wwPDB EM Validation Summary Report

Aug 6, 2022 – 07:13 am BST

PDB ID	:	7Z3A
EMDB ID	:	EMD-14474
Title	:	AMC009 SOSIPv5.2 in complex with Fabs ACS101 and ACS124
Authors	:	van Schooten, J.; Ward, A.
Deposited on	:	2022-03-02
Resolution	:	3.95 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:

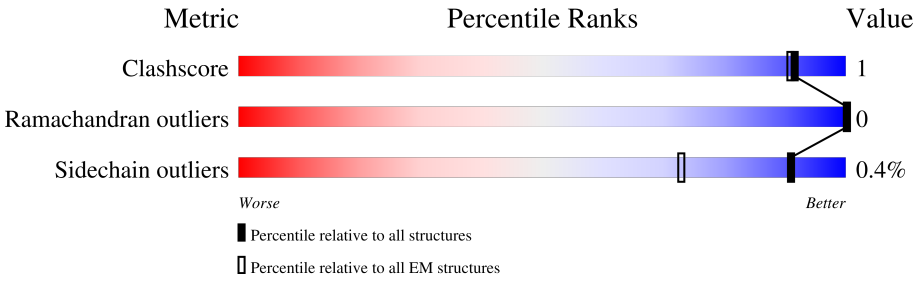
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.95 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	482	83% 6% 11%
1	C	482	82% 7% 11%
1	D	482	81% 8% 11%
2	B	154	75% 19%
2	E	154	70% 27%
2	F	154	69% 5% 26%
3	G	124	11% 90% 6%
3	M	124	6% 90% 6%

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Mol	Chain	Length	Quality of chain
4	I	108	16% 95%
4	O	108	6% 96%
5	H	126	90% 9%
5	J	126	21% 92% 7%
5	K	126	87% 8%
6	L	108	95%
6	N	108	35% 94% 5%
6	P	108	94%
7	2	2	50% 100%
7	9	2	100% 100%
7	AA	2	50% 100%
7	Q	2	50% 100%
7	W	2	50% 100%
7	g	2	100% 100%
7	l	2	50% 100%
7	s	2	50% 100%
7	u	2	100% 100%
7	v	2	50% 100%
8	0	3	100%
8	1	3	100%
8	3	3	67% 100%
8	4	3	33% 100%
8	5	3	33% 100%
8	6	3	33% 100%
8	7	3	67% 100%

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Mol	Chain	Length	Quality of chain
8	8	3	67% 100%
8	R	3	67% 100%
8	T	3	67% 100%
8	U	3	100%
8	V	3	100%
8	X	3	67% 100%
8	Y	3	33% 100%
8	Z	3	33% 100%
8	a	3	67% 100%
8	b	3	67% 100%
8	c	3	67% 100%
8	e	3	67% 100%
8	f	3	67% 100%
8	h	3	67% 100%
8	i	3	67% 100%
8	j	3	100%
8	k	3	100%
8	m	3	67% 100%
8	n	3	67% 100%
8	o	3	100%
8	p	3	67% 100%
8	q	3	67% 100%
8	r	3	67% 100%
8	t	3	67% 100%
8	w	3	67% 100%

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Mol	Chain	Length	Quality of chain
8	x	3	100%
8	z	3	67% 100%
9	S	5	80% 100%
9	y	5	60% 100%
10	d	3	67% 100%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 24000 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 AMC009 SOSIPv5.2 envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	429	Total	C	N	O	S	0	0
			3403	2149	598	629	27		
1	C	429	Total	C	N	O	S	0	0
			3403	2149	598	629	27		
1	D	429	Total	C	N	O	S	0	0
			3403	2149	598	629	27		

- Molecule 2 is a protein called AMC009 SOSIP.v5.2 envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	124	Total	C	N	O	S	0	0
			992	623	172	190	7		
2	E	113	Total	C	N	O	S	0	0
			898	566	158	167	7		
2	F	114	Total	C	N	O	S	0	0
			907	571	159	170	7		

- Molecule 3 is a protein called ACS124 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	123	Total	C	N	O	S	0	0
			969	618	164	183	4		
3	M	123	Total	C	N	O	S	0	0
			969	618	164	183	4		

- Molecule 4 is a protein called ACS124 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	108	Total	C	N	O	S	0	0
			820	510	142	165	3		
4	O	108	Total	C	N	O	S	0	0
			820	510	142	165	3		

- Molecule 5 is a protein called ACS101 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	125	Total	C	N	O	S	0	0
			990	630	171	186	3		
5	J	125	Total	C	N	O	S	0	0
			990	630	171	186	3		
5	K	125	Total	C	N	O	S	0	0
			990	630	171	186	3		

- Molecule 6 is a protein called ACS101 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	106	Total	C	N	O	S	0	0
			795	502	130	160	3		
6	N	106	Total	C	N	O	S	0	0
			795	502	130	160	3		
6	P	106	Total	C	N	O	S	0	0
			795	502	130	160	3		

- Molecule 7 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
7	Q	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	g	2	Total	C	N	O	0	0
			28	16	2	10		
7	l	2	Total	C	N	O	0	0
			28	16	2	10		
7	s	2	Total	C	N	O	0	0
			28	16	2	10		
7	u	2	Total	C	N	O	0	0
			28	16	2	10		
7	v	2	Total	C	N	O	0	0
			28	16	2	10		
7	2	2	Total	C	N	O	0	0
			28	16	2	10		

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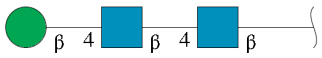
Mol	Chain	Residues	Atoms				AltConf	Trace
7	9	2	Total 28	C 16	N 2	O 10	0	0
7	AA	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	R	3	Total 39	C 22	N 2	O 15	0	0
8	T	3	Total 39	C 22	N 2	O 15	0	0
8	U	3	Total 39	C 22	N 2	O 15	0	0
8	V	3	Total 39	C 22	N 2	O 15	0	0
8	X	3	Total 39	C 22	N 2	O 15	0	0
8	Y	3	Total 39	C 22	N 2	O 15	0	0
8	Z	3	Total 39	C 22	N 2	O 15	0	0
8	a	3	Total 39	C 22	N 2	O 15	0	0
8	b	3	Total 39	C 22	N 2	O 15	0	0
8	c	3	Total 39	C 22	N 2	O 15	0	0
8	e	3	Total 39	C 22	N 2	O 15	0	0
8	f	3	Total 39	C 22	N 2	O 15	0	0
8	h	3	Total 39	C 22	N 2	O 15	0	0
8	i	3	Total 39	C 22	N 2	O 15	0	0
8	j	3	Total 39	C 22	N 2	O 15	0	0

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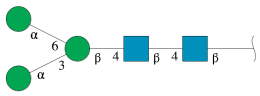
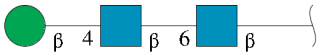
Mol	Chain	Residues	Atoms				AltConf	Trace
8	k	3	Total	C	N	O	0	0
			39	22	2	15		
8	m	3	Total	C	N	O	0	0
			39	22	2	15		
8	n	3	Total	C	N	O	0	0
			39	22	2	15		
8	o	3	Total	C	N	O	0	0
			39	22	2	15		
8	p	3	Total	C	N	O	0	0
			39	22	2	15		
8	q	3	Total	C	N	O	0	0
			39	22	2	15		
8	r	3	Total	C	N	O	0	0
			39	22	2	15		
8	t	3	Total	C	N	O	0	0
			39	22	2	15		
8	w	3	Total	C	N	O	0	0
			39	22	2	15		
8	x	3	Total	C	N	O	0	0
			39	22	2	15		
8	z	3	Total	C	N	O	0	0
			39	22	2	15		
8	0	3	Total	C	N	O	0	0
			39	22	2	15		
8	1	3	Total	C	N	O	0	0
			39	22	2	15		
8	3	3	Total	C	N	O	0	0
			39	22	2	15		
8	4	3	Total	C	N	O	0	0
			39	22	2	15		
8	5	3	Total	C	N	O	0	0
			39	22	2	15		
8	6	3	Total	C	N	O	0	0
			39	22	2	15		
8	7	3	Total	C	N	O	0	0
			39	22	2	15		
8	8	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



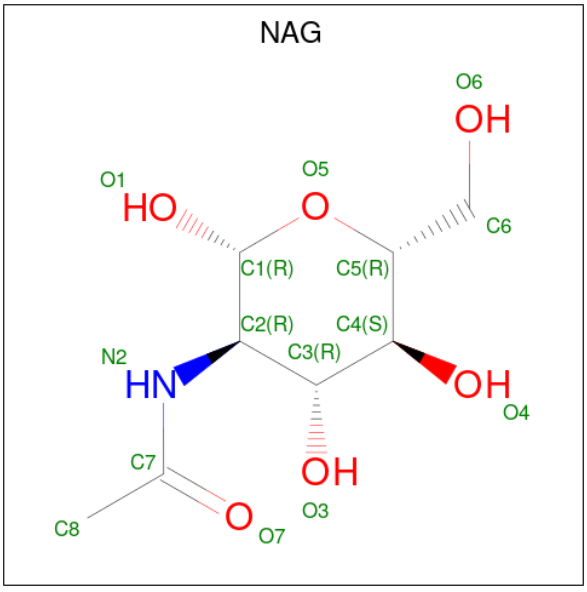
Mol	Chain	Residues	Atoms				AltConf	Trace
9	S	5	Total	C	N	O	0	0
			61	34	2	25		
9	y	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 10 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
10	d	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	N	O	0
			70	40	5	25	

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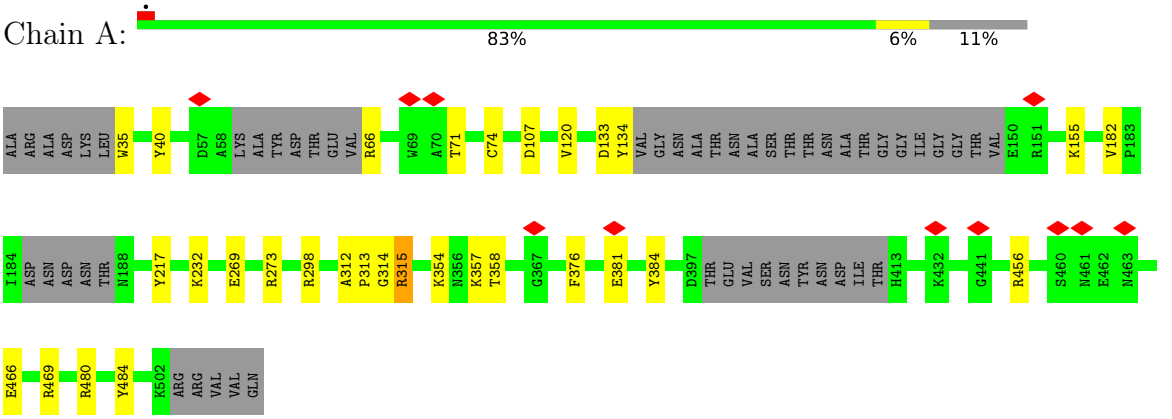
Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	N	O	0
			70	40	5	25	
11	A	1	Total	C	N	O	0
			70	40	5	25	
11	A	1	Total	C	N	O	0
			70	40	5	25	
11	A	1	Total	C	N	O	0
			70	40	5	25	
11	B	1	Total	C	N	O	0
			42	24	3	15	
11	B	1	Total	C	N	O	0
			42	24	3	15	
11	B	1	Total	C	N	O	0
			42	24	3	15	
11	C	1	Total	C	N	O	0
			42	24	3	15	
11	C	1	Total	C	N	O	0
			42	24	3	15	
11	C	1	Total	C	N	O	0
			42	24	3	15	
11	E	1	Total	C	N	O	0
			28	16	2	10	
11	E	1	Total	C	N	O	0
			28	16	2	10	
11	D	1	Total	C	N	O	0
			84	48	6	30	
11	D	1	Total	C	N	O	0
			84	48	6	30	
11	D	1	Total	C	N	O	0
			84	48	6	30	
11	D	1	Total	C	N	O	0
			84	48	6	30	
11	D	1	Total	C	N	O	0
			84	48	6	30	
11	D	1	Total	C	N	O	0
			84	48	6	30	
11	F	1	Total	C	N	O	0
			28	16	2	10	
11	F	1	Total	C	N	O	0
			28	16	2	10	

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.

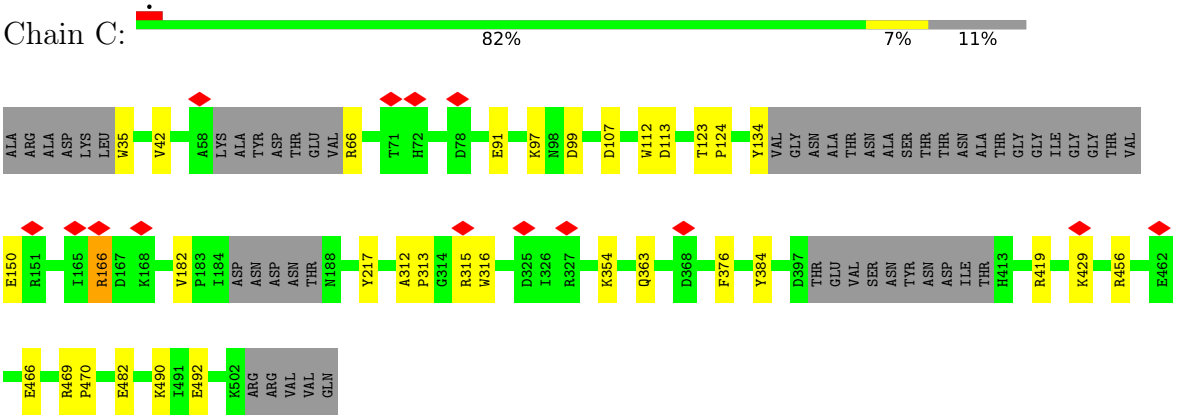
• Molecule 1: AMC009 SOSIPv5.2 envelope glycoprotein gp120

Chain A:



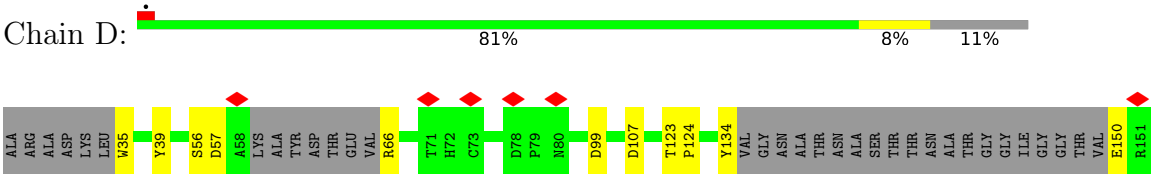
• Molecule 1: AMC009 SOSIPv5.2 envelope glycoprotein gp120

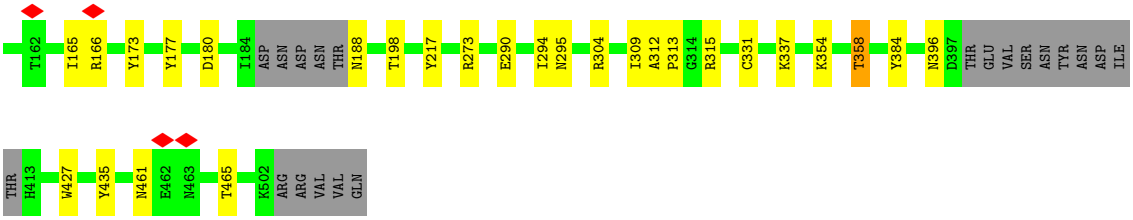
Chain C:



• Molecule 1: AMC009 SOSIPv5.2 envelope glycoprotein gp120

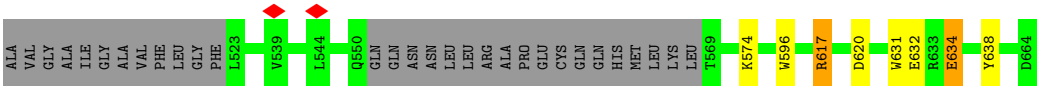
Chain D:





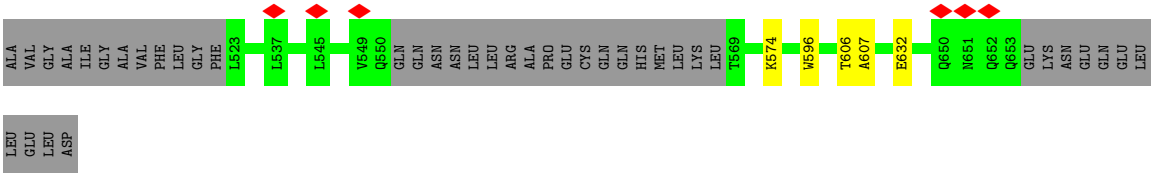
• Molecule 2: AMC009 SOSIP.v5.2 envelope glycoprotein gp41

Chain B:



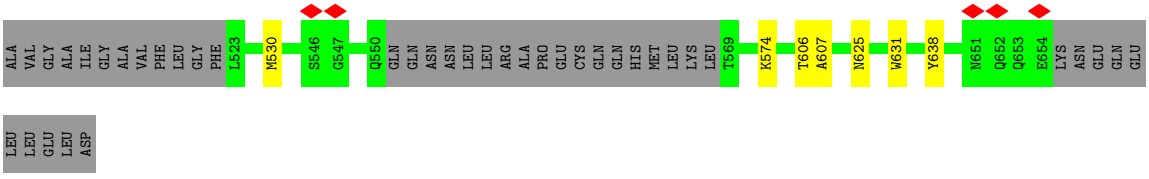
• Molecule 2: AMC009 SOSIP.v5.2 envelope glycoprotein gp41

Chain E:



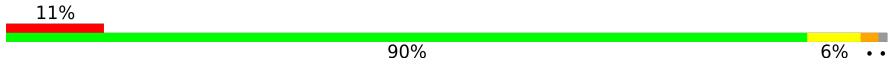
• Molecule 2: AMC009 SOSIP.v5.2 envelope glycoprotein gp41

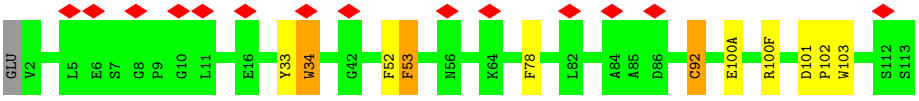
Chain F:



• Molecule 3: ACS124 heavy chain

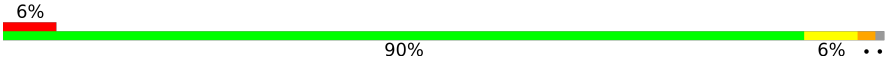
Chain G:

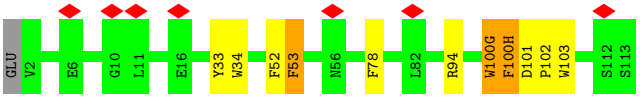




• Molecule 3: ACS124 heavy chain

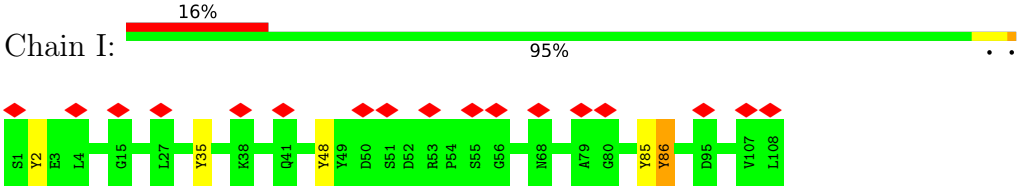
Chain M:





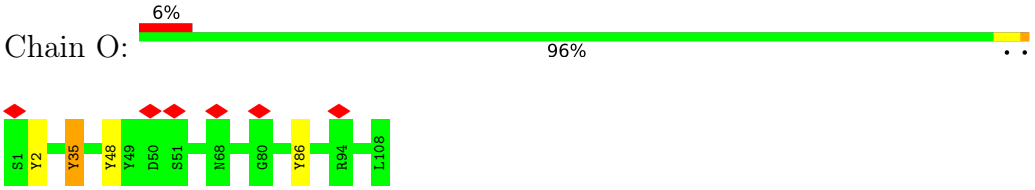
• Molecule 4: ACS124 light chain

Chain I:



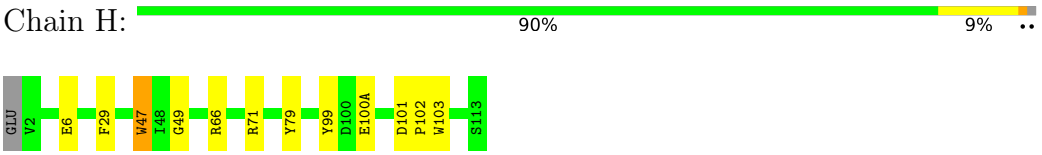
• Molecule 4: ACS124 light chain

Chain O:



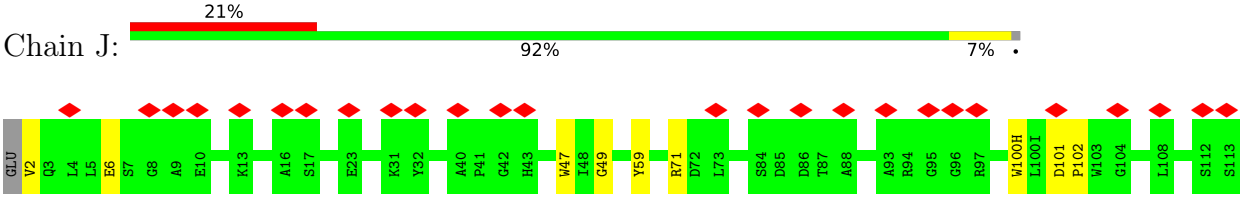
• Molecule 5: ACS101 heavy chain

Chain H:



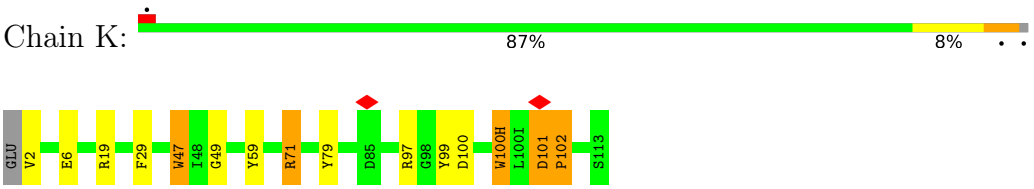
• Molecule 5: ACS101 heavy chain

Chain J:



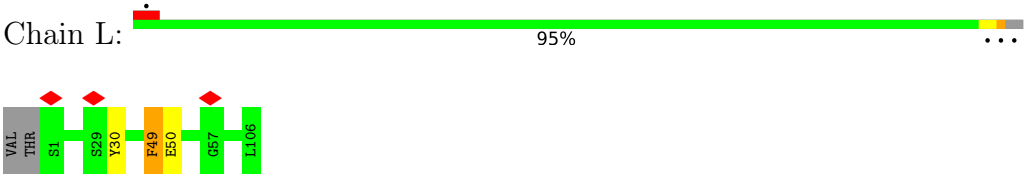
• Molecule 5: ACS101 heavy chain

Chain K:



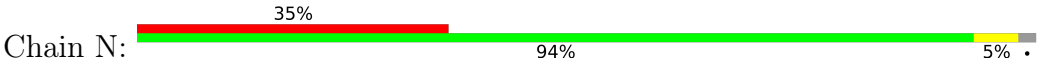
• Molecule 6: ACS101 light chain

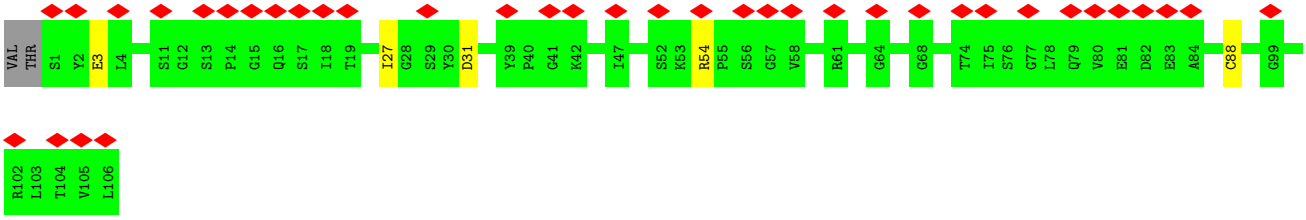
Chain L:



• Molecule 6: ACS101 light chain

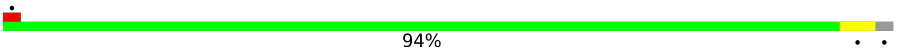
Chain N:





• Molecule 6: ACS101 light chain

Chain P:

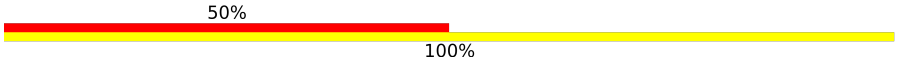


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

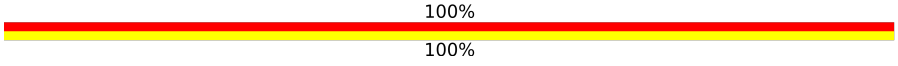
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



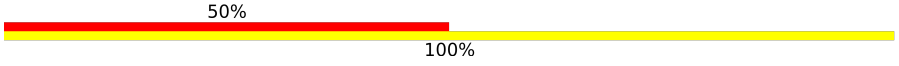
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



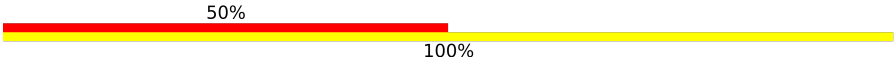
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



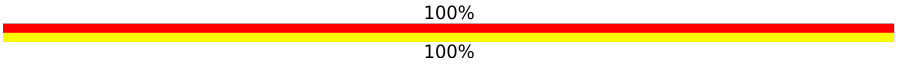
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:



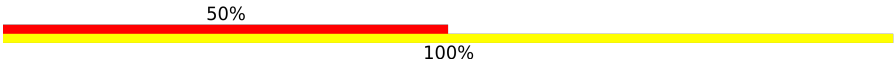
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:



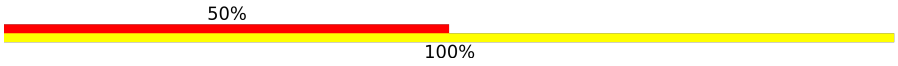
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:

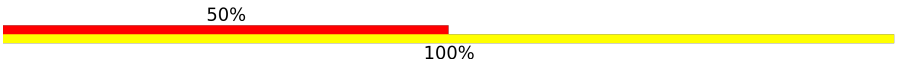


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9:

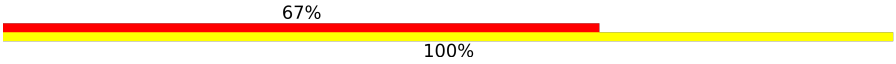
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA:



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

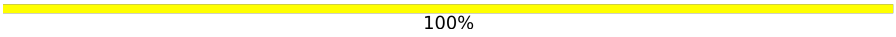


• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

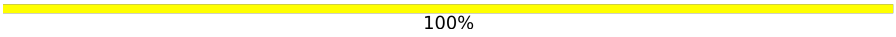
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

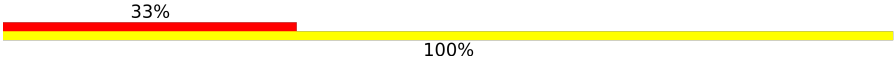


• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

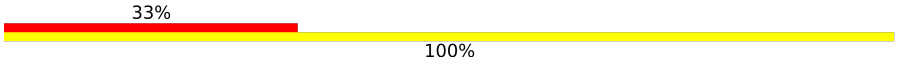
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



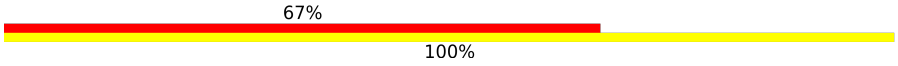
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



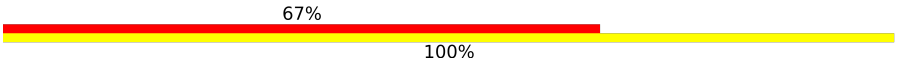
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

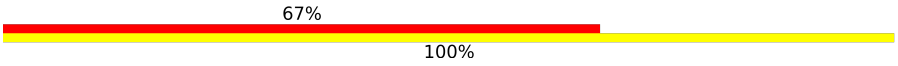
Chain e:

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:

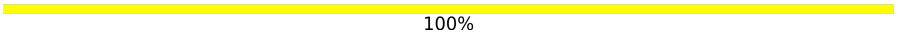


• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:

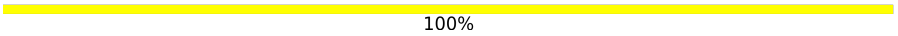
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

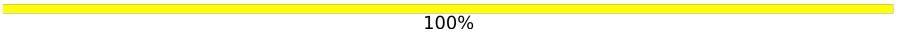
Chain m:

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:

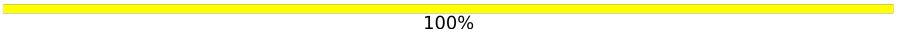
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w: 

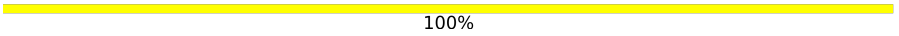
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x: 

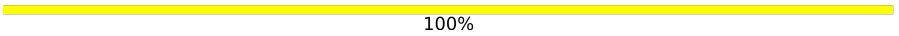
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z: 

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0: 

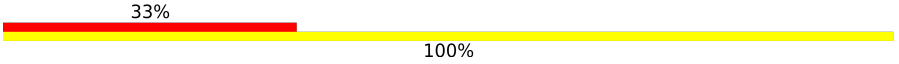
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1: 

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

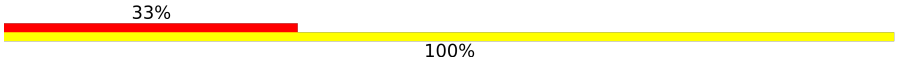
Chain 3: 

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4: 

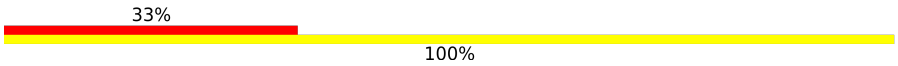
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5:



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6:



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7:

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8:

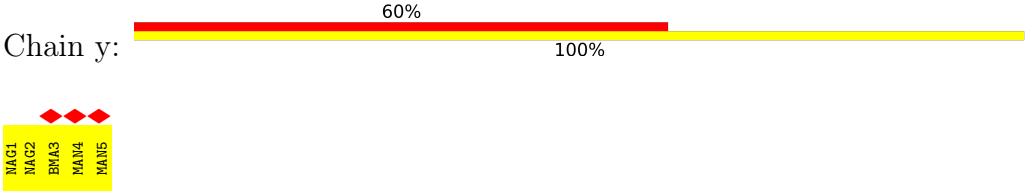
• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra

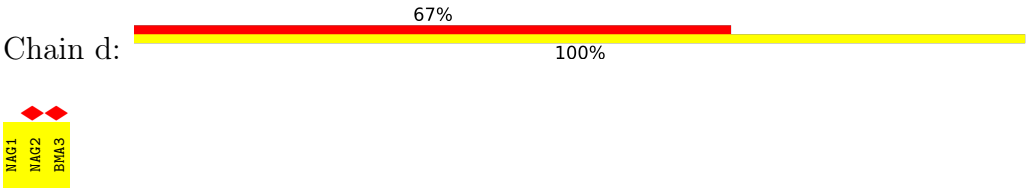
nose

Chain y:



• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	95062	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	49	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.860	Depositor
Minimum map value	-0.373	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	345.0, 345.0, 345.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.16	13/3476 (0.4%)	0.95	10/4718 (0.2%)
1	C	1.15	19/3476 (0.5%)	0.94	6/4718 (0.1%)
1	D	1.17	15/3476 (0.4%)	0.92	7/4718 (0.1%)
2	B	1.32	5/1008 (0.5%)	0.90	1/1367 (0.1%)
2	E	1.20	2/914 (0.2%)	0.89	0/1241
2	F	1.22	1/923 (0.1%)	0.86	2/1253 (0.2%)
3	G	1.35	8/994 (0.8%)	0.98	2/1355 (0.1%)
3	M	1.37	11/994 (1.1%)	0.94	0/1355
4	I	1.18	6/839 (0.7%)	0.97	2/1143 (0.2%)
4	O	1.22	3/839 (0.4%)	0.93	2/1143 (0.2%)
5	H	1.36	7/1018 (0.7%)	1.01	2/1387 (0.1%)
5	J	1.18	4/1018 (0.4%)	0.99	0/1387
5	K	1.31	9/1018 (0.9%)	1.04	4/1387 (0.3%)
6	L	1.14	1/813 (0.1%)	0.98	2/1103 (0.2%)
6	N	1.10	3/813 (0.4%)	1.01	1/1103 (0.1%)
6	P	1.11	0/813	0.97	1/1103 (0.1%)
All	All	1.21	107/22432 (0.5%)	0.95	42/30481 (0.1%)

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	48	TYR	CB-CG	-11.48	1.34	1.51
3	G	92	CYS	CB-SG	-10.80	1.63	1.82
3	M	78	PHE	CB-CG	-8.92	1.36	1.51
1	A	376	PHE	CB-CG	-8.75	1.36	1.51
3	M	53	PHE	CB-CG	-8.30	1.37	1.51

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	66	ARG	NE-CZ-NH2	-9.23	115.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	273	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	D	273	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	C	166	ARG	NE-CZ-NH2	-8.51	116.05	120.30
3	G	100(F)	ARG	NE-CZ-NH2	-8.29	116.16	120.30

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	3403	0	3351	8	0
1	C	3403	0	3352	12	0
1	D	3403	0	3351	15	0
2	B	992	0	967	4	0
2	E	898	0	879	2	0
2	F	907	0	885	2	0
3	G	969	0	948	3	0
3	M	969	0	948	7	0
4	I	820	0	788	1	0
4	O	820	0	788	3	0
5	H	990	0	942	2	0
5	J	990	0	942	2	0
5	K	990	0	942	9	0
6	L	795	0	773	1	0
6	N	795	0	773	1	0
6	P	795	0	773	5	0
7	2	28	0	25	0	0
7	9	28	0	25	0	0
7	AA	28	0	25	0	0
7	Q	28	0	25	0	0
7	W	28	0	25	0	0
7	g	28	0	25	0	0
7	l	28	0	25	0	0
7	s	28	0	25	0	0
7	u	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	v	28	0	25	0	0
8	0	39	0	34	0	0
8	1	39	0	34	0	0
8	3	39	0	34	0	0
8	4	39	0	34	0	0
8	5	39	0	34	0	0
8	6	39	0	34	0	0
8	7	39	0	34	0	0
8	8	39	0	34	0	0
8	R	39	0	34	0	0
8	T	39	0	34	0	0
8	U	39	0	34	0	0
8	V	39	0	33	0	0
8	X	39	0	34	0	0
8	Y	39	0	34	0	0
8	Z	39	0	34	0	0
8	a	39	0	34	0	0
8	b	39	0	34	0	0
8	c	39	0	34	0	0
8	e	39	0	34	0	0
8	f	39	0	34	0	0
8	h	39	0	34	0	0
8	i	39	0	34	0	0
8	j	39	0	34	0	0
8	k	39	0	34	0	0
8	m	39	0	34	0	0
8	n	39	0	34	0	0
8	o	39	0	34	0	0
8	p	39	0	34	0	0
8	q	39	0	34	0	0
8	r	39	0	34	0	0
8	t	39	0	34	0	0
8	w	39	0	34	0	0
8	x	39	0	34	0	0
8	z	39	0	34	0	0
9	S	61	0	52	0	0
9	y	61	0	52	0	0
10	d	39	0	34	0	0
11	A	70	0	65	0	0
11	B	42	0	39	2	0
11	C	42	0	39	0	0
11	D	84	0	78	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	E	28	0	26	0	0
11	F	28	0	26	0	0
All	All	24000	0	23218	67	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 1.

