wwPDB EM Validation Summary Report (i)

Nov 3, 2024 – 08:38 AM EST

PDB ID	:	6VY2
EMDB ID	:	EMD-21456
Title	:	Cryo-EM structure of M1214_N1 Fab in complex with CH505 TF chimeric SOSIP.664 Env trimer
Authors	:	Chan, K.-W.; Kong, X.P.
Deposited on	:	2020-02-25
Resolution	:	4.86 Å(reported)
Based on initial model	:	6UDA

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

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

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

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

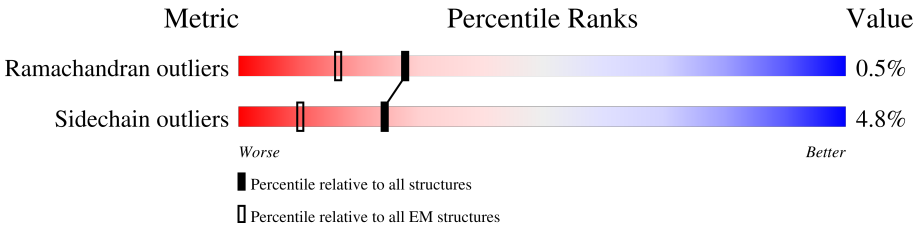
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 4.86 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	A	487	8% 89% 5% 6%
1	C	487	7% 89% 6% 6%
1	E	487	7% 89% 5% 6%
2	B	160	74% 24%
2	D	160	74% 24%
2	F	160	74% 24%
3	H	226	52% 45%
3	I	226	52% 45%
3	J	226	52% 45%

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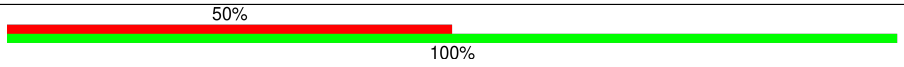
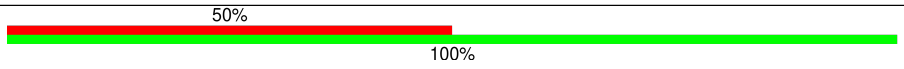
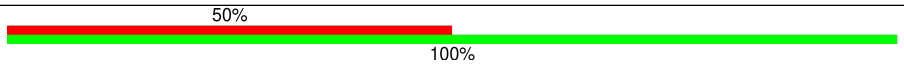
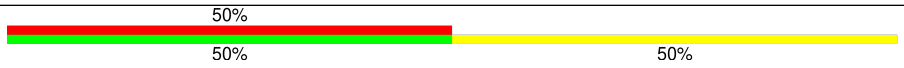
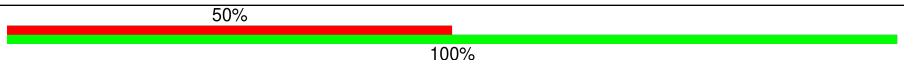
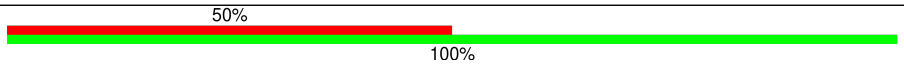
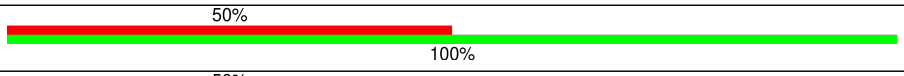
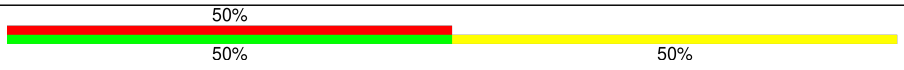
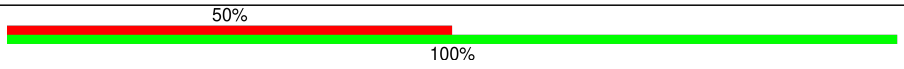
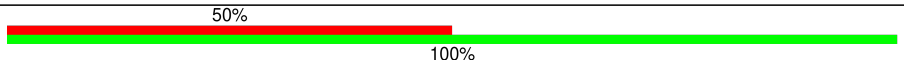
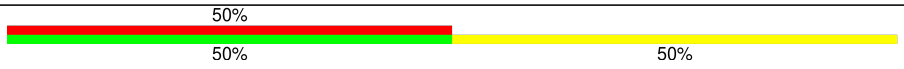
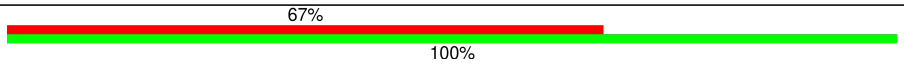
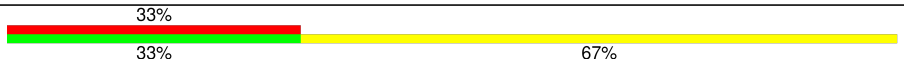
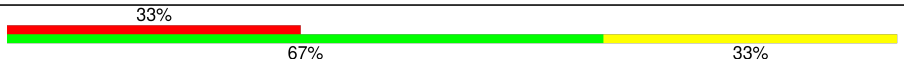
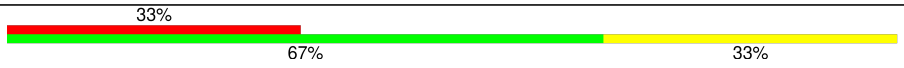
Mol	Chain	Length	Quality of chain
4	L	214	
4	M	214	
4	N	214	
5	2	2	
5	7	2	
5	G	2	
5	K	2	
5	P	2	
5	W	2	
5	b	2	
5	c	2	
5	d	2	
5	f	2	
5	m	2	
5	r	2	
5	s	2	
5	t	2	
5	v	2	
6	0	3	
6	1	3	
6	3	3	
6	5	3	
6	6	3	
6	O	3	
6	R	3	

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Mol	Chain	Length	Quality of chain
6	U	3	67% 100%
6	V	3	33% 33% 67%
6	X	3	33% 67% 33%
6	Z	3	67% 67% 33%
6	a	3	67% 67% 33%
6	e	3	67% 67% 33%
6	h	3	33% 67% 33%
6	k	3	67% 100%
6	l	3	33% 33% 67%
6	n	3	33% 33% 67%
6	p	3	67% 67% 33%
6	q	3	67% 67% 33%
6	u	3	67% 67% 33%
6	x	3	33% 67% 33%
7	Q	5	40% 60%
7	g	5	40% 60%
7	w	5	40% 60%
8	S	4	50% 25% 75%
8	i	4	50% 25% 75%
8	y	4	50% 25% 75%
9	T	5	40% 40% 60%
9	j	5	40% 40% 60%
9	z	5	40% 40% 60%
10	4	7	14% 29% 71%
10	Y	7	14% 29% 71%

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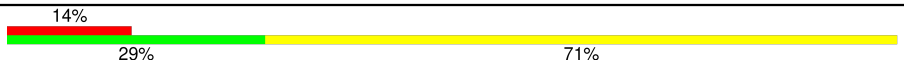
Mol	Chain	Length	Quality of chain
10	o	7	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 21426 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 Glycoprotein 120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	458	Total 3601	C 2261	N 627	O 684	S 29	0	0
1	C	458	Total 3601	C 2261	N 627	O 684	S 29	0	0
1	E	458	Total 3601	C 2261	N 627	O 684	S 29	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	initiating methionine	UNP A0A0A7I3C6
A	8	PRO	-	expression tag	UNP A0A0A7I3C6
A	9	MET	-	expression tag	UNP A0A0A7I3C6
A	10	GLY	-	expression tag	UNP A0A0A7I3C6
A	11	SER	-	expression tag	UNP A0A0A7I3C6
A	12	LEU	-	expression tag	UNP A0A0A7I3C6
A	13	GLN	-	expression tag	UNP A0A0A7I3C6
A	14	PRO	-	expression tag	UNP A0A0A7I3C6
A	15	LEU	-	expression tag	UNP A0A0A7I3C6
A	16	ALA	-	expression tag	UNP A0A0A7I3C6
A	17	THR	-	expression tag	UNP A0A0A7I3C6
A	18	LEU	-	expression tag	UNP A0A0A7I3C6
A	19	TYR	-	expression tag	UNP A0A0A7I3C6
A	20	LEU	-	expression tag	UNP A0A0A7I3C6
A	21	LEU	-	expression tag	UNP A0A0A7I3C6
A	22	GLY	-	expression tag	UNP A0A0A7I3C6
A	23	MET	-	expression tag	UNP A0A0A7I3C6
A	24	LEU	-	expression tag	UNP A0A0A7I3C6
A	25	VAL	-	expression tag	UNP A0A0A7I3C6
A	26	ALA	-	expression tag	UNP A0A0A7I3C6
A	27	SER	-	expression tag	UNP A0A0A7I3C6
A	28	VAL	-	expression tag	UNP A0A0A7I3C6
A	29	LEU	-	expression tag	UNP A0A0A7I3C6
A	30	ALA	-	expression tag	UNP A0A0A7I3C6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ALA	-	expression tag	UNP A0A0A7I3C6
A	32	GLU	-	expression tag	UNP A0A0A7I3C6
A	33	ASN	-	expression tag	UNP A0A0A7I3C6
A	34	LEU	-	expression tag	UNP A0A0A7I3C6
A	64	LYS	GLU	conflict	UNP A0A0A7I3C6
A	316	TRP	ALA	conflict	UNP A0A0A7I3C6
A	490	LYS	GLU	conflict	UNP A0A0A7I3C6
A	491	ILE	VAL	conflict	UNP A0A0A7I3C6
A	492	GLU	LYS	conflict	UNP A0A0A7I3C6
A	500	ARG	ASN	conflict	UNP A0A0A7I3C6
A	501	CYS	ALA	conflict	UNP A0A0A7I3C6
A	502	LYS	ARG	conflict	UNP A0A0A7I3C6
C	7	MET	-	initiating methionine	UNP A0A0A7I3C6
C	8	PRO	-	expression tag	UNP A0A0A7I3C6
C	9	MET	-	expression tag	UNP A0A0A7I3C6
C	10	GLY	-	expression tag	UNP A0A0A7I3C6
C	11	SER	-	expression tag	UNP A0A0A7I3C6
C	12	LEU	-	expression tag	UNP A0A0A7I3C6
C	13	GLN	-	expression tag	UNP A0A0A7I3C6
C	14	PRO	-	expression tag	UNP A0A0A7I3C6
C	15	LEU	-	expression tag	UNP A0A0A7I3C6
C	16	ALA	-	expression tag	UNP A0A0A7I3C6
C	17	THR	-	expression tag	UNP A0A0A7I3C6
C	18	LEU	-	expression tag	UNP A0A0A7I3C6
C	19	TYR	-	expression tag	UNP A0A0A7I3C6
C	20	LEU	-	expression tag	UNP A0A0A7I3C6
C	21	LEU	-	expression tag	UNP A0A0A7I3C6
C	22	GLY	-	expression tag	UNP A0A0A7I3C6
C	23	MET	-	expression tag	UNP A0A0A7I3C6
C	24	LEU	-	expression tag	UNP A0A0A7I3C6
C	25	VAL	-	expression tag	UNP A0A0A7I3C6
C	26	ALA	-	expression tag	UNP A0A0A7I3C6
C	27	SER	-	expression tag	UNP A0A0A7I3C6
C	28	VAL	-	expression tag	UNP A0A0A7I3C6
C	29	LEU	-	expression tag	UNP A0A0A7I3C6
C	30	ALA	-	expression tag	UNP A0A0A7I3C6
C	31	ALA	-	expression tag	UNP A0A0A7I3C6
C	32	GLU	-	expression tag	UNP A0A0A7I3C6
C	33	ASN	-	expression tag	UNP A0A0A7I3C6
C	34	LEU	-	expression tag	UNP A0A0A7I3C6
C	64	LYS	GLU	conflict	UNP A0A0A7I3C6
C	316	TRP	ALA	conflict	UNP A0A0A7I3C6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	490	LYS	GLU	conflict	UNP A0A0A7I3C6
C	491	ILE	VAL	conflict	UNP A0A0A7I3C6
C	492	GLU	LYS	conflict	UNP A0A0A7I3C6
C	500	ARG	ASN	conflict	UNP A0A0A7I3C6
C	501	CYS	ALA	conflict	UNP A0A0A7I3C6
C	502	LYS	ARG	conflict	UNP A0A0A7I3C6
E	7	MET	-	initiating methionine	UNP A0A0A7I3C6
E	8	PRO	-	expression tag	UNP A0A0A7I3C6
E	9	MET	-	expression tag	UNP A0A0A7I3C6
E	10	GLY	-	expression tag	UNP A0A0A7I3C6
E	11	SER	-	expression tag	UNP A0A0A7I3C6
E	12	LEU	-	expression tag	UNP A0A0A7I3C6
E	13	GLN	-	expression tag	UNP A0A0A7I3C6
E	14	PRO	-	expression tag	UNP A0A0A7I3C6
E	15	LEU	-	expression tag	UNP A0A0A7I3C6
E	16	ALA	-	expression tag	UNP A0A0A7I3C6
E	17	THR	-	expression tag	UNP A0A0A7I3C6
E	18	LEU	-	expression tag	UNP A0A0A7I3C6
E	19	TYR	-	expression tag	UNP A0A0A7I3C6
E	20	LEU	-	expression tag	UNP A0A0A7I3C6
E	21	LEU	-	expression tag	UNP A0A0A7I3C6
E	22	GLY	-	expression tag	UNP A0A0A7I3C6
E	23	MET	-	expression tag	UNP A0A0A7I3C6
E	24	LEU	-	expression tag	UNP A0A0A7I3C6
E	25	VAL	-	expression tag	UNP A0A0A7I3C6
E	26	ALA	-	expression tag	UNP A0A0A7I3C6
E	27	SER	-	expression tag	UNP A0A0A7I3C6
E	28	VAL	-	expression tag	UNP A0A0A7I3C6
E	29	LEU	-	expression tag	UNP A0A0A7I3C6
E	30	ALA	-	expression tag	UNP A0A0A7I3C6
E	31	ALA	-	expression tag	UNP A0A0A7I3C6
E	32	GLU	-	expression tag	UNP A0A0A7I3C6
E	33	ASN	-	expression tag	UNP A0A0A7I3C6
E	34	LEU	-	expression tag	UNP A0A0A7I3C6
E	64	LYS	GLU	conflict	UNP A0A0A7I3C6
E	316	TRP	ALA	conflict	UNP A0A0A7I3C6
E	490	LYS	GLU	conflict	UNP A0A0A7I3C6
E	491	ILE	VAL	conflict	UNP A0A0A7I3C6
E	492	GLU	LYS	conflict	UNP A0A0A7I3C6
E	500	ARG	ASN	conflict	UNP A0A0A7I3C6
E	501	CYS	ALA	conflict	UNP A0A0A7I3C6
E	502	LYS	ARG	conflict	UNP A0A0A7I3C6

- Molecule 2 is a protein called Glycoprotein 41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	121	Total	C	N	O	S	0	0
			965	606	167	186	6		
2	D	121	Total	C	N	O	S	0	0
			965	606	167	186	6		
2	F	121	Total	C	N	O	S	0	0
			965	606	167	186	6		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	505	GLY	-	expression tag	UNP Q2N0S5
B	506	ARG	-	expression tag	UNP Q2N0S5
B	507	ARG	-	expression tag	UNP Q2N0S5
B	508	ARG	-	expression tag	UNP Q2N0S5
B	509	ARG	-	expression tag	UNP Q2N0S5
B	510	ARG	-	expression tag	UNP Q2N0S5
B	559	PRO	ILE	conflict	UNP Q2N0S5
B	605	CYS	THR	conflict	UNP Q2N0S5
D	505	GLY	-	expression tag	UNP Q2N0S5
D	506	ARG	-	expression tag	UNP Q2N0S5
D	507	ARG	-	expression tag	UNP Q2N0S5
D	508	ARG	-	expression tag	UNP Q2N0S5
D	509	ARG	-	expression tag	UNP Q2N0S5
D	510	ARG	-	expression tag	UNP Q2N0S5
D	559	PRO	ILE	conflict	UNP Q2N0S5
D	605	CYS	THR	conflict	UNP Q2N0S5
F	505	GLY	-	expression tag	UNP Q2N0S5
F	506	ARG	-	expression tag	UNP Q2N0S5
F	507	ARG	-	expression tag	UNP Q2N0S5
F	508	ARG	-	expression tag	UNP Q2N0S5
F	509	ARG	-	expression tag	UNP Q2N0S5
F	510	ARG	-	expression tag	UNP Q2N0S5
F	559	PRO	ILE	conflict	UNP Q2N0S5
F	605	CYS	THR	conflict	UNP Q2N0S5

- Molecule 3 is a protein called M1214 N1 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	125	Total	C	N	O	S	0	0
			969	604	176	183	6		
3	I	125	Total	C	N	O	S	0	0
			969	604	176	183	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	125	Total	C	N	O	S	0	0
			969	604	176	183	6		

- Molecule 4 is a protein called M1214 N1 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	110	Total	C	N	O	S	0	0
			827	521	142	161	3		
4	M	110	Total	C	N	O	S	0	0
			827	521	142	161	3		
4	N	110	Total	C	N	O	S	0	0
			827	521	142	161	3		

- Molecule 5 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
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	b	2	Total	C	N	O	0	0
			28	16	2	10		
5	c	2	Total	C	N	O	0	0
			28	16	2	10		
5	d	2	Total	C	N	O	0	0
			28	16	2	10		
5	f	2	Total	C	N	O	0	0
			28	16	2	10		
5	m	2	Total	C	N	O	0	0
			28	16	2	10		
5	r	2	Total	C	N	O	0	0
			28	16	2	10		

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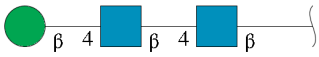
Mol	Chain	Residues	Atoms	AltConf	Trace
5	s	2	Total C N O 28 16 2 10	0	0
5	t	2	Total C N O 28 16 2 10	0	0
5	v	2	Total C N O 28 16 2 10	0	0
5	2	2	Total C N O 28 16 2 10	0	0
5	7	2	Total C N O 28 16 2 10	0	0

- Molecule 6 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
6	O	3	Total C N O 39 22 2 15	0	0
6	R	3	Total C N O 39 22 2 15	0	0
6	U	3	Total C N O 39 22 2 15	0	0
6	V	3	Total C N O 39 22 2 15	0	0
6	X	3	Total C N O 39 22 2 15	0	0
6	Z	3	Total C N O 39 22 2 15	0	0
6	a	3	Total C N O 39 22 2 15	0	0
6	e	3	Total C N O 39 22 2 15	0	0
6	h	3	Total C N O 39 22 2 15	0	0
6	k	3	Total C N O 39 22 2 15	0	0
6	l	3	Total C N O 39 22 2 15	0	0
6	n	3	Total C N O 39 22 2 15	0	0

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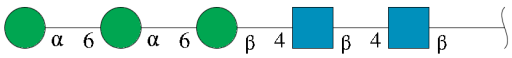
Mol	Chain	Residues	Atoms				AltConf	Trace
6	p	3	Total	C	N	O	0	0
			39	22	2	15		
6	q	3	Total	C	N	O	0	0
			39	22	2	15		
6	u	3	Total	C	N	O	0	0
			39	22	2	15		
6	x	3	Total	C	N	O	0	0
			39	22	2	15		
6	0	3	Total	C	N	O	0	0
			39	22	2	15		
6	1	3	Total	C	N	O	0	0
			39	22	2	15		
6	3	3	Total	C	N	O	0	0
			39	22	2	15		
6	5	3	Total	C	N	O	0	0
			39	22	2	15		
6	6	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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.

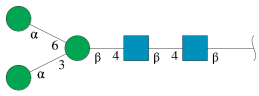


Mol	Chain	Residues	Atoms				AltConf	Trace
7	Q	5	Total	C	N	O	0	0
			61	34	2	25		
7	g	5	Total	C	N	O	0	0
			61	34	2	25		
7	w	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is an oligosaccharide called 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.

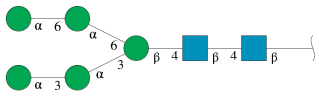
Mol	Chain	Residues	Atoms	AltConf	Trace
8	S	4	Total C N O 50 28 2 20	0	0
8	i	4	Total C N O 50 28 2 20	0	0
8	y	4	Total C N O 50 28 2 20	0	0

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



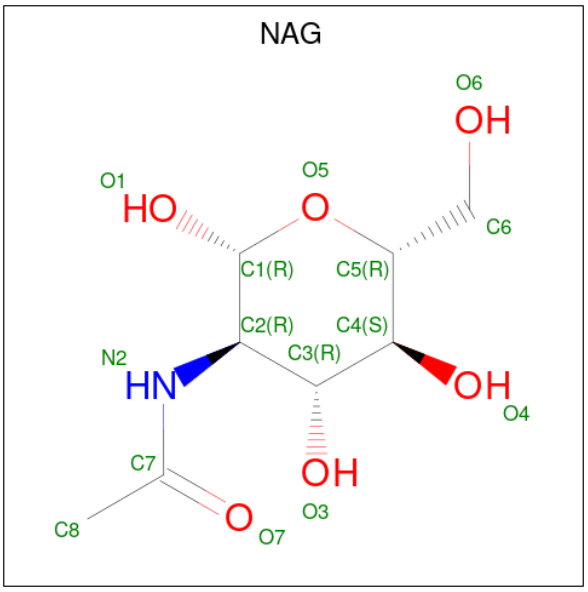
Mol	Chain	Residues	Atoms	AltConf	Trace
9	T	5	Total C N O 61 34 2 25	0	0
9	j	5	Total C N O 61 34 2 25	0	0
9	z	5	Total C N O 61 34 2 25	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-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.



Mol	Chain	Residues	Atoms	AltConf	Trace
10	Y	7	Total C N O 83 46 2 35	0	0
10	o	7	Total C N O 83 46 2 35	0	0
10	4	7	Total C N O 83 46 2 35	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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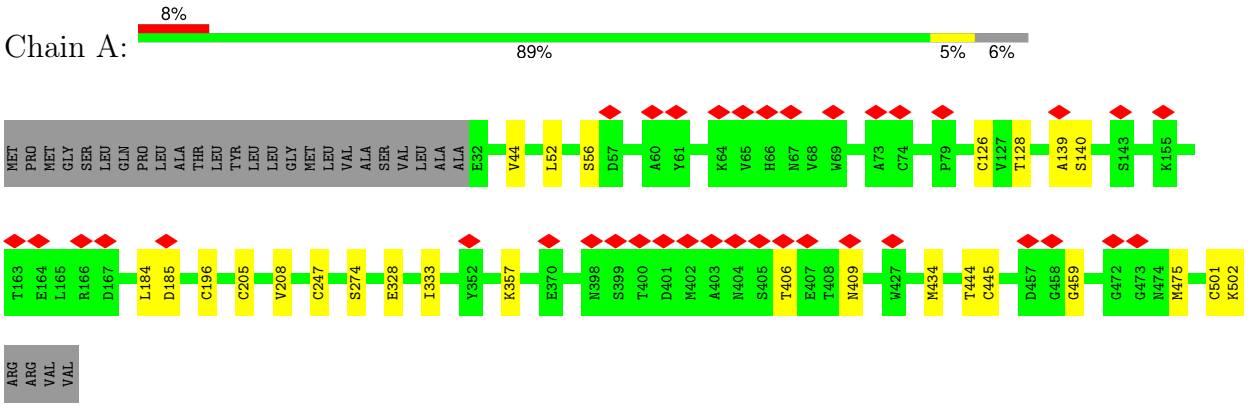
Mol	Chain	Residues	Atoms				AltConf
11	D	1	Total	C	N	O	0
			14	8	1	5	
11	D	1	Total	C	N	O	0
			14	8	1	5	
11	E	1	Total	C	N	O	0
			14	8	1	5	
11	E	1	Total	C	N	O	0
			14	8	1	5	
11	E	1	Total	C	N	O	0
			14	8	1	5	
11	E	1	Total	C	N	O	0
			14	8	1	5	
11	E	1	Total	C	N	O	0
			14	8	1	5	
11	F	1	Total	C	N	O	0
			14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

3 Residue-property plots

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.

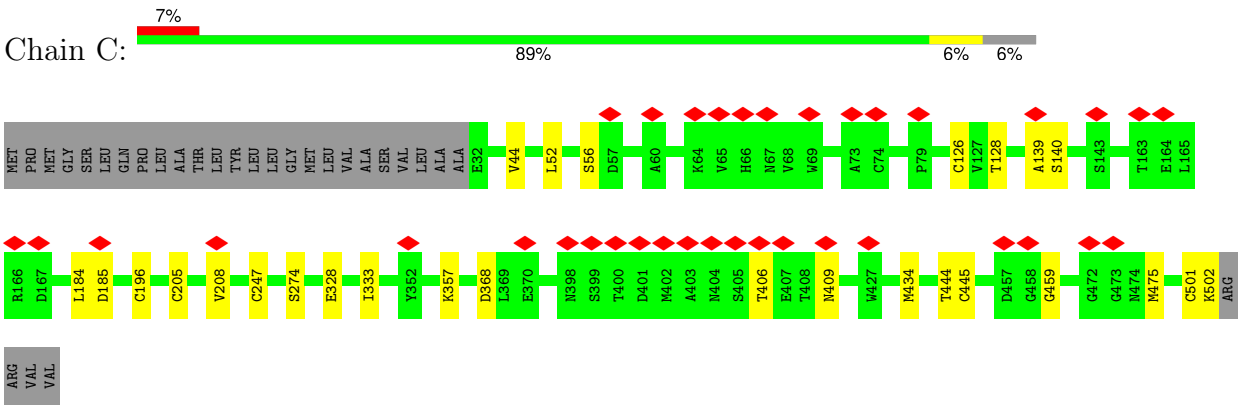
• Molecule 1: Glycoprotein 120

Chain A:



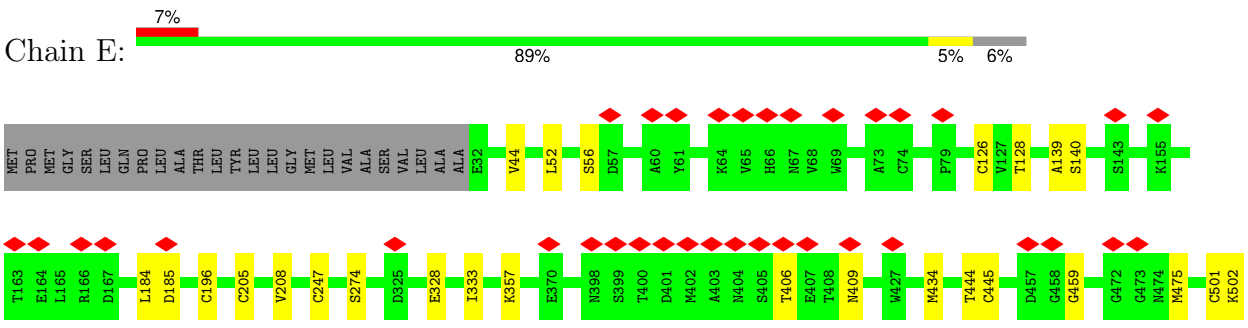
• Molecule 1: Glycoprotein 120

Chain C:



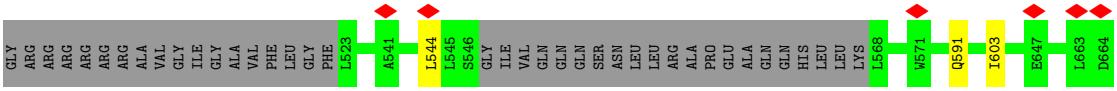
• Molecule 1: Glycoprotein 120

Chain E:



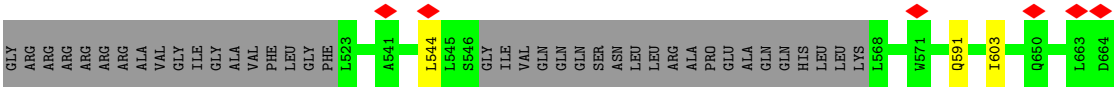
• Molecule 2: Glycoprotein 41

Chain B:



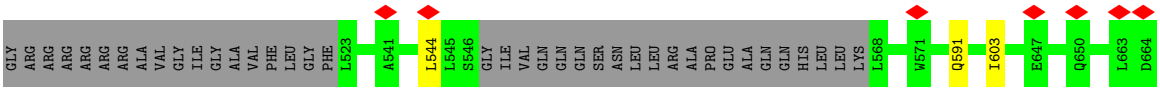
• Molecule 2: Glycoprotein 41

Chain D:



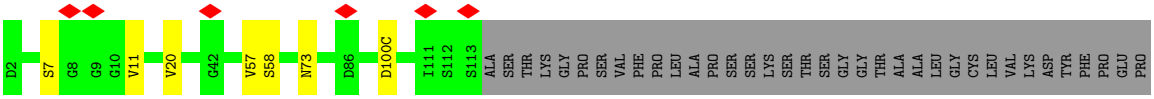
• Molecule 2: Glycoprotein 41

Chain F:



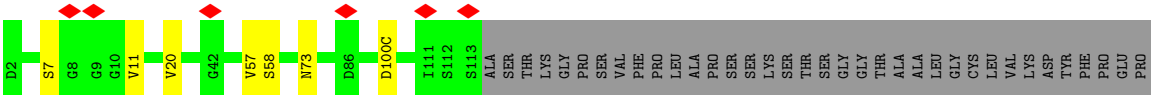
• Molecule 3: M1214 N1 Fab heavy chain

Chain H:



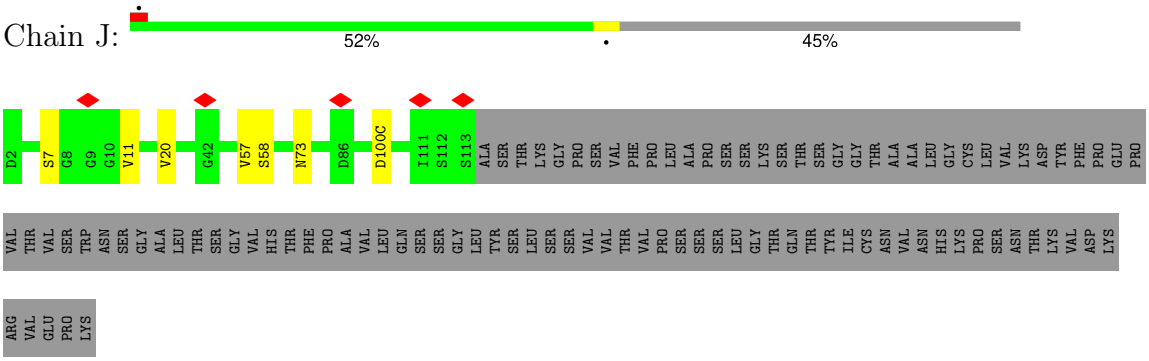
• Molecule 3: M1214 N1 Fab heavy chain

Chain I:



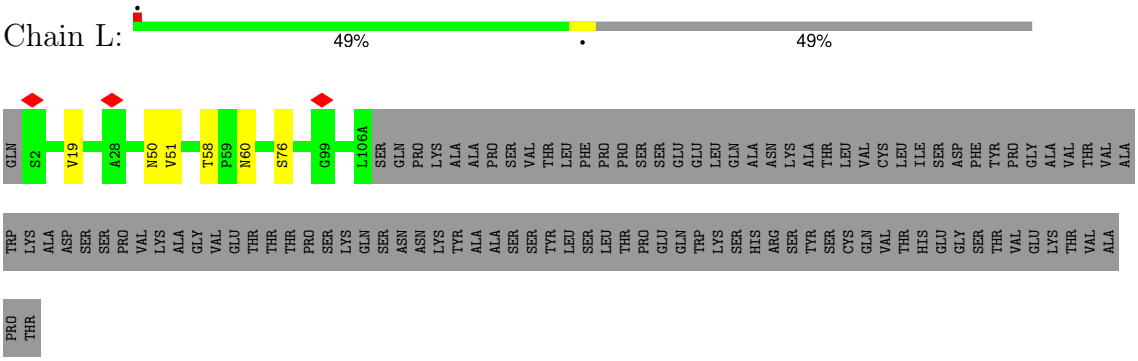
• Molecule 3: M1214 N1 Fab heavy chain

Chain J:



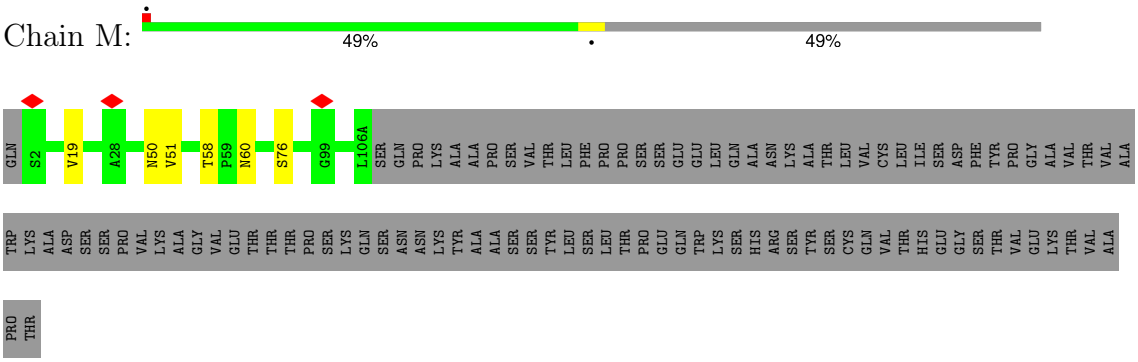
• Molecule 4: M1214 N1 Fab light chain

Chain L:



