wwPDB EM Validation Summary Report (i)

Mar 7, 2026 – 04:28 AM UTC

PDB ID	:	9YGU / pdb_00009ygu
EMDB ID	:	EMD-72942
Title	:	Flagella filament structure in H. pylori composed of flagellin FlaA
Authors	:	Kumar, R.; Yu, H.; Tachiyama, S.; Liu, J.
Deposited on	:	2025-09-29
Resolution	:	2.88 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

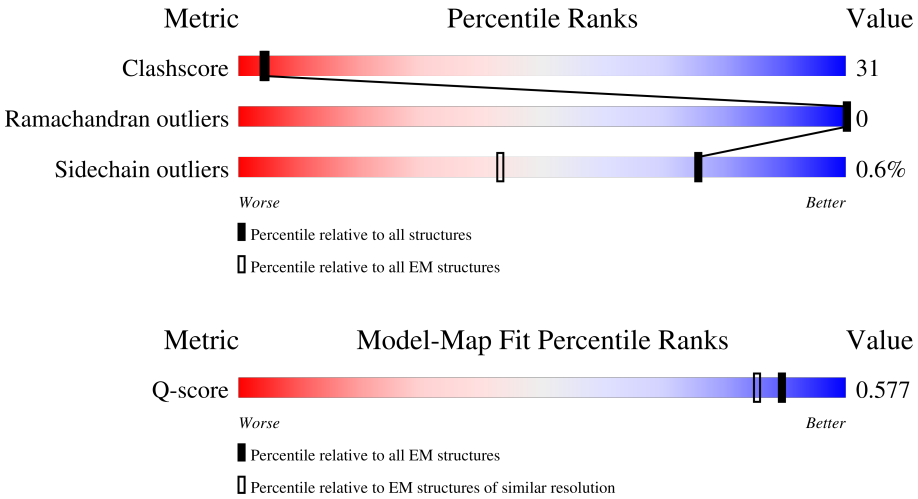
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 (i)

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

The reported resolution of this entry is 2.88 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	12111 (2.38 - 3.38)

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	A7	508	55% 44%
1	BJ	508	53% 47%
1	CT	508	55% 45%
1	DN	508	55% 44%

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Mol	Chain	Length	Quality of chain
1	EX	508	53% 47%
1	FB	508	55% 45%
1	GQ	508	54% 45%
1	HL	508	53% 47%
1	I3	508	56% 43%
1	JD	508	55% 45%
1	KE	508	53% 47%
1	LF	508	55% 45%
1	MO	508	55% 45%
1	NI	508	53% 47%
1	OA	508	57% 43%
1	PU	508	55% 45%
1	Q2	508	53% 47%
1	R4	508	55% 44%
1	S5	508	55% 45%
1	TP	508	53% 47%
1	UH	508	57% 43%
1	VR	508	55% 45%
1	WG	508	53% 47%
1	XM	508	55% 44%
1	Y1	508	54% 46%
1	Z9	508	53% 47%
1	aW	508	56% 44%
1	bS	508	55% 45%
1	cV	508	52% 47%

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Mol	Chain	Length	Quality of chain
1	dC	508	
1	e8	508	
1	fK	508	
1	g6	508	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	P8E	A7	605	X	-	-	-
2	P8E	BJ	605	X	-	-	-
2	P8E	CT	605	X	-	-	-
2	P8E	DN	605	X	-	-	-
2	P8E	EX	605	X	-	-	-
2	P8E	FB	605	X	-	-	-
2	P8E	GQ	605	X	-	-	-
2	P8E	HL	605	X	-	-	-
2	P8E	I3	605	X	-	-	-
2	P8E	JD	605	X	-	-	-
2	P8E	KE	605	X	-	-	-
2	P8E	LF	605	X	-	-	-
2	P8E	MO	605	X	-	-	-
2	P8E	NI	605	X	-	-	-
2	P8E	OA	605	X	-	-	-
2	P8E	PU	605	X	-	-	-
2	P8E	Q2	605	X	-	-	-
2	P8E	R4	605	X	-	-	-
2	P8E	S5	605	X	-	-	-
2	P8E	TP	605	X	-	-	-
2	P8E	UH	605	X	-	-	-
2	P8E	VR	605	X	-	-	-
2	P8E	WG	605	X	-	-	-
2	P8E	XM	605	X	-	-	-
2	P8E	Y1	605	X	-	-	-
2	P8E	Z9	605	X	-	-	-
2	P8E	aW	605	X	-	-	-
2	P8E	bS	605	X	-	-	-
2	P8E	cV	605	X	-	-	-
2	P8E	dC	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	P8E	e8	605	X	-	-	-
2	P8E	fK	605	X	-	-	-
2	P8E	g6	605	X	-	-	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 129921 atoms, of which 3696 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Y1	508	Total	C	N	O	S	0	0
			3713	2256	669	778	10		
1	Q2	508	Total	C	N	O	S	0	0
			3713	2256	669	778	10		
1	I3	508	Total	C	N	O	S	0	0
			3713	2256	669	778	10		
1	R4	508	Total	C	N	O	S	0	0
			3713	2256	669	778	10		
1	S5	508	Total	C	N	O	S	0	0
			3713	2256	669	778	10		
1	g6	508	Total	C	N	O	S	0	0
			3713	2256	669	778	10		
1	A7	508	Total	C	N	O	S	0	0
			3713	2256	669	778	10		
1	e8	508	Total	C	N	O	S	0	0
			3713	2256	669	778	10		
1	Z9	508	Total	C	N	O	S	0	0
			3713	2256	669	778	10		
1	OA	508	Total	C	N	O	S	0	0
			3713	2256	669	778	10		
1	FB	508	Total	C	N	O	S	0	0
			3713	2256	669	778	10		
1	dC	508	Total	C	N	O	S	0	0
			3713	2256	669	778	10		
1	JD	508	Total	C	N	O	S	0	0
			3713	2256	669	778	10		
1	KE	508	Total	C	N	O	S	0	0
			3713	2256	669	778	10		
1	LF	508	Total	C	N	O	S	0	0
			3713	2256	669	778	10		
1	WG	508	Total	C	N	O	S	0	0
			3713	2256	669	778	10		
1	UH	508	Total	C	N	O	S	0	0
			3713	2256	669	778	10		

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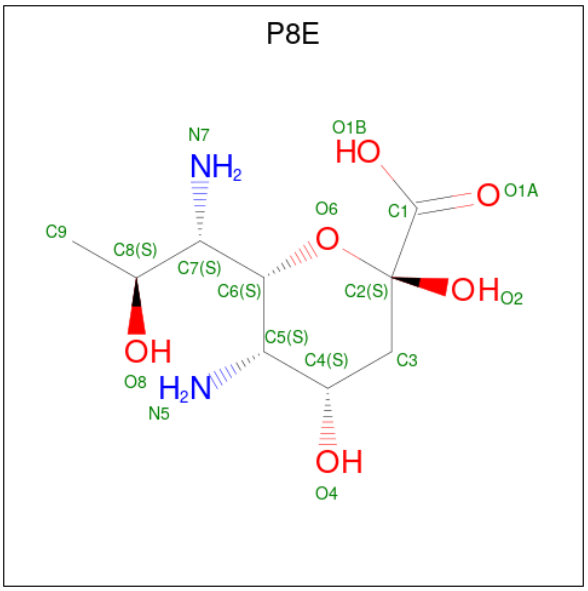
Mol	Chain	Residues	Atoms					AltConf	Trace
1	NI	508	Total 3713	C 2256	N 669	O 778	S 10	0	0
1	BJ	508	Total 3713	C 2256	N 669	O 778	S 10	0	0
1	fK	508	Total 3713	C 2256	N 669	O 778	S 10	0	0
1	HL	508	Total 3713	C 2256	N 669	O 778	S 10	0	0
1	XM	508	Total 3713	C 2256	N 669	O 778	S 10	0	0
1	DN	508	Total 3713	C 2256	N 669	O 778	S 10	0	0
1	MO	508	Total 3713	C 2256	N 669	O 778	S 10	0	0
1	TP	508	Total 3713	C 2256	N 669	O 778	S 10	0	0
1	GQ	508	Total 3713	C 2256	N 669	O 778	S 10	0	0
1	VR	508	Total 3713	C 2256	N 669	O 778	S 10	0	0
1	bS	508	Total 3713	C 2256	N 669	O 778	S 10	0	0
1	CT	508	Total 3713	C 2256	N 669	O 778	S 10	0	0
1	PU	508	Total 3713	C 2256	N 669	O 778	S 10	0	0
1	cV	508	Total 3713	C 2256	N 669	O 778	S 10	0	0
1	aW	508	Total 3713	C 2256	N 669	O 778	S 10	0	0
1	EX	508	Total 3713	C 2256	N 669	O 778	S 10	0	0

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



Mol	Chain	Residues	Atoms					AltConf
2	Y1	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Y1	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Y1	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Y1	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Y1	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Y1	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Y1	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Q2	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Q2	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Q2	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Q2	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Q2	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Q2	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	I3	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	I3	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	I3	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	I3	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	I3	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	I3	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	I3	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	R4	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	R4	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	R4	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	R4	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	R4	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	R4	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	R4	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	S5	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	S5	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	S5	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	S5	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	S5	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	S5	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	g6	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	g6	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	g6	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	g6	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	g6	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	g6	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	g6	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A7	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A7	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A7	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A7	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A7	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A7	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	A7	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	e8	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	e8	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	e8	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	e8	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	e8	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	e8	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	Z9	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Z9	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Z9	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Z9	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Z9	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Z9	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	Z9	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	OA	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	OA	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	OA	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	OA	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	OA	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	OA	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	OA	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	FB	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	FB	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	FB	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	FB	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	FB	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	FB	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	dC	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	dC	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	dC	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	dC	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	dC	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	dC	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	dC	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	JD	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	JD	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	JD	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	JD	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	JD	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	JD	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	JD	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	KE	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	KE	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	KE	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	KE	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	KE	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	KE	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	KE	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	LF	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	LF	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	LF	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	LF	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	LF	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	LF	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	LF	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	WG	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	WG	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	WG	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	WG	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	WG	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	WG	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	WG	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	UH	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	UH	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	UH	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	UH	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	UH	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	UH	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	UH	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	NI	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	NI	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	NI	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	NI	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	NI	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	NI	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	NI	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	BJ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	BJ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	BJ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	BJ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	BJ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	BJ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	BJ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	fK	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	fK	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	fK	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	fK	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	fK	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	fK	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	fK	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	HL	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	HL	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	HL	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	HL	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	HL	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	HL	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	HL	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	XM	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	XM	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	XM	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	XM	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	XM	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	XM	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	XM	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	DN	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	DN	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	DN	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	DN	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	DN	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	DN	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	MO	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	MO	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	MO	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	MO	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	MO	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	MO	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	MO	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	TP	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	TP	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	TP	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	TP	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	TP	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	TP	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	TP	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	GQ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	GQ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	GQ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	GQ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	GQ	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	GQ	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	VR	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	VR	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	VR	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	VR	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	VR	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	VR	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	VR	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	bS	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	bS	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	bS	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	bS	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	bS	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	bS	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	bS	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	CT	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	CT	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	CT	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	CT	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	CT	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	CT	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	CT	1	Total	C	H	N	O	0
			32	9	16	2	5	

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Mol	Chain	Residues	Atoms					AltConf
2	PU	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	PU	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	PU	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	PU	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	PU	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	PU	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	PU	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	cV	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	cV	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	cV	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	cV	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	cV	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	cV	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	cV	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	aW	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	aW	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	aW	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	aW	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	aW	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	aW	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	aW	1	Total	C	H	N	O	0
			32	9	16	2	5	

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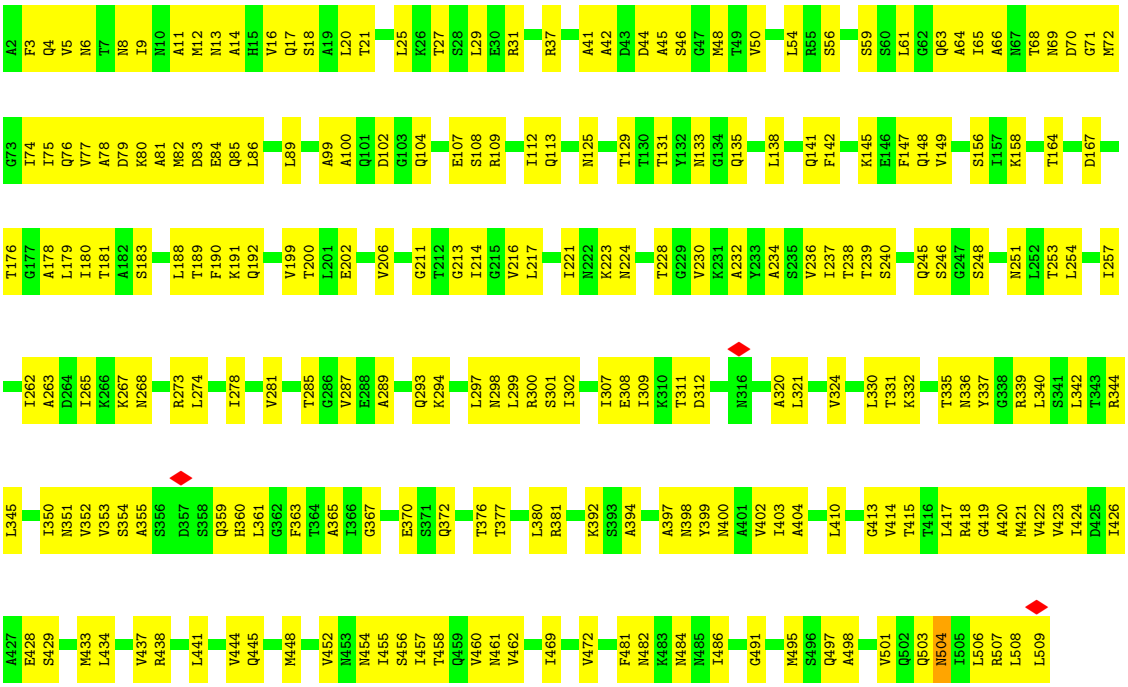
Mol	Chain	Residues	Atoms					AltConf
2	EX	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	EX	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	EX	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	EX	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	EX	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	EX	1	Total	C	H	N	O	0
			32	9	16	2	5	
2	EX	1	Total	C	H	N	O	0
			32	9	16	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.

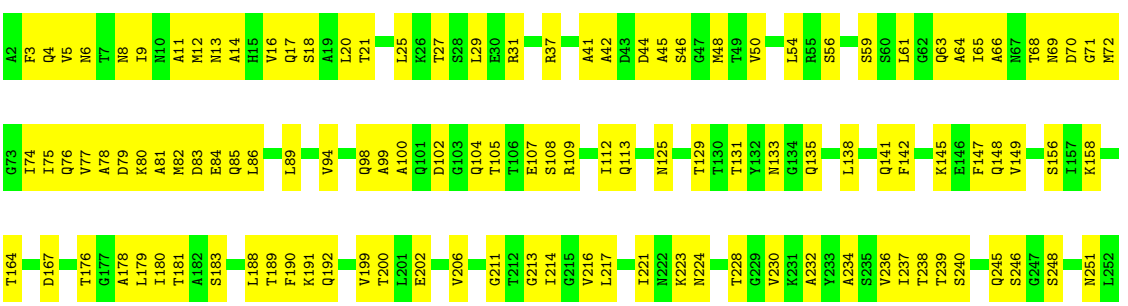
• Molecule 1: Flagellin

Chain Y1:



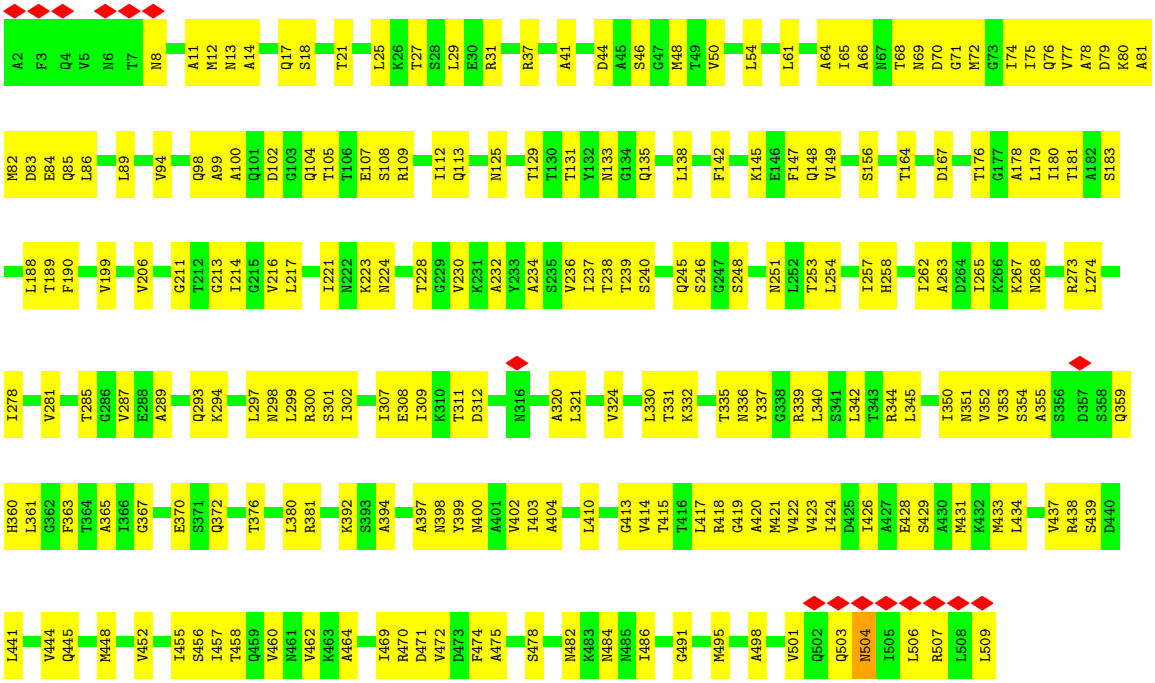
• Molecule 1: Flagellin

Chain Q2:



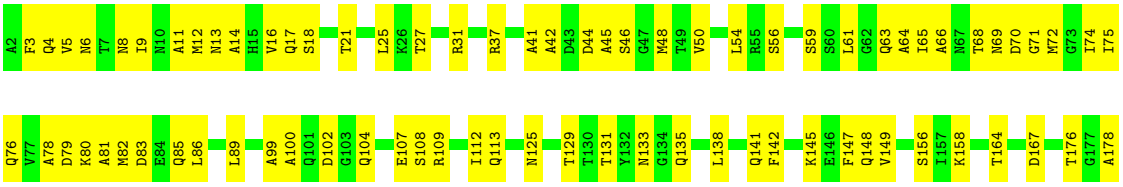
• Molecule 1: Flagellin

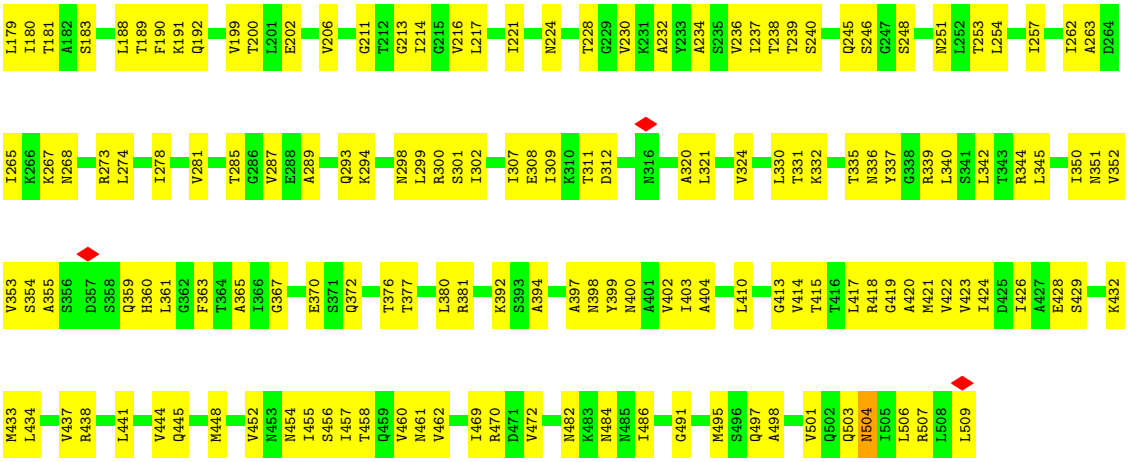
Chain I3:



• Molecule 1: Flagellin

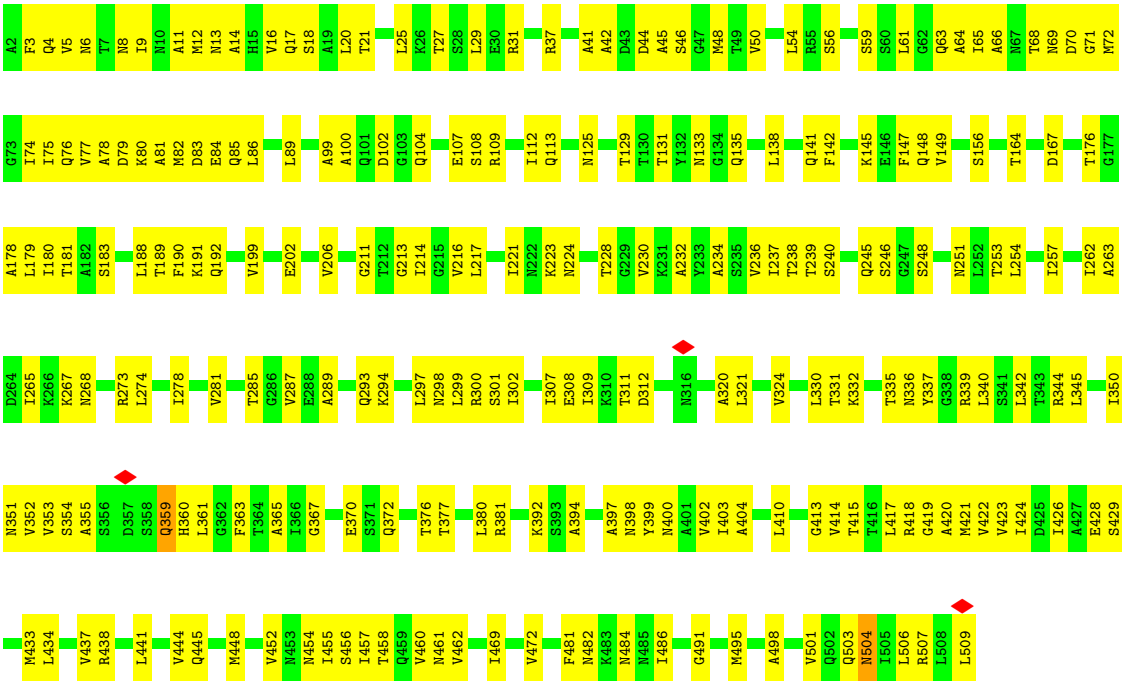
Chain R4:





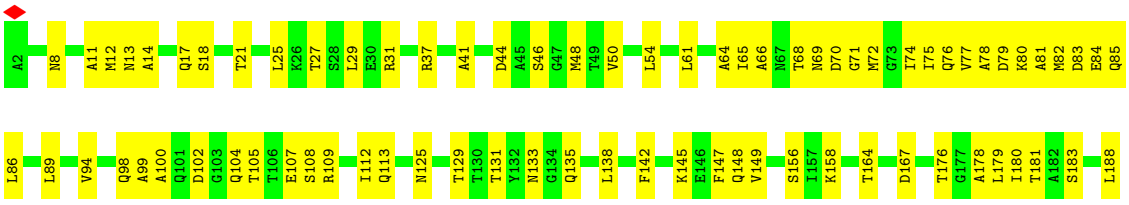
• Molecule 1: Flagellin

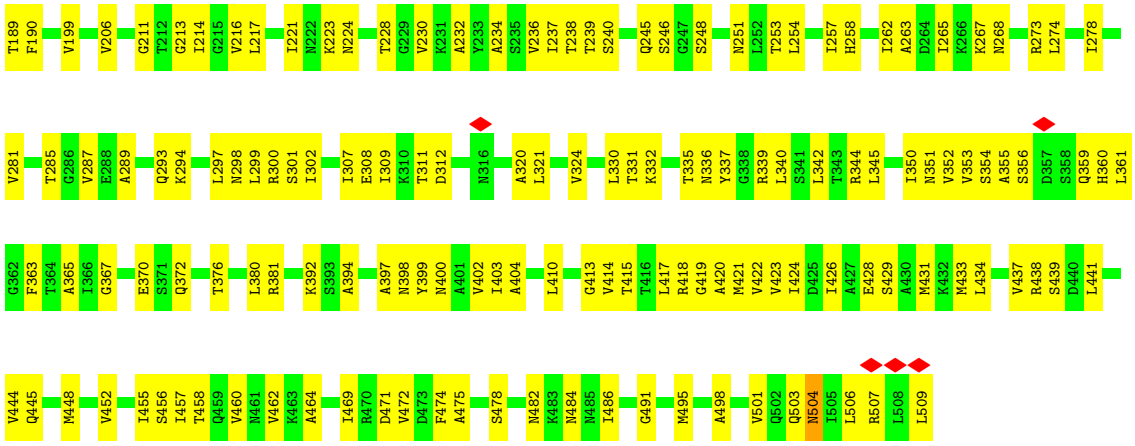
Chain S5:



• Molecule 1: Flagellin

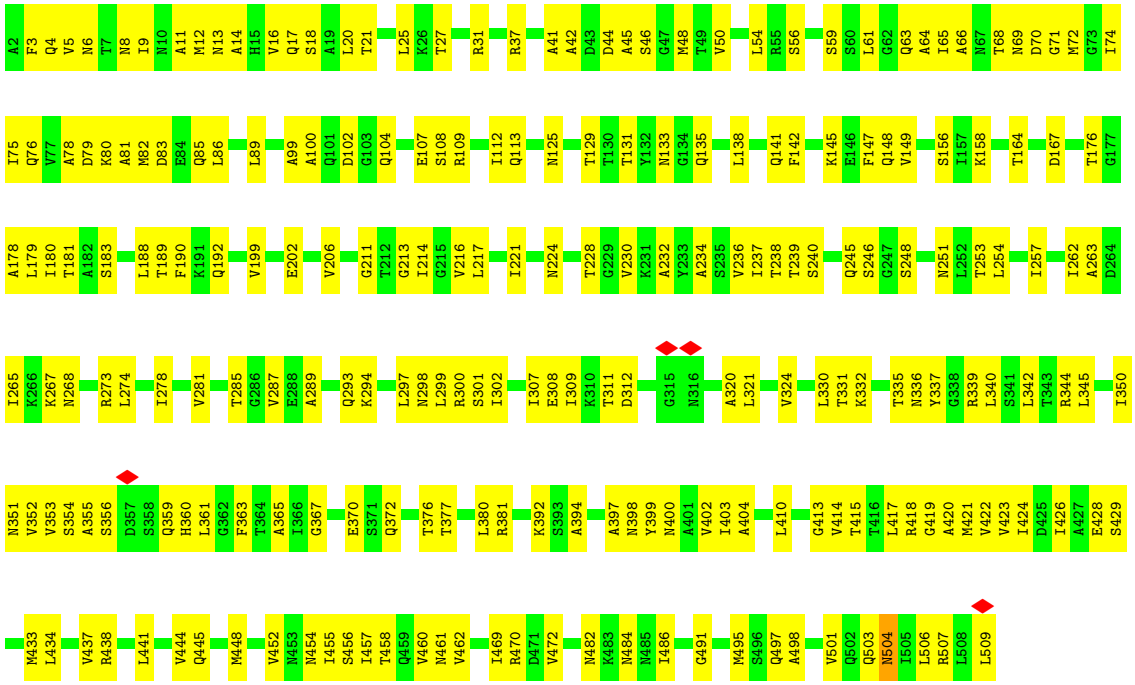
Chain g6:





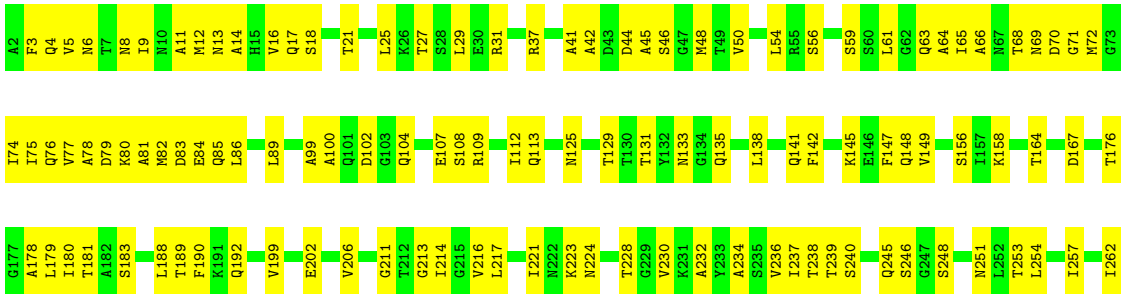
• Molecule 1: Flagellin

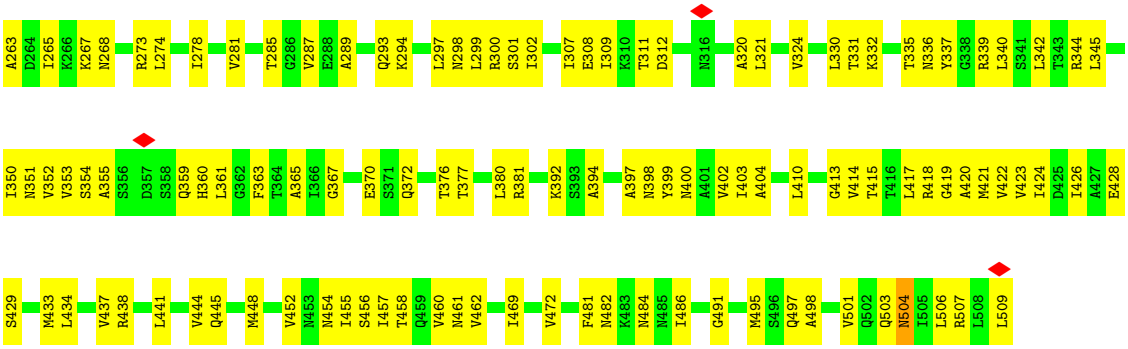
Chain A7:



• Molecule 1: Flagellin

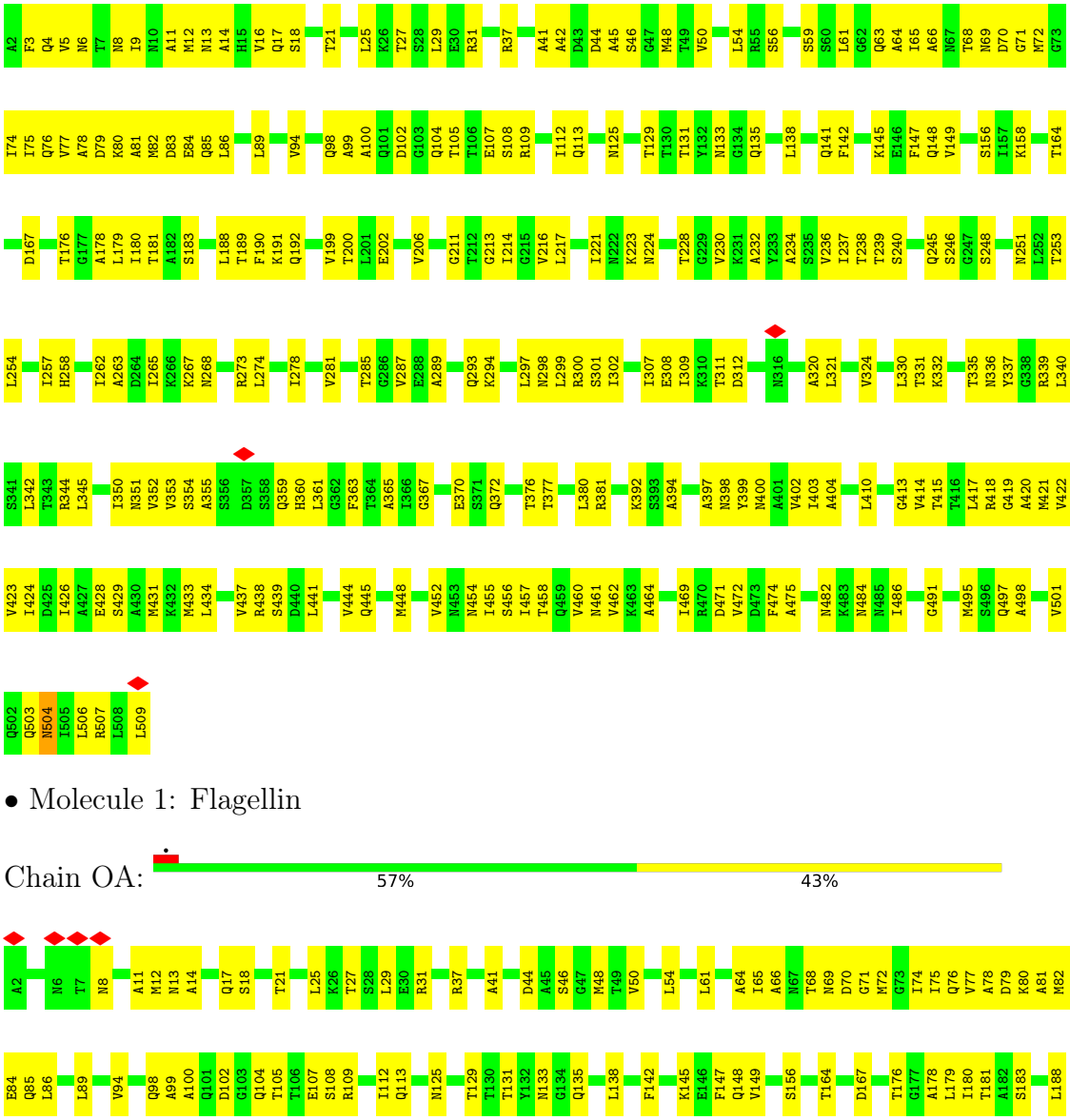
Chain e8:





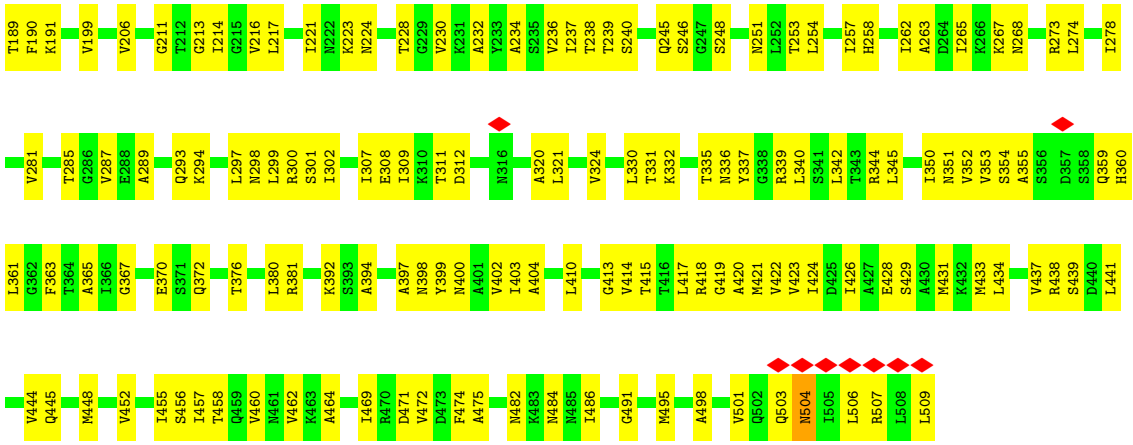
• Molecule 1: Flagellin

Chain Z9:



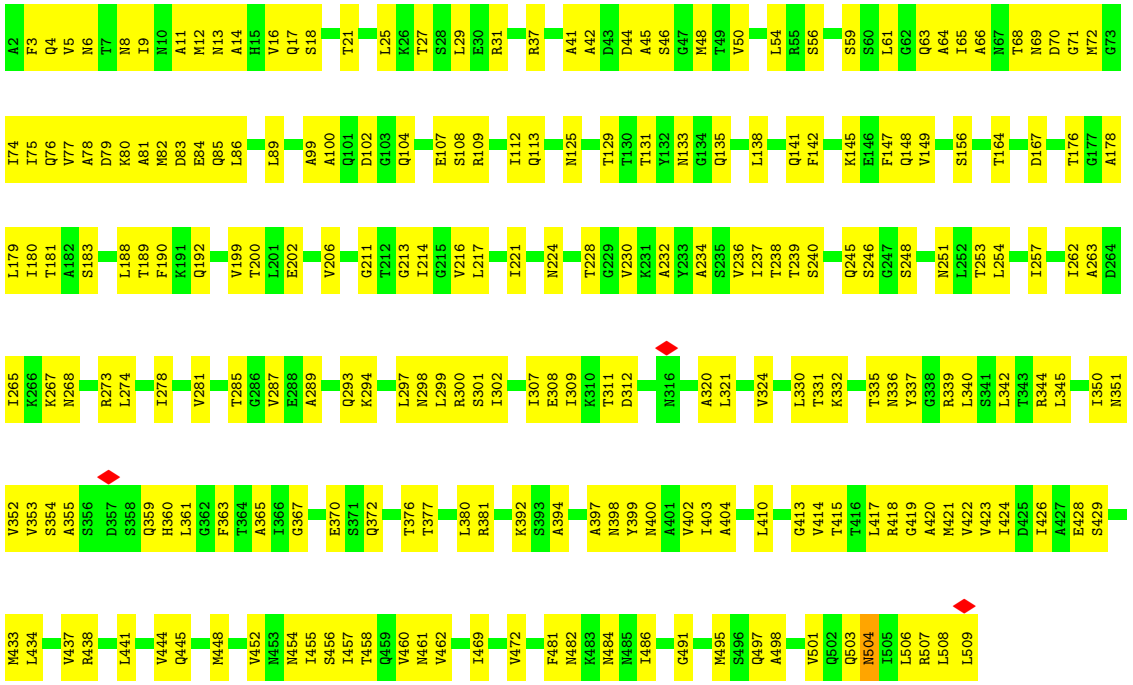
• Molecule 1: Flagellin

Chain OA:



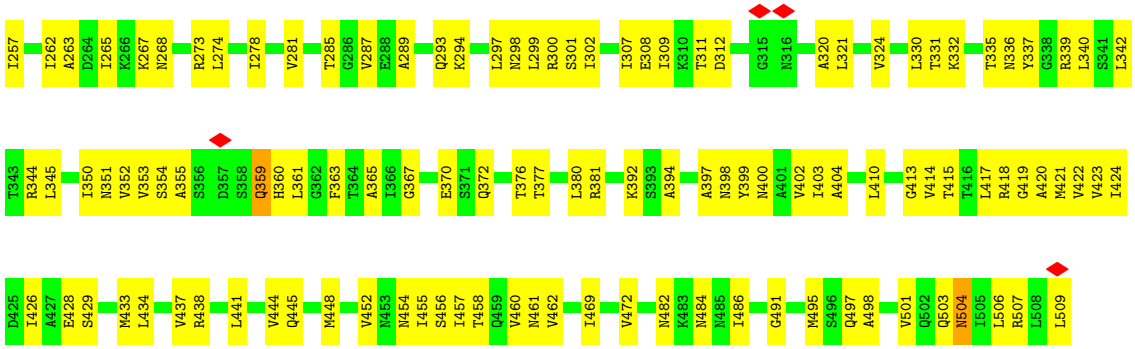
• Molecule 1: Flagellin

Chain FB:



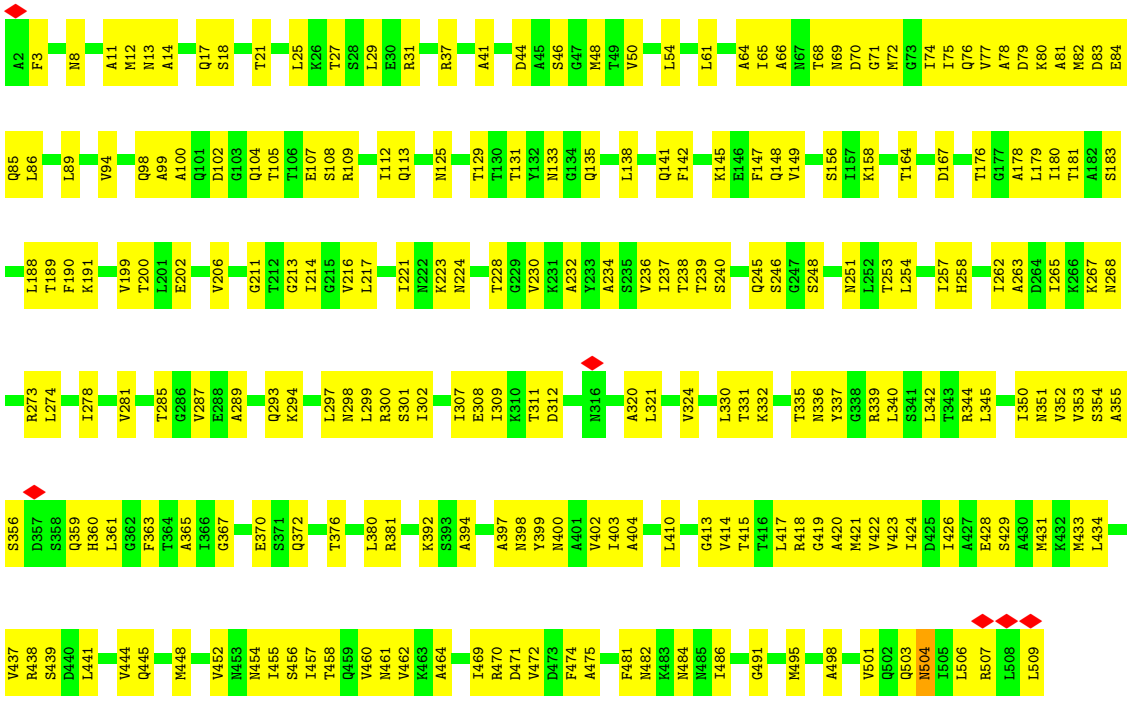
• Molecule 1: Flagellin

Chain dC:



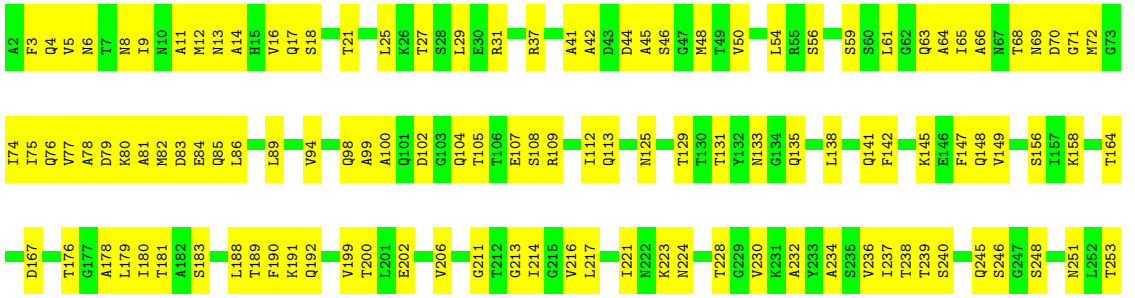
• Molecule 1: Flagellin

Chain JD:



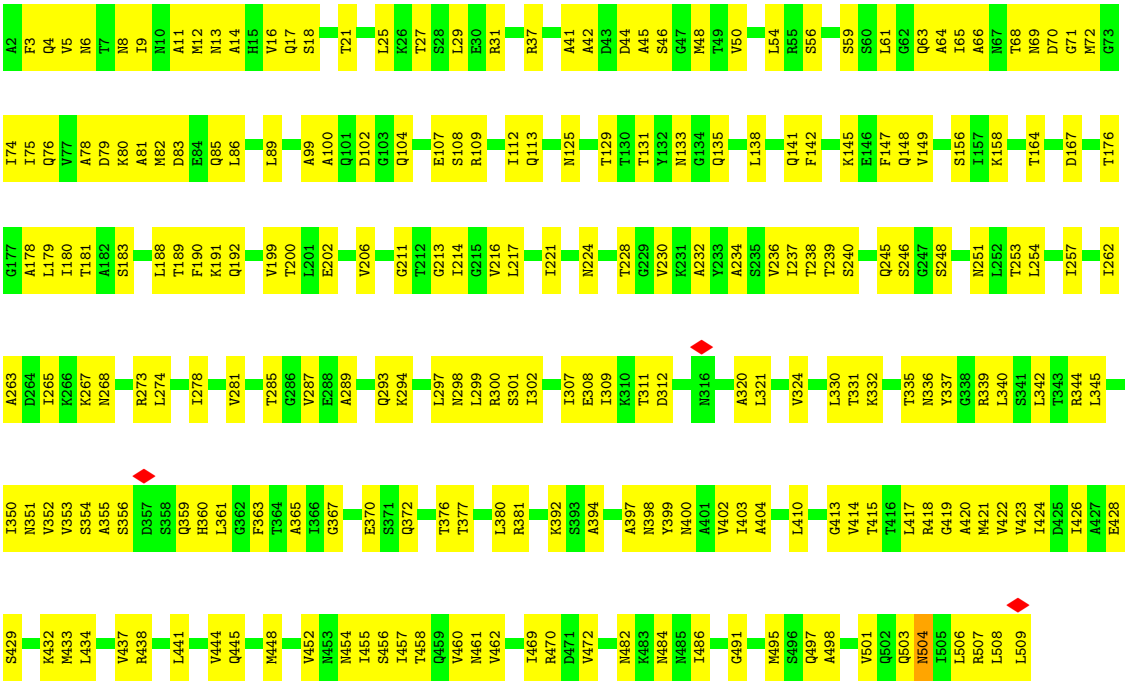
• Molecule 1: Flagellin

Chain KE:



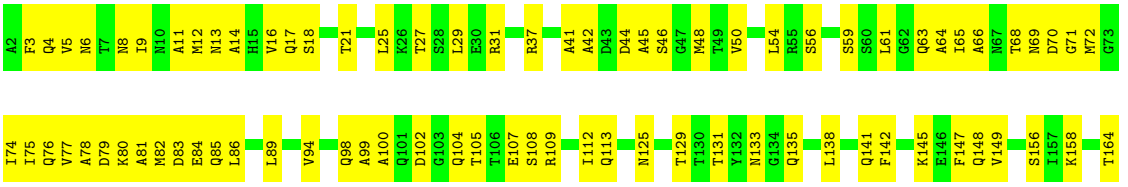
• Molecule 1: Flagellin

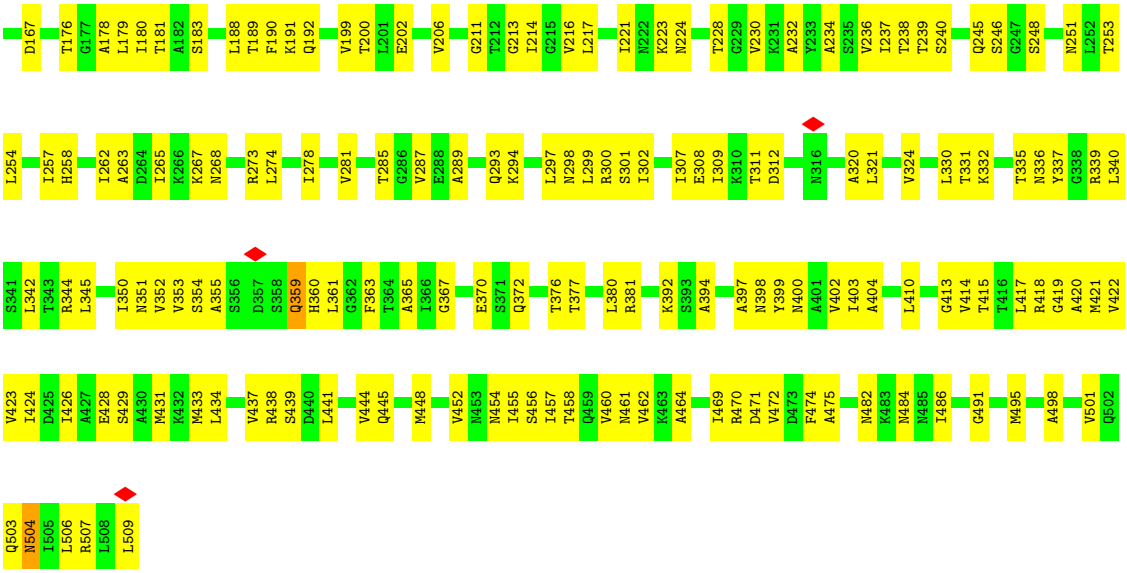
Chain LF:

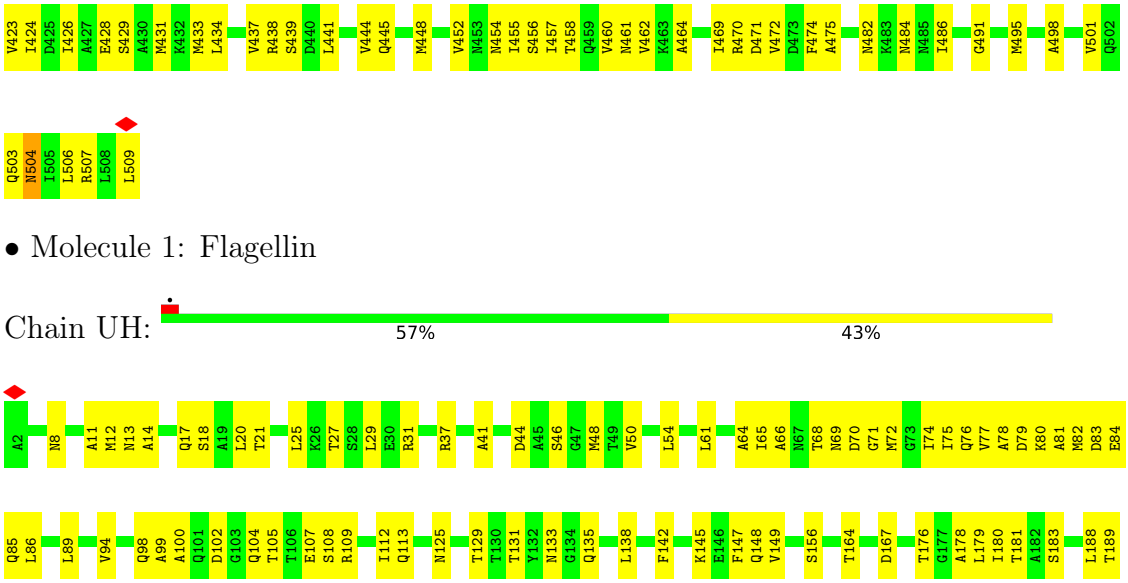


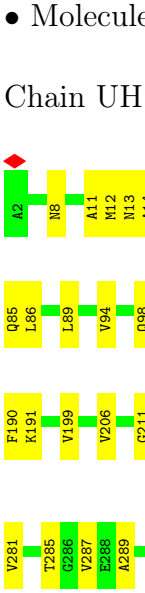
• Molecule 1: Flagellin

Chain WG:



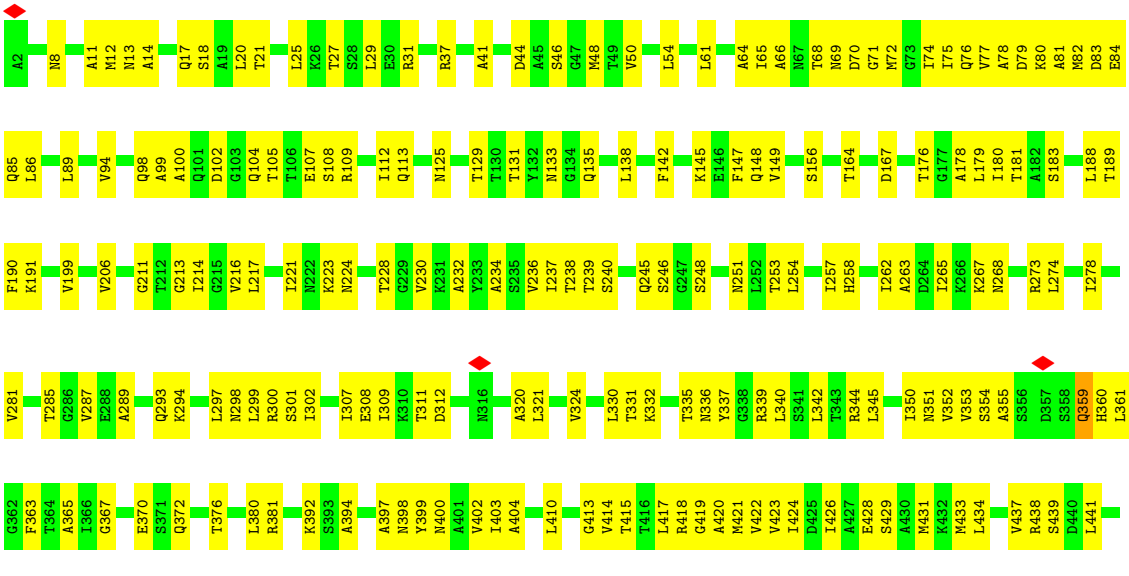


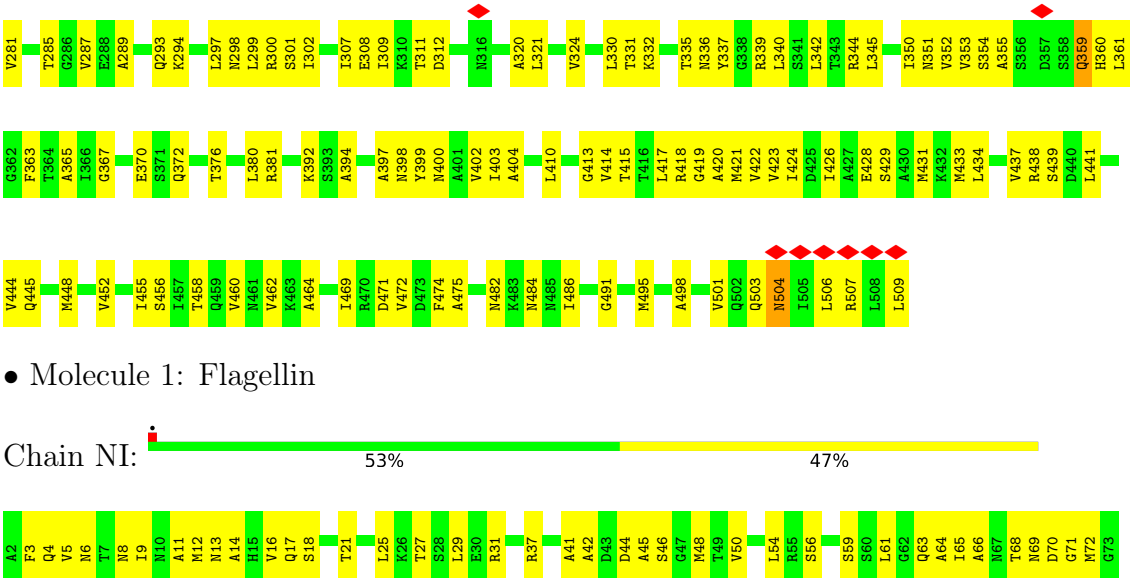


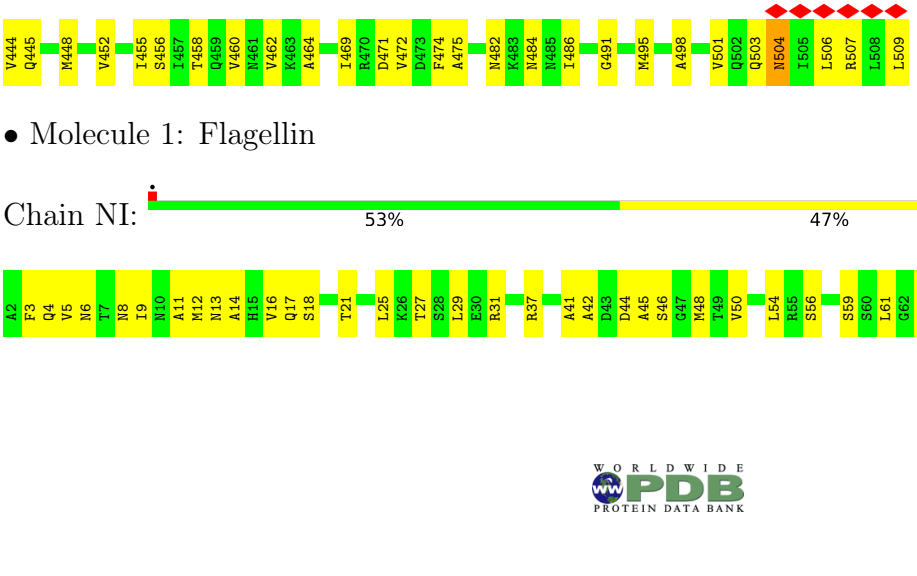


• Molecule 1: Flagellin

Chain UH:

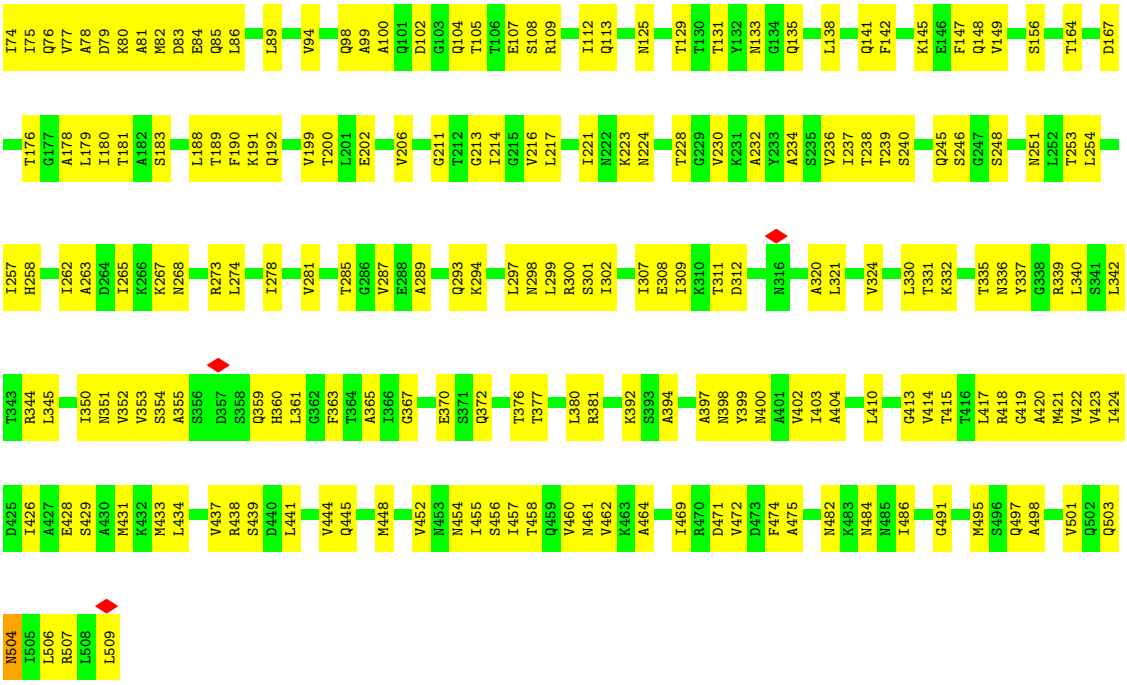






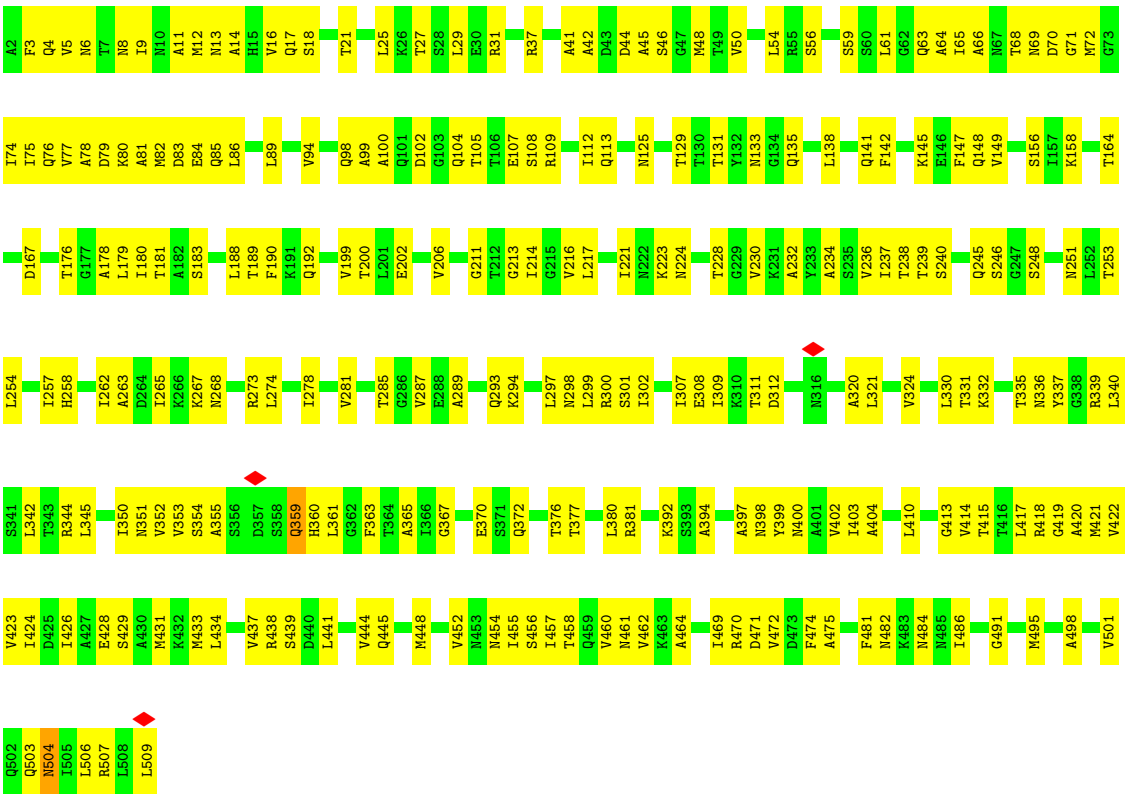
• Molecule 1: Flagellin

Chain NI:



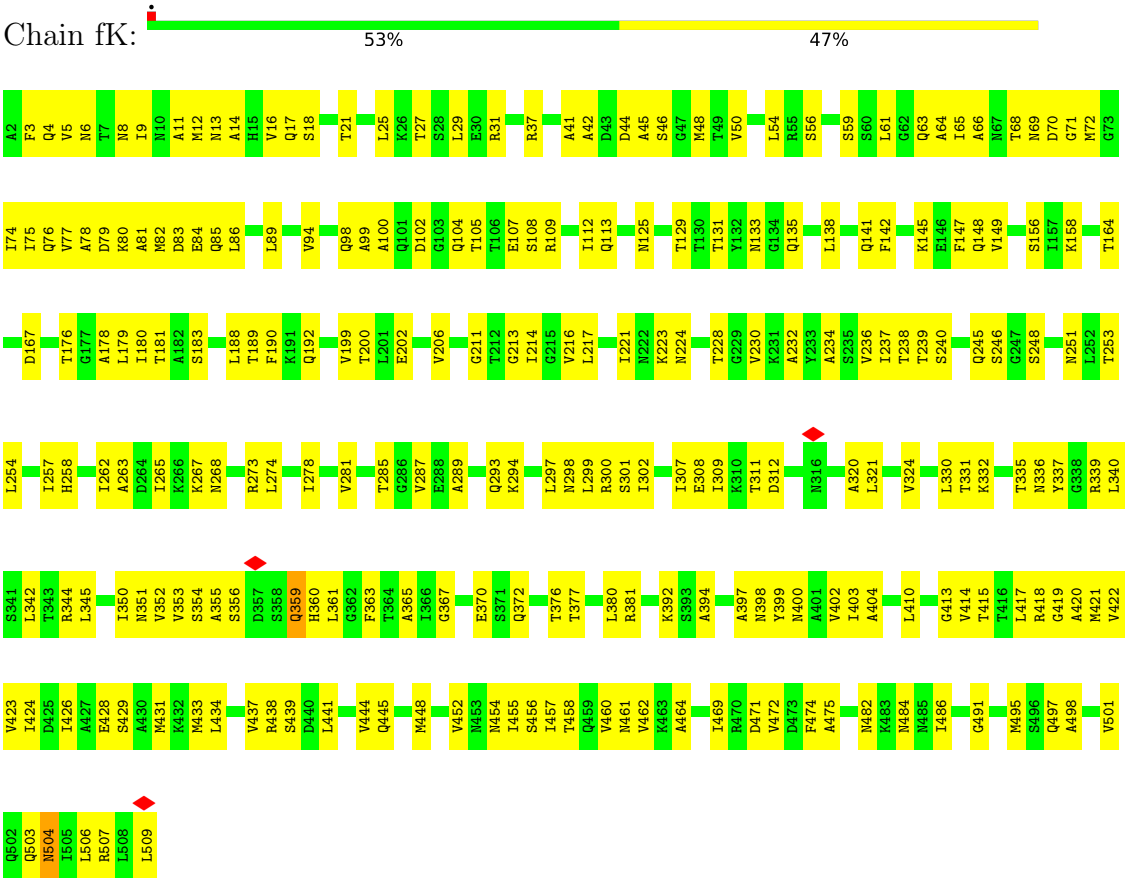
• Molecule 1: Flagellin

Chain BJ:



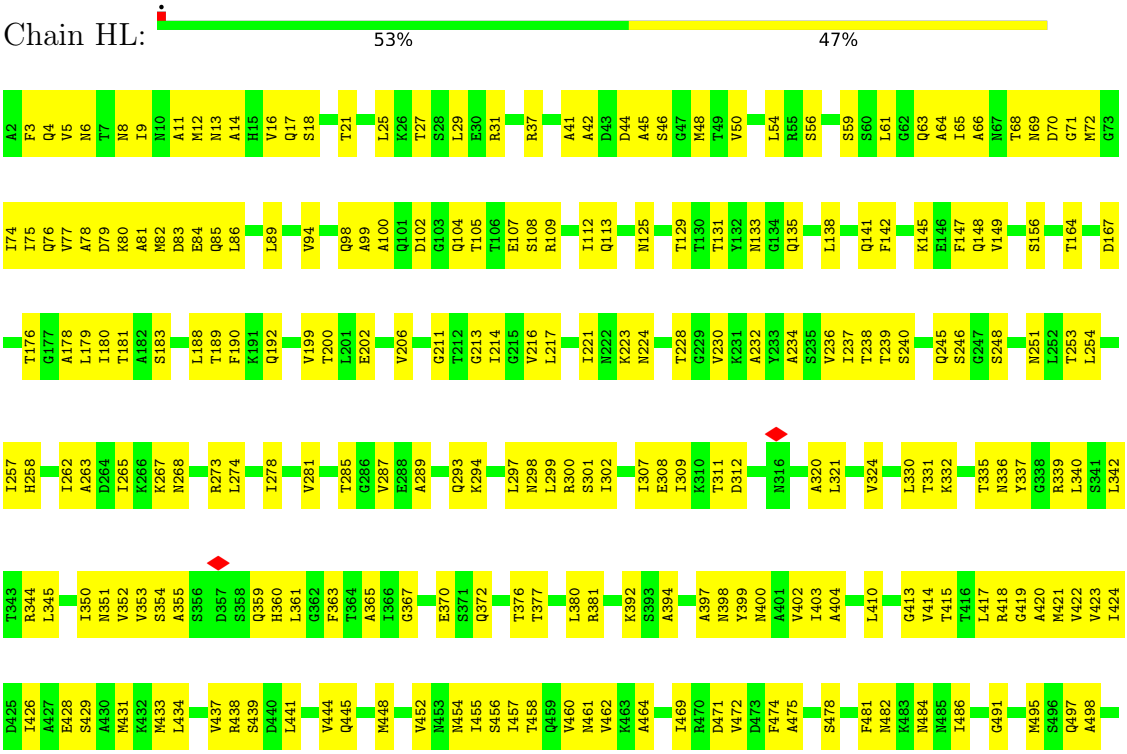
• Molecule 1: Flagellin

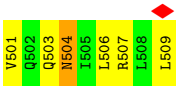
Chain fK:



• Molecule 1: Flagellin

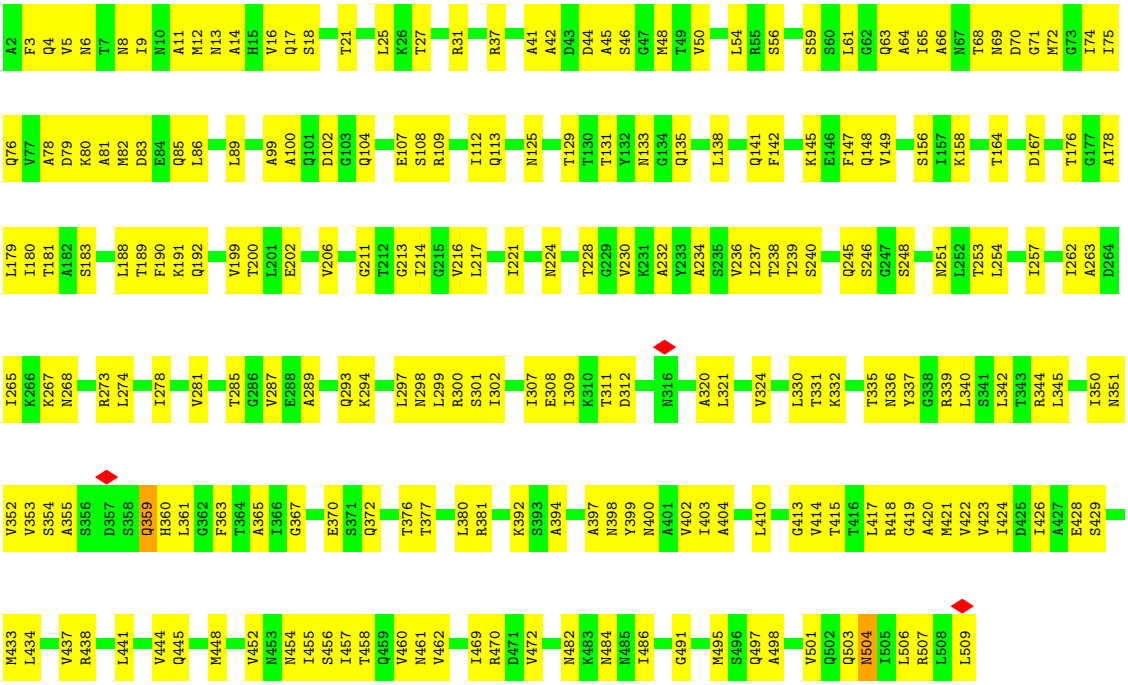
Chain HL:





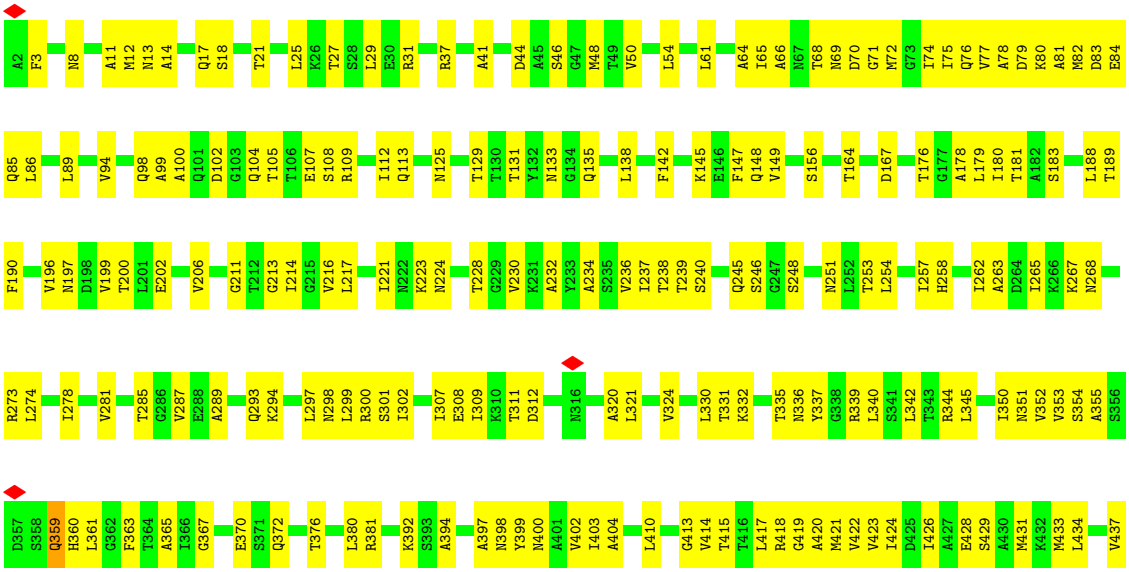
• Molecule 1: Flagellin

Chain XM:



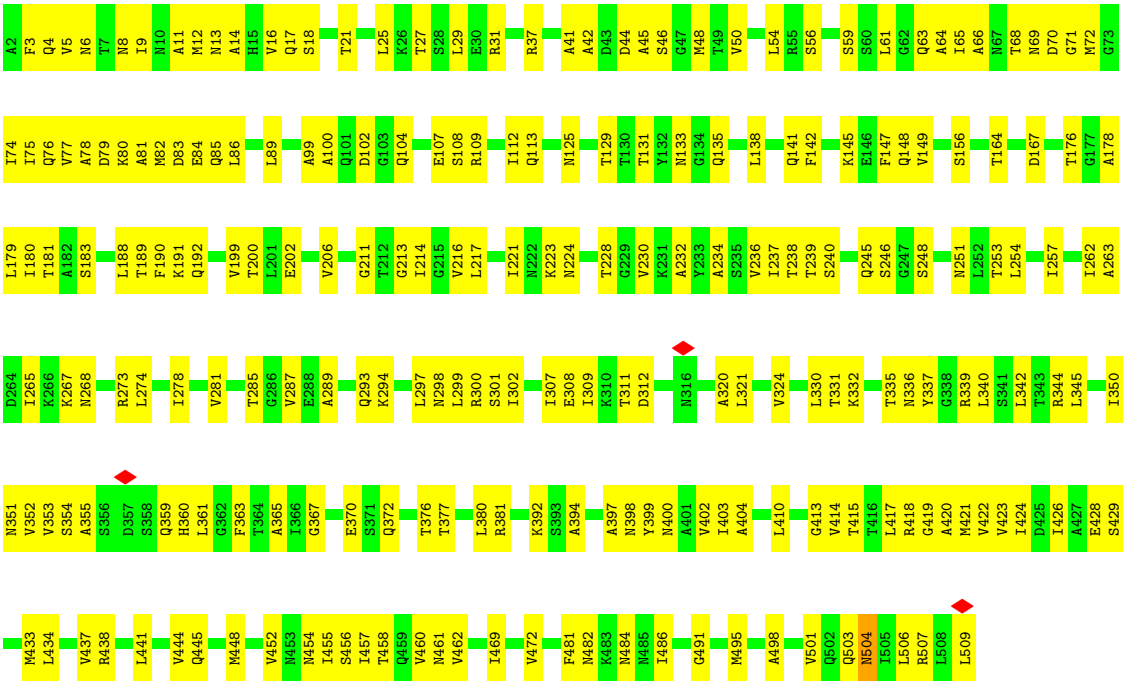
• Molecule 1: Flagellin

Chain DN:



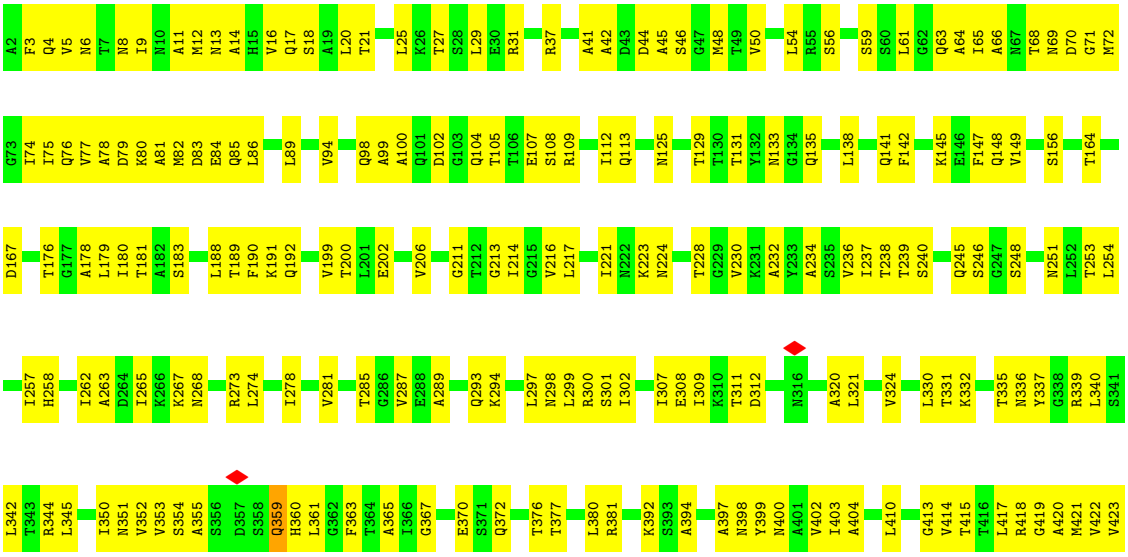
• Molecule 1: Flagellin

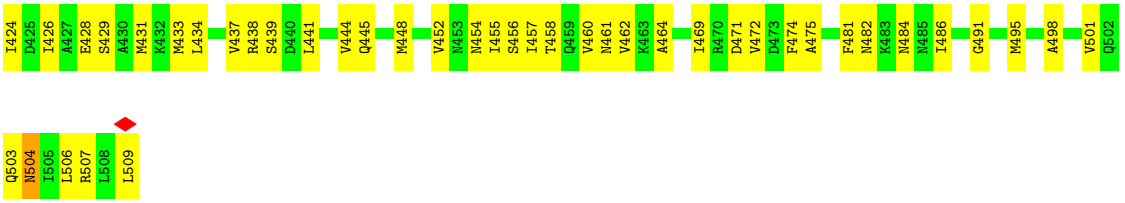
Chain MO:



• Molecule 1: Flagellin

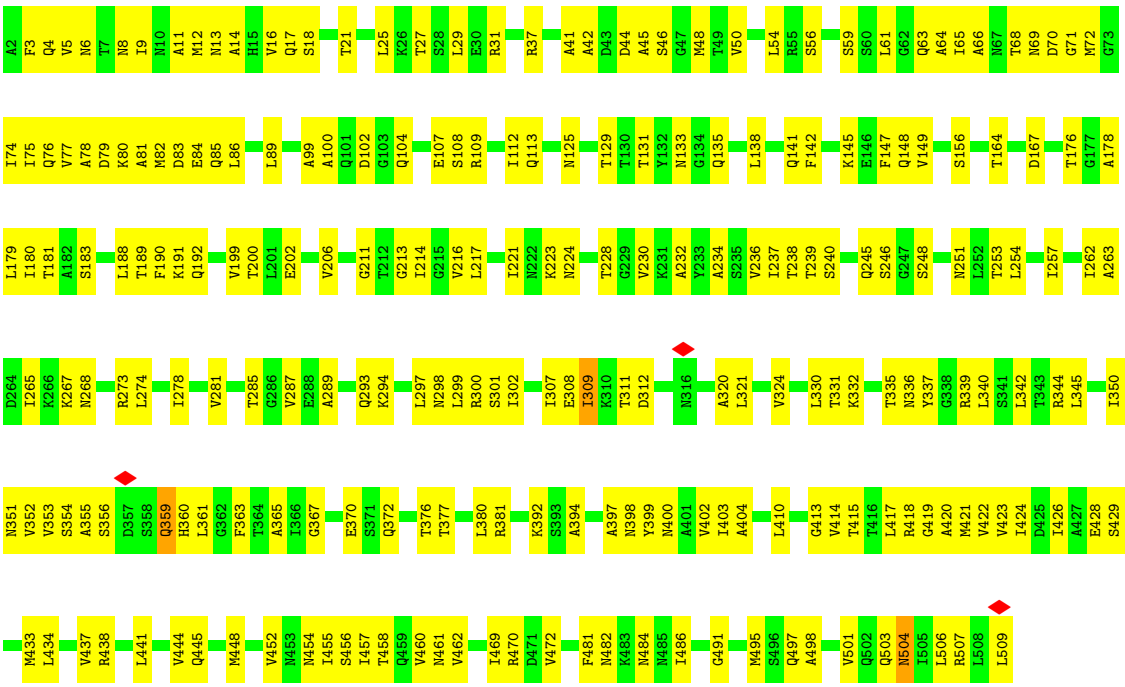
Chain TP:





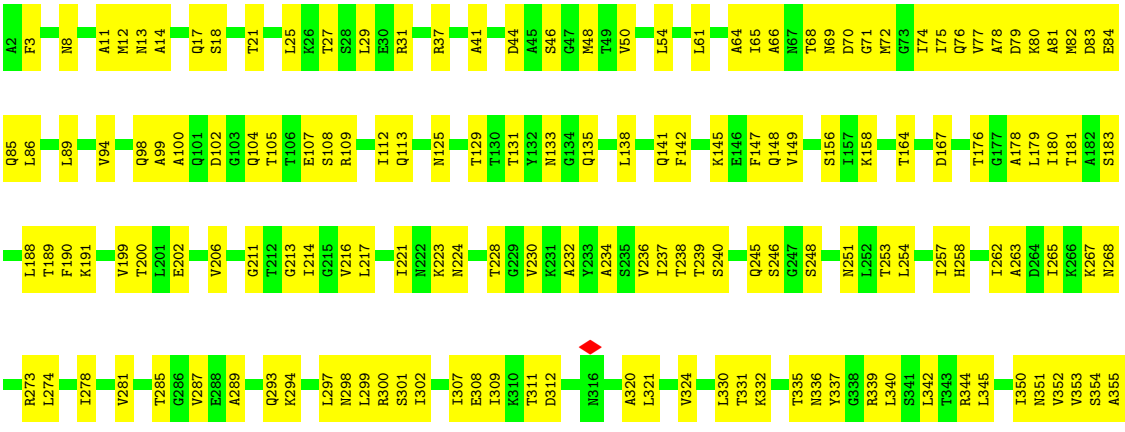
• Molecule 1: Flagellin

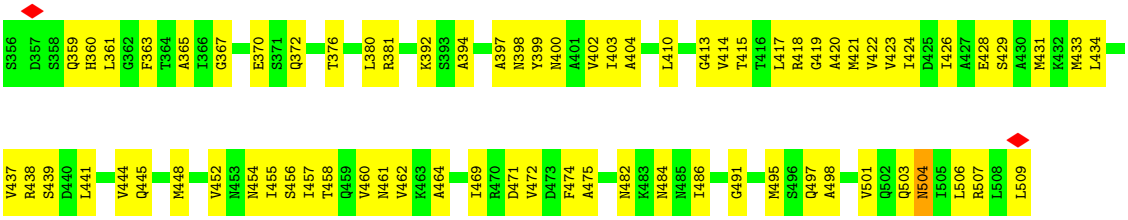
Chain GQ:



• Molecule 1: Flagellin

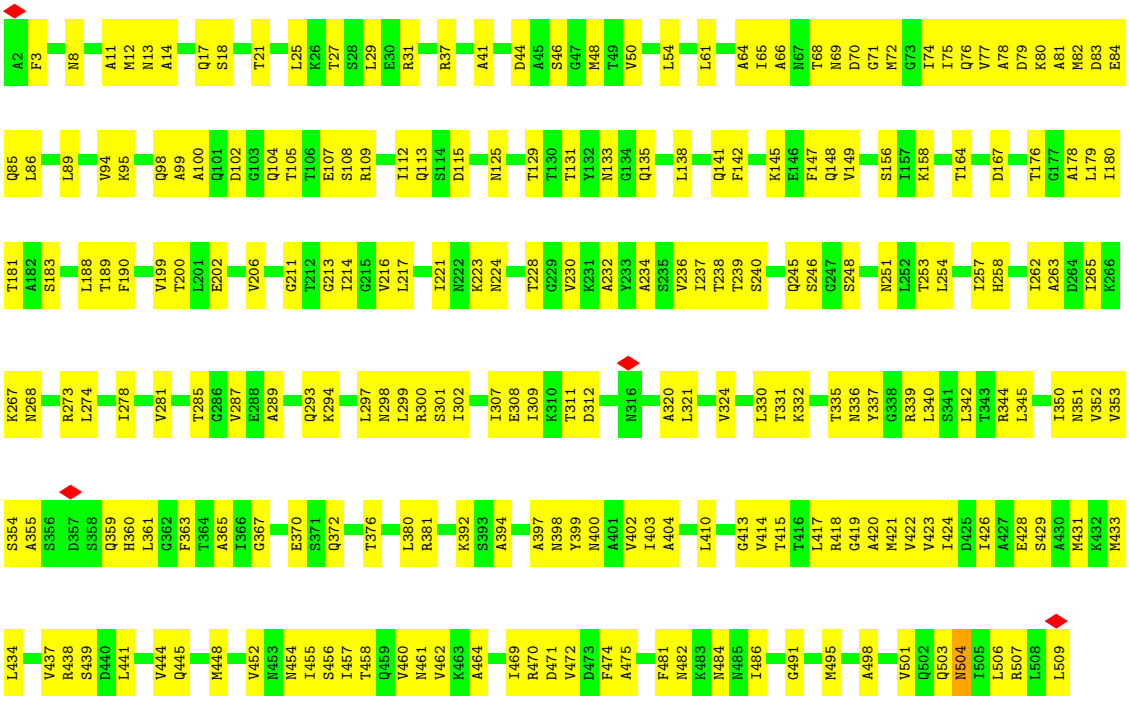
Chain VR:





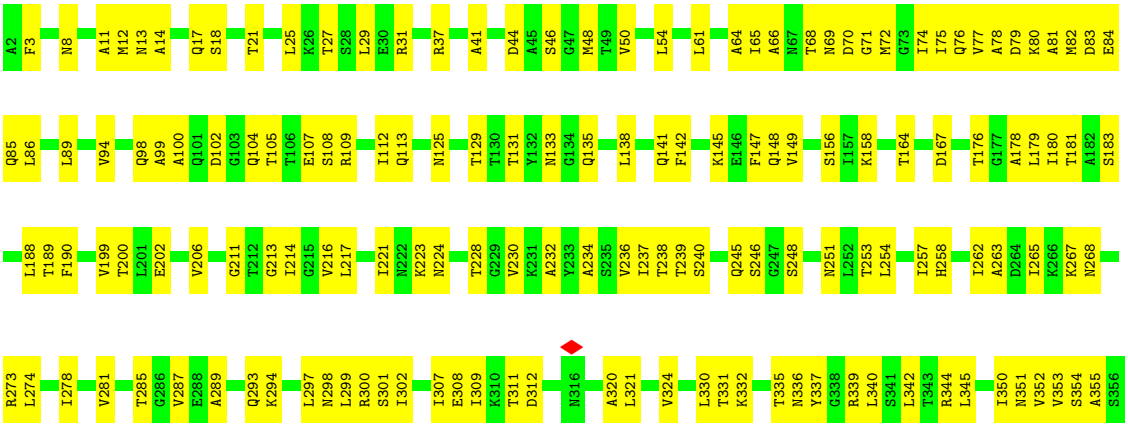
• Molecule 1: Flagellin

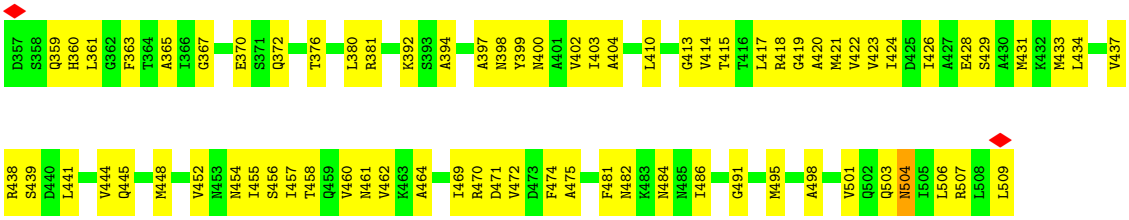
Chain bS:



• Molecule 1: Flagellin

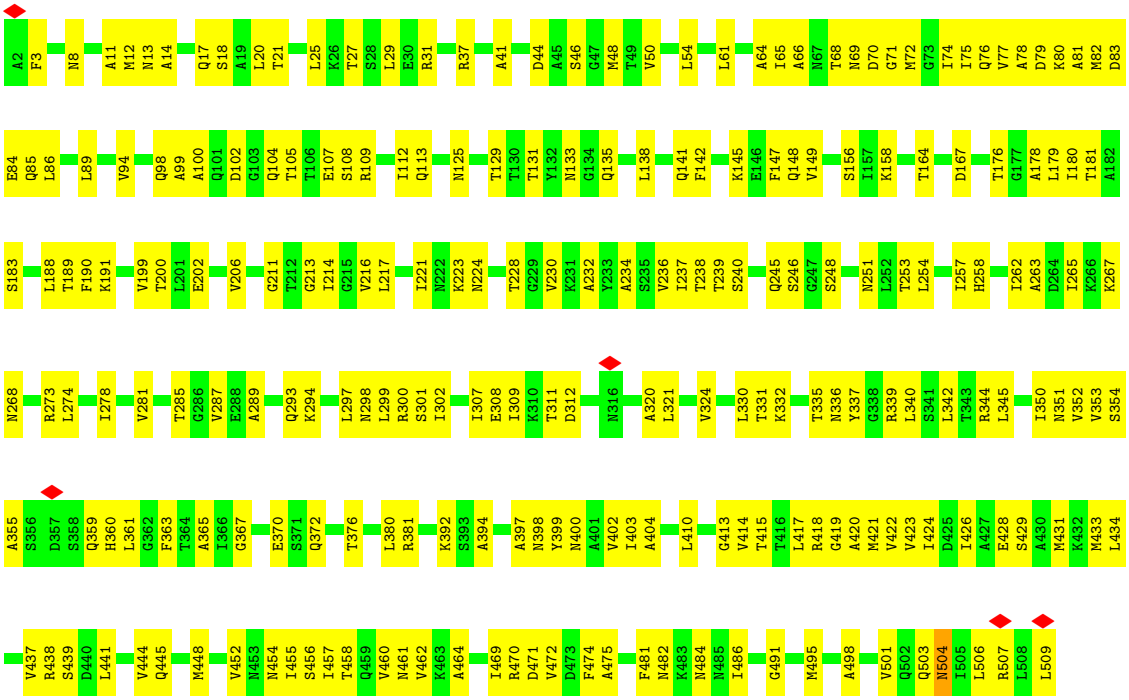
Chain CT:





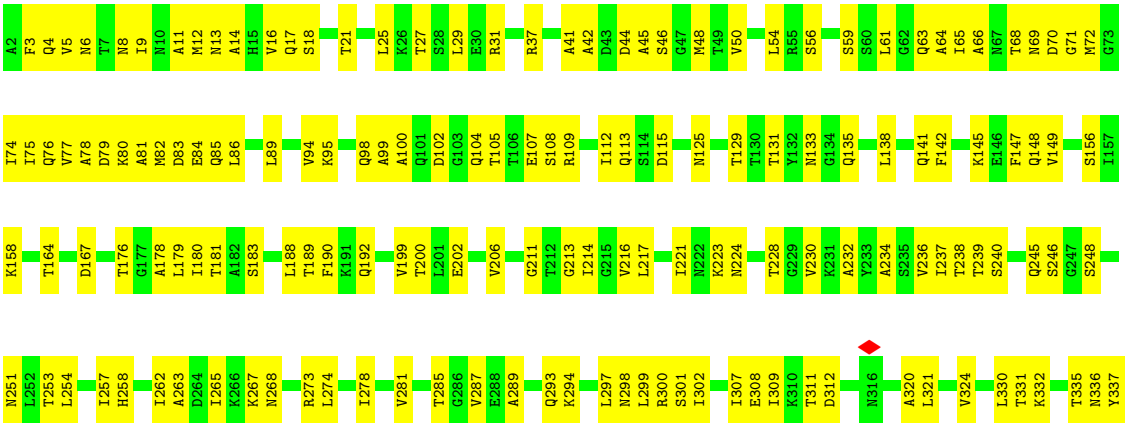
• Molecule 1: Flagellin

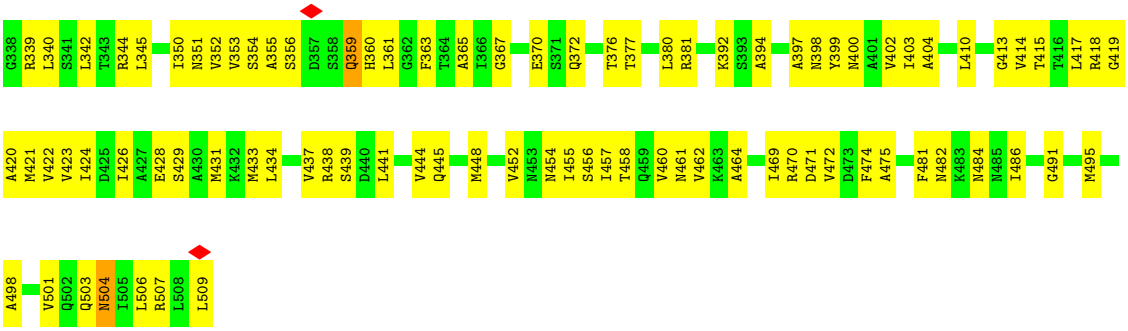
Chain PU:



• Molecule 1: Flagellin

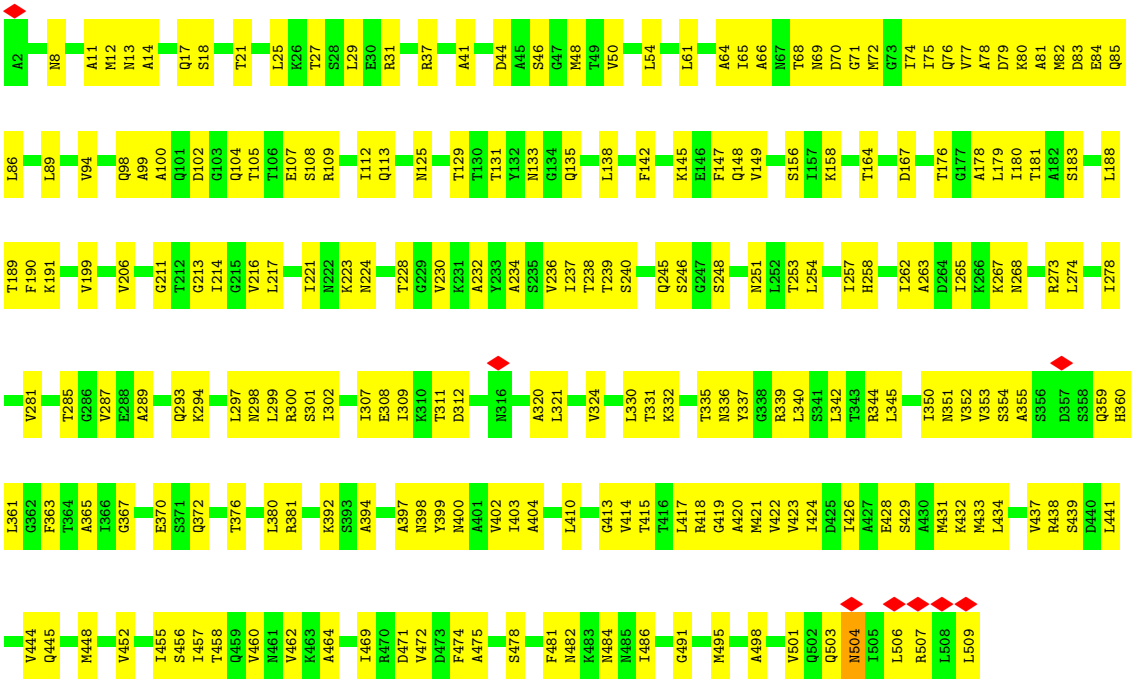
Chain cV:





• Molecule 1: Flagellin

Chain aW:



• Molecule 1: Flagellin

Chain EX:

T253 L254 I257 H258 I262 A263 D264 I265 K266 K267 N268 R273 L274 I278 V281 T285 G286 V287 E288 A289 Q293 K294 L297 N298 L299 R300 S301 I302 I307 E308 I309 K310 T311 D312 N316 A320 L321 V324 L330 T331 K332 T335 N336 Y337 G338 R339
L340 S341 L342 T343 R344 L345 I350 N351 V352 V353 S354 A355 S356 D357 S358 Q359 H360 L361 G362 F363 T364 A365 I366 G367 E370 S371 Q372 T376 T377 L380 R381 K392 S393 A394 A397 N398 Y399 N400 A401 V402 I403 A404 L410 G413 V414 T415 T416 L417 R418 G419 A420 M421
V422 V423 I424 D425 I426 A427 E428 S429 A430 M431 K432 M433 L434 V437 R438 S439 D440 L441 V444 Q445 M448 V452 N453 N454 I455 S456 I457 T458 Q459 V460 N461 V462 K463 A464 I469 R470 D471 V472 D473 F474 A475 N482 K483 N484 N485 I486 G491 M495 S496 Q497 A498
V501 Q502 Q503 N504 I505 L506 R507 L508 L509

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	228410	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.777	Depositor
Minimum map value	-0.363	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.111	Depositor
Map size (Å)	427.19998, 427.19998, 427.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	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	A7	0.08	0/3732	0.21	0/5046
1	BJ	0.08	0/3732	0.21	0/5046
1	CT	0.08	0/3732	0.21	0/5046
1	DN	0.08	0/3732	0.21	0/5046
1	EX	0.08	0/3732	0.21	0/5046
1	FB	0.08	0/3732	0.21	0/5046
1	GQ	0.08	0/3732	0.21	0/5046
1	HL	0.08	0/3732	0.21	0/5046
1	I3	0.08	0/3732	0.21	0/5046
1	JD	0.08	0/3732	0.21	0/5046
1	KE	0.08	0/3732	0.21	0/5046
1	LF	0.08	0/3732	0.21	0/5046
1	MO	0.08	0/3732	0.21	0/5046
1	NI	0.08	0/3732	0.21	0/5046
1	OA	0.08	0/3732	0.21	0/5046
1	PU	0.08	0/3732	0.21	0/5046
1	Q2	0.08	0/3732	0.21	0/5046
1	R4	0.08	0/3732	0.21	0/5046
1	S5	0.08	0/3732	0.21	0/5046
1	TP	0.08	0/3732	0.21	0/5046
1	UH	0.08	0/3732	0.21	0/5046
1	VR	0.08	0/3732	0.21	0/5046
1	WG	0.08	0/3732	0.21	0/5046
1	XM	0.08	0/3732	0.21	0/5046
1	Y1	0.08	0/3732	0.21	0/5046
1	Z9	0.08	0/3732	0.21	0/5046
1	aW	0.08	0/3732	0.21	0/5046
1	bS	0.08	0/3732	0.21	0/5046
1	cV	0.08	0/3732	0.21	0/5046
1	dC	0.08	0/3732	0.21	0/5046
1	e8	0.08	0/3732	0.21	0/5046
1	fK	0.08	0/3732	0.21	0/5046

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	g6	0.08	0/3732	0.21	0/5046
All	All	0.08	0/123156	0.21	0/166518

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A7	3713	0	3729	251	0
1	BJ	3713	0	3729	292	0
1	CT	3713	0	3729	268	0
1	DN	3713	0	3729	260	0
1	EX	3713	0	3729	288	0
1	FB	3713	0	3729	260	0
1	GQ	3713	0	3729	266	0
1	HL	3713	0	3729	288	0
1	I3	3713	0	3729	245	0
1	JD	3713	0	3729	263	0
1	KE	3713	0	3729	288	0
1	LF	3713	0	3729	249	0
1	MO	3713	0	3729	266	0
1	NI	3713	0	3729	285	0
1	OA	3713	0	3729	245	0
1	PU	3713	0	3729	267	0
1	Q2	3713	0	3729	289	0
1	R4	3713	0	3729	250	0
1	S5	3713	0	3729	262	0
1	TP	3713	0	3729	284	0
1	UH	3713	0	3729	243	0
1	VR	3713	0	3729	264	0
1	WG	3713	0	3729	285	0
1	XM	3713	0	3729	251	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y1	3713	0	3729	268	0
1	Z9	3713	0	3729	289	0
1	aW	3713	0	3729	252	0
1	bS	3713	0	3729	270	0
1	cV	3713	0	3729	289	0
1	dC	3713	0	3729	247	0
1	e8	3713	0	3729	266	0
1	fK	3713	0	3729	292	0
1	g6	3713	0	3729	252	0
2	A7	112	112	0	0	0
2	BJ	112	112	0	0	0
2	CT	112	112	0	0	0
2	DN	112	112	0	0	0
2	EX	112	112	0	0	0
2	FB	112	112	0	0	0
2	GQ	112	112	0	0	0
2	HL	112	112	0	0	0
2	I3	112	112	0	0	0
2	JD	112	112	0	0	0
2	KE	112	112	0	0	0
2	LF	112	112	0	0	0
2	MO	112	112	0	0	0
2	NI	112	112	0	0	0
2	OA	112	112	0	0	0
2	PU	112	112	0	0	0
2	Q2	112	112	0	0	0
2	R4	112	112	0	0	0
2	S5	112	112	0	0	0
2	TP	112	112	0	0	0
2	UH	112	112	0	0	0
2	VR	112	112	0	0	0
2	WG	112	112	0	0	0
2	XM	112	112	0	0	0
2	Y1	112	112	0	0	0
2	Z9	112	112	0	0	0
2	aW	112	112	0	0	0
2	bS	112	112	0	0	0
2	cV	112	112	0	0	0
2	dC	112	112	0	0	0
2	e8	112	112	0	0	0
2	fK	112	112	0	0	0
2	g6	112	112	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	126225	3696	123057	7830	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 31.

The worst 5 of 7830 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:S5:82:MET:HE1	1:S5:441:LEU:HD12	1.29	1.15
1:UH:82:MET:HE1	1:UH:441:LEU:HD12	1.29	1.15
1:TP:82:MET:HE1	1:TP:441:LEU:HD12	1.29	1.15
1:aW:82:MET:HE1	1:aW:441:LEU:HD12	1.29	1.14
1:Y1:82:MET:HE1	1:Y1:441:LEU:HD12	1.29	1.14

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	A7	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	BJ	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	CT	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	DN	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	EX	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	FB	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	GQ	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	HL	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	I3	506/508 (100%)	492 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	JD	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	KE	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	LF	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	MO	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	NI	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	OA	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	PU	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	Q2	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	R4	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	S5	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	TP	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	UH	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	VR	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	WG	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	XM	506/508 (100%)	493 (97%)	13 (3%)	0	100	100
1	Y1	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	Z9	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	aW	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	bS	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	cV	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	dC	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	e8	506/508 (100%)	493 (97%)	13 (3%)	0	100	100
1	fK	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
1	g6	506/508 (100%)	492 (97%)	14 (3%)	0	100	100
All	All	16698/16764 (100%)	16238 (97%)	460 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A7	409/409 (100%)	406 (99%)	3 (1%)	76	90
1	BJ	409/409 (100%)	406 (99%)	3 (1%)	76	90
1	CT	409/409 (100%)	407 (100%)	2 (0%)	81	93
1	DN	409/409 (100%)	406 (99%)	3 (1%)	76	90
1	EX	409/409 (100%)	407 (100%)	2 (0%)	81	93
1	FB	409/409 (100%)	407 (100%)	2 (0%)	81	93
1	GQ	409/409 (100%)	404 (99%)	5 (1%)	63	84
1	HL	409/409 (100%)	407 (100%)	2 (0%)	81	93
1	I3	409/409 (100%)	407 (100%)	2 (0%)	81	93
1	JD	409/409 (100%)	406 (99%)	3 (1%)	76	90
1	KE	409/409 (100%)	407 (100%)	2 (0%)	81	93
1	LF	409/409 (100%)	406 (99%)	3 (1%)	76	90
1	MO	409/409 (100%)	407 (100%)	2 (0%)	81	93
1	NI	409/409 (100%)	407 (100%)	2 (0%)	81	93
1	OA	409/409 (100%)	407 (100%)	2 (0%)	81	93
1	PU	409/409 (100%)	407 (100%)	2 (0%)	81	93
1	Q2	409/409 (100%)	407 (100%)	2 (0%)	81	93
1	R4	409/409 (100%)	407 (100%)	2 (0%)	81	93
1	S5	409/409 (100%)	406 (99%)	3 (1%)	76	90
1	TP	409/409 (100%)	406 (99%)	3 (1%)	76	90
1	UH	409/409 (100%)	406 (99%)	3 (1%)	76	90
1	VR	409/409 (100%)	407 (100%)	2 (0%)	81	93
1	WG	409/409 (100%)	406 (99%)	3 (1%)	76	90
1	XM	409/409 (100%)	406 (99%)	3 (1%)	76	90
1	Y1	409/409 (100%)	407 (100%)	2 (0%)	81	93
1	Z9	409/409 (100%)	407 (100%)	2 (0%)	81	93
1	aW	409/409 (100%)	407 (100%)	2 (0%)	81	93
1	bS	409/409 (100%)	407 (100%)	2 (0%)	81	93
1	cV	409/409 (100%)	405 (99%)	4 (1%)	68	87
1	dC	409/409 (100%)	406 (99%)	3 (1%)	76	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	e8	409/409 (100%)	407 (100%)	2 (0%)	81 93
1	fK	409/409 (100%)	405 (99%)	4 (1%)	68 87
1	g6	409/409 (100%)	406 (99%)	3 (1%)	76 90
All	All	13497/13497 (100%)	13412 (99%)	85 (1%)	76 92

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DN	359	GLN
1	bS	302	ILE
1	MO	302	ILE
1	GQ	309	ILE
1	PU	302	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 230 such sidechains are listed below:

Mol	Chain	Res	Type
1	UH	76	GLN
1	aW	454	ASN
1	HL	63	GLN
1	aW	155	GLN
1	CT	155	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

231 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	g6	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	R4	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	MO	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	Q2	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	Y1	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	dC	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	Z9	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	OA	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.98	3 (17%)
2	P8E	NI	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	XM	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	HL	601	-	15,16,17	1.12	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	HL	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.09	2 (11%)
2	P8E	Q2	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.09	2 (11%)
2	P8E	R4	601	-	15,16,17	1.13	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	e8	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	HL	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	XM	601	-	15,16,17	1.13	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	KE	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	PU	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	KE	601	-	15,16,17	1.12	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	HL	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	g6	601	-	15,16,17	1.12	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	Z9	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	Q2	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	dC	601	-	15,16,17	1.12	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	Z9	601	-	15,16,17	1.12	1 (6%)	17,23,26	2.20	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	P8E	WG	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	KE	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	JD	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	PU	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.98	3 (17%)
2	P8E	fK	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	VR	601	-	15,16,17	1.12	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	dC	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	cV	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	FB	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.98	3 (17%)
2	P8E	NI	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	GQ	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	FB	601	-	15,16,17	1.13	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	VR	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	bS	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	LF	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	NI	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	GQ	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	g6	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.98	3 (17%)
2	P8E	DN	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	Q2	601	-	15,16,17	1.12	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	DN	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	LF	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	g6	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	FB	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	MO	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.09	2 (11%)
2	P8E	JD	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	S5	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	XM	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	e8	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	LF	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.09	2 (11%)
2	P8E	g6	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	CT	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	UH	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	JD	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	UH	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	P8E	CT	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	WG	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	BJ	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	LF	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	fK	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	aW	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	I3	601	-	15,16,17	1.13	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	TP	601	-	15,16,17	1.12	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	KE	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	aW	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	A7	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	S5	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.98	3 (17%)
2	P8E	NI	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	HL	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	PU	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	R4	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	fK	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	cV	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	aW	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	BJ	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	DN	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	KE	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	JD	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	BJ	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	GQ	601	-	15,16,17	1.12	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	GQ	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	bS	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	BJ	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	WG	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	e8	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	cV	601	-	15,16,17	1.13	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	BJ	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.98	3 (17%)
2	P8E	XM	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	CT	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.98	3 (17%)
2	P8E	UH	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	P8E	Y1	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	dC	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	I3	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	MO	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	GQ	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	S5	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	S5	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	A7	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	TP	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	PU	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	I3	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	VR	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	WG	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	Q2	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	I3	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	TP	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	CT	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	e8	601	-	15,16,17	1.13	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	fK	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	e8	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	fK	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	cV	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	OA	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	JD	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	aW	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.98	3 (17%)
2	P8E	Y1	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	Y1	601	-	15,16,17	1.12	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	FB	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	Y1	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.09	2 (11%)
2	P8E	GQ	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	KE	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	VR	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	A7	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	OA	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	dC	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	P8E	g6	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	fK	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	Y1	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	dC	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.98	3 (17%)
2	P8E	NI	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	XM	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	Z9	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	JD	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	DN	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	MO	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	MO	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	VR	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.98	3 (17%)
2	P8E	UH	601	-	15,16,17	1.13	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	JD	601	-	15,16,17	1.12	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	CT	601	-	15,16,17	1.12	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	S5	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	EX	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.09	2 (11%)
2	P8E	TP	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	A7	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	DN	601	-	15,16,17	1.12	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	DN	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	TP	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	HL	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.98	3 (17%)
2	P8E	TP	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	VR	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.09	2 (11%)
2	P8E	Q2	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	g6	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	fK	601	-	15,16,17	1.13	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	EX	601	-	15,16,17	1.13	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	Z9	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	OA	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	bS	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	HL	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	XM	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.98	3 (17%)
2	P8E	PU	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	P8E	aW	601	-	15,16,17	1.12	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	MO	601	-	15,16,17	1.13	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	LF	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	R4	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	bS	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	CT	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	UH	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	R4	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.09	2 (11%)
2	P8E	GQ	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	e8	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	UH	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.09	2 (11%)
2	P8E	CT	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	EX	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	MO	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	OA	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	S5	601	-	15,16,17	1.12	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	DN	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	A7	601	-	15,16,17	1.12	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	I3	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	Z9	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.09	2 (11%)
2	P8E	LF	601	-	15,16,17	1.13	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	WG	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	A7	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	LF	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	EX	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	S5	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	cV	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	XM	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	aW	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	TP	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	aW	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	OA	601	-	15,16,17	1.12	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	bS	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	bS	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	R4	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	P8E	BJ	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.09	2 (11%)
2	P8E	FB	602	-	15,16,17	1.06	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	Q2	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	UH	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	EX	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	dC	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	NI	601	-	15,16,17	1.13	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	PU	601	-	15,16,17	1.13	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	OA	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	R4	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	FB	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	bS	601	-	15,16,17	1.13	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	NI	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	EX	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	PU	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	Z9	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	EX	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	FB	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.09	2 (11%)
2	P8E	BJ	601	-	15,16,17	1.13	1 (6%)	17,23,26	2.20	3 (17%)
2	P8E	cV	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	WG	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	I3	604	-	15,16,17	1.11	1 (6%)	17,23,26	1.99	3 (17%)
2	P8E	Y1	603	-	15,16,17	1.06	1 (6%)	17,23,26	2.14	3 (17%)
2	P8E	cV	607	-	15,16,17	1.05	1 (6%)	17,23,26	2.11	3 (17%)
2	P8E	KE	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.10	2 (11%)
2	P8E	VR	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	e8	605	-	15,16,17	1.10	1 (6%)	17,23,26	2.09	2 (11%)
2	P8E	A7	606	-	15,16,17	1.05	1 (6%)	17,23,26	2.16	2 (11%)
2	P8E	I3	602	-	15,16,17	1.07	1 (6%)	17,23,26	2.04	2 (11%)
2	P8E	WG	601	-	15,16,17	1.13	1 (6%)	17,23,26	2.20	3 (17%)

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	g6	602	-	-	0/11/28/32	0/1/1/1
2	P8E	R4	602	-	-	0/11/28/32	0/1/1/1
2	P8E	MO	603	-	-	0/11/28/32	0/1/1/1
2	P8E	Q2	606	-	-	2/11/28/32	0/1/1/1
2	P8E	Y1	607	-	-	3/11/28/32	0/1/1/1
2	P8E	dC	607	-	-	3/11/28/32	0/1/1/1
2	P8E	Z9	602	-	-	0/11/28/32	0/1/1/1
2	P8E	OA	604	-	-	3/11/28/32	0/1/1/1
2	P8E	NI	604	-	-	3/11/28/32	0/1/1/1
2	P8E	XM	606	-	-	2/11/28/32	0/1/1/1
2	P8E	HL	601	-	-	0/11/28/32	0/1/1/1
2	P8E	HL	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	Q2	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	R4	601	-	-	0/11/28/32	0/1/1/1
2	P8E	e8	602	-	-	0/11/28/32	0/1/1/1
2	P8E	HL	603	-	-	0/11/28/32	0/1/1/1
2	P8E	XM	601	-	-	0/11/28/32	0/1/1/1
2	P8E	KE	604	-	-	3/11/28/32	0/1/1/1
2	P8E	PU	602	-	-	0/11/28/32	0/1/1/1
2	P8E	KE	601	-	-	0/11/28/32	0/1/1/1
2	P8E	HL	602	-	-	0/11/28/32	0/1/1/1
2	P8E	g6	601	-	-	0/11/28/32	0/1/1/1
2	P8E	Z9	603	-	-	0/11/28/32	0/1/1/1
2	P8E	Q2	607	-	-	3/11/28/32	0/1/1/1
2	P8E	dC	601	-	-	0/11/28/32	0/1/1/1
2	P8E	Z9	601	-	-	0/11/28/32	0/1/1/1
2	P8E	WG	604	-	-	3/11/28/32	0/1/1/1
2	P8E	KE	606	-	-	2/11/28/32	0/1/1/1
2	P8E	JD	604	-	-	3/11/28/32	0/1/1/1
2	P8E	PU	604	-	-	3/11/28/32	0/1/1/1
2	P8E	fK	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	cV	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	dC	603	-	-	0/11/28/32	0/1/1/1
2	P8E	VR	601	-	-	0/11/28/32	0/1/1/1
2	P8E	FB	604	-	-	3/11/28/32	0/1/1/1
2	P8E	NI	606	-	-	2/11/28/32	0/1/1/1
2	P8E	GQ	603	-	-	0/11/28/32	0/1/1/1
2	P8E	FB	601	-	-	0/11/28/32	0/1/1/1
2	P8E	VR	603	-	-	0/11/28/32	0/1/1/1
2	P8E	bS	603	-	-	0/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	LF	602	-	-	0/11/28/32	0/1/1/1
2	P8E	NI	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	GQ	607	-	-	3/11/28/32	0/1/1/1
2	P8E	g6	604	-	-	3/11/28/32	0/1/1/1
2	P8E	DN	603	-	-	0/11/28/32	0/1/1/1
2	P8E	Q2	601	-	-	0/11/28/32	0/1/1/1
2	P8E	DN	607	-	-	3/11/28/32	0/1/1/1
2	P8E	LF	604	-	-	3/11/28/32	0/1/1/1
2	P8E	g6	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	FB	603	-	-	0/11/28/32	0/1/1/1
2	P8E	MO	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	JD	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	S5	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	XM	603	-	-	0/11/28/32	0/1/1/1
2	P8E	e8	604	-	-	3/11/28/32	0/1/1/1
2	P8E	LF	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	g6	603	-	-	0/11/28/32	0/1/1/1
2	P8E	CT	602	-	-	0/11/28/32	0/1/1/1
2	P8E	UH	602	-	-	0/11/28/32	0/1/1/1
2	P8E	JD	602	-	-	0/11/28/32	0/1/1/1
2	P8E	UH	603	-	-	0/11/28/32	0/1/1/1
2	P8E	CT	607	-	-	3/11/28/32	0/1/1/1
2	P8E	WG	603	-	-	0/11/28/32	0/1/1/1
2	P8E	BJ	607	-	-	3/11/28/32	0/1/1/1
2	P8E	LF	607	-	-	3/11/28/32	0/1/1/1
2	P8E	fK	603	-	-	0/11/28/32	0/1/1/1
2	P8E	aW	603	-	-	0/11/28/32	0/1/1/1
2	P8E	I3	601	-	-	0/11/28/32	0/1/1/1
2	P8E	TP	601	-	-	0/11/28/32	0/1/1/1
2	P8E	KE	602	-	-	0/11/28/32	0/1/1/1
2	P8E	aW	607	-	-	3/11/28/32	0/1/1/1
2	P8E	A7	604	-	-	3/11/28/32	0/1/1/1
2	P8E	S5	604	-	-	3/11/28/32	0/1/1/1
2	P8E	NI	607	-	-	3/11/28/32	0/1/1/1
2	P8E	HL	607	-	-	3/11/28/32	0/1/1/1
2	P8E	PU	607	-	-	3/11/28/32	0/1/1/1
2	P8E	R4	607	-	-	3/11/28/32	0/1/1/1
2	P8E	fK	602	-	-	0/11/28/32	0/1/1/1
2	P8E	cV	602	-	-	0/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	aW	602	-	-	0/11/28/32	0/1/1/1
2	P8E	BJ	602	-	-	0/11/28/32	0/1/1/1
2	P8E	DN	606	-	-	2/11/28/32	0/1/1/1
2	P8E	KE	603	-	-	0/11/28/32	0/1/1/1
2	P8E	JD	603	-	-	0/11/28/32	0/1/1/1
2	P8E	BJ	603	-	-	0/11/28/32	0/1/1/1
2	P8E	GQ	601	-	-	0/11/28/32	0/1/1/1
2	P8E	GQ	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	bS	604	-	-	3/11/28/32	0/1/1/1
2	P8E	BJ	606	-	-	2/11/28/32	0/1/1/1
2	P8E	WG	606	-	-	2/11/28/32	0/1/1/1
2	P8E	e8	603	-	-	0/11/28/32	0/1/1/1
2	P8E	cV	601	-	-	0/11/28/32	0/1/1/1
2	P8E	BJ	604	-	-	3/11/28/32	0/1/1/1
2	P8E	XM	607	-	-	3/11/28/32	0/1/1/1
2	P8E	CT	604	-	-	3/11/28/32	0/1/1/1
2	P8E	UH	604	-	-	3/11/28/32	0/1/1/1
2	P8E	Y1	602	-	-	0/11/28/32	0/1/1/1
2	P8E	dC	602	-	-	0/11/28/32	0/1/1/1
2	P8E	I3	607	-	-	3/11/28/32	0/1/1/1
2	P8E	MO	602	-	-	0/11/28/32	0/1/1/1
2	P8E	GQ	604	-	-	3/11/28/32	0/1/1/1
2	P8E	S5	602	-	-	0/11/28/32	0/1/1/1
2	P8E	S5	607	-	-	3/11/28/32	0/1/1/1
2	P8E	A7	602	-	-	0/11/28/32	0/1/1/1
2	P8E	TP	606	-	-	2/11/28/32	0/1/1/1
2	P8E	PU	603	-	-	0/11/28/32	0/1/1/1
2	P8E	I3	606	-	-	2/11/28/32	0/1/1/1
2	P8E	VR	607	-	-	3/11/28/32	0/1/1/1
2	P8E	WG	607	-	-	3/11/28/32	0/1/1/1
2	P8E	Q2	603	-	-	0/11/28/32	0/1/1/1
2	P8E	I3	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	TP	602	-	-	0/11/28/32	0/1/1/1
2	P8E	CT	603	-	-	0/11/28/32	0/1/1/1
2	P8E	e8	601	-	-	0/11/28/32	0/1/1/1
2	P8E	fK	606	-	-	2/11/28/32	0/1/1/1
2	P8E	e8	606	-	-	2/11/28/32	0/1/1/1
2	P8E	fK	604	-	-	3/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	cV	604	-	-	3/11/28/32	0/1/1/1
2	P8E	OA	607	-	-	3/11/28/32	0/1/1/1
2	P8E	JD	607	-	-	3/11/28/32	0/1/1/1
2	P8E	aW	604	-	-	3/11/28/32	0/1/1/1
2	P8E	Y1	606	-	-	2/11/28/32	0/1/1/1
2	P8E	Y1	601	-	-	0/11/28/32	0/1/1/1
2	P8E	FB	606	-	-	2/11/28/32	0/1/1/1
2	P8E	Y1	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	GQ	602	-	-	0/11/28/32	0/1/1/1
2	P8E	KE	607	-	-	3/11/28/32	0/1/1/1
2	P8E	VR	602	-	-	0/11/28/32	0/1/1/1
2	P8E	OA	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	A7	607	-	-	3/11/28/32	0/1/1/1
2	P8E	dC	606	-	-	2/11/28/32	0/1/1/1
2	P8E	g6	606	-	-	2/11/28/32	0/1/1/1
2	P8E	XM	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	Y1	604	-	-	3/11/28/32	0/1/1/1
2	P8E	dC	604	-	-	3/11/28/32	0/1/1/1
2	P8E	NI	602	-	-	0/11/28/32	0/1/1/1
2	P8E	fK	607	-	-	3/11/28/32	0/1/1/1
2	P8E	Z9	607	-	-	3/11/28/32	0/1/1/1
2	P8E	JD	606	-	-	2/11/28/32	0/1/1/1
2	P8E	DN	602	-	-	0/11/28/32	0/1/1/1
2	P8E	MO	604	-	-	3/11/28/32	0/1/1/1
2	P8E	MO	606	-	-	2/11/28/32	0/1/1/1
2	P8E	VR	604	-	-	3/11/28/32	0/1/1/1
2	P8E	UH	601	-	-	0/11/28/32	0/1/1/1
2	P8E	JD	601	-	-	0/11/28/32	0/1/1/1
2	P8E	CT	601	-	-	0/11/28/32	0/1/1/1
2	P8E	EX	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	S5	606	-	-	2/11/28/32	0/1/1/1
2	P8E	TP	603	-	-	0/11/28/32	0/1/1/1
2	P8E	A7	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	DN	601	-	-	0/11/28/32	0/1/1/1
2	P8E	DN	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	VR	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	HL	604	-	-	3/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	TP	604	-	-	3/11/28/32	0/1/1/1
2	P8E	TP	607	-	-	3/11/28/32	0/1/1/1
2	P8E	Q2	604	-	-	3/11/28/32	0/1/1/1
2	P8E	g6	607	-	-	3/11/28/32	0/1/1/1
2	P8E	fK	601	-	-	0/11/28/32	0/1/1/1
2	P8E	EX	601	-	-	0/11/28/32	0/1/1/1
2	P8E	Z9	604	-	-	3/11/28/32	0/1/1/1
2	P8E	OA	606	-	-	2/11/28/32	0/1/1/1
2	P8E	bS	606	-	-	2/11/28/32	0/1/1/1
2	P8E	HL	606	-	-	2/11/28/32	0/1/1/1
2	P8E	XM	604	-	-	3/11/28/32	0/1/1/1
2	P8E	PU	606	-	-	2/11/28/32	0/1/1/1
2	P8E	aW	601	-	-	0/11/28/32	0/1/1/1
2	P8E	MO	601	-	-	0/11/28/32	0/1/1/1
2	P8E	LF	606	-	-	2/11/28/32	0/1/1/1
2	P8E	bS	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	R4	606	-	-	2/11/28/32	0/1/1/1
2	P8E	CT	606	-	-	2/11/28/32	0/1/1/1
2	P8E	UH	606	-	-	2/11/28/32	0/1/1/1
2	P8E	R4	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	GQ	606	-	-	2/11/28/32	0/1/1/1
2	P8E	CT	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	UH	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	e8	607	-	-	3/11/28/32	0/1/1/1
2	P8E	EX	606	-	-	2/11/28/32	0/1/1/1
2	P8E	MO	607	-	-	3/11/28/32	0/1/1/1
2	P8E	OA	603	-	-	0/11/28/32	0/1/1/1
2	P8E	S5	601	-	-	0/11/28/32	0/1/1/1
2	P8E	DN	604	-	-	3/11/28/32	0/1/1/1
2	P8E	A7	601	-	-	0/11/28/32	0/1/1/1
2	P8E	Z9	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	I3	603	-	-	0/11/28/32	0/1/1/1
2	P8E	WG	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	LF	601	-	-	0/11/28/32	0/1/1/1
2	P8E	A7	603	-	-	0/11/28/32	0/1/1/1
2	P8E	LF	603	-	-	0/11/28/32	0/1/1/1
2	P8E	EX	607	-	-	3/11/28/32	0/1/1/1
2	P8E	S5	603	-	-	0/11/28/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P8E	cV	606	-	-	2/11/28/32	0/1/1/1
2	P8E	XM	602	-	-	0/11/28/32	0/1/1/1
2	P8E	aW	606	-	-	2/11/28/32	0/1/1/1
2	P8E	TP	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	aW	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	OA	601	-	-	0/11/28/32	0/1/1/1
2	P8E	bS	602	-	-	0/11/28/32	0/1/1/1
2	P8E	bS	607	-	-	3/11/28/32	0/1/1/1
2	P8E	R4	603	-	-	0/11/28/32	0/1/1/1
2	P8E	BJ	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	FB	602	-	-	0/11/28/32	0/1/1/1
2	P8E	Q2	602	-	-	0/11/28/32	0/1/1/1
2	P8E	UH	607	-	-	3/11/28/32	0/1/1/1
2	P8E	EX	603	-	-	0/11/28/32	0/1/1/1
2	P8E	dC	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	NI	601	-	-	0/11/28/32	0/1/1/1
2	P8E	PU	601	-	-	0/11/28/32	0/1/1/1
2	P8E	OA	602	-	-	0/11/28/32	0/1/1/1
2	P8E	R4	604	-	-	3/11/28/32	0/1/1/1
2	P8E	FB	607	-	-	3/11/28/32	0/1/1/1
2	P8E	bS	601	-	-	0/11/28/32	0/1/1/1
2	P8E	NI	603	-	-	0/11/28/32	0/1/1/1
2	P8E	EX	602	-	-	0/11/28/32	0/1/1/1
2	P8E	PU	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	Z9	606	-	-	2/11/28/32	0/1/1/1
2	P8E	EX	604	-	-	3/11/28/32	0/1/1/1
2	P8E	FB	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	BJ	601	-	-	0/11/28/32	0/1/1/1
2	P8E	cV	603	-	-	0/11/28/32	0/1/1/1
2	P8E	WG	602	-	-	0/11/28/32	0/1/1/1
2	P8E	I3	604	-	-	3/11/28/32	0/1/1/1
2	P8E	Y1	603	-	-	0/11/28/32	0/1/1/1
2	P8E	cV	607	-	-	3/11/28/32	0/1/1/1
2	P8E	KE	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	VR	606	-	-	2/11/28/32	0/1/1/1
2	P8E	e8	605	-	1/1/7/7	1/11/28/32	0/1/1/1
2	P8E	A7	606	-	-	2/11/28/32	0/1/1/1
2	P8E	I3	602	-	-	0/11/28/32	0/1/1/1
2	P8E	WG	601	-	-	0/11/28/32	0/1/1/1

The worst 5 of 231 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	LF	601	P8E	O6-C6	-2.51	1.40	1.44
2	PU	601	P8E	O6-C6	-2.51	1.40	1.44
2	e8	601	P8E	O6-C6	-2.51	1.40	1.44
2	dC	601	P8E	O6-C6	-2.51	1.40	1.44
2	WG	601	P8E	O6-C6	-2.51	1.40	1.44

The worst 5 of 594 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	JD	606	P8E	O6-C2-C1	7.75	122.36	107.72
2	DN	606	P8E	O6-C2-C1	7.75	122.36	107.72
2	aW	606	P8E	O6-C2-C1	7.75	122.36	107.72
2	EX	606	P8E	O6-C2-C1	7.75	122.36	107.72
2	FB	606	P8E	O6-C2-C1	7.75	122.35	107.72

5 of 33 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	Y1	605	P8E	C2
2	Q2	605	P8E	C2
2	I3	605	P8E	C2
2	R4	605	P8E	C2
2	S5	605	P8E	C2

5 of 297 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Y1	604	P8E	O1A-C1-C2-C3
2	Y1	604	P8E	O1B-C1-C2-C3
2	Y1	606	P8E	N7-C7-C8-C9
2	Q2	604	P8E	O1A-C1-C2-C3
2	Q2	604	P8E	O1B-C1-C2-C3

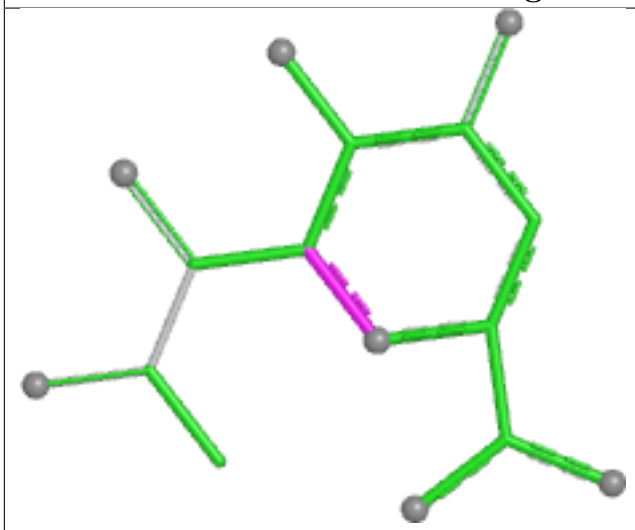
There are no ring outliers.

No monomer is involved in short contacts.

