Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 08:12 PM EDT

PDB ID	:	8FAD
EMDB ID	:	EMD-28953
Title	:	Asymmetric structure of cleaved HIV-1 AD8 envelope glycoprotein trimer in styrene-maleic acid lipid nanoparticles
Authors	:	Wang, K.; Zhang, S.; Sodroski, J.; Mao, Y.
Deposited on	:	2022-11-26
Resolution	:	4.00 Å(reported)

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

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

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

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

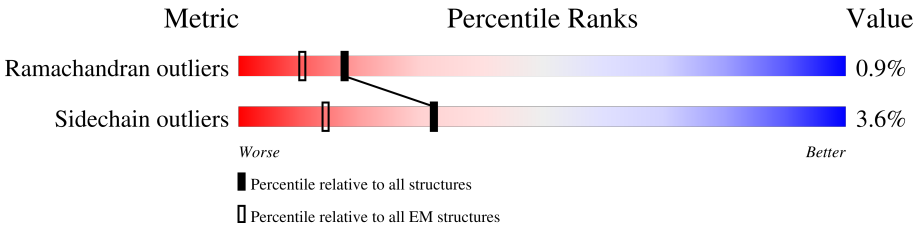
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.00 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	B	138	10% 97%
1	D	138	12% 96%
1	F	138	13% 80% 9% 11%
2	A	469	7% 94% 5%
2	C	469	7% 97%
2	E	469	10% 96%
3	0	2	50% 50% 50%
3	1	2	50% 50% 50%
3	G	2	50% 100%

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Mol	Chain	Length	Quality of chain
3	H	2	50% 50% 50%
3	I	2	50% 50%
3	K	2	100%
3	L	2	50% 100%
3	O	2	50% 100%
3	P	2	100%
3	S	2	50% 100%
3	U	2	50% 50%
3	V	2	100%
3	W	2	50% 50% 50%
3	X	2	50% 50% 50%
3	Y	2	50% 50% 50%
3	a	2	50% 100%
3	b	2	50% 100%
3	d	2	100%
3	e	2	50% 100%
3	f	2	100%
3	i	2	50% 100%
3	k	2	50% 50% 50%
3	l	2	50% 50% 50%
3	m	2	100% 50% 50%
3	n	2	50% 50% 50%
3	o	2	50% 100%
3	p	2	50% 100%
3	q	2	50% 100%

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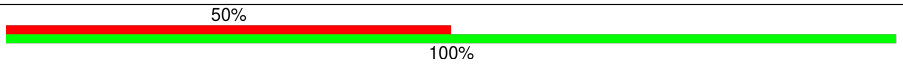
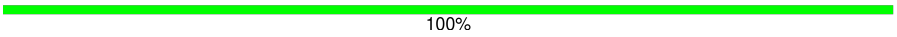
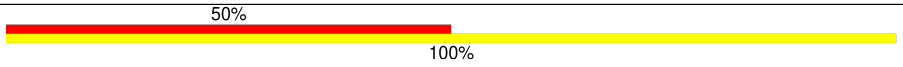
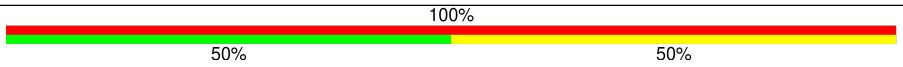
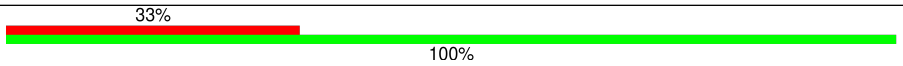
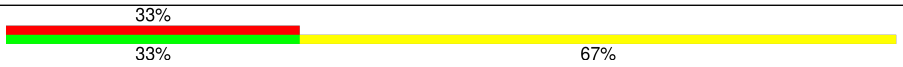
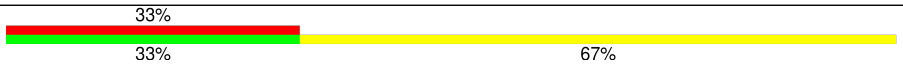
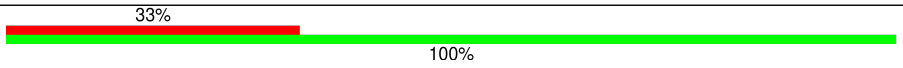
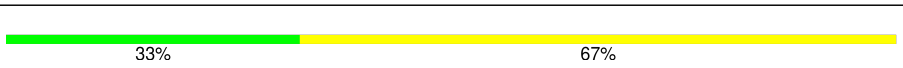
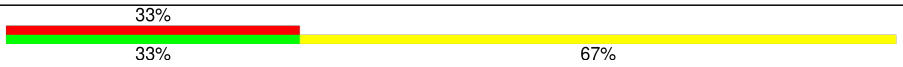
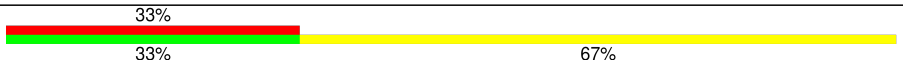
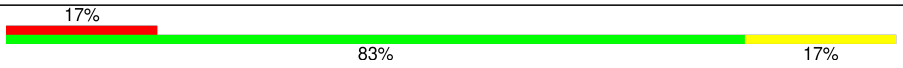
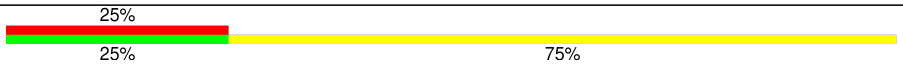
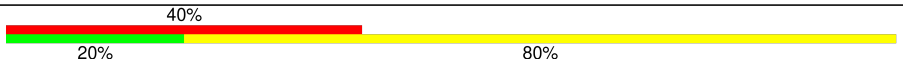
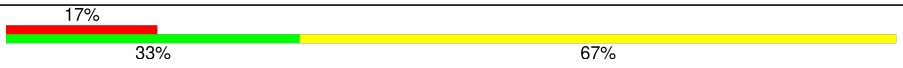
Mol	Chain	Length	Quality of chain
3	s	2	
3	t	2	
3	u	2	
3	v	2	
3	x	2	
3	y	2	
3	z	2	
4	J	3	
4	N	3	
4	Q	3	
4	T	3	
4	Z	3	
4	g	3	
4	j	3	
4	w	3	
5	M	6	
6	R	4	
7	c	5	
8	h	5	
9	r	6	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 16210 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 Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	138	Total	C	N	O	S	0	0
			1100	697	192	205	6		
1	D	138	Total	C	N	O	S	0	0
			1100	697	192	205	6		
1	F	123	Total	C	N	O	S	0	0
			979	623	168	182	6		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	533	ALA	ARG	conflict	UNP P19550
B	535	ILE	LEU	conflict	UNP P19550
B	543	LEU	GLN	conflict	UNP P19550
B	588	ARG	LYS	conflict	UNP P19550
B	618	THR	SER	conflict	UNP P19550
B	621	MET	GLN	conflict	UNP P19550
B	640	GLY	ASN	conflict	UNP P19550
D	533	ALA	ARG	conflict	UNP P19550
D	535	ILE	LEU	conflict	UNP P19550
D	543	LEU	GLN	conflict	UNP P19550
D	588	ARG	LYS	conflict	UNP P19550
D	618	THR	SER	conflict	UNP P19550
D	621	MET	GLN	conflict	UNP P19550
D	640	GLY	ASN	conflict	UNP P19550
F	533	ALA	ARG	conflict	UNP P19550
F	535	ILE	LEU	conflict	UNP P19550
F	543	LEU	GLN	conflict	UNP P19550
F	588	ARG	LYS	conflict	UNP P19550
F	618	THR	SER	conflict	UNP P19550
F	621	MET	GLN	conflict	UNP P19550
F	640	GLY	ASN	conflict	UNP P19550

- Molecule 2 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	466	Total	C	N	O	S	0	0
			3675	2301	648	700	26		
2	E	466	Total	C	N	O	S	0	0
			3675	2301	648	700	26		
2	A	466	Total	C	N	O	S	0	0
			3675	2301	648	700	26		

- Molecule 3 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
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	a	2	Total	C	N	O	0	0
			28	16	2	10		

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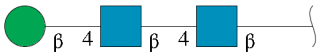
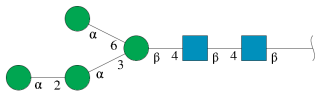
Mol	Chain	Residues	Atoms				AltConf	Trace
3	b	2	Total	C	N	O	0	0
			28	16	2	10		
3	d	2	Total	C	N	O	0	0
			28	16	2	10		
3	e	2	Total	C	N	O	0	0
			28	16	2	10		
3	f	2	Total	C	N	O	0	0
			28	16	2	10		
3	i	2	Total	C	N	O	0	0
			28	16	2	10		
3	k	2	Total	C	N	O	0	0
			28	16	2	10		
3	l	2	Total	C	N	O	0	0
			28	16	2	10		
3	m	2	Total	C	N	O	0	0
			28	16	2	10		
3	n	2	Total	C	N	O	0	0
			28	16	2	10		
3	o	2	Total	C	N	O	0	0
			28	16	2	10		
3	p	2	Total	C	N	O	0	0
			28	16	2	10		
3	q	2	Total	C	N	O	0	0
			28	16	2	10		
3	s	2	Total	C	N	O	0	0
			28	16	2	10		
3	t	2	Total	C	N	O	0	0
			28	16	2	10		
3	u	2	Total	C	N	O	0	0
			28	16	2	10		
3	v	2	Total	C	N	O	0	0
			28	16	2	10		
3	x	2	Total	C	N	O	0	0
			28	16	2	10		
3	y	2	Total	C	N	O	0	0
			28	16	2	10		
3	z	2	Total	C	N	O	0	0
			28	16	2	10		
3	0	2	Total	C	N	O	0	0
			28	16	2	10		
3	1	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 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
4	J	3	Total	C	N	O	0	0
			39	22	2	15		
4	N	3	Total	C	N	O	0	0
			39	22	2	15		
4	Q	3	Total	C	N	O	0	0
			39	22	2	15		
4	T	3	Total	C	N	O	0	0
			39	22	2	15		
4	Z	3	Total	C	N	O	0	0
			39	22	2	15		
4	g	3	Total	C	N	O	0	0
			39	22	2	15		
4	j	3	Total	C	N	O	0	0
			39	22	2	15		
4	w	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.

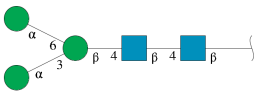


Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 6 is an oligosaccharide called 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.

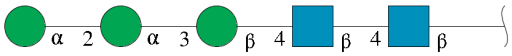
Mol	Chain	Residues	Atoms				AltConf	Trace
6	R	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 7 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.



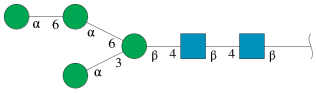
Mol	Chain	Residues	Atoms				AltConf	Trace
7	c	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



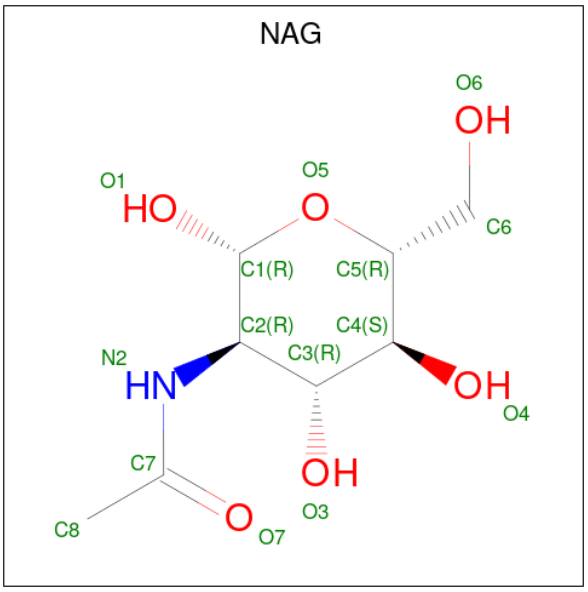
Mol	Chain	Residues	Atoms				AltConf	Trace
8	h	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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	r	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 10 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
10	B	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	D	1	Total	C	N	O	0
			14	8	1	5	
10	D	1	Total	C	N	O	0
			14	8	1	5	
10	D	1	Total	C	N	O	0
			14	8	1	5	
10	E	1	Total	C	N	O	0
			14	8	1	5	
10	E	1	Total	C	N	O	0
			14	8	1	5	
10	E	1	Total	C	N	O	0
			14	8	1	5	

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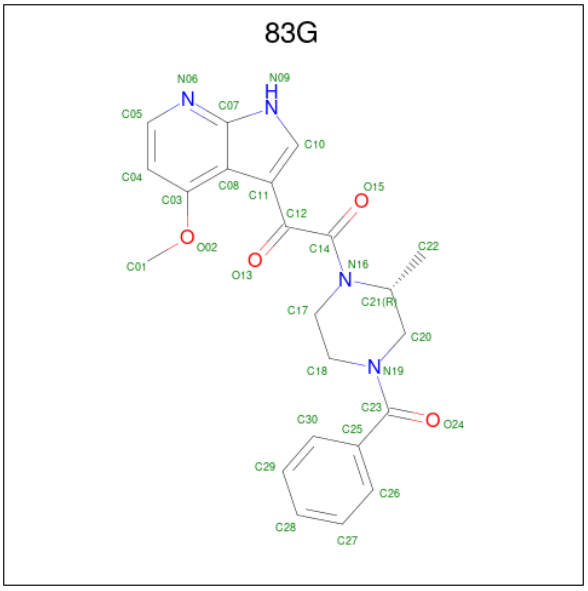
Mol	Chain	Residues	Atoms	AltConf
10	E	1	Total C N O 14 8 1 5	0
10	A	1	Total C N O 14 8 1 5	0
10	A	1	Total C N O 14 8 1 5	0
10	A	1	Total C N O 14 8 1 5	0
10	A	1	Total C N O 14 8 1 5	0
10	F	1	Total C N O 14 8 1 5	0
10	F	1	Total C N O 14 8 1 5	0
10	F	1	Total C N O 14 8 1 5	0

- Molecule 11 is 1-[(2R)-4-(benzenecarbonyl)-2-methylpiperazin-1-yl]-2-(4-methoxy-1H-pyrrolo[2,3-b]pyridin-3-yl)ethane-1,2-dione (three-letter code: 83G) (formula: $C_{22}H_{22}N_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
11	C	1	Total C N O 30 22 4 4	0
11	E	1	Total C N O 30 22 4 4	0

Continued on next page...

Continued from previous page...

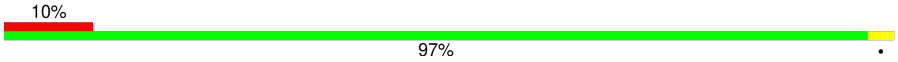
Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	N	O	0
			30	22	4	4	

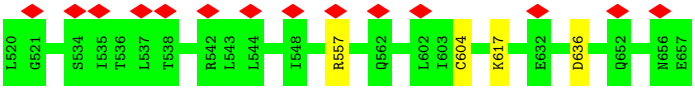
3 Residue-property plots (i)

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: Transmembrane protein gp41

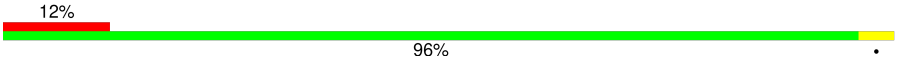
Chain B:

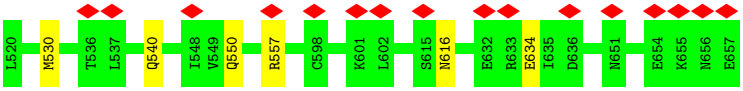




• Molecule 1: Transmembrane protein gp41

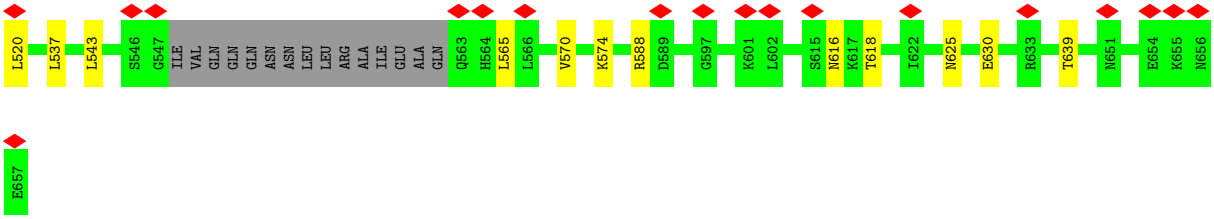
Chain D:





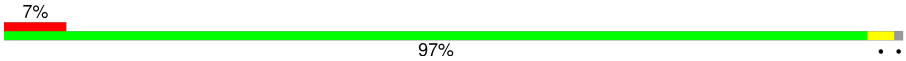
• Molecule 1: Transmembrane protein gp41

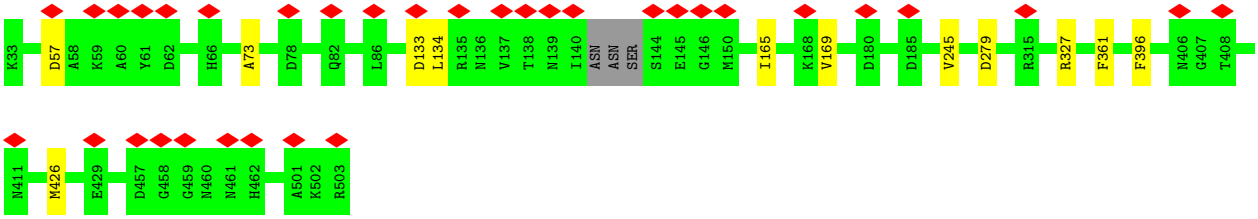
Chain F:



• Molecule 2: Envelope glycoprotein gp120

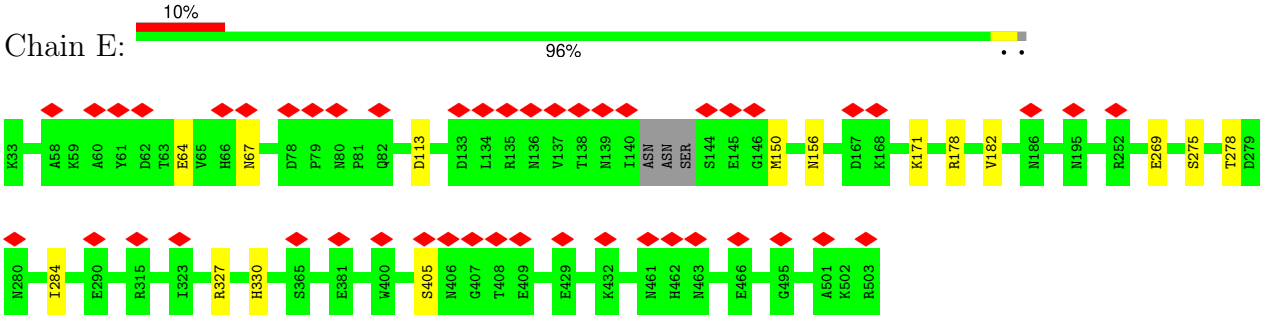
Chain C:





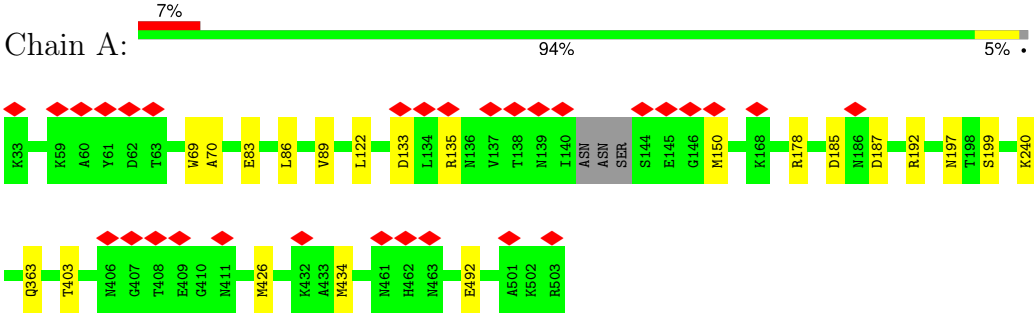
• Molecule 2: Envelope glycoprotein gp120

Chain E:



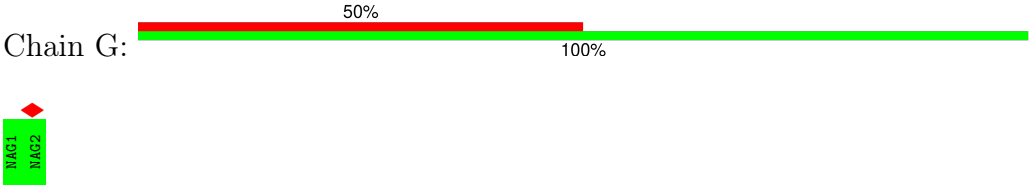
• Molecule 2: Envelope glycoprotein gp120

Chain A:



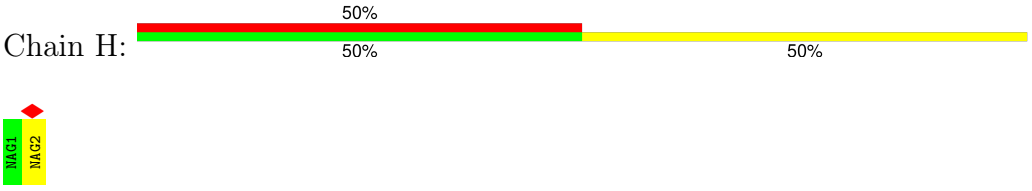
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

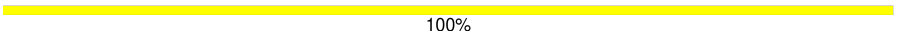


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

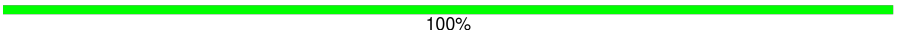
Chain L:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

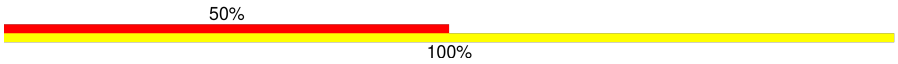
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

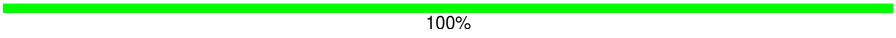


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

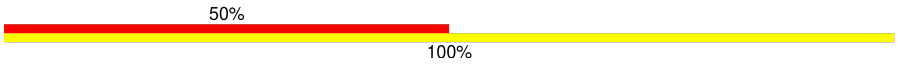
Chain X:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

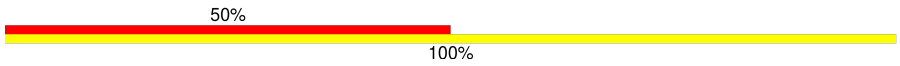
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

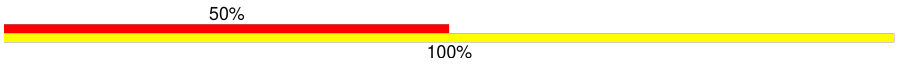
Chain e:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

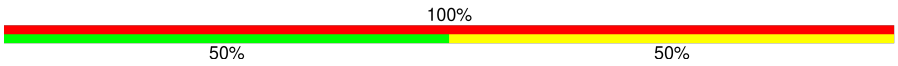
Chain k:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:

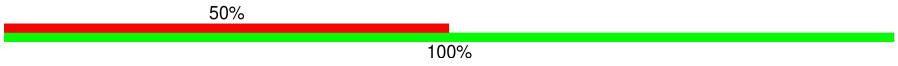


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:

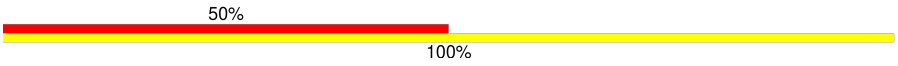
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

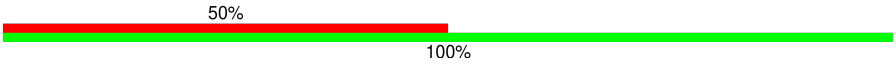
Chain q:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:

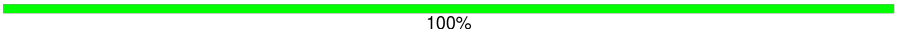
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

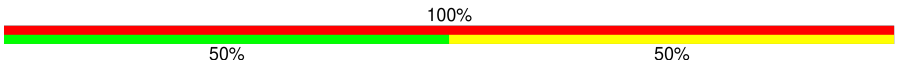
Chain x:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

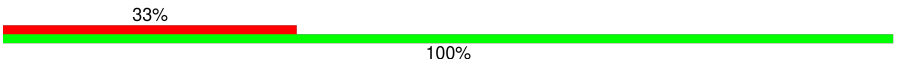
Chain 0:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:

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

Chain J:



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

Chain N:

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

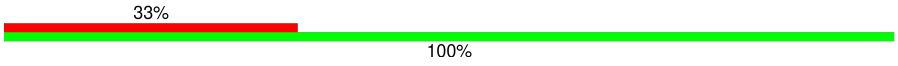
Chain Q:

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

Chain T:

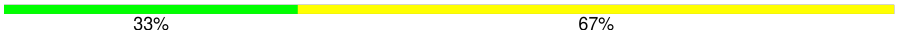
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



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

Chain g:



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

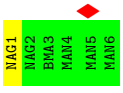
Chain j:

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

Chain w:

• Molecule 5: alpha-D-mannopyranose-(1-2)-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 M:



• Molecule 6: 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

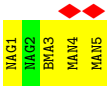
Chain R:

• Molecule 7: 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 c:

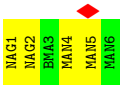
• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



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

Chain r:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	365824	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	54	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.113	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	230.16, 230.16, 230.16	wwPDB
Map dimensions	168, 168, 168	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 83G, NAG, BMA, MAN

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	B	0.59	0/1119	0.64	1/1520 (0.1%)
1	D	0.59	0/1119	0.67	0/1520
1	F	0.63	0/997	0.68	0/1353
2	A	0.48	0/3753	0.61	0/5100
2	C	0.51	0/3753	0.63	0/5100
2	E	0.54	0/3753	0.64	0/5100
All	All	0.53	0/14494	0.64	1/19693 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	604	CYS	CB-CA-C	-5.24	99.93	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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	B	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	19	55
1	D	136/138 (99%)	128 (94%)	6 (4%)	2 (2%)	8	40
1	F	119/138 (86%)	100 (84%)	18 (15%)	1 (1%)	16	53
2	A	462/469 (98%)	395 (86%)	61 (13%)	6 (1%)	10	42
2	C	462/469 (98%)	418 (90%)	40 (9%)	4 (1%)	14	49
2	E	462/469 (98%)	425 (92%)	35 (8%)	2 (0%)	30	66
All	All	1777/1821 (98%)	1590 (90%)	171 (10%)	16 (1%)	17	49

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	69	TRP
2	A	70	ALA
1	B	636	ASP
2	C	57	ASP
2	C	73	ALA
2	C	396	PHE
1	D	530	MET
1	D	616	ASN
2	A	133	ASP
2	A	187	ASP
2	C	133	ASP
2	E	156	ASN
2	E	405	SER
2	A	185	ASP
2	A	199	SER
1	F	570	VAL

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	B	117/117 (100%)	115 (98%)	2 (2%)	56 72
1	D	117/117 (100%)	113 (97%)	4 (3%)	32 54
1	F	104/117 (89%)	93 (89%)	11 (11%)	5 22
2	A	418/421 (99%)	399 (96%)	19 (4%)	23 46
2	C	418/421 (99%)	410 (98%)	8 (2%)	52 70
2	E	418/421 (99%)	405 (97%)	13 (3%)	35 56
All	All	1592/1614 (99%)	1535 (96%)	57 (4%)	32 52

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	557	ARG
1	B	617	LYS
2	C	134	LEU
2	C	165	ILE
2	C	169	VAL
2	C	245	VAL
2	C	279	ASP
2	C	327	ARG
2	C	361	PHE
2	C	426	MET
1	D	540	GLN
1	D	550	GLN
1	D	557	ARG
1	D	634	GLU
2	E	64	GLU
2	E	67	ASN
2	E	113	ASP
2	E	150	MET
2	E	171	LYS
2	E	178	ARG
2	E	182	VAL
2	E	269	GLU
2	E	275	SER
2	E	278	THR
2	E	284	ILE
2	E	327	ARG
2	E	330	HIS
2	A	83	GLU
2	A	86	LEU
2	A	89	VAL

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Mol	Chain	Res	Type
2	A	122	LEU
2	A	135	ARG
2	A	150	MET
2	A	178	ARG
2	A	192	ARG
2	A	197	ASN
2	A	240	LYS
2	A	245	VAL
2	A	270	VAL
2	A	275	SER
2	A	327	ARG
2	A	363	GLN
2	A	403	THR
2	A	426	MET
2	A	434	MET
2	A	492	GLU
1	F	520	LEU
1	F	537	LEU
1	F	543	LEU
1	F	565	LEU
1	F	574	LYS
1	F	588	ARG
1	F	616	ASN
1	F	618	THR
1	F	625	ASN
1	F	630	GLU
1	F	639	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	554	ASN
1	D	591	GLN
1	D	624	ASN
1	D	656	ASN
2	E	66	HIS
2	E	67	ASN
2	E	330	HIS
2	E	428	GLN
2	E	442	GLN
2	A	186	ASN
2	A	343	ASN

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Mol	Chain	Res	Type
2	A	363	GLN
2	A	428	GLN
2	A	442	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

120 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	$\#\|Z\| > 2$
3	NAG	0	1	3,2	14,14,15	0.92	1 (7%)	17,19,21	0.76	0
3	NAG	0	2	3	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	1	1	1,3	14,14,15	0.31	0	17,19,21	0.51	0
3	NAG	1	2	3	14,14,15	0.28	0	17,19,21	0.79	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.31	0	17,19,21	0.55	0
3	NAG	G	2	3	14,14,15	0.30	0	17,19,21	0.60	0
3	NAG	H	1	3,2	14,14,15	0.27	0	17,19,21	0.50	0
3	NAG	H	2	3	14,14,15	0.40	0	17,19,21	1.35	2 (11%)
3	NAG	I	1	3,2	14,14,15	0.30	0	17,19,21	1.24	2 (11%)
3	NAG	I	2	3	14,14,15	0.28	0	17,19,21	0.63	0
4	NAG	J	1	4,2	14,14,15	0.41	0	17,19,21	0.46	0
4	NAG	J	2	4	14,14,15	0.19	0	17,19,21	0.48	0
4	BMA	J	3	4	11,11,12	0.65	0	15,15,17	0.65	0
3	NAG	K	1	3,2	14,14,15	0.36	0	17,19,21	1.32	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	K	2	3	14,14,15	0.50	0	17,19,21	1.27	2 (11%)
3	NAG	L	1	3,2	14,14,15	0.34	0	17,19,21	0.82	1 (5%)
3	NAG	L	2	3	14,14,15	0.24	0	17,19,21	1.09	2 (11%)
5	NAG	M	1	5,2	14,14,15	0.23	0	17,19,21	0.64	1 (5%)
5	NAG	M	2	5	14,14,15	0.30	0	17,19,21	0.60	0
5	BMA	M	3	5	11,11,12	0.23	0	15,15,17	0.71	0
5	MAN	M	4	5	11,11,12	0.17	0	15,15,17	0.64	0
5	MAN	M	5	5	11,11,12	0.20	0	15,15,17	0.55	0
5	MAN	M	6	5	11,11,12	0.21	0	15,15,17	0.57	0
4	NAG	N	1	4,2	14,14,15	0.39	0	17,19,21	1.12	2 (11%)
4	NAG	N	2	4	14,14,15	0.46	0	17,19,21	1.36	1 (5%)
4	BMA	N	3	4	11,11,12	0.21	0	15,15,17	0.65	0
3	NAG	O	1	3,2	14,14,15	0.35	0	17,19,21	0.45	0
3	NAG	O	2	3	14,14,15	0.26	0	17,19,21	0.45	0
3	NAG	P	1	3,2	14,14,15	0.21	0	17,19,21	0.50	0
3	NAG	P	2	3	14,14,15	0.26	0	17,19,21	0.53	0
4	NAG	Q	1	4,2	14,14,15	0.36	0	17,19,21	1.58	2 (11%)
4	NAG	Q	2	4	14,14,15	0.34	0	17,19,21	0.41	0
4	BMA	Q	3	4	11,11,12	0.65	0	15,15,17	1.07	1 (6%)
6	NAG	R	1	6,2	14,14,15	0.83	1 (7%)	17,19,21	2.52	6 (35%)
6	NAG	R	2	6	14,14,15	0.71	0	17,19,21	1.76	3 (17%)
6	BMA	R	3	6	11,11,12	0.53	0	15,15,17	0.89	0
6	MAN	R	4	6	11,11,12	0.61	0	15,15,17	1.23	2 (13%)
3	NAG	S	1	3,2	14,14,15	0.39	0	17,19,21	0.85	2 (11%)
3	NAG	S	2	3	14,14,15	0.53	0	17,19,21	0.81	1 (5%)
4	NAG	T	1	4,2	14,14,15	0.30	0	17,19,21	1.38	2 (11%)
4	NAG	T	2	4	14,14,15	0.31	0	17,19,21	1.07	2 (11%)
4	BMA	T	3	4	11,11,12	0.23	0	15,15,17	0.65	0
3	NAG	U	1	3,2	14,14,15	0.51	0	17,19,21	0.90	1 (5%)
3	NAG	U	2	3	14,14,15	0.28	0	17,19,21	0.60	0
3	NAG	V	1	3,2	14,14,15	0.36	0	17,19,21	0.85	0
3	NAG	V	2	3	14,14,15	0.34	0	17,19,21	0.74	0
3	NAG	W	1	1,3	14,14,15	0.29	0	17,19,21	1.12	1 (5%)
3	NAG	W	2	3	14,14,15	0.30	0	17,19,21	0.59	0
3	NAG	X	1	3,2	14,14,15	0.30	0	17,19,21	0.52	0
3	NAG	X	2	3	14,14,15	0.43	0	17,19,21	1.35	2 (11%)
3	NAG	Y	1	3,2	14,14,15	0.30	0	17,19,21	1.23	2 (11%)
3	NAG	Y	2	3	14,14,15	0.32	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	Z	1	4,2	14,14,15	0.44	0	17,19,21	0.47	0
4	NAG	Z	2	4	14,14,15	0.20	0	17,19,21	0.46	0
4	BMA	Z	3	4	11,11,12	0.64	0	15,15,17	0.65	0
3	NAG	a	1	3,2	14,14,15	0.85	1 (7%)	17,19,21	0.71	0
3	NAG	a	2	3	14,14,15	0.39	0	17,19,21	0.96	2 (11%)
3	NAG	b	1	3,2	14,14,15	0.35	0	17,19,21	0.77	1 (5%)
3	NAG	b	2	3	14,14,15	0.23	0	17,19,21	1.09	2 (11%)
7	NAG	c	1	7,2	14,14,15	0.22	0	17,19,21	0.64	1 (5%)
7	NAG	c	2	7	14,14,15	0.28	0	17,19,21	0.60	0
7	BMA	c	3	7	11,11,12	0.61	0	15,15,17	0.67	1 (6%)
7	MAN	c	4	7	11,11,12	0.53	0	15,15,17	3.49	4 (26%)
7	MAN	c	5	7	11,11,12	1.02	0	15,15,17	1.41	2 (13%)
3	NAG	d	1	3,2	14,14,15	0.34	0	17,19,21	1.50	3 (17%)
3	NAG	d	2	3	14,14,15	0.48	0	17,19,21	1.22	1 (5%)
3	NAG	e	1	3,2	14,14,15	0.34	0	17,19,21	0.46	0
3	NAG	e	2	3	14,14,15	0.26	0	17,19,21	0.45	0
3	NAG	f	1	3,2	14,14,15	0.24	0	17,19,21	0.52	0
3	NAG	f	2	3	14,14,15	0.24	0	17,19,21	0.54	0
4	NAG	g	1	4,2	14,14,15	0.36	0	17,19,21	1.58	2 (11%)
4	NAG	g	2	4	14,14,15	0.32	0	17,19,21	0.42	0
4	BMA	g	3	4	11,11,12	0.65	0	15,15,17	1.08	1 (6%)
8	NAG	h	1	8,2	14,14,15	0.70	1 (7%)	17,19,21	0.79	0
8	NAG	h	2	8	14,14,15	0.19	0	17,19,21	0.40	0
8	BMA	h	3	8	11,11,12	0.92	1 (9%)	15,15,17	1.09	1 (6%)
8	MAN	h	4	8	11,11,12	1.32	2 (18%)	15,15,17	1.85	2 (13%)
8	MAN	h	5	8	11,11,12	0.84	1 (9%)	15,15,17	1.04	2 (13%)
3	NAG	i	1	3,2	14,14,15	0.36	0	17,19,21	0.85	2 (11%)
3	NAG	i	2	3	14,14,15	0.51	0	17,19,21	0.79	1 (5%)
4	NAG	j	1	4,2	14,14,15	0.32	0	17,19,21	1.50	3 (17%)
4	NAG	j	2	4	14,14,15	0.34	0	17,19,21	0.71	0
4	BMA	j	3	4	11,11,12	0.22	0	15,15,17	0.67	1 (6%)
3	NAG	k	1	3,2	14,14,15	0.34	0	17,19,21	0.72	1 (5%)
3	NAG	k	2	3	14,14,15	0.28	0	17,19,21	0.60	0
3	NAG	l	1	3,2	14,14,15	0.30	0	17,19,21	0.73	1 (5%)
3	NAG	l	2	3	14,14,15	0.31	0	17,19,21	0.61	0
3	NAG	m	1	3,2	14,14,15	0.33	0	17,19,21	0.64	0
3	NAG	m	2	3	14,14,15	0.29	0	17,19,21	1.28	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	n	1	3,2	14,14,15	0.30	0	17,19,21	1.24	2 (11%)
3	NAG	n	2	3	14,14,15	0.30	0	17,19,21	0.62	0
3	NAG	o	1	3,2	14,14,15	0.42	0	17,19,21	0.46	0
3	NAG	o	2	3	14,14,15	0.21	0	17,19,21	0.47	0
3	NAG	p	1	3,2	14,14,15	0.34	0	17,19,21	1.31	1 (5%)
3	NAG	p	2	3	14,14,15	0.50	0	17,19,21	1.27	2 (11%)
3	NAG	q	1	3,2	14,14,15	0.34	0	17,19,21	1.03	2 (11%)
3	NAG	q	2	3	14,14,15	0.29	0	17,19,21	1.43	2 (11%)
9	NAG	r	1	9,2	14,14,15	1.15	1 (7%)	17,19,21	2.92	4 (23%)
9	NAG	r	2	9	14,14,15	0.27	0	17,19,21	0.90	1 (5%)
9	BMA	r	3	9	11,11,12	0.24	0	15,15,17	0.59	0
9	MAN	r	4	9	11,11,12	1.01	0	15,15,17	1.41	2 (13%)
9	MAN	r	5	9	11,11,12	0.70	0	15,15,17	0.99	2 (13%)
9	MAN	r	6	9	11,11,12	0.20	0	15,15,17	0.63	0
3	NAG	s	1	3,2	14,14,15	0.61	1 (7%)	17,19,21	0.70	0
3	NAG	s	2	3	14,14,15	0.20	0	17,19,21	0.84	0
3	NAG	t	1	3,2	14,14,15	0.35	0	17,19,21	0.46	0
3	NAG	t	2	3	14,14,15	0.30	0	17,19,21	0.46	0
3	NAG	u	1	3,2	14,14,15	0.23	0	17,19,21	0.51	0
3	NAG	u	2	3	14,14,15	0.26	0	17,19,21	0.53	0
3	NAG	v	1	3,2	14,14,15	0.34	0	17,19,21	1.58	2 (11%)
3	NAG	v	2	3	14,14,15	0.31	0	17,19,21	0.43	0
4	NAG	w	1	4,2	14,14,15	0.83	0	17,19,21	2.52	6 (35%)
4	NAG	w	2	4	14,14,15	0.69	0	17,19,21	1.76	3 (17%)
4	BMA	w	3	4	11,11,12	0.50	0	15,15,17	0.85	0
3	NAG	x	1	3,2	14,14,15	0.38	0	17,19,21	0.84	2 (11%)
3	NAG	x	2	3	14,14,15	0.50	0	17,19,21	0.81	1 (5%)
3	NAG	y	1	3,2	14,14,15	0.30	0	17,19,21	1.46	3 (17%)
3	NAG	y	2	3	14,14,15	0.28	0	17,19,21	0.61	0
3	NAG	z	1	3,2	14,14,15	0.32	0	17,19,21	0.72	1 (5%)
3	NAG	z	2	3	14,14,15	0.28	0	17,19,21	0.52	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
3	NAG	0	1	3,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	0	2	3	-	0/6/23/26	0/1/1/1
3	NAG	1	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	1	2	3	-	3/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	6/6/23/26	0/1/1/1
3	NAG	I	1	3,2	-	3/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
4	NAG	J	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
3	NAG	K	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	3/6/23/26	0/1/1/1
3	NAG	L	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	4/6/23/26	0/1/1/1
5	NAG	M	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	0/2/19/22	0/1/1/1
5	MAN	M	5	5	-	1/2/19/22	0/1/1/1
5	MAN	M	6	5	-	0/2/19/22	0/1/1/1
4	NAG	N	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	BMA	N	3	4	-	2/2/19/22	0/1/1/1
3	NAG	O	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	BMA	Q	3	4	-	0/2/19/22	0/1/1/1
6	NAG	R	1	6,2	-	6/6/23/26	0/1/1/1
6	NAG	R	2	6	-	3/6/23/26	0/1/1/1
6	BMA	R	3	6	-	2/2/19/22	0/1/1/1
6	MAN	R	4	6	-	0/2/19/22	0/1/1/1
3	NAG	S	1	3,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
4	NAG	T	1	4,2	-	3/6/23/26	0/1/1/1
4	NAG	T	2	4	-	3/6/23/26	0/1/1/1
4	BMA	T	3	4	-	2/2/19/22	0/1/1/1
3	NAG	U	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	U	2	3	-	4/6/23/26	0/1/1/1
3	NAG	V	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	NAG	X	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	6/6/23/26	0/1/1/1
3	NAG	Y	1	3,2	-	3/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	0/6/23/26	0/1/1/1
4	NAG	Z	1	4,2	-	1/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	1/6/23/26	0/1/1/1
4	BMA	Z	3	4	-	0/2/19/22	0/1/1/1
3	NAG	a	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	1/6/23/26	0/1/1/1
3	NAG	b	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	4/6/23/26	0/1/1/1
7	NAG	c	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	c	2	7	-	2/6/23/26	0/1/1/1
7	BMA	c	3	7	-	0/2/19/22	0/1/1/1
7	MAN	c	4	7	-	0/2/19/22	0/1/1/1
7	MAN	c	5	7	-	1/2/19/22	0/1/1/1
3	NAG	d	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	d	2	3	-	1/6/23/26	0/1/1/1
3	NAG	e	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	e	2	3	-	2/6/23/26	0/1/1/1
3	NAG	f	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	f	2	3	-	2/6/23/26	0/1/1/1
4	NAG	g	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	g	2	4	-	2/6/23/26	0/1/1/1
4	BMA	g	3	4	-	0/2/19/22	0/1/1/1
8	NAG	h	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	h	2	8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	h	3	8	-	2/2/19/22	0/1/1/1
8	MAN	h	4	8	-	0/2/19/22	0/1/1/1
8	MAN	h	5	8	-	0/2/19/22	0/1/1/1
3	NAG	i	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	i	2	3	-	2/6/23/26	0/1/1/1
4	NAG	j	1	4,2	-	3/6/23/26	0/1/1/1
4	NAG	j	2	4	-	2/6/23/26	0/1/1/1
4	BMA	j	3	4	-	0/2/19/22	0/1/1/1
3	NAG	k	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	k	2	3	-	4/6/23/26	0/1/1/1
3	NAG	l	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	l	2	3	-	0/6/23/26	0/1/1/1
3	NAG	m	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	m	2	3	-	5/6/23/26	0/1/1/1
3	NAG	n	1	3,2	-	3/6/23/26	0/1/1/1
3	NAG	n	2	3	-	0/6/23/26	0/1/1/1
3	NAG	o	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	o	2	3	-	1/6/23/26	0/1/1/1
3	NAG	p	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	p	2	3	-	3/6/23/26	0/1/1/1
3	NAG	q	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	q	2	3	-	5/6/23/26	0/1/1/1
9	NAG	r	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	r	2	9	-	5/6/23/26	0/1/1/1
9	BMA	r	3	9	-	2/2/19/22	0/1/1/1
9	MAN	r	4	9	-	1/2/19/22	0/1/1/1
9	MAN	r	5	9	-	0/2/19/22	0/1/1/1
9	MAN	r	6	9	-	0/2/19/22	0/1/1/1
3	NAG	s	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	s	2	3	-	4/6/23/26	0/1/1/1
3	NAG	t	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	t	2	3	-	2/6/23/26	0/1/1/1
3	NAG	u	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	u	2	3	-	2/6/23/26	0/1/1/1
3	NAG	v	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	v	2	3	-	2/6/23/26	0/1/1/1

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	1	NAG	C1-C2	3.84	1.57	1.52
8	h	4	MAN	C1-C2	3.20	1.59	1.52
3	a	1	NAG	O5-C1	-3.08	1.38	1.43
3	0	1	NAG	O5-C1	-3.07	1.38	1.43
8	h	1	NAG	O5-C1	-2.48	1.39	1.43
8	h	4	MAN	O5-C1	2.44	1.47	1.43
8	h	3	BMA	C4-C3	2.07	1.57	1.52
6	R	1	NAG	C1-C2	2.06	1.55	1.52
3	s	1	NAG	O5-C1	-2.04	1.40	1.43
8	h	5	MAN	C1-C2	2.02	1.57	1.52

