wwPDB EM Validation Summary Report

Mar 19, 2026 – 10:11 PM UTC

PDB ID	:	7DWX / pdb_00007dwx
EMDB ID	:	EMD-30888
Title	:	Conformation 1 of S-ACE2-B0AT1 ternary complex
Authors	:	Yan, R.H.; Zhang, Y.Y.; Li, Y.N.; Ye, F.F.; Guo, Y.Y.; Xia, L.; Zhong, X.Y.; Chi, X.M.; Zhou, Q.
Deposited on	:	2021-01-18
Resolution	:	8.30 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 ⓘ symbol.

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

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

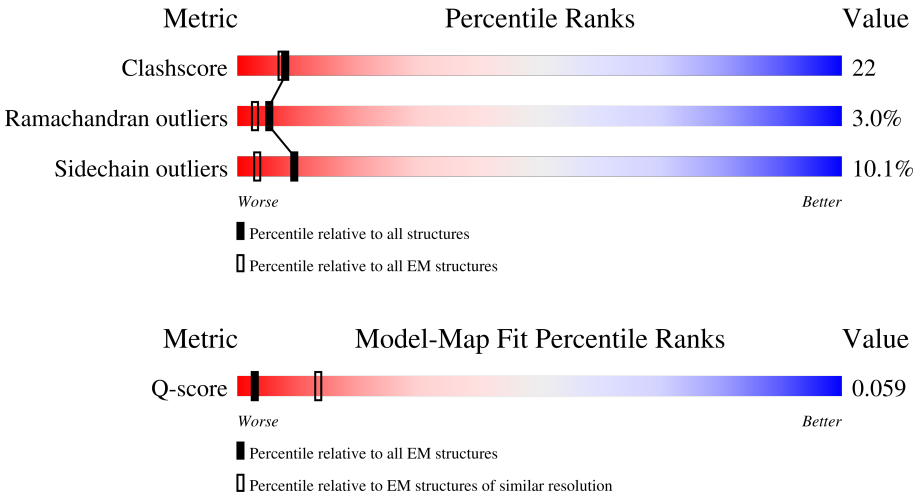
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 8.30 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	280 (7.82 - 8.80)

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

Mol	Chain	Length	Quality of chain
1	A	654	5% 71% 18% • 7%
1	C	654	6% 72% 17% • 7%
2	B	817	• 76% 12% • 8%
2	D	817	5% 76% 12% • • 8%

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Mol	Chain	Length	Quality of chain
3	E	1283	49% 23% 6% 22%
3	F	1283	51% 20% 6% 22%
3	G	1283	5% 50% 22% 5% 22%
3	H	1283	31% 49% 23% 6% 22%
3	I	1283	43% 52% 20% 6% 22%
3	J	1283	65% 50% 22% 6% 22%
4	0	2	100% 50% 50%
4	1	2	100% 50% 50%
4	2	2	100% 50% 50%
4	3	2	100% 100%
4	4	2	100% 50% 50%
4	5	2	50% 50%
4	6	2	100% 100%
4	7	2	100% 100%
4	8	2	100% 100%
4	9	2	100% 100%
4	AA	2	100% 50% 50%
4	BA	2	100% 50% 50%
4	CA	2	100% 100%
4	DA	2	100% 50% 50%
4	EA	2	100% 100%
4	FA	2	100% 100%
4	K	2	100%
4	L	2	100%
4	M	2	50% 50%

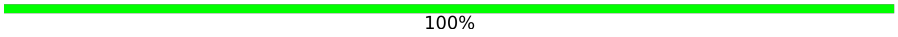
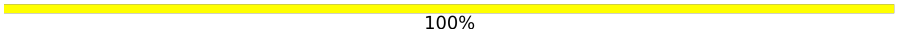
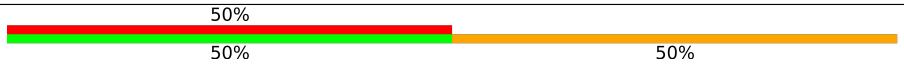
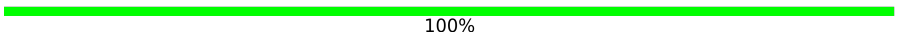
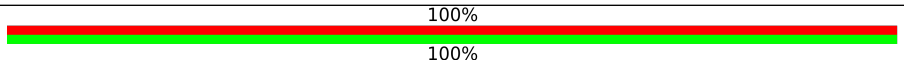
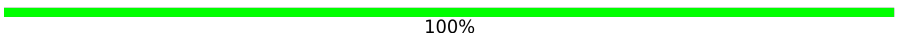
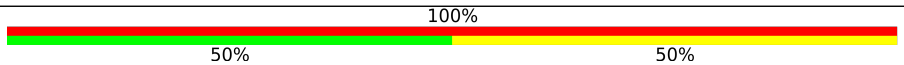
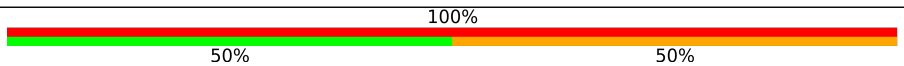
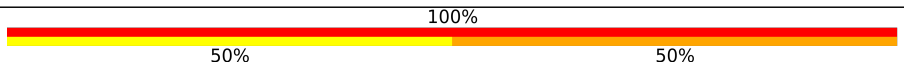
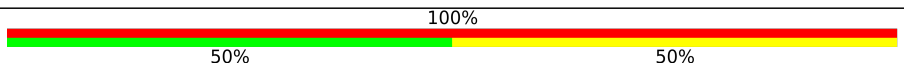
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Mol	Chain	Length	Quality of chain
4	N	2	100%
4	O	2	50% 100%
4	P	2	50% 50%
4	Q	2	100%
4	R	2	100%
4	S	2	50% 100%
4	T	2	50% 50%
4	U	2	100%
4	V	2	50% 100%
4	W	2	50% 50%
4	X	2	100%
4	Y	2	100%
4	Z	2	100%
4	a	2	100%
4	b	2	50% 50%
4	c	2	50% 50% 50%
4	d	2	50% 50% 50%
4	e	2	50% 50%
4	f	2	50% 50% 50%
4	g	2	100%
4	h	2	100%
4	i	2	50% 50%
4	j	2	50% 50% 50%
4	k	2	50% 100%
4	l	2	100%

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Mol	Chain	Length	Quality of chain
4	m	2	
4	n	2	
4	o	2	
4	p	2	
4	q	2	
4	r	2	
4	s	2	
4	t	2	
4	u	2	
4	v	2	
4	w	2	
4	x	2	
4	y	2	
4	z	2	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 71532 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sodium-dependent neutral amino acid transporter B(0)AT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	605	Total 4799	C 3171	N 744	O 854	S 30	0	0
1	C	605	Total 4799	C 3171	N 744	O 854	S 30	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q695T7
A	-18	ALA	-	expression tag	UNP Q695T7
A	-17	ASP	-	expression tag	UNP Q695T7
A	-16	TYR	-	expression tag	UNP Q695T7
A	-15	LYS	-	expression tag	UNP Q695T7
A	-14	ASP	-	expression tag	UNP Q695T7
A	-13	ASP	-	expression tag	UNP Q695T7
A	-12	ASP	-	expression tag	UNP Q695T7
A	-11	ASP	-	expression tag	UNP Q695T7
A	-10	LYS	-	expression tag	UNP Q695T7
A	-9	SER	-	expression tag	UNP Q695T7
A	-8	GLY	-	expression tag	UNP Q695T7
A	-7	PRO	-	expression tag	UNP Q695T7
A	-6	ASP	-	expression tag	UNP Q695T7
A	-5	GLU	-	expression tag	UNP Q695T7
A	-4	VAL	-	expression tag	UNP Q695T7
A	-3	ASP	-	expression tag	UNP Q695T7
A	-2	ALA	-	expression tag	UNP Q695T7
A	-1	SER	-	expression tag	UNP Q695T7
A	0	GLY	-	expression tag	UNP Q695T7
A	1	ARG	-	expression tag	UNP Q695T7
C	-19	MET	-	initiating methionine	UNP Q695T7
C	-18	ALA	-	expression tag	UNP Q695T7
C	-17	ASP	-	expression tag	UNP Q695T7
C	-16	TYR	-	expression tag	UNP Q695T7
C	-15	LYS	-	expression tag	UNP Q695T7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	ASP	-	expression tag	UNP Q695T7
C	-13	ASP	-	expression tag	UNP Q695T7
C	-12	ASP	-	expression tag	UNP Q695T7
C	-11	ASP	-	expression tag	UNP Q695T7
C	-10	LYS	-	expression tag	UNP Q695T7
C	-9	SER	-	expression tag	UNP Q695T7
C	-8	GLY	-	expression tag	UNP Q695T7
C	-7	PRO	-	expression tag	UNP Q695T7
C	-6	ASP	-	expression tag	UNP Q695T7
C	-5	GLU	-	expression tag	UNP Q695T7
C	-4	VAL	-	expression tag	UNP Q695T7
C	-3	ASP	-	expression tag	UNP Q695T7
C	-2	ALA	-	expression tag	UNP Q695T7
C	-1	SER	-	expression tag	UNP Q695T7
C	0	GLY	-	expression tag	UNP Q695T7
C	1	ARG	-	expression tag	UNP Q695T7

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	748	Total	C	N	O	S	0	0
			6089	3906	1018	1131	34		
2	D	748	Total	C	N	O	S	0	0
			6089	3906	1018	1131	34		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	expression tag	UNP Q9BYF1
B	-10	ALA	-	expression tag	UNP Q9BYF1
B	-9	SER	-	expression tag	UNP Q9BYF1
B	-8	GLY	-	expression tag	UNP Q9BYF1
B	-7	ARG	-	expression tag	UNP Q9BYF1
B	10	TRP	-	insertion	UNP Q9BYF1
B	11	SER	-	insertion	UNP Q9BYF1
B	12	HIS	-	insertion	UNP Q9BYF1
B	13	PRO	-	insertion	UNP Q9BYF1
B	14	GLN	-	insertion	UNP Q9BYF1
B	15	PHE	-	insertion	UNP Q9BYF1
B	16	GLU	-	insertion	UNP Q9BYF1
B	17	LYS	-	insertion	UNP Q9BYF1
D	-11	MET	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	ALA	-	expression tag	UNP Q9BYF1
D	-9	SER	-	expression tag	UNP Q9BYF1
D	-8	GLY	-	expression tag	UNP Q9BYF1
D	-7	ARG	-	expression tag	UNP Q9BYF1
D	10	TRP	-	insertion	UNP Q9BYF1
D	11	SER	-	insertion	UNP Q9BYF1
D	12	HIS	-	insertion	UNP Q9BYF1
D	13	PRO	-	insertion	UNP Q9BYF1
D	14	GLN	-	insertion	UNP Q9BYF1
D	15	PHE	-	insertion	UNP Q9BYF1
D	16	GLU	-	insertion	UNP Q9BYF1
D	17	LYS	-	insertion	UNP Q9BYF1

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	1007	Total	C	N	O	S	0	0
			7872	5025	1310	1501	36		
3	F	1006	Total	C	N	O	S	0	0
			7866	5022	1309	1499	36		
3	G	1006	Total	C	N	O	S	0	0
			7866	5022	1309	1499	36		
3	H	1007	Total	C	N	O	S	0	0
			7872	5025	1310	1501	36		
3	I	1006	Total	C	N	O	S	0	0
			7866	5022	1309	1499	36		
3	J	1006	Total	C	N	O	S	0	0
			7866	5022	1309	1499	36		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	986	PRO	LYS	engineered mutation	UNP P0DTC2
E	987	PRO	VAL	engineered mutation	UNP P0DTC2
E	1274	LEU	-	expression tag	UNP P0DTC2
E	1275	GLU	-	expression tag	UNP P0DTC2
E	1276	ASP	-	expression tag	UNP P0DTC2
E	1277	TYR	-	expression tag	UNP P0DTC2
E	1278	LYS	-	expression tag	UNP P0DTC2
E	1279	ASP	-	expression tag	UNP P0DTC2
E	1280	ASP	-	expression tag	UNP P0DTC2
E	1281	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1282	ASP	-	expression tag	UNP P0DTC2
E	1283	LYS	-	expression tag	UNP P0DTC2
F	986	PRO	LYS	engineered mutation	UNP P0DTC2
F	987	PRO	VAL	engineered mutation	UNP P0DTC2
F	1274	LEU	-	expression tag	UNP P0DTC2
F	1275	GLU	-	expression tag	UNP P0DTC2
F	1276	ASP	-	expression tag	UNP P0DTC2
F	1277	TYR	-	expression tag	UNP P0DTC2
F	1278	LYS	-	expression tag	UNP P0DTC2
F	1279	ASP	-	expression tag	UNP P0DTC2
F	1280	ASP	-	expression tag	UNP P0DTC2
F	1281	ASP	-	expression tag	UNP P0DTC2
F	1282	ASP	-	expression tag	UNP P0DTC2
F	1283	LYS	-	expression tag	UNP P0DTC2
G	986	PRO	LYS	engineered mutation	UNP P0DTC2
G	987	PRO	VAL	engineered mutation	UNP P0DTC2
G	1274	LEU	-	expression tag	UNP P0DTC2
G	1275	GLU	-	expression tag	UNP P0DTC2
G	1276	ASP	-	expression tag	UNP P0DTC2
G	1277	TYR	-	expression tag	UNP P0DTC2
G	1278	LYS	-	expression tag	UNP P0DTC2
G	1279	ASP	-	expression tag	UNP P0DTC2
G	1280	ASP	-	expression tag	UNP P0DTC2
G	1281	ASP	-	expression tag	UNP P0DTC2
G	1282	ASP	-	expression tag	UNP P0DTC2
G	1283	LYS	-	expression tag	UNP P0DTC2
H	986	PRO	LYS	engineered mutation	UNP P0DTC2
H	987	PRO	VAL	engineered mutation	UNP P0DTC2
H	1274	LEU	-	expression tag	UNP P0DTC2
H	1275	GLU	-	expression tag	UNP P0DTC2
H	1276	ASP	-	expression tag	UNP P0DTC2
H	1277	TYR	-	expression tag	UNP P0DTC2
H	1278	LYS	-	expression tag	UNP P0DTC2
H	1279	ASP	-	expression tag	UNP P0DTC2
H	1280	ASP	-	expression tag	UNP P0DTC2
H	1281	ASP	-	expression tag	UNP P0DTC2
H	1282	ASP	-	expression tag	UNP P0DTC2
H	1283	LYS	-	expression tag	UNP P0DTC2
I	986	PRO	LYS	engineered mutation	UNP P0DTC2
I	987	PRO	VAL	engineered mutation	UNP P0DTC2
I	1274	LEU	-	expression tag	UNP P0DTC2
I	1275	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	1276	ASP	-	expression tag	UNP P0DTC2
I	1277	TYR	-	expression tag	UNP P0DTC2
I	1278	LYS	-	expression tag	UNP P0DTC2
I	1279	ASP	-	expression tag	UNP P0DTC2
I	1280	ASP	-	expression tag	UNP P0DTC2
I	1281	ASP	-	expression tag	UNP P0DTC2
I	1282	ASP	-	expression tag	UNP P0DTC2
I	1283	LYS	-	expression tag	UNP P0DTC2
J	986	PRO	LYS	engineered mutation	UNP P0DTC2
J	987	PRO	VAL	engineered mutation	UNP P0DTC2
J	1274	LEU	-	expression tag	UNP P0DTC2
J	1275	GLU	-	expression tag	UNP P0DTC2
J	1276	ASP	-	expression tag	UNP P0DTC2
J	1277	TYR	-	expression tag	UNP P0DTC2
J	1278	LYS	-	expression tag	UNP P0DTC2
J	1279	ASP	-	expression tag	UNP P0DTC2
J	1280	ASP	-	expression tag	UNP P0DTC2
J	1281	ASP	-	expression tag	UNP P0DTC2
J	1282	ASP	-	expression tag	UNP P0DTC2
J	1283	LYS	-	expression tag	UNP P0DTC2

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		
4	d	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		
4	f	2	Total	C	N	O	0	0
			28	16	2	10		
4	g	2	Total	C	N	O	0	0
			28	16	2	10		
4	h	2	Total	C	N	O	0	0
			28	16	2	10		
4	i	2	Total	C	N	O	0	0
			28	16	2	10		
4	j	2	Total	C	N	O	0	0
			28	16	2	10		
4	k	2	Total	C	N	O	0	0
			28	16	2	10		

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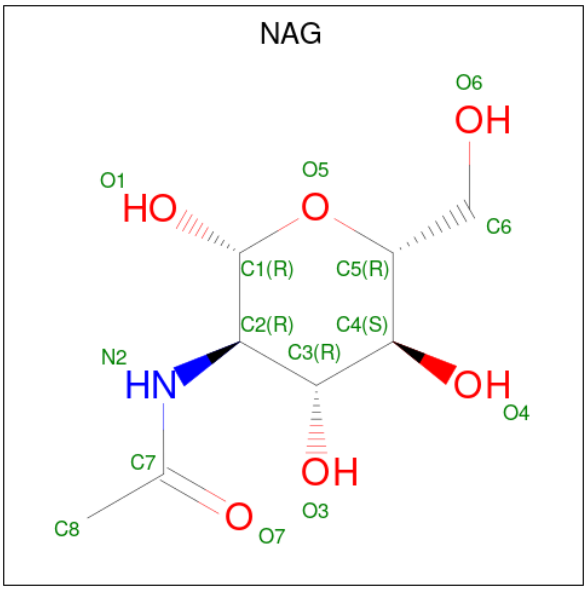
Mol	Chain	Residues	Atoms				AltConf	Trace
4	l	2	Total	C	N	O	0	0
			28	16	2	10		
4	m	2	Total	C	N	O	0	0
			28	16	2	10		
4	n	2	Total	C	N	O	0	0
			28	16	2	10		
4	o	2	Total	C	N	O	0	0
			28	16	2	10		
4	p	2	Total	C	N	O	0	0
			28	16	2	10		
4	q	2	Total	C	N	O	0	0
			28	16	2	10		
4	r	2	Total	C	N	O	0	0
			28	16	2	10		
4	s	2	Total	C	N	O	0	0
			28	16	2	10		
4	t	2	Total	C	N	O	0	0
			28	16	2	10		
4	u	2	Total	C	N	O	0	0
			28	16	2	10		
4	v	2	Total	C	N	O	0	0
			28	16	2	10		
4	w	2	Total	C	N	O	0	0
			28	16	2	10		
4	x	2	Total	C	N	O	0	0
			28	16	2	10		
4	y	2	Total	C	N	O	0	0
			28	16	2	10		
4	z	2	Total	C	N	O	0	0
			28	16	2	10		
4	0	2	Total	C	N	O	0	0
			28	16	2	10		
4	1	2	Total	C	N	O	0	0
			28	16	2	10		
4	2	2	Total	C	N	O	0	0
			28	16	2	10		
4	3	2	Total	C	N	O	0	0
			28	16	2	10		
4	4	2	Total	C	N	O	0	0
			28	16	2	10		
4	5	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms	AltConf	Trace
4	6	2	Total C N O 28 16 2 10	0	0
4	7	2	Total C N O 28 16 2 10	0	0
4	8	2	Total C N O 28 16 2 10	0	0
4	9	2	Total C N O 28 16 2 10	0	0
4	AA	2	Total C N O 28 16 2 10	0	0
4	BA	2	Total C N O 28 16 2 10	0	0
4	CA	2	Total C N O 28 16 2 10	0	0
4	DA	2	Total C N O 28 16 2 10	0	0
4	EA	2	Total C N O 28 16 2 10	0	0
4	FA	2	Total C N O 28 16 2 10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C N O 14 8 1 5	0

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Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	

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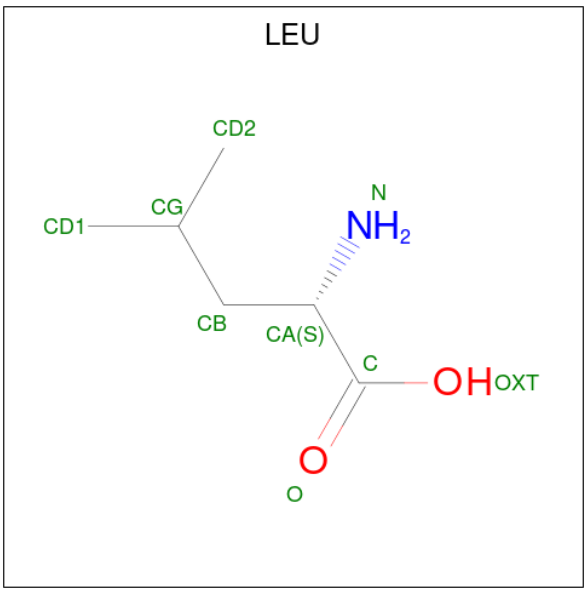
Mol	Chain	Residues	Atoms				AltConf
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is LEUCINE (CCD ID: LEU) (formula: $C_6H_{13}NO_2$).



Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C N O 9 6 1 2	0
6	C	1	Total C N O 9 6 1 2	0

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
7	B	1	Total Zn 1 1	0
7	D	1	Total Zn 1 1	0

- Molecule 8 is water.

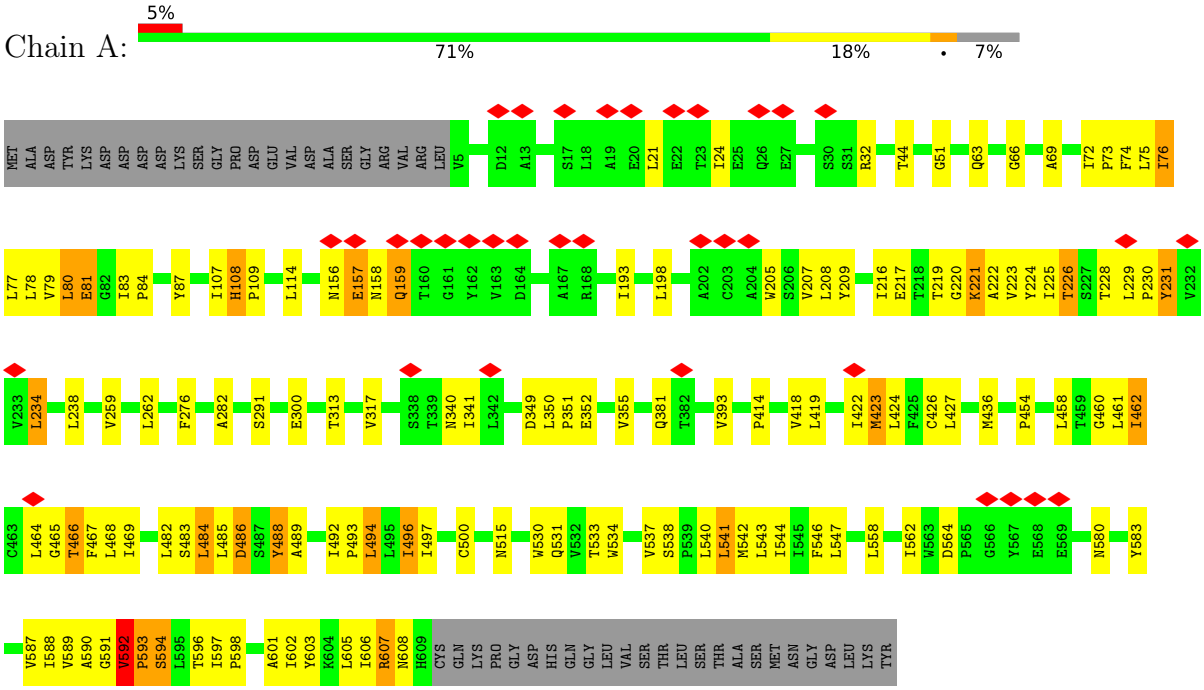
Mol	Chain	Residues	Atoms	AltConf
8	B	4	Total O 4 4	0
8	D	4	Total O 4 4	0

3 Residue-property plots (i)

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

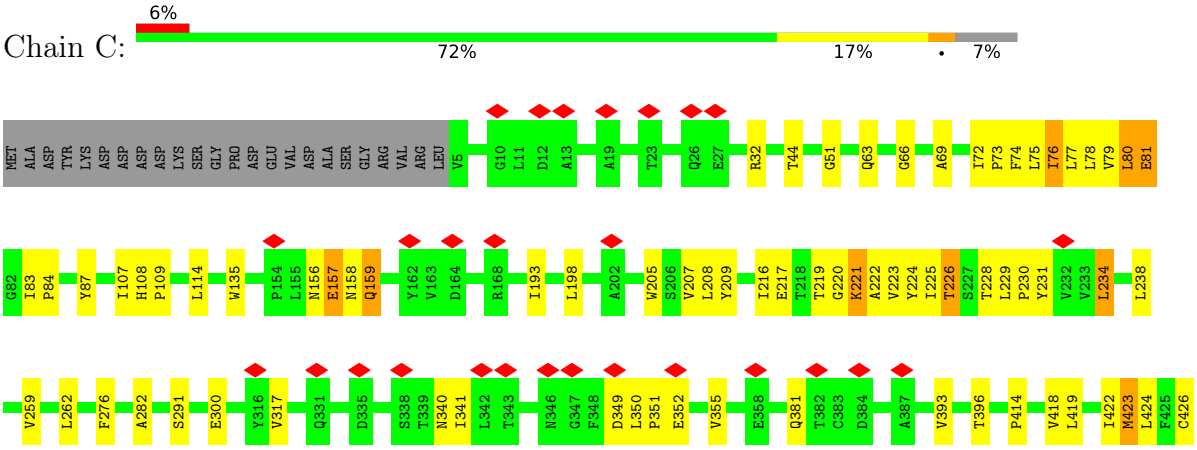
• Molecule 1: Sodium-dependent neutral amino acid transporter B(0)AT1

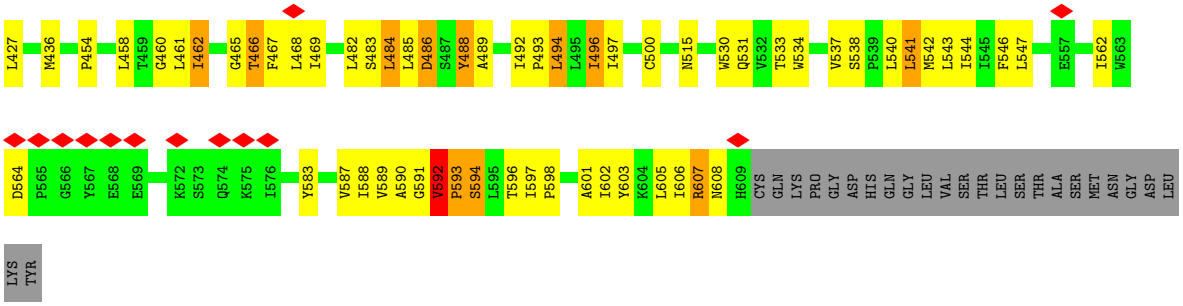
Chain A:



• Molecule 1: Sodium-dependent neutral amino acid transporter B(0)AT1

Chain C:

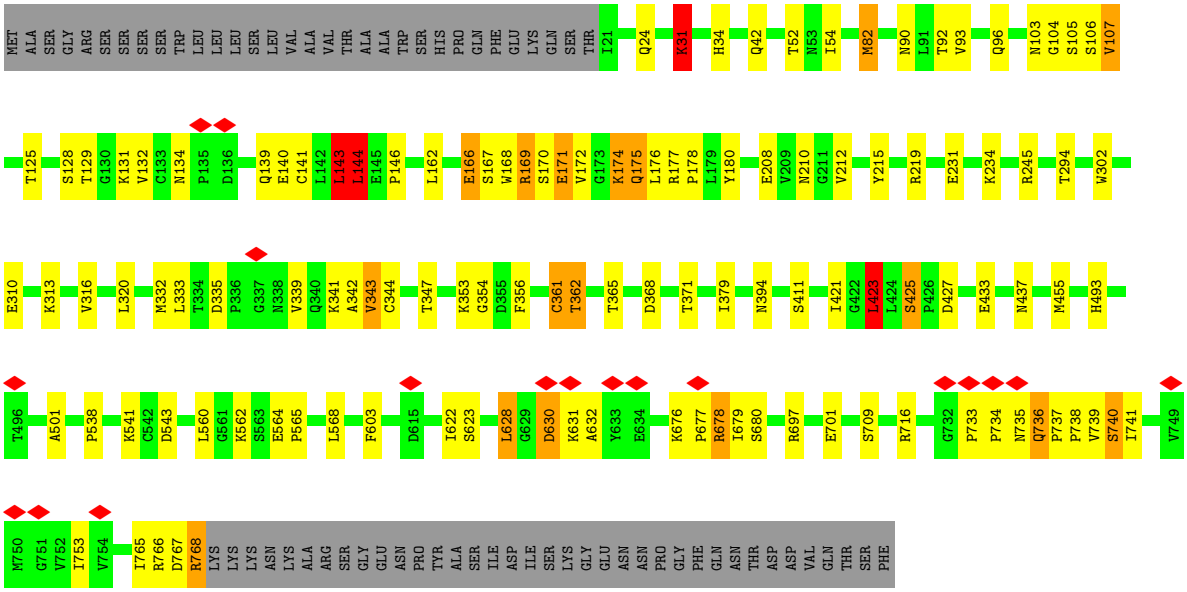




• Molecule 2: Angiotensin-converting enzyme 2

Chain B:

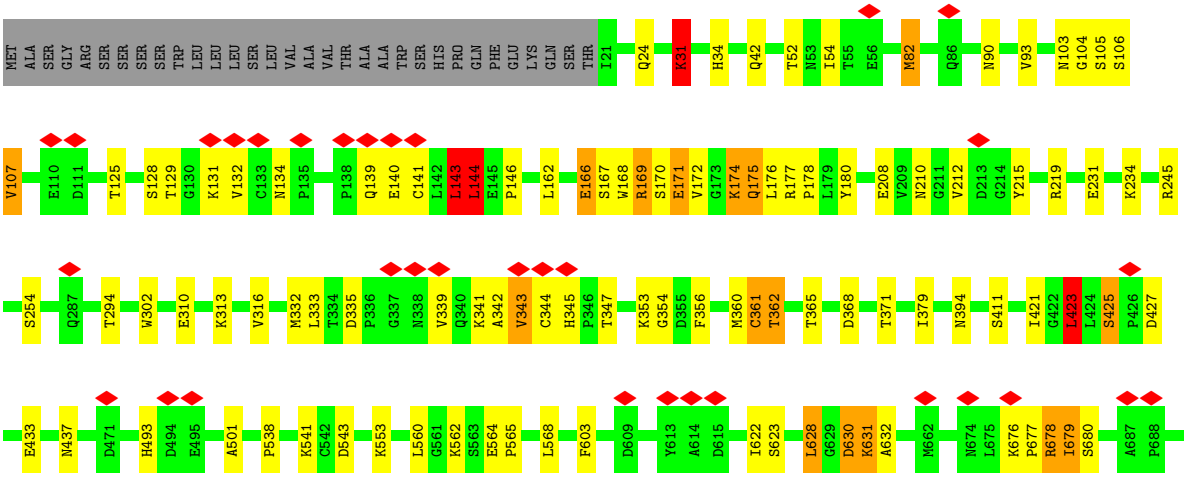


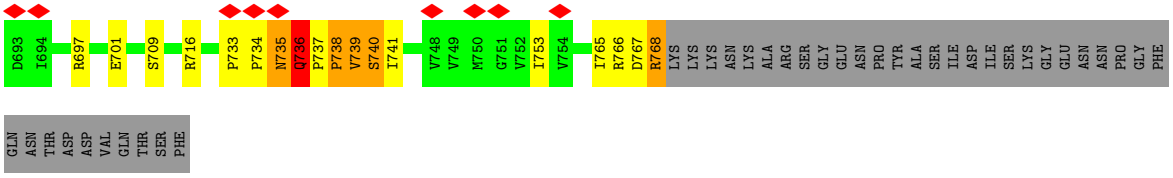


• Molecule 2: Angiotensin-converting enzyme 2

Chain D:



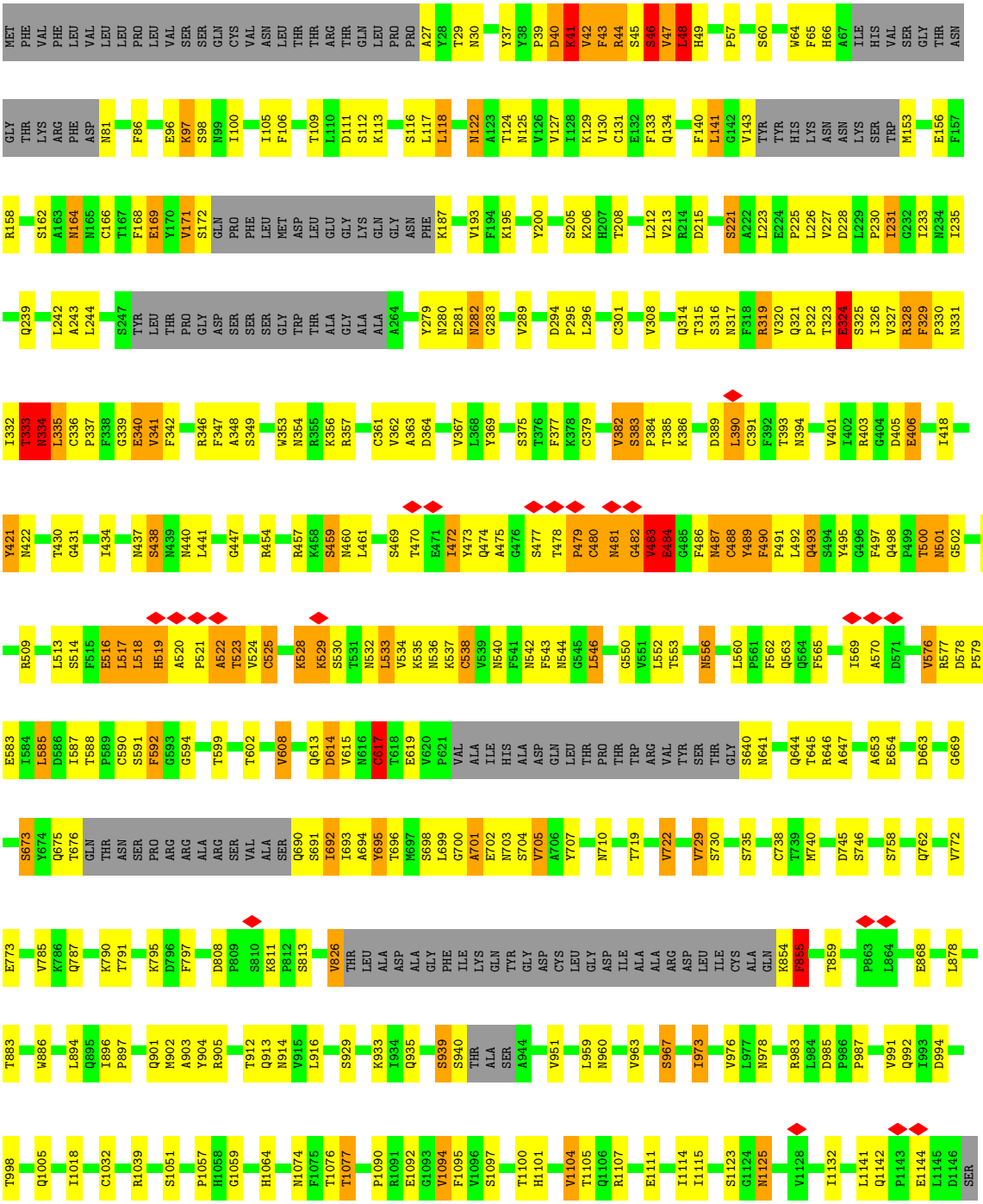


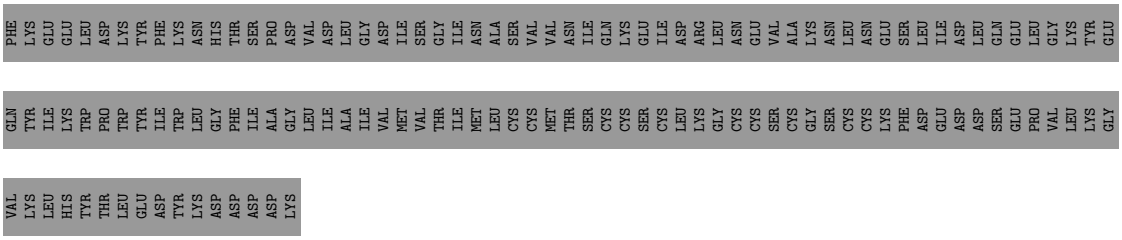


• Molecule 3: Spike glycoprotein

Chain E:



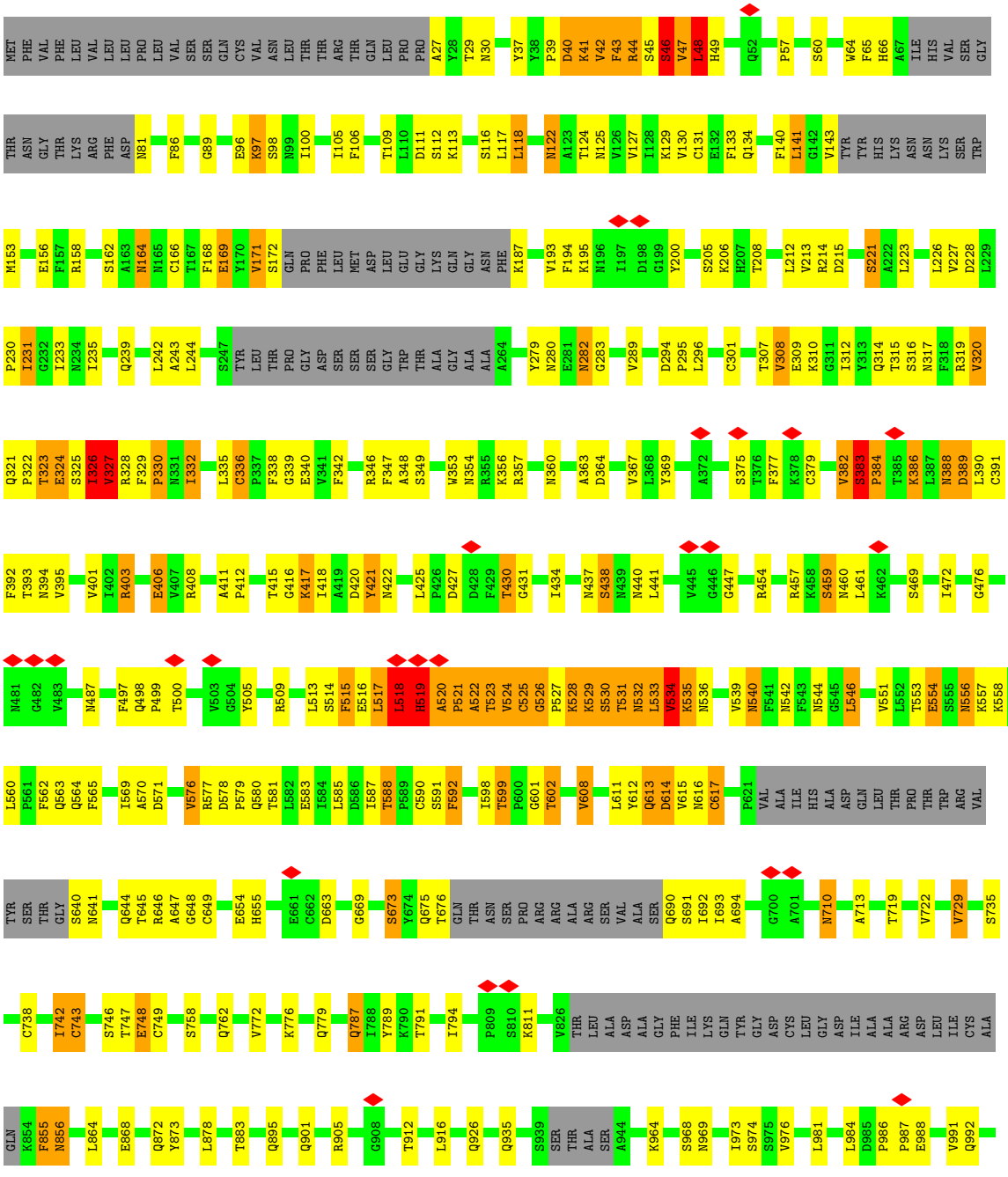


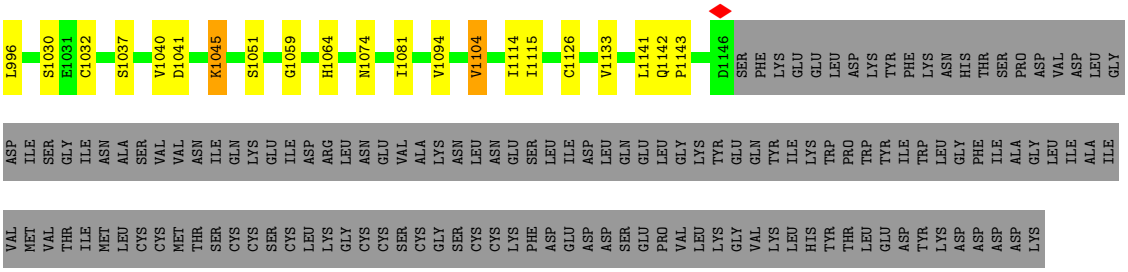


• Molecule 3: Spike glycoprotein

Chain F:



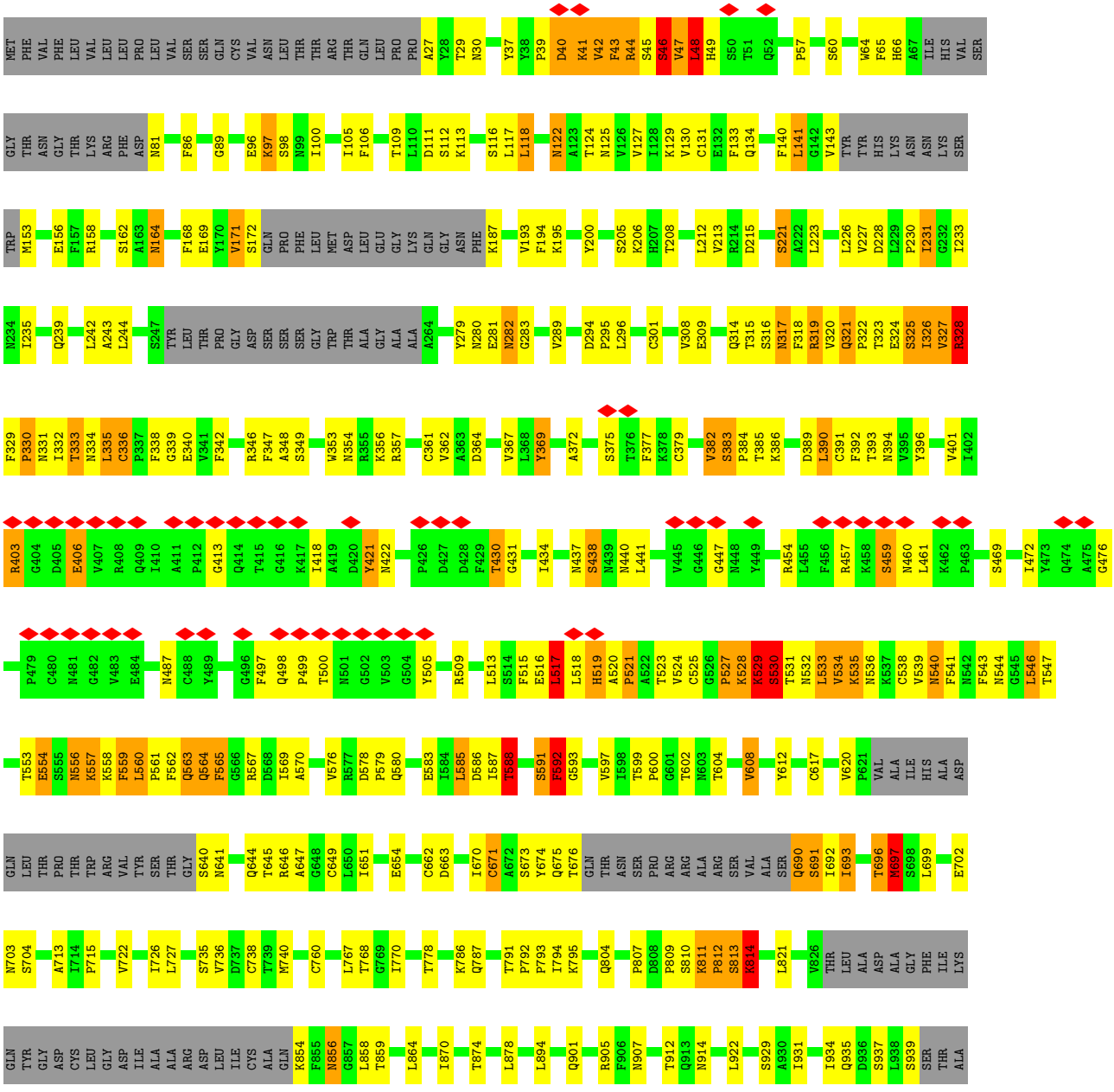


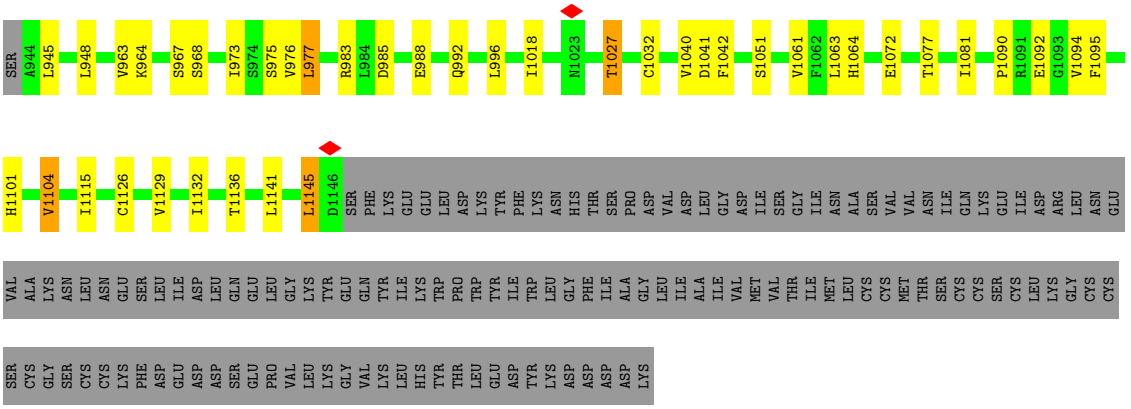


• Molecule 3: Spike glycoprotein

Chain G:



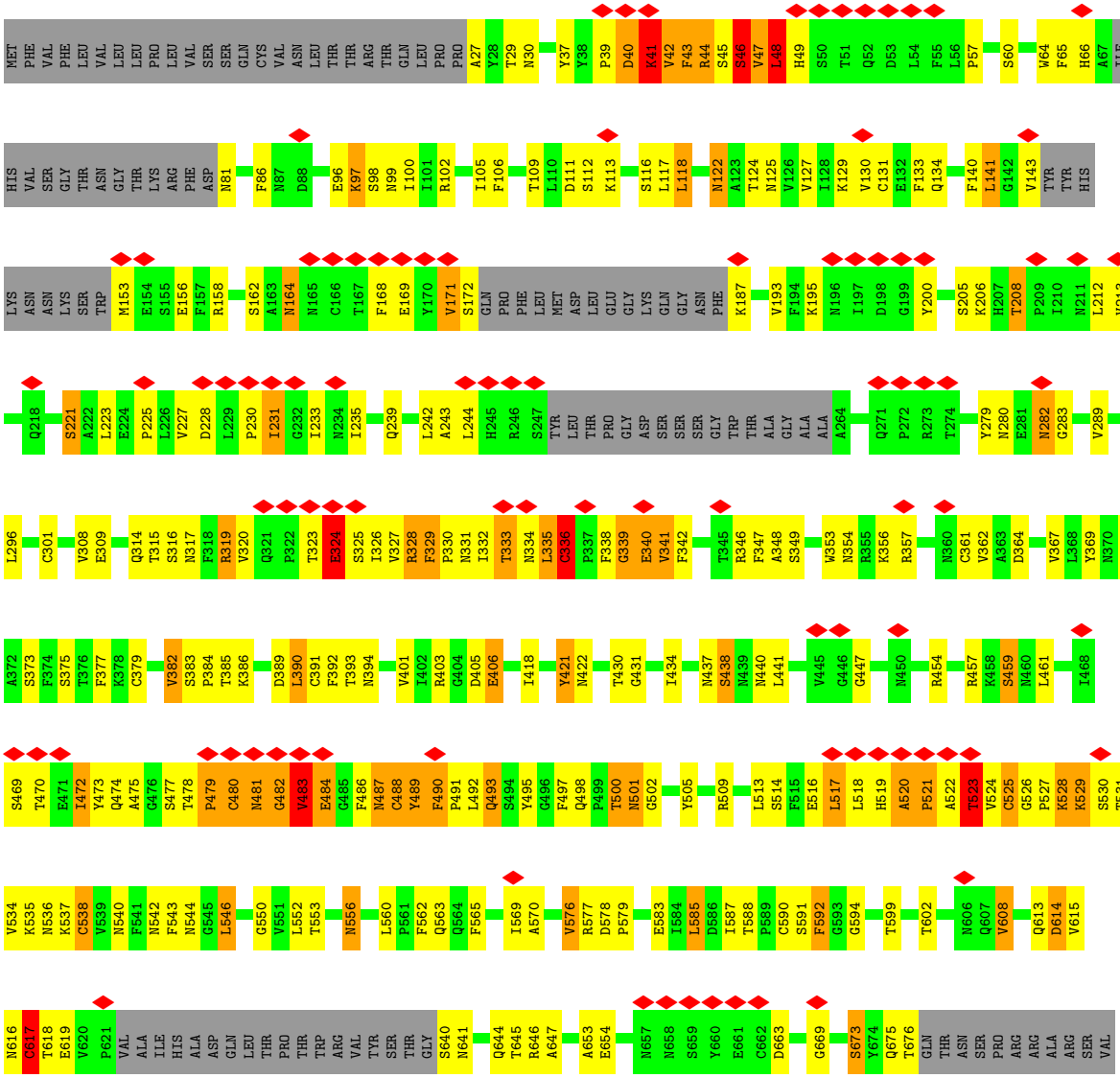


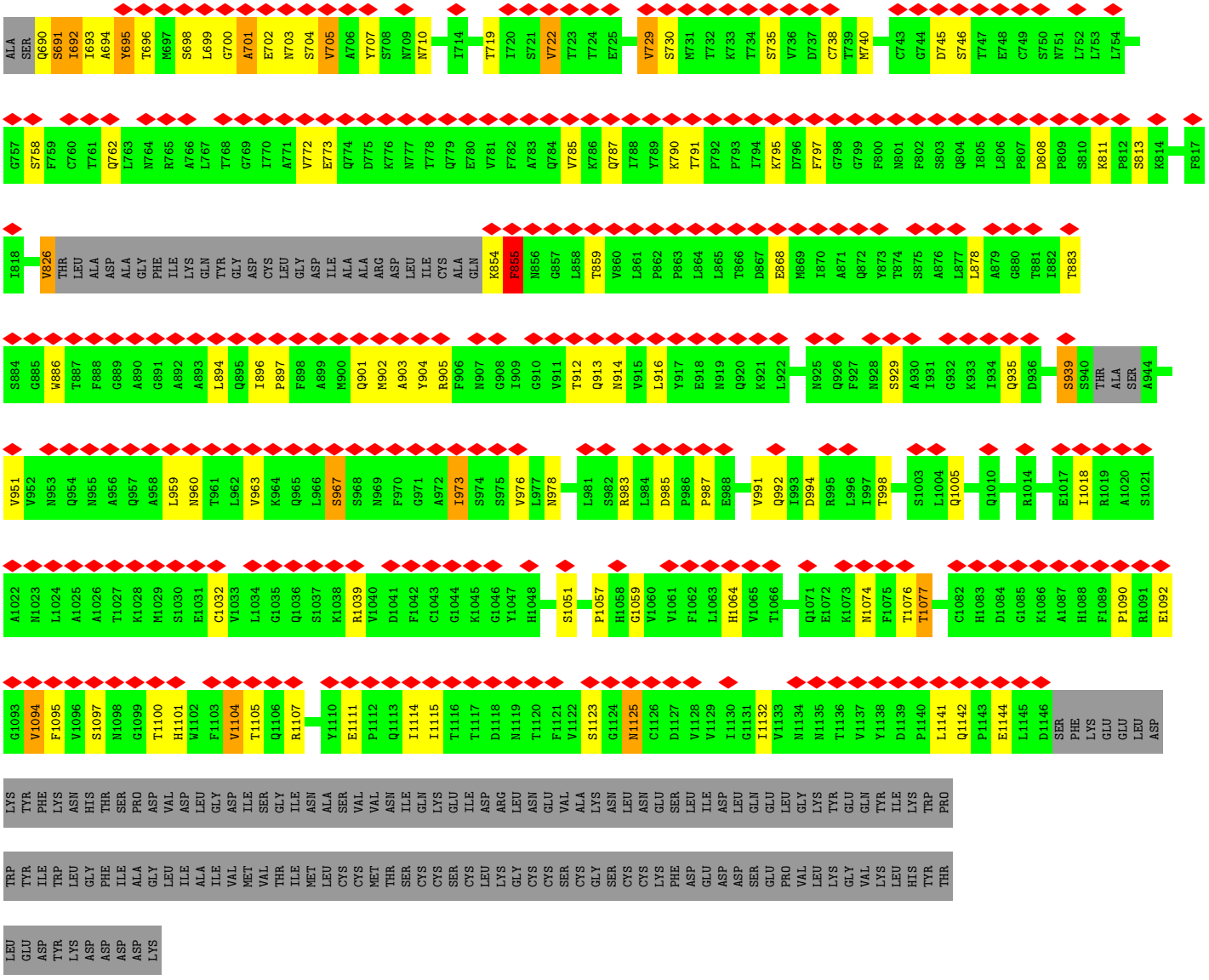


• Molecule 3: Spike glycoprotein

Chain H:



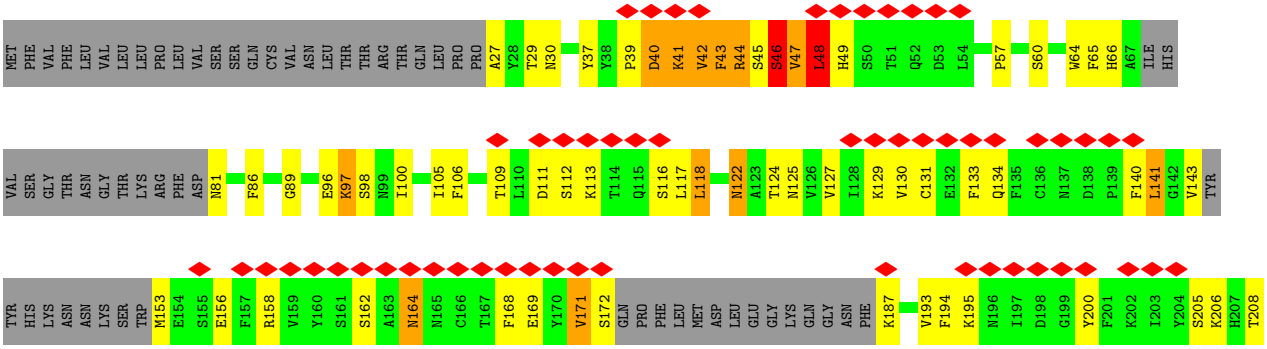


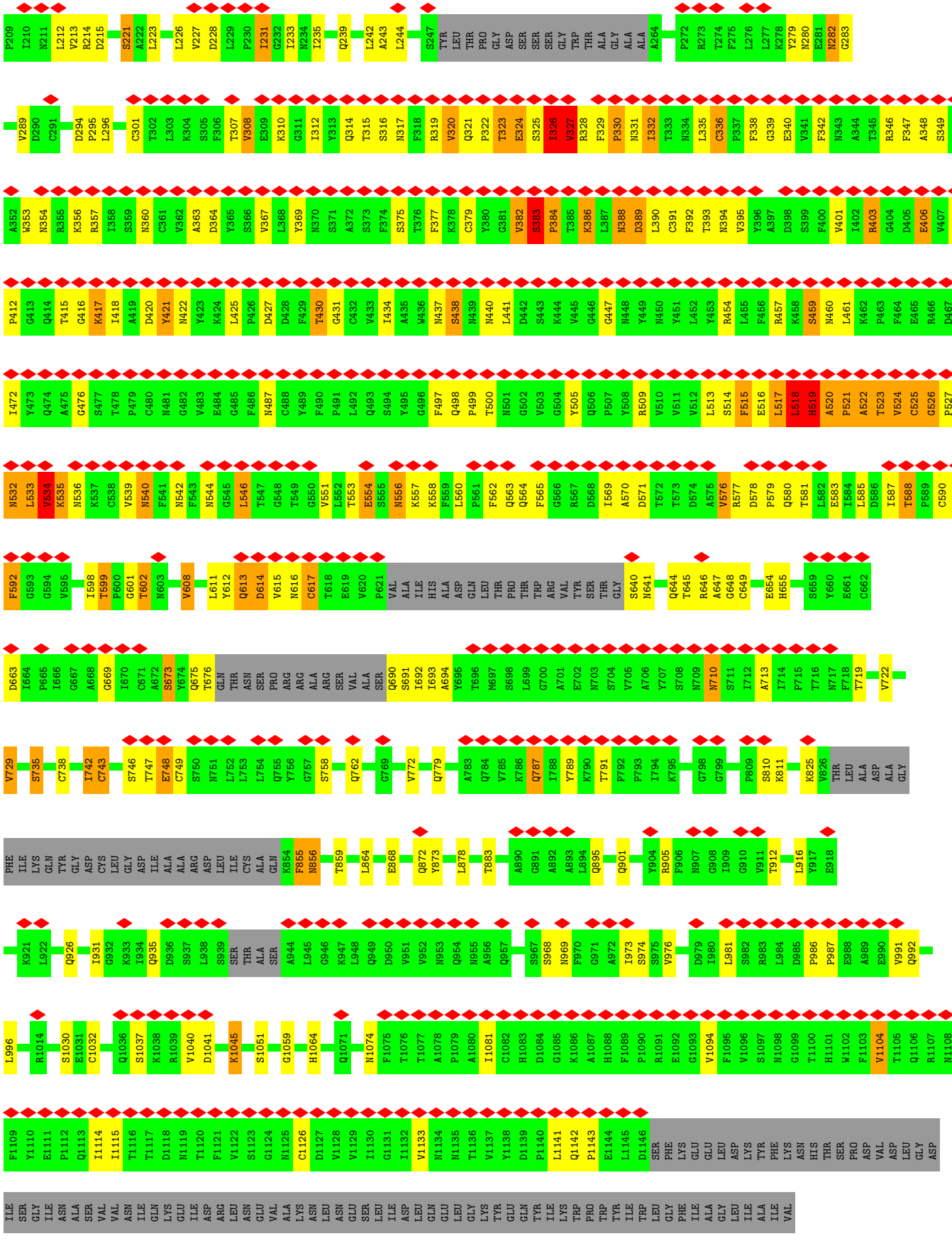


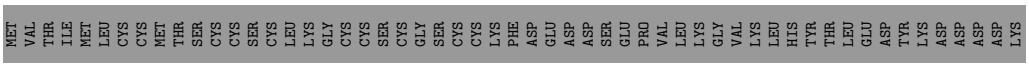
• Molecule 3: Spike glycoprotein

Chain I:





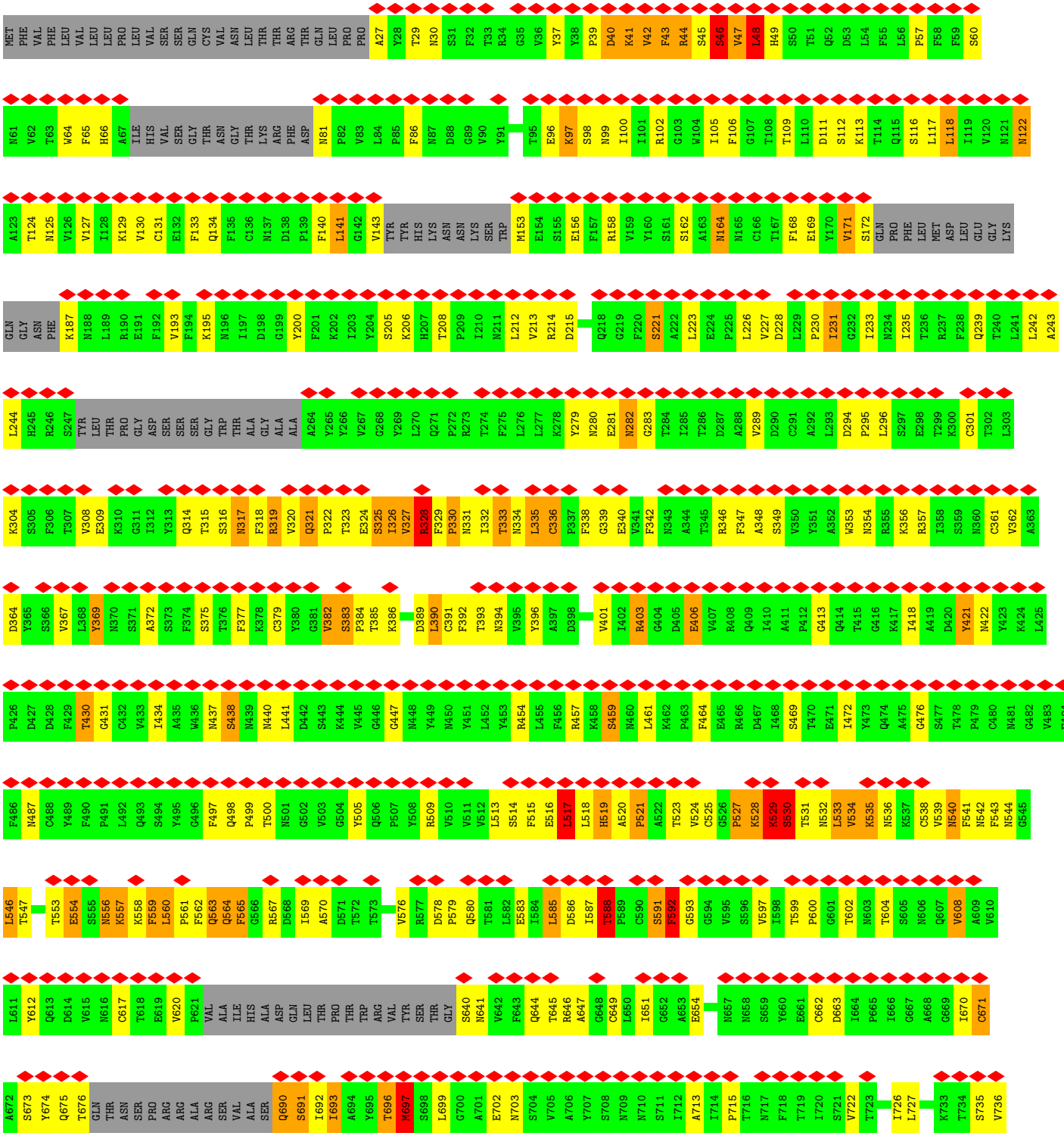

P209 I210 N211 L212 V213 R214 D215 S221 A222 L223 L226 V227 D228 L229 P230 I231 G232 I233 N234 I235 Q239 L242 A243 L244 S247 TYR LEU THR PRO GLY ASP SER SER SER GLY TRP THR ALA GLY ALA ALA A264 P272 R273 T274 F275 L276 L277 K278 Y279 N280 E281 N282 G283
V289 D290 C291 D294 P295 L296 C301 T302 L303 K304 S305 F306 T307 V308 E309 K310 G311 I312 Y313 Q314 T315 S316 N317 F318 R319 V320 Q321 P322 T323 E324 S325 T326 V327 R328 F329 P330 N331 I332 T333 N334 L335 C336 P337 F338 G339 E340 V341 F342 N343 A344 T345 R346 F347 A348 S349 V350 Y351
A352 W353 N354 R355 K356 R357 I358 S359 N360 C361 V362 A363 D364 Y365 S366 V367 L368 Y369 N370 S371 A372 S373 F374 S375 T376 F377 K378 C379 Y380 G381 V382 S383 P384 T385 K386 L387 N388 D389 L390 C391 F392 T393 N394 V395 Y396 A397 D398 S399 F400 V401 I402 R403 G404 D405 E406 V407 R408 Q409 I410 A411
P412 G413 Q414 T415 G416 K417 I418 A419 D420 Y421 N422 Y423 K424 L425 P426 D427 D428 F429 T430 G431 C432 V433 I434 A435 W436 N437 S438 N439 N440 L441 D442 S443 K444 V445 G446 G447 N448 Y449 N450 Y451 L452 Y453 R454 L455 F456 R457 K458 S459 N460 L461 K462 P463 F464 E465 R466 D467 I468 S469 T470 E471
I472 Y473 Q474 A475 G476 S477 T478 P479 C480 N481 G482 V483 E484 G485 F486 N487 C488 Y489 F490 P491 L492 Q493 S494 Y495 G496 F497 Q498 P499 T500 N501 G502 V503 G504 Y505 Q506 P507 Y508 R509 V510 V511 V512 L513 S514 F515 E516 L517 L518 H519 A520 P521 A522 T523 V524 C525 G526 P527 K528 K529 S530 T531
N532 L533 V534 K535 N536 K537 C538 V539 N540 F541 N542 F543 N544 G545 L546 T547 G548 T549 G550 V551 L552 T553 E554 S555 N556 K557 K558 F559 L560 P561 F562 Q563 Q564 F565 G566 R567 D568 I569 A570 D571 T572 T573 D574 A575 V576 R577 D578 P579 Q580 T581 L582 E583 I584 L585 D586 I587 T588 P589 C590 S591
F592 G593 G594 V595 I598 T599 P600 G601 T602 N603 V608 L611 Y612 Q613 D614 V615 N616 C617 T618 E619 V620 P621 VAL ALA ILE HIS ALA ASP GLN LEU THR PRO THR TRP ARG VAL TYR SER THR GLY S640 N641 Q644 T645 R646 A647 G648 C649 E654 H655 S659 Y660 E661 C662
D663 I664 P665 I666 G667 A668 G669 I670 C671 A672 S673 Y674 Q675 T676 GLN THR ASN SER PRO ARG ARG ALA ARG SER VAL ALA SER Q690 S691 I692 I693 A694 Y696 T696 M697 S698 L699 G700 A701 E702 N703 S704 V705 A706 Y707 S708 N709 N710 S711 I712 A713 I714 P715 T716 N717 F718 T719 V722
V729 S735 C738 I742 C743 S746 T747 E748 C749 S750 N751 L752 L753 L754 Q755 Y756 G757 S758 Q762 G769 V772 Q779 A783 Q784 V785 K786 Q787 I788 Y789 K790 T791 P792 P793 I794 K795 G798 G799 P809 S810 K811 K825 V826 THR LEU ALA ASP ALA GLY
PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG ASP LEU ILE LEU CYS ALA GLN K854 F855 N856 T859 L864 E868 Q872 Y873 L878 T883 A890 G891 A892 A893 L894 Q895 Q901 Y904 R905 F906 N907 G908 I909 G910 V911 T912 L916 Y917 E918
K921 L922 Q926 I931 G932 K933 I934 Q935 D936 S937 L938 S939 SER THR ALA SER A944 L945 G946 K947 L948 Q949 D950 V951 V952 N953 Q954 N955 A956 Q957 S967 S968 N969 F970 G971 A972 I973 S974 S975 V976 D979 I980 L981 S982 R983 L984 D985 P986 P987 E988 A989 E990 V991 Q992
L996 R1014 S1030 E1031 C1032 Q1036 S1037 K1038 R1039 V1040 D1041 K1045 S1051 G1059 H1064 Q1071 N1074 F1075 T1076 T1077 A1078 P1079 A1080 I1081 C1082 H1083 D1084 G1085 K1086 A1087 H1088 F1089 P1090 R1091 E1092 G1093 V1094 F1095 V1096 S1097 N1098 G1099 T1100 H1101 W1102 F1103 V1104 T1105 Q1106 R1107 N1108
F1109 Y1110 E1111 P1112 Q1113 I1114 I1115 T1116 T1117 D1118 N1119 T1120 F1121 V1122 S1123 G1124 N1125 C1126 D1127 V1128 V1129 I1130 G1131 I1132 V1133 N1134 N1135 T1136 V1137 Y1138 D1139 P1140 L1141 Q1142 P1143 E1144 L1145 D1146 SER PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP
ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN D1127 LEU ASN GLU SER LEU ILE ASP LEU GLN LEU GLU LEU GLY LYS TYR GLU GLN TYR ILE LYS TRP PRO TRP TYR ILE TRP LEU GLY PHE ILE ALA GLY LEU ILE ALA ILE VAL

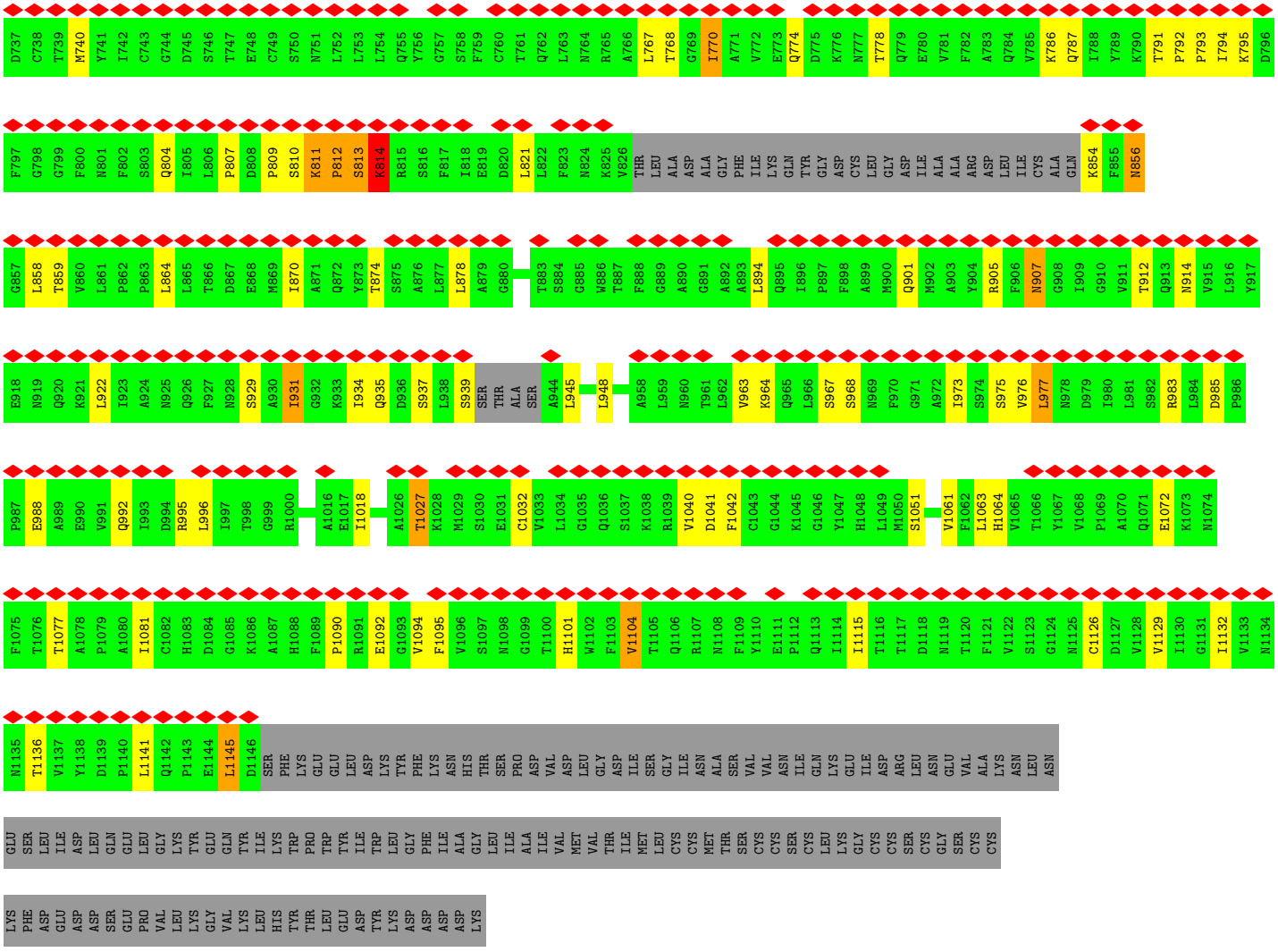


• Molecule 3: Spike glycoprotein

Chain J:

