wwPDB EM Validation Summary Report

Oct 12, 2024 – 07:22 PM EDT

PDB ID	:	6UDJ
EMDB ID	:	EMD-20739
Title	:	HIV-1 bNAb 1-18 in complex with BG505 SOSIP.664 and 10-1074
Authors	:	Abernathy, M.E.; Barnes, C.O.; Gristick, H.B.; Bjorkman, P.J.
Deposited on	:	2019-09-19
Resolution	:	2.50 Å(reported)
Based on initial models	:	5T3Z, 6MTJ, 4RWY

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

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

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

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

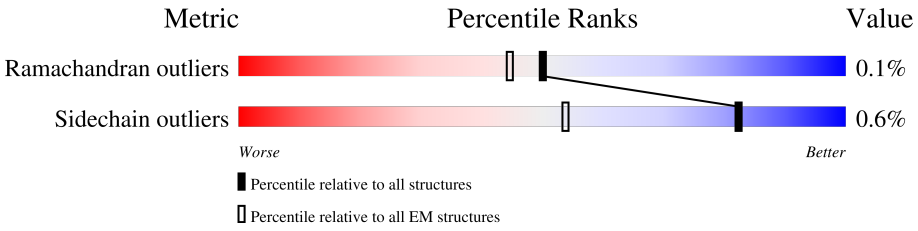
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.50 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	238	26% 55% 44%
1	K	238	25% 55% 44%
1	Q	238	24% 55% 44%
2	E	234	45% 54%
2	I	234	46% 54%
2	O	234	46% 54%
3	B	214	7% 50% 50%
3	L	214	7% 50% 50%
3	R	214	7% 50% 50%

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Mol	Chain	Length	Quality of chain
4	D	480	27% 73%
4	H	480	27% 73%
4	N	480	27% 73%
5	C	153	5% 80% 20%
5	F	153	6% 80% 20%
5	M	153	5% 80% 20%
6	G	479	88% 10%
6	J	479	89% 10%
6	P	479	89% 10%
7	S	9	22% 100%
7	T	9	22% 11% 89%
7	U	9	22% 100%
8	0	2	50% 100%
8	2	2	50% 50% 50%
8	4	2	50% 100%
8	7	2	50% 50% 50%
8	V	2	50% 100%
8	W	2	100% 100%
8	Y	2	50% 100%
8	a	2	50% 50% 50%
8	c	2	50% 100%
8	f	2	50% 50% 50%
8	j	2	50% 100%
8	k	2	100% 100%
8	m	2	50% 100%

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Mol	Chain	Length	Quality of chain
8	o	2	50% 100%
8	q	2	50% 100%
8	t	2	50% 50% 50%
8	x	2	50% 50% 50%
8	y	2	50% 100%
9	AA	5	40% 20% 80%
9	X	5	60% 40% 60%
9	i	5	40% 100%
9	l	5	60% 40% 60%
9	w	5	40% 100%
9	z	5	60% 40% 60%
10	1	4	50% 25% 75%
10	5	4	50% 25% 75%
10	Z	4	50% 25% 75%
10	d	4	50% 25% 75%
10	n	4	50% 25% 75%
10	r	4	50% 25% 75%
11	3	6	50% 33% 67%
11	b	6	50% 50% 50%
11	p	6	67% 33% 67%
12	6	3	67% 33% 67%
12	8	3	67% 100%
12	9	3	67% 33% 67%
12	e	3	67% 33% 67%
12	g	3	67% 100%

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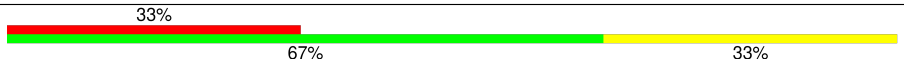
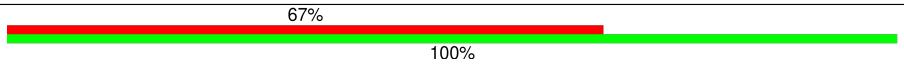
Mol	Chain	Length	Quality of chain
12	h	3	
12	s	3	
12	u	3	
12	v	3	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 26592 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 10-1074 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		
1	K	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		
1	Q	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		

- Molecule 2 is a protein called 1-18 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	108	Total	C	N	O	S	0	0
			820	514	146	158	2		
2	O	108	Total	C	N	O	S	0	0
			820	514	146	158	2		
2	I	108	Total	C	N	O	S	0	0
			820	514	146	158	2		

- Molecule 3 is a protein called 10-1074 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	107	Total	C	N	O	S	0	0
			824	515	152	154	3		
3	L	107	Total	C	N	O	S	0	0
			824	515	152	154	3		
3	R	107	Total	C	N	O	S	0	0
			824	515	152	154	3		

- Molecule 4 is a protein called 1-18 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	130	Total	C	N	O	S	0	0
			1050	667	187	193	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	130	Total	C	N	O	S	0	0
			1050	667	187	193	3		
4	H	130	Total	C	N	O	S	0	0
			1050	667	187	193	3		

- Molecule 5 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	123	Total	C	N	O	S	0	0
			982	622	169	185	6		
5	M	123	Total	C	N	O	S	0	0
			982	622	169	185	6		
5	F	123	Total	C	N	O	S	0	0
			982	622	169	185	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	559	PRO	ILE	conflict	UNP Q2N0S6
C	605	CYS	THR	conflict	UNP Q2N0S6
M	559	PRO	ILE	conflict	UNP Q2N0S6
M	605	CYS	THR	conflict	UNP Q2N0S6
F	559	PRO	ILE	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 6 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	429	Total	C	N	O	S	0	0
			3378	2126	597	628	27		
6	J	429	Total	C	N	O	S	0	0
			3378	2126	597	628	27		
6	P	429	Total	C	N	O	S	0	0
			3378	2126	597	628	27		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6

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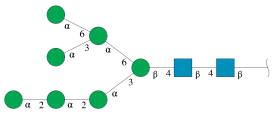
Chain	Residue	Modelled	Actual	Comment	Reference
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6
J	332	ASN	THR	conflict	UNP Q2N0S6
J	501	CYS	ALA	conflict	UNP Q2N0S6
J	509	ARG	-	expression tag	UNP Q2N0S6
J	510	ARG	-	expression tag	UNP Q2N0S6
J	511	ARG	-	expression tag	UNP Q2N0S6
J	512	ARG	-	expression tag	UNP Q2N0S6
J	513	ARG	-	expression tag	UNP Q2N0S6
P	332	ASN	THR	conflict	UNP Q2N0S6
P	501	CYS	ALA	conflict	UNP Q2N0S6
P	509	ARG	-	expression tag	UNP Q2N0S6
P	510	ARG	-	expression tag	UNP Q2N0S6
P	511	ARG	-	expression tag	UNP Q2N0S6
P	512	ARG	-	expression tag	UNP Q2N0S6
P	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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.

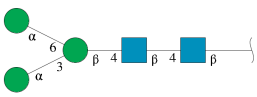


Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	9	Total 105	C 58	N 2	O 45	0	0
7	T	9	Total 105	C 58	N 2	O 45	0	0
7	U	9	Total 105	C 58	N 2	O 45	0	0

- Molecule 8 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
8	V	2	Total	C	N	O	0	0
			28	16	2	10		
8	W	2	Total	C	N	O	0	0
			28	16	2	10		
8	Y	2	Total	C	N	O	0	0
			28	16	2	10		
8	a	2	Total	C	N	O	0	0
			28	16	2	10		
8	c	2	Total	C	N	O	0	0
			28	16	2	10		
8	f	2	Total	C	N	O	0	0
			28	16	2	10		
8	j	2	Total	C	N	O	0	0
			28	16	2	10		
8	k	2	Total	C	N	O	0	0
			28	16	2	10		
8	m	2	Total	C	N	O	0	0
			28	16	2	10		
8	o	2	Total	C	N	O	0	0
			28	16	2	10		
8	q	2	Total	C	N	O	0	0
			28	16	2	10		
8	t	2	Total	C	N	O	0	0
			28	16	2	10		
8	x	2	Total	C	N	O	0	0
			28	16	2	10		
8	y	2	Total	C	N	O	0	0
			28	16	2	10		
8	0	2	Total	C	N	O	0	0
			28	16	2	10		
8	2	2	Total	C	N	O	0	0
			28	16	2	10		
8	4	2	Total	C	N	O	0	0
			28	16	2	10		
8	7	2	Total	C	N	O	0	0
			28	16	2	10		

- 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.

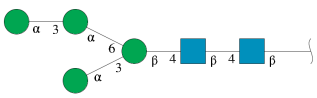


Mol	Chain	Residues	Atoms				AltConf	Trace
9	X	5	Total	C	N	O	0	0
			61	34	2	25		
9	i	5	Total	C	N	O	0	0
			61	34	2	25		
9	l	5	Total	C	N	O	0	0
			61	34	2	25		
9	w	5	Total	C	N	O	0	0
			61	34	2	25		
9	z	5	Total	C	N	O	0	0
			61	34	2	25		
9	AA	5	Total	C	N	O	0	0
			61	34	2	25		

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

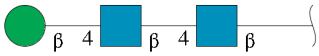
Mol	Chain	Residues	Atoms				AltConf	Trace
10	Z	4	Total	C	N	O	0	0
			50	28	2	20		
10	d	4	Total	C	N	O	0	0
			50	28	2	20		
10	n	4	Total	C	N	O	0	0
			50	28	2	20		
10	r	4	Total	C	N	O	0	0
			50	28	2	20		
10	1	4	Total	C	N	O	0	0
			50	28	2	20		
10	5	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



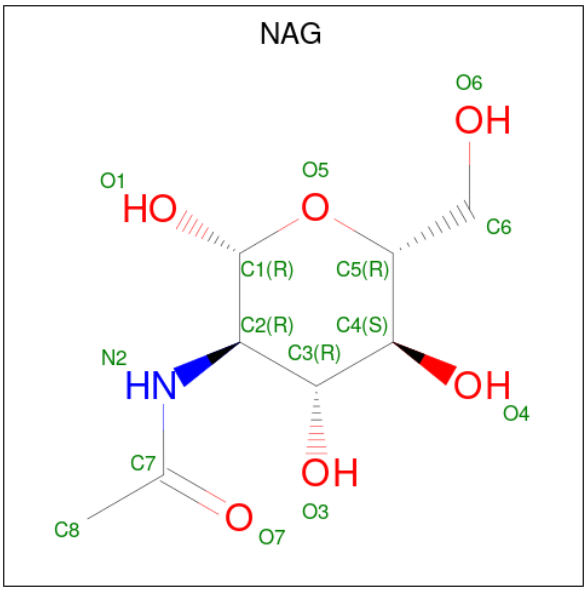
Mol	Chain	Residues	Atoms	AltConf	Trace
11	b	6	Total C N O 72 40 2 30	0	0
11	p	6	Total C N O 72 40 2 30	0	0
11	3	6	Total C N O 72 40 2 30	0	0

- Molecule 12 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
12	e	3	Total C N O 39 22 2 15	0	0
12	g	3	Total C N O 39 22 2 15	0	0
12	h	3	Total C N O 39 22 2 15	0	0
12	s	3	Total C N O 39 22 2 15	0	0
12	u	3	Total C N O 39 22 2 15	0	0
12	v	3	Total C N O 39 22 2 15	0	0
12	6	3	Total C N O 39 22 2 15	0	0
12	8	3	Total C N O 39 22 2 15	0	0
12	9	3	Total C N O 39 22 2 15	0	0

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
13	C	1	Total	C	N	O	0
			14	8	1	5	
13	C	1	Total	C	N	O	0
			14	8	1	5	
13	C	1	Total	C	N	O	0
			14	8	1	5	
13	G	1	Total	C	N	O	0
			14	8	1	5	
13	G	1	Total	C	N	O	0
			14	8	1	5	
13	M	1	Total	C	N	O	0
			14	8	1	5	
13	M	1	Total	C	N	O	0
			14	8	1	5	
13	M	1	Total	C	N	O	0
			14	8	1	5	
13	J	1	Total	C	N	O	0
			14	8	1	5	
13	J	1	Total	C	N	O	0
			14	8	1	5	
13	F	1	Total	C	N	O	0
			14	8	1	5	
13	F	1	Total	C	N	O	0
			14	8	1	5	
13	F	1	Total	C	N	O	0
			14	8	1	5	
13	P	1	Total	C	N	O	0
			14	8	1	5	

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

- Molecule 14 is water.

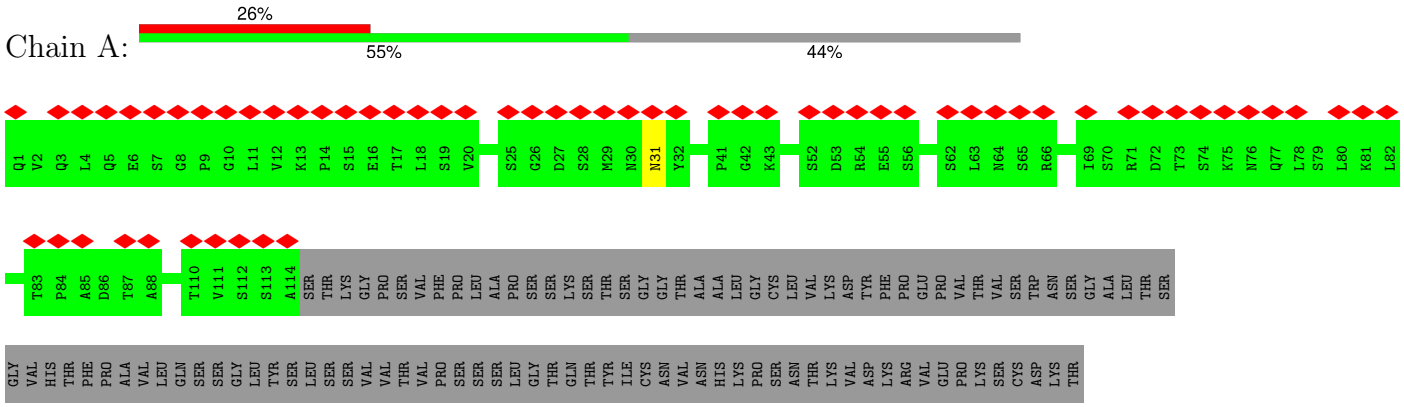
Mol	Chain	Residues	Atoms		AltConf
14	G	15	Total	O	0
			15	15	
14	J	15	Total	O	0
			15	15	
14	P	15	Total	O	0
			15	15	

3 Residue-property plots (i)

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

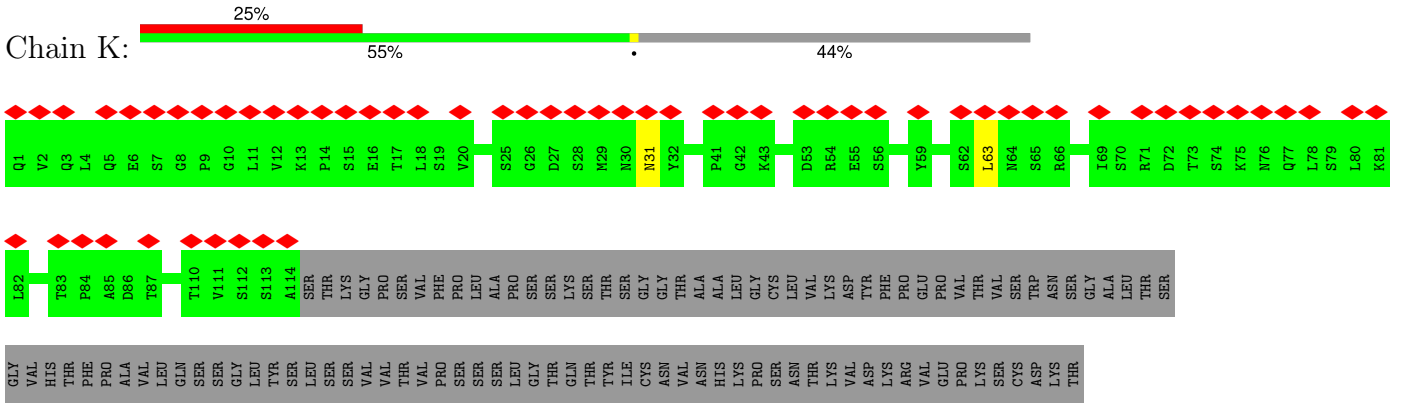
• Molecule 1: 10-1074 Fab Heavy Chain

Chain A:



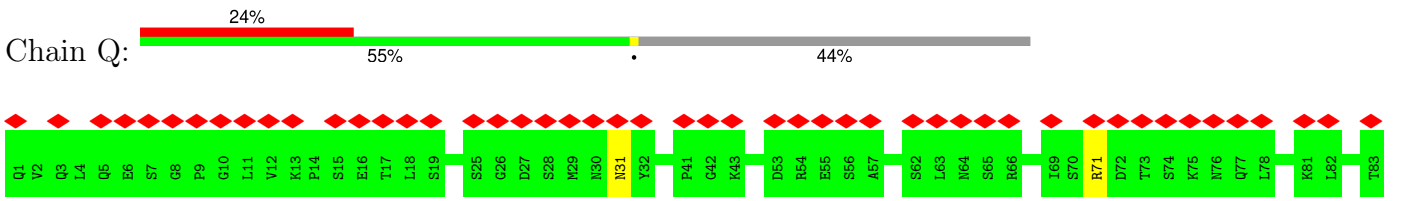
• Molecule 1: 10-1074 Fab Heavy Chain

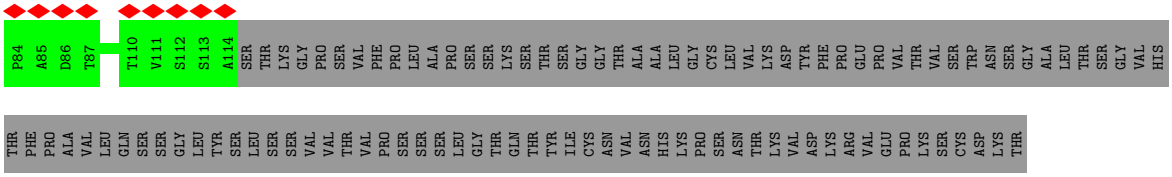
Chain K:



• Molecule 1: 10-1074 Fab Heavy Chain

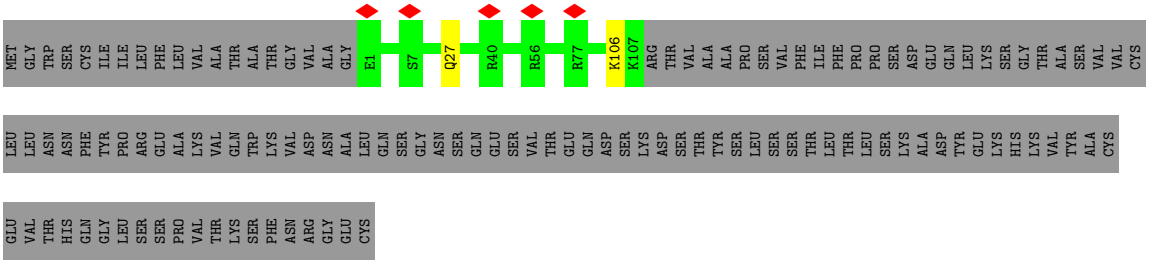
Chain Q:





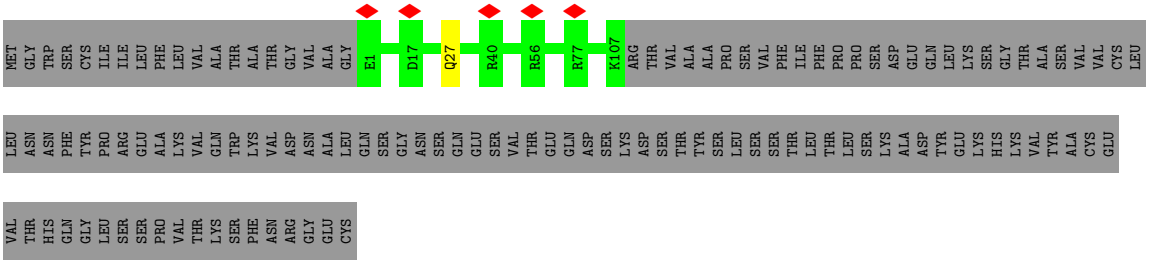
• Molecule 2: 1-18 Fab Light Chain

Chain E:



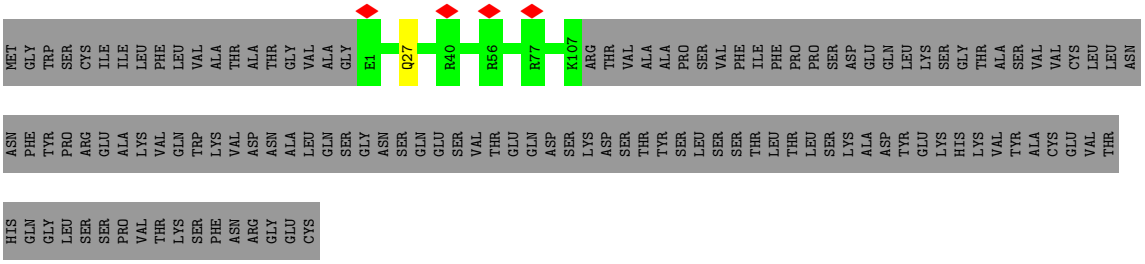
• Molecule 2: 1-18 Fab Light Chain

Chain O:



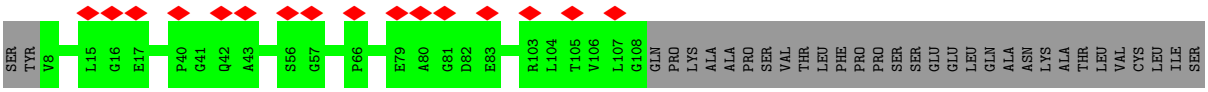
• Molecule 2: 1-18 Fab Light Chain

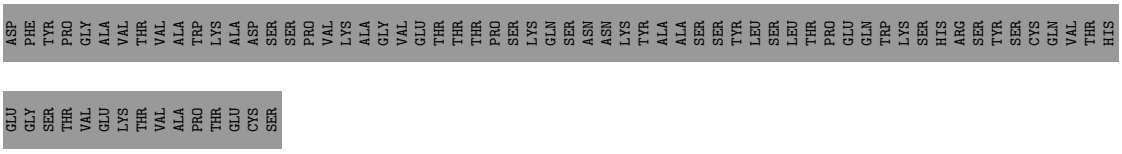
Chain I:



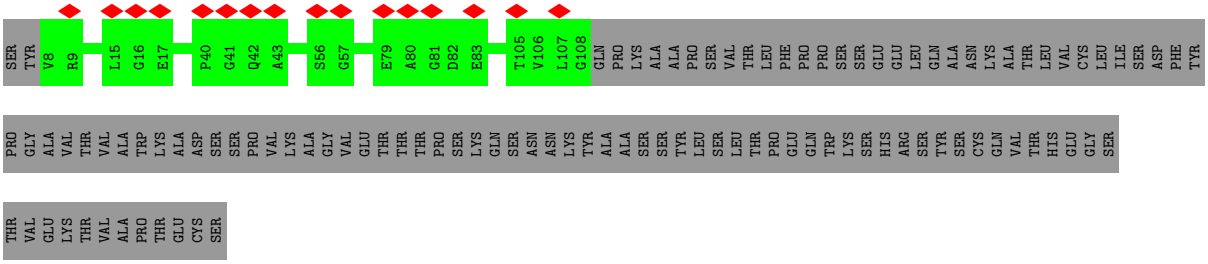
• Molecule 3: 10-1074 Fab Light Chain

Chain B:

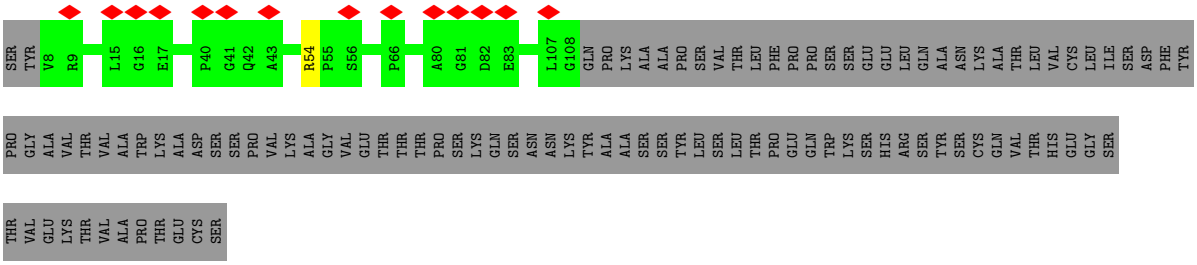




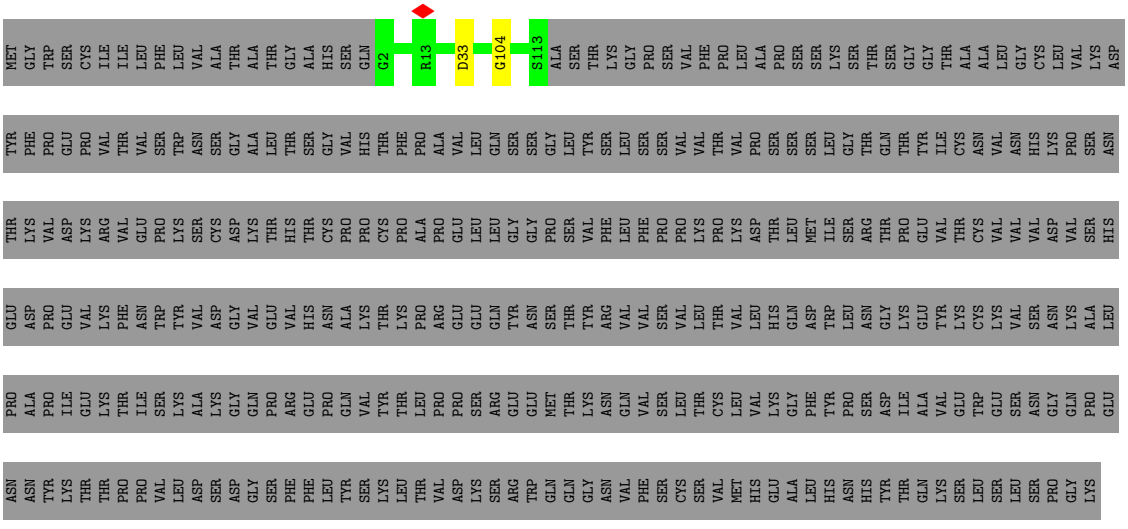
• Molecule 3: 10-1074 Fab Light Chain



• Molecule 3: 10-1074 Fab Light Chain

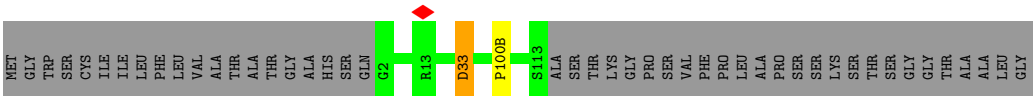


• Molecule 4: 1-18 Fab Heavy Chain



• Molecule 4: 1-18 Fab Heavy Chain

Chain N:

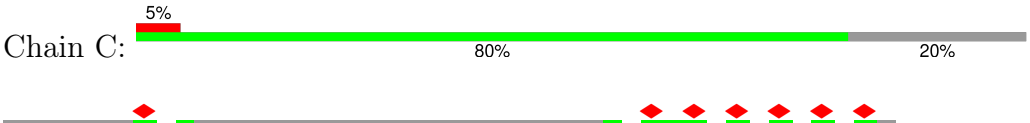


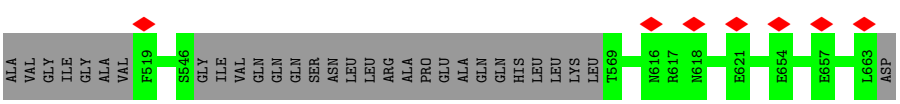
• Molecule 4: 1-18 Fab Heavy Chain

Chain H:

• Molecule 5: Envelope glycoprotein gp41

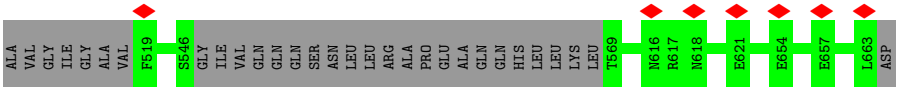
Chain C:





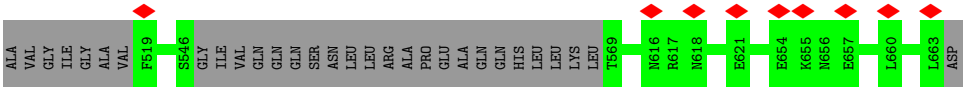
• Molecule 5: Envelope glycoprotein gp41

Chain M:



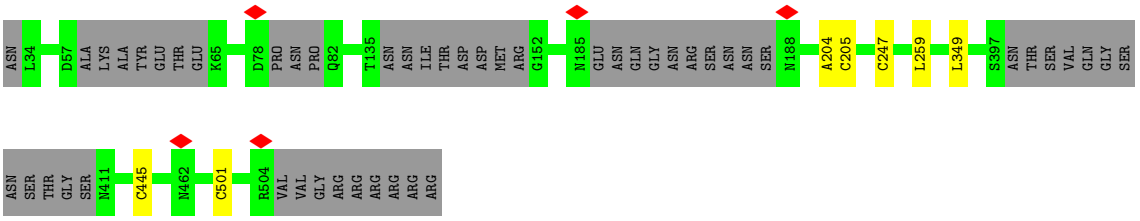
• Molecule 5: Envelope glycoprotein gp41

Chain F:



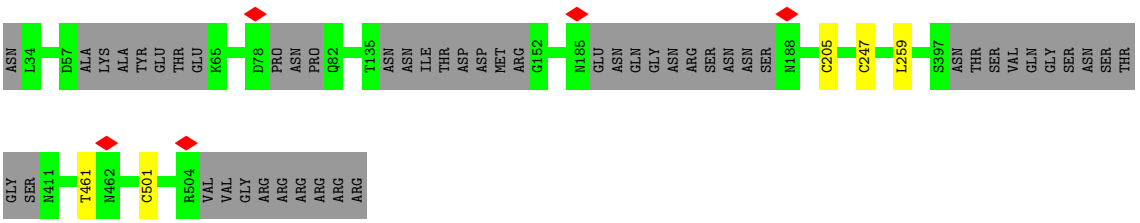
• Molecule 6: Envelope glycoprotein gp120

Chain G:



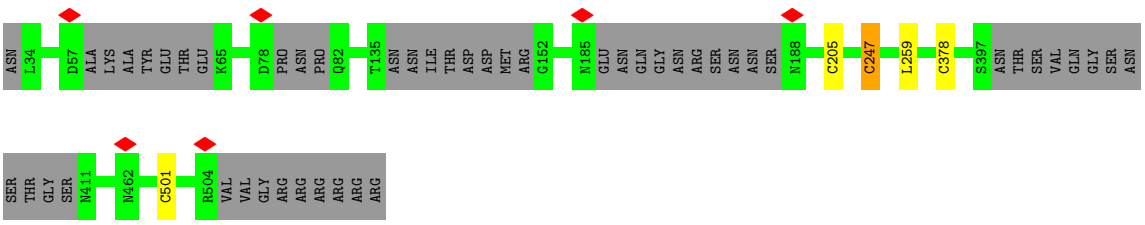
• Molecule 6: Envelope glycoprotein gp120

Chain J:



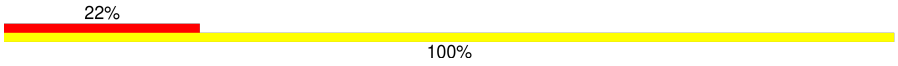
• Molecule 6: Envelope glycoprotein gp120

Chain P:



• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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 S:

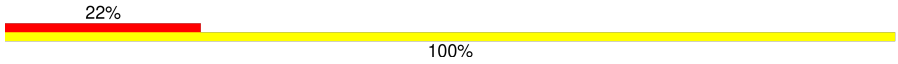


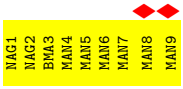
• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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

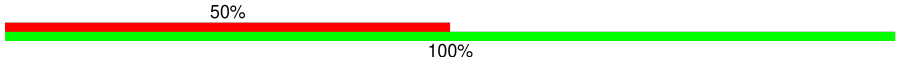
Chain U:





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

Chain V:

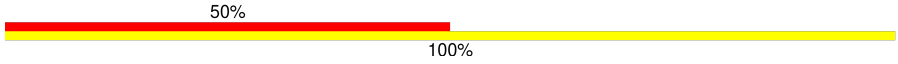


• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

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

Chain Y:



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

Chain a:

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

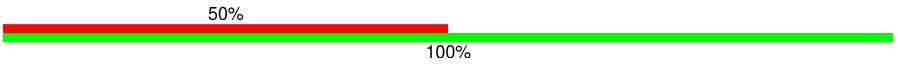
Chain c:

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

Chain f:

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

Chain j:



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

Chain k:

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

Chain m:

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

Chain o:

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

Chain q:

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

Chain t:

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

Chain x:

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

Chain y:

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

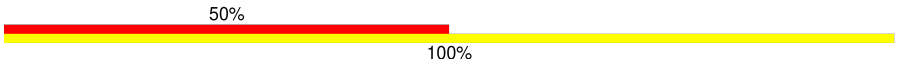
Chain 0:

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

Chain 2:

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

Chain 4:

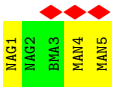


• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7:

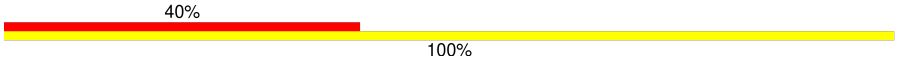
• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



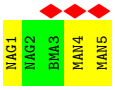
• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:



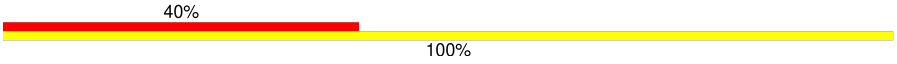
• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



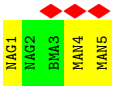
• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:



