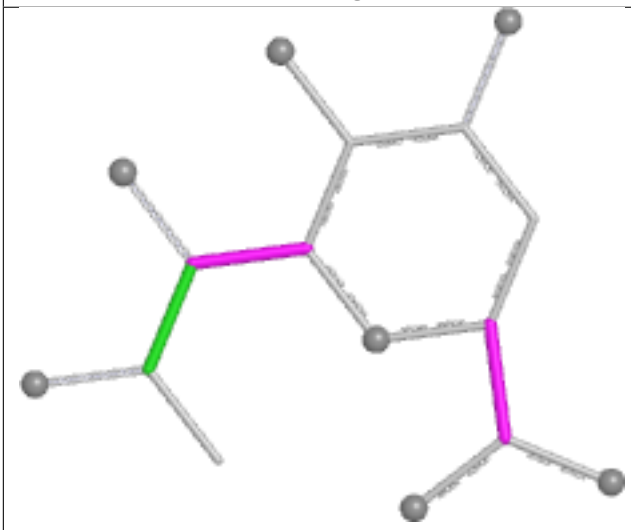
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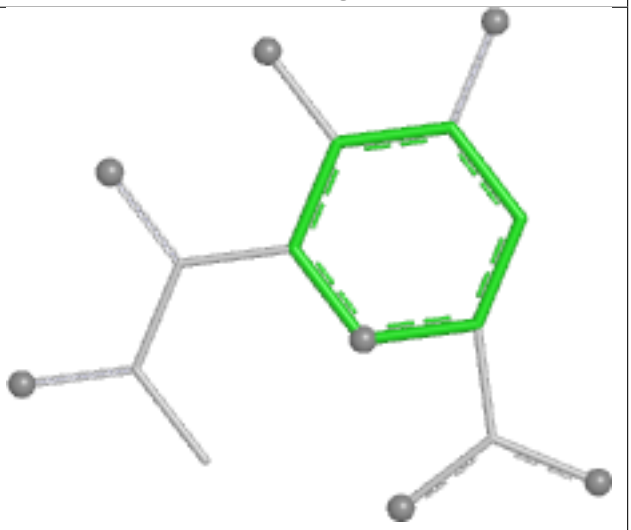
Bond lengths



Bond angles

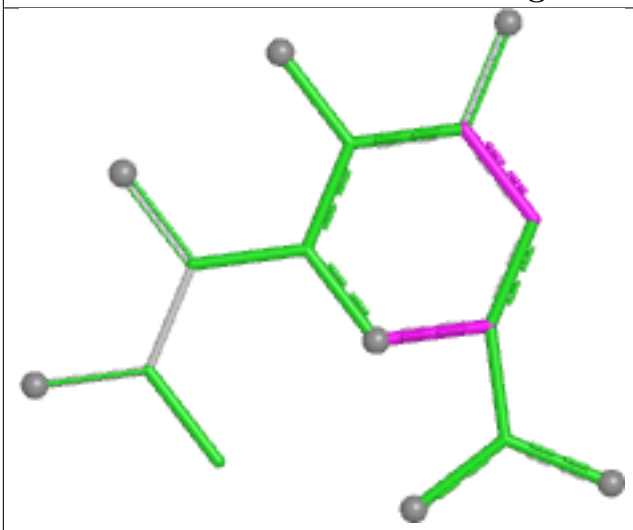


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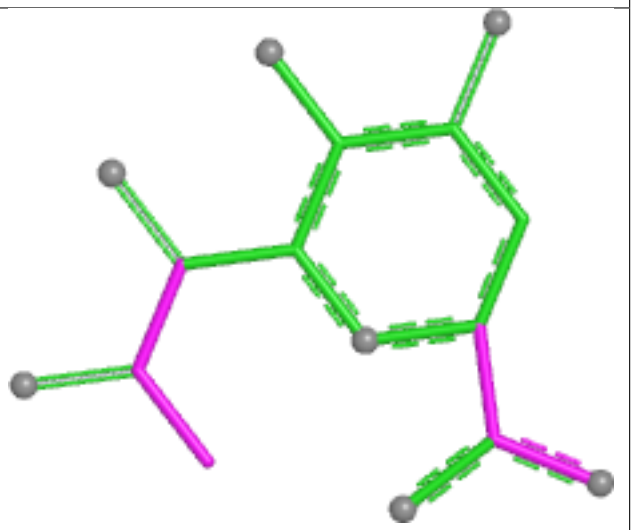


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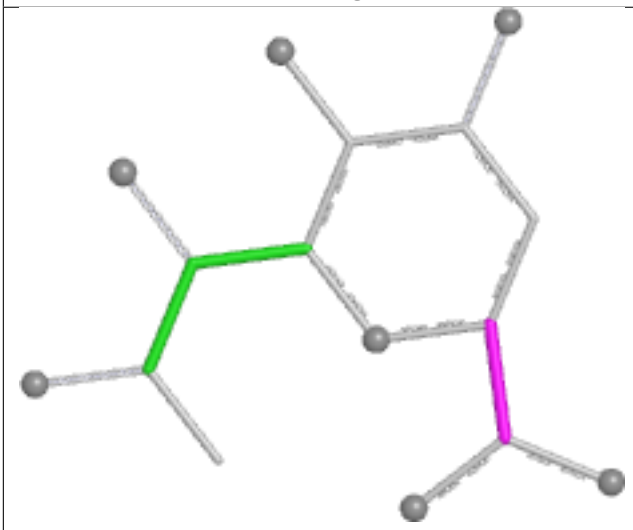
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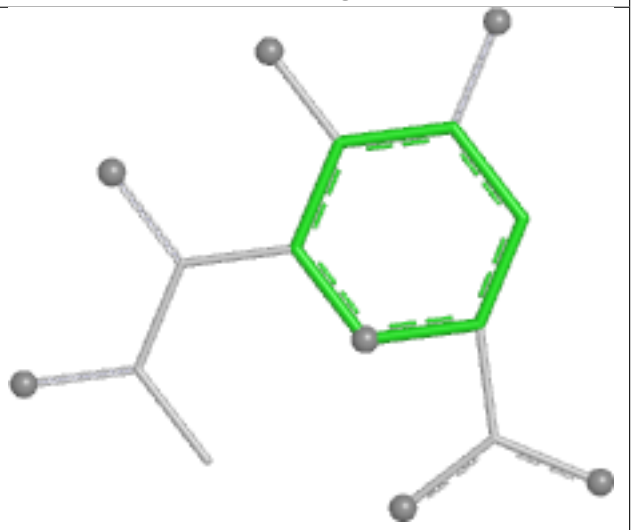
Bond lengths



Bond angles

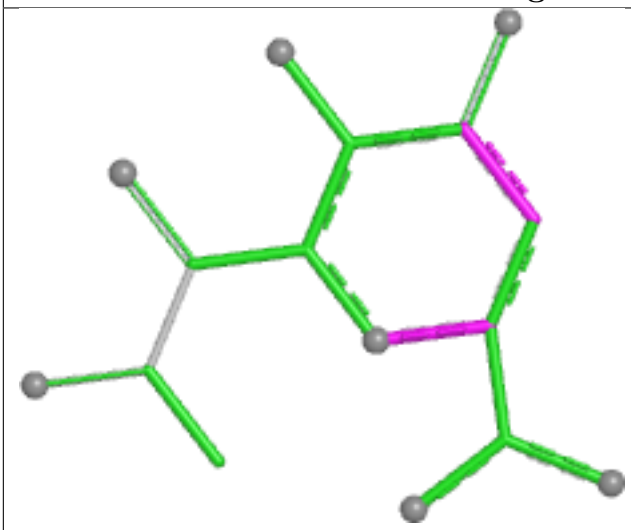


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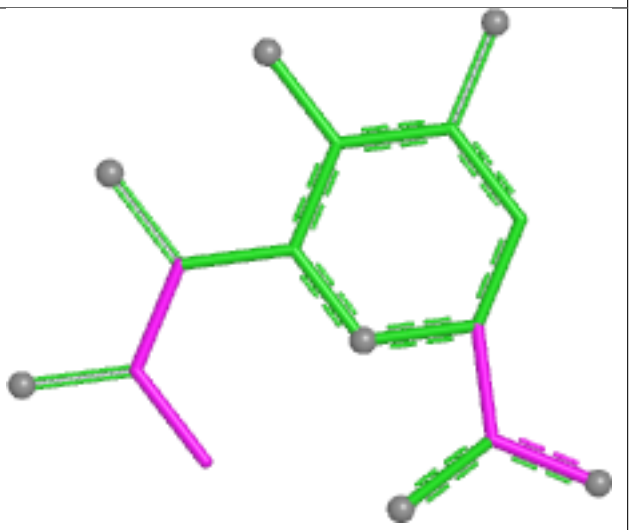


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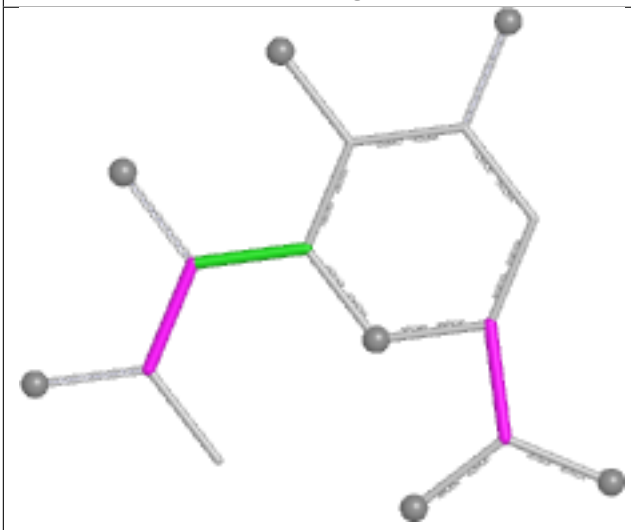
Ligand P8E U 614