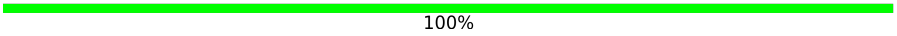






• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

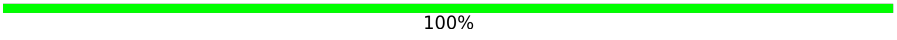
Chain K:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

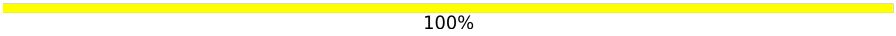
Chain M:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

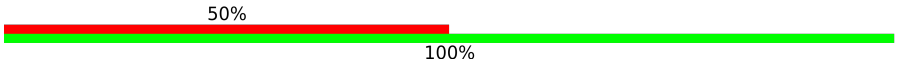
Chain N:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

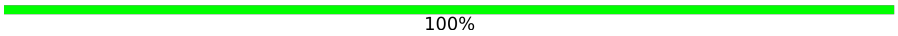
Chain P:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

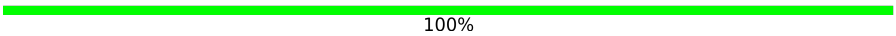
Chain Q:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

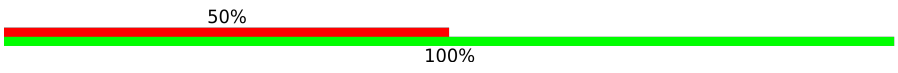
Chain R:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

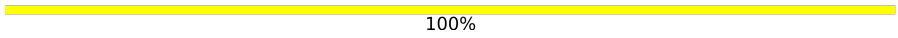
Chain T:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

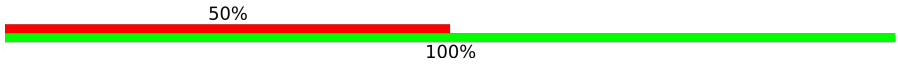
Chain U:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

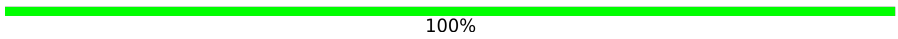
Chain W:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

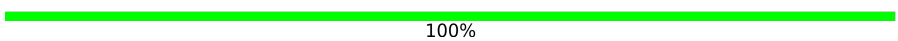
Chain X:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

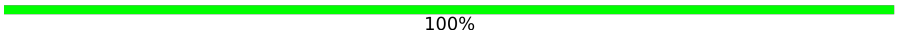
Chain Y:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

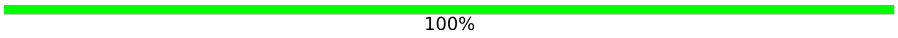
Chain Z:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

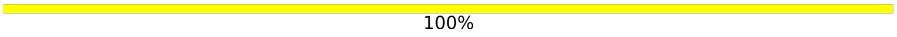
Chain f:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

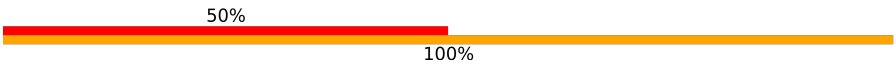
Chain j:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

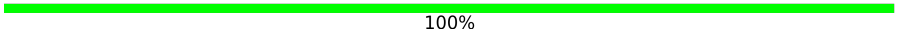
Chain l:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

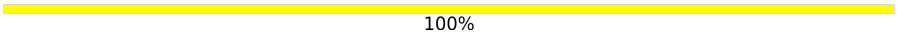
Chain m:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

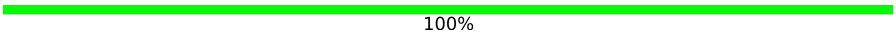
Chain s:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

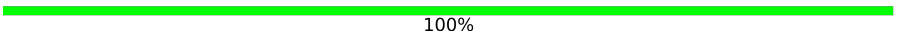
Chain u:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

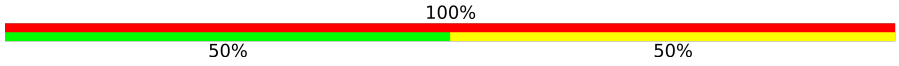
Chain v:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

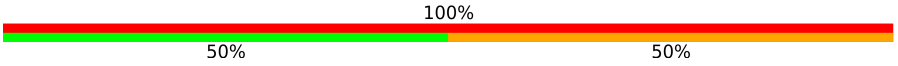
Chain w:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

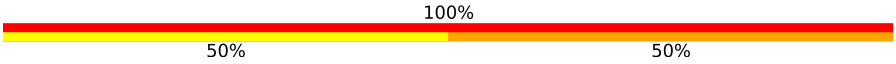
Chain x:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

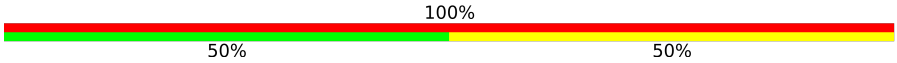
Chain y:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

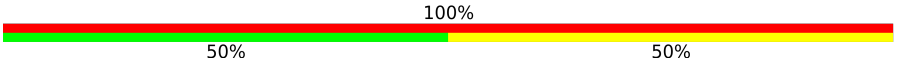
Chain z:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

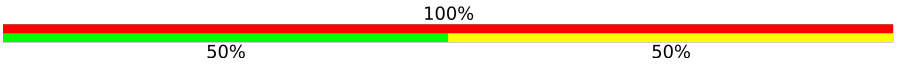
Chain 0:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

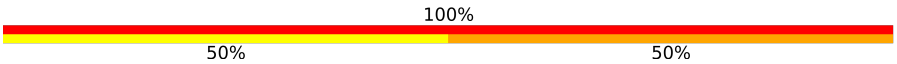
Chain 1:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

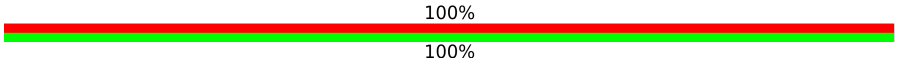
Chain 2:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

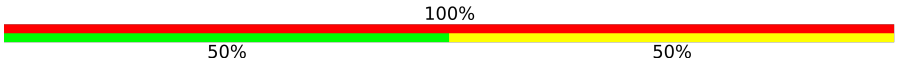
Chain 3:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

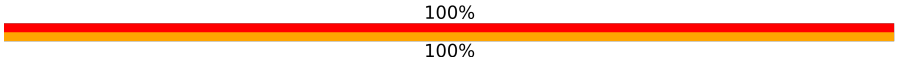
Chain 5:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

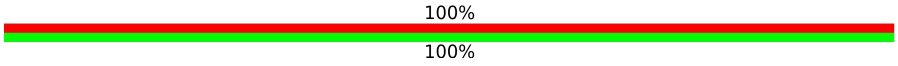
Chain 6:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

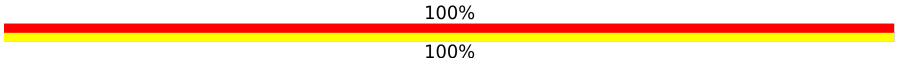
Chain 8:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

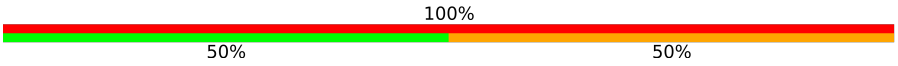
Chain 9:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

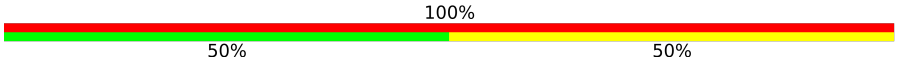
Chain AA:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

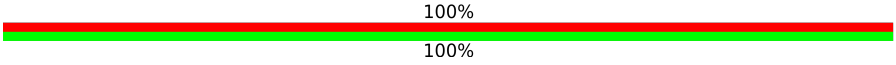
Chain BA:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

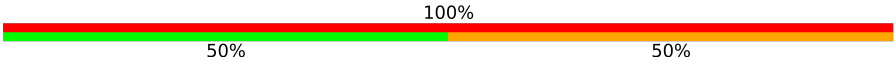
Chain CA:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DA:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain EA:





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53141	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.786	Depositor
Minimum map value	-0.869	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	521.76, 521.76, 521.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.35	0/4940	0.70	9/6748 (0.1%)
1	C	0.34	0/4940	0.70	9/6748 (0.1%)
2	B	0.33	0/6252	0.61	4/8488 (0.0%)
2	D	0.33	0/6252	0.61	4/8488 (0.0%)
3	E	0.53	1/8048 (0.0%)	0.64	5/10947 (0.0%)
3	F	0.51	0/8042	0.63	2/10939 (0.0%)
3	G	0.51	0/8042	0.61	3/10939 (0.0%)
3	H	0.53	1/8048 (0.0%)	0.64	5/10947 (0.0%)
3	I	0.51	0/8042	0.63	2/10939 (0.0%)
3	J	0.51	0/8042	0.61	3/10939 (0.0%)
All	All	0.47	2/70648 (0.0%)	0.63	46/96122 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	698	SER	CA-C	-6.59	1.44	1.52
3	E	698	SER	CA-C	-6.51	1.44	1.52

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	157	GLU	N-CA-C	-10.67	99.18	111.03
1	A	157	GLU	N-CA-C	-10.63	99.23	111.03
2	D	143	LEU	N-CA-C	6.41	120.24	107.62
2	B	143	LEU	N-CA-C	6.40	120.23	107.62
3	H	538	CYS	N-CA-C	-6.40	100.83	110.24

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	A	4799	0	4762	156	0
1	C	4799	0	4762	153	0
2	B	6089	0	5901	157	0
2	D	6089	0	5901	152	0
3	E	7872	0	7674	441	0
3	F	7866	0	7663	458	0
3	G	7866	0	7663	504	0
3	H	7872	0	7670	453	0
3	I	7866	0	7663	458	0
3	J	7866	0	7663	503	0
4	0	28	0	25	0	0
4	1	28	0	25	1	0
4	2	28	0	25	3	0
4	3	28	0	25	0	0
4	4	28	0	25	0	0
4	5	28	0	25	0	0
4	6	28	0	25	1	0
4	7	28	0	25	0	0
4	8	28	0	25	0	0
4	9	28	0	25	3	0
4	AA	28	0	25	1	0
4	BA	28	0	25	0	0
4	CA	28	0	25	0	0
4	DA	28	0	25	1	0
4	EA	28	0	25	2	0
4	FA	28	0	25	0	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	6	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	V	28	0	25	0	0
4	W	28	0	25	0	0
4	X	28	0	25	0	0
4	Y	28	0	25	0	0
4	Z	28	0	25	0	0
4	a	28	0	25	0	0
4	b	28	0	25	1	0
4	c	28	0	25	1	0
4	d	28	0	25	0	0
4	e	28	0	25	0	0
4	f	28	0	25	1	0
4	g	28	0	25	3	0
4	h	28	0	25	0	0
4	i	28	0	25	0	0
4	j	28	0	25	0	0
4	k	28	0	25	1	0
4	l	28	0	25	0	0
4	m	28	0	25	0	0
4	n	28	0	25	3	0
4	o	28	0	25	1	0
4	p	28	0	25	0	0
4	q	28	0	25	0	0
4	r	28	0	25	1	0
4	s	28	0	25	2	0
4	t	28	0	25	0	0
4	u	28	0	25	0	0
4	v	28	0	25	0	0
4	w	28	0	25	0	0
4	x	28	0	25	1	0
4	y	28	0	25	1	0
4	z	28	0	25	0	0
5	A	56	0	52	0	0
5	B	14	0	13	0	0
5	C	56	0	52	0	0
5	D	14	0	13	0	0
5	E	126	0	117	5	0
5	F	140	0	129	8	0
5	G	112	0	104	8	0
5	H	126	0	117	5	0
5	I	140	0	129	8	0
5	J	112	0	104	8	0
6	A	9	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	9	0	10	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	B	4	0	0	0	0
8	D	4	0	0	0	0
All	All	71532	0	69622	3146	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 22.

The worst 5 of 3146 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)
3:F:431:GLY:HA2	3:F:515:PHE:CE1	1.25	1.71
3:I:431:GLY:HA2	3:I:515:PHE:CE1	1.25	1.62
3:H:740:MET:HE1	3:J:592:PHE:CD2	1.44	1.53
3:E:740:MET:HE1	3:G:592:PHE:CD2	1.44	1.52
3:G:431:GLY:HA2	3:G:515:PHE:CD1	1.51	1.45

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	603/654 (92%)	540 (90%)	59 (10%)	4 (1%)	18 56
1	C	531/654 (81%)	483 (91%)	45 (8%)	3 (1%)	21 59
2	B	394/817 (48%)	356 (90%)	34 (9%)	4 (1%)	12 49
2	D	731/817 (90%)	671 (92%)	50 (7%)	10 (1%)	9 40
3	E	989/1283 (77%)	841 (85%)	113 (11%)	35 (4%)	3 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	988/1283 (77%)	855 (86%)	96 (10%)	37 (4%)	2	20
3	G	988/1283 (77%)	842 (85%)	106 (11%)	40 (4%)	2	18
3	H	989/1283 (77%)	841 (85%)	112 (11%)	36 (4%)	2	20
3	I	988/1283 (77%)	855 (86%)	96 (10%)	37 (4%)	2	20
3	J	988/1283 (77%)	842 (85%)	106 (11%)	40 (4%)	2	18
All	All	8189/10640 (77%)	7126 (87%)	817 (10%)	246 (3%)	5	23

5 of 246 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	144	LEU
2	D	144	LEU
2	D	631	LYS
2	D	736	GLN
3	E	48	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	531/572 (93%)	510 (96%)	21 (4%)	28	49
1	C	531/572 (93%)	510 (96%)	21 (4%)	28	49
2	B	662/721 (92%)	637 (96%)	25 (4%)	29	50
2	D	662/721 (92%)	636 (96%)	26 (4%)	28	49
3	E	882/1122 (79%)	756 (86%)	126 (14%)	3	13
3	F	881/1122 (78%)	771 (88%)	110 (12%)	4	16
3	G	881/1122 (78%)	776 (88%)	105 (12%)	5	18
3	H	882/1122 (79%)	757 (86%)	125 (14%)	3	13
3	I	881/1122 (78%)	771 (88%)	110 (12%)	4	16
3	J	881/1122 (78%)	776 (88%)	105 (12%)	5	18
All	All	7674/9318 (82%)	6900 (90%)	774 (10%)	9	23

5 of 774 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	319	ARG
3	I	169	GLU
3	H	421	TYR
3	H	315	THR
3	H	746	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 252 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	920	GLN
3	J	317	ASN
3	G	804	GLN
3	J	239	GLN
3	J	804	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)

116 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	0	1	3,4	14,14,15	0.25	0	17,19,21	0.70	1 (5%)
4	NAG	0	2	4	14,14,15	0.15	0	17,19,21	0.50	0
4	NAG	1	1	3,4	14,14,15	0.28	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	1	2	4	14,14,15	0.24	0	17,19,21	0.60	0
4	NAG	2	1	3,4	14,14,15	0.58	1 (7%)	17,19,21	0.58	0
4	NAG	2	2	4	14,14,15	0.31	0	17,19,21	0.48	0
4	NAG	3	1	3,4	14,14,15	0.29	0	17,19,21	0.42	0
4	NAG	3	2	4	14,14,15	0.43	0	17,19,21	0.38	0
4	NAG	4	1	3,4	14,14,15	0.37	0	17,19,21	1.16	1 (5%)
4	NAG	4	2	4	14,14,15	0.28	0	17,19,21	0.50	0
4	NAG	5	1	3,4	14,14,15	0.31	0	17,19,21	0.72	1 (5%)
4	NAG	5	2	4	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	6	1	3,4	14,14,15	0.73	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	6	2	4	14,14,15	0.33	0	17,19,21	0.73	1 (5%)
4	NAG	7	1	3,4	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	7	2	4	14,14,15	0.27	0	17,19,21	0.38	0
4	NAG	8	1	3,4	14,14,15	0.52	0	17,19,21	0.51	0
4	NAG	8	2	4	14,14,15	0.25	0	17,19,21	0.59	0
4	NAG	9	1	3,4	14,14,15	0.55	0	17,19,21	0.58	0
4	NAG	9	2	4	14,14,15	0.29	0	17,19,21	0.48	0
4	NAG	AA	1	3,4	14,14,15	0.23	0	17,19,21	1.45	2 (11%)
4	NAG	AA	2	4	14,14,15	0.19	0	17,19,21	0.53	0
4	NAG	BA	1	3,4	14,14,15	0.52	0	17,19,21	0.73	1 (5%)
4	NAG	BA	2	4	14,14,15	0.41	0	17,19,21	0.48	0
4	NAG	CA	1	3,4	14,14,15	0.37	0	17,19,21	0.41	0
4	NAG	CA	2	4	14,14,15	0.19	0	17,19,21	0.77	0
4	NAG	DA	1	3,4	14,14,15	0.36	0	17,19,21	0.49	0
4	NAG	DA	2	4	14,14,15	0.60	0	17,19,21	1.39	2 (11%)
4	NAG	EA	1	3,4	14,14,15	0.63	1 (7%)	17,19,21	0.44	0
4	NAG	EA	2	4	14,14,15	0.33	0	17,19,21	1.44	2 (11%)
4	NAG	FA	1	3,4	14,14,15	0.39	0	17,19,21	0.46	0
4	NAG	FA	2	4	14,14,15	0.24	0	17,19,21	0.52	0
4	NAG	K	1	4,1	14,14,15	0.33	0	17,19,21	0.53	0
4	NAG	K	2	4	14,14,15	0.33	0	17,19,21	0.51	0
4	NAG	L	1	2,4	14,14,15	0.58	0	17,19,21	0.73	0
4	NAG	L	2	4	14,14,15	0.55	0	17,19,21	0.38	0
4	NAG	M	1	2,4	14,14,15	0.40	0	17,19,21	0.66	0
4	NAG	M	2	4	14,14,15	0.29	0	17,19,21	0.71	1 (5%)
4	NAG	N	1	2,4	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	N	2	4	14,14,15	0.30	0	17,19,21	0.56	0
4	NAG	O	1	2,4	14,14,15	0.31	0	17,19,21	0.53	0
4	NAG	O	2	4	14,14,15	0.37	0	17,19,21	0.48	0
4	NAG	P	1	2,4	14,14,15	0.24	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	P	2	4	14,14,15	0.33	0	17,19,21	0.61	1 (5%)
4	NAG	Q	1	2,4	14,14,15	0.24	0	17,19,21	0.58	0
4	NAG	Q	2	4	14,14,15	0.23	0	17,19,21	0.59	0
4	NAG	R	1	4,1	14,14,15	0.34	0	17,19,21	0.53	0
4	NAG	R	2	4	14,14,15	0.33	0	17,19,21	0.49	0
4	NAG	S	1	2,4	14,14,15	0.57	0	17,19,21	0.74	0
4	NAG	S	2	4	14,14,15	0.54	0	17,19,21	0.37	0
4	NAG	T	1	2,4	14,14,15	0.39	0	17,19,21	0.66	0
4	NAG	T	2	4	14,14,15	0.28	0	17,19,21	0.71	1 (5%)
4	NAG	U	1	2,4	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	U	2	4	14,14,15	0.30	0	17,19,21	0.56	0
4	NAG	V	1	2,4	14,14,15	0.33	0	17,19,21	0.53	0
4	NAG	V	2	4	14,14,15	0.35	0	17,19,21	0.48	0
4	NAG	W	1	2,4	14,14,15	0.23	0	17,19,21	0.63	0
4	NAG	W	2	4	14,14,15	0.34	0	17,19,21	0.61	1 (5%)
4	NAG	X	1	2,4	14,14,15	0.25	0	17,19,21	0.58	0
4	NAG	X	2	4	14,14,15	0.23	0	17,19,21	0.59	0
4	NAG	Y	1	3,4	14,14,15	0.51	0	17,19,21	0.52	0
4	NAG	Y	2	4	14,14,15	0.25	0	17,19,21	0.61	0
4	NAG	Z	1	3,4	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	Z	2	4	14,14,15	0.29	0	17,19,21	0.56	0
4	NAG	a	1	3,4	14,14,15	0.31	0	17,19,21	0.64	0
4	NAG	a	2	4	14,14,15	0.51	0	17,19,21	0.49	0
4	NAG	b	1	3,4	14,14,15	0.35	0	17,19,21	0.74	0
4	NAG	b	2	4	14,14,15	0.31	0	17,19,21	1.40	2 (11%)
4	NAG	c	1	3,4	14,14,15	0.68	1 (7%)	17,19,21	0.71	0
4	NAG	c	2	4	14,14,15	0.41	0	17,19,21	1.49	3 (17%)
4	NAG	d	1	3,4	14,14,15	0.66	1 (7%)	17,19,21	0.68	0
4	NAG	d	2	4	14,14,15	0.28	0	17,19,21	0.67	0
4	NAG	e	1	3,4	14,14,15	0.24	0	17,19,21	0.71	1 (5%)
4	NAG	e	2	4	14,14,15	0.18	0	17,19,21	0.50	0
4	NAG	f	1	3,4	14,14,15	0.29	0	17,19,21	0.56	0
4	NAG	f	2	4	14,14,15	0.24	0	17,19,21	0.60	0
4	NAG	g	1	3,4	14,14,15	0.56	0	17,19,21	0.58	0
4	NAG	g	2	4	14,14,15	0.31	0	17,19,21	0.48	0
4	NAG	h	1	3,4	14,14,15	0.31	0	17,19,21	0.41	0
4	NAG	h	2	4	14,14,15	0.42	0	17,19,21	0.38	0
4	NAG	i	1	3,4	14,14,15	0.37	0	17,19,21	1.17	1 (5%)
4	NAG	i	2	4	14,14,15	0.25	0	17,19,21	0.49	0
4	NAG	j	1	3,4	14,14,15	0.30	0	17,19,21	0.72	1 (5%)
4	NAG	j	2	4	14,14,15	0.21	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	k	1	3,4	14,14,15	0.73	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	k	2	4	14,14,15	0.33	0	17,19,21	0.73	1 (5%)
4	NAG	l	1	3,4	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	l	2	4	14,14,15	0.29	0	17,19,21	0.39	0
4	NAG	m	1	3,4	14,14,15	0.53	0	17,19,21	0.51	0
4	NAG	m	2	4	14,14,15	0.24	0	17,19,21	0.60	0
4	NAG	n	1	3,4	14,14,15	0.56	0	17,19,21	0.58	0
4	NAG	n	2	4	14,14,15	0.29	0	17,19,21	0.47	0
4	NAG	o	1	3,4	14,14,15	0.22	0	17,19,21	1.45	2 (11%)
4	NAG	o	2	4	14,14,15	0.20	0	17,19,21	0.53	0
4	NAG	p	1	3,4	14,14,15	0.53	0	17,19,21	0.74	1 (5%)
4	NAG	p	2	4	14,14,15	0.41	0	17,19,21	0.48	0
4	NAG	q	1	3,4	14,14,15	0.38	0	17,19,21	0.40	0
4	NAG	q	2	4	14,14,15	0.20	0	17,19,21	0.77	0
4	NAG	r	1	3,4	14,14,15	0.35	0	17,19,21	0.48	0
4	NAG	r	2	4	14,14,15	0.60	0	17,19,21	1.39	2 (11%)
4	NAG	s	1	3,4	14,14,15	0.63	1 (7%)	17,19,21	0.45	0
4	NAG	s	2	4	14,14,15	0.33	0	17,19,21	1.44	2 (11%)
4	NAG	t	1	3,4	14,14,15	0.38	0	17,19,21	0.47	0
4	NAG	t	2	4	14,14,15	0.23	0	17,19,21	0.52	0
4	NAG	u	1	3,4	14,14,15	0.51	0	17,19,21	0.51	0
4	NAG	u	2	4	14,14,15	0.24	0	17,19,21	0.61	0
4	NAG	v	1	3,4	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	v	2	4	14,14,15	0.29	0	17,19,21	0.56	0
4	NAG	w	1	3,4	14,14,15	0.32	0	17,19,21	0.65	1 (5%)
4	NAG	w	2	4	14,14,15	0.51	0	17,19,21	0.49	0
4	NAG	x	1	3,4	14,14,15	0.36	0	17,19,21	0.74	0
4	NAG	x	2	4	14,14,15	0.33	0	17,19,21	1.40	2 (11%)
4	NAG	y	1	3,4	14,14,15	0.68	1 (7%)	17,19,21	0.71	0
4	NAG	y	2	4	14,14,15	0.40	0	17,19,21	1.48	3 (17%)
4	NAG	z	1	3,4	14,14,15	0.66	1 (7%)	17,19,21	0.68	0
4	NAG	z	2	4	14,14,15	0.27	0	17,19,21	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	0	1	3,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	0	2	4	-	0/6/23/26	0/1/1/1
4	NAG	1	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	1	2	4	-	2/6/23/26	0/1/1/1
4	NAG	2	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	2	2	4	-	3/6/23/26	0/1/1/1
4	NAG	3	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	3	2	4	-	1/6/23/26	0/1/1/1
4	NAG	4	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	4	2	4	-	0/6/23/26	0/1/1/1
4	NAG	5	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	5	2	4	-	3/6/23/26	0/1/1/1
4	NAG	6	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	6	2	4	-	3/6/23/26	0/1/1/1
4	NAG	7	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	7	2	4	-	2/6/23/26	0/1/1/1
4	NAG	8	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	8	2	4	-	2/6/23/26	0/1/1/1
4	NAG	9	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	9	2	4	-	3/6/23/26	0/1/1/1
4	NAG	AA	1	3,4	-	6/6/23/26	0/1/1/1
4	NAG	AA	2	4	-	2/6/23/26	0/1/1/1
4	NAG	BA	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	BA	2	4	-	2/6/23/26	0/1/1/1
4	NAG	CA	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	CA	2	4	-	2/6/23/26	0/1/1/1
4	NAG	DA	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	DA	2	4	-	6/6/23/26	0/1/1/1
4	NAG	EA	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	EA	2	4	-	5/6/23/26	0/1/1/1
4	NAG	FA	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	FA	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	L	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	NAG	M	1	2,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	3/6/23/26	0/1/1/1
4	NAG	O	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	NAG	P	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	NAG	S	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	3/6/23/26	0/1/1/1
4	NAG	V	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	NAG	W	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Y	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Z	1	3,4	-	3/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	4/6/23/26	0/1/1/1
4	NAG	a	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	a	2	4	-	2/6/23/26	0/1/1/1
4	NAG	b	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	b	2	4	-	4/6/23/26	0/1/1/1
4	NAG	c	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	c	2	4	-	6/6/23/26	0/1/1/1
4	NAG	d	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	d	2	4	-	4/6/23/26	0/1/1/1
4	NAG	e	1	3,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	e	2	4	-	0/6/23/26	0/1/1/1
4	NAG	f	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	f	2	4	-	2/6/23/26	0/1/1/1
4	NAG	g	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	g	2	4	-	3/6/23/26	0/1/1/1
4	NAG	h	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	h	2	4	-	1/6/23/26	0/1/1/1
4	NAG	i	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	i	2	4	-	0/6/23/26	0/1/1/1
4	NAG	j	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	j	2	4	-	3/6/23/26	0/1/1/1
4	NAG	k	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	k	2	4	-	3/6/23/26	0/1/1/1
4	NAG	l	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	l	2	4	-	2/6/23/26	0/1/1/1
4	NAG	m	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	m	2	4	-	2/6/23/26	0/1/1/1
4	NAG	n	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	n	2	4	-	3/6/23/26	0/1/1/1
4	NAG	o	1	3,4	-	6/6/23/26	0/1/1/1
4	NAG	o	2	4	-	2/6/23/26	0/1/1/1
4	NAG	p	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	p	2	4	-	2/6/23/26	0/1/1/1
4	NAG	q	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	r	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	r	2	4	-	6/6/23/26	0/1/1/1
4	NAG	s	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	s	2	4	-	5/6/23/26	0/1/1/1
4	NAG	t	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	t	2	4	-	2/6/23/26	0/1/1/1
4	NAG	u	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	u	2	4	-	2/6/23/26	0/1/1/1
4	NAG	v	1	3,4	-	3/6/23/26	0/1/1/1
4	NAG	v	2	4	-	4/6/23/26	0/1/1/1
4	NAG	w	1	3,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	w	2	4	-	2/6/23/26	0/1/1/1
4	NAG	x	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	x	2	4	-	4/6/23/26	0/1/1/1
4	NAG	y	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	y	2	4	-	6/6/23/26	0/1/1/1
4	NAG	z	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	z	2	4	-	4/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	6	1	NAG	O5-C1	-2.63	1.39	1.43
4	k	1	NAG	O5-C1	-2.62	1.39	1.43
4	d	1	NAG	O5-C1	-2.39	1.39	1.43
4	z	1	NAG	O5-C1	-2.39	1.39	1.43
4	c	1	NAG	O5-C1	-2.22	1.40	1.43

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	AA	1	NAG	C2-N2-C7	4.99	129.59	122.90
4	o	1	NAG	C2-N2-C7	4.99	129.59	122.90
4	c	2	NAG	C2-N2-C7	4.72	129.22	122.90
4	y	2	NAG	C2-N2-C7	4.65	129.13	122.90
4	s	2	NAG	C2-N2-C7	4.64	129.12	122.90

There are no chirality outliers.

5 of 230 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	1	NAG	O7-C7-N2-C2
4	N	2	NAG	C3-C2-N2-C7
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	U	1	NAG	O7-C7-N2-C2

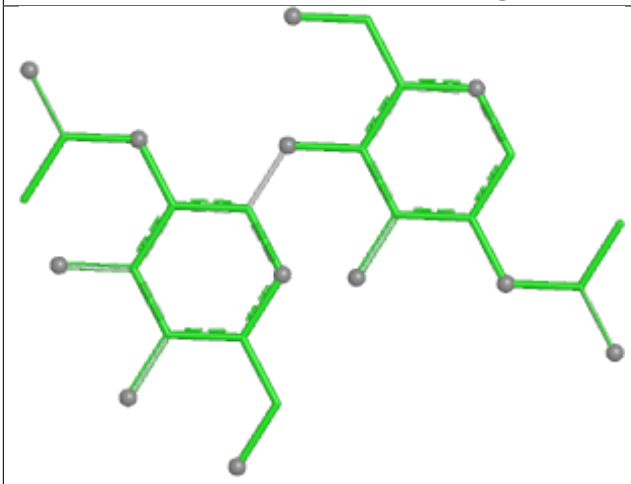
There are no ring outliers.

30 monomers are involved in 40 short contacts:

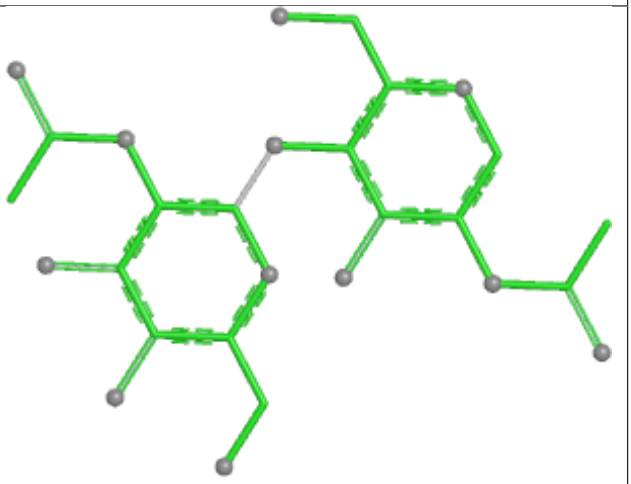
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	s	1	NAG	1	0
4	2	1	NAG	3	0
4	s	2	NAG	1	0
4	r	2	NAG	1	0
4	EA	1	NAG	1	0
4	9	1	NAG	3	0
4	b	2	NAG	1	0
4	k	2	NAG	1	0
4	N	2	NAG	5	0
4	EA	2	NAG	1	0
4	U	2	NAG	5	0
4	n	2	NAG	2	0
4	c	2	NAG	1	0
4	f	1	NAG	1	0
4	U	1	NAG	4	0
4	AA	1	NAG	1	0
4	DA	2	NAG	1	0
4	k	1	NAG	1	0
4	9	2	NAG	2	0
4	n	1	NAG	3	0
4	y	2	NAG	1	0
4	o	1	NAG	1	0
4	x	2	NAG	1	0
4	6	1	NAG	1	0
4	6	2	NAG	1	0
4	N	1	NAG	4	0
4	2	2	NAG	2	0
4	g	1	NAG	3	0
4	g	2	NAG	2	0
4	1	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

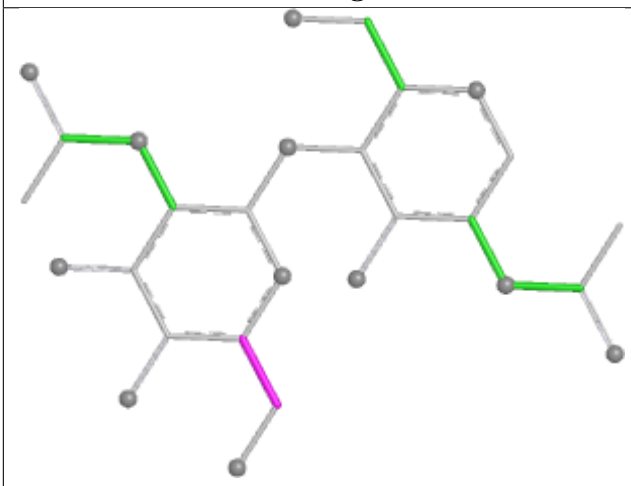
Oligosaccharide Chain K



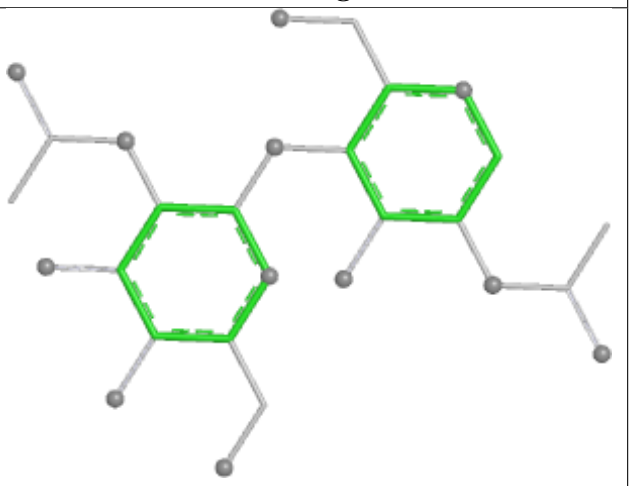
Bond lengths



Bond angles

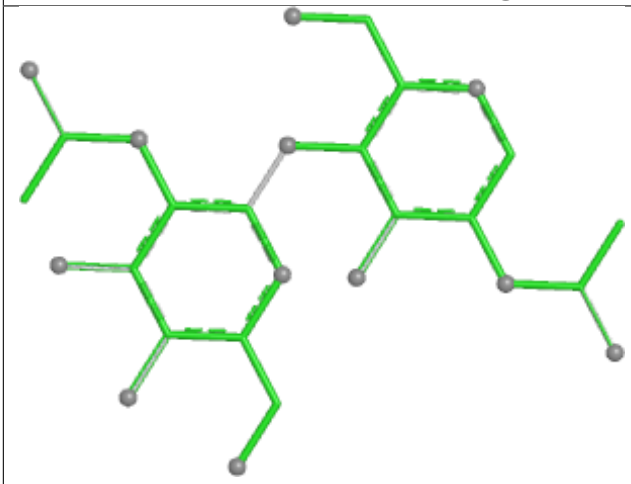


Torsions

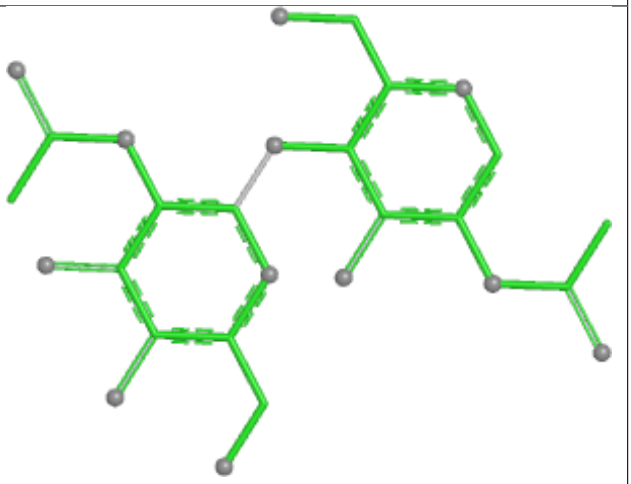


Rings

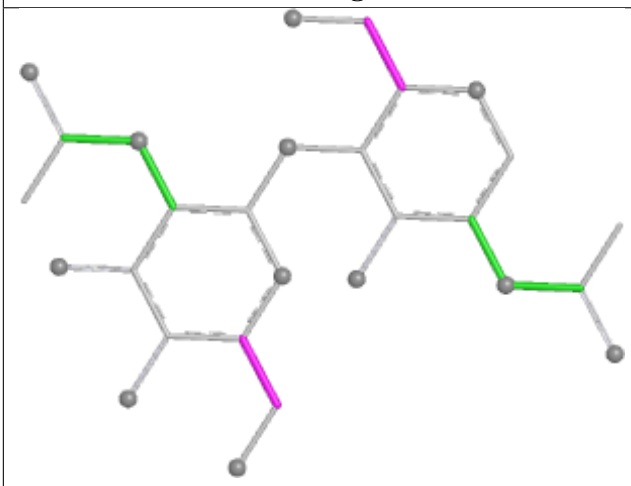
Oligosaccharide Chain L



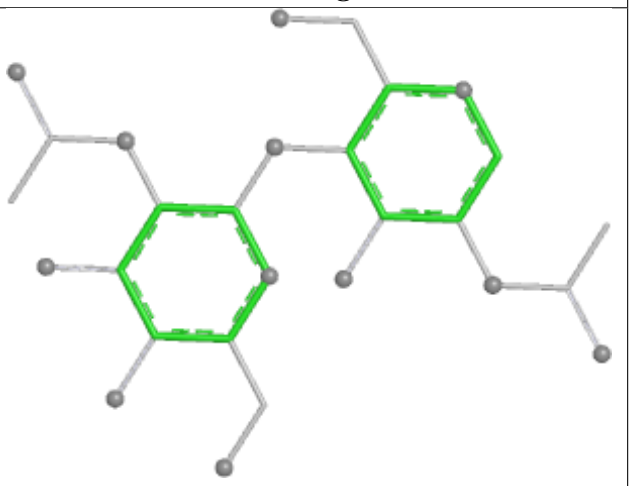
Bond lengths



Bond angles

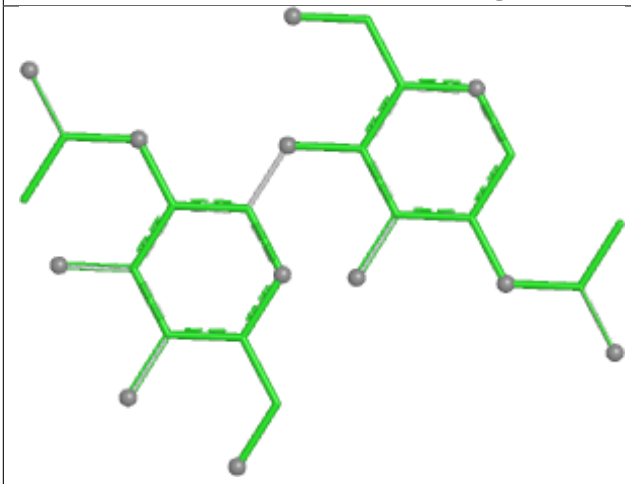


Torsions

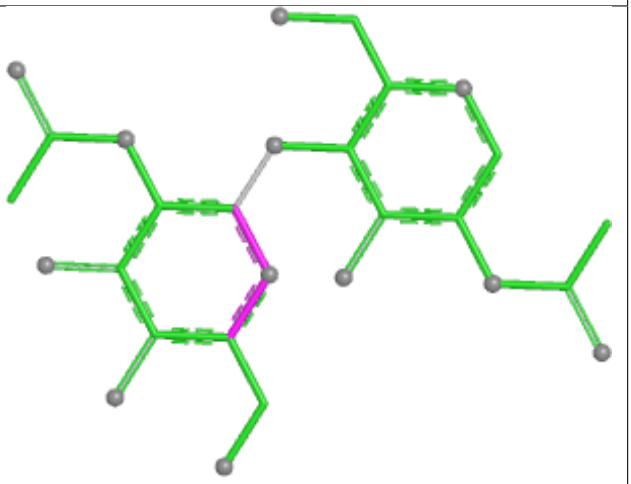


Rings

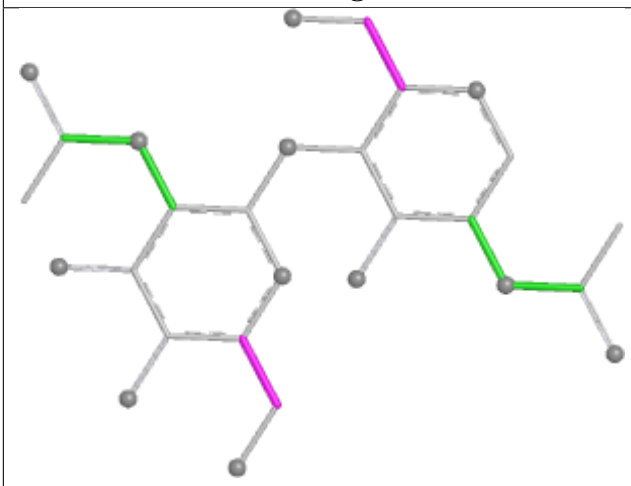
Oligosaccharide Chain M



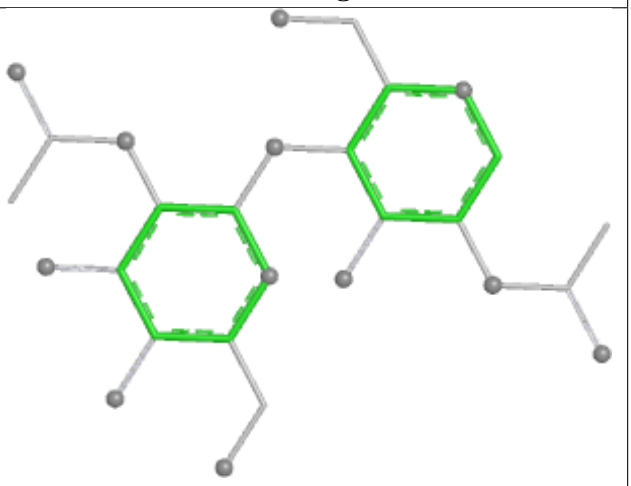
Bond lengths



Bond angles

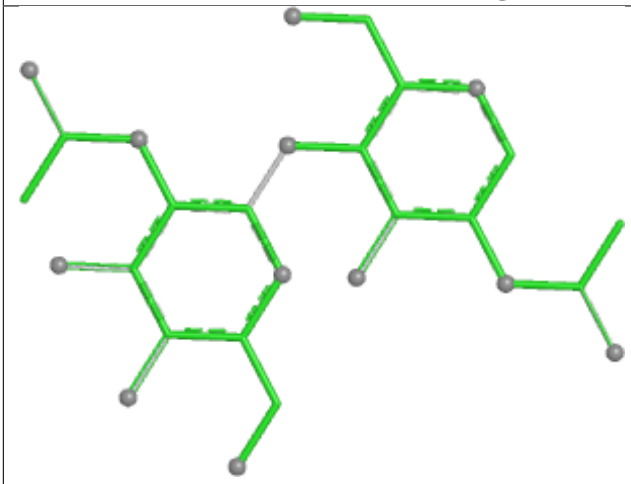


Torsions

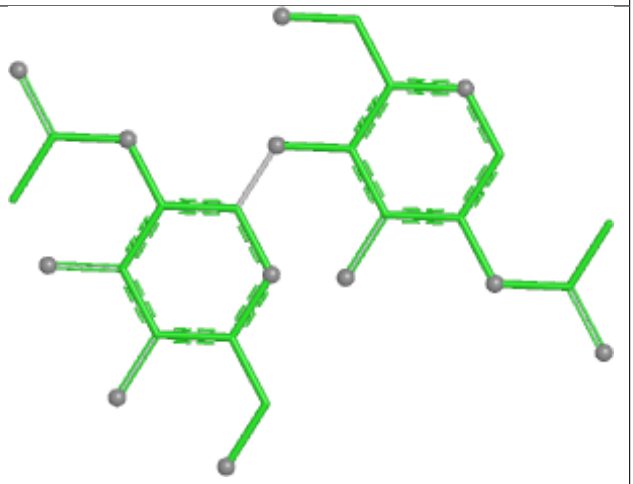


Rings

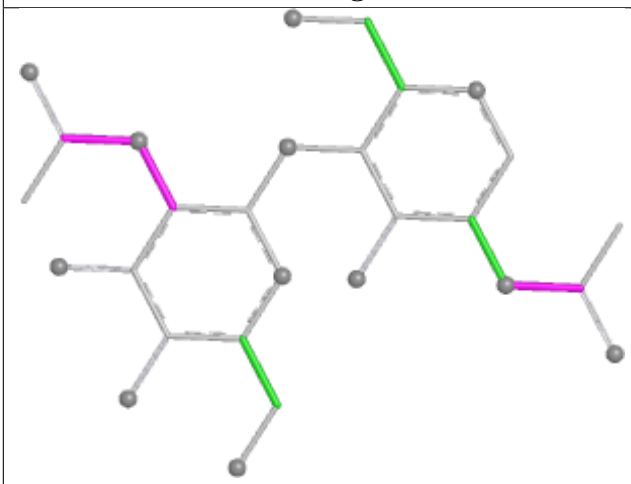
Oligosaccharide Chain N



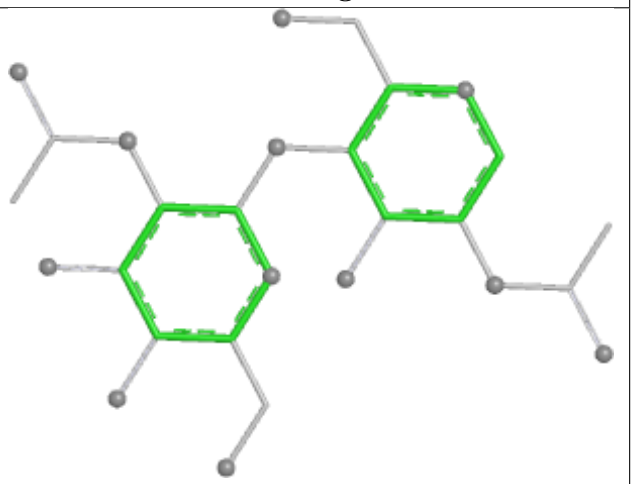
Bond lengths



Bond angles

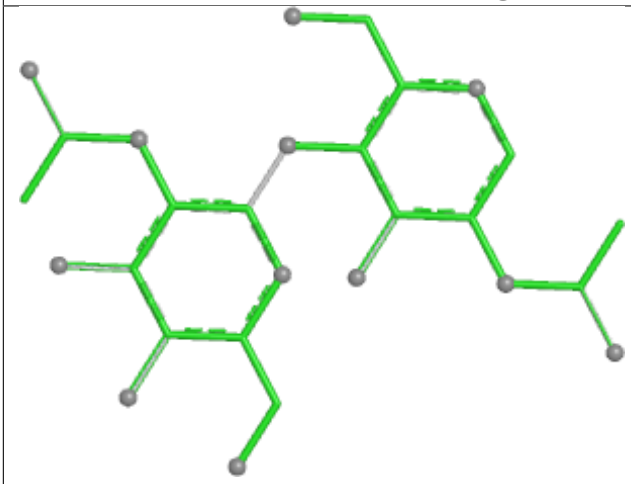


Torsions

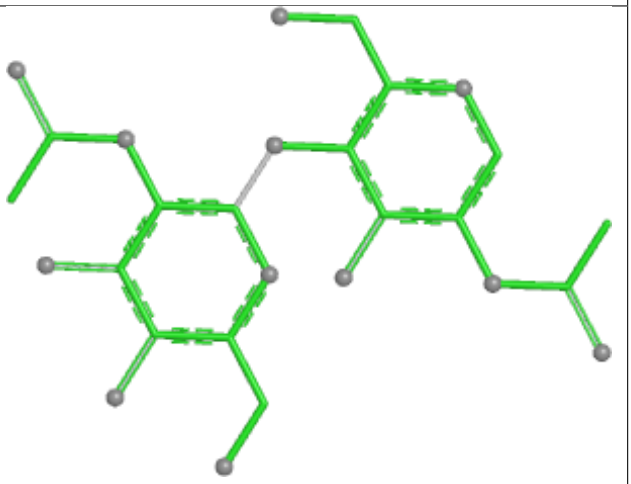


Rings

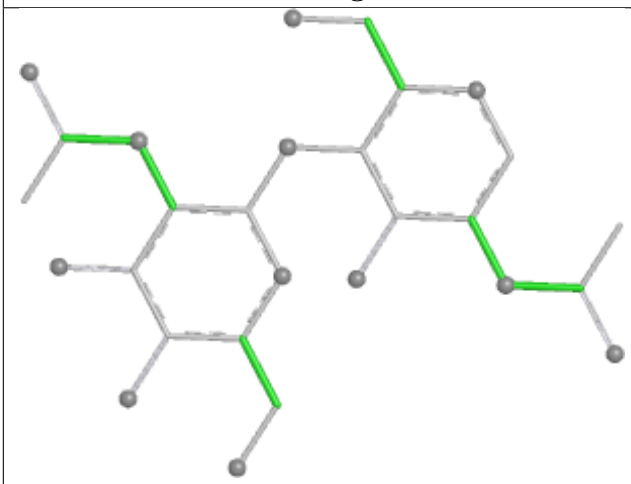
Oligosaccharide Chain O



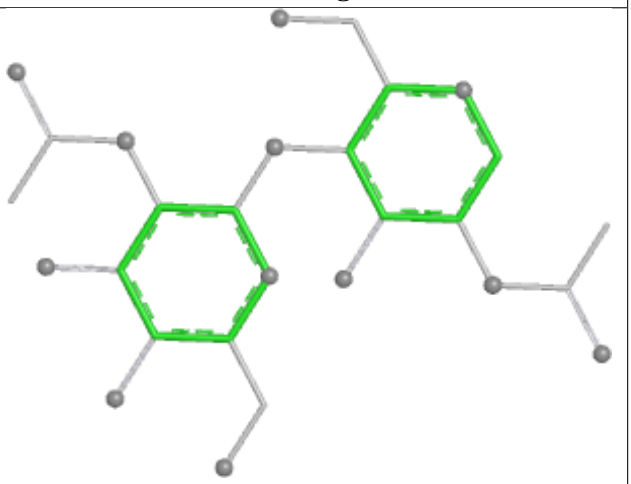
Bond lengths



Bond angles

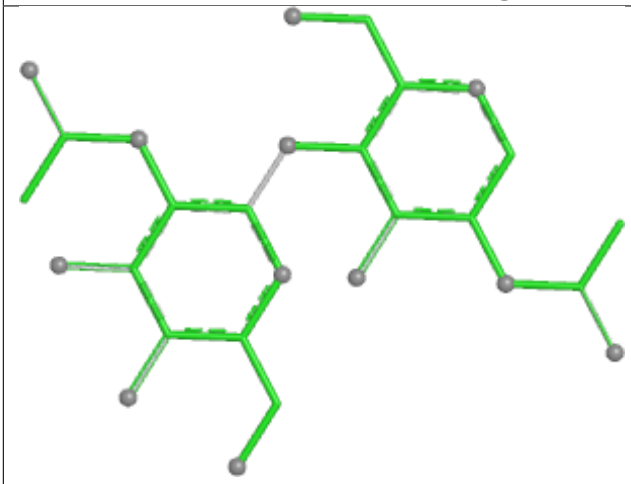


Torsions

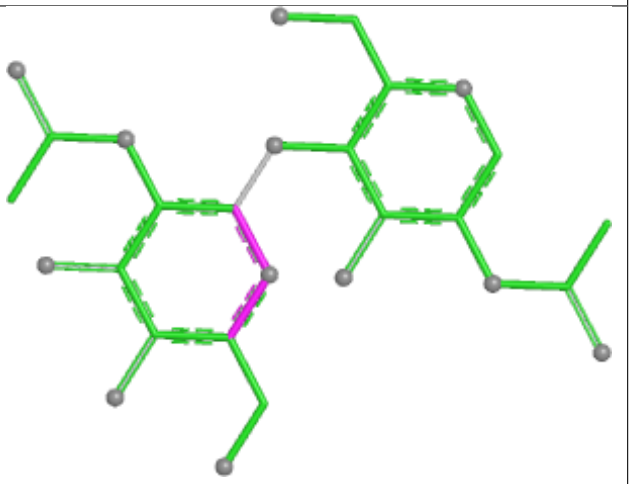


Rings

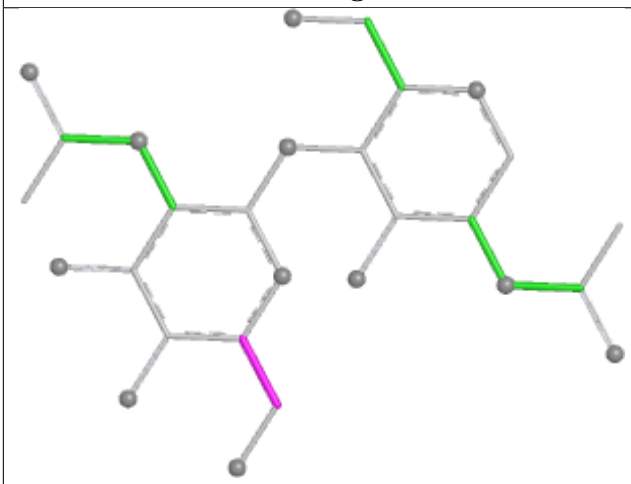
Oligosaccharide Chain P



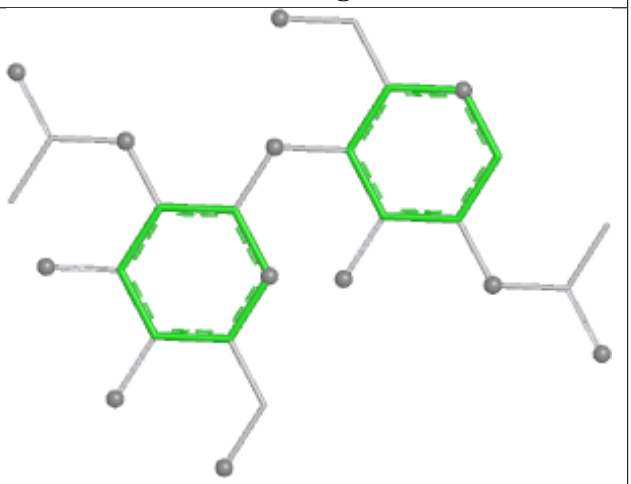
Bond lengths



Bond angles

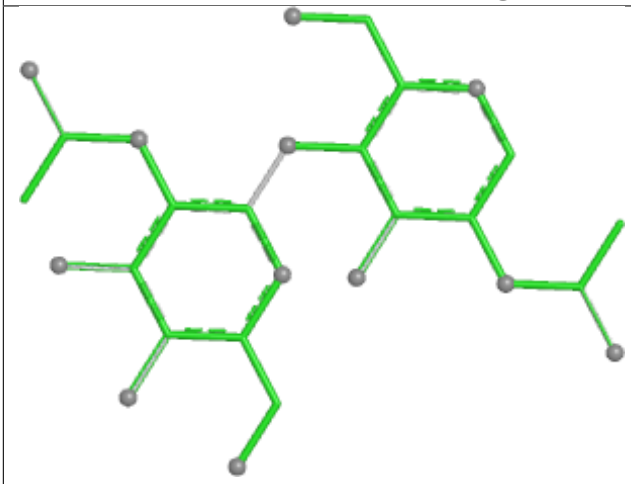


Torsions

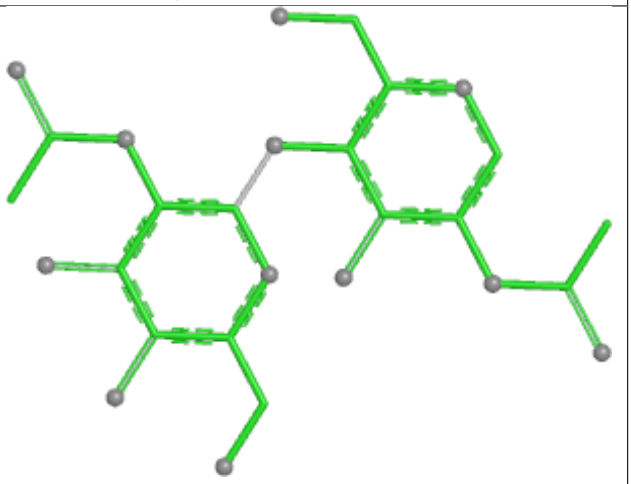


Rings

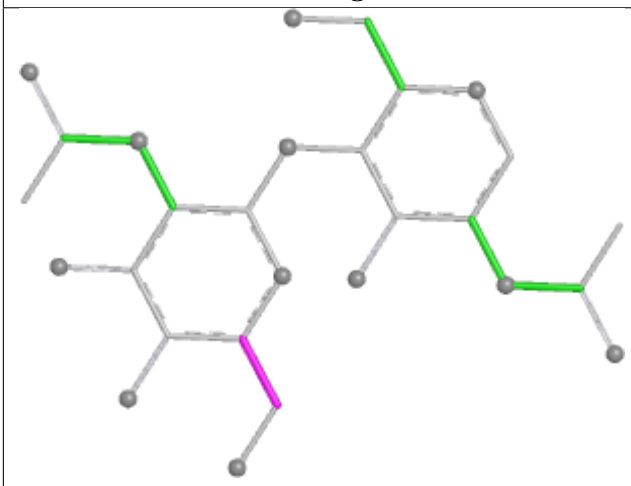
Oligosaccharide Chain Q



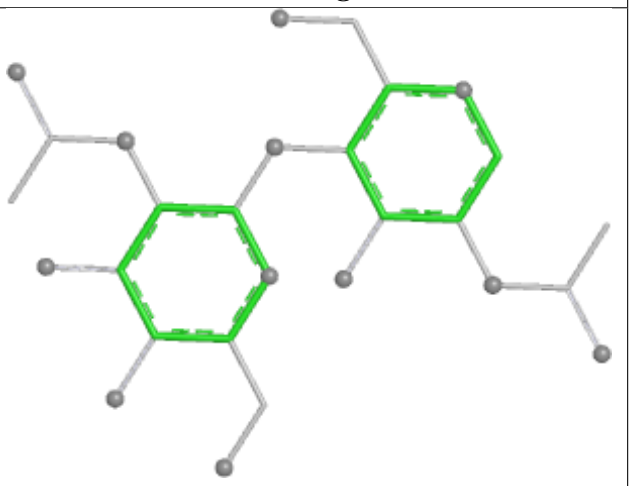
Bond lengths



Bond angles

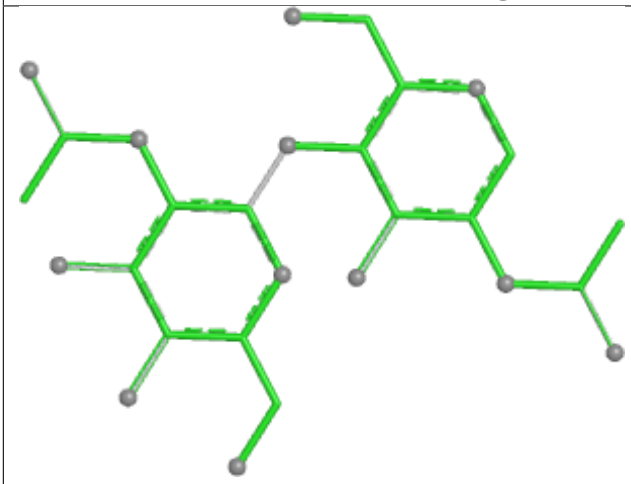


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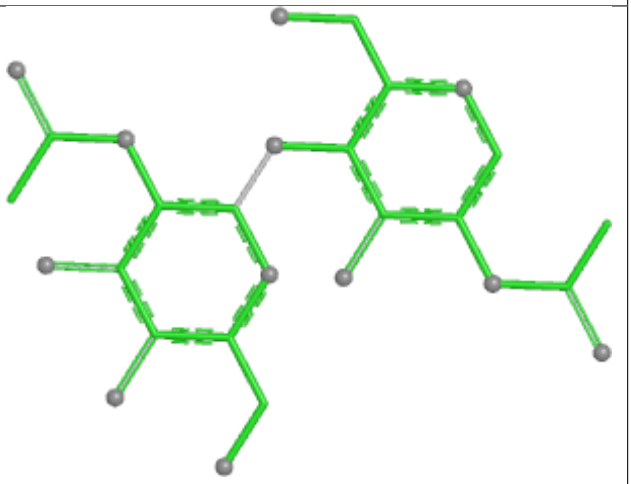


Rings

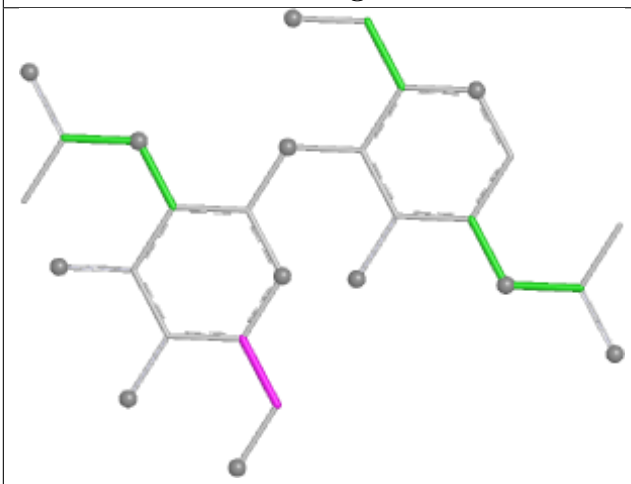
Oligosaccharide Chain R



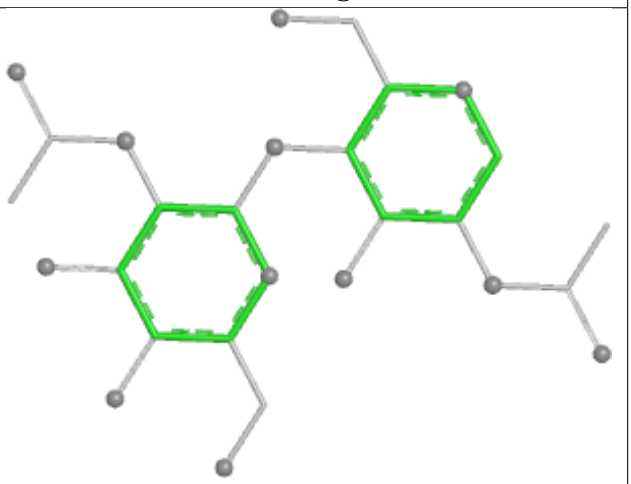
Bond lengths



Bond angles

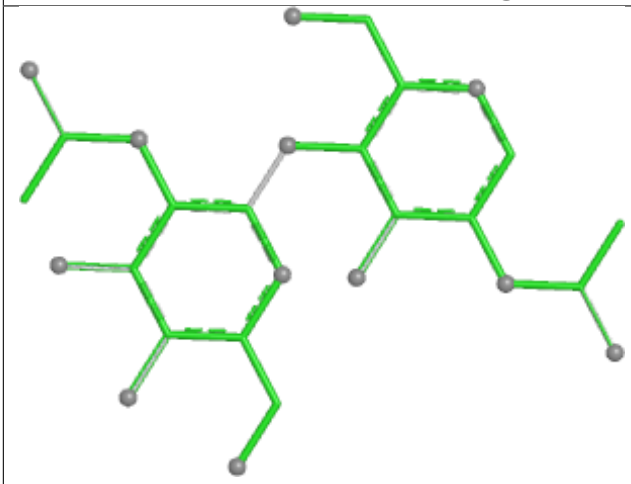


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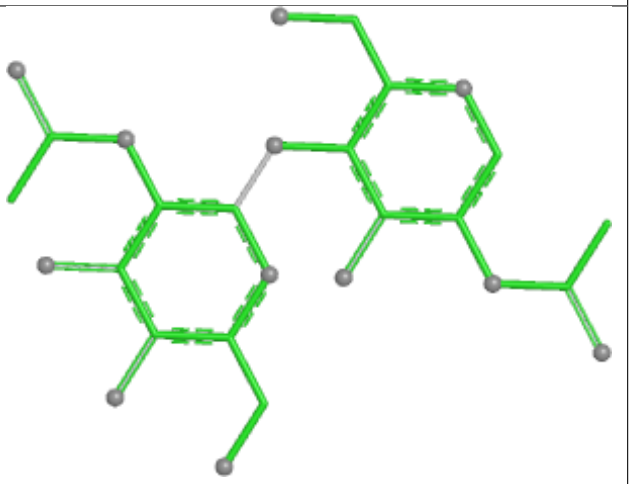


Rings

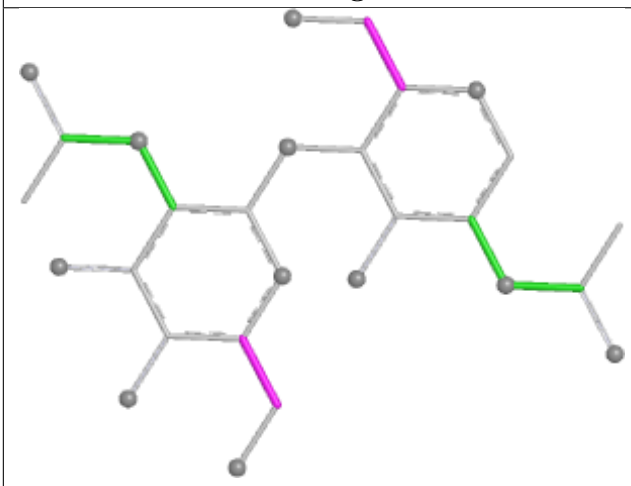
Oligosaccharide Chain S



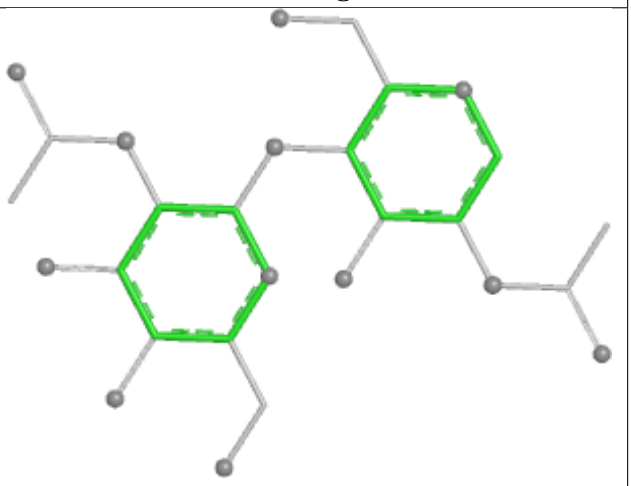
Bond lengths



Bond angles

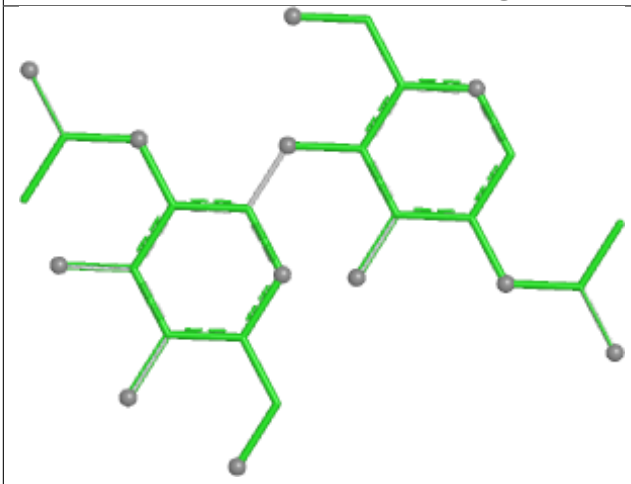


Torsions

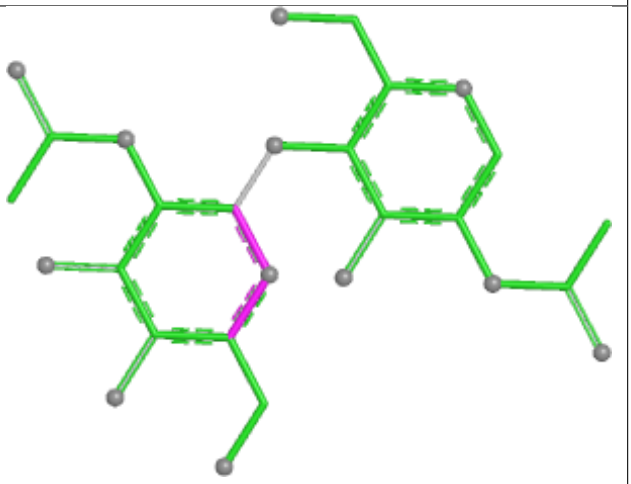


Rings

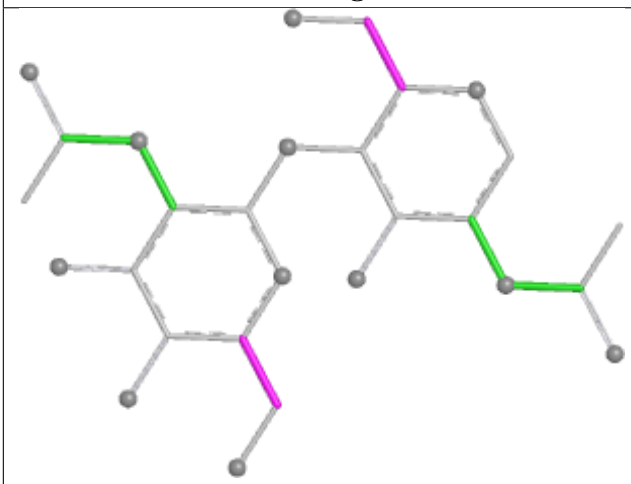
Oligosaccharide Chain T



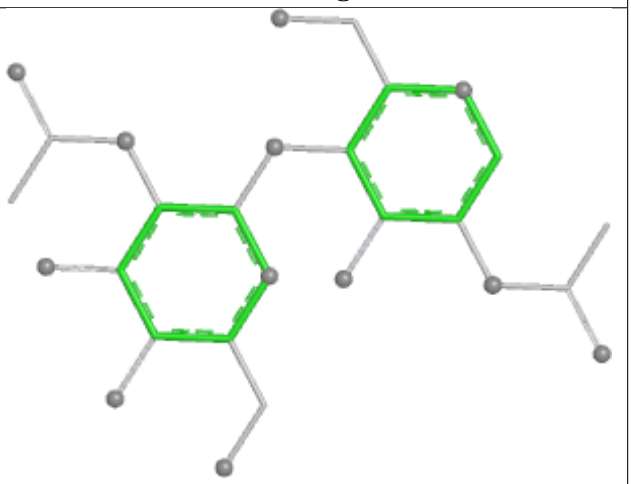
Bond lengths



Bond angles

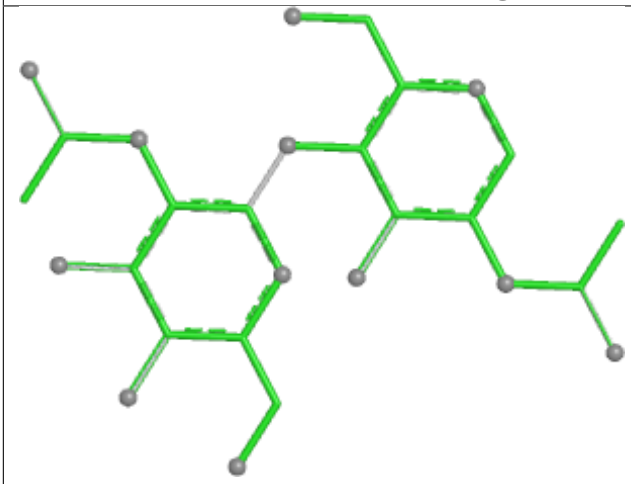


Torsions

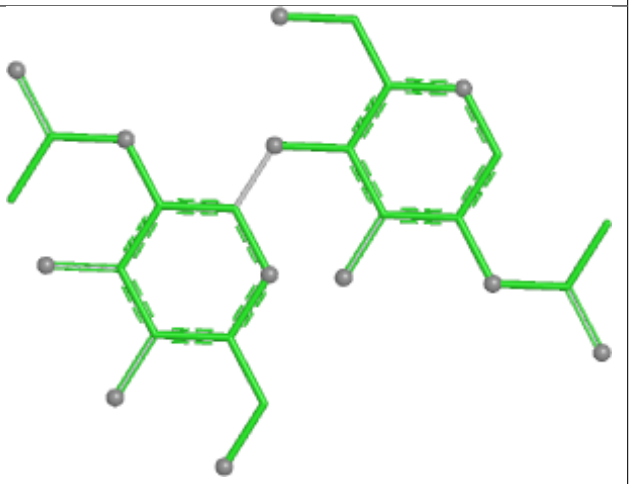


Rings

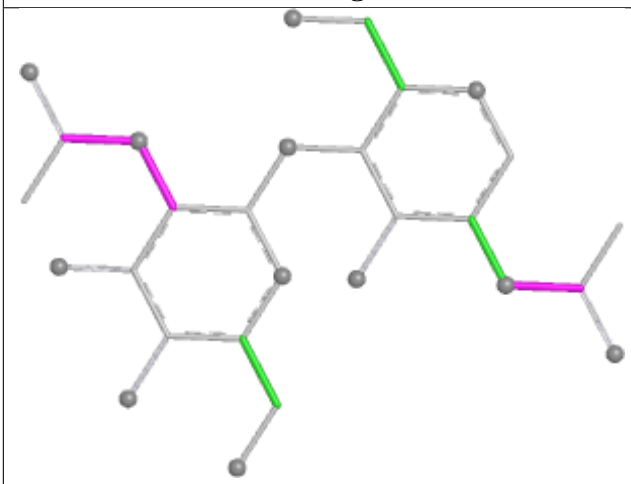
Oligosaccharide Chain U



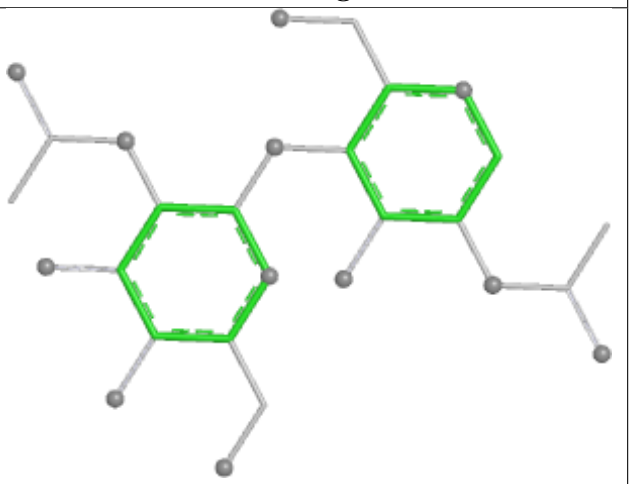
Bond lengths



Bond angles

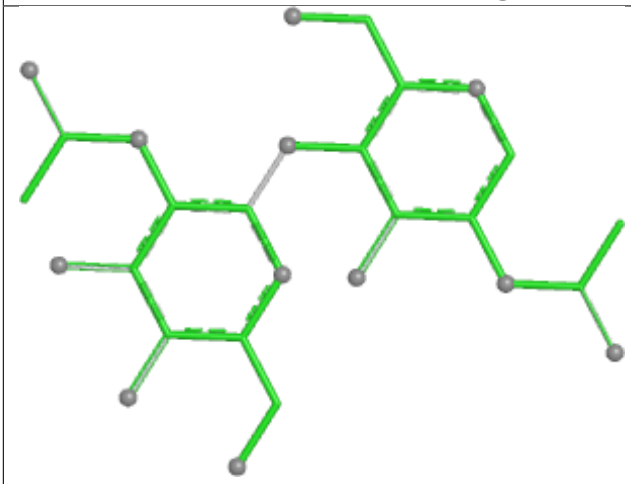


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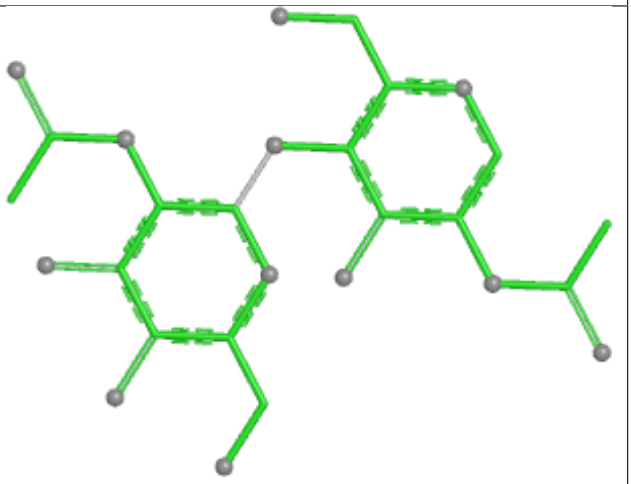