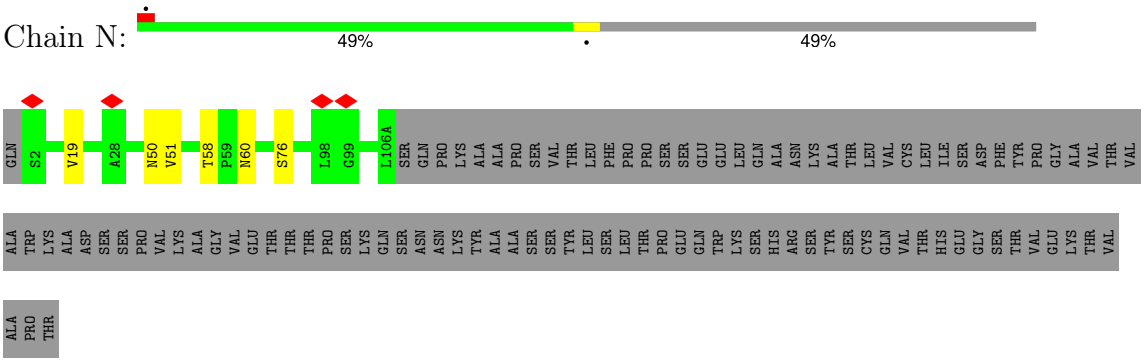
• Molecule 4: M1214 N1 Fab light chain

Chain M:



• Molecule 4: M1214 N1 Fab light chain

Chain N:

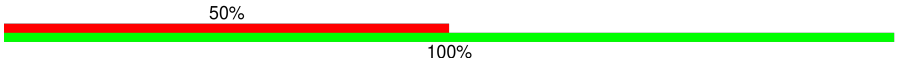


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

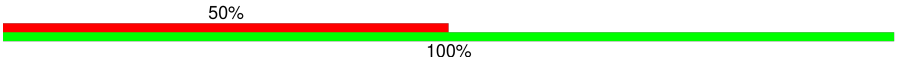
Chain b:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

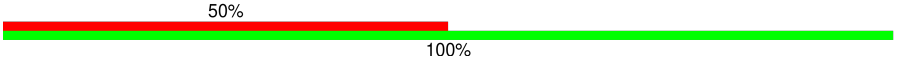
Chain r:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:

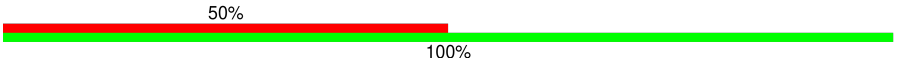


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7:

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

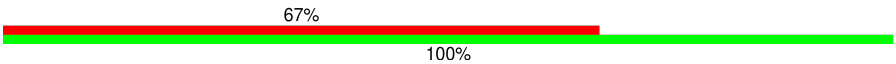
Chain O:

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

Chain U:



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

Chain V:

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

Chain X:

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

Chain Z:

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

Chain a:

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

Chain e:

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

Chain h:

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

Chain k:

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

Chain l:

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

Chain n:

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

Chain p:

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

Chain q:

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

Chain u:

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

Chain x:

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

Chain 0:

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

Chain 1:

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

Chain 3:

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

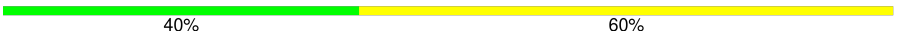
Chain 5:

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

Chain 6:

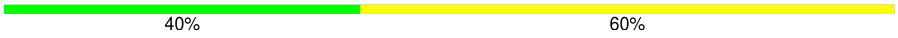
• Molecule 7: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



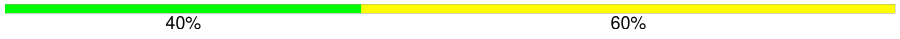
• Molecule 7: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



• Molecule 7: alpha-D-mannopyranose-(1-6)-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 w:



• Molecule 8: 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 S:

• Molecule 8: 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

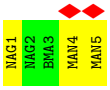
Chain i:

• Molecule 8: 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 y:

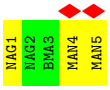
• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



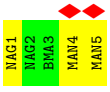
• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



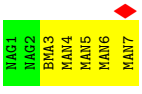
• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:



• Molecule 10: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-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 Y:

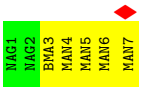


• Molecule 10: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:

• Molecule 10: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-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 4:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	94839	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.124	Depositor
Minimum map value	-0.571	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	417.59998, 417.59998, 417.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.33	0/3677	0.58	0/4994
1	C	0.33	0/3677	0.58	1/4994 (0.0%)
1	E	0.34	0/3677	0.58	0/4994
2	B	0.31	0/981	0.47	0/1330
2	D	0.31	0/981	0.47	0/1330
2	F	0.31	0/981	0.47	0/1330
3	H	0.35	0/991	0.50	0/1338
3	I	0.35	0/991	0.50	0/1338
3	J	0.35	0/991	0.50	0/1338
4	L	0.35	0/848	0.51	0/1153
4	M	0.35	0/848	0.51	0/1153
4	N	0.35	0/848	0.51	0/1153
All	All	0.34	0/19491	0.55	1/26445 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	3
1	E	0	3
4	L	0	1
4	M	0	1
4	N	0	1
All	All	0	12

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	C	368	ASP	CB-CG-OD1	5.02	122.81	118.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ALA	Peptide
1	A	406	THR	Peptide
1	A	459	GLY	Peptide
1	C	139	ALA	Peptide
1	C	406	THR	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	456/487 (94%)	416 (91%)	37 (8%)	3 (1%)	19	56
1	C	456/487 (94%)	415 (91%)	38 (8%)	3 (1%)	19	56
1	E	456/487 (94%)	415 (91%)	38 (8%)	3 (1%)	19	56
2	B	117/160 (73%)	115 (98%)	2 (2%)	0	100	100
2	D	117/160 (73%)	115 (98%)	2 (2%)	0	100	100
2	F	117/160 (73%)	115 (98%)	2 (2%)	0	100	100
3	H	123/226 (54%)	122 (99%)	1 (1%)	0	100	100
3	I	123/226 (54%)	122 (99%)	1 (1%)	0	100	100
3	J	123/226 (54%)	122 (99%)	1 (1%)	0	100	100
4	L	108/214 (50%)	102 (94%)	5 (5%)	1 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	M	108/214 (50%)	102 (94%)	5 (5%)	1 (1%)	14	50
4	N	108/214 (50%)	102 (94%)	5 (5%)	1 (1%)	14	50
All	All	2412/3261 (74%)	2263 (94%)	137 (6%)	12 (0%)	27	63

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	51	VAL
4	M	51	VAL
4	N	51	VAL
1	A	357	LYS
1	A	409	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/433 (95%)	390 (95%)	20 (5%)	21	42
1	C	410/433 (95%)	390 (95%)	20 (5%)	21	42
1	E	410/433 (95%)	390 (95%)	20 (5%)	21	42
2	B	105/135 (78%)	102 (97%)	3 (3%)	37	57
2	D	105/135 (78%)	102 (97%)	3 (3%)	37	57
2	F	105/135 (78%)	102 (97%)	3 (3%)	37	57
3	H	101/188 (54%)	94 (93%)	7 (7%)	13	34
3	I	101/188 (54%)	94 (93%)	7 (7%)	13	34
3	J	101/188 (54%)	94 (93%)	7 (7%)	13	34
4	L	90/180 (50%)	86 (96%)	4 (4%)	24	46
4	M	90/180 (50%)	86 (96%)	4 (4%)	24	46
4	N	90/180 (50%)	86 (96%)	4 (4%)	24	46
All	All	2118/2808 (75%)	2016 (95%)	102 (5%)	24	43

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	274	SER
3	H	20	VAL
4	N	58	THR
1	E	333	ILE
1	E	502	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	591	GLN
1	E	195	ASN
2	F	611	ASN
1	E	374	HIS
2	F	591	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)

156 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	$\#\|Z\| > 2$
6	NAG	0	1	6,1	14,14,15	0.38	0	17,19,21	0.47	0
6	NAG	0	2	6	14,14,15	0.22	0	17,19,21	0.44	0
6	BMA	0	3	6	11,11,12	0.51	0	15,15,17	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	1	1	6,1	14,14,15	0.53	0	17,19,21	0.51	0
6	NAG	1	2	6	14,14,15	0.35	0	17,19,21	0.91	1 (5%)
6	BMA	1	3	6	11,11,12	0.64	0	15,15,17	0.87	1 (6%)
5	NAG	2	1	5	14,14,15	0.27	0	17,19,21	0.52	0
5	NAG	2	2	5	14,14,15	0.34	0	17,19,21	0.46	0
6	NAG	3	1	6,1	14,14,15	0.97	1 (7%)	17,19,21	0.89	1 (5%)
6	NAG	3	2	6	14,14,15	0.57	0	17,19,21	0.50	0
6	BMA	3	3	6	11,11,12	0.48	0	15,15,17	0.67	0
10	NAG	4	1	1,10	14,14,15	0.37	0	17,19,21	0.46	0
10	NAG	4	2	10	14,14,15	0.30	0	17,19,21	0.51	0
10	BMA	4	3	10	11,11,12	0.78	1 (9%)	15,15,17	0.81	0
10	MAN	4	4	10	11,11,12	0.74	0	15,15,17	1.30	2 (13%)
10	MAN	4	5	10	11,11,12	0.78	1 (9%)	15,15,17	0.90	1 (6%)
10	MAN	4	6	10	11,11,12	0.48	0	15,15,17	0.98	1 (6%)
10	MAN	4	7	10	11,11,12	0.71	0	15,15,17	1.00	1 (6%)
6	NAG	5	1	6,1	14,14,15	0.65	1 (7%)	17,19,21	0.49	0
6	NAG	5	2	6	14,14,15	0.20	0	17,19,21	0.56	0
6	BMA	5	3	6	11,11,12	0.47	0	15,15,17	0.79	0
6	NAG	6	1	6,1	14,14,15	0.59	0	17,19,21	1.33	2 (11%)
6	NAG	6	2	6	14,14,15	0.16	0	17,19,21	0.54	0
6	BMA	6	3	6	11,11,12	0.56	0	15,15,17	0.67	0
5	NAG	7	1	1,5	14,14,15	0.58	0	17,19,21	1.18	3 (17%)
5	NAG	7	2	5	14,14,15	0.26	0	17,19,21	0.41	0
5	NAG	G	1	1,5	14,14,15	0.30	0	17,19,21	0.78	0
5	NAG	G	2	5	14,14,15	0.26	0	17,19,21	0.40	0
5	NAG	K	1	1,5	14,14,15	0.20	0	17,19,21	0.36	0
5	NAG	K	2	5	14,14,15	0.28	0	17,19,21	0.48	0
6	NAG	O	1	6,1	14,14,15	0.92	1 (7%)	17,19,21	1.64	3 (17%)
6	NAG	O	2	6	14,14,15	0.26	0	17,19,21	0.59	0
6	BMA	O	3	6	11,11,12	0.68	0	15,15,17	0.74	0
5	NAG	P	1	1,5	14,14,15	0.56	1 (7%)	17,19,21	0.59	0
5	NAG	P	2	5	14,14,15	0.18	0	17,19,21	0.50	0
7	NAG	Q	1	1,7	14,14,15	0.78	1 (7%)	17,19,21	0.99	2 (11%)
7	NAG	Q	2	7	14,14,15	0.19	0	17,19,21	0.50	0
7	BMA	Q	3	7	11,11,12	0.56	0	15,15,17	0.76	0
7	MAN	Q	4	7	11,11,12	0.57	0	15,15,17	1.10	2 (13%)
7	MAN	Q	5	7	11,11,12	0.79	1 (9%)	15,15,17	0.83	1 (6%)
6	NAG	R	1	6,1	14,14,15	0.50	0	17,19,21	1.34	2 (11%)
6	NAG	R	2	6	14,14,15	0.36	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BMA	R	3	6	11,11,12	0.54	0	15,15,17	0.67	0
8	NAG	S	1	1,8	14,14,15	0.66	1 (7%)	17,19,21	1.68	3 (17%)
8	NAG	S	2	8	14,14,15	0.28	0	17,19,21	0.47	0
8	BMA	S	3	8	11,11,12	0.46	0	15,15,17	1.06	1 (6%)
8	MAN	S	4	8	11,11,12	0.83	0	15,15,17	1.34	2 (13%)
9	NAG	T	1	9,1	14,14,15	1.36	2 (14%)	17,19,21	1.28	2 (11%)
9	NAG	T	2	9	14,14,15	0.20	0	17,19,21	0.57	0
9	BMA	T	3	9	11,11,12	0.49	0	15,15,17	0.74	0
9	MAN	T	4	9	11,11,12	0.61	0	15,15,17	0.87	1 (6%)
9	MAN	T	5	9	11,11,12	0.55	0	15,15,17	1.08	2 (13%)
6	NAG	U	1	6,1	14,14,15	0.37	0	17,19,21	0.46	0
6	NAG	U	2	6	14,14,15	0.23	0	17,19,21	0.45	0
6	BMA	U	3	6	11,11,12	0.50	0	15,15,17	0.70	0
6	NAG	V	1	6,1	14,14,15	0.54	0	17,19,21	0.52	0
6	NAG	V	2	6	14,14,15	0.35	0	17,19,21	0.91	1 (5%)
6	BMA	V	3	6	11,11,12	0.64	0	15,15,17	0.86	1 (6%)
5	NAG	W	1	1,5	14,14,15	0.26	0	17,19,21	0.51	0
5	NAG	W	2	5	14,14,15	0.33	0	17,19,21	0.46	0
6	NAG	X	1	6,1	14,14,15	0.99	1 (7%)	17,19,21	0.88	1 (5%)
6	NAG	X	2	6	14,14,15	0.54	0	17,19,21	0.49	0
6	BMA	X	3	6	11,11,12	0.48	0	15,15,17	0.67	0
10	NAG	Y	1	1,10	14,14,15	0.34	0	17,19,21	0.46	0
10	NAG	Y	2	10	14,14,15	0.28	0	17,19,21	0.52	0
10	BMA	Y	3	10	11,11,12	0.77	1 (9%)	15,15,17	0.81	0
10	MAN	Y	4	10	11,11,12	0.73	0	15,15,17	1.30	2 (13%)
10	MAN	Y	5	10	11,11,12	0.79	1 (9%)	15,15,17	0.89	1 (6%)
10	MAN	Y	6	10	11,11,12	0.46	0	15,15,17	0.98	1 (6%)
10	MAN	Y	7	10	11,11,12	0.69	0	15,15,17	1.01	1 (6%)
6	NAG	Z	1	6,1	14,14,15	0.65	1 (7%)	17,19,21	0.49	0
6	NAG	Z	2	6	14,14,15	0.18	0	17,19,21	0.55	0
6	BMA	Z	3	6	11,11,12	0.48	0	15,15,17	0.79	0
6	NAG	a	1	6,1	14,14,15	0.61	0	17,19,21	1.33	2 (11%)
6	NAG	a	2	6	14,14,15	0.17	0	17,19,21	0.55	0
6	BMA	a	3	6	11,11,12	0.56	0	15,15,17	0.68	0
5	NAG	b	1	1,5	14,14,15	0.60	1 (7%)	17,19,21	1.17	3 (17%)
5	NAG	b	2	5	14,14,15	0.26	0	17,19,21	0.41	0
5	NAG	c	1	1,5	14,14,15	0.31	0	17,19,21	0.78	0
5	NAG	c	2	5	14,14,15	0.26	0	17,19,21	0.40	0
5	NAG	d	1	1,5	14,14,15	0.19	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	d	2	5	14,14,15	0.28	0	17,19,21	0.48	0
6	NAG	e	1	6,1	14,14,15	0.91	1 (7%)	17,19,21	1.64	3 (17%)
6	NAG	e	2	6	14,14,15	0.26	0	17,19,21	0.59	0
6	BMA	e	3	6	11,11,12	0.68	0	15,15,17	0.75	0
5	NAG	f	1	1,5	14,14,15	0.58	1 (7%)	17,19,21	0.59	0
5	NAG	f	2	5	14,14,15	0.19	0	17,19,21	0.51	0
7	NAG	g	1	1,7	14,14,15	0.78	1 (7%)	17,19,21	0.99	2 (11%)
7	NAG	g	2	7	14,14,15	0.19	0	17,19,21	0.50	0
7	BMA	g	3	7	11,11,12	0.56	0	15,15,17	0.76	0
7	MAN	g	4	7	11,11,12	0.57	0	15,15,17	1.10	2 (13%)
7	MAN	g	5	7	11,11,12	0.80	1 (9%)	15,15,17	0.84	1 (6%)
6	NAG	h	1	6,1	14,14,15	0.51	0	17,19,21	1.34	2 (11%)
6	NAG	h	2	6	14,14,15	0.36	0	17,19,21	0.55	0
6	BMA	h	3	6	11,11,12	0.55	0	15,15,17	0.67	0
8	NAG	i	1	1,8	14,14,15	0.66	1 (7%)	17,19,21	1.69	3 (17%)
8	NAG	i	2	8	14,14,15	0.28	0	17,19,21	0.47	0
8	BMA	i	3	8	11,11,12	0.47	0	15,15,17	1.07	1 (6%)
8	MAN	i	4	8	11,11,12	0.83	0	15,15,17	1.34	2 (13%)
9	NAG	j	1	9,1	14,14,15	1.36	2 (14%)	17,19,21	1.28	2 (11%)
9	NAG	j	2	9	14,14,15	0.20	0	17,19,21	0.57	0
9	BMA	j	3	9	11,11,12	0.49	0	15,15,17	0.75	0
9	MAN	j	4	9	11,11,12	0.59	0	15,15,17	0.88	1 (6%)
9	MAN	j	5	9	11,11,12	0.54	0	15,15,17	1.08	2 (13%)
6	NAG	k	1	6,1	14,14,15	0.37	0	17,19,21	0.47	0
6	NAG	k	2	6	14,14,15	0.22	0	17,19,21	0.44	0
6	BMA	k	3	6	11,11,12	0.50	0	15,15,17	0.70	0
6	NAG	l	1	6,1	14,14,15	0.54	0	17,19,21	0.50	0
6	NAG	l	2	6	14,14,15	0.35	0	17,19,21	0.89	1 (5%)
6	BMA	l	3	6	11,11,12	0.64	0	15,15,17	0.87	1 (6%)
5	NAG	m	1	1,5	14,14,15	0.29	0	17,19,21	0.51	0
5	NAG	m	2	5	14,14,15	0.34	0	17,19,21	0.47	0
6	NAG	n	1	6,1	14,14,15	0.99	1 (7%)	17,19,21	0.89	1 (5%)
6	NAG	n	2	6	14,14,15	0.57	1 (7%)	17,19,21	0.50	0
6	BMA	n	3	6	11,11,12	0.49	0	15,15,17	0.67	0
10	NAG	o	1	1,10	14,14,15	0.33	0	17,19,21	0.47	0
10	NAG	o	2	10	14,14,15	0.27	0	17,19,21	0.52	0
10	BMA	o	3	10	11,11,12	0.79	1 (9%)	15,15,17	0.81	0
10	MAN	o	4	10	11,11,12	0.72	0	15,15,17	1.30	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	MAN	o	5	10	11,11,12	0.77	1 (9%)	15,15,17	0.88	1 (6%)
10	MAN	o	6	10	11,11,12	0.48	0	15,15,17	0.98	1 (6%)
10	MAN	o	7	10	11,11,12	0.71	0	15,15,17	0.99	1 (6%)
6	NAG	p	1	6,1	14,14,15	0.64	1 (7%)	17,19,21	0.50	0
6	NAG	p	2	6	14,14,15	0.20	0	17,19,21	0.55	0
6	BMA	p	3	6	11,11,12	0.48	0	15,15,17	0.78	0
6	NAG	q	1	6,1	14,14,15	0.58	0	17,19,21	1.34	2 (11%)
6	NAG	q	2	6	14,14,15	0.17	0	17,19,21	0.53	0
6	BMA	q	3	6	11,11,12	0.56	0	15,15,17	0.67	0
5	NAG	r	1	1,5	14,14,15	0.57	0	17,19,21	1.17	3 (17%)
5	NAG	r	2	5	14,14,15	0.26	0	17,19,21	0.40	0
5	NAG	s	1	1,5	14,14,15	0.30	0	17,19,21	0.79	0
5	NAG	s	2	5	14,14,15	0.25	0	17,19,21	0.39	0
5	NAG	t	1	1,5	14,14,15	0.20	0	17,19,21	0.37	0
5	NAG	t	2	5	14,14,15	0.30	0	17,19,21	0.49	0
6	NAG	u	1	6,1	14,14,15	0.91	1 (7%)	17,19,21	1.64	4 (23%)
6	NAG	u	2	6	14,14,15	0.26	0	17,19,21	0.60	0
6	BMA	u	3	6	11,11,12	0.68	0	15,15,17	0.74	0
5	NAG	v	1	1,5	14,14,15	0.56	1 (7%)	17,19,21	0.59	0
5	NAG	v	2	5	14,14,15	0.21	0	17,19,21	0.51	0
7	NAG	w	1	7	14,14,15	0.80	1 (7%)	17,19,21	0.99	2 (11%)
7	NAG	w	2	7	14,14,15	0.19	0	17,19,21	0.50	0
7	BMA	w	3	7	11,11,12	0.56	0	15,15,17	0.76	0
7	MAN	w	4	7	11,11,12	0.58	0	15,15,17	1.10	2 (13%)
7	MAN	w	5	7	11,11,12	0.79	1 (9%)	15,15,17	0.83	1 (6%)
6	NAG	x	1	6,1	14,14,15	0.51	0	17,19,21	1.34	2 (11%)
6	NAG	x	2	6	14,14,15	0.36	0	17,19,21	0.56	0
6	BMA	x	3	6	11,11,12	0.54	0	15,15,17	0.67	0
8	NAG	y	1	1,8	14,14,15	0.65	1 (7%)	17,19,21	1.69	3 (17%)
8	NAG	y	2	8	14,14,15	0.28	0	17,19,21	0.47	0
8	BMA	y	3	8	11,11,12	0.47	0	15,15,17	1.07	1 (6%)
8	MAN	y	4	8	11,11,12	0.83	0	15,15,17	1.33	2 (13%)
9	NAG	z	1	9,1	14,14,15	1.36	2 (14%)	17,19,21	1.27	2 (11%)
9	NAG	z	2	9	14,14,15	0.20	0	17,19,21	0.57	0
9	BMA	z	3	9	11,11,12	0.47	0	15,15,17	0.75	0
9	MAN	z	4	9	11,11,12	0.62	0	15,15,17	0.88	1 (6%)
9	MAN	z	5	9	11,11,12	0.55	0	15,15,17	1.05	2 (13%)

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
6	NAG	0	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	0	2	6	-	0/6/23/26	0/1/1/1
6	BMA	0	3	6	-	1/2/19/22	0/1/1/1
6	NAG	1	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	1	2	6	-	1/6/23/26	0/1/1/1
6	BMA	1	3	6	-	2/2/19/22	0/1/1/1
5	NAG	2	1	5	-	2/6/23/26	0/1/1/1
5	NAG	2	2	5	-	0/6/23/26	0/1/1/1
6	NAG	3	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	3	2	6	-	0/6/23/26	0/1/1/1
6	BMA	3	3	6	-	0/2/19/22	0/1/1/1
10	NAG	4	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	4	2	10	-	0/6/23/26	0/1/1/1
10	BMA	4	3	10	-	1/2/19/22	0/1/1/1
10	MAN	4	4	10	-	0/2/19/22	1/1/1/1
10	MAN	4	5	10	-	0/2/19/22	0/1/1/1
10	MAN	4	6	10	-	0/2/19/22	0/1/1/1
10	MAN	4	7	10	-	0/2/19/22	0/1/1/1
6	NAG	5	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	5	2	6	-	1/6/23/26	0/1/1/1
6	BMA	5	3	6	-	0/2/19/22	0/1/1/1
6	NAG	6	1	6,1	-	5/6/23/26	0/1/1/1
6	NAG	6	2	6	-	0/6/23/26	0/1/1/1
6	BMA	6	3	6	-	0/2/19/22	0/1/1/1
5	NAG	7	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	7	2	5	-	1/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	K	2	5	-	1/6/23/26	0/1/1/1
6	NAG	O	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	BMA	O	3	6	-	1/2/19/22	0/1/1/1
5	NAG	P	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
7	NAG	Q	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	Q	3	7	-	2/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	1/2/19/22	0/1/1/1
7	MAN	Q	5	7	-	0/2/19/22	0/1/1/1
6	NAG	R	1	6,1	-	6/6/23/26	0/1/1/1
6	NAG	R	2	6	-	2/6/23/26	0/1/1/1
6	BMA	R	3	6	-	0/2/19/22	0/1/1/1
8	NAG	S	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	S	2	8	-	2/6/23/26	0/1/1/1
8	BMA	S	3	8	-	2/2/19/22	0/1/1/1
8	MAN	S	4	8	-	0/2/19/22	0/1/1/1
9	NAG	T	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	T	2	9	-	0/6/23/26	0/1/1/1
9	BMA	T	3	9	-	0/2/19/22	0/1/1/1
9	MAN	T	4	9	-	0/2/19/22	0/1/1/1
9	MAN	T	5	9	-	0/2/19/22	0/1/1/1
6	NAG	U	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	BMA	U	3	6	-	1/2/19/22	0/1/1/1
6	NAG	V	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	V	2	6	-	1/6/23/26	0/1/1/1
6	BMA	V	3	6	-	2/2/19/22	0/1/1/1
5	NAG	W	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	0/6/23/26	0/1/1/1
6	NAG	X	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	X	2	6	-	0/6/23/26	0/1/1/1
6	BMA	X	3	6	-	0/2/19/22	0/1/1/1
10	NAG	Y	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	Y	2	10	-	0/6/23/26	0/1/1/1
10	BMA	Y	3	10	-	1/2/19/22	0/1/1/1
10	MAN	Y	4	10	-	0/2/19/22	1/1/1/1
10	MAN	Y	5	10	-	0/2/19/22	0/1/1/1
10	MAN	Y	6	10	-	0/2/19/22	0/1/1/1
10	MAN	Y	7	10	-	0/2/19/22	0/1/1/1
6	NAG	Z	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	1/6/23/26	0/1/1/1
6	BMA	Z	3	6	-	0/2/19/22	0/1/1/1
6	NAG	a	1	6,1	-	5/6/23/26	0/1/1/1
6	NAG	a	2	6	-	0/6/23/26	0/1/1/1
6	BMA	a	3	6	-	0/2/19/22	0/1/1/1
5	NAG	b	1	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	b	2	5	-	1/6/23/26	0/1/1/1
5	NAG	c	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
5	NAG	d	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	d	2	5	-	1/6/23/26	0/1/1/1
6	NAG	e	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	e	2	6	-	2/6/23/26	0/1/1/1
6	BMA	e	3	6	-	1/2/19/22	0/1/1/1
5	NAG	f	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	f	2	5	-	2/6/23/26	0/1/1/1
7	NAG	g	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	g	2	7	-	2/6/23/26	0/1/1/1
7	BMA	g	3	7	-	2/2/19/22	0/1/1/1
7	MAN	g	4	7	-	1/2/19/22	0/1/1/1
7	MAN	g	5	7	-	0/2/19/22	0/1/1/1
6	NAG	h	1	6,1	-	6/6/23/26	0/1/1/1
6	NAG	h	2	6	-	2/6/23/26	0/1/1/1
6	BMA	h	3	6	-	0/2/19/22	0/1/1/1
8	NAG	i	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	i	2	8	-	2/6/23/26	0/1/1/1
8	BMA	i	3	8	-	2/2/19/22	0/1/1/1
8	MAN	i	4	8	-	0/2/19/22	0/1/1/1
9	NAG	j	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	j	2	9	-	0/6/23/26	0/1/1/1
9	BMA	j	3	9	-	0/2/19/22	0/1/1/1
9	MAN	j	4	9	-	0/2/19/22	0/1/1/1
9	MAN	j	5	9	-	0/2/19/22	0/1/1/1
6	NAG	k	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	k	2	6	-	0/6/23/26	0/1/1/1
6	BMA	k	3	6	-	1/2/19/22	0/1/1/1
6	NAG	l	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	l	2	6	-	1/6/23/26	0/1/1/1
6	BMA	l	3	6	-	2/2/19/22	0/1/1/1
5	NAG	m	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	m	2	5	-	0/6/23/26	0/1/1/1
6	NAG	n	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	n	2	6	-	0/6/23/26	0/1/1/1
6	BMA	n	3	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	o	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	o	2	10	-	0/6/23/26	0/1/1/1
10	BMA	o	3	10	-	1/2/19/22	0/1/1/1
10	MAN	o	4	10	-	0/2/19/22	1/1/1/1
10	MAN	o	5	10	-	0/2/19/22	0/1/1/1
10	MAN	o	6	10	-	0/2/19/22	0/1/1/1
10	MAN	o	7	10	-	0/2/19/22	0/1/1/1
6	NAG	p	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	p	2	6	-	1/6/23/26	0/1/1/1
6	BMA	p	3	6	-	0/2/19/22	0/1/1/1
6	NAG	q	1	6,1	-	5/6/23/26	0/1/1/1
6	NAG	q	2	6	-	0/6/23/26	0/1/1/1
6	BMA	q	3	6	-	0/2/19/22	0/1/1/1
5	NAG	r	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	r	2	5	-	1/6/23/26	0/1/1/1
5	NAG	s	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	s	2	5	-	2/6/23/26	0/1/1/1
5	NAG	t	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	t	2	5	-	1/6/23/26	0/1/1/1
6	NAG	u	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	u	2	6	-	2/6/23/26	0/1/1/1
6	BMA	u	3	6	-	1/2/19/22	0/1/1/1
5	NAG	v	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	v	2	5	-	2/6/23/26	0/1/1/1
7	NAG	w	1	7	-	2/6/23/26	0/1/1/1
7	NAG	w	2	7	-	2/6/23/26	0/1/1/1
7	BMA	w	3	7	-	2/2/19/22	0/1/1/1
7	MAN	w	4	7	-	1/2/19/22	0/1/1/1
7	MAN	w	5	7	-	0/2/19/22	0/1/1/1
6	NAG	x	1	6,1	-	6/6/23/26	0/1/1/1
6	NAG	x	2	6	-	2/6/23/26	0/1/1/1
6	BMA	x	3	6	-	0/2/19/22	0/1/1/1
8	NAG	y	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	y	2	8	-	2/6/23/26	0/1/1/1
8	BMA	y	3	8	-	2/2/19/22	0/1/1/1
8	MAN	y	4	8	-	0/2/19/22	0/1/1/1
9	NAG	z	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	z	2	9	-	0/6/23/26	0/1/1/1
9	BMA	z	3	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	z	4	9	-	0/2/19/22	0/1/1/1
9	MAN	z	5	9	-	0/2/19/22	0/1/1/1

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	z	1	NAG	O5-C1	-4.32	1.36	1.43
9	T	1	NAG	O5-C1	-4.29	1.36	1.43
9	j	1	NAG	O5-C1	-4.28	1.36	1.43
6	n	1	NAG	O5-C1	-3.52	1.37	1.43
6	X	1	NAG	O5-C1	-3.50	1.37	1.43

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	u	1	NAG	C2-N2-C7	4.52	128.95	122.90
6	R	1	NAG	C2-N2-C7	4.48	128.90	122.90
6	O	1	NAG	C2-N2-C7	4.47	128.88	122.90
6	e	1	NAG	C2-N2-C7	4.47	128.88	122.90
6	6	1	NAG	C2-N2-C7	4.43	128.84	122.90

There are no chirality outliers.

5 of 174 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	S	1	NAG	C1-C2-N2-C7
8	i	1	NAG	C1-C2-N2-C7
8	y	1	NAG	C1-C2-N2-C7
8	S	3	BMA	O5-C5-C6-O6
8	i	3	BMA	O5-C5-C6-O6

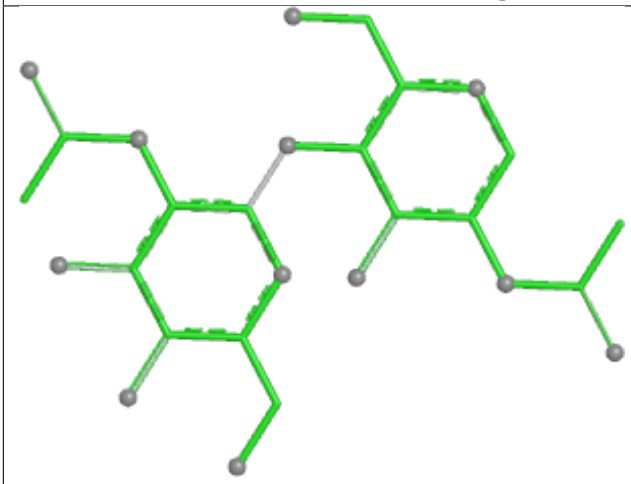
All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	o	4	MAN	C1-C2-C3-C4-C5-O5
10	4	4	MAN	C1-C2-C3-C4-C5-O5
10	Y	4	MAN	C1-C2-C3-C4-C5-O5

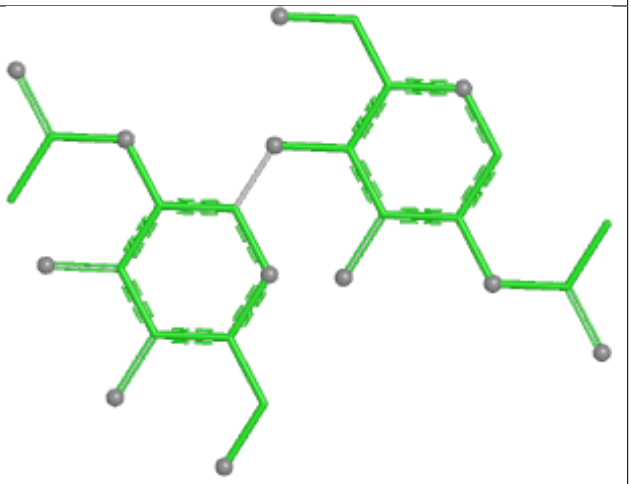
No monomer is involved in short contacts.