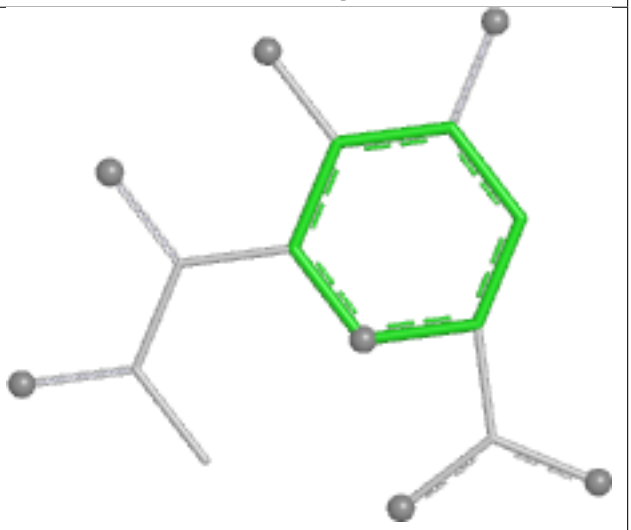
Bond lengths



Bond angles

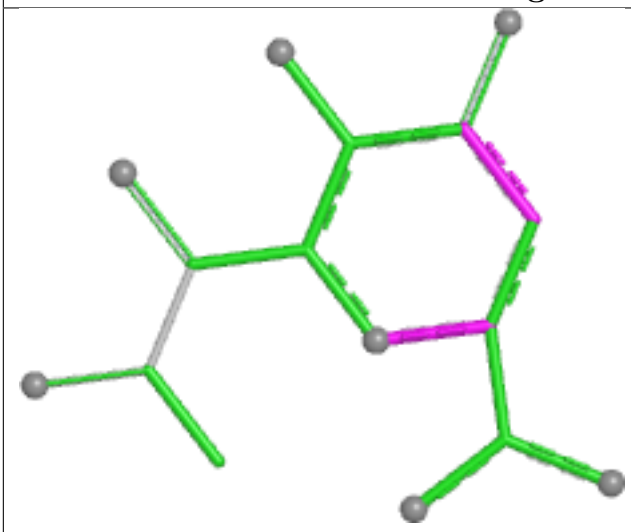


Torsions

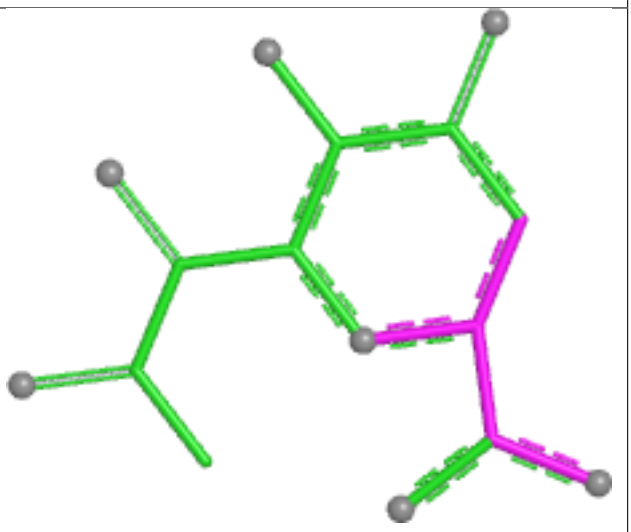


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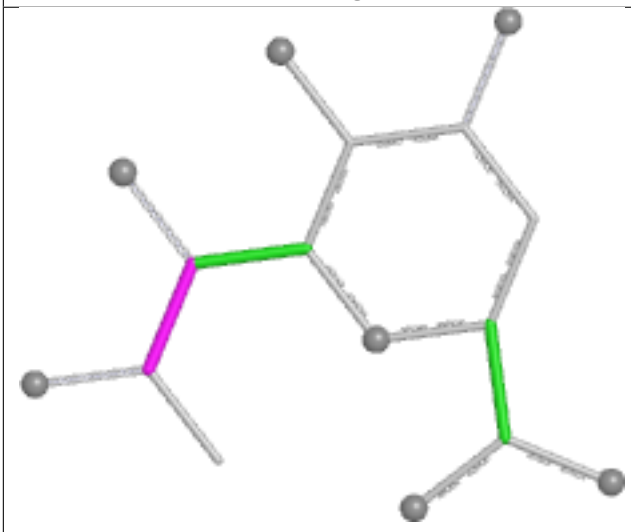
Ligand P8E D 603



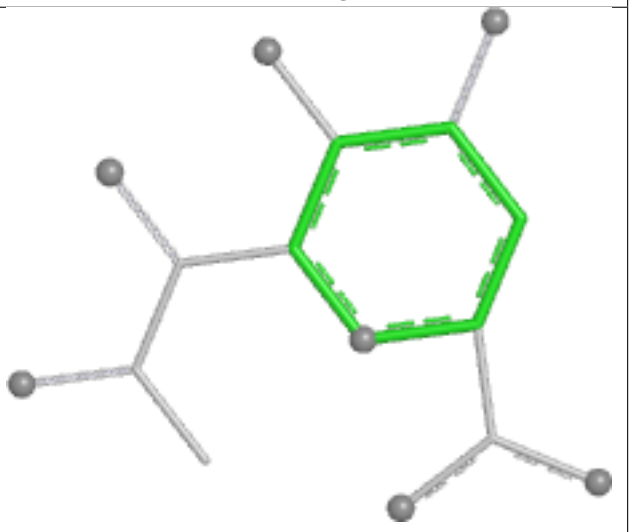
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Bond angles

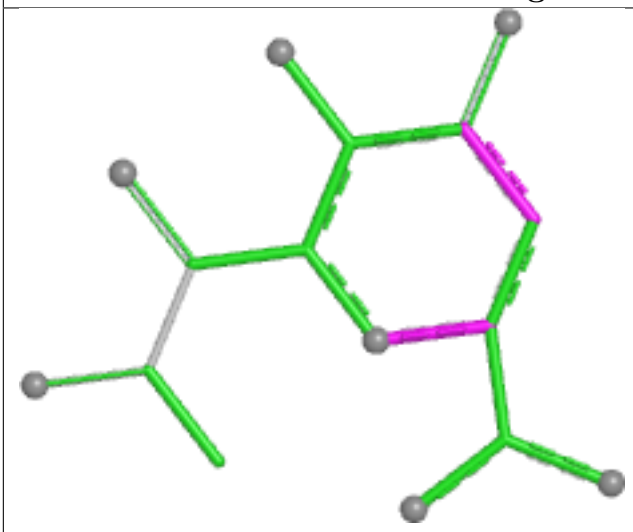


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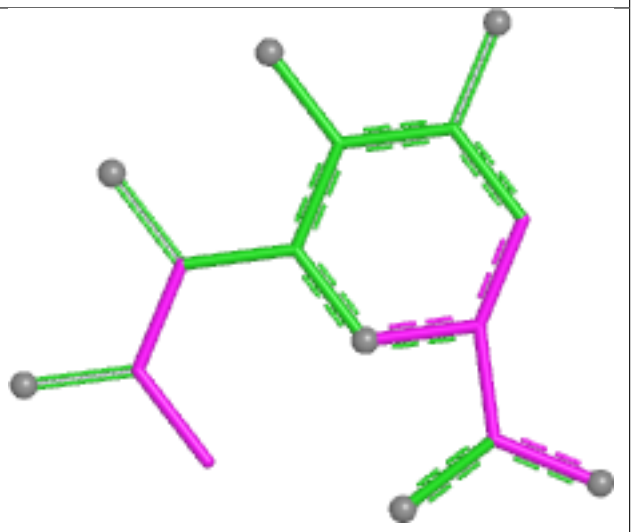


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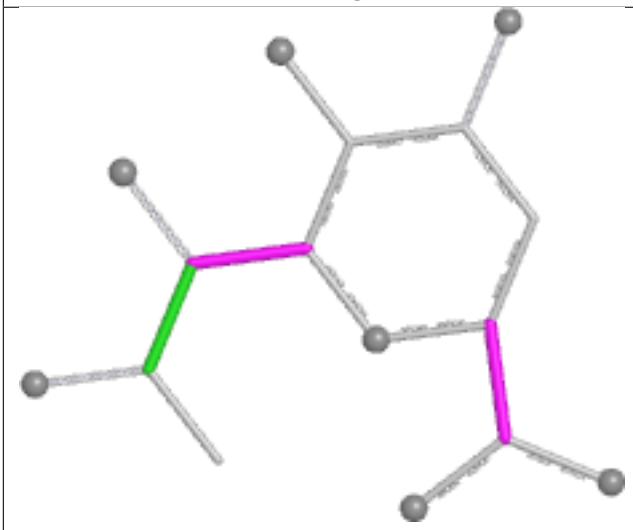
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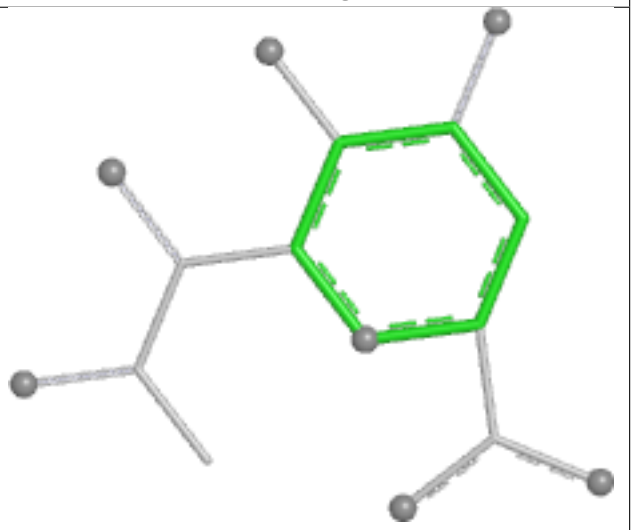
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Bond angles

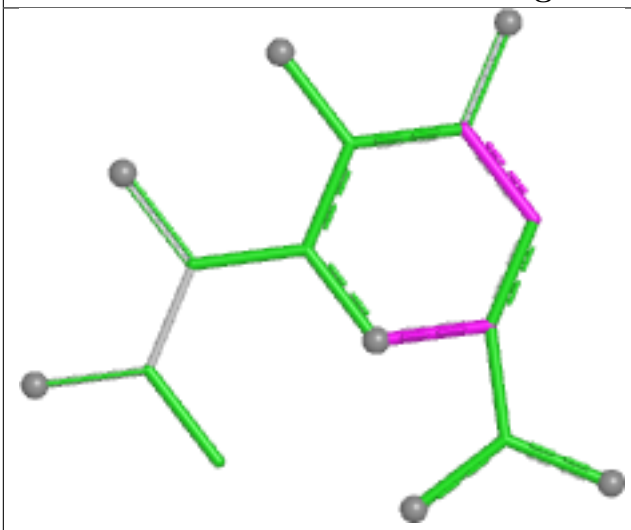


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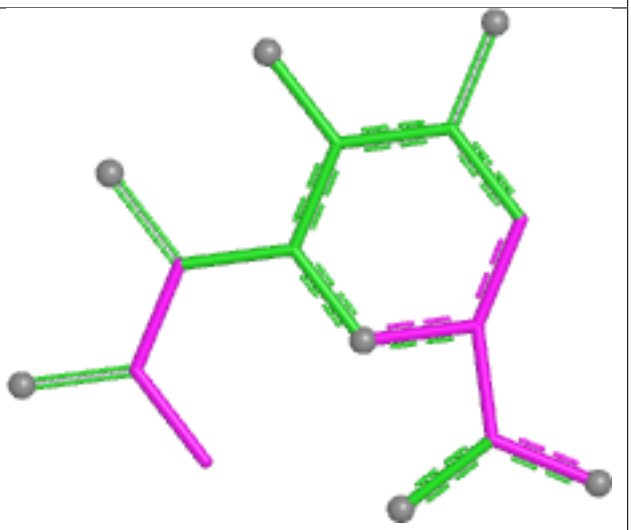


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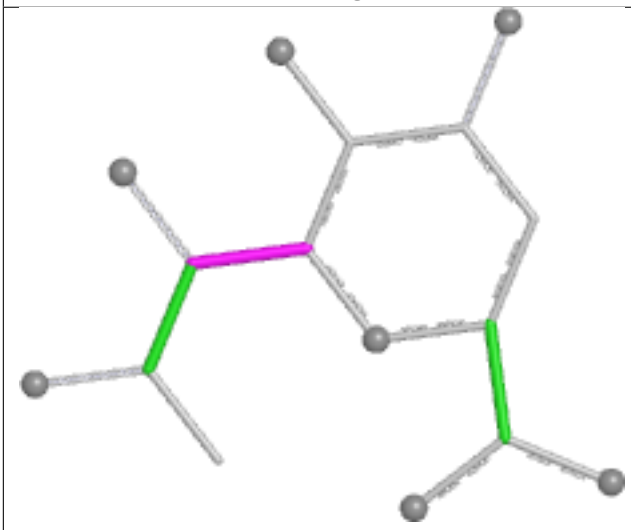
Ligand P8E I 615