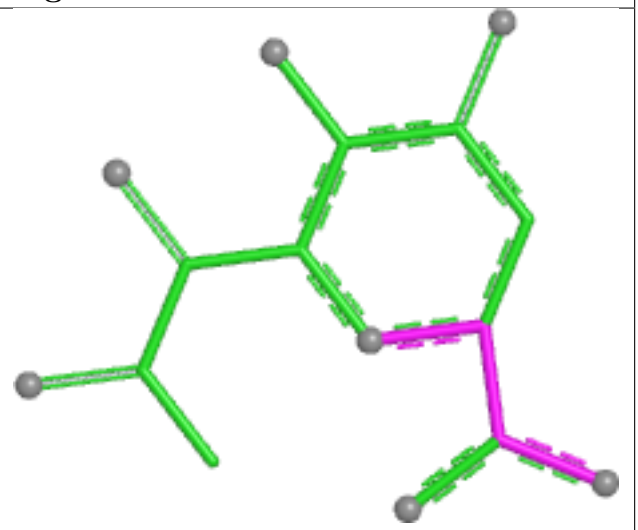
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

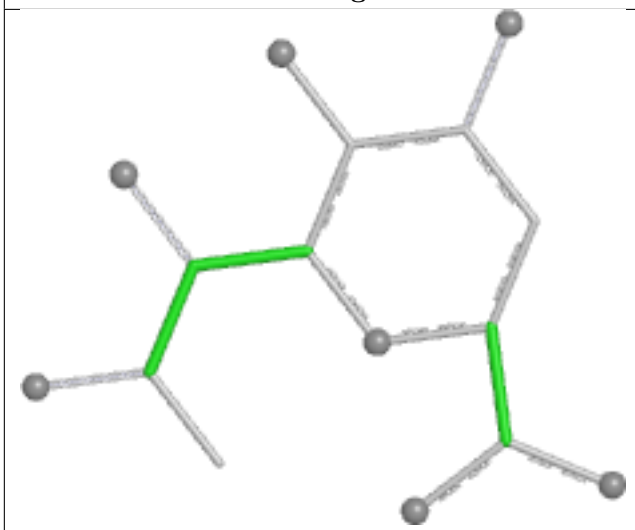
Ligand P8E g6 602



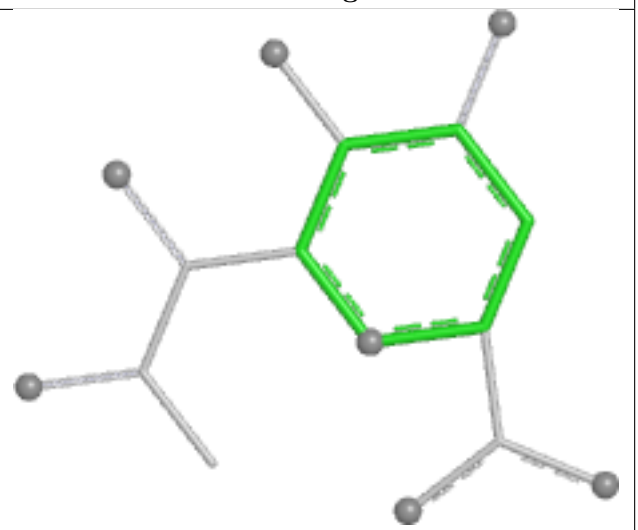
Bond lengths



Bond angles

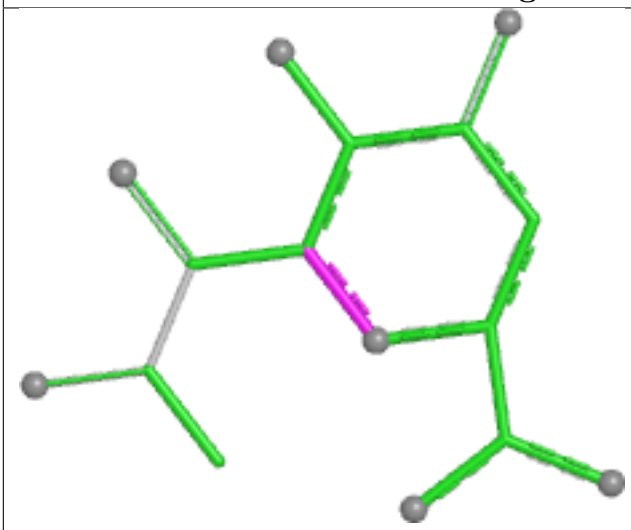


Torsions

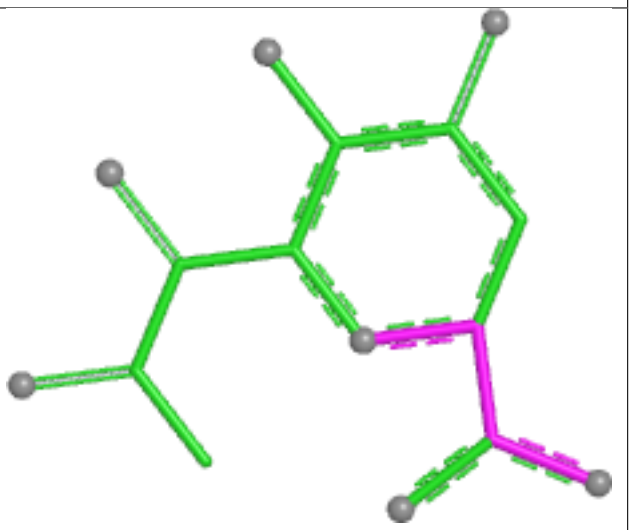


Rings

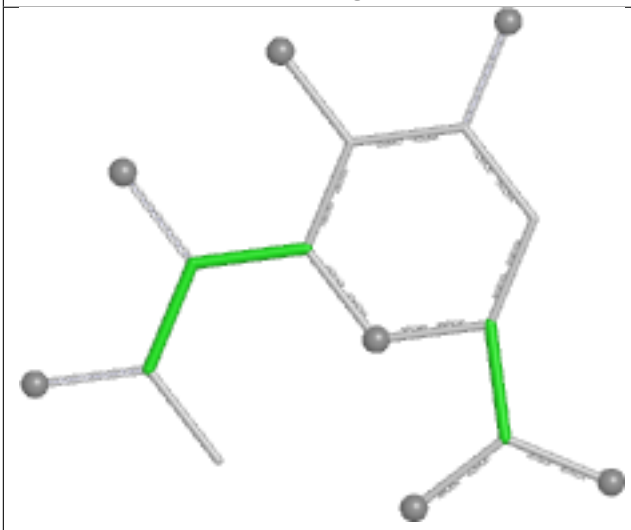
Ligand P8E R4 602



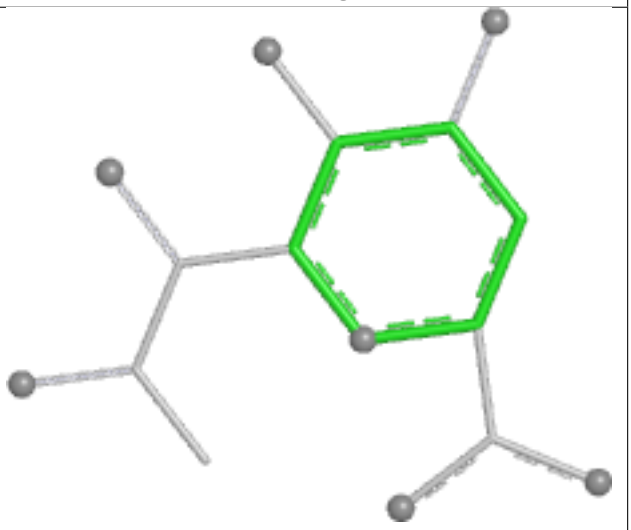
Bond lengths



Bond angles

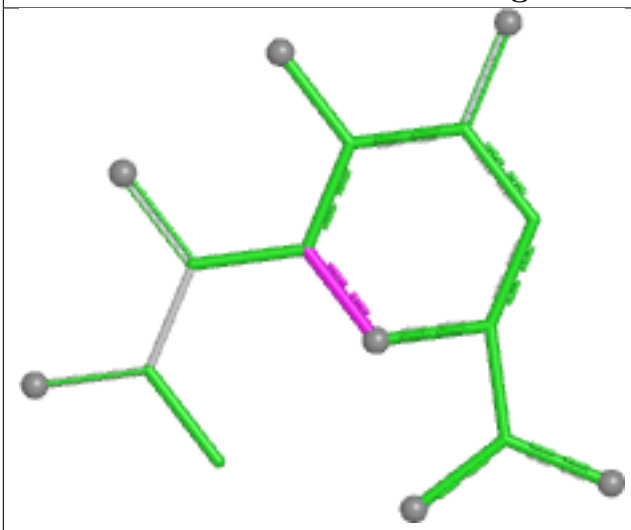


Torsions

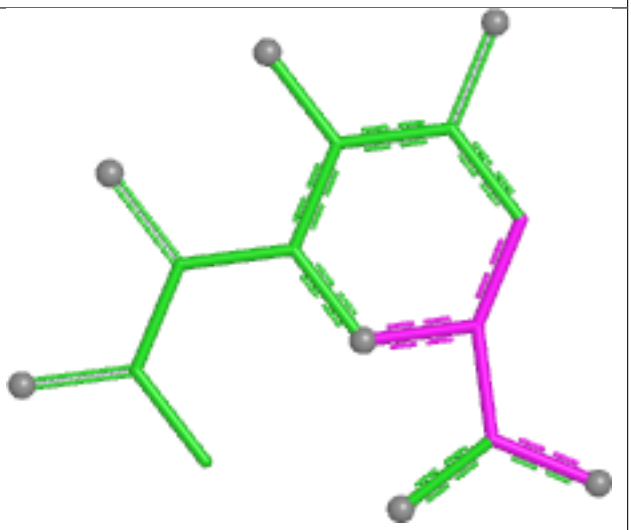


Rings

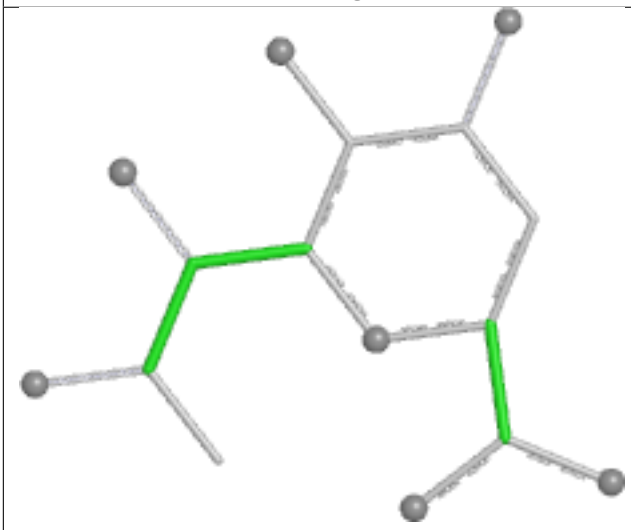
Ligand P8E MO 603



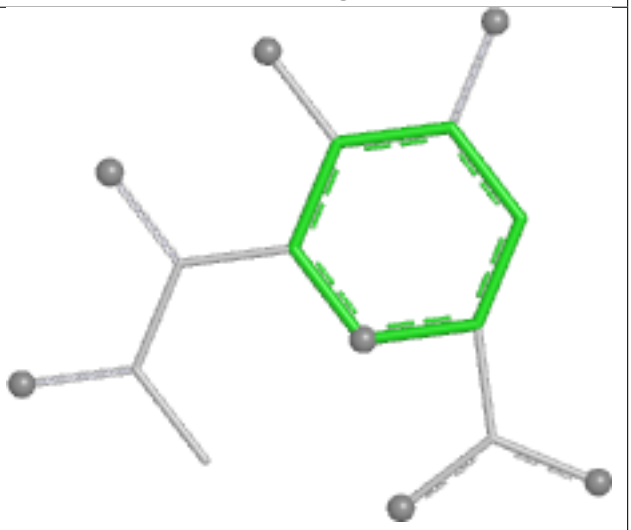
Bond lengths



Bond angles

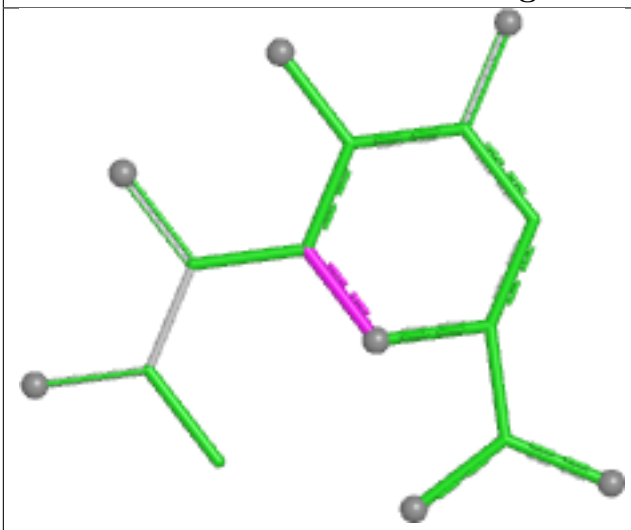


Torsions

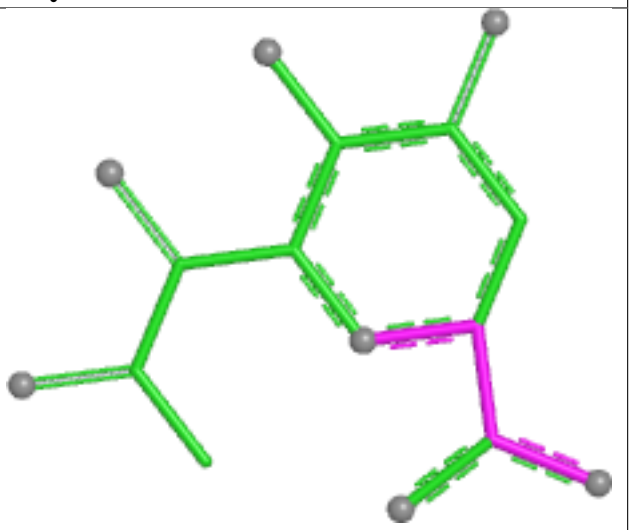


Rings

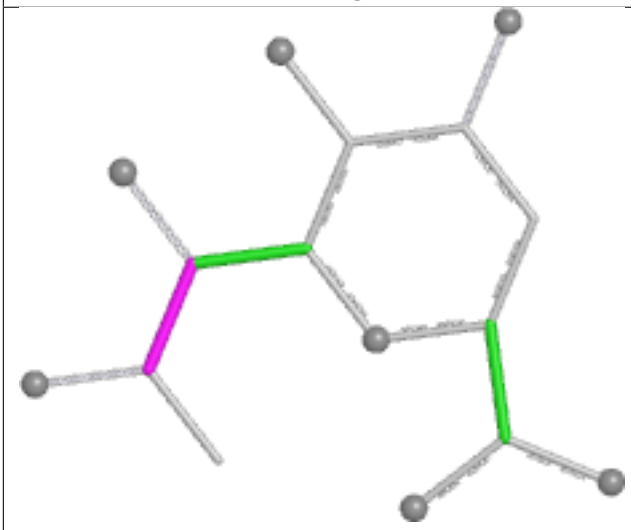
Ligand P8E Q2 606



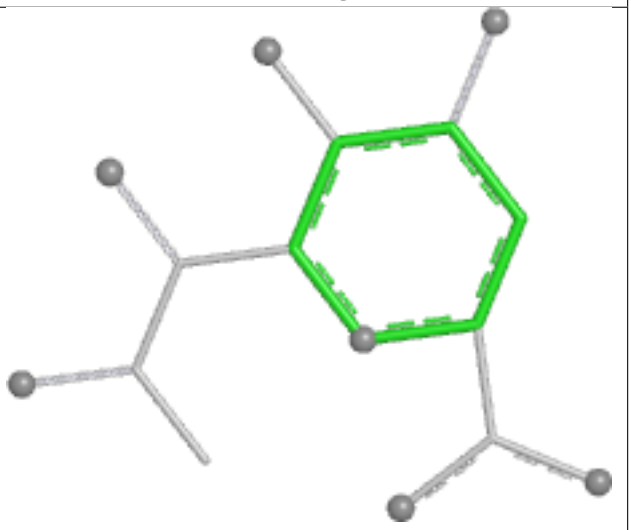
Bond lengths



Bond angles

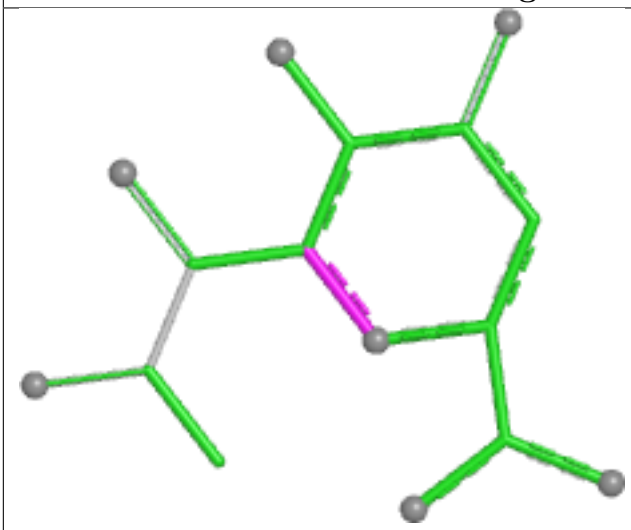


Torsions

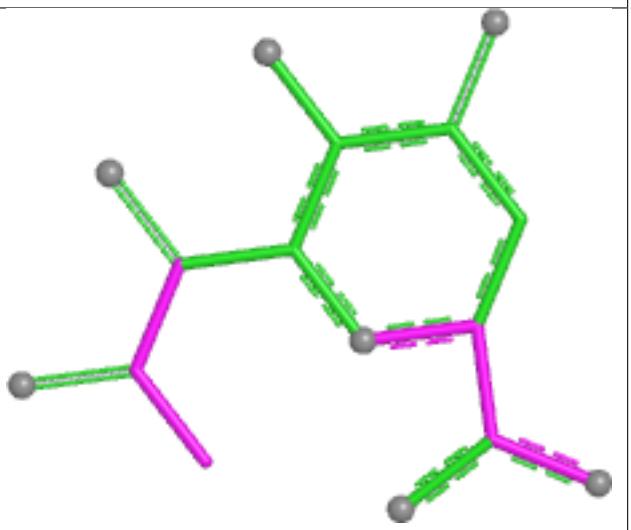


Rings

Ligand P8E Y1 607



Bond lengths



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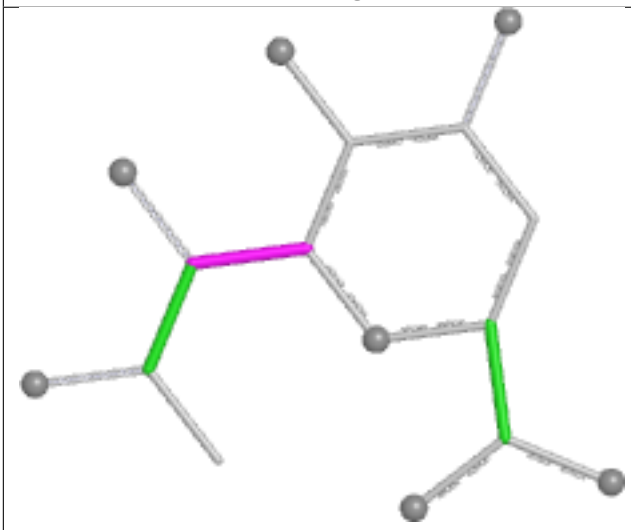

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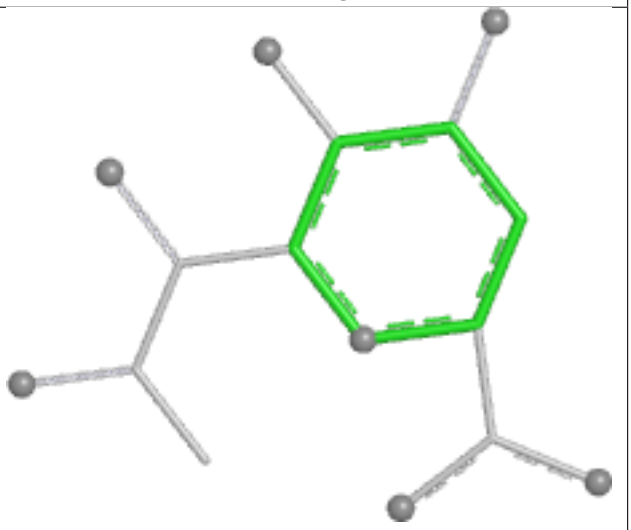
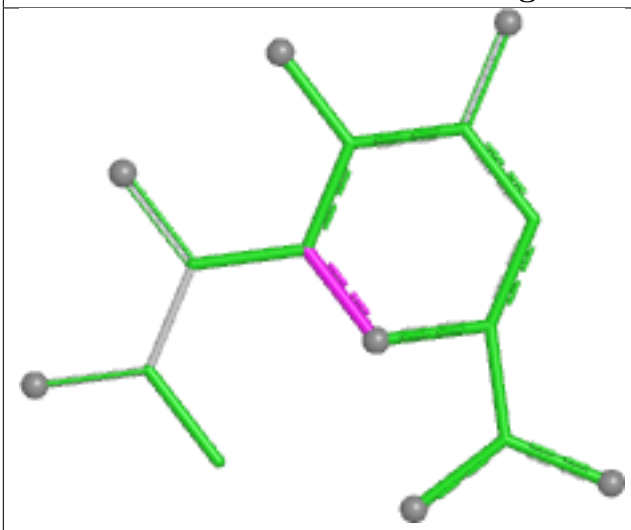
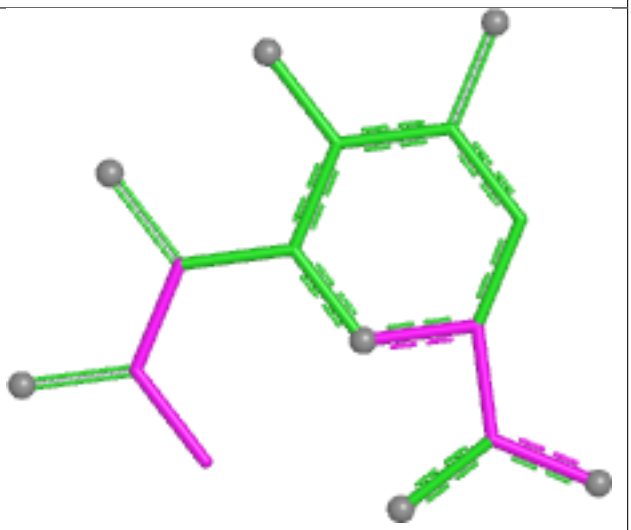


Rings

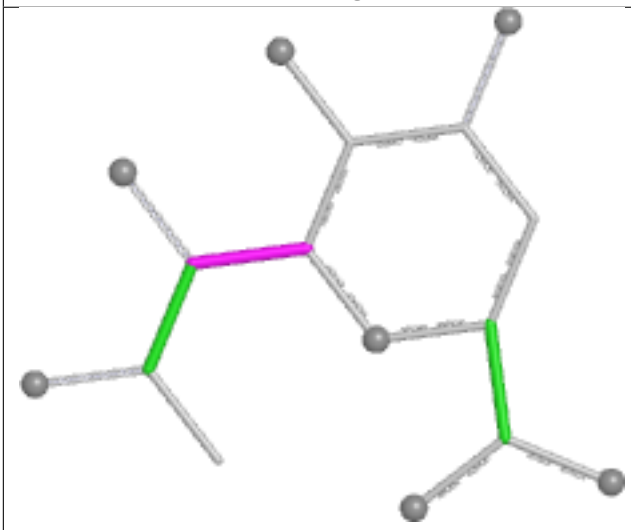
Ligand P8E dC 607



Bond lengths



Bond angles



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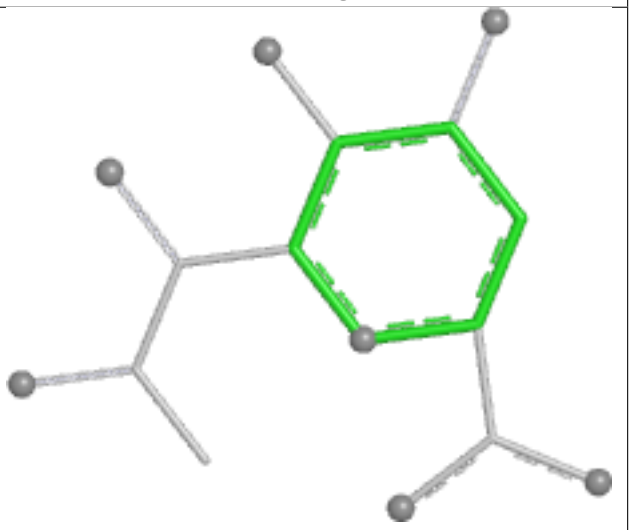
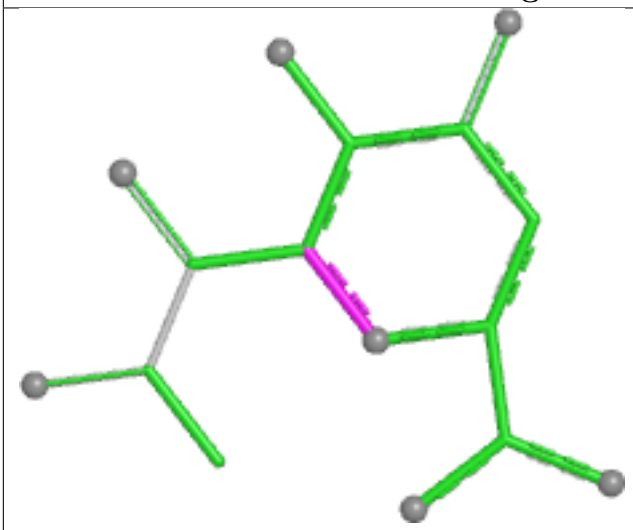
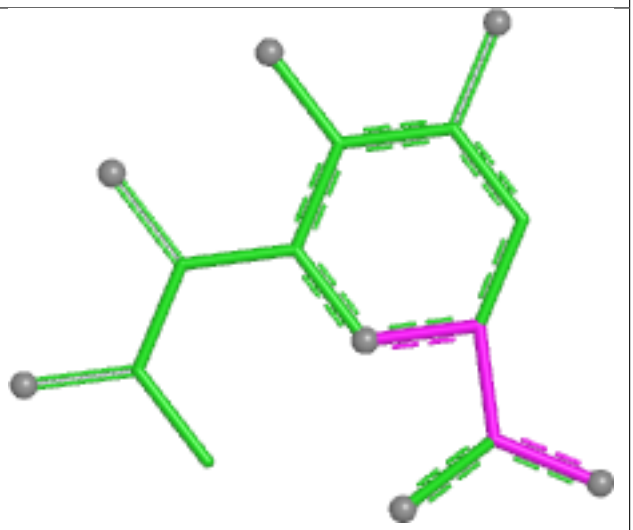


Rings

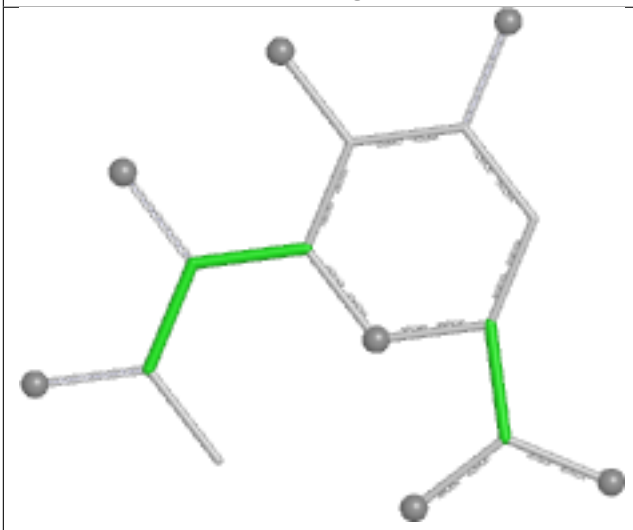
Ligand P8E Z9 602



Bond lengths



Bond angles



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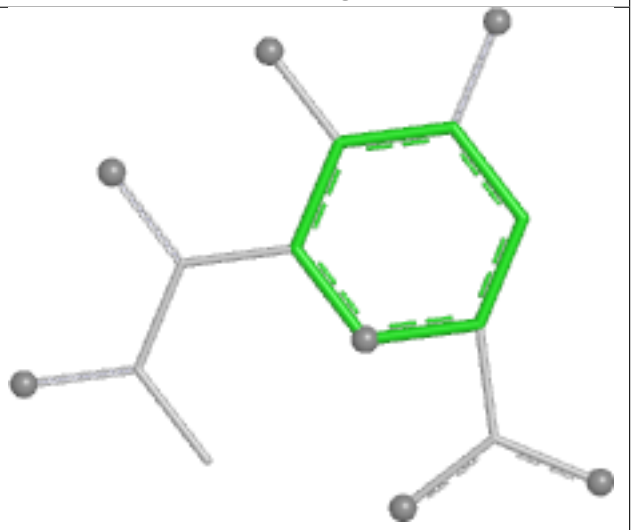

Rings

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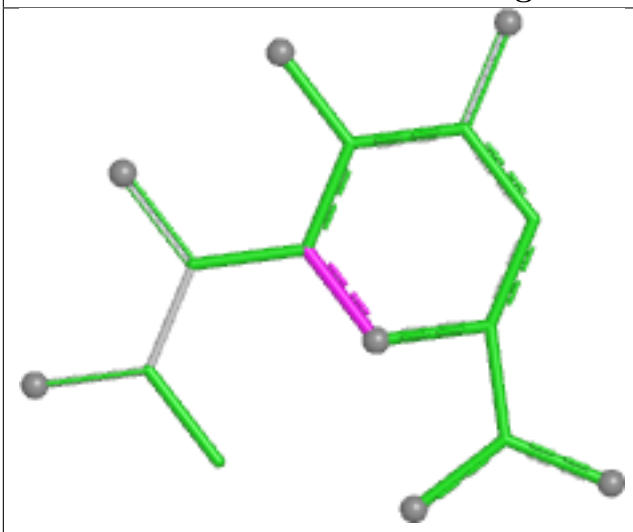
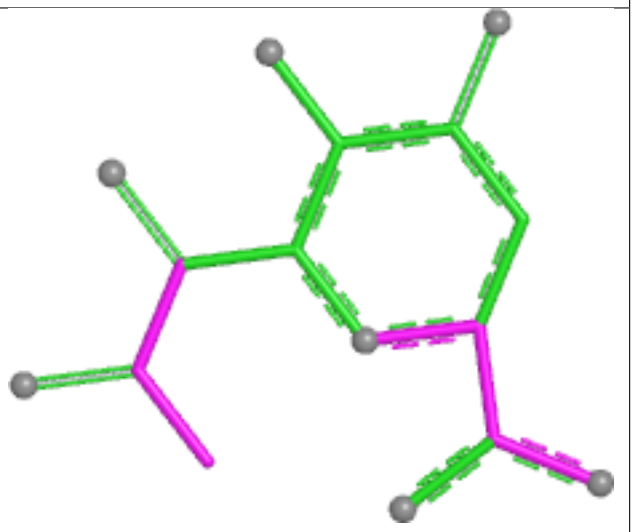
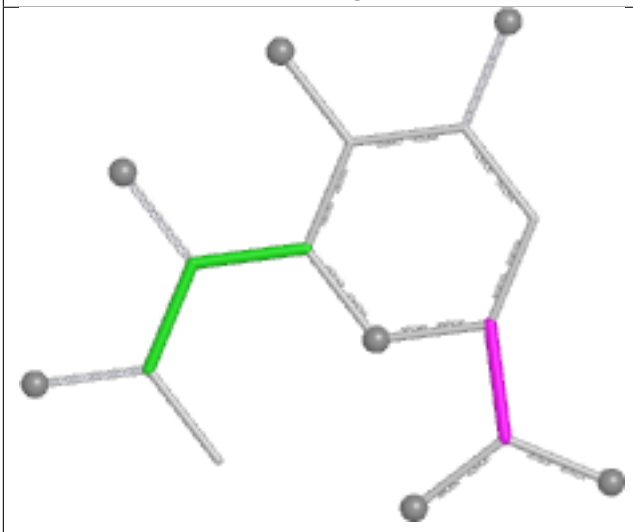


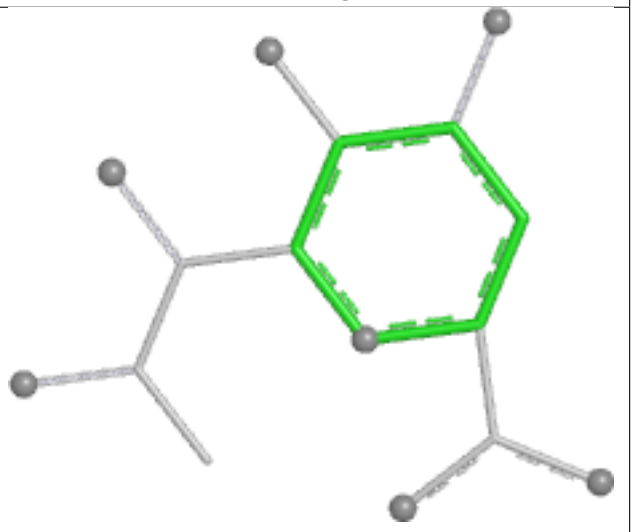
Bond lengths



Bond angles

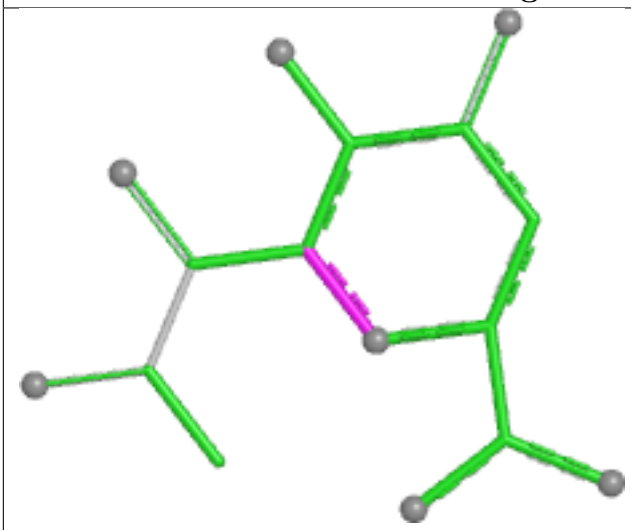


Torsions

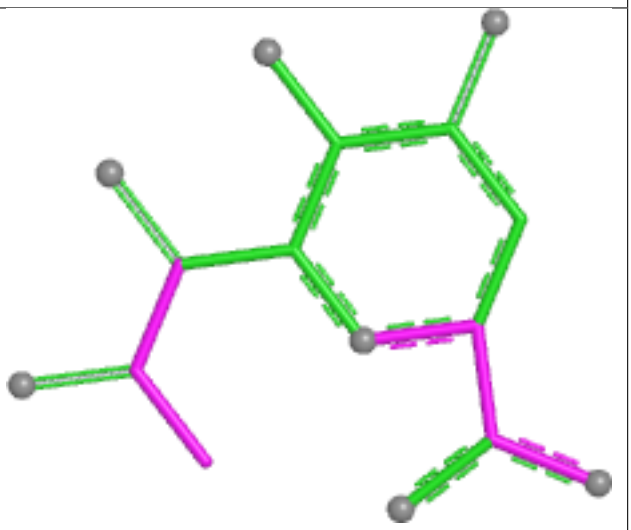


Rings

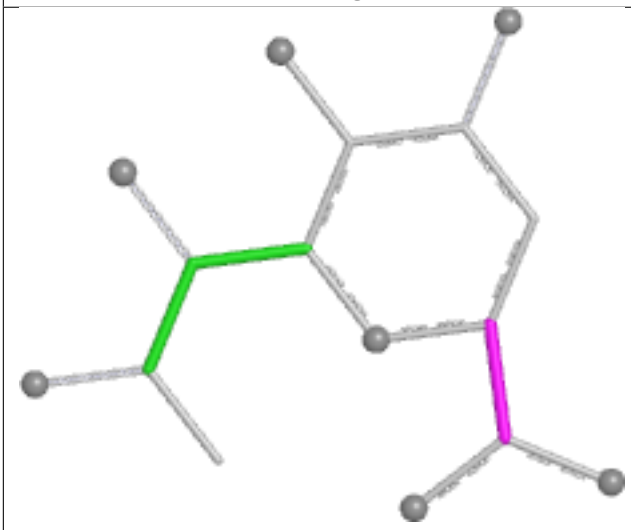
Ligand P8E NI 604



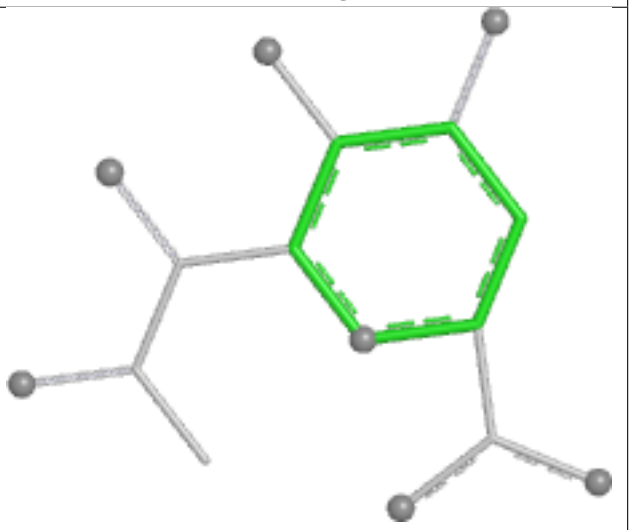
Bond lengths



Bond angles

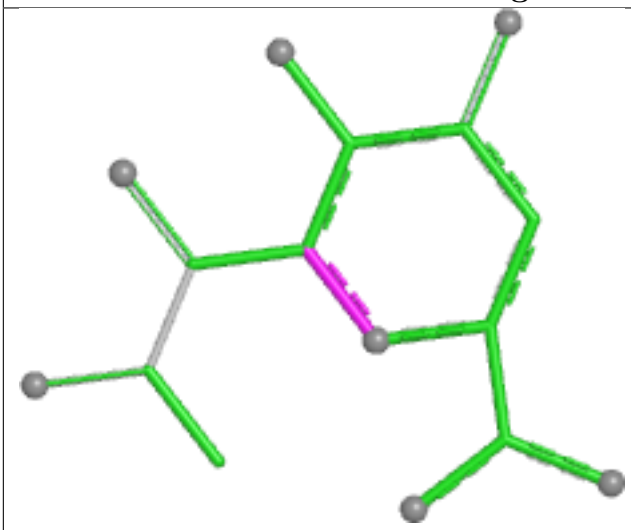


Torsions



Rings

Ligand P8E XM 606



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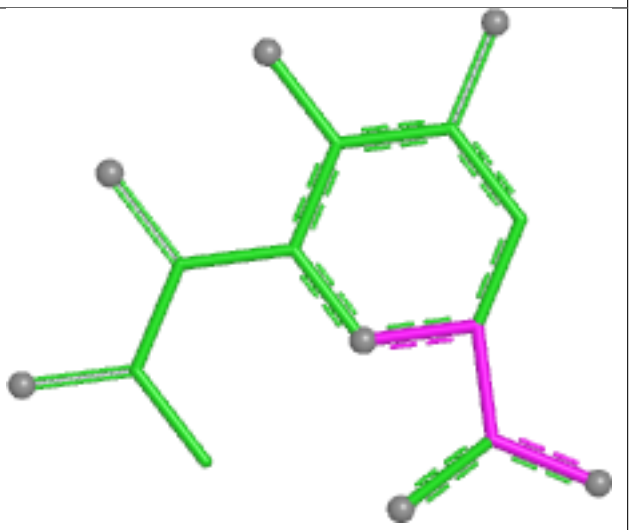

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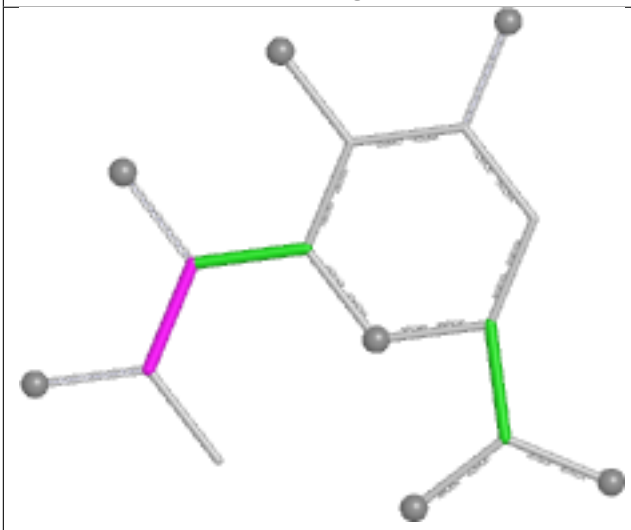

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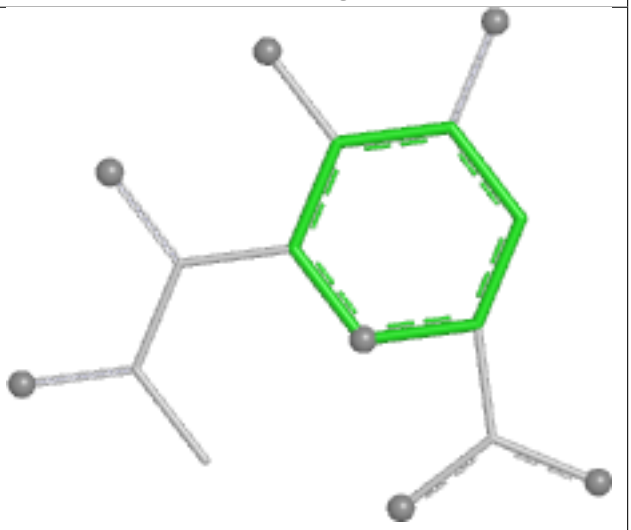
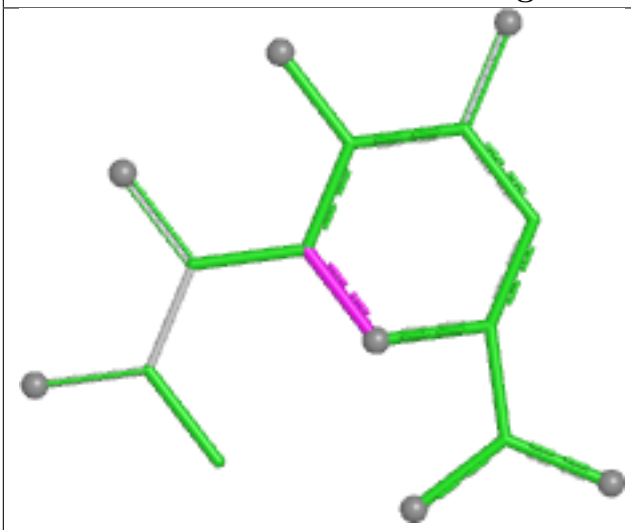


Rings

Ligand P8E HL 601



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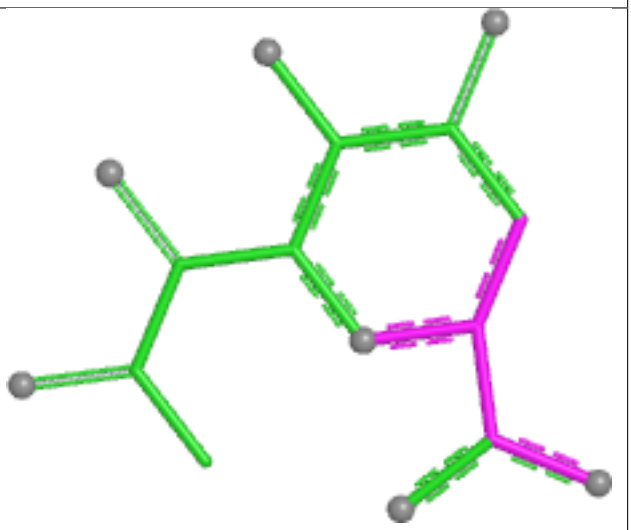

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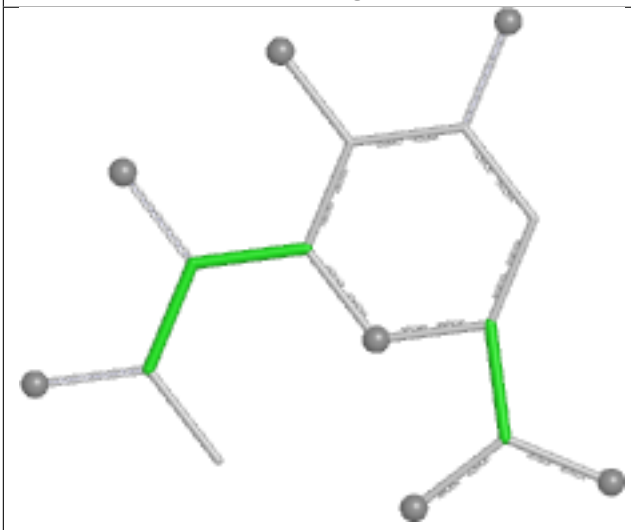

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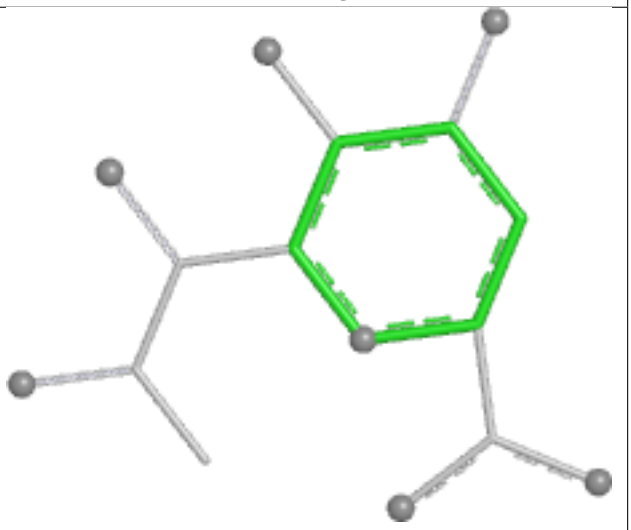

Rings

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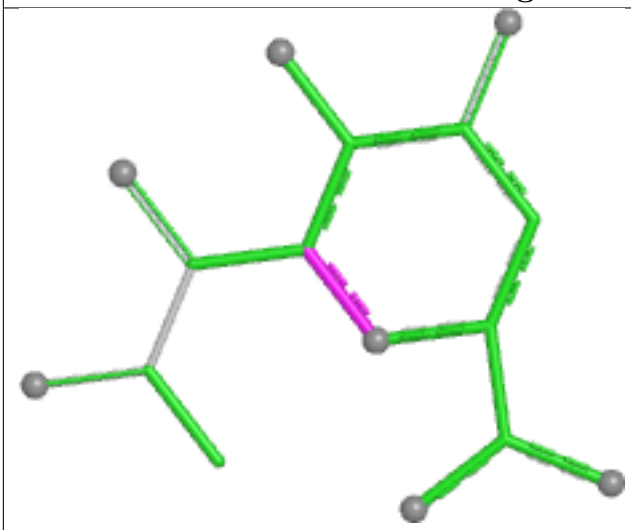

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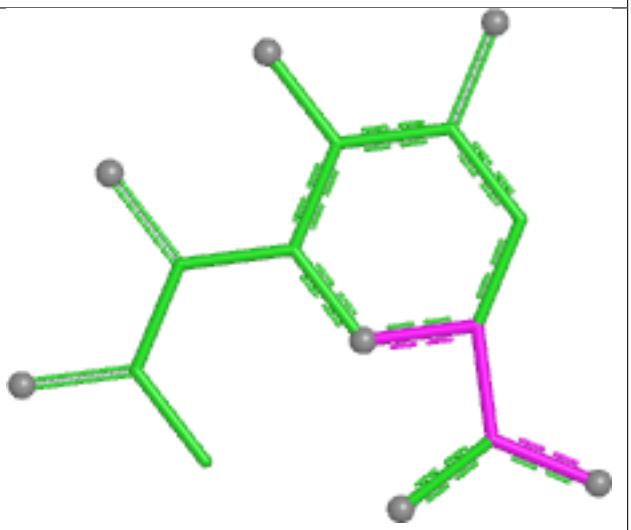

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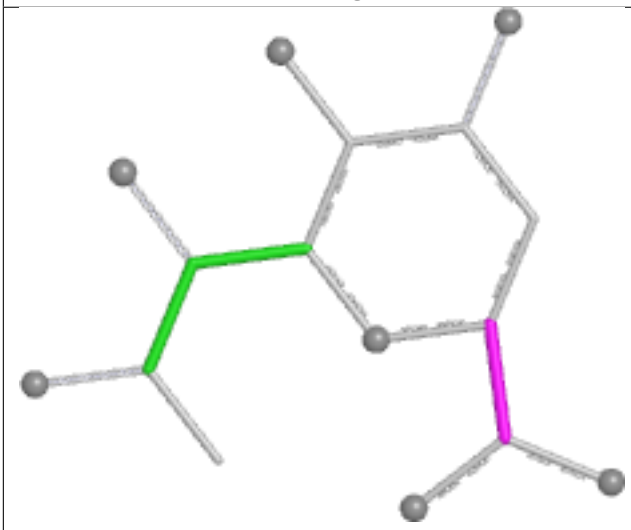

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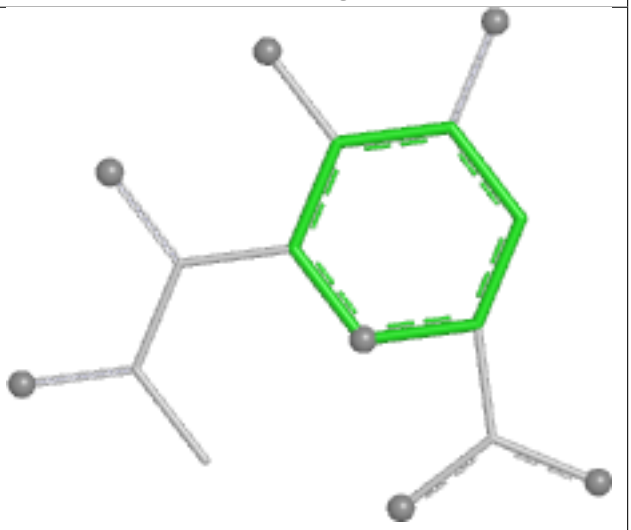

Rings

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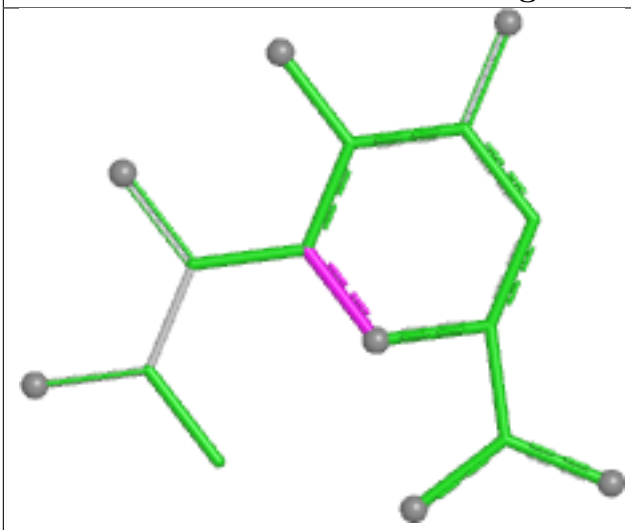

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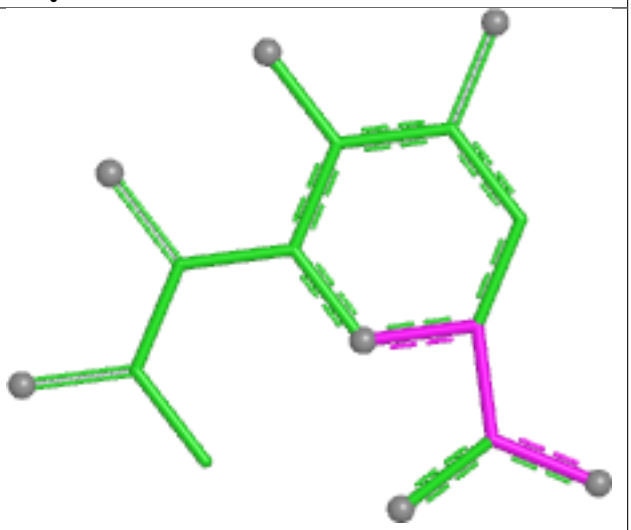

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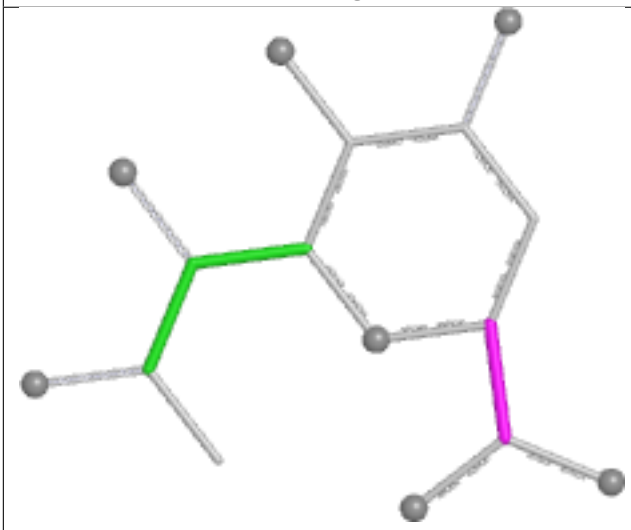

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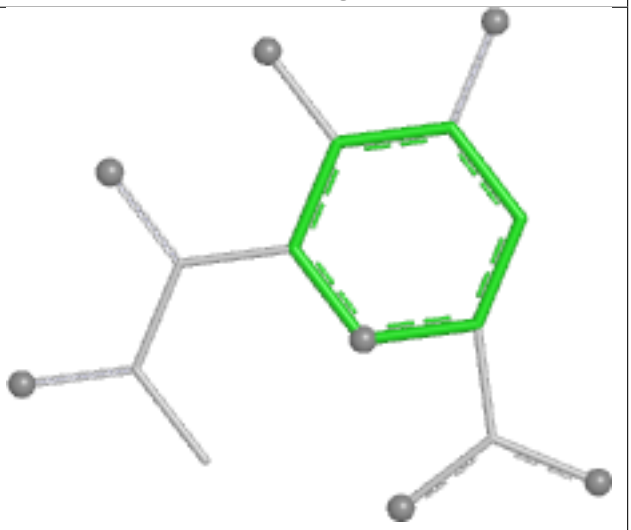
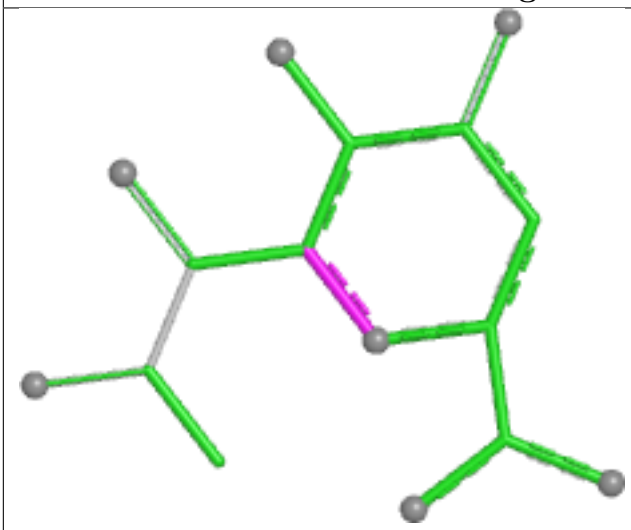


Rings

Ligand P8E R4 601



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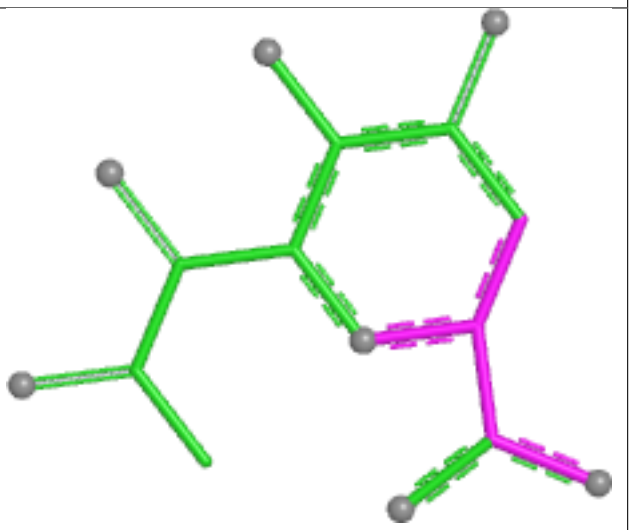

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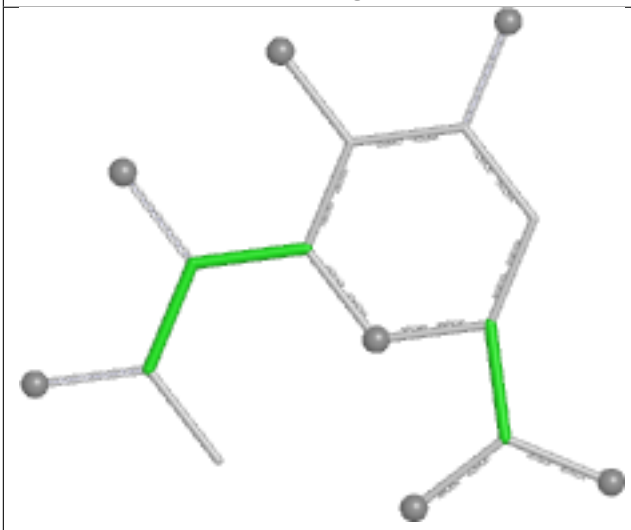

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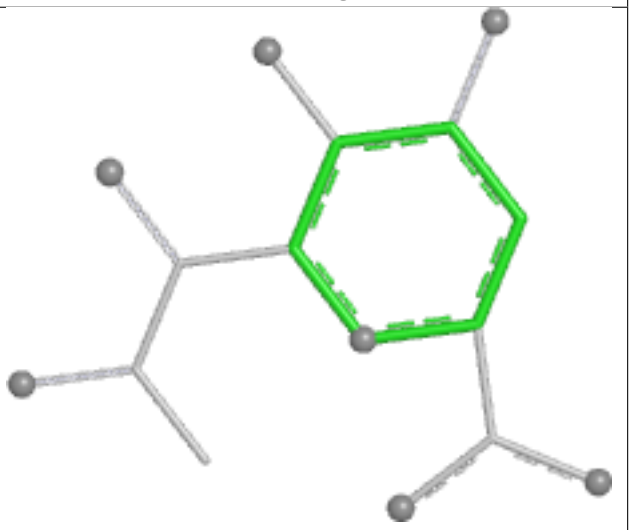
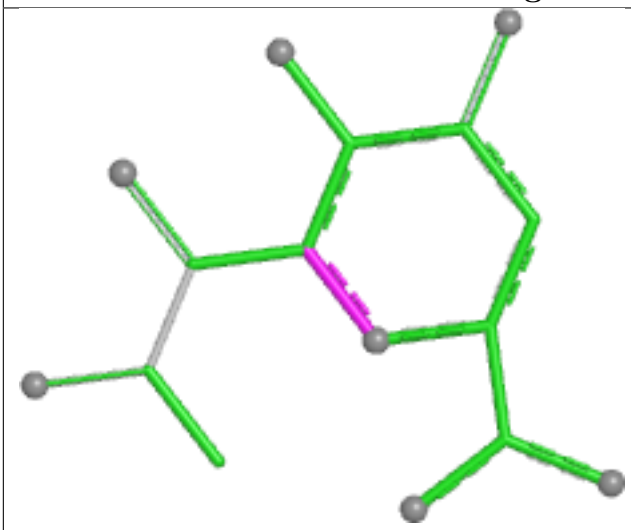


Rings

Ligand P8E e8 602



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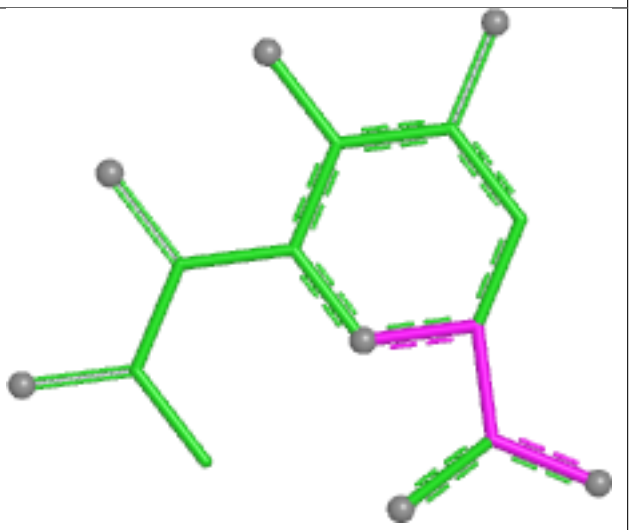

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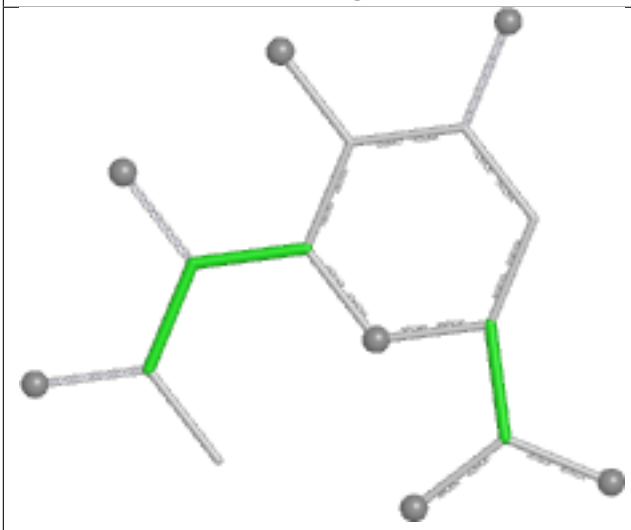

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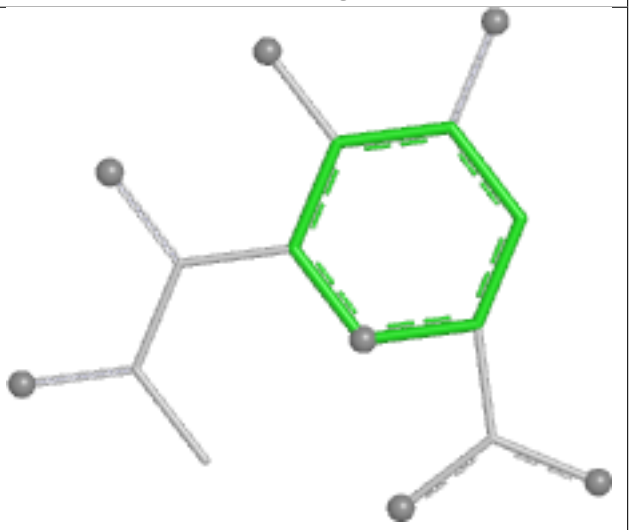
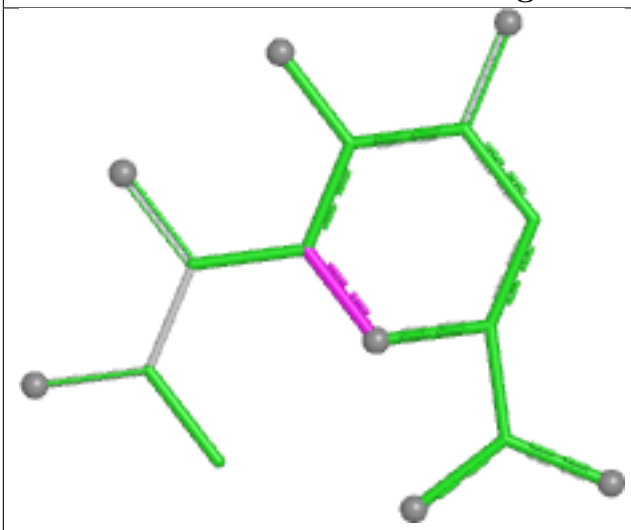


Rings

Ligand P8E HL 603



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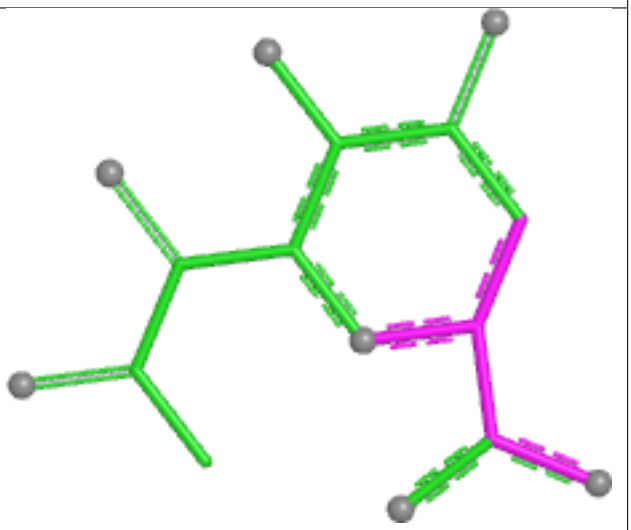

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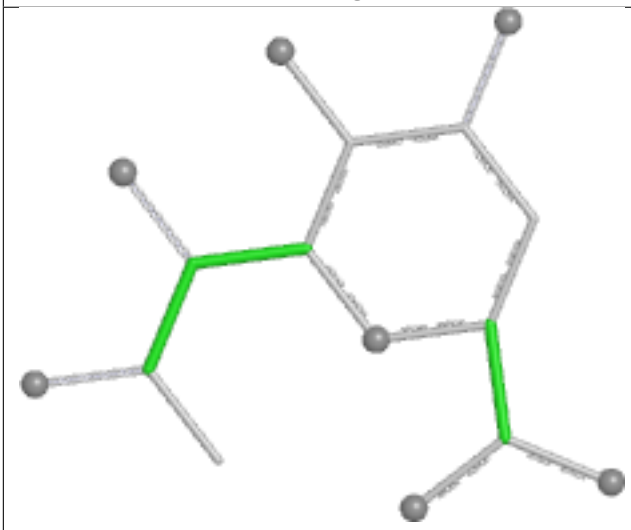

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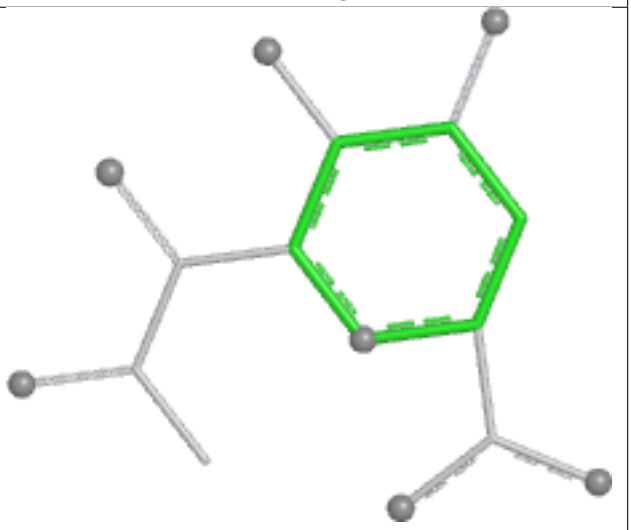
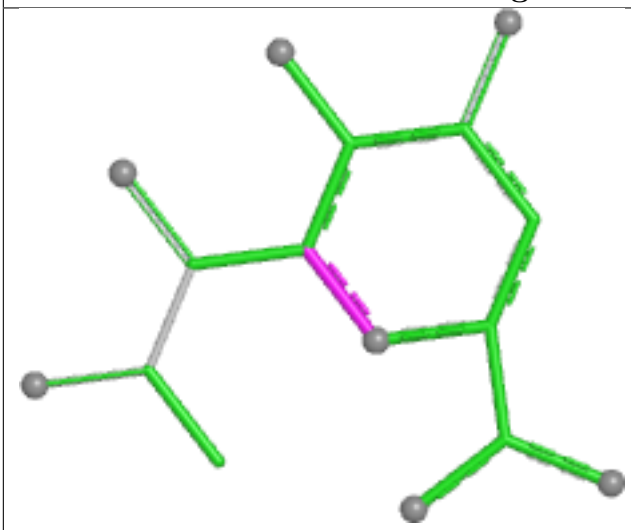


Rings

Ligand P8E XM 601



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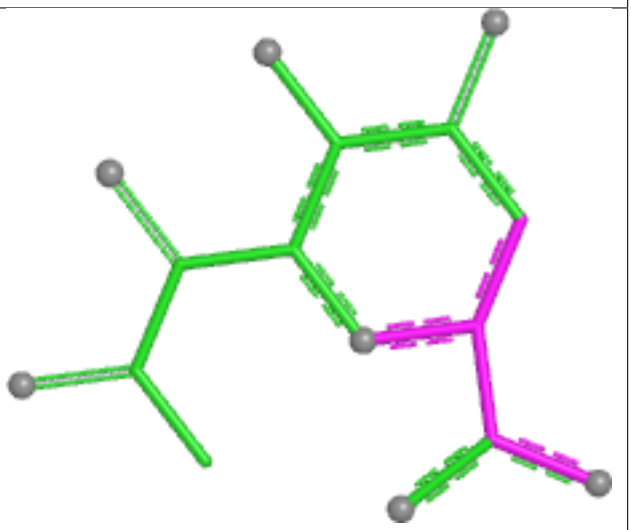

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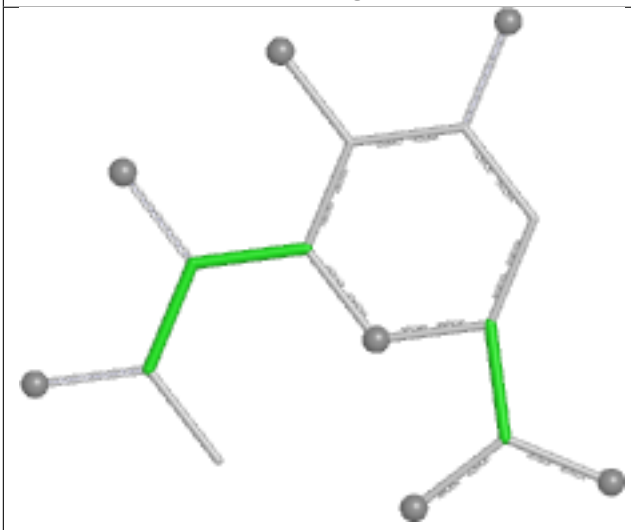

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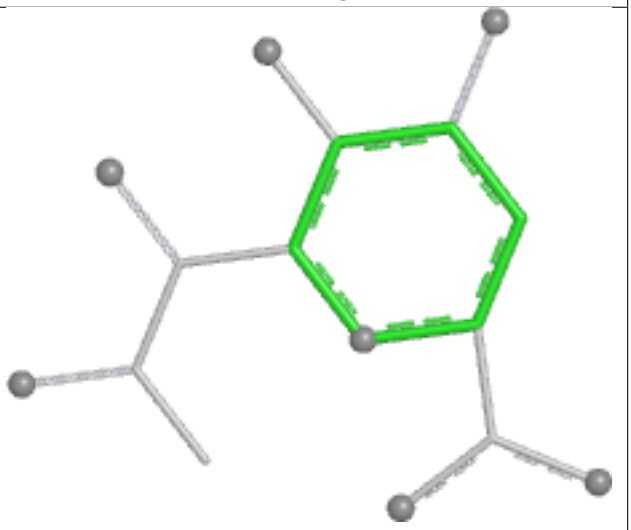
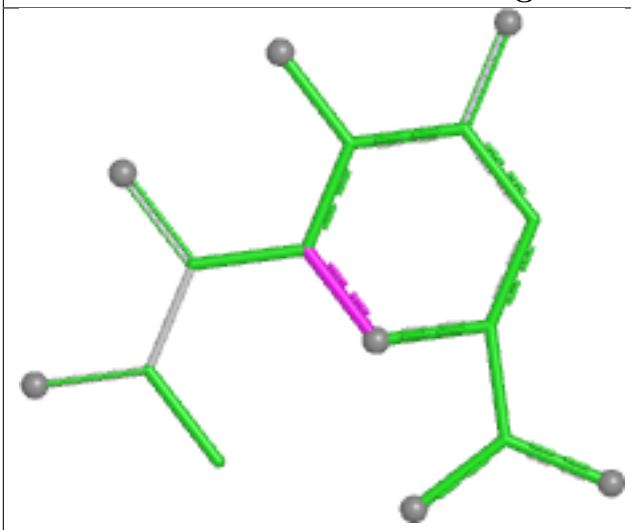


Rings

Ligand P8E KE 604



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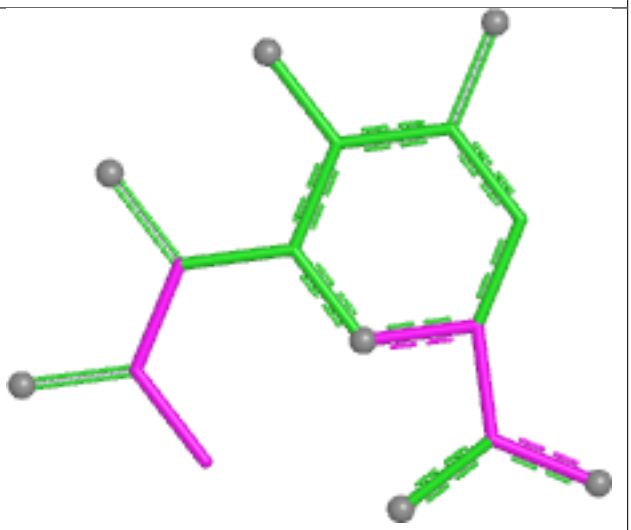

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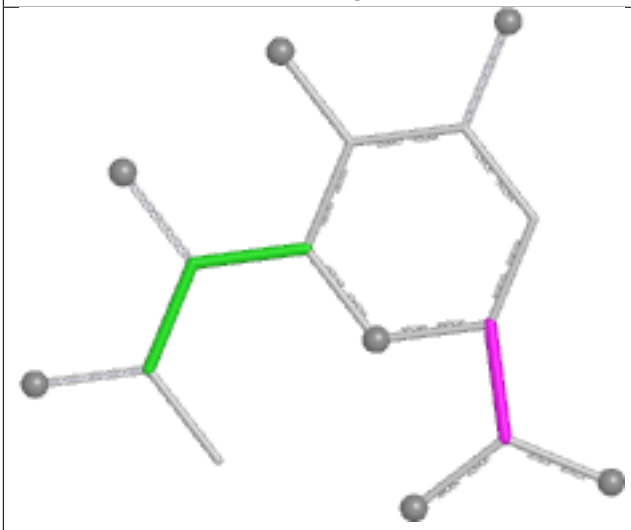

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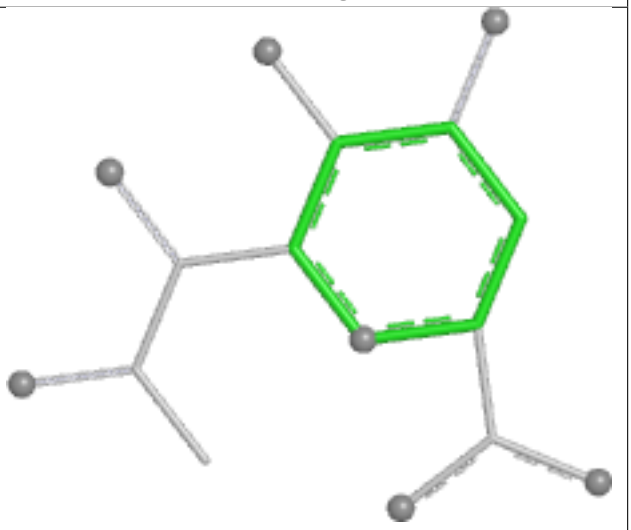
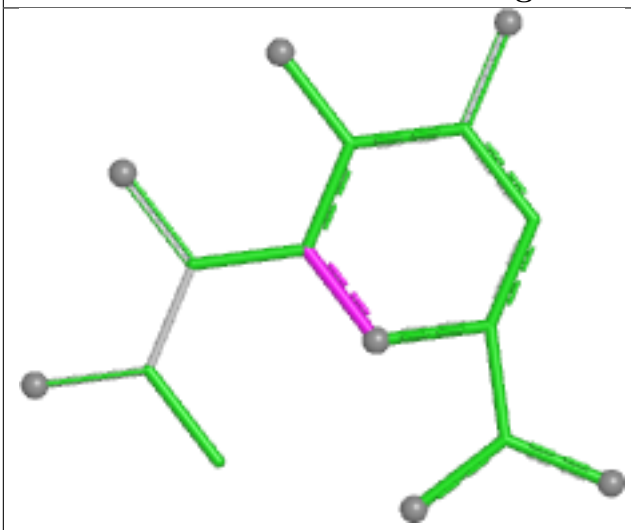


Rings

Ligand P8E PU 602



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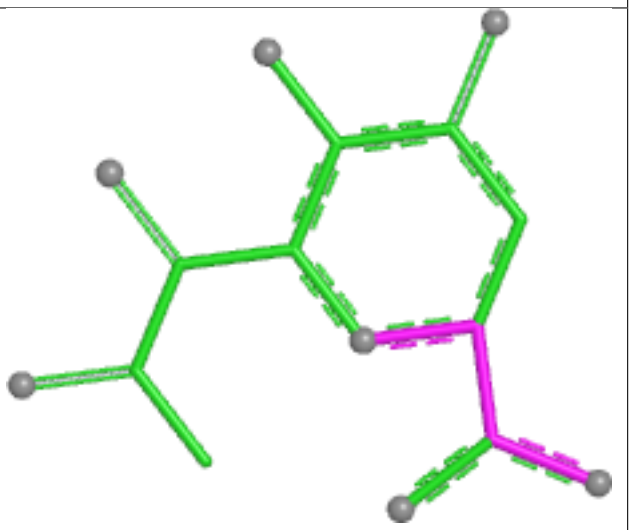

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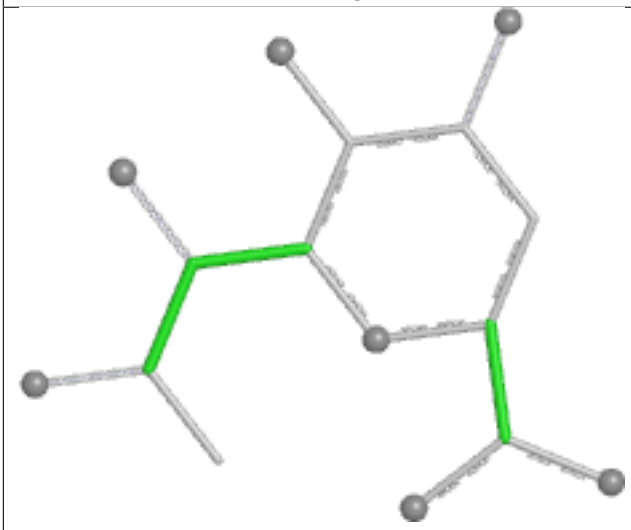

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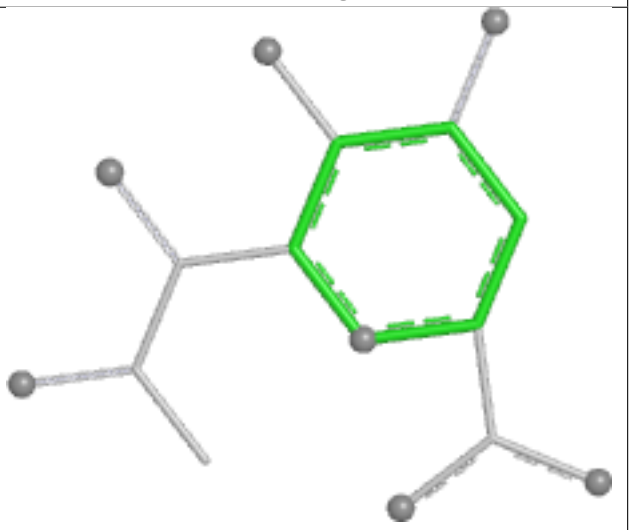
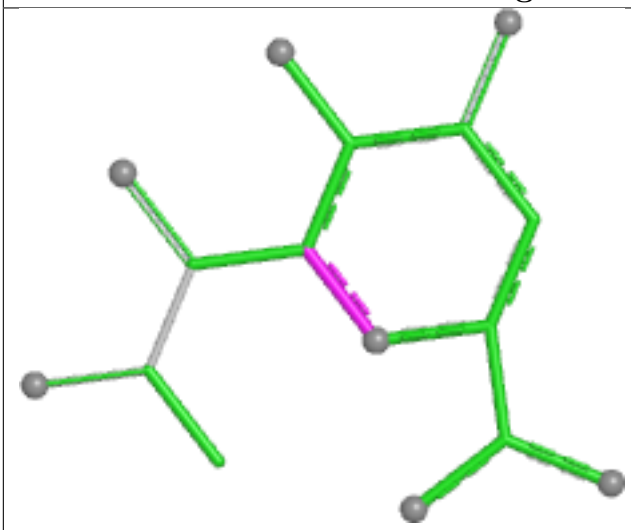


Rings

Ligand P8E KE 601



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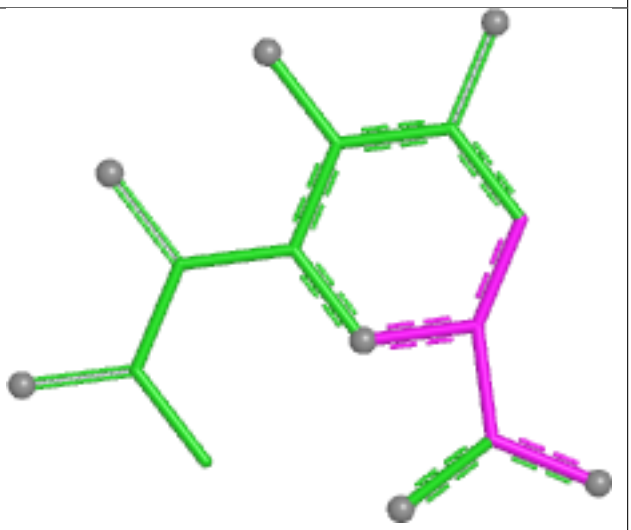

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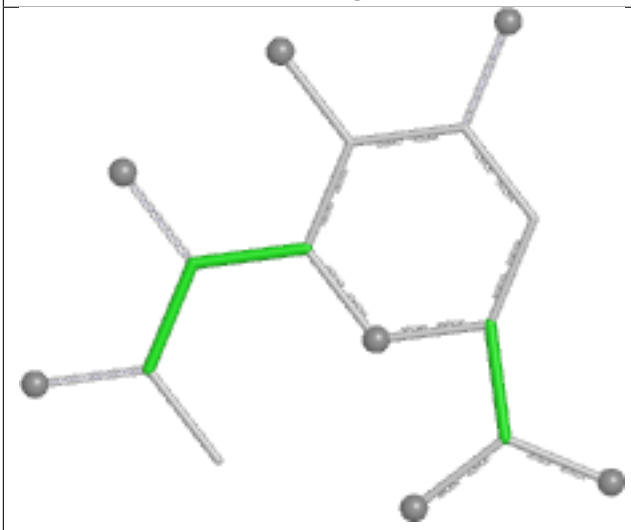

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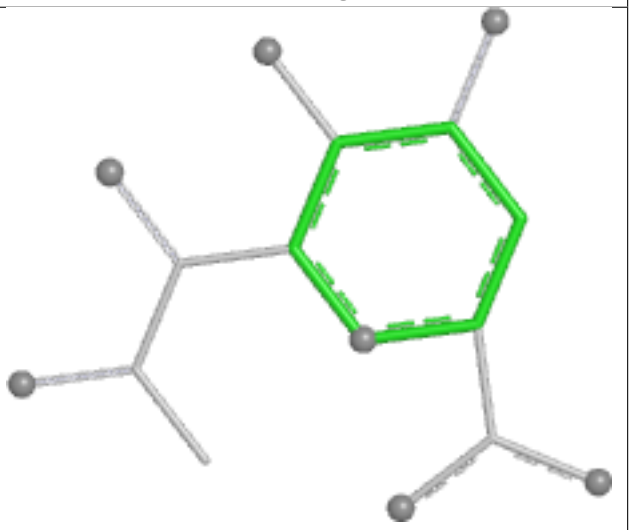
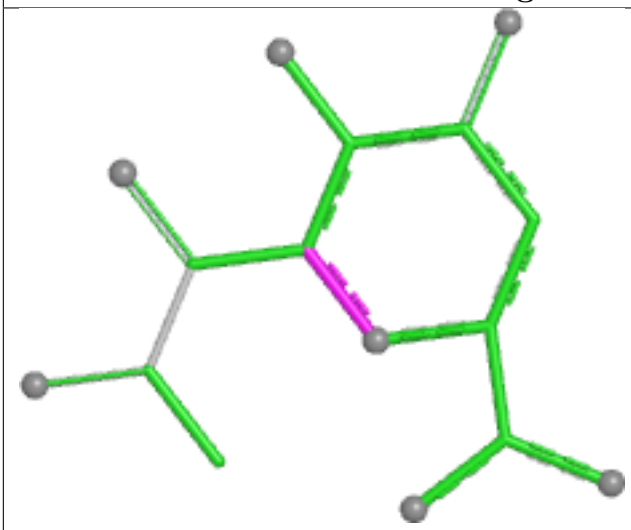


Rings

Ligand P8E HL 602



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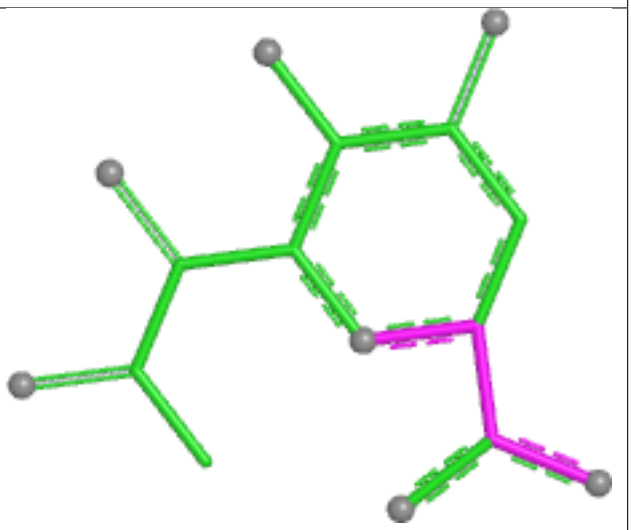
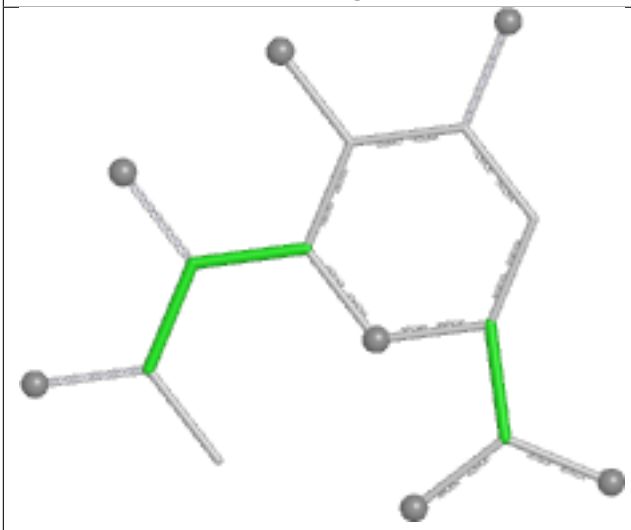


Bond angles



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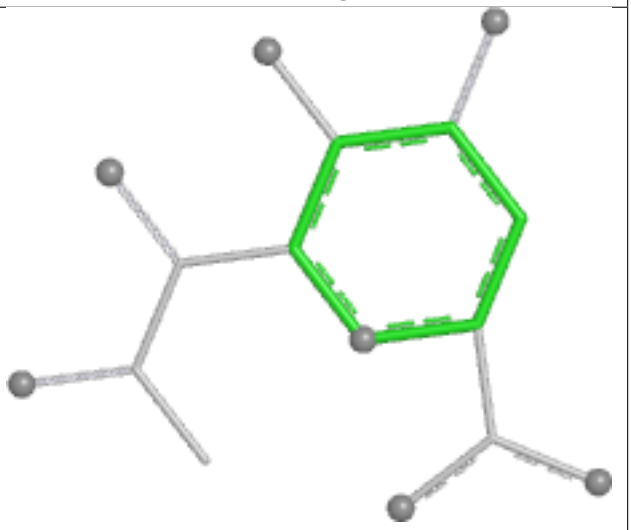
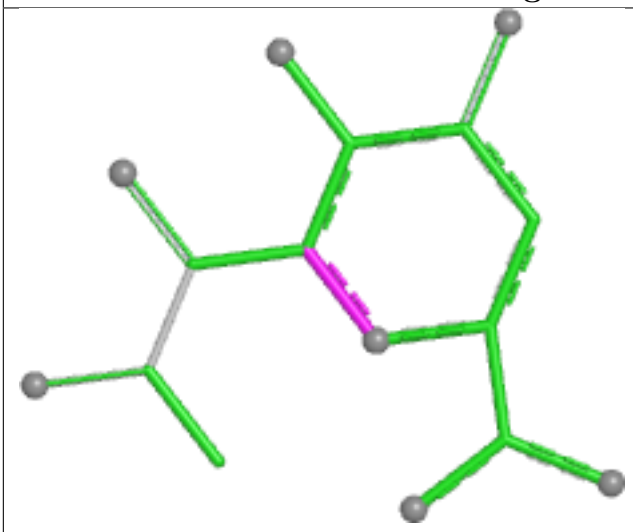
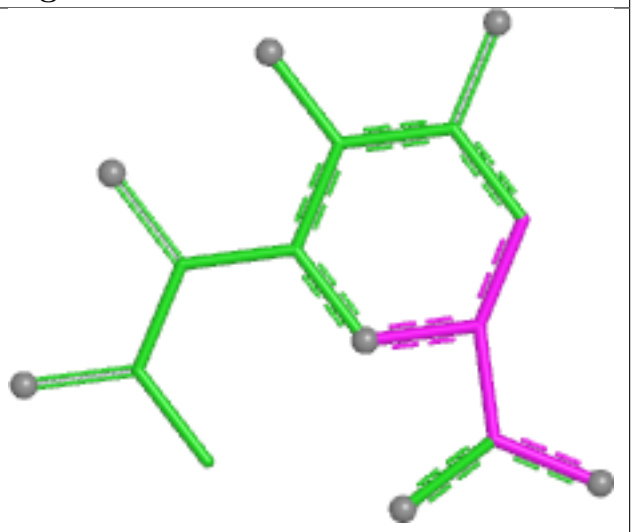


Rings

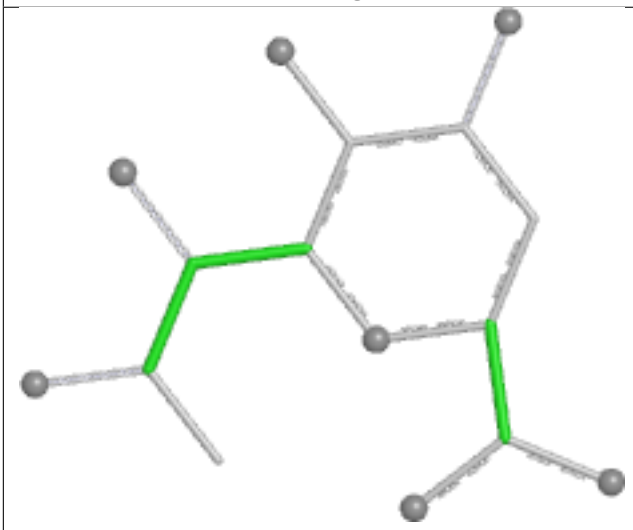
Ligand P8E g6 601



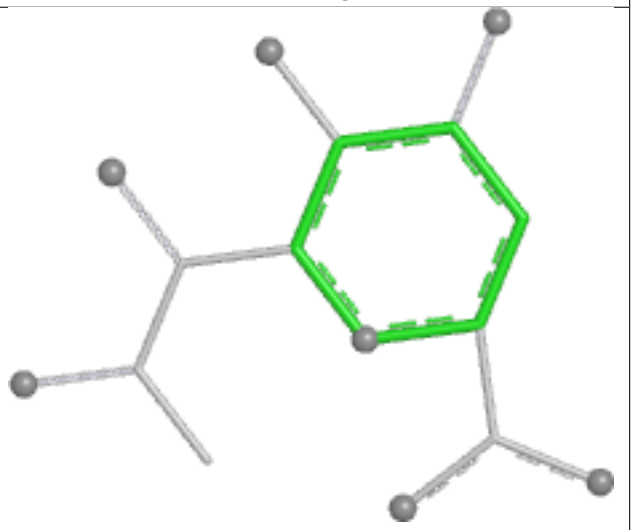
Bond lengths



Bond angles

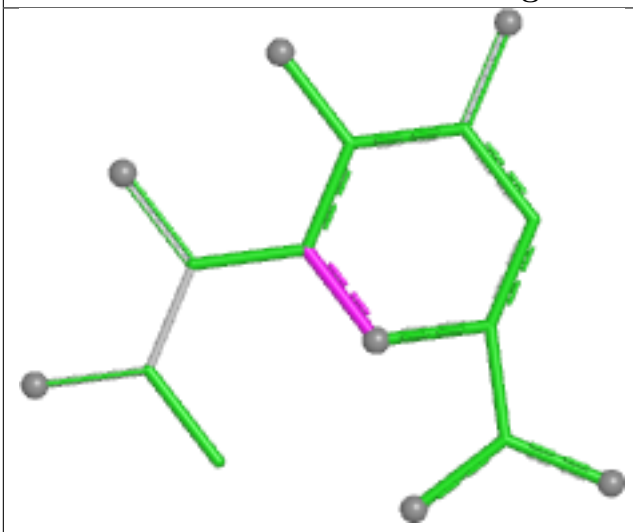


Torsions



Rings

Ligand P8E Z9 603



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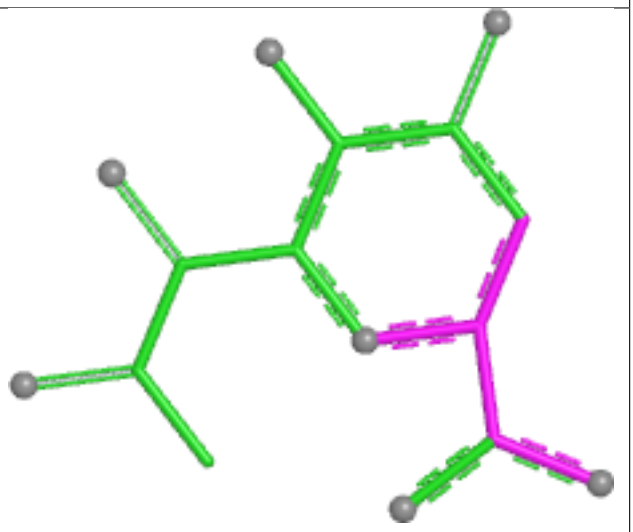

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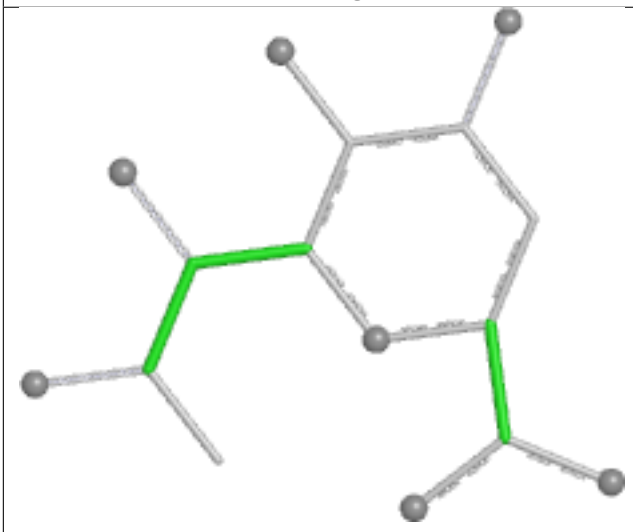

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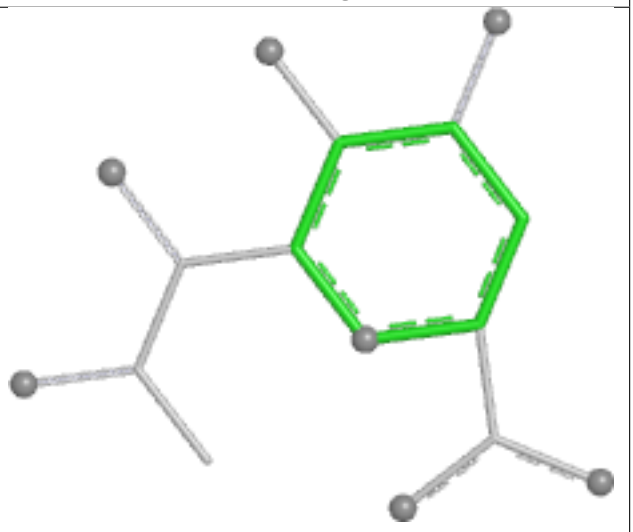
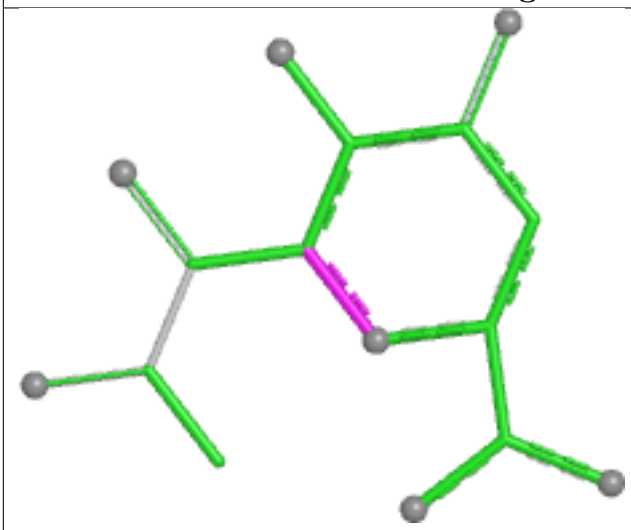


Rings

Ligand P8E Q2 607



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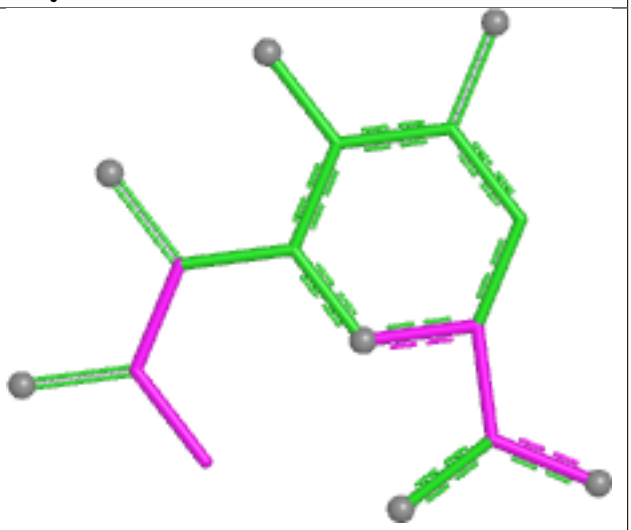

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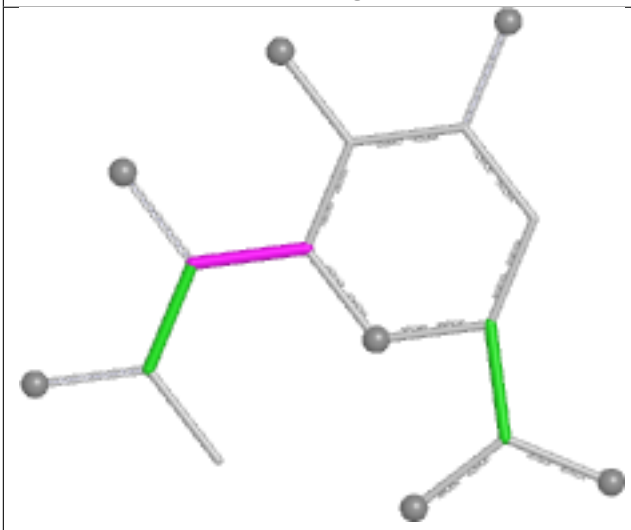

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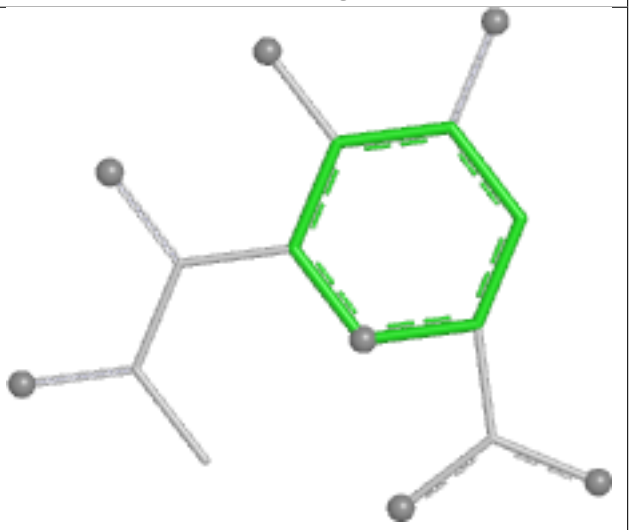
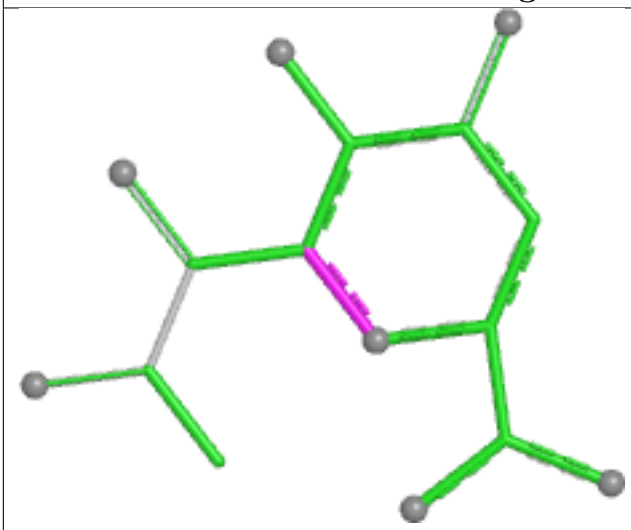


Rings

Ligand P8E dC 601



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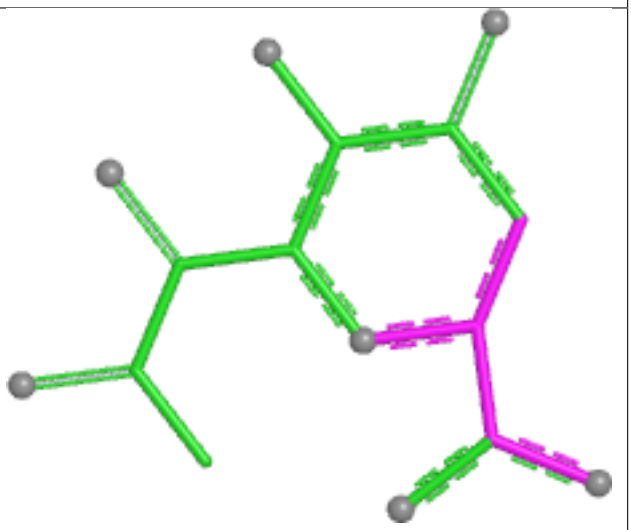
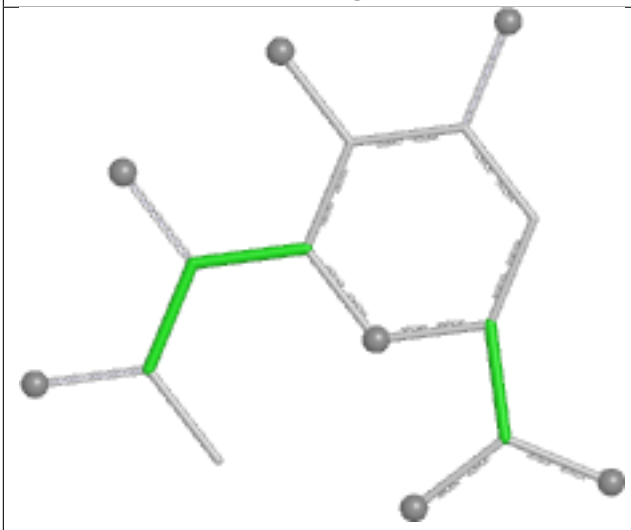


Bond angles



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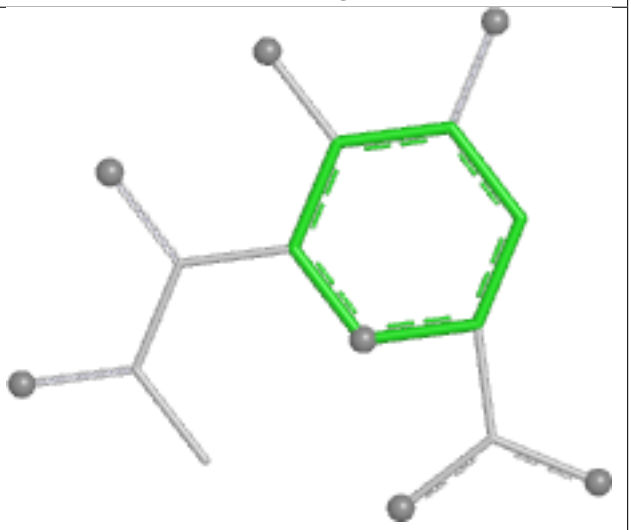
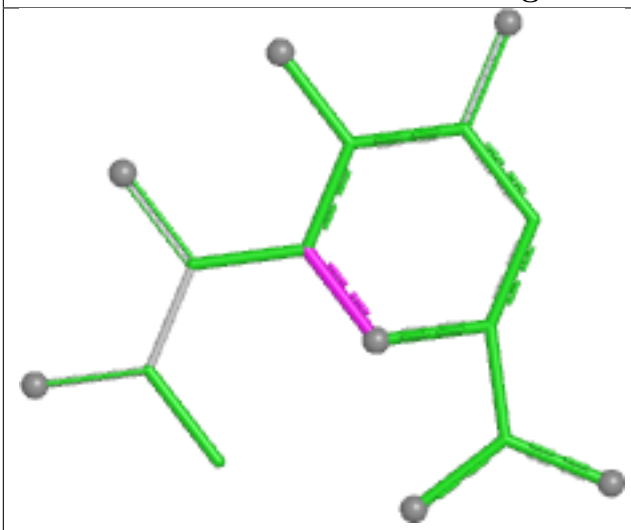


Rings

Ligand P8E Z9 601



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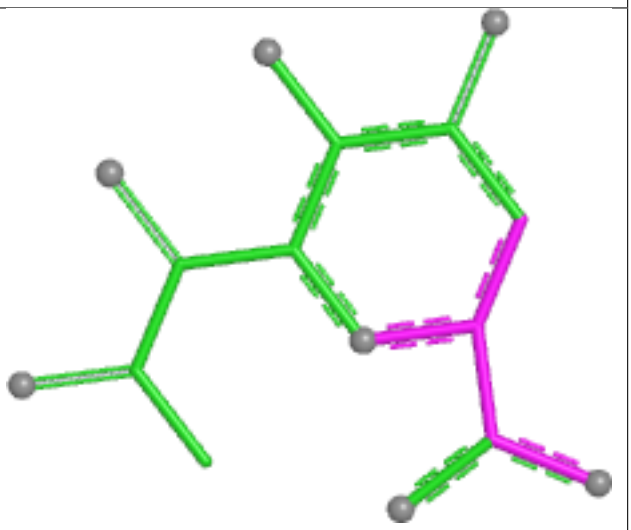

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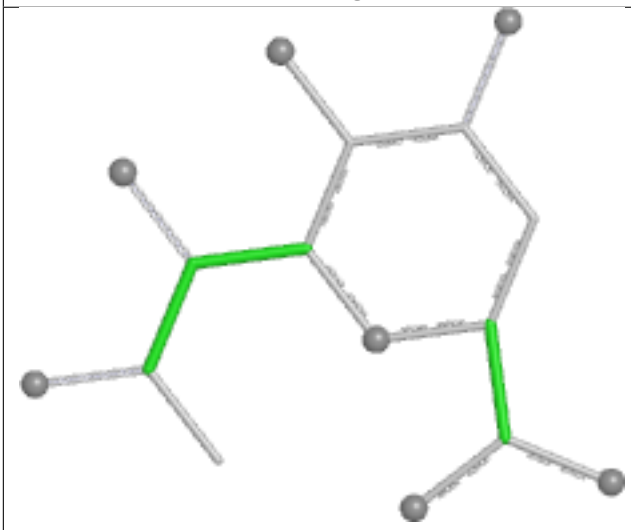

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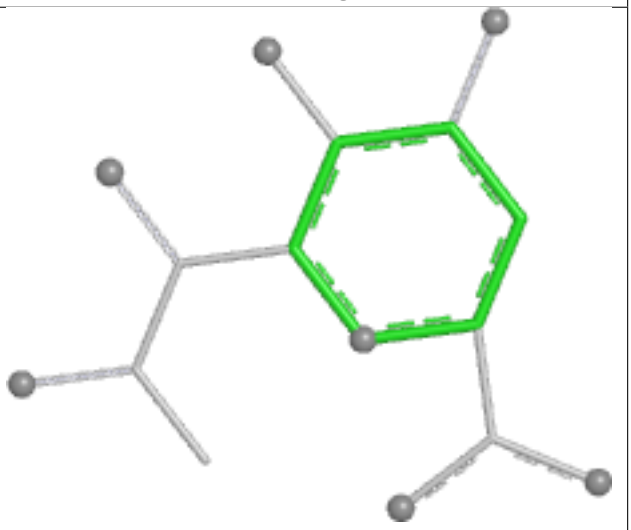
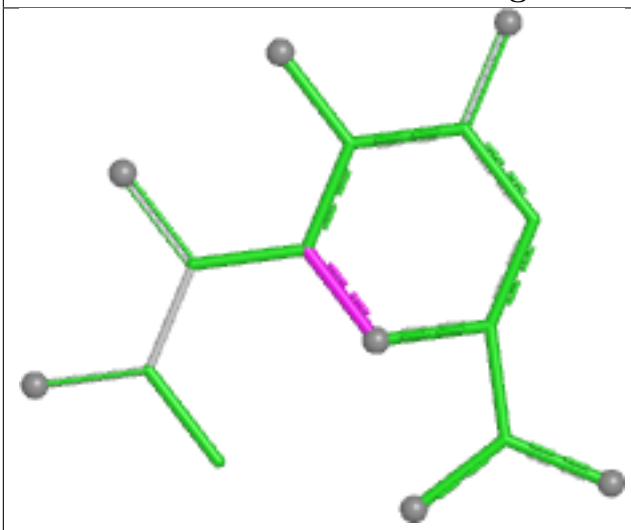


Rings

Ligand P8E WG 604



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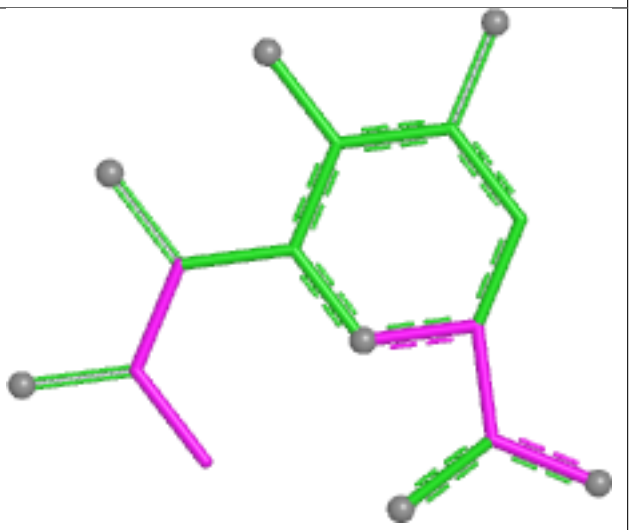

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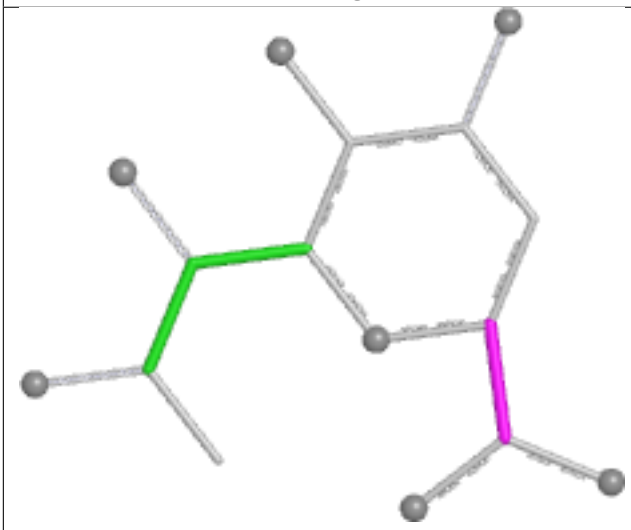

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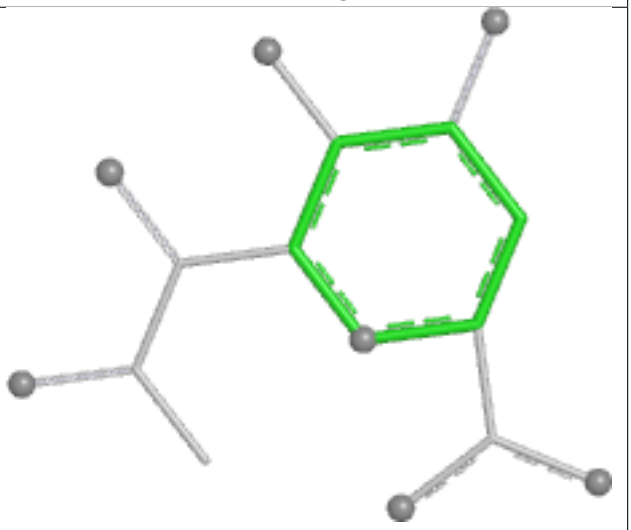
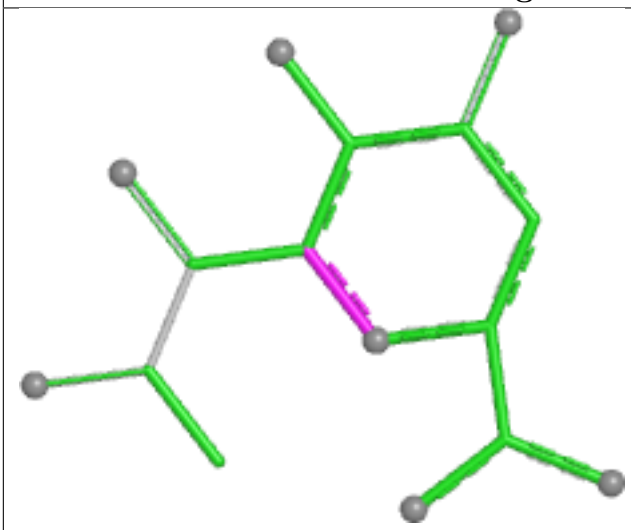


Rings

Ligand P8E KE 606



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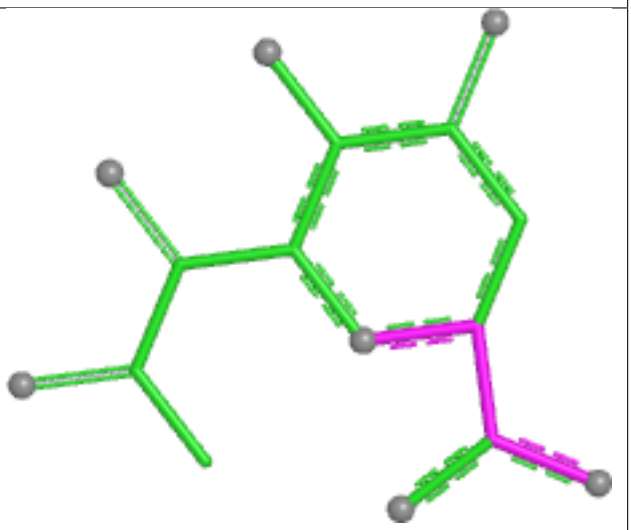

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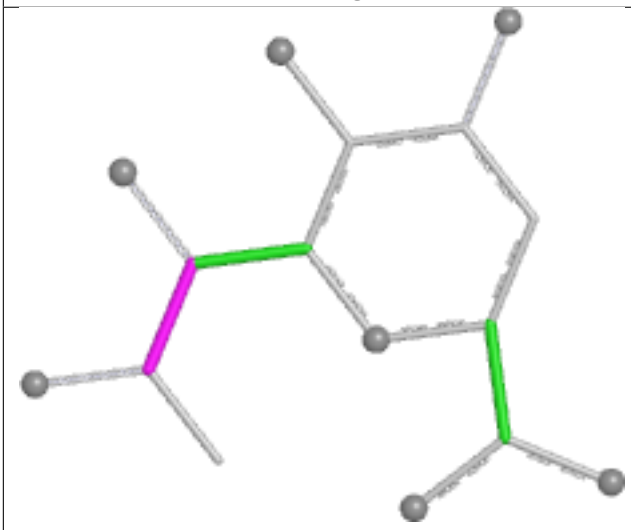

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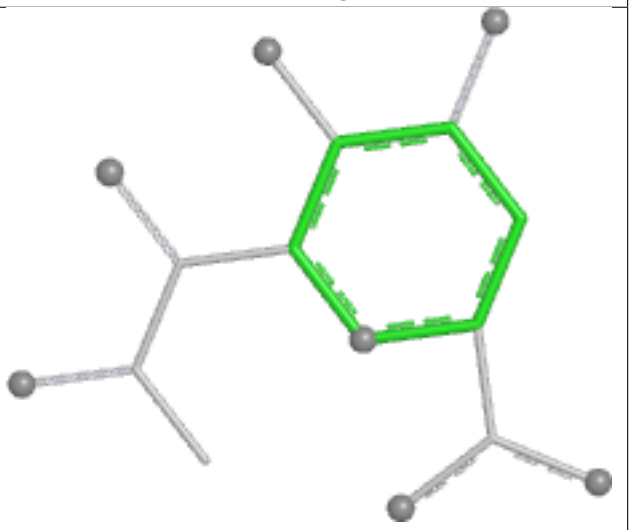
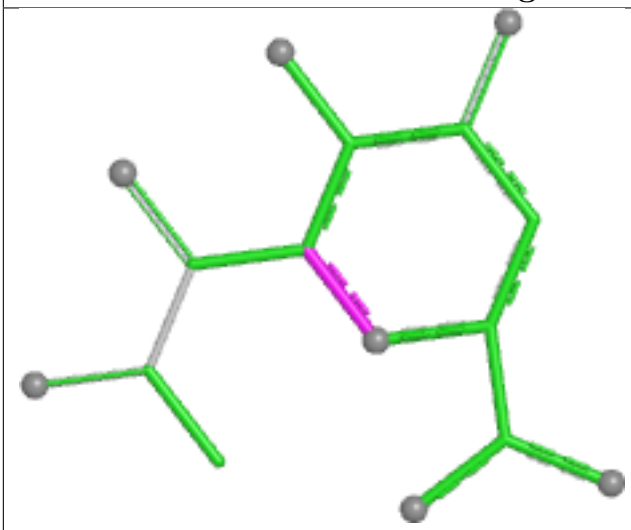


Rings

Ligand P8E JD 604



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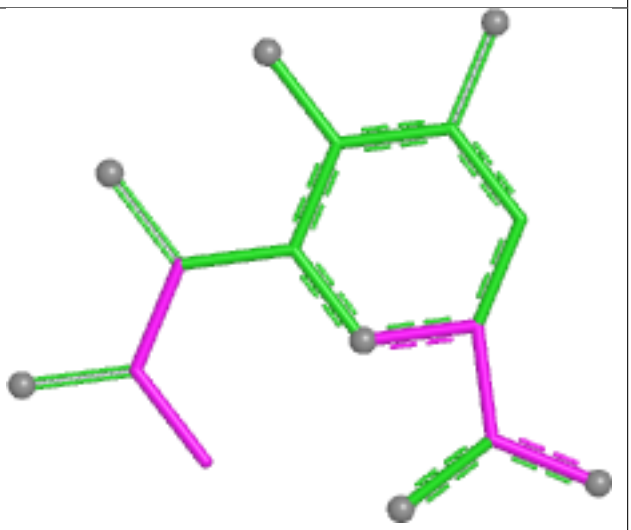

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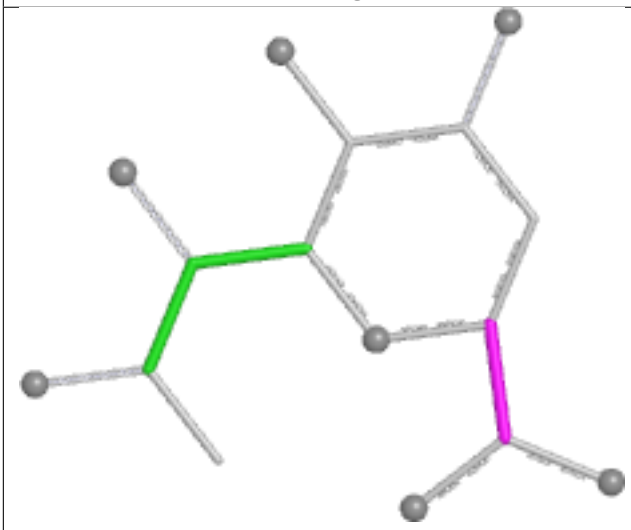

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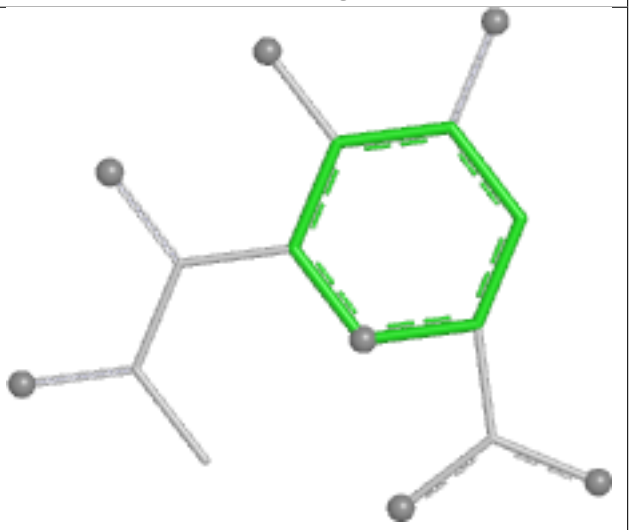

Rings

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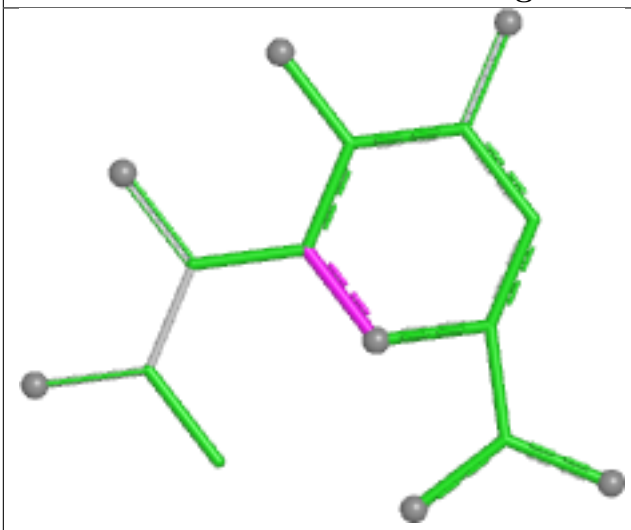

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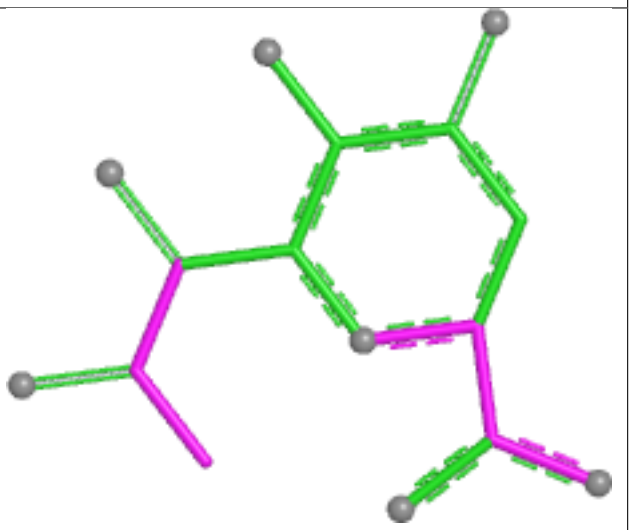

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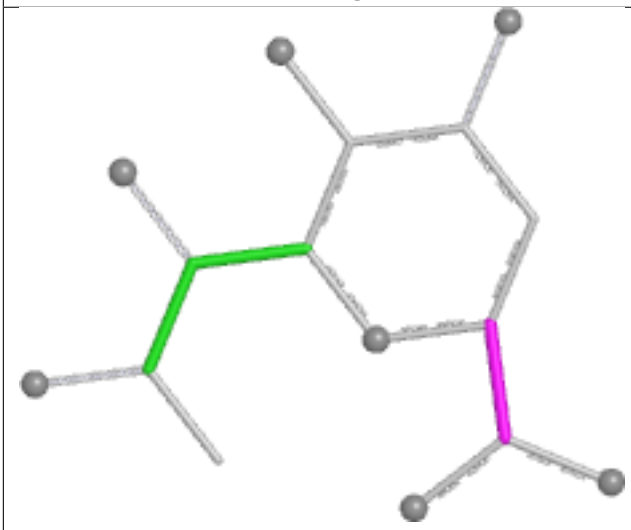

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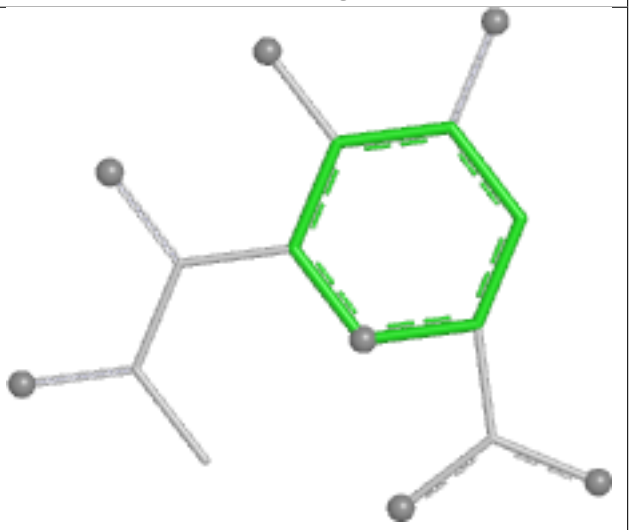
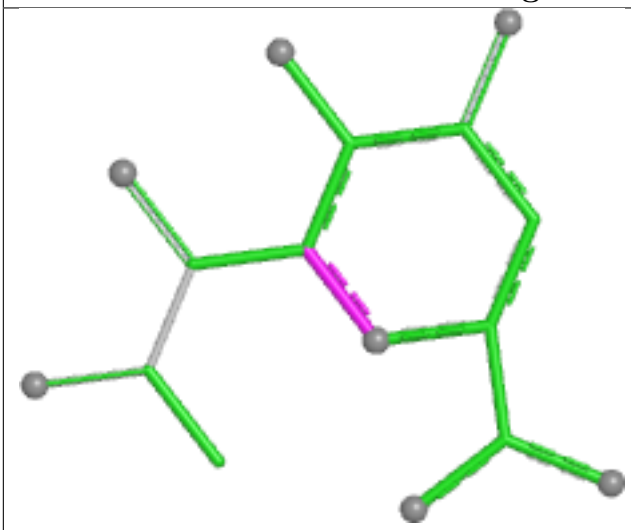


Rings

Ligand P8E fK 605



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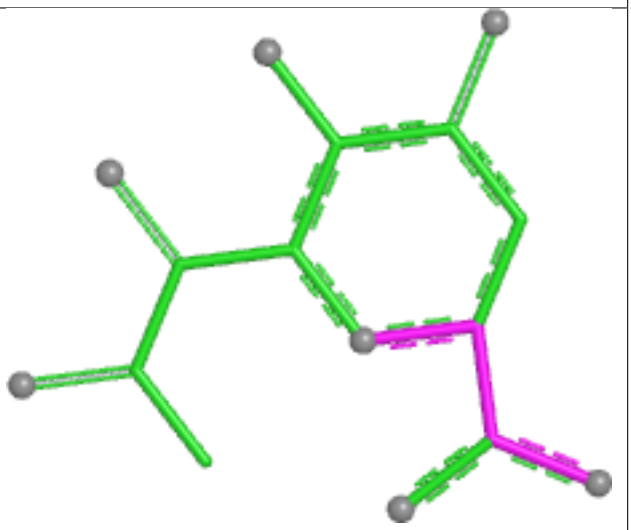

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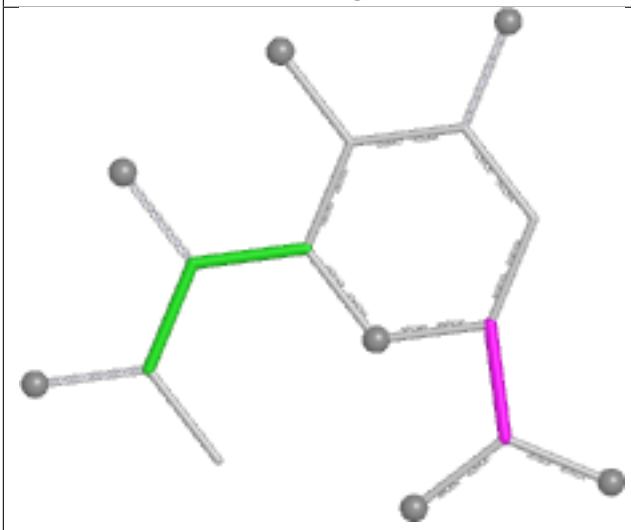

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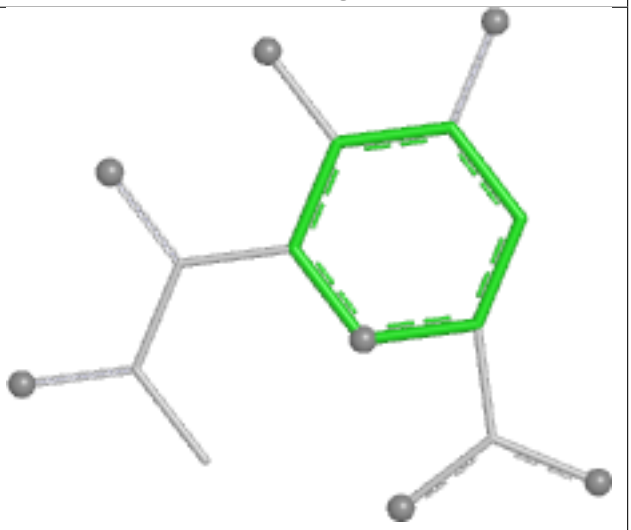
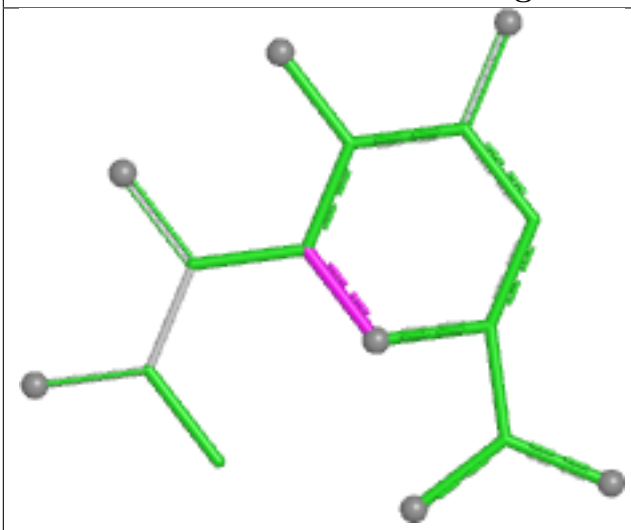


Rings

Ligand P8E VR 601



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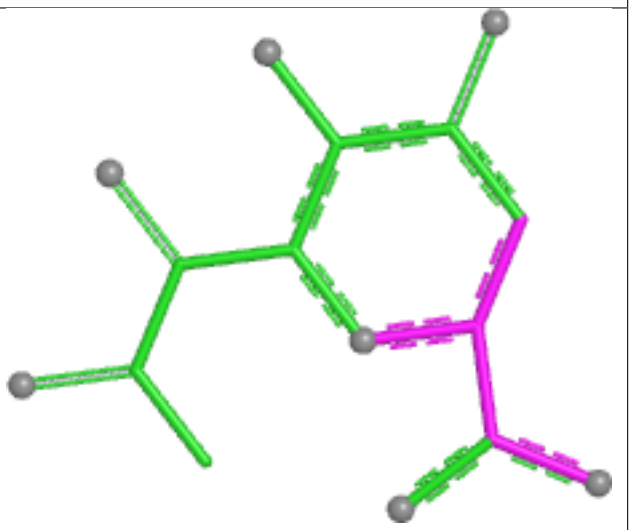

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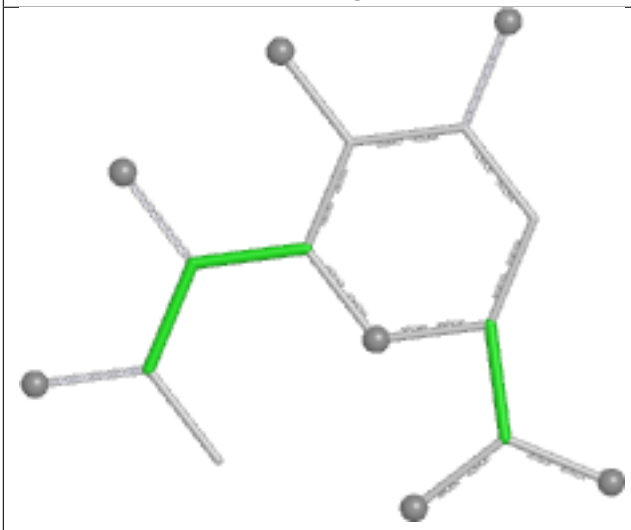

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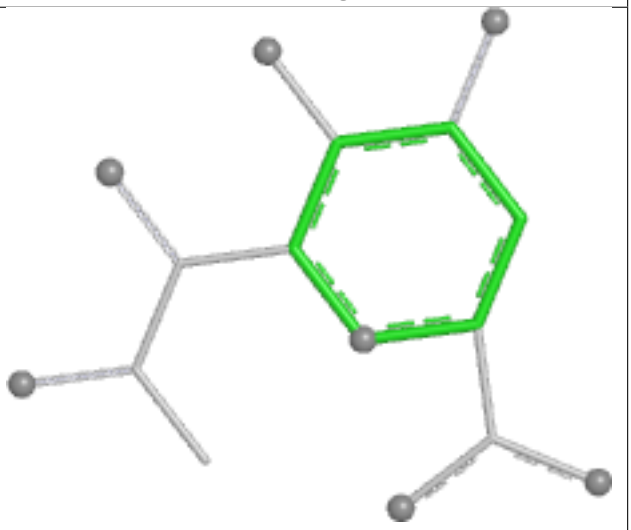
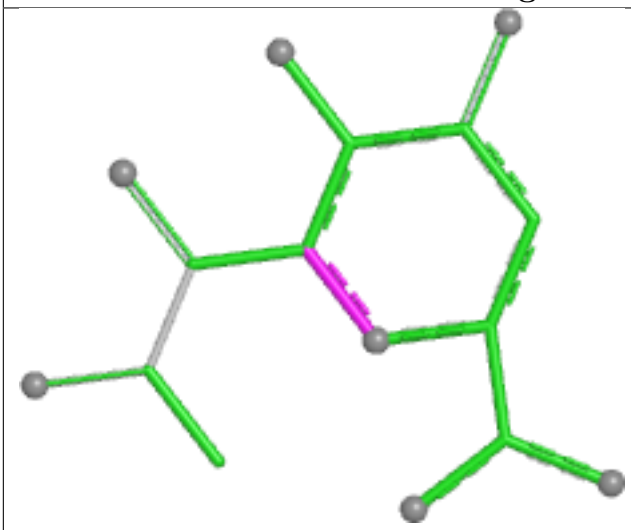


Rings

Ligand P8E dC 603



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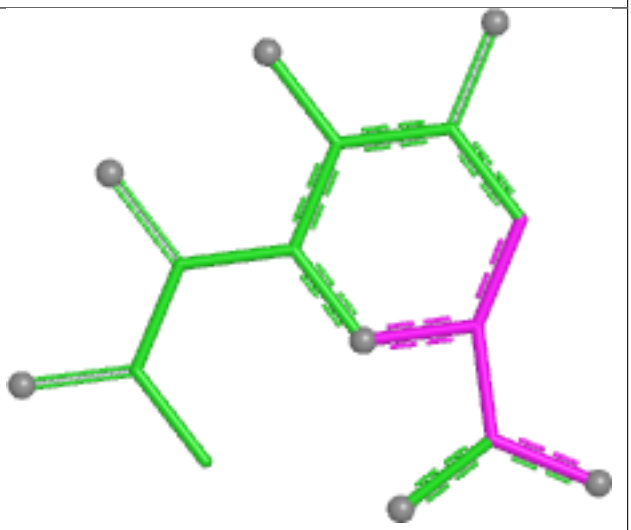
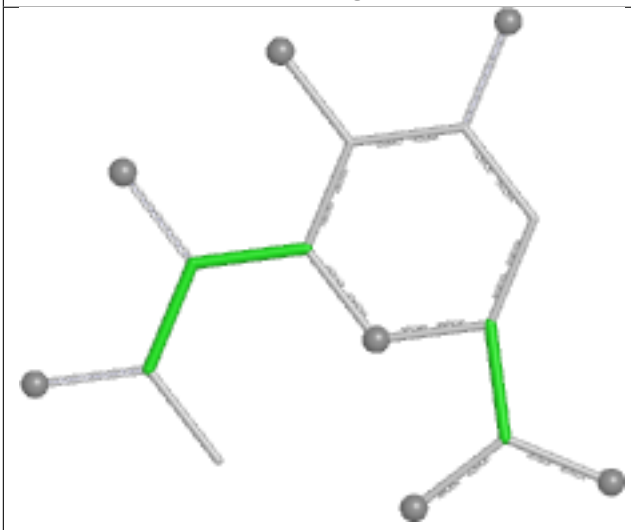


Bond angles



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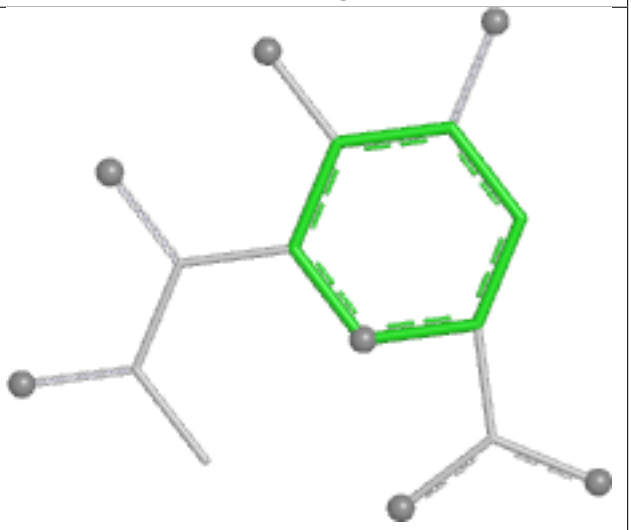
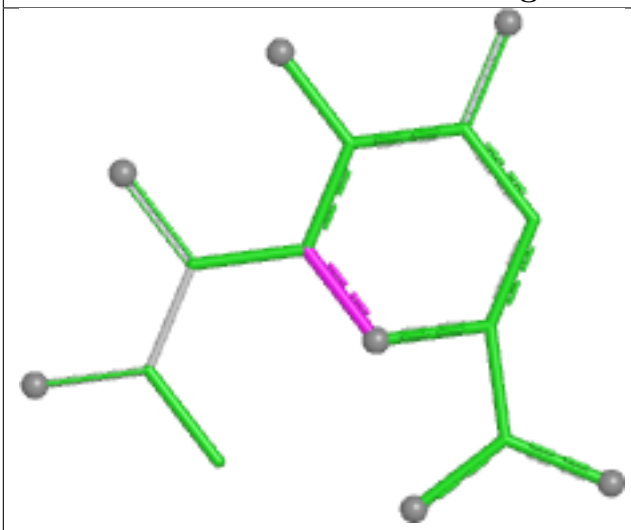


Rings

Ligand P8E cV 605



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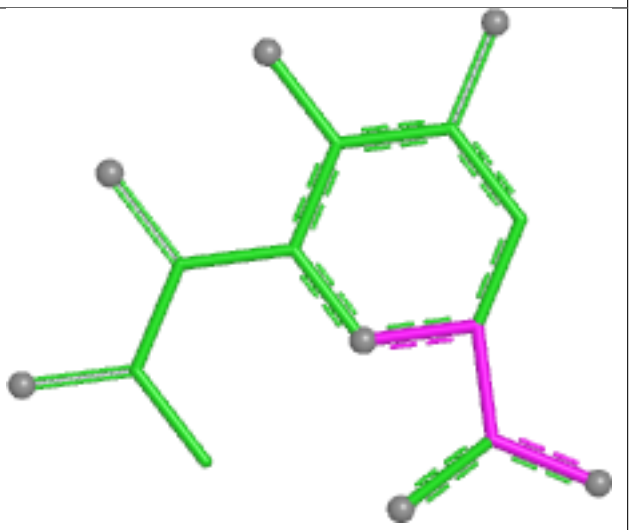
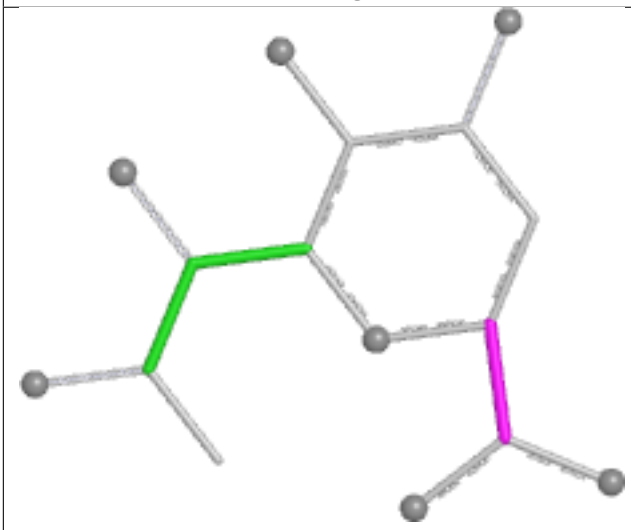


Bond angles



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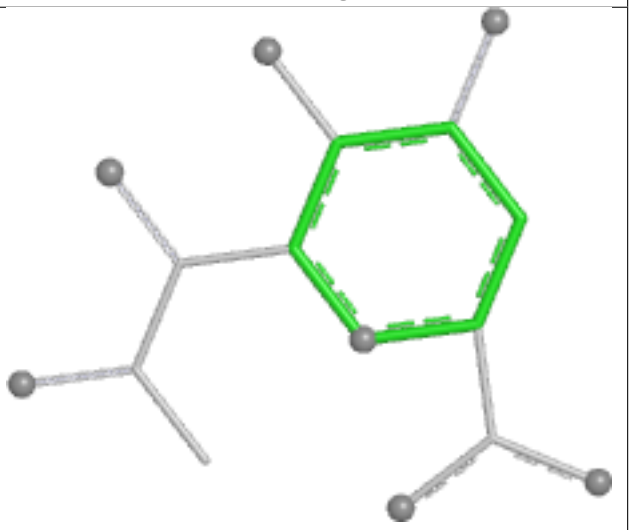
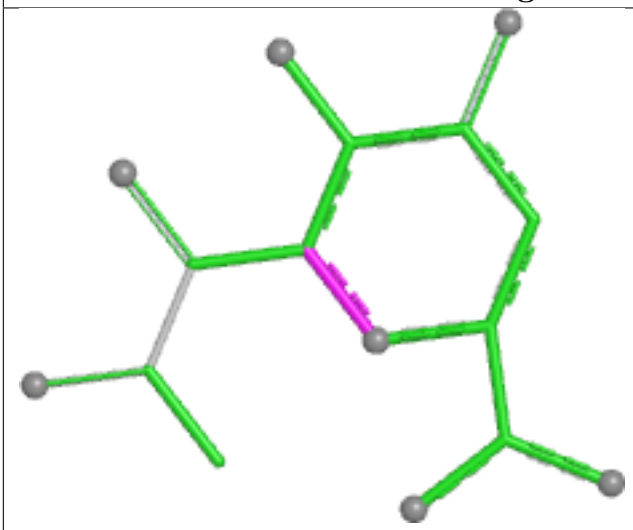


Rings

Ligand P8E FB 604



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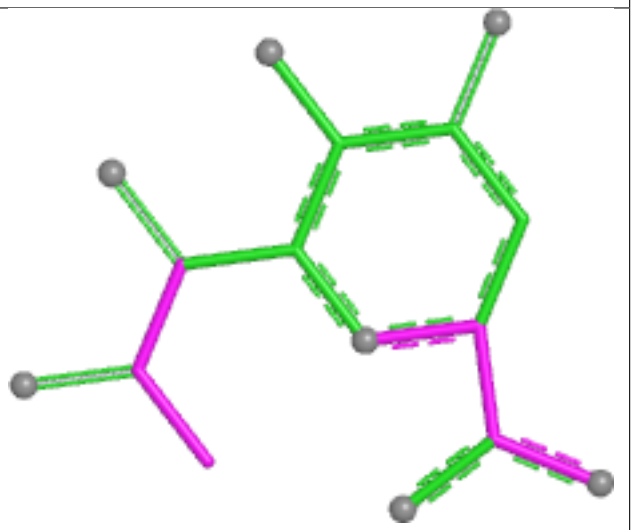
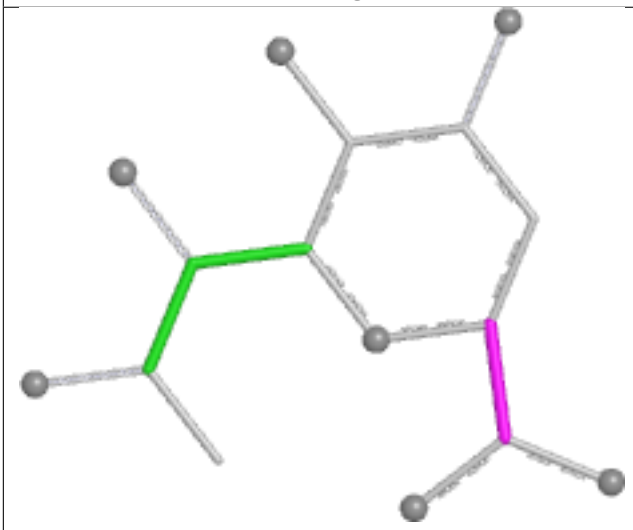
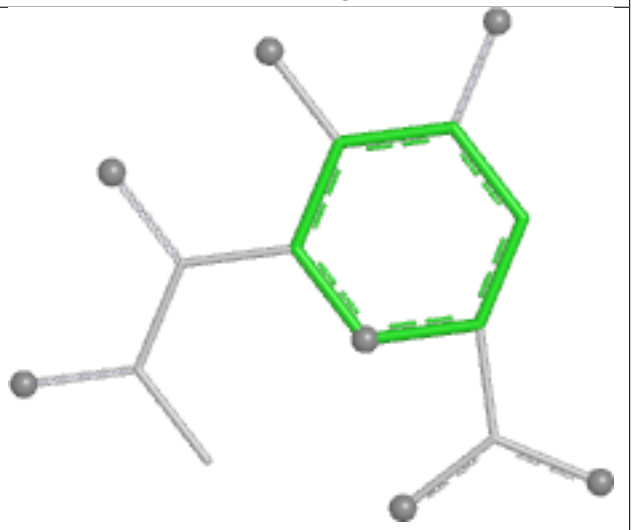


Bond angles

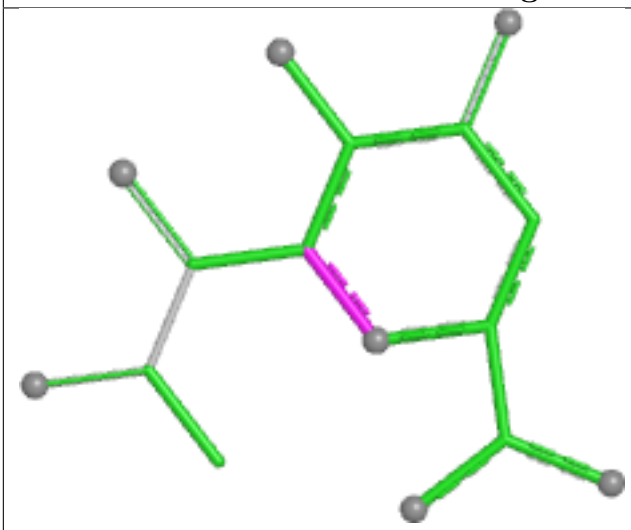


Torsions

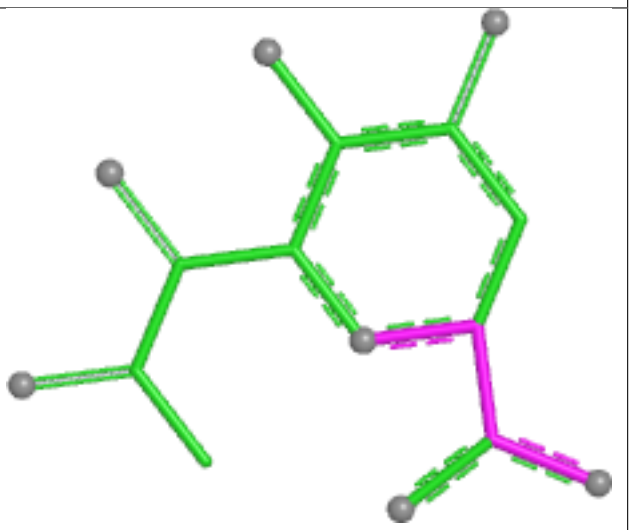


Rings

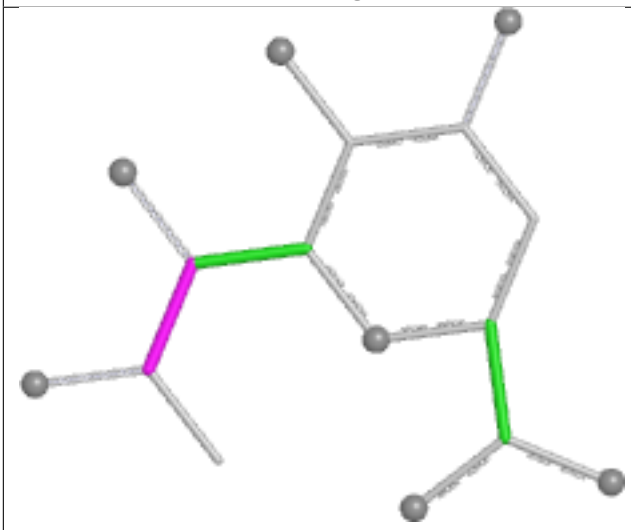
Ligand P8E NI 606



Bond lengths



Bond angles



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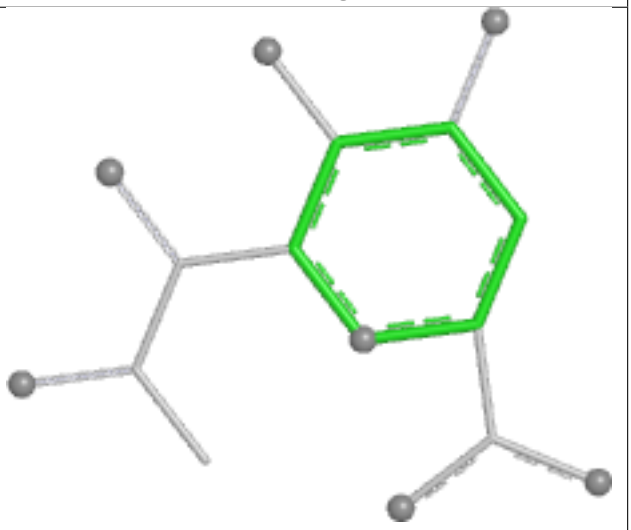
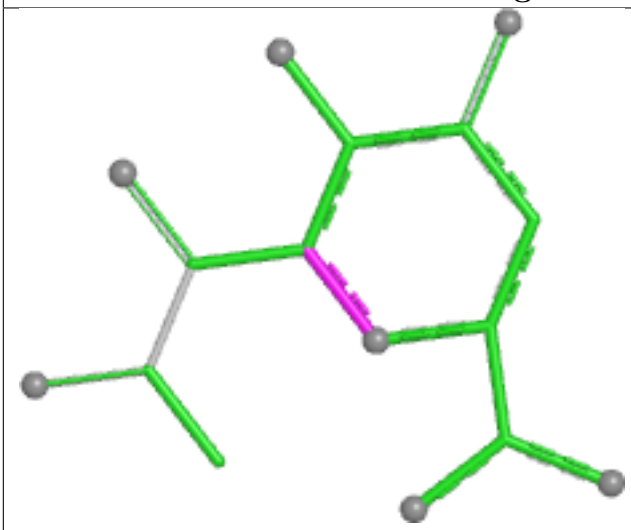


Rings

Ligand P8E GQ 603



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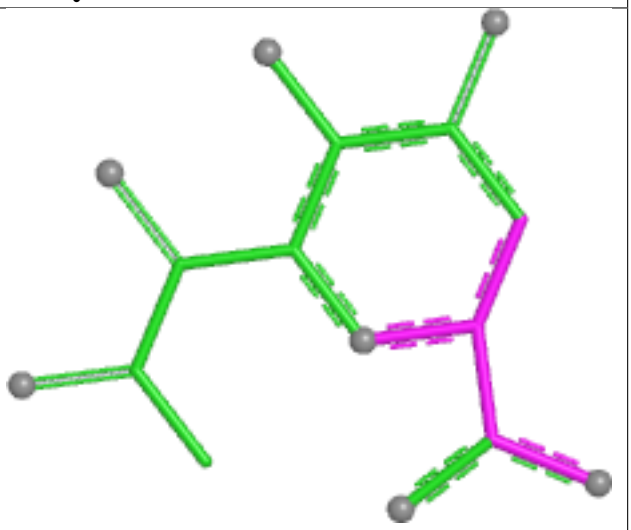
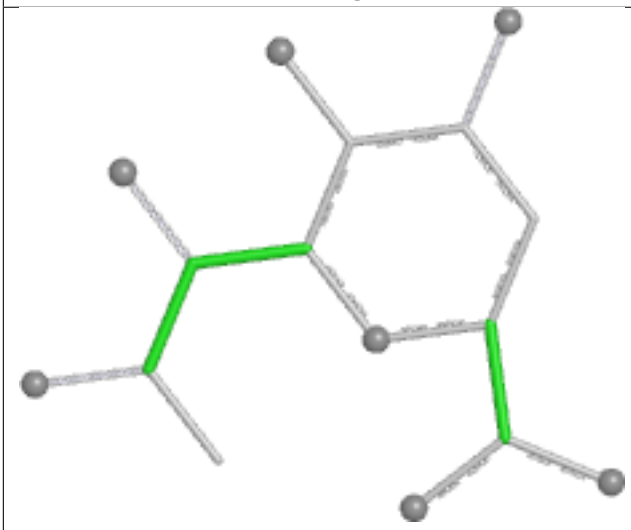


Bond angles



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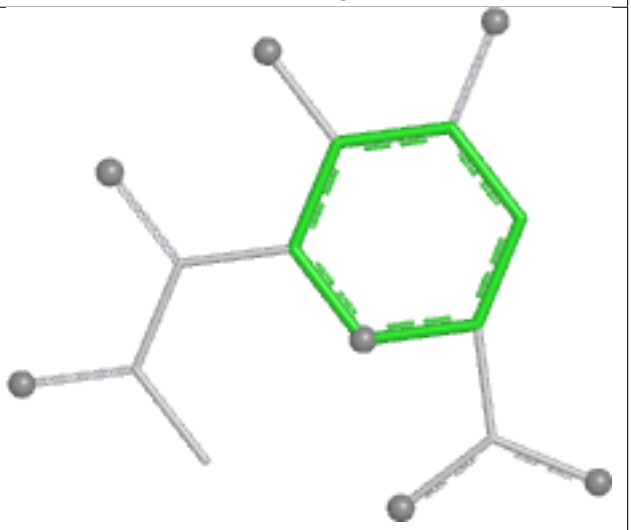
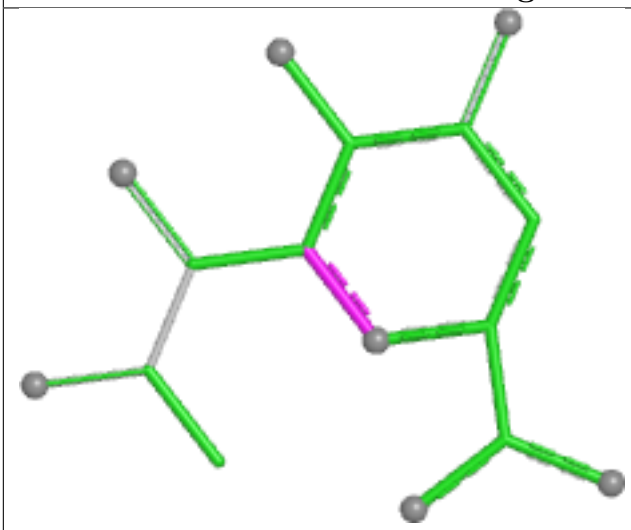