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

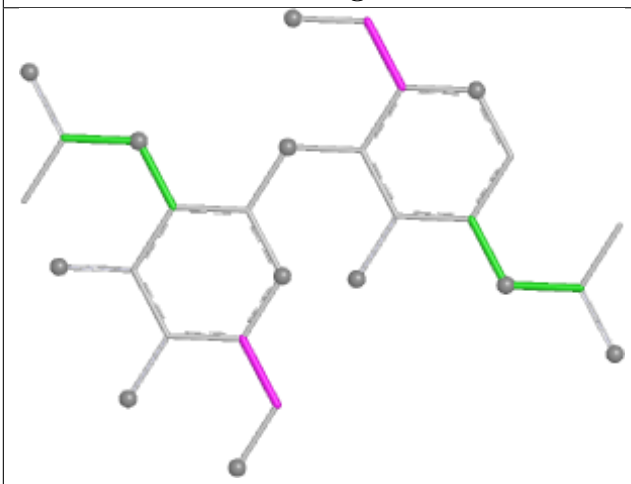
Oligosaccharide Chain G



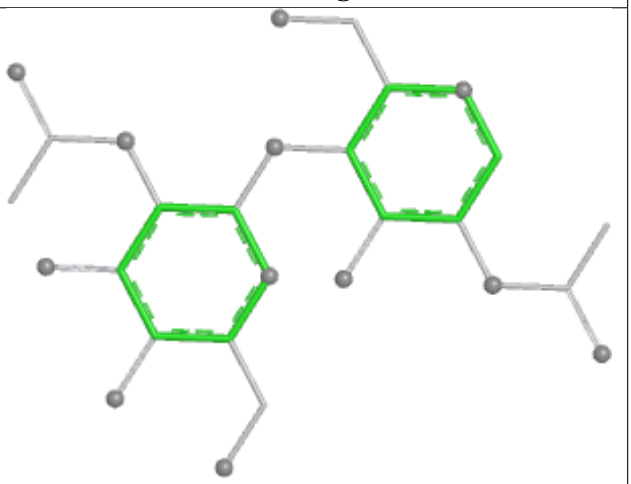
Bond lengths



Bond angles

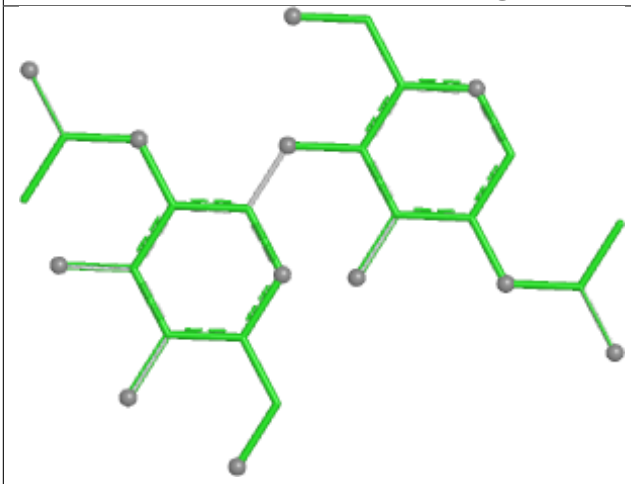


Torsions

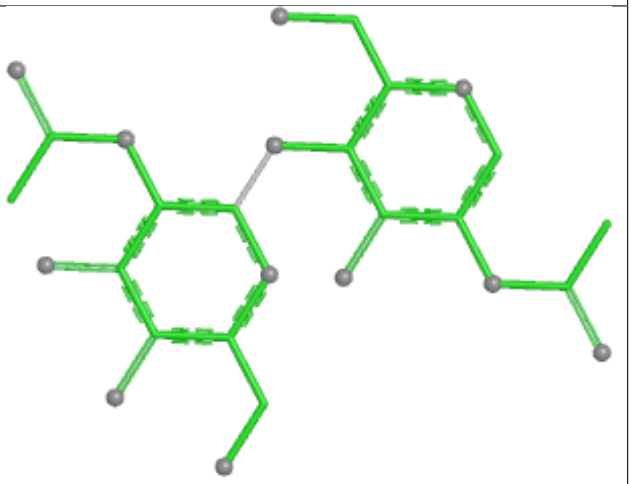


Rings

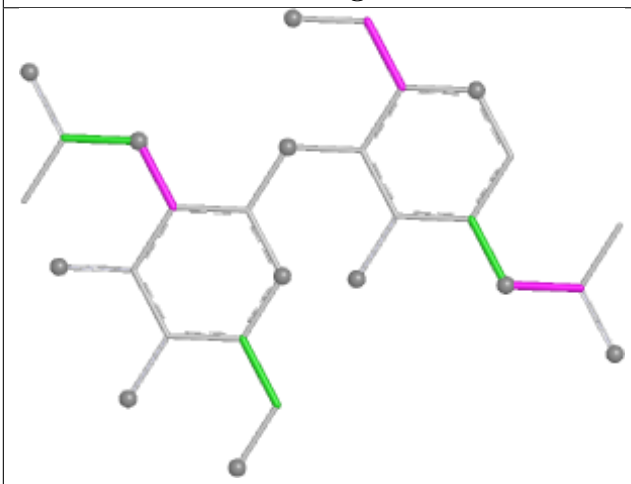
Oligosaccharide Chain K



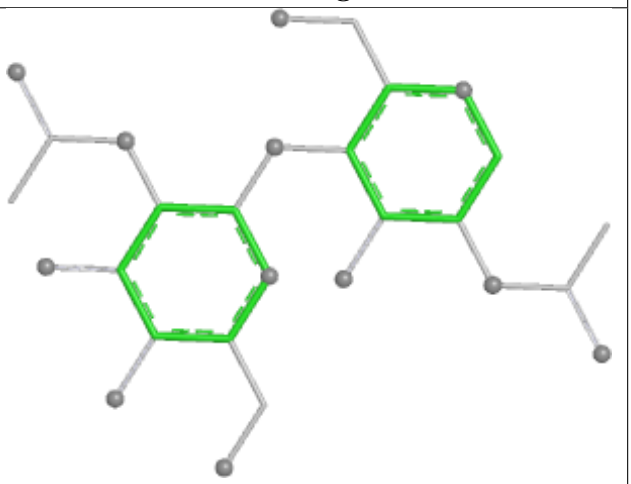
Bond lengths



Bond angles

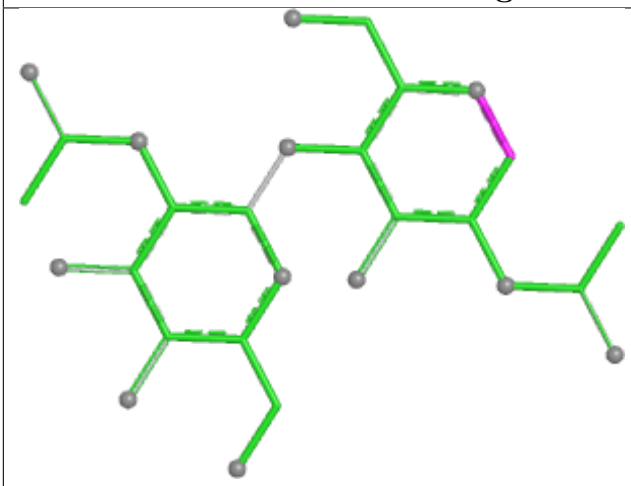


Torsions

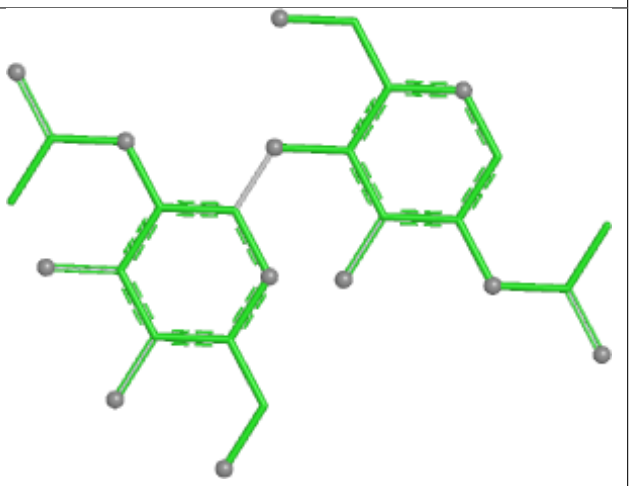


Rings

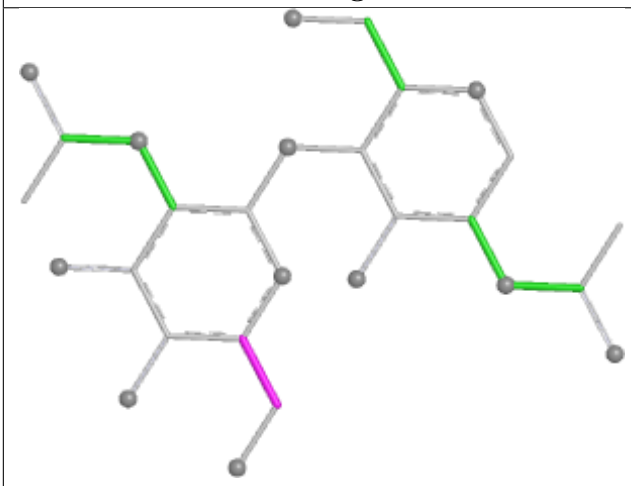
Oligosaccharide Chain P



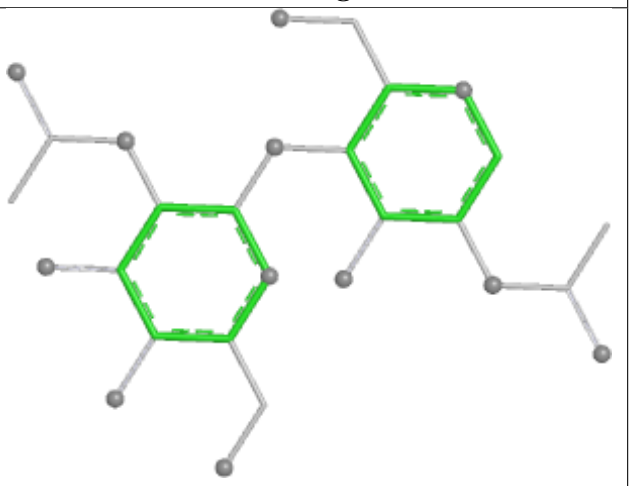
Bond lengths



Bond angles

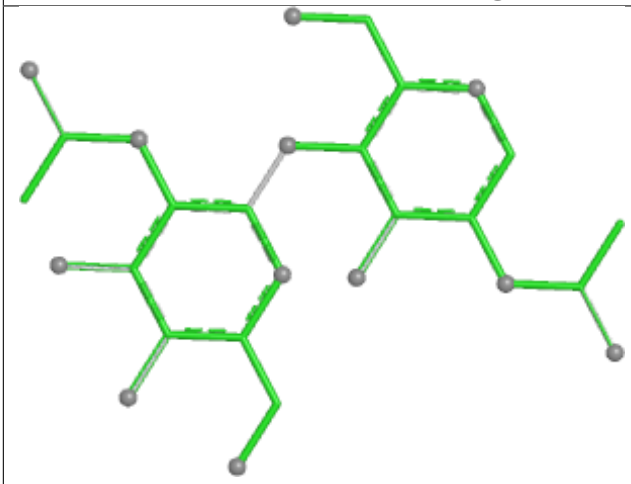


Torsions

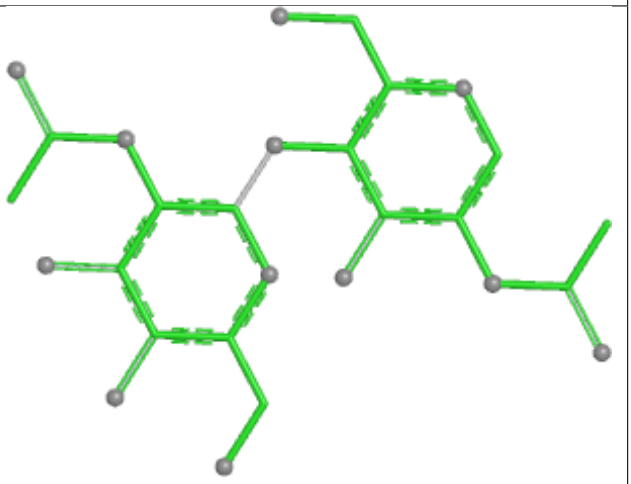


Rings

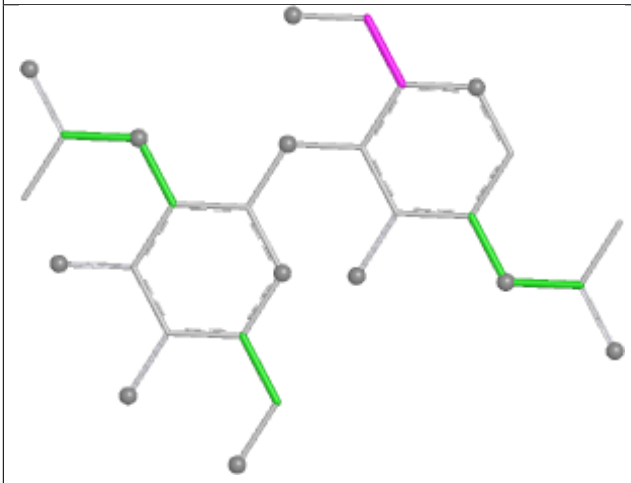
Oligosaccharide Chain W



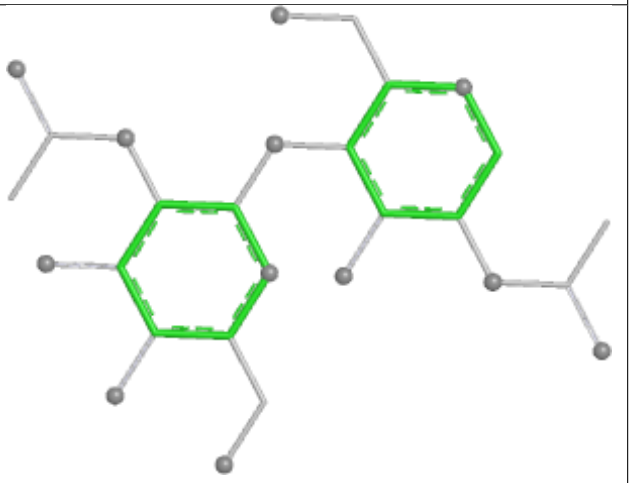
Bond lengths



Bond angles

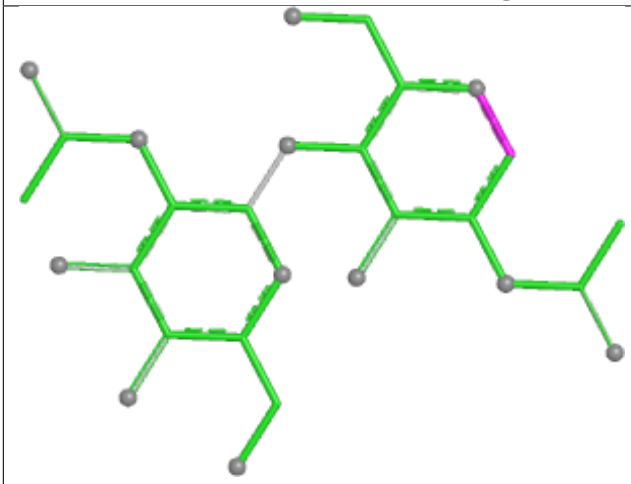


Torsions

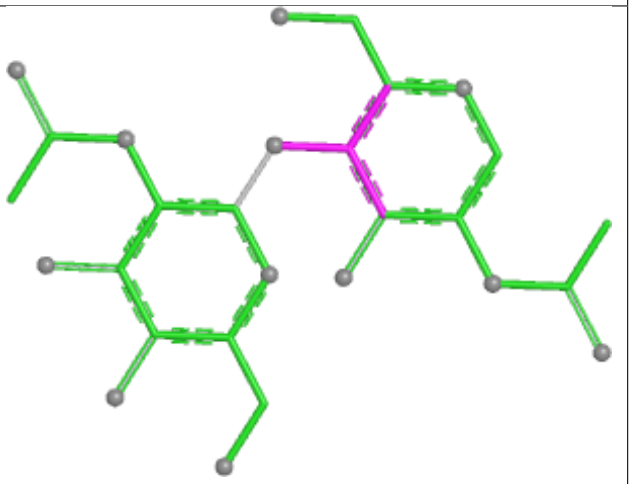


Rings

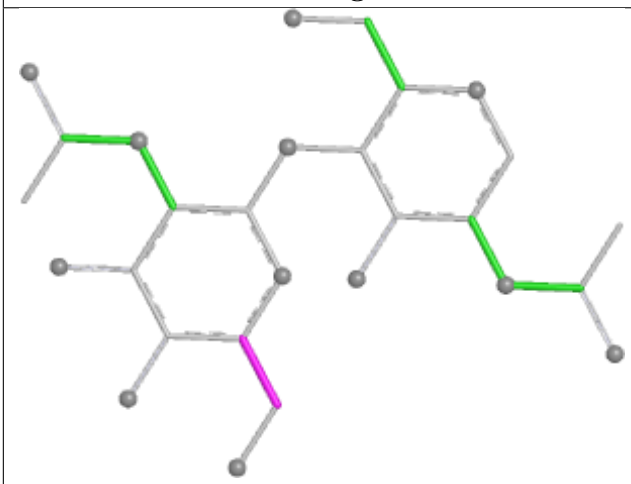
Oligosaccharide Chain b



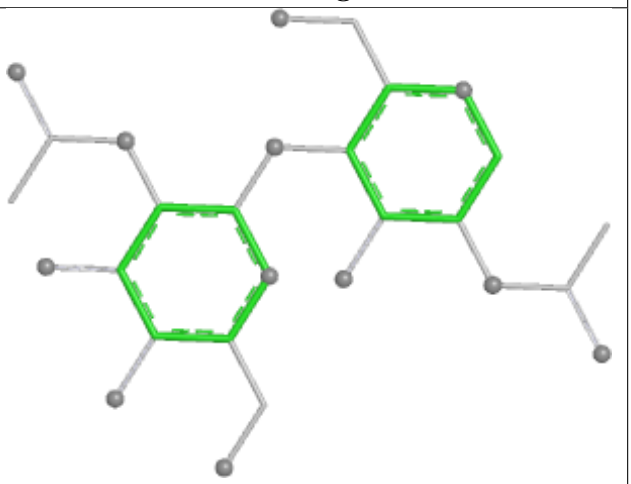
Bond lengths



Bond angles

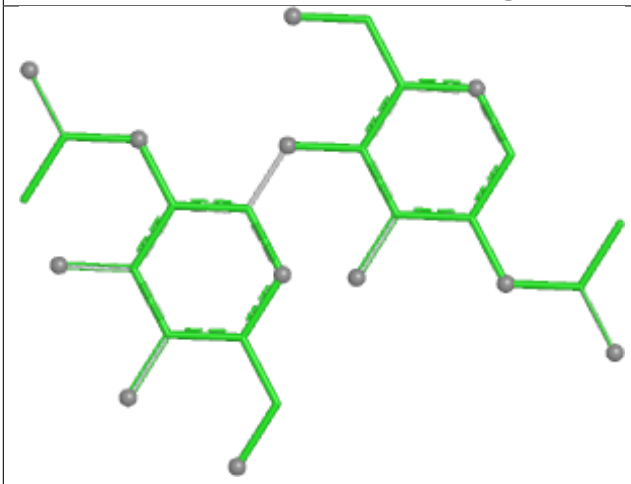


Torsions

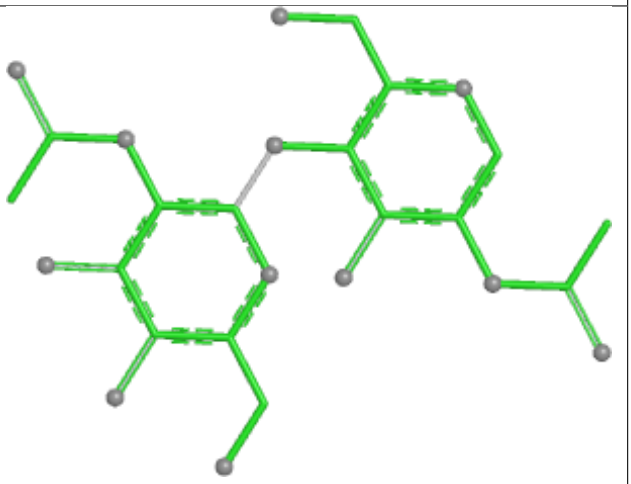


Rings

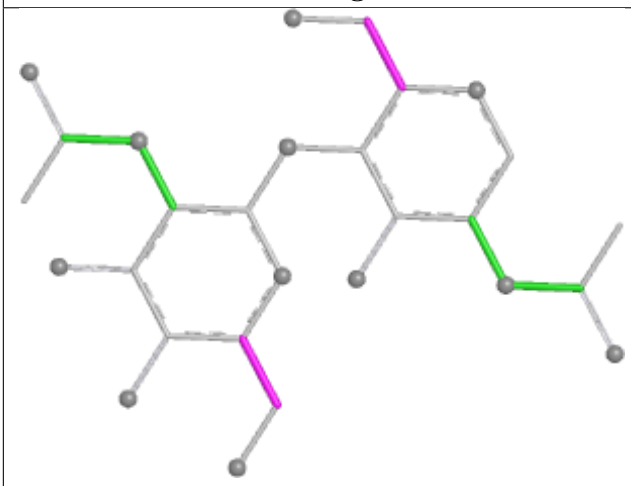
Oligosaccharide Chain c



Bond lengths



Bond angles



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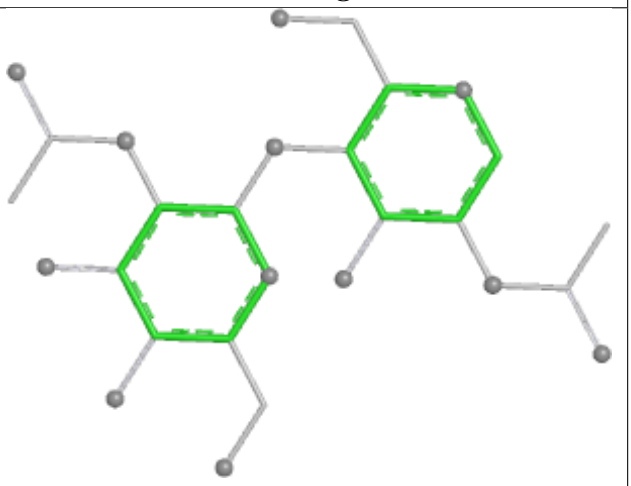
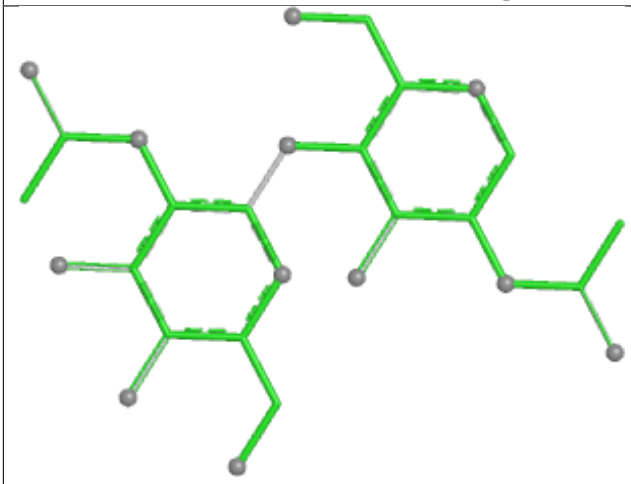
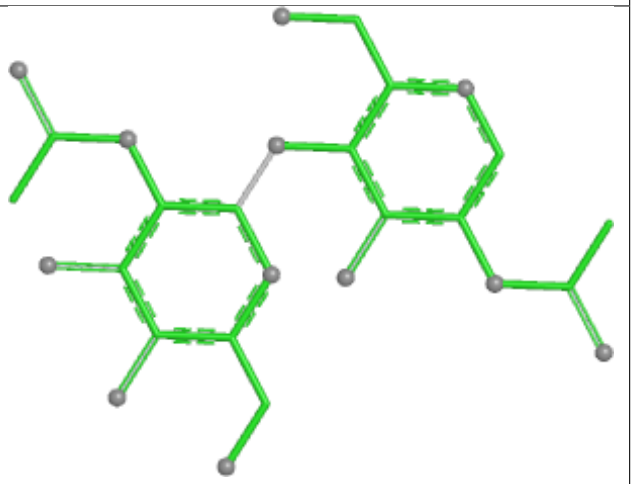


Rings

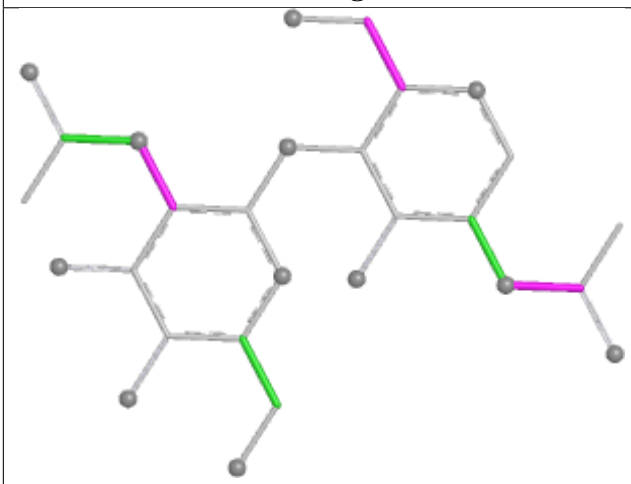
Oligosaccharide Chain d



Bond lengths



Bond angles



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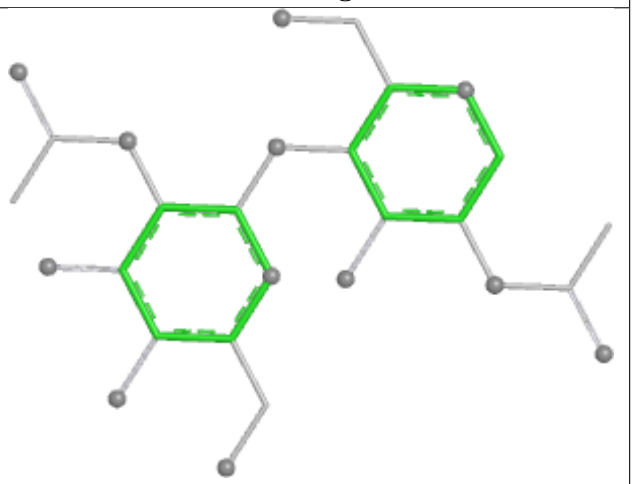
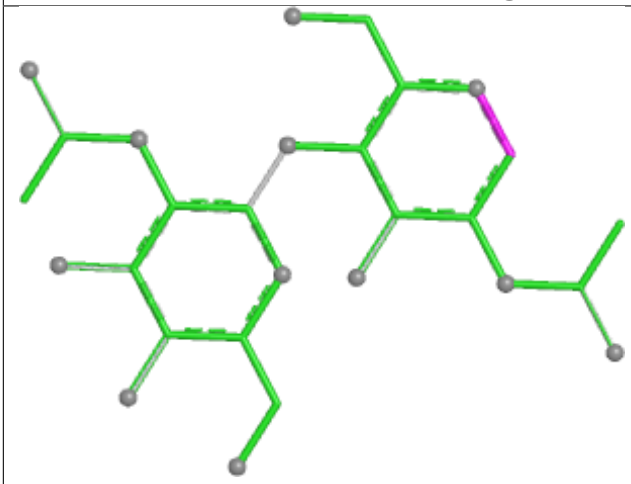


Rings

Oligosaccharide Chain f



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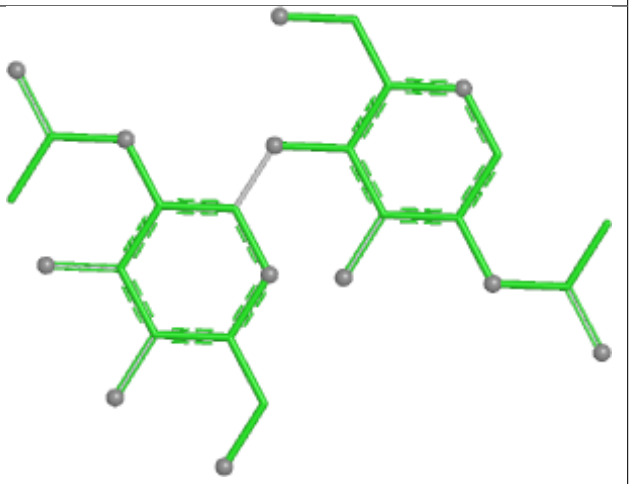
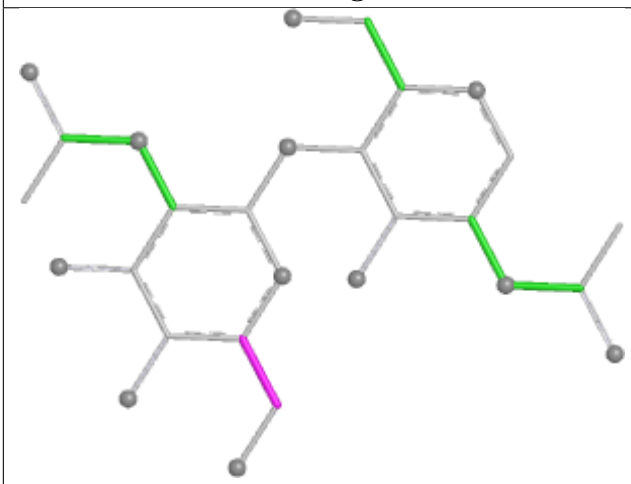
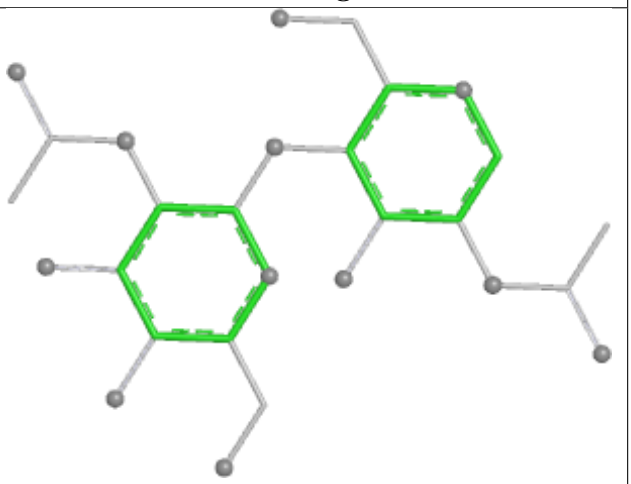