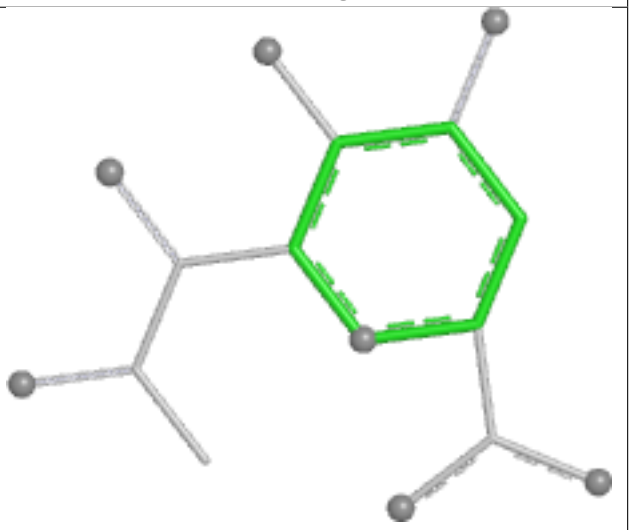
Bond lengths



Bond angles

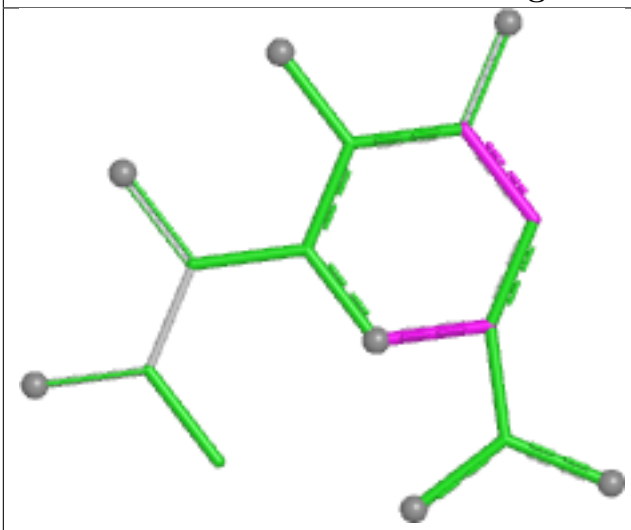


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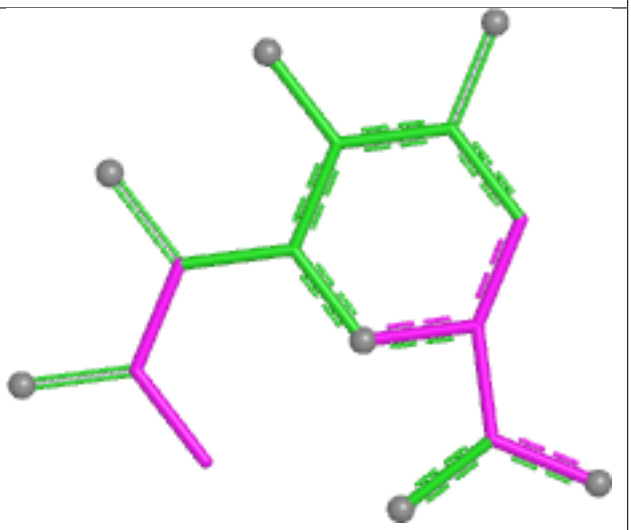


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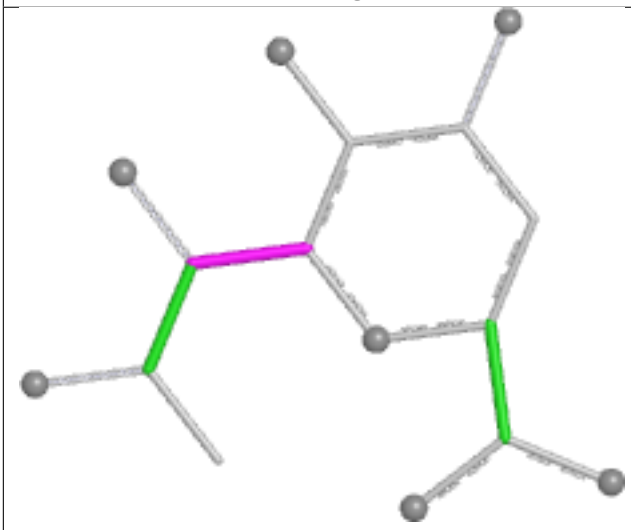
Ligand P8E V 613



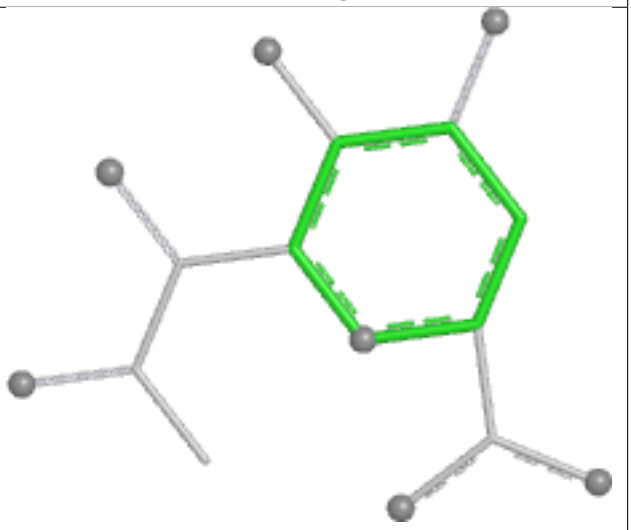
Bond lengths



Bond angles

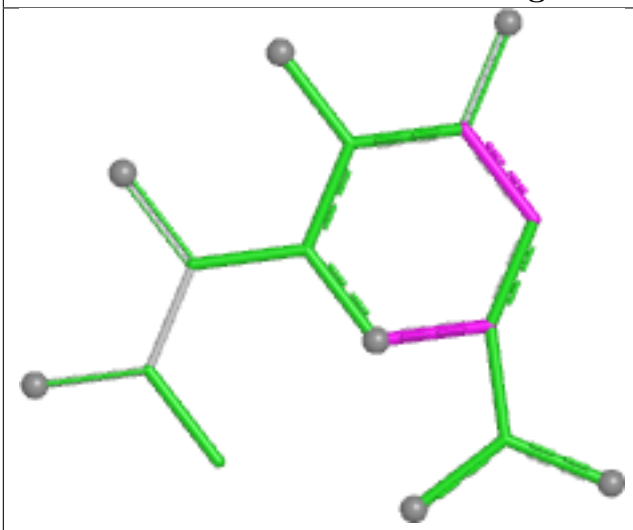


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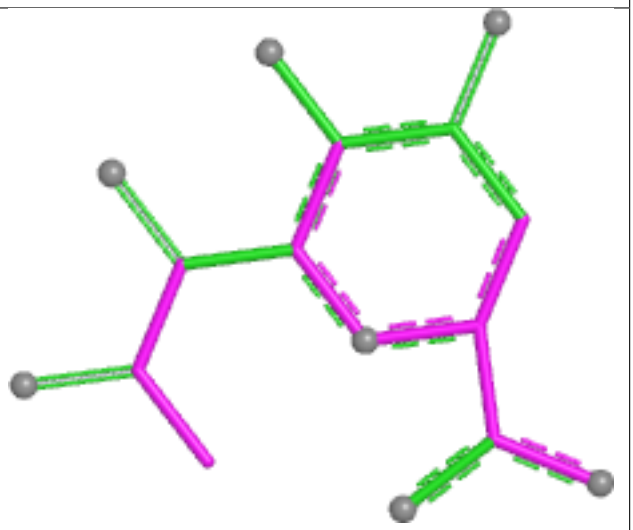


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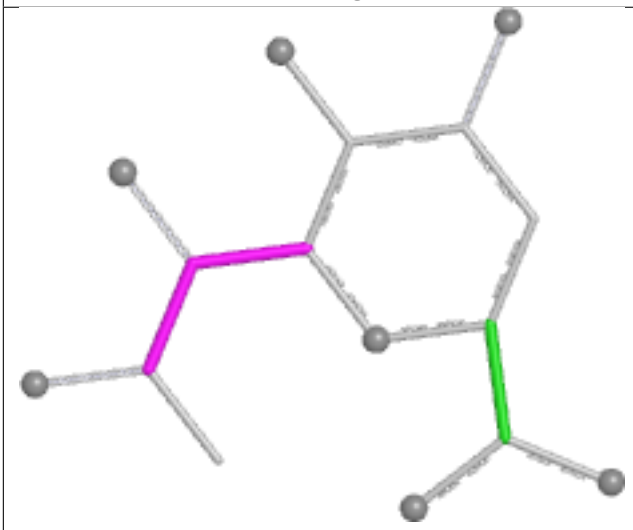
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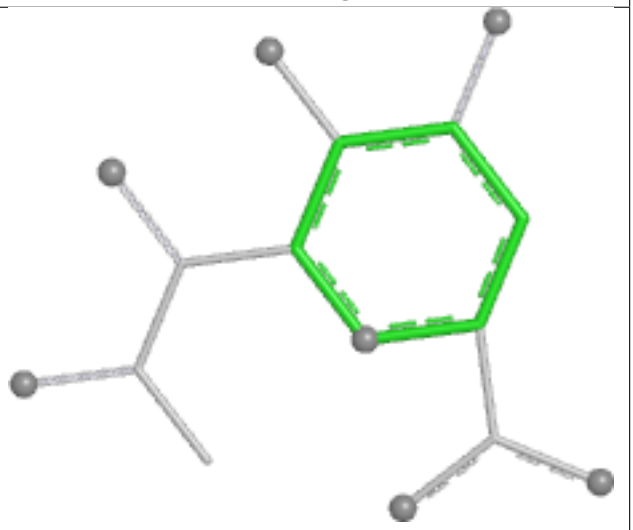
Bond lengths



Bond angles

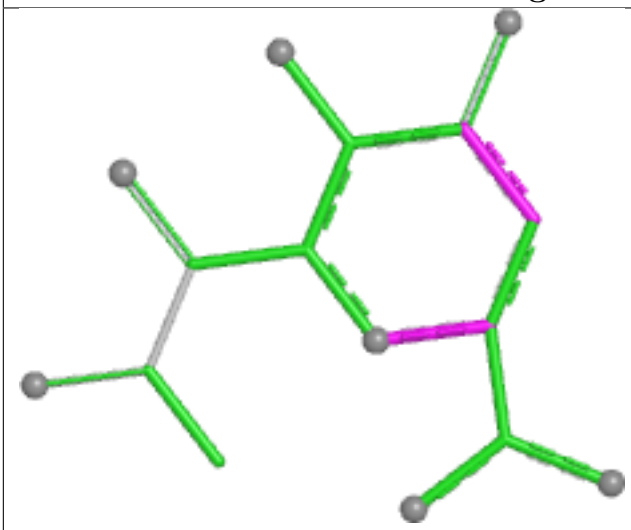


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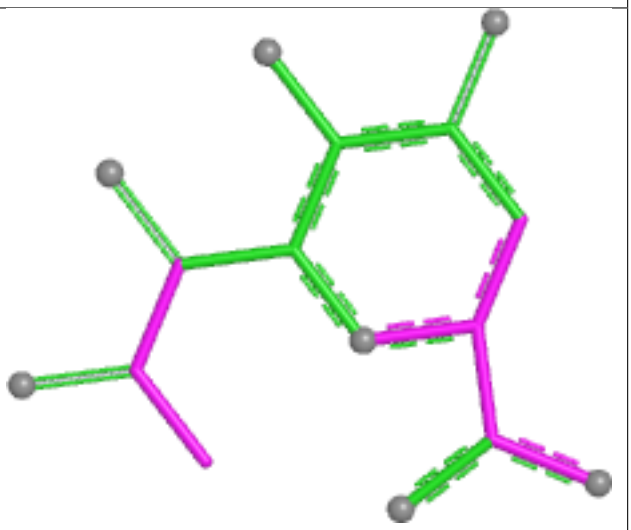