Rings

Ligand P8E FB 601



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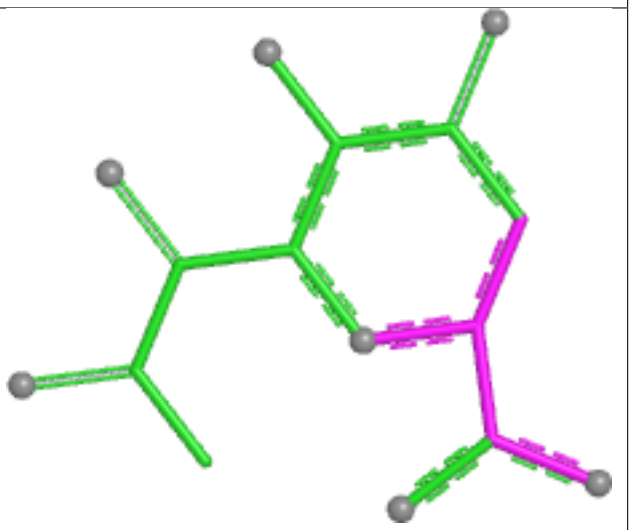
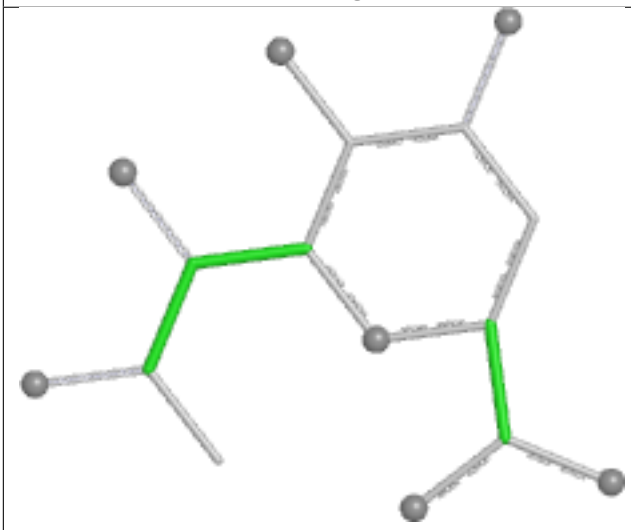


Bond angles



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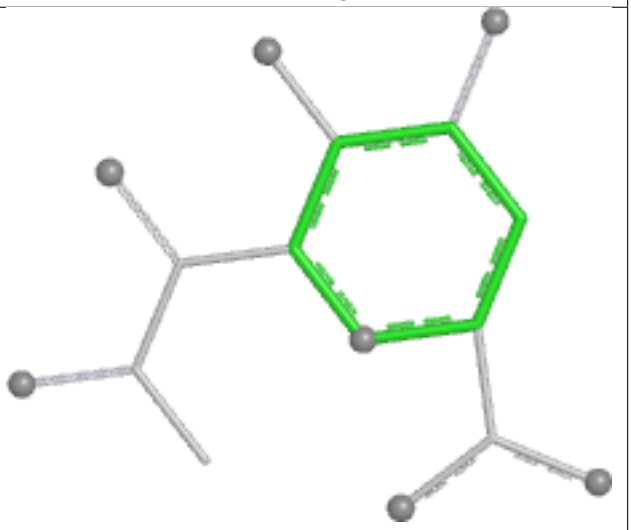
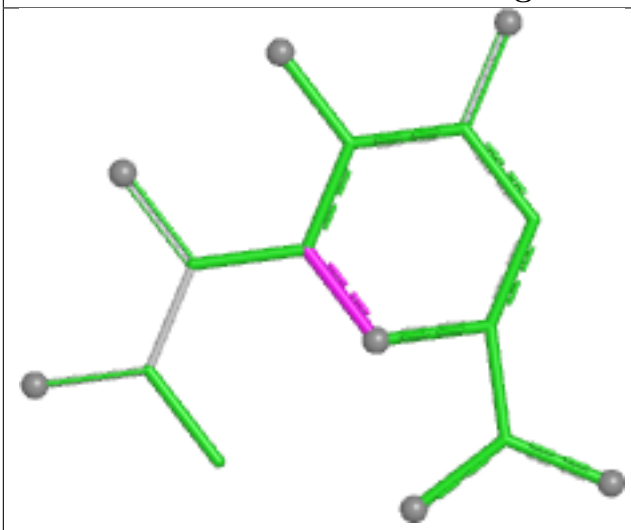


Rings

Ligand P8E VR 603



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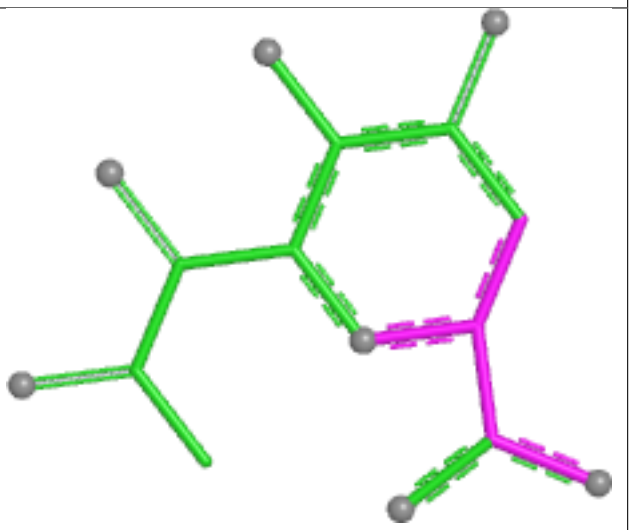
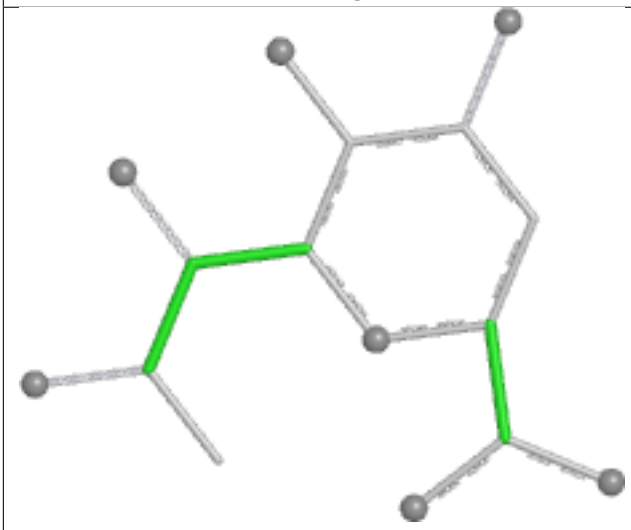


Bond angles



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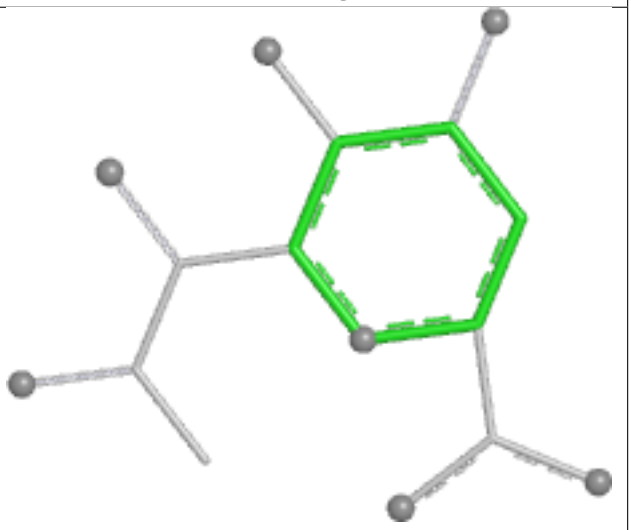
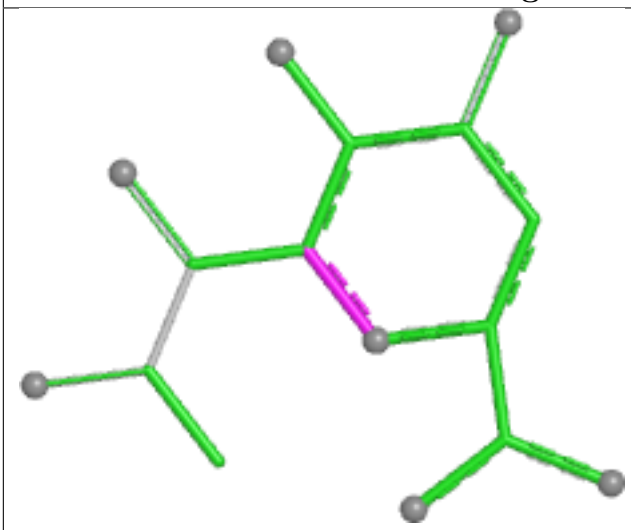


Rings

Ligand P8E bS 603



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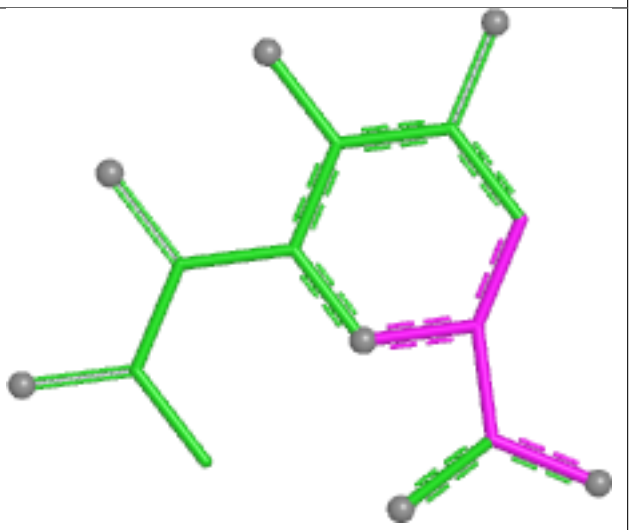

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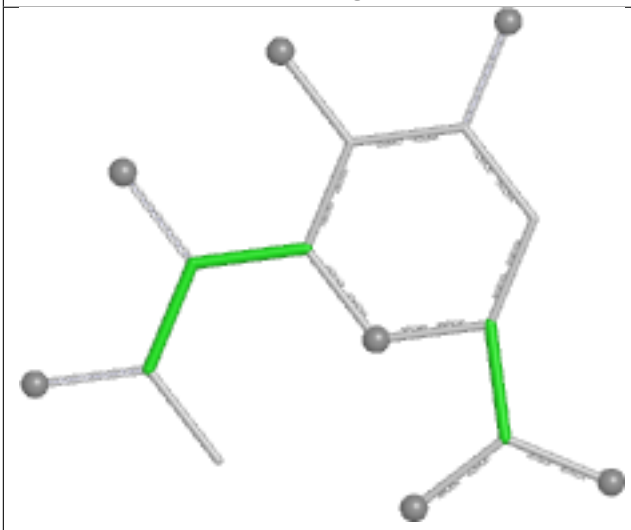

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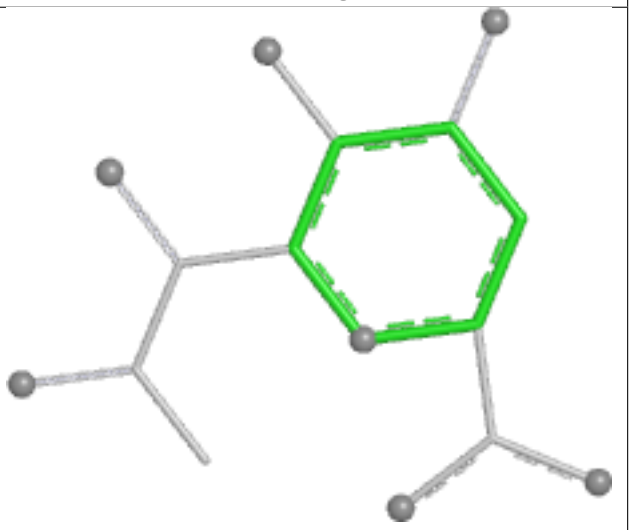
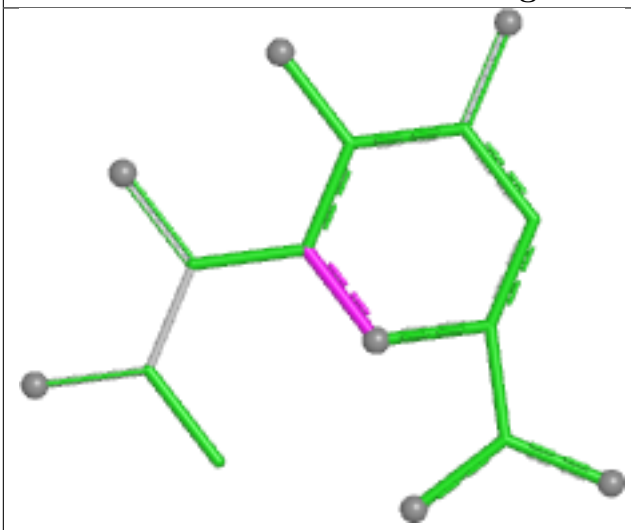


Rings

Ligand P8E LF 602



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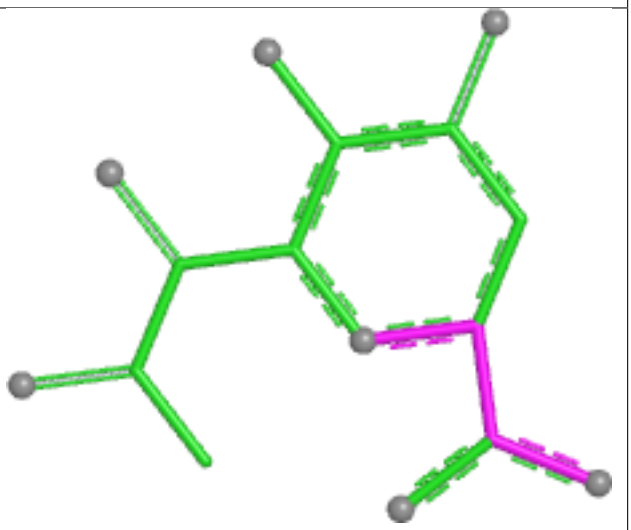
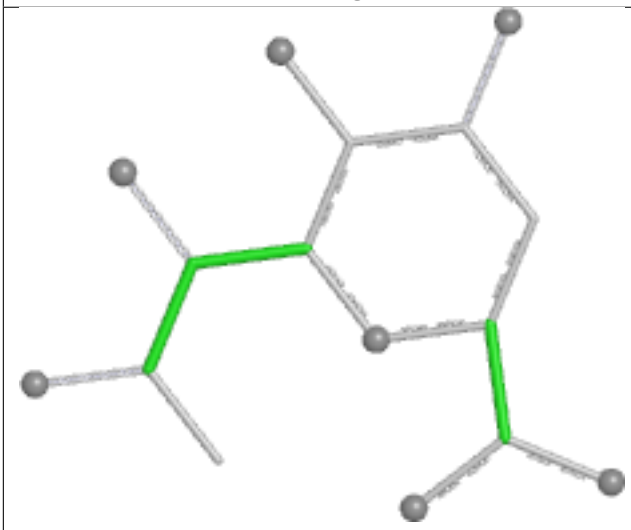


Bond angles



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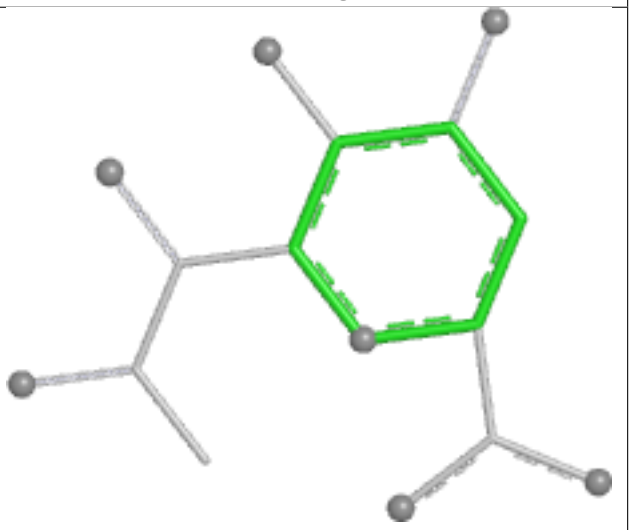
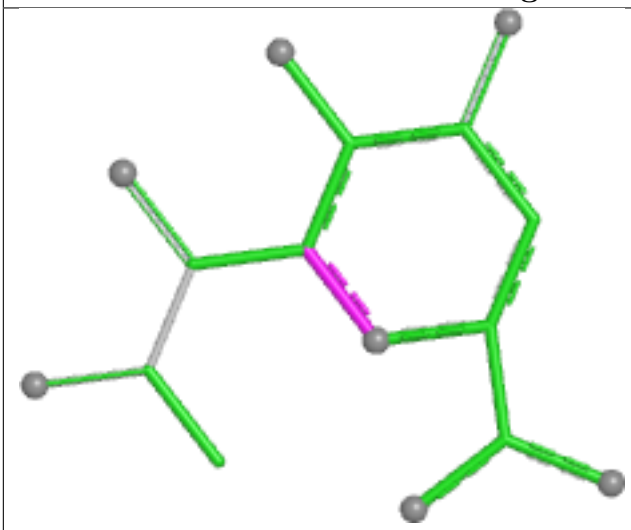


Rings

Ligand P8E NI 605



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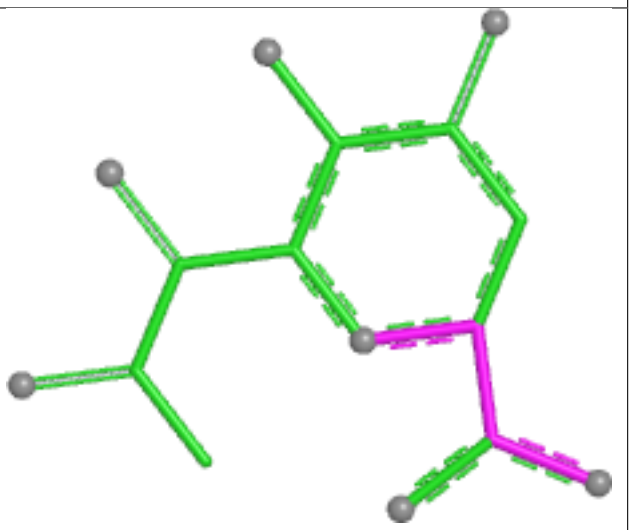

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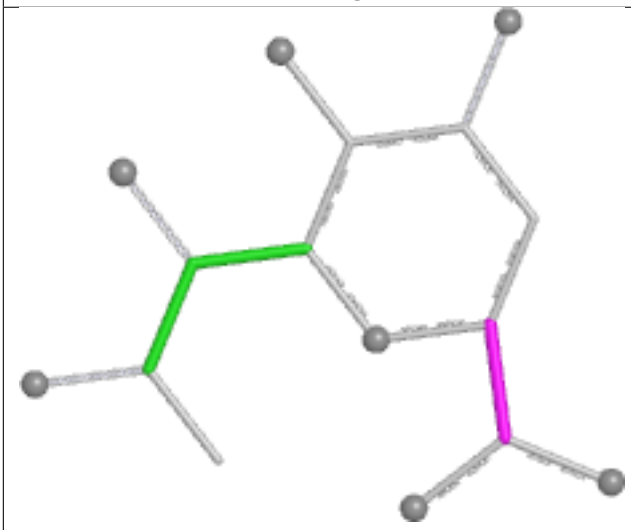

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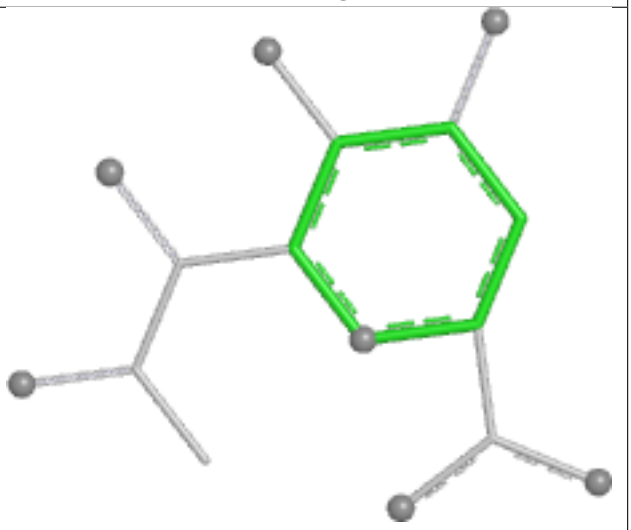
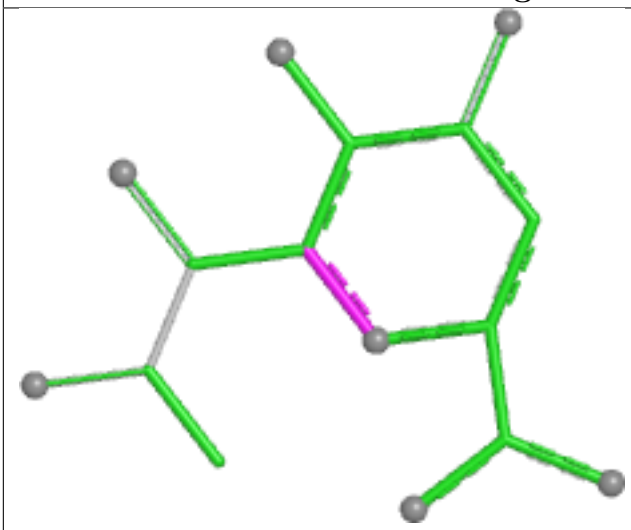


Rings

Ligand P8E GQ 607



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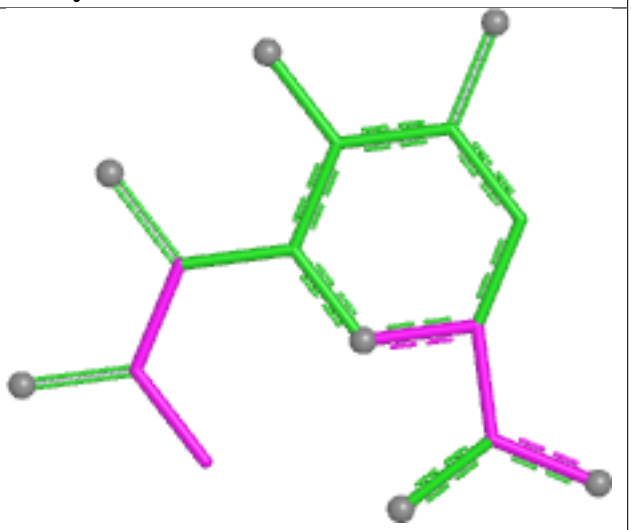
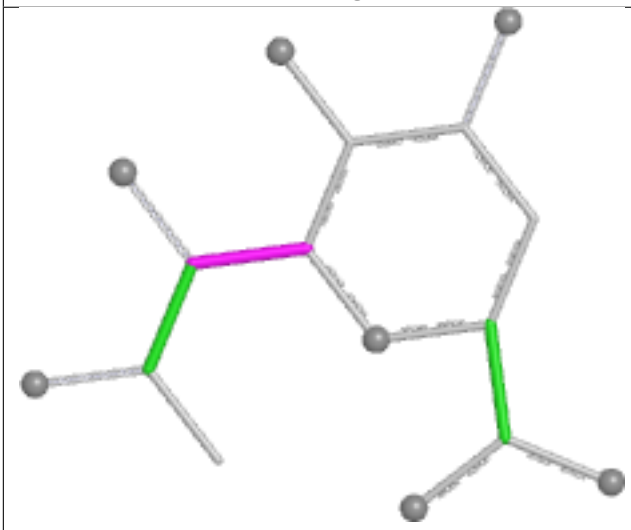


Bond angles



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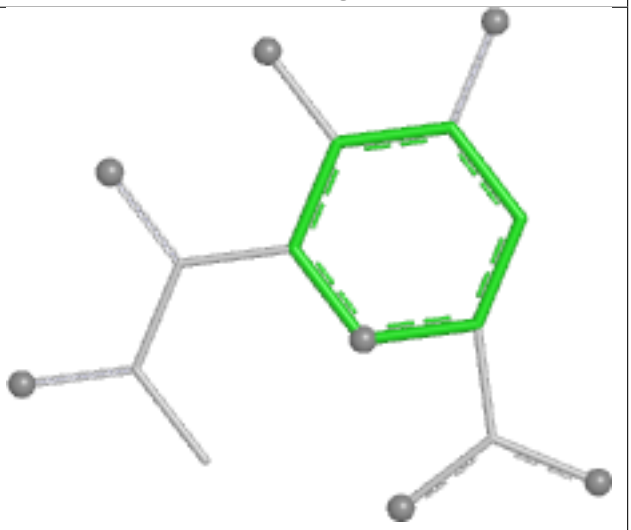
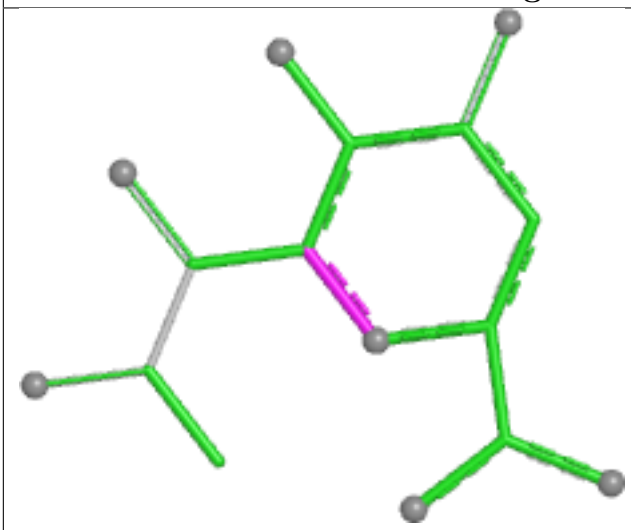


Rings

Ligand P8E g6 604



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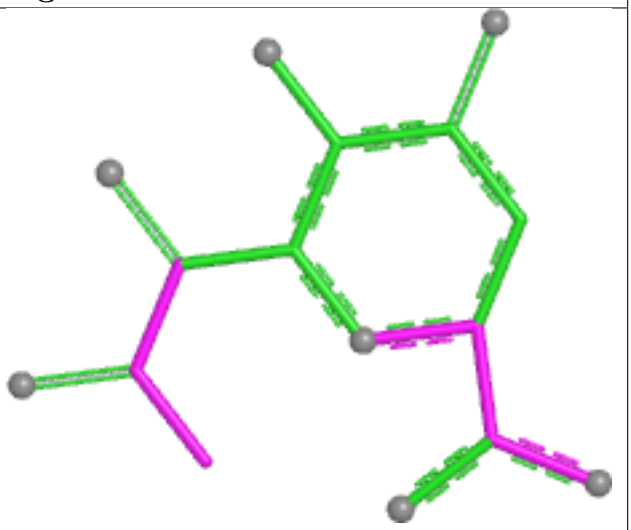
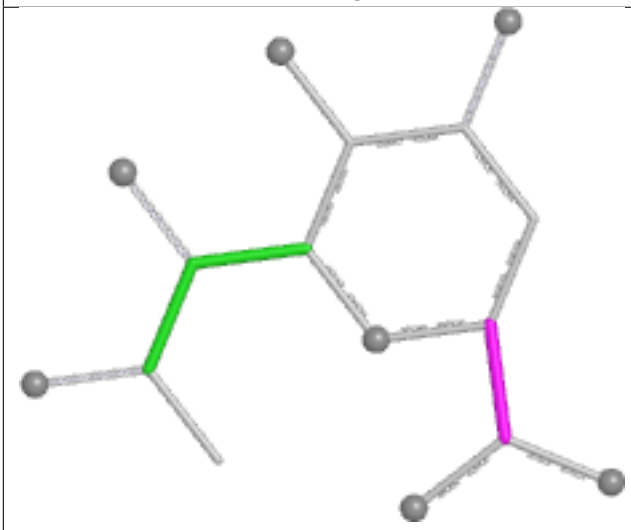


Bond angles



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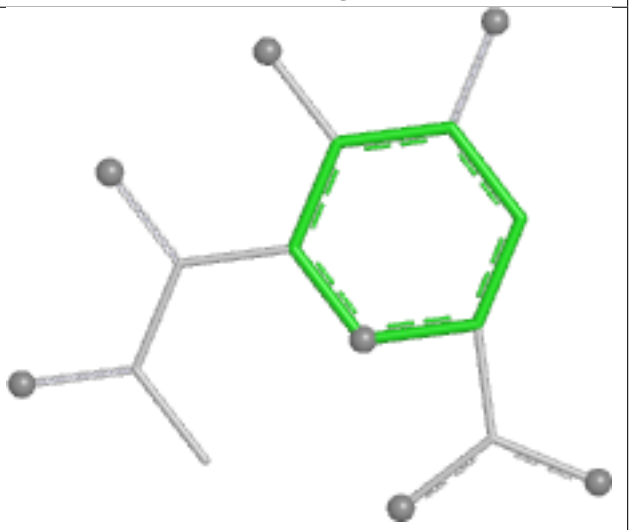
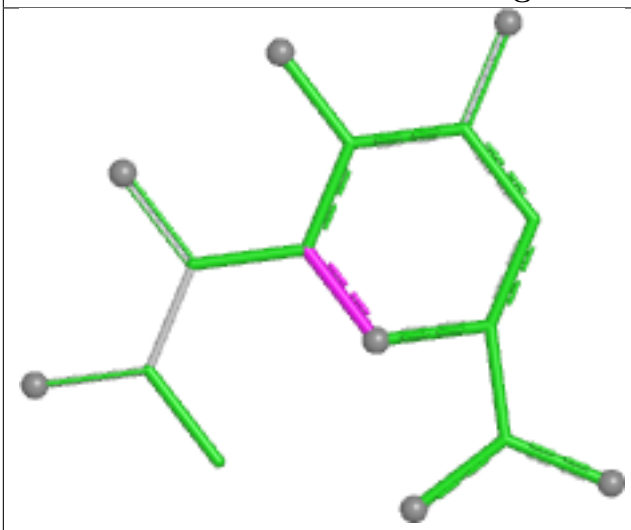


Rings

Ligand P8E DN 603



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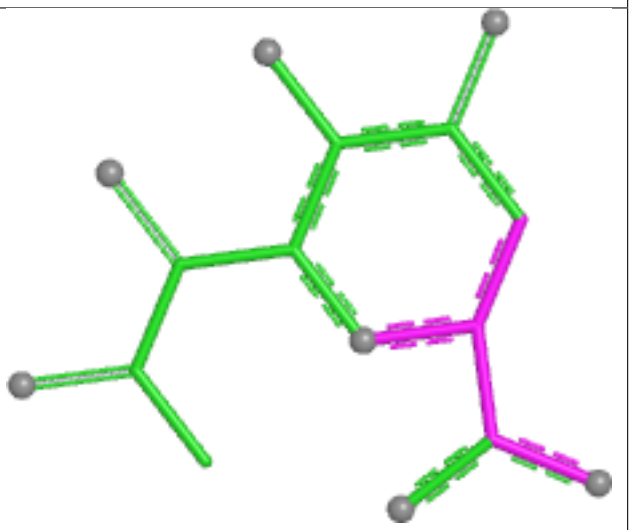
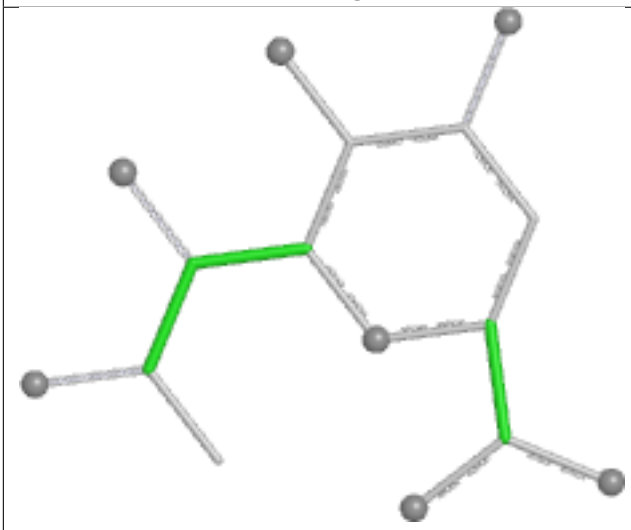


Bond angles



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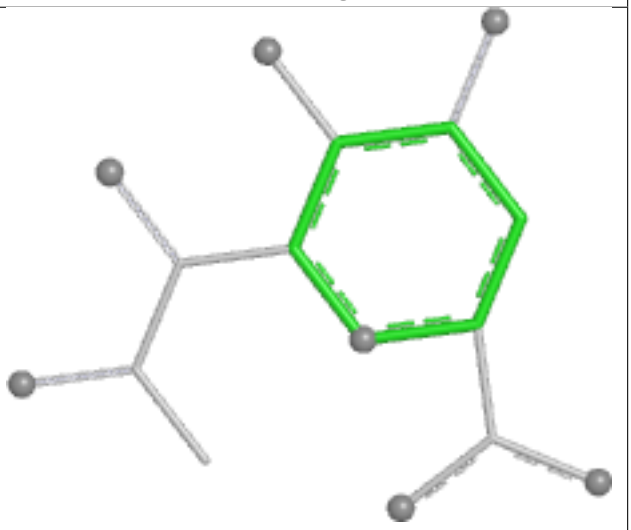
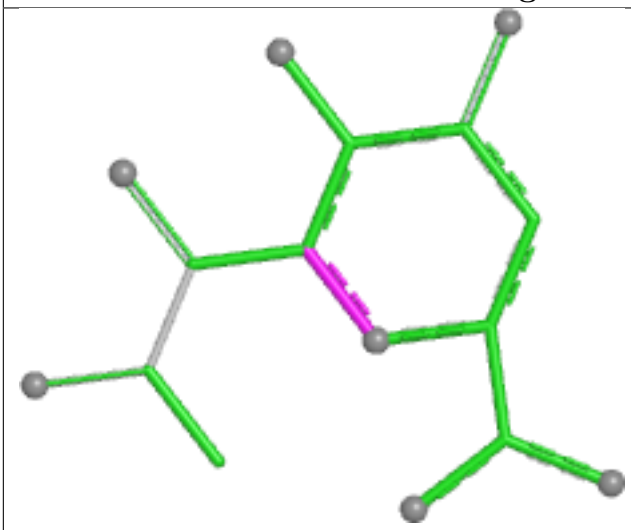


Rings

Ligand P8E Q2 601



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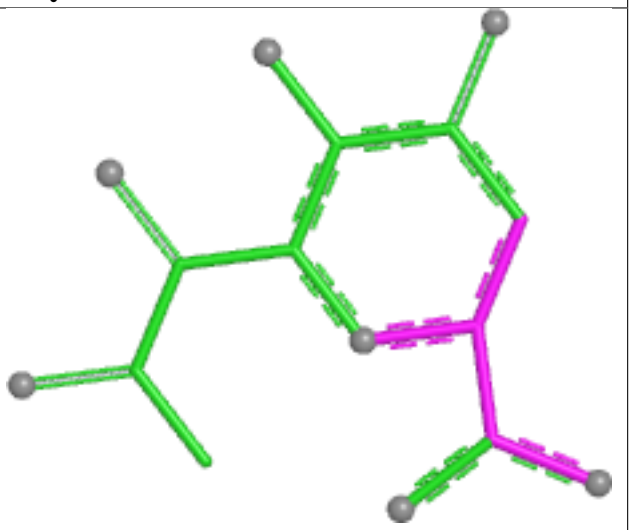

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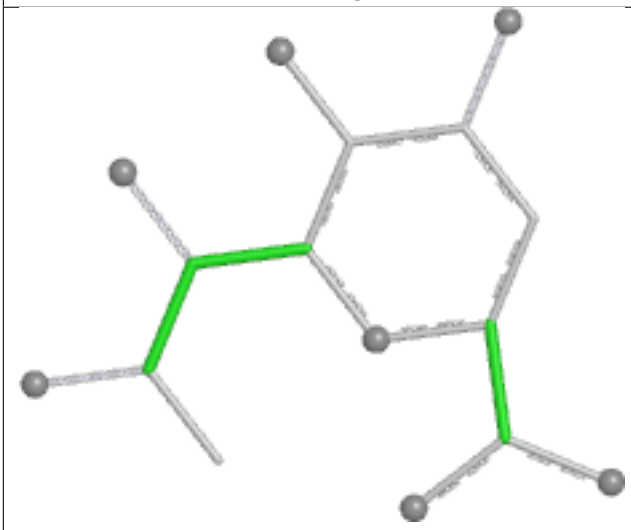

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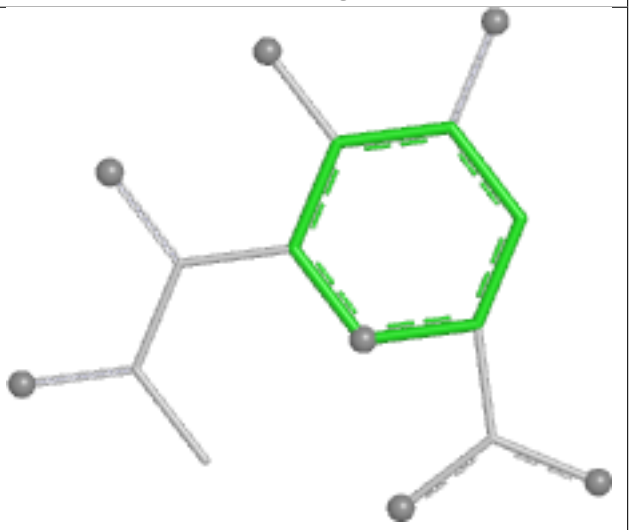
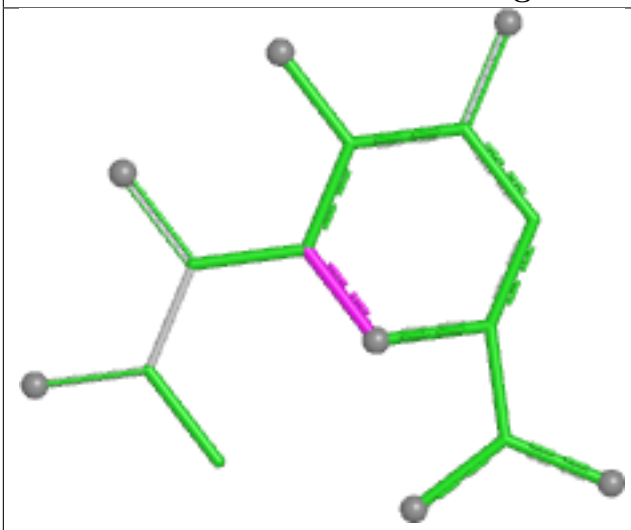


Rings

Ligand P8E DN 607



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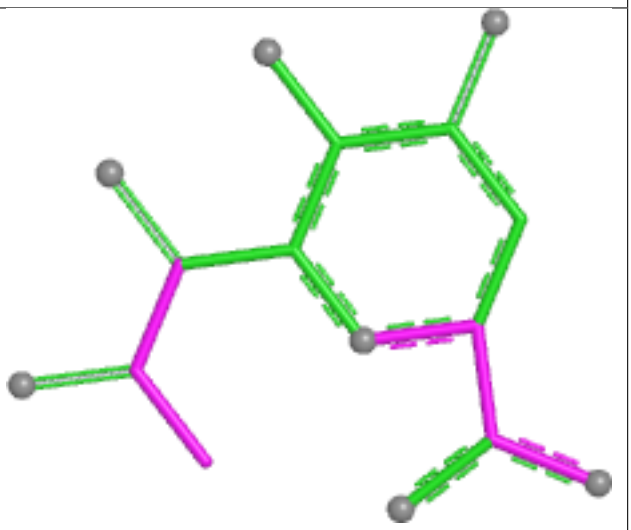
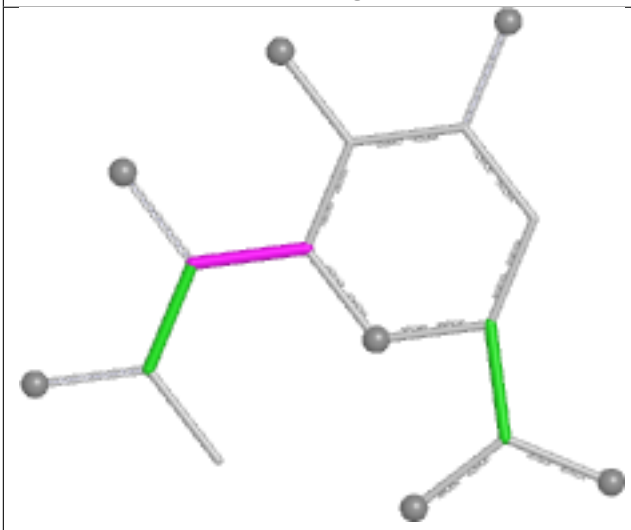


Bond angles



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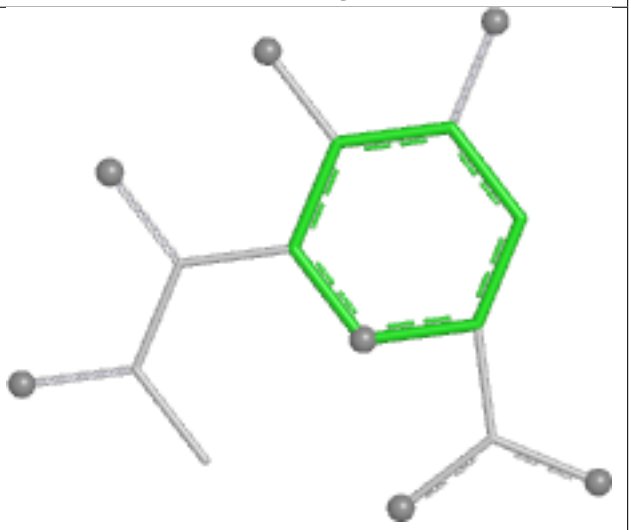
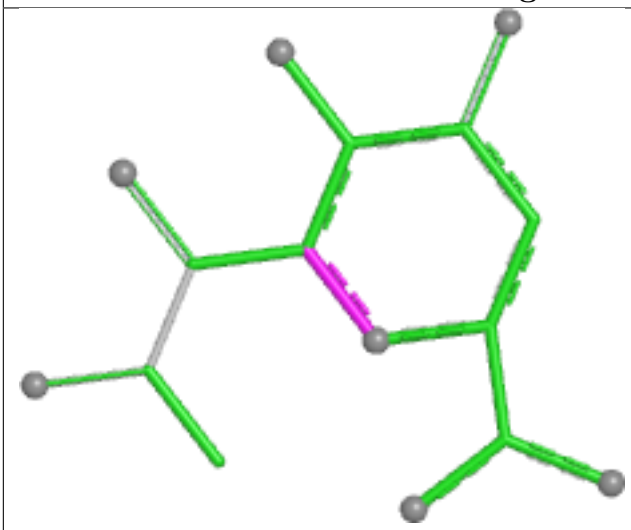


Rings

Ligand P8E LF 604



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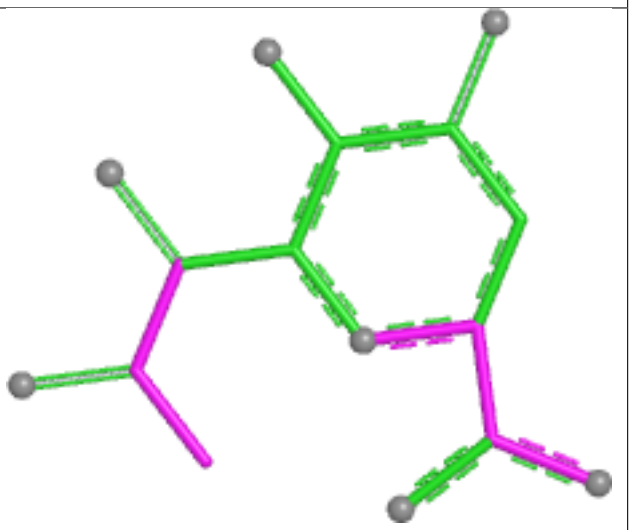
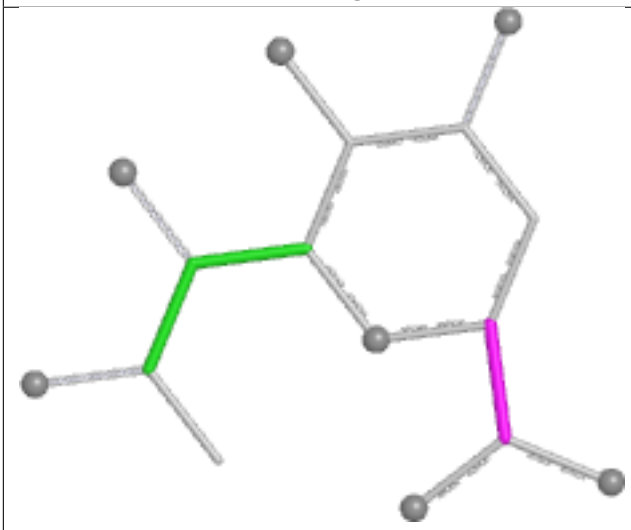


Bond angles



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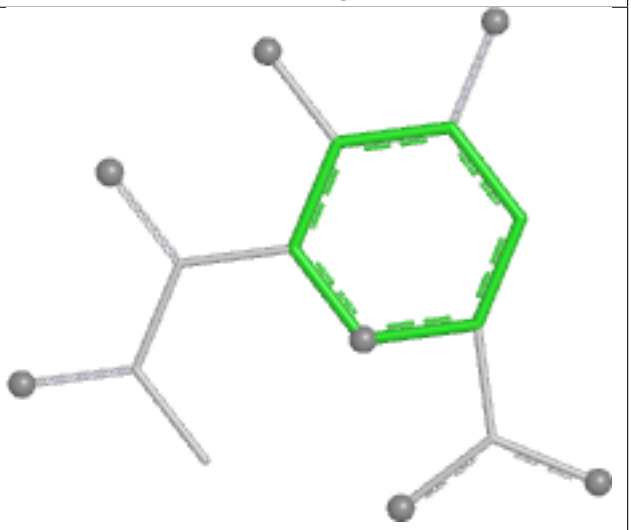
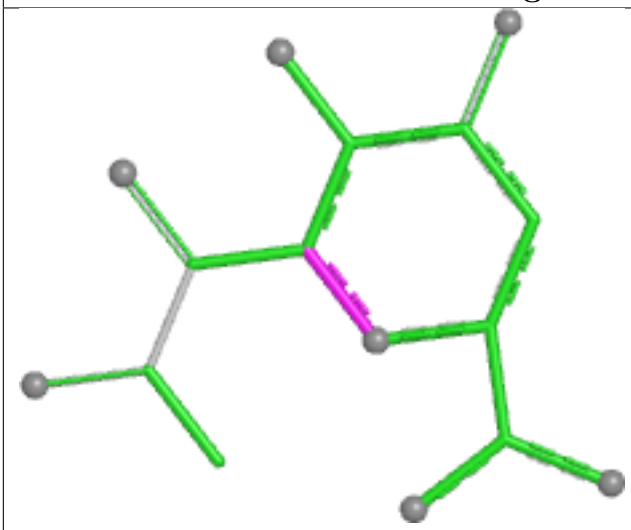


Rings

Ligand P8E g6 605



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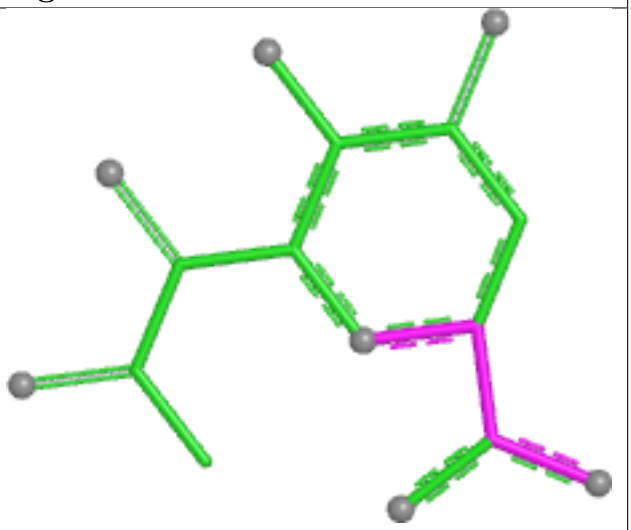

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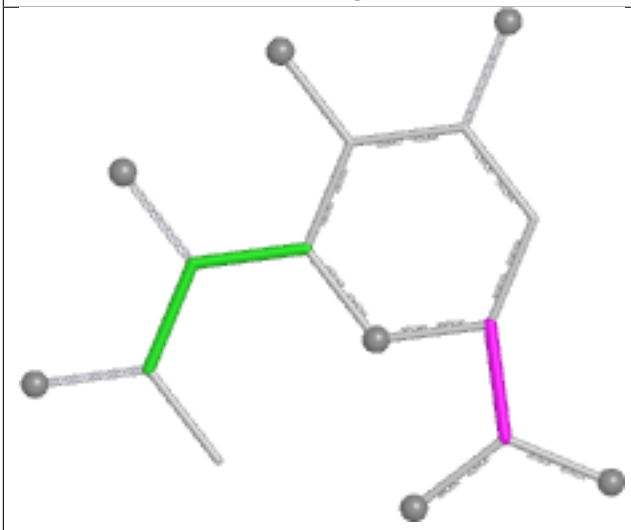
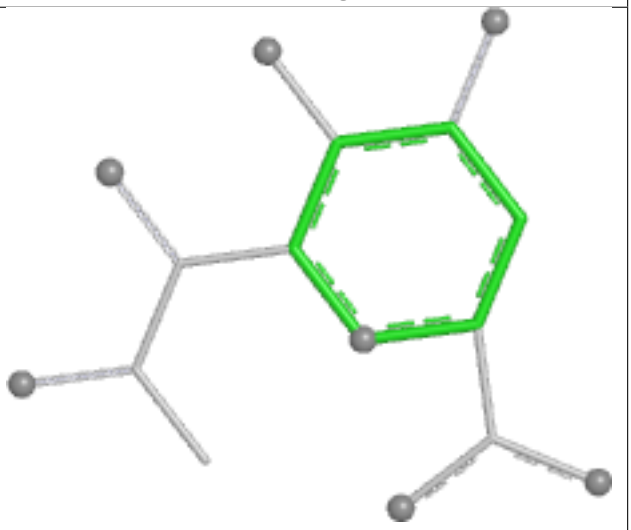
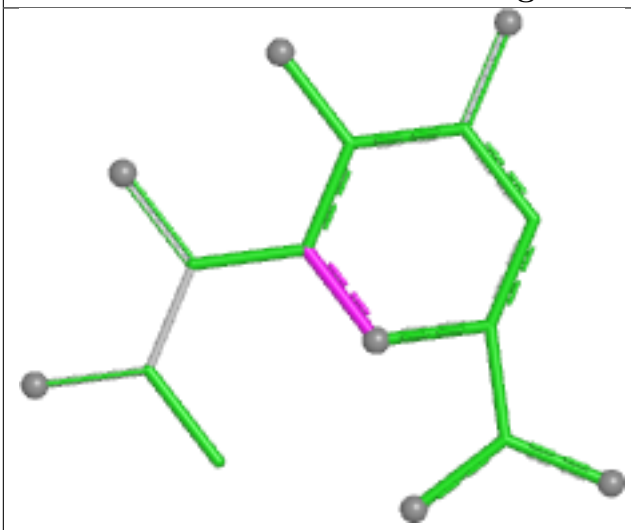


Torsions



Rings

Ligand P8E FB 603



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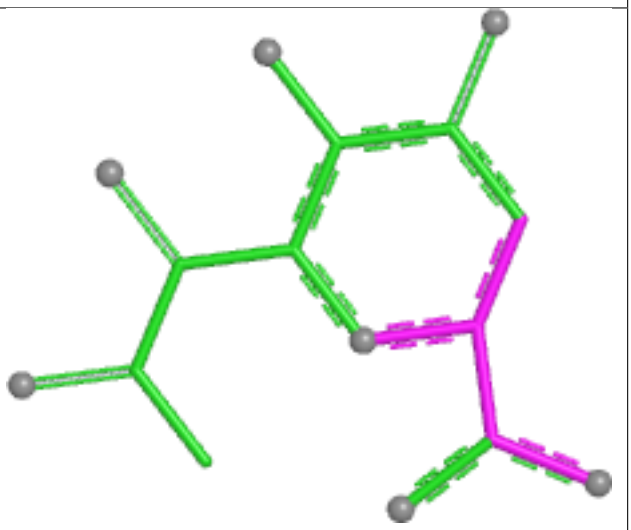

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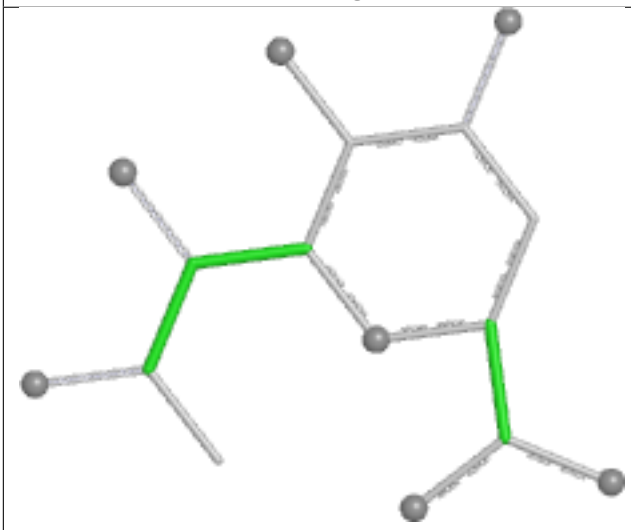

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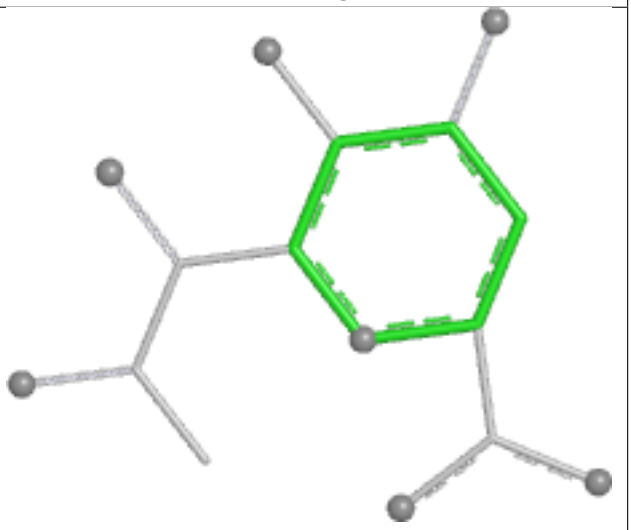

Rings

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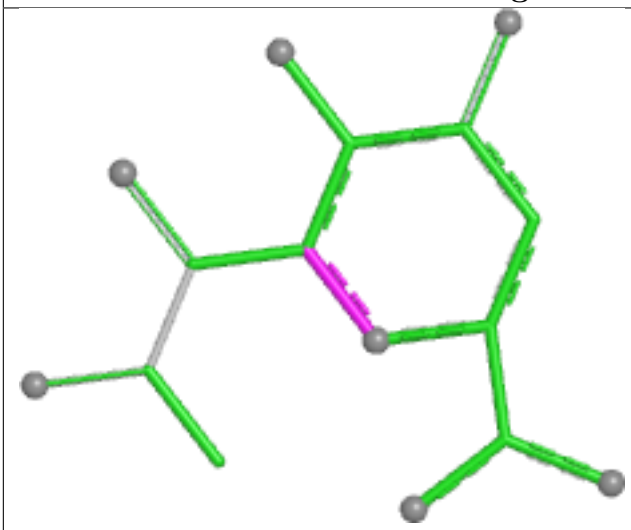

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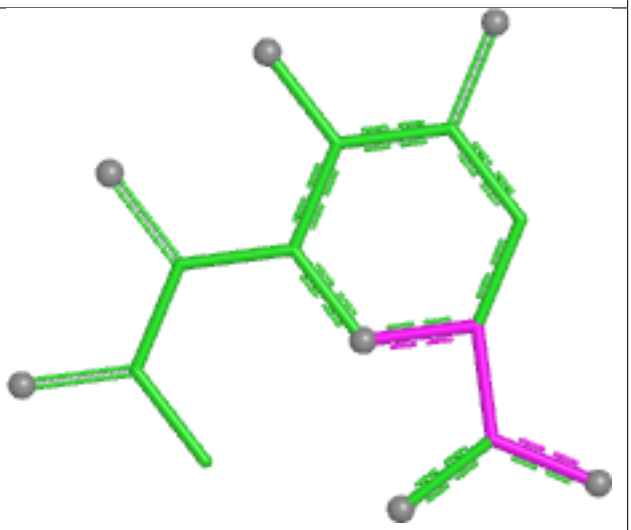

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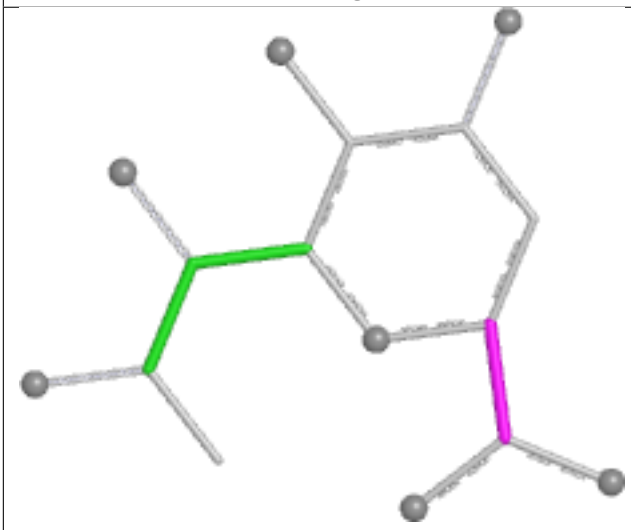

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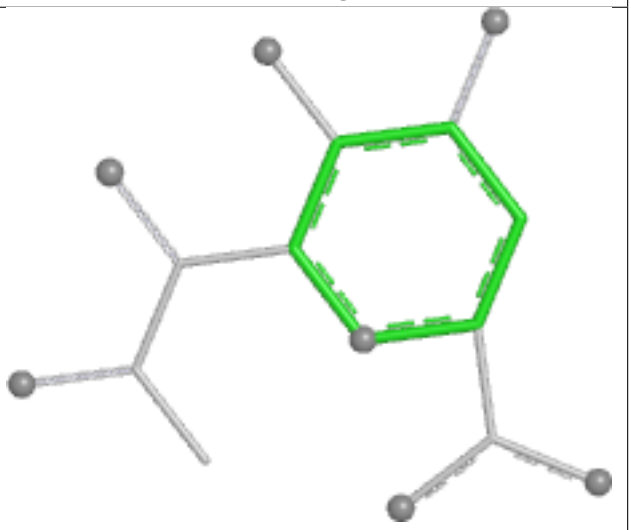

Rings

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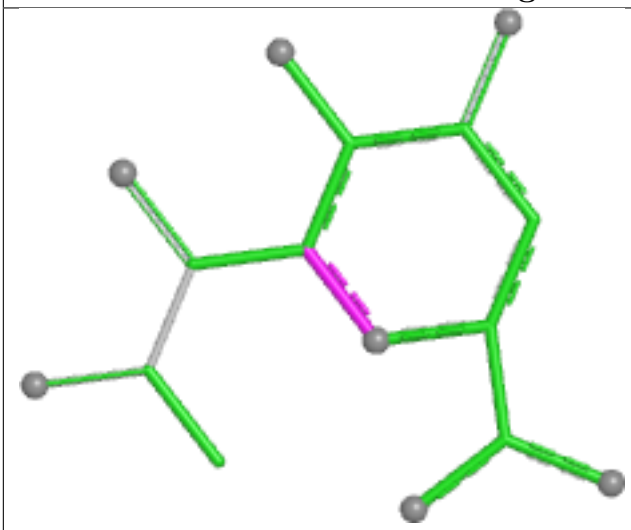

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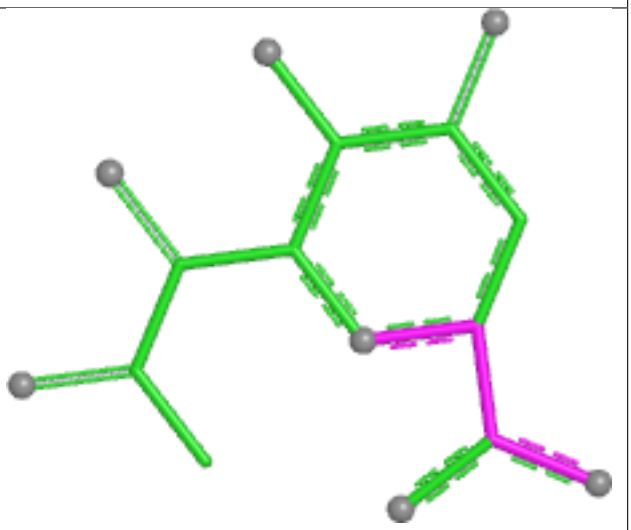

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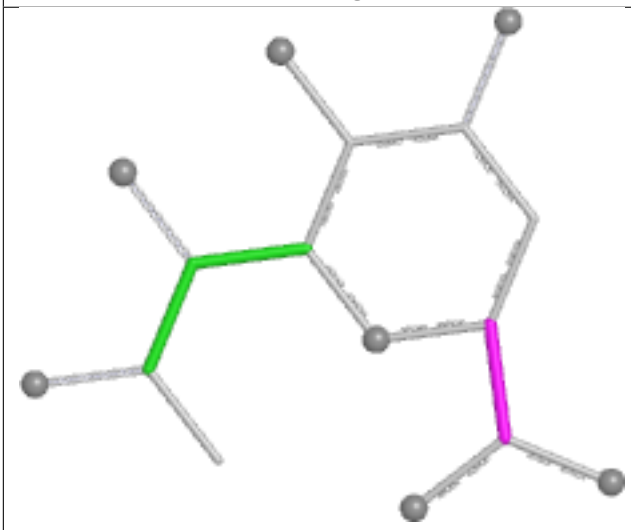

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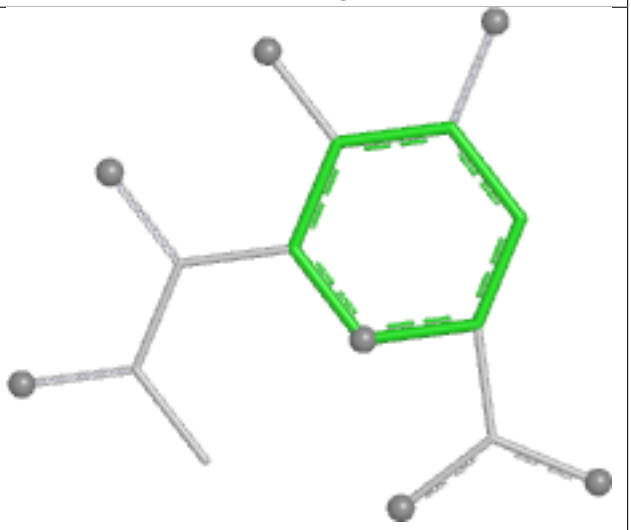
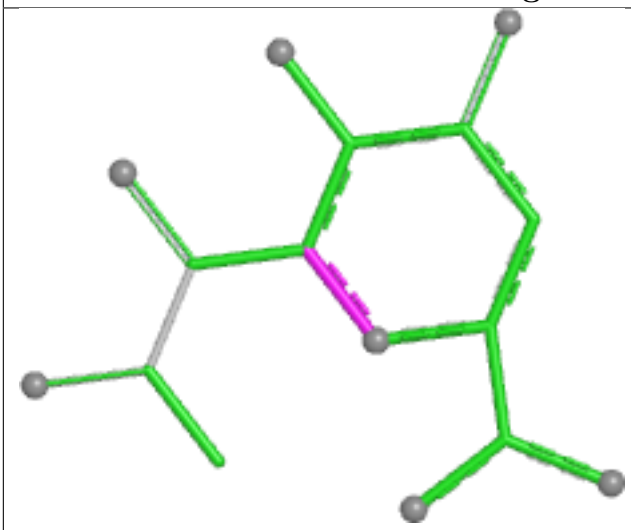


Rings

Ligand P8E S5 605



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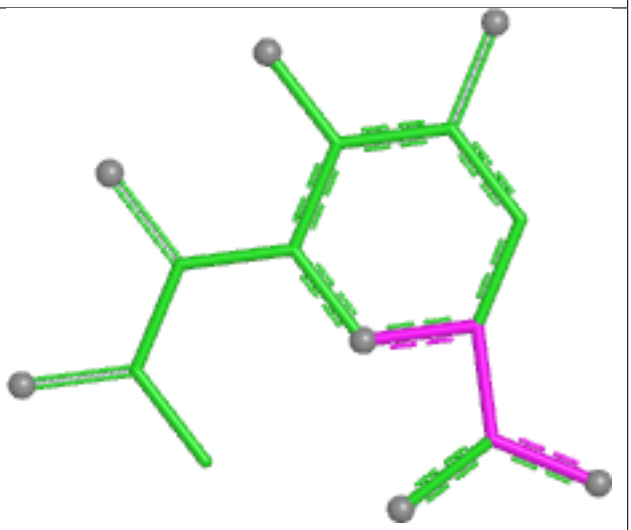

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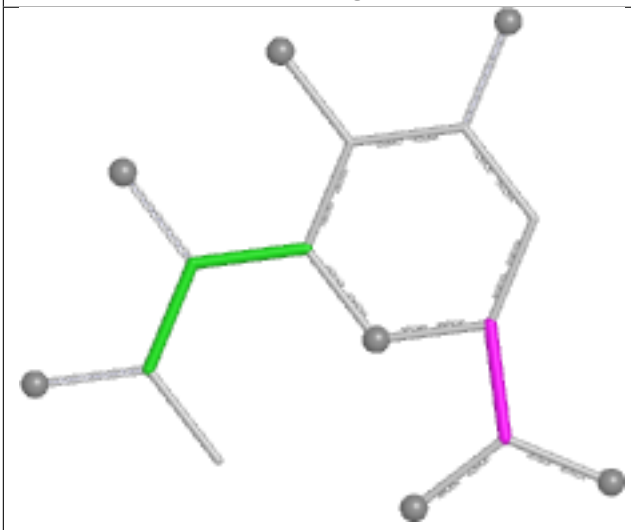

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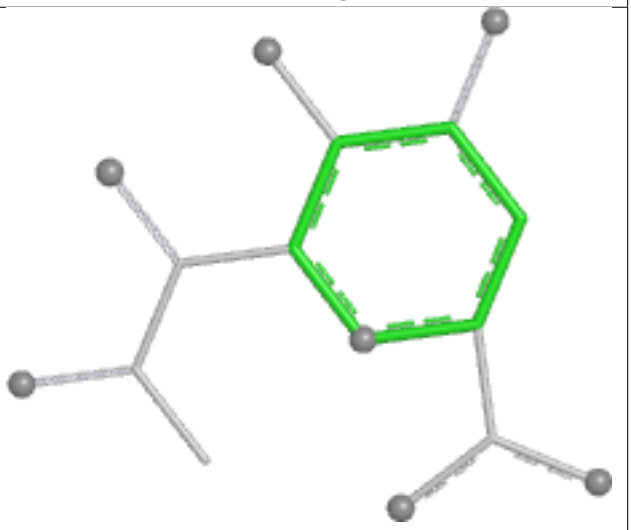
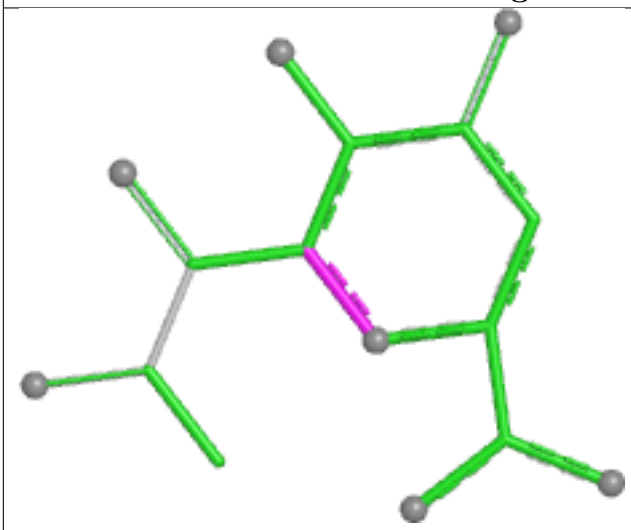


Rings

Ligand P8E XM 603



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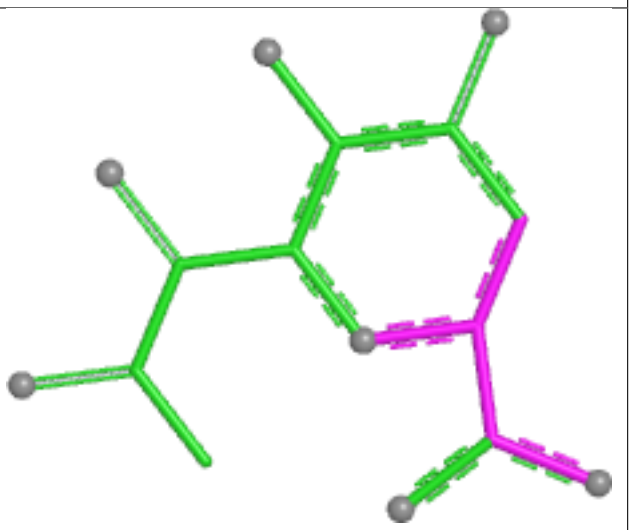

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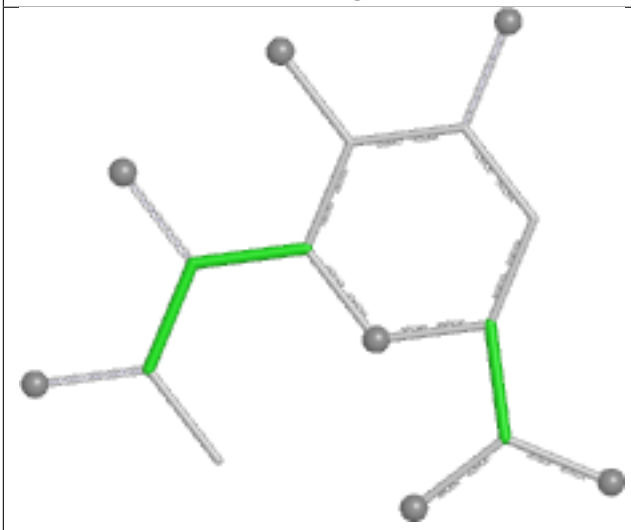

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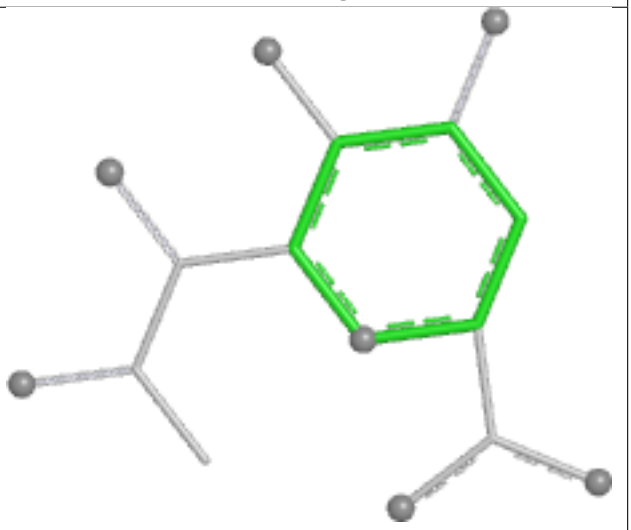
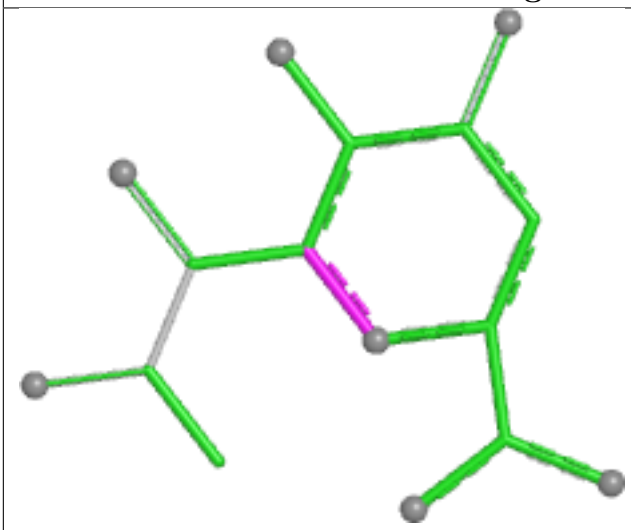


Rings

Ligand P8E e8 604



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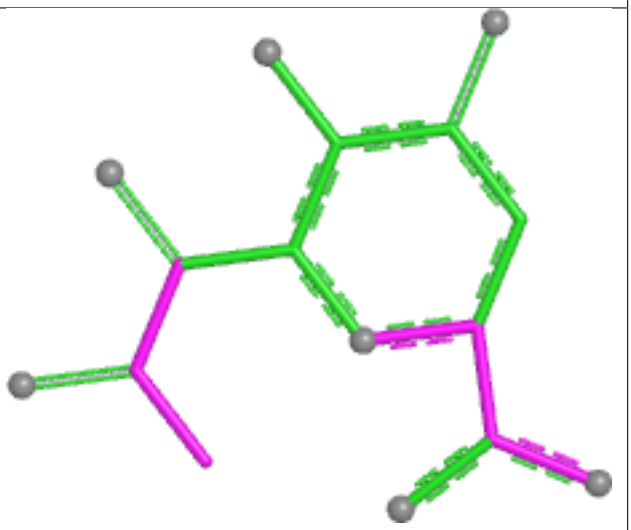

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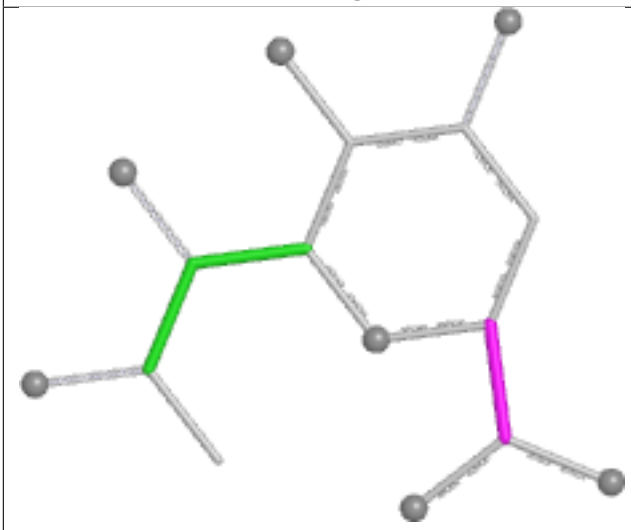

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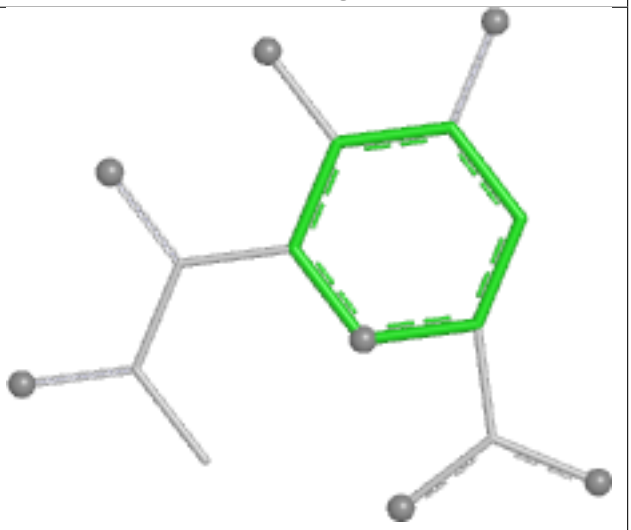

Rings

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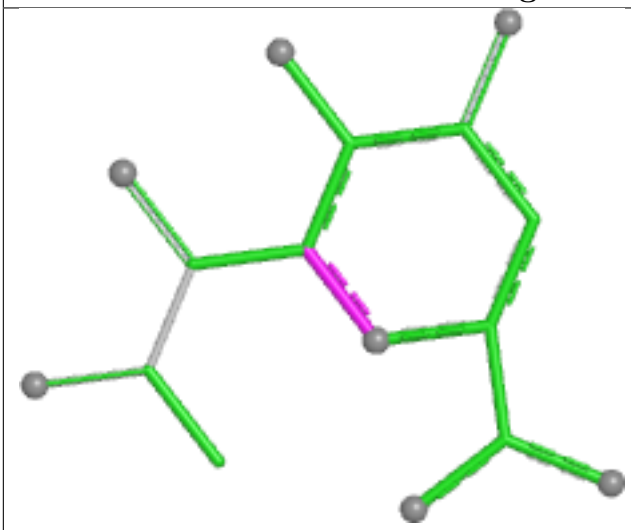

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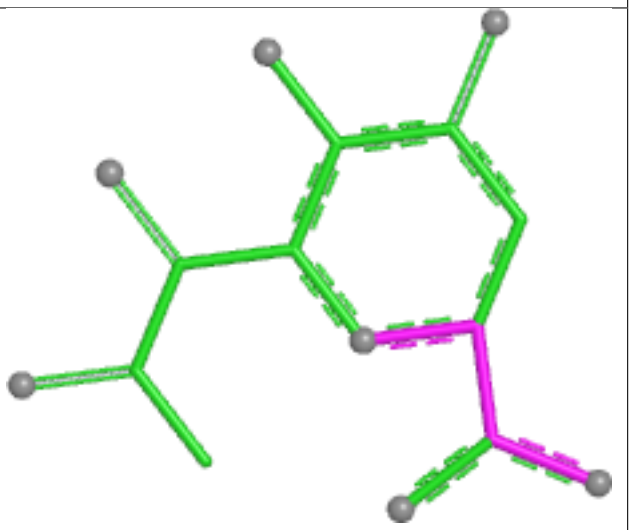

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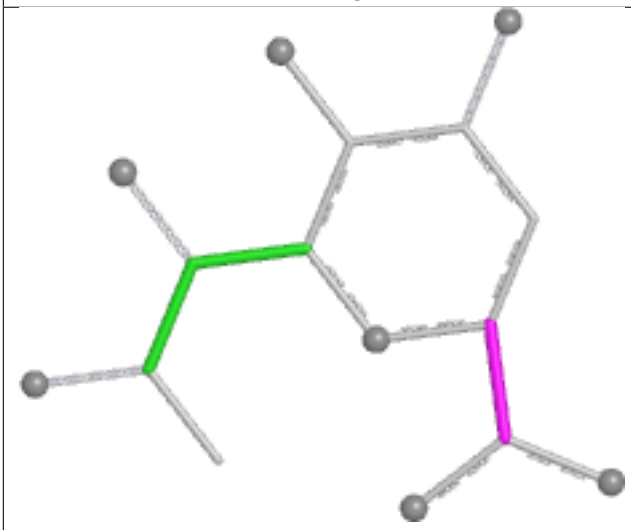

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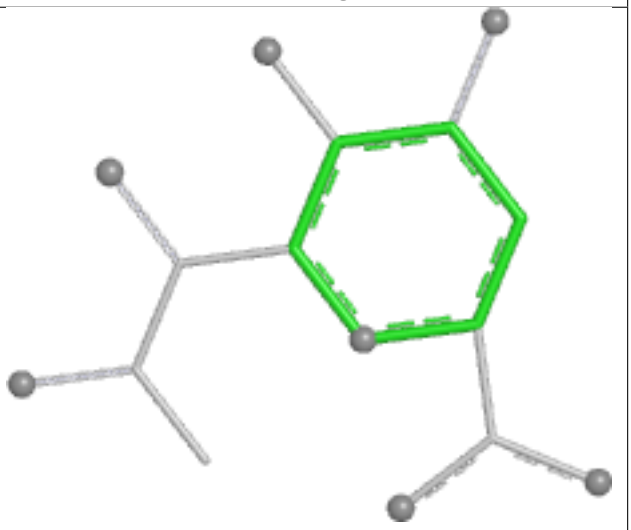
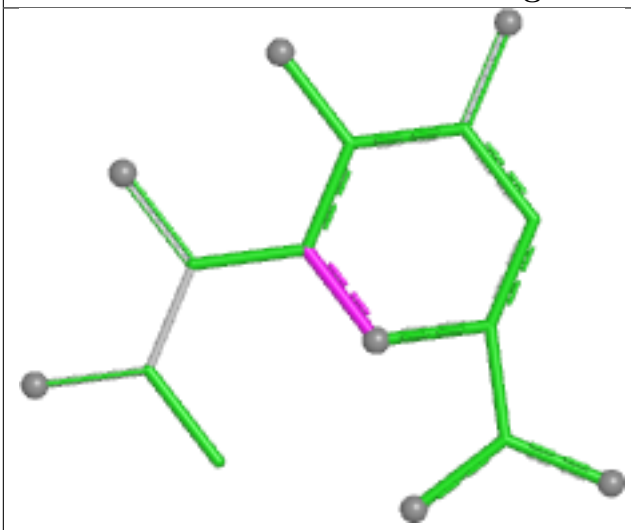


Rings

Ligand P8E g6 603



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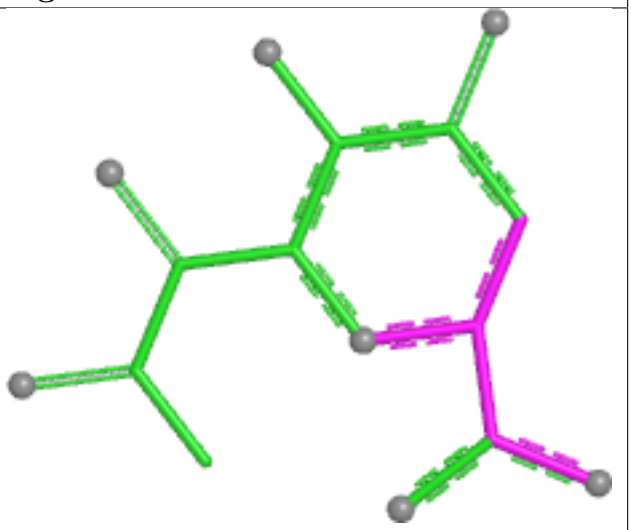

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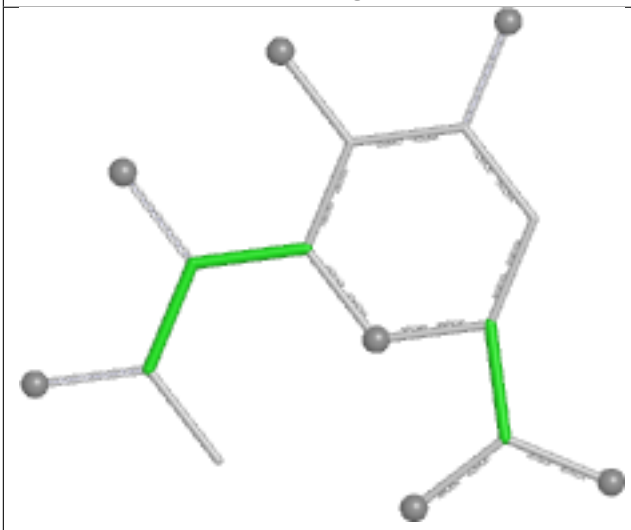

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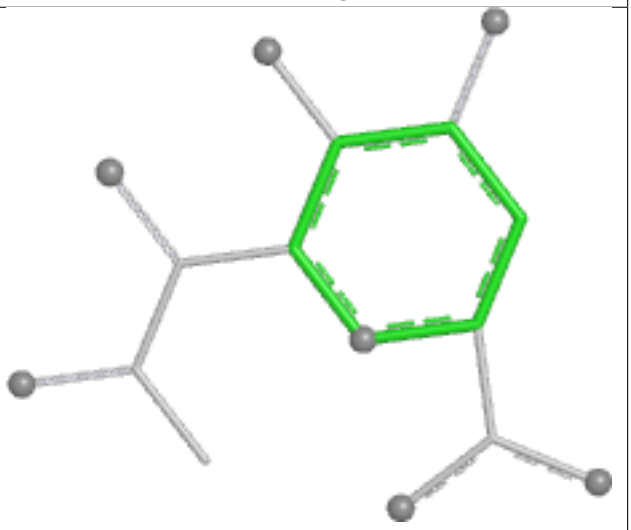
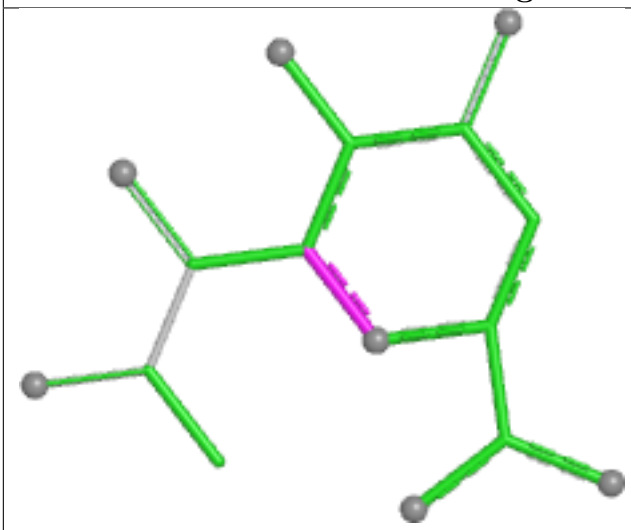


Rings

Ligand P8E CT 602



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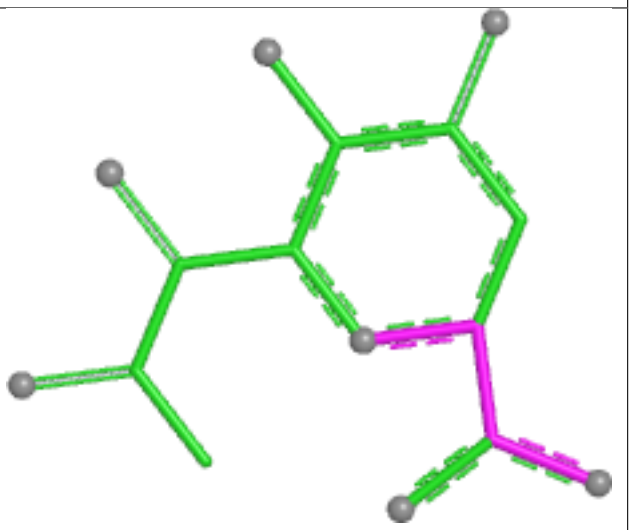

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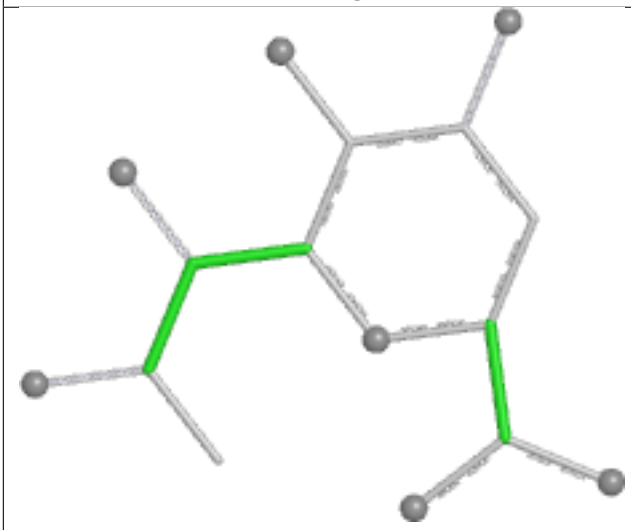

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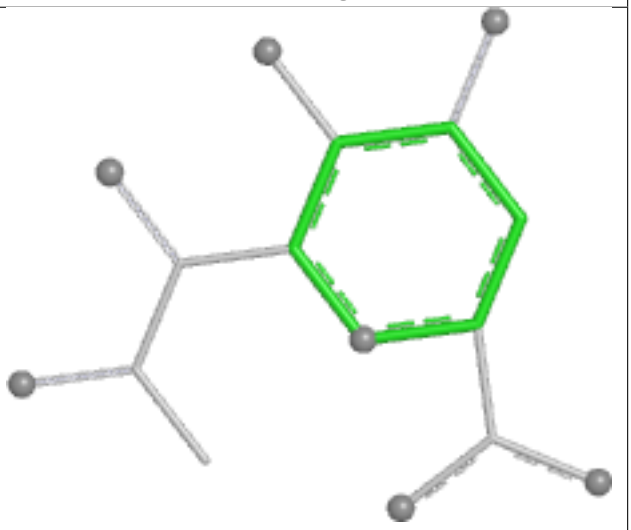
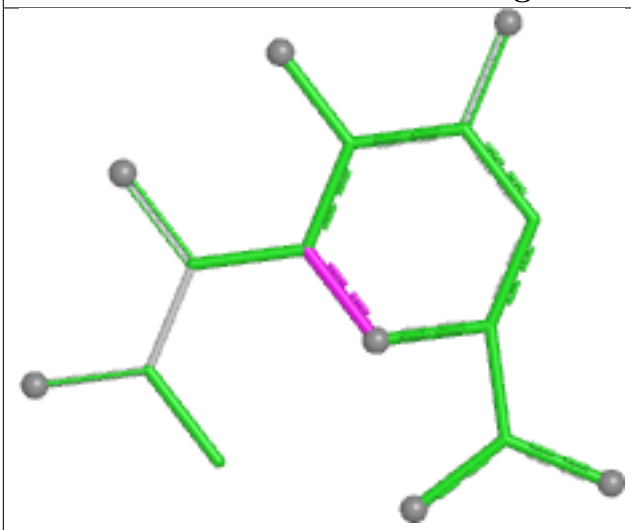


Rings

Ligand P8E UH 602



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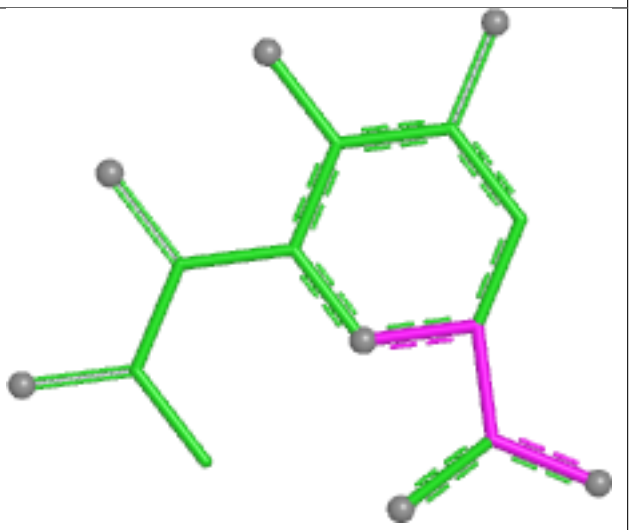

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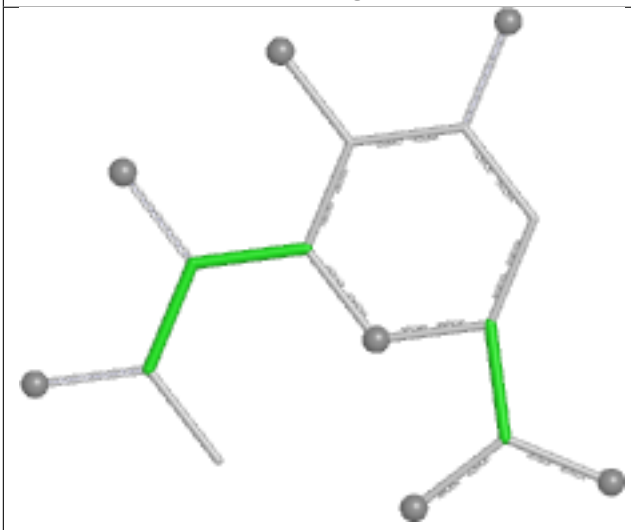

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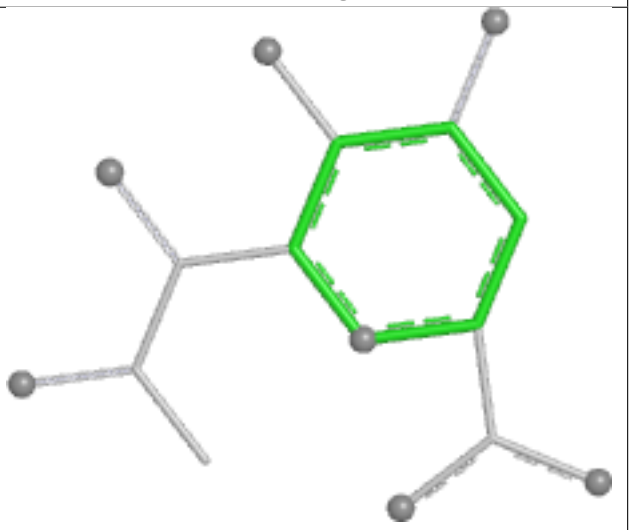
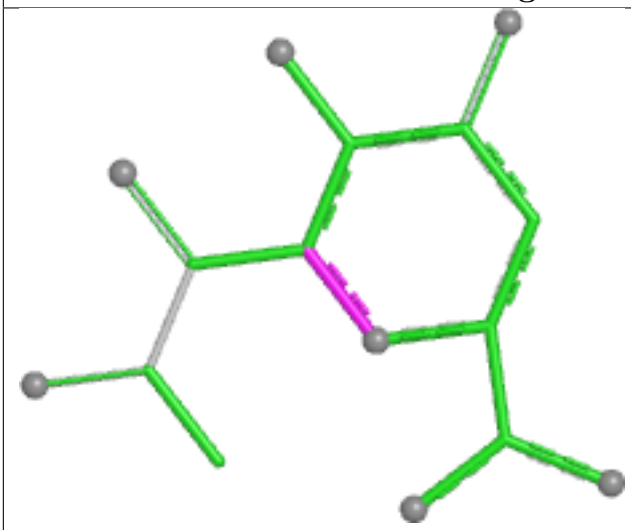


Rings

Ligand P8E JD 602



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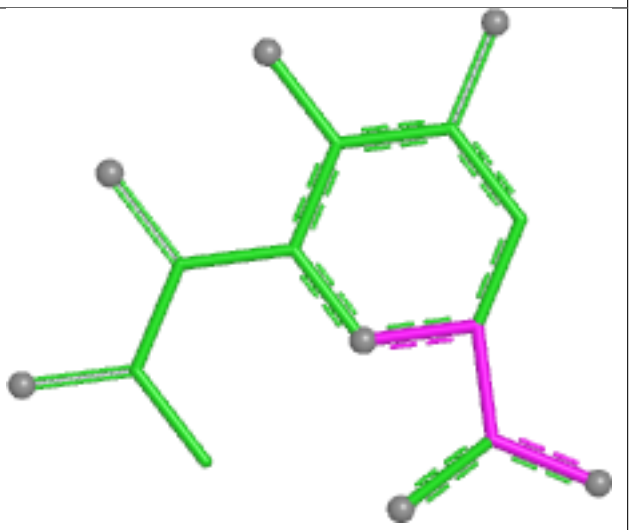

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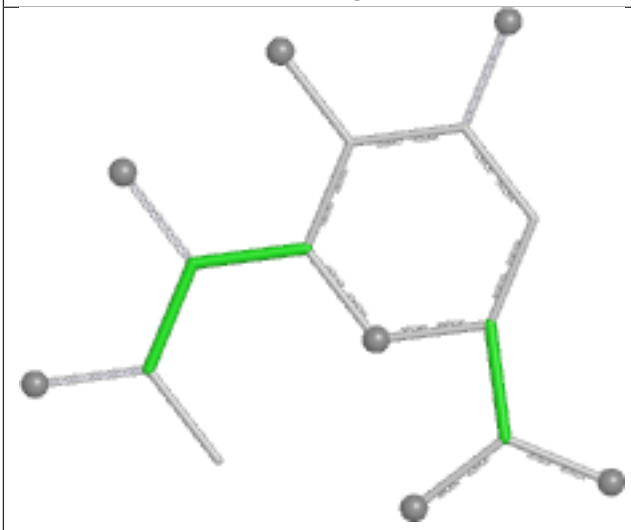

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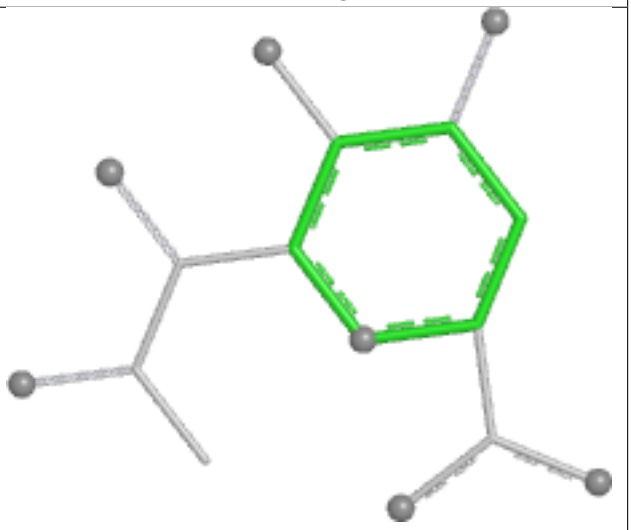
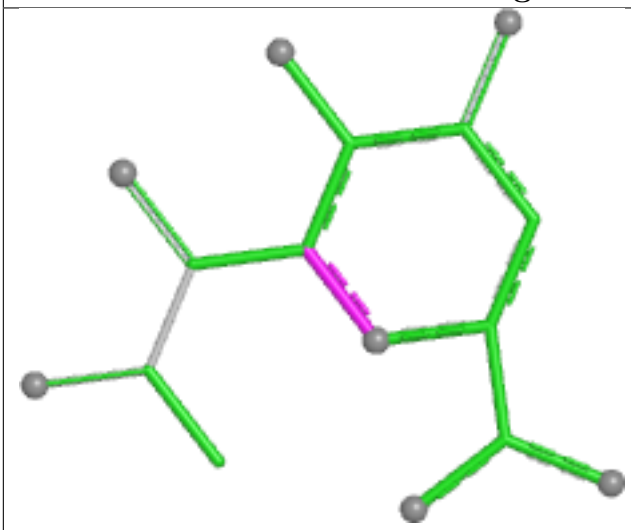


Rings

Ligand P8E UH 603



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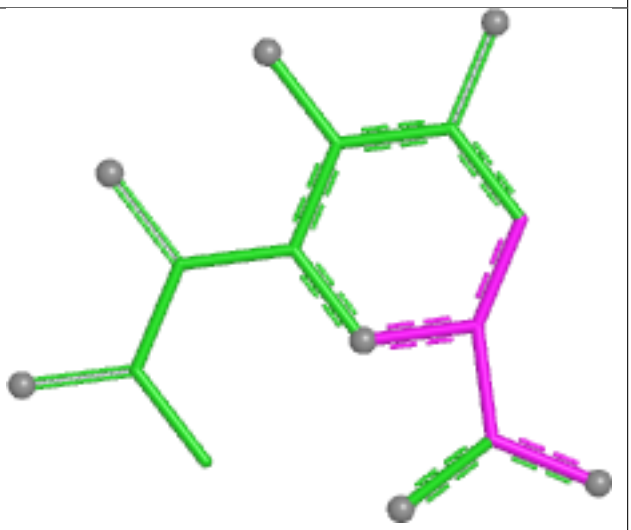

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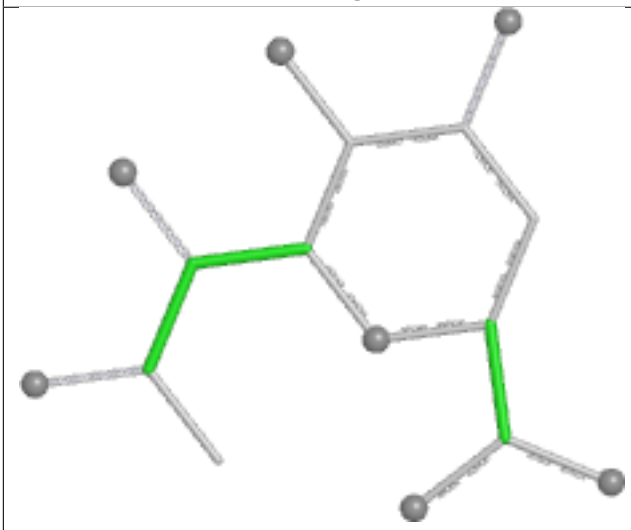

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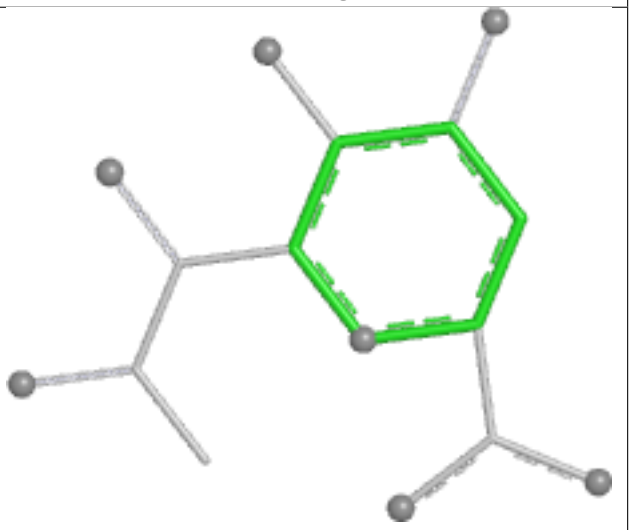
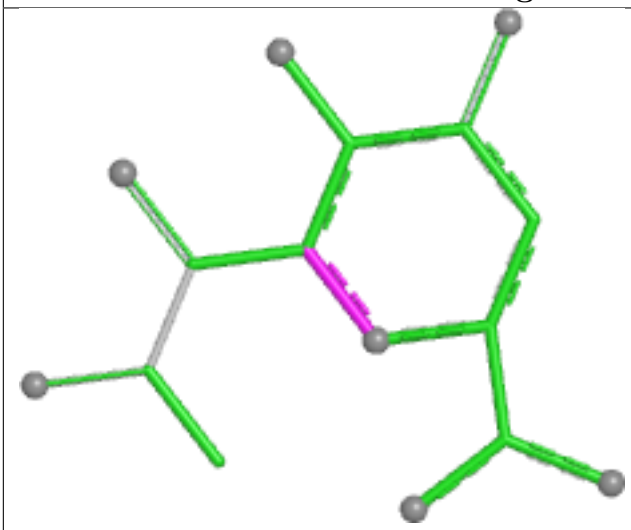


Rings

Ligand P8E CT 607



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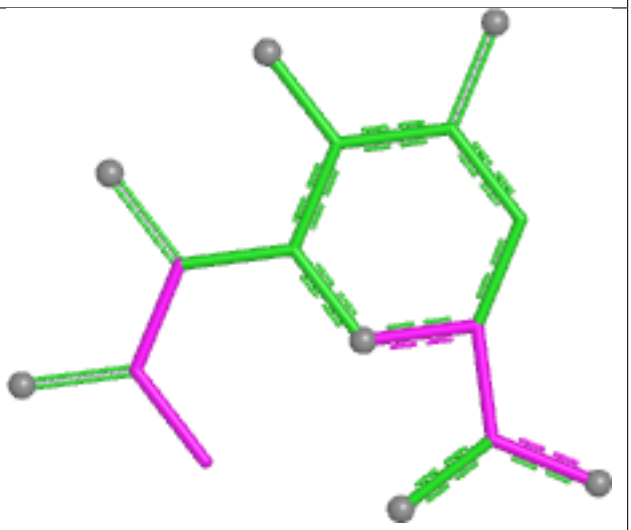
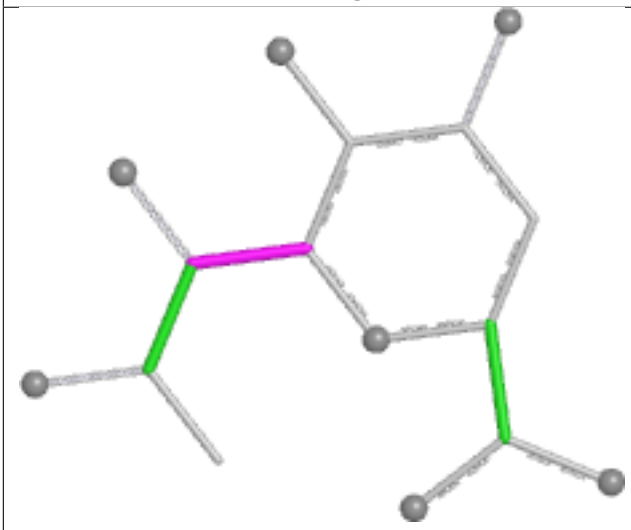
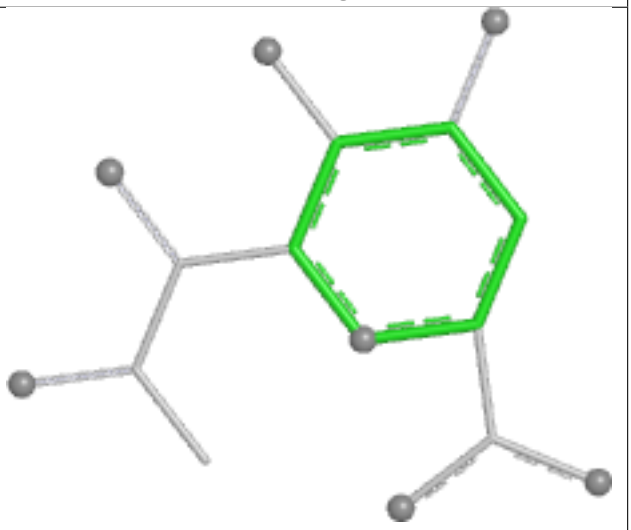


Bond angles

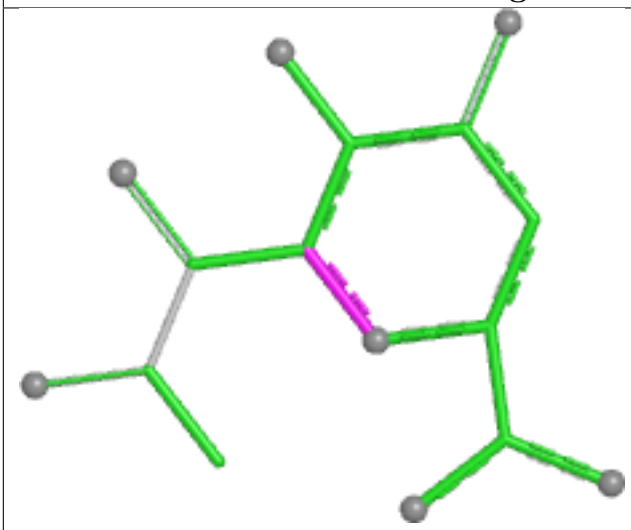


Torsions



Rings

Ligand P8E WG 603



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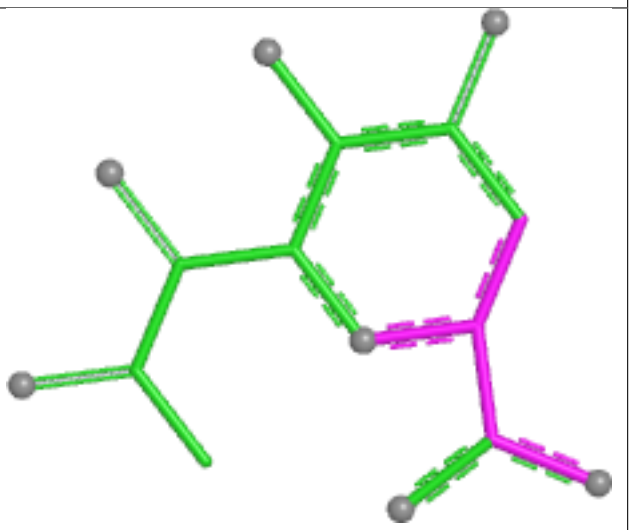
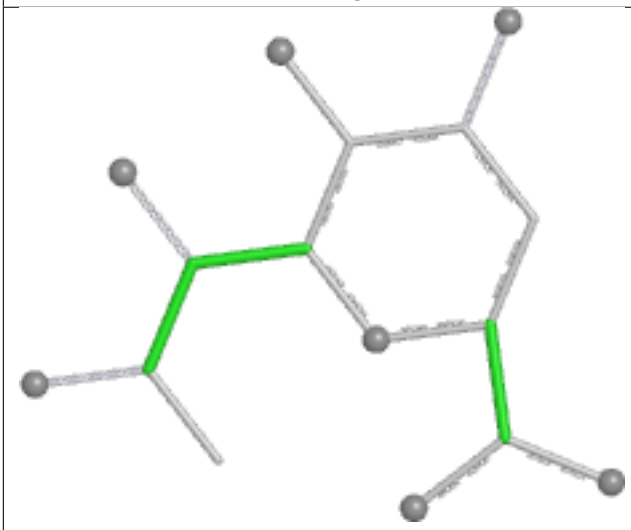


Bond angles



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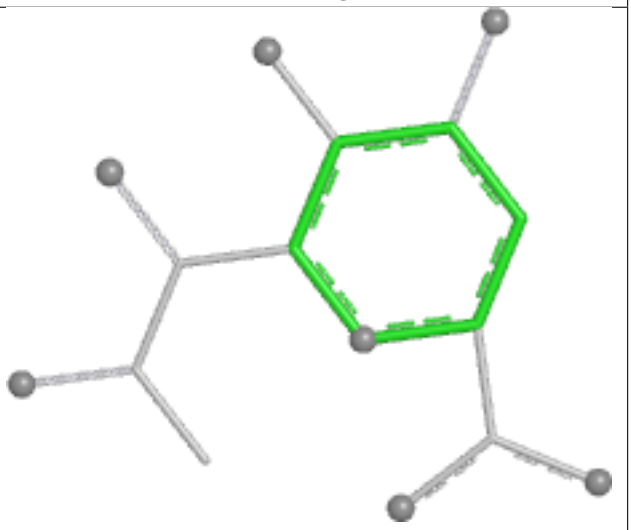
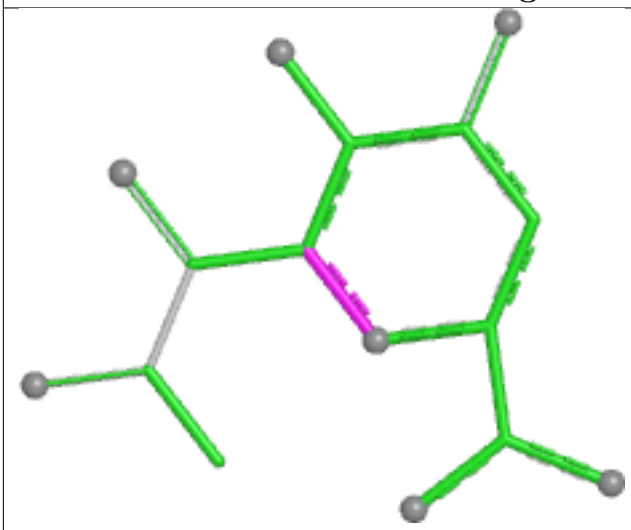


Rings

Ligand P8E BJ 607



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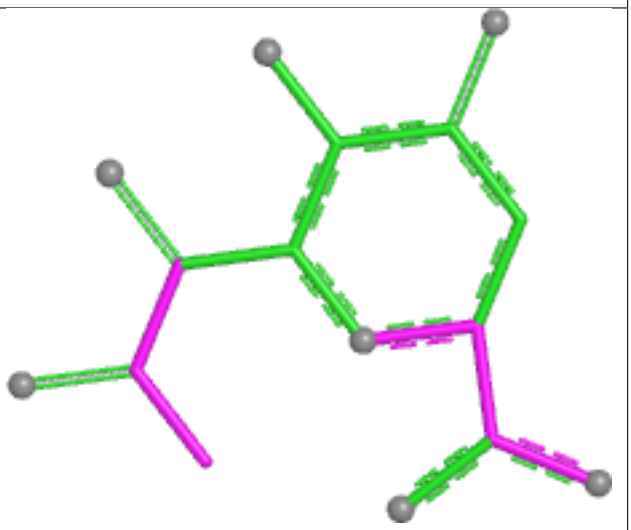

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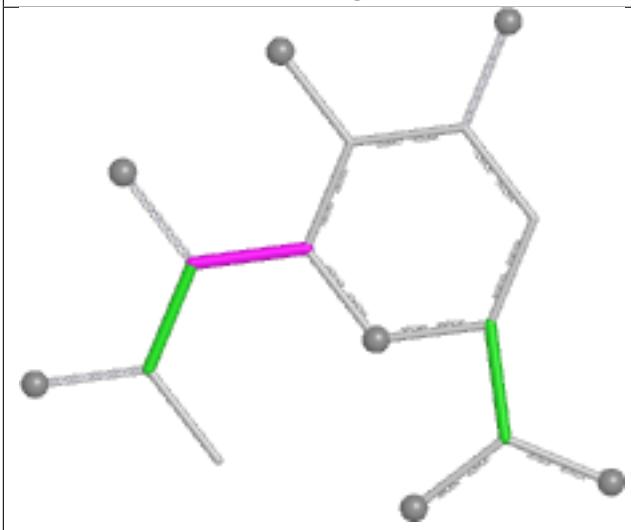

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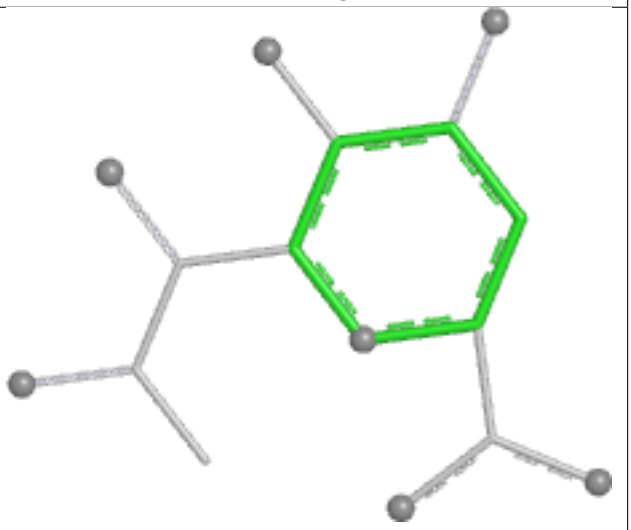
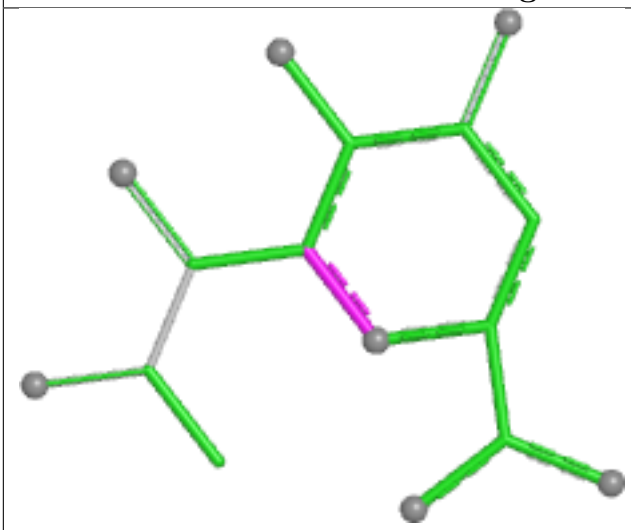


Rings

Ligand P8E LF 607



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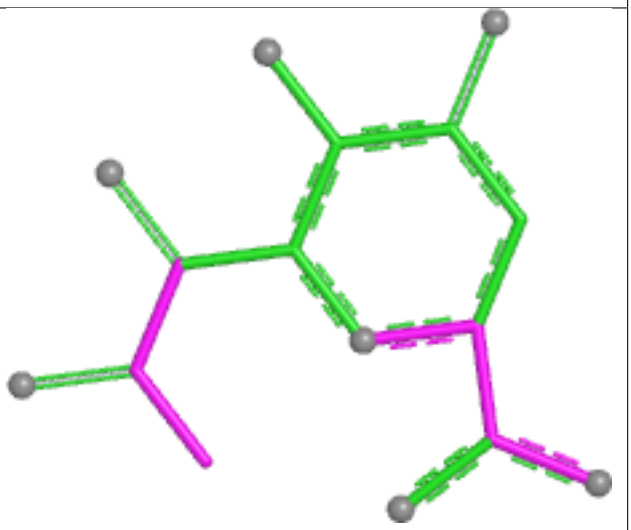

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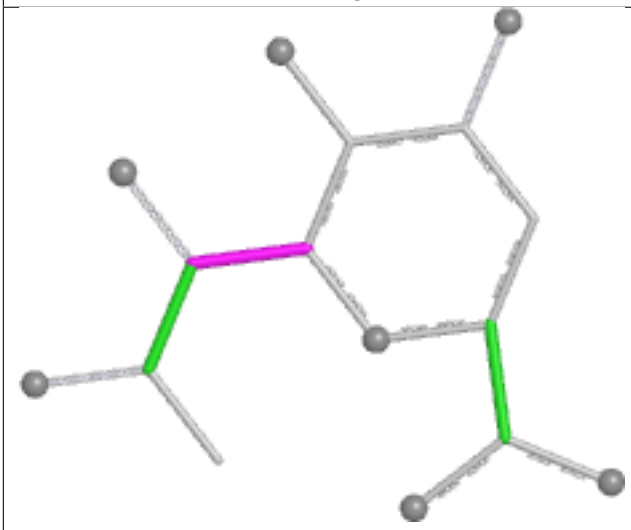

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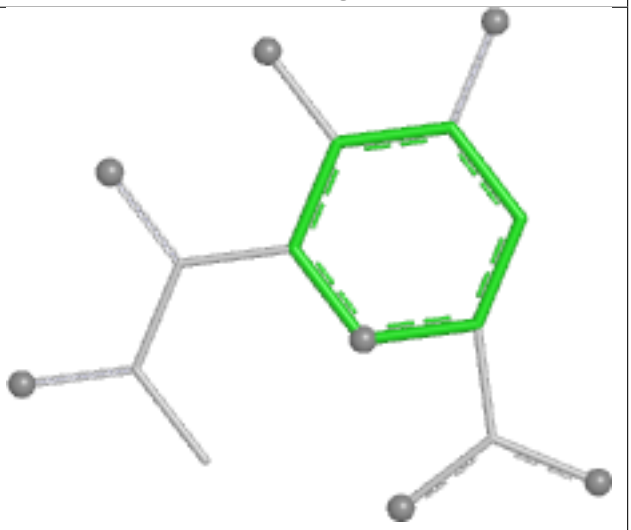
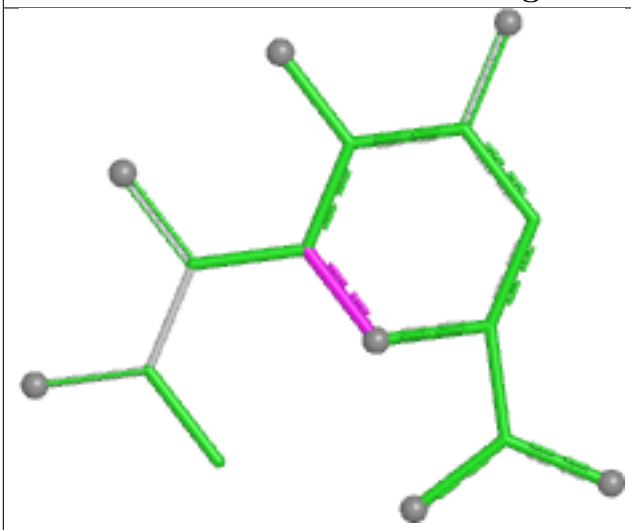


Rings

Ligand P8E fK 603



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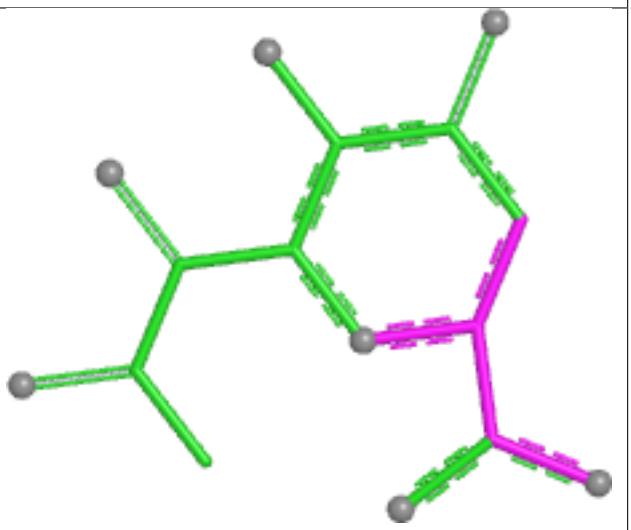

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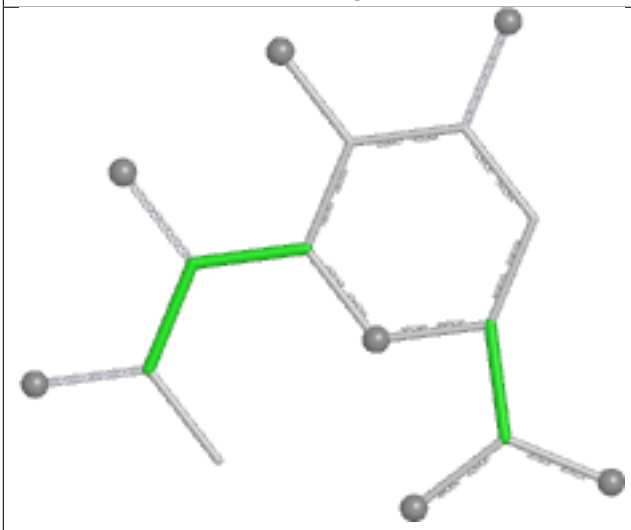

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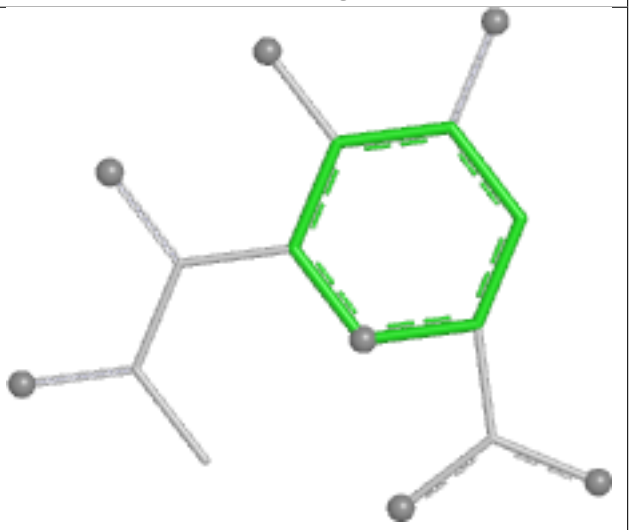
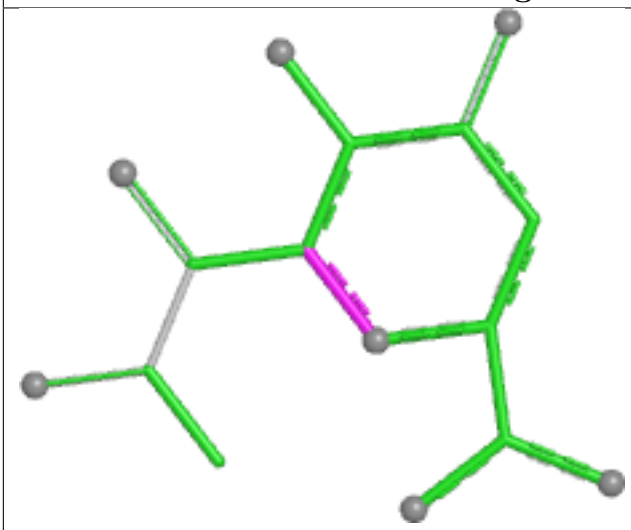


Rings

Ligand P8E aW 603



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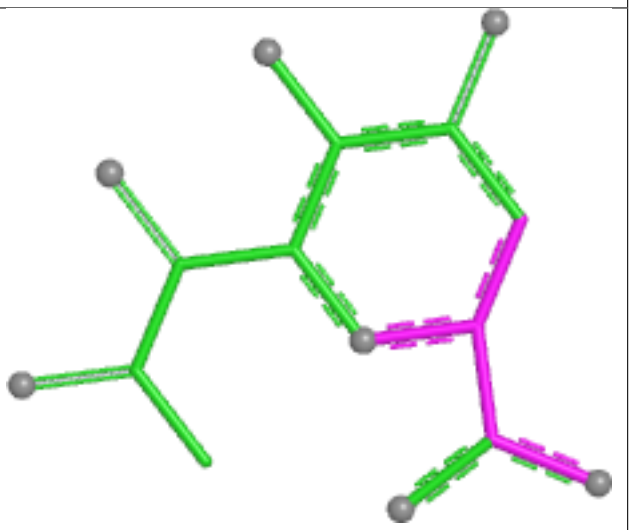

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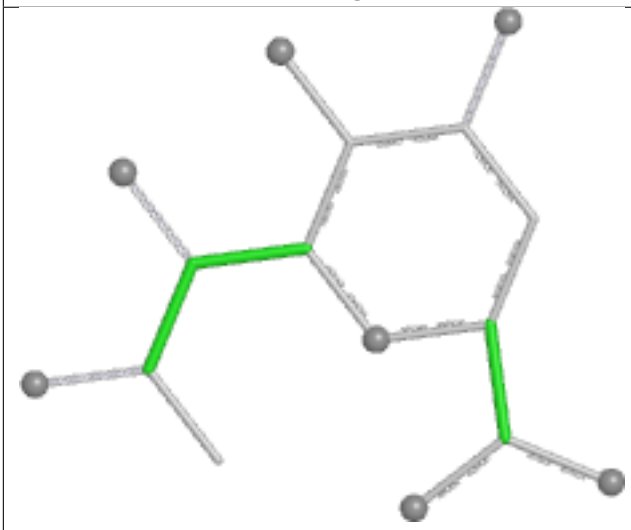

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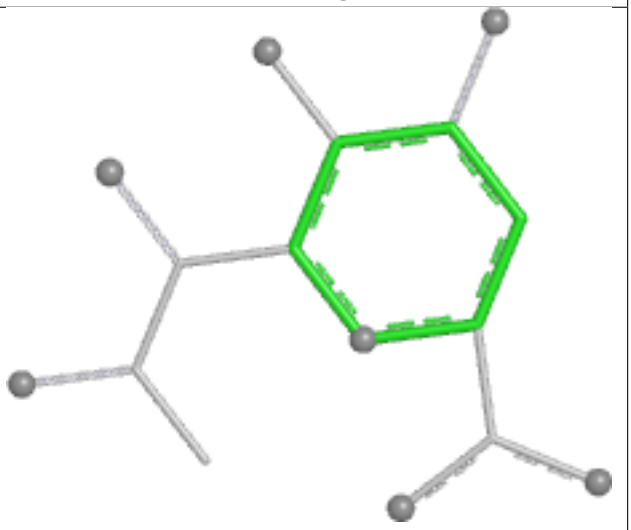
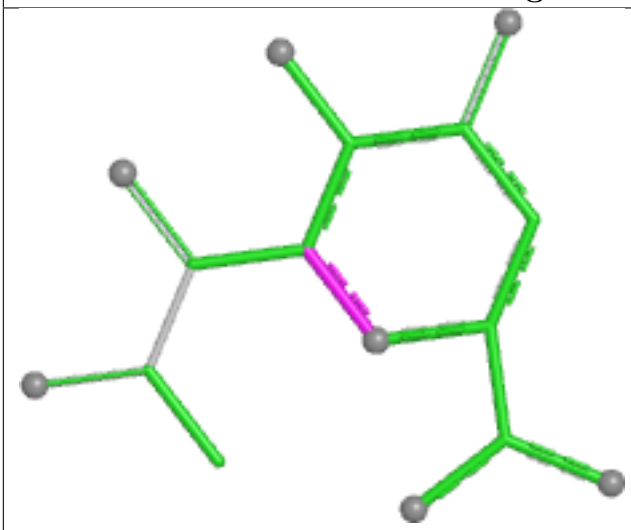


Rings

Ligand P8E I3 601



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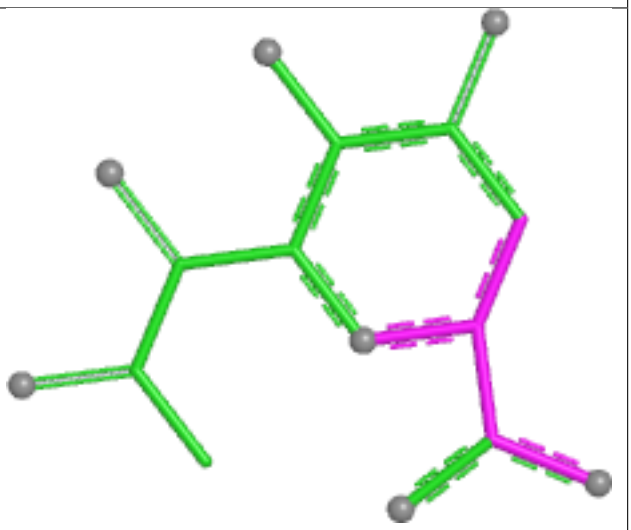

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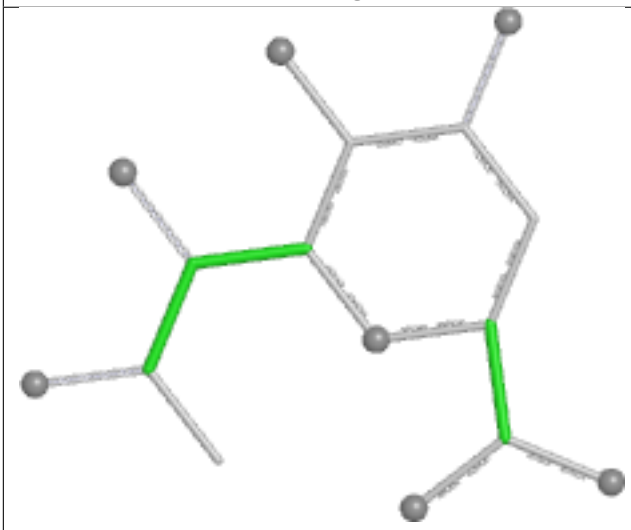

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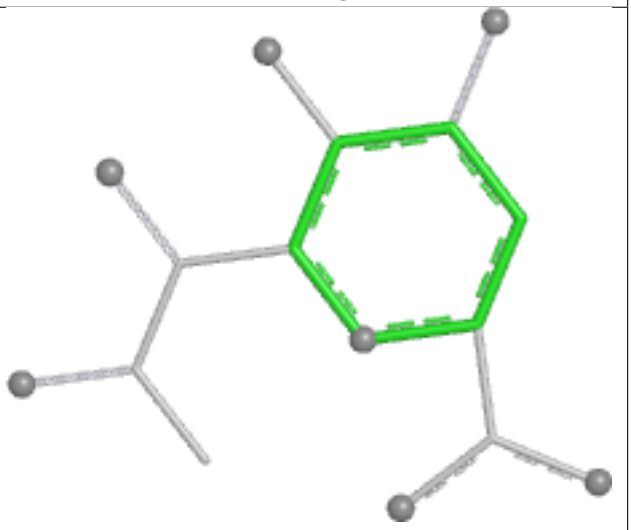
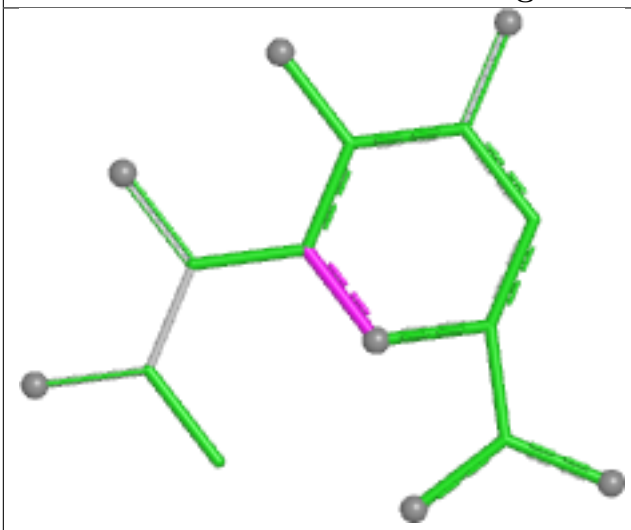


Rings

Ligand P8E TP 601



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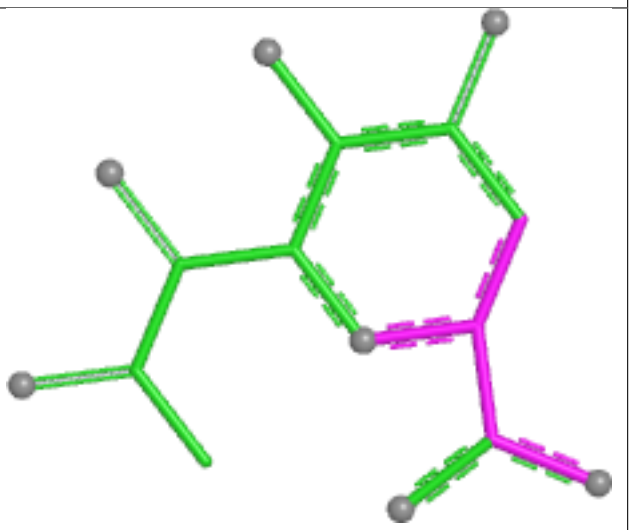

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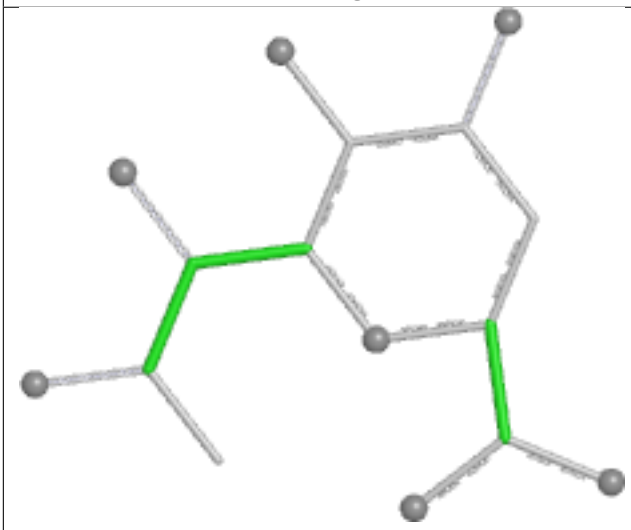

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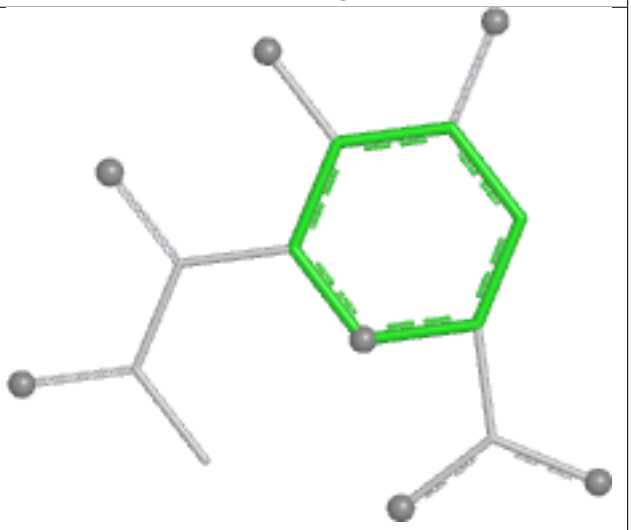
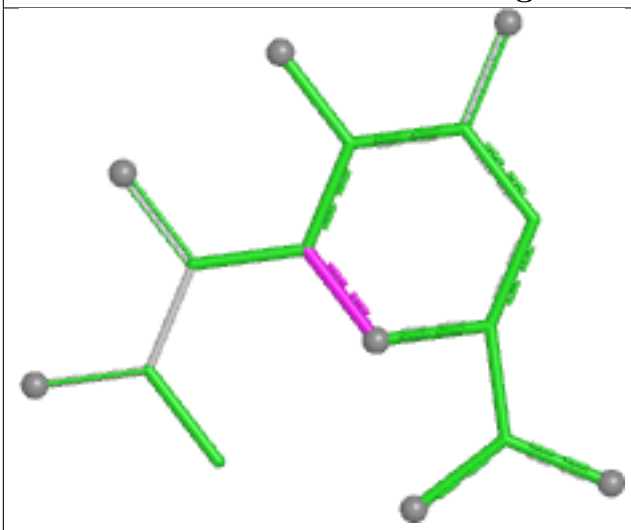


Rings

Ligand P8E KE 602



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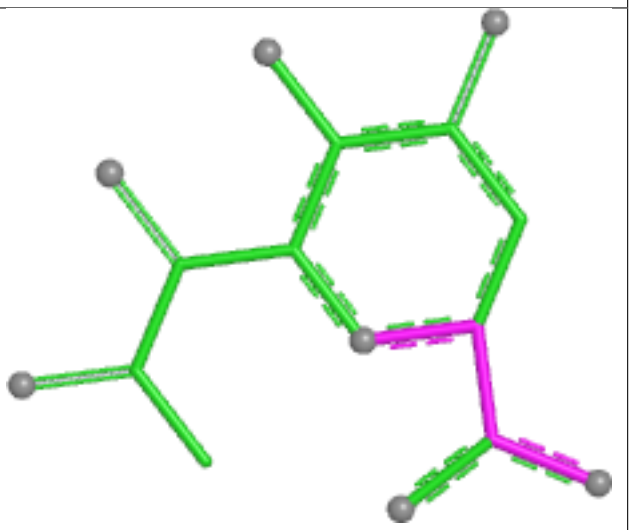

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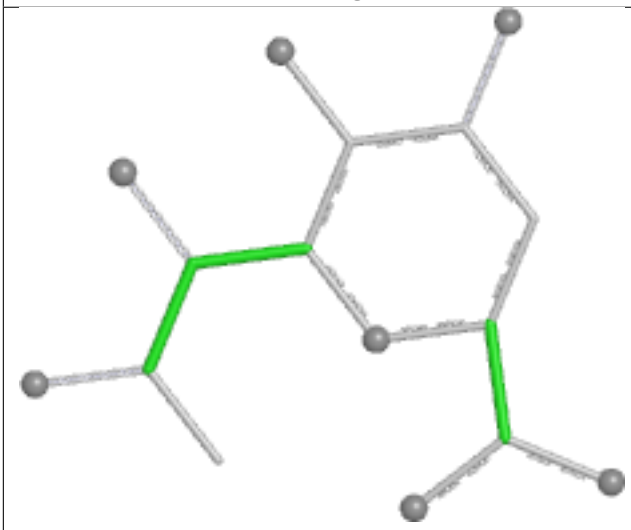

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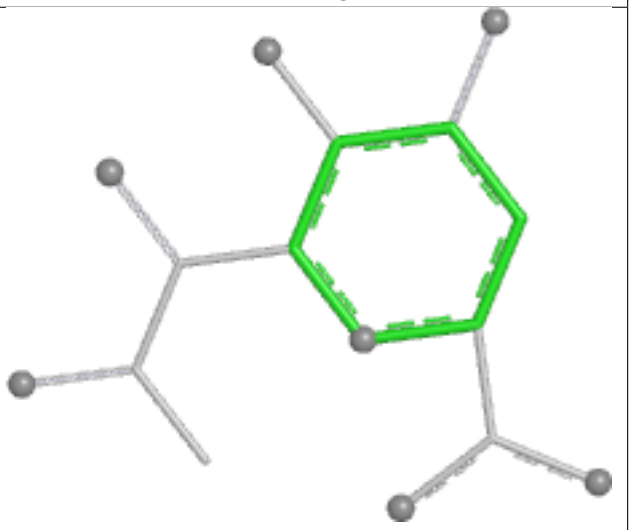
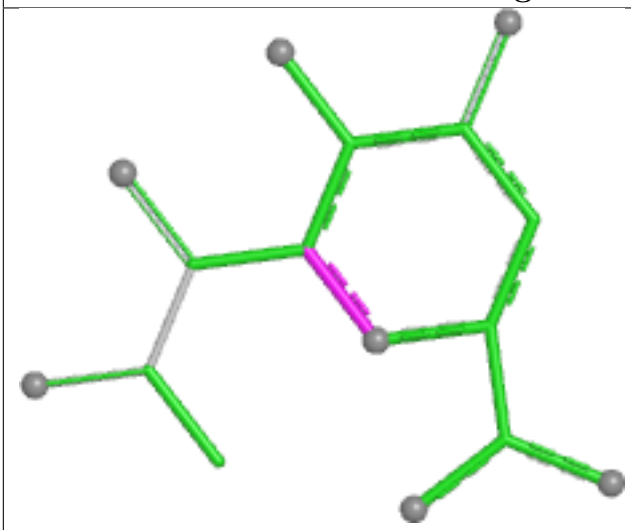


Rings

Ligand P8E aW 607



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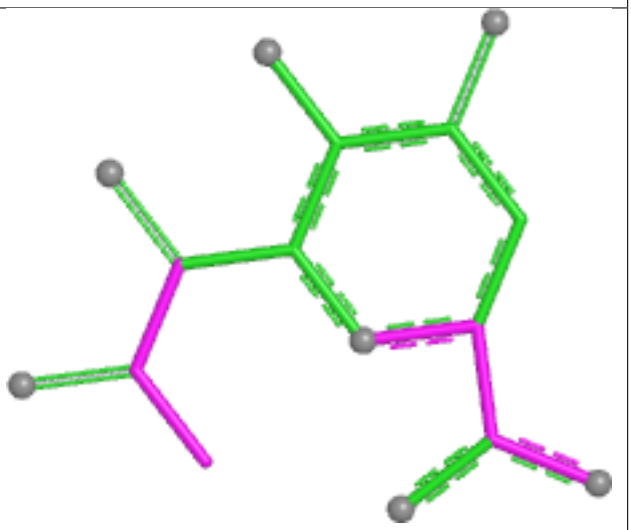

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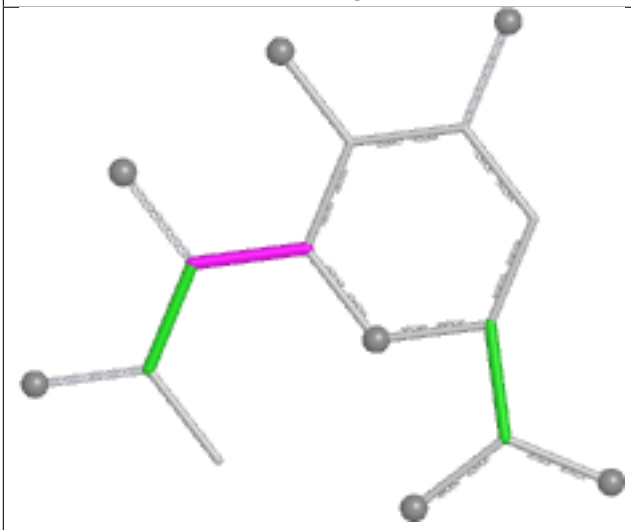

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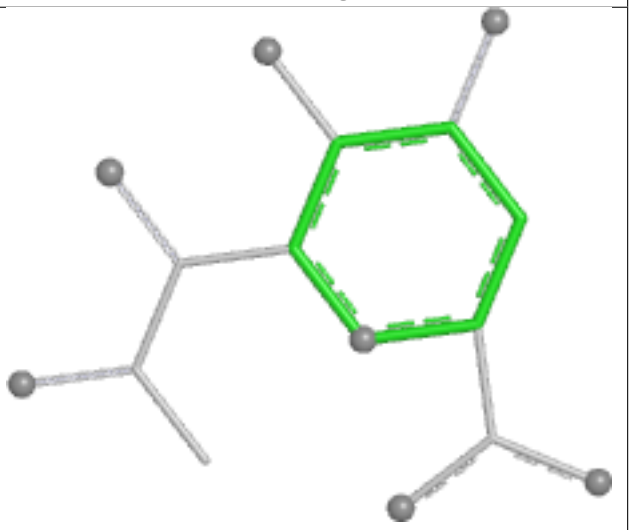
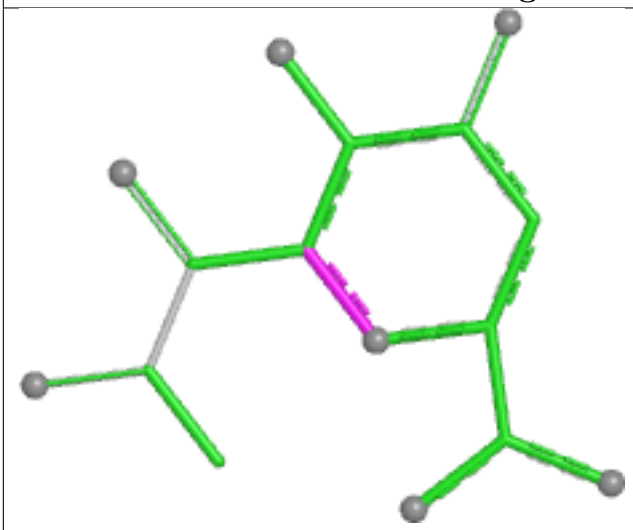