Bond angles

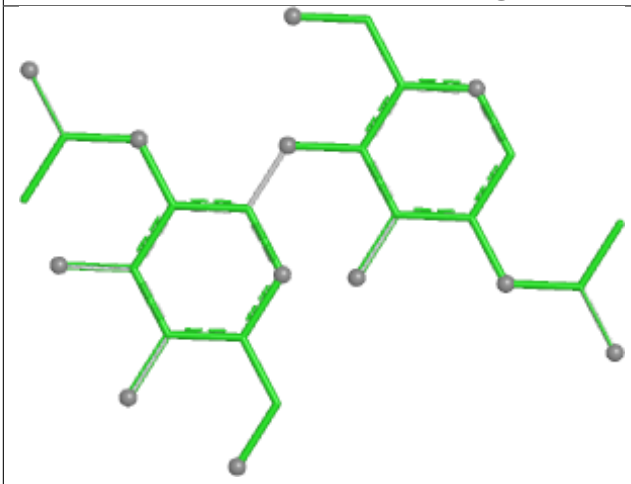


Torsions

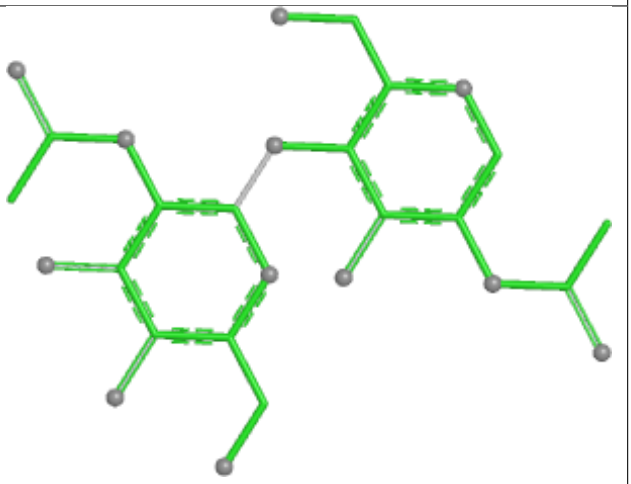


Rings

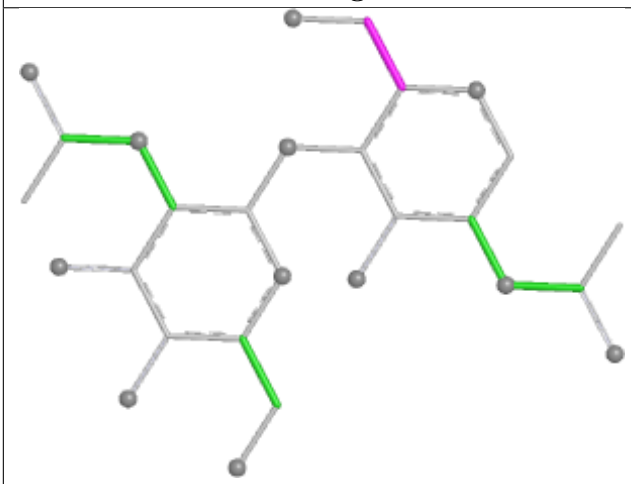
Oligosaccharide Chain m



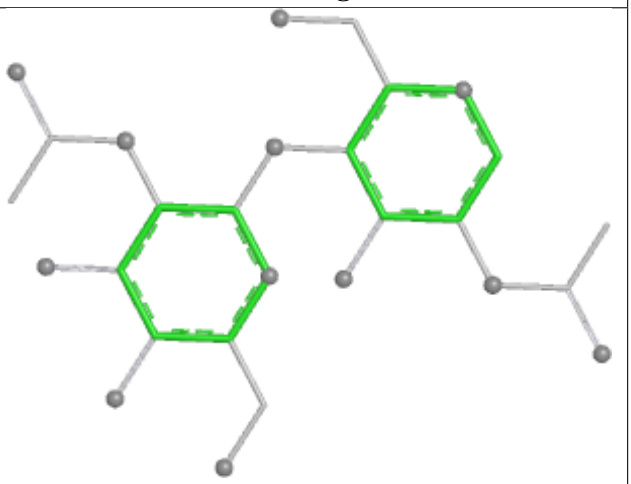
Bond lengths



Bond angles

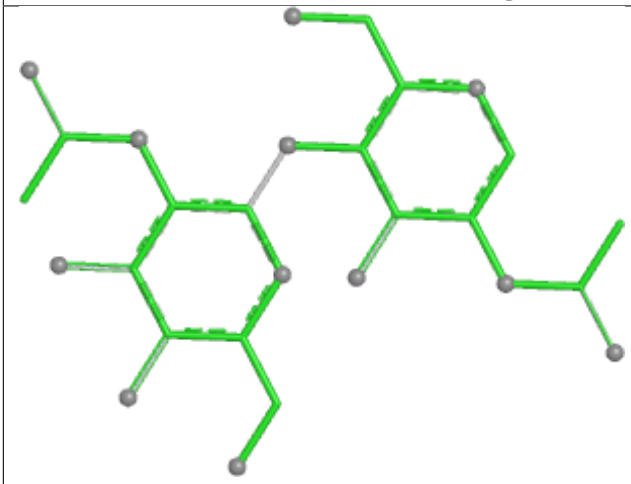


Torsions

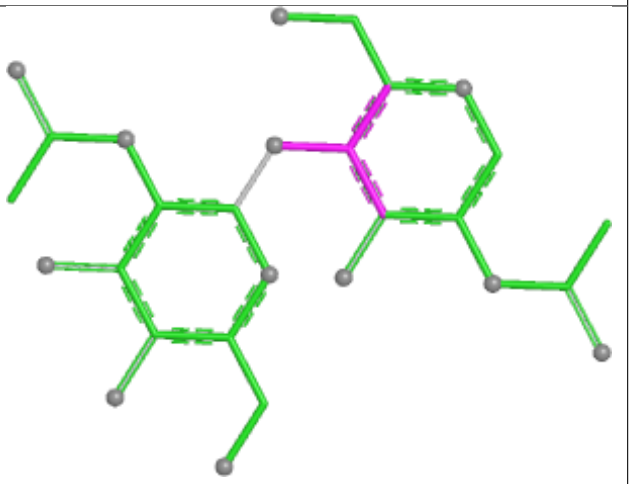


Rings

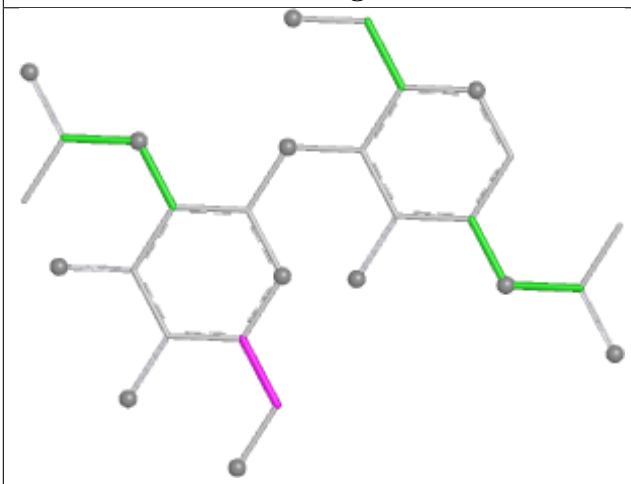
Oligosaccharide Chain r



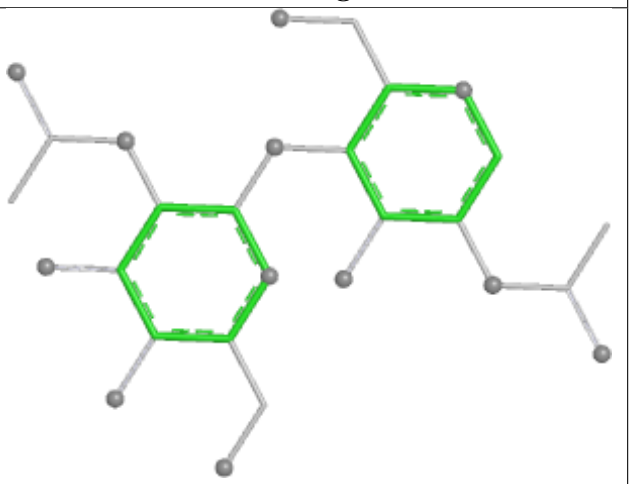
Bond lengths



Bond angles

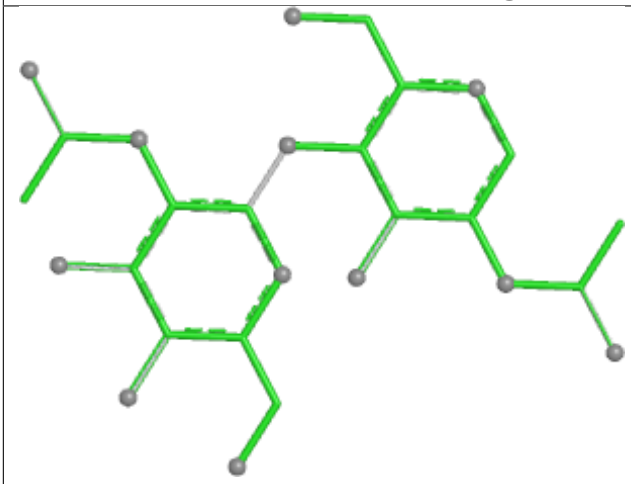


Torsions

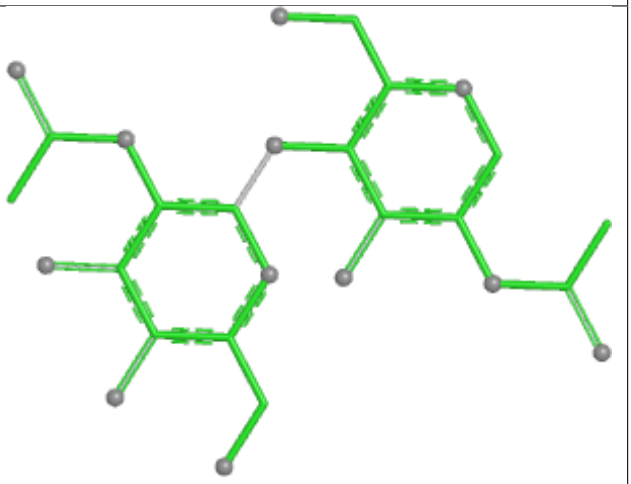


Rings

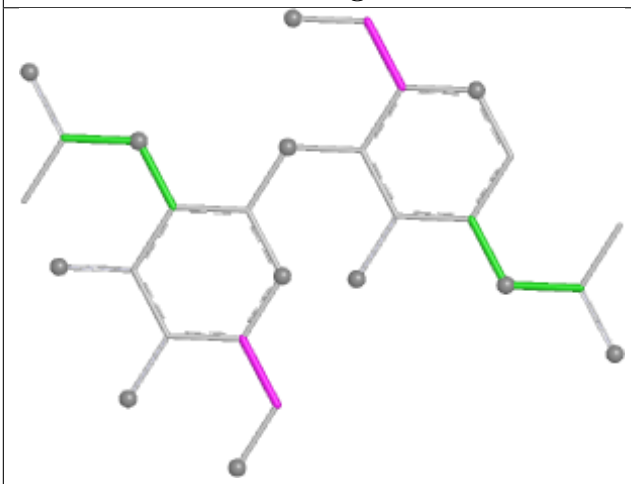
Oligosaccharide Chain s



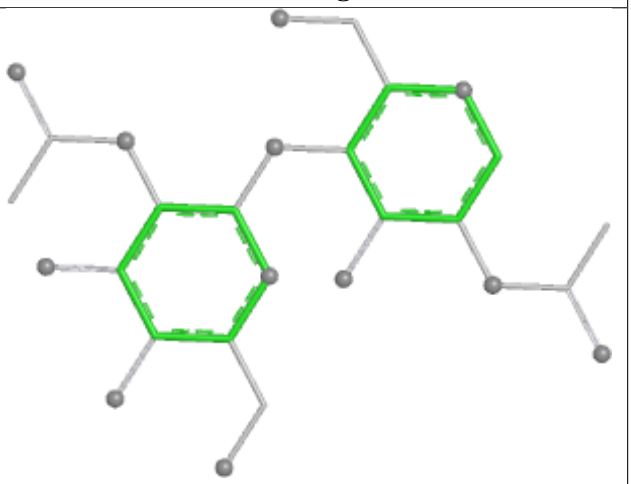
Bond lengths



Bond angles

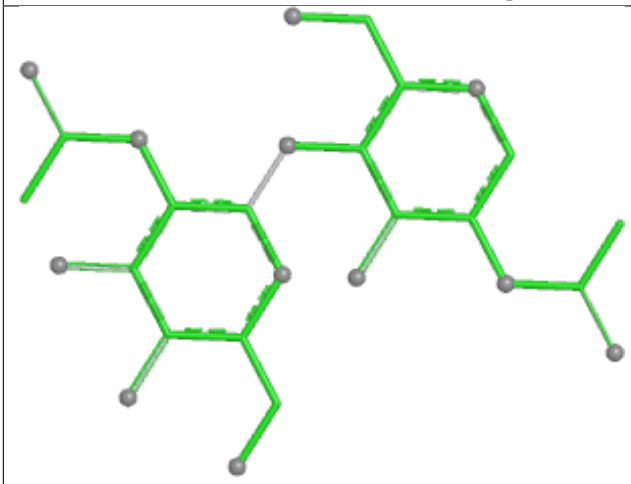


Torsions

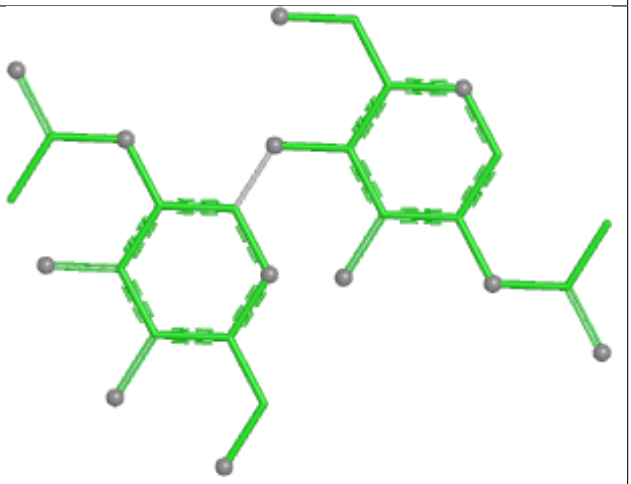


Rings

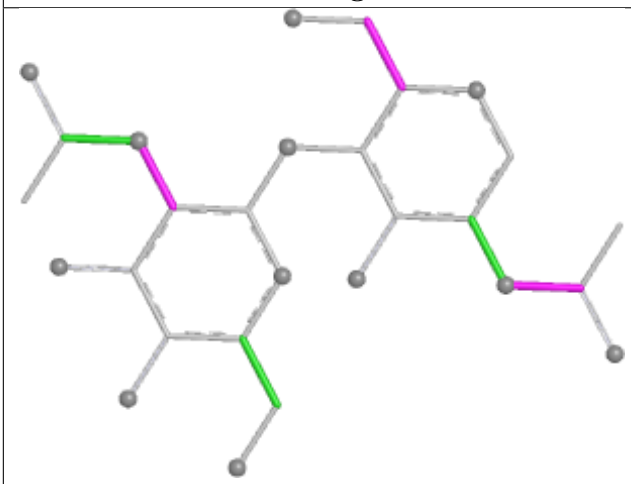
Oligosaccharide Chain t



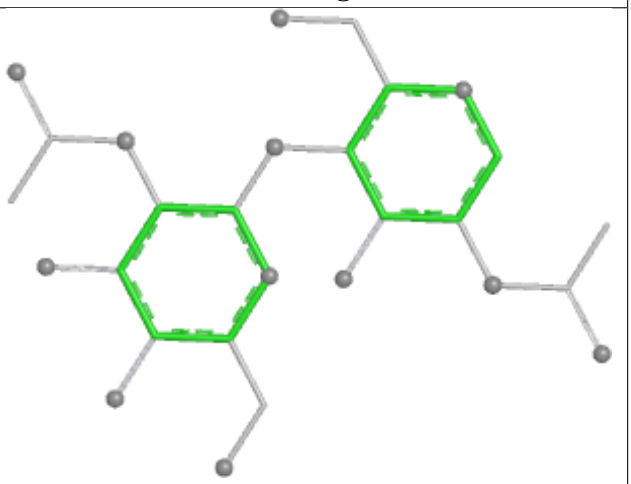
Bond lengths



Bond angles

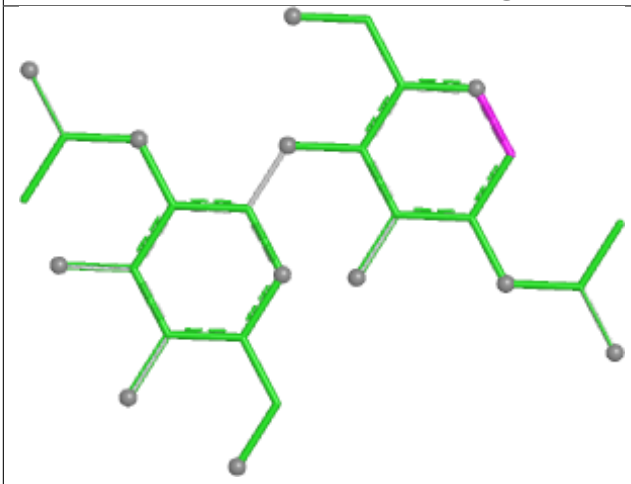


Torsions

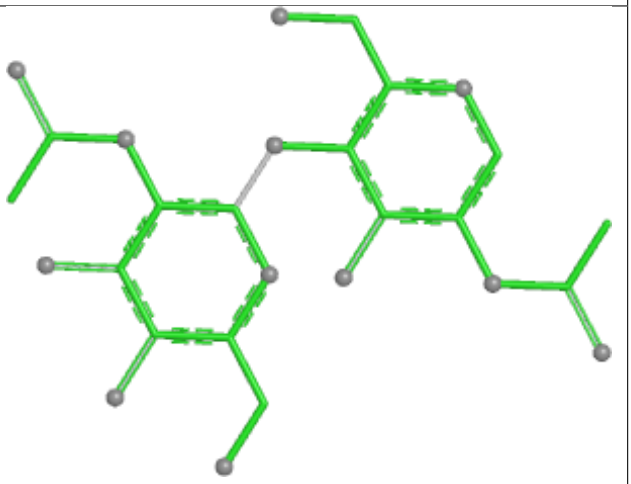


Rings

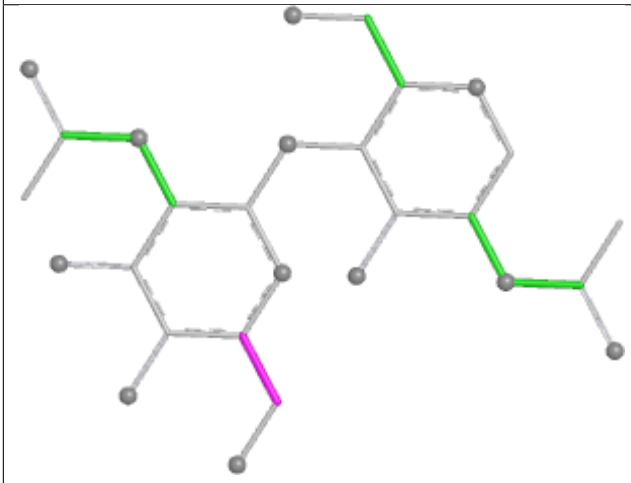
Oligosaccharide Chain v



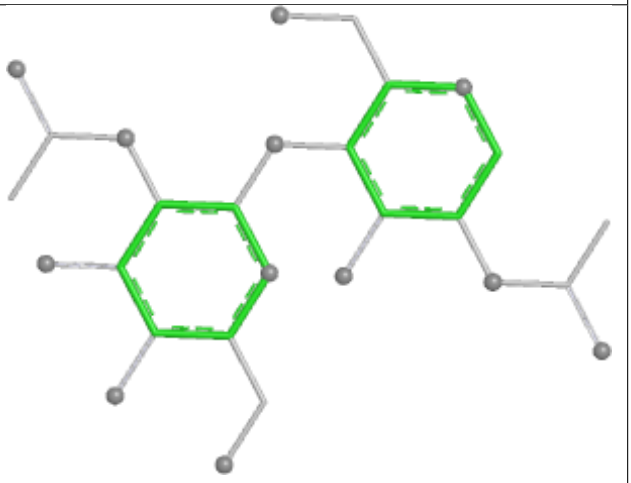
Bond lengths



Bond angles

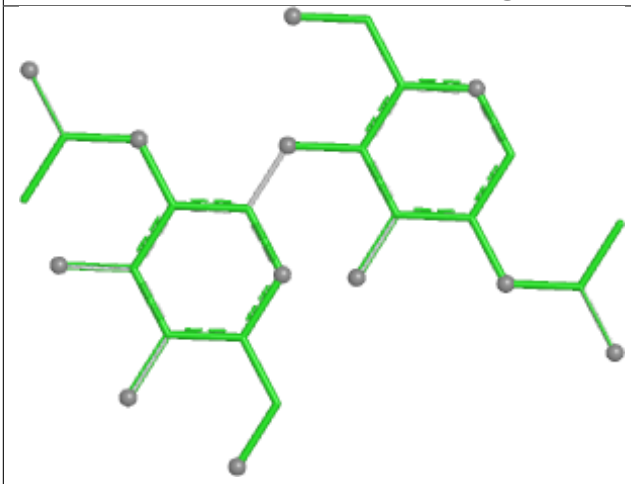


Torsions

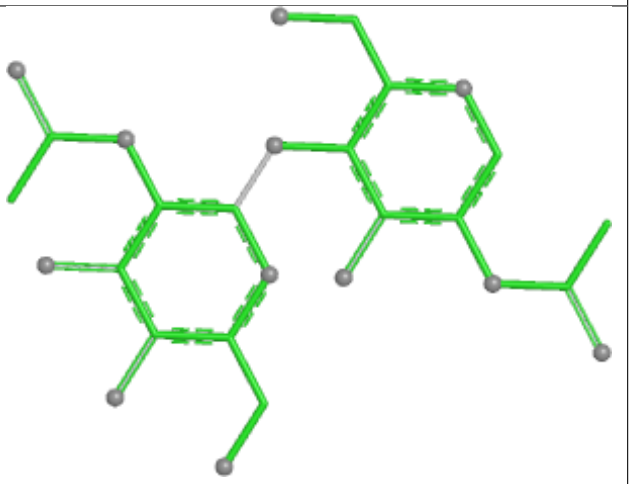


Rings

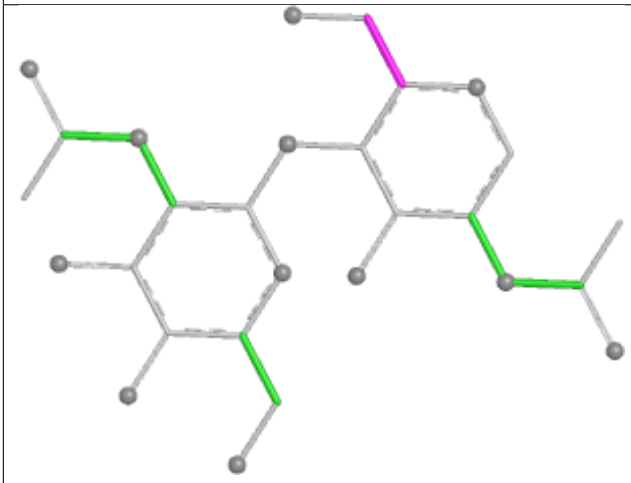
Oligosaccharide Chain 2



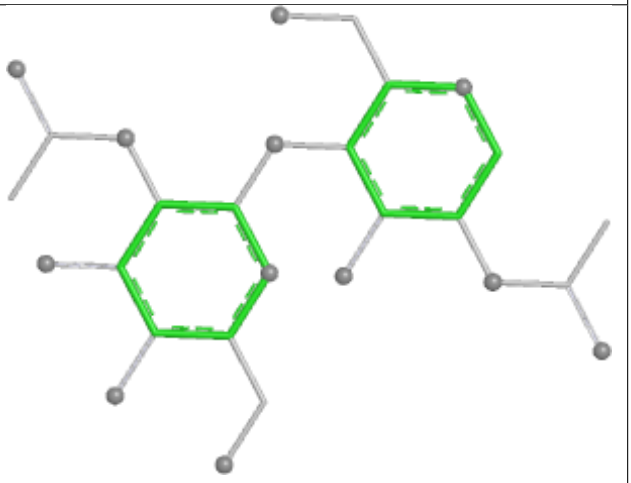
Bond lengths



Bond angles

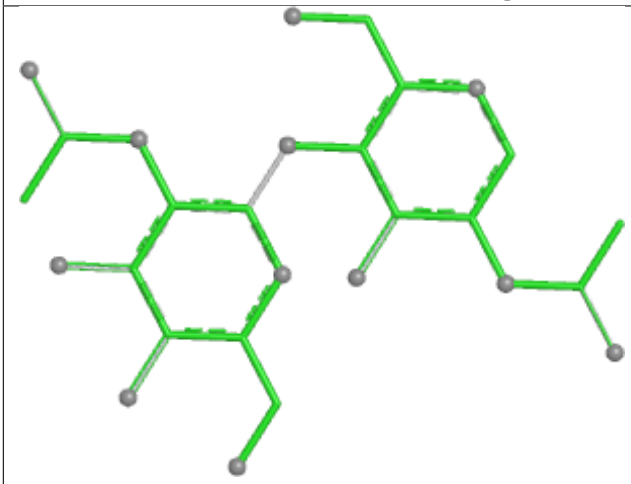


Torsions

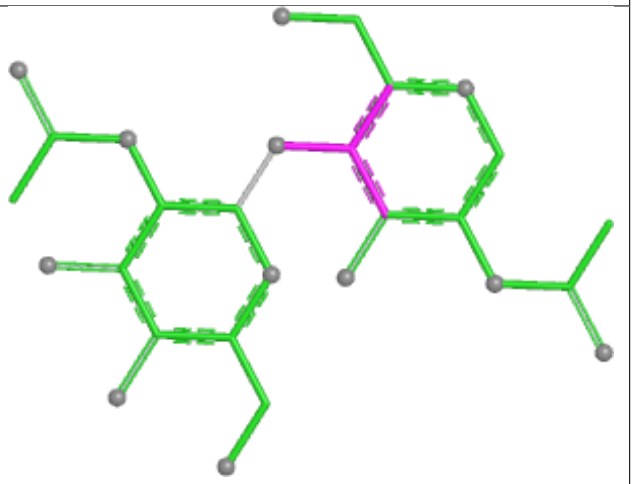


Rings

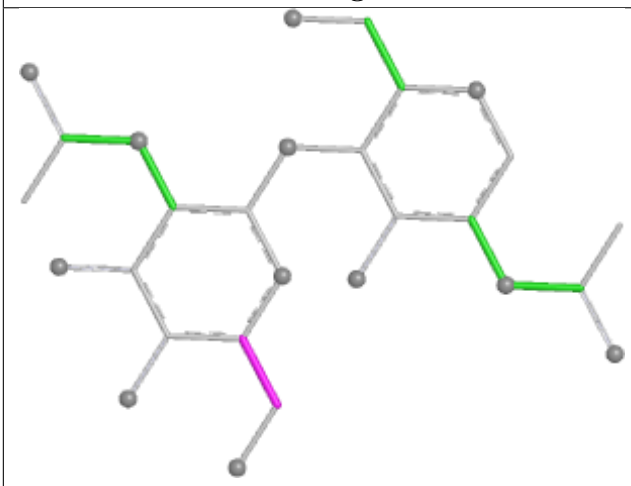
Oligosaccharide Chain 7



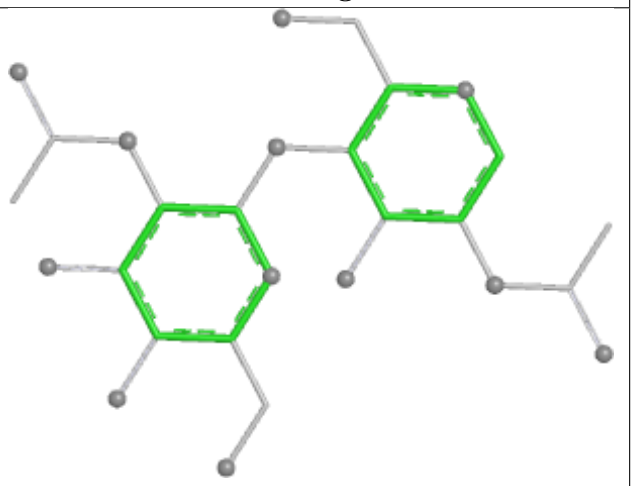
Bond lengths



Bond angles

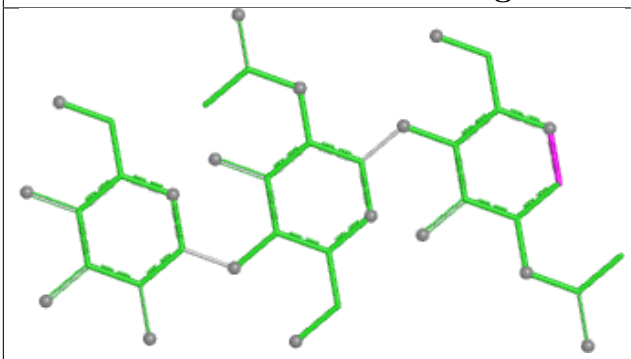


Torsions

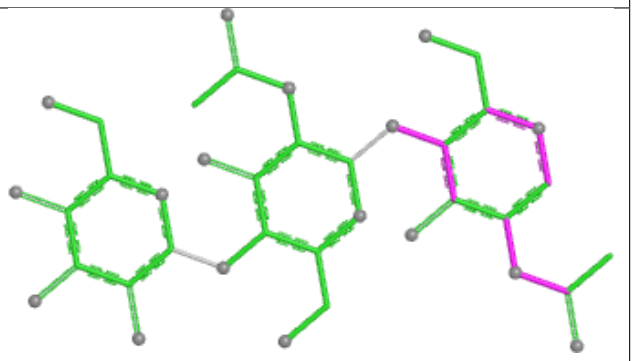


Rings

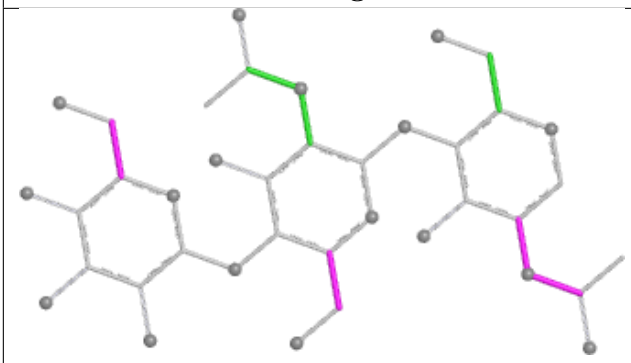
Oligosaccharide Chain O



Bond lengths



Bond angles



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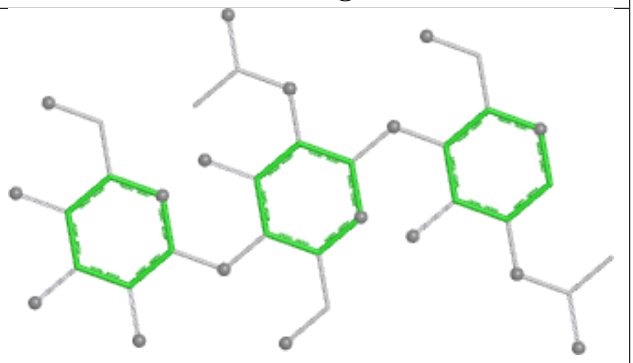
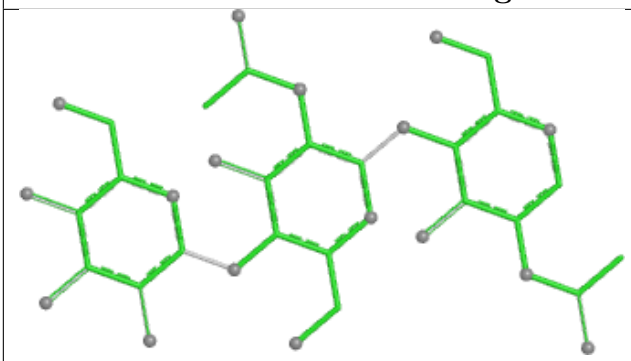


Rings

Oligosaccharide Chain R



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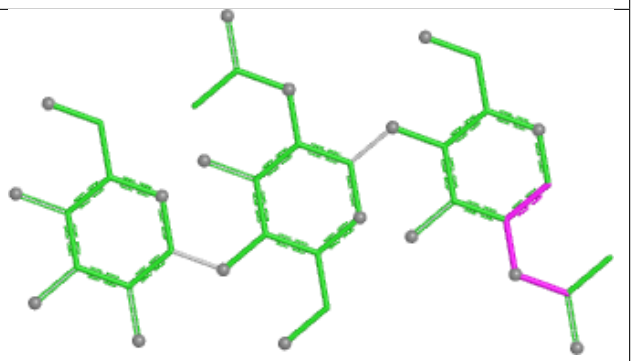
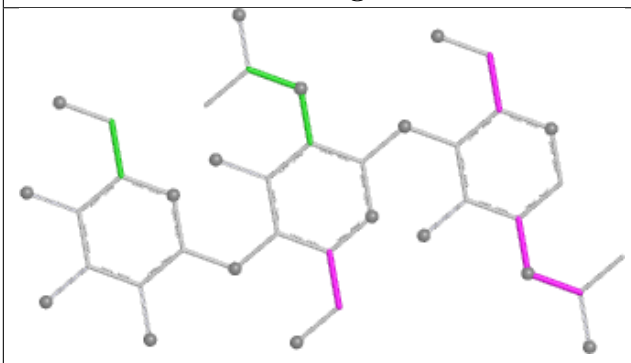


Bond angles



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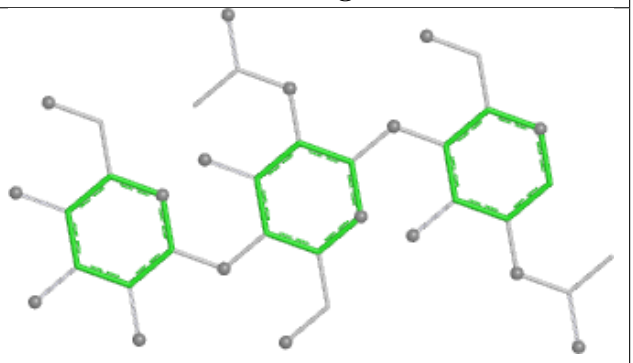
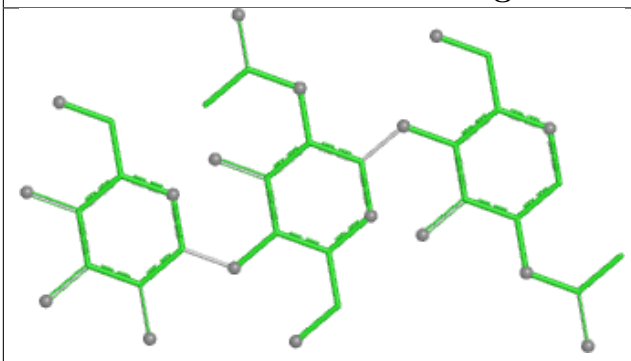