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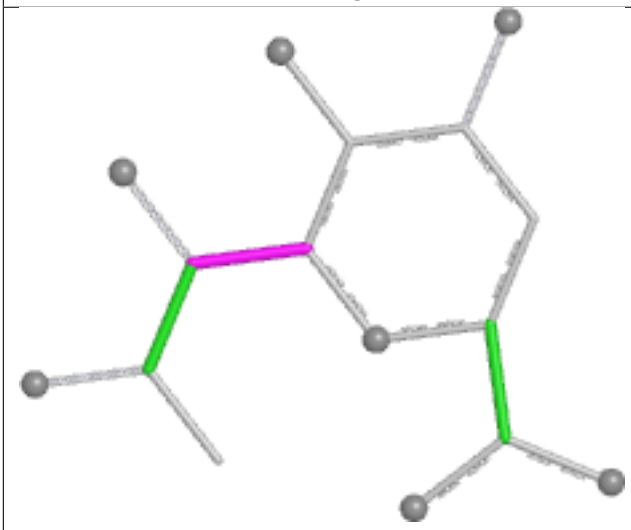
Ligand P8E T 612



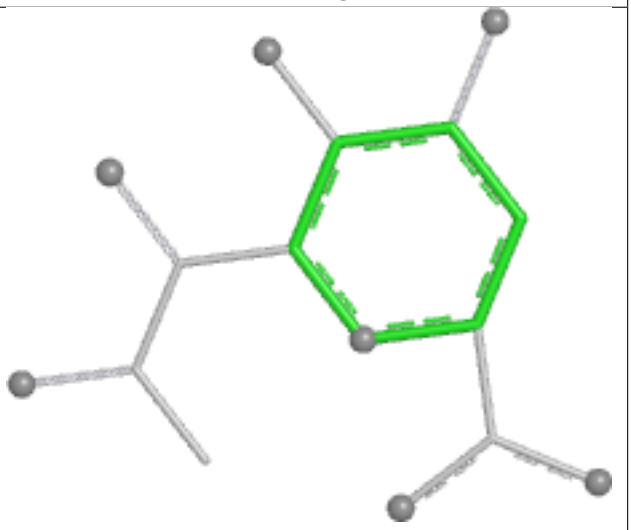
Bond lengths



Bond angles

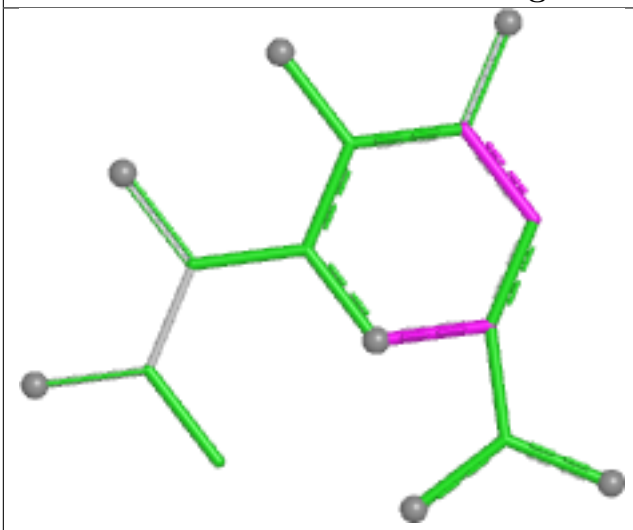


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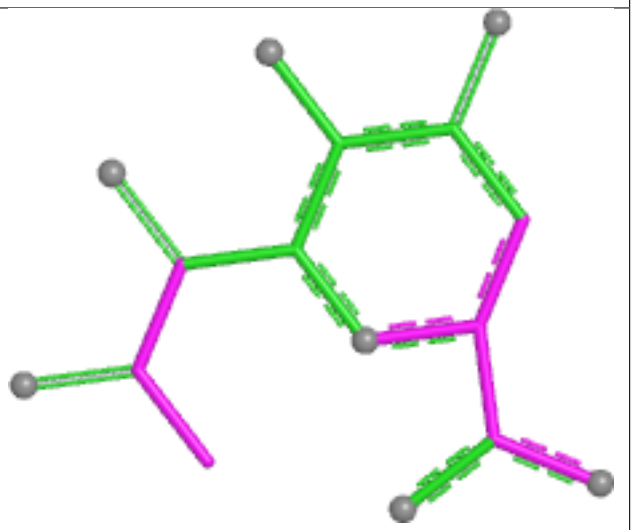


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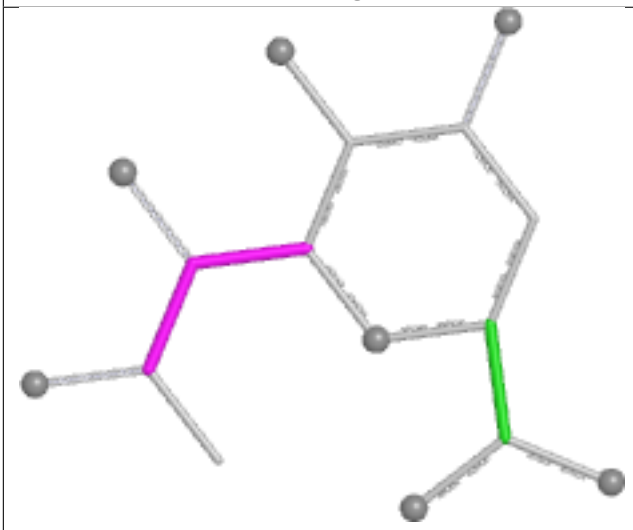
Ligand P8E C 605



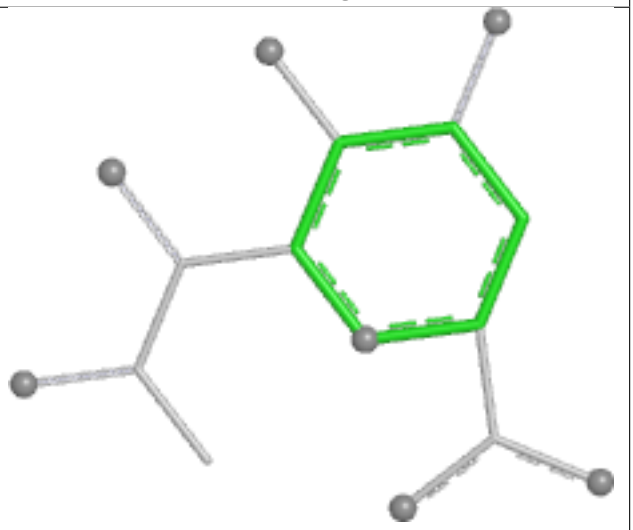
Bond lengths



Bond angles

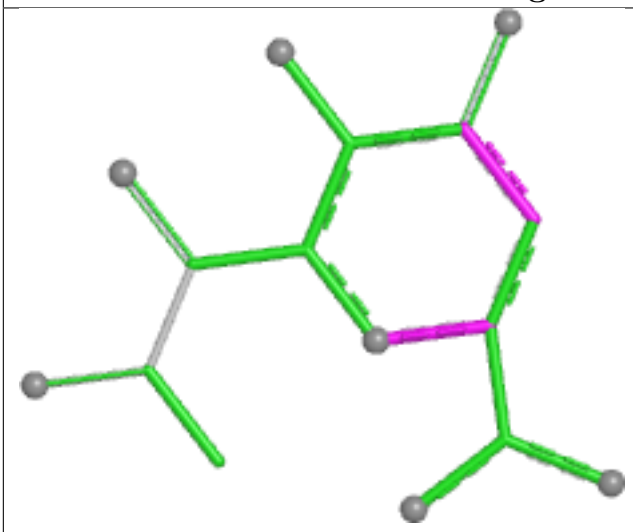


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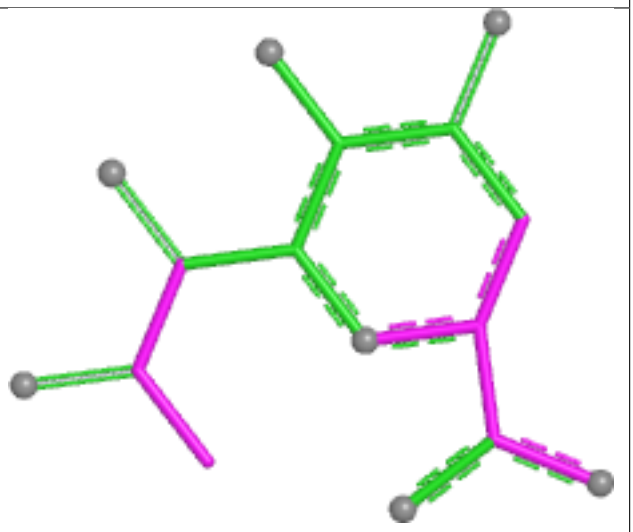


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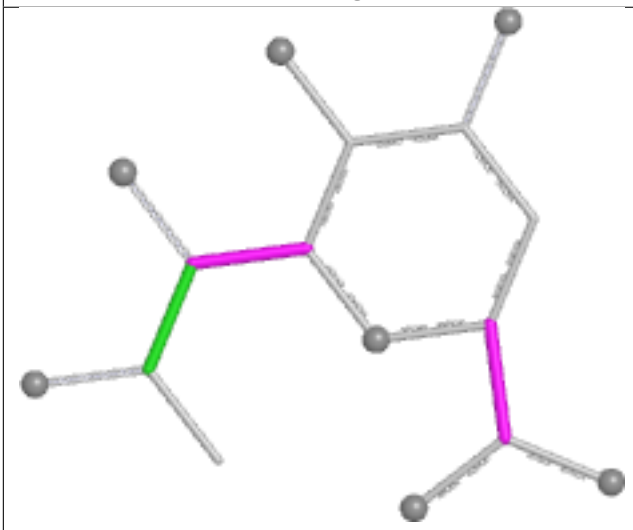
Ligand P8E B 607



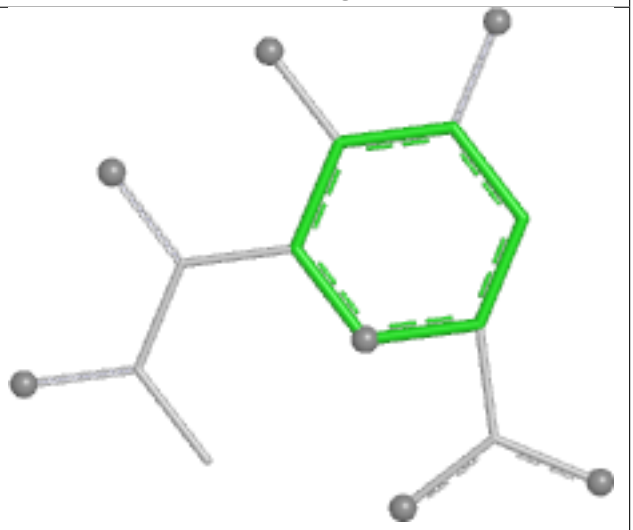
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Bond angles