The worst 5 of 67 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)
5:K:101:ASP:OD1	6:P:46:VAL:HG21	1.43	1.17
5:K:101:ASP:OD1	6:P:46:VAL:CG2	1.98	1.10
1:D:358:THR:HG23	1:D:396:ASN:HB3	1.59	0.82
5:K:100(H):TRP:NE1	5:K:101:ASP:OD2	2.12	0.82
1:C:312:ALA:HB3	1:C:315:ARG:HB3	1.74	0.69

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	419/482 (87%)	410 (98%)	9 (2%)	0	100	100
1	C	419/482 (87%)	404 (96%)	15 (4%)	0	100	100
1	D	419/482 (87%)	408 (97%)	11 (3%)	0	100	100
2	B	120/154 (78%)	118 (98%)	2 (2%)	0	100	100
2	E	109/154 (71%)	106 (97%)	3 (3%)	0	100	100
2	F	110/154 (71%)	108 (98%)	2 (2%)	0	100	100
3	G	121/124 (98%)	117 (97%)	4 (3%)	0	100	100
3	M	121/124 (98%)	115 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	I	106/108 (98%)	106 (100%)	0	0	100	100
4	O	106/108 (98%)	106 (100%)	0	0	100	100
5	H	123/126 (98%)	119 (97%)	4 (3%)	0	100	100
5	J	123/126 (98%)	119 (97%)	4 (3%)	0	100	100
5	K	123/126 (98%)	120 (98%)	3 (2%)	0	100	100
6	L	104/108 (96%)	99 (95%)	5 (5%)	0	100	100
6	N	104/108 (96%)	101 (97%)	3 (3%)	0	100	100
6	P	104/108 (96%)	102 (98%)	2 (2%)	0	100	100
All	All	2731/3074 (89%)	2658 (97%)	73 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	387/429 (90%)	385 (100%)	2 (0%)	88	93
1	C	387/429 (90%)	386 (100%)	1 (0%)	92	95
1	D	387/429 (90%)	384 (99%)	3 (1%)	81	88
2	B	107/130 (82%)	107 (100%)	0	100	100
2	E	96/130 (74%)	96 (100%)	0	100	100
2	F	97/130 (75%)	96 (99%)	1 (1%)	76	85
3	G	109/110 (99%)	109 (100%)	0	100	100
3	M	109/110 (99%)	109 (100%)	0	100	100
4	I	91/91 (100%)	91 (100%)	0	100	100
4	O	91/91 (100%)	91 (100%)	0	100	100
5	H	103/104 (99%)	102 (99%)	1 (1%)	76	85
5	J	103/104 (99%)	102 (99%)	1 (1%)	76	85
5	K	103/104 (99%)	102 (99%)	1 (1%)	76	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	L	89/91 (98%)	89 (100%)	0	100	100
6	N	89/91 (98%)	89 (100%)	0	100	100
6	P	89/91 (98%)	89 (100%)	0	100	100
All	All	2437/2664 (92%)	2427 (100%)	10 (0%)	91	94

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	H	71	ARG
5	J	71	ARG
5	K	71	ARG
1	D	295	ASN
1	D	354	LYS

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

135 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	$\#\|Z\| > 2$
8	NAG	0	1	1,8	14,14,15	2.24	6 (42%)	17,19,21	1.36	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	0	2	8	14,14,15	1.99	4 (28%)	17,19,21	1.02	1 (5%)
8	BMA	0	3	8	11,11,12	1.94	4 (36%)	15,15,17	0.75	0
8	NAG	1	1	1,8	14,14,15	1.92	6 (42%)	17,19,21	1.46	2 (11%)
8	NAG	1	2	8	14,14,15	1.85	5 (35%)	17,19,21	1.06	2 (11%)
8	BMA	1	3	8	11,11,12	1.92	5 (45%)	15,15,17	0.79	1 (6%)
7	NAG	2	1	1,7	14,14,15	2.00	5 (35%)	17,19,21	1.23	2 (11%)
7	NAG	2	2	7	14,14,15	2.19	6 (42%)	17,19,21	1.11	2 (11%)
8	NAG	3	1	1,8	14,14,15	2.16	5 (35%)	17,19,21	1.71	4 (23%)
8	NAG	3	2	8	14,14,15	2.21	7 (50%)	17,19,21	1.21	3 (17%)
8	BMA	3	3	8	11,11,12	2.05	6 (54%)	15,15,17	0.70	0
8	NAG	4	1	1,8	14,14,15	1.96	5 (35%)	17,19,21	1.08	1 (5%)
8	NAG	4	2	8	14,14,15	1.99	5 (35%)	17,19,21	0.98	1 (5%)
8	BMA	4	3	8	11,11,12	1.97	6 (54%)	15,15,17	0.68	0
8	NAG	5	1	1,8	14,14,15	1.90	5 (35%)	17,19,21	1.14	1 (5%)
8	NAG	5	2	8	14,14,15	2.00	6 (42%)	17,19,21	0.96	1 (5%)
8	BMA	5	3	8	11,11,12	1.98	6 (54%)	15,15,17	0.77	0
8	NAG	6	1	1,8	14,14,15	2.15	5 (35%)	17,19,21	1.24	2 (11%)
8	NAG	6	2	8	14,14,15	2.31	7 (50%)	17,19,21	1.31	3 (17%)
8	BMA	6	3	8	11,11,12	2.01	6 (54%)	15,15,17	0.72	0
8	NAG	7	1	1,8	14,14,15	2.07	6 (42%)	17,19,21	1.01	1 (5%)
8	NAG	7	2	8	14,14,15	2.03	5 (35%)	17,19,21	0.92	1 (5%)
8	BMA	7	3	8	11,11,12	2.01	6 (54%)	15,15,17	0.79	0
8	NAG	8	1	1,8	14,14,15	0.56	0	17,19,21	1.24	2 (11%)
8	NAG	8	2	8	14,14,15	0.31	0	17,19,21	1.47	3 (17%)
8	BMA	8	3	8	11,11,12	0.20	0	15,15,17	0.86	1 (6%)
7	NAG	9	1	2,7	14,14,15	2.26	4 (28%)	17,19,21	1.16	1 (5%)
7	NAG	9	2	7	14,14,15	2.18	7 (50%)	17,19,21	0.88	2 (11%)
7	NAG	AA	1	2,7	14,14,15	2.16	7 (50%)	17,19,21	1.24	2 (11%)
7	NAG	AA	2	7	14,14,15	2.22	7 (50%)	17,19,21	0.87	1 (5%)
7	NAG	Q	1	1,7	14,14,15	2.24	6 (42%)	17,19,21	1.16	1 (5%)
7	NAG	Q	2	7	14,14,15	2.02	7 (50%)	17,19,21	0.89	1 (5%)
8	NAG	R	1	1,8	14,14,15	2.18	7 (50%)	17,19,21	1.51	3 (17%)
8	NAG	R	2	8	14,14,15	2.01	5 (35%)	17,19,21	1.11	2 (11%)
8	BMA	R	3	8	11,11,12	2.03	6 (54%)	15,15,17	0.77	0
9	NAG	S	1	9,1	14,14,15	2.03	5 (35%)	17,19,21	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	S	2	9	14,14,15	1.96	5 (35%)	17,19,21	1.00	1 (5%)
9	BMA	S	3	9	11,11,12	1.60	3 (27%)	15,15,17	0.90	1 (6%)
9	MAN	S	4	9	11,11,12	2.04	5 (45%)	15,15,17	0.76	0
9	MAN	S	5	9	11,11,12	1.88	5 (45%)	15,15,17	0.85	0
8	NAG	T	1	1,8	14,14,15	1.89	5 (35%)	17,19,21	1.10	1 (5%)
8	NAG	T	2	8	14,14,15	2.02	6 (42%)	17,19,21	0.98	1 (5%)
8	BMA	T	3	8	11,11,12	2.00	6 (54%)	15,15,17	0.68	0
8	NAG	U	1	1,8	14,14,15	2.07	5 (35%)	17,19,21	1.15	1 (5%)
8	NAG	U	2	8	14,14,15	2.09	6 (42%)	17,19,21	1.32	3 (17%)
8	BMA	U	3	8	11,11,12	2.05	4 (36%)	15,15,17	0.70	0
8	NAG	V	1	1,8	14,14,15	2.12	6 (42%)	17,19,21	0.95	1 (5%)
8	NAG	V	2	8	14,14,15	1.85	5 (35%)	17,19,21	12.05	4 (23%)
8	BMA	V	3	8	11,11,12	1.91	5 (45%)	15,15,17	0.82	0
7	NAG	W	1	1,7	14,14,15	1.88	5 (35%)	17,19,21	1.26	2 (11%)
7	NAG	W	2	7	14,14,15	2.02	5 (35%)	17,19,21	0.92	1 (5%)
8	NAG	X	1	1,8	14,14,15	1.94	7 (50%)	17,19,21	1.26	2 (11%)
8	NAG	X	2	8	14,14,15	2.09	5 (35%)	17,19,21	0.92	1 (5%)
8	BMA	X	3	8	11,11,12	2.03	6 (54%)	15,15,17	0.68	0
8	NAG	Y	1	1,8	14,14,15	1.98	6 (42%)	17,19,21	1.08	1 (5%)
8	NAG	Y	2	8	14,14,15	1.94	5 (35%)	17,19,21	0.99	2 (11%)
8	BMA	Y	3	8	11,11,12	1.98	6 (54%)	15,15,17	0.78	0
8	NAG	Z	1	1,8	14,14,15	1.93	4 (28%)	17,19,21	0.97	0
8	NAG	Z	2	8	14,14,15	1.96	6 (42%)	17,19,21	0.93	1 (5%)
8	BMA	Z	3	8	11,11,12	1.98	6 (54%)	15,15,17	0.77	0
8	NAG	a	1	1,8	14,14,15	2.14	5 (35%)	17,19,21	1.15	2 (11%)
8	NAG	a	2	8	14,14,15	2.33	7 (50%)	17,19,21	1.24	2 (11%)
8	BMA	a	3	8	11,11,12	2.06	6 (54%)	15,15,17	0.67	0
8	NAG	b	1	1,8	14,14,15	2.08	4 (28%)	17,19,21	0.93	1 (5%)
8	NAG	b	2	8	14,14,15	1.98	5 (35%)	17,19,21	0.95	1 (5%)
8	BMA	b	3	8	11,11,12	2.02	6 (54%)	15,15,17	0.72	0
8	NAG	c	1	1,8	14,14,15	2.05	5 (35%)	17,19,21	1.13	1 (5%)
8	NAG	c	2	8	14,14,15	2.33	6 (42%)	17,19,21	1.11	2 (11%)
8	BMA	c	3	8	11,11,12	2.06	6 (54%)	15,15,17	0.67	0
10	NAG	d	1	10,1	14,14,15	2.04	4 (28%)	17,19,21	1.10	2 (11%)
10	NAG	d	2	10	14,14,15	2.17	8 (57%)	17,19,21	1.30	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	BMA	d	3	10	11,11,12	1.99	6 (54%)	15,15,17	0.73	0
8	NAG	e	1	8,2	14,14,15	2.11	6 (42%)	17,19,21	1.70	4 (23%)
8	NAG	e	2	8	14,14,15	2.09	6 (42%)	17,19,21	0.89	1 (5%)
8	BMA	e	3	8	11,11,12	2.03	6 (54%)	15,15,17	0.67	0
8	NAG	f	1	1,8	14,14,15	2.03	6 (42%)	17,19,21	1.08	1 (5%)
8	NAG	f	2	8	14,14,15	2.03	7 (50%)	17,19,21	1.27	1 (5%)
8	BMA	f	3	8	11,11,12	1.99	6 (54%)	15,15,17	0.73	0
7	NAG	g	1	1,7	14,14,15	2.25	6 (42%)	17,19,21	0.83	0
7	NAG	g	2	7	14,14,15	1.91	6 (42%)	17,19,21	0.96	2 (11%)
8	NAG	h	1	1,8	14,14,15	1.99	5 (35%)	17,19,21	1.21	3 (17%)
8	NAG	h	2	8	14,14,15	2.00	6 (42%)	17,19,21	0.97	1 (5%)
8	BMA	h	3	8	11,11,12	2.04	6 (54%)	15,15,17	0.67	0
8	NAG	i	1	1,8	14,14,15	2.08	6 (42%)	17,19,21	1.40	3 (17%)
8	NAG	i	2	8	14,14,15	2.12	6 (42%)	17,19,21	1.23	4 (23%)
8	BMA	i	3	8	11,11,12	2.01	6 (54%)	15,15,17	0.69	0
8	NAG	j	1	1,8	14,14,15	2.18	7 (50%)	17,19,21	1.30	3 (17%)
8	NAG	j	2	8	14,14,15	1.94	4 (28%)	17,19,21	1.03	1 (5%)
8	BMA	j	3	8	11,11,12	1.99	4 (36%)	15,15,17	0.79	0
8	NAG	k	1	1,8	14,14,15	1.95	6 (42%)	17,19,21	1.21	2 (11%)
8	NAG	k	2	8	14,14,15	1.88	6 (42%)	17,19,21	1.08	1 (5%)
8	BMA	k	3	8	11,11,12	1.99	5 (45%)	15,15,17	0.71	0
7	NAG	l	1	1,7	14,14,15	1.93	5 (35%)	17,19,21	1.34	4 (23%)
7	NAG	l	2	7	14,14,15	1.94	6 (42%)	17,19,21	0.87	1 (5%)
8	NAG	m	1	1,8	14,14,15	1.99	6 (42%)	17,19,21	1.13	2 (11%)
8	NAG	m	2	8	14,14,15	2.03	5 (35%)	17,19,21	0.87	1 (5%)
8	BMA	m	3	8	11,11,12	2.01	6 (54%)	15,15,17	0.77	0
8	NAG	n	1	1,8	14,14,15	2.30	6 (42%)	17,19,21	1.58	4 (23%)
8	NAG	n	2	8	14,14,15	2.14	6 (42%)	17,19,21	1.07	1 (5%)
8	BMA	n	3	8	11,11,12	2.10	6 (54%)	15,15,17	0.71	0
8	NAG	o	1	1,8	14,14,15	2.04	6 (42%)	17,19,21	1.32	3 (17%)
8	NAG	o	2	8	14,14,15	2.11	7 (50%)	17,19,21	1.23	4 (23%)
8	BMA	o	3	8	11,11,12	2.01	6 (54%)	15,15,17	0.73	0
8	NAG	p	1	1,8	14,14,15	2.02	5 (35%)	17,19,21	1.07	0
8	NAG	p	2	8	14,14,15	2.31	7 (50%)	17,19,21	1.31	4 (23%)
8	BMA	p	3	8	11,11,12	2.03	6 (54%)	15,15,17	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	q	1	1,8	14,14,15	2.03	7 (50%)	17,19,21	1.12	2 (11%)
8	NAG	q	2	8	14,14,15	2.18	7 (50%)	17,19,21	0.94	0
8	BMA	q	3	8	11,11,12	2.03	6 (54%)	15,15,17	0.73	0
8	NAG	r	1	1,8	14,14,15	2.14	5 (35%)	17,19,21	1.06	1 (5%)
8	NAG	r	2	8	14,14,15	2.01	6 (42%)	17,19,21	1.02	2 (11%)
8	BMA	r	3	8	11,11,12	2.02	6 (54%)	15,15,17	0.67	0
7	NAG	s	1	1,7	14,14,15	2.11	5 (35%)	17,19,21	1.11	0
7	NAG	s	2	7	14,14,15	1.99	4 (28%)	17,19,21	0.85	1 (5%)
8	NAG	t	1	1,8	14,14,15	2.06	5 (35%)	17,19,21	1.09	2 (11%)
8	NAG	t	2	8	14,14,15	2.14	6 (42%)	17,19,21	1.30	4 (23%)
8	BMA	t	3	8	11,11,12	2.09	6 (54%)	15,15,17	0.73	0
7	NAG	u	1	2,7	14,14,15	2.20	7 (50%)	17,19,21	1.50	3 (17%)
7	NAG	u	2	7	14,14,15	2.16	7 (50%)	17,19,21	0.92	1 (5%)
7	NAG	v	1	2,7	14,14,15	2.29	6 (42%)	17,19,21	1.04	1 (5%)
7	NAG	v	2	7	14,14,15	1.98	6 (42%)	17,19,21	0.87	1 (5%)
8	NAG	w	1	1,8	14,14,15	1.94	5 (35%)	17,19,21	1.08	1 (5%)
8	NAG	w	2	8	14,14,15	2.02	6 (42%)	17,19,21	1.00	2 (11%)
8	BMA	w	3	8	11,11,12	2.00	6 (54%)	15,15,17	0.67	0
8	NAG	x	1	1,8	14,14,15	2.28	6 (42%)	17,19,21	1.31	1 (5%)
8	NAG	x	2	8	14,14,15	2.11	6 (42%)	17,19,21	1.22	3 (17%)
8	BMA	x	3	8	11,11,12	2.03	6 (54%)	15,15,17	0.69	0
9	NAG	y	1	9,1	14,14,15	2.20	6 (42%)	17,19,21	1.19	2 (11%)
9	NAG	y	2	9	14,14,15	2.17	7 (50%)	17,19,21	1.73	4 (23%)
9	BMA	y	3	9	11,11,12	1.44	3 (27%)	15,15,17	0.69	0
9	MAN	y	4	9	11,11,12	1.97	6 (54%)	15,15,17	0.69	0
9	MAN	y	5	9	11,11,12	1.93	5 (45%)	15,15,17	0.75	0
8	NAG	z	1	1,8	14,14,15	2.12	5 (35%)	17,19,21	1.07	2 (11%)
8	NAG	z	2	8	14,14,15	2.19	6 (42%)	17,19,21	1.05	1 (5%)
8	BMA	z	3	8	11,11,12	2.02	6 (54%)	15,15,17	0.68	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
8	NAG	0	1	1,8	-	4/6/23/26	0/1/1/1
8	NAG	0	2	8	-	0/6/23/26	0/1/1/1
8	BMA	0	3	8	-	1/2/19/22	0/1/1/1
8	NAG	1	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	1	2	8	-	0/6/23/26	0/1/1/1
8	BMA	1	3	8	-	0/2/19/22	0/1/1/1
7	NAG	2	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	2	2	7	-	0/6/23/26	0/1/1/1
8	NAG	3	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	3	2	8	-	0/6/23/26	0/1/1/1
8	BMA	3	3	8	-	0/2/19/22	0/1/1/1
8	NAG	4	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	4	2	8	-	0/6/23/26	0/1/1/1
8	BMA	4	3	8	-	0/2/19/22	0/1/1/1
8	NAG	5	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	5	2	8	-	0/6/23/26	0/1/1/1
8	BMA	5	3	8	-	1/2/19/22	0/1/1/1
8	NAG	6	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	6	2	8	-	0/6/23/26	0/1/1/1
8	BMA	6	3	8	-	1/2/19/22	0/1/1/1
8	NAG	7	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	7	2	8	-	0/6/23/26	0/1/1/1
8	BMA	7	3	8	-	1/2/19/22	0/1/1/1
8	NAG	8	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	8	2	8	-	3/6/23/26	0/1/1/1
8	BMA	8	3	8	-	1/2/19/22	0/1/1/1
7	NAG	9	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	9	2	7	-	0/6/23/26	0/1/1/1
7	NAG	AA	1	2,7	-	1/6/23/26	0/1/1/1
7	NAG	AA	2	7	-	0/6/23/26	0/1/1/1
7	NAG	Q	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	0/6/23/26	0/1/1/1
8	NAG	R	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	R	2	8	-	0/6/23/26	0/1/1/1
8	BMA	R	3	8	-	1/2/19/22	0/1/1/1
9	NAG	S	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	S	2	9	-	0/6/23/26	0/1/1/1
9	BMA	S	3	9	-	0/2/19/22	0/1/1/1
9	MAN	S	4	9	-	1/2/19/22	0/1/1/1
9	MAN	S	5	9	-	1/2/19/22	0/1/1/1
8	NAG	T	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	T	2	8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	T	3	8	-	0/2/19/22	0/1/1/1
8	NAG	U	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	U	2	8	-	0/6/23/26	0/1/1/1
8	BMA	U	3	8	-	0/2/19/22	0/1/1/1
8	NAG	V	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	V	2	8	-	2/6/23/26	0/1/1/1
8	BMA	V	3	8	-	1/2/19/22	0/1/1/1
7	NAG	W	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	W	2	7	-	0/6/23/26	0/1/1/1
8	NAG	X	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	X	2	8	-	0/6/23/26	0/1/1/1
8	BMA	X	3	8	-	0/2/19/22	0/1/1/1
8	NAG	Y	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	1/2/19/22	0/1/1/1
8	NAG	Z	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Z	3	8	-	1/2/19/22	0/1/1/1
8	NAG	a	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	a	2	8	-	0/6/23/26	0/1/1/1
8	BMA	a	3	8	-	0/2/19/22	0/1/1/1
8	NAG	b	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	b	2	8	-	0/6/23/26	0/1/1/1
8	BMA	b	3	8	-	1/2/19/22	0/1/1/1
8	NAG	c	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	c	2	8	-	0/6/23/26	0/1/1/1
8	BMA	c	3	8	-	0/2/19/22	0/1/1/1
10	NAG	d	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	d	2	10	-	0/6/23/26	0/1/1/1
10	BMA	d	3	10	-	0/2/19/22	0/1/1/1
8	NAG	e	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	e	2	8	-	0/6/23/26	0/1/1/1
8	BMA	e	3	8	-	0/2/19/22	0/1/1/1
8	NAG	f	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	f	2	8	-	0/6/23/26	0/1/1/1
8	BMA	f	3	8	-	1/2/19/22	0/1/1/1
7	NAG	g	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	g	2	7	-	0/6/23/26	0/1/1/1
8	NAG	h	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	h	2	8	-	0/6/23/26	0/1/1/1
8	BMA	h	3	8	-	0/2/19/22	0/1/1/1
8	NAG	i	1	1,8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	i	2	8	-	0/6/23/26	0/1/1/1
8	BMA	i	3	8	-	0/2/19/22	0/1/1/1
8	NAG	j	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	j	2	8	-	0/6/23/26	0/1/1/1
8	BMA	j	3	8	-	1/2/19/22	0/1/1/1
8	NAG	k	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	k	2	8	-	0/6/23/26	0/1/1/1
8	BMA	k	3	8	-	1/2/19/22	0/1/1/1
7	NAG	l	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	l	2	7	-	0/6/23/26	0/1/1/1
8	NAG	m	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	m	2	8	-	0/6/23/26	0/1/1/1
8	BMA	m	3	8	-	1/2/19/22	0/1/1/1
8	NAG	n	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	n	2	8	-	0/6/23/26	0/1/1/1
8	BMA	n	3	8	-	0/2/19/22	0/1/1/1
8	NAG	o	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	o	2	8	-	0/6/23/26	0/1/1/1
8	BMA	o	3	8	-	1/2/19/22	0/1/1/1
8	NAG	p	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	p	2	8	-	0/6/23/26	0/1/1/1
8	BMA	p	3	8	-	1/2/19/22	0/1/1/1
8	NAG	q	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	q	2	8	-	0/6/23/26	0/1/1/1
8	BMA	q	3	8	-	1/2/19/22	0/1/1/1
8	NAG	r	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	r	2	8	-	0/6/23/26	0/1/1/1
8	BMA	r	3	8	-	0/2/19/22	0/1/1/1
7	NAG	s	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	s	2	7	-	0/6/23/26	0/1/1/1
8	NAG	t	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	t	2	8	-	0/6/23/26	0/1/1/1
8	BMA	t	3	8	-	1/2/19/22	0/1/1/1
7	NAG	u	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	u	2	7	-	0/6/23/26	0/1/1/1
7	NAG	v	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	v	2	7	-	0/6/23/26	0/1/1/1
8	NAG	w	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	w	2	8	-	0/6/23/26	0/1/1/1
8	BMA	w	3	8	-	0/2/19/22	0/1/1/1
8	NAG	x	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	x	2	8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	x	3	8	-	1/2/19/22	0/1/1/1
9	NAG	y	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	y	2	9	-	1/6/23/26	0/1/1/1
9	BMA	y	3	9	-	2/2/19/22	0/1/1/1
9	MAN	y	4	9	-	0/2/19/22	0/1/1/1
9	MAN	y	5	9	-	0/2/19/22	0/1/1/1
8	NAG	z	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	z	2	8	-	0/6/23/26	0/1/1/1
8	BMA	z	3	8	-	0/2/19/22	0/1/1/1

The worst 5 of 750 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	c	2	NAG	C1-C2	5.95	1.61	1.52
7	g	1	NAG	C1-C2	5.91	1.61	1.52
8	p	2	NAG	C1-C2	5.76	1.60	1.52
7	9	1	NAG	C1-C2	5.73	1.60	1.52
8	a	2	NAG	C1-C2	5.71	1.60	1.52

The worst 5 of 172 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	V	2	NAG	C8-C7-N2	27.73	163.04	116.10
8	V	2	NAG	C2-N2-C7	26.61	160.79	122.90
8	V	2	NAG	O7-C7-N2	-25.05	75.90	121.95
8	V	2	NAG	O7-C7-C8	-18.80	87.14	122.06
8	3	1	NAG	O4-C4-C3	-4.87	99.10	110.35

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

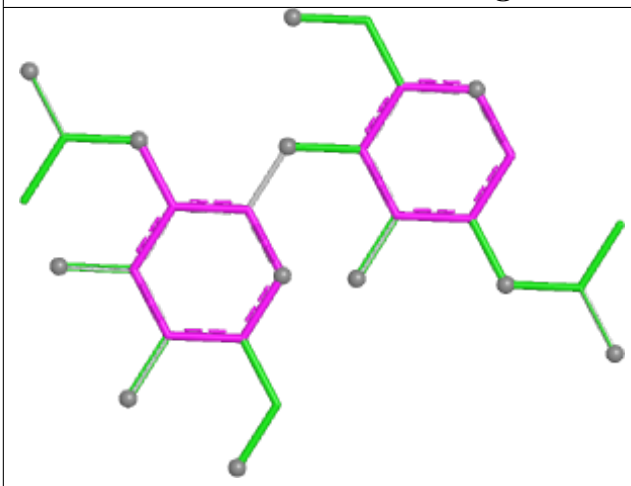
Mol	Chain	Res	Type	Atoms
8	8	1	NAG	C8-C7-N2-C2
8	8	1	NAG	O7-C7-N2-C2
8	8	2	NAG	C8-C7-N2-C2
8	8	2	NAG	O7-C7-N2-C2
8	p	1	NAG	O5-C5-C6-O6

There are no ring outliers.

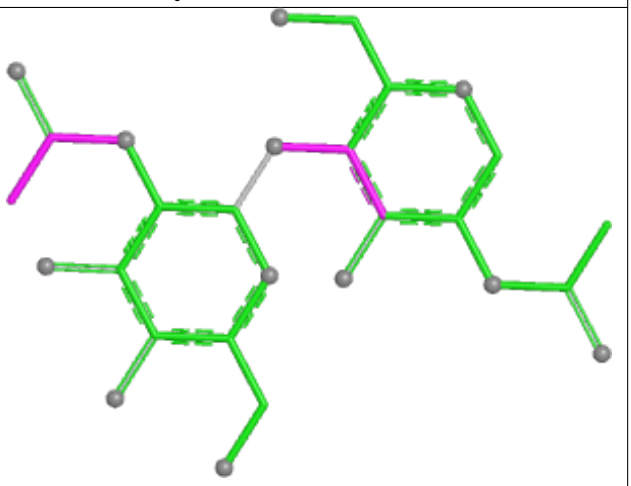
No monomer is involved in short contacts.

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

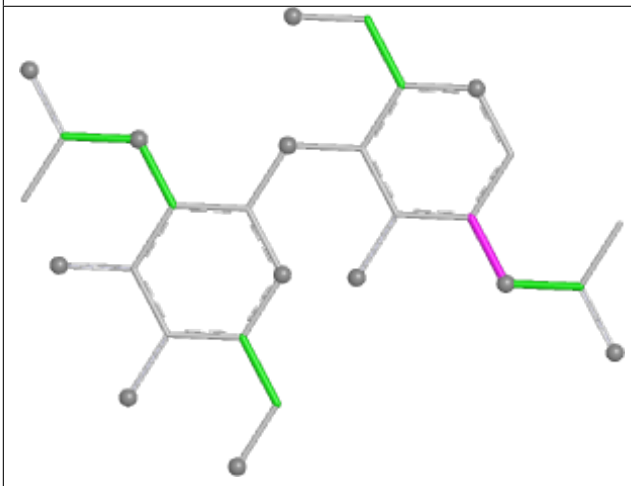
Oligosaccharide Chain Q



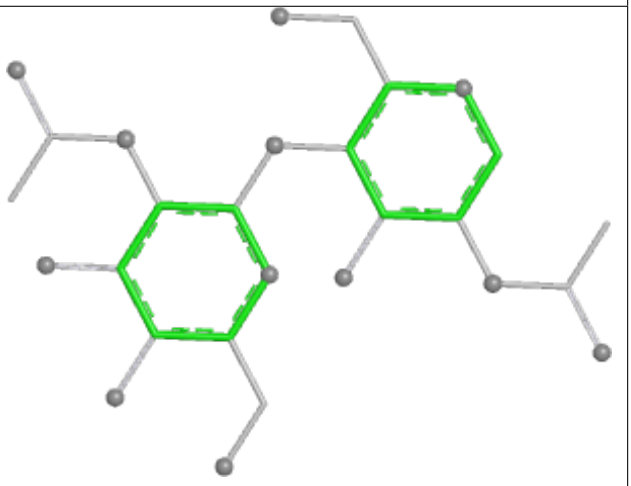
Bond lengths



Bond angles

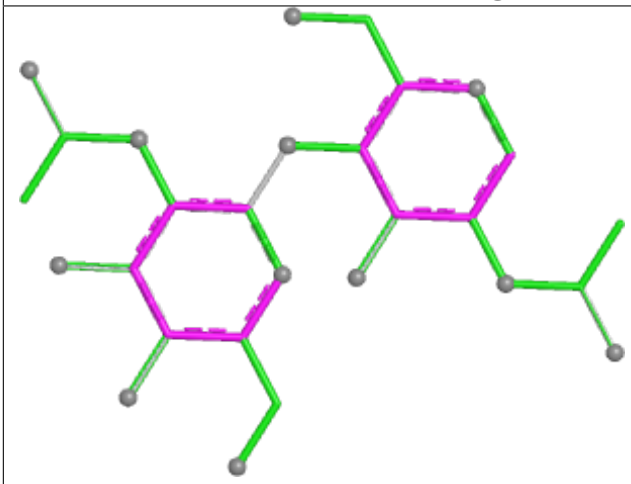


Torsions

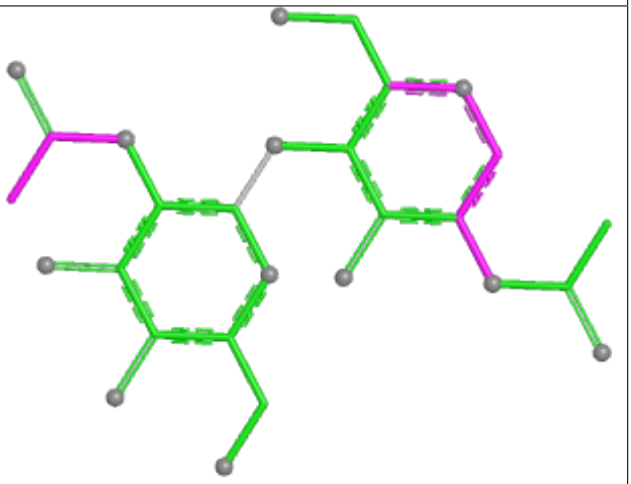


Rings

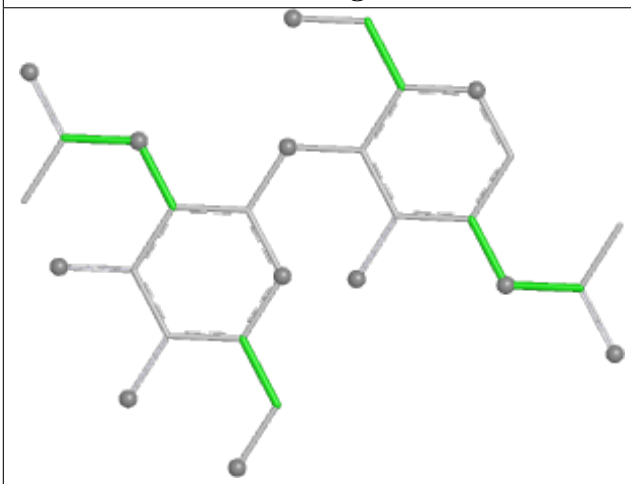
Oligosaccharide Chain W



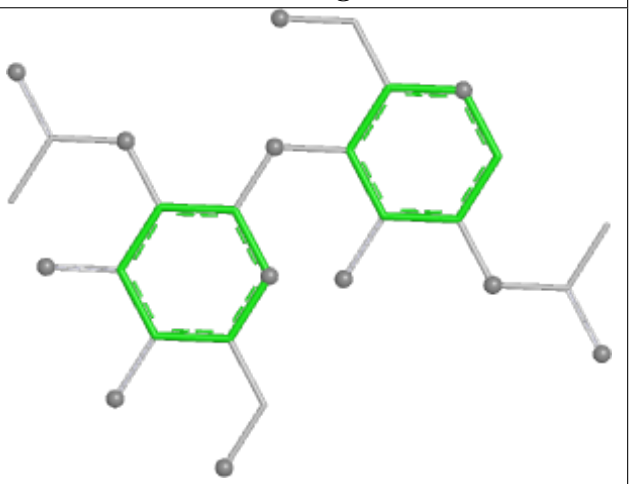
Bond lengths



Bond angles

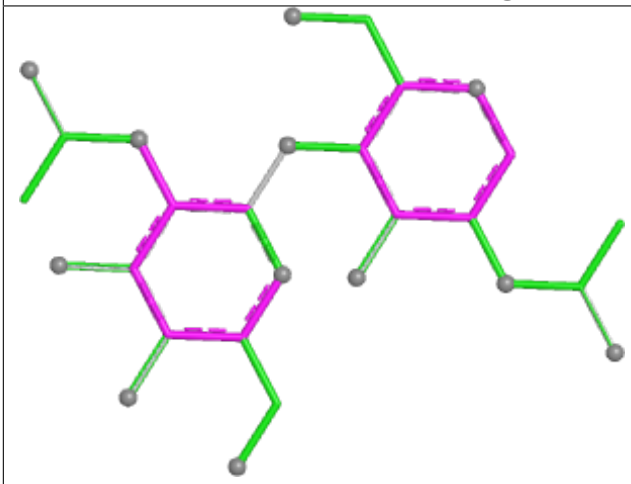


Torsions

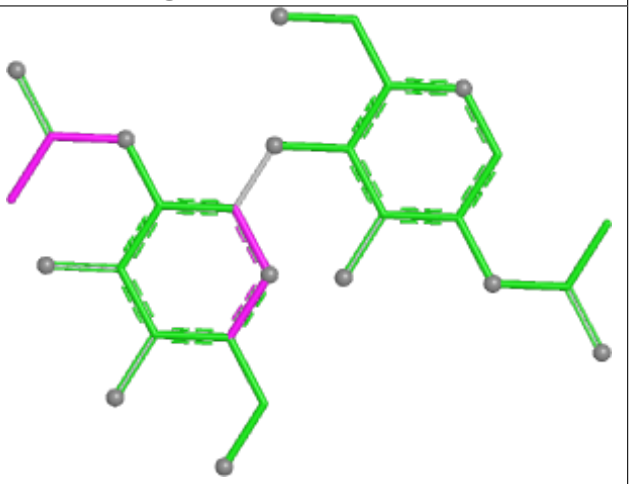


Rings

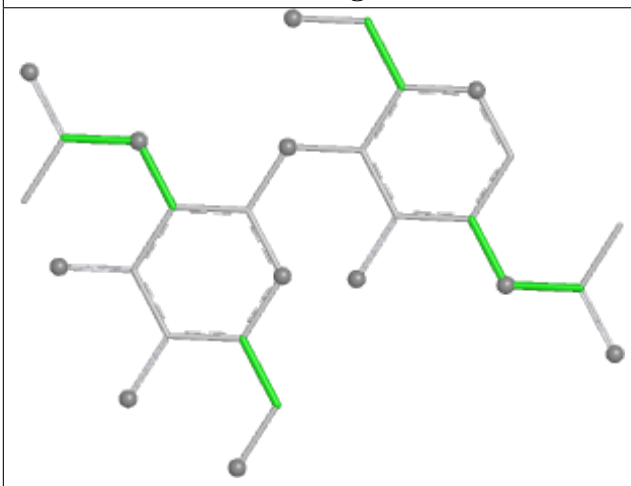
Oligosaccharide Chain g



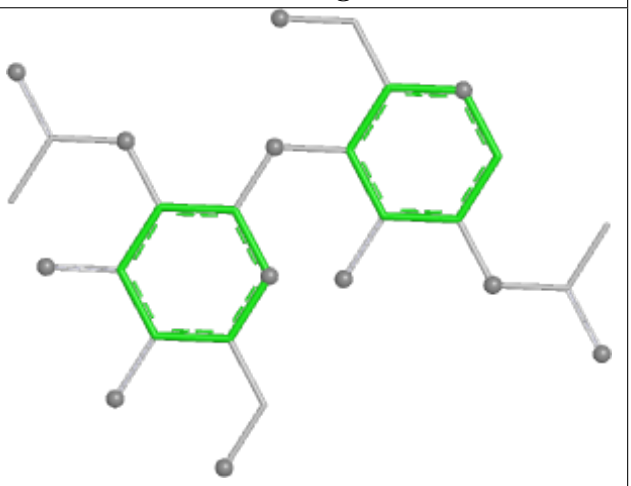
Bond lengths



Bond angles

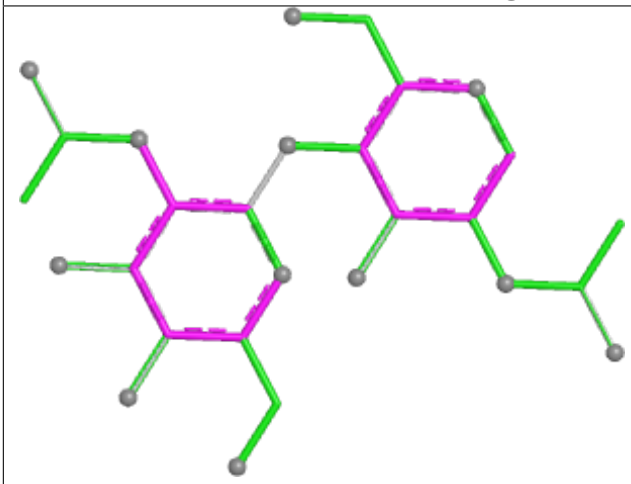


Torsions

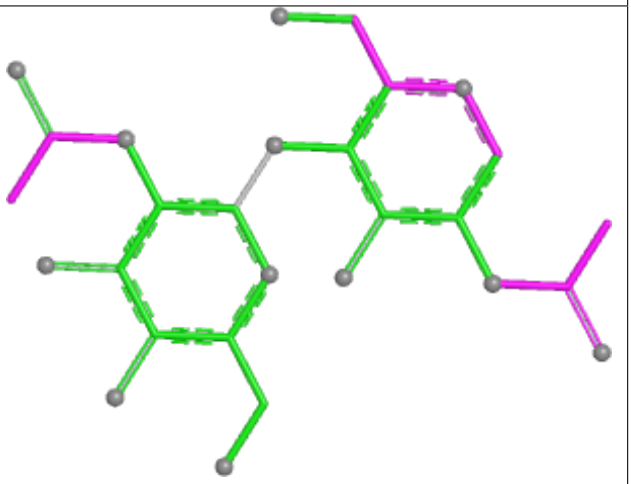


Rings

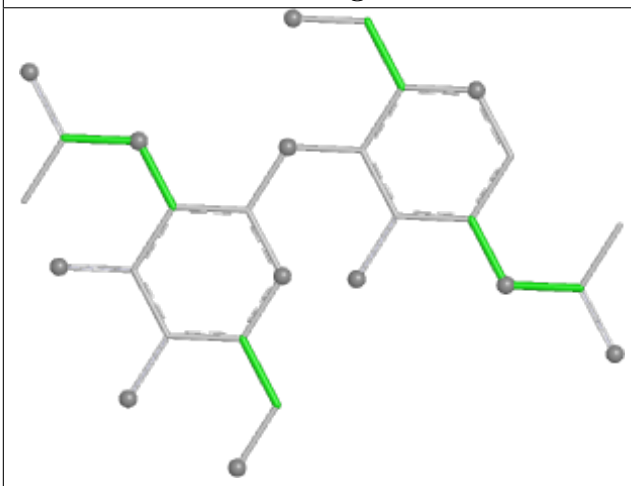
Oligosaccharide Chain l



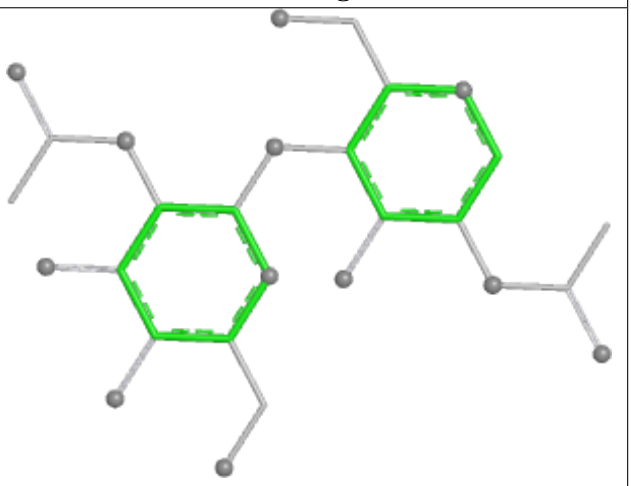
Bond lengths



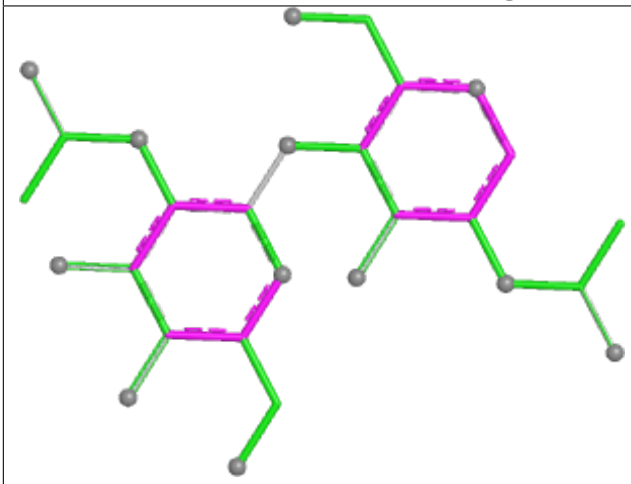
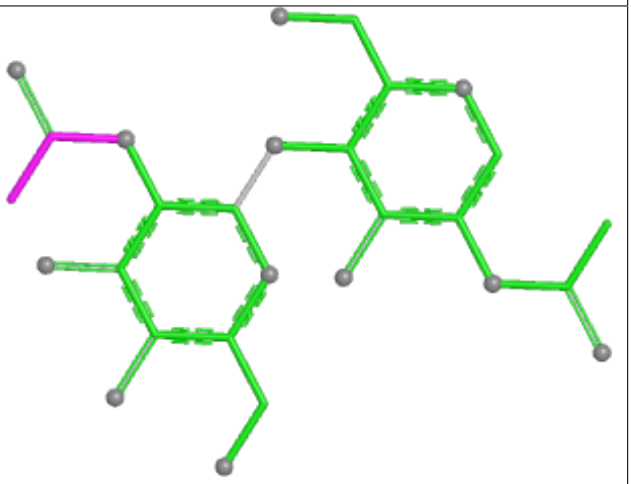
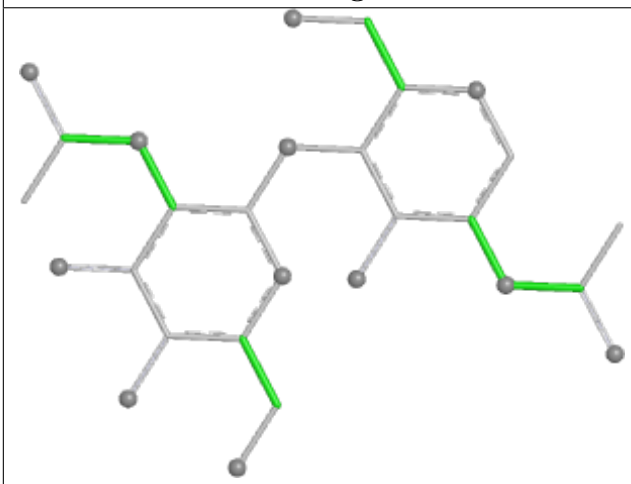
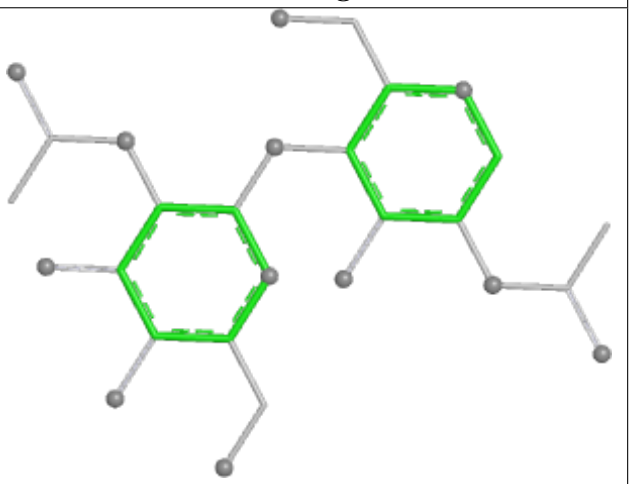
Bond angles