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	c	4	MAN	O2-C2-C3	9.46	129.75	110.15
9	r	1	NAG	O5-C1-C2	-8.96	97.43	111.29
4	w	1	NAG	C2-N2-C7	7.15	132.48	122.90
6	R	1	NAG	C2-N2-C7	7.12	132.44	122.90
8	h	4	MAN	C1-O5-C5	6.04	120.28	112.19
7	c	4	MAN	O3-C3-C4	-5.84	96.61	110.38
7	c	4	MAN	O4-C4-C5	-5.79	95.06	109.32
9	r	1	NAG	C2-N2-C7	-4.93	116.30	122.90
3	v	1	NAG	C2-N2-C7	4.92	129.49	122.90
4	g	1	NAG	C2-N2-C7	4.91	129.48	122.90
4	N	2	NAG	C1-O5-C5	4.91	118.76	112.19
4	Q	1	NAG	C2-N2-C7	4.91	129.48	122.90
9	r	1	NAG	C1-O5-C5	4.60	118.35	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	2	NAG	C2-N2-C7	4.56	129.02	122.90
3	X	2	NAG	C2-N2-C7	4.53	128.97	122.90
3	q	2	NAG	C2-N2-C7	4.51	128.94	122.90
4	w	2	NAG	C1-O5-C5	4.38	118.06	112.19
6	R	2	NAG	C1-O5-C5	4.38	118.05	112.19
7	c	4	MAN	O5-C5-C6	-4.31	99.28	107.66
3	d	2	NAG	C1-O5-C5	4.18	117.79	112.19
7	c	5	MAN	C1-O5-C5	4.11	117.69	112.19
9	r	4	MAN	C1-O5-C5	4.09	117.67	112.19
4	T	1	NAG	C2-N2-C7	3.93	128.16	122.90
3	y	1	NAG	C2-N2-C7	3.89	128.11	122.90
6	R	4	MAN	C1-O5-C5	3.83	117.32	112.19
4	w	1	NAG	C1-C2-N2	3.81	116.44	110.43
6	R	1	NAG	C1-C2-N2	3.74	116.33	110.43
4	j	1	NAG	C2-N2-C7	3.73	127.91	122.90
3	n	1	NAG	C2-N2-C7	3.64	127.77	122.90
3	I	1	NAG	C2-N2-C7	3.61	127.73	122.90
3	m	2	NAG	C2-N2-C7	3.58	127.69	122.90
3	Y	1	NAG	C2-N2-C7	3.56	127.67	122.90
3	d	1	NAG	O4-C4-C5	3.46	117.84	109.32
3	W	1	NAG	C2-N2-C7	3.43	127.49	122.90
3	p	2	NAG	C1-O5-C5	3.39	116.73	112.19
9	r	1	NAG	C3-C4-C5	-3.37	104.11	110.23
3	K	2	NAG	C1-O5-C5	3.36	116.69	112.19
6	R	2	NAG	C4-C3-C2	3.34	115.92	111.02
4	w	2	NAG	C4-C3-C2	3.32	115.89	111.02
3	K	1	NAG	O4-C4-C5	3.23	117.29	109.32
3	p	1	NAG	O4-C4-C5	3.21	117.22	109.32
4	g	1	NAG	C1-C2-N2	2.98	115.12	110.43
4	Q	1	NAG	C1-C2-N2	2.97	115.12	110.43
4	w	2	NAG	O5-C5-C4	2.97	118.04	110.83
3	v	1	NAG	C1-C2-N2	2.96	115.09	110.43
6	R	2	NAG	O5-C5-C4	2.95	117.99	110.83
3	b	2	NAG	C2-N2-C7	2.89	126.77	122.90
9	r	4	MAN	O3-C3-C2	2.86	115.90	110.05
7	c	5	MAN	O3-C3-C2	2.86	115.89	110.05
3	L	2	NAG	C2-N2-C7	2.85	126.72	122.90
4	j	1	NAG	C1-O5-C5	2.81	115.95	112.19
4	N	1	NAG	O4-C4-C5	2.79	116.19	109.32
3	d	1	NAG	O5-C1-C2	-2.77	107.01	111.29
4	T	2	NAG	C2-N2-C7	2.77	126.61	122.90
8	h	5	MAN	C1-O5-C5	2.76	115.89	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	2	NAG	C1-C2-N2	2.75	114.76	110.43
3	p	2	NAG	C1-C2-N2	2.74	114.74	110.43
4	T	2	NAG	C1-O5-C5	2.73	115.84	112.19
4	w	1	NAG	O5-C5-C4	2.70	117.40	110.83
6	R	1	NAG	O5-C5-C4	2.70	117.39	110.83
3	y	1	NAG	C1-O5-C5	2.68	115.78	112.19
3	m	2	NAG	C1-O5-C5	2.65	115.74	112.19
6	R	1	NAG	C6-C5-C4	-2.58	106.70	113.02
4	w	1	NAG	C6-C5-C4	-2.54	106.77	113.02
8	h	4	MAN	C1-C2-C3	2.48	113.26	109.64
4	T	1	NAG	C1-C2-N2	2.44	114.28	110.43
3	a	2	NAG	C3-C4-C5	2.44	114.66	110.23
4	w	1	NAG	C4-C3-C2	-2.43	107.45	111.02
4	g	3	BMA	C1-O5-C5	2.43	115.45	112.19
4	j	1	NAG	C1-C2-N2	2.43	114.27	110.43
6	R	1	NAG	C4-C3-C2	-2.42	107.47	111.02
4	Q	3	BMA	C1-O5-C5	2.42	115.43	112.19
4	N	1	NAG	C2-N2-C7	-2.33	119.78	122.90
3	m	2	NAG	C1-C2-N2	2.32	114.09	110.43
3	q	2	NAG	C4-C3-C2	-2.31	107.63	111.02
3	I	1	NAG	C1-C2-N2	2.28	114.02	110.43
3	b	2	NAG	C1-O5-C5	2.26	115.22	112.19
3	Y	1	NAG	C1-C2-N2	2.26	113.99	110.43
3	L	2	NAG	C1-O5-C5	2.25	115.21	112.19
3	1	2	NAG	C2-N2-C7	2.25	125.92	122.90
3	n	1	NAG	C1-C2-N2	2.24	113.96	110.43
3	H	2	NAG	C1-C2-N2	2.24	113.96	110.43
3	z	1	NAG	C1-O5-C5	2.23	115.18	112.19
9	r	5	MAN	C1-O5-C5	2.23	115.18	112.19
3	X	2	NAG	C1-C2-N2	2.23	113.94	110.43
9	r	5	MAN	O2-C2-C3	-2.21	105.56	110.15
6	R	4	MAN	O2-C2-C3	-2.21	105.58	110.15
3	S	1	NAG	O4-C4-C5	-2.19	103.93	109.32
6	R	1	NAG	O7-C7-N2	2.18	125.83	121.98
3	k	1	NAG	C1-O5-C5	2.18	115.10	112.19
3	x	1	NAG	O4-C4-C5	-2.18	103.97	109.32
4	w	1	NAG	O7-C7-N2	2.16	125.79	121.98
3	l	1	NAG	C1-O5-C5	2.16	115.08	112.19
3	i	1	NAG	O4-C4-C5	-2.15	104.02	109.32
3	S	2	NAG	C1-O5-C5	2.15	115.07	112.19
3	U	1	NAG	O5-C5-C4	-2.12	105.66	110.83
3	x	2	NAG	C1-O5-C5	2.12	115.03	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	1	NAG	C4-C3-C2	-2.12	107.92	111.02
5	M	1	NAG	C1-O5-C5	2.11	115.02	112.19
3	q	1	NAG	C4-C3-C2	-2.11	107.92	111.02
8	h	5	MAN	O2-C2-C3	-2.11	105.79	110.15
8	h	3	BMA	C1-C2-C3	-2.11	106.58	109.64
3	q	1	NAG	C3-C4-C5	-2.10	106.42	110.23
3	i	1	NAG	O4-C4-C3	2.10	115.33	110.38
7	c	1	NAG	C1-O5-C5	2.09	114.98	112.19
3	a	2	NAG	O4-C4-C5	-2.05	104.28	109.32
4	j	3	BMA	C1-O5-C5	2.03	114.91	112.19
3	y	1	NAG	O7-C7-N2	2.03	125.57	121.98
3	x	1	NAG	O4-C4-C3	2.03	115.15	110.38
3	S	1	NAG	O4-C4-C3	2.03	115.15	110.38
3	b	1	NAG	C4-C3-C2	-2.02	108.06	111.02
3	i	2	NAG	C1-O5-C5	2.01	114.87	112.19
7	c	3	BMA	O2-C2-C3	-2.01	106.00	110.15
9	r	2	NAG	C1-O5-C5	2.00	114.87	112.19
3	d	1	NAG	C4-C3-C2	-2.00	108.08	111.02

There are no chirality outliers.

All (230) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C1-C2-N2-C7
3	I	1	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	L	1	NAG	O7-C7-N2-C2
3	L	2	NAG	C3-C2-N2-C7
3	L	2	NAG	O7-C7-N2-C2
3	U	2	NAG	O7-C7-N2-C2
3	W	1	NAG	C1-C2-N2-C7
3	W	1	NAG	O7-C7-N2-C2
3	Y	1	NAG	C1-C2-N2-C7
3	Y	1	NAG	O7-C7-N2-C2
3	b	1	NAG	O7-C7-N2-C2
3	b	2	NAG	C3-C2-N2-C7
3	b	2	NAG	O7-C7-N2-C2
3	k	2	NAG	C8-C7-N2-C2
3	k	2	NAG	O7-C7-N2-C2
3	l	1	NAG	C8-C7-N2-C2
3	l	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	m	1	NAG	C8-C7-N2-C2
3	m	1	NAG	O7-C7-N2-C2
3	m	2	NAG	C1-C2-N2-C7
3	m	2	NAG	C8-C7-N2-C2
3	m	2	NAG	O7-C7-N2-C2
3	n	1	NAG	C1-C2-N2-C7
3	n	1	NAG	O7-C7-N2-C2
3	p	2	NAG	C8-C7-N2-C2
3	p	2	NAG	O7-C7-N2-C2
3	q	1	NAG	C8-C7-N2-C2
3	q	1	NAG	O7-C7-N2-C2
3	q	2	NAG	C3-C2-N2-C7
3	q	2	NAG	C8-C7-N2-C2
3	q	2	NAG	O7-C7-N2-C2
3	y	1	NAG	C1-C2-N2-C7
3	z	2	NAG	C8-C7-N2-C2
3	z	2	NAG	O7-C7-N2-C2
3	1	2	NAG	C1-C2-N2-C7
3	1	2	NAG	C8-C7-N2-C2
3	1	2	NAG	O7-C7-N2-C2
4	T	1	NAG	C1-C2-N2-C7
4	T	2	NAG	C3-C2-N2-C7
4	T	2	NAG	C8-C7-N2-C2
4	T	2	NAG	O7-C7-N2-C2
4	j	1	NAG	C1-C2-N2-C7
4	w	2	NAG	C8-C7-N2-C2
4	w	2	NAG	O7-C7-N2-C2
6	R	2	NAG	C8-C7-N2-C2
6	R	2	NAG	O7-C7-N2-C2
9	r	2	NAG	C3-C2-N2-C7
3	m	2	NAG	O5-C5-C6-O6
4	T	3	BMA	O5-C5-C6-O6
3	I	1	NAG	C8-C7-N2-C2
3	L	1	NAG	C8-C7-N2-C2
3	L	2	NAG	C8-C7-N2-C2
3	U	2	NAG	C8-C7-N2-C2
3	W	1	NAG	C8-C7-N2-C2
3	Y	1	NAG	C8-C7-N2-C2
3	b	1	NAG	C8-C7-N2-C2
3	b	2	NAG	C8-C7-N2-C2
3	n	1	NAG	C8-C7-N2-C2
3	z	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	z	1	NAG	O7-C7-N2-C2
9	r	2	NAG	C8-C7-N2-C2
9	r	2	NAG	O7-C7-N2-C2
3	U	1	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
7	c	1	NAG	O5-C5-C6-O6
4	j	1	NAG	O7-C7-N2-C2
3	H	2	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	k	2	NAG	O5-C5-C6-O6
4	N	3	BMA	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	e	1	NAG	O5-C5-C6-O6
3	t	1	NAG	O5-C5-C6-O6
3	v	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	g	2	NAG	O5-C5-C6-O6
8	h	3	BMA	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
7	c	2	NAG	O5-C5-C6-O6
3	q	2	NAG	O5-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	k	2	NAG	C4-C5-C6-O6
3	m	2	NAG	C4-C5-C6-O6
4	N	3	BMA	C4-C5-C6-O6
4	T	3	BMA	C4-C5-C6-O6
3	s	2	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
3	U	1	NAG	C8-C7-N2-C2
4	T	1	NAG	C8-C7-N2-C2
4	T	1	NAG	O7-C7-N2-C2
4	j	1	NAG	C8-C7-N2-C2
9	r	2	NAG	O5-C5-C6-O6
3	k	1	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	f	2	NAG	O5-C5-C6-O6
3	u	2	NAG	O5-C5-C6-O6
3	z	1	NAG	O5-C5-C6-O6
3	k	1	NAG	C4-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	c	2	NAG	C4-C5-C6-O6
3	s	2	NAG	C4-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
8	h	3	BMA	C4-C5-C6-O6
6	R	3	BMA	O5-C5-C6-O6
3	z	1	NAG	C4-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
7	c	1	NAG	C4-C5-C6-O6
3	d	1	NAG	C8-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
4	j	2	NAG	C8-C7-N2-C2
3	O	1	NAG	C4-C5-C6-O6
3	e	1	NAG	C4-C5-C6-O6
3	i	2	NAG	C4-C5-C6-O6
3	t	1	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	f	2	NAG	C4-C5-C6-O6
3	u	2	NAG	C4-C5-C6-O6
3	x	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	v	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	g	2	NAG	C4-C5-C6-O6
4	w	3	BMA	O5-C5-C6-O6
6	R	3	BMA	C4-C5-C6-O6
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	U	1	NAG	O7-C7-N2-C2
3	V	1	NAG	C8-C7-N2-C2
3	X	2	NAG	C8-C7-N2-C2
3	X	2	NAG	O7-C7-N2-C2
3	d	1	NAG	O7-C7-N2-C2
3	v	1	NAG	C8-C7-N2-C2
3	v	1	NAG	O7-C7-N2-C2
3	y	1	NAG	C8-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
4	Q	1	NAG	C8-C7-N2-C2
4	Q	1	NAG	O7-C7-N2-C2
4	g	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	g	1	NAG	O7-C7-N2-C2
4	j	2	NAG	O7-C7-N2-C2
9	r	1	NAG	C8-C7-N2-C2
3	S	2	NAG	O5-C5-C6-O6
3	i	2	NAG	O5-C5-C6-O6
3	x	2	NAG	O5-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	q	2	NAG	C4-C5-C6-O6
4	w	3	BMA	C4-C5-C6-O6
3	y	1	NAG	O7-C7-N2-C2
3	a	1	NAG	C4-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	e	2	NAG	O5-C5-C6-O6
3	t	2	NAG	O5-C5-C6-O6
3	K	1	NAG	C8-C7-N2-C2
3	V	1	NAG	O7-C7-N2-C2
3	p	1	NAG	C8-C7-N2-C2
9	r	1	NAG	O7-C7-N2-C2
3	d	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	f	1	NAG	O5-C5-C6-O6
3	u	1	NAG	O5-C5-C6-O6
3	K	1	NAG	O7-C7-N2-C2
3	p	1	NAG	O7-C7-N2-C2
3	y	2	NAG	O5-C5-C6-O6
4	w	1	NAG	O5-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
4	w	2	NAG	C3-C2-N2-C7
6	R	2	NAG	C3-C2-N2-C7
3	K	2	NAG	O5-C5-C6-O6
3	d	2	NAG	O5-C5-C6-O6
3	p	2	NAG	O5-C5-C6-O6
5	M	5	MAN	O5-C5-C6-O6
6	R	1	NAG	C4-C5-C6-O6
4	w	1	NAG	C4-C5-C6-O6
3	1	1	NAG	C8-C7-N2-C2
9	r	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	v	1	NAG	C1-C2-N2-C7
4	Q	1	NAG	C1-C2-N2-C7
4	g	1	NAG	C1-C2-N2-C7
9	r	3	BMA	C4-C5-C6-O6
3	o	1	NAG	C4-C5-C6-O6
4	w	1	NAG	C8-C7-N2-C2
3	d	1	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
3	1	1	NAG	O7-C7-N2-C2
6	R	1	NAG	C8-C7-N2-C2
3	s	1	NAG	C3-C2-N2-C7
3	s	2	NAG	C3-C2-N2-C7
4	w	1	NAG	C3-C2-N2-C7
6	R	1	NAG	C3-C2-N2-C7
9	r	4	MAN	O5-C5-C6-O6
7	c	5	MAN	O5-C5-C6-O6
9	r	3	BMA	O5-C5-C6-O6
4	w	1	NAG	O7-C7-N2-C2
6	R	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C1-C2-N2-C7
3	X	2	NAG	C1-C2-N2-C7
3	o	1	NAG	C1-C2-N2-C7
3	o	2	NAG	C1-C2-N2-C7
3	s	1	NAG	C1-C2-N2-C7
3	s	2	NAG	C1-C2-N2-C7
3	1	1	NAG	C1-C2-N2-C7
4	J	1	NAG	C1-C2-N2-C7
4	J	2	NAG	C1-C2-N2-C7
4	Z	2	NAG	C1-C2-N2-C7
4	w	1	NAG	C1-C2-N2-C7
6	R	1	NAG	C1-C2-N2-C7
3	H	2	NAG	C3-C2-N2-C7
3	X	2	NAG	C3-C2-N2-C7
3	v	1	NAG	C3-C2-N2-C7
4	Q	1	NAG	C3-C2-N2-C7
4	g	1	NAG	C3-C2-N2-C7
3	O	2	NAG	C4-C5-C6-O6
3	e	2	NAG	C4-C5-C6-O6
3	t	2	NAG	C4-C5-C6-O6
3	f	1	NAG	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6

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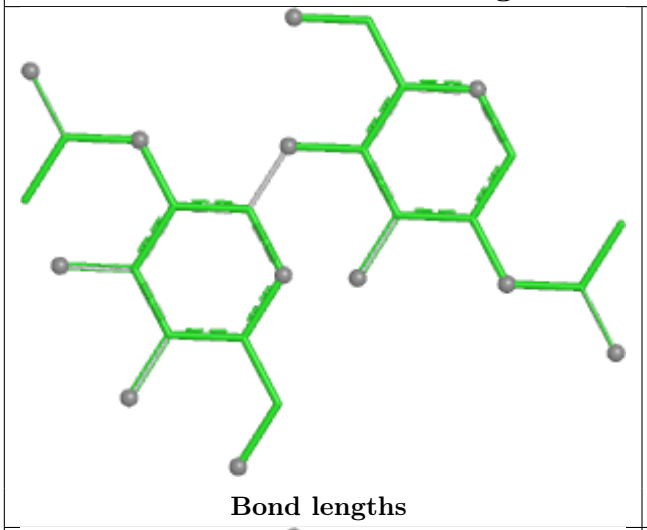
Mol	Chain	Res	Type	Atoms
3	u	1	NAG	C4-C5-C6-O6

There are no ring outliers.

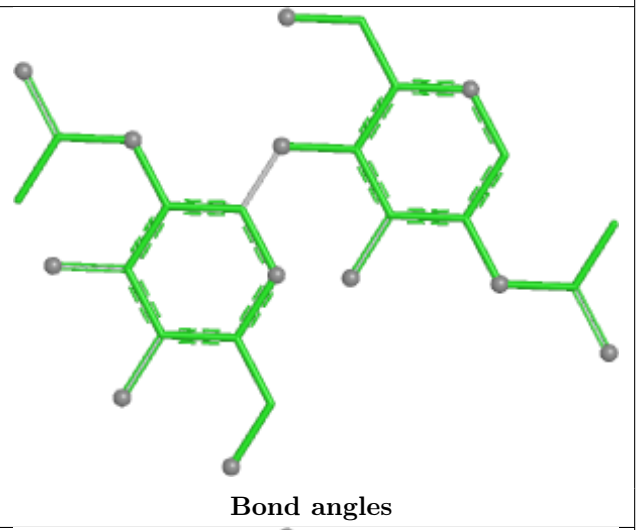
No monomer is involved in short contacts.