Rings

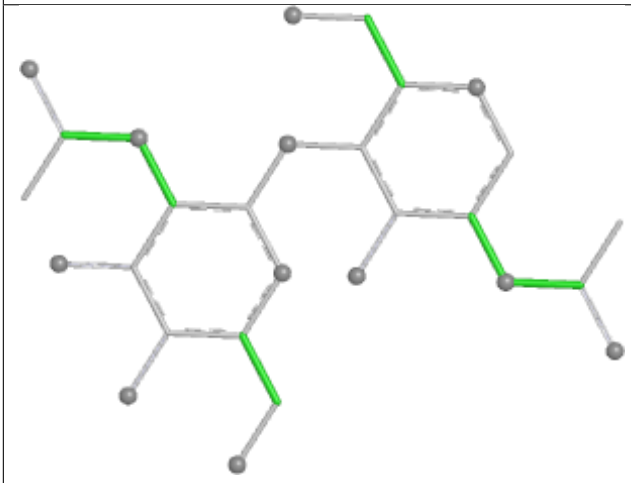
Oligosaccharide Chain V



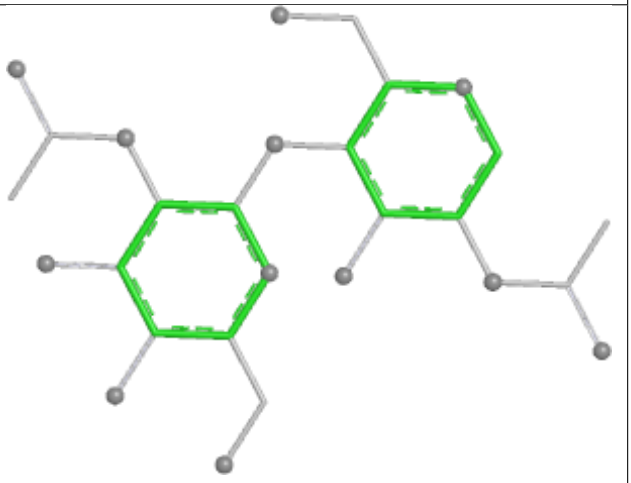
Bond lengths



Bond angles

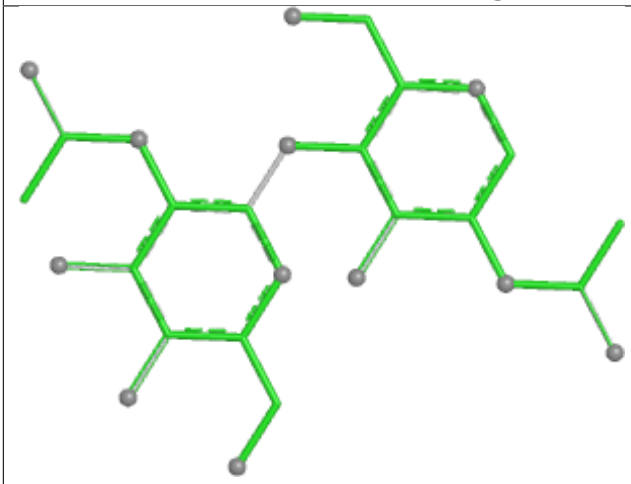


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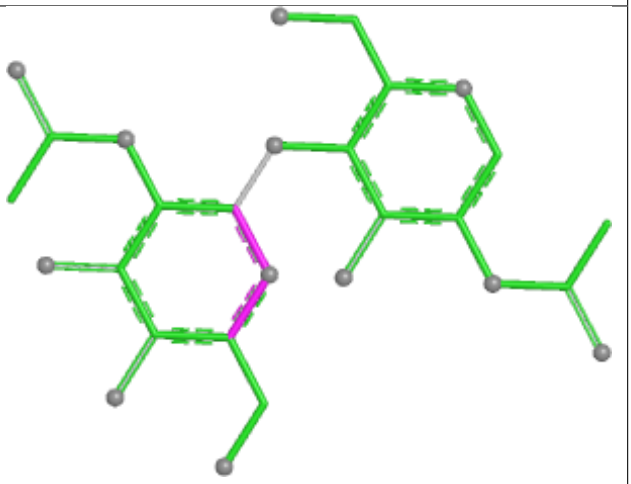


Rings

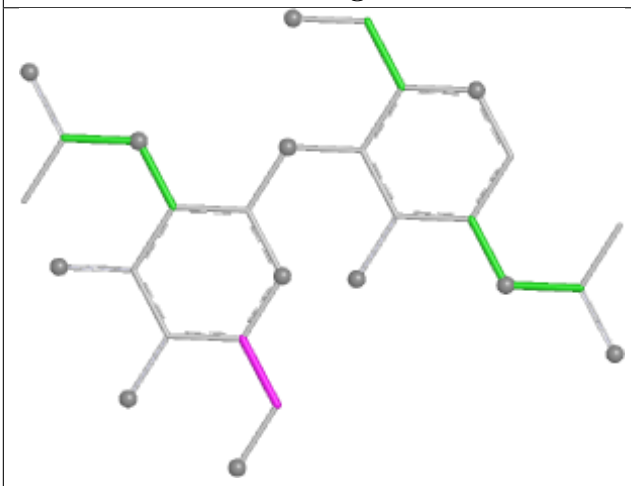
Oligosaccharide Chain W



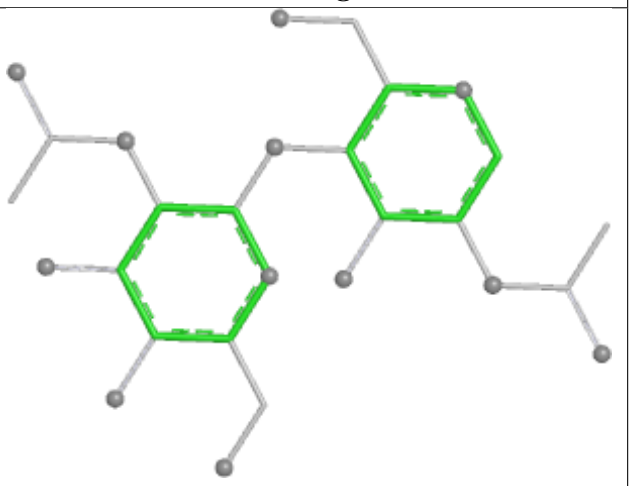
Bond lengths



Bond angles

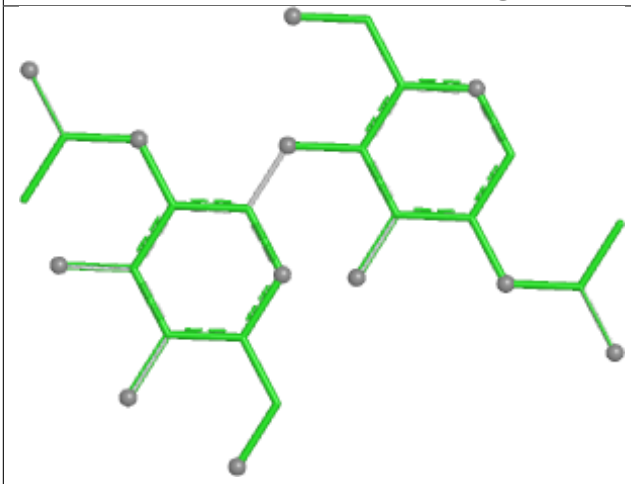


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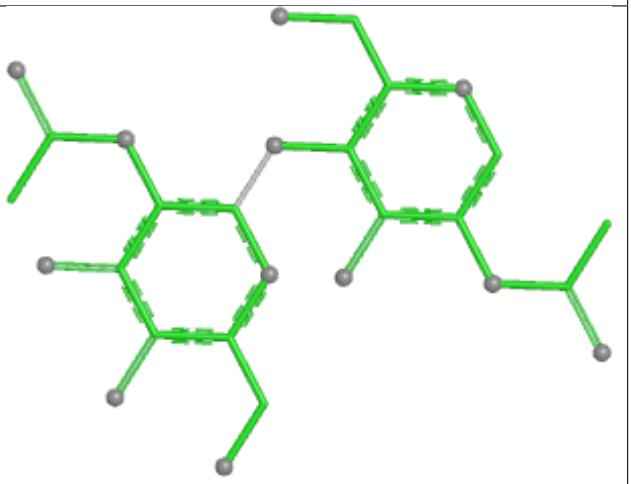


Rings

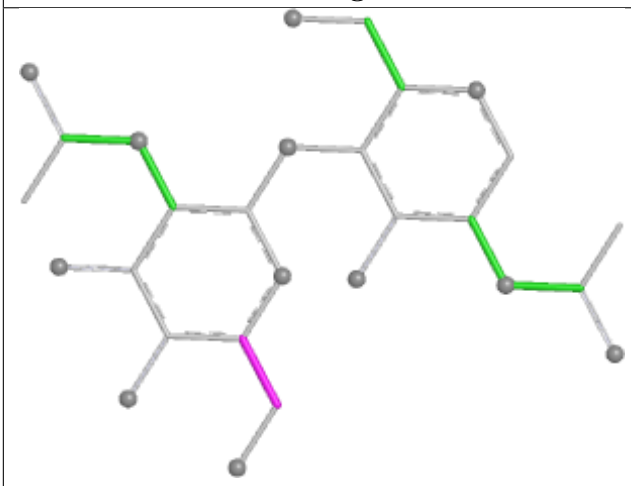
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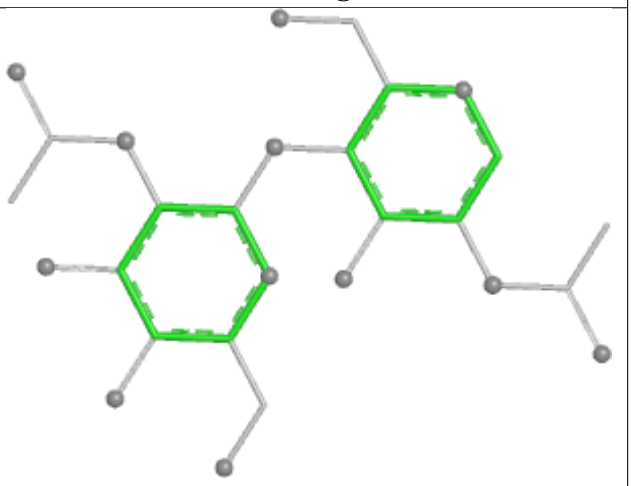
Bond lengths



Bond angles

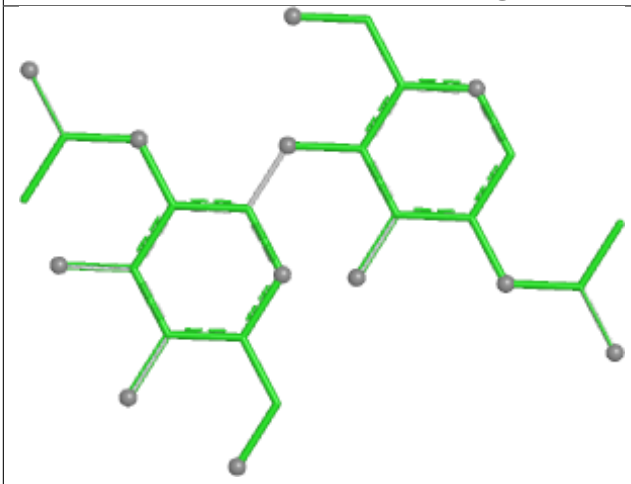


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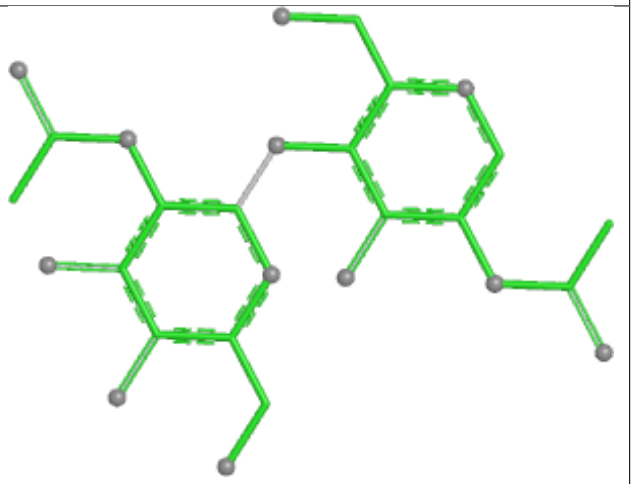


Rings

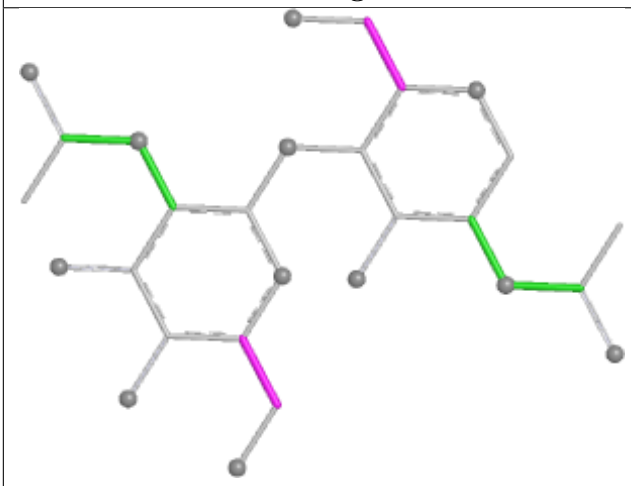
Oligosaccharide Chain Y



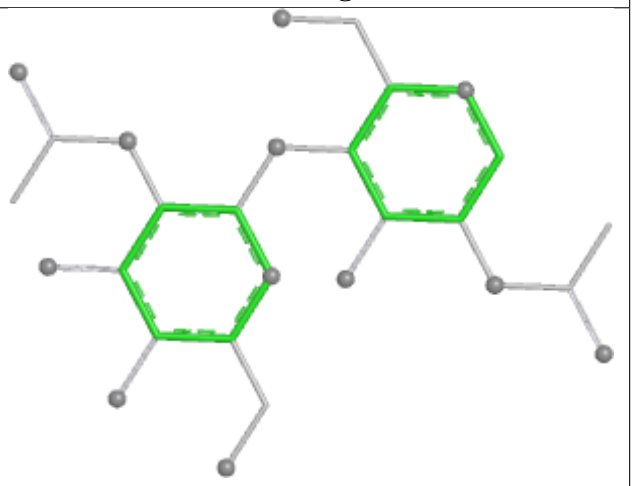
Bond lengths



Bond angles

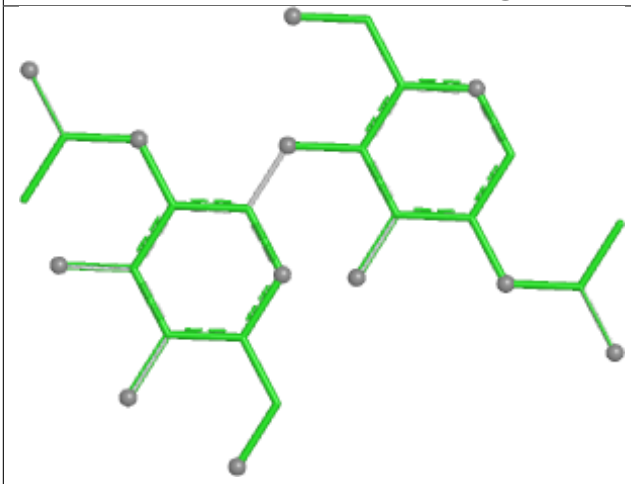


Torsions

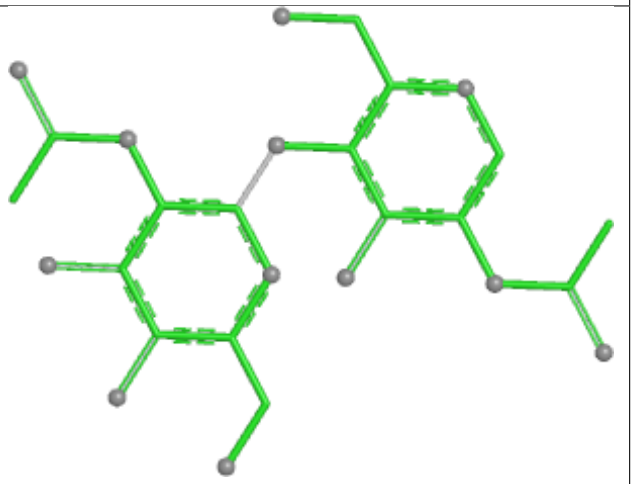


Rings

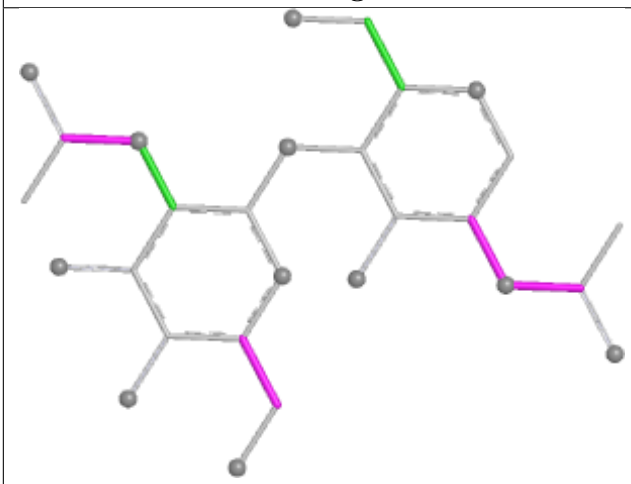
Oligosaccharide Chain Z



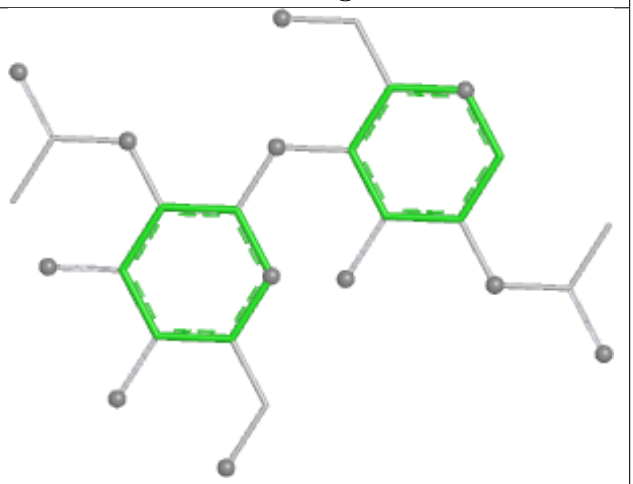
Bond lengths



Bond angles

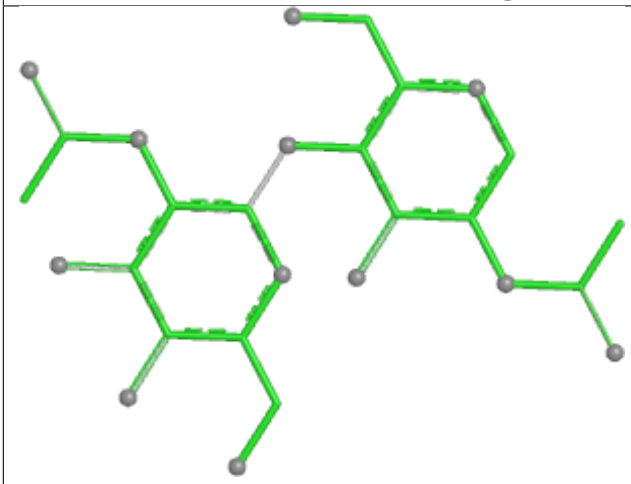


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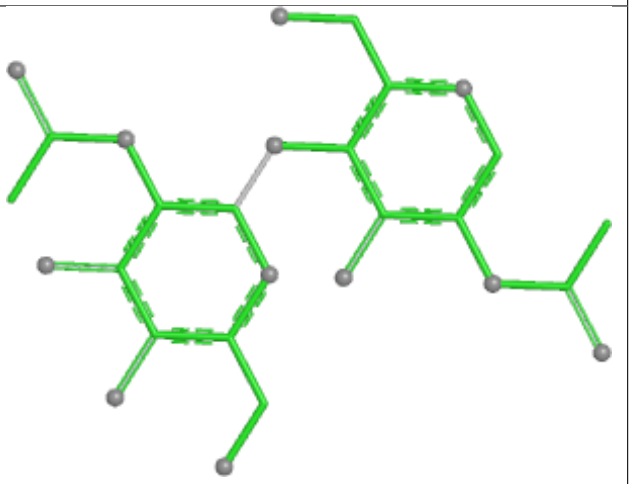


Rings

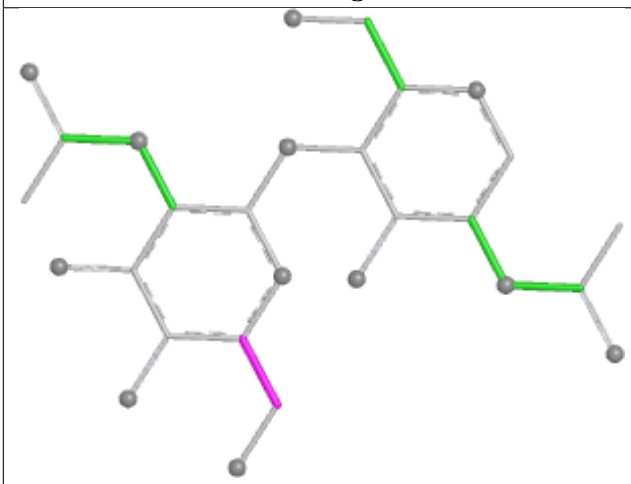
Oligosaccharide Chain a



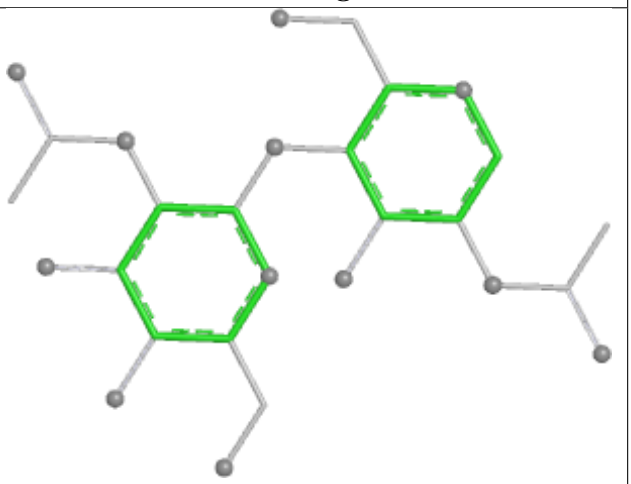
Bond lengths



Bond angles

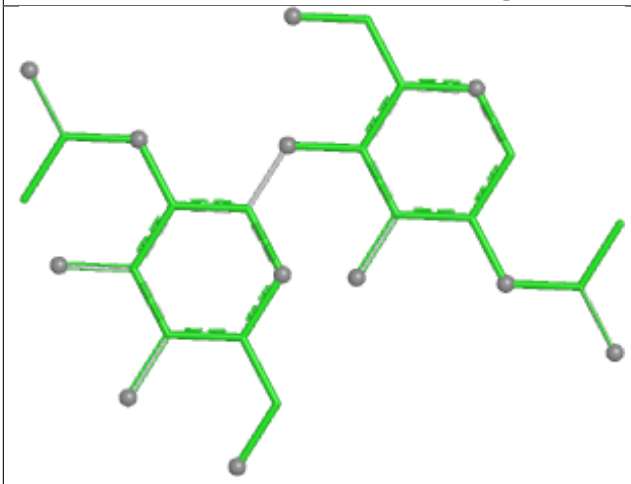


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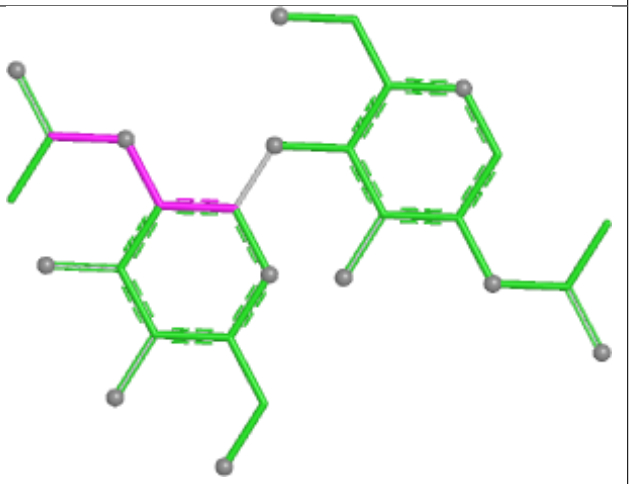


Rings

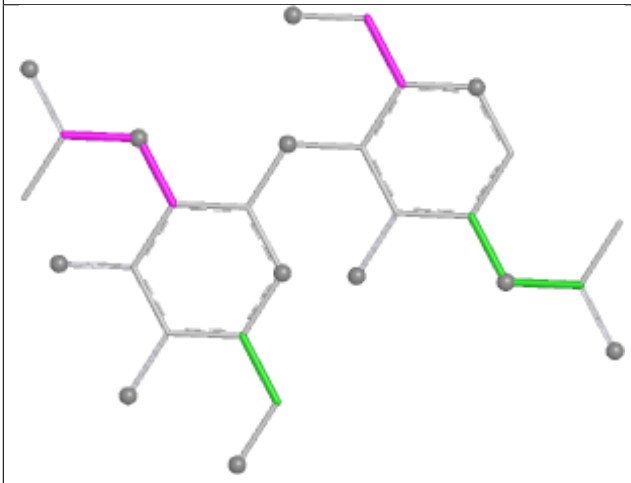
Oligosaccharide Chain b



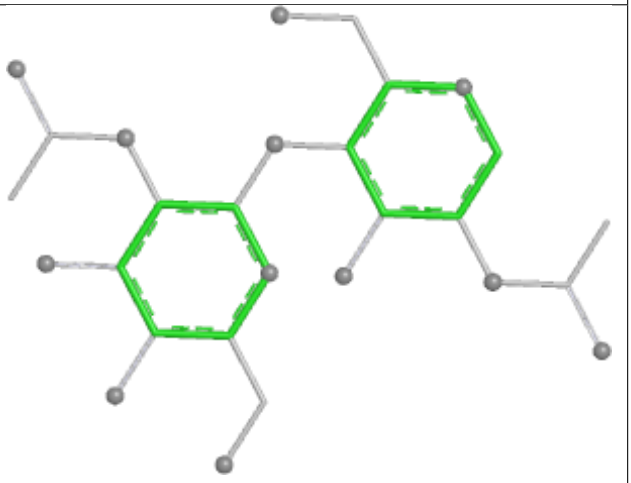
Bond lengths



Bond angles

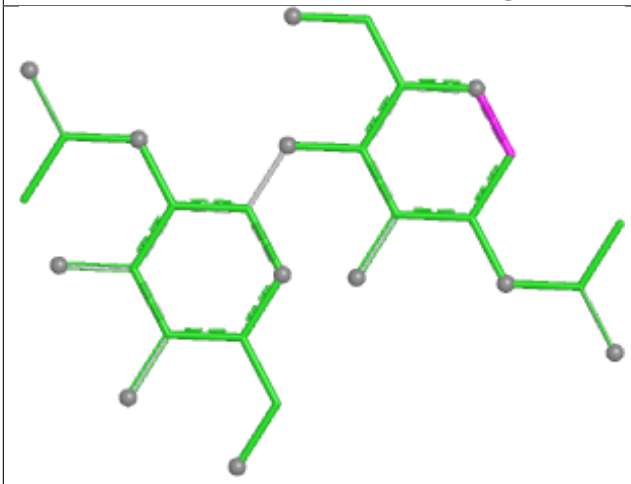


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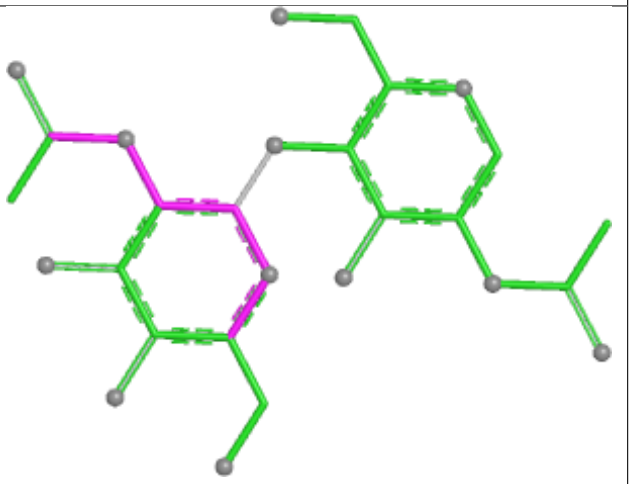


Rings

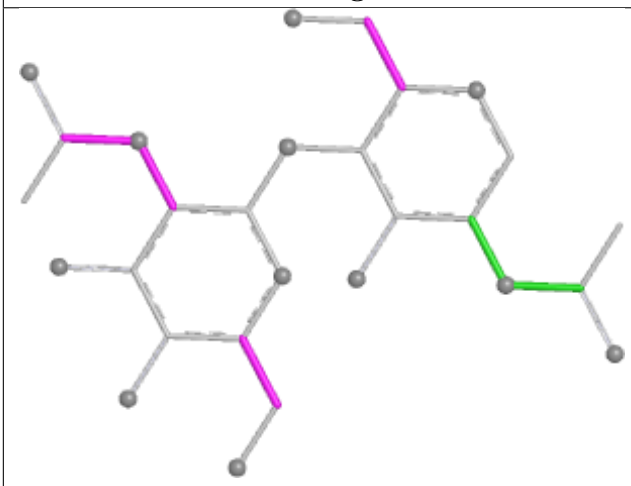
Oligosaccharide Chain c



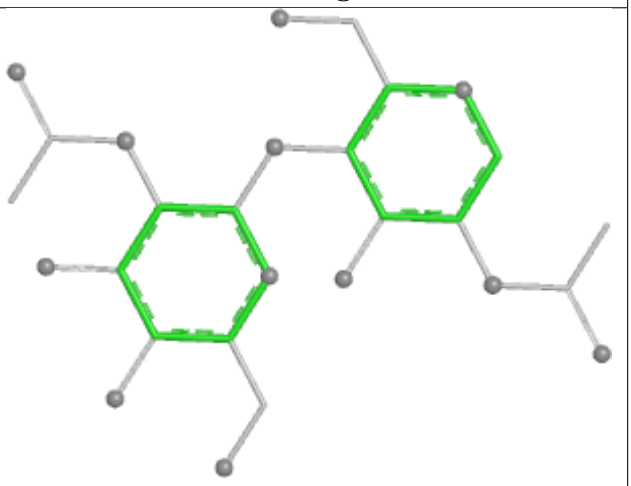
Bond lengths



Bond angles

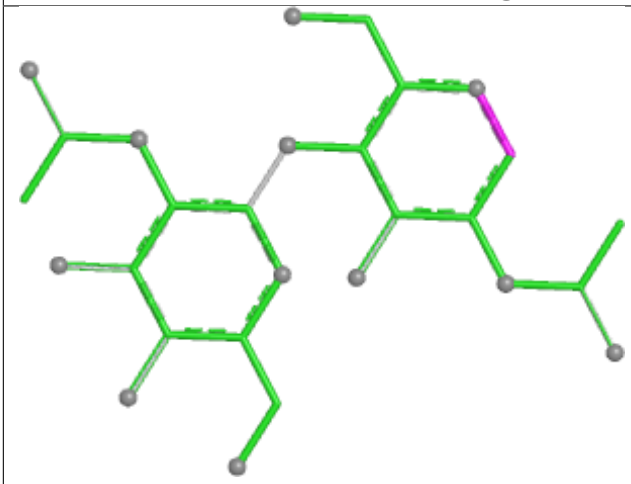


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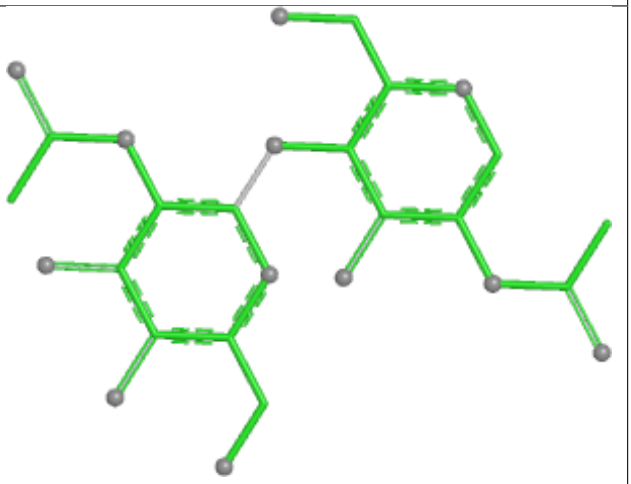


Rings

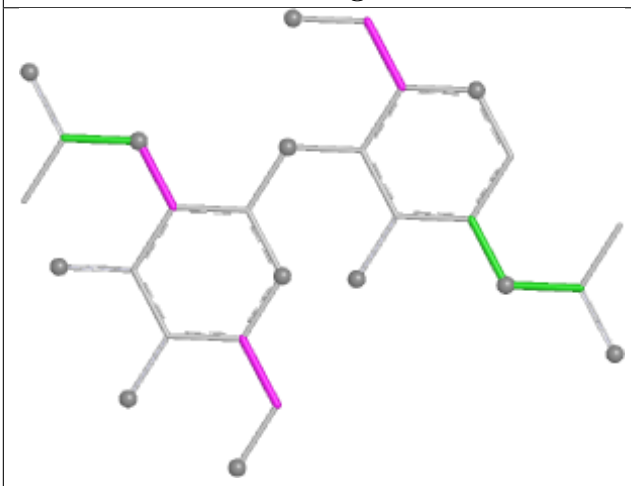
Oligosaccharide Chain d



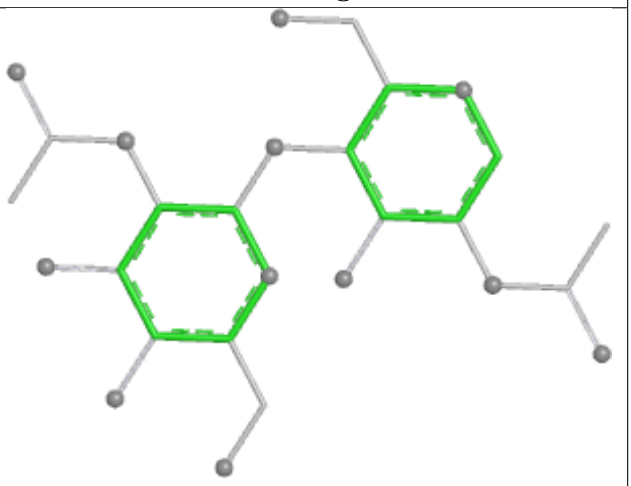
Bond lengths



Bond angles

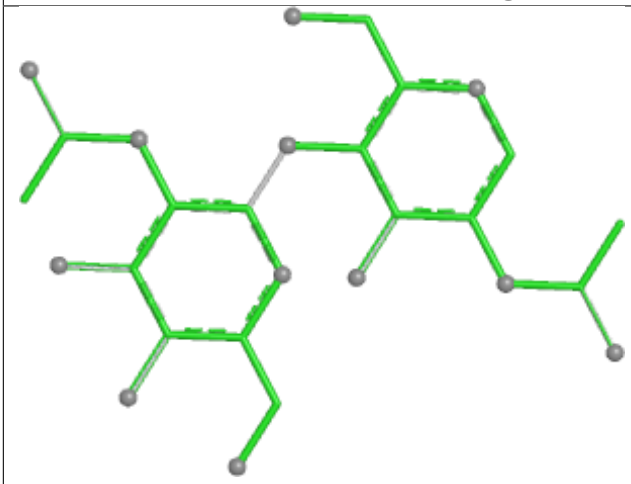


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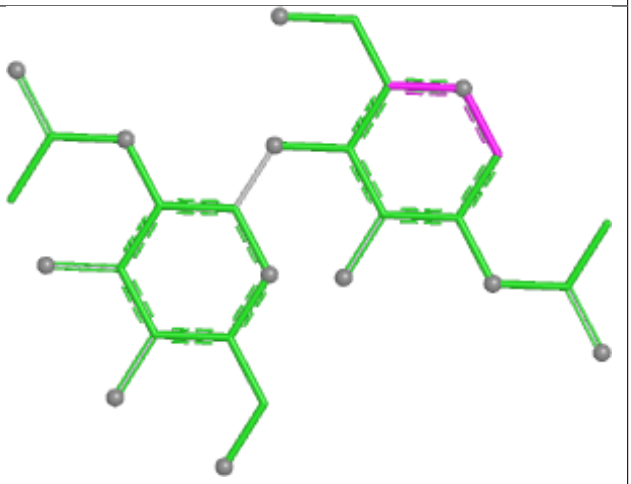


Rings

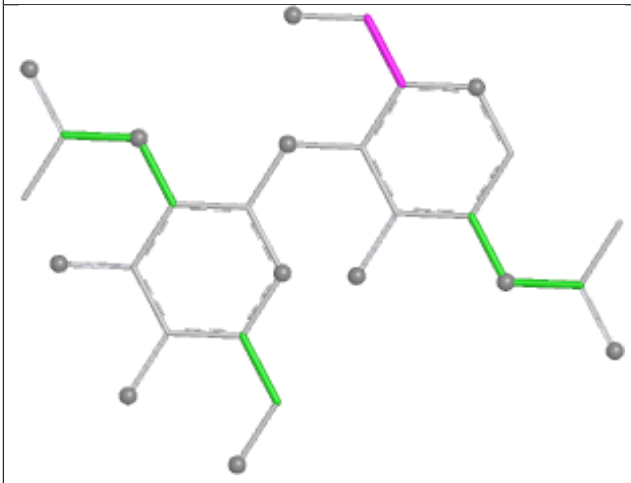
Oligosaccharide Chain e



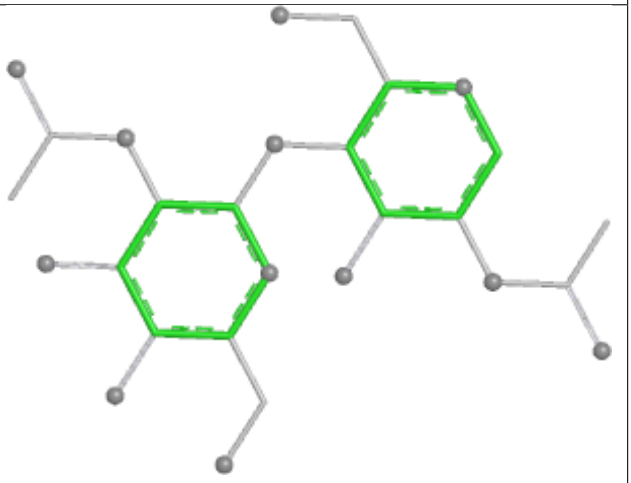
Bond lengths



Bond angles

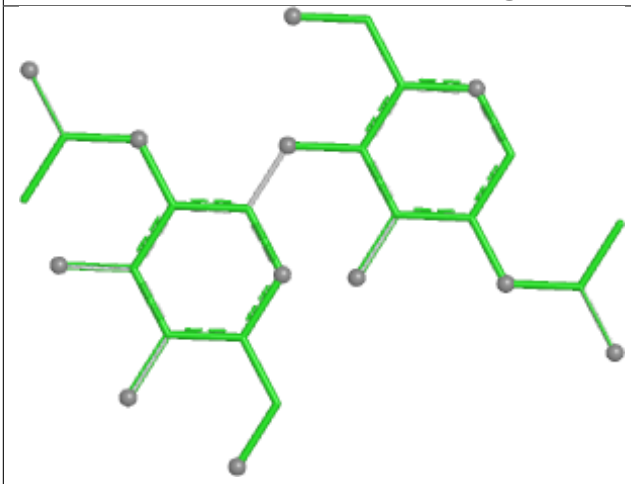


Torsions

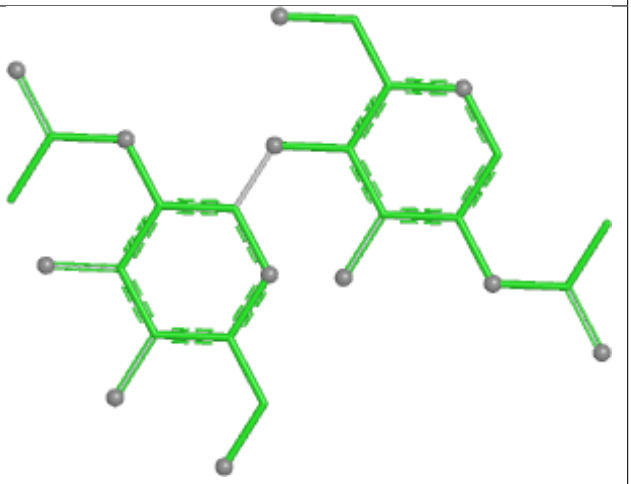


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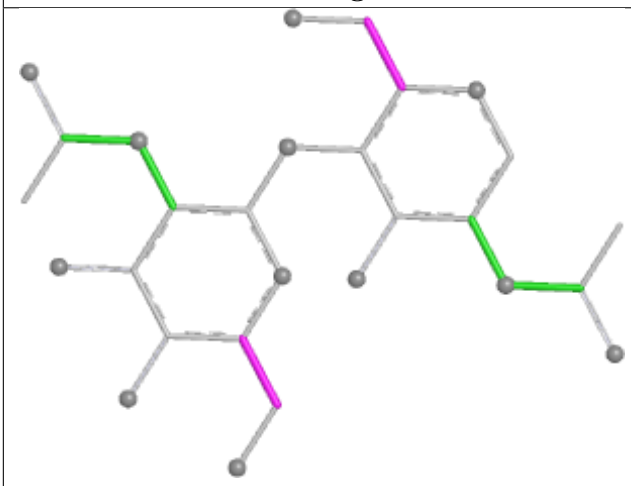
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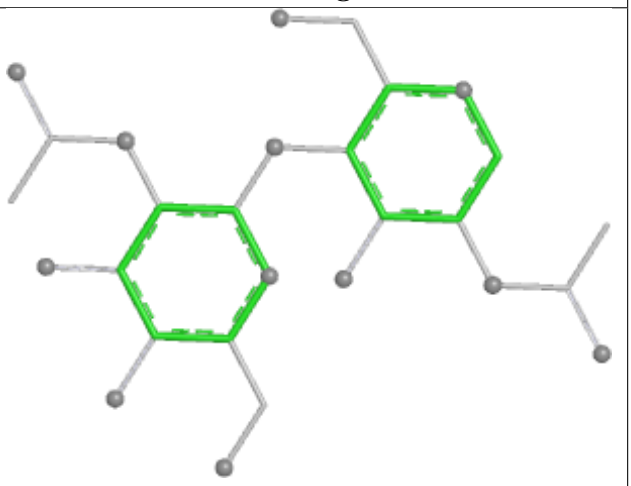
Bond lengths



Bond angles

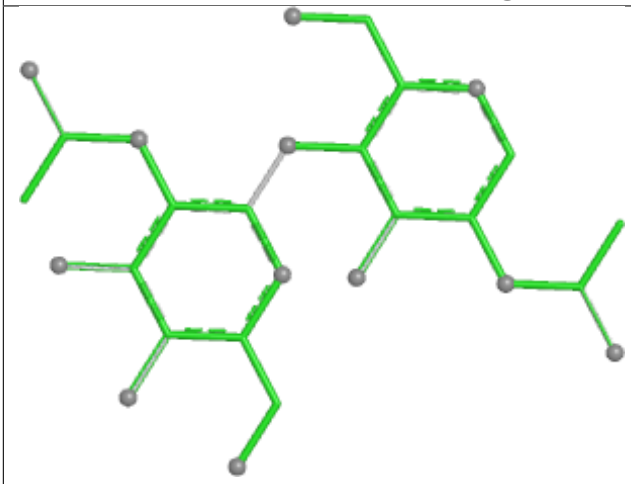


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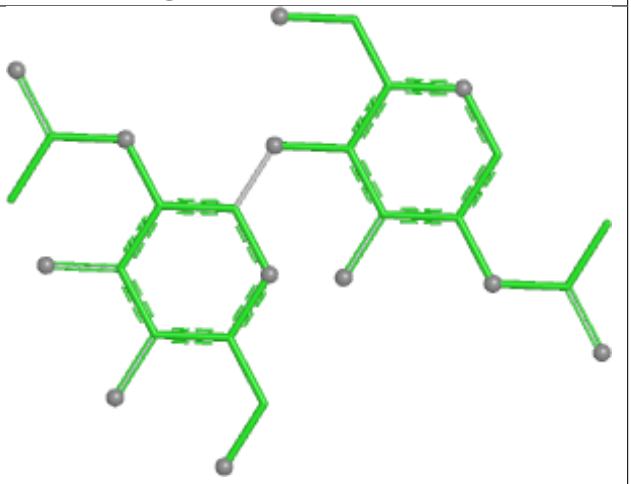


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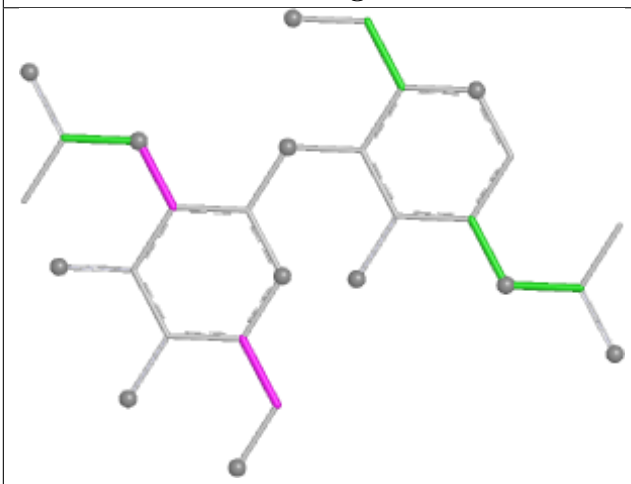
Oligosaccharide Chain g



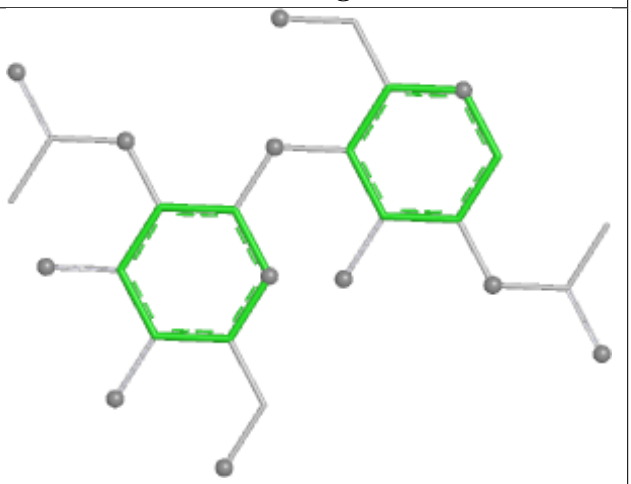
Bond lengths



Bond angles

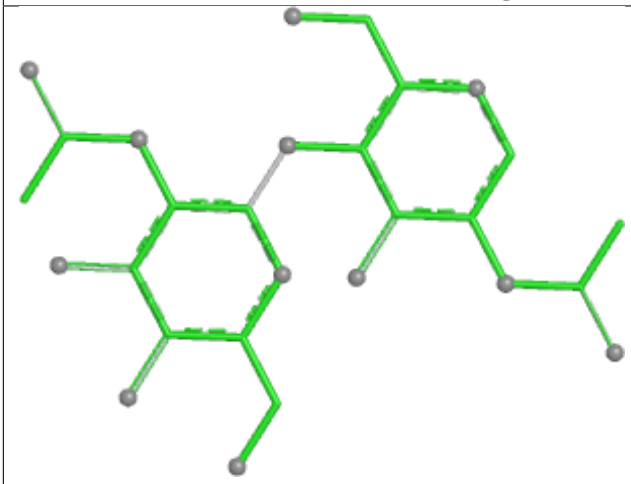


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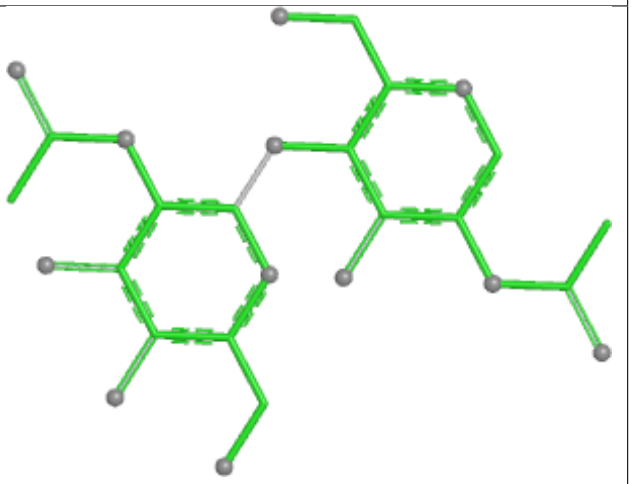


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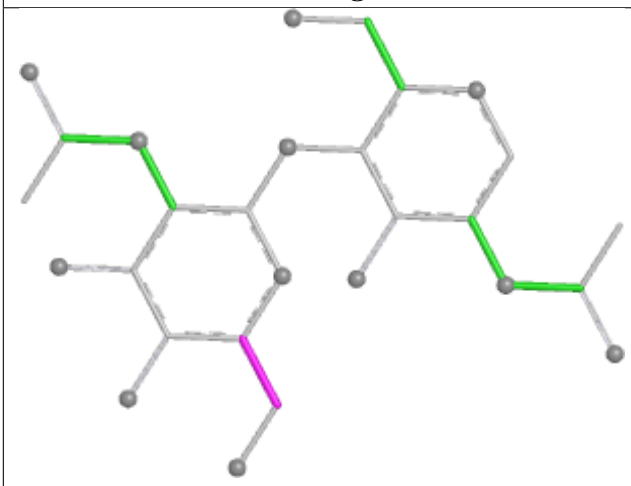
Oligosaccharide Chain h



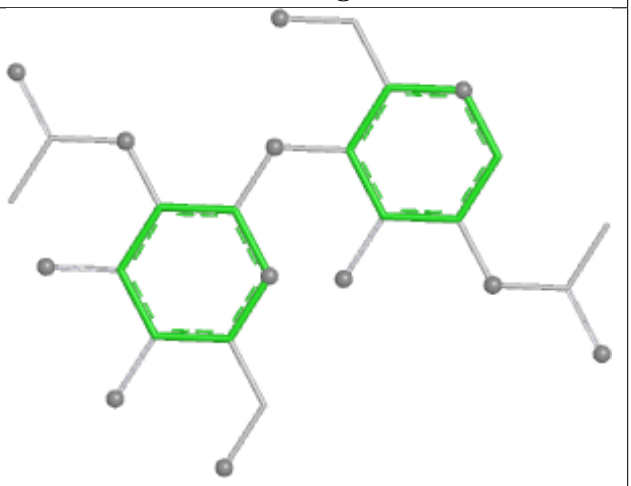
Bond lengths



Bond angles

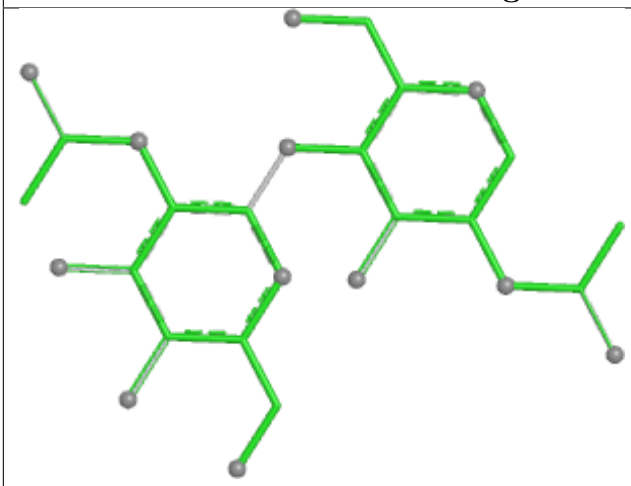


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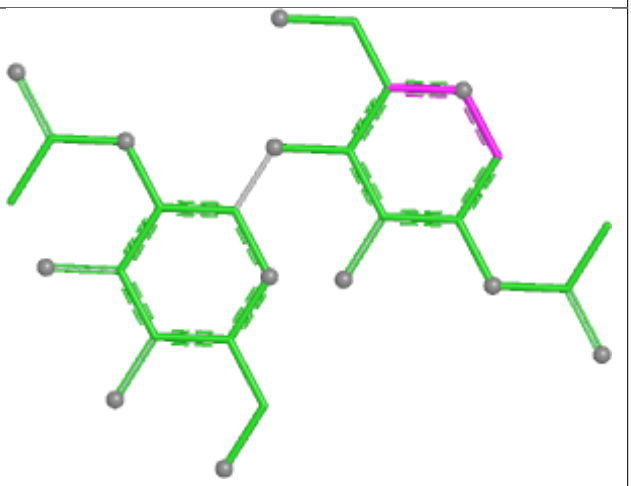


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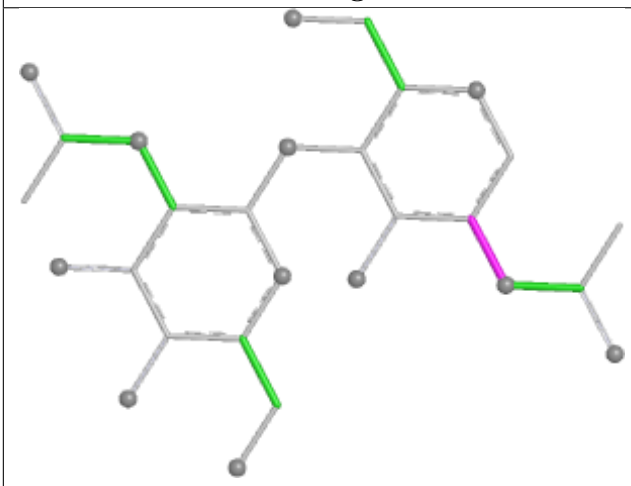
Oligosaccharide Chain i



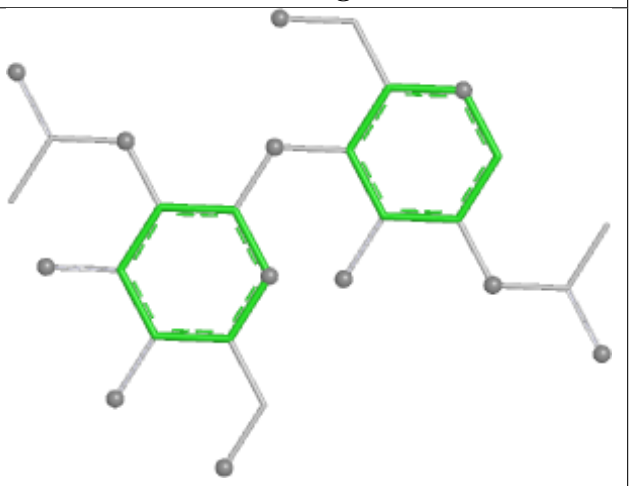
Bond lengths



Bond angles

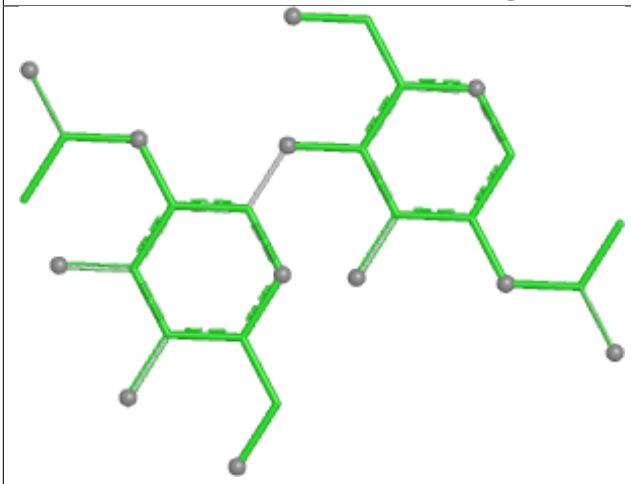


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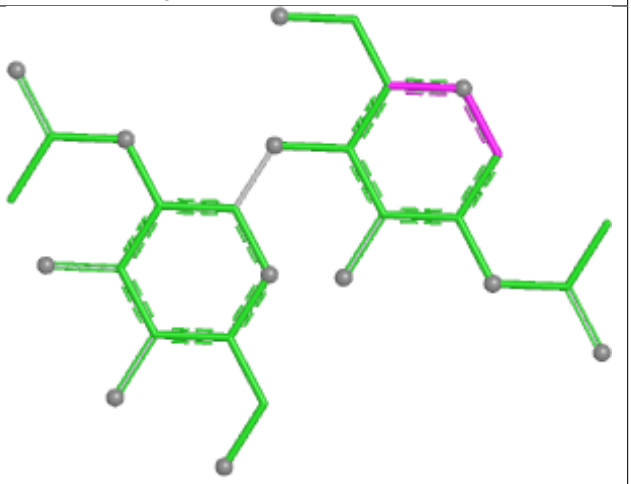


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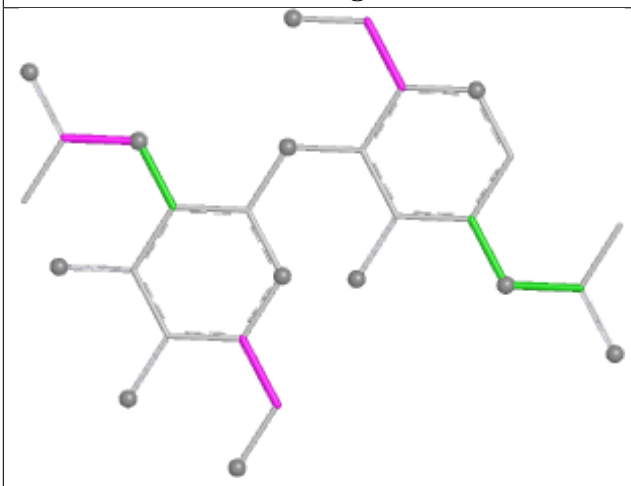
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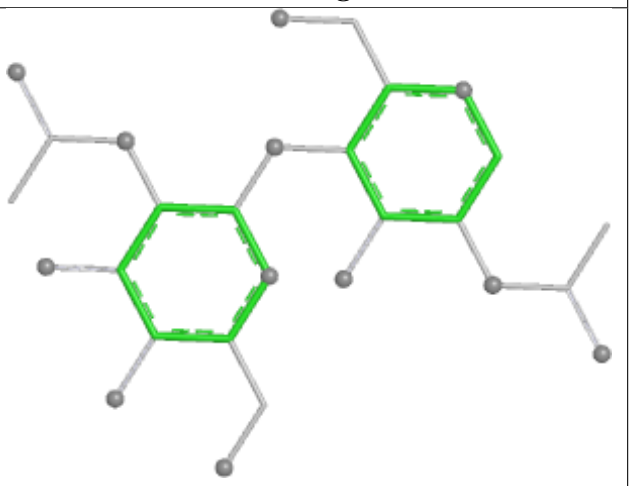
Bond lengths



Bond angles

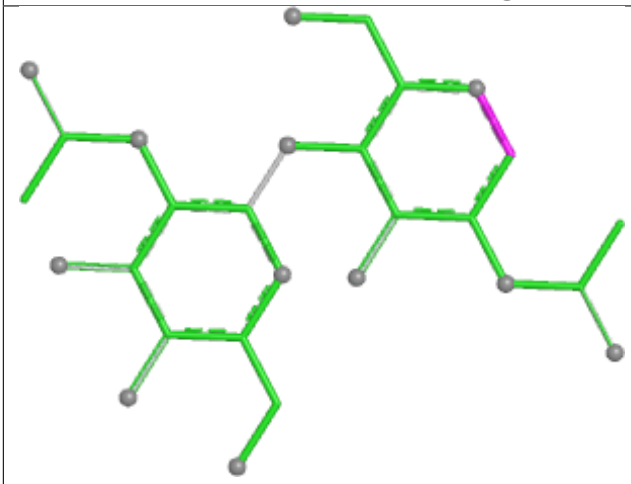


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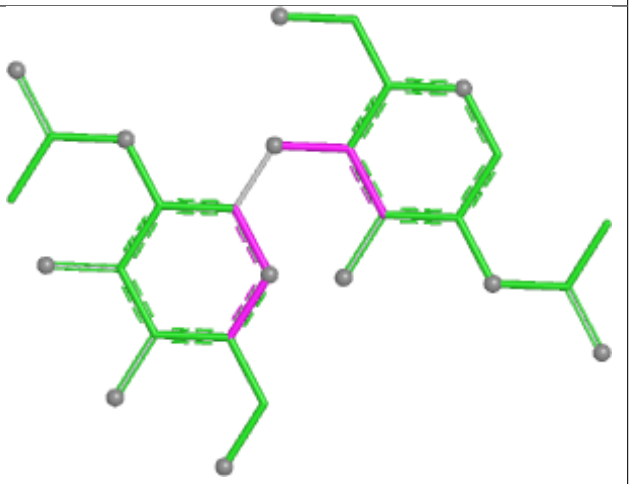


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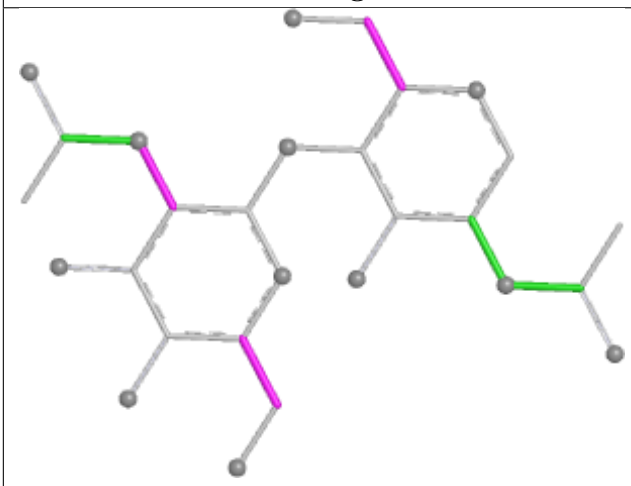
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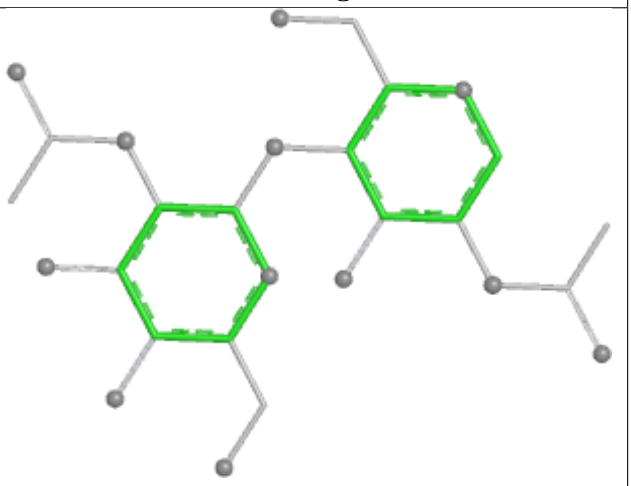
Bond lengths



Bond angles

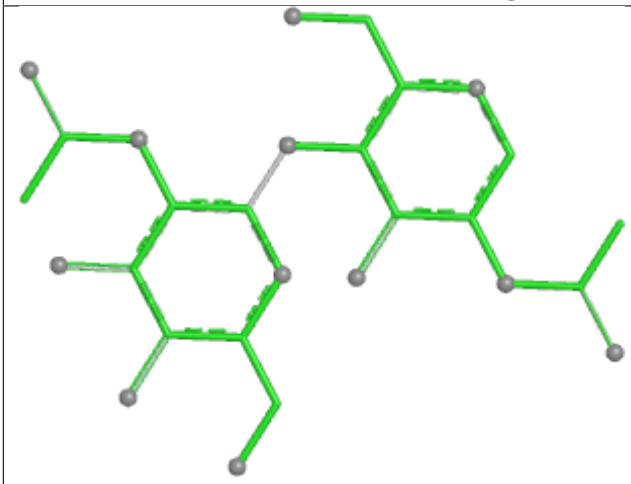


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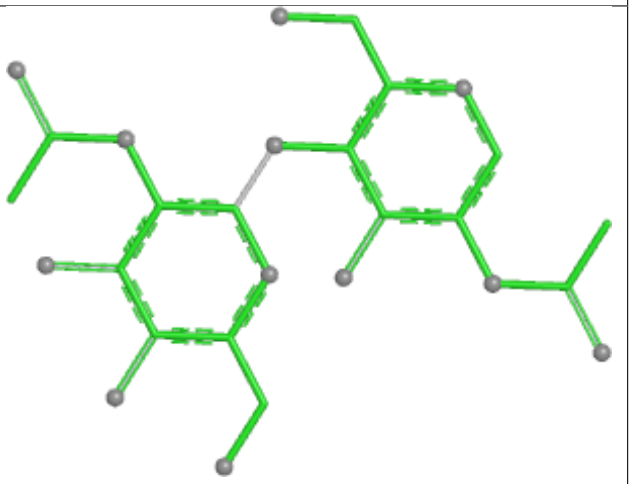


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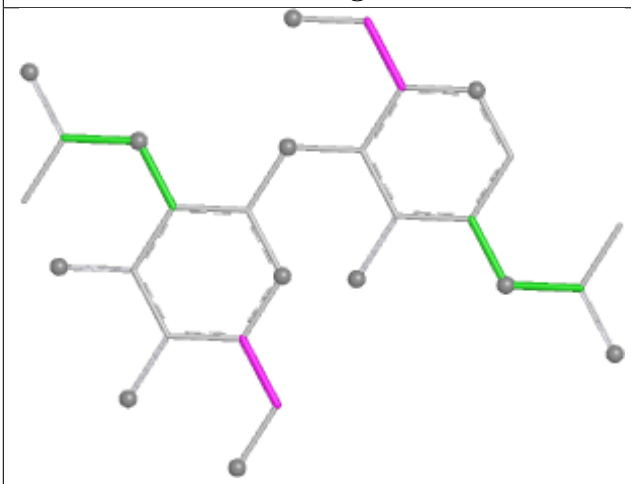
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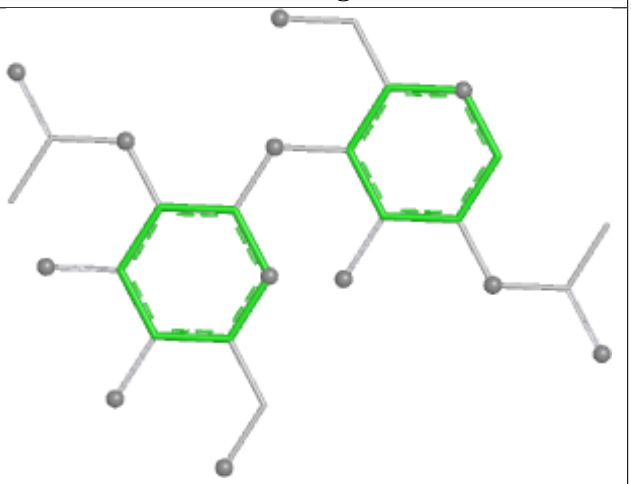
Bond lengths