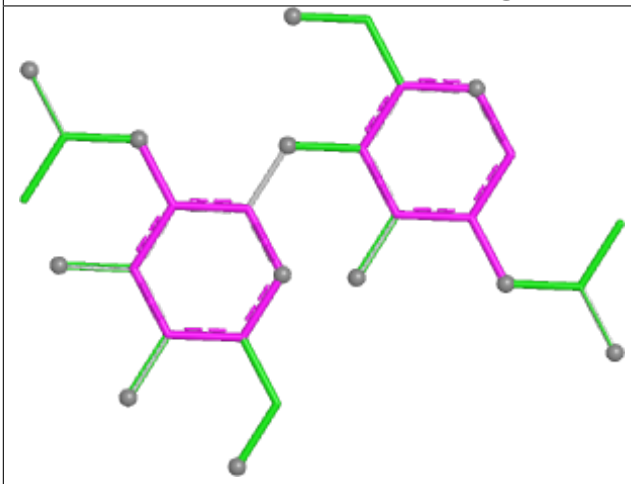
Torsions



Rings

Oligosaccharide Chain s	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain u



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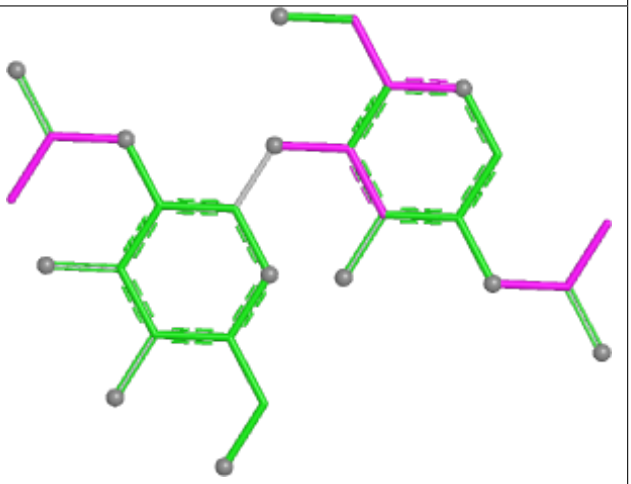
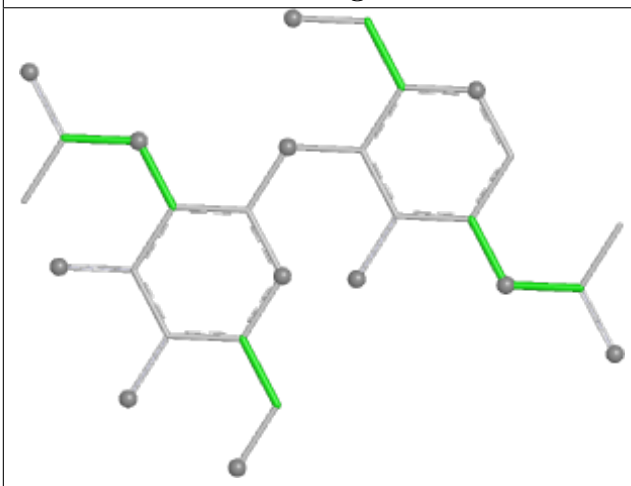


Bond angles



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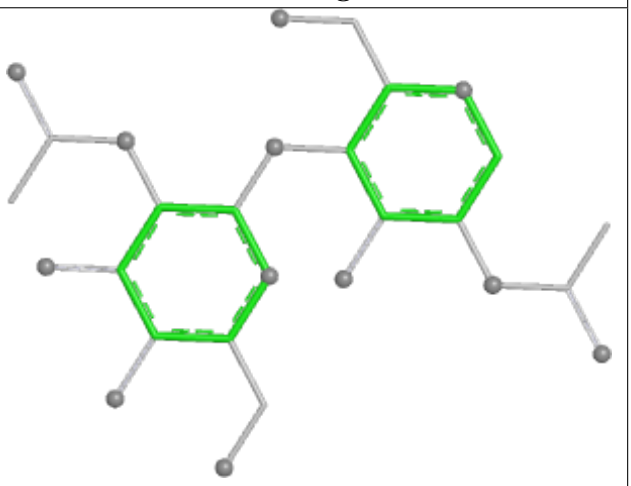
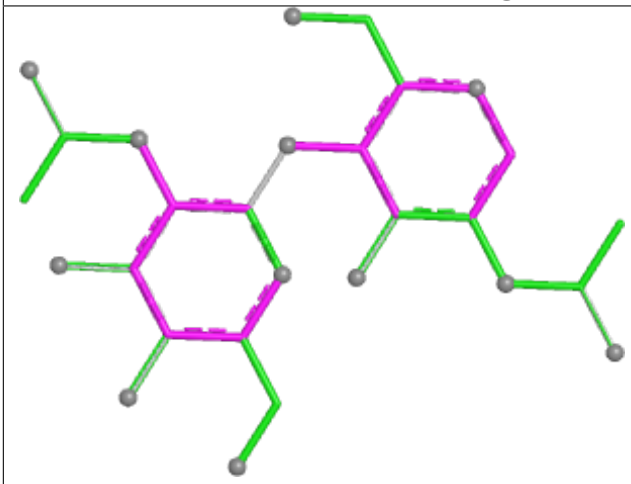


Rings

Oligosaccharide Chain v



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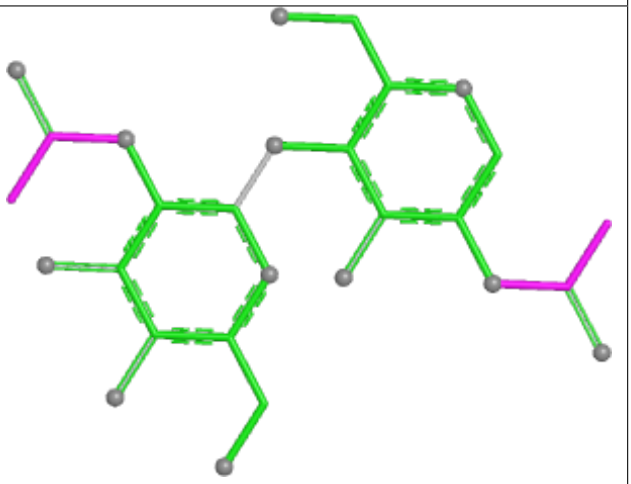

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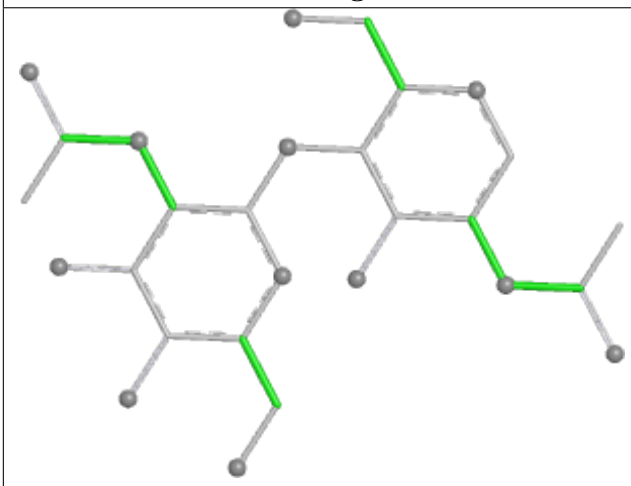

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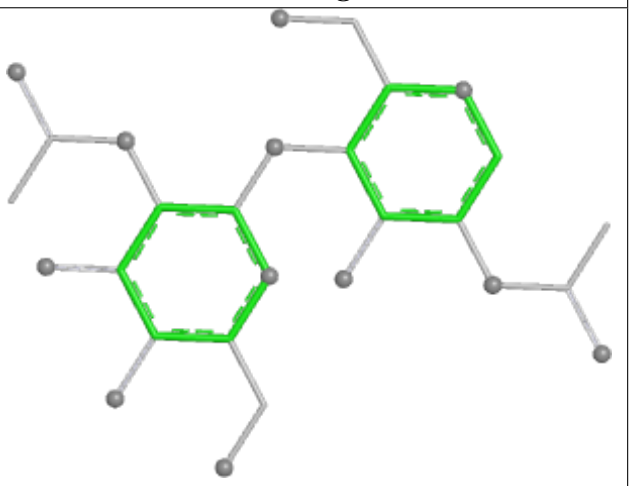
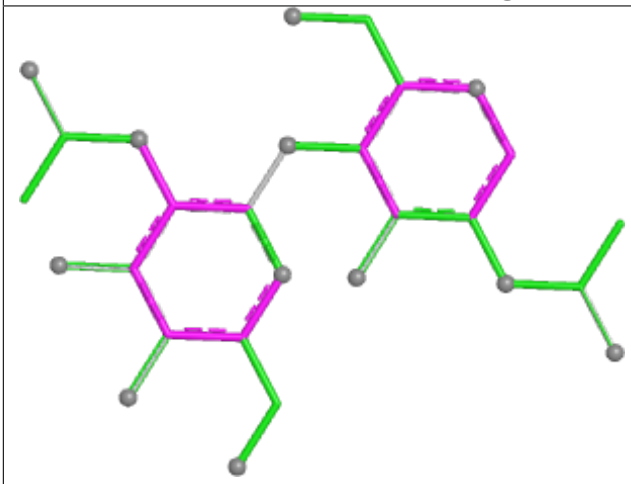
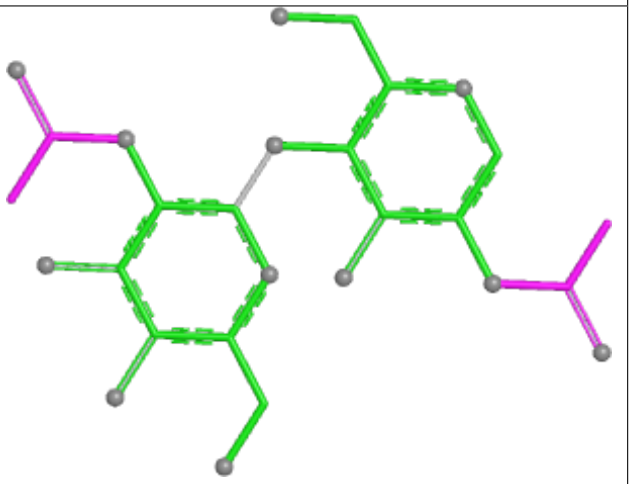


Rings

Oligosaccharide Chain 2



Bond lengths



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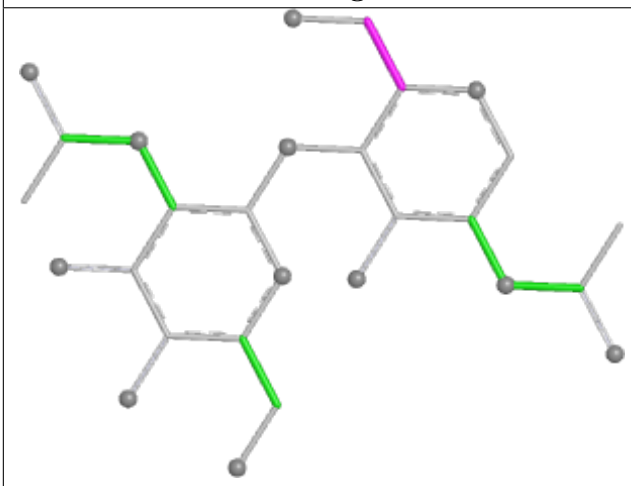

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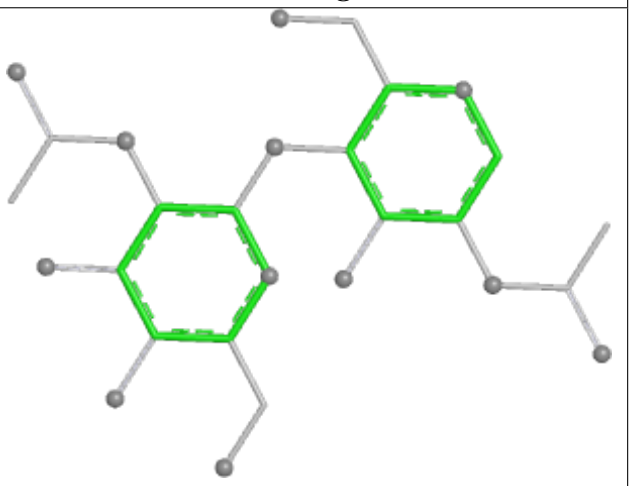
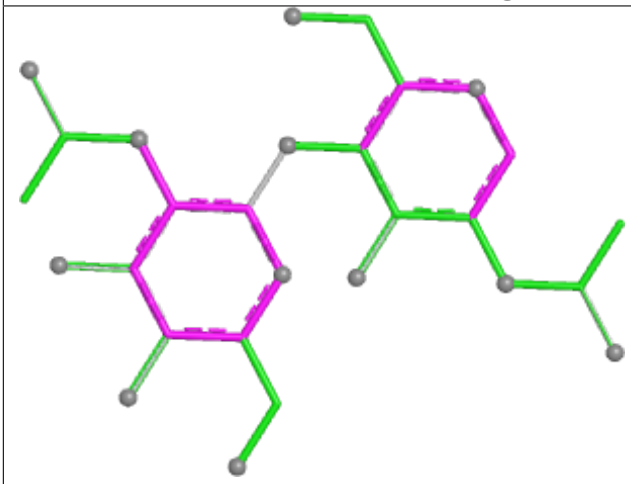


Rings

Oligosaccharide Chain 9



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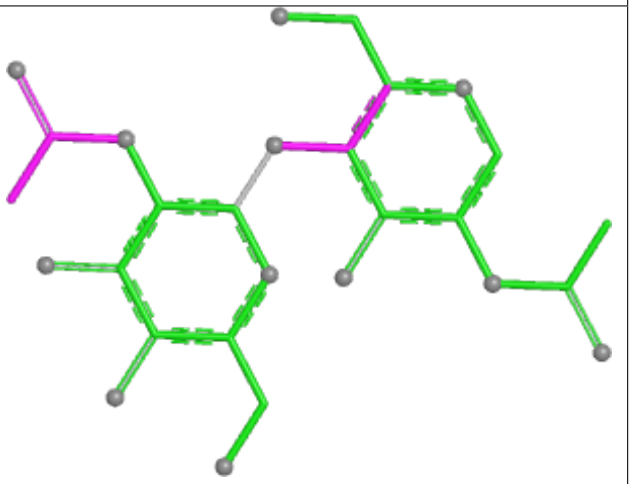

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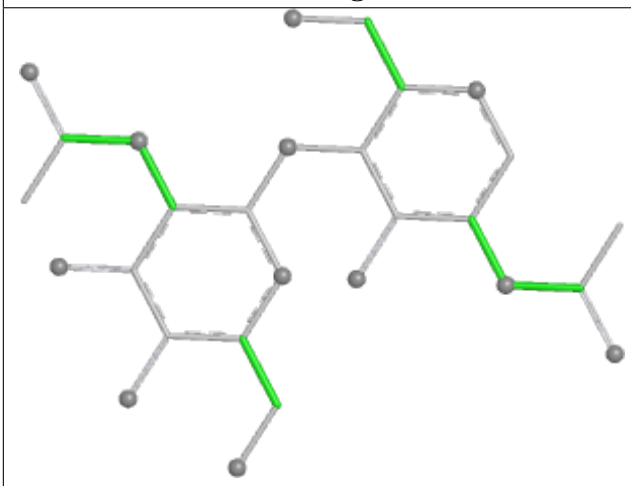

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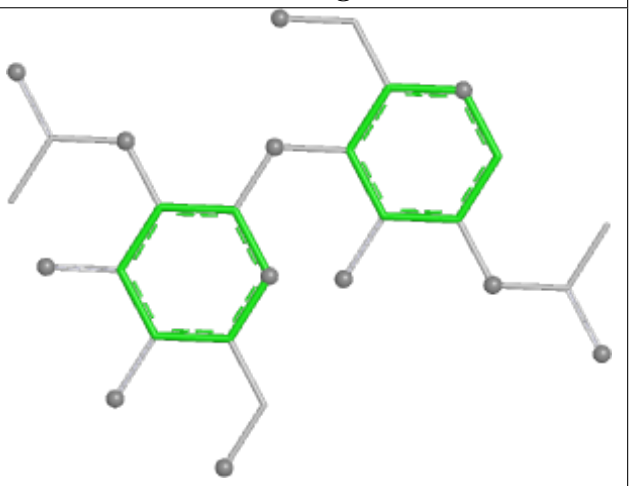
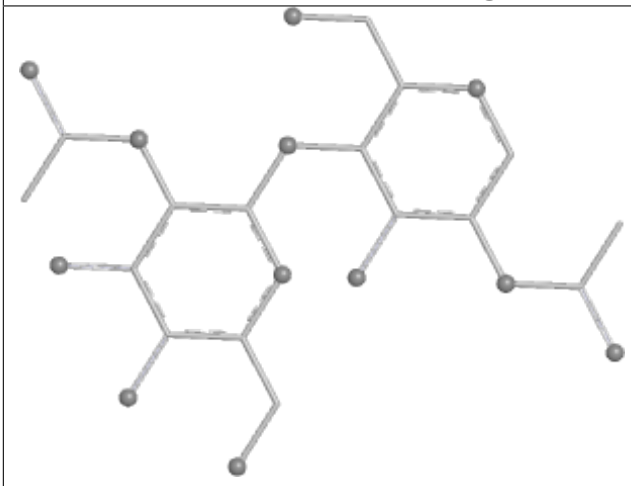


Rings

Oligosaccharide Chain AA



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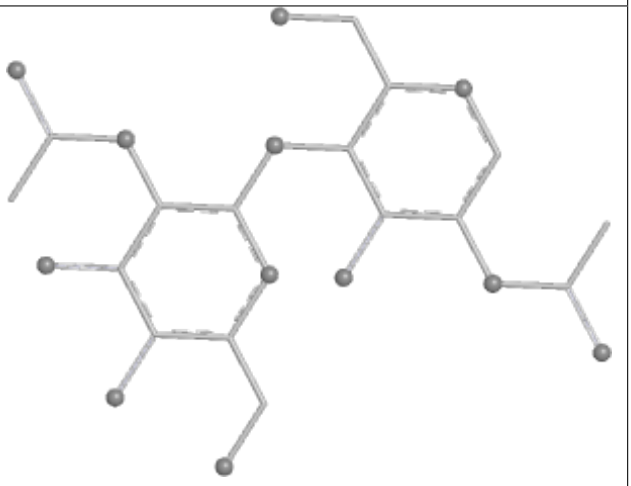
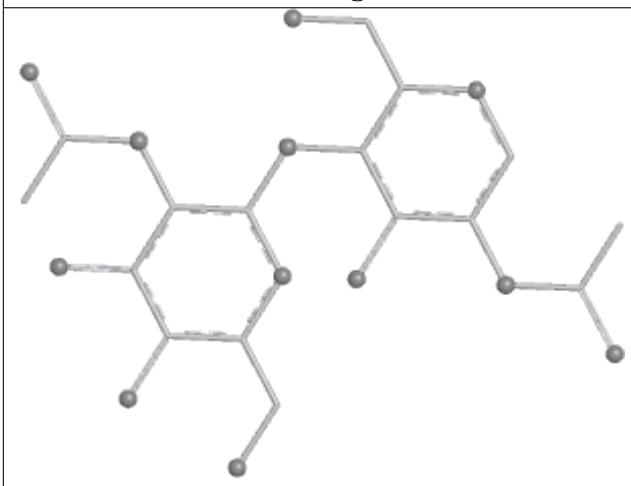


Bond angles



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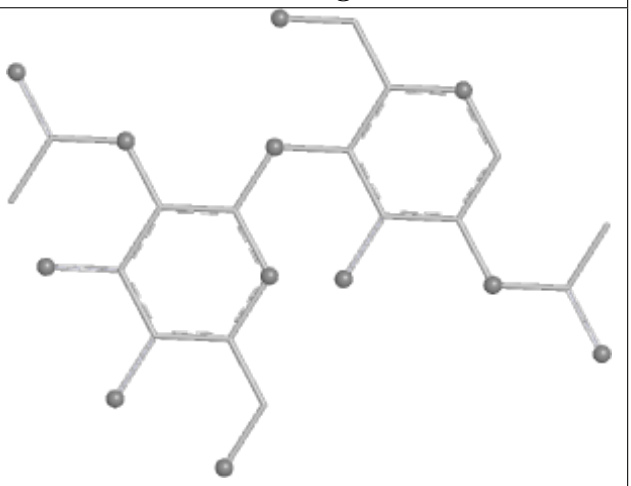
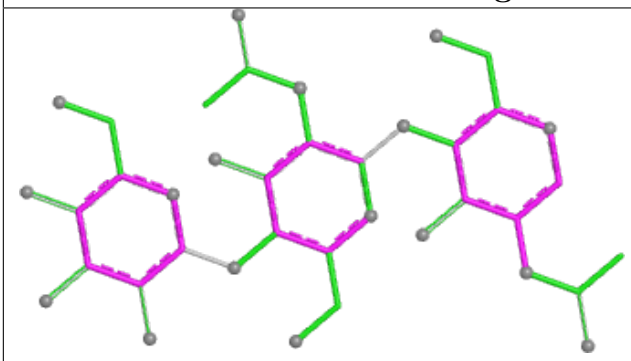


Rings

Oligosaccharide Chain R



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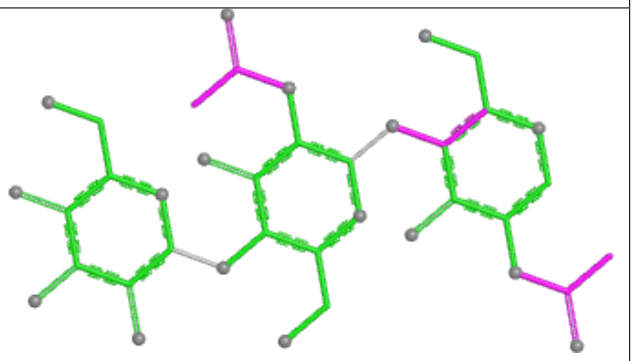
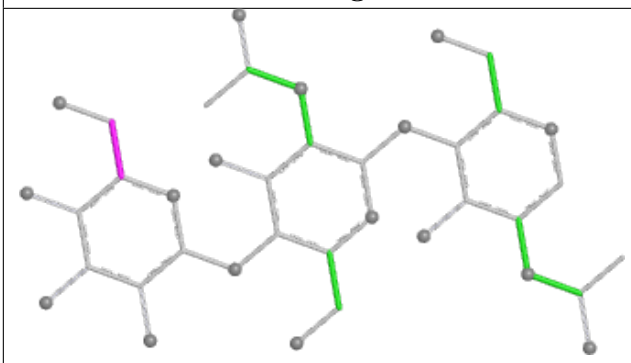


Bond angles



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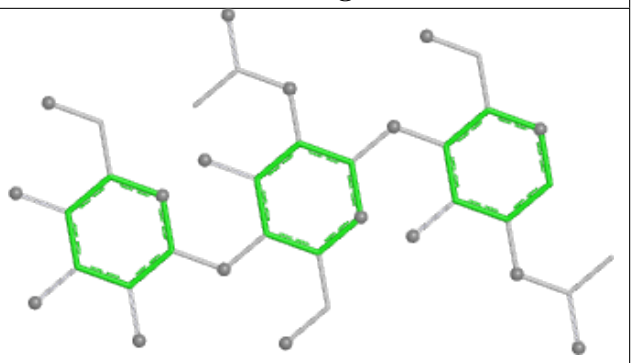
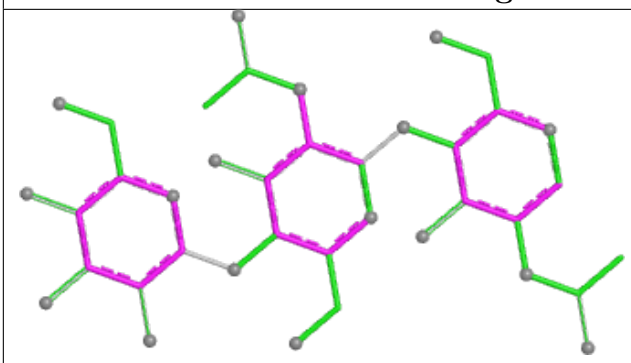


Rings

Oligosaccharide Chain T



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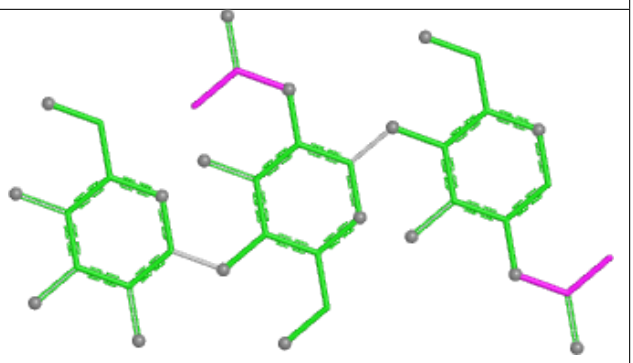
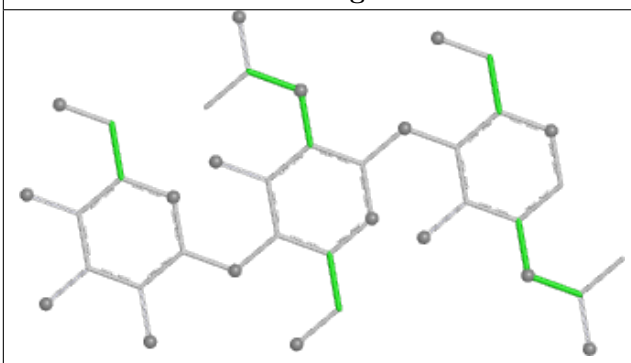
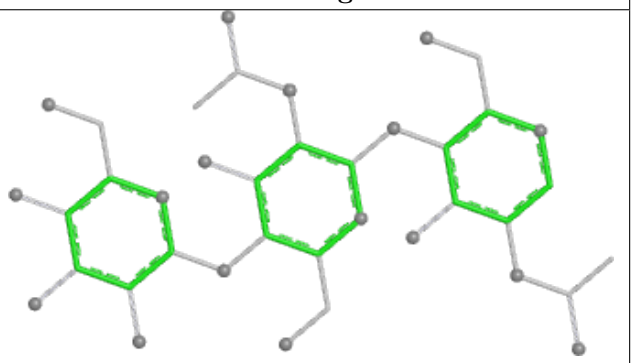


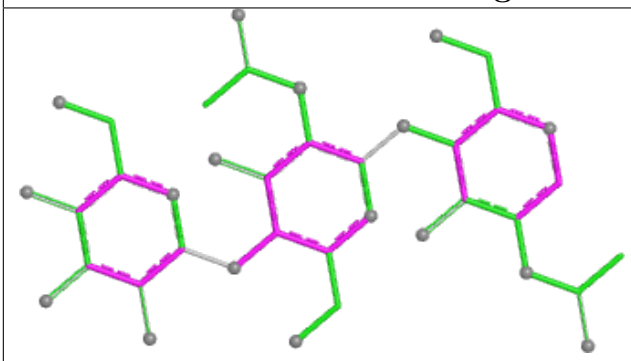
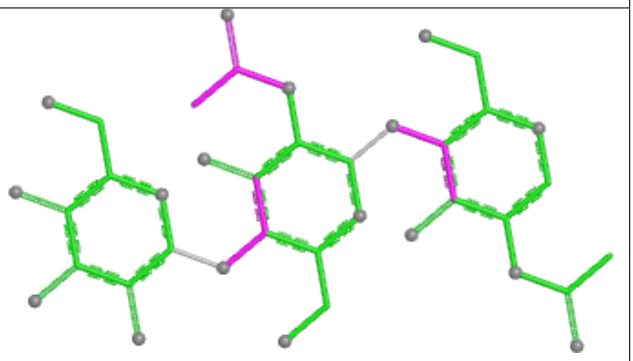
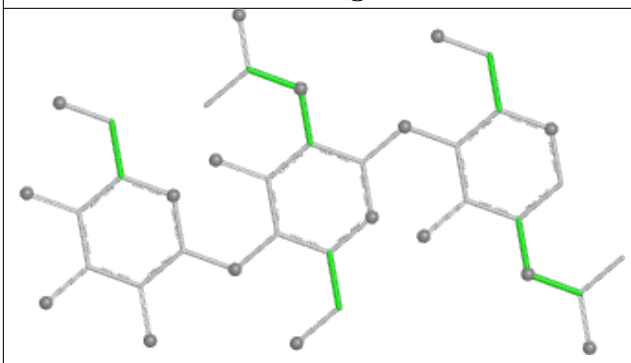
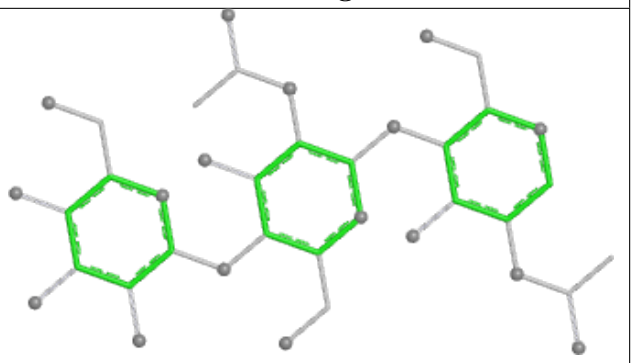
Bond angles



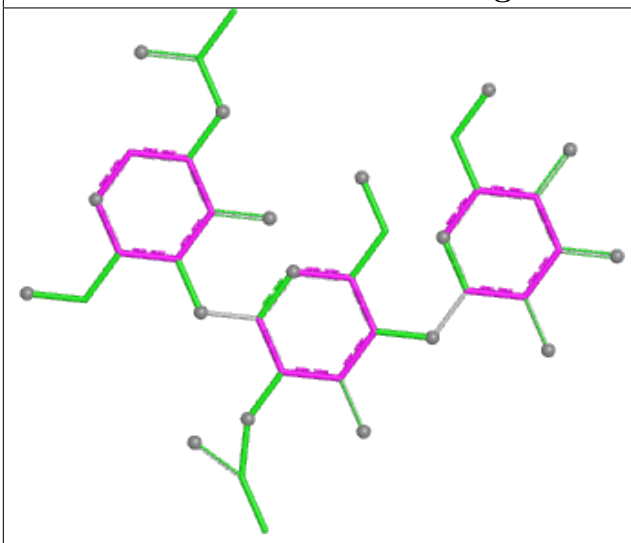
Torsions



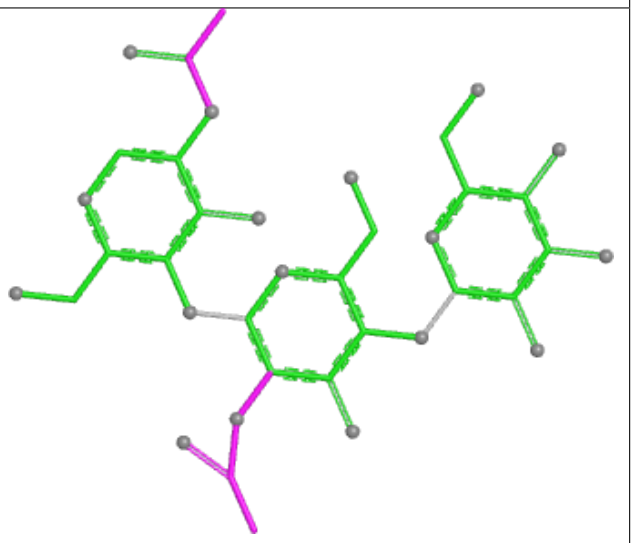
Rings

Oligosaccharide Chain U	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

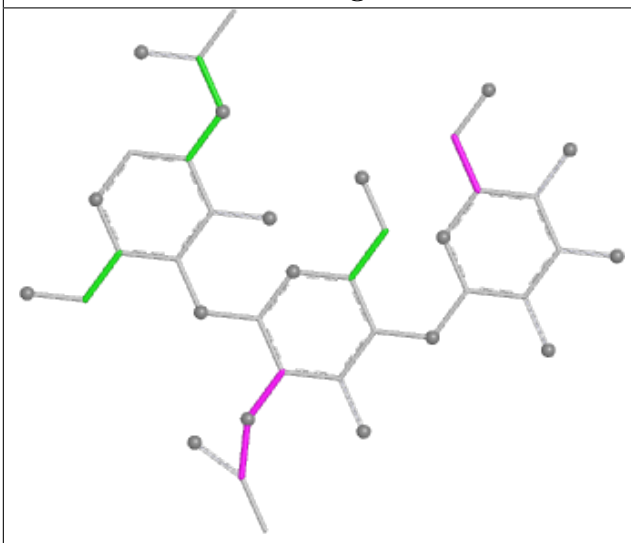
Oligosaccharide Chain V



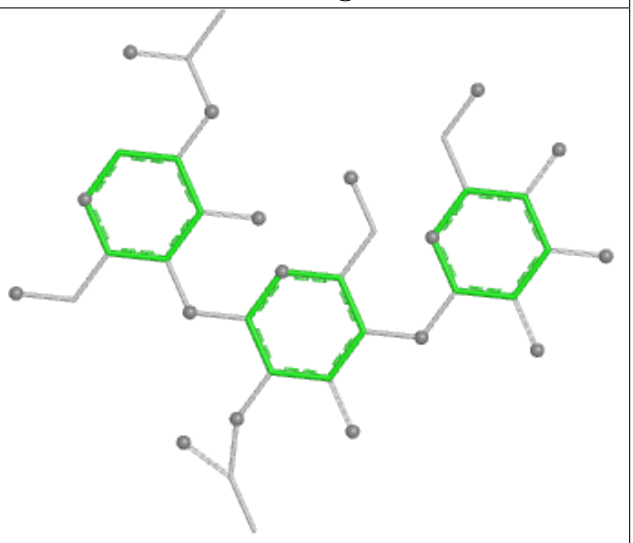
Bond lengths



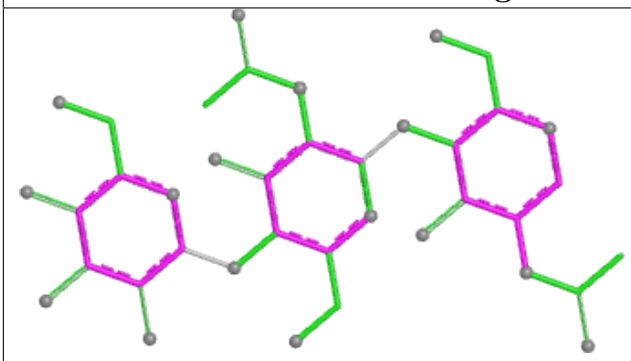
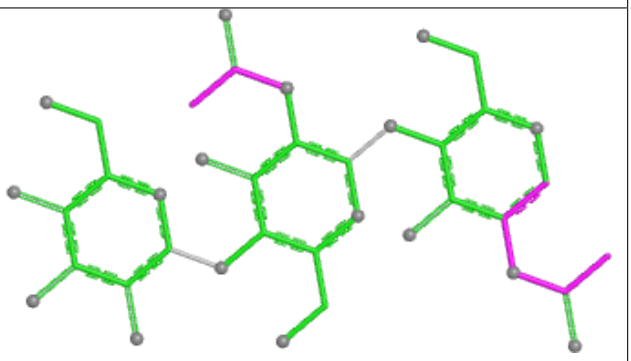
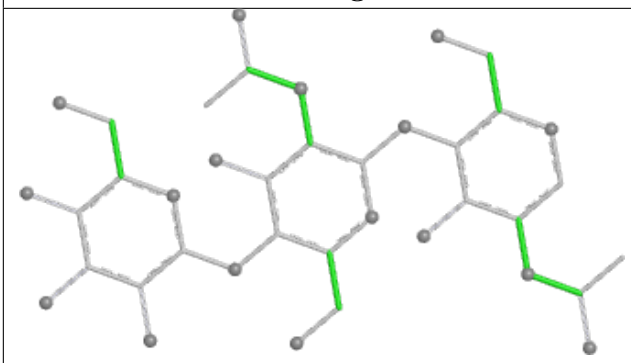
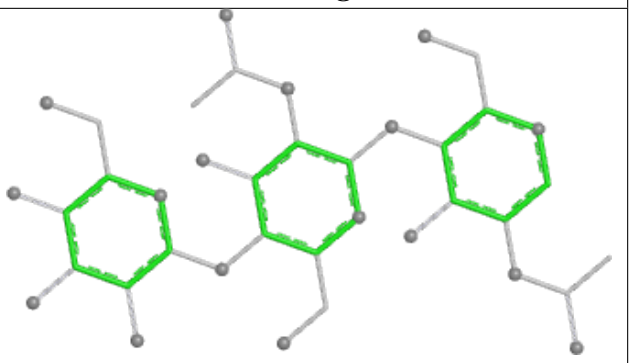
Bond angles