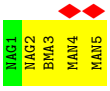
• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:



• Molecule 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 AA:



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

Chain d:

• Molecule 10: 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 n:

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

Chain r:

• Molecule 10: 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

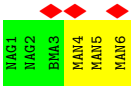
Chain 1:

• Molecule 10: 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 5:

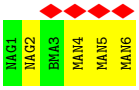
• Molecule 11: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



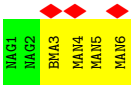
• Molecule 11: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:



• Molecule 11: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3:



• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6:

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8:

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9:


NAG1
NAG2
BMA3

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	230924	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.254	Depositor
Minimum map value	-0.143	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0302	Depositor
Map size (Å)	304.41602, 304.41602, 304.41602	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.057, 1.057, 1.057	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.41	0/1066	0.59	0/1451
1	K	0.41	0/1066	0.60	0/1451
1	Q	0.40	0/1066	0.58	0/1451
2	E	0.44	0/838	0.62	0/1135
2	I	0.43	0/838	0.61	0/1135
2	O	0.46	0/838	0.63	0/1135
3	B	0.37	0/845	0.57	0/1148
3	L	0.37	0/845	0.58	0/1148
3	R	0.38	0/845	0.56	0/1148
4	D	0.53	0/1084	0.70	1/1475 (0.1%)
4	H	0.51	0/1084	0.70	2/1475 (0.1%)
4	N	0.51	0/1084	0.71	2/1475 (0.1%)
5	C	0.37	0/1000	0.51	0/1356
5	F	0.37	0/1000	0.53	0/1356
5	M	0.39	0/1000	0.51	0/1356
6	G	0.54	2/3446 (0.1%)	0.63	2/4672 (0.0%)
6	J	0.53	0/3446	0.62	1/4672 (0.0%)
6	P	0.52	0/3446	0.62	2/4672 (0.0%)
All	All	0.47	2/24837 (0.0%)	0.61	10/33711 (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	1
1	K	0	1
1	Q	0	1
2	E	0	1
2	I	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	O	0	1
4	D	0	1
4	N	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	445	CYS	CB-SG	-5.85	1.72	1.81
6	G	204	ALA	C-N	-5.47	1.21	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	33	ASP	CB-CG-OD1	10.31	127.58	118.30
4	D	33	ASP	CB-CG-OD1	10.26	127.53	118.30
4	H	33	ASP	CB-CG-OD1	9.93	127.24	118.30
6	G	349	LEU	CA-CB-CG	5.86	128.78	115.30
6	P	247	CYS	CA-CB-SG	5.81	124.47	114.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	ASN	Peptide
2	E	27	GLN	Peptide
1	K	31	ASN	Peptide
2	O	27	GLN	Peptide
1	Q	31	ASN	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	131/238 (55%)	123 (94%)	8 (6%)	0	100	100
1	K	131/238 (55%)	123 (94%)	8 (6%)	0	100	100
1	Q	131/238 (55%)	125 (95%)	6 (5%)	0	100	100
2	E	106/234 (45%)	97 (92%)	9 (8%)	0	100	100
2	I	106/234 (45%)	99 (93%)	7 (7%)	0	100	100
2	O	106/234 (45%)	95 (90%)	11 (10%)	0	100	100
3	B	105/214 (49%)	97 (92%)	8 (8%)	0	100	100
3	L	105/214 (49%)	98 (93%)	7 (7%)	0	100	100
3	R	105/214 (49%)	99 (94%)	6 (6%)	0	100	100
4	D	128/480 (27%)	124 (97%)	4 (3%)	0	100	100
4	H	128/480 (27%)	124 (97%)	3 (2%)	1 (1%)	16	31
4	N	128/480 (27%)	123 (96%)	4 (3%)	1 (1%)	16	31
5	C	119/153 (78%)	116 (98%)	3 (2%)	0	100	100
5	F	119/153 (78%)	117 (98%)	2 (2%)	0	100	100
5	M	119/153 (78%)	117 (98%)	2 (2%)	0	100	100
6	G	417/479 (87%)	404 (97%)	13 (3%)	0	100	100
6	J	417/479 (87%)	405 (97%)	12 (3%)	0	100	100
6	P	417/479 (87%)	406 (97%)	11 (3%)	0	100	100
All	All	3018/5394 (56%)	2892 (96%)	124 (4%)	2 (0%)	50	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	N	100(B)	PRO
4	H	100(B)	PRO

5.3.2 Protein sidechains ⓘ

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	116/208 (56%)	116 (100%)	0	100	100
1	K	116/208 (56%)	115 (99%)	1 (1%)	75	90
1	Q	116/208 (56%)	115 (99%)	1 (1%)	75	90
2	E	88/198 (44%)	87 (99%)	1 (1%)	70	87
2	I	88/198 (44%)	88 (100%)	0	100	100
2	O	88/198 (44%)	88 (100%)	0	100	100
3	B	85/178 (48%)	85 (100%)	0	100	100
3	L	85/178 (48%)	85 (100%)	0	100	100
3	R	85/178 (48%)	84 (99%)	1 (1%)	67	86
4	D	110/424 (26%)	110 (100%)	0	100	100
4	H	110/424 (26%)	110 (100%)	0	100	100
4	N	110/424 (26%)	110 (100%)	0	100	100
5	C	106/129 (82%)	106 (100%)	0	100	100
5	F	106/129 (82%)	106 (100%)	0	100	100
5	M	106/129 (82%)	106 (100%)	0	100	100
6	G	383/427 (90%)	380 (99%)	3 (1%)	79	91
6	J	383/427 (90%)	379 (99%)	4 (1%)	73	88
6	P	383/427 (90%)	379 (99%)	4 (1%)	73	88
All	All	2664/4692 (57%)	2649 (99%)	15 (1%)	82	94

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	J	205	CYS
6	P	378	CYS
6	J	247	CYS
6	P	501	CYS
6	P	205	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
5	C	577	GLN
6	G	280	ASN

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Mol	Chain	Res	Type
6	J	411	ASN
6	G	85	HIS
6	G	411	ASN

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)

162 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	0	1	8,6	14,14,15	0.56	0	17,19,21	0.98	1 (5%)
8	NAG	0	2	8	14,14,15	0.56	0	17,19,21	0.94	1 (5%)
10	NAG	1	1	10,6	14,14,15	0.71	1 (7%)	17,19,21	0.75	0
10	NAG	1	2	10	14,14,15	0.28	0	17,19,21	1.27	3 (17%)
10	BMA	1	3	10	11,11,12	0.85	0	15,15,17	0.77	0
10	MAN	1	4	10	11,11,12	1.07	2 (18%)	15,15,17	1.14	1 (6%)
8	NAG	2	1	8,6	14,14,15	0.29	0	17,19,21	0.62	1 (5%)
8	NAG	2	2	8	14,14,15	0.36	0	17,19,21	0.48	0
11	NAG	3	1	11,6	14,14,15	0.38	0	17,19,21	0.54	0
11	NAG	3	2	11	14,14,15	0.44	0	17,19,21	0.63	0
11	BMA	3	3	11	11,11,12	1.12	1 (9%)	15,15,17	0.87	0
11	MAN	3	4	11	11,11,12	0.77	0	15,15,17	1.35	2 (13%)
11	MAN	3	5	11	11,11,12	0.68	0	15,15,17	1.20	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	MAN	3	6	11	11,11,12	0.78	0	15,15,17	1.10	2 (13%)
8	NAG	4	1	8,6	14,14,15	0.79	1 (7%)	17,19,21	0.63	0
8	NAG	4	2	8	14,14,15	0.46	0	17,19,21	1.06	1 (5%)
10	NAG	5	1	10,6	14,14,15	0.45	0	17,19,21	0.58	0
10	NAG	5	2	10	14,14,15	0.28	0	17,19,21	0.69	1 (5%)
10	BMA	5	3	10	11,11,12	0.60	0	15,15,17	0.87	1 (6%)
10	MAN	5	4	10	11,11,12	0.74	0	15,15,17	1.19	2 (13%)
12	NAG	6	1	12,6	14,14,15	0.32	0	17,19,21	0.88	1 (5%)
12	NAG	6	2	12	14,14,15	0.26	0	17,19,21	0.46	0
12	BMA	6	3	12	11,11,12	0.75	0	15,15,17	0.82	1 (6%)
8	NAG	7	1	8,6	14,14,15	0.56	0	17,19,21	0.53	0
8	NAG	7	2	8	14,14,15	0.48	0	17,19,21	1.05	1 (5%)
12	NAG	8	1	12,6	14,14,15	0.28	0	17,19,21	0.44	0
12	NAG	8	2	12	14,14,15	0.37	0	17,19,21	0.59	0
12	BMA	8	3	12	11,11,12	0.95	0	15,15,17	0.89	0
12	NAG	9	1	12,6	14,14,15	0.47	0	17,19,21	0.81	1 (5%)
12	NAG	9	2	12	14,14,15	0.47	0	17,19,21	1.01	1 (5%)
12	BMA	9	3	12	11,11,12	0.89	0	15,15,17	0.81	0
9	NAG	AA	1	9,6	14,14,15	0.60	0	17,19,21	0.68	0
9	NAG	AA	2	9	14,14,15	0.61	1 (7%)	17,19,21	0.81	1 (5%)
9	BMA	AA	3	9	11,11,12	0.89	0	15,15,17	1.02	1 (6%)
9	MAN	AA	4	9	11,11,12	0.58	0	15,15,17	1.03	1 (6%)
9	MAN	AA	5	9	11,11,12	0.90	0	15,15,17	1.05	1 (6%)
7	NAG	S	1	7,6	14,14,15	0.81	1 (7%)	17,19,21	0.57	0
7	NAG	S	2	7	14,14,15	0.43	0	17,19,21	0.87	1 (5%)
7	BMA	S	3	7	11,11,12	1.48	2 (18%)	15,15,17	1.16	0
7	MAN	S	4	7	11,11,12	0.96	0	15,15,17	1.65	2 (13%)
7	MAN	S	5	7	11,11,12	0.91	0	15,15,17	1.38	2 (13%)
7	MAN	S	6	7	11,11,12	0.90	0	15,15,17	1.31	3 (20%)
7	MAN	S	7	7	11,11,12	0.81	0	15,15,17	1.07	2 (13%)
7	MAN	S	8	7	11,11,12	0.90	0	15,15,17	0.93	1 (6%)
7	MAN	S	9	7	11,11,12	0.84	0	15,15,17	0.94	1 (6%)
7	NAG	T	1	7,6	14,14,15	0.81	1 (7%)	17,19,21	0.58	0
7	NAG	T	2	7	14,14,15	0.59	1 (7%)	17,19,21	0.86	1 (5%)
7	BMA	T	3	7	11,11,12	1.51	2 (18%)	15,15,17	1.24	2 (13%)
7	MAN	T	4	7	11,11,12	1.00	0	15,15,17	1.60	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MAN	T	5	7	11,11,12	0.88	0	15,15,17	1.34	2 (13%)
7	MAN	T	6	7	11,11,12	0.83	0	15,15,17	1.23	3 (20%)
7	MAN	T	7	7	11,11,12	0.88	0	15,15,17	1.05	2 (13%)
7	MAN	T	8	7	11,11,12	0.97	0	15,15,17	0.94	0
7	MAN	T	9	7	11,11,12	0.85	0	15,15,17	0.95	2 (13%)
7	NAG	U	1	7,6	14,14,15	0.75	1 (7%)	17,19,21	0.57	0
7	NAG	U	2	7	14,14,15	0.59	1 (7%)	17,19,21	0.89	1 (5%)
7	BMA	U	3	7	11,11,12	1.47	2 (18%)	15,15,17	1.24	2 (13%)
7	MAN	U	4	7	11,11,12	0.93	0	15,15,17	1.58	2 (13%)
7	MAN	U	5	7	11,11,12	0.92	0	15,15,17	1.35	2 (13%)
7	MAN	U	6	7	11,11,12	0.85	0	15,15,17	1.17	1 (6%)
7	MAN	U	7	7	11,11,12	0.85	0	15,15,17	1.02	2 (13%)
7	MAN	U	8	7	11,11,12	0.92	0	15,15,17	0.93	1 (6%)
7	MAN	U	9	7	11,11,12	0.87	0	15,15,17	0.95	1 (6%)
8	NAG	V	1	8,6	14,14,15	0.42	0	17,19,21	0.53	0
8	NAG	V	2	8	14,14,15	0.24	0	17,19,21	0.54	0
8	NAG	W	1	8,6	14,14,15	0.18	0	17,19,21	0.60	0
8	NAG	W	2	8	14,14,15	0.30	0	17,19,21	0.44	0
9	NAG	X	1	9,6	14,14,15	0.34	0	17,19,21	0.69	1 (5%)
9	NAG	X	2	9	14,14,15	0.34	0	17,19,21	0.52	0
9	BMA	X	3	9	11,11,12	0.76	0	15,15,17	0.81	0
9	MAN	X	4	9	11,11,12	1.00	1 (9%)	15,15,17	1.33	2 (13%)
9	MAN	X	5	9	11,11,12	0.94	1 (9%)	15,15,17	0.89	0
8	NAG	Y	1	8,6	14,14,15	0.62	0	17,19,21	0.98	1 (5%)
8	NAG	Y	2	8	14,14,15	0.54	0	17,19,21	0.95	1 (5%)
10	NAG	Z	1	10,6	14,14,15	0.74	1 (7%)	17,19,21	0.75	0
10	NAG	Z	2	10	14,14,15	0.30	0	17,19,21	1.27	3 (17%)
10	BMA	Z	3	10	11,11,12	0.89	0	15,15,17	0.77	0
10	MAN	Z	4	10	11,11,12	1.07	2 (18%)	15,15,17	1.10	1 (6%)
8	NAG	a	1	8,6	14,14,15	0.31	0	17,19,21	0.64	1 (5%)
8	NAG	a	2	8	14,14,15	0.36	0	17,19,21	0.47	0
11	NAG	b	1	11,6	14,14,15	0.30	0	17,19,21	0.57	0
11	NAG	b	2	11	14,14,15	0.49	0	17,19,21	0.65	0
11	BMA	b	3	11	11,11,12	0.99	0	15,15,17	0.81	0
11	MAN	b	4	11	11,11,12	0.73	0	15,15,17	1.39	2 (13%)
11	MAN	b	5	11	11,11,12	0.62	0	15,15,17	1.18	1 (6%)
11	MAN	b	6	11	11,11,12	0.74	0	15,15,17	1.01	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	c	1	8,6	14,14,15	0.89	1 (7%)	17,19,21	0.60	0
8	NAG	c	2	8	14,14,15	0.49	0	17,19,21	1.05	1 (5%)
10	NAG	d	1	10,6	14,14,15	0.45	0	17,19,21	0.63	0
10	NAG	d	2	10	14,14,15	0.29	0	17,19,21	0.78	1 (5%)
10	BMA	d	3	10	11,11,12	0.59	0	15,15,17	0.88	1 (6%)
10	MAN	d	4	10	11,11,12	0.73	0	15,15,17	1.26	2 (13%)
12	NAG	e	1	12,6	14,14,15	0.31	0	17,19,21	0.92	1 (5%)
12	NAG	e	2	12	14,14,15	0.26	0	17,19,21	0.44	0
12	BMA	e	3	12	11,11,12	0.77	0	15,15,17	0.82	1 (6%)
8	NAG	f	1	8,6	14,14,15	0.45	0	17,19,21	0.57	0
8	NAG	f	2	8	14,14,15	0.62	0	17,19,21	1.03	1 (5%)
12	NAG	g	1	12,6	14,14,15	0.26	0	17,19,21	0.46	0
12	NAG	g	2	12	14,14,15	0.41	0	17,19,21	0.62	0
12	BMA	g	3	12	11,11,12	0.98	0	15,15,17	0.92	0
12	NAG	h	1	12,6	14,14,15	0.56	0	17,19,21	0.79	1 (5%)
12	NAG	h	2	12	14,14,15	0.42	0	17,19,21	1.01	1 (5%)
12	BMA	h	3	12	11,11,12	0.92	0	15,15,17	0.84	0
9	NAG	i	1	9,6	14,14,15	0.56	0	17,19,21	0.83	1 (5%)
9	NAG	i	2	9	14,14,15	0.48	0	17,19,21	0.70	1 (5%)
9	BMA	i	3	9	11,11,12	0.85	0	15,15,17	1.06	1 (6%)
9	MAN	i	4	9	11,11,12	0.63	0	15,15,17	1.01	2 (13%)
9	MAN	i	5	9	11,11,12	0.87	0	15,15,17	1.07	1 (6%)
8	NAG	j	1	8,6	14,14,15	0.44	0	17,19,21	0.52	0
8	NAG	j	2	8	14,14,15	0.24	0	17,19,21	0.57	0
8	NAG	k	1	8,6	14,14,15	0.19	0	17,19,21	0.62	0
8	NAG	k	2	8	14,14,15	0.35	0	17,19,21	0.45	0
9	NAG	l	1	9,6	14,14,15	0.23	0	17,19,21	0.70	1 (5%)
9	NAG	l	2	9	14,14,15	0.38	0	17,19,21	0.50	0
9	BMA	l	3	9	11,11,12	0.77	0	15,15,17	0.79	0
9	MAN	l	4	9	11,11,12	1.05	1 (9%)	15,15,17	1.33	2 (13%)
9	MAN	l	5	9	11,11,12	0.93	1 (9%)	15,15,17	0.92	0
8	NAG	m	1	8,6	14,14,15	0.59	0	17,19,21	0.95	1 (5%)
8	NAG	m	2	8	14,14,15	0.51	0	17,19,21	0.95	1 (5%)
10	NAG	n	1	10,6	14,14,15	0.68	1 (7%)	17,19,21	0.76	0
10	NAG	n	2	10	14,14,15	0.33	0	17,19,21	1.29	3 (17%)
10	BMA	n	3	10	11,11,12	0.96	0	15,15,17	0.78	0
10	MAN	n	4	10	11,11,12	1.05	2 (18%)	15,15,17	1.18	1 (6%)
8	NAG	o	1	8,6	14,14,15	0.26	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	o	2	8	14,14,15	0.33	0	17,19,21	0.51	0
11	NAG	p	1	11,6	14,14,15	0.36	0	17,19,21	0.53	0
11	NAG	p	2	11	14,14,15	0.42	0	17,19,21	0.67	1 (5%)
11	BMA	p	3	11	11,11,12	1.05	0	15,15,17	0.80	0
11	MAN	p	4	11	11,11,12	0.79	0	15,15,17	1.38	2 (13%)
11	MAN	p	5	11	11,11,12	0.71	0	15,15,17	1.21	2 (13%)
11	MAN	p	6	11	11,11,12	0.78	0	15,15,17	1.05	2 (13%)
8	NAG	q	1	8,6	14,14,15	1.00	1 (7%)	17,19,21	0.64	0
8	NAG	q	2	8	14,14,15	0.47	0	17,19,21	1.04	1 (5%)
10	NAG	r	1	10,6	14,14,15	0.35	0	17,19,21	0.62	0
10	NAG	r	2	10	14,14,15	0.27	0	17,19,21	0.75	1 (5%)
10	BMA	r	3	10	11,11,12	0.62	0	15,15,17	0.89	1 (6%)
10	MAN	r	4	10	11,11,12	0.73	0	15,15,17	1.23	2 (13%)
12	NAG	s	1	12,6	14,14,15	0.37	0	17,19,21	0.92	1 (5%)
12	NAG	s	2	12	14,14,15	0.26	0	17,19,21	0.44	0
12	BMA	s	3	12	11,11,12	0.78	0	15,15,17	0.82	0
8	NAG	t	1	8,6	14,14,15	0.55	0	17,19,21	0.54	0
8	NAG	t	2	8	14,14,15	0.52	0	17,19,21	1.02	1 (5%)
12	NAG	u	1	12,6	14,14,15	0.25	0	17,19,21	0.48	0
12	NAG	u	2	12	14,14,15	0.33	0	17,19,21	0.56	0
12	BMA	u	3	12	11,11,12	0.95	0	15,15,17	0.82	0
12	NAG	v	1	12,6	14,14,15	0.46	0	17,19,21	0.77	1 (5%)
12	NAG	v	2	12	14,14,15	0.44	0	17,19,21	1.01	1 (5%)
12	BMA	v	3	12	11,11,12	0.88	0	15,15,17	0.82	0
9	NAG	w	1	9,6	14,14,15	0.59	0	17,19,21	0.73	1 (5%)
9	NAG	w	2	9	14,14,15	0.52	0	17,19,21	0.78	1 (5%)
9	BMA	w	3	9	11,11,12	0.89	0	15,15,17	1.05	1 (6%)
9	MAN	w	4	9	11,11,12	0.63	0	15,15,17	1.02	2 (13%)
9	MAN	w	5	9	11,11,12	0.93	0	15,15,17	1.05	1 (6%)
8	NAG	x	1	8,6	14,14,15	0.43	0	17,19,21	0.52	0
8	NAG	x	2	8	14,14,15	0.23	0	17,19,21	0.60	1 (5%)
8	NAG	y	1	8,6	14,14,15	0.19	0	17,19,21	0.61	0
8	NAG	y	2	8	14,14,15	0.28	0	17,19,21	0.42	0
9	NAG	z	1	9,6	14,14,15	0.30	0	17,19,21	0.70	1 (5%)
9	NAG	z	2	9	14,14,15	0.43	0	17,19,21	0.55	0
9	BMA	z	3	9	11,11,12	0.83	0	15,15,17	0.79	0
9	MAN	z	4	9	11,11,12	1.00	1 (9%)	15,15,17	1.31	2 (13%)
9	MAN	z	5	9	11,11,12	0.94	1 (9%)	15,15,17	0.91	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	0	1	8,6	-	4/6/23/26	0/1/1/1
8	NAG	0	2	8	-	2/6/23/26	0/1/1/1
10	NAG	1	1	10,6	-	0/6/23/26	0/1/1/1
10	NAG	1	2	10	-	2/6/23/26	0/1/1/1
10	BMA	1	3	10	-	2/2/19/22	0/1/1/1
10	MAN	1	4	10	-	0/2/19/22	0/1/1/1
8	NAG	2	1	8,6	-	0/6/23/26	0/1/1/1
8	NAG	2	2	8	-	2/6/23/26	0/1/1/1
11	NAG	3	1	11,6	-	0/6/23/26	0/1/1/1
11	NAG	3	2	11	-	2/6/23/26	0/1/1/1
11	BMA	3	3	11	-	0/2/19/22	0/1/1/1
11	MAN	3	4	11	-	2/2/19/22	0/1/1/1
11	MAN	3	5	11	-	0/2/19/22	0/1/1/1
11	MAN	3	6	11	-	2/2/19/22	0/1/1/1
8	NAG	4	1	8,6	-	0/6/23/26	0/1/1/1
8	NAG	4	2	8	-	4/6/23/26	0/1/1/1
10	NAG	5	1	10,6	-	2/6/23/26	0/1/1/1
10	NAG	5	2	10	-	2/6/23/26	0/1/1/1
10	BMA	5	3	10	-	0/2/19/22	0/1/1/1
10	MAN	5	4	10	-	2/2/19/22	0/1/1/1
12	NAG	6	1	12,6	-	2/6/23/26	0/1/1/1
12	NAG	6	2	12	-	2/6/23/26	0/1/1/1
12	BMA	6	3	12	-	2/2/19/22	0/1/1/1
8	NAG	7	1	8,6	-	0/6/23/26	0/1/1/1
8	NAG	7	2	8	-	2/6/23/26	0/1/1/1
12	NAG	8	1	12,6	-	2/6/23/26	0/1/1/1
12	NAG	8	2	12	-	2/6/23/26	0/1/1/1
12	BMA	8	3	12	-	0/2/19/22	0/1/1/1
12	NAG	9	1	12,6	-	0/6/23/26	0/1/1/1
12	NAG	9	2	12	-	4/6/23/26	0/1/1/1
12	BMA	9	3	12	-	2/2/19/22	0/1/1/1
9	NAG	AA	1	9,6	-	0/6/23/26	0/1/1/1
9	NAG	AA	2	9	-	2/6/23/26	0/1/1/1
9	BMA	AA	3	9	-	2/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	Y	1	8,6	-	4/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	3/6/23/26	0/1/1/1
10	NAG	Z	1	10,6	-	0/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	2/6/23/26	0/1/1/1
10	BMA	Z	3	10	-	2/2/19/22	0/1/1/1
10	MAN	Z	4	10	-	0/2/19/22	0/1/1/1
8	NAG	a	1	8,6	-	0/6/23/26	0/1/1/1
8	NAG	a	2	8	-	2/6/23/26	0/1/1/1
11	NAG	b	1	11,6	-	0/6/23/26	0/1/1/1
11	NAG	b	2	11	-	2/6/23/26	0/1/1/1
11	BMA	b	3	11	-	0/2/19/22	0/1/1/1
11	MAN	b	4	11	-	2/2/19/22	0/1/1/1
11	MAN	b	5	11	-	0/2/19/22	0/1/1/1
11	MAN	b	6	11	-	2/2/19/22	0/1/1/1
8	NAG	c	1	8,6	-	0/6/23/26	0/1/1/1
8	NAG	c	2	8	-	4/6/23/26	0/1/1/1
10	NAG	d	1	10,6	-	2/6/23/26	0/1/1/1
10	NAG	d	2	10	-	2/6/23/26	0/1/1/1
10	BMA	d	3	10	-	0/2/19/22	0/1/1/1
10	MAN	d	4	10	-	2/2/19/22	0/1/1/1
12	NAG	e	1	12,6	-	2/6/23/26	0/1/1/1
12	NAG	e	2	12	-	2/6/23/26	0/1/1/1
12	BMA	e	3	12	-	0/2/19/22	0/1/1/1
8	NAG	f	1	8,6	-	0/6/23/26	0/1/1/1
8	NAG	f	2	8	-	2/6/23/26	0/1/1/1
12	NAG	g	1	12,6	-	0/6/23/26	0/1/1/1
12	NAG	g	2	12	-	2/6/23/26	0/1/1/1
12	BMA	g	3	12	-	0/2/19/22	0/1/1/1
12	NAG	h	1	12,6	-	0/6/23/26	0/1/1/1
12	NAG	h	2	12	-	2/6/23/26	0/1/1/1
12	BMA	h	3	12	-	2/2/19/22	0/1/1/1
9	NAG	i	1	9,6	-	0/6/23/26	0/1/1/1
9	NAG	i	2	9	-	2/6/23/26	0/1/1/1
9	BMA	i	3	9	-	2/2/19/22	0/1/1/1
9	MAN	i	4	9	-	1/2/19/22	0/1/1/1
9	MAN	i	5	9	-	0/2/19/22	0/1/1/1
8	NAG	j	1	8,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	j	2	8	-	2/6/23/26	0/1/1/1
8	NAG	k	1	8,6	-	0/6/23/26	0/1/1/1
8	NAG	k	2	8	-	2/6/23/26	0/1/1/1
9	NAG	l	1	9,6	-	2/6/23/26	0/1/1/1
9	NAG	l	2	9	-	0/6/23/26	0/1/1/1
9	BMA	l	3	9	-	0/2/19/22	0/1/1/1
9	MAN	l	4	9	-	0/2/19/22	0/1/1/1
9	MAN	l	5	9	-	0/2/19/22	0/1/1/1
8	NAG	m	1	8,6	-	4/6/23/26	0/1/1/1
8	NAG	m	2	8	-	2/6/23/26	0/1/1/1
10	NAG	n	1	10,6	-	0/6/23/26	0/1/1/1
10	NAG	n	2	10	-	3/6/23/26	0/1/1/1
10	BMA	n	3	10	-	2/2/19/22	0/1/1/1
10	MAN	n	4	10	-	0/2/19/22	0/1/1/1
8	NAG	o	1	8,6	-	0/6/23/26	0/1/1/1
8	NAG	o	2	8	-	2/6/23/26	0/1/1/1
11	NAG	p	1	11,6	-	0/6/23/26	0/1/1/1
11	NAG	p	2	11	-	2/6/23/26	0/1/1/1
11	BMA	p	3	11	-	0/2/19/22	0/1/1/1
11	MAN	p	4	11	-	2/2/19/22	0/1/1/1
11	MAN	p	5	11	-	0/2/19/22	0/1/1/1
11	MAN	p	6	11	-	2/2/19/22	0/1/1/1
8	NAG	q	1	8,6	-	0/6/23/26	0/1/1/1
8	NAG	q	2	8	-	4/6/23/26	0/1/1/1
10	NAG	r	1	10,6	-	2/6/23/26	0/1/1/1
10	NAG	r	2	10	-	2/6/23/26	0/1/1/1
10	BMA	r	3	10	-	0/2/19/22	0/1/1/1
10	MAN	r	4	10	-	2/2/19/22	0/1/1/1
12	NAG	s	1	12,6	-	2/6/23/26	0/1/1/1
12	NAG	s	2	12	-	2/6/23/26	0/1/1/1
12	BMA	s	3	12	-	1/2/19/22	0/1/1/1
8	NAG	t	1	8,6	-	0/6/23/26	0/1/1/1
8	NAG	t	2	8	-	4/6/23/26	0/1/1/1
12	NAG	u	1	12,6	-	0/6/23/26	0/1/1/1
12	NAG	u	2	12	-	2/6/23/26	0/1/1/1
12	BMA	u	3	12	-	0/2/19/22	0/1/1/1
12	NAG	v	1	12,6	-	0/6/23/26	0/1/1/1
12	NAG	v	2	12	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BMA	v	3	12	-	2/2/19/22	0/1/1/1
9	NAG	w	1	9,6	-	0/6/23/26	0/1/1/1
9	NAG	w	2	9	-	2/6/23/26	0/1/1/1
9	BMA	w	3	9	-	2/2/19/22	0/1/1/1
9	MAN	w	4	9	-	1/2/19/22	0/1/1/1
9	MAN	w	5	9	-	0/2/19/22	0/1/1/1
8	NAG	x	1	8,6	-	0/6/23/26	0/1/1/1
8	NAG	x	2	8	-	2/6/23/26	0/1/1/1
8	NAG	y	1	8,6	-	0/6/23/26	0/1/1/1
8	NAG	y	2	8	-	2/6/23/26	0/1/1/1
9	NAG	z	1	9,6	-	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
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 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	q	1	NAG	O5-C1	-3.57	1.37	1.43
8	c	1	NAG	O5-C1	-3.20	1.38	1.43
7	T	1	NAG	O5-C1	-2.86	1.38	1.43
8	4	1	NAG	O5-C1	-2.84	1.38	1.43
7	S	1	NAG	O5-C1	-2.80	1.39	1.43

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	S	4	MAN	C1-O5-C5	5.22	119.19	112.19
7	U	4	MAN	C1-O5-C5	5.08	118.99	112.19
7	T	4	MAN	C1-O5-C5	4.80	118.62	112.19
11	b	4	MAN	C1-O5-C5	4.12	117.70	112.19
9	X	4	MAN	C1-O5-C5	4.08	117.65	112.19

There are no chirality outliers.

5 of 195 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	s	2	NAG	O5-C5-C6-O6
10	d	2	NAG	O5-C5-C6-O6

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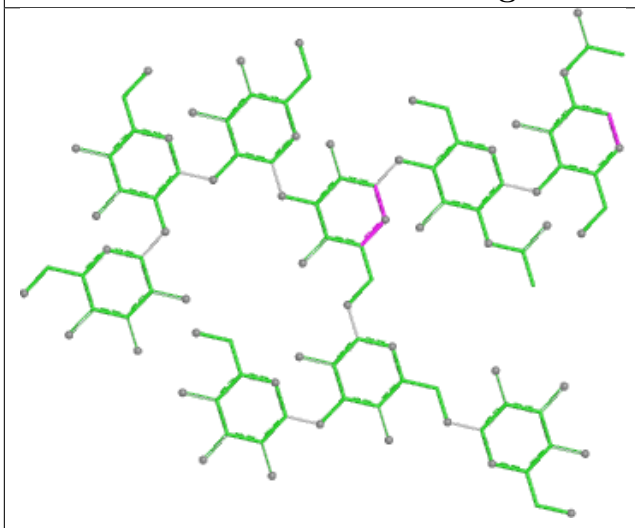
Mol	Chain	Res	Type	Atoms
10	d	4	MAN	O5-C5-C6-O6
12	e	2	NAG	O5-C5-C6-O6
12	s	1	NAG	O5-C5-C6-O6

There are no ring outliers.

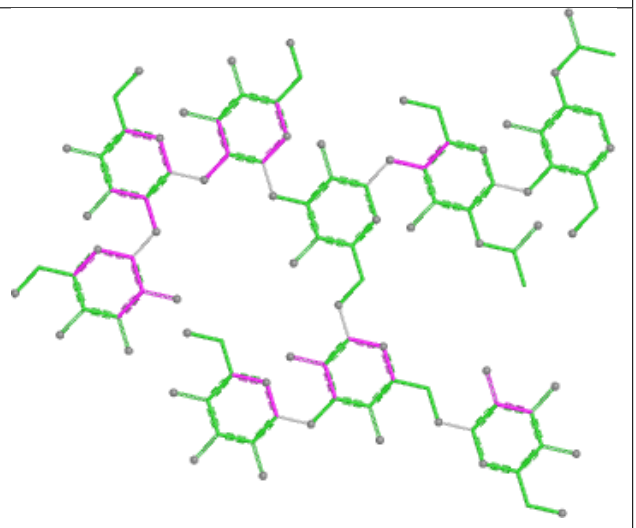
No monomer is involved in short contacts.