Bond angles

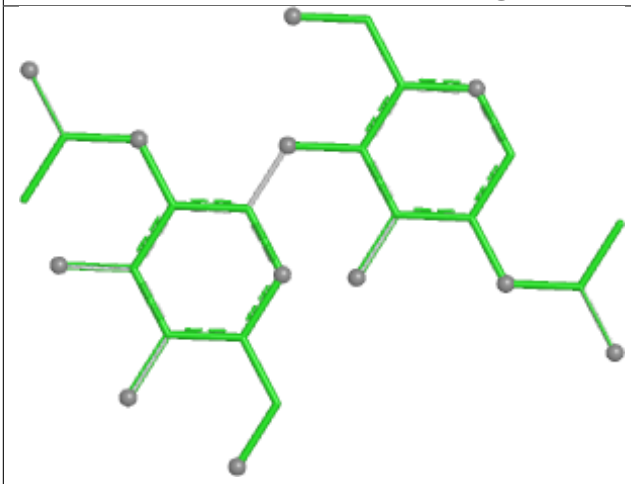


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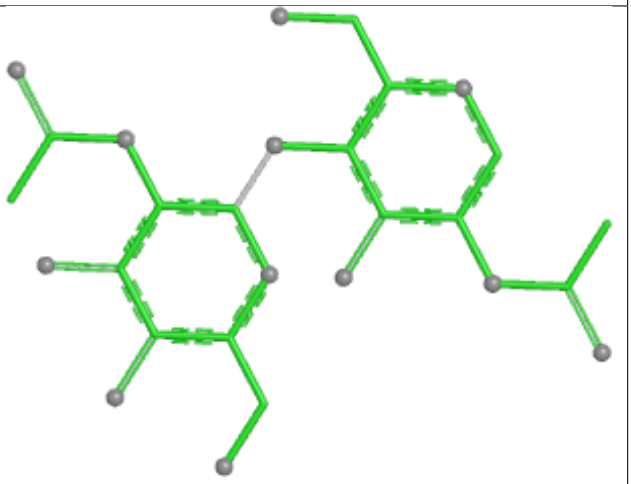


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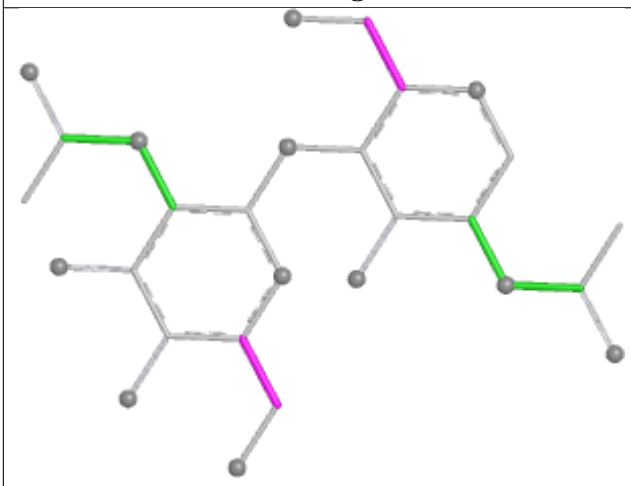
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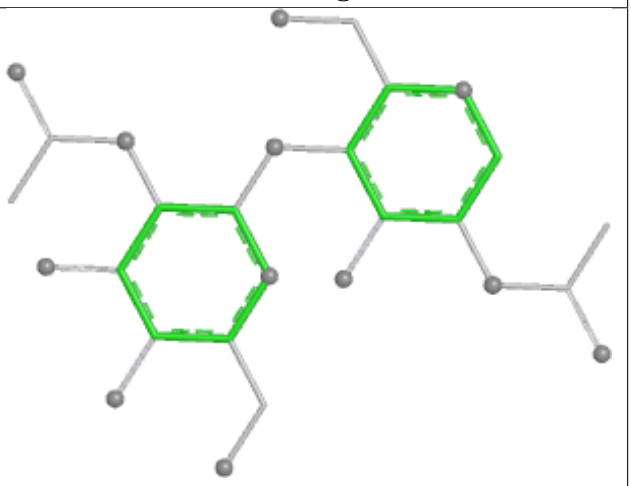
Bond lengths



Bond angles

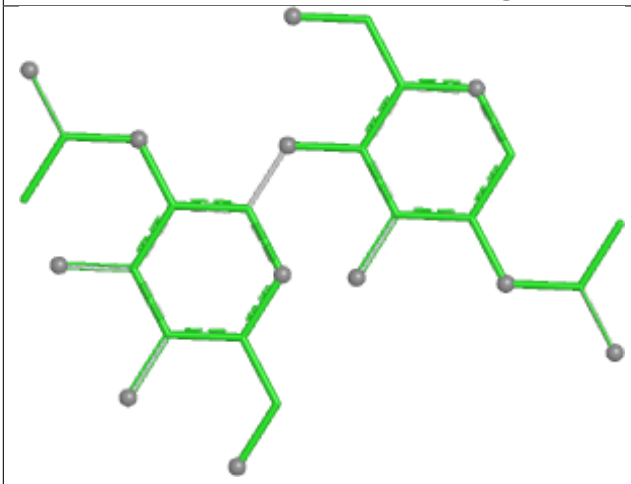


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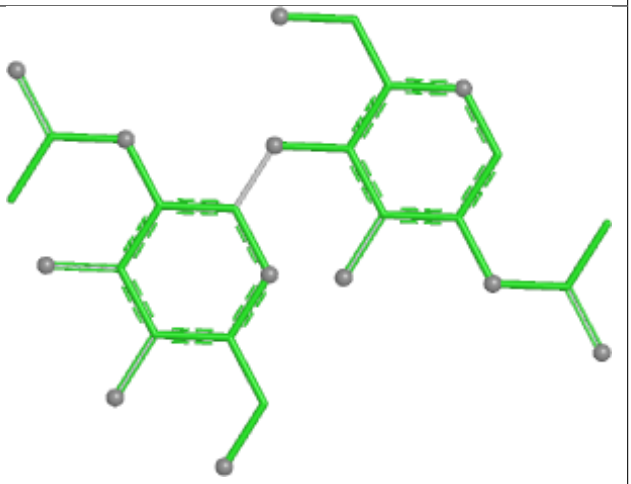


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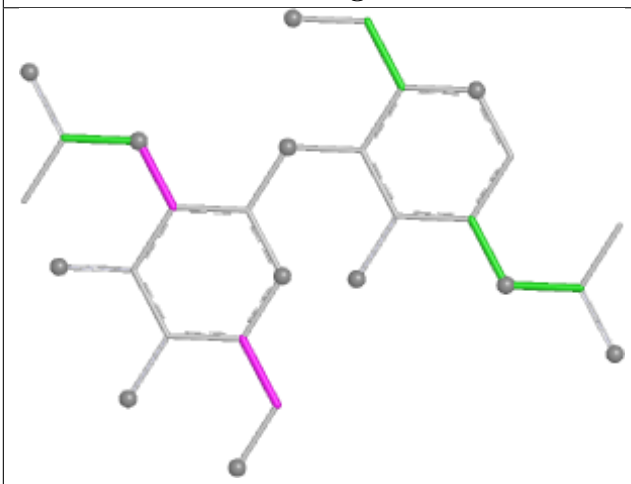
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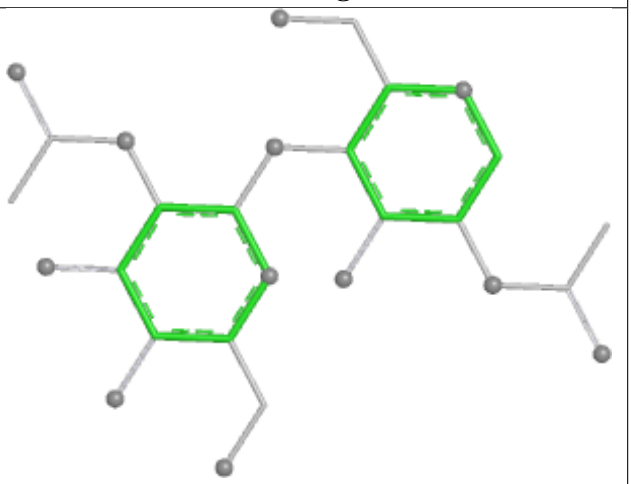
Bond lengths



Bond angles

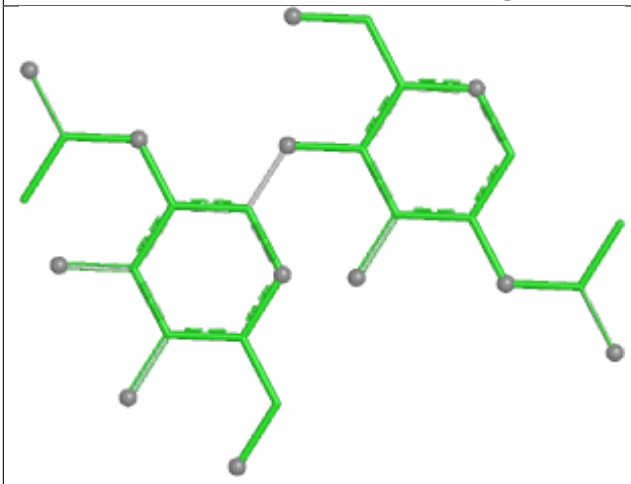


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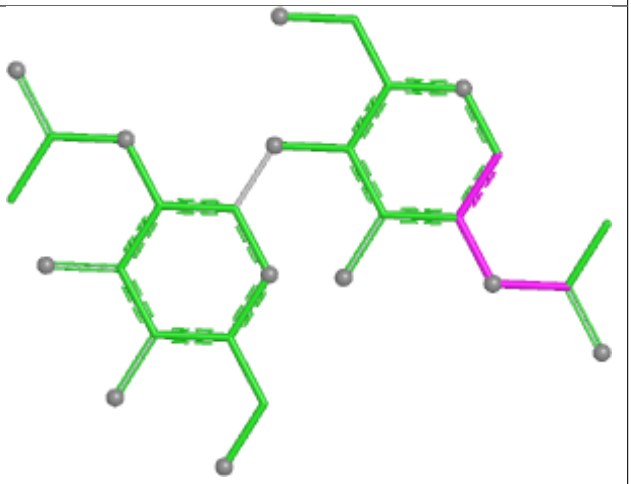


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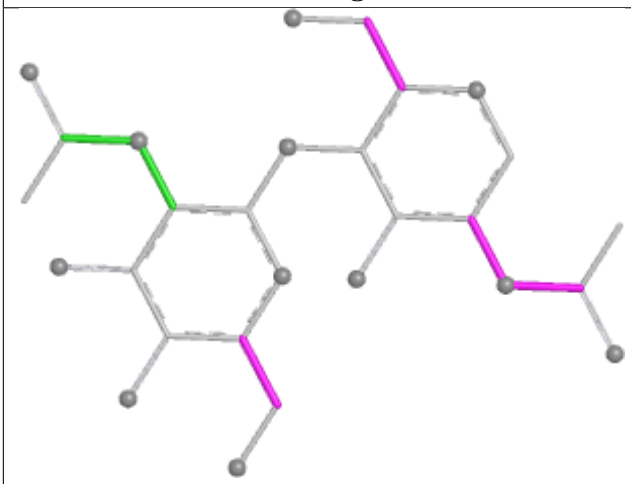
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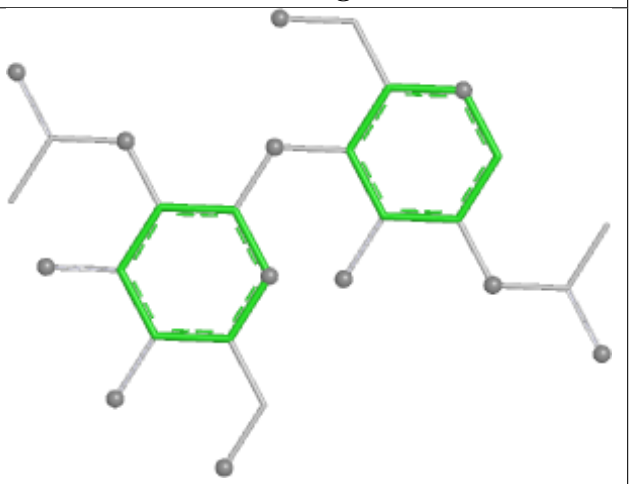
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Bond angles

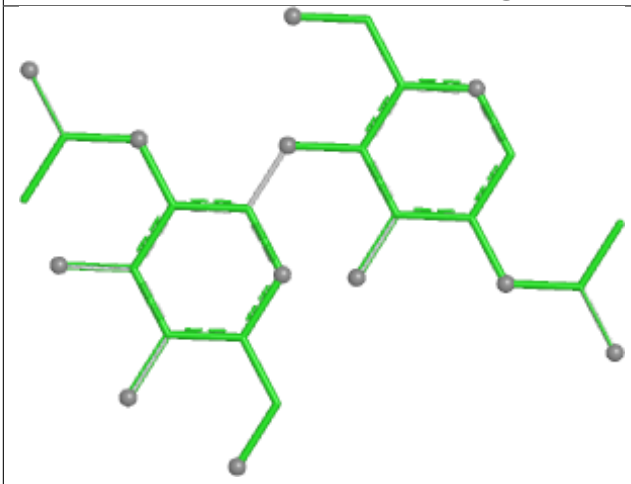


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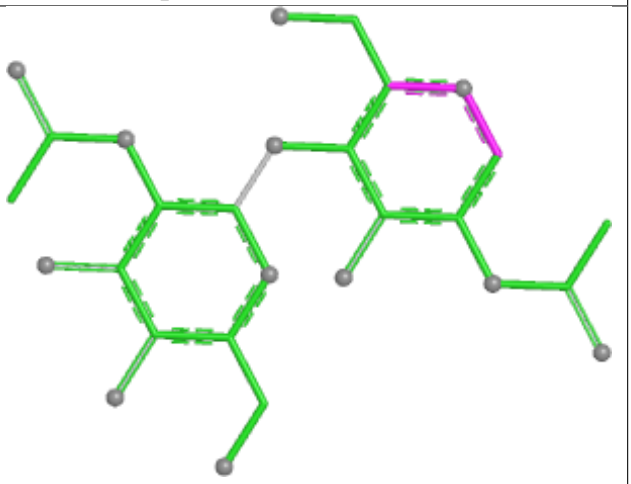


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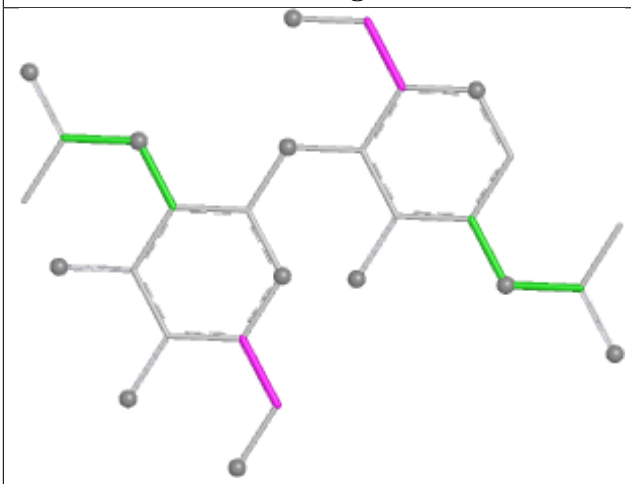
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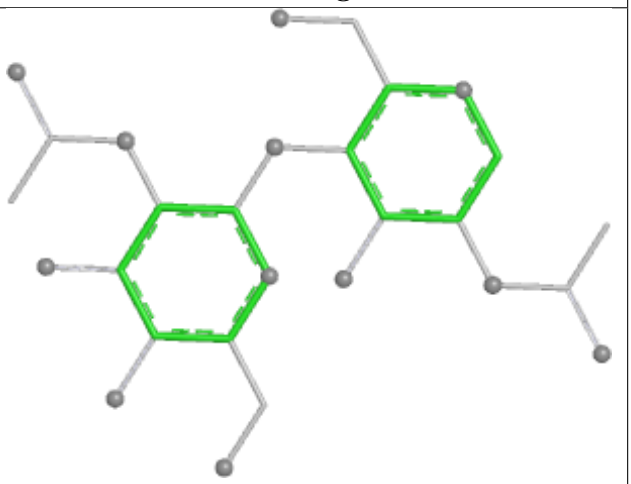
Bond lengths



Bond angles

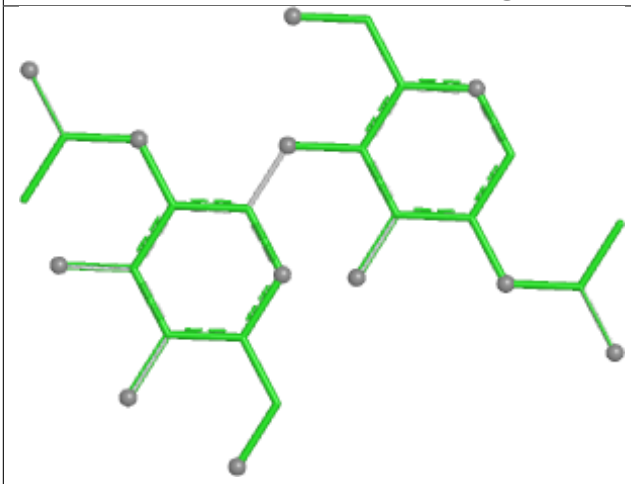


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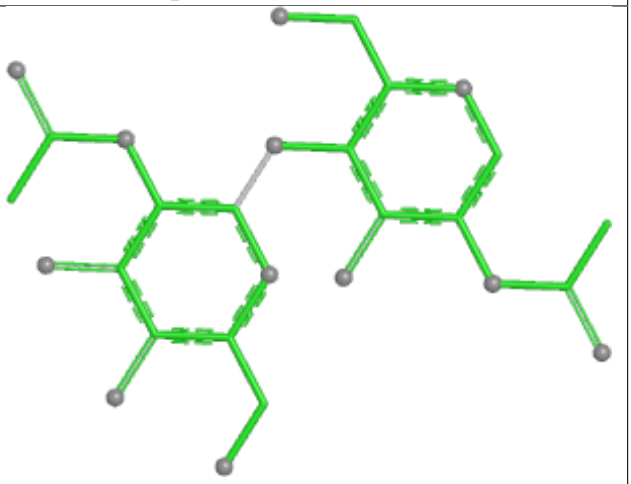


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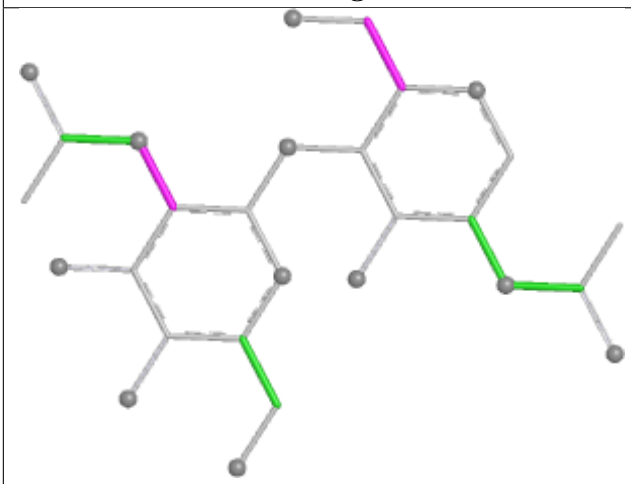
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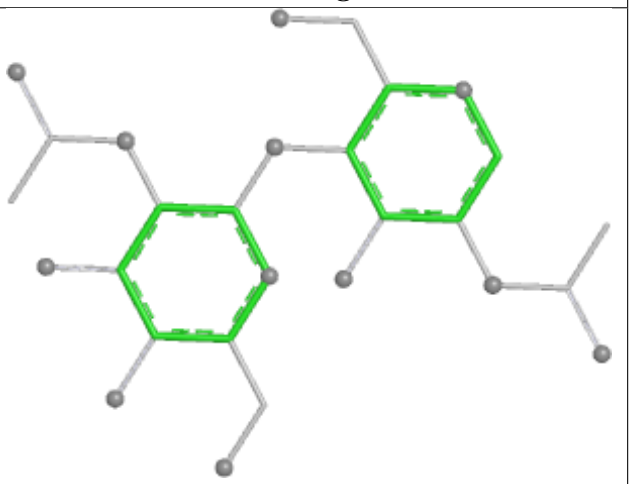
Bond lengths



Bond angles

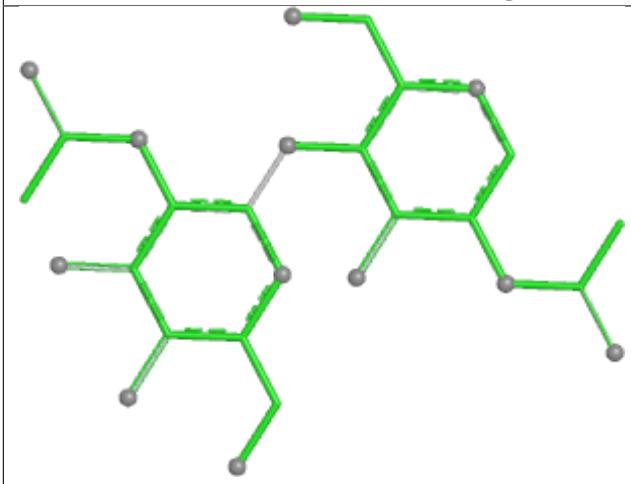


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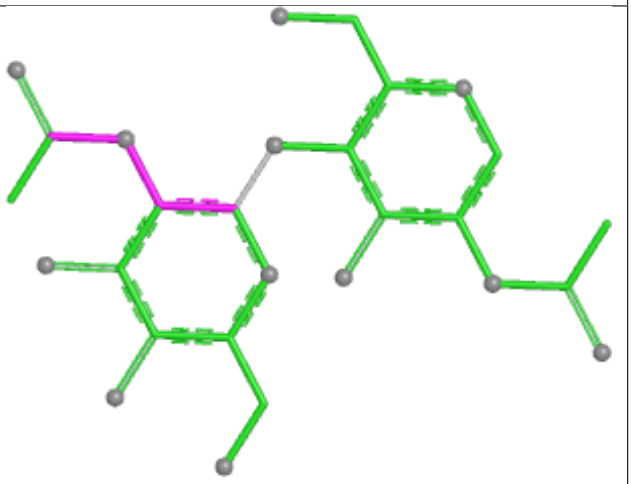


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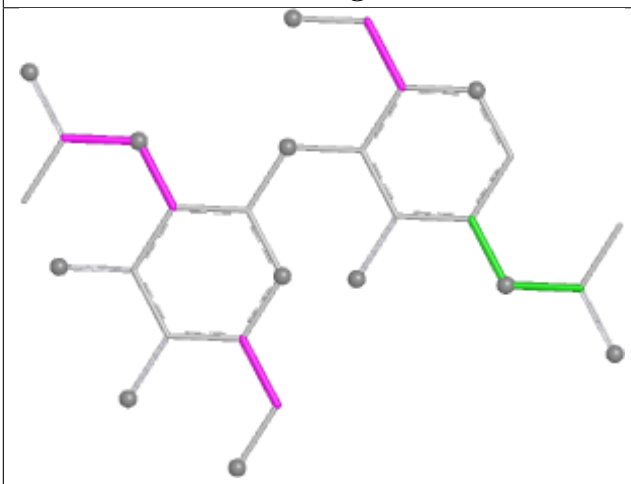
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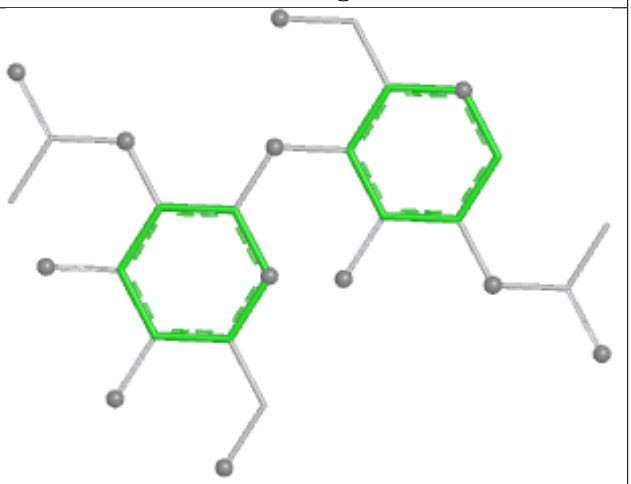
Bond lengths



Bond angles

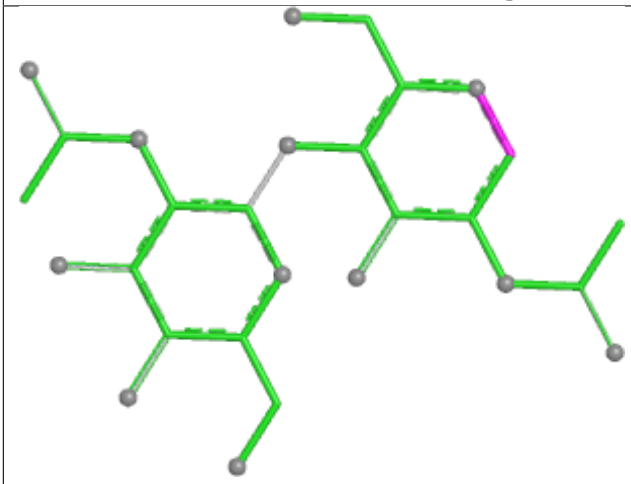


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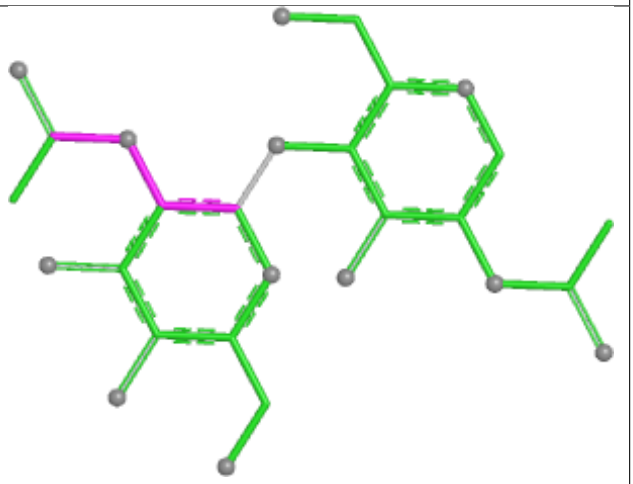


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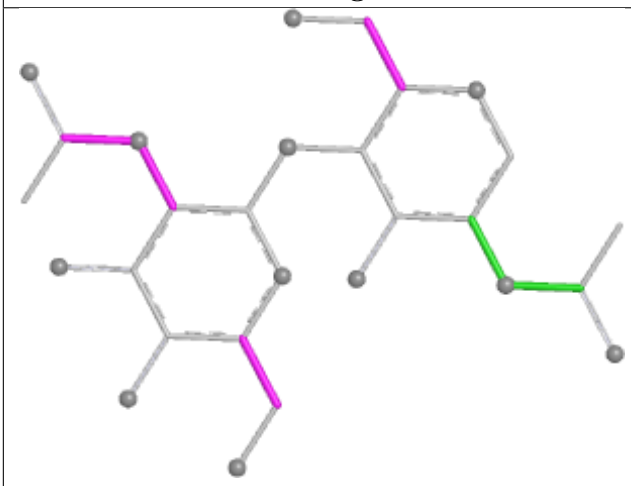
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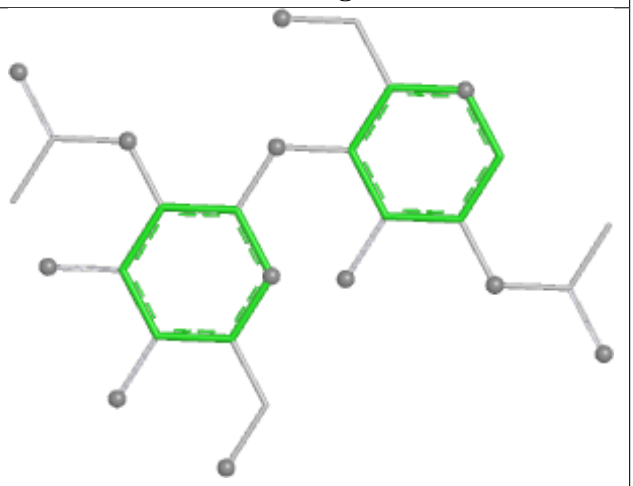
Bond lengths



Bond angles

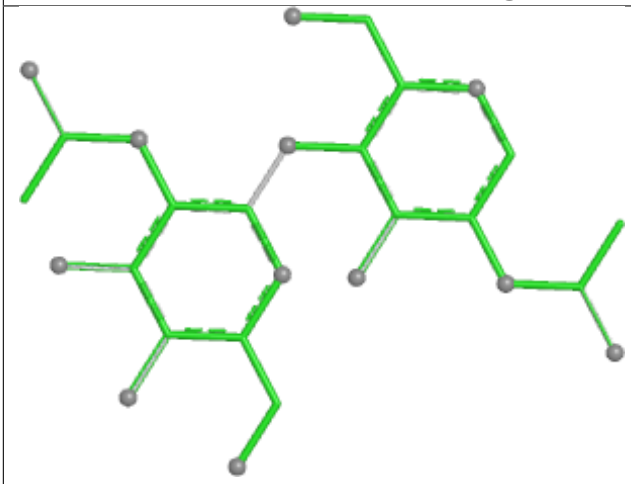


Torsions

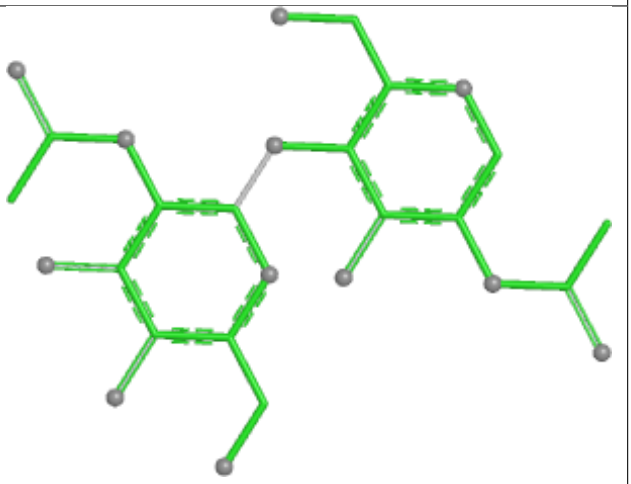


Rings

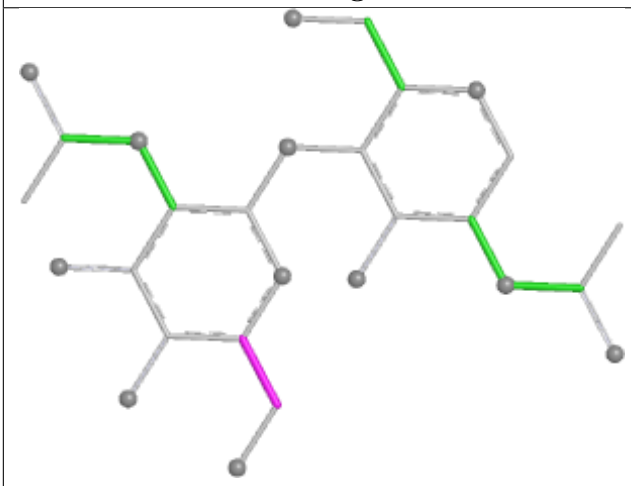
Oligosaccharide Chain t



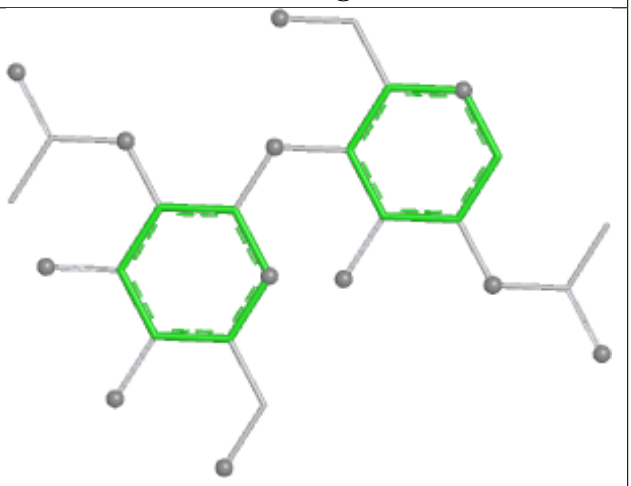
Bond lengths



Bond angles

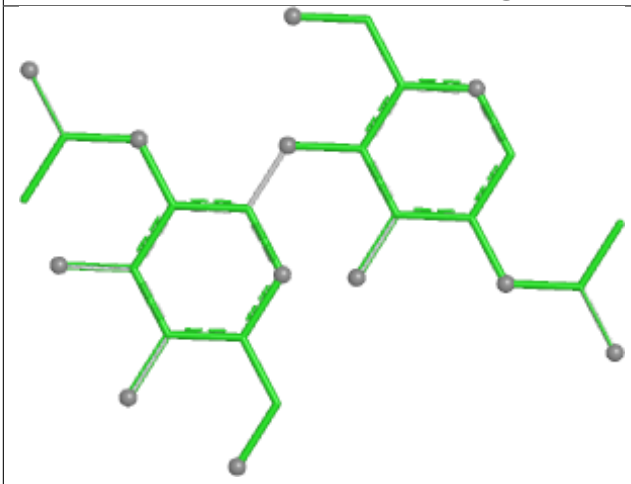


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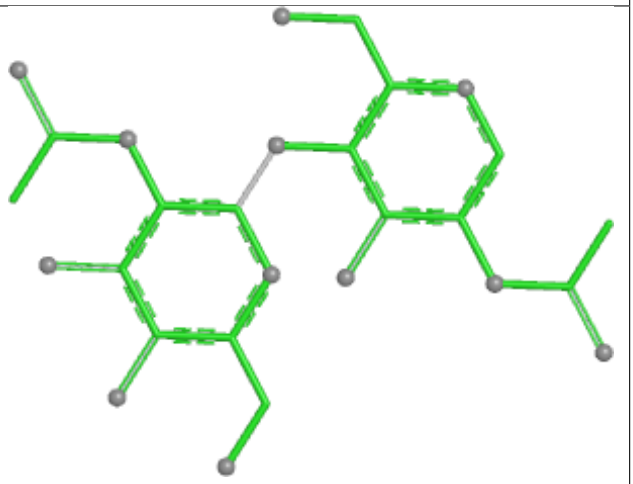


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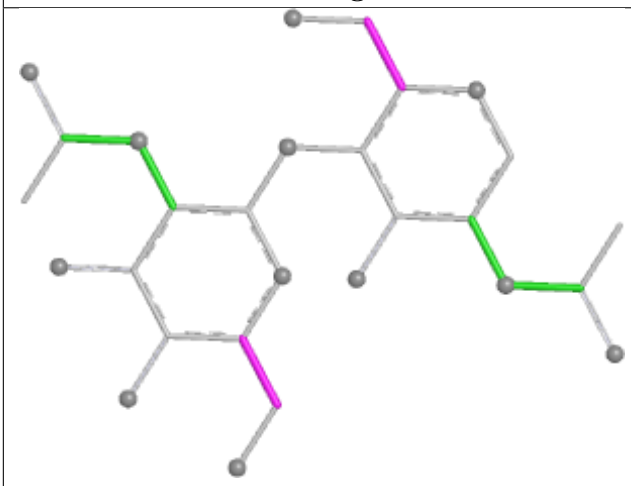
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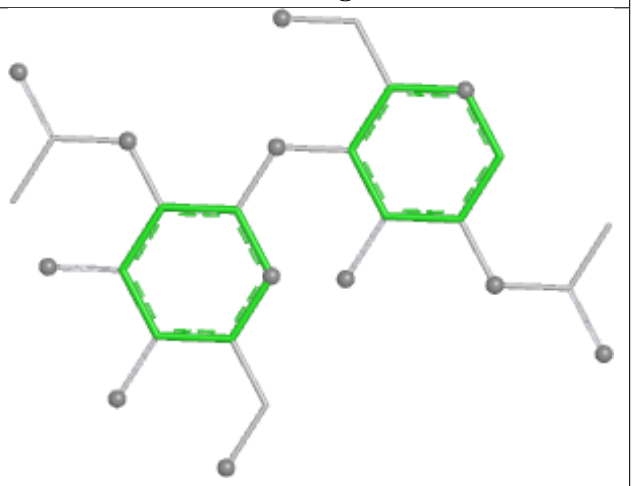
Bond lengths



Bond angles

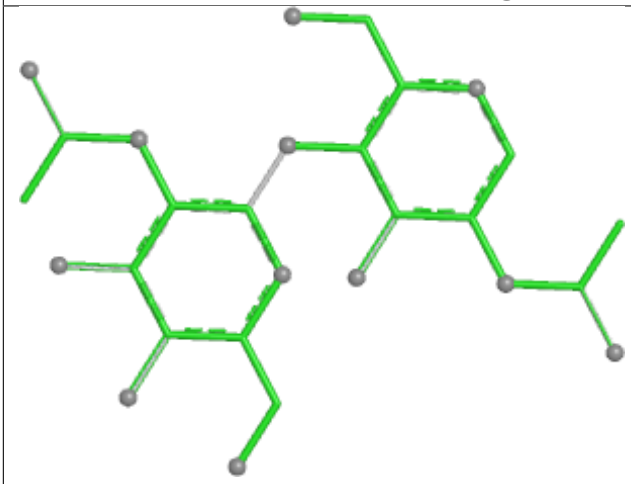


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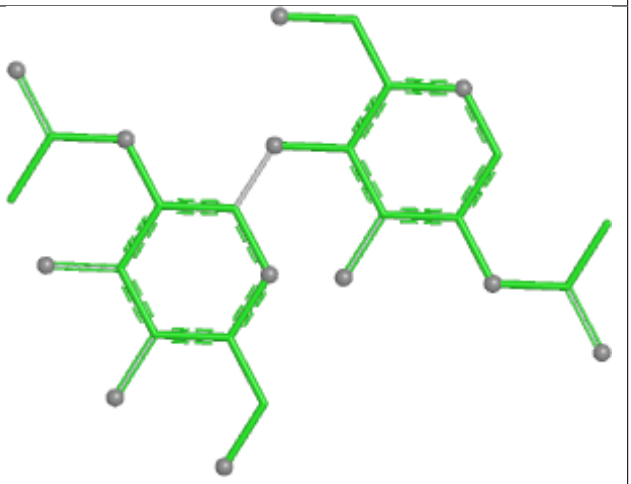


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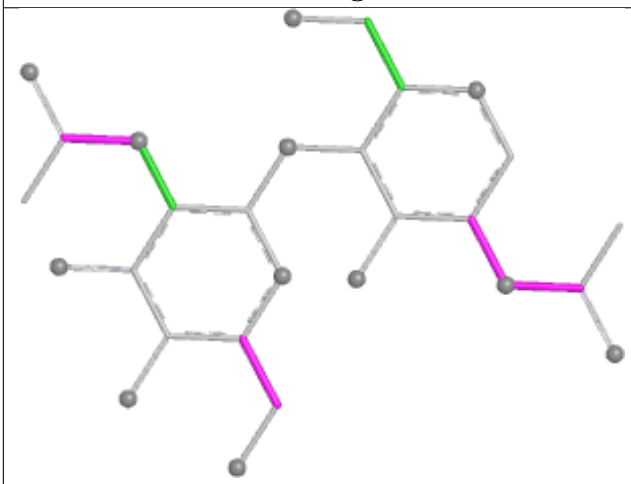
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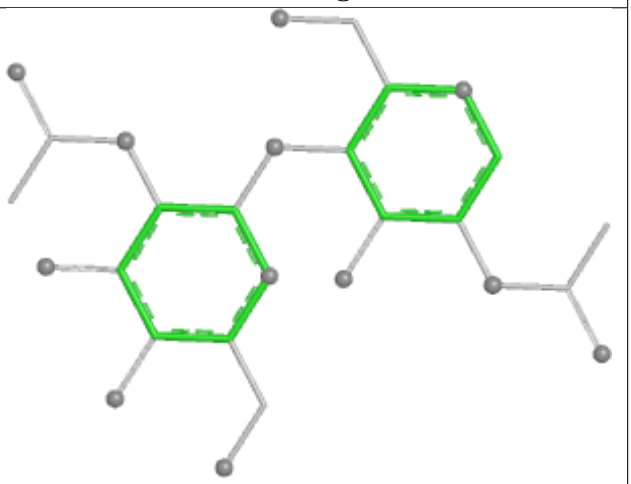
Bond lengths



Bond angles

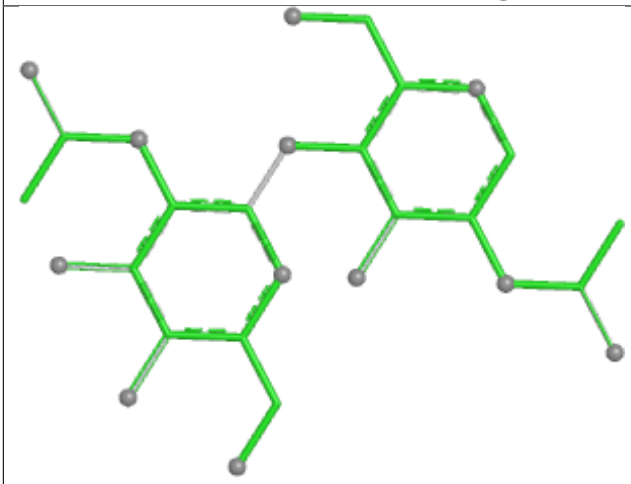


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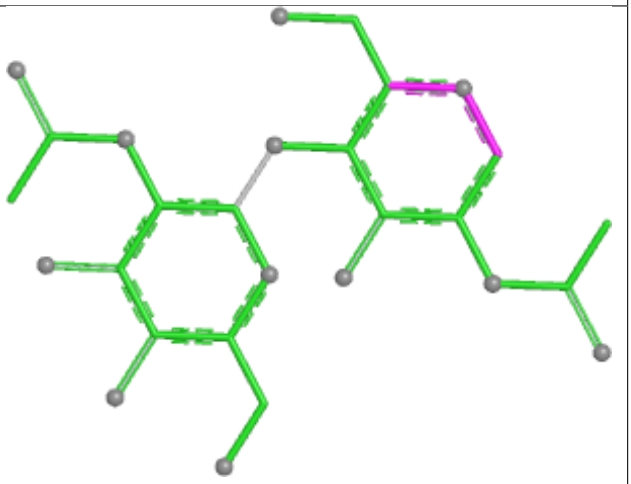


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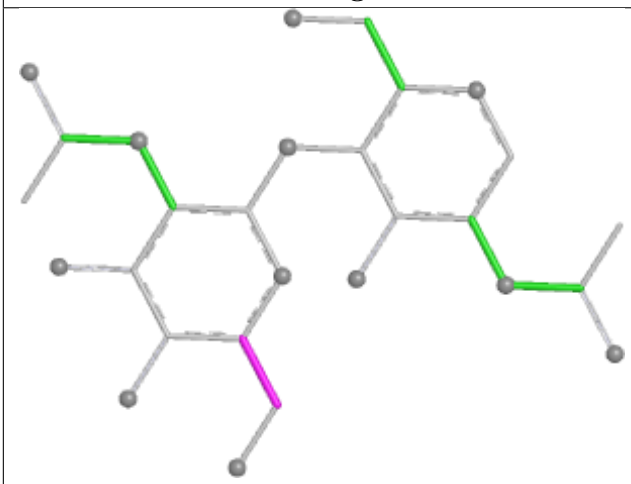
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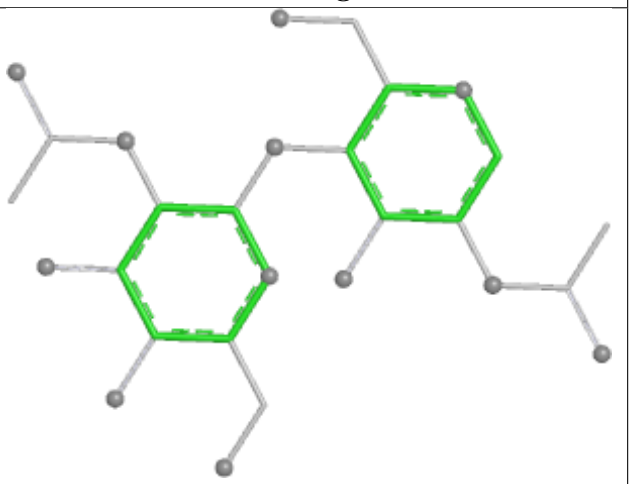
Bond lengths



Bond angles

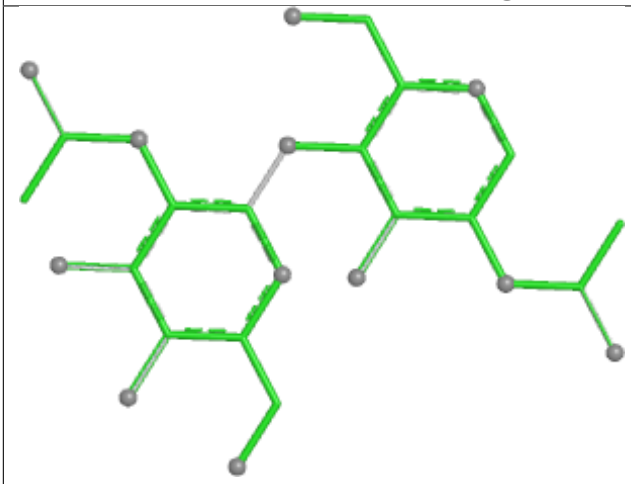


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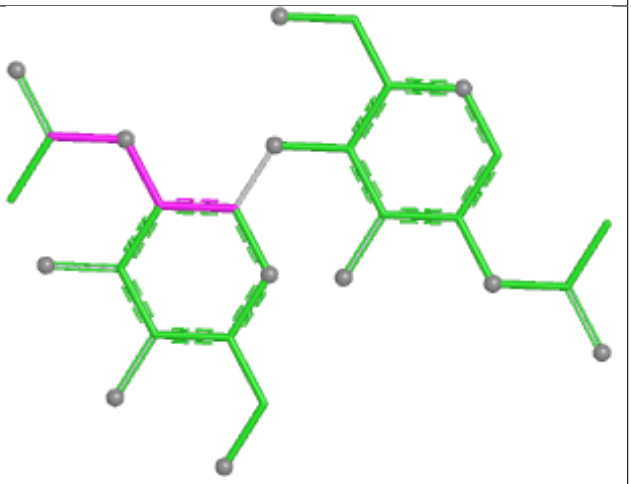


Rings

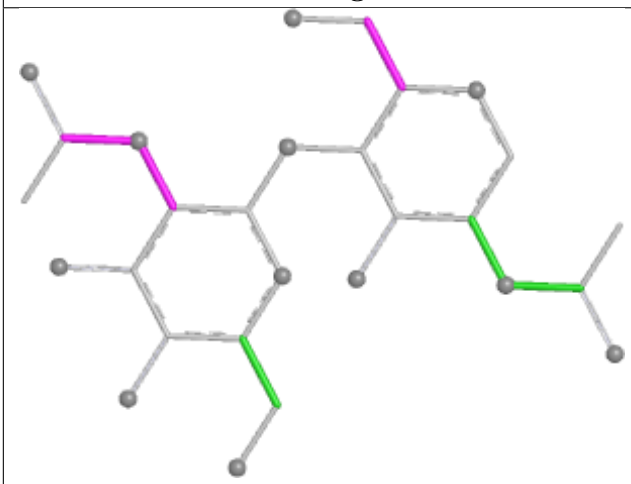
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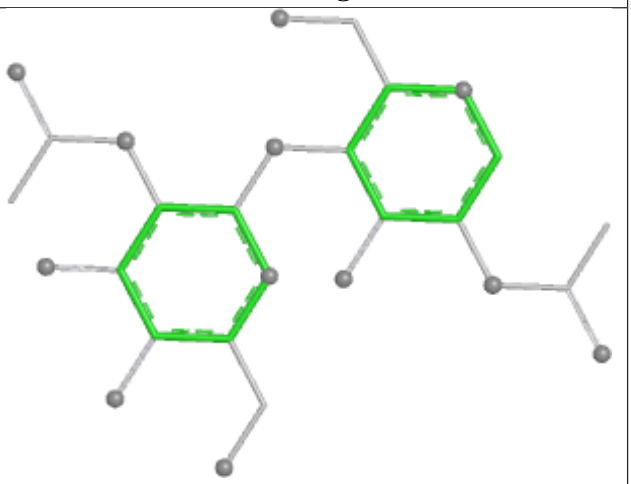
Bond lengths



Bond angles

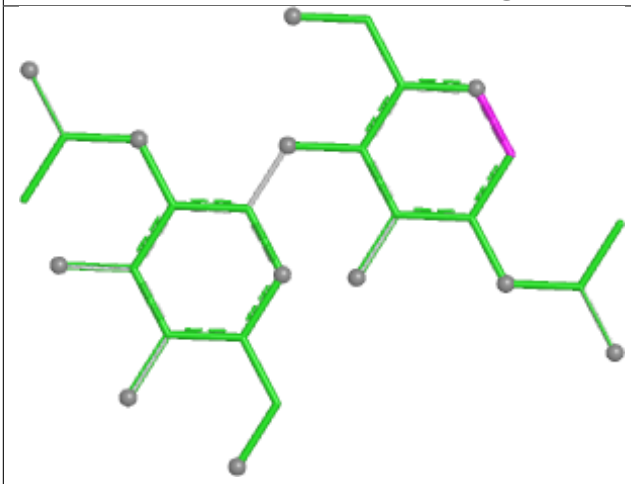


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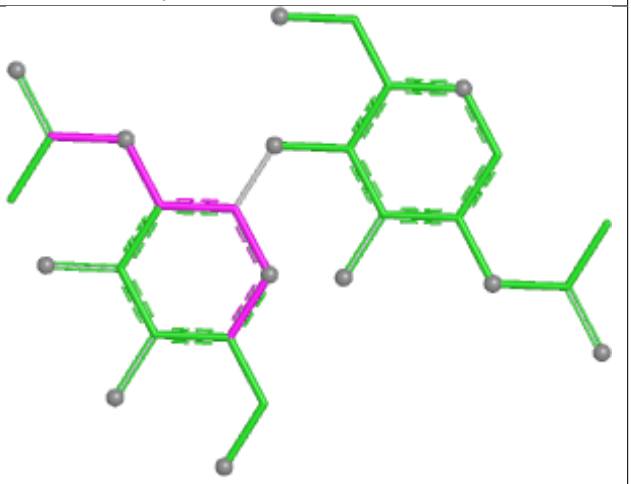


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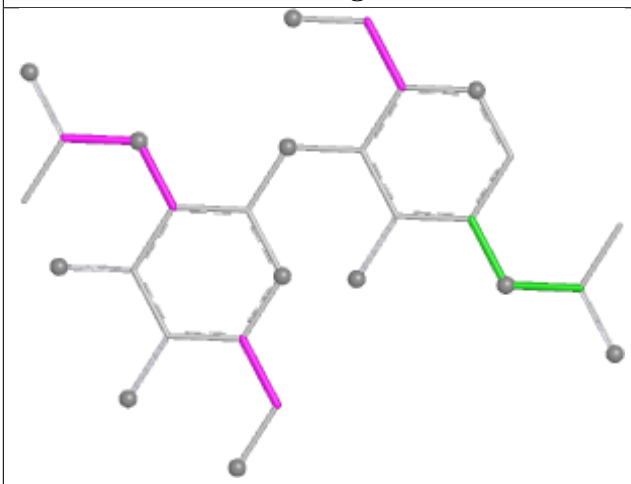
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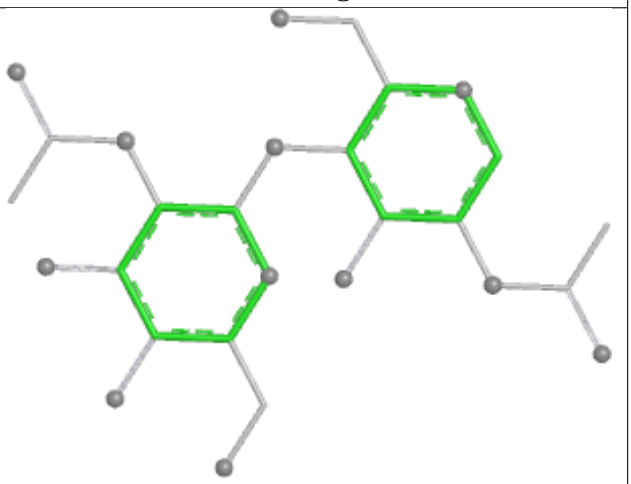
Bond lengths



Bond angles

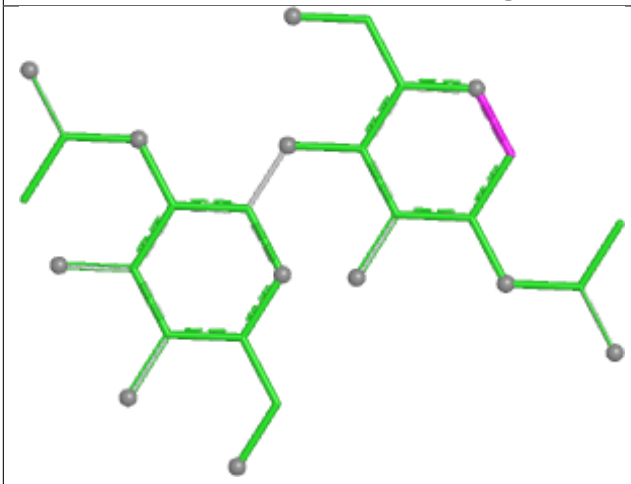


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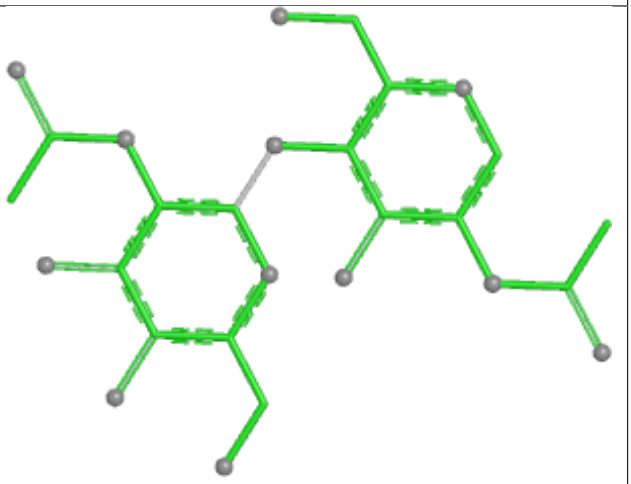


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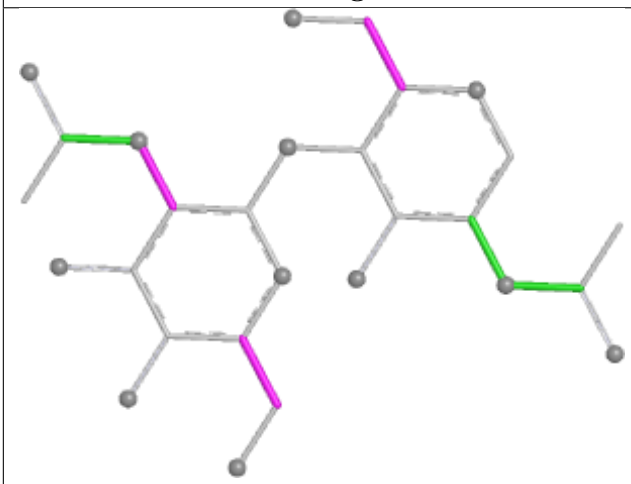
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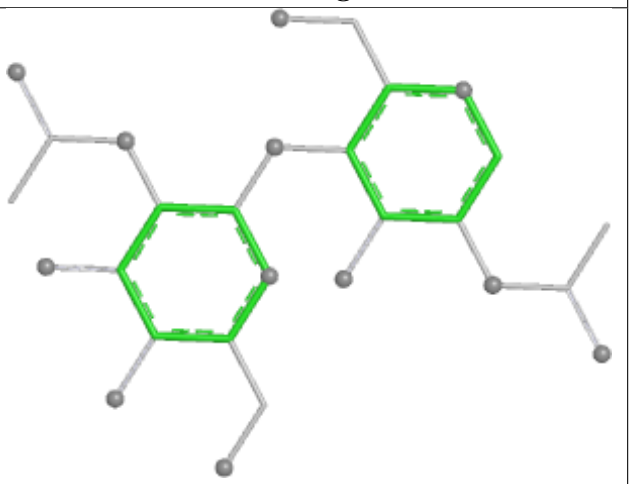
Bond lengths



Bond angles

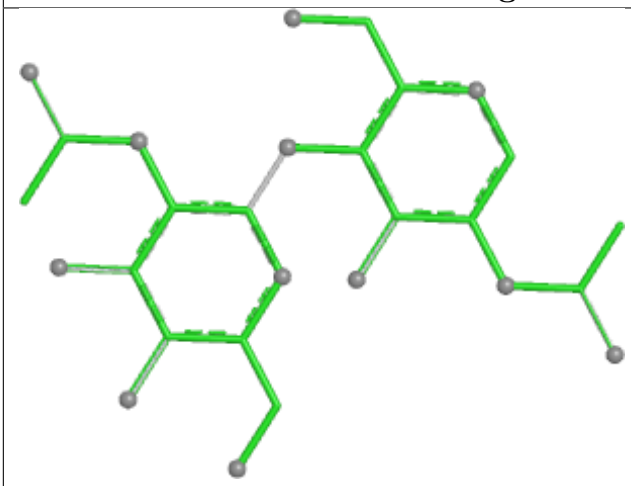


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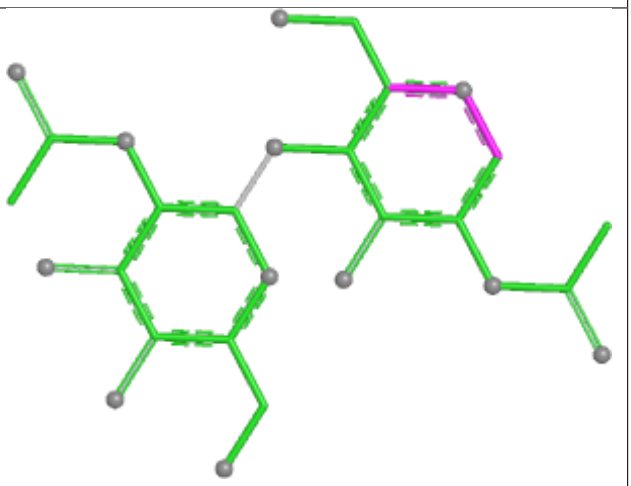


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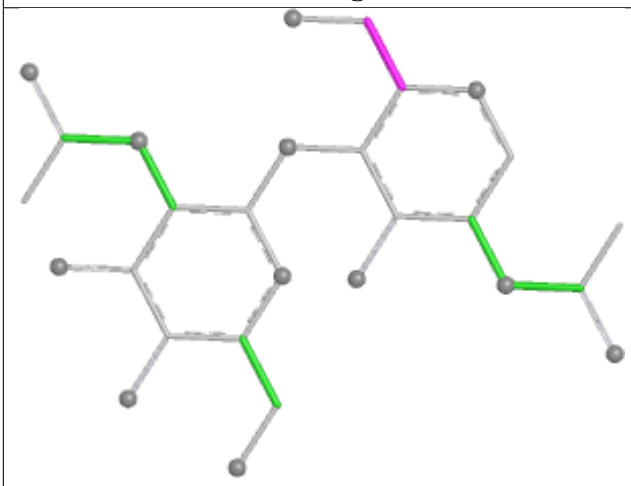
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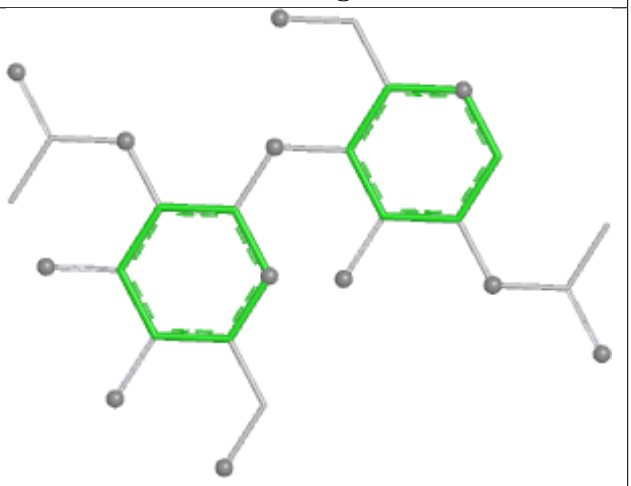
Bond lengths



Bond angles

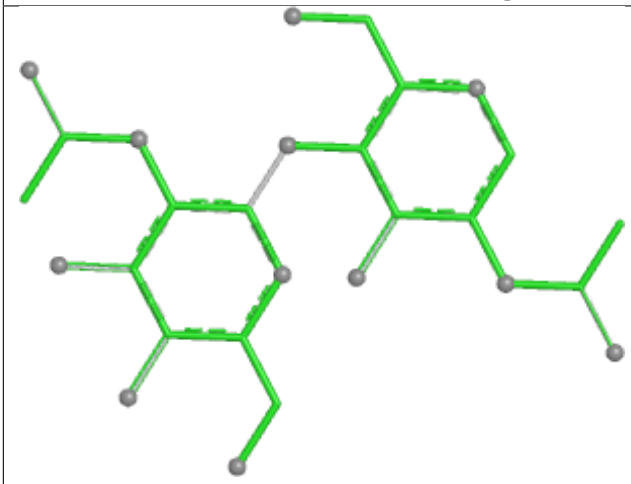


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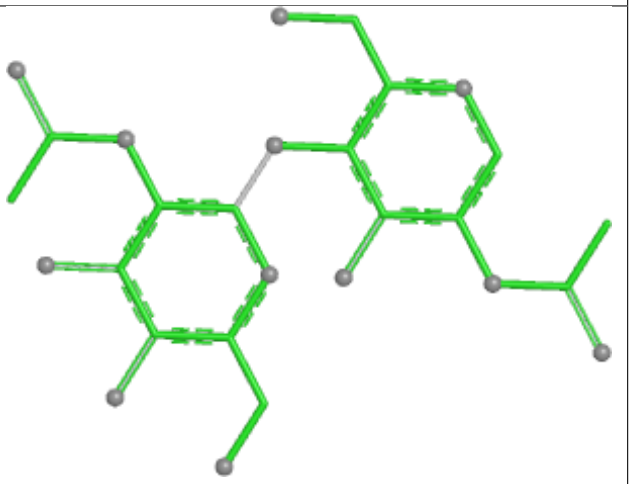


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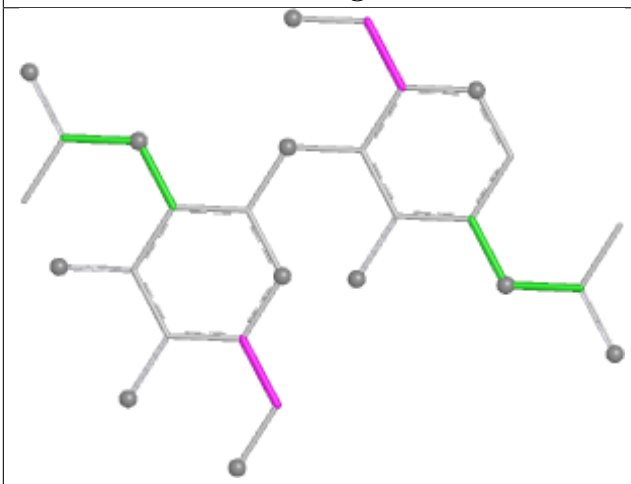
Oligosaccharide Chain 1



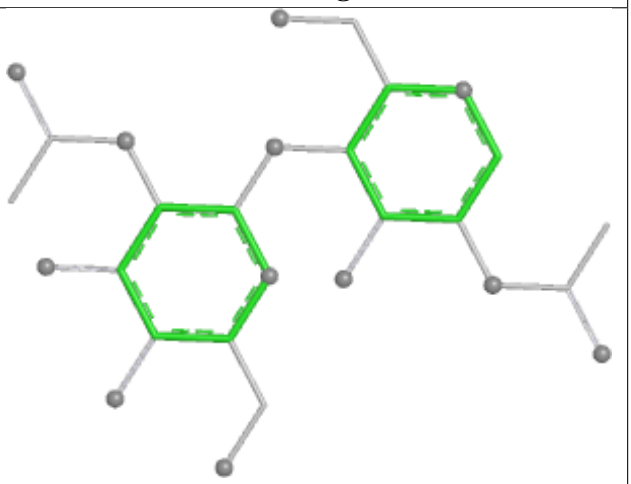
Bond lengths



Bond angles

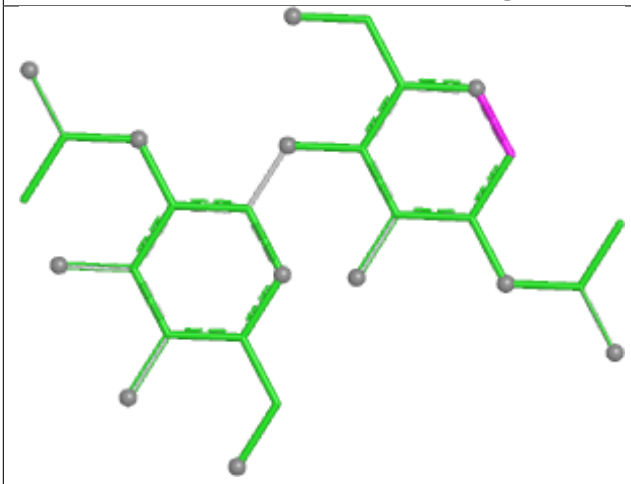


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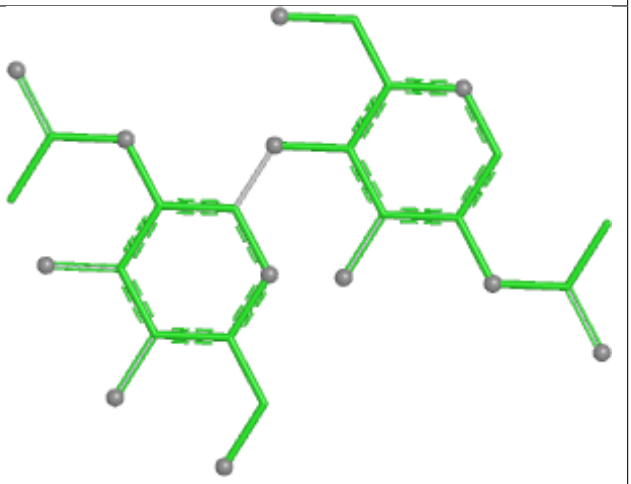


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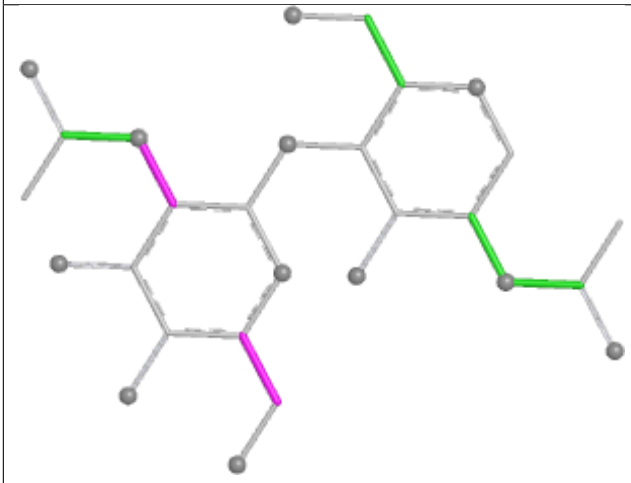
Oligosaccharide Chain 2



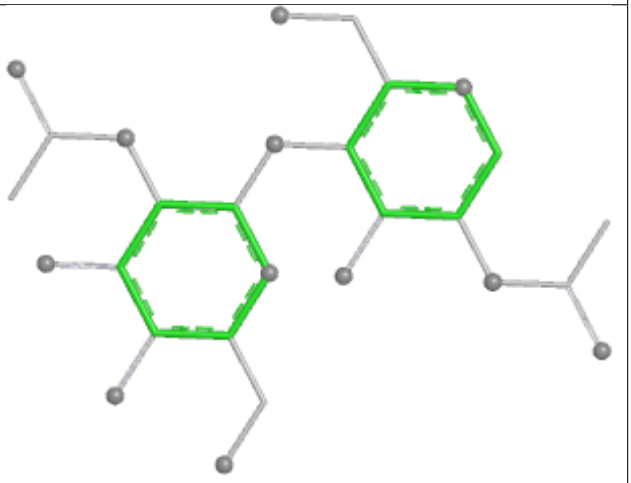
Bond lengths



Bond angles

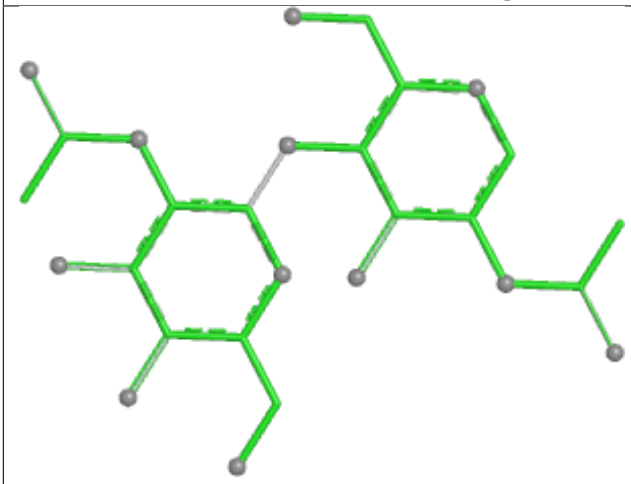


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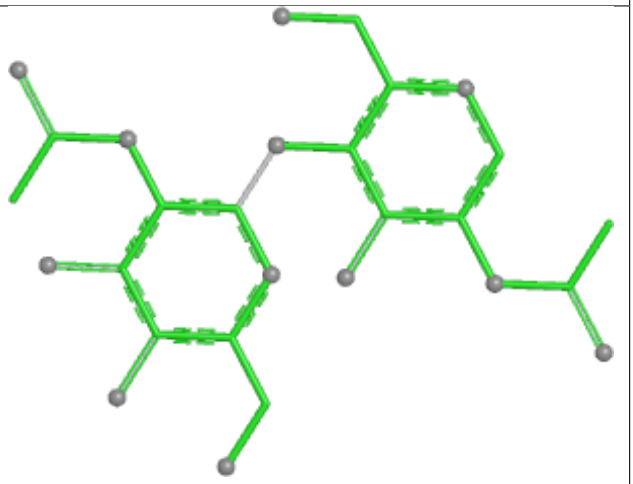