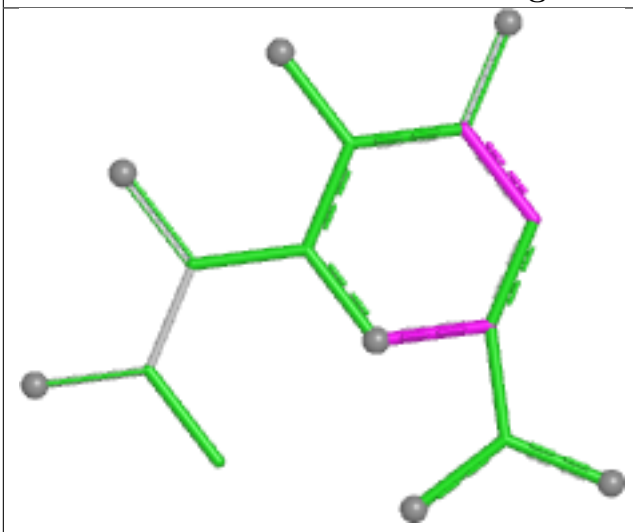


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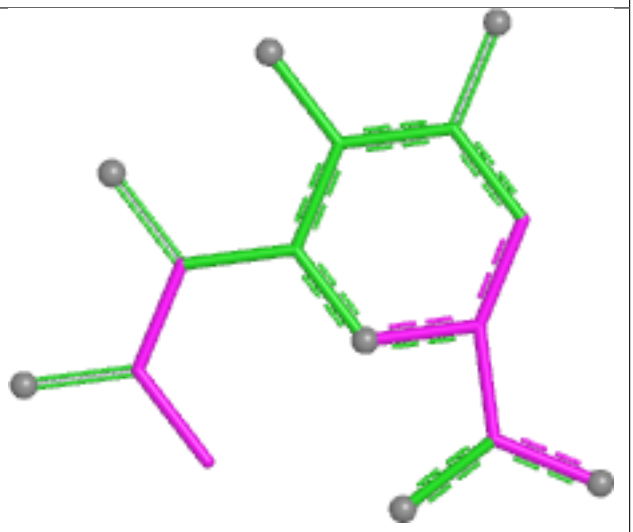


Rings

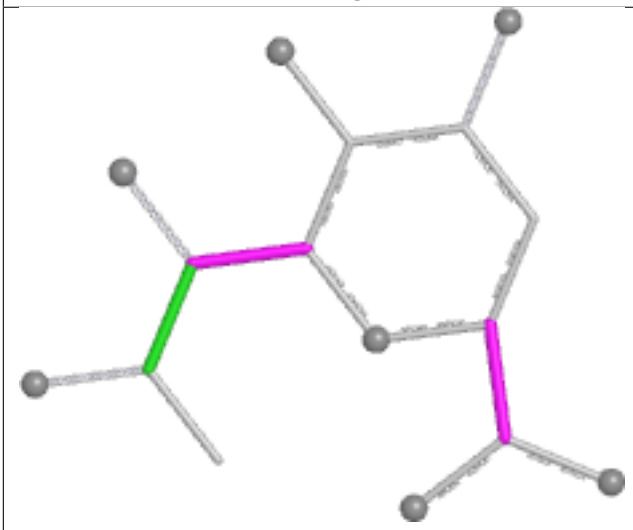
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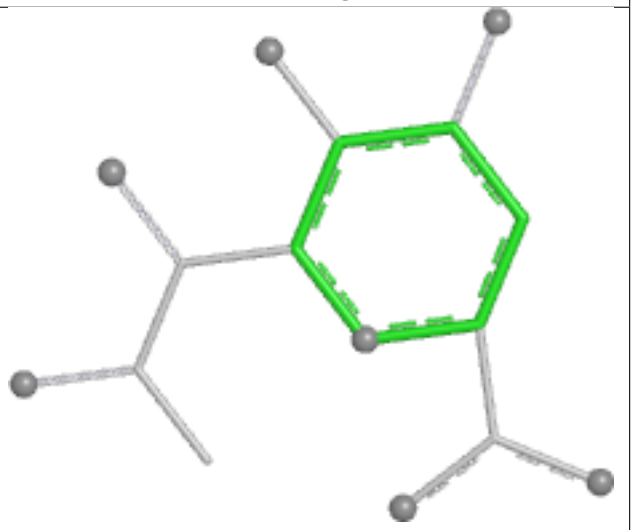
Bond lengths



Bond angles

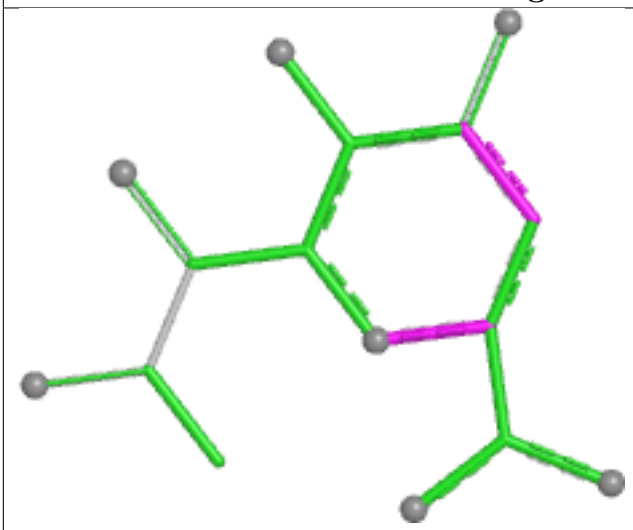


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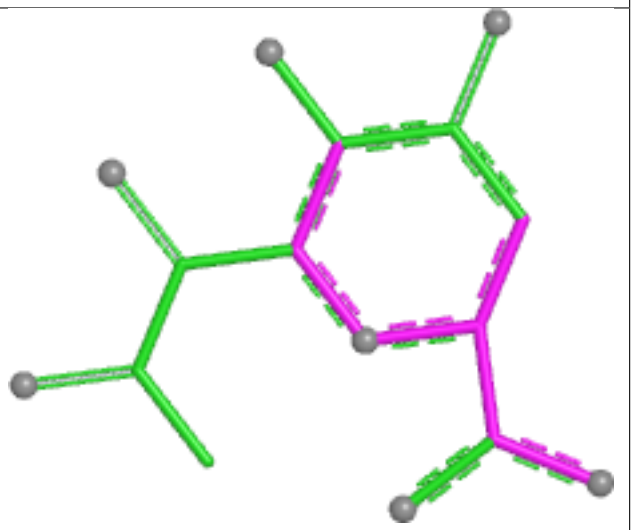


Rings

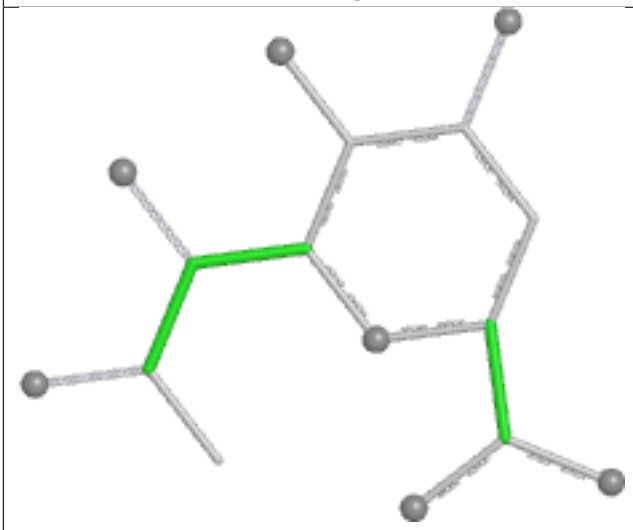
Ligand P8E D 617



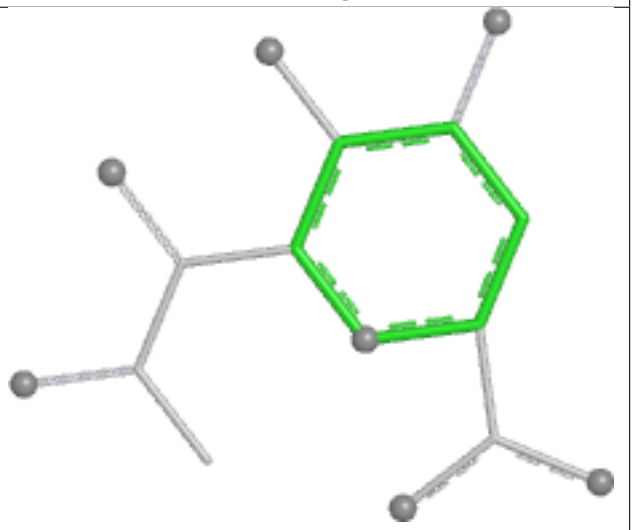
Bond lengths



Bond angles

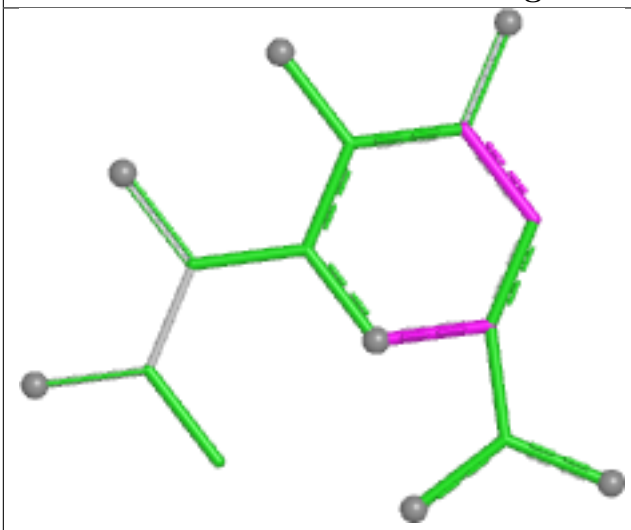


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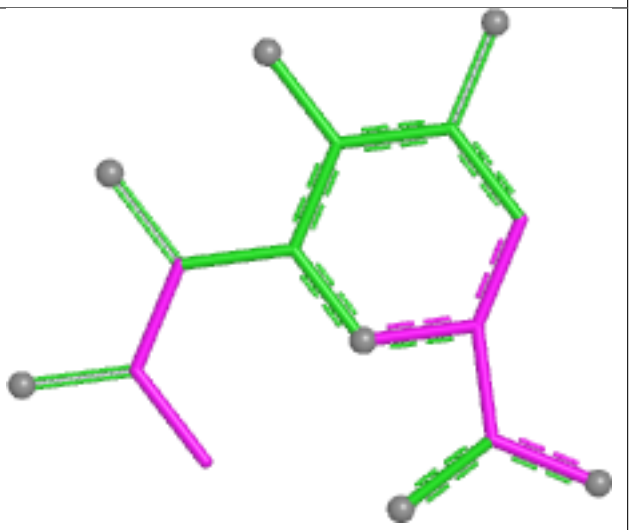


Rings

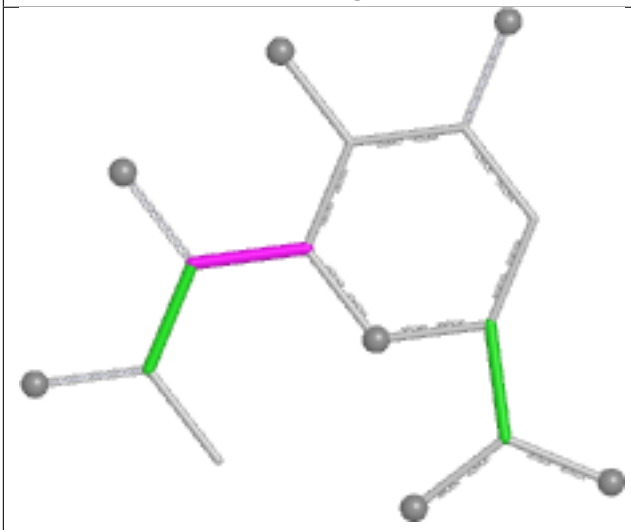
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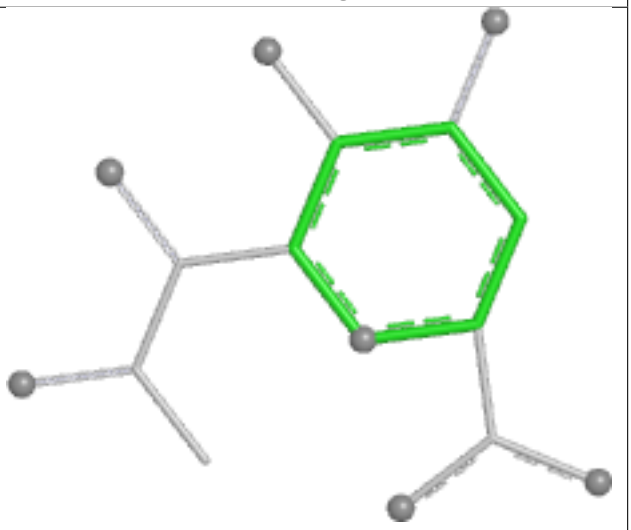
Bond lengths