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

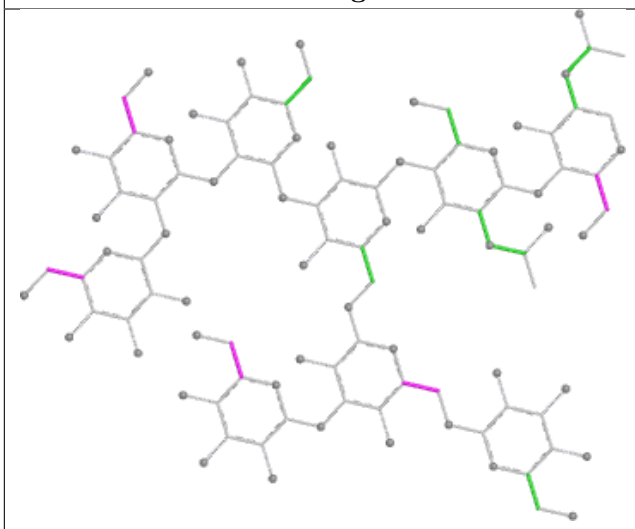
Oligosaccharide Chain S



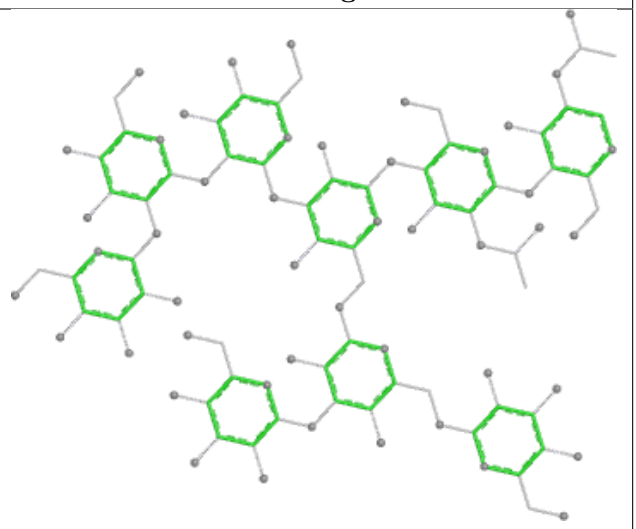
Bond lengths



Bond angles

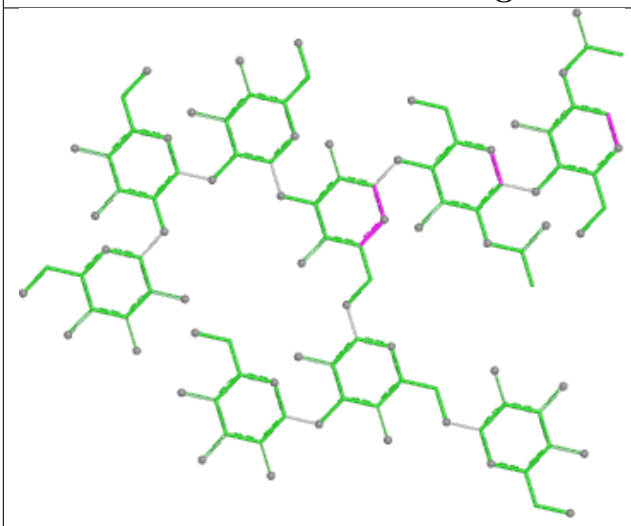


Torsions

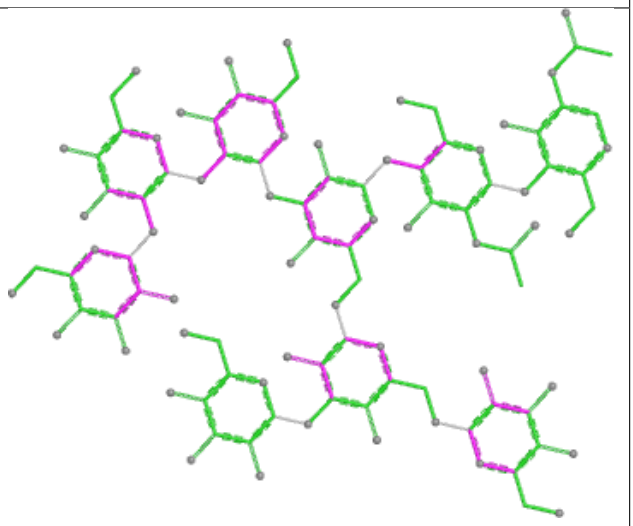


Rings

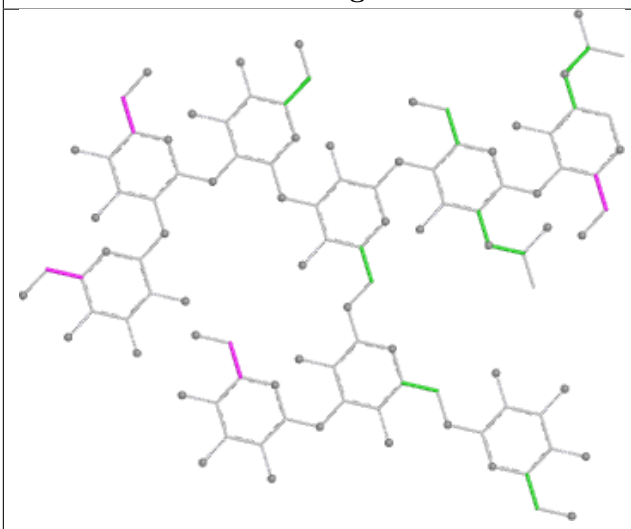
Oligosaccharide Chain T



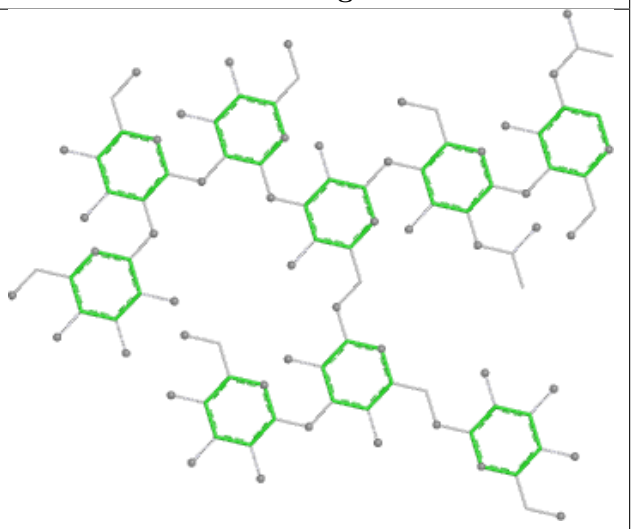
Bond lengths



Bond angles

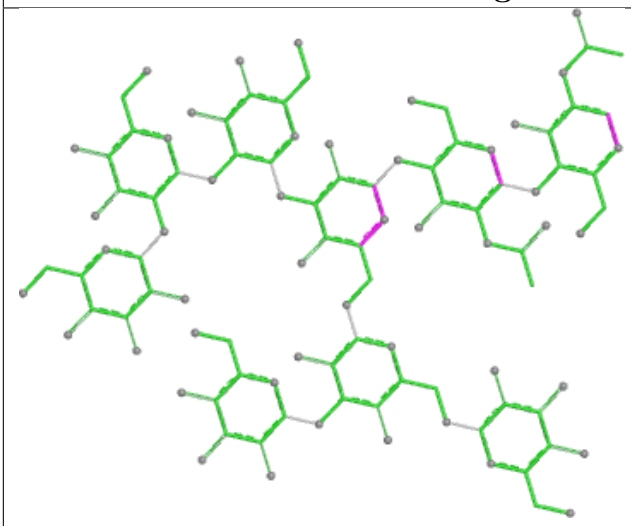


Torsions

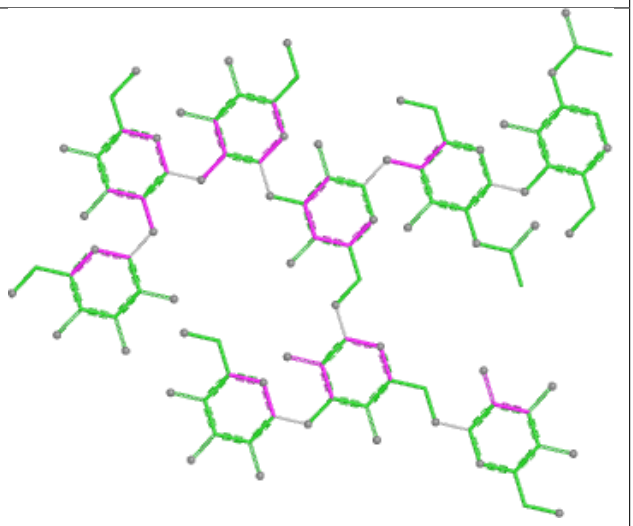


Rings

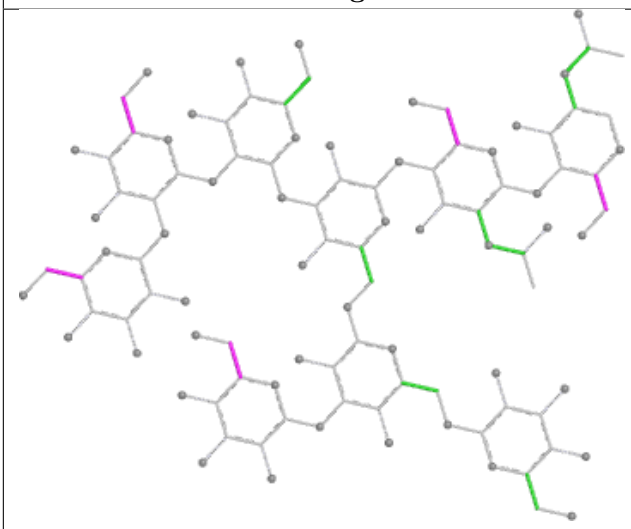
Oligosaccharide Chain U



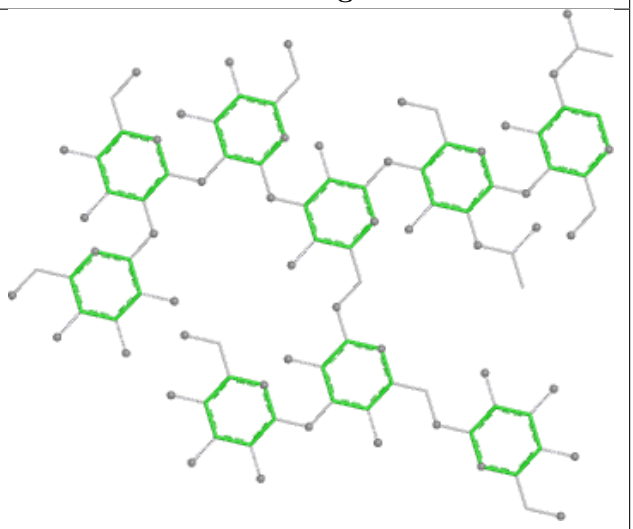
Bond lengths



Bond angles

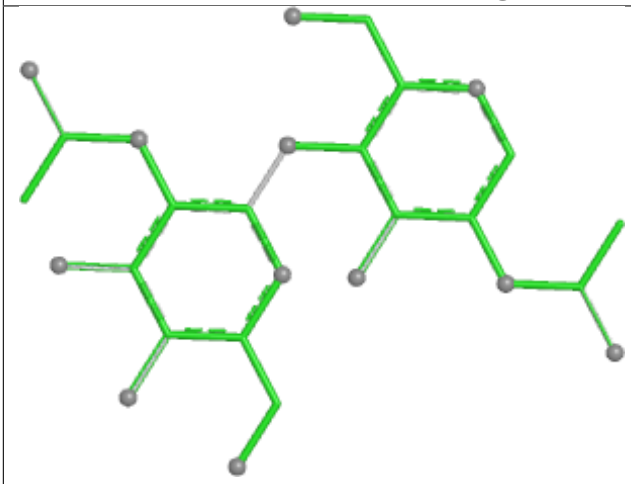


Torsions



Rings

Oligosaccharide Chain V



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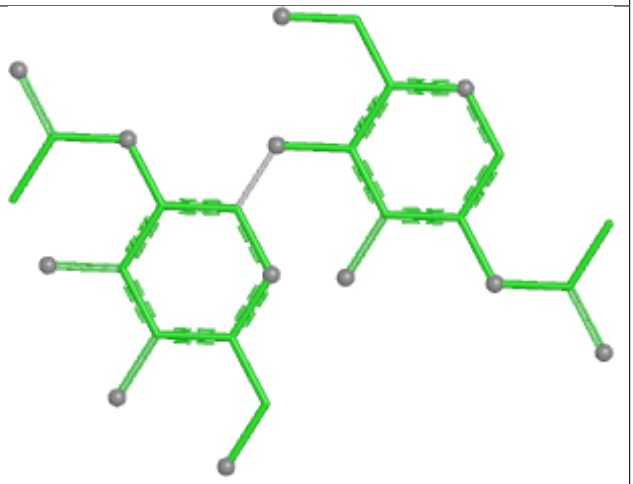
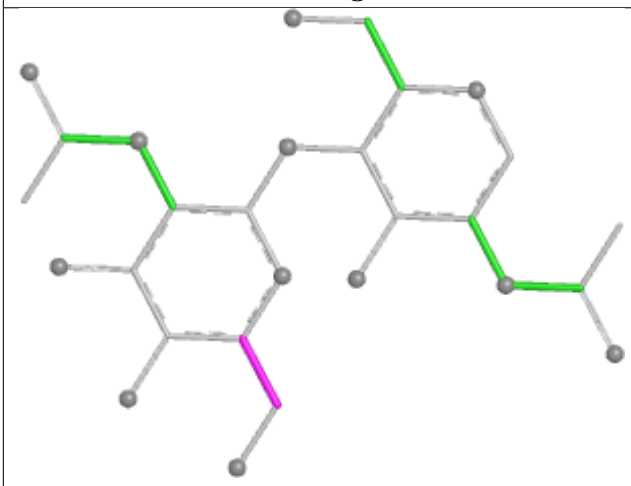


Bond angles



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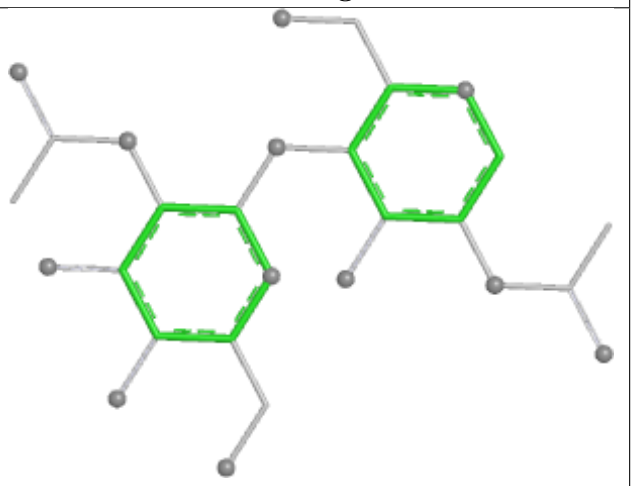
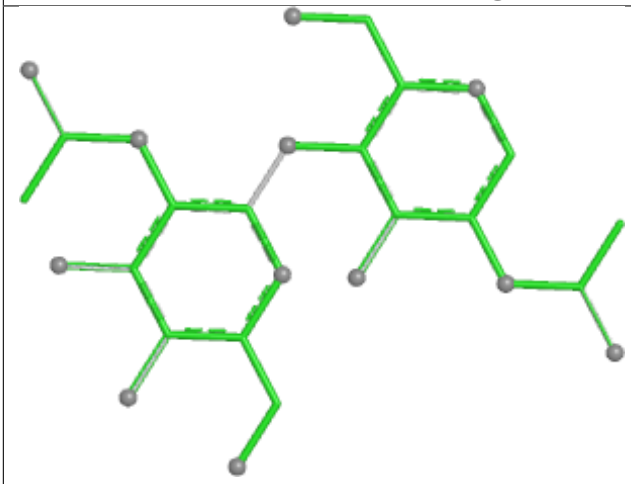


Rings

Oligosaccharide Chain W



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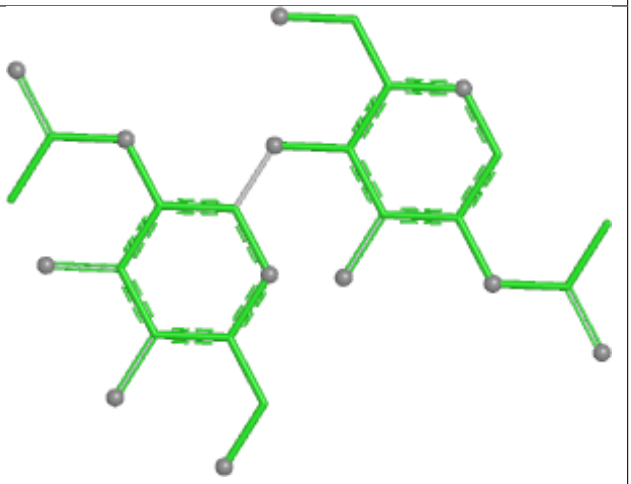
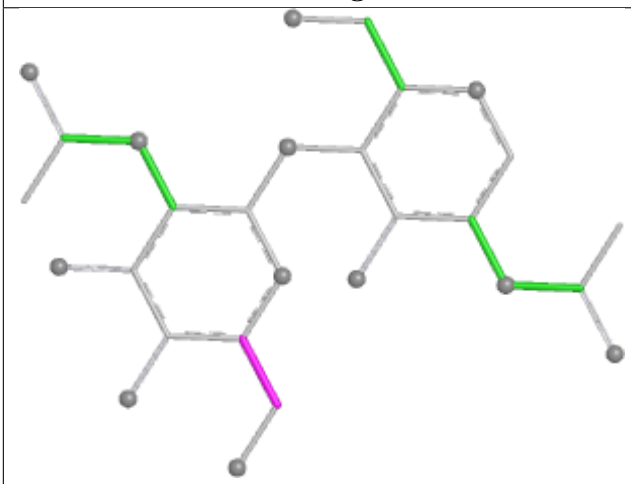


Bond angles



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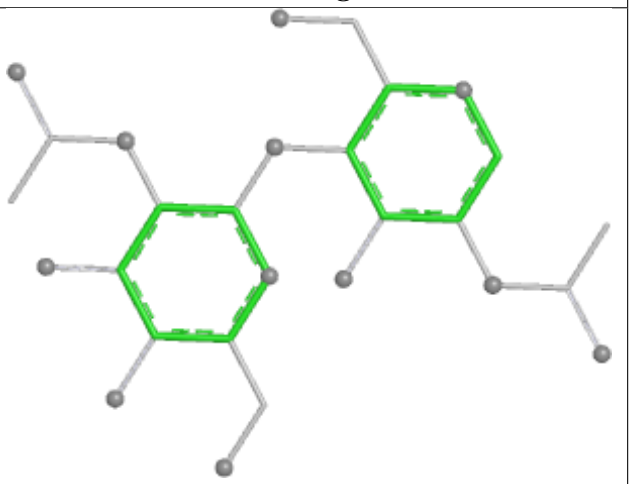
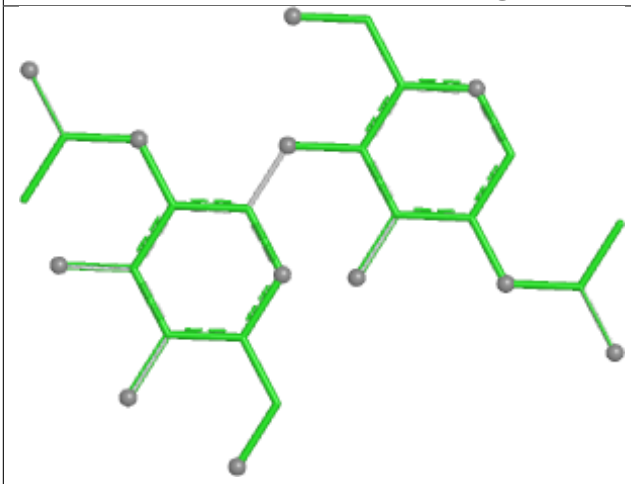


Rings

Oligosaccharide Chain Y



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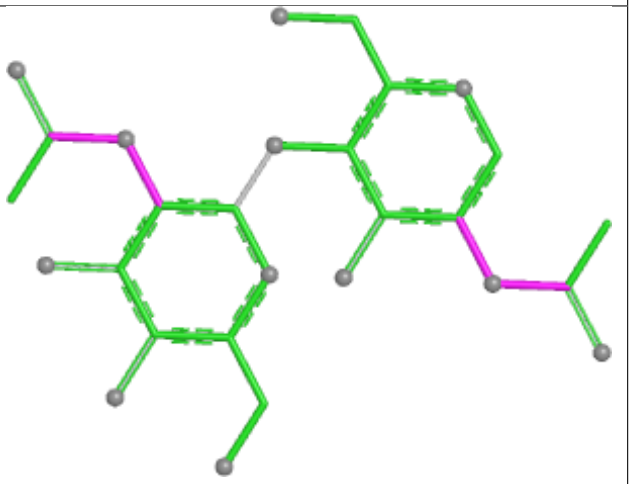
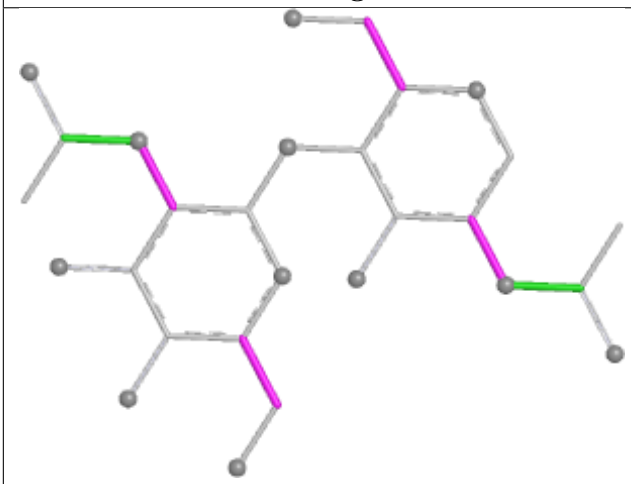


Bond angles



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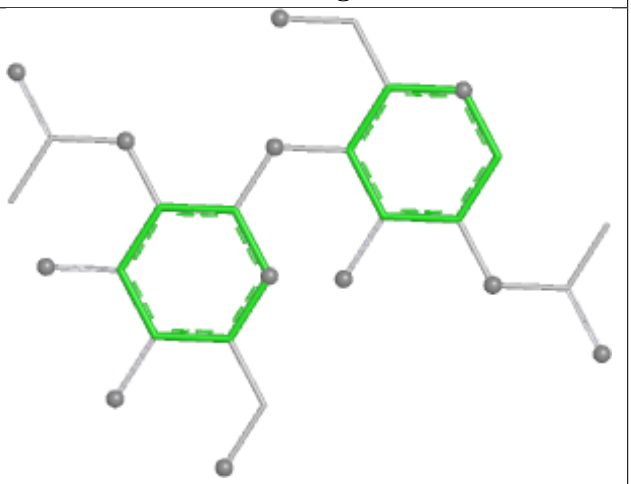
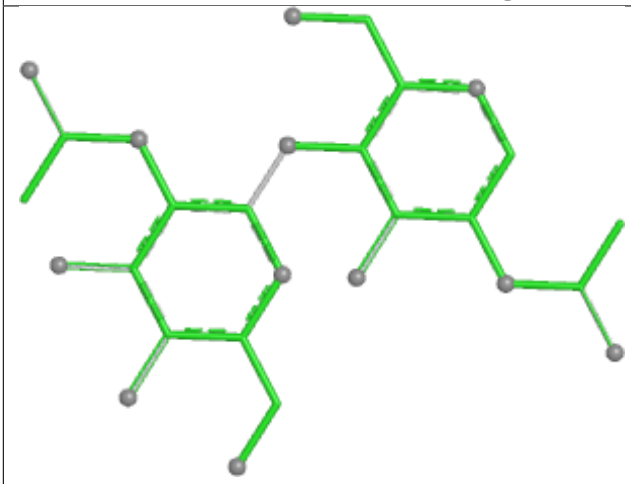


Rings

Oligosaccharide Chain a



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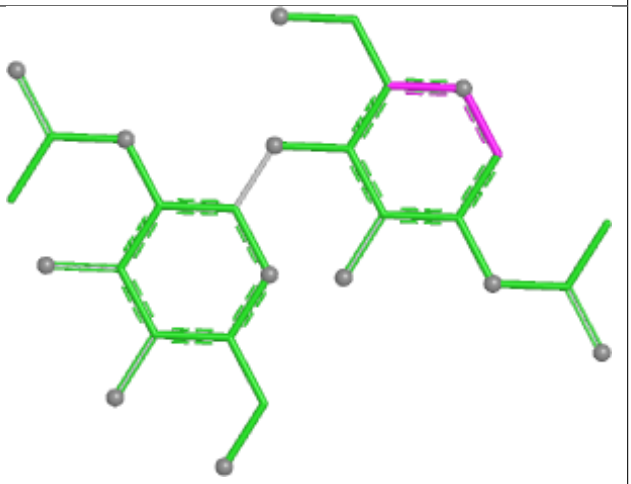
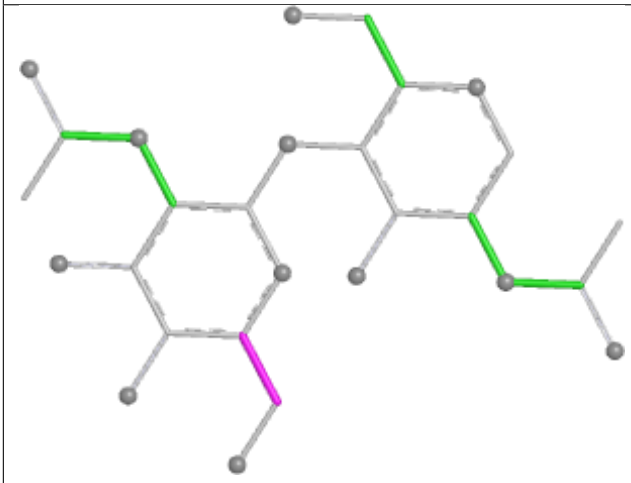


Bond angles



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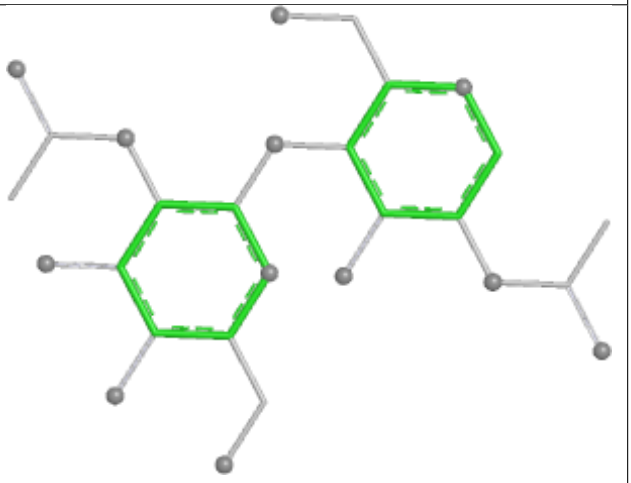
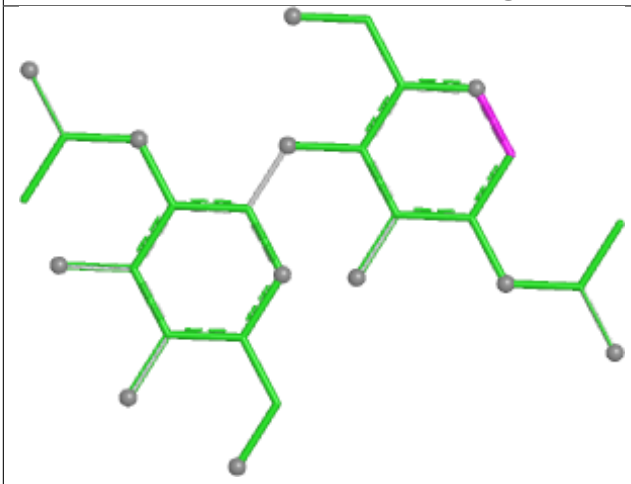


Rings

Oligosaccharide Chain c



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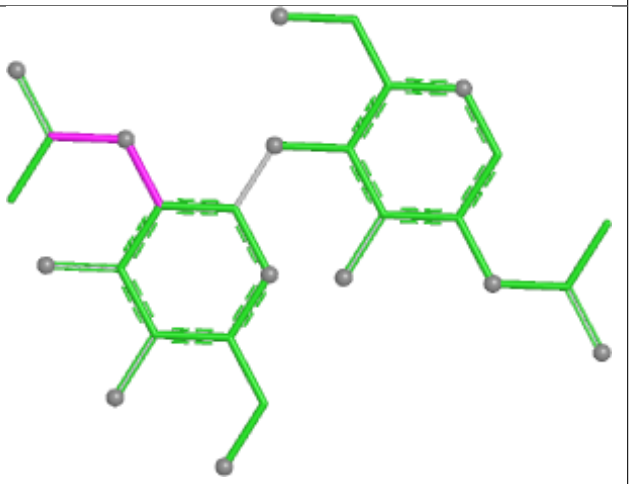
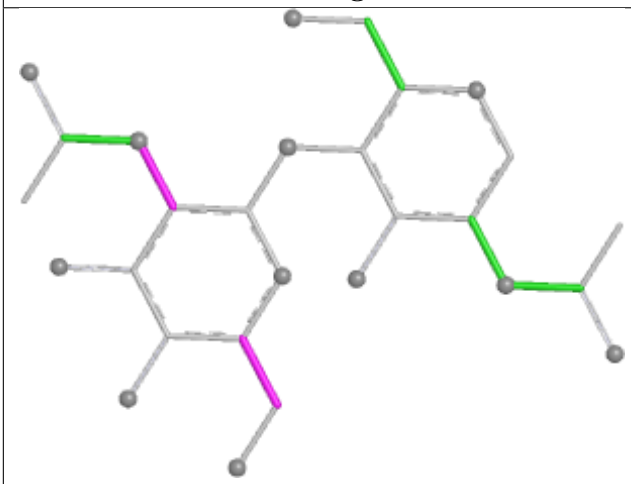


Bond angles



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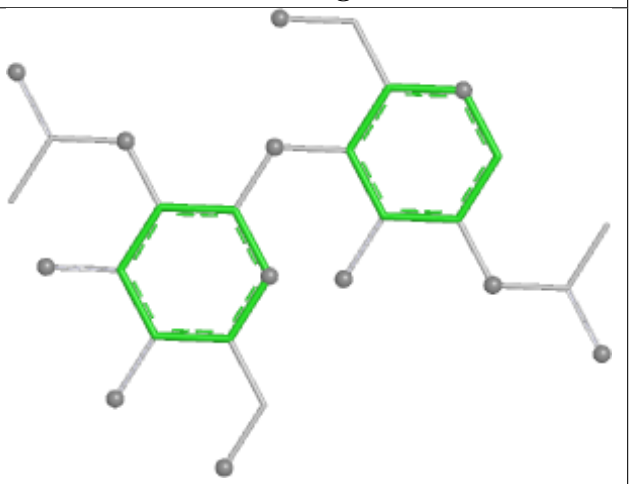
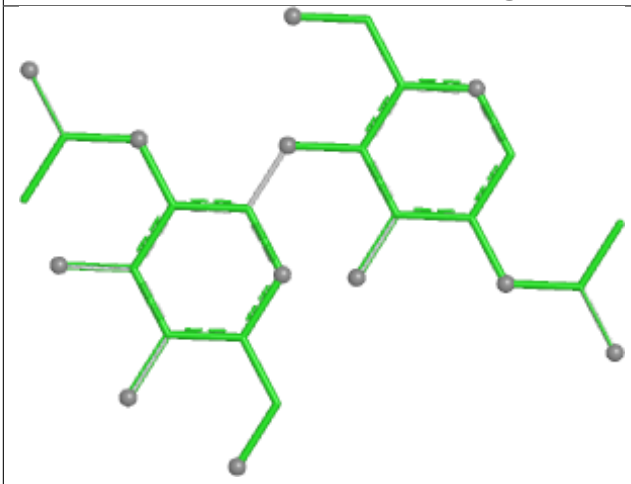


Rings

Oligosaccharide Chain f



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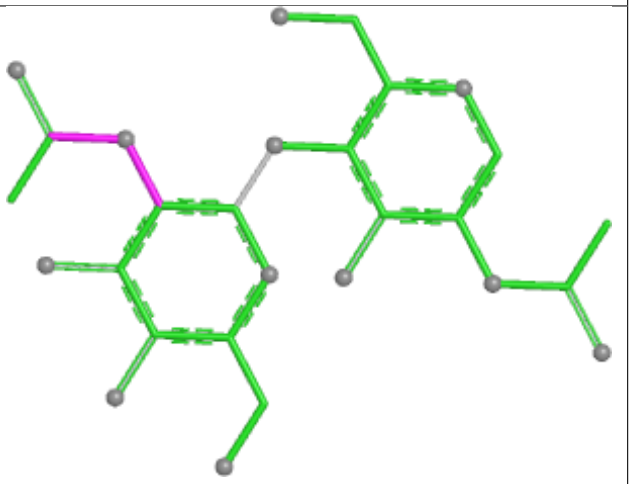
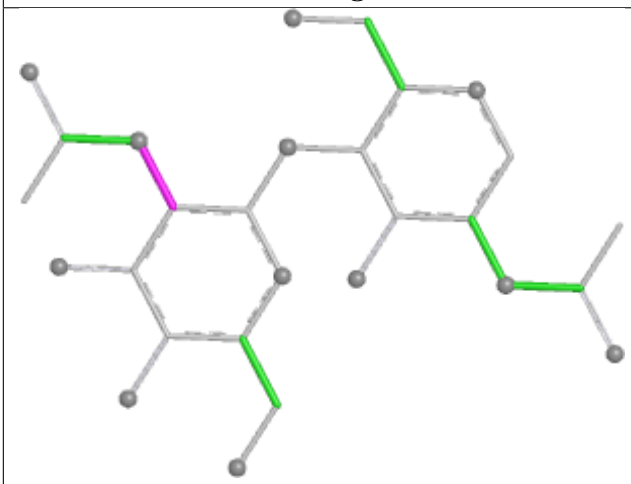