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

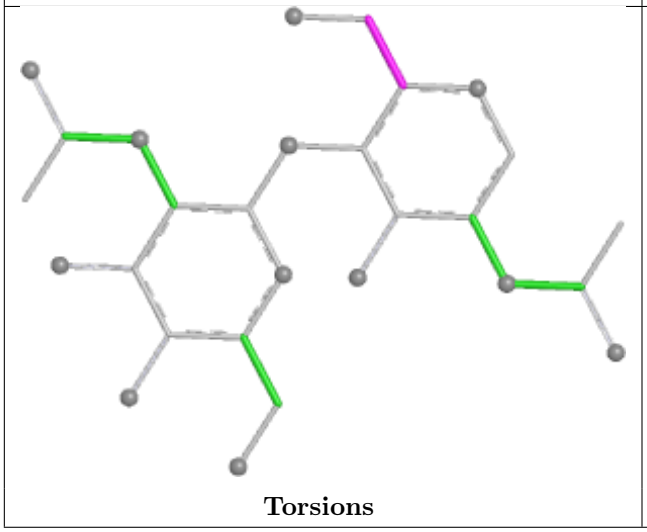
Oligosaccharide Chain G



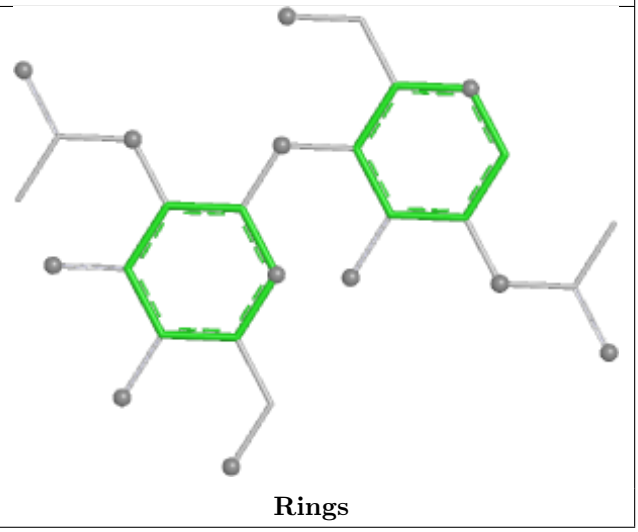
Bond lengths



Bond angles

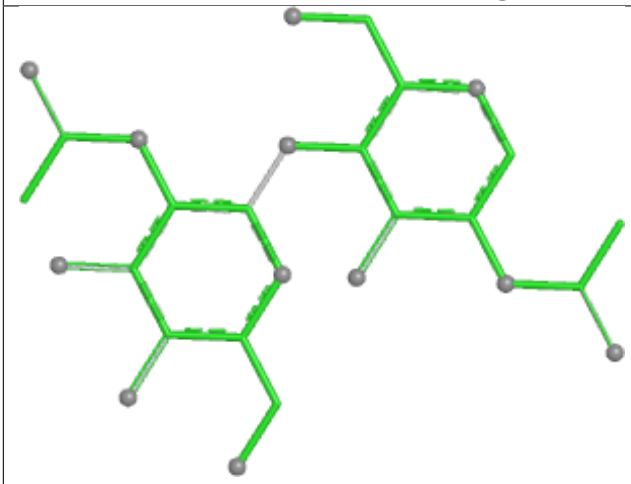


Torsions

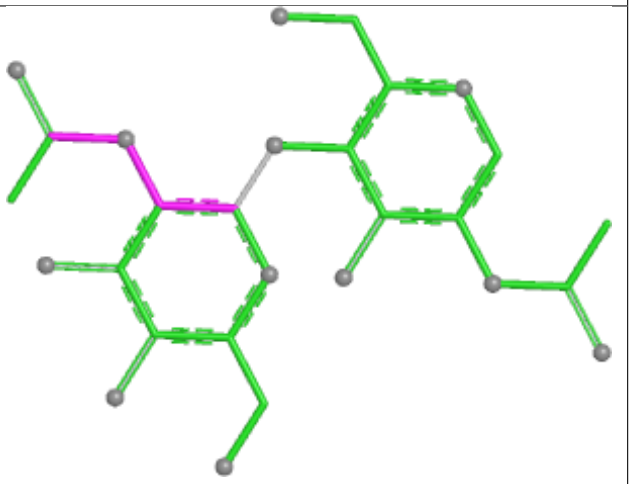


Rings

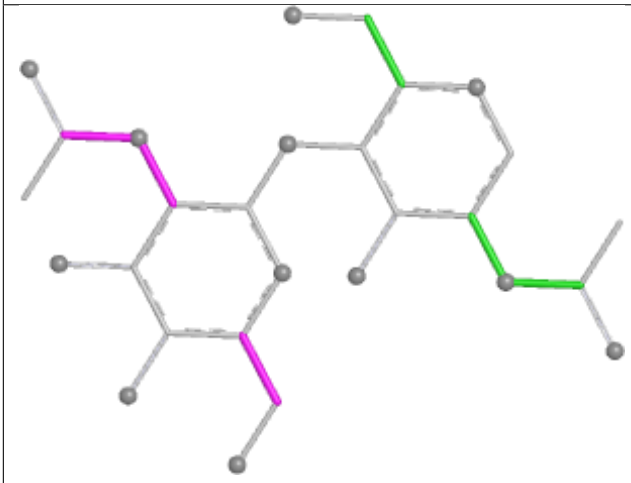
Oligosaccharide Chain H



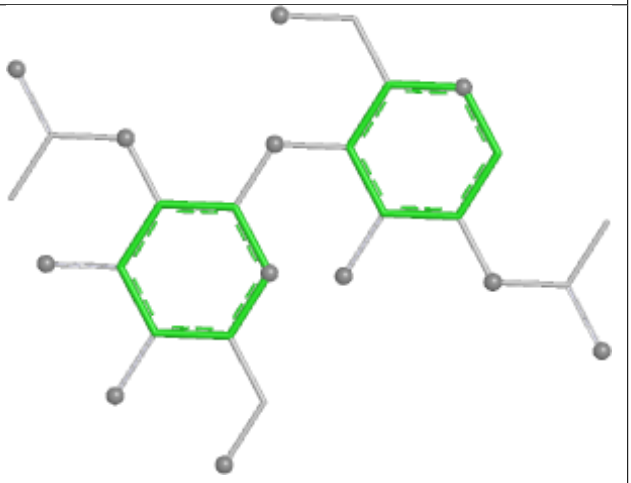
Bond lengths



Bond angles

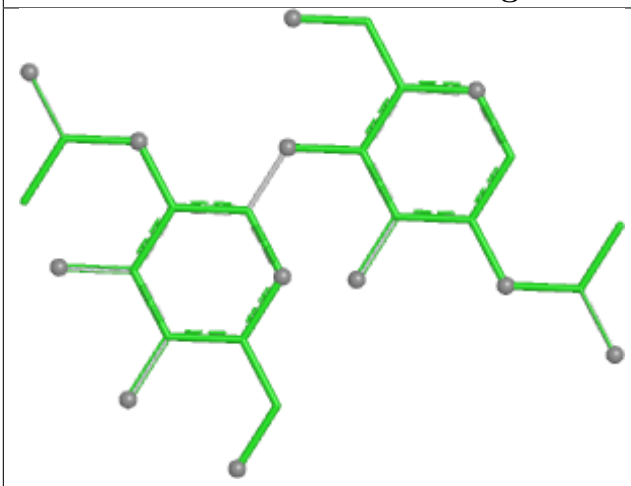


Torsions

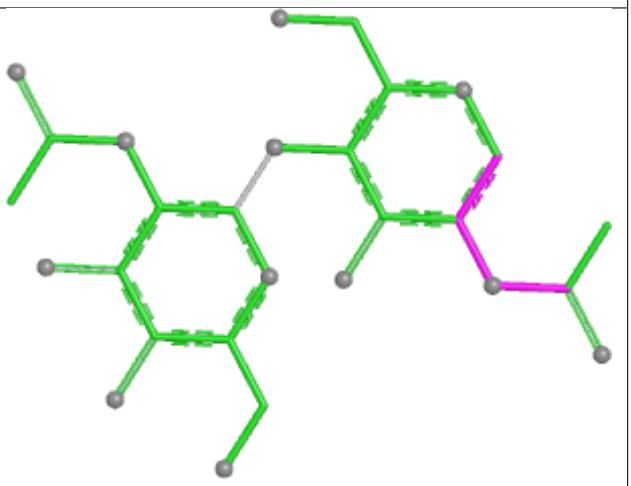


Rings

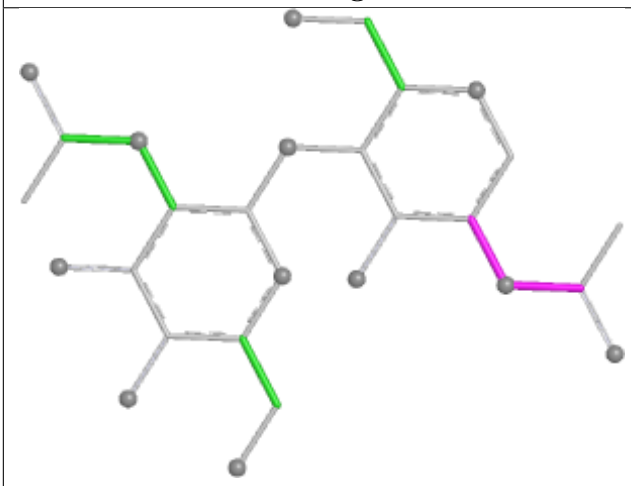
Oligosaccharide Chain I



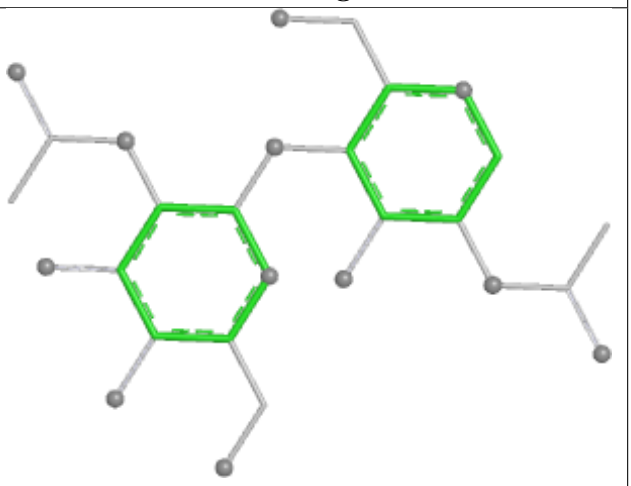
Bond lengths



Bond angles

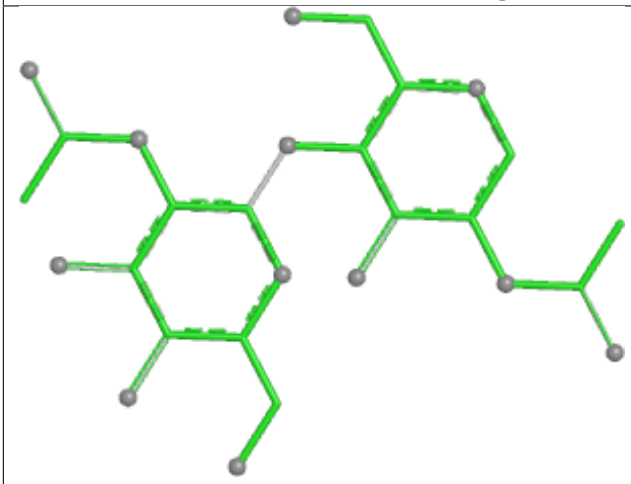


Torsions

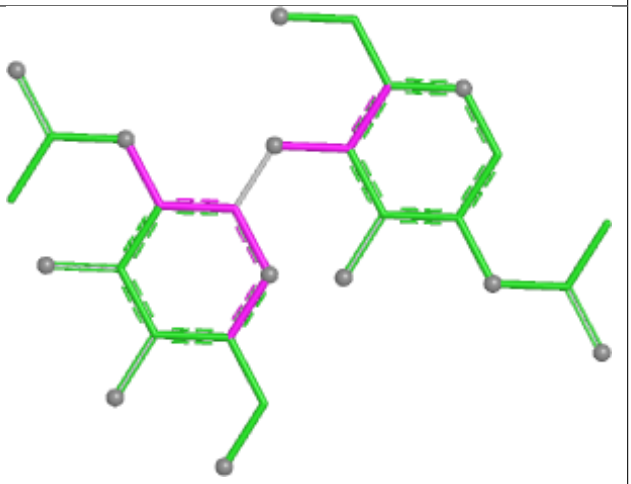


Rings

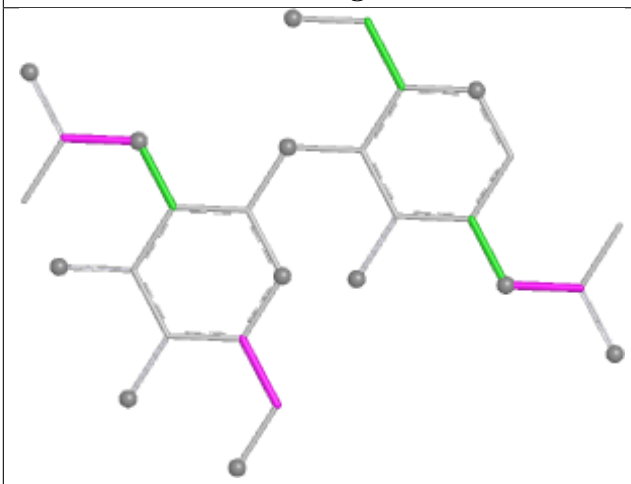
Oligosaccharide Chain K



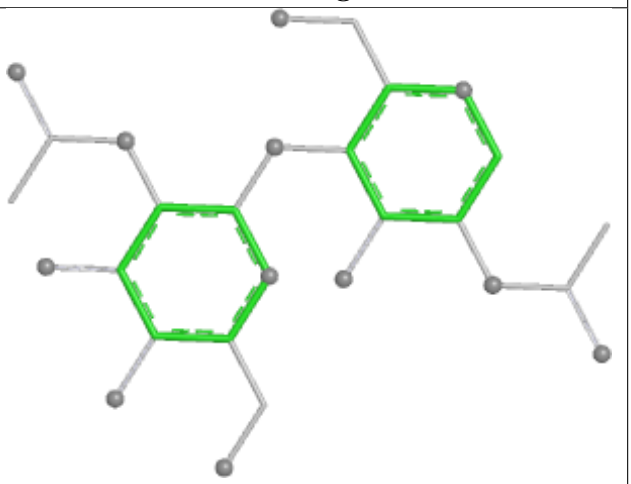
Bond lengths



Bond angles

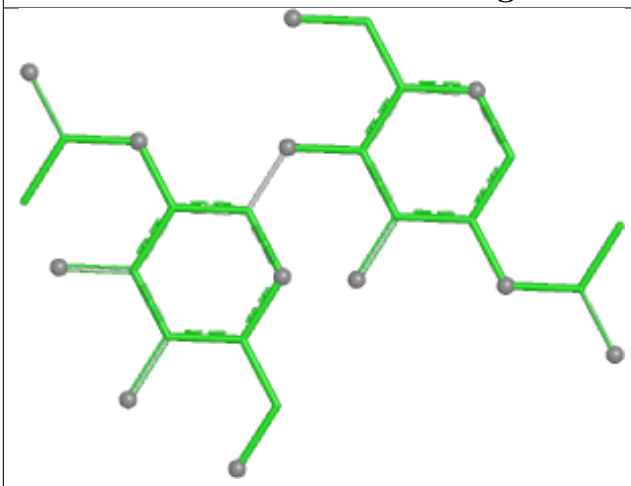


Torsions

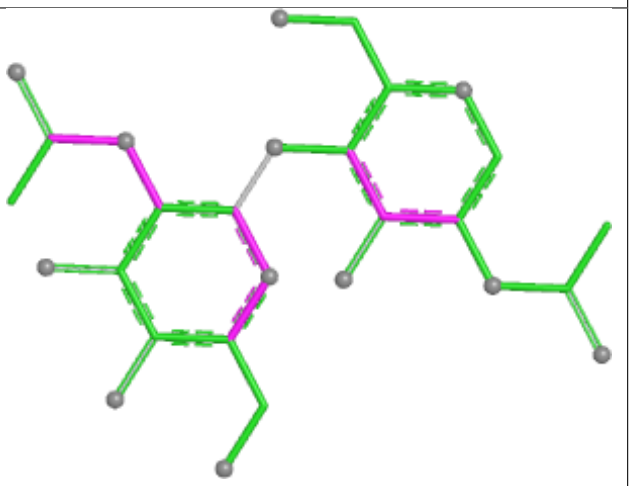


Rings

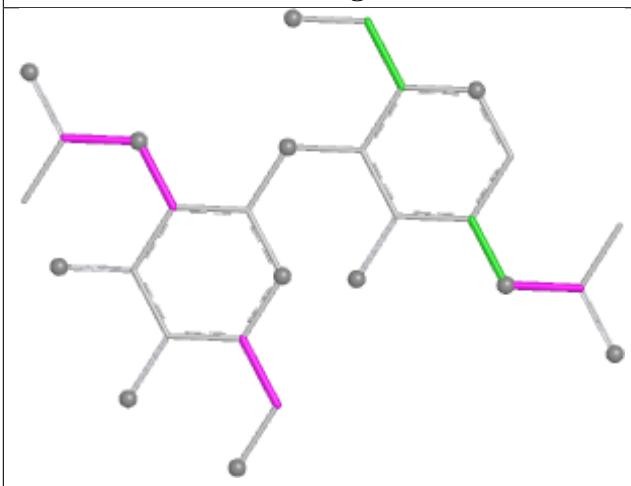
Oligosaccharide Chain L



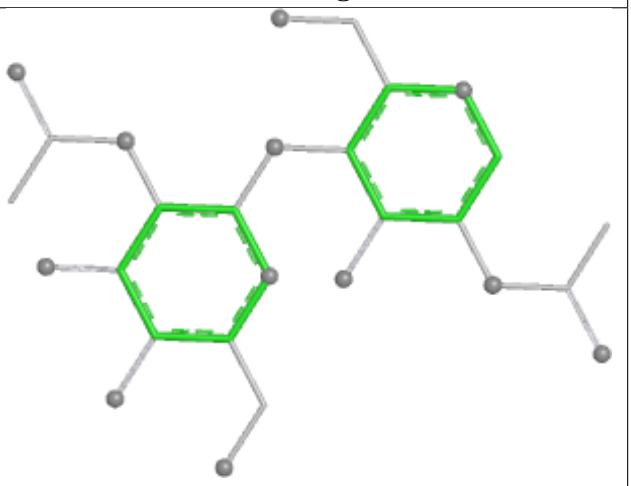
Bond lengths



Bond angles

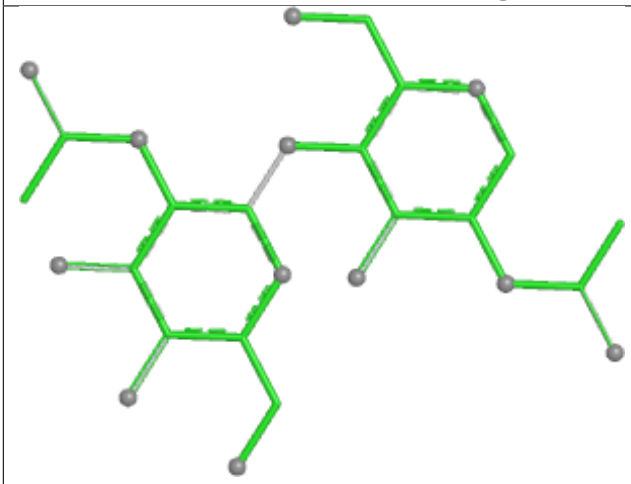


Torsions

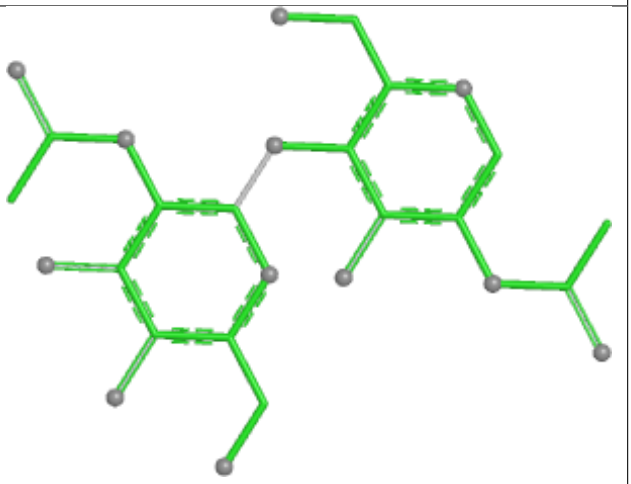


Rings

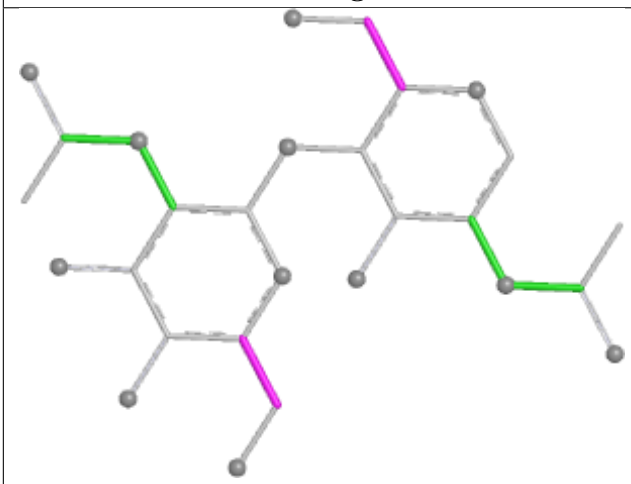
Oligosaccharide Chain O



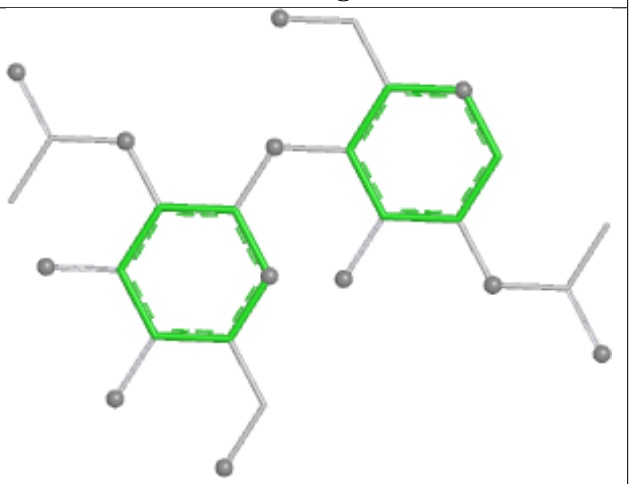
Bond lengths



Bond angles

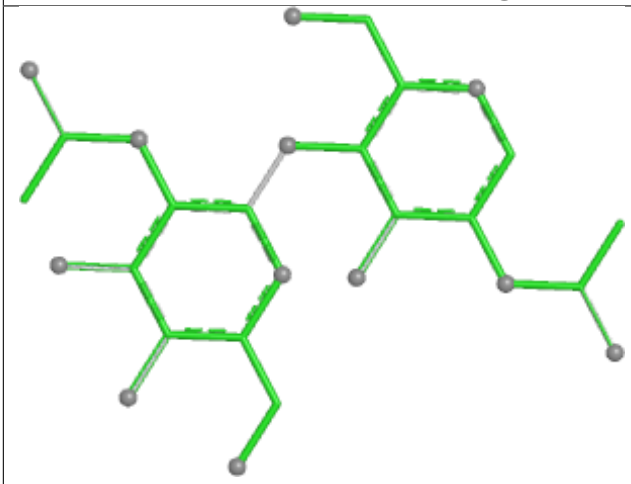


Torsions

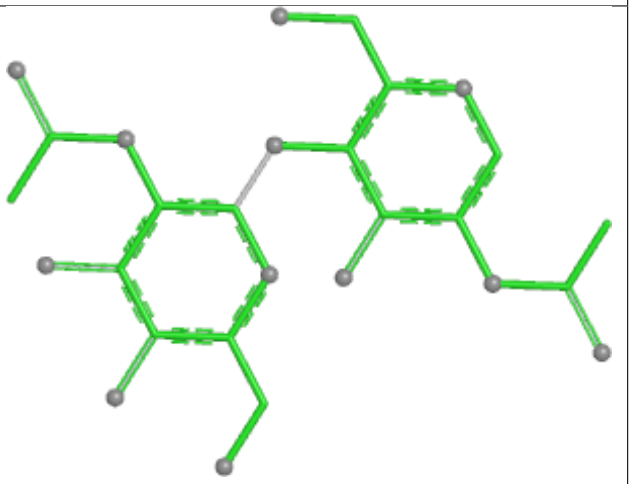


Rings

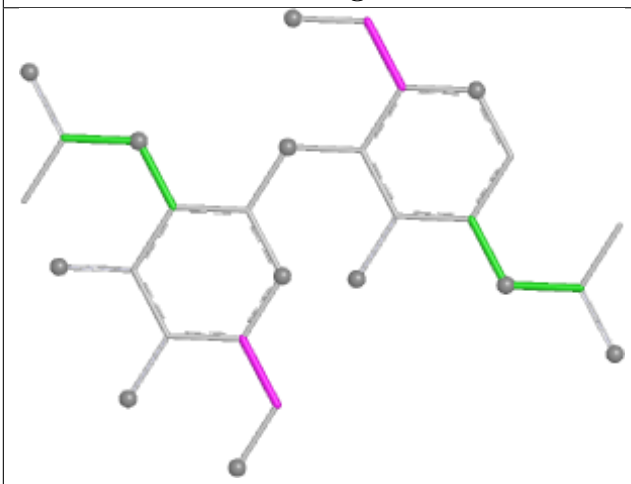
Oligosaccharide Chain P



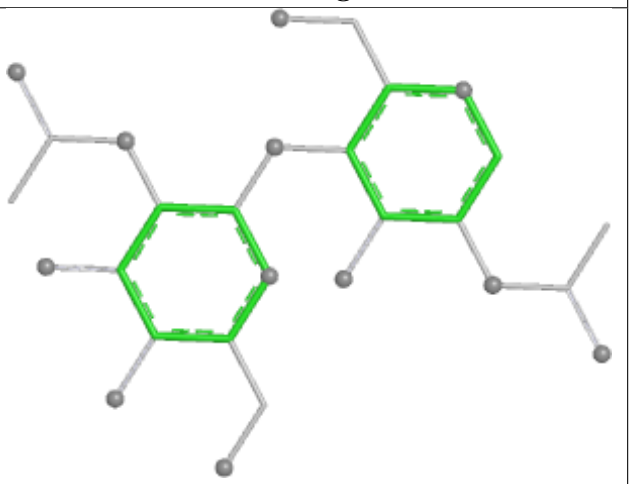
Bond lengths



Bond angles

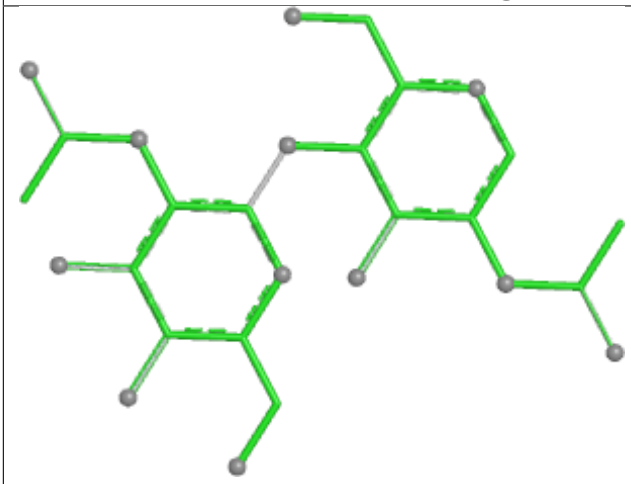


Torsions

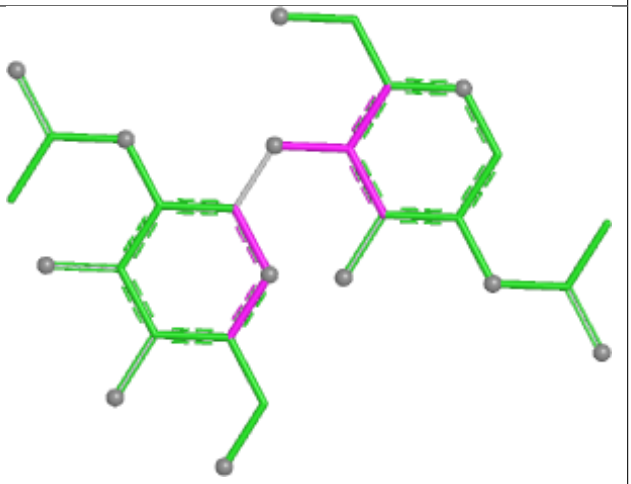


Rings

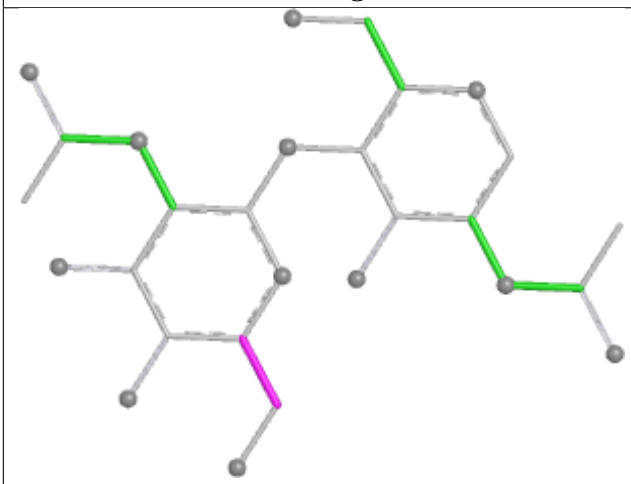
Oligosaccharide Chain S



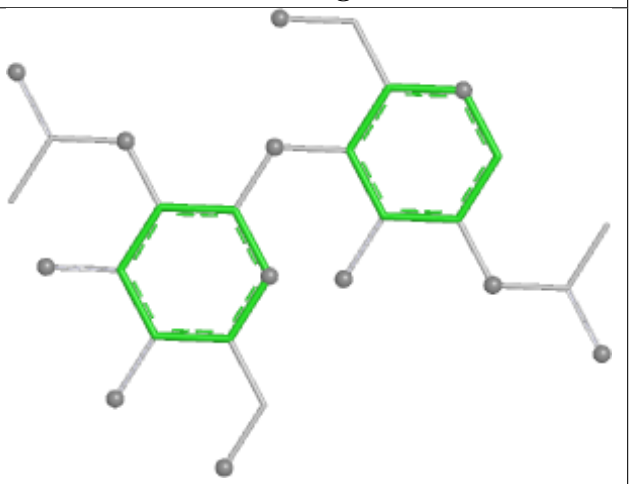
Bond lengths



Bond angles

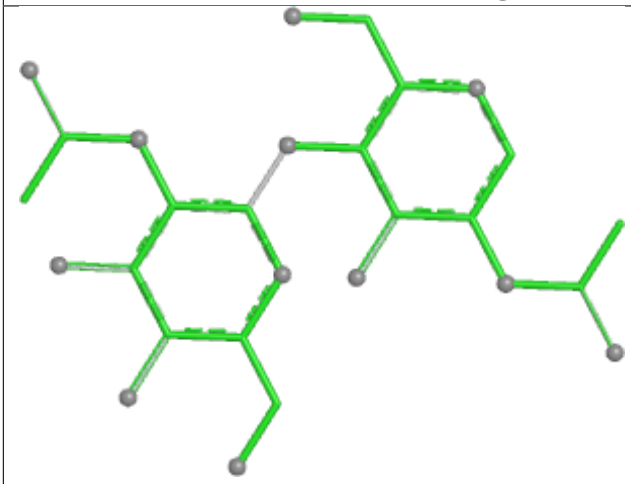


Torsions

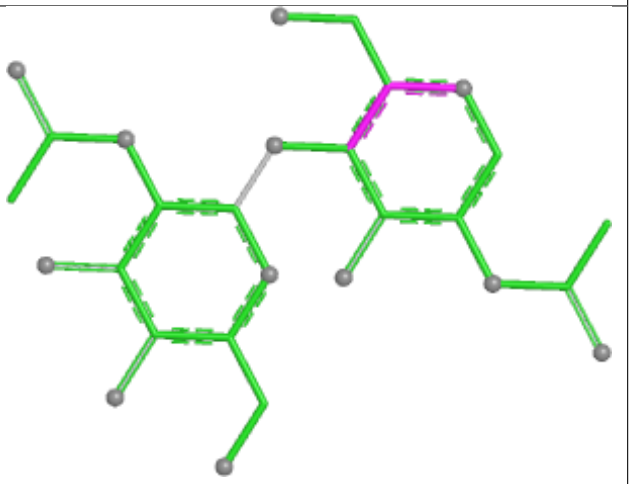


Rings

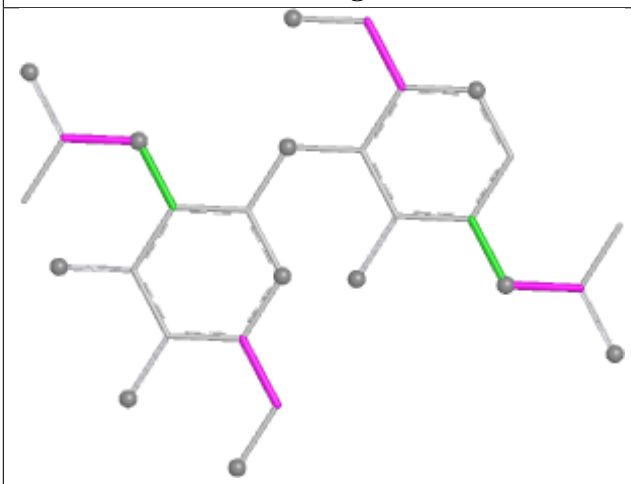
Oligosaccharide Chain U



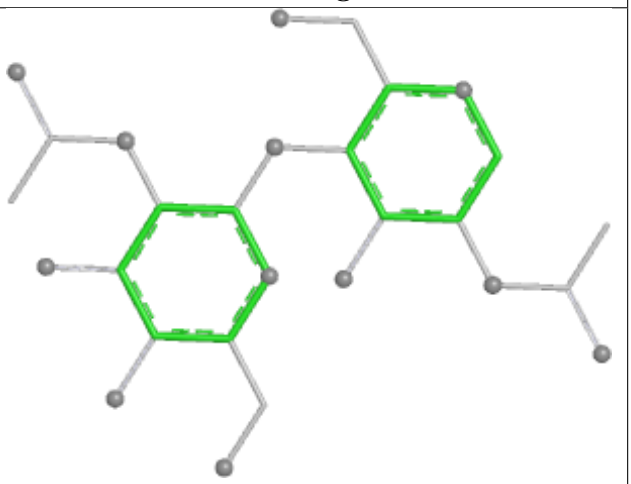
Bond lengths



Bond angles

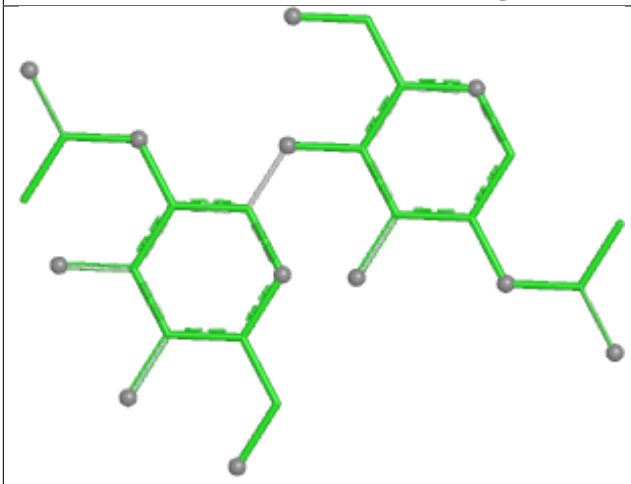


Torsions



Rings

Oligosaccharide Chain V



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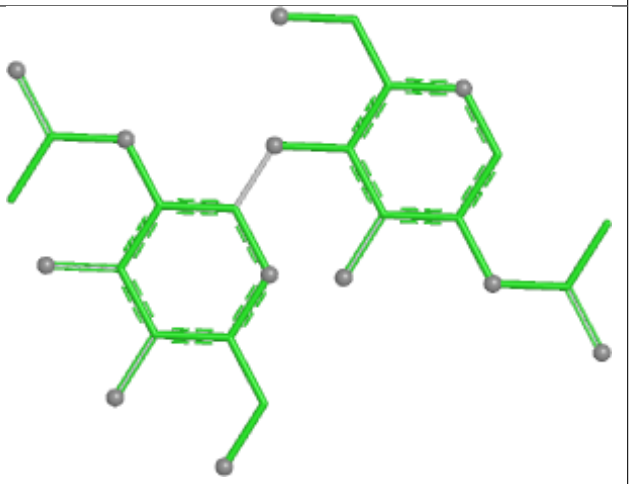

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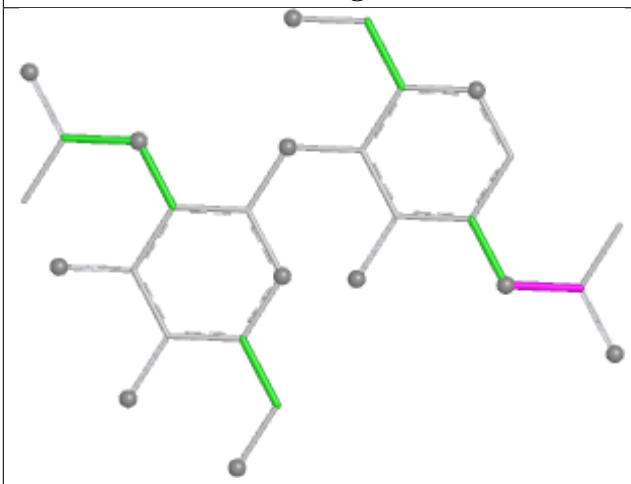

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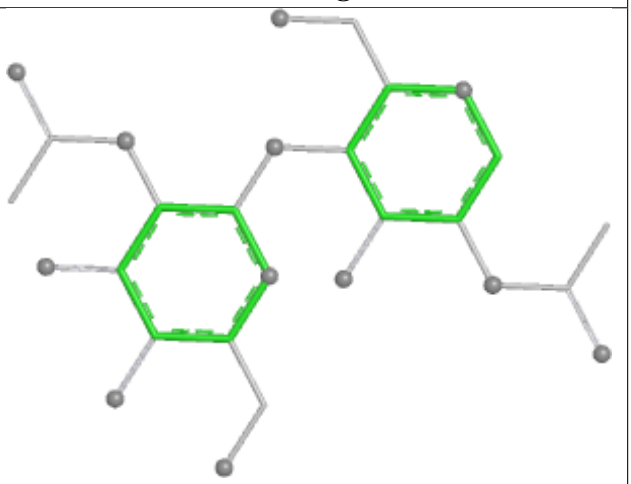
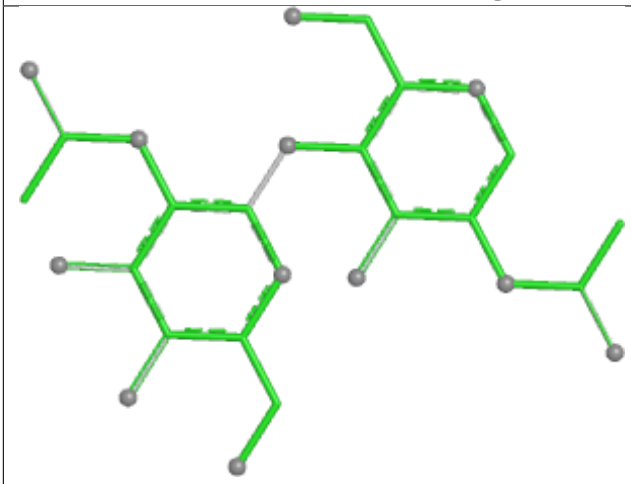
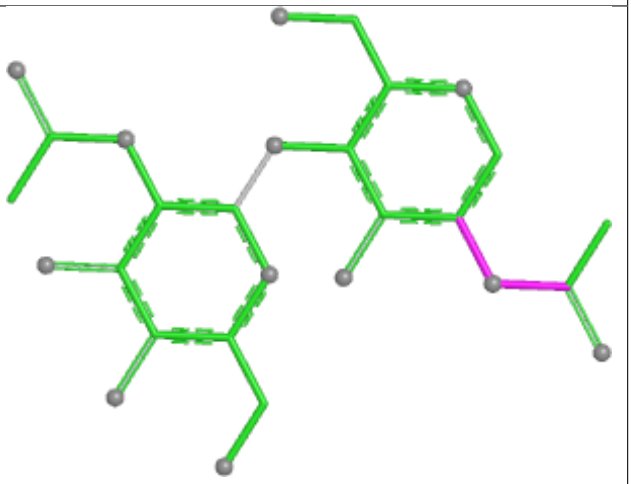


Rings

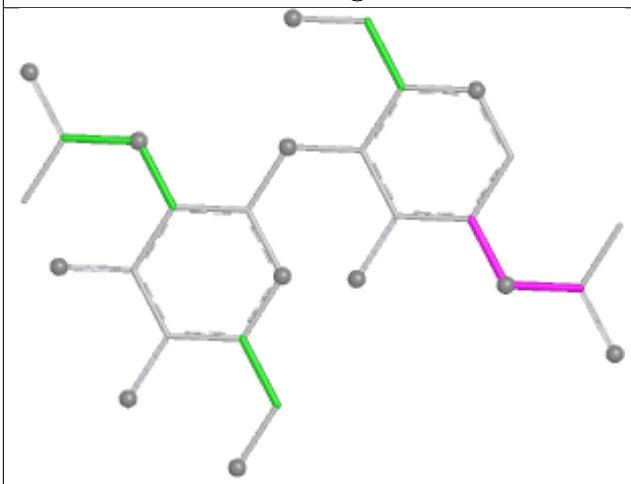
Oligosaccharide Chain W



Bond lengths



Bond angles



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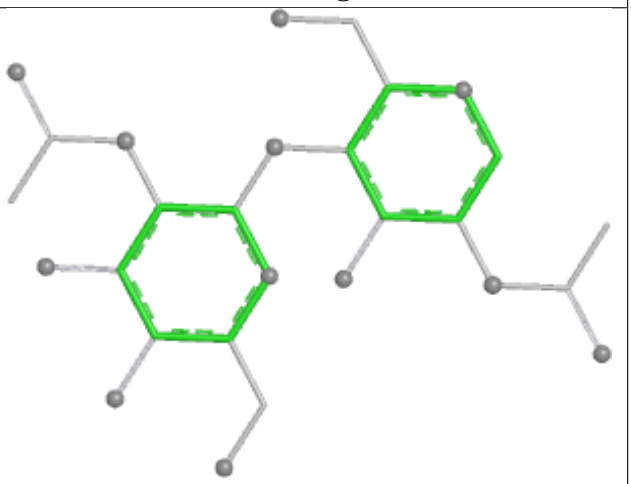
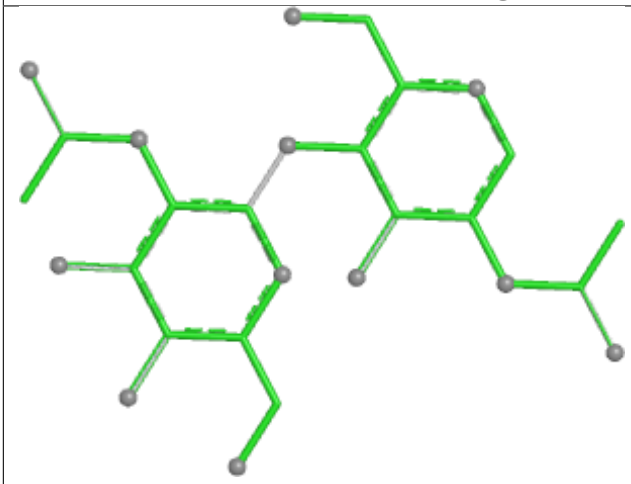


Rings

Oligosaccharide Chain X



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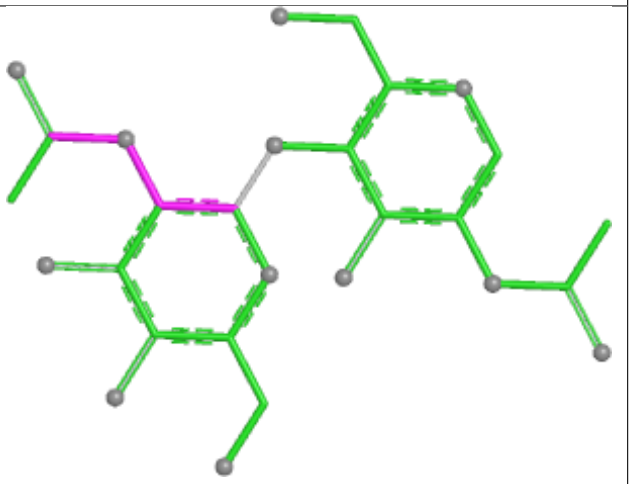

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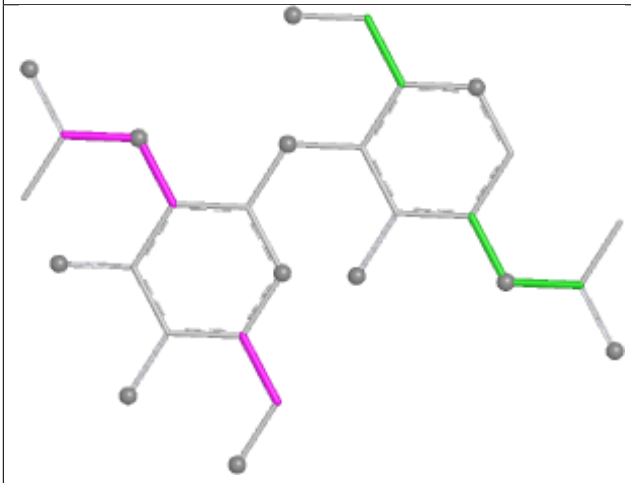

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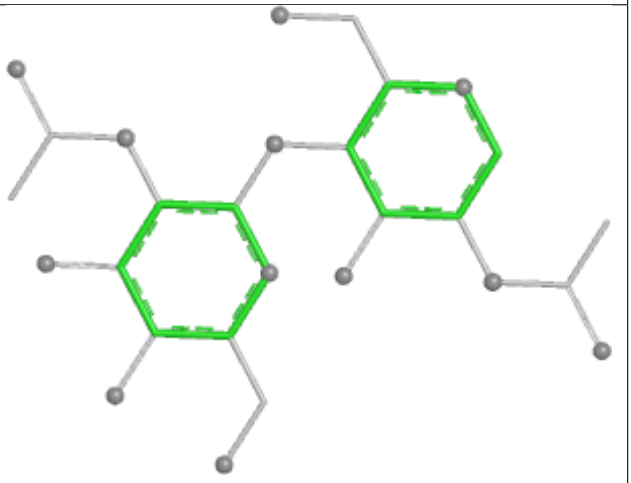
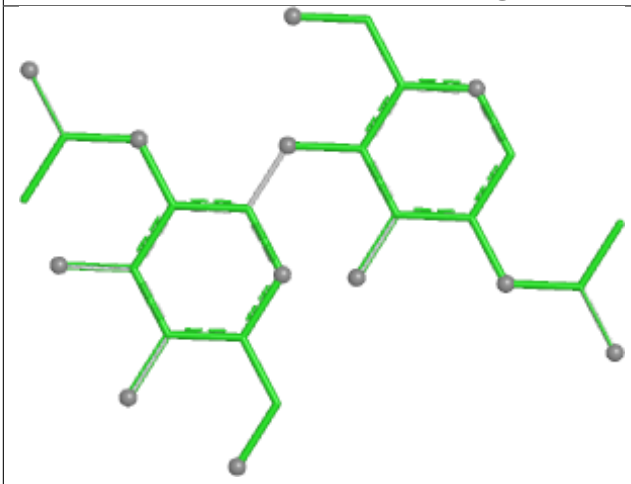


Rings

Oligosaccharide Chain Y



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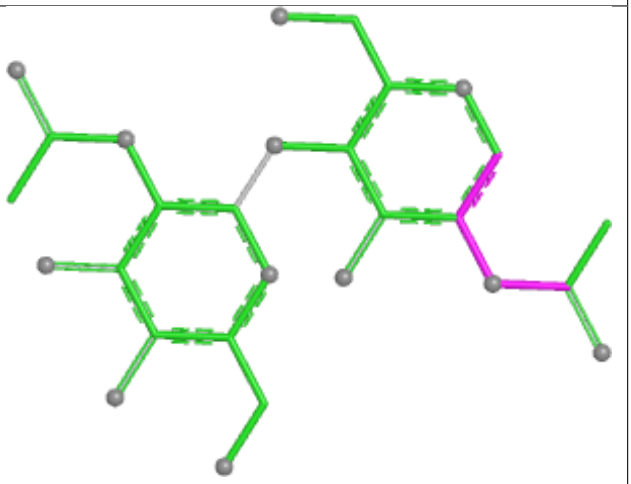
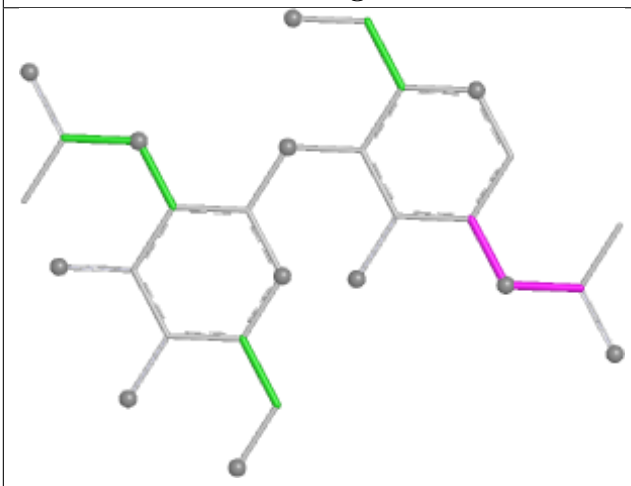


Bond angles



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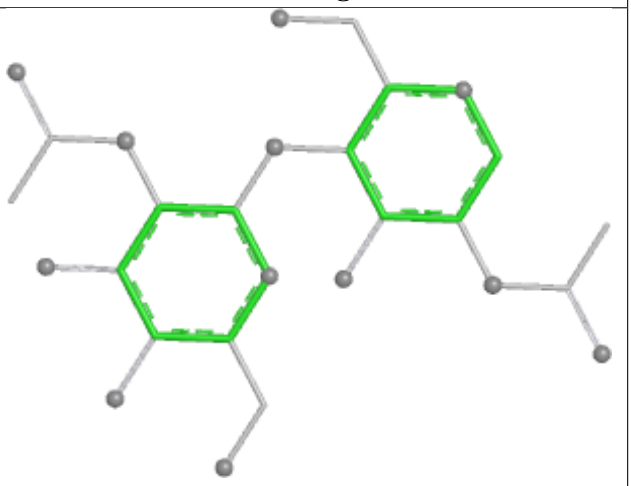
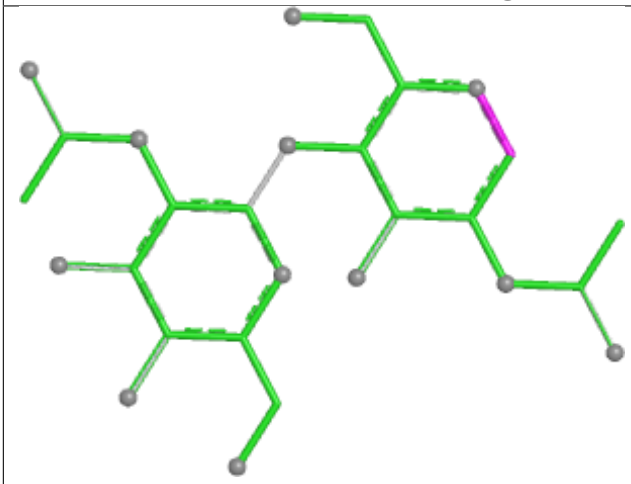


Rings

Oligosaccharide Chain a



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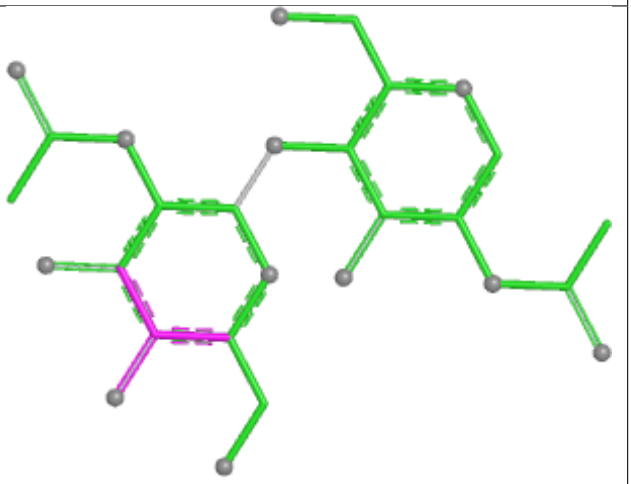

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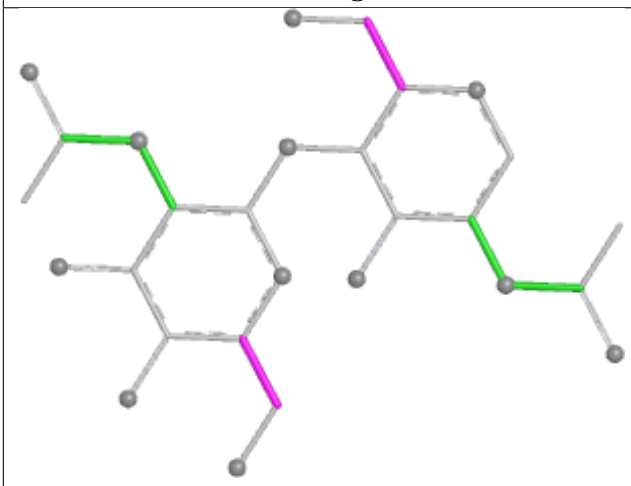

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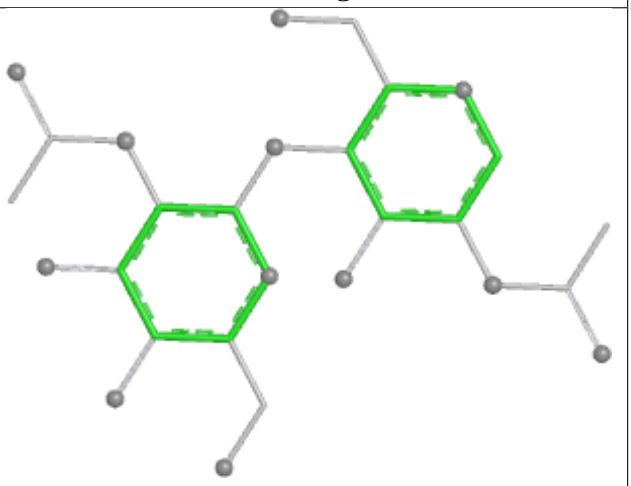
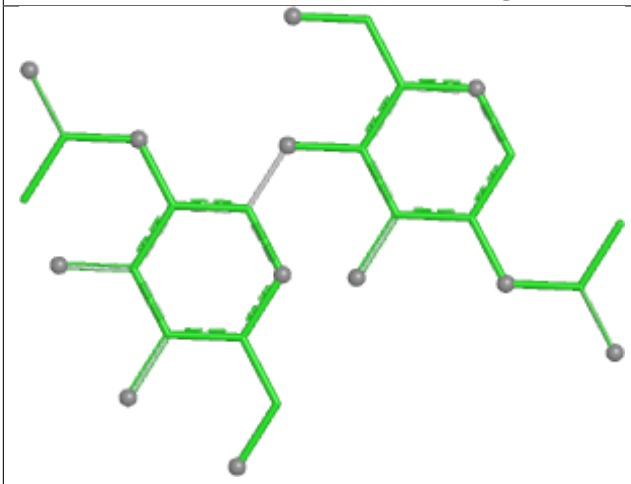


Rings

Oligosaccharide Chain b



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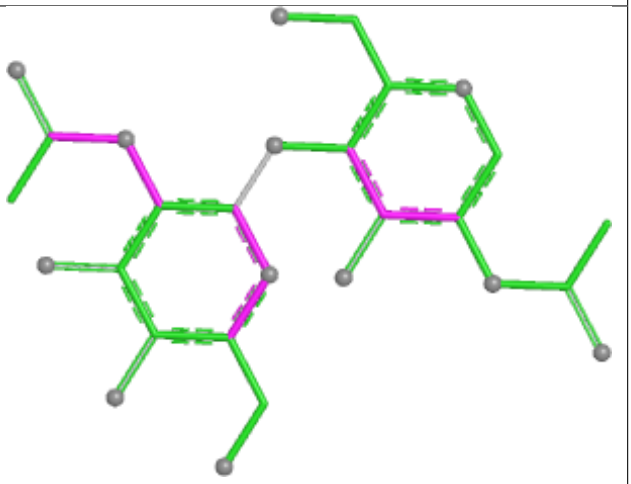
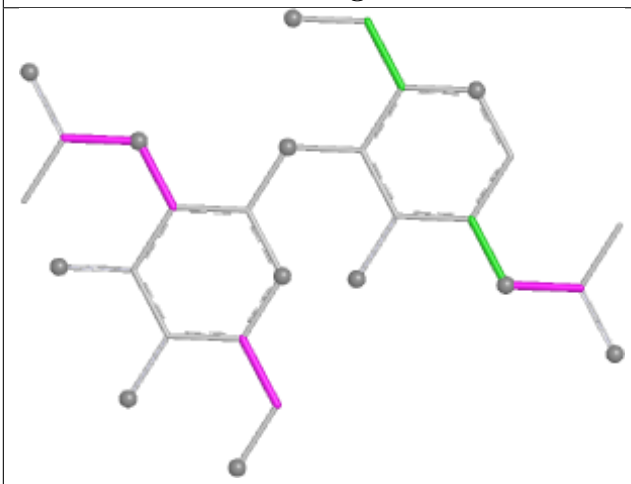


Bond angles



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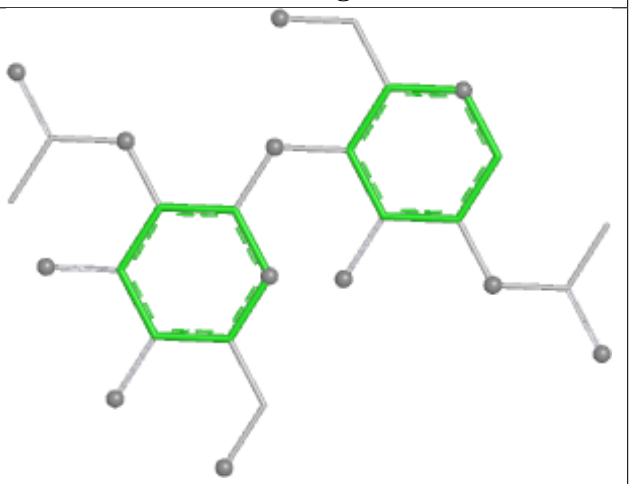
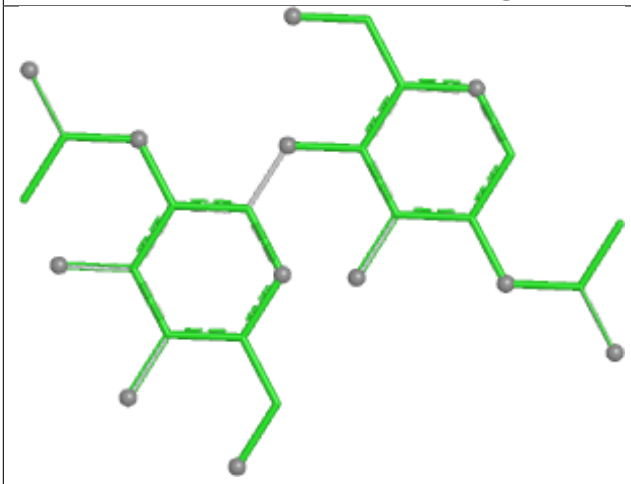


Rings

Oligosaccharide Chain d



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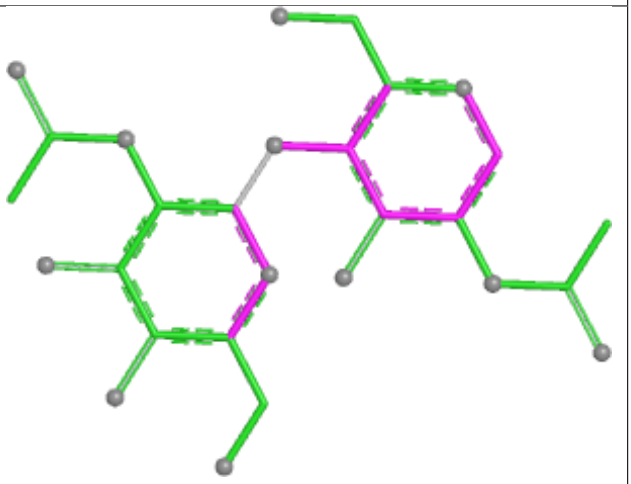
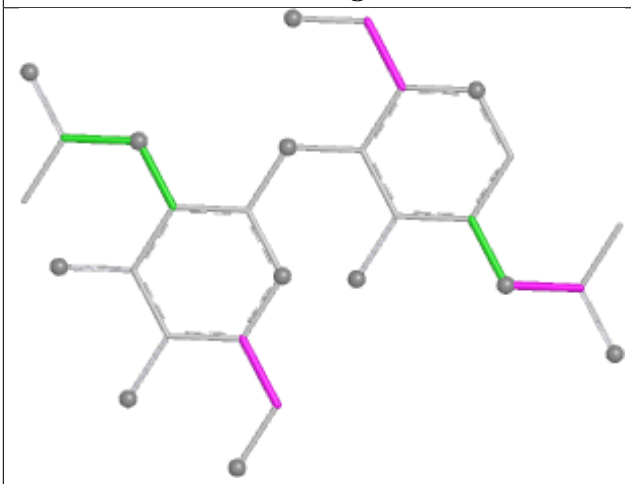


Bond angles



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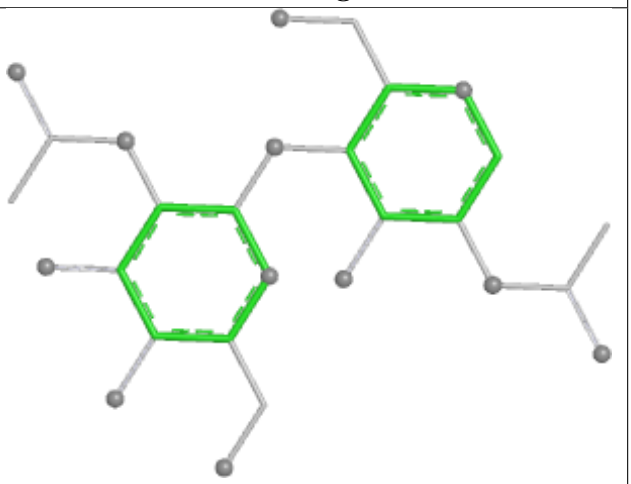
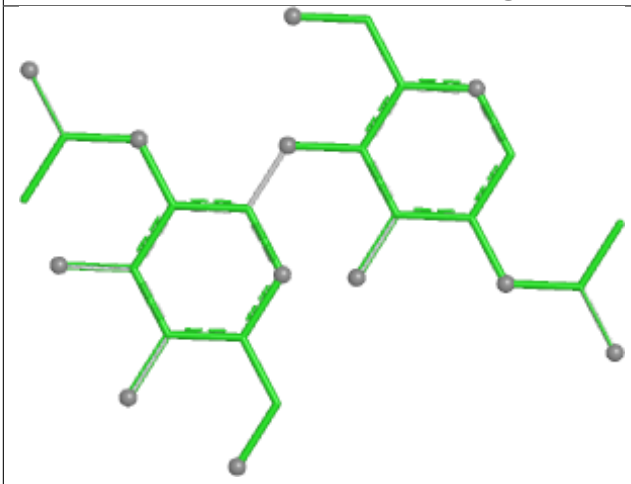


Rings

Oligosaccharide Chain e



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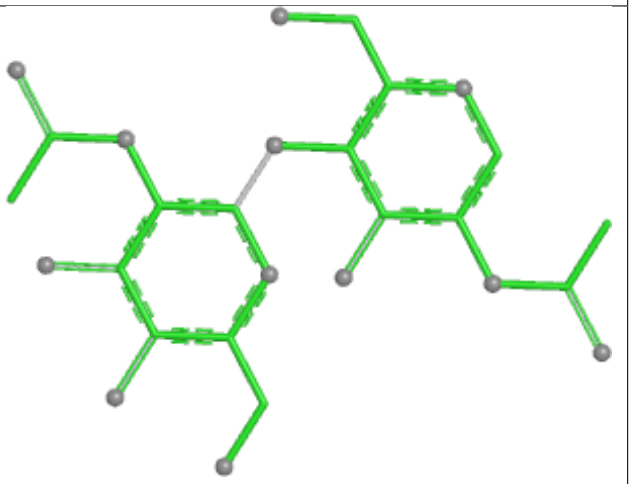
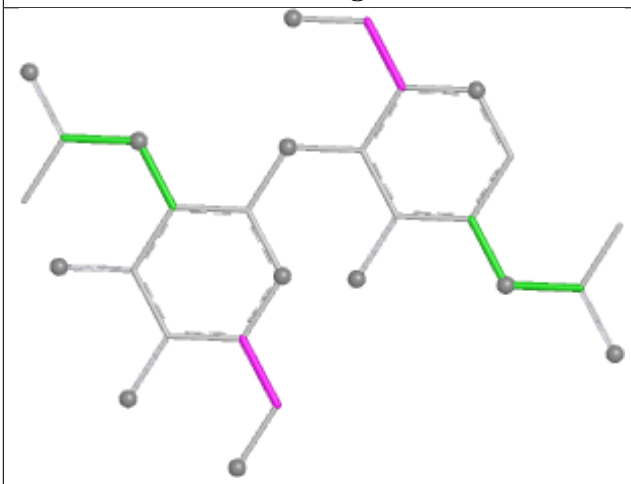
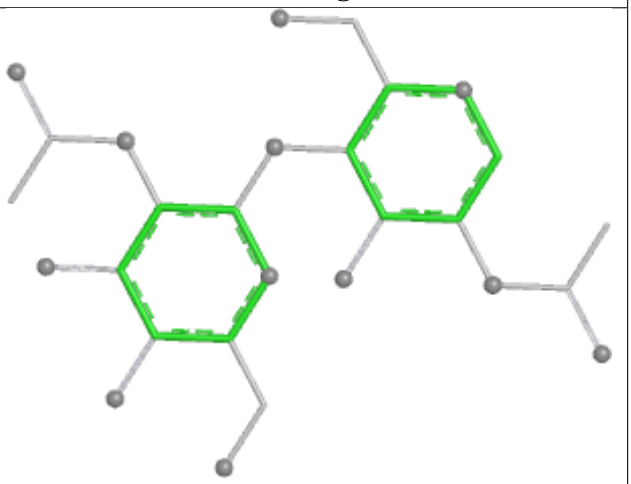


Bond angles

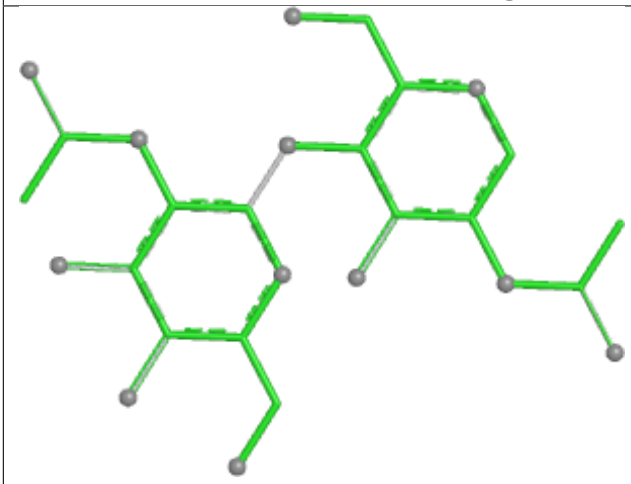


Torsions



Rings

Oligosaccharide Chain f



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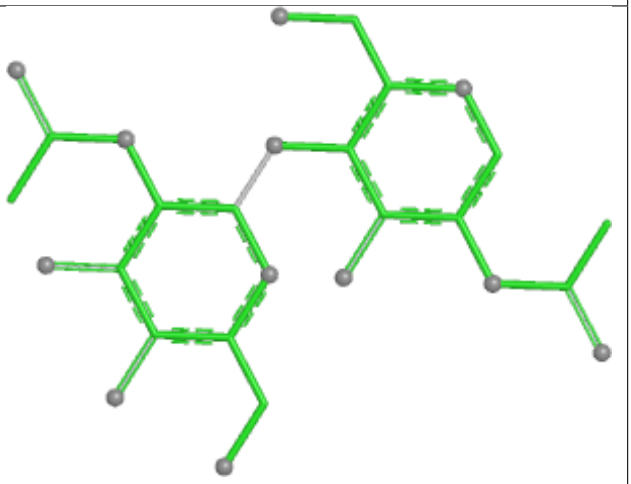
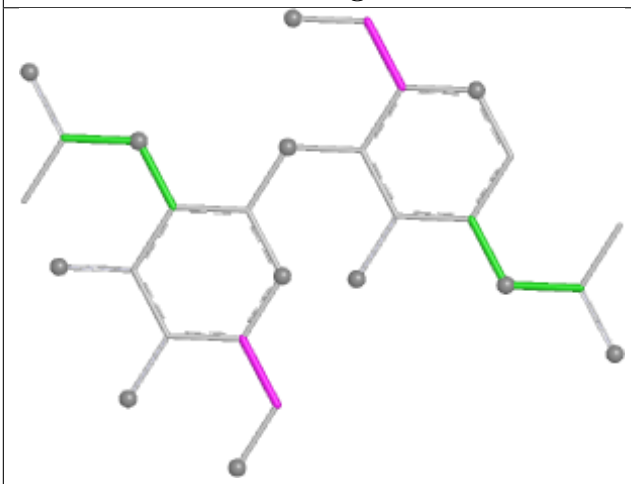


Bond angles



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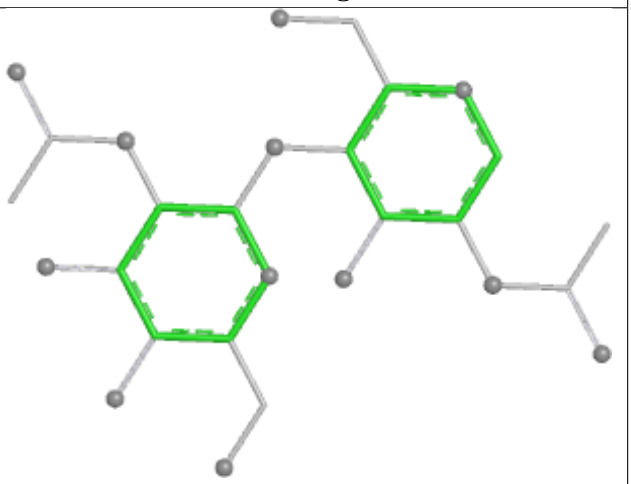
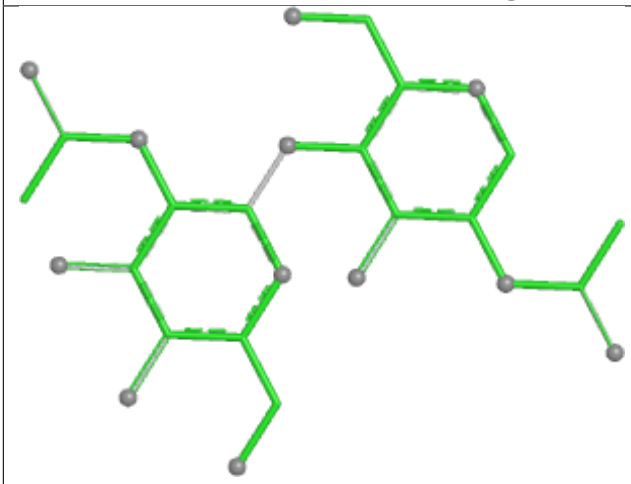


Rings

Oligosaccharide Chain i



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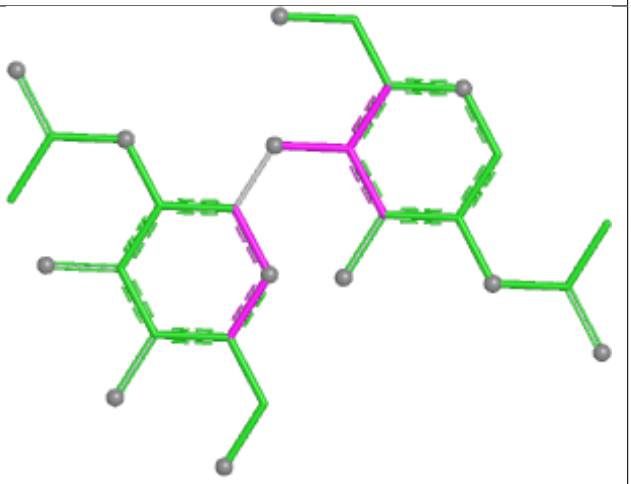
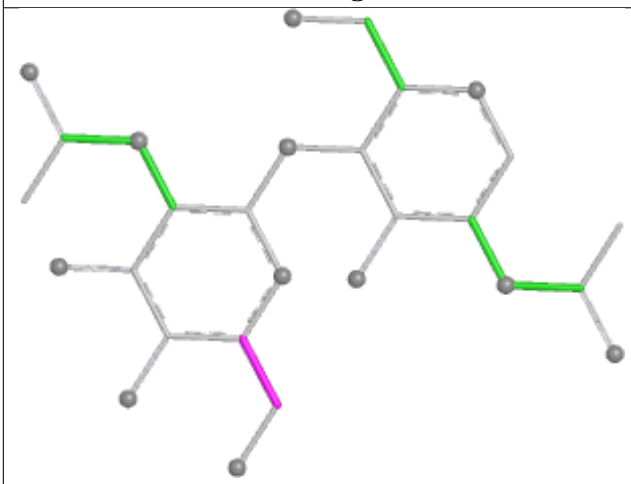