Rings

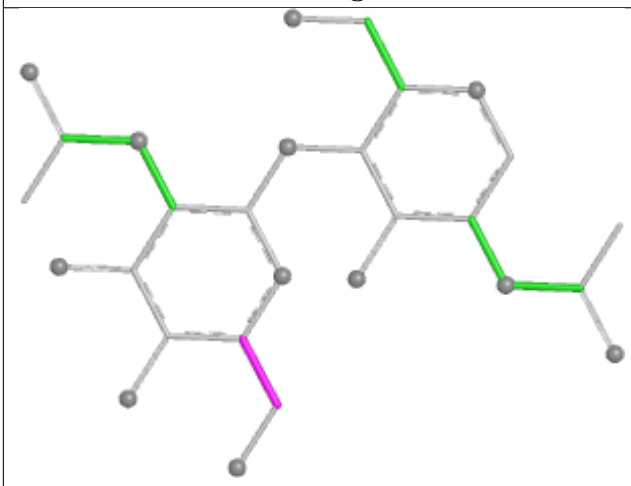
Oligosaccharide Chain 3



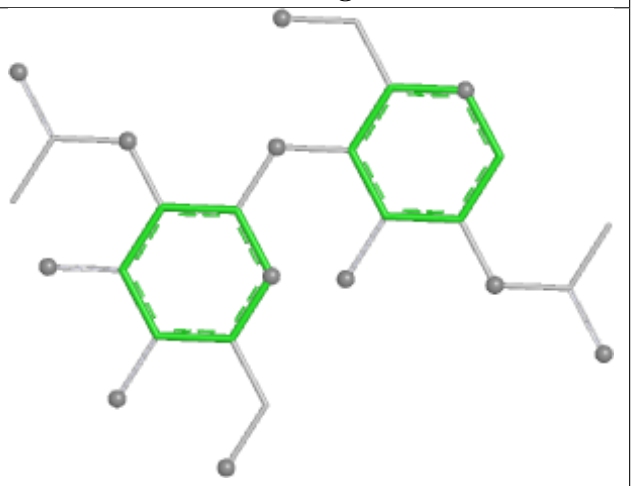
Bond lengths



Bond angles

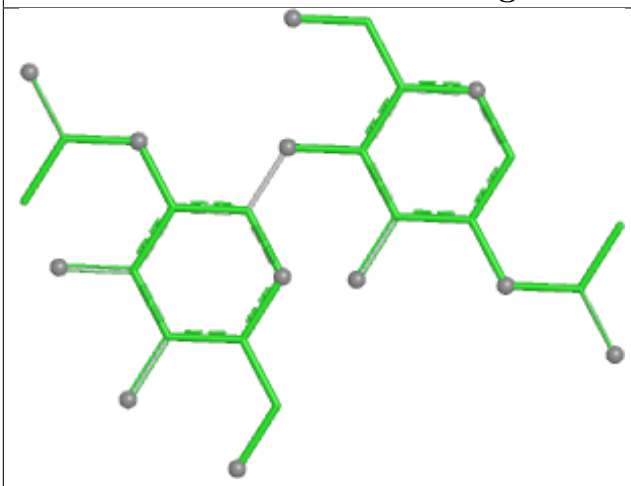


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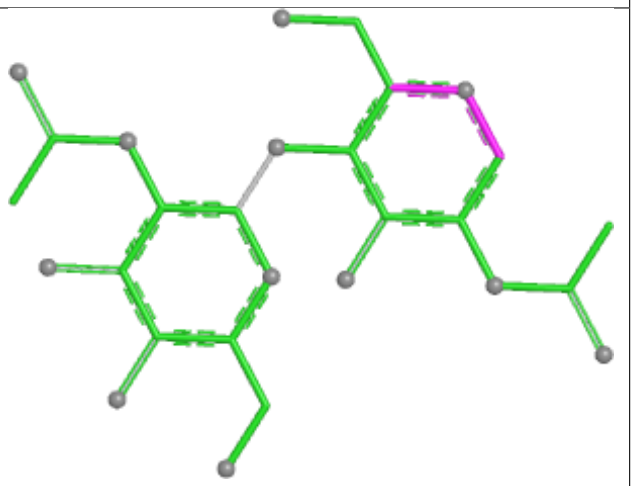


Rings

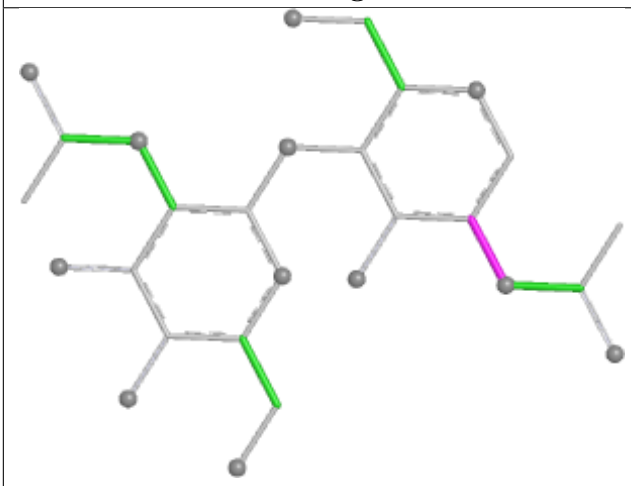
Oligosaccharide Chain 4



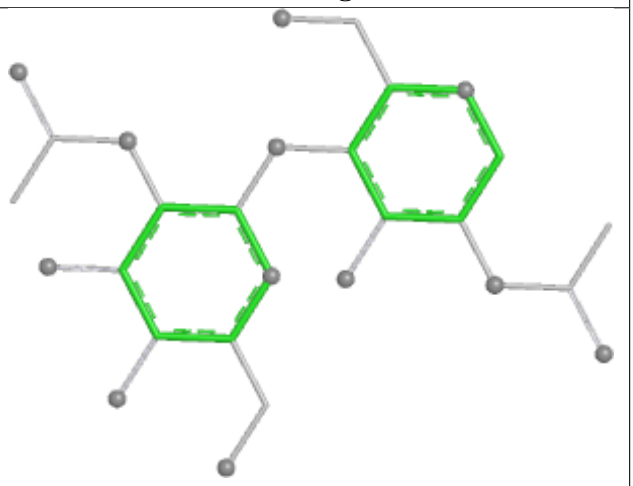
Bond lengths



Bond angles

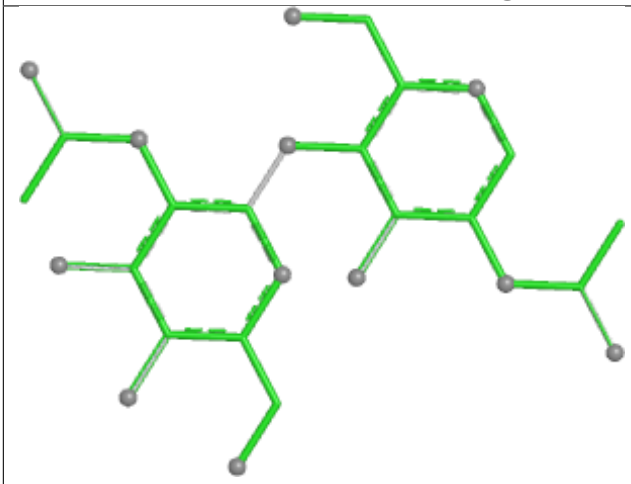


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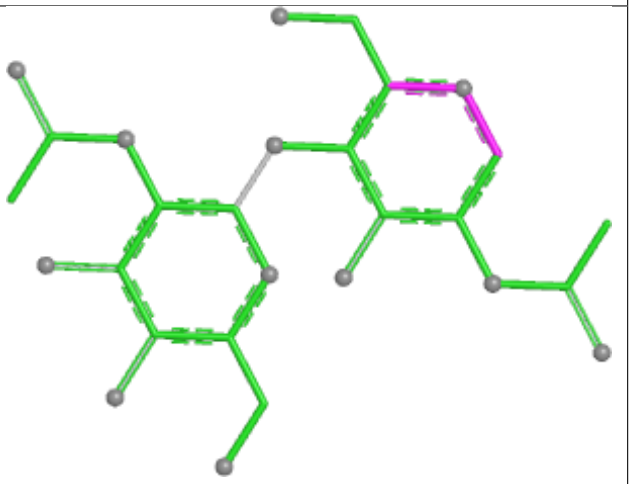


Rings

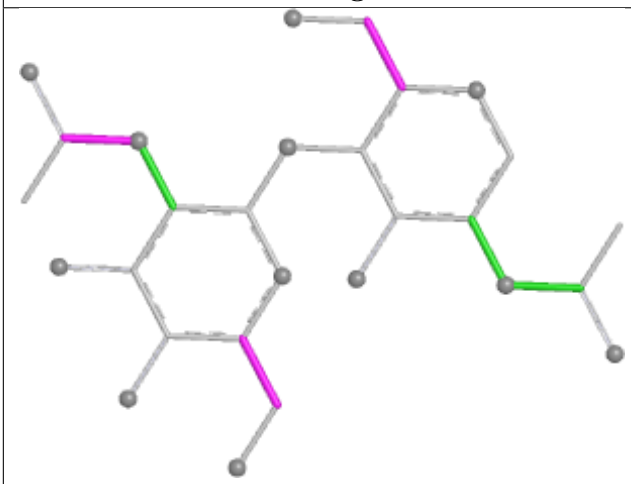
Oligosaccharide Chain 5



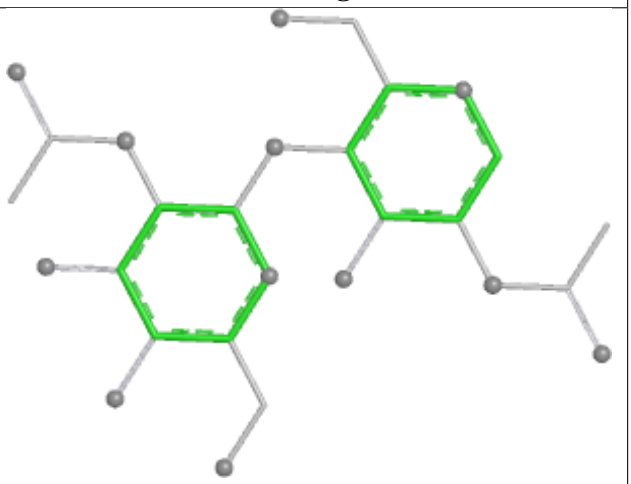
Bond lengths



Bond angles

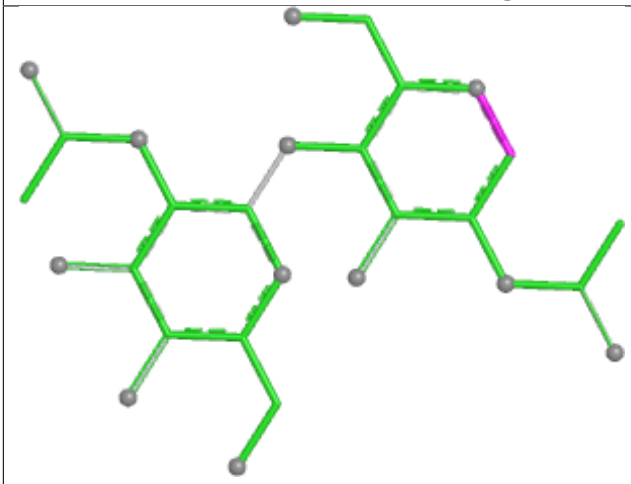


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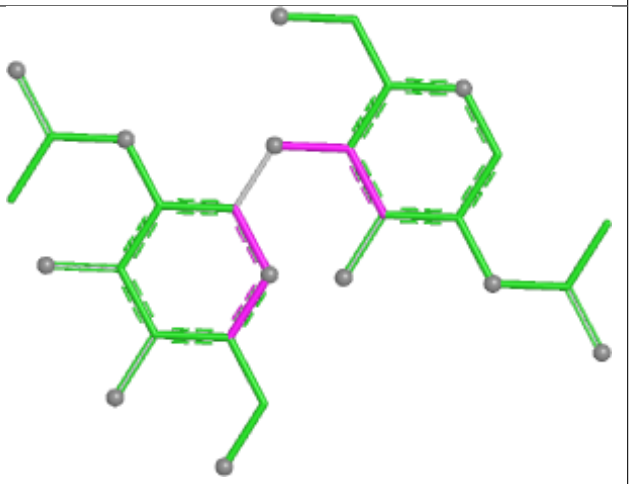


Rings

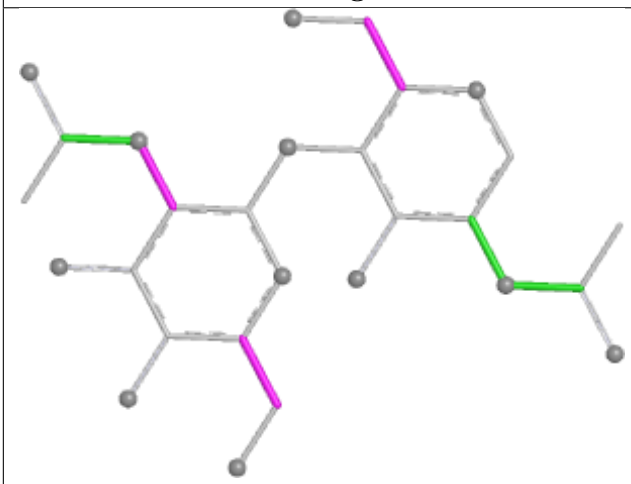
Oligosaccharide Chain 6



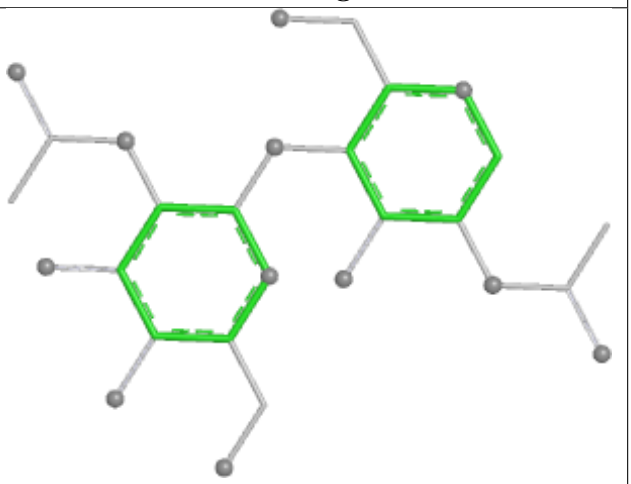
Bond lengths



Bond angles

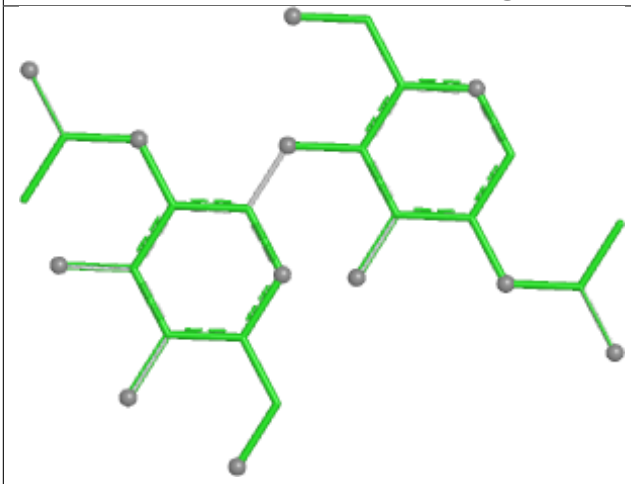


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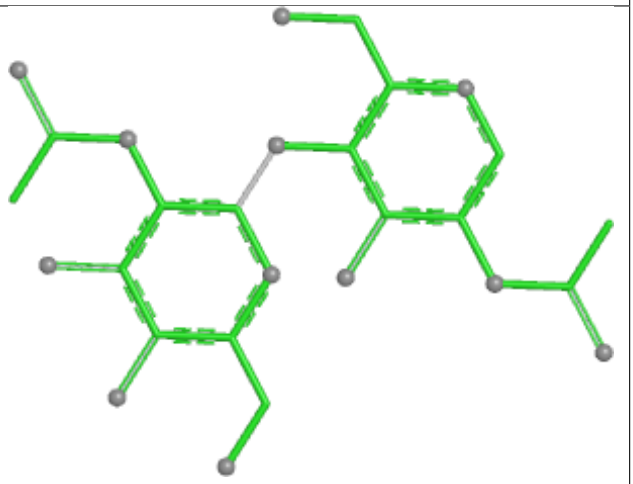


Rings

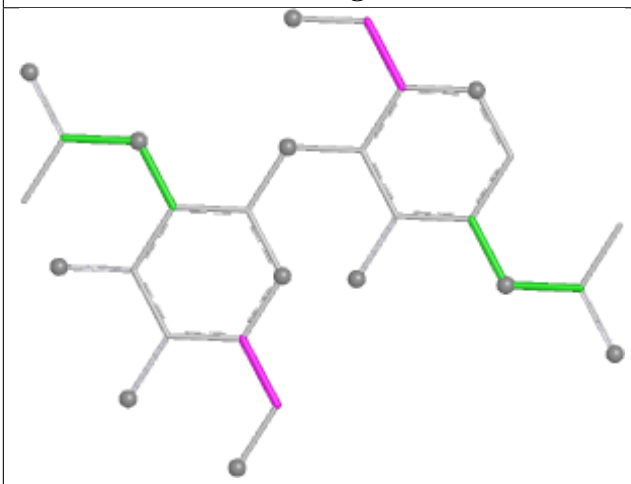
Oligosaccharide Chain 7



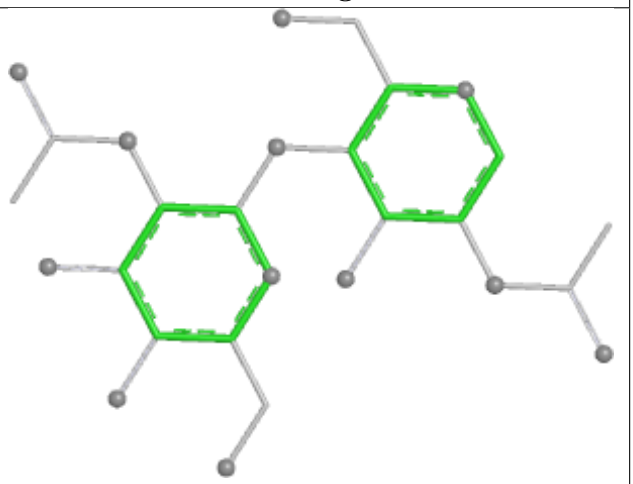
Bond lengths



Bond angles

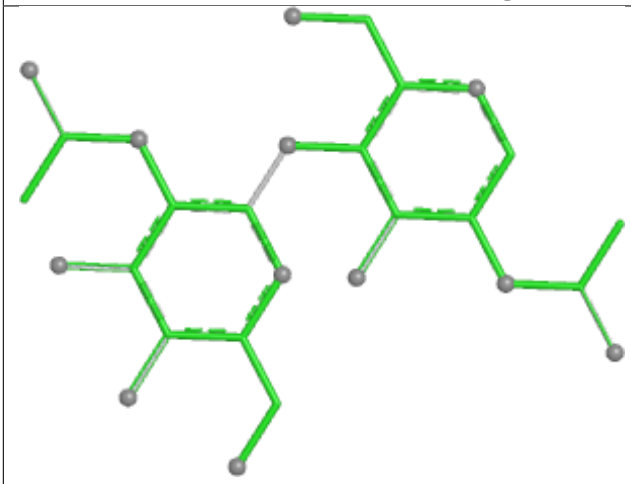


Torsions

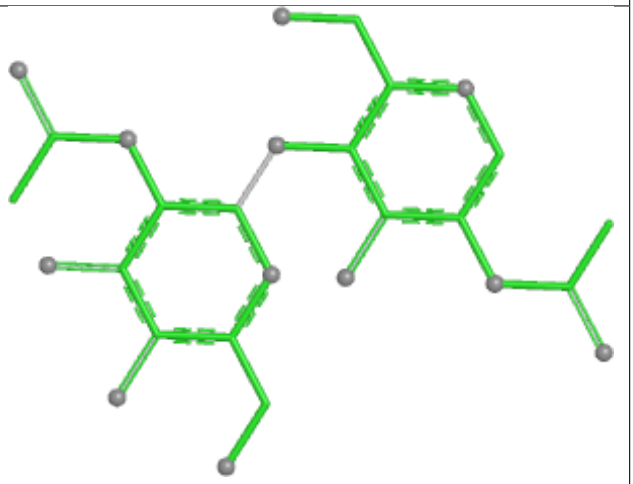


Rings

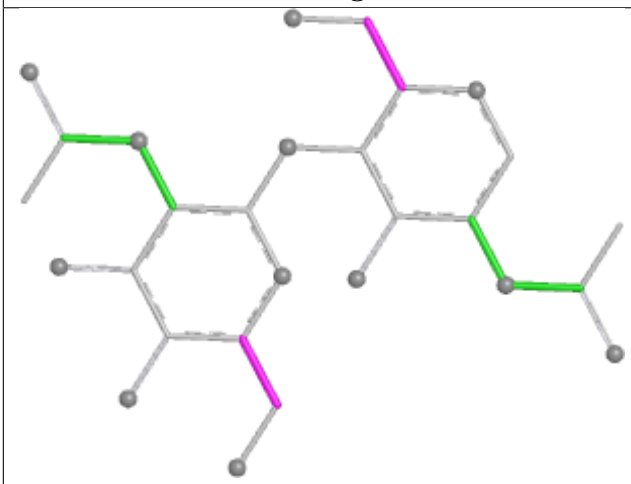
Oligosaccharide Chain 8



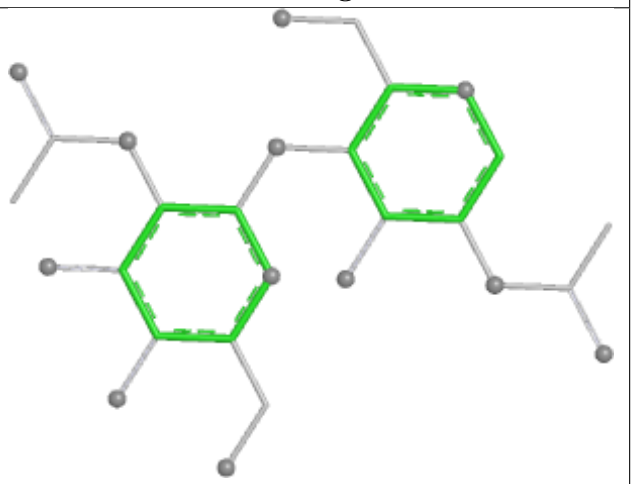
Bond lengths



Bond angles

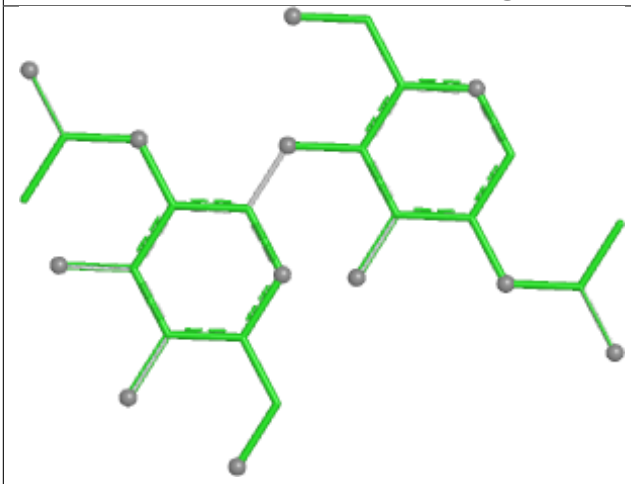


Torsions

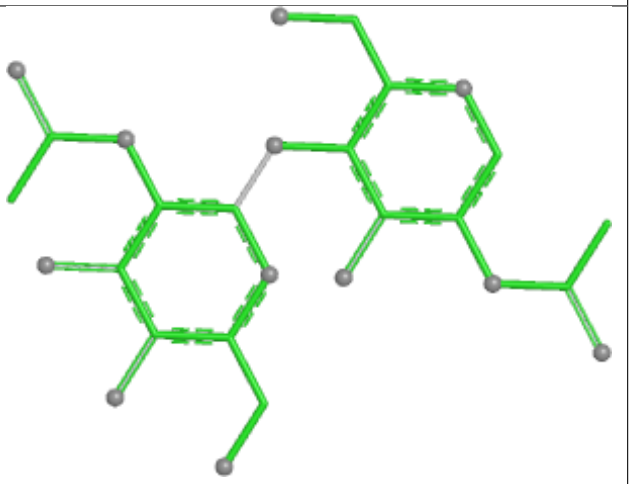


Rings

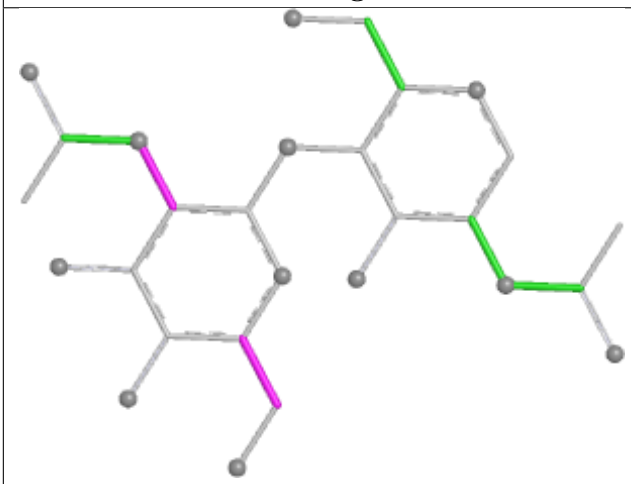
Oligosaccharide Chain 9



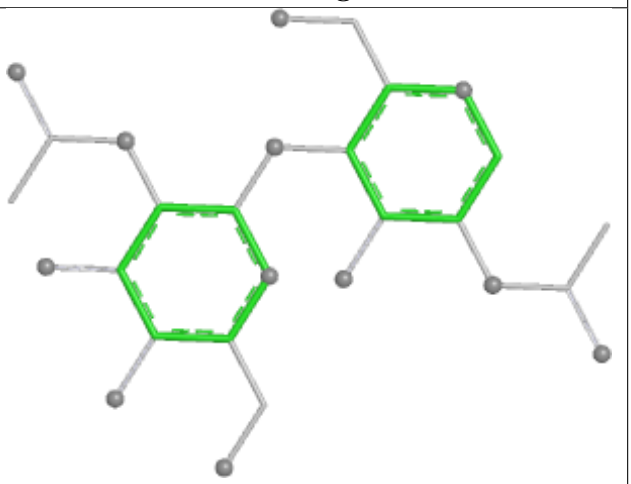
Bond lengths



Bond angles

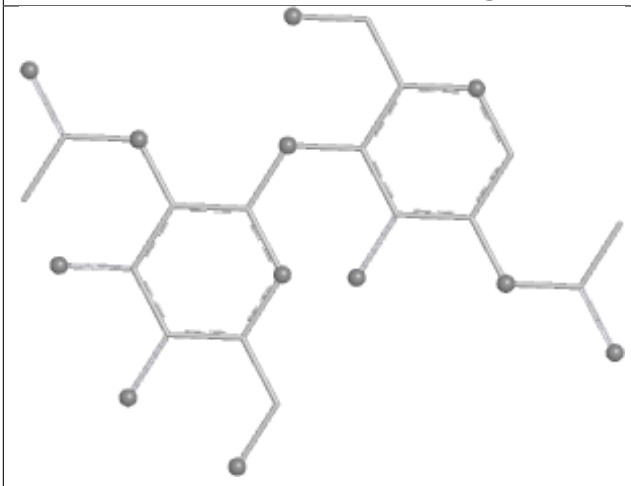


Torsions

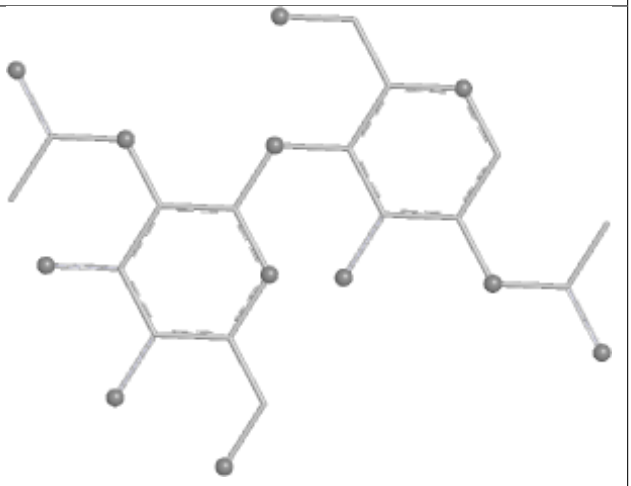


Rings

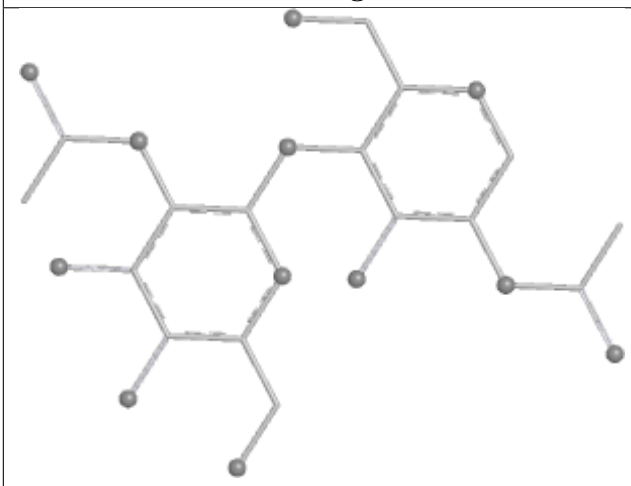
Oligosaccharide Chain AA



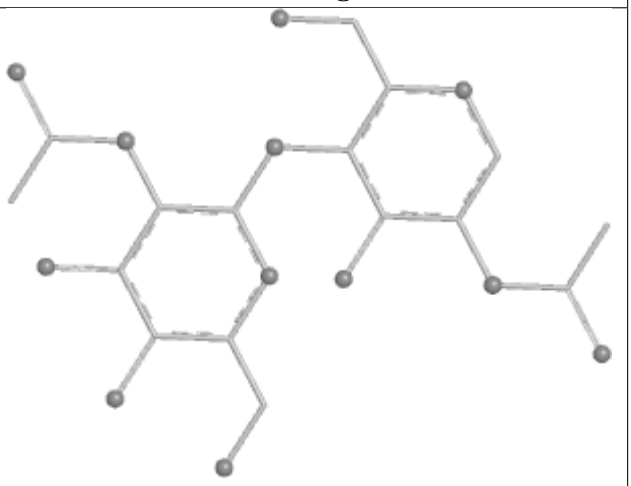
Bond lengths



Bond angles

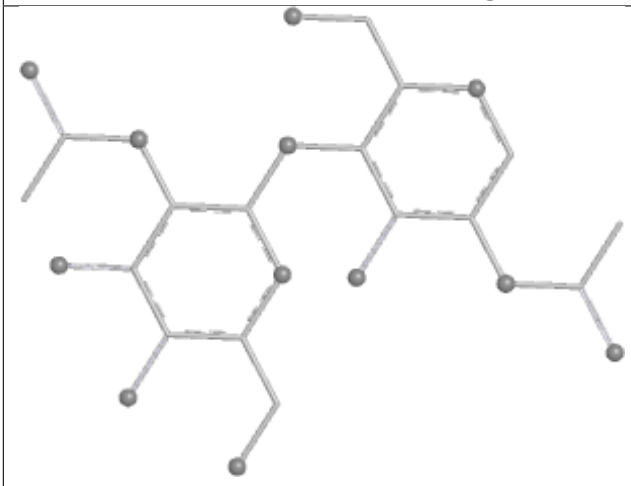


Torsions

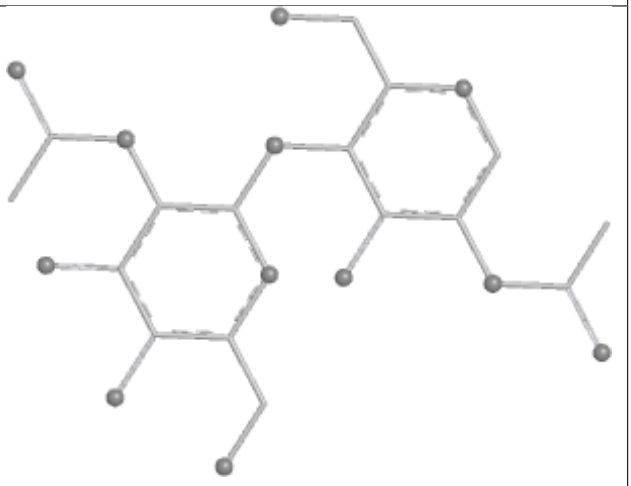


Rings

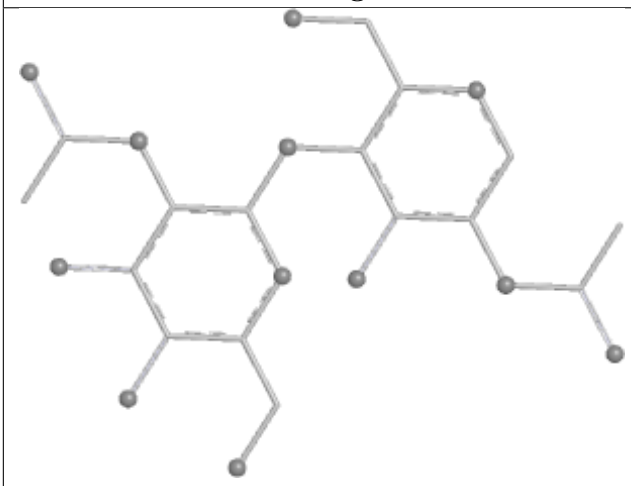
Oligosaccharide Chain BA



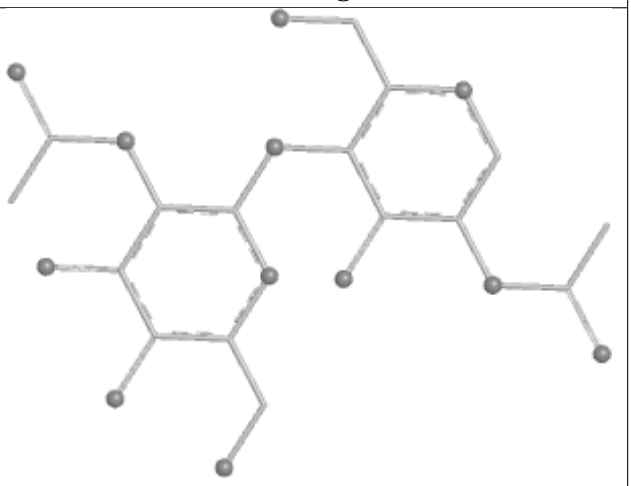
Bond lengths



Bond angles

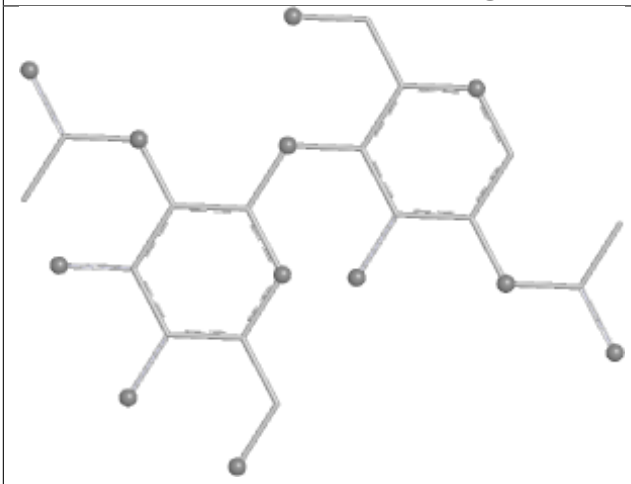


Torsions

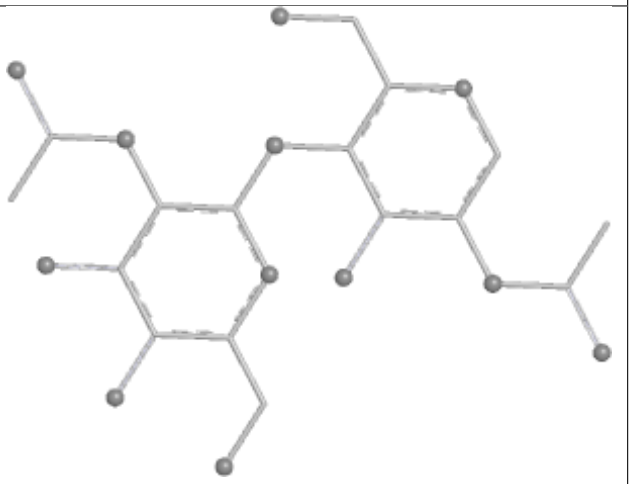


Rings

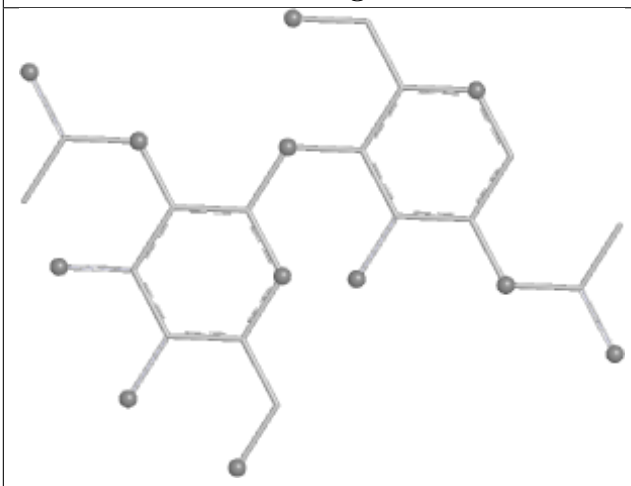
Oligosaccharide Chain CA



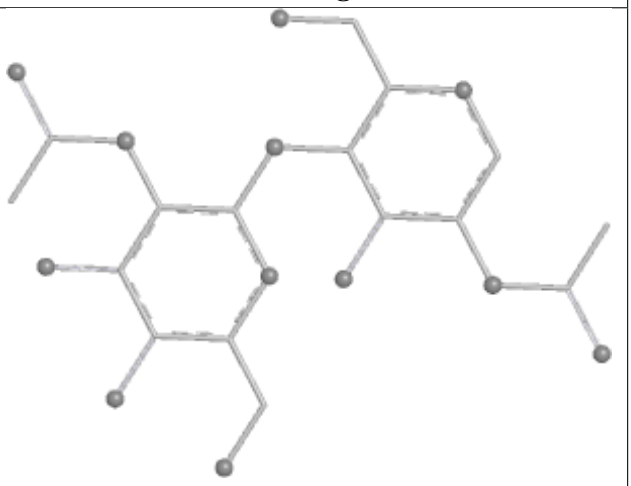
Bond lengths



Bond angles

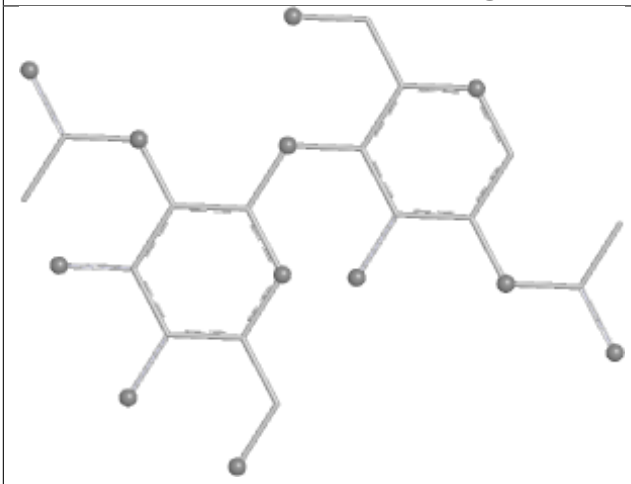


Torsions

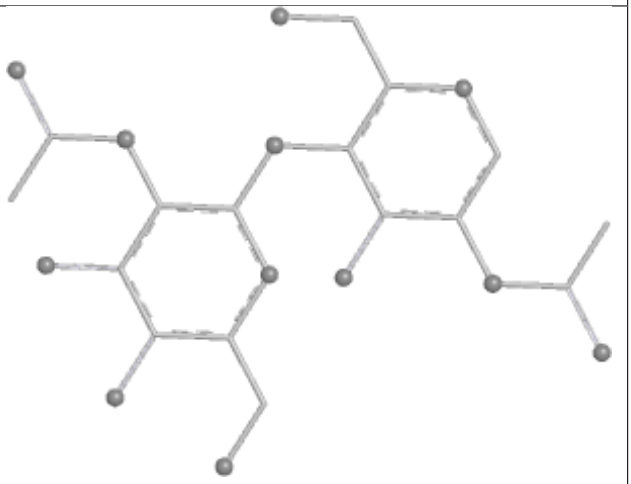


Rings

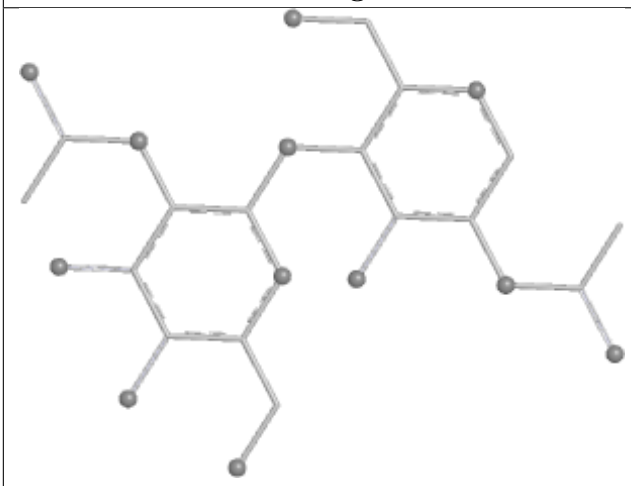
Oligosaccharide Chain DA



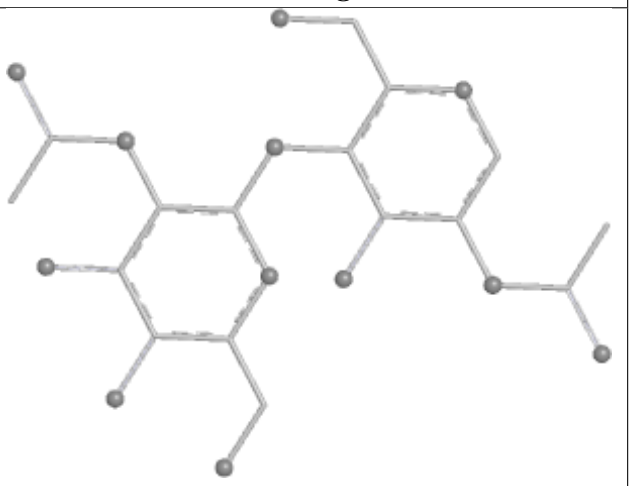
Bond lengths



Bond angles

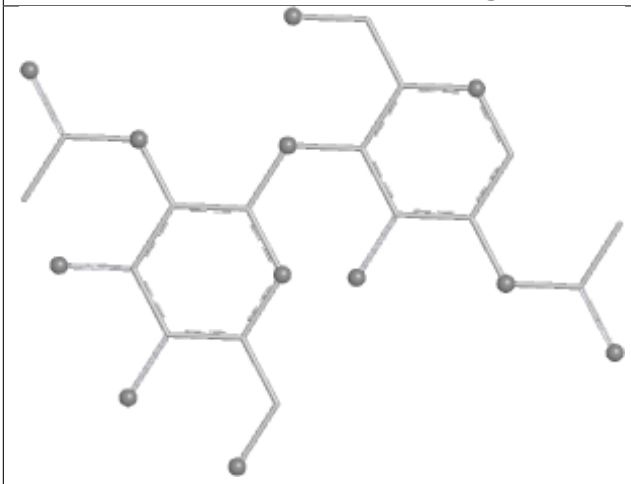


Torsions

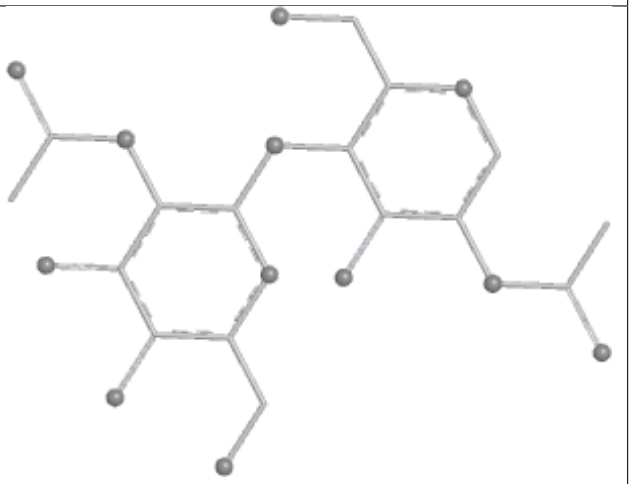


Rings

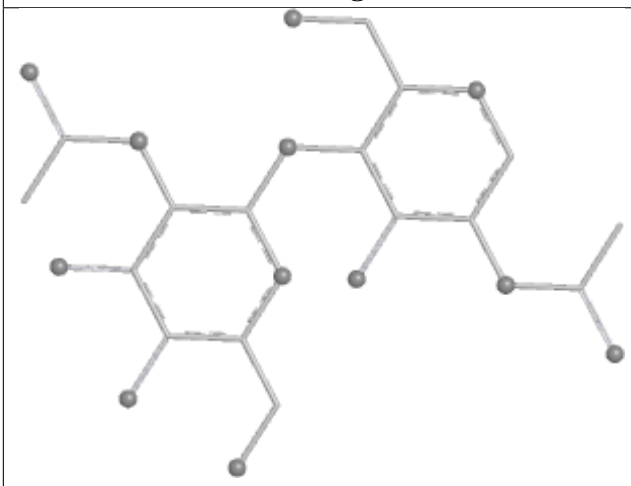
Oligosaccharide Chain EA



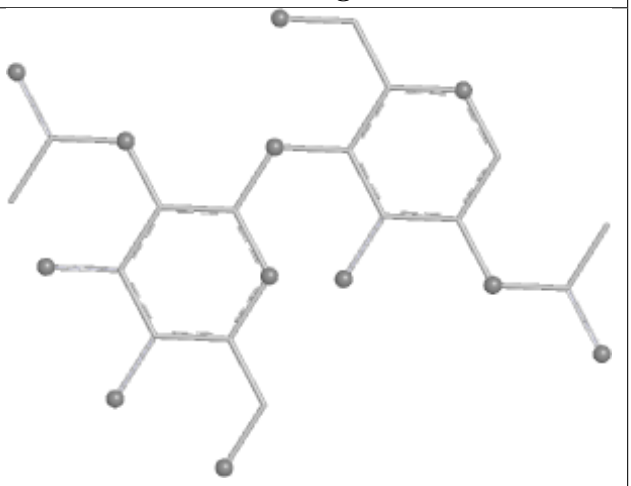
Bond lengths



Bond angles

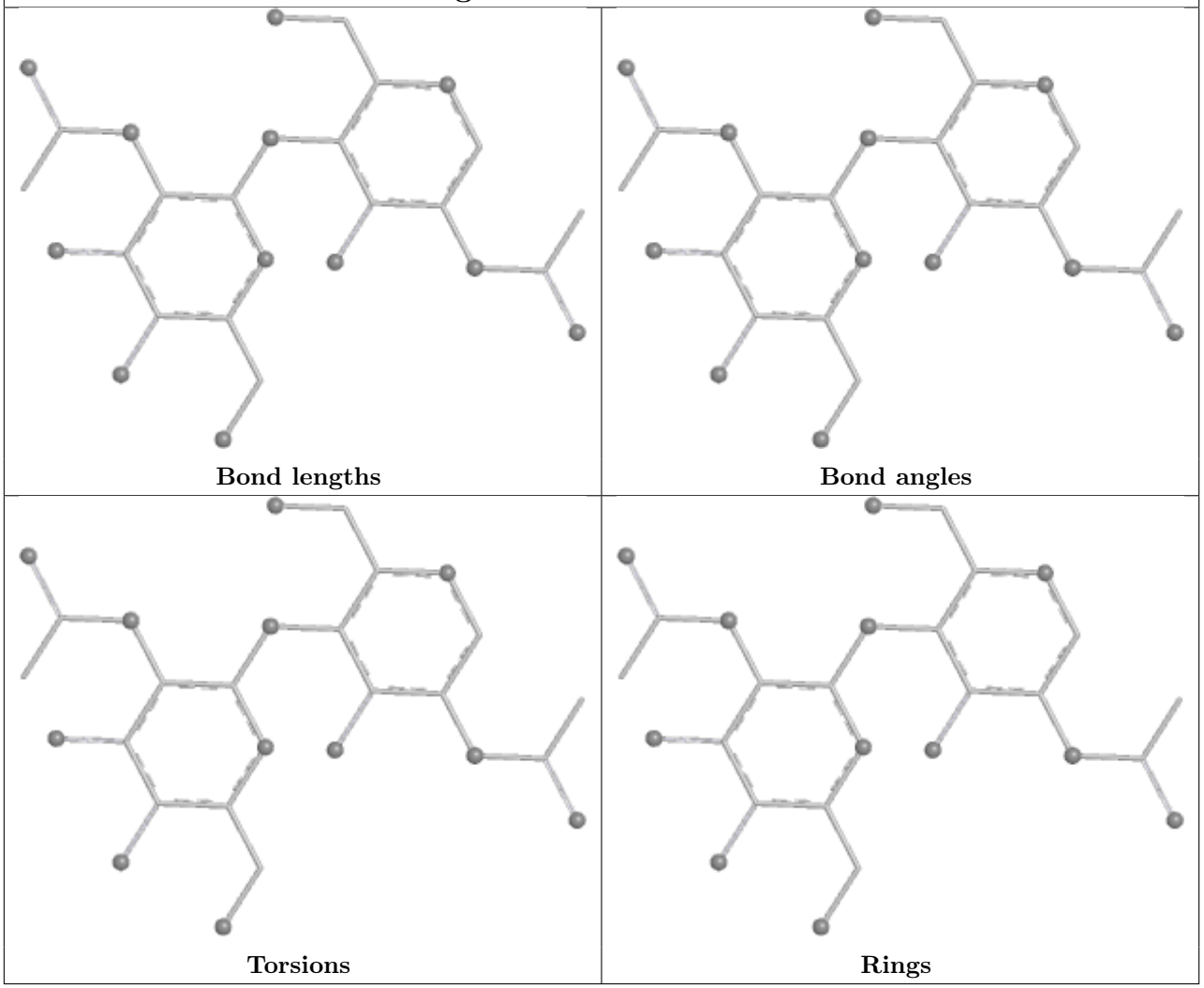


Torsions



Rings

Oligosaccharide Chain FA



5.6 Ligand geometry (i)

Of 68 ligands modelled in this entry, 2 are monoatomic - leaving 66 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	E	1403	3	14,14,15	0.18	0	17,19,21	0.44	0
5	NAG	G	1402	3	14,14,15	0.21	0	17,19,21	0.67	0
5	NAG	B	901	2	14,14,15	0.39	0	17,19,21	0.61	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	F	1407	3	14,14,15	0.26	0	17,19,21	0.52	0
5	NAG	E	1409	3	14,14,15	0.48	0	17,19,21	0.38	0
5	NAG	F	1402	3	14,14,15	0.22	0	17,19,21	0.66	0
5	NAG	I	1410	-	14,14,15	0.37	0	17,19,21	0.43	0
5	NAG	F	1405	3	14,14,15	0.60	0	17,19,21	1.34	2 (11%)
5	NAG	I	1404	3	14,14,15	0.50	0	17,19,21	0.54	0
5	NAG	H	1405	3	14,14,15	0.60	0	17,19,21	1.34	2 (11%)
5	NAG	E	1404	3	14,14,15	0.51	0	17,19,21	0.55	0
5	NAG	J	1404	3	14,14,15	0.51	0	17,19,21	0.55	0
5	NAG	G	1405	3	14,14,15	0.60	0	17,19,21	1.34	2 (11%)
5	NAG	I	1406	3	14,14,15	0.29	0	17,19,21	0.41	0
5	NAG	C	701	1	14,14,15	0.37	0	17,19,21	0.45	0
6	LEU	C	705	-	6,8,8	1.02	1 (16%)	5,10,10	1.27	1 (20%)
5	NAG	J	1401	3	14,14,15	0.32	0	17,19,21	0.34	0
5	NAG	G	1407	3	14,14,15	0.24	0	17,19,21	0.51	0
5	NAG	J	1406	3	14,14,15	0.29	0	17,19,21	0.40	0
5	NAG	G	1403	3	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	F	1406	3	14,14,15	0.30	0	17,19,21	0.41	0
5	NAG	H	1407	3	14,14,15	0.25	0	17,19,21	0.51	0
5	NAG	H	1406	3	14,14,15	0.28	0	17,19,21	0.40	0
5	NAG	I	1401	3	14,14,15	0.31	0	17,19,21	0.36	0
5	NAG	H	1409	3	14,14,15	0.48	0	17,19,21	0.38	0
5	NAG	F	1409	3	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
5	NAG	J	1403	3	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	J	1405	3	14,14,15	0.62	0	17,19,21	1.34	2 (11%)
5	NAG	C	702	1	14,14,15	0.36	0	17,19,21	0.42	0
5	NAG	I	1408	3	14,14,15	0.34	0	17,19,21	0.39	0
5	NAG	J	1408	3	14,14,15	0.33	0	17,19,21	0.40	0
5	NAG	E	1407	3	14,14,15	0.25	0	17,19,21	0.52	0
5	NAG	F	1403	3	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	H	1402	3	14,14,15	0.22	0	17,19,21	0.66	0
5	NAG	H	1401	3	14,14,15	0.32	0	17,19,21	0.35	0
5	NAG	A	701	1	14,14,15	0.36	0	17,19,21	0.45	0
5	NAG	E	1405	3	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
5	NAG	G	1406	3	14,14,15	0.27	0	17,19,21	0.40	0
5	NAG	A	702	1	14,14,15	0.37	0	17,19,21	0.42	0
5	NAG	H	1403	3	14,14,15	0.17	0	17,19,21	0.44	0
5	NAG	F	1401	3	14,14,15	0.32	0	17,19,21	0.35	0
5	NAG	D	901	2	14,14,15	0.39	0	17,19,21	0.61	1 (5%)
5	NAG	G	1401	3	14,14,15	0.30	0	17,19,21	0.34	0
5	NAG	F	1408	3	14,14,15	0.32	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	G	1408	3	14,14,15	0.33	0	17,19,21	0.41	0
5	NAG	I	1409	3	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
5	NAG	F	1404	3	14,14,15	0.51	0	17,19,21	0.55	0
5	NAG	H	1408	3	14,14,15	0.34	0	17,19,21	0.40	0
5	NAG	A	704	1	14,14,15	0.38	0	17,19,21	0.57	0
5	NAG	E	1408	3	14,14,15	0.34	0	17,19,21	0.40	0
5	NAG	A	703	1	14,14,15	0.41	0	17,19,21	0.67	1 (5%)
5	NAG	I	1403	3	14,14,15	0.20	0	17,19,21	0.45	0
5	NAG	F	1410	-	14,14,15	0.38	0	17,19,21	0.44	0
5	NAG	E	1401	3	14,14,15	0.31	0	17,19,21	0.36	0
5	NAG	E	1402	3	14,14,15	0.22	0	17,19,21	0.66	0
5	NAG	E	1406	3	14,14,15	0.28	0	17,19,21	0.40	0
5	NAG	G	1404	3	14,14,15	0.50	0	17,19,21	0.55	0
5	NAG	I	1402	3	14,14,15	0.21	0	17,19,21	0.66	0
5	NAG	I	1407	3	14,14,15	0.28	0	17,19,21	0.52	0
5	NAG	J	1402	3	14,14,15	0.20	0	17,19,21	0.66	0
5	NAG	H	1404	3	14,14,15	0.50	0	17,19,21	0.54	0
5	NAG	I	1405	3	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
5	NAG	J	1407	3	14,14,15	0.24	0	17,19,21	0.52	0
6	LEU	A	705	-	6,8,8	1.03	1 (16%)	5,10,10	1.27	1 (20%)
5	NAG	C	704	1	14,14,15	0.38	0	17,19,21	0.57	0
5	NAG	C	703	1	14,14,15	0.40	0	17,19,21	0.66	1 (5%)

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
5	NAG	E	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	B	901	2	-	2/6/23/26	0/1/1/1
5	NAG	F	1407	3	-	0/6/23/26	0/1/1/1
5	NAG	E	1409	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	I	1410	-	-	0/6/23/26	0/1/1/1
5	NAG	F	1405	3	-	6/6/23/26	0/1/1/1
5	NAG	I	1404	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1405	3	-	6/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1404	3	-	2/6/23/26	0/1/1/1
5	NAG	J	1404	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1405	3	-	6/6/23/26	0/1/1/1
5	NAG	I	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	C	701	1	-	2/6/23/26	0/1/1/1
6	LEU	C	705	-	-	2/8/8/8	-
5	NAG	J	1401	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1407	3	-	0/6/23/26	0/1/1/1
5	NAG	J	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1407	3	-	0/6/23/26	0/1/1/1
5	NAG	H	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	I	1401	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1409	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1409	3	-	0/6/23/26	0/1/1/1
5	NAG	J	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	J	1405	3	-	6/6/23/26	0/1/1/1
5	NAG	C	702	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1408	3	-	2/6/23/26	0/1/1/1
5	NAG	J	1408	3	-	2/6/23/26	0/1/1/1
5	NAG	E	1407	3	-	0/6/23/26	0/1/1/1
5	NAG	F	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1401	3	-	2/6/23/26	0/1/1/1
5	NAG	A	701	1	-	2/6/23/26	0/1/1/1
5	NAG	E	1405	3	-	6/6/23/26	0/1/1/1
5	NAG	G	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	A	702	1	-	2/6/23/26	0/1/1/1
5	NAG	H	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1401	3	-	2/6/23/26	0/1/1/1
5	NAG	D	901	2	-	2/6/23/26	0/1/1/1
5	NAG	G	1401	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1408	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1408	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1409	3	-	0/6/23/26	0/1/1/1
5	NAG	F	1404	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1408	3	-	2/6/23/26	0/1/1/1
5	NAG	A	704	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1408	3	-	2/6/23/26	0/1/1/1
5	NAG	A	703	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1410	-	-	0/6/23/26	0/1/1/1
5	NAG	E	1401	3	-	2/6/23/26	0/1/1/1
5	NAG	E	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	E	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1404	3	-	2/6/23/26	0/1/1/1
5	NAG	I	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	I	1407	3	-	0/6/23/26	0/1/1/1
5	NAG	J	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1404	3	-	2/6/23/26	0/1/1/1
5	NAG	I	1405	3	-	6/6/23/26	0/1/1/1
5	NAG	J	1407	3	-	0/6/23/26	0/1/1/1
6	LEU	A	705	-	-	2/8/8/8	-
5	NAG	C	704	1	-	0/6/23/26	0/1/1/1
5	NAG	C	703	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	705	LEU	OXT-C	-2.41	1.23	1.30
6	C	705	LEU	OXT-C	-2.38	1.23	1.30

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1405	NAG	C2-N2-C7	4.62	129.09	122.90
5	I	1405	NAG	C2-N2-C7	4.61	129.08	122.90
5	H	1405	NAG	C2-N2-C7	4.61	129.07	122.90
5	G	1405	NAG	C2-N2-C7	4.59	129.05	122.90
5	F	1405	NAG	C2-N2-C7	4.59	129.04	122.90

There are no chirality outliers.

5 of 132 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	705	LEU	N-CA-CB-CG
6	C	705	LEU	N-CA-CB-CG
5	A	701	NAG	O5-C5-C6-O6
5	C	701	NAG	O5-C5-C6-O6
5	E	1406	NAG	O5-C5-C6-O6

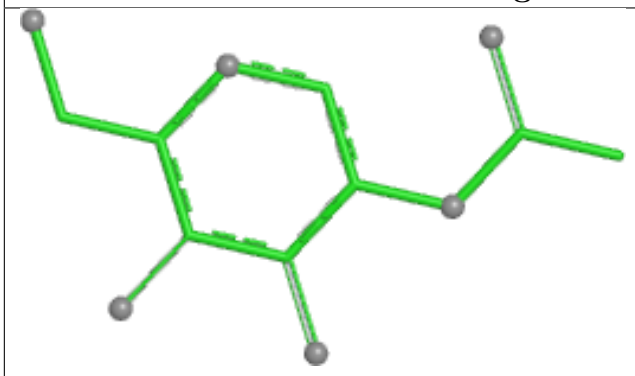
There are no ring outliers.

16 monomers are involved in 42 short contacts:

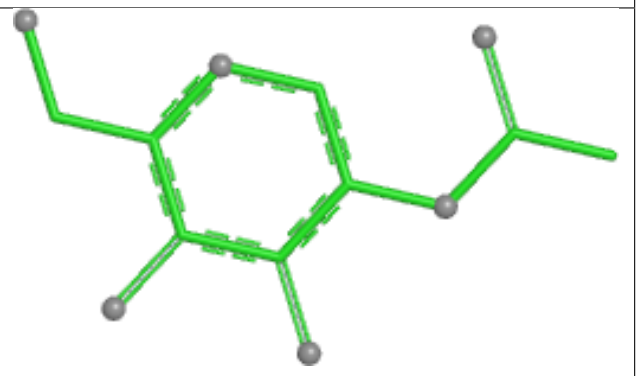
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1402	NAG	3	0
5	F	1402	NAG	3	0
5	I	1410	NAG	4	0
5	F	1405	NAG	1	0
5	H	1405	NAG	2	0
5	G	1405	NAG	5	0
5	F	1409	NAG	4	0
5	J	1405	NAG	5	0
5	H	1402	NAG	3	0
5	E	1405	NAG	2	0
5	I	1409	NAG	4	0
5	F	1410	NAG	4	0
5	E	1402	NAG	3	0
5	I	1402	NAG	3	0
5	J	1402	NAG	3	0
5	I	1405	NAG	1	0

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

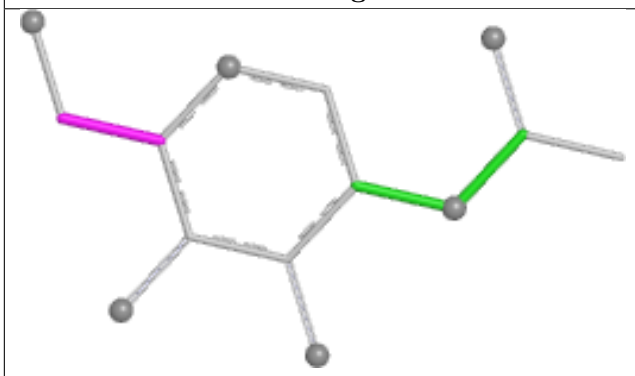
Ligand NAG E 1403



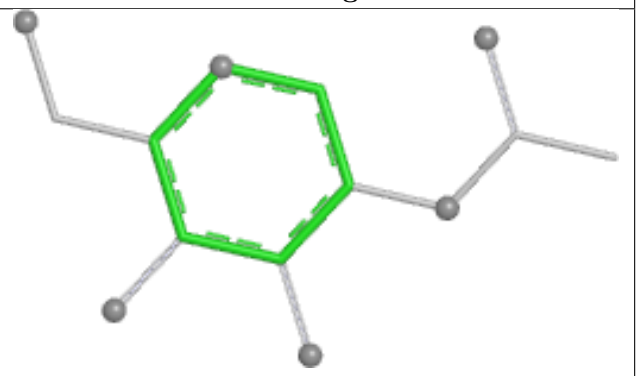
Bond lengths



Bond angles

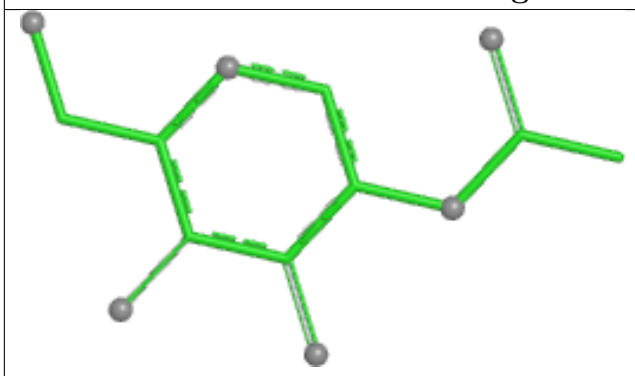


Torsions

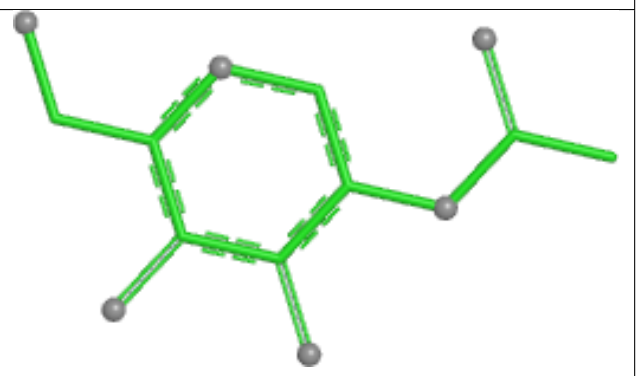


Rings

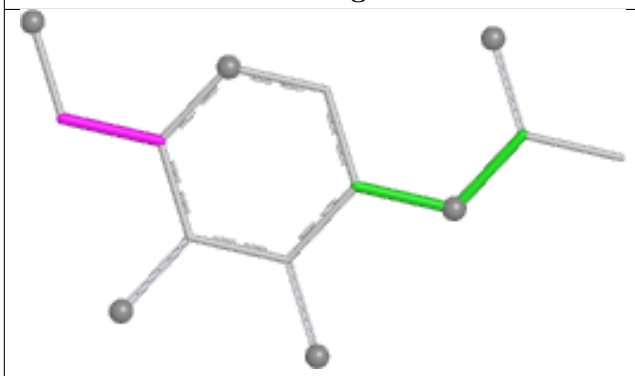
Ligand NAG G 1402



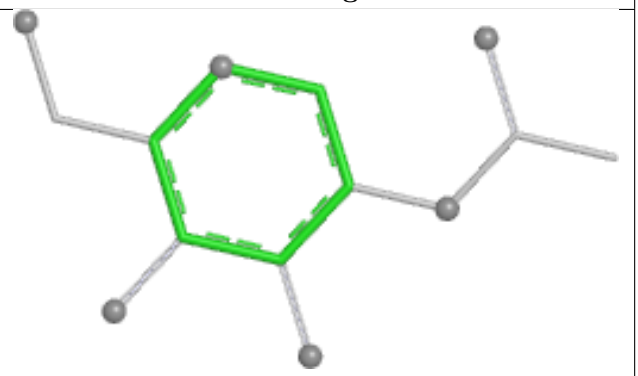
Bond lengths



Bond angles

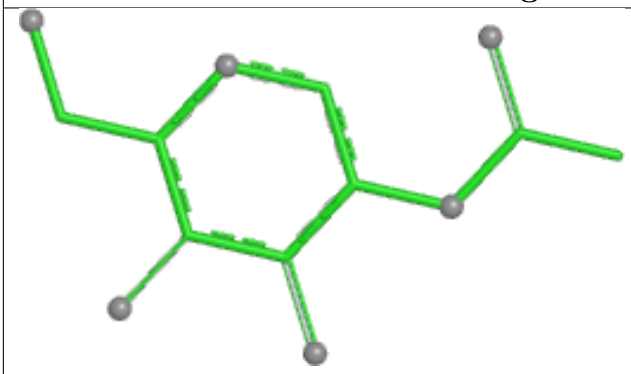


Torsions

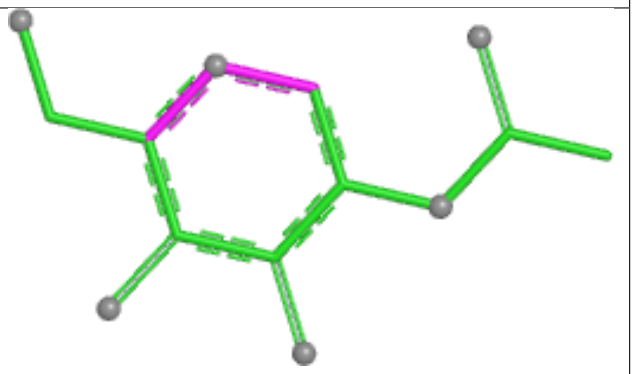


Rings

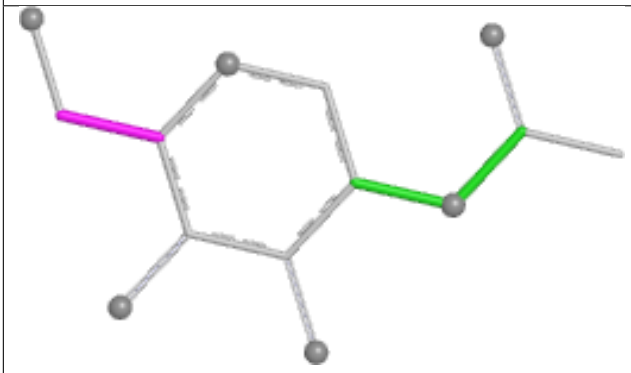
Ligand NAG B 901



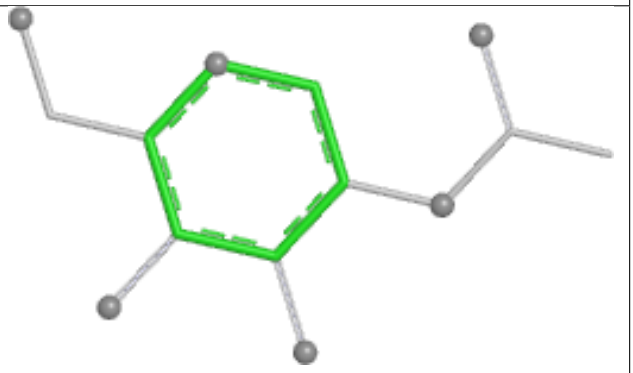
Bond lengths



Bond angles

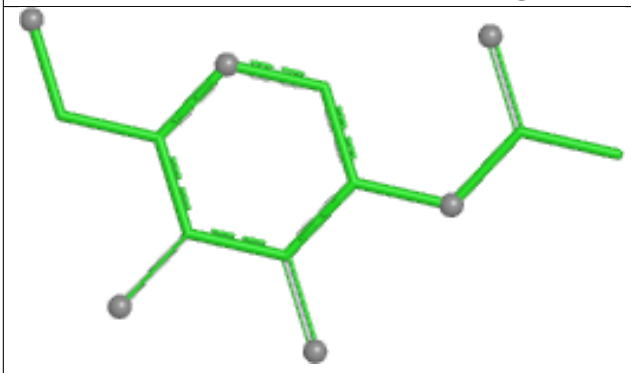


Torsions

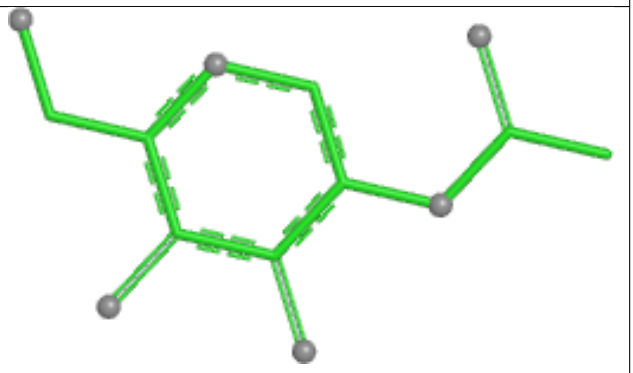


Rings

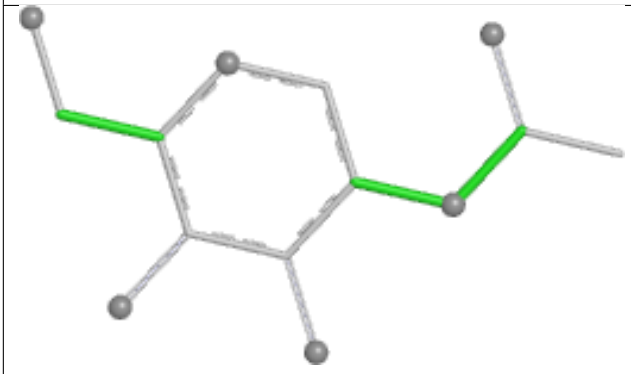
Ligand NAG F 1407



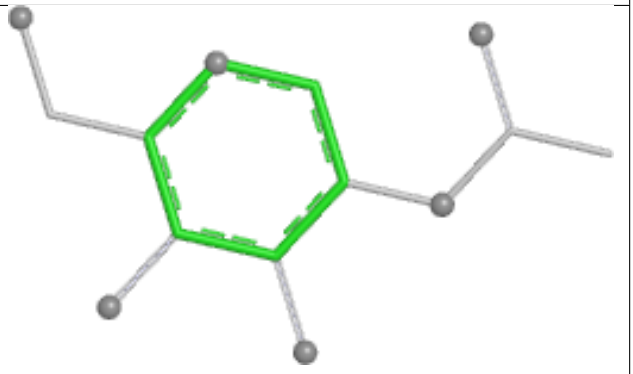
Bond lengths



Bond angles

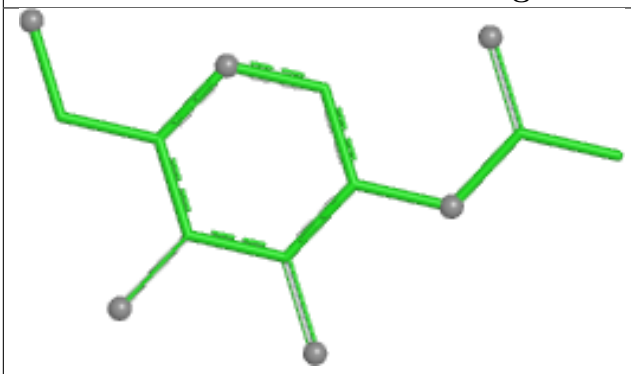


Torsions

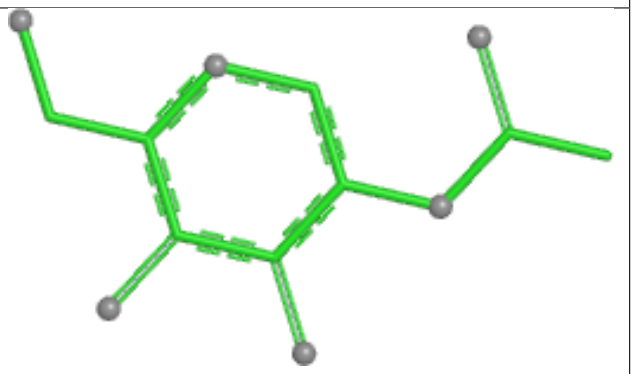


Rings

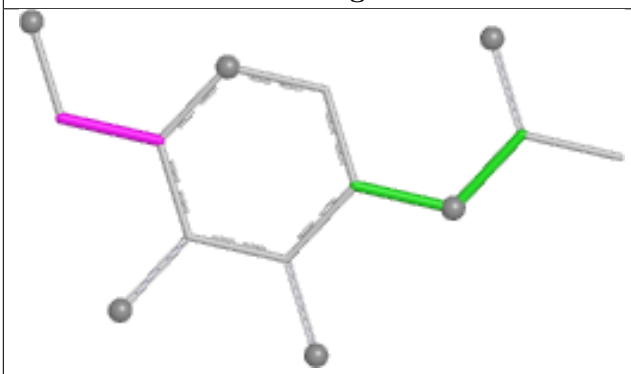
Ligand NAG E 1409



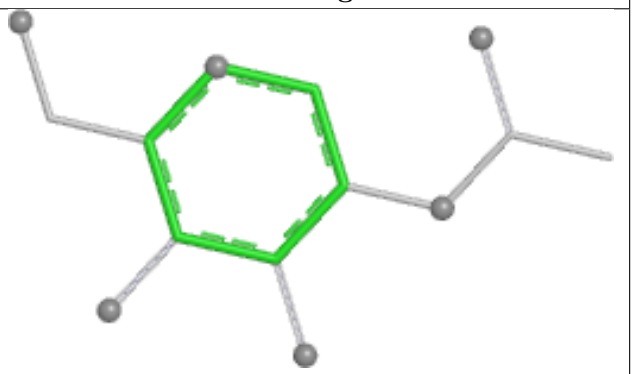
Bond lengths



Bond angles

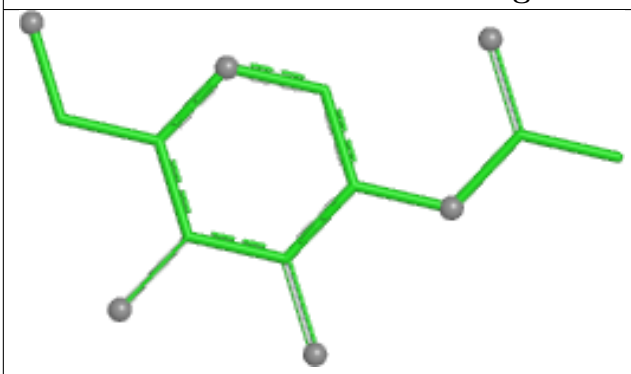


Torsions

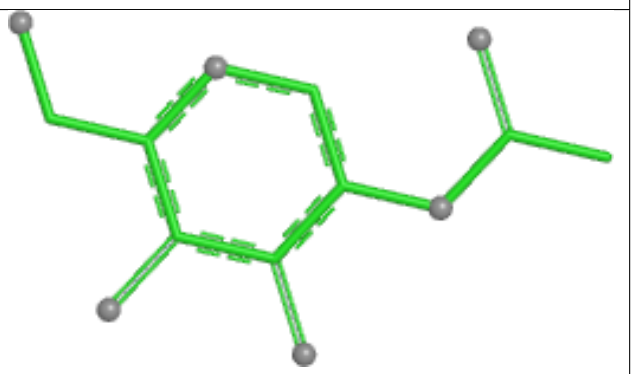


Rings

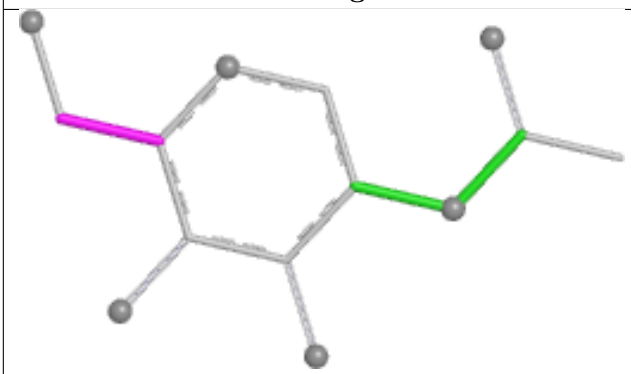
Ligand NAG F 1402



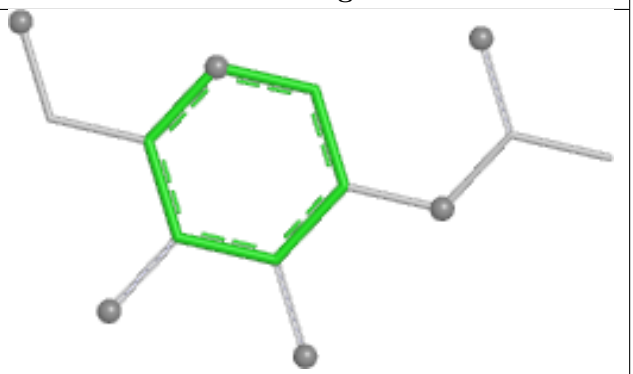
Bond lengths



Bond angles

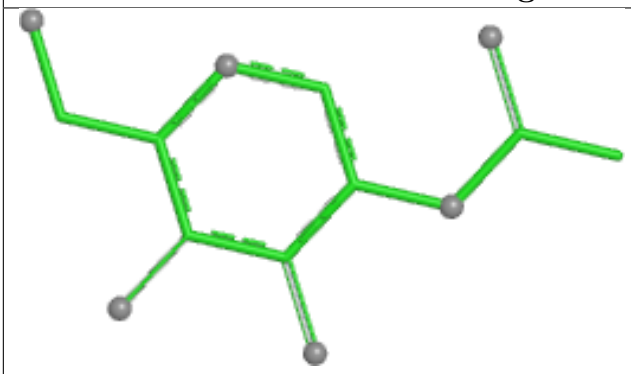


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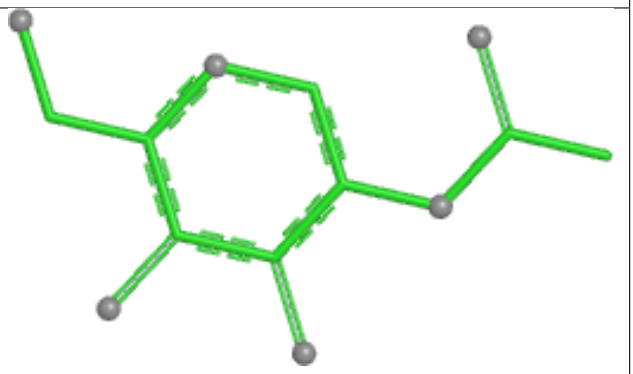