Bond angles



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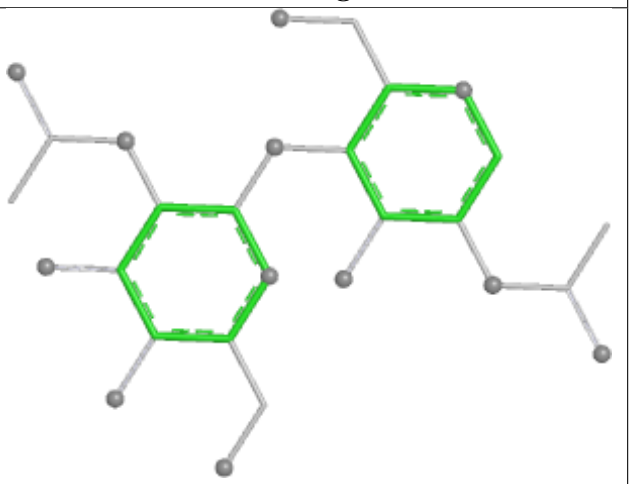
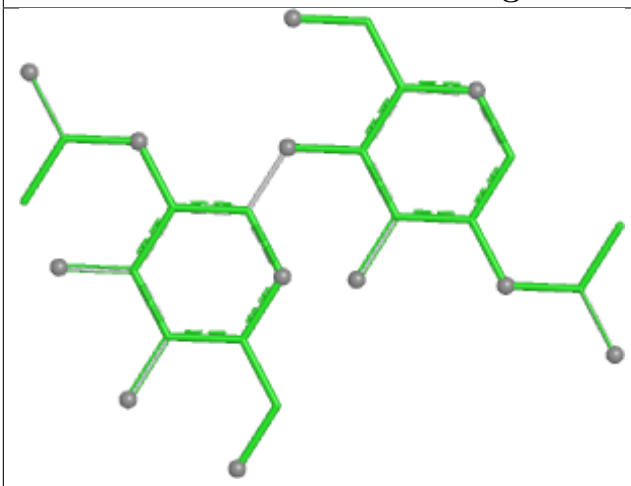


Rings

Oligosaccharide Chain j



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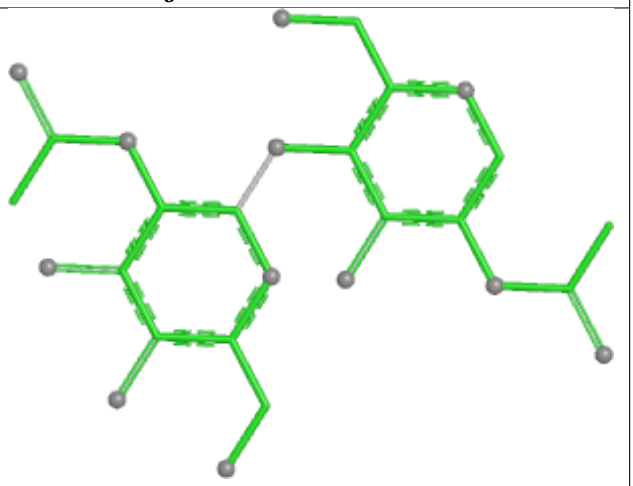
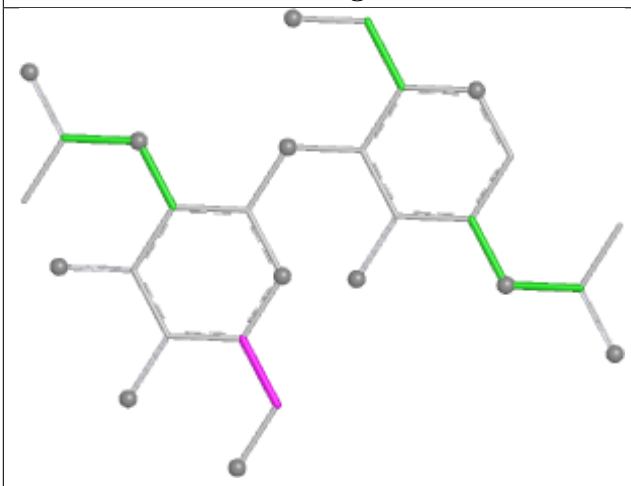


Bond angles



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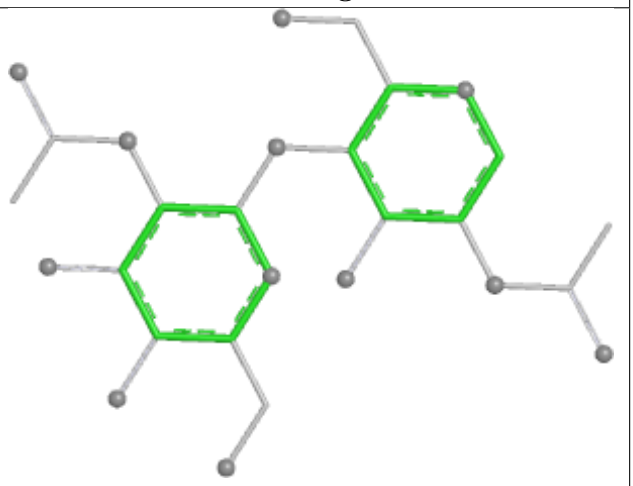
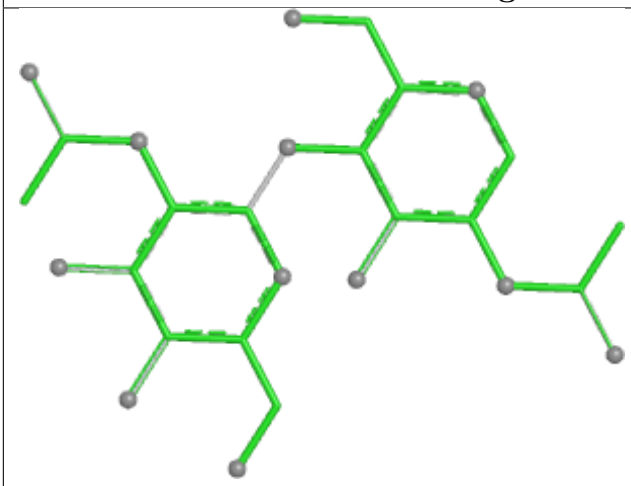


Rings

Oligosaccharide Chain k



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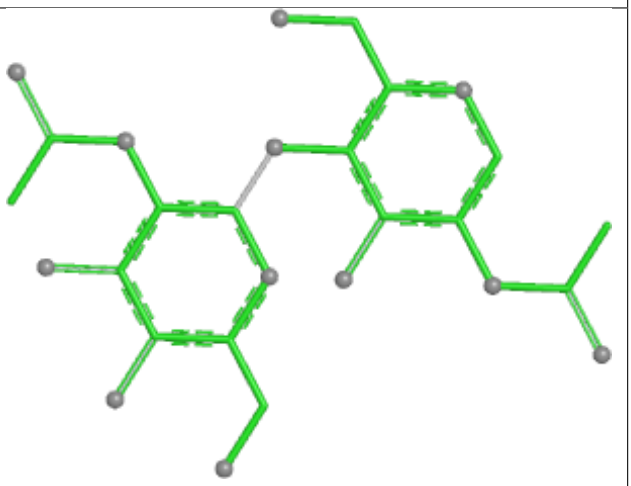
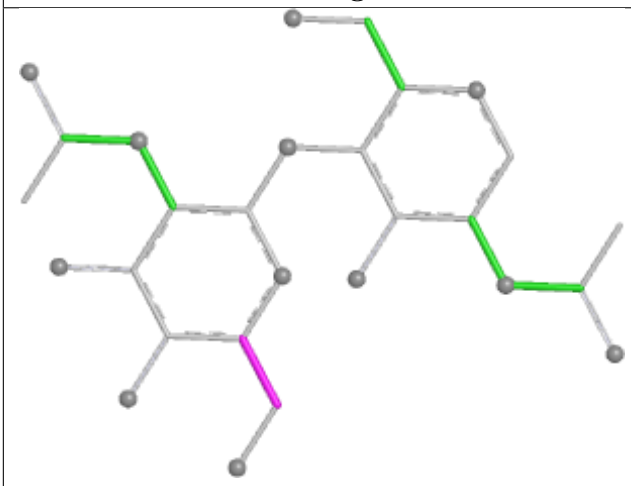


Bond angles



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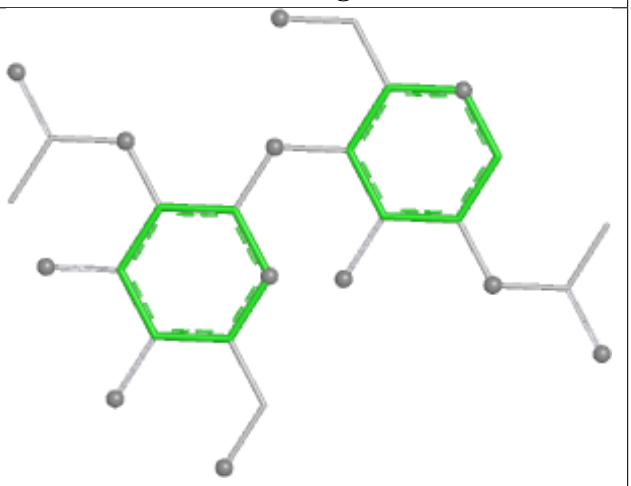
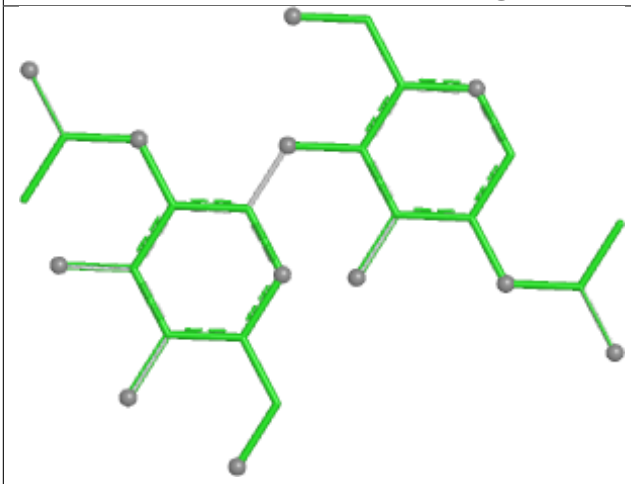


Rings

Oligosaccharide Chain m



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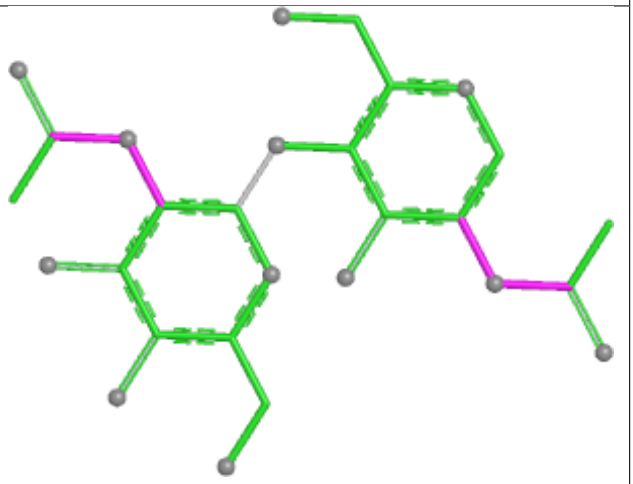
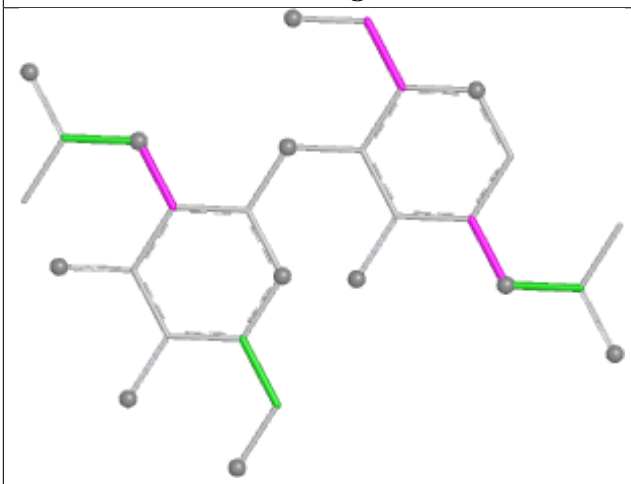


Bond angles



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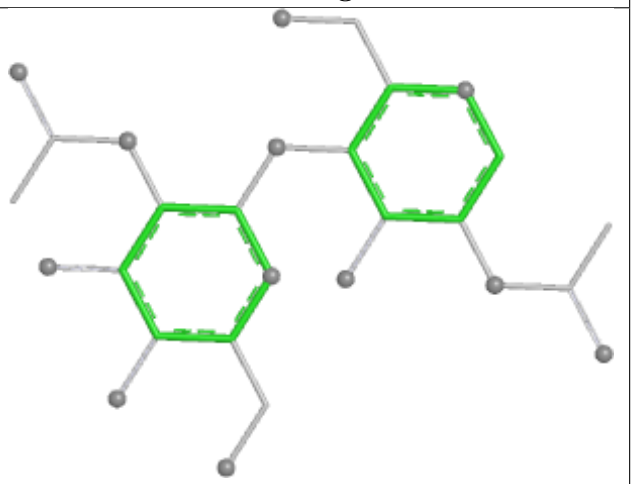
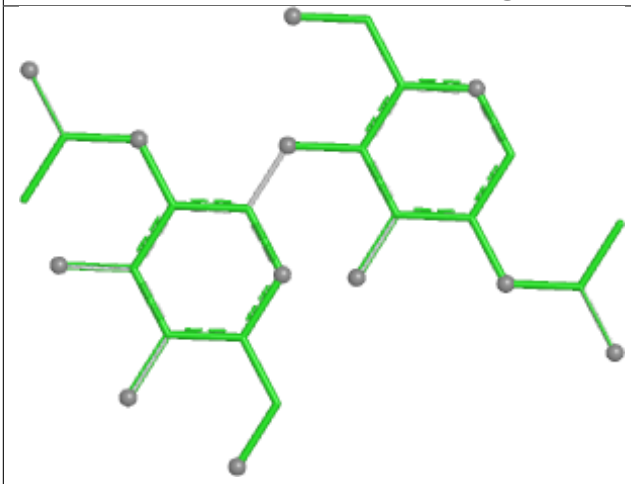


Rings

Oligosaccharide Chain o



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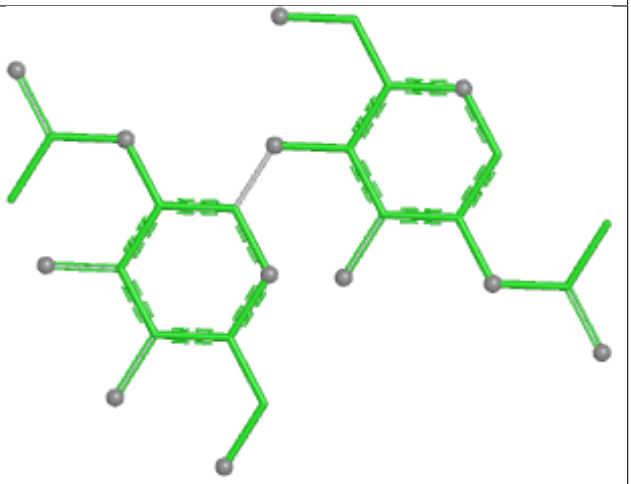
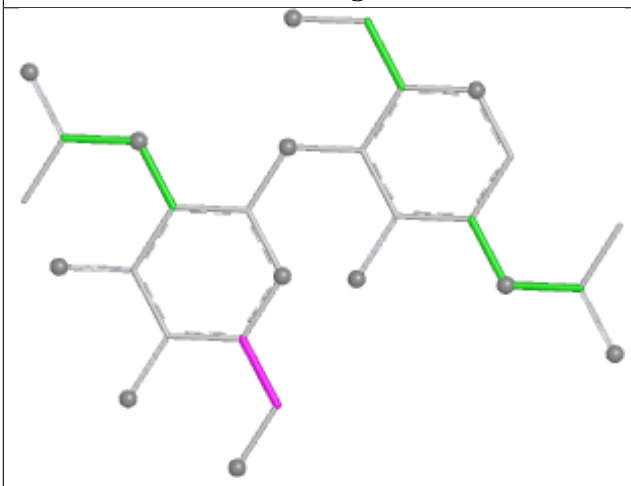


Bond angles



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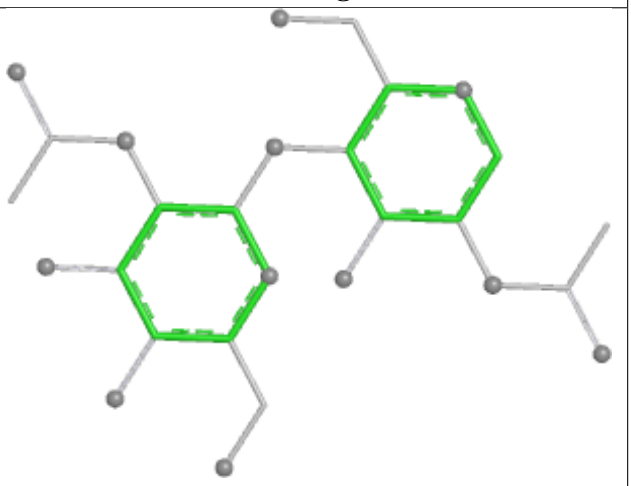
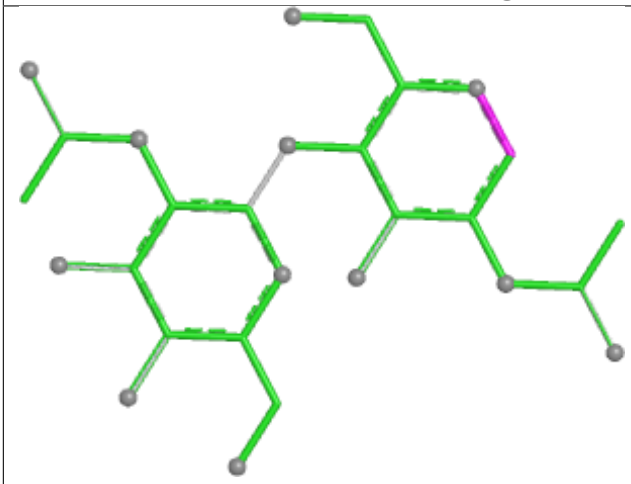


Rings

Oligosaccharide Chain q



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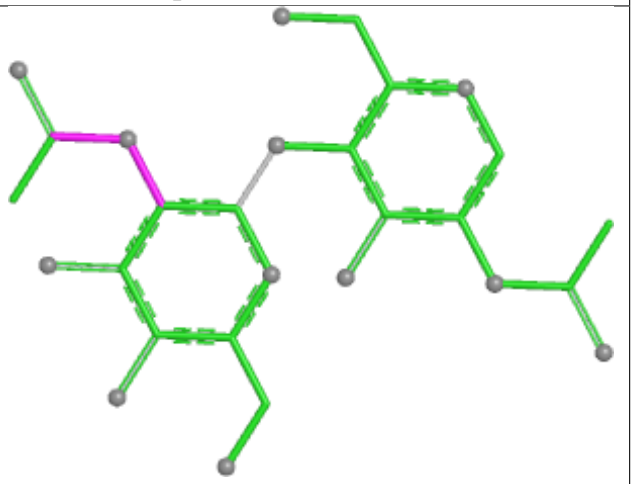
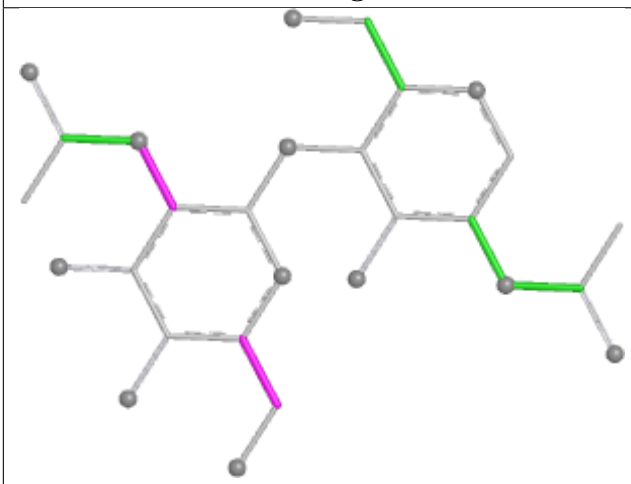


Bond angles



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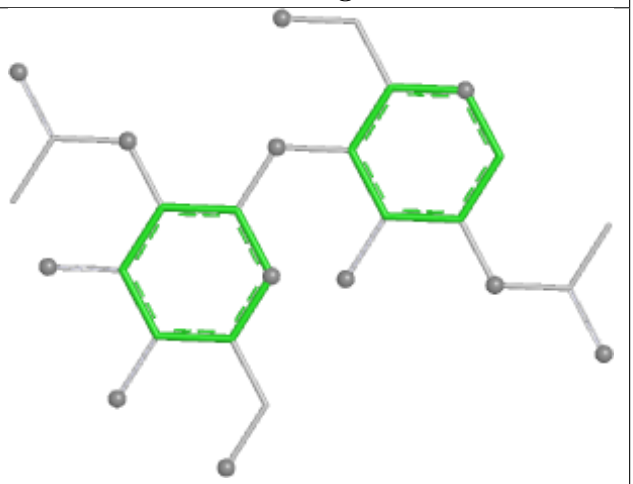
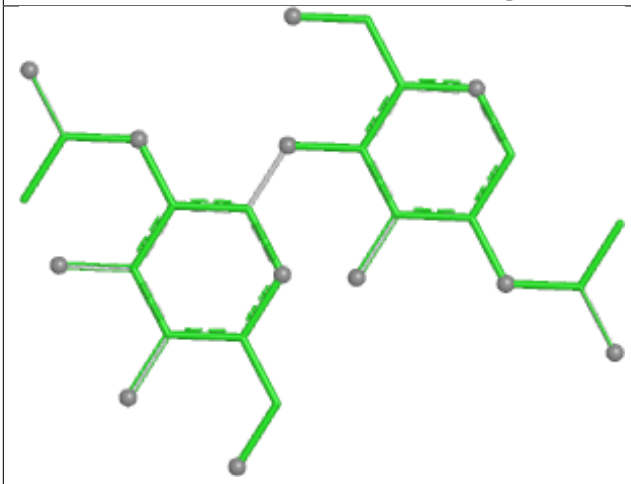


Rings

Oligosaccharide Chain t



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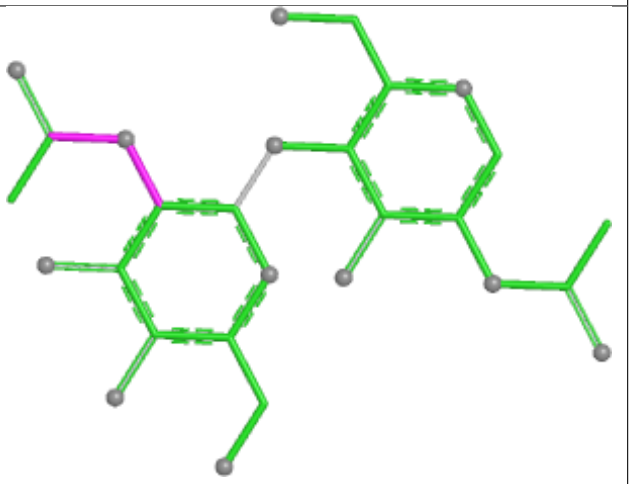
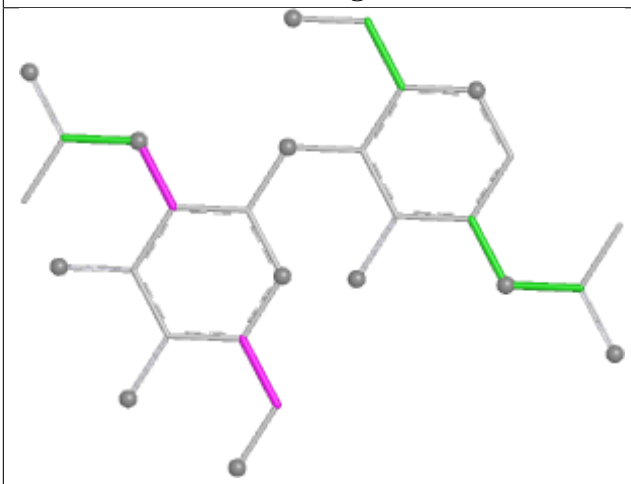


Bond angles



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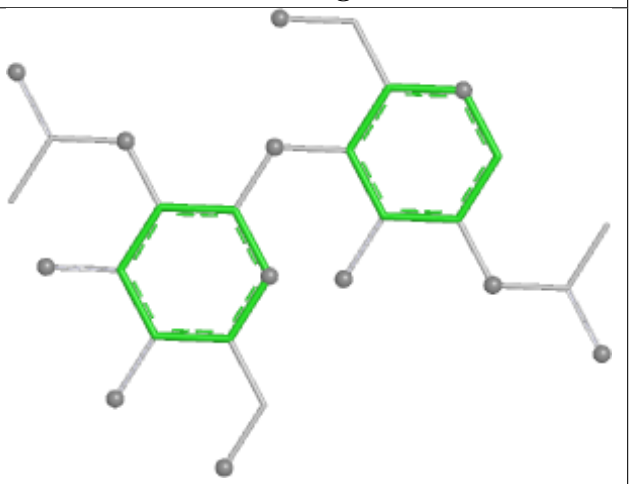
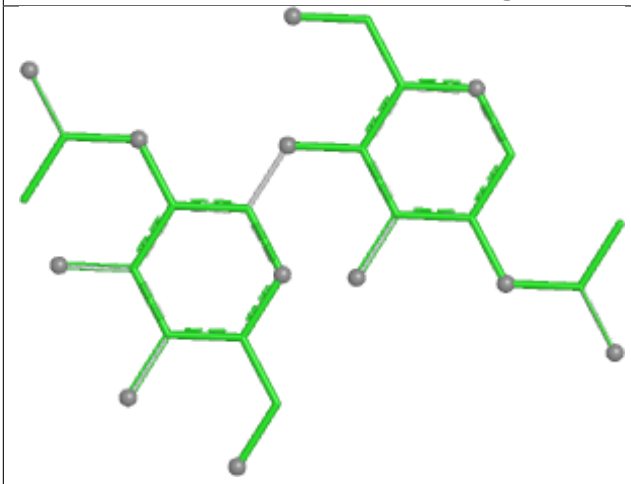


Rings

Oligosaccharide Chain x



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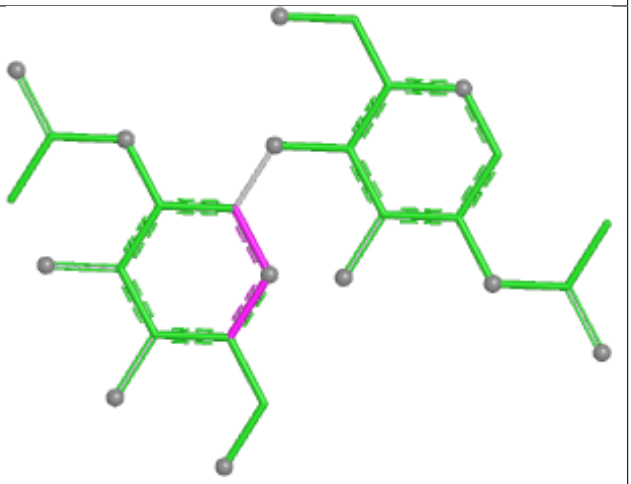
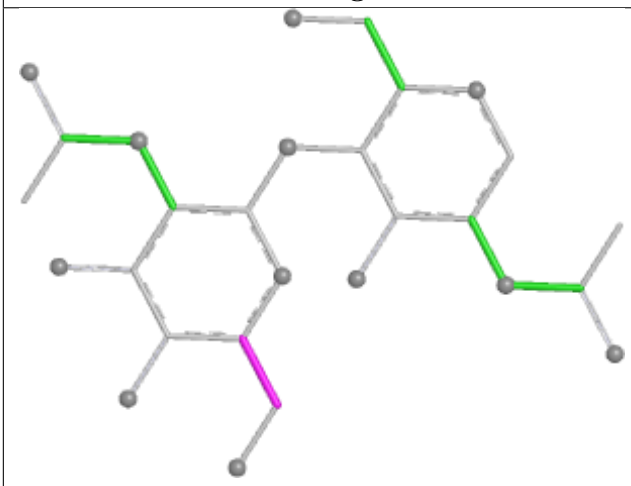


Bond angles



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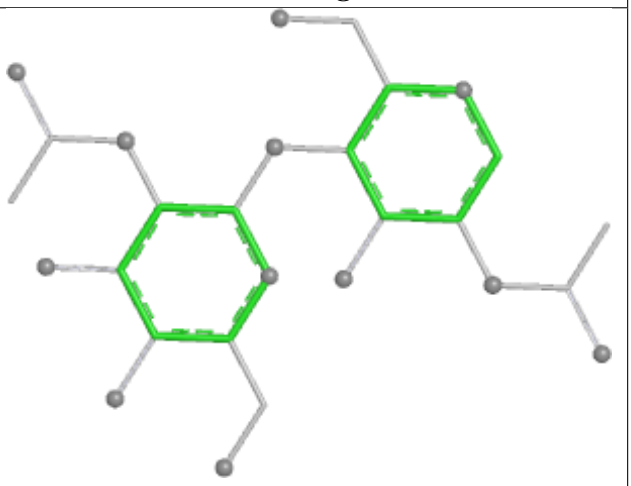
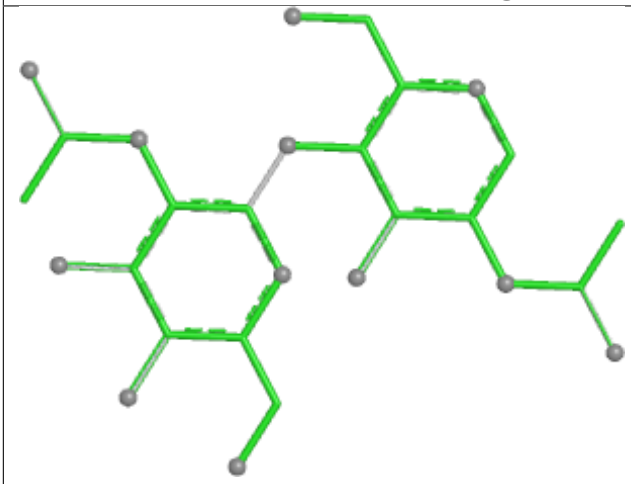


Rings

Oligosaccharide Chain y



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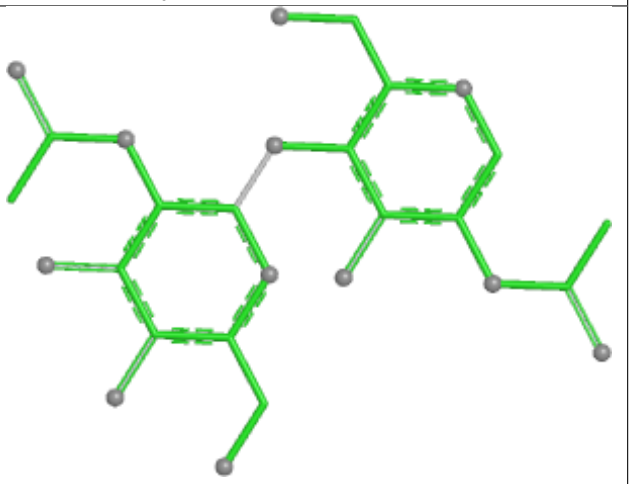
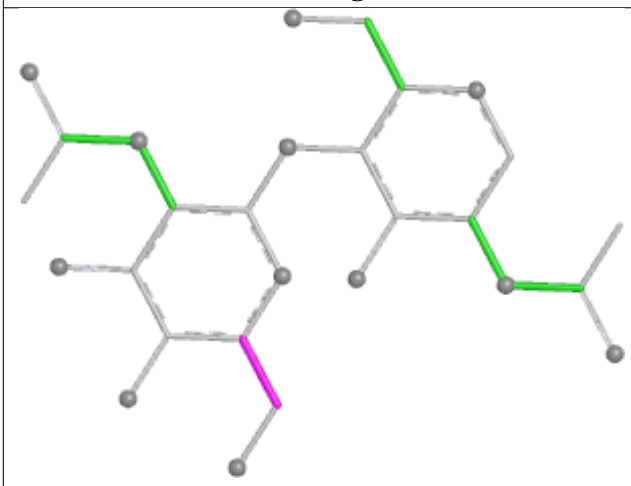
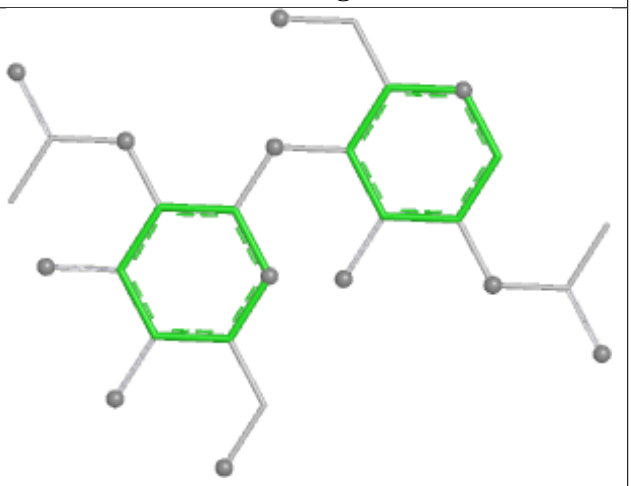