Bond angles



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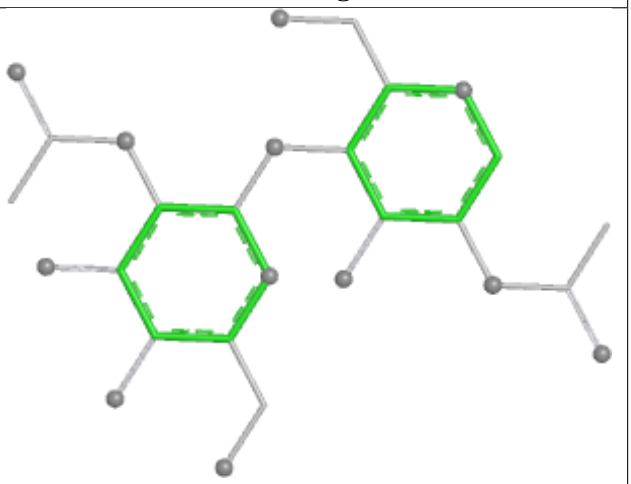
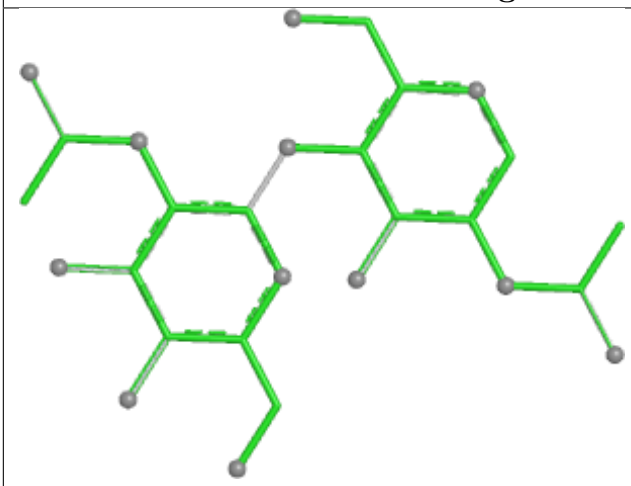


Rings

Oligosaccharide Chain k



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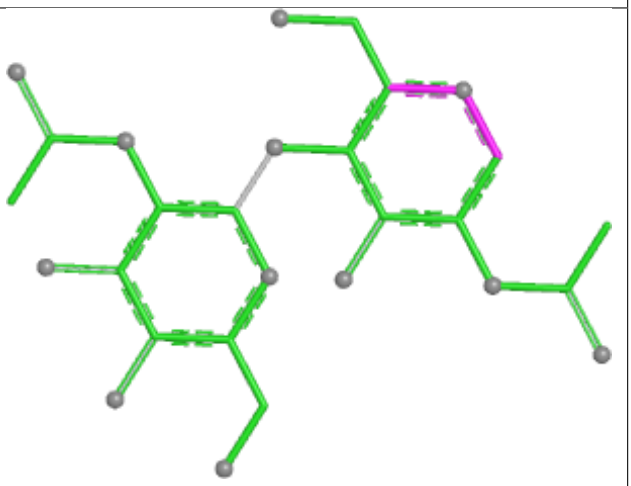
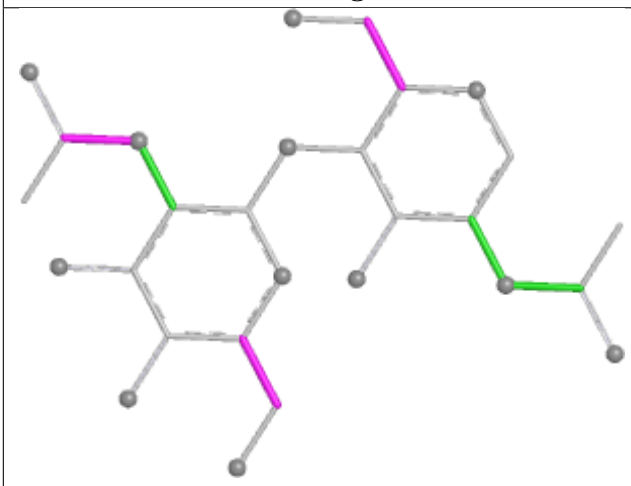


Bond angles



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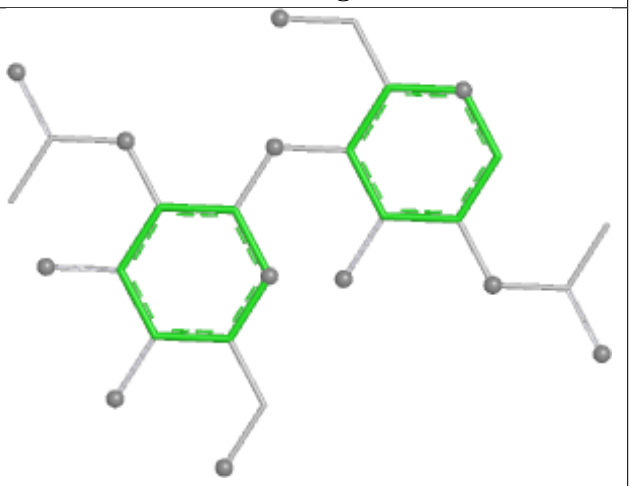
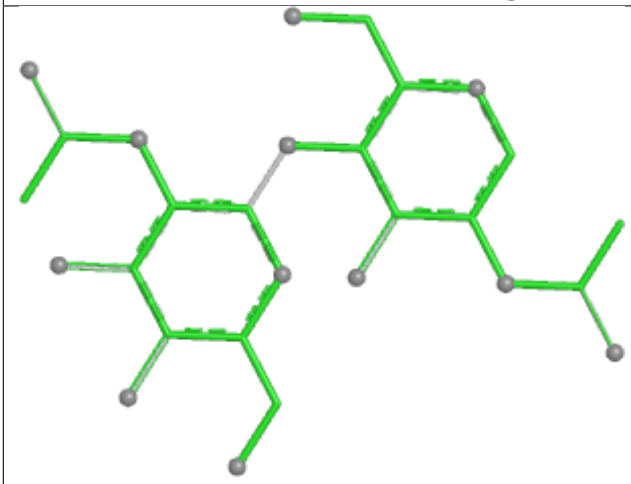
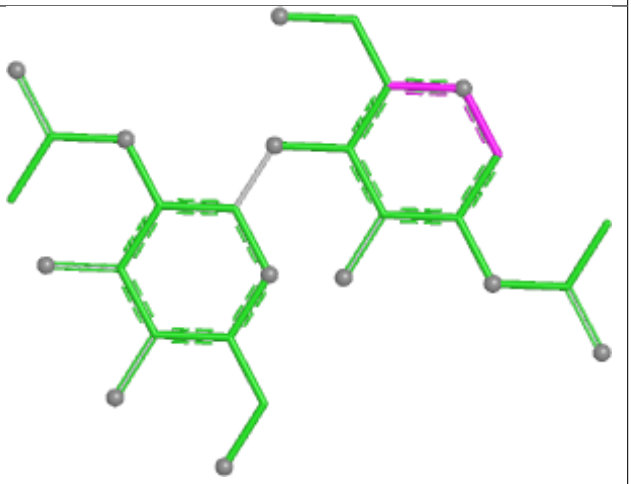


Rings

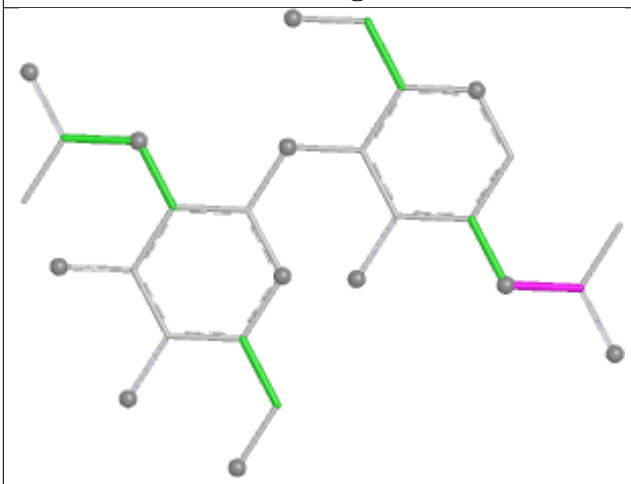
Oligosaccharide Chain l



Bond lengths



Bond angles



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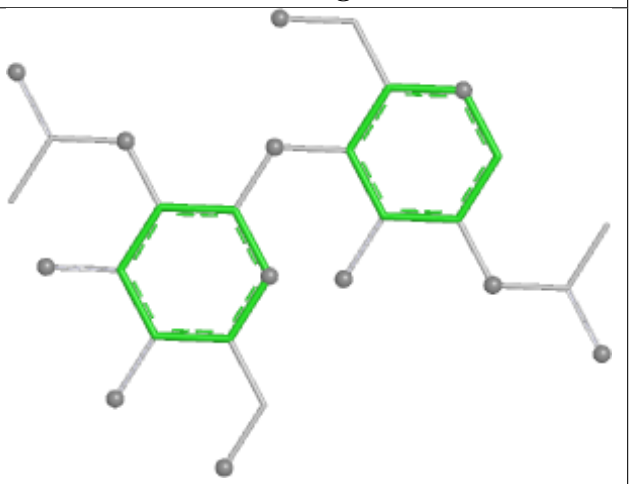
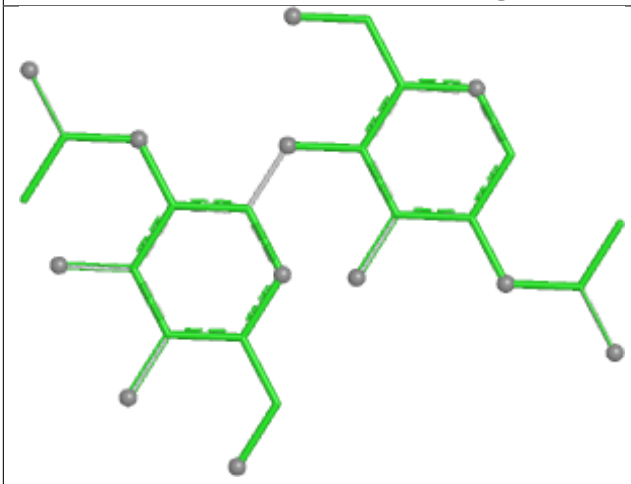
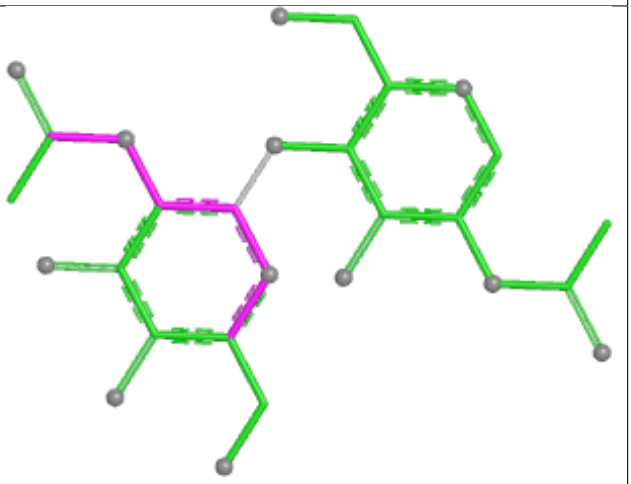


Rings

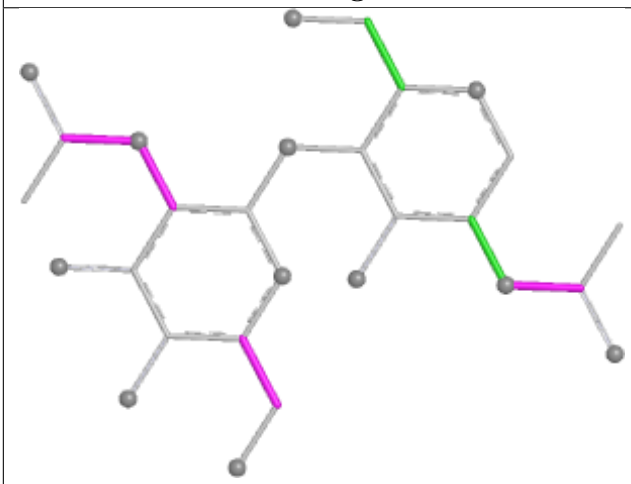
Oligosaccharide Chain m



Bond lengths



Bond angles



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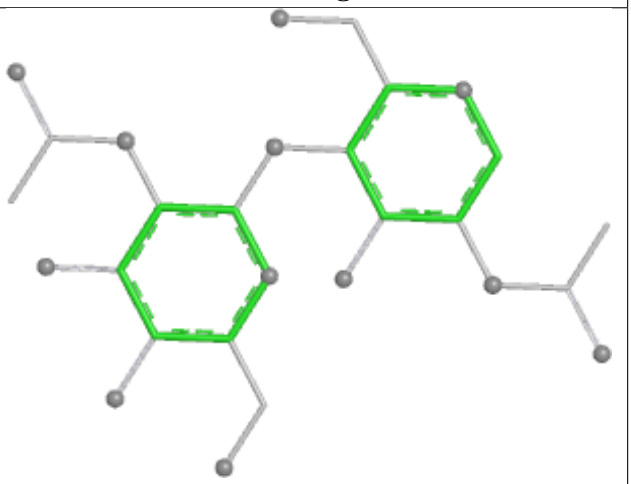
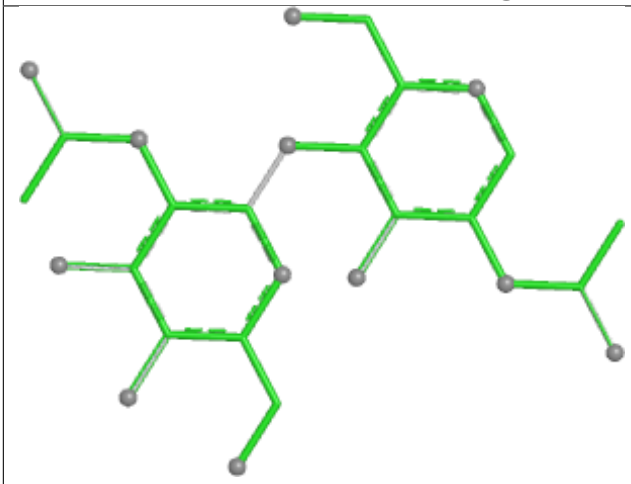
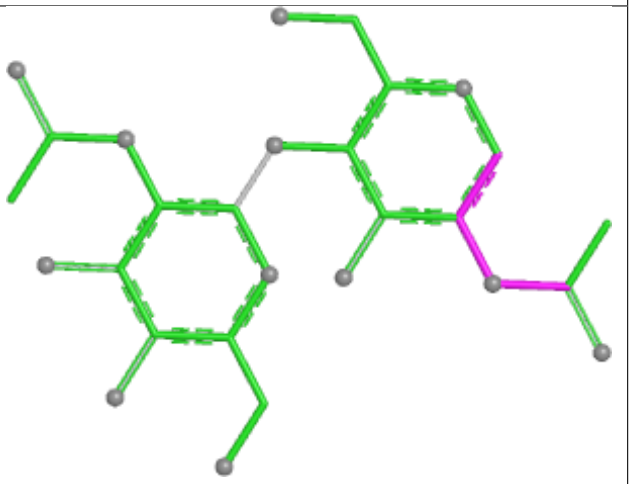


Rings

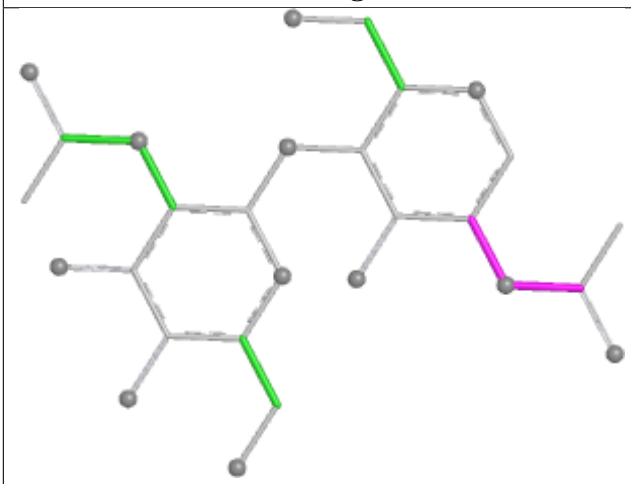
Oligosaccharide Chain n



Bond lengths



Bond angles



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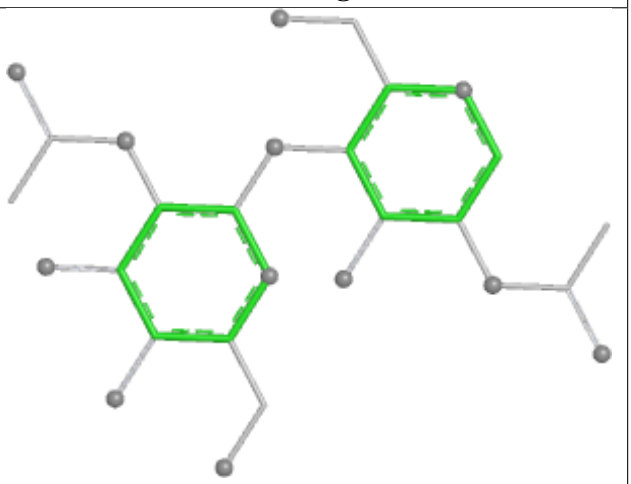
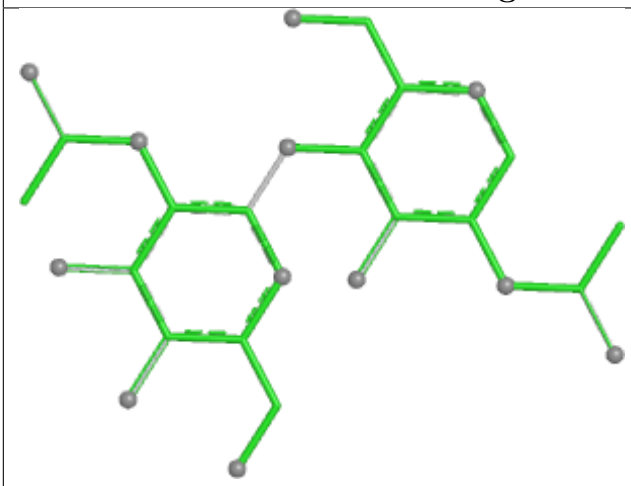
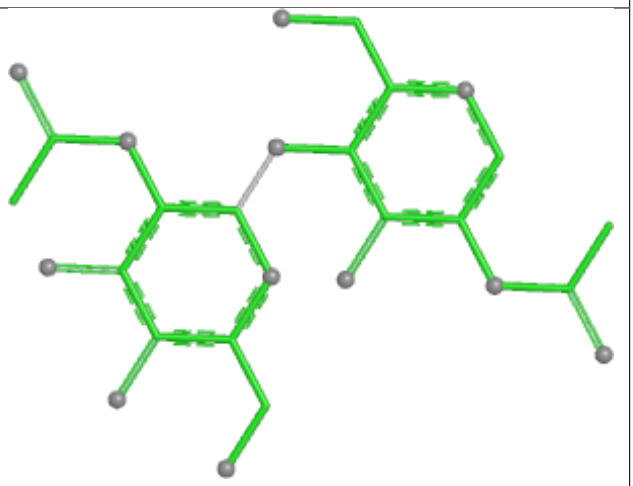


Rings

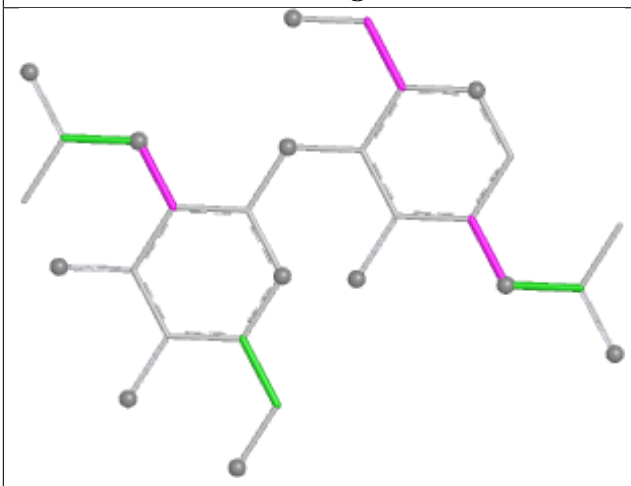
Oligosaccharide Chain o



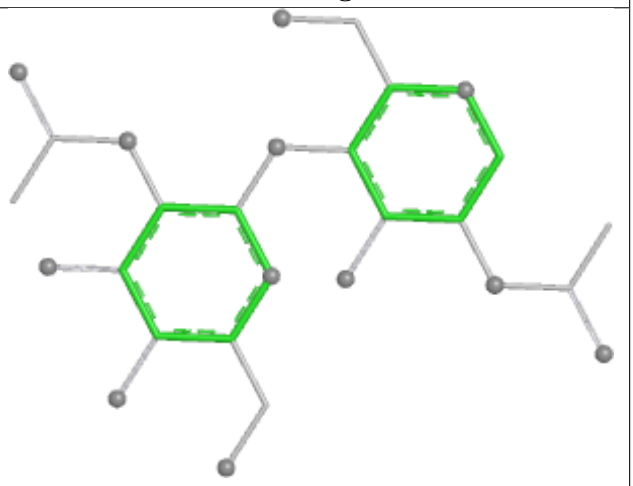
Bond lengths



Bond angles

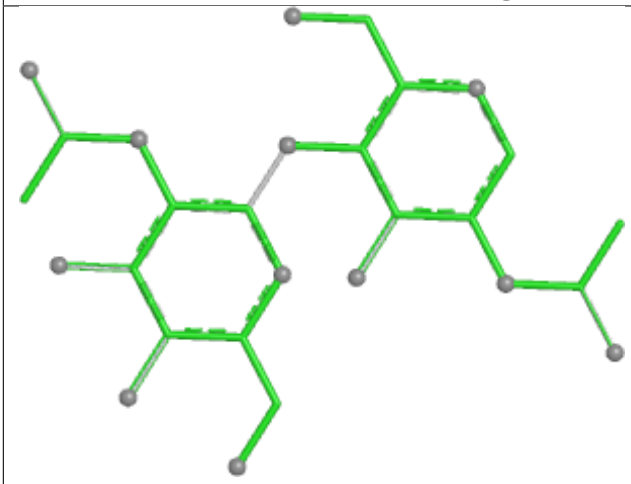


Torsions

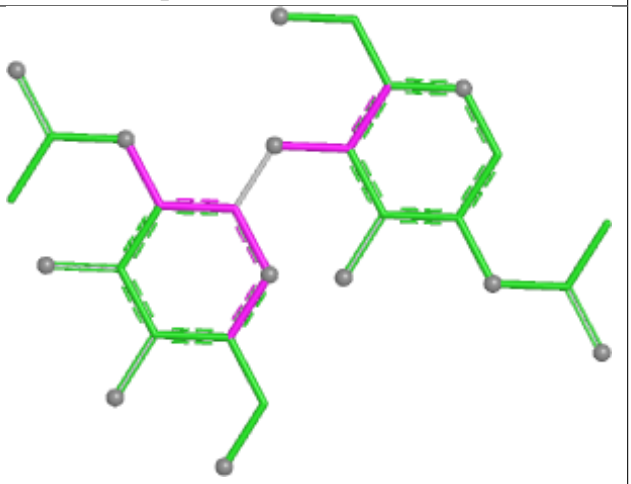


Rings

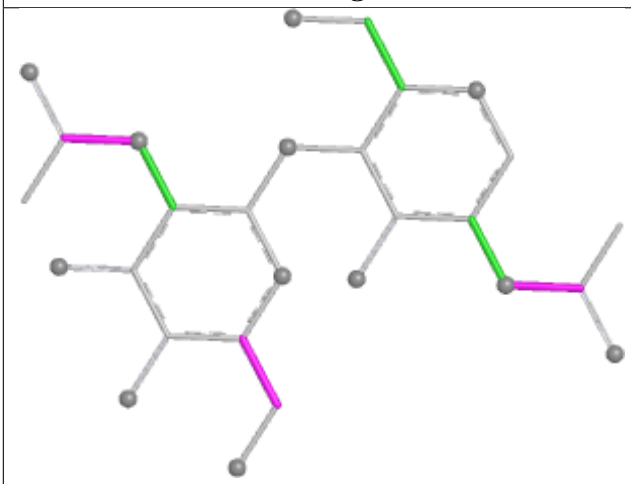
Oligosaccharide Chain p



Bond lengths



Bond angles



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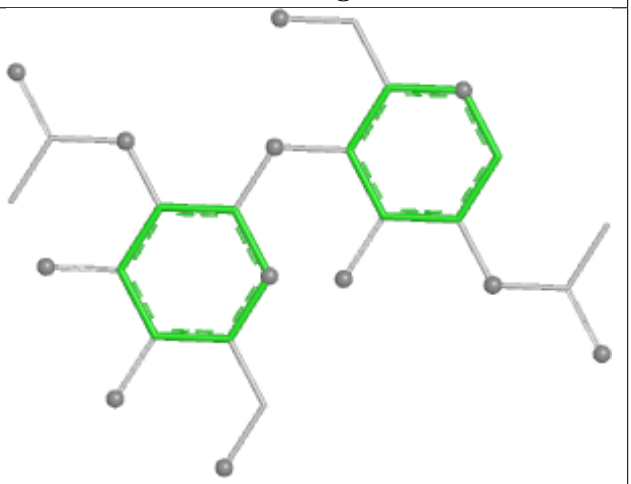
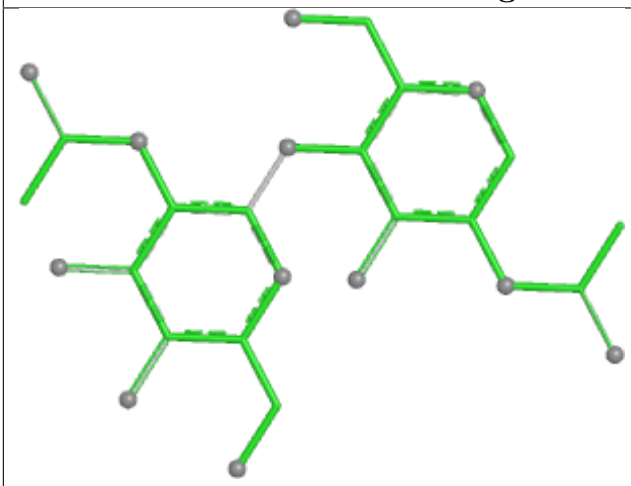


Rings

Oligosaccharide Chain q



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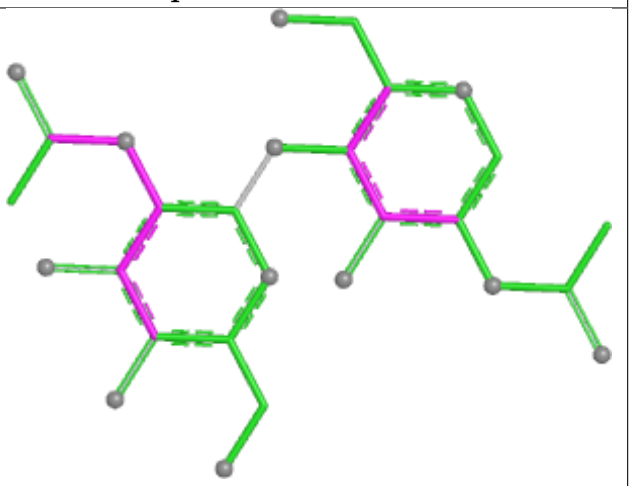

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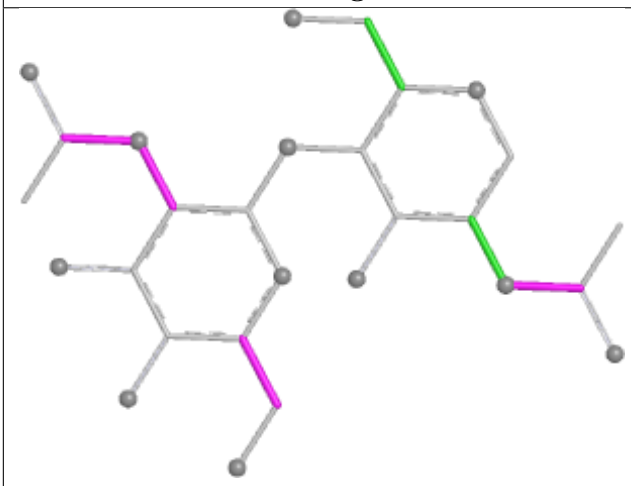

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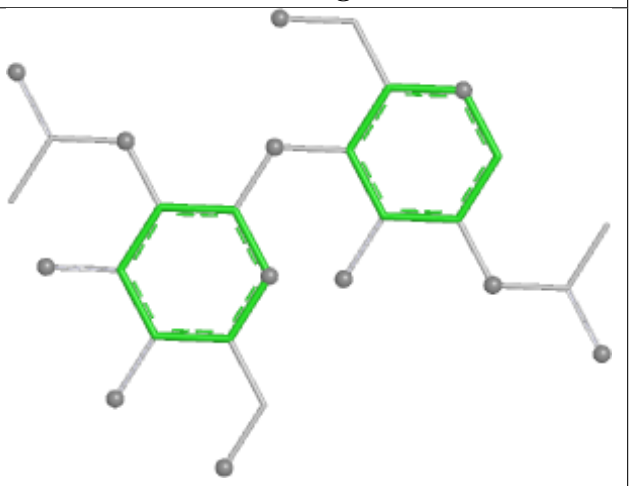
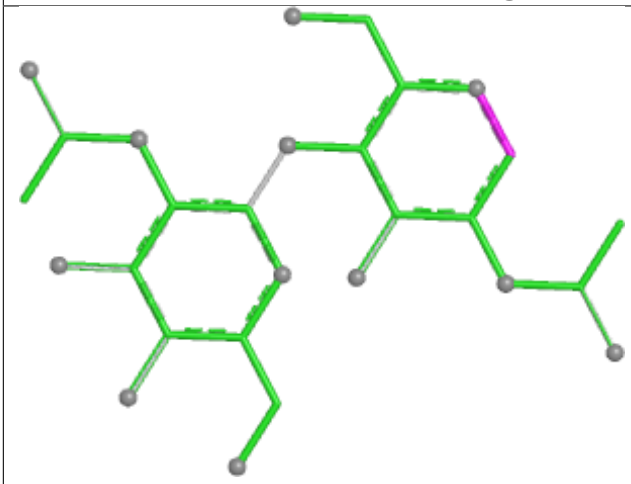


Rings

Oligosaccharide Chain s



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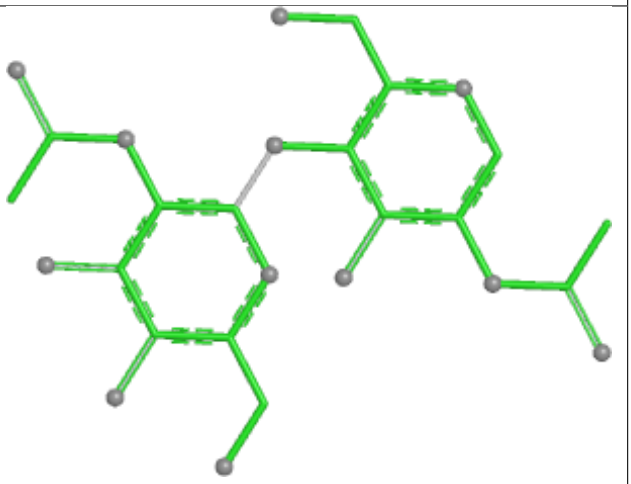

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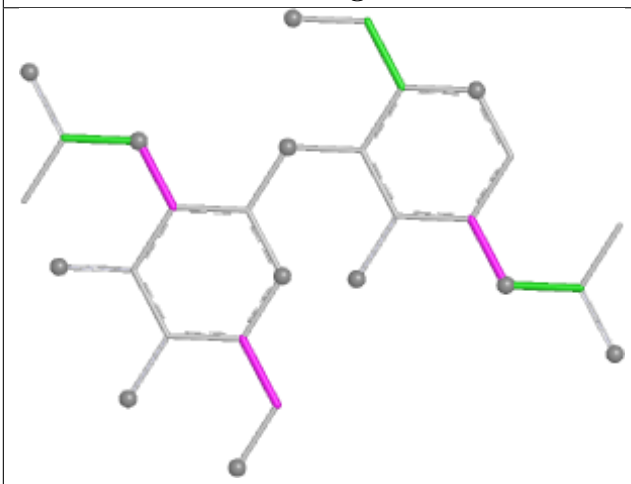

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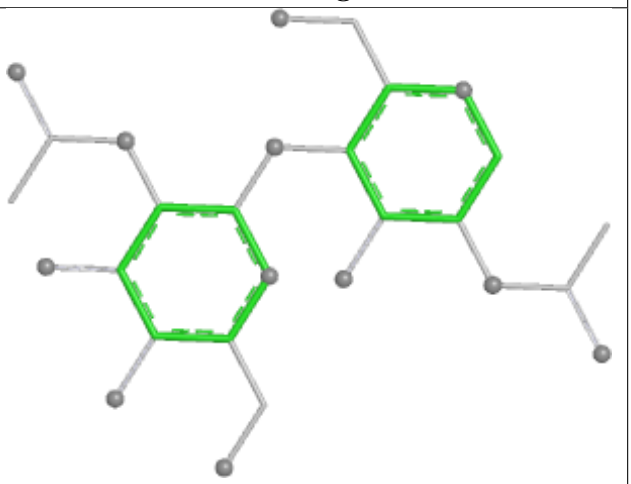
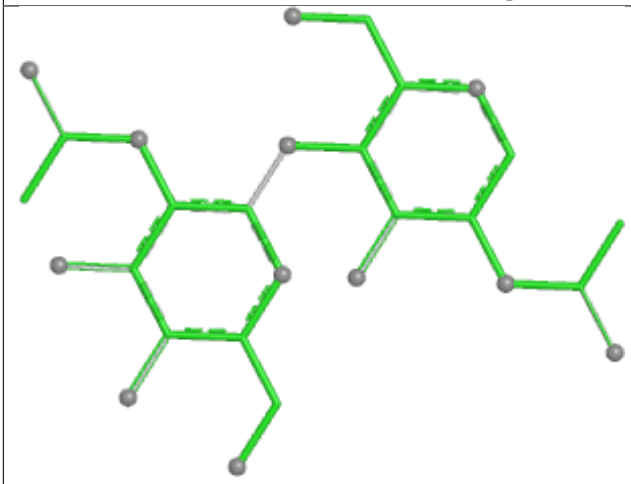


Rings

Oligosaccharide Chain t



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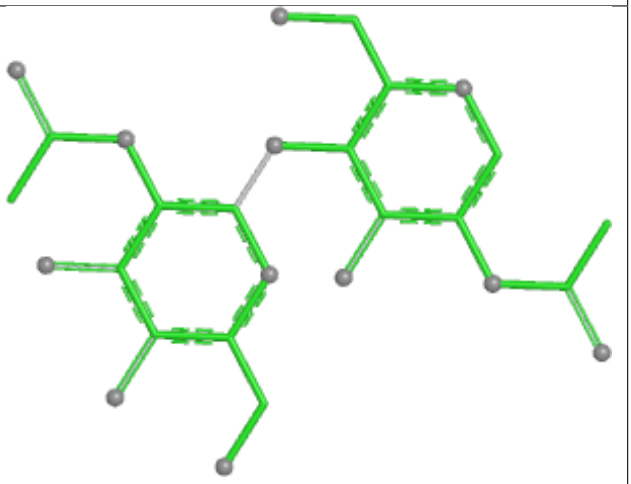
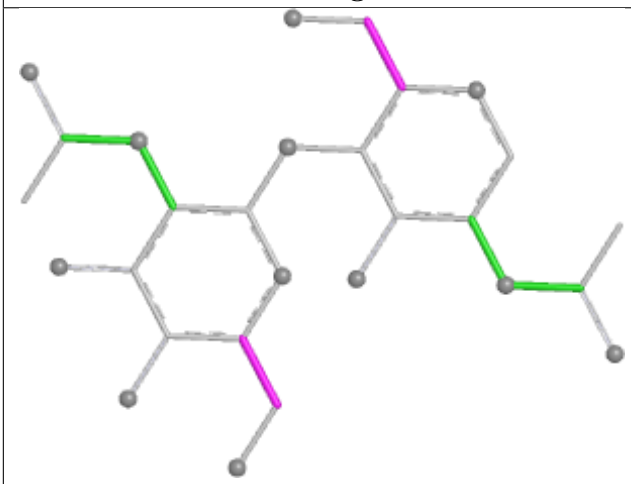


Bond angles



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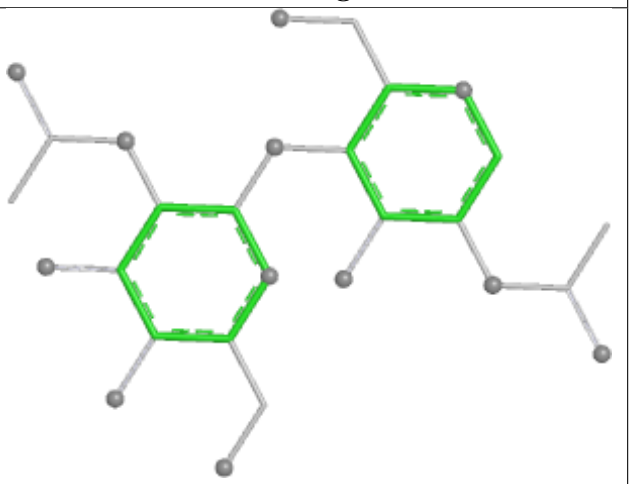
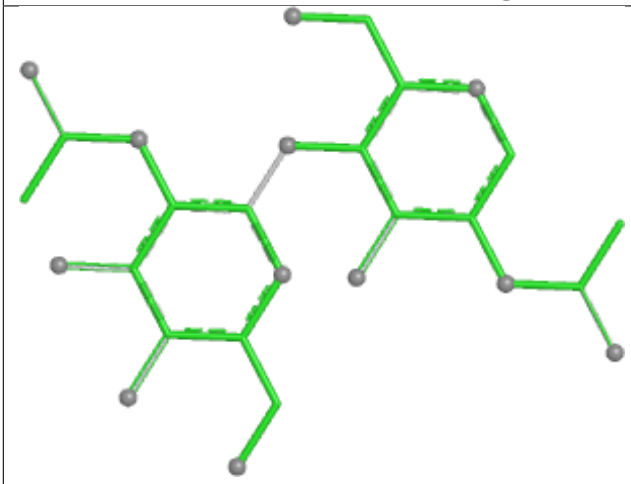


Rings

Oligosaccharide Chain u



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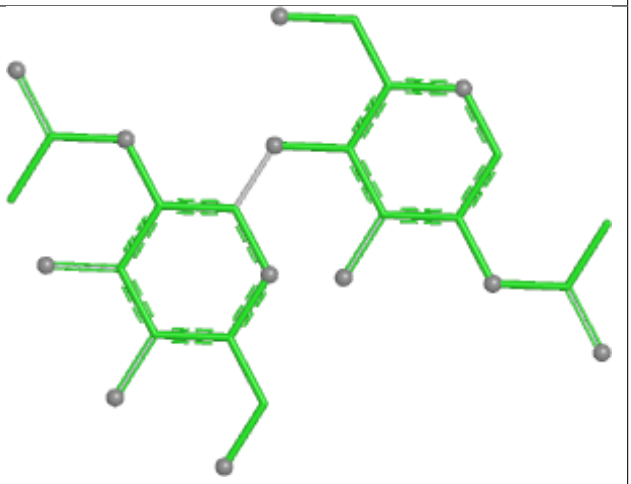
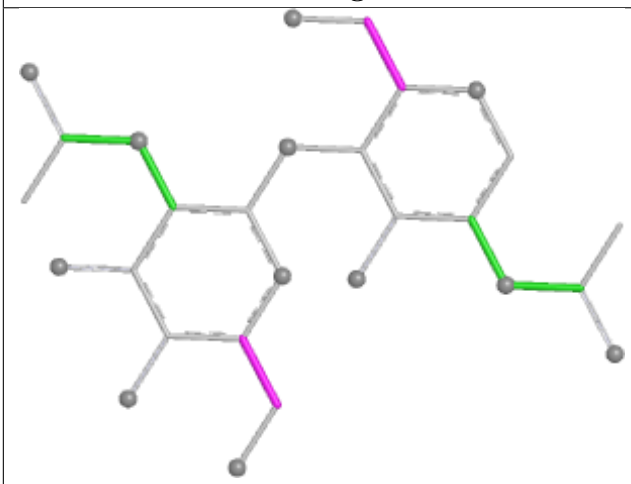


Bond angles



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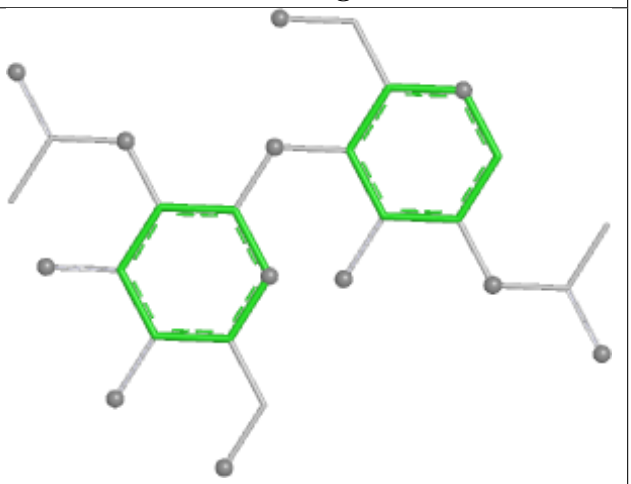
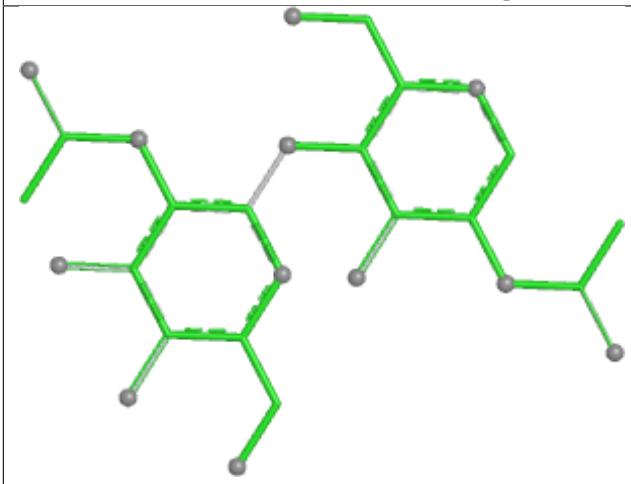


Rings

Oligosaccharide Chain v



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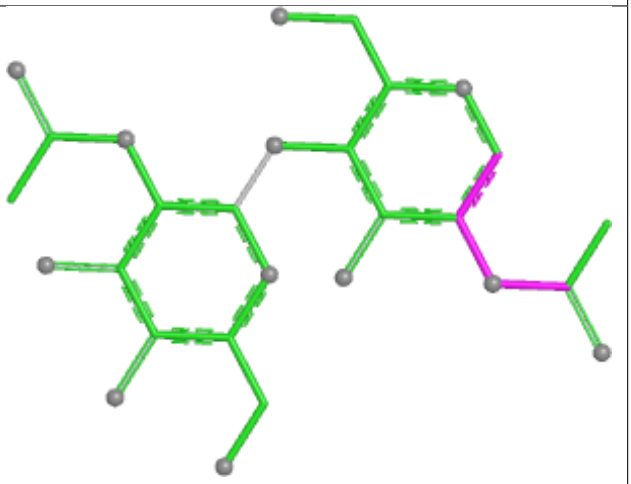
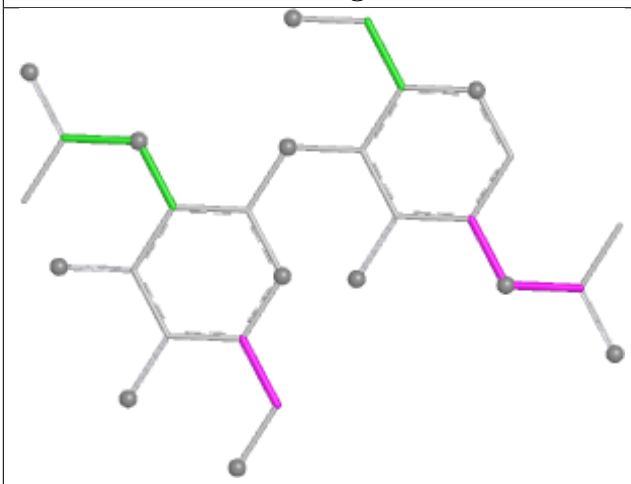


Bond angles



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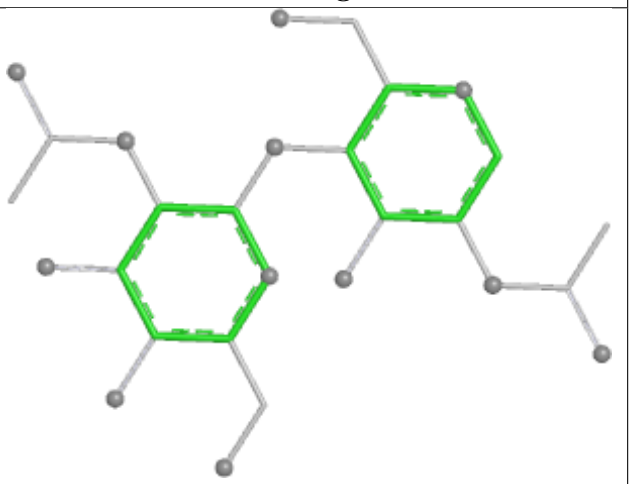
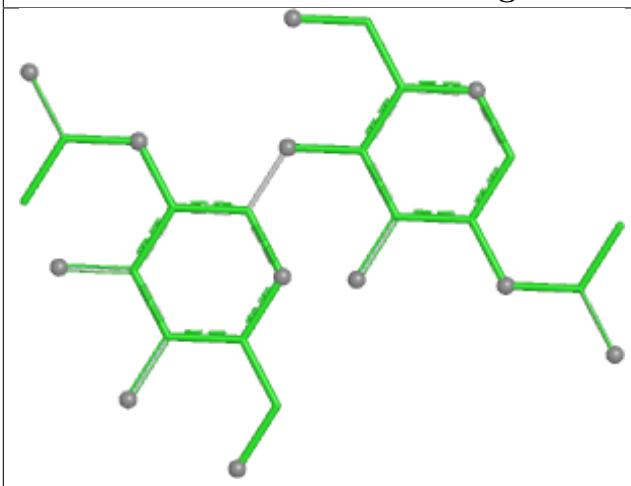