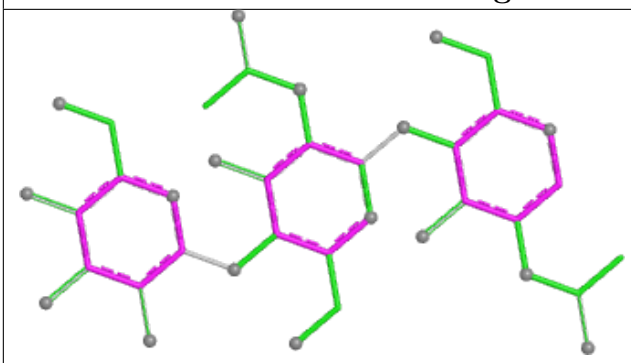
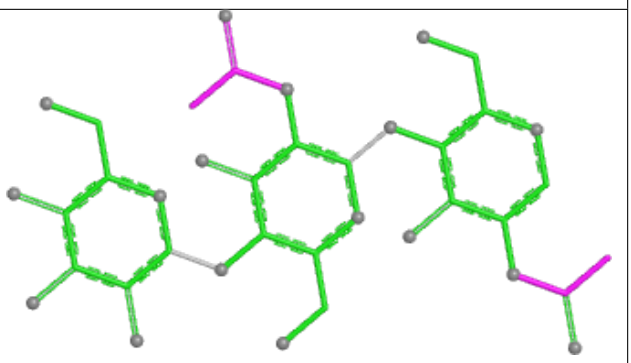
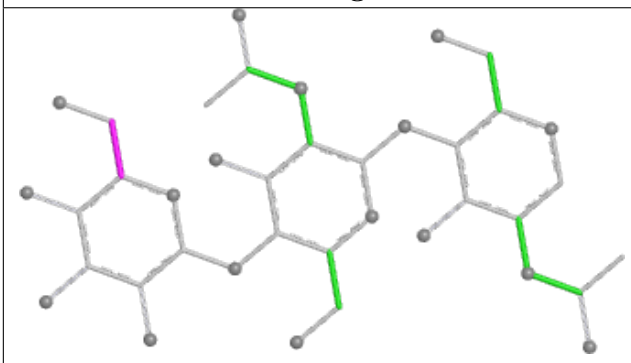
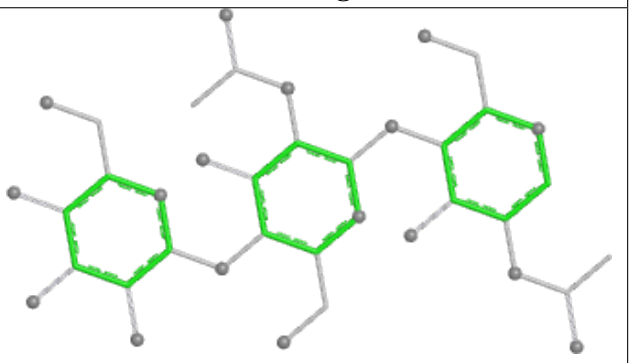


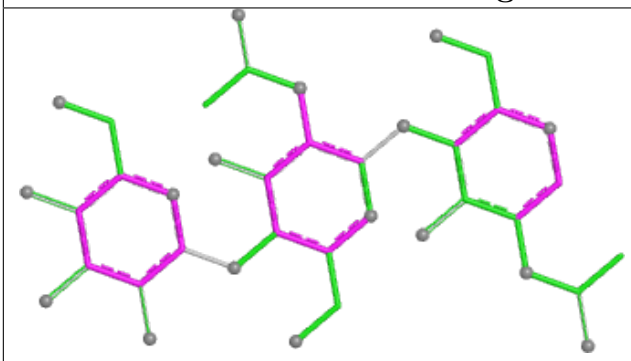
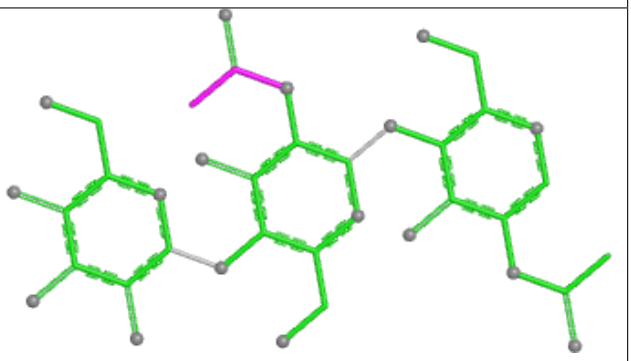
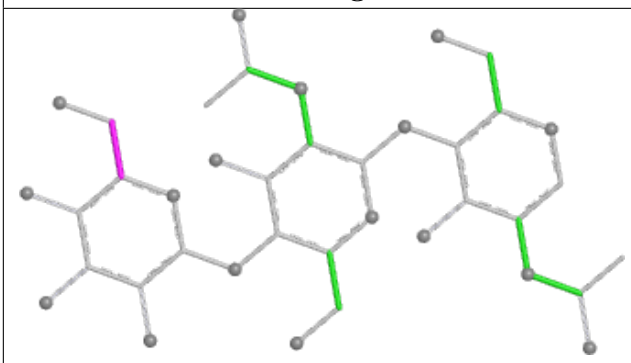
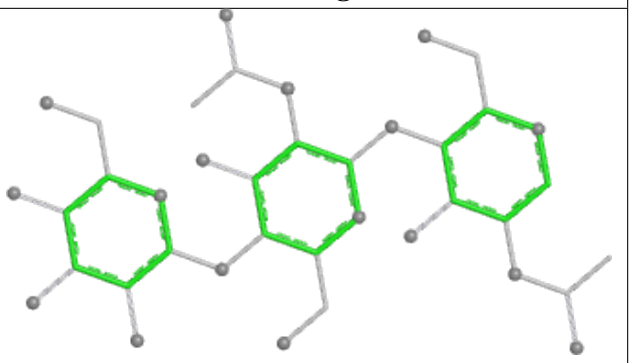
Torsions

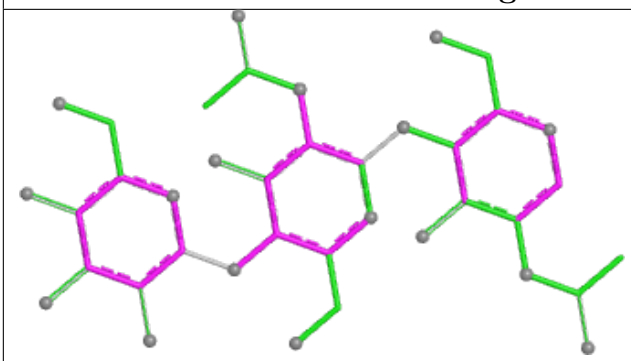
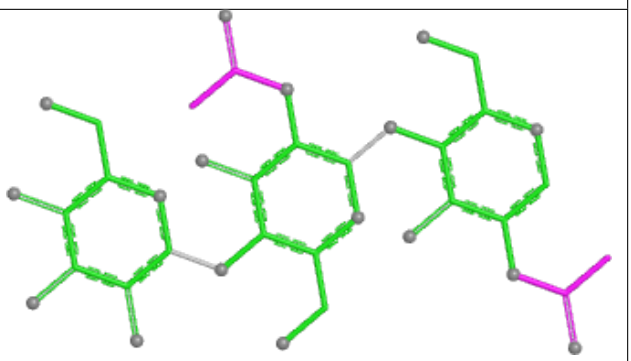
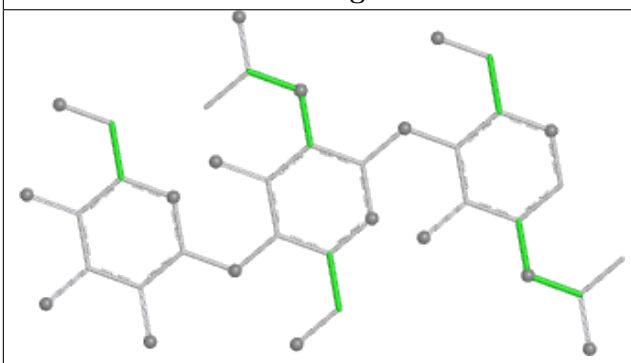
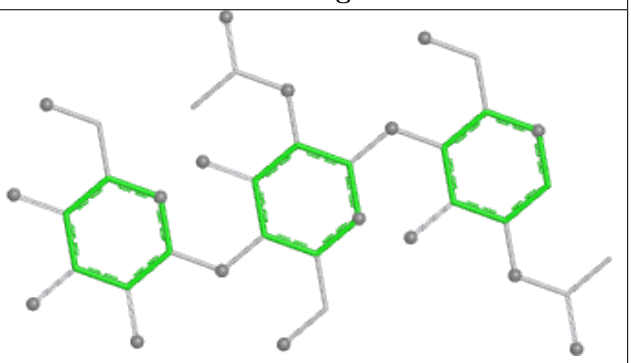


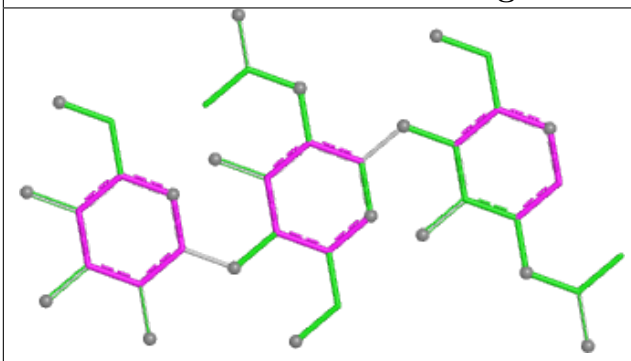
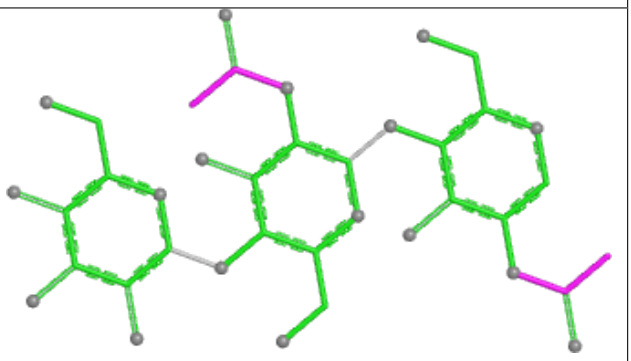
Rings

Oligosaccharide Chain X	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain Y	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain Z	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain a	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain b	
	
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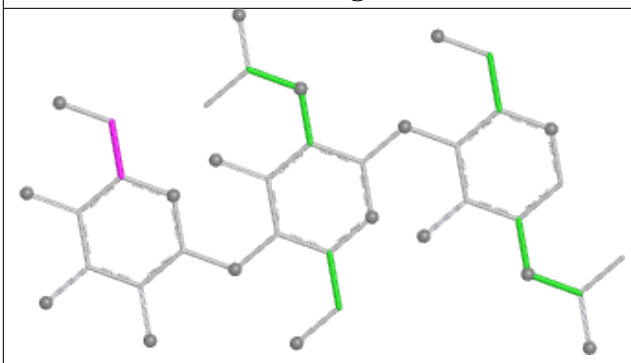	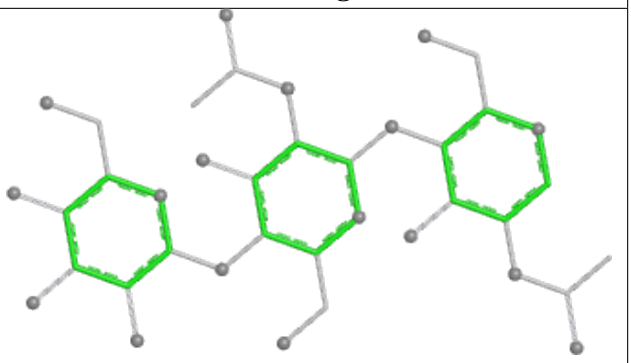
Torsions	Rings

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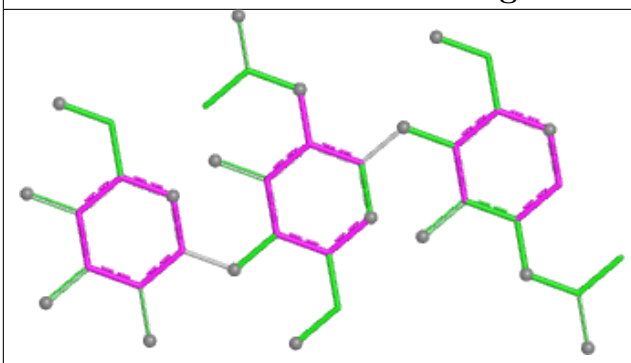	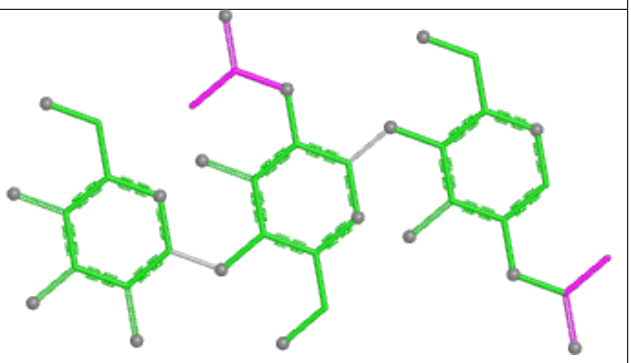
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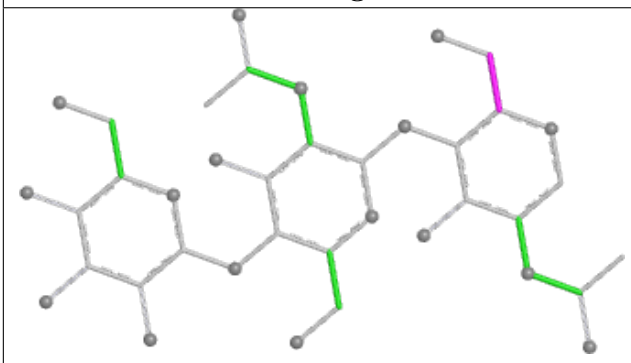	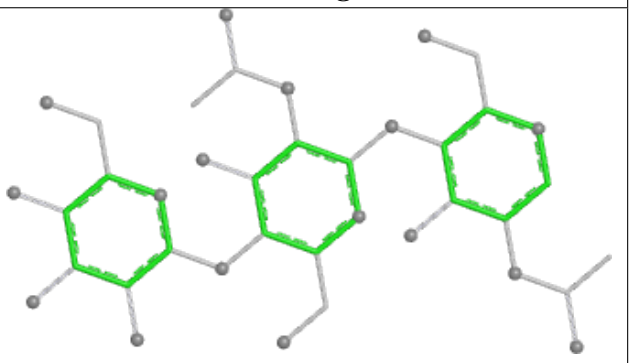
Torsions	Rings

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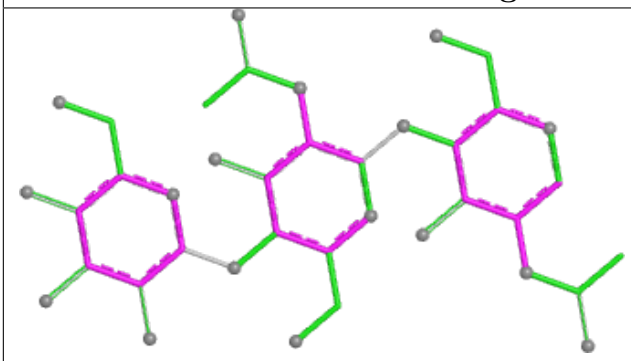	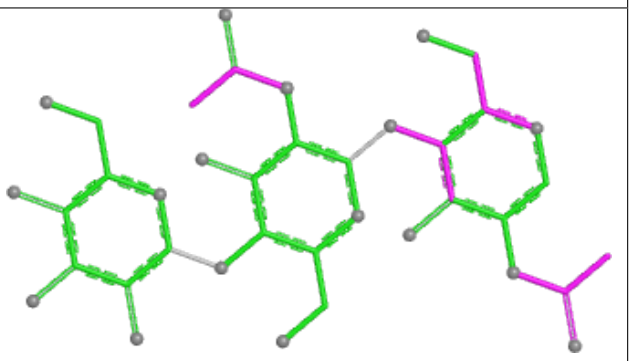
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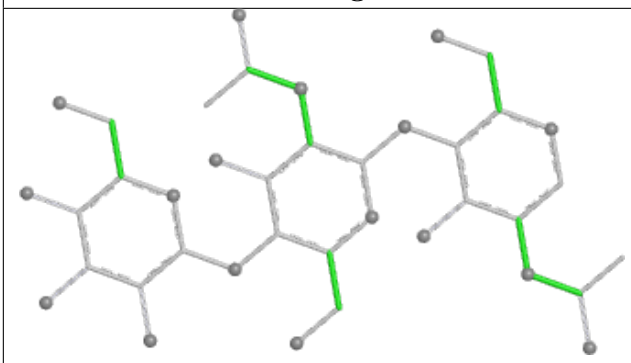	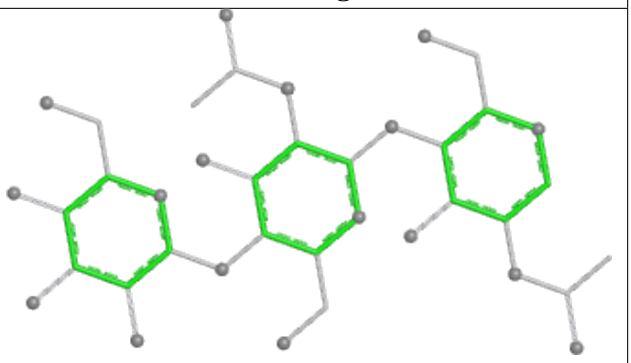
Torsions	Rings

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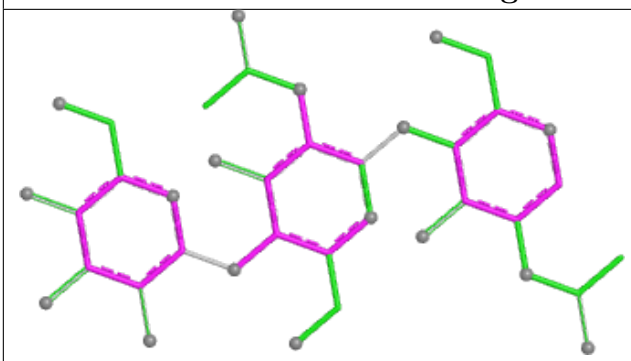	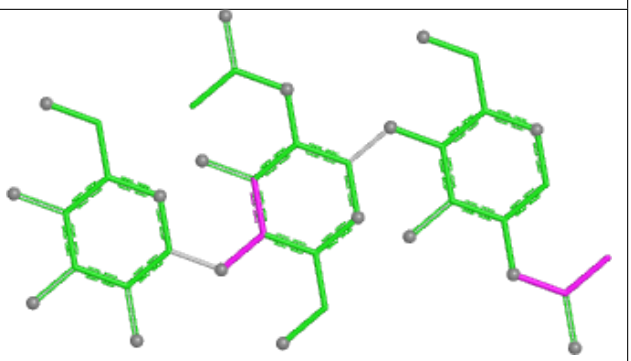
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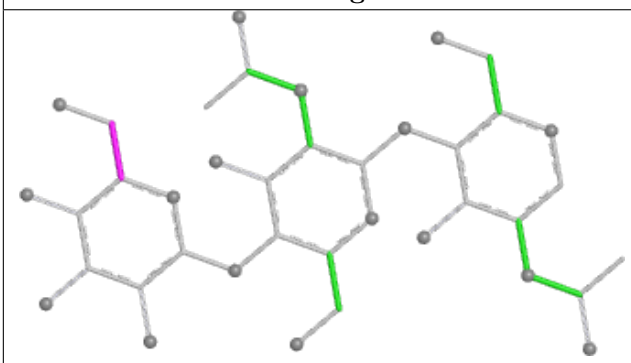	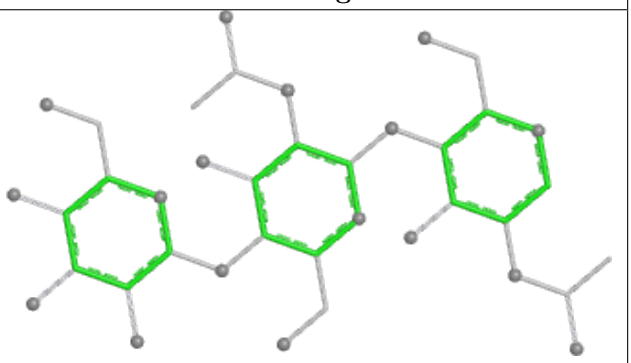
Torsions	Rings

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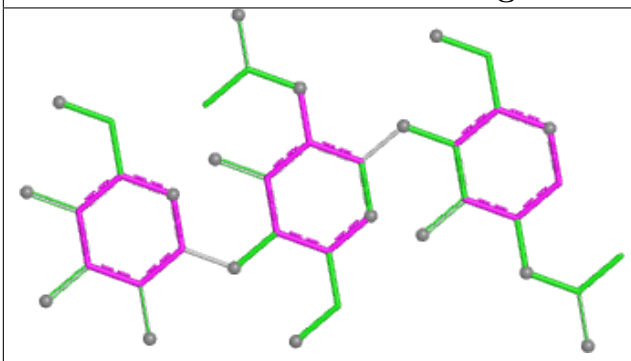
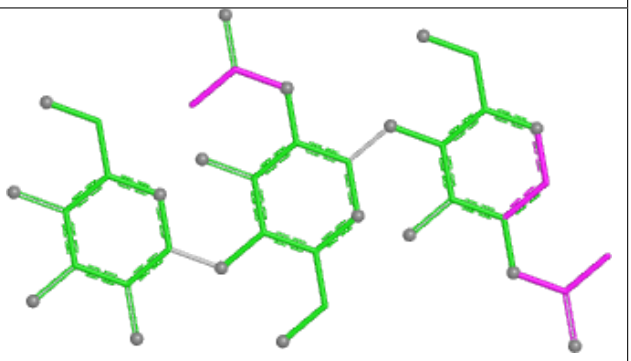
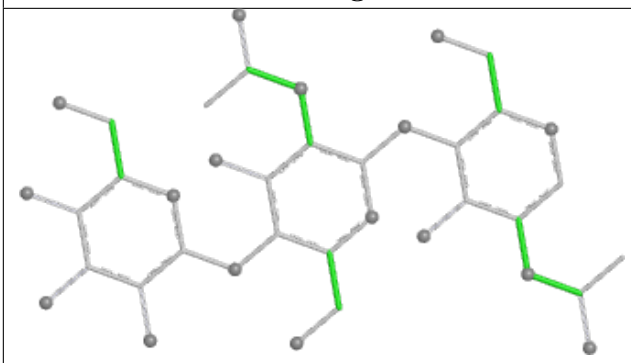
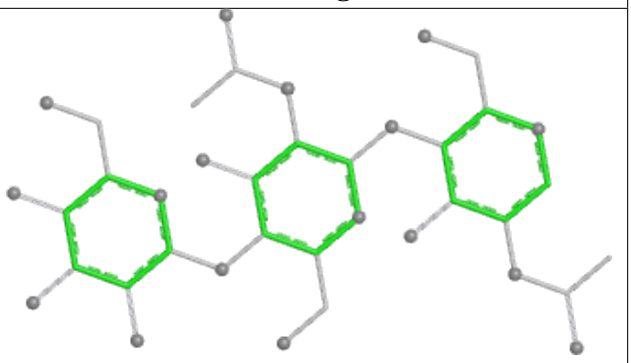
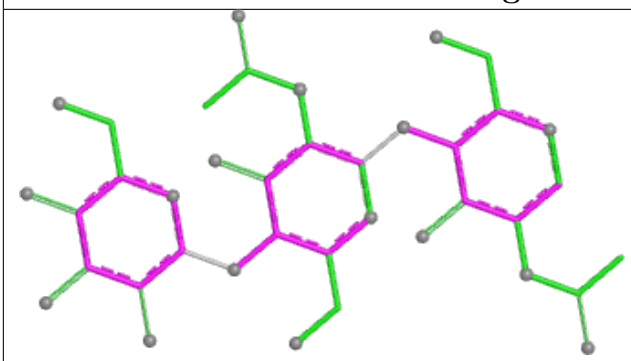
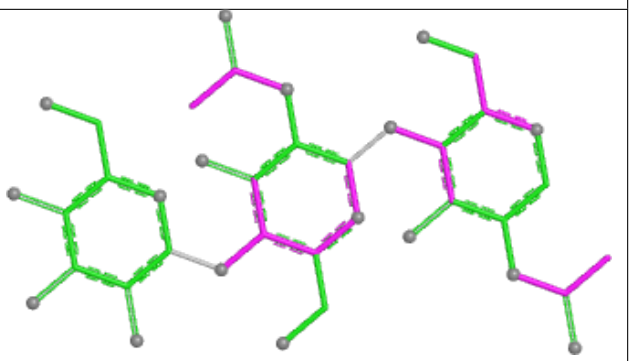
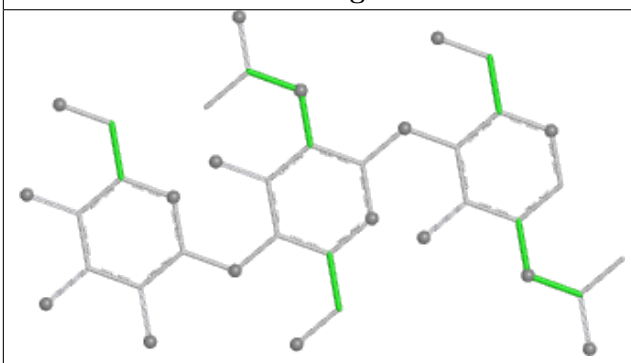
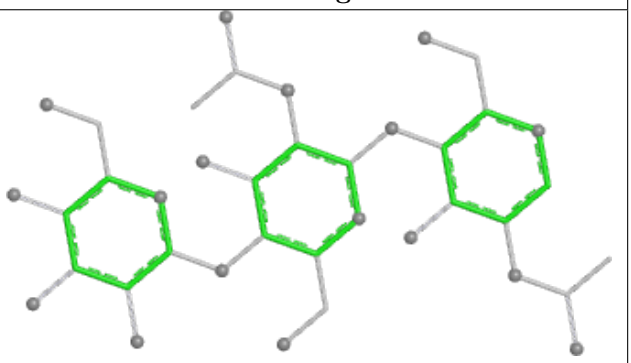
	
Bond lengths	Bond angles
	
Torsions	Rings

Oligosaccharide Chain i	
	
Bond lengths	Bond angles
	
Torsions	Rings

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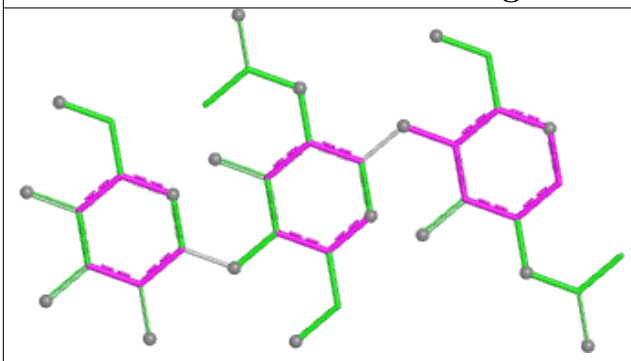
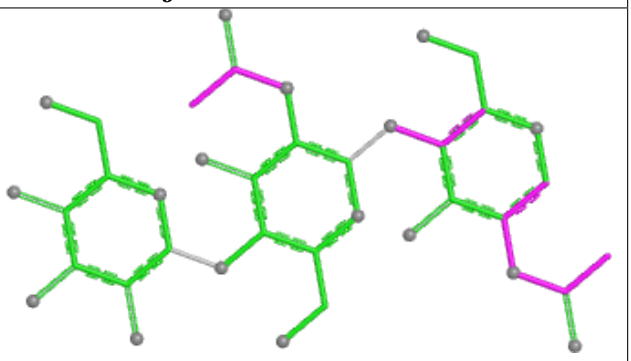
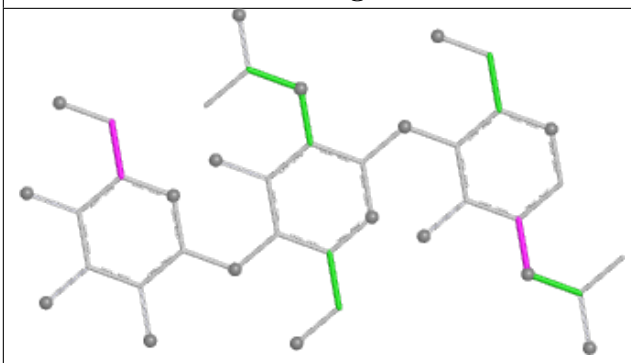
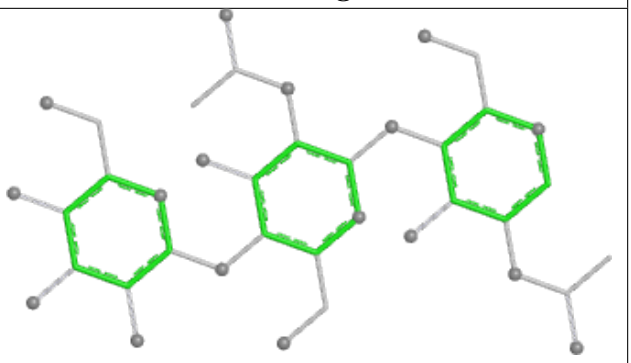
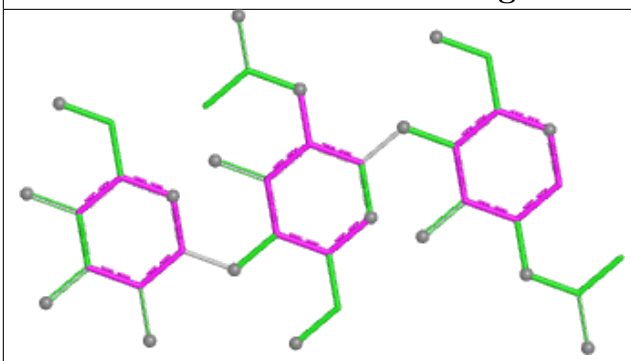
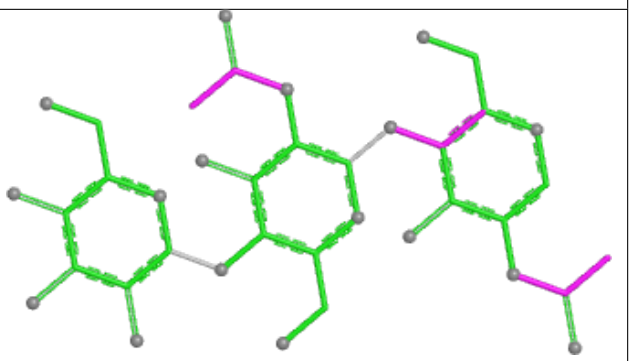
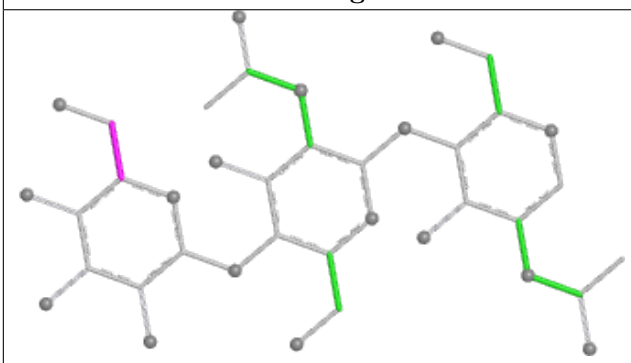
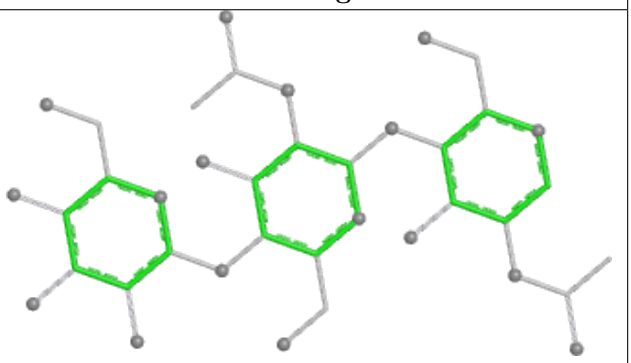
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain k	
 Bond lengths	 Bond angles
 Torsions	 Rings