Rings

Ligand P8E A7 604



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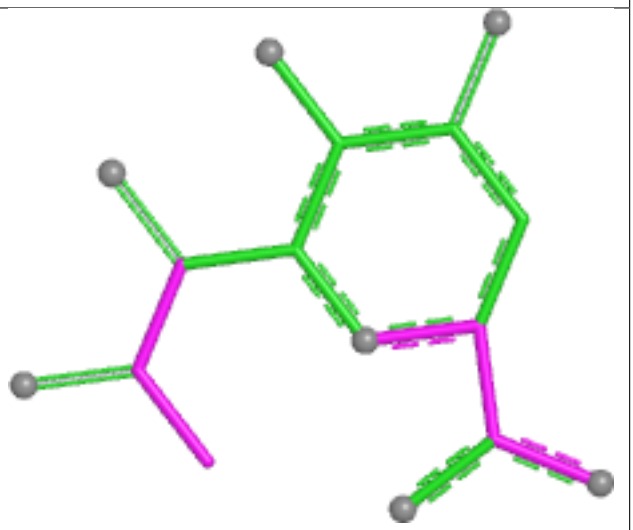

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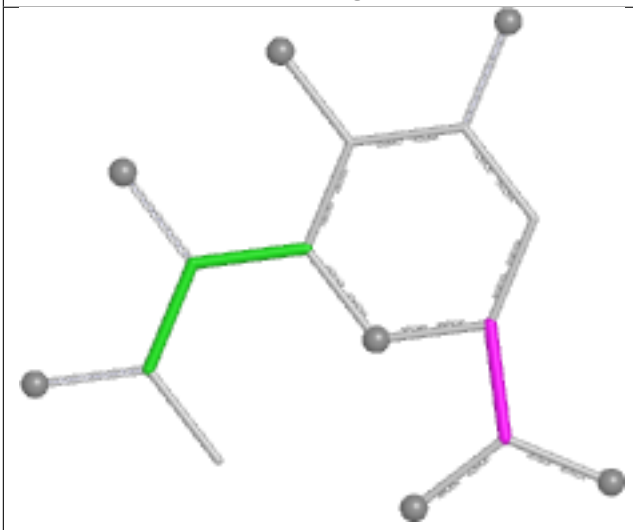

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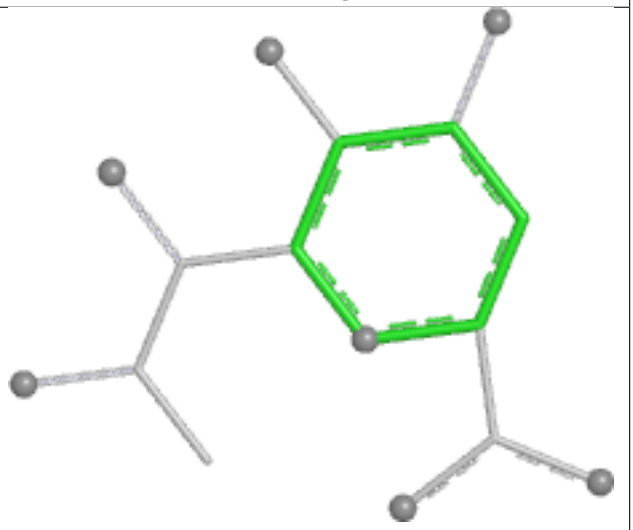
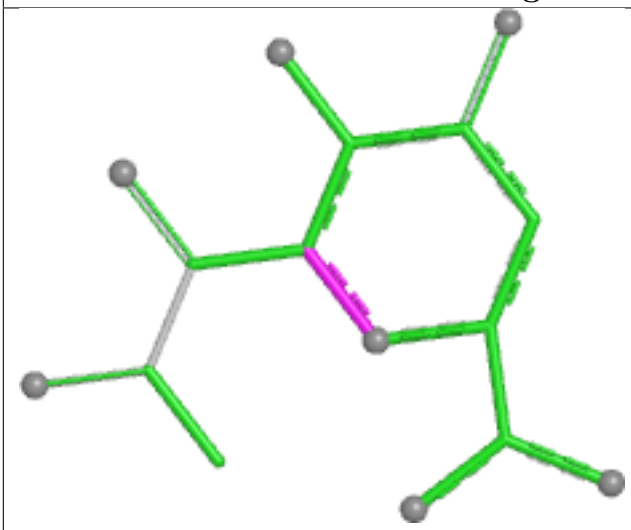


Rings

Ligand P8E S5 604



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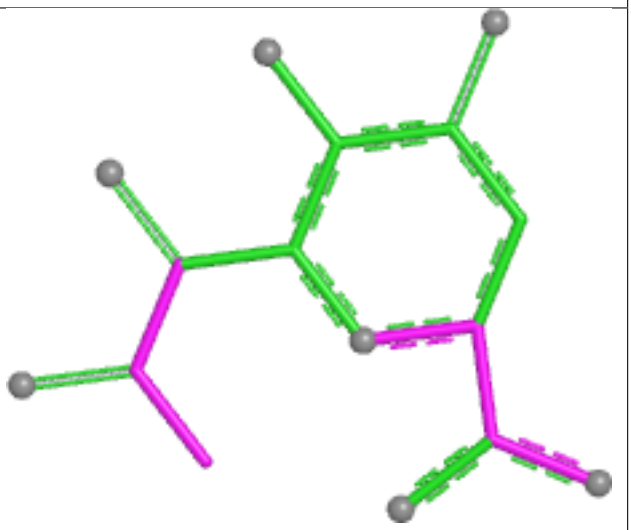

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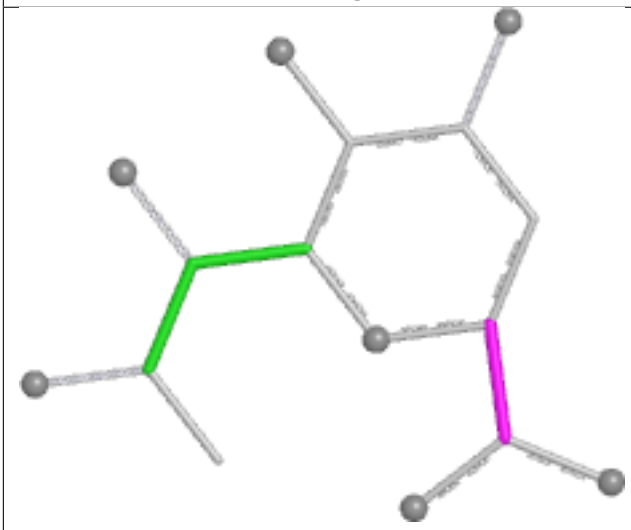

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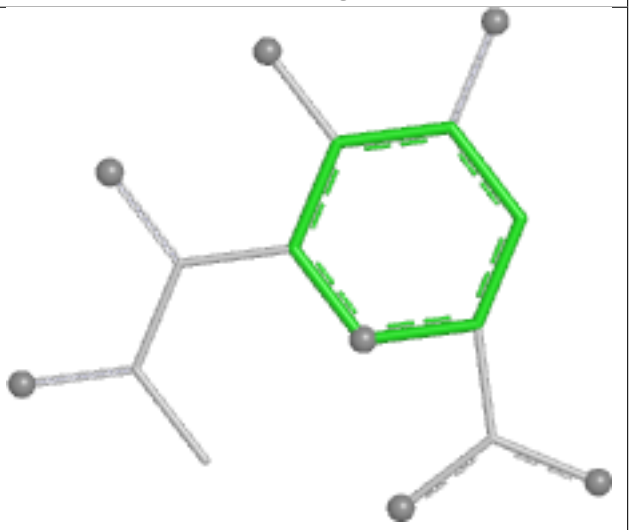
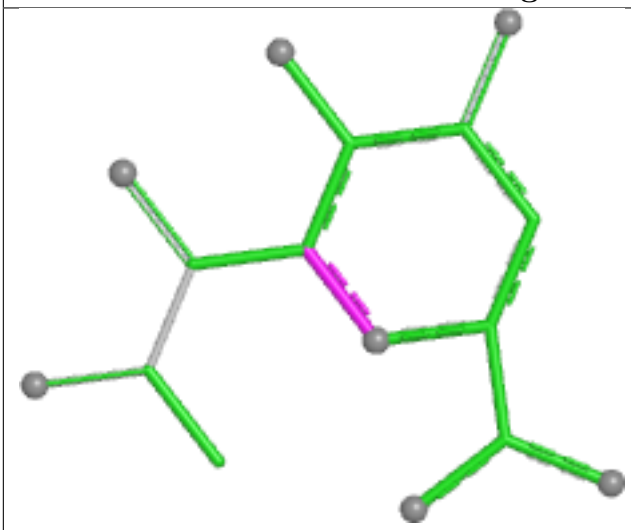


Rings

Ligand P8E NI 607



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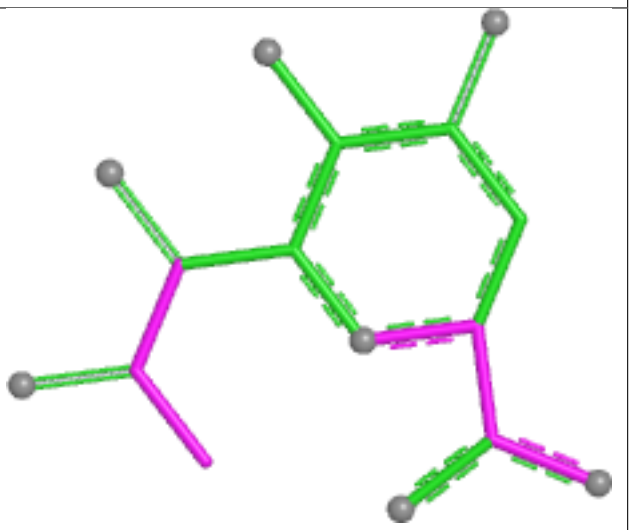
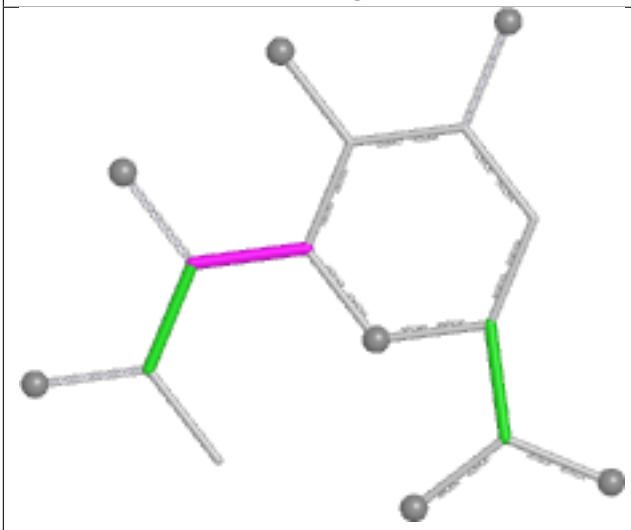


Bond angles



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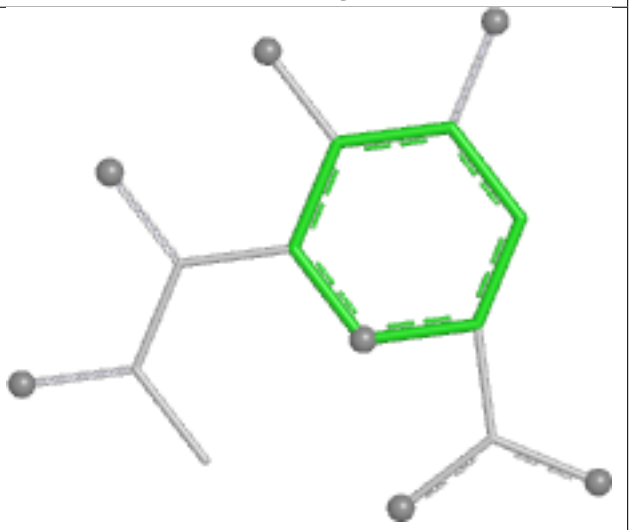
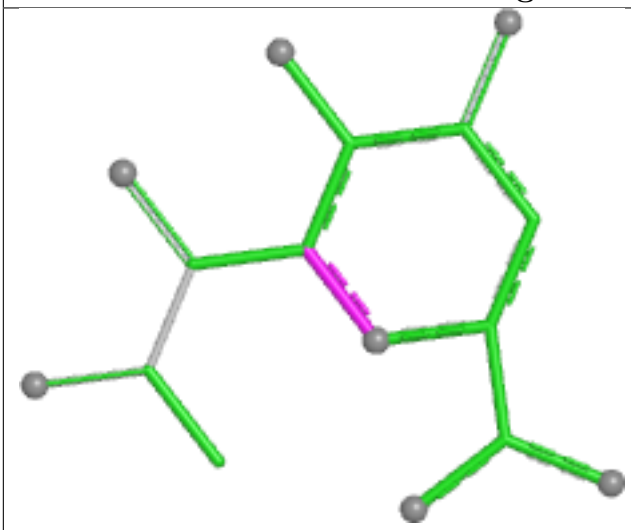


Rings

Ligand P8E HL 607



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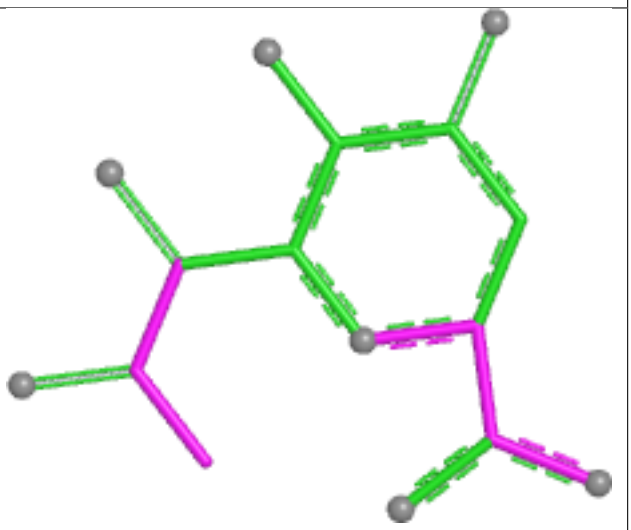

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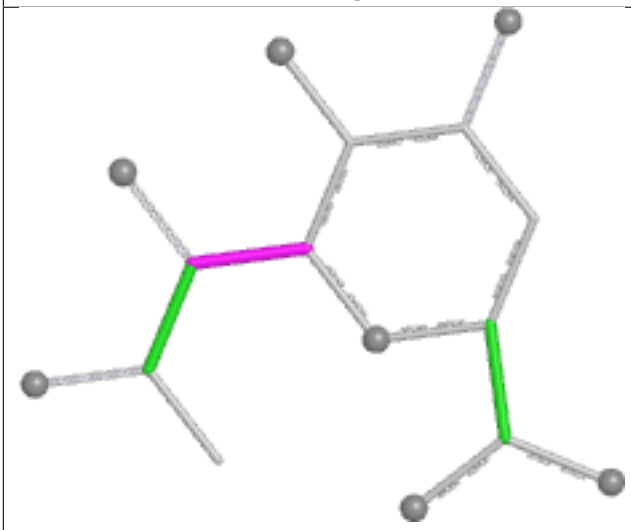
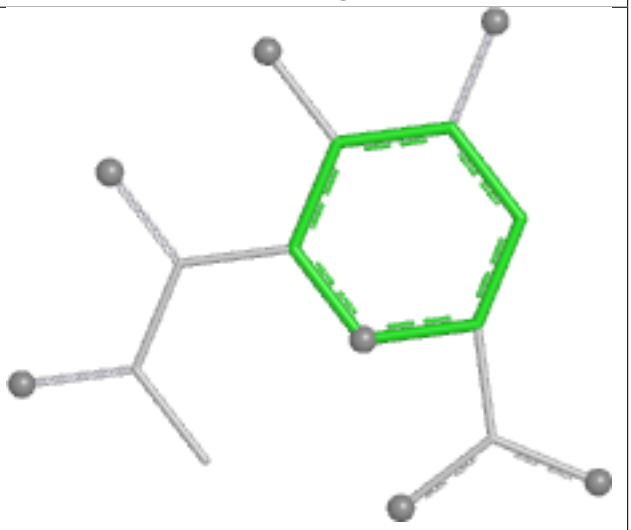
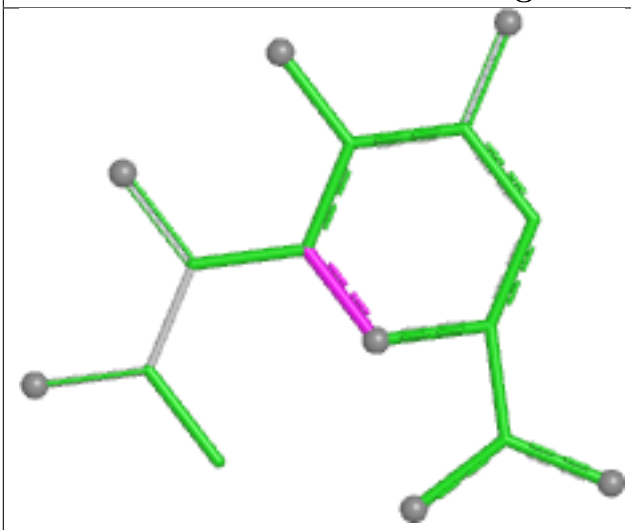


Torsions

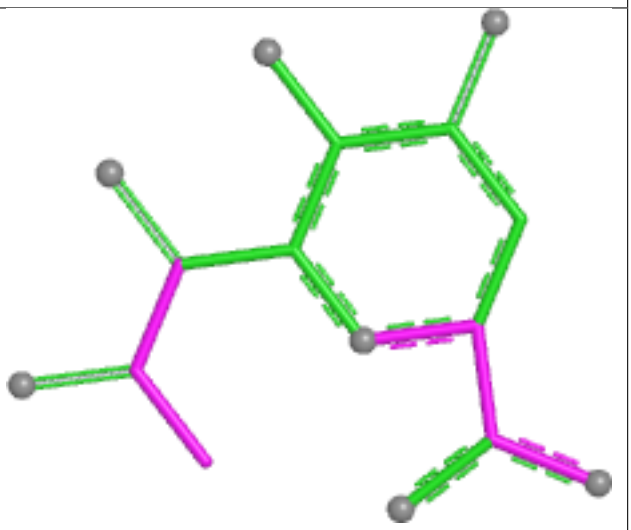


Rings

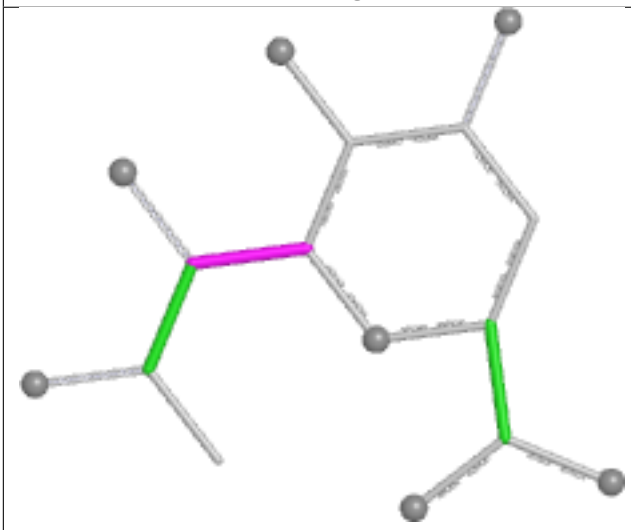
Ligand P8E PU 607



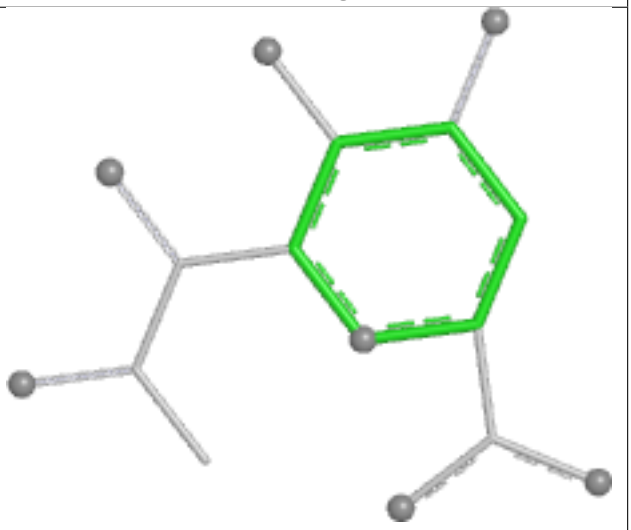
Bond lengths



Bond angles

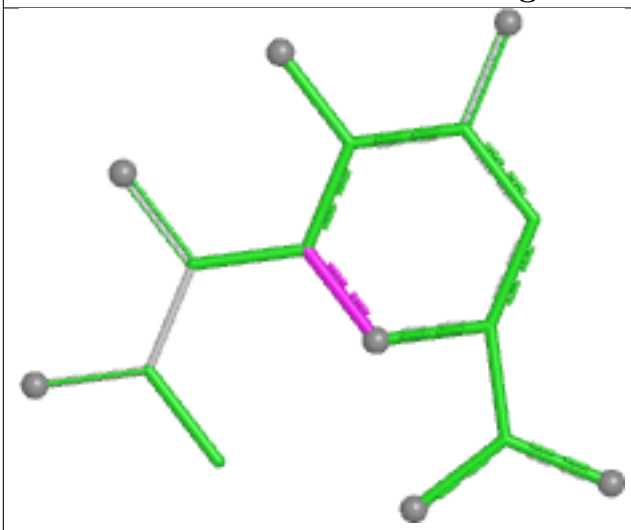


Torsions



Rings

Ligand P8E R4 607



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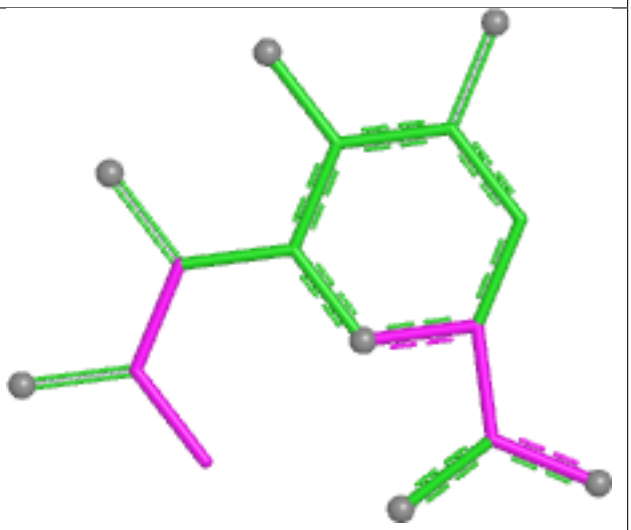

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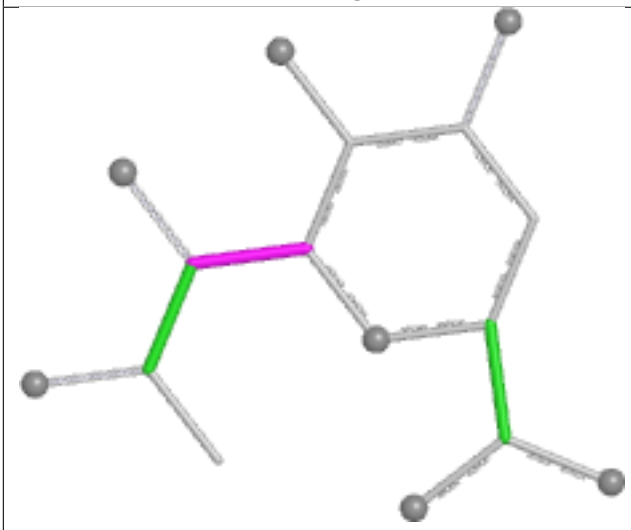

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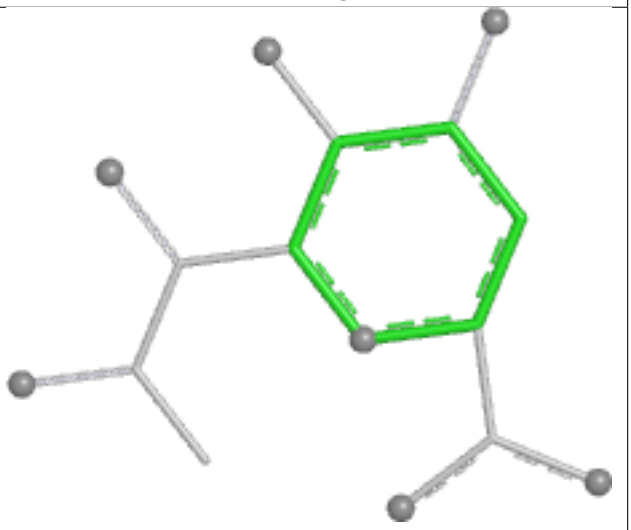
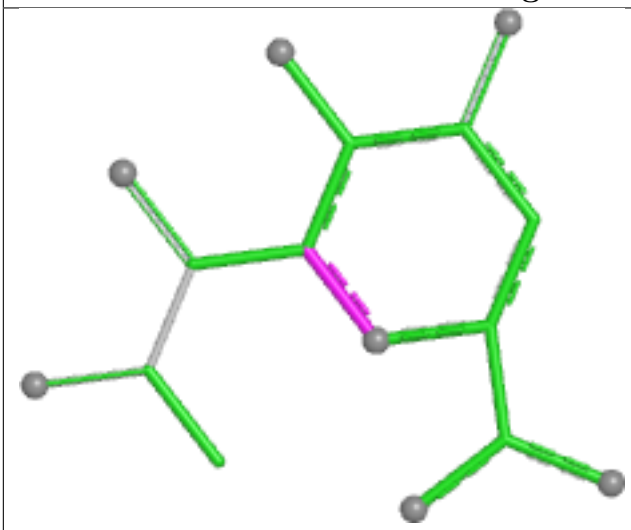


Rings

Ligand P8E fK 602



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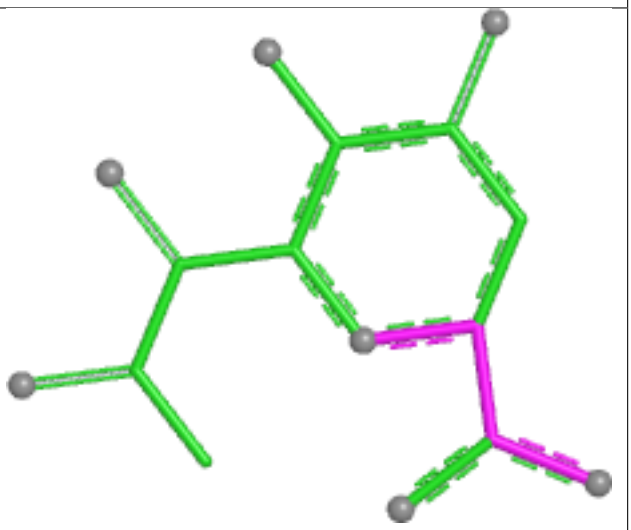

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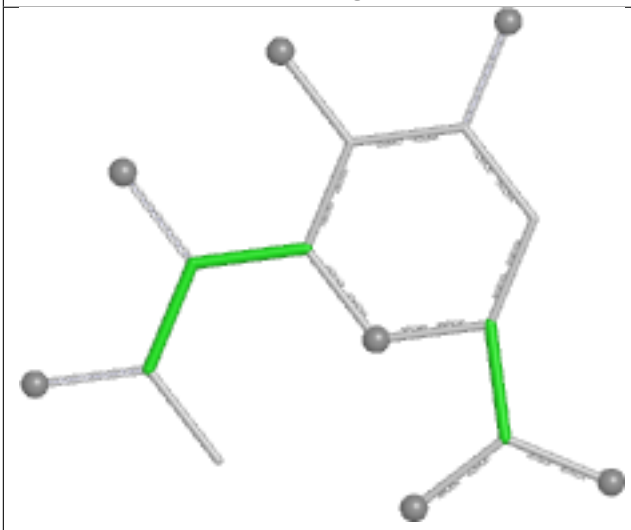

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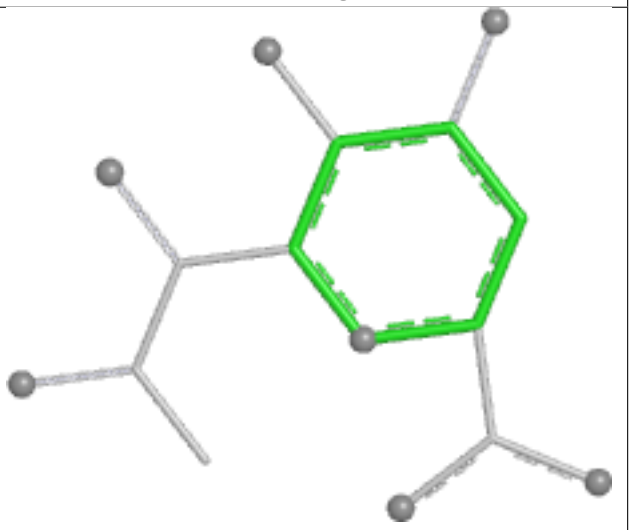
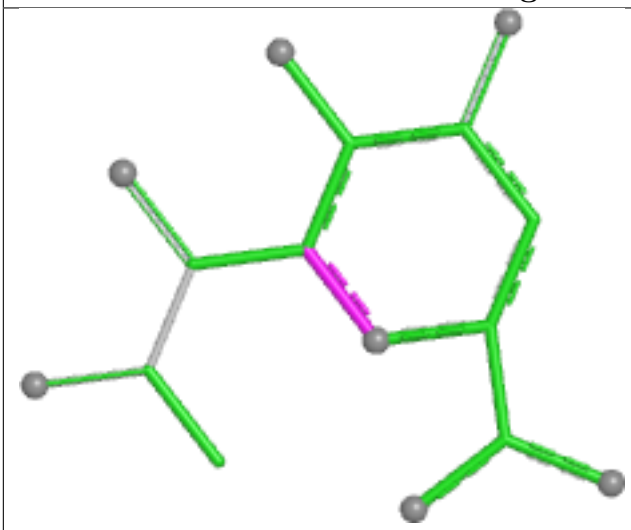


Rings

Ligand P8E cV 602



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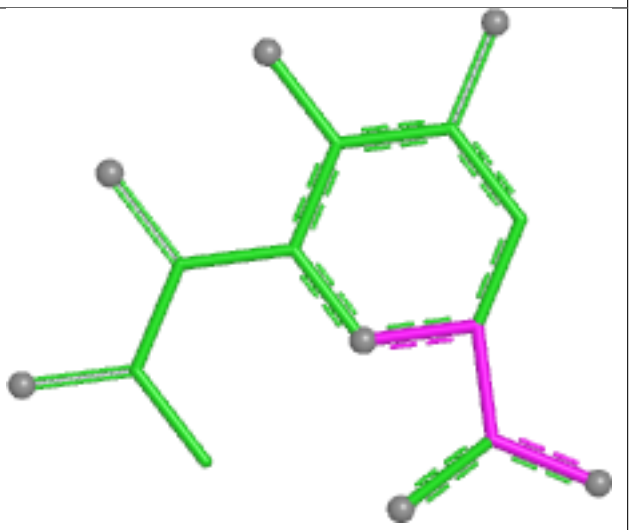

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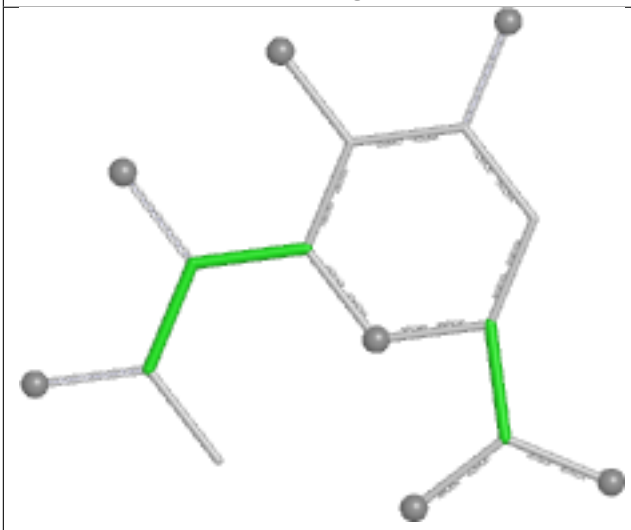

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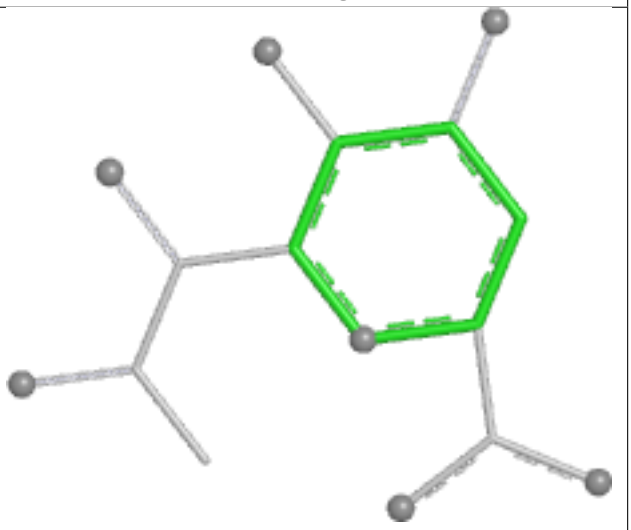
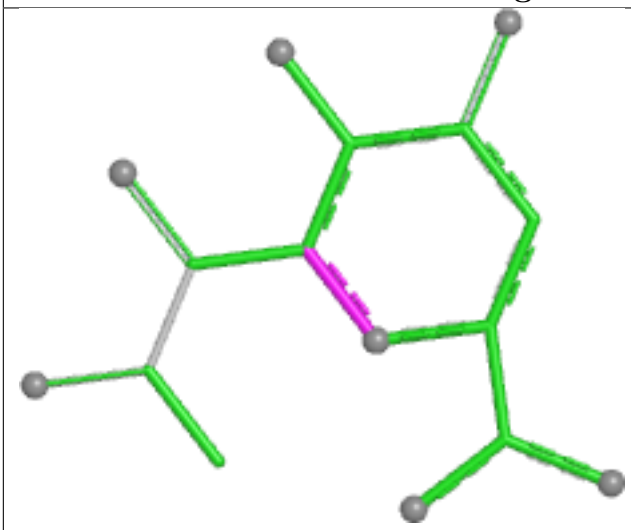


Rings

Ligand P8E aW 602



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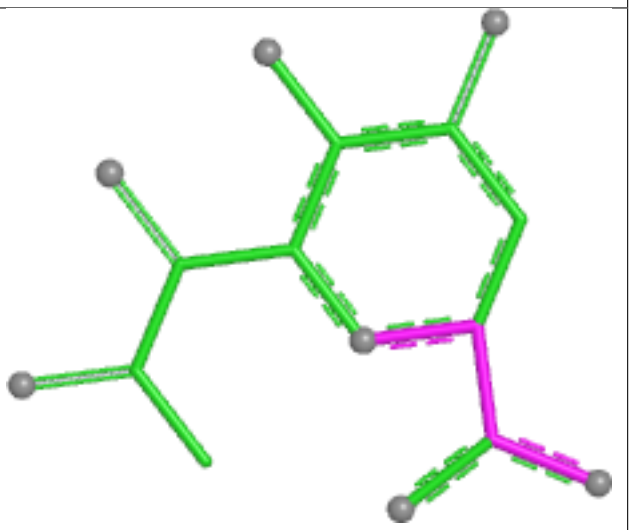

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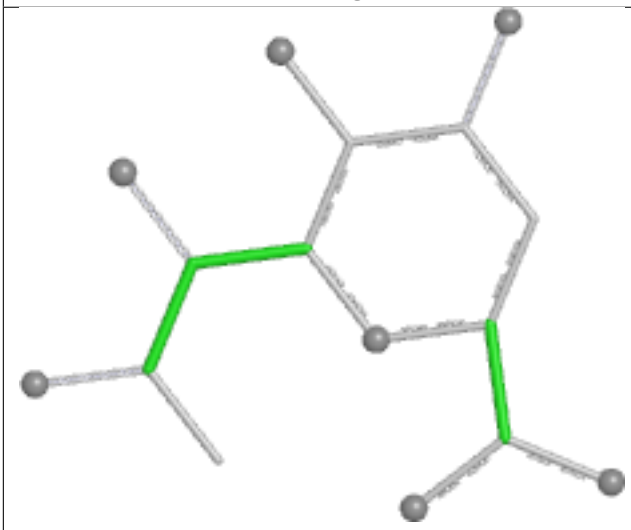

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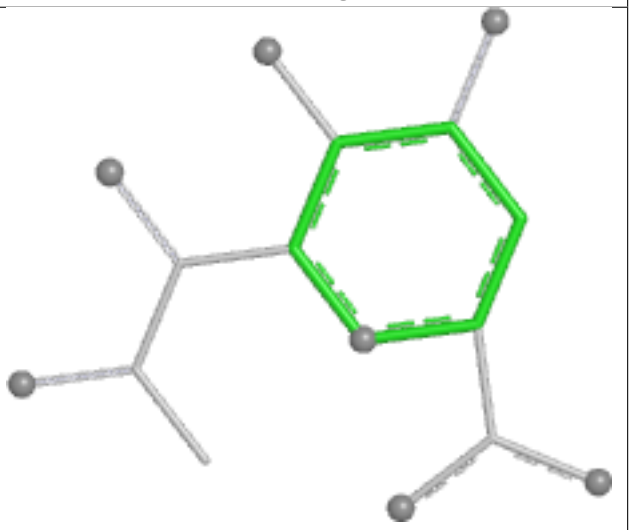
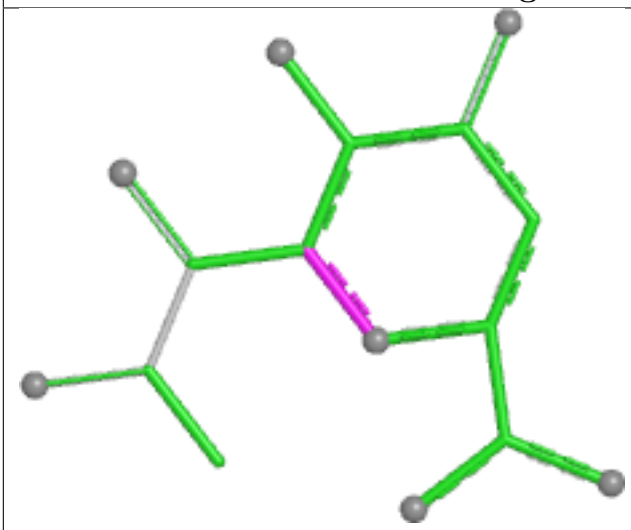


Rings

Ligand P8E BJ 602



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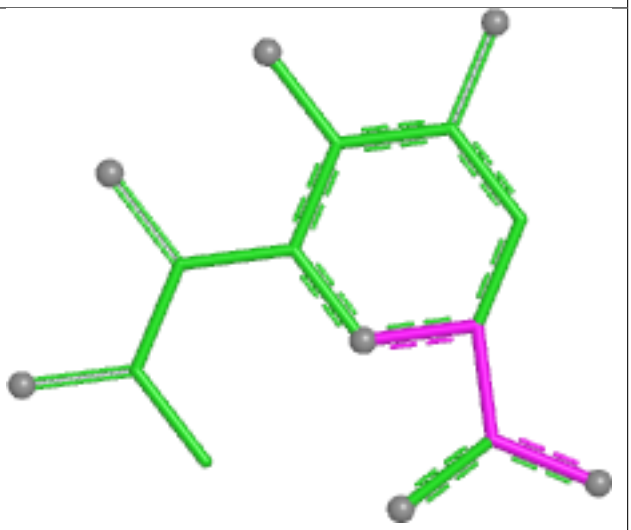

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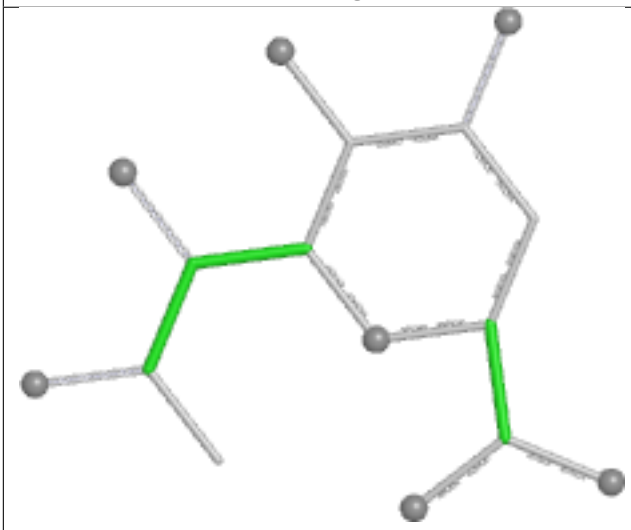

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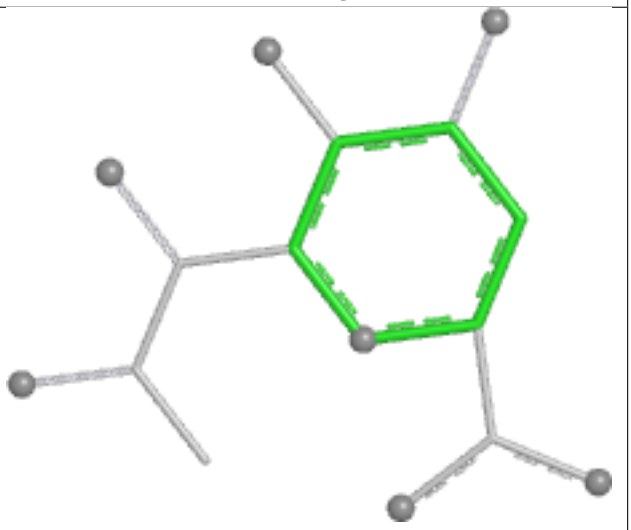
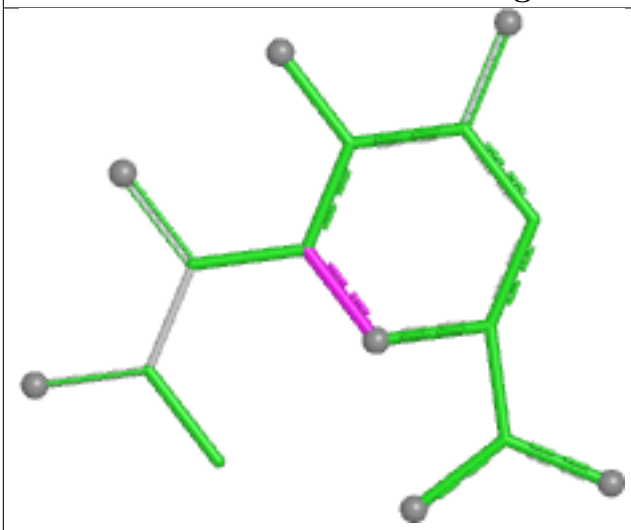


Rings

Ligand P8E DN 606



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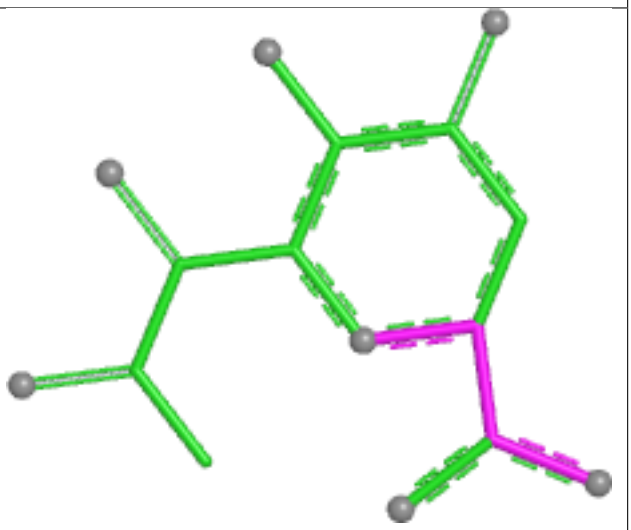

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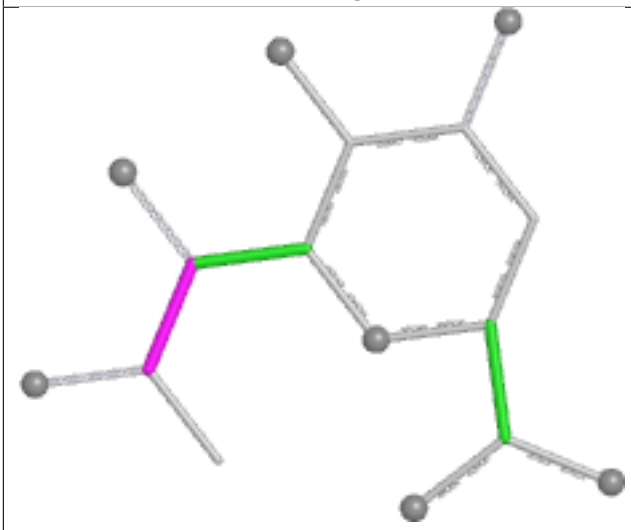

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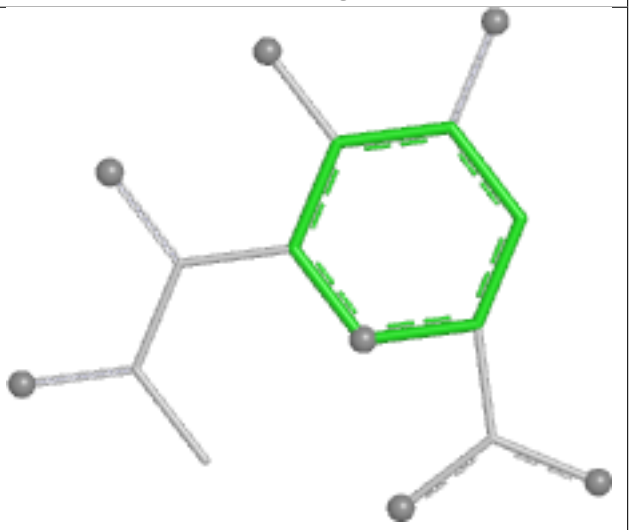
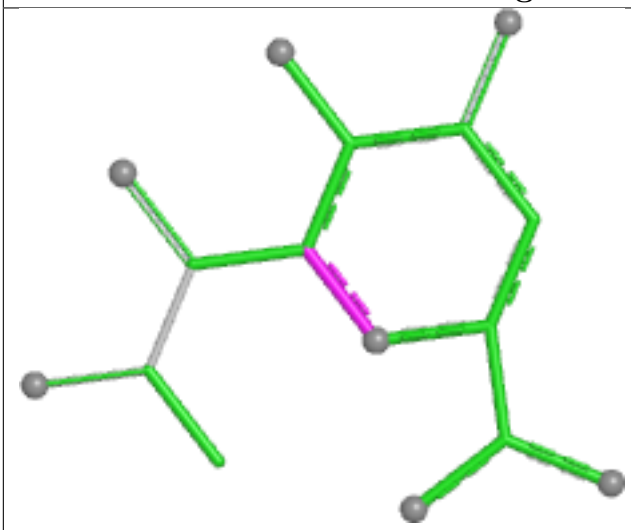


Rings

Ligand P8E KE 603



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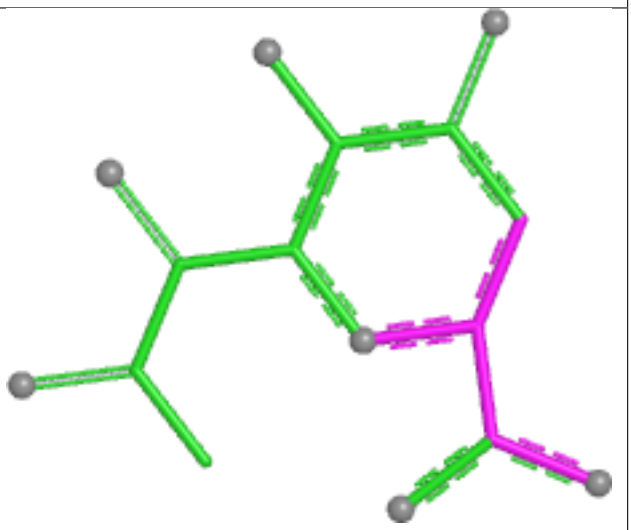

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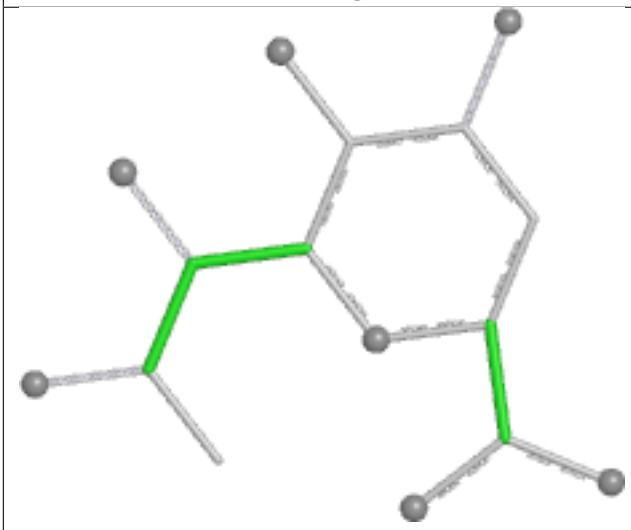

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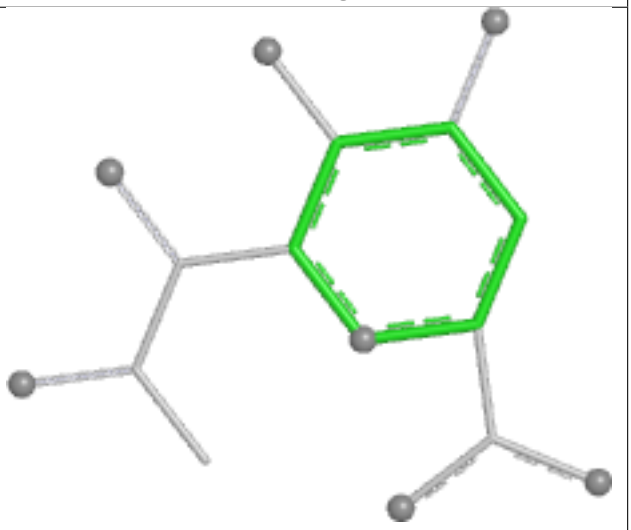
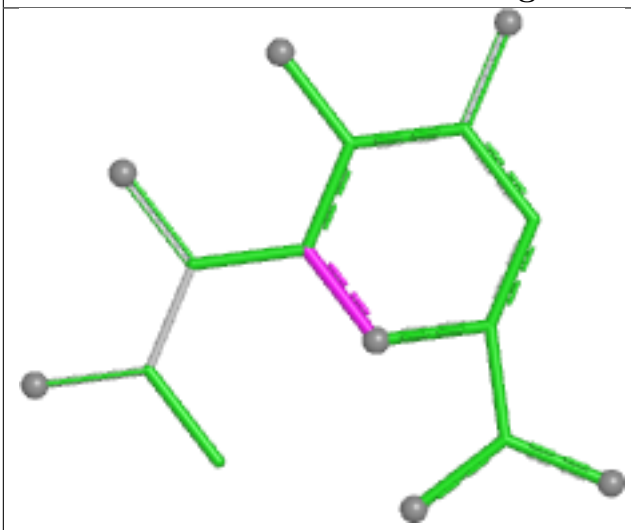


Rings

Ligand P8E JD 603



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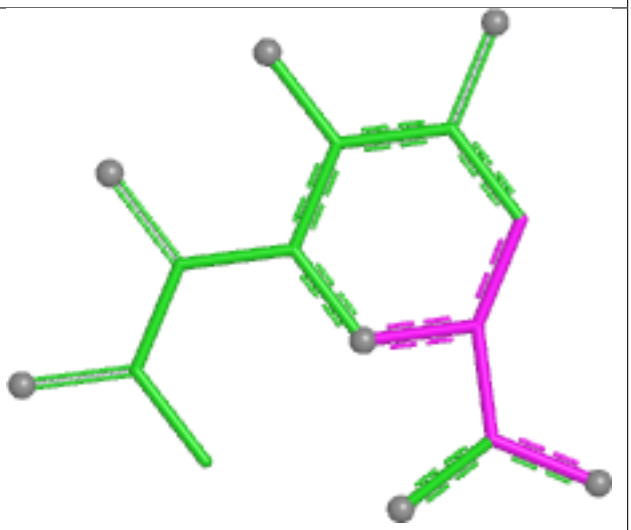

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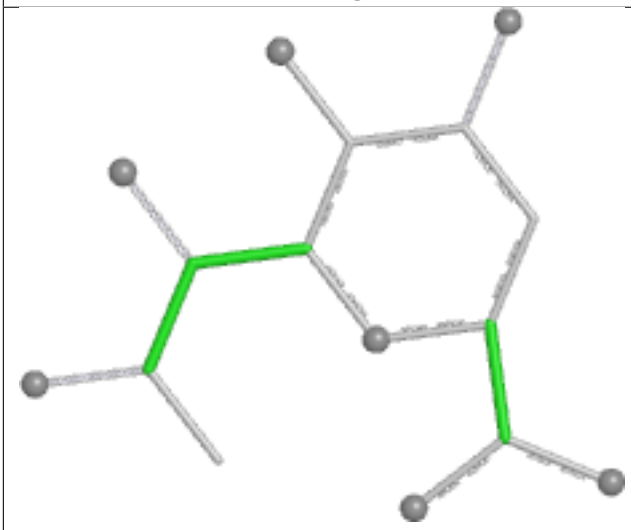

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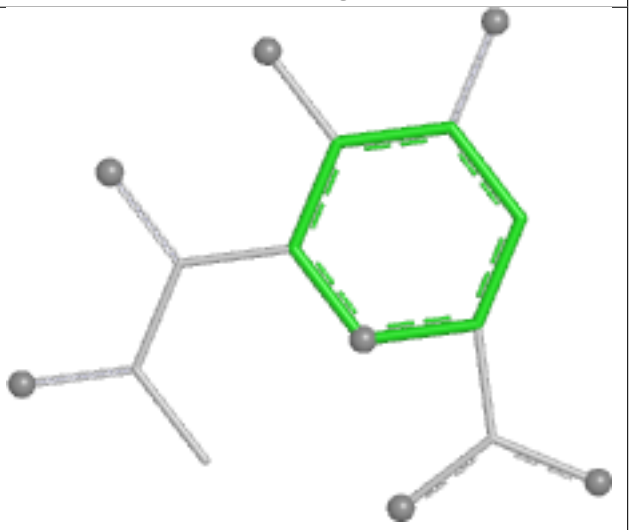
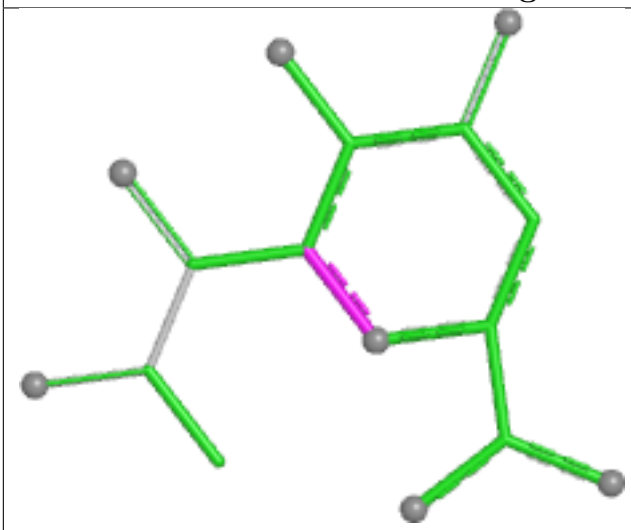


Rings

Ligand P8E BJ 603



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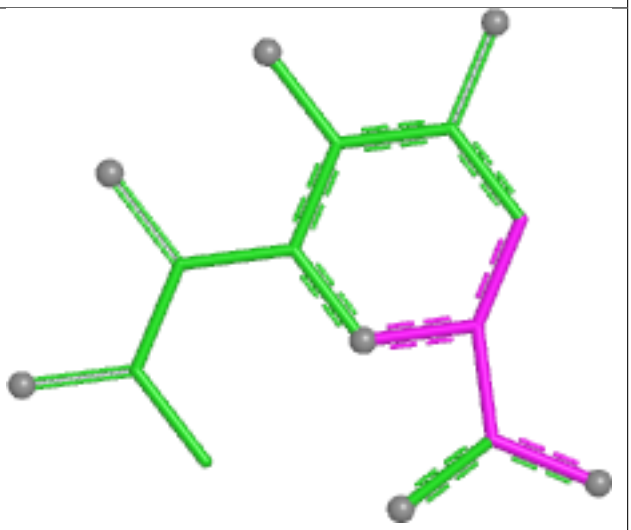

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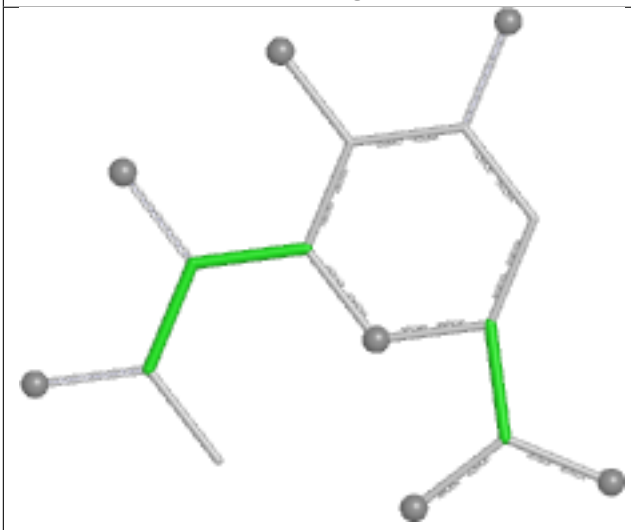

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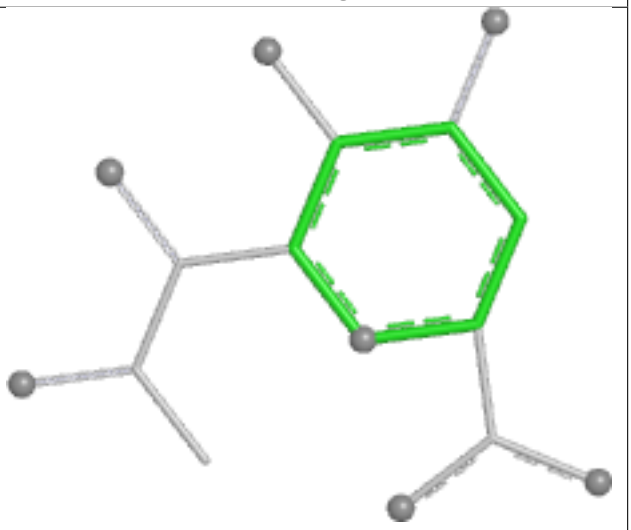
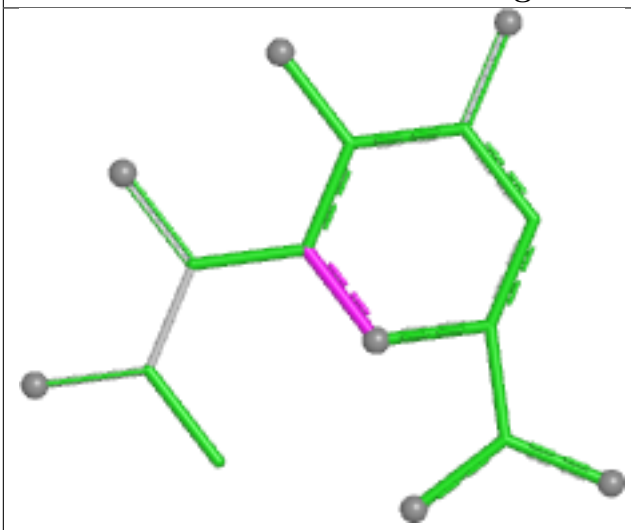


Rings

Ligand P8E GQ 601



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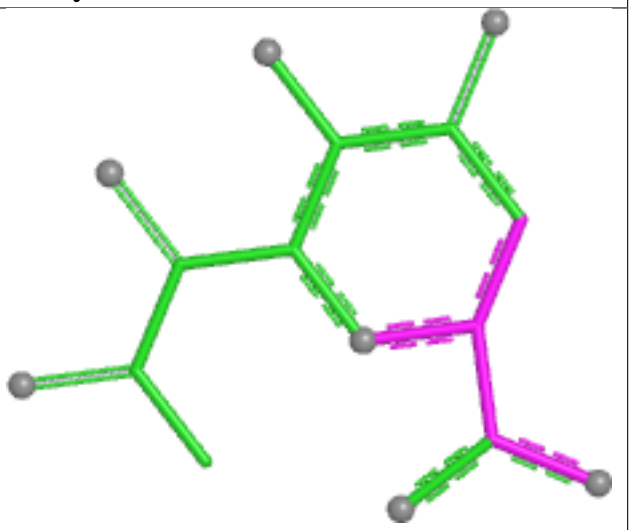

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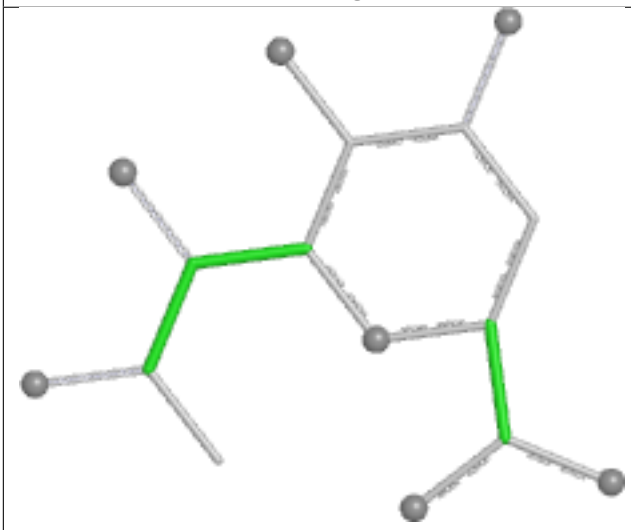

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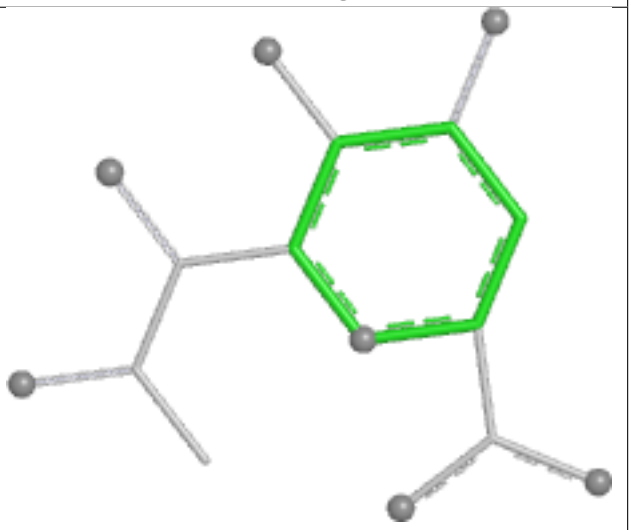
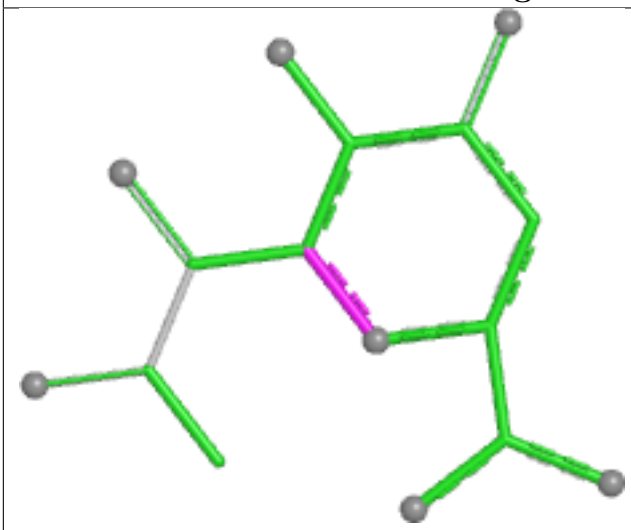


Rings

Ligand P8E GQ 605



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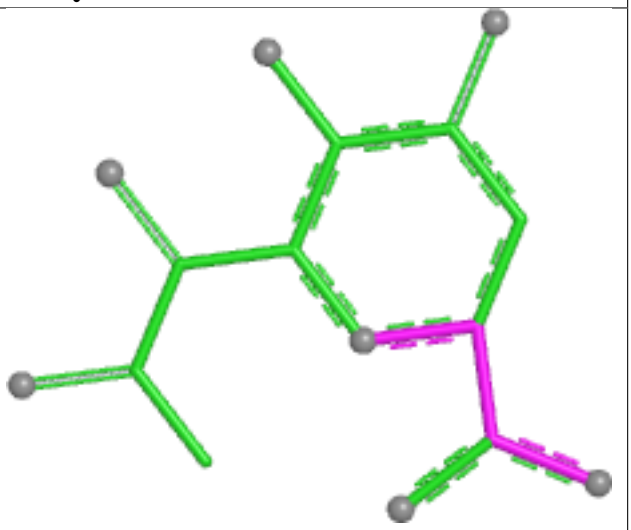

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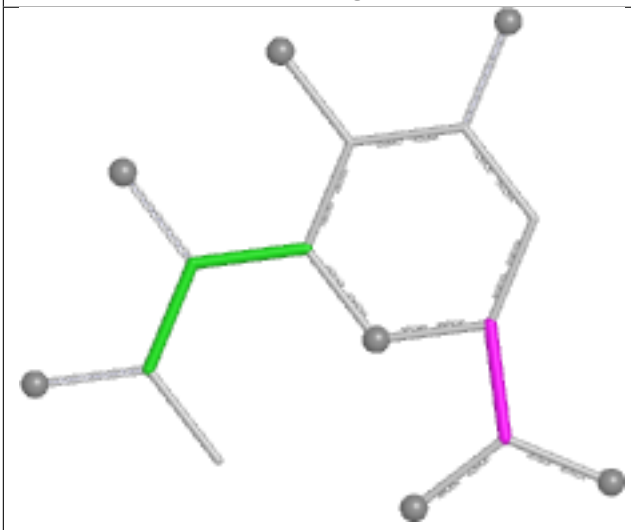

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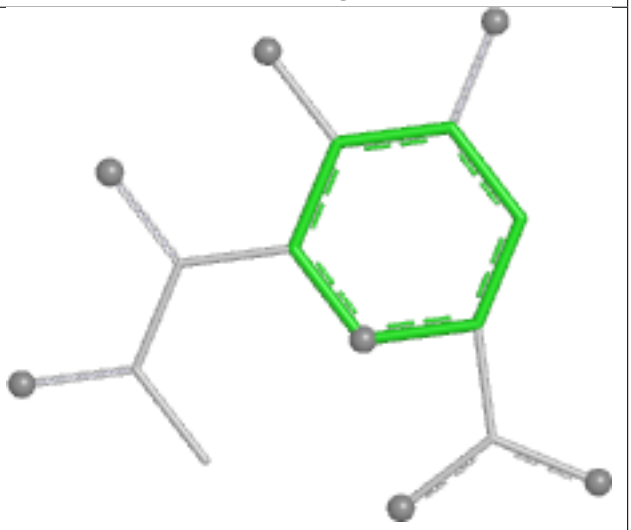
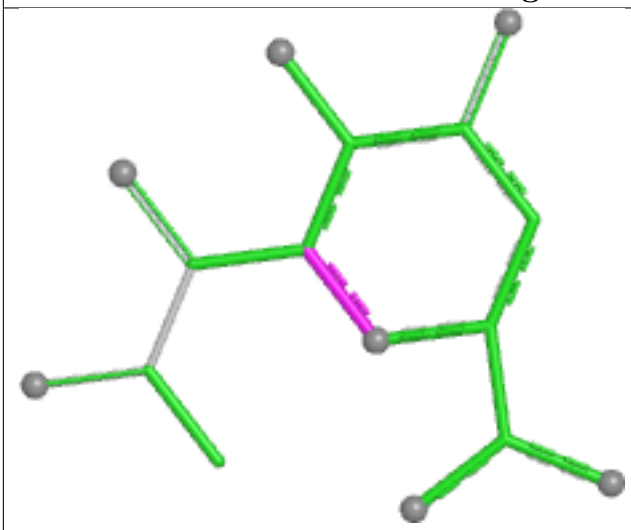


Rings

Ligand P8E bS 604



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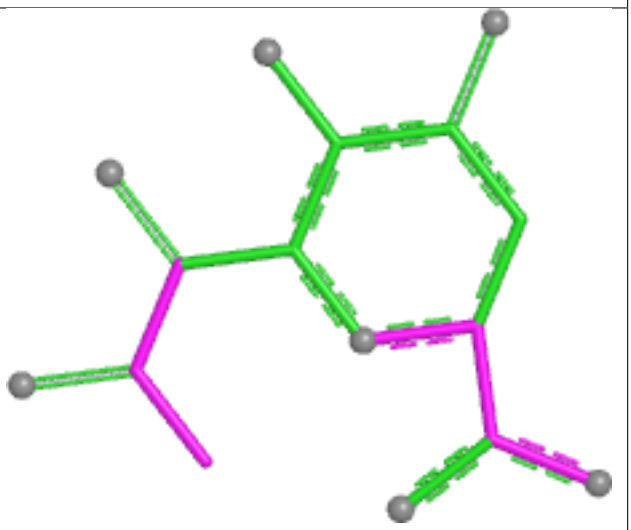

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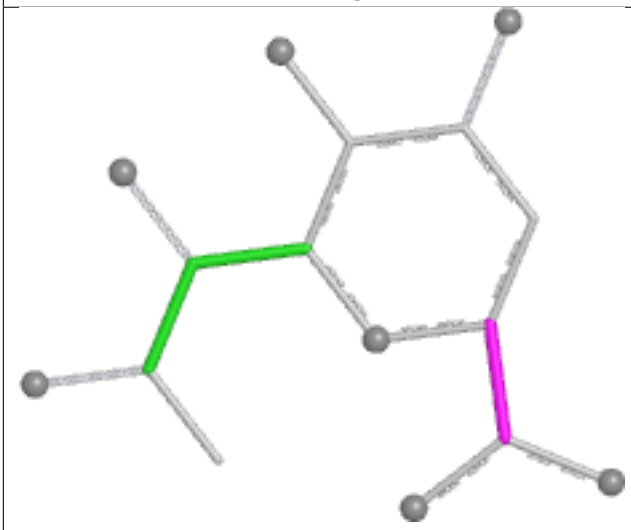

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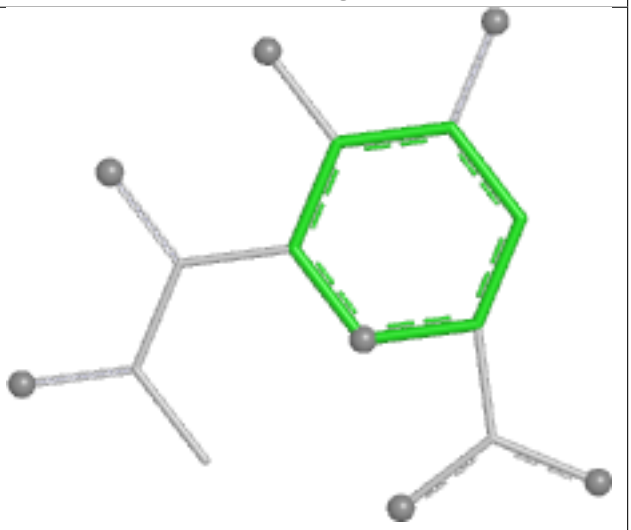
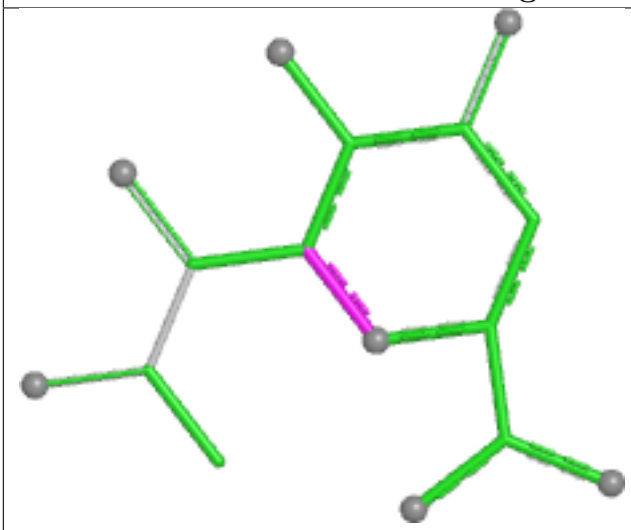


Rings

Ligand P8E BJ 606



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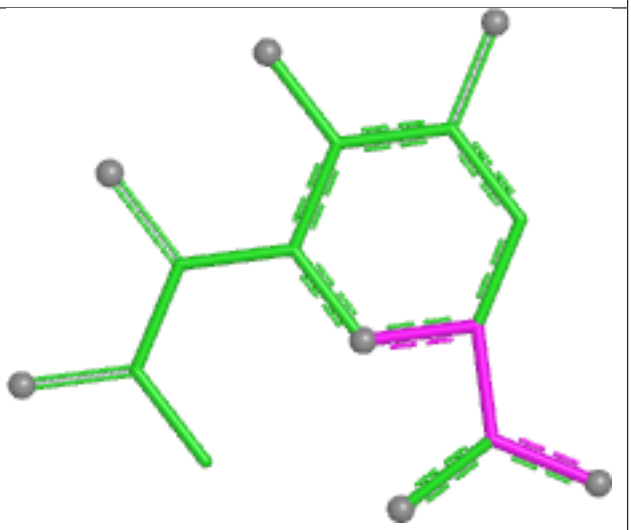

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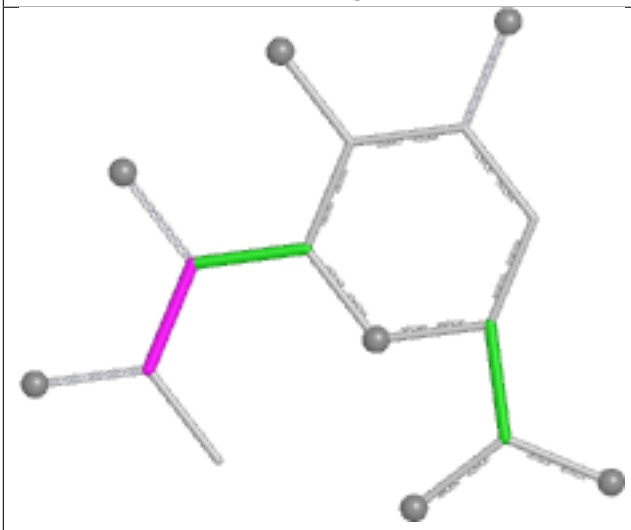
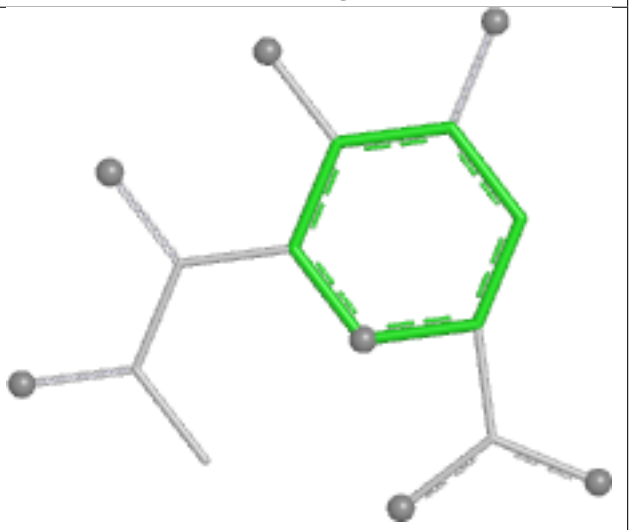
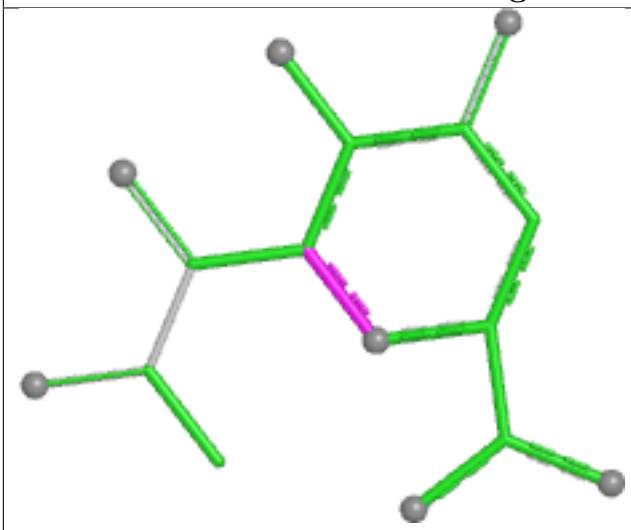


Torsions



Rings

Ligand P8E WG 606



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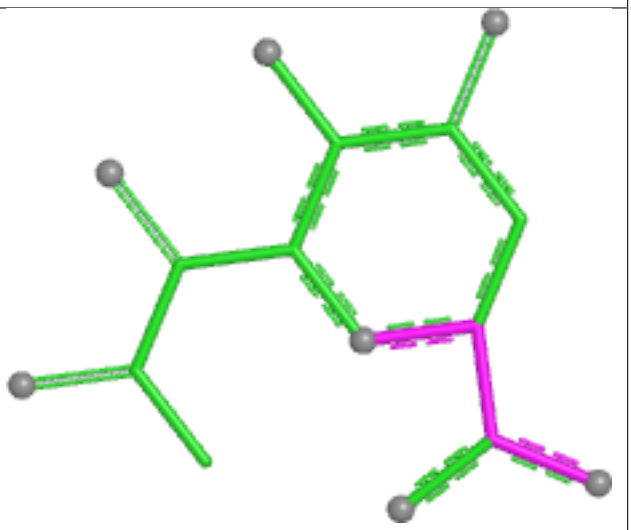

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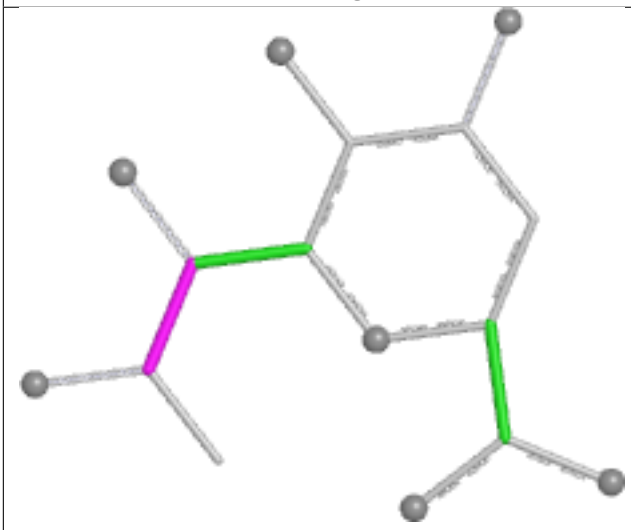

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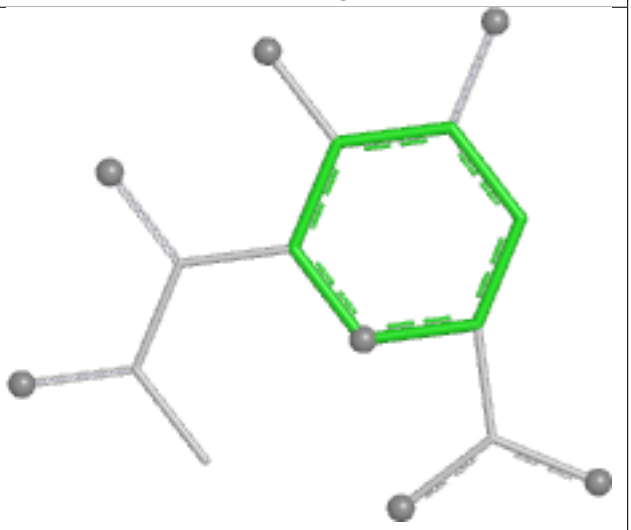
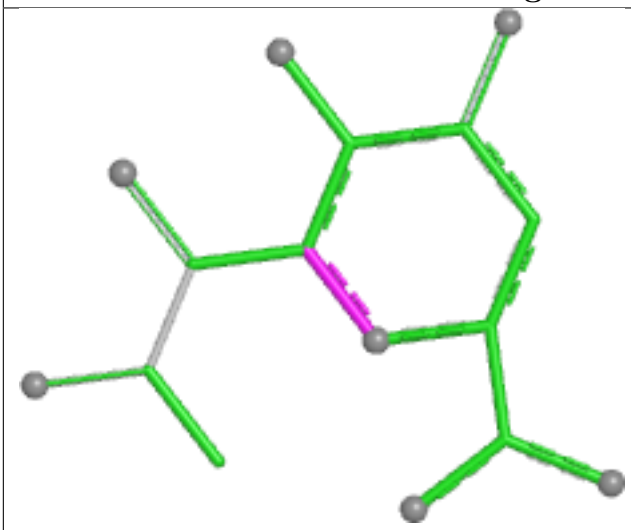


Rings

Ligand P8E e8 603



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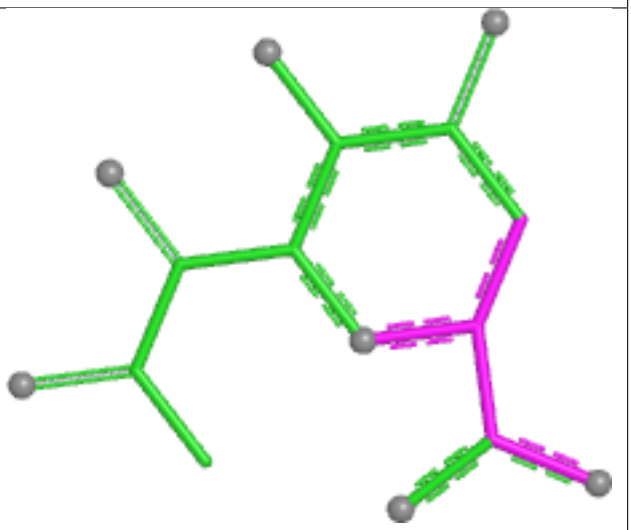

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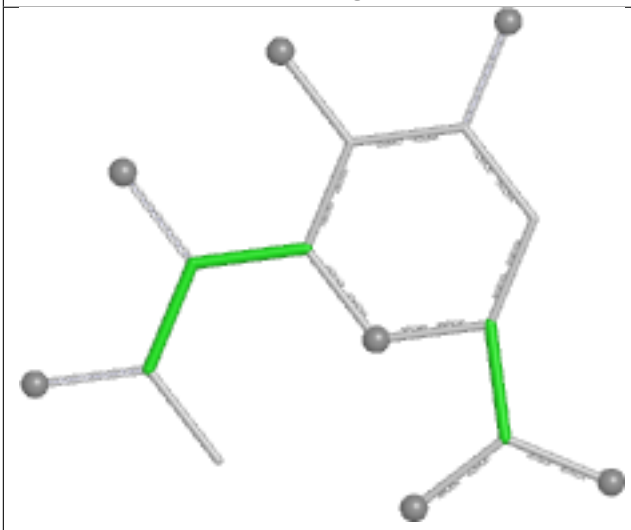

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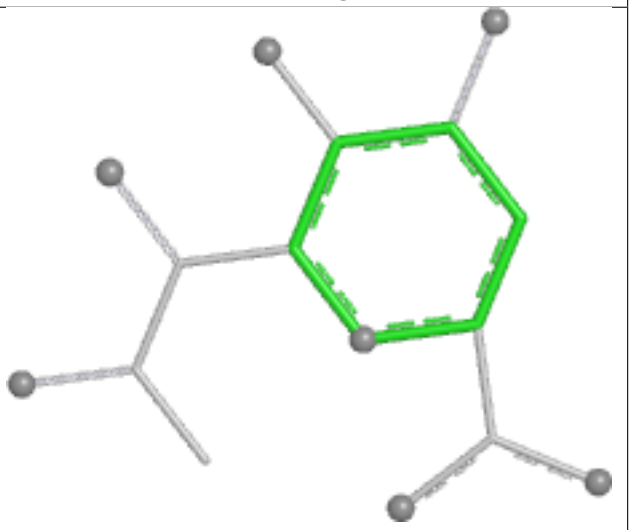
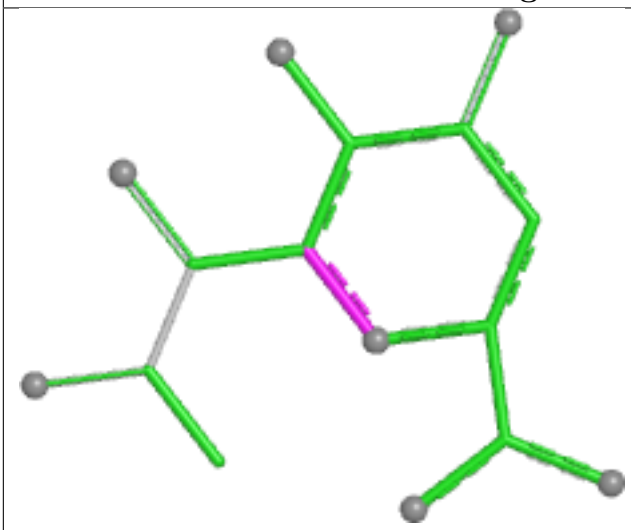


Rings

Ligand P8E cV 601



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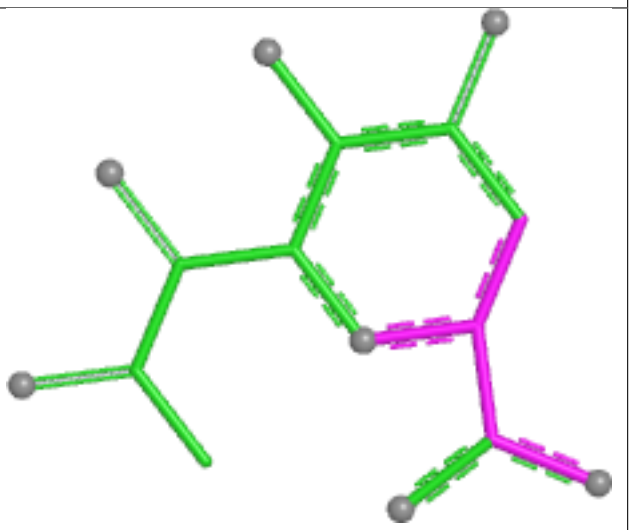

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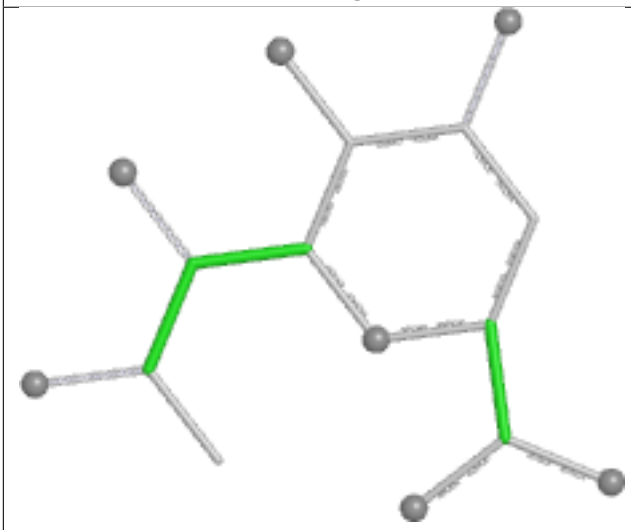

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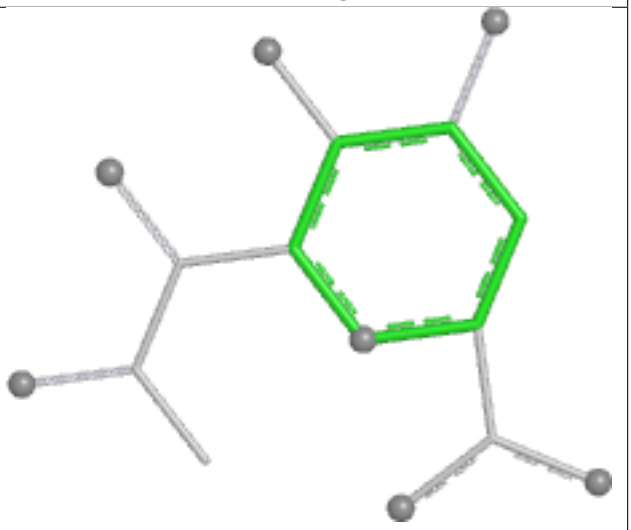
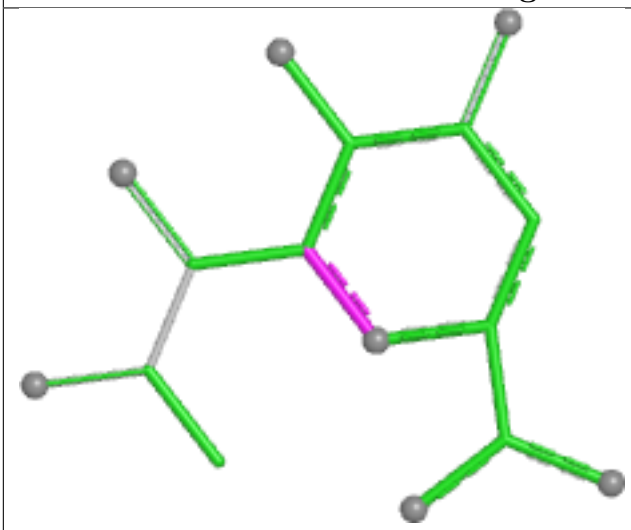


Rings

Ligand P8E BJ 604



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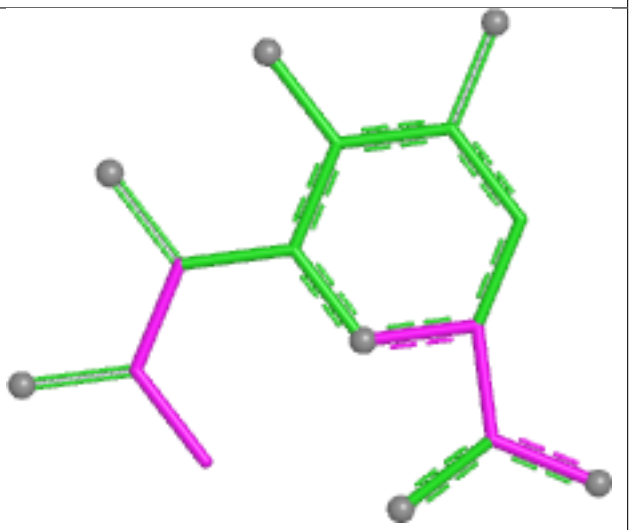

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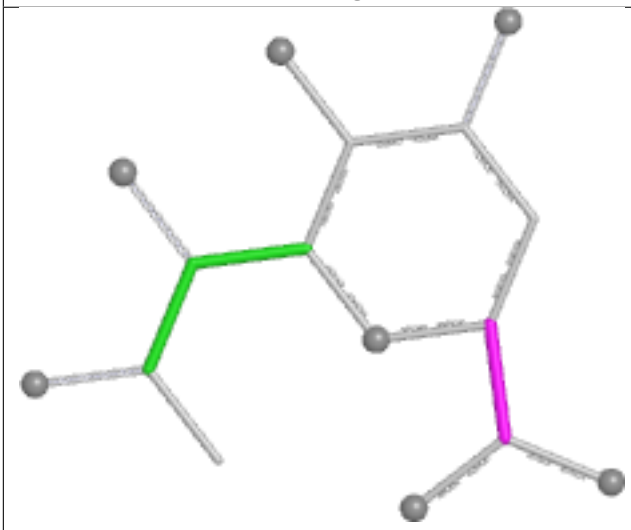

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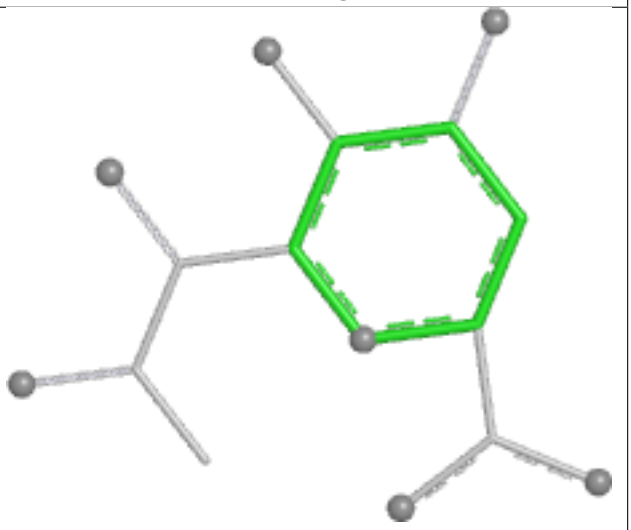

Rings

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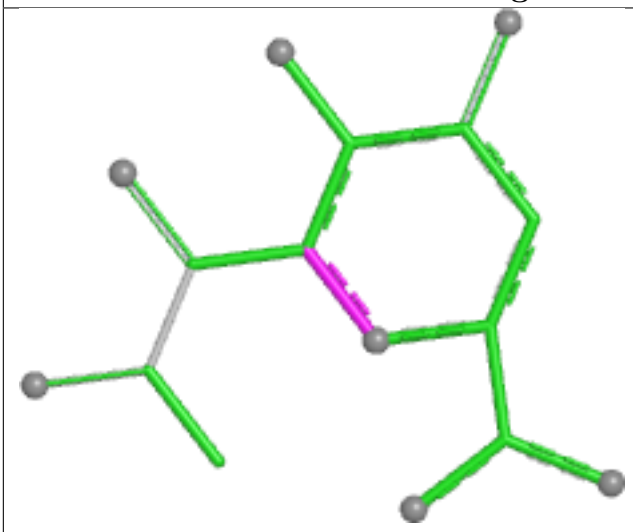

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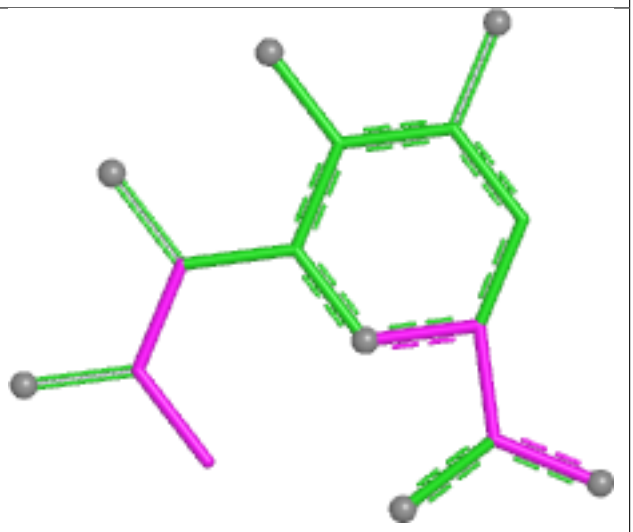

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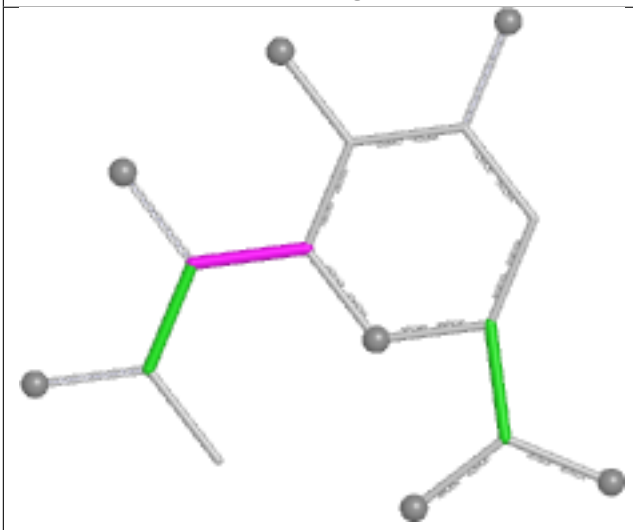

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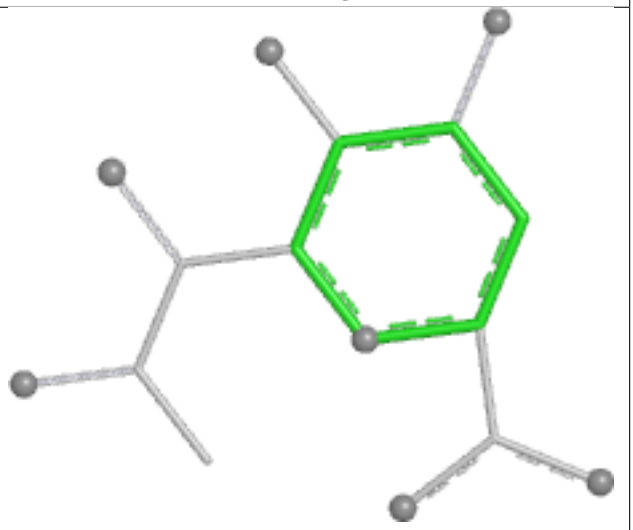

Rings

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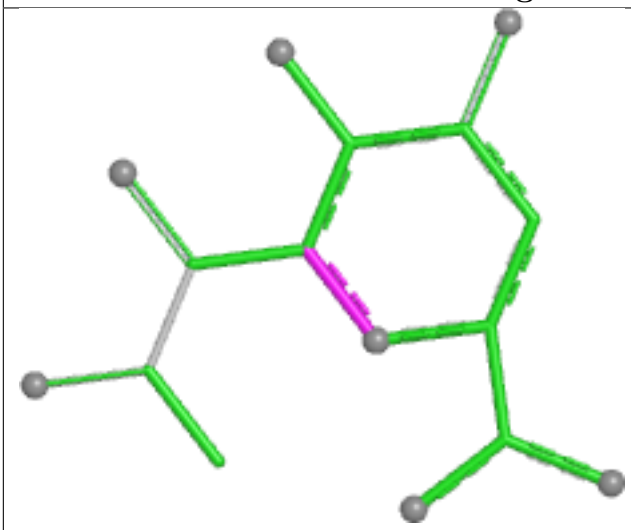

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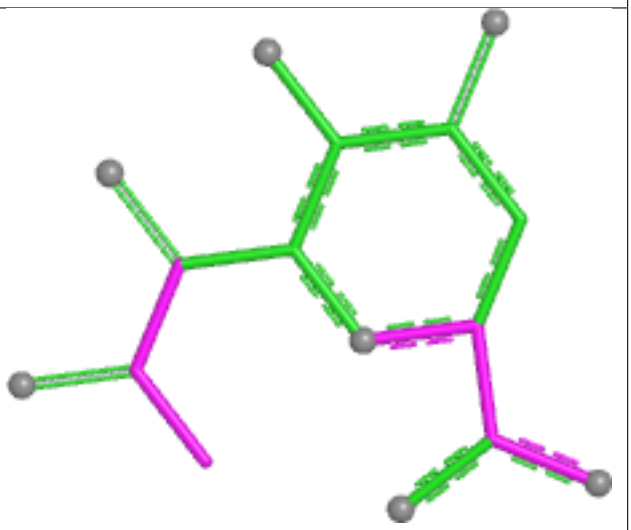

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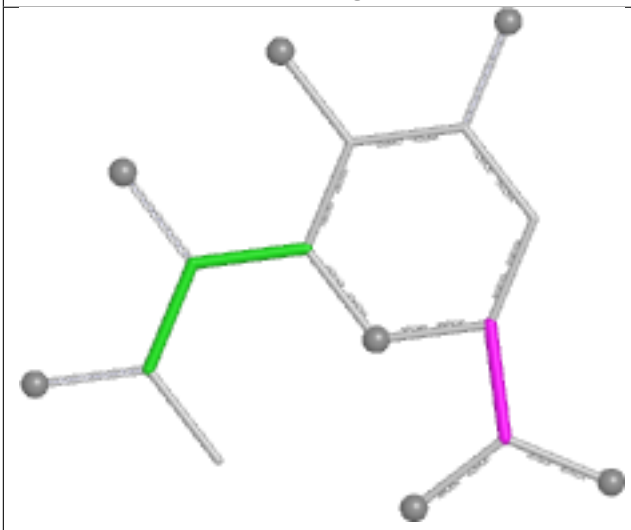

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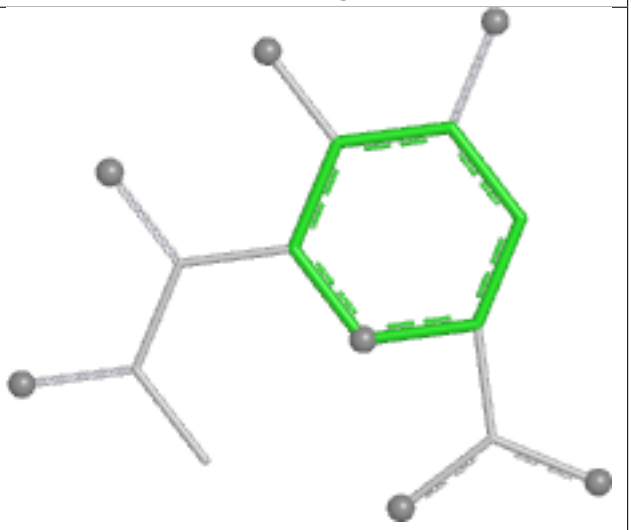

Rings

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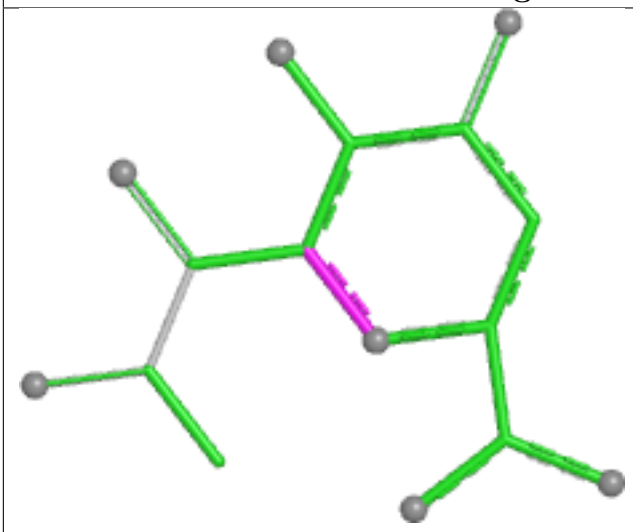

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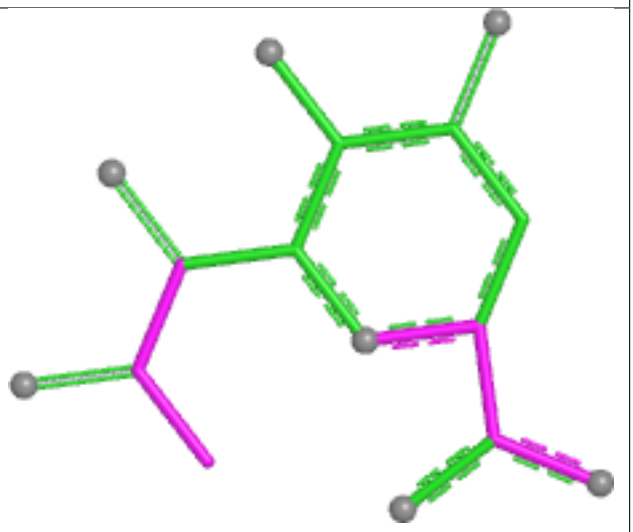

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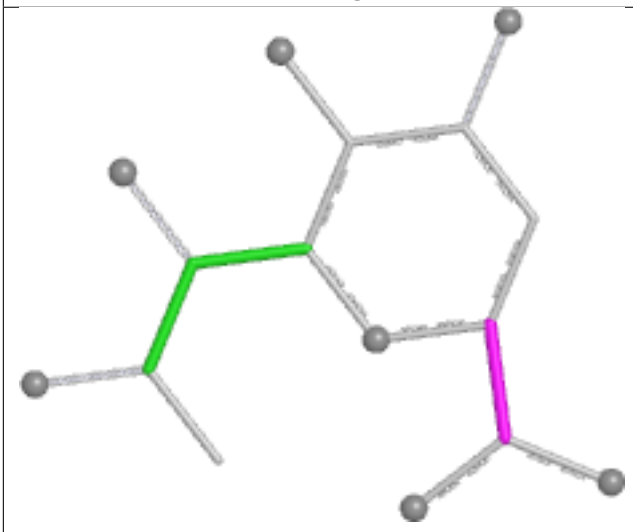

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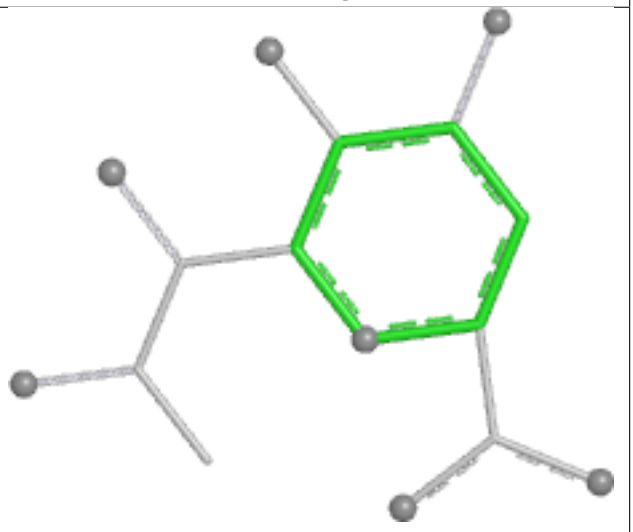
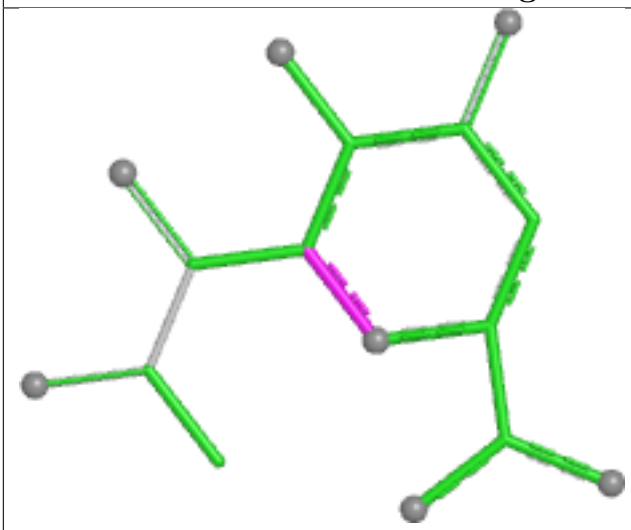


Rings

Ligand P8E Y1 602



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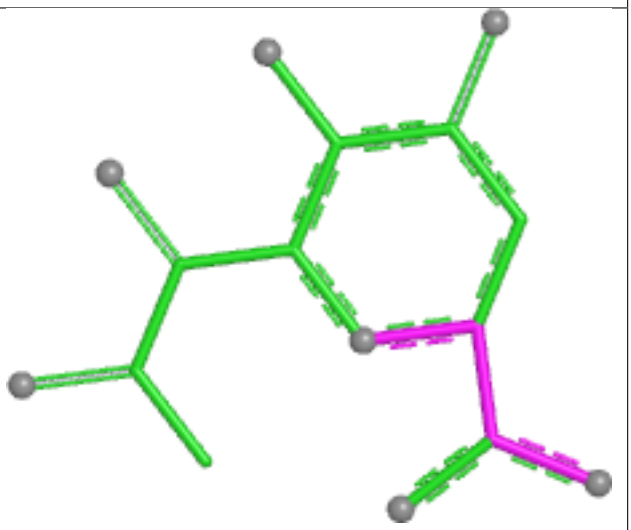

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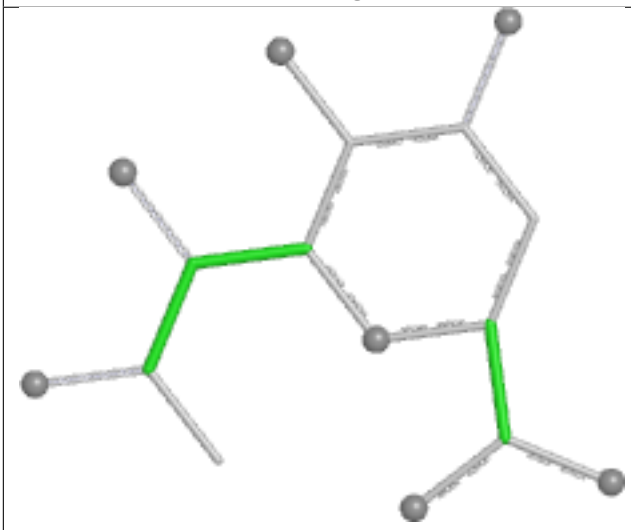

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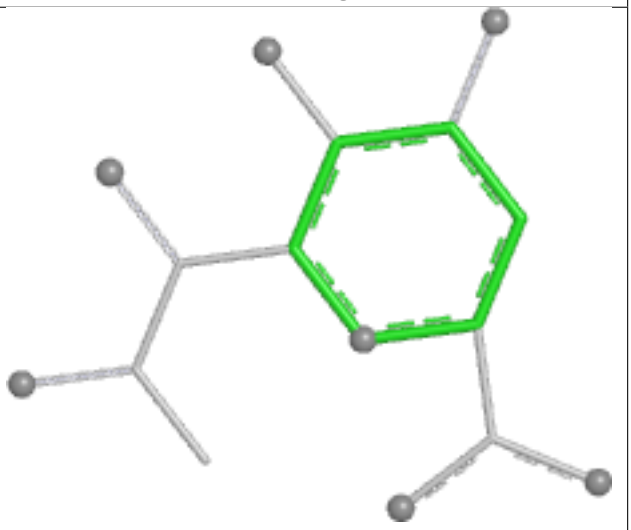
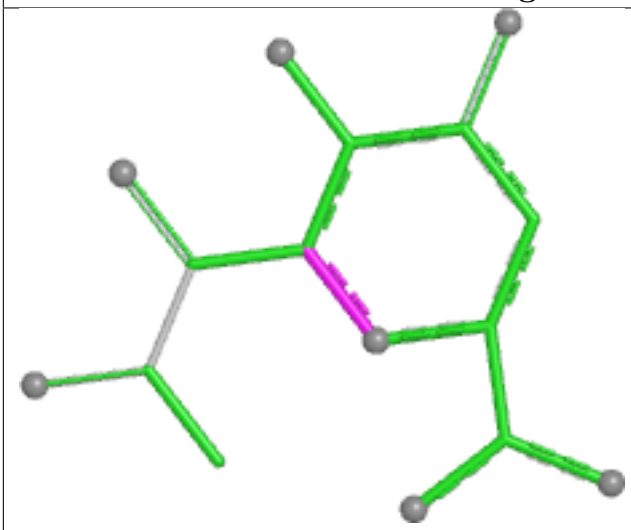


Rings

Ligand P8E dC 602



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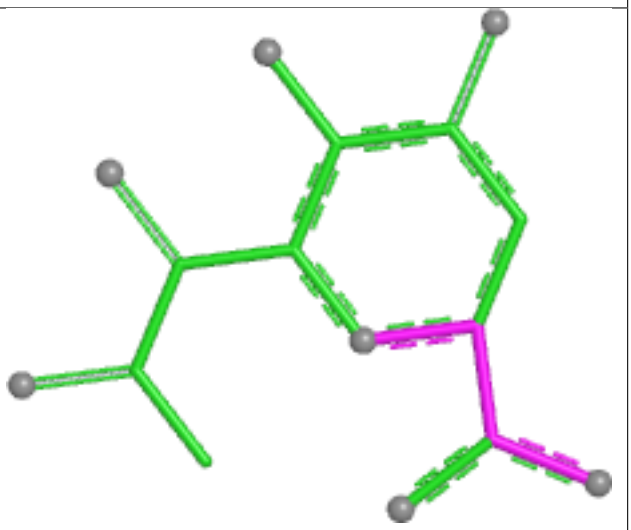

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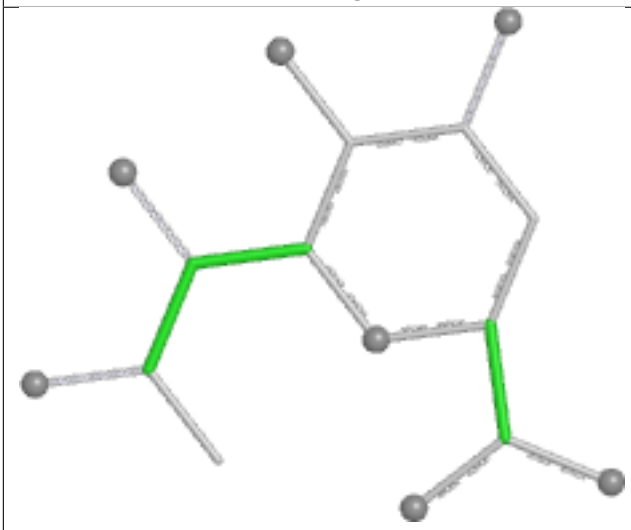

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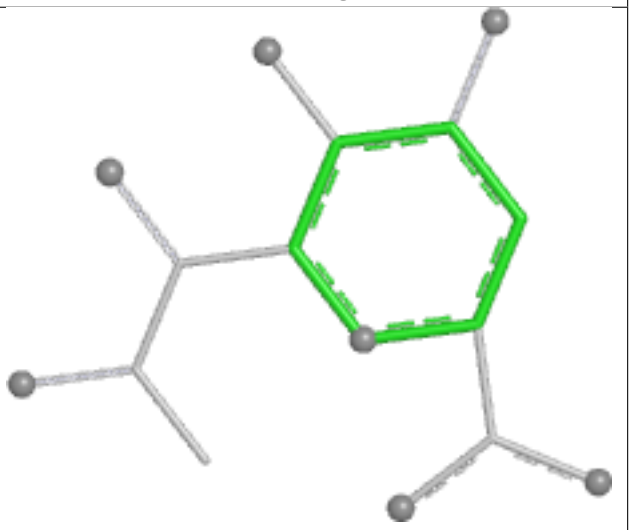
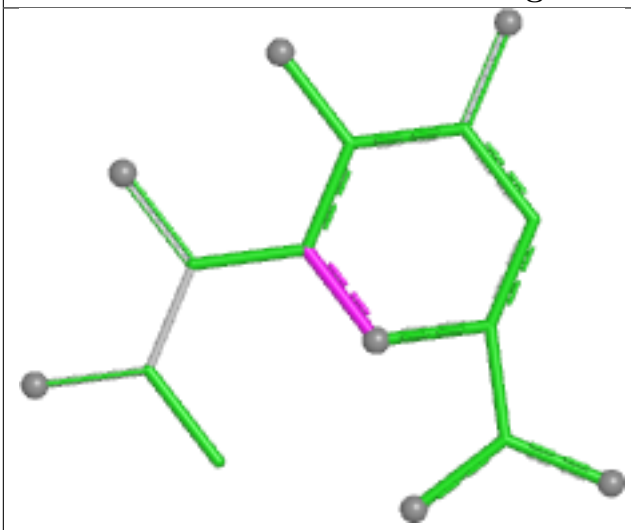


Rings

Ligand P8E I3 607



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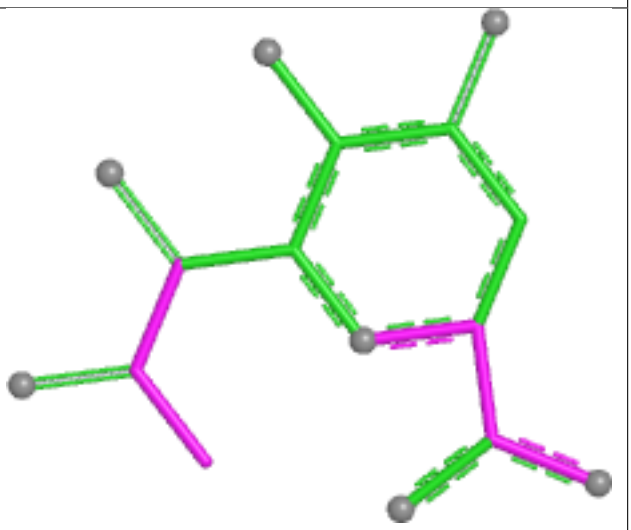

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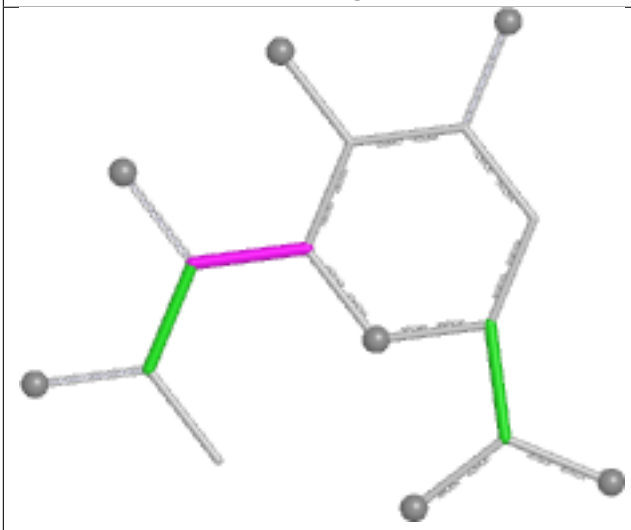

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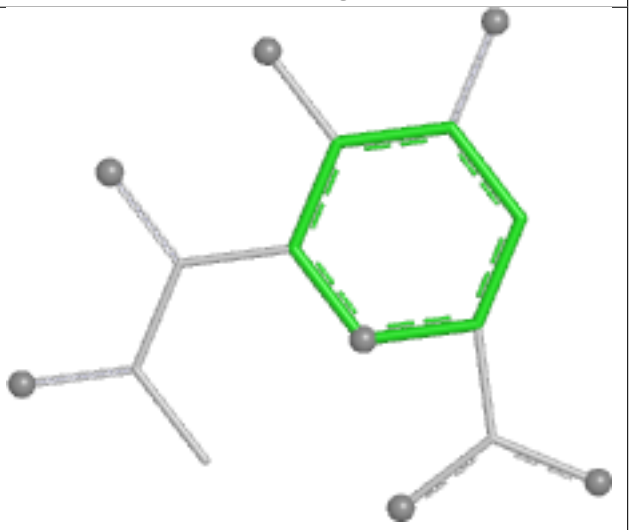
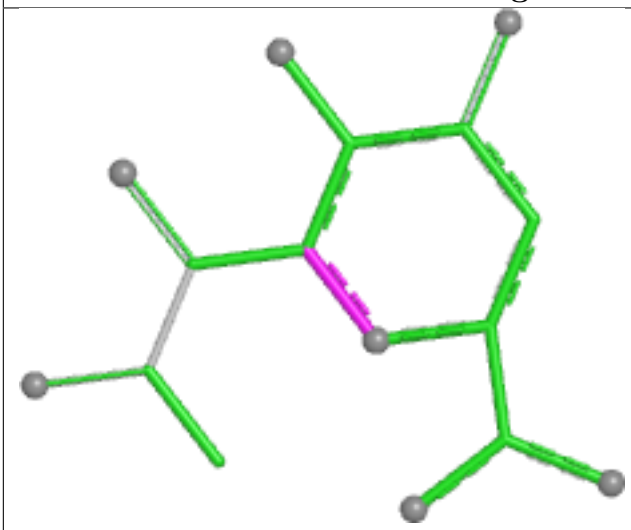


Rings

Ligand P8E MO 602



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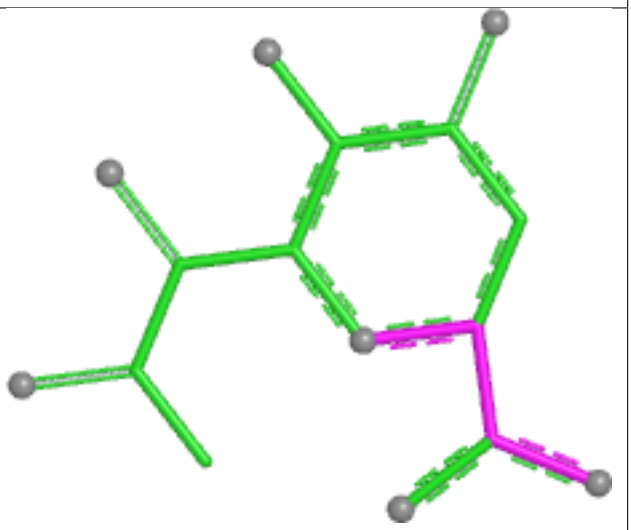

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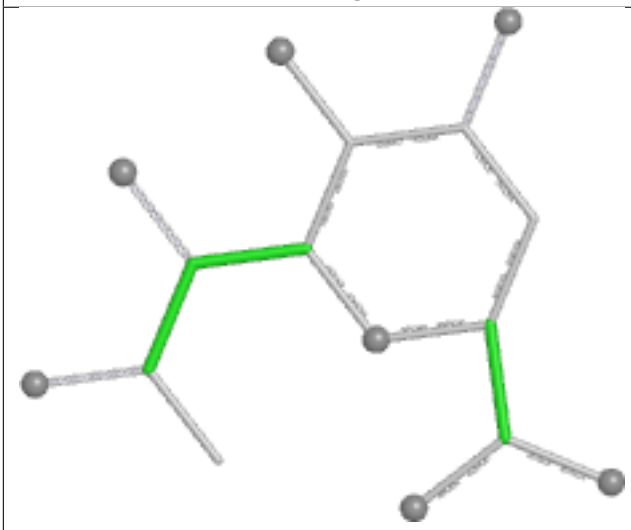

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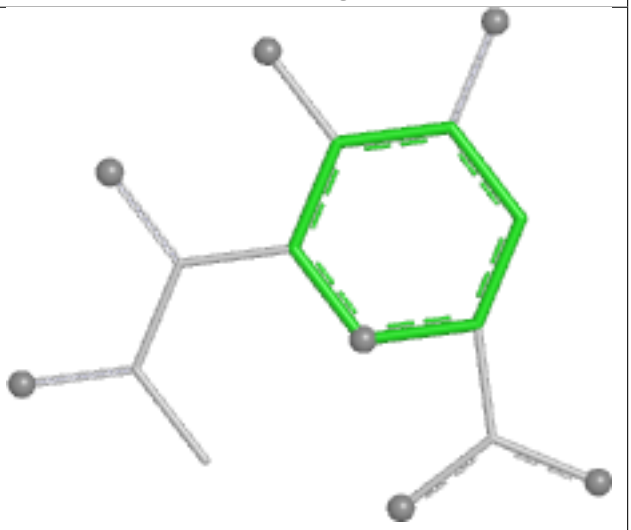
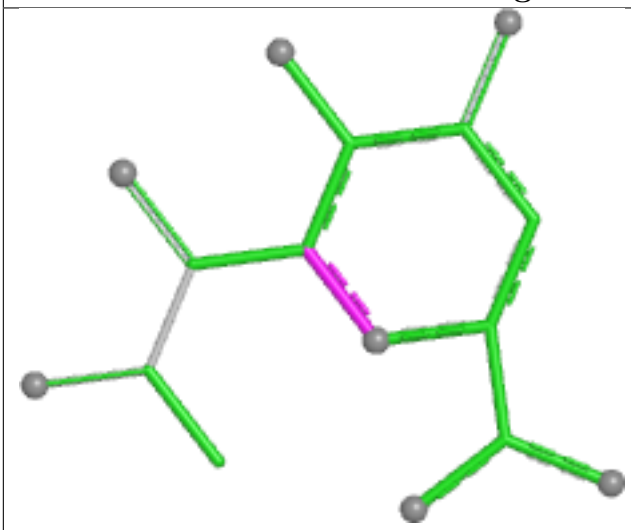


Rings

Ligand P8E GQ 604



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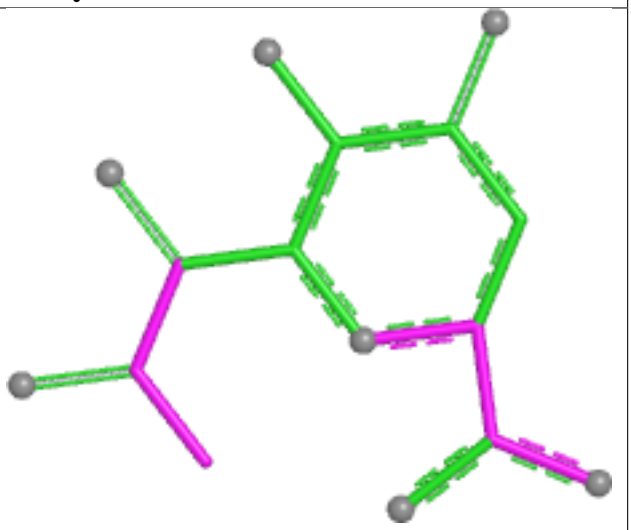
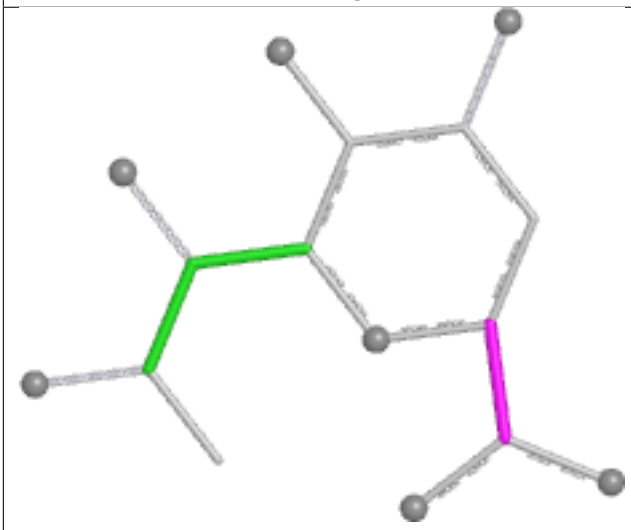


Bond angles



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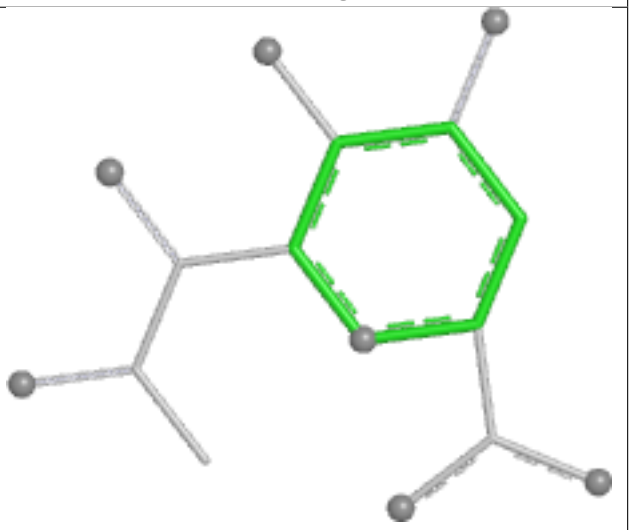
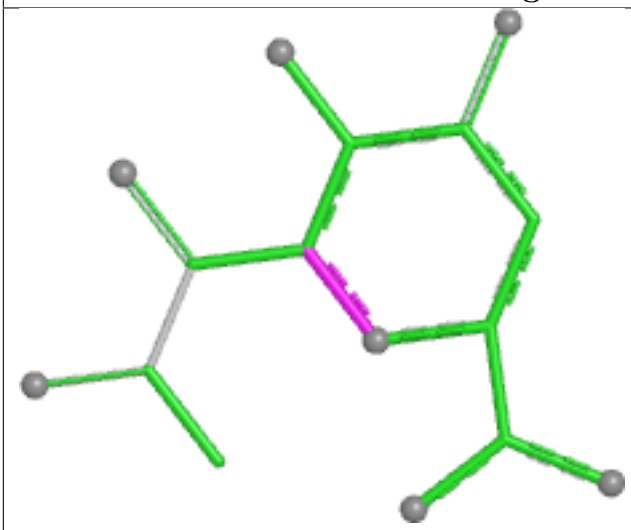


Rings

Ligand P8E S5 602



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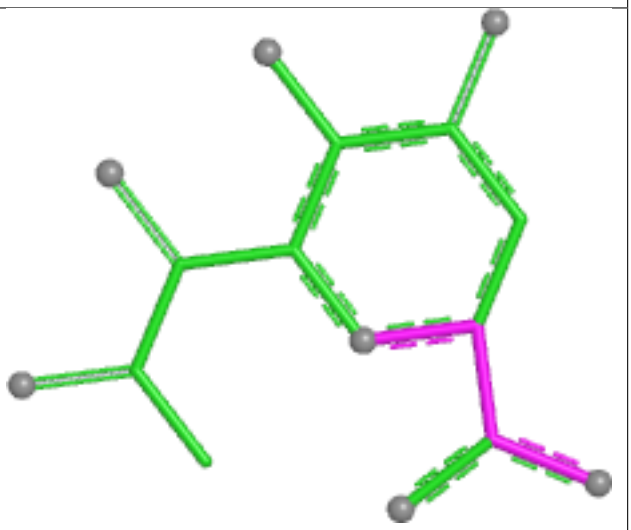
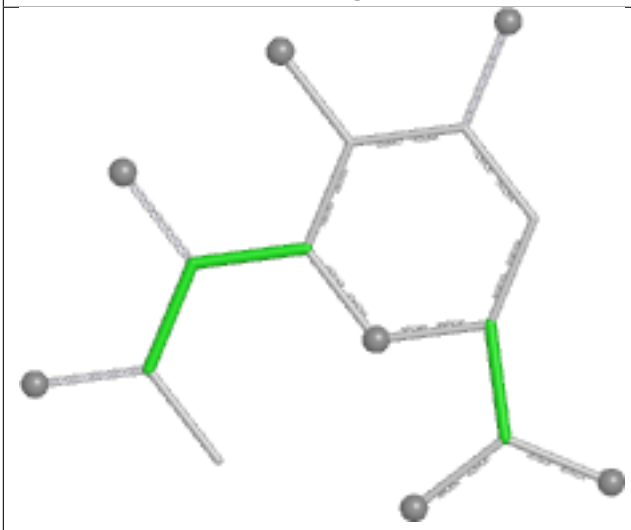
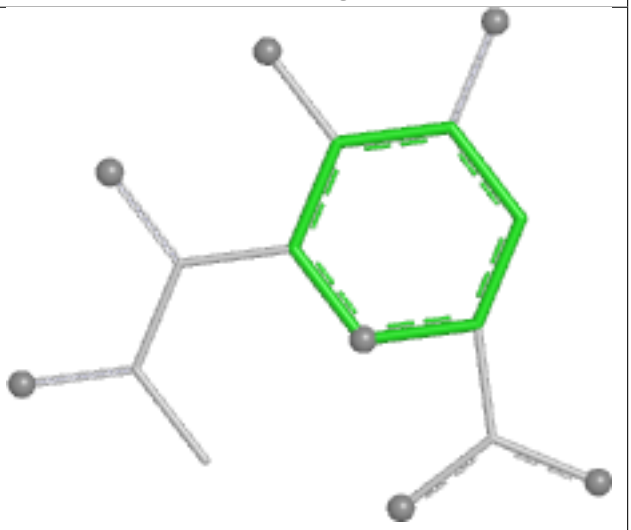


Bond angles

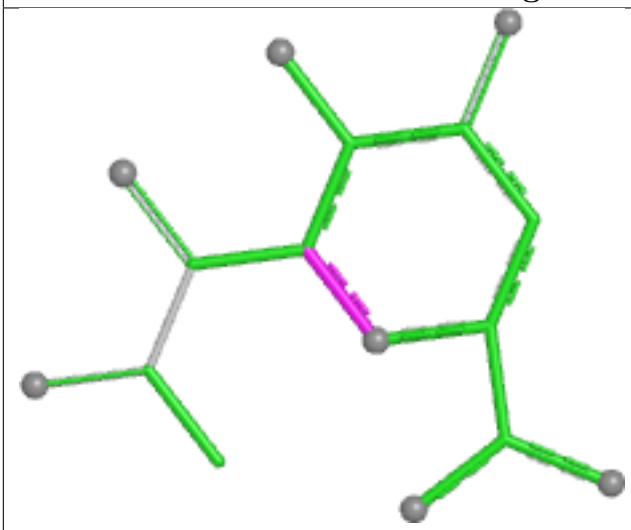


Torsions



Rings

Ligand P8E S5 607



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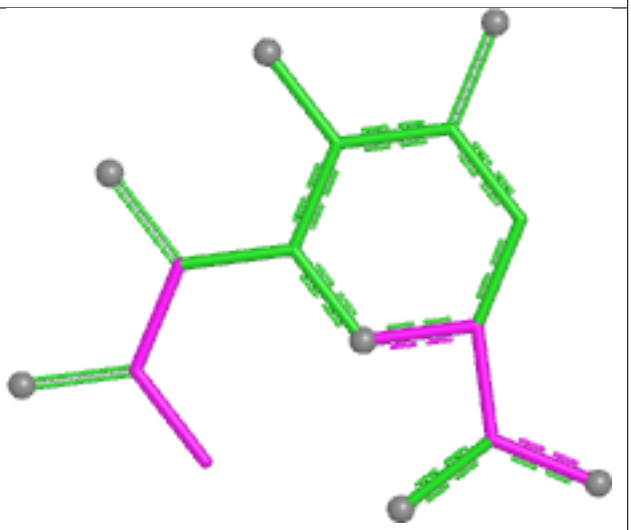

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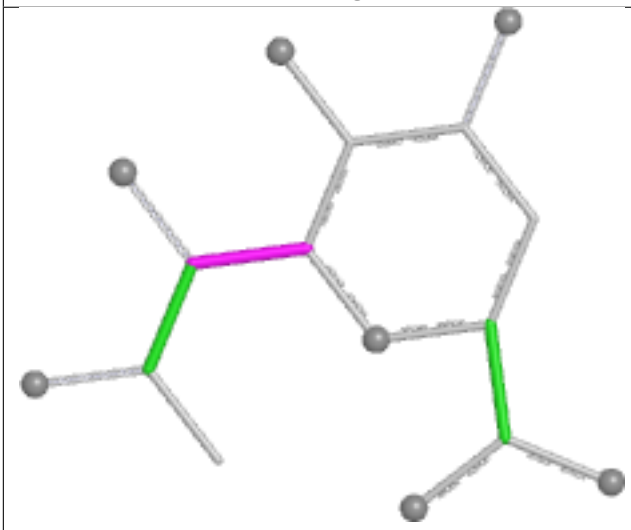

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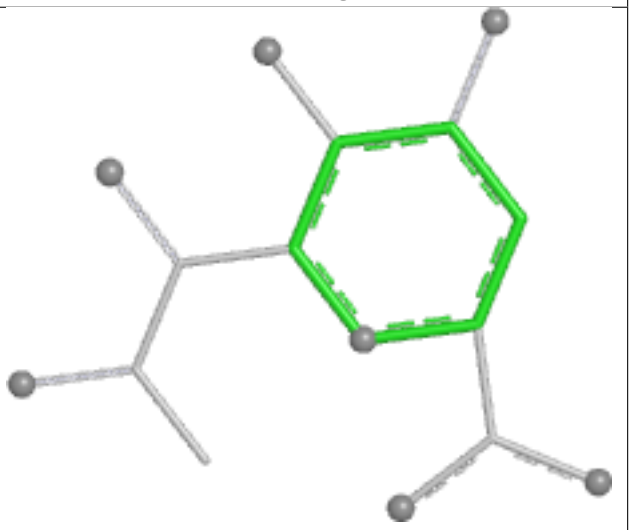
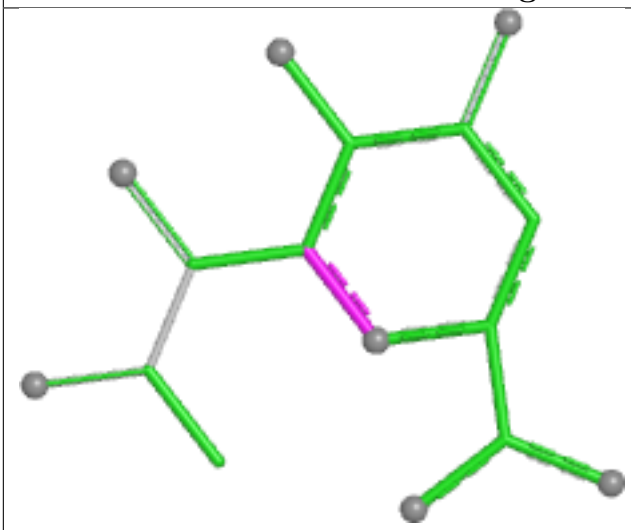


Rings

Ligand P8E A7 602



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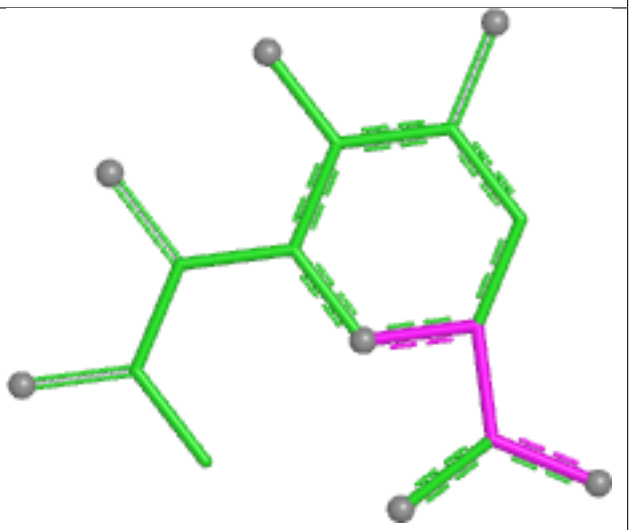

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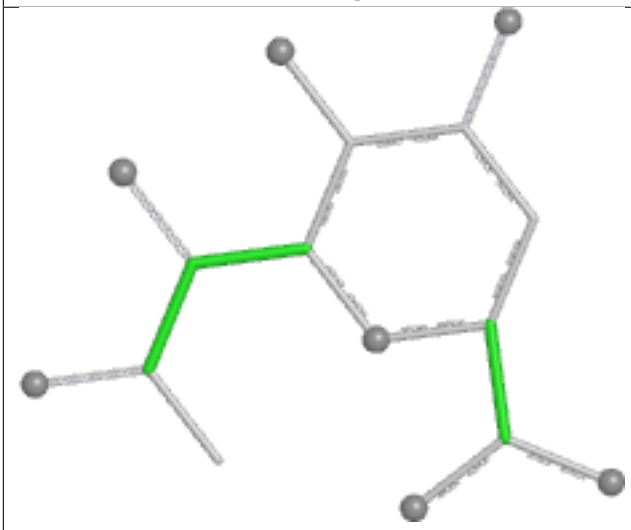

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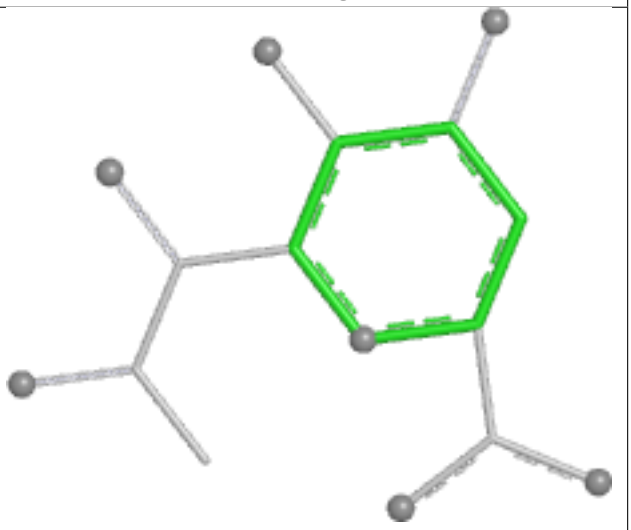
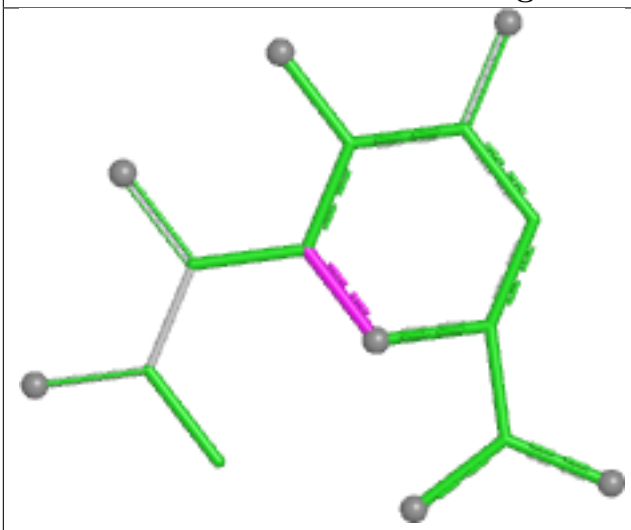


Rings

Ligand P8E TP 606



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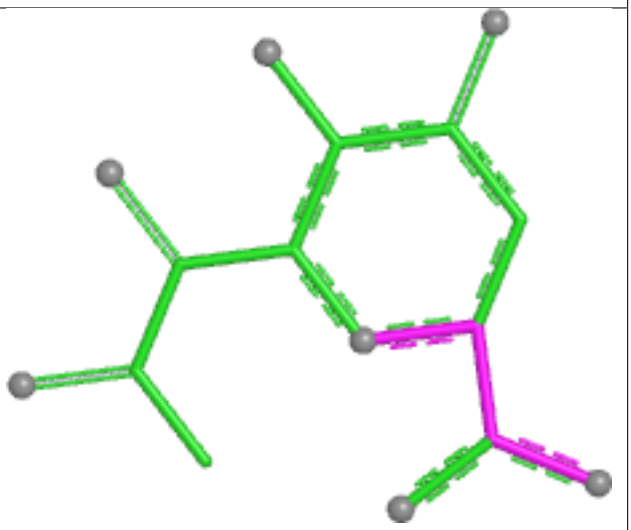

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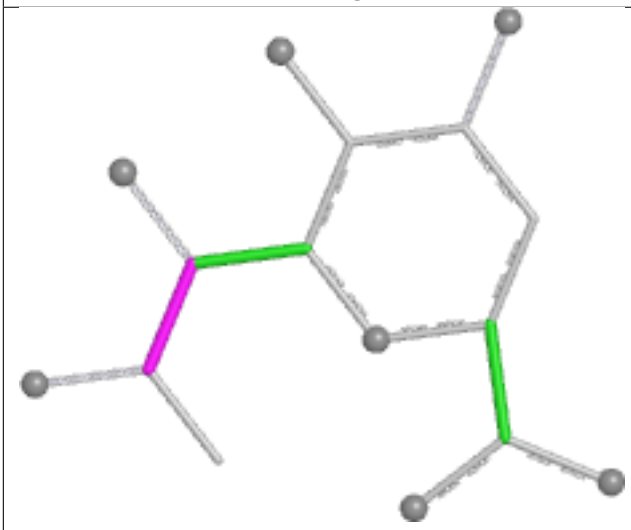