Rings

Oligosaccharide Chain x



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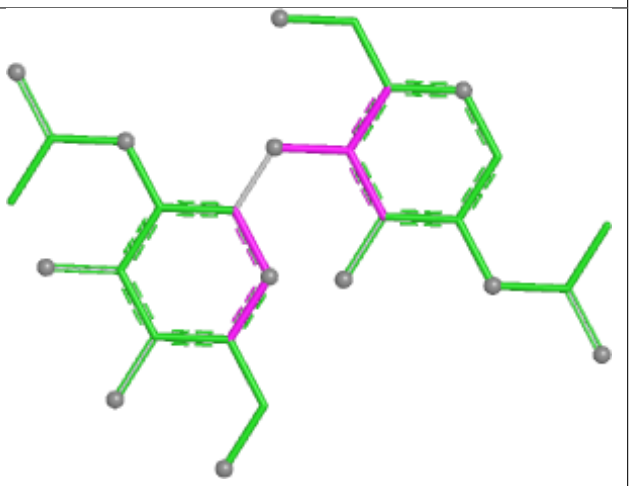
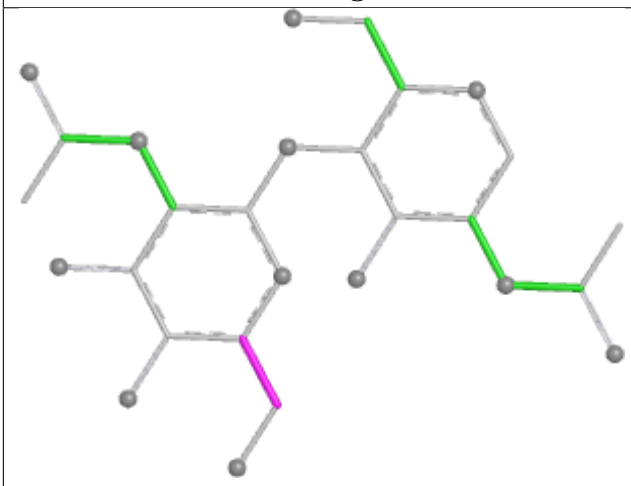


Bond angles



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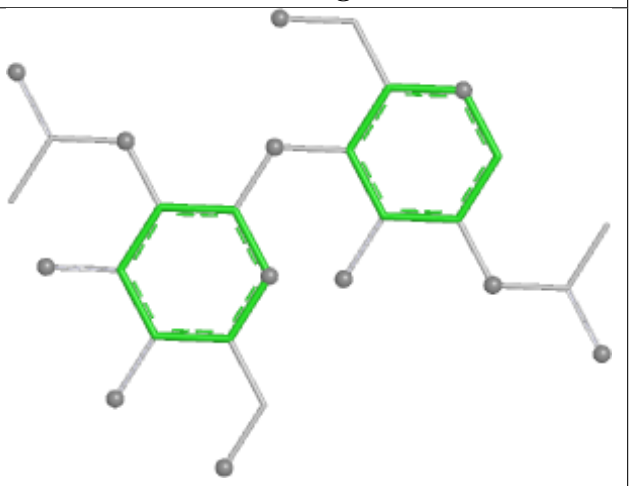
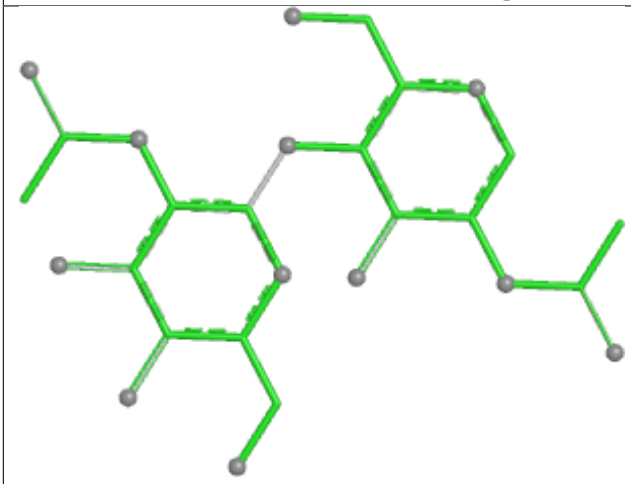


Rings

Oligosaccharide Chain y



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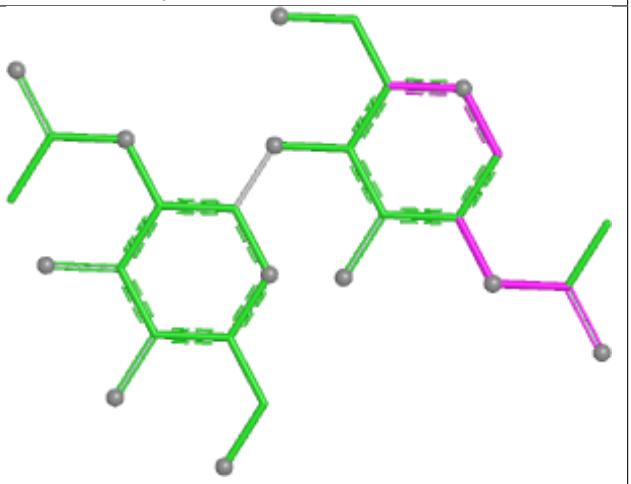
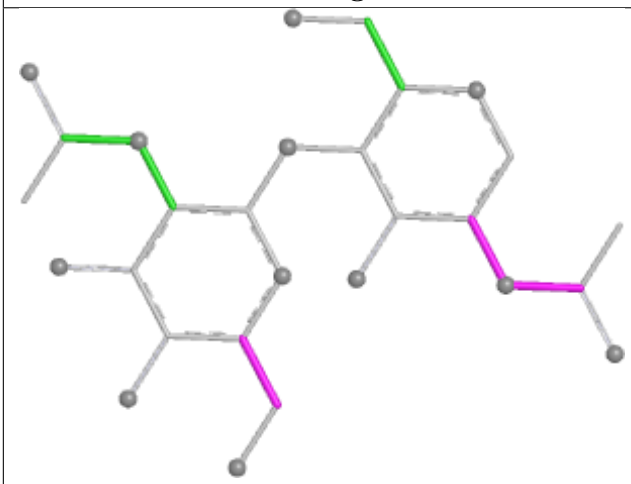


Bond angles



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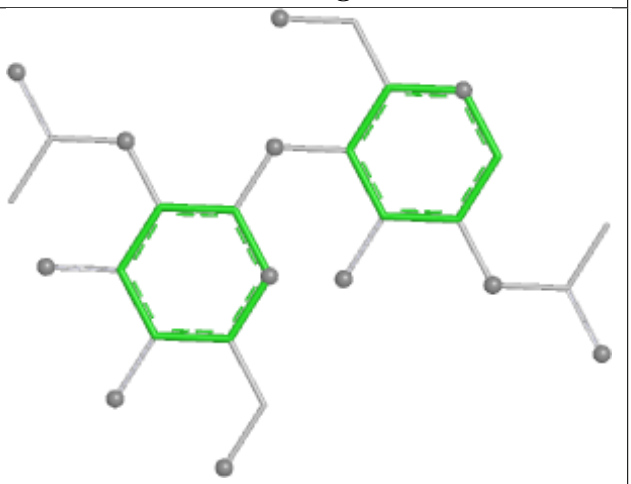
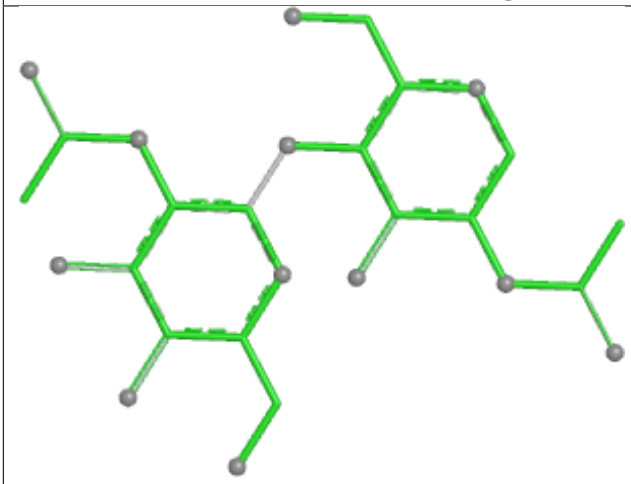


Rings

Oligosaccharide Chain z



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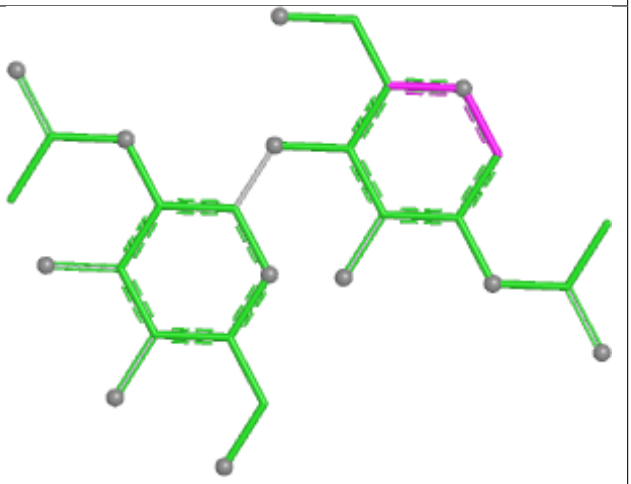
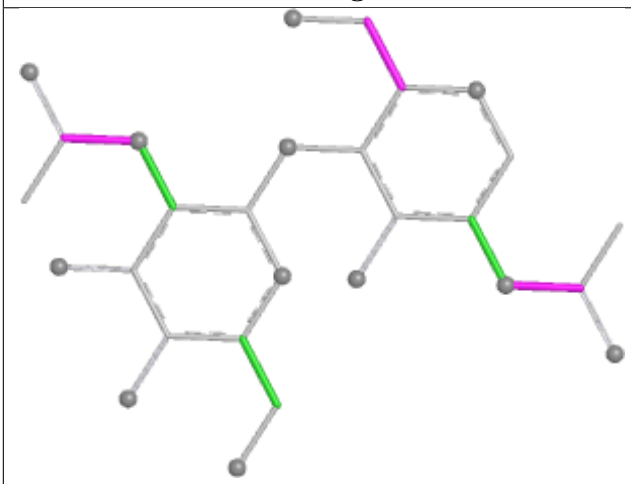


Bond angles



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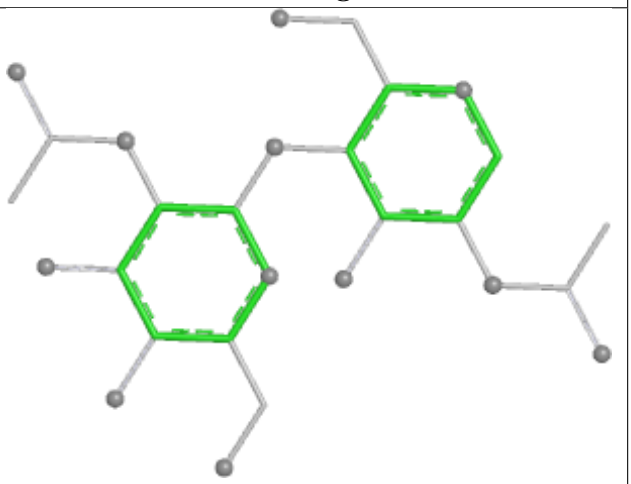
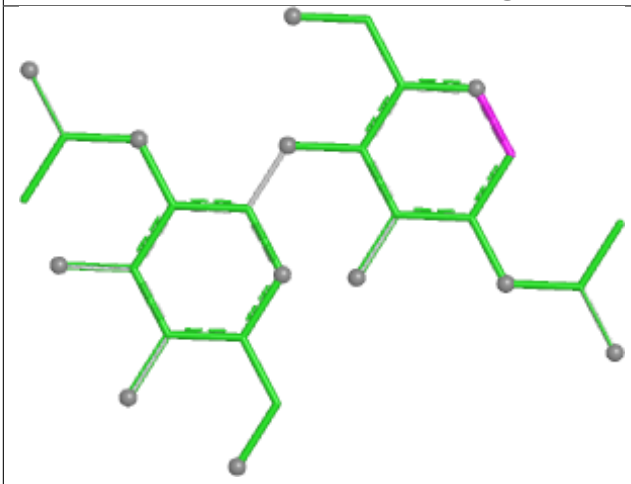


Rings

Oligosaccharide Chain 0



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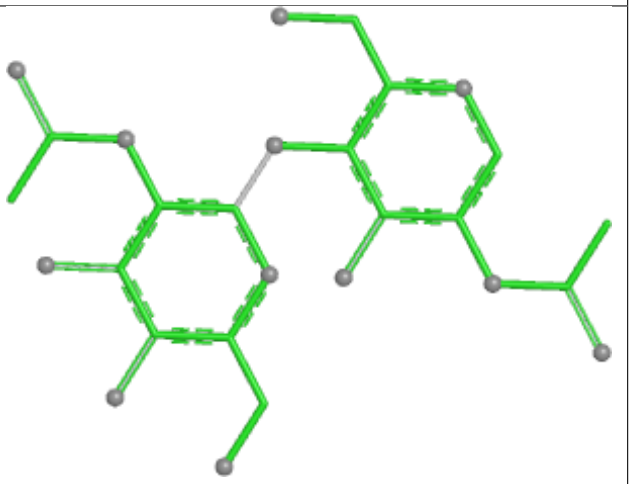
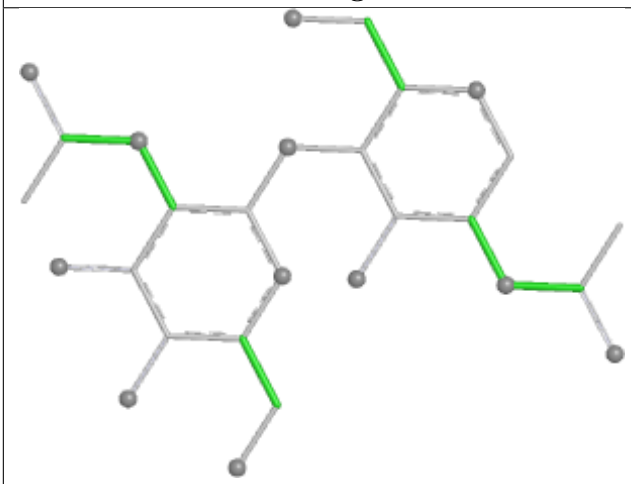
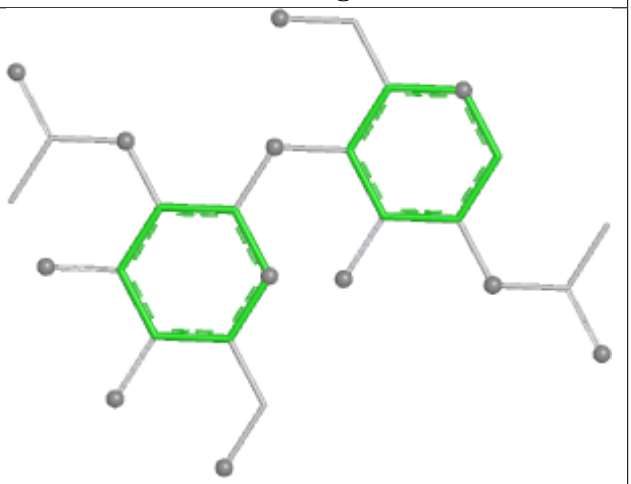


Bond angles

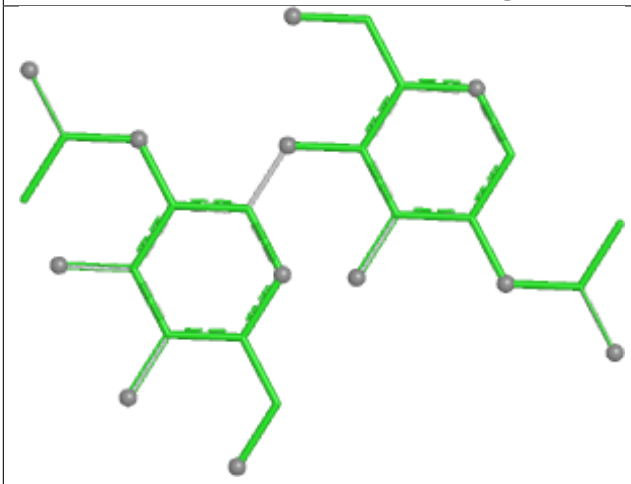


Torsions



Rings

Oligosaccharide Chain 1



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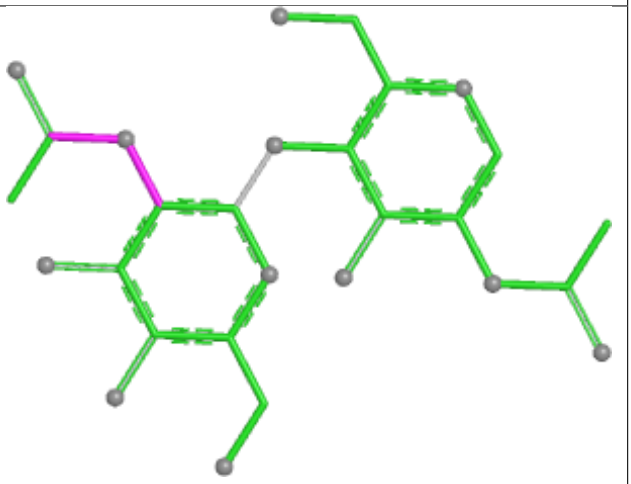
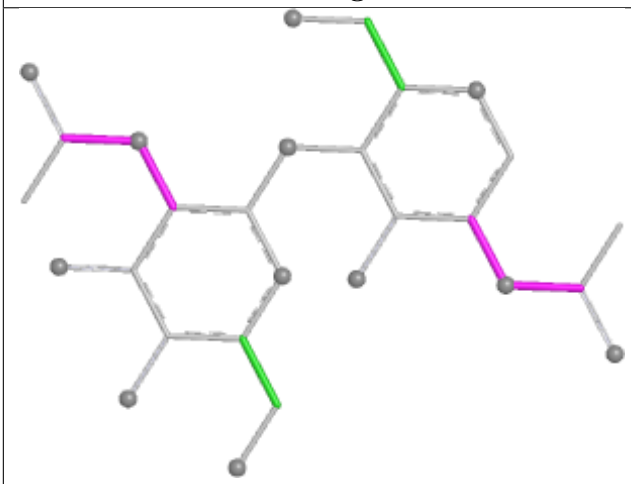
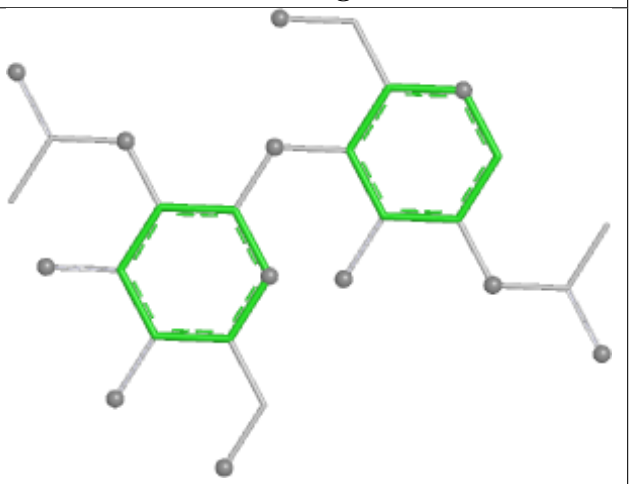