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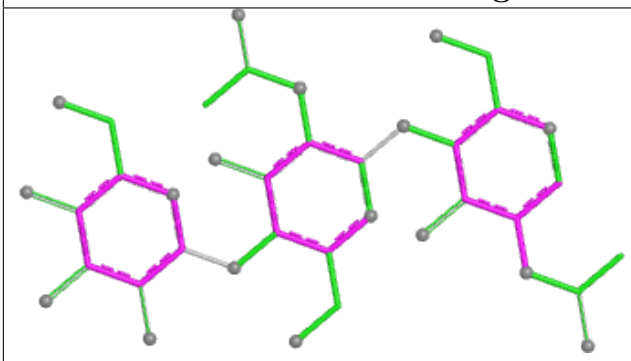
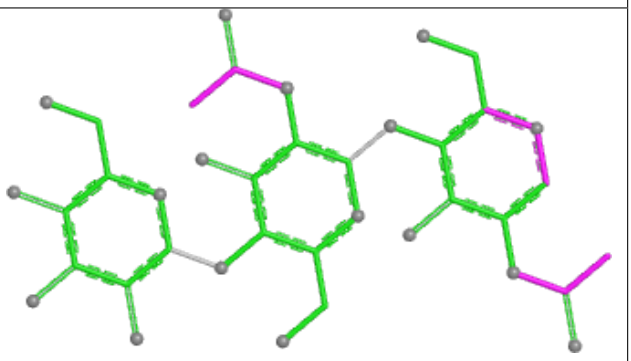
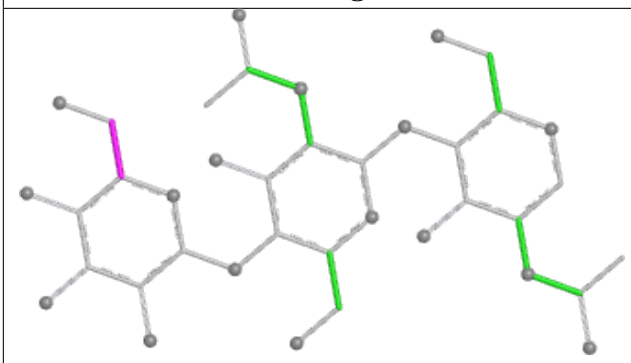
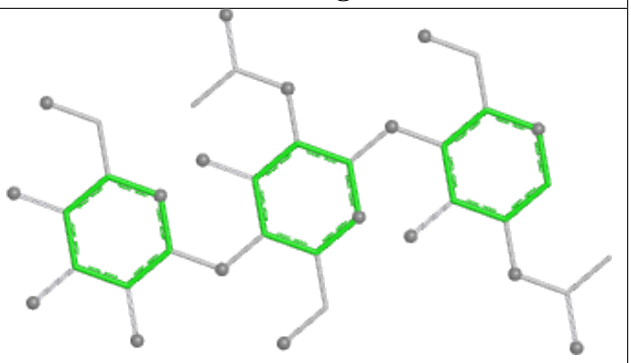
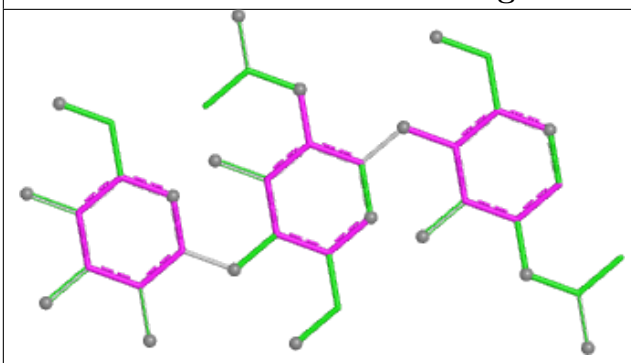
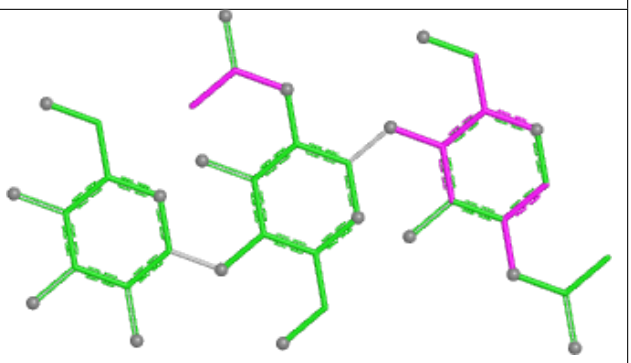
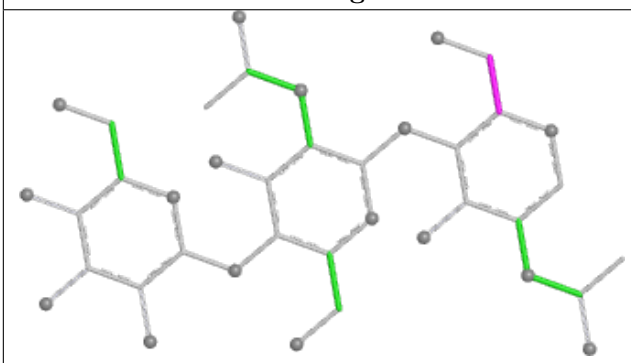
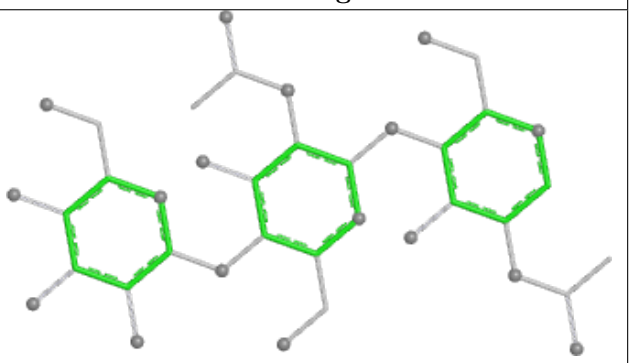
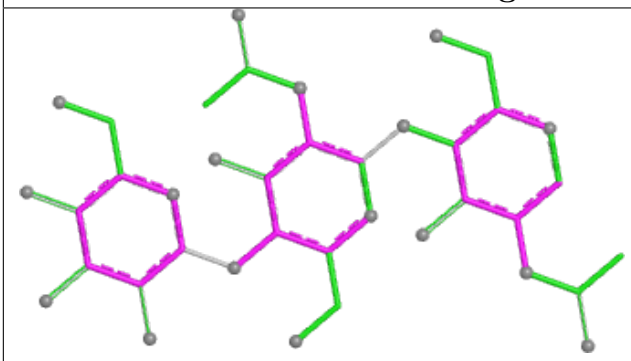
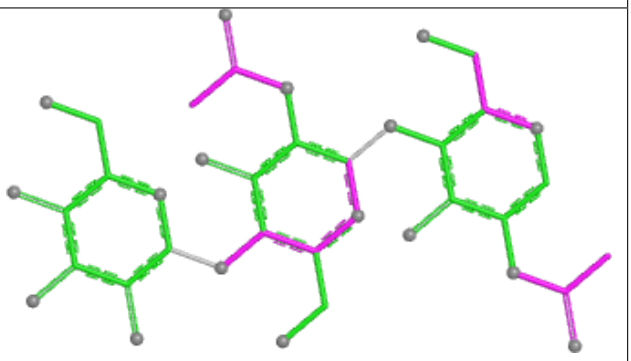
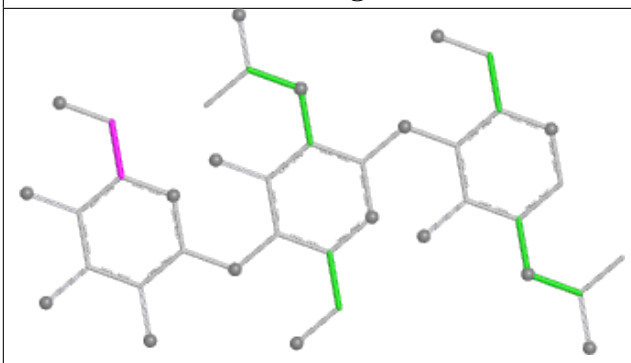
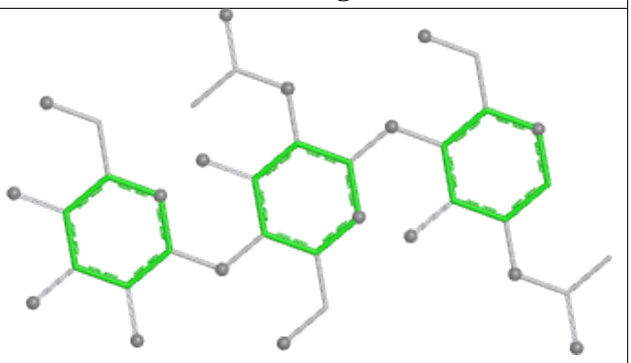
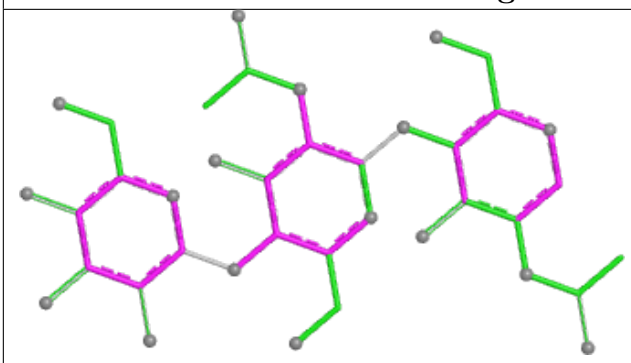
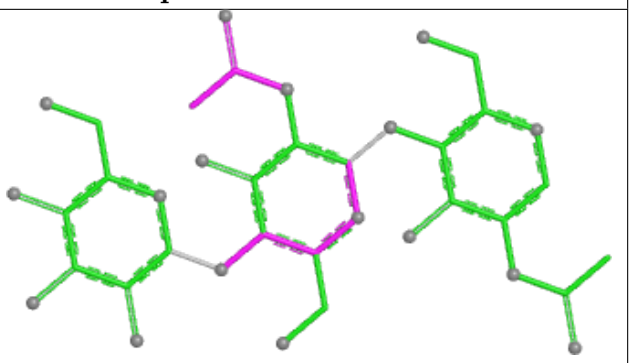
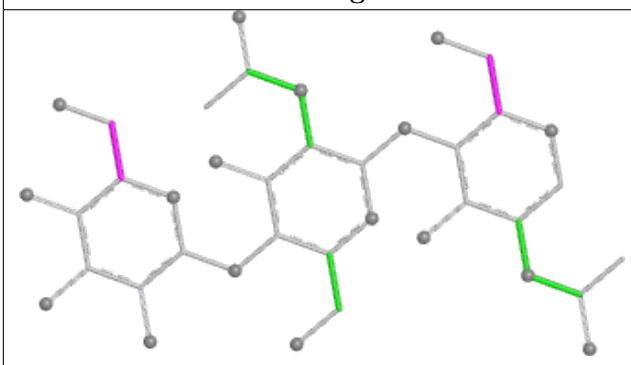
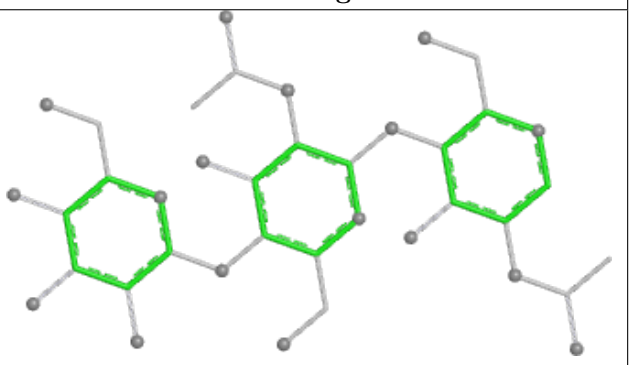
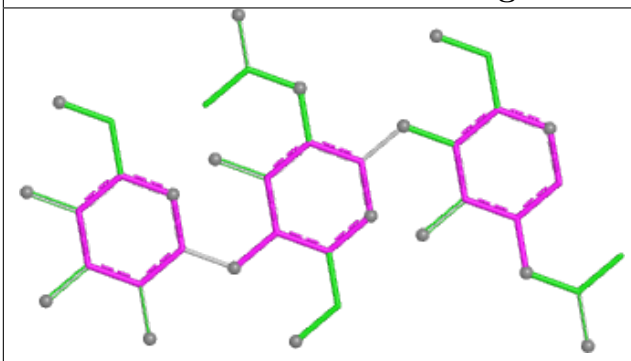
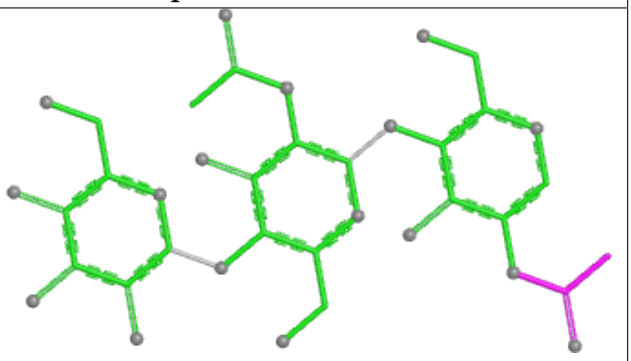
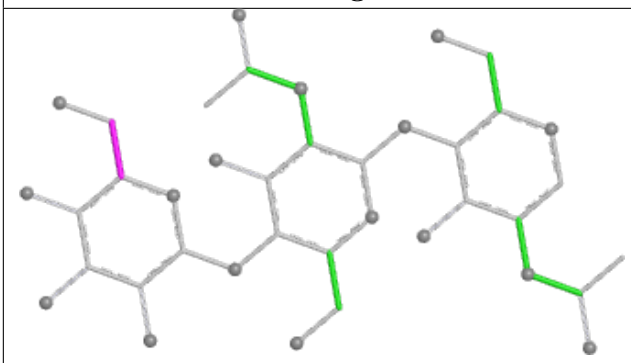
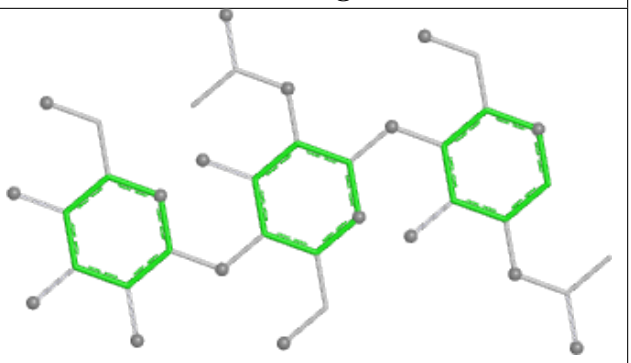
	
Bond lengths	Bond angles
	
Torsions	Rings

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
 Torsions	 Rings

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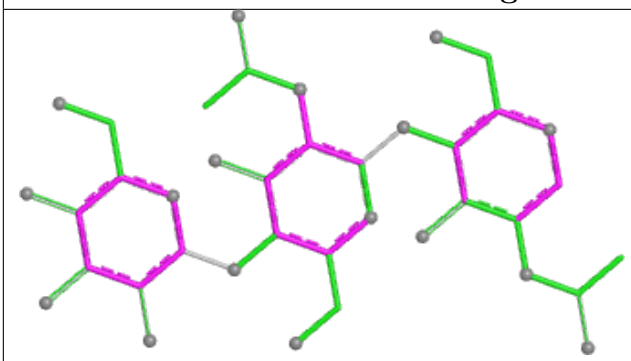
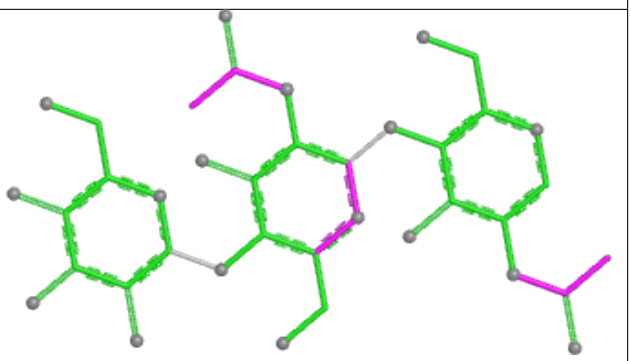
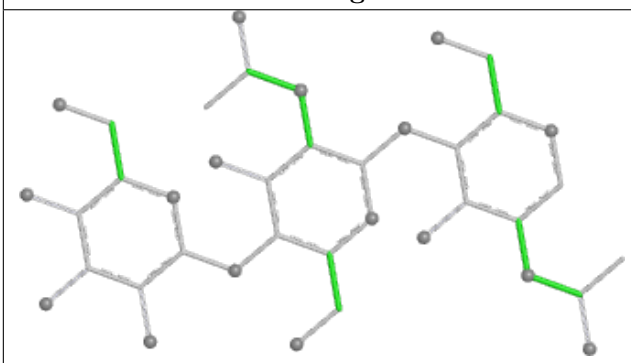
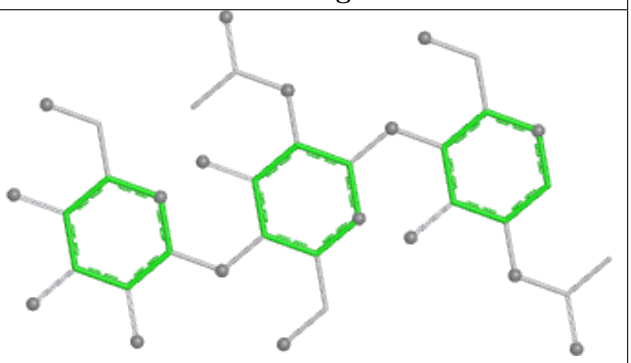
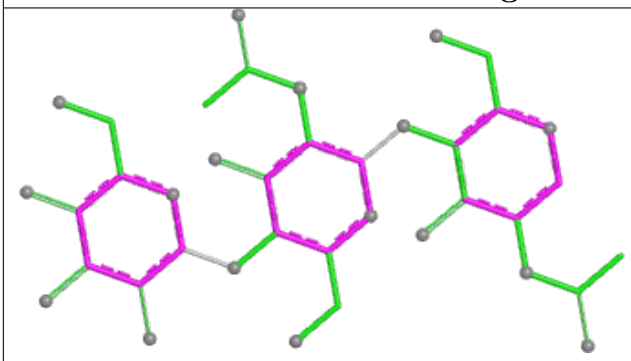
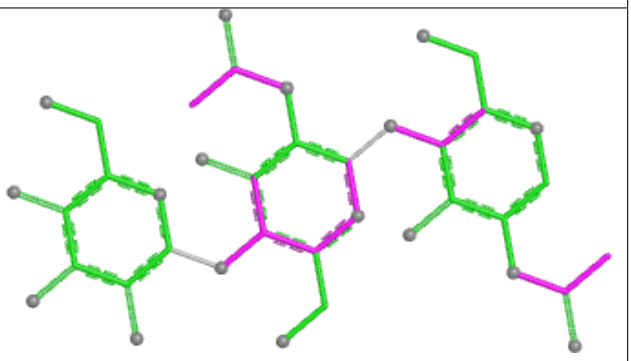
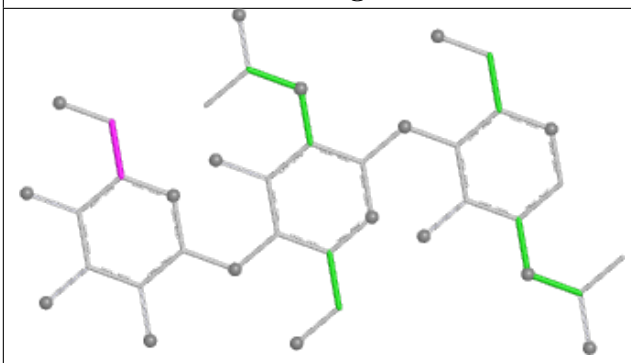
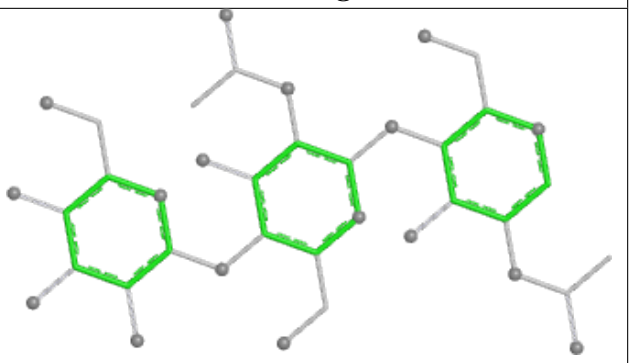
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain t	
	
Bond lengths	Bond angles
	
Torsions	Rings

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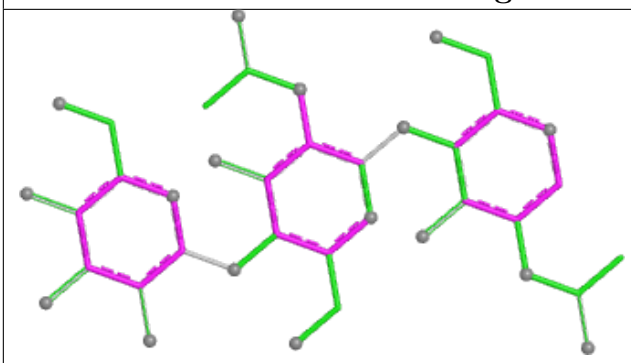
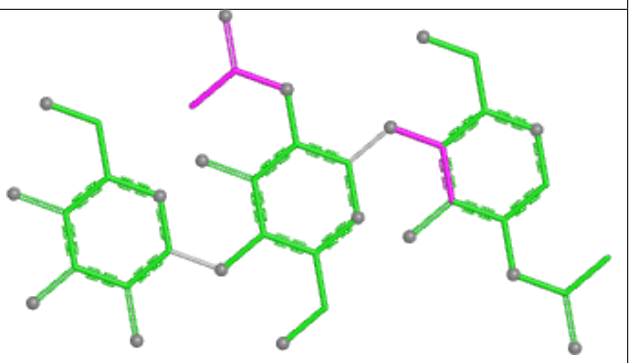
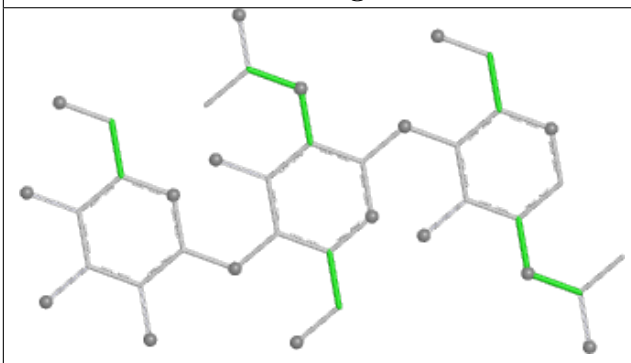
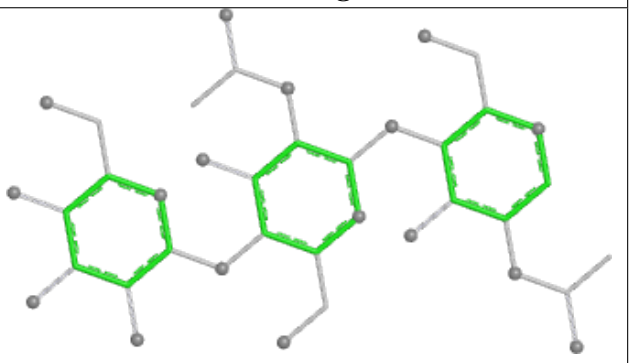
	
Bond lengths	Bond angles
	
Torsions	Rings

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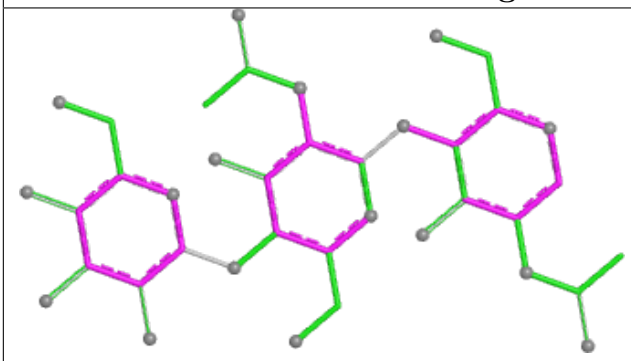
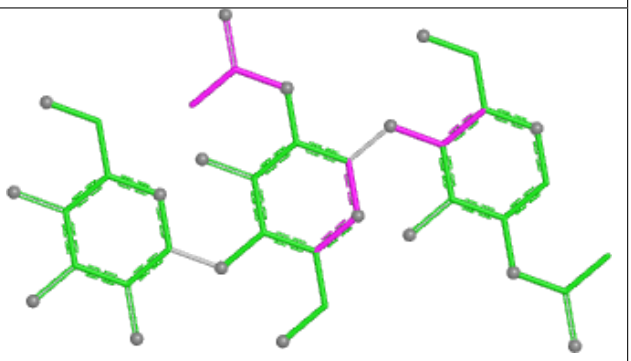
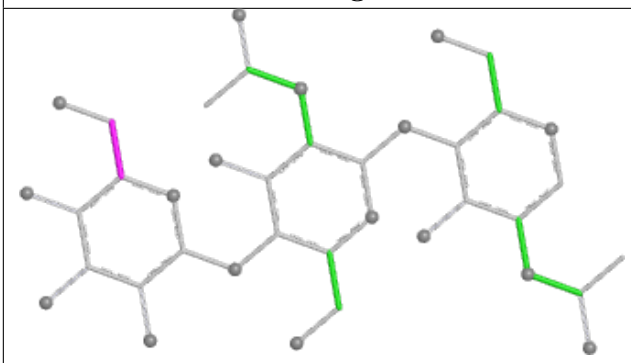
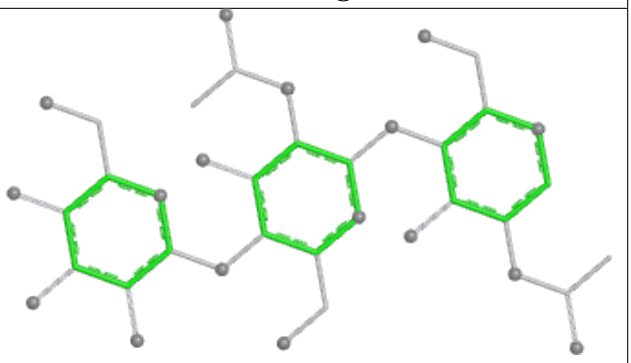
 Bond lengths	 Bond angles
 Torsions	 Rings

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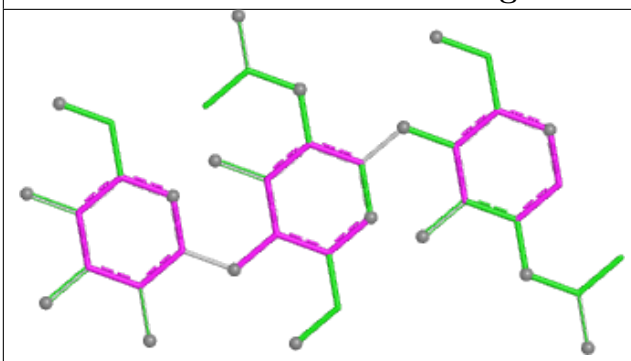
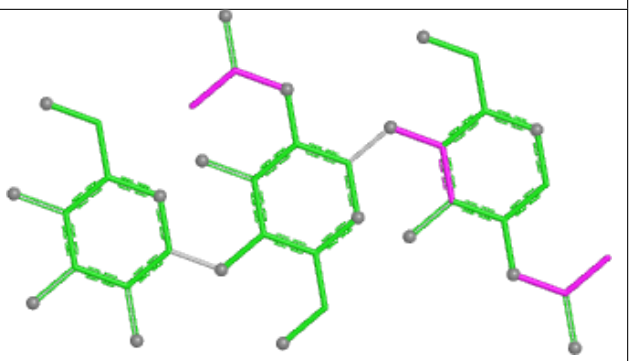
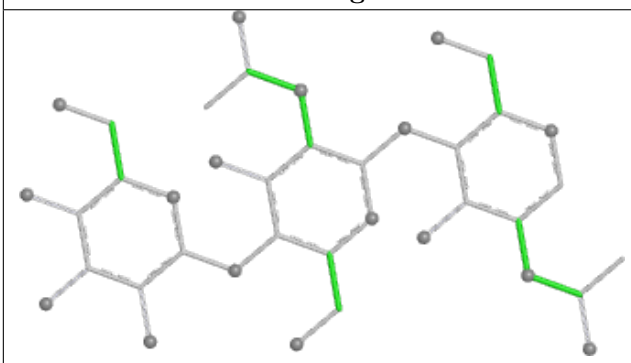
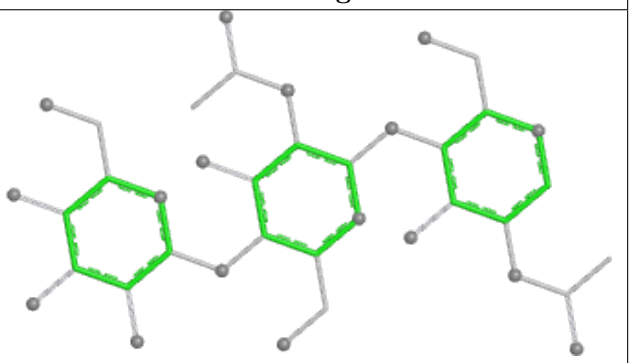
 Bond lengths	 Bond angles
 Torsions	 Rings

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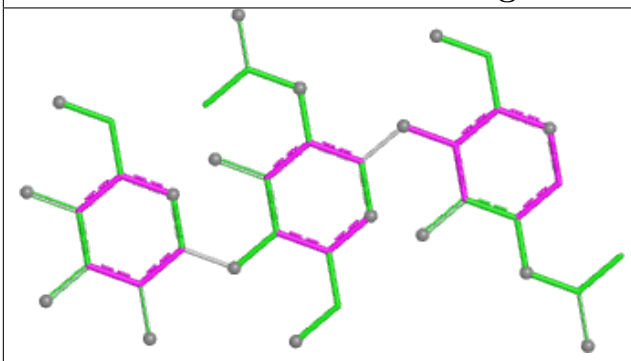
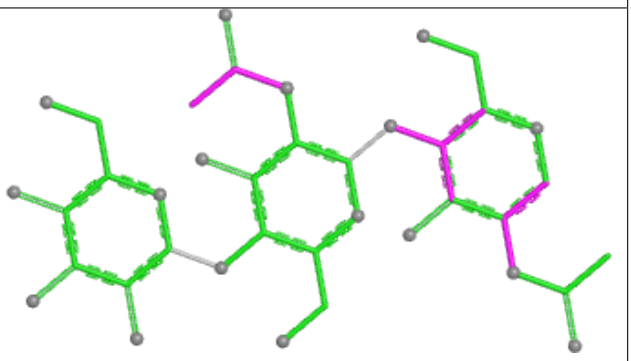
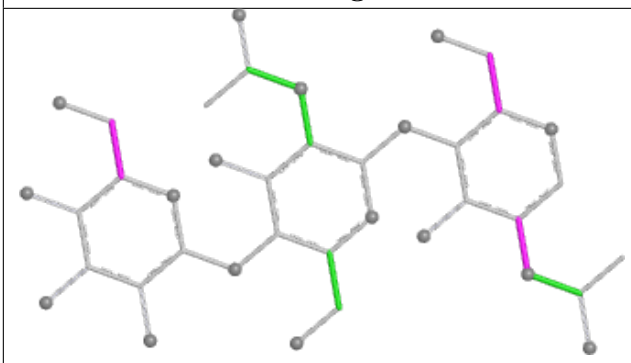
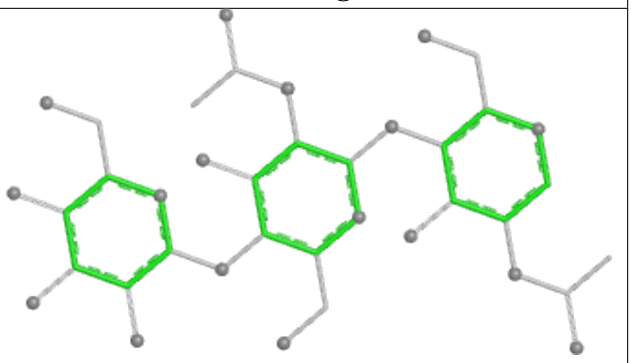
 Bond lengths	 Bond angles
 Torsions	 Rings

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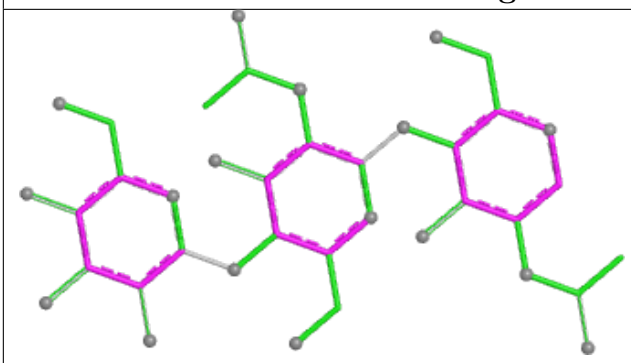
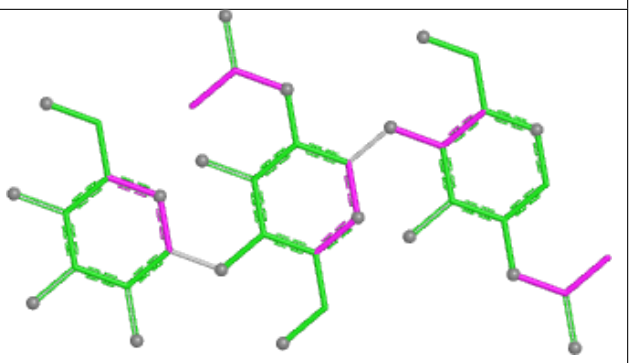
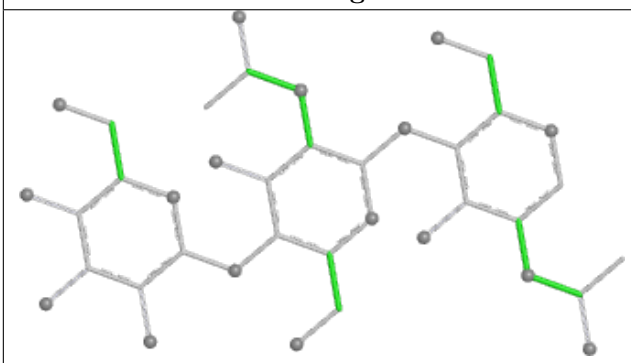
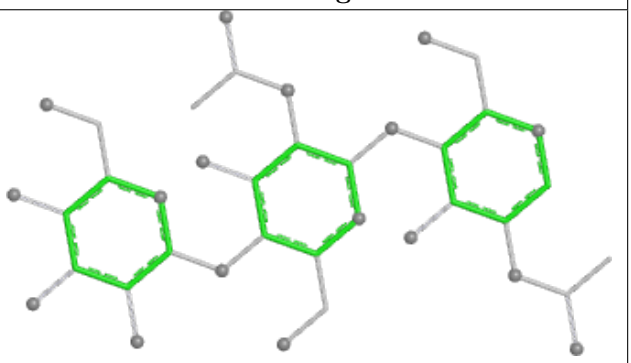
 Bond lengths	 Bond angles
 Torsions	 Rings

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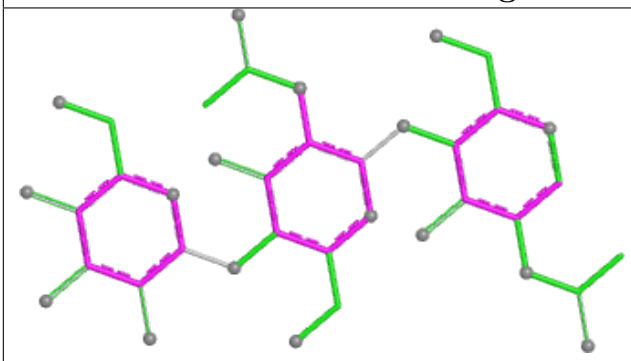
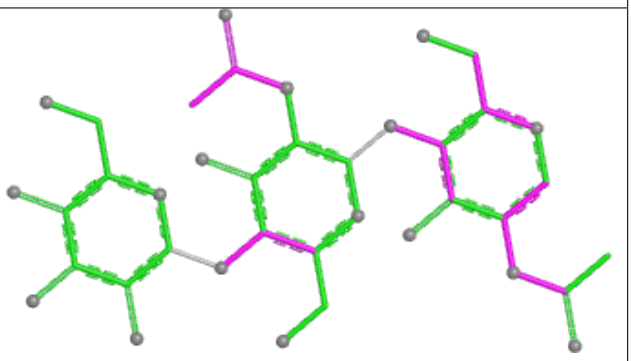
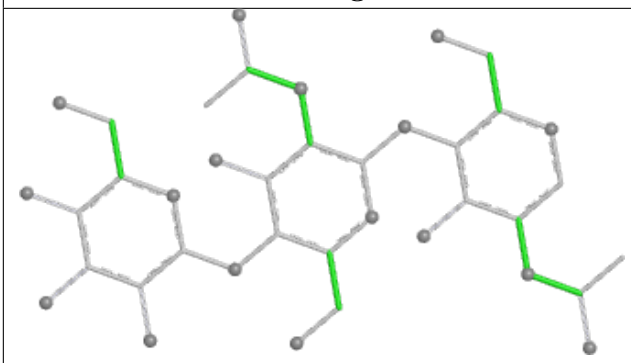
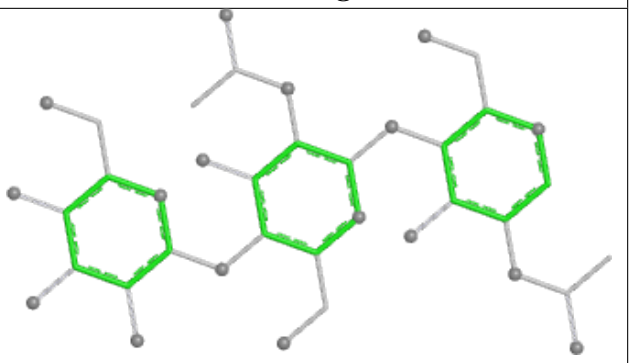
	
Bond lengths	Bond angles
	
Torsions	Rings

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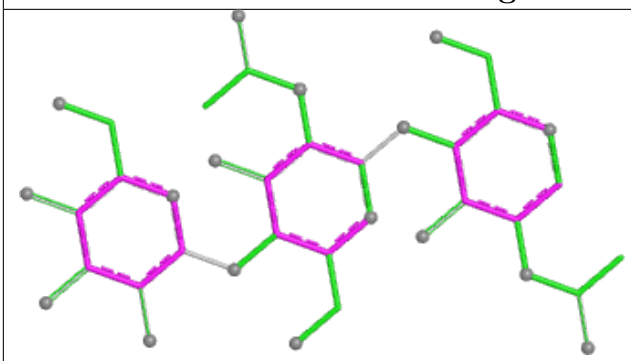
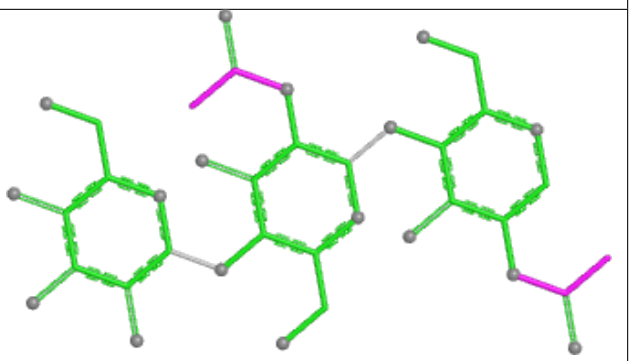
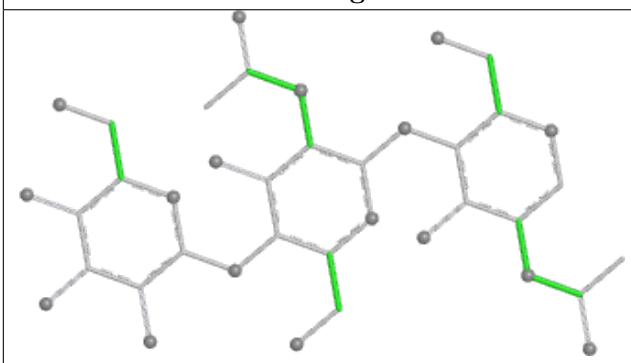
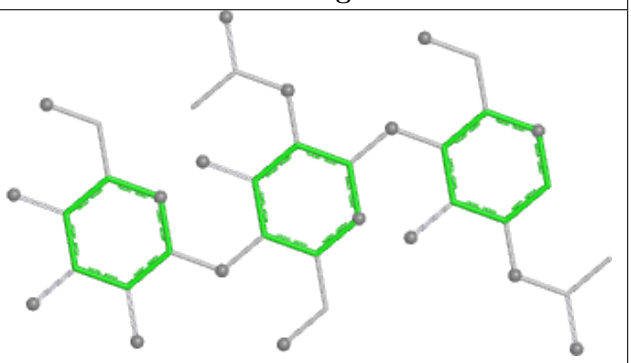
	
Bond lengths	Bond angles
	
Torsions	Rings

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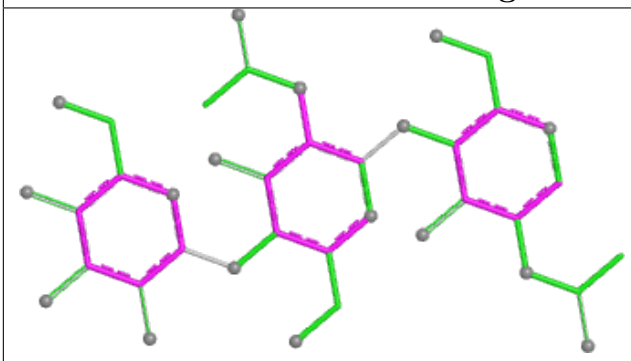
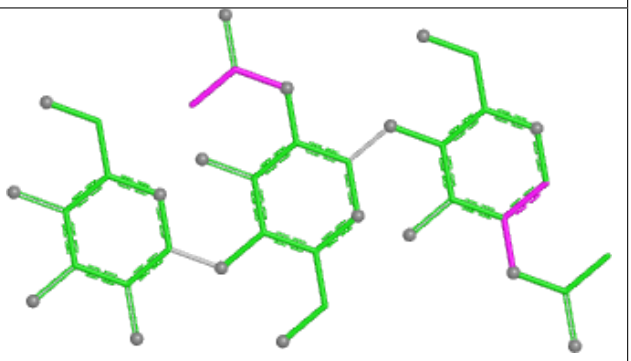
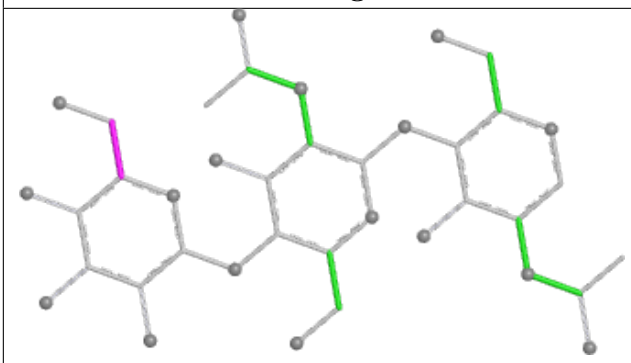
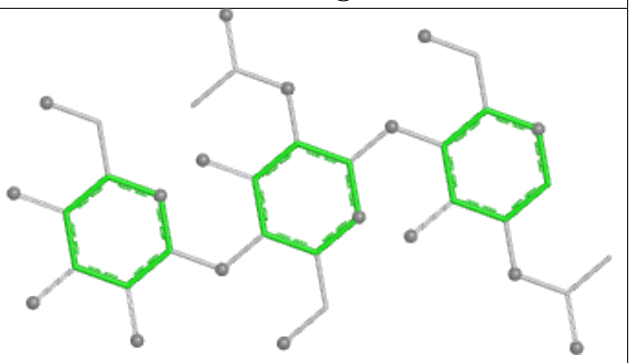
 Bond lengths	 Bond angles
 Torsions	 Rings