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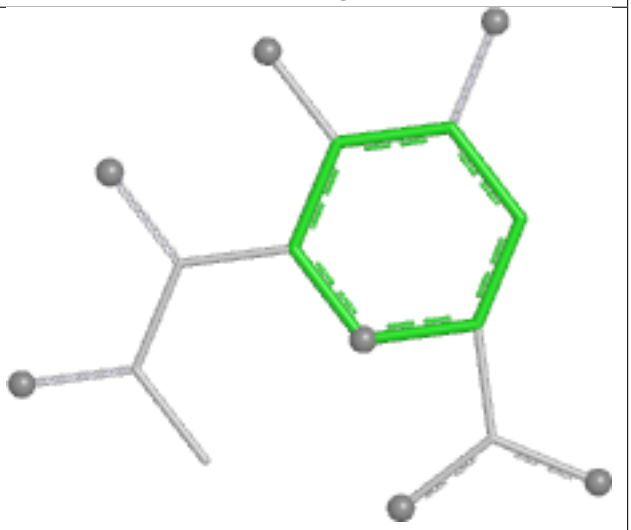
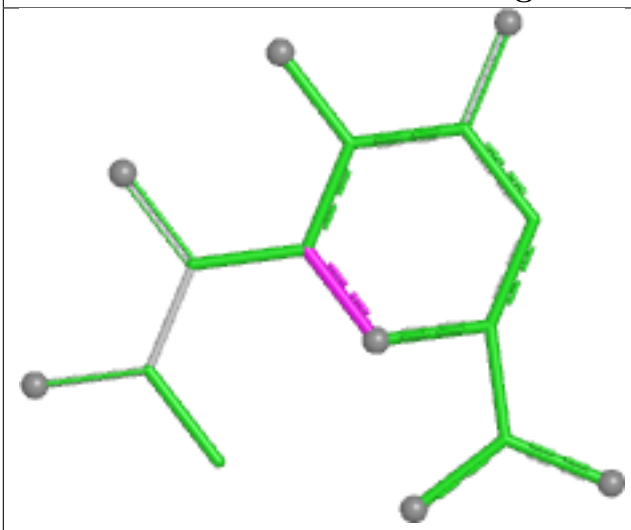


Rings

Ligand P8E PU 603



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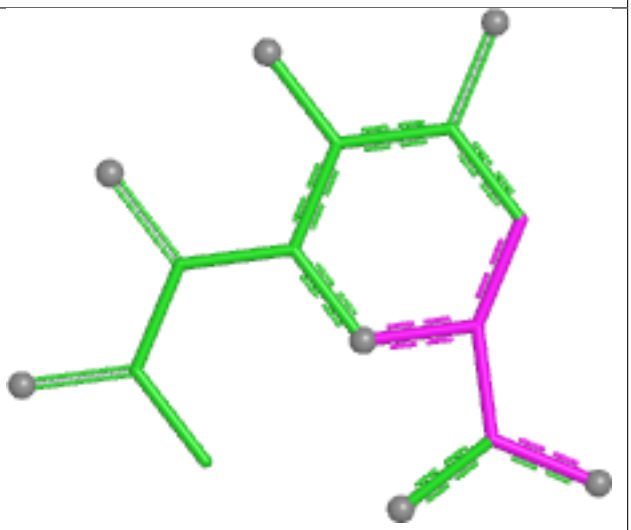

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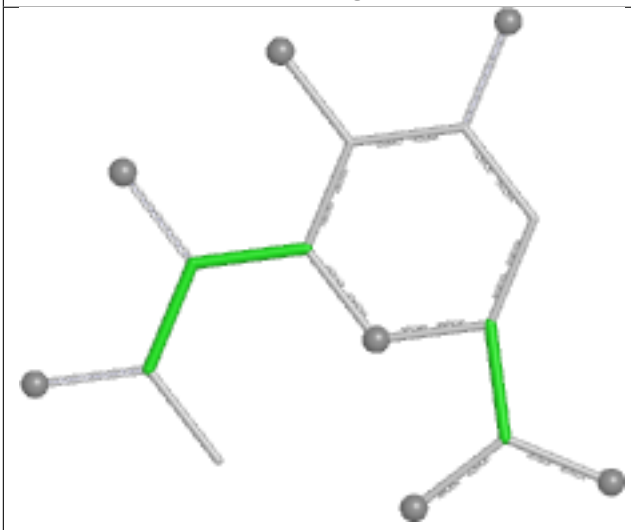

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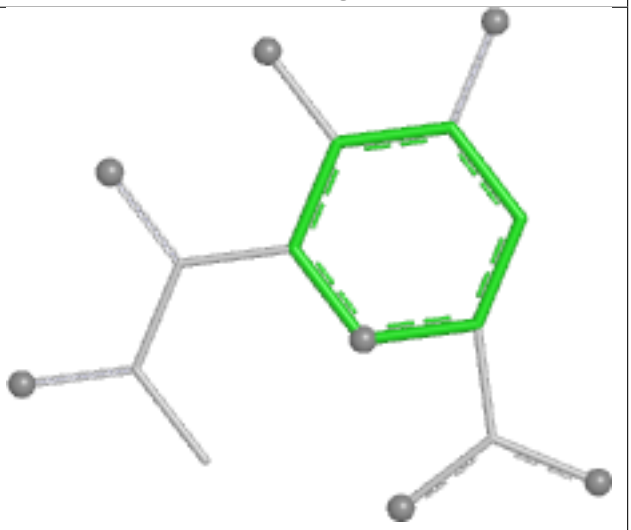
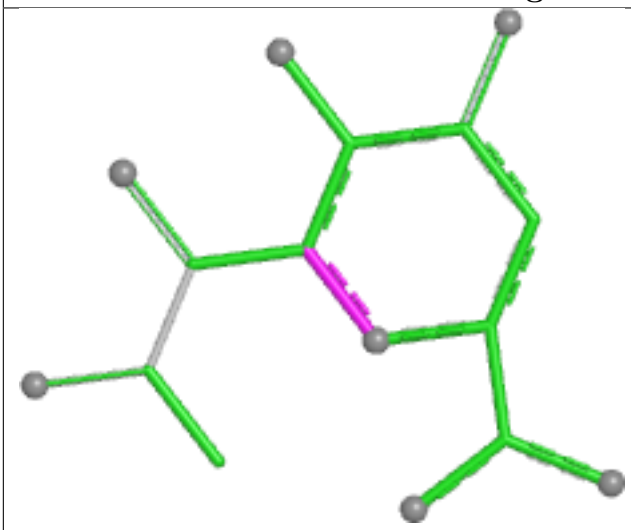


Rings

Ligand P8E I3 606



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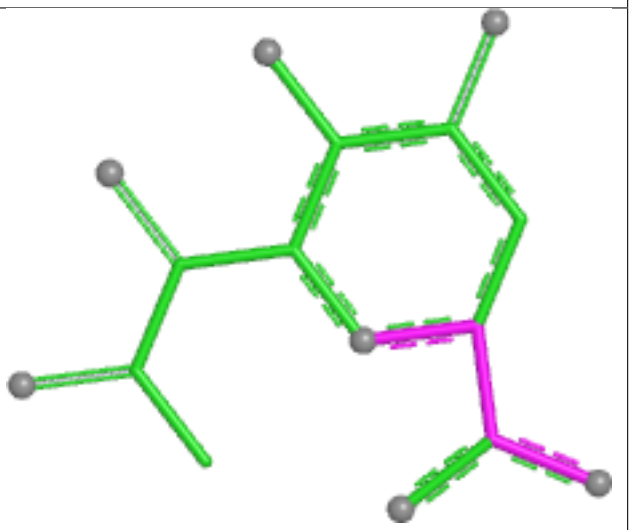

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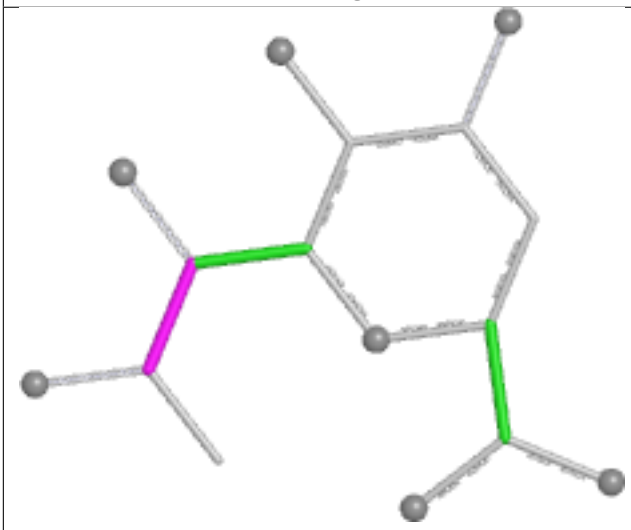

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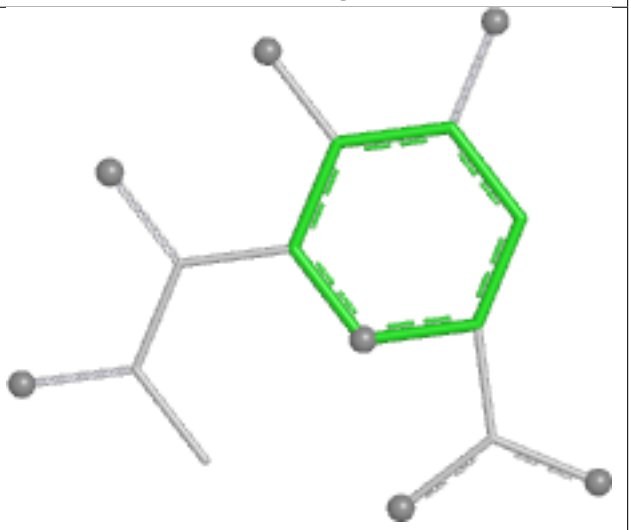
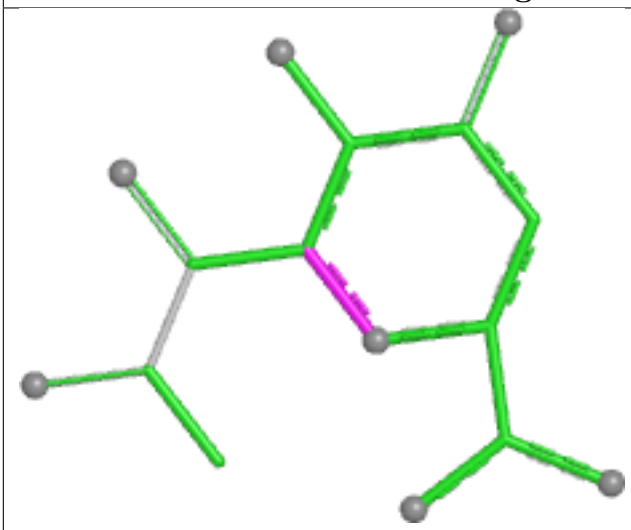


Rings

Ligand P8E VR 607



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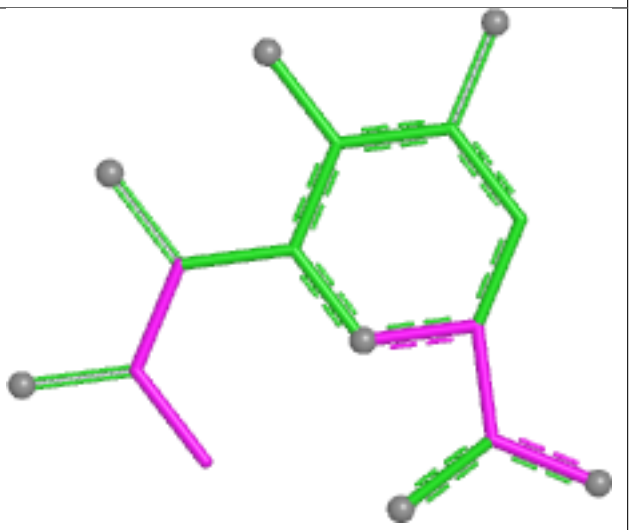

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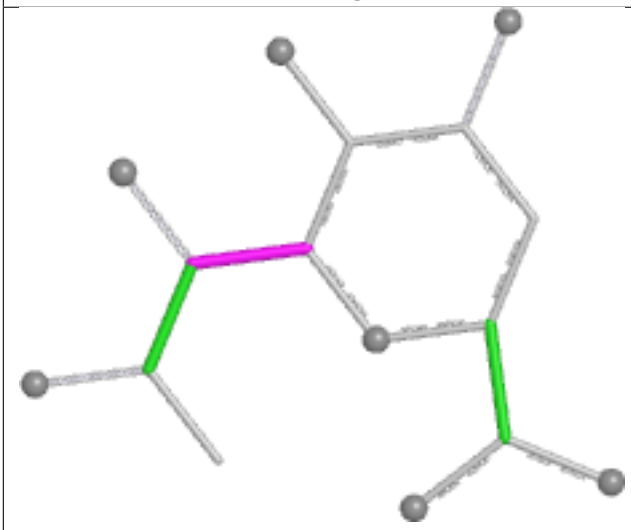

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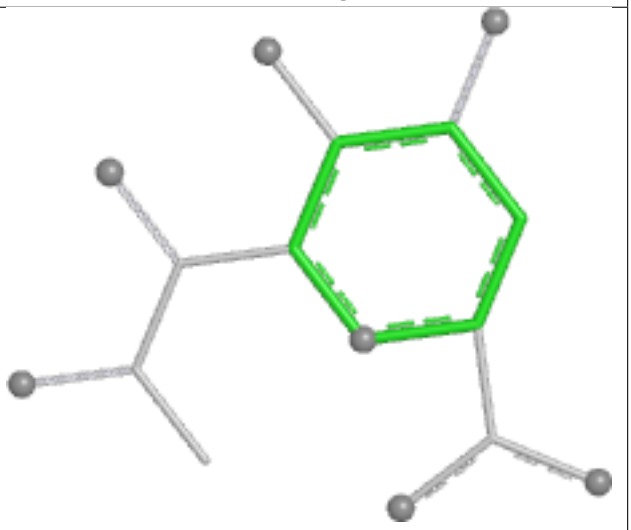
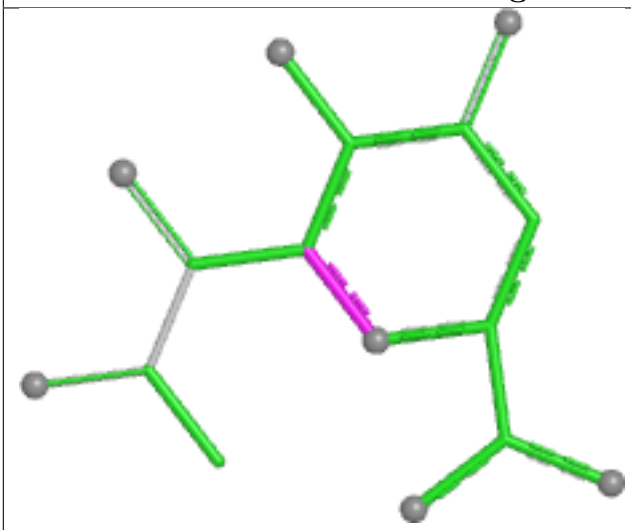


Rings

Ligand P8E WG 607



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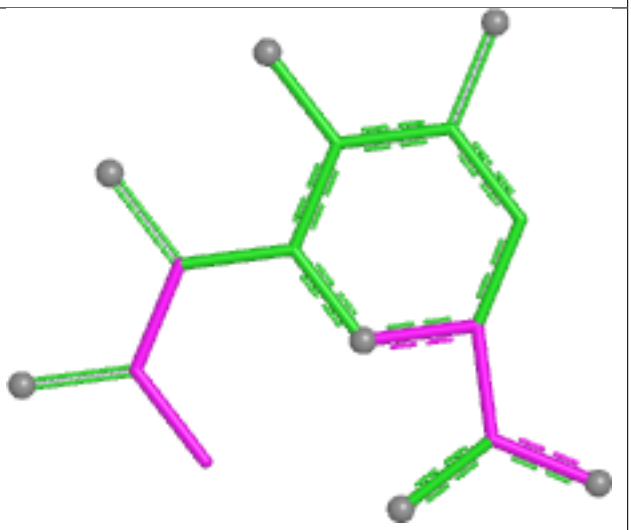

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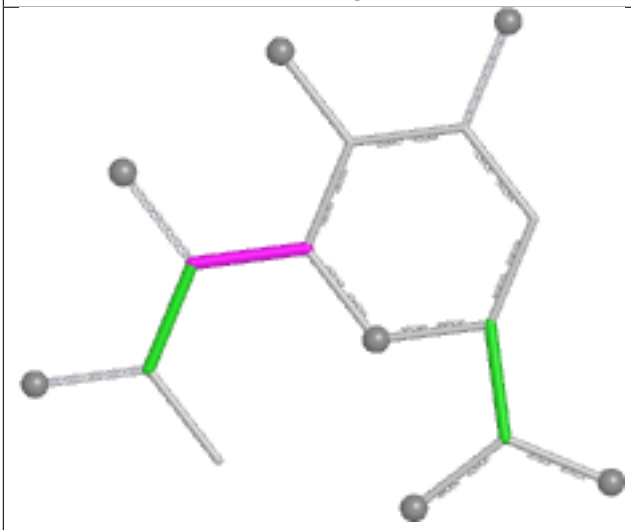

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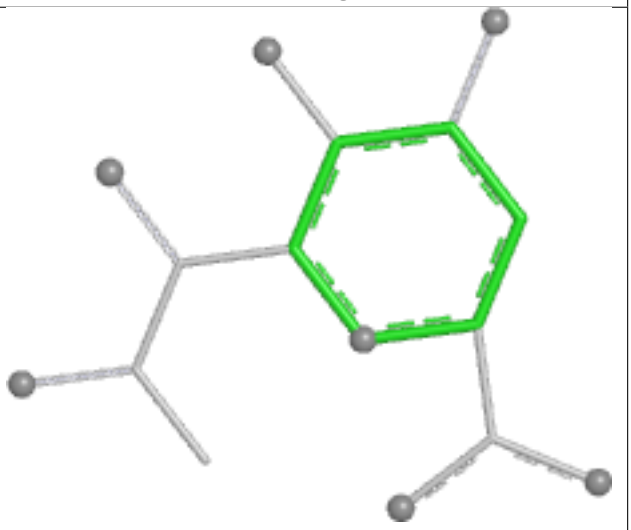
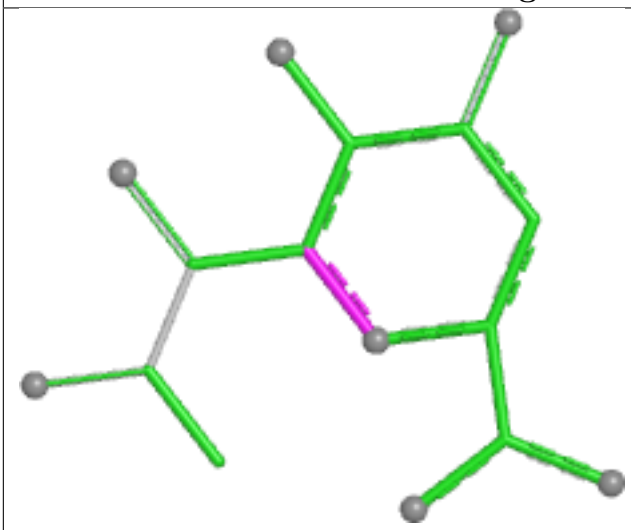


Rings

Ligand P8E Q2 603



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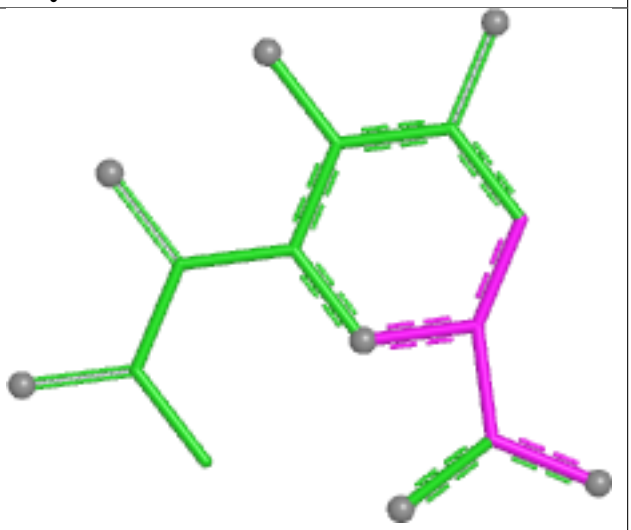
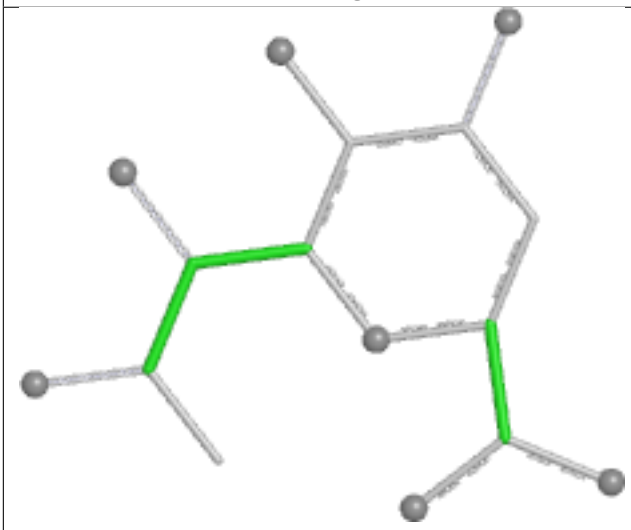


Bond angles



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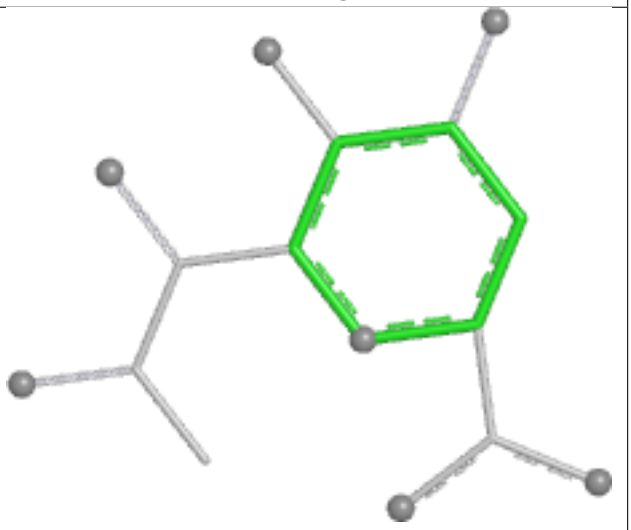
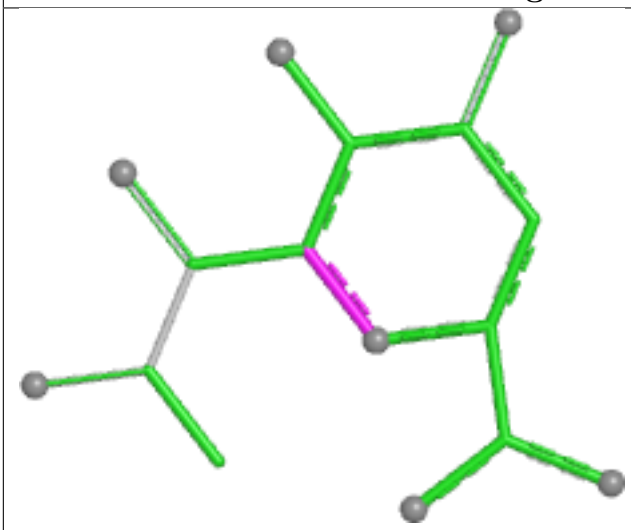


Rings

Ligand P8E I3 605



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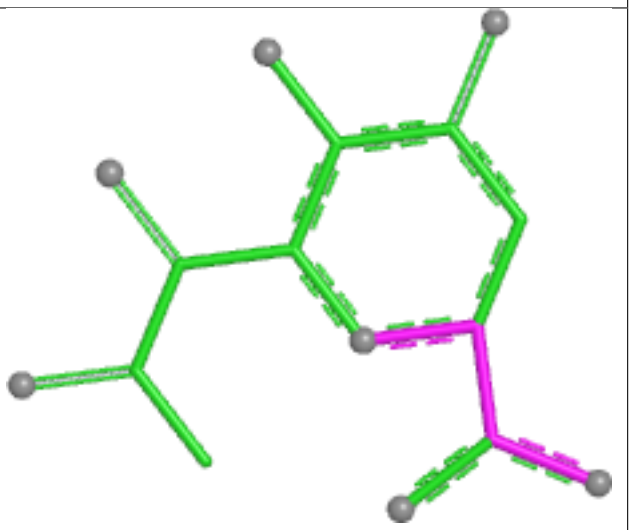

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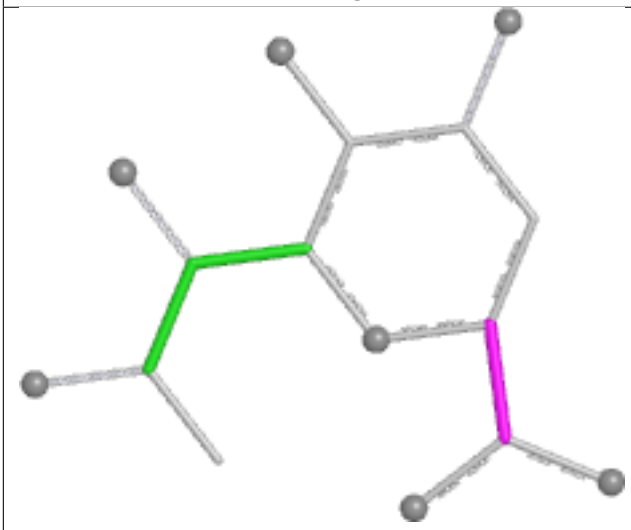

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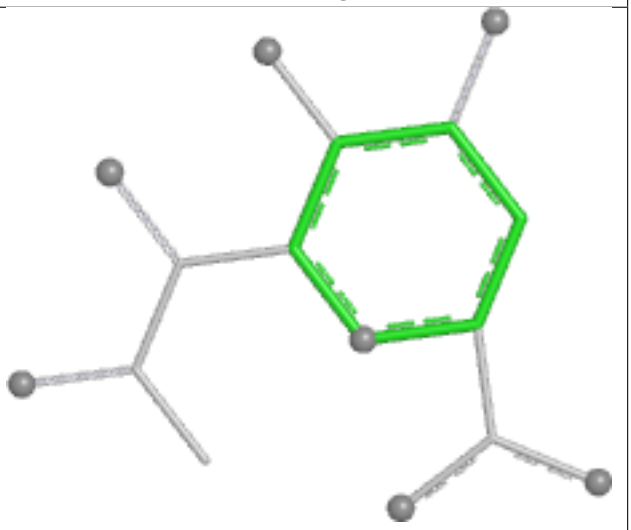
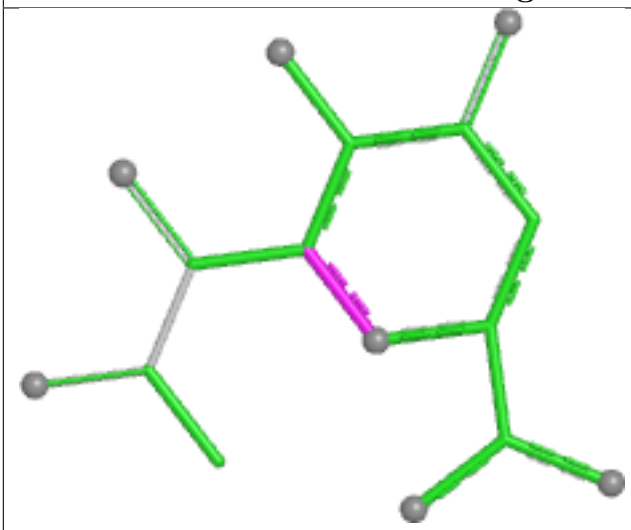


Rings

Ligand P8E TP 602



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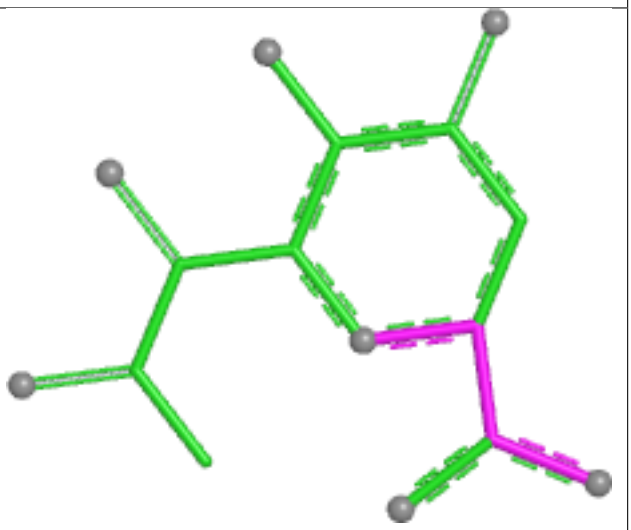

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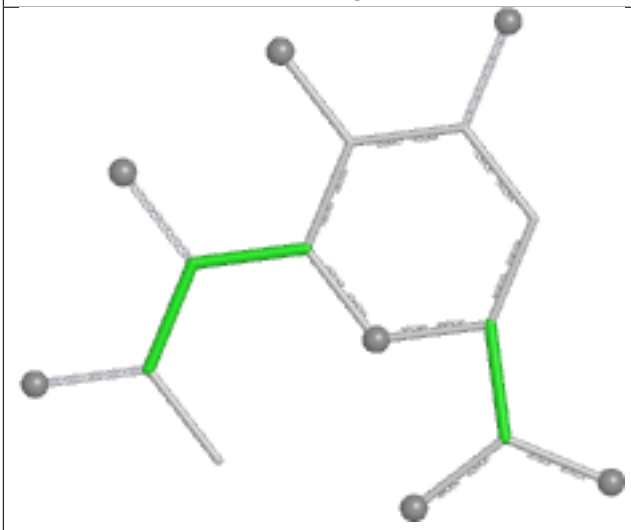

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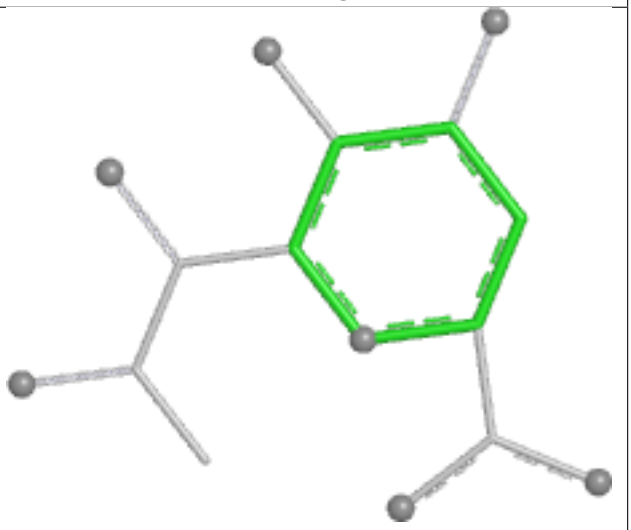
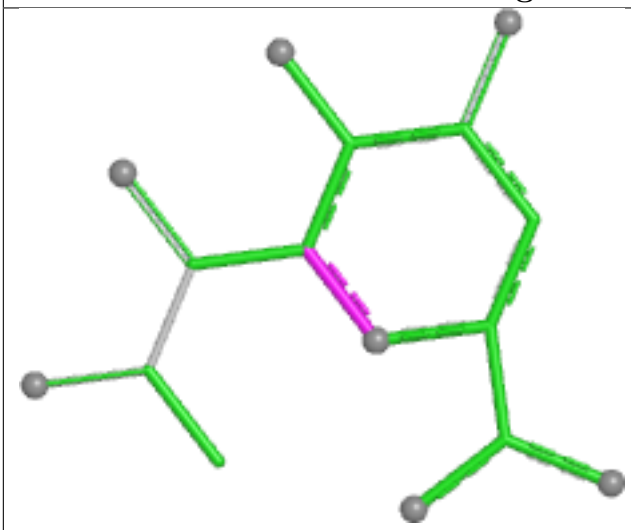


Rings

Ligand P8E CT 603



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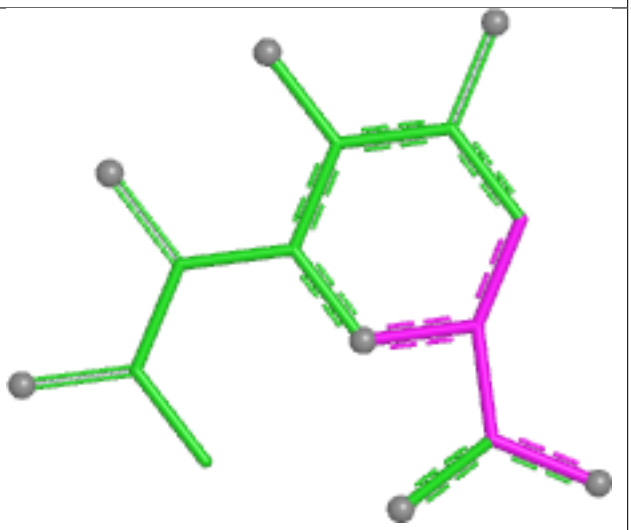

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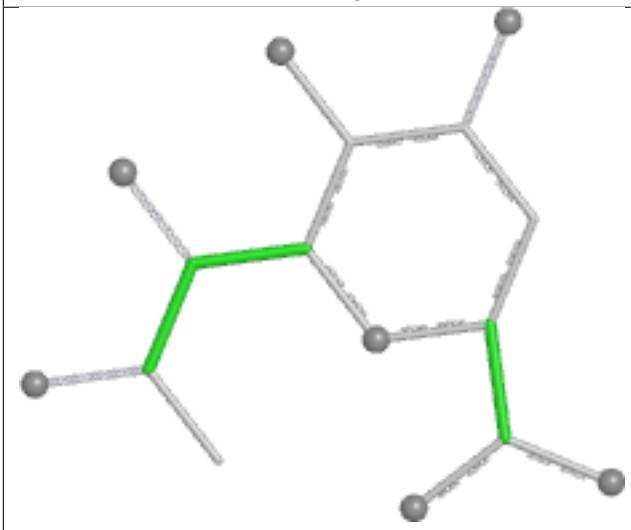

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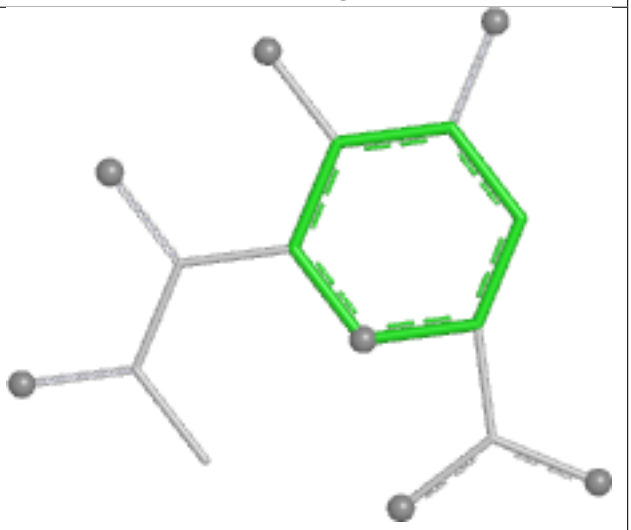
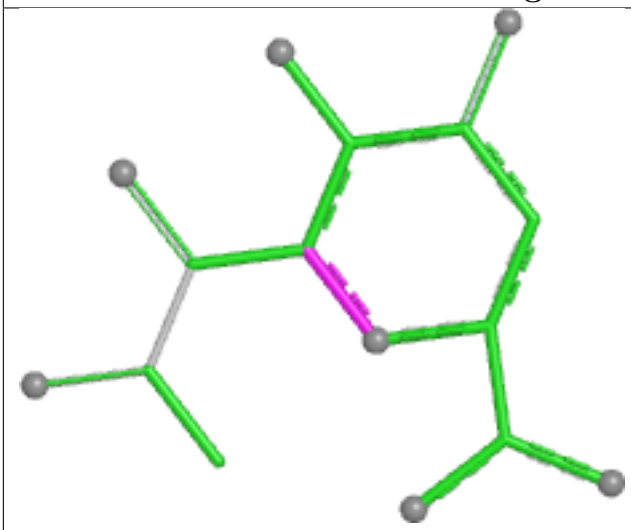


Rings

Ligand P8E e8 601



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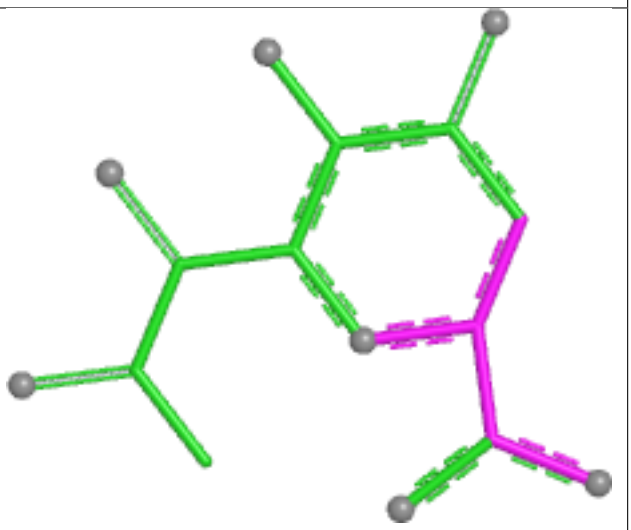
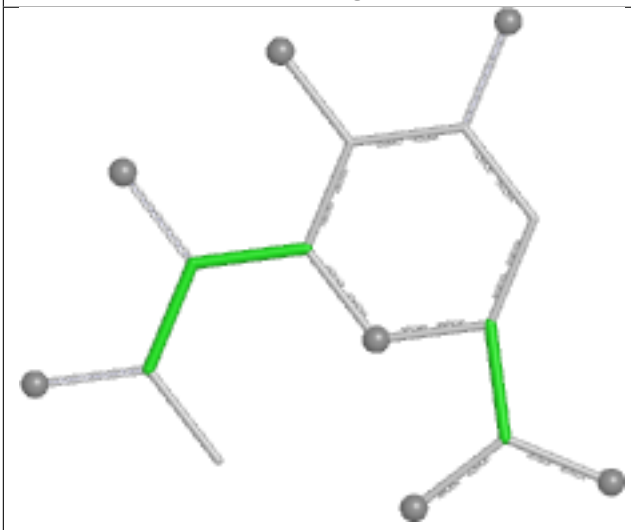


Bond angles



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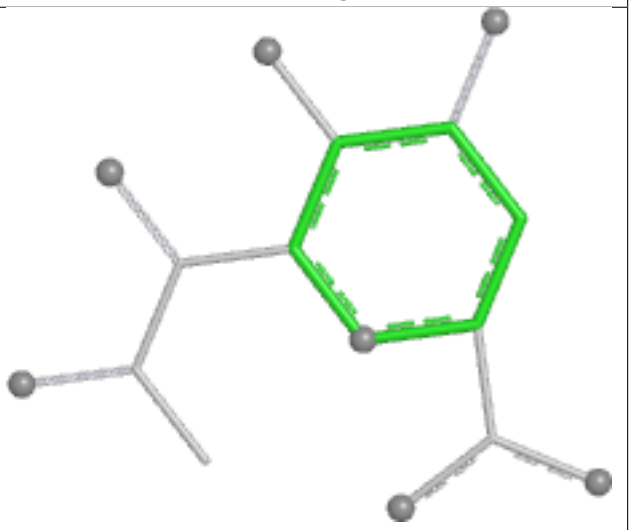
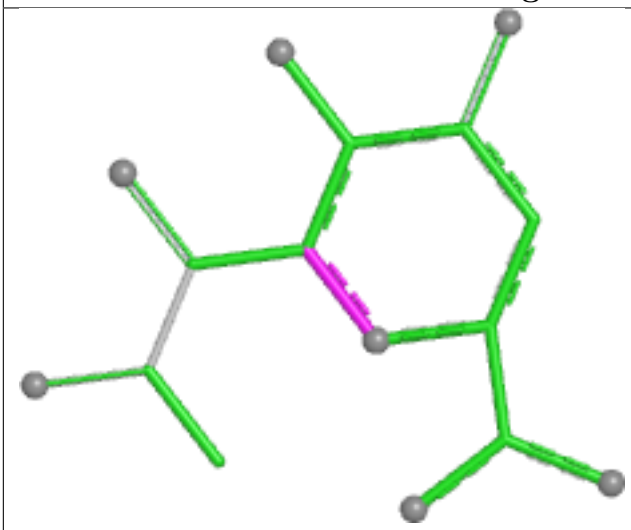


Rings

Ligand P8E fK 606



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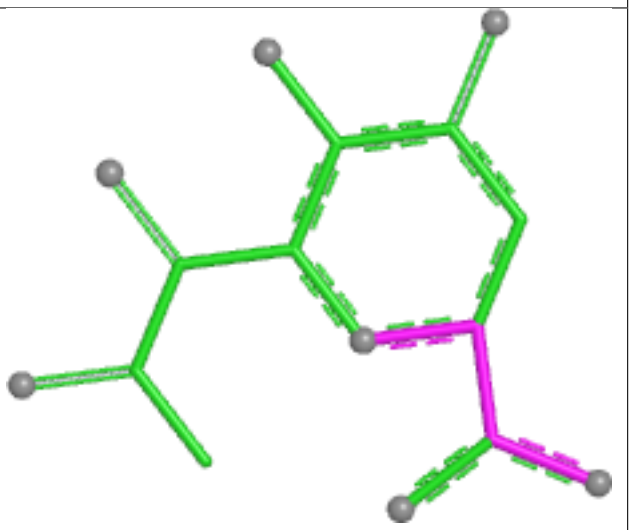
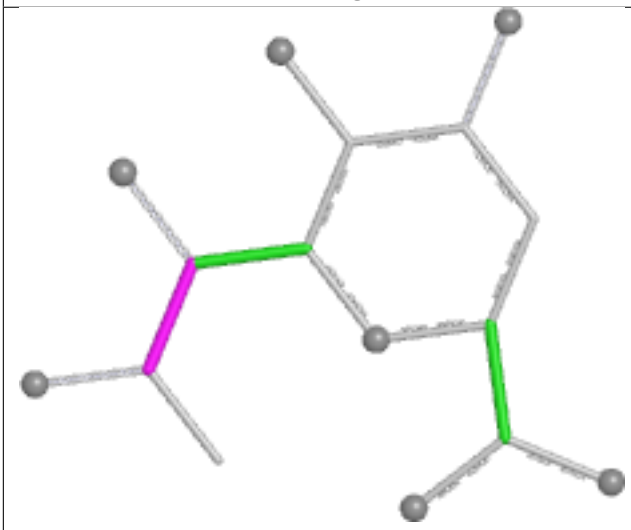
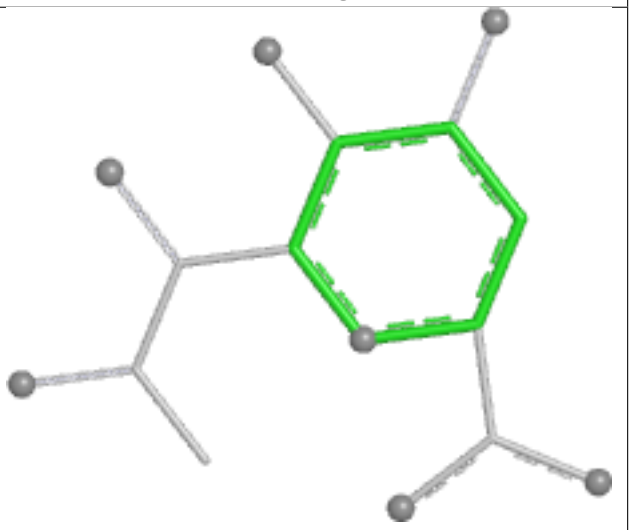


Bond angles

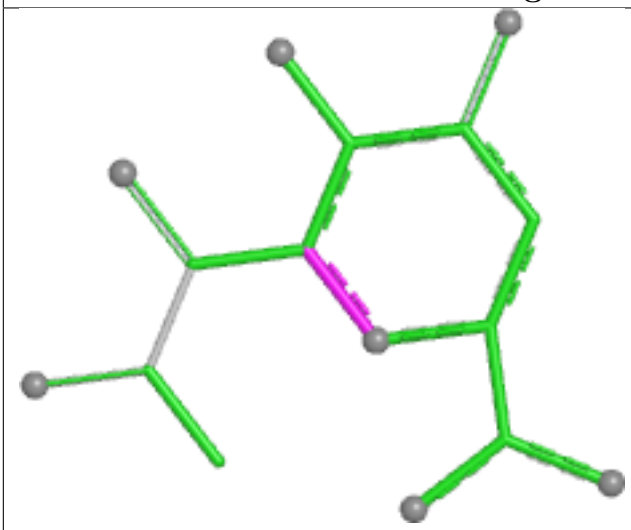


Torsions

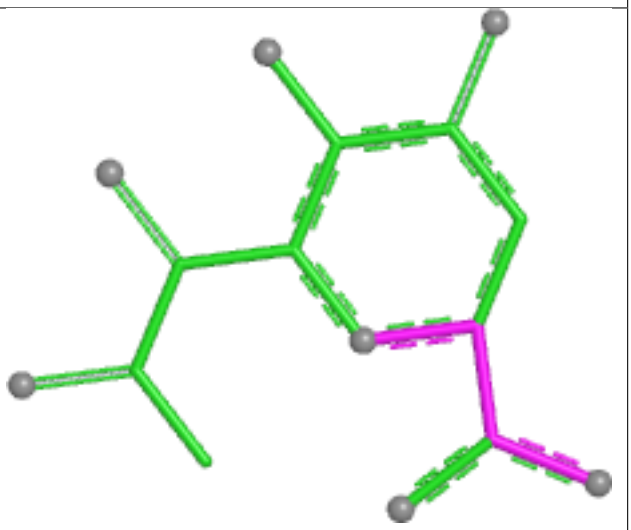


Rings

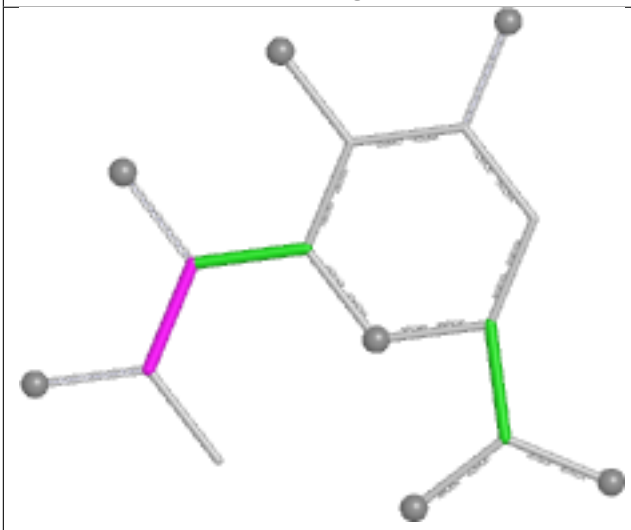
Ligand P8E e8 606



Bond lengths



Bond angles



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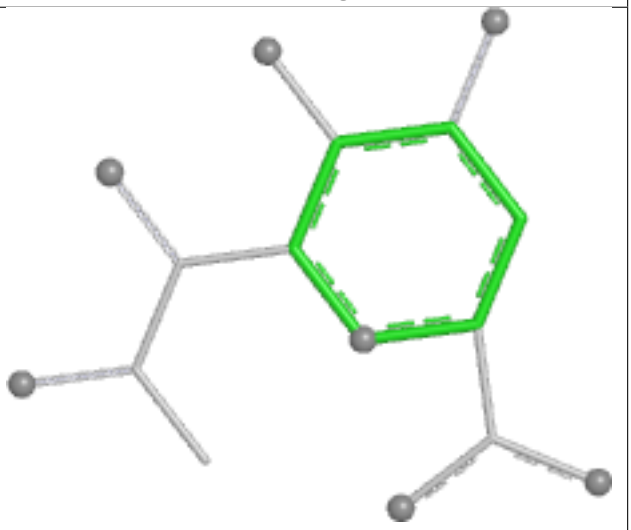
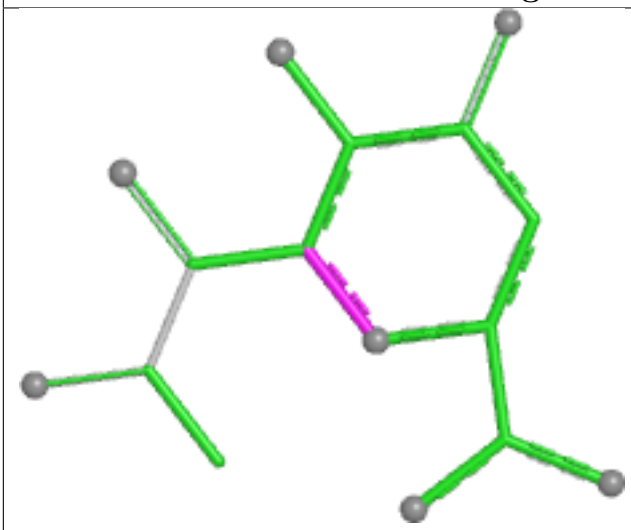


Rings

Ligand P8E fK 604



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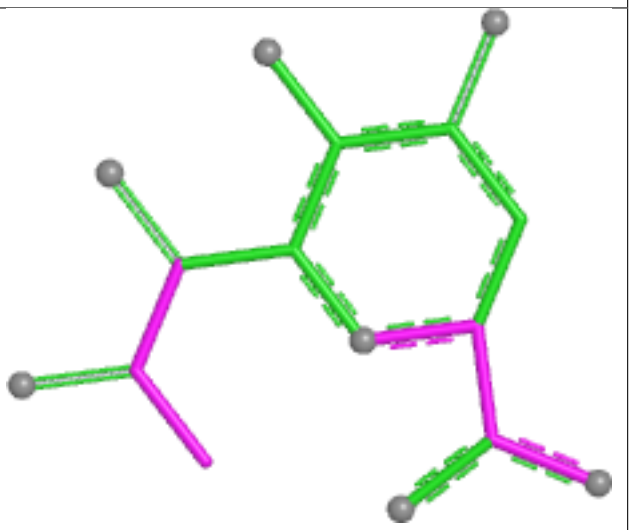

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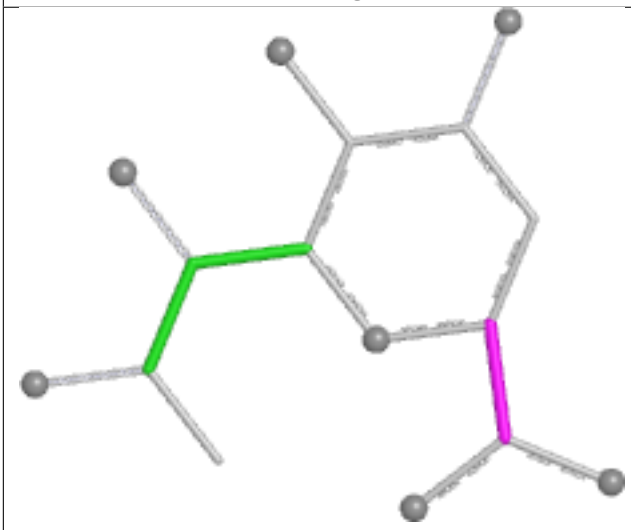

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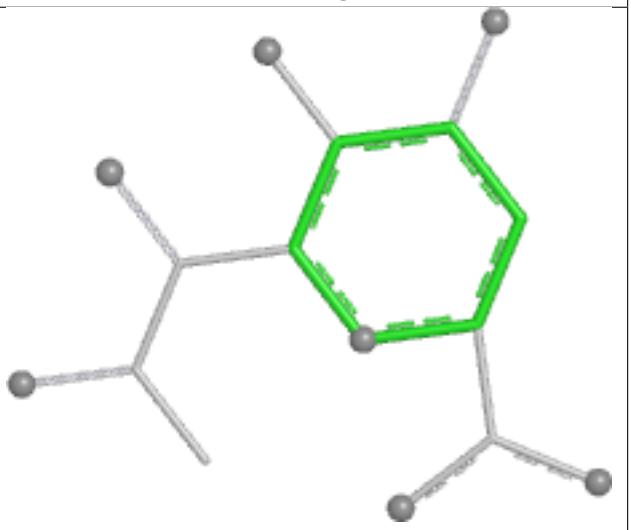
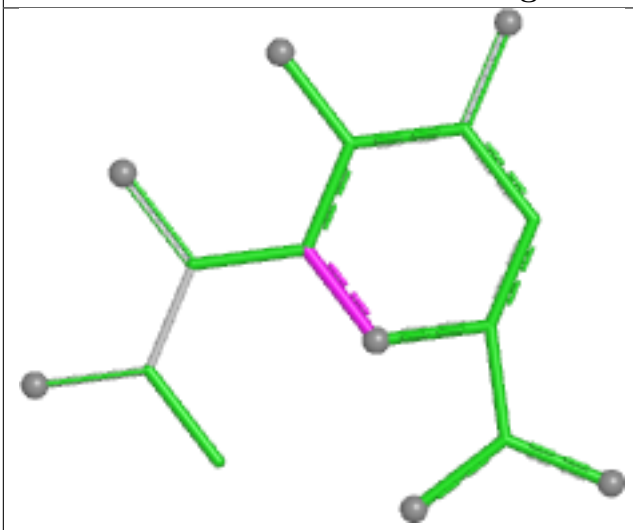


Rings

Ligand P8E cV 604



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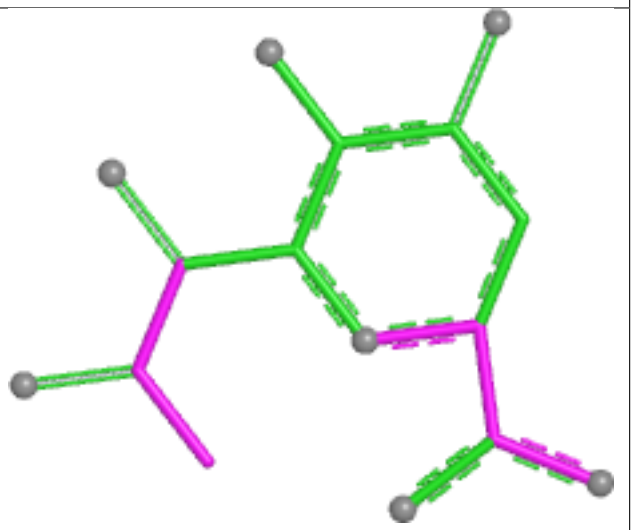

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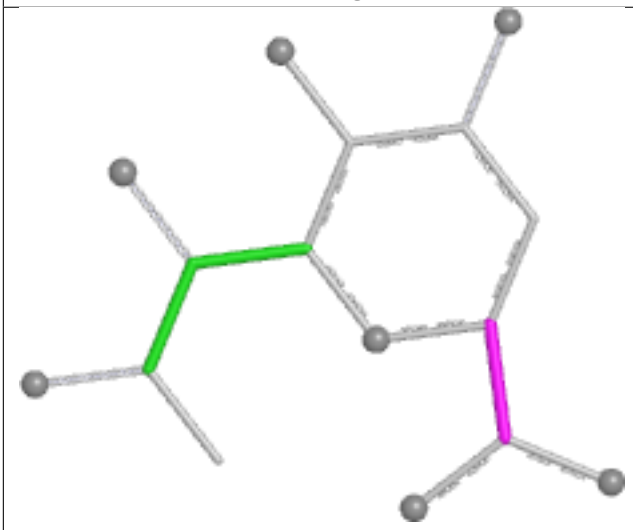

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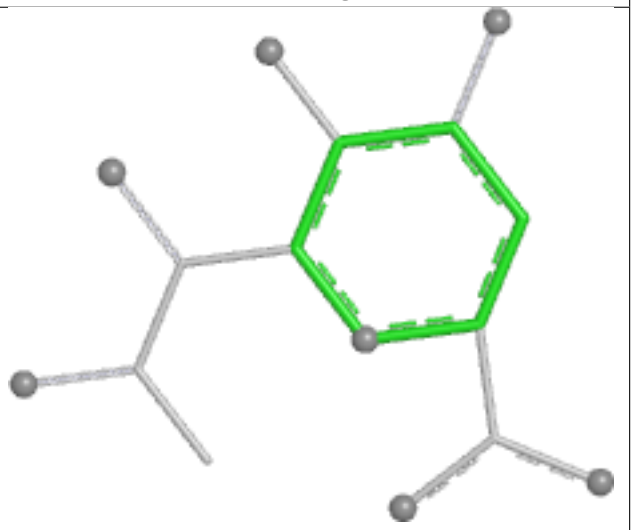
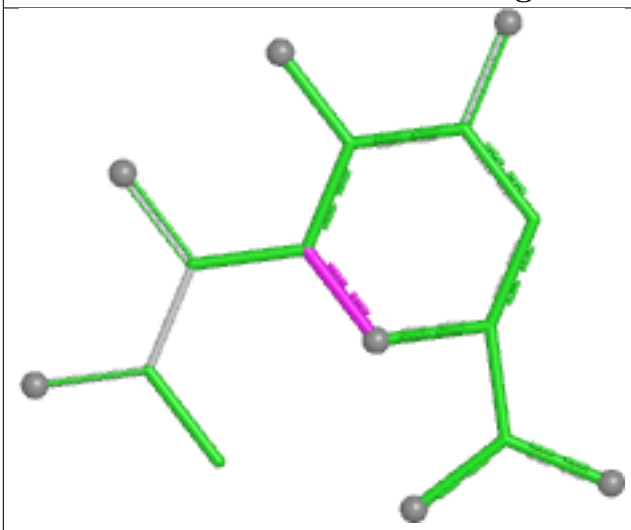


Rings

Ligand P8E OA 607



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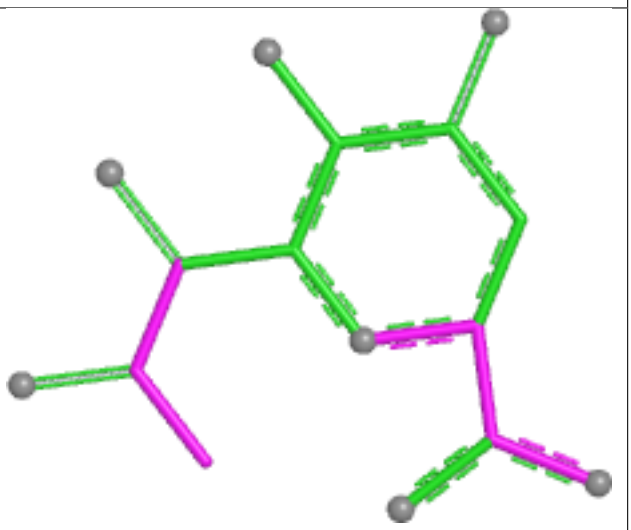

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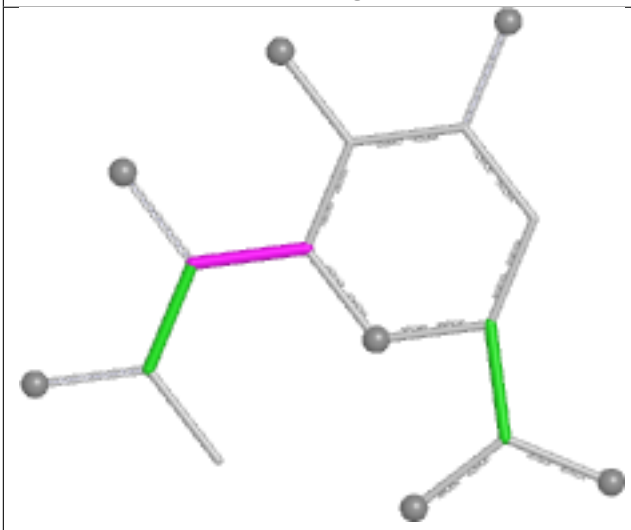

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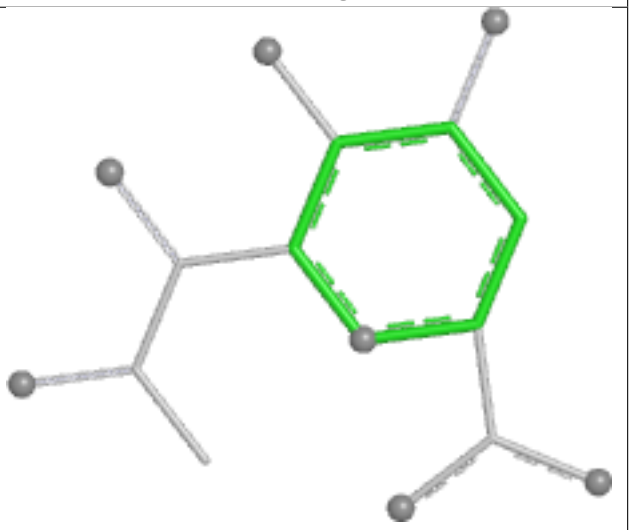

Rings

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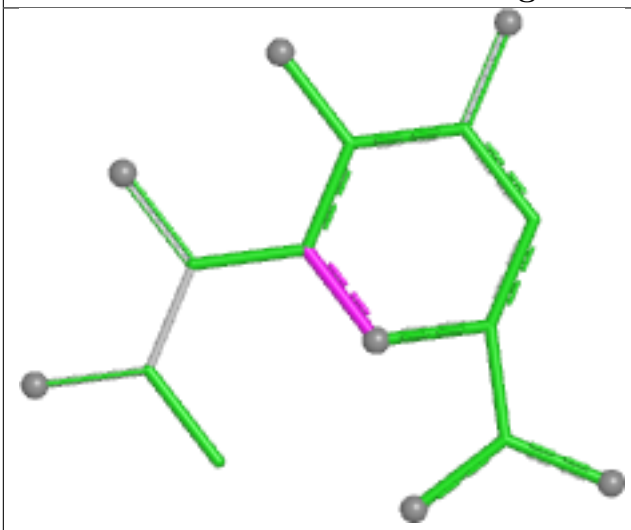

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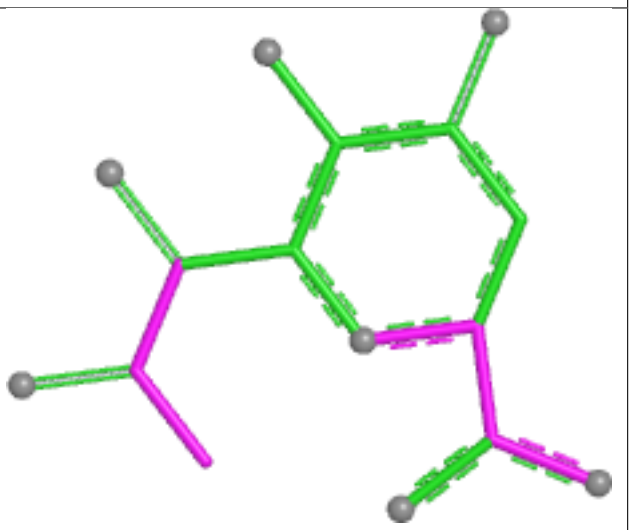

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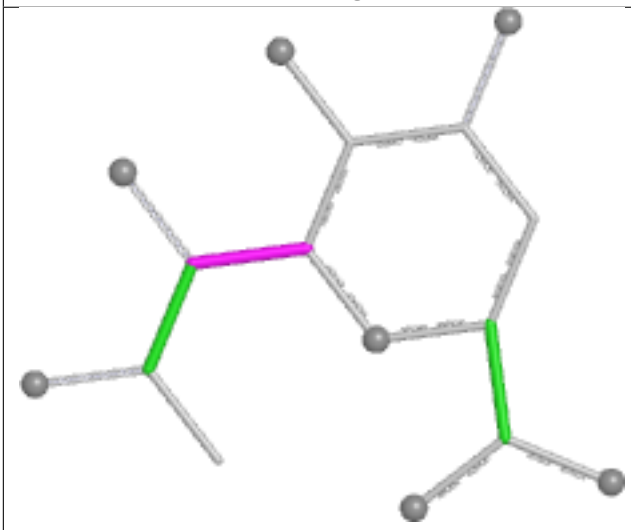

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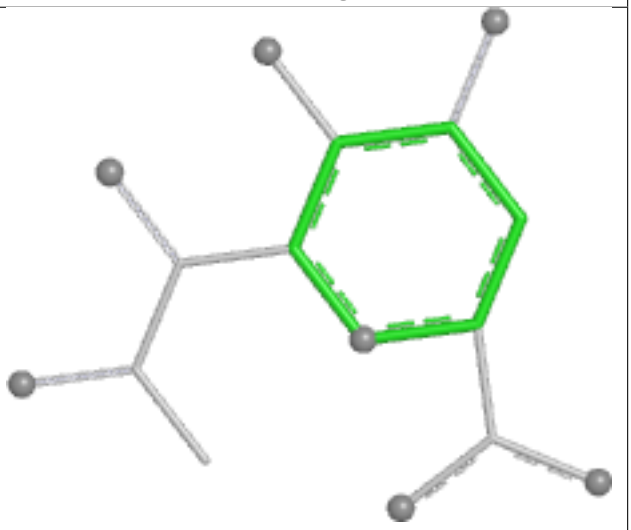

Rings

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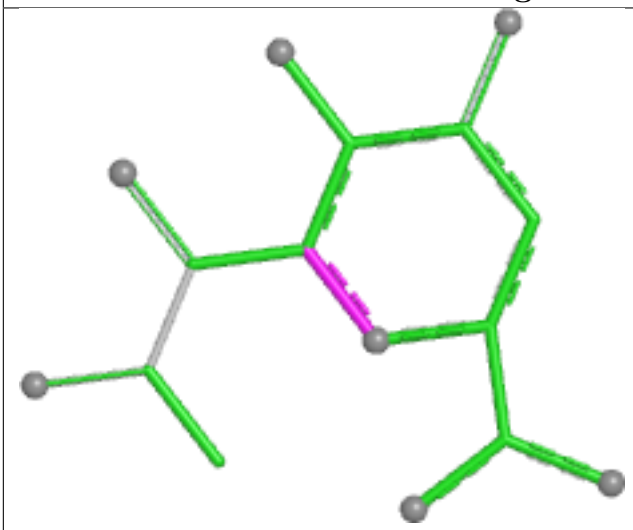

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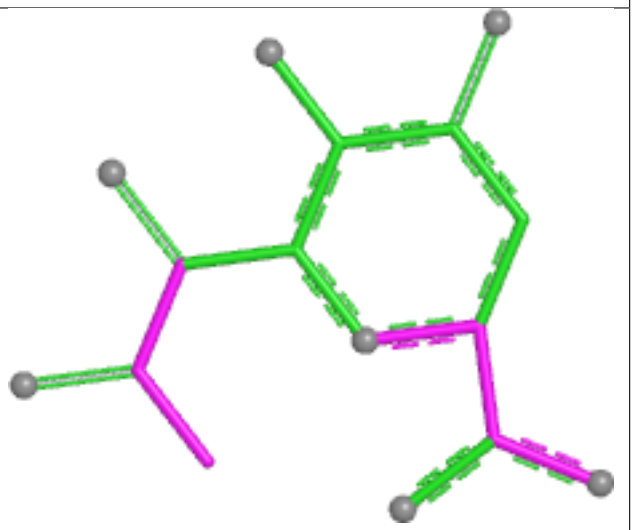

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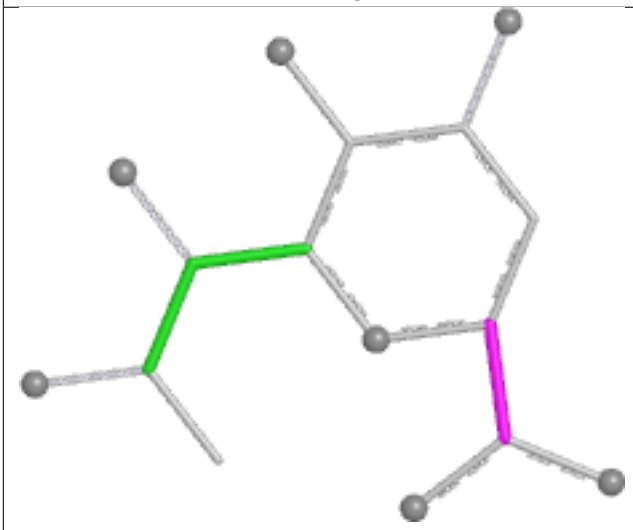

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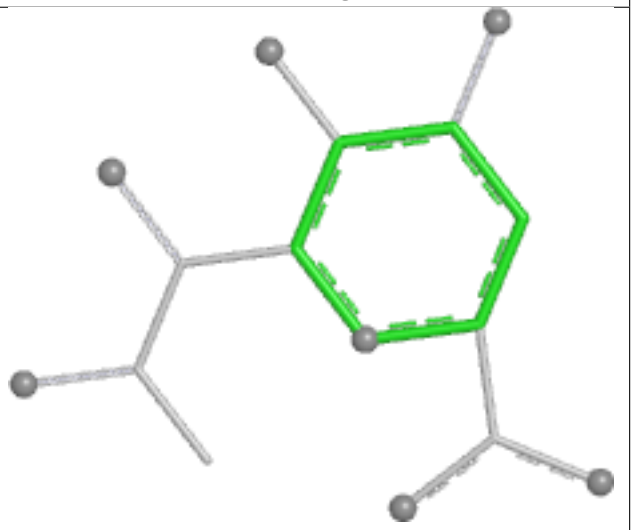
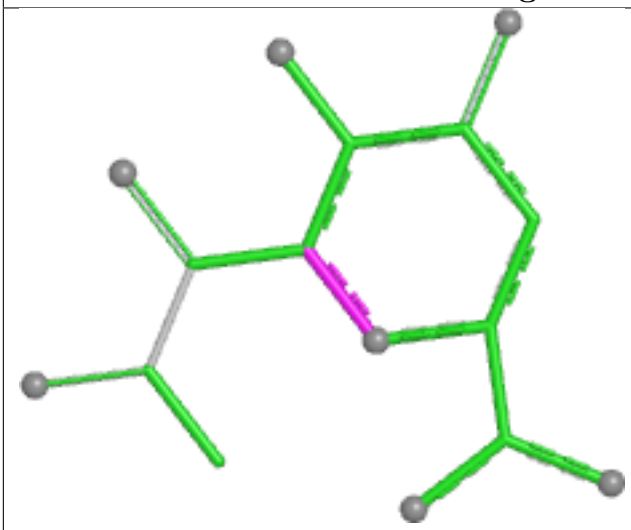


Rings

Ligand P8E Y1 606



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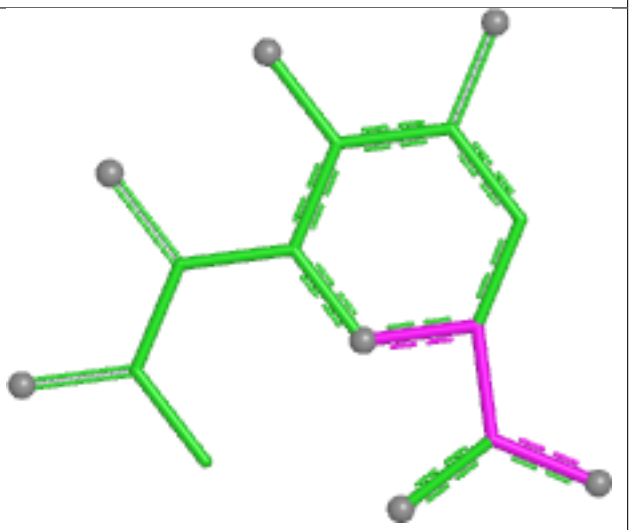

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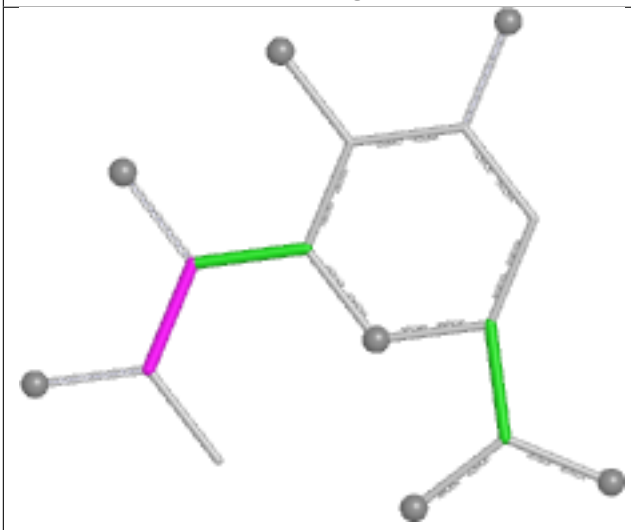

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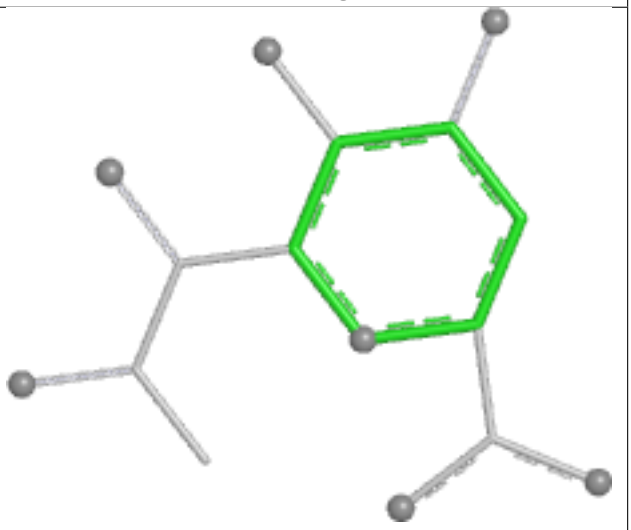

Rings

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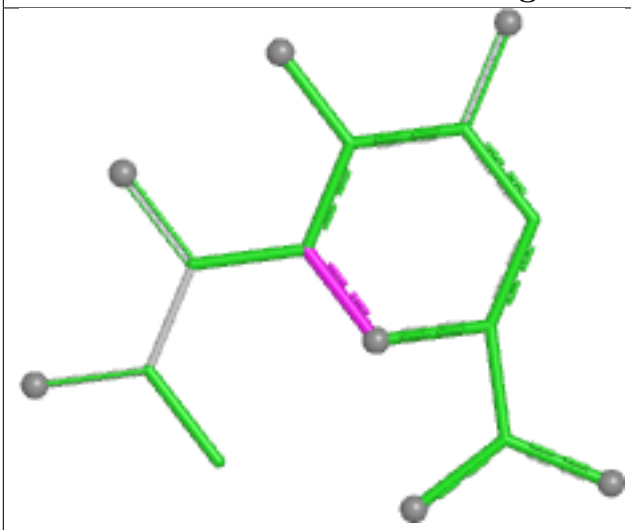

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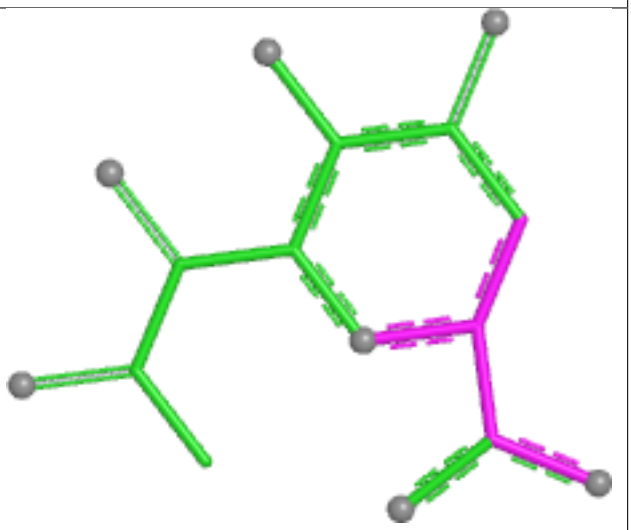

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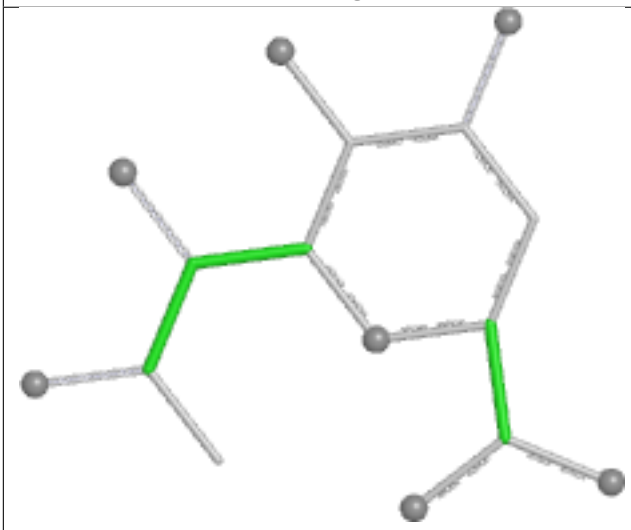

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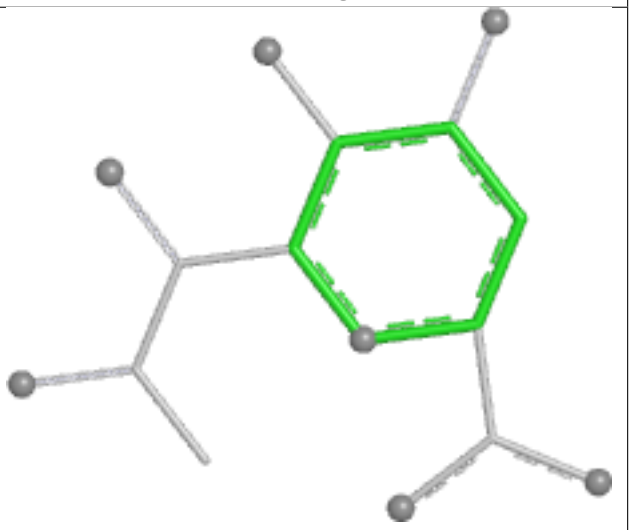
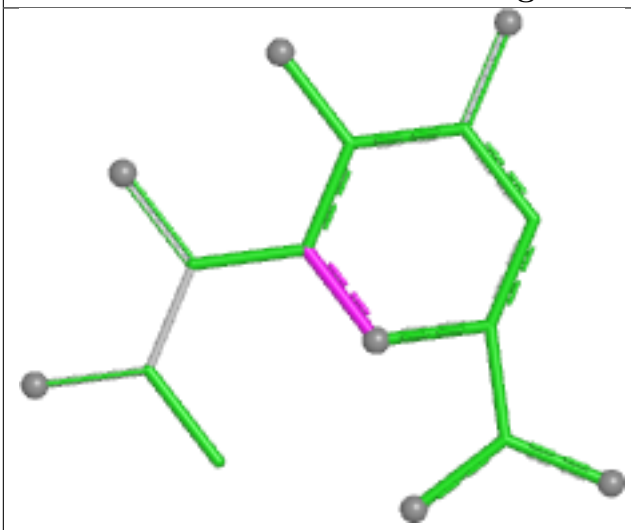


Rings

Ligand P8E FB 606



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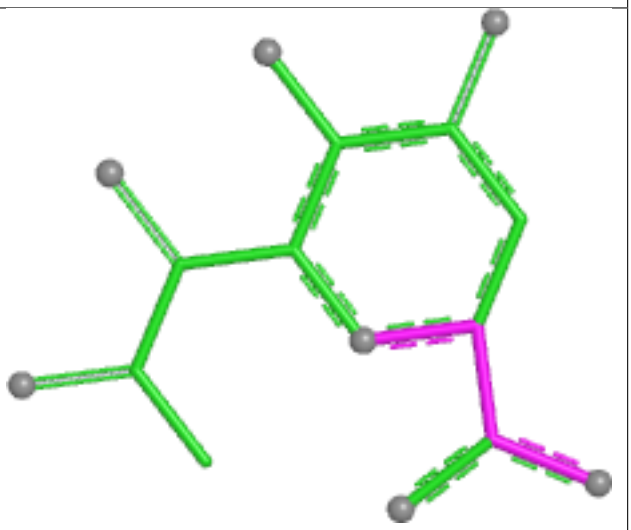

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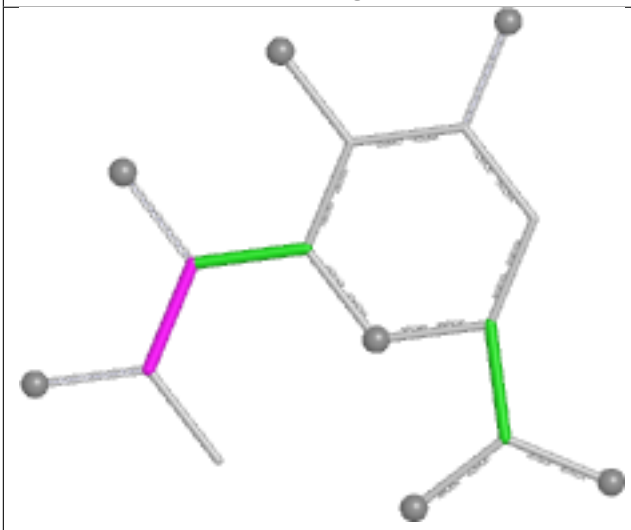

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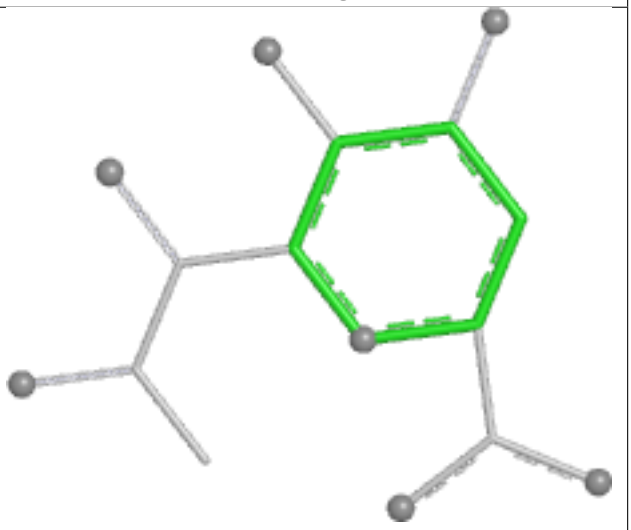

Rings

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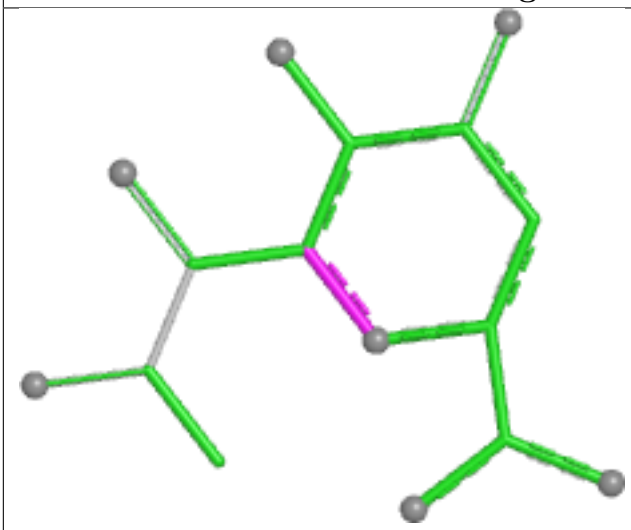

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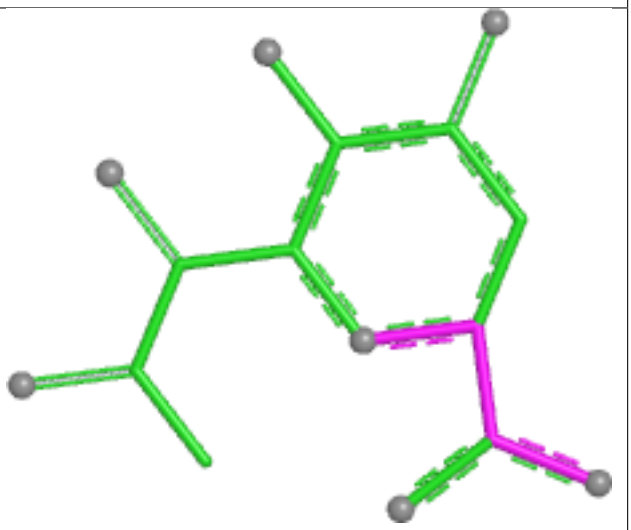

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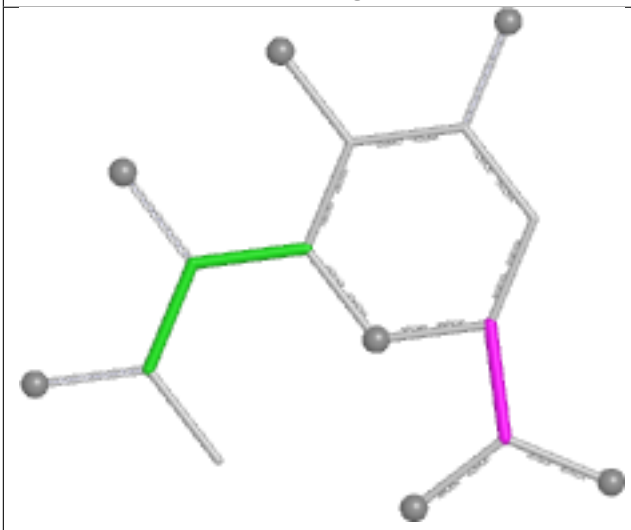

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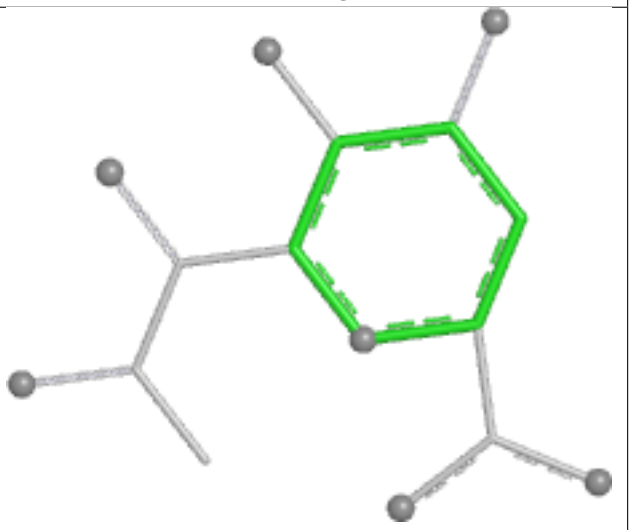
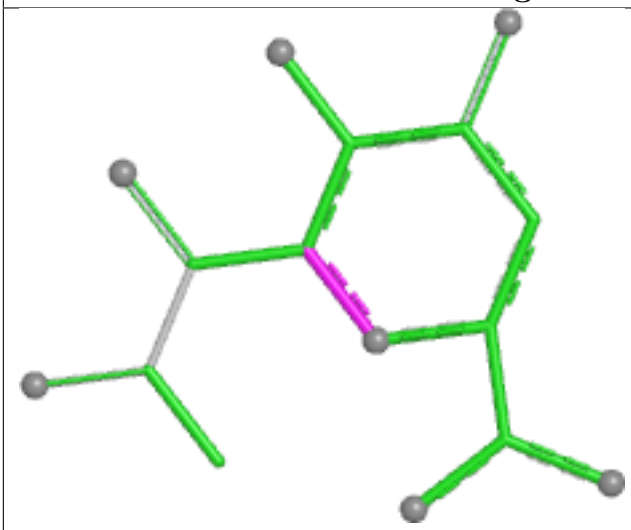


Rings

Ligand P8E GQ 602



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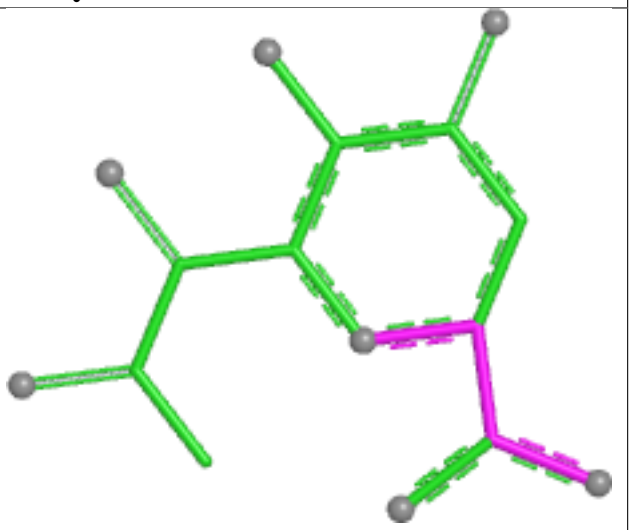

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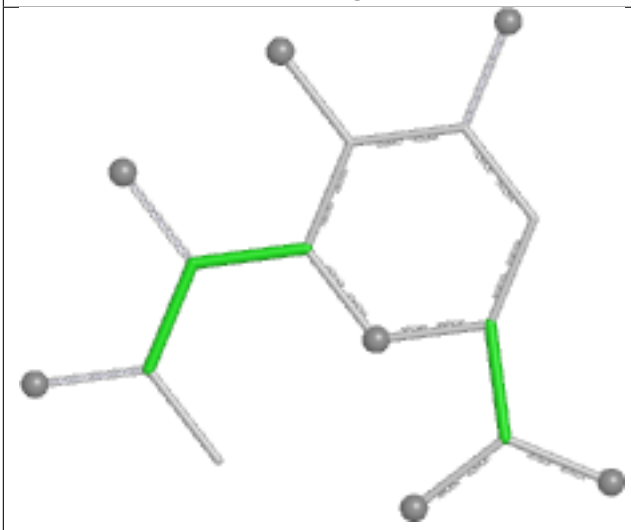

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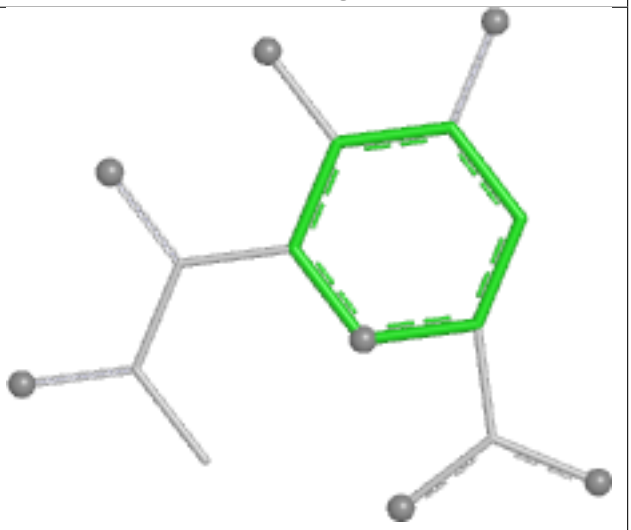
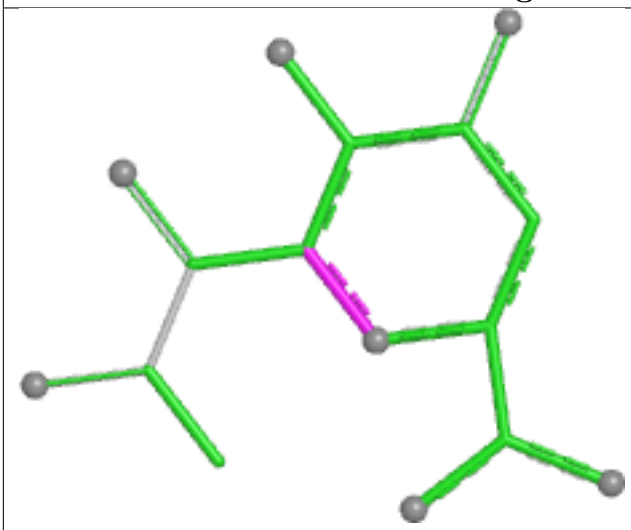


Rings

Ligand P8E KE 607



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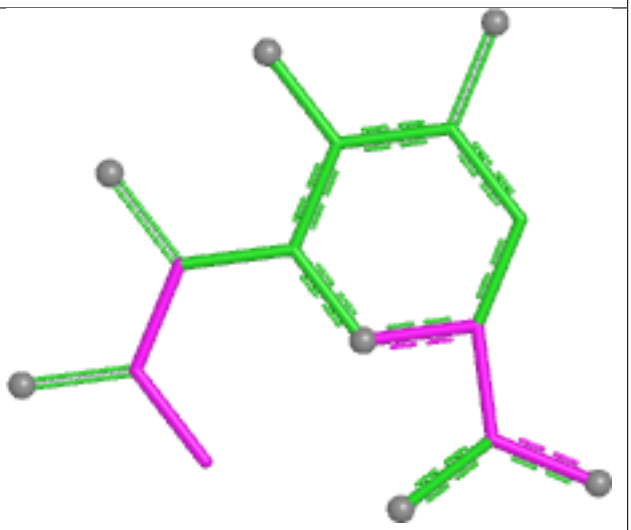
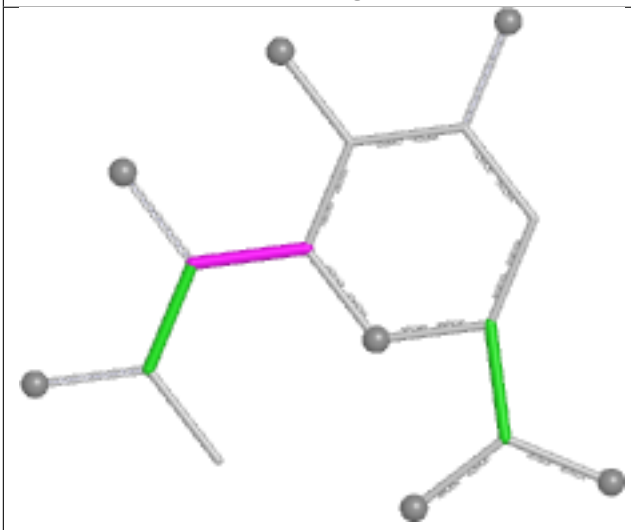


Bond angles



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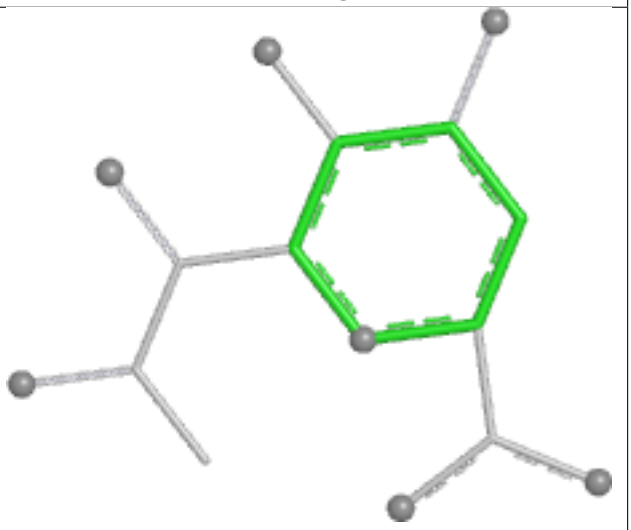
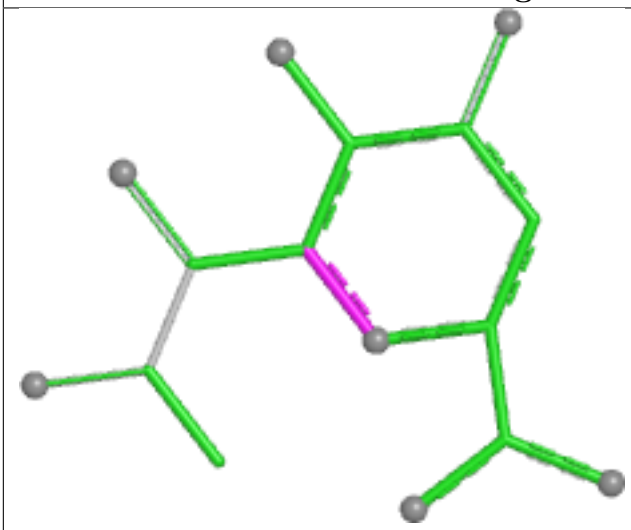


Rings

Ligand P8E VR 602



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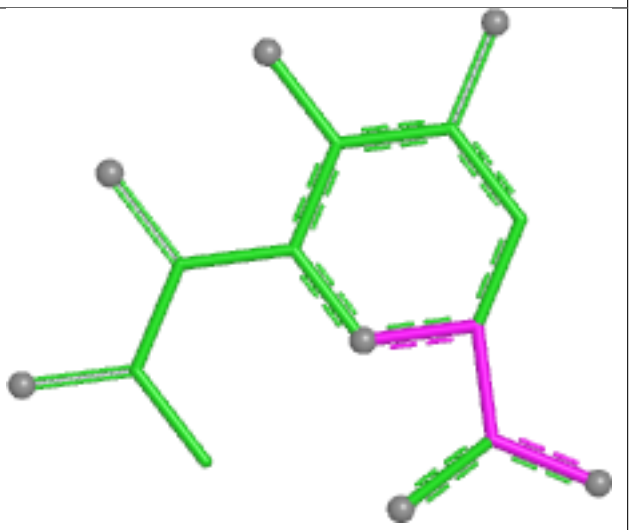
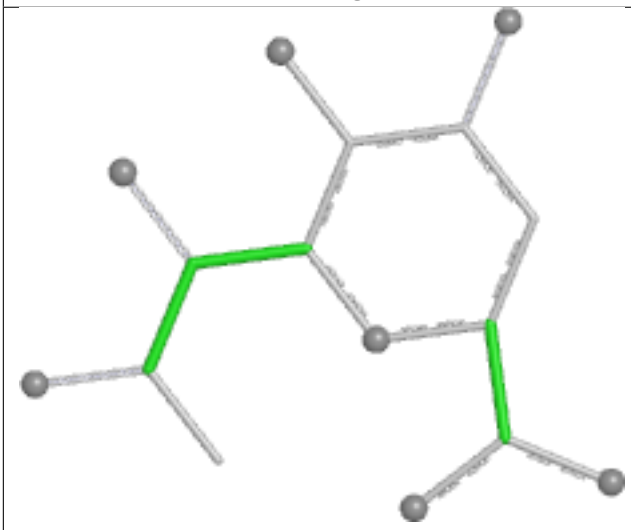


Bond angles



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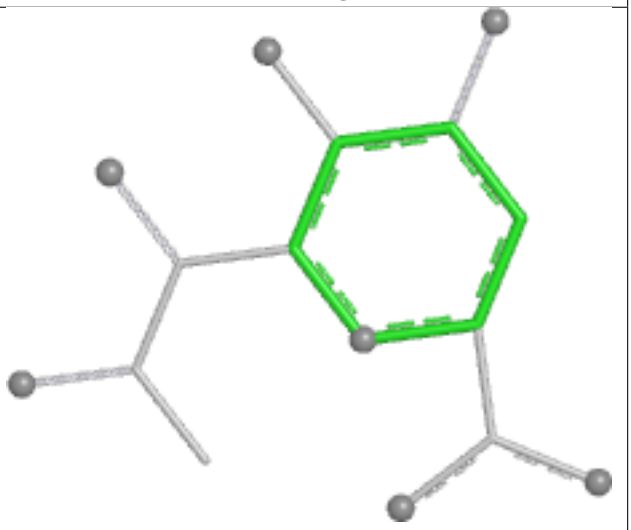
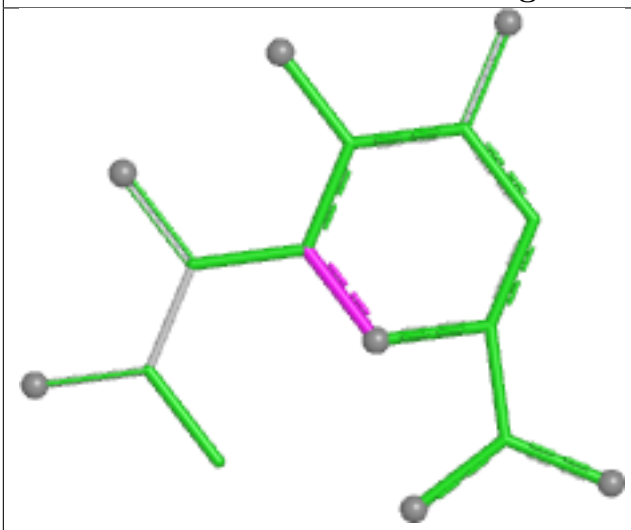


Rings

Ligand P8E A7 607



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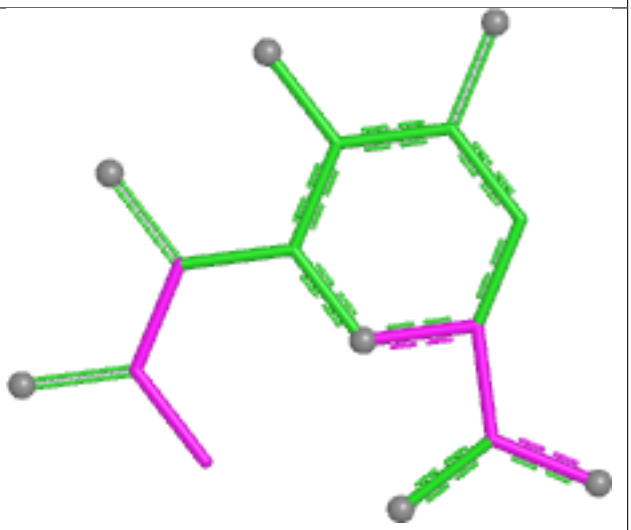

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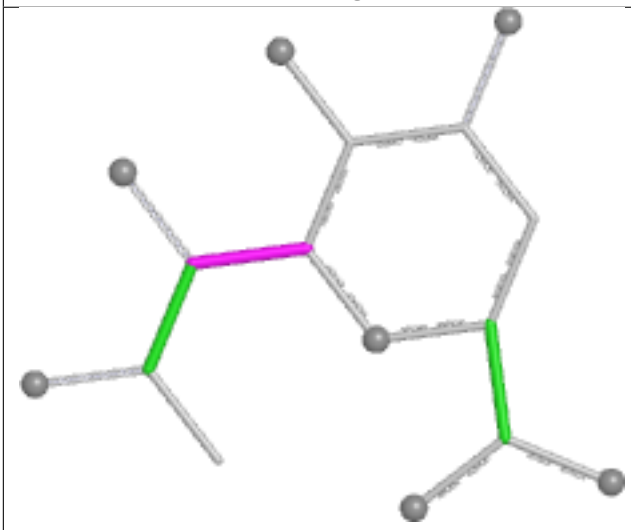
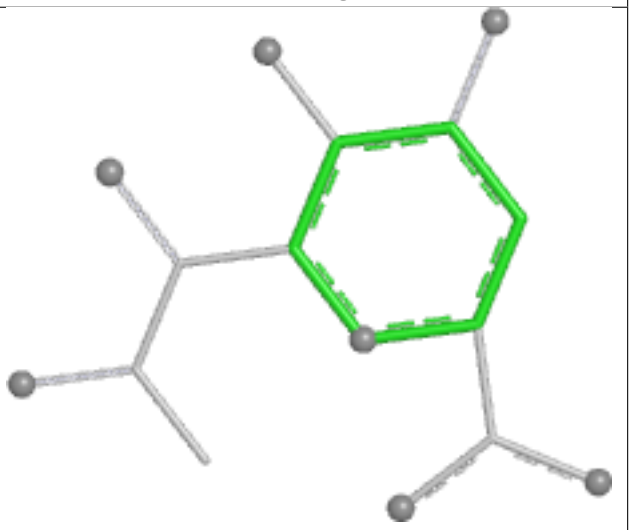
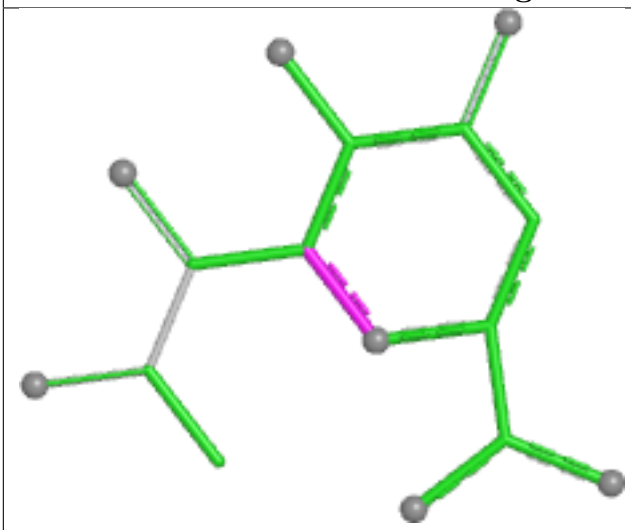


Torsions



Rings

Ligand P8E OA 605



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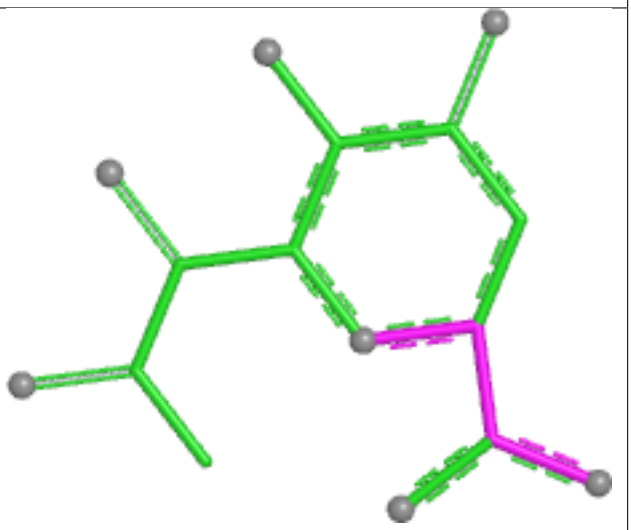

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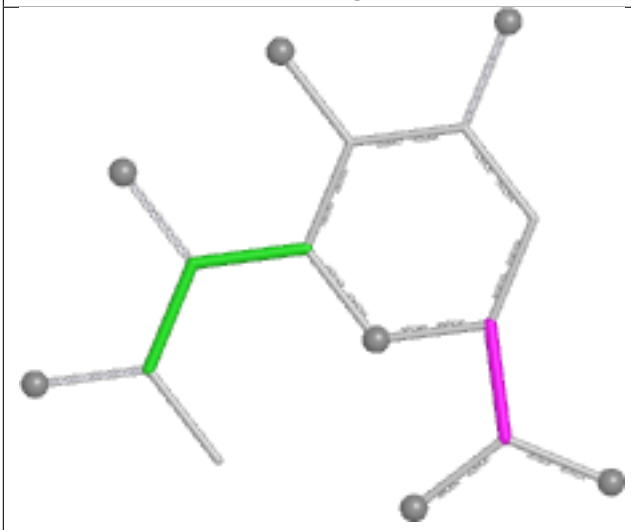

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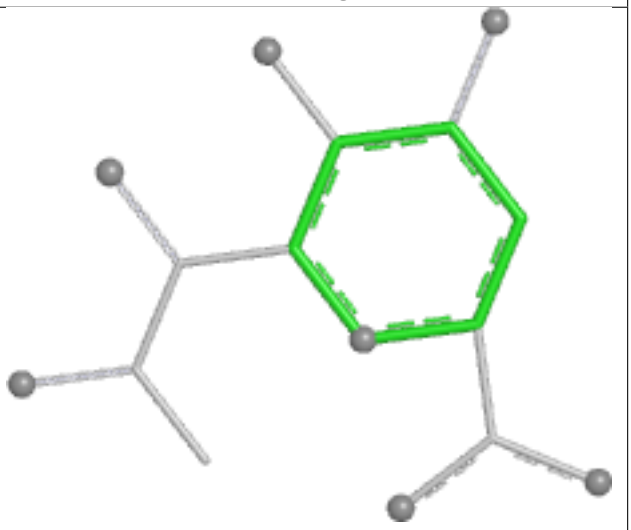
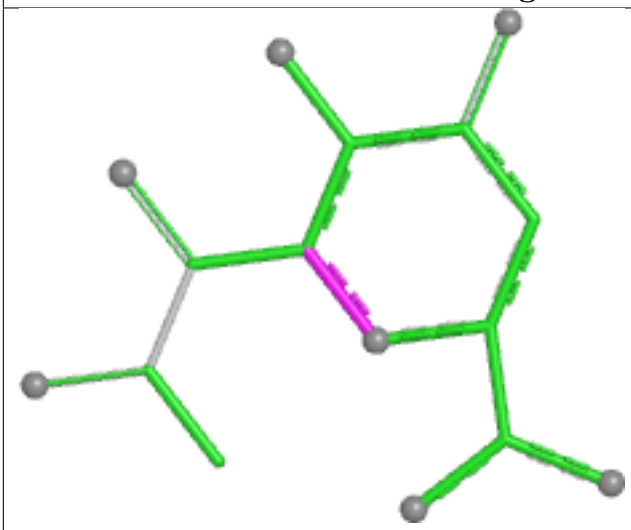


Rings

Ligand P8E dC 606



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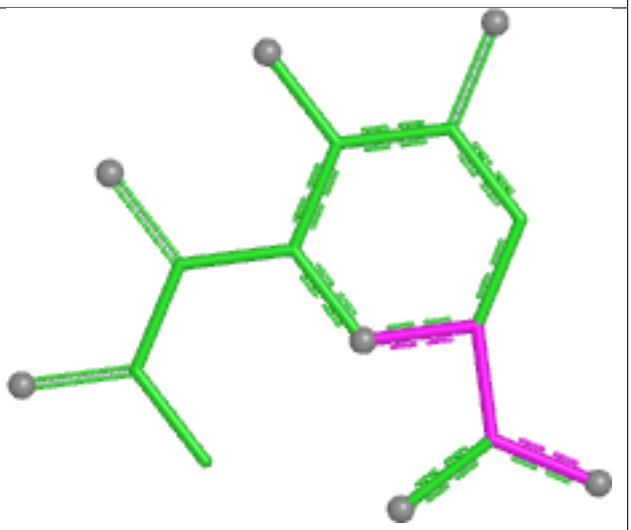

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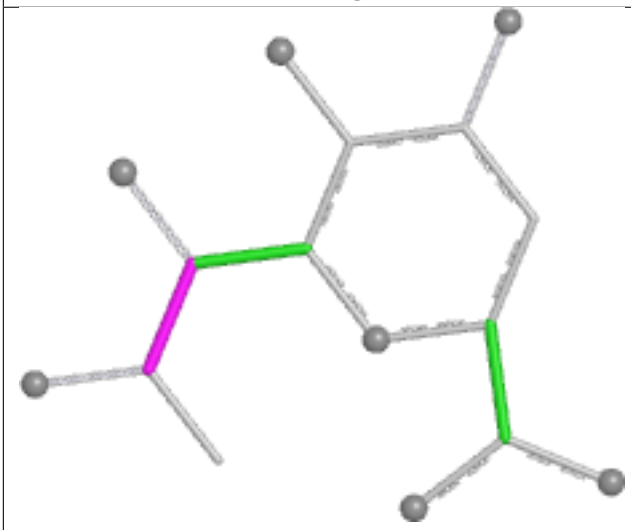

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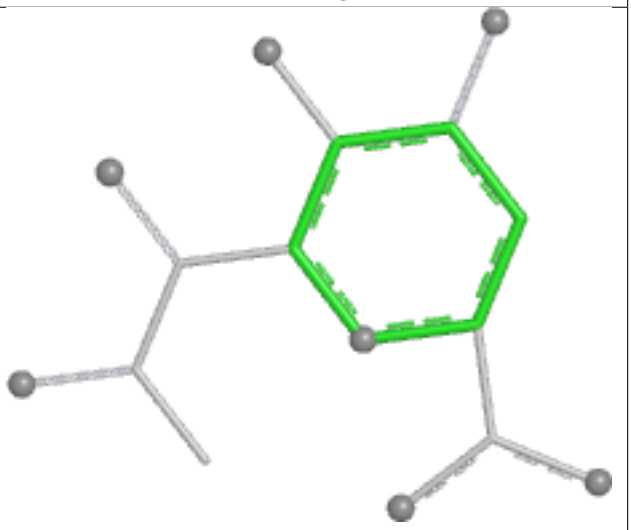
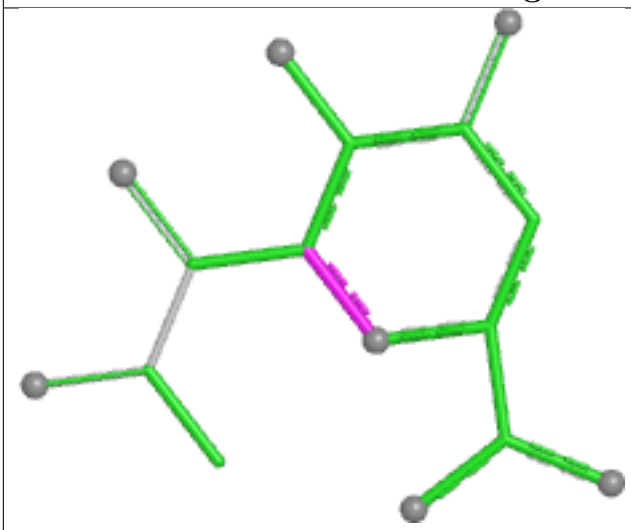


Rings

Ligand P8E g6 606



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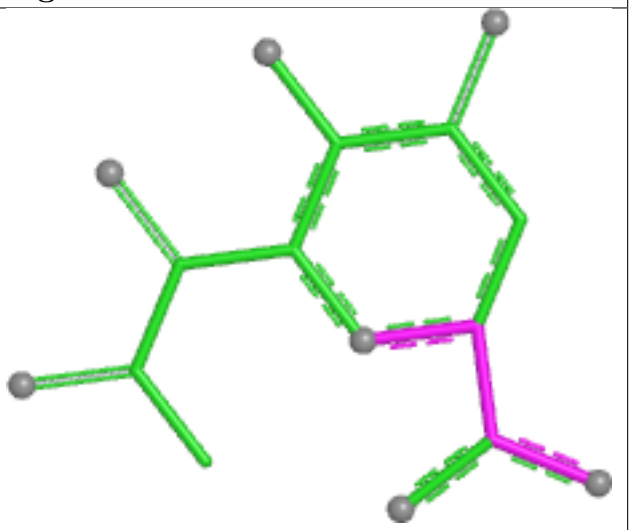

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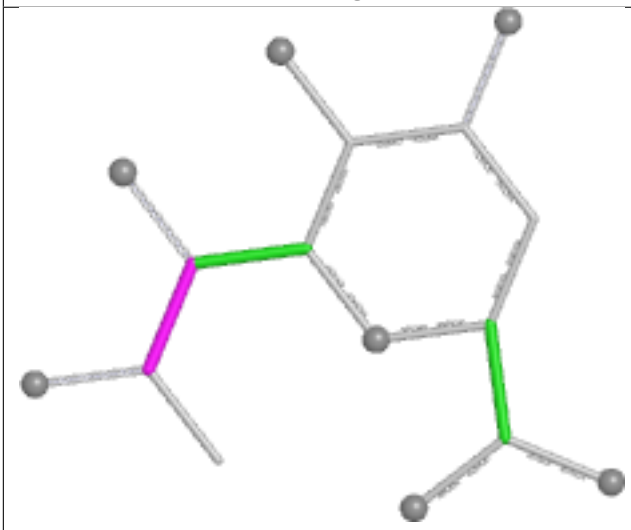

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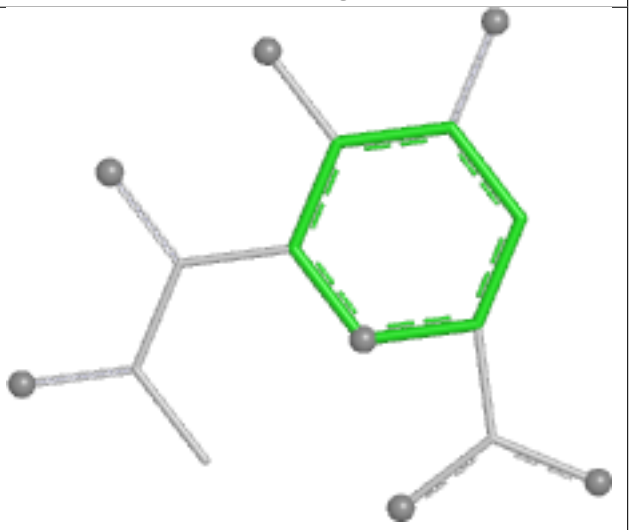
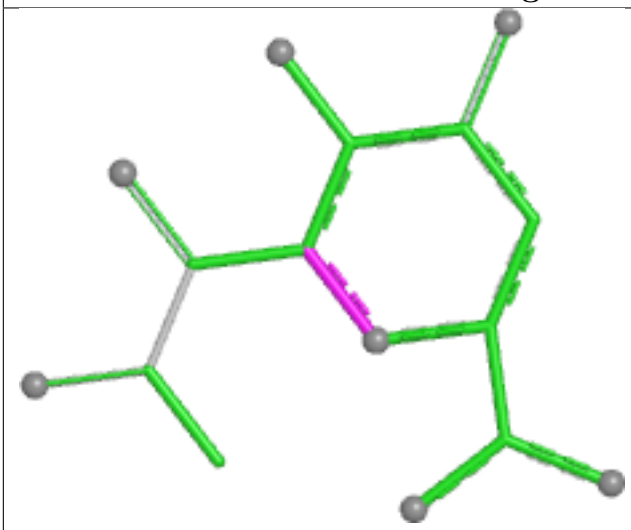


Rings

Ligand P8E fK 607



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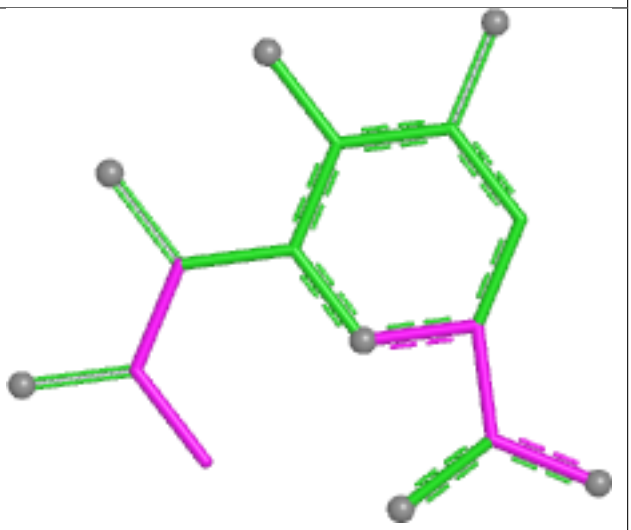

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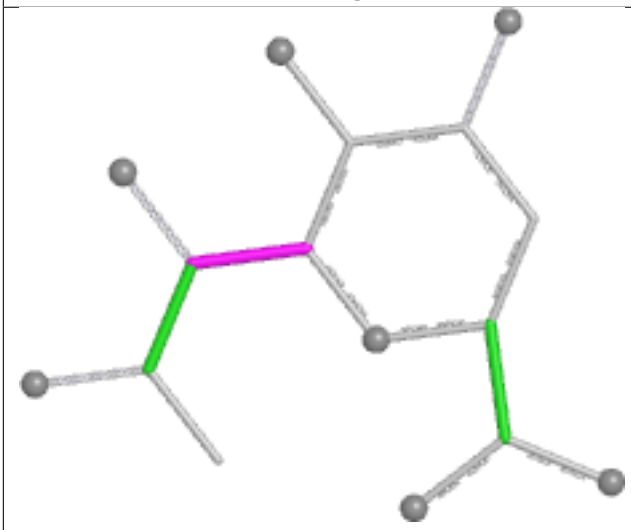

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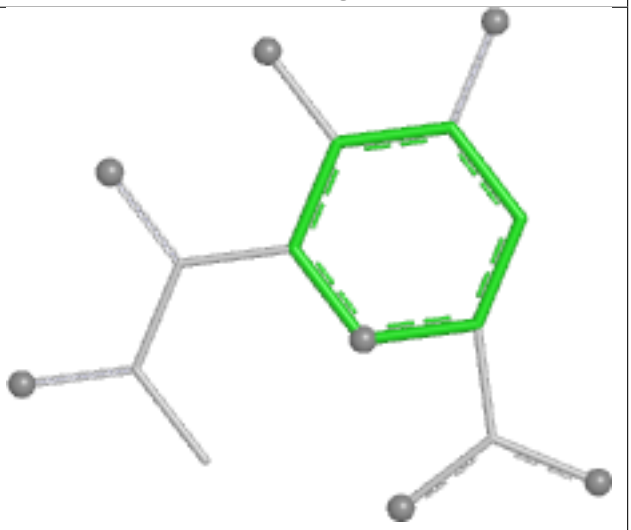

Rings

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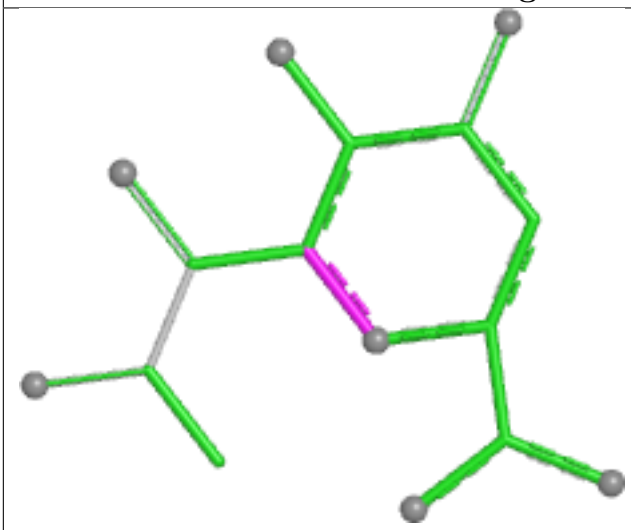

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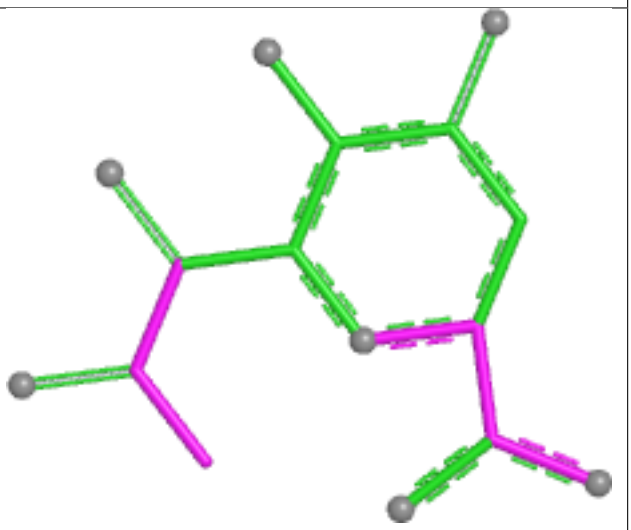

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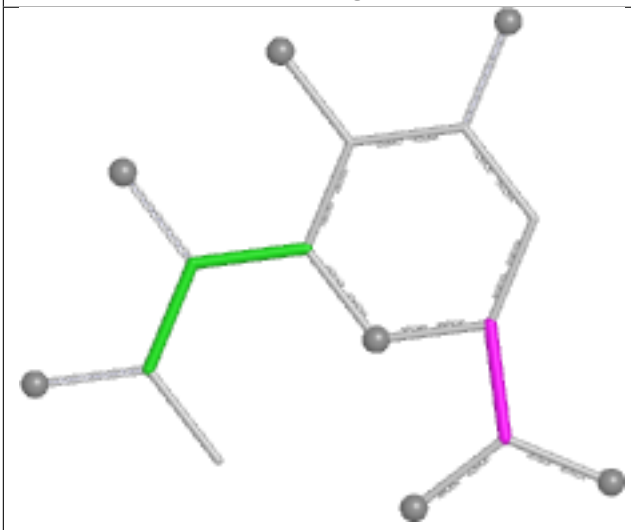

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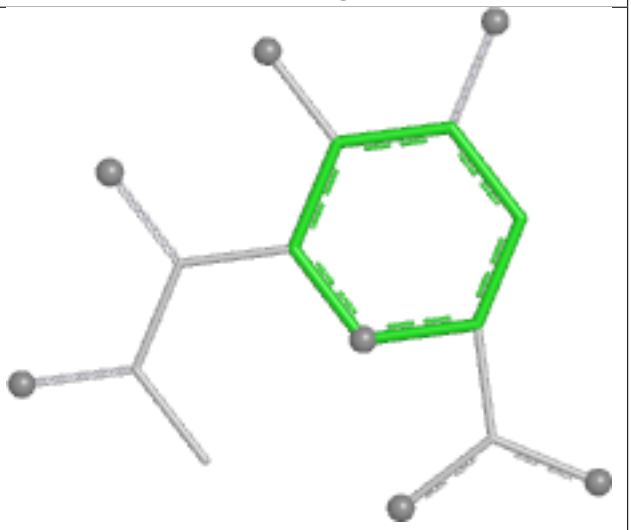

Rings

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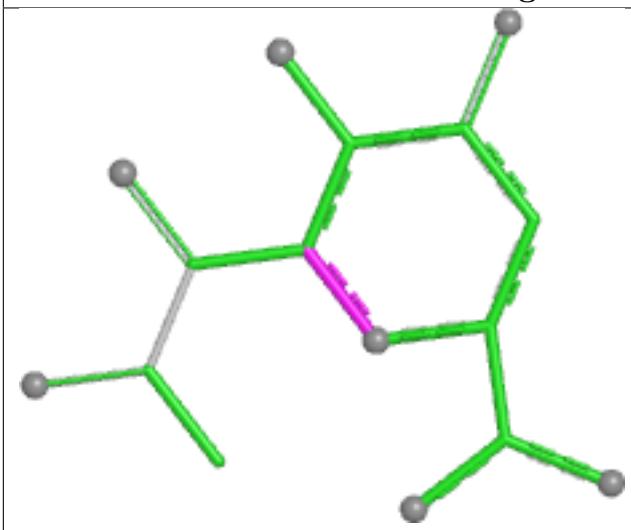

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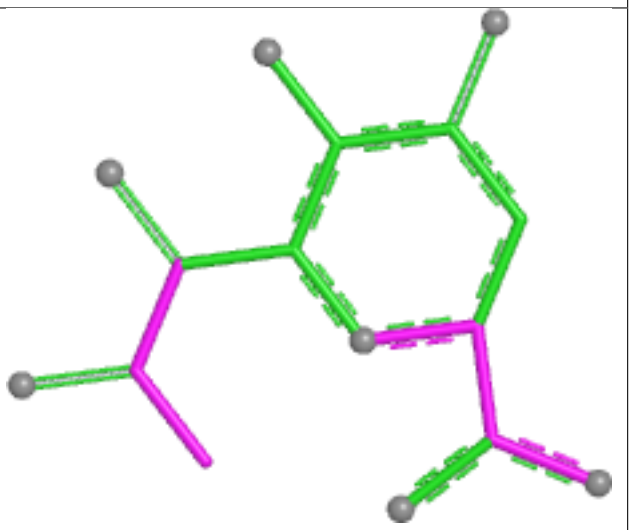

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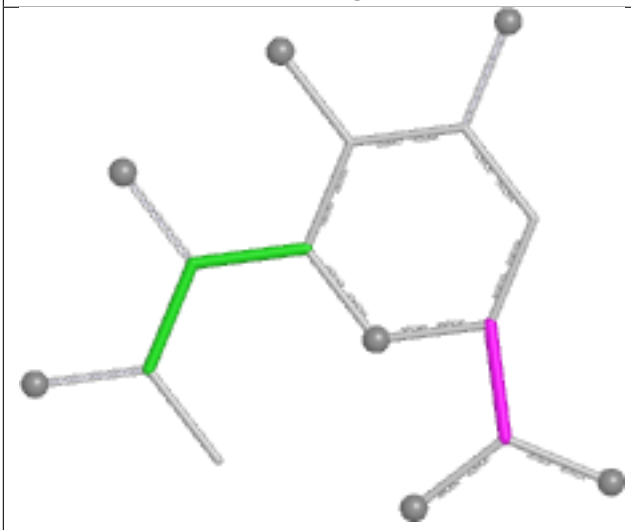

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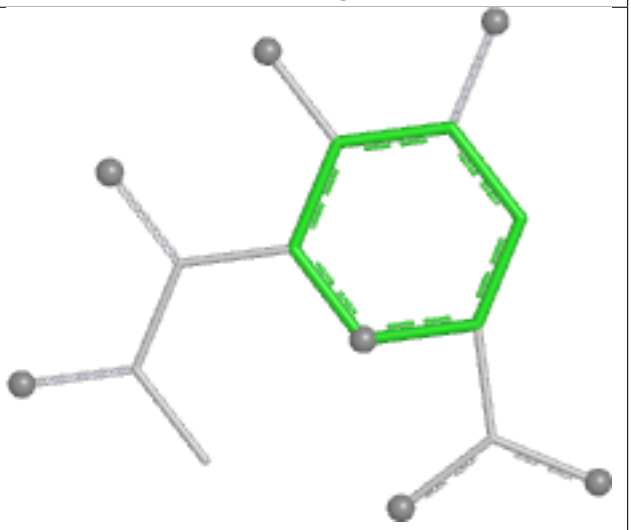

Rings

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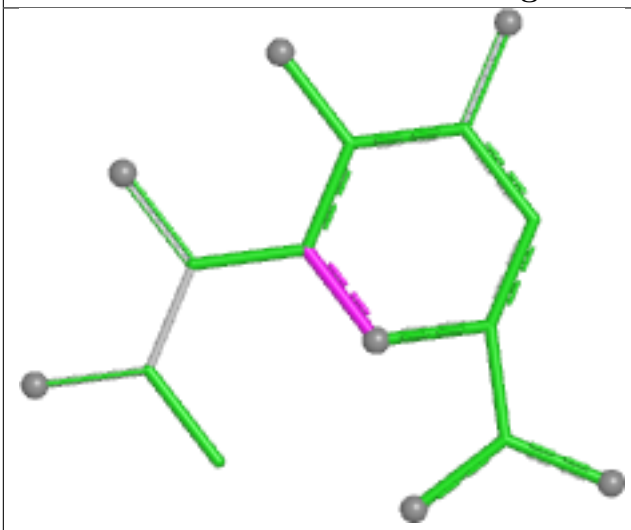

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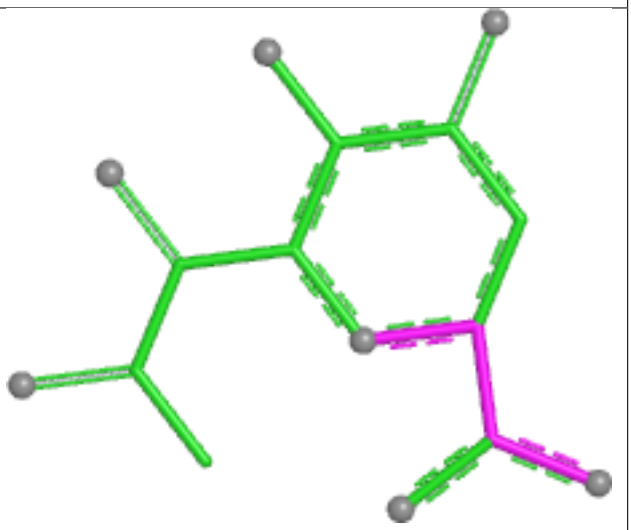

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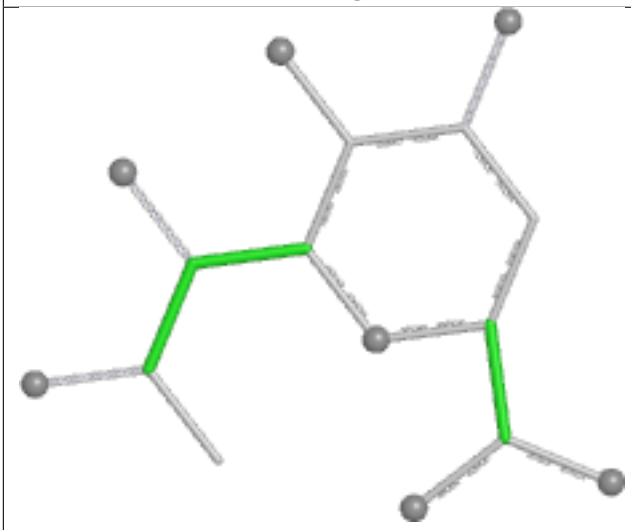

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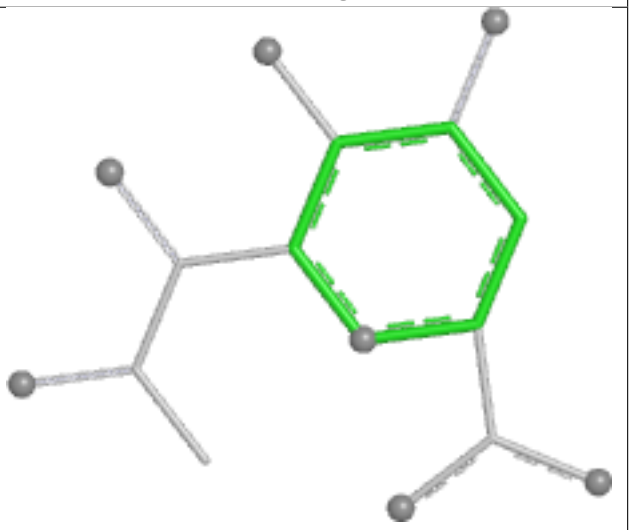

Rings

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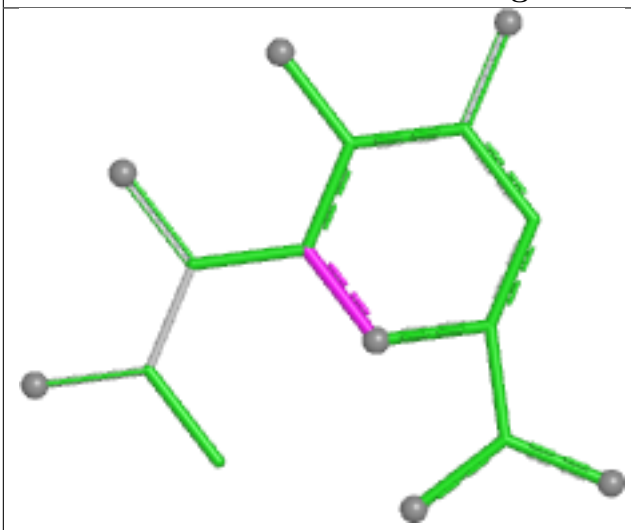

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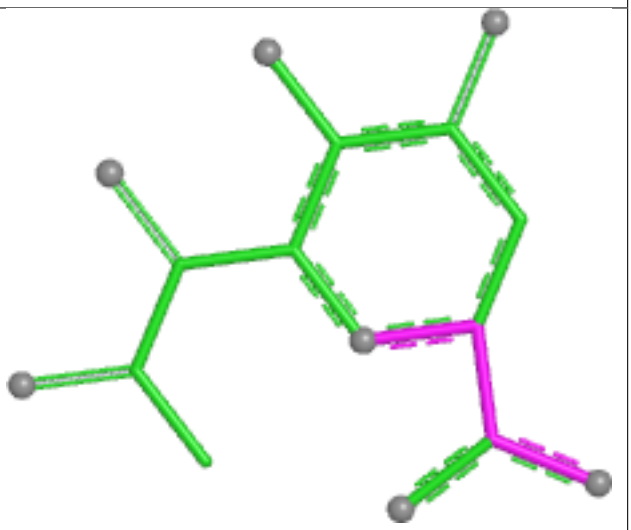

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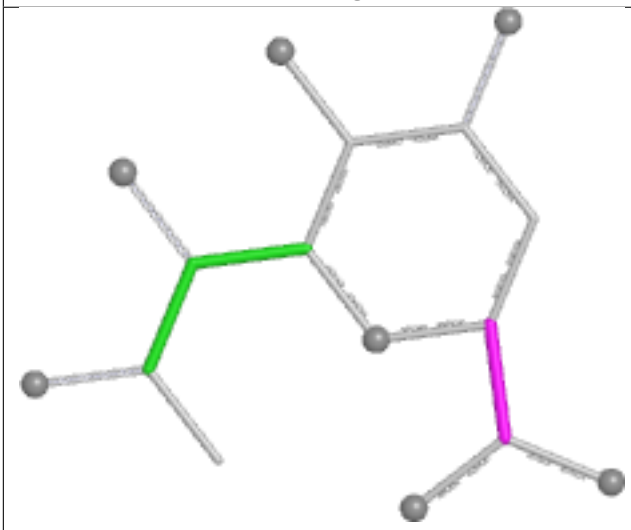

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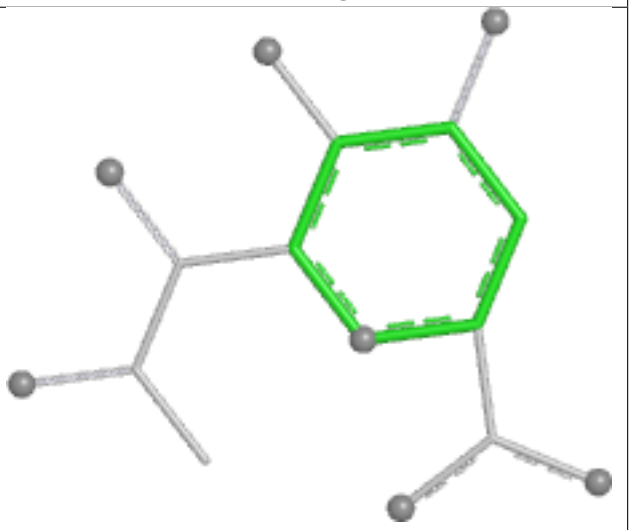
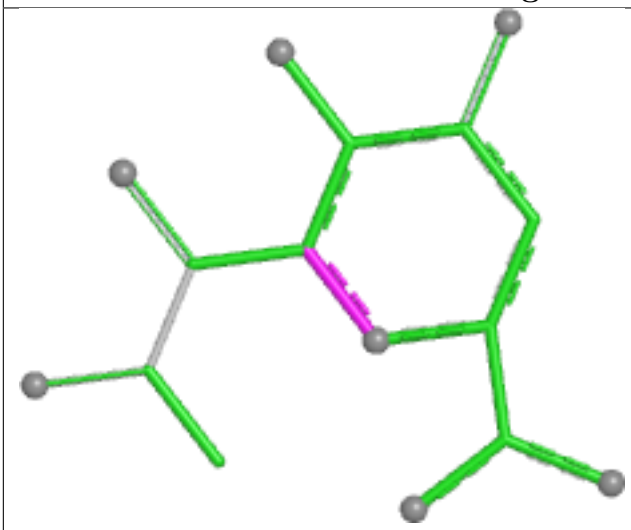


Rings

Ligand P8E Z9 607



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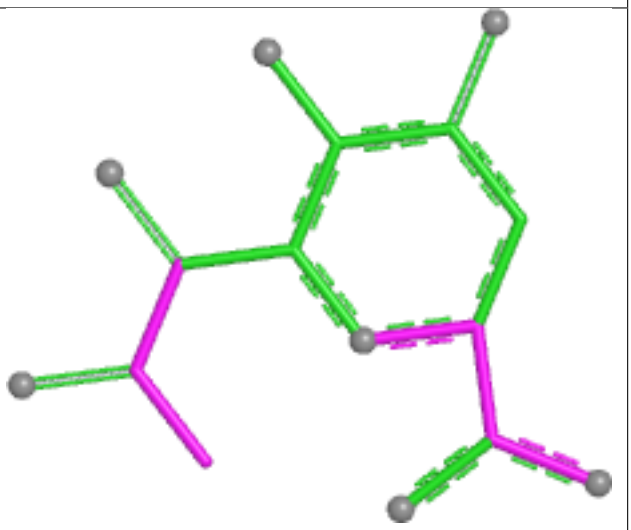

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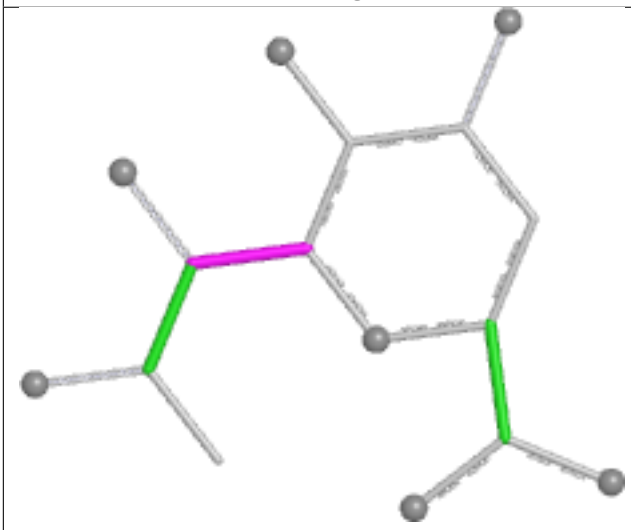

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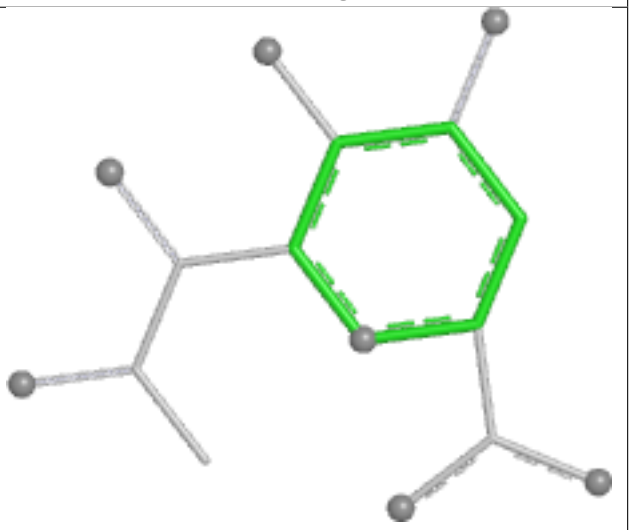
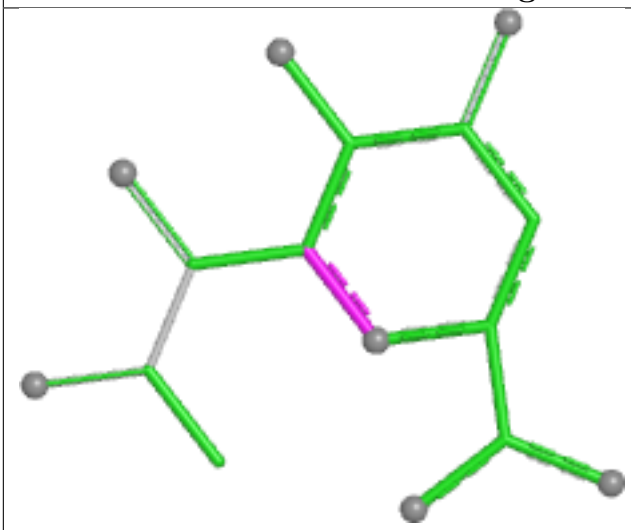


Rings

Ligand P8E JD 606



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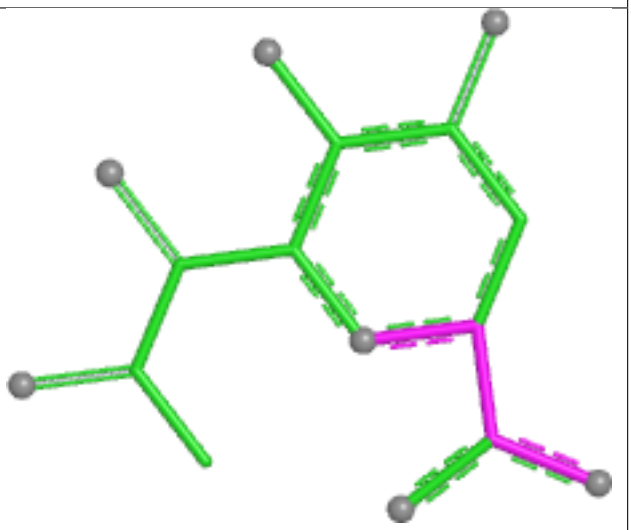

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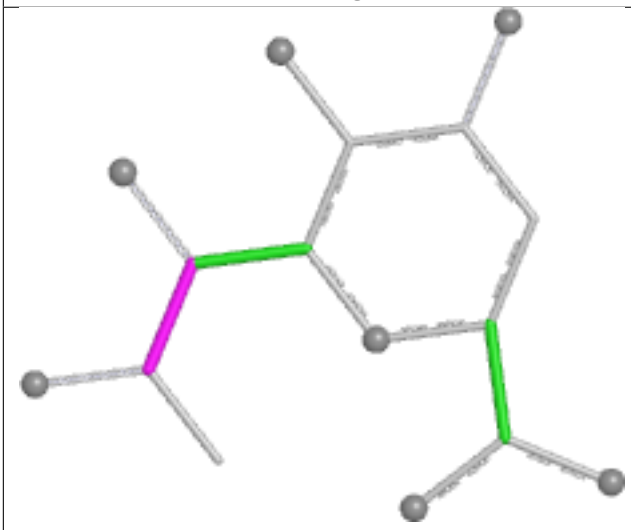