Rings

Oligosaccharide Chain U



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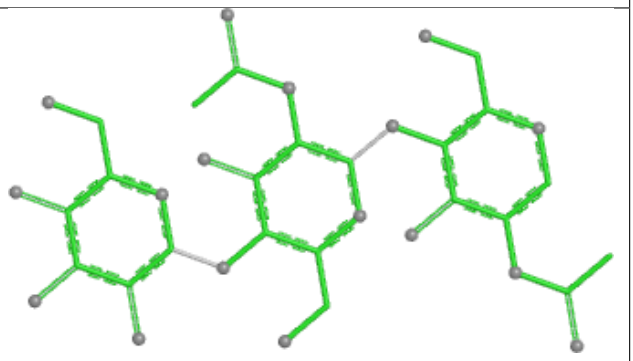

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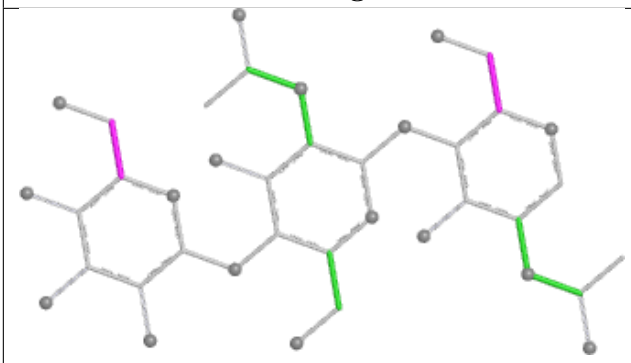

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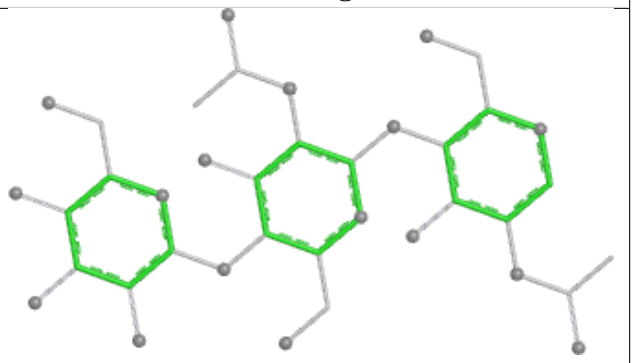
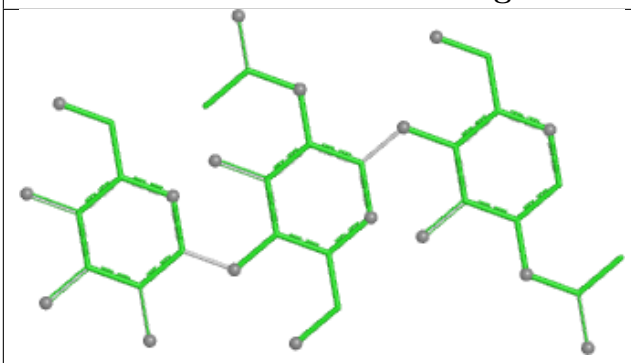


Rings

Oligosaccharide Chain V



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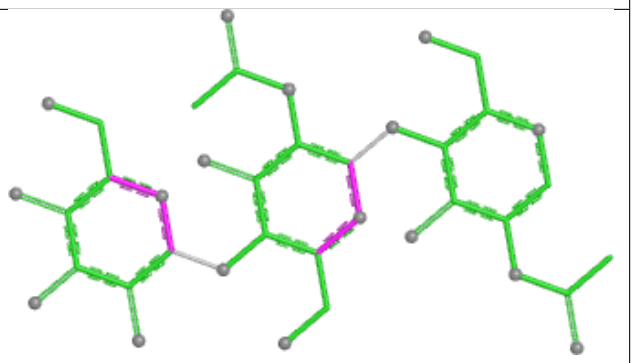
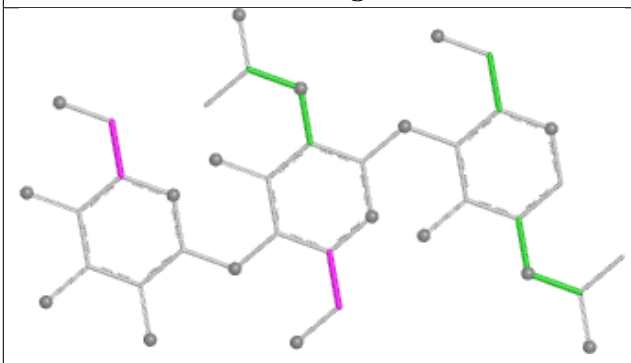


Bond angles



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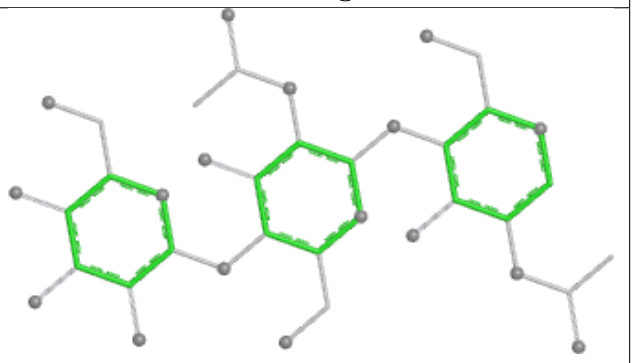
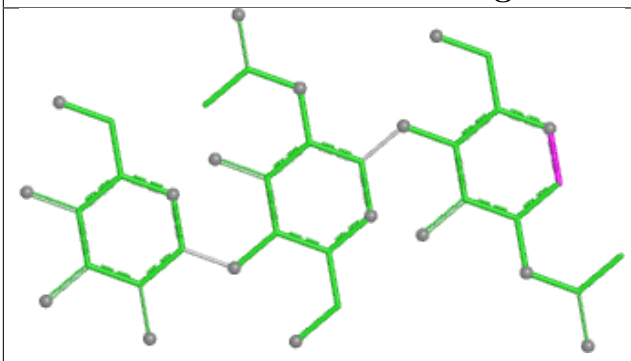


Rings

Oligosaccharide Chain X



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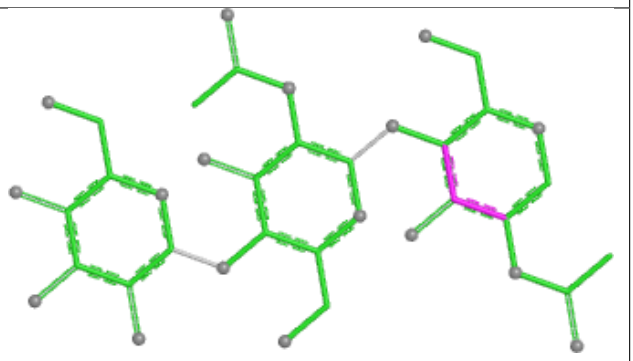
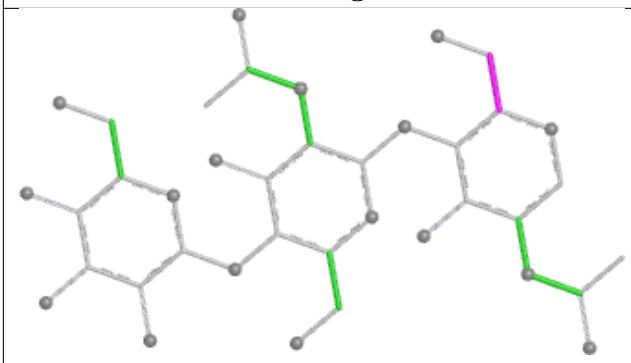


Bond angles



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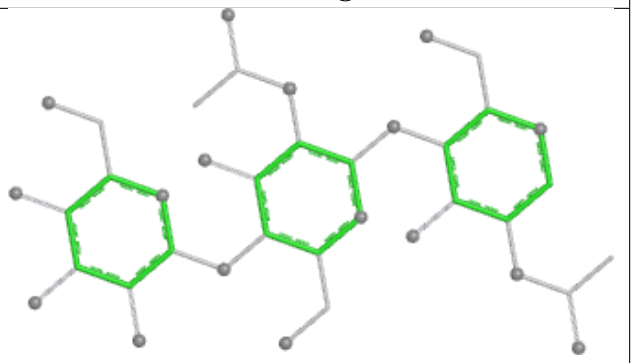
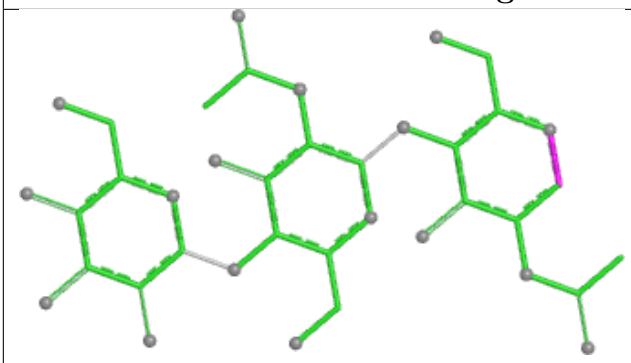


Rings

Oligosaccharide Chain Z



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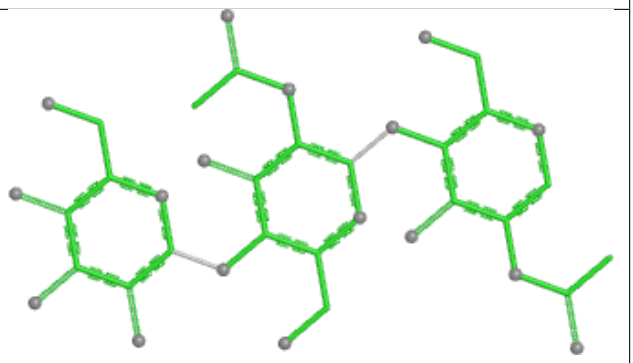
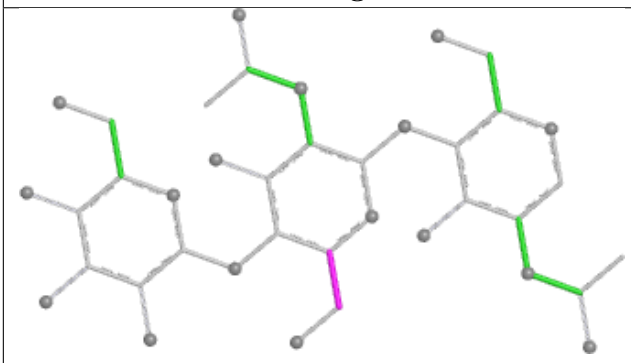


Bond angles



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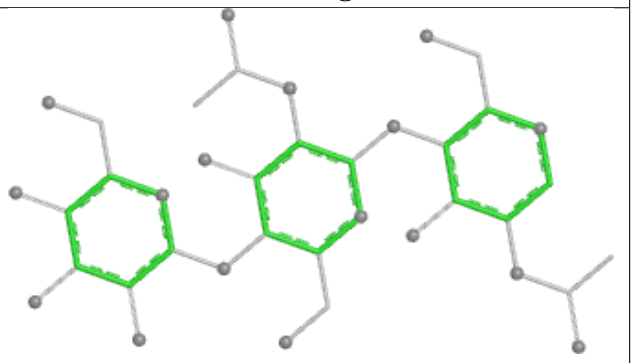
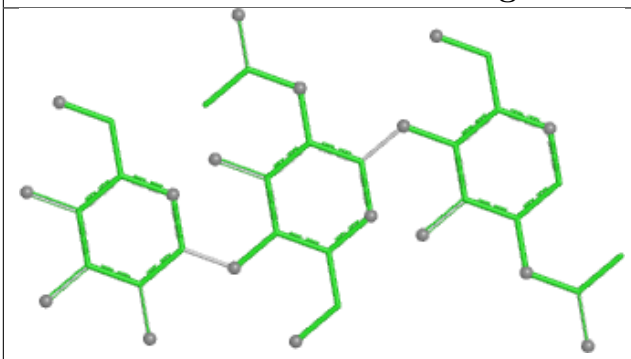


Rings

Oligosaccharide Chain a



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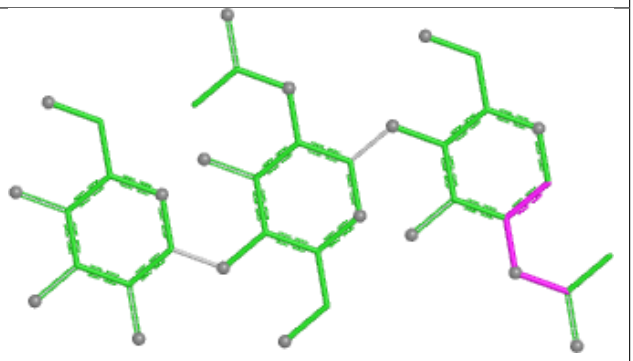

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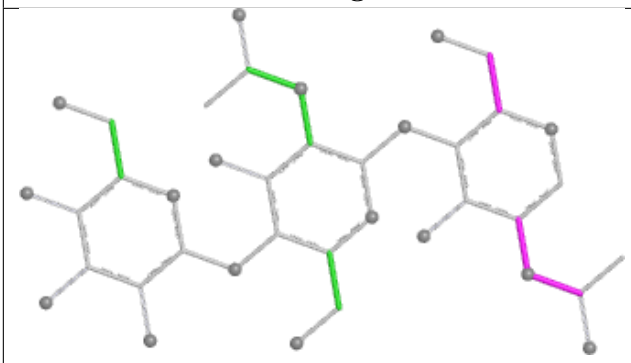

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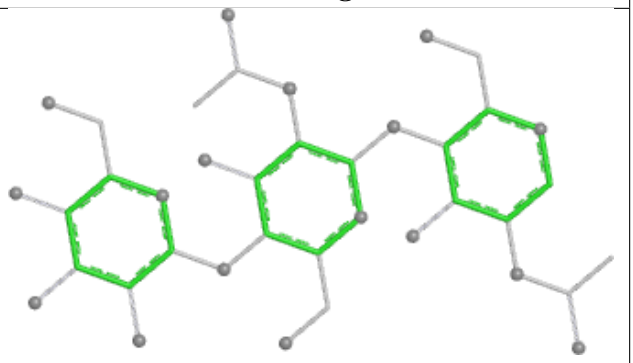
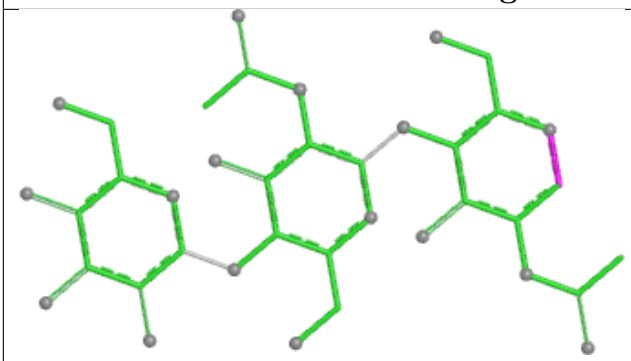


Rings

Oligosaccharide Chain e



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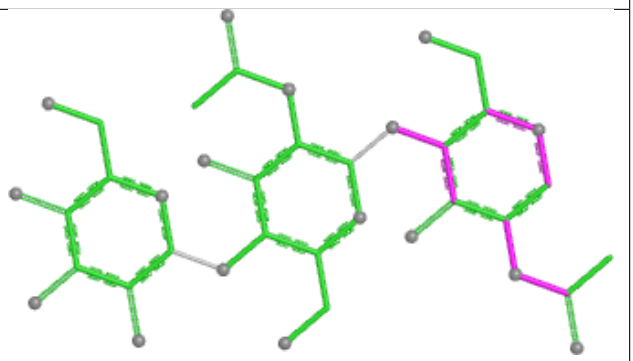
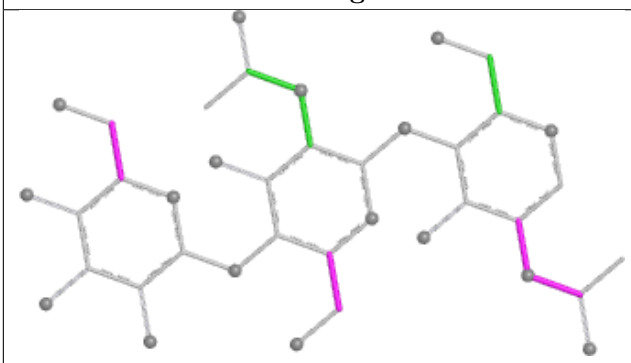


Bond angles



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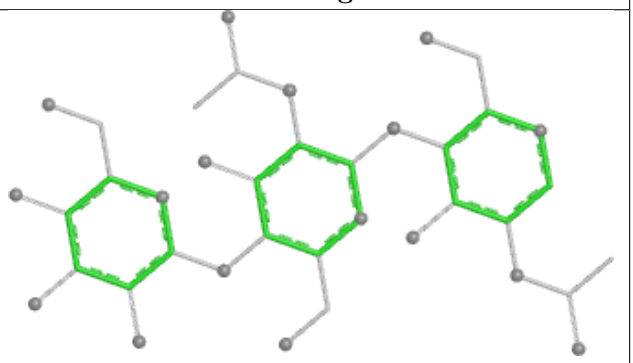
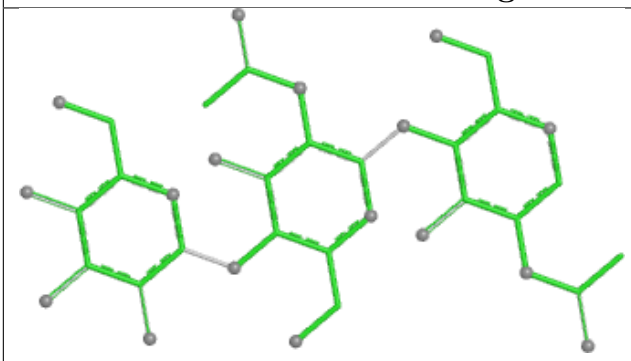
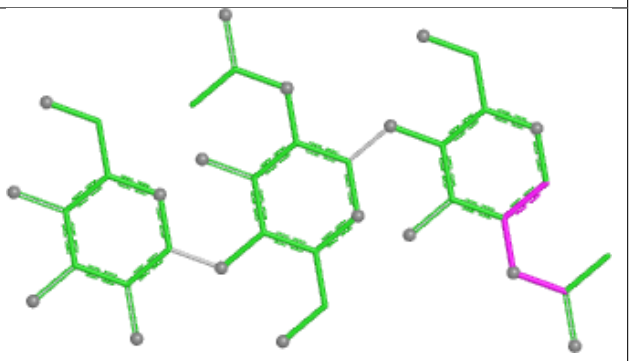


Rings

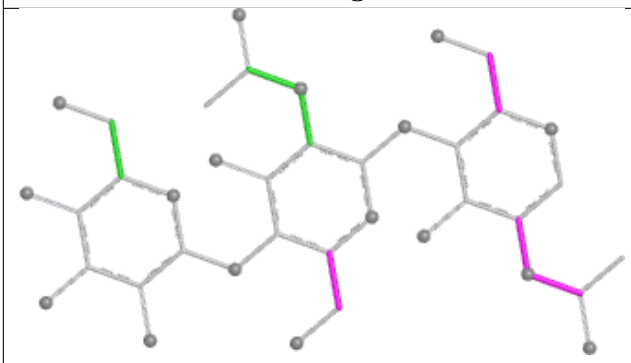
Oligosaccharide Chain h



Bond lengths



Bond angles



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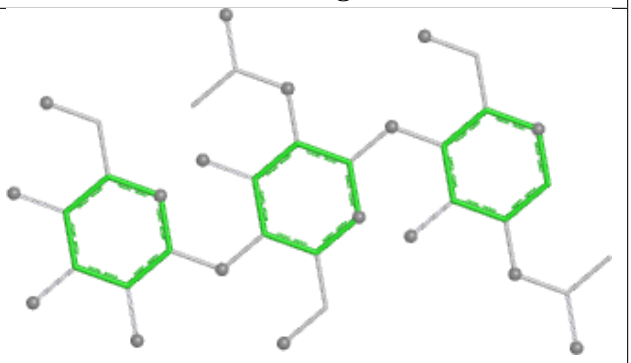
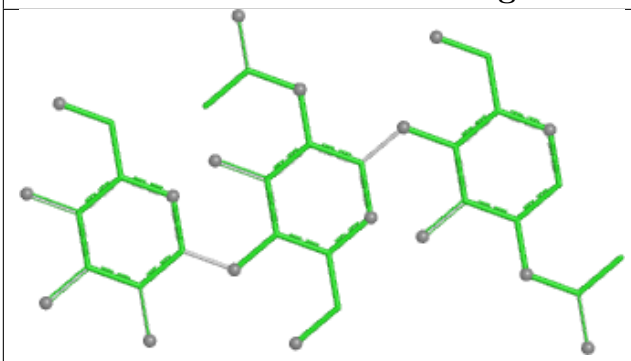


Rings

Oligosaccharide Chain k



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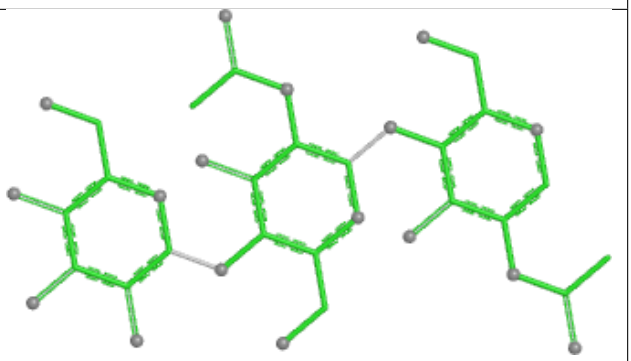

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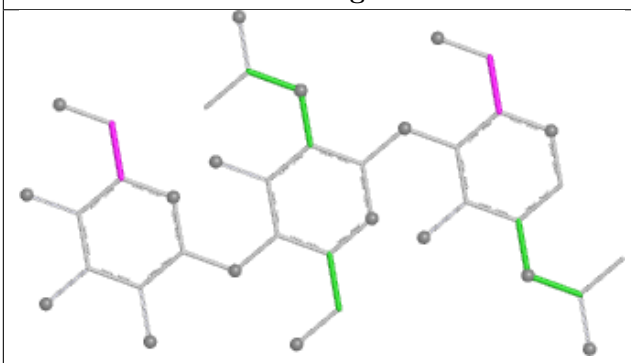

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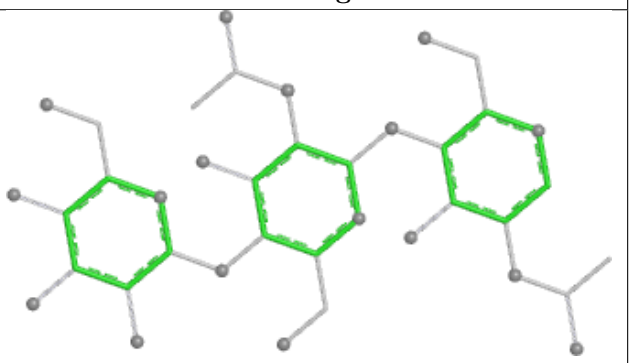
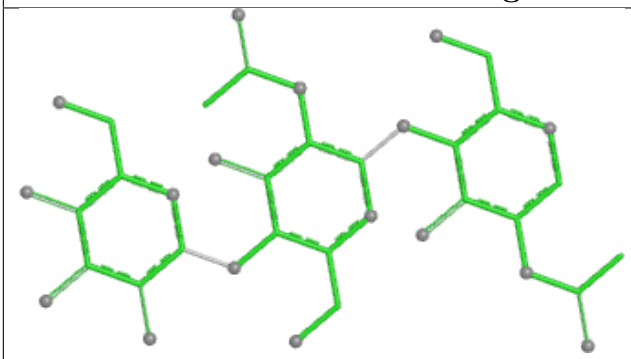


Rings

Oligosaccharide Chain l



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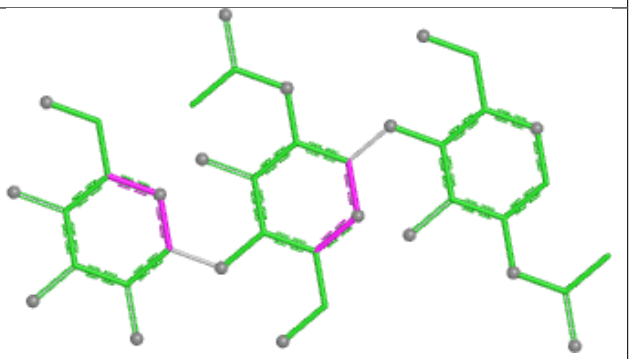
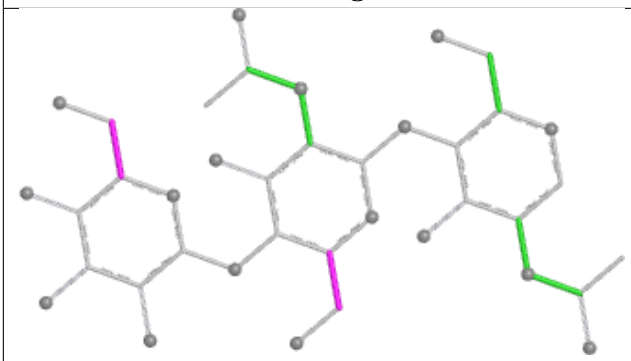


Bond angles



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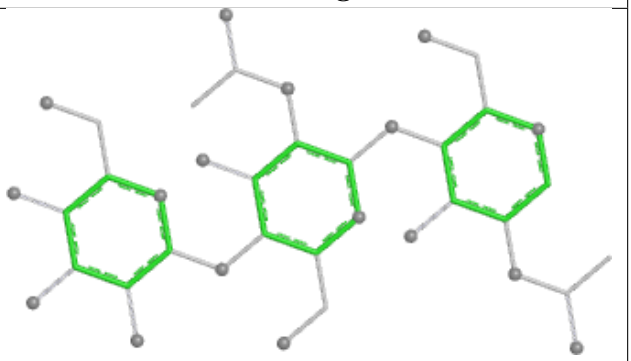
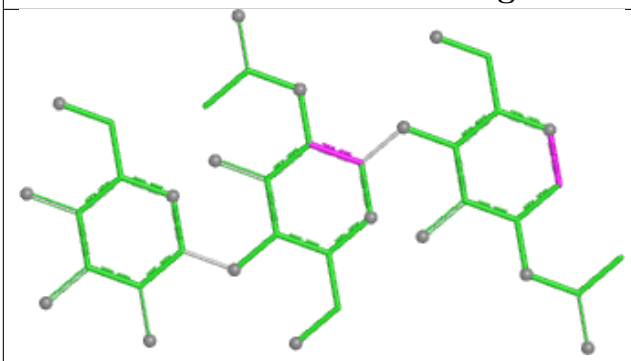
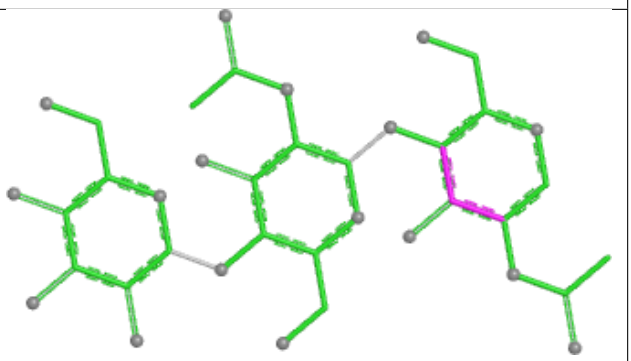