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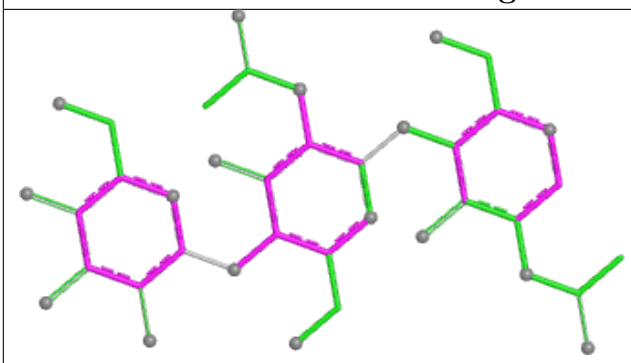
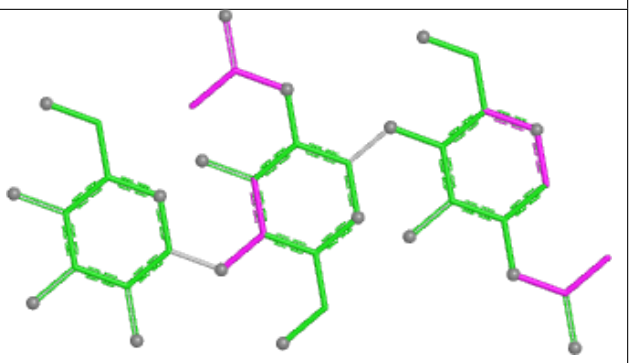
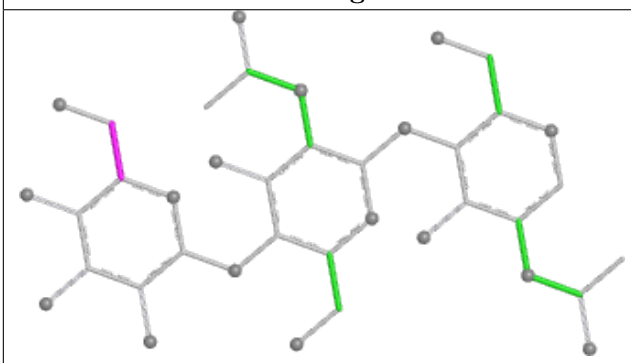
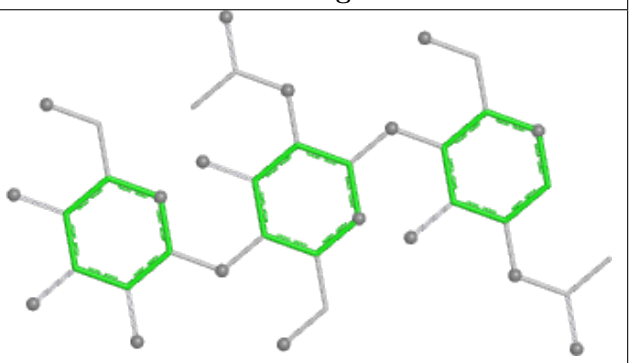
 Bond lengths	 Bond angles
 Torsions	 Rings

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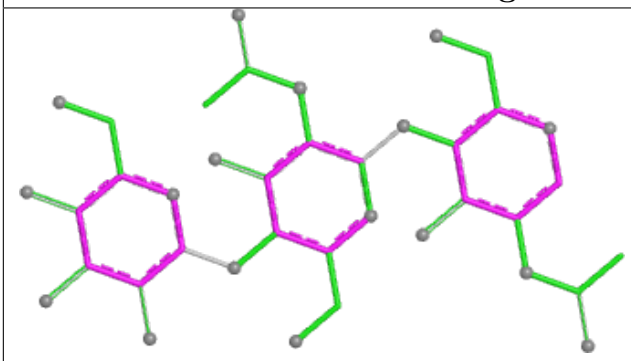
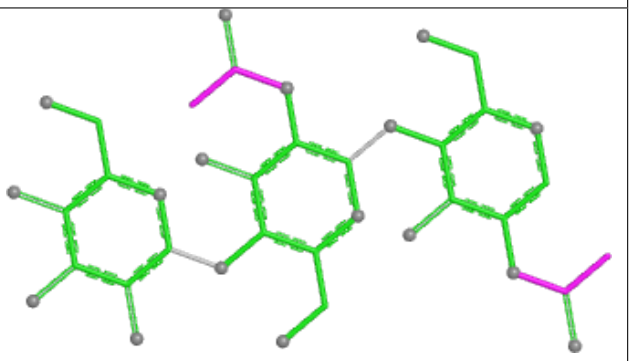
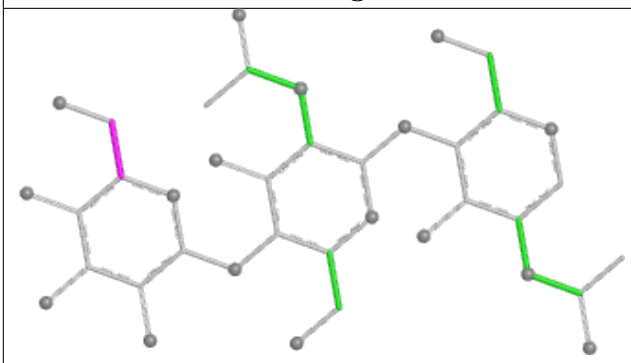
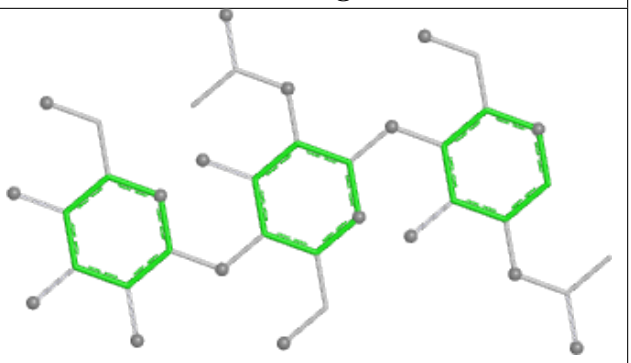
 Bond lengths	 Bond angles
 Torsions	 Rings

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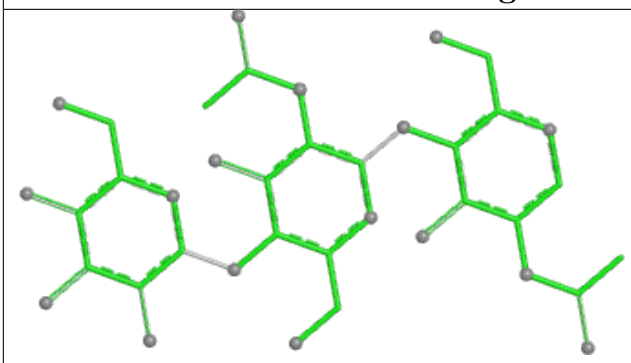
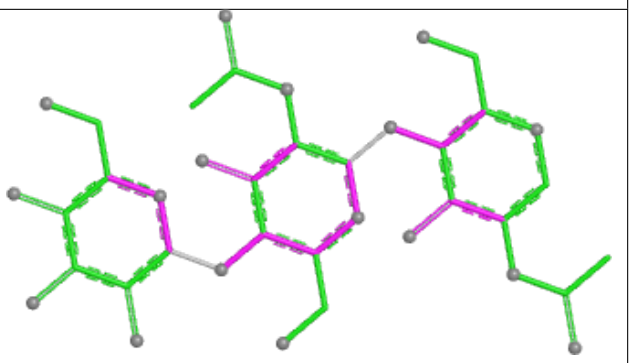
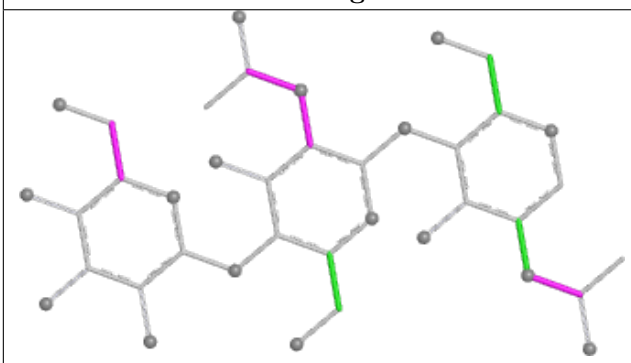
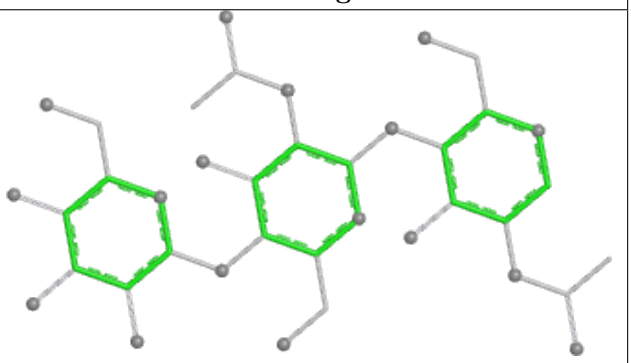
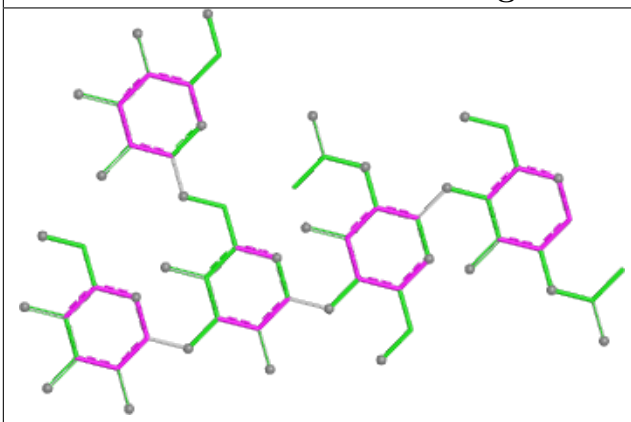
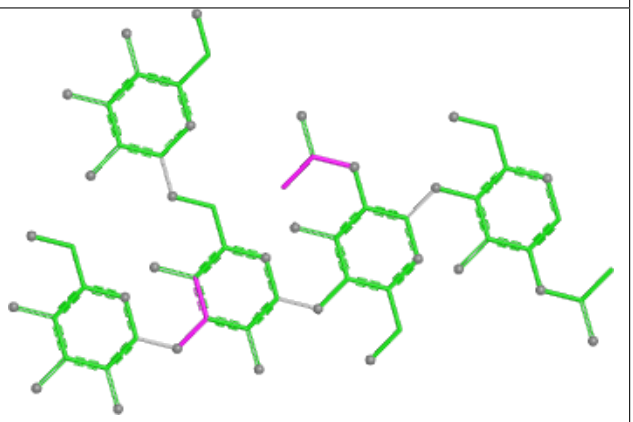
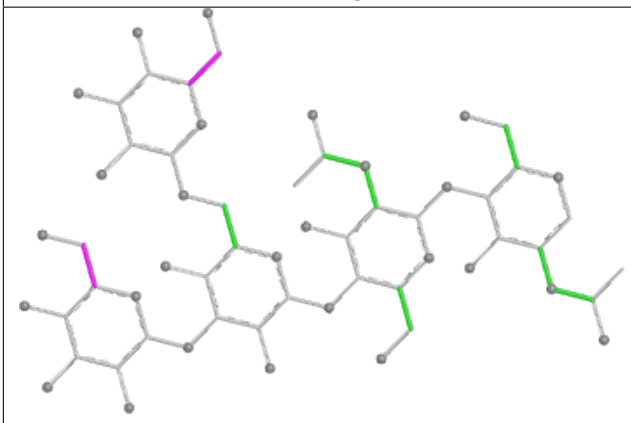
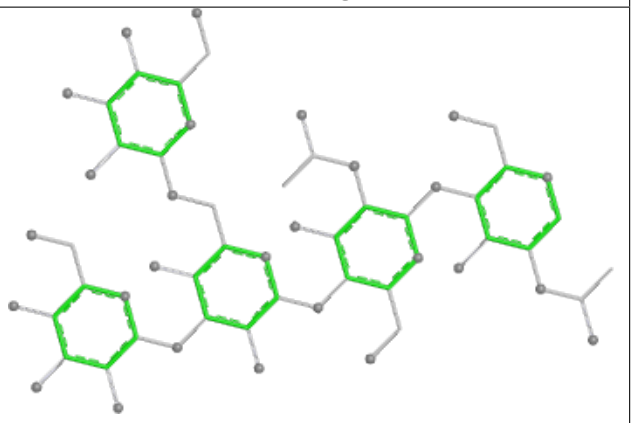
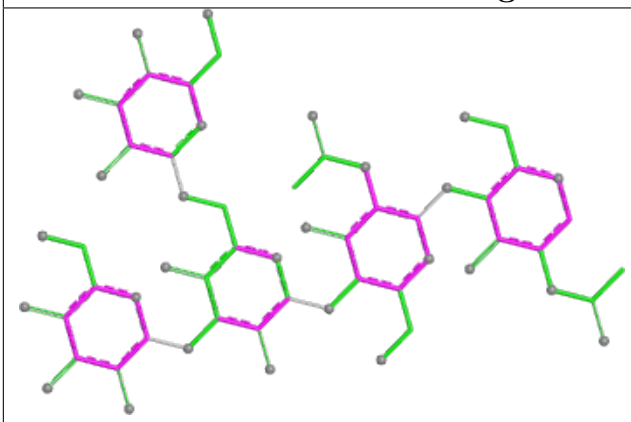
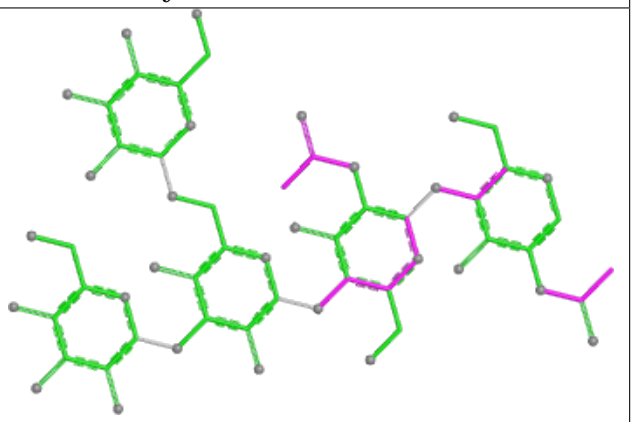
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain S	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

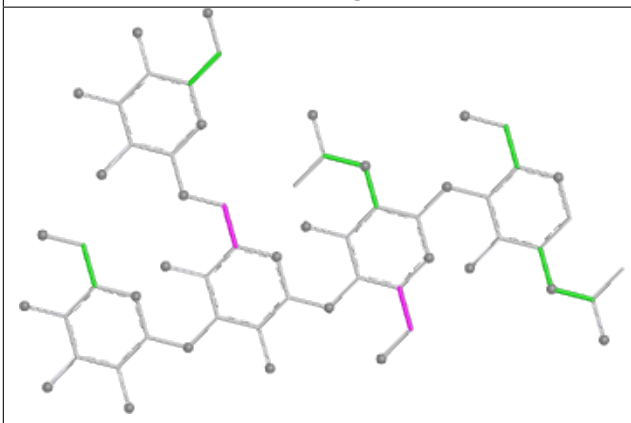
Oligosaccharide Chain y



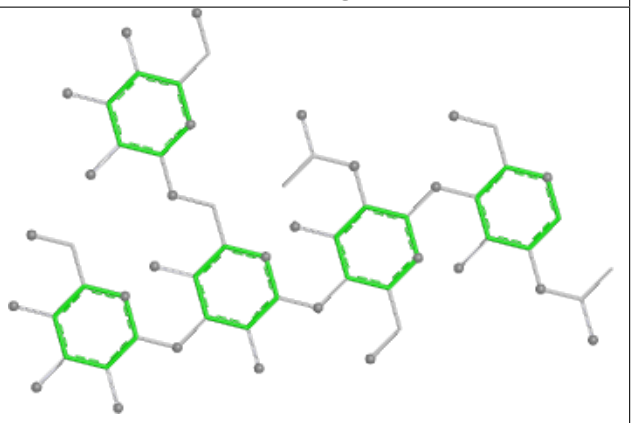
Bond lengths



Bond angles

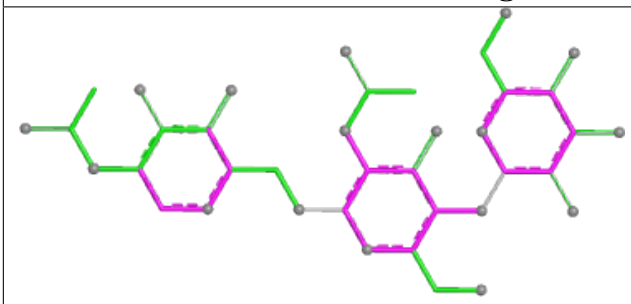


Torsions

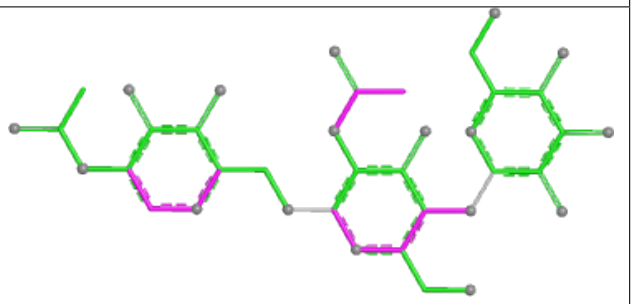


Rings

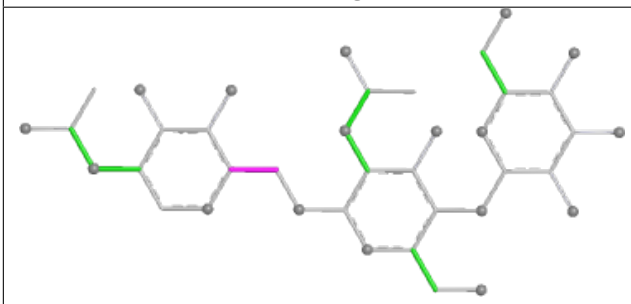
Oligosaccharide Chain d



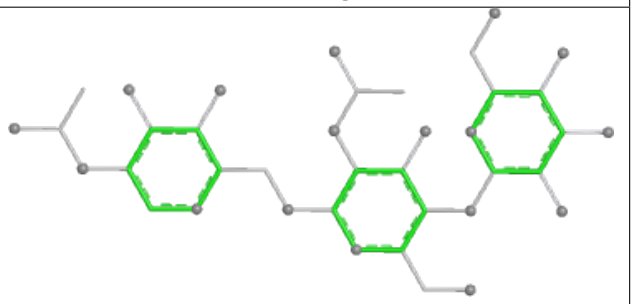
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	NAG	B	702	2	14,14,15	2.34	6 (42%)	17,19,21	1.48	5 (29%)
11	NAG	F	701	2	14,14,15	2.21	6 (42%)	17,19,21	0.91	0
11	NAG	A	605	1	14,14,15	2.39	6 (42%)	17,19,21	1.80	4 (23%)
11	NAG	D	605	1	14,14,15	2.10	5 (35%)	17,19,21	0.93	0
11	NAG	D	606	1	14,14,15	0.34	0	17,19,21	0.65	0
11	NAG	B	701	2	14,14,15	2.14	6 (42%)	17,19,21	0.94	0
11	NAG	D	603	1	14,14,15	2.01	6 (42%)	17,19,21	1.02	1 (5%)
11	NAG	F	702	2	14,14,15	2.24	7 (50%)	17,19,21	1.10	2 (11%)
11	NAG	D	604	1	14,14,15	2.19	7 (50%)	17,19,21	1.18	2 (11%)
11	NAG	C	603	1	14,14,15	1.96	6 (42%)	17,19,21	1.58	2 (11%)
11	NAG	A	604	1	14,14,15	2.21	7 (50%)	17,19,21	0.92	0
11	NAG	C	601	1	14,14,15	2.09	5 (35%)	17,19,21	0.90	0
11	NAG	A	601	1	14,14,15	2.20	6 (42%)	17,19,21	1.34	4 (23%)
11	NAG	B	703	2	14,14,15	2.25	5 (35%)	17,19,21	1.08	1 (5%)
11	NAG	D	602	1	14,14,15	2.05	5 (35%)	17,19,21	0.96	0
11	NAG	A	602	1	14,14,15	2.10	5 (35%)	17,19,21	0.92	0
11	NAG	E	701	2	14,14,15	2.23	5 (35%)	17,19,21	0.87	1 (5%)
11	NAG	E	702	2	14,14,15	2.11	7 (50%)	17,19,21	1.05	1 (5%)
11	NAG	A	603	1	14,14,15	2.00	5 (35%)	17,19,21	1.02	2 (11%)
11	NAG	D	601	1	14,14,15	2.02	5 (35%)	17,19,21	1.06	1 (5%)
11	NAG	C	602	1	14,14,15	2.27	7 (50%)	17,19,21	1.27	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	B	702	2	-	0/6/23/26	0/1/1/1
11	NAG	F	701	2	-	0/6/23/26	0/1/1/1
11	NAG	A	605	1	-	1/6/23/26	0/1/1/1
11	NAG	D	605	1	-	0/6/23/26	0/1/1/1
11	NAG	D	606	1	-	2/6/23/26	0/1/1/1
11	NAG	B	701	2	-	0/6/23/26	0/1/1/1
11	NAG	D	603	1	-	0/6/23/26	0/1/1/1
11	NAG	F	702	2	-	0/6/23/26	0/1/1/1
11	NAG	D	604	1	-	2/6/23/26	0/1/1/1
11	NAG	C	603	1	-	1/6/23/26	0/1/1/1
11	NAG	A	604	1	-	1/6/23/26	0/1/1/1
11	NAG	C	601	1	-	1/6/23/26	0/1/1/1
11	NAG	A	601	1	-	2/6/23/26	0/1/1/1
11	NAG	B	703	2	-	0/6/23/26	0/1/1/1
11	NAG	D	602	1	-	0/6/23/26	0/1/1/1
11	NAG	A	602	1	-	1/6/23/26	0/1/1/1
11	NAG	E	701	2	-	0/6/23/26	0/1/1/1
11	NAG	E	702	2	-	0/6/23/26	0/1/1/1
11	NAG	A	603	1	-	0/6/23/26	0/1/1/1
11	NAG	D	601	1	-	0/6/23/26	0/1/1/1
11	NAG	C	602	1	-	1/6/23/26	0/1/1/1

The worst 5 of 117 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	605	NAG	C1-C2	6.22	1.61	1.52
11	B	703	NAG	C1-C2	6.09	1.61	1.52
11	C	602	NAG	C1-C2	5.65	1.60	1.52
11	F	702	NAG	C1-C2	5.65	1.60	1.52
11	F	701	NAG	C1-C2	5.62	1.60	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	603	NAG	C2-N2-C7	4.59	129.44	122.90
11	A	605	NAG	C2-N2-C7	4.50	129.31	122.90
11	A	605	NAG	C1-C2-N2	3.87	117.09	110.49
11	B	702	NAG	O7-C7-C8	-3.05	116.39	122.06
11	B	702	NAG	C8-C7-N2	3.03	121.23	116.10

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

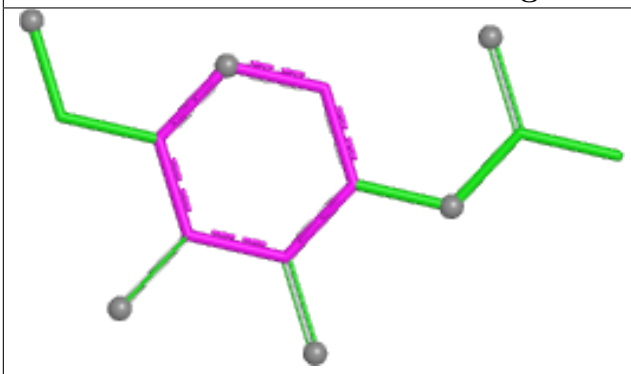
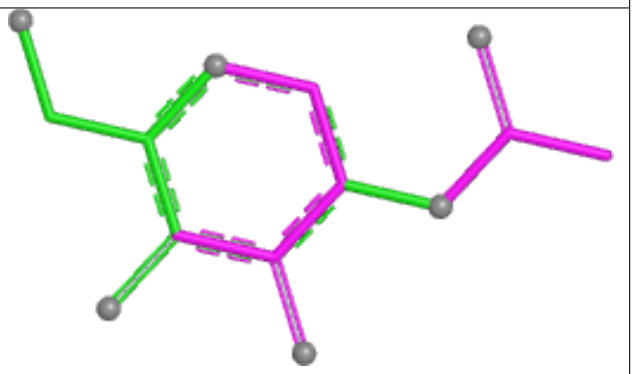
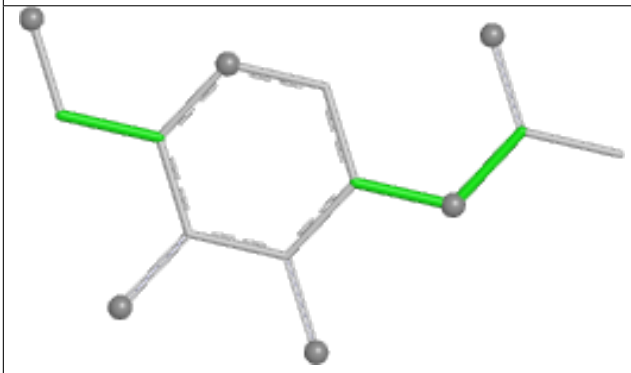
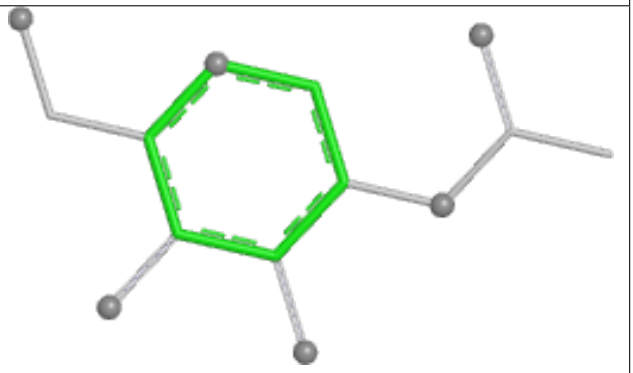
Mol	Chain	Res	Type	Atoms
11	A	605	NAG	C1-C2-N2-C7
11	C	603	NAG	C3-C2-N2-C7
11	D	606	NAG	C8-C7-N2-C2
11	D	606	NAG	O7-C7-N2-C2
11	C	601	NAG	O5-C5-C6-O6

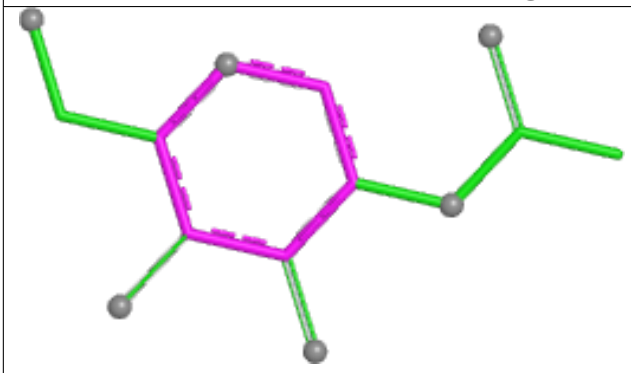
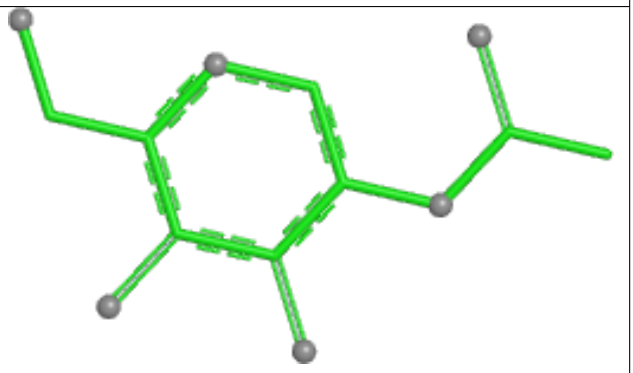
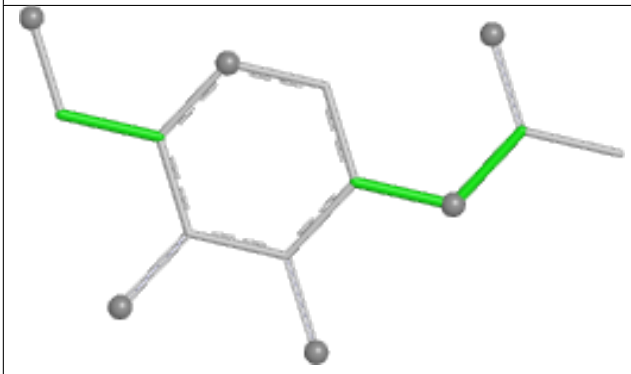
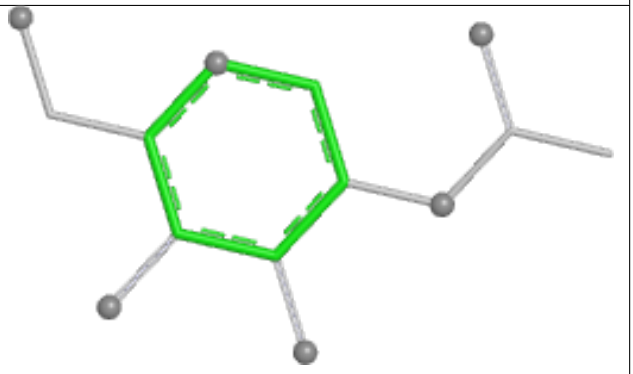
There are no ring outliers.

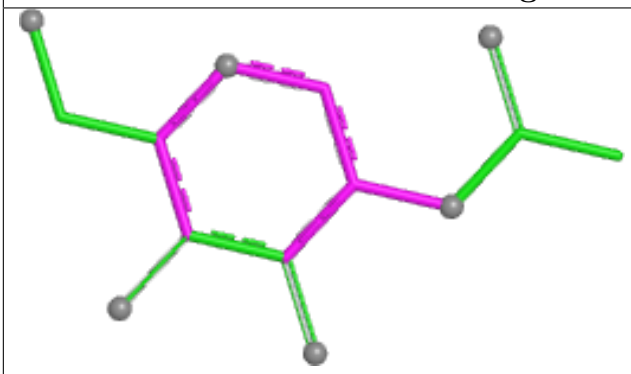
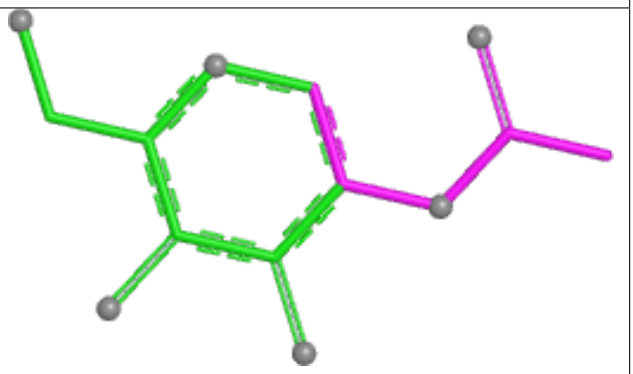
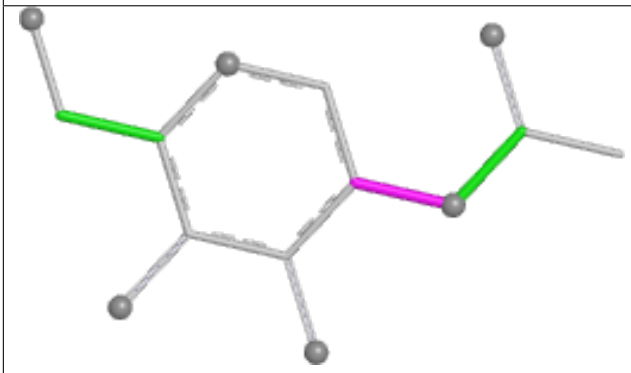
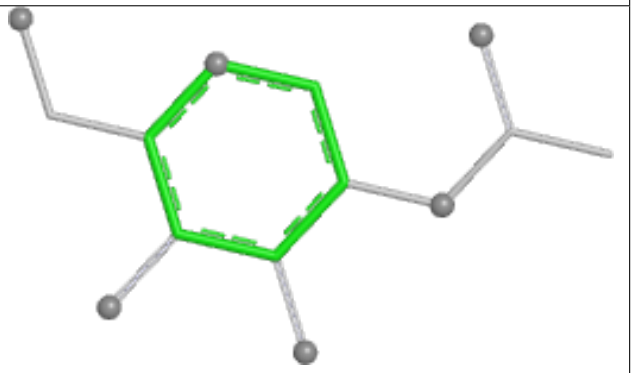
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	702	NAG	1	0
11	B	701	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 B 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG F 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

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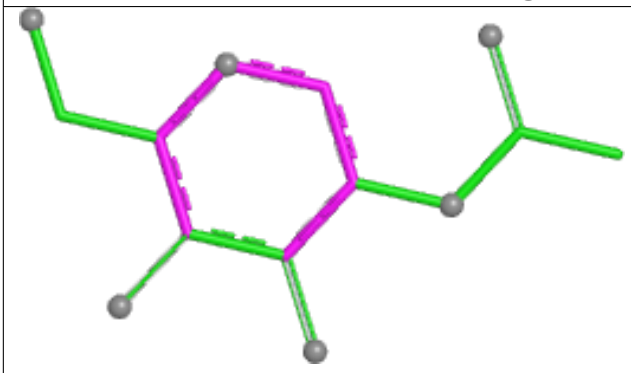
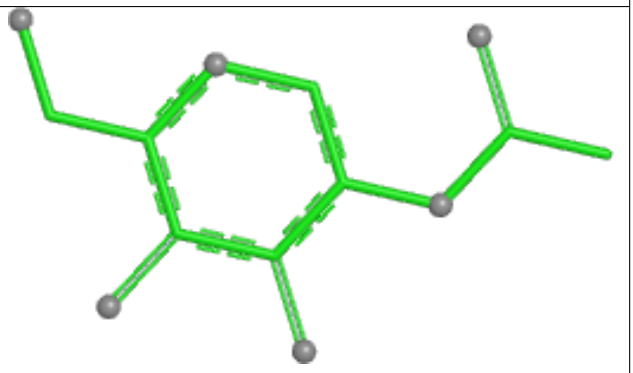
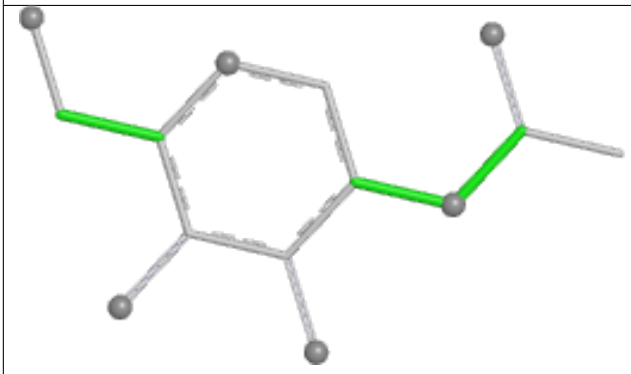
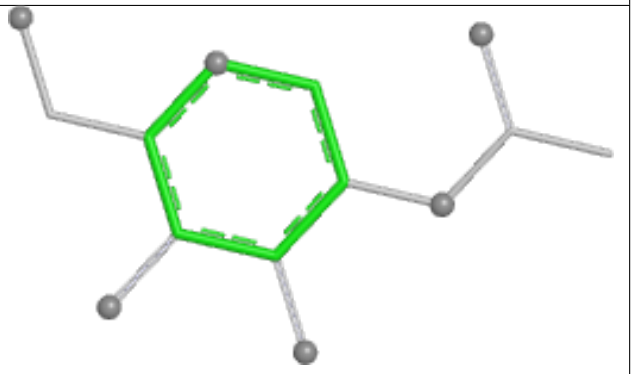
	
Bond lengths	Bond angles
	
Torsions	Rings

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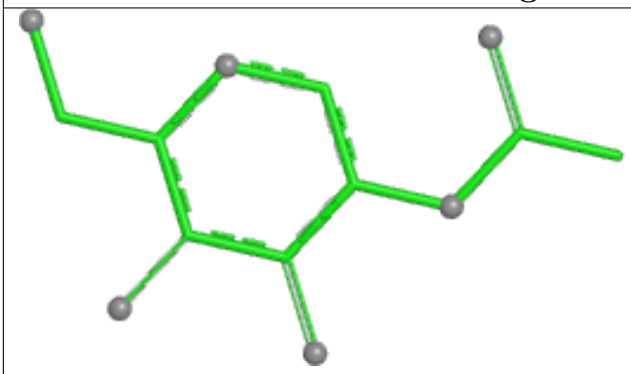
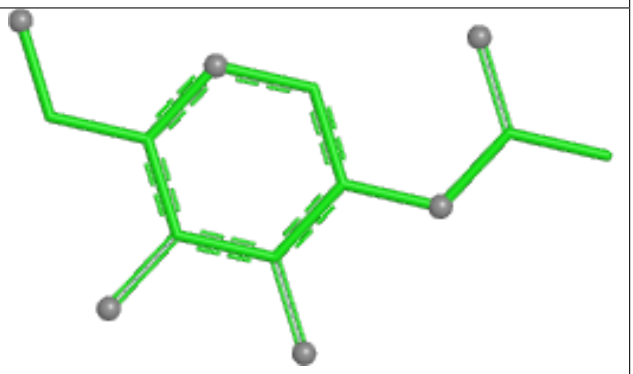
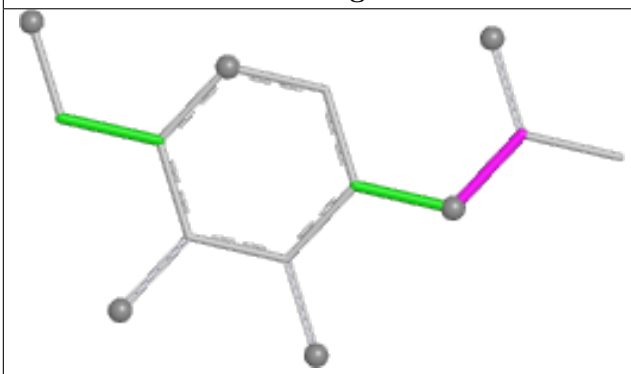


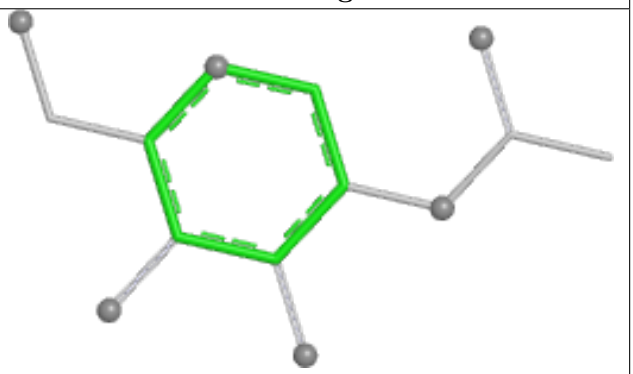
Bond lengths



Bond angles

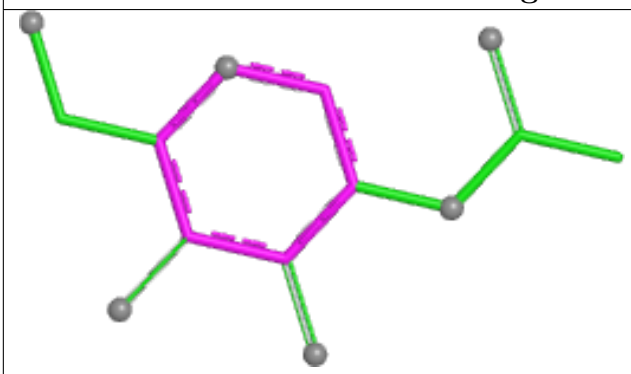


Torsions



Rings

Ligand NAG B 701



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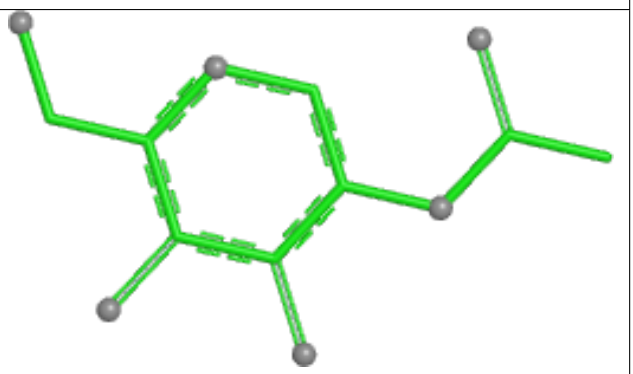