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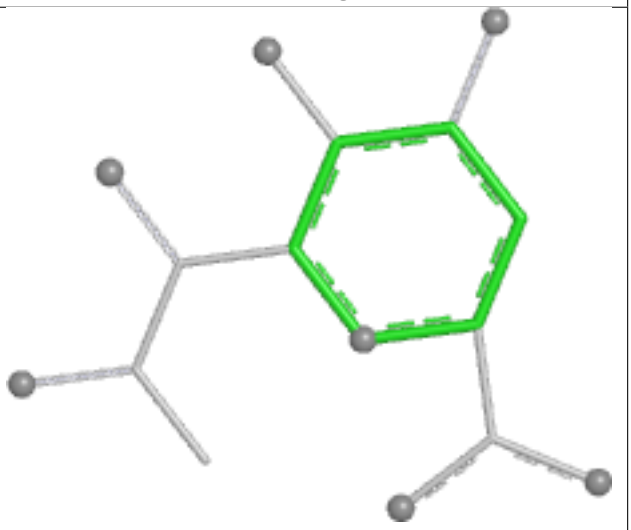
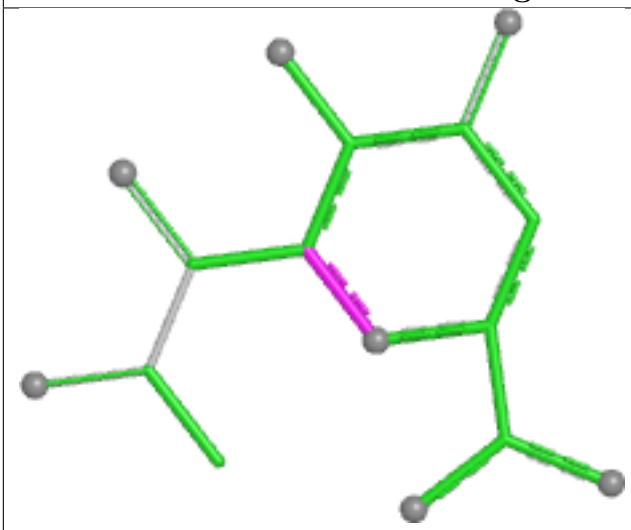


Rings

Ligand P8E DN 602



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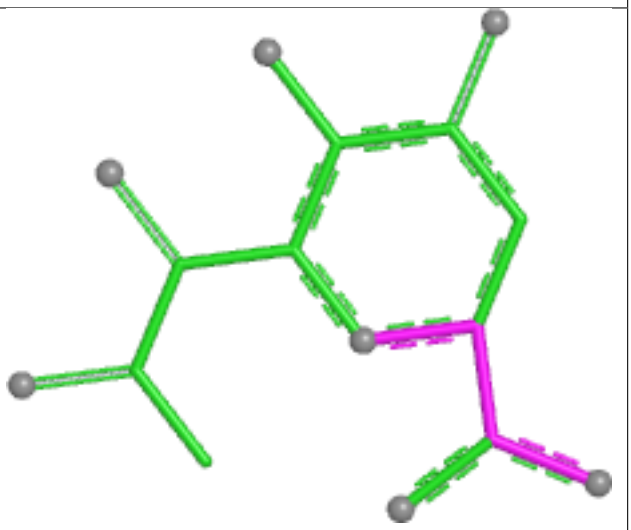

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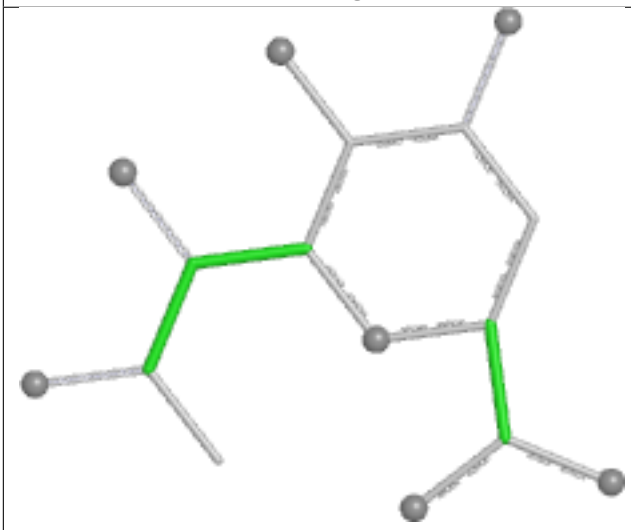

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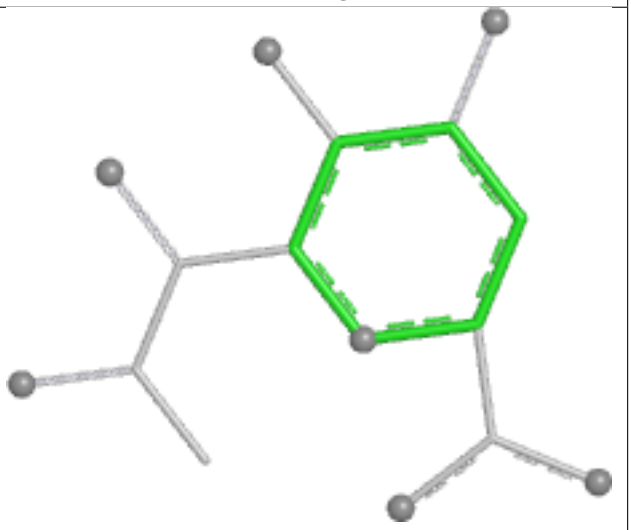
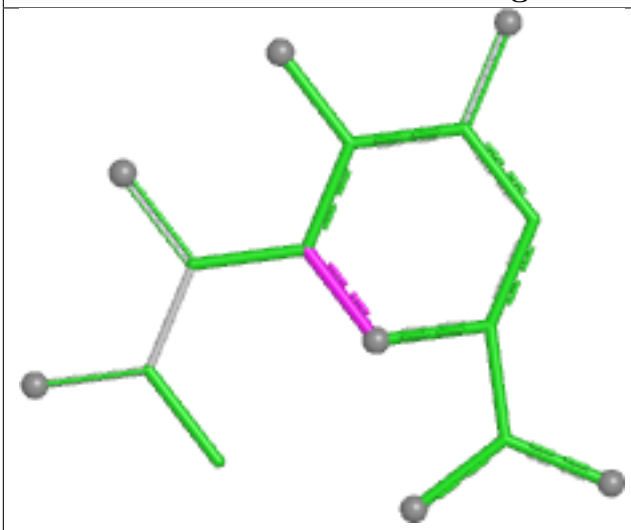


Rings

Ligand P8E MO 604



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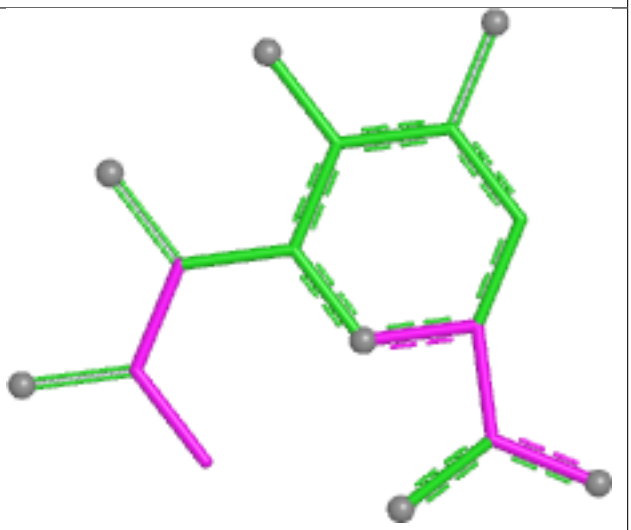
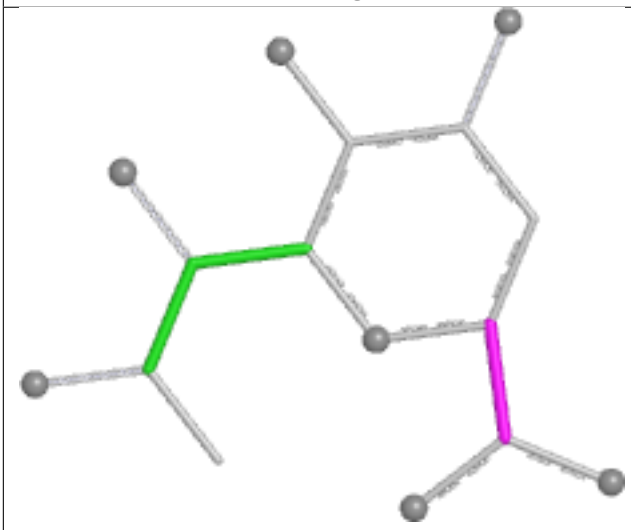


Bond angles



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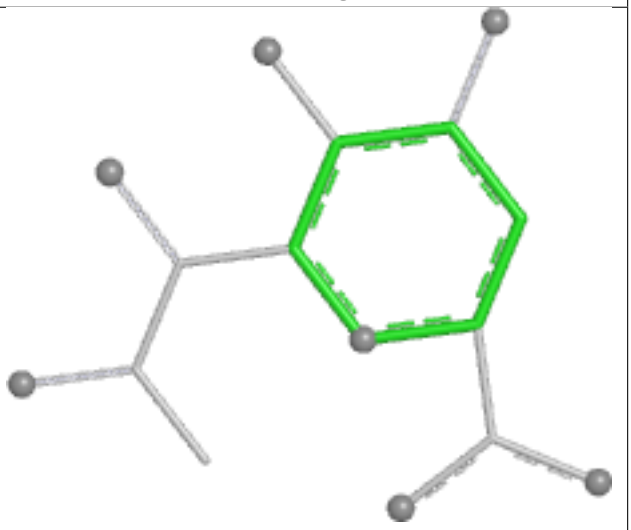

Rings

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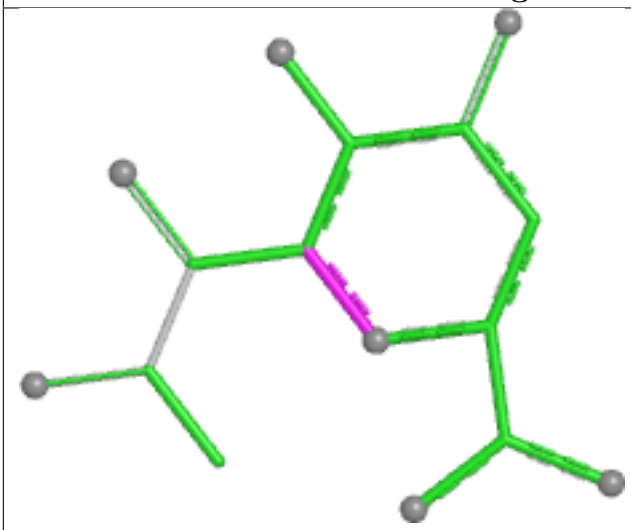

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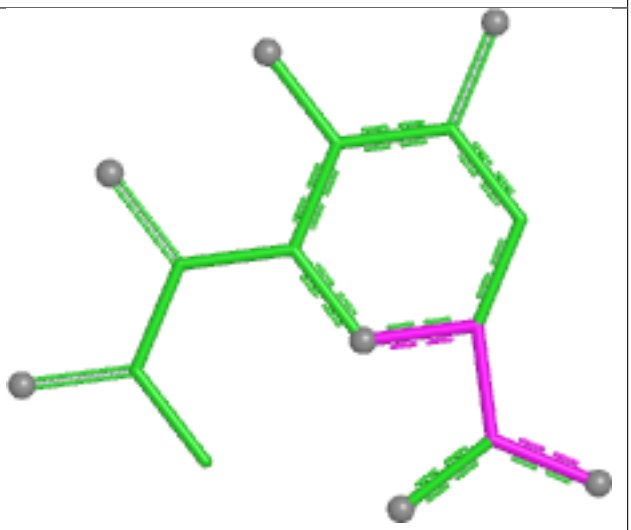
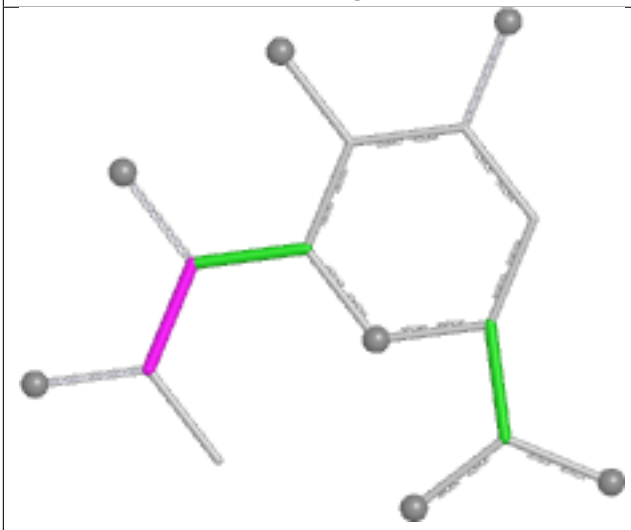
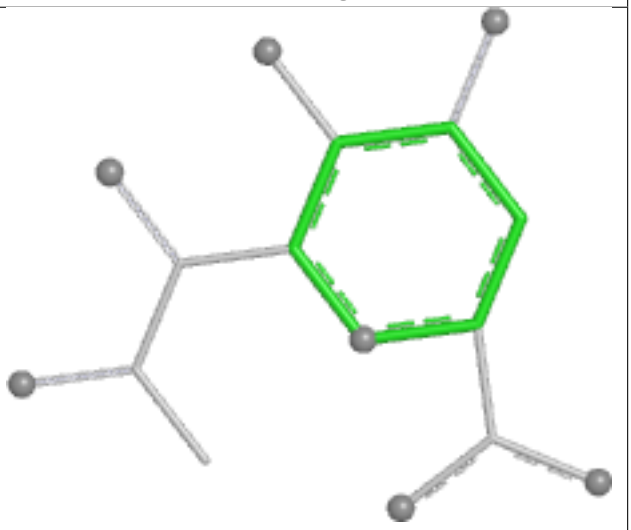


Bond angles

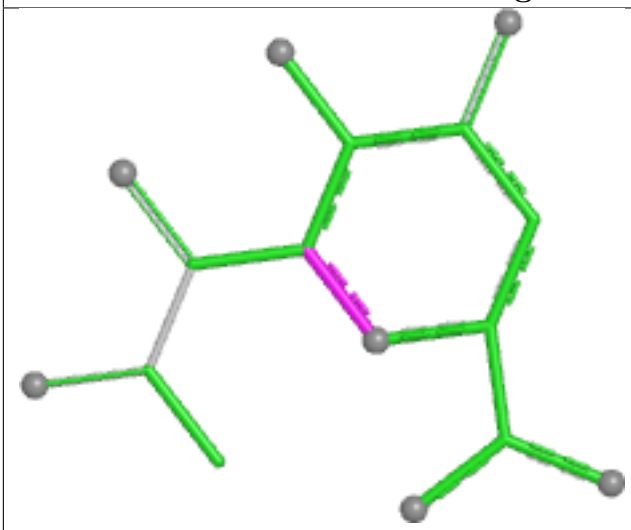


Torsions

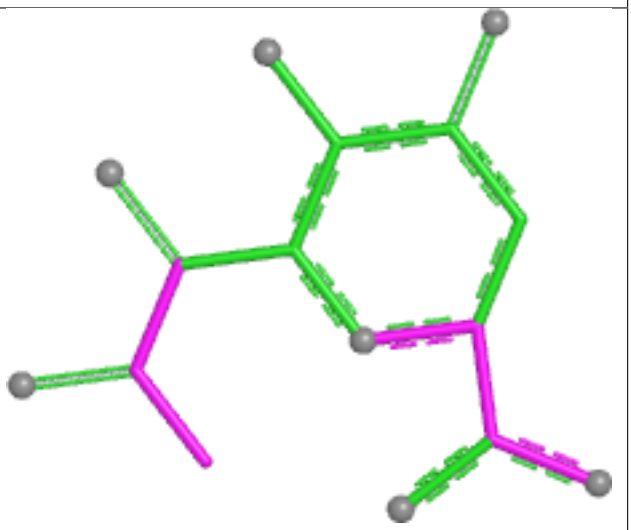


Rings

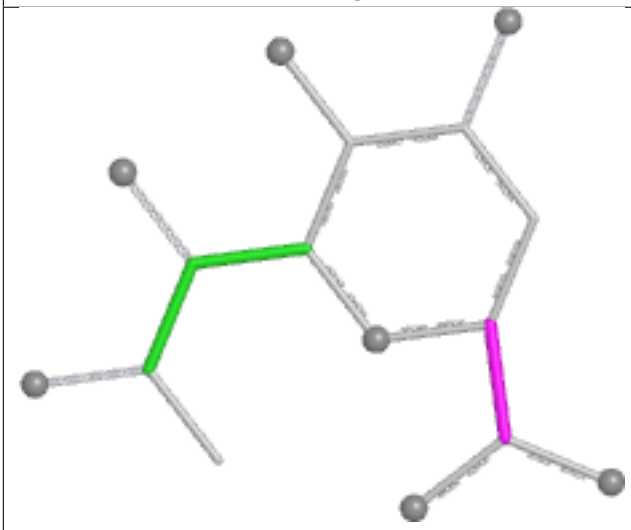
Ligand P8E VR 604



Bond lengths



Bond angles



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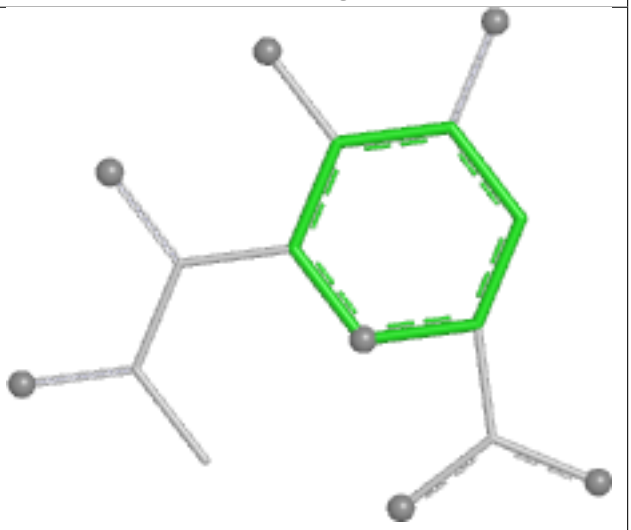
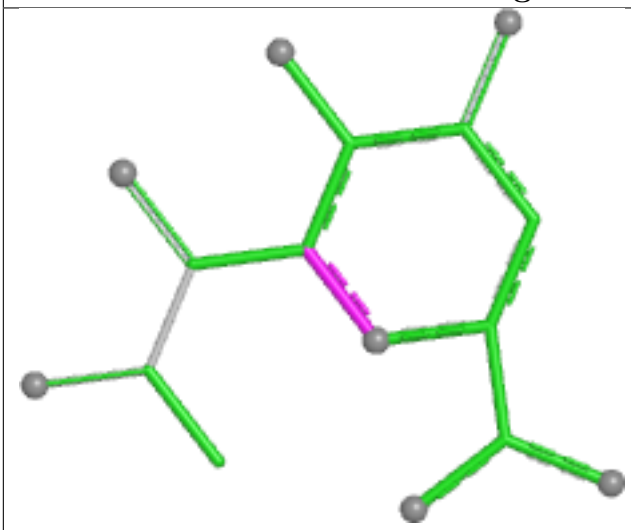


Rings

Ligand P8E UH 601



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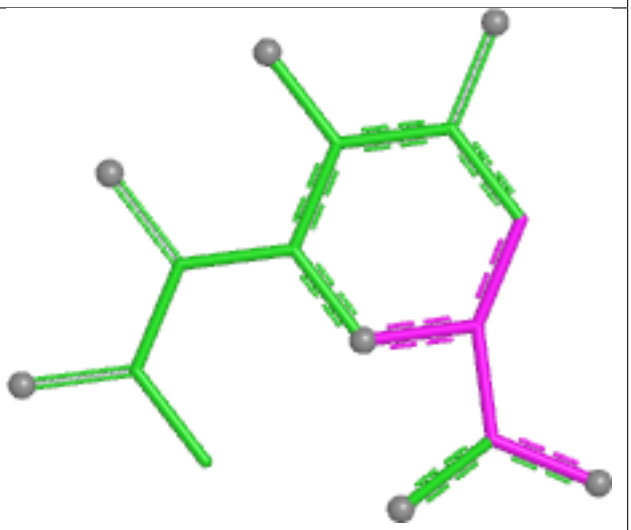
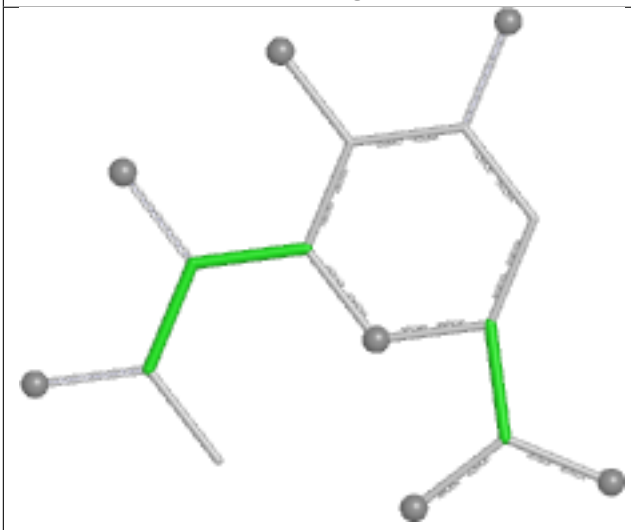


Bond angles



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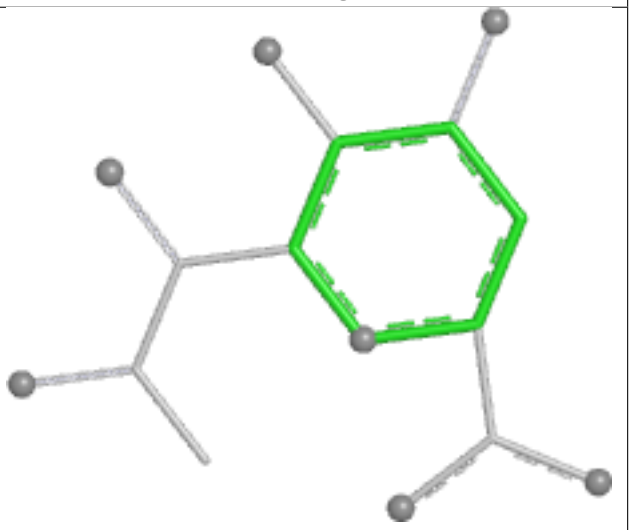
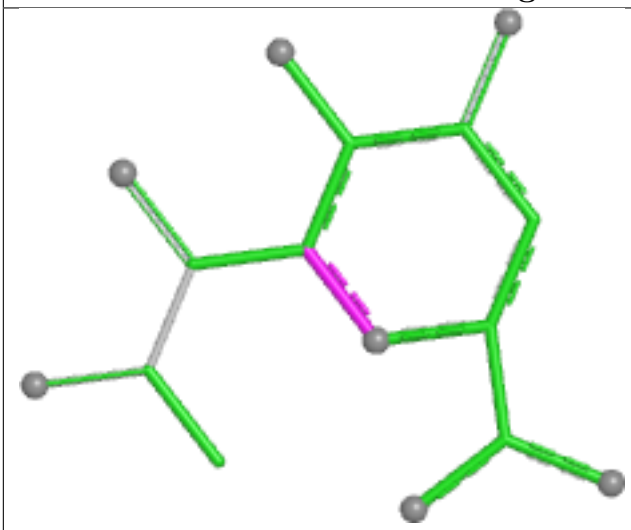


Rings

Ligand P8E JD 601



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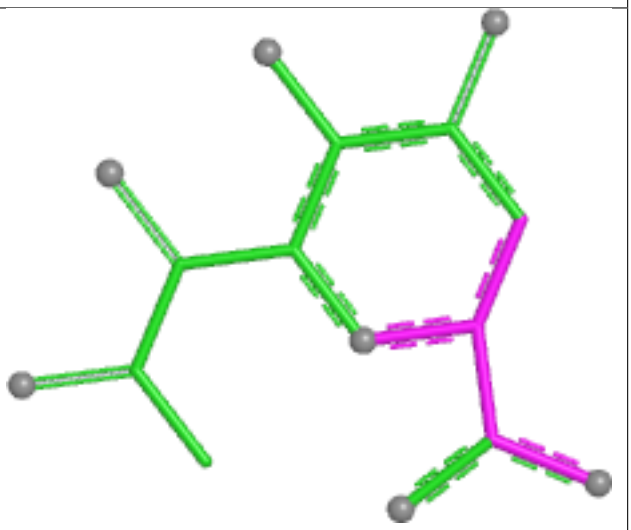

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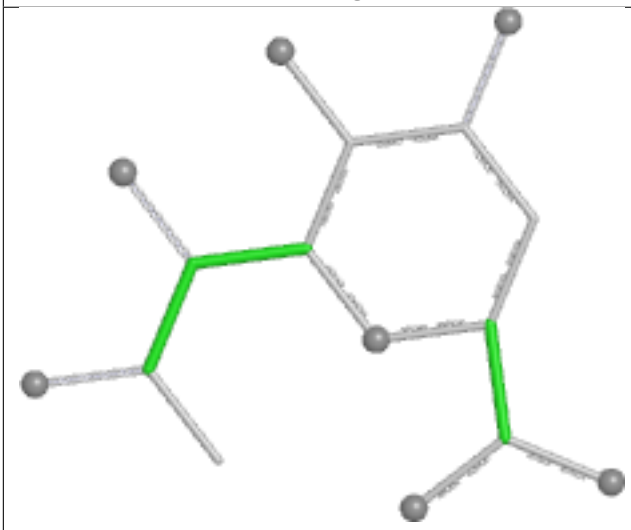

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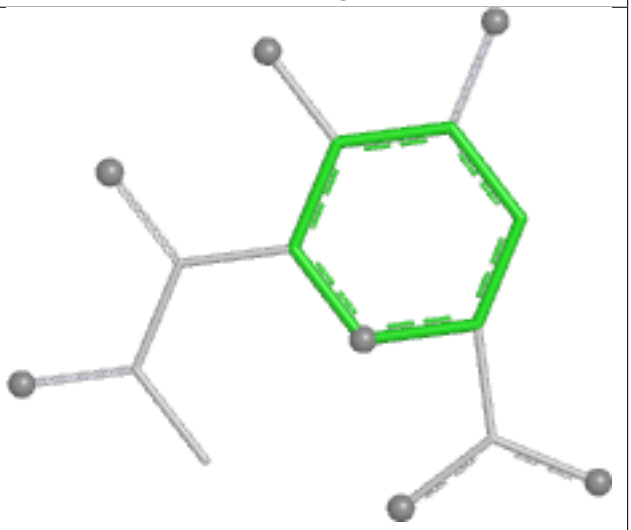
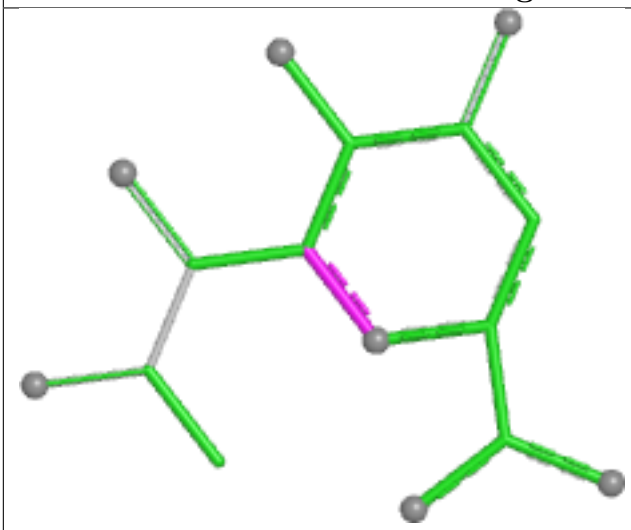


Rings

Ligand P8E CT 601



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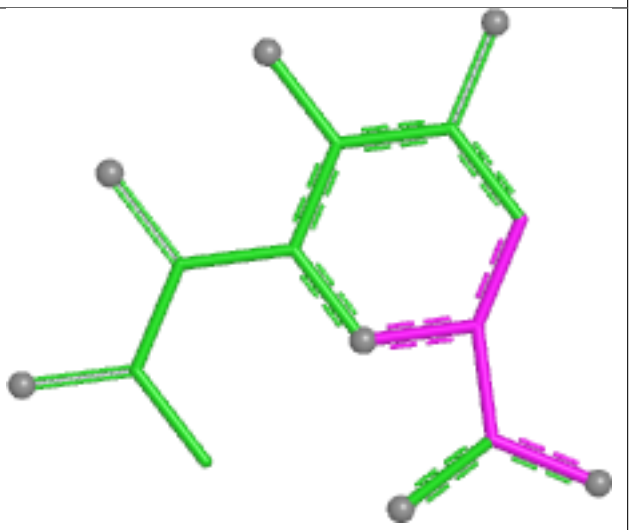

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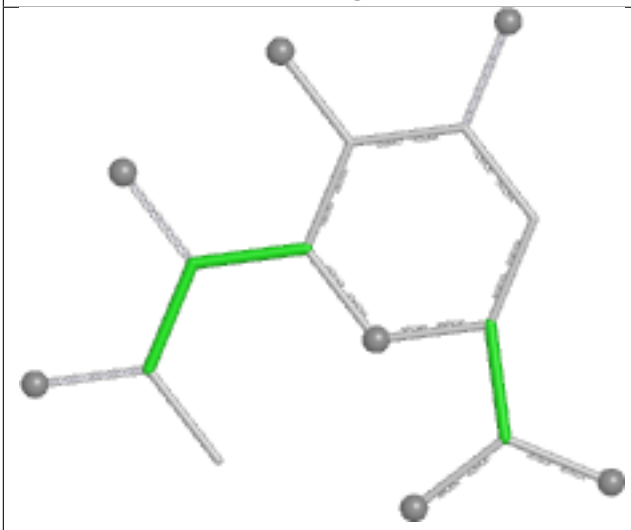

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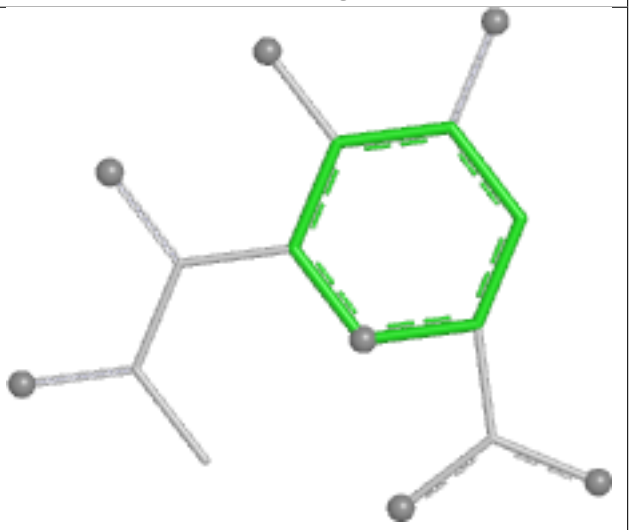
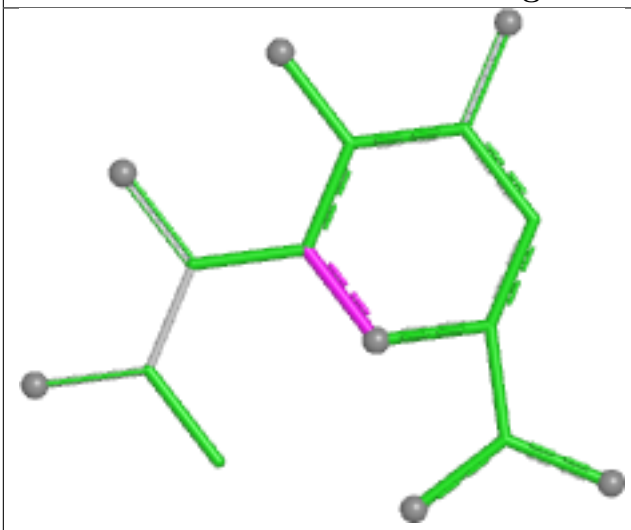


Rings

Ligand P8E S5 606



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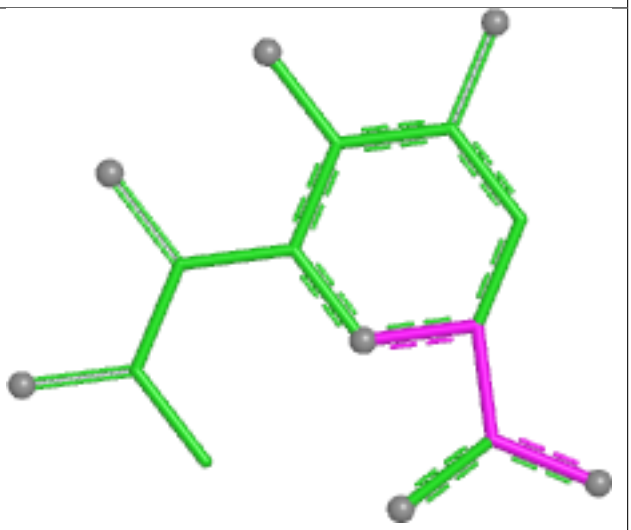

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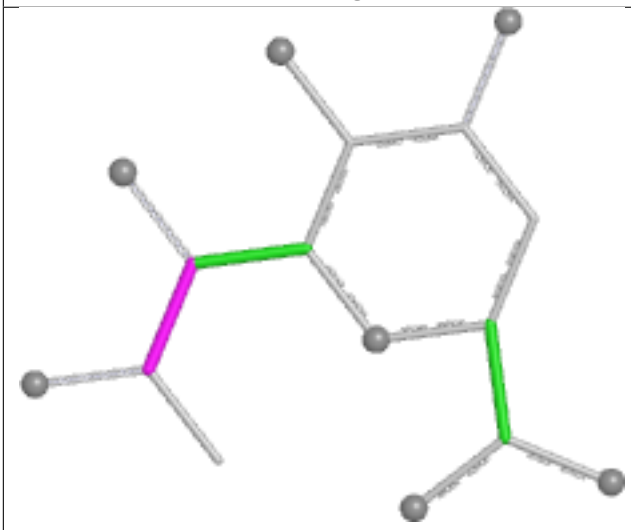

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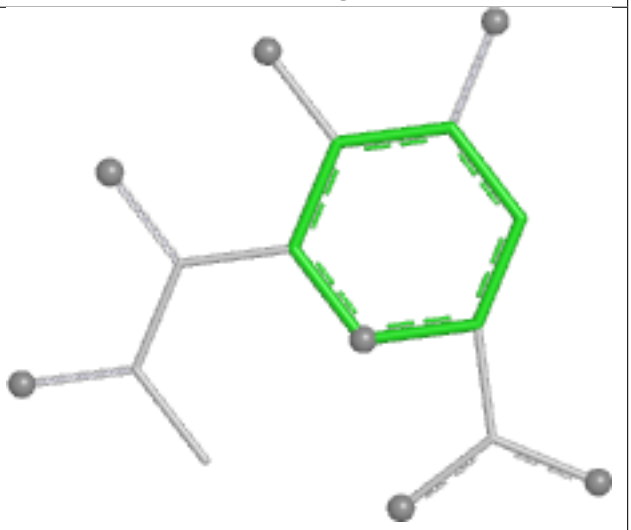
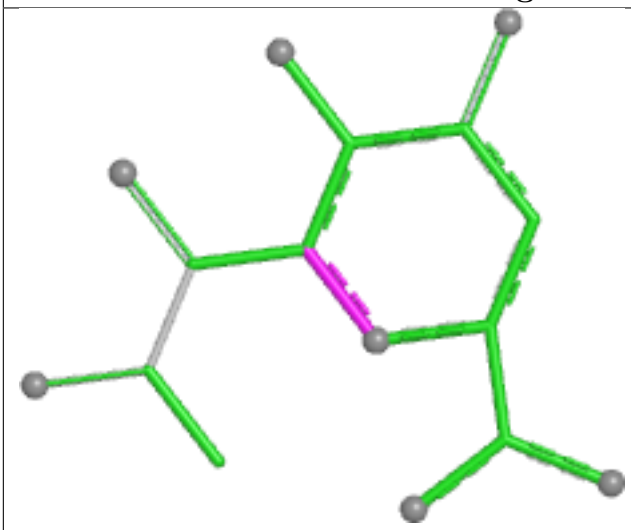


Rings

Ligand P8E EX 605



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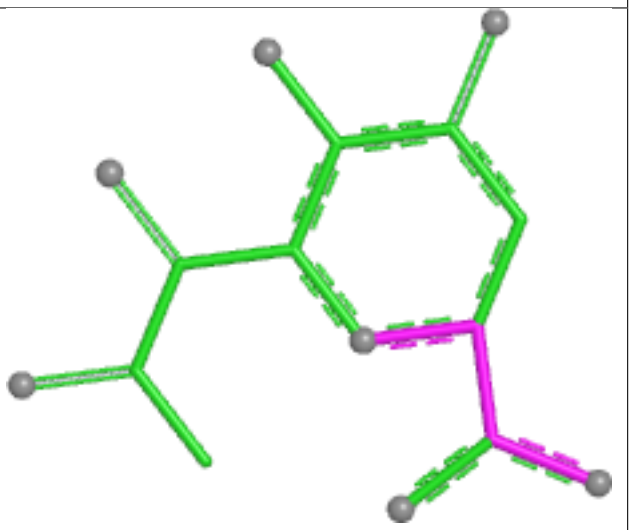
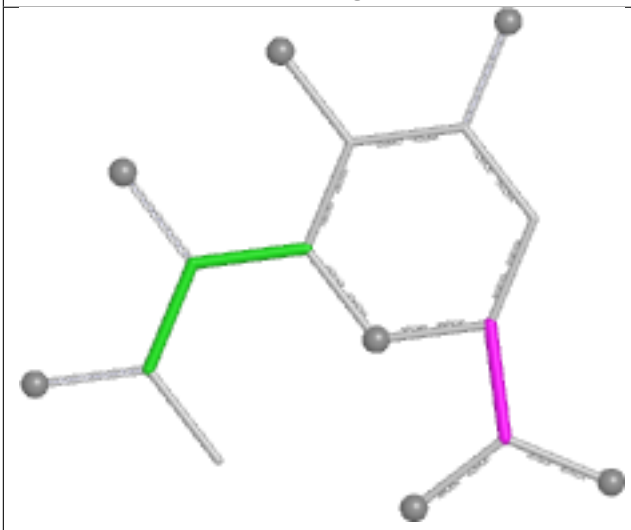


Bond angles



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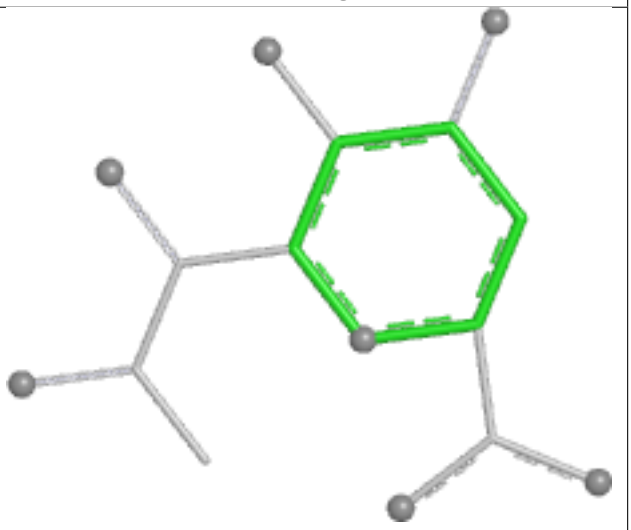
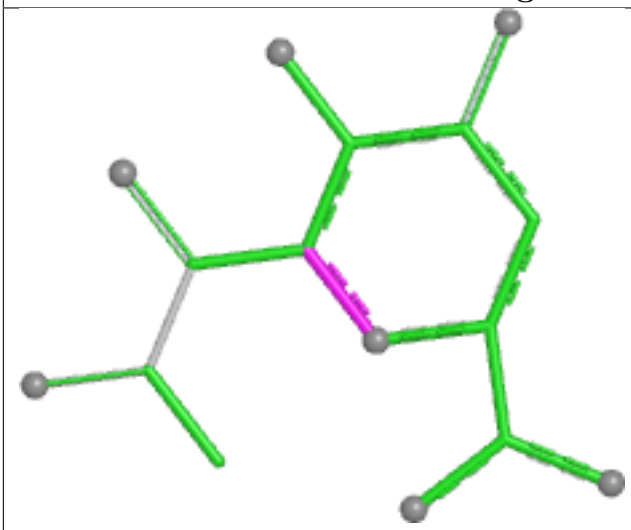


Rings

Ligand P8E TP 603



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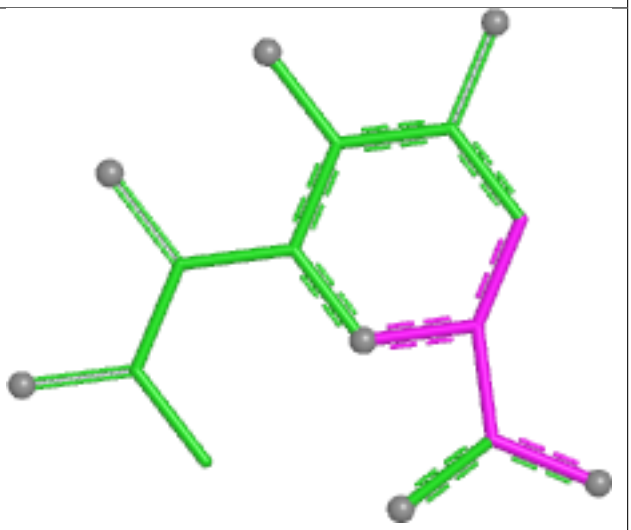
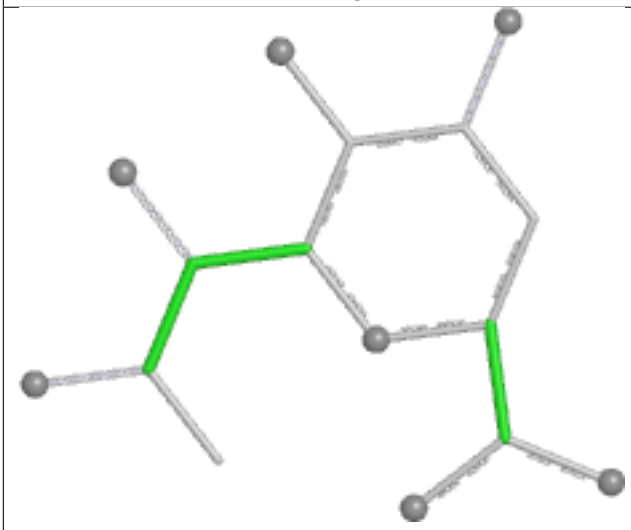


Bond angles



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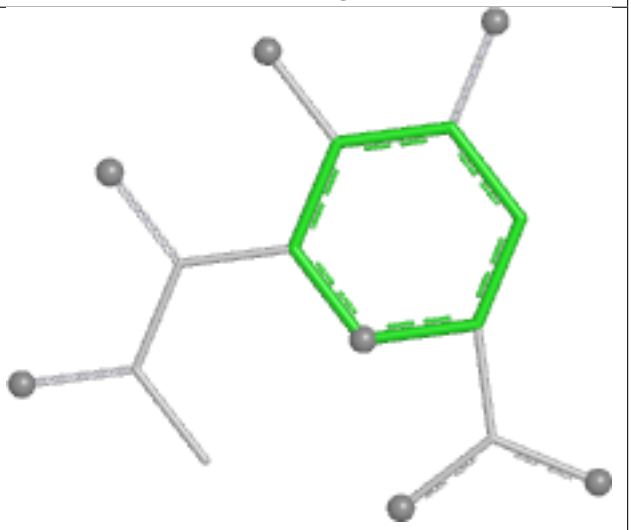
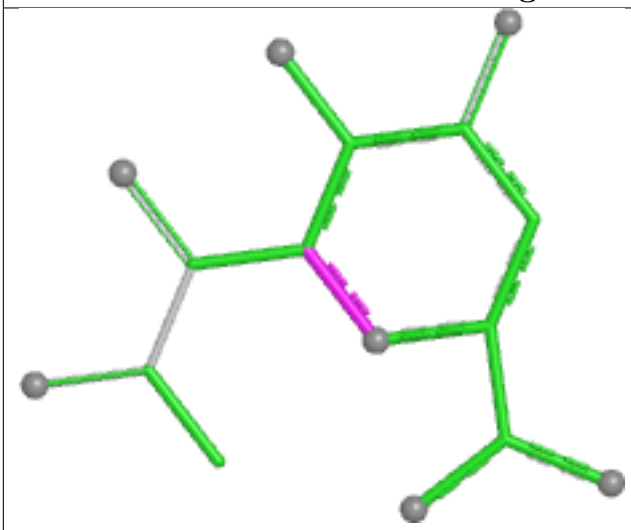


Rings

Ligand P8E A7 605



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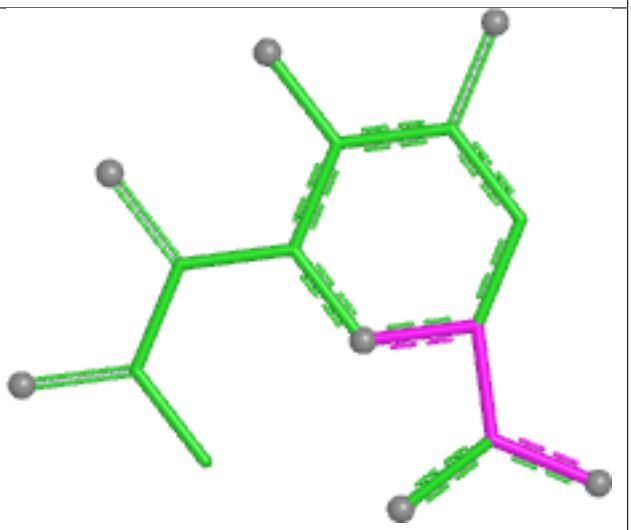
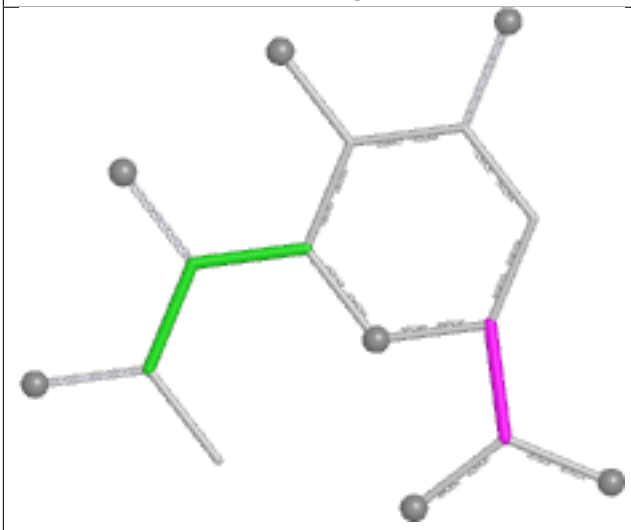


Bond angles



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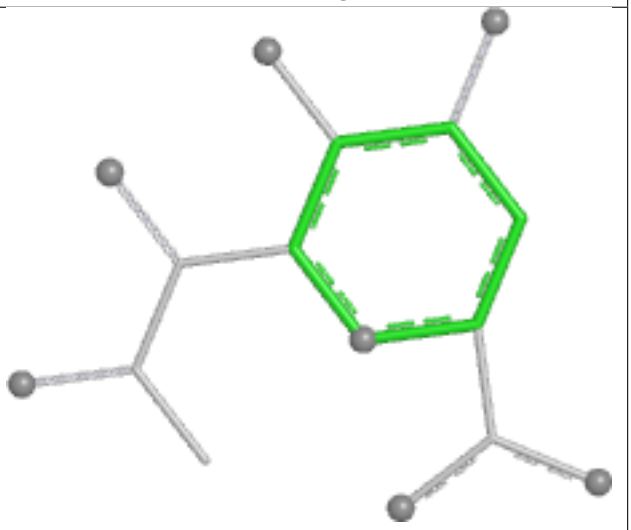
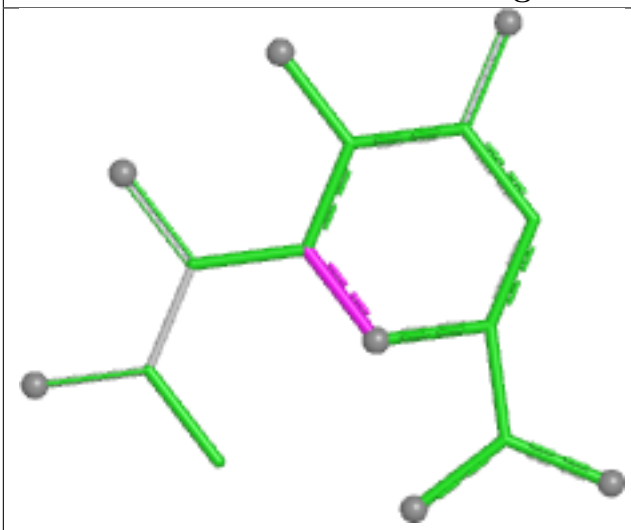


Rings

Ligand P8E DN 601



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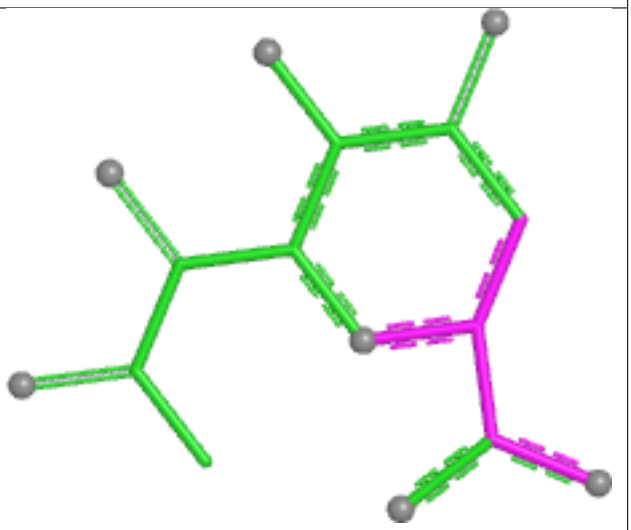

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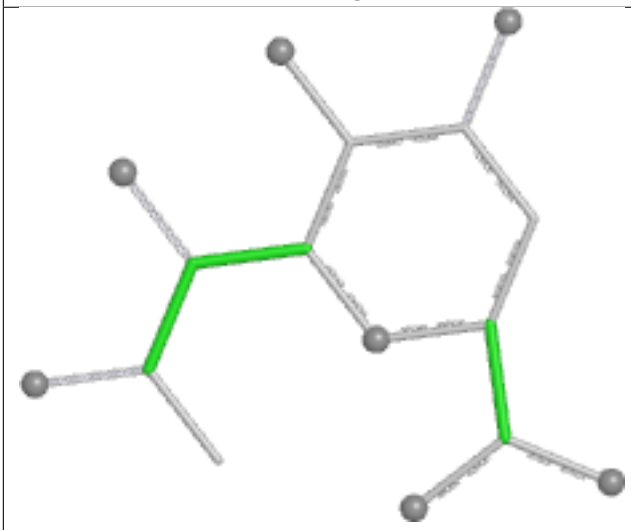

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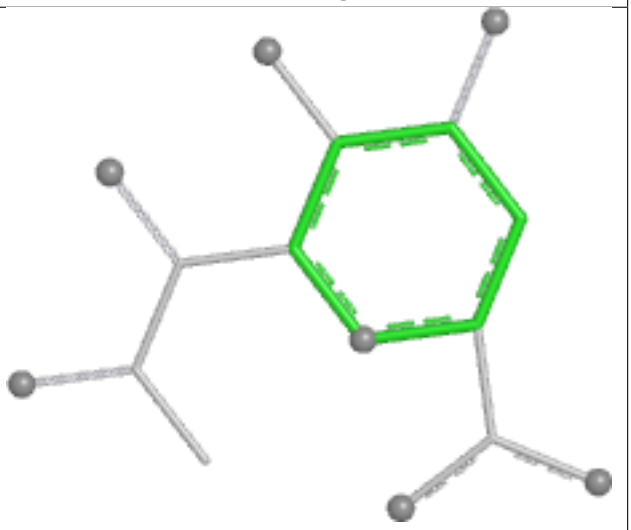
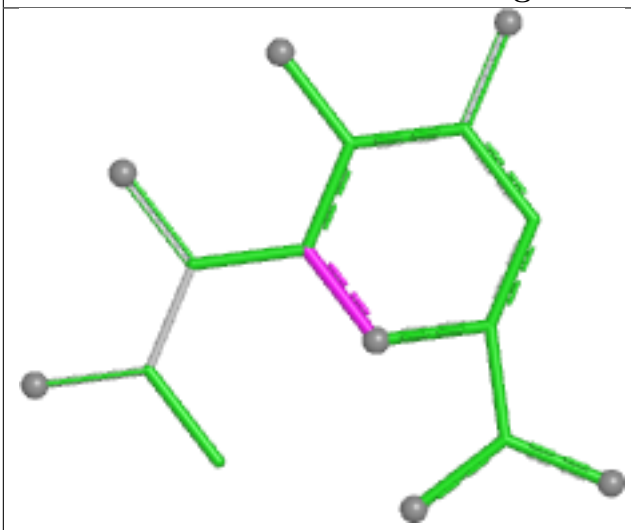


Rings

Ligand P8E DN 605



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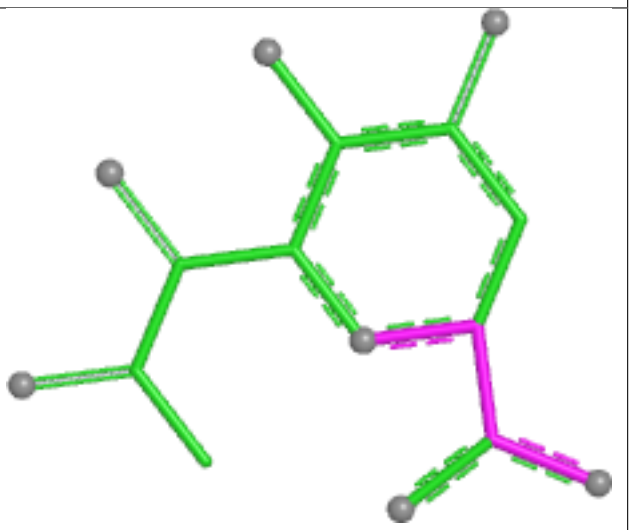

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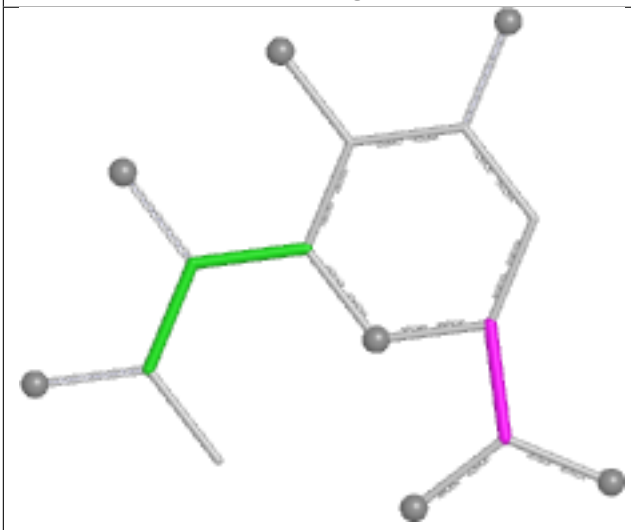

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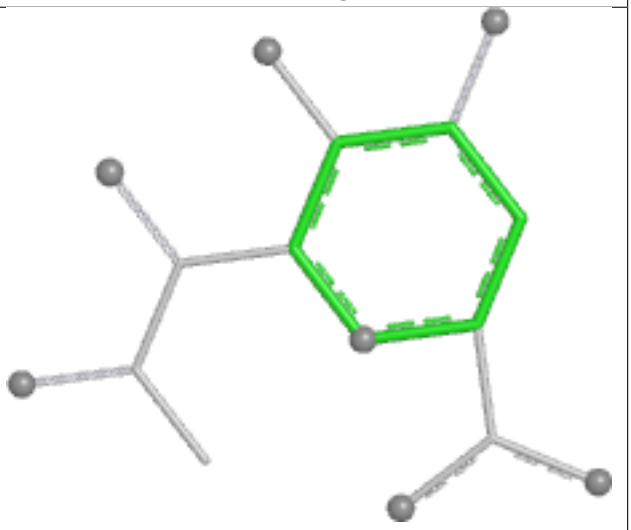
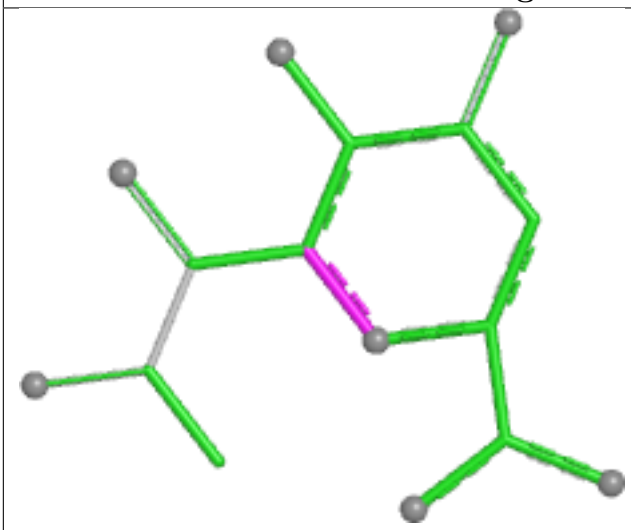


Rings

Ligand P8E TP 607



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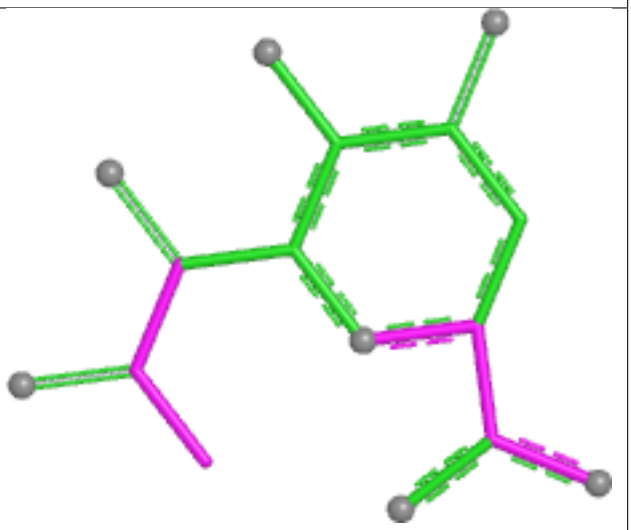

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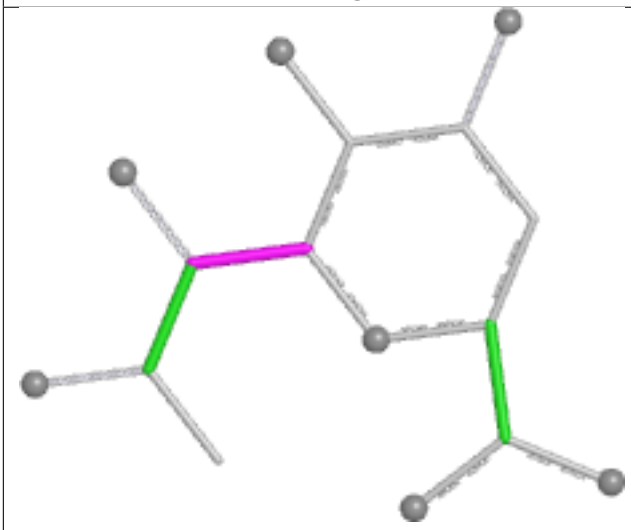

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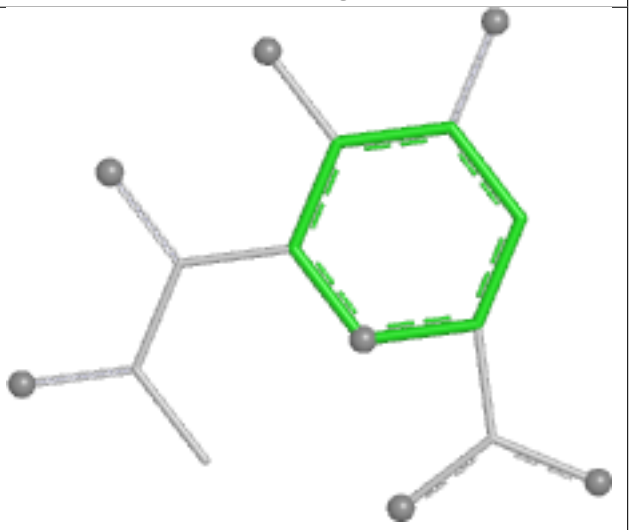
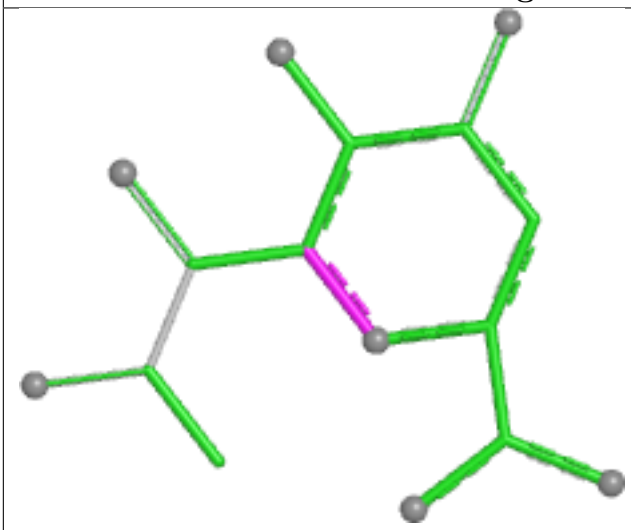


Rings

Ligand P8E HL 604



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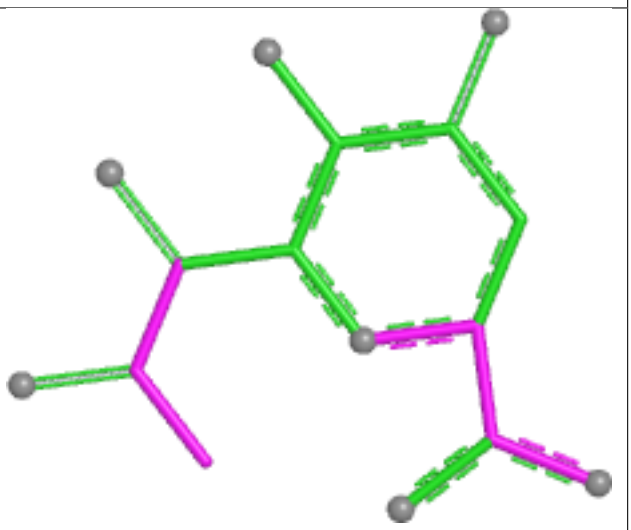
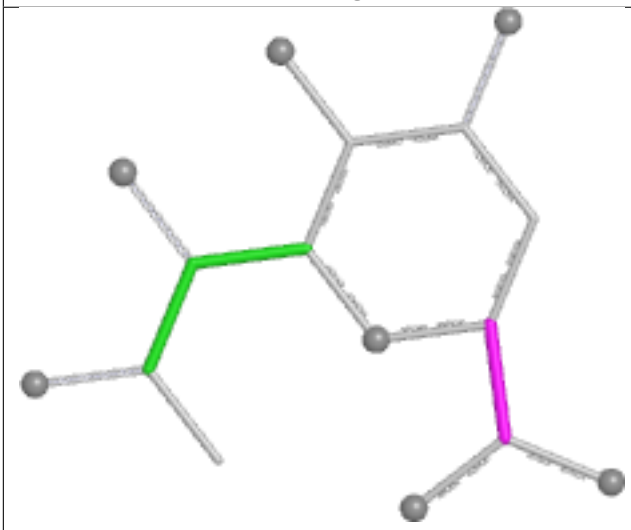


Bond angles



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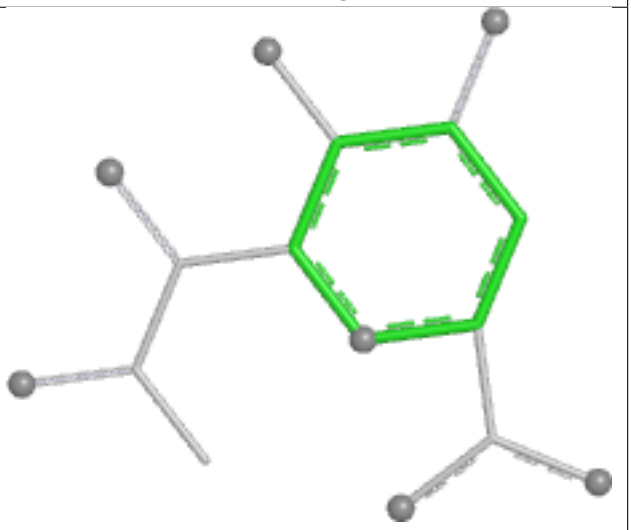
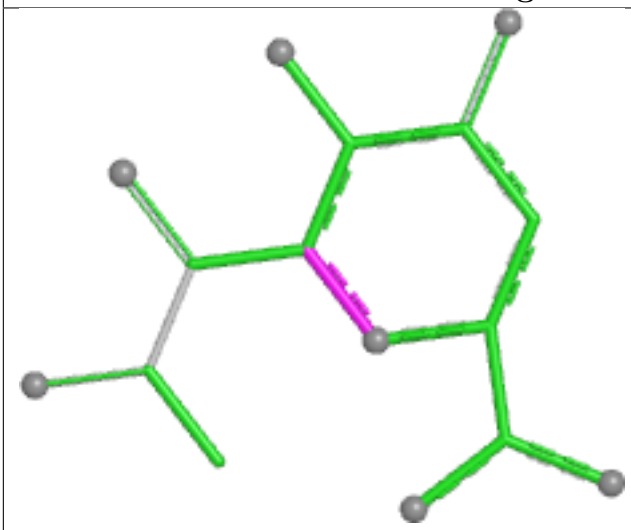


Rings

Ligand P8E TP 604



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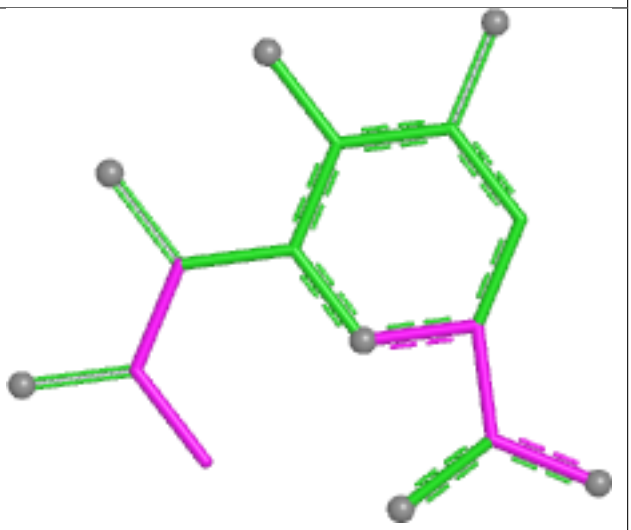
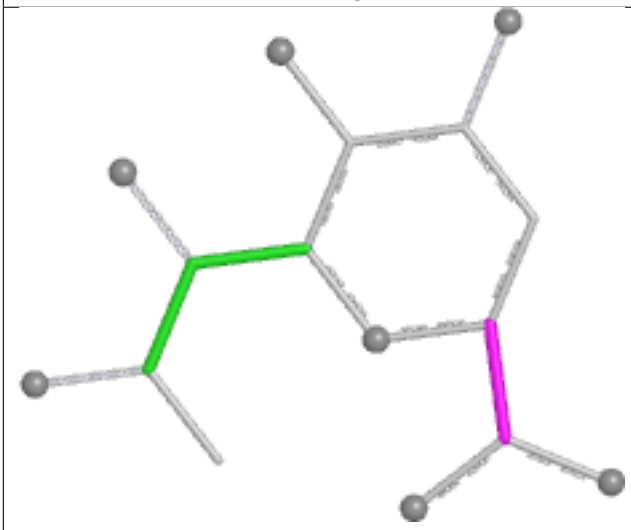
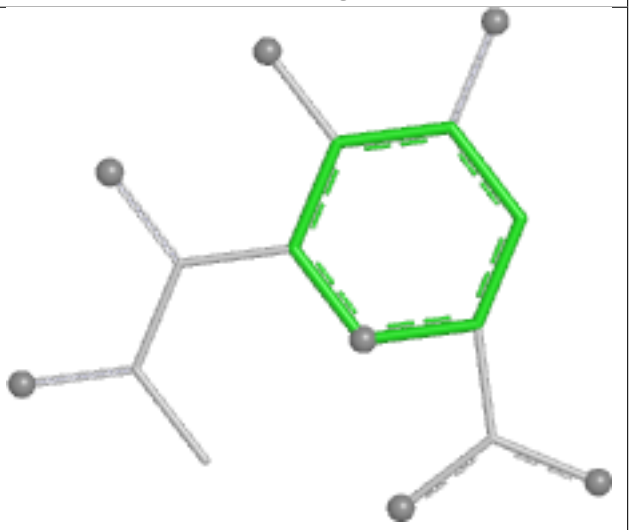


Bond angles

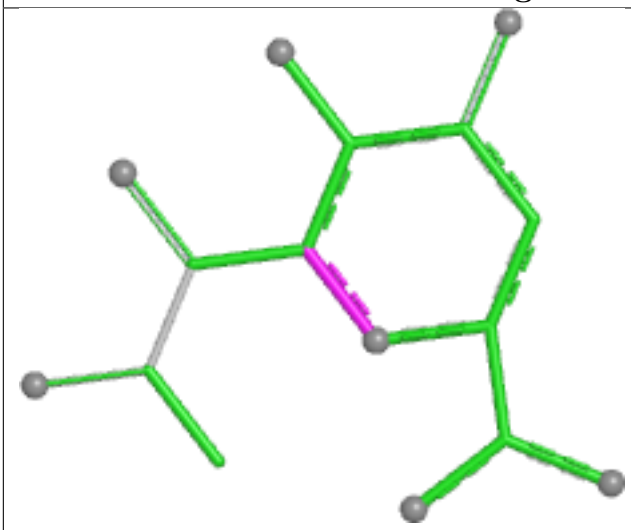


Torsions

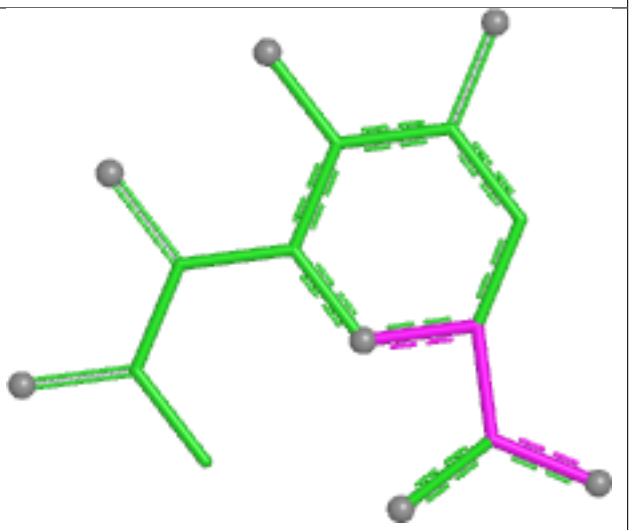


Rings

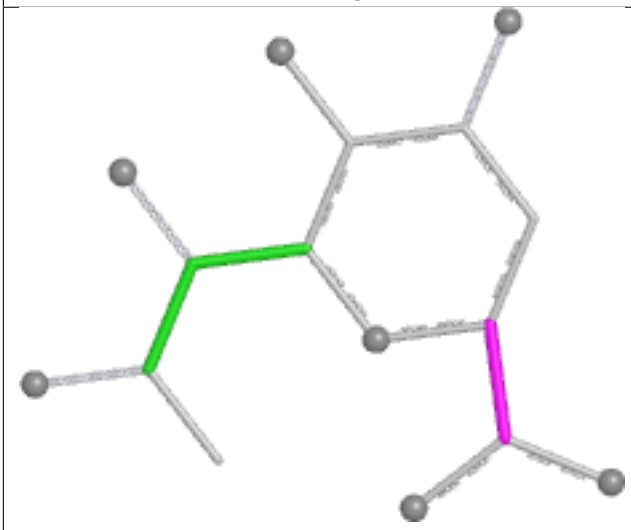
Ligand P8E VR 605



Bond lengths



Bond angles



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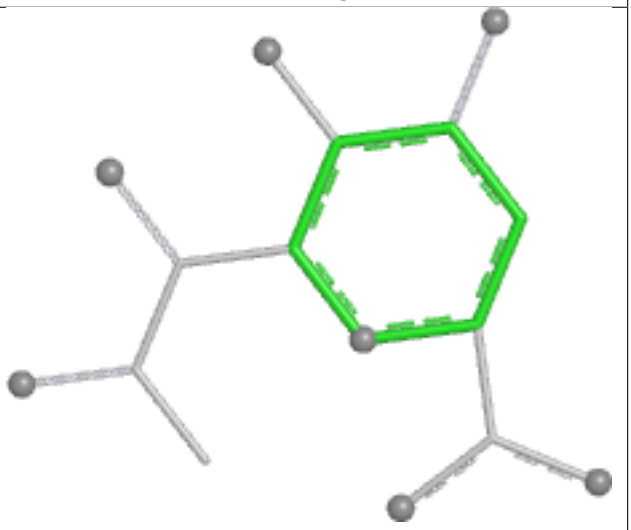
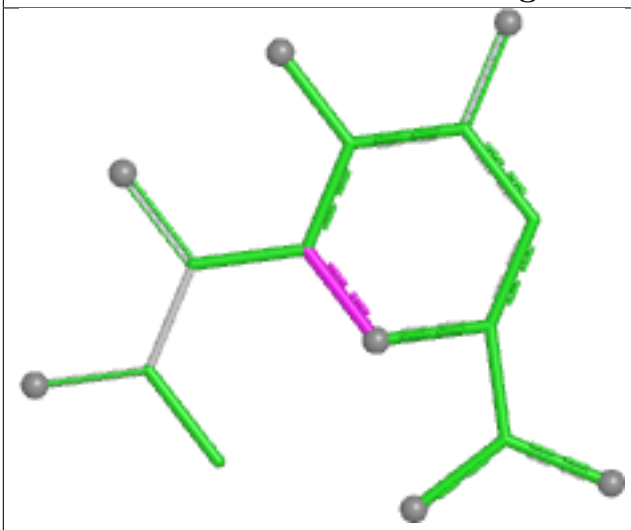


Rings

Ligand P8E Q2 604



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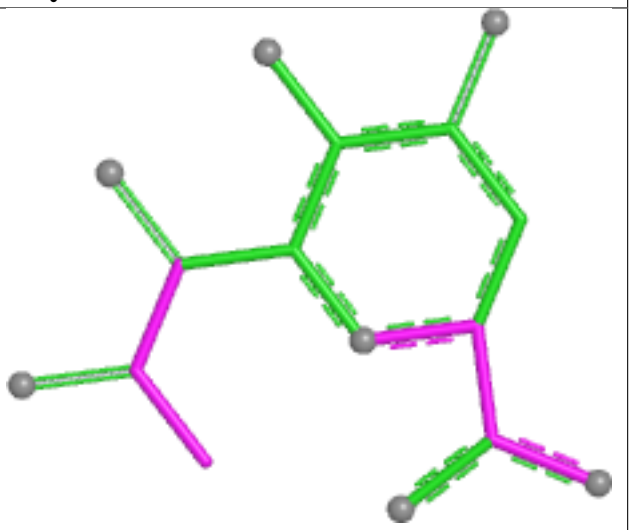

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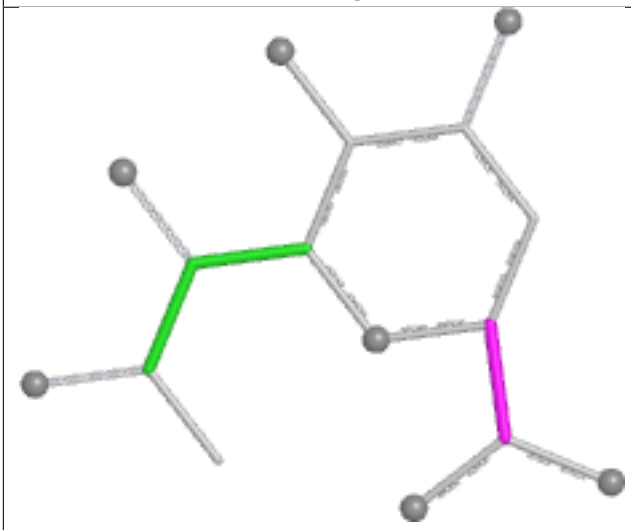

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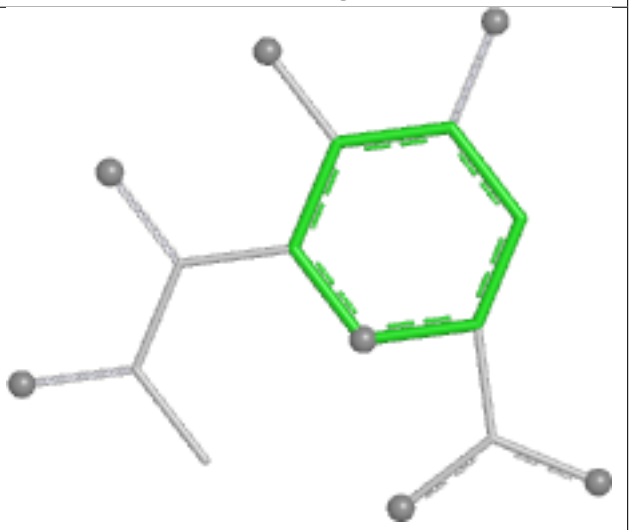
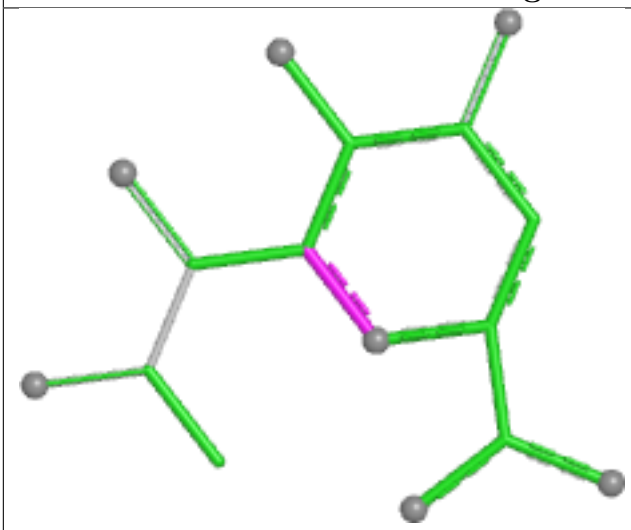


Rings

Ligand P8E g6 607



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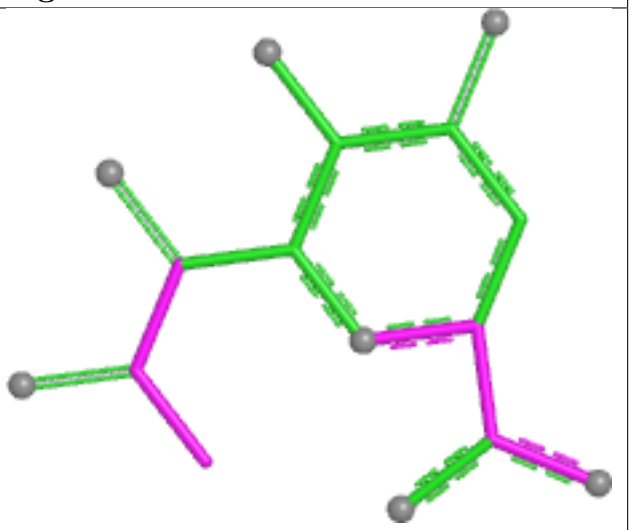
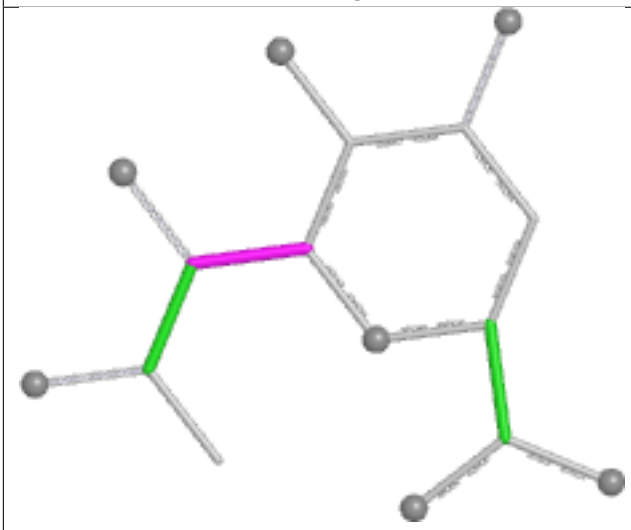


Bond angles



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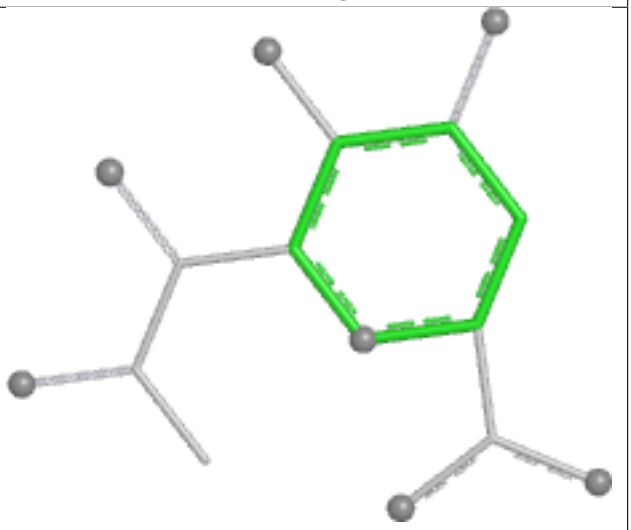
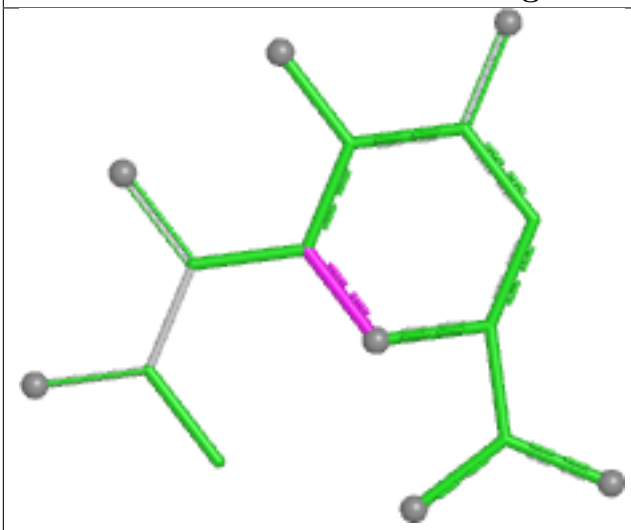


Rings

Ligand P8E fK 601



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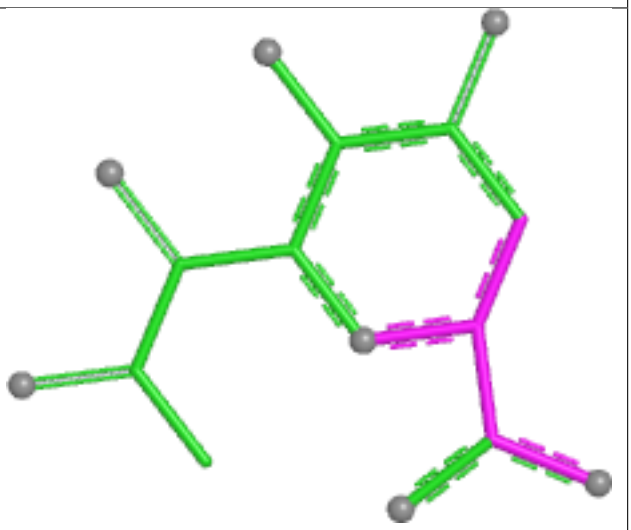
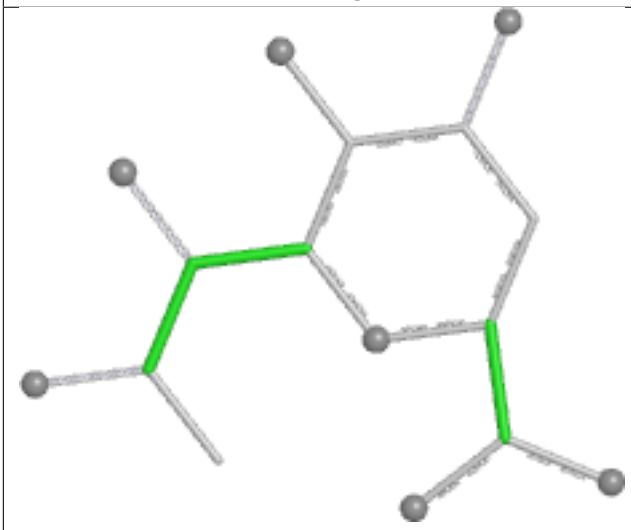


Bond angles



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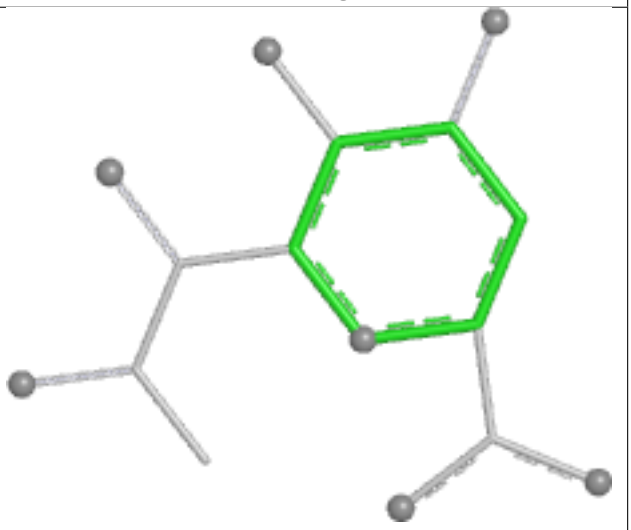
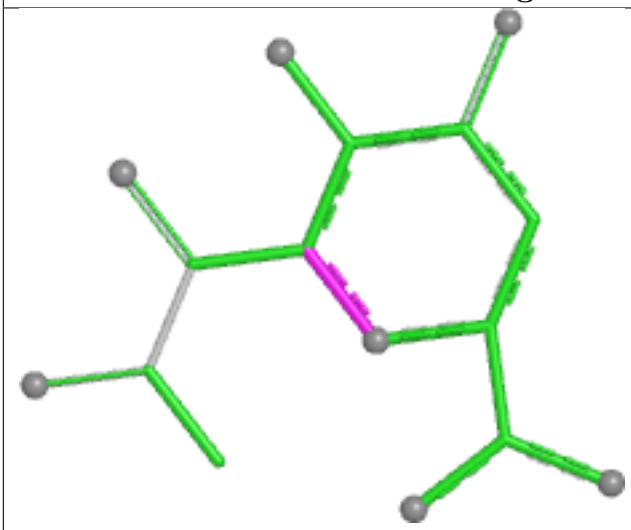


Rings

Ligand P8E EX 601



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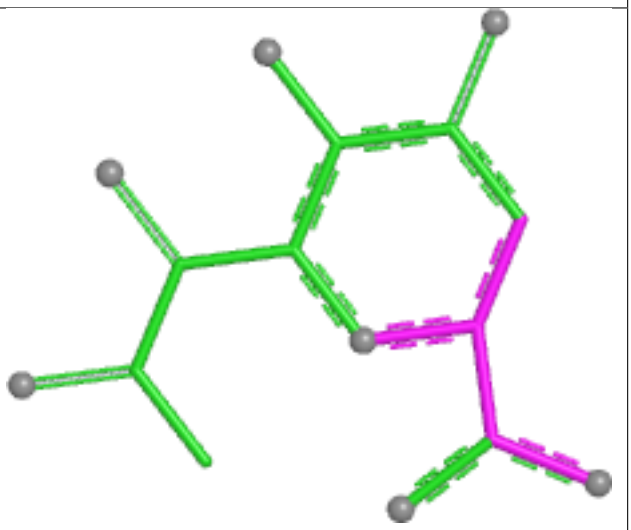

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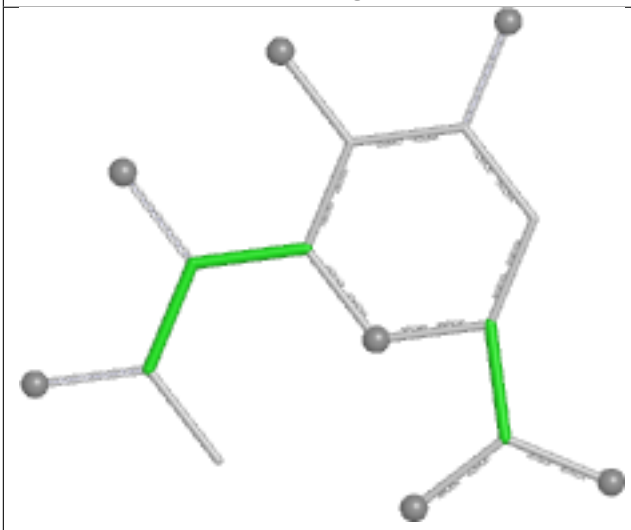

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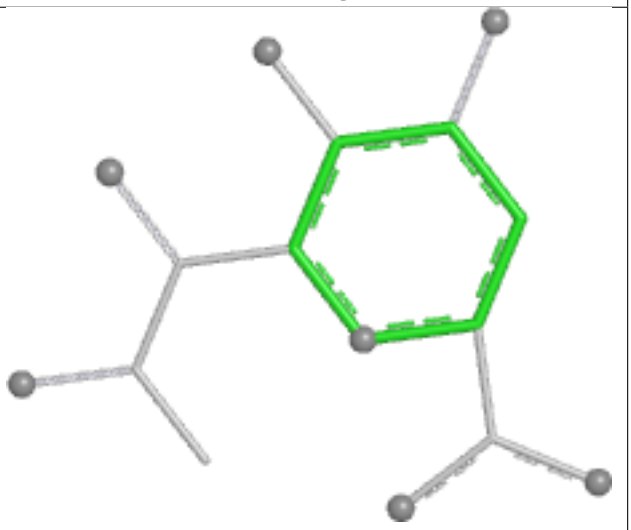
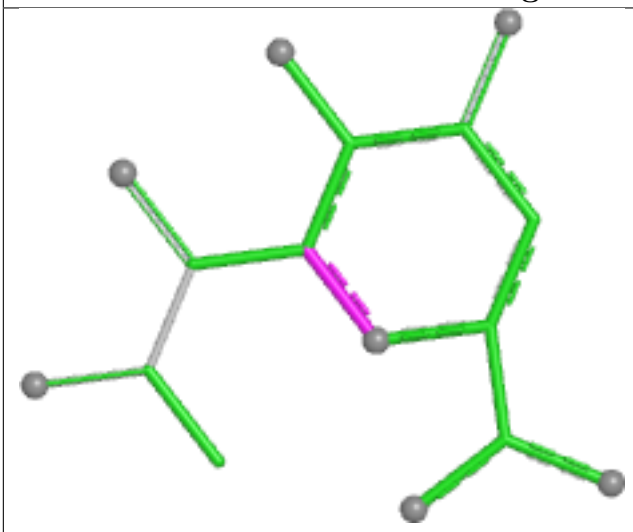


Rings

Ligand P8E Z9 604



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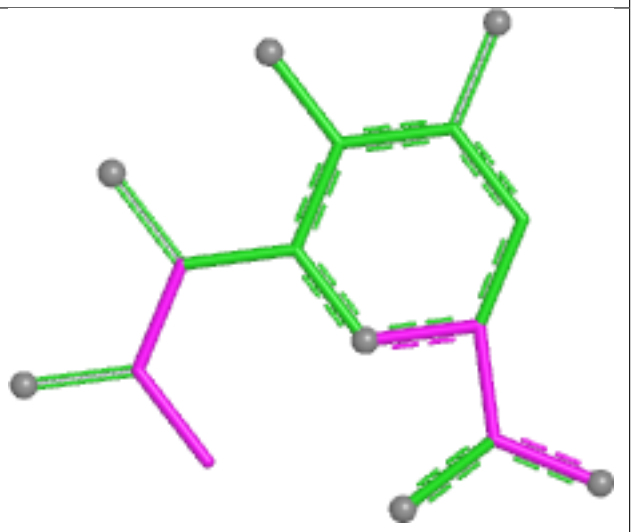

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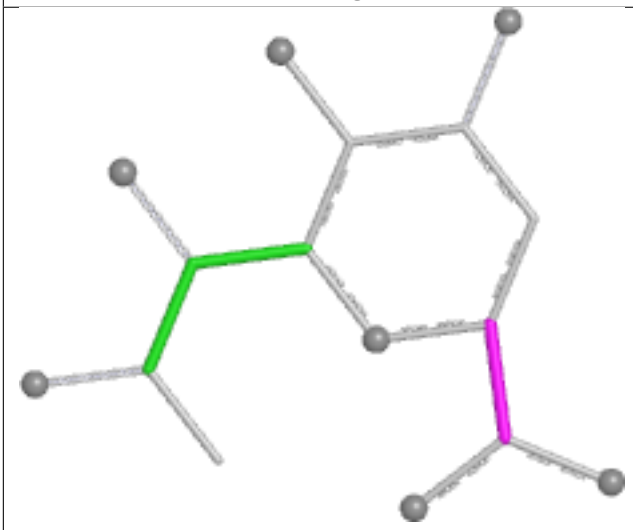

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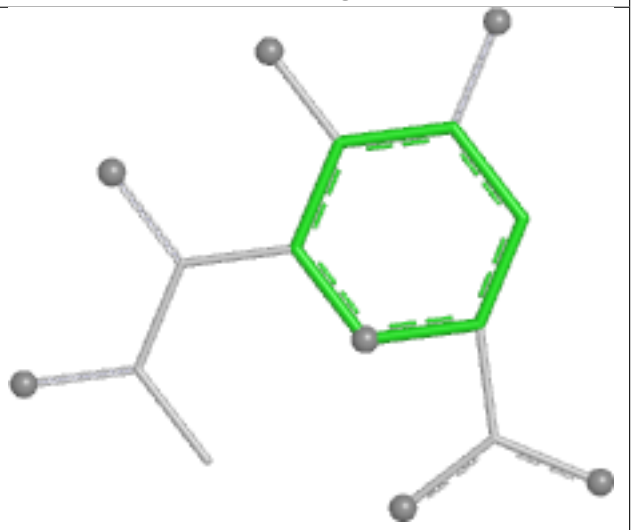
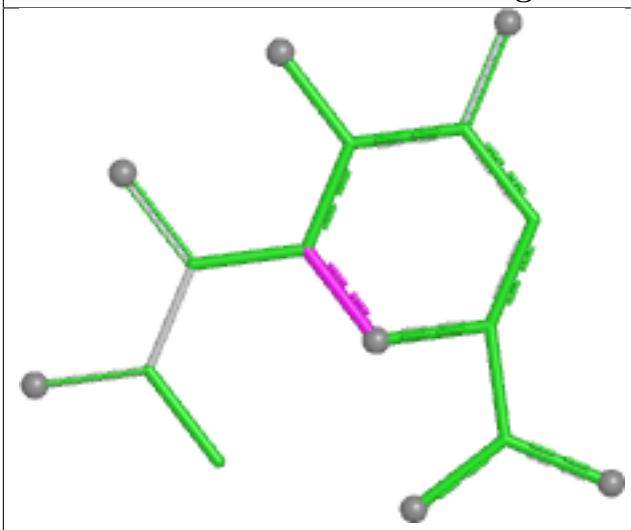


Rings

Ligand P8E OA 606



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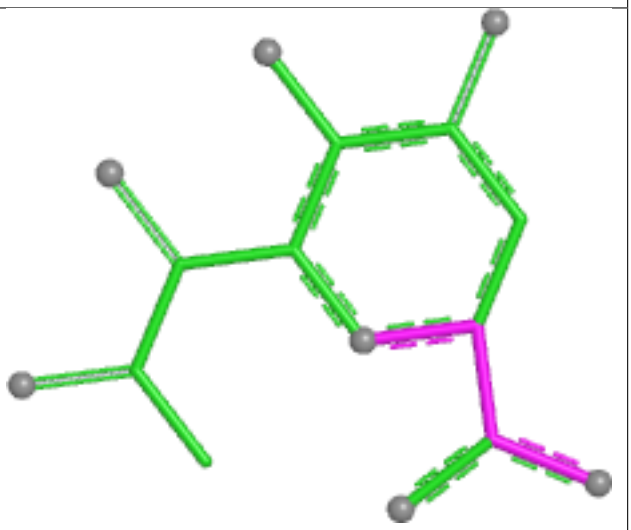

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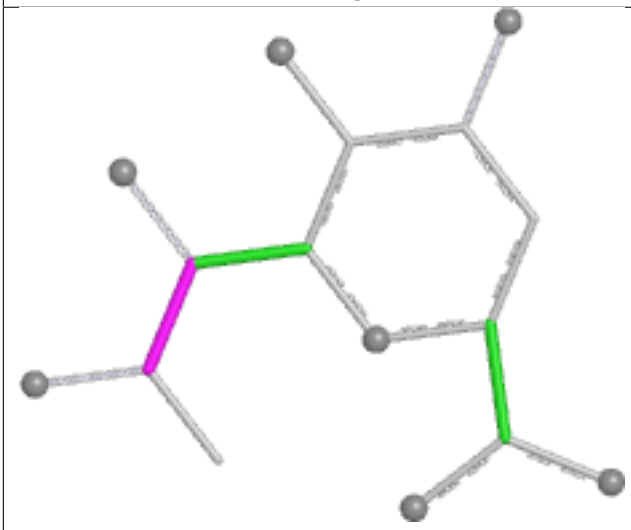

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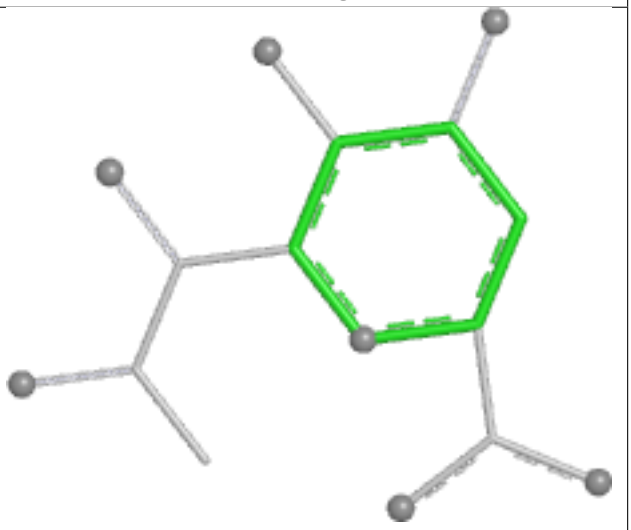
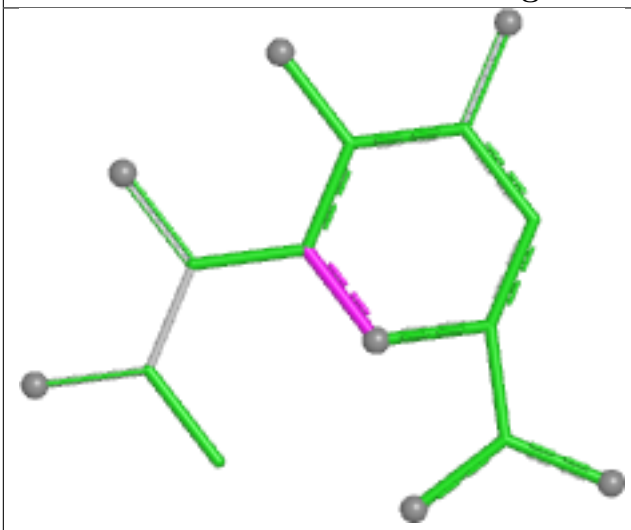


Rings

Ligand P8E bS 606



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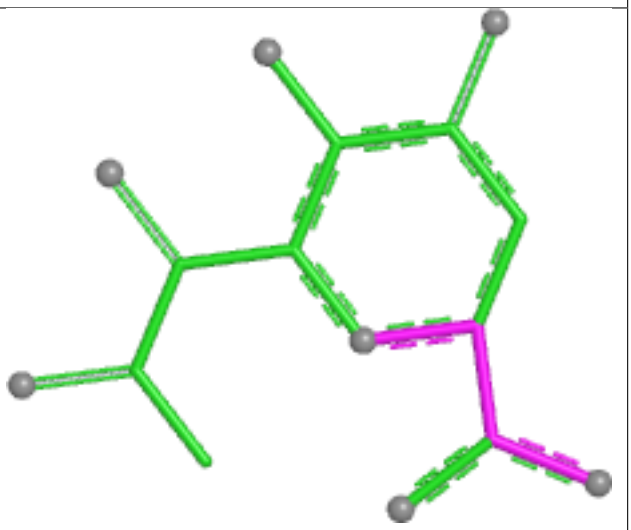

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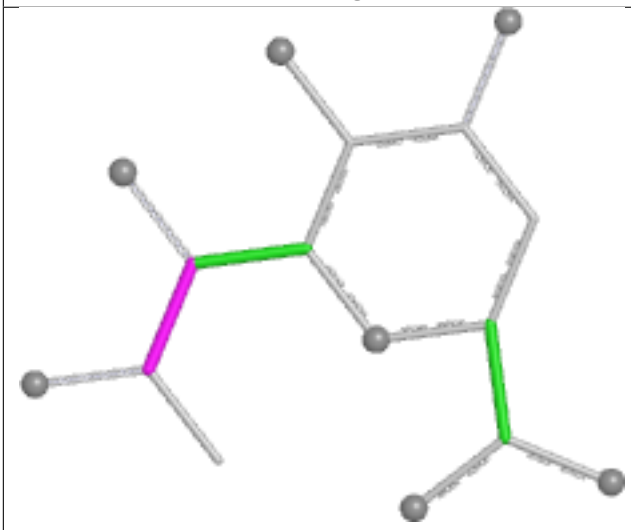

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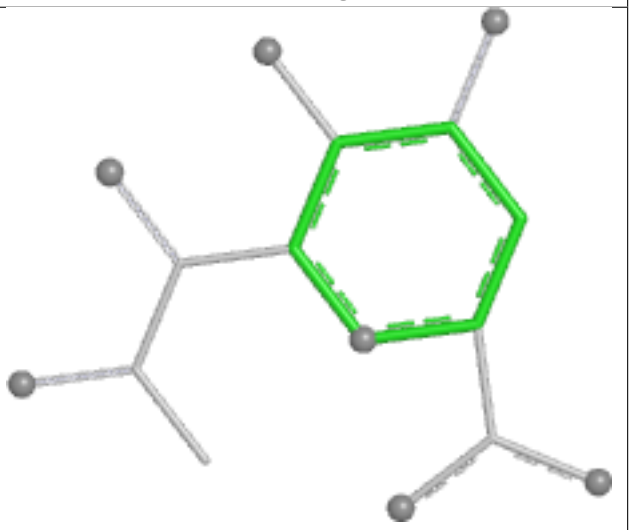
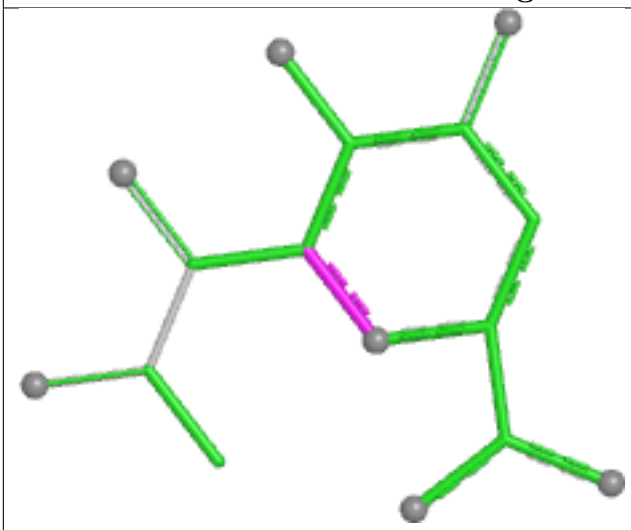


Rings

Ligand P8E HL 606



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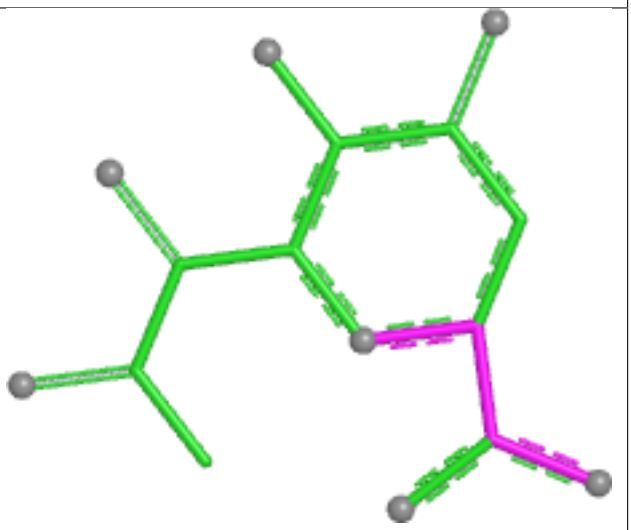

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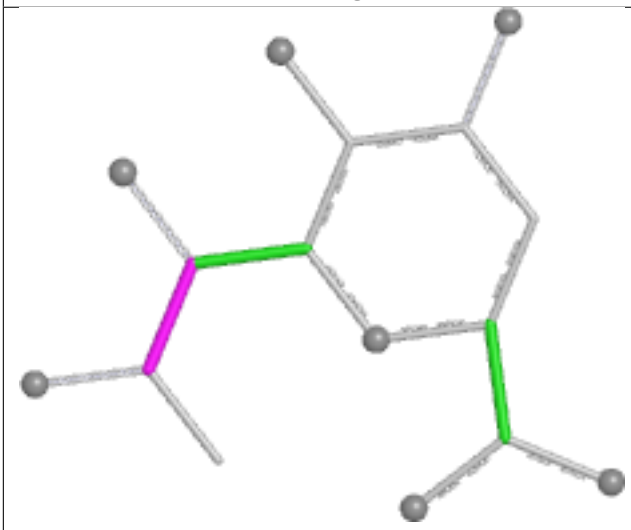

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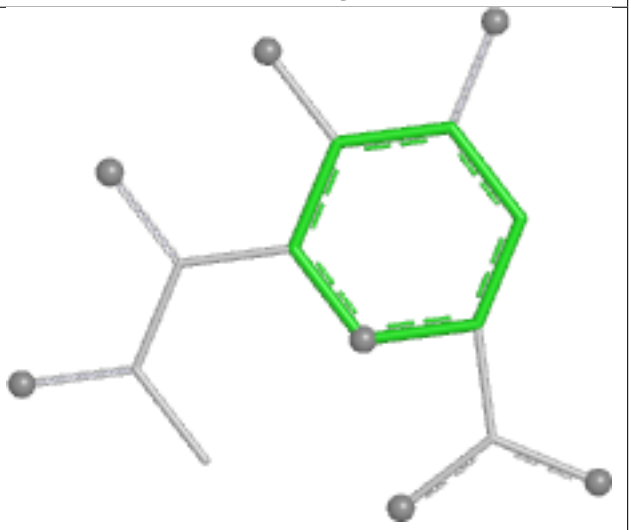
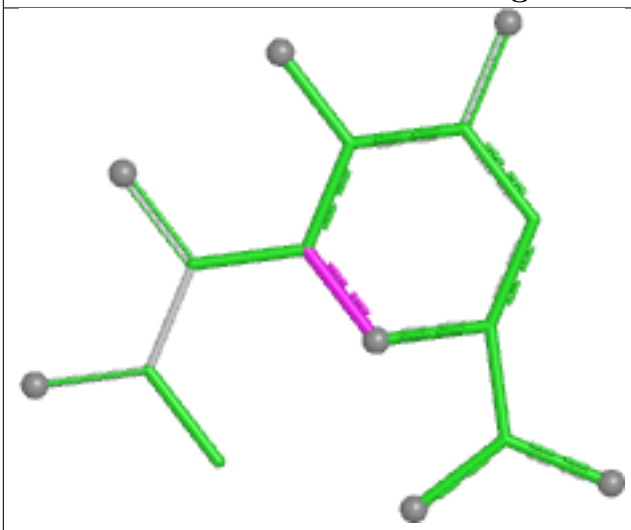


Rings

Ligand P8E XM 604



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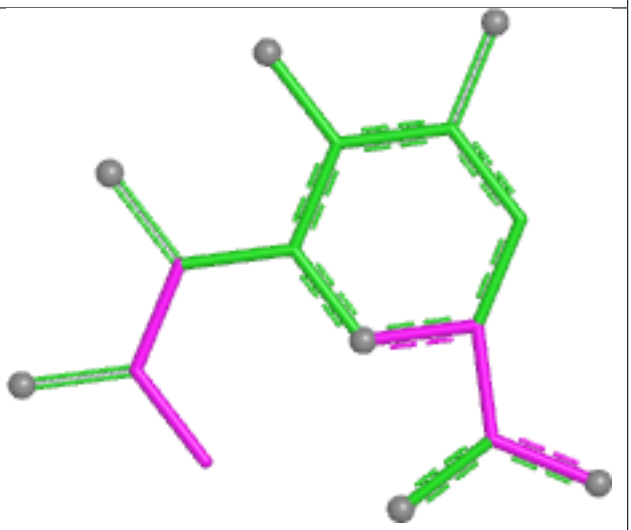

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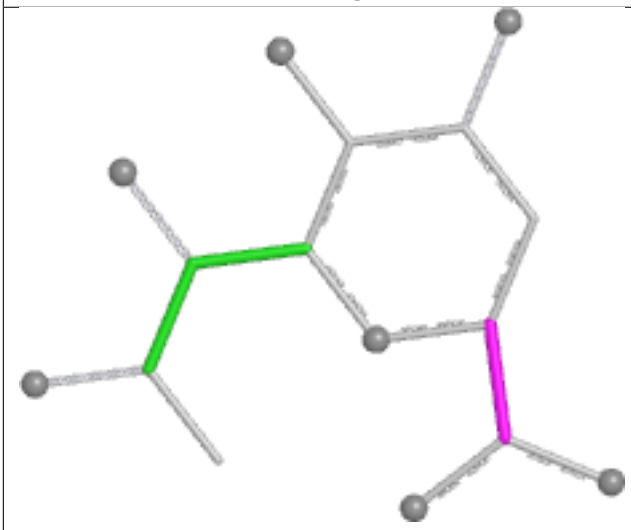

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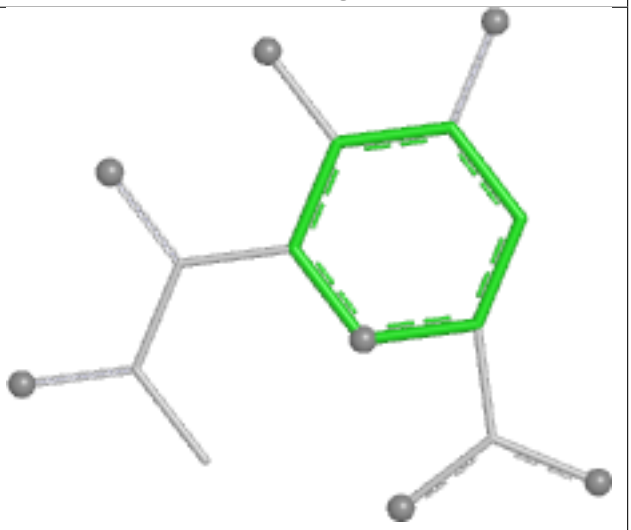
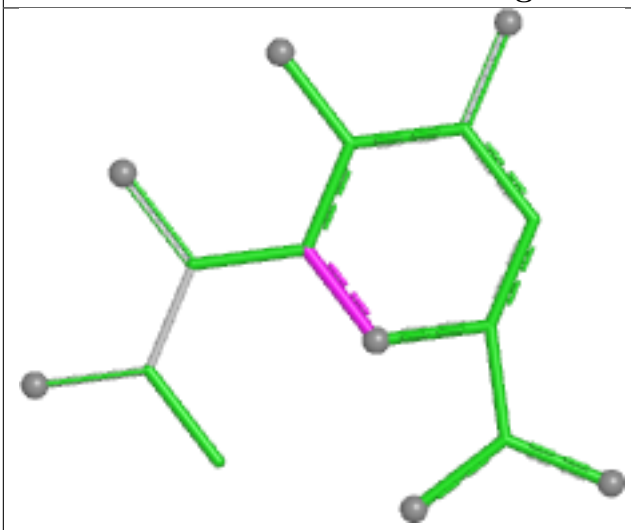


Rings

Ligand P8E PU 606



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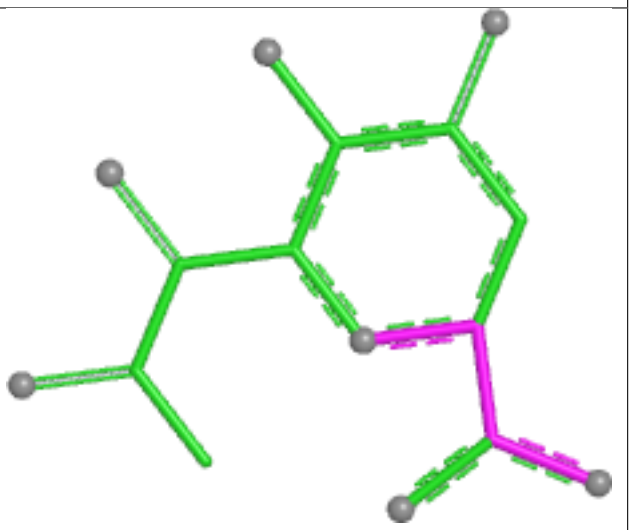

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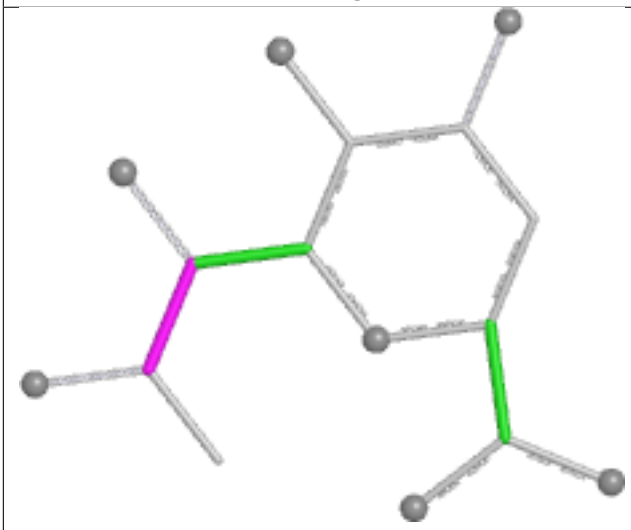

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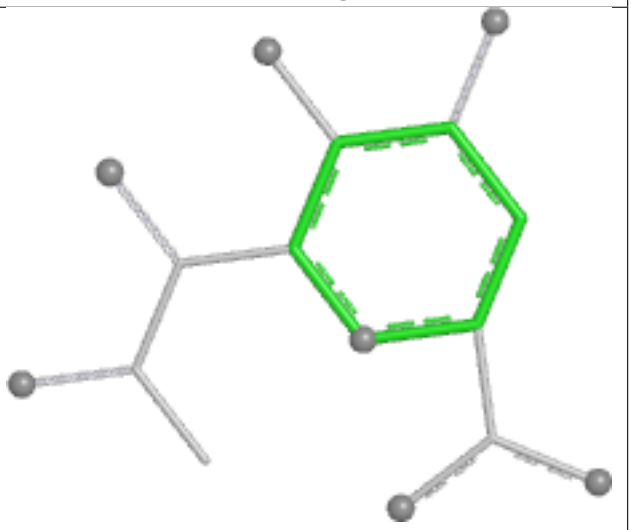
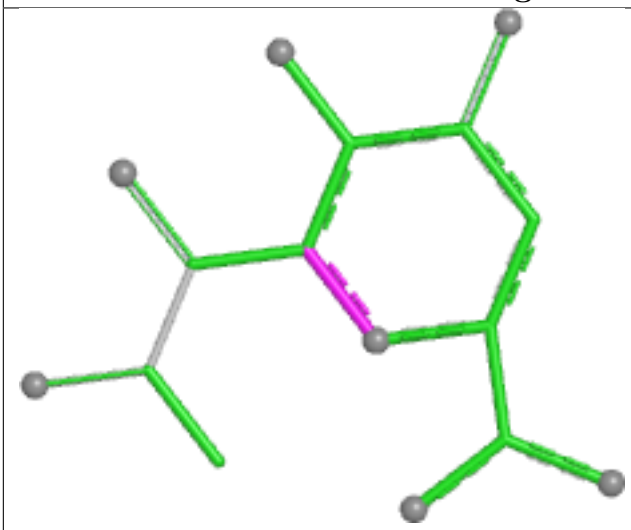


Rings

Ligand P8E aW 601



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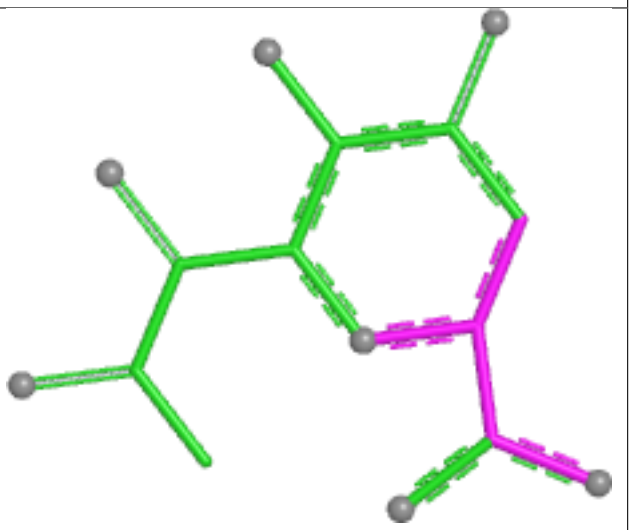
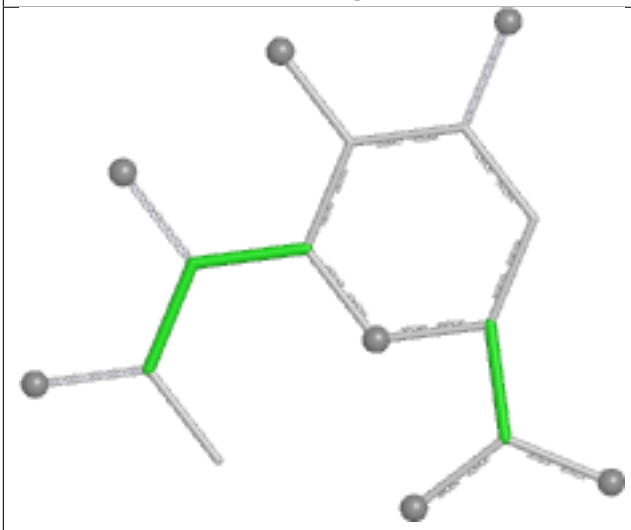


Bond angles



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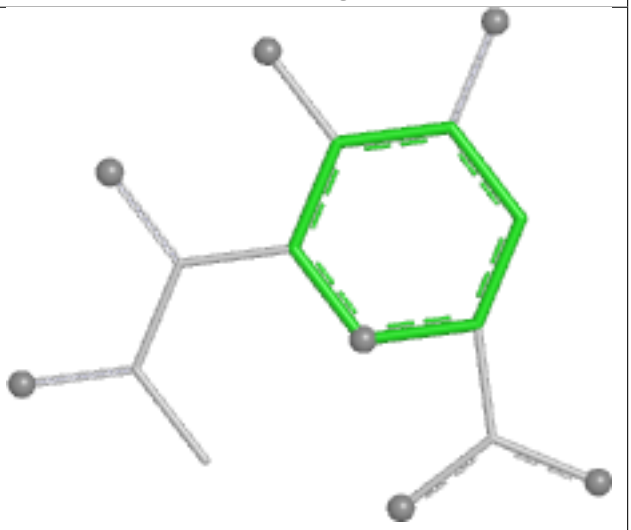
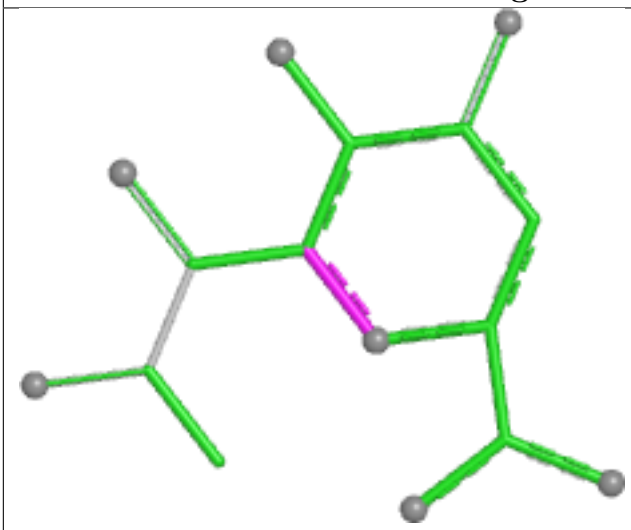


Rings

Ligand P8E MO 601



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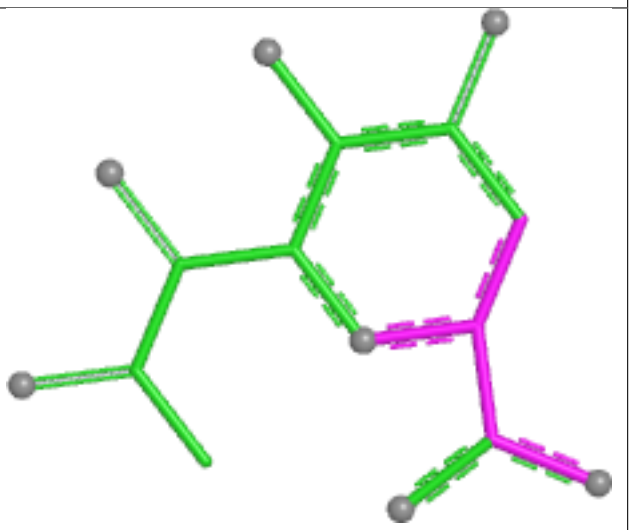
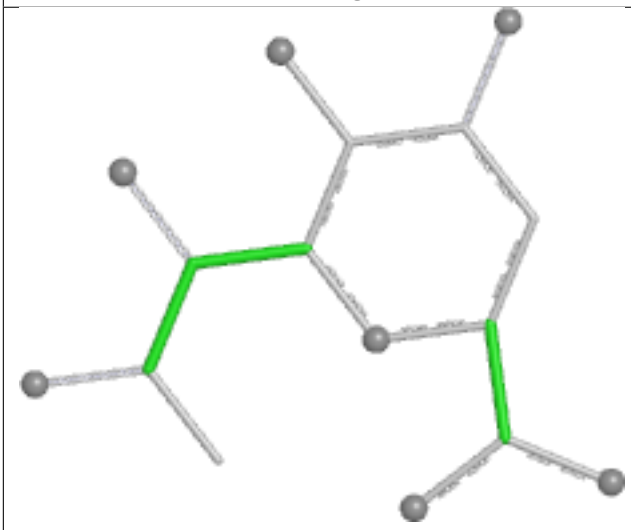


Bond angles



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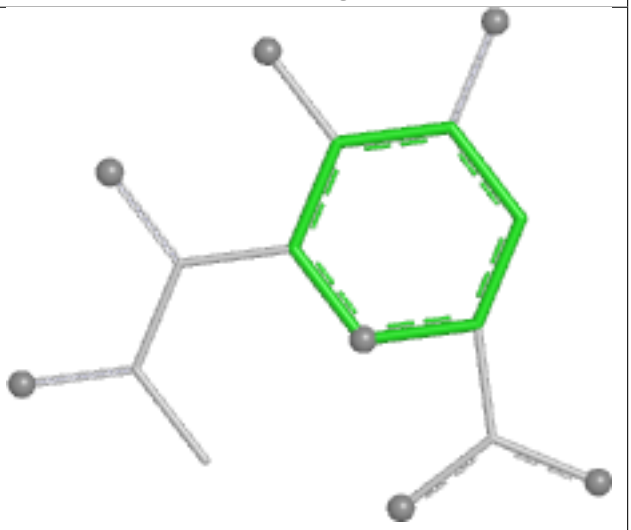
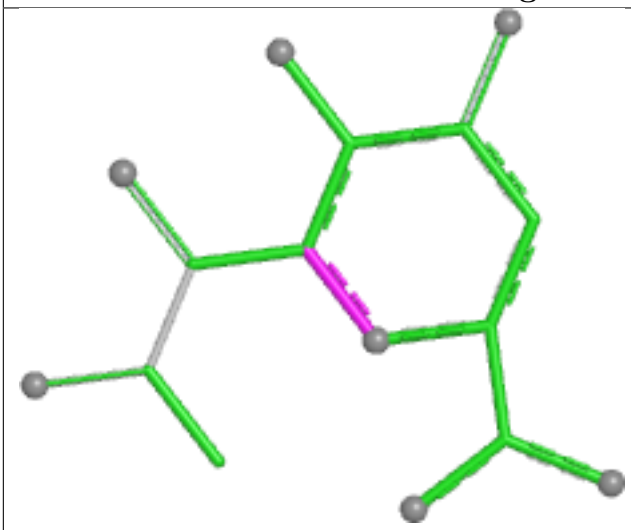


Rings

Ligand P8E LF 606



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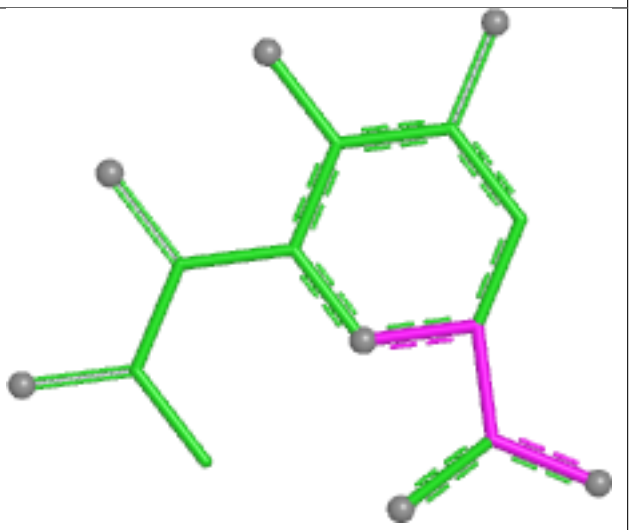
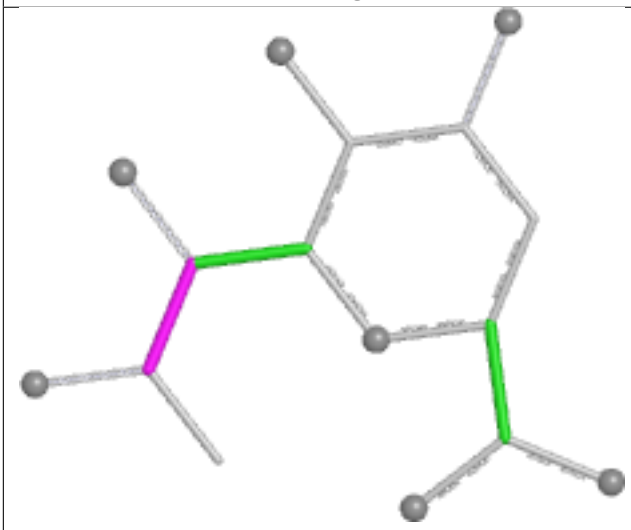
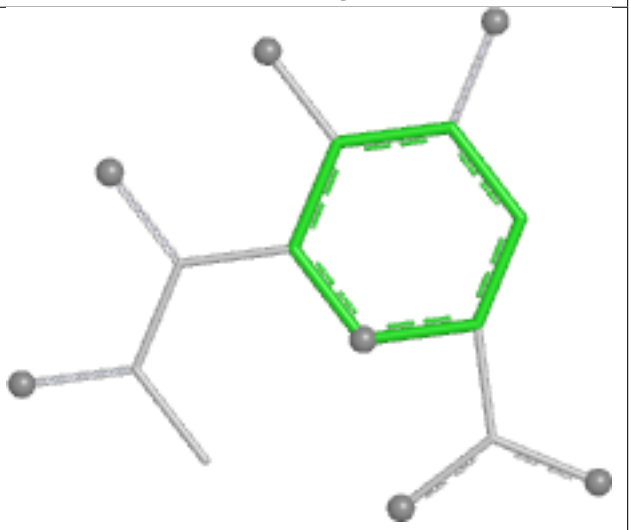


Bond angles

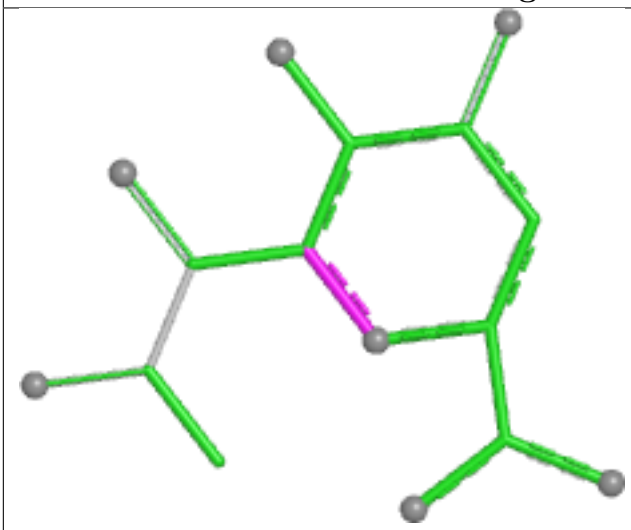


Torsions



Rings

Ligand P8E R4 606



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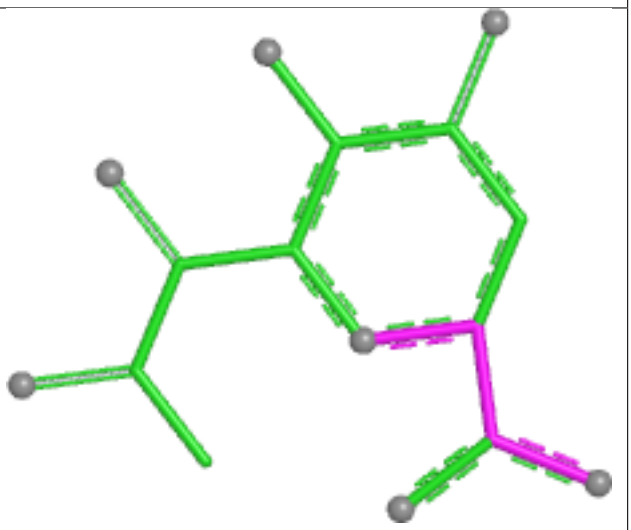

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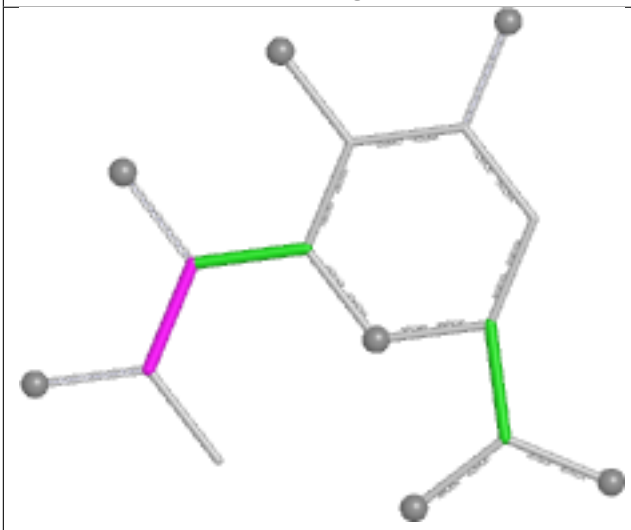

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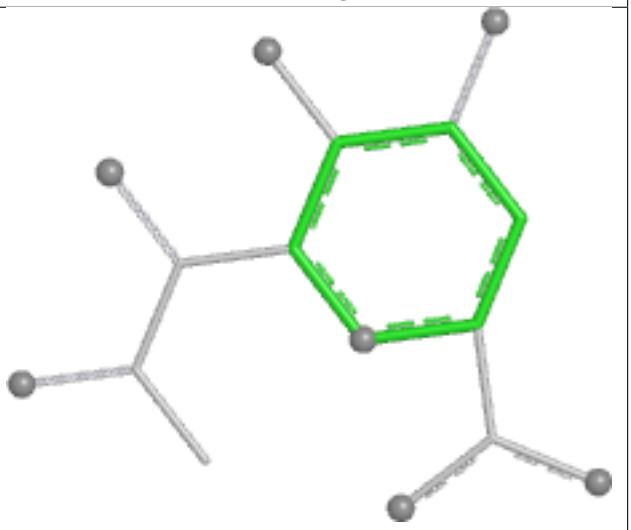
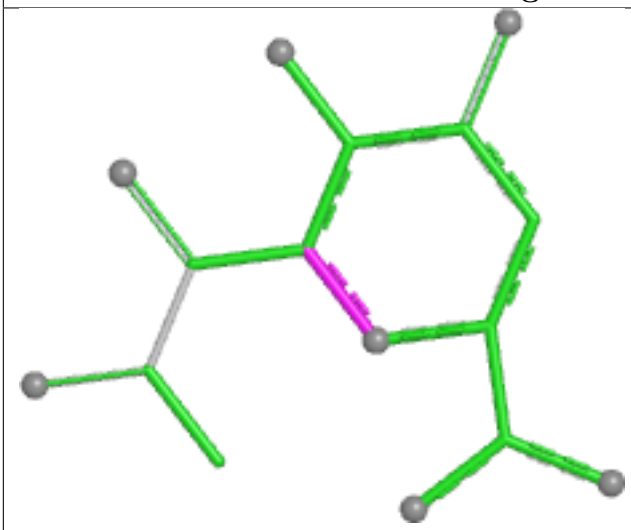


Rings

Ligand P8E bS 605



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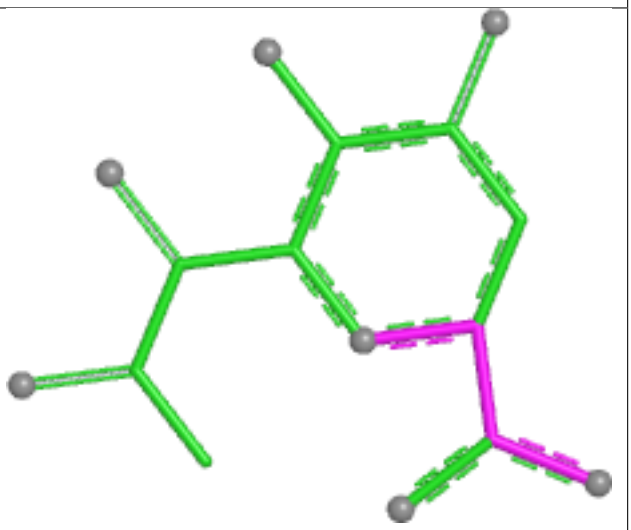

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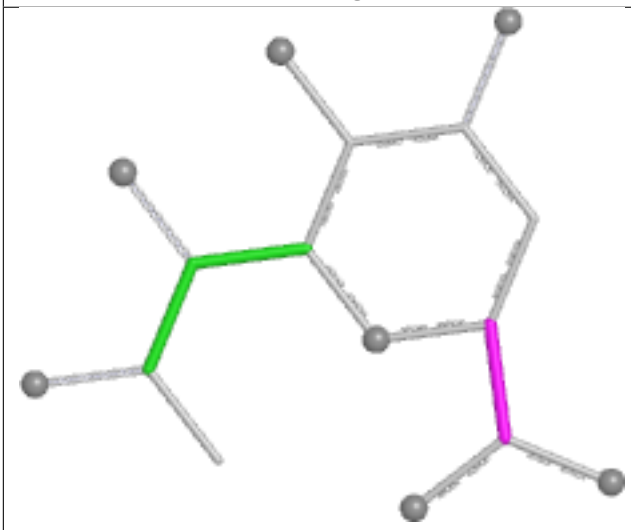

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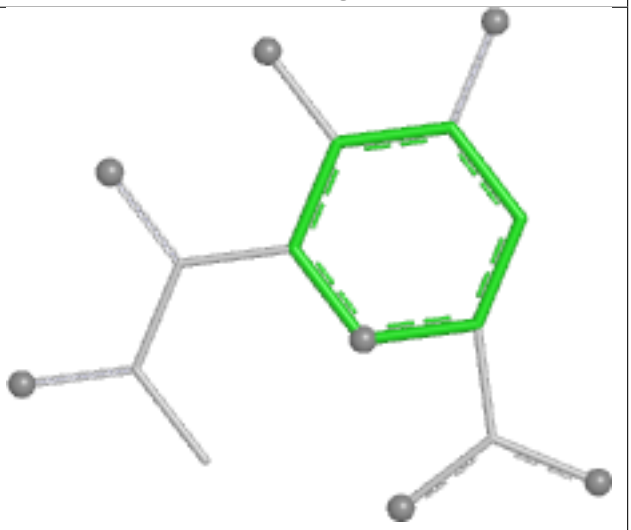
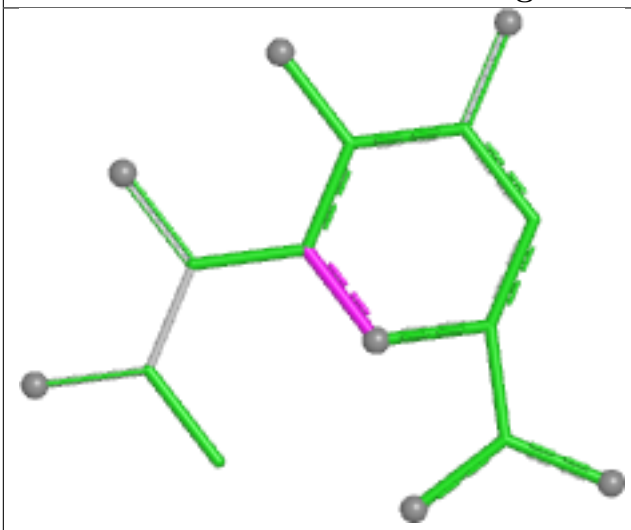


Rings

Ligand P8E CT 606



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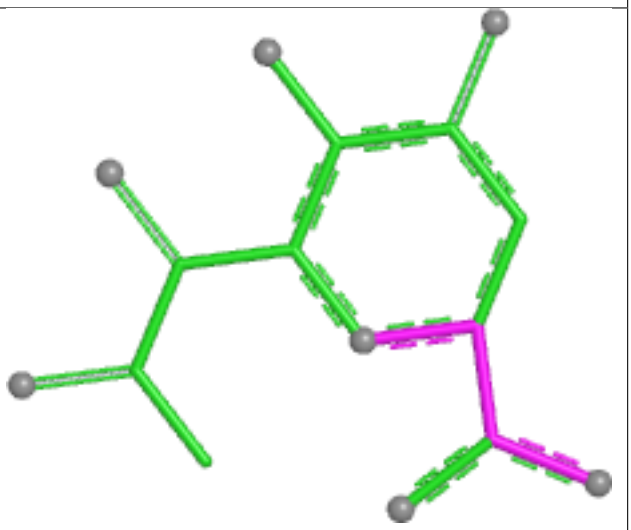

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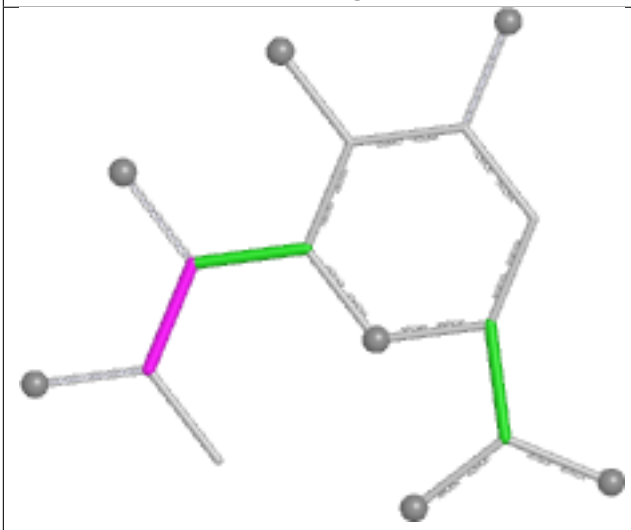

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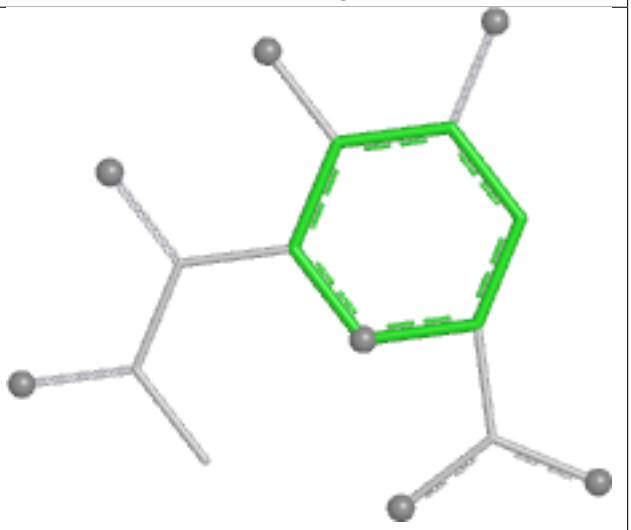
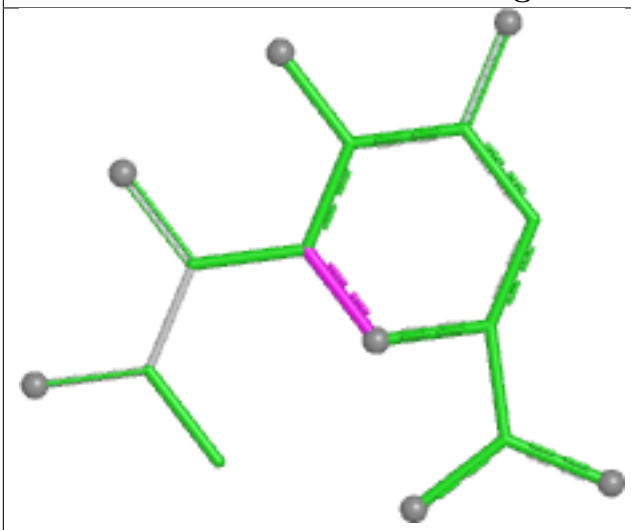


Rings

Ligand P8E UH 606



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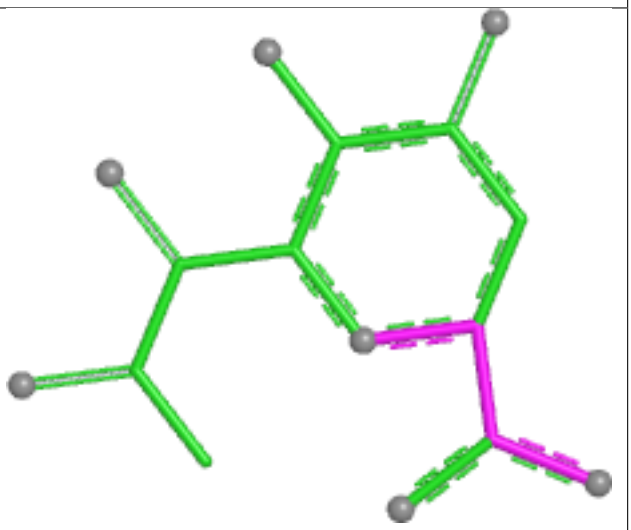