Bond angles

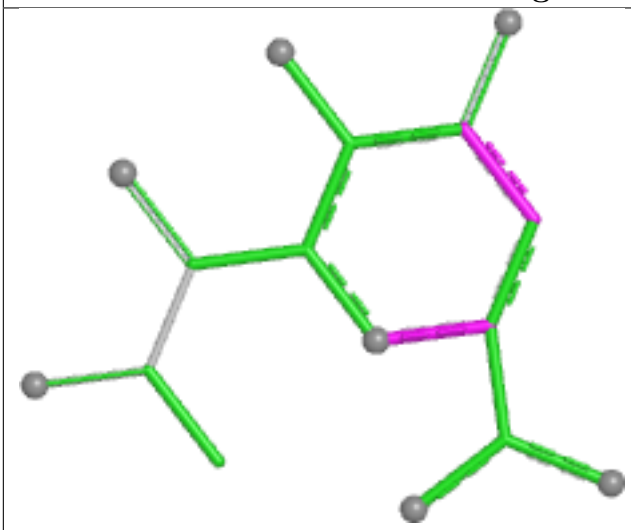


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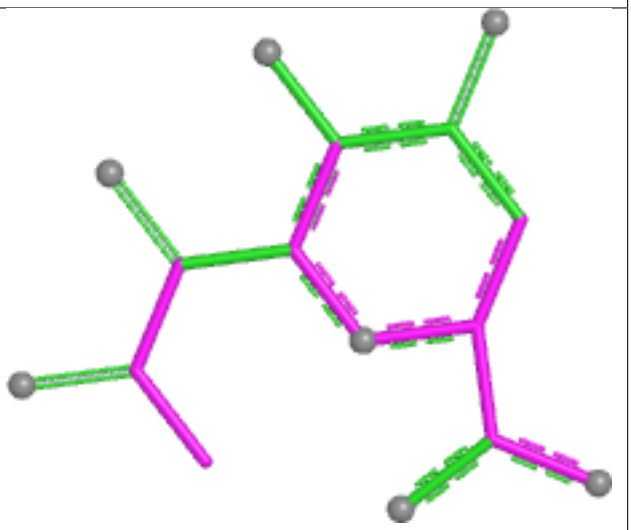


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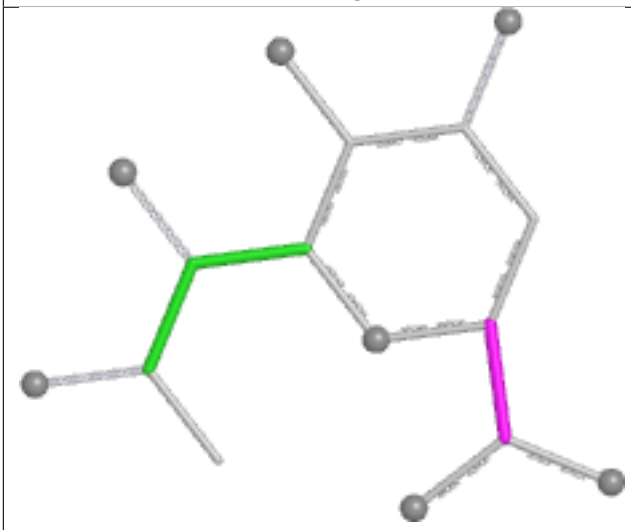
Ligand P8E J 617



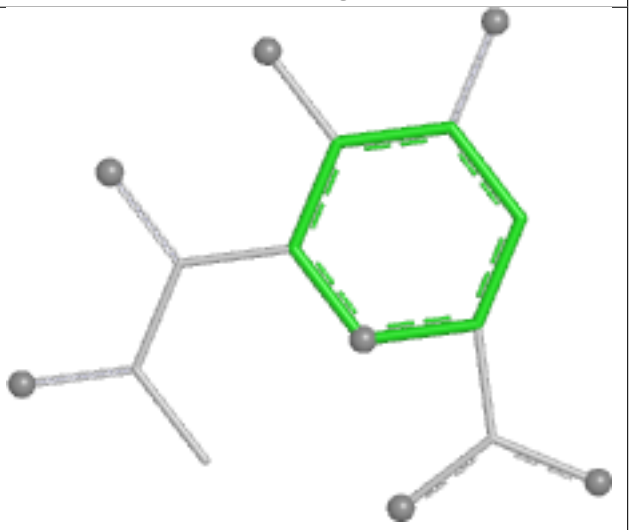
Bond lengths



Bond angles

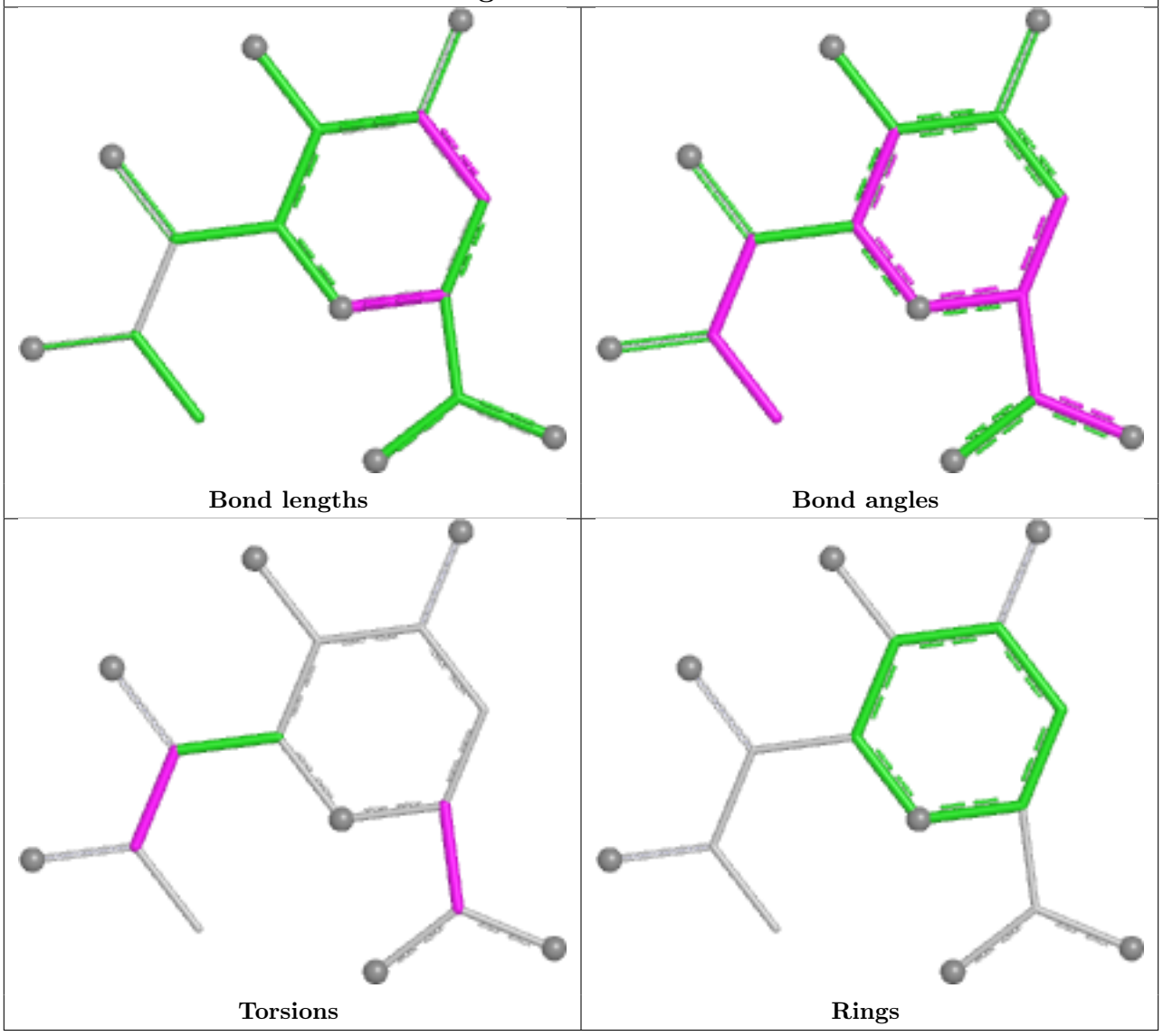


Torsions



Rings

Ligand P8E U 617



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.

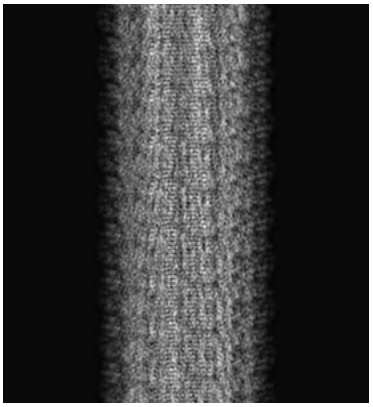
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22088. These allow visual inspection of the internal detail of the map and identification of artifacts.

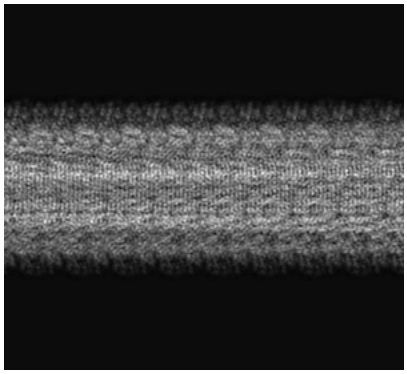
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

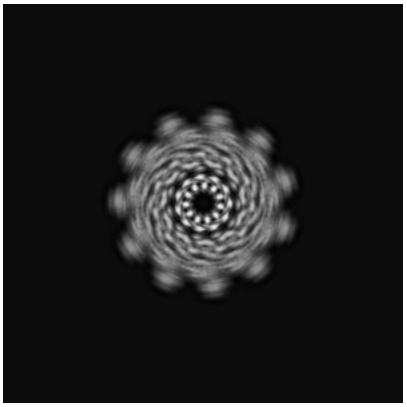
6.1.1 Primary map



X



Y

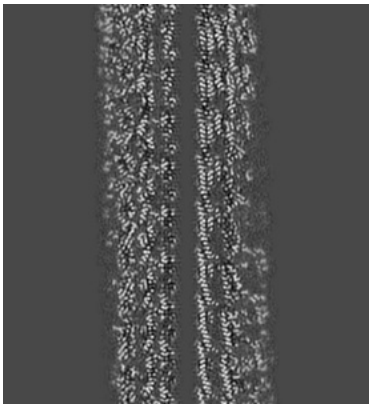


Z

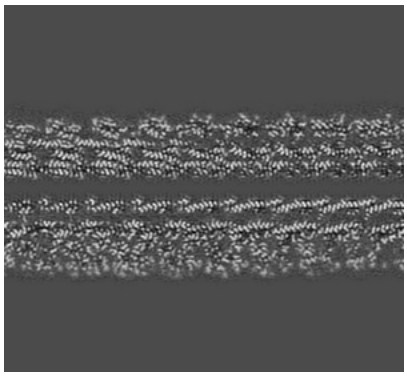
The images above show the map projected in three orthogonal directions.