Bond angles

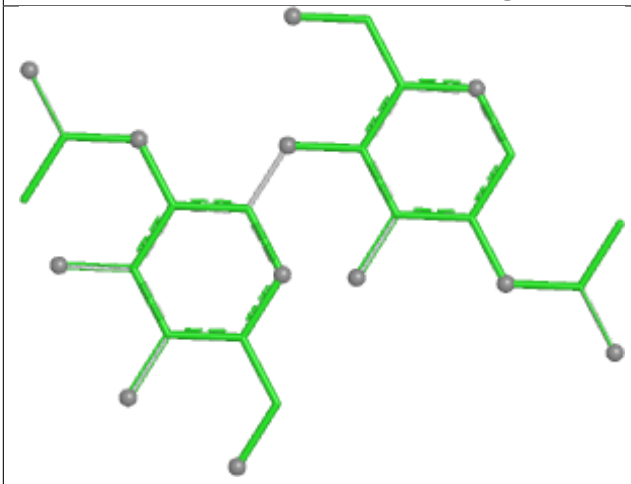


Torsions

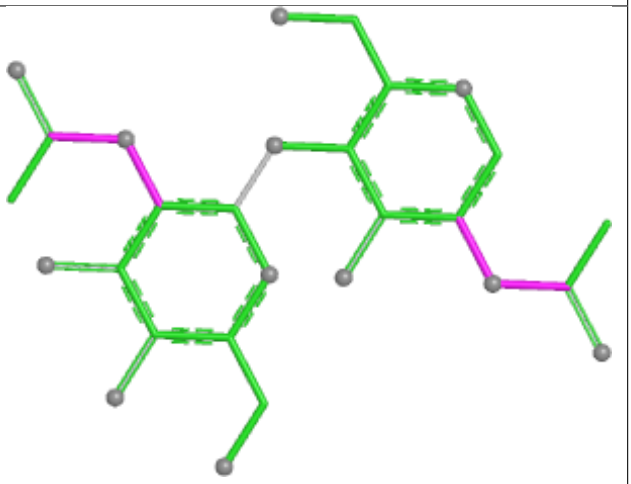


Rings

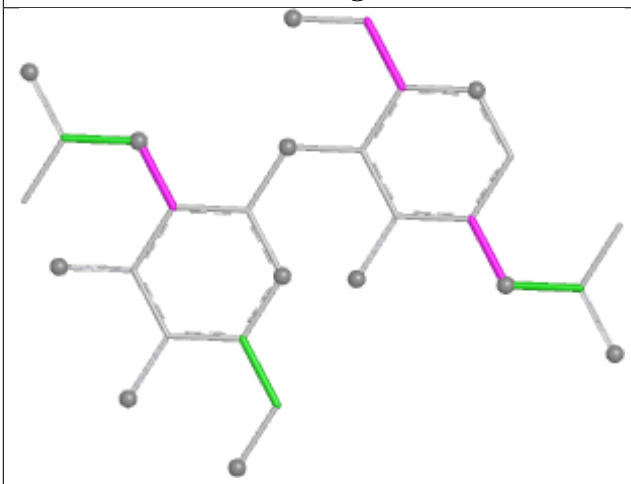
Oligosaccharide Chain 0



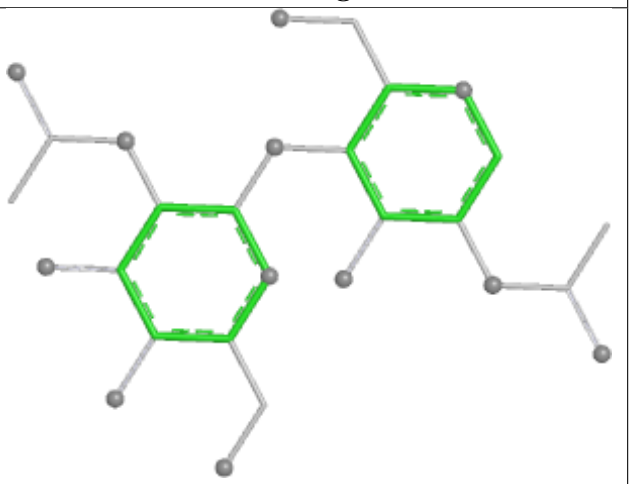
Bond lengths



Bond angles

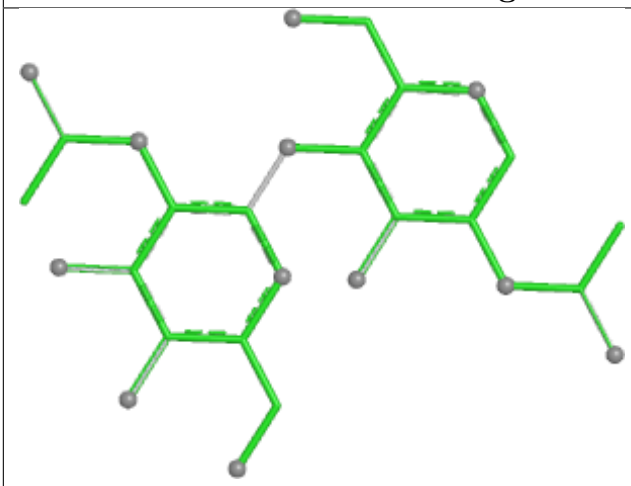


Torsions



Rings

Oligosaccharide Chain 2



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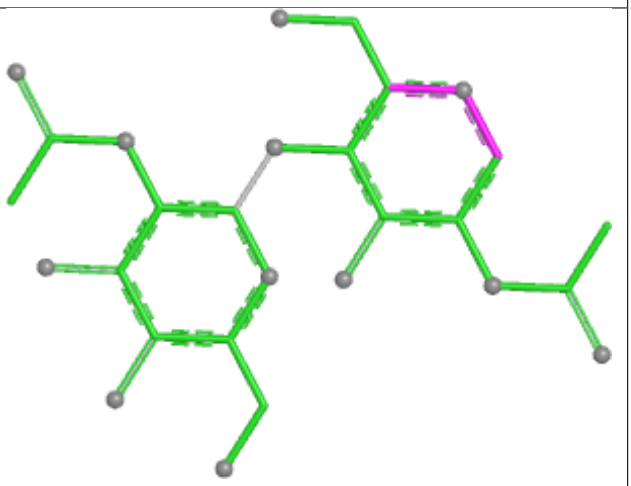
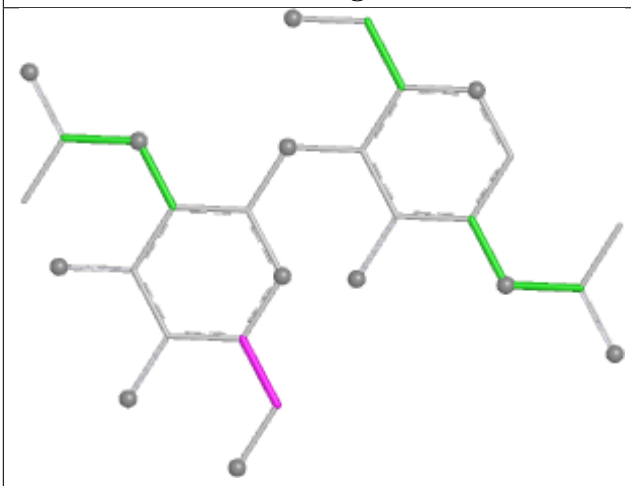


Bond angles



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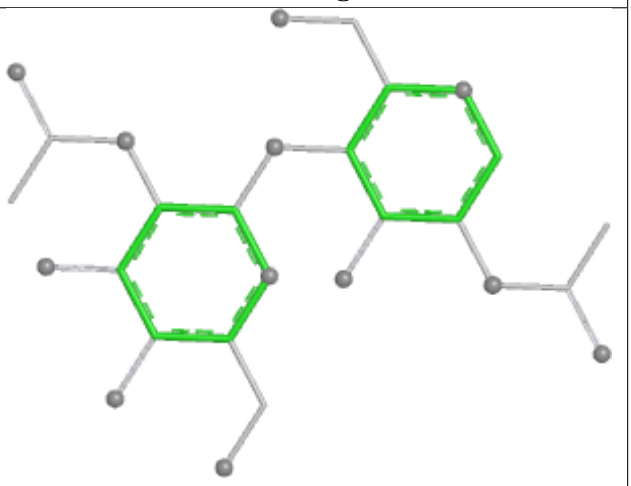
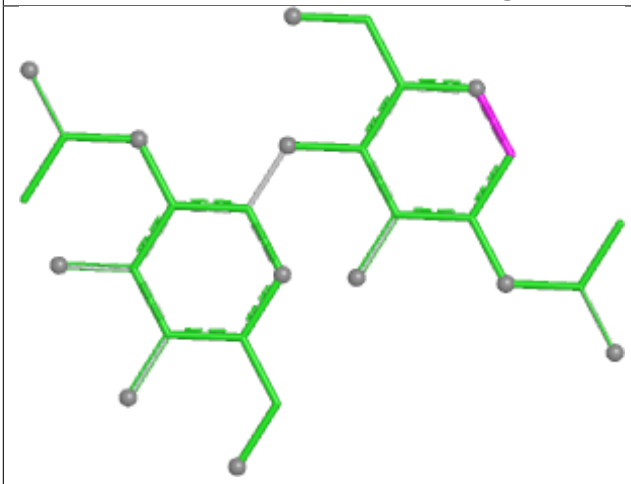


Rings

Oligosaccharide Chain 4



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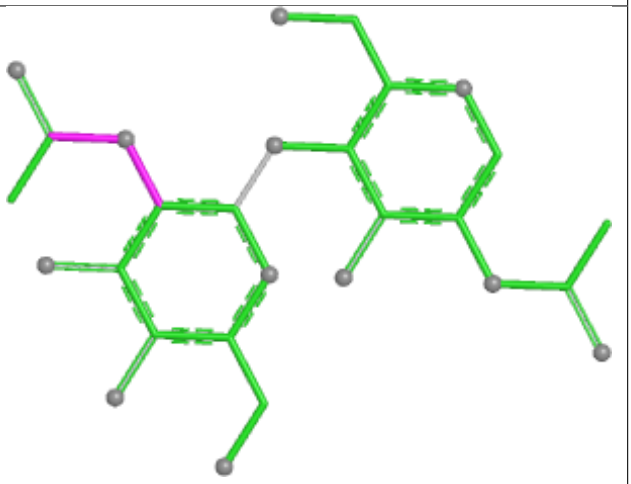
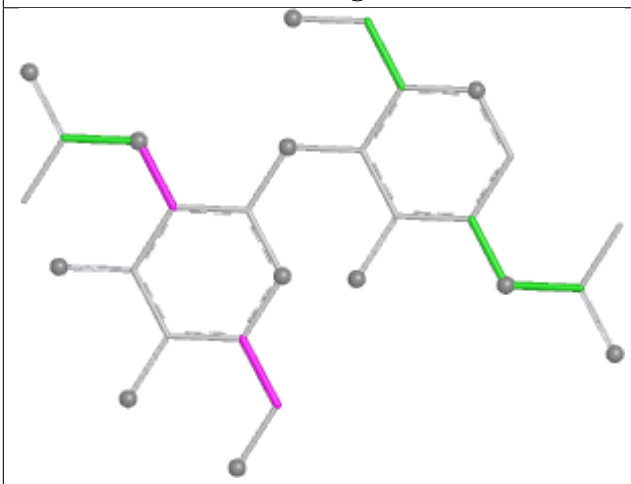


Bond angles



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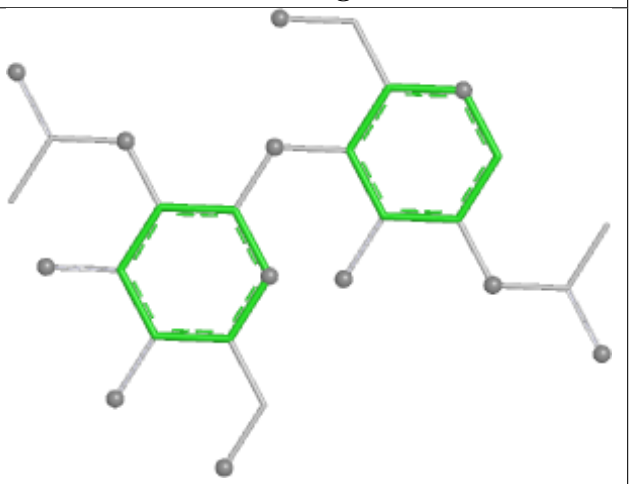
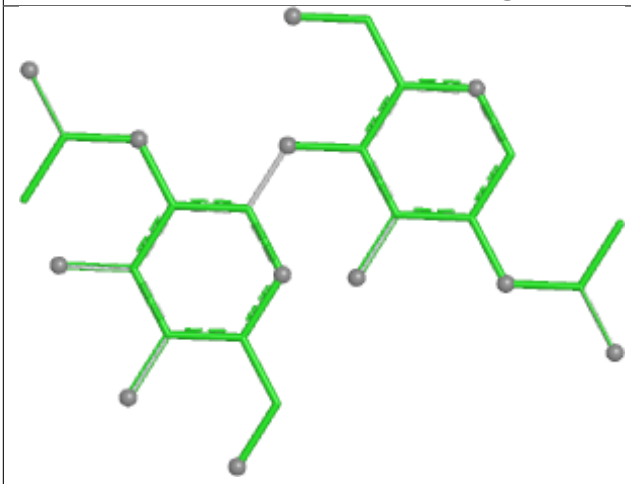


Rings

Oligosaccharide Chain 7



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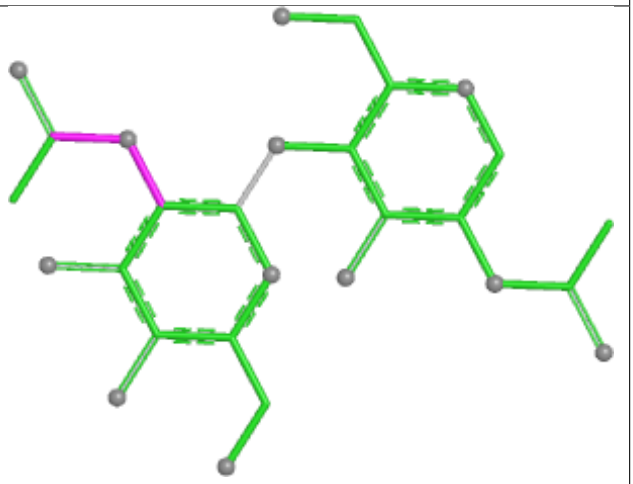
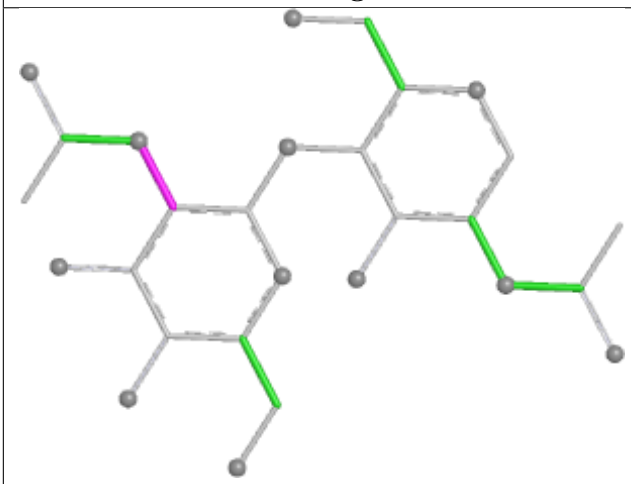


Bond angles



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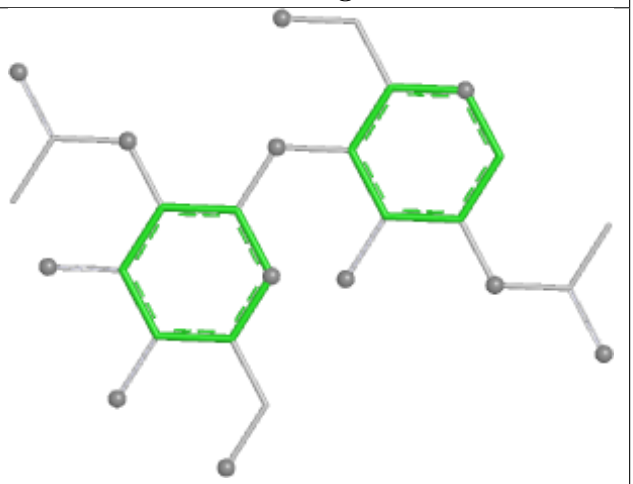
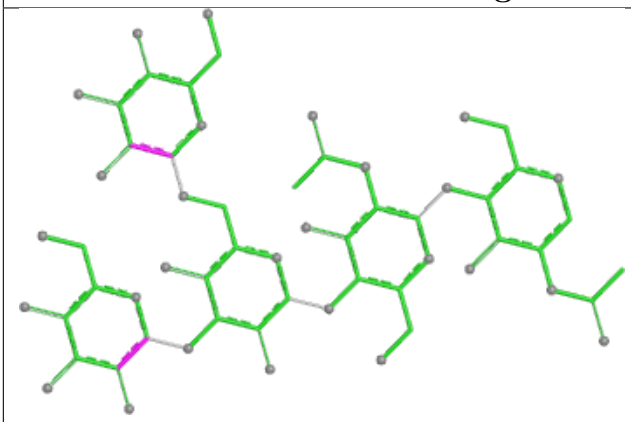


Rings

Oligosaccharide Chain X



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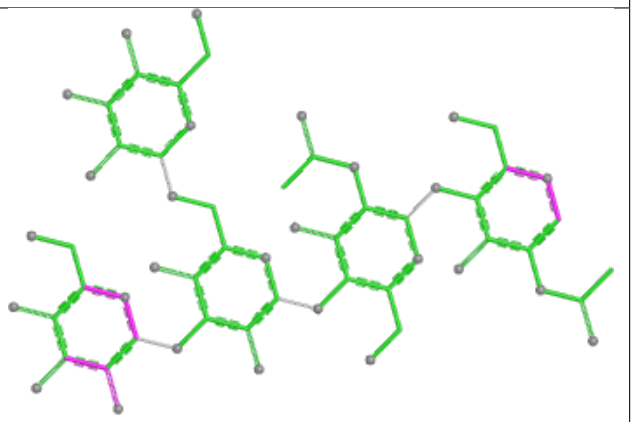
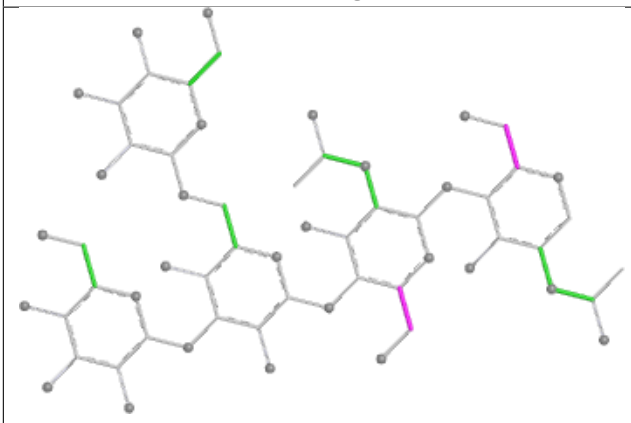


Bond angles



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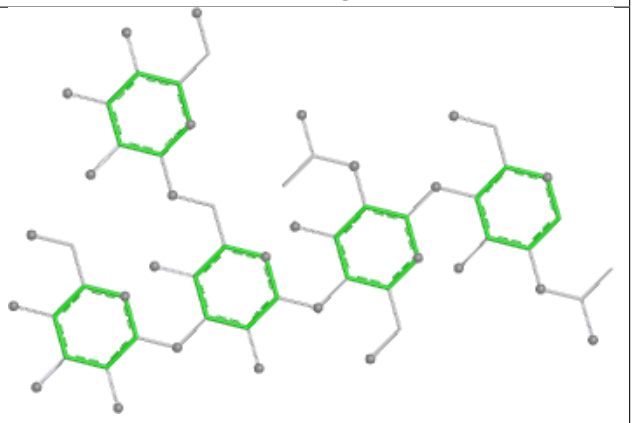
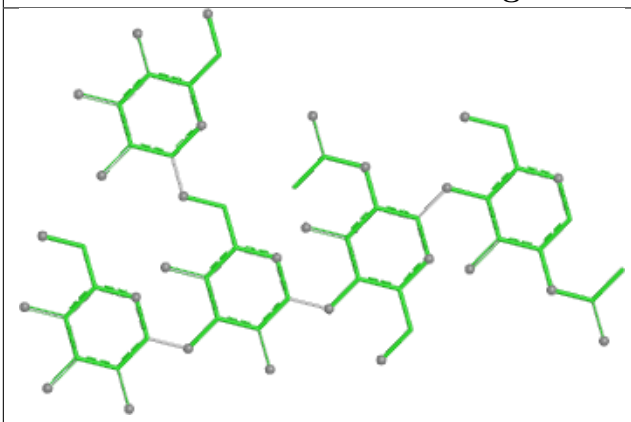


Rings

Oligosaccharide Chain i



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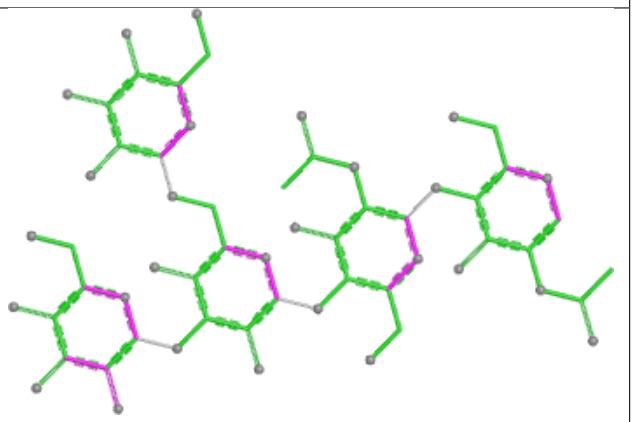
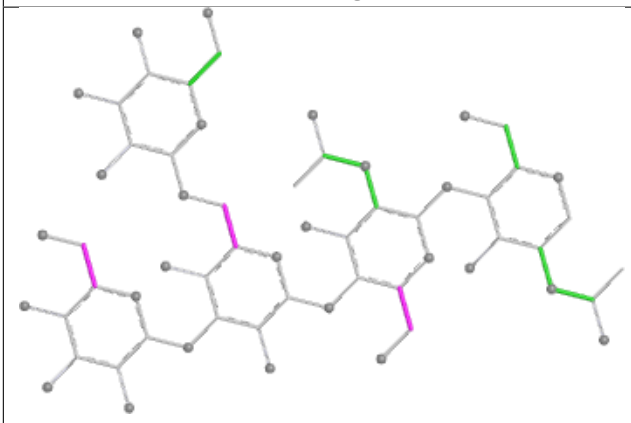


Bond angles



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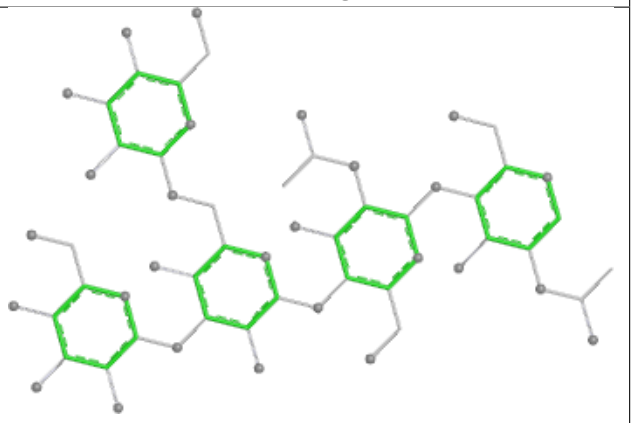
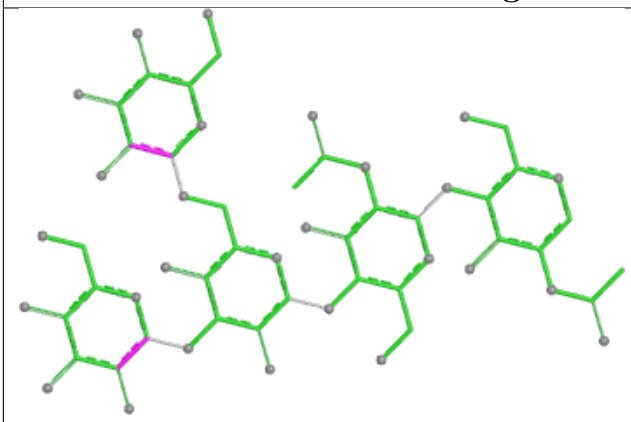


Rings

Oligosaccharide Chain l



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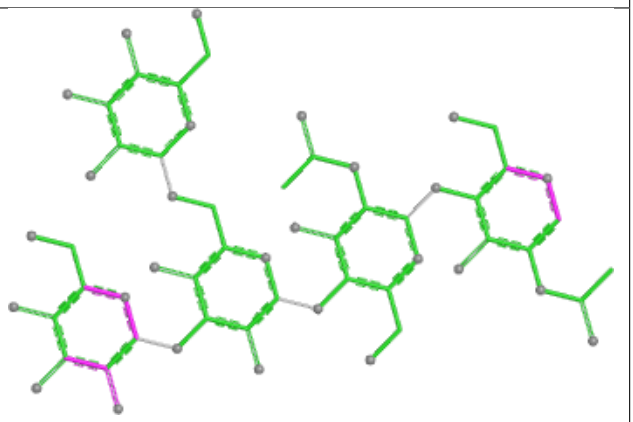
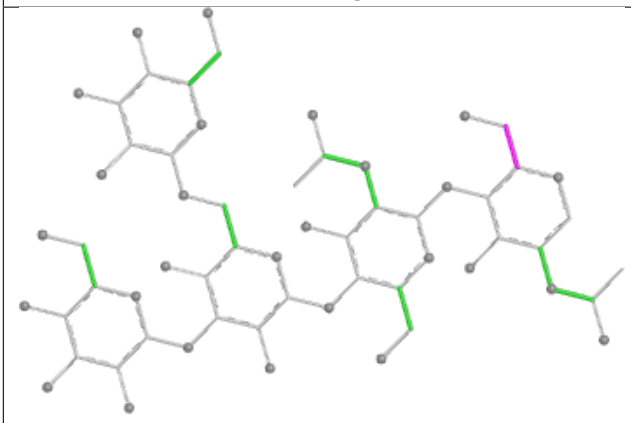


Bond angles



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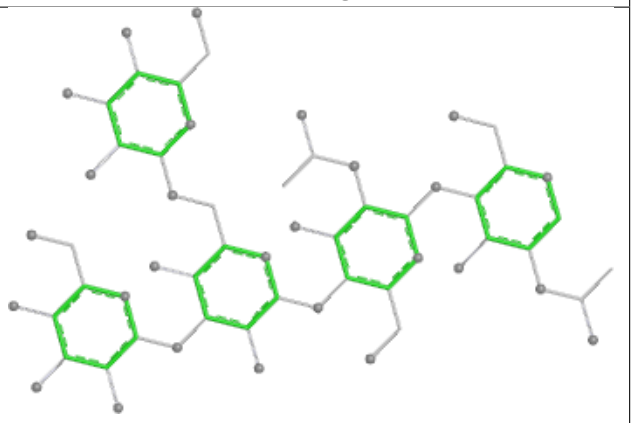
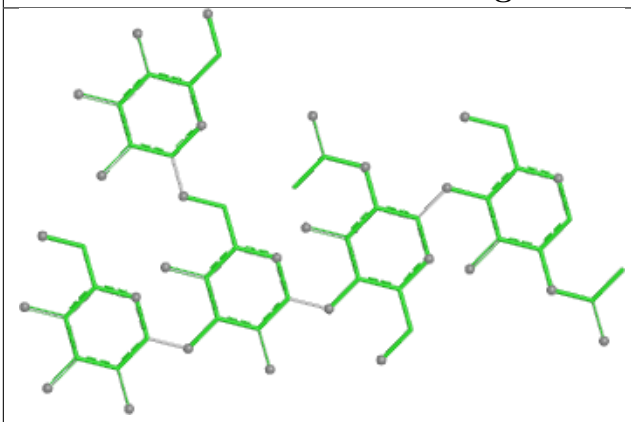


Rings

Oligosaccharide Chain w



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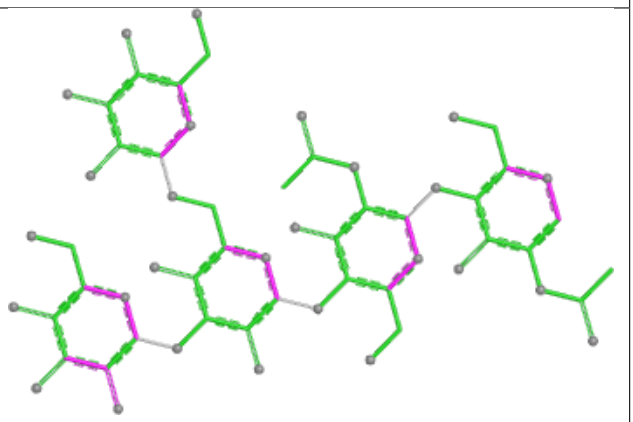
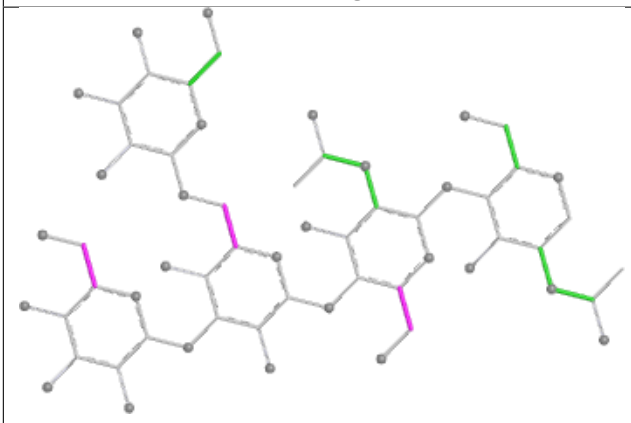


Bond angles



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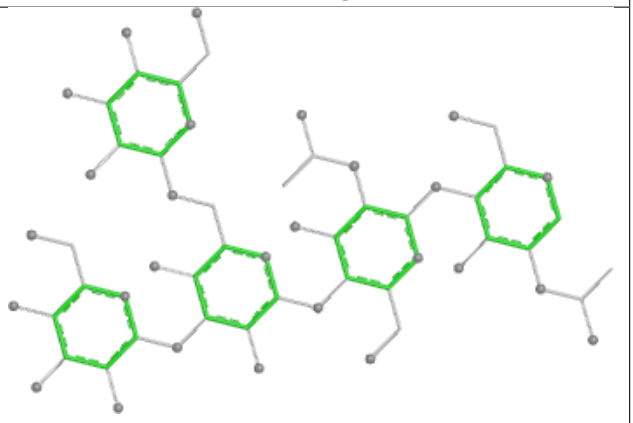
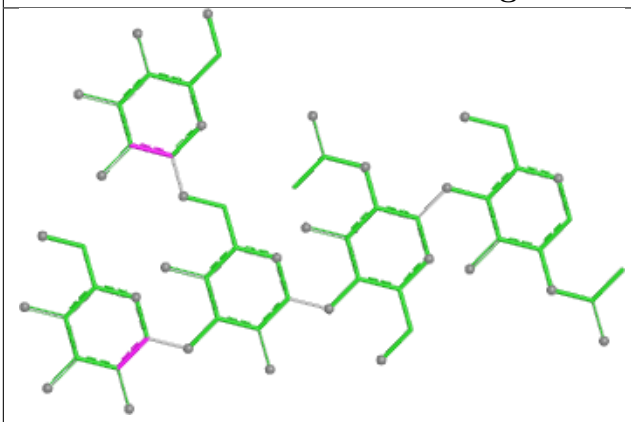


Rings

Oligosaccharide Chain z



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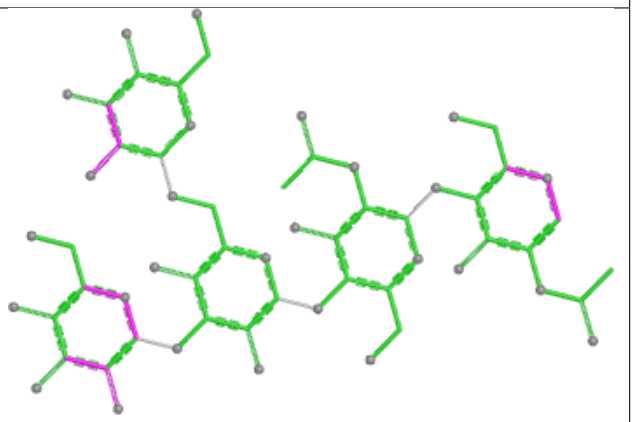
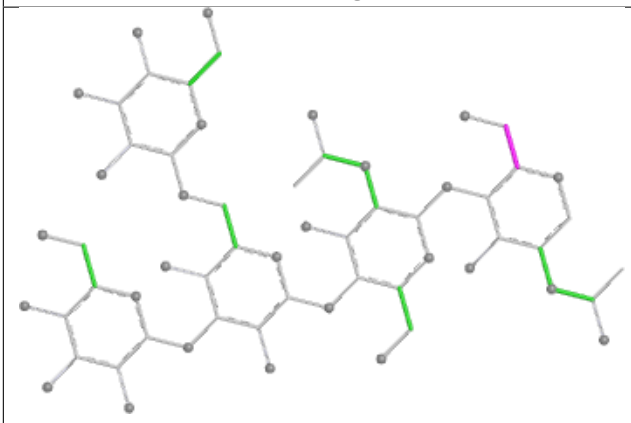
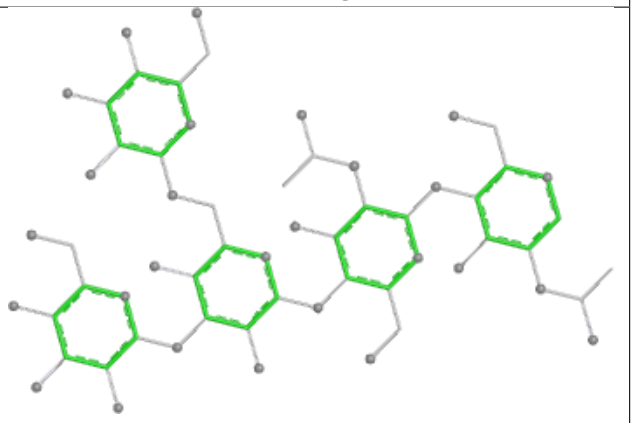