Rings

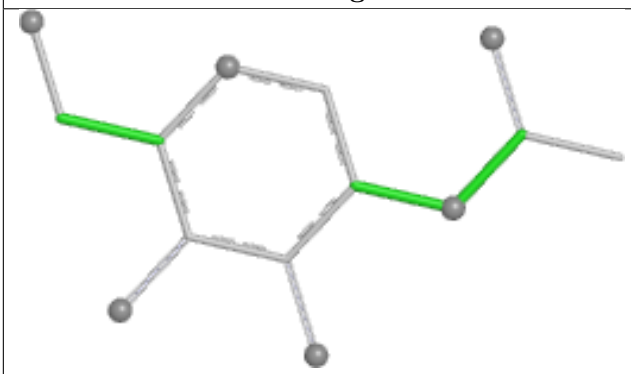
Ligand NAG I 1410



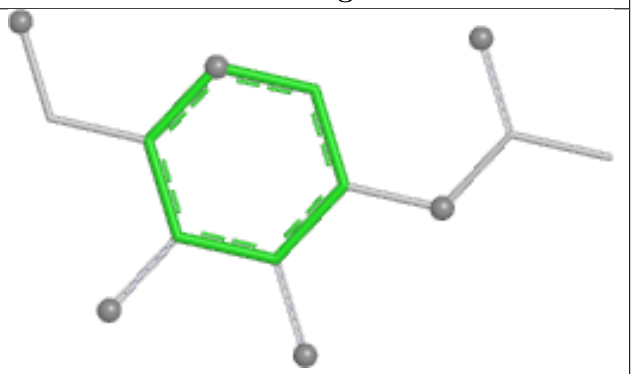
Bond lengths



Bond angles

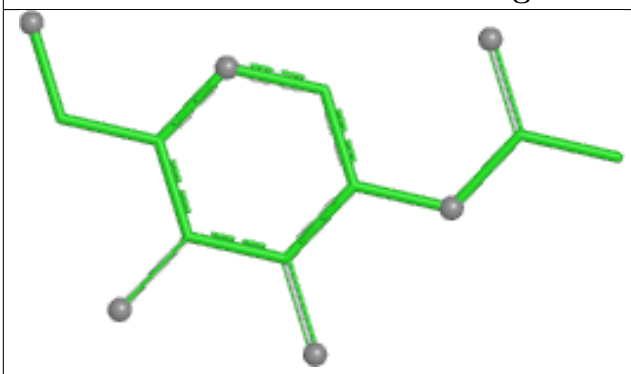


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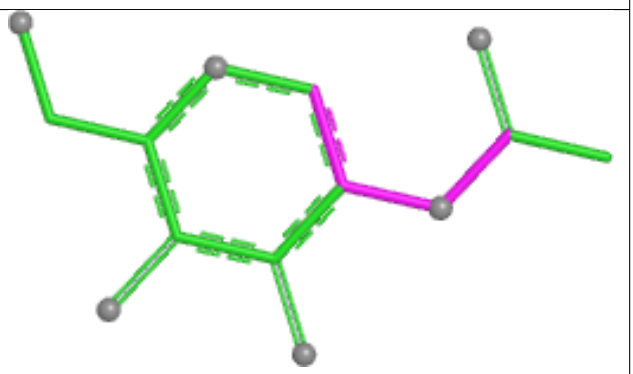


Rings

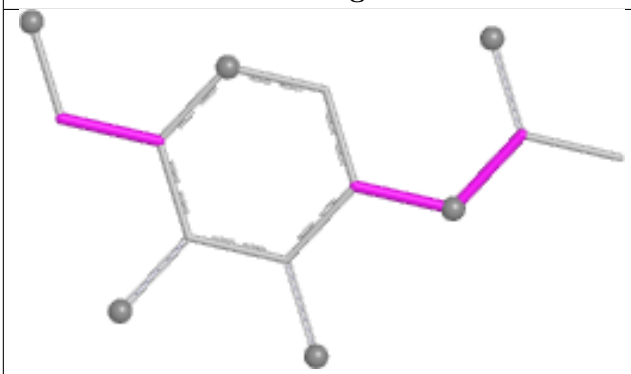
Ligand NAG F 1405



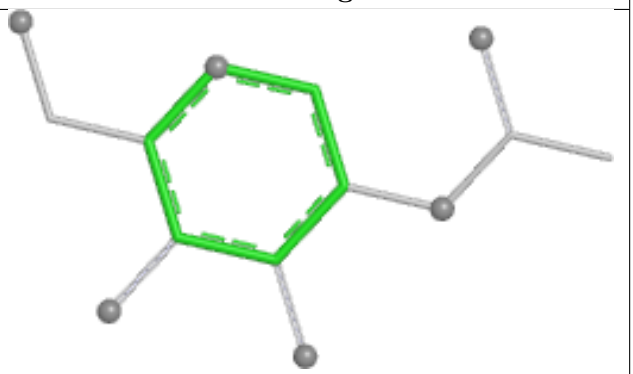
Bond lengths



Bond angles

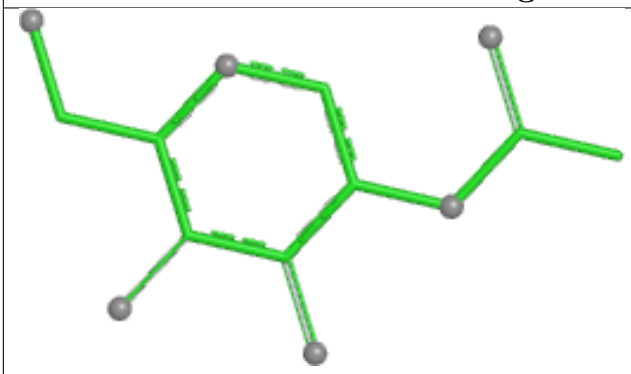


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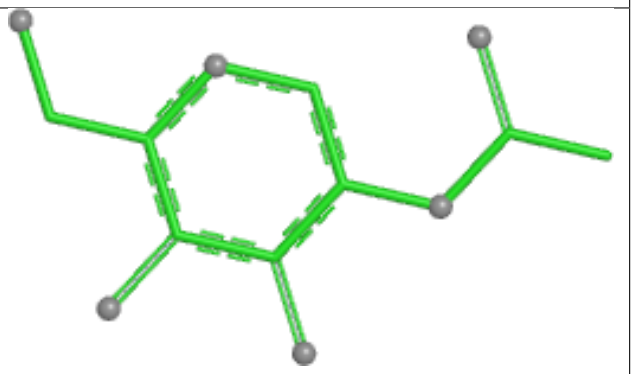


Rings

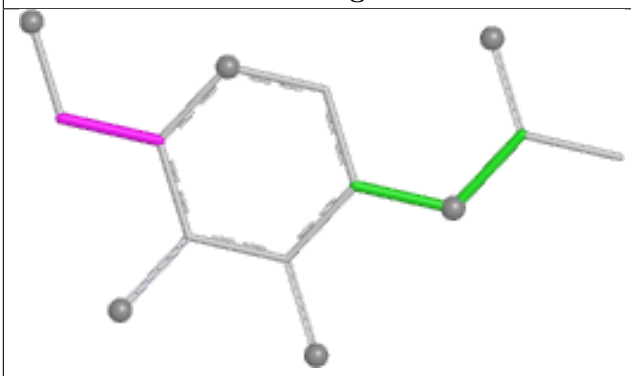
Ligand NAG I 1404



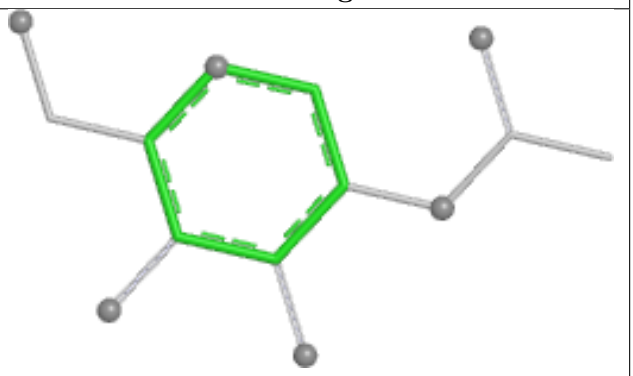
Bond lengths



Bond angles

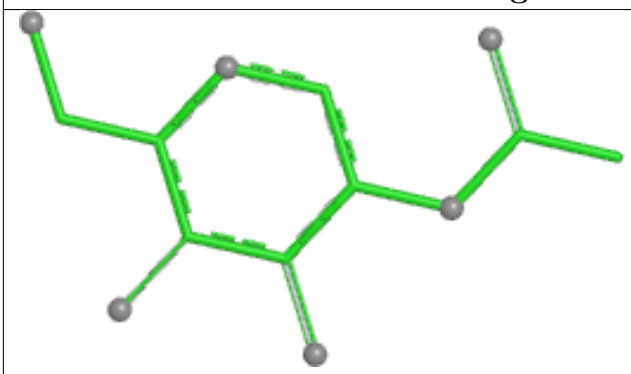


Torsions

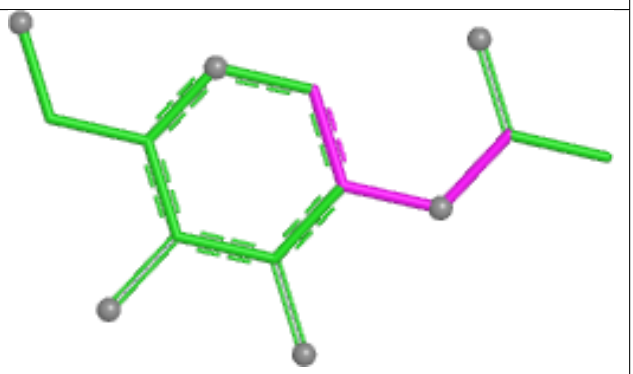


Rings

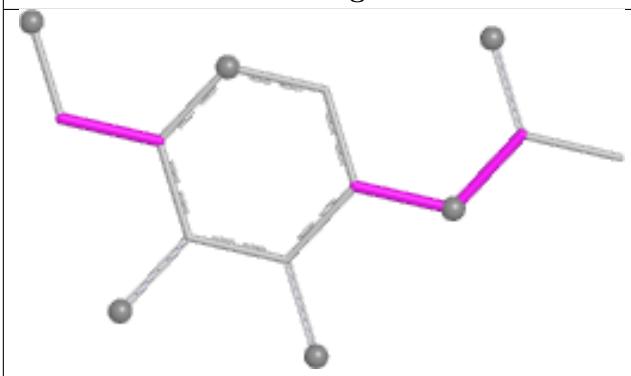
Ligand NAG H 1405



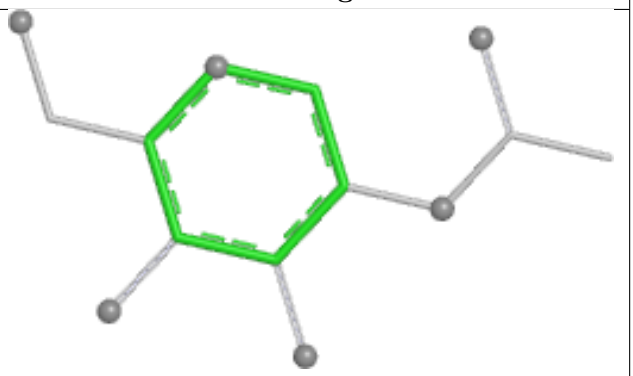
Bond lengths



Bond angles

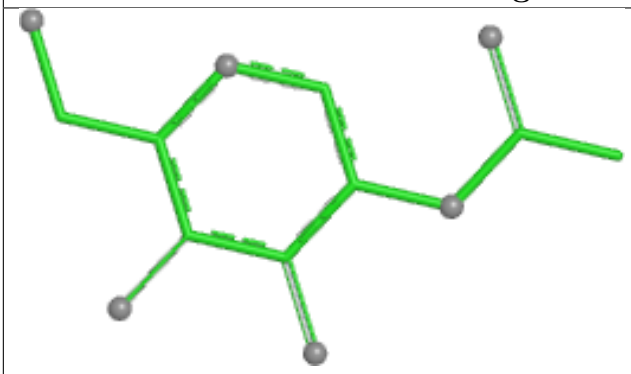


Torsions

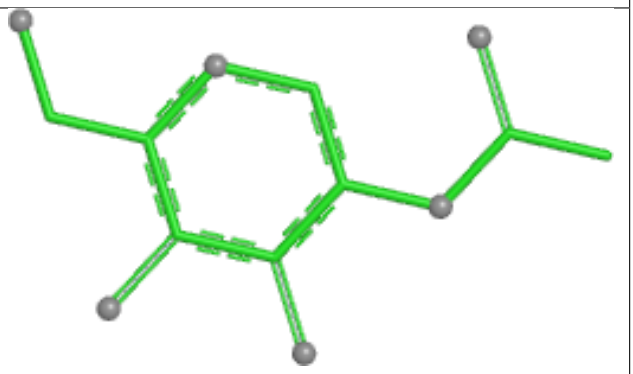


Rings

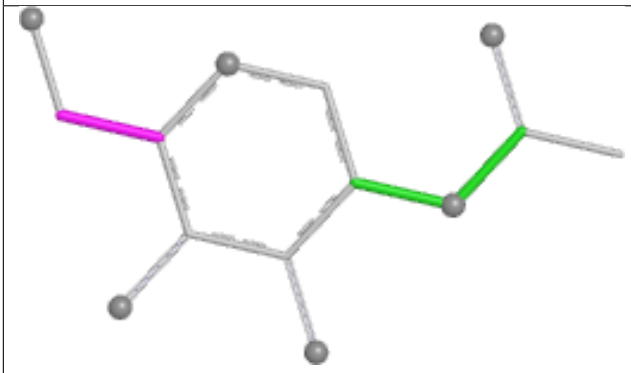
Ligand NAG E 1404



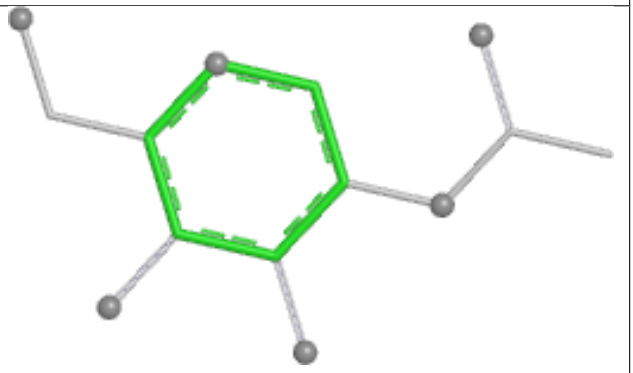
Bond lengths



Bond angles

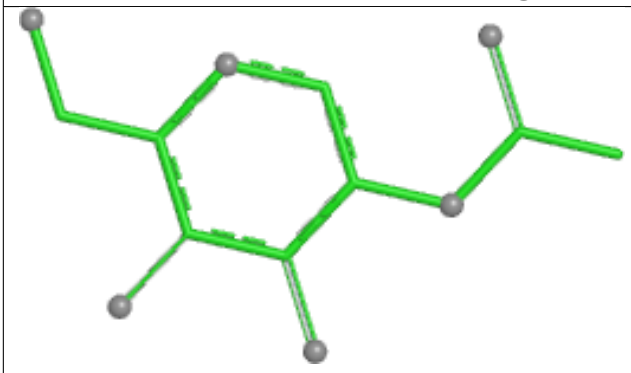


Torsions

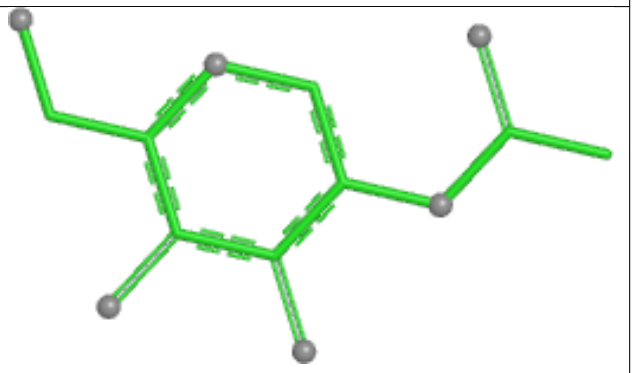


Rings

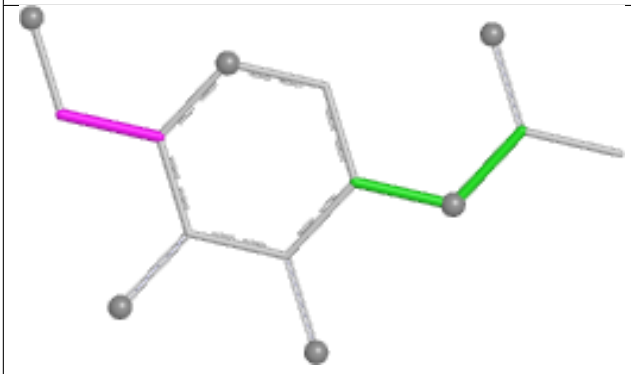
Ligand NAG J 1404



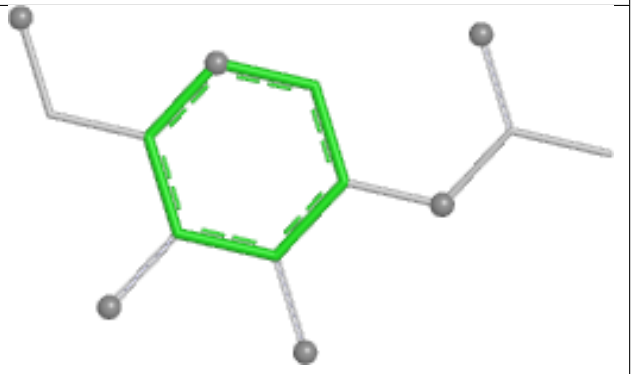
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Bond angles

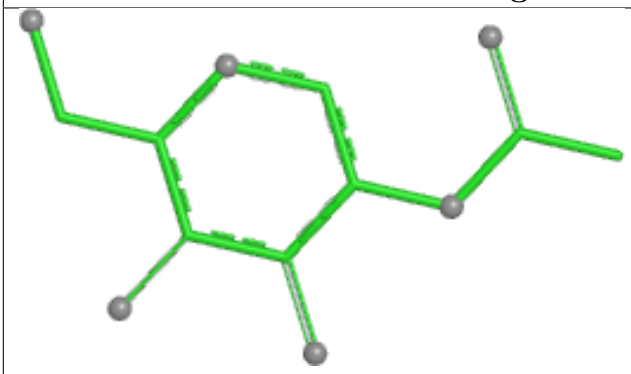


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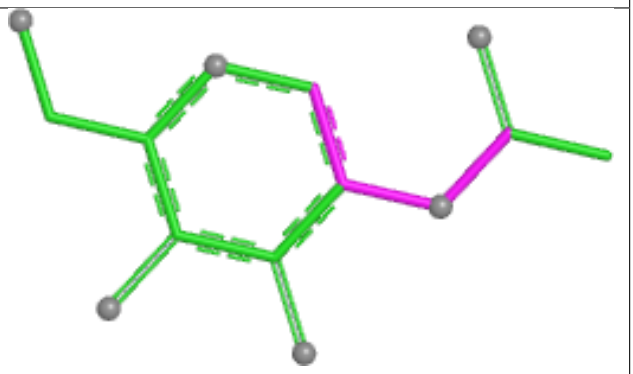


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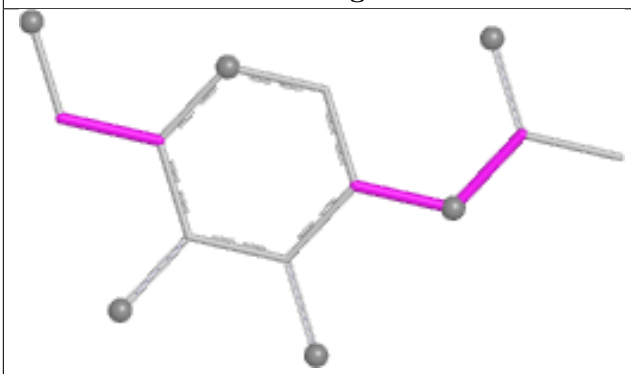
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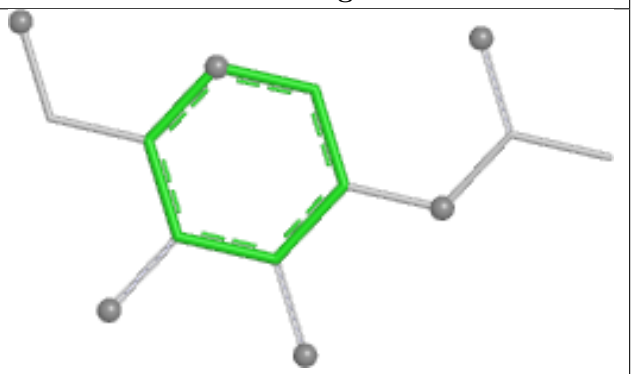
Bond lengths



Bond angles

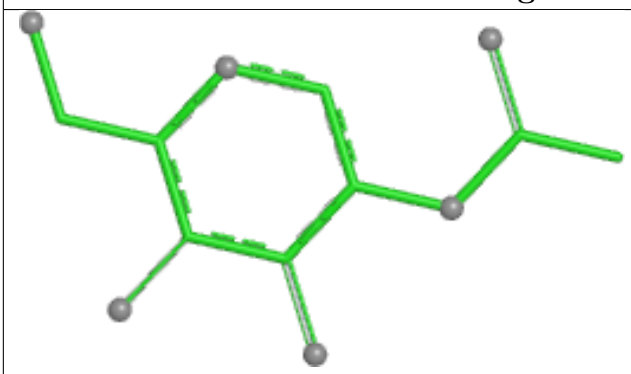


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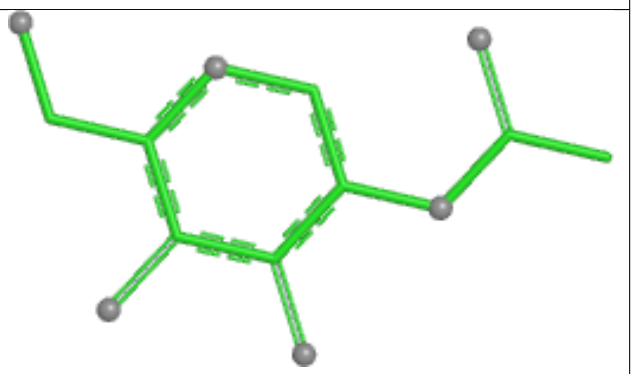


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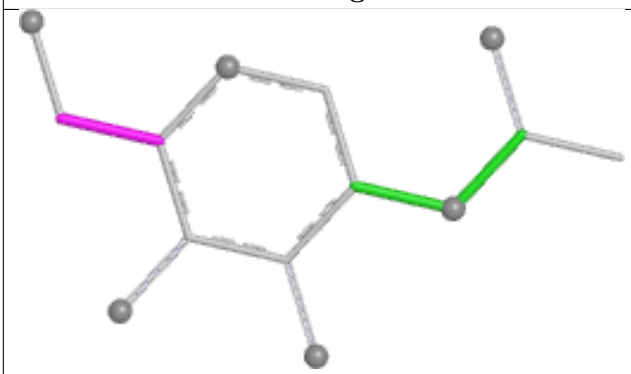
Ligand NAG I 1406



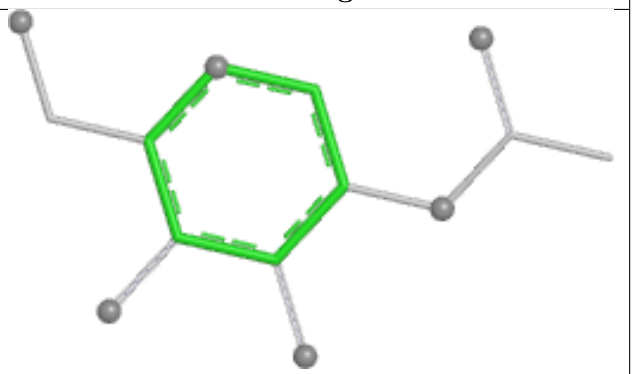
Bond lengths



Bond angles

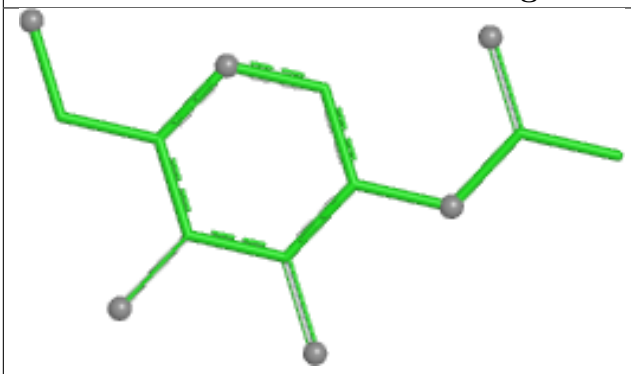


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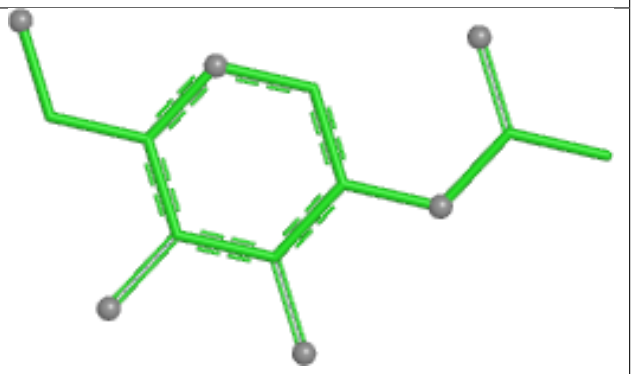


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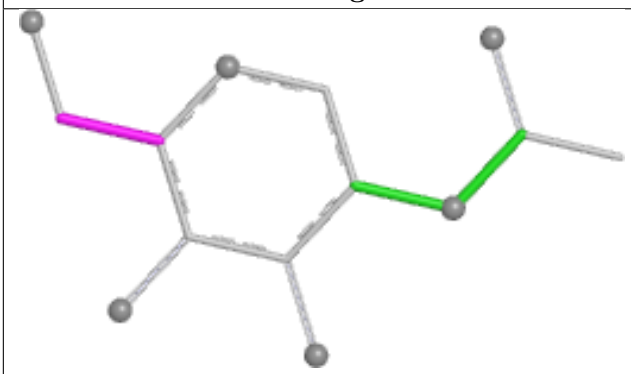
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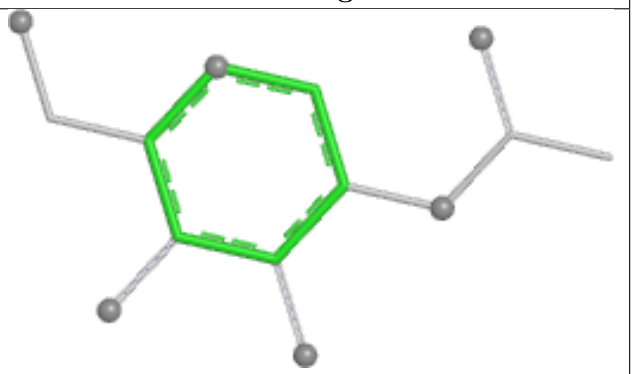
Bond lengths



Bond angles

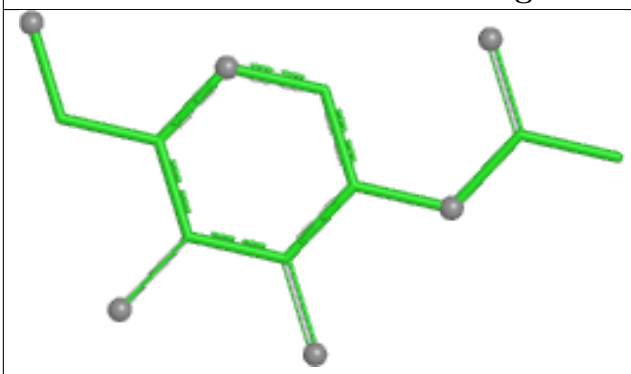


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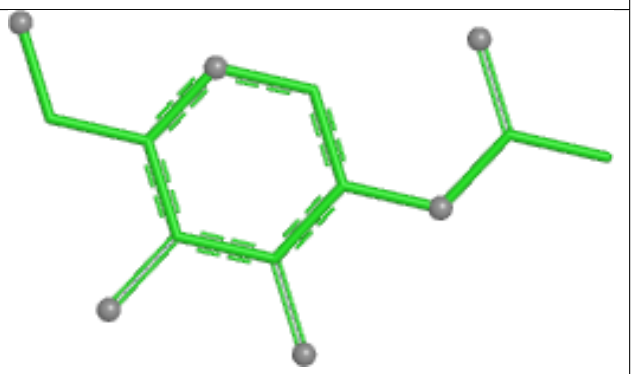


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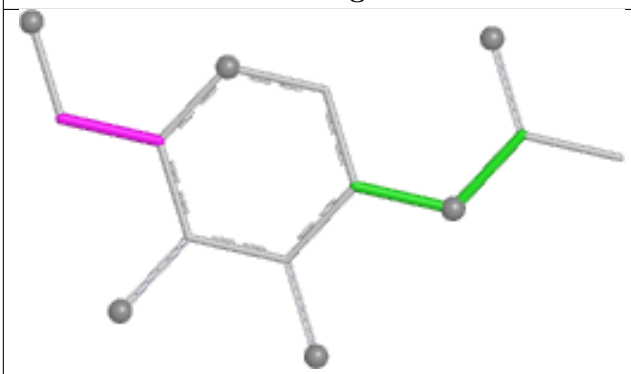
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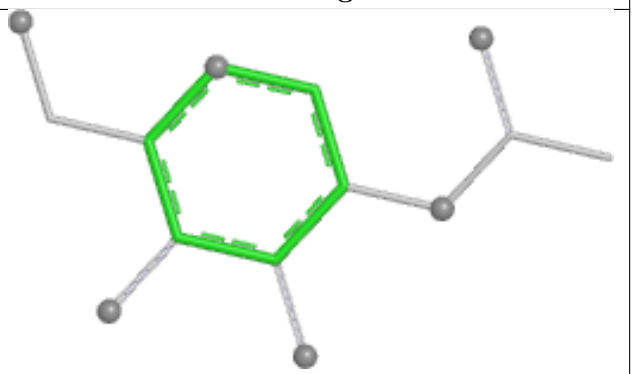
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Bond angles

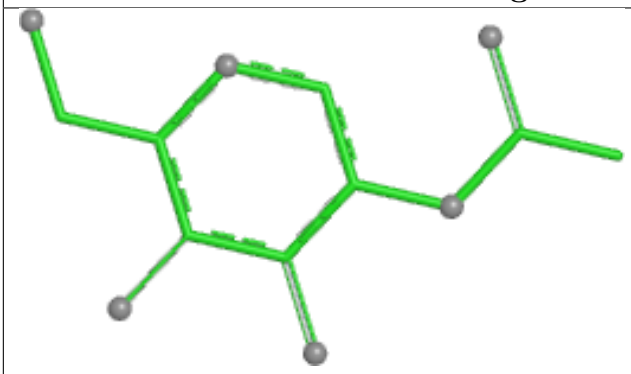


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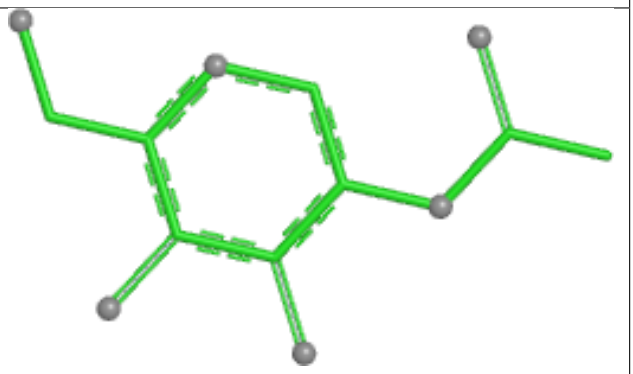


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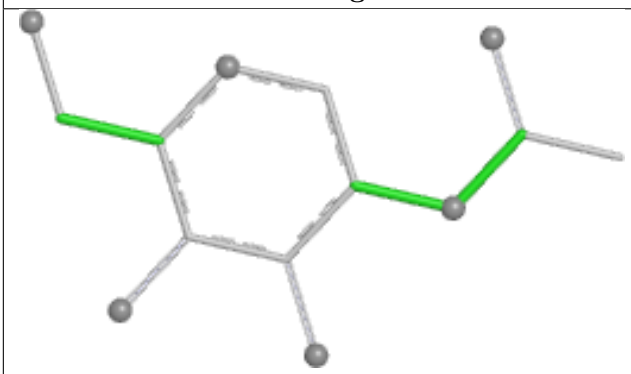
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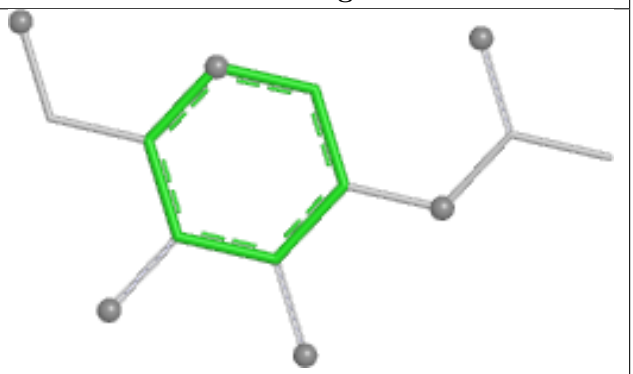
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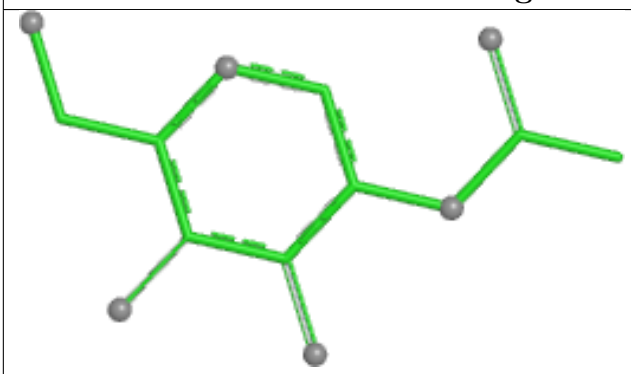


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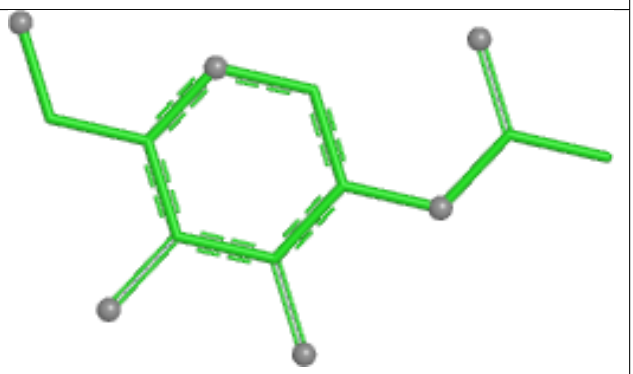


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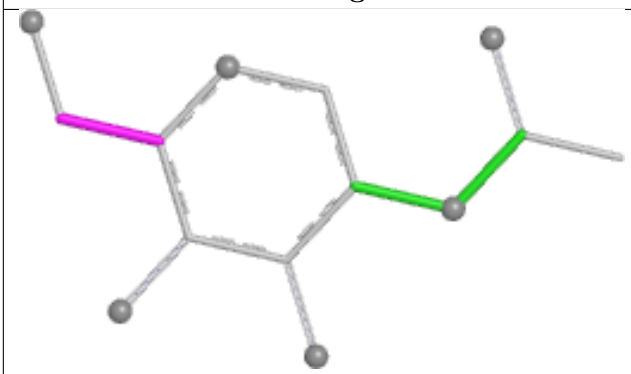
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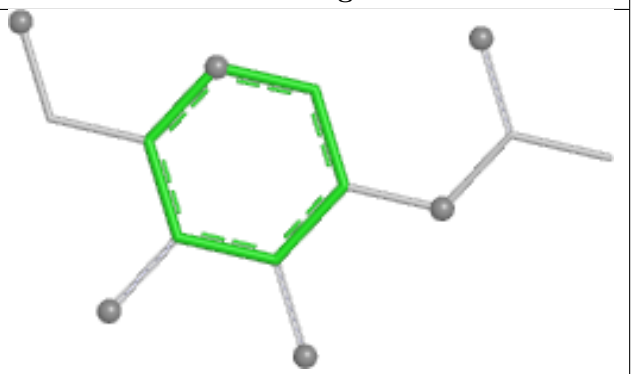
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Bond angles

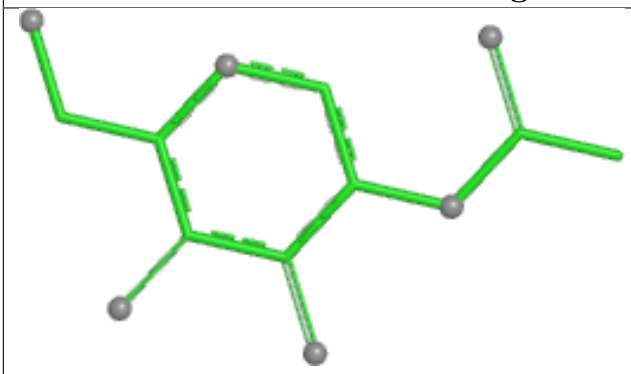


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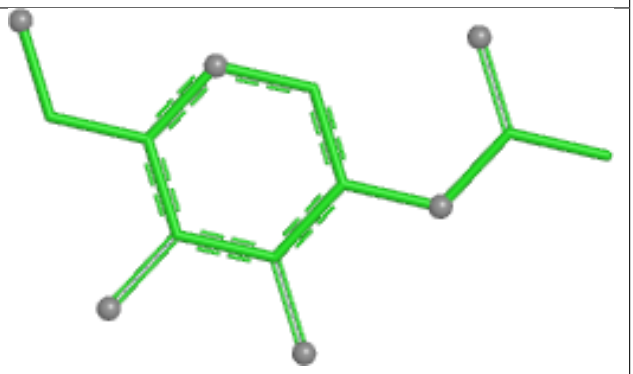


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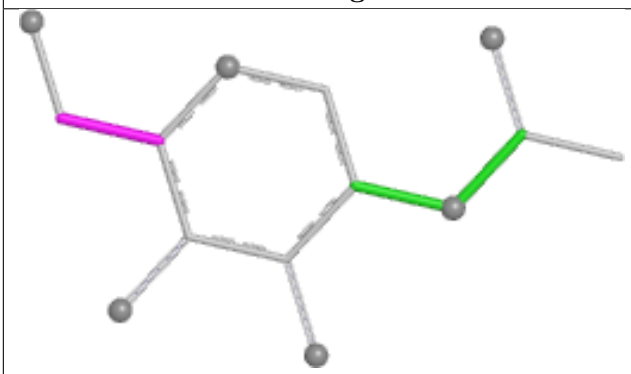
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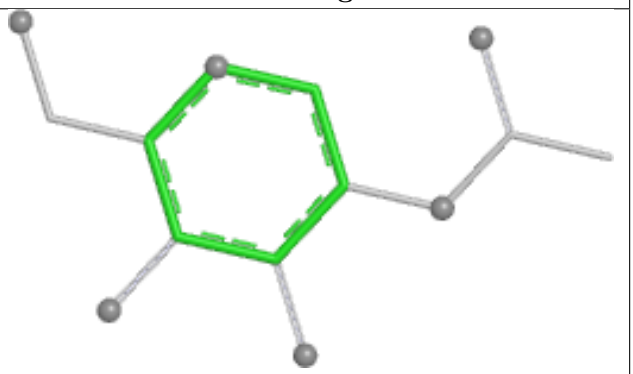
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Bond angles

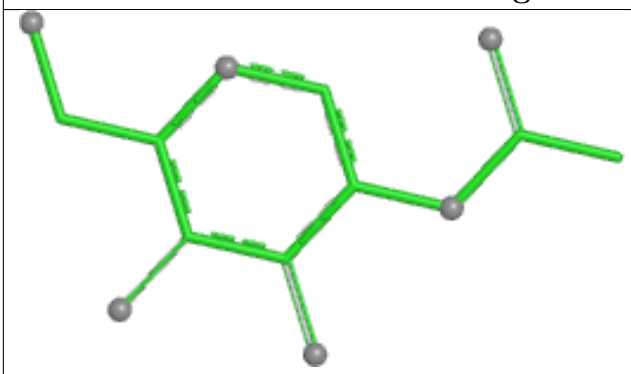


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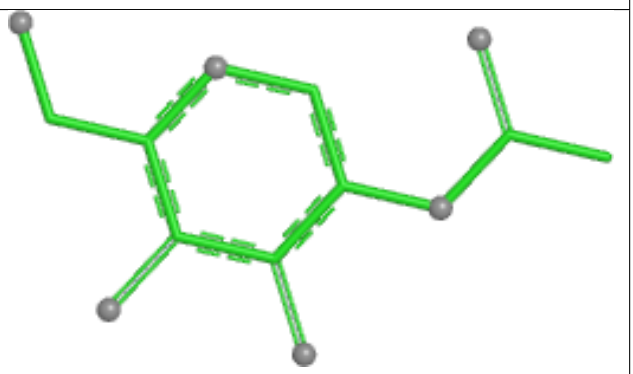


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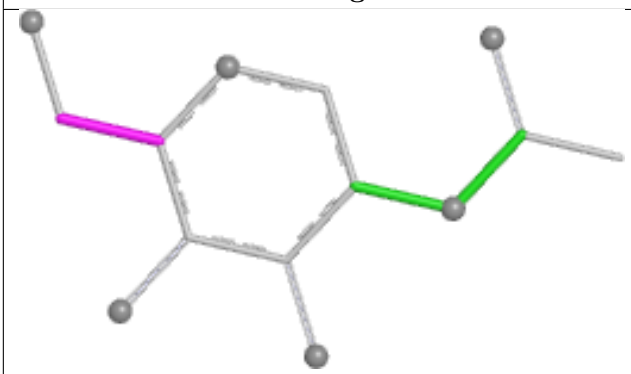
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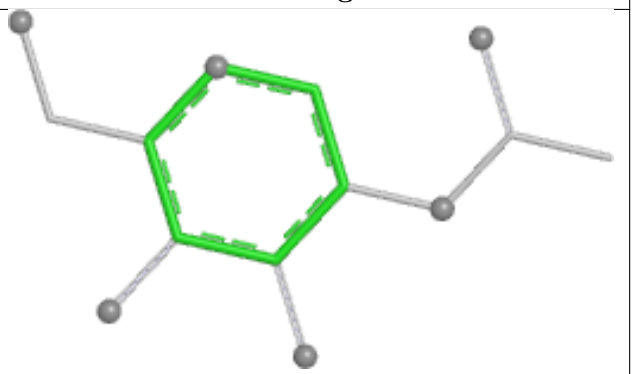
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Bond angles

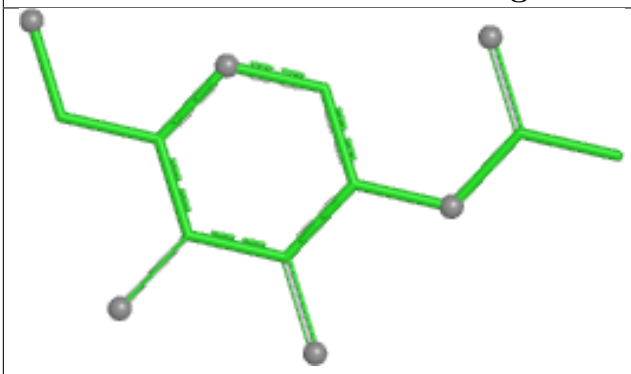


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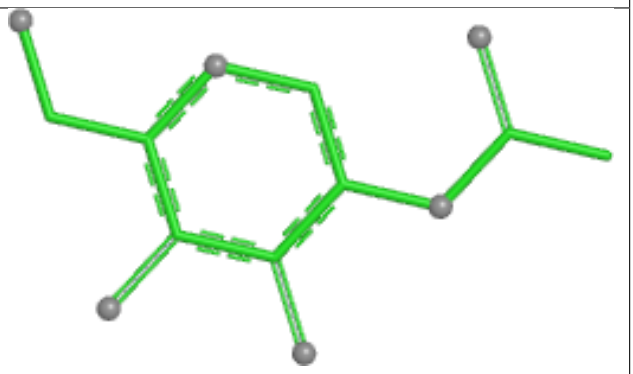


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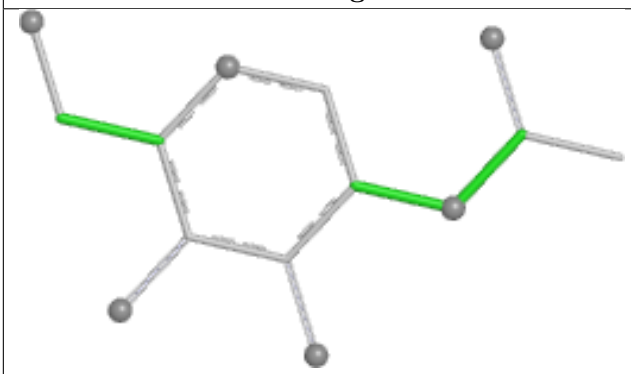
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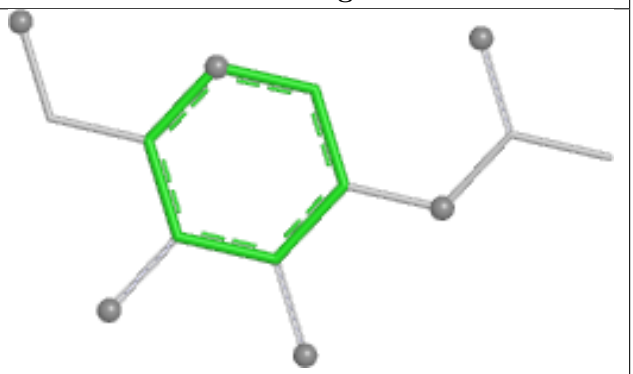
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Bond angles

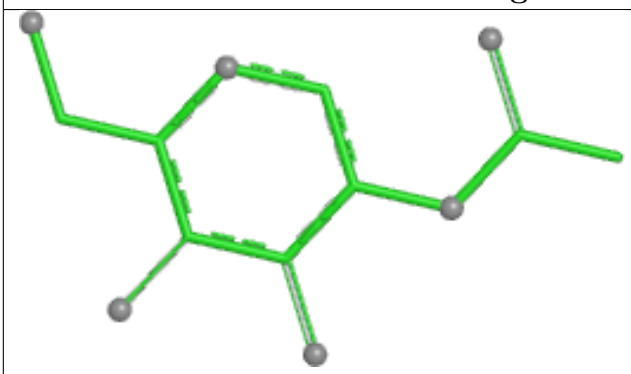


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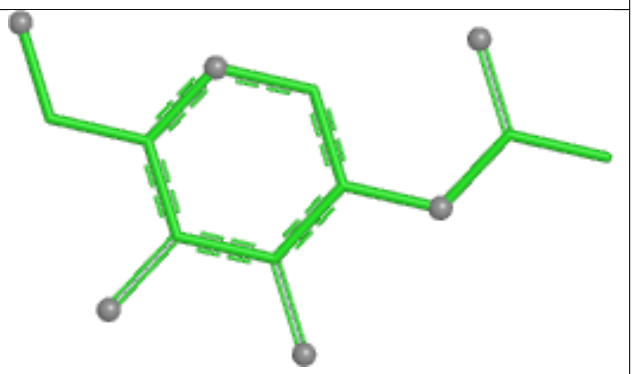


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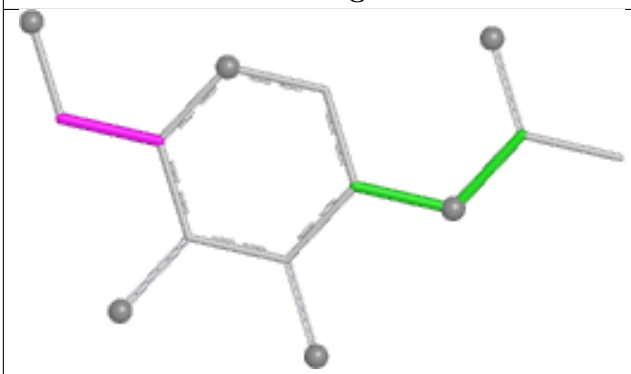
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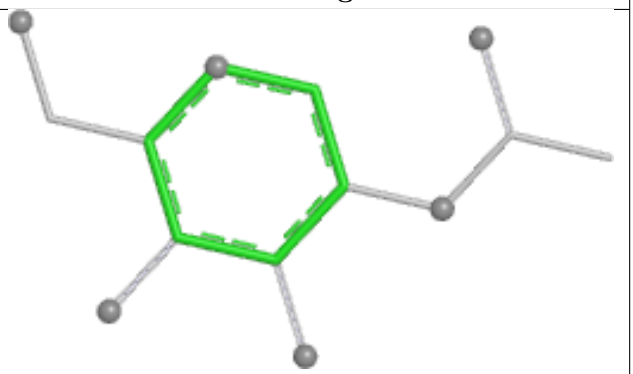
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Bond angles

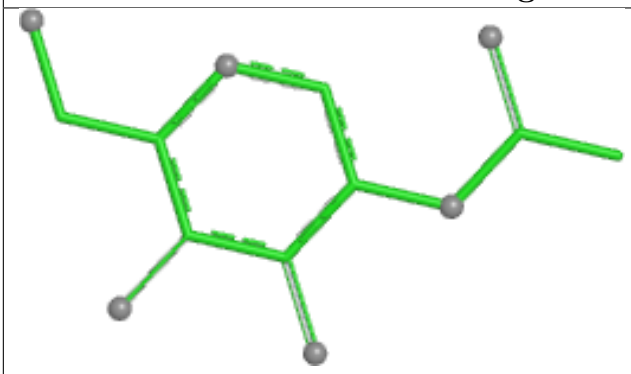


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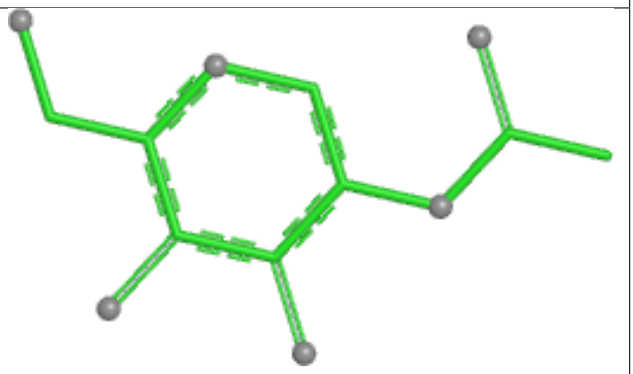


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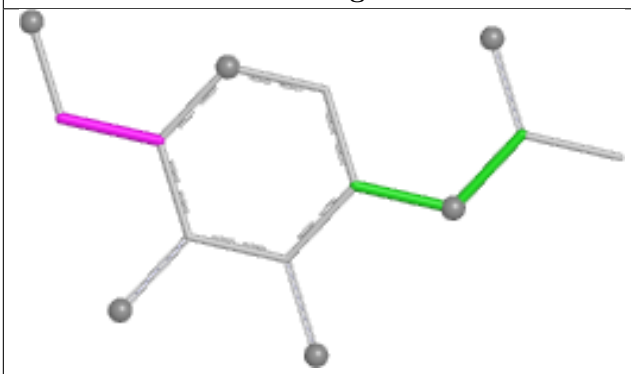
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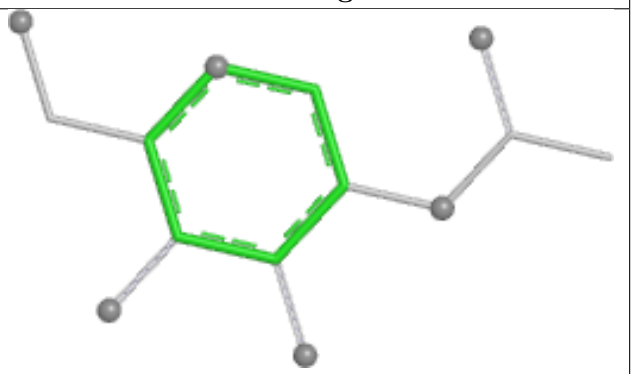
Bond lengths



Bond angles

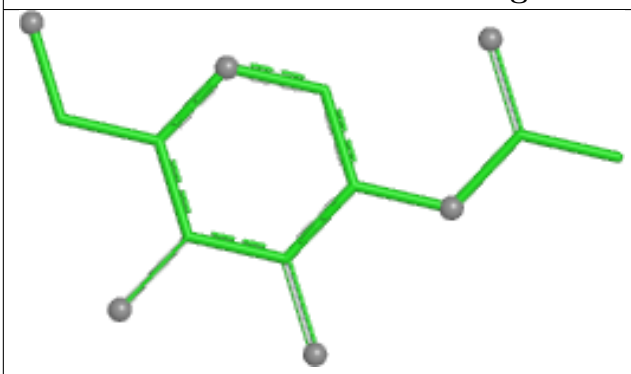


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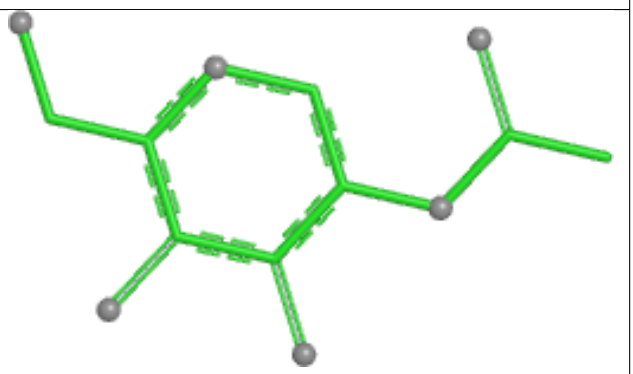


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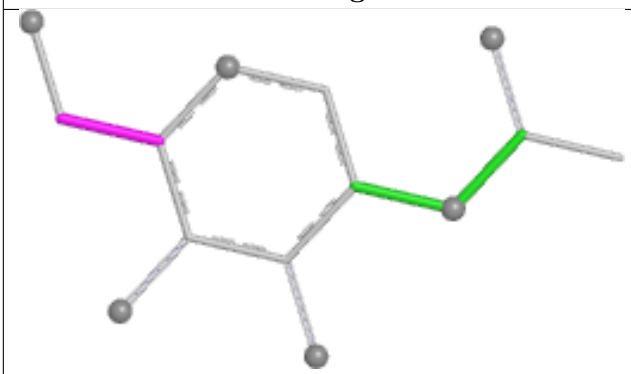
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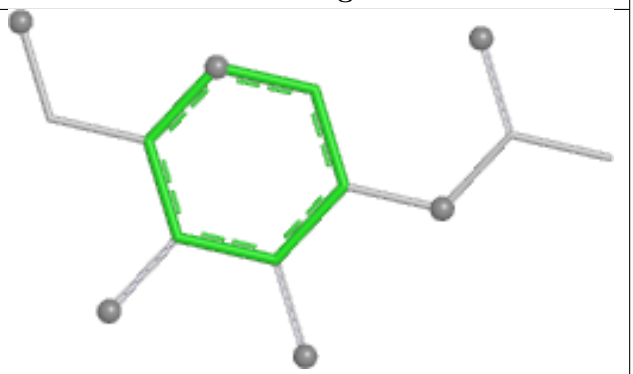
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Bond angles

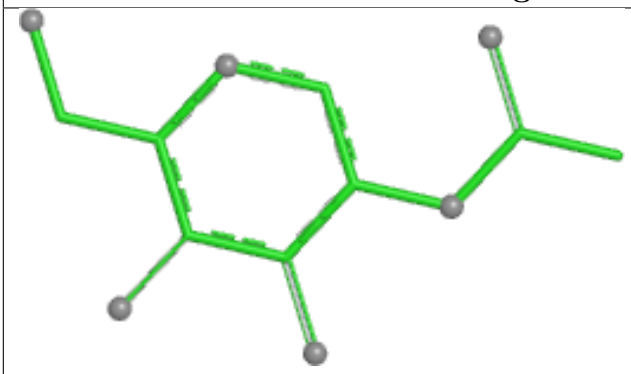


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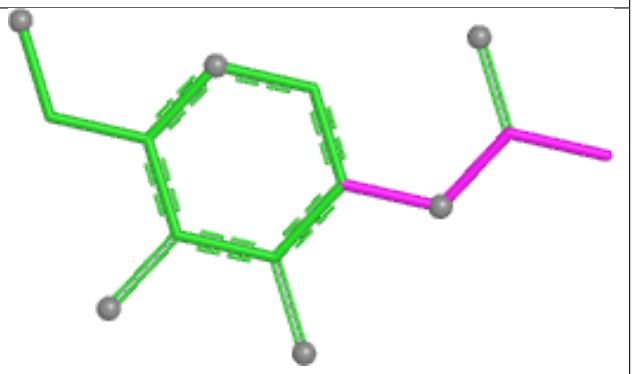


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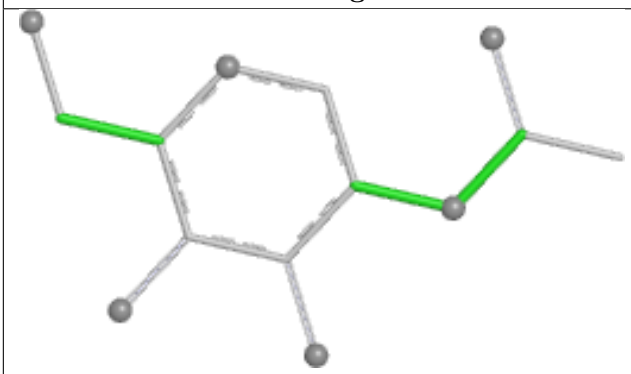
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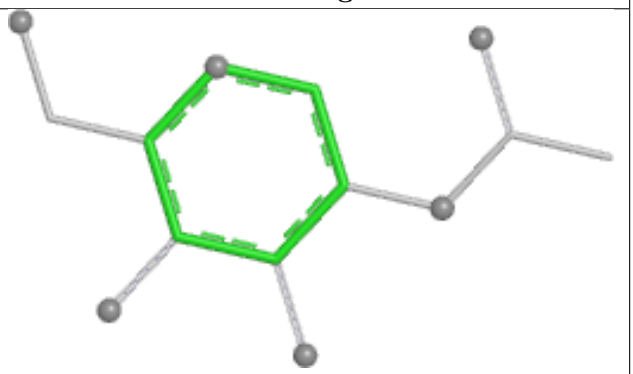
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Bond angles

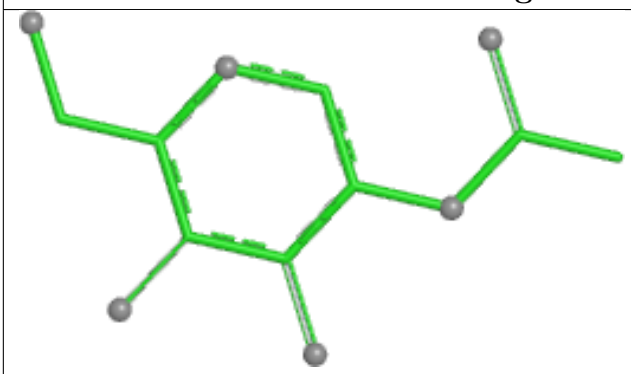


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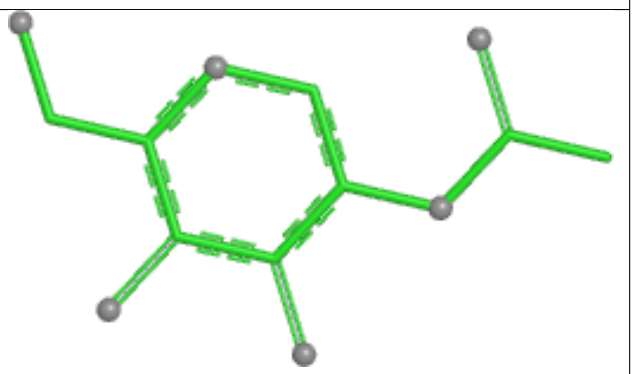


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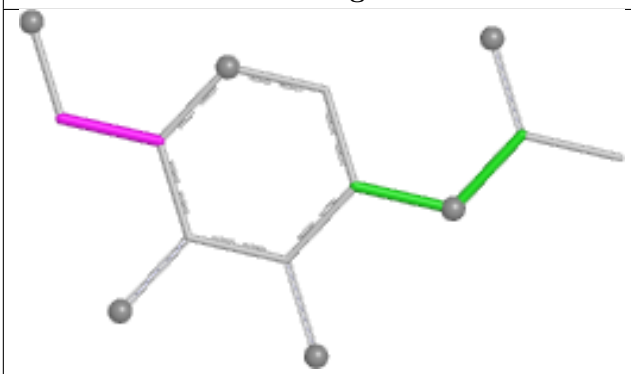
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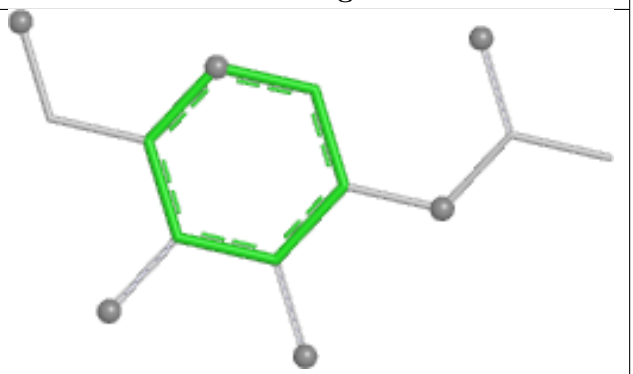
Bond lengths



Bond angles

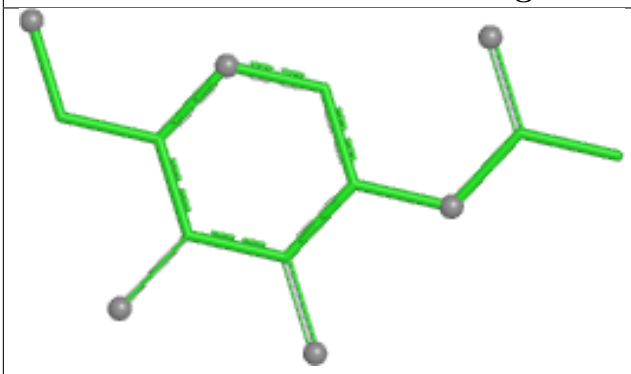


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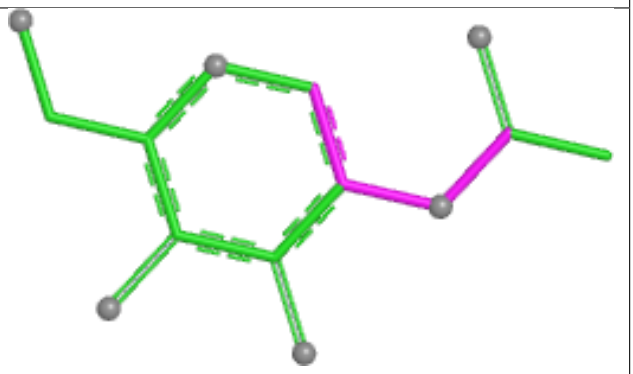


Rings

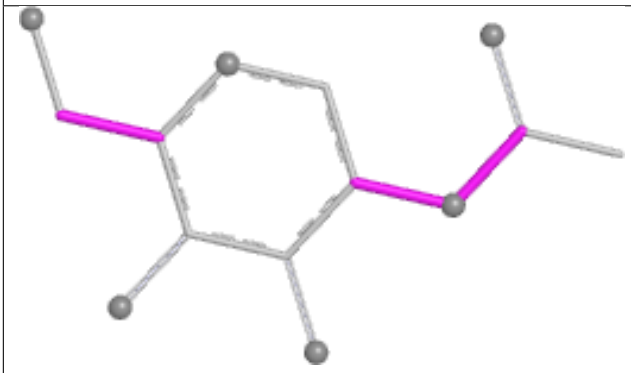
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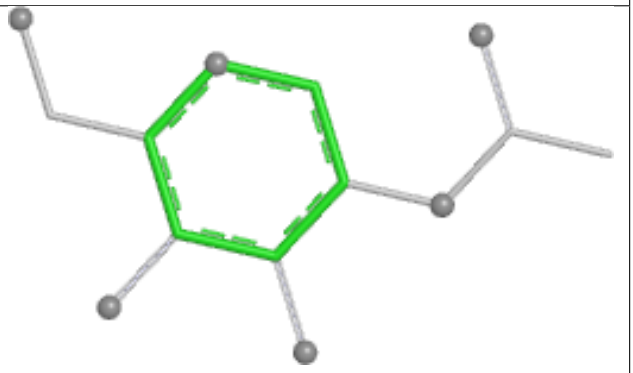
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Bond angles