Bond angles

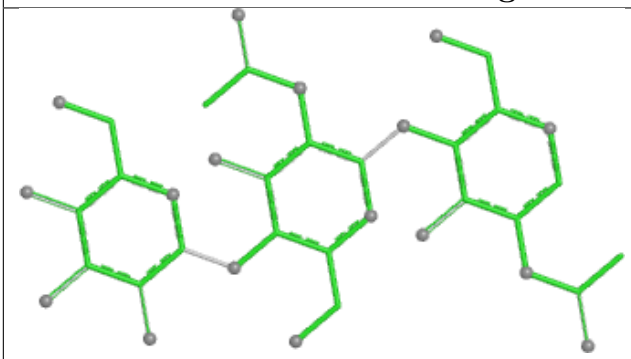


Torsions

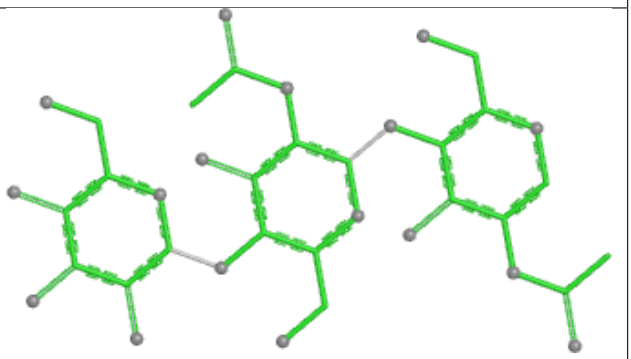


Rings

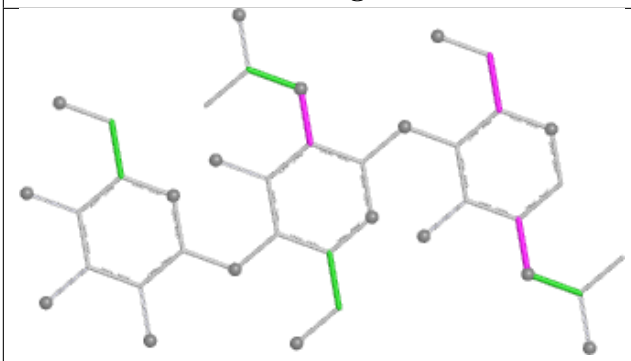
Oligosaccharide Chain J



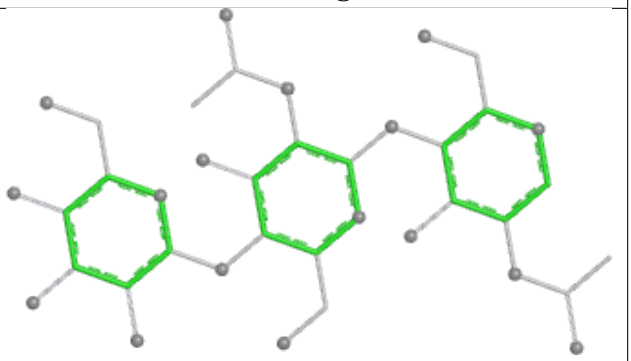
Bond lengths



Bond angles

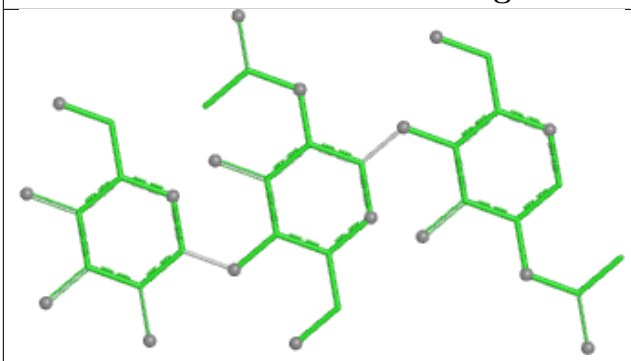


Torsions

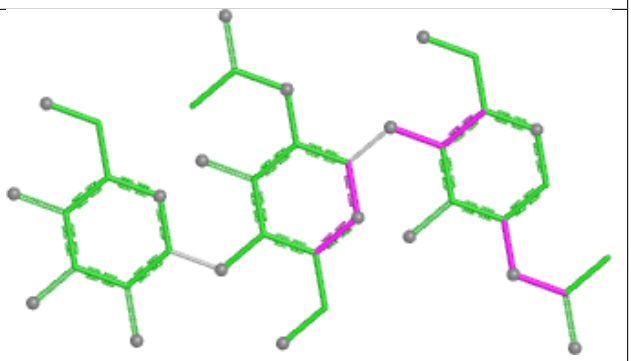


Rings

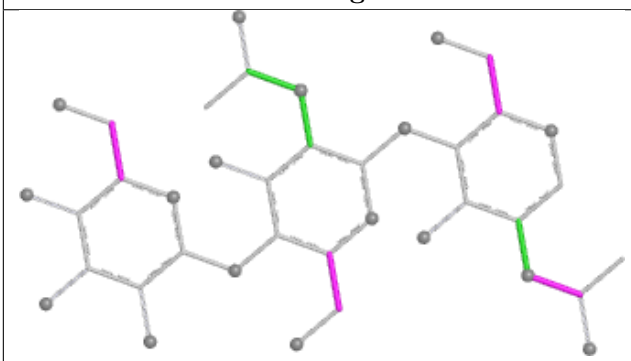
Oligosaccharide Chain N



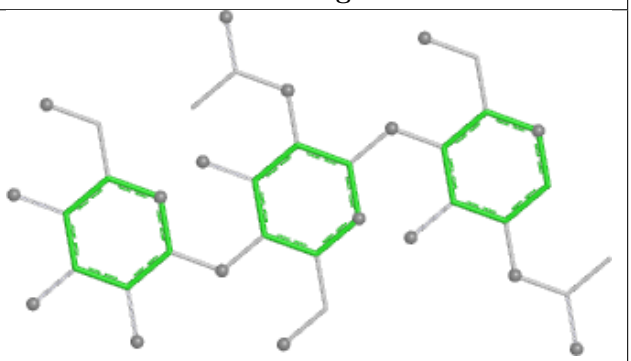
Bond lengths



Bond angles

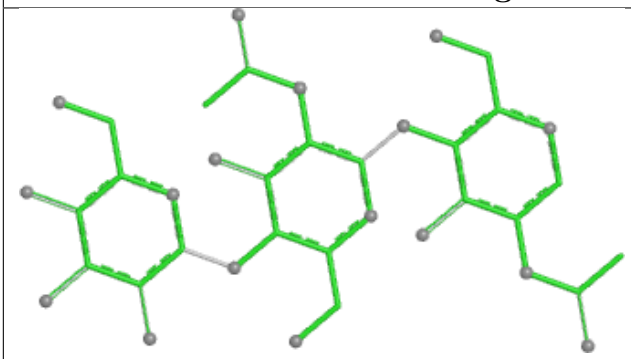


Torsions

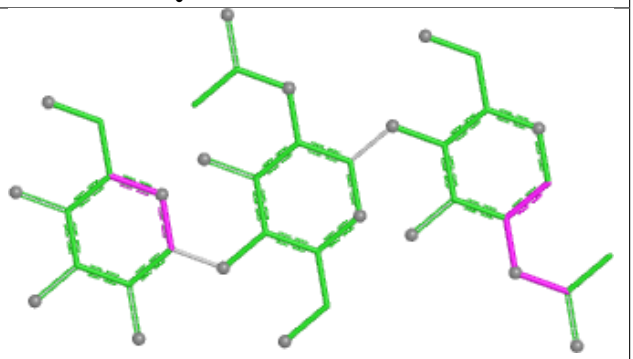


Rings

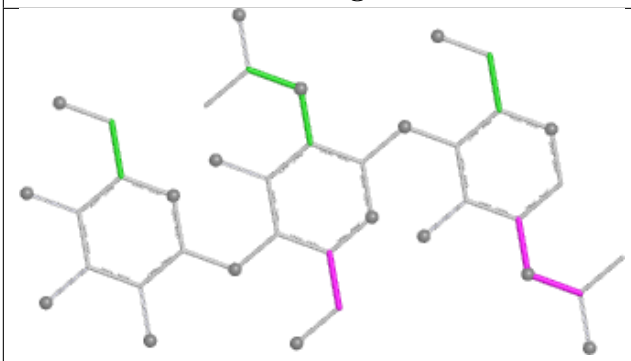
Oligosaccharide Chain Q



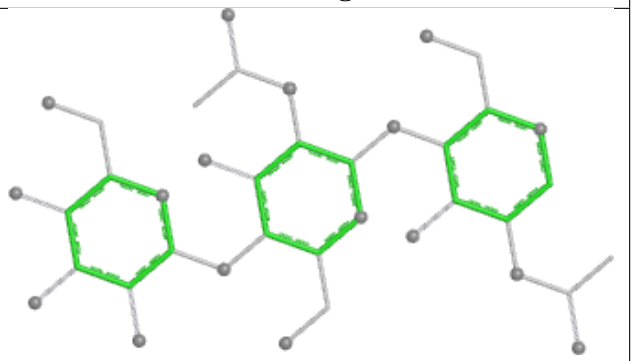
Bond lengths



Bond angles

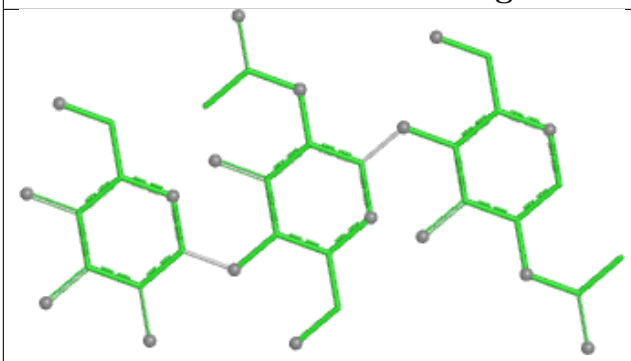


Torsions

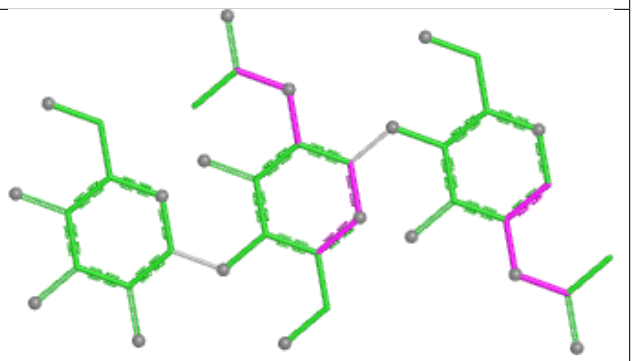


Rings

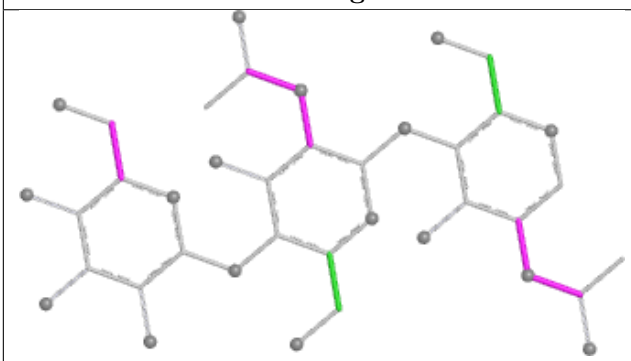
Oligosaccharide Chain T



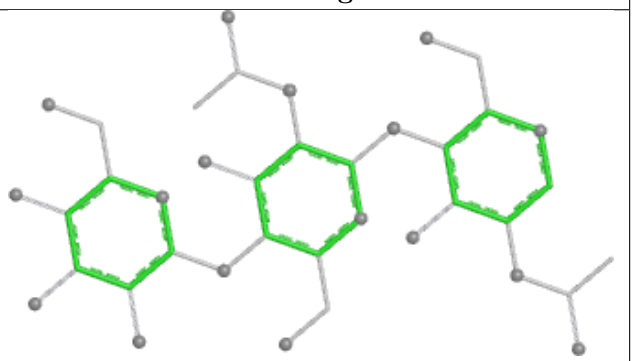
Bond lengths



Bond angles

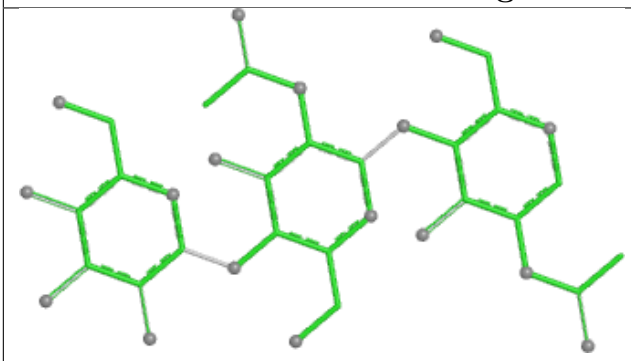


Torsions

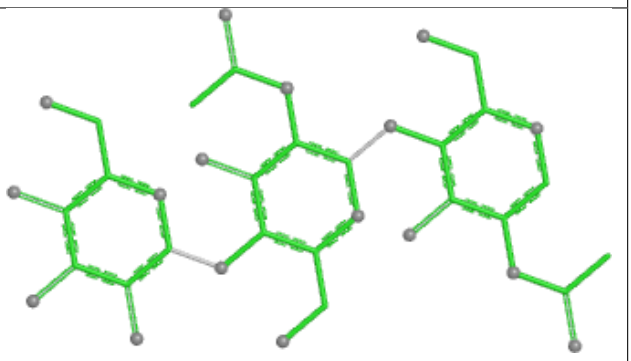


Rings

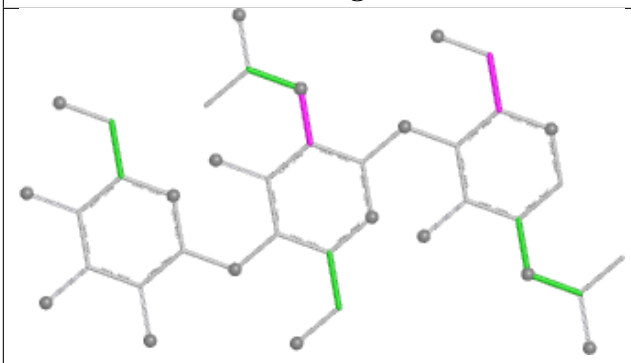
Oligosaccharide Chain Z



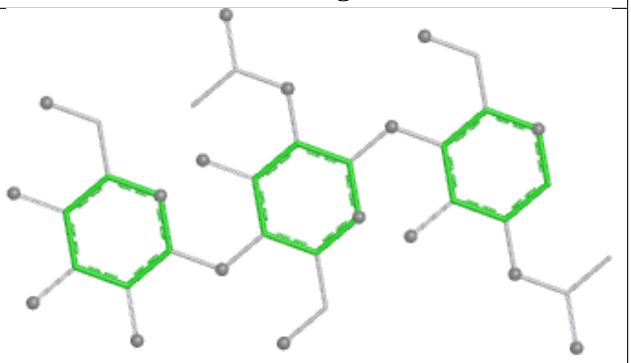
Bond lengths



Bond angles

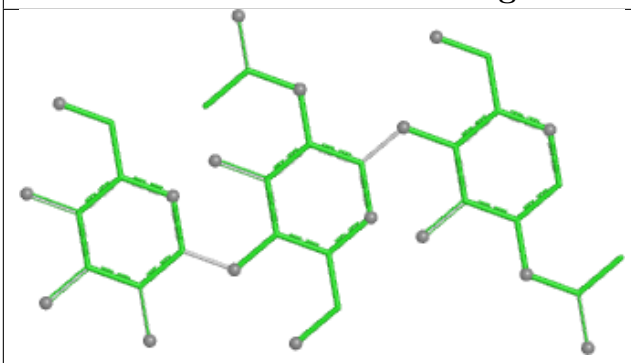


Torsions

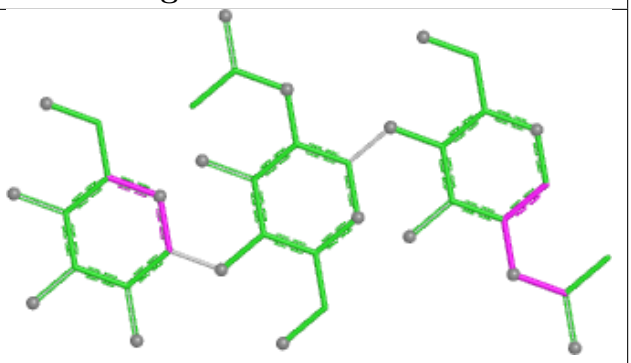


Rings

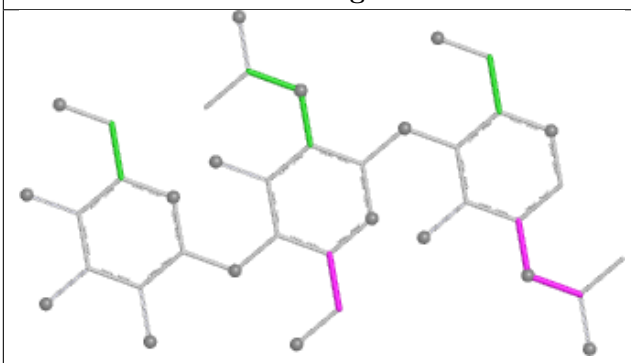
Oligosaccharide Chain g



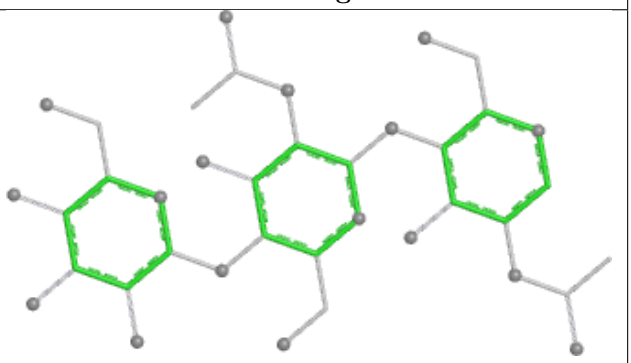
Bond lengths



Bond angles

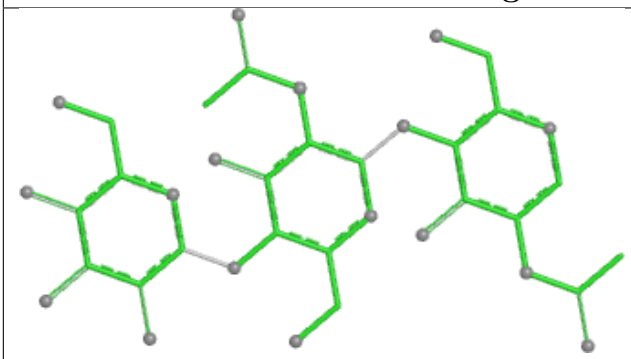


Torsions

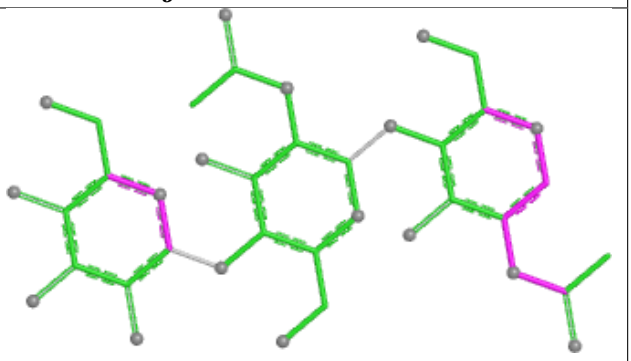


Rings

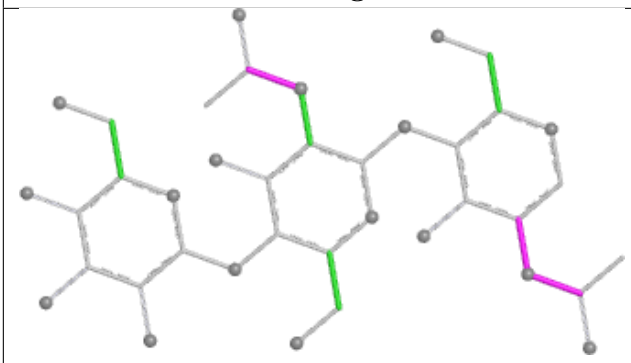
Oligosaccharide Chain j



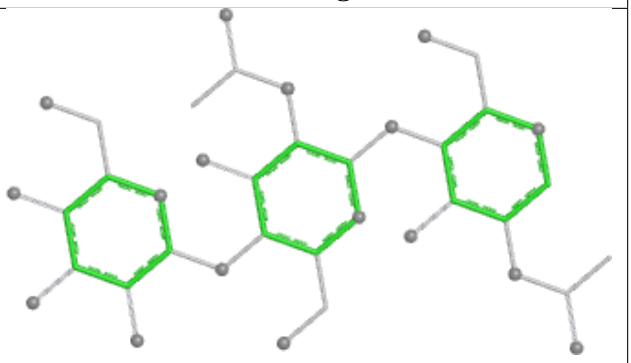
Bond lengths



Bond angles

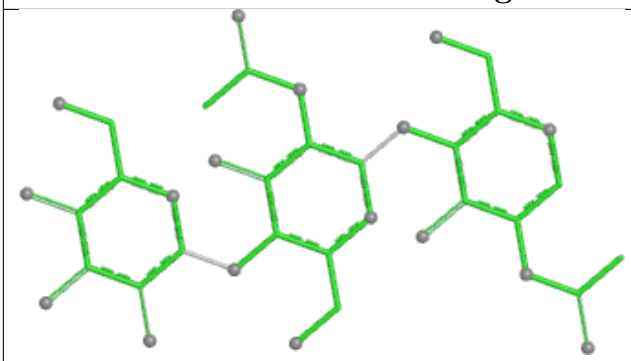


Torsions

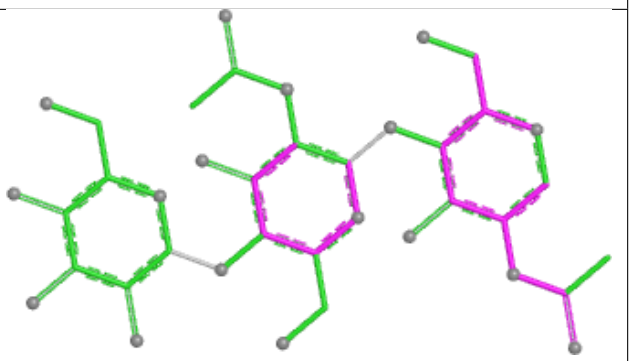


Rings

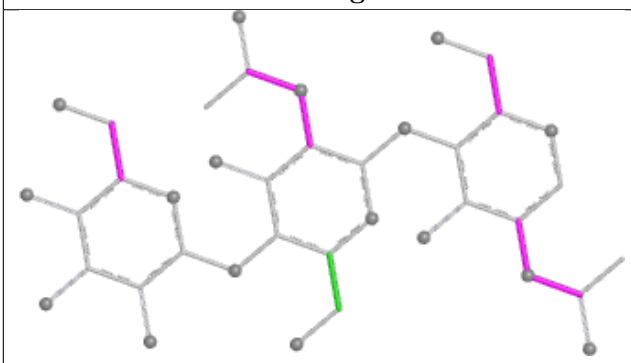
Oligosaccharide Chain w



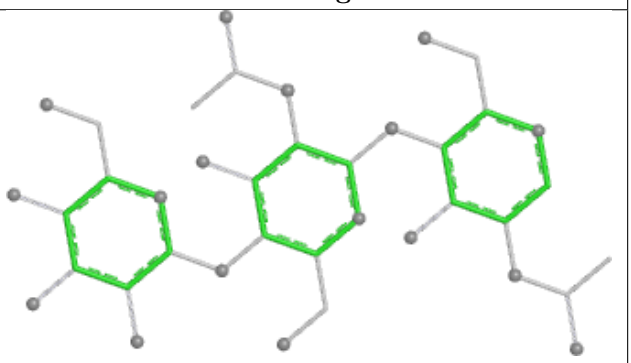
Bond lengths



Bond angles

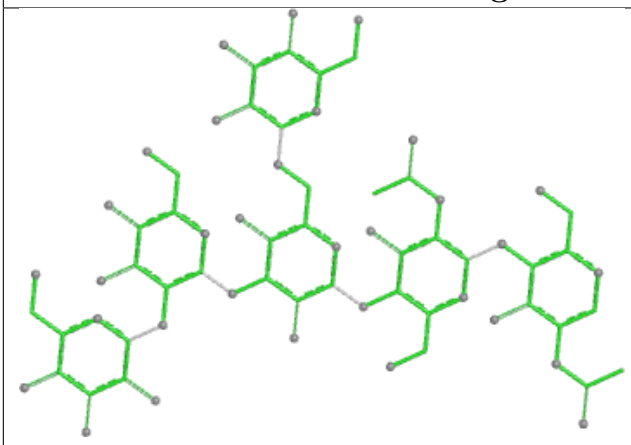


Torsions

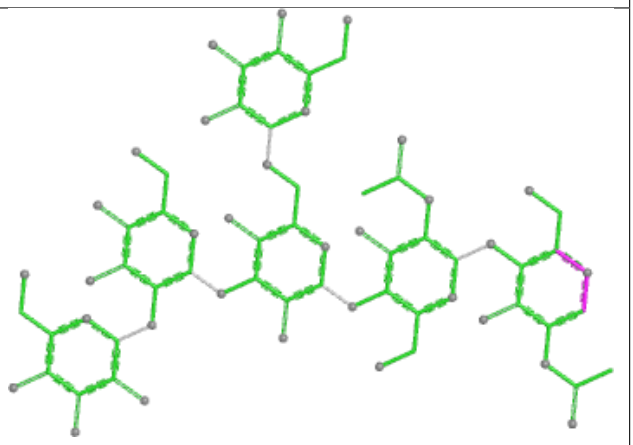


Rings

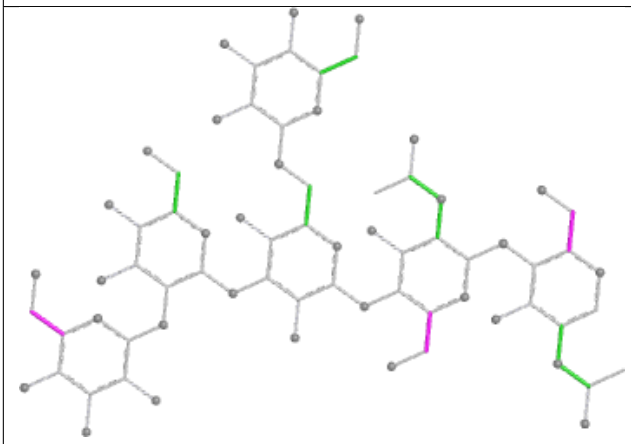
Oligosaccharide Chain M



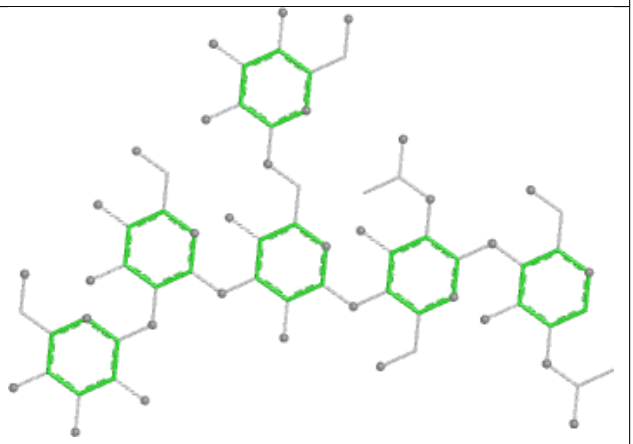
Bond lengths



Bond angles

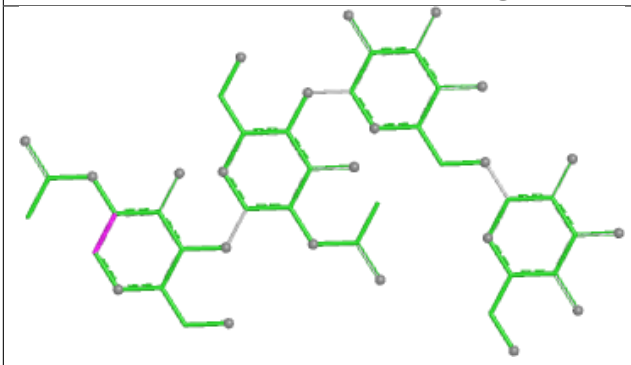


Torsions

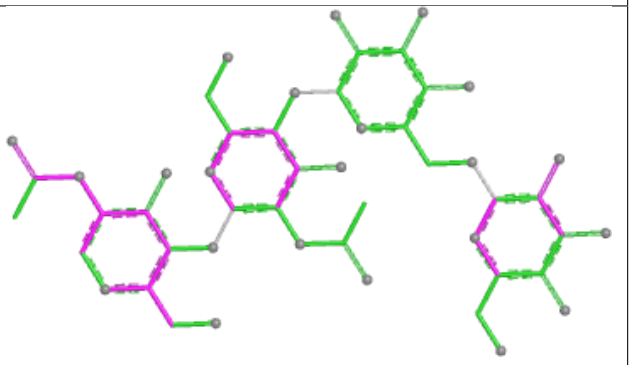


Rings

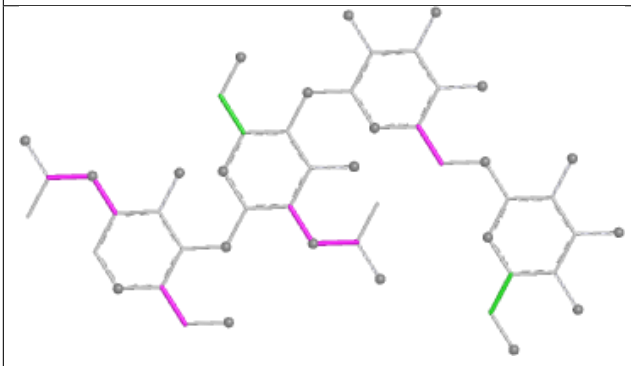
Oligosaccharide Chain R



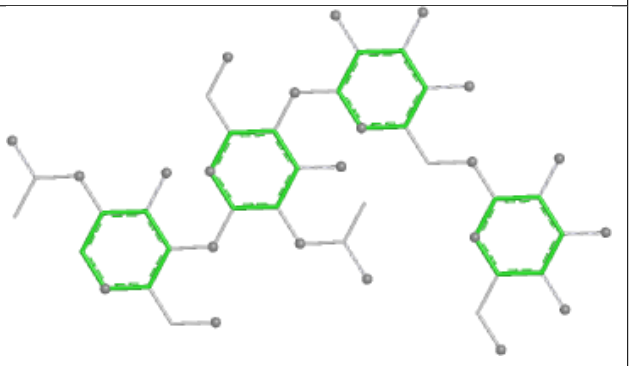
Bond lengths



Bond angles

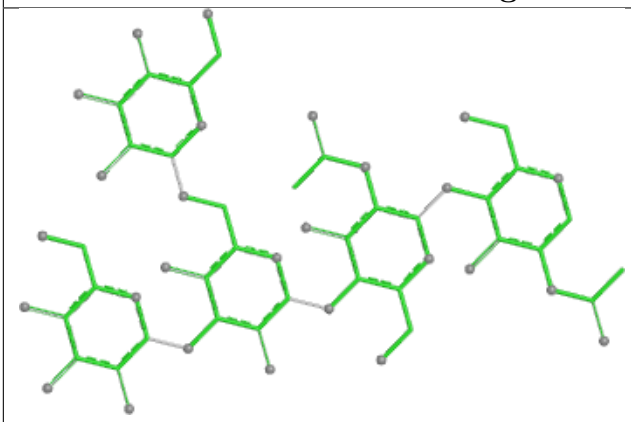


Torsions

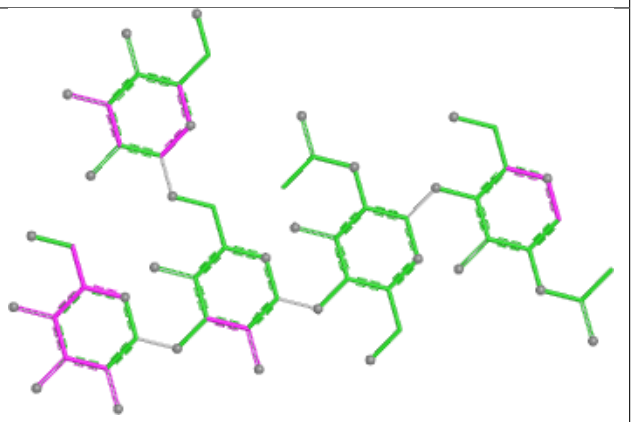


Rings

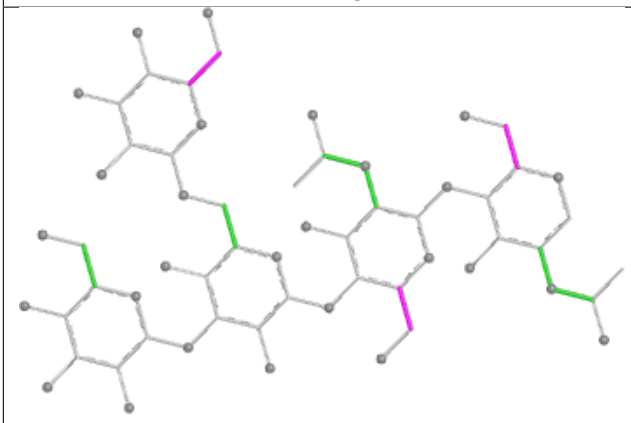
Oligosaccharide Chain c



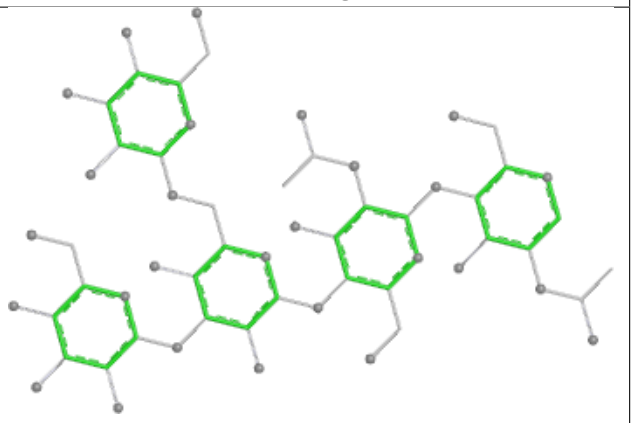
Bond lengths



Bond angles

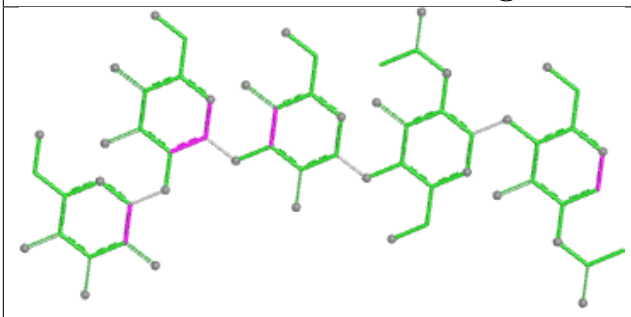


Torsions

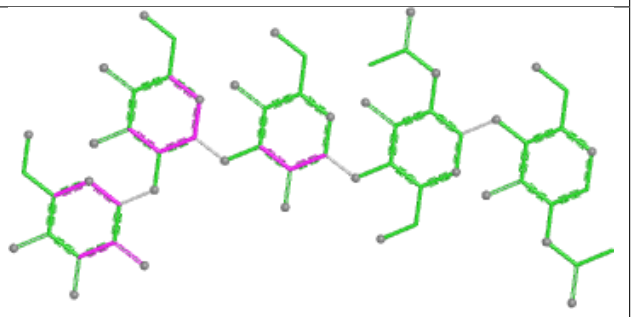


Rings

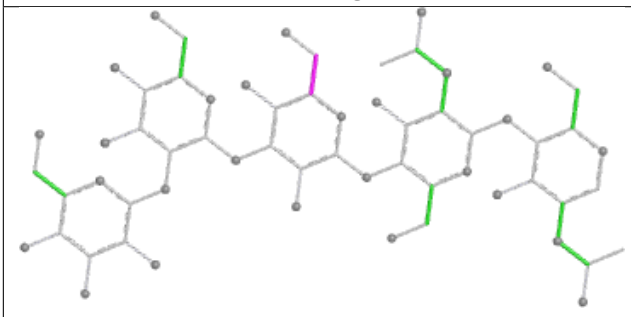
Oligosaccharide Chain h



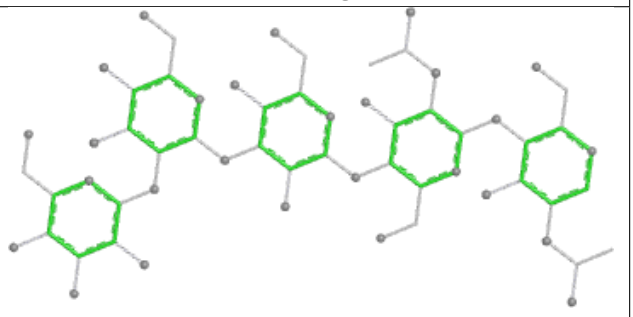
Bond lengths



Bond angles

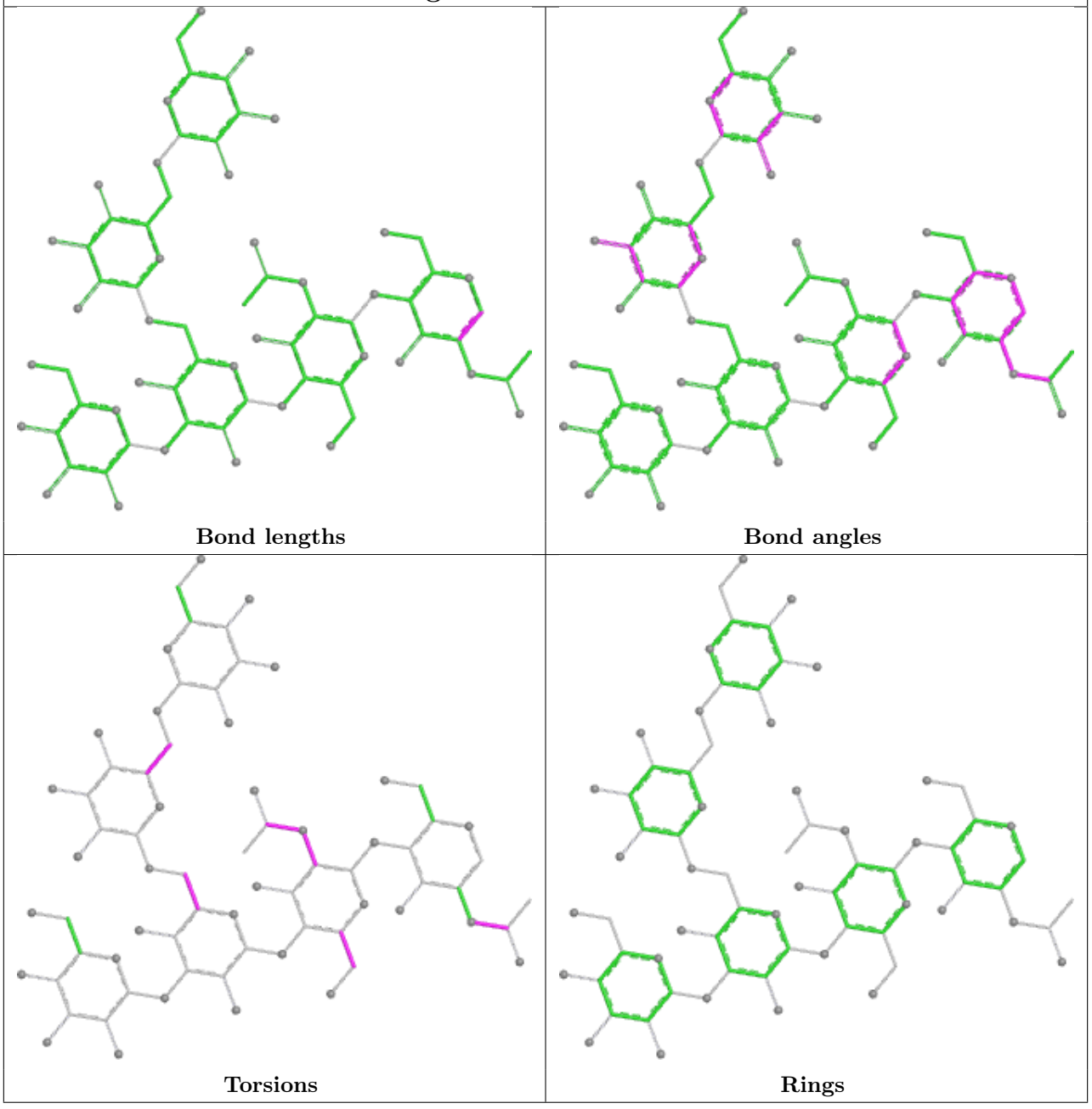


Torsions



Rings

Oligosaccharide Chain r



5.6 Ligand geometry (i)

25 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	$\#\|Z\|>2$
10	NAG	E	604	2	14,14,15	0.30	0	17,19,21	0.63	0
10	NAG	A	604	2	14,14,15	0.29	0	17,19,21	0.63	0
10	NAG	A	605	2	14,14,15	0.39	0	17,19,21	0.75	0
10	NAG	D	703	1	14,14,15	0.31	0	17,19,21	0.47	0
10	NAG	B	701	1	14,14,15	0.32	0	17,19,21	0.71	0
10	NAG	C	606	2	14,14,15	0.39	0	17,19,21	0.76	0
10	NAG	D	702	1	14,14,15	0.37	0	17,19,21	0.52	0
10	NAG	A	603	2	14,14,15	0.28	0	17,19,21	0.58	0
10	NAG	F	701	1	14,14,15	0.32	0	17,19,21	0.89	1 (5%)
10	NAG	E	605	2	14,14,15	0.40	0	17,19,21	0.76	0
11	83G	C	601	-	32,33,33	0.94	4 (12%)	39,47,47	0.94	2 (5%)
10	NAG	B	702	1	14,14,15	0.36	0	17,19,21	0.52	0
10	NAG	C	604	2	14,14,15	0.31	0	17,19,21	0.93	1 (5%)
10	NAG	A	602	2	14,14,15	0.36	0	17,19,21	0.48	0
10	NAG	C	603	2	14,14,15	0.31	0	17,19,21	0.72	0
10	NAG	D	701	1	14,14,15	0.30	0	17,19,21	0.71	0
11	83G	A	601	-	32,33,33	0.94	3 (9%)	39,47,47	0.89	2 (5%)
10	NAG	C	602	2	14,14,15	0.35	0	17,19,21	0.47	0
10	NAG	E	603	2	14,14,15	0.26	0	17,19,21	0.56	0
10	NAG	F	702	1	14,14,15	0.27	0	17,19,21	0.43	0
10	NAG	F	703	1	14,14,15	0.31	0	17,19,21	0.64	0
11	83G	E	601	-	32,33,33	0.99	4 (12%)	39,47,47	1.08	3 (7%)
10	NAG	B	703	1	14,14,15	0.29	0	17,19,21	0.47	0
10	NAG	E	602	2	14,14,15	0.36	0	17,19,21	0.48	0
10	NAG	C	605	2	14,14,15	0.41	0	17,19,21	0.75	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
10	NAG	E	604	2	-	2/6/23/26	0/1/1/1
10	NAG	A	604	2	-	2/6/23/26	0/1/1/1
10	NAG	A	605	2	-	1/6/23/26	0/1/1/1
10	NAG	D	703	1	-	1/6/23/26	0/1/1/1
10	NAG	B	701	1	-	3/6/23/26	0/1/1/1
10	NAG	C	606	2	-	1/6/23/26	0/1/1/1
10	NAG	D	702	1	-	2/6/23/26	0/1/1/1
10	NAG	A	603	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	F	701	1	-	3/6/23/26	0/1/1/1
10	NAG	E	605	2	-	1/6/23/26	0/1/1/1
11	83G	C	601	-	-	6/18/35/35	0/4/4/4
10	NAG	B	702	1	-	2/6/23/26	0/1/1/1
10	NAG	C	604	2	-	4/6/23/26	0/1/1/1
10	NAG	A	602	2	-	0/6/23/26	0/1/1/1
10	NAG	C	603	2	-	2/6/23/26	0/1/1/1
10	NAG	D	701	1	-	3/6/23/26	0/1/1/1
11	83G	A	601	-	-	10/18/35/35	0/4/4/4
10	NAG	C	602	2	-	0/6/23/26	0/1/1/1
10	NAG	E	603	2	-	2/6/23/26	0/1/1/1
10	NAG	F	702	1	-	1/6/23/26	0/1/1/1
10	NAG	F	703	1	-	2/6/23/26	0/1/1/1
11	83G	E	601	-	-	4/18/35/35	0/4/4/4
10	NAG	B	703	1	-	1/6/23/26	0/1/1/1
10	NAG	E	602	2	-	0/6/23/26	0/1/1/1
10	NAG	C	605	2	-	1/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	601	83G	C11-C12	-3.10	1.43	1.49
11	A	601	83G	C11-C12	-3.09	1.43	1.49
11	E	601	83G	C11-C12	-3.05	1.43	1.49
11	E	601	83G	C14-C12	-2.62	1.50	1.53
11	C	601	83G	C11-C08	2.20	1.45	1.42
11	E	601	83G	C11-C08	2.13	1.45	1.42
11	C	601	83G	C14-C12	-2.13	1.50	1.53
11	E	601	83G	C07-N06	-2.10	1.34	1.37
11	A	601	83G	C11-C08	2.06	1.44	1.42
11	A	601	83G	C07-N06	-2.05	1.34	1.37
11	C	601	83G	C07-N06	-2.00	1.34	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	604	NAG	C2-N2-C7	2.73	126.55	122.90
10	F	701	NAG	C2-N2-C7	-2.57	119.46	122.90
11	C	601	83G	O02-C03-C08	2.50	119.47	115.91
11	C	601	83G	C11-C08-C07	-2.38	105.64	107.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	E	601	83G	O02-C03-C08	2.37	119.29	115.91
11	E	601	83G	C11-C08-C07	-2.35	105.66	107.54
11	A	601	83G	C12-C14-N16	2.09	120.95	118.81
11	A	601	83G	C11-C08-C07	-2.07	105.89	107.54
11	E	601	83G	C21-N16-C14	2.02	125.35	120.32

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	604	NAG	C8-C7-N2-C2
10	C	604	NAG	O7-C7-N2-C2
10	E	603	NAG	C8-C7-N2-C2
10	E	603	NAG	O7-C7-N2-C2
10	F	703	NAG	C8-C7-N2-C2
10	F	703	NAG	O7-C7-N2-C2
11	C	601	83G	O15-C14-N16-C17
11	A	601	83G	O15-C14-N16-C17
10	A	603	NAG	O7-C7-N2-C2
11	A	601	83G	C08-C03-O02-C01
10	B	702	NAG	O5-C5-C6-O6
10	D	702	NAG	O5-C5-C6-O6
10	A	603	NAG	C8-C7-N2-C2
11	A	601	83G	C04-C03-O02-C01
10	E	604	NAG	C8-C7-N2-C2
10	A	604	NAG	C8-C7-N2-C2
10	E	604	NAG	O7-C7-N2-C2
10	A	604	NAG	O7-C7-N2-C2
11	A	601	83G	C25-C23-N19-C20
11	E	601	83G	C08-C03-O02-C01
11	A	601	83G	O24-C23-N19-C20
10	B	701	NAG	C8-C7-N2-C2
10	D	701	NAG	C8-C7-N2-C2
11	C	601	83G	C12-C14-N16-C17
11	E	601	83G	O15-C14-N16-C17
10	F	701	NAG	C8-C7-N2-C2
10	B	701	NAG	O7-C7-N2-C2
10	D	701	NAG	O7-C7-N2-C2
10	C	603	NAG	C4-C5-C6-O6
11	E	601	83G	C04-C03-O02-C01
10	B	703	NAG	O5-C5-C6-O6
10	D	703	NAG	O5-C5-C6-O6

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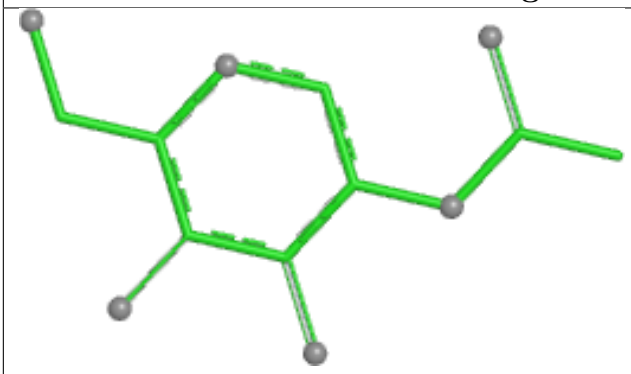
Mol	Chain	Res	Type	Atoms
10	F	701	NAG	O5-C5-C6-O6
10	B	701	NAG	O5-C5-C6-O6
10	D	701	NAG	O5-C5-C6-O6
10	F	702	NAG	O5-C5-C6-O6
11	A	601	83G	C12-C14-N16-C17
11	C	601	83G	O13-C12-C14-O15
11	A	601	83G	O13-C12-C14-O15
10	C	604	NAG	C1-C2-N2-C7
10	F	701	NAG	O7-C7-N2-C2
10	D	702	NAG	C4-C5-C6-O6
10	B	702	NAG	C4-C5-C6-O6
10	C	603	NAG	O5-C5-C6-O6
11	A	601	83G	C11-C12-C14-O15
10	C	604	NAG	C3-C2-N2-C7
11	C	601	83G	C12-C14-N16-C21
11	E	601	83G	C12-C14-N16-C21
11	A	601	83G	C12-C14-N16-C21
11	C	601	83G	O24-C23-N19-C20
10	C	605	NAG	C1-C2-N2-C7
10	C	606	NAG	C1-C2-N2-C7
10	E	605	NAG	C1-C2-N2-C7
10	A	605	NAG	C1-C2-N2-C7
11	C	601	83G	C11-C12-C14-O15
11	A	601	83G	O13-C12-C14-N16

There are no ring outliers.

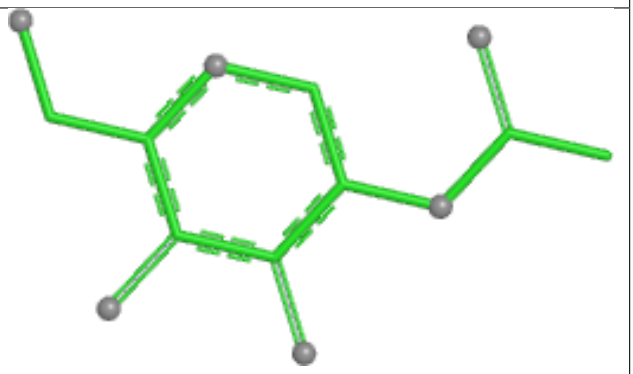
No monomer is involved in short contacts.

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

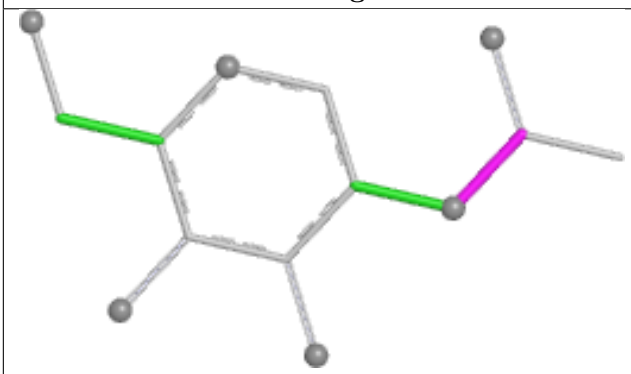
Ligand NAG E 604



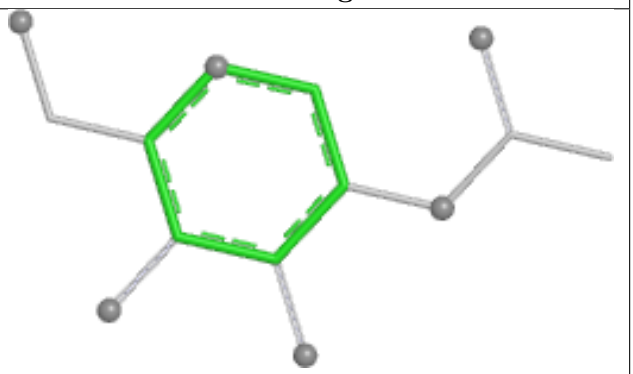
Bond lengths



Bond angles

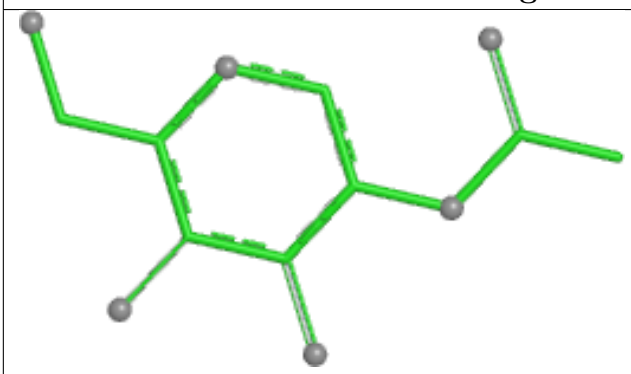


Torsions

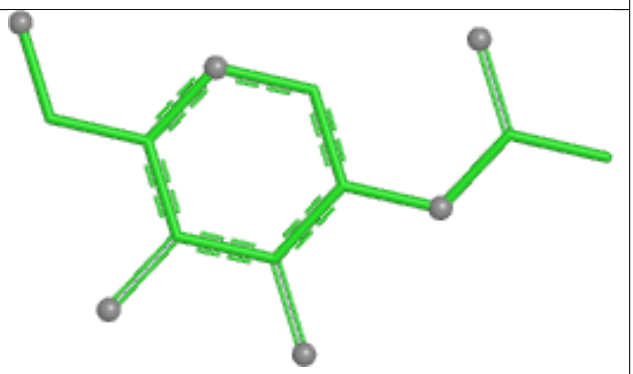


Rings

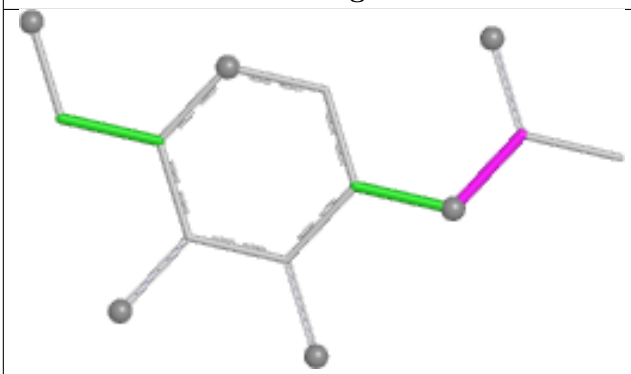
Ligand NAG A 604



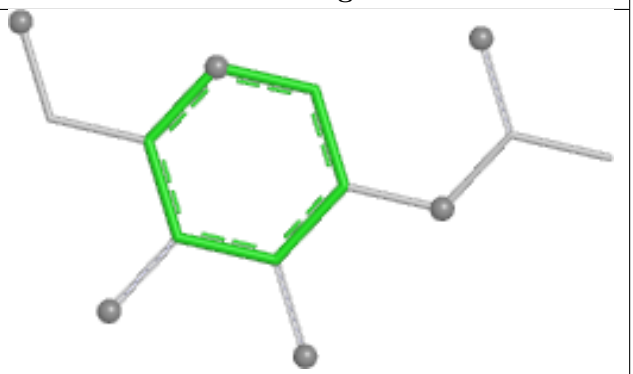
Bond lengths



Bond angles

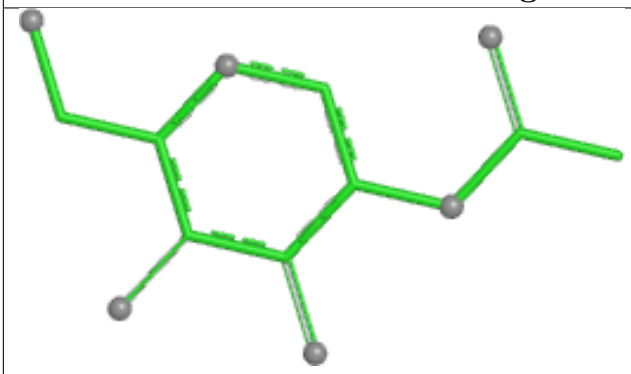


Torsions

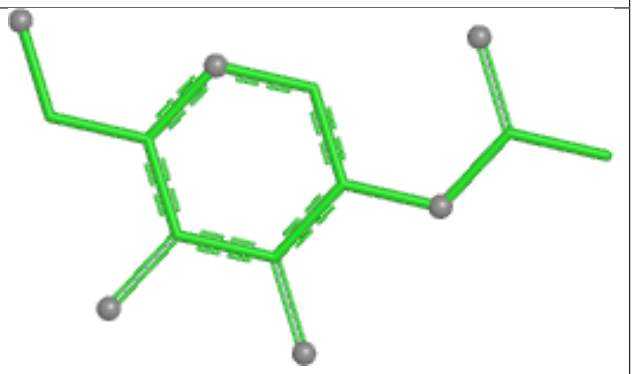


Rings

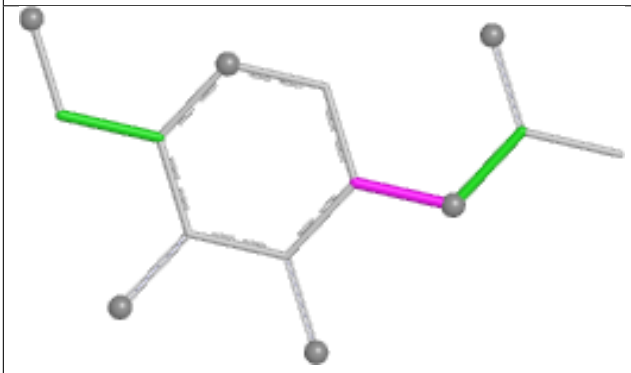
Ligand NAG A 605



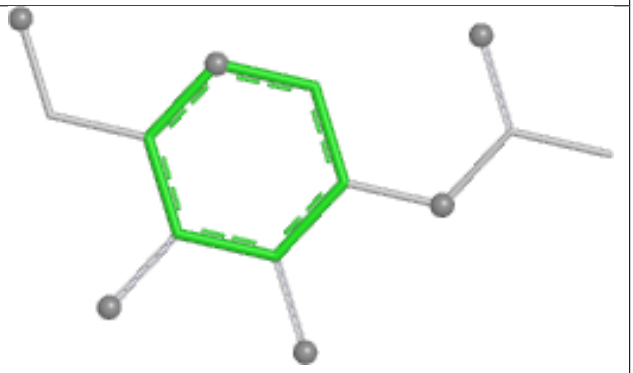
Bond lengths



Bond angles

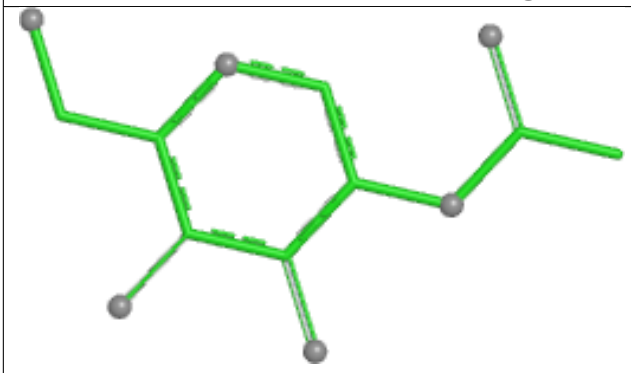


Torsions

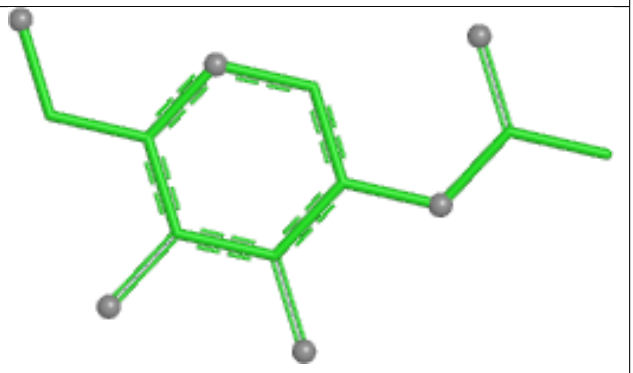


Rings

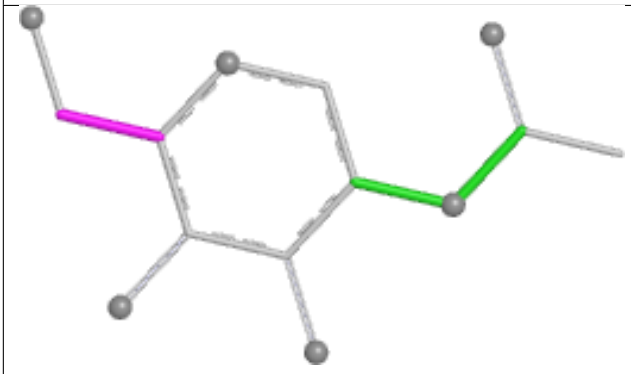
Ligand NAG D 703



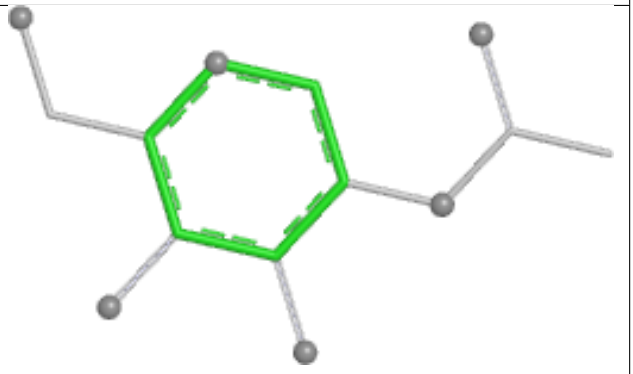
Bond lengths



Bond angles

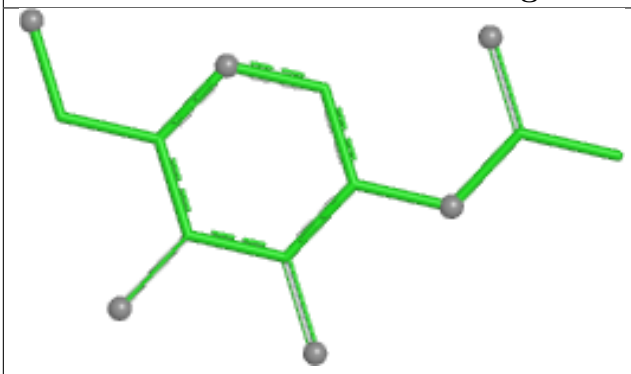


Torsions

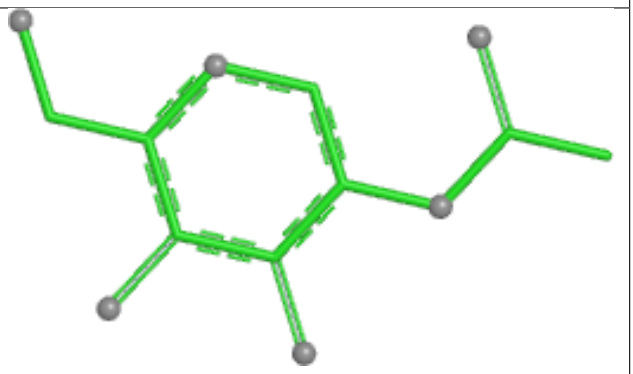


Rings

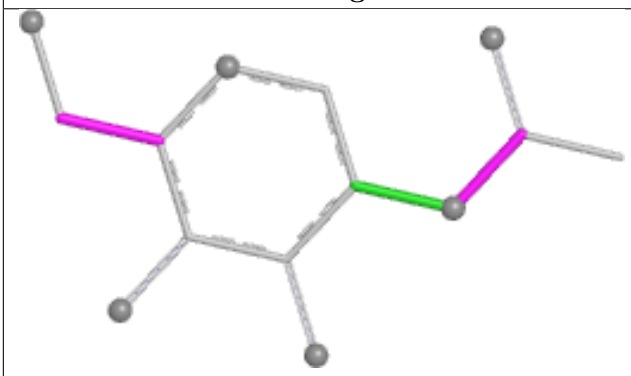
Ligand NAG B 701



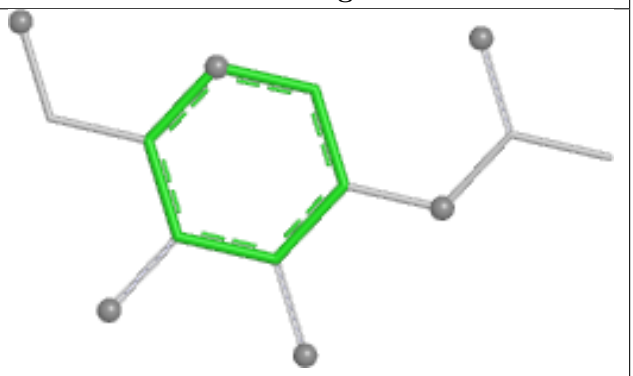
Bond lengths



Bond angles

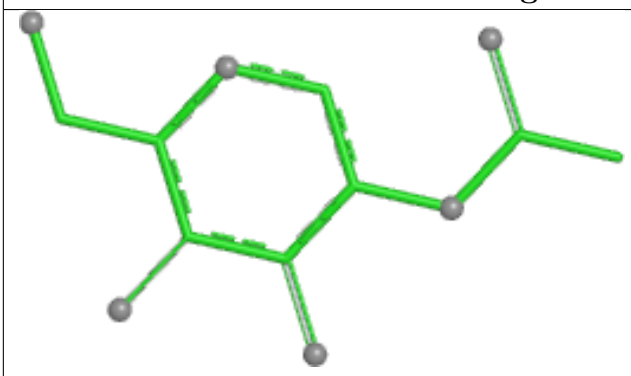


Torsions



Rings

Ligand NAG C 606



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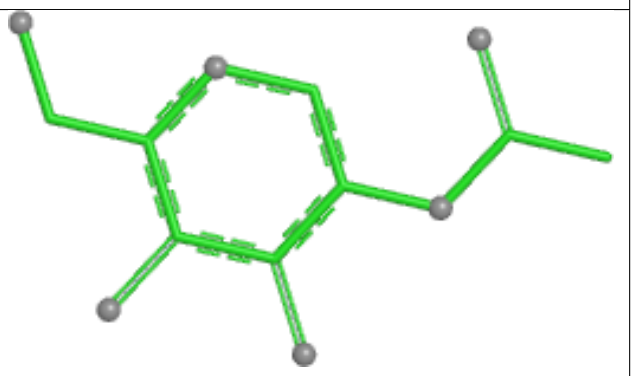
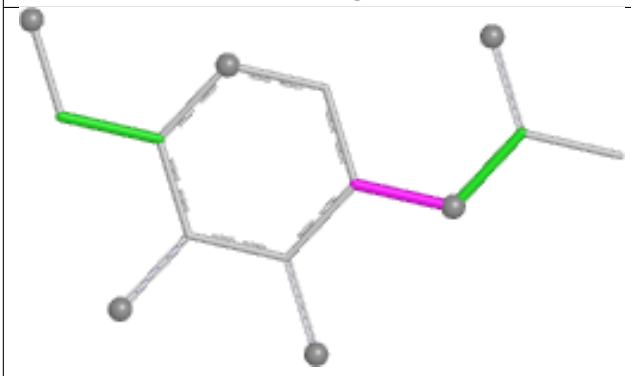
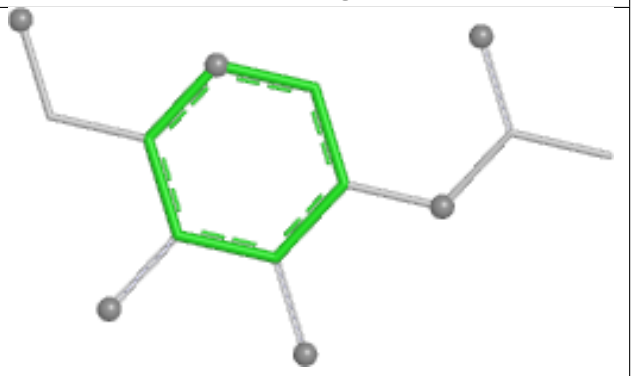


Bond angles

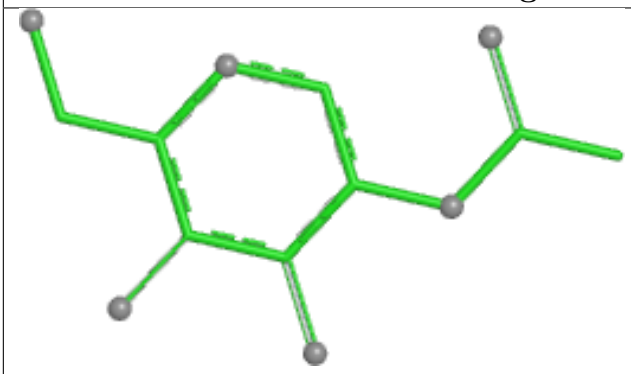


Torsions

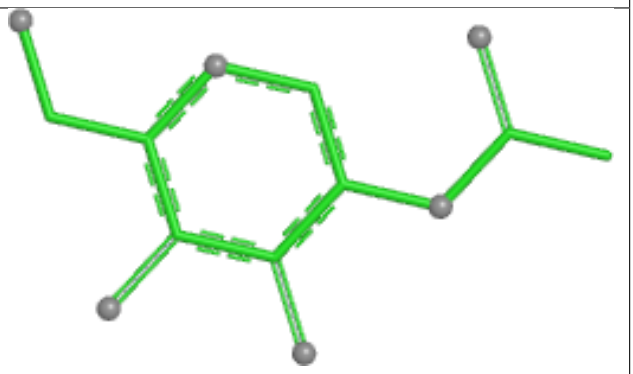


Rings

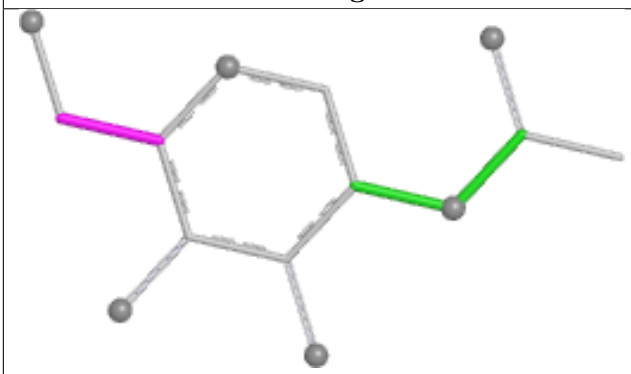
Ligand NAG D 702



Bond lengths



Bond angles



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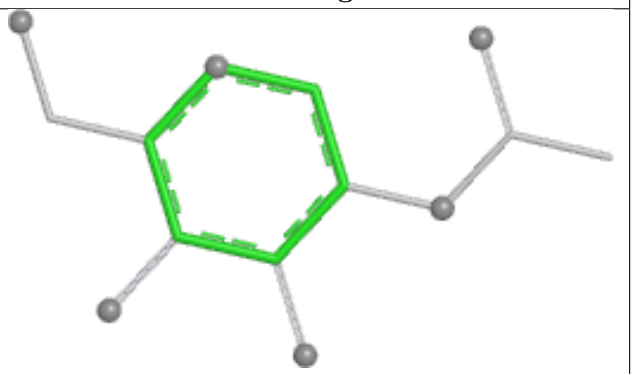
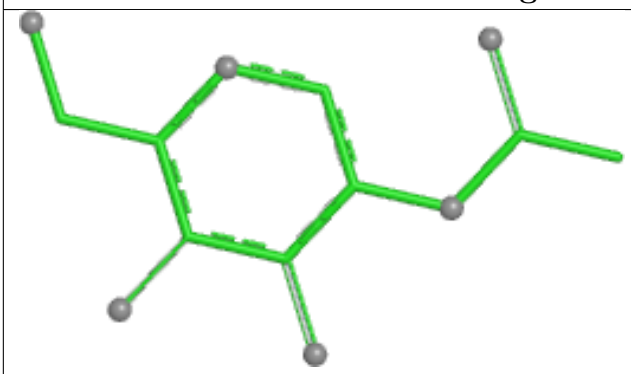