Bond angles

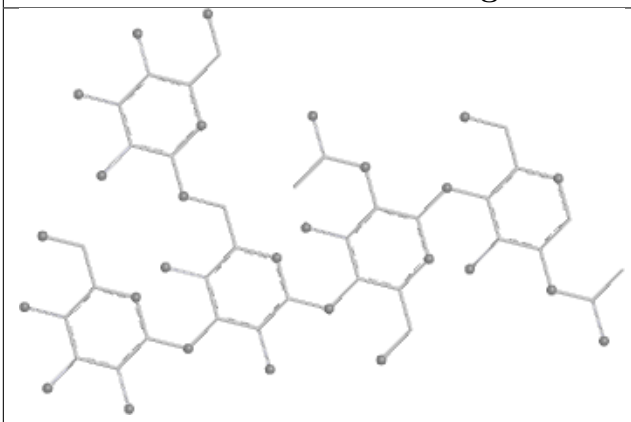


Torsions



Rings

Oligosaccharide Chain AA



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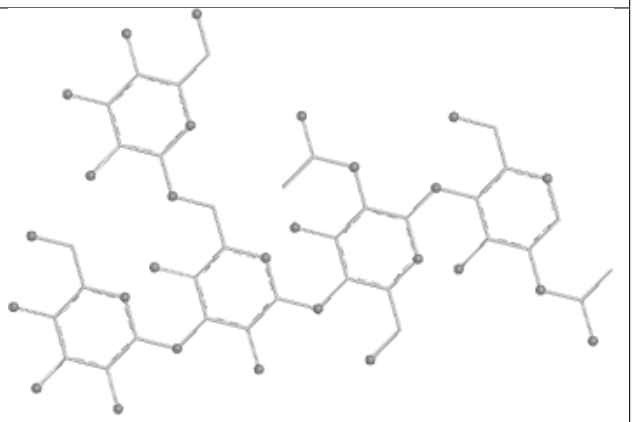
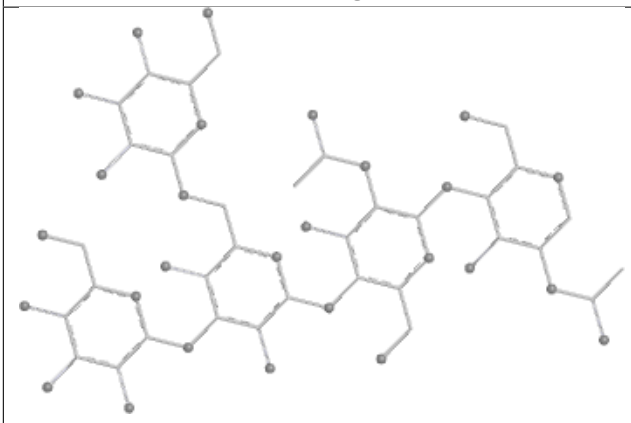
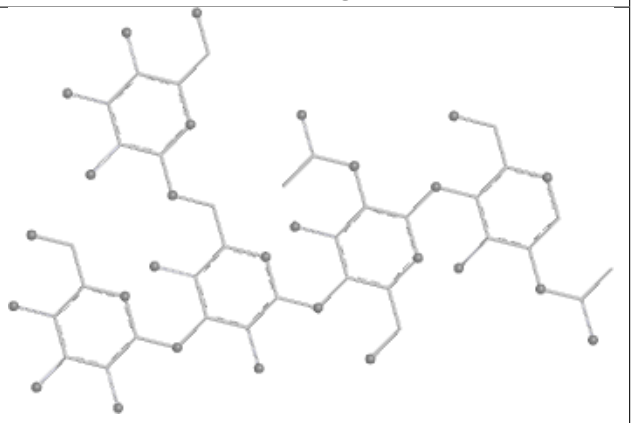


Bond angles

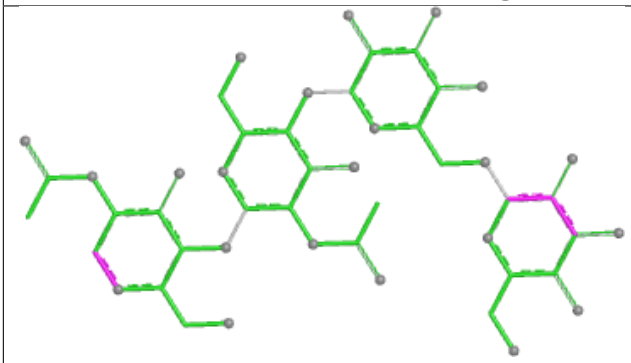


Torsions



Rings

Oligosaccharide Chain Z



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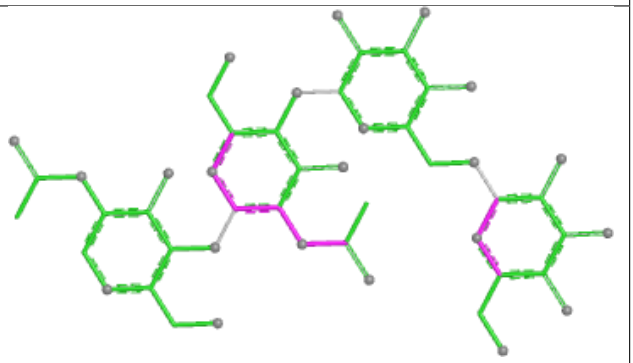
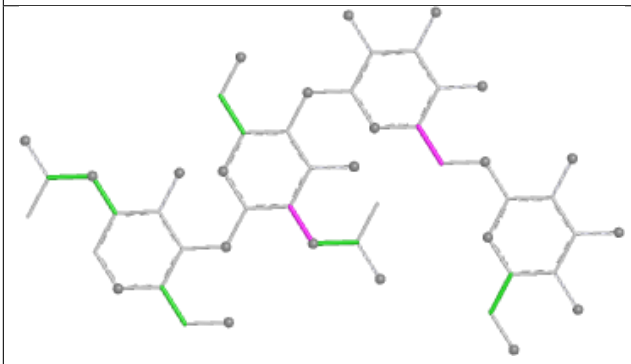


Bond angles



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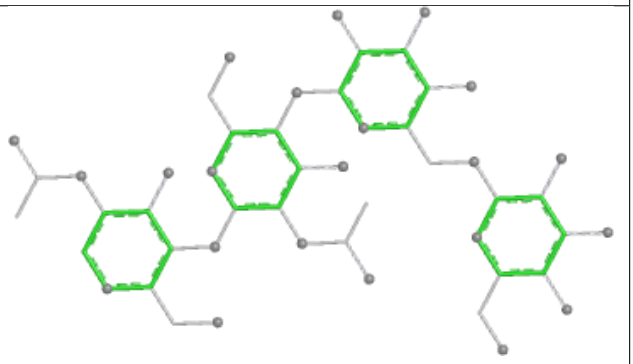
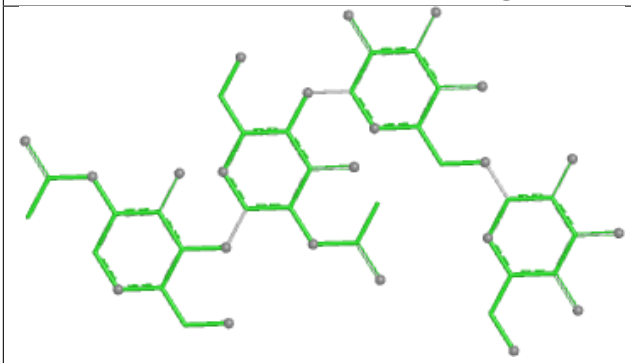


Rings

Oligosaccharide Chain d



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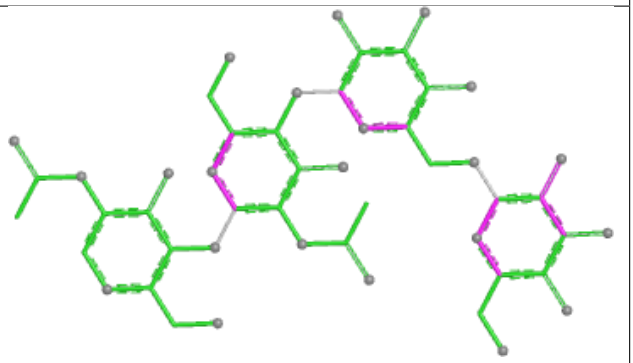
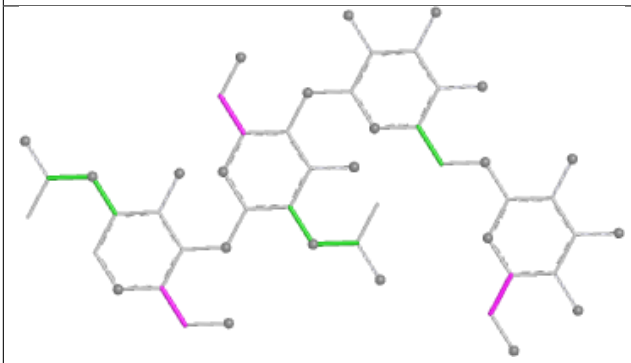


Bond angles



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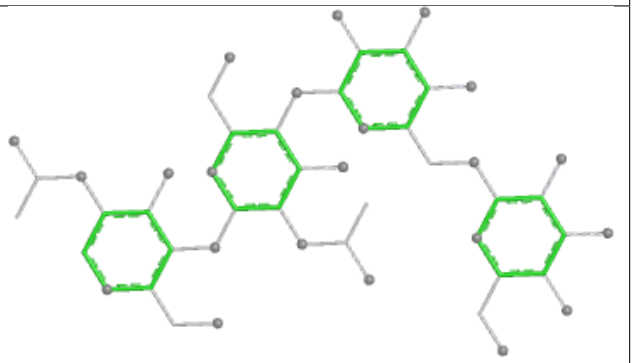
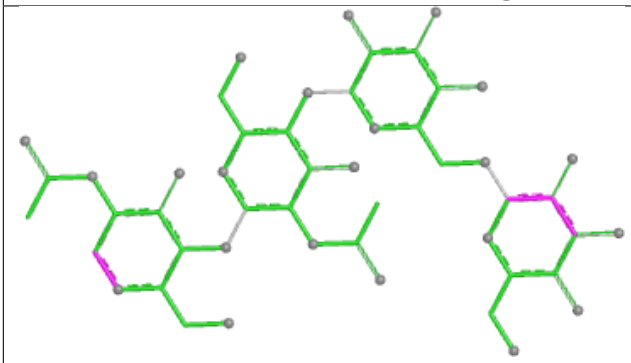
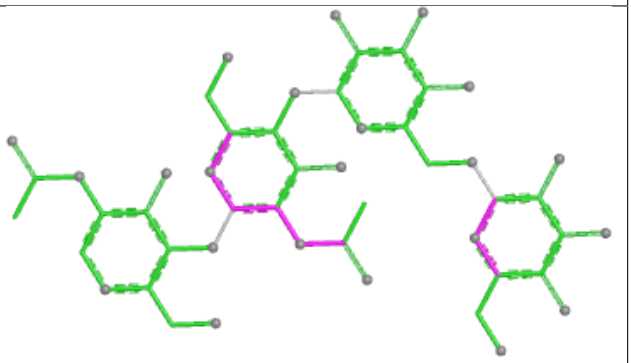


Rings

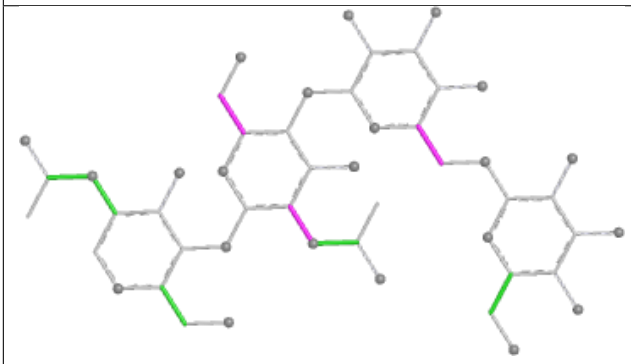
Oligosaccharide Chain n



Bond lengths



Bond angles



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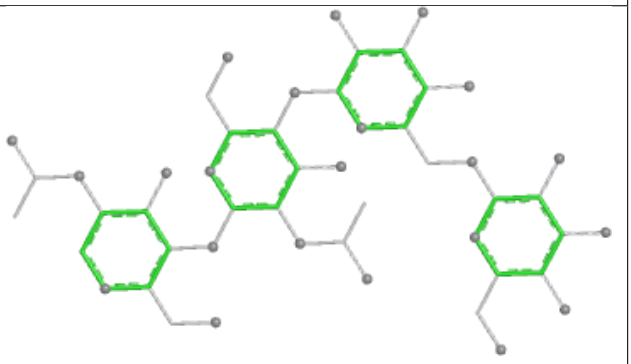
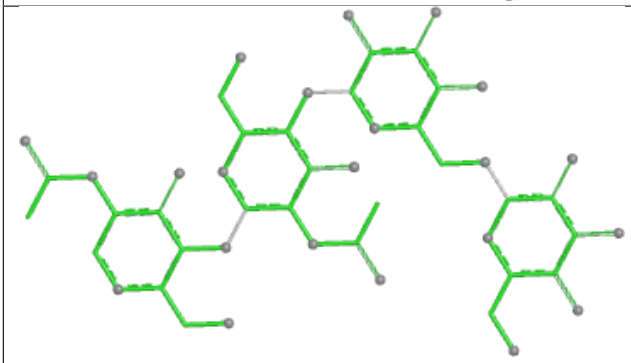


Rings

Oligosaccharide Chain r



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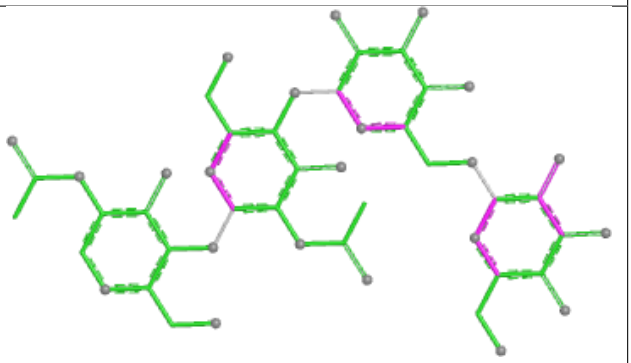
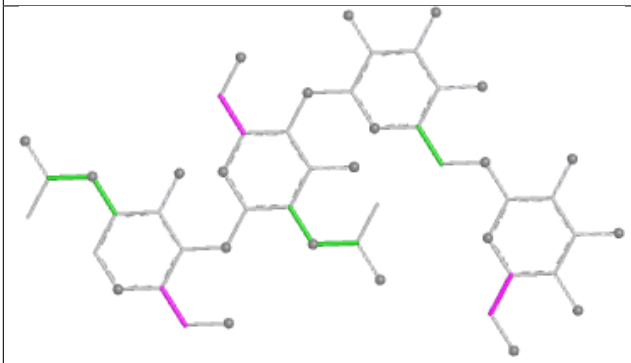


Bond angles



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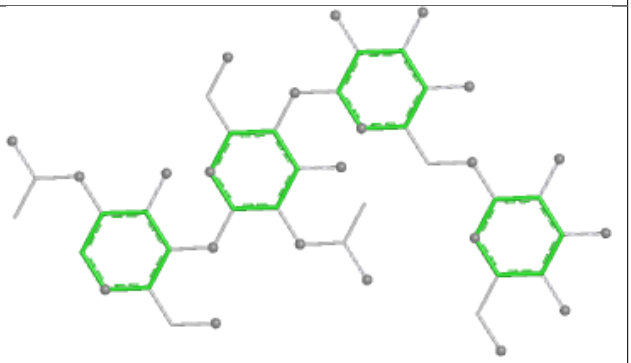
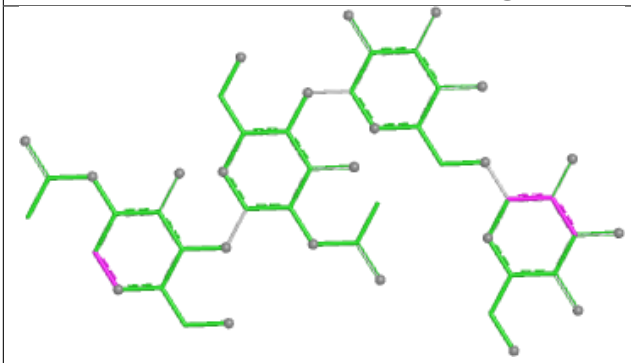
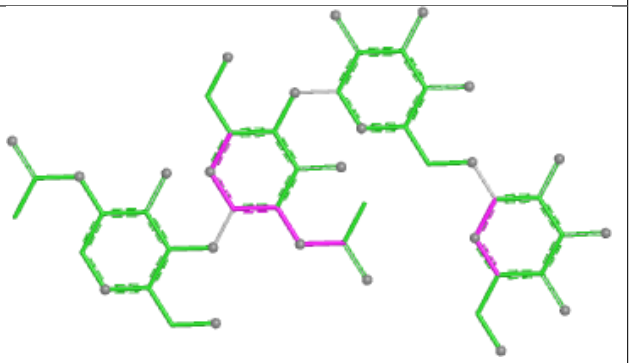


Rings

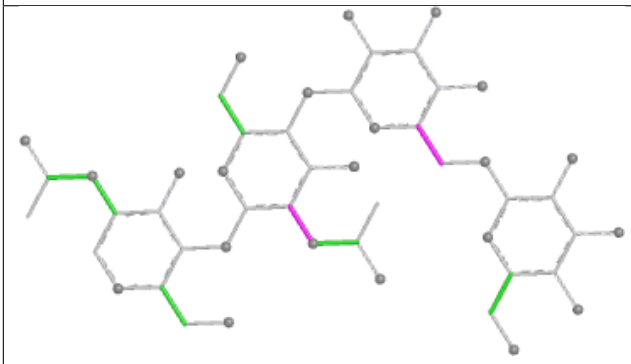
Oligosaccharide Chain 1



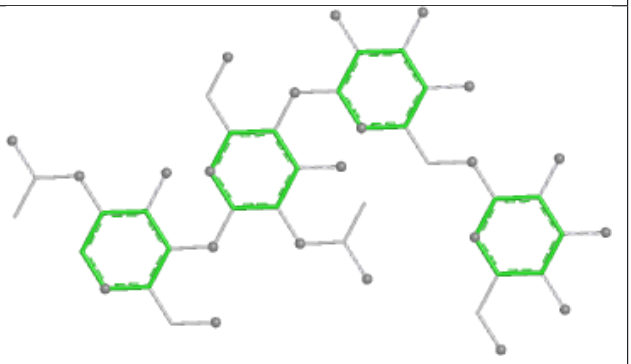
Bond lengths



Bond angles

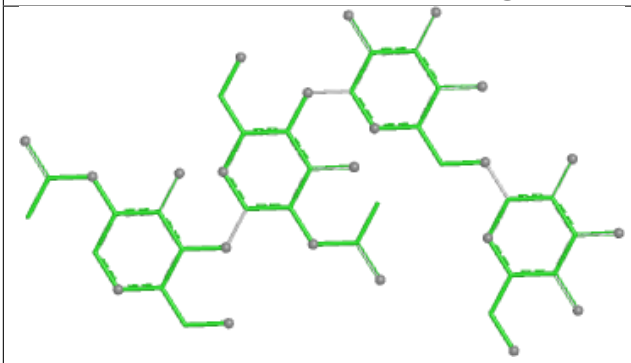


Torsions



Rings

Oligosaccharide Chain 5



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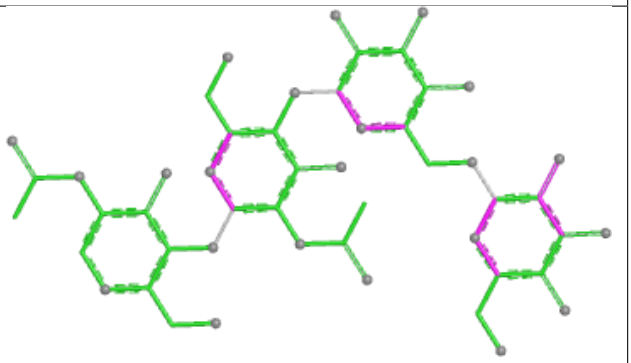
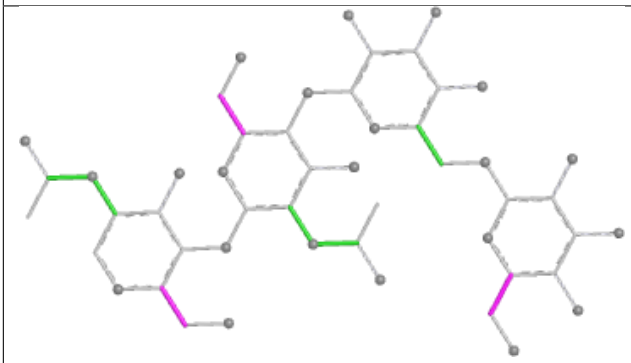


Bond angles



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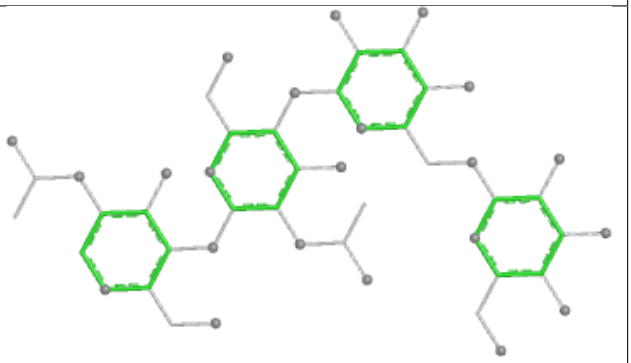
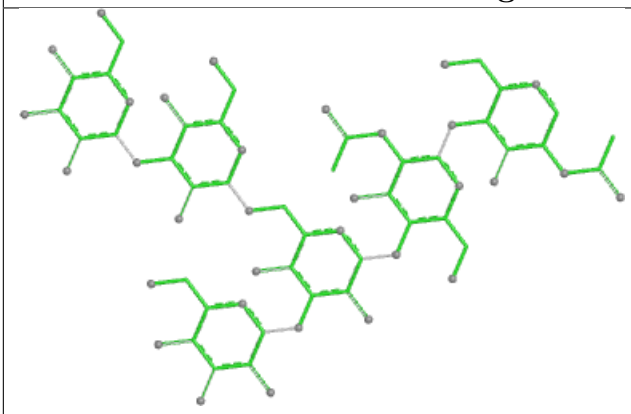


Rings

Oligosaccharide Chain b



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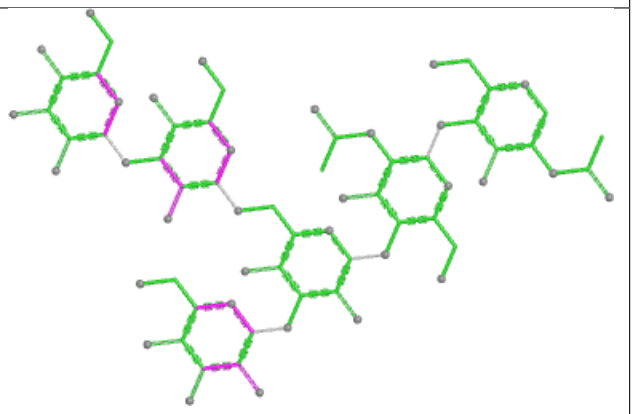
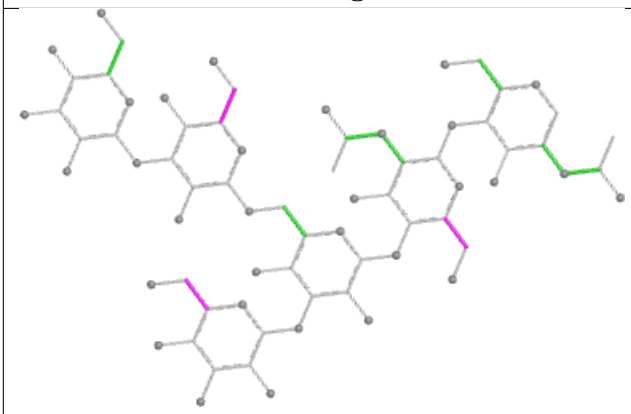
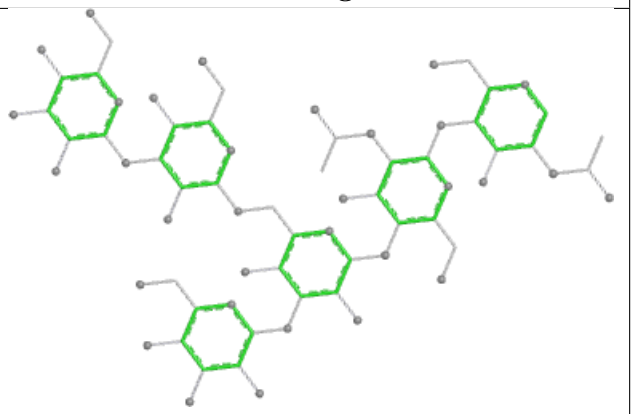


Bond angles

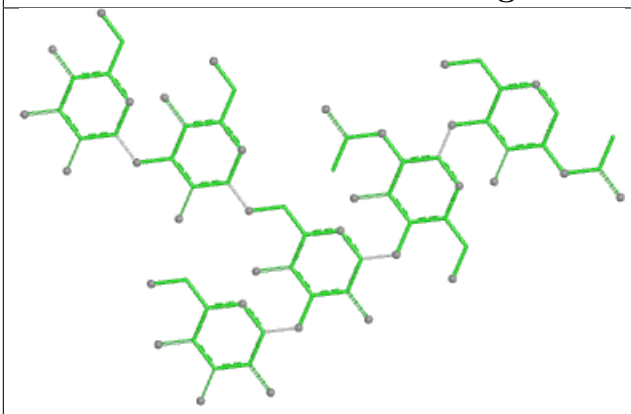


Torsions



Rings

Oligosaccharide Chain p



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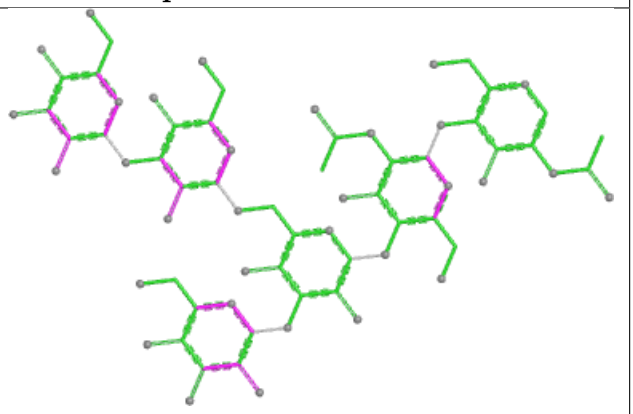
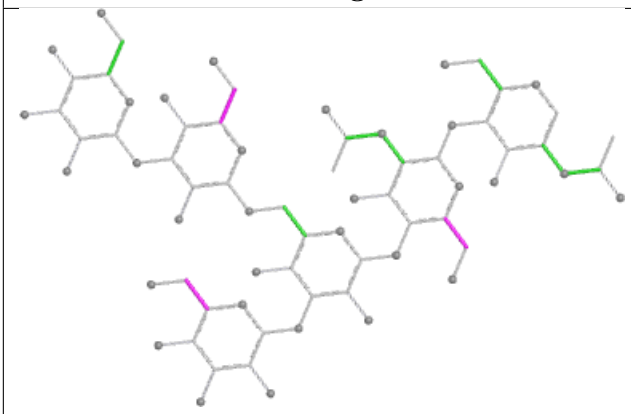
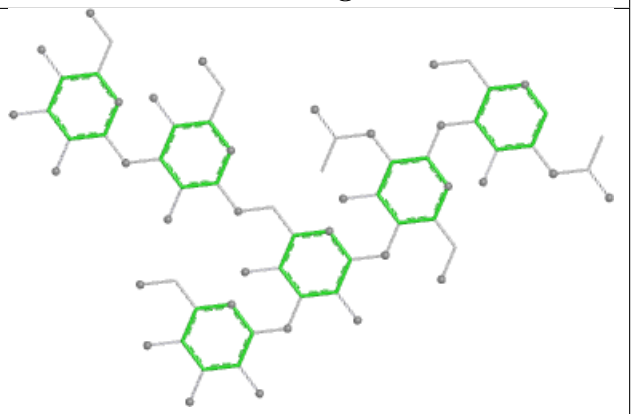


Bond angles

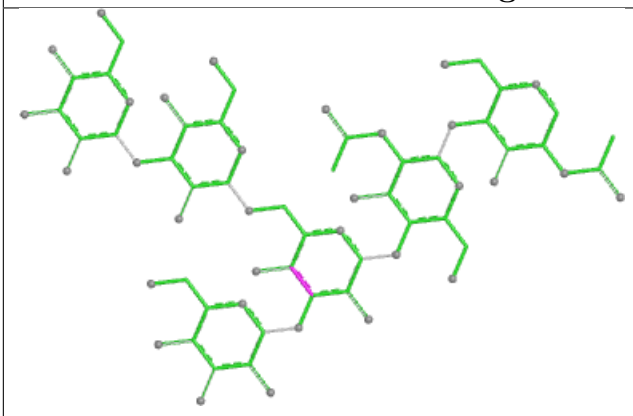


Torsions

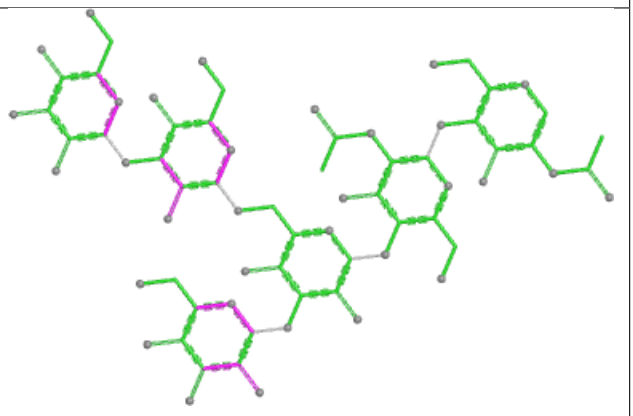


Rings

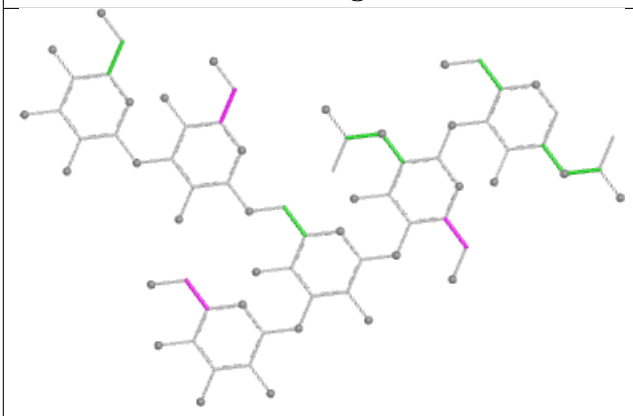
Oligosaccharide Chain 3



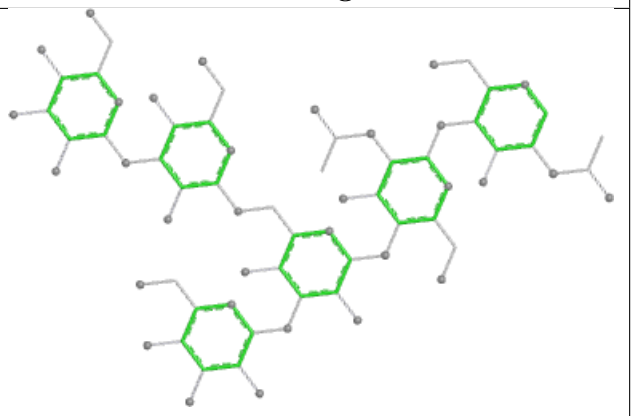
Bond lengths



Bond angles

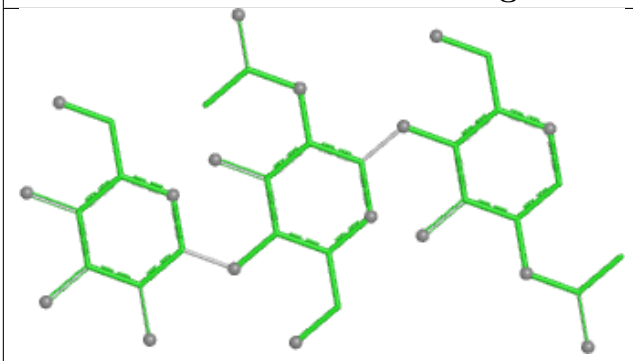


Torsions

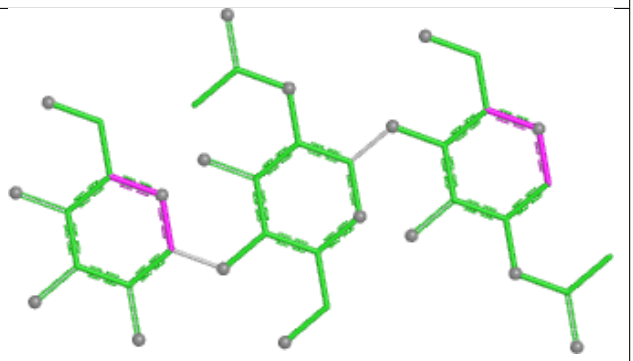


Rings

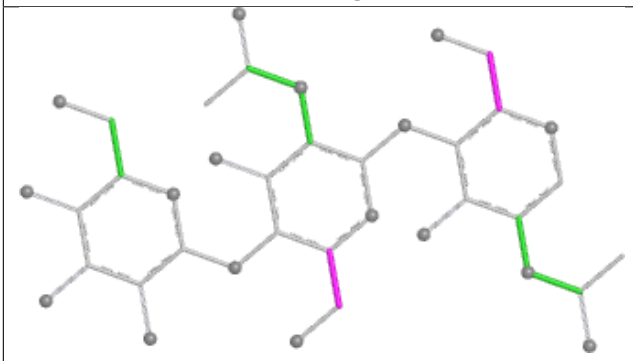
Oligosaccharide Chain e



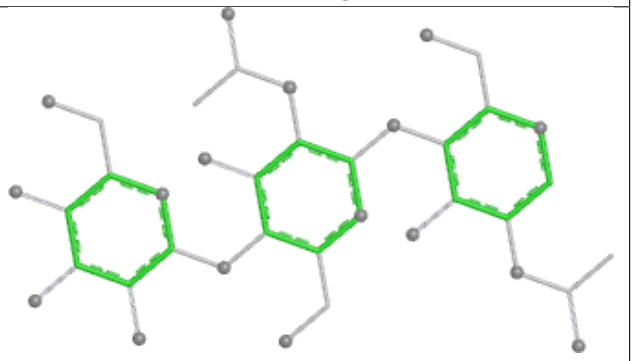
Bond lengths



Bond angles

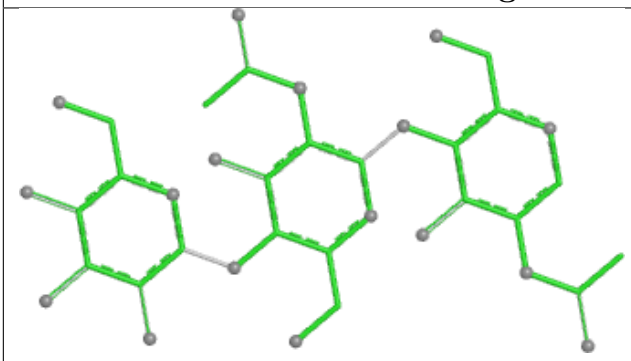


Torsions

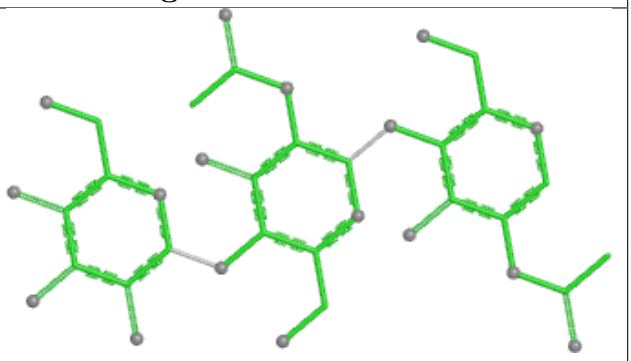


Rings

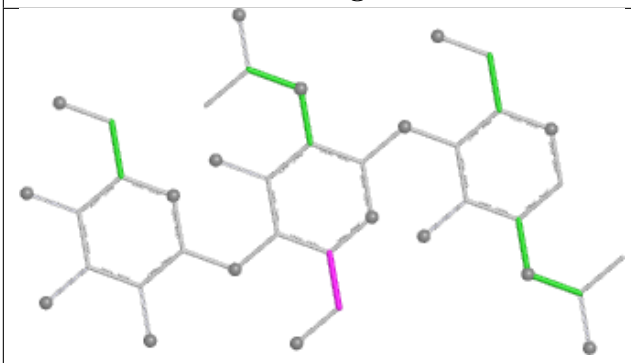
Oligosaccharide Chain g



Bond lengths



Bond angles



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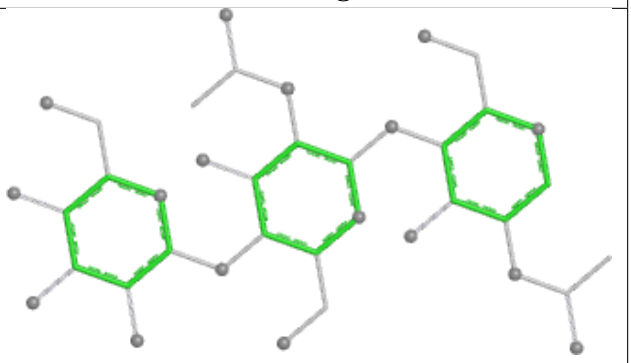
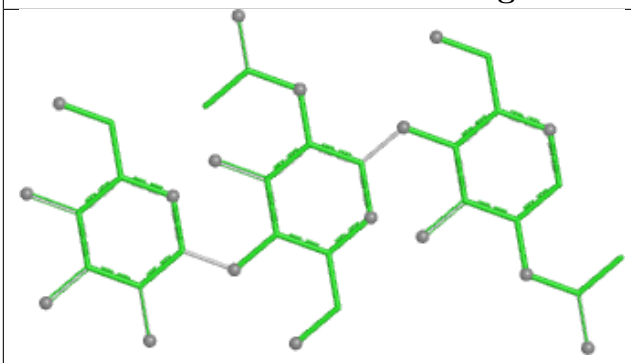
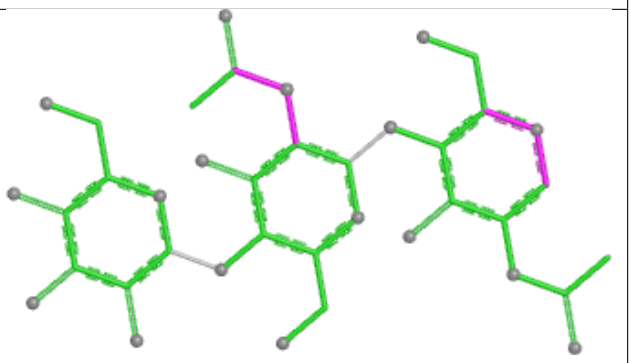