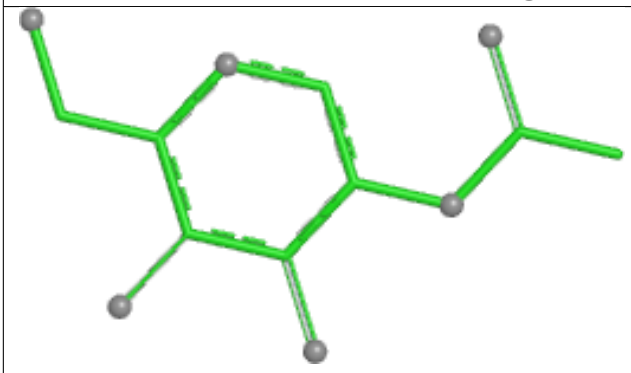


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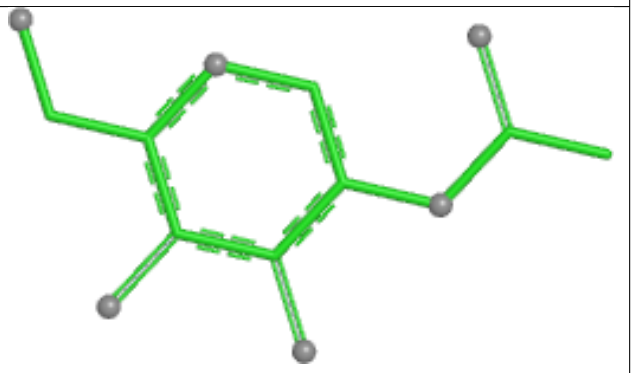


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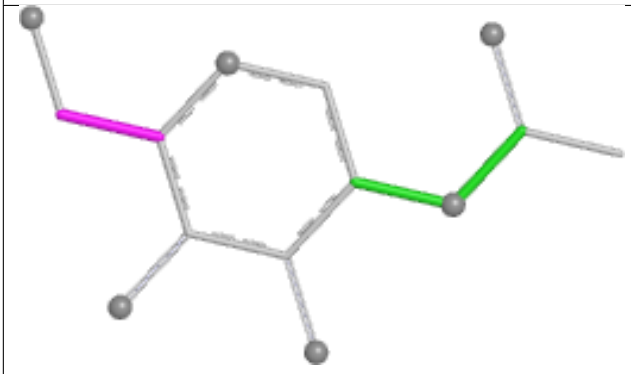
Ligand NAG C 702



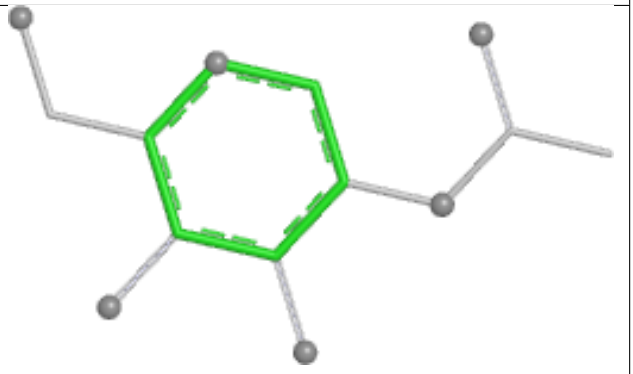
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Bond angles

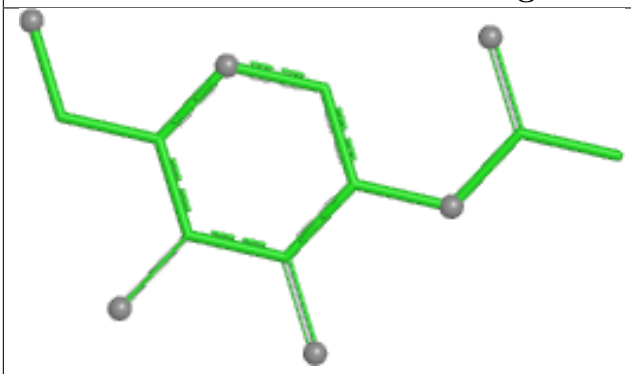


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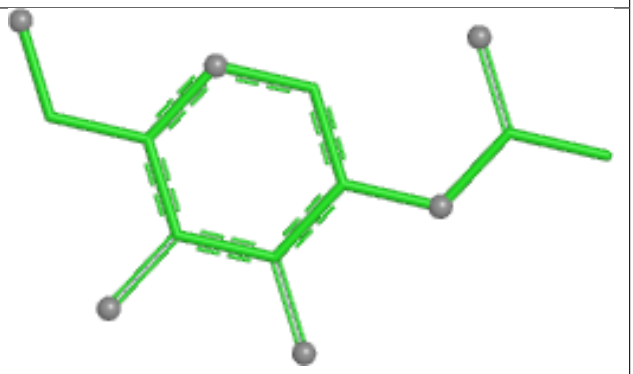


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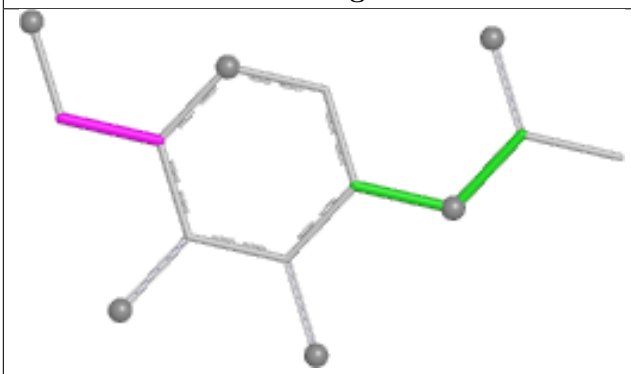
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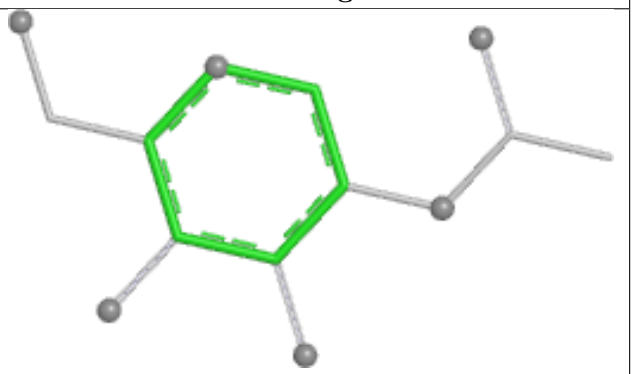
Bond lengths



Bond angles

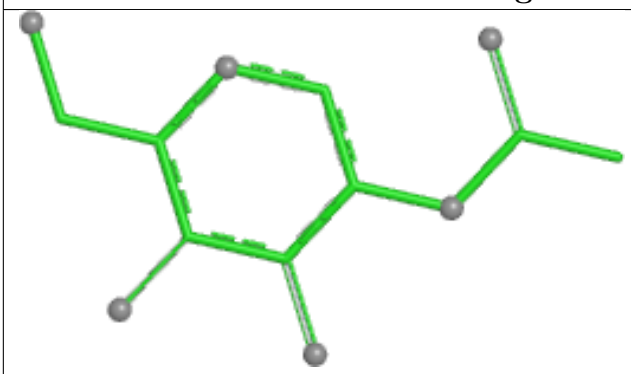


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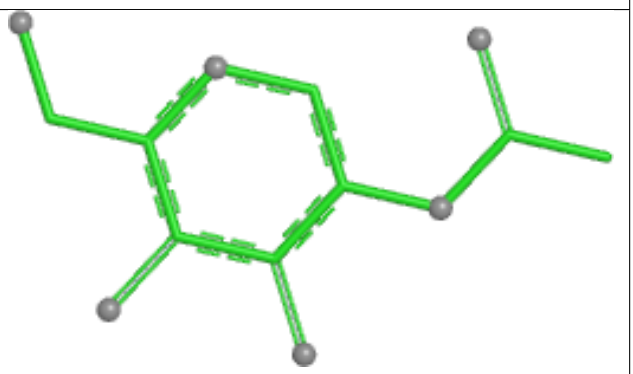


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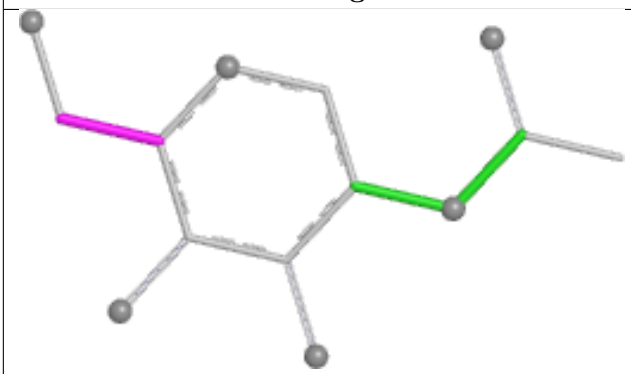
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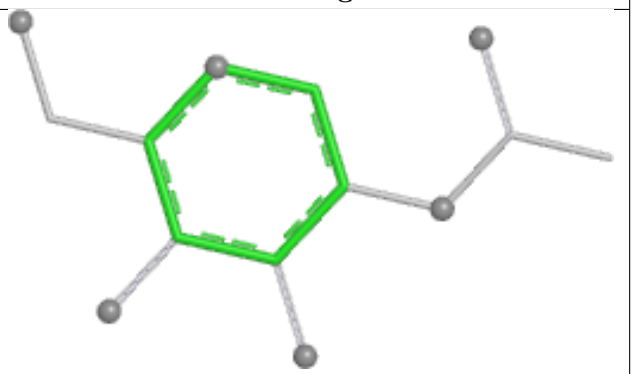
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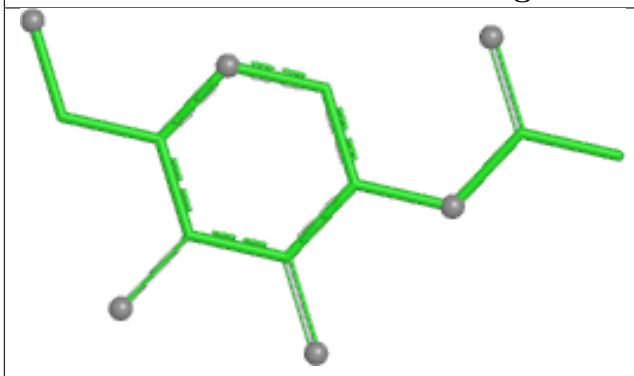


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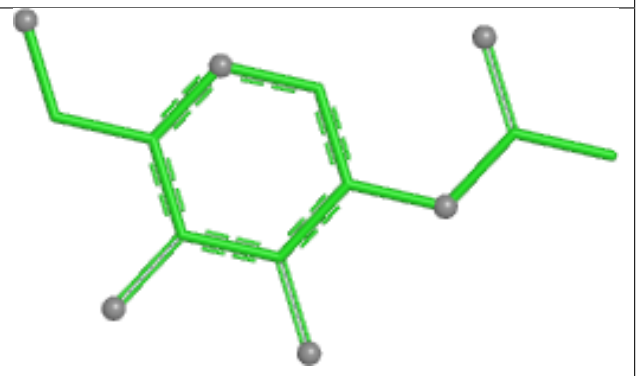


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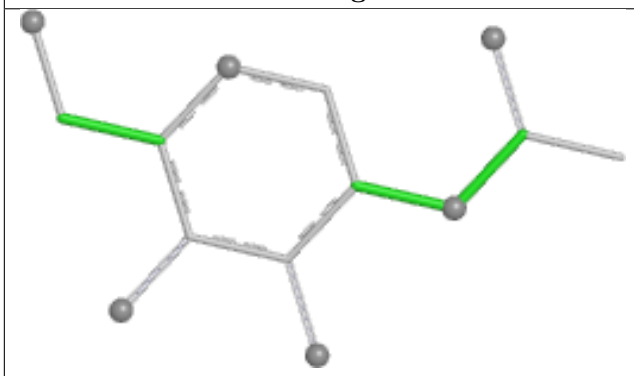
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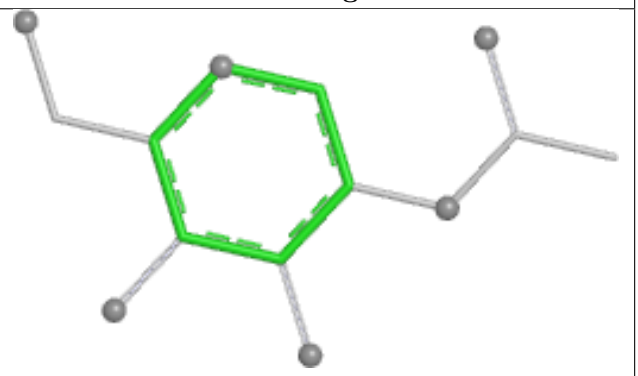
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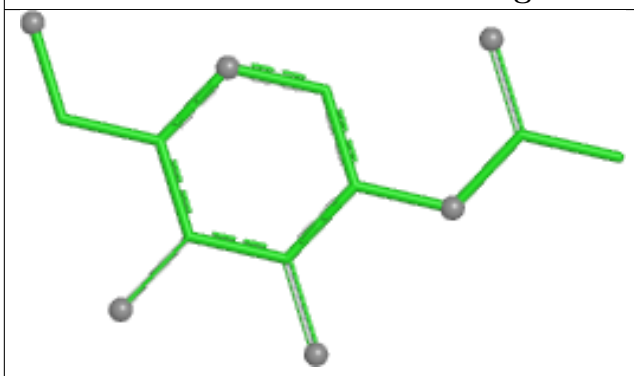


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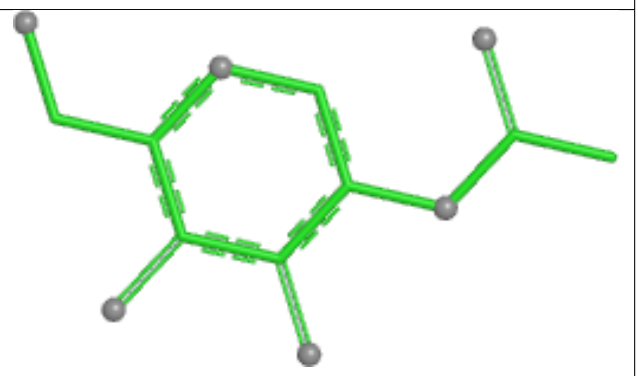


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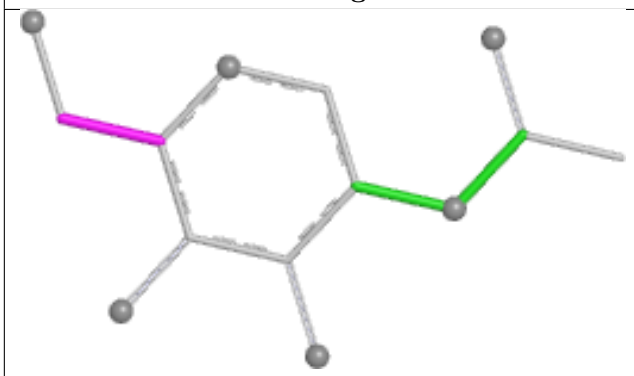
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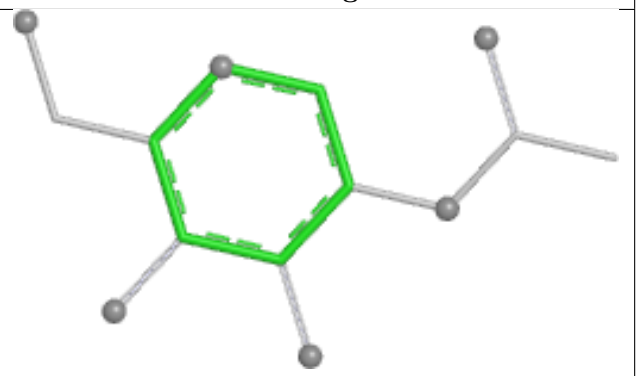
Bond lengths



Bond angles

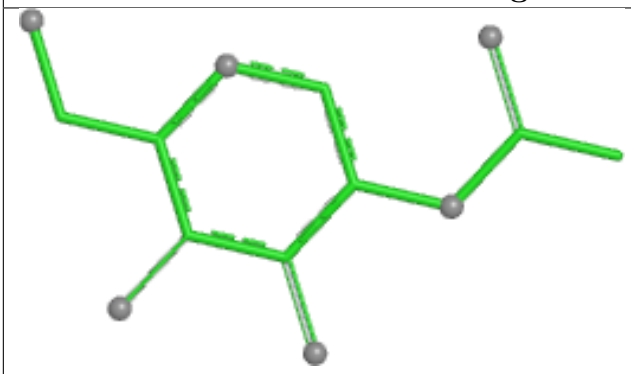


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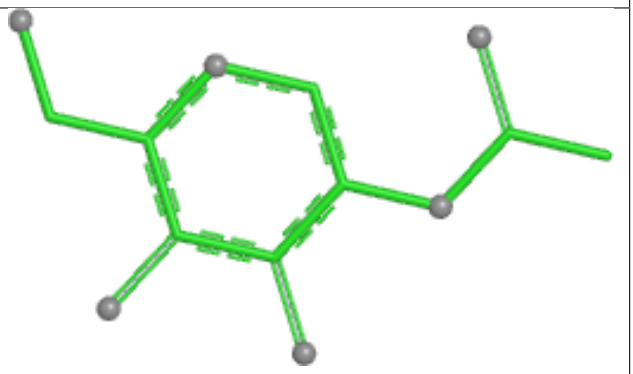


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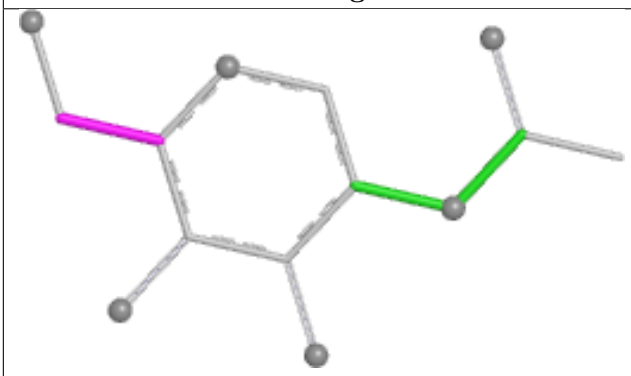
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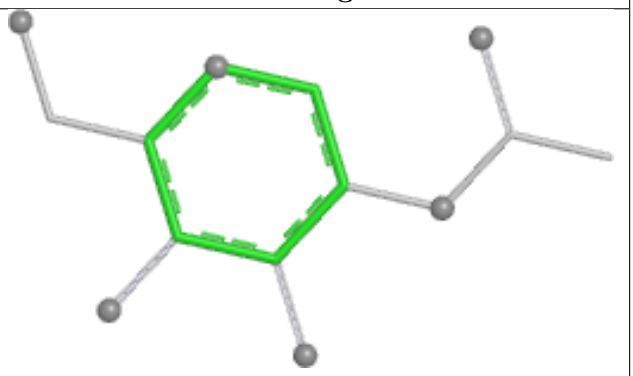
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Bond angles

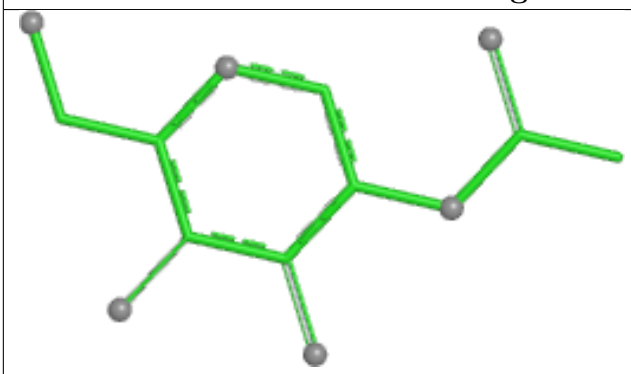


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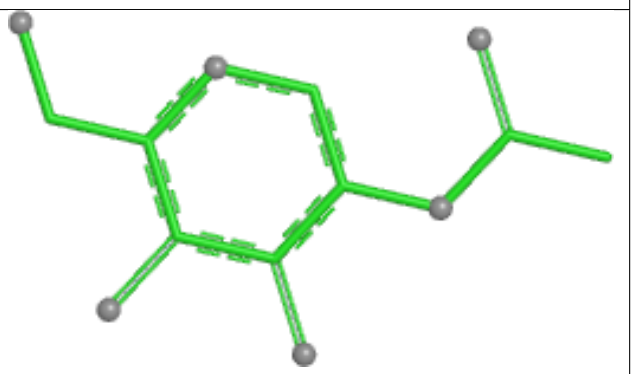


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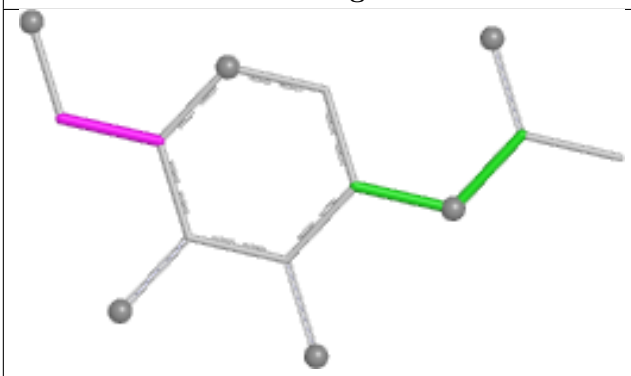
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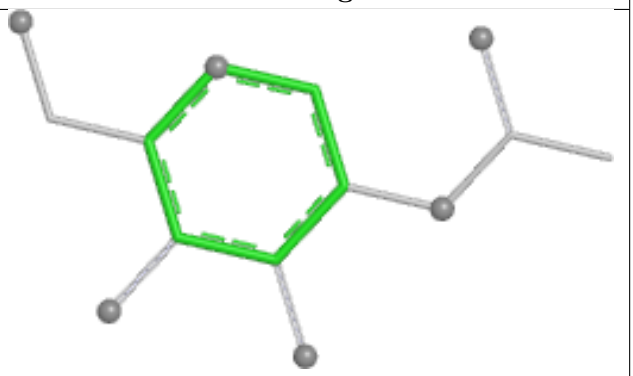
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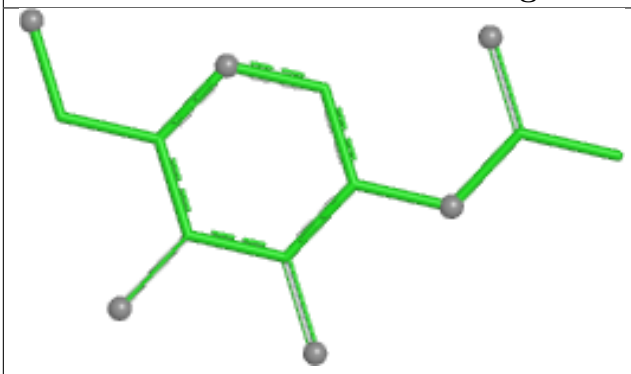


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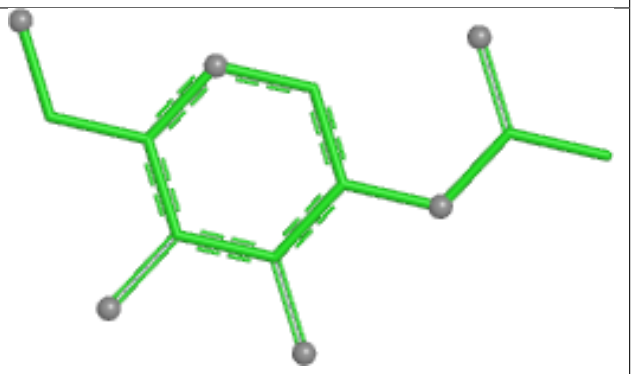


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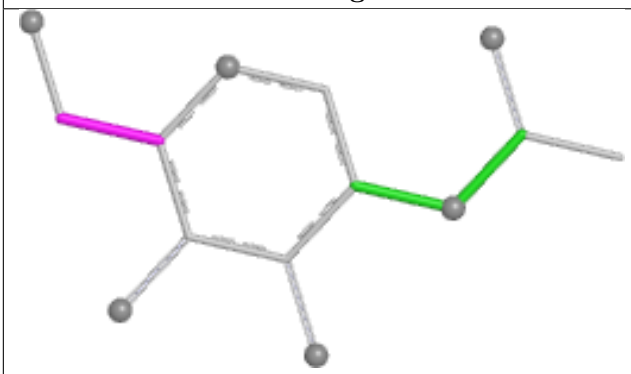
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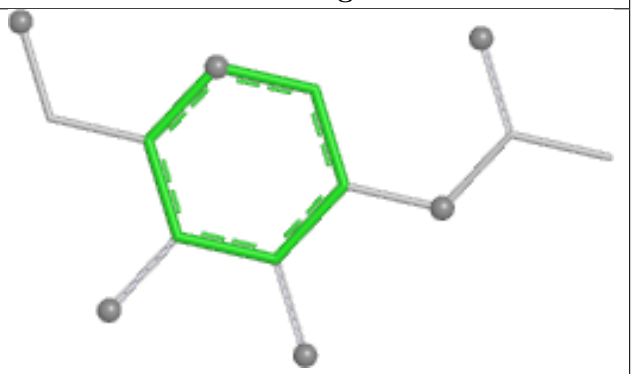
Bond lengths



Bond angles

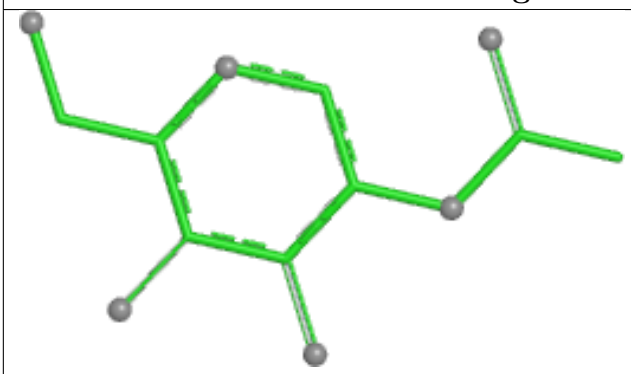


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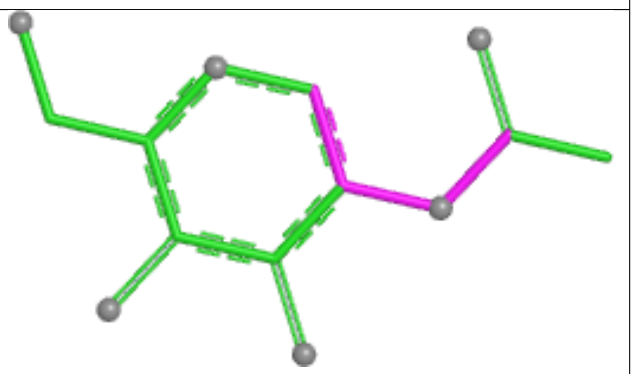


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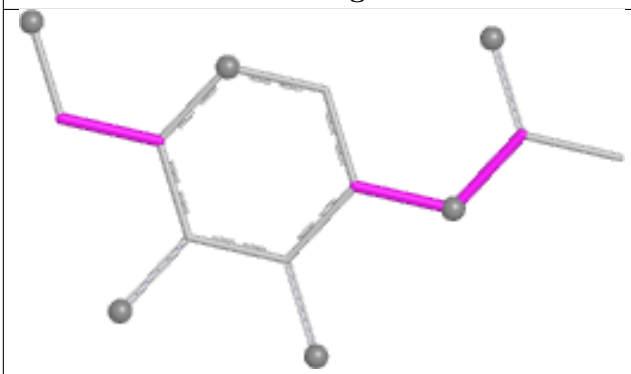
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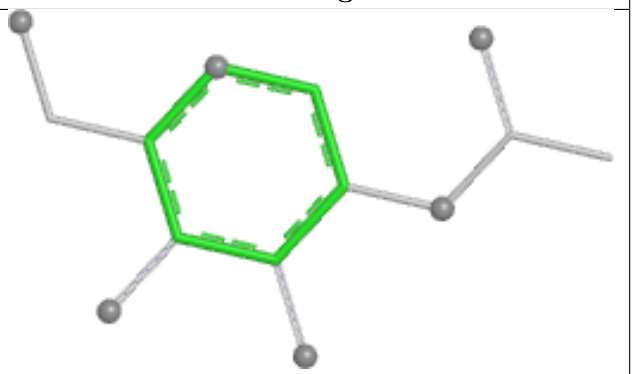
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Bond angles

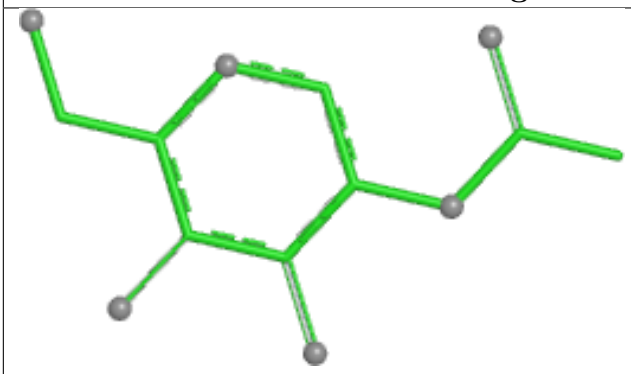


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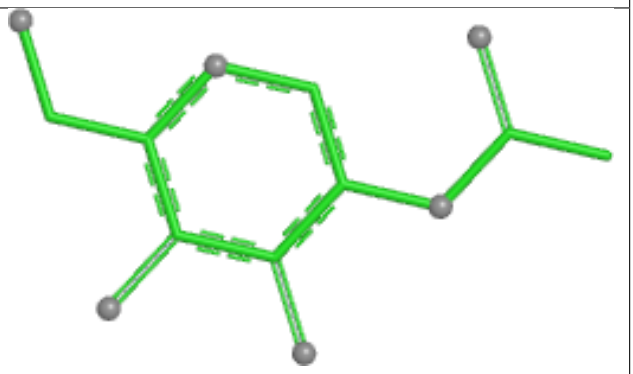


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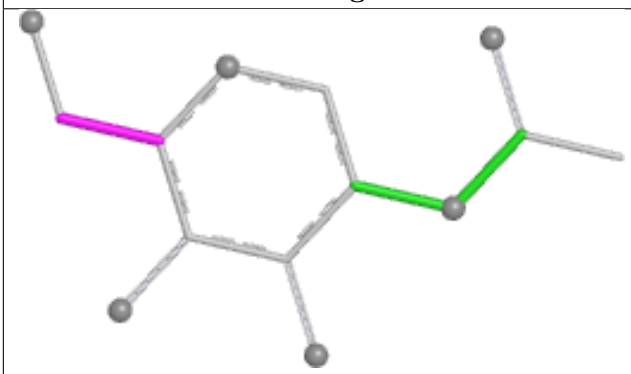
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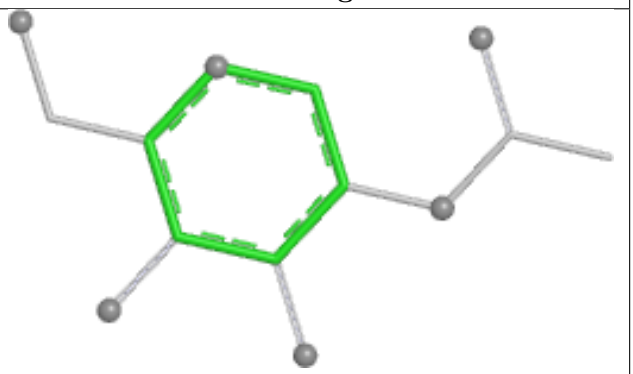
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Bond angles

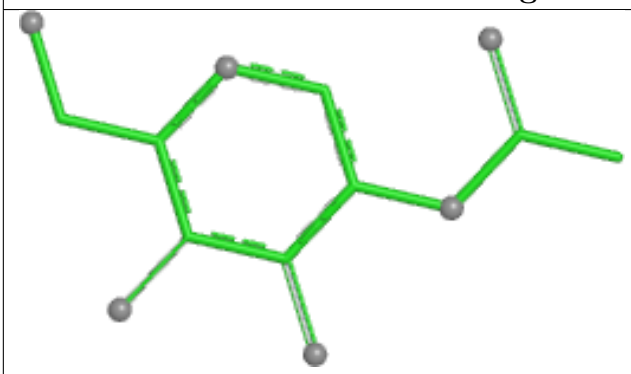


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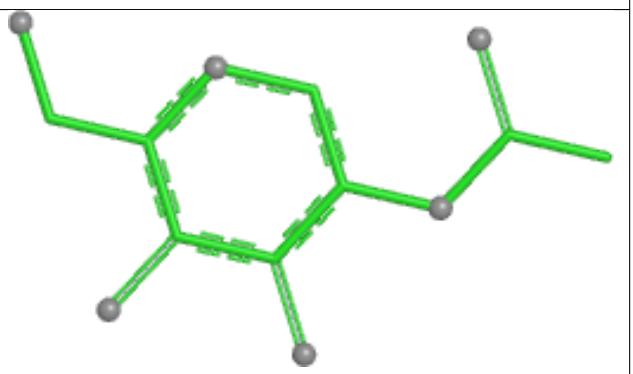


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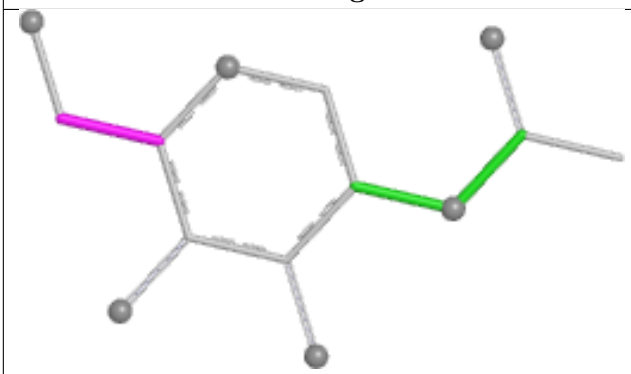
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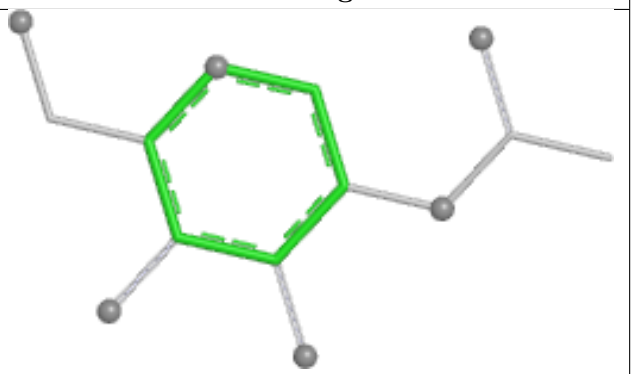
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Bond angles

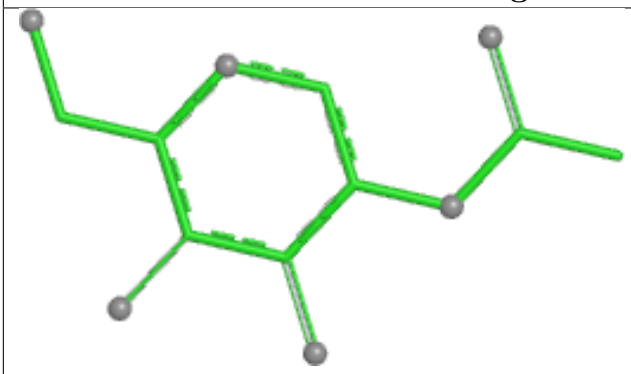


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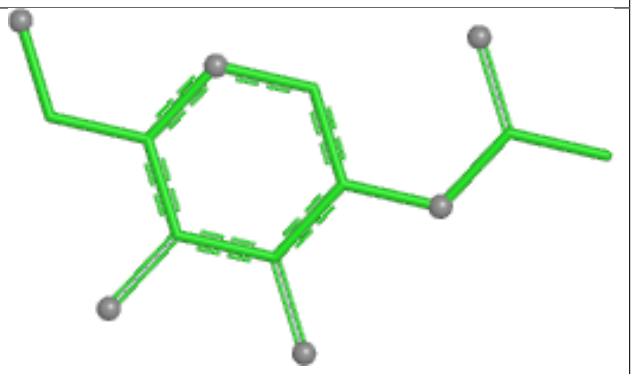


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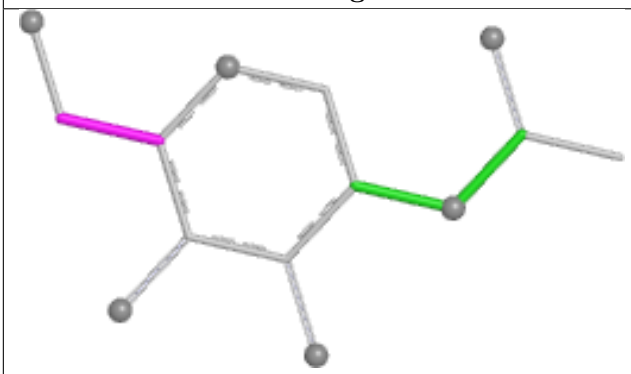
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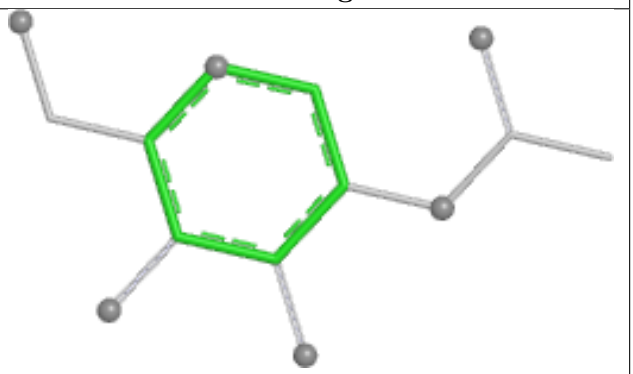
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Bond angles

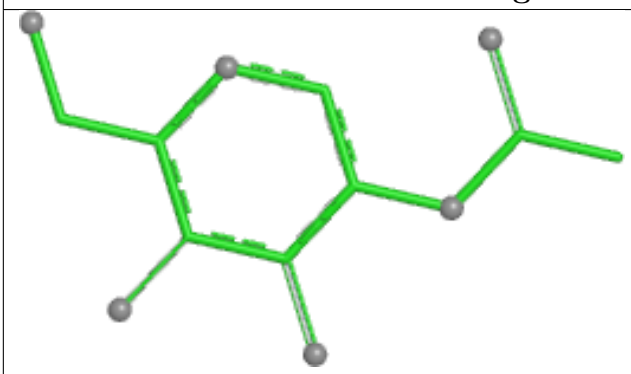


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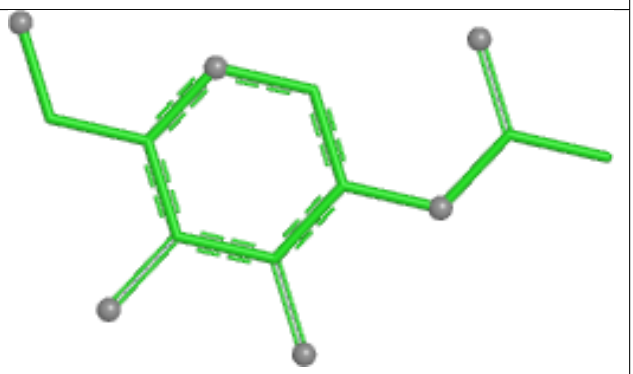


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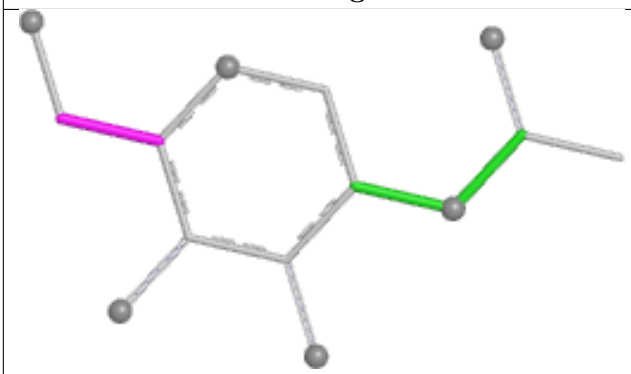
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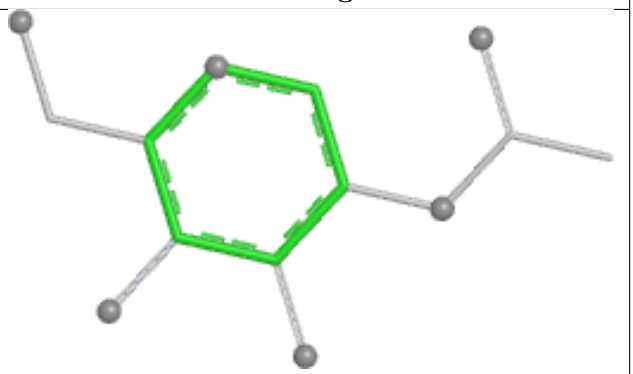
Bond lengths



Bond angles

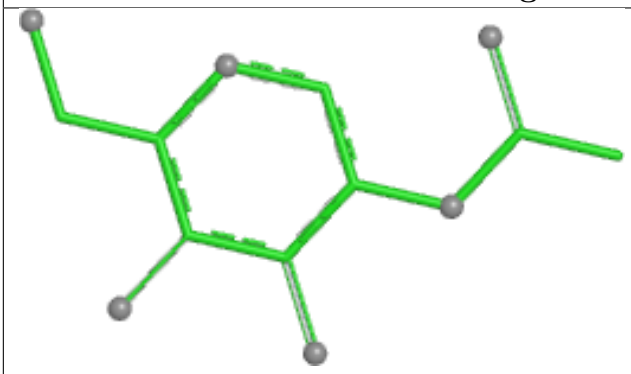


Torsions

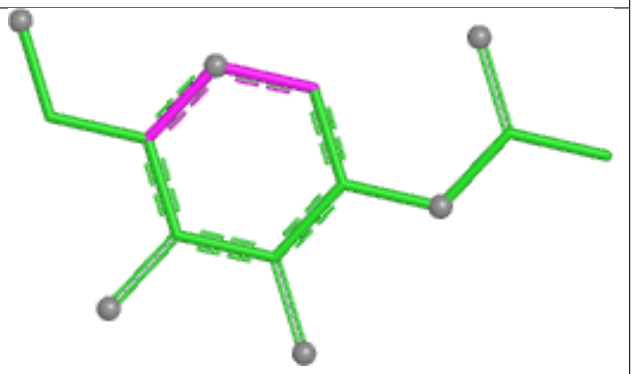


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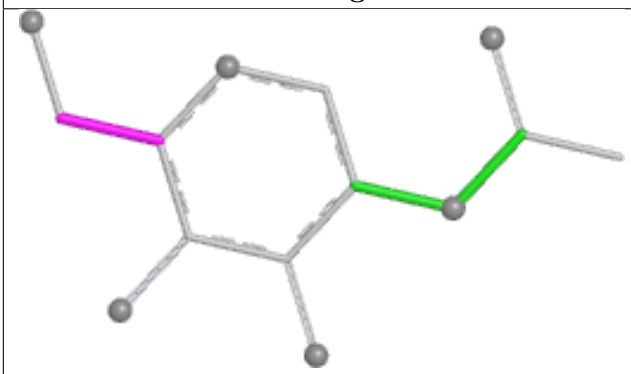
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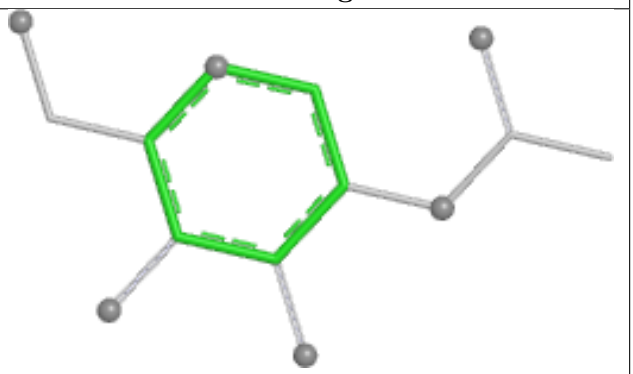
Bond lengths



Bond angles

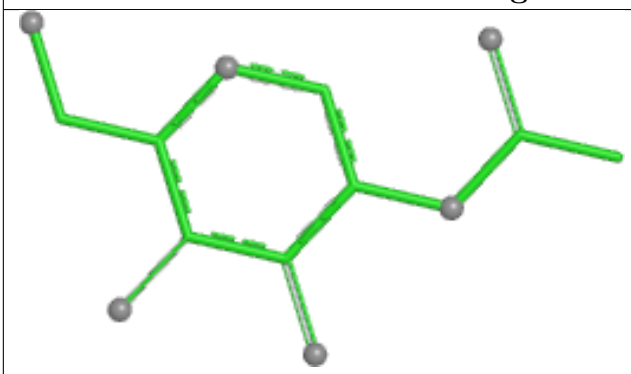


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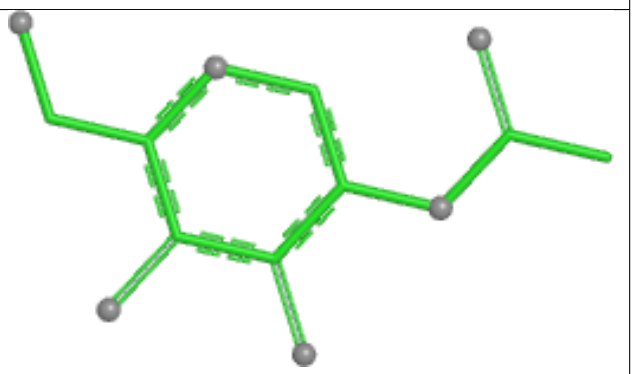


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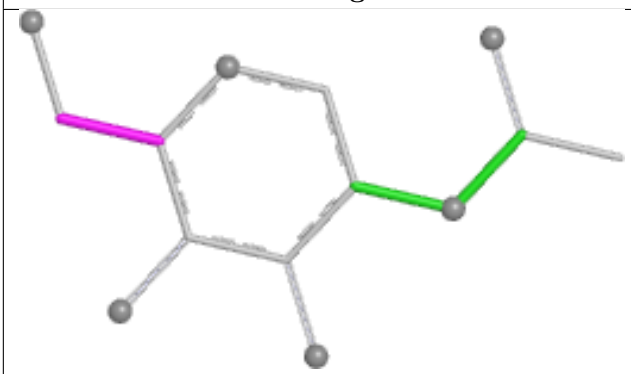
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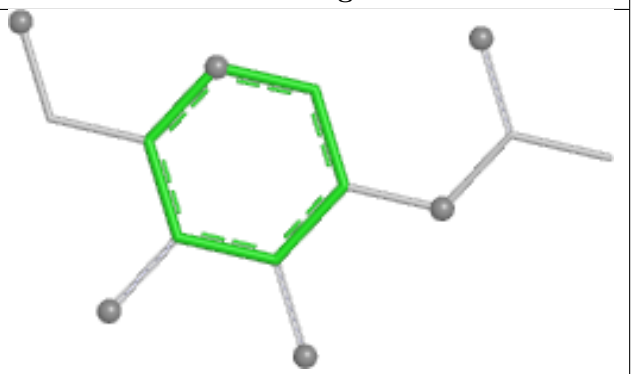
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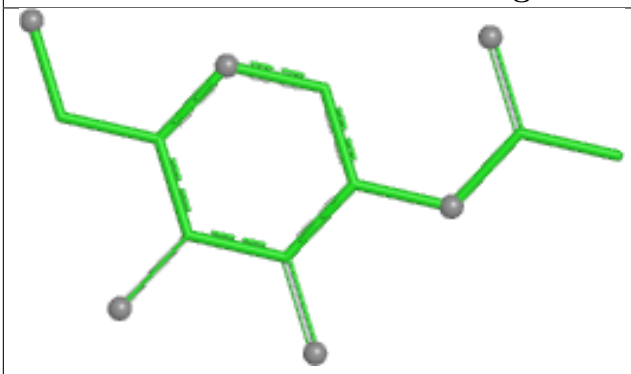


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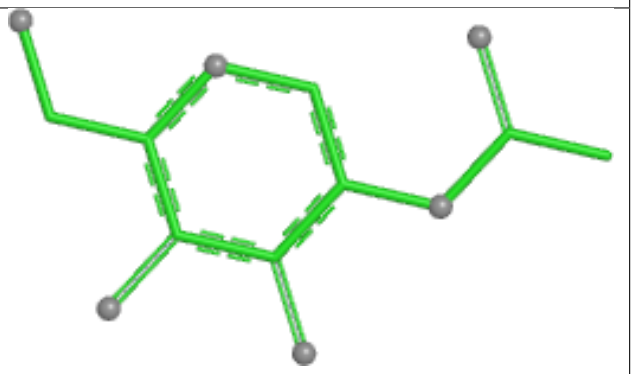


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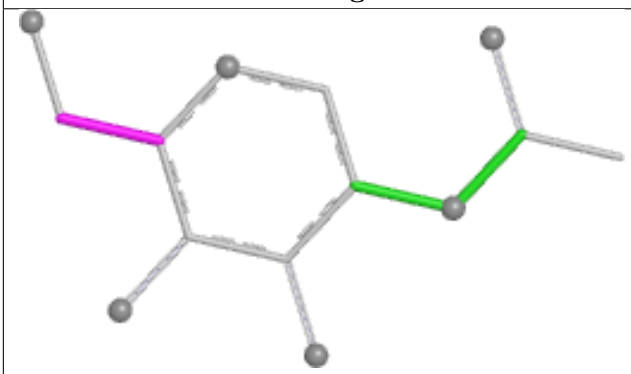
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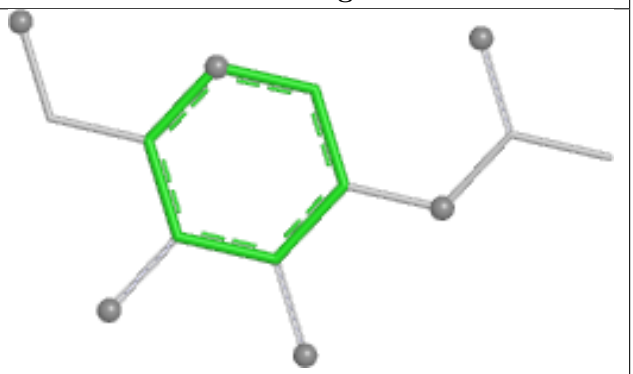
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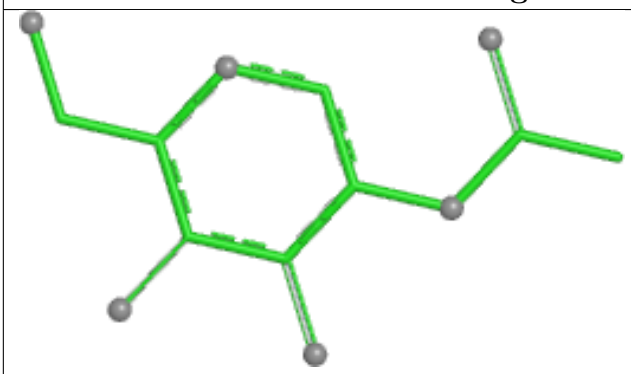


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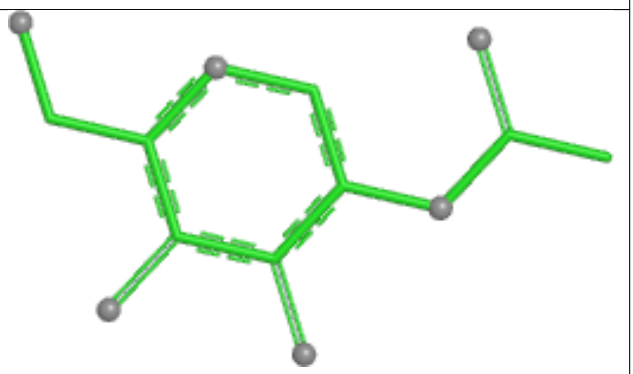


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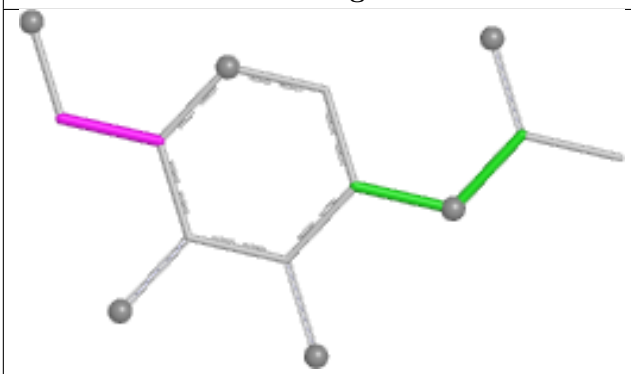
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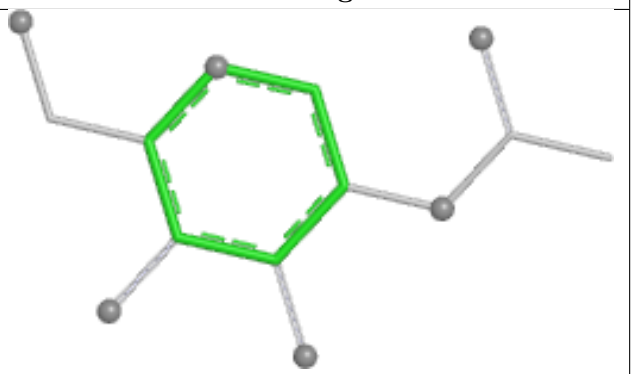
Bond lengths



Bond angles

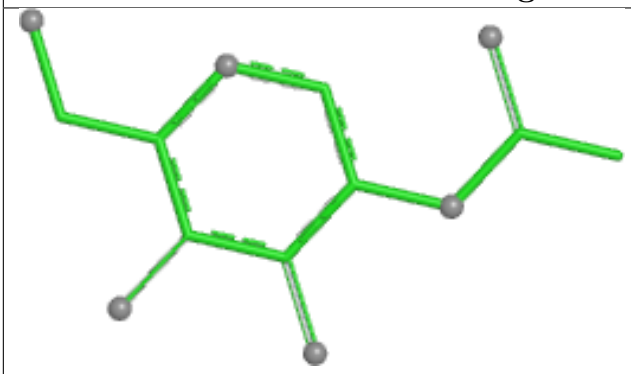


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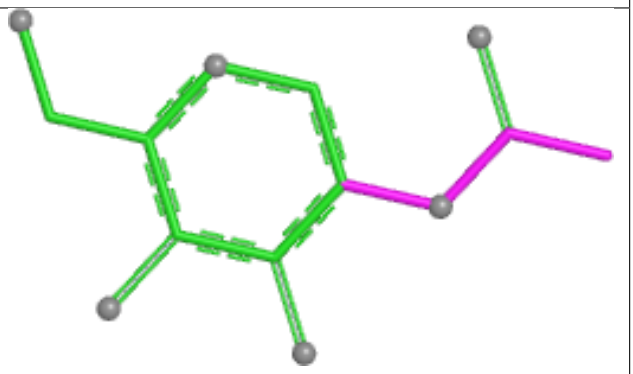


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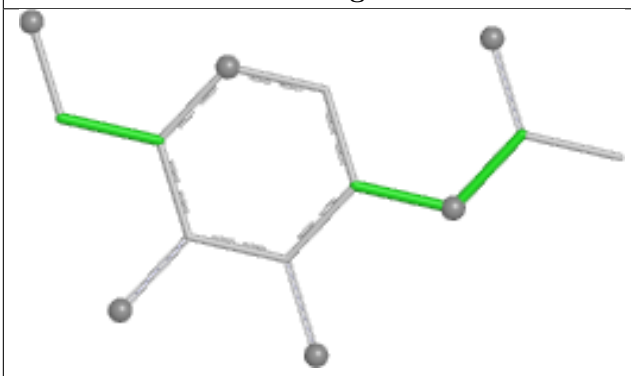
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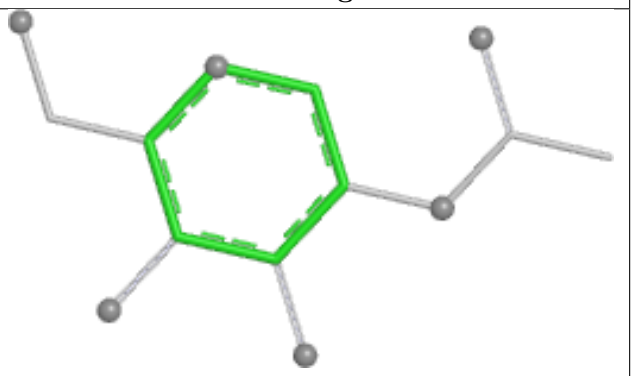
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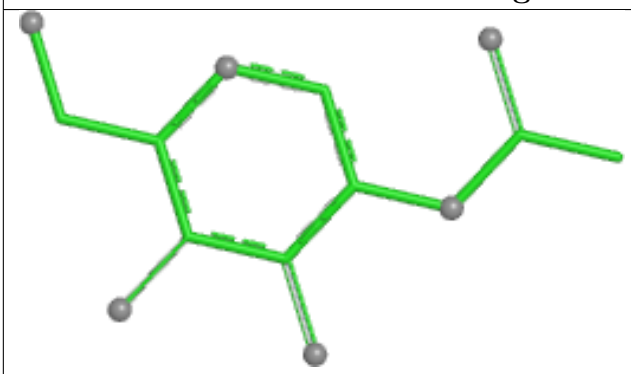


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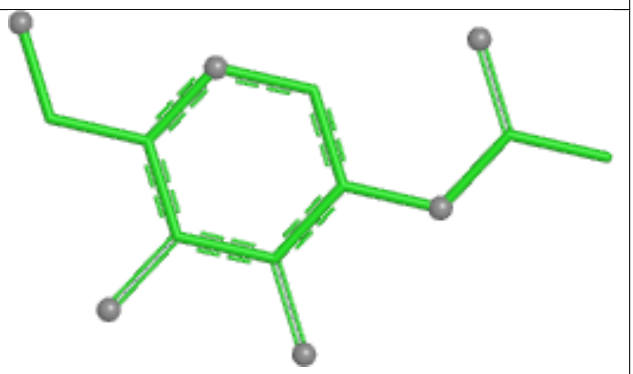


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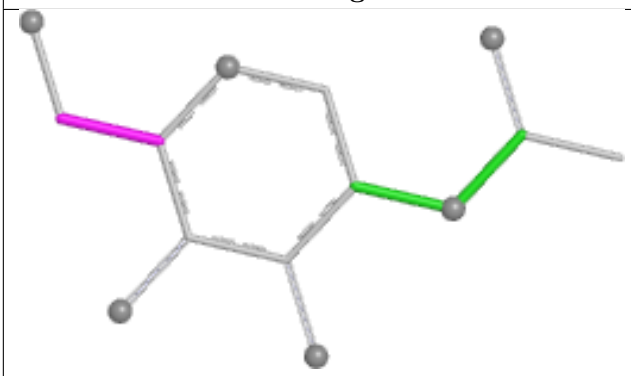
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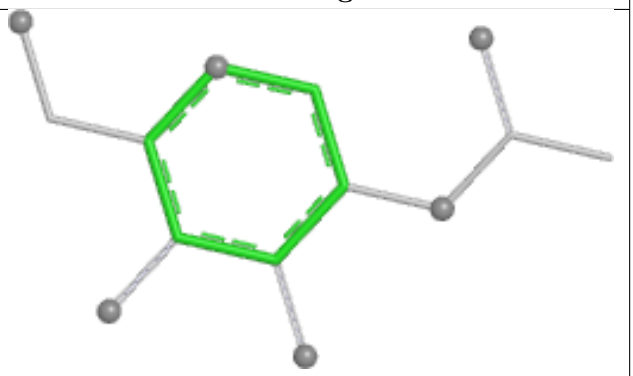
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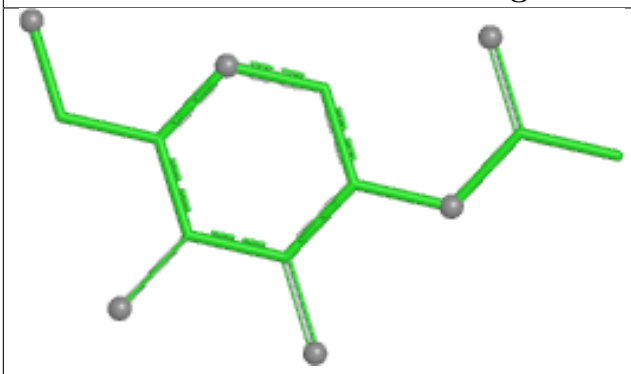


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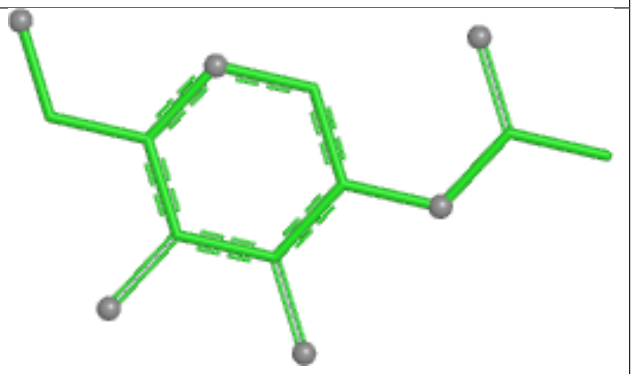


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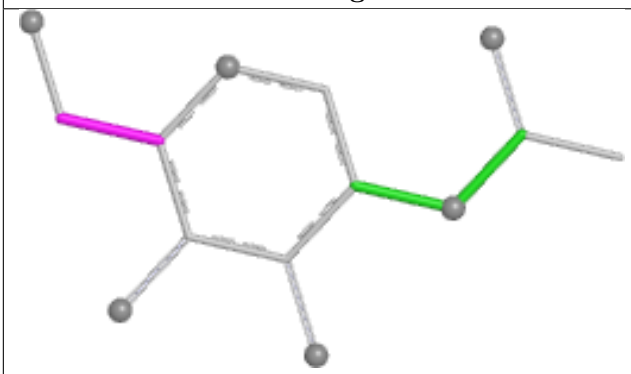
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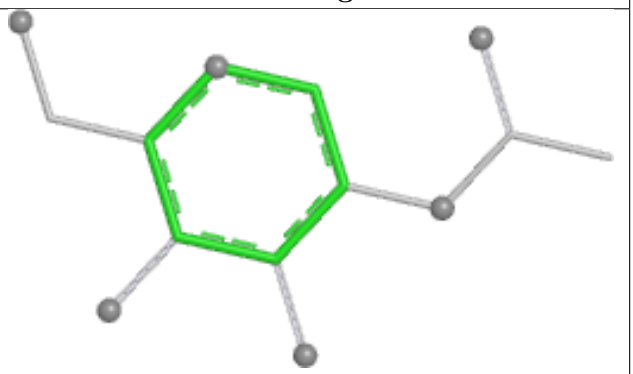
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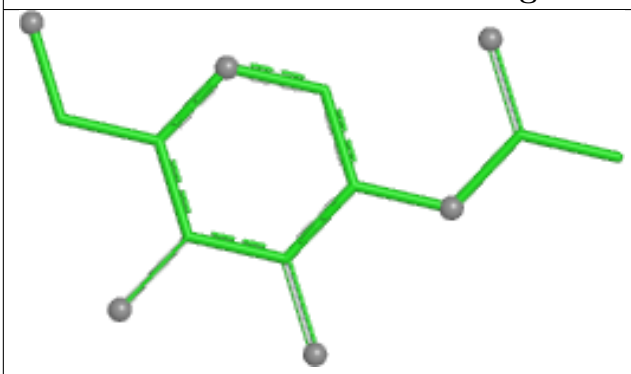


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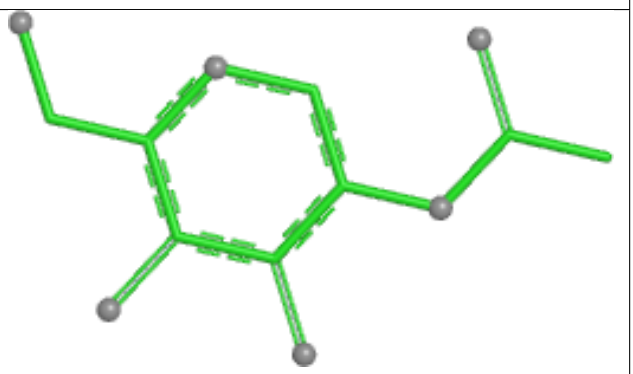


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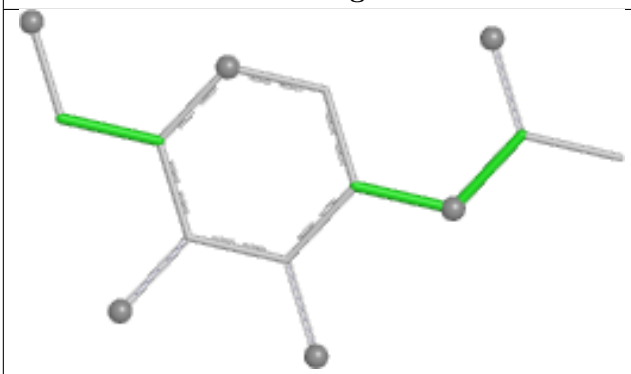
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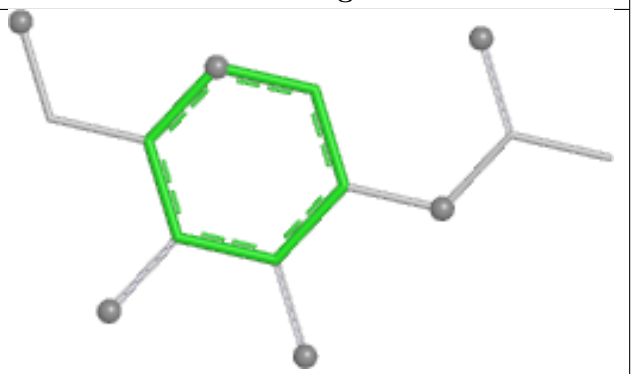
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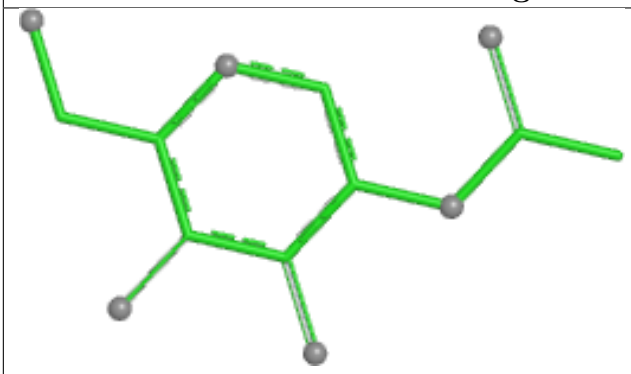


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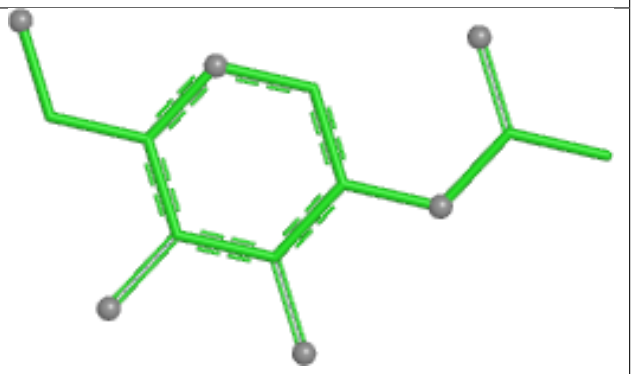


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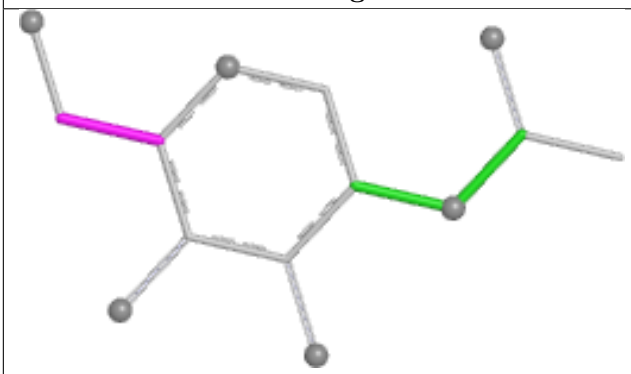
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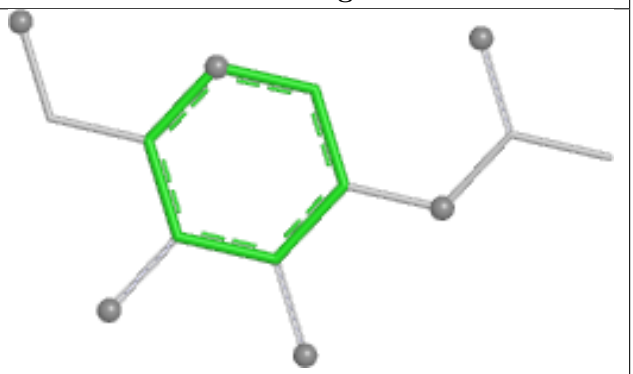
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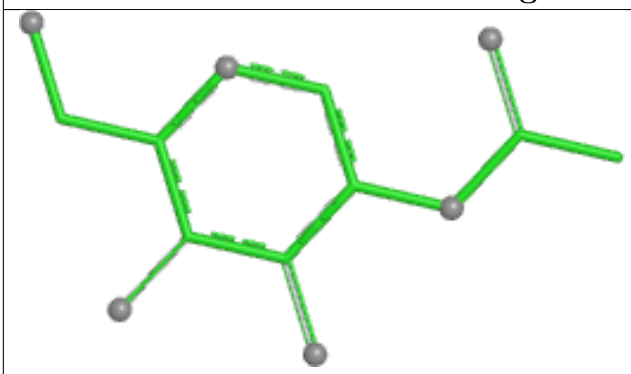


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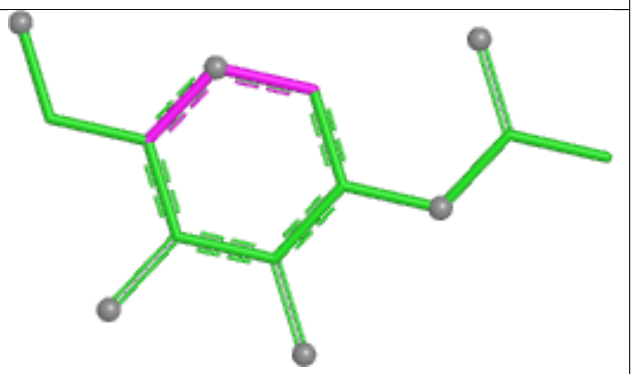


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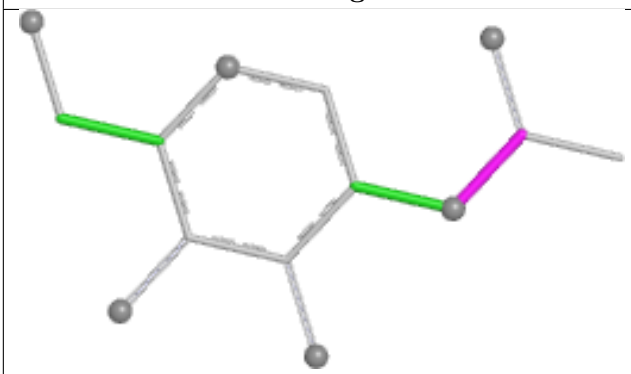
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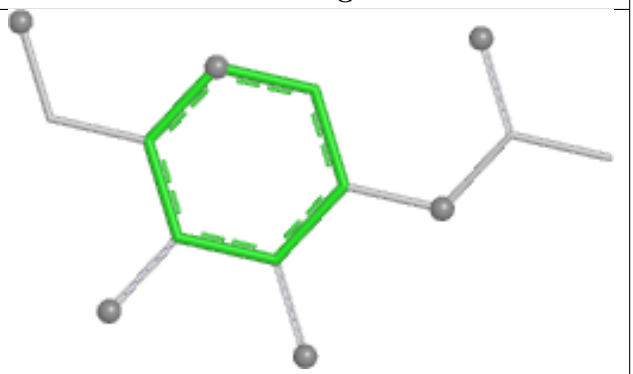
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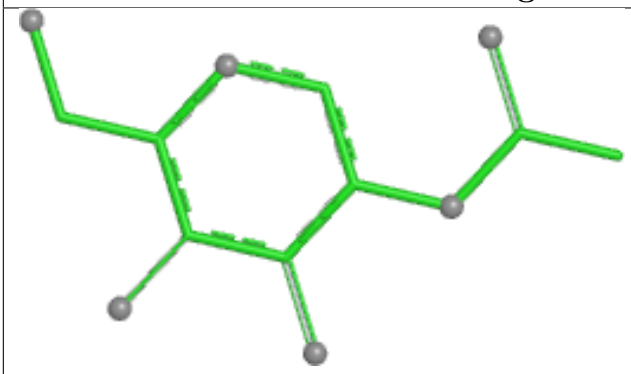