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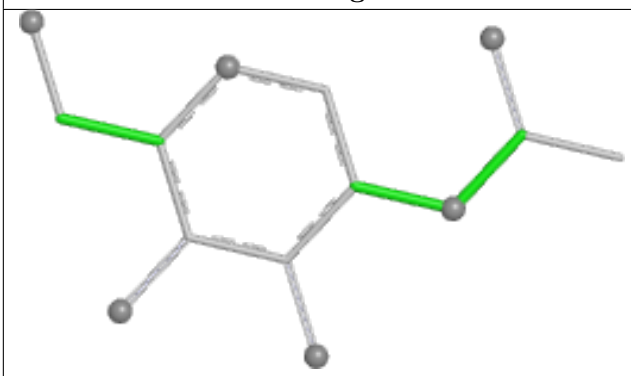

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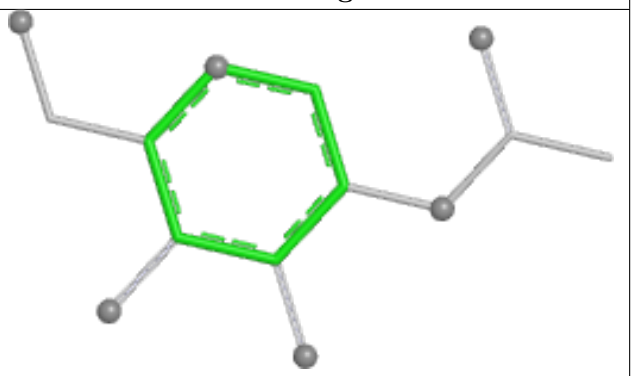
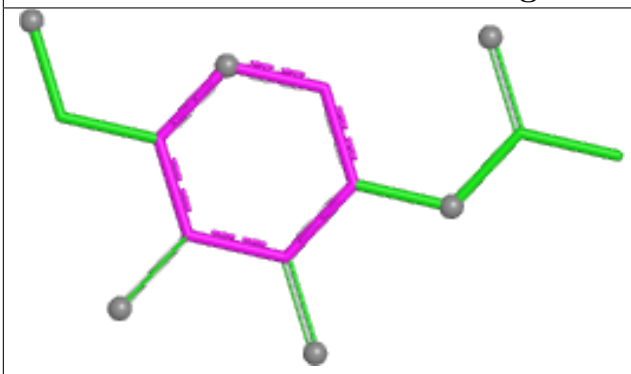


Rings

Ligand NAG D 603



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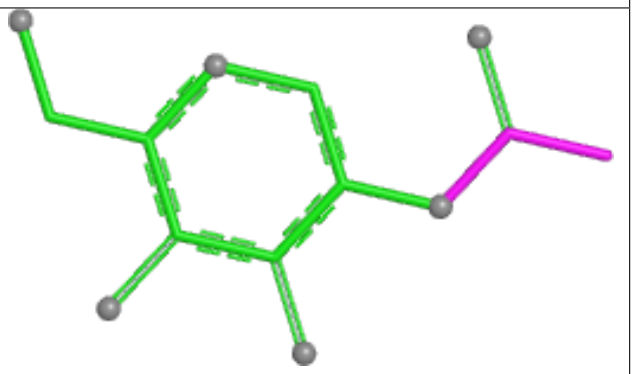

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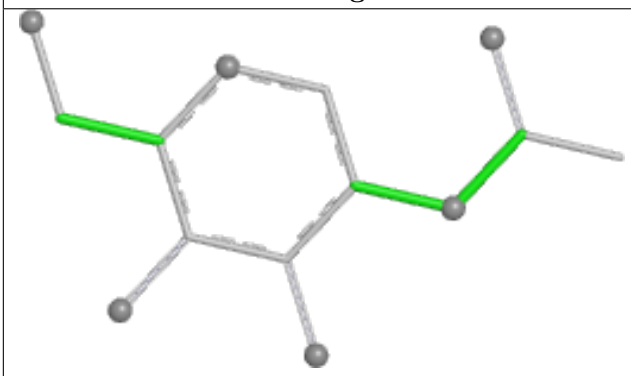

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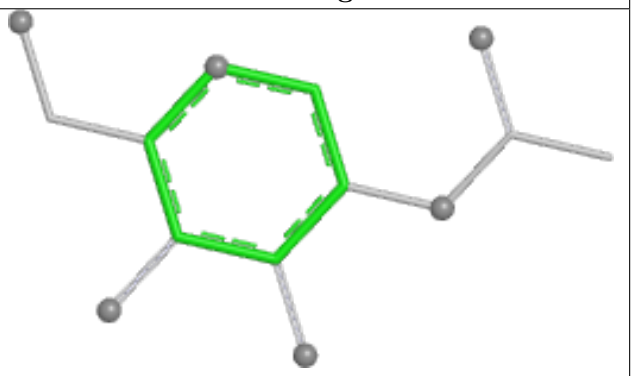

Rings

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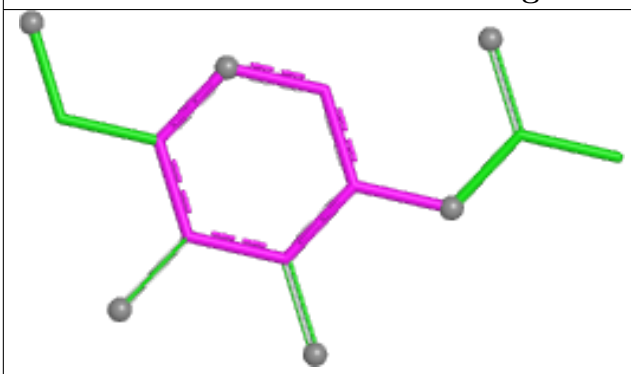

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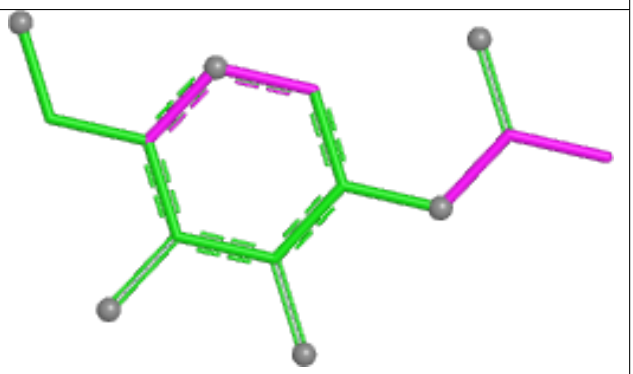

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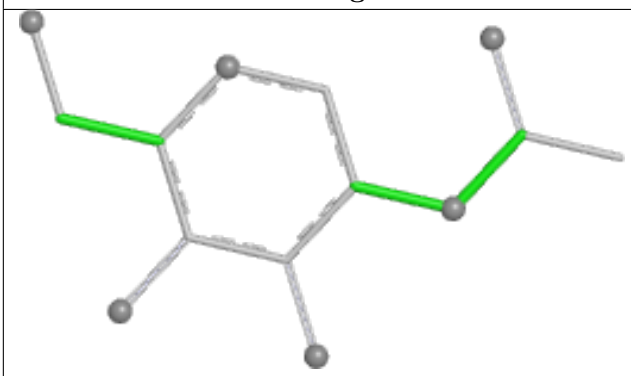

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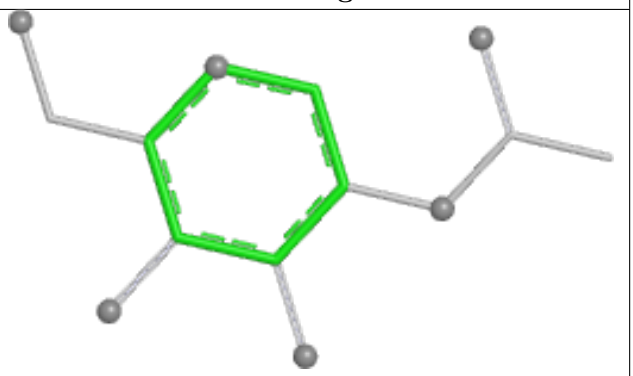
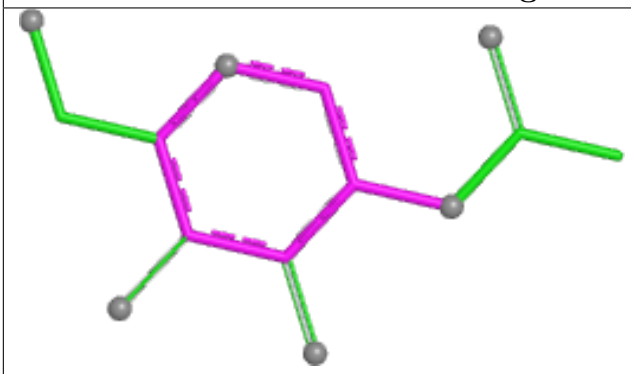


Rings

Ligand NAG D 604



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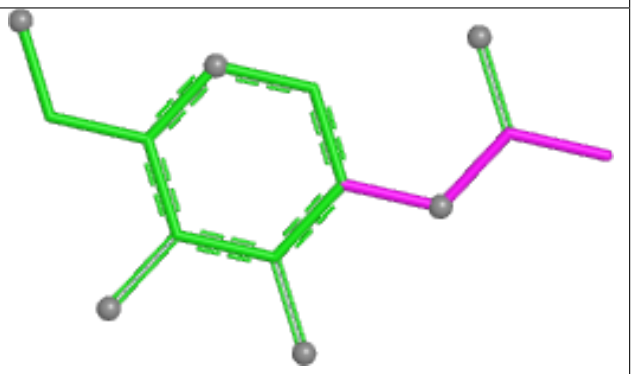
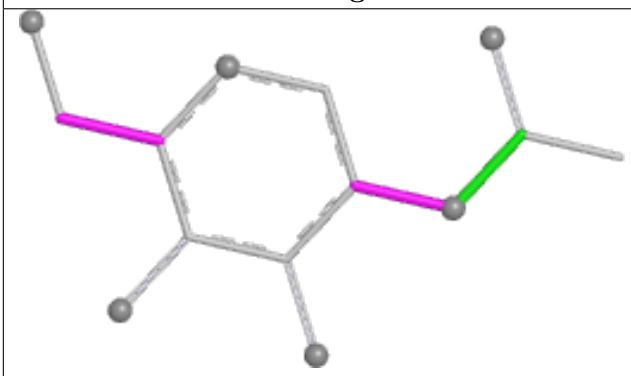
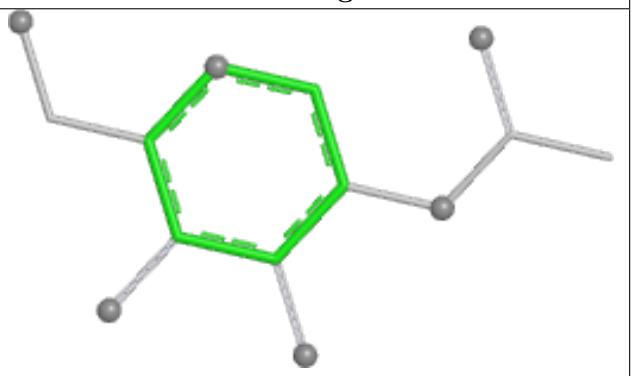


Bond angles

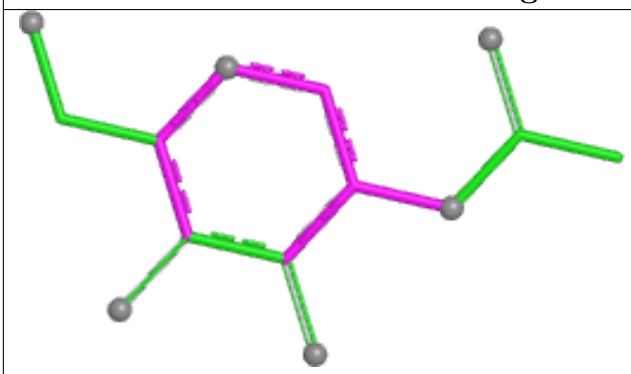


Torsions

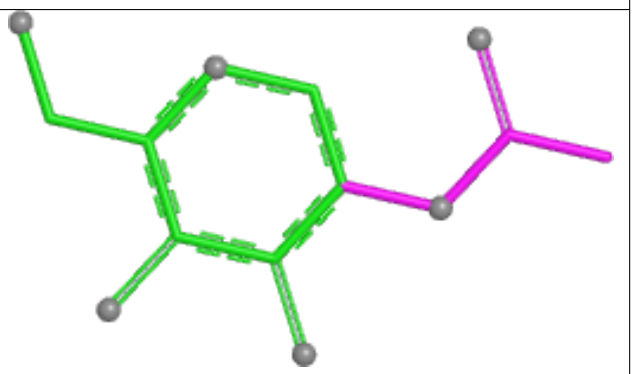


Rings

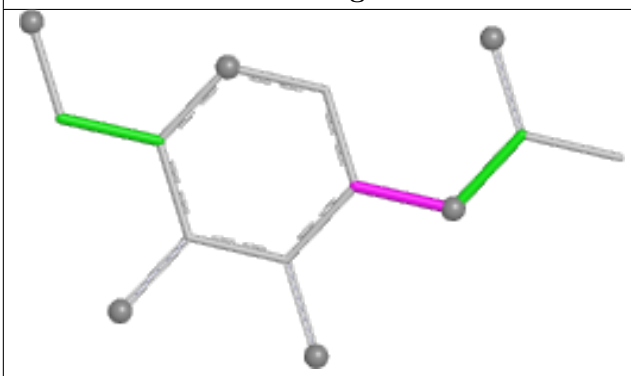
Ligand NAG C 603



Bond lengths



Bond angles



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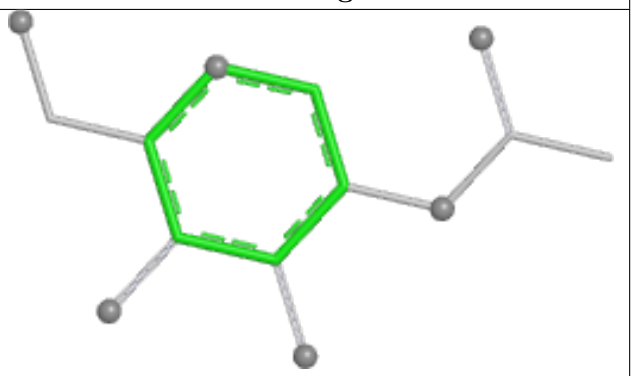
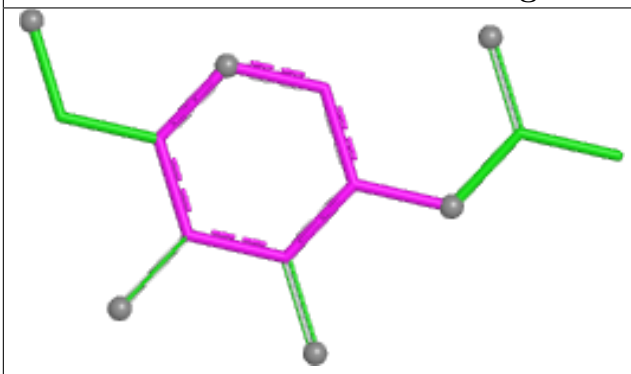
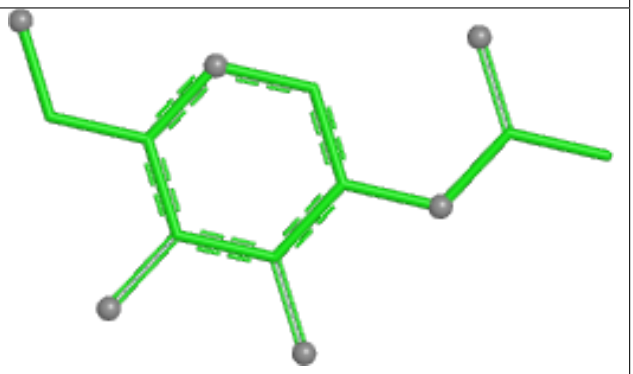


Rings

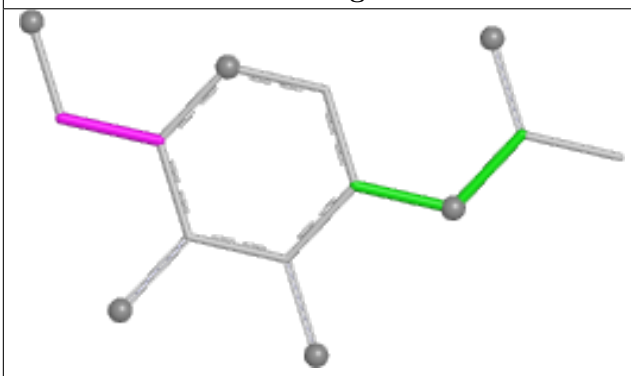
Ligand NAG A 604



Bond lengths



Bond angles



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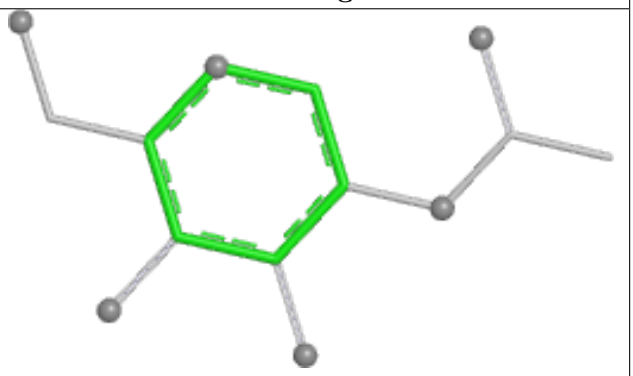
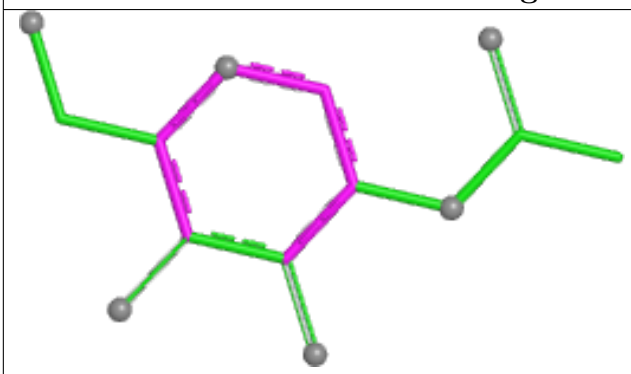
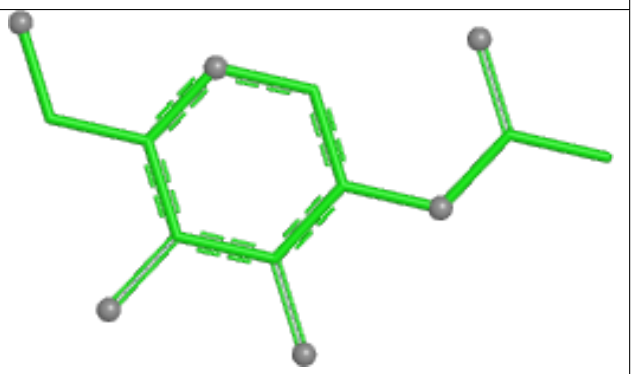


Rings

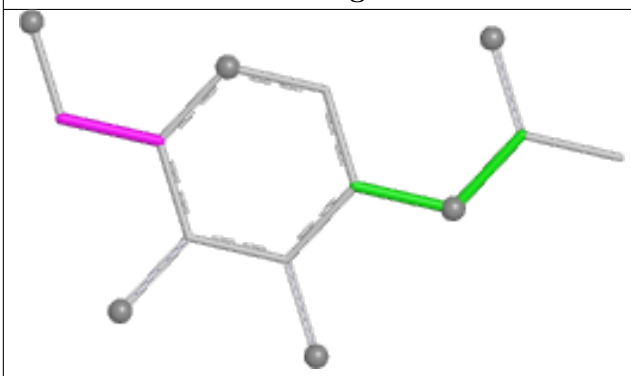
Ligand NAG C 601



Bond lengths



Bond angles



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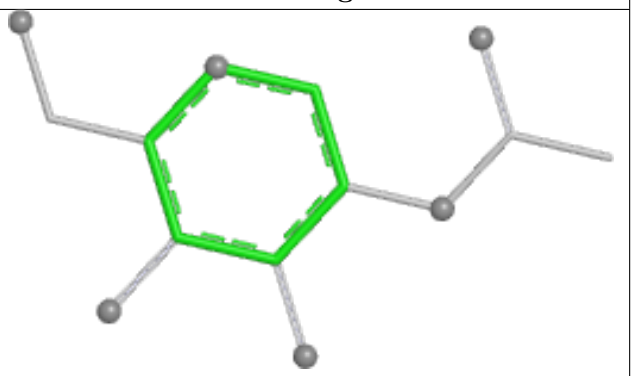
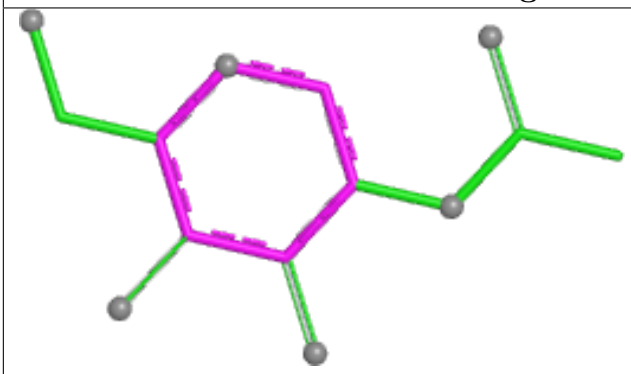
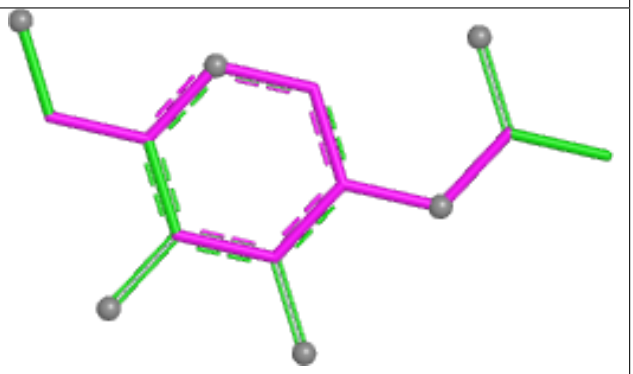
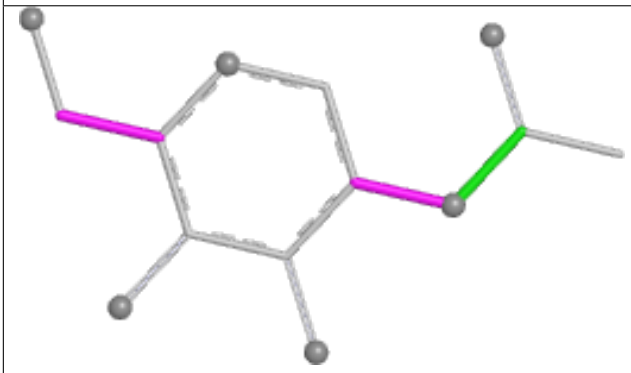
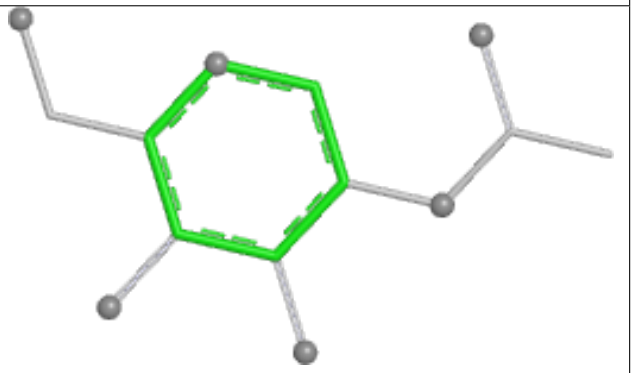
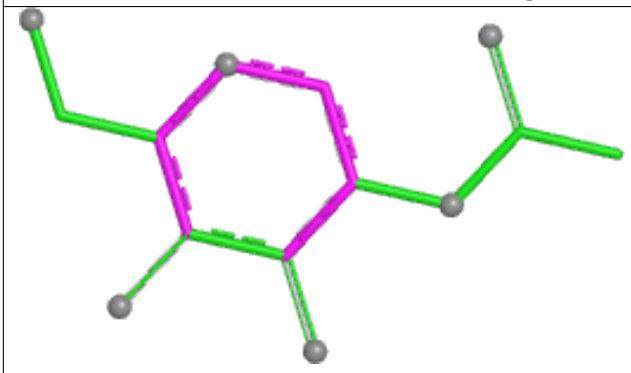
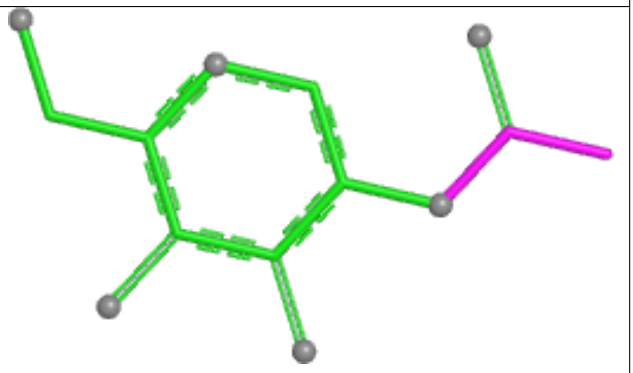
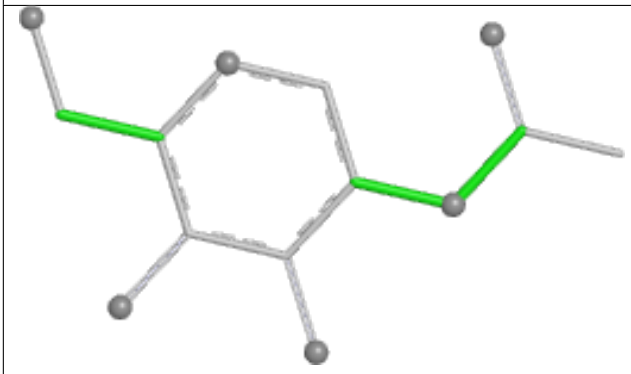
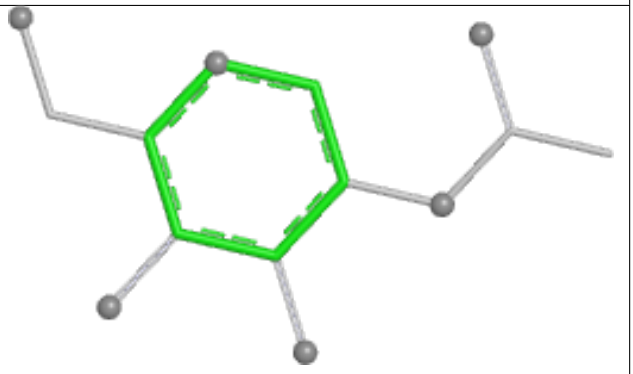
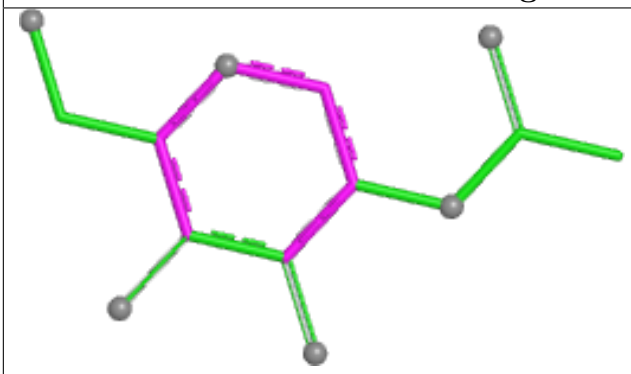


Rings

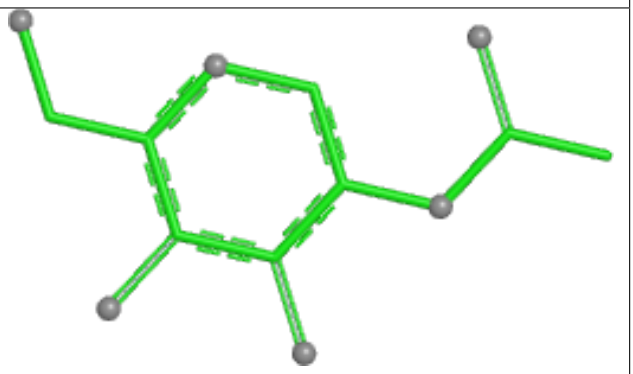
Ligand NAG A 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

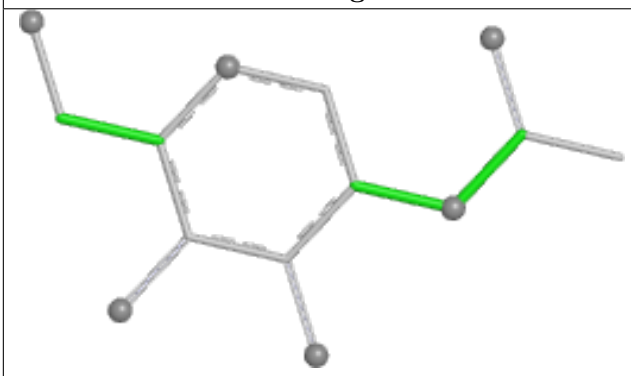
Ligand NAG D 602



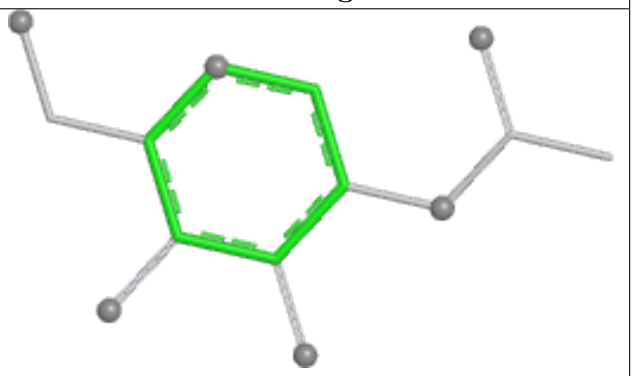
Bond lengths



Bond angles

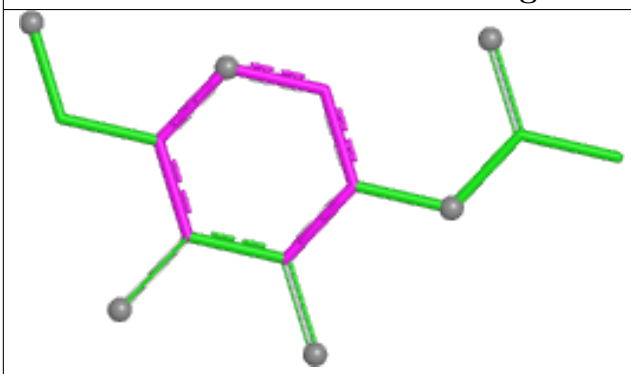


Torsions



Rings

Ligand NAG A 602



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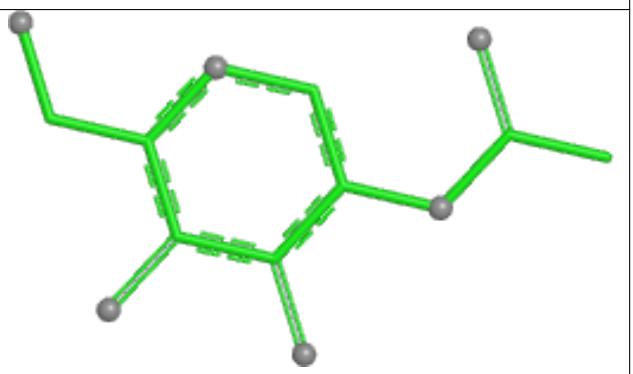
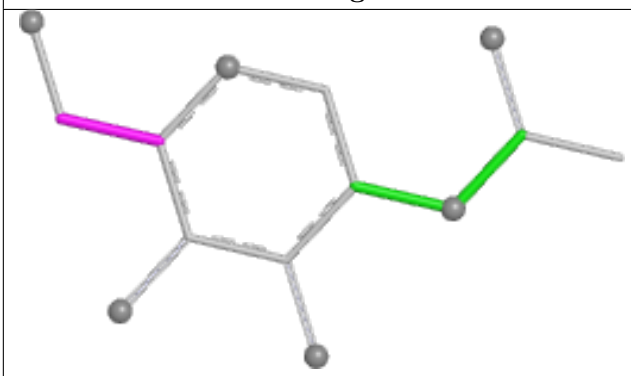
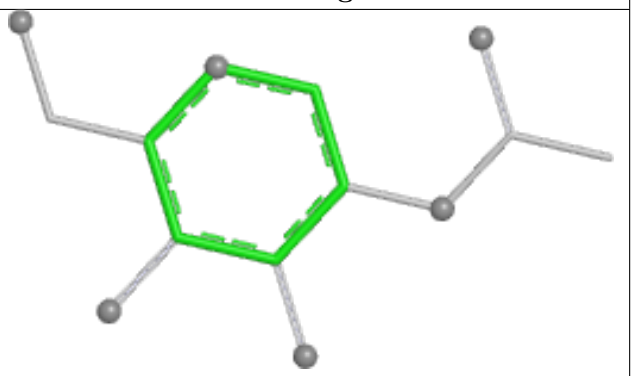


Bond angles

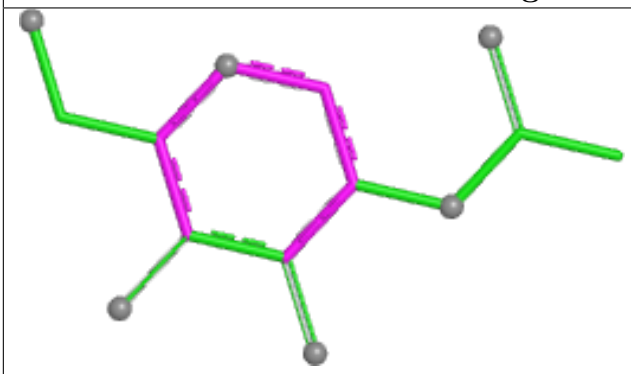


Torsions

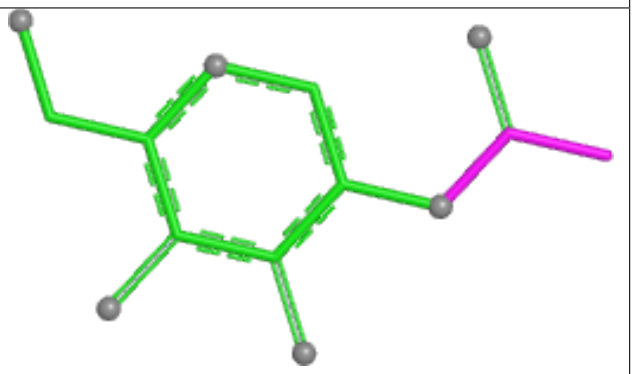


Rings

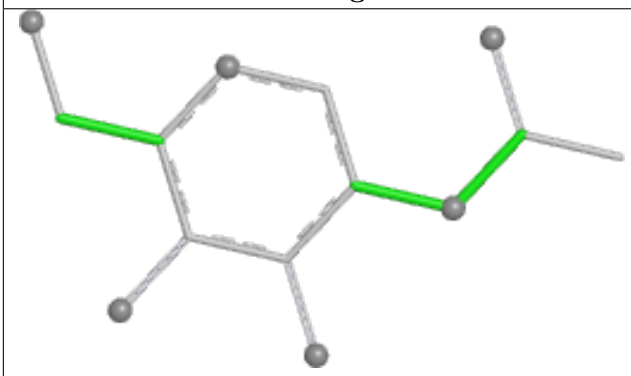
Ligand NAG E 701



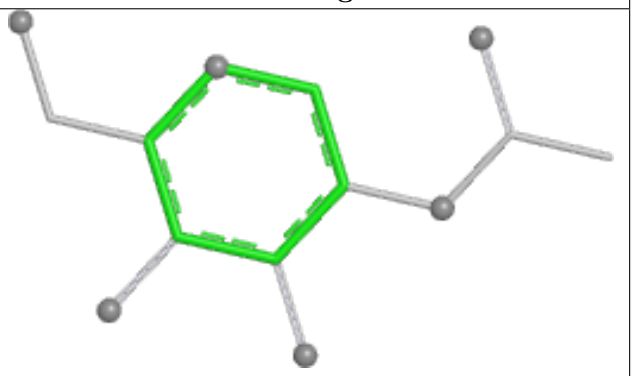
Bond lengths



Bond angles

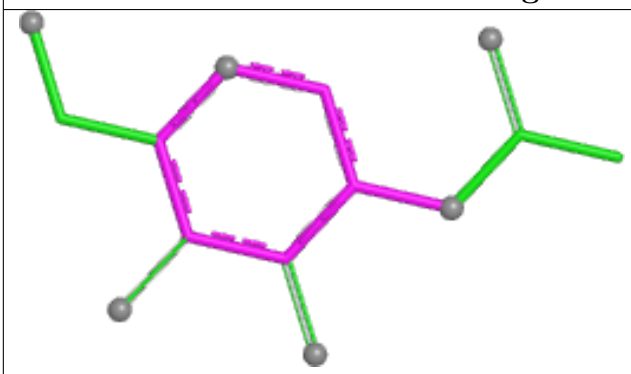


Torsions

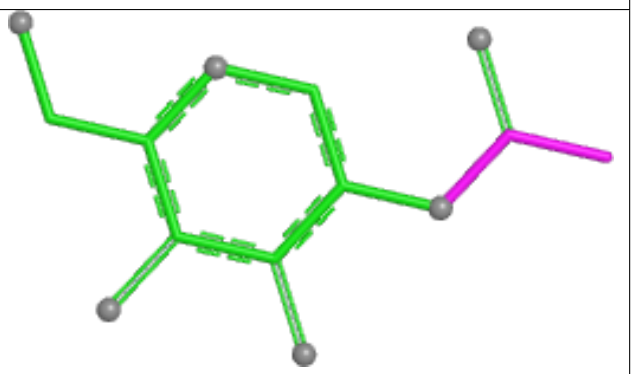


Rings

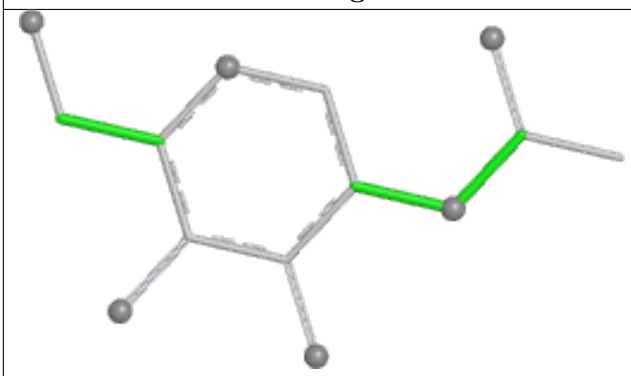
Ligand NAG E 702



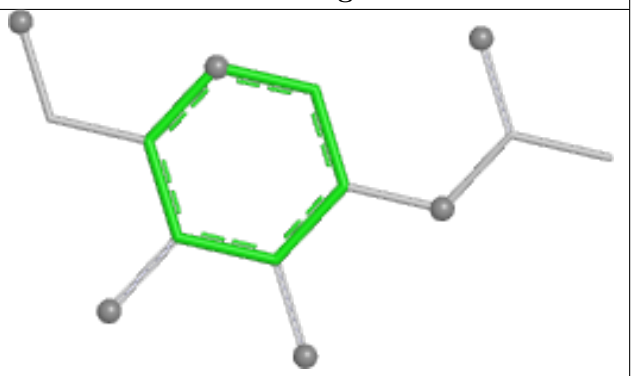
Bond lengths



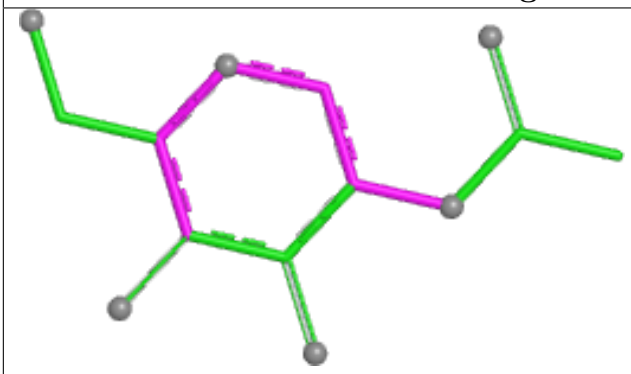
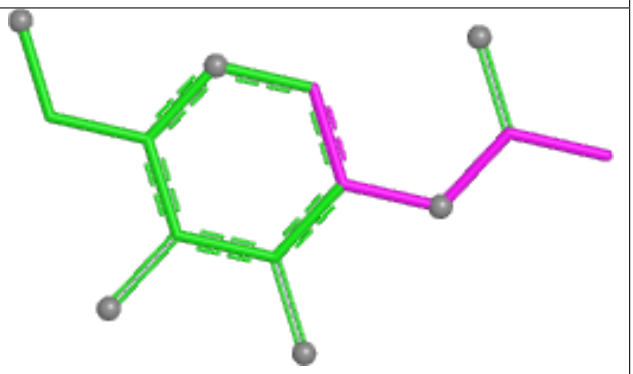
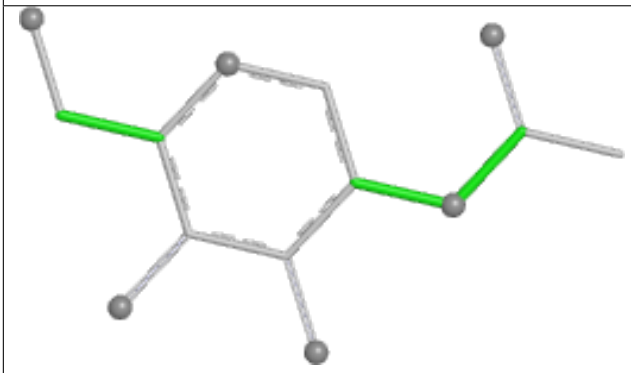
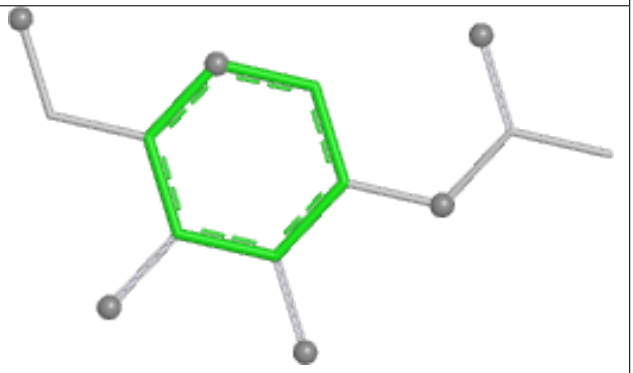
Bond angles