6.2 Central slices

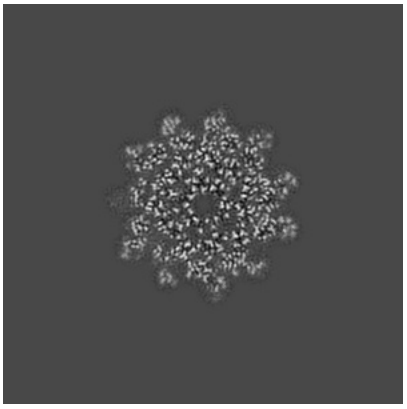
6.2.1 Primary map



X Index: 192



Y Index: 192

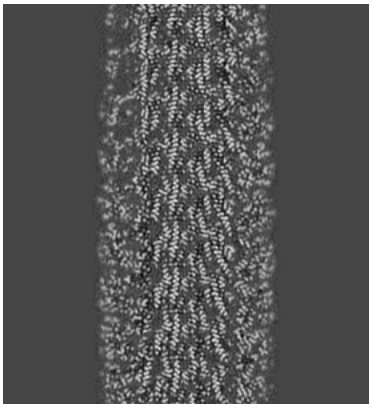


Z Index: 210

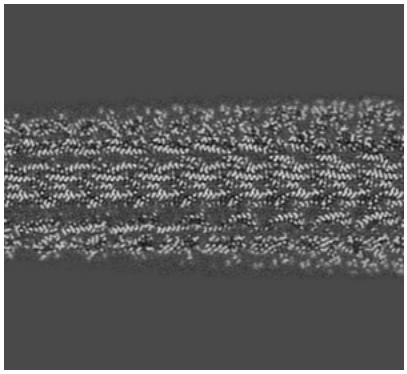
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

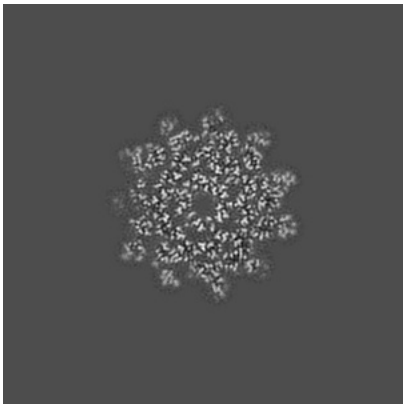
6.3.1 Primary map



X Index: 205



Y Index: 206

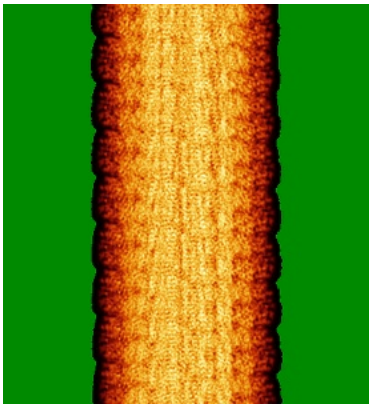


Z Index: 159

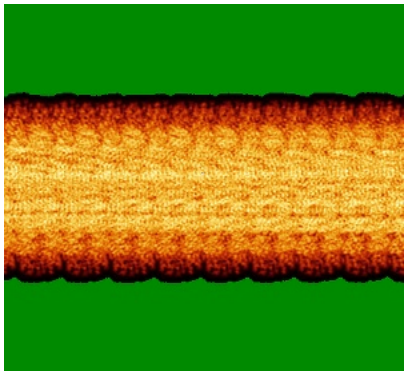
The images above show the largest variance slices of the map in three orthogonal directions.

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

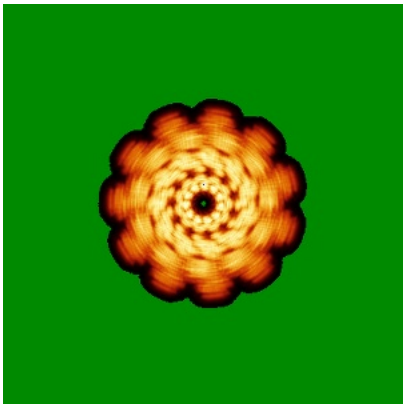
6.4.1 Primary map



X



Y

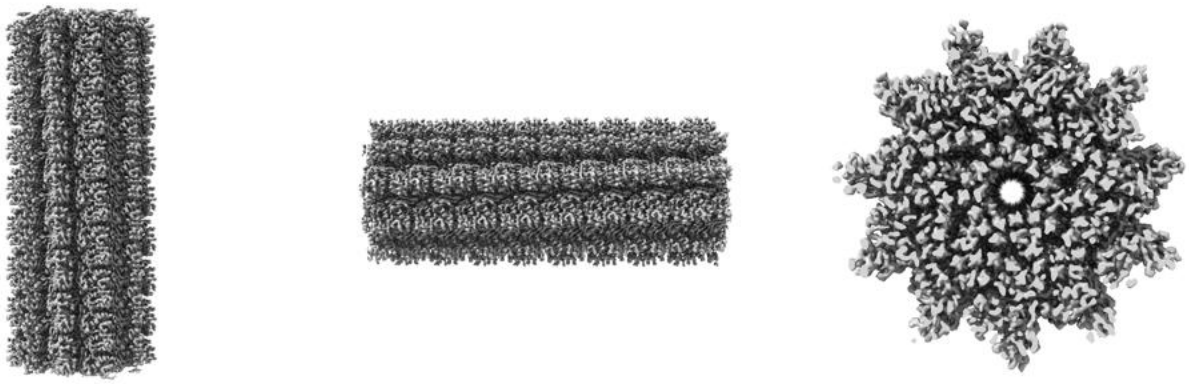


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0054. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

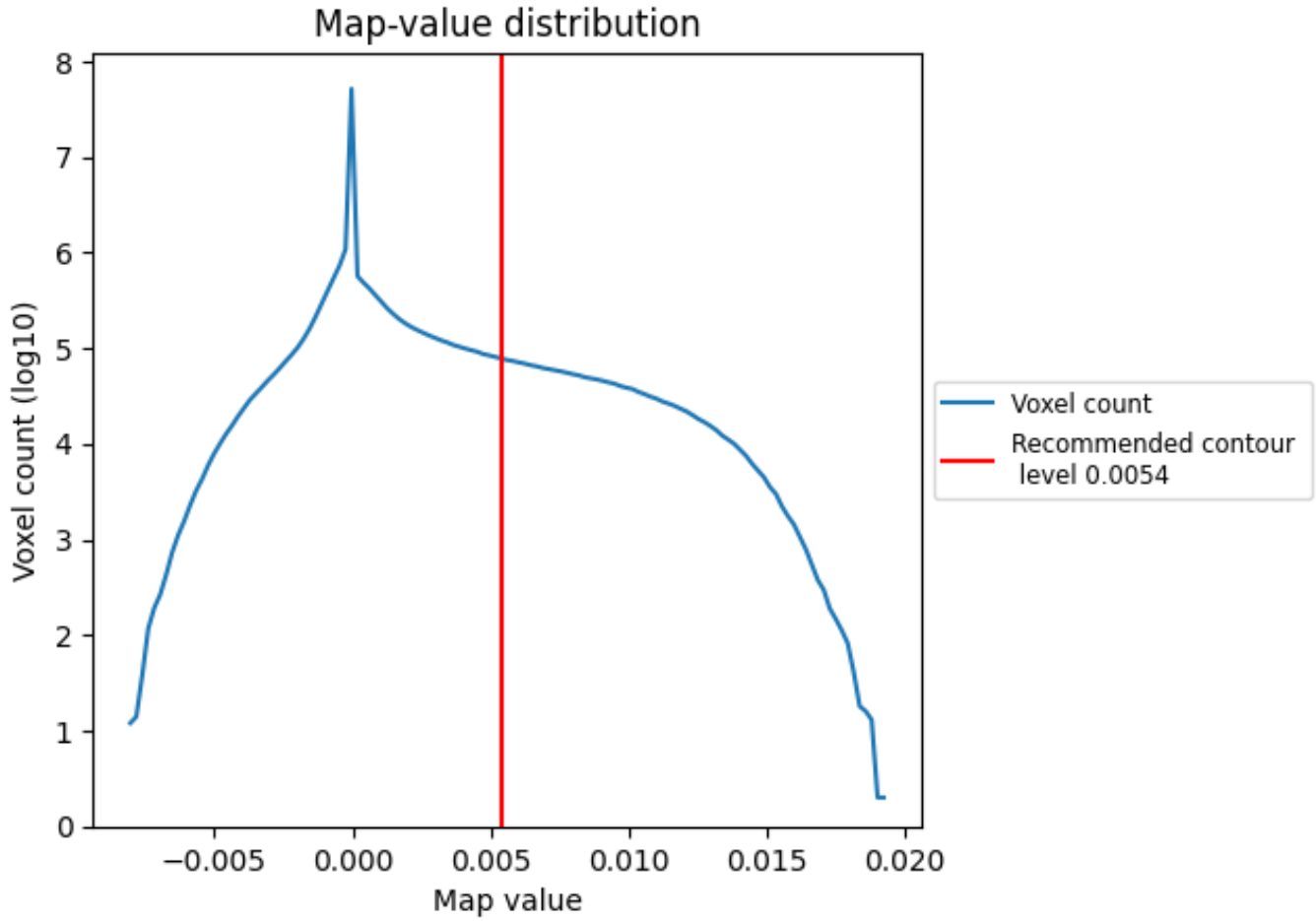
6.6 Mask visualisation (i)