Rings

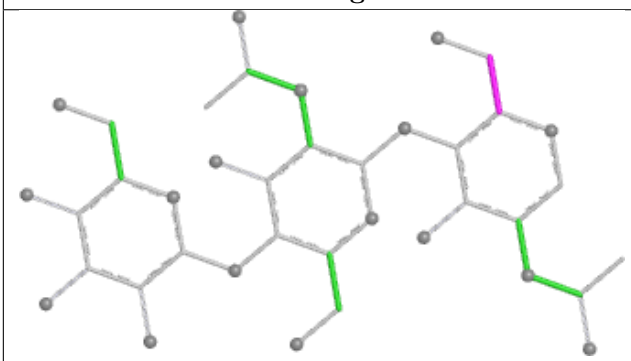
Oligosaccharide Chain n



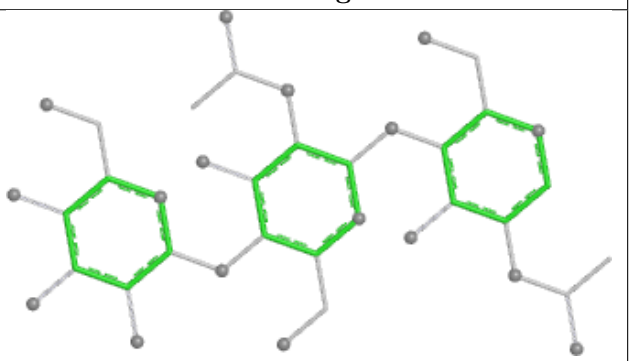
Bond lengths



Bond angles

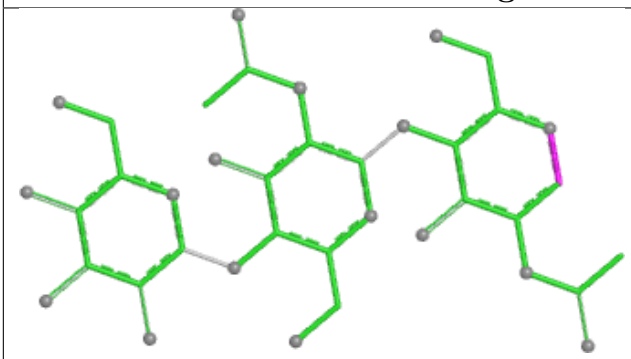


Torsions

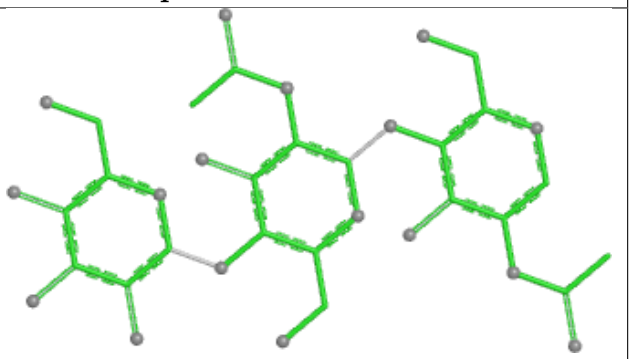


Rings

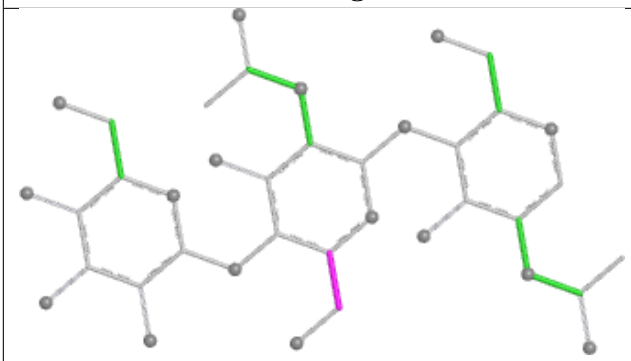
Oligosaccharide Chain p



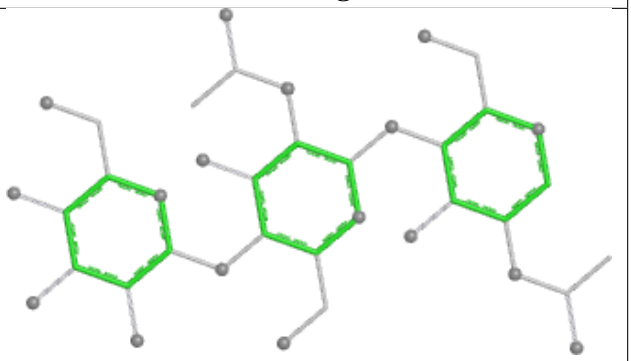
Bond lengths



Bond angles

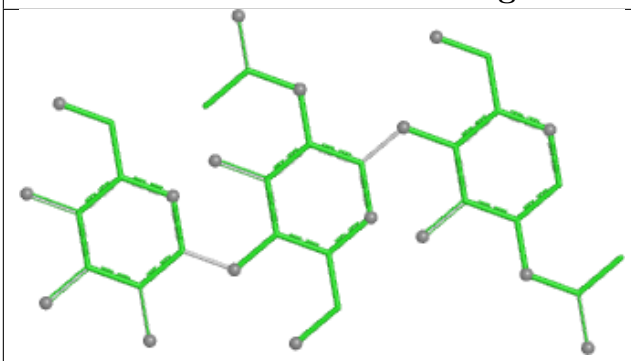


Torsions

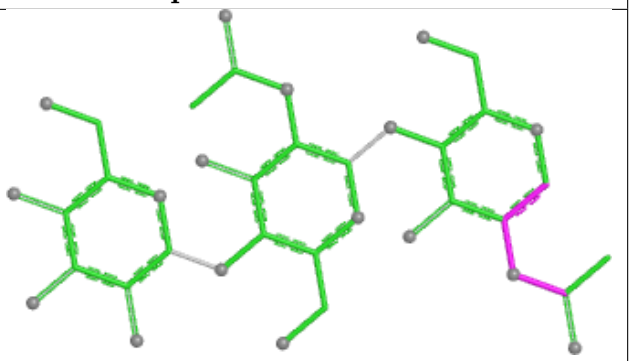


Rings

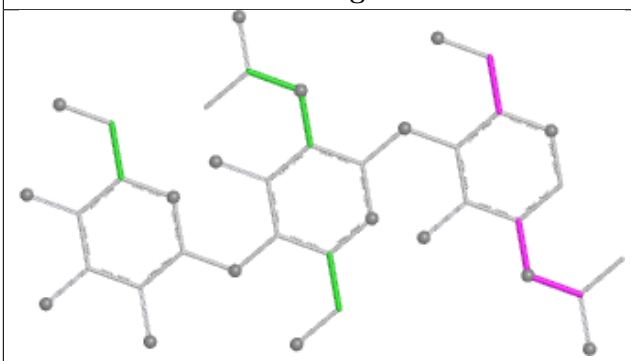
Oligosaccharide Chain q



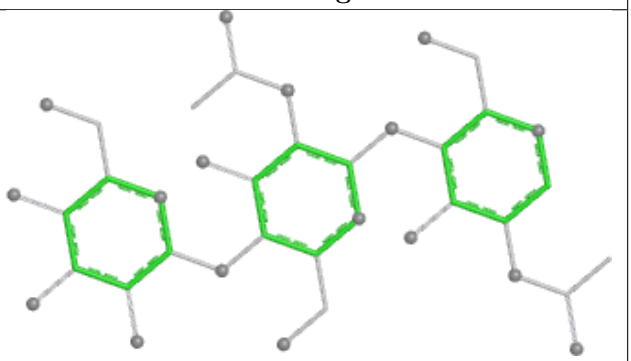
Bond lengths



Bond angles

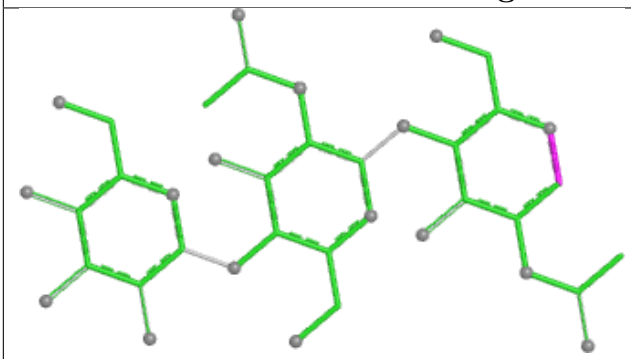


Torsions

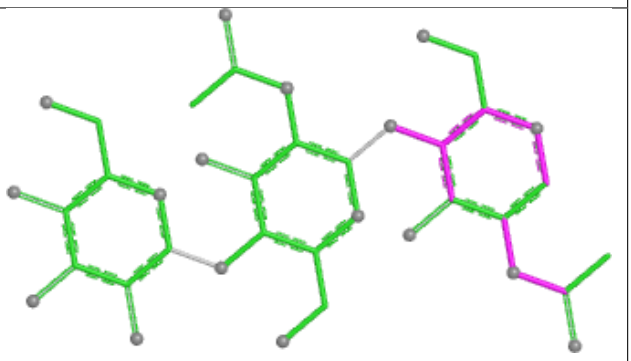


Rings

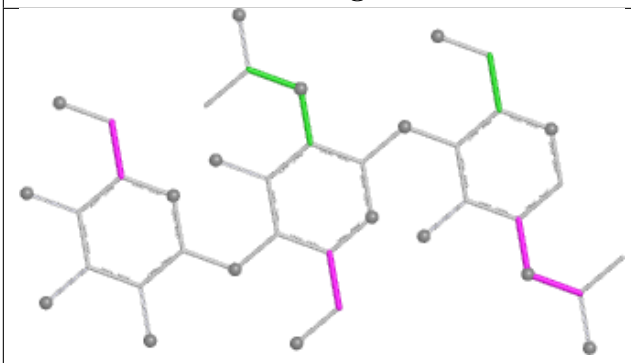
Oligosaccharide Chain u



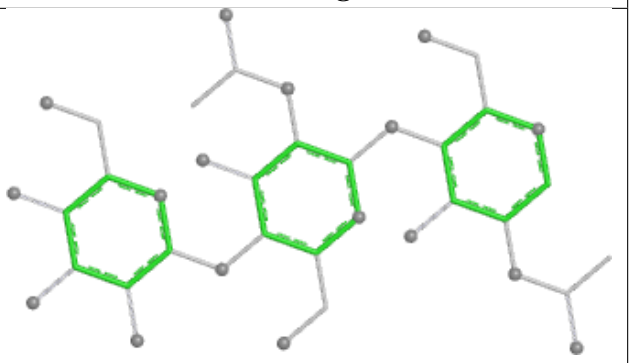
Bond lengths



Bond angles

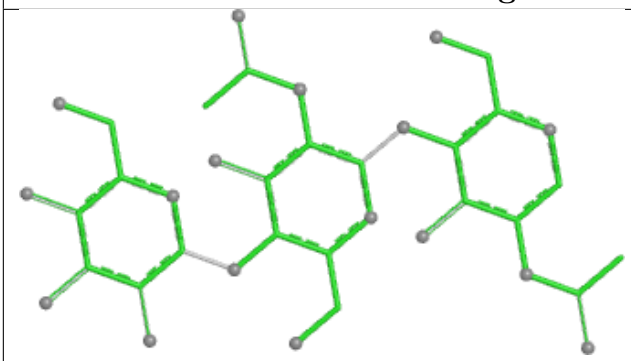


Torsions



Rings

Oligosaccharide Chain x



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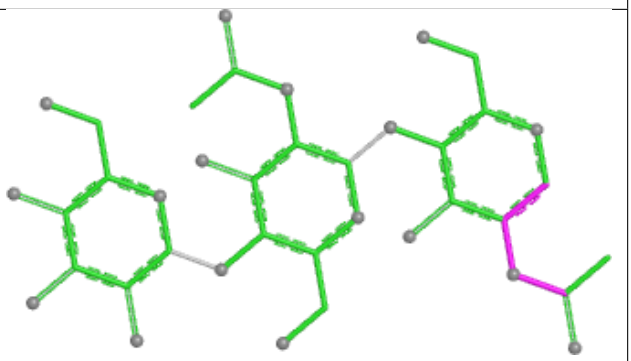
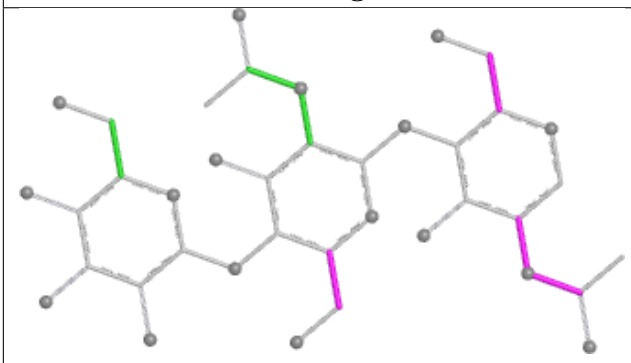


Bond angles



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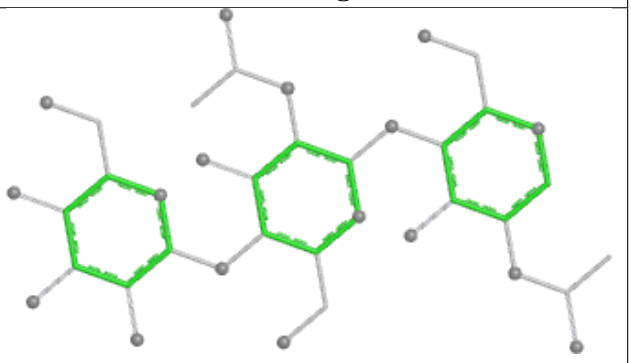
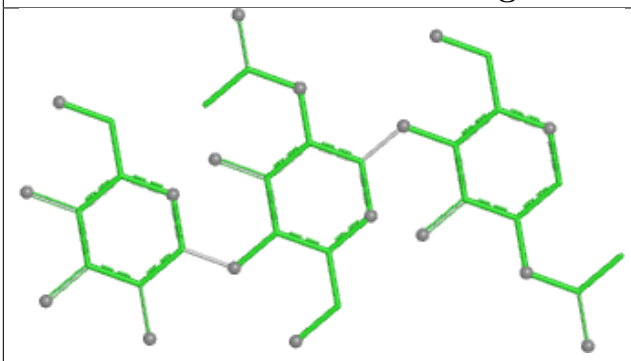
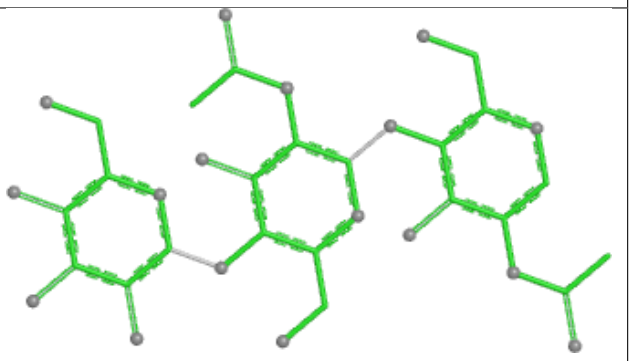


Rings

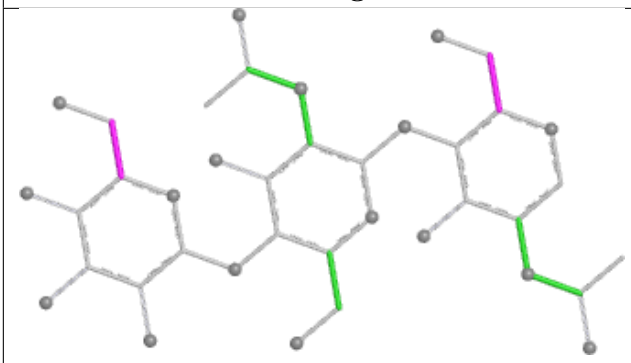
Oligosaccharide Chain 0



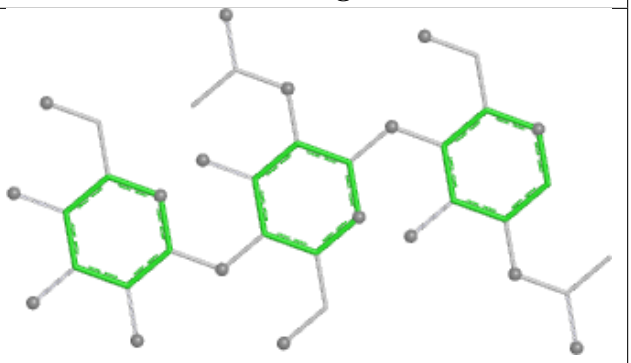
Bond lengths



Bond angles

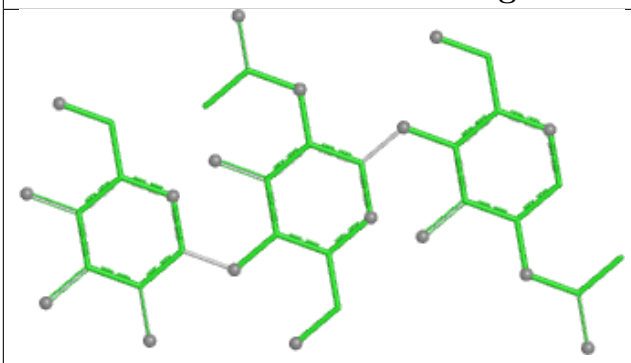


Torsions



Rings

Oligosaccharide Chain 1



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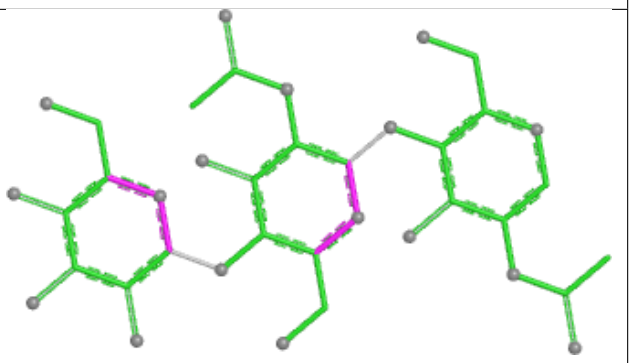
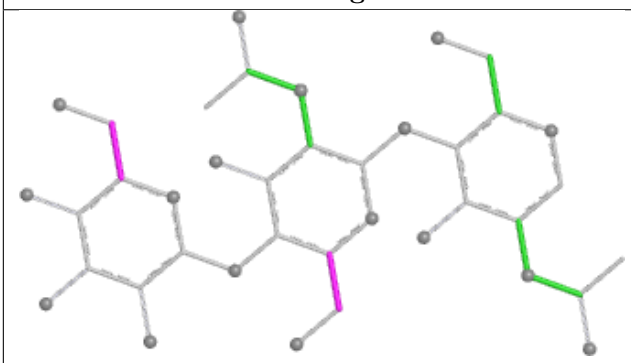
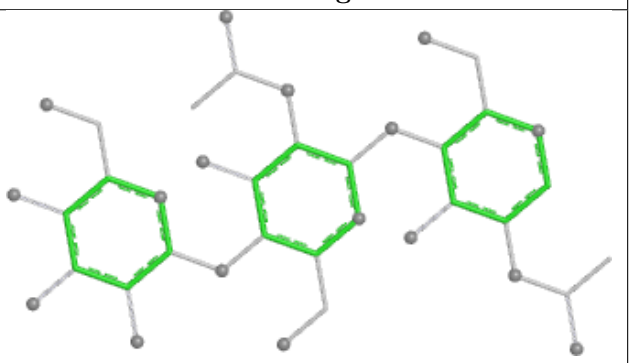


Bond angles

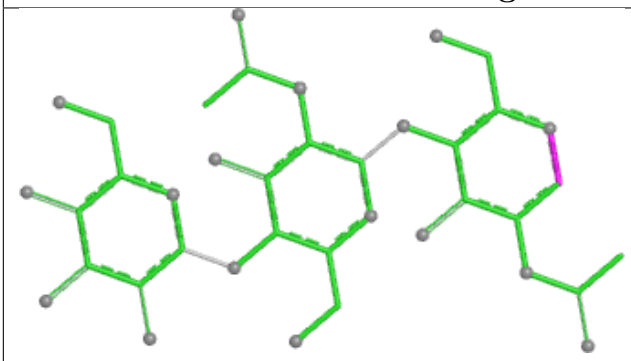


Torsions



Rings

Oligosaccharide Chain 3



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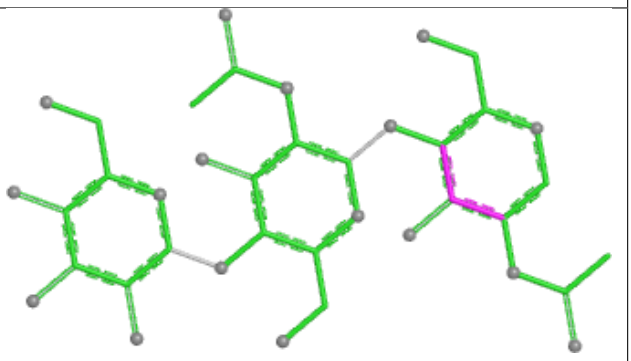
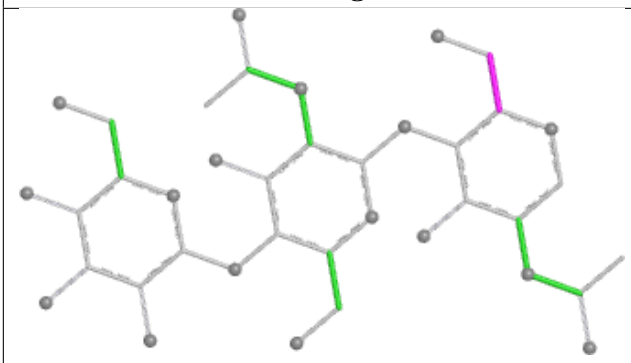
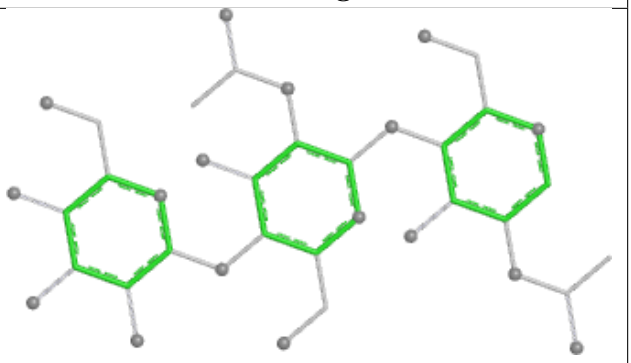


Bond angles

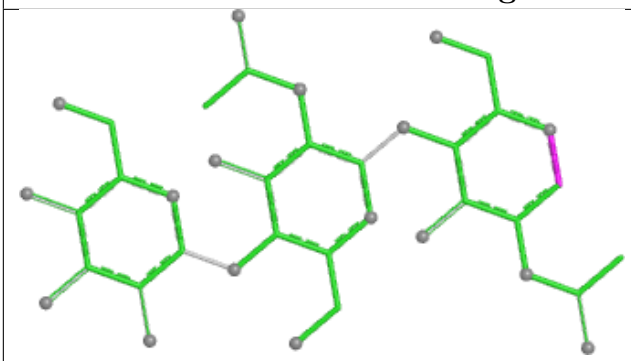


Torsions



Rings

Oligosaccharide Chain 5



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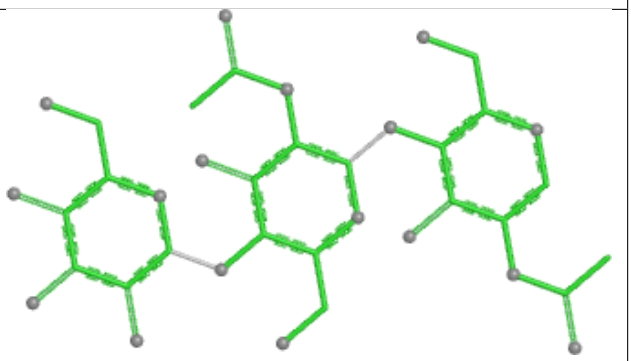
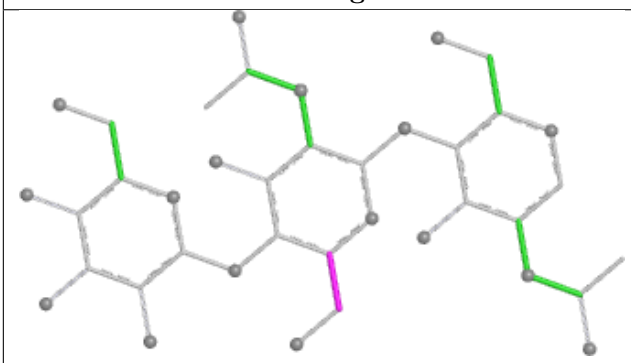
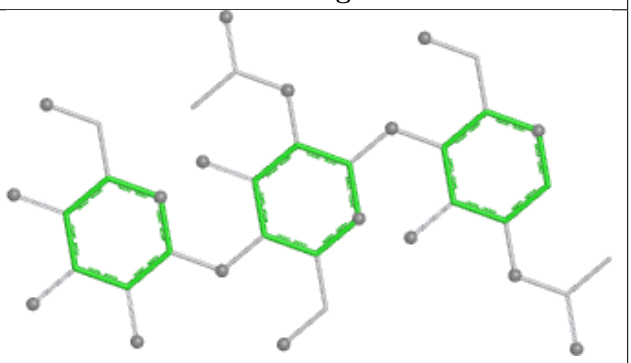


Bond angles

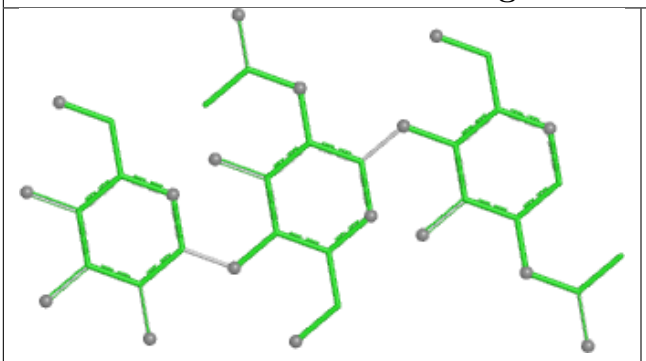


Torsions



Rings

Oligosaccharide Chain 6



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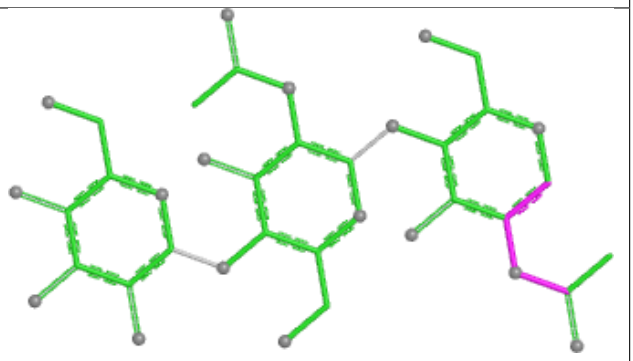
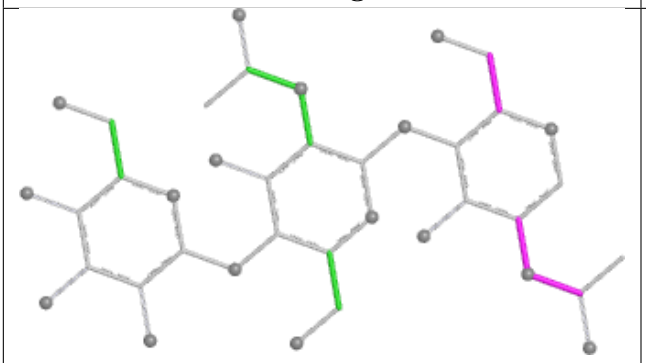


Bond angles



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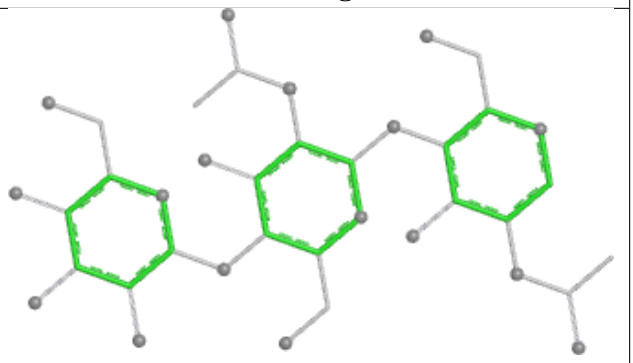
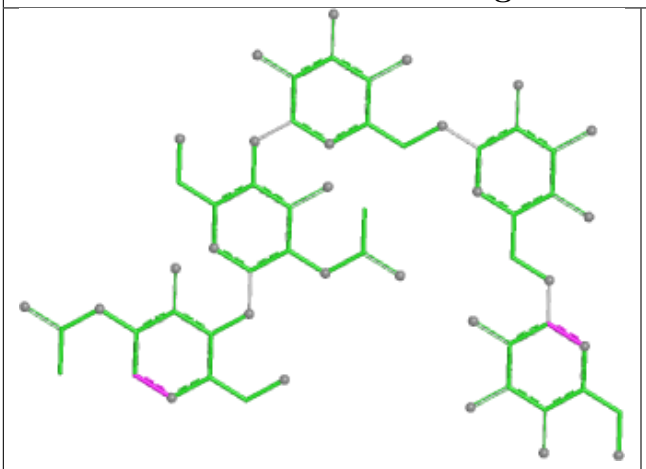


Rings

Oligosaccharide Chain Q



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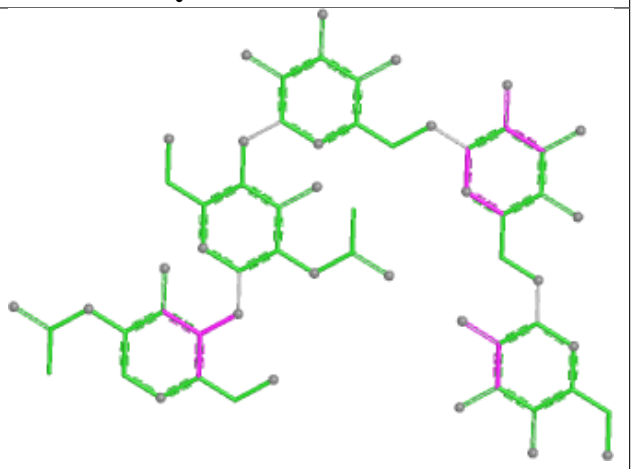
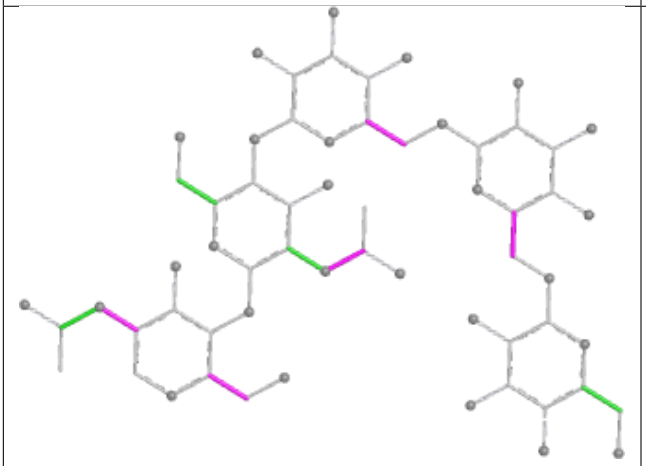


Bond angles



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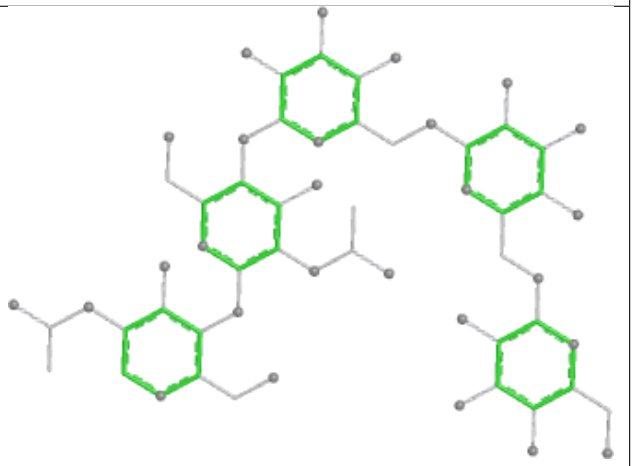
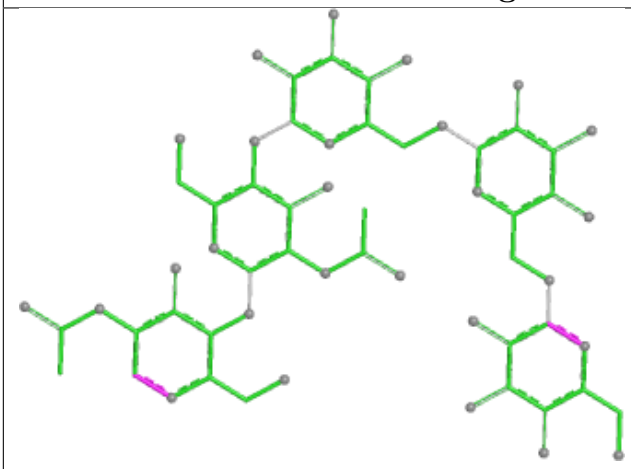


Rings

Oligosaccharide Chain g



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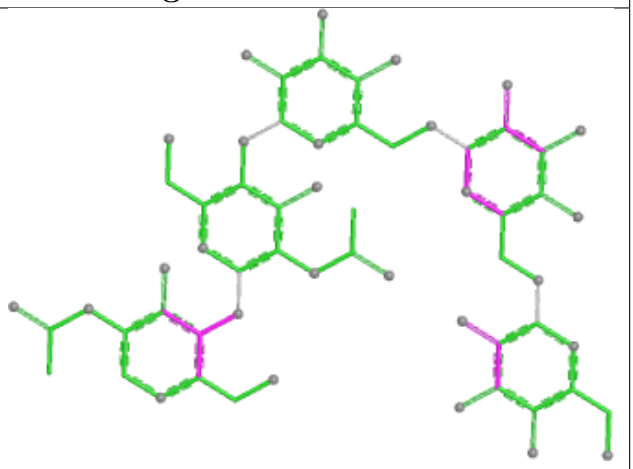
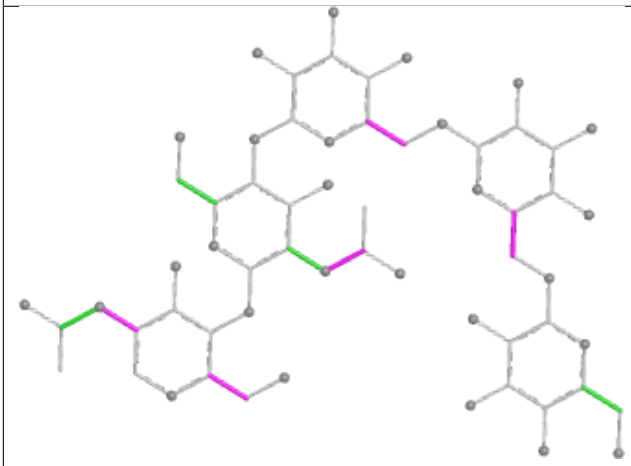
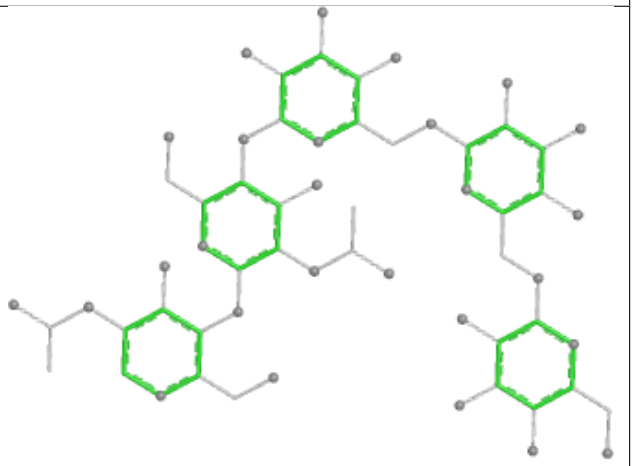


Bond angles

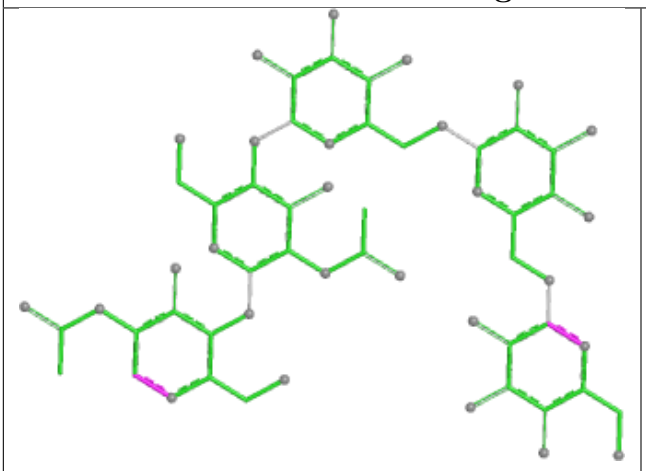


Torsions

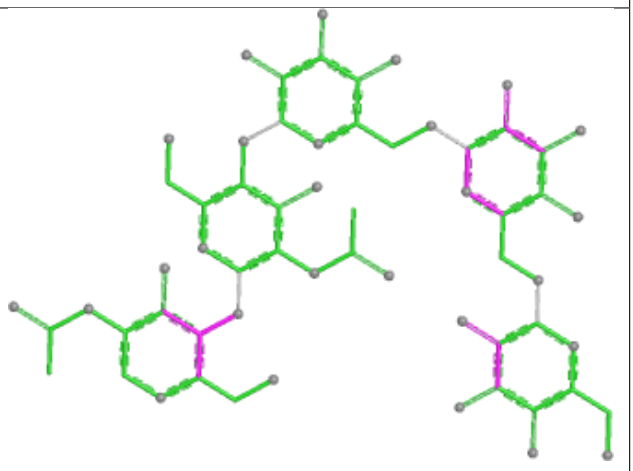


Rings

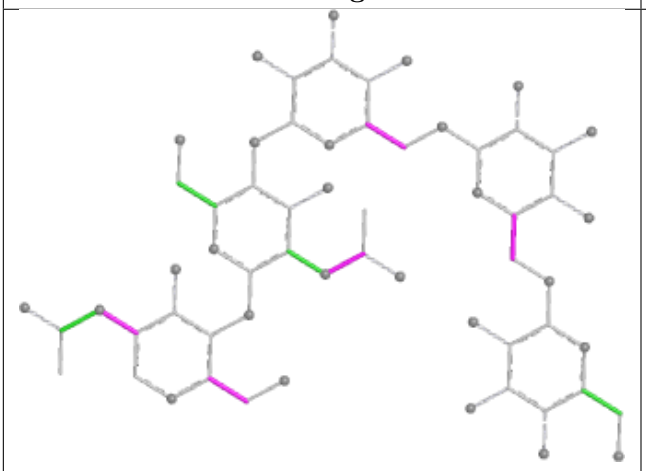
Oligosaccharide Chain w



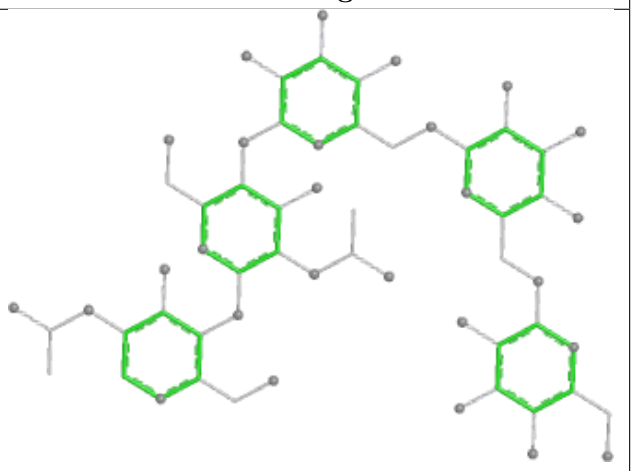
Bond lengths



Bond angles

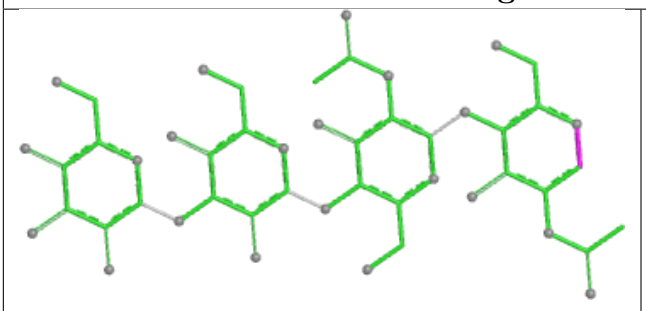


Torsions



Rings

Oligosaccharide Chain S



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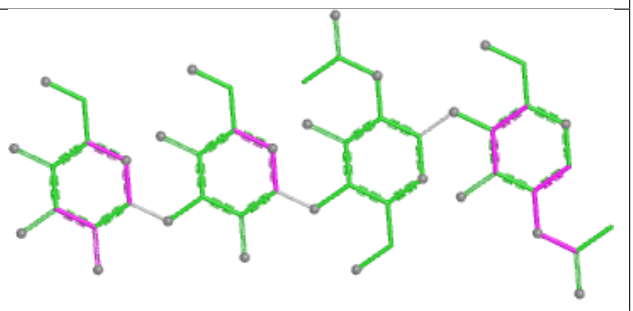
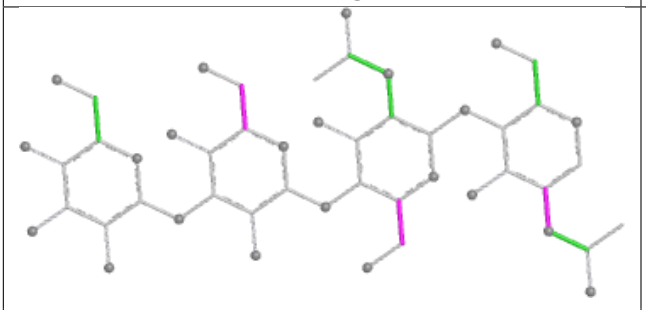