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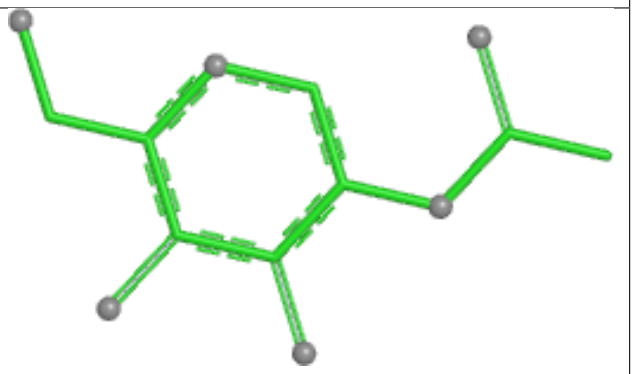


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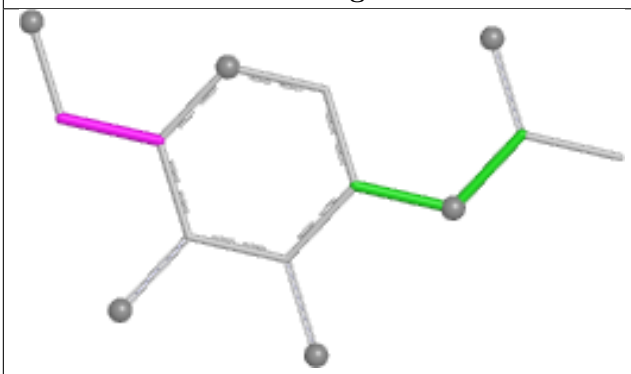
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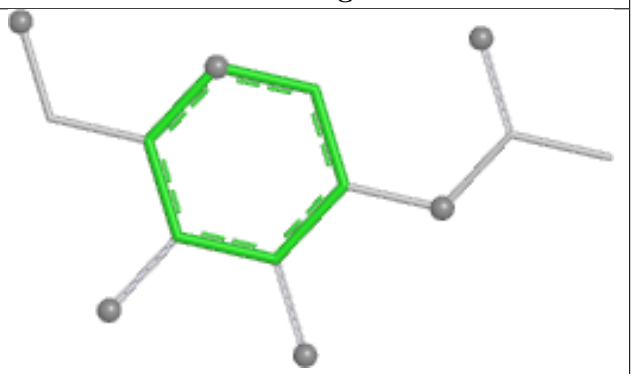
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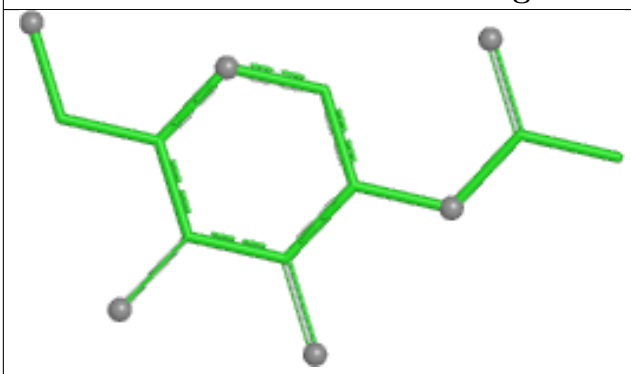


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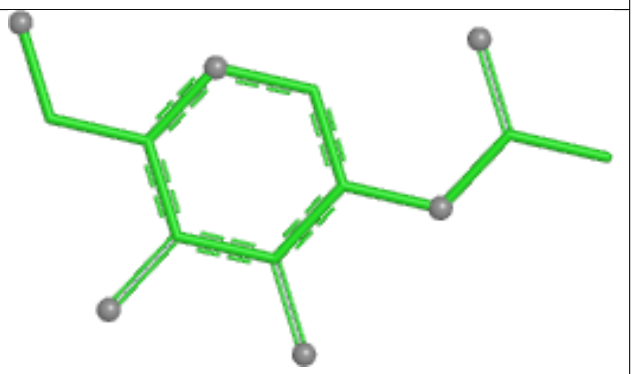


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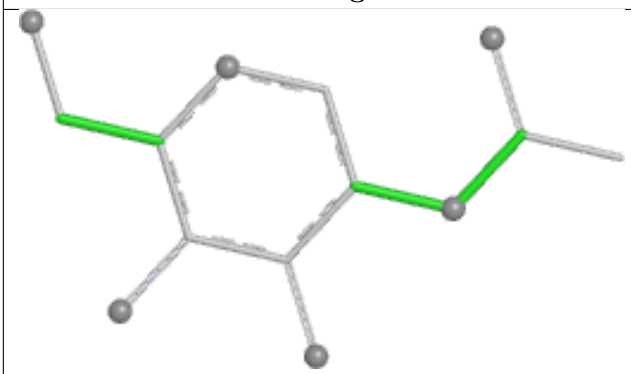
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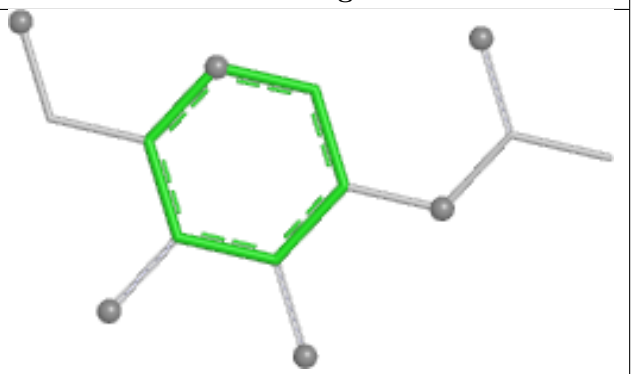
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Bond angles

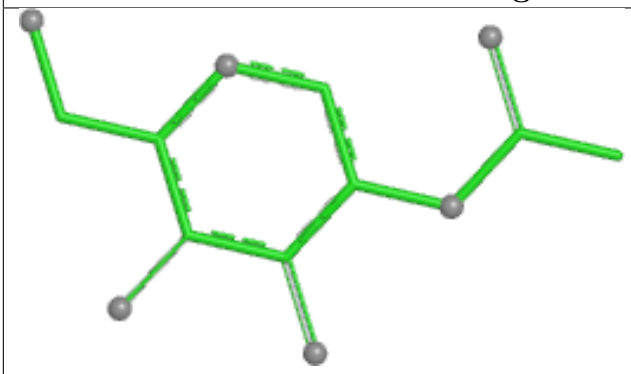


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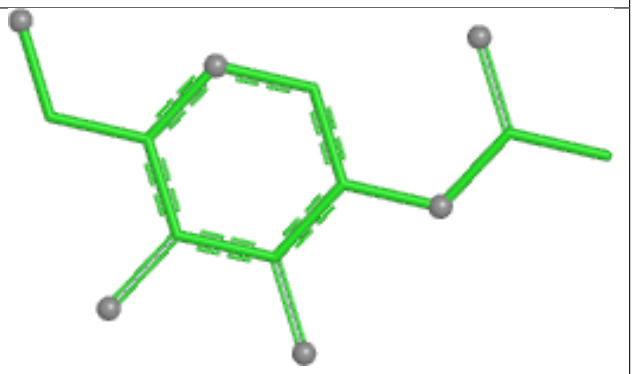


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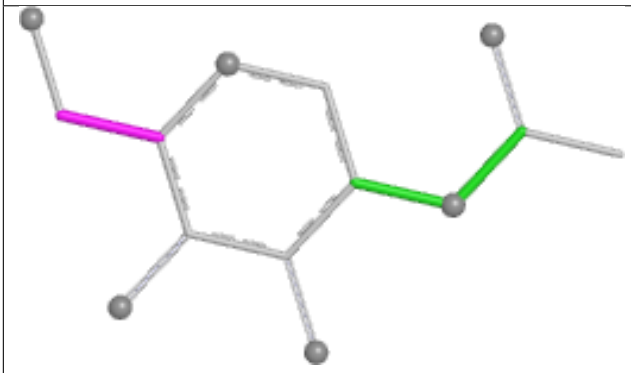
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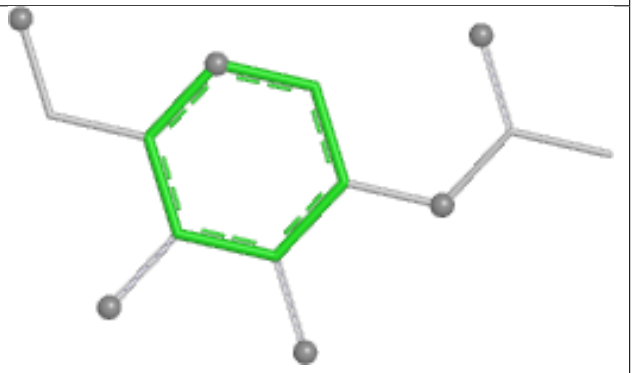
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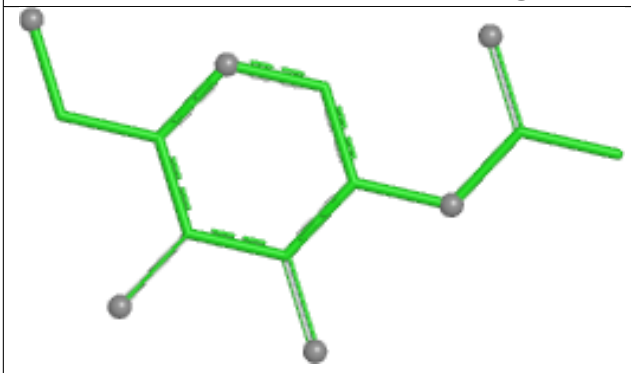


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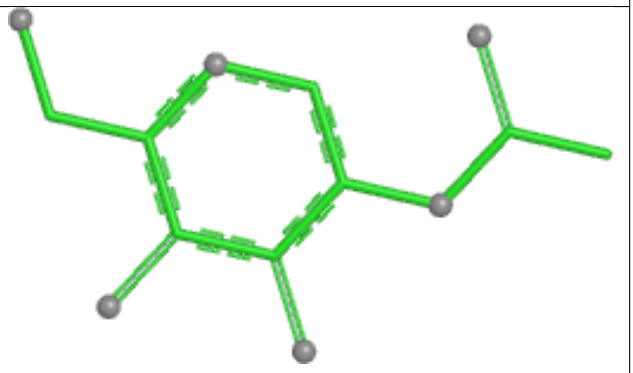


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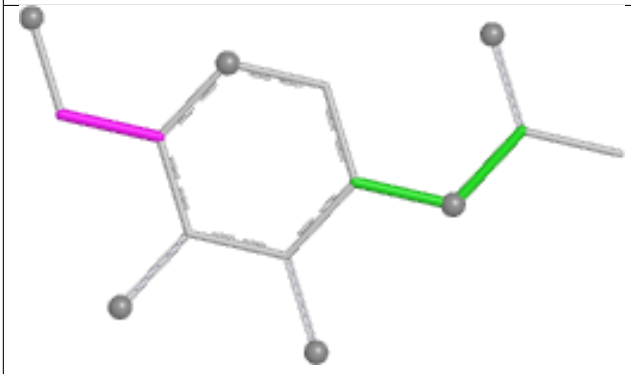
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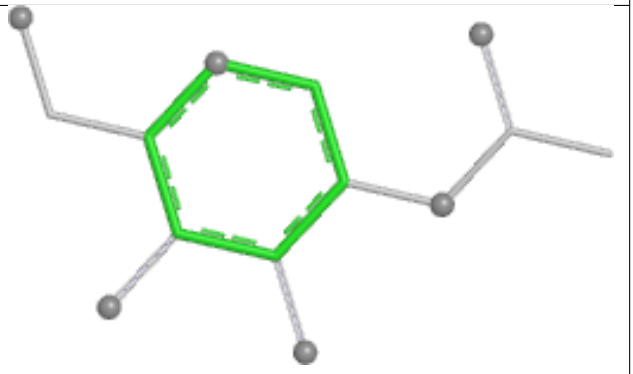
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Bond angles

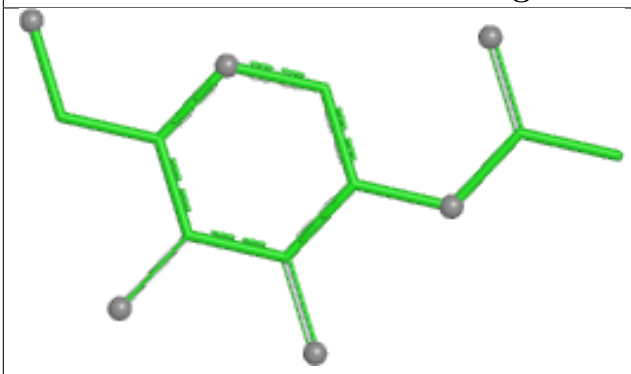


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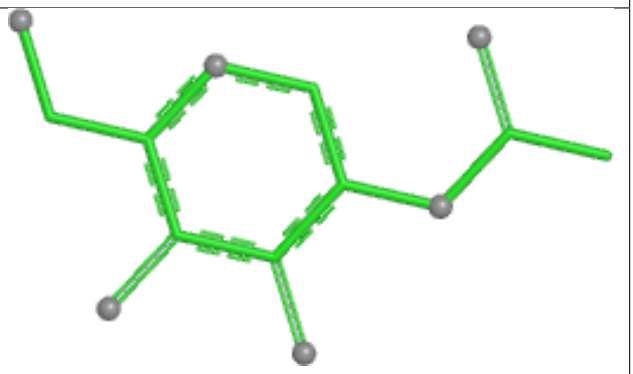


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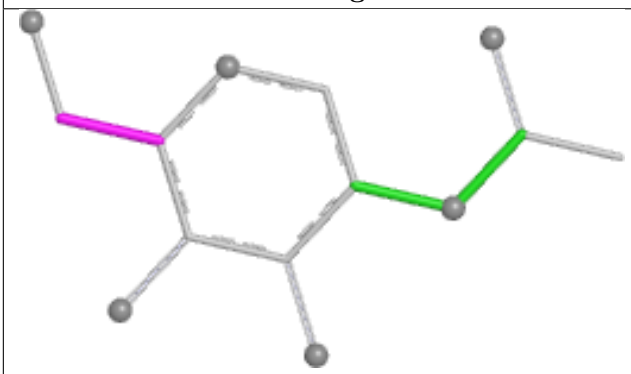
Ligand NAG E 1406



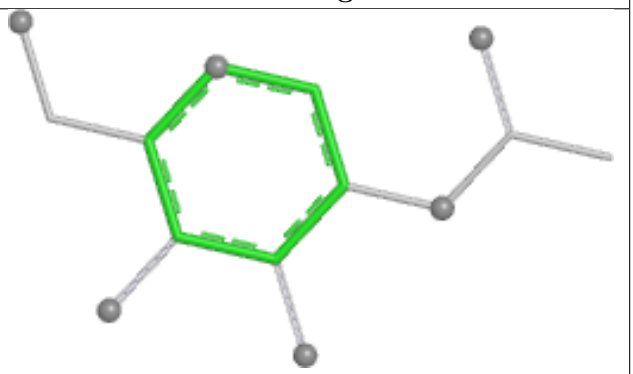
Bond lengths



Bond angles

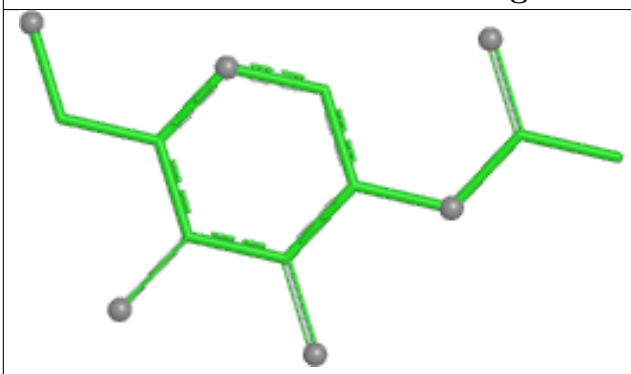


Torsions

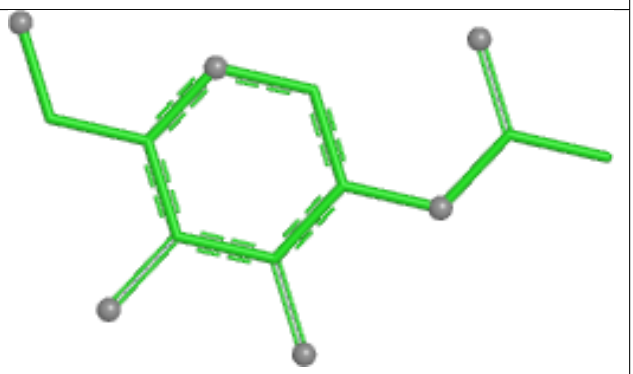


Rings

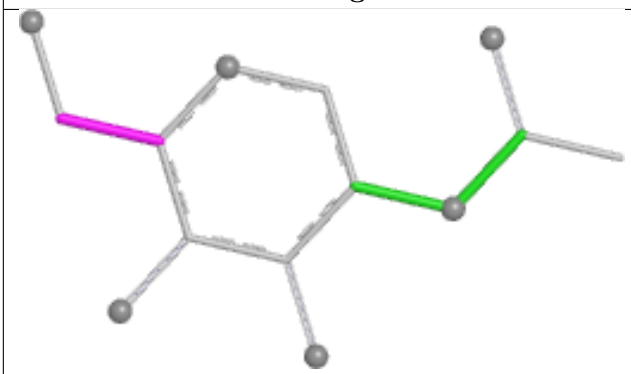
Ligand NAG G 1404



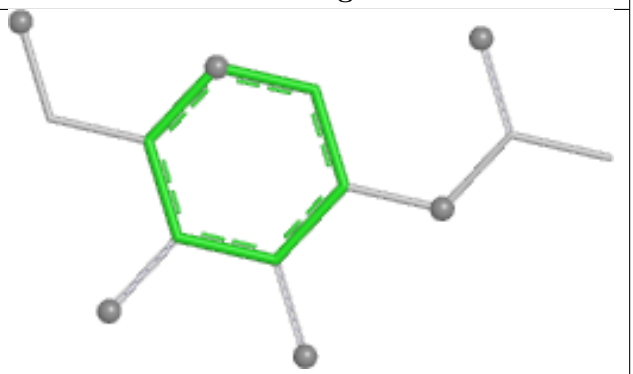
Bond lengths



Bond angles

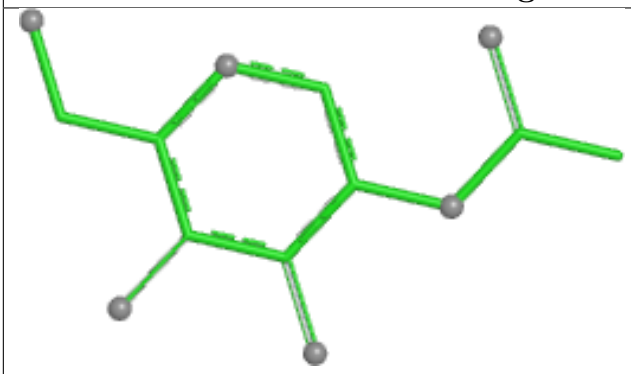


Torsions

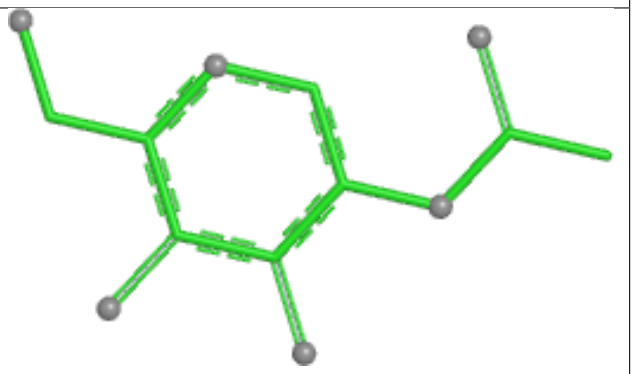


Rings

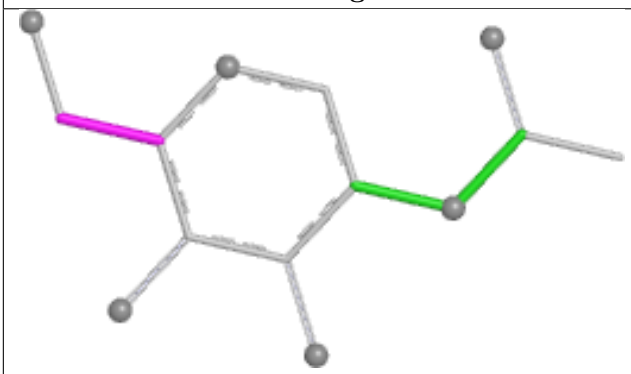
Ligand NAG I 1402



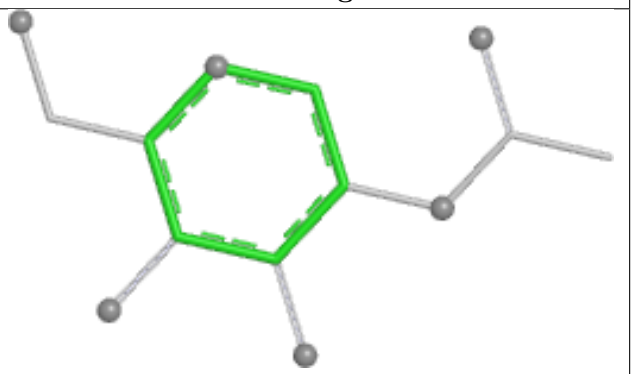
Bond lengths



Bond angles

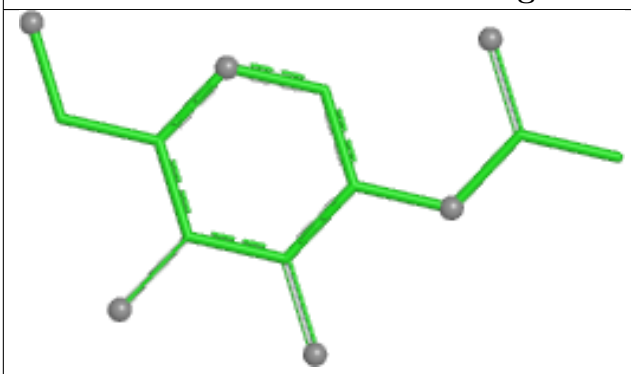


Torsions

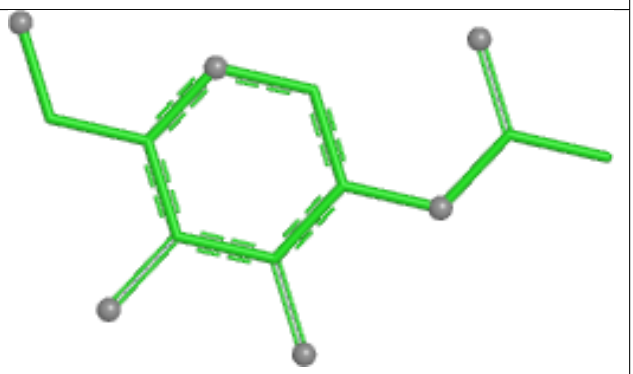


Rings

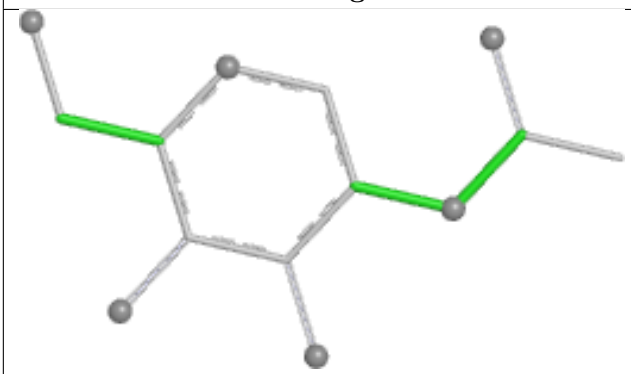
Ligand NAG I 1407



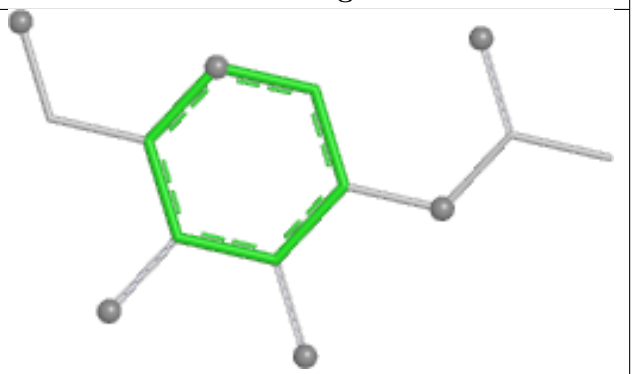
Bond lengths



Bond angles

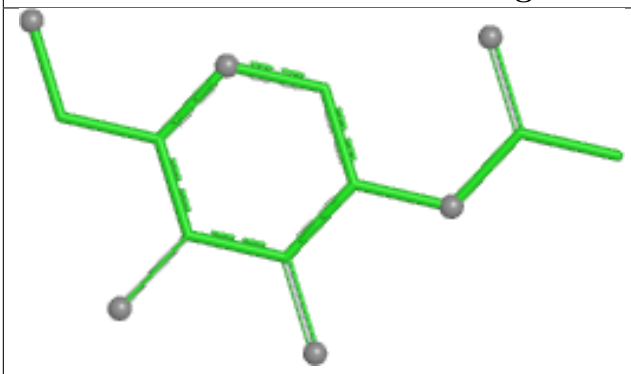


Torsions

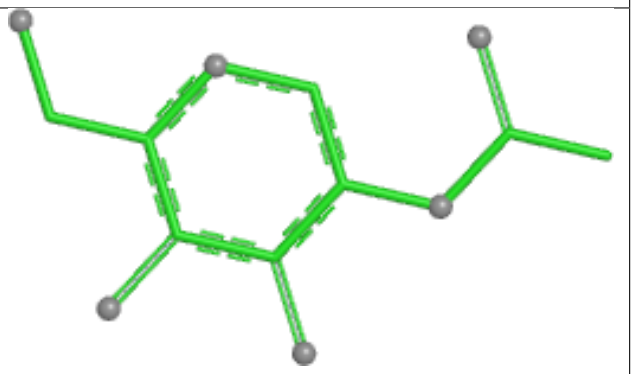


Rings

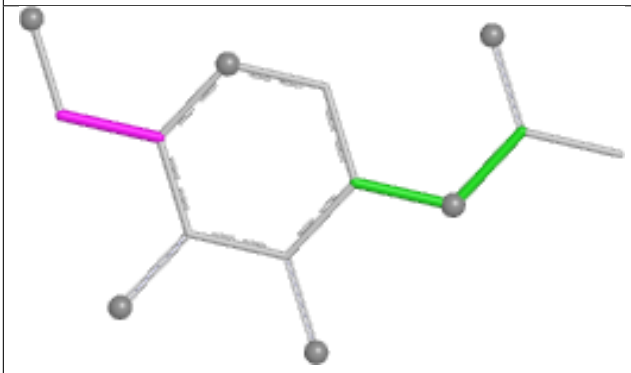
Ligand NAG J 1402



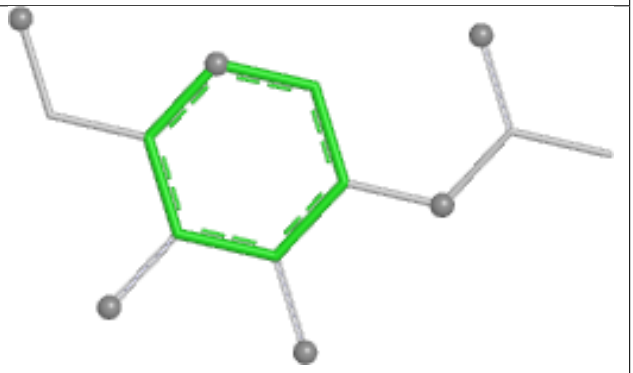
Bond lengths



Bond angles

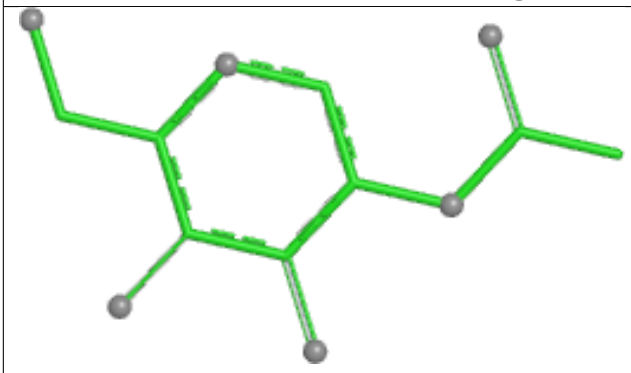


Torsions

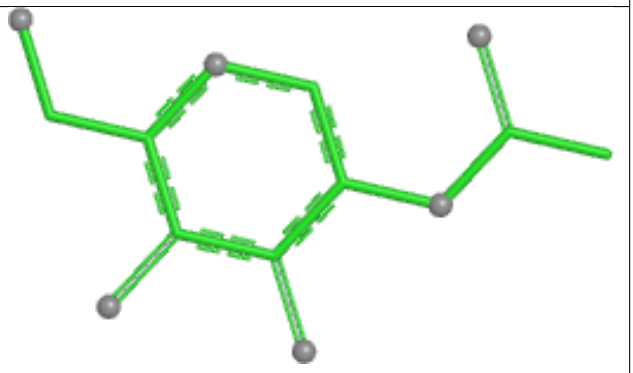


Rings

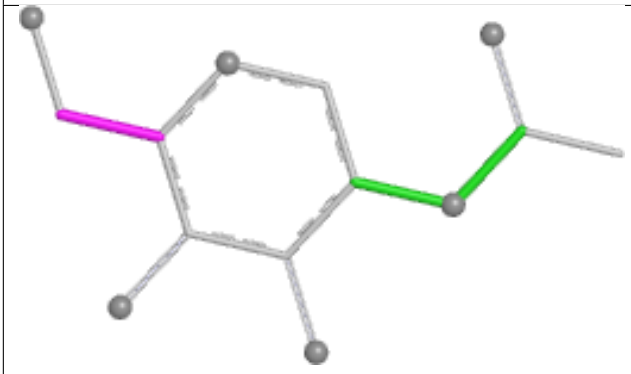
Ligand NAG H 1404



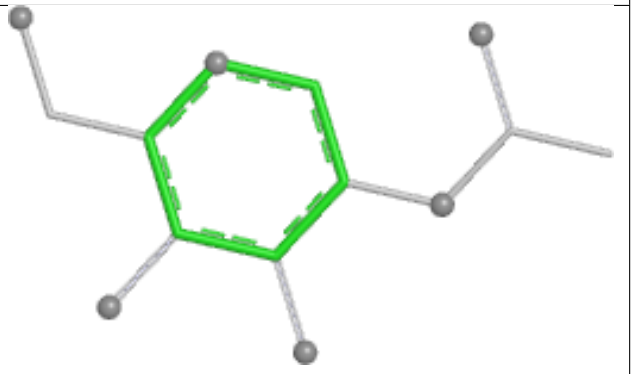
Bond lengths



Bond angles

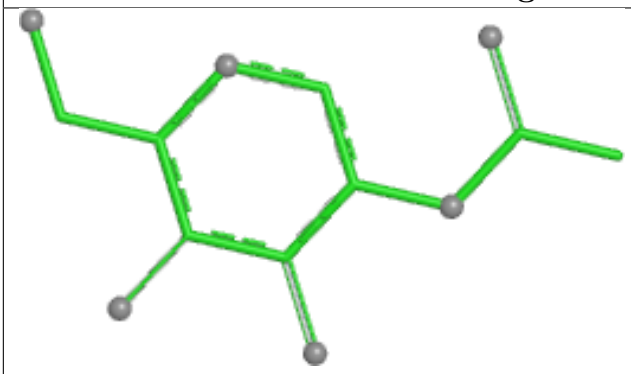


Torsions

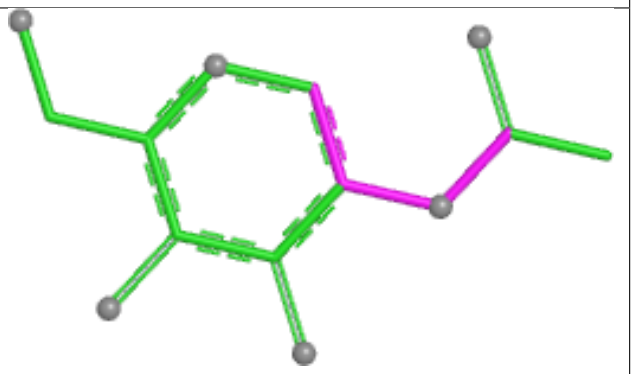


Rings

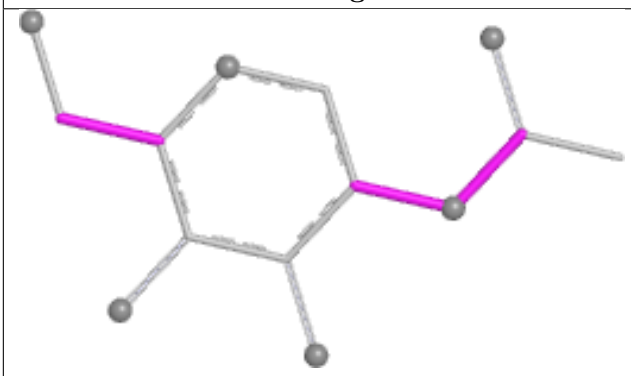
Ligand NAG I 1405



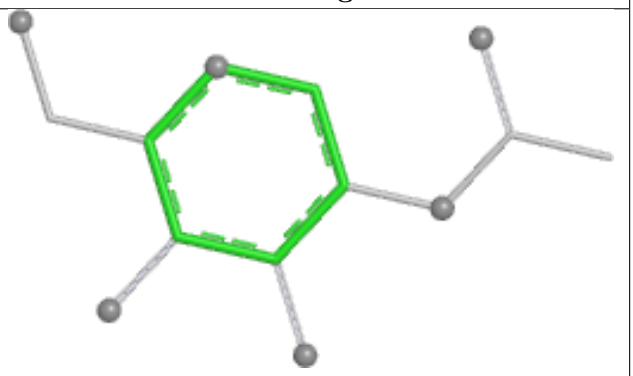
Bond lengths



Bond angles

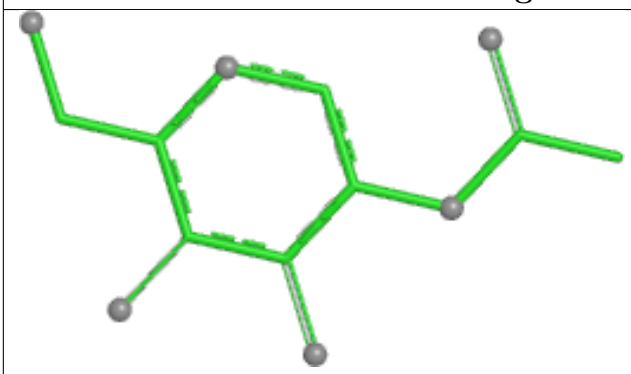


Torsions

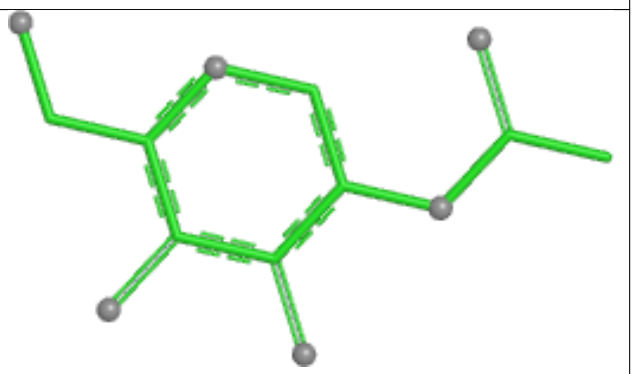


Rings

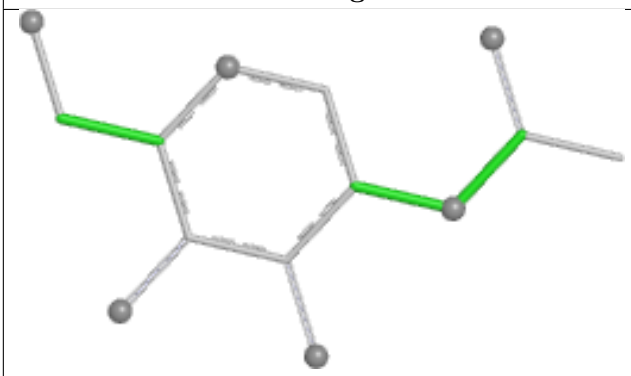
Ligand NAG J 1407



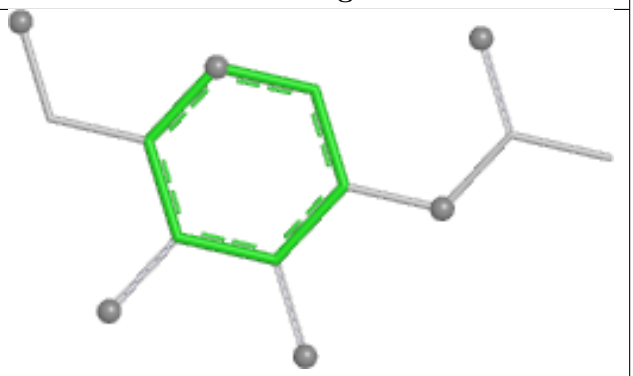
Bond lengths



Bond angles

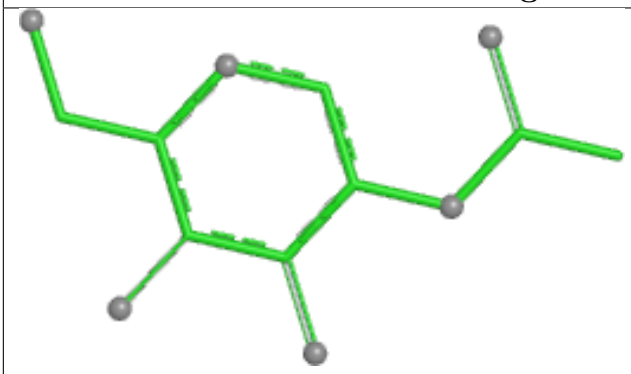


Torsions

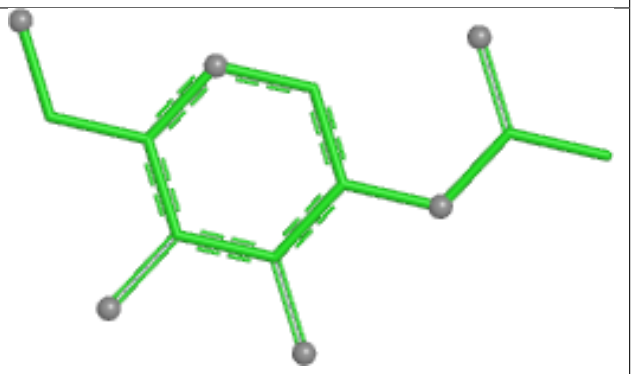


Rings

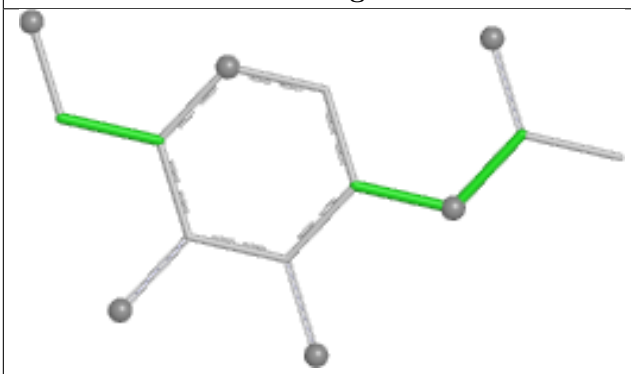
Ligand NAG C 704



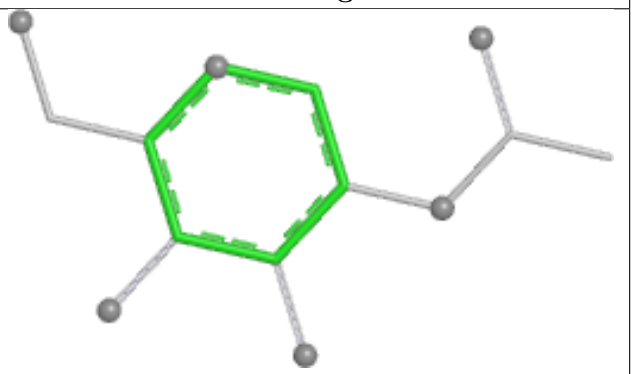
Bond lengths



Bond angles

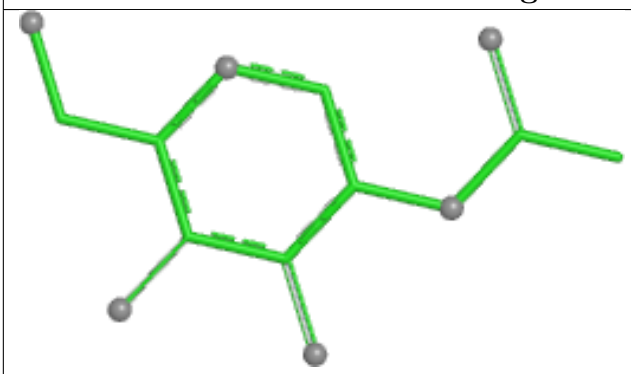


Torsions

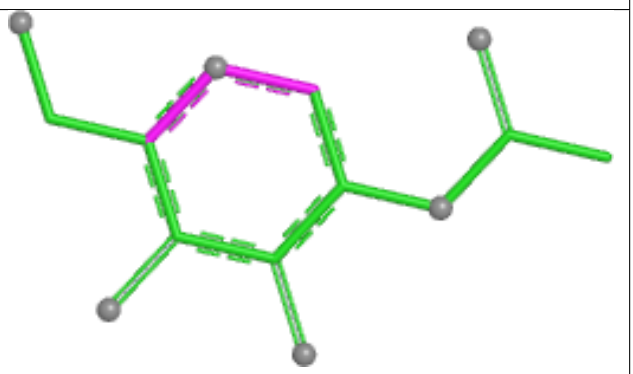


Rings

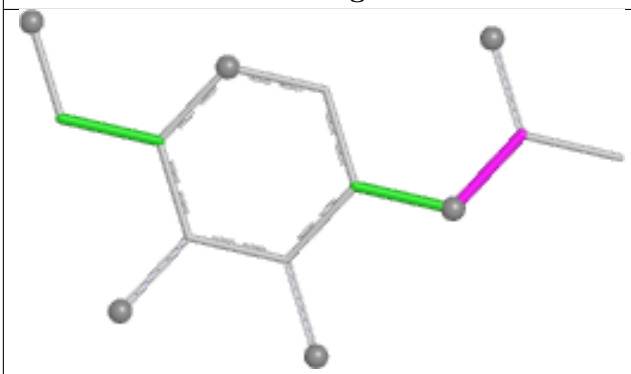
Ligand NAG C 703



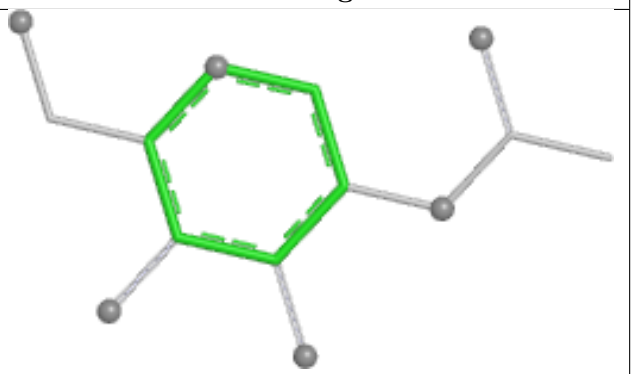
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

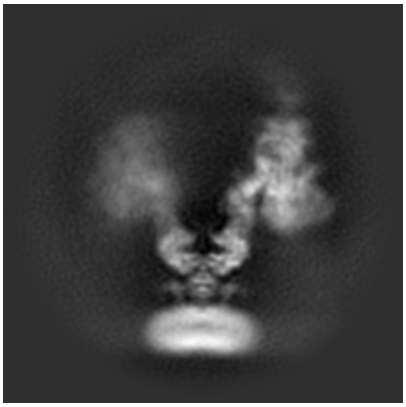
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30888. These allow visual inspection of the internal detail of the map and identification of artifacts.

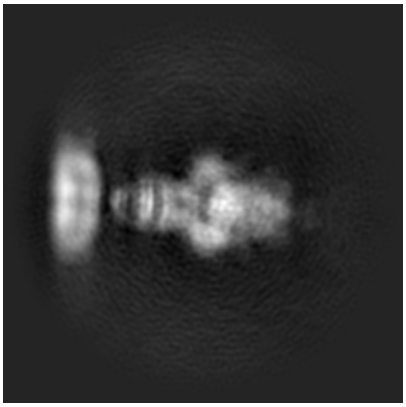
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

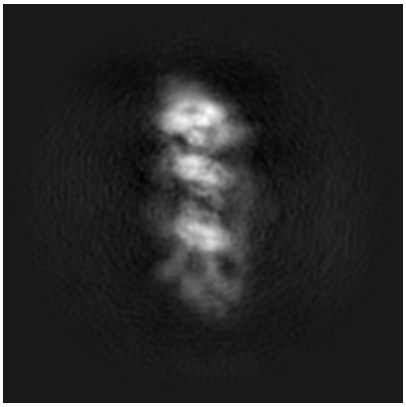
6.1.1 Primary map



X



Y

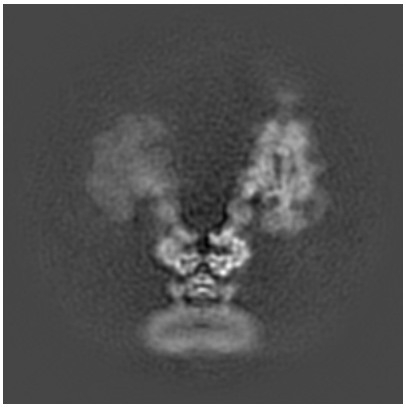


Z

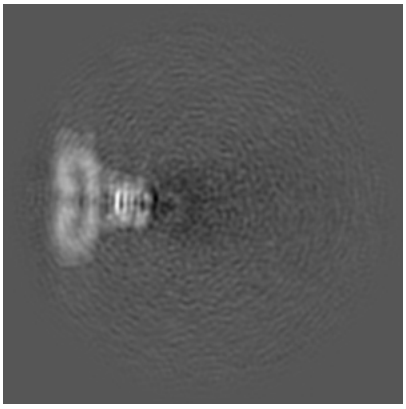
The images above show the map projected in three orthogonal directions.

6.2 Central slices

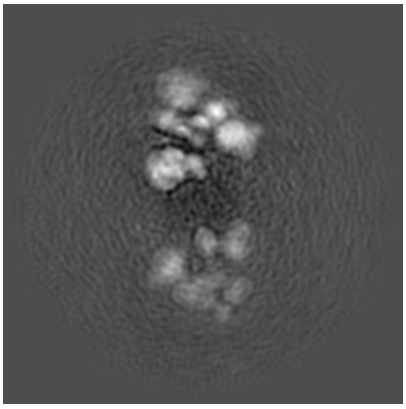
6.2.1 Primary map



X Index: 240



Y Index: 240

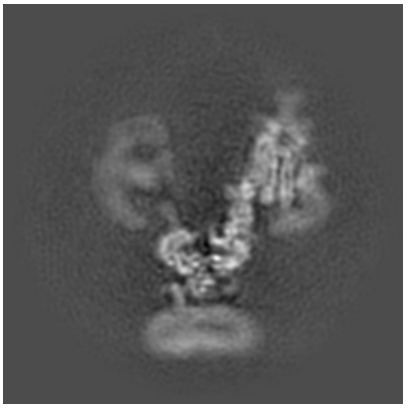


Z Index: 240

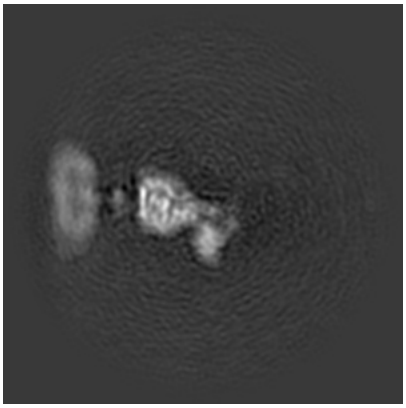
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

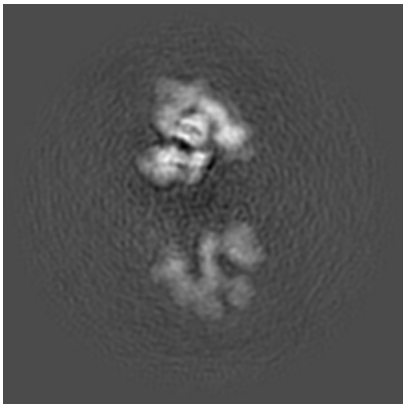
6.3.1 Primary map



X Index: 231



Y Index: 279



Z Index: 253

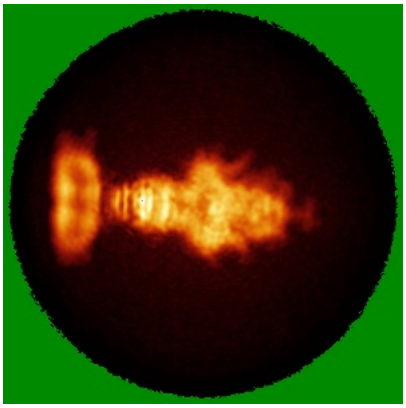
The images above show the largest variance slices of the map in three orthogonal directions.

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

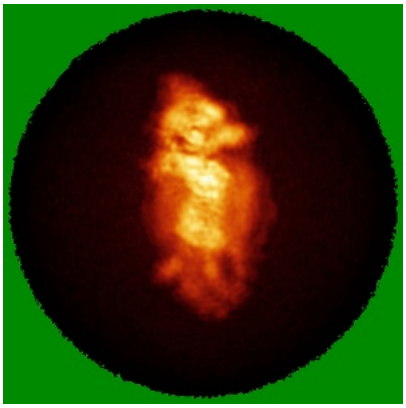
6.4.1 Primary map



X



Y

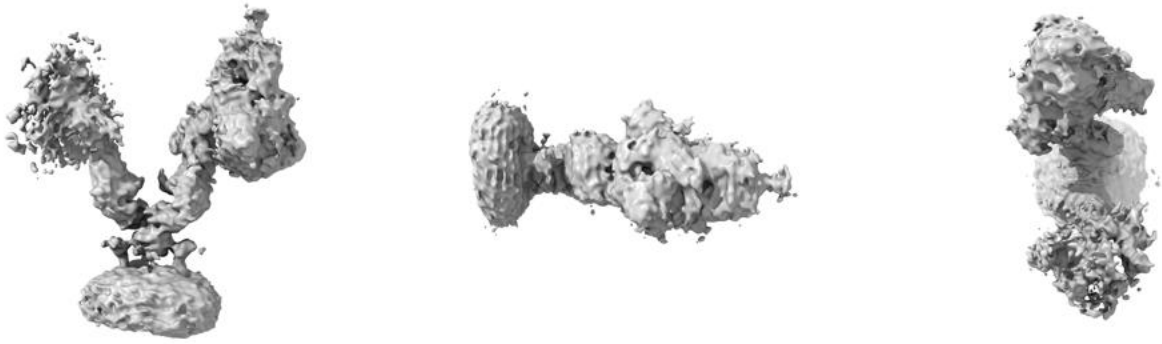


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

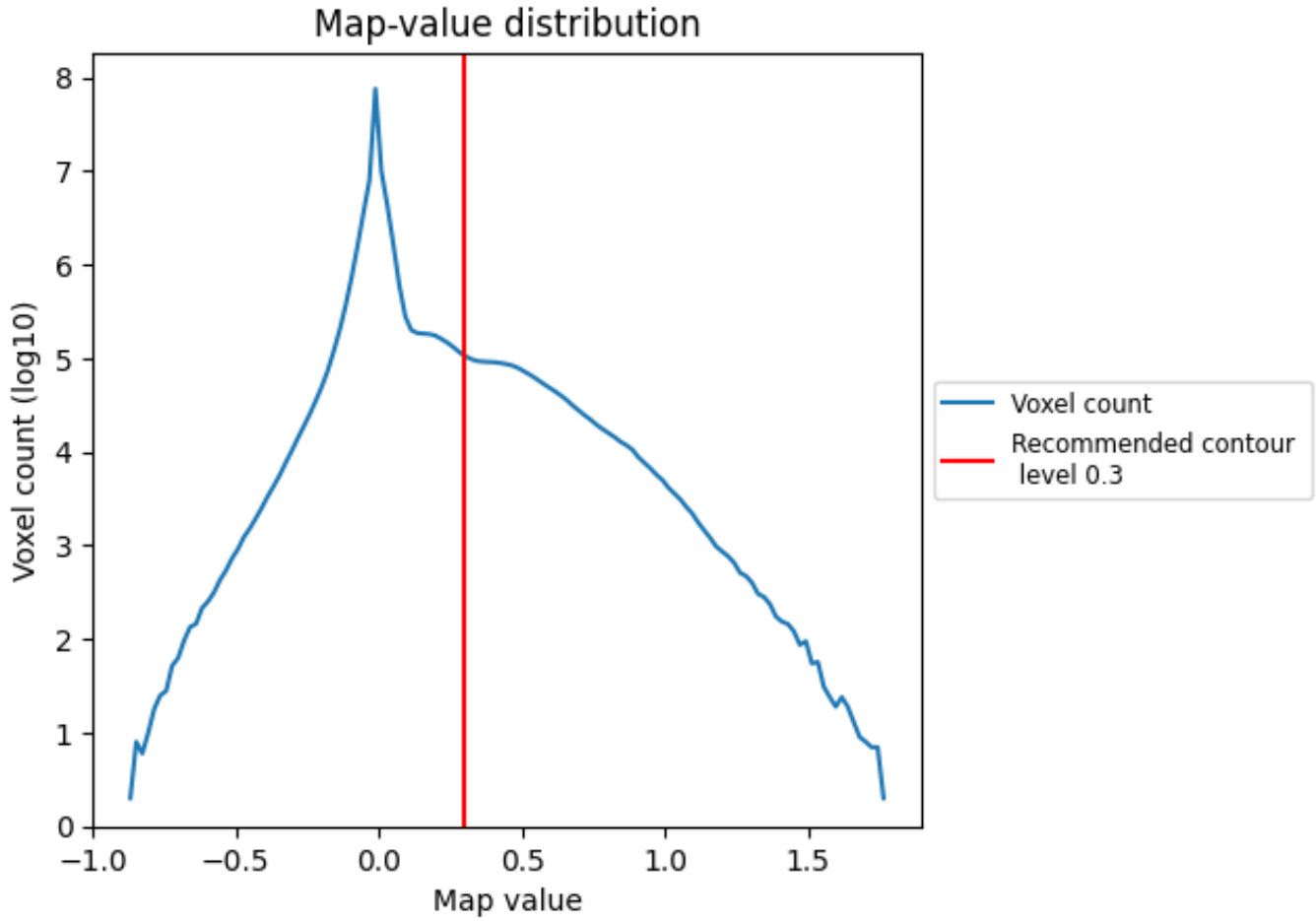
6.6 Mask visualisation (i)

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

7 Map analysis

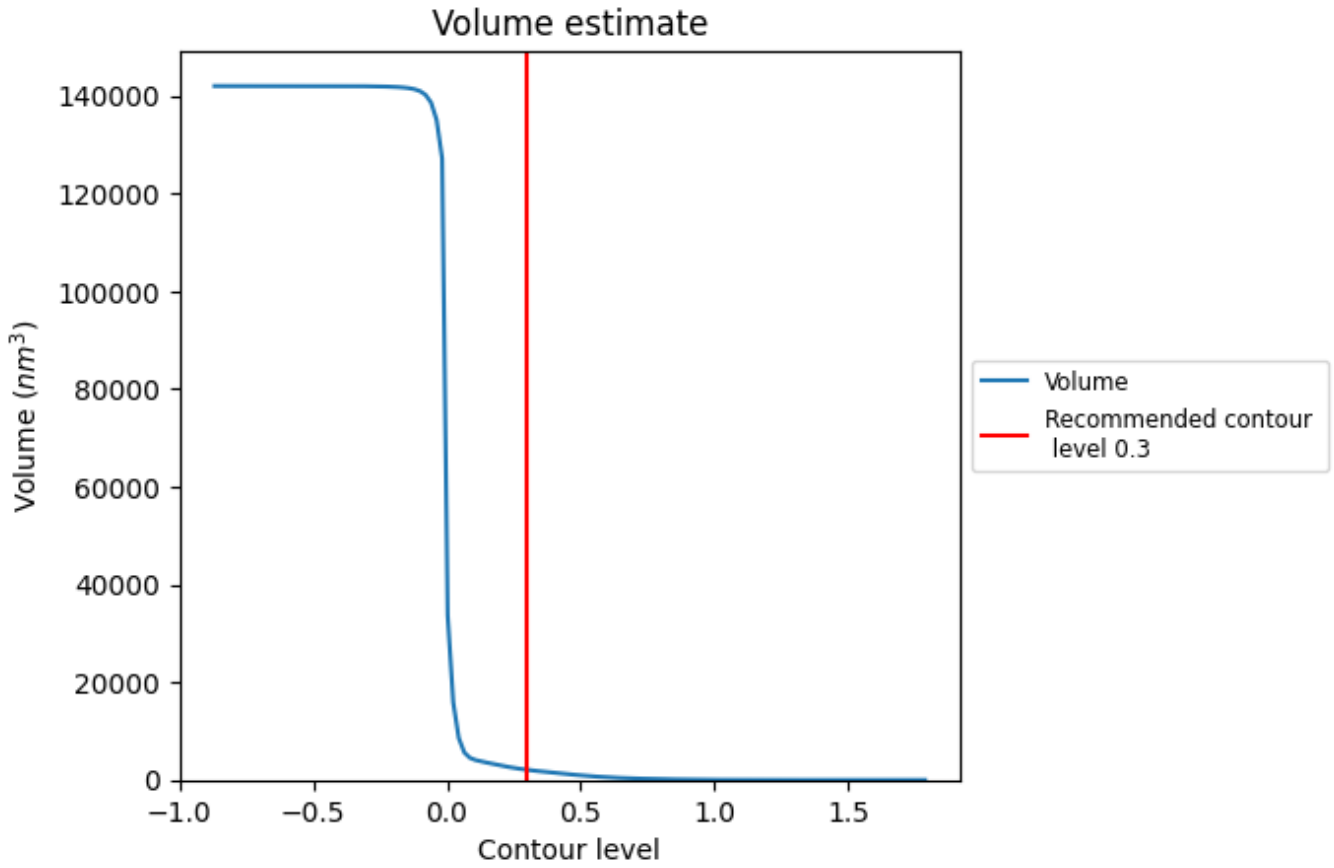
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

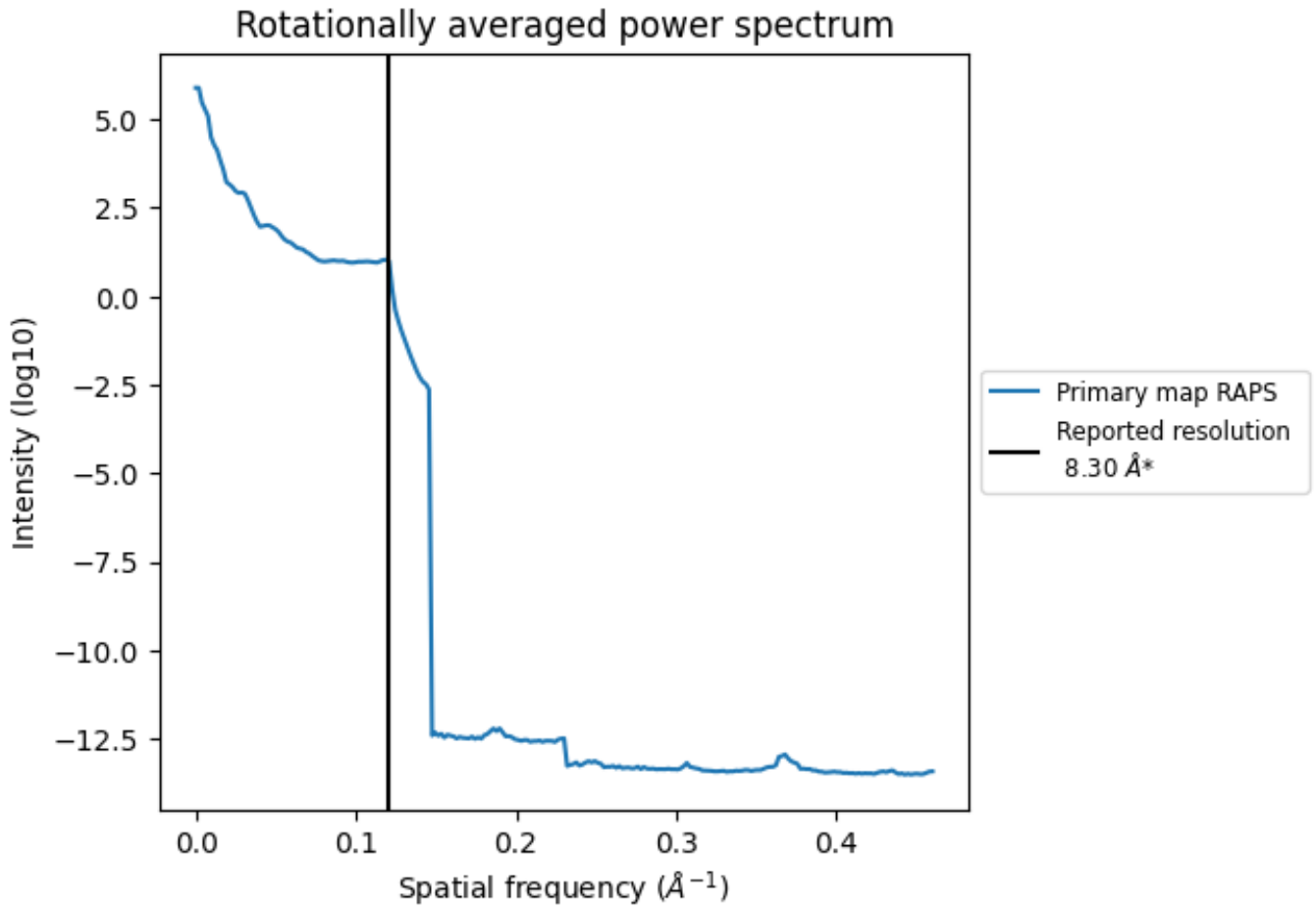
7.2 Volume estimate



The volume at the recommended contour level is 2071 nm^3; this corresponds to an approximate mass of 1871 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 0.120 $Å^{-1}$

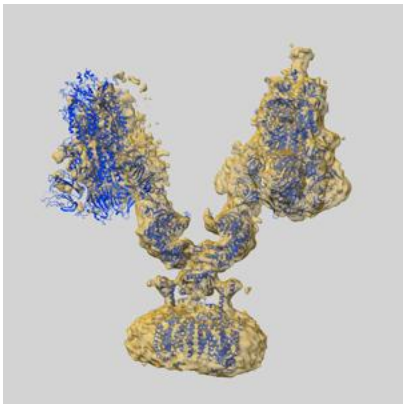
8 Fourier-Shell correlation

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

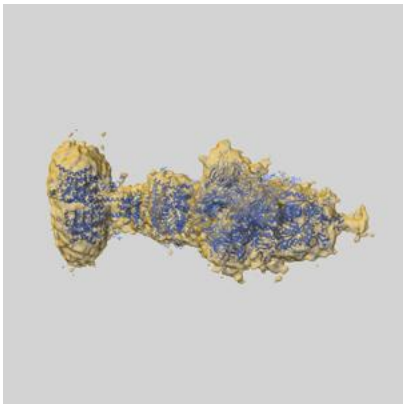
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30888 and PDB model 7DWX. Per-residue inclusion information can be found in section 3 on page 18.

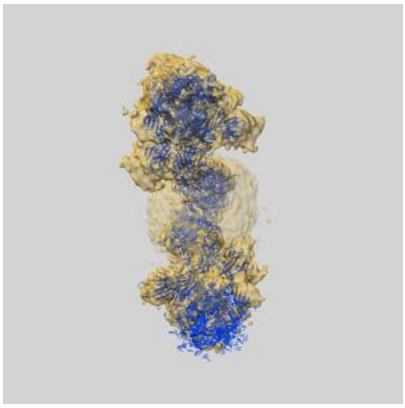
9.1 Map-model overlay



X



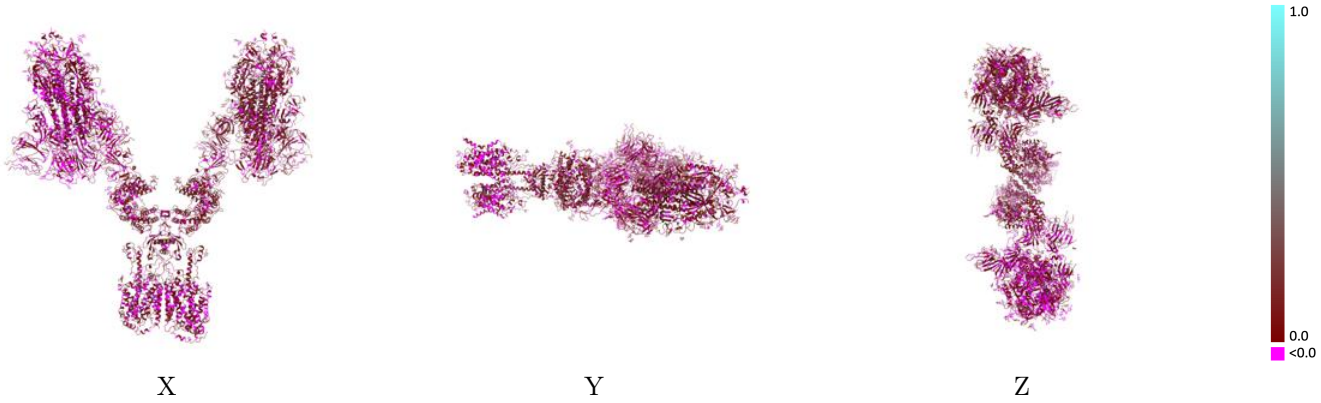
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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)

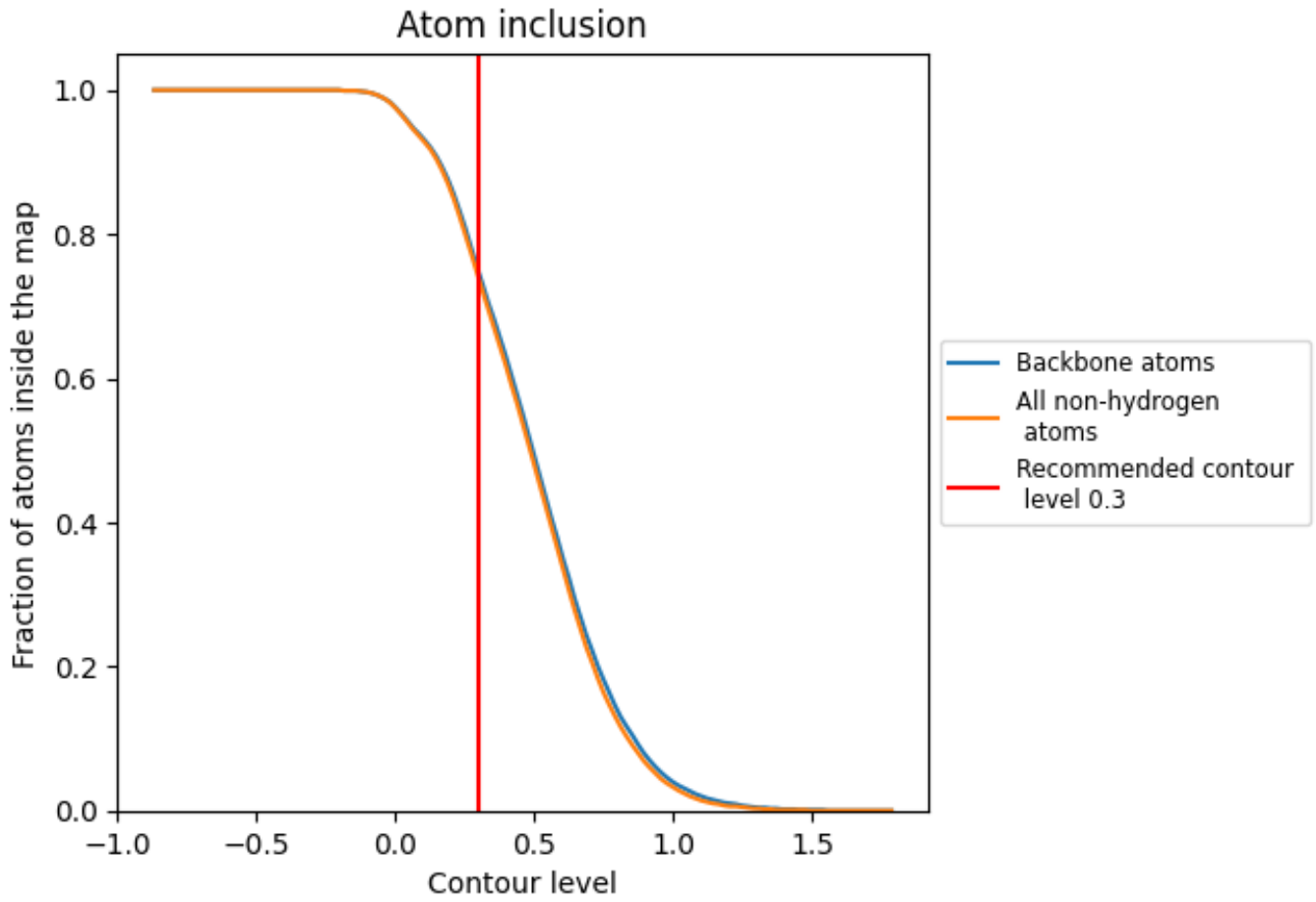


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 74% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7380	0.0590
0	0.0000	-0.1670
1	0.0000	0.2380
2	0.0000	-0.0390
3	0.0000	0.0190
4	0.0360	0.2120
5	0.6070	0.0500
6	0.0000	0.0020
7	0.0000	-0.2070
8	0.1070	-0.0560
9	0.0360	-0.0570
A	0.9270	0.0490
AA	0.0000	-0.0820
B	0.9440	0.1070
BA	0.0000	-0.0660
C	0.9090	0.0470
CA	0.0000	0.1500
D	0.9070	0.0910
DA	0.0000	-0.0150
E	0.9640	0.0800
EA	0.0000	-0.0910
F	0.9470	0.0870
FA	0.0000	-0.0470
G	0.9250	0.0690
H	0.5640	0.0340
I	0.4230	0.0240
J	0.1580	0.0150
K	0.5360	0.0770
L	0.7140	0.0810
M	0.8210	0.0720
N	1.0000	0.0400
O	0.2140	-0.0370
P	0.8210	0.0760
Q	0.8210	0.0990
R	0.5360	0.0400



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Chain	Atom inclusion	Q-score
S	0.2860	0.1170
T	0.7860	0.0600
U	0.7860	0.0600
V	0.2500	0.0480
W	0.9290	0.0700
X	1.0000	0.2210
Y	1.0000	0.2510
Z	1.0000	0.1410
a	0.8930	0.0060
b	0.8210	0.0300
c	0.5710	0.0880
d	0.4640	-0.0740
e	0.5710	0.1110
f	0.3930	0.0910
g	0.8210	-0.0920
h	0.9290	0.0370
i	0.8210	0.1070
j	0.5710	0.0380
k	0.4290	-0.0010
l	0.7860	0.0880
m	0.9640	0.1240
n	1.0000	0.1630
o	0.5000	-0.0350
p	1.0000	0.1070
q	1.0000	0.1420
r	0.7500	0.0740
s	0.6790	0.0080
t	0.7500	0.0860
u	0.2500	0.0420
v	0.6430	0.0270
w	0.1430	-0.0040
x	0.0000	0.1240
y	0.0000	-0.1520
z	0.0000	-0.1580