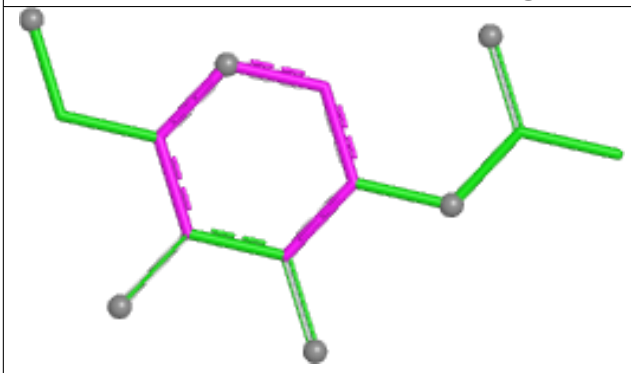
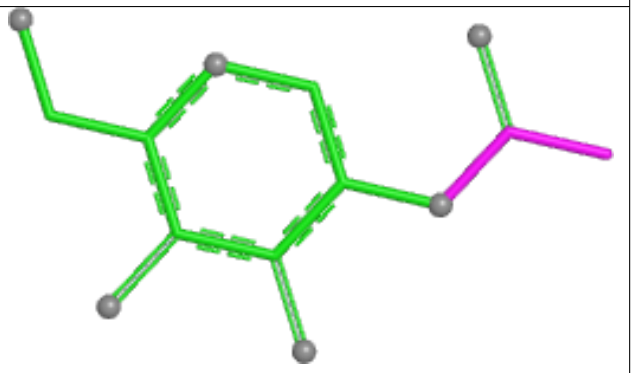
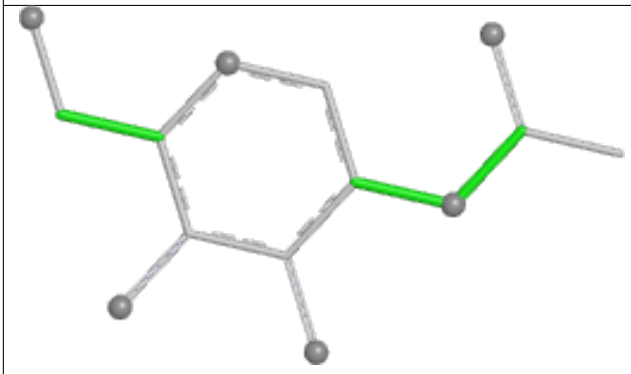
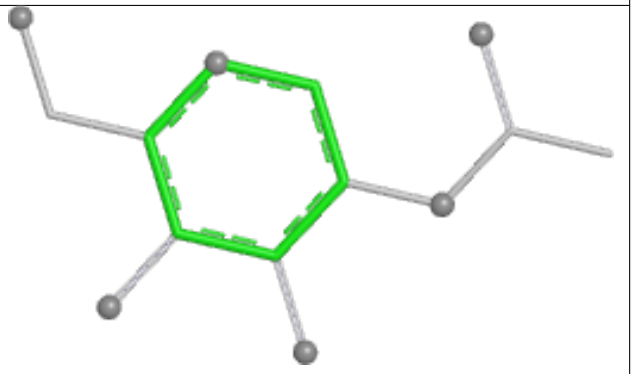


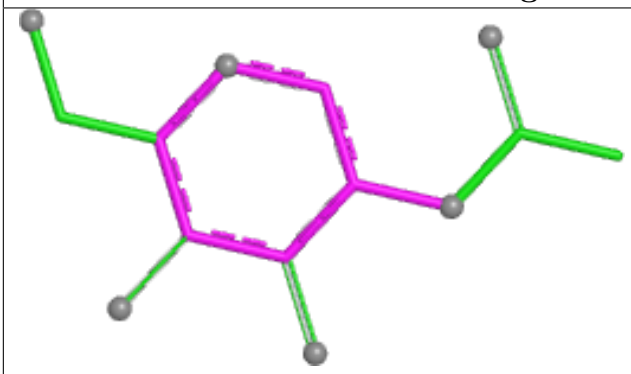
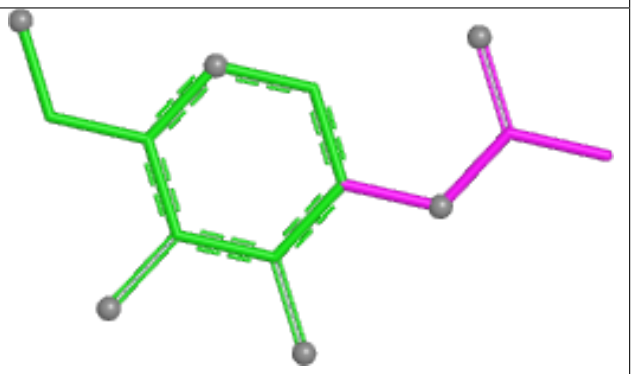
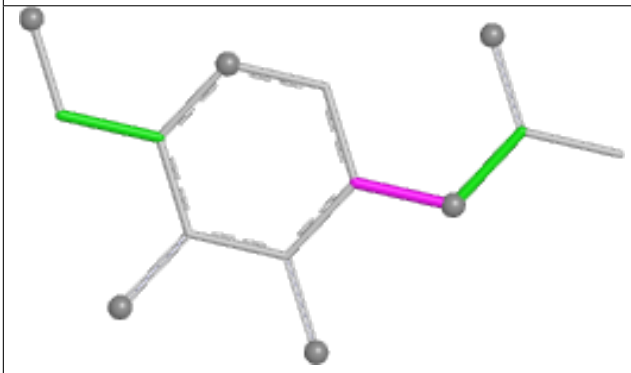
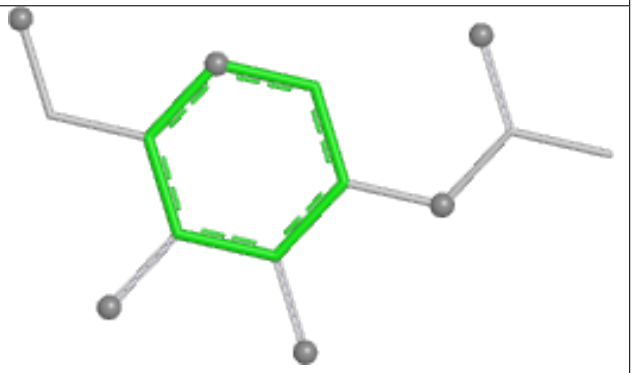
Torsions



Rings

Ligand NAG A 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG D 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

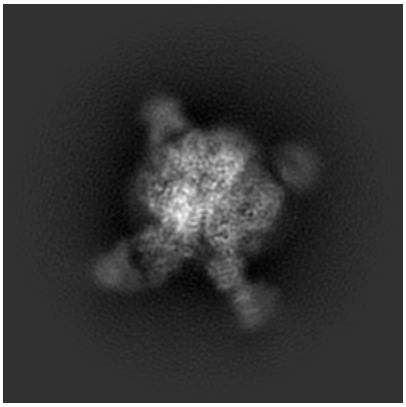
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14474. These allow visual inspection of the internal detail of the map and identification of artifacts.

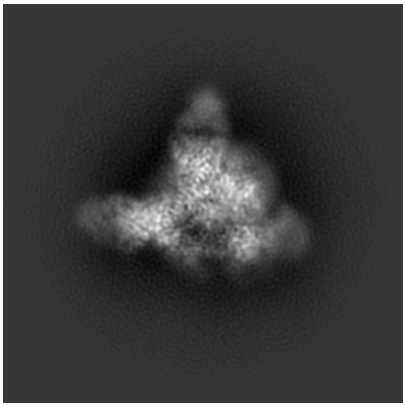
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

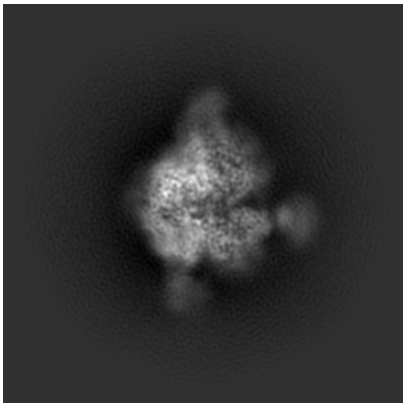
6.1.1 Primary map



X



Y

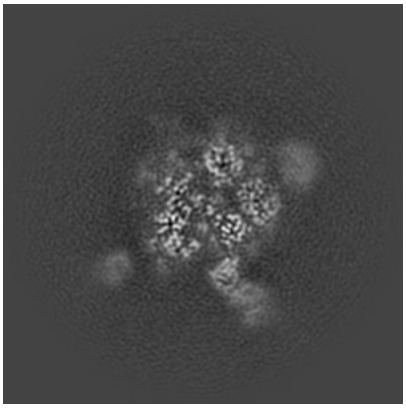


Z

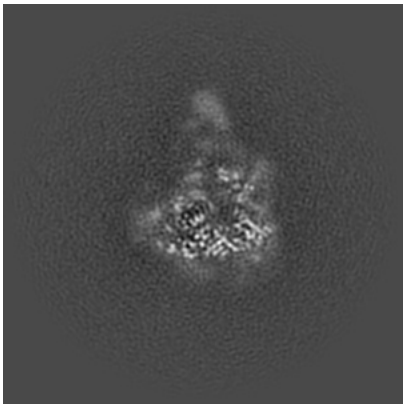
The images above show the map projected in three orthogonal directions.

6.2 Central slices

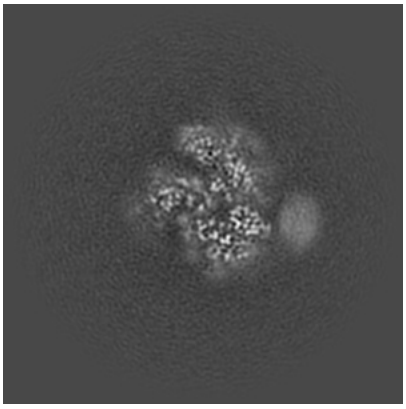
6.2.1 Primary map



X Index: 150



Y Index: 150

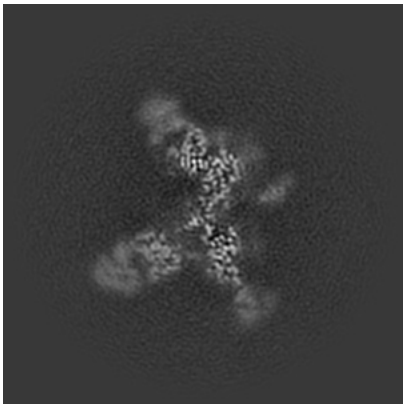


Z Index: 150

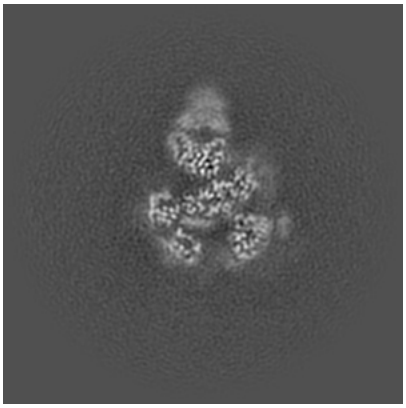
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

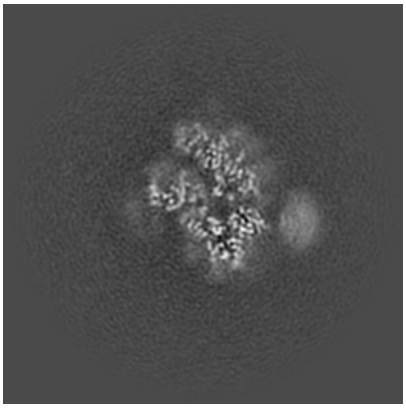
6.3.1 Primary map



X Index: 131



Y Index: 137



Z Index: 153

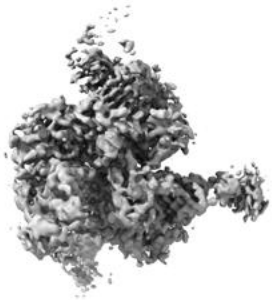
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

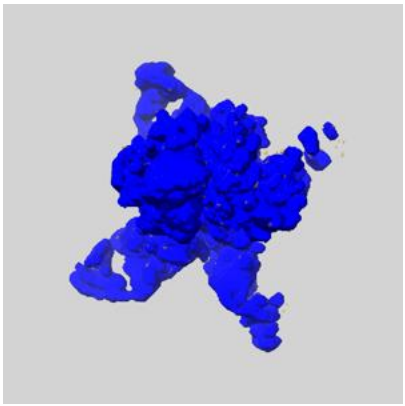
6.5 Mask visualisation

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

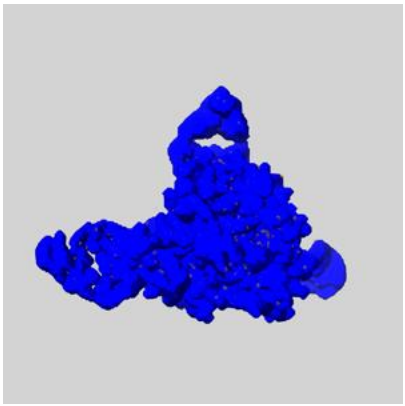
A mask typically either:

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

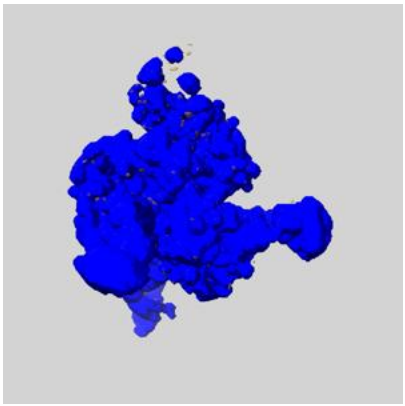
6.5.1 emd_14474_msk_1.map



X



Y

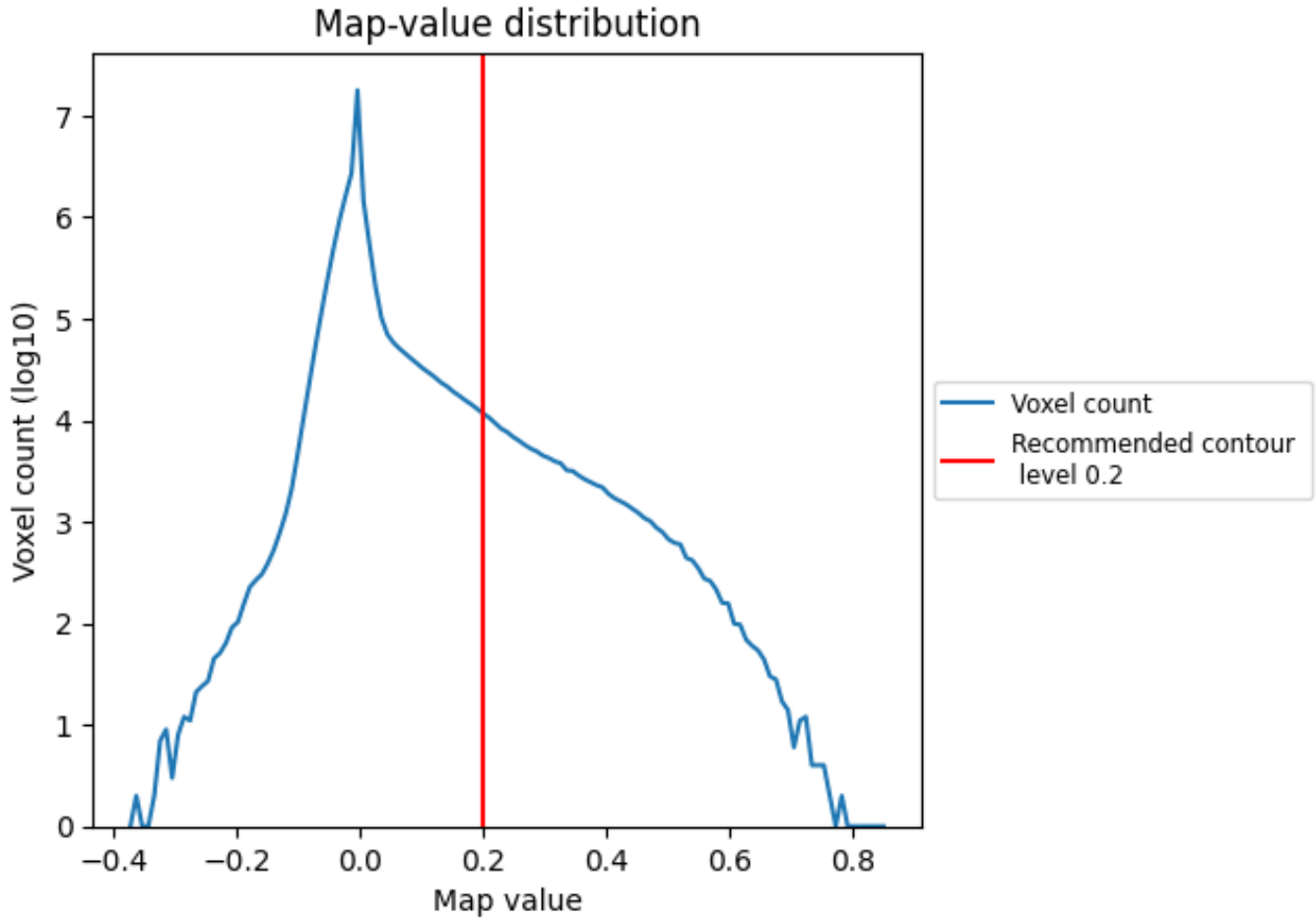


Z

7 Map analysis

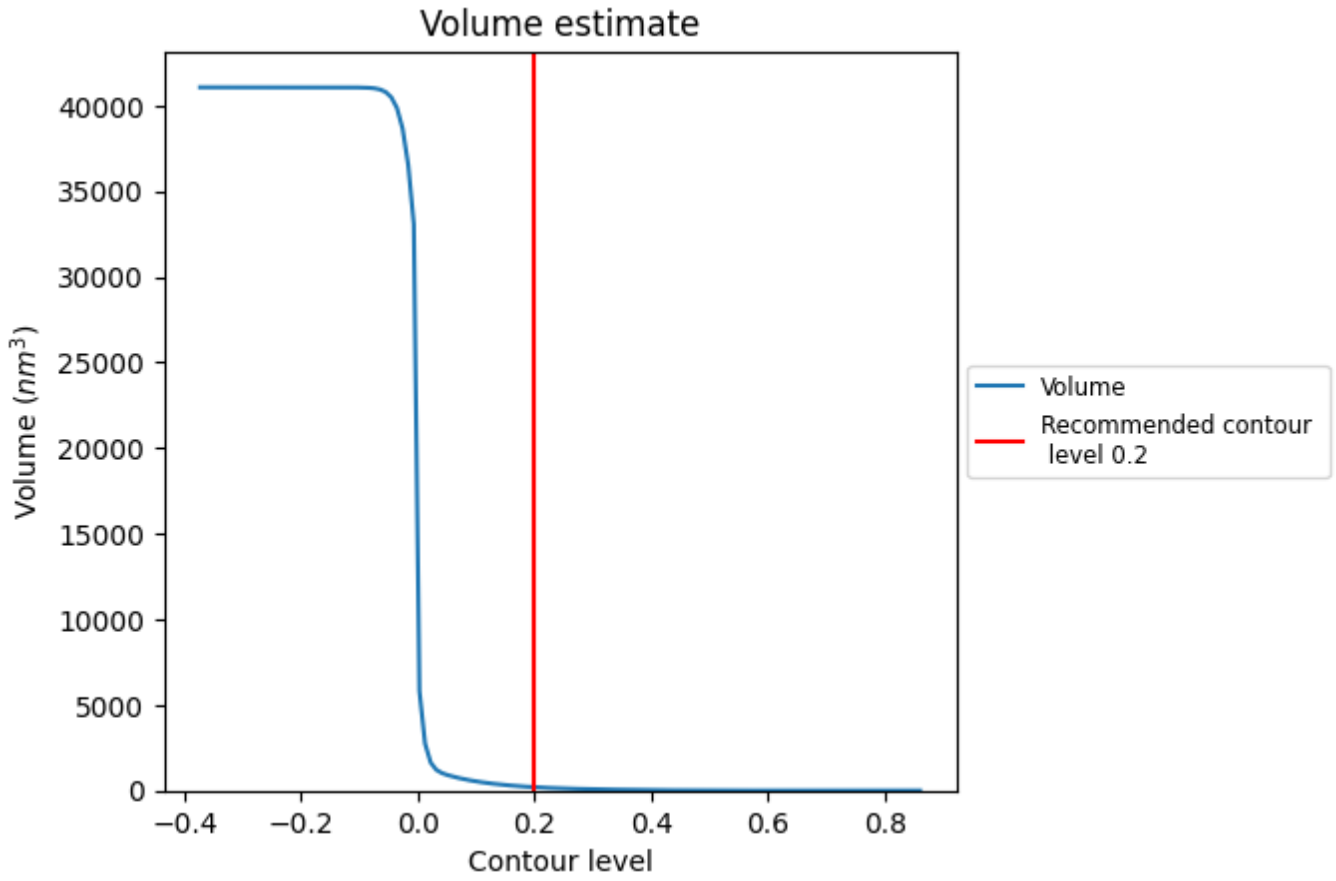
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

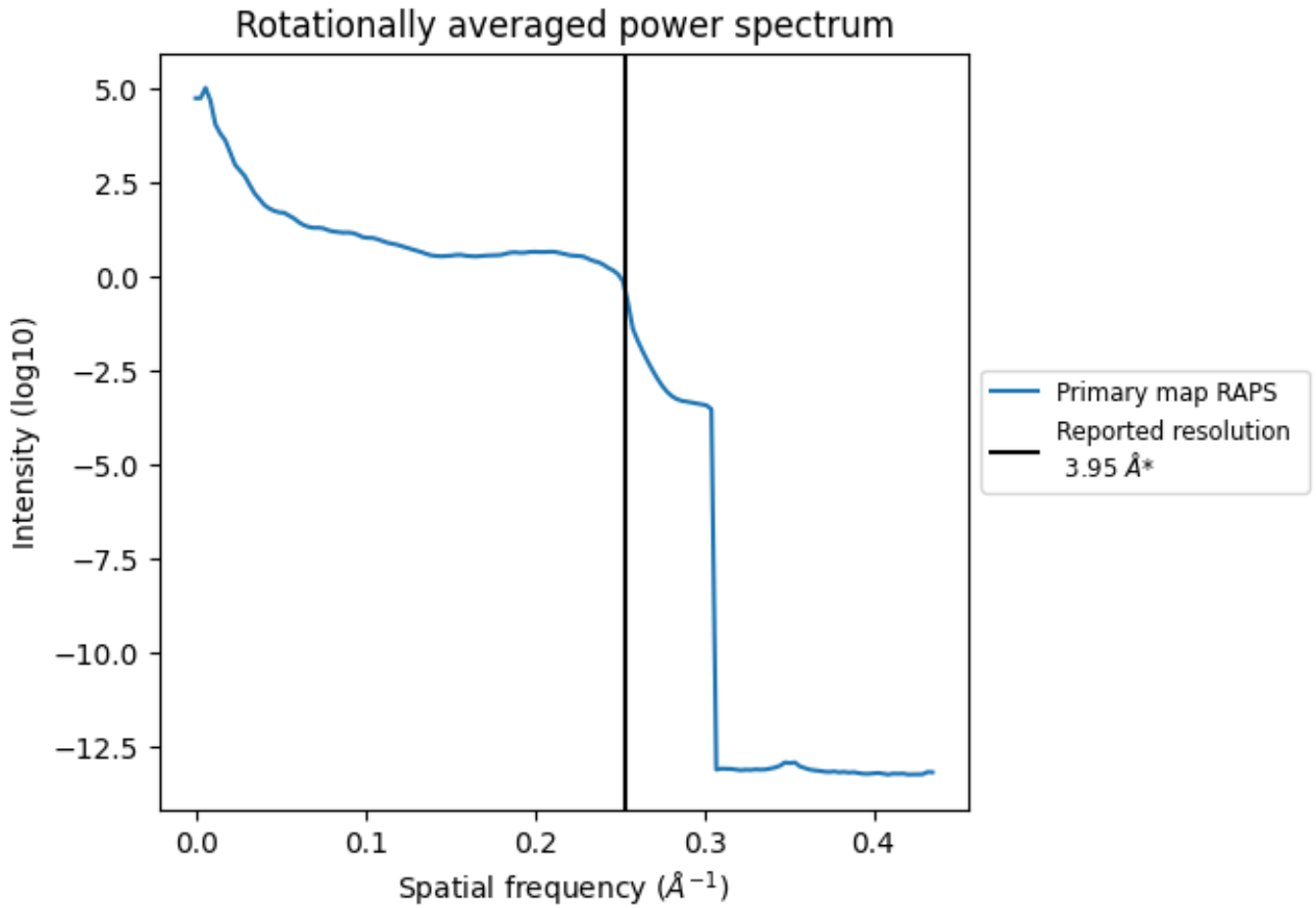
7.2 Volume estimate (i)



The volume at the recommended contour level is 197 nm^3; this corresponds to an approximate mass of 178 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)

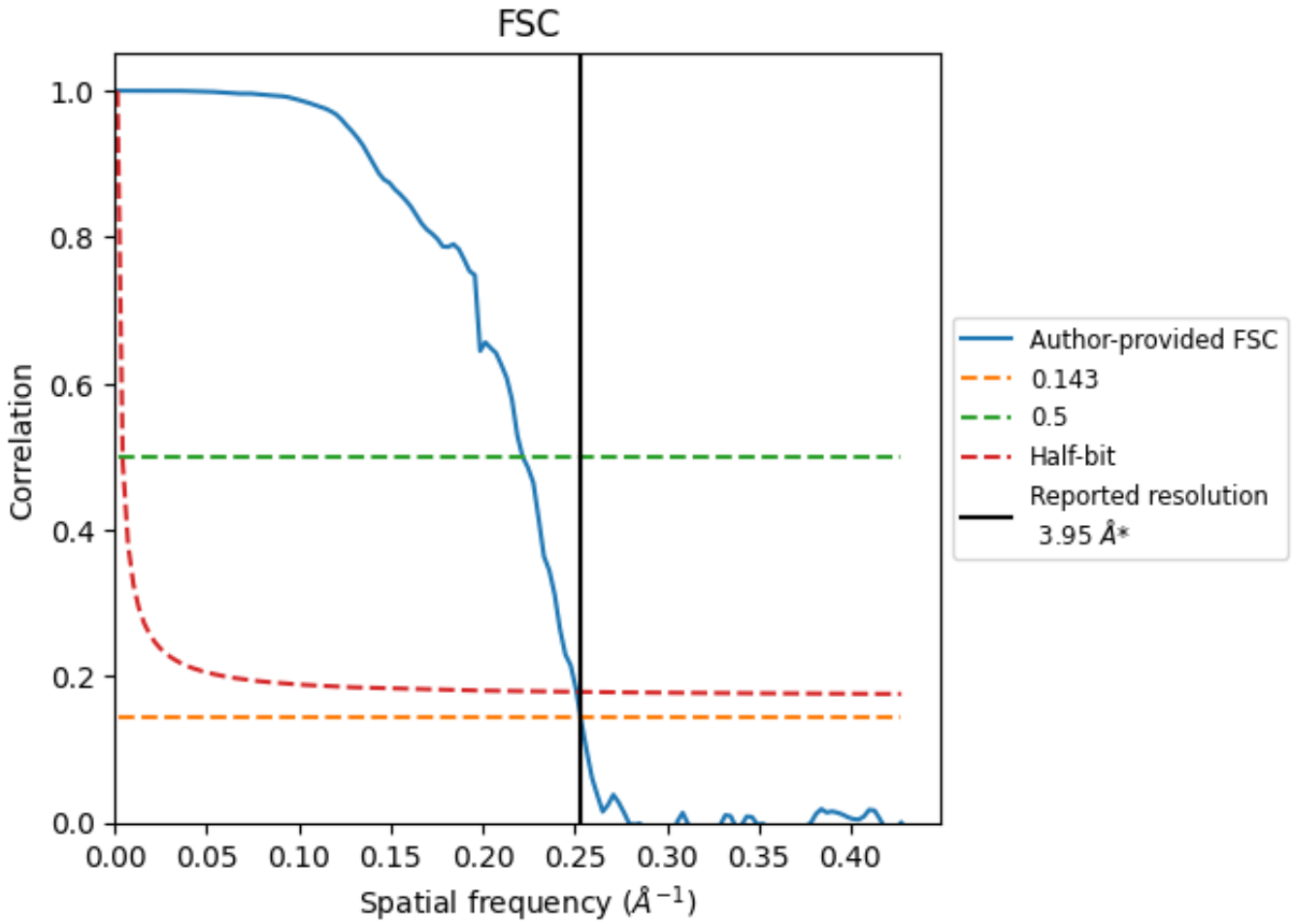


*Reported resolution corresponds to spatial frequency of 0.253 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.253 Å^{-1}

8.2 Resolution estimates (i)

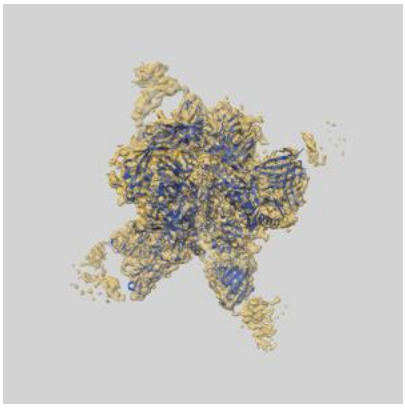
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.95	-	-
Author-provided FSC curve	3.95	4.51	3.98
Unmasked-calculated*	-	-	-

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

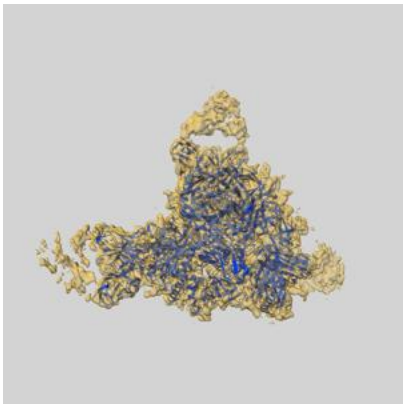
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14474 and PDB model 7Z3A. Per-residue inclusion information can be found in section 3 on page 12.

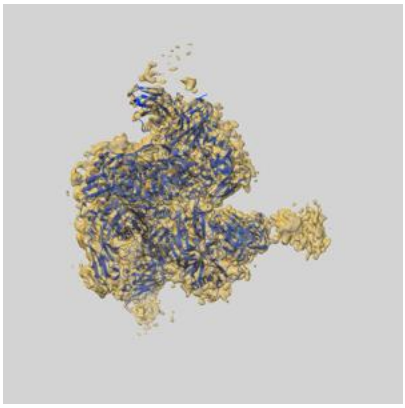
9.1 Map-model overlay



X



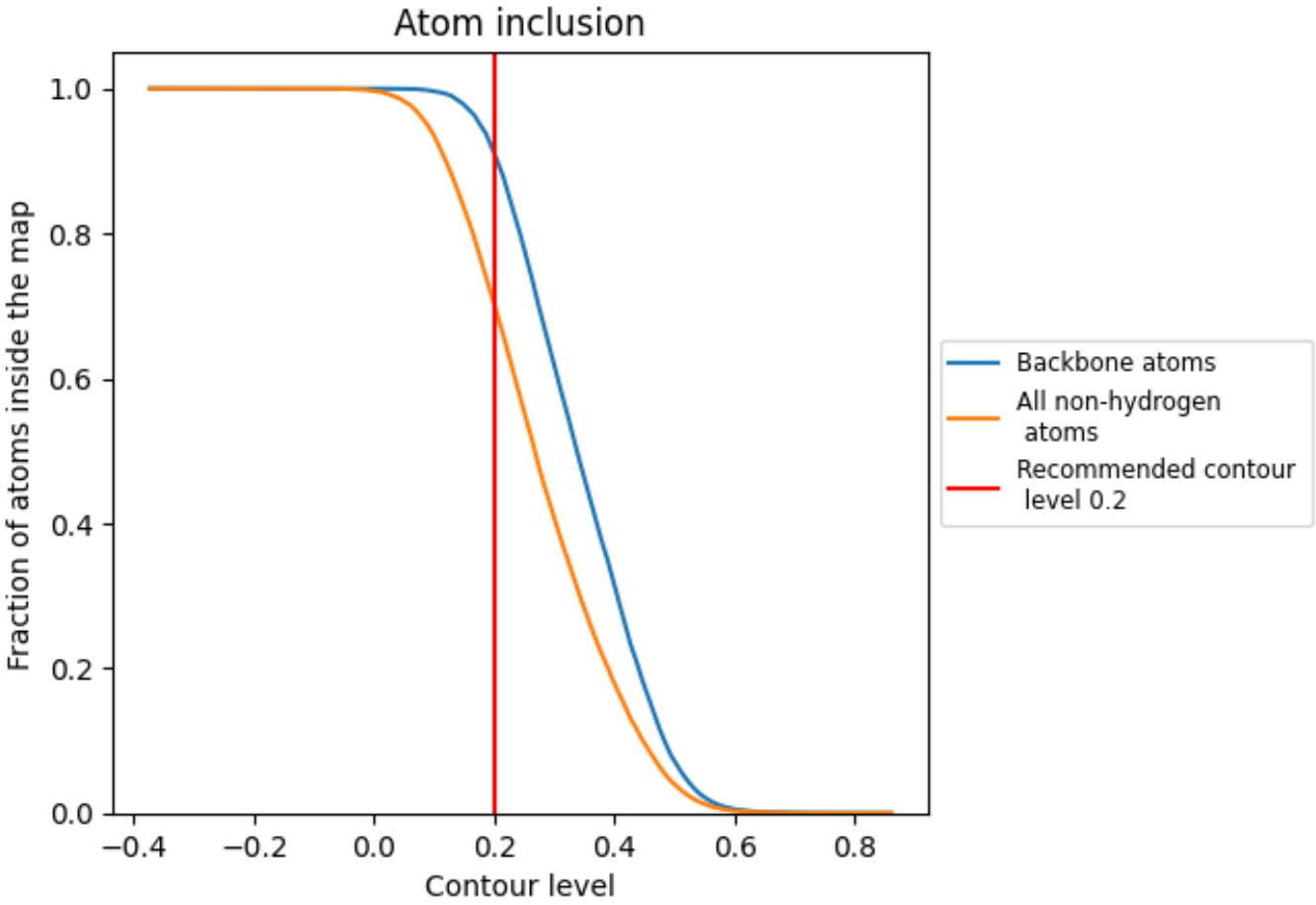
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.