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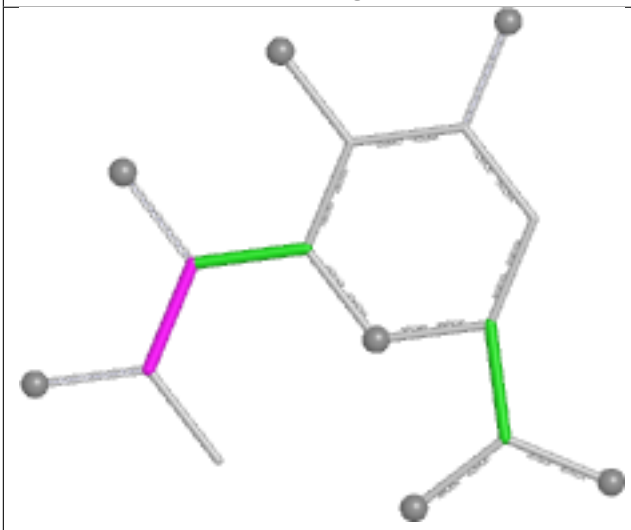

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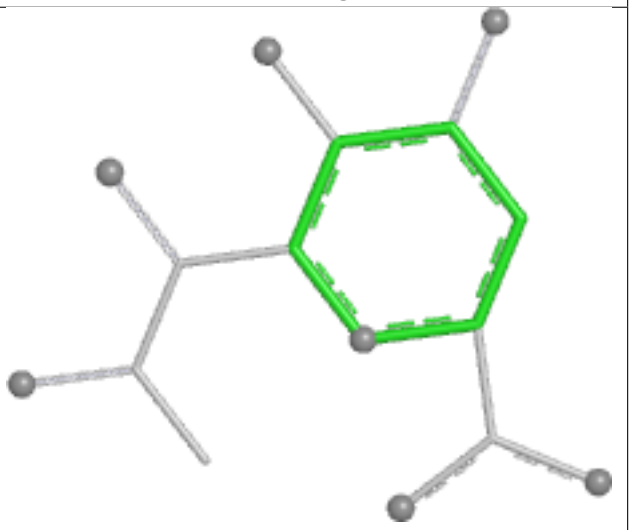
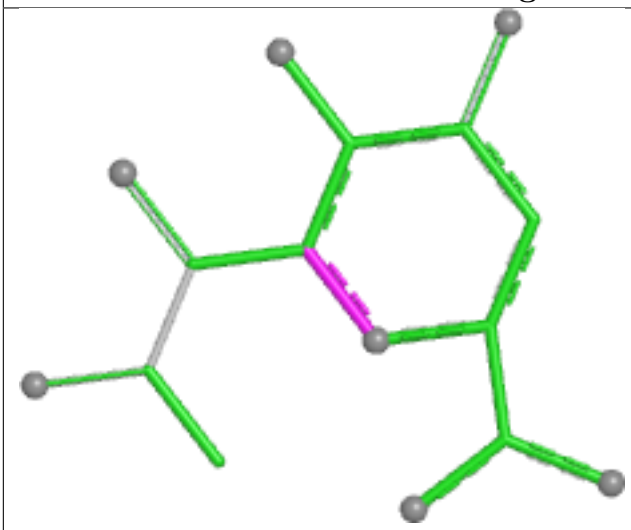


Rings

Ligand P8E R4 605



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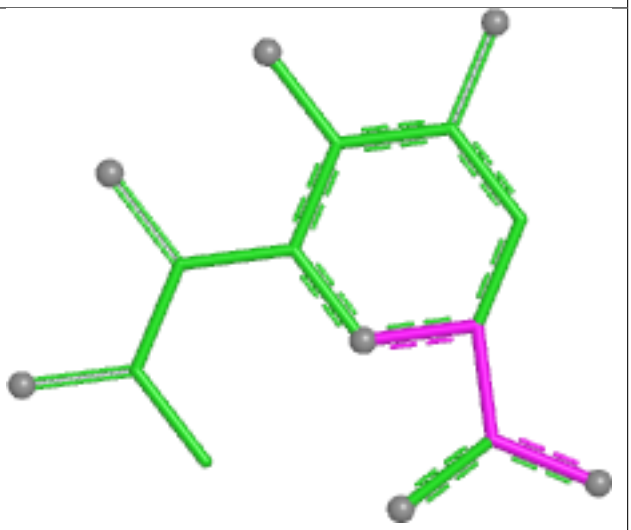

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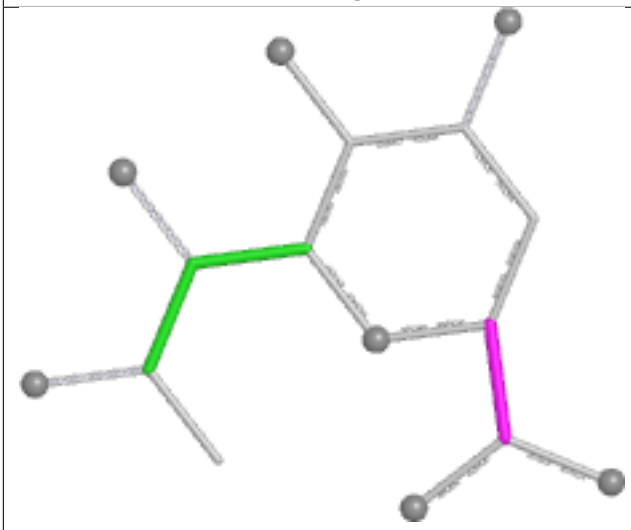

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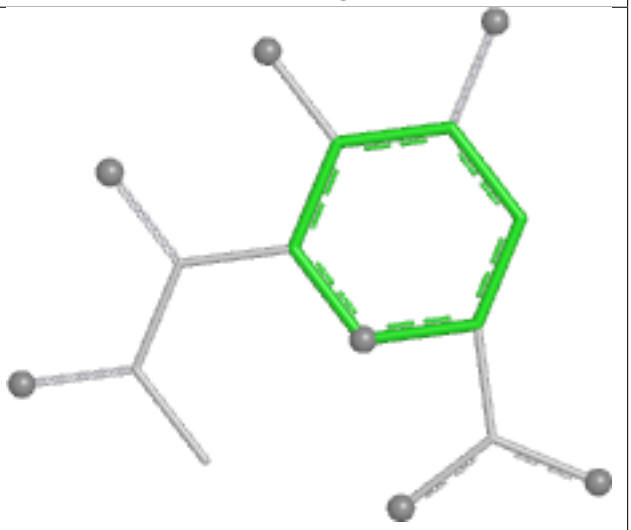

Rings

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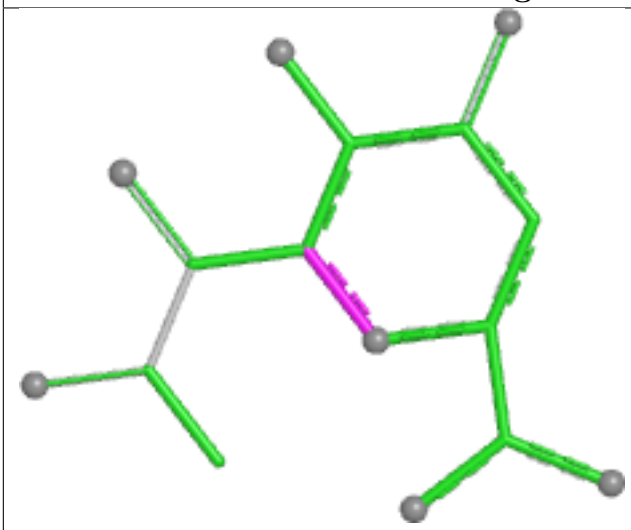

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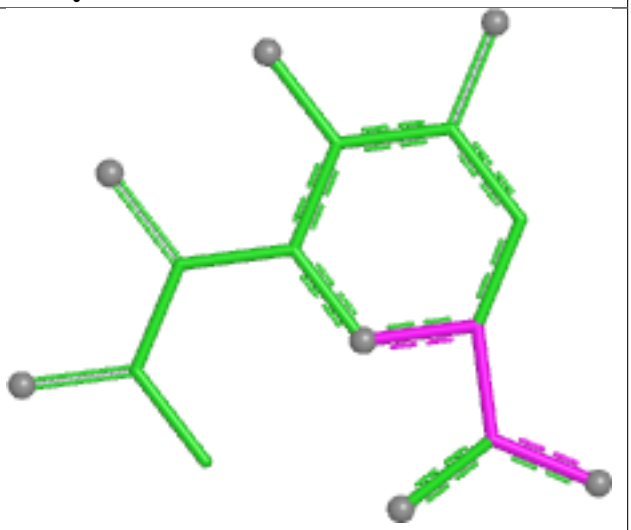

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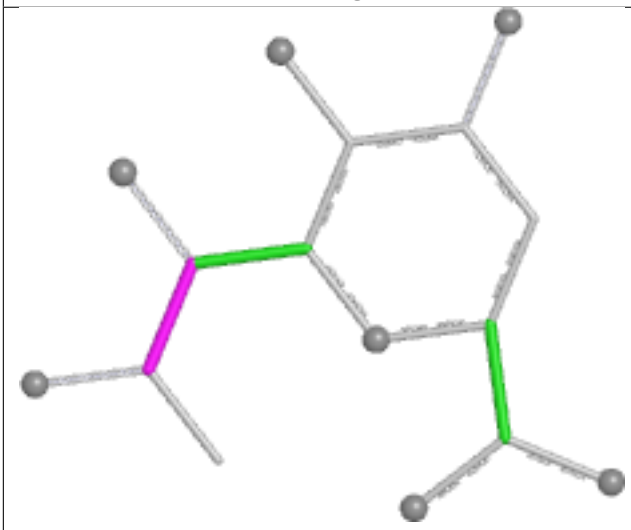

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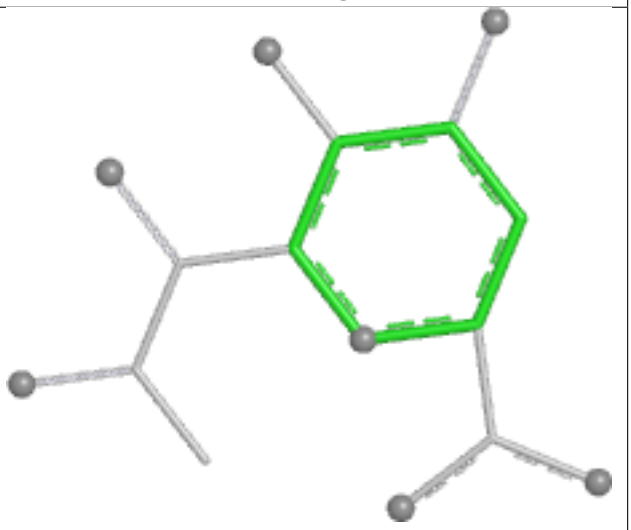
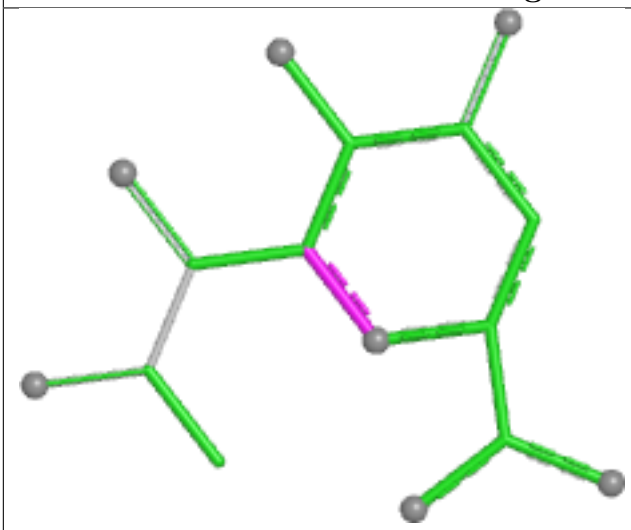


Rings

Ligand P8E e8 607



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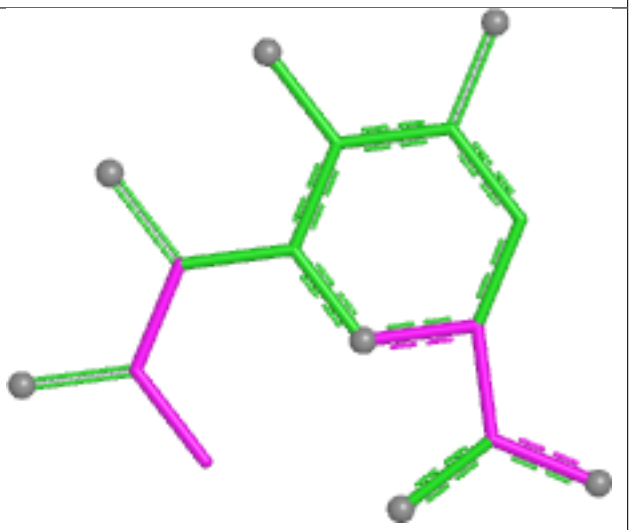

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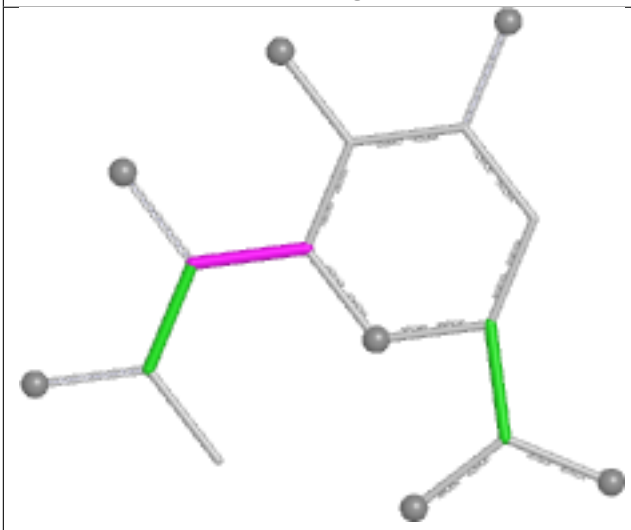

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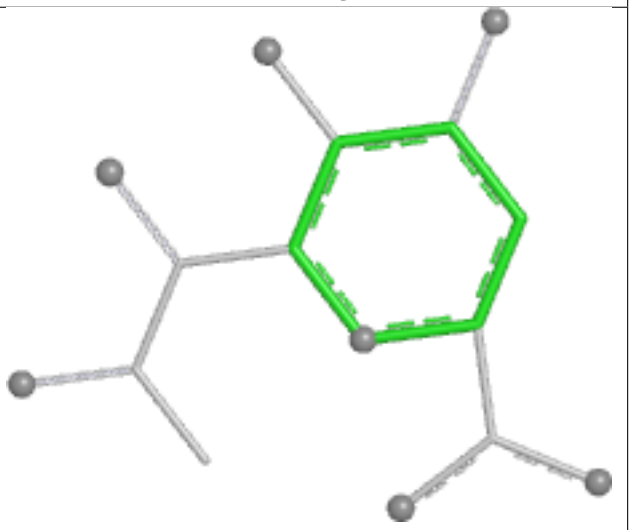
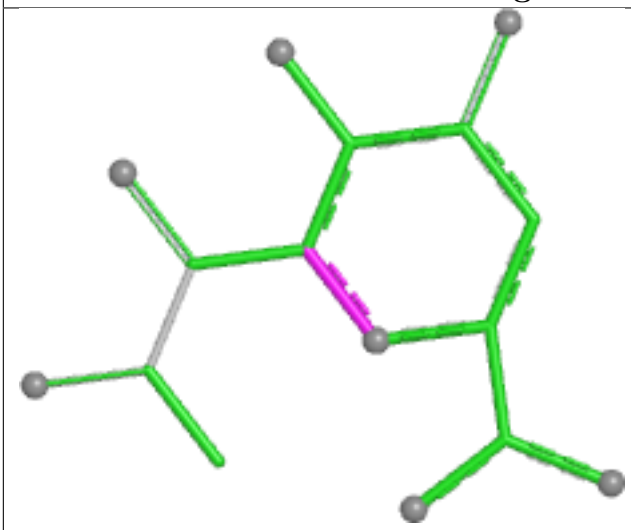


Rings

Ligand P8E UH 605



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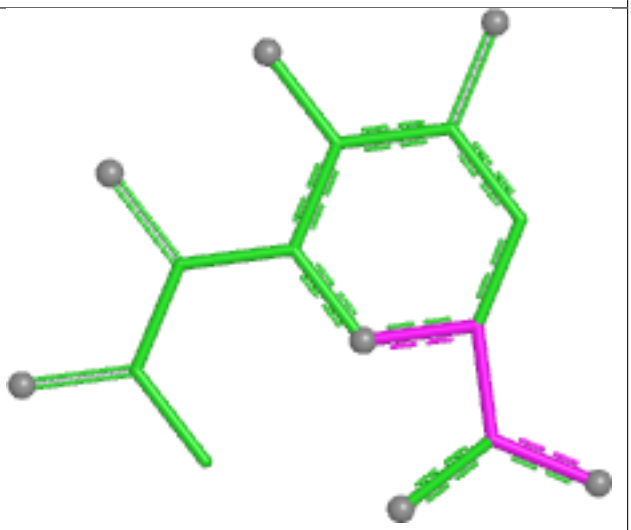

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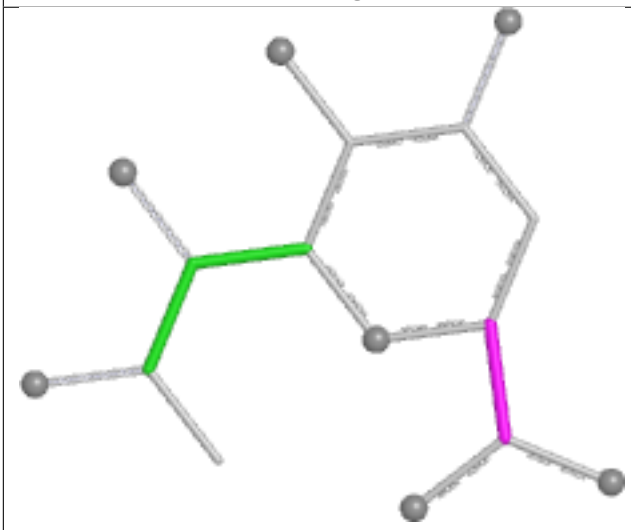

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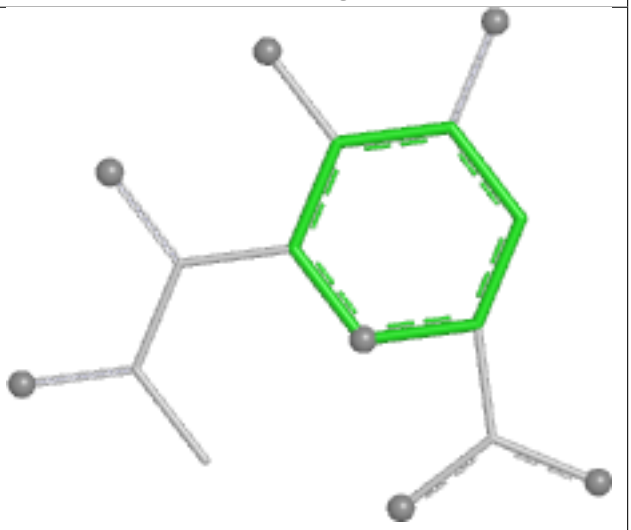
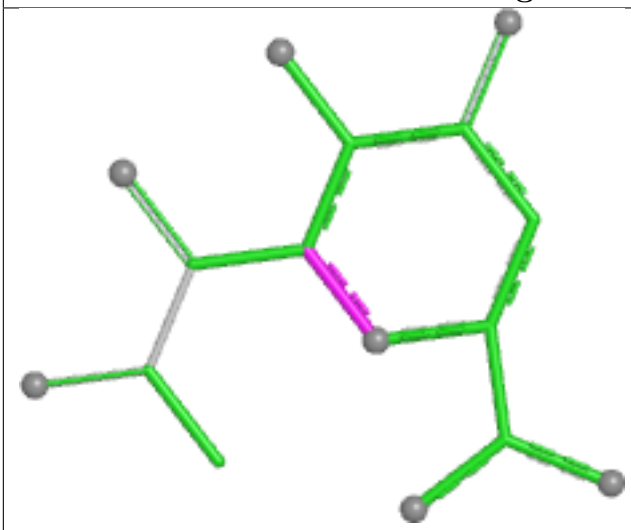


Rings

Ligand P8E CT 605



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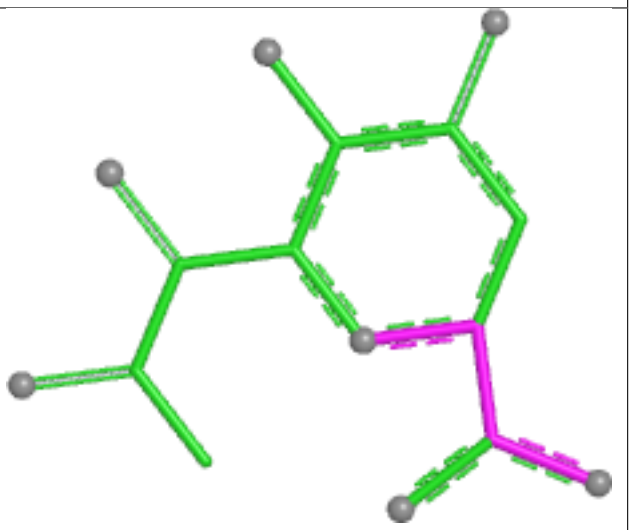

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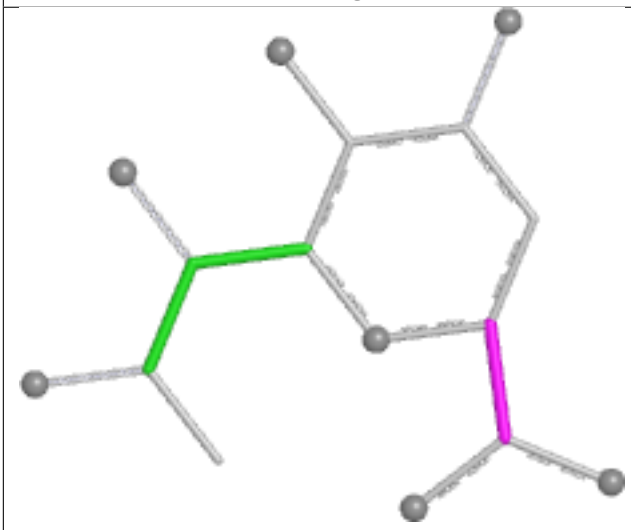

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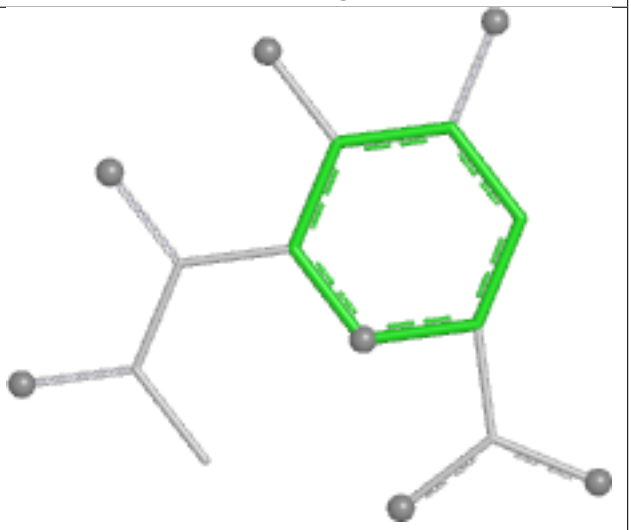
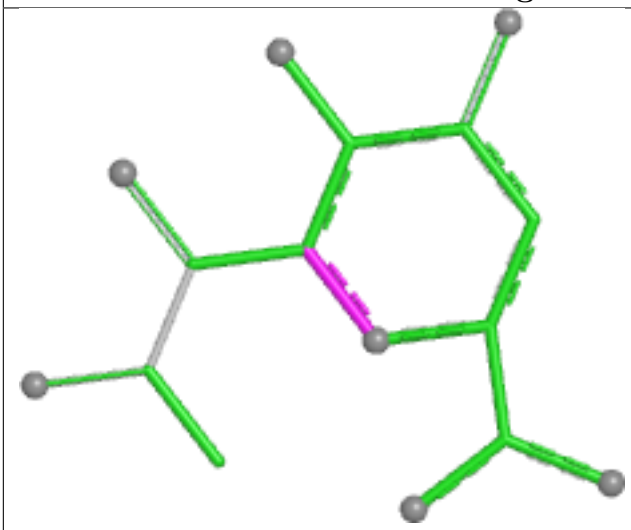


Rings

Ligand P8E EX 606



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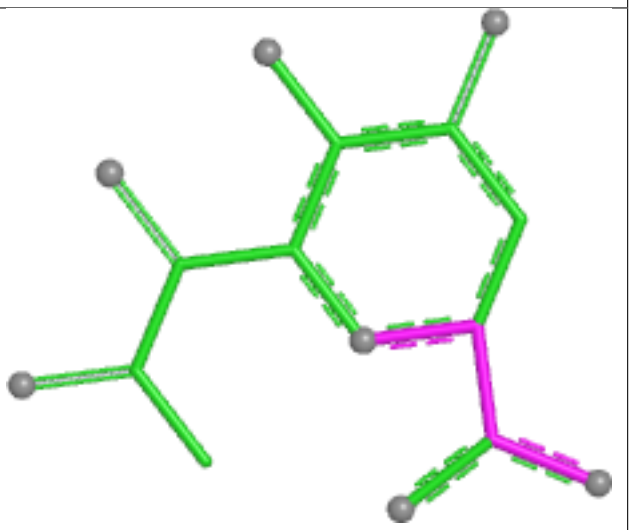

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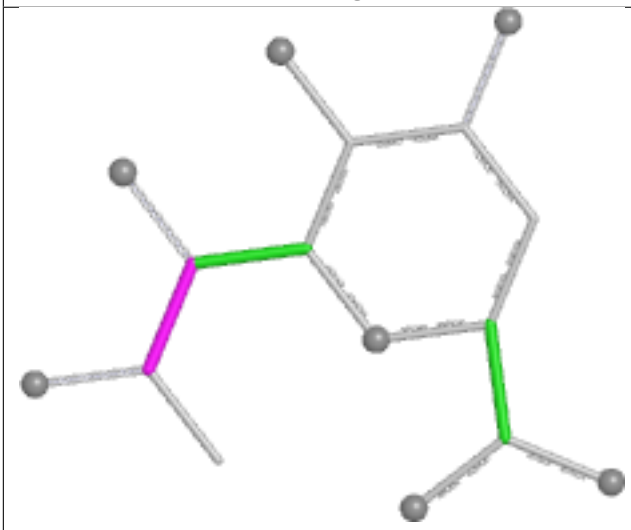

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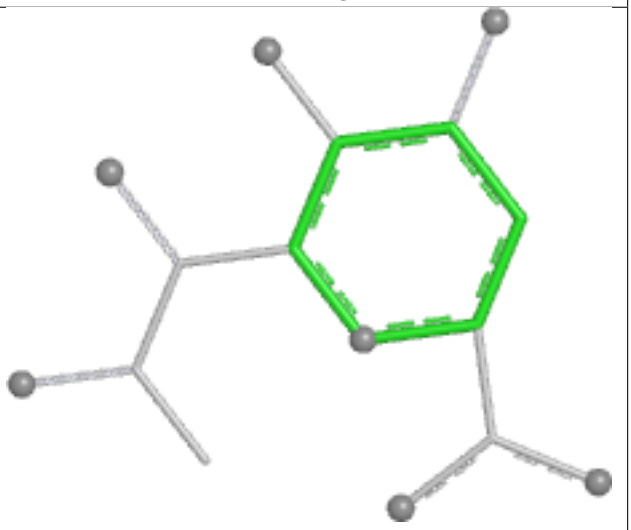
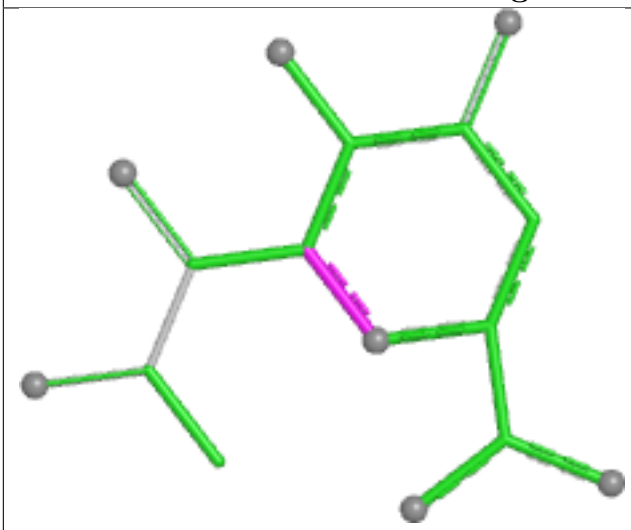


Rings

Ligand P8E MO 607



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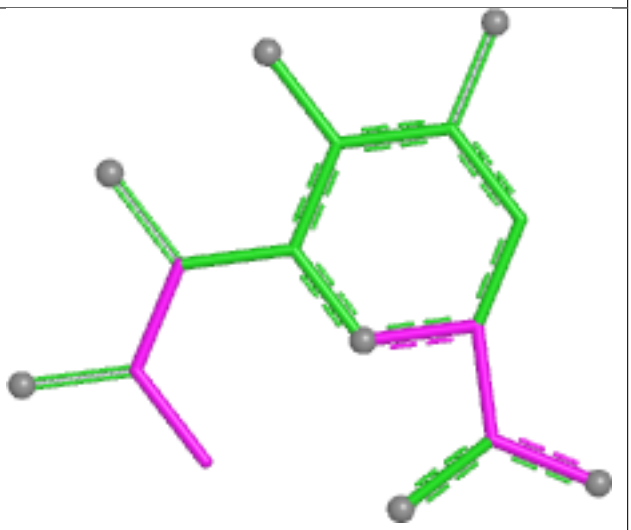
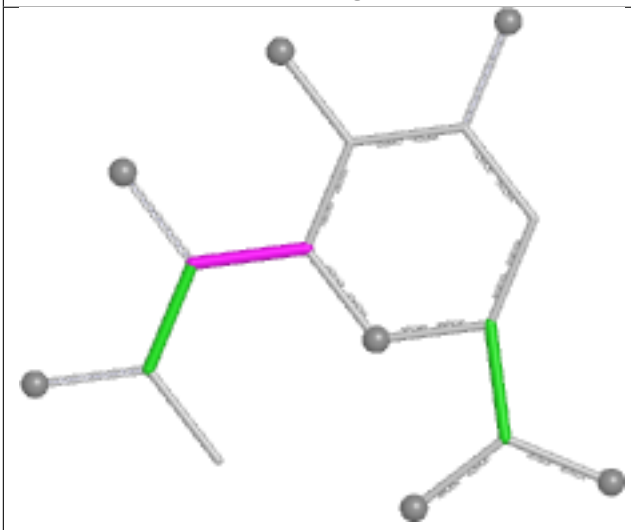


Bond angles



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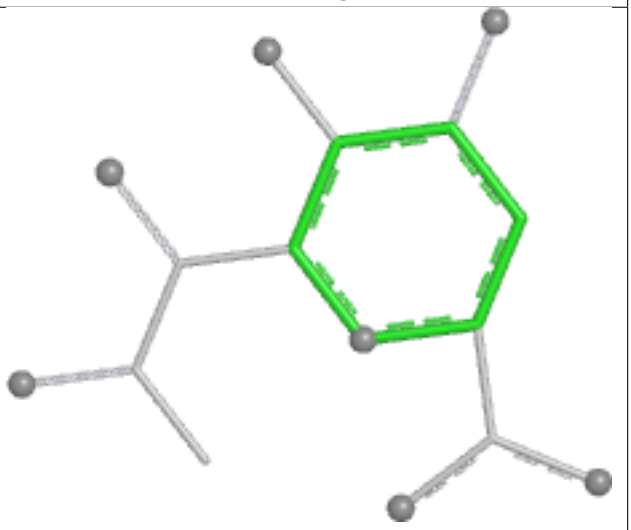
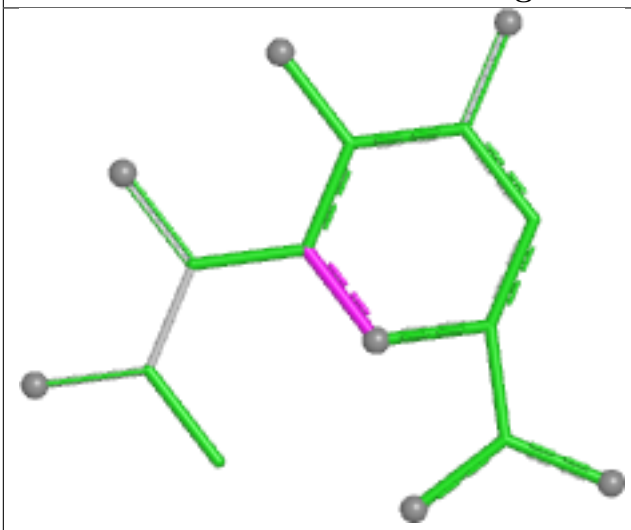


Rings

Ligand P8E OA 603



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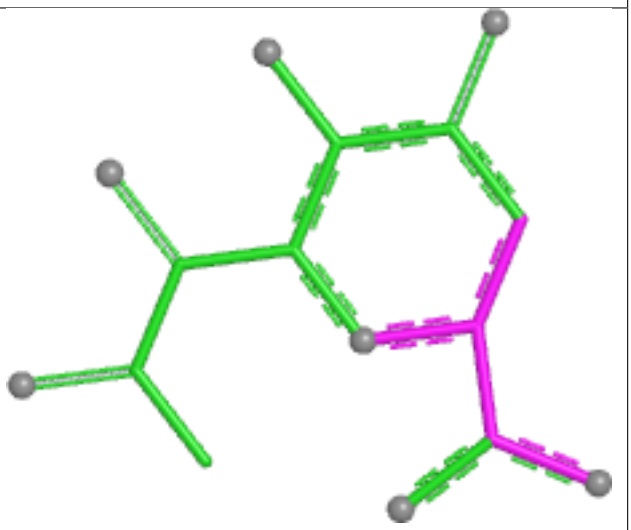
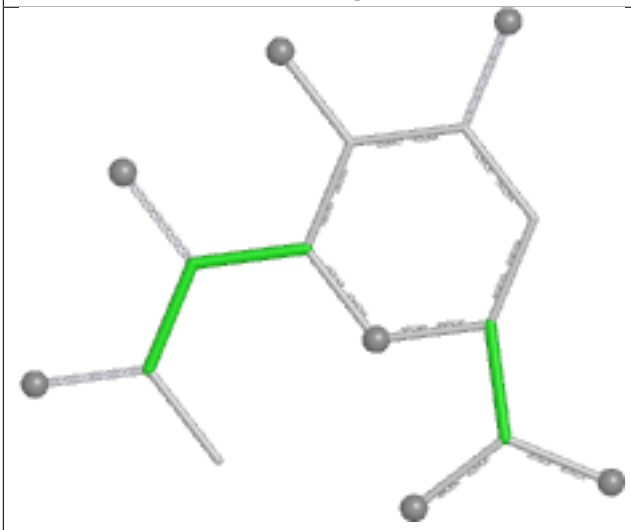


Bond angles



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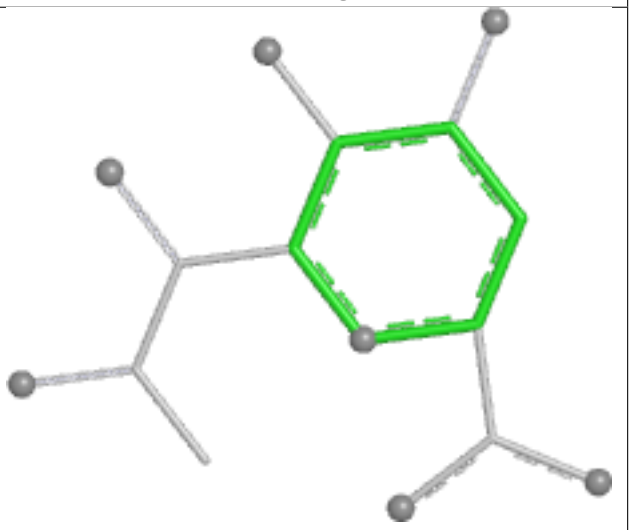
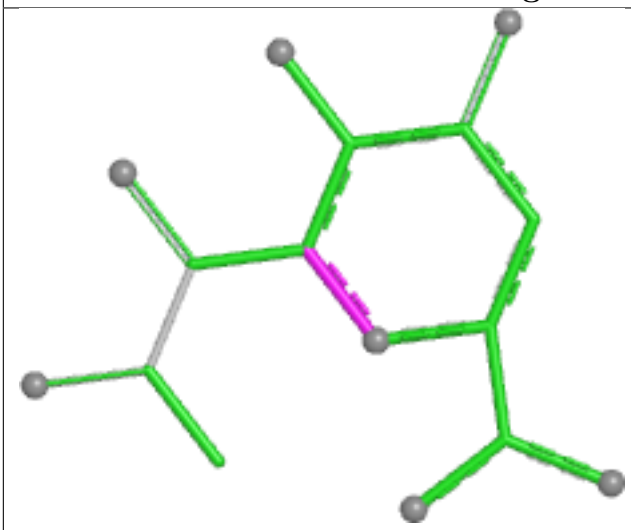


Rings

Ligand P8E S5 601



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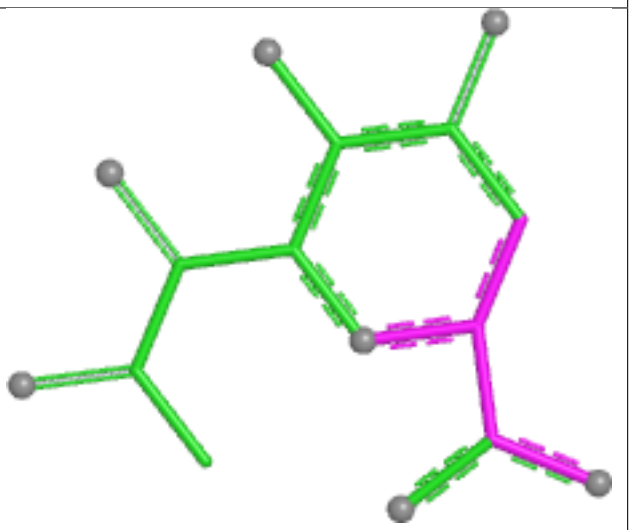
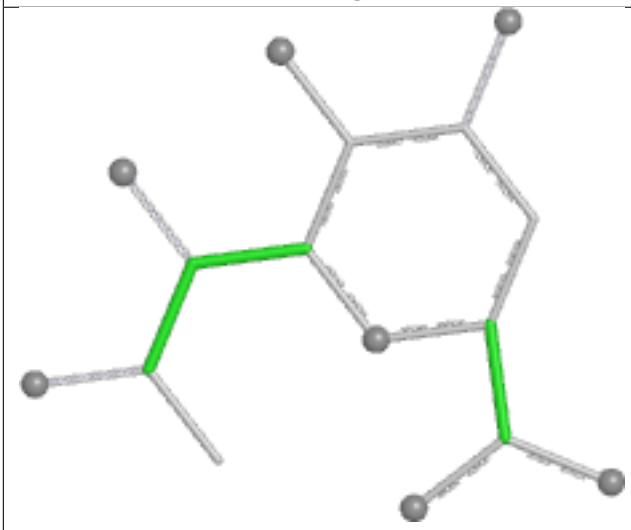
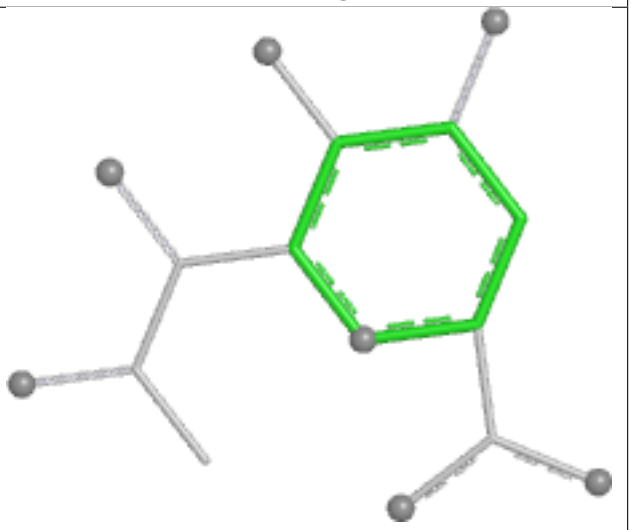


Bond angles

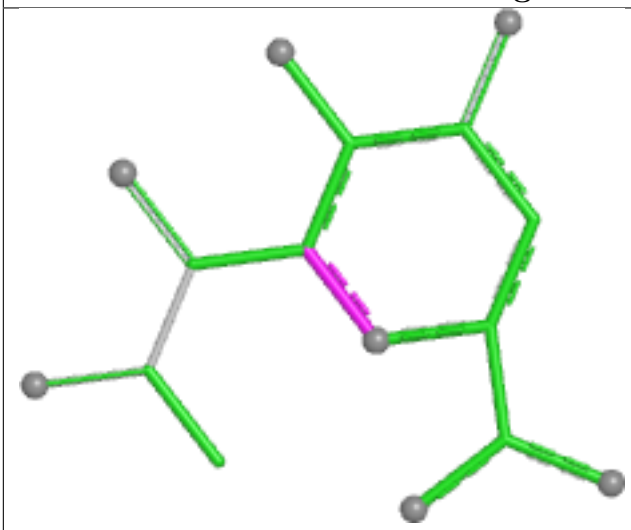


Torsions

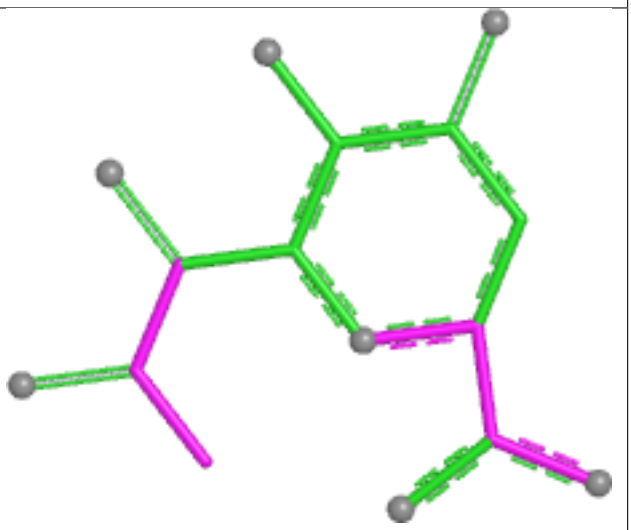


Rings

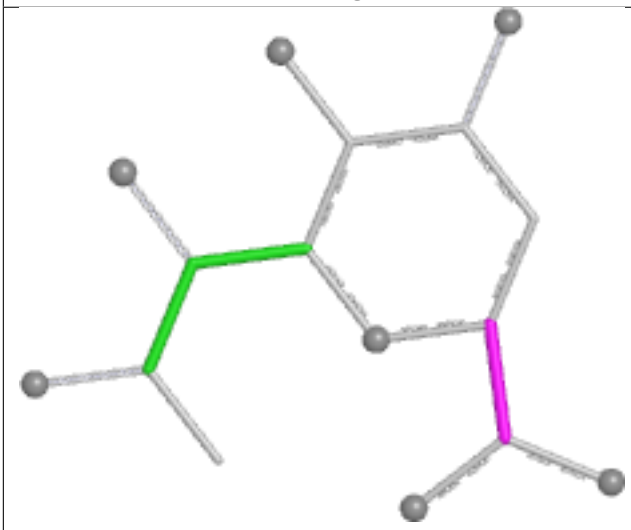
Ligand P8E DN 604



Bond lengths



Bond angles



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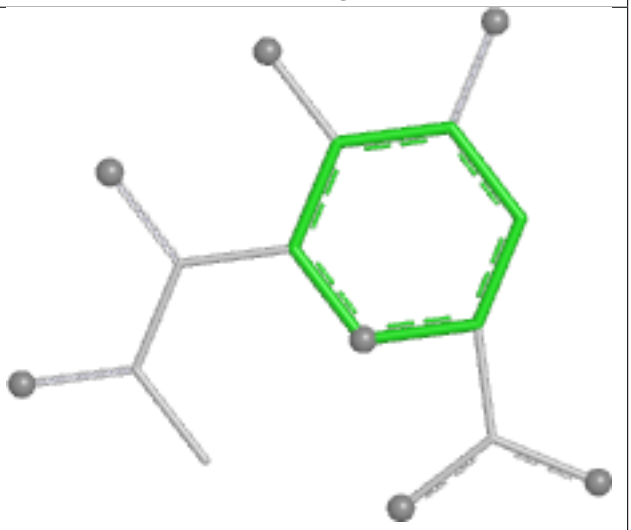
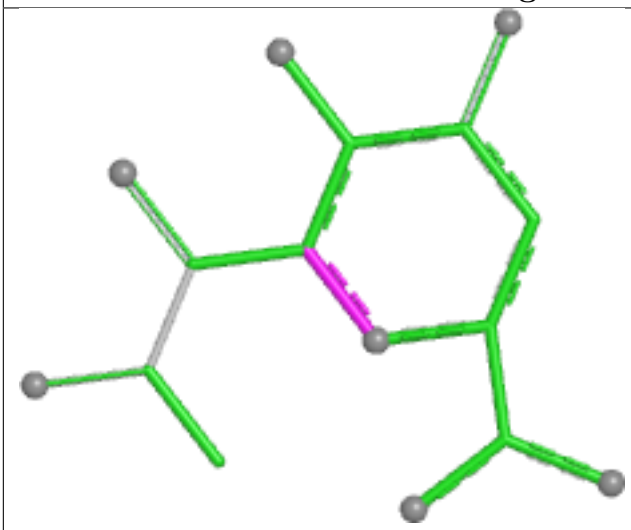


Rings

Ligand P8E A7 601



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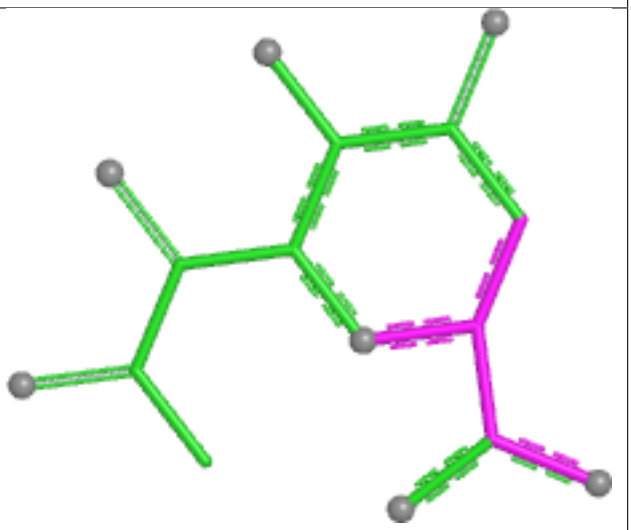

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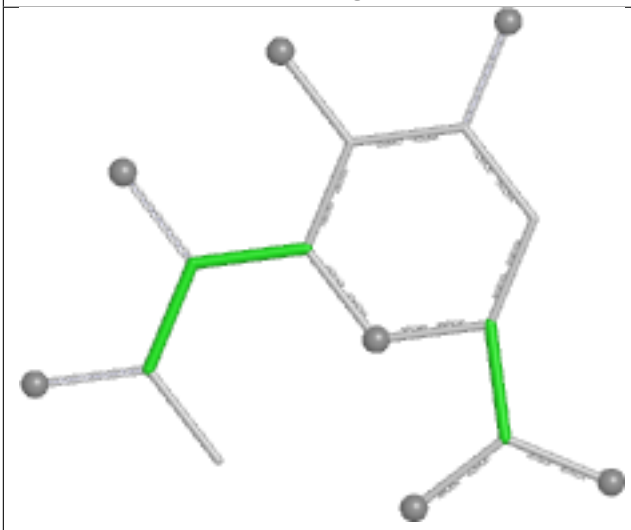
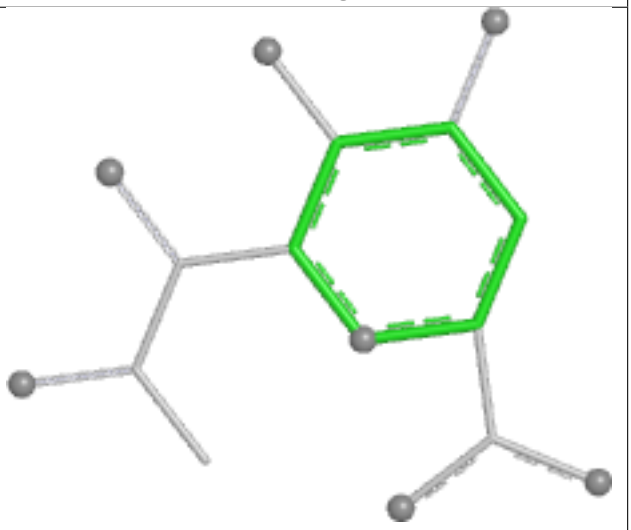
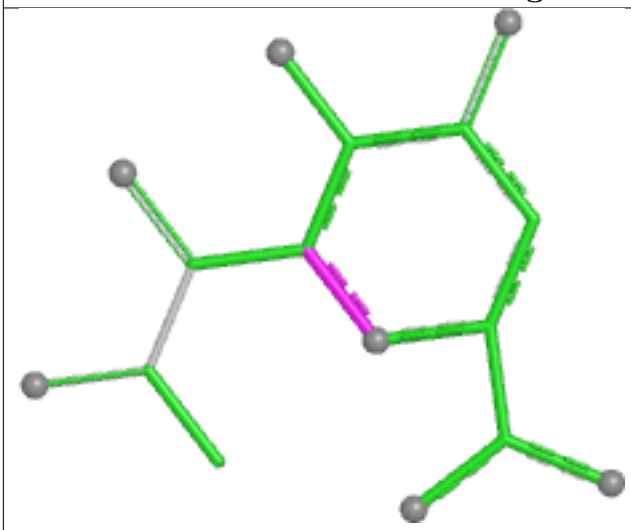


Torsions



Rings

Ligand P8E I3 603



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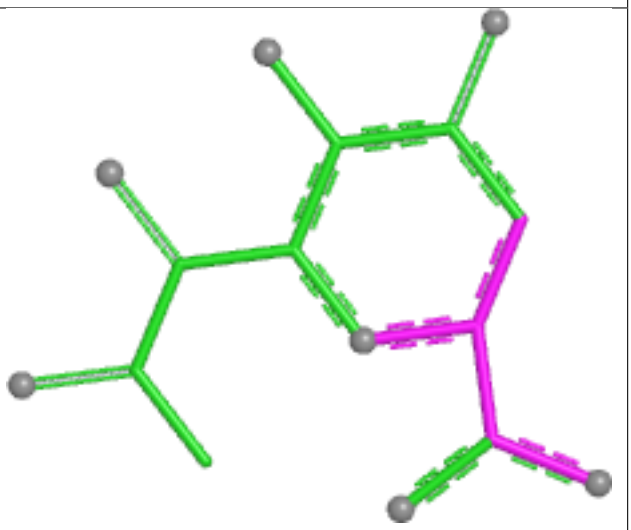
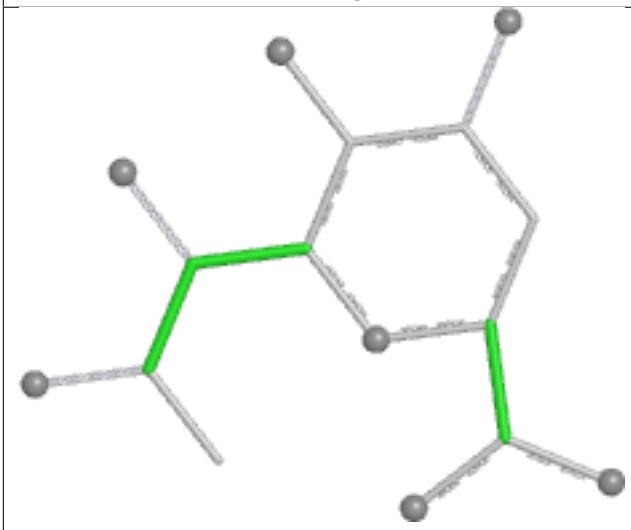


Bond angles



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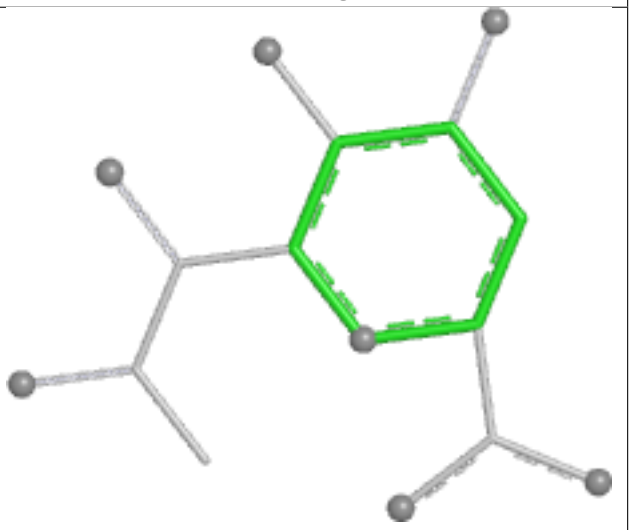
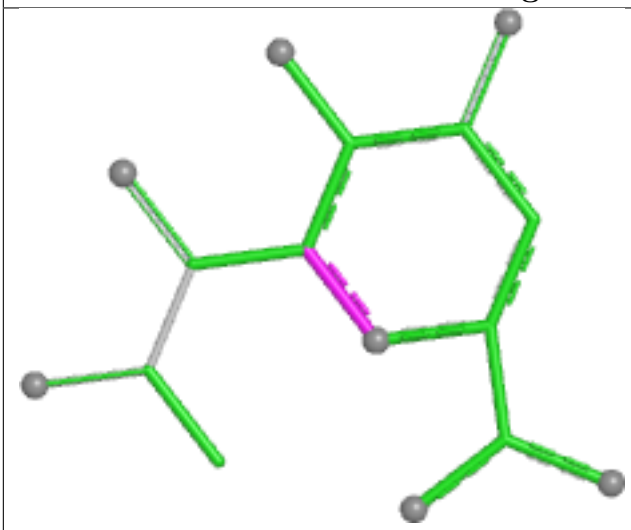


Rings

Ligand P8E Z9 605



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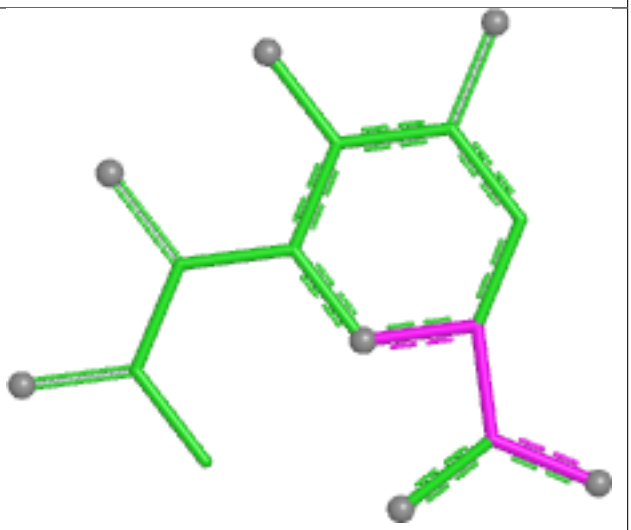
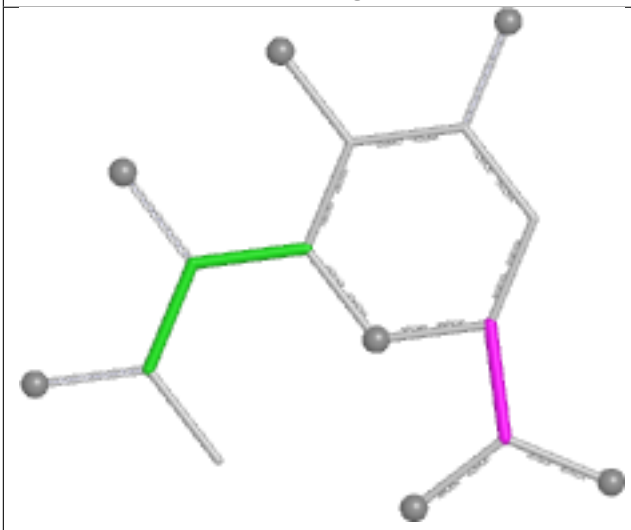


Bond angles



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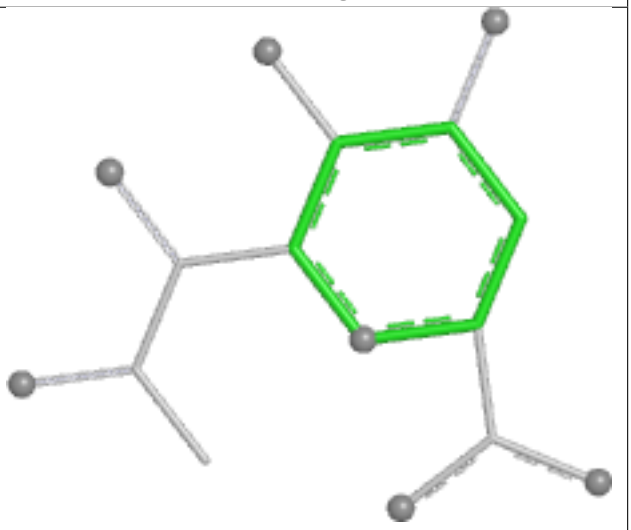
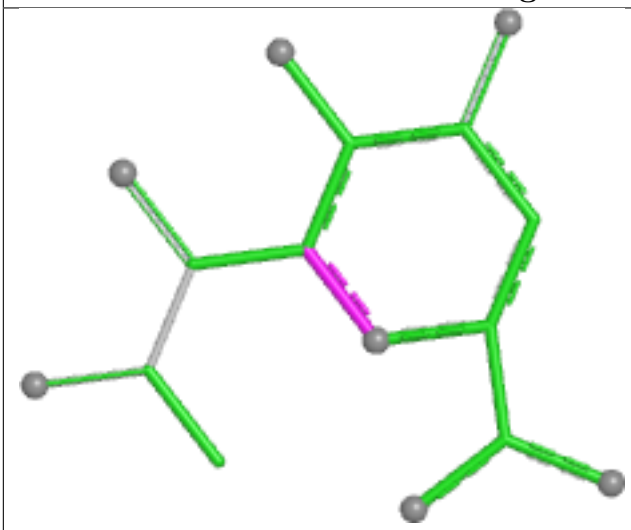


Rings

Ligand P8E LF 601



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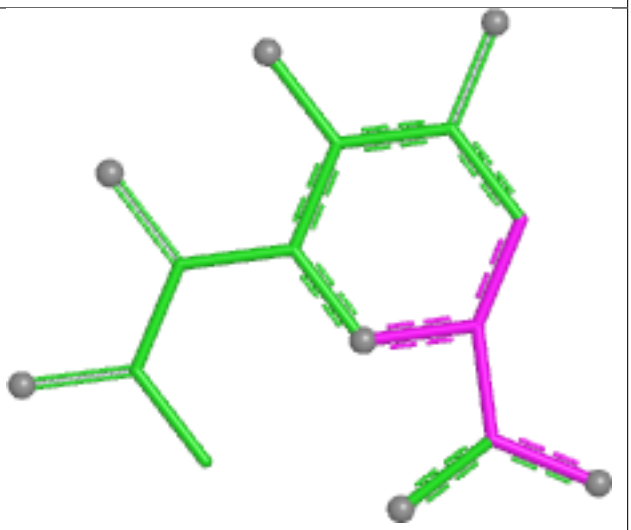

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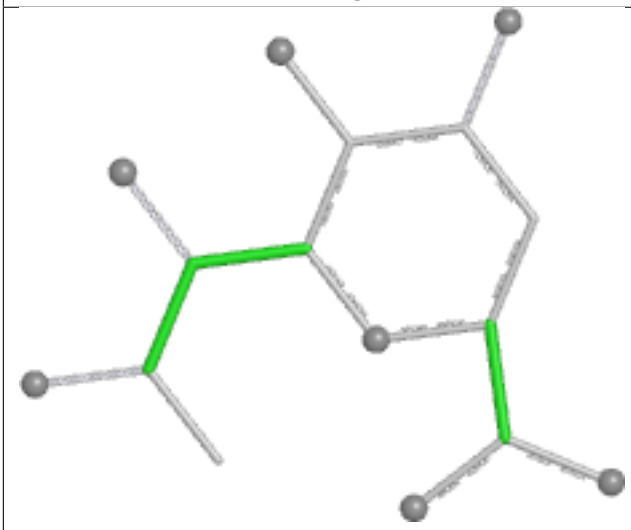

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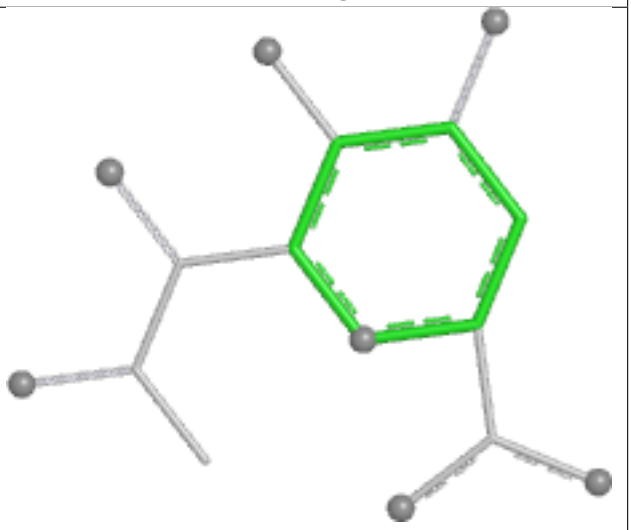
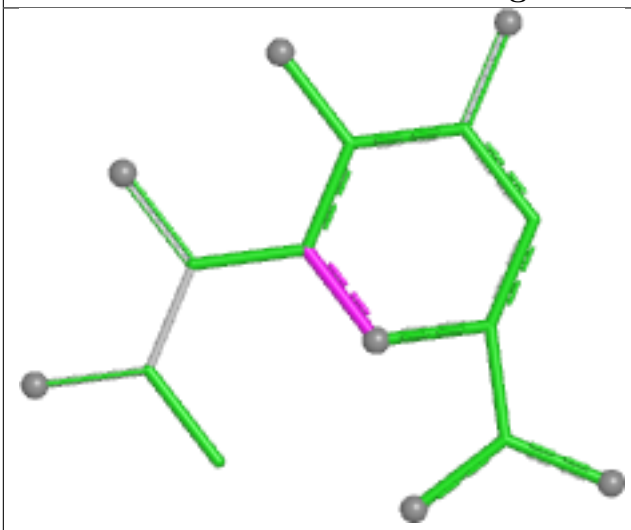


Rings

Ligand P8E WG 605



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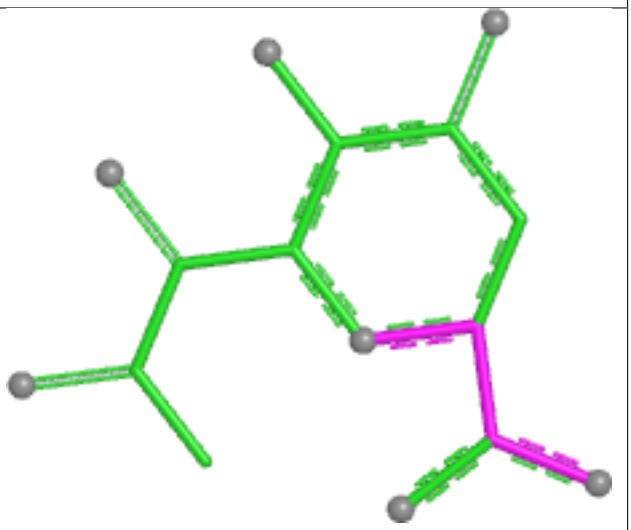

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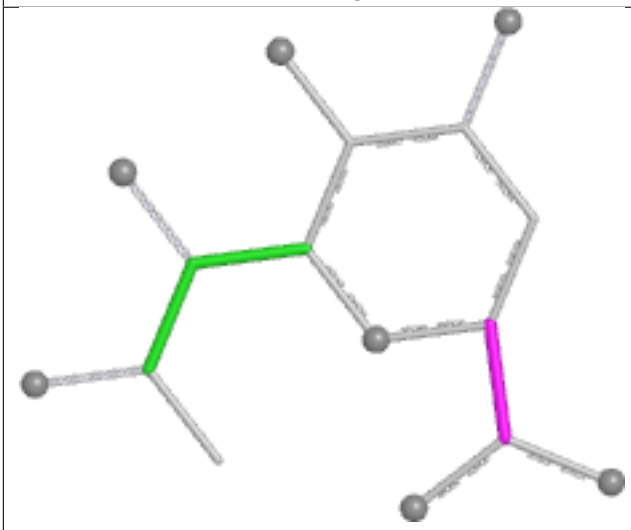

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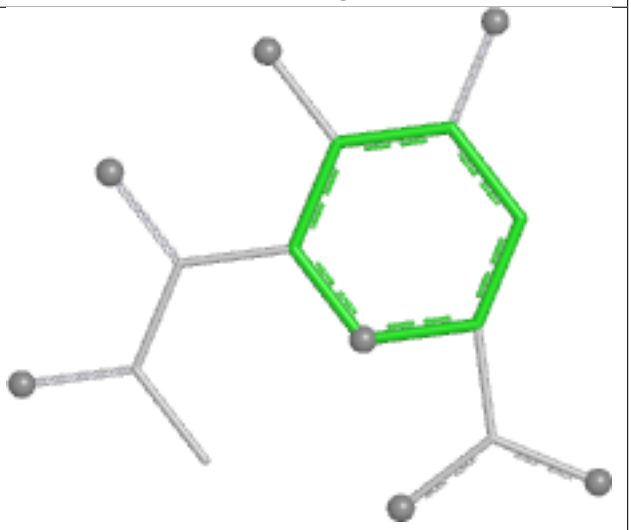
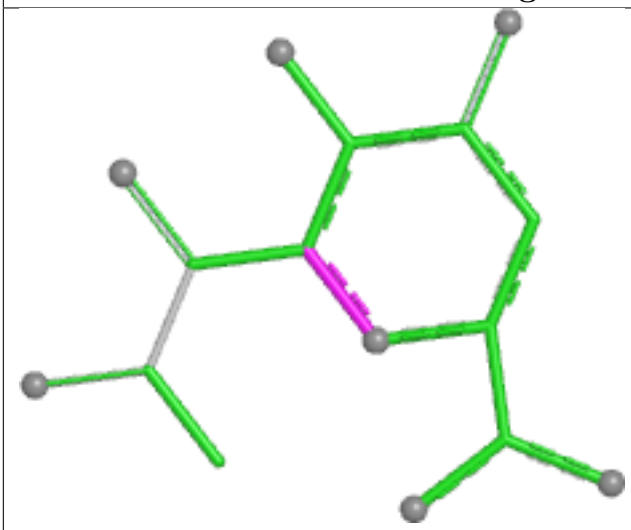


Rings

Ligand P8E A7 603



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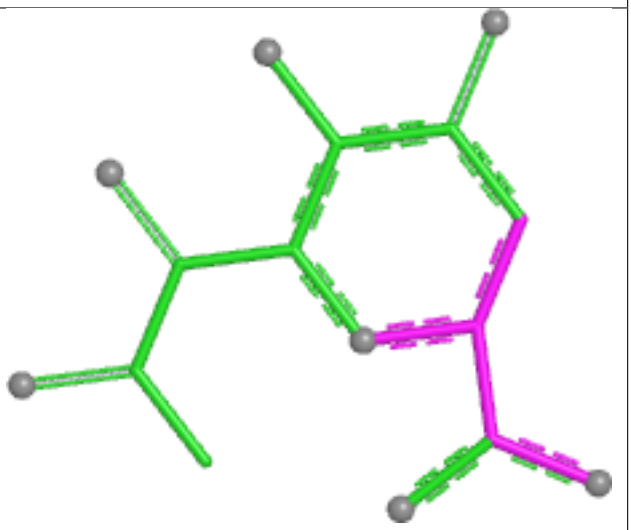

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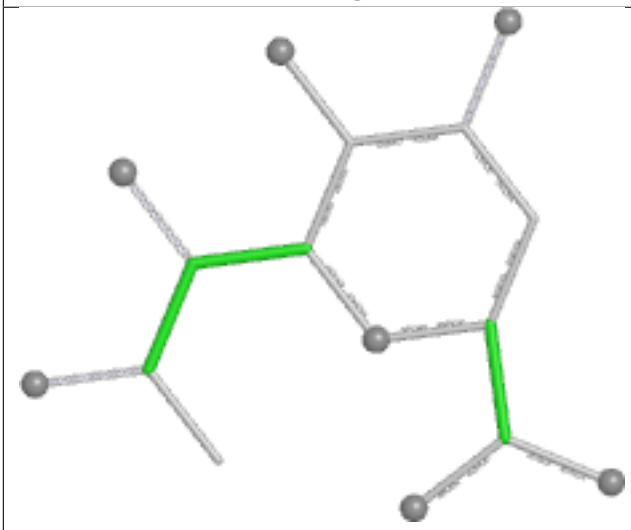

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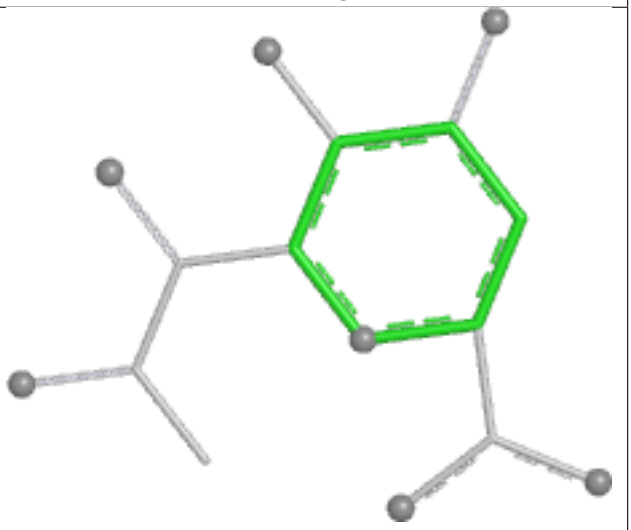
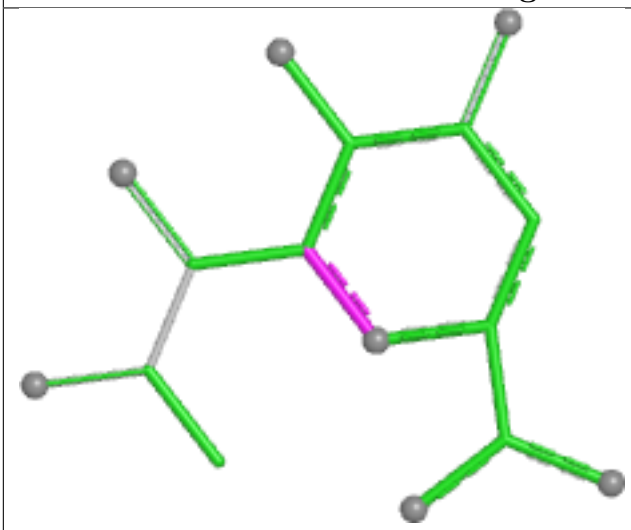


Rings

Ligand P8E LF 603



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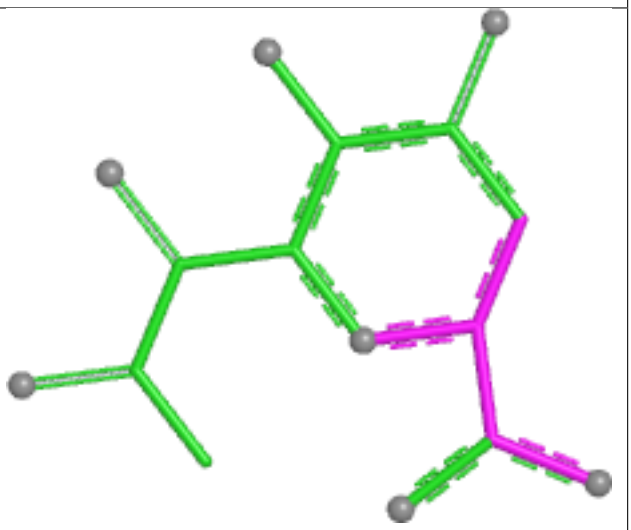
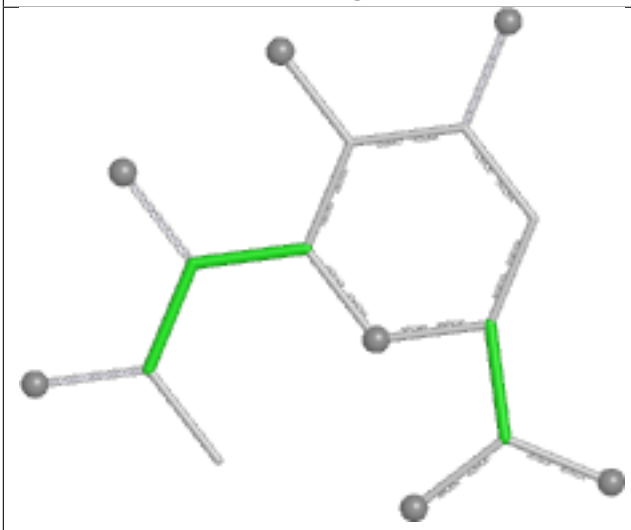


Bond angles



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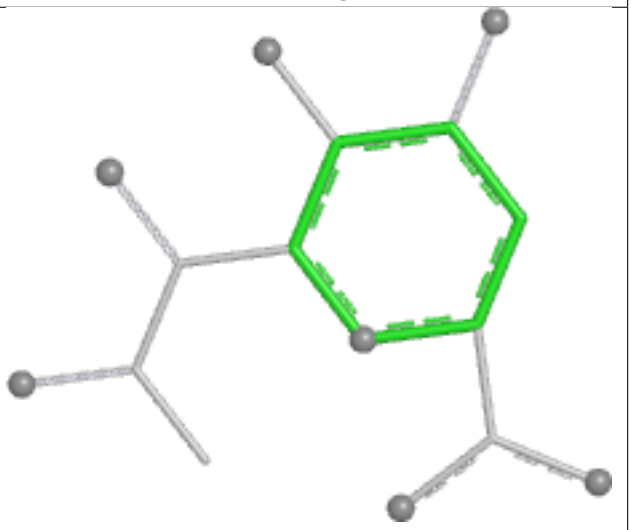
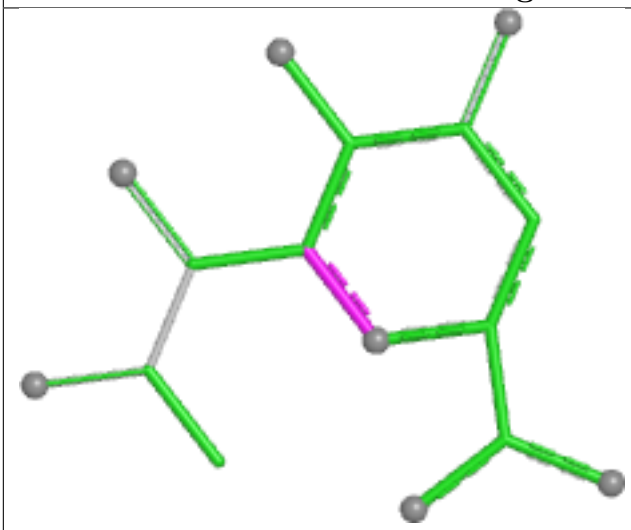


Rings

Ligand P8E EX 607



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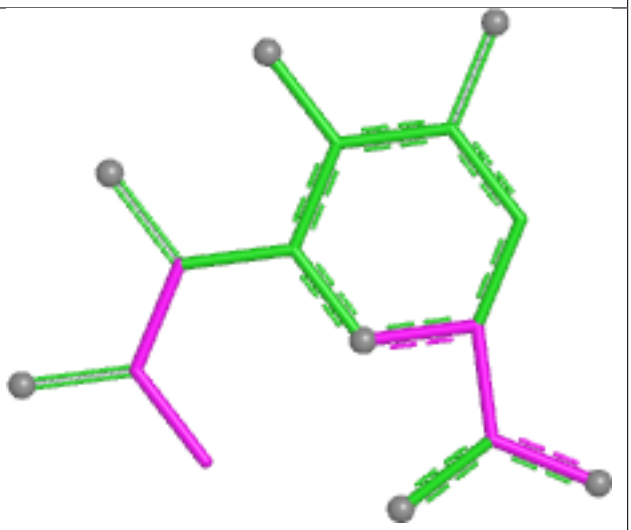
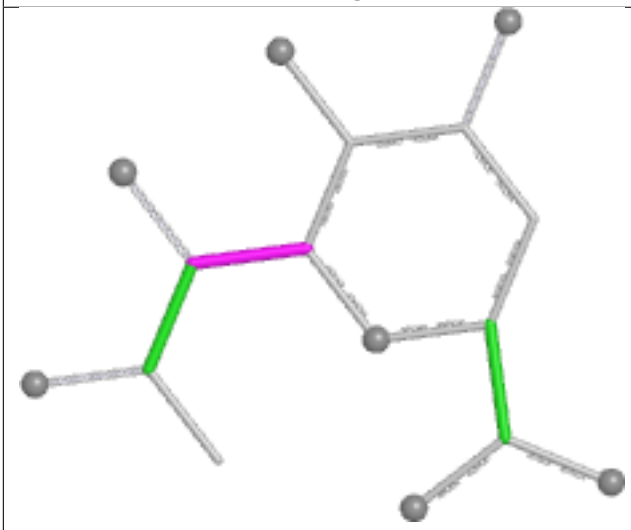


Bond angles



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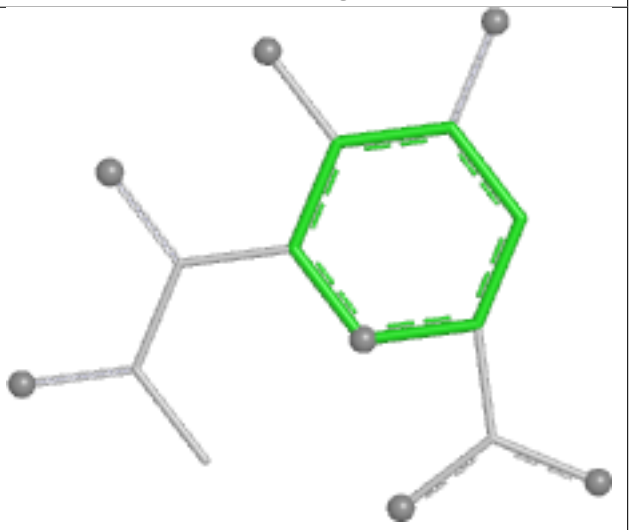
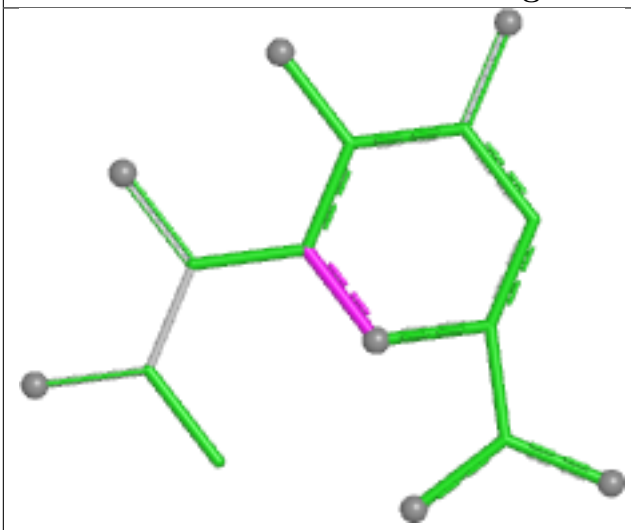


Rings

Ligand P8E S5 603



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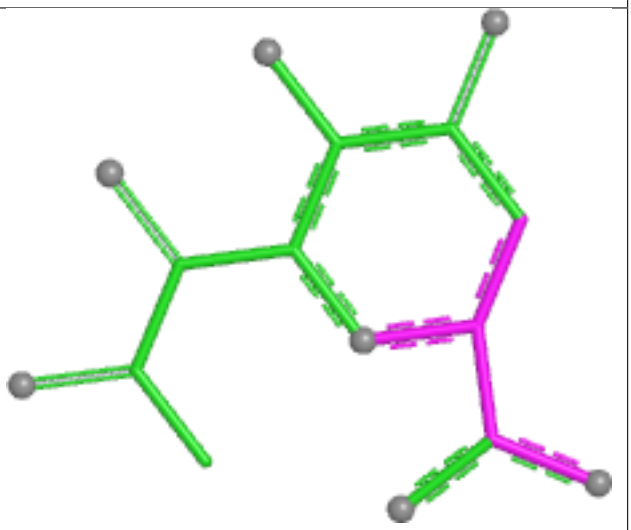

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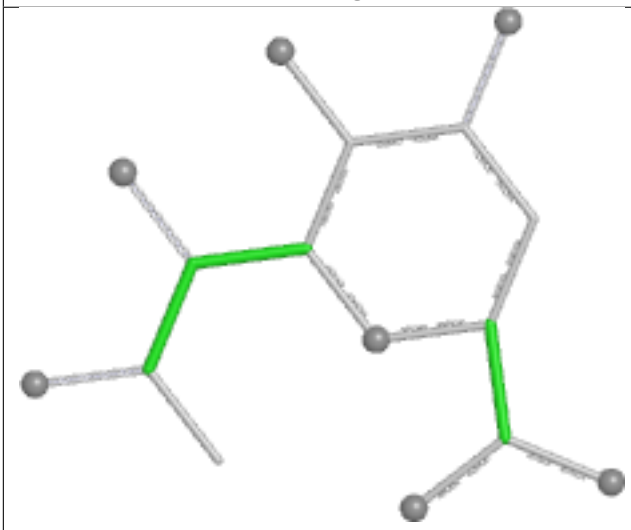

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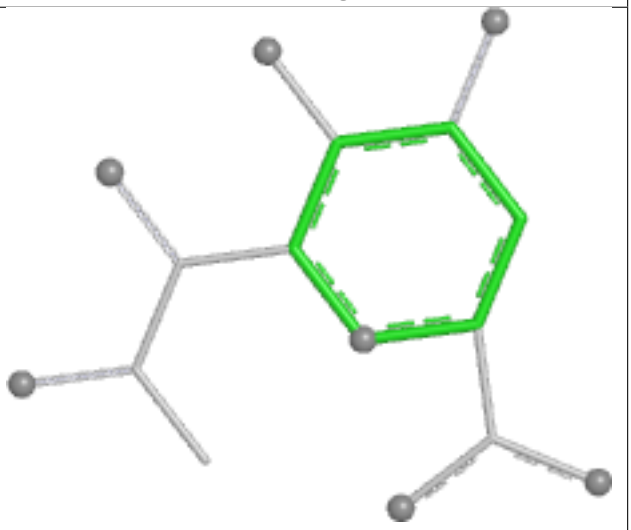
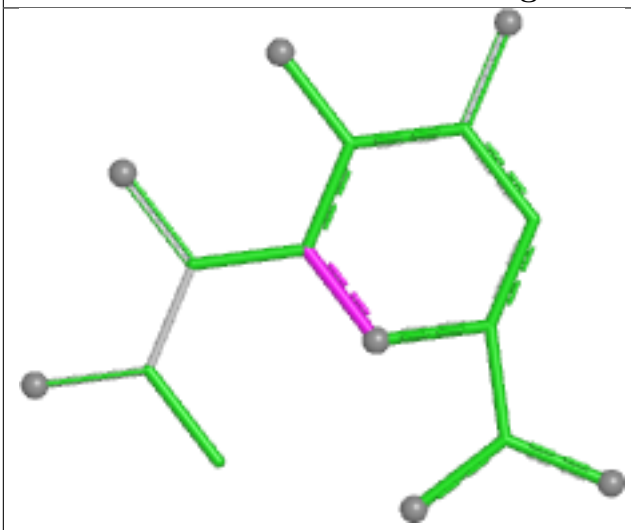


Rings

Ligand P8E cV 606



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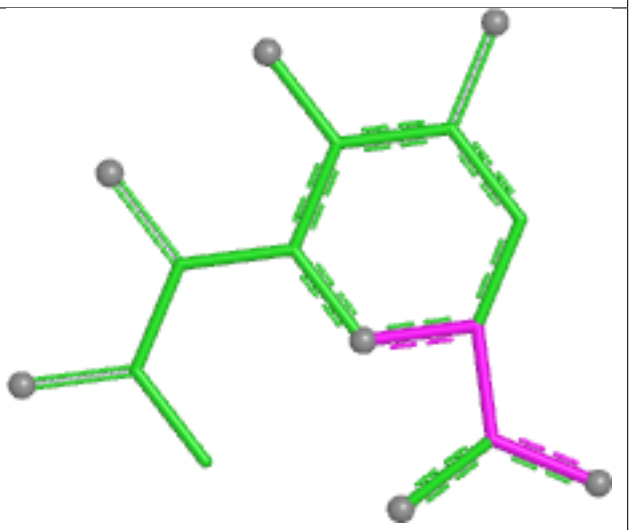
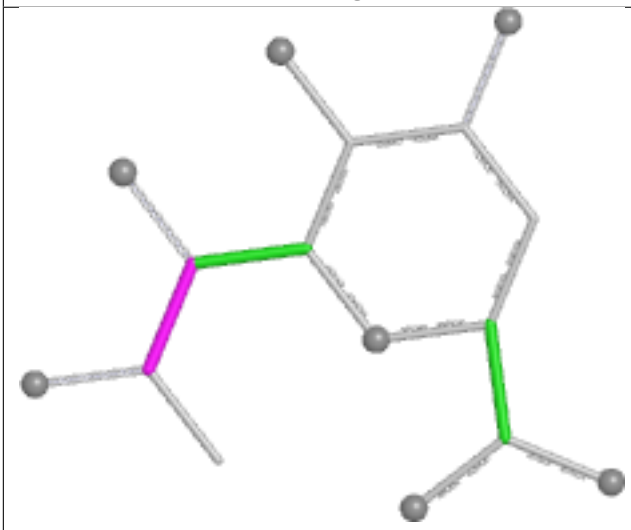


Bond angles



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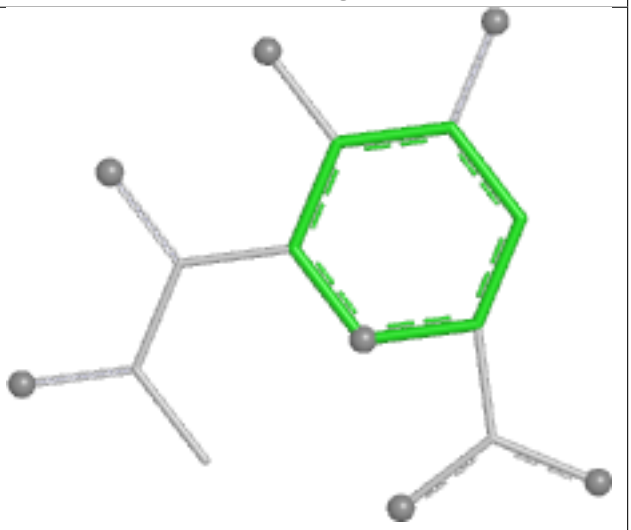
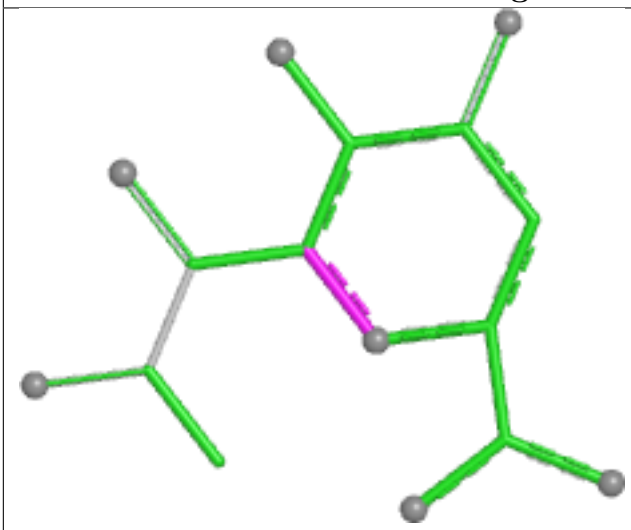


Rings

Ligand P8E XM 602



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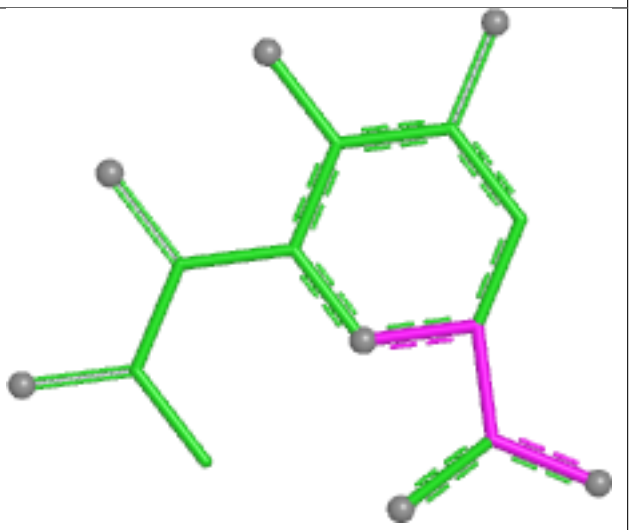
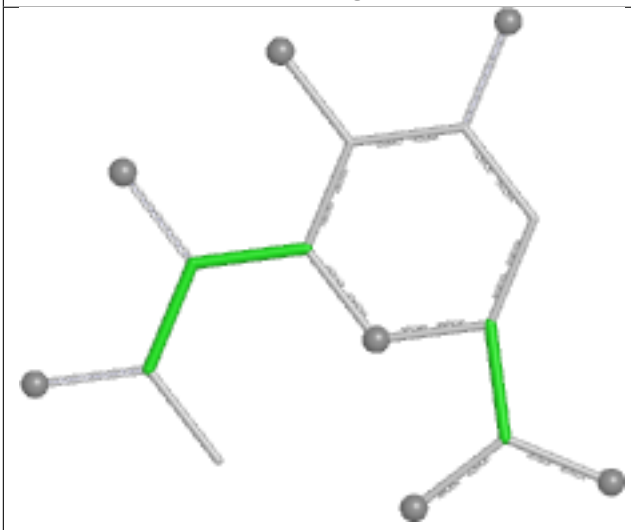


Bond angles



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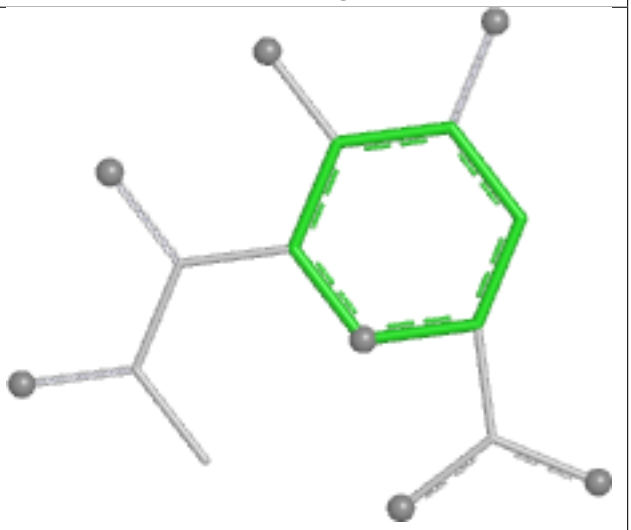
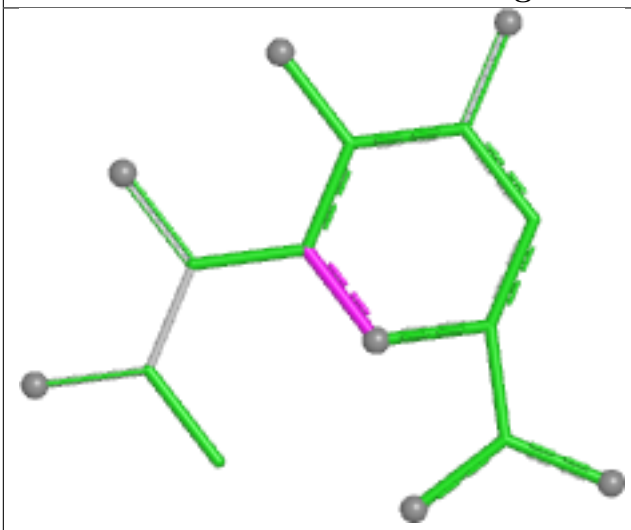


Rings

Ligand P8E aW 606



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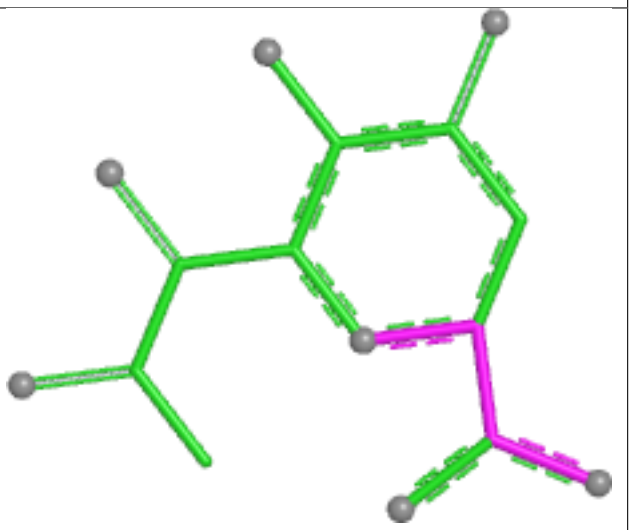
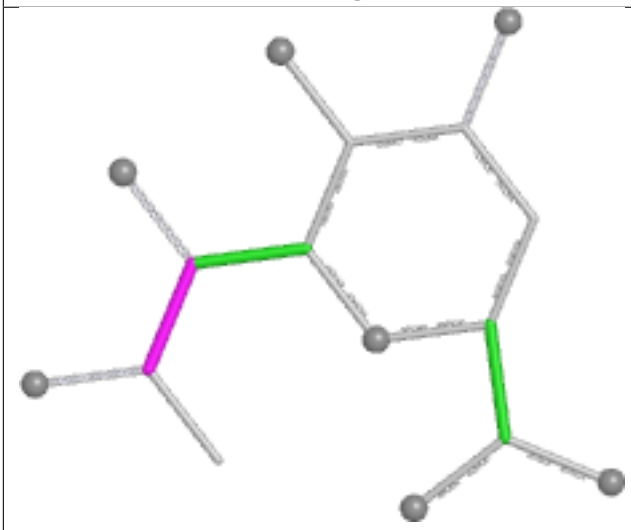
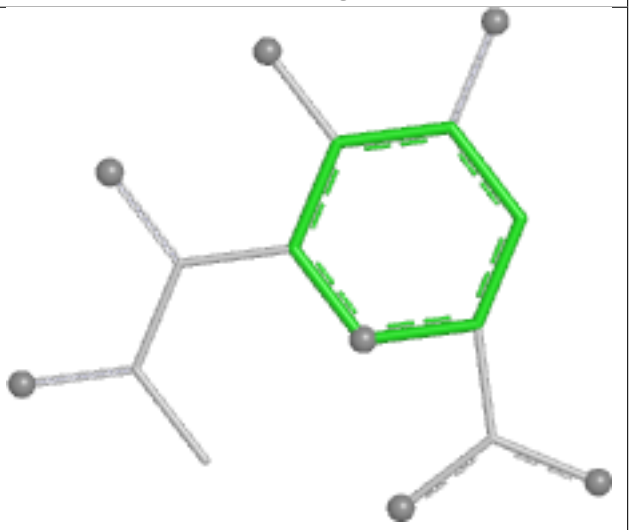


Bond angles

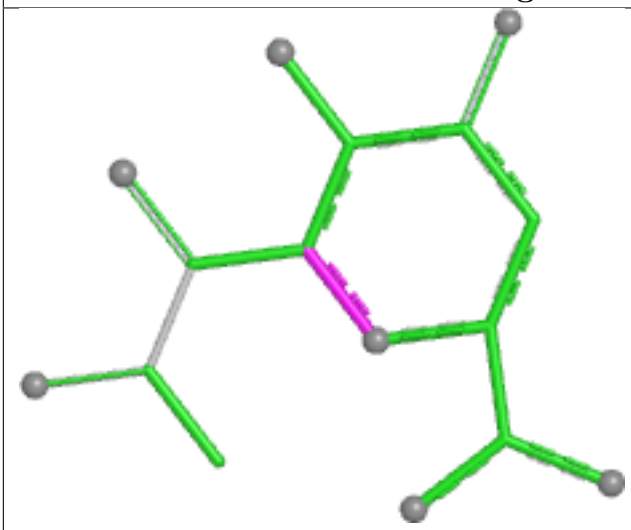


Torsions



Rings

Ligand P8E TP 605



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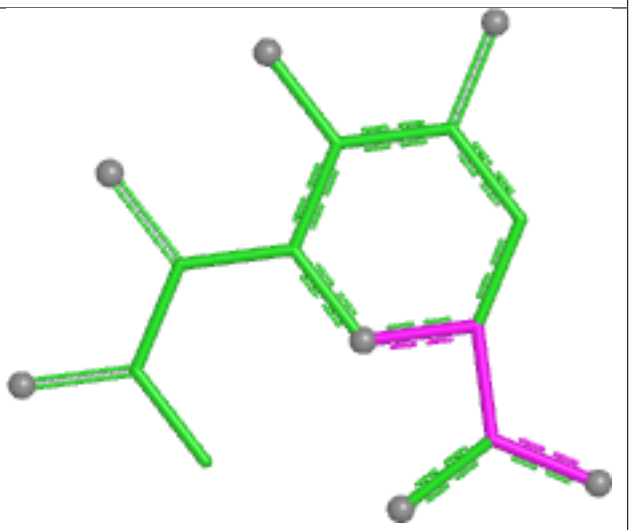
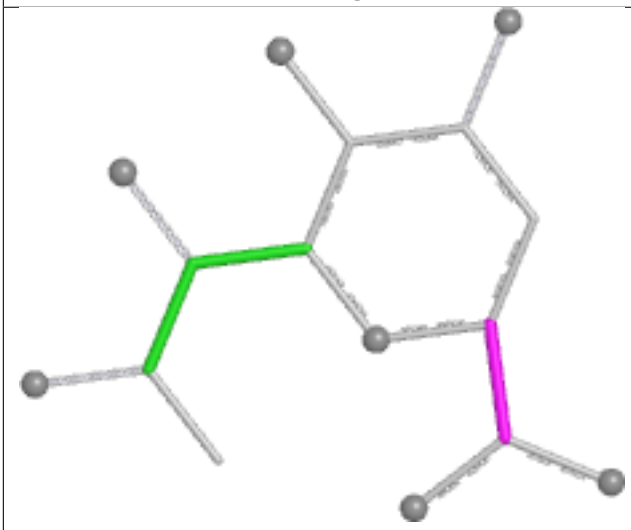


Bond angles



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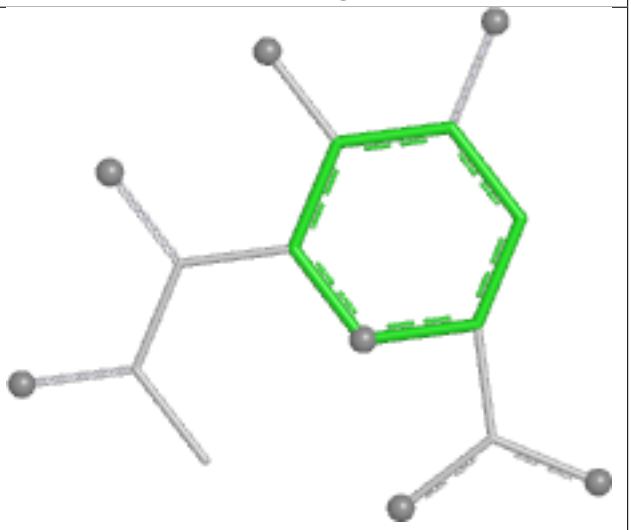
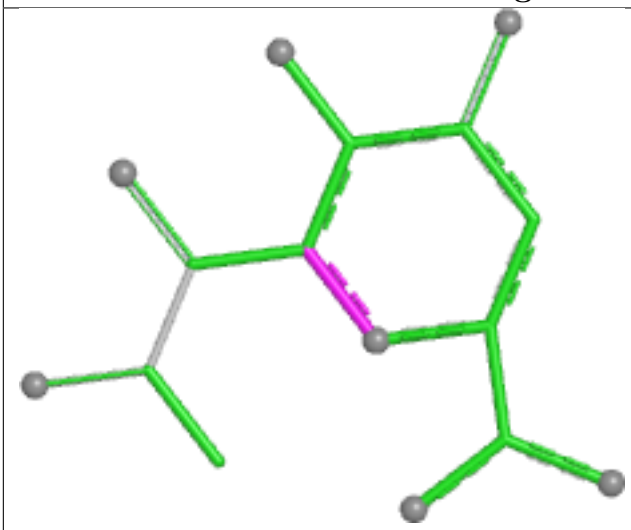


Rings

Ligand P8E aW 605



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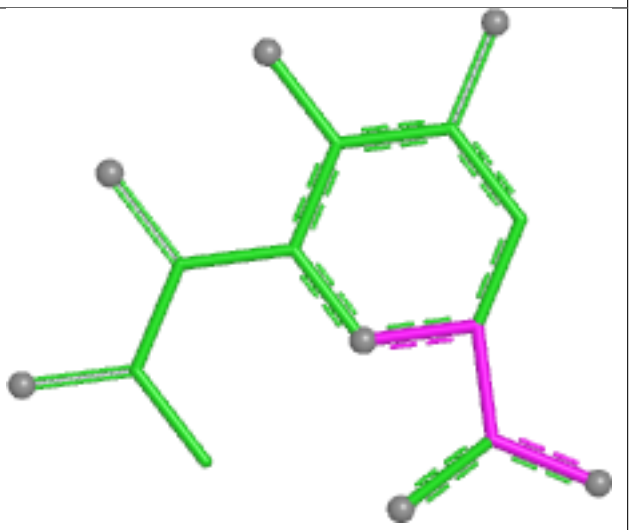

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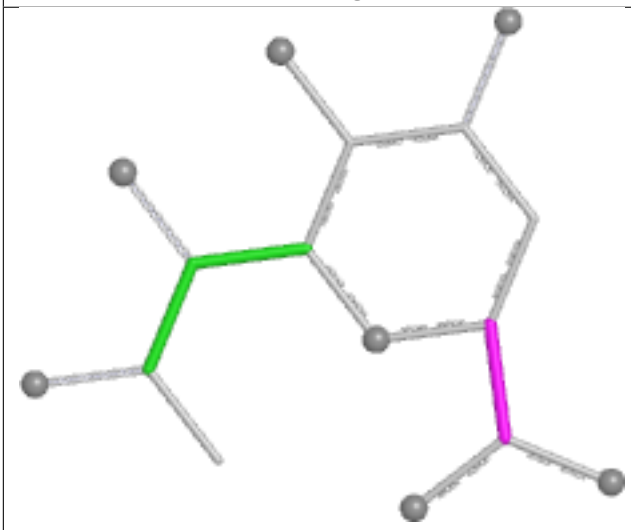

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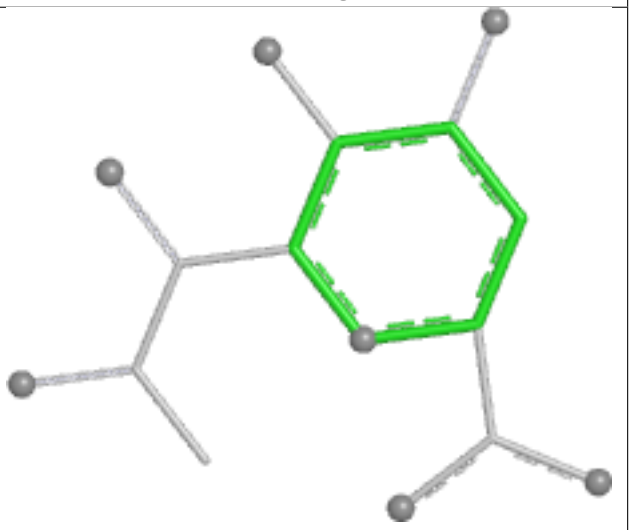
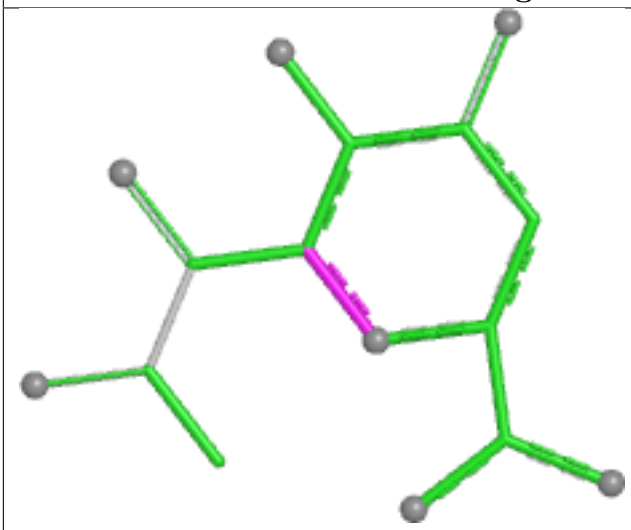


Rings

Ligand P8E OA 601



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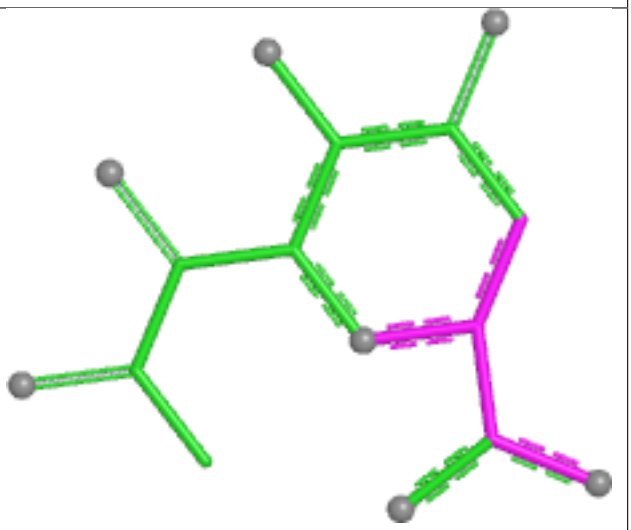
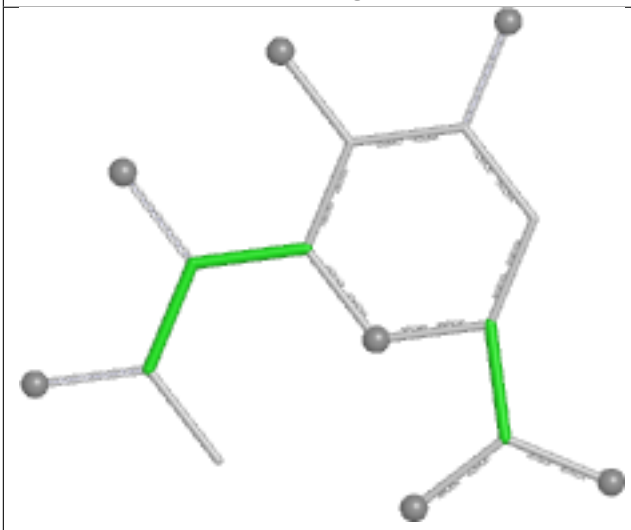


Bond angles



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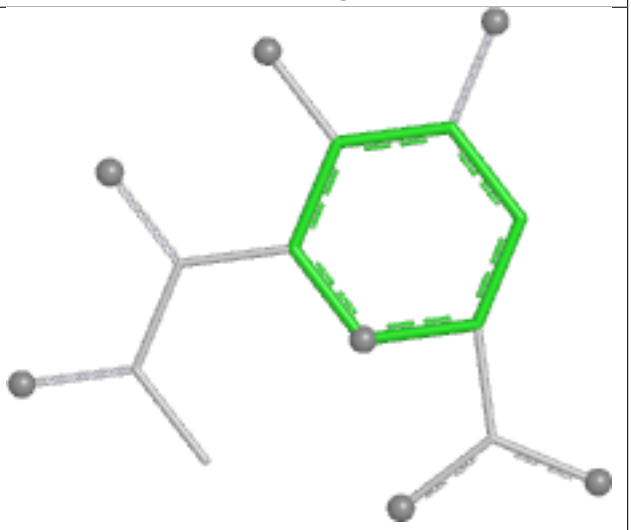
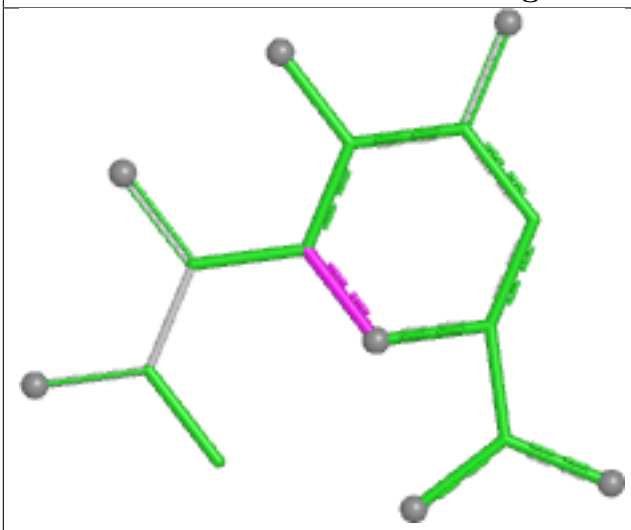


Rings

Ligand P8E bS 602



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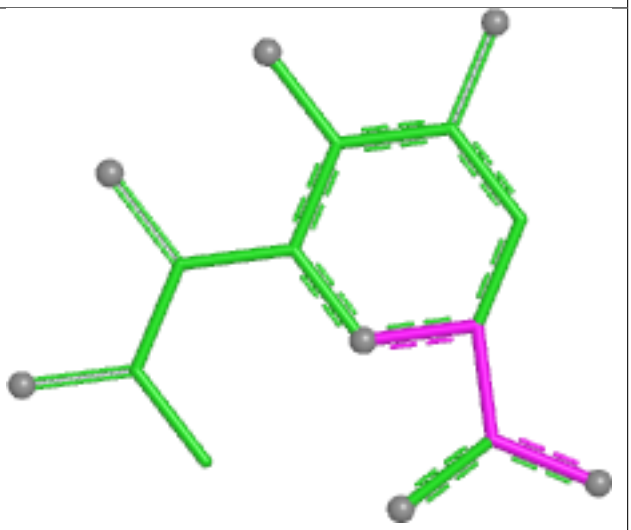
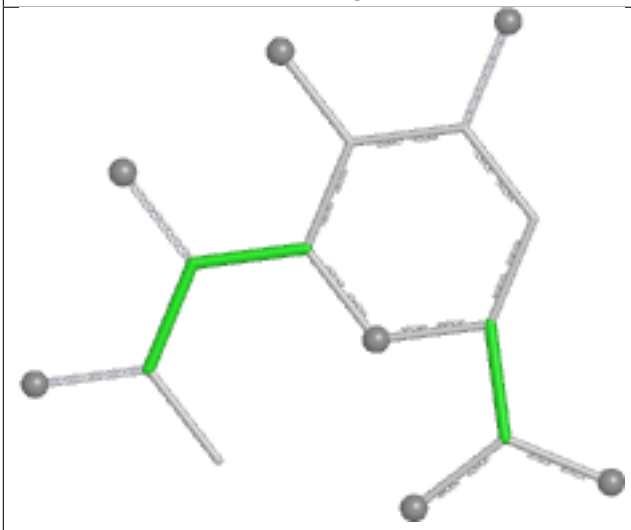


Bond angles



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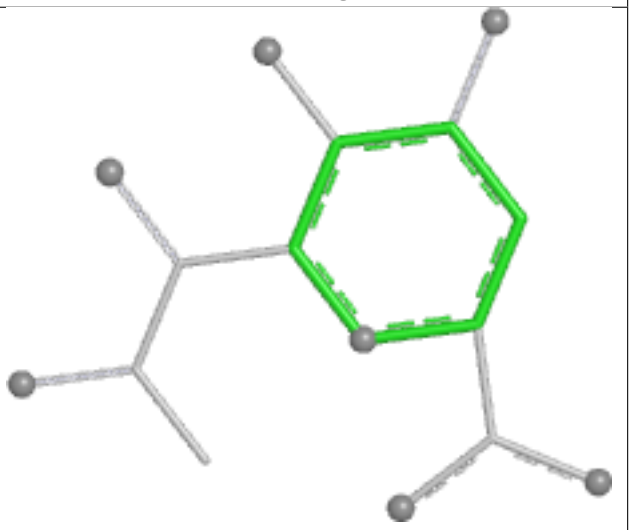
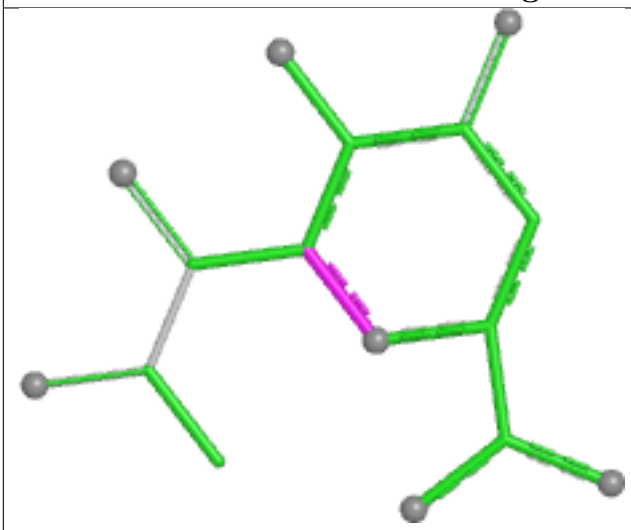


Rings

Ligand P8E bS 607



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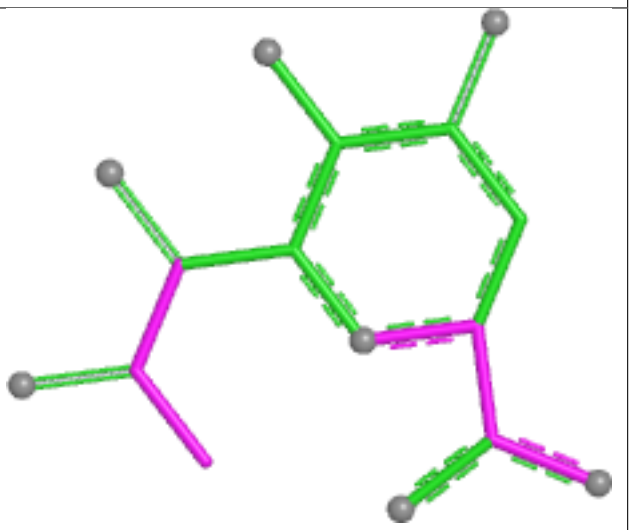

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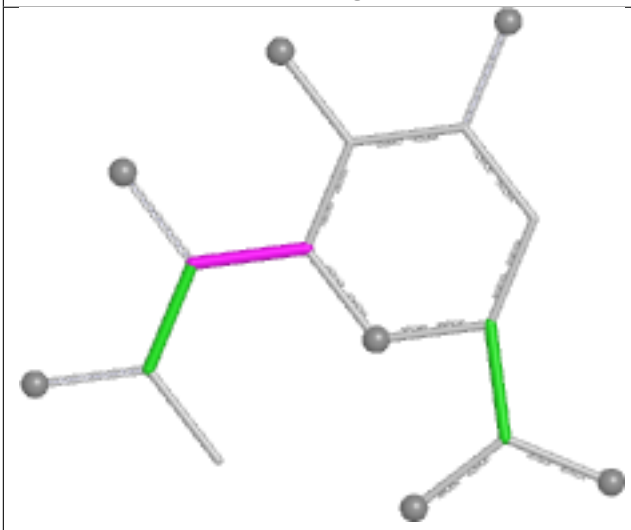

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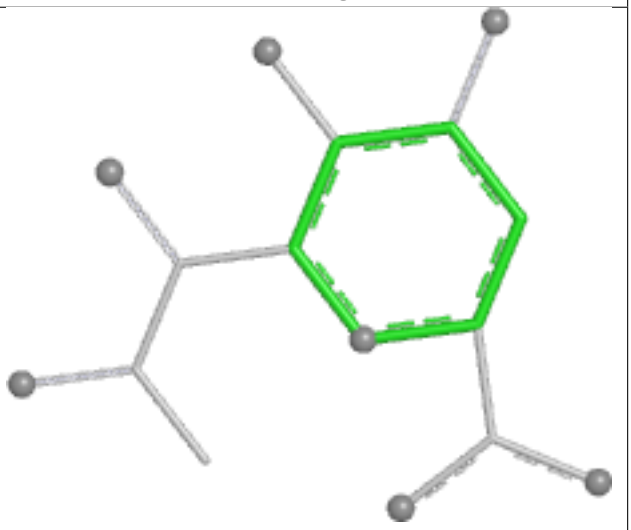
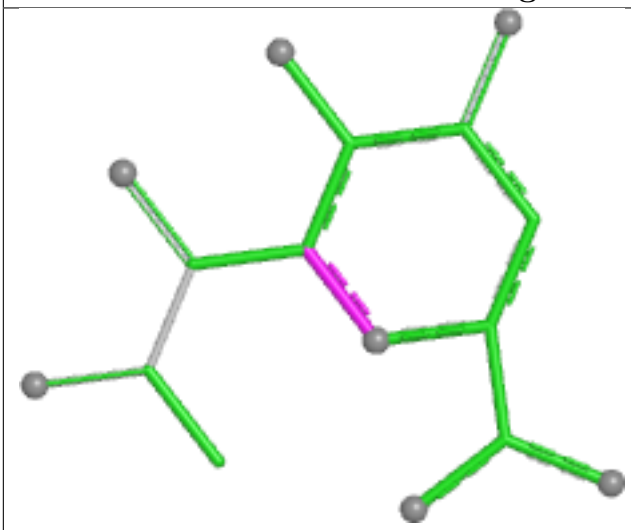


Rings

Ligand P8E R4 603



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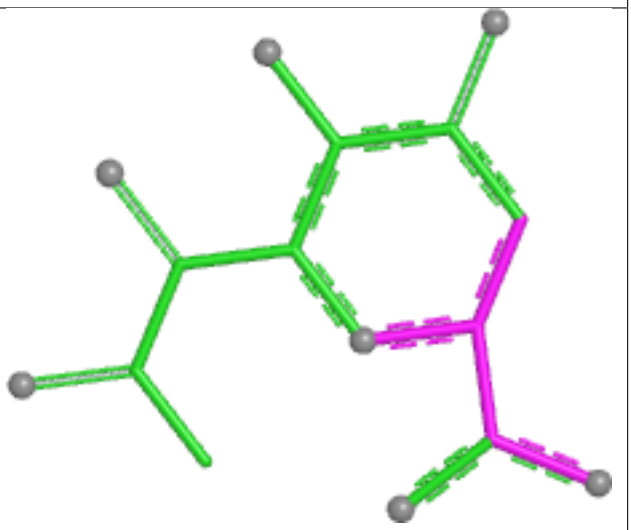

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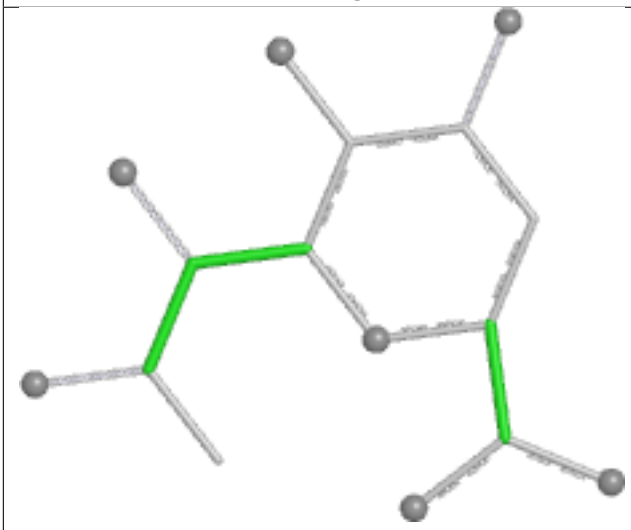

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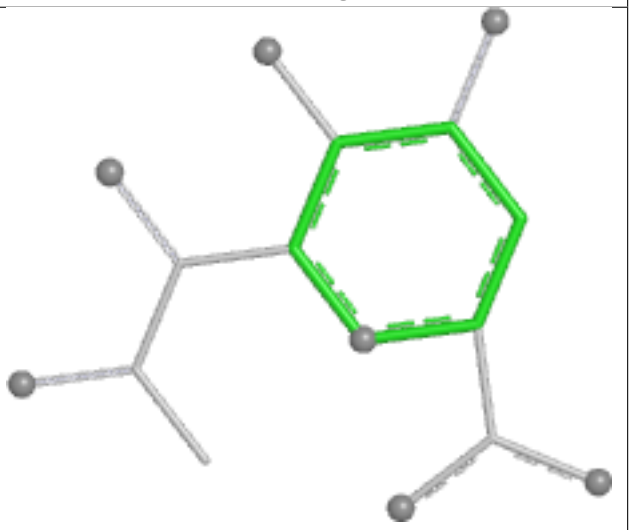
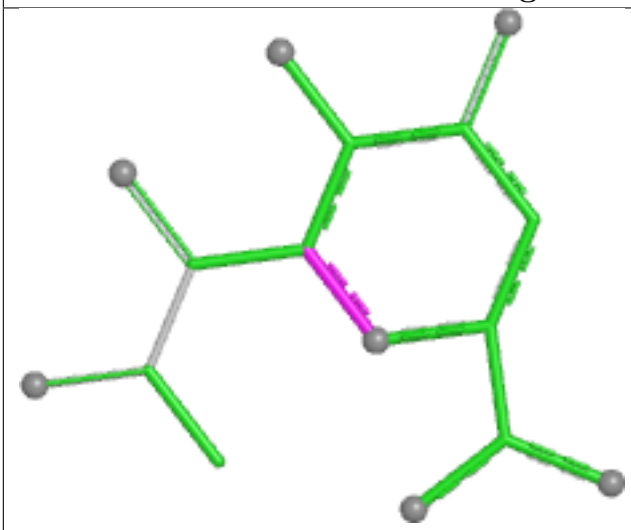


Rings

Ligand P8E BJ 605



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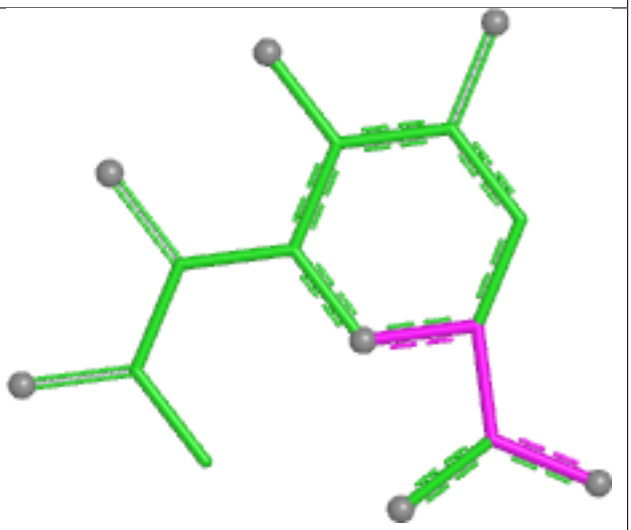

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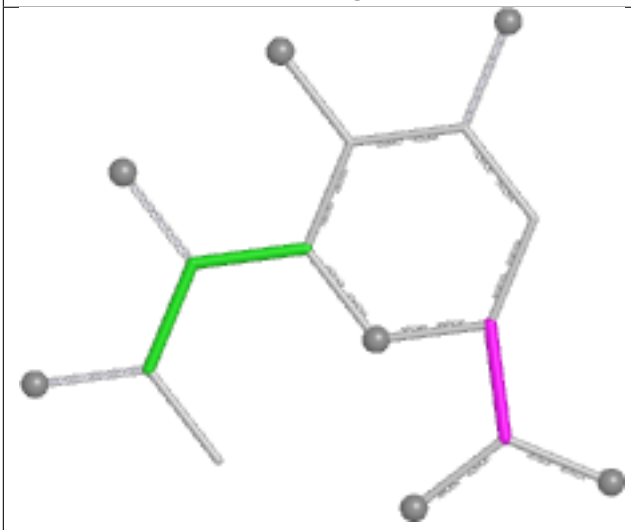

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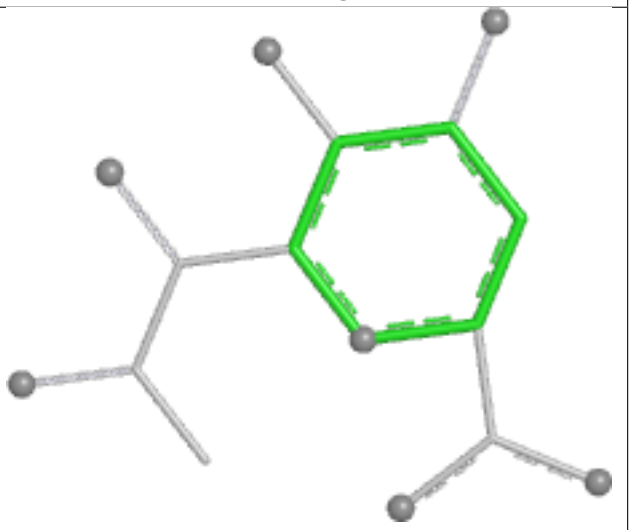

Rings

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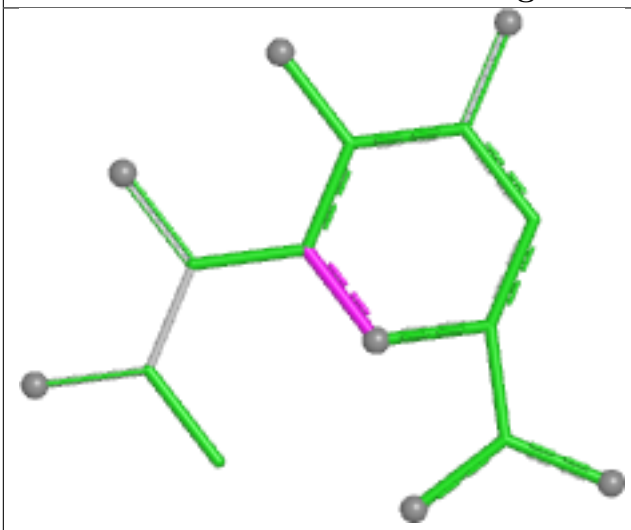

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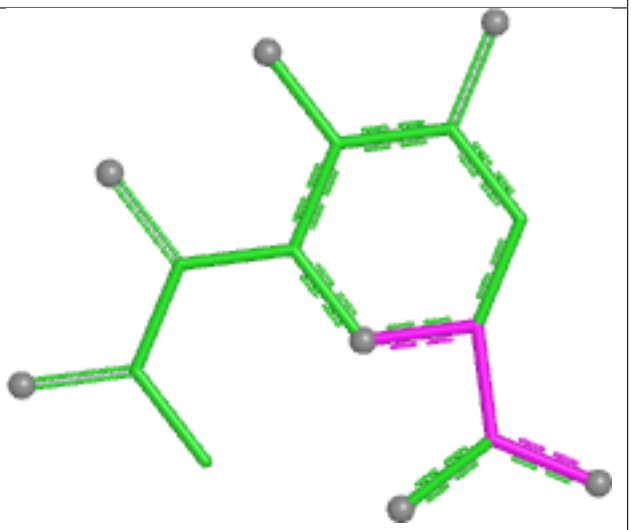
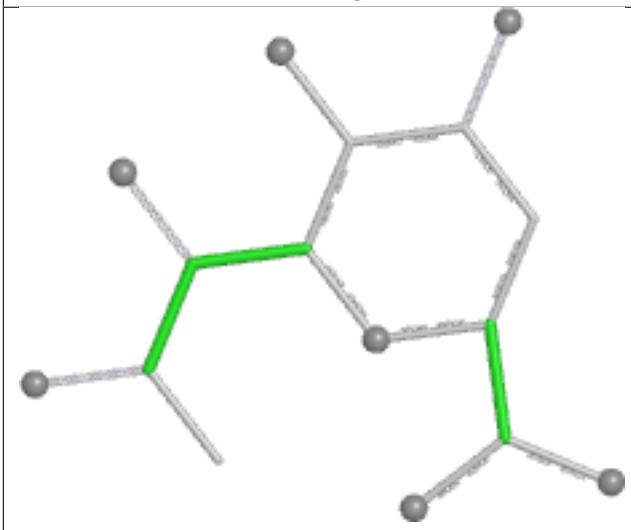


Bond angles



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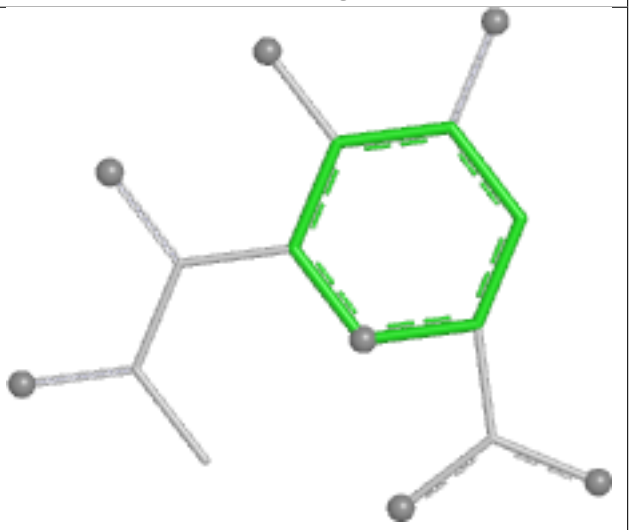
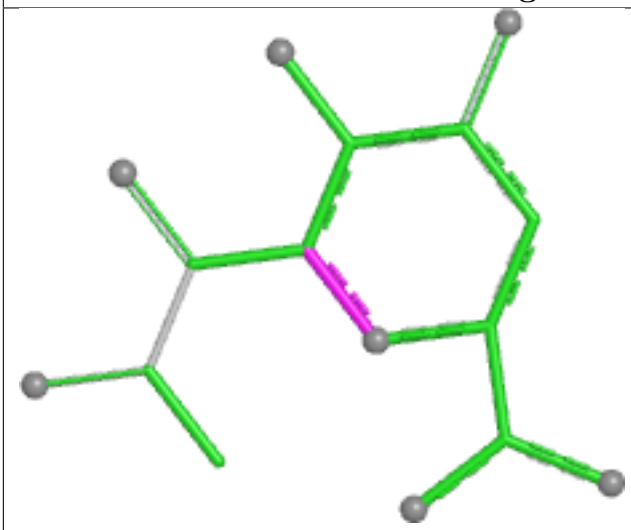


Rings

Ligand P8E Q2 602



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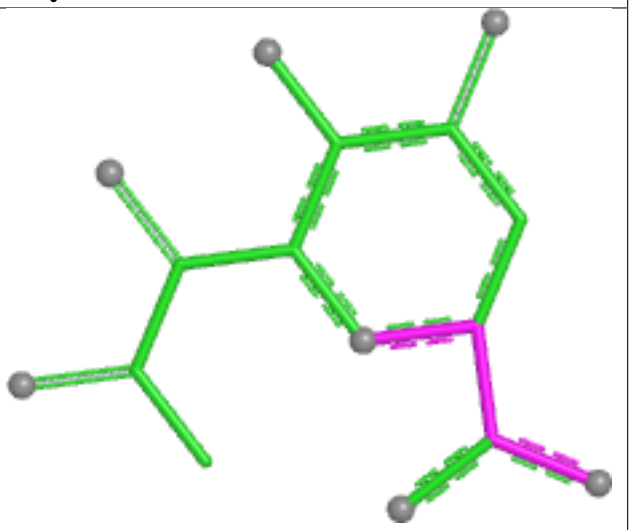

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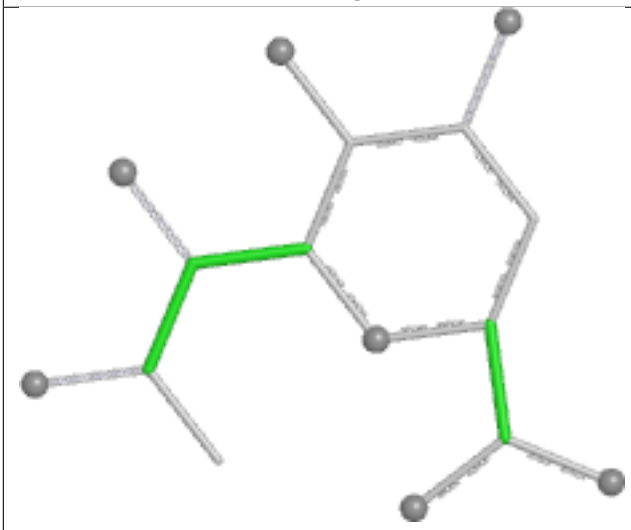

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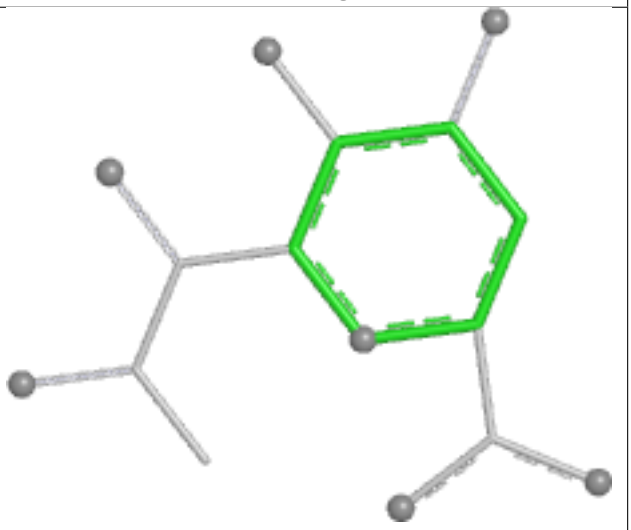

Rings

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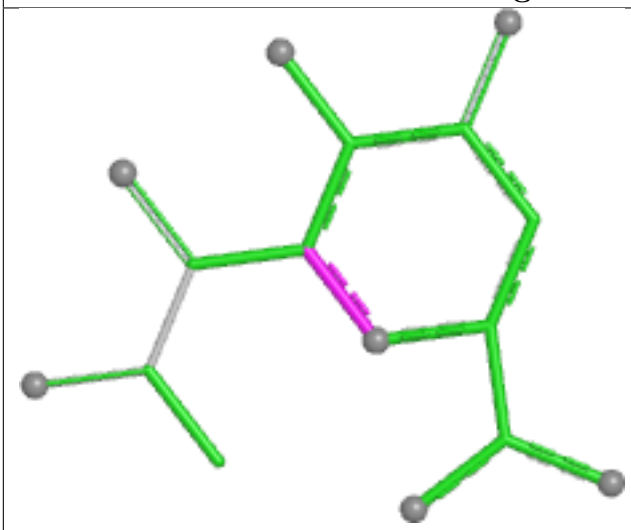

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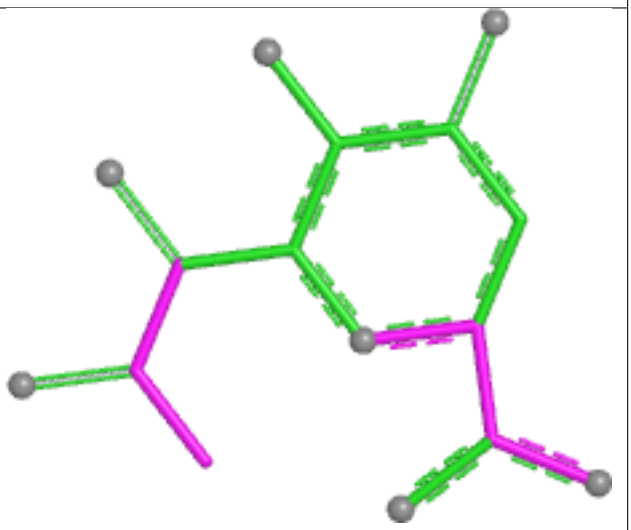

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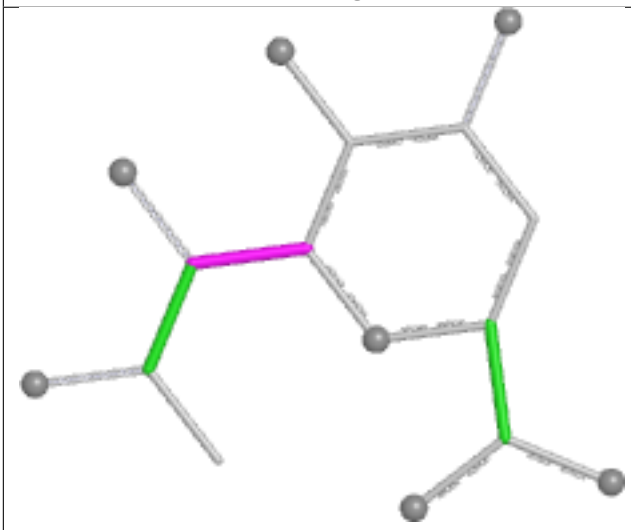

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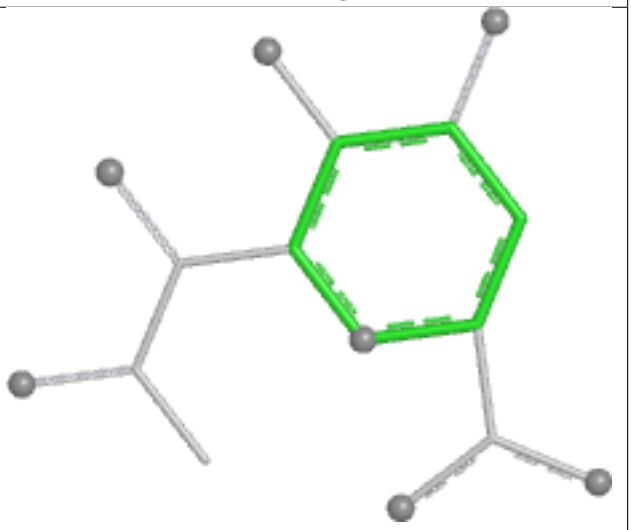
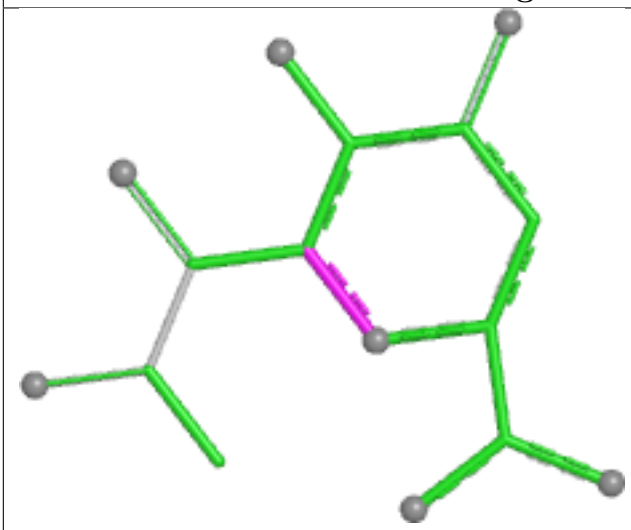


Rings

Ligand P8E EX 603



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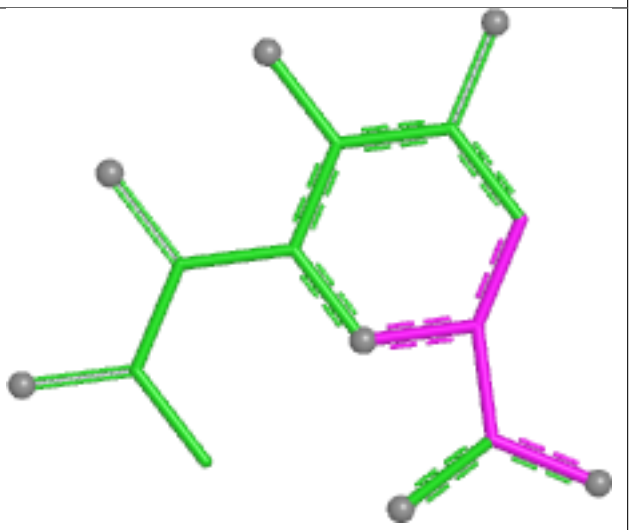

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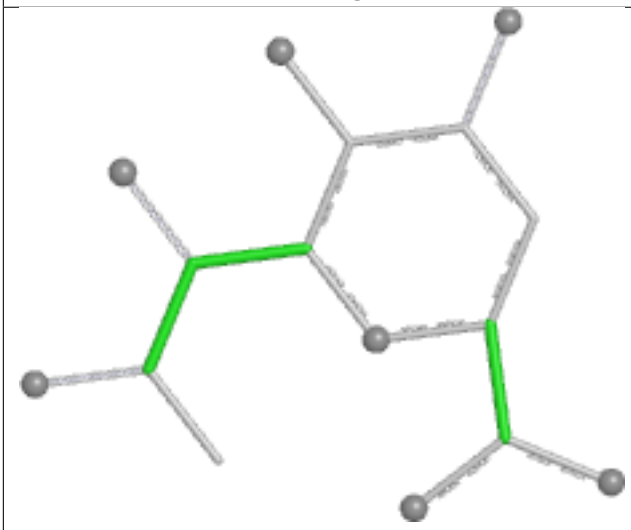

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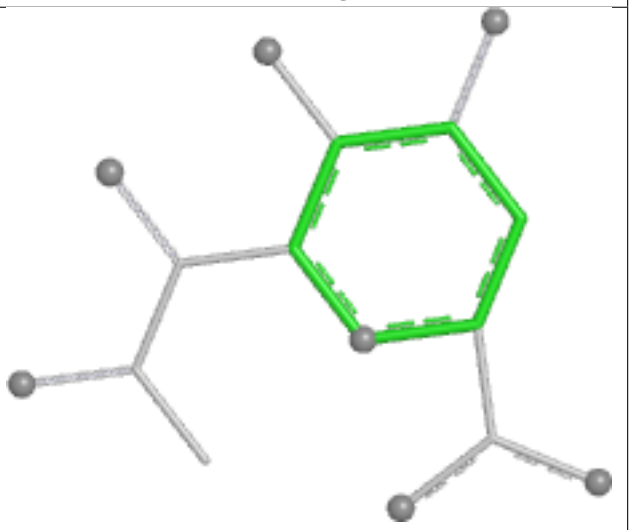
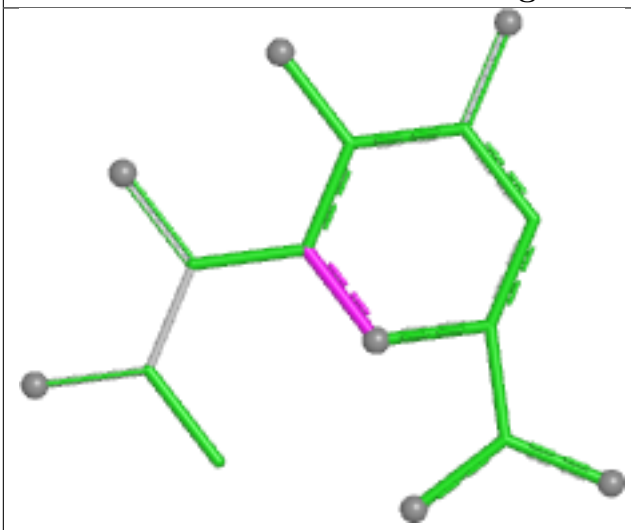