Rings

Ligand NAG A 603



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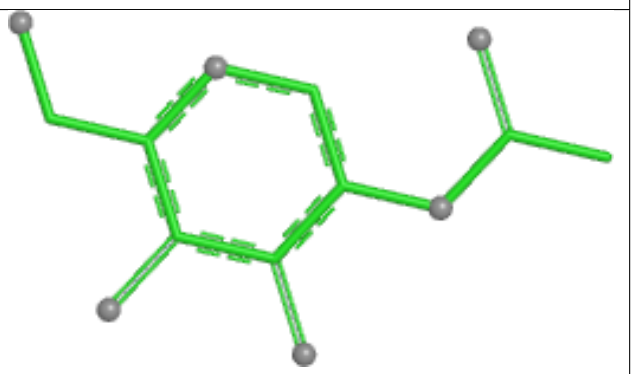
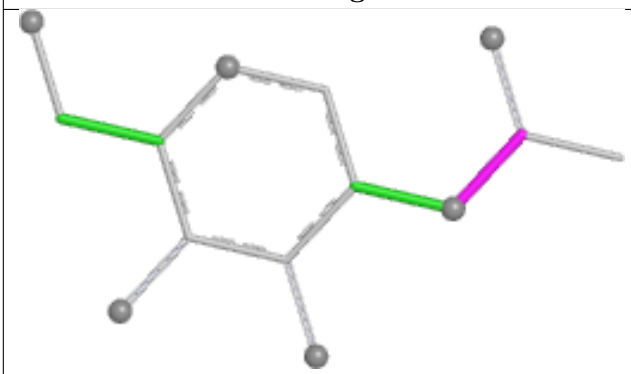


Bond angles



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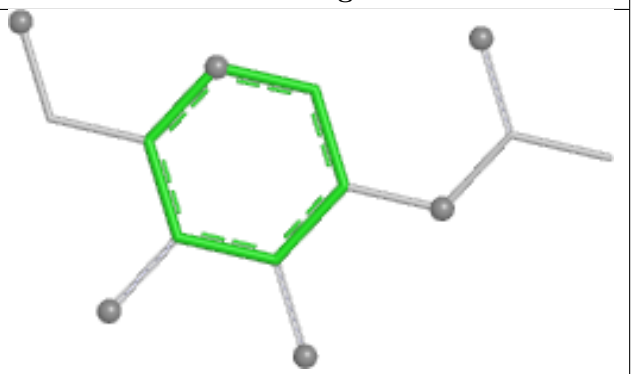
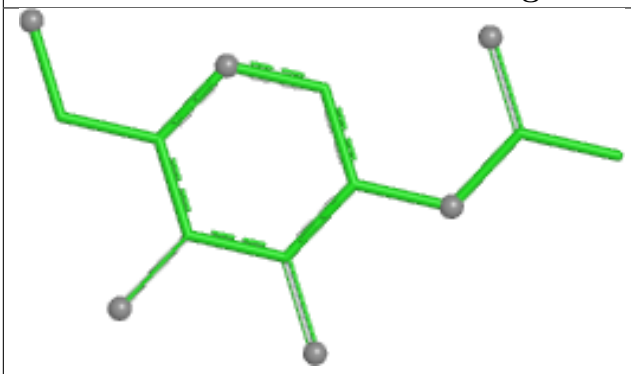
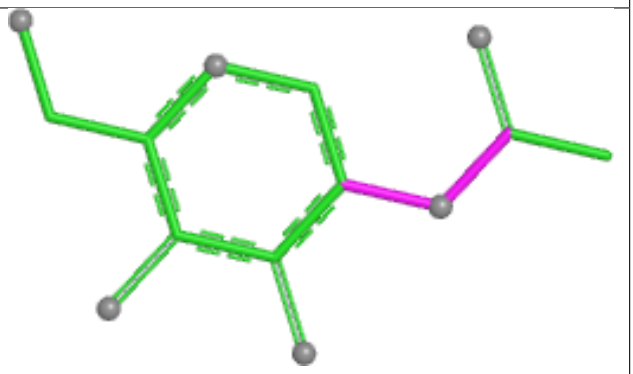


Rings

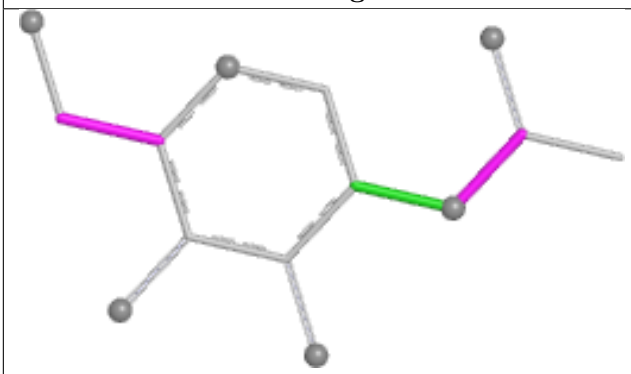
Ligand NAG F 701



Bond lengths



Bond angles



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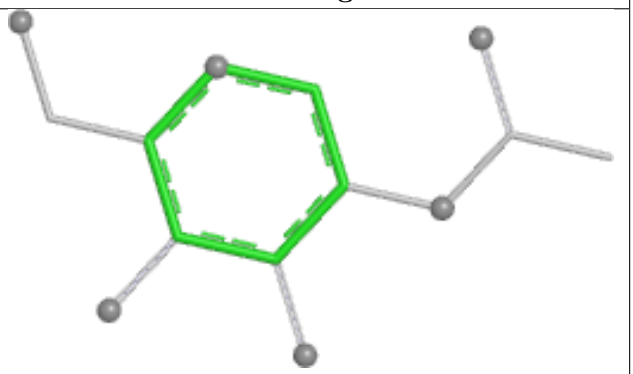
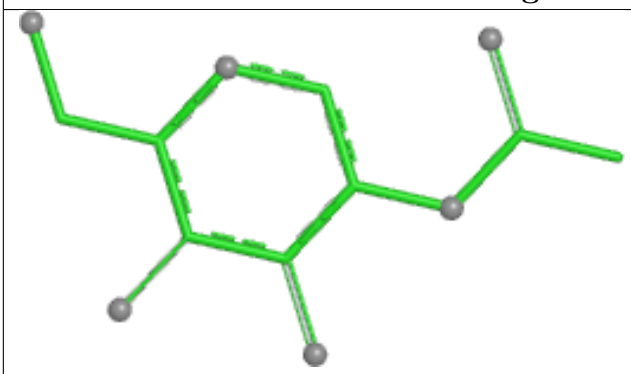
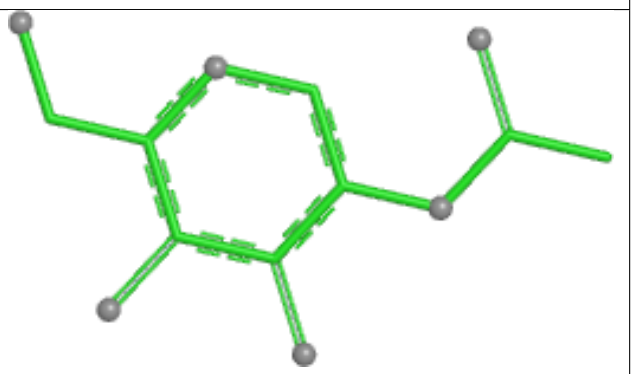


Rings

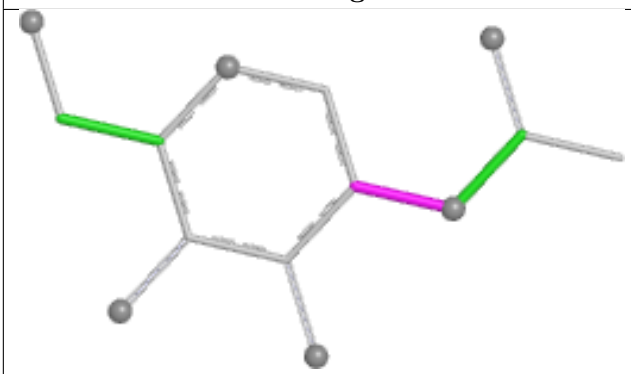
Ligand NAG E 605



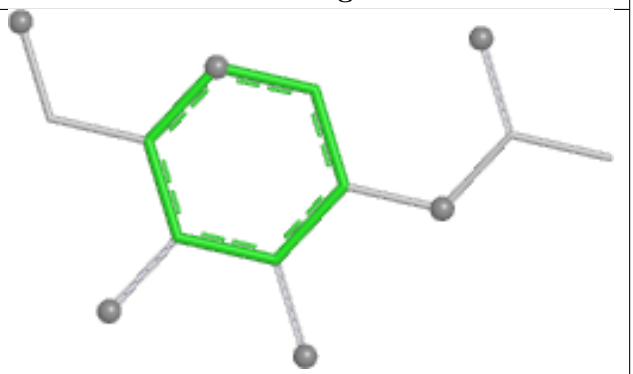
Bond lengths



Bond angles

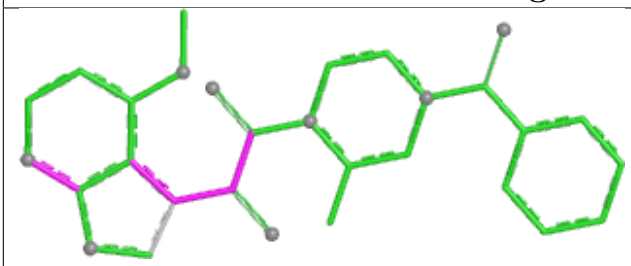


Torsions



Rings

Ligand 83G C 601



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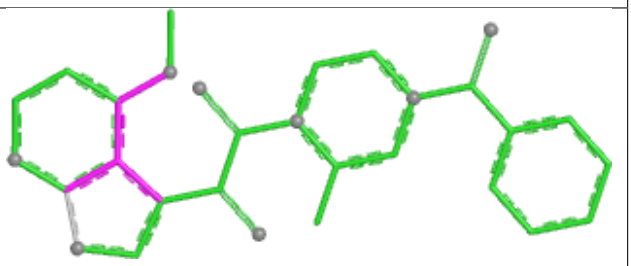
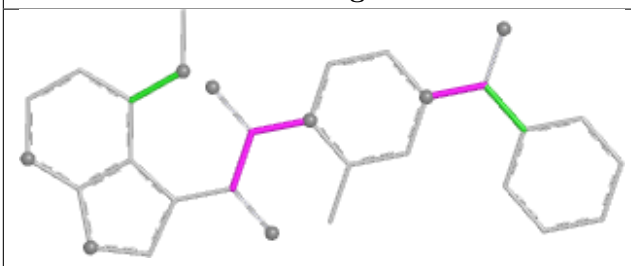


Bond angles



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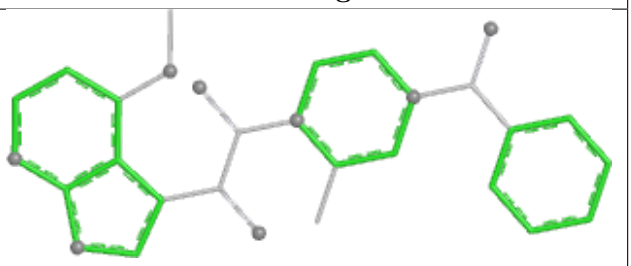
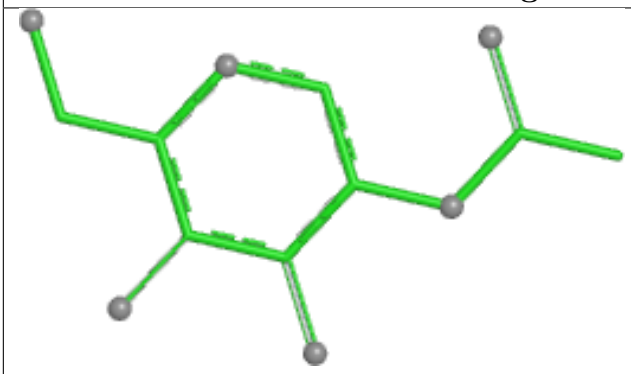
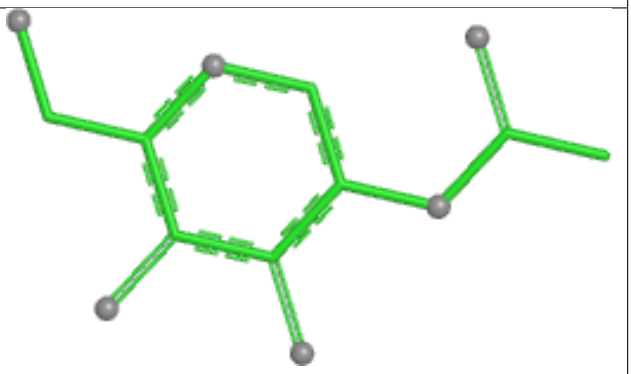