Bond angles



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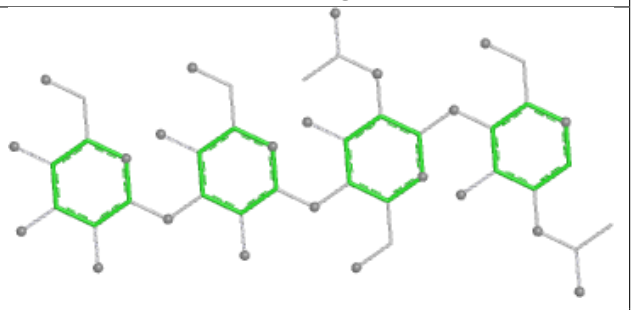
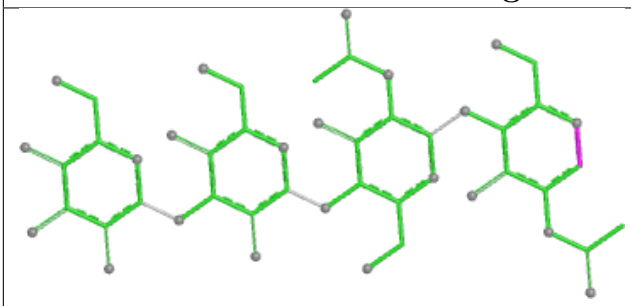


Rings

Oligosaccharide Chain i



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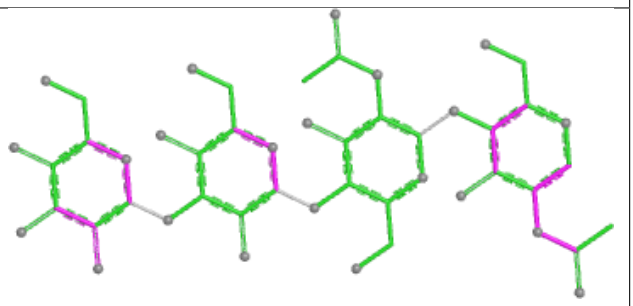
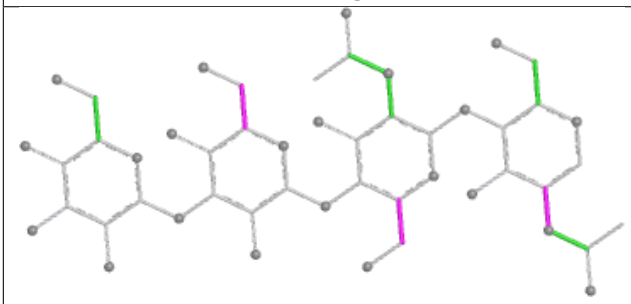
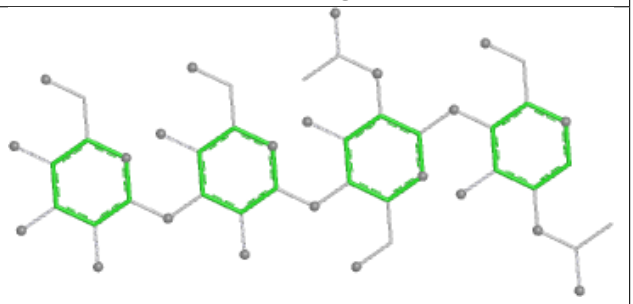


Bond angles

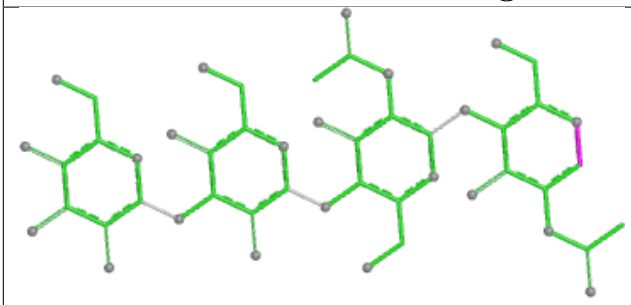


Torsions



Rings

Oligosaccharide Chain y



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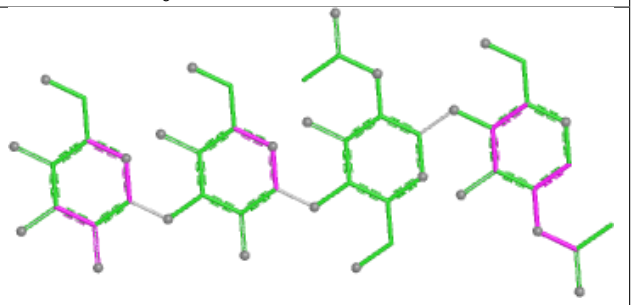
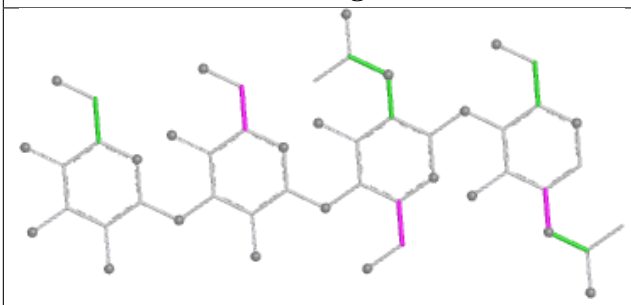
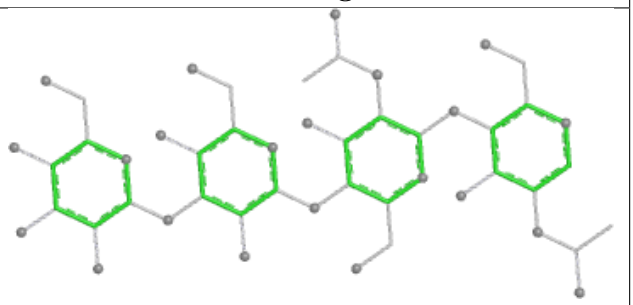


Bond angles

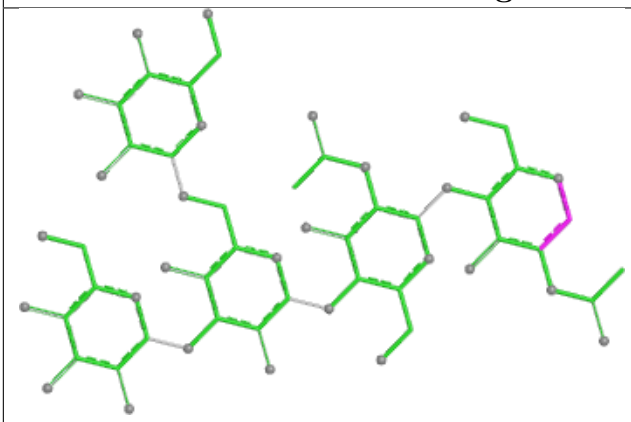


Torsions

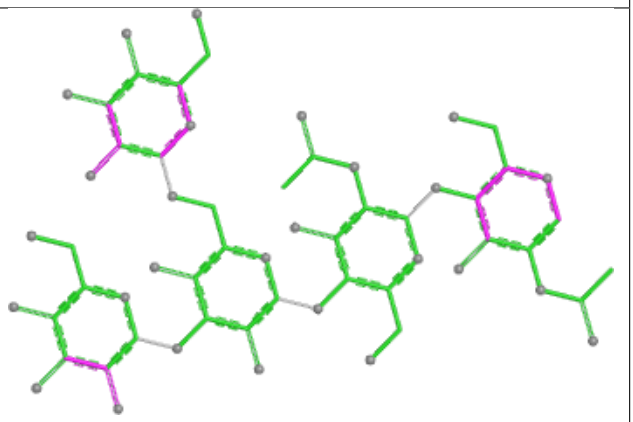


Rings

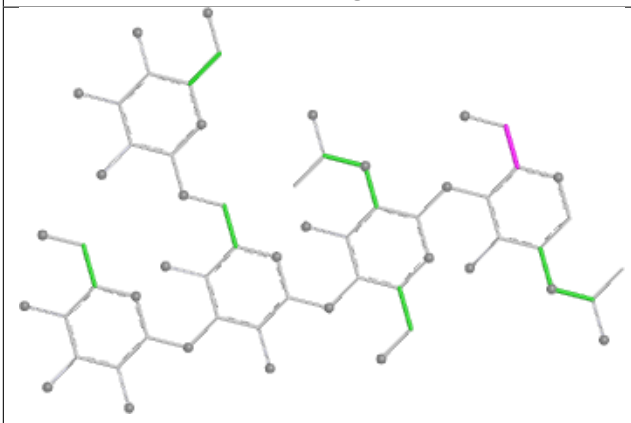
Oligosaccharide Chain T



Bond lengths



Bond angles



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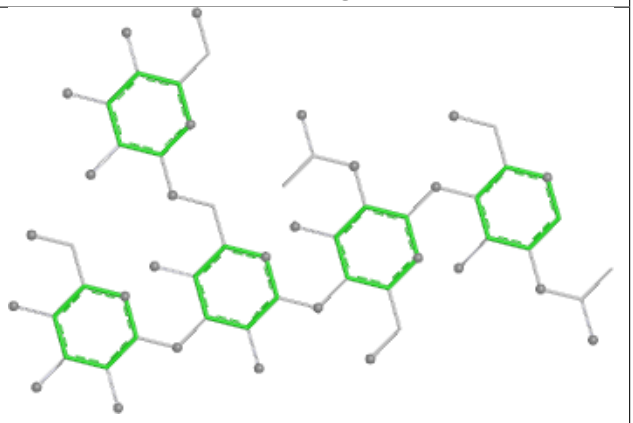
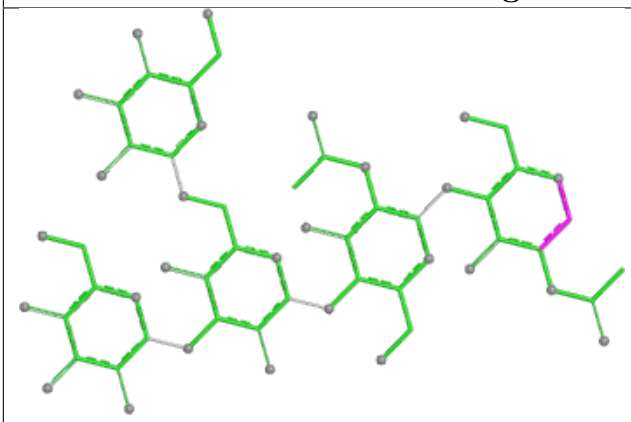
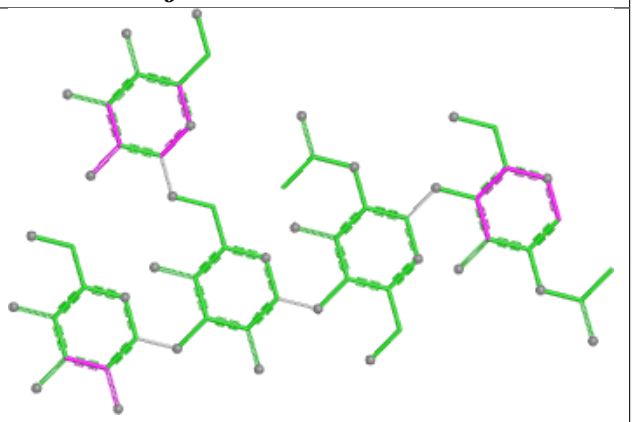


Rings

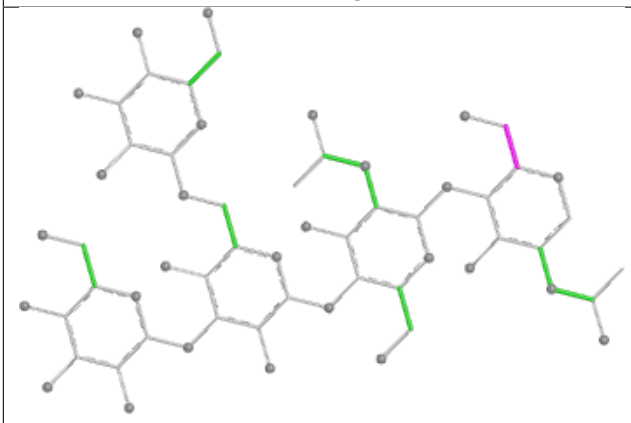
Oligosaccharide Chain j



Bond lengths



Bond angles



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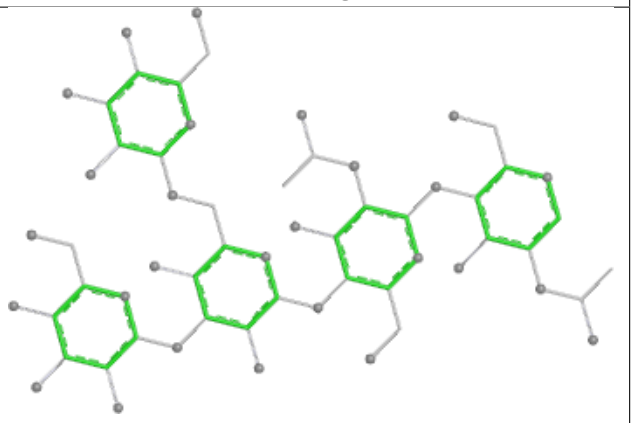
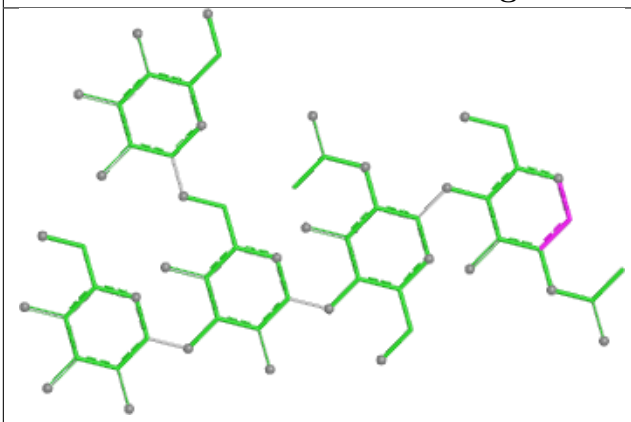
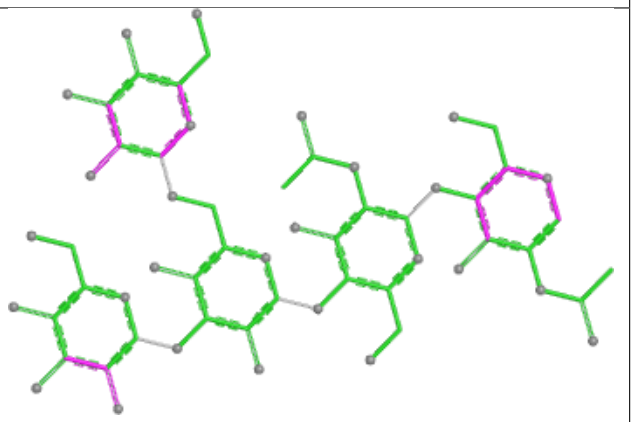


Rings

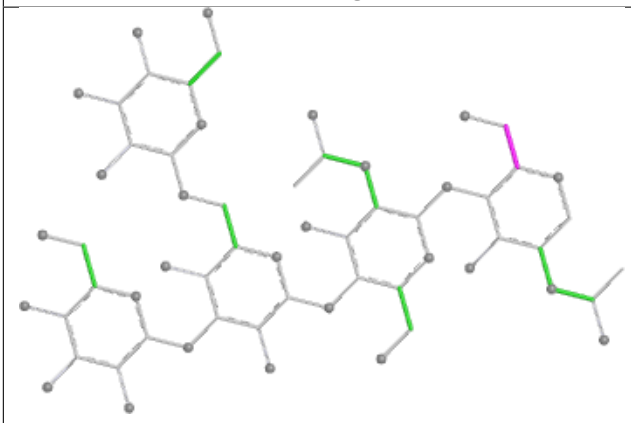
Oligosaccharide Chain z



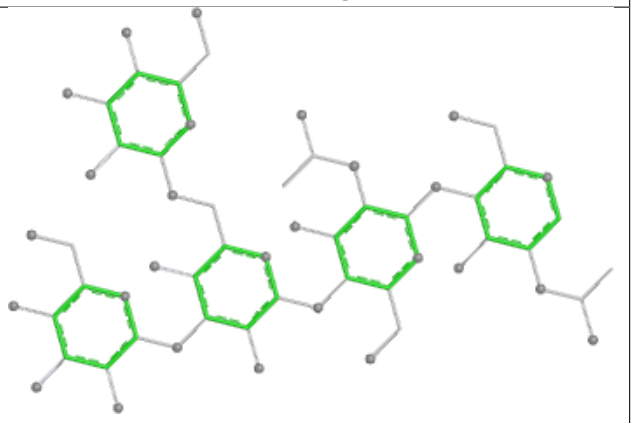
Bond lengths



Bond angles

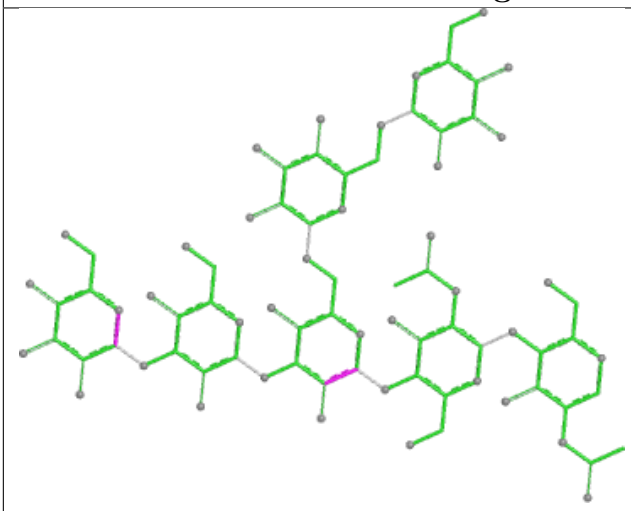


Torsions

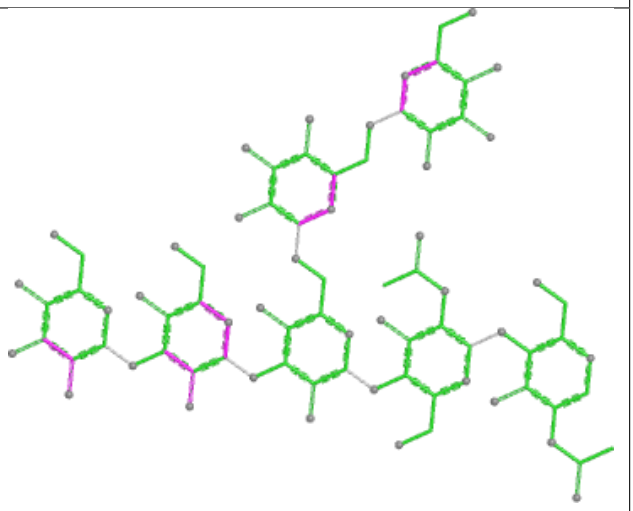


Rings

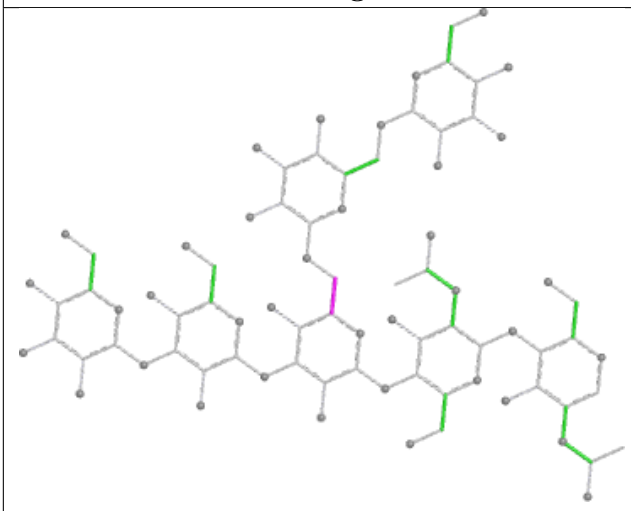
Oligosaccharide Chain Y



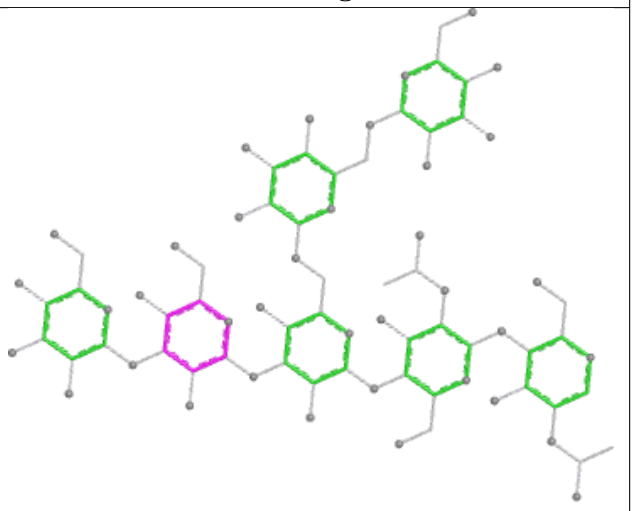
Bond lengths



Bond angles

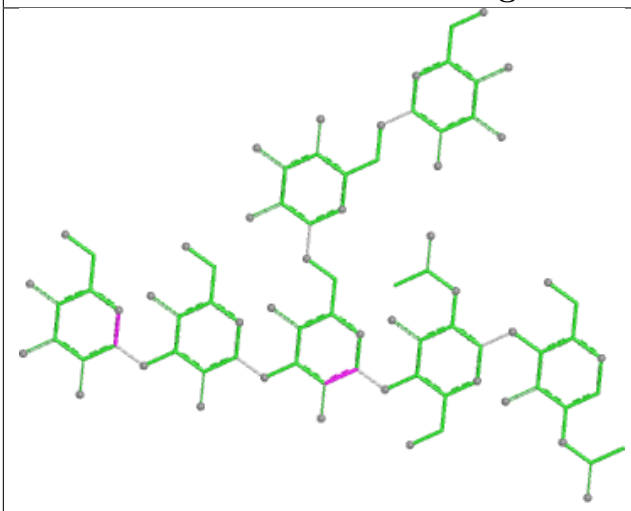


Torsions

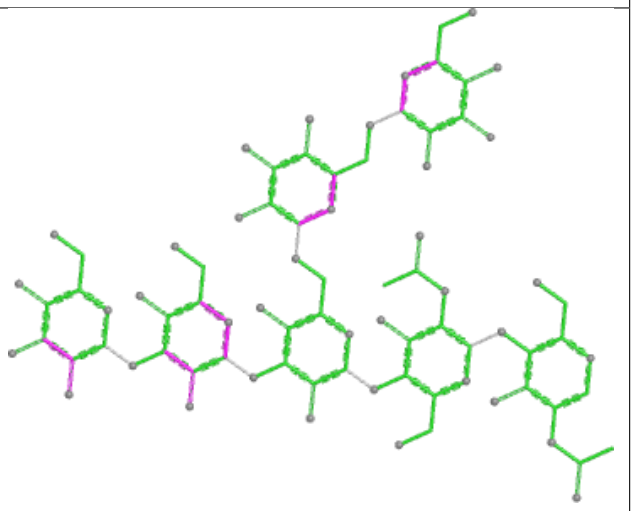


Rings

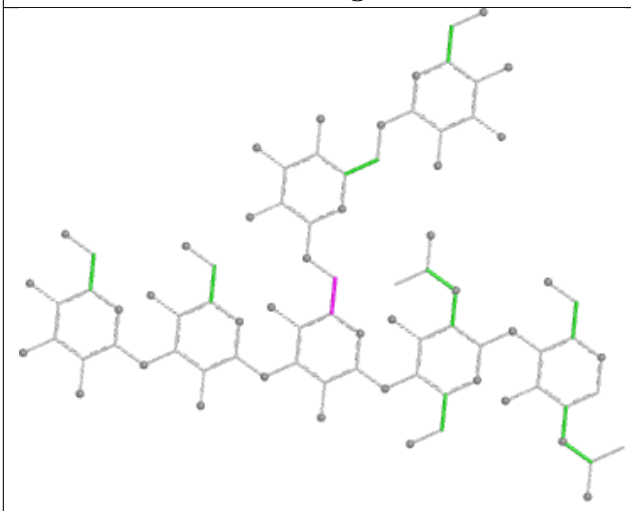
Oligosaccharide Chain o



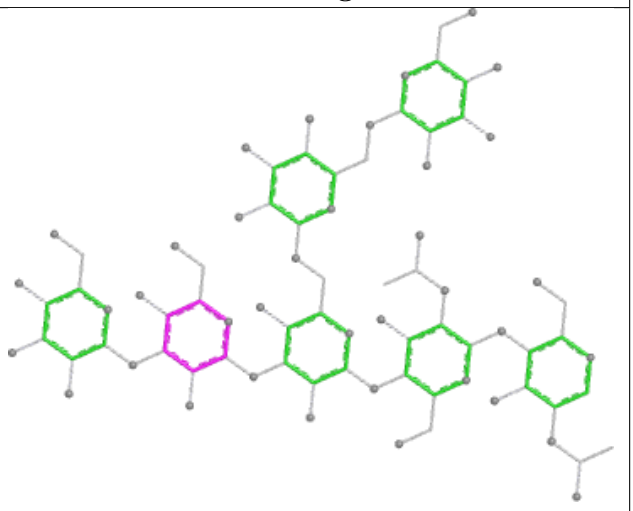
Bond lengths



Bond angles

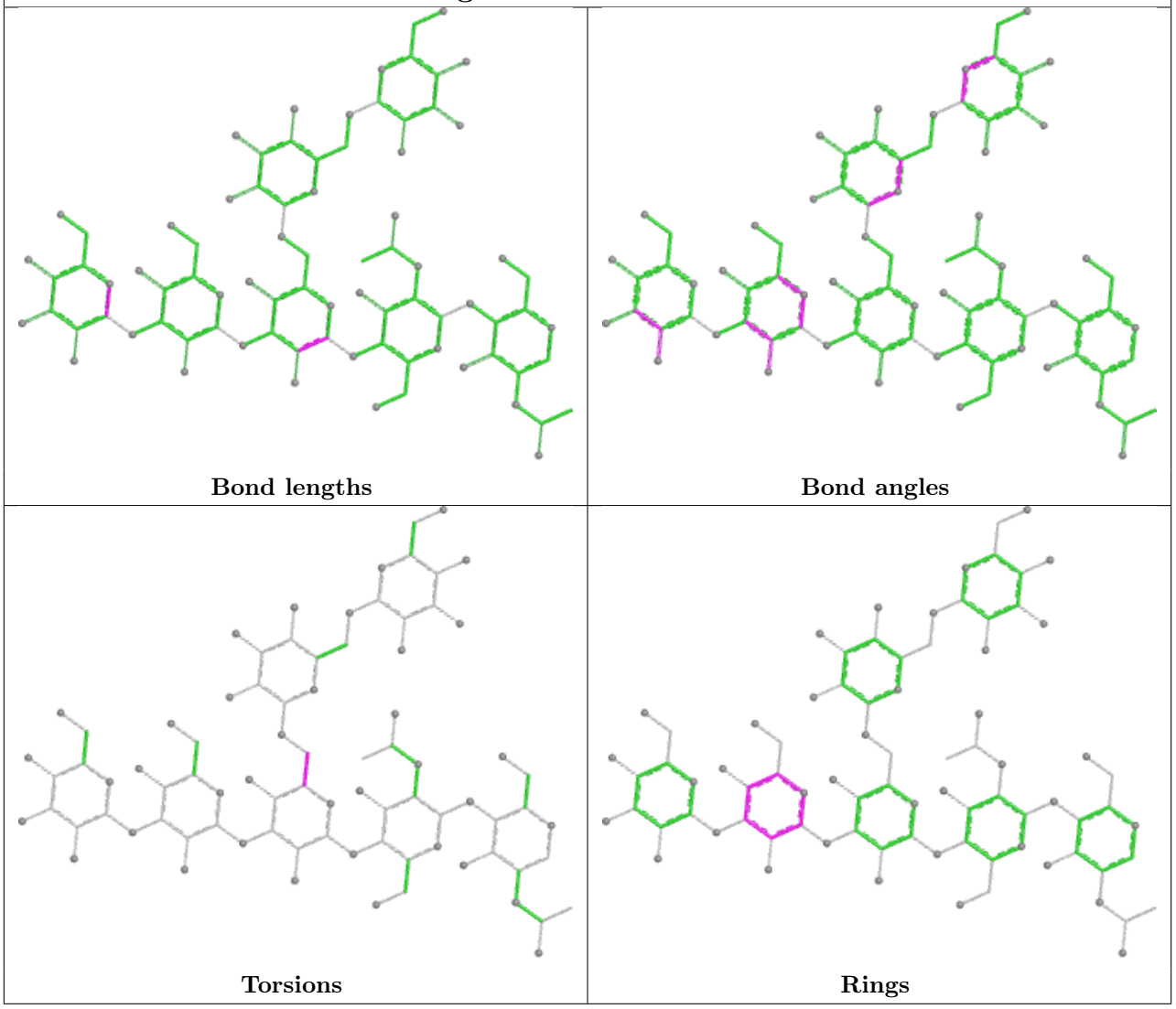


Torsions



Rings

Oligosaccharide Chain 4



5.6 Ligand geometry (i)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	NAG	A	652	1	14,14,15	0.32	0	17,19,21	0.68	1 (5%)
11	NAG	A	641	1	14,14,15	1.10	1 (7%)	17,19,21	0.90	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	NAG	D	701	2	14,14,15	1.20	2 (14%)	17,19,21	1.42	1 (5%)
11	NAG	F	702	-	14,14,15	0.48	0	17,19,21	1.54	2 (11%)
11	NAG	E	641	1	14,14,15	1.11	1 (7%)	17,19,21	0.89	1 (5%)
11	NAG	A	635	1	14,14,15	0.31	0	17,19,21	0.89	1 (5%)
11	NAG	C	635	1	14,14,15	0.33	0	17,19,21	0.89	1 (5%)
11	NAG	B	702	2	14,14,15	0.47	0	17,19,21	1.54	2 (11%)
11	NAG	A	608	1	14,14,15	0.21	0	17,19,21	0.57	0
11	NAG	C	608	1	14,14,15	0.23	0	17,19,21	0.58	0
11	NAG	E	652	1	14,14,15	0.31	0	17,19,21	0.67	1 (5%)
11	NAG	C	652	1	14,14,15	0.31	0	17,19,21	0.67	0
11	NAG	F	703	2	14,14,15	0.19	0	17,19,21	0.45	0
11	NAG	C	611	1	14,14,15	1.04	1 (7%)	17,19,21	0.68	0
11	NAG	A	611	1	14,14,15	1.04	1 (7%)	17,19,21	0.67	0
11	NAG	B	703	2	14,14,15	0.18	0	17,19,21	0.46	0
11	NAG	C	641	1	14,14,15	1.09	1 (7%)	17,19,21	0.90	1 (5%)
11	NAG	E	608	1	14,14,15	0.21	0	17,19,21	0.58	0
11	NAG	E	635	1	14,14,15	0.32	0	17,19,21	0.89	1 (5%)
11	NAG	D	703	2	14,14,15	0.18	0	17,19,21	0.46	0
11	NAG	D	702	2	14,14,15	0.46	0	17,19,21	1.53	2 (11%)
11	NAG	B	701	2	14,14,15	1.19	2 (14%)	17,19,21	1.41	1 (5%)
11	NAG	F	701	-	14,14,15	1.19	2 (14%)	17,19,21	1.41	1 (5%)
11	NAG	E	611	1	14,14,15	1.03	1 (7%)	17,19,21	0.68	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	A	652	1	-	2/6/23/26	0/1/1/1
11	NAG	A	641	1	-	0/6/23/26	0/1/1/1
11	NAG	D	701	2	-	1/6/23/26	0/1/1/1
11	NAG	F	702	-	-	6/6/23/26	0/1/1/1
11	NAG	E	641	1	-	0/6/23/26	0/1/1/1
11	NAG	A	635	1	-	0/6/23/26	0/1/1/1
11	NAG	C	635	1	-	0/6/23/26	0/1/1/1
11	NAG	B	702	2	-	6/6/23/26	0/1/1/1
11	NAG	A	608	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	C	608	1	-	4/6/23/26	0/1/1/1
11	NAG	E	652	1	-	2/6/23/26	0/1/1/1
11	NAG	C	652	1	-	2/6/23/26	0/1/1/1
11	NAG	F	703	2	-	0/6/23/26	0/1/1/1
11	NAG	C	611	1	-	2/6/23/26	0/1/1/1
11	NAG	A	611	1	-	2/6/23/26	0/1/1/1
11	NAG	B	703	2	-	0/6/23/26	0/1/1/1
11	NAG	C	641	1	-	0/6/23/26	0/1/1/1
11	NAG	E	608	1	-	4/6/23/26	0/1/1/1
11	NAG	E	635	1	-	0/6/23/26	0/1/1/1
11	NAG	D	703	2	-	0/6/23/26	0/1/1/1
11	NAG	D	702	2	-	6/6/23/26	0/1/1/1
11	NAG	B	701	2	-	1/6/23/26	0/1/1/1
11	NAG	F	701	-	-	1/6/23/26	0/1/1/1
11	NAG	E	611	1	-	2/6/23/26	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	701	NAG	O5-C1	3.68	1.49	1.43
11	D	701	NAG	O5-C1	3.67	1.49	1.43
11	B	701	NAG	O5-C1	3.62	1.49	1.43
11	E	641	NAG	C1-C2	3.61	1.57	1.52
11	A	611	NAG	O5-C1	3.59	1.49	1.43

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	701	NAG	C1-O5-C5	5.33	119.33	112.19
11	F	701	NAG	C1-O5-C5	5.31	119.30	112.19
11	B	701	NAG	C1-O5-C5	5.31	119.30	112.19
11	B	702	NAG	C2-N2-C7	4.97	129.57	122.90
11	F	702	NAG	C2-N2-C7	4.97	129.55	122.90

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	611	NAG	C4-C5-C6-O6
11	C	611	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	E	611	NAG	C4-C5-C6-O6
11	A	611	NAG	O5-C5-C6-O6
11	C	611	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

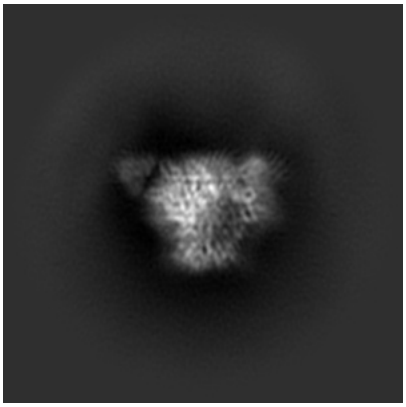
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21456. These allow visual inspection of the internal detail of the map and identification of artifacts.