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

7 Map analysis

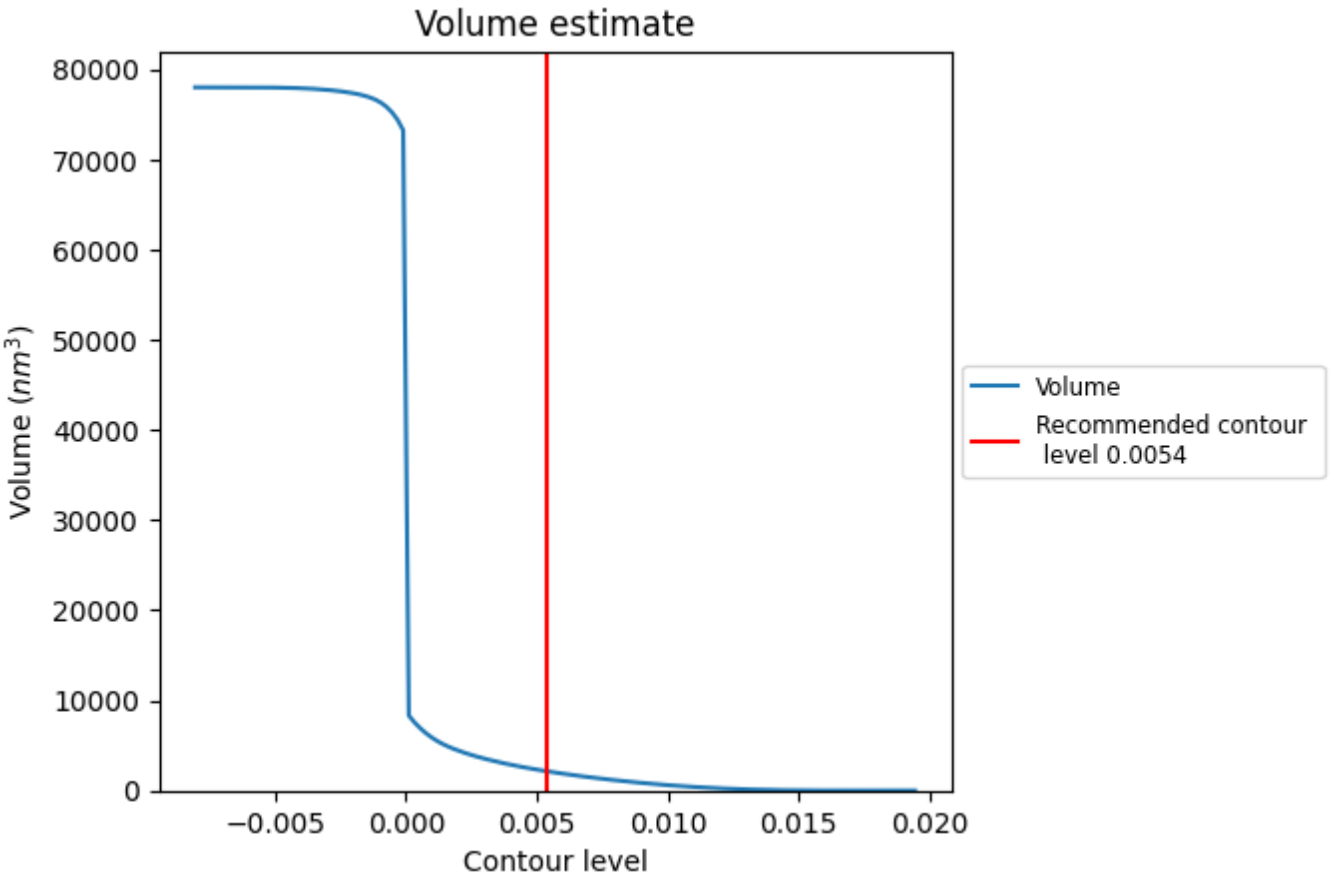
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate



The volume at the recommended contour level is 2138 nm^3; this corresponds to an approximate mass of 1932 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

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

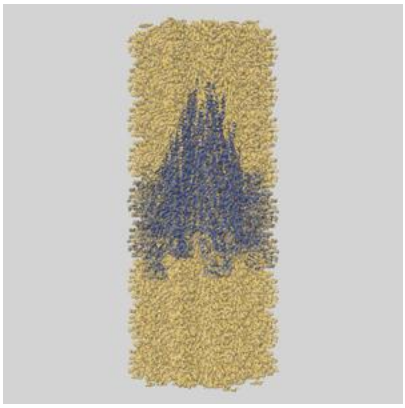
8 Fourier-Shell correlation

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

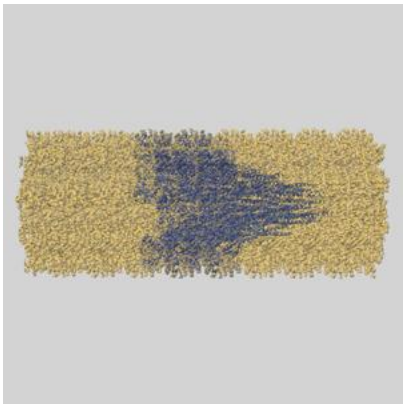
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22088 and PDB model 6X80. Per-residue inclusion information can be found in section 3 on page 25.

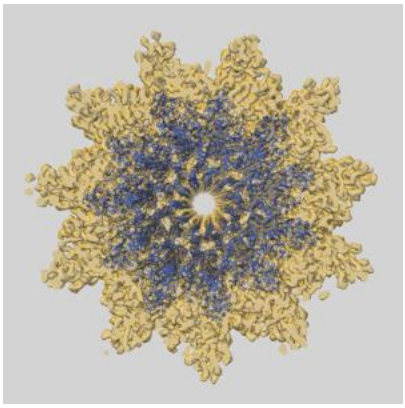
9.1 Map-model overlay



X



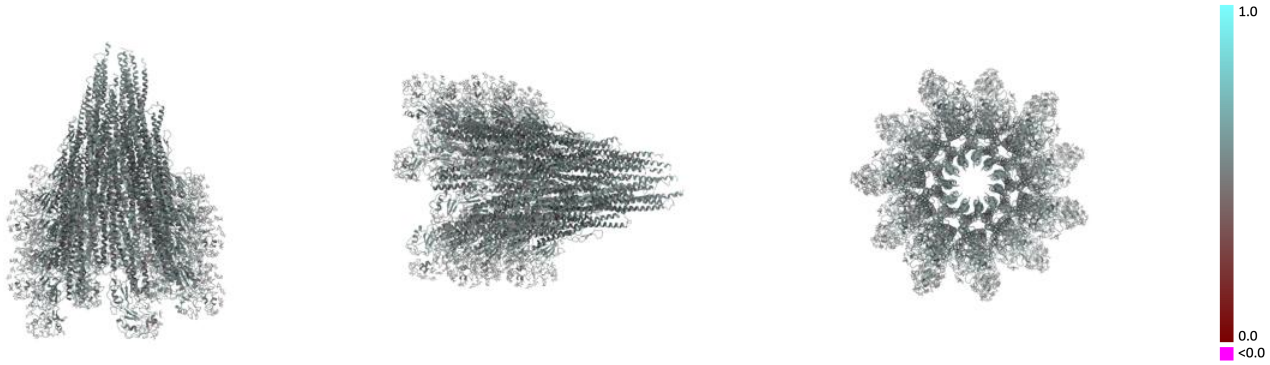
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0054 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

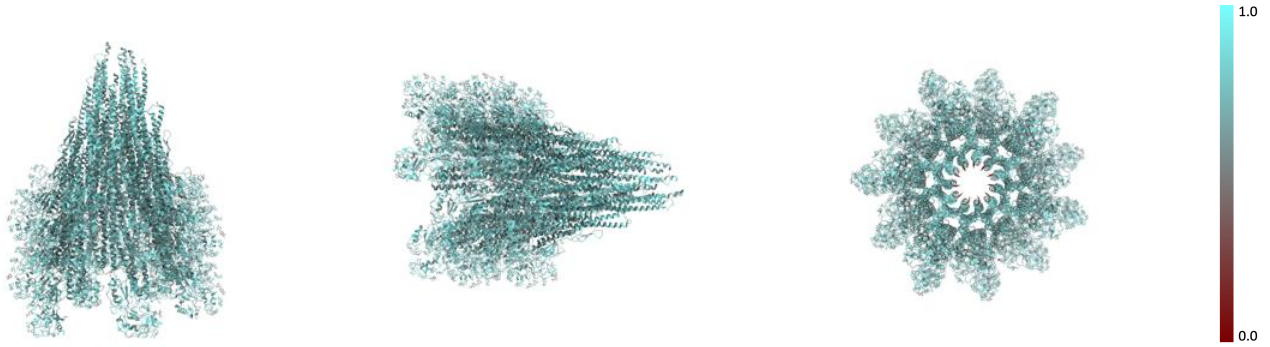
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

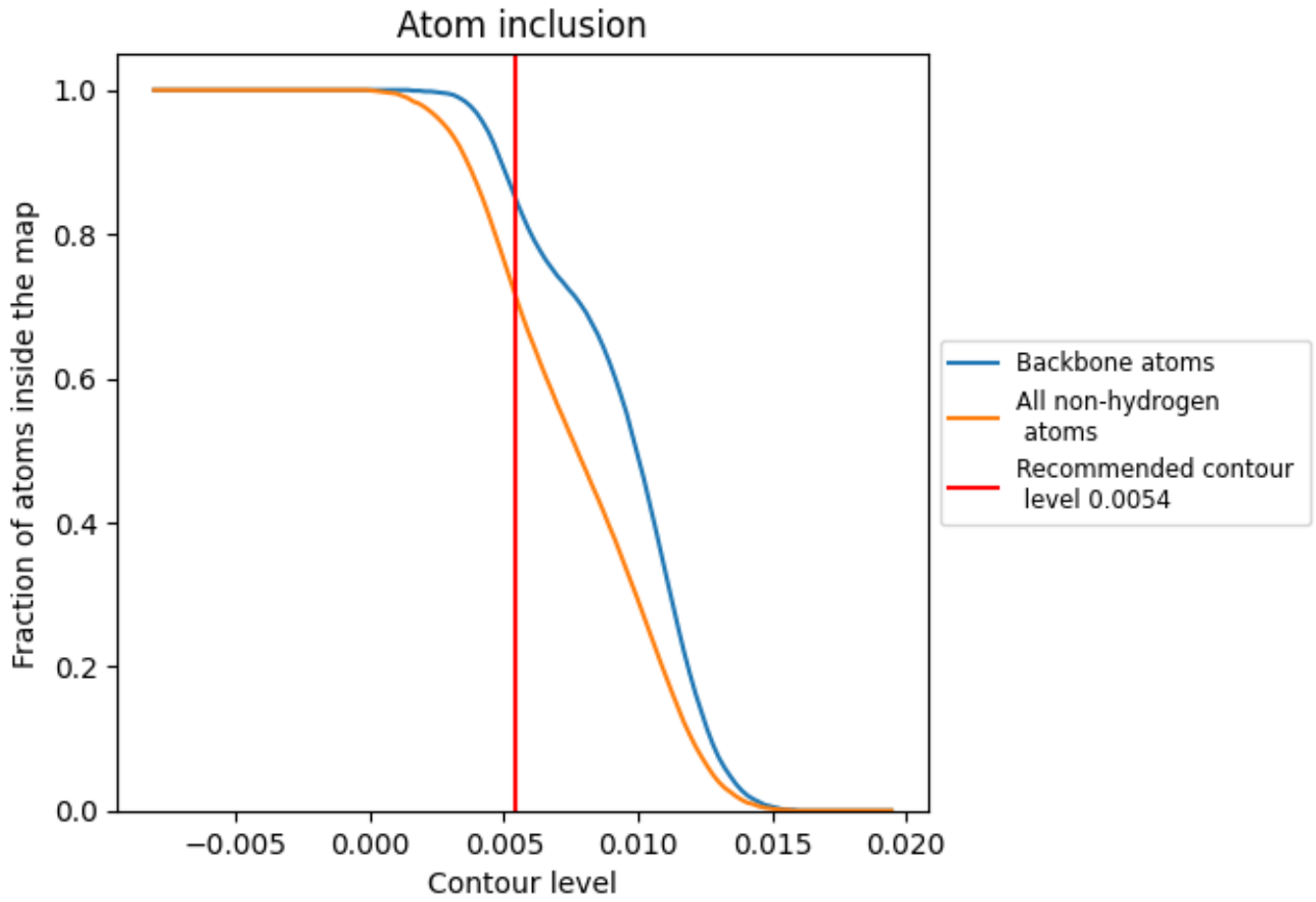
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0054).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 72% 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 (0.0054) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7180	0.5240
A	0.7220	0.5230
B	0.7170	0.5230
C	0.7180	0.5240
D	0.7170	0.5230
E	0.7220	0.5230
F	0.7180	0.5230
G	0.7170	0.5230
H	0.7150	0.5230
I	0.7220	0.5250
J	0.7180	0.5230
K	0.7160	0.5250
L	0.7140	0.5240
M	0.7220	0.5240
N	0.7200	0.5240
O	0.7160	0.5230
P	0.7100	0.5220
Q	0.7150	0.5240
R	0.7160	0.5230
S	0.7200	0.5230
T	0.7170	0.5230
U	0.7210	0.5240
V	0.7190	0.5270