Rings

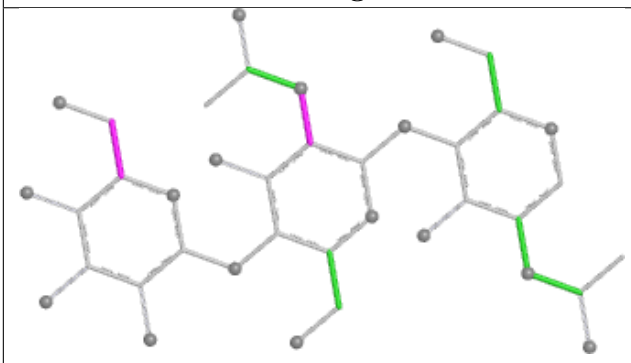
Oligosaccharide Chain h



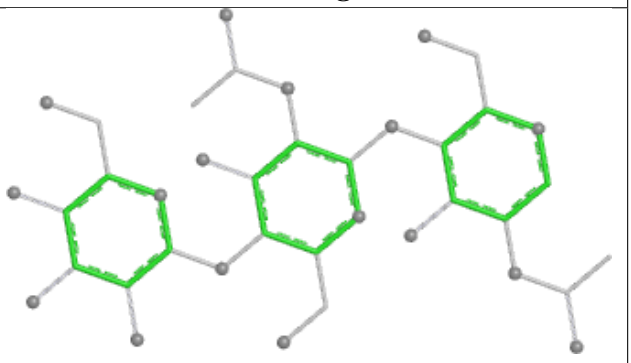
Bond lengths



Bond angles

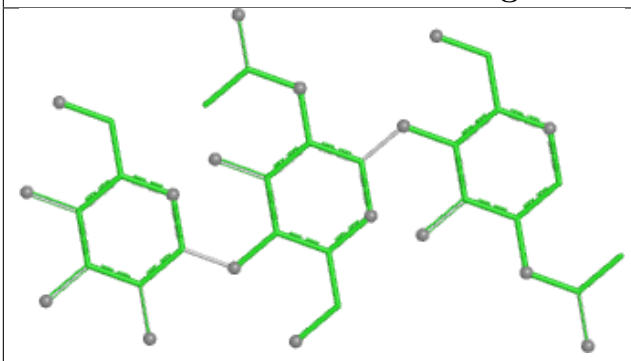


Torsions

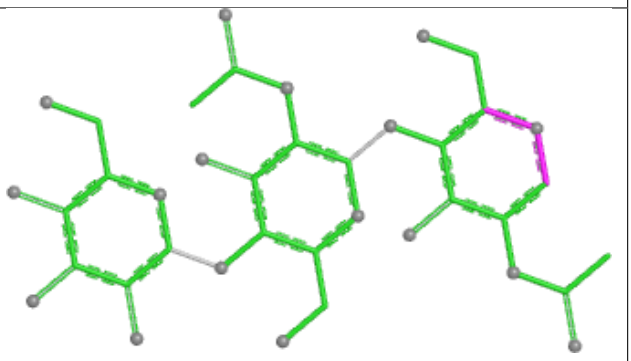


Rings

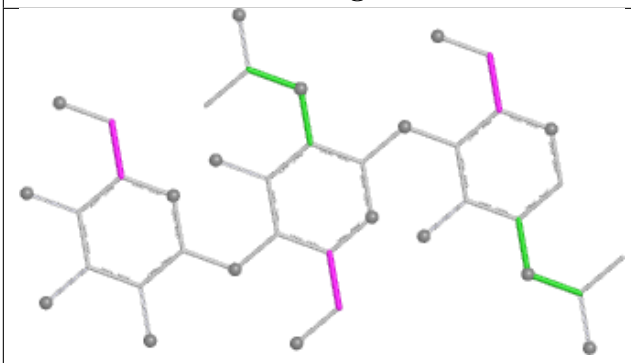
Oligosaccharide Chain s



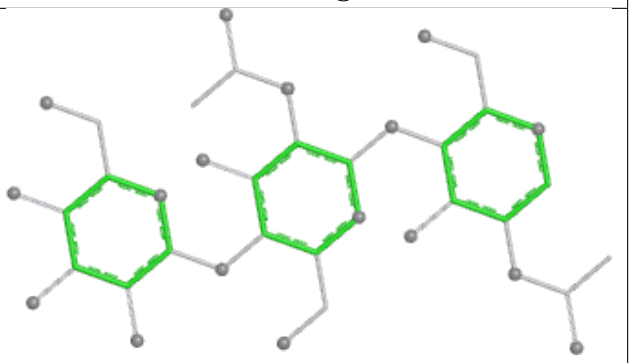
Bond lengths



Bond angles

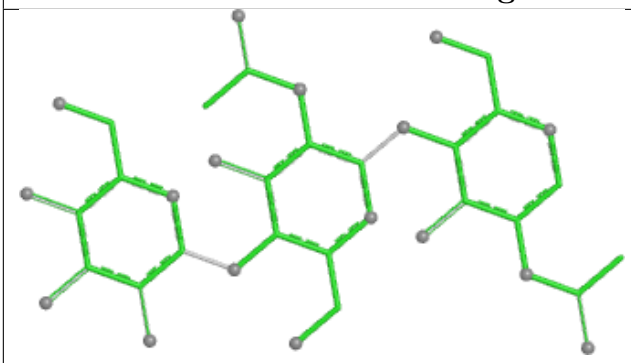


Torsions

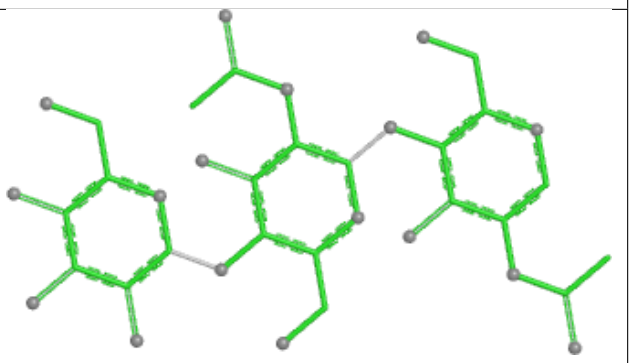


Rings

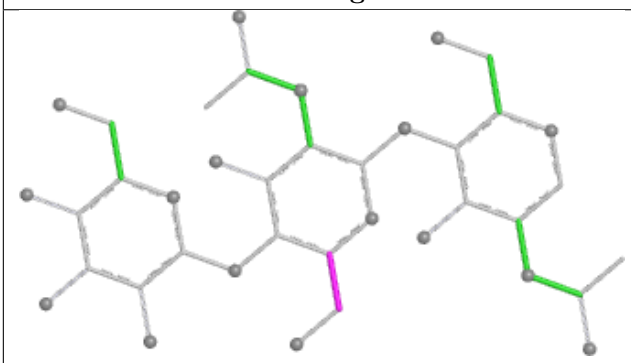
Oligosaccharide Chain u



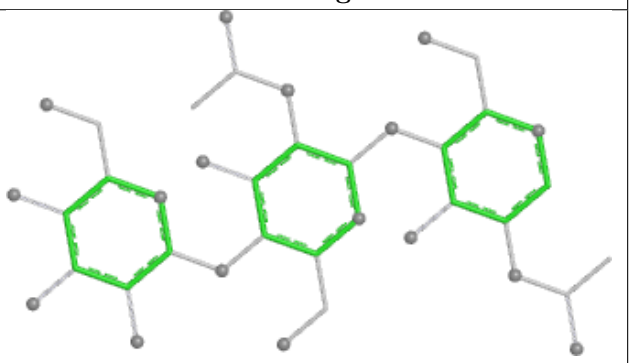
Bond lengths



Bond angles

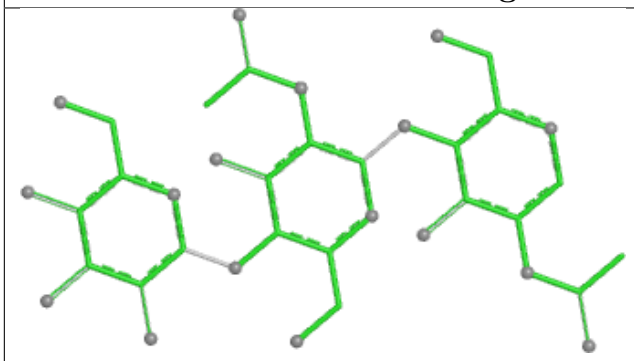


Torsions

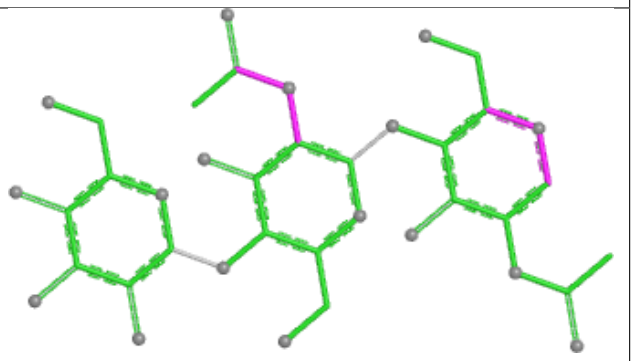


Rings

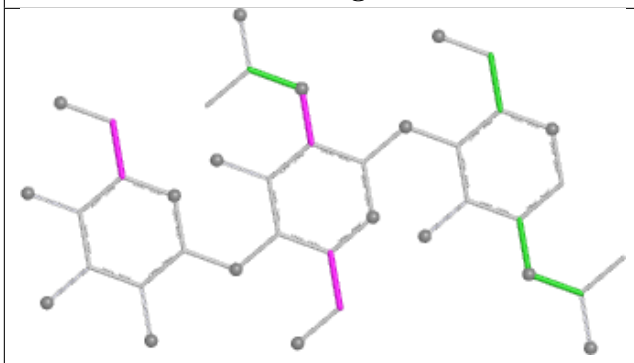
Oligosaccharide Chain v



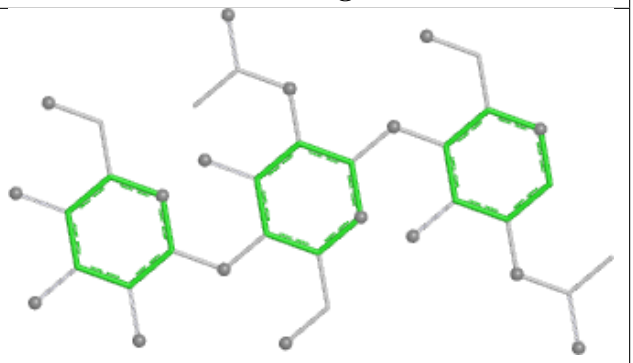
Bond lengths



Bond angles

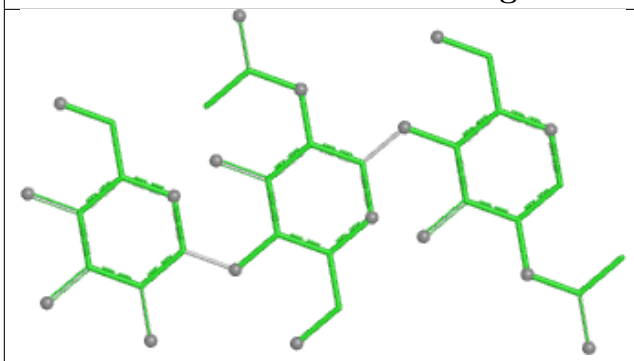


Torsions

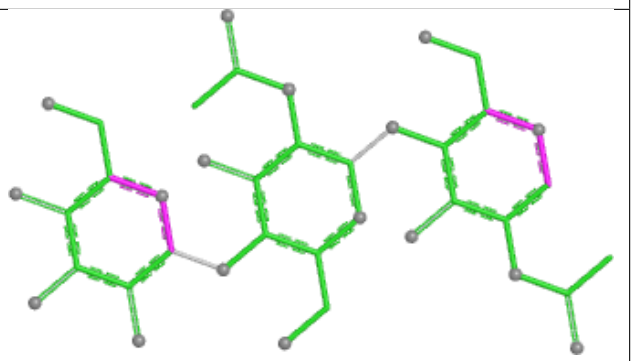


Rings

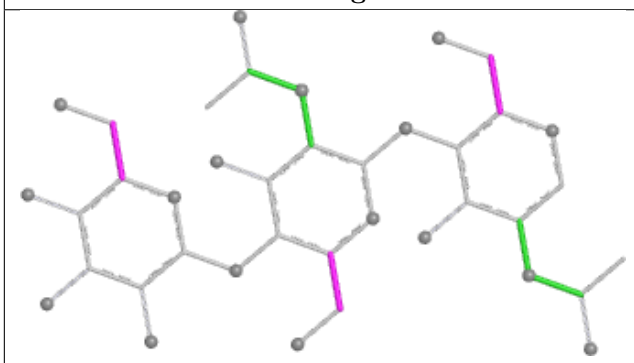
Oligosaccharide Chain 6



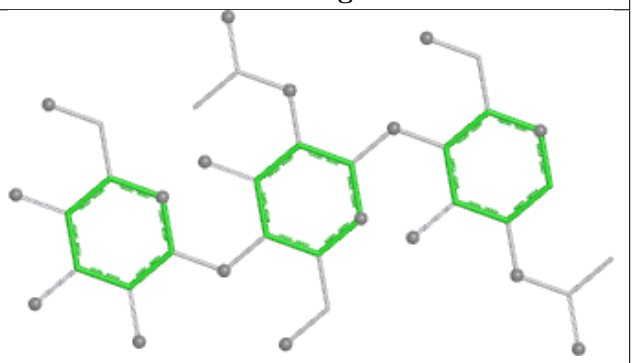
Bond lengths



Bond angles

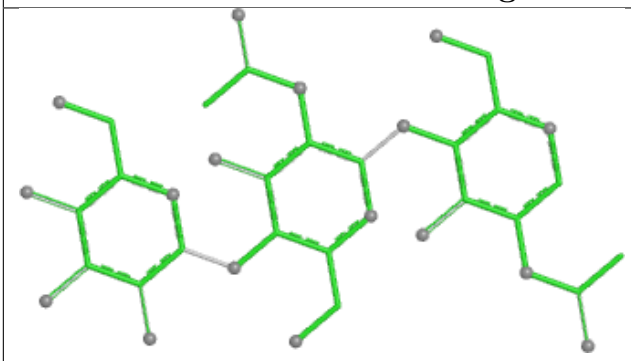


Torsions

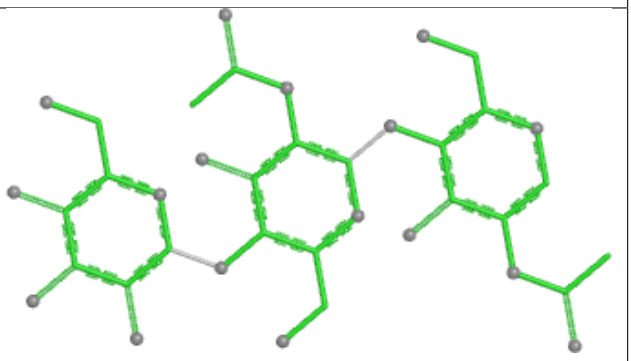


Rings

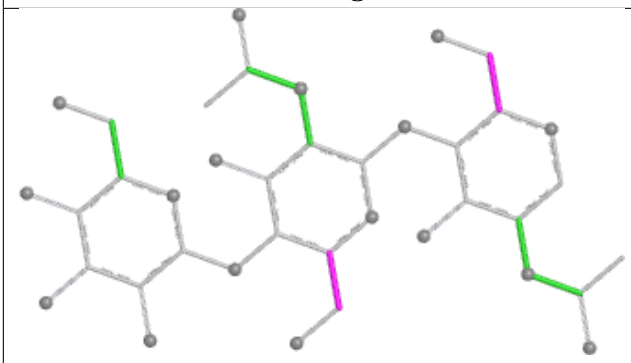
Oligosaccharide Chain 8



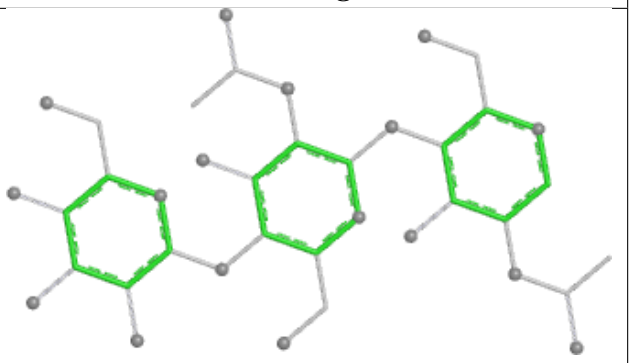
Bond lengths



Bond angles

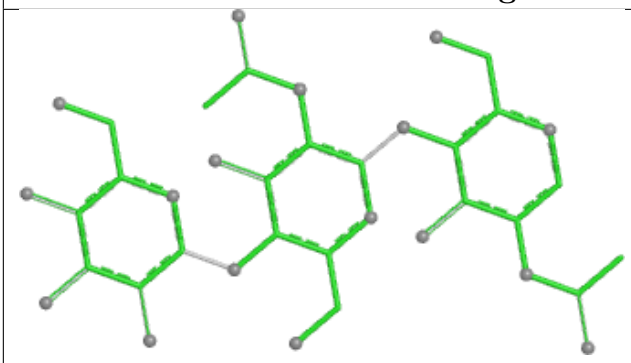


Torsions

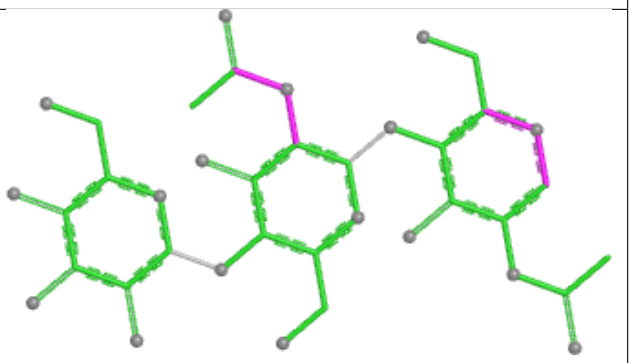


Rings

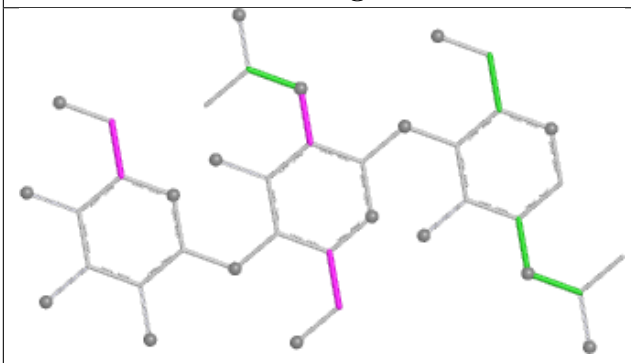
Oligosaccharide Chain 9



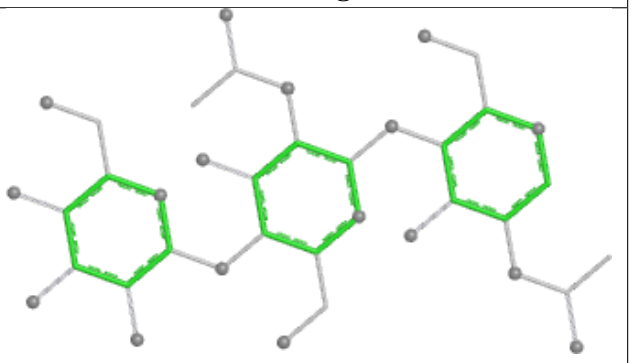
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

15 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	$\#\|Z\| > 2$
13	NAG	F	702	5	14,14,15	0.37	0	17,19,21	0.41	0
13	NAG	C	703	5	14,14,15	0.39	0	17,19,21	0.50	0
13	NAG	G	631	6	14,14,15	0.24	0	17,19,21	0.46	0
13	NAG	P	630	6	14,14,15	0.42	0	17,19,21	0.62	0
13	NAG	G	630	6	14,14,15	0.44	0	17,19,21	0.61	0
13	NAG	C	701	5	14,14,15	0.45	0	17,19,21	0.50	0
13	NAG	F	701	5	14,14,15	0.48	0	17,19,21	0.52	0
13	NAG	M	701	5	14,14,15	0.42	0	17,19,21	0.49	0
13	NAG	C	702	5	14,14,15	0.37	0	17,19,21	0.38	0
13	NAG	P	631	6	14,14,15	0.29	0	17,19,21	0.46	0
13	NAG	M	702	5	14,14,15	0.37	0	17,19,21	0.39	0
13	NAG	F	703	5	14,14,15	0.26	0	17,19,21	0.49	0
13	NAG	M	703	5	14,14,15	0.31	0	17,19,21	0.51	0
13	NAG	J	631	6	14,14,15	0.24	0	17,19,21	0.57	0
13	NAG	J	630	6	14,14,15	0.36	0	17,19,21	0.60	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
13	NAG	F	702	5	-	1/6/23/26	0/1/1/1
13	NAG	C	703	5	-	0/6/23/26	0/1/1/1
13	NAG	G	631	6	-	2/6/23/26	0/1/1/1
13	NAG	P	630	6	-	2/6/23/26	0/1/1/1
13	NAG	G	630	6	-	2/6/23/26	0/1/1/1
13	NAG	C	701	5	-	2/6/23/26	0/1/1/1
13	NAG	F	701	5	-	2/6/23/26	0/1/1/1
13	NAG	M	701	5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	C	702	5	-	2/6/23/26	0/1/1/1
13	NAG	P	631	6	-	2/6/23/26	0/1/1/1
13	NAG	M	702	5	-	2/6/23/26	0/1/1/1
13	NAG	F	703	5	-	0/6/23/26	0/1/1/1
13	NAG	M	703	5	-	0/6/23/26	0/1/1/1
13	NAG	J	631	6	-	2/6/23/26	0/1/1/1
13	NAG	J	630	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	P	630	NAG	O5-C5-C6-O6
13	C	702	NAG	O5-C5-C6-O6
13	G	630	NAG	O5-C5-C6-O6
13	J	630	NAG	O5-C5-C6-O6
13	M	702	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.

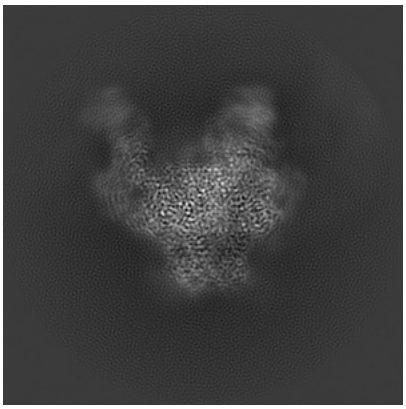
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20739. These allow visual inspection of the internal detail of the map and identification of artifacts.

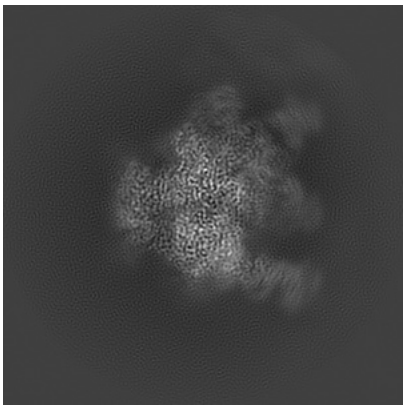
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

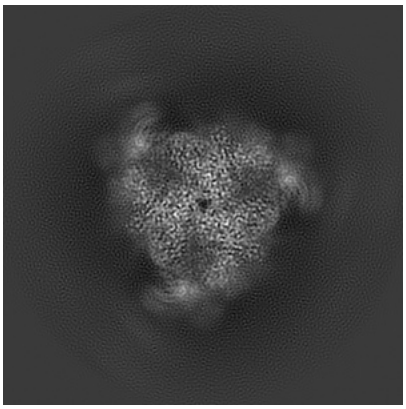
6.1.1 Primary map



X

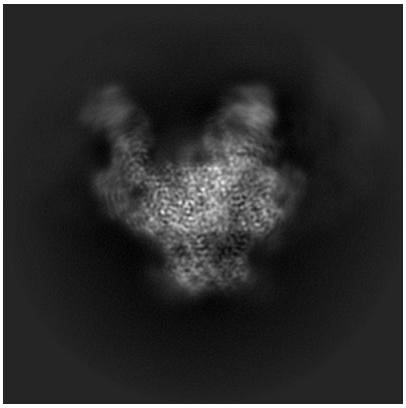


Y

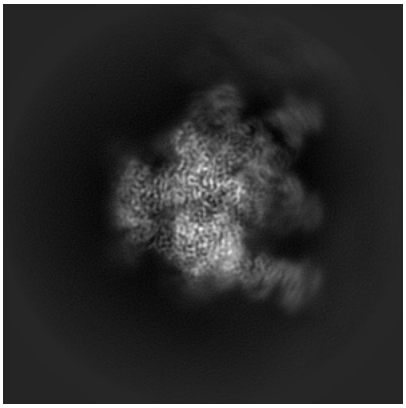


Z

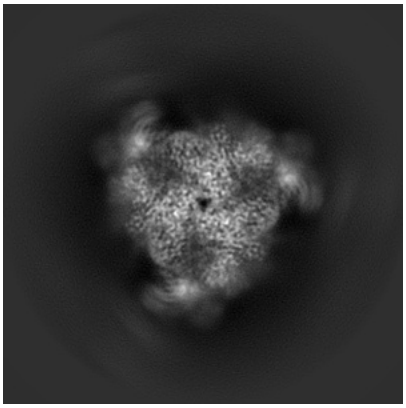
6.1.2 Raw map



X



Y

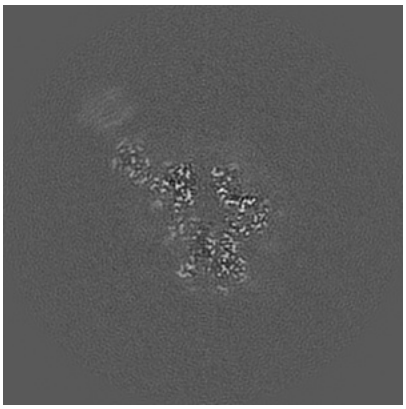


Z

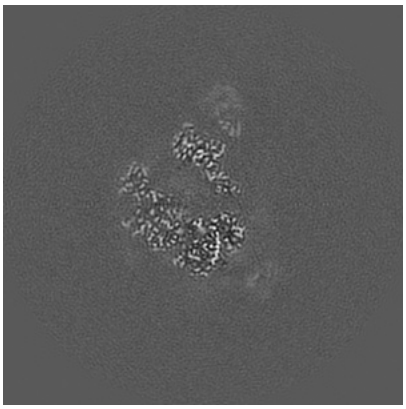
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

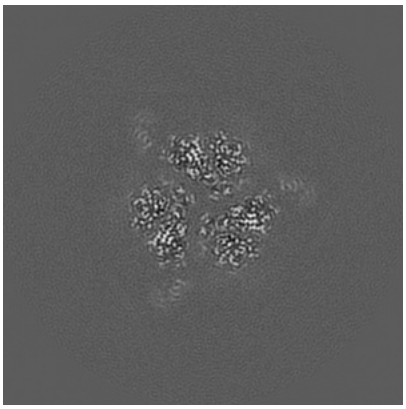
6.2.1 Primary map



X Index: 144

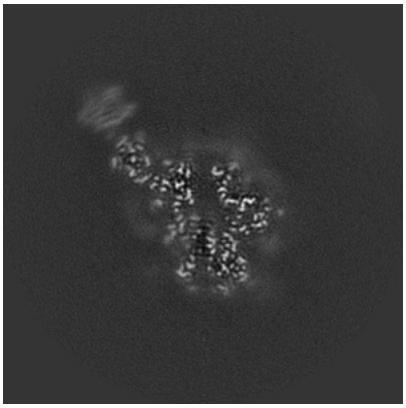


Y Index: 144

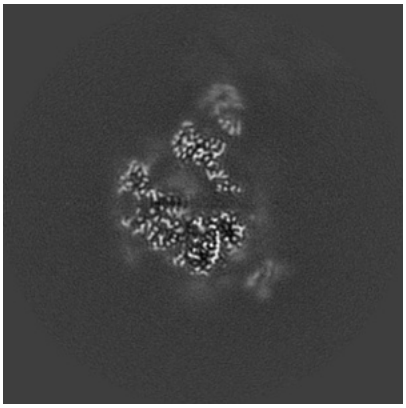


Z Index: 144

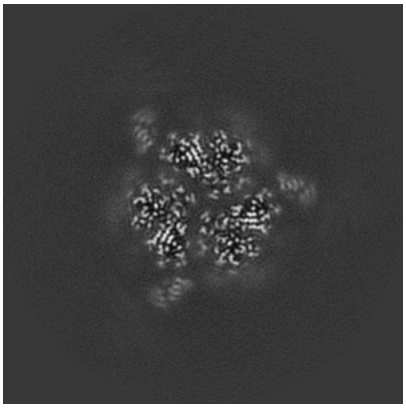
6.2.2 Raw map



X Index: 144



Y Index: 144

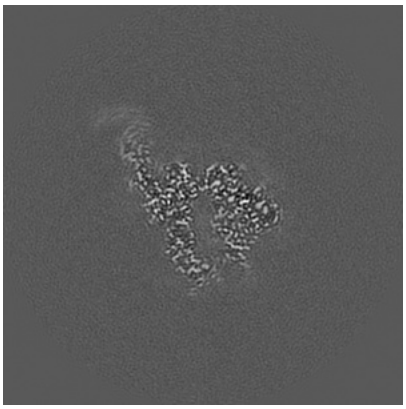


Z Index: 144

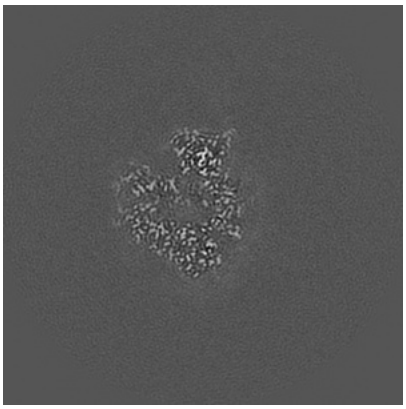
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

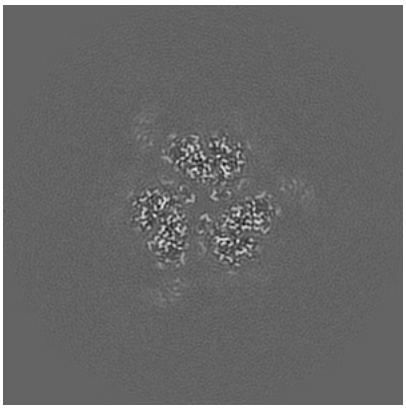
6.3.1 Primary map



X Index: 157

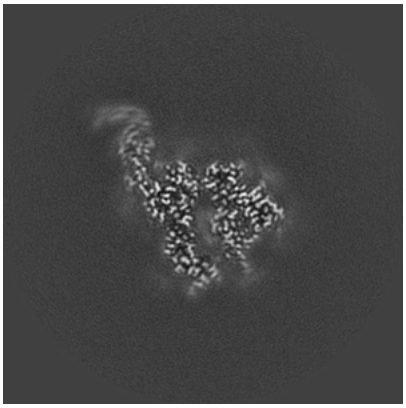


Y Index: 136

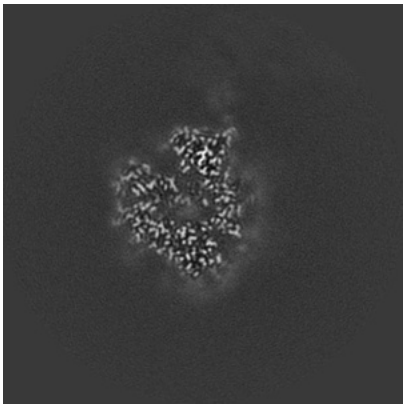


Z Index: 145

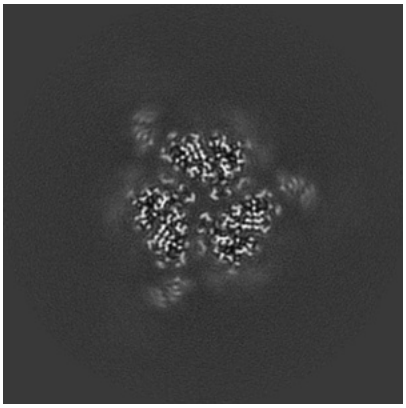
6.3.2 Raw map



X Index: 158



Y Index: 136

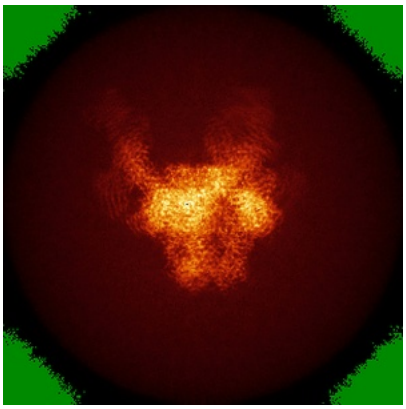


Z Index: 145

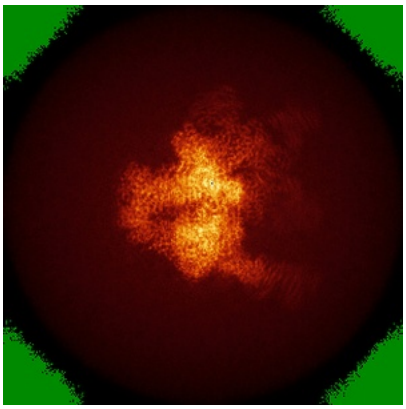
The images above show the largest variance slices of the map in three orthogonal directions.