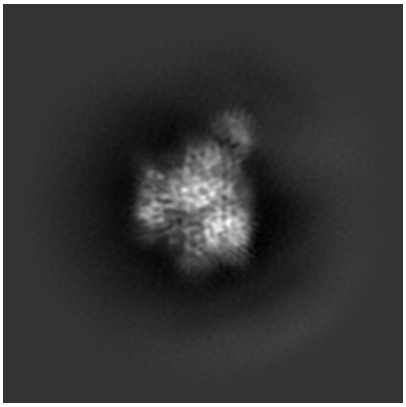
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

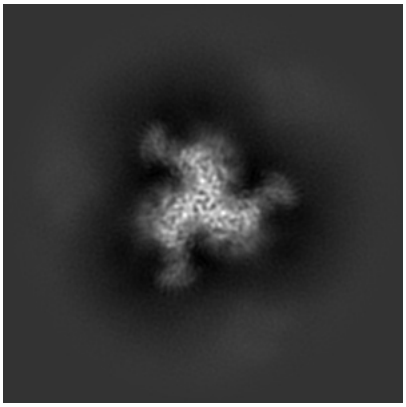
6.1.1 Primary map



X



Y

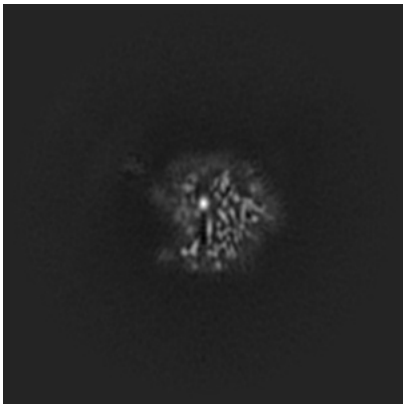


Z

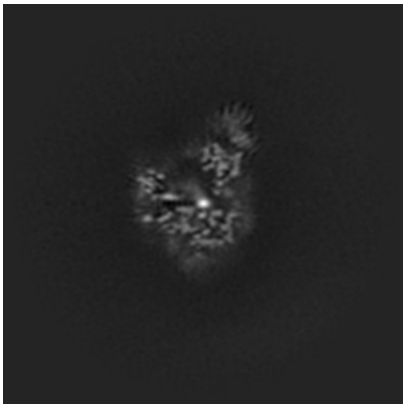
The images above show the map projected in three orthogonal directions.

6.2 Central slices

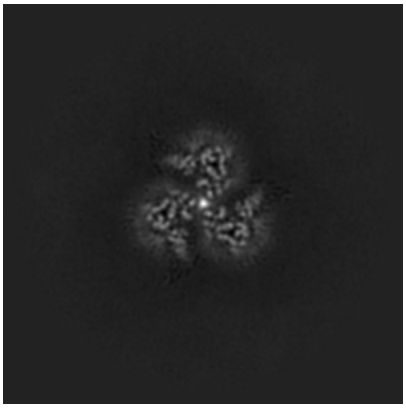
6.2.1 Primary map



X Index: 180



Y Index: 180

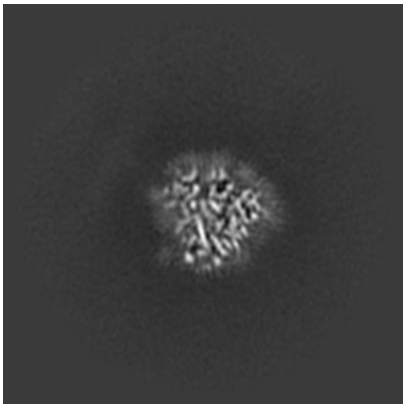


Z Index: 180

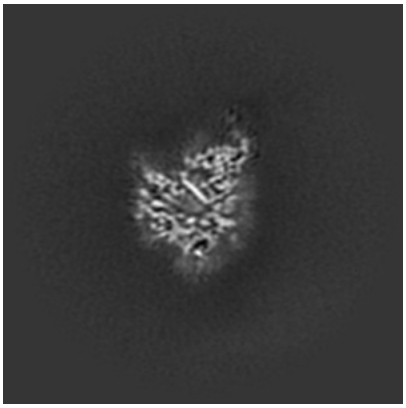
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

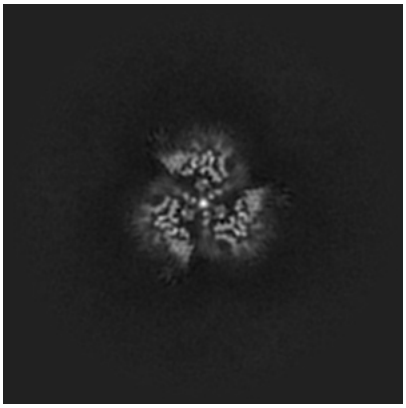
6.3.1 Primary map



X Index: 185



Y Index: 171

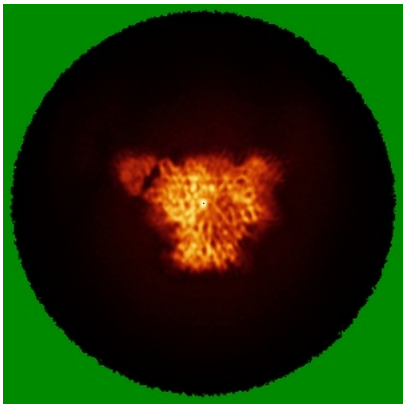


Z Index: 183

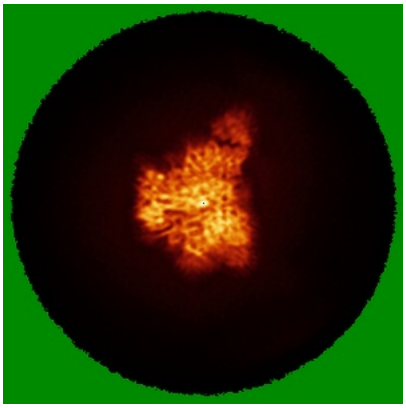
The images above show the largest variance slices of the map in three orthogonal directions.

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

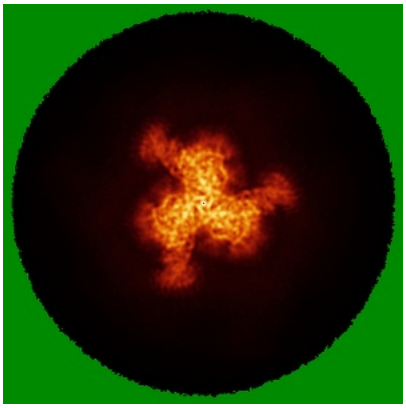
6.4.1 Primary map



X



Y

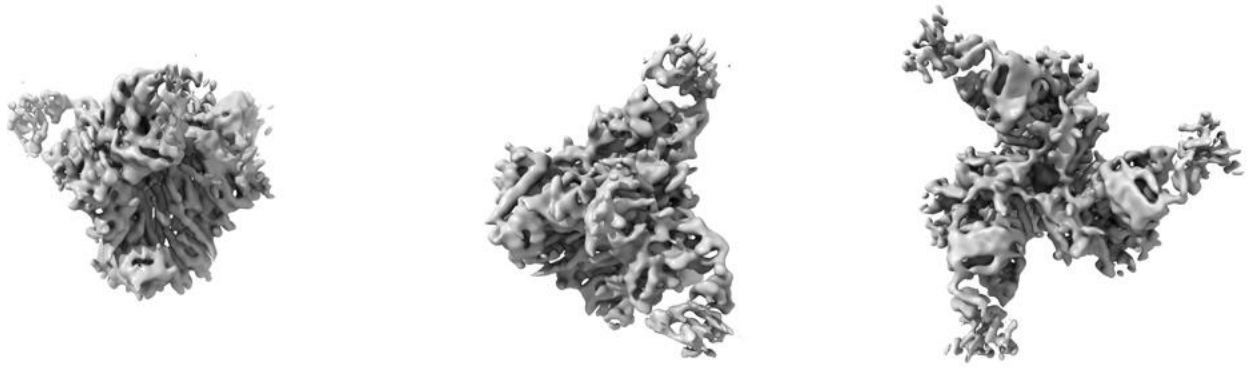


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

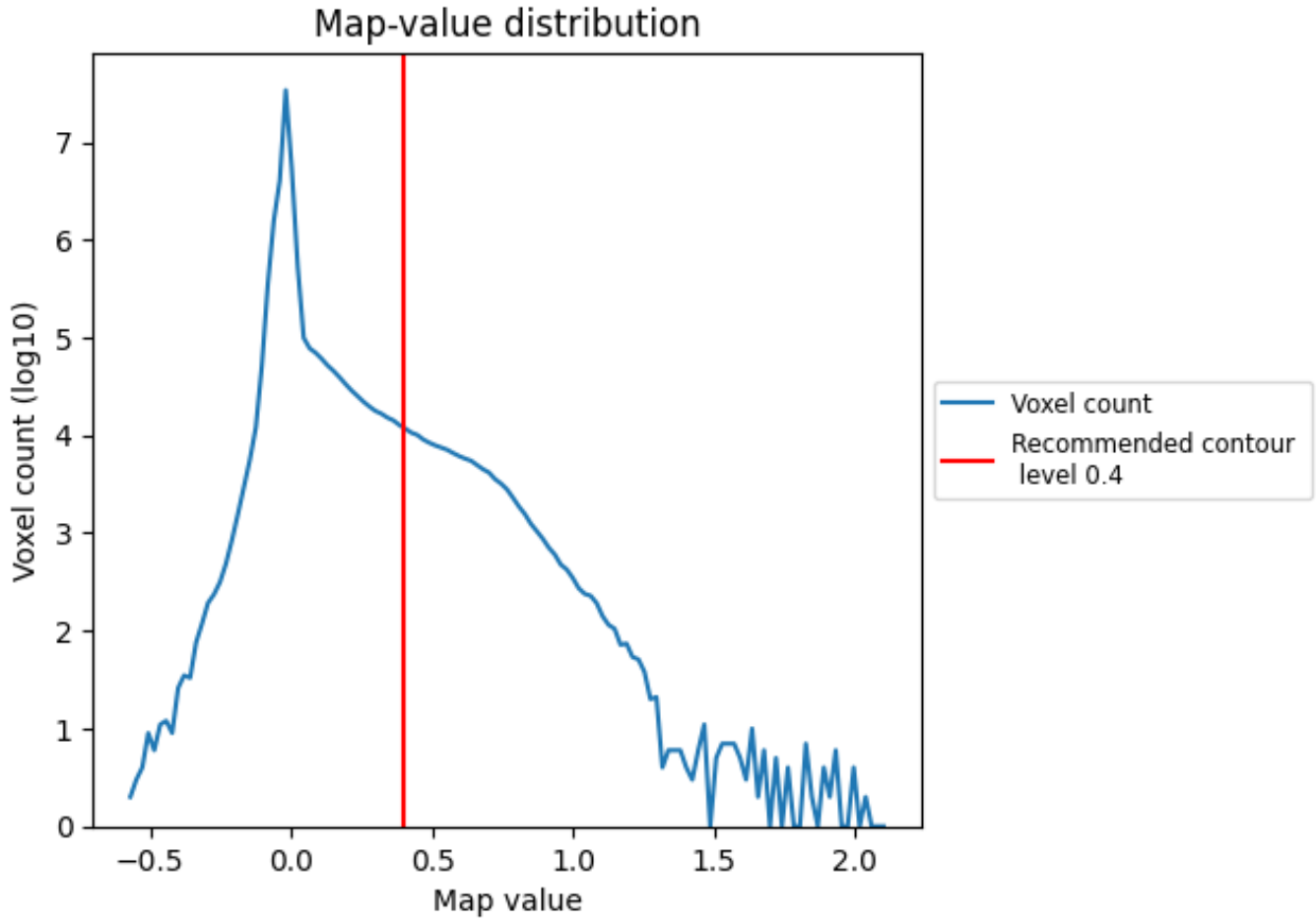
6.6 Mask visualisation (i)

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

7 Map analysis

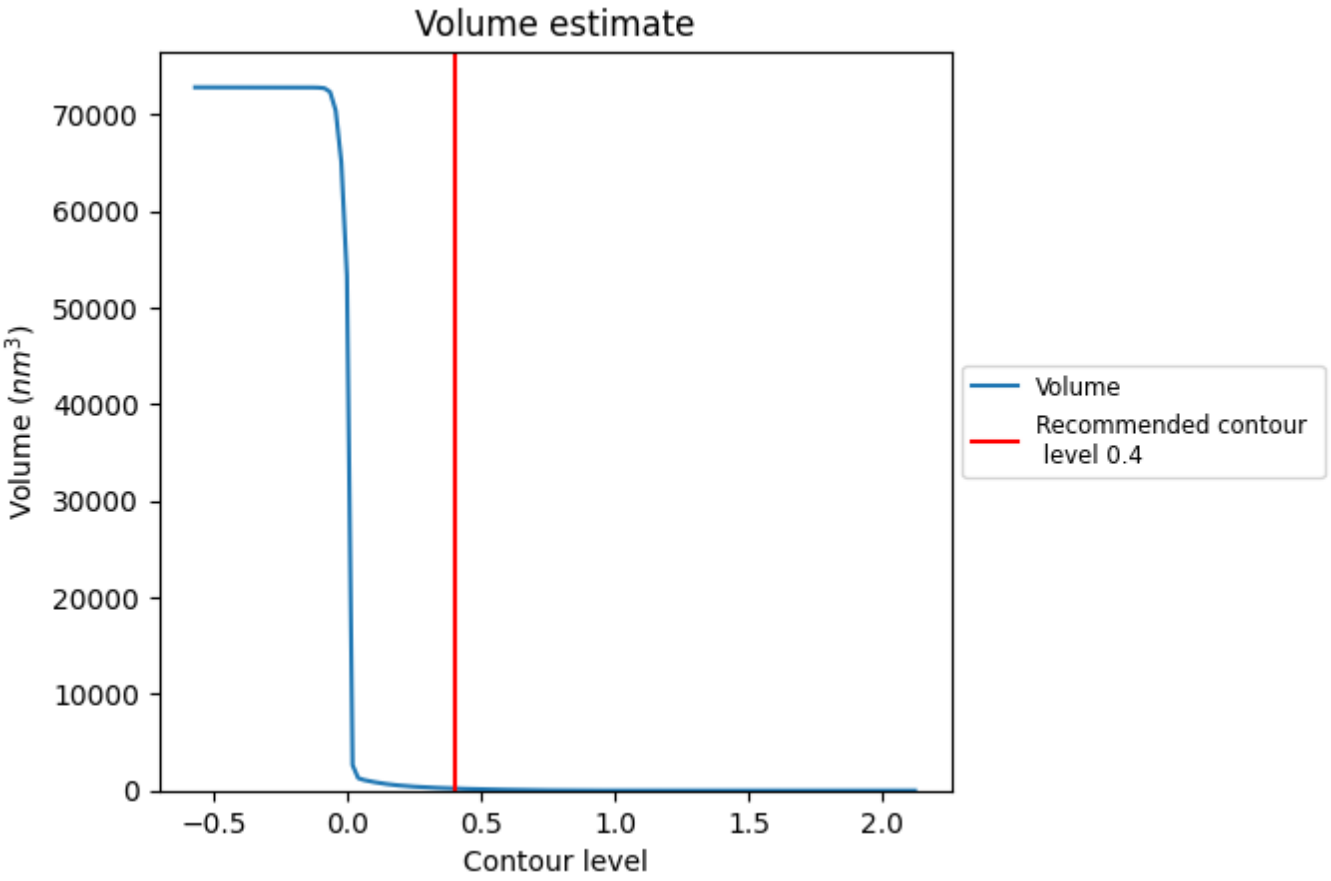
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

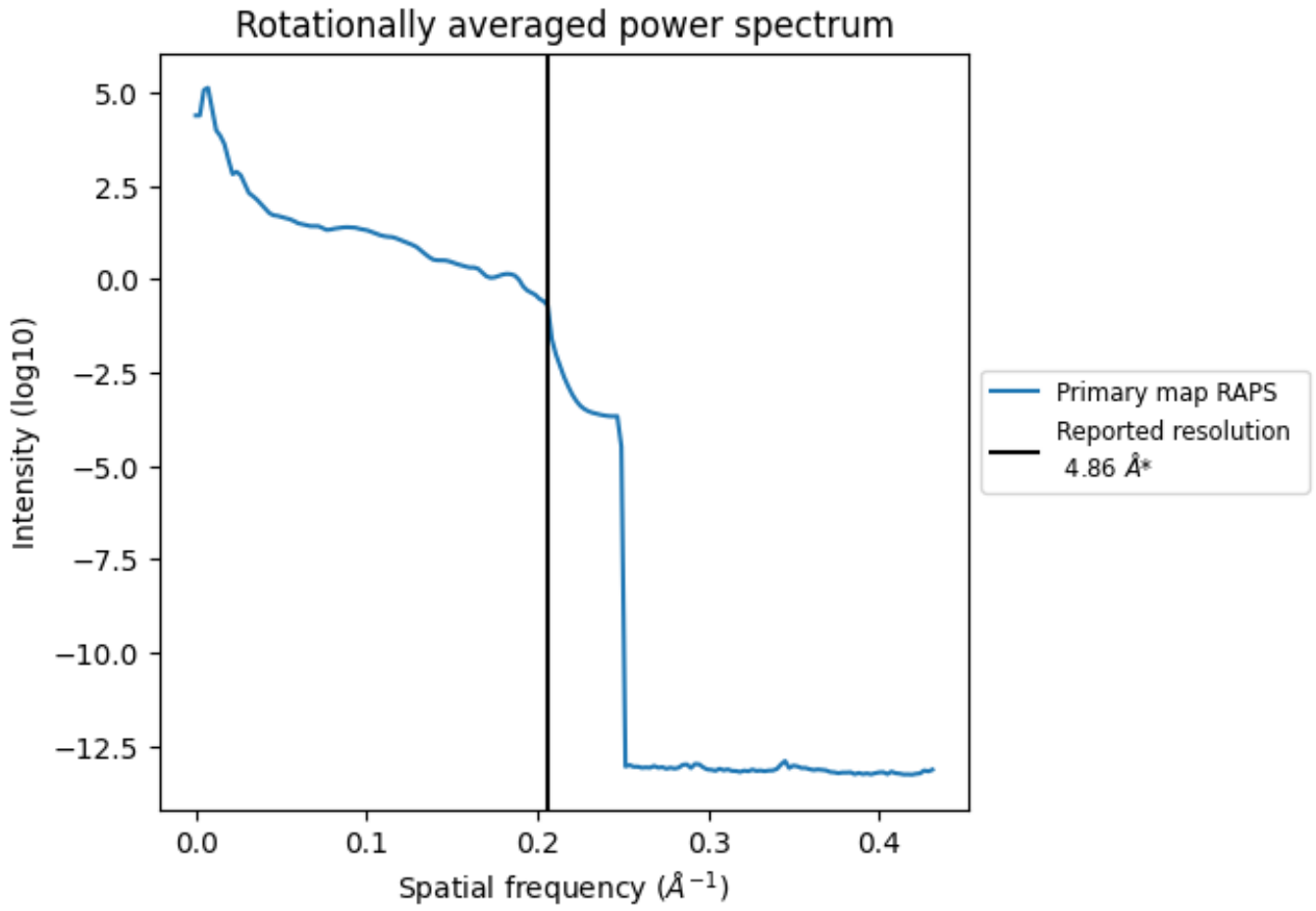
7.2 Volume estimate (i)



The volume at the recommended contour level is 212 nm^3; this corresponds to an approximate mass of 191 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 0.206 $Å^{-1}$

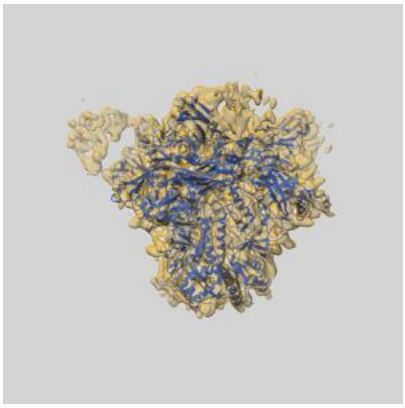
8 Fourier-Shell correlation (i)

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

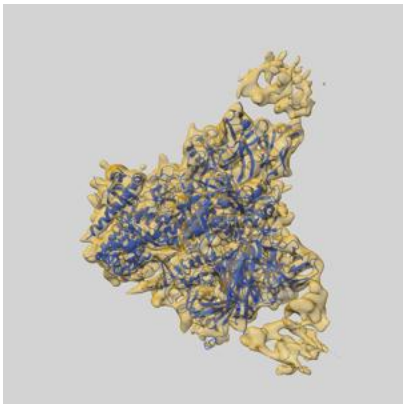
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21456 and PDB model 6VY2. Per-residue inclusion information can be found in section 3 on page 16.

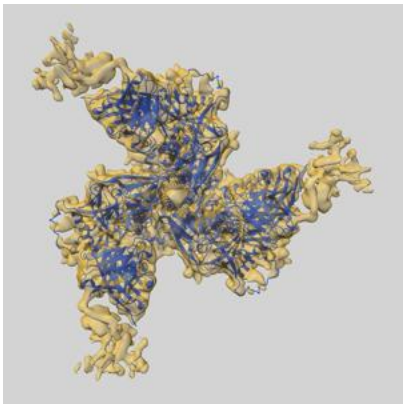
9.1 Map-model overlay



X



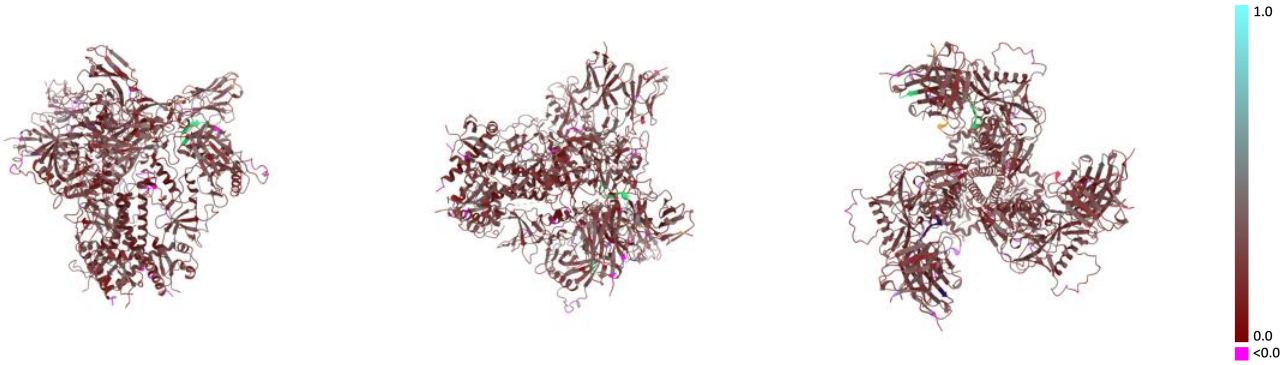
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

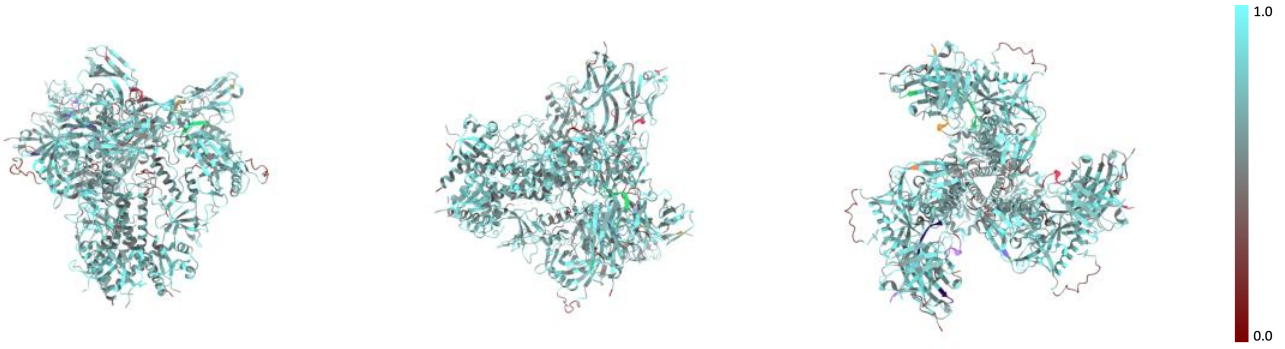
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

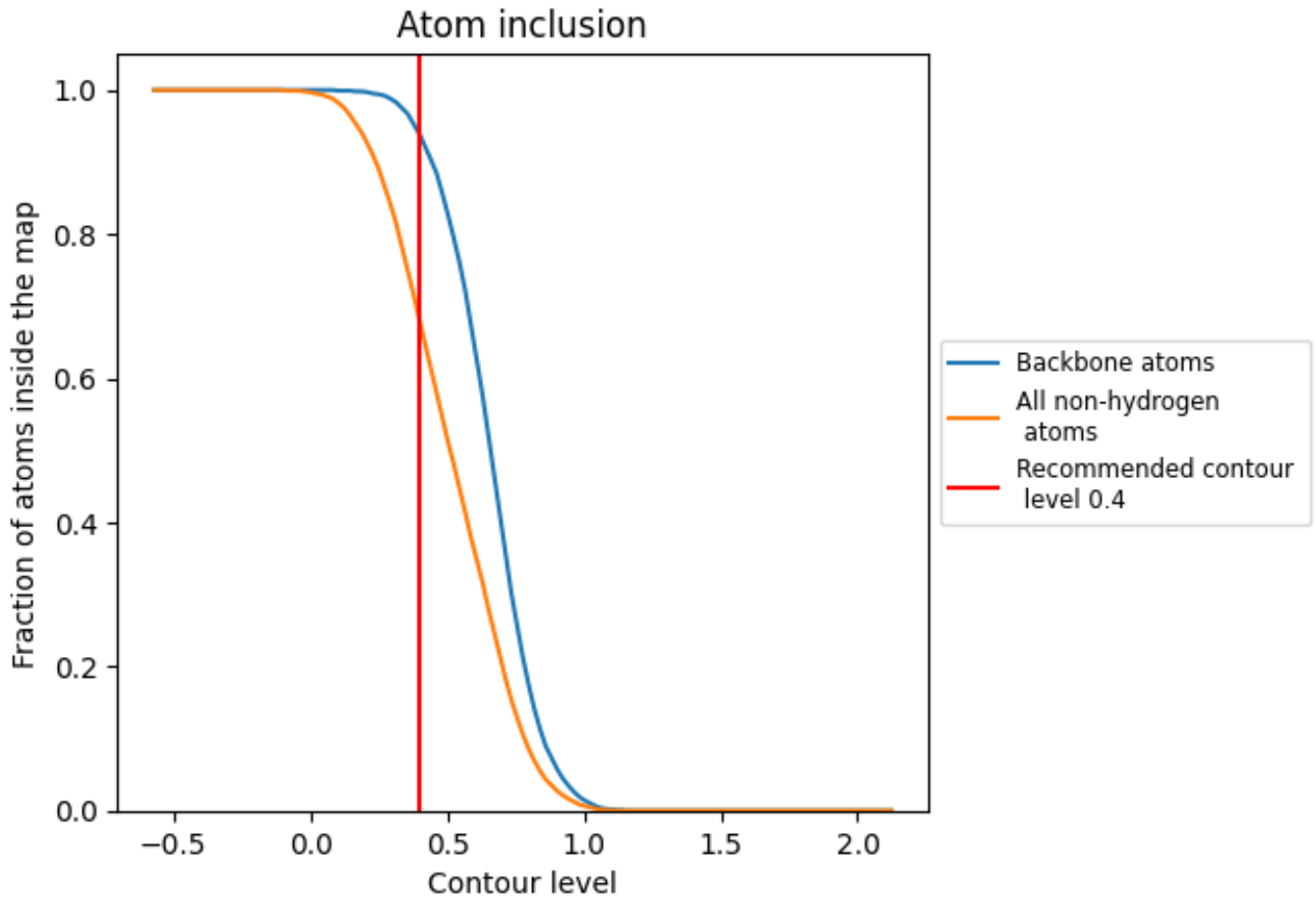
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 68% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6790	0.2600
0	0.3080	0.3210
1	0.5380	0.3220
2	0.4290	0.3360
3	0.4870	0.3030
4	0.6630	0.2990
5	0.3330	0.3110
6	0.2310	0.2930
7	0.4290	0.3060
A	0.6880	0.2540
B	0.6970	0.2280
C	0.6910	0.2550
D	0.6970	0.2270
E	0.6900	0.2520
F	0.6990	0.2310
G	0.2500	0.2230
H	0.7210	0.2630
I	0.7210	0.2650
J	0.7280	0.2650
K	0.3930	0.3310
L	0.7240	0.2730
M	0.7330	0.2760
N	0.7300	0.2740
O	0.3080	0.2730
P	0.4290	0.2850
Q	0.8200	0.4210
R	0.5130	0.2690
S	0.4200	0.3460
T	0.5250	0.3130
U	0.3080	0.3000
V	0.5380	0.3250
W	0.4290	0.3340
X	0.4870	0.3040
Y	0.6510	0.3110
Z	0.3330	0.3340

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Chain	Atom inclusion	Q-score
a	0.2310	0.2980
b	0.4290	0.3350
c	0.2500	0.2270
d	0.3570	0.3430
e	0.2820	0.2790
f	0.3930	0.2850
g	0.8030	0.4120
h	0.5130	0.2780
i	0.4200	0.3380
j	0.5080	0.2980
k	0.3080	0.3050
l	0.5380	0.3250
m	0.4290	0.3290
n	0.5130	0.3230
o	0.6510	0.3090
p	0.3330	0.3270
q	0.2310	0.3070
r	0.4290	0.3270
s	0.1790	0.2150
t	0.3570	0.3480
u	0.2820	0.2740
v	0.4290	0.2970
w	0.8360	0.4140
x	0.5380	0.2650
y	0.4200	0.3440
z	0.5250	0.3120