Rings

Ligand P8E dC 605



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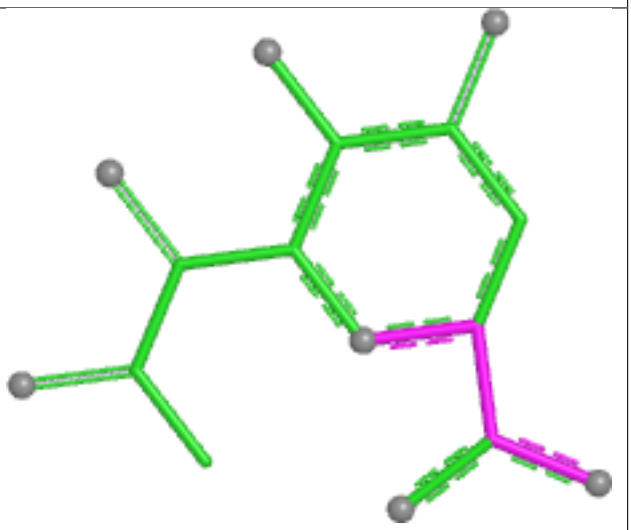

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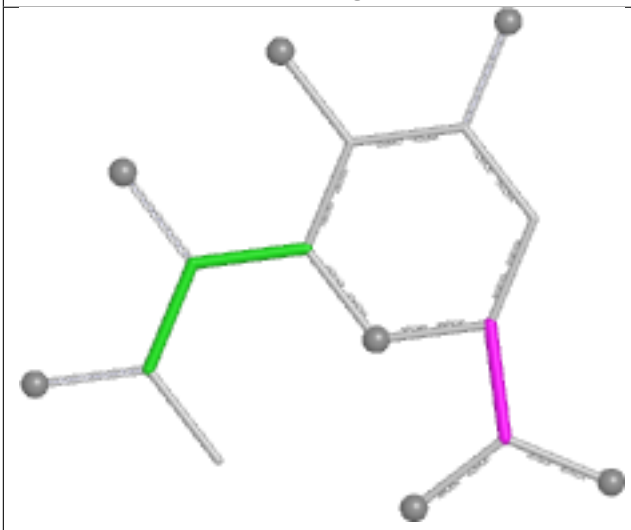

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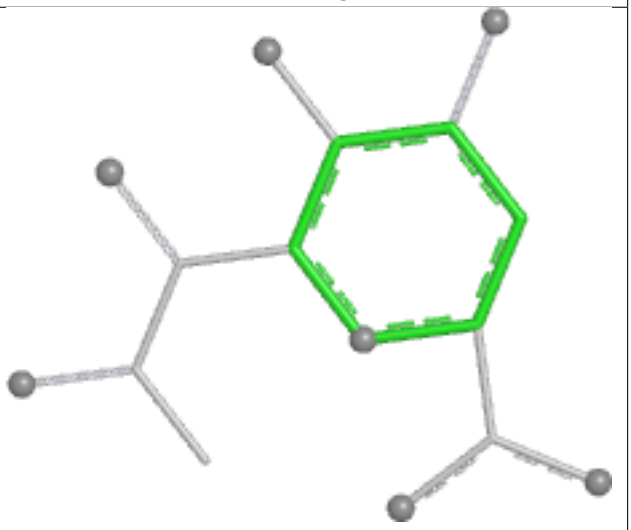
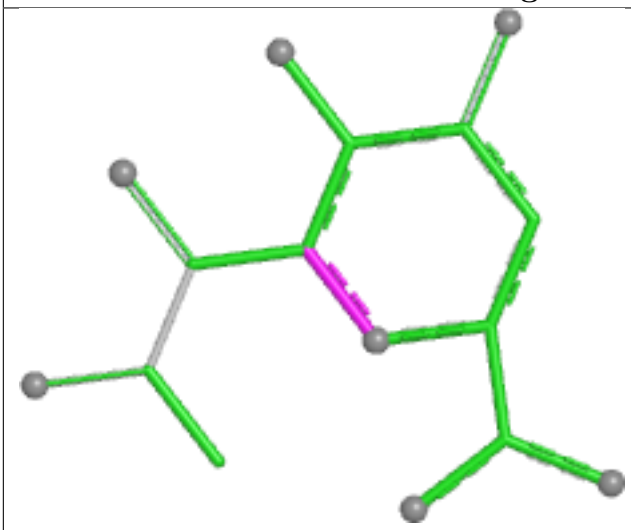


Rings

Ligand P8E NI 601



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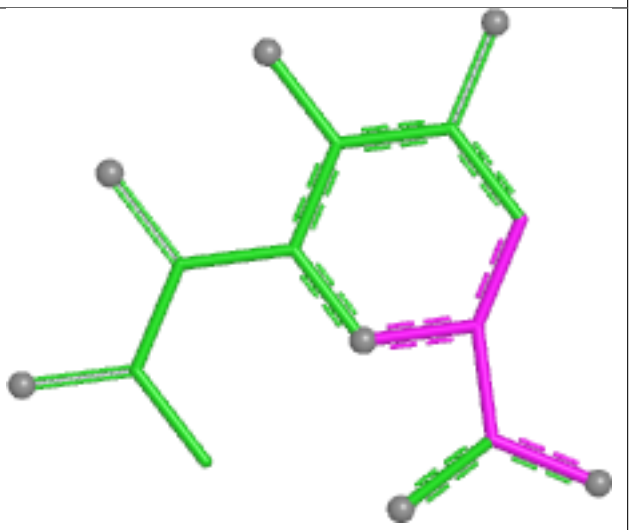
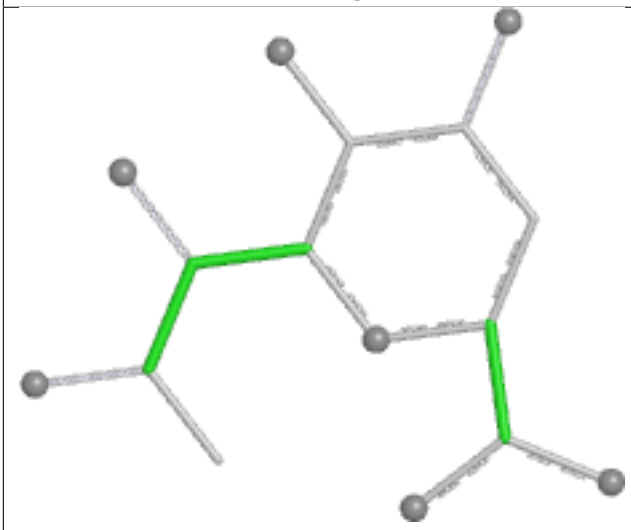


Bond angles



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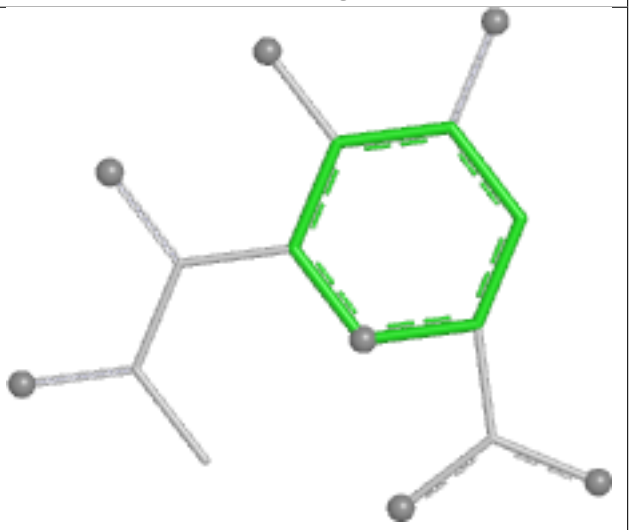
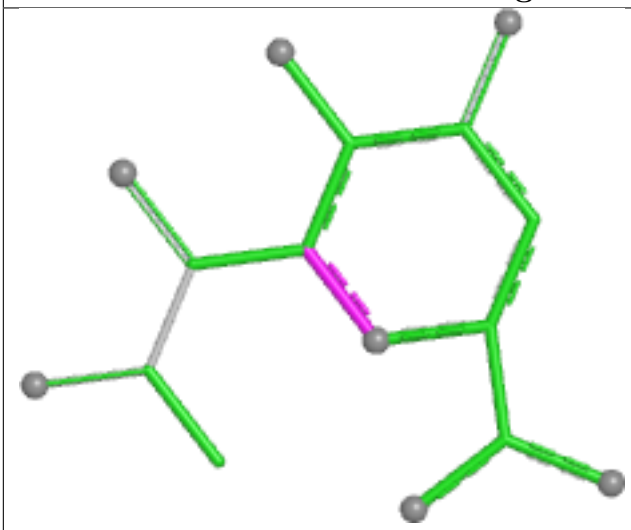
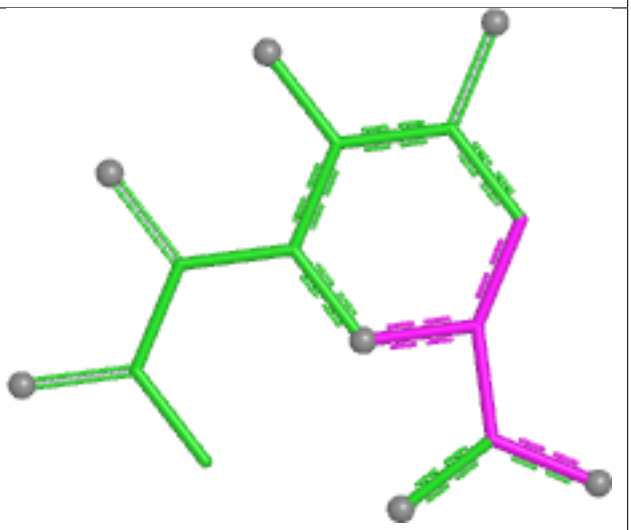


Rings

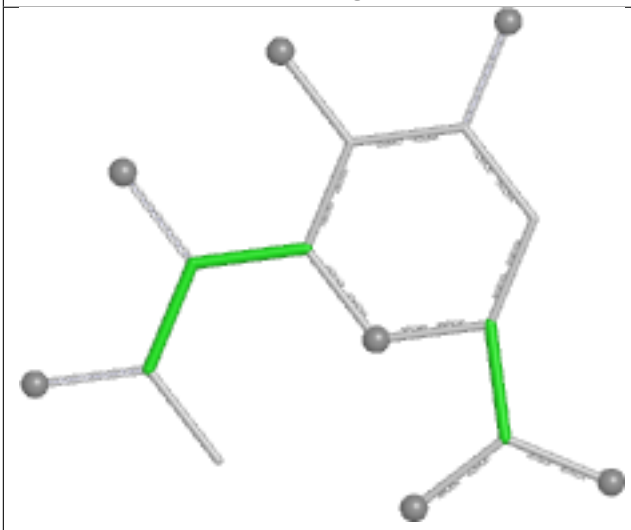
Ligand P8E PU 601



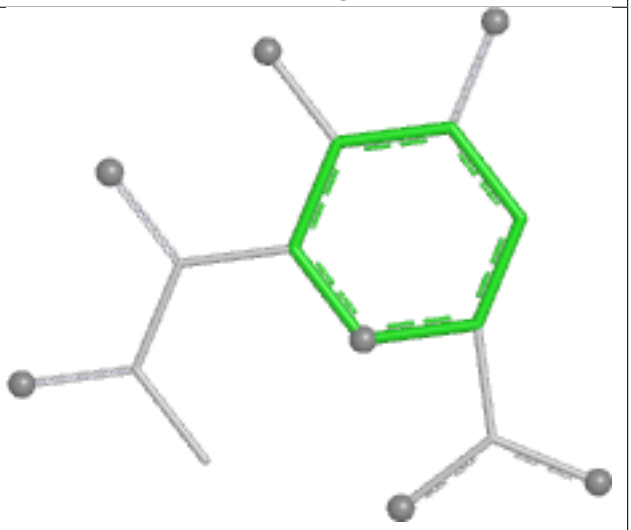
Bond lengths



Bond angles

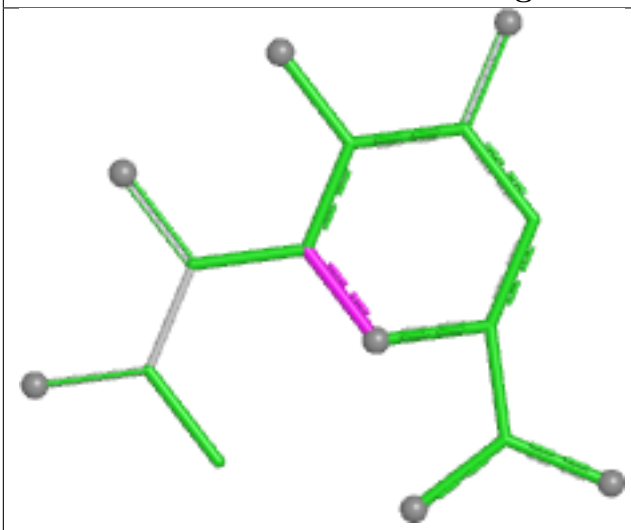


Torsions



Rings

Ligand P8E OA 602



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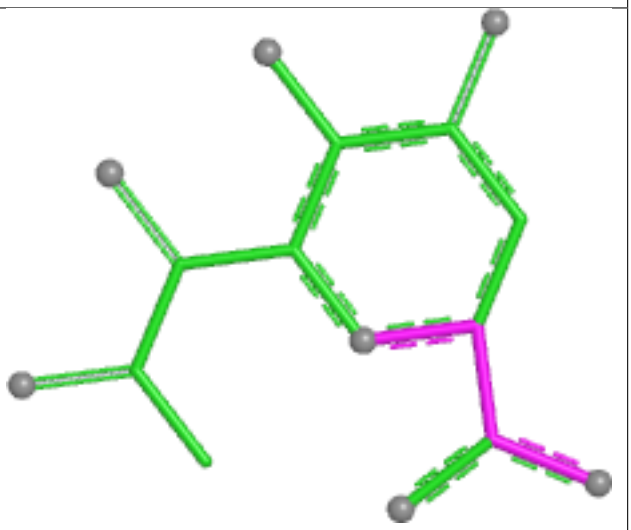

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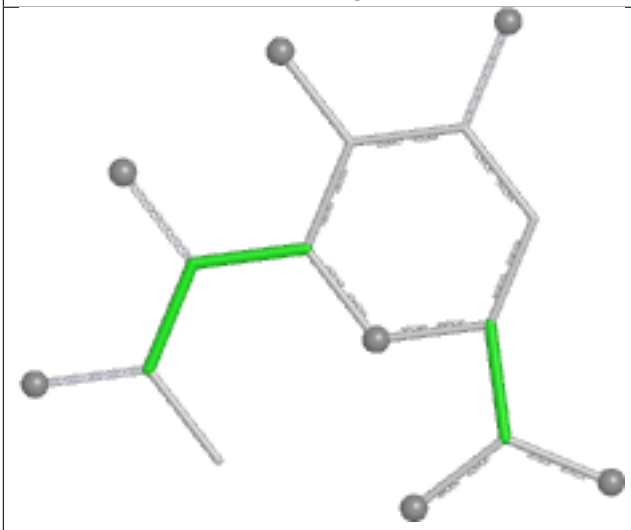

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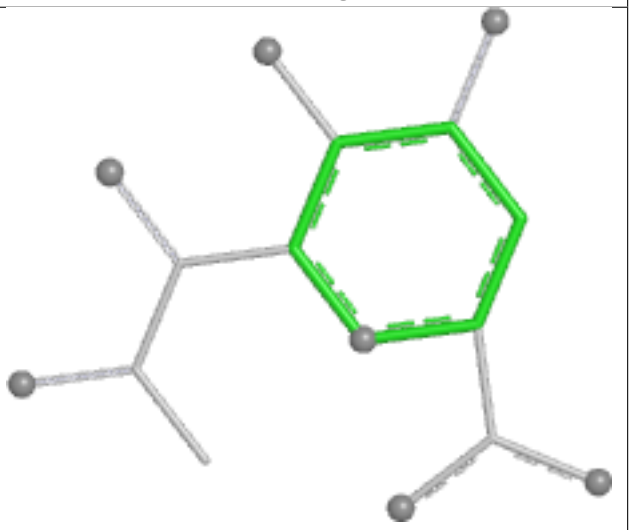
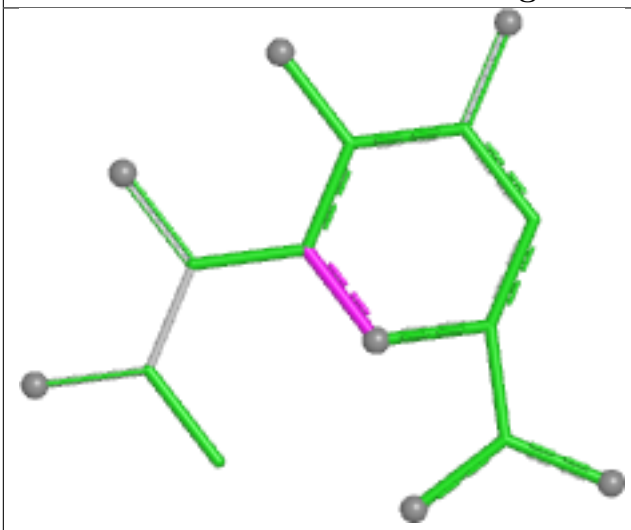


Rings

Ligand P8E R4 604



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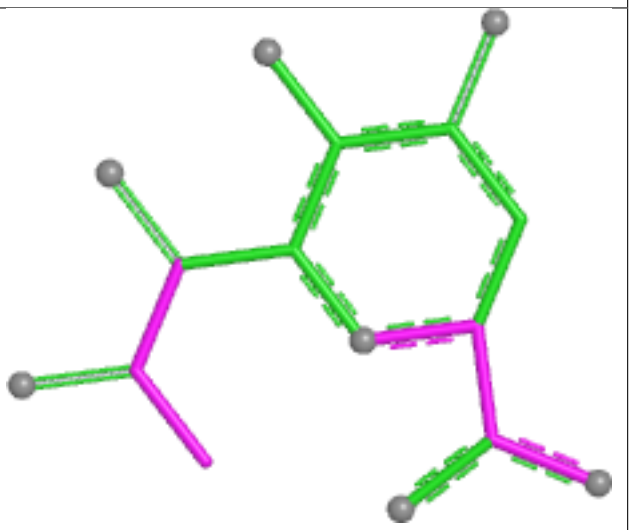

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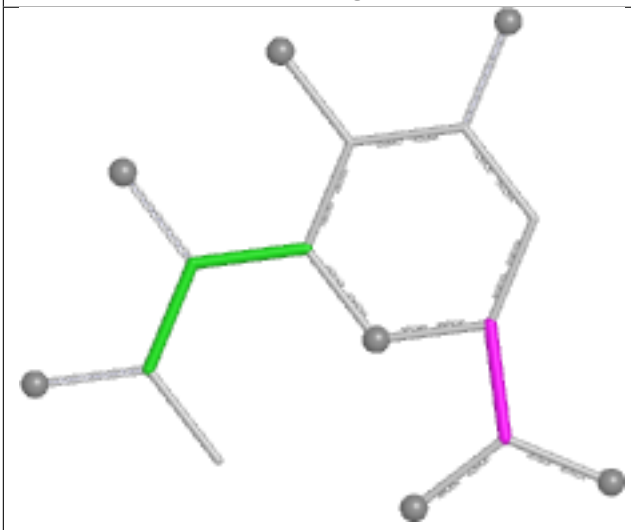

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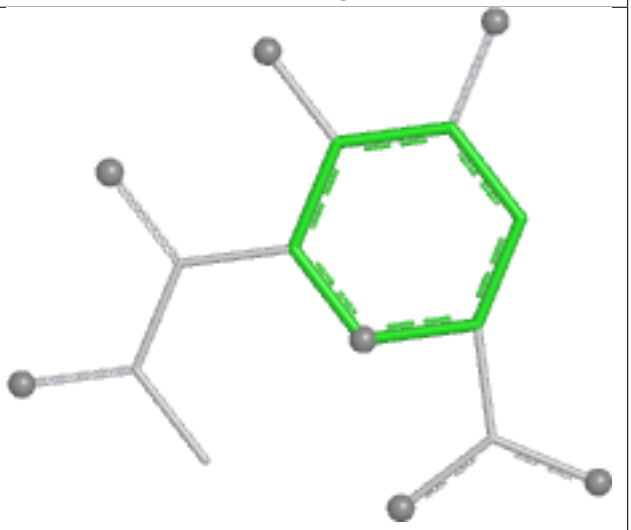

Rings

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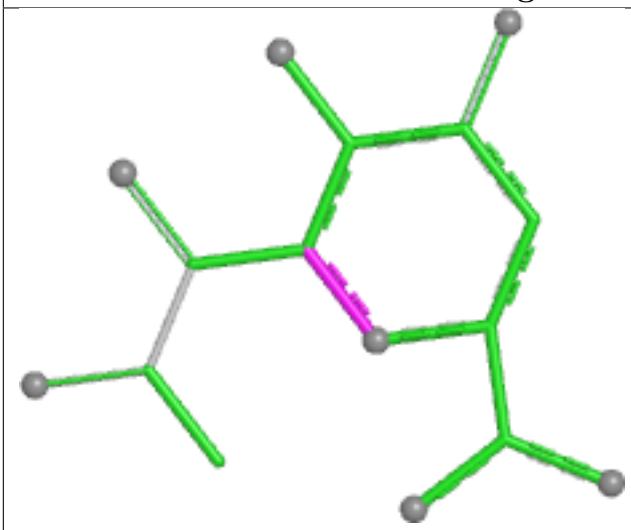

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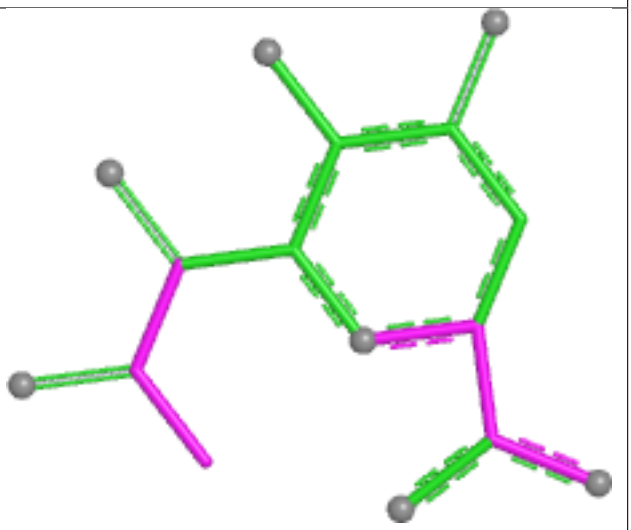

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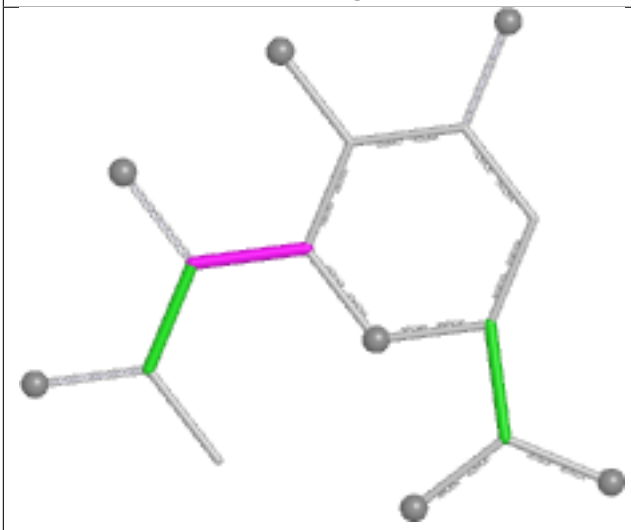

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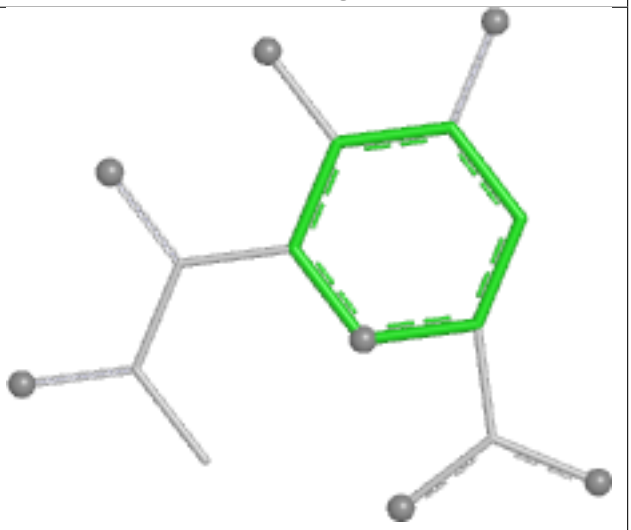

Rings

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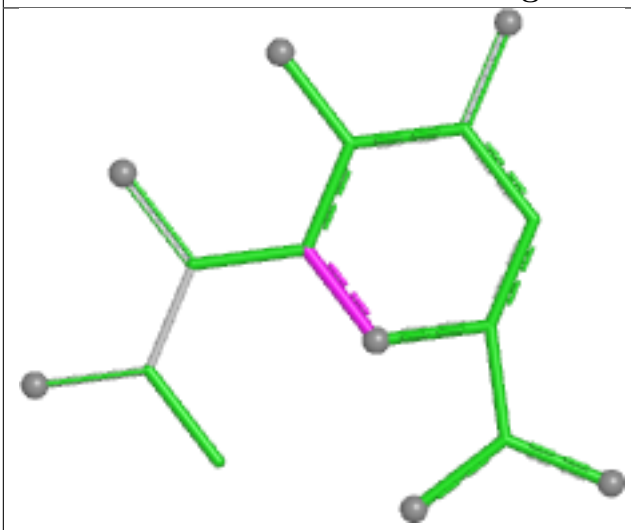

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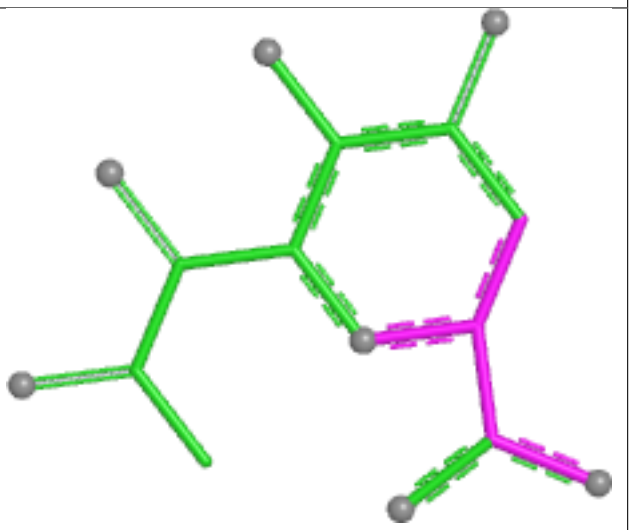

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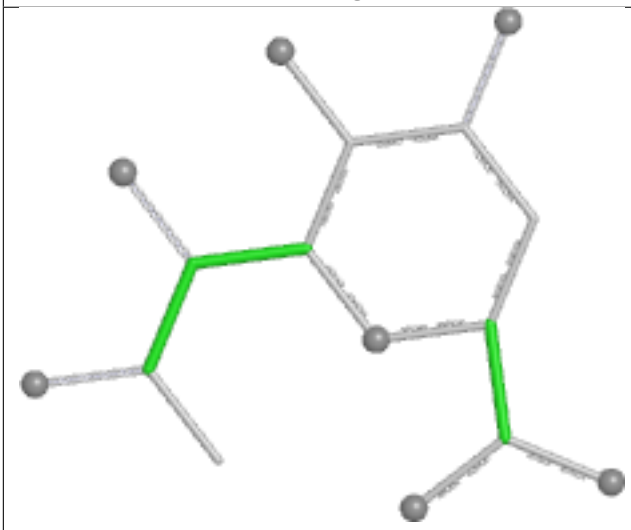

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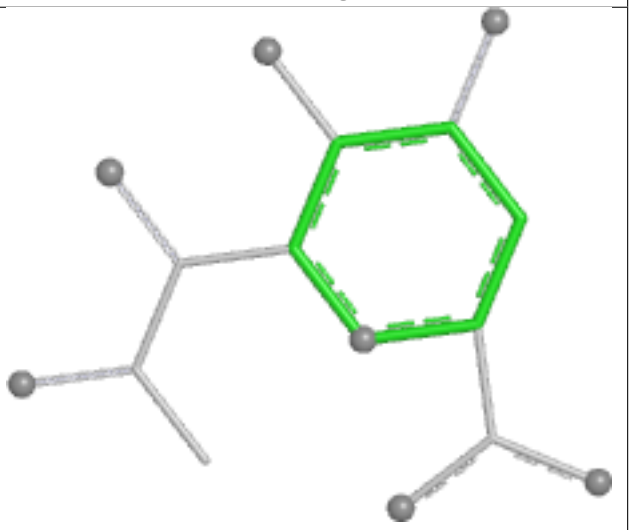
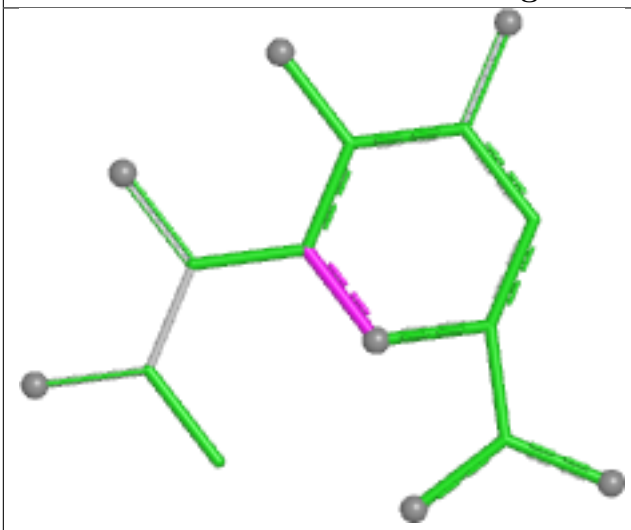


Rings

Ligand P8E NI 603



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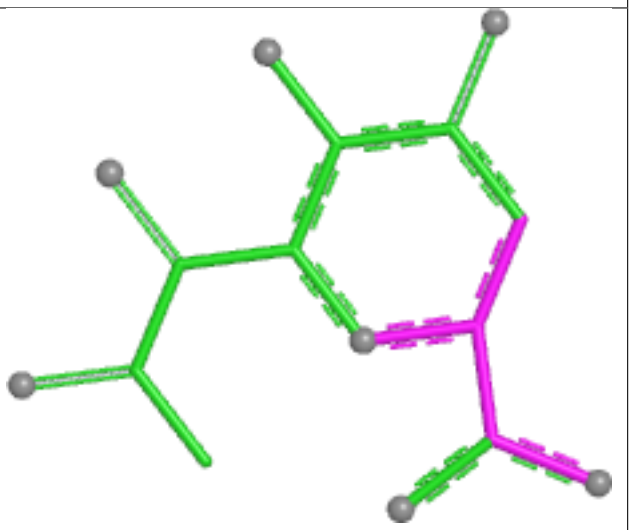

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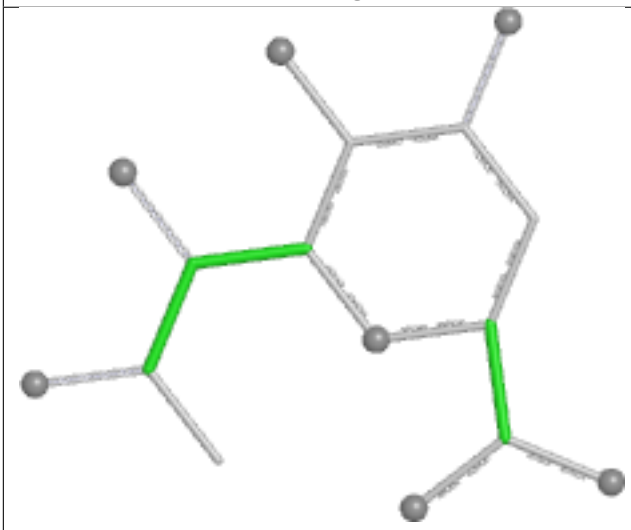

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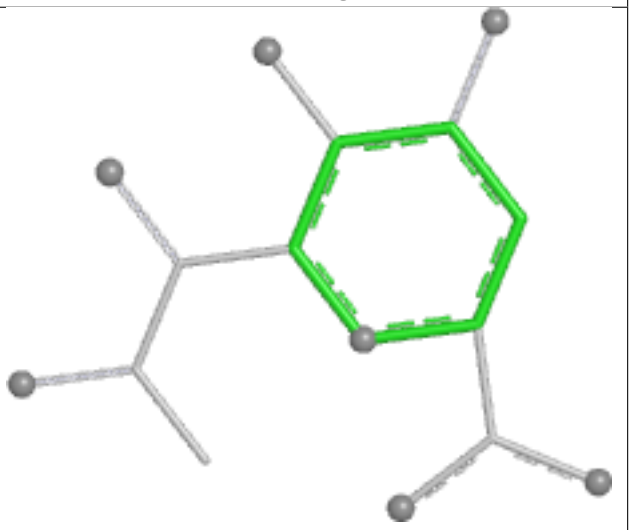
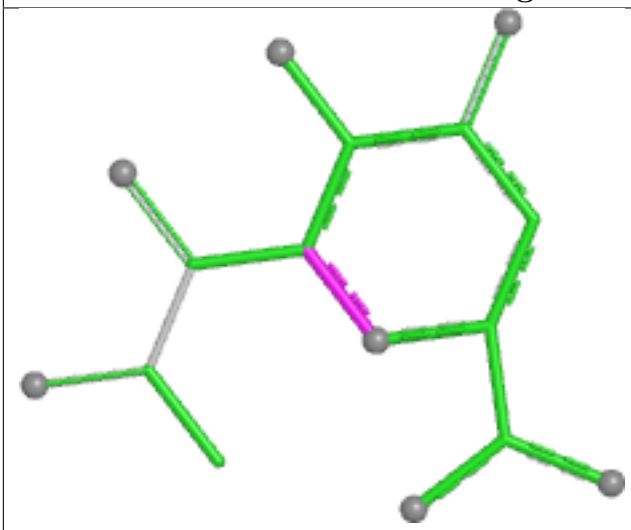


Rings

Ligand P8E EX 602



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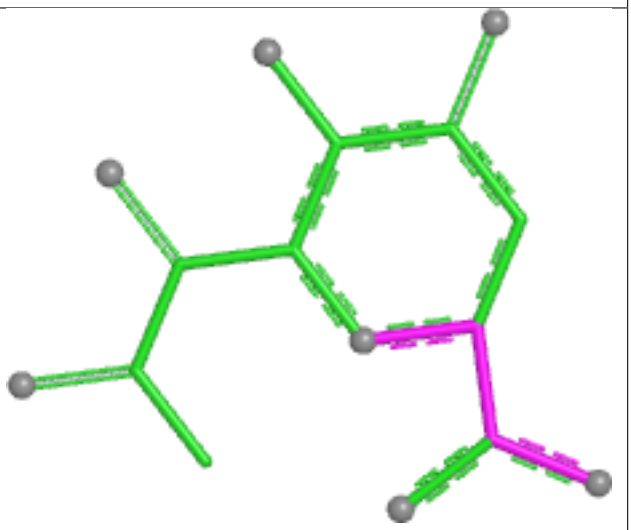

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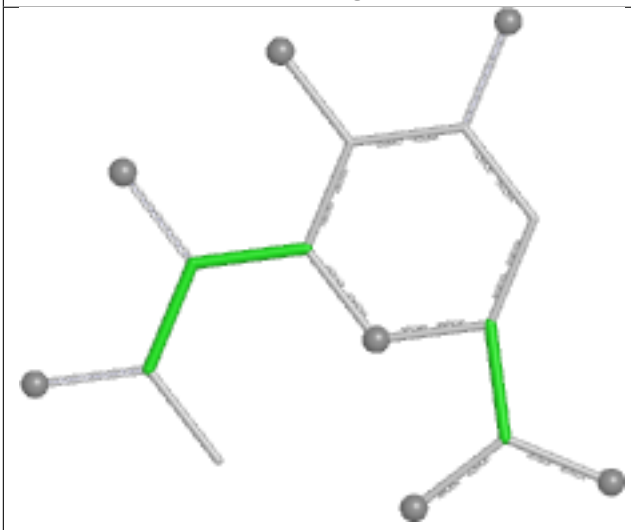

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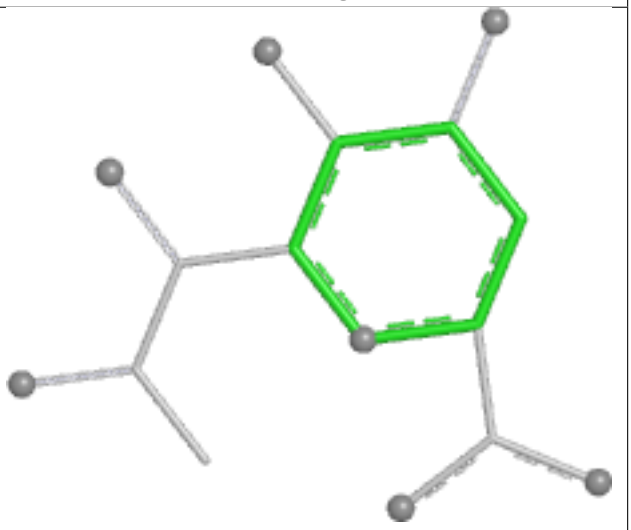

Rings

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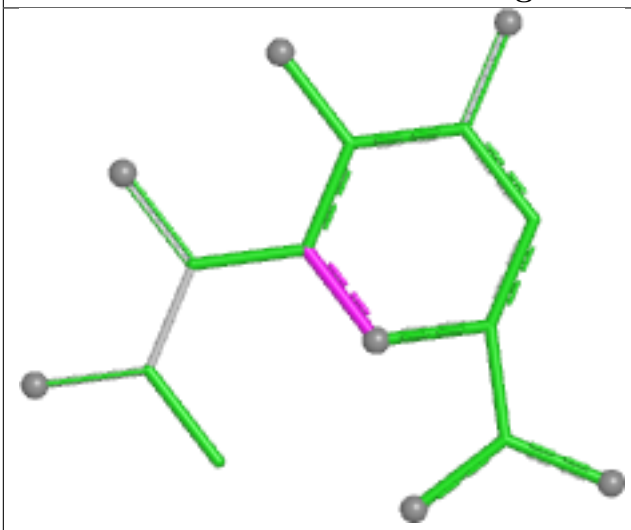

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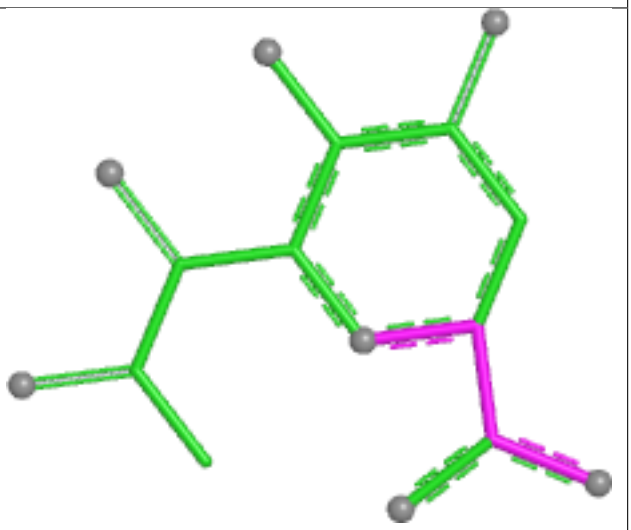

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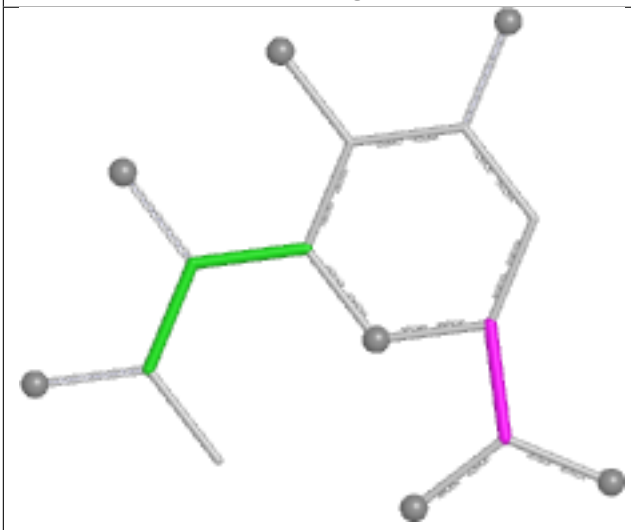

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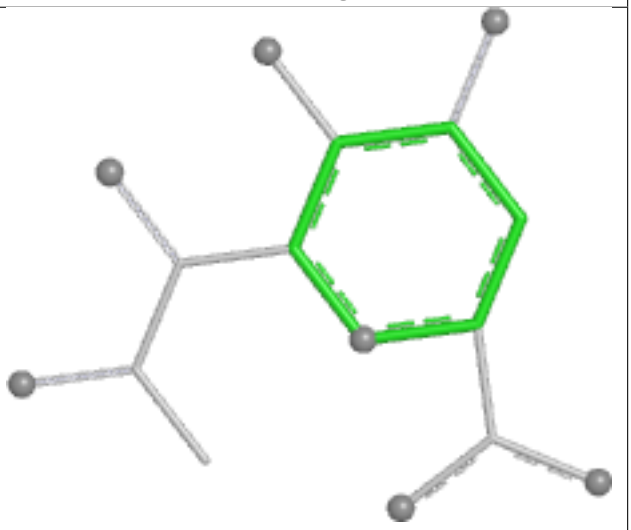
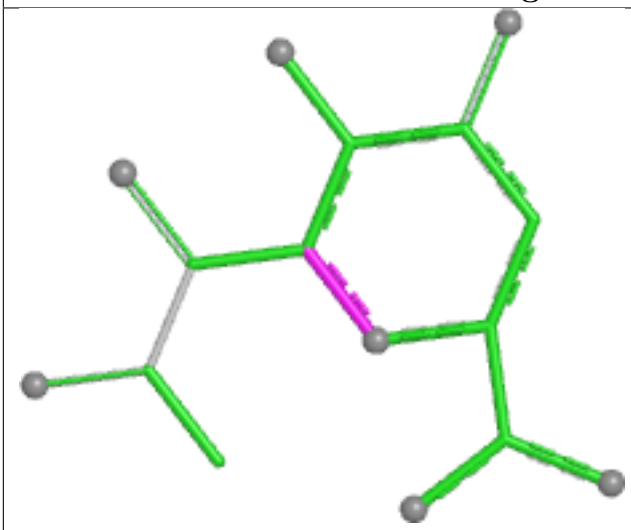


Rings

Ligand P8E Z9 606



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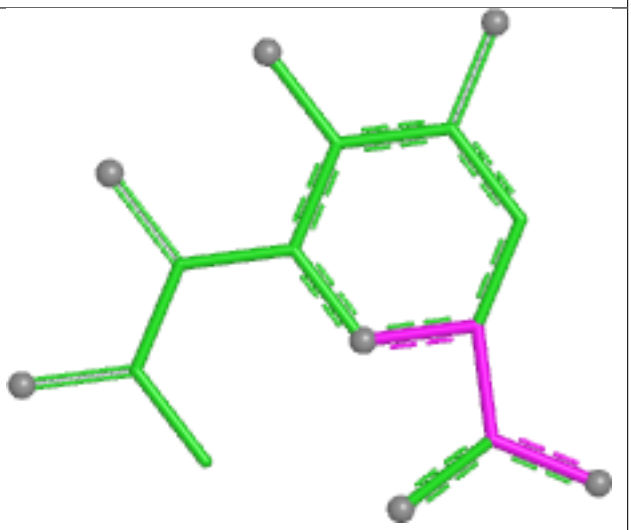

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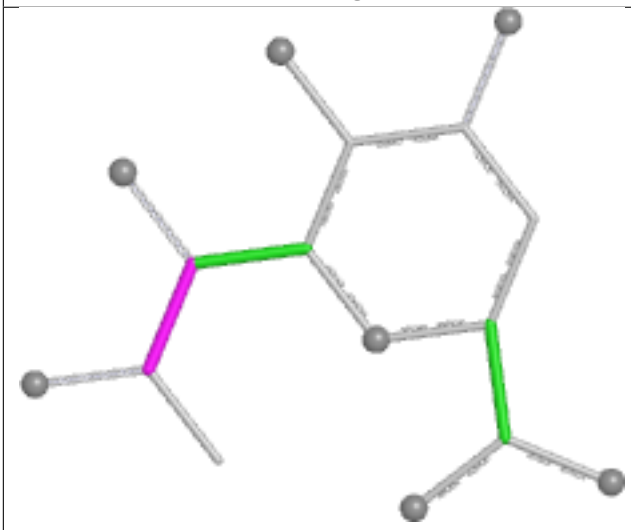

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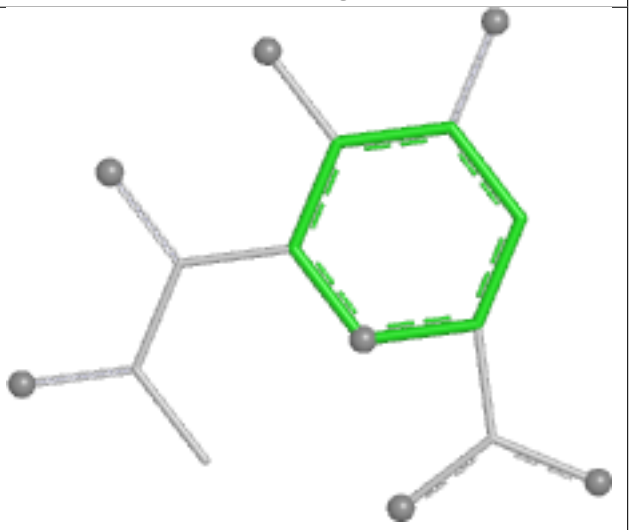
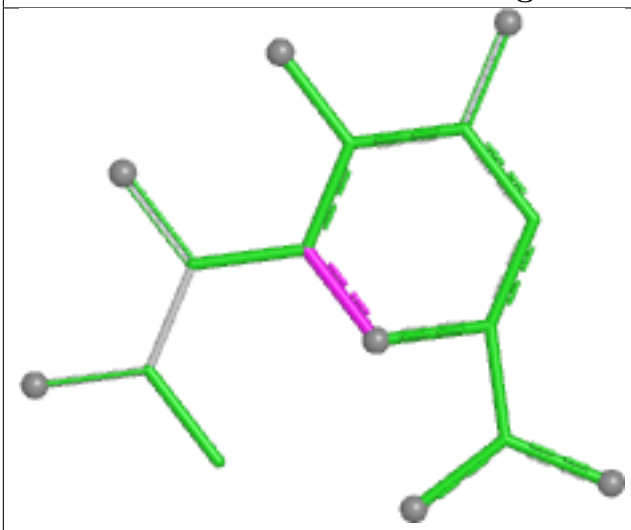


Rings

Ligand P8E EX 604



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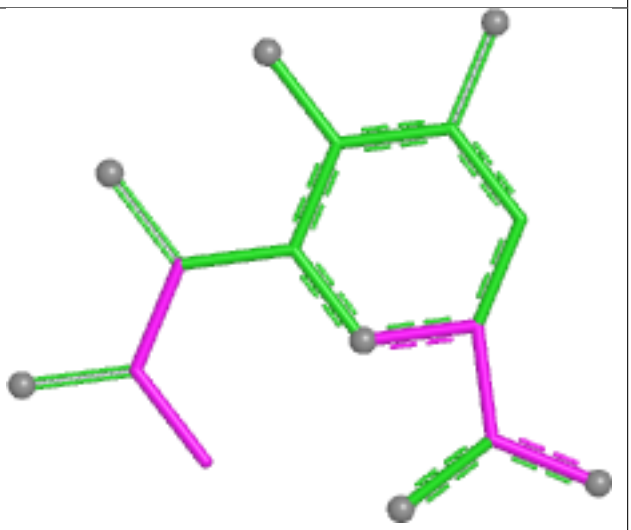

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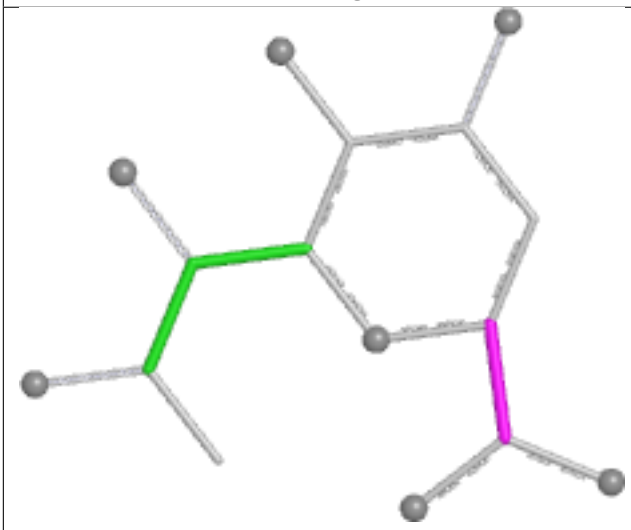

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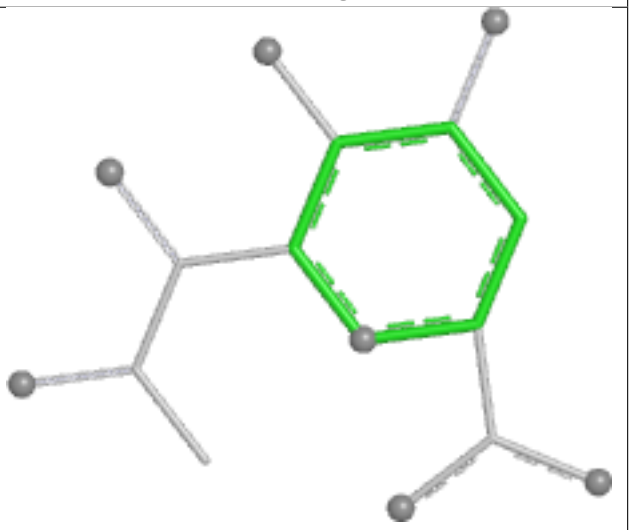
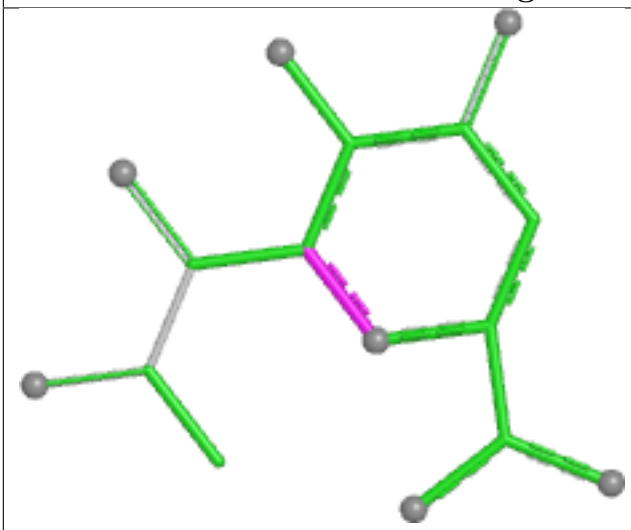


Rings

Ligand P8E FB 605



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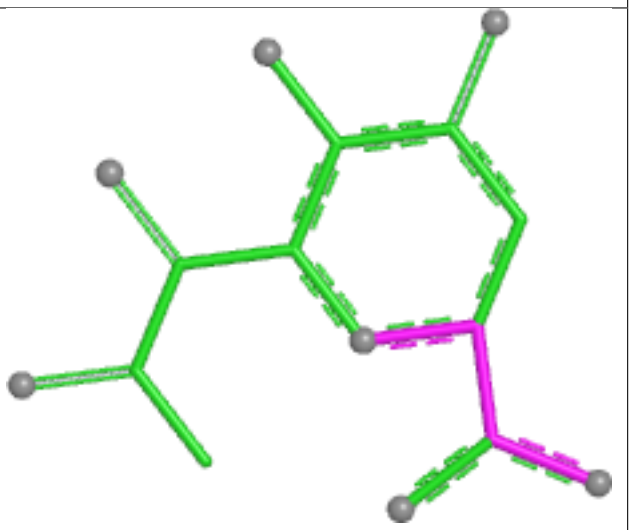

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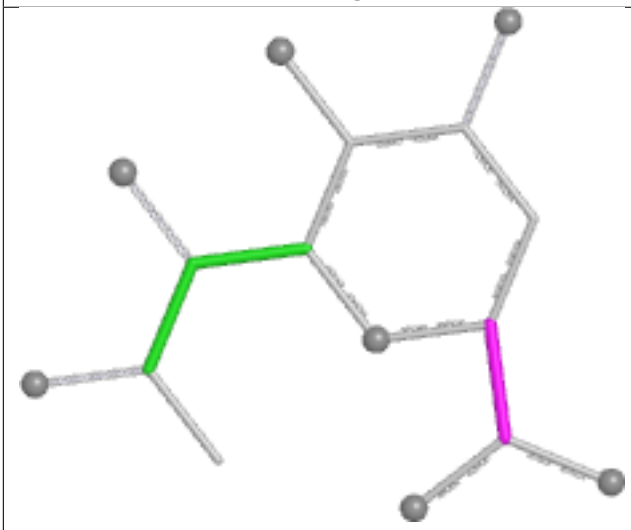

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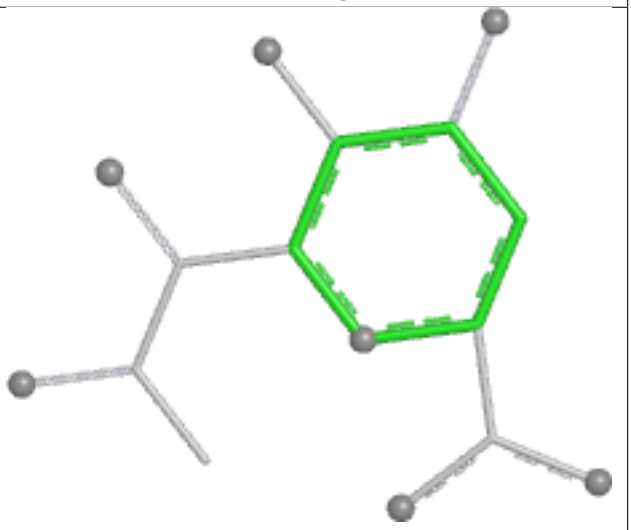
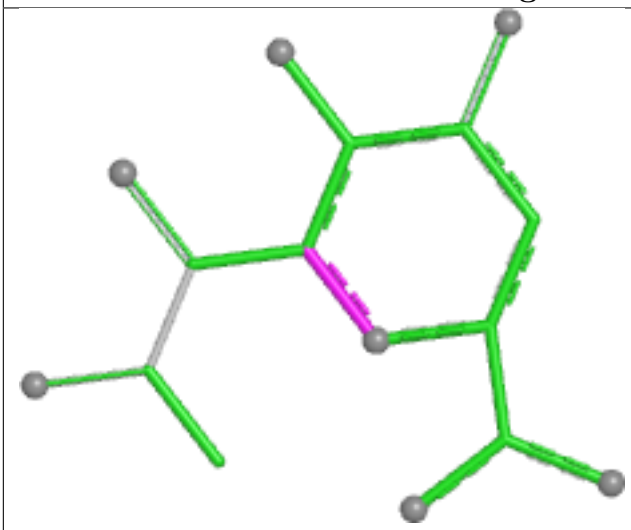


Rings

Ligand P8E BJ 601



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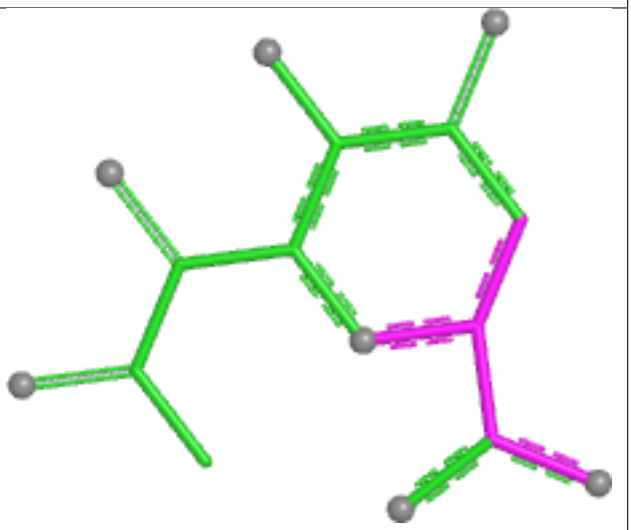
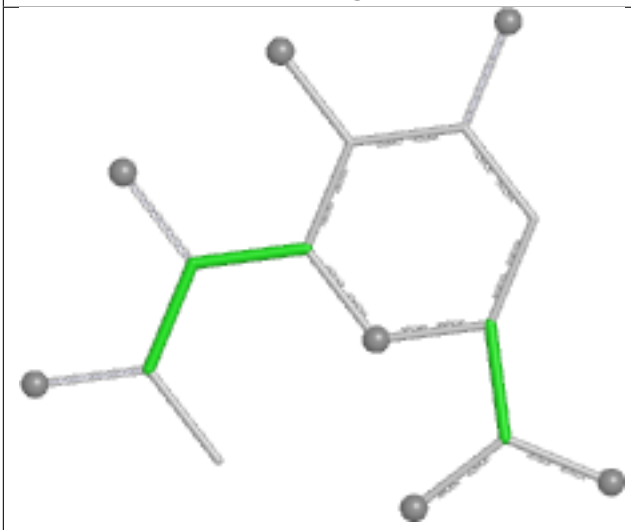


Bond angles



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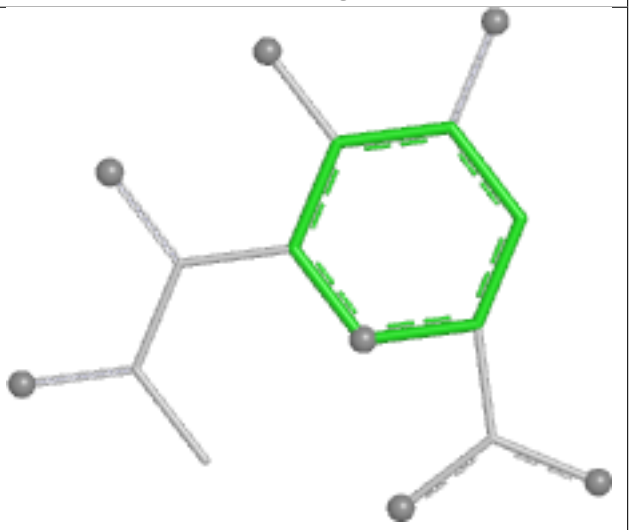
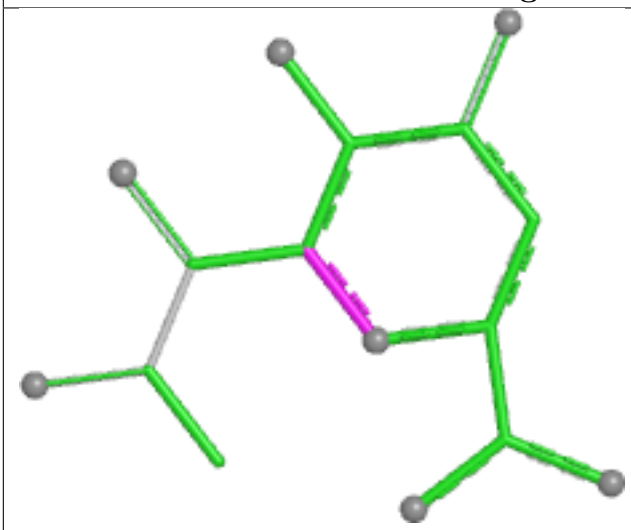


Rings

Ligand P8E cV 603



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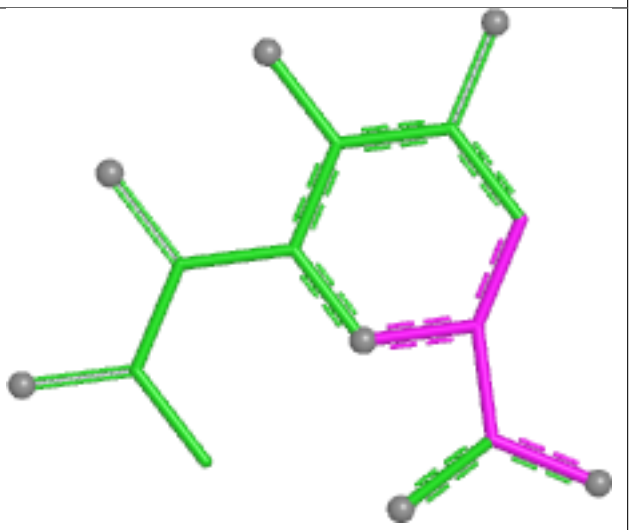
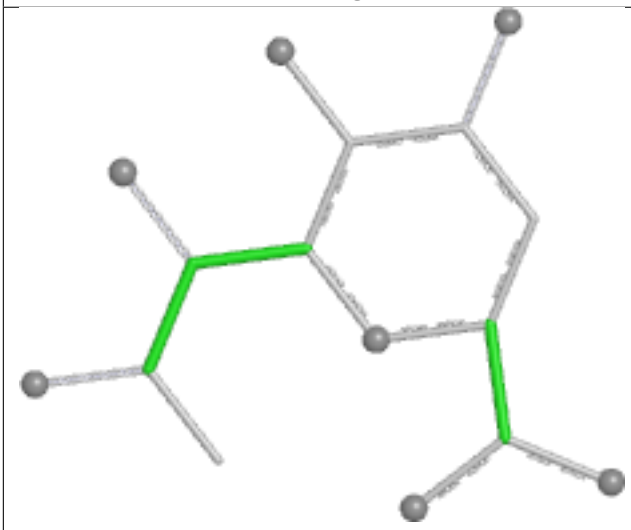


Bond angles



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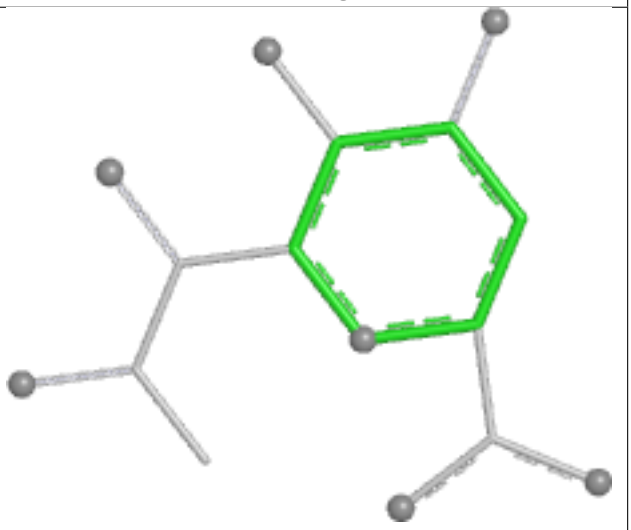
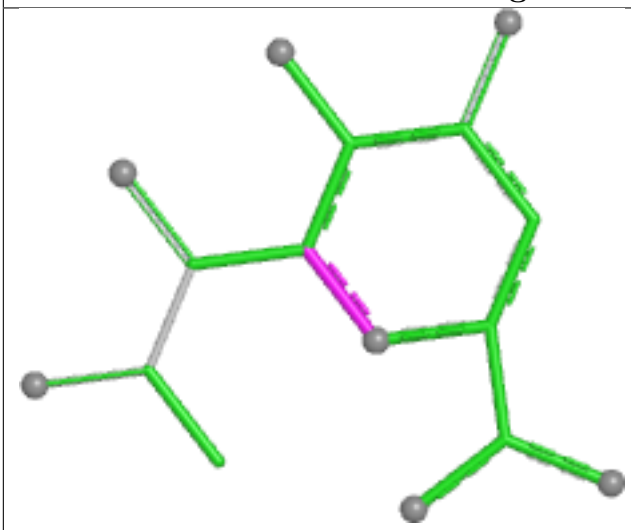


Rings

Ligand P8E WG 602



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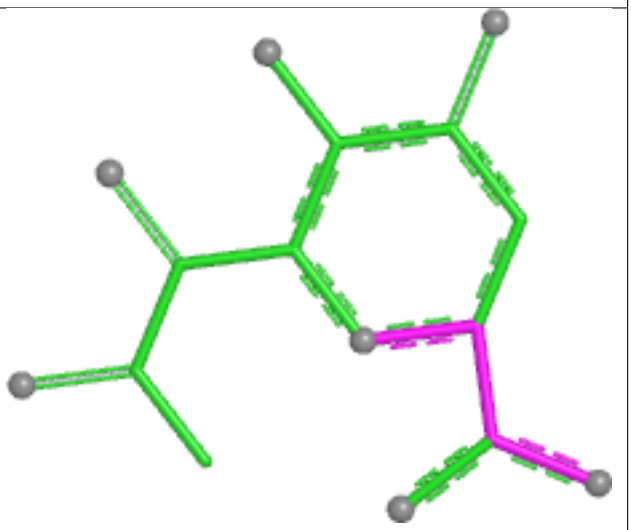
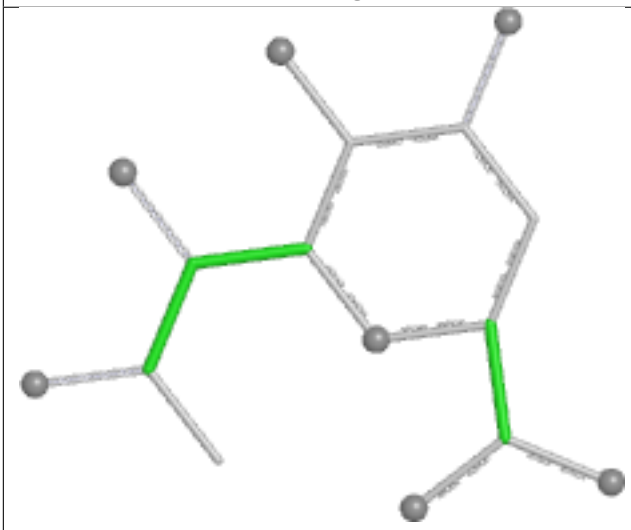
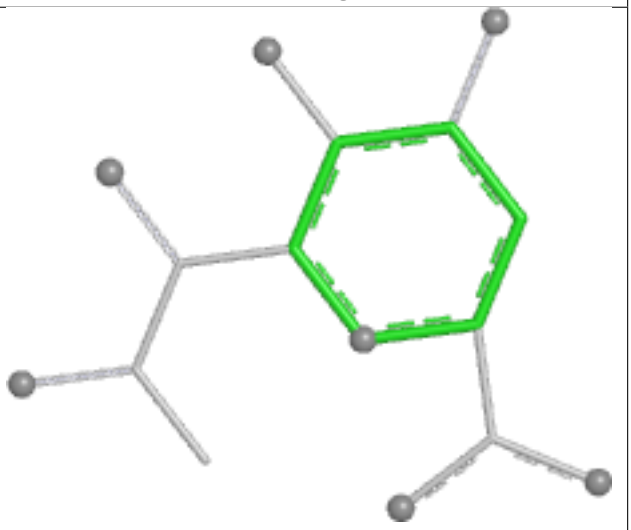


Bond angles

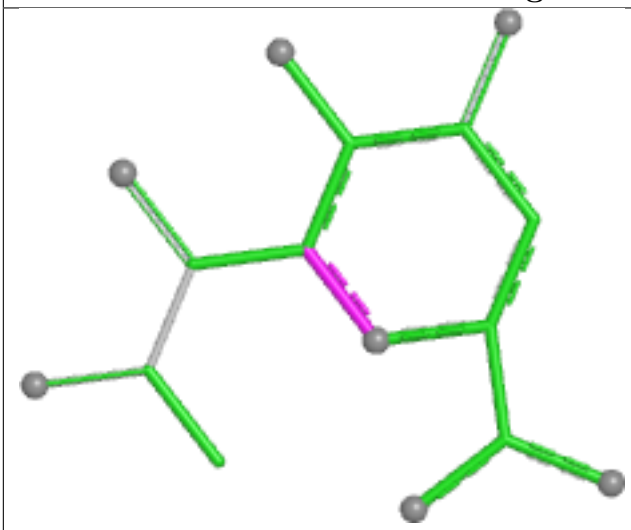


Torsions

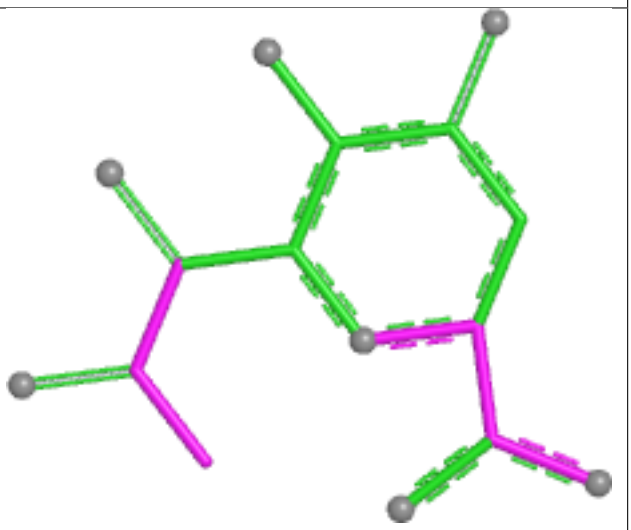


Rings

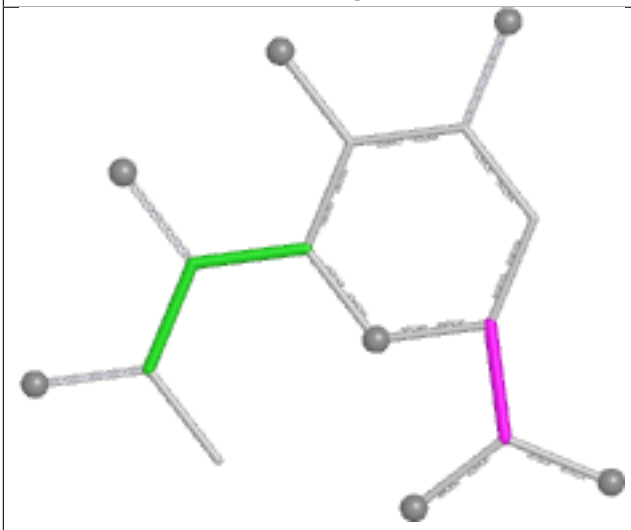
Ligand P8E I3 604



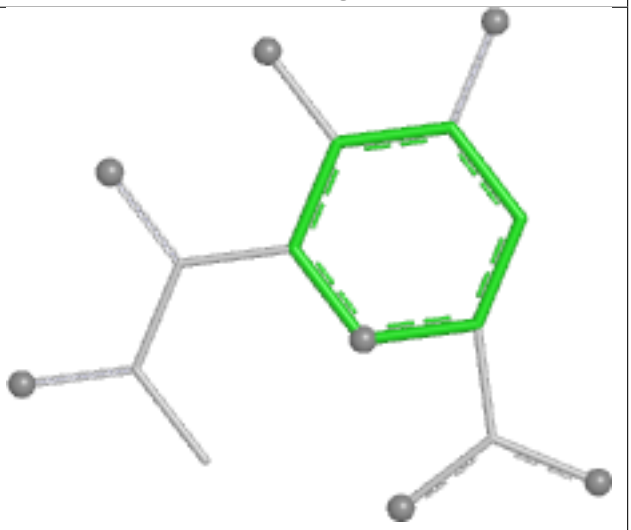
Bond lengths



Bond angles

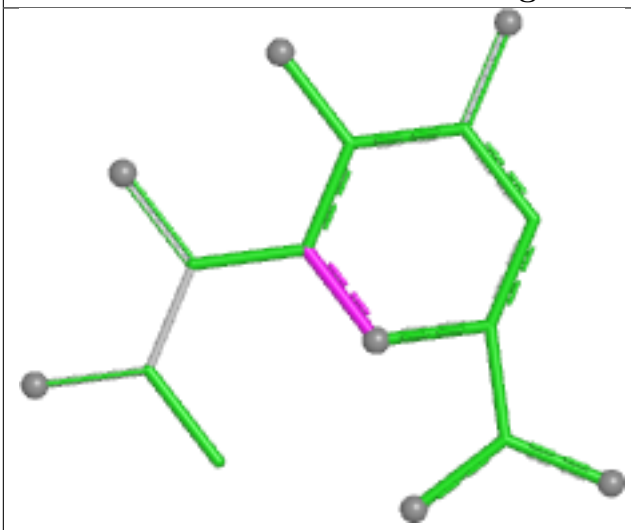


Torsions

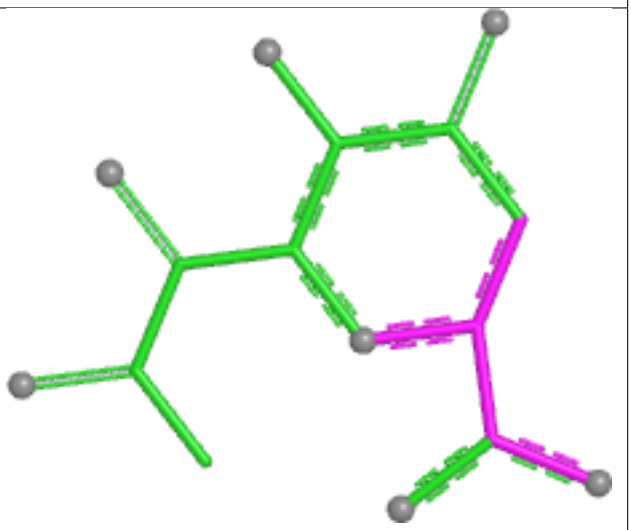


Rings

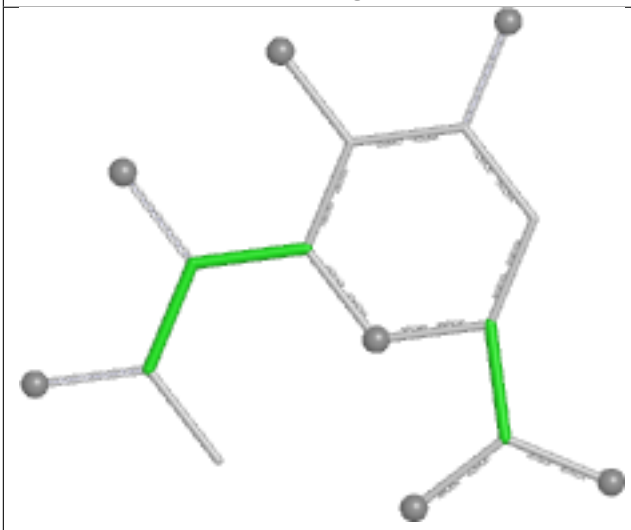
Ligand P8E Y1 603



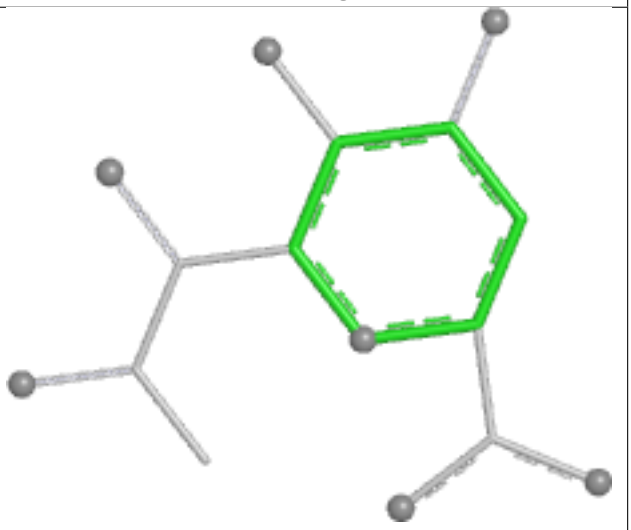
Bond lengths



Bond angles

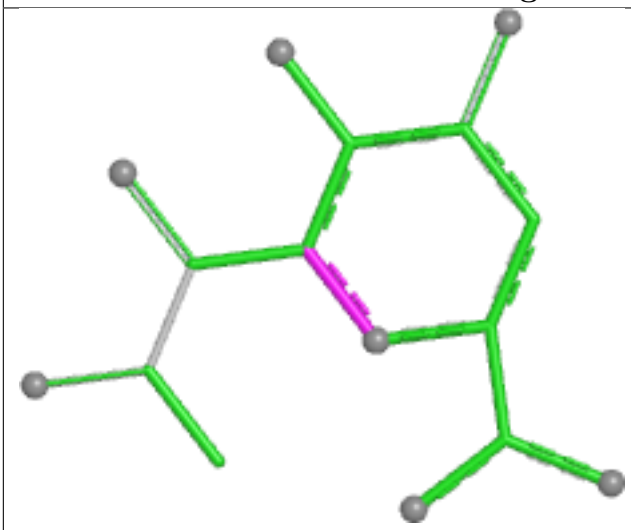


Torsions

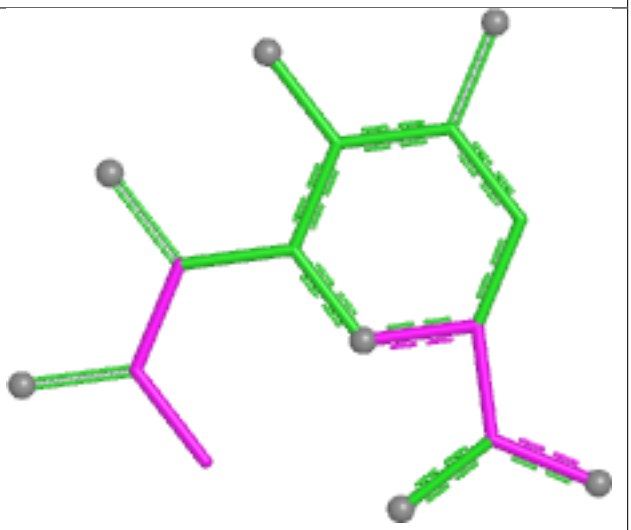


Rings

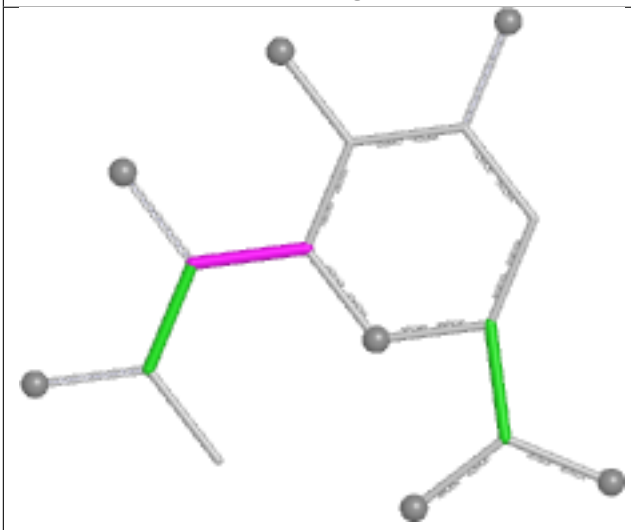
Ligand P8E cV 607



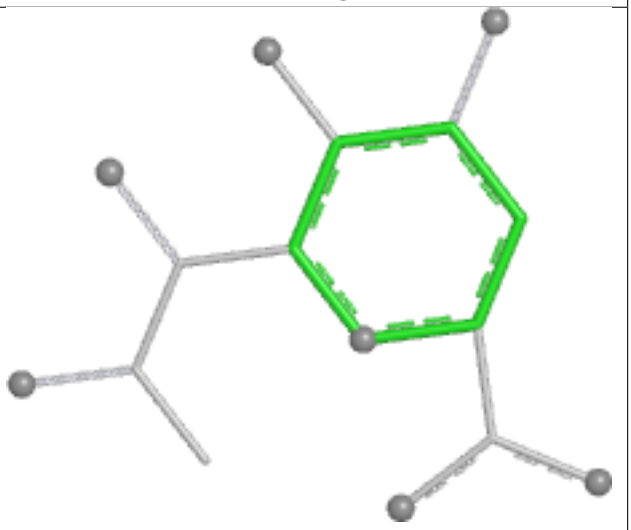
Bond lengths



Bond angles

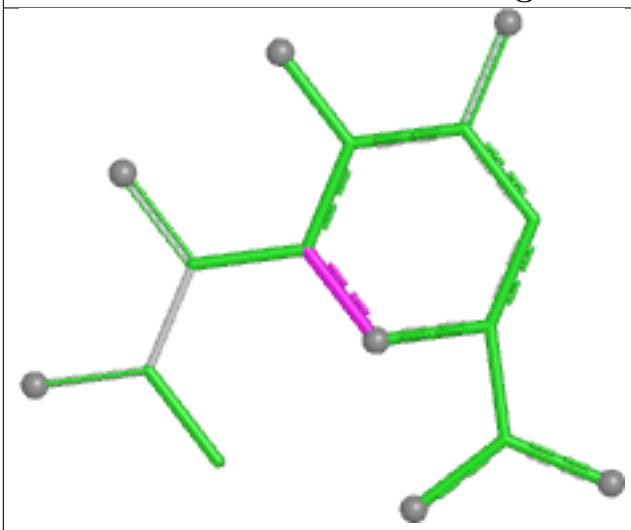


Torsions

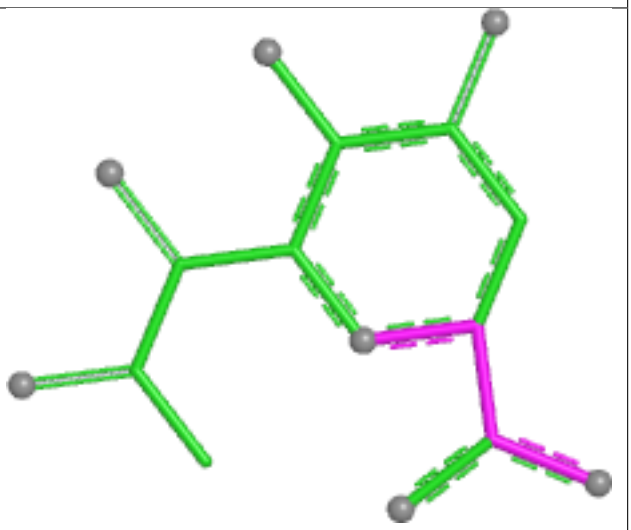


Rings

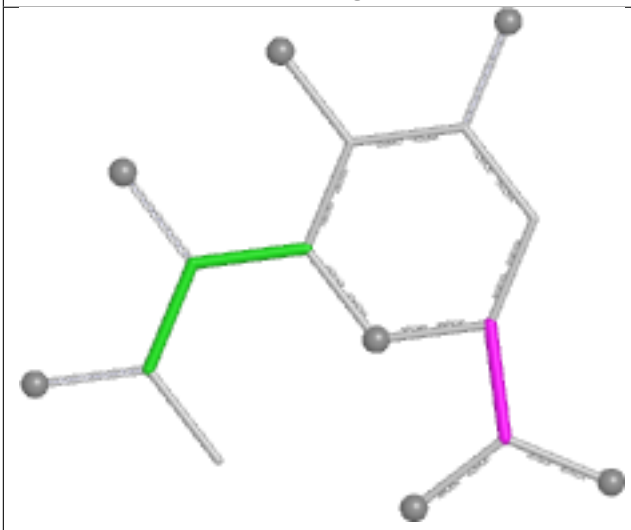
Ligand P8E KE 605



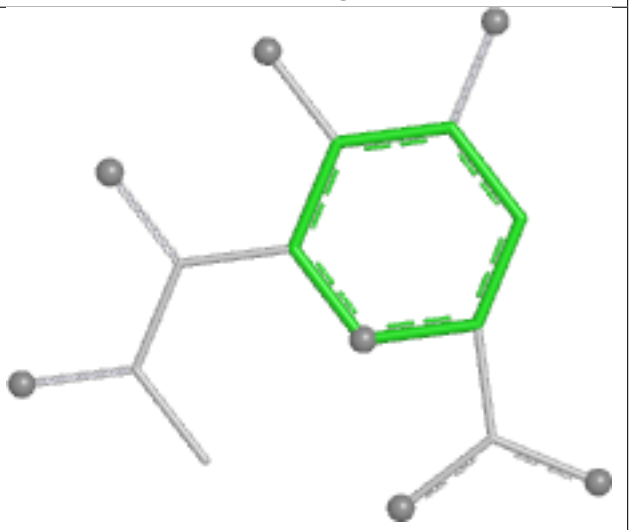
Bond lengths



Bond angles

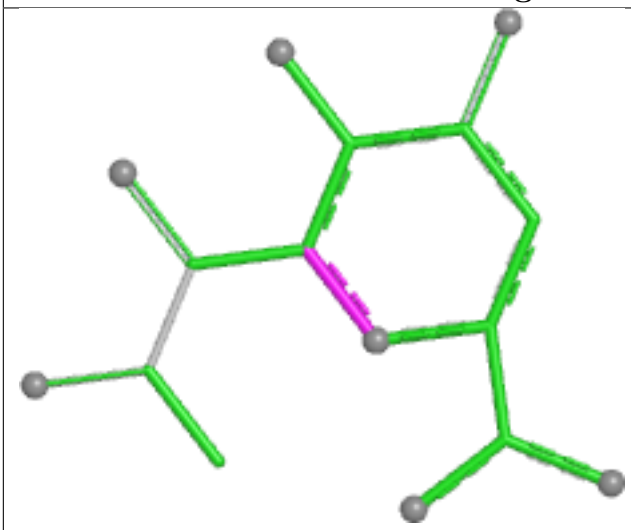


Torsions

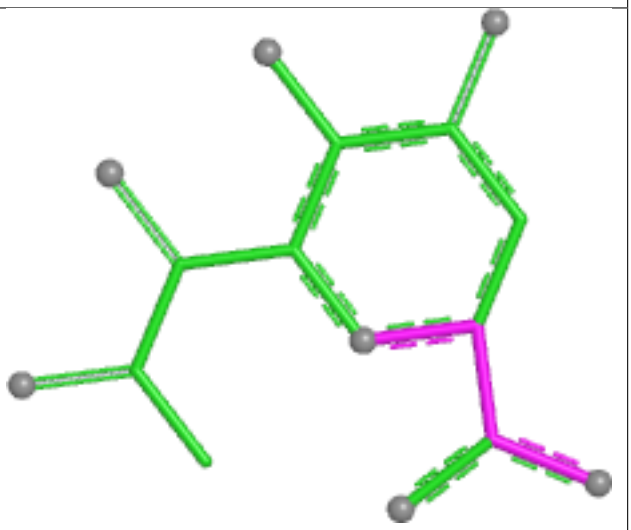


Rings

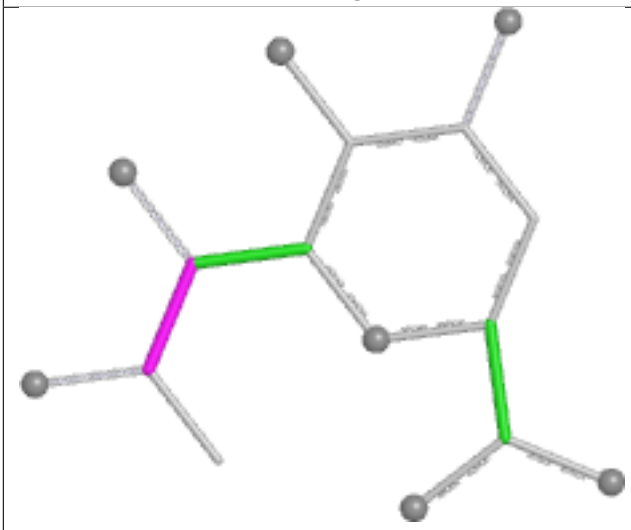
Ligand P8E VR 606



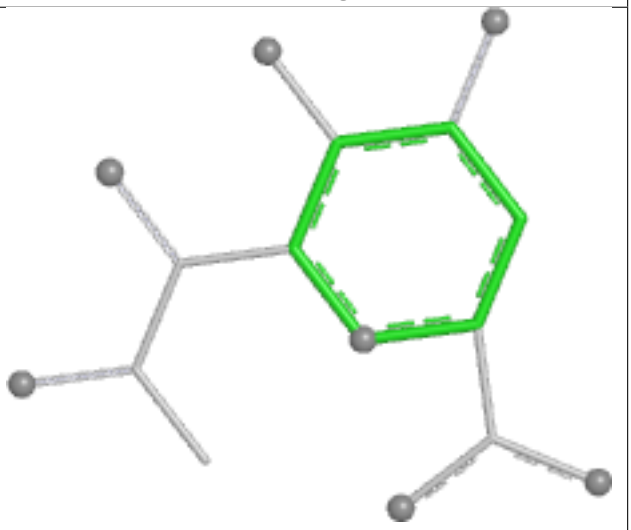
Bond lengths



Bond angles

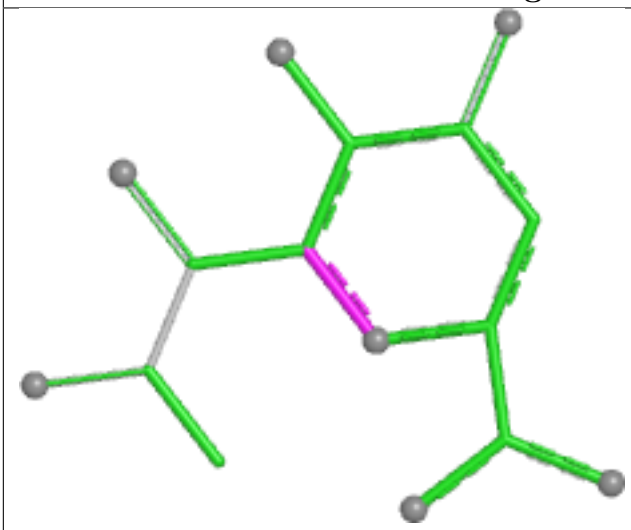


Torsions

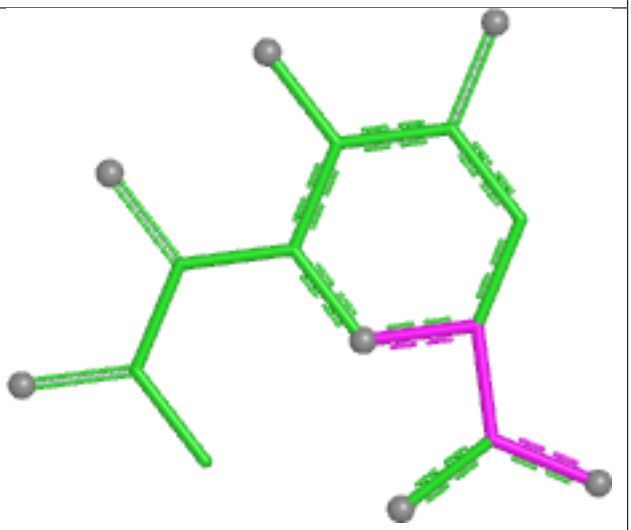


Rings

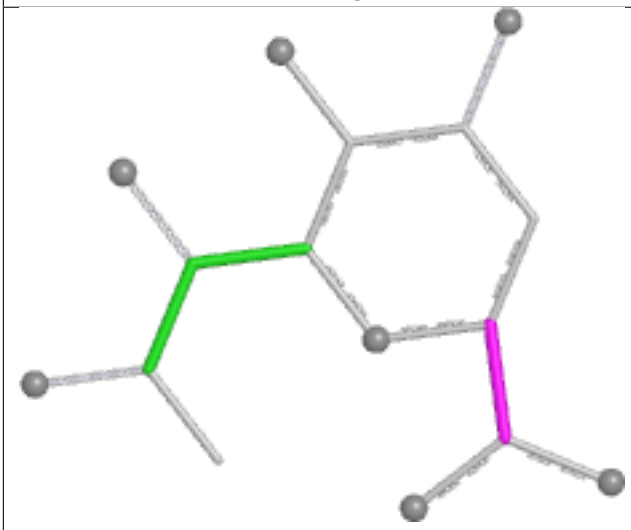
Ligand P8E e8 605



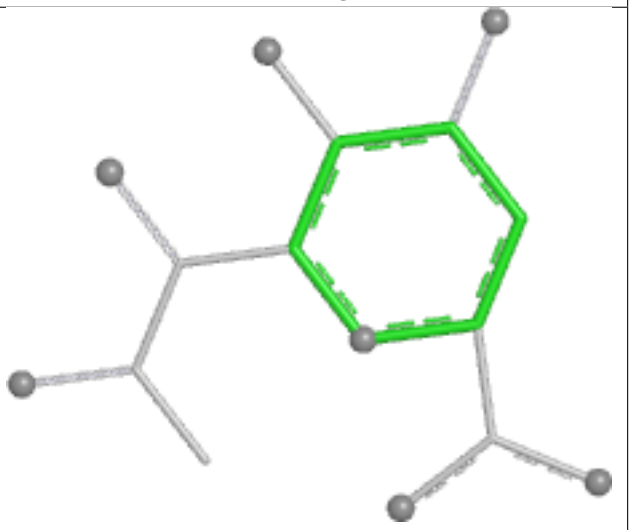
Bond lengths



Bond angles

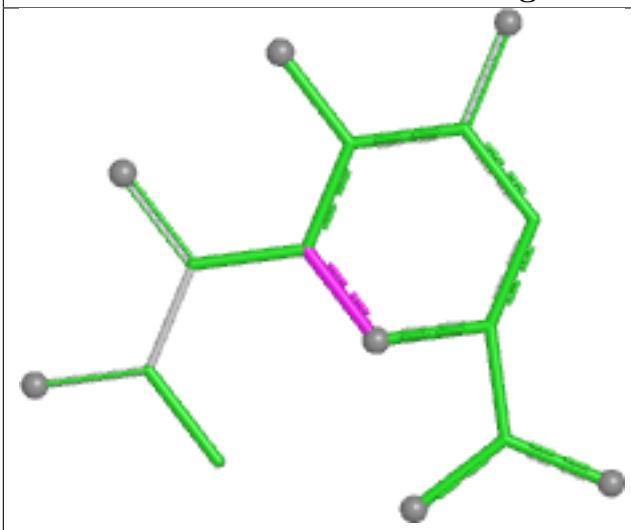


Torsions

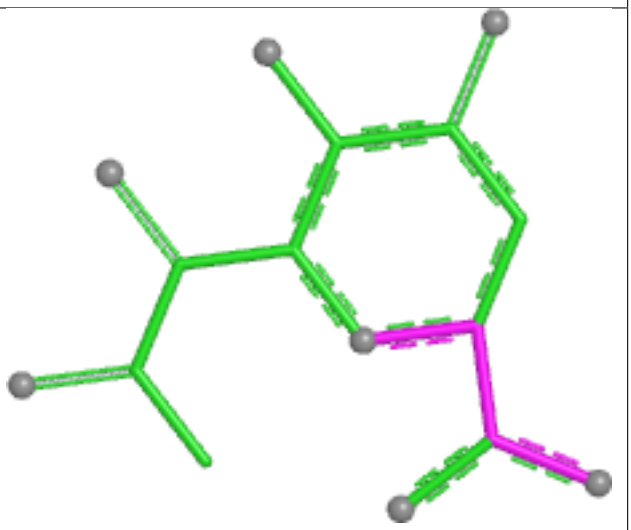


Rings

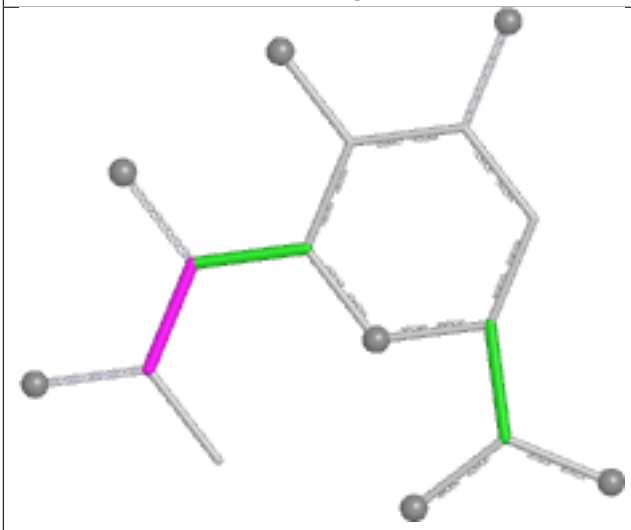
Ligand P8E A7 606



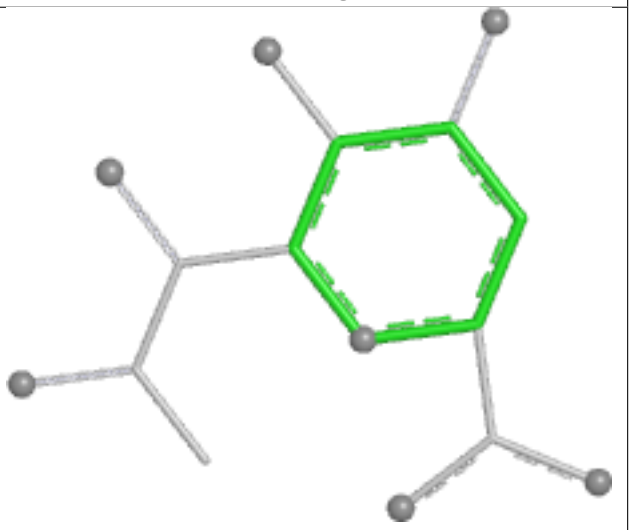
Bond lengths



Bond angles

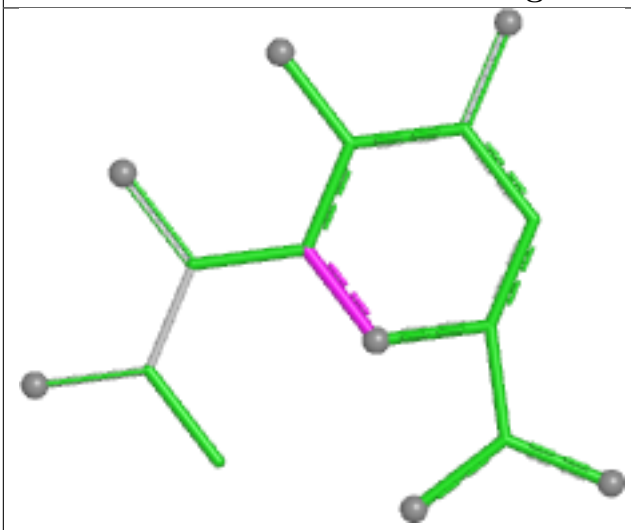


Torsions

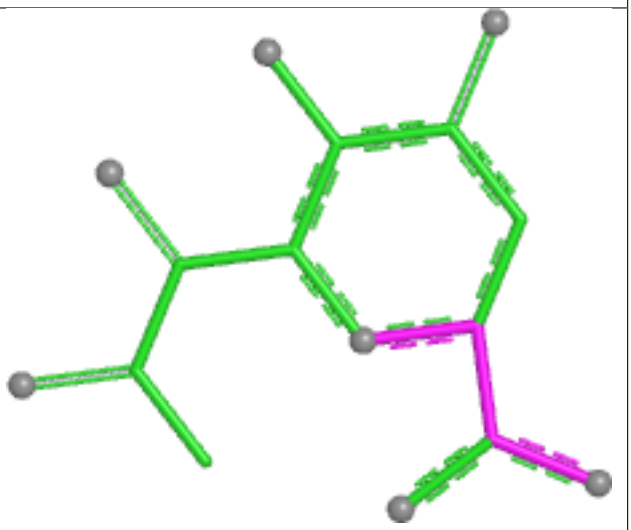


Rings

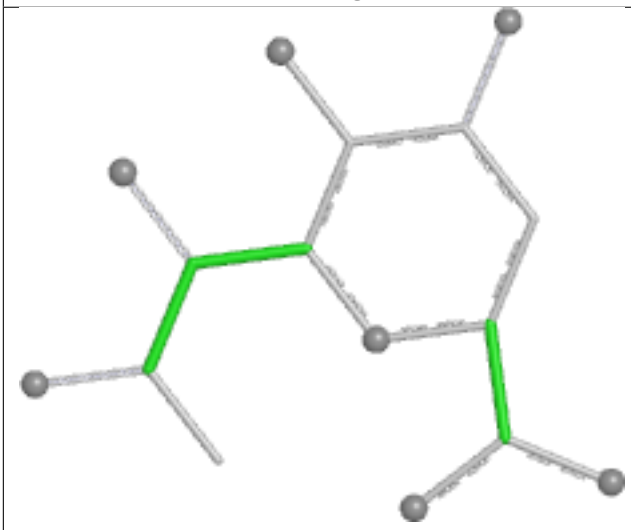
Ligand P8E I3 602



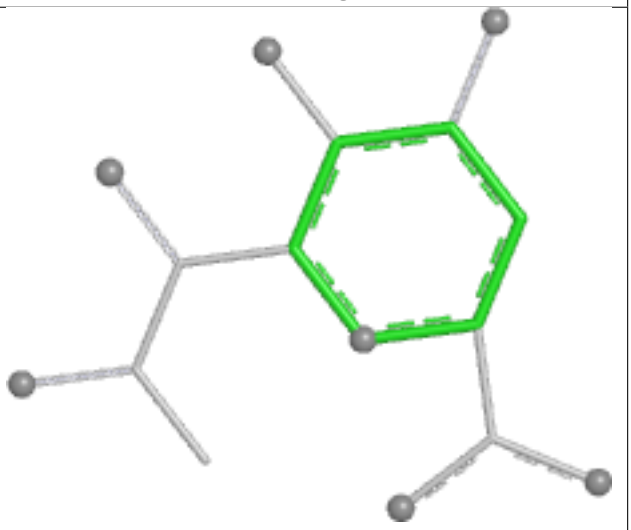
Bond lengths



Bond angles

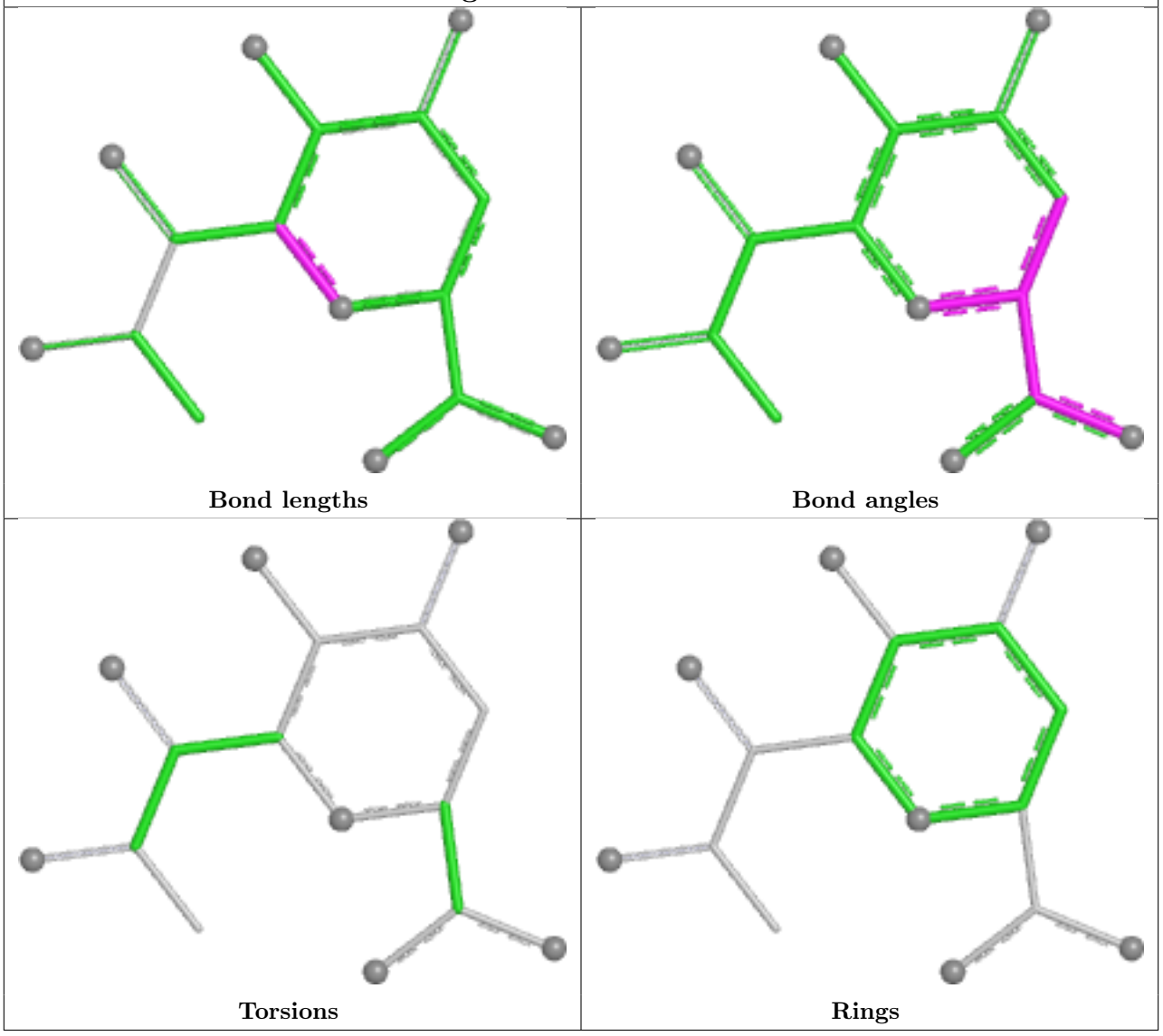


Torsions



Rings

Ligand P8E WG 601



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.

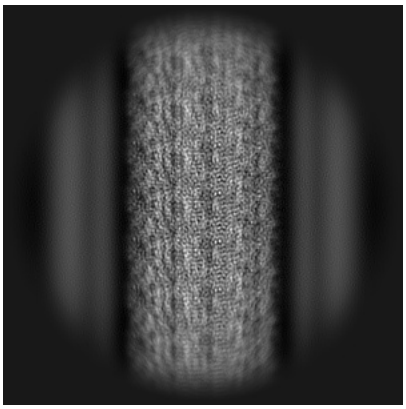
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-72942. These allow visual inspection of the internal detail of the map and identification of artifacts.

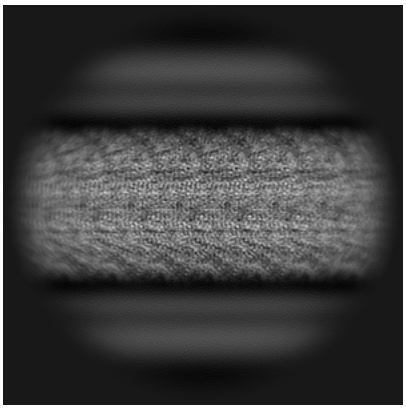
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

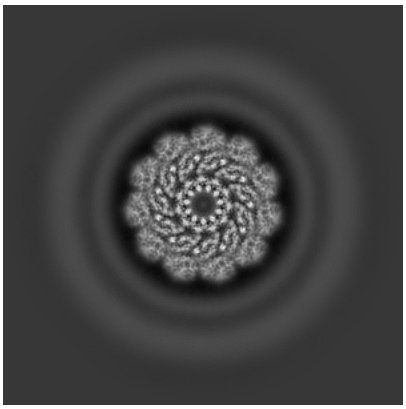
6.1.1 Primary map



X

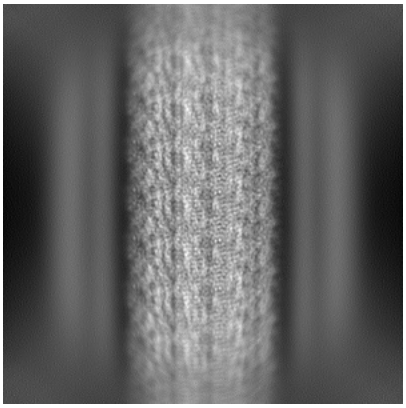


Y

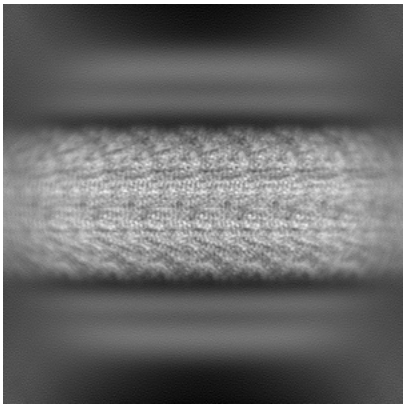


Z

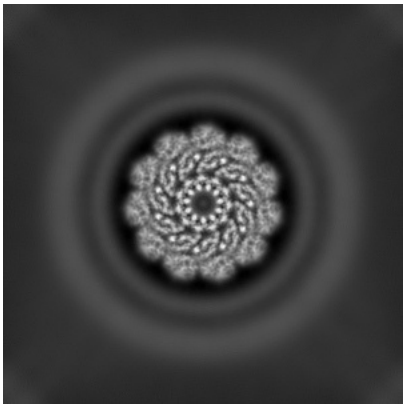
6.1.2 Raw map



X



Y

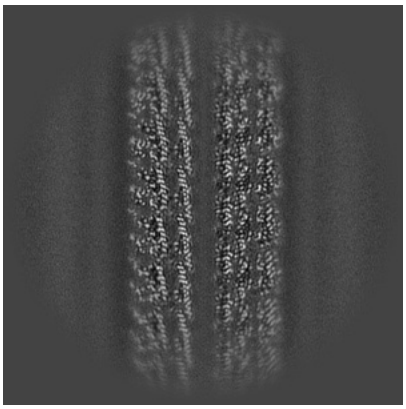


Z

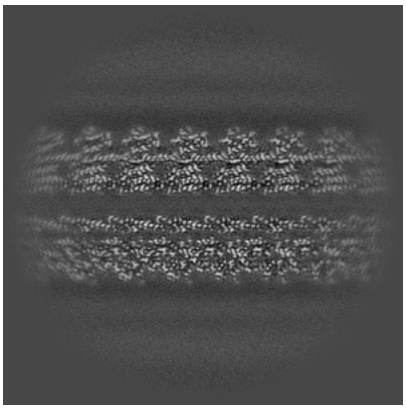
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

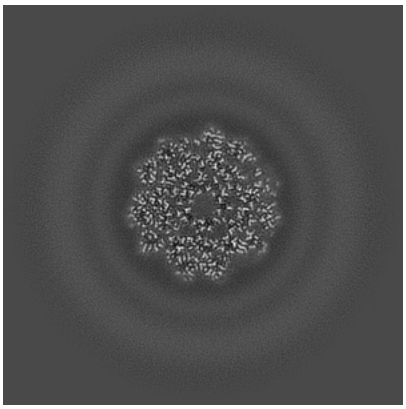
6.2.1 Primary map



X Index: 200

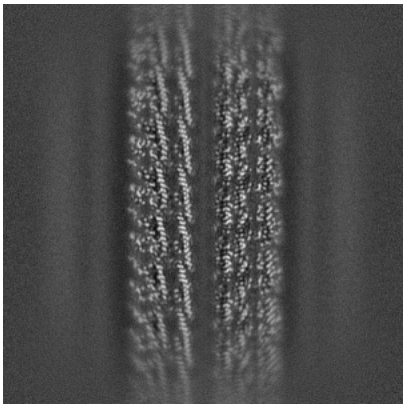


Y Index: 200

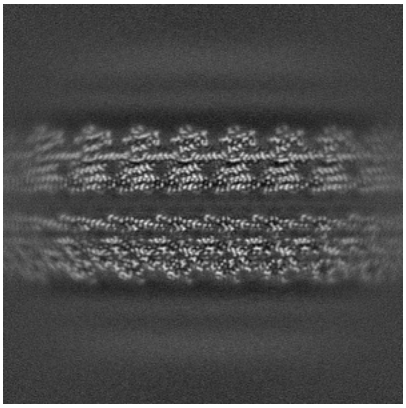


Z Index: 200

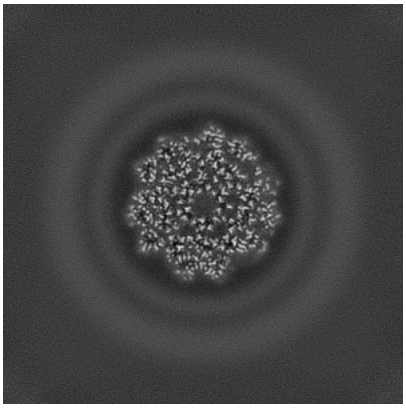
6.2.2 Raw map



X Index: 200



Y Index: 200

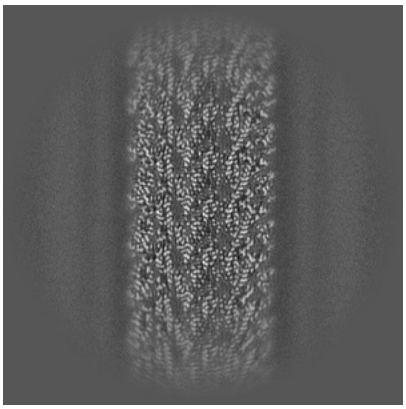


Z Index: 200

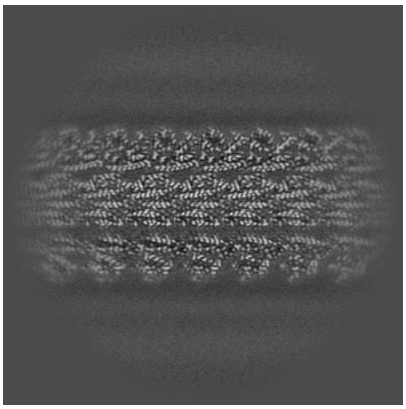
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

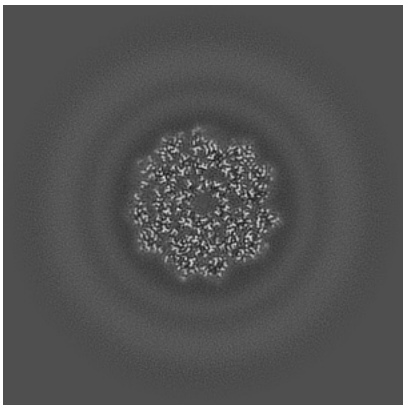
6.3.1 Primary map



X Index: 180

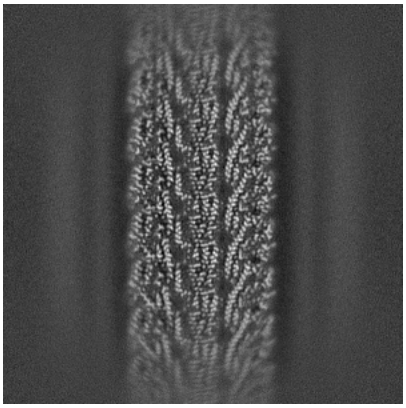


Y Index: 184

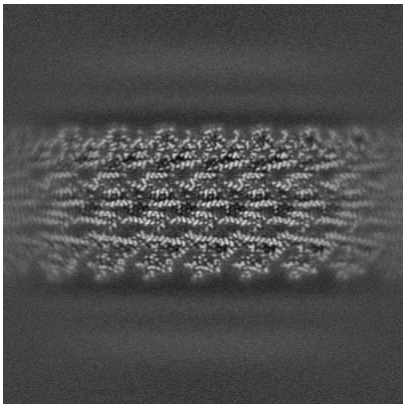


Z Index: 208

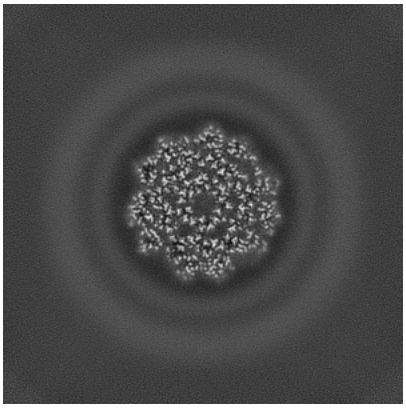
6.3.2 Raw map



X Index: 178



Y Index: 182

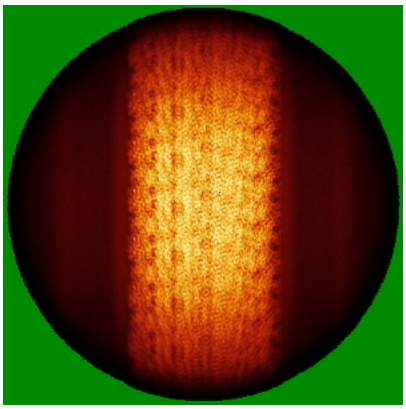


Z Index: 199

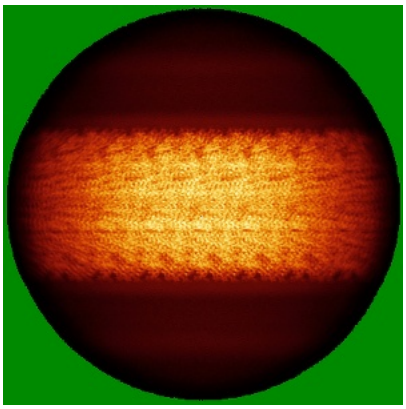
The images above show the largest variance slices of the map in three orthogonal directions.

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

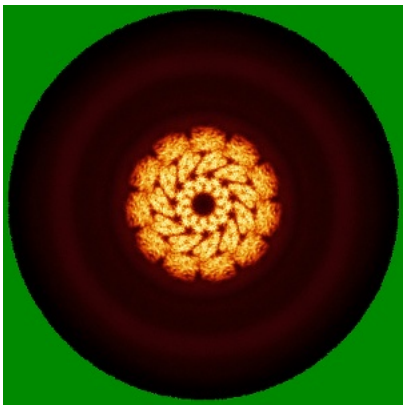
6.4.1 Primary map



X

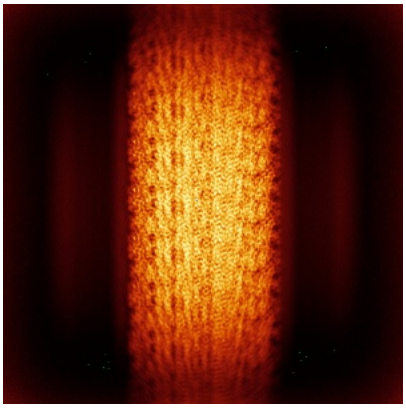


Y

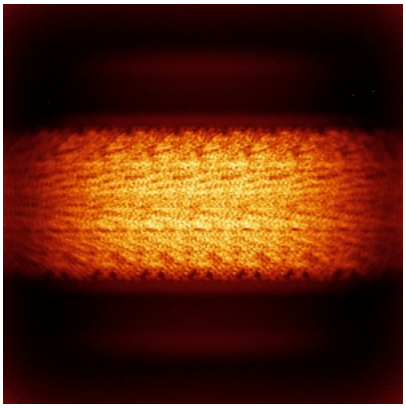


Z

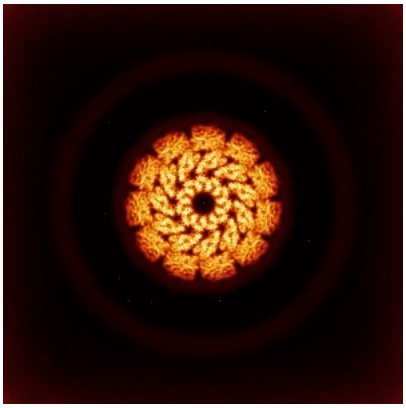
6.4.2 Raw map



X



Y



Z

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

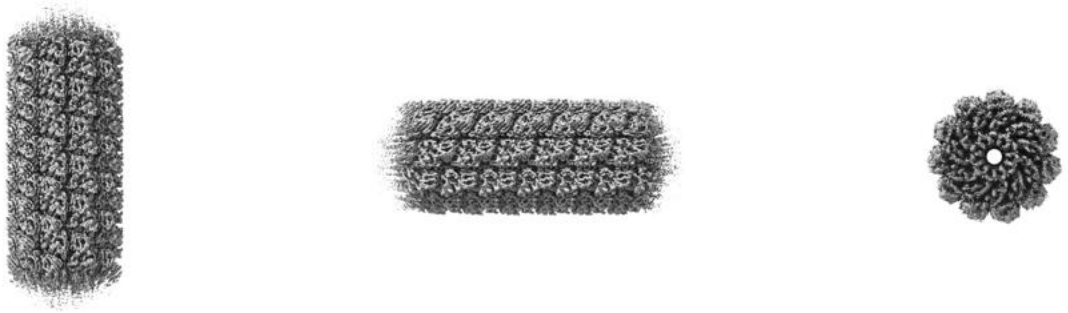
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.111. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

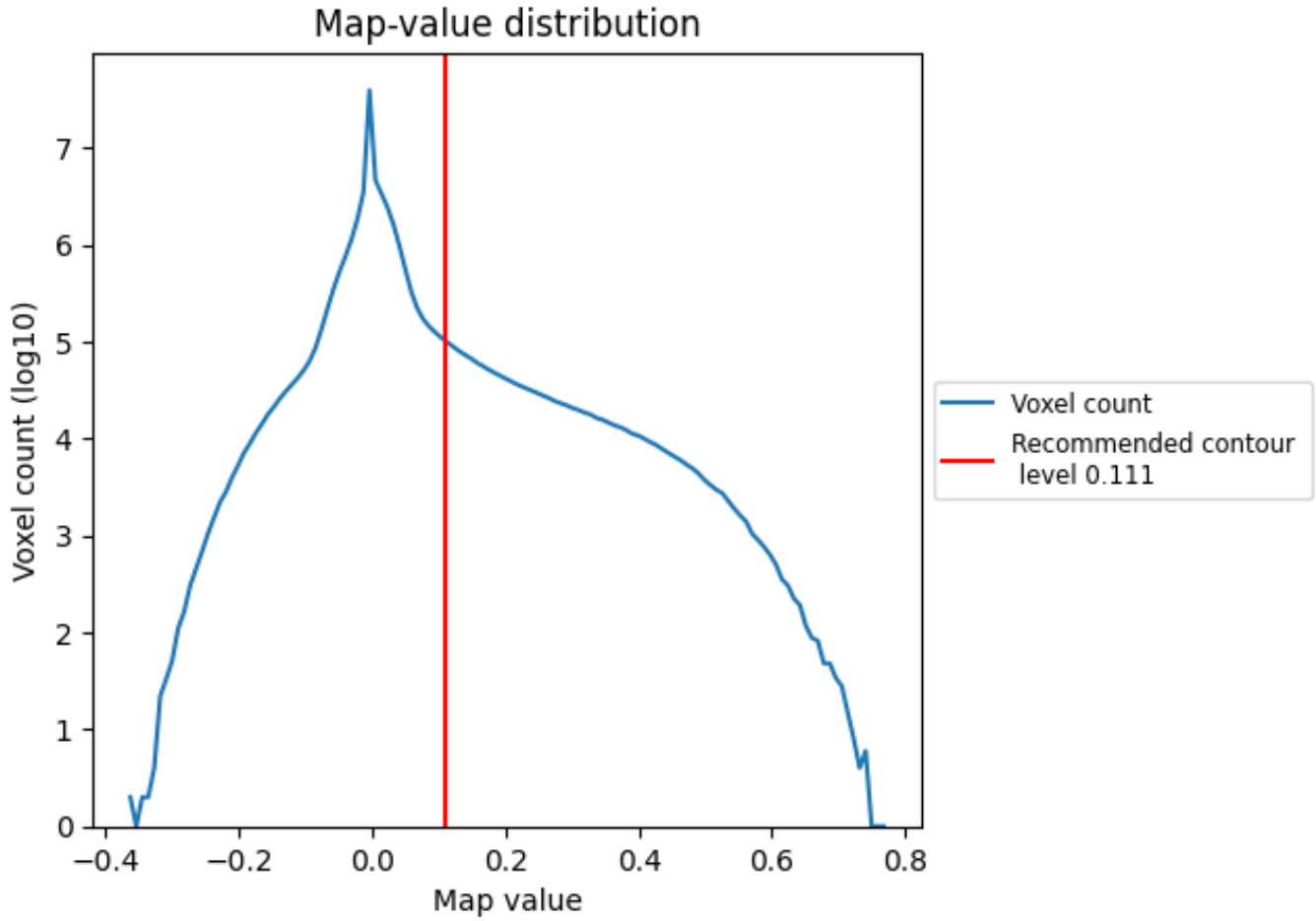
6.6 Mask visualisation (i)

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

7 Map analysis

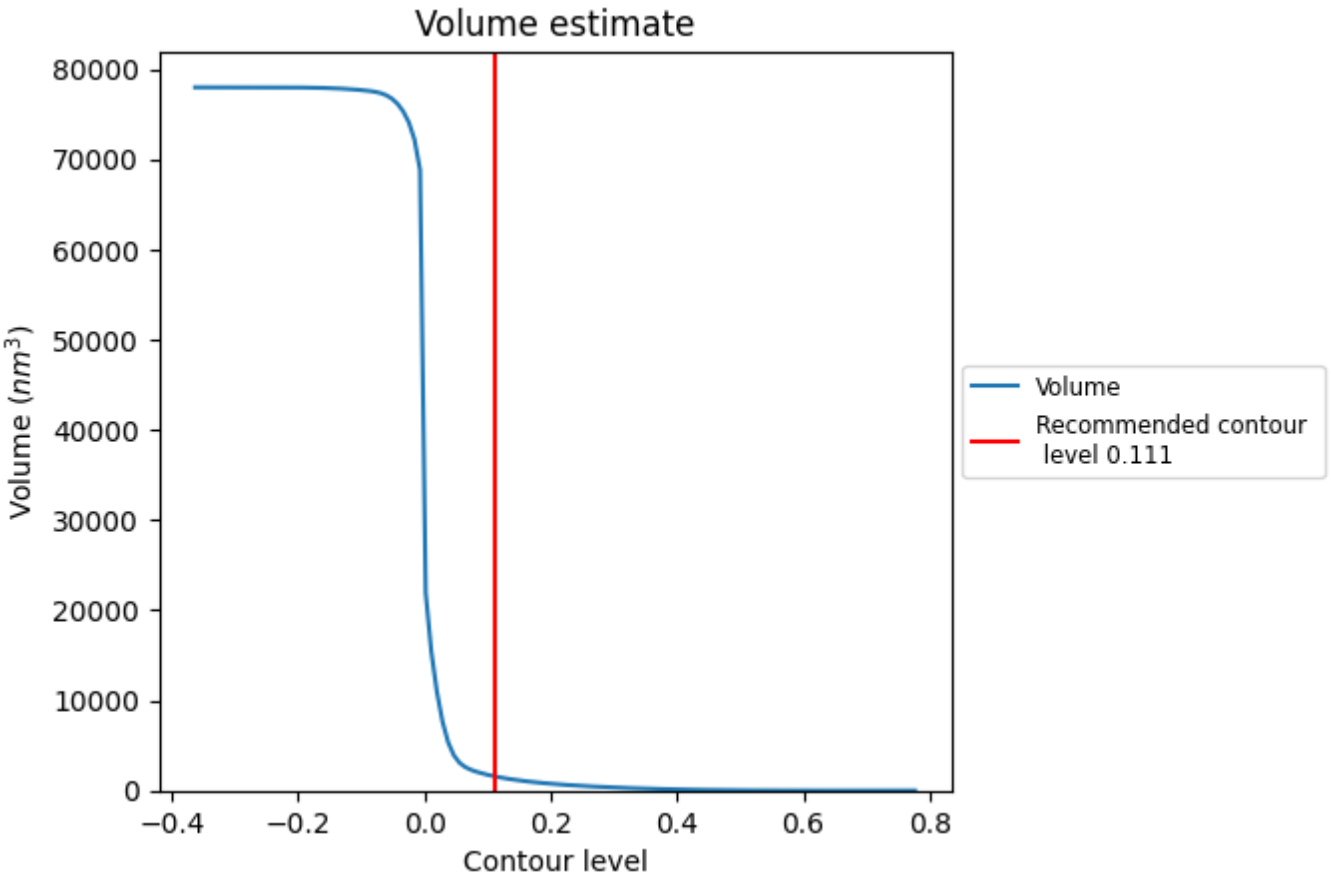
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

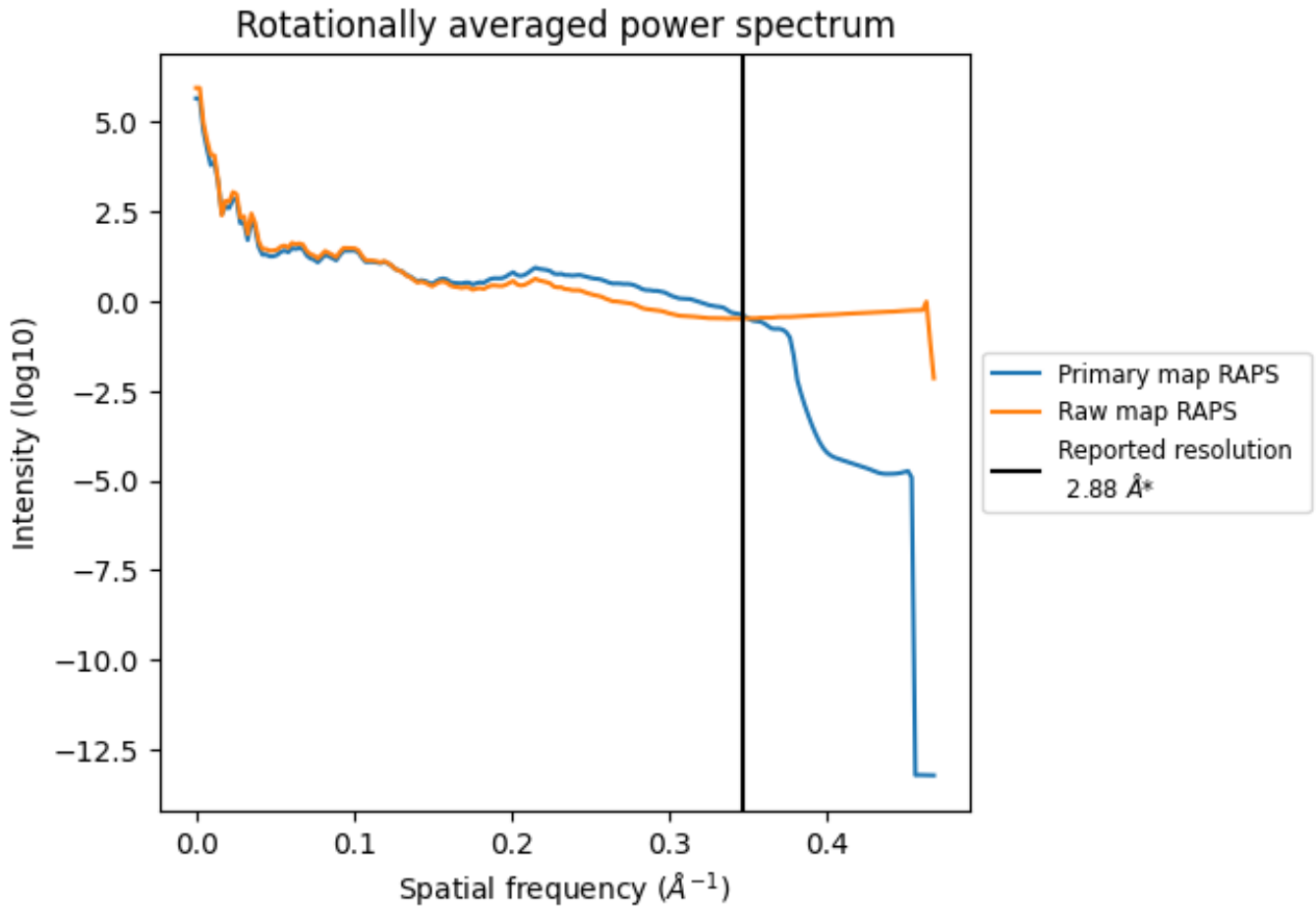
7.2 Volume estimate



The volume at the recommended contour level is 1578 nm^3; this corresponds to an approximate mass of 1426 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

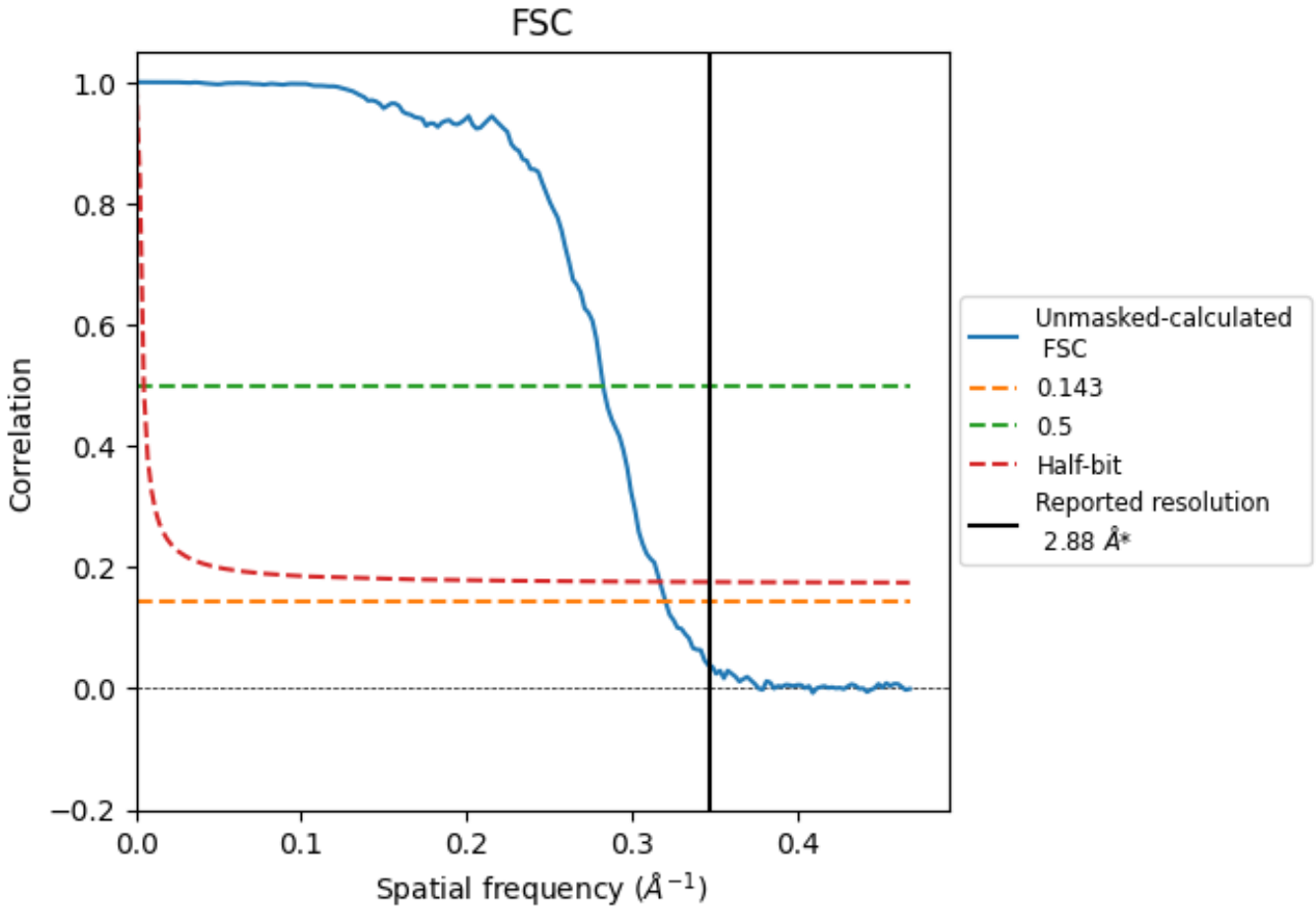


*Reported resolution corresponds to spatial frequency of 0.347 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.347 Å^{-1}

8.2 Resolution estimates (i)

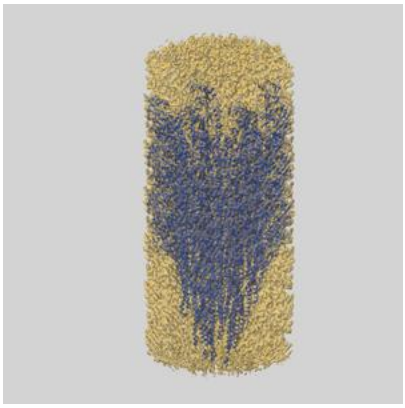
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.12	3.54	3.15

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

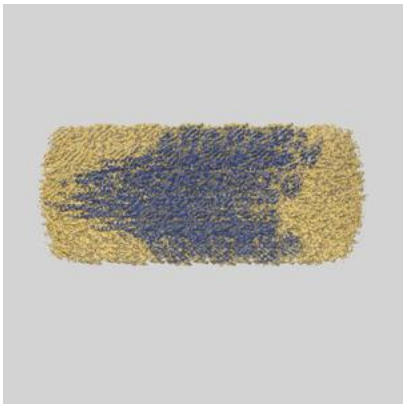
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-72942 and PDB model 9YGU. Per-residue inclusion information can be found in section 3 on page 20.

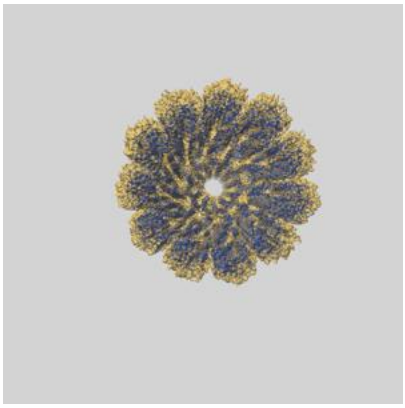
9.1 Map-model overlay



X



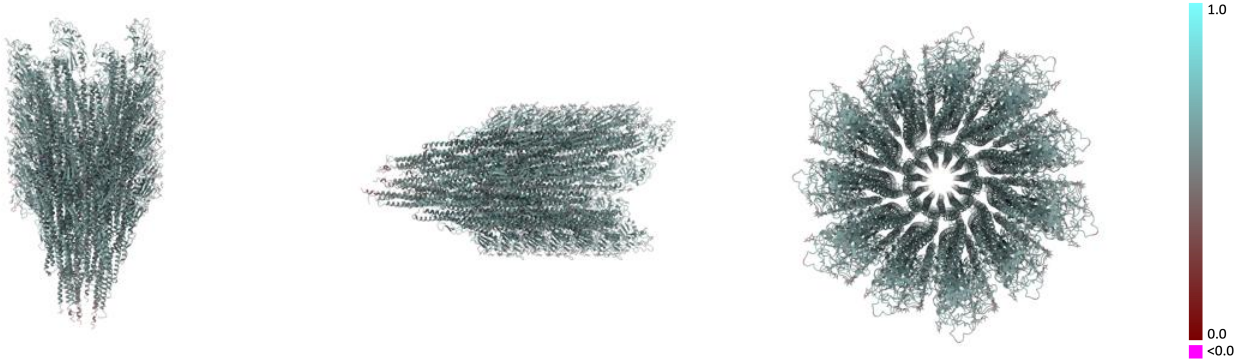
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.111 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

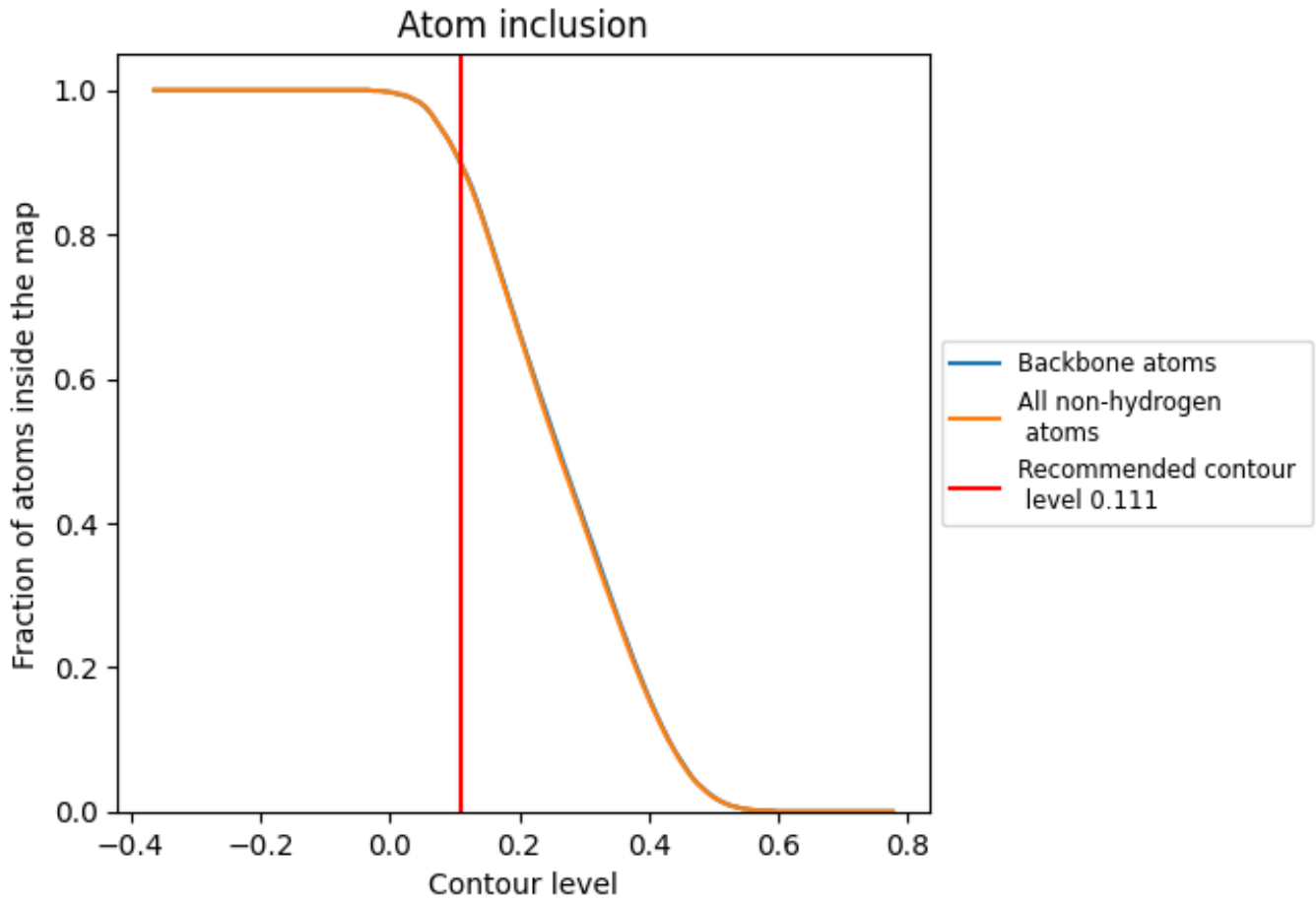
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.111).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (0.111) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8960	0.5770
A7	0.8830	0.5730
BJ	0.9120	0.5840
CT	0.9010	0.5780
DN	0.8880	0.5710
EX	0.9120	0.5840
FB	0.9030	0.5800
GQ	0.9090	0.5840
HL	0.9030	0.5800
I3	0.8490	0.5550
JD	0.8910	0.5730
KE	0.9120	0.5850
LF	0.8980	0.5800
MO	0.9130	0.5840
NI	0.9050	0.5810
OA	0.8590	0.5600
PU	0.8950	0.5750
Q2	0.9130	0.5840
R4	0.8970	0.5780
S5	0.9080	0.5830
TP	0.9080	0.5810
UH	0.8680	0.5620
VR	0.8960	0.5770
WG	0.9120	0.5840
XM	0.8880	0.5760
Y1	0.9060	0.5800
Z9	0.9080	0.5810
aW	0.8740	0.5650
bS	0.8990	0.5770
cV	0.9130	0.5840
dC	0.8900	0.5740
e8	0.9040	0.5800
fK	0.9110	0.5810
g6	0.8790	0.5670