Rings

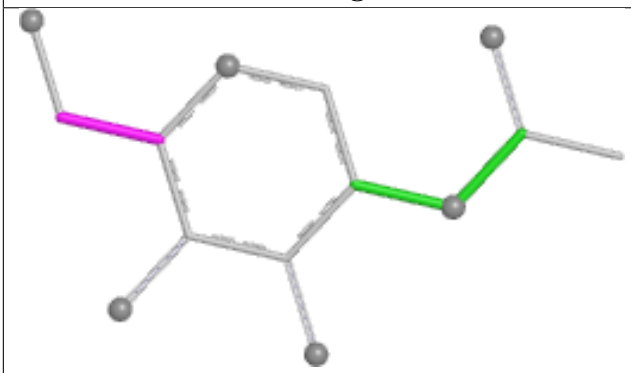
Ligand NAG B 702



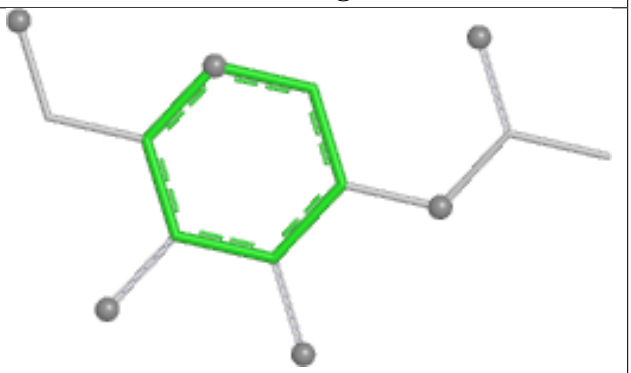
Bond lengths



Bond angles

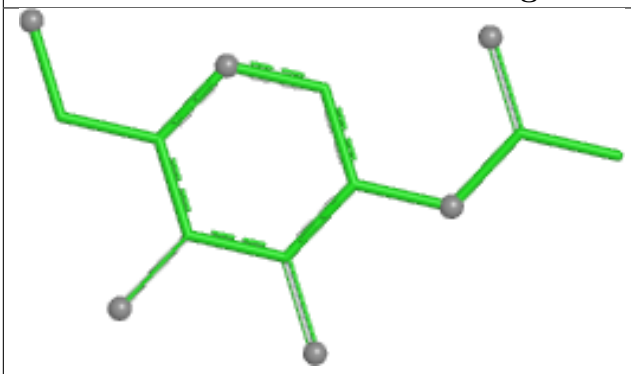


Torsions

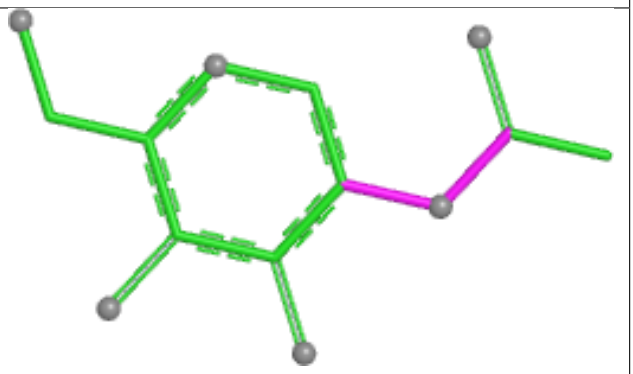


Rings

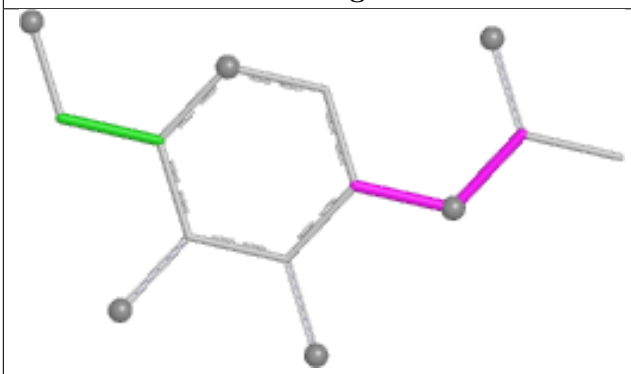
Ligand NAG C 604



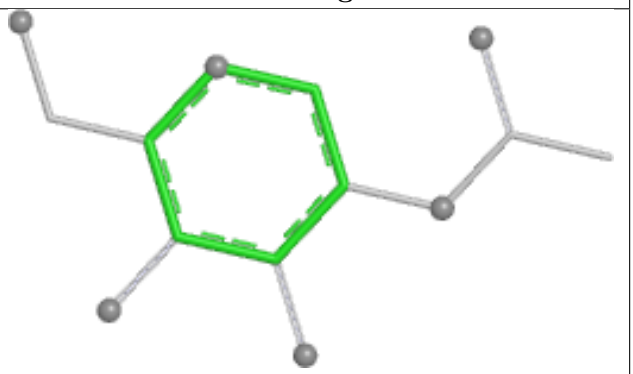
Bond lengths



Bond angles

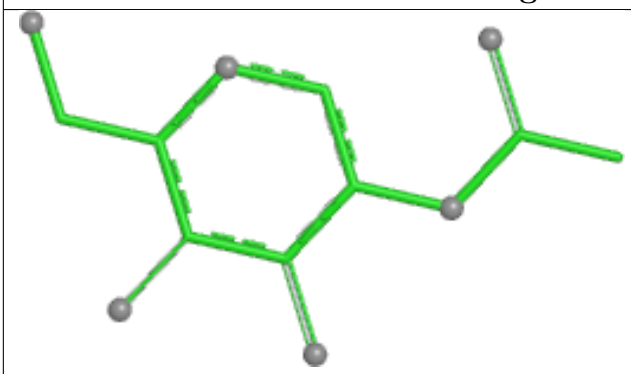


Torsions

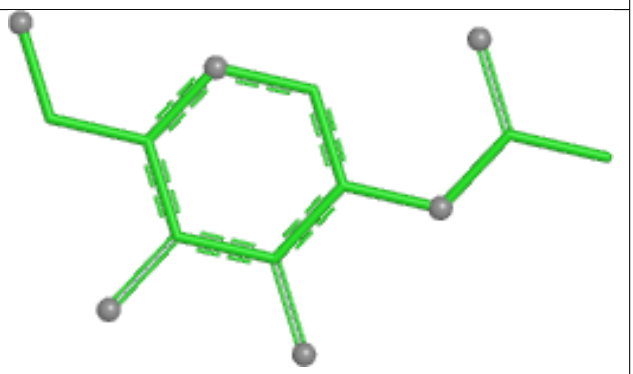


Rings

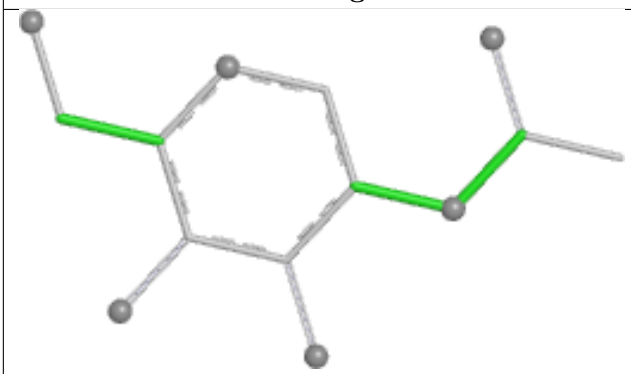
Ligand NAG A 602



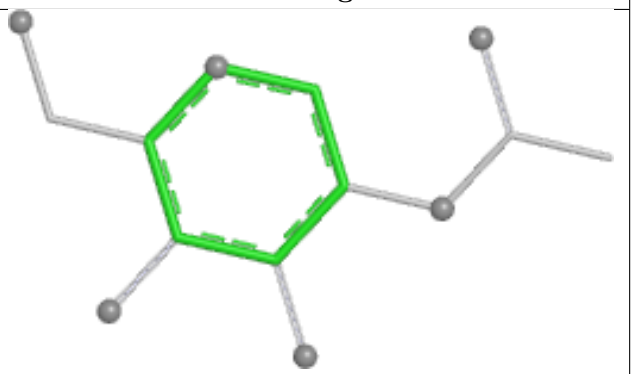
Bond lengths



Bond angles

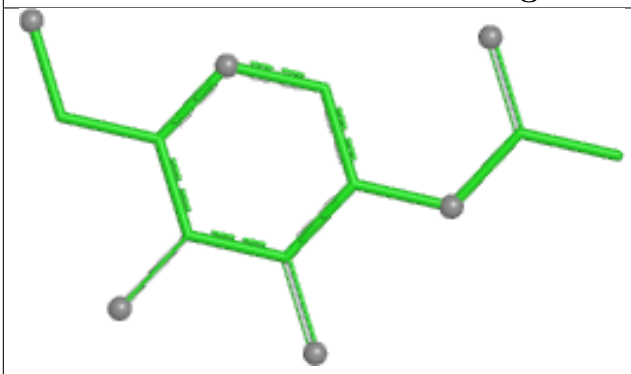


Torsions

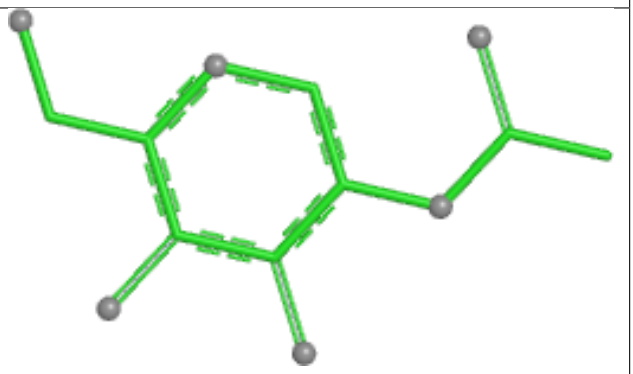


Rings

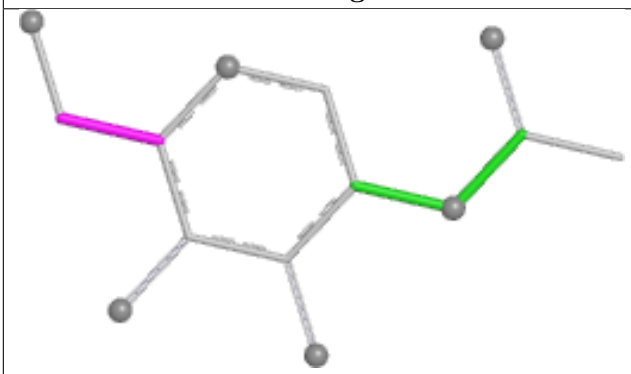
Ligand NAG C 603



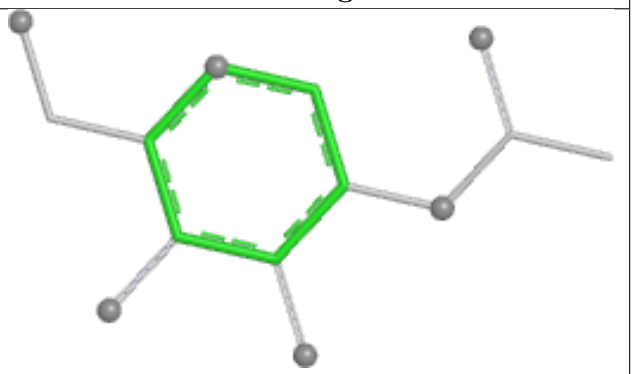
Bond lengths



Bond angles

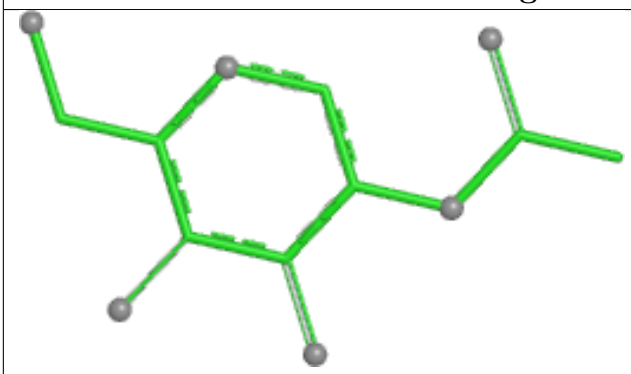


Torsions

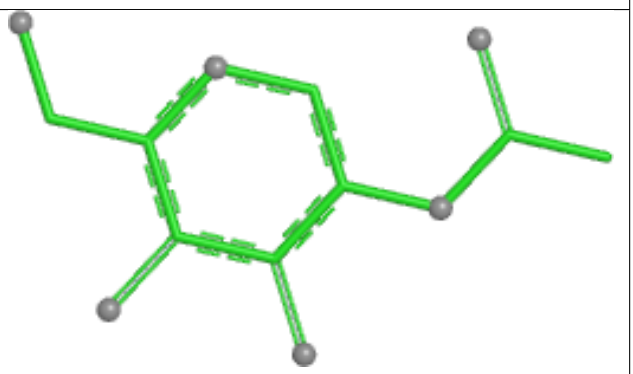


Rings

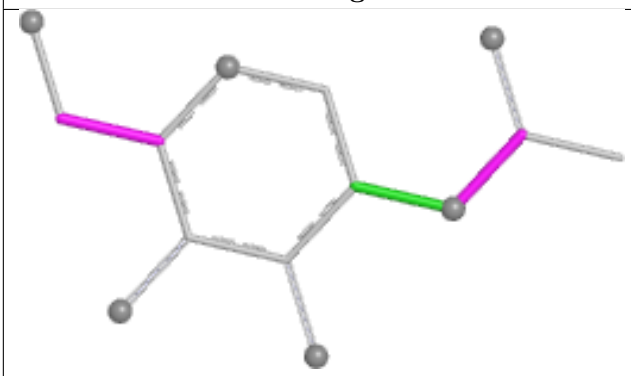
Ligand NAG D 701



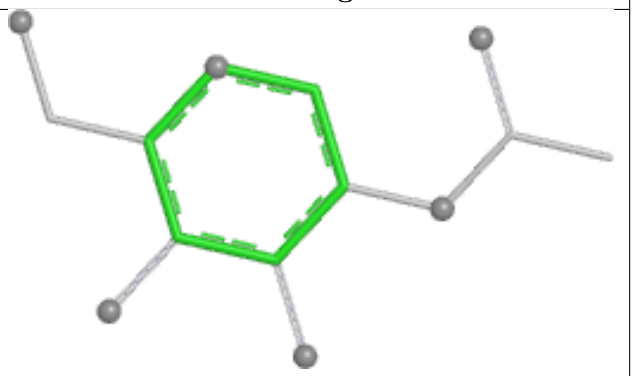
Bond lengths



Bond angles

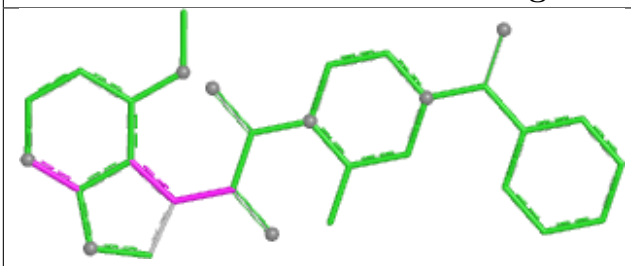


Torsions

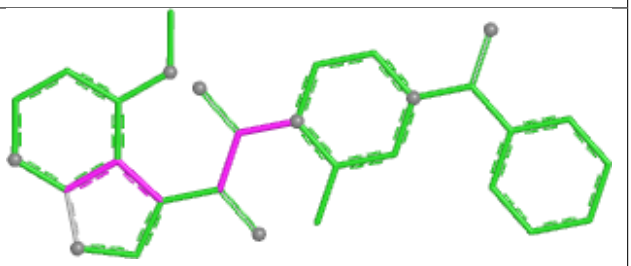


Rings

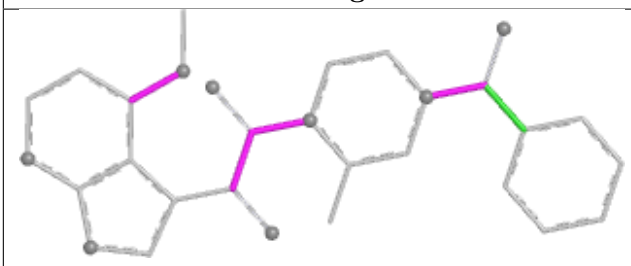
Ligand 83G A 601



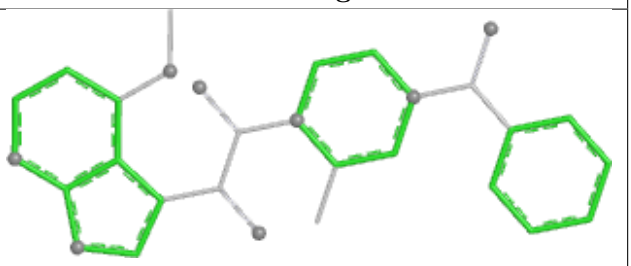
Bond lengths



Bond angles

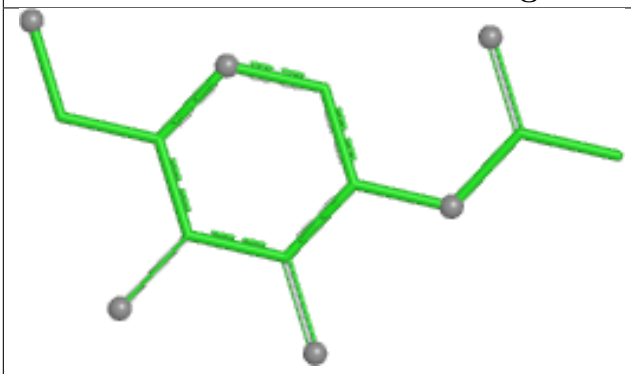


Torsions

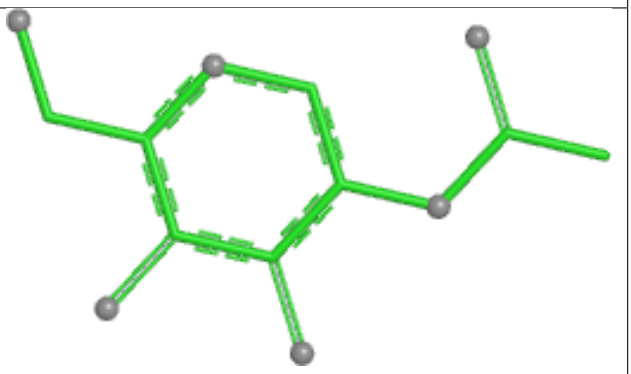


Rings

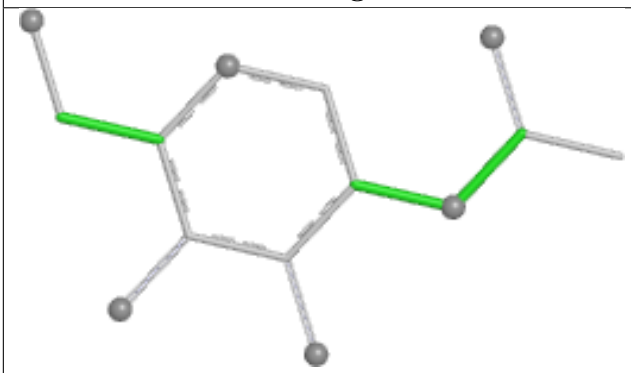
Ligand NAG C 602



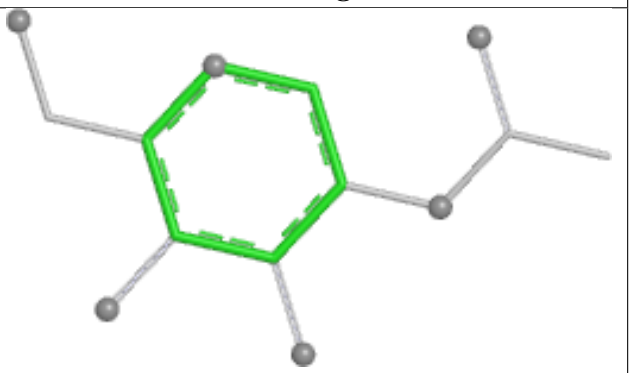
Bond lengths



Bond angles

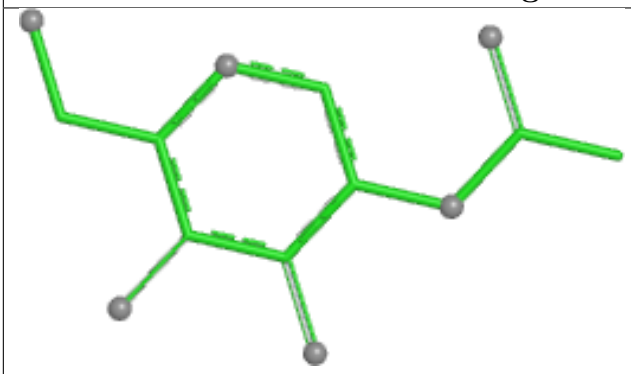


Torsions

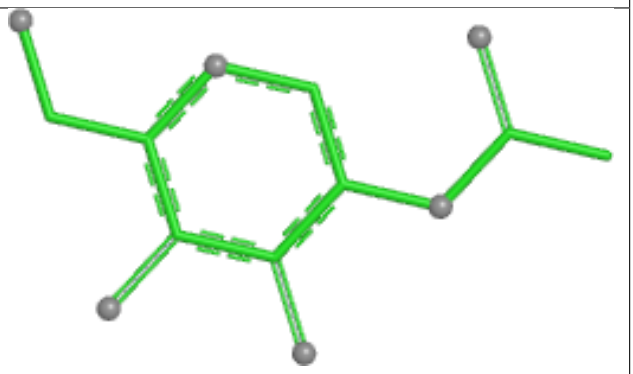


Rings

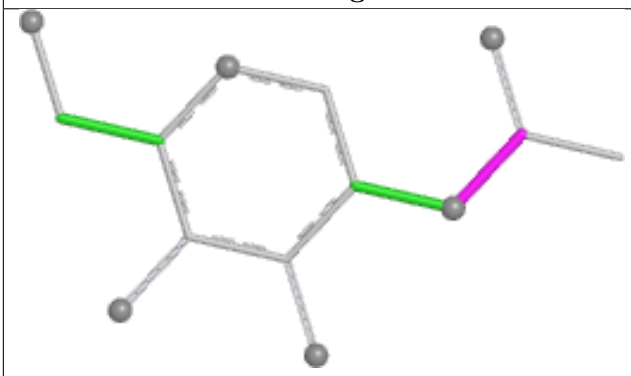
Ligand NAG E 603



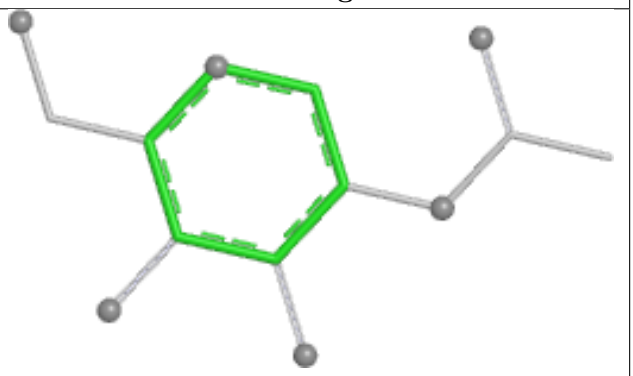
Bond lengths



Bond angles

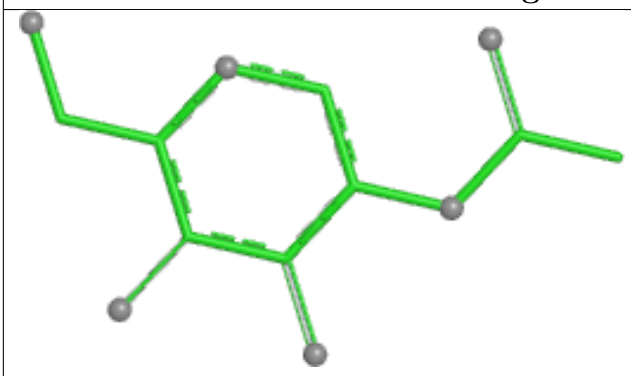


Torsions

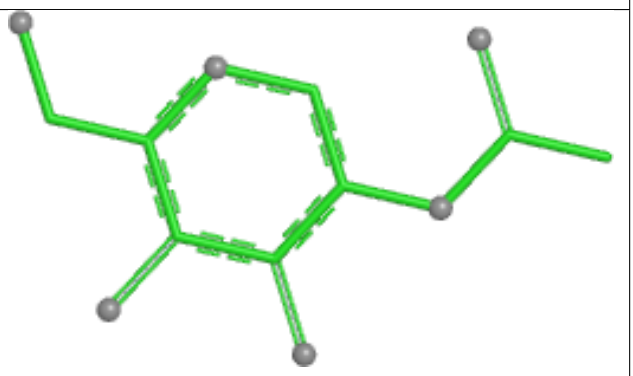


Rings

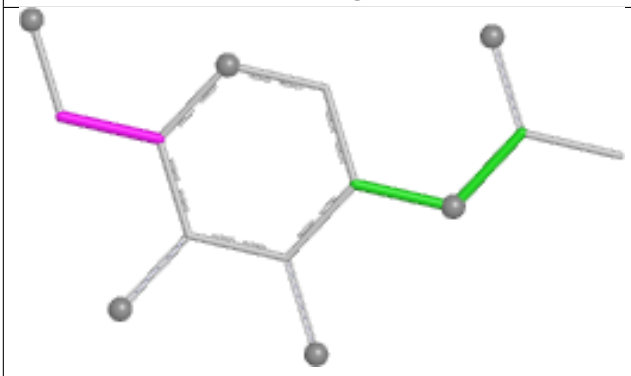
Ligand NAG F 702



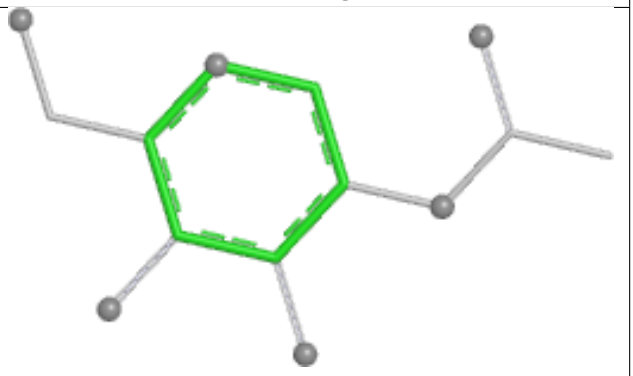
Bond lengths



Bond angles

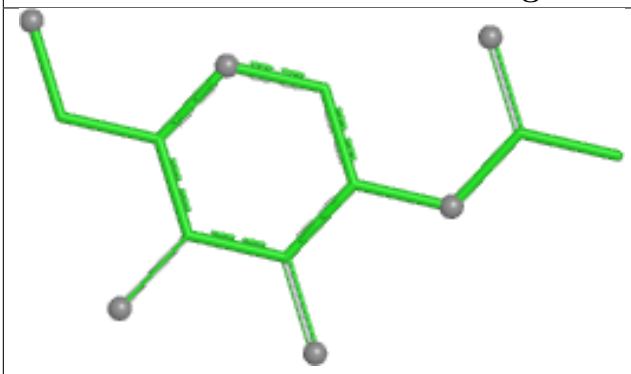


Torsions

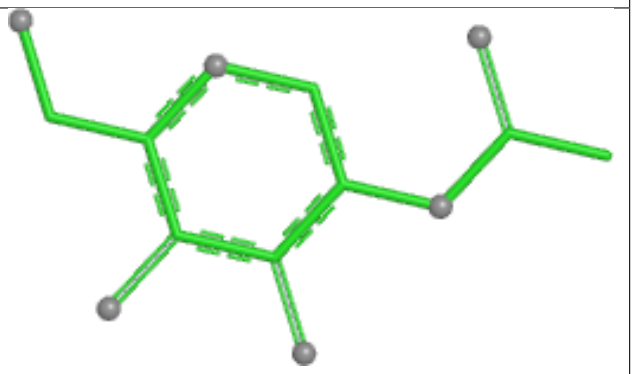


Rings

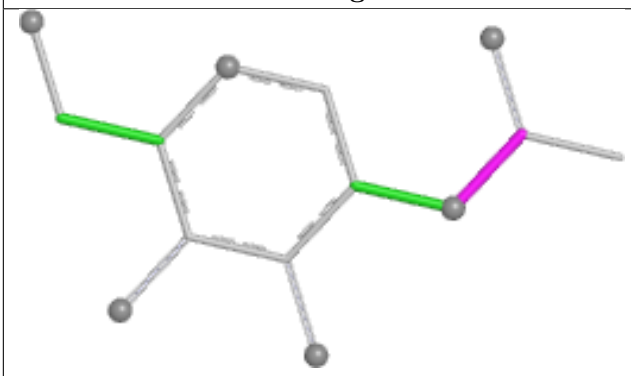
Ligand NAG F 703



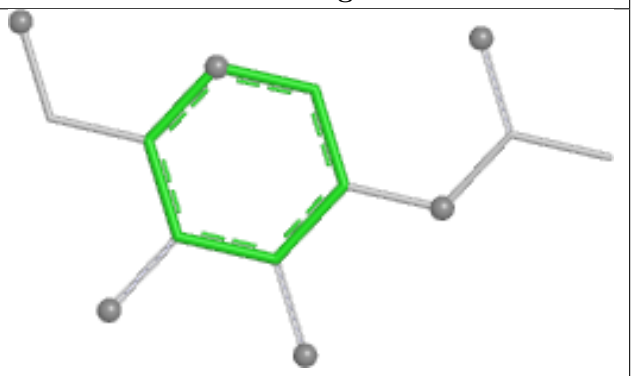
Bond lengths



Bond angles

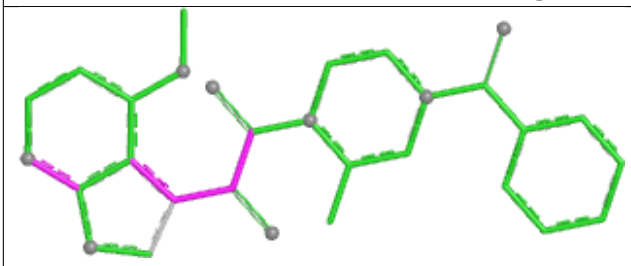


Torsions

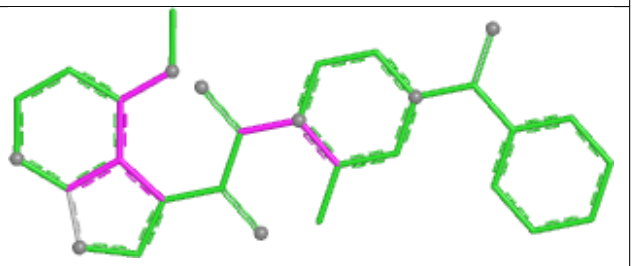


Rings

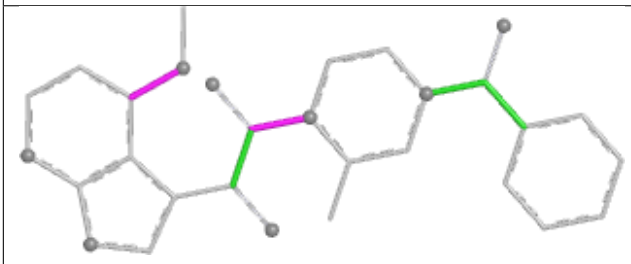
Ligand 83G E 601



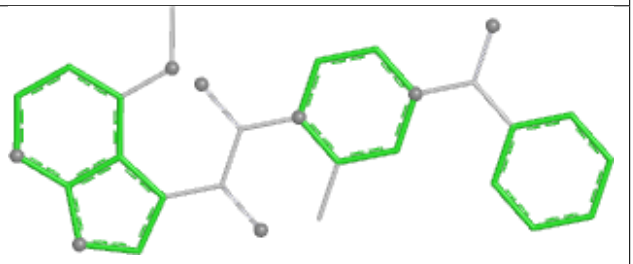
Bond lengths



Bond angles

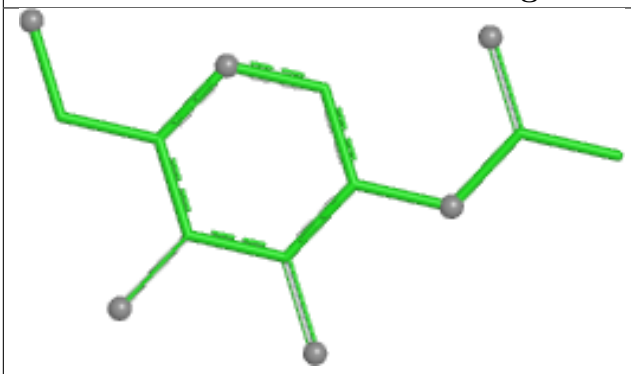


Torsions

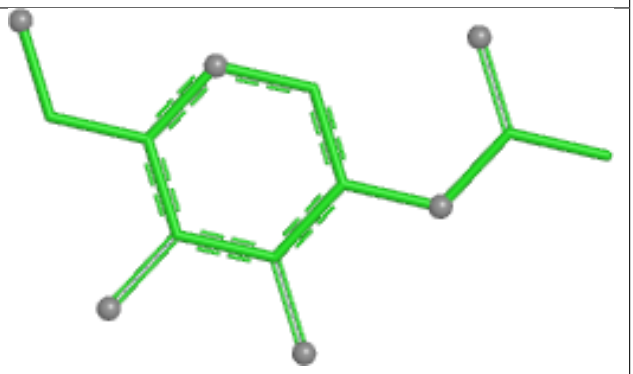


Rings

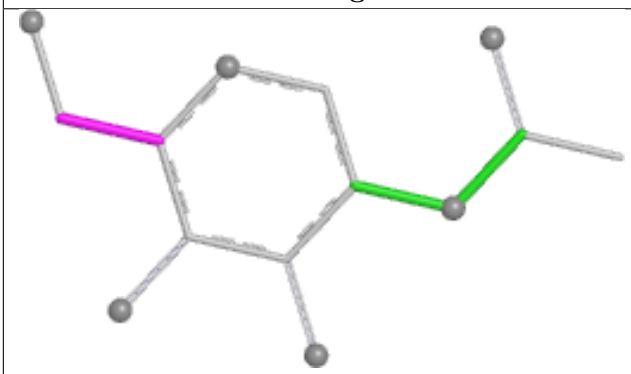
Ligand NAG B 703



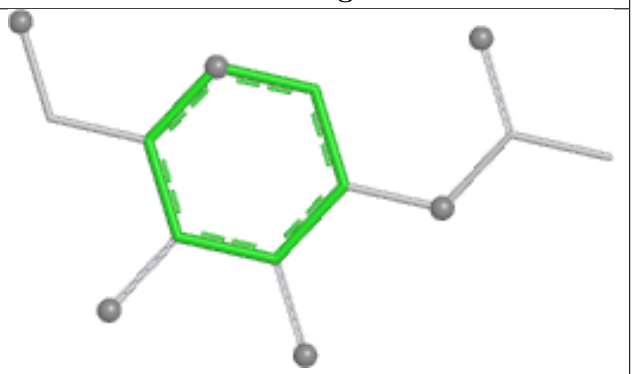
Bond lengths



Bond angles

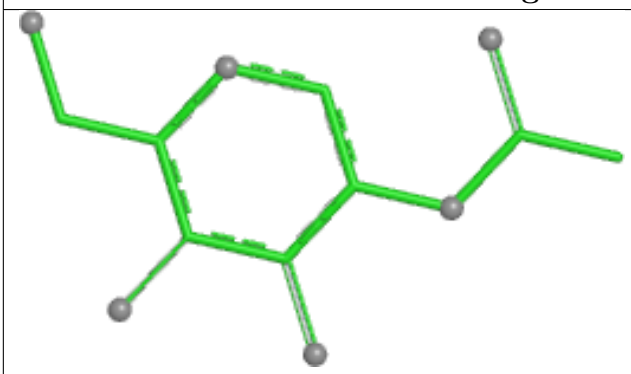


Torsions

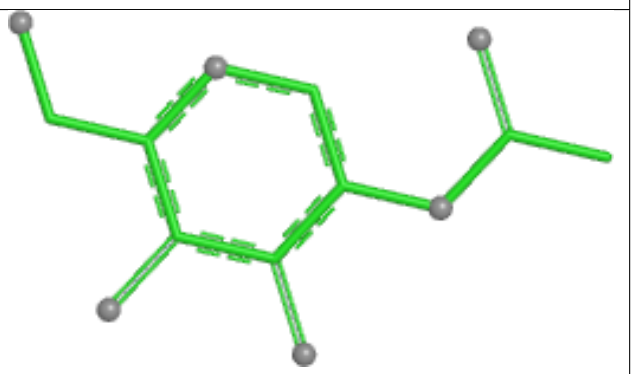


Rings

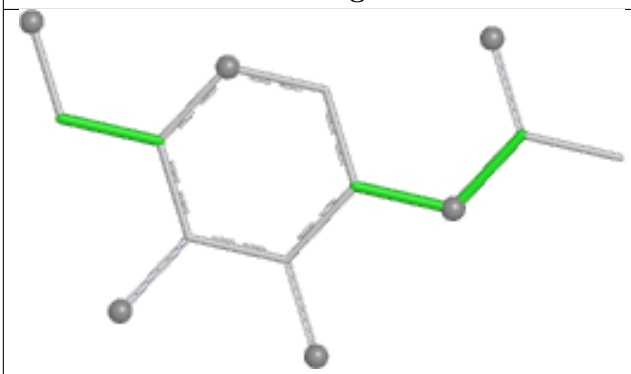
Ligand NAG E 602



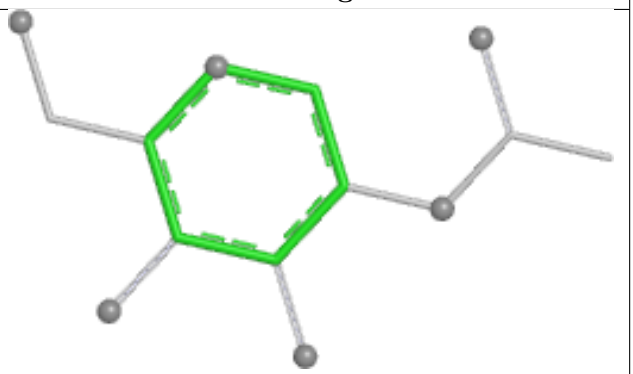
Bond lengths



Bond angles

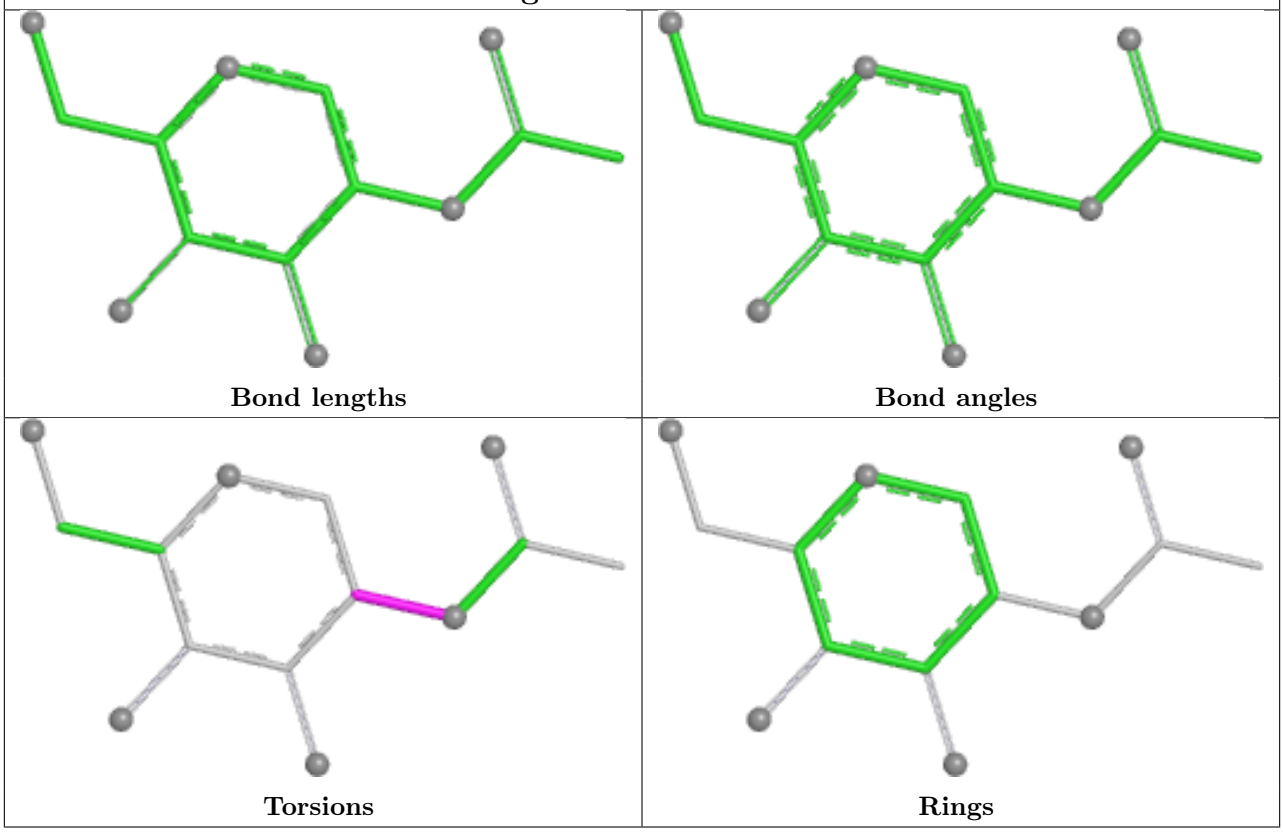


Torsions



Rings

Ligand NAG C 605



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.

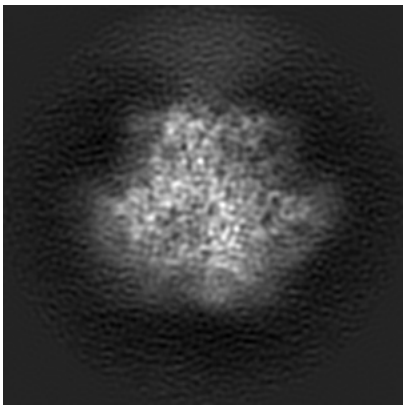
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28953. These allow visual inspection of the internal detail of the map and identification of artifacts.

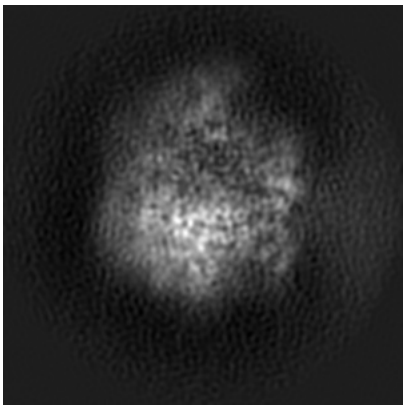
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

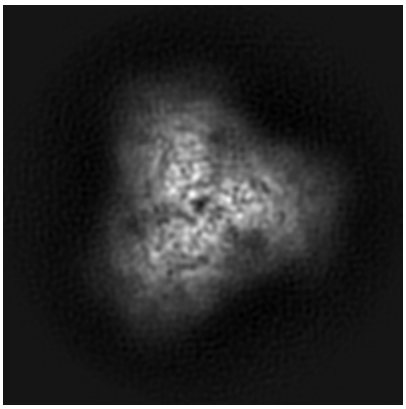
6.1.1 Primary map



X

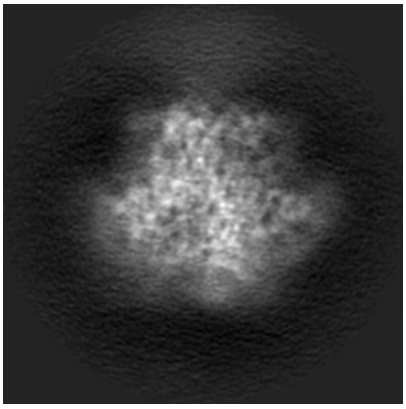


Y

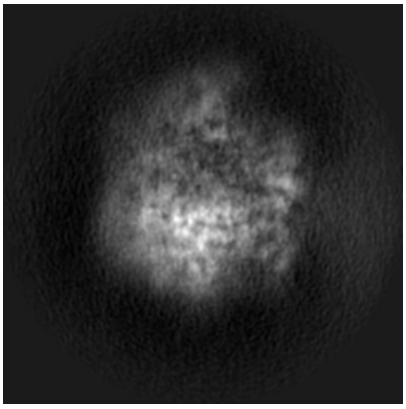


Z

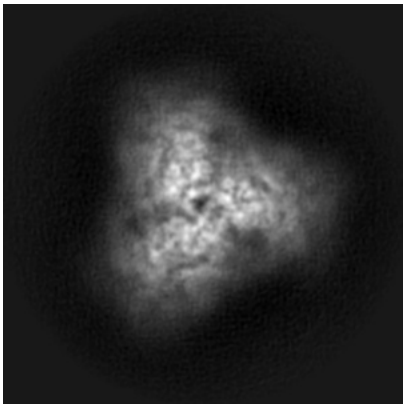
6.1.2 Raw map



X



Y

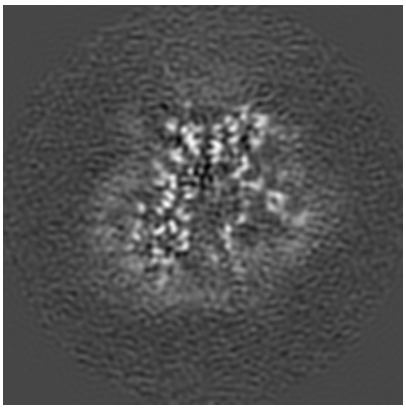


Z

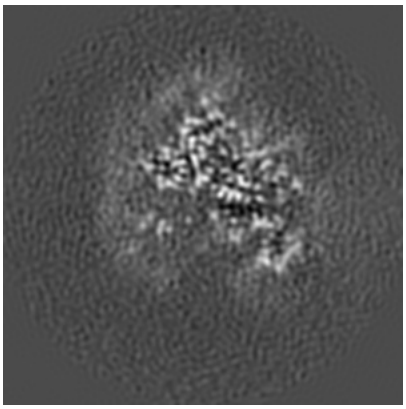
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

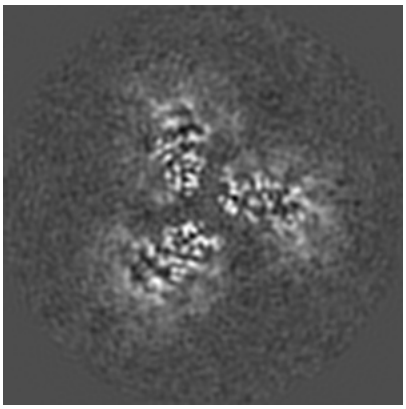
6.2.1 Primary map



X Index: 84

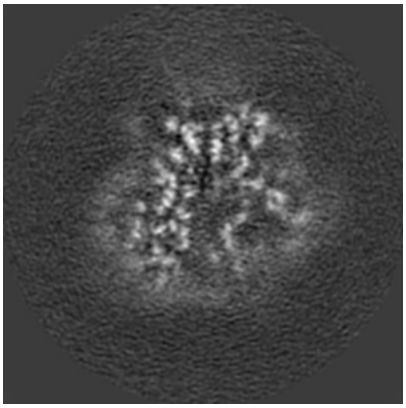


Y Index: 84

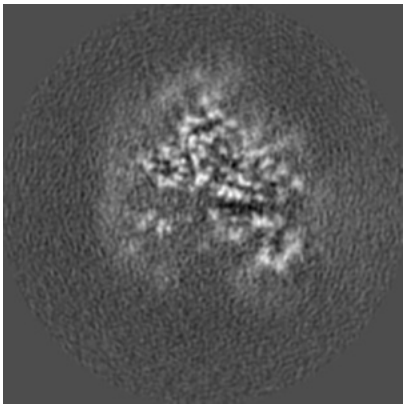


Z Index: 84

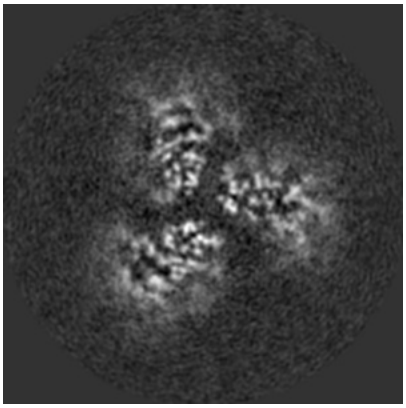
6.2.2 Raw map



X Index: 84



Y Index: 84

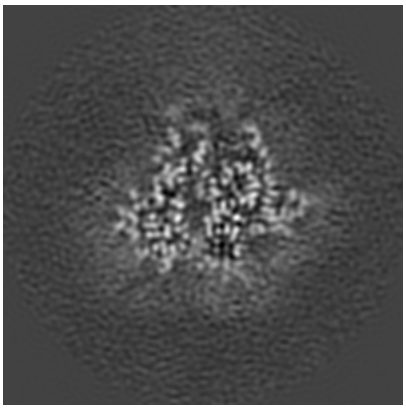


Z Index: 84

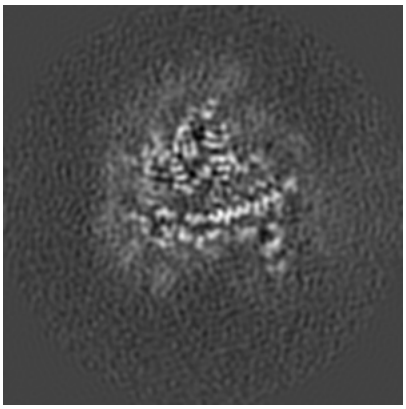
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

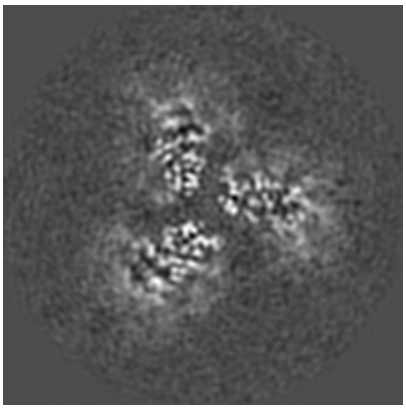
6.3.1 Primary map



X Index: 77

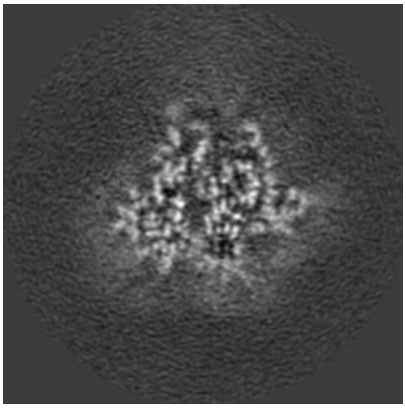


Y Index: 88

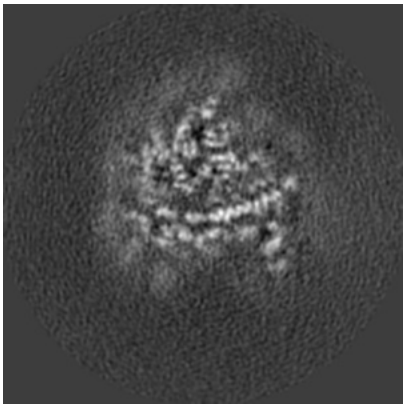


Z Index: 84

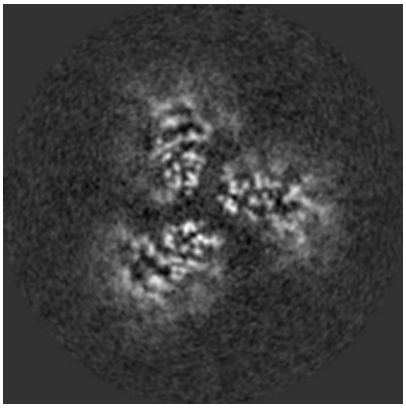
6.3.2 Raw map



X Index: 77



Y Index: 88

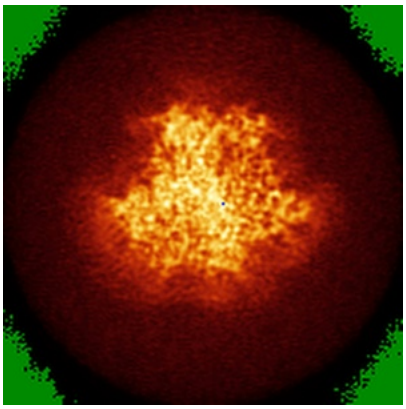


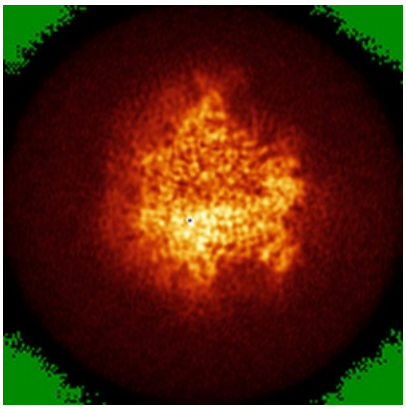
Z Index: 84

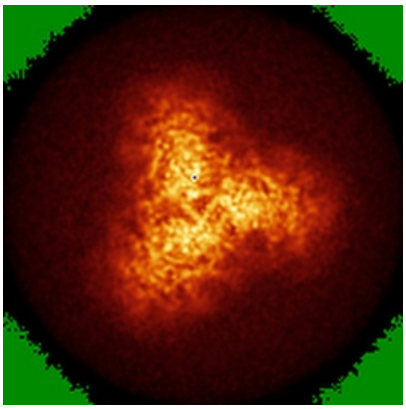
The images above show the largest variance slices of the map in three orthogonal directions.

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

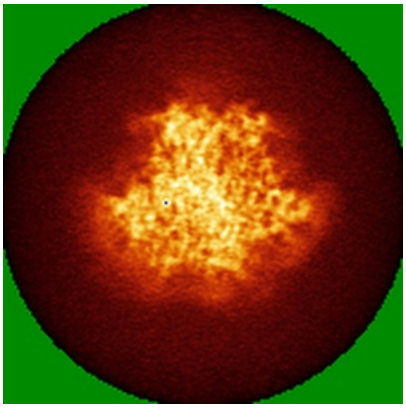
6.4.1 Primary map

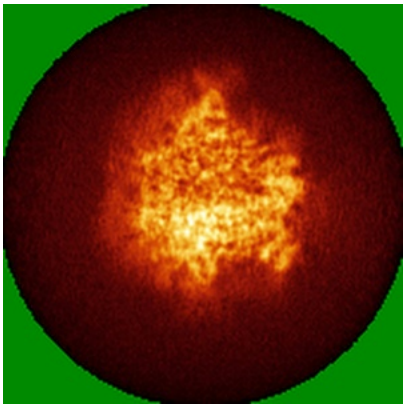

X

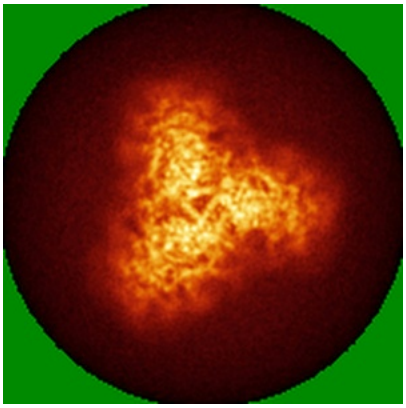

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

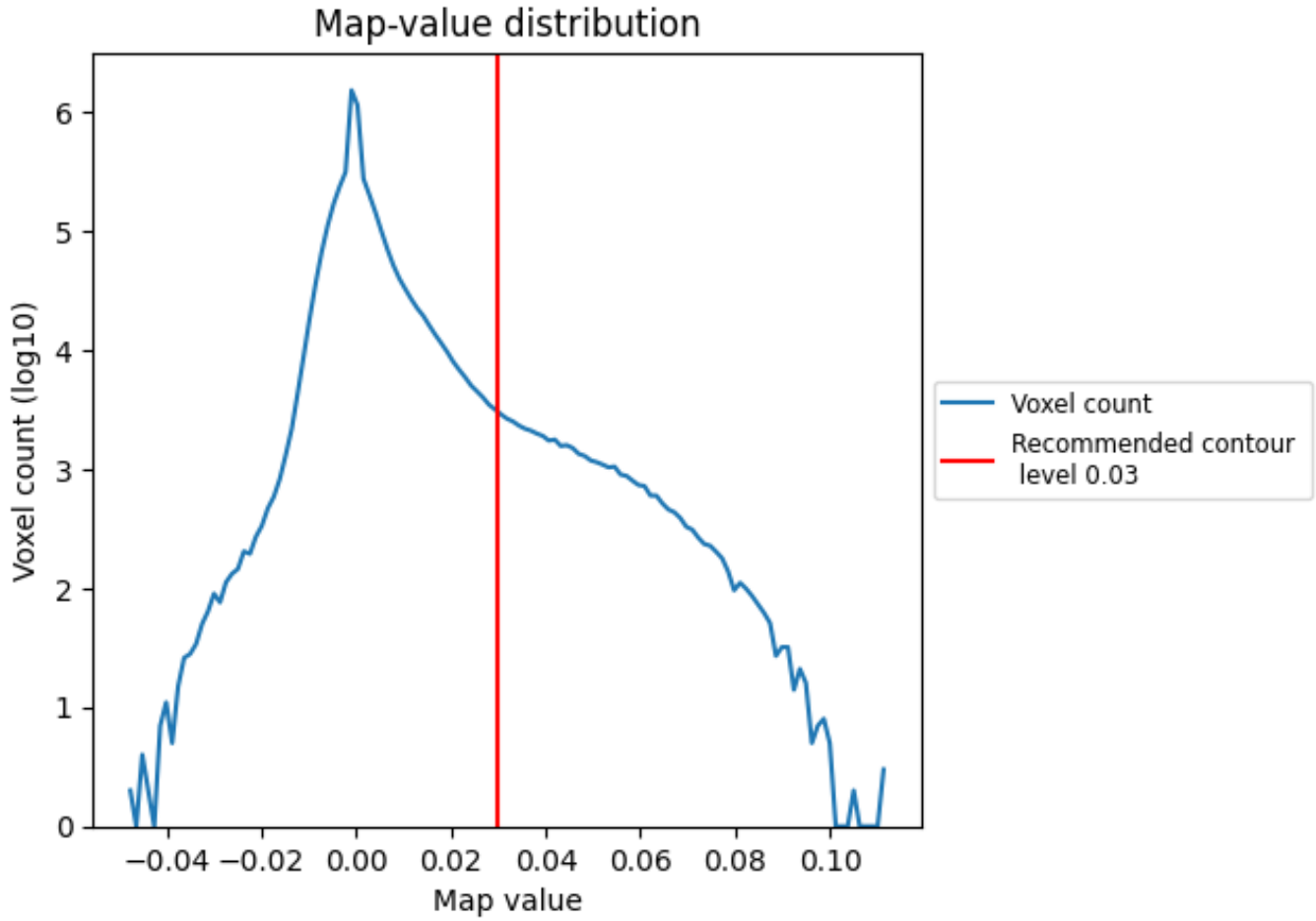
6.6 Mask visualisation (i)

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

7 Map analysis

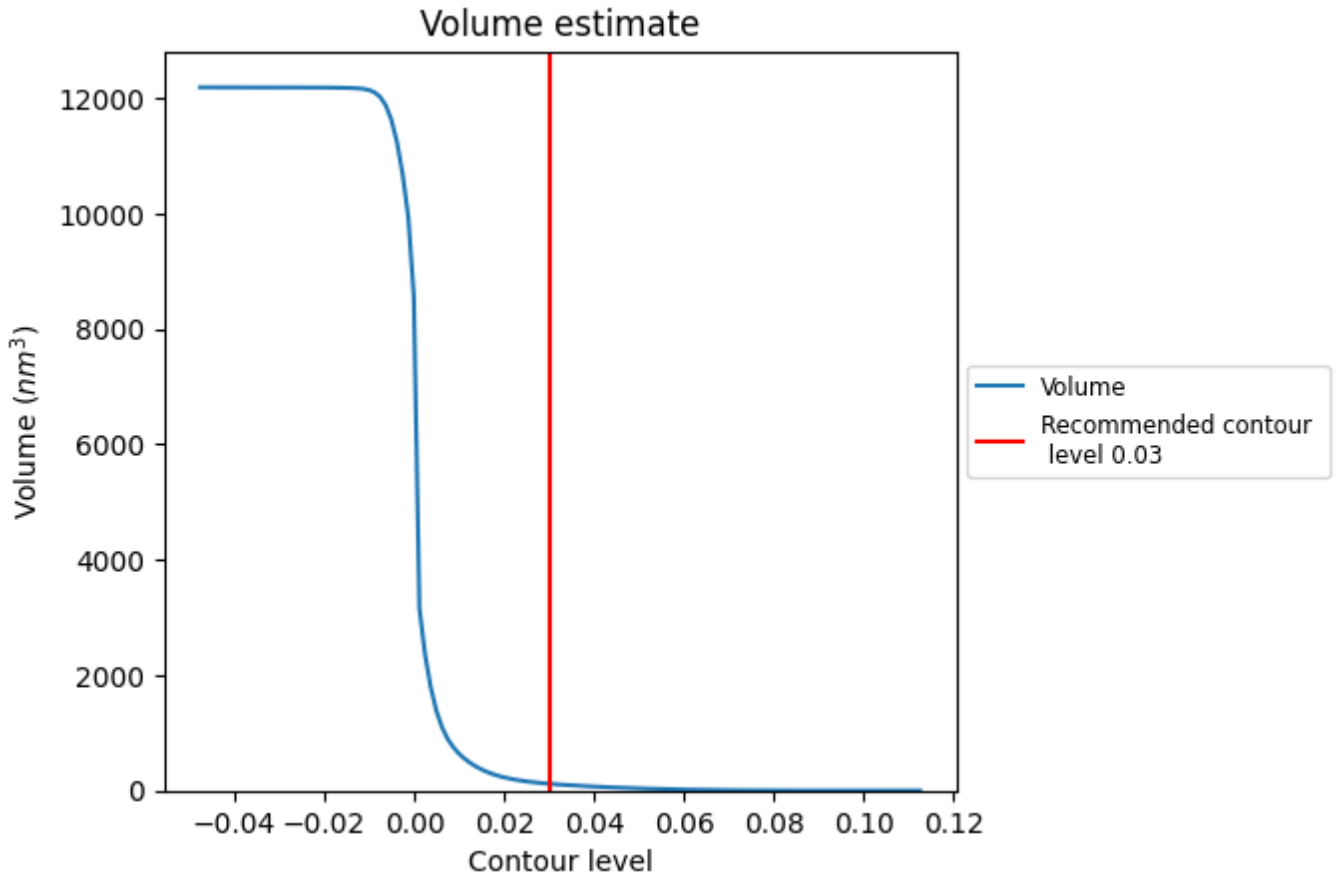
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

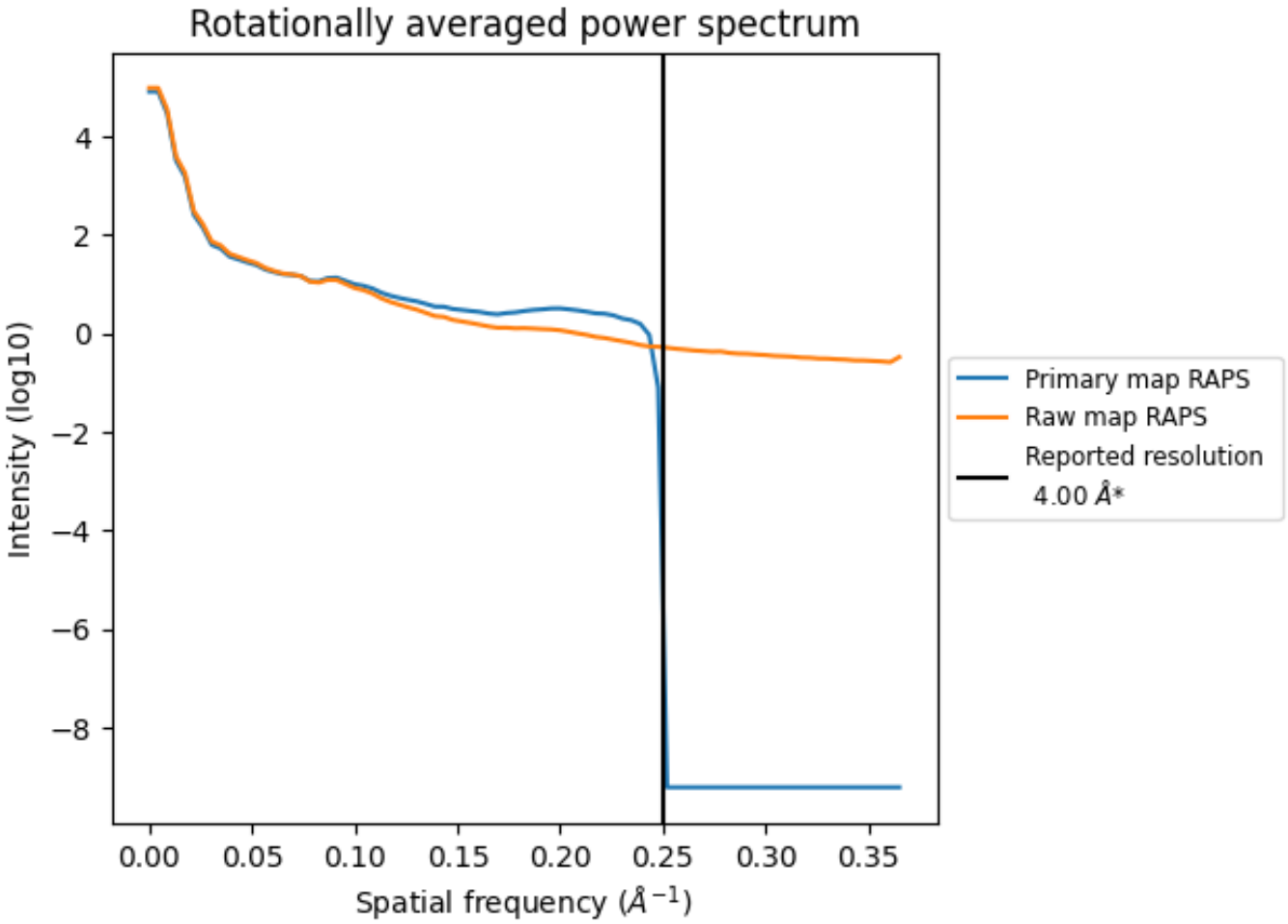
7.2 Volume estimate



The volume at the recommended contour level is 118 nm^3; this corresponds to an approximate mass of 107 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)

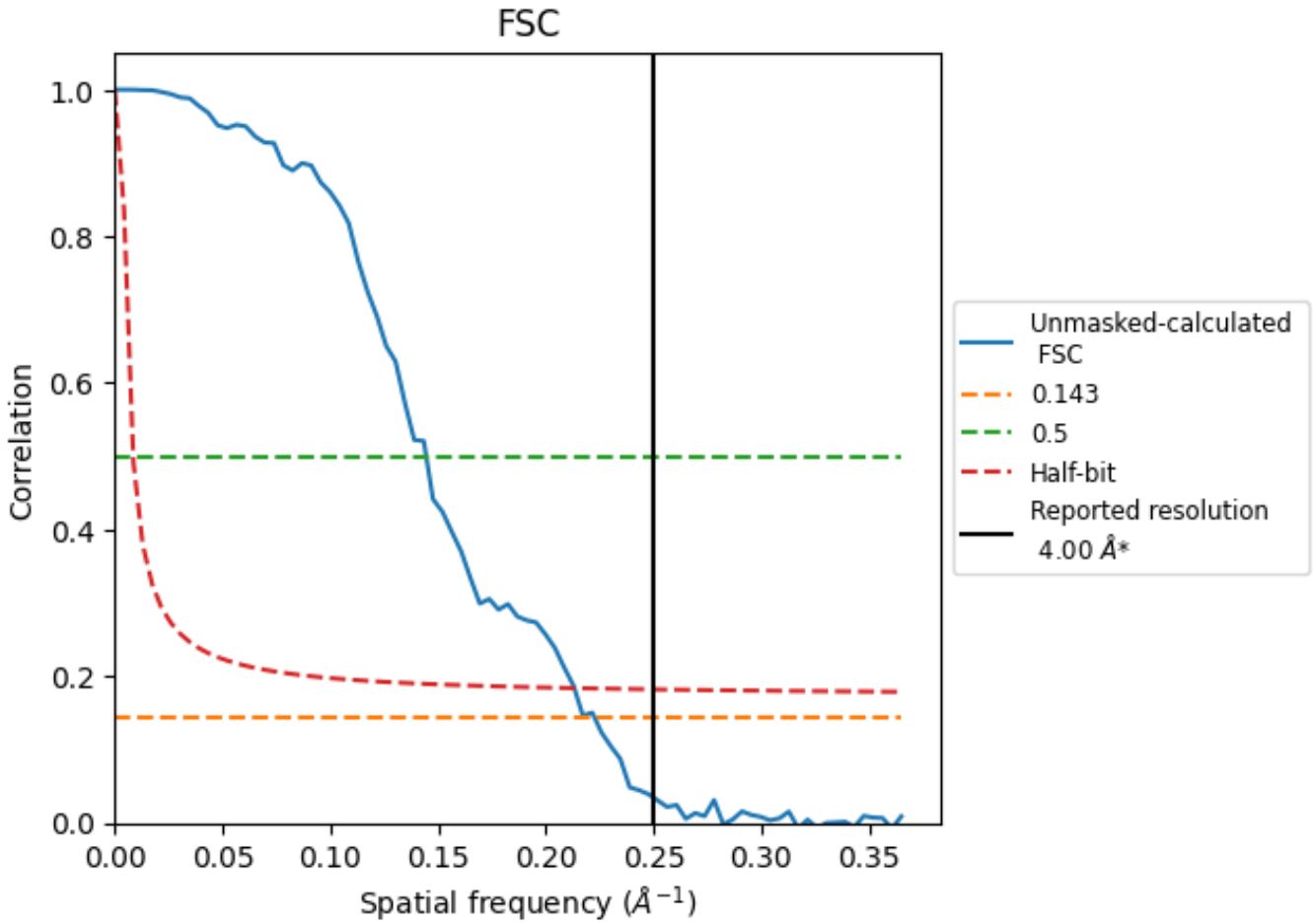


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

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 0.250 Å^{-1}

8.2 Resolution estimates (i)

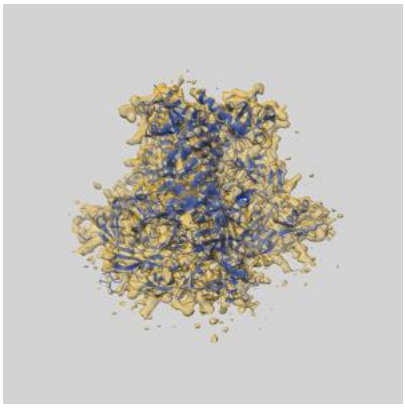
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.49	6.92	4.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.49 differs from the reported value 4.0 by more than 10 %

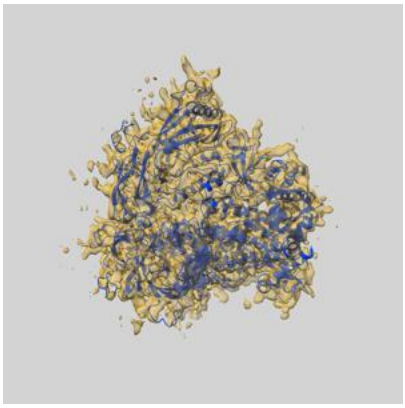
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28953 and PDB model 8FAD. Per-residue inclusion information can be found in section 3 on page 13.

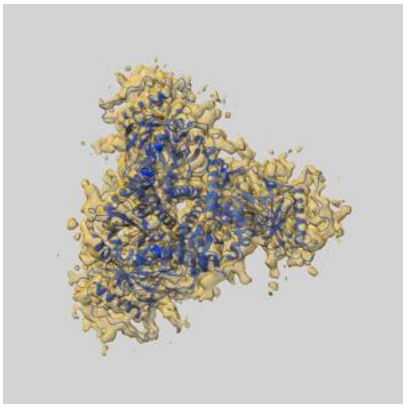
9.1 Map-model overlay



X



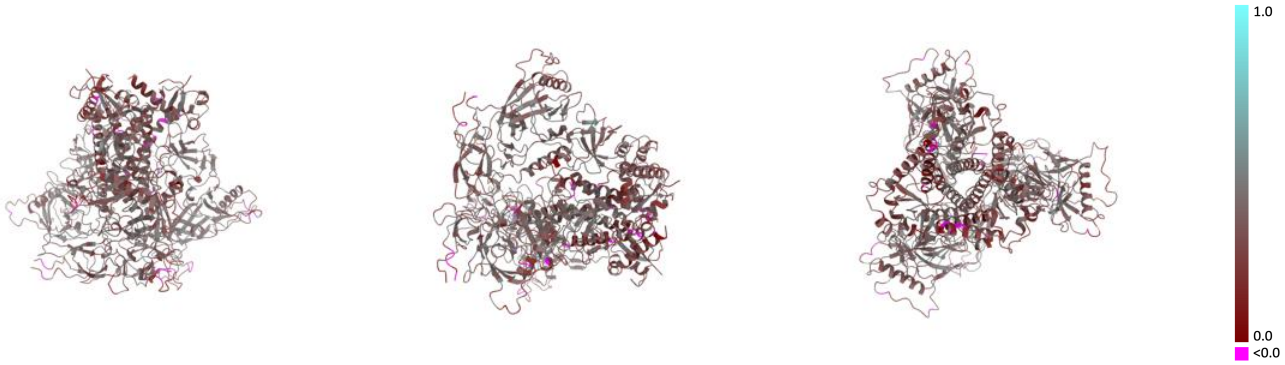
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

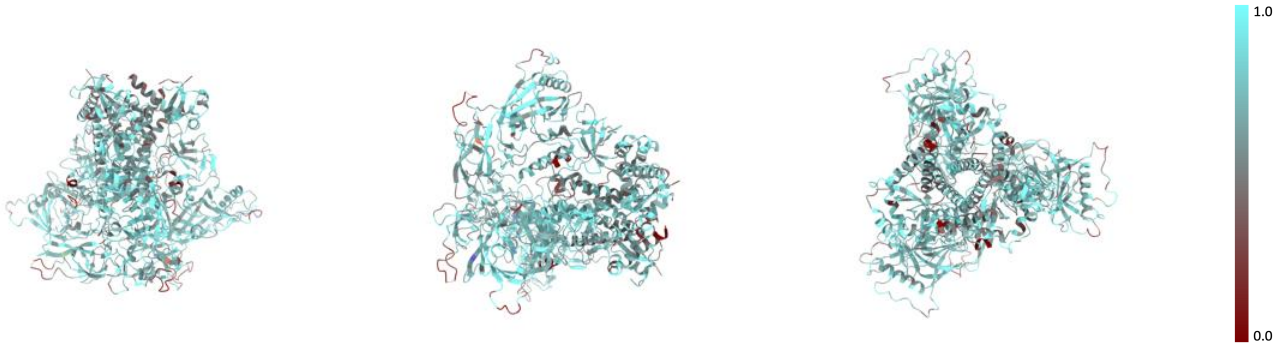
9.2 Q-score mapped to coordinate model



X Y Z

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

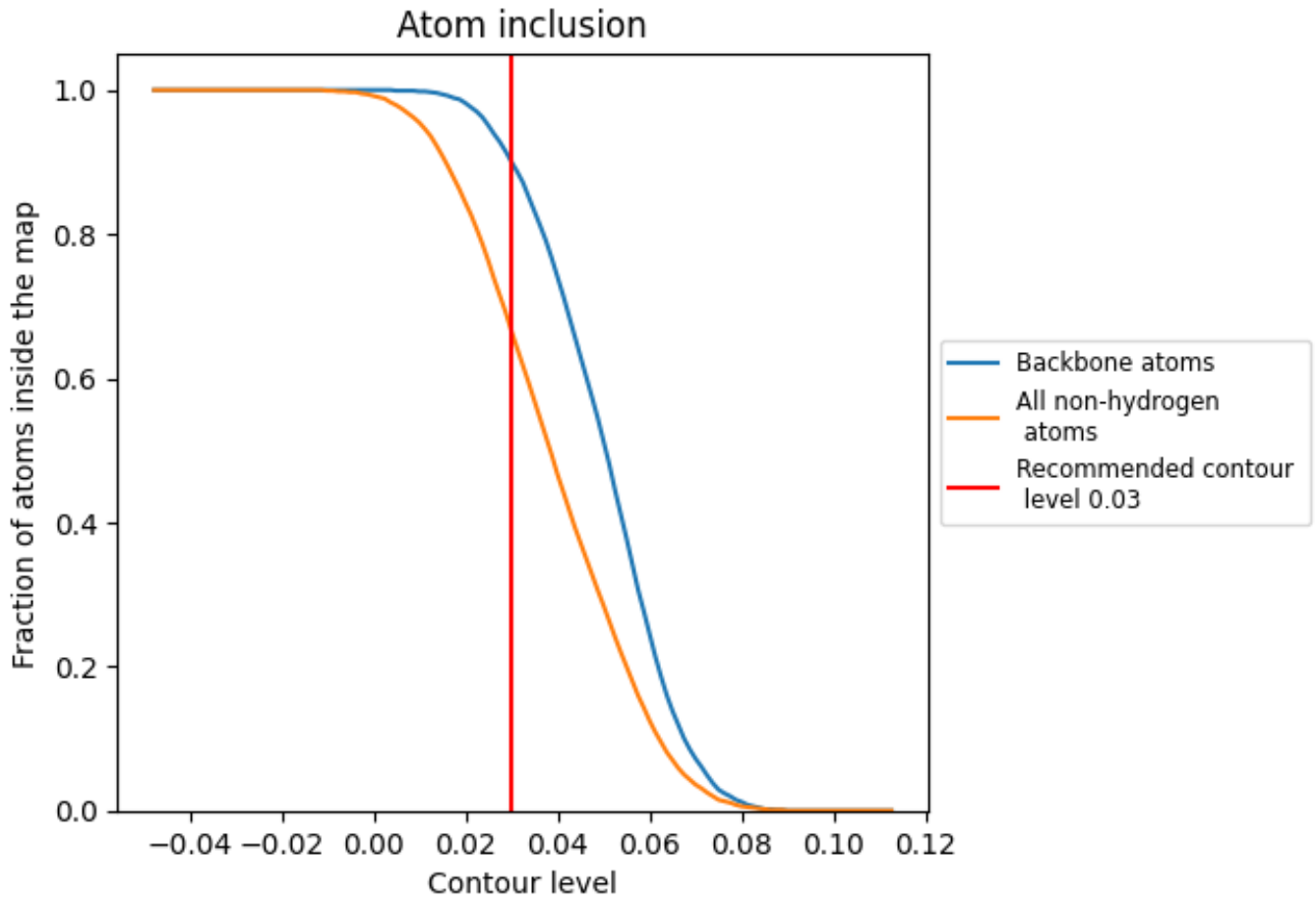
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6650	0.3320
0	0.3930	0.2670
1	0.5000	0.1870
A	0.7060	0.3540
B	0.6430	0.2900
C	0.7070	0.3600
D	0.6380	0.2780
E	0.6880	0.3430
F	0.6010	0.2770
G	0.5360	0.2880
H	0.3570	0.2770
I	0.5710	0.3930
J	0.4100	0.2790
K	0.5360	0.3370
L	0.3570	0.3160
M	0.6530	0.3000
N	0.3590	0.2460
O	0.5360	0.4380
P	0.5000	0.3340
Q	0.5130	0.3580
R	0.5400	0.2210
S	0.5000	0.2300
T	0.4870	0.2560
U	0.5360	0.3300
V	0.5360	0.3960
W	0.4640	0.2640
X	0.4290	0.3100
Y	0.3570	0.2600
Z	0.4360	0.1850
a	0.6070	0.2640
b	0.3570	0.2830
c	0.7050	0.3650
d	0.4640	0.2670
e	0.4290	0.2770
f	0.6430	0.4330

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Chain	Atom inclusion	Q-score
g	0.6410	0.3880
h	0.5080	0.2460
i	0.4640	0.2660
j	0.5380	0.3320
k	0.3570	0.3460
l	0.4290	0.2670
m	0.2500	0.1870
n	0.3930	0.2320
o	0.5360	0.2790
p	0.4290	0.1080
q	0.5000	0.4070
r	0.5690	0.2820
s	0.5710	0.2890
t	0.3930	0.3070
u	0.6790	0.3640
v	0.4640	0.2170
w	0.5640	0.2970
x	0.4640	0.1620
y	0.6070	0.3960
z	0.2860	0.1980