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

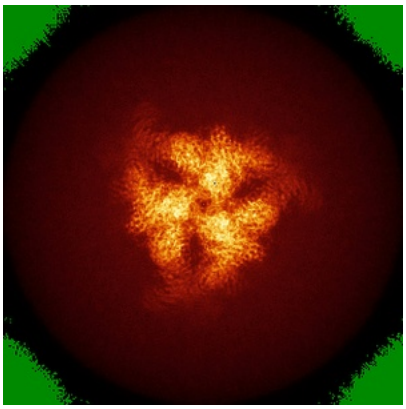
6.4.1 Primary map



X

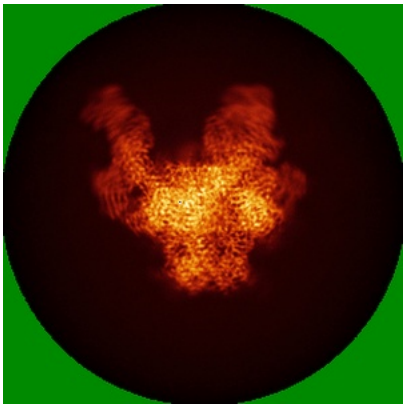


Y

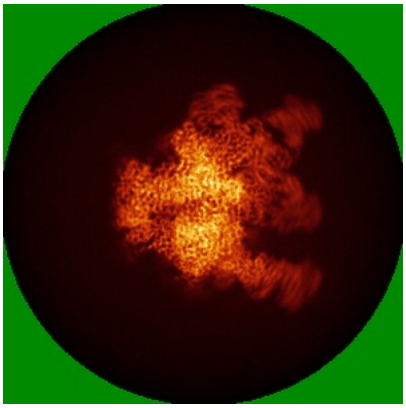


Z

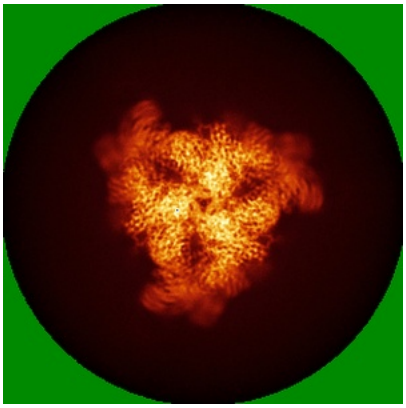
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0302. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

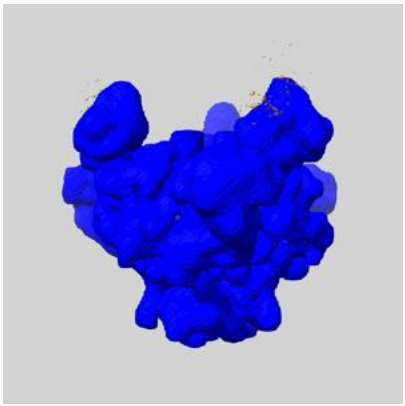
6.6 Mask visualisation (i)

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

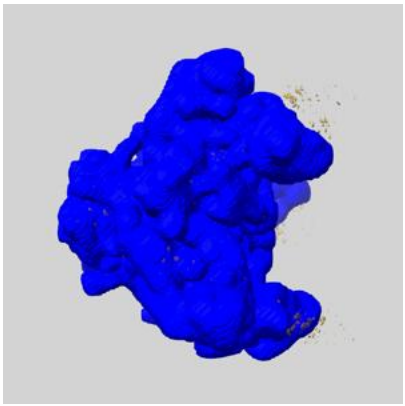
A mask typically either:

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

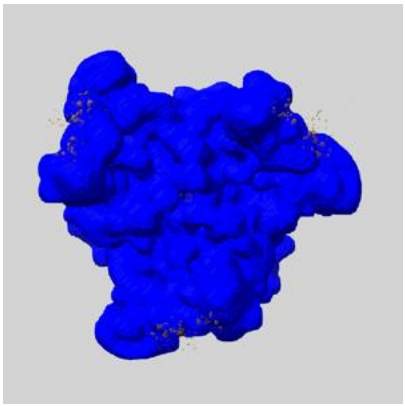
6.6.1 emd_20739_msk_1.map (i)



X



Y

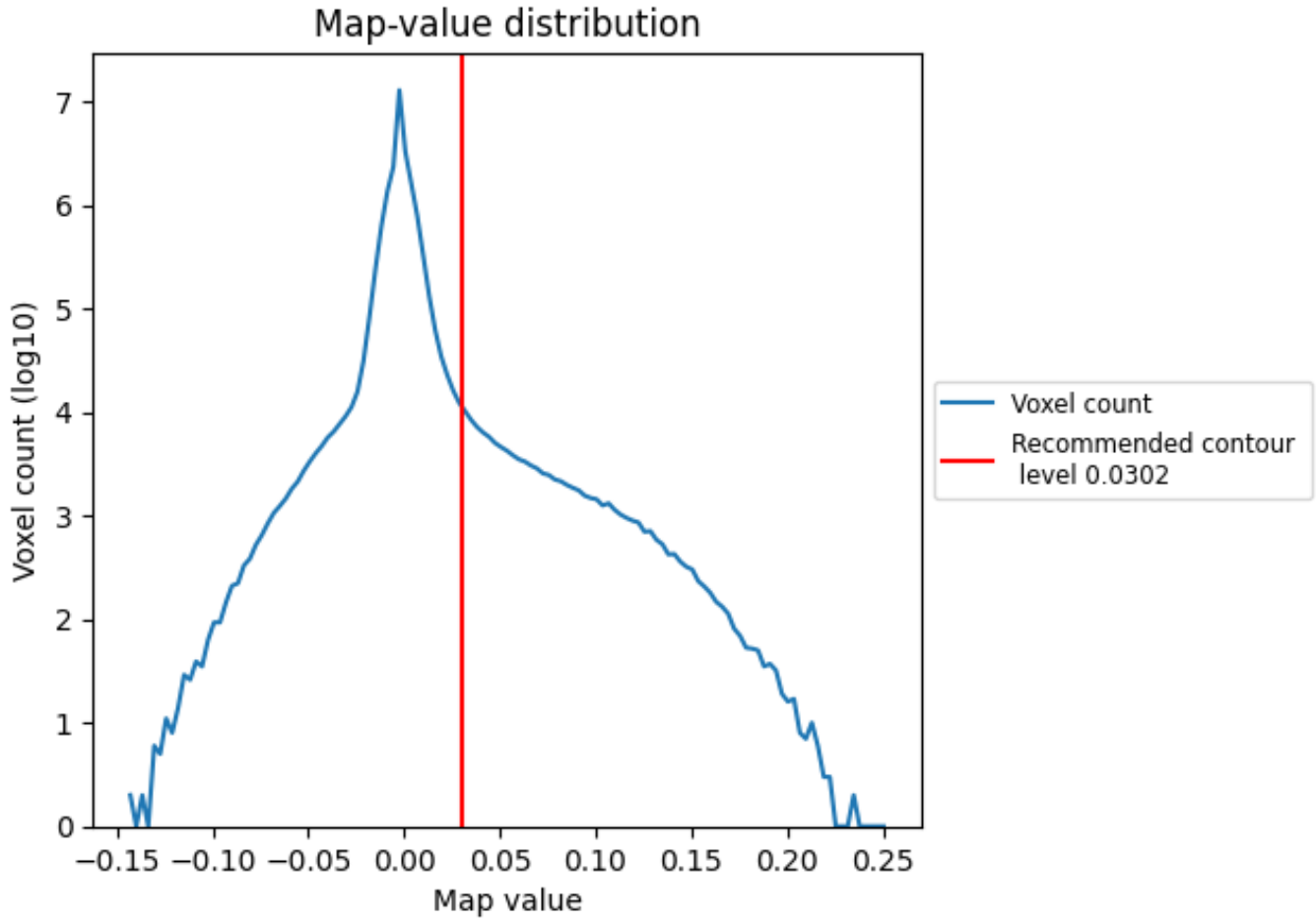


Z

7 Map analysis

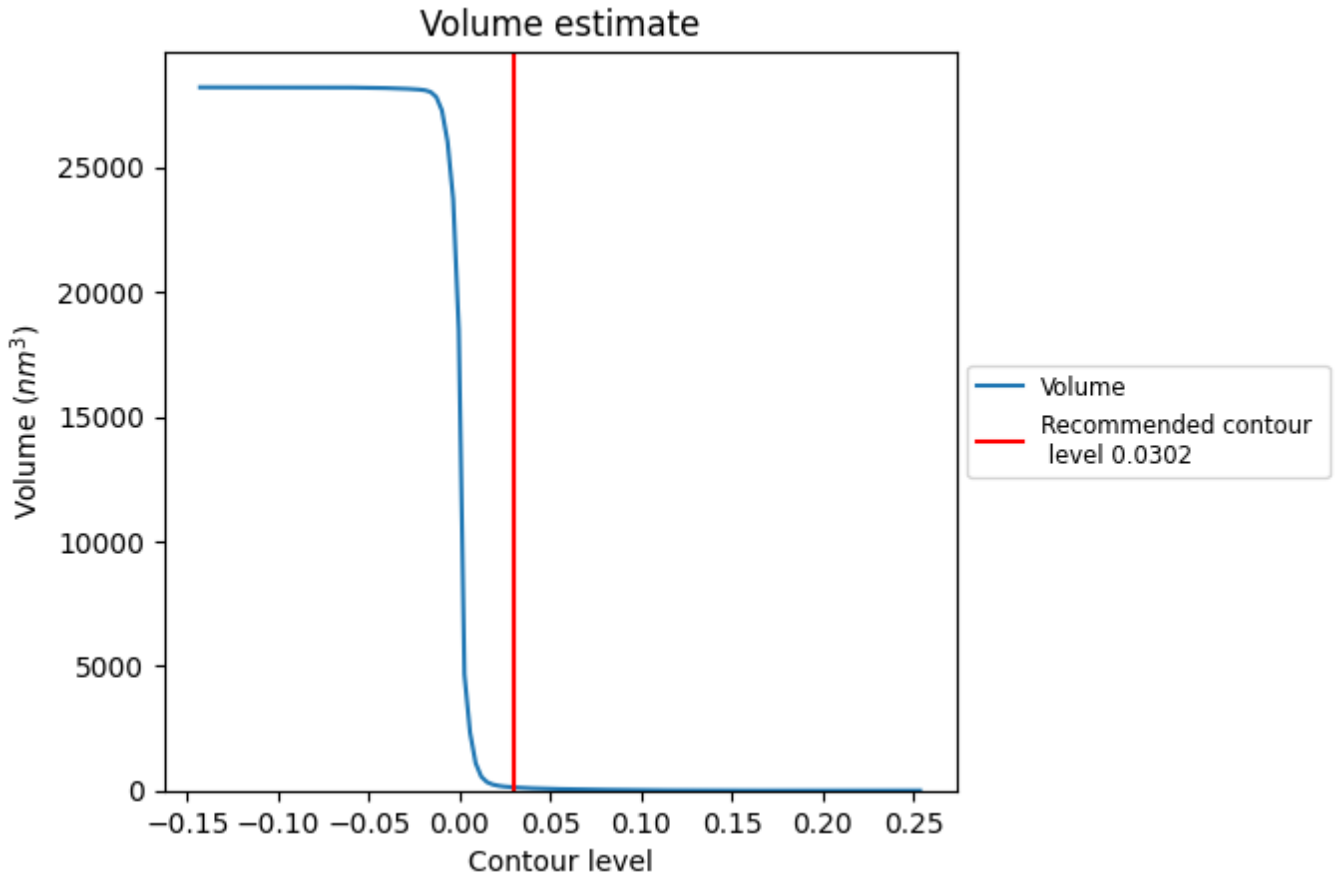
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

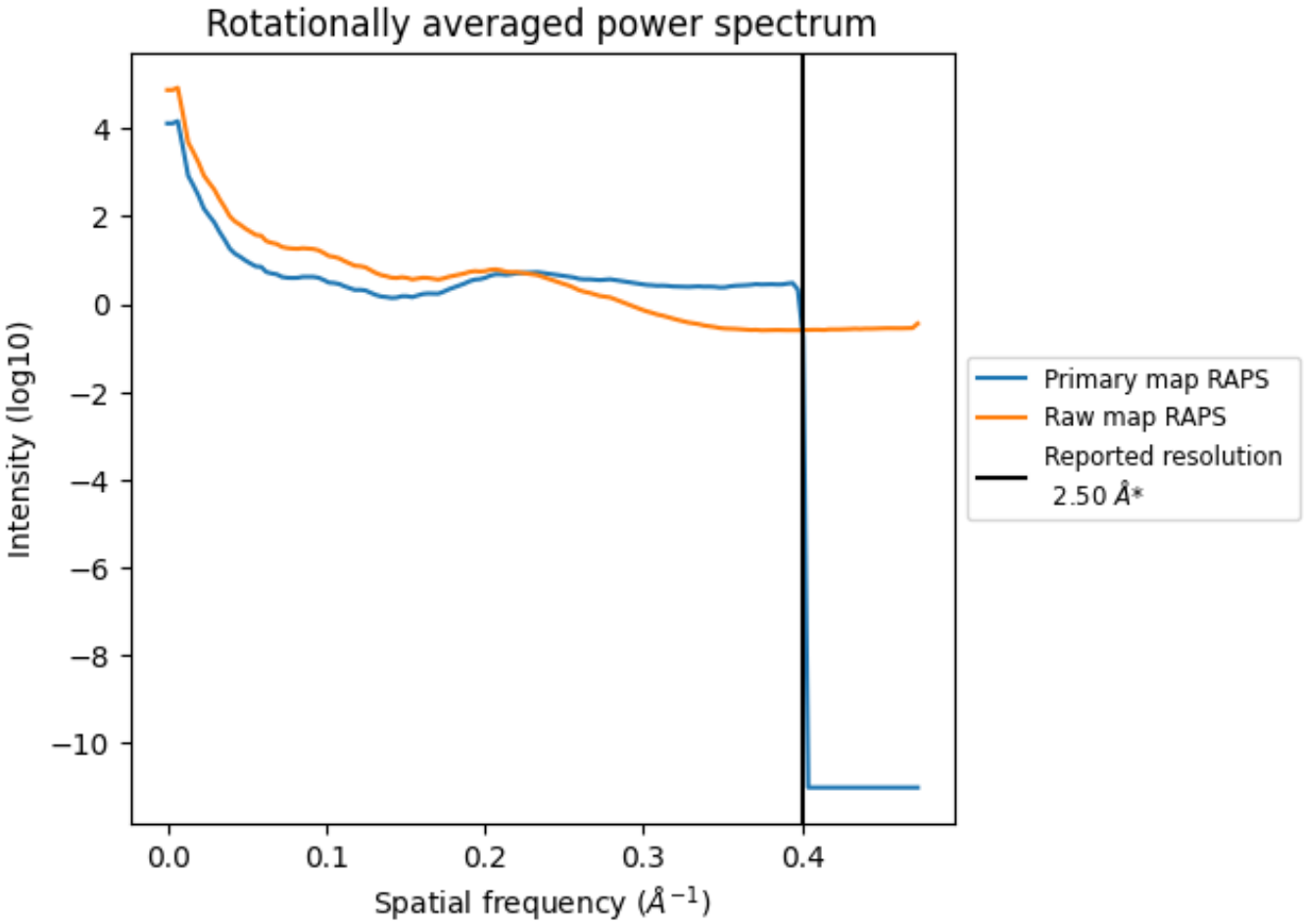
7.2 Volume estimate (i)



The volume at the recommended contour level is 127 nm^3; this corresponds to an approximate mass of 115 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)

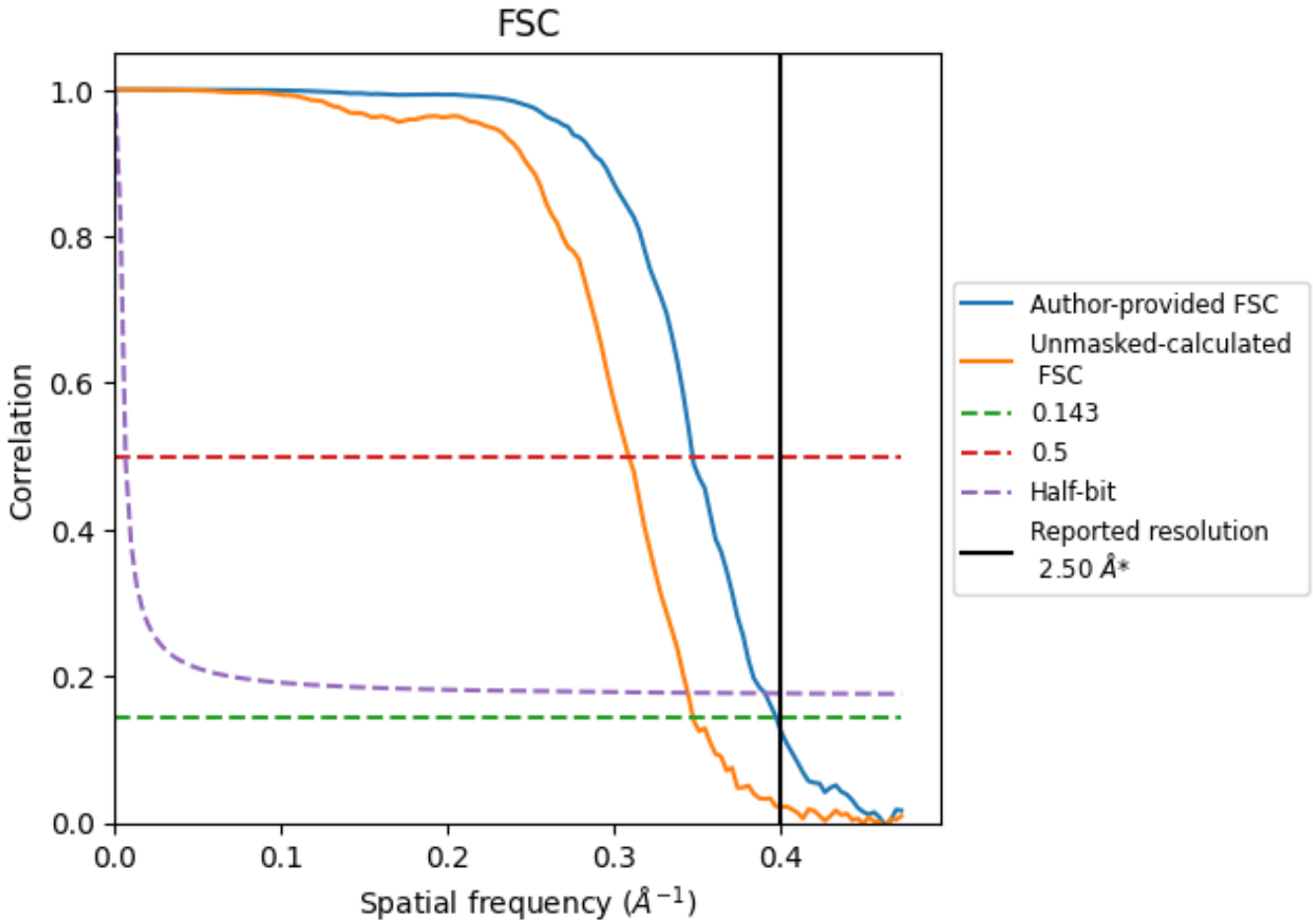


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates (i)

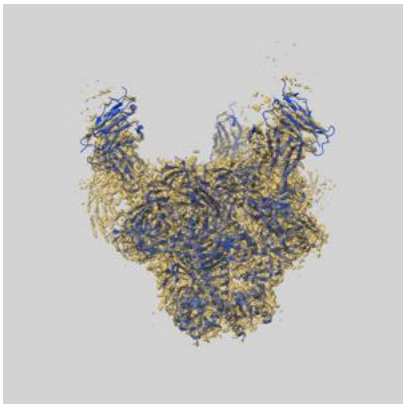
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.51	2.88	2.56
Unmasked-calculated*	2.88	3.24	2.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.88 differs from the reported value 2.5 by more than 10 %

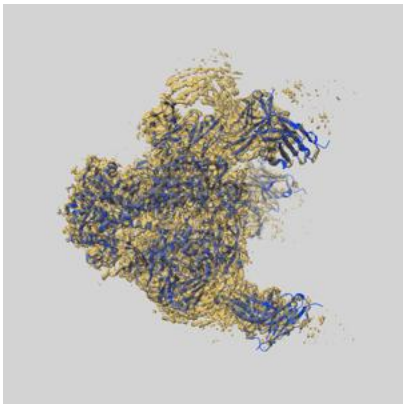
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20739 and PDB model 6UDJ. Per-residue inclusion information can be found in section 3 on page 14.

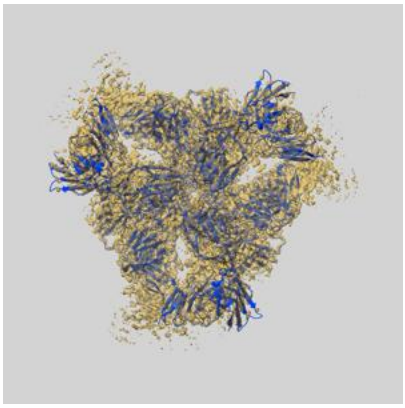
9.1 Map-model overlay



X



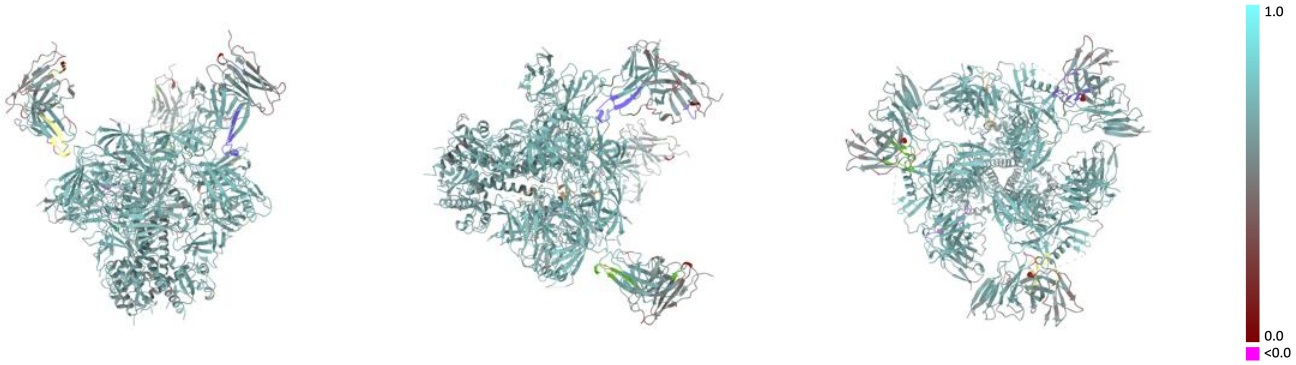
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0302 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.

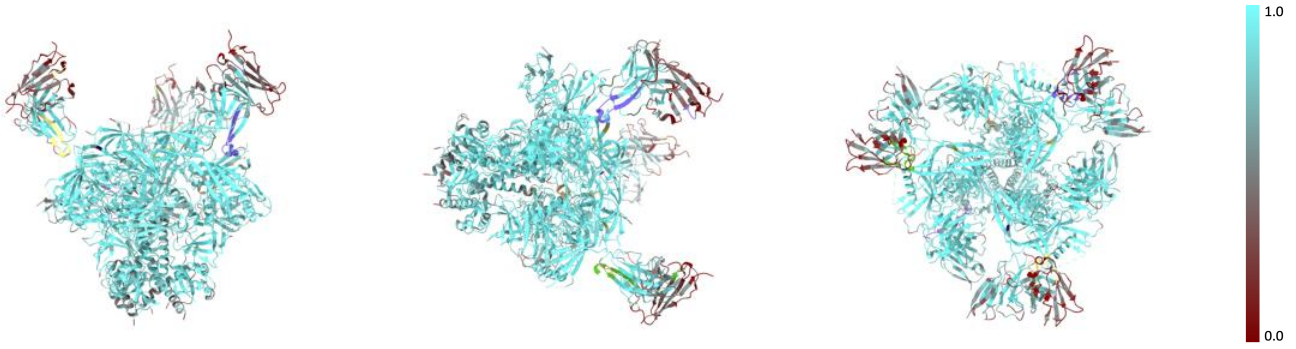
9.2 Q-score mapped to coordinate model (i)



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.

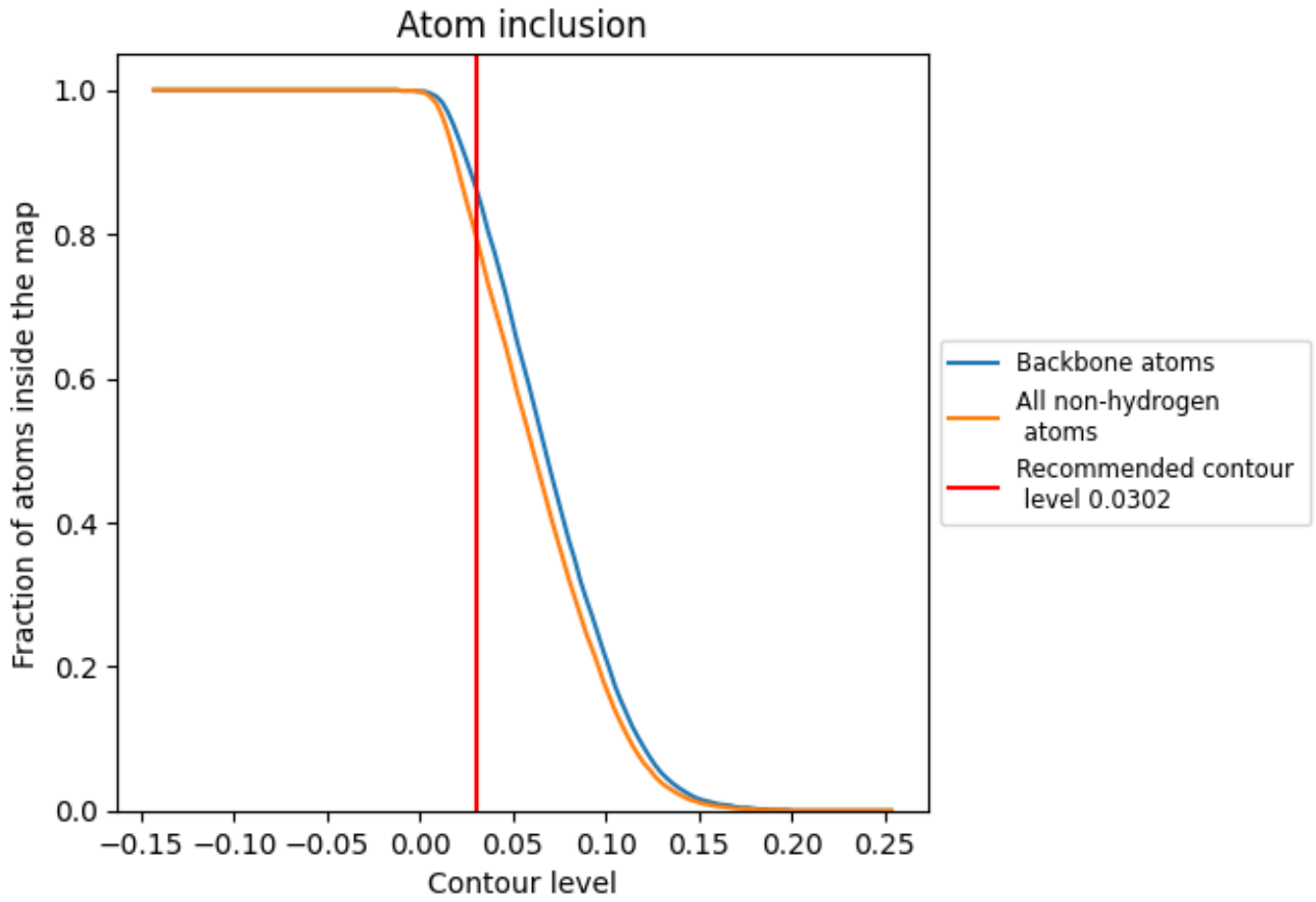
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0302).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.0302) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7970	0.6320
0	0.4290	0.5380
1	0.5000	0.5650
2	0.2140	0.5290
3	0.4860	0.5960
4	0.5000	0.5420
5	0.3800	0.4870
6	0.4620	0.5650
7	0.2860	0.5450
8	0.3850	0.5070
9	0.4360	0.5330
A	0.4840	0.5270
AA	0.6560	0.5880
B	0.7670	0.6190
C	0.7680	0.6170
D	0.9370	0.6810
E	0.8310	0.6340
F	0.7630	0.6170
G	0.9210	0.6750
H	0.9330	0.6750
I	0.8380	0.6330
J	0.9210	0.6750
K	0.4870	0.5220
L	0.7700	0.6270
M	0.7610	0.6120
N	0.9350	0.6810
O	0.8330	0.6330
P	0.9210	0.6750
Q	0.4870	0.5190
R	0.7690	0.6220
S	0.8090	0.6080
T	0.8090	0.6150
U	0.7900	0.6130
V	0.3930	0.5250
W	0.2140	0.4920

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
X	0.3770	0.4890
Y	0.4290	0.5210
Z	0.4800	0.5440
a	0.2500	0.5350
b	0.5000	0.5970
c	0.5360	0.5640
d	0.3800	0.4690
e	0.4100	0.5430
f	0.3570	0.5490
g	0.3590	0.5150
h	0.4620	0.5400
i	0.6560	0.5900
j	0.3570	0.5580
k	0.2500	0.5060
l	0.3770	0.4850
m	0.4290	0.5270
n	0.5000	0.5550
o	0.2500	0.5180
p	0.4580	0.5980
q	0.5000	0.5360
r	0.4200	0.4890
s	0.4620	0.5690
t	0.3210	0.5510
u	0.4100	0.5140
v	0.4360	0.5450
w	0.6560	0.5860
x	0.3570	0.5500
y	0.2500	0.5080
z	0.3770